Full wwPDB EM Validation Report

Mar 23, 2026 – 10:20 AM UTC

PDB ID	:	7DZ7 / pdb_00007dz7
EMDB ID	:	EMD-30925
Title	:	State transition supercomplex PSI-LHCI-LHCII from double phosphatase mutant pph1;pbcp of green alga Chlamydomonas reinhardtii
Authors	:	Pan, X.W.; Li, A.J.; Liu, Z.F.; Li, M.
Deposited on	:	2021-01-23
Resolution	:	2.84 Å(reported)

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

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

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

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

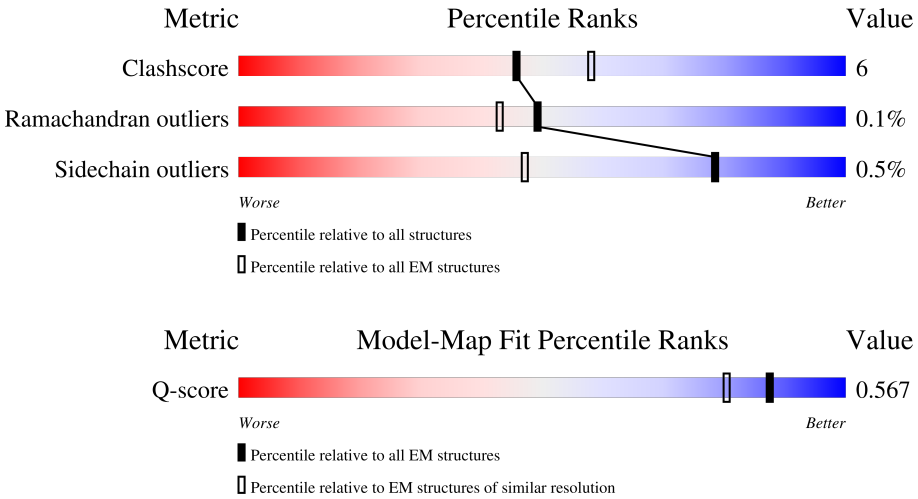
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.84 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11884 (2.34 - 3.34)

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	751	87% 12% •
2	B	735	88% 11%
3	C	81	5% 86% 12% •
4	D	196	68% 5% 27%

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Mol	Chain	Length	Quality of chain
5	E	97	60% 35%
6	F	227	64% 9% 27%
7	G	126	67% 8% 25%
8	H	130	65% 12% 23%
9	I	106	34% 6% 60%
10	J	41	83% 17%
11	K	113	67% 9% 24%
12	L	196	72% 9% 19%
13	O	126	68% 9% 23%
14	1	228	78% 7% 15%
14	a	228	75% 10% 15%
15	2	246	82% 6% 12%
16	3	298	66% 7% 26%
17	4	264	74% 5% 20%
18	5	257	80% 8% 12%
19	6	257	81% 9% 11%
20	7	241	80% 8% 12%
21	8	243	77% 12% 11%
22	9	213	76% 10% 14%
23	W	249	24% 78% 10% 12%
23	X	249	44% 76% 12% 12%
24	U	257	14% 72% 12% 15%
24	Y	257	33% 75% 9% 14%
25	Z	256	6% 85% 5% 9%
26	V	268	82% 7% 11%

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
27	CLA	1	602	X	-	-	-
27	CLA	1	603	X	-	-	-
27	CLA	1	604	X	-	-	-
27	CLA	1	606	X	-	-	-
27	CLA	1	607	X	-	-	-
27	CLA	1	608	X	-	-	-
27	CLA	1	609	X	-	-	-
27	CLA	1	610	X	-	-	-
27	CLA	1	611	X	-	-	-
27	CLA	1	612	X	-	-	-
27	CLA	1	613	X	-	-	-
27	CLA	1	614	X	-	-	-
27	CLA	1	616	X	-	-	-
27	CLA	2	601	X	-	-	-
27	CLA	2	602	X	-	-	-
27	CLA	2	603	X	-	-	-
27	CLA	2	604	X	-	-	-
27	CLA	2	606	X	-	-	-
27	CLA	2	607	X	-	-	-
27	CLA	2	609	X	-	-	-
27	CLA	2	610	X	-	-	-
27	CLA	2	611	X	-	-	-
27	CLA	2	612	X	-	-	-
27	CLA	2	613	X	-	-	-
27	CLA	2	614	X	-	-	-
27	CLA	2	616	X	-	-	-
27	CLA	3	602	X	-	-	-
27	CLA	3	603	X	-	-	-
27	CLA	3	604	X	-	-	-
27	CLA	3	606	X	-	-	-
27	CLA	3	607	X	-	-	-
27	CLA	3	608	X	-	-	-
27	CLA	3	609	X	-	-	-
27	CLA	3	610	X	-	-	-
27	CLA	3	611	X	-	-	-
27	CLA	3	612	X	-	-	-
27	CLA	3	613	X	-	-	-
27	CLA	3	614	X	-	-	-
27	CLA	3	615	X	-	-	-
27	CLA	3	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	4	601	X	-	-	-
27	CLA	4	602	X	-	-	-
27	CLA	4	603	X	-	-	-
27	CLA	4	604	X	-	-	-
27	CLA	4	606	X	-	-	-
27	CLA	4	607	X	-	-	-
27	CLA	4	608	X	-	-	-
27	CLA	4	609	X	-	-	-
27	CLA	4	610	X	-	-	-
27	CLA	4	611	X	-	-	-
27	CLA	4	612	X	-	-	-
27	CLA	4	613	X	-	-	-
27	CLA	4	614	X	-	-	-
27	CLA	4	616	X	-	-	-
27	CLA	4	618	X	-	-	-
27	CLA	5	601	X	-	-	-
27	CLA	5	603	X	-	-	-
27	CLA	5	604	X	-	-	-
27	CLA	5	607	X	-	-	-
27	CLA	5	608	X	-	-	-
27	CLA	5	609	X	-	-	-
27	CLA	5	610	X	-	-	-
27	CLA	5	611	X	-	-	-
27	CLA	5	612	X	-	-	-
27	CLA	5	613	X	-	-	-
27	CLA	5	614	X	-	-	-
27	CLA	5	616	X	-	-	-
27	CLA	5	617	X	-	-	-
27	CLA	5	618	X	-	-	-
27	CLA	5	619	X	-	-	-
27	CLA	6	601	X	-	-	-
27	CLA	6	602	X	-	-	-
27	CLA	6	603	X	-	-	-
27	CLA	6	606	X	-	-	-
27	CLA	6	607	X	-	-	-
27	CLA	6	608	X	-	-	-
27	CLA	6	609	X	-	-	-
27	CLA	6	610	X	-	-	-
27	CLA	6	611	X	-	-	-
27	CLA	6	612	X	-	-	-
27	CLA	6	613	X	-	-	-
27	CLA	6	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	6	616	X	-	-	-
27	CLA	6	617	X	-	-	-
27	CLA	6	618	X	-	-	-
27	CLA	6	620	X	-	-	-
27	CLA	7	601	X	-	-	-
27	CLA	7	602	X	-	-	-
27	CLA	7	603	X	-	-	-
27	CLA	7	604	X	-	-	-
27	CLA	7	607	X	-	-	-
27	CLA	7	608	X	-	-	-
27	CLA	7	609	X	-	-	-
27	CLA	7	610	X	-	-	-
27	CLA	7	611	X	-	-	-
27	CLA	7	612	X	-	-	-
27	CLA	7	613	X	-	-	-
27	CLA	7	614	X	-	-	-
27	CLA	7	615	X	-	-	-
27	CLA	7	616	X	-	-	-
27	CLA	8	601	X	-	-	-
27	CLA	8	602	X	-	-	-
27	CLA	8	603	X	-	-	-
27	CLA	8	604	X	-	-	-
27	CLA	8	606	X	-	-	-
27	CLA	8	607	X	-	-	-
27	CLA	8	608	X	-	-	-
27	CLA	8	609	X	-	-	-
27	CLA	8	610	X	-	-	-
27	CLA	8	611	X	-	-	-
27	CLA	8	612	X	-	-	-
27	CLA	8	613	X	-	-	-
27	CLA	8	614	X	-	-	-
27	CLA	8	616	X	-	-	-
27	CLA	9	601	X	-	-	-
27	CLA	9	603	X	-	-	-
27	CLA	9	604	X	-	-	-
27	CLA	9	606	X	-	-	-
27	CLA	9	609	X	-	-	-
27	CLA	9	610	X	-	-	-
27	CLA	9	611	X	-	-	-
27	CLA	9	612	X	-	-	-
27	CLA	9	613	X	-	-	-
27	CLA	9	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	801	X	-	-	-
27	CLA	A	802	X	-	-	-
27	CLA	A	803	X	-	-	-
27	CLA	A	804	X	-	-	-
27	CLA	A	806	X	-	-	-
27	CLA	A	807	X	-	-	-
27	CLA	A	809	X	-	-	-
27	CLA	A	810	X	-	-	-
27	CLA	A	811	X	-	-	-
27	CLA	A	812	X	-	-	-
27	CLA	A	813	X	-	-	-
27	CLA	A	814	X	-	-	-
27	CLA	A	815	X	-	-	-
27	CLA	A	816	X	-	-	-
27	CLA	A	819	X	-	-	-
27	CLA	A	820	X	-	-	-
27	CLA	A	821	X	-	-	-
27	CLA	A	822	X	-	-	-
27	CLA	A	823	X	-	-	-
27	CLA	A	824	X	-	-	-
27	CLA	A	825	X	-	-	-
27	CLA	A	826	X	-	-	-
27	CLA	A	827	X	-	-	-
27	CLA	A	828	X	-	-	-
27	CLA	A	829	X	-	-	-
27	CLA	A	830	X	-	-	-
27	CLA	A	831	X	-	-	-
27	CLA	A	832	X	-	-	-
27	CLA	A	833	X	-	-	-
27	CLA	A	834	X	-	-	-
27	CLA	A	836	X	-	-	-
27	CLA	A	838	X	-	-	-
27	CLA	A	839	X	-	-	-
27	CLA	A	841	X	-	-	-
27	CLA	A	842	X	-	-	-
27	CLA	A	843	X	-	-	-
27	CLA	A	845	X	-	-	-
27	CLA	A	854	X	-	-	-
27	CLA	B	802	X	-	-	-
27	CLA	B	803	X	-	-	-
27	CLA	B	804	X	-	-	-
27	CLA	B	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	806	X	-	-	-
27	CLA	B	808	X	-	-	-
27	CLA	B	809	X	-	-	-
27	CLA	B	810	X	-	-	-
27	CLA	B	811	X	-	-	-
27	CLA	B	812	X	-	-	-
27	CLA	B	813	X	-	-	-
27	CLA	B	814	X	-	-	-
27	CLA	B	815	X	-	-	-
27	CLA	B	816	X	-	-	-
27	CLA	B	817	X	-	-	-
27	CLA	B	819	X	-	-	-
27	CLA	B	820	X	-	-	-
27	CLA	B	821	X	-	-	-
27	CLA	B	823	X	-	-	-
27	CLA	B	824	X	-	-	-
27	CLA	B	826	X	-	-	-
27	CLA	B	827	X	-	-	-
27	CLA	B	828	X	-	-	-
27	CLA	B	829	X	-	-	-
27	CLA	B	830	X	-	-	-
27	CLA	B	831	X	-	-	-
27	CLA	B	833	X	-	-	-
27	CLA	B	834	X	-	-	-
27	CLA	B	835	X	-	-	-
27	CLA	B	836	X	-	-	-
27	CLA	B	839	X	-	-	-
27	CLA	B	840	X	-	-	-
27	CLA	B	841	X	-	-	-
27	CLA	F	301	X	-	-	-
27	CLA	G	203	X	-	-	-
27	CLA	G	204	X	-	-	-
27	CLA	H	202	X	-	-	-
27	CLA	J	101	X	-	-	-
27	CLA	K	201	X	-	-	-
27	CLA	K	204	X	-	-	-
27	CLA	K	206	X	-	-	-
27	CLA	L	302	X	-	-	-
27	CLA	L	304	X	-	-	-
27	CLA	L	306	X	-	-	-
27	CLA	L	307	X	-	-	-
27	CLA	O	2001	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	O	2002	X	-	-	-
27	CLA	O	2003	X	-	-	-
27	CLA	U	602	X	-	-	-
27	CLA	U	603	X	-	-	-
27	CLA	U	604	X	-	-	-
27	CLA	U	610	X	-	-	-
27	CLA	U	611	X	-	-	-
27	CLA	U	612	X	-	-	-
27	CLA	U	613	X	-	-	-
27	CLA	U	614	X	-	-	-
27	CLA	V	602	X	-	-	-
27	CLA	V	603	X	-	-	-
27	CLA	V	604	X	-	-	-
27	CLA	V	610	X	-	-	-
27	CLA	V	611	X	-	-	-
27	CLA	V	612	X	-	-	-
27	CLA	V	613	X	-	-	-
27	CLA	V	614	X	-	-	-
27	CLA	W	602	X	-	-	-
27	CLA	W	603	X	-	-	-
27	CLA	W	604	X	-	-	-
27	CLA	W	610	X	-	-	-
27	CLA	W	611	X	-	-	-
27	CLA	W	612	X	-	-	-
27	CLA	W	613	X	-	-	-
27	CLA	W	614	X	-	-	-
27	CLA	X	602	X	-	-	-
27	CLA	X	603	X	-	-	-
27	CLA	X	604	X	-	-	-
27	CLA	X	610	X	-	-	-
27	CLA	X	611	X	-	-	-
27	CLA	X	612	X	-	-	-
27	CLA	X	613	X	-	-	-
27	CLA	X	614	X	-	-	-
27	CLA	Y	602	X	-	-	-
27	CLA	Y	603	X	-	-	-
27	CLA	Y	604	X	-	-	-
27	CLA	Y	610	X	-	-	-
27	CLA	Y	611	X	-	-	-
27	CLA	Y	612	X	-	-	-
27	CLA	Y	613	X	-	-	-
27	CLA	Y	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	Z	602	X	-	-	-
27	CLA	Z	603	X	-	-	-
27	CLA	Z	604	X	-	-	-
27	CLA	Z	610	X	-	-	-
27	CLA	Z	611	X	-	-	-
27	CLA	Z	612	X	-	-	-
27	CLA	Z	613	X	-	-	-
27	CLA	Z	614	X	-	-	-
27	CLA	a	602	X	-	-	-
27	CLA	a	603	X	-	-	-
27	CLA	a	604	X	-	-	-
27	CLA	a	606	X	-	-	-
27	CLA	a	607	X	-	-	-
27	CLA	a	608	X	-	-	-
27	CLA	a	609	X	-	-	-
27	CLA	a	610	X	-	-	-
27	CLA	a	611	X	-	-	-
27	CLA	a	612	X	-	-	-
27	CLA	a	613	X	-	-	-
27	CLA	a	614	X	-	-	-
27	CLA	a	616	X	-	-	-
38	CHL	U	601	X	-	-	-
38	CHL	U	605	X	-	-	-
38	CHL	U	606	X	-	-	-
38	CHL	U	607	X	-	-	-
38	CHL	U	608	X	-	-	-
38	CHL	U	609	X	-	-	-
38	CHL	V	601	X	-	-	-
38	CHL	V	605	X	-	-	-
38	CHL	V	606	X	-	-	-
38	CHL	V	607	X	-	-	-
38	CHL	V	608	X	-	-	-
38	CHL	V	609	X	-	-	-
38	CHL	W	601	X	-	-	-
38	CHL	W	605	X	-	-	-
38	CHL	W	606	X	-	-	-
38	CHL	W	607	X	-	-	-
38	CHL	W	608	X	-	-	-
38	CHL	W	609	X	-	-	-
38	CHL	X	601	X	-	-	-
38	CHL	X	605	X	-	-	-
38	CHL	X	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
38	CHL	X	607	X	-	-	-
38	CHL	X	608	X	-	-	-
38	CHL	X	609	X	-	-	-
38	CHL	Y	601	X	-	-	-
38	CHL	Y	605	X	-	-	-
38	CHL	Y	606	X	-	-	-
38	CHL	Y	607	X	-	-	-
38	CHL	Y	608	X	-	-	-
38	CHL	Y	609	X	-	-	-
38	CHL	Z	601	X	-	-	-
38	CHL	Z	605	X	-	-	-
38	CHL	Z	606	X	-	-	-
38	CHL	Z	607	X	-	-	-
38	CHL	Z	608	X	-	-	-
38	CHL	Z	609	X	-	-	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 69647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5819	3805	993	999	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5824	3825	977	1004	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	116	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1124	719	199	199	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	63	Total	C	N	O	0	0
			496	316	87	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1265	817	213	232	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	94	Total	C	N	O	0	0
			699	449	118	132		

- Molecule 8 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	100	Total	C	N	O	S	0	0
			776	482	138	154	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	42	Total	C	N	O	S	0	0
			316	217	45	53	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			337	231	47	58	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	86	Total	C	N	O	S	0	0
			582	370	100	110	2		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	159	Total	C	N	O	S	0	0
			1161	757	189	212	3		

- Molecule 13 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	O	97	Total	C	N	O	0	0
			758	503	123	132		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
14	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2	217	Total	C	N	O	S	0	0
			1682	1094	274	304	10		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	220	Total	C	N	O	S	0	0
			1678	1097	270	303	8		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	4	210	Total	C	N	O	S	0	0
			1631	1071	263	292	5		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	227	Total	C	N	O	S	0	0
			1774	1154	297	315	8		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	230	Total	C	N	O	S	0	0
			1771	1167	293	305	6		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	7	213	Total	C	N	O	S	0	0
			1649	1072	274	297	6		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	8	217	Total	C	N	O	S	0	0
			1649	1073	280	292	4		

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	9	183	Total	C	N	O	S	0	0
			1403	909	235	252	7		

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	220	Total	C	N	O	S	0	0
			1675	1088	273	309	5		
23	W	220	Total	C	N	O	S	0	0
			1671	1085	273	308	5		

- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	220	Total	C	N	O	S	0	0
			1679	1086	273	315	5		
24	U	219	Total	C	N	O	S	0	0
			1670	1080	272	313	5		

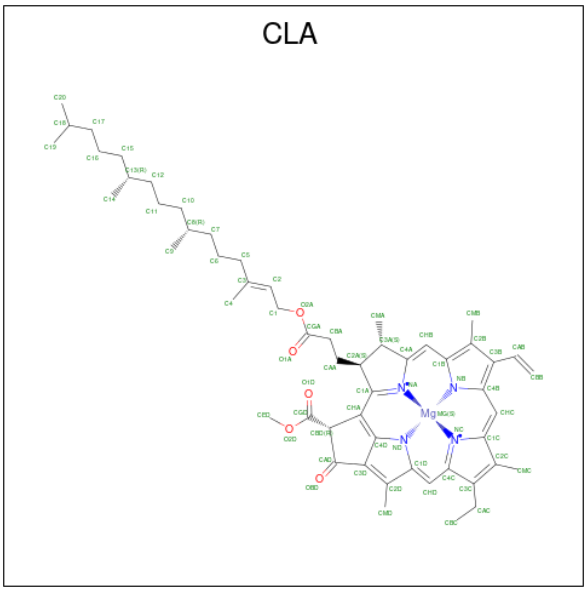
- Molecule 25 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	232	Total	C	N	O	P	S	0	0
			1780	1154	291	329	1	5		

- Molecule 26 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	V	238	Total	C	N	O	P	S	0	0
			1815	1176	300	333	1	5		

- Molecule 27 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
27	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
27	B	1	Total	C	Mg	N	O	0
			52	43	1	4	4	
27	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	B	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
27	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
27	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
27	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
27	O	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
27	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
27	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
27	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
27	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
27	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
27	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			37	29	1	4	3	
27	1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	2	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
27	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	3	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
27	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
27	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
27	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
27	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
27	7	1	Total	C	Mg	N	O	0
			43	33	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	9	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	Y	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
27	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Y	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Y	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			48	39	1	4	4	
27	U	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	U	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	U	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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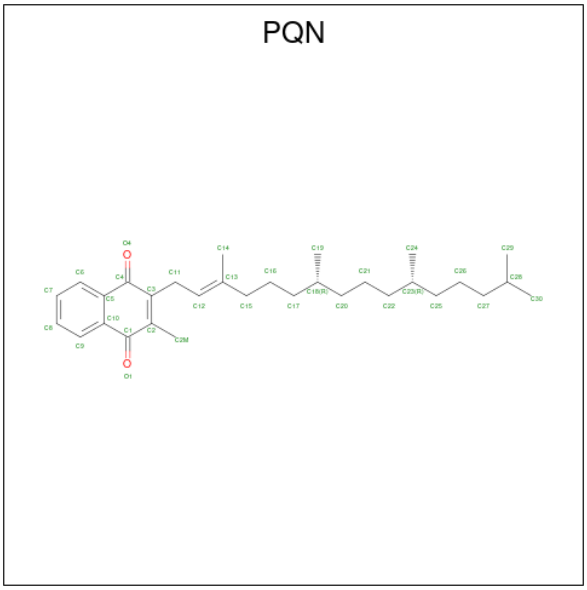
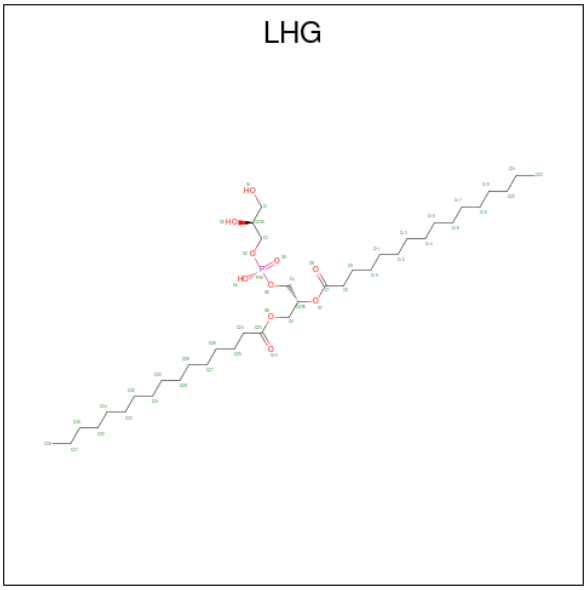
Mol	Chain	Residues	Atoms					AltConf
27	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			33	31	2	
28	B	1	Total	C	O	0
			33	31	2	

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	P	0
			49	38	10	1	
29	A	1	Total	C	O	P	0
			30	19	10	1	
29	B	1	Total	C	O	P	0
			38	27	10	1	
29	B	1	Total	C	O	P	0
			49	38	10	1	
29	H	1	Total	C	O	P	0
			49	38	10	1	
29	O	1	Total	C	O	P	0
			36	25	10	1	
29	a	1	Total	C	O	P	0
			43	32	10	1	
29	1	1	Total	C	O	P	0
			49	38	10	1	
29	2	1	Total	C	O	P	0
			36	25	10	1	

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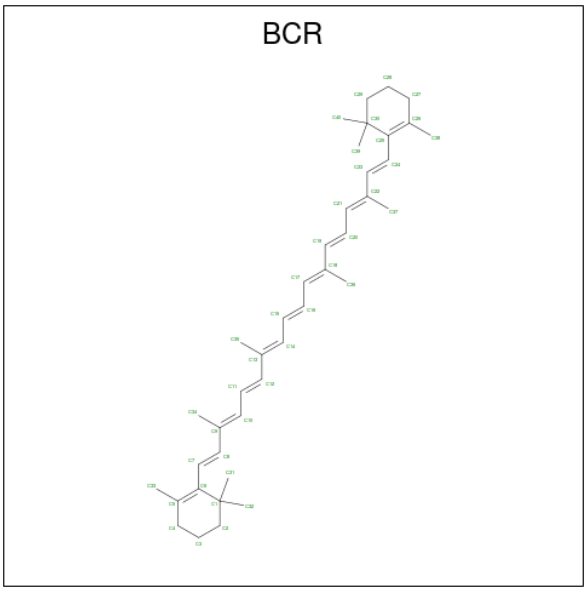
Mol	Chain	Residues	Atoms				AltConf
29	3	1	Total	C	O	P	0
			45	34	10	1	
29	3	1	Total	C	O	P	0
			49	38	10	1	
29	4	1	Total	C	O	P	0
			49	38	10	1	
29	5	1	Total	C	O	P	0
			49	38	10	1	
29	5	1	Total	C	O	P	0
			49	38	10	1	
29	6	1	Total	C	O	P	0
			48	37	10	1	
29	7	1	Total	C	O	P	0
			37	26	10	1	
29	8	1	Total	C	O	P	0
			49	38	10	1	
29	8	1	Total	C	O	P	0
			40	29	10	1	
29	9	1	Total	C	O	P	0
			30	19	10	1	
29	9	1	Total	C	O	P	0
			49	38	10	1	
29	9	1	Total	C	O	P	0
			49	38	10	1	
29	X	1	Total	C	O	P	0
			49	38	10	1	
29	Y	1	Total	C	O	P	0
			49	38	10	1	
29	Z	1	Total	C	O	P	0
			49	38	10	1	
29	U	1	Total	C	O	P	0
			49	38	10	1	
29	V	1	Total	C	O	P	0
			48	37	10	1	
29	W	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	G	1	Total C 40 40	0
30	J	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	O	1	Total C 40 40	0
30	O	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	1	1	Total C 40 40	0
30	2	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	4	1	Total C 40 40	0
30	5	1	Total C 40 40	0

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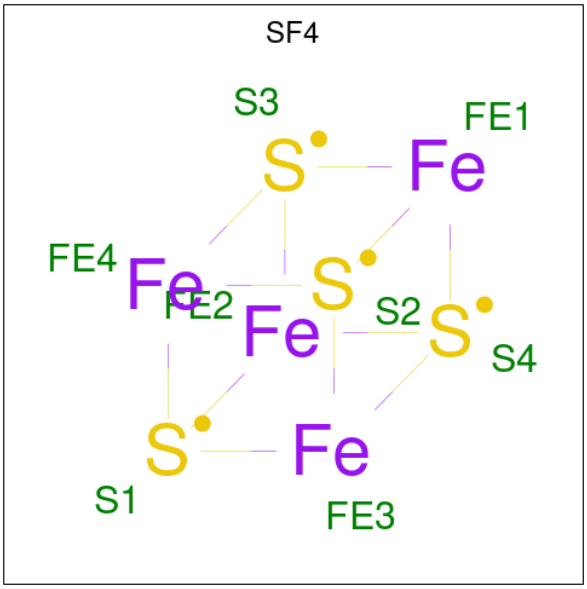
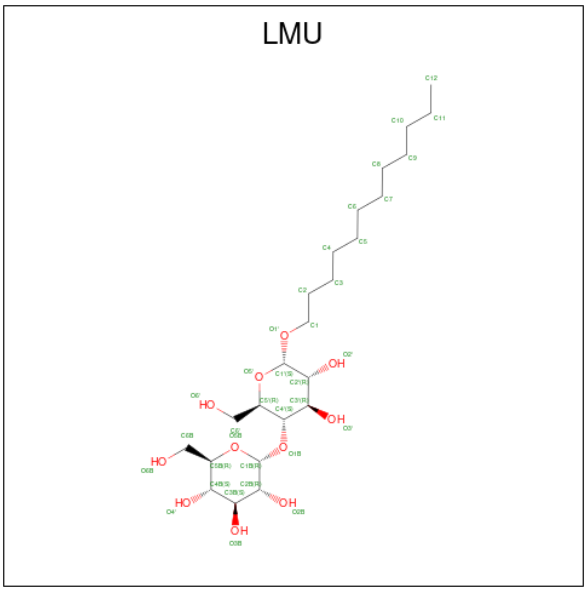
Mol	Chain	Residues	Atoms	AltConf
30	6	1	Total C 40 40	0
30	7	1	Total C 40 40	0
30	7	1	Total C 40 40	0
30	8	1	Total C 40 40	0
30	9	1	Total C 40 40	0

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



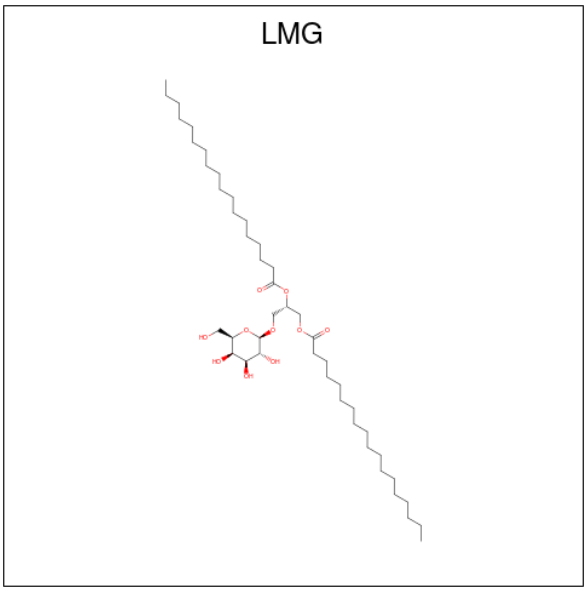
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total Fe S 8 4 4	0
31	C	1	Total Fe S 8 4 4	0
31	C	1	Total Fe S 8 4 4	0

- Molecule 32 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



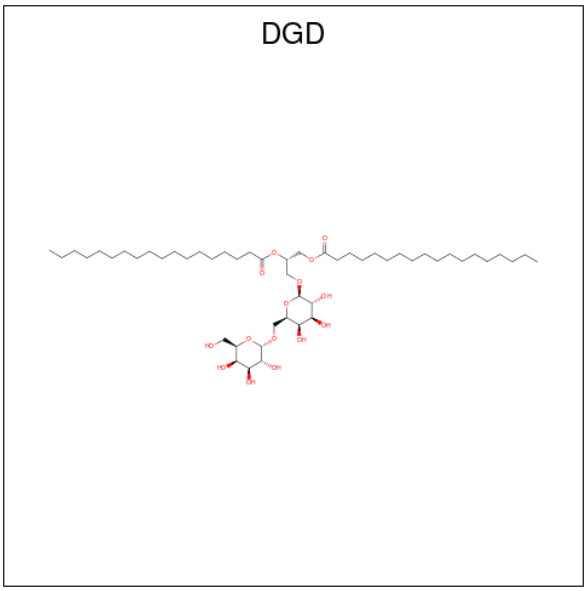
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			35	24	11	
32	A	1	Total	C	O	0
			34	24	10	
32	K	1	Total	C	O	0
			35	24	11	
32	1	1	Total	C	O	0
			35	24	11	
32	5	1	Total	C	O	0
			33	22	11	
32	5	1	Total	C	O	0
			32	21	11	
32	8	1	Total	C	O	0
			35	24	11	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



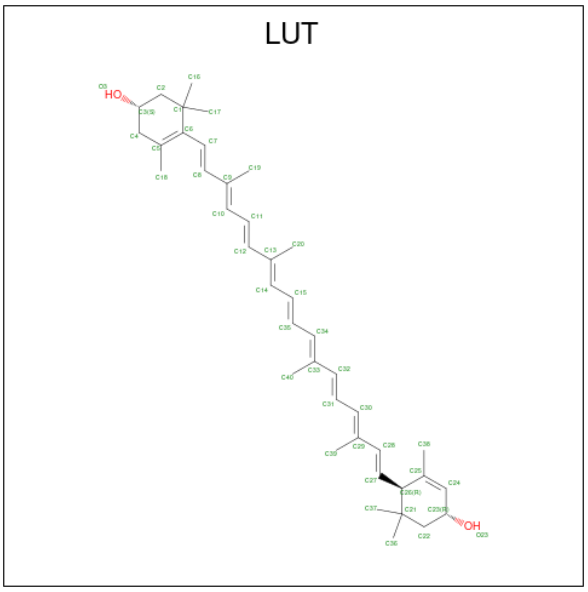
Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C O 40 30 10	0
33	H	1	Total C O 55 45 10	0
33	J	1	Total C O 42 32 10	0
33	J	1	Total C O 40 30 10	0
33	L	1	Total C O 37 27 10	0
33	4	1	Total C O 40 30 10	0
33	4	1	Total C O 40 30 10	0
33	5	1	Total C O 40 30 10	0
33	8	1	Total C O 46 36 10	0
33	9	1	Total C O 55 45 10	0
33	V	1	Total C O 41 31 10	0

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			62	47	15	

- Molecule 35 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
35	a	1	Total	C	O	0
			42	40	2	
35	1	1	Total	C	O	0
			42	40	2	

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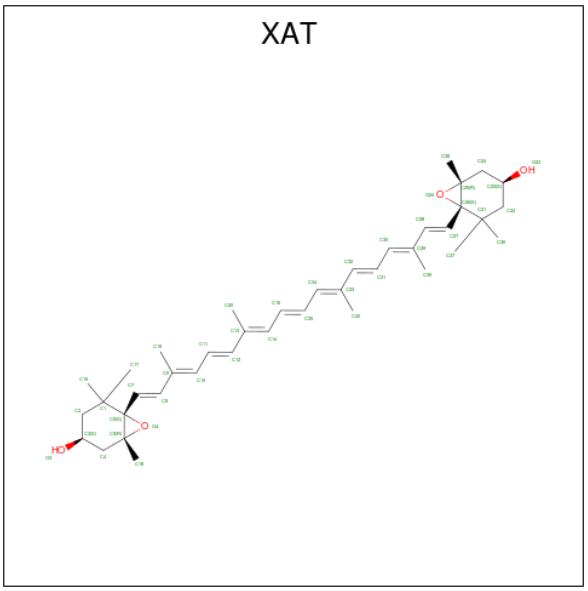
Mol	Chain	Residues	Atoms			AltConf
35	2	1	Total	C	O	0
			42	40	2	
35	3	1	Total	C	O	0
			42	40	2	
35	4	1	Total	C	O	0
			42	40	2	
35	5	1	Total	C	O	0
			42	40	2	
35	6	1	Total	C	O	0
			42	40	2	
35	7	1	Total	C	O	0
			42	40	2	
35	8	1	Total	C	O	0
			42	40	2	
35	9	1	Total	C	O	0
			42	40	2	
35	X	1	Total	C	O	0
			42	40	2	
35	X	1	Total	C	O	0
			42	40	2	
35	Y	1	Total	C	O	0
			42	40	2	
35	Y	1	Total	C	O	0
			42	40	2	
35	Z	1	Total	C	O	0
			42	40	2	
35	Z	1	Total	C	O	0
			42	40	2	
35	U	1	Total	C	O	0
			42	40	2	
35	U	1	Total	C	O	0
			42	40	2	
35	V	1	Total	C	O	0
			42	40	2	
35	V	1	Total	C	O	0
			42	40	2	
35	W	1	Total	C	O	0
			42	40	2	
35	W	1	Total	C	O	0
			42	40	2	

- Molecule 36 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
36	a	1	Total	C	O	0
			44	40	4	
36	1	1	Total	C	O	0
			44	40	4	
36	2	1	Total	C	O	0
			44	40	4	
36	3	1	Total	C	O	0
			44	40	4	
36	4	1	Total	C	O	0
			44	40	4	
36	5	1	Total	C	O	0
			44	40	4	
36	6	1	Total	C	O	0
			44	40	4	
36	7	1	Total	C	O	0
			44	40	4	
36	8	1	Total	C	O	0
			44	40	4	
36	9	1	Total	C	O	0
			44	40	4	
36	X	1	Total	C	O	0
			44	40	4	
36	Y	1	Total	C	O	0
			44	40	4	
36	Z	1	Total	C	O	0
			44	40	4	
36	U	1	Total	C	O	0
			44	40	4	

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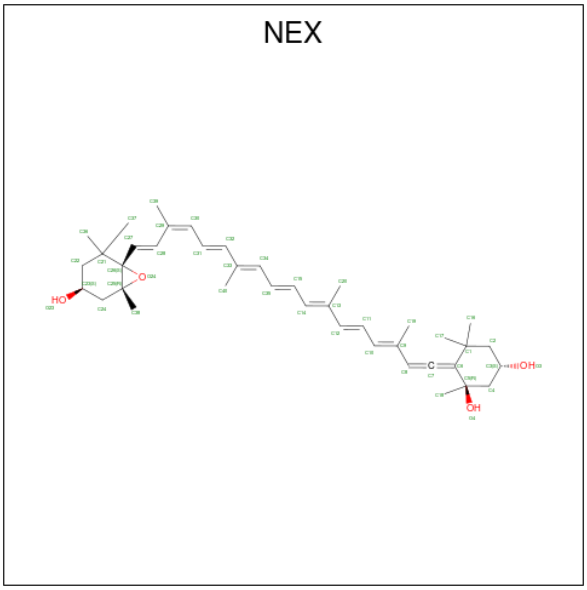
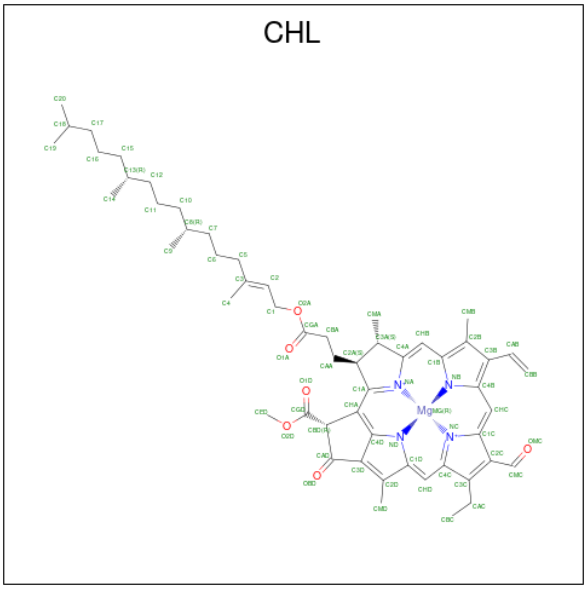
Mol	Chain	Residues	Atoms	AltConf
36	V	1	Total C O 44 40 4	0
36	W	1	Total C O 44 40 4	0

- Molecule 37 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	AltConf
37	5	1	Total C O 44 40 4	0
37	6	1	Total C O 44 40 4	0
37	X	1	Total C O 44 40 4	0
37	Y	1	Total C O 43 40 3	0
37	Z	1	Total C O 44 40 4	0
37	U	1	Total C O 44 40 4	0
37	V	1	Total C O 44 40 4	0
37	W	1	Total C O 44 40 4	0

- Molecule 38 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
38	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	X	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
38	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
38	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
38	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
38	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Z	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
38	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	Z	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	U	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
38	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
38	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
38	U	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
38	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
38	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
38	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	V	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	V	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
38	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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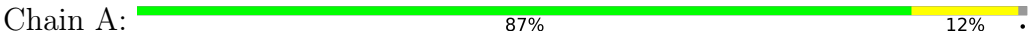
Mol	Chain	Residues	Atoms					AltConf
38	W	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
38	W	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
38	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

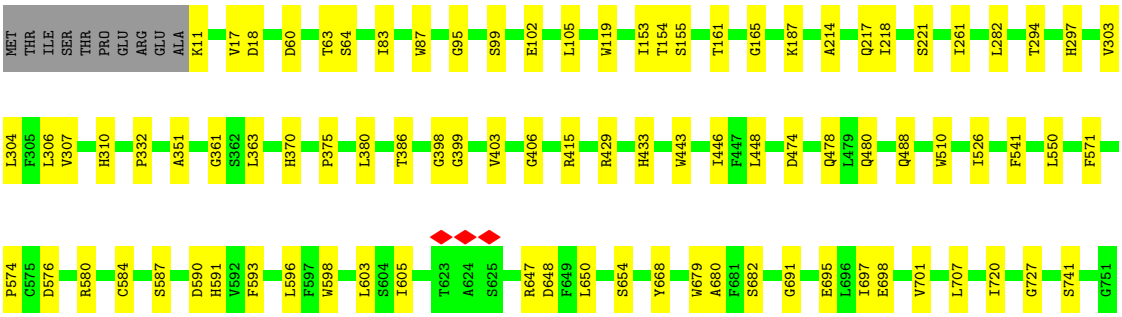
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

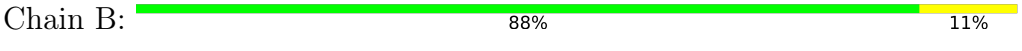
Chain A:

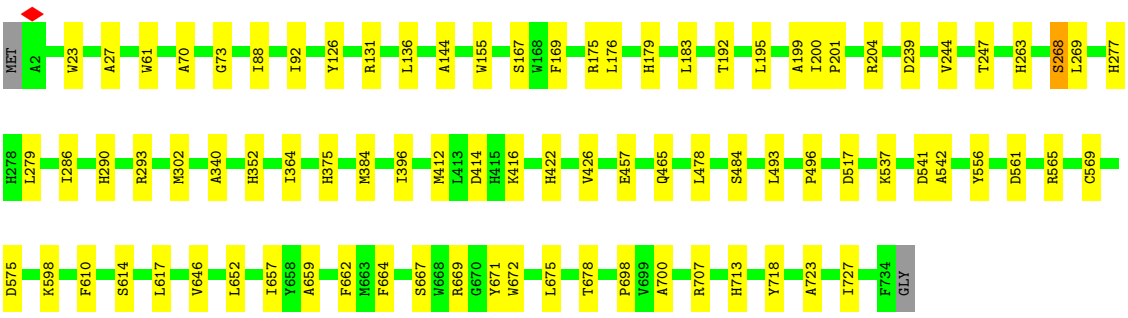




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

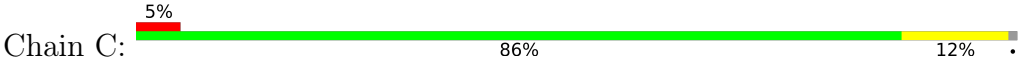
Chain B:

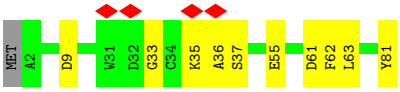




• Molecule 3: Photosystem I iron-sulfur center

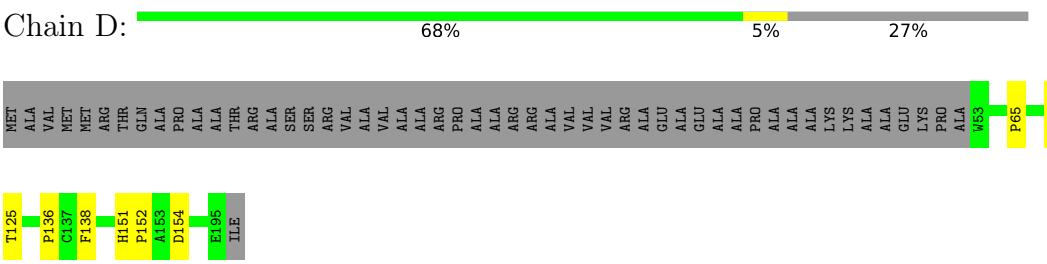
Chain C:





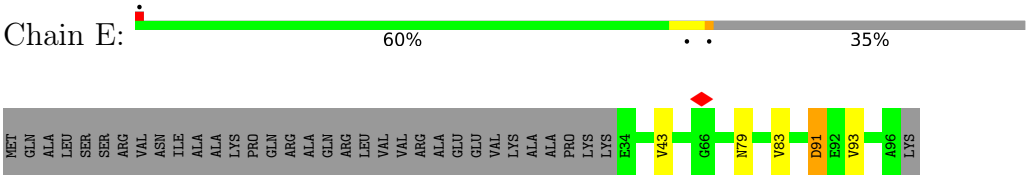
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:



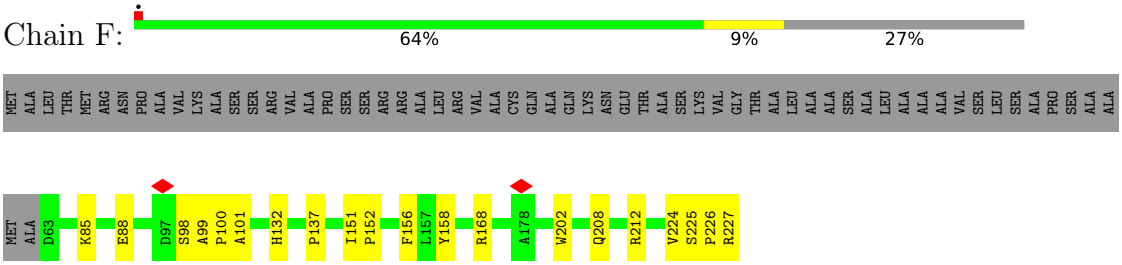
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



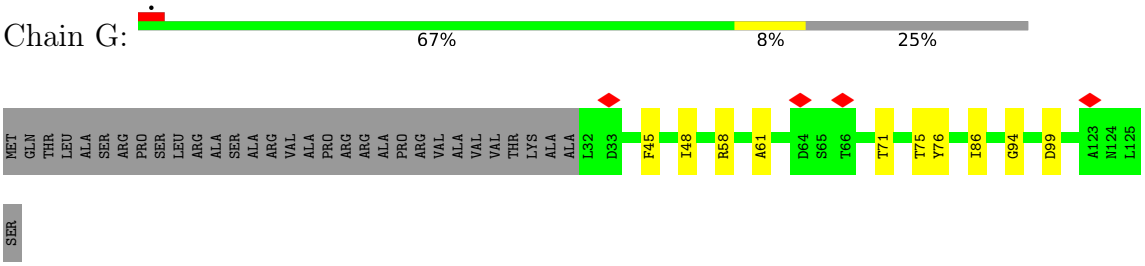
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:



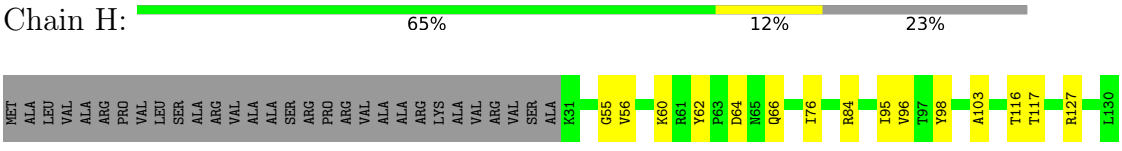
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:



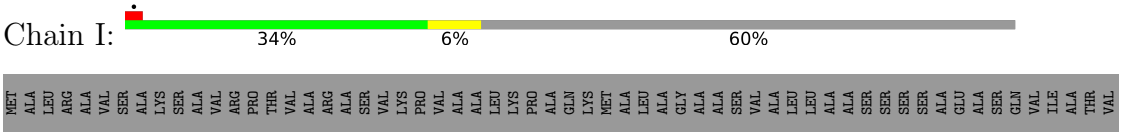
• Molecule 8: Photosystem I reaction center subunit VI, chloroplastic

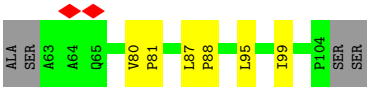
Chain H:



• Molecule 9: Photosystem I reaction center subunit VIII

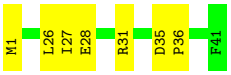
Chain I:





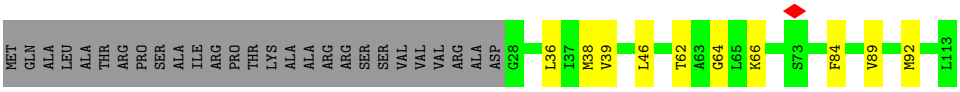
• Molecule 10: Photosystem I reaction center subunit IX

Chain J:



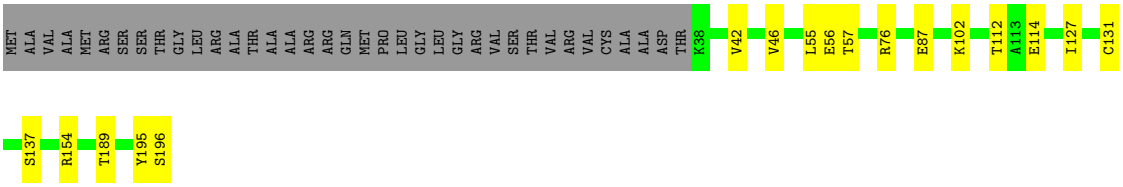
• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:



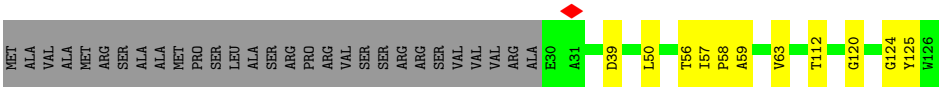
• Molecule 12: PSI subunit V

Chain L:



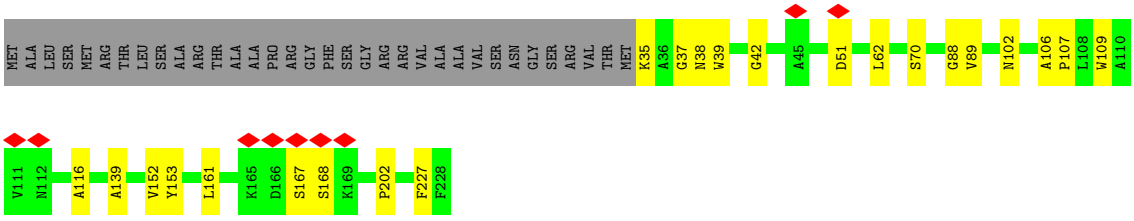
• Molecule 13: Photosystem I subunit O

Chain O:



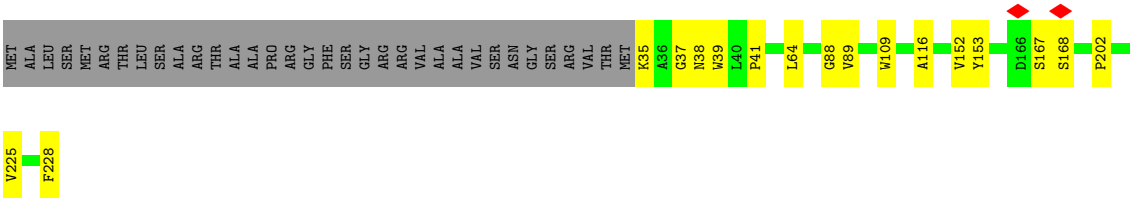
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain a:



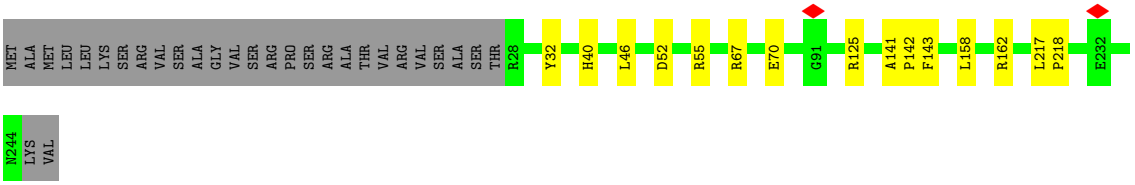
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



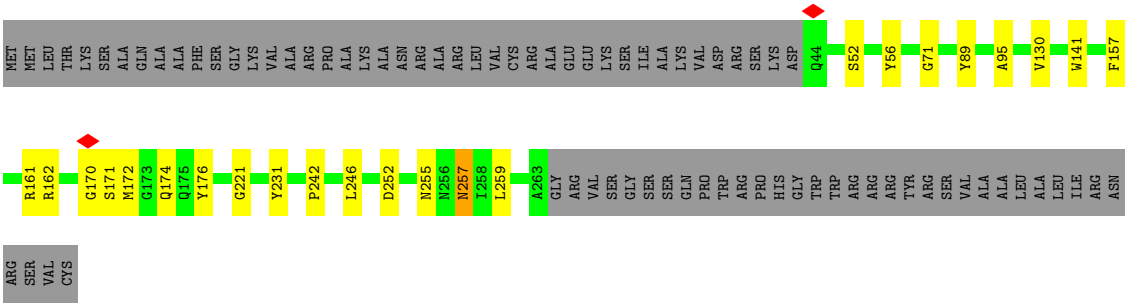
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



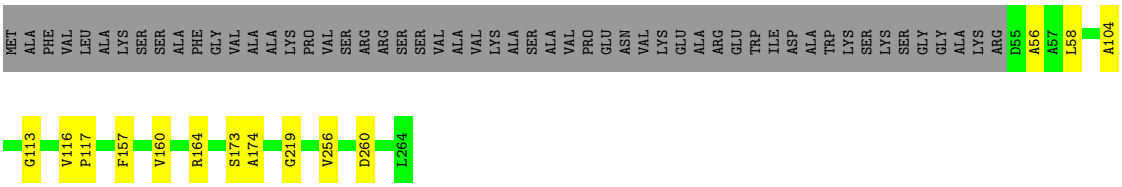
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



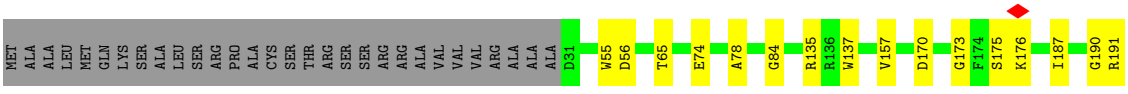
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

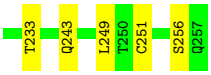
Chain 4:



• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

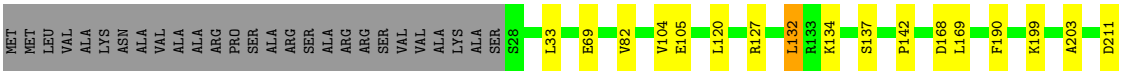
Chain 5:





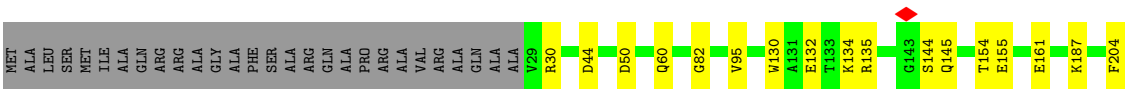
• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

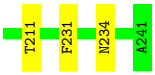
Chain 6:



• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



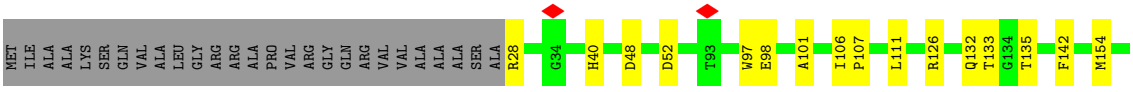


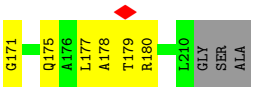
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 8:

• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

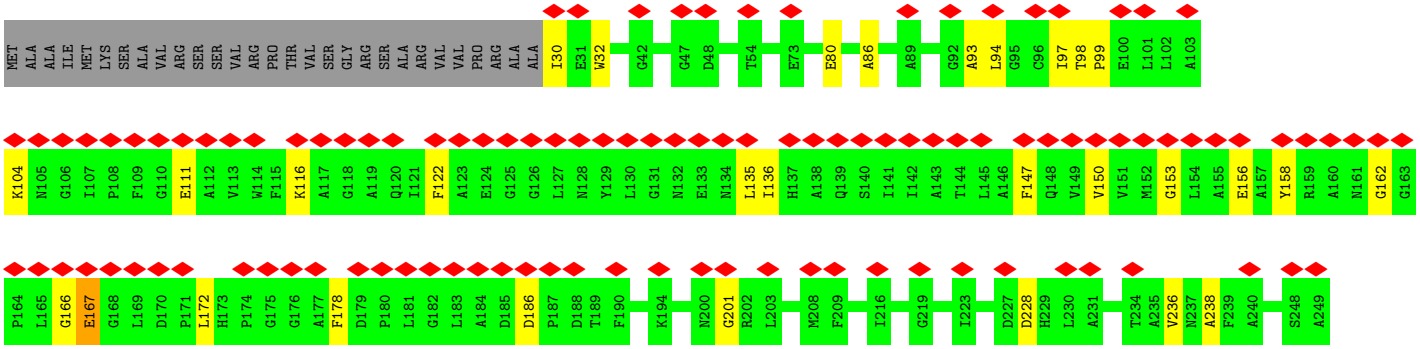
Chain 9:





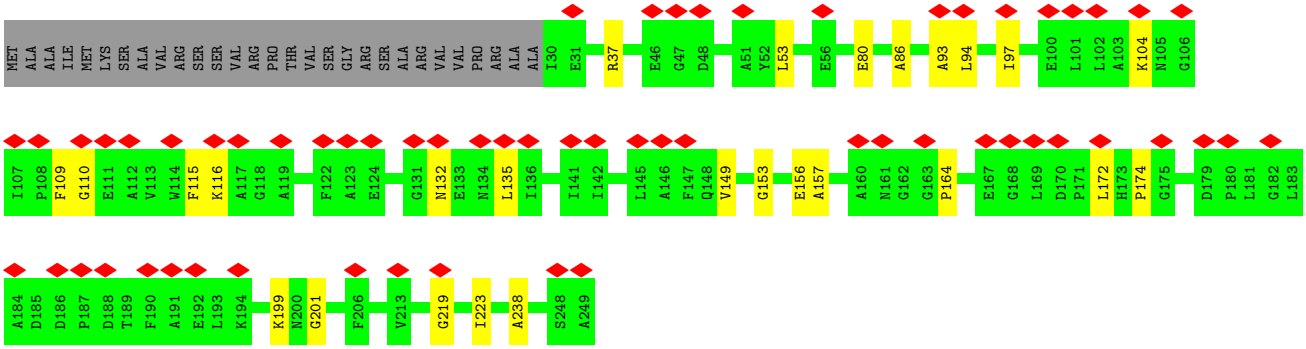
• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain X:



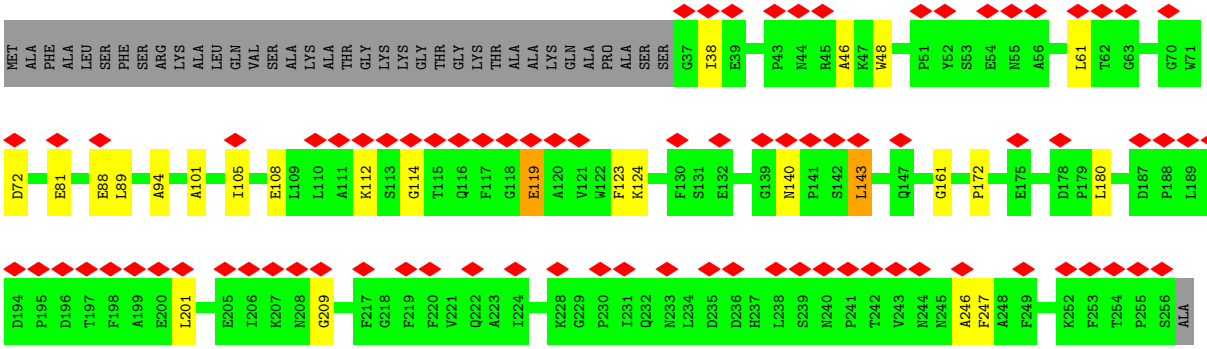
• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain W:



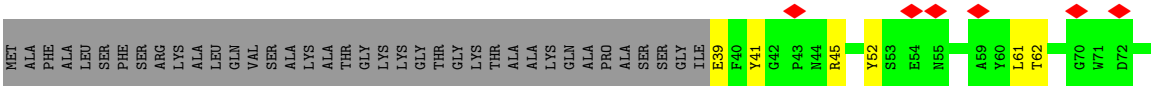
• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

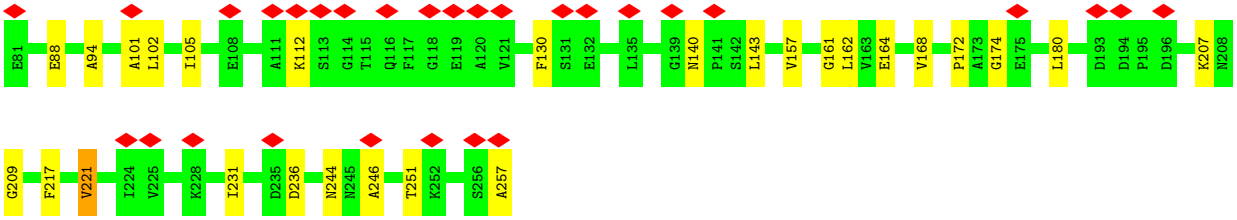
Chain Y:



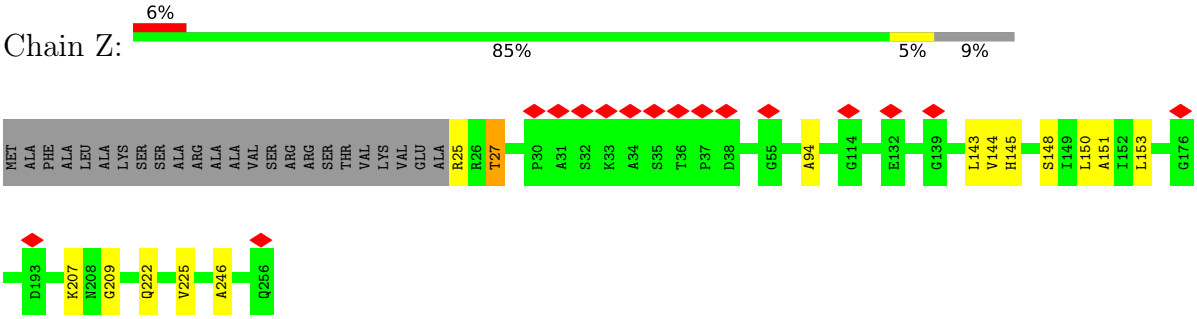
• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain U:

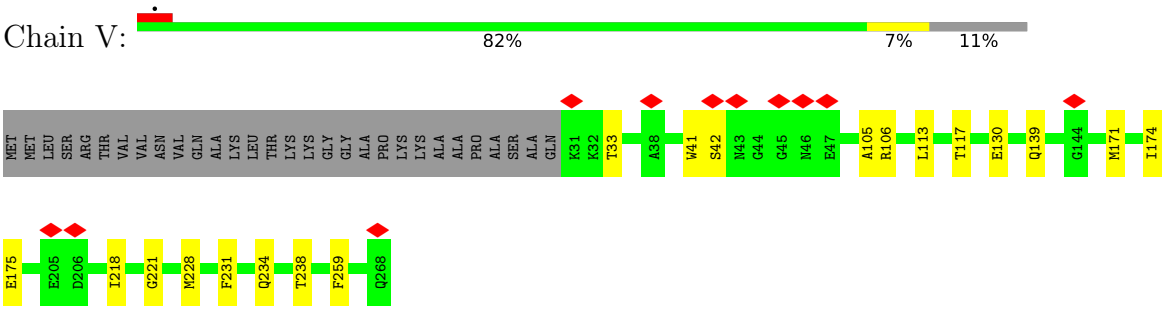




• Molecule 25: Chlorophyll a-b binding protein, chloroplastic



• Molecule 26: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1.5625	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.216	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, NEX, BCR, SF4, DGD, LMG, LMU, TPO, XAT, PQN, CLA, CHL, LUT

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	0.31	0/6015	0.32	0/8201
2	B	0.29	0/6036	0.34	0/8242
3	C	0.24	0/610	0.37	0/826
4	D	0.24	0/1152	0.36	0/1556
5	E	0.21	0/506	0.30	0/689
6	F	0.23	0/1291	0.33	0/1747
7	G	0.20	0/714	0.33	0/972
8	H	0.23	0/788	0.32	0/1059
9	I	0.28	0/329	0.35	0/456
10	J	0.27	0/349	0.30	0/478
11	K	0.24	0/587	0.38	0/795
12	L	0.27	0/1190	0.36	0/1628
13	O	0.25	0/784	0.35	0/1069
14	1	0.29	0/1490	0.41	0/2028
14	a	0.32	0/1490	0.44	0/2028
15	2	0.22	0/1730	0.35	0/2353
16	3	0.26	0/1726	0.34	0/2342
17	4	0.22	0/1686	0.33	0/2300
18	5	0.24	0/1829	0.36	0/2492
19	6	0.29	0/1833	0.42	0/2505
20	7	0.27	0/1701	0.34	0/2310
21	8	0.27	0/1700	0.35	0/2315
22	9	0.23	0/1444	0.39	0/1964
23	W	0.39	0/1721	0.43	0/2341
23	X	0.24	0/1725	0.47	1/2348 (0.0%)
24	U	0.42	0/1718	0.48	0/2338
24	Y	0.25	0/1727	0.46	0/2350
25	Z	0.13	0/1822	0.30	0/2474
26	V	0.40	0/1856	0.40	0/2518
All	All	0.28	0/47549	0.37	1/64724 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	X	166	GLY	CA-C-O	-6.01	118.31	122.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5819	0	5670	68	0
2	B	5824	0	5579	72	0
3	C	600	0	581	6	0
4	D	1124	0	1139	6	0
5	E	496	0	491	4	0
6	F	1265	0	1301	16	0
7	G	699	0	681	9	0
8	H	776	0	765	17	0
9	I	316	0	321	3	0
10	J	337	0	336	5	0
11	K	582	0	620	13	0
12	L	1161	0	1184	16	0
13	O	758	0	740	10	0
14	1	1444	0	1396	12	0
14	a	1444	0	1396	20	0
15	2	1682	0	1665	15	0
16	3	1678	0	1637	19	0
17	4	1631	0	1587	11	0
18	5	1774	0	1746	18	0
19	6	1771	0	1770	19	0
20	7	1649	0	1589	15	0
21	8	1649	0	1629	32	0
22	9	1403	0	1381	21	0
23	W	1671	0	1604	28	0
23	X	1675	0	1617	27	0
24	U	1670	0	1604	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Y	1679	0	1620	26	0
25	Z	1780	0	1723	14	0
26	V	1815	0	1765	32	0
27	1	666	0	522	1	0
27	2	641	0	533	9	0
27	3	724	0	628	9	0
27	4	778	0	678	8	0
27	5	878	0	758	9	0
27	6	903	0	831	6	0
27	7	756	0	635	5	0
27	8	724	0	629	4	0
27	9	595	0	491	5	0
27	A	2669	0	2693	40	0
27	B	2282	0	2232	40	0
27	F	140	0	113	1	0
27	G	87	0	64	0	0
27	H	104	0	93	1	0
27	J	42	0	31	0	0
27	K	191	0	150	7	0
27	L	235	0	184	4	0
27	O	116	0	61	0	0
27	U	401	0	344	4	0
27	V	415	0	365	4	0
27	W	426	0	377	5	0
27	X	436	0	415	5	0
27	Y	429	0	389	6	0
27	Z	496	0	520	2	0
27	a	710	0	591	2	0
28	A	33	0	46	0	0
28	B	33	0	46	2	0
29	1	49	0	74	0	0
29	2	36	0	42	0	0
29	3	94	0	137	1	0
29	4	49	0	74	0	0
29	5	98	0	148	1	0
29	6	48	0	69	0	0
29	7	37	0	44	1	0
29	8	89	0	124	0	0
29	9	128	0	178	2	0
29	A	79	0	104	0	0
29	B	87	0	120	1	0
29	H	49	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	O	36	0	42	0	0
29	U	49	0	74	0	0
29	V	48	0	69	2	0
29	W	44	0	61	0	0
29	X	49	0	74	0	0
29	Y	49	0	74	0	0
29	Z	49	0	74	2	0
29	a	43	0	59	0	0
30	1	40	0	56	2	0
30	2	40	0	56	9	0
30	3	120	0	168	15	0
30	4	40	0	56	3	0
30	5	40	0	56	3	0
30	6	40	0	56	3	0
30	7	80	0	112	10	0
30	8	40	0	56	3	0
30	9	40	0	56	5	0
30	A	240	0	336	38	0
30	B	400	0	560	50	0
30	F	40	0	56	8	0
30	G	40	0	56	2	0
30	J	40	0	56	10	0
30	K	80	0	112	17	0
30	L	160	0	224	20	0
30	O	80	0	112	11	0
30	a	40	0	56	2	0
31	A	8	0	0	0	0
31	C	16	0	0	0	0
32	1	35	0	46	0	0
32	5	65	0	76	0	0
32	8	35	0	46	0	0
32	A	69	0	90	1	0
32	K	35	0	46	1	0
33	4	80	0	100	0	0
33	5	40	0	50	1	0
33	8	46	0	65	0	0
33	9	55	0	86	0	0
33	A	40	0	50	1	0
33	H	55	0	86	0	0
33	J	82	0	107	0	0
33	L	37	0	44	1	0
33	V	41	0	52	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B	62	0	85	3	0
35	1	42	0	56	3	0
35	2	42	0	56	2	0
35	3	42	0	56	3	0
35	4	42	0	56	4	0
35	5	42	0	56	0	0
35	6	42	0	56	3	0
35	7	42	0	56	2	0
35	8	42	0	56	3	0
35	9	42	0	56	2	0
35	U	84	0	112	2	0
35	V	84	0	112	2	0
35	W	84	0	112	2	0
35	X	84	0	112	5	0
35	Y	84	0	112	3	0
35	Z	84	0	112	4	0
35	a	42	0	56	4	0
36	1	44	0	56	1	0
36	2	44	0	56	0	0
36	3	44	0	56	1	0
36	4	44	0	56	0	0
36	5	44	0	56	3	0
36	6	44	0	56	1	0
36	7	44	0	56	2	0
36	8	44	0	56	0	0
36	9	44	0	56	0	0
36	U	44	0	56	3	0
36	V	44	0	56	0	0
36	W	44	0	56	1	0
36	X	44	0	56	0	0
36	Y	44	0	56	1	0
36	Z	44	0	56	1	0
36	a	44	0	56	1	0
37	5	44	0	56	2	0
37	6	44	0	56	1	0
37	U	44	0	56	0	0
37	V	44	0	56	1	0
37	W	44	0	56	2	0
37	X	44	0	56	2	0
37	Y	43	0	55	2	0
37	Z	44	0	56	4	0
38	U	303	0	248	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	V	309	0	253	28	0
38	W	336	0	298	19	0
38	X	354	0	342	16	0
38	Y	335	0	302	19	0
38	Z	338	0	309	17	0
All	All	69647	0	68867	860	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (860) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:140:ASN:CB	24:U:143:LEU:HD13	1.49	1.42
12:L:114:GLU:HG2	12:L:189:THR:CG2	1.67	1.24
22:9:133:THR:HG22	22:9:135:THR:CG2	1.71	1.20
22:9:133:THR:CG2	22:9:135:THR:HG22	1.74	1.18
12:L:114:GLU:CG	12:L:189:THR:HG21	1.75	1.16
21:8:78:CYS:SG	21:8:201:MET:HE2	1.89	1.12
18:5:233:THR:HA	18:5:256:SER:OG	1.48	1.11
24:U:140:ASN:HB3	24:U:143:LEU:HD13	1.32	1.11
1:A:95:GLY:HA2	1:A:99:SER:OG	1.52	1.09
24:U:140:ASN:HB2	24:U:143:LEU:HD13	1.12	1.08
11:K:89:VAL:HG21	27:K:201:CLA:HMD1	1.33	1.07
11:K:89:VAL:HG21	27:K:201:CLA:CMD	1.85	1.06
2:B:244:VAL:HG23	2:B:247:THR:OG1	1.58	1.03
24:U:140:ASN:CB	24:U:143:LEU:CD1	2.35	1.03
24:Y:140:ASN:HD22	24:Y:143:LEU:HD13	1.20	1.03
24:Y:140:ASN:HD22	24:Y:143:LEU:CD1	1.72	1.01
23:X:135:LEU:CD2	23:X:136:ILE:HG12	1.91	1.00
26:V:174:ILE:HD11	38:V:608:CHL:C4A	1.93	0.98
12:L:55:LEU:O	12:L:57:THR:HG23	1.67	0.94
24:U:140:ASN:HB3	24:U:143:LEU:CD1	1.97	0.91
26:V:174:ILE:HD11	38:V:608:CHL:CHB	2.00	0.90
21:8:164:THR:HG22	21:8:165:SER:H	1.36	0.90
26:V:171:MET:HA	26:V:174:ILE:HG22	1.50	0.90
26:V:171:MET:HA	26:V:174:ILE:CG2	2.03	0.88
30:B:843:BCR:H362	30:G:205:BCR:H312	1.53	0.88
30:7:623:BCR:H321	30:7:623:BCR:HC8	1.56	0.87
21:8:164:THR:HG22	21:8:165:SER:N	1.90	0.86
30:7:623:BCR:H323	21:8:230:TRP:CE2	2.11	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:135:LEU:HD23	23:X:136:ILE:HG12	1.54	0.86
23:W:132:ASN:HB2	23:W:135:LEU:CD1	2.07	0.85
30:B:843:BCR:HC8	30:B:843:BCR:H331	1.59	0.83
24:U:140:ASN:HB2	24:U:143:LEU:CD1	2.01	0.82
27:A:808:CLA:HBB2	30:J:102:BCR:H312	1.60	0.82
26:V:171:MET:CA	26:V:174:ILE:HG22	2.10	0.82
23:X:135:LEU:HD22	23:X:136:ILE:HG12	1.59	0.82
26:V:174:ILE:HD11	38:V:608:CHL:CMA	2.10	0.81
11:K:89:VAL:CG2	27:K:201:CLA:CMD	2.59	0.80
30:A:850:BCR:H321	30:A:850:BCR:HC8	1.63	0.80
12:L:114:GLU:HG2	12:L:189:THR:HG21	0.83	0.80
21:8:78:CYS:SG	21:8:201:MET:CE	2.68	0.80
22:9:133:THR:CG2	22:9:135:THR:CG2	2.46	0.80
30:B:843:BCR:H383	30:B:843:BCR:H23C	1.64	0.79
26:V:171:MET:C	26:V:174:ILE:HG22	2.06	0.79
26:V:171:MET:O	26:V:174:ILE:HG22	1.82	0.79
24:Y:140:ASN:ND2	24:Y:143:LEU:HD13	1.97	0.79
30:L:309:BCR:HC8	30:L:309:BCR:H311	1.66	0.77
30:A:856:BCR:H321	30:A:856:BCR:HC8	1.66	0.76
27:2:613:CLA:HMB1	35:2:619:LUT:H7	1.68	0.76
30:B:801:BCR:H312	27:B:833:CLA:H62	1.65	0.76
27:B:821:CLA:CAD	30:B:843:BCR:H312	2.16	0.76
11:K:89:VAL:CG2	27:K:201:CLA:HMD1	2.15	0.76
30:B:845:BCR:H383	30:B:845:BCR:H23C	1.69	0.75
27:B:821:CLA:C3D	30:B:843:BCR:H312	2.16	0.74
30:O:2004:BCR:H383	30:O:2004:BCR:H23C	1.68	0.74
21:8:164:THR:CG2	21:8:165:SER:H	2.01	0.74
14:a:227:PHE:HE1	21:8:100:LEU:HD21	1.52	0.74
26:V:174:ILE:CD1	38:V:608:CHL:CMA	2.65	0.74
30:L:301:BCR:HC8	30:L:301:BCR:H311	1.71	0.73
20:7:234:ASN:ND2	27:7:613:CLA:OBD	2.21	0.73
23:X:111:GLU:OE2	23:X:116:LYS:HD2	1.88	0.73
30:B:852:BCR:H383	30:B:852:BCR:H23C	1.71	0.72
30:L:305:BCR:H311	30:L:305:BCR:HC8	1.69	0.72
37:Z:1623:NEX:H163	24:U:162:LEU:HD21	1.71	0.72
24:U:217:PHE:O	24:U:221:VAL:HG23	1.89	0.72
26:V:174:ILE:CD1	38:V:608:CHL:CHB	2.67	0.72
12:L:189:THR:HG23	12:L:195:TYR:CE2	2.25	0.72
22:9:133:THR:HG22	22:9:135:THR:HG22	0.84	0.72
8:H:84:ARG:HH22	12:L:137:SER:HB2	1.54	0.71
30:A:852:BCR:H362	27:A:854:CLA:C4	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLY:CA	1:A:99:SER:OG	2.36	0.71
2:B:244:VAL:HG23	2:B:247:THR:HG1	1.55	0.71
30:L:301:BCR:H383	30:L:301:BCR:H23C	1.72	0.71
15:2:141:ALA:HB3	15:2:142:PRO:HD3	1.72	0.71
27:A:808:CLA:CBB	30:J:102:BCR:H312	2.21	0.70
30:A:852:BCR:H362	27:A:854:CLA:H42	1.73	0.70
6:F:137:PRO:CD	30:F:305:BCR:H312	2.21	0.70
33:A:860:LMG:HC1	20:7:60:GLN:HE22	1.57	0.70
10:J:1:MET:N	20:7:60:GLN:OE1	2.25	0.70
27:A:829:CLA:H11	30:A:852:BCR:H323	1.74	0.69
15:2:67:ARG:NH1	15:2:70:GLU:OE1	2.24	0.69
30:7:621:BCR:H312	27:8:611:CLA:HAB	1.73	0.69
30:B:848:BCR:H382	30:B:848:BCR:H23C	1.74	0.69
2:B:244:VAL:CG2	2:B:247:THR:OG1	2.38	0.69
27:B:808:CLA:CMC	30:B:848:BCR:HC22	2.23	0.69
23:W:132:ASN:HB2	23:W:135:LEU:HD12	1.73	0.69
38:X:607:CHL:HBB2	35:X:1621:LUT:H193	1.75	0.69
30:B:844:BCR:HC8	30:B:844:BCR:H311	1.75	0.69
14:a:227:PHE:CE1	21:8:100:LEU:HD21	2.28	0.68
7:G:58:ARG:NH2	7:G:94:GLY:O	2.26	0.68
29:B:851:LHG:HC12	14:1:64:LEU:HA	1.74	0.68
8:H:116:THR:HG22	8:H:117:THR:N	2.08	0.68
22:9:107:PRO:O	22:9:111:LEU:HG	1.93	0.68
19:6:127:ARG:HH11	27:6:618:CLA:HMC2	1.59	0.68
27:A:816:CLA:C1C	30:K:202:BCR:H312	2.24	0.67
38:Y:607:CHL:H142	38:Y:607:CHL:HMB2	1.77	0.67
18:5:65:THR:HG22	27:5:619:CLA:HBA1	1.75	0.67
21:8:164:THR:CG2	21:8:165:SER:N	2.58	0.67
1:A:707:LEU:O	6:F:168:ARG:NH1	2.28	0.66
17:4:256:VAL:N	27:4:613:CLA:O1A	2.29	0.66
1:A:11:LYS:N	16:3:52:SER:HG	1.94	0.66
30:B:844:BCR:H382	30:B:844:BCR:H23C	1.77	0.66
30:7:623:BCR:H323	21:8:230:TRP:CD2	2.31	0.66
23:X:94:LEU:O	23:X:98:THR:HG23	1.96	0.66
27:3:617:CLA:HBB2	30:3:621:BCR:HC22	1.78	0.66
1:A:60:ASP:OD2	1:A:415:ARG:NH1	2.29	0.66
4:D:151:HIS:HB3	4:D:152:PRO:HD3	1.76	0.66
2:B:465:GLN:NE2	27:B:836:CLA:OBD	2.30	0.65
30:B:801:BCR:H321	6:F:156:PHE:HB2	1.77	0.65
30:3:622:BCR:H321	30:3:622:BCR:HC8	1.78	0.65
5:E:43:VAL:HG21	5:E:93:VAL:HB	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:63:VAL:HG11	30:O:2005:BCR:HC21	1.79	0.65
30:O:2005:BCR:H23C	30:O:2005:BCR:H383	1.78	0.65
2:B:167:SER:OG	7:G:71:THR:CG2	2.45	0.65
16:3:130:VAL:HG21	36:3:619:XAT:H172	1.78	0.65
30:5:622:BCR:H403	30:5:622:BCR:H23C	1.79	0.65
26:V:174:ILE:CD1	38:V:608:CHL:HMA3	2.28	0.64
30:O:2004:BCR:HC8	30:O:2004:BCR:H331	1.78	0.64
27:3:617:CLA:CBB	30:3:621:BCR:HC22	2.27	0.64
19:6:69:GLU:HG2	19:6:132:LEU:HD11	1.80	0.64
27:a:603:CLA:H2	21:8:155:LEU:HB2	1.79	0.64
15:2:46:LEU:O	15:2:67:ARG:NH2	2.30	0.64
18:5:74:GLU:OE2	18:5:191:ARG:NH2	2.31	0.64
2:B:575:ASP:OD1	2:B:707:ARG:NH2	2.31	0.64
11:K:89:VAL:CG2	27:K:201:CLA:HMD2	2.27	0.64
8:H:76:ILE:HD12	27:H:203:CLA:HMA1	1.81	0.63
23:X:98:THR:OG1	23:X:99:PRO:HD3	1.98	0.63
30:K:202:BCR:H331	30:K:202:BCR:HC8	1.79	0.63
18:5:135:ARG:NH2	27:6:601:CLA:OBD	2.32	0.63
23:X:135:LEU:HD22	23:X:136:ILE:CG1	2.28	0.63
26:V:171:MET:O	26:V:174:ILE:CG2	2.47	0.63
1:A:119:TRP:CD2	30:A:856:BCR:H323	2.34	0.63
23:W:132:ASN:CB	23:W:135:LEU:HG	2.29	0.63
11:K:84:PHE:HE2	11:K:89:VAL:HG22	1.65	0.62
27:9:610:CLA:HAB	35:9:619:LUT:H32	1.81	0.62
1:A:474:ASP:OD1	1:A:480:GLN:NE2	2.32	0.62
27:A:816:CLA:NC	30:K:202:BCR:H312	2.13	0.62
6:F:137:PRO:HD3	30:F:305:BCR:HC22	1.82	0.62
24:Y:172:PRO:HG2	38:Y:608:CHL:CBB	2.29	0.62
26:V:174:ILE:HD11	38:V:608:CHL:HMA3	1.81	0.62
27:B:826:CLA:H142	30:B:846:BCR:C21	2.29	0.62
23:W:132:ASN:HB2	23:W:135:LEU:HG	1.82	0.62
21:8:78:CYS:HB3	21:8:197:GLY:HA3	1.81	0.62
30:8:621:BCR:H321	30:8:621:BCR:HC8	1.81	0.62
2:B:340:ALA:HB2	30:B:847:BCR:H372	1.82	0.61
30:4:621:BCR:H403	30:4:621:BCR:H23C	1.81	0.61
30:J:102:BCR:HC8	30:J:102:BCR:H331	1.82	0.61
22:9:28:ARG:NH1	22:9:48:ASP:OD1	2.34	0.61
38:Z:606:CHL:HBB2	38:Z:609:CHL:HBC1	1.83	0.61
26:V:174:ILE:CD1	38:V:608:CHL:HMA1	2.31	0.61
22:9:106:ILE:HB	22:9:111:LEU:HD21	1.80	0.61
1:A:406:GLY:HA2	30:A:851:BCR:HC21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:PHE:O	2:B:175:ARG:NH2	2.33	0.60
19:6:82:VAL:HG11	35:6:619:LUT:H12	1.82	0.60
23:W:132:ASN:HB2	23:W:135:LEU:CG	2.31	0.60
16:3:141:TRP:HA	29:3:623:LHG:HC12	1.83	0.60
30:A:850:BCR:HC8	30:A:850:BCR:C32	2.31	0.60
30:B:853:BCR:H383	30:B:853:BCR:H23C	1.82	0.60
2:B:669:ARG:NH1	2:B:700:ALA:O	2.35	0.60
30:L:309:BCR:H311	30:L:309:BCR:C8	2.31	0.60
38:X:607:CHL:CBB	35:X:1621:LUT:H193	2.31	0.60
1:A:119:TRP:CG	30:A:856:BCR:H323	2.36	0.59
14:a:35:LYS:NZ	14:a:37:GLY:O	2.35	0.59
30:2:623:BCR:H321	38:V:605:CHL:CGA	2.33	0.59
24:U:251:THR:HA	38:W:607:CHL:HED3	1.84	0.59
26:V:171:MET:HA	26:V:174:ILE:HG21	1.84	0.59
30:K:202:BCR:H331	30:K:202:BCR:C8	2.32	0.59
20:7:204:PHE:HE1	35:7:619:LUT:H41	1.67	0.59
30:7:623:BCR:HC8	30:7:623:BCR:C32	2.31	0.59
27:4:610:CLA:H52	35:4:619:LUT:H30	1.85	0.59
30:L:305:BCR:H311	30:L:305:BCR:C8	2.30	0.58
17:4:56:ALA:HB3	17:4:58:LEU:HD13	1.86	0.58
27:5:603:CLA:HBC3	36:5:621:XAT:H203	1.85	0.58
38:Z:606:CHL:CBB	38:Z:609:CHL:HBC1	2.34	0.58
8:H:55:GLY:O	25:Z:25:ARG:NH2	2.36	0.58
1:A:87:TRP:HZ3	30:A:849:BCR:H322	1.68	0.58
2:B:352:HIS:ND1	27:B:817:CLA:OBD	2.35	0.58
20:7:30:ARG:NH2	20:7:50:ASP:OD1	2.36	0.58
16:3:252:ASP:OD2	16:3:255:ASN:ND2	2.37	0.58
14:1:35:LYS:NZ	14:1:37:GLY:O	2.35	0.58
22:9:171:GLY:O	22:9:175:GLN:HB2	2.04	0.58
30:1:619:BCR:H403	30:1:619:BCR:H23C	1.86	0.58
30:a:619:BCR:H23C	30:a:619:BCR:H403	1.86	0.58
1:A:119:TRP:HB3	30:A:856:BCR:H322	1.85	0.58
23:X:135:LEU:CD2	23:X:136:ILE:CG1	2.77	0.57
30:A:851:BCR:H23C	30:A:851:BCR:H403	1.86	0.57
5:E:43:VAL:CG2	5:E:93:VAL:HB	2.33	0.57
14:1:228:PHE:CE1	21:8:124:LEU:HD23	2.38	0.57
15:2:32:TYR:HB2	27:2:601:CLA:HED2	1.87	0.57
27:A:843:CLA:H3A	30:L:301:BCR:H322	1.87	0.57
2:B:286:ILE:O	2:B:290:HIS:ND1	2.35	0.56
7:G:58:ARG:NH2	7:G:99:ASP:OD2	2.36	0.56
16:3:257:ASN:N	16:3:257:ASN:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:801:BCR:H23C	30:B:801:BCR:C38	2.36	0.56
15:2:218:PRO:HG3	27:2:601:CLA:HED3	1.87	0.56
19:6:211:ASP:O	19:6:215:THR:OG1	2.22	0.56
14:1:41:PRO:O	21:8:148:GLN:NE2	2.39	0.56
8:H:64:ASP:CG	26:V:41:TRP:HA	2.31	0.56
30:B:801:BCR:H331	30:B:801:BCR:C8	2.35	0.56
30:3:621:BCR:C23	30:3:621:BCR:H383	2.36	0.56
19:6:127:ARG:NH1	19:6:142:PRO:HD3	2.21	0.56
22:9:133:THR:HG21	22:9:142:PHE:HB3	1.88	0.56
14:a:70:SER:OG	21:8:156:GLY:O	2.20	0.56
27:L:307:CLA:HMC1	30:L:309:BCR:H12C	1.87	0.56
30:9:621:BCR:H382	30:9:621:BCR:H23C	1.88	0.56
30:A:850:BCR:H313	13:O:112:THR:HG21	1.88	0.55
30:3:621:BCR:H383	30:3:621:BCR:H23C	1.87	0.55
17:4:116:VAL:HG22	17:4:117:PRO:HD3	1.86	0.55
24:U:105:ILE:HG23	24:U:231:ILE:HD11	1.88	0.55
30:3:622:BCR:H321	30:3:622:BCR:C8	2.36	0.55
20:7:132:GLU:OE1	20:7:135:ARG:NH2	2.34	0.55
8:H:60:LYS:HB3	26:V:41:TRP:HZ2	1.70	0.55
34:B:850:DGD:O5D	34:B:850:DGD:O4D	2.21	0.55
6:F:137:PRO:HD2	30:F:305:BCR:H312	1.88	0.55
14:a:227:PHE:HE1	21:8:100:LEU:CD2	2.17	0.55
37:5:624:NEX:H172	19:6:229:VAL:HG11	1.87	0.55
24:U:236:ASP:O	24:U:244:ASN:ND2	2.40	0.55
30:B:801:BCR:H312	27:B:833:CLA:C6	2.34	0.55
30:J:102:BCR:H331	30:J:102:BCR:C8	2.37	0.55
30:5:622:BCR:H311	27:6:611:CLA:HAB	1.89	0.55
35:X:1620:LUT:H171	35:X:1620:LUT:H8	1.90	0.54
30:7:621:BCR:H23C	30:7:621:BCR:H403	1.90	0.54
25:Z:222:GLN:NE2	35:Z:1620:LUT:O3	2.40	0.54
23:W:80:GLU:HA	23:W:172:LEU:HD21	1.90	0.54
1:A:474:ASP:O	1:A:478:GLN:NE2	2.39	0.54
2:B:667:SER:OG	2:B:672:TRP:NE1	2.40	0.54
30:B:801:BCR:H331	30:B:801:BCR:HC8	1.88	0.54
30:L:309:BCR:H23C	30:L:309:BCR:H392	1.90	0.54
38:V:605:CHL:HHD	38:V:606:CHL:OBD	2.07	0.54
23:W:97:ILE:HG23	23:W:223:ILE:HD11	1.88	0.54
30:L:305:BCR:H392	30:L:305:BCR:H23C	1.89	0.54
23:X:178:PHE:HD1	38:X:608:CHL:H2	1.71	0.54
30:2:623:BCR:H343	33:V:2631:LMG:O10	2.07	0.54
1:A:576:ASP:OD2	1:A:580:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:88:GLU:HA	24:U:180:LEU:HD21	1.90	0.54
27:A:816:CLA:C4C	30:K:202:BCR:H312	2.37	0.54
24:U:157:VAL:HG13	38:U:609:CHL:HBB2	1.90	0.54
30:J:102:BCR:C23	30:J:102:BCR:H382	2.38	0.53
35:Y:1620:LUT:H171	35:Y:1620:LUT:H8	1.89	0.53
29:5:625:LHG:HC11	33:5:627:LMG:O2	2.07	0.53
35:Z:1620:LUT:C8	35:Z:1620:LUT:H181	2.38	0.53
1:A:217:GLN:HA	1:A:221:SER:HB3	1.90	0.53
30:3:622:BCR:HC8	30:3:622:BCR:H311	1.90	0.53
30:B:843:BCR:H331	30:B:843:BCR:C8	2.31	0.53
14:a:38:ASN:O	14:a:39:TRP:CD1	2.61	0.53
2:B:126:TYR:O	2:B:131:ARG:NH1	2.40	0.53
27:4:610:CLA:H2	35:4:619:LUT:H28	1.91	0.53
27:B:825:CLA:HMA1	30:B:847:BCR:H14C	1.89	0.53
27:A:854:CLA:H11	2:B:617:LEU:HD12	1.91	0.53
2:B:671:TYR:OH	27:B:803:CLA:OBD	2.25	0.53
27:B:837:CLA:H41	30:F:305:BCR:H321	1.90	0.53
12:L:154:ARG:NH2	25:Z:27:TPO:O1P	2.42	0.53
14:1:38:ASN:O	14:1:39:TRP:CD1	2.61	0.53
25:Z:153:LEU:HD21	36:Z:1622:XAT:H202	1.91	0.53
8:H:116:THR:CG2	8:H:117:THR:N	2.72	0.53
27:X:613:CLA:HMB1	35:X:1620:LUT:H7	1.91	0.53
30:7:623:BCR:C32	21:8:230:TRP:CE2	2.90	0.53
30:B:845:BCR:H321	22:9:177:LEU:HD21	1.91	0.52
30:K:207:BCR:H331	30:K:207:BCR:C8	2.39	0.52
2:B:23:TRP:HB3	34:B:850:DGD:HA21	1.91	0.52
20:7:231:PHE:N	27:7:613:CLA:O1A	2.41	0.52
21:8:218:PRO:O	35:8:619:LUT:O3	2.25	0.52
30:A:856:BCR:H23C	30:A:856:BCR:H392	1.92	0.52
27:L:307:CLA:HMC1	30:L:309:BCR:C12	2.39	0.52
2:B:713:HIS:NE2	27:B:840:CLA:NA	2.58	0.52
35:V:1620:LUT:C8	35:V:1620:LUT:H181	2.38	0.52
18:5:233:THR:CA	18:5:256:SER:OG	2.40	0.52
20:7:161:GLU:OE1	20:7:187:LYS:NZ	2.42	0.52
2:B:277:HIS:HE2	27:B:818:CLA:C1B	2.22	0.52
27:B:804:CLA:HAC1	30:L:305:BCR:HC21	1.92	0.52
5:E:79:ASN:OD1	5:E:83:VAL:N	2.42	0.52
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.91	0.52
8:H:60:LYS:HB3	26:V:41:TRP:CZ2	2.45	0.52
24:U:39:GLU:CD	24:U:41:TYR:O	2.53	0.52
30:B:844:BCR:H311	30:B:844:BCR:C8	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:612:CLA:HHC	27:3:612:CLA:HBB1	1.93	0.51
14:1:228:PHE:HE1	21:8:124:LEU:HD23	1.75	0.51
16:3:95:ALA:HB1	16:3:221:GLY:HA3	1.90	0.51
24:Y:124:LYS:HA	38:Y:607:CHL:O1D	2.10	0.51
26:V:105:ALA:HB1	26:V:221:GLY:HA3	1.92	0.51
30:B:852:BCR:H23C	30:B:852:BCR:C38	2.40	0.51
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.93	0.51
1:A:584:CYS:N	2:B:669:ARG:O	2.43	0.51
2:B:493:LEU:O	2:B:496:PRO:HD2	2.10	0.51
30:B:847:BCR:C23	30:B:847:BCR:H383	2.41	0.51
27:Y:613:CLA:HMB1	35:Y:1620:LUT:H7	1.91	0.51
26:V:106:ARG:NH1	38:V:608:CHL:OBD	2.36	0.51
27:A:829:CLA:HBC3	30:A:852:BCR:H313	1.92	0.51
24:U:246:ALA:N	27:U:613:CLA:O1A	2.39	0.51
30:F:305:BCR:C33	30:F:305:BCR:HC8	2.41	0.51
36:Y:1622:XAT:H193	25:Z:246:ALA:HB3	1.91	0.51
23:W:115:PHE:HA	38:W:607:CHL:HMA2	1.91	0.51
23:W:156:GLU:OE1	38:W:609:CHL:NA	2.43	0.51
22:9:97:TRP:CH2	22:9:179:THR:HA	2.46	0.51
30:A:856:BCR:HC8	30:A:856:BCR:C32	2.39	0.51
11:K:38:MET:HG3	27:K:204:CLA:HMD3	1.93	0.51
23:X:162:GLY:HA3	23:X:167:GLU:HA	1.93	0.51
38:Z:606:CHL:HBB1	38:Z:606:CHL:HMB3	1.91	0.51
23:W:238:ALA:N	27:W:613:CLA:O1A	2.39	0.51
35:1:617:LUT:H41	35:1:617:LUT:H173	1.93	0.50
35:8:619:LUT:H41	35:8:619:LUT:H173	1.92	0.50
24:Y:46:ALA:HB1	38:Y:601:CHL:HBC1	1.93	0.50
24:U:140:ASN:ND2	24:U:143:LEU:HD11	2.26	0.50
14:a:139:ALA:HB1	27:1:611:CLA:H43	1.93	0.50
14:1:167:SER:OG	14:1:168:SER:N	2.44	0.50
23:X:158:TYR:HB3	38:X:608:CHL:CMC	2.42	0.50
38:U:601:CHL:H161	38:W:607:CHL:H161	1.92	0.50
1:A:361:GLY:HA2	1:A:398:GLY:HA2	1.92	0.50
25:Z:246:ALA:N	27:Z:613:CLA:O1A	2.42	0.50
23:W:104:LYS:NZ	23:W:223:ILE:HG21	2.27	0.50
30:B:849:BCR:C23	30:B:849:BCR:H383	2.42	0.50
14:a:167:SER:OG	14:a:168:SER:N	2.44	0.50
25:Z:94:ALA:HB1	25:Z:209:GLY:HA3	1.94	0.50
1:A:306:LEU:O	1:A:310:HIS:ND1	2.39	0.50
30:B:843:BCR:H23C	30:B:843:BCR:C38	2.39	0.50
23:X:86:ALA:HB1	23:X:201:GLY:HA3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:88:GLU:HA	24:Y:180:LEU:HD21	1.93	0.50
13:O:56:THR:HA	13:O:59:ALA:HB3	1.94	0.50
30:4:621:BCR:H23C	30:4:621:BCR:C40	2.42	0.50
1:A:83:ILE:HG23	30:J:102:BCR:HC21	1.93	0.50
23:X:80:GLU:HA	23:X:172:LEU:HD21	1.93	0.50
14:a:202:PRO:O	35:a:617:LUT:O3	2.30	0.50
22:9:178:ALA:O	22:9:180:ARG:N	2.41	0.50
23:X:30:ILE:CD1	27:X:611:CLA:HMA1	2.41	0.50
2:B:179:HIS:CD2	27:B:813:CLA:NB	2.79	0.49
2:B:517:ASP:OD2	2:B:598:LYS:NZ	2.42	0.49
27:B:839:CLA:H93	30:B:849:BCR:H333	1.94	0.49
8:H:98:TYR:O	8:H:103:ALA:N	2.40	0.49
11:K:89:VAL:HG23	27:K:201:CLA:HMD2	1.93	0.49
18:5:243:GLN:O	37:5:624:NEX:O4	2.26	0.49
14:1:202:PRO:O	35:1:617:LUT:O3	2.30	0.49
30:2:623:BCR:H321	38:V:605:CHL:CBA	2.42	0.49
24:U:94:ALA:HB1	24:U:209:GLY:HA3	1.93	0.49
1:A:17:VAL:HG11	27:A:811:CLA:HED3	1.95	0.49
23:X:30:ILE:HD13	27:X:611:CLA:CMA	2.43	0.49
23:X:238:ALA:N	27:X:613:CLA:O1A	2.42	0.49
24:Y:38:ILE:CD1	27:Y:611:CLA:HMA1	2.41	0.49
25:Z:222:GLN:HA	25:Z:225:VAL:HG22	1.94	0.49
2:B:144:ALA:HB1	30:B:852:BCR:C21	2.42	0.49
27:9:613:CLA:H2	27:9:614:CLA:HMD1	1.94	0.49
38:Y:606:CHL:CBB	38:Y:607:CHL:HHC	2.42	0.49
26:V:174:ILE:HG23	26:V:175:GLU:N	2.26	0.49
35:a:617:LUT:H173	35:a:617:LUT:H41	1.93	0.49
21:8:41:LEU:HD11	21:8:56:ASP:HB2	1.95	0.49
30:A:856:BCR:H311	30:A:856:BCR:C8	2.43	0.49
32:K:208:LMU:H5'	16:3:259:LEU:HB3	1.94	0.49
23:W:153:GLY:CA	38:W:609:CHL:HAB	2.42	0.49
2:B:412:MET:HE1	27:B:830:CLA:C4C	2.42	0.49
22:9:126:ARG:HD3	30:9:621:BCR:H292	1.93	0.49
24:U:161:GLY:CA	38:U:609:CHL:HAB	2.43	0.49
1:A:550:LEU:HD13	30:A:851:BCR:H322	1.94	0.49
24:U:164:GLU:OE1	38:U:609:CHL:NA	2.45	0.49
23:W:86:ALA:HB1	23:W:201:GLY:HA3	1.93	0.49
30:A:856:BCR:H311	10:J:27:ILE:CG2	2.43	0.49
24:U:112:LYS:NZ	24:U:231:ILE:HG21	2.27	0.49
24:U:172:PRO:HG2	38:U:608:CHL:CBB	2.43	0.49
21:8:68:ARG:NH2	21:8:142:ILE:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:42:GLY:HA3	17:4:173:SER:HB3	1.95	0.48
14:1:89:VAL:HG11	35:1:617:LUT:H12	1.94	0.48
30:8:621:BCR:H403	30:8:621:BCR:H23C	1.95	0.48
22:9:40:HIS:NE2	22:9:52:ASP:OD2	2.40	0.48
22:9:106:ILE:HB	22:9:111:LEU:CD2	2.42	0.48
23:X:98:THR:OG1	23:X:99:PRO:CD	2.60	0.48
24:Y:94:ALA:HB1	24:Y:209:GLY:HA3	1.94	0.48
38:Z:607:CHL:CBB	35:Z:1621:LUT:H193	2.43	0.48
1:A:214:ALA:O	1:A:218:ILE:HG12	2.13	0.48
1:A:691:GLY:N	2:B:569:CYS:O	2.37	0.48
27:A:809:CLA:H93	30:J:102:BCR:H343	1.95	0.48
15:2:52:ASP:O	15:2:55:ARG:NH1	2.44	0.48
16:3:171:SER:OG	16:3:172:MET:N	2.46	0.48
24:Y:38:ILE:HD13	27:Y:611:CLA:CMA	2.43	0.48
27:A:802:CLA:CGA	27:A:802:CLA:H3A	2.43	0.48
12:L:56:GLU:C	12:L:57:THR:HG23	2.39	0.48
13:O:63:VAL:CG1	30:O:2005:BCR:HC21	2.43	0.48
27:4:614:CLA:H2	19:6:120:LEU:HD21	1.95	0.48
18:5:65:THR:HG22	27:5:619:CLA:CBA	2.40	0.48
38:Y:607:CHL:H61	38:Y:607:CHL:H92	1.64	0.48
2:B:396:ILE:HD13	2:B:556:TYR:HA	1.95	0.48
37:6:624:NEX:C28	37:6:624:NEX:H381	2.43	0.48
24:Y:140:ASN:ND2	24:Y:143:LEU:CD1	2.57	0.48
30:L:301:BCR:H312	27:L:303:CLA:C2C	2.44	0.48
13:O:57:ILE:HB	13:O:58:PRO:HD3	1.95	0.48
16:3:89:TYR:OH	16:3:162:ARG:HG2	2.14	0.48
24:U:140:ASN:HD22	24:U:143:LEU:HD11	1.76	0.48
1:A:370:HIS:ND1	27:A:819:CLA:OBD	2.41	0.48
1:A:647:ARG:NH1	1:A:648:ASP:OD2	2.46	0.48
2:B:293:ARG:NH1	7:G:61:ALA:O	2.47	0.48
30:K:207:BCR:H331	30:K:207:BCR:HC8	1.93	0.48
14:a:89:VAL:HG11	35:a:617:LUT:H12	1.94	0.48
18:5:233:THR:HA	18:5:256:SER:HG	1.68	0.48
19:6:254:GLY:HA2	20:7:95:VAL:HG21	1.96	0.48
24:Y:161:GLY:CA	38:Y:609:CHL:HAB	2.44	0.48
2:B:561:ASP:OD2	2:B:565:ARG:NH2	2.39	0.48
30:K:207:BCR:H383	30:K:207:BCR:H23C	1.95	0.48
30:K:202:BCR:HC8	30:K:202:BCR:C33	2.42	0.48
30:K:207:BCR:H383	30:K:207:BCR:C23	2.44	0.48
15:2:40:HIS:NE2	15:2:52:ASP:OD2	2.43	0.48
27:4:601:CLA:OBD	19:6:127:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:153:GLY:CA	38:X:609:CHL:HAB	2.44	0.48
30:A:852:BCR:H362	27:A:854:CLA:H41	1.93	0.48
27:A:854:CLA:C1	2:B:617:LEU:HD12	2.44	0.48
25:Z:207:LYS:NZ	29:Z:2630:LHG:O4	2.43	0.48
23:W:164:PRO:HG2	38:W:608:CHL:CBB	2.43	0.48
1:A:363:LEU:HD21	27:A:820:CLA:H72	1.96	0.48
2:B:610:PHE:O	2:B:614:SER:OG	2.29	0.48
2:B:61:TRP:NE1	27:B:827:CLA:OBD	2.46	0.47
27:B:808:CLA:HBB2	30:B:848:BCR:H311	1.96	0.47
15:2:217:LEU:N	15:2:218:PRO:HD2	2.29	0.47
21:8:234:TYR:N	27:8:613:CLA:O1A	2.45	0.47
2:B:263:HIS:N	2:B:268:SER:O	2.39	0.47
30:J:102:BCR:HC8	30:J:102:BCR:C33	2.43	0.47
27:5:607:CLA:CBB	36:5:621:XAT:H193	2.44	0.47
20:7:144:SER:OG	20:7:145:GLN:N	2.47	0.47
23:X:147:PHE:O	23:X:150:VAL:HG12	2.14	0.47
24:Y:161:GLY:HA2	38:Y:609:CHL:HAB	1.96	0.47
9:I:80:VAL:HB	9:I:81:PRO:HD3	1.95	0.47
12:L:189:THR:HG23	12:L:195:TYR:CZ	2.48	0.47
33:L:2631:LMG:O5	33:L:2631:LMG:O4	2.25	0.47
30:O:2004:BCR:H23C	30:O:2004:BCR:C38	2.43	0.47
38:X:601:CHL:H41	38:X:601:CHL:H62	1.54	0.47
38:Z:601:CHL:H202	38:Z:601:CHL:H161	1.65	0.47
6:F:99:ALA:HB3	6:F:100:PRO:HD3	1.96	0.47
8:H:116:THR:HG22	8:H:117:THR:H	1.78	0.47
19:6:199:LYS:HE2	19:6:203:ALA:HB1	1.97	0.47
23:X:228:ASP:HB3	23:X:236:VAL:HG11	1.97	0.47
38:Y:609:CHL:HHC	38:Z:601:CHL:H52	1.96	0.47
38:W:601:CHL:H101	38:W:601:CHL:H61	1.30	0.47
30:J:102:BCR:H382	30:J:102:BCR:H23C	1.96	0.47
14:a:227:PHE:HE1	21:8:100:LEU:CG	2.27	0.47
22:9:101:ALA:HA	29:9:623:LHG:HC12	1.97	0.47
27:B:826:CLA:H142	30:B:846:BCR:C22	2.45	0.47
6:F:158:TYR:O	6:F:202:TRP:NE1	2.48	0.47
30:F:305:BCR:H331	30:F:305:BCR:C8	2.44	0.47
18:5:175:SER:O	18:5:176:LYS:HG3	2.14	0.47
2:B:70:ALA:HB2	2:B:136:LEU:HB2	1.97	0.47
11:K:62:THR:OG1	11:K:64:GLY:O	2.26	0.47
13:O:50:LEU:HD13	30:O:2005:BCR:H372	1.97	0.47
30:O:2005:BCR:H383	30:O:2005:BCR:C23	2.44	0.47
6:F:137:PRO:HD3	30:F:305:BCR:H312	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:V:607:CHL:HBB2	38:V:609:CHL:HBC1	1.96	0.46
23:W:149:VAL:HG13	38:W:609:CHL:HBB2	1.96	0.46
21:8:237:ASN:ND2	27:8:613:CLA:OBD	2.48	0.46
36:U:1622:XAT:H15	27:V:613:CLA:H203	1.97	0.46
30:B:848:BCR:H331	30:B:848:BCR:C8	2.44	0.46
38:V:609:CHL:H71	38:V:609:CHL:H111	1.54	0.46
30:A:848:BCR:C23	30:A:848:BCR:H383	2.45	0.46
6:F:225:SER:HB2	6:F:226:PRO:HD3	1.96	0.46
13:O:120:GLY:O	13:O:124:GLY:O	2.34	0.46
16:3:141:TRP:NE1	27:3:606:CLA:OBD	2.43	0.46
37:Z:1623:NEX:H192	37:Z:1623:NEX:H183	1.97	0.46
11:K:84:PHE:HE2	11:K:89:VAL:CG2	2.28	0.46
26:V:174:ILE:HD13	38:V:608:CHL:HMA3	1.98	0.46
1:A:18:ASP:OD1	1:A:187:LYS:NZ	2.47	0.46
6:F:85:LYS:HA	6:F:88:GLU:HG2	1.97	0.46
10:J:28:GLU:OE1	10:J:31:ARG:NH2	2.40	0.46
15:2:70:GLU:CD	15:2:158:LEU:HD11	2.41	0.46
30:2:623:BCR:H382	30:2:623:BCR:H23C	1.97	0.46
16:3:246:LEU:HB2	35:3:618:LUT:H21	1.97	0.46
24:U:257:ALA:H	23:W:219:GLY:HA3	1.80	0.46
26:V:174:ILE:HD11	38:V:608:CHL:C3A	2.41	0.46
2:B:144:ALA:HB1	30:B:852:BCR:C22	2.45	0.46
23:W:132:ASN:HB3	23:W:135:LEU:HG	1.97	0.46
2:B:27:ALA:HB2	34:B:850:DGD:HA22	1.98	0.46
2:B:167:SER:OG	7:G:71:THR:HG23	2.15	0.46
2:B:659:ALA:O	2:B:662:PHE:HB2	2.16	0.46
3:C:9:ASP:HA	3:C:35:LYS:HZ1	1.81	0.46
3:C:33:GLY:HA3	3:C:35:LYS:NZ	2.30	0.46
7:G:86:ILE:O	7:G:86:ILE:HG13	2.16	0.46
19:6:104:VAL:HG23	19:6:105:GLU:N	2.31	0.46
38:Z:601:CHL:HBA1	38:Z:601:CHL:H3A	1.71	0.46
1:A:590:ASP:HA	1:A:593:PHE:HB3	1.98	0.46
2:B:277:HIS:HE2	27:B:818:CLA:C2B	2.29	0.46
27:B:808:CLA:CBB	30:B:848:BCR:C31	2.93	0.46
30:B:844:BCR:HC8	30:B:844:BCR:H321	1.98	0.46
13:O:59:ALA:HA	30:O:2005:BCR:HC42	1.97	0.46
24:Y:108:GLU:O	24:Y:112:LYS:HG3	2.15	0.46
30:A:848:BCR:C8	30:A:848:BCR:H331	2.45	0.46
16:3:170:GLY:O	16:3:174:GLN:NE2	2.48	0.46
30:6:622:BCR:H23C	30:6:622:BCR:C39	2.46	0.46
22:9:132:GLN:O	22:9:133:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:621:BCR:H382	30:9:621:BCR:C23	2.45	0.46
23:X:30:ILE:CD1	27:X:611:CLA:CMA	2.94	0.46
38:X:608:CHL:H111	38:X:608:CHL:H71	1.36	0.46
38:Z:601:CHL:H43	38:Z:601:CHL:HMA2	1.98	0.46
1:A:153:ILE:O	1:A:154:THR:OG1	2.29	0.45
19:6:168:ASP:OD1	19:6:169:LEU:N	2.49	0.45
1:A:119:TRP:HB3	30:A:856:BCR:C32	2.46	0.45
1:A:574:PRO:HB3	1:A:720:ILE:HB	1.97	0.45
27:V:610:CLA:HBB1	27:V:610:CLA:HMB3	1.97	0.45
2:B:155:TRP:HB2	30:B:853:BCR:H312	1.98	0.45
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.98	0.45
24:Y:38:ILE:CD1	27:Y:611:CLA:CMA	2.94	0.45
38:Y:606:CHL:HBB1	38:Y:607:CHL:HHC	1.98	0.45
37:V:1623:NEX:H15	37:V:1623:NEX:H201	1.75	0.45
23:W:199:LYS:NZ	27:W:611:CLA:O1D	2.37	0.45
38:W:607:CHL:H193	38:W:607:CHL:H162	1.74	0.45
2:B:416:LYS:NZ	2:B:541:ASP:OD1	2.43	0.45
7:G:75:THR:HG22	7:G:76:TYR:N	2.32	0.45
19:6:134:LYS:HB2	19:6:137:SER:OG	2.16	0.45
29:9:623:LHG:O1	29:9:624:LHG:O5	2.32	0.45
38:X:601:CHL:HBA2	38:Z:609:CHL:HBA1	1.99	0.45
38:U:601:CHL:H61	38:U:601:CHL:H101	1.51	0.45
4:D:151:HIS:CB	4:D:152:PRO:HD3	2.45	0.45
16:3:161:ARG:HB3	27:3:608:CLA:HMC2	1.98	0.45
20:7:130:TRP:O	20:7:134:LYS:HG2	2.16	0.45
38:Y:601:CHL:HBA1	38:Y:601:CHL:H3A	1.68	0.45
37:Z:1623:NEX:H163	24:U:162:LEU:CD2	2.44	0.45
24:U:207:LYS:NZ	27:U:611:CLA:O1D	2.37	0.45
38:V:607:CHL:HBB2	38:V:609:CHL:CBC	2.47	0.45
27:A:809:CLA:H91	27:A:812:CLA:H193	1.98	0.45
27:A:854:CLA:H43	27:A:854:CLA:CGA	2.46	0.45
2:B:669:ARG:HB2	28:B:842:PQN:H7	1.99	0.45
2:B:713:HIS:CE1	27:B:840:CLA:ND	2.85	0.45
19:6:82:VAL:HG13	19:6:190:PHE:CE2	2.52	0.45
1:A:682:SER:HB2	1:A:727:GLY:O	2.16	0.45
21:8:74:GLU:O	21:8:78:CYS:SG	2.75	0.45
23:X:111:GLU:HG2	23:X:116:LYS:HB2	1.98	0.45
30:A:849:BCR:H382	30:A:849:BCR:H23C	1.99	0.45
2:B:200:ILE:HB	2:B:201:PRO:HD3	1.99	0.45
21:8:222:LEU:HB2	35:8:619:LUT:H21	1.99	0.45
38:X:608:CHL:H92	38:X:608:CHL:H62	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:164:GLU:O	24:U:168:VAL:HG13	2.17	0.45
38:U:609:CHL:H91	38:U:609:CHL:H111	1.62	0.45
38:V:605:CHL:HHC	38:V:605:CHL:HBB1	1.99	0.45
27:A:803:CLA:H203	30:B:848:BCR:H321	1.98	0.45
27:A:841:CLA:H91	27:F:303:CLA:HBC3	1.99	0.45
21:8:50:ALA:HB2	21:8:190:LYS:HB3	1.99	0.45
24:Y:140:ASN:HB2	24:Y:143:LEU:HD13	1.98	0.45
24:Y:246:ALA:N	27:Y:613:CLA:O1A	2.42	0.45
27:A:825:CLA:H43	30:A:851:BCR:H363	1.99	0.44
30:B:801:BCR:HC8	30:B:801:BCR:C33	2.46	0.44
11:K:64:GLY:O	11:K:66:LYS:N	2.48	0.44
37:W:1623:NEX:H35	37:W:1623:NEX:H401	1.81	0.44
1:A:332:PRO:HB2	12:L:42:VAL:HG23	1.98	0.44
30:A:852:BCR:H20C	30:A:852:BCR:H361	1.73	0.44
26:V:113:LEU:O	26:V:117:THR:OG1	2.28	0.44
30:A:852:BCR:H382	30:A:852:BCR:H23C	1.98	0.44
30:B:846:BCR:H331	30:B:846:BCR:C8	2.46	0.44
30:2:623:BCR:C19	33:V:2631:LMG:H181	2.47	0.44
38:X:607:CHL:H92	38:X:607:CHL:H61	1.59	0.44
24:U:45:ARG:NH2	24:U:61:LEU:O	2.51	0.44
38:V:608:CHL:HHC	38:V:608:CHL:HBB1	1.97	0.44
30:A:852:BCR:H331	30:A:852:BCR:C8	2.47	0.44
14:a:88:GLY:HA2	36:a:618:XAT:H181	2.00	0.44
37:X:1623:NEX:H401	37:X:1623:NEX:H35	1.80	0.44
37:Y:1623:NEX:H35	37:Y:1623:NEX:H401	1.81	0.44
23:W:104:LYS:HZ3	23:W:223:ILE:HG21	1.83	0.44
30:B:801:BCR:H353	27:B:832:CLA:CGA	2.48	0.44
27:B:834:CLA:H2	27:B:835:CLA:HMB1	1.98	0.44
30:G:205:BCR:H383	30:G:205:BCR:C23	2.48	0.44
14:1:88:GLY:HA2	36:1:618:XAT:H181	2.00	0.44
16:3:161:ARG:HD3	27:7:601:CLA:OBD	2.18	0.44
24:Y:123:PHE:HA	38:Y:607:CHL:HMA2	2.00	0.44
38:Z:605:CHL:HHC	38:Z:605:CHL:HBB1	2.00	0.44
37:W:1623:NEX:H15	37:W:1623:NEX:H201	1.76	0.44
27:A:803:CLA:OBD	27:B:802:CLA:HMB3	2.17	0.44
9:I:95:LEU:O	9:I:99:ILE:HG12	2.16	0.44
15:2:70:GLU:OE2	15:2:162:ARG:NE	2.36	0.44
30:3:621:BCR:C23	30:3:621:BCR:C38	2.93	0.44
17:4:174:ALA:HB1	27:4:608:CLA:HMC1	2.00	0.44
21:8:144:LYS:HB2	21:8:147:SER:HB3	2.00	0.44
26:V:130:GLU:HB2	26:V:139:GLN:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:818:CLA:H101	30:K:207:BCR:HC21	2.00	0.44
13:O:39:ASP:OD1	13:O:39:ASP:N	2.47	0.44
38:Z:607:CHL:H92	38:Z:607:CHL:H61	1.74	0.44
30:A:852:BCR:C33	30:A:852:BCR:HC8	2.48	0.44
30:B:846:BCR:H392	30:B:847:BCR:C38	2.48	0.44
27:2:601:CLA:HHD	27:2:601:CLA:HBC2	2.00	0.44
21:8:154:PHE:HB2	21:8:158:GLU:HB3	1.99	0.44
23:X:30:ILE:HG21	23:X:32:TRP:CZ2	2.53	0.44
38:X:606:CHL:HHC	38:X:606:CHL:HBB1	1.98	0.44
38:Y:606:CHL:HBB1	38:Y:606:CHL:HHC	1.98	0.44
2:B:176:LEU:HD21	27:B:819:CLA:HMA3	2.00	0.44
2:B:364:ILE:O	8:H:127:ARG:NH1	2.46	0.44
2:B:457:GLU:OE1	6:F:132:HIS:ND1	2.45	0.44
27:3:617:CLA:HBB2	30:3:621:BCR:H312	2.00	0.44
30:5:622:BCR:H23C	30:5:622:BCR:C40	2.46	0.44
27:A:834:CLA:HAA1	30:L:301:BCR:C14	2.48	0.43
38:Z:609:CHL:H92	38:Z:609:CHL:H61	1.75	0.43
10:J:35:ASP:N	10:J:36:PRO:HD3	2.33	0.43
11:K:46:LEU:HD23	11:K:92:MET:HB2	2.00	0.43
27:a:611:CLA:HHC	30:4:621:BCR:H313	1.99	0.43
18:5:84:GLY:HA2	36:5:621:XAT:H181	2.00	0.43
38:X:601:CHL:H101	38:X:601:CHL:H61	1.33	0.43
38:Z:608:CHL:HHC	38:Z:608:CHL:HBB1	2.00	0.43
1:A:351:ALA:HB1	30:A:850:BCR:C39	2.49	0.43
1:A:380:LEU:HD12	1:A:386:THR:HG21	1.99	0.43
27:B:803:CLA:CGA	27:B:803:CLA:H3A	2.48	0.43
4:D:125:THR:HG23	4:D:136:PRO:HG2	2.00	0.43
12:L:46:VAL:HA	12:L:56:GLU:CG	2.47	0.43
27:2:603:CLA:HHC	27:2:603:CLA:HBB1	2.00	0.43
25:Z:150:LEU:HD23	25:Z:150:LEU:H	1.84	0.43
23:W:135:LEU:O	38:W:605:CHL:CGD	2.66	0.43
1:A:403:VAL:HG11	1:A:596:LEU:HG	2.01	0.43
2:B:675:LEU:O	2:B:678:THR:OG1	2.33	0.43
17:4:56:ALA:HB3	17:4:58:LEU:CD1	2.49	0.43
19:6:250:CYS:HB2	19:6:253:GLN:HB2	2.01	0.43
24:U:143:LEU:O	38:U:605:CHL:CGD	2.66	0.43
23:W:37:ARG:NH2	23:W:53:LEU:O	2.51	0.43
1:A:297:HIS:HE2	27:A:820:CLA:C2B	2.31	0.43
30:A:850:BCR:C23	30:A:850:BCR:H383	2.49	0.43
2:B:723:ALA:O	2:B:727:ILE:HG12	2.19	0.43
24:U:164:GLU:OE1	38:U:609:CHL:C4A	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:U:605:CHL:HHD	38:U:606:CHL:OBD	2.18	0.43
27:U:613:CLA:HMB1	35:U:1620:LUT:H7	2.01	0.43
1:A:87:TRP:CZ3	30:A:849:BCR:H322	2.51	0.43
1:A:584:CYS:O	2:B:669:ARG:O	2.36	0.43
2:B:718:TYR:CE1	27:B:802:CLA:HED1	2.53	0.43
38:U:605:CHL:HHC	38:U:605:CHL:HBB1	2.00	0.43
27:B:808:CLA:CBB	30:B:848:BCR:H311	2.48	0.43
17:4:164:ARG:NH1	27:4:609:CLA:O1D	2.45	0.43
27:6:613:CLA:HMB1	35:6:619:LUT:H7	2.01	0.43
22:9:133:THR:HG22	22:9:133:THR:O	2.19	0.43
38:V:601:CHL:H61	38:V:601:CHL:H102	1.30	0.43
38:W:605:CHL:HHD	38:W:606:CHL:OBD	2.18	0.43
1:A:571:PHE:O	1:A:587:SER:OG	2.37	0.43
1:A:580:ARG:O	2:B:669:ARG:NH2	2.50	0.43
30:L:309:BCR:H23C	30:L:309:BCR:H403	2.00	0.43
17:4:104:ALA:HB1	17:4:219:GLY:HA3	2.00	0.43
38:W:605:CHL:HHC	38:W:605:CHL:HBB1	2.00	0.43
2:B:657:ILE:HG22	2:B:713:HIS:O	2.18	0.43
8:H:62:TYR:OH	12:L:87:GLU:OE1	2.34	0.43
30:L:301:BCR:H383	30:L:301:BCR:C23	2.42	0.43
14:a:109:TRP:CE2	14:a:116:ALA:HB2	2.54	0.43
20:7:154:THR:OG1	20:7:155:GLU:N	2.52	0.43
24:U:130:PHE:HZ	26:V:259:PHE:HB3	1.84	0.43
3:C:55:GLU:HB2	3:C:63:LEU:HD13	2.00	0.43
30:O:2005:BCR:C33	30:O:2005:BCR:HC8	2.48	0.43
14:a:62:LEU:CD2	21:8:176:PRO:HA	2.49	0.43
23:X:135:LEU:HD23	23:X:135:LEU:C	2.44	0.43
38:Y:605:CHL:HHC	38:Y:605:CHL:HBB1	2.01	0.43
35:Y:1620:LUT:H8	35:Y:1620:LUT:C17	2.49	0.43
1:A:261:ILE:HG21	30:K:202:BCR:HC21	2.00	0.42
1:A:488:GLN:NE2	1:A:526:ILE:O	2.50	0.42
30:3:622:BCR:C8	30:3:622:BCR:H311	2.49	0.42
35:4:619:LUT:H15	35:4:619:LUT:H201	1.93	0.42
19:6:82:VAL:HG13	19:6:190:PHE:CZ	2.54	0.42
30:6:622:BCR:C23	30:6:622:BCR:H402	2.48	0.42
22:9:133:THR:HG21	22:9:142:PHE:CB	2.48	0.42
5:E:91:ASP:OD1	5:E:91:ASP:N	2.51	0.42
15:2:143:PHE:N	27:2:610:CLA:OBD	2.49	0.42
27:3:602:CLA:H71	27:3:603:CLA:HMB3	2.01	0.42
17:4:113:GLY:O	17:4:117:PRO:HG2	2.19	0.42
38:X:605:CHL:HHC	38:X:605:CHL:HBB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:W:607:CHL:H92	38:W:607:CHL:H61	1.73	0.42
1:A:63:THR:OG1	1:A:64:SER:N	2.53	0.42
1:A:303:VAL:CG1	30:K:207:BCR:HC22	2.50	0.42
27:L:303:CLA:H141	27:L:303:CLA:H161	1.94	0.42
14:1:109:TRP:CE2	14:1:116:ALA:HB2	2.54	0.42
19:6:120:LEU:HD12	27:6:606:CLA:HMA2	2.01	0.42
27:7:613:CLA:HMB1	35:7:619:LUT:H7	2.01	0.42
35:X:1620:LUT:H8	35:X:1620:LUT:C17	2.49	0.42
35:U:1620:LUT:C8	35:U:1620:LUT:H171	2.49	0.42
38:V:601:CHL:H141	38:V:601:CHL:H161	1.58	0.42
38:W:606:CHL:HBB1	38:W:606:CHL:HHC	2.00	0.42
38:W:606:CHL:HBB1	38:W:607:CHL:HHC	2.01	0.42
1:A:161:THR:HG21	27:A:817:CLA:HAA2	2.01	0.42
20:7:44:ASP:OD1	20:7:44:ASP:N	2.52	0.42
36:7:620:XAT:C28	36:7:620:XAT:H381	2.49	0.42
23:X:122:PHE:HZ	24:Y:247:PHE:HB3	1.83	0.42
25:Z:148:SER:OG	25:Z:151:ALA:HB3	2.19	0.42
26:V:174:ILE:HG23	26:V:175:GLU:HG2	2.01	0.42
1:A:153:ILE:HG22	1:A:155:SER:H	1.85	0.42
1:A:680:ALA:HB3	27:A:802:CLA:HBB2	2.00	0.42
2:B:179:HIS:HA	2:B:183:LEU:HB3	2.01	0.42
2:B:384:MET:HE1	30:B:847:BCR:H361	2.01	0.42
18:5:78:ALA:HB1	18:5:190:GLY:HA3	2.01	0.42
18:5:170:ASP:OD2	18:5:173:GLY:HA2	2.19	0.42
19:6:120:LEU:HD22	30:6:622:BCR:C14	2.50	0.42
22:9:154:MET:HG3	27:9:610:CLA:HHB	2.01	0.42
24:U:112:LYS:HZ1	24:U:231:ILE:HG21	1.84	0.42
38:U:606:CHL:HHC	38:U:606:CHL:HBB1	2.00	0.42
36:U:1622:XAT:H403	29:V:2630:LHG:H281	2.02	0.42
26:V:234:GLN:O	26:V:238:THR:HB	2.19	0.42
1:A:598:TRP:HE1	27:B:803:CLA:C1D	2.32	0.42
8:H:116:THR:CG2	8:H:117:THR:H	2.33	0.42
30:K:207:BCR:H11C	30:K:207:BCR:H341	1.84	0.42
30:O:2005:BCR:C33	30:O:2005:BCR:C8	2.96	0.42
16:3:176:TYR:HB3	29:7:622:LHG:HC12	2.01	0.42
30:3:621:BCR:H11C	30:3:621:BCR:H341	1.83	0.42
18:5:65:THR:CG2	27:5:619:CLA:CBA	2.97	0.42
24:Y:119:GLU:HG3	24:Y:124:LYS:HB2	2.01	0.42
2:B:167:SER:OG	7:G:71:THR:HG22	2.19	0.42
7:G:45:PHE:HA	7:G:48:ILE:HG12	2.01	0.42
10:J:26:LEU:HD22	30:J:102:BCR:H402	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:8:150:GLU:O	21:8:153:SER:OG	2.27	0.42
37:Y:1623:NEX:H15	37:Y:1623:NEX:H201	1.75	0.42
27:W:613:CLA:HMB1	35:W:1620:LUT:H7	2.01	0.42
27:B:808:CLA:CGA	27:B:808:CLA:C1A	2.98	0.42
35:W:1620:LUT:H171	35:W:1620:LUT:C8	2.49	0.42
1:A:488:GLN:HG2	1:A:510:TRP:HA	2.00	0.42
2:B:422:HIS:O	2:B:426:VAL:HG23	2.20	0.42
4:D:65:PRO:HD2	4:D:113:LEU:HD13	2.01	0.42
4:D:88:TRP:HB3	4:D:136:PRO:HB3	2.01	0.42
17:4:260:ASP:HB3	27:4:616:CLA:C1B	2.50	0.42
22:9:97:TRP:CE3	22:9:98:GLU:HG3	2.55	0.42
38:X:607:CHL:HMB2	38:X:607:CHL:H142	2.02	0.42
24:Y:89:LEU:HD23	38:Y:609:CHL:O2D	2.20	0.42
24:Y:172:PRO:HG2	38:Y:608:CHL:HBB2	2.02	0.42
38:U:601:CHL:H3A	38:U:601:CHL:HBA1	1.76	0.42
38:V:606:CHL:HHC	38:V:606:CHL:HBB1	2.01	0.42
38:V:607:CHL:CBB	38:V:609:CHL:HBC1	2.50	0.42
1:A:679:TRP:O	1:A:682:SER:OG	2.35	0.42
8:H:64:ASP:OD2	26:V:41:TRP:HA	2.19	0.42
15:2:32:TYR:HB2	27:2:601:CLA:CED	2.48	0.42
24:U:102:LEU:HD23	27:U:604:CLA:HMC1	2.01	0.42
26:V:218:ILE:HD12	26:V:218:ILE:HA	1.92	0.42
38:V:607:CHL:HHC	38:V:607:CHL:HBB1	2.01	0.42
23:W:94:LEU:HD23	27:W:604:CLA:HMC1	2.01	0.42
3:C:61:ASP:HA	3:C:62:PHE:HA	1.87	0.41
30:L:301:BCR:C23	30:L:301:BCR:C38	2.98	0.41
13:O:124:GLY:O	13:O:125:TYR:HB2	2.20	0.41
30:1:619:BCR:H15C	30:1:619:BCR:H351	1.84	0.41
30:2:623:BCR:C21	33:V:2631:LMG:H192	2.50	0.41
18:5:55:TRP:O	18:5:56:ASP:C	2.63	0.41
30:7:623:BCR:H383	30:7:623:BCR:H23C	2.02	0.41
23:X:156:GLU:OE1	38:X:609:CHL:NA	2.52	0.41
38:Y:609:CHL:H91	38:Y:609:CHL:H112	1.75	0.41
38:V:601:CHL:H3A	38:V:601:CHL:HBA1	1.75	0.41
38:V:601:CHL:HED3	29:V:2630:LHG:H282	2.02	0.41
38:V:606:CHL:HBB2	38:V:607:CHL:CBB	2.49	0.41
27:A:803:CLA:O2A	2:B:652:LEU:HB3	2.20	0.41
12:L:127:ILE:O	12:L:131:CYS:SG	2.74	0.41
15:2:70:GLU:OE2	15:2:158:LEU:HD11	2.20	0.41
20:7:82:GLY:HA2	36:7:620:XAT:H181	2.01	0.41
27:V:602:CLA:CGA	27:V:602:CLA:H3A	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:V:611:CLA:O1D	27:V:611:CLA:H2A	2.20	0.41
23:W:116:LYS:HA	38:W:607:CHL:O1D	2.20	0.41
1:A:102:GLU:HA	1:A:105:LEU:HD12	2.01	0.41
30:A:848:BCR:H11C	30:A:848:BCR:H341	1.87	0.41
2:B:302:MET:HG2	27:B:819:CLA:HED2	2.01	0.41
2:B:713:HIS:HE1	27:B:840:CLA:ND	2.18	0.41
6:F:151:ILE:N	6:F:152:PRO:HD2	2.35	0.41
6:F:224:VAL:HG23	6:F:226:PRO:HD2	2.01	0.41
30:L:309:BCR:H403	30:L:309:BCR:C23	2.50	0.41
16:3:231:TYR:HE1	35:3:618:LUT:C4	2.33	0.41
18:5:191:ARG:HD3	27:5:602:CLA:CHD	2.50	0.41
25:Z:143:LEU:O	25:Z:144:VAL:C	2.63	0.41
23:W:109:PHE:O	23:W:110:GLY:C	2.63	0.41
1:A:446:ILE:HD11	30:B:848:BCR:H402	2.01	0.41
2:B:204:ARG:NH2	2:B:239:ASP:OD1	2.45	0.41
38:Z:601:CHL:H162	29:Z:2630:LHG:H212	2.02	0.41
35:Z:1620:LUT:C8	35:Z:1620:LUT:C18	2.98	0.41
30:B:849:BCR:H11C	30:B:849:BCR:H341	1.89	0.41
24:U:101:ALA:O	24:U:105:ILE:HG13	2.21	0.41
23:W:174:PRO:HD2	27:W:610:CLA:OBD	2.21	0.41
1:A:650:LEU:O	1:A:654:SER:OG	2.22	0.41
1:A:668:TYR:O	1:A:741:SER:HB3	2.21	0.41
30:F:305:BCR:C33	30:F:305:BCR:C8	2.98	0.41
14:a:35:LYS:HB2	14:a:51:ASP:OD1	2.20	0.41
35:4:619:LUT:H35	35:4:619:LUT:H401	1.80	0.41
24:Y:101:ALA:O	24:Y:105:ILE:HG13	2.21	0.41
24:Y:201:LEU:HD13	27:Y:610:CLA:O1A	2.20	0.41
36:U:1622:XAT:H31	36:U:1622:XAT:H391	1.92	0.41
36:W:1622:XAT:H31	36:W:1622:XAT:H391	1.92	0.41
1:A:304:LEU:O	1:A:307:VAL:HG22	2.19	0.41
1:A:697:ILE:O	1:A:701:VAL:HG23	2.21	0.41
15:2:125:ARG:HD3	30:2:623:BCR:H292	2.02	0.41
16:3:242:PRO:O	35:3:618:LUT:O3	2.38	0.41
19:6:33:LEU:HD23	19:6:33:LEU:HA	1.97	0.41
30:9:621:BCR:H11C	30:9:621:BCR:H341	1.92	0.41
25:Z:144:VAL:HG23	25:Z:145:HIS:N	2.36	0.41
23:W:156:GLU:OE1	38:W:609:CHL:C4A	2.68	0.41
38:W:601:CHL:H3A	38:W:601:CHL:HBA1	1.53	0.41
2:B:414:ASP:HA	6:F:227:ARG:HB3	2.02	0.41
16:3:157:PHE:O	16:3:161:ARG:HG2	2.21	0.41
27:9:610:CLA:H2	35:9:619:LUT:H28	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:X:608:CHL:H152	37:X:1623:NEX:H402	2.02	0.41
1:A:443:TRP:NE1	27:A:834:CLA:OBD	2.46	0.41
1:A:587:SER:O	1:A:591:HIS:ND1	2.42	0.41
1:A:695:GLU:O	1:A:698:GLU:HG2	2.20	0.41
30:A:852:BCR:H391	27:B:832:CLA:HMA1	2.03	0.41
30:A:856:BCR:H392	30:A:856:BCR:C23	2.51	0.41
2:B:73:GLY:HA2	2:B:88:ILE:HB	2.02	0.41
2:B:92:ILE:CD1	27:B:809:CLA:HMD1	2.50	0.41
2:B:268:SER:OG	2:B:269:LEU:N	2.54	0.41
2:B:396:ILE:HD11	2:B:542:ALA:HB1	2.03	0.41
2:B:478:LEU:O	2:B:484:SER:OG	2.31	0.41
30:B:852:BCR:C38	30:B:852:BCR:C23	2.98	0.41
3:C:36:ALA:O	3:C:37:SER:C	2.63	0.41
8:H:56:VAL:HG21	12:L:76:ARG:NH2	2.36	0.41
11:K:36:LEU:HA	11:K:39:VAL:HG22	2.03	0.41
12:L:131:CYS:HB3	30:L:305:BCR:C19	2.51	0.41
14:a:161:LEU:HD12	35:a:617:LUT:H222	2.02	0.41
18:5:65:THR:CG2	27:5:619:CLA:HBA1	2.47	0.41
27:5:617:CLA:HMB1	27:6:616:CLA:H171	2.03	0.41
35:6:619:LUT:C8	35:6:619:LUT:H181	2.51	0.41
30:7:623:BCR:H15C	30:7:623:BCR:H351	1.93	0.41
38:Z:609:CHL:H143	38:Z:609:CHL:H161	1.74	0.41
37:Z:1623:NEX:H15	37:Z:1623:NEX:H201	1.92	0.41
24:U:52:TYR:CB	23:W:157:ALA:HB1	2.50	0.41
38:U:607:CHL:HBB2	38:U:609:CHL:HBC1	2.02	0.41
1:A:165:GLY:HA3	30:A:848:BCR:H313	2.03	0.41
27:A:803:CLA:H91	27:B:803:CLA:H101	2.02	0.41
30:A:849:BCR:C33	30:A:849:BCR:HC8	2.50	0.41
2:B:698:PRO:O	3:C:81:TYR:OH	2.33	0.41
27:B:818:CLA:H93	27:B:818:CLA:H61	1.92	0.41
8:H:95:ILE:HG13	8:H:96:VAL:N	2.36	0.41
9:I:87:LEU:N	9:I:88:PRO:HD2	2.36	0.41
30:L:305:BCR:H15C	30:L:305:BCR:H351	1.92	0.41
14:a:102:ASN:OD1	14:a:102:ASN:N	2.47	0.41
27:3:609:CLA:C2C	30:3:621:BCR:H322	2.50	0.41
18:5:187:ILE:O	18:5:191:ARG:HG3	2.22	0.41
27:9:609:CLA:H91	27:9:609:CLA:H112	1.94	0.41
30:9:621:BCR:H15C	30:9:621:BCR:H351	1.88	0.41
24:Y:61:LEU:HD11	24:Y:72:ASP:HB2	2.03	0.41
38:Y:609:CHL:CHC	38:Z:601:CHL:H52	2.51	0.41
38:U:607:CHL:CBB	38:U:609:CHL:HBC1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:V:601:CHL:H111	38:V:601:CHL:H151	1.72	0.41
1:A:294:THR:HG23	27:A:820:CLA:HMA3	2.03	0.40
1:A:429:ARG:O	1:A:433:HIS:ND1	2.45	0.40
1:A:448:LEU:HB3	1:A:541:PHE:HB2	2.03	0.40
2:B:195:LEU:HA	2:B:199:ALA:HB3	2.03	0.40
2:B:375:HIS:HE2	27:B:828:CLA:C1B	2.33	0.40
30:K:207:BCR:H15C	30:K:207:BCR:H351	1.95	0.40
12:L:102:LYS:NZ	12:L:196:SER:O	2.54	0.40
15:2:218:PRO:CG	27:2:601:CLA:HED3	2.51	0.40
30:2:623:BCR:H11C	30:2:623:BCR:H341	1.95	0.40
16:3:56:TYR:OH	16:3:71:GLY:HA2	2.21	0.40
21:8:82:MET:HG3	21:8:197:GLY:HA2	2.03	0.40
27:8:604:CLA:HMA1	27:8:606:CLA:HMC3	2.02	0.40
30:8:621:BCR:HC8	30:8:621:BCR:C32	2.50	0.40
23:X:93:ALA:O	23:X:97:ILE:HG13	2.21	0.40
27:A:829:CLA:H143	27:A:829:CLA:H112	1.83	0.40
2:B:664:PHE:HA	28:B:842:PQN:H9	2.03	0.40
4:D:138:PHE:CZ	4:D:151:HIS:HB2	2.56	0.40
6:F:208:GLN:O	6:F:212:ARG:HG2	2.21	0.40
30:a:619:BCR:H351	30:a:619:BCR:H15C	1.84	0.40
14:1:152:VAL:HG13	14:1:153:TYR:CD2	2.56	0.40
27:3:606:CLA:H3A	30:3:620:BCR:C21	2.52	0.40
30:7:621:BCR:H11C	30:7:621:BCR:H341	1.94	0.40
35:V:1620:LUT:C8	35:V:1620:LUT:C18	2.98	0.40
1:A:541:PHE:HZ	27:A:803:CLA:CBB	2.33	0.40
1:A:605:ILE:HD12	27:A:801:CLA:H122	2.03	0.40
27:A:801:CLA:HMB3	27:A:854:CLA:OBD	2.21	0.40
27:A:834:CLA:HMA1	30:B:849:BCR:HC31	2.03	0.40
30:B:845:BCR:H23C	30:B:845:BCR:C38	2.44	0.40
8:H:64:ASP:HB2	26:V:42:SER:H	1.86	0.40
30:2:623:BCR:H382	30:2:623:BCR:C23	2.51	0.40
30:3:620:BCR:H351	30:3:620:BCR:H15C	1.88	0.40
17:4:157:PHE:HA	17:4:160:VAL:HG22	2.03	0.40
36:6:621:XAT:C28	36:6:621:XAT:H381	2.51	0.40
20:7:135:ARG:HG2	27:7:608:CLA:CHD	2.50	0.40
24:Y:48:TRP:HE3	38:Y:601:CHL:HAA1	1.87	0.40
25:Z:225:VAL:HG21	27:Z:613:CLA:HMD2	2.03	0.40
38:Z:601:CHL:H61	38:Z:601:CHL:H102	1.61	0.40
23:W:93:ALA:O	23:W:97:ILE:HG13	2.21	0.40
32:A:857:LMU:H122	30:3:621:BCR:H383	2.03	0.40
6:F:98:SER:H	6:F:101:ALA:HB3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2:619:LUT:H11	35:2:619:LUT:H191	1.95	0.40
38:W:601:CHL:H41	38:W:601:CHL:H62	1.57	0.40
1:A:303:VAL:HG13	30:K:207:BCR:HC22	2.03	0.40
27:A:816:CLA:C4C	30:K:202:BCR:C31	3.00	0.40
27:A:829:CLA:CBC	30:A:852:BCR:H313	2.51	0.40
2:B:646:VAL:HG21	27:B:808:CLA:HAC1	2.03	0.40
30:B:801:BCR:H371	30:B:801:BCR:H24C	1.90	0.40
14:a:106:ALA:N	14:a:107:PRO:CD	2.85	0.40
14:a:152:VAL:HG13	14:a:153:TYR:CD2	2.56	0.40
27:2:603:CLA:HHC	27:2:603:CLA:CBB	2.51	0.40
18:5:137:TRP:NE1	27:5:619:CLA:OBD	2.47	0.40
26:V:228:MET:SD	26:V:231:PHE:CD2	3.15	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	720 (97%)	19 (3%)	0	100	100
2	B	731/735 (100%)	714 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	141/196 (72%)	135 (96%)	6 (4%)	0	100	100
5	E	61/97 (63%)	59 (97%)	2 (3%)	0	100	100
6	F	163/227 (72%)	155 (95%)	8 (5%)	0	100	100
7	G	92/126 (73%)	86 (94%)	6 (6%)	0	100	100
8	H	98/130 (75%)	92 (94%)	6 (6%)	0	100	100
9	I	40/106 (38%)	35 (88%)	5 (12%)	0	100	100
10	J	39/41 (95%)	38 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	84/113 (74%)	79 (94%)	5 (6%)	0	100	100
12	L	157/196 (80%)	150 (96%)	7 (4%)	0	100	100
13	O	95/126 (75%)	87 (92%)	8 (8%)	0	100	100
14	1	192/228 (84%)	185 (96%)	7 (4%)	0	100	100
14	a	192/228 (84%)	185 (96%)	7 (4%)	0	100	100
15	2	215/246 (87%)	202 (94%)	13 (6%)	0	100	100
16	3	218/298 (73%)	213 (98%)	5 (2%)	0	100	100
17	4	208/264 (79%)	201 (97%)	7 (3%)	0	100	100
18	5	225/257 (88%)	212 (94%)	13 (6%)	0	100	100
19	6	228/257 (89%)	206 (90%)	22 (10%)	0	100	100
20	7	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
21	8	215/243 (88%)	209 (97%)	6 (3%)	0	100	100
22	9	181/213 (85%)	167 (92%)	14 (8%)	0	100	100
23	W	218/249 (88%)	204 (94%)	14 (6%)	0	100	100
23	X	218/249 (88%)	204 (94%)	13 (6%)	1 (0%)	24	43
24	U	217/257 (84%)	197 (91%)	19 (9%)	1 (0%)	24	43
24	Y	218/257 (85%)	202 (93%)	15 (7%)	1 (0%)	24	43
25	Z	229/256 (90%)	223 (97%)	6 (3%)	0	100	100
26	V	235/268 (88%)	220 (94%)	15 (6%)	0	100	100
All	All	5938/6936 (86%)	5655 (95%)	280 (5%)	3 (0%)	49	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	X	167	GLU
24	Y	114	GLY
24	U	174	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	601/610 (98%)	601 (100%)	0	100	100
2	B	596/597 (100%)	594 (100%)	2 (0%)	86	94
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	120/152 (79%)	119 (99%)	1 (1%)	73	86
5	E	54/81 (67%)	53 (98%)	1 (2%)	50	73
6	F	127/169 (75%)	127 (100%)	0	100	100
7	G	70/94 (74%)	70 (100%)	0	100	100
8	H	81/102 (79%)	80 (99%)	1 (1%)	63	80
9	I	33/76 (43%)	33 (100%)	0	100	100
10	J	37/37 (100%)	37 (100%)	0	100	100
11	K	59/80 (74%)	59 (100%)	0	100	100
12	L	121/148 (82%)	120 (99%)	1 (1%)	73	86
13	O	78/101 (77%)	78 (100%)	0	100	100
14	1	137/162 (85%)	136 (99%)	1 (1%)	76	88
14	a	137/162 (85%)	137 (100%)	0	100	100
15	2	173/198 (87%)	173 (100%)	0	100	100
16	3	167/230 (73%)	166 (99%)	1 (1%)	78	89
17	4	165/205 (80%)	165 (100%)	0	100	100
18	5	184/206 (89%)	181 (98%)	3 (2%)	55	76
19	6	184/203 (91%)	182 (99%)	2 (1%)	65	81
20	7	164/181 (91%)	163 (99%)	1 (1%)	78	89
21	8	163/183 (89%)	162 (99%)	1 (1%)	78	89
22	9	140/159 (88%)	140 (100%)	0	100	100
23	W	163/187 (87%)	163 (100%)	0	100	100
23	X	165/187 (88%)	163 (99%)	2 (1%)	63	80
24	U	168/194 (87%)	166 (99%)	2 (1%)	63	80
24	Y	170/194 (88%)	167 (98%)	3 (2%)	51	74
25	Z	178/195 (91%)	178 (100%)	0	100	100
26	V	178/201 (89%)	178 (100%)	0	100	100
All	All	4682/5364 (87%)	4660 (100%)	22 (0%)	78	90

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	268	SER
2	B	537	LYS
4	D	154	ASP
5	E	91	ASP
8	H	66	GLN
12	L	112	THR
14	1	225	VAL
16	3	257	ASN
18	5	157	VAL
18	5	249	LEU
18	5	251	CYS
19	6	132	LEU
19	6	233	CYS
20	7	211	THR
21	8	154	PHE
23	X	104	LYS
23	X	186	ASP
24	Y	81	GLU
24	Y	119	GLU
24	Y	143	LEU
24	U	62	THR
24	U	221	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	268	ASN
1	A	609	HIS
2	B	77	GLN
2	B	253	GLN
2	B	334	GLN
2	B	504	ASN
2	B	506	GLN
2	B	628	ASN
2	B	705	GLN
3	C	16	GLN
4	D	120	GLN
4	D	162	ASN
5	E	87	ASN
7	G	62	ASN
7	G	90	ASN
8	H	66	GLN

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Mol	Chain	Res	Type
8	H	72	GLN
9	I	65	GLN
10	J	30	ASN
12	L	71	ASN
12	L	190	GLN
13	O	60	ASN
13	O	69	GLN
13	O	119	GLN
13	O	123	GLN
14	a	144	GLN
14	1	144	GLN
15	2	240	ASN
16	3	256	ASN
17	4	166	GLN
17	4	259	ASN
18	5	138	GLN
18	5	238	HIS
19	6	41	HIS
20	7	113	ASN
20	7	184	GLN
21	8	140	GLN
22	9	109	GLN
23	X	128	ASN
23	X	137	HIS
23	X	139	GLN
24	Y	140	ASN
24	Y	145	HIS
24	Y	147	GLN
25	Z	131	GLN
25	Z	169	ASN
24	U	169	ASN
26	V	156	HIS
26	V	158	GLN
23	W	161	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
25	TPO	Z	27	25	8,10,11	1.12	0	10,14,16	1.81	1 (10%)
26	TPO	V	33	26	8,10,11	1.60	1 (12%)	10,14,16	1.95	2 (20%)

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
25	TPO	Z	27	25	-	1/9/11/13	-
26	TPO	V	33	26	-	5/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	33	TPO	P-O1P	3.31	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	33	TPO	P-OG1-CB	-5.16	109.31	123.33
25	Z	27	TPO	P-OG1-CB	-5.12	109.42	123.33
26	V	33	TPO	CG2-CB-CA	-2.34	108.70	113.26

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	V	33	TPO	N-CA-CB-CG2
26	V	33	TPO	CB-OG1-P-O1P
26	V	33	TPO	CB-OG1-P-O2P
26	V	33	TPO	CB-OG1-P-O3P
25	Z	27	TPO	C-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
26	V	33	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	27	TPO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

471 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
27	CLA	3	613	16	56,61,73	1.29	8 (14%)	65,98,113	1.17	5 (7%)
27	CLA	J	101	10	46,50,73	1.40	8 (17%)	53,85,113	1.26	5 (9%)
27	CLA	A	812	-	69,73,73	1.15	7 (10%)	82,113,113	1.12	4 (4%)
27	CLA	2	602	15	67,72,73	1.17	9 (13%)	79,112,113	1.15	4 (5%)
27	CLA	A	819	-	63,67,73	1.21	8 (12%)	74,105,113	1.27	6 (8%)
27	CLA	B	807	-	56,60,73	1.28	7 (12%)	65,97,113	1.30	7 (10%)
35	LUT	X	1621	-	42,43,43	0.81	1 (2%)	51,60,60	1.86	16 (31%)
27	CLA	B	803	-	69,73,73	1.15	8 (11%)	82,113,113	1.12	4 (4%)
38	CHL	Z	601	25	60,74,74	3.40	20 (33%)	58,114,114	2.41	15 (25%)
27	CLA	2	603	15	47,52,73	1.43	8 (17%)	55,88,113	1.29	5 (9%)
35	LUT	5	620	-	42,43,43	0.84	1 (2%)	51,60,60	2.16	12 (23%)
27	CLA	B	836	-	54,58,73	1.31	9 (16%)	64,95,113	1.32	6 (9%)
27	CLA	1	607	-	43,48,73	1.40	7 (16%)	51,83,113	1.27	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	XAT	W	1622	-	41,47,47	0.97	3 (7%)	54,74,74	3.86	25 (46%)
27	CLA	Y	602	24	62,66,73	1.25	7 (11%)	73,104,113	1.14	4 (5%)
27	CLA	L	302	12	49,53,73	1.36	7 (14%)	58,89,113	1.26	5 (8%)
27	CLA	2	612	15	48,52,73	1.40	7 (14%)	57,88,113	1.28	4 (7%)
30	BCR	K	202	-	41,41,41	0.80	0	56,56,56	2.18	18 (32%)
32	LMU	A	857	-	36,36,36	1.14	2 (5%)	47,47,47	0.99	1 (2%)
33	LMG	8	626	-	46,46,55	0.97	2 (4%)	54,54,63	1.11	4 (7%)
38	CHL	W	606	-	40,54,74	3.96	19 (47%)	34,90,114	5.43	19 (55%)
37	NEX	Z	1623	-	40,46,46	1.27	4 (10%)	50,70,70	2.24	16 (32%)
27	CLA	A	802	-	69,73,73	1.15	8 (11%)	82,113,113	1.21	6 (7%)
27	CLA	8	609	21	49,53,73	1.36	7 (14%)	58,89,113	1.24	4 (6%)
27	CLA	7	613	20	69,73,73	1.16	7 (10%)	82,113,113	1.08	6 (7%)
27	CLA	H	203	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	5 (6%)
27	CLA	A	823	-	46,50,73	1.39	7 (15%)	53,85,113	1.23	4 (7%)
27	CLA	A	831	-	69,73,73	1.16	6 (8%)	82,113,113	1.09	6 (7%)
38	CHL	W	605	23	40,54,74	4.03	19 (47%)	34,90,114	3.22	17 (50%)
27	CLA	4	609	17	61,65,73	1.22	7 (11%)	72,103,113	1.20	6 (8%)
27	CLA	9	613	22	69,73,73	1.17	7 (10%)	82,113,113	1.13	5 (6%)
38	CHL	U	607	-	40,54,74	3.95	19 (47%)	34,90,114	3.00	15 (44%)
27	CLA	B	810	-	68,72,73	1.17	9 (13%)	80,111,113	1.15	4 (5%)
27	CLA	9	601	22	49,53,73	1.38	7 (14%)	58,89,113	1.26	4 (6%)
27	CLA	A	821	-	57,61,73	1.28	7 (12%)	67,98,113	1.27	5 (7%)
27	CLA	Z	614	-	58,62,73	1.28	6 (10%)	68,99,113	1.15	4 (5%)
36	XAT	6	621	-	41,47,47	0.88	2 (4%)	54,74,74	2.36	20 (37%)
38	CHL	V	609	26	55,69,74	3.59	19 (34%)	52,108,114	2.21	15 (28%)
38	CHL	Z	608	-	44,58,74	4.00	19 (43%)	37,94,114	2.93	18 (48%)
27	CLA	B	821	-	47,51,73	1.45	9 (19%)	54,86,113	1.28	5 (9%)
27	CLA	8	616	-	47,51,73	1.50	9 (19%)	58,87,113	1.31	6 (10%)
27	CLA	V	611	29	47,51,73	1.35	7 (14%)	55,86,113	1.33	4 (7%)
38	CHL	U	609	24	54,68,74	3.58	20 (37%)	50,106,114	2.47	15 (30%)
31	SF4	C	101	3	0,12,12	-	-	-		
27	CLA	2	604	-	46,50,73	1.40	8 (17%)	54,85,113	1.22	4 (7%)
38	CHL	Y	606	-	40,54,74	4.15	18 (45%)	34,90,114	3.10	15 (44%)
27	CLA	Y	614	-	52,56,73	1.36	7 (13%)	61,92,113	1.20	5 (8%)
27	CLA	W	613	23	69,73,73	1.16	6 (8%)	82,113,113	1.17	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	a	609	14	67,72,73	1.18	7 (10%)	79,112,113	1.11	4 (5%)
30	BCR	B	852	-	41,41,41	0.78	0	56,56,56	3.62	24 (42%)
30	BCR	7	621	-	41,41,41	0.76	1 (2%)	56,56,56	2.37	22 (39%)
27	CLA	Y	604	-	54,58,73	1.33	7 (12%)	64,95,113	1.17	6 (9%)
27	CLA	8	608	-	55,59,73	1.31	8 (14%)	64,96,113	1.30	5 (7%)
27	CLA	L	307	-	43,48,73	1.45	7 (16%)	49,83,113	1.32	4 (8%)
27	CLA	A	808	-	54,58,73	1.30	7 (12%)	64,95,113	1.25	6 (9%)
27	CLA	7	608	-	54,58,73	1.29	7 (12%)	64,95,113	1.22	4 (6%)
27	CLA	4	604	-	58,62,73	1.34	8 (13%)	71,100,113	1.22	6 (8%)
27	CLA	U	603	-	56,60,73	1.29	8 (14%)	65,97,113	1.34	6 (9%)
27	CLA	7	616	20	47,51,73	1.50	8 (17%)	58,87,113	1.28	6 (10%)
27	CLA	A	801	-	69,73,73	1.18	6 (8%)	82,113,113	1.19	8 (9%)
27	CLA	4	613	17	69,73,73	1.16	8 (11%)	82,113,113	1.11	5 (6%)
27	CLA	6	610	19	69,73,73	1.17	8 (11%)	82,113,113	1.08	5 (6%)
27	CLA	Z	610	25	69,73,73	1.17	6 (8%)	82,113,113	1.15	7 (8%)
27	CLA	G	204	7	49,53,73	1.38	8 (16%)	58,89,113	1.33	5 (8%)
27	CLA	3	609	16	64,68,73	1.20	6 (9%)	76,107,113	1.32	7 (9%)
27	CLA	Y	603	-	59,63,73	1.29	7 (11%)	70,101,113	1.23	5 (7%)
35	LUT	V	1621	-	42,43,43	0.98	2 (4%)	51,60,60	1.82	12 (23%)
36	XAT	Y	1622	-	41,47,47	0.91	1 (2%)	54,74,74	3.78	26 (48%)
27	CLA	2	601	15	69,73,73	1.16	8 (11%)	82,113,113	1.36	9 (10%)
33	LMG	A	860	-	40,40,55	1.04	2 (5%)	48,48,63	1.10	4 (8%)
27	CLA	6	602	19	69,73,73	1.17	8 (11%)	82,113,113	1.14	7 (8%)
32	LMU	A	858	-	35,35,36	1.22	3 (8%)	44,45,47	0.92	1 (2%)
27	CLA	2	610	15	59,63,73	1.24	8 (13%)	70,101,113	1.29	8 (11%)
32	LMU	8	625	-	36,36,36	1.15	2 (5%)	47,47,47	1.03	3 (6%)
27	CLA	B	818	-	64,68,73	1.19	7 (10%)	76,107,113	1.33	6 (7%)
27	CLA	B	812	-	47,51,73	1.37	8 (17%)	55,86,113	1.28	6 (10%)
35	LUT	2	619	-	42,43,43	0.82	2 (4%)	51,60,60	2.02	12 (23%)
27	CLA	4	616	17	47,51,73	1.51	9 (19%)	58,87,113	1.28	6 (10%)
27	CLA	Y	611	29	47,51,73	1.40	7 (14%)	55,86,113	1.27	4 (7%)
27	CLA	6	608	-	49,53,73	1.37	8 (16%)	58,89,113	1.27	5 (8%)
27	CLA	A	804	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	5 (6%)
30	BCR	A	856	-	41,41,41	0.75	0	56,56,56	2.17	18 (32%)
27	CLA	B	835	-	49,53,73	1.37	7 (14%)	58,89,113	1.21	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	O	2001	-	41,46,73	1.48	8 (19%)	47,80,113	1.34	4 (8%)
27	CLA	4	608	-	69,73,73	1.17	7 (10%)	82,113,113	1.15	5 (6%)
27	CLA	a	610	14	63,67,73	1.20	7 (11%)	75,106,113	1.19	6 (8%)
27	CLA	A	817	-	49,53,73	1.36	7 (14%)	58,89,113	1.40	6 (10%)
27	CLA	A	827	-	62,66,73	1.22	8 (12%)	73,104,113	1.20	5 (6%)
29	LHG	A	847	27	29,29,48	1.18	2 (6%)	32,35,54	1.05	2 (6%)
37	NEX	5	624	-	40,46,46	1.23	3 (7%)	50,70,70	2.14	15 (30%)
30	BCR	3	621	-	41,41,41	0.82	2 (4%)	56,56,56	1.81	14 (25%)
33	LMG	J	104	-	40,40,55	1.06	2 (5%)	48,48,63	1.18	5 (10%)
27	CLA	5	606	-	43,48,73	1.45	8 (18%)	49,83,113	1.21	3 (6%)
33	LMG	L	2631	-	37,37,55	1.10	2 (5%)	45,45,63	1.12	3 (6%)
35	LUT	U	1620	-	42,43,43	0.89	1 (2%)	51,60,60	1.89	10 (19%)
27	CLA	B	824	-	69,73,73	1.17	8 (11%)	82,113,113	1.15	4 (4%)
27	CLA	5	604	-	67,71,73	1.26	8 (11%)	82,111,113	1.17	7 (8%)
29	LHG	9	624	-	48,48,48	0.95	2 (4%)	51,54,54	1.01	2 (3%)
27	CLA	U	604	-	52,56,73	1.43	8 (15%)	61,91,113	1.26	6 (9%)
27	CLA	5	614	-	48,52,73	1.39	8 (16%)	53,87,113	1.27	4 (7%)
27	CLA	A	822	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	8 (9%)
30	BCR	a	619	-	41,41,41	0.72	0	56,56,56	2.44	21 (37%)
36	XAT	7	620	-	41,47,47	0.90	2 (4%)	54,74,74	2.35	23 (42%)
29	LHG	2	622	27	35,35,48	1.08	2 (5%)	38,41,54	0.99	2 (5%)
30	BCR	7	623	-	41,41,41	0.67	0	56,56,56	2.24	25 (44%)
38	CHL	Y	609	24	60,74,74	3.41	20 (33%)	58,114,114	2.16	16 (27%)
27	CLA	5	616	18	44,50,73	1.52	8 (18%)	57,85,113	1.23	6 (10%)
35	LUT	Y	1621	-	42,43,43	0.79	0	51,60,60	1.86	16 (31%)
27	CLA	5	607	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	4 (4%)
29	LHG	1	620	27	48,48,48	0.92	2 (4%)	51,54,54	0.98	4 (7%)
27	CLA	6	613	-	67,72,73	1.18	8 (11%)	79,112,113	1.08	4 (5%)
27	CLA	B	813	-	69,73,73	1.18	9 (13%)	82,113,113	1.20	6 (7%)
30	BCR	4	621	-	41,41,41	0.78	1 (2%)	56,56,56	2.50	23 (41%)
29	LHG	9	623	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	3 (5%)
27	CLA	A	828	-	69,73,73	1.16	9 (13%)	82,113,113	1.17	6 (7%)
27	CLA	B	825	-	53,57,73	1.29	7 (13%)	61,93,113	1.22	6 (9%)
27	CLA	L	304	-	49,53,73	1.35	7 (14%)	58,89,113	1.20	4 (6%)
30	BCR	G	205	-	41,41,41	0.81	1 (2%)	56,56,56	1.97	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	BCR	3	622	-	41,41,41	0.74	0	56,56,56	2.32	19 (33%)
38	CHL	X	609	23	60,74,74	3.41	19 (31%)	58,114,114	2.30	17 (29%)
27	CLA	V	603	-	49,53,73	1.38	7 (14%)	58,89,113	1.38	3 (5%)
29	LHG	4	622	27	48,48,48	0.93	2 (4%)	51,54,54	0.90	2 (3%)
27	CLA	A	806	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
27	CLA	1	610	14	43,47,73	1.42	7 (16%)	50,81,113	1.51	7 (14%)
27	CLA	2	609	15	49,53,73	1.37	8 (16%)	58,89,113	1.25	4 (6%)
27	CLA	X	610	23	69,73,73	1.19	7 (10%)	82,113,113	1.11	6 (7%)
27	CLA	3	602	16	64,68,73	1.19	8 (12%)	76,107,113	1.12	5 (6%)
27	CLA	4	607	-	49,53,73	1.35	7 (14%)	58,89,113	1.29	4 (6%)
27	CLA	A	820	-	69,73,73	1.16	7 (10%)	82,113,113	1.21	6 (7%)
27	CLA	W	611	29	61,65,73	1.22	8 (13%)	72,103,113	1.22	5 (6%)
27	CLA	9	611	29	46,50,73	1.39	8 (17%)	53,85,113	1.23	4 (7%)
30	BCR	B	849	-	41,41,41	0.73	0	56,56,56	2.52	24 (42%)
27	CLA	G	203	-	46,50,73	1.38	8 (17%)	53,85,113	1.30	4 (7%)
38	CHL	Z	607	-	60,74,74	3.39	19 (31%)	58,114,114	2.49	18 (31%)
27	CLA	B	811	-	56,60,73	1.45	10 (17%)	70,97,113	1.22	6 (8%)
27	CLA	3	612	16	47,51,73	1.40	7 (14%)	55,86,113	1.30	5 (9%)
27	CLA	A	841	-	69,73,73	1.14	9 (13%)	82,113,113	1.16	4 (4%)
27	CLA	B	809	2	69,73,73	1.18	7 (10%)	82,113,113	1.20	5 (6%)
27	CLA	1	611	29	61,65,73	1.24	7 (11%)	72,103,113	1.16	4 (5%)
27	CLA	A	854	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	7 (8%)
27	CLA	3	604	-	69,73,73	1.15	7 (10%)	82,113,113	1.17	5 (6%)
27	CLA	1	616	14	47,51,73	1.49	7 (14%)	58,87,113	1.36	7 (12%)
27	CLA	A	845	29	54,58,73	1.30	7 (12%)	64,95,113	1.19	4 (6%)
27	CLA	7	609	20	46,52,73	1.38	7 (15%)	57,87,113	1.21	5 (8%)
38	CHL	X	601	23	60,74,74	3.39	20 (33%)	58,114,114	2.46	15 (25%)
27	CLA	7	615	-	44,50,73	1.54	8 (18%)	57,85,113	1.28	5 (8%)
27	CLA	6	607	-	45,49,73	1.48	9 (20%)	54,84,113	1.33	5 (9%)
27	CLA	1	604	-	53,57,73	1.30	7 (13%)	61,93,113	1.18	3 (4%)
29	LHG	A	846	-	48,48,48	0.92	2 (4%)	51,54,54	0.91	2 (3%)
27	CLA	X	614	-	46,50,73	1.41	7 (15%)	53,85,113	1.24	4 (7%)
27	CLA	B	805	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	6 (7%)
27	CLA	9	603	22	48,52,73	1.49	9 (18%)	59,88,113	1.30	5 (8%)
29	LHG	Z	2630	27	48,48,48	0.94	2 (4%)	51,54,54	0.86	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LHG	O	2631	-	35,35,48	1.09	2 (5%)	38,41,54	1.09	3 (7%)
35	LUT	U	1621	-	42,43,43	0.96	2 (4%)	51,60,60	1.82	14 (27%)
27	CLA	9	606	-	43,48,73	1.46	8 (18%)	49,83,113	1.28	4 (8%)
38	CHL	Y	607	-	60,74,74	3.45	19 (31%)	58,114,114	2.14	18 (31%)
35	LUT	V	1620	-	42,43,43	0.90	2 (4%)	51,60,60	1.79	13 (25%)
27	CLA	V	602	26	64,68,73	1.21	9 (14%)	76,107,113	1.23	7 (9%)
32	LMU	K	208	-	36,36,36	1.14	2 (5%)	47,47,47	0.98	2 (4%)
27	CLA	A	810	1	54,58,73	1.33	9 (16%)	64,95,113	1.33	6 (9%)
27	CLA	4	603	17	48,52,73	1.49	8 (16%)	59,88,113	1.39	5 (8%)
27	CLA	5	611	29	46,50,73	1.37	7 (15%)	53,85,113	1.23	4 (7%)
27	CLA	W	604	-	51,55,73	1.34	7 (13%)	60,91,113	1.22	4 (6%)
33	LMG	J	103	-	42,42,55	1.02	2 (4%)	50,50,63	1.09	3 (6%)
35	LUT	W	1621	-	42,43,43	0.97	2 (4%)	51,60,60	1.82	14 (27%)
38	CHL	X	608	-	60,74,74	3.44	18 (30%)	58,114,114	2.01	15 (25%)
27	CLA	Z	602	25	64,68,73	1.22	6 (9%)	76,107,113	1.13	6 (7%)
27	CLA	3	608	-	59,63,73	1.30	8 (13%)	70,101,113	1.18	5 (7%)
38	CHL	Z	606	-	40,54,74	4.17	19 (47%)	34,90,114	3.08	16 (47%)
27	CLA	4	606	-	43,48,73	1.44	8 (18%)	49,83,113	1.27	4 (8%)
27	CLA	A	833	-	49,53,73	1.36	8 (16%)	58,89,113	1.32	5 (8%)
27	CLA	8	611	29	46,50,73	1.37	8 (17%)	53,85,113	1.22	4 (7%)
29	LHG	V	2630	27	47,47,48	0.90	2 (4%)	50,53,54	1.13	3 (6%)
27	CLA	6	601	19	69,73,73	1.17	7 (10%)	82,113,113	1.19	6 (7%)
30	BCR	O	2005	-	41,41,41	0.83	1 (2%)	56,56,56	3.07	25 (44%)
27	CLA	B	833	-	69,73,73	1.15	8 (11%)	82,113,113	1.14	9 (10%)
27	CLA	Y	612	24	49,53,73	1.40	7 (14%)	58,89,113	1.29	4 (6%)
30	BCR	F	305	-	41,41,41	0.80	0	56,56,56	2.27	27 (48%)
38	CHL	U	608	-	38,52,74	4.01	18 (47%)	31,87,114	3.05	14 (45%)
36	XAT	9	620	-	41,47,47	0.90	3 (7%)	54,74,74	2.33	21 (38%)
38	CHL	Z	605	25	38,52,74	4.26	17 (44%)	31,87,114	3.17	18 (58%)
27	CLA	Z	604	-	61,65,73	1.25	6 (9%)	72,103,113	1.17	4 (5%)
32	LMU	5	629	-	33,33,36	1.17	2 (6%)	44,44,47	1.10	3 (6%)
33	LMG	4	623	-	40,40,55	1.05	2 (5%)	48,48,63	1.15	4 (8%)
27	CLA	B	815	-	47,51,73	1.37	6 (12%)	55,86,113	1.24	3 (5%)
30	BCR	L	301	-	41,41,41	0.71	0	56,56,56	2.27	27 (48%)
27	CLA	A	840	-	56,60,73	1.29	8 (14%)	65,97,113	1.32	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	NEX	Y	1623	-	41,45,46	1.03	3 (7%)	50,67,70	2.35	18 (36%)
33	LMG	5	627	-	40,40,55	1.05	2 (5%)	48,48,63	1.02	2 (4%)
27	CLA	V	604	-	54,58,73	1.32	6 (11%)	64,95,113	1.25	5 (7%)
33	LMG	V	2631	-	41,41,55	1.02	3 (7%)	49,49,63	1.17	4 (8%)
27	CLA	2	613	15	69,73,73	1.14	7 (10%)	82,113,113	1.09	5 (6%)
37	NEX	6	624	-	40,46,46	1.39	3 (7%)	50,70,70	2.02	15 (30%)
27	CLA	V	610	26	66,70,73	1.19	7 (10%)	78,109,113	1.14	6 (7%)
27	CLA	A	807	1	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
27	CLA	9	612	22	44,49,73	1.42	7 (15%)	50,84,113	1.28	3 (6%)
27	CLA	A	814	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
30	BCR	2	623	-	41,41,41	0.80	0	56,56,56	2.34	22 (39%)
29	LHG	5	623	27	48,48,48	0.92	2 (4%)	51,54,54	0.84	2 (3%)
27	CLA	U	610	24	60,64,73	1.26	8 (13%)	71,102,113	1.16	6 (8%)
27	CLA	7	611	29	63,67,73	1.19	7 (11%)	74,105,113	1.12	5 (6%)
36	XAT	1	618	-	41,47,47	0.89	2 (4%)	54,74,74	2.42	23 (42%)
27	CLA	Z	613	25	69,73,73	1.17	8 (11%)	82,113,113	1.12	5 (6%)
27	CLA	1	612	14	49,53,73	1.37	7 (14%)	58,89,113	1.26	3 (5%)
35	LUT	Y	1620	-	42,43,43	0.80	1 (2%)	51,60,60	2.04	12 (23%)
38	CHL	V	601	26	60,74,74	3.37	19 (31%)	58,114,114	2.40	14 (24%)
27	CLA	A	803	-	69,73,73	1.16	7 (10%)	82,113,113	1.14	2 (2%)
27	CLA	B	816	-	58,62,73	1.24	7 (12%)	68,99,113	1.22	5 (7%)
27	CLA	F	304	6	45,49,73	1.39	8 (17%)	54,84,113	1.29	4 (7%)
27	CLA	4	618	17	43,48,73	1.52	7 (16%)	51,83,113	1.39	5 (9%)
35	LUT	9	619	-	42,43,43	0.72	0	51,60,60	1.88	14 (27%)
27	CLA	3	607	16	60,64,73	1.31	8 (13%)	73,102,113	1.28	8 (10%)
27	CLA	B	839	-	69,73,73	1.15	7 (10%)	82,113,113	1.08	4 (4%)
27	CLA	B	841	29	69,73,73	1.16	9 (13%)	82,113,113	1.19	5 (6%)
30	BCR	6	622	-	41,41,41	0.73	1 (2%)	56,56,56	3.56	27 (48%)
27	CLA	a	601	14	57,62,73	1.27	7 (12%)	67,100,113	1.18	5 (7%)
27	CLA	A	811	-	69,73,73	1.15	7 (10%)	82,113,113	1.11	6 (7%)
27	CLA	B	808	-	69,73,73	1.13	7 (10%)	82,113,113	1.15	7 (8%)
29	LHG	8	622	27	48,48,48	0.93	2 (4%)	51,54,54	0.86	2 (3%)
30	BCR	B	848	-	41,41,41	0.74	0	56,56,56	2.23	20 (35%)
27	CLA	7	612	20	48,52,73	1.40	7 (14%)	57,88,113	1.32	3 (5%)
27	CLA	5	603	-	58,62,73	1.36	9 (15%)	71,100,113	1.28	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	XAT	8	620	-	41,47,47	0.89	2 (4%)	54,74,74	2.46	26 (48%)
30	BCR	B	846	-	41,41,41	0.76	1 (2%)	56,56,56	2.26	20 (35%)
27	CLA	W	602	23	64,68,73	1.21	8 (12%)	76,107,113	1.23	4 (5%)
29	LHG	3	624	27	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
27	CLA	B	834	-	64,68,73	1.19	7 (10%)	76,107,113	1.19	5 (6%)
27	CLA	1	603	-	56,61,73	1.28	8 (14%)	65,98,113	1.30	5 (7%)
29	LHG	U	2630	27	48,48,48	0.92	2 (4%)	51,54,54	0.93	2 (3%)
27	CLA	A	843	-	68,72,73	1.17	8 (11%)	80,111,113	1.13	6 (7%)
27	CLA	A	815	-	54,58,73	1.31	8 (14%)	64,95,113	1.29	4 (6%)
27	CLA	V	613	26	69,73,73	1.18	6 (8%)	82,113,113	1.16	5 (6%)
38	CHL	U	605	24	37,51,74	4.11	18 (48%)	30,86,114	3.38	16 (53%)
27	CLA	O	2002	-	41,46,73	1.58	8 (19%)	51,81,113	1.28	5 (9%)
27	CLA	U	612	24	47,51,73	1.38	8 (17%)	55,86,113	1.30	4 (7%)
29	LHG	B	851	27	37,37,48	1.08	2 (5%)	40,43,54	1.15	3 (7%)
30	BCR	J	102	-	41,41,41	0.74	0	56,56,56	2.20	22 (39%)
27	CLA	1	602	14	65,69,73	1.20	8 (12%)	77,108,113	1.18	6 (7%)
31	SF4	A	853	2,1	0,12,12	-	-	-		
27	CLA	6	604	-	69,73,73	1.16	7 (10%)	82,113,113	1.10	6 (7%)
38	CHL	U	601	24	60,74,74	3.40	19 (31%)	58,114,114	2.46	16 (27%)
27	CLA	5	610	18	58,62,73	1.24	8 (13%)	68,99,113	1.21	6 (8%)
27	CLA	9	607	-	49,53,73	1.38	7 (14%)	58,89,113	1.28	4 (6%)
36	XAT	Z	1622	-	41,47,47	0.93	1 (2%)	54,74,74	3.72	25 (46%)
27	CLA	L	306	-	43,48,73	1.42	7 (16%)	49,83,113	1.30	3 (6%)
27	CLA	Z	612	25	69,73,73	1.18	6 (8%)	82,113,113	1.11	3 (3%)
29	LHG	9	622	27	29,29,48	1.19	2 (6%)	32,35,54	1.05	2 (6%)
35	LUT	3	618	-	42,43,43	0.82	2 (4%)	51,60,60	1.83	12 (23%)
27	CLA	H	202	8	42,47,73	1.46	7 (16%)	50,82,113	1.22	3 (6%)
27	CLA	B	830	-	47,51,73	1.37	7 (14%)	55,86,113	1.21	6 (10%)
38	CHL	V	608	-	42,56,74	3.80	19 (45%)	36,92,114	2.93	14 (38%)
27	CLA	4	611	29	46,50,73	1.38	7 (15%)	53,85,113	1.25	4 (7%)
27	CLA	B	802	-	69,73,73	1.16	7 (10%)	82,113,113	1.08	5 (6%)
27	CLA	1	613	-	69,73,73	1.16	7 (10%)	82,113,113	1.10	6 (7%)
36	XAT	3	619	-	41,47,47	0.87	2 (4%)	54,74,74	2.46	23 (42%)
27	CLA	U	602	24	63,67,73	1.21	7 (11%)	74,105,113	1.24	4 (5%)
29	LHG	7	622	27	36,36,48	1.05	2 (5%)	39,42,54	0.86	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	CHL	W	601	23	60,74,74	3.39	19 (31%)	58,114,114	2.46	17 (29%)
27	CLA	Z	611	29	69,73,73	1.16	5 (7%)	82,113,113	1.12	4 (4%)
35	LUT	8	619	-	42,43,43	0.80	1 (2%)	51,60,60	1.78	14 (27%)
27	CLA	7	607	-	46,50,73	1.37	7 (15%)	53,85,113	1.24	4 (7%)
27	CLA	U	613	24	63,67,73	1.20	6 (9%)	74,105,113	1.21	5 (6%)
27	CLA	K	204	-	49,53,73	1.37	8 (16%)	58,89,113	1.37	5 (8%)
27	CLA	8	602	21	64,68,73	1.20	9 (14%)	76,107,113	1.18	5 (6%)
27	CLA	B	840	-	69,73,73	1.17	7 (10%)	82,113,113	1.19	3 (3%)
36	XAT	V	1622	-	41,47,47	0.94	4 (9%)	54,74,74	2.47	19 (35%)
27	CLA	V	612	26	49,53,73	1.37	8 (16%)	58,89,113	1.33	6 (10%)
27	CLA	8	603	-	48,52,73	1.49	9 (18%)	59,88,113	1.43	5 (8%)
27	CLA	A	826	-	68,72,73	1.17	9 (13%)	80,111,113	1.24	6 (7%)
27	CLA	6	618	19	43,48,73	1.52	10 (23%)	51,83,113	1.38	5 (9%)
29	LHG	a	620	27	42,42,48	0.98	2 (4%)	45,48,54	1.03	4 (8%)
35	LUT	a	617	-	42,43,43	0.81	1 (2%)	51,60,60	1.92	15 (29%)
27	CLA	A	825	-	69,73,73	1.15	6 (8%)	82,113,113	1.14	6 (7%)
33	LMG	4	624	-	40,40,55	1.05	2 (5%)	48,48,63	1.21	7 (14%)
38	CHL	X	607	-	60,74,74	3.41	19 (31%)	58,114,114	2.38	19 (32%)
27	CLA	1	608	-	47,52,73	1.40	7 (14%)	55,88,113	1.23	4 (7%)
27	CLA	8	606	-	68,72,73	1.17	8 (11%)	81,112,113	1.13	5 (6%)
27	CLA	8	612	21	44,49,73	1.42	7 (15%)	50,84,113	1.30	3 (6%)
27	CLA	8	601	21	69,73,73	1.16	7 (10%)	82,113,113	1.18	6 (7%)
27	CLA	a	611	29	41,46,73	1.57	9 (21%)	51,81,113	1.33	6 (11%)
27	CLA	F	301	-	61,65,73	1.25	9 (14%)	72,103,113	1.14	4 (5%)
27	CLA	O	2003	-	43,48,73	1.46	8 (18%)	49,83,113	1.22	3 (6%)
27	CLA	8	610	21	64,68,73	1.18	8 (12%)	76,107,113	1.28	7 (9%)
30	BCR	B	843	-	41,41,41	0.73	0	56,56,56	1.83	16 (28%)
38	CHL	W	607	-	59,73,74	3.23	19 (32%)	59,113,114	2.15	17 (28%)
35	LUT	6	619	-	42,43,43	0.80	2 (4%)	51,60,60	1.98	16 (31%)
27	CLA	6	603	-	55,59,73	1.39	7 (12%)	66,96,113	1.29	5 (7%)
38	CHL	U	606	-	38,52,74	3.97	18 (47%)	31,87,114	3.21	16 (51%)
30	BCR	A	852	-	41,41,41	0.80	1 (2%)	56,56,56	2.46	25 (44%)
27	CLA	a	613	-	58,62,73	1.25	7 (12%)	68,99,113	1.16	5 (7%)
27	CLA	3	615	-	43,48,73	1.45	7 (16%)	49,83,113	1.39	5 (10%)
35	LUT	7	619	-	42,43,43	0.86	2 (4%)	51,60,60	1.99	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	A	837	1	49,53,73	1.36	8 (16%)	58,89,113	1.33	4 (6%)
27	CLA	A	824	-	69,73,73	1.14	7 (10%)	82,113,113	1.19	7 (8%)
27	CLA	3	606	-	57,62,73	1.27	7 (12%)	67,100,113	1.18	5 (7%)
27	CLA	A	809	1	69,73,73	1.13	6 (8%)	82,113,113	1.21	5 (6%)
34	DGD	B	850	-	63,63,67	0.85	2 (3%)	77,77,81	1.04	4 (5%)
27	CLA	7	610	20	69,73,73	1.14	7 (10%)	82,113,113	1.16	7 (8%)
27	CLA	Z	603	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	4 (4%)
30	BCR	A	850	-	41,41,41	0.77	1 (2%)	56,56,56	2.19	22 (39%)
27	CLA	6	617	-	49,53,73	1.36	7 (14%)	58,89,113	1.23	4 (6%)
27	CLA	6	616	19	69,73,73	1.16	8 (11%)	82,113,113	1.26	8 (9%)
27	CLA	9	604	-	54,58,73	1.40	9 (16%)	65,95,113	1.24	6 (9%)
27	CLA	2	607	-	49,53,73	1.37	9 (18%)	58,89,113	1.33	4 (6%)
27	CLA	7	603	-	47,52,73	1.40	8 (17%)	55,88,113	1.40	4 (7%)
38	CHL	X	605	23	40,54,74	4.21	19 (47%)	34,90,114	3.23	16 (47%)
27	CLA	B	832	-	64,68,73	1.20	7 (10%)	76,107,113	1.20	6 (7%)
27	CLA	W	610	23	59,63,73	1.26	8 (13%)	70,101,113	1.16	6 (8%)
29	LHG	5	625	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
27	CLA	B	837	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	8 (9%)
27	CLA	5	618	18	43,48,73	1.53	8 (18%)	51,83,113	1.36	6 (11%)
27	CLA	7	606	-	45,49,73	1.42	8 (17%)	52,84,113	1.28	3 (5%)
35	LUT	Z	1621	-	42,43,43	0.77	1 (2%)	51,60,60	1.89	16 (31%)
38	CHL	W	609	23	60,74,74	3.40	20 (33%)	58,114,114	2.34	16 (27%)
30	BCR	B	801	-	41,41,41	0.76	0	56,56,56	2.13	21 (37%)
27	CLA	A	829	-	69,73,73	1.15	9 (13%)	82,113,113	1.14	6 (7%)
27	CLA	2	606	-	49,53,73	1.38	8 (16%)	58,89,113	1.34	4 (6%)
27	CLA	a	608	-	47,52,73	1.39	7 (14%)	55,88,113	1.22	4 (7%)
27	CLA	8	607	-	45,49,73	1.50	8 (17%)	54,84,113	1.34	5 (9%)
27	CLA	8	613	21	69,73,73	1.17	8 (11%)	82,113,113	1.12	5 (6%)
27	CLA	W	603	-	56,60,73	1.29	9 (16%)	65,97,113	1.35	6 (9%)
29	LHG	6	623	27	47,47,48	0.93	2 (4%)	50,53,54	0.91	3 (6%)
27	CLA	X	602	23	69,73,73	1.19	7 (10%)	82,113,113	1.11	4 (4%)
27	CLA	7	604	-	54,58,73	1.32	8 (14%)	63,95,113	1.21	6 (9%)
32	LMU	5	628	-	34,34,36	1.15	2 (5%)	45,45,47	1.17	6 (13%)
27	CLA	6	609	19	49,53,73	1.37	8 (16%)	58,89,113	1.27	4 (6%)
30	BCR	B	847	-	41,41,41	0.83	1 (2%)	56,56,56	2.10	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	4	610	17	65,69,73	1.18	7 (10%)	77,108,113	1.17	7 (9%)
36	XAT	U	1622	-	41,47,47	0.98	3 (7%)	54,74,74	3.86	25 (46%)
27	CLA	7	614	-	46,50,73	1.37	9 (19%)	53,85,113	1.24	5 (9%)
27	CLA	2	616	-	47,51,73	1.49	9 (19%)	58,87,113	1.28	5 (8%)
27	CLA	A	835	-	65,69,73	1.20	7 (10%)	77,108,113	1.19	5 (6%)
30	BCR	B	844	-	41,41,41	0.79	1 (2%)	56,56,56	2.13	20 (35%)
35	LUT	X	1620	-	42,43,43	0.80	1 (2%)	51,60,60	2.03	11 (21%)
37	NEX	W	1623	-	40,46,46	1.00	2 (5%)	50,70,70	2.35	17 (34%)
27	CLA	2	614	-	45,50,73	1.40	7 (15%)	52,85,113	1.19	4 (7%)
27	CLA	B	823	-	49,53,73	1.38	8 (16%)	58,89,113	1.19	4 (6%)
27	CLA	5	617	-	54,58,73	1.30	6 (11%)	64,95,113	1.21	5 (7%)
38	CHL	X	606	-	38,52,74	4.20	17 (44%)	31,87,114	3.23	15 (48%)
27	CLA	a	607	-	49,53,73	1.37	7 (14%)	58,89,113	1.23	5 (8%)
27	CLA	X	613	23	69,73,73	1.18	8 (11%)	82,113,113	1.14	6 (7%)
30	BCR	B	845	-	41,41,41	0.78	1 (2%)	56,56,56	2.08	22 (39%)
27	CLA	9	614	-	49,53,73	1.37	7 (14%)	58,89,113	1.30	5 (8%)
35	LUT	4	619	-	42,43,43	0.71	1 (2%)	51,60,60	1.90	15 (29%)
27	CLA	9	602	22	64,68,73	1.19	9 (14%)	76,107,113	1.22	7 (9%)
27	CLA	B	827	-	66,70,73	1.17	8 (12%)	78,109,113	1.19	5 (6%)
32	LMU	1	621	-	36,36,36	1.17	2 (5%)	47,47,47	0.97	1 (2%)
29	LHG	H	204	-	48,48,48	0.90	2 (4%)	51,54,54	0.91	1 (1%)
27	CLA	A	813	-	58,62,73	1.26	7 (12%)	68,99,113	1.27	7 (10%)
27	CLA	3	611	29	41,46,73	1.57	8 (19%)	51,81,113	1.30	6 (11%)
27	CLA	1	609	14	44,48,73	1.52	8 (18%)	55,83,113	1.37	6 (10%)
27	CLA	W	614	-	49,53,73	1.37	8 (16%)	58,89,113	1.31	4 (6%)
27	CLA	a	616	14	49,53,73	1.38	8 (16%)	58,89,113	1.26	5 (8%)
30	BCR	L	309	-	41,41,41	0.65	0	56,56,56	1.99	18 (32%)
27	CLA	3	617	16	43,48,73	1.42	7 (16%)	51,83,113	1.35	5 (9%)
27	CLA	K	206	11	49,53,73	1.39	7 (14%)	58,89,113	1.30	3 (5%)
37	NEX	V	1623	-	40,46,46	0.96	3 (7%)	50,70,70	2.10	13 (26%)
27	CLA	4	614	-	60,64,73	1.25	8 (13%)	71,102,113	1.21	7 (9%)
33	LMG	9	625	-	55,55,55	0.89	2 (3%)	63,63,63	0.95	2 (3%)
30	BCR	L	305	-	41,41,41	0.70	0	56,56,56	2.10	23 (41%)
38	CHL	W	608	-	41,55,74	3.94	19 (46%)	35,91,114	2.93	15 (42%)
38	CHL	Y	601	24	60,74,74	3.39	19 (31%)	58,114,114	2.45	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	BCR	8	621	-	41,41,41	0.86	1 (2%)	56,56,56	2.56	18 (32%)
30	BCR	A	849	-	41,41,41	0.75	0	56,56,56	2.26	20 (35%)
29	LHG	X	2630	27	48,48,48	0.96	2 (4%)	51,54,54	0.98	2 (3%)
27	CLA	B	804	-	45,49,73	1.38	7 (15%)	54,84,113	1.24	4 (7%)
27	CLA	V	614	-	49,53,73	1.38	8 (16%)	58,89,113	1.26	4 (6%)
27	CLA	6	606	-	43,48,73	1.45	8 (18%)	49,83,113	1.21	4 (8%)
27	CLA	1	601	14	57,62,73	1.27	9 (15%)	67,100,113	1.17	5 (7%)
30	BCR	9	621	-	41,41,41	0.77	0	56,56,56	2.08	18 (32%)
27	CLA	B	828	-	69,73,73	1.16	8 (11%)	82,113,113	1.12	8 (9%)
27	CLA	A	832	-	54,58,73	1.33	7 (12%)	64,95,113	1.21	8 (12%)
27	CLA	A	836	-	69,73,73	1.15	7 (10%)	82,113,113	1.15	6 (7%)
27	CLA	6	614	-	64,68,73	1.22	7 (10%)	76,107,113	1.14	5 (6%)
27	CLA	F	303	-	46,50,73	1.41	9 (19%)	53,85,113	1.33	4 (7%)
27	CLA	8	604	-	54,58,73	1.28	7 (12%)	64,95,113	1.27	6 (9%)
27	CLA	1	606	-	41,47,73	1.44	8 (19%)	50,80,113	1.42	6 (12%)
36	XAT	a	618	-	41,47,47	0.89	1 (2%)	54,74,74	2.42	23 (42%)
27	CLA	a	612	14	49,53,73	1.37	7 (14%)	58,89,113	1.26	3 (5%)
27	CLA	A	842	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	7 (8%)
27	CLA	8	614	-	57,61,73	1.27	9 (15%)	67,98,113	1.25	6 (8%)
37	NEX	U	1623	-	40,46,46	1.02	3 (7%)	50,70,70	2.35	17 (34%)
27	CLA	Y	613	24	69,73,73	1.18	8 (11%)	82,113,113	1.14	6 (7%)
27	CLA	a	602	14	65,69,73	1.19	8 (12%)	77,108,113	1.17	6 (7%)
27	CLA	4	602	17	64,68,73	1.20	8 (12%)	76,107,113	1.24	7 (9%)
38	CHL	V	605	26	38,52,74	4.05	18 (47%)	31,87,114	3.09	13 (41%)
27	CLA	B	820	-	54,58,73	1.29	8 (14%)	64,95,113	1.29	6 (9%)
27	CLA	L	303	-	69,73,73	1.15	6 (8%)	82,113,113	1.19	7 (8%)
38	CHL	Y	605	24	36,50,74	4.37	18 (50%)	29,85,114	3.18	15 (51%)
27	CLA	9	610	22	61,65,73	1.24	8 (13%)	72,103,113	1.18	7 (9%)
27	CLA	B	831	-	69,73,73	1.15	8 (11%)	82,113,113	1.25	7 (8%)
27	CLA	B	838	-	50,54,73	1.32	8 (16%)	59,90,113	1.33	5 (8%)
27	CLA	A	834	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
27	CLA	U	614	-	46,50,73	1.39	8 (17%)	53,85,113	1.29	4 (7%)
35	LUT	Z	1620	-	42,43,43	0.75	1 (2%)	51,60,60	1.87	12 (23%)
27	CLA	B	822	-	46,50,73	1.37	7 (15%)	53,85,113	1.23	5 (9%)
27	CLA	B	819	-	59,63,73	1.27	7 (11%)	70,101,113	1.22	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	5	609	18	69,73,73	1.17	7 (10%)	82,113,113	1.15	5 (6%)
27	CLA	a	603	-	58,62,73	1.27	8 (13%)	68,99,113	1.31	5 (7%)
27	CLA	A	818	-	64,68,73	1.18	7 (10%)	76,107,113	1.20	7 (9%)
27	CLA	W	612	23	49,53,73	1.38	8 (16%)	58,89,113	1.30	4 (6%)
27	CLA	6	620	-	68,72,73	1.15	8 (11%)	80,111,113	1.10	5 (6%)
36	XAT	X	1622	-	41,47,47	0.92	2 (4%)	54,74,74	3.78	26 (48%)
27	CLA	2	611	29	46,50,73	1.38	8 (17%)	53,85,113	1.27	4 (7%)
27	CLA	X	612	23	47,51,73	1.40	7 (14%)	55,86,113	1.28	4 (7%)
35	LUT	1	617	-	42,43,43	0.82	1 (2%)	51,60,60	1.92	15 (29%)
30	BCR	1	619	-	41,41,41	0.71	0	56,56,56	2.44	21 (37%)
27	CLA	a	606	-	46,52,73	1.40	8 (17%)	57,87,113	1.26	4 (7%)
30	BCR	3	620	-	41,41,41	0.86	0	56,56,56	4.43	32 (57%)
29	LHG	Y	2630	27	48,48,48	0.95	2 (4%)	51,54,54	0.98	2 (3%)
38	CHL	V	606	-	38,52,74	3.97	19 (50%)	31,87,114	3.18	13 (41%)
36	XAT	5	621	-	41,47,47	0.90	3 (7%)	54,74,74	2.39	22 (40%)
27	CLA	Y	610	24	69,73,73	1.20	7 (10%)	82,113,113	1.11	6 (7%)
36	XAT	4	620	-	41,47,47	0.87	2 (4%)	54,74,74	2.42	23 (42%)
27	CLA	5	612	18	44,49,73	1.41	7 (15%)	50,84,113	1.25	3 (6%)
27	CLA	B	806	2	69,73,73	1.18	8 (11%)	82,113,113	1.20	4 (4%)
30	BCR	L	308	-	41,41,41	0.82	2 (4%)	56,56,56	2.34	26 (46%)
27	CLA	B	826	-	66,70,73	1.19	9 (13%)	78,109,113	1.27	7 (8%)
31	SF4	C	102	3	0,12,12	-	-	-		
27	CLA	3	610	16	69,73,73	1.15	8 (11%)	82,113,113	1.12	7 (8%)
27	CLA	5	613	18	68,72,73	1.16	7 (10%)	80,111,113	1.11	5 (6%)
30	BCR	5	622	-	41,41,41	0.75	0	56,56,56	2.37	20 (35%)
28	PQN	B	842	-	34,34,34	3.48	10 (29%)	43,45,45	1.54	6 (13%)
29	LHG	8	623	-	39,39,48	1.03	2 (5%)	42,45,54	1.10	3 (7%)
27	CLA	5	602	18	69,73,73	1.15	9 (13%)	82,113,113	1.15	5 (6%)
30	BCR	A	851	-	41,41,41	0.80	1 (2%)	56,56,56	2.12	23 (41%)
27	CLA	B	817	-	63,67,73	1.21	8 (12%)	74,105,113	1.30	7 (9%)
27	CLA	7	601	20	64,68,73	1.18	8 (12%)	76,107,113	1.29	7 (9%)
27	CLA	3	614	-	43,48,73	1.44	9 (20%)	51,83,113	1.28	4 (7%)
29	LHG	3	623	-	44,44,48	0.96	2 (4%)	47,50,54	1.07	3 (6%)
27	CLA	6	611	29	46,50,73	1.38	8 (17%)	53,85,113	1.25	4 (7%)
27	CLA	A	839	-	59,63,73	1.25	8 (13%)	70,101,113	1.21	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	1	614	-	40,45,73	1.61	9 (22%)	47,79,113	1.43	6 (12%)
35	LUT	W	1620	-	42,43,43	0.89	1 (2%)	51,60,60	1.89	9 (17%)
30	BCR	A	848	-	41,41,41	0.85	1 (2%)	56,56,56	1.98	14 (25%)
36	XAT	2	620	-	41,47,47	0.90	2 (4%)	54,74,74	2.43	21 (38%)
27	CLA	5	619	-	47,51,73	1.52	8 (17%)	58,87,113	1.35	8 (13%)
27	CLA	X	611	29	49,53,73	1.40	7 (14%)	58,89,113	1.30	6 (10%)
38	CHL	Y	608	-	43,57,74	4.06	18 (41%)	37,93,114	2.89	16 (43%)
30	BCR	O	2004	-	41,41,41	0.78	1 (2%)	56,56,56	2.44	19 (33%)
27	CLA	A	838	-	54,58,73	1.28	8 (14%)	64,95,113	1.36	8 (12%)
27	CLA	B	814	-	66,70,73	1.16	8 (12%)	78,109,113	1.11	6 (7%)
27	CLA	K	201	11	49,53,73	1.37	7 (14%)	58,89,113	1.16	3 (5%)
27	CLA	3	603	-	59,63,73	1.26	8 (13%)	70,101,113	1.39	7 (10%)
27	CLA	4	612	17	44,49,73	1.42	7 (15%)	50,84,113	1.28	3 (6%)
30	BCR	B	853	-	41,41,41	0.75	1 (2%)	56,56,56	1.71	14 (25%)
29	LHG	B	854	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
27	CLA	9	609	22	65,69,73	1.20	7 (10%)	77,108,113	1.14	4 (5%)
30	BCR	K	207	-	41,41,41	0.76	1 (2%)	56,56,56	3.01	24 (42%)
27	CLA	X	604	-	53,57,73	1.33	7 (13%)	61,93,113	1.17	5 (8%)
27	CLA	U	611	29	46,50,73	1.36	8 (17%)	53,85,113	1.32	4 (7%)
27	CLA	B	829	-	69,73,73	1.15	6 (8%)	82,113,113	1.13	5 (6%)
27	CLA	K	203	-	60,64,73	1.26	8 (13%)	71,102,113	1.31	8 (11%)
27	CLA	5	608	-	54,58,73	1.31	8 (14%)	63,95,113	1.19	5 (7%)
27	CLA	6	612	19	44,49,73	1.41	7 (15%)	50,84,113	1.26	3 (6%)
27	CLA	A	830	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	5 (6%)
27	CLA	a	604	-	53,57,73	1.31	7 (13%)	61,93,113	1.18	3 (4%)
27	CLA	X	603	-	66,70,73	1.22	7 (10%)	78,109,113	1.19	5 (6%)
27	CLA	a	614	-	58,62,73	1.27	8 (13%)	65,99,113	1.24	6 (9%)
27	CLA	A	805	-	56,60,73	1.27	7 (12%)	65,97,113	1.36	6 (9%)
28	PQN	A	844	-	34,34,34	3.54	10 (29%)	43,45,45	1.54	4 (9%)
27	CLA	A	816	-	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
37	NEX	X	1623	-	40,46,46	1.03	3 (7%)	50,70,70	2.33	17 (34%)
27	CLA	5	601	18	60,64,73	1.24	7 (11%)	71,102,113	1.32	7 (9%)
29	LHG	W	2630	27	43,43,48	0.96	2 (4%)	46,49,54	0.97	2 (4%)
38	CHL	Z	609	25	60,74,74	3.47	20 (33%)	58,114,114	2.02	16 (27%)
38	CHL	V	607	-	40,54,74	3.94	19 (47%)	34,90,114	2.93	14 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	7	602	20	69,73,73	1.15	9 (13%)	82,113,113	1.13	4 (4%)
27	CLA	4	601	17	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)
33	LMG	H	205	-	55,55,55	0.89	2 (3%)	63,63,63	1.12	7 (11%)

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
27	CLA	3	613	16	1/1/12/20	9/23/99/115	-
27	CLA	J	101	10	1/1/10/20	5/12/88/115	-
27	CLA	A	812	-	1/1/15/20	4/39/115/115	-
27	CLA	2	602	15	1/1/15/20	8/37/113/115	-
27	CLA	A	819	-	1/1/13/20	5/32/108/115	-
27	CLA	B	807	-	-	3/24/100/115	-
35	LUT	X	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	B	803	-	1/1/15/20	11/39/115/115	-
38	CHL	Z	601	25	3/3/20/26	19/39/137/137	-
27	CLA	2	603	15	1/1/11/20	3/13/89/115	-
35	LUT	5	620	-	-	1/29/67/67	0/2/2/2
27	CLA	B	836	-	1/1/12/20	2/21/97/115	-
27	CLA	1	607	-	1/1/10/20	2/8/84/115	-
36	XAT	W	1622	-	-	1/31/93/93	0/4/4/4
27	CLA	Y	602	24	1/1/13/20	6/31/107/115	-
27	CLA	L	302	12	1/1/11/20	4/15/91/115	-
27	CLA	2	612	15	1/1/11/20	7/13/89/115	-
30	BCR	K	202	-	-	4/29/63/63	0/2/2/2
32	LMU	A	857	-	-	3/21/61/61	0/2/2/2
33	LMG	8	626	-	-	16/41/61/70	0/1/1/1
38	CHL	W	606	-	3/3/16/26	2/15/113/137	-
37	NEX	Z	1623	-	-	3/27/83/83	0/3/3/3
27	CLA	A	802	-	1/1/15/20	10/39/115/115	-
27	CLA	8	609	21	1/1/11/20	6/15/91/115	-
27	CLA	7	613	20	1/1/15/20	10/39/115/115	-
27	CLA	H	203	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	823	-	1/1/10/20	4/12/88/115	-
27	CLA	A	831	-	1/1/15/20	11/39/115/115	-
38	CHL	W	605	23	3/3/16/26	3/15/113/137	-
27	CLA	4	609	17	1/1/13/20	4/30/106/115	-
27	CLA	9	613	22	1/1/15/20	6/39/115/115	-
38	CHL	U	607	-	3/3/16/26	4/15/113/137	-
27	CLA	B	810	-	1/1/14/20	15/37/113/115	-
27	CLA	9	601	22	1/1/11/20	4/15/91/115	-
27	CLA	A	821	-	1/1/12/20	15/25/101/115	-
27	CLA	Z	614	-	1/1/12/20	7/26/102/115	-
36	XAT	6	621	-	-	0/31/93/93	0/4/4/4
38	CHL	V	609	26	3/3/19/26	17/33/131/137	-
38	CHL	Z	608	-	3/3/16/26	5/20/118/137	-
27	CLA	B	821	-	1/1/11/20	4/13/89/115	-
27	CLA	8	616	-	1/1/11/20	5/11/87/115	-
27	CLA	V	611	29	1/1/10/20	4/13/89/115	-
38	CHL	U	609	24	3/3/18/26	12/32/130/137	-
31	SF4	C	101	3	-	-	0/6/5/5
27	CLA	2	604	-	1/1/10/20	4/11/87/115	-
38	CHL	Y	606	-	3/3/16/26	2/15/113/137	-
27	CLA	Y	614	-	1/1/11/20	8/19/95/115	-
27	CLA	W	613	23	1/1/15/20	12/39/115/115	-
27	CLA	a	609	14	1/1/15/20	13/37/113/115	-
30	BCR	B	852	-	-	6/29/63/63	0/2/2/2
30	BCR	7	621	-	-	5/29/63/63	0/2/2/2
27	CLA	Y	604	-	1/1/12/20	4/21/97/115	-
27	CLA	8	608	-	1/1/12/20	8/23/99/115	-
27	CLA	L	307	-	1/1/10/20	2/8/84/115	-
27	CLA	A	808	-	-	4/21/97/115	-
27	CLA	7	608	-	1/1/12/20	3/21/97/115	-
27	CLA	4	604	-	1/1/13/20	8/25/101/115	-
27	CLA	U	603	-	1/1/12/20	11/24/100/115	-
27	CLA	7	616	20	1/1/11/20	2/11/87/115	-
27	CLA	A	801	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	4	613	17	1/1/15/20	12/39/115/115	-
27	CLA	6	610	19	1/1/15/20	8/39/115/115	-
27	CLA	Z	610	25	1/1/15/20	10/39/115/115	-
27	CLA	G	204	7	1/1/11/20	4/15/91/115	-
27	CLA	3	609	16	1/1/14/20	15/33/109/115	-
27	CLA	Y	603	-	1/1/13/20	11/27/103/115	-
35	LUT	V	1621	-	-	2/29/67/67	0/2/2/2
36	XAT	Y	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	2	601	15	1/1/15/20	13/39/115/115	-
33	LMG	A	860	-	-	10/35/55/70	0/1/1/1
27	CLA	6	602	19	1/1/15/20	9/39/115/115	-
32	LMU	A	858	-	-	12/21/57/61	0/2/2/2
27	CLA	2	610	15	1/1/13/20	9/27/103/115	-
32	LMU	8	625	-	-	8/21/61/61	0/2/2/2
27	CLA	B	818	-	-	14/33/109/115	-
27	CLA	B	812	-	1/1/10/20	2/13/89/115	-
35	LUT	2	619	-	-	1/29/67/67	0/2/2/2
27	CLA	4	616	17	1/1/11/20	7/11/87/115	-
27	CLA	Y	611	29	1/1/10/20	6/13/89/115	-
27	CLA	6	608	-	1/1/11/20	6/15/91/115	-
27	CLA	A	804	-	1/1/15/20	16/39/115/115	-
30	BCR	A	856	-	-	2/29/63/63	0/2/2/2
27	CLA	B	835	-	1/1/11/20	4/15/91/115	-
27	CLA	O	2001	-	1/1/9/20	1/6/78/115	-
27	CLA	4	608	-	1/1/15/20	10/39/115/115	-
27	CLA	a	610	14	1/1/14/20	2/31/107/115	-
27	CLA	A	827	-	1/1/13/20	6/31/107/115	-
27	CLA	A	817	-	-	2/15/91/115	-
29	LHG	A	847	27	-	4/34/34/53	-
37	NEX	5	624	-	-	2/27/83/83	0/3/3/3
30	BCR	3	621	-	-	0/29/63/63	0/2/2/2
33	LMG	J	104	-	-	13/35/55/70	0/1/1/1
27	CLA	5	606	-	-	3/8/84/115	-
33	LMG	L	2631	-	-	8/32/52/70	0/1/1/1
35	LUT	U	1620	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	824	-	1/1/15/20	12/39/115/115	-
27	CLA	5	604	-	1/1/15/20	15/35/111/115	-
29	LHG	9	624	-	-	19/53/53/53	-
27	CLA	U	604	-	1/1/10/20	6/20/92/115	-
27	CLA	5	614	-	1/1/10/20	10/15/87/115	-
27	CLA	A	822	-	1/1/15/20	7/39/115/115	-
30	BCR	a	619	-	-	4/29/63/63	0/2/2/2
36	XAT	7	620	-	-	0/31/93/93	0/4/4/4
29	LHG	2	622	27	-	13/40/40/53	-
30	BCR	7	623	-	-	4/29/63/63	0/2/2/2
38	CHL	Y	609	24	3/3/20/26	14/39/137/137	-
27	CLA	5	616	18	1/1/10/20	2/8/84/115	-
35	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	5	607	-	1/1/15/20	12/39/115/115	-
29	LHG	1	620	27	-	9/53/53/53	-
27	CLA	6	613	-	1/1/15/20	13/37/113/115	-
27	CLA	B	813	-	1/1/15/20	18/39/115/115	-
30	BCR	4	621	-	-	4/29/63/63	0/2/2/2
29	LHG	9	623	-	-	16/53/53/53	-
27	CLA	A	828	-	1/1/15/20	9/39/115/115	-
27	CLA	B	825	-	-	4/20/96/115	-
27	CLA	L	304	-	1/1/11/20	0/15/91/115	-
30	BCR	G	205	-	-	0/29/63/63	0/2/2/2
30	BCR	3	622	-	-	2/29/63/63	0/2/2/2
38	CHL	X	609	23	3/3/20/26	17/39/137/137	-
27	CLA	V	603	-	1/1/11/20	4/15/91/115	-
29	LHG	4	622	27	-	10/53/53/53	-
27	CLA	A	806	-	1/1/15/20	14/39/115/115	-
27	CLA	1	610	14	1/1/9/20	1/8/80/115	-
27	CLA	2	609	15	1/1/11/20	2/15/91/115	-
27	CLA	X	610	23	1/1/15/20	9/39/115/115	-
27	CLA	3	602	16	1/1/14/20	3/33/109/115	-
27	CLA	4	607	-	1/1/11/20	6/15/91/115	-
27	CLA	A	820	-	1/1/15/20	10/39/115/115	-
27	CLA	W	611	29	1/1/13/20	12/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	9	611	29	1/1/10/20	3/12/88/115	-
30	BCR	B	849	-	-	3/29/63/63	0/2/2/2
27	CLA	G	203	-	1/1/10/20	4/12/88/115	-
38	CHL	Z	607	-	3/3/20/26	19/39/137/137	-
27	CLA	B	811	-	1/1/12/20	8/23/95/115	-
27	CLA	3	612	16	1/1/10/20	1/13/89/115	-
27	CLA	A	841	-	1/1/15/20	17/39/115/115	-
27	CLA	B	809	2	1/1/15/20	15/39/115/115	-
27	CLA	1	611	29	1/1/13/20	7/30/106/115	-
27	CLA	A	854	-	1/1/15/20	8/39/115/115	-
27	CLA	3	604	-	1/1/15/20	8/39/115/115	-
27	CLA	1	616	14	1/1/11/20	5/11/87/115	-
27	CLA	A	845	29	1/1/12/20	3/21/97/115	-
27	CLA	7	609	20	1/1/10/20	4/12/88/115	-
38	CHL	X	601	23	3/3/20/26	21/39/137/137	-
27	CLA	7	615	-	1/1/10/20	6/8/84/115	-
27	CLA	6	607	-	1/1/10/20	2/10/86/115	-
27	CLA	1	604	-	1/1/11/20	10/20/96/115	-
29	LHG	A	846	-	-	12/53/53/53	-
27	CLA	X	614	-	1/1/10/20	5/12/88/115	-
27	CLA	B	805	-	1/1/15/20	14/39/115/115	-
27	CLA	9	603	22	1/1/11/20	2/13/89/115	-
29	LHG	Z	2630	27	-	17/53/53/53	-
29	LHG	O	2631	-	-	15/40/40/53	-
35	LUT	U	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	9	606	-	1/1/10/20	4/8/84/115	-
38	CHL	Y	607	-	3/3/20/26	21/39/137/137	-
35	LUT	V	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	V	602	26	1/1/14/20	5/33/109/115	-
32	LMU	K	208	-	-	14/21/61/61	0/2/2/2
27	CLA	A	810	1	1/1/12/20	10/21/97/115	-
27	CLA	4	603	17	1/1/11/20	2/13/89/115	-
27	CLA	5	611	29	1/1/10/20	5/12/88/115	-
27	CLA	W	604	-	1/1/11/20	2/18/94/115	-
33	LMG	J	103	-	-	5/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LUT	W	1621	-	-	1/29/67/67	0/2/2/2
38	CHL	X	608	-	3/3/20/26	21/39/137/137	-
27	CLA	Z	602	25	1/1/14/20	3/33/109/115	-
27	CLA	3	608	-	1/1/13/20	4/27/103/115	-
38	CHL	Z	606	-	3/3/16/26	4/15/113/137	-
27	CLA	4	606	-	1/1/10/20	4/8/84/115	-
27	CLA	A	833	-	1/1/11/20	5/15/91/115	-
27	CLA	8	611	29	1/1/10/20	4/12/88/115	-
29	LHG	V	2630	27	-	7/52/52/53	-
27	CLA	6	601	19	1/1/15/20	10/39/115/115	-
30	BCR	O	2005	-	-	4/29/63/63	0/2/2/2
27	CLA	B	833	-	1/1/15/20	11/39/115/115	-
27	CLA	Y	612	24	1/1/11/20	6/15/91/115	-
38	CHL	U	608	-	3/3/15/26	3/13/111/137	-
30	BCR	F	305	-	-	6/29/63/63	0/2/2/2
36	XAT	9	620	-	-	0/31/93/93	0/4/4/4
38	CHL	Z	605	25	3/3/15/26	1/13/111/137	-
27	CLA	Z	604	-	1/1/13/20	6/30/106/115	-
32	LMU	5	629	-	-	11/18/58/61	0/2/2/2
33	LMG	4	623	-	-	5/35/55/70	0/1/1/1
27	CLA	B	815	-	1/1/10/20	2/13/89/115	-
30	BCR	L	301	-	-	4/29/63/63	0/2/2/2
27	CLA	A	840	-	-	4/24/100/115	-
37	NEX	Y	1623	-	-	3/27/80/83	0/3/3/3
33	LMG	5	627	-	-	12/35/55/70	0/1/1/1
27	CLA	V	604	-	1/1/12/20	5/21/97/115	-
33	LMG	V	2631	-	-	9/36/56/70	0/1/1/1
27	CLA	2	613	15	1/1/15/20	6/39/115/115	-
37	NEX	6	624	-	-	2/27/83/83	0/3/3/3
27	CLA	V	610	26	1/1/14/20	6/36/112/115	-
27	CLA	A	807	1	1/1/15/20	19/39/115/115	-
27	CLA	9	612	22	1/1/10/20	2/10/86/115	-
27	CLA	A	814	-	1/1/15/20	14/39/115/115	-
30	BCR	2	623	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	5	623	27	-	14/53/53/53	-
27	CLA	U	610	24	1/1/13/20	8/29/105/115	-
27	CLA	7	611	29	1/1/13/20	6/31/107/115	-
36	XAT	1	618	-	-	0/31/93/93	0/4/4/4
27	CLA	Z	613	25	1/1/15/20	16/39/115/115	-
27	CLA	1	612	14	1/1/11/20	5/15/91/115	-
35	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
38	CHL	V	601	26	3/3/20/26	13/39/137/137	-
27	CLA	A	803	-	1/1/15/20	3/39/115/115	-
27	CLA	B	816	-	1/1/12/20	11/25/101/115	-
27	CLA	F	304	6	-	4/10/86/115	-
27	CLA	4	618	17	1/1/10/20	2/8/84/115	-
35	LUT	9	619	-	-	0/29/67/67	0/2/2/2
27	CLA	3	607	16	1/1/13/20	10/28/104/115	-
27	CLA	B	839	-	1/1/15/20	14/39/115/115	-
27	CLA	B	841	29	1/1/15/20	9/39/115/115	-
30	BCR	6	622	-	-	5/29/63/63	0/2/2/2
27	CLA	a	601	14	-	4/25/101/115	-
27	CLA	A	811	-	1/1/15/20	10/39/115/115	-
27	CLA	B	808	-	1/1/15/20	14/39/115/115	-
29	LHG	8	622	27	-	8/53/53/53	-
30	BCR	B	848	-	-	3/29/63/63	0/2/2/2
27	CLA	7	612	20	1/1/11/20	4/13/89/115	-
27	CLA	5	603	-	1/1/13/20	6/25/101/115	-
36	XAT	8	620	-	-	0/31/93/93	0/4/4/4
30	BCR	B	846	-	-	2/29/63/63	0/2/2/2
27	CLA	W	602	23	1/1/14/20	6/33/109/115	-
29	LHG	3	624	27	-	22/53/53/53	-
27	CLA	B	834	-	1/1/14/20	7/33/109/115	-
27	CLA	1	603	-	1/1/12/20	3/23/99/115	-
29	LHG	U	2630	27	-	12/53/53/53	-
27	CLA	A	843	-	1/1/14/20	12/37/113/115	-
27	CLA	A	815	-	1/1/12/20	8/21/97/115	-
27	CLA	V	613	26	1/1/15/20	16/39/115/115	-
38	CHL	U	605	24	3/3/15/26	0/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
27	CLA	U	612	24	1/1/10/20	4/13/89/115	-
29	LHG	B	851	27	-	11/42/42/53	-
30	BCR	J	102	-	-	2/29/63/63	0/2/2/2
27	CLA	1	602	14	1/1/14/20	3/35/111/115	-
31	SF4	A	853	2,1	-	-	0/6/5/5
27	CLA	6	604	-	-	13/39/115/115	-
38	CHL	U	601	24	3/3/20/26	20/39/137/137	-
27	CLA	5	610	18	1/1/12/20	3/26/102/115	-
27	CLA	9	607	-	-	8/15/91/115	-
36	XAT	Z	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	L	306	-	1/1/10/20	0/8/84/115	-
27	CLA	Z	612	25	1/1/15/20	6/39/115/115	-
29	LHG	9	622	27	-	11/34/34/53	-
35	LUT	3	618	-	-	0/29/67/67	0/2/2/2
27	CLA	H	202	8	1/1/10/20	2/6/82/115	-
27	CLA	B	830	-	1/1/10/20	4/13/89/115	-
38	CHL	V	608	-	3/3/16/26	5/18/116/137	-
27	CLA	4	611	29	1/1/10/20	4/12/88/115	-
27	CLA	B	802	-	1/1/15/20	19/39/115/115	-
27	CLA	1	613	-	1/1/15/20	12/39/115/115	-
36	XAT	3	619	-	-	0/31/93/93	0/4/4/4
27	CLA	U	602	24	1/1/13/20	6/32/108/115	-
29	LHG	7	622	27	-	21/41/41/53	-
38	CHL	W	601	23	3/3/20/26	20/39/137/137	-
27	CLA	Z	611	29	1/1/15/20	5/39/115/115	-
35	LUT	8	619	-	-	1/29/67/67	0/2/2/2
27	CLA	7	607	-	1/1/10/20	3/12/88/115	-
27	CLA	U	613	24	1/1/13/20	10/32/108/115	-
27	CLA	K	204	-	1/1/11/20	4/15/91/115	-
27	CLA	8	602	21	1/1/14/20	7/33/109/115	-
27	CLA	B	840	-	1/1/15/20	5/39/115/115	-
36	XAT	V	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	V	612	26	1/1/11/20	4/15/91/115	-
27	CLA	8	603	-	1/1/11/20	5/13/89/115	-
27	CLA	A	826	-	1/1/14/20	12/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	6	618	19	1/1/10/20	0/8/84/115	-
29	LHG	a	620	27	-	9/47/47/53	-
35	LUT	a	617	-	-	0/29/67/67	0/2/2/2
27	CLA	A	825	-	1/1/15/20	20/39/115/115	-
38	CHL	X	607	-	3/3/20/26	17/39/137/137	-
33	LMG	4	624	-	-	8/35/55/70	0/1/1/1
27	CLA	1	608	-	1/1/11/20	5/13/89/115	-
27	CLA	8	606	-	1/1/15/20	8/37/113/115	-
27	CLA	8	612	21	1/1/10/20	2/10/86/115	-
27	CLA	8	601	21	1/1/15/20	14/39/115/115	-
27	CLA	a	611	29	1/1/10/20	2/4/80/115	-
27	CLA	F	301	-	1/1/13/20	10/30/106/115	-
27	CLA	O	2003	-	1/1/10/20	2/8/84/115	-
27	CLA	8	610	21	1/1/14/20	8/33/109/115	-
30	BCR	B	843	-	-	4/29/63/63	0/2/2/2
38	CHL	W	607	-	3/3/20/26	25/37/135/137	-
35	LUT	6	619	-	-	0/29/67/67	0/2/2/2
27	CLA	6	603	-	1/1/12/20	3/22/98/115	-
38	CHL	U	606	-	3/3/15/26	0/13/111/137	-
30	BCR	A	852	-	-	8/29/63/63	0/2/2/2
27	CLA	a	613	-	1/1/12/20	8/26/102/115	-
27	CLA	3	615	-	1/1/10/20	2/8/84/115	-
35	LUT	7	619	-	-	1/29/67/67	0/2/2/2
27	CLA	A	837	1	-	9/15/91/115	-
27	CLA	A	824	-	1/1/15/20	9/39/115/115	-
27	CLA	3	606	-	1/1/13/20	6/25/101/115	-
27	CLA	A	809	1	1/1/15/20	10/39/115/115	-
34	DGD	B	850	-	-	16/51/91/95	0/2/2/2
27	CLA	7	610	20	1/1/15/20	2/39/115/115	-
27	CLA	Z	603	-	1/1/15/20	20/39/115/115	-
30	BCR	A	850	-	-	2/29/63/63	0/2/2/2
27	CLA	6	617	-	1/1/11/20	8/15/91/115	-
27	CLA	6	616	19	1/1/15/20	20/39/115/115	-
27	CLA	9	604	-	1/1/12/20	2/20/96/115	-
27	CLA	2	607	-	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	7	603	-	1/1/11/20	3/13/89/115	-
38	CHL	X	605	23	3/3/16/26	1/15/113/137	-
27	CLA	B	832	-	-	9/33/109/115	-
27	CLA	W	610	23	1/1/13/20	8/27/103/115	-
29	LHG	5	625	-	-	15/53/53/53	-
27	CLA	B	837	-	-	12/39/115/115	-
27	CLA	5	618	18	1/1/10/20	0/8/84/115	-
27	CLA	7	606	-	-	2/10/86/115	-
35	LUT	Z	1621	-	-	2/29/67/67	0/2/2/2
38	CHL	W	609	23	3/3/20/26	15/39/137/137	-
30	BCR	B	801	-	-	3/29/63/63	0/2/2/2
27	CLA	A	829	-	1/1/15/20	13/39/115/115	-
27	CLA	2	606	-	1/1/11/20	4/15/91/115	-
27	CLA	a	608	-	1/1/11/20	5/13/89/115	-
27	CLA	8	607	-	1/1/10/20	4/10/86/115	-
27	CLA	8	613	21	1/1/15/20	11/39/115/115	-
27	CLA	W	603	-	1/1/12/20	11/24/100/115	-
29	LHG	6	623	27	-	24/52/52/53	-
27	CLA	X	602	23	1/1/15/20	9/39/115/115	-
27	CLA	7	604	-	1/1/12/20	9/21/97/115	-
32	LMU	5	628	-	-	9/19/59/61	0/2/2/2
27	CLA	6	609	19	1/1/11/20	2/15/91/115	-
30	BCR	B	847	-	-	2/29/63/63	0/2/2/2
27	CLA	4	610	17	1/1/14/20	7/35/111/115	-
36	XAT	U	1622	-	-	1/31/93/93	0/4/4/4
27	CLA	7	614	-	1/1/10/20	3/12/88/115	-
27	CLA	2	616	-	1/1/11/20	4/11/87/115	-
27	CLA	A	835	-	-	11/35/111/115	-
30	BCR	B	844	-	-	2/29/63/63	0/2/2/2
35	LUT	X	1620	-	-	2/29/67/67	0/2/2/2
37	NEX	W	1623	-	-	4/27/83/83	0/3/3/3
27	CLA	2	614	-	1/1/10/20	1/11/87/115	-
27	CLA	B	823	-	1/1/11/20	6/15/91/115	-
27	CLA	5	617	-	1/1/12/20	8/21/97/115	-
38	CHL	X	606	-	3/3/15/26	0/13/111/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	607	-	1/1/11/20	3/15/91/115	-
27	CLA	X	613	23	1/1/15/20	14/39/115/115	-
30	BCR	B	845	-	-	9/29/63/63	0/2/2/2
27	CLA	9	614	-	1/1/11/20	7/15/91/115	-
35	LUT	4	619	-	-	4/29/67/67	0/2/2/2
27	CLA	9	602	22	-	7/33/109/115	-
27	CLA	B	827	-	1/1/14/20	15/36/112/115	-
32	LMU	1	621	-	-	7/21/61/61	0/2/2/2
29	LHG	H	204	-	-	16/53/53/53	-
27	CLA	A	813	-	1/1/12/20	5/26/102/115	-
27	CLA	3	611	29	1/1/10/20	2/4/80/115	-
27	CLA	1	609	14	1/1/10/20	2/8/84/115	-
27	CLA	W	614	-	1/1/11/20	4/15/91/115	-
27	CLA	a	616	14	1/1/11/20	5/15/91/115	-
30	BCR	L	309	-	-	1/29/63/63	0/2/2/2
27	CLA	3	617	16	1/1/10/20	2/8/84/115	-
27	CLA	K	206	11	1/1/11/20	4/15/91/115	-
37	NEX	V	1623	-	-	4/27/83/83	0/3/3/3
27	CLA	4	614	-	1/1/13/20	11/29/105/115	-
33	LMG	9	625	-	-	16/50/70/70	0/1/1/1
30	BCR	L	305	-	-	2/29/63/63	0/2/2/2
38	CHL	W	608	-	3/3/16/26	5/17/115/137	-
38	CHL	Y	601	24	3/3/20/26	21/39/137/137	-
30	BCR	8	621	-	-	4/29/63/63	0/2/2/2
30	BCR	A	849	-	-	5/29/63/63	0/2/2/2
29	LHG	X	2630	27	-	11/53/53/53	-
27	CLA	B	804	-	1/1/10/20	0/10/86/115	-
27	CLA	V	614	-	1/1/11/20	5/15/91/115	-
27	CLA	6	606	-	1/1/10/20	0/8/84/115	-
27	CLA	1	601	14	-	4/25/101/115	-
30	BCR	9	621	-	-	4/29/63/63	0/2/2/2
27	CLA	B	828	-	1/1/15/20	13/39/115/115	-
27	CLA	A	832	-	1/1/12/20	7/21/97/115	-
27	CLA	A	836	-	1/1/15/20	5/39/115/115	-
27	CLA	6	614	-	1/1/14/20	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	F	303	-	-	6/12/88/115	-
27	CLA	8	604	-	1/1/12/20	3/21/97/115	-
27	CLA	1	606	-	1/1/8/20	3/7/79/115	-
36	XAT	a	618	-	-	0/31/93/93	0/4/4/4
27	CLA	a	612	14	1/1/11/20	5/15/91/115	-
27	CLA	A	842	-	1/1/15/20	17/39/115/115	-
27	CLA	8	614	-	1/1/12/20	9/25/101/115	-
37	NEX	U	1623	-	-	5/27/83/83	0/3/3/3
27	CLA	Y	613	24	1/1/15/20	14/39/115/115	-
27	CLA	a	602	14	1/1/14/20	3/35/111/115	-
27	CLA	4	602	17	1/1/14/20	5/33/109/115	-
38	CHL	V	605	26	3/3/15/26	0/13/111/137	-
27	CLA	B	820	-	1/1/12/20	3/21/97/115	-
38	CHL	Y	605	24	3/3/15/26	0/10/108/137	-
27	CLA	L	303	-	-	12/39/115/115	-
27	CLA	9	610	22	1/1/13/20	3/30/106/115	-
27	CLA	B	831	-	1/1/15/20	13/39/115/115	-
27	CLA	B	838	-	-	2/17/93/115	-
27	CLA	A	834	-	1/1/15/20	15/39/115/115	-
27	CLA	U	614	-	1/1/10/20	5/12/88/115	-
35	LUT	Z	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	B	822	-	-	4/12/88/115	-
27	CLA	B	819	-	1/1/13/20	9/27/103/115	-
27	CLA	5	609	18	1/1/15/20	13/39/115/115	-
27	CLA	a	603	-	1/1/12/20	2/25/101/115	-
27	CLA	A	818	-	-	12/33/109/115	-
27	CLA	W	612	23	1/1/11/20	6/15/91/115	-
27	CLA	6	620	-	1/1/14/20	10/37/113/115	-
36	XAT	X	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	2	611	29	1/1/10/20	5/12/88/115	-
27	CLA	X	612	23	1/1/10/20	4/13/89/115	-
35	LUT	1	617	-	-	0/29/67/67	0/2/2/2
30	BCR	1	619	-	-	4/29/63/63	0/2/2/2
27	CLA	a	606	-	1/1/10/20	5/12/88/115	-
30	BCR	3	620	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	Y	2630	27	-	11/53/53/53	-
38	CHL	V	606	-	3/3/15/26	2/13/111/137	-
36	XAT	5	621	-	-	0/31/93/93	0/4/4/4
27	CLA	Y	610	24	1/1/15/20	9/39/115/115	-
36	XAT	4	620	-	-	0/31/93/93	0/4/4/4
27	CLA	5	612	18	1/1/10/20	4/10/86/115	-
27	CLA	B	806	2	1/1/15/20	16/39/115/115	-
30	BCR	L	308	-	-	2/29/63/63	0/2/2/2
27	CLA	B	826	-	1/1/14/20	7/36/112/115	-
31	SF4	C	102	3	-	-	0/6/5/5
27	CLA	3	610	16	1/1/15/20	12/39/115/115	-
27	CLA	5	613	18	1/1/14/20	15/37/113/115	-
30	BCR	5	622	-	-	3/29/63/63	0/2/2/2
28	PQN	B	842	-	-	5/23/43/43	0/2/2/2
29	LHG	8	623	-	-	10/44/44/53	-
27	CLA	5	602	18	-	12/39/115/115	-
30	BCR	A	851	-	-	2/29/63/63	0/2/2/2
27	CLA	B	817	-	1/1/13/20	10/32/108/115	-
27	CLA	7	601	20	1/1/14/20	10/33/109/115	-
27	CLA	3	614	-	1/1/10/20	3/8/84/115	-
29	LHG	3	623	-	-	19/49/49/53	-
27	CLA	6	611	29	1/1/10/20	4/12/88/115	-
27	CLA	A	839	-	1/1/13/20	6/27/103/115	-
27	CLA	1	614	-	1/1/9/20	4/4/76/115	-
35	LUT	W	1620	-	-	2/29/67/67	0/2/2/2
30	BCR	A	848	-	-	0/29/63/63	0/2/2/2
36	XAT	2	620	-	-	0/31/93/93	0/4/4/4
27	CLA	5	619	-	1/1/11/20	6/11/87/115	-
27	CLA	X	611	29	1/1/11/20	8/15/91/115	-
38	CHL	Y	608	-	3/3/16/26	6/19/117/137	-
30	BCR	O	2004	-	-	3/29/63/63	0/2/2/2
27	CLA	A	838	-	1/1/12/20	7/21/97/115	-
27	CLA	B	814	-	1/1/14/20	9/36/112/115	-
27	CLA	K	201	11	1/1/11/20	7/15/91/115	-
27	CLA	3	603	-	1/1/13/20	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	4	612	17	1/1/10/20	2/10/86/115	-
30	BCR	B	853	-	-	4/29/63/63	0/2/2/2
29	LHG	B	854	-	-	16/53/53/53	-
27	CLA	9	609	22	1/1/14/20	7/35/111/115	-
30	BCR	K	207	-	-	0/29/63/63	0/2/2/2
27	CLA	X	604	-	1/1/11/20	6/20/96/115	-
27	CLA	U	611	29	1/1/10/20	6/12/88/115	-
27	CLA	B	829	-	1/1/15/20	11/39/115/115	-
27	CLA	K	203	-	-	8/29/105/115	-
27	CLA	5	608	-	1/1/12/20	6/21/97/115	-
27	CLA	6	612	19	1/1/10/20	2/10/86/115	-
27	CLA	A	830	-	1/1/15/20	11/39/115/115	-
27	CLA	a	604	-	1/1/11/20	10/20/96/115	-
27	CLA	X	603	-	1/1/14/20	11/36/112/115	-
27	CLA	a	614	-	1/1/12/20	5/27/99/115	-
27	CLA	A	805	-	-	5/24/100/115	-
28	PQN	A	844	-	-	10/23/43/43	0/2/2/2
27	CLA	A	816	-	1/1/15/20	9/39/115/115	-
37	NEX	X	1623	-	-	3/27/83/83	0/3/3/3
27	CLA	5	601	18	1/1/13/20	4/29/105/115	-
29	LHG	W	2630	27	-	10/48/48/53	-
38	CHL	Z	609	25	3/3/20/26	20/39/137/137	-
38	CHL	V	607	-	3/3/16/26	2/15/113/137	-
27	CLA	7	602	20	1/1/15/20	13/39/115/115	-
27	CLA	4	601	17	1/1/15/20	14/39/115/115	-
33	LMG	H	205	-	-	8/50/70/70	0/1/1/1

All (3162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	Y	608	CHL	C2C-C3C	11.50	1.47	1.36
38	Z	606	CHL	C2C-C3C	11.35	1.47	1.36
38	X	606	CHL	C2C-C3C	11.14	1.47	1.36
38	Y	606	CHL	C2C-C3C	11.12	1.47	1.36
38	Z	609	CHL	C2C-C3C	11.10	1.47	1.36
38	Z	605	CHL	C2C-C3C	11.07	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	X	605	CHL	C2C-C3C	10.96	1.47	1.36
38	Z	608	CHL	C2C-C3C	10.96	1.47	1.36
38	Y	605	CHL	C2C-C3C	10.95	1.47	1.36
38	X	608	CHL	C2C-C3C	10.92	1.46	1.36
38	V	609	CHL	C2C-C3C	10.86	1.46	1.36
38	X	609	CHL	C2C-C3C	10.72	1.46	1.36
38	W	609	CHL	C2C-C3C	10.68	1.46	1.36
38	W	608	CHL	C2C-C3C	10.68	1.46	1.36
38	Y	609	CHL	C2C-C3C	10.68	1.46	1.36
38	Y	607	CHL	C2C-C3C	10.67	1.46	1.36
38	U	601	CHL	C2C-C3C	10.66	1.46	1.36
38	X	607	CHL	C2C-C3C	10.64	1.46	1.36
38	V	605	CHL	C2C-C3C	10.63	1.46	1.36
38	U	608	CHL	C2C-C3C	10.63	1.46	1.36
38	W	605	CHL	C2C-C3C	10.58	1.46	1.36
38	V	607	CHL	C2C-C3C	10.57	1.46	1.36
38	U	605	CHL	C2C-C3C	10.56	1.46	1.36
38	Z	601	CHL	C2C-C3C	10.54	1.46	1.36
38	Y	601	CHL	C2C-C3C	10.54	1.46	1.36
38	U	609	CHL	C2C-C3C	10.53	1.46	1.36
38	U	607	CHL	C2C-C3C	10.49	1.46	1.36
38	W	606	CHL	C2C-C3C	10.47	1.46	1.36
38	V	601	CHL	C2C-C3C	10.45	1.46	1.36
38	U	606	CHL	C2C-C3C	10.44	1.46	1.36
38	X	601	CHL	C2C-C3C	10.42	1.46	1.36
38	V	606	CHL	C2C-C3C	10.40	1.46	1.36
38	Z	609	CHL	C1D-C2D	10.36	1.51	1.39
38	V	609	CHL	C1D-C2D	10.35	1.51	1.39
38	W	601	CHL	C2C-C3C	10.35	1.46	1.36
38	Z	607	CHL	C2C-C3C	10.32	1.46	1.36
38	W	609	CHL	C1D-C2D	10.24	1.51	1.39
38	Y	601	CHL	C1D-C2D	10.22	1.51	1.39
38	U	609	CHL	C1D-C2D	10.20	1.51	1.39
38	X	601	CHL	C1D-C2D	10.20	1.51	1.39
38	W	601	CHL	C1D-C2D	10.20	1.51	1.39
38	U	601	CHL	C1D-C2D	10.19	1.51	1.39
28	A	844	PQN	C12-C13	10.18	1.56	1.33
38	Y	609	CHL	C1D-C2D	10.16	1.51	1.39
38	X	609	CHL	C1D-C2D	10.14	1.51	1.39
38	X	608	CHL	C1D-C2D	10.07	1.51	1.39
38	V	608	CHL	C2C-C3C	10.01	1.46	1.36
38	Z	601	CHL	C1D-C2D	10.01	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	842	PQN	C12-C13	10.01	1.56	1.33
38	Z	607	CHL	C1D-C2D	9.93	1.50	1.39
38	V	601	CHL	C1D-C2D	9.93	1.50	1.39
38	X	607	CHL	C1D-C2D	9.91	1.50	1.39
38	Y	607	CHL	C1D-C2D	9.74	1.50	1.39
38	X	606	CHL	C3B-C4B	9.71	1.50	1.41
38	Y	606	CHL	C3B-C4B	9.71	1.50	1.41
38	Y	608	CHL	C3B-C4B	9.66	1.50	1.41
38	X	605	CHL	C3B-C4B	9.63	1.50	1.41
38	W	607	CHL	C1D-C2D	9.62	1.50	1.39
38	Z	608	CHL	C3B-C4B	9.60	1.50	1.41
38	Z	605	CHL	C3B-C4B	9.56	1.50	1.41
38	Y	605	CHL	C3B-C4B	9.50	1.50	1.41
38	W	606	CHL	C3B-C4B	9.17	1.50	1.41
38	W	608	CHL	C3B-C4B	9.03	1.50	1.41
38	W	607	CHL	C1A-CHA	9.01	1.50	1.40
38	U	606	CHL	C3B-C4B	9.00	1.50	1.41
38	W	605	CHL	C3B-C4B	8.94	1.50	1.41
38	U	608	CHL	C3B-C4B	8.93	1.50	1.41
38	U	605	CHL	C3B-C4B	8.92	1.50	1.41
38	V	606	CHL	C3B-C4B	8.88	1.50	1.41
38	Y	607	CHL	C1A-CHA	8.76	1.50	1.40
38	Z	609	CHL	C1B-C2B	8.67	1.49	1.39
38	U	607	CHL	C3B-C4B	8.63	1.49	1.41
38	V	608	CHL	C3B-C4B	8.58	1.49	1.41
38	X	608	CHL	C1B-C2B	8.58	1.49	1.39
38	Z	606	CHL	C1B-C2B	8.54	1.49	1.39
38	V	605	CHL	C3B-C4B	8.48	1.49	1.41
38	X	609	CHL	C1B-C2B	8.47	1.49	1.39
38	Z	607	CHL	C1B-C2B	8.45	1.49	1.39
38	Z	605	CHL	C1D-C2D	8.42	1.49	1.39
38	V	607	CHL	C3B-C4B	8.41	1.49	1.41
38	Z	601	CHL	C1B-C2B	8.40	1.49	1.39
38	Z	606	CHL	C1D-C2D	8.40	1.49	1.39
38	X	601	CHL	C1B-C2B	8.39	1.49	1.39
38	W	601	CHL	C1B-C2B	8.38	1.49	1.39
38	Y	601	CHL	C1B-C2B	8.38	1.49	1.39
38	W	607	CHL	C1B-C2B	8.37	1.49	1.39
38	V	601	CHL	C1B-C2B	8.33	1.49	1.39
38	U	609	CHL	C1B-C2B	8.33	1.49	1.39
38	W	609	CHL	C1B-C2B	8.32	1.49	1.39
38	Z	608	CHL	C1D-C2D	8.31	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	Y	609	CHL	C1B-C2B	8.30	1.49	1.39
38	X	608	CHL	C1A-CHA	8.30	1.49	1.40
38	U	601	CHL	C1B-C2B	8.20	1.48	1.39
38	Y	605	CHL	C1A-CHA	8.20	1.49	1.40
38	X	605	CHL	C1A-CHA	8.20	1.49	1.40
38	Z	607	CHL	C1A-CHA	8.17	1.49	1.40
38	Z	605	CHL	C1B-C2B	8.16	1.48	1.39
38	X	607	CHL	C1A-CHA	8.15	1.49	1.40
38	V	609	CHL	C1B-C2B	8.14	1.48	1.39
38	U	607	CHL	C1A-CHA	8.13	1.49	1.40
38	X	605	CHL	C1D-C2D	8.12	1.48	1.39
38	Y	605	CHL	C1D-C2D	8.09	1.48	1.39
38	Z	601	CHL	C1A-CHA	8.09	1.49	1.40
38	X	605	CHL	C1B-C2B	8.08	1.48	1.39
38	Y	605	CHL	C1B-C2B	8.07	1.48	1.39
38	Y	606	CHL	C1D-C2D	8.06	1.48	1.39
38	Y	609	CHL	C1A-CHA	8.05	1.49	1.40
38	X	607	CHL	C1B-C2B	8.03	1.48	1.39
38	Y	608	CHL	C1D-C2D	8.03	1.48	1.39
38	Y	607	CHL	C1B-C2B	8.02	1.48	1.39
38	Z	608	CHL	C1A-CHA	7.99	1.49	1.40
38	Z	609	CHL	C1A-CHA	7.98	1.49	1.40
28	B	842	PQN	O4-C4	7.95	1.39	1.23
28	A	844	PQN	O4-C4	7.92	1.39	1.23
38	X	606	CHL	C1D-C2D	7.90	1.48	1.39
38	V	609	CHL	C1A-CHA	7.86	1.48	1.40
38	V	601	CHL	C1A-CHA	7.86	1.48	1.40
38	X	601	CHL	C1A-CHA	7.85	1.48	1.40
38	V	607	CHL	C1A-CHA	7.84	1.48	1.40
38	W	601	CHL	C1A-CHA	7.84	1.48	1.40
38	X	609	CHL	C1A-CHA	7.83	1.48	1.40
38	Y	601	CHL	C1A-CHA	7.82	1.48	1.40
38	Z	606	CHL	C3B-C4B	7.82	1.49	1.41
38	V	605	CHL	C1D-C2D	7.77	1.48	1.39
28	A	844	PQN	O1-C1	7.75	1.39	1.23
38	Z	605	CHL	C1A-CHA	7.72	1.48	1.40
28	B	842	PQN	O1-C1	7.69	1.39	1.23
38	W	609	CHL	C1A-CHA	7.69	1.48	1.40
38	W	605	CHL	C1A-CHA	7.68	1.48	1.40
38	U	601	CHL	C1A-CHA	7.67	1.48	1.40
38	U	605	CHL	C1A-CHA	7.67	1.48	1.40
38	U	609	CHL	C1A-CHA	7.67	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	Z	608	CHL	C1B-C2B	7.64	1.48	1.39
38	Y	608	CHL	C1A-CHA	7.62	1.48	1.40
38	W	605	CHL	C1B-C2B	7.59	1.48	1.39
38	Y	607	CHL	C3B-C4B	7.54	1.48	1.41
38	U	601	CHL	C3B-C4B	7.52	1.48	1.41
38	Y	608	CHL	C1B-C2B	7.52	1.48	1.39
38	X	607	CHL	C3B-C4B	7.50	1.48	1.41
38	Z	601	CHL	C3B-C4B	7.50	1.48	1.41
38	U	605	CHL	C1B-C2B	7.48	1.48	1.39
38	X	606	CHL	C1A-CHA	7.46	1.48	1.40
28	A	844	PQN	C9-C10	7.44	1.51	1.39
38	Y	606	CHL	C1B-C2B	7.44	1.48	1.39
38	Z	606	CHL	C1A-CHA	7.42	1.48	1.40
38	X	608	CHL	C3B-C4B	7.39	1.48	1.41
38	W	608	CHL	C1D-C2D	7.39	1.48	1.39
38	X	606	CHL	C1B-C2B	7.38	1.48	1.39
38	W	605	CHL	C1D-C2D	7.38	1.47	1.39
38	V	607	CHL	C1D-C2D	7.38	1.47	1.39
38	U	609	CHL	C3B-C4B	7.32	1.48	1.41
38	W	601	CHL	C3B-C4B	7.29	1.48	1.41
38	U	605	CHL	C1D-C2D	7.28	1.47	1.39
38	W	608	CHL	C1A-CHA	7.28	1.48	1.40
38	Y	606	CHL	C1A-CHA	7.27	1.48	1.40
38	V	607	CHL	C1B-C2B	7.27	1.47	1.39
38	U	608	CHL	C1D-C2D	7.27	1.47	1.39
38	Y	601	CHL	C3B-C4B	7.26	1.48	1.41
38	W	607	CHL	C3B-C4B	7.26	1.48	1.41
28	A	844	PQN	C6-C5	7.24	1.50	1.39
38	X	601	CHL	C3B-C4B	7.23	1.48	1.41
38	Z	607	CHL	C3B-C4B	7.23	1.48	1.41
38	V	601	CHL	C3B-C4B	7.22	1.48	1.41
38	V	605	CHL	C1B-C2B	7.21	1.47	1.39
38	W	606	CHL	C1A-CHA	7.19	1.48	1.40
38	W	606	CHL	C1D-C2D	7.18	1.47	1.39
38	V	608	CHL	C1A-CHA	7.17	1.48	1.40
38	V	605	CHL	C1A-CHA	7.14	1.48	1.40
38	X	609	CHL	C3B-C4B	7.13	1.48	1.41
38	U	606	CHL	C1A-CHA	7.12	1.48	1.40
38	U	607	CHL	C1B-C2B	7.12	1.47	1.39
38	Y	609	CHL	C3B-C4B	7.11	1.48	1.41
28	B	842	PQN	C6-C5	7.11	1.50	1.39
38	U	606	CHL	C1D-C2D	7.10	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	V	609	CHL	C3B-C4B	7.10	1.48	1.41
38	U	608	CHL	C1A-CHA	7.09	1.48	1.40
28	B	842	PQN	C9-C10	7.06	1.50	1.39
38	W	609	CHL	C3B-C4B	7.05	1.48	1.41
38	V	606	CHL	C1D-C2D	7.03	1.47	1.39
38	V	606	CHL	C1A-CHA	6.93	1.47	1.40
38	V	608	CHL	C1B-C2B	6.89	1.47	1.39
38	V	608	CHL	C1D-C2D	6.88	1.47	1.39
38	U	607	CHL	C1D-C2D	6.87	1.47	1.39
38	Z	609	CHL	C3B-C4B	6.85	1.48	1.41
28	B	842	PQN	C10-C5	-6.74	1.29	1.40
38	U	608	CHL	C1B-C2B	6.65	1.47	1.39
38	W	608	CHL	C1B-C2B	6.59	1.47	1.39
38	W	606	CHL	C1B-C2B	6.59	1.47	1.39
38	V	606	CHL	C1B-C2B	6.57	1.47	1.39
28	A	844	PQN	C10-C5	-6.56	1.30	1.40
38	U	606	CHL	C1B-C2B	6.52	1.47	1.39
38	V	606	CHL	C3A-C2A	-6.35	1.49	1.54
38	U	608	CHL	C3A-C2A	-6.01	1.49	1.54
38	V	608	CHL	C3A-C2A	-6.01	1.49	1.54
38	V	605	CHL	C3A-C2A	-5.97	1.49	1.54
38	W	605	CHL	C3A-C2A	-5.93	1.49	1.54
38	W	608	CHL	C3A-C2A	-5.91	1.49	1.54
38	Z	606	CHL	C3B-C2B	5.84	1.48	1.40
38	U	605	CHL	C3A-C2A	-5.75	1.49	1.54
38	Z	605	CHL	C3B-C2B	5.67	1.48	1.40
38	U	606	CHL	C3A-C2A	-5.64	1.49	1.54
38	W	606	CHL	C3A-C2A	-5.62	1.49	1.54
38	X	605	CHL	C3B-C2B	5.60	1.48	1.40
38	Y	605	CHL	C2A-C3A	-5.57	1.50	1.54
38	U	606	CHL	CHB-C4A	-5.56	1.31	1.38
38	Y	605	CHL	C3B-C2B	5.54	1.47	1.40
38	W	606	CHL	CHB-C4A	-5.54	1.31	1.38
38	Z	606	CHL	C3D-C2D	5.54	1.49	1.39
38	Z	609	CHL	C3D-C4D	-5.51	1.33	1.41
38	V	601	CHL	C3D-C4D	-5.48	1.33	1.41
38	U	601	CHL	C3D-C4D	-5.47	1.33	1.41
38	Y	607	CHL	C3D-C4D	-5.46	1.33	1.41
38	U	609	CHL	C3D-C4D	-5.44	1.33	1.41
38	Y	609	CHL	C3D-C4D	-5.44	1.33	1.41
38	Y	608	CHL	C3D-C2D	5.44	1.48	1.39
37	6	624	NEX	C7-C6	-5.42	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	X	601	CHL	C3D-C4D	-5.42	1.33	1.41
38	W	609	CHL	C3D-C4D	-5.41	1.33	1.41
38	V	609	CHL	C3D-C4D	-5.41	1.33	1.41
38	X	605	CHL	C3D-C2D	5.41	1.48	1.39
38	Z	608	CHL	C3D-C2D	5.40	1.48	1.39
38	Y	605	CHL	C3D-C2D	5.40	1.48	1.39
38	Z	605	CHL	C3D-C2D	5.39	1.48	1.39
38	W	601	CHL	C3D-C4D	-5.39	1.33	1.41
38	X	607	CHL	C3D-C4D	-5.38	1.33	1.41
38	Z	601	CHL	C3D-C4D	-5.38	1.33	1.41
38	X	606	CHL	CHC-C4B	5.37	1.48	1.39
38	Y	601	CHL	C3D-C4D	-5.37	1.33	1.41
38	X	608	CHL	C3D-C4D	-5.37	1.33	1.41
38	X	609	CHL	C3D-C4D	-5.36	1.33	1.41
38	Y	606	CHL	CHC-C4B	5.32	1.48	1.39
38	X	606	CHL	C3D-C2D	5.30	1.48	1.39
38	V	609	CHL	C3B-C2B	5.29	1.47	1.40
38	Z	609	CHL	C3B-C2B	5.28	1.47	1.40
38	W	607	CHL	C3D-C4D	-5.25	1.33	1.41
38	Y	606	CHL	C3D-C2D	5.25	1.48	1.39
38	Z	608	CHL	C3B-C2B	5.24	1.47	1.40
38	Z	607	CHL	C3D-C4D	-5.23	1.33	1.41
38	U	607	CHL	CHB-C4A	-5.22	1.32	1.38
38	V	606	CHL	CHB-C4A	-5.21	1.32	1.38
38	V	607	CHL	CHB-C4A	-5.21	1.32	1.38
38	U	608	CHL	CHB-C4A	-5.20	1.32	1.38
38	W	608	CHL	CHB-C4A	-5.20	1.32	1.38
38	X	608	CHL	C3B-C2B	5.18	1.47	1.40
38	U	609	CHL	C3B-C2B	5.18	1.47	1.40
38	Y	606	CHL	O2D-CGD	5.17	1.46	1.33
38	U	607	CHL	C3A-C2A	-5.17	1.50	1.54
38	Y	608	CHL	OBD-CAD	5.14	1.29	1.22
38	X	609	CHL	C3B-C2B	5.14	1.47	1.40
38	Y	608	CHL	CHC-C4B	5.14	1.47	1.39
38	Y	607	CHL	C3B-C2B	5.14	1.47	1.40
38	X	606	CHL	C3B-C2B	5.13	1.47	1.40
38	Z	606	CHL	O2D-CGD	5.13	1.45	1.33
38	Y	608	CHL	C3A-C2A	-5.13	1.50	1.54
38	Y	608	CHL	C3B-C2B	5.13	1.47	1.40
38	Y	609	CHL	C3B-C2B	5.13	1.47	1.40
38	Z	608	CHL	O2D-CGD	5.12	1.45	1.33
38	Z	605	CHL	O2D-CGD	5.12	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	V	605	CHL	CHB-C4A	-5.12	1.32	1.38
38	W	607	CHL	CHB-C4A	-5.12	1.32	1.38
38	X	606	CHL	O2D-CGD	5.11	1.45	1.33
38	V	608	CHL	CHB-C4A	-5.11	1.32	1.38
38	U	607	CHL	C3D-C2D	5.11	1.48	1.39
38	X	605	CHL	C3A-C2A	-5.10	1.50	1.54
38	W	609	CHL	O2D-CGD	5.10	1.45	1.33
38	Y	607	CHL	O2D-CGD	5.10	1.45	1.33
38	W	609	CHL	C3B-C2B	5.10	1.47	1.40
38	Z	608	CHL	C3A-C2A	-5.10	1.50	1.54
38	W	601	CHL	O2D-CGD	5.10	1.45	1.33
38	Y	601	CHL	O2D-CGD	5.09	1.45	1.33
38	U	605	CHL	C3B-C2B	5.09	1.47	1.40
38	Y	605	CHL	OBD-CAD	5.09	1.29	1.22
38	Z	609	CHL	CHB-C1B	5.09	1.47	1.39
38	X	605	CHL	O2D-CGD	5.09	1.45	1.33
38	Z	606	CHL	C3A-C2A	-5.08	1.50	1.54
38	Y	608	CHL	O2D-CGD	5.08	1.45	1.33
38	X	607	CHL	C3B-C2B	5.08	1.47	1.40
38	X	609	CHL	O2D-CGD	5.08	1.45	1.33
38	Z	607	CHL	O2D-CGD	5.07	1.45	1.33
38	Y	605	CHL	O2D-CGD	5.07	1.45	1.33
38	U	601	CHL	O2D-CGD	5.07	1.45	1.33
38	X	608	CHL	O2D-CGD	5.07	1.45	1.33
38	X	607	CHL	O2D-CGD	5.07	1.45	1.33
38	Y	606	CHL	C3B-C2B	5.06	1.47	1.40
38	Y	607	CHL	CHB-C4A	-5.06	1.32	1.38
38	X	605	CHL	OBD-CAD	5.06	1.28	1.22
38	U	609	CHL	O2D-CGD	5.06	1.45	1.33
38	W	605	CHL	C3B-C2B	5.06	1.47	1.40
38	V	605	CHL	C3B-C2B	5.05	1.47	1.40
38	W	607	CHL	O2D-CGD	5.05	1.45	1.33
38	Y	609	CHL	O2D-CGD	5.04	1.45	1.33
38	Z	609	CHL	O2D-CGD	5.04	1.45	1.33
38	Z	608	CHL	OBD-CAD	5.03	1.28	1.22
38	V	601	CHL	O2D-CGD	5.03	1.45	1.33
38	V	606	CHL	CHC-C4B	5.01	1.47	1.39
38	Z	601	CHL	O2D-CGD	5.00	1.45	1.33
38	U	605	CHL	C3D-C2D	5.00	1.48	1.39
38	V	609	CHL	O2D-CGD	5.00	1.45	1.33
38	Z	607	CHL	OBD-CAD	4.99	1.28	1.22
38	X	606	CHL	C3A-C2A	-4.99	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	W	605	CHL	C3D-C2D	4.98	1.48	1.39
38	X	601	CHL	C3B-C2B	4.97	1.47	1.40
38	Z	605	CHL	CHC-C4B	4.97	1.47	1.39
38	W	606	CHL	O2D-CGD	4.96	1.45	1.33
38	X	607	CHL	CHB-C4A	-4.96	1.32	1.38
38	Z	607	CHL	C3A-C2A	-4.95	1.50	1.54
38	Y	606	CHL	C3A-C2A	-4.94	1.50	1.54
38	Y	605	CHL	CHC-C4B	4.94	1.47	1.39
38	W	607	CHL	OBD-CAD	4.94	1.28	1.22
38	X	601	CHL	O2D-CGD	4.94	1.45	1.33
38	U	601	CHL	C3A-C2A	-4.94	1.50	1.54
38	W	606	CHL	C3D-C2D	4.93	1.48	1.39
38	W	605	CHL	O2D-CGD	4.93	1.45	1.33
38	U	606	CHL	O2D-CGD	4.93	1.45	1.33
38	Z	605	CHL	OBD-CAD	4.92	1.28	1.22
38	W	608	CHL	OBD-CAD	4.92	1.28	1.22
38	W	605	CHL	OBD-CAD	4.91	1.28	1.22
38	Y	606	CHL	CHB-C4A	-4.91	1.32	1.38
38	V	607	CHL	C3D-C2D	4.91	1.48	1.39
38	U	605	CHL	O2D-CGD	4.90	1.45	1.33
38	U	606	CHL	CHC-C4B	4.90	1.47	1.39
38	Z	607	CHL	C3B-C2B	4.89	1.47	1.40
38	U	605	CHL	OBD-CAD	4.89	1.28	1.22
38	V	605	CHL	OBD-CAD	4.89	1.28	1.22
38	Z	609	CHL	CHD-C1D	4.89	1.47	1.39
38	V	606	CHL	C3D-C2D	4.89	1.48	1.39
38	W	606	CHL	CHC-C4B	4.88	1.47	1.39
38	U	606	CHL	C3D-C2D	4.88	1.48	1.39
38	X	605	CHL	CHC-C4B	4.88	1.47	1.39
38	V	605	CHL	C3D-C2D	4.88	1.48	1.39
38	Z	606	CHL	OBD-CAD	4.88	1.28	1.22
38	V	608	CHL	OBD-CAD	4.87	1.28	1.22
38	V	609	CHL	CHB-C1B	4.87	1.47	1.39
38	Y	607	CHL	CHC-C4B	4.87	1.47	1.39
38	U	608	CHL	OBD-CAD	4.86	1.28	1.22
38	V	606	CHL	O2D-CGD	4.86	1.45	1.33
38	X	607	CHL	OBD-CAD	4.85	1.28	1.22
38	Z	601	CHL	OBD-CAD	4.85	1.28	1.22
38	Y	601	CHL	C3A-C2A	-4.85	1.50	1.54
38	V	609	CHL	CHC-C4B	4.85	1.47	1.39
38	Y	609	CHL	CHB-C1B	4.84	1.47	1.39
38	V	601	CHL	C3B-C2B	4.84	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	W	601	CHL	C3A-C2A	-4.84	1.50	1.54
38	V	605	CHL	O2D-CGD	4.84	1.45	1.33
38	Y	601	CHL	C3B-C2B	4.84	1.46	1.40
38	Z	605	CHL	C3A-C2A	-4.84	1.50	1.54
38	X	606	CHL	CHB-C4A	-4.83	1.32	1.38
38	Y	607	CHL	OBD-CAD	4.83	1.28	1.22
38	V	608	CHL	C3D-C2D	4.82	1.47	1.39
38	V	607	CHL	OBD-CAD	4.82	1.28	1.22
38	Z	601	CHL	C3B-C2B	4.82	1.46	1.40
38	U	607	CHL	OBD-CAD	4.82	1.28	1.22
38	Y	608	CHL	CHB-C4A	-4.80	1.32	1.38
38	W	601	CHL	C3B-C2B	4.80	1.46	1.40
38	X	609	CHL	CHB-C1B	4.80	1.47	1.39
38	X	601	CHL	OBD-CAD	4.80	1.28	1.22
38	U	608	CHL	C3D-C2D	4.79	1.47	1.39
38	W	601	CHL	OBD-CAD	4.79	1.28	1.22
38	W	609	CHL	CHB-C1B	4.78	1.47	1.39
38	V	601	CHL	C3A-C2A	-4.78	1.50	1.54
38	V	607	CHL	C3A-C2A	-4.78	1.50	1.54
38	W	607	CHL	C3B-C2B	4.78	1.46	1.40
38	X	606	CHL	OBD-CAD	4.77	1.28	1.22
38	W	608	CHL	C3D-C2D	4.77	1.47	1.39
38	W	608	CHL	O2D-CGD	4.77	1.44	1.33
38	U	605	CHL	CHB-C4A	-4.76	1.32	1.38
38	U	601	CHL	OBD-CAD	4.76	1.28	1.22
38	Z	609	CHL	CHD-C4C	4.76	1.48	1.39
38	U	601	CHL	C3B-C2B	4.76	1.46	1.40
38	Z	601	CHL	C3A-C2A	-4.76	1.50	1.54
38	Y	606	CHL	OBD-CAD	4.76	1.28	1.22
38	V	607	CHL	O2D-CGD	4.75	1.44	1.33
38	U	608	CHL	O2D-CGD	4.75	1.44	1.33
38	Z	608	CHL	CHC-C4B	4.74	1.47	1.39
38	V	609	CHL	CHD-C1D	4.73	1.47	1.39
38	X	607	CHL	C3A-C2A	-4.73	1.50	1.54
38	U	609	CHL	CHB-C1B	4.73	1.47	1.39
38	X	601	CHL	C3A-C2A	-4.72	1.50	1.54
38	V	608	CHL	O2D-CGD	4.72	1.44	1.33
38	U	601	CHL	CHB-C4A	-4.72	1.32	1.38
38	V	601	CHL	OBD-CAD	4.71	1.28	1.22
38	V	608	CHL	C3B-C2B	4.70	1.46	1.40
38	W	607	CHL	C2C-C3C	4.70	1.46	1.37
38	Y	601	CHL	OBD-CAD	4.70	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	X	608	CHL	CHC-C4B	4.70	1.47	1.39
38	V	609	CHL	CHD-C4C	4.70	1.48	1.39
38	Z	609	CHL	CHC-C4B	4.69	1.47	1.39
38	X	608	CHL	OBD-CAD	4.69	1.28	1.22
38	Z	606	CHL	CHD-C1D	4.69	1.47	1.39
38	W	609	CHL	C3A-C2A	-4.68	1.50	1.54
38	X	609	CHL	CHC-C4B	4.68	1.47	1.39
38	Z	608	CHL	CHB-C4A	-4.67	1.33	1.38
38	W	607	CHL	CHD-C1D	4.65	1.47	1.39
38	Z	609	CHL	OBD-CAD	4.65	1.28	1.22
38	U	607	CHL	O2D-CGD	4.64	1.44	1.33
38	U	605	CHL	CHC-C4B	4.64	1.47	1.39
38	Y	609	CHL	CHD-C1D	4.64	1.47	1.39
38	X	609	CHL	OBD-CAD	4.63	1.28	1.22
38	W	609	CHL	CHD-C4C	4.63	1.48	1.39
38	V	609	CHL	OBD-CAD	4.63	1.28	1.22
38	V	601	CHL	CHB-C1B	4.63	1.47	1.39
38	W	605	CHL	CHC-C4B	4.63	1.47	1.39
38	W	605	CHL	CHB-C4A	-4.62	1.33	1.38
38	W	607	CHL	CHC-C4B	4.61	1.47	1.39
38	U	609	CHL	CHC-C4B	4.61	1.47	1.39
38	Y	607	CHL	CHD-C1D	4.61	1.47	1.39
38	X	609	CHL	CHD-C4C	4.61	1.48	1.39
38	X	608	CHL	CHC-C1C	4.60	1.48	1.39
38	Z	607	CHL	CHC-C4B	4.60	1.47	1.39
38	Y	609	CHL	CHD-C4C	4.60	1.48	1.39
38	Z	608	CHL	CHD-C4C	4.59	1.48	1.39
38	Z	601	CHL	CHB-C1B	4.59	1.47	1.39
38	U	609	CHL	CHD-C4C	4.59	1.48	1.39
38	X	601	CHL	CHC-C4B	4.58	1.47	1.39
38	X	607	CHL	CHC-C4B	4.58	1.47	1.39
38	X	601	CHL	CHB-C1B	4.58	1.47	1.39
38	Y	609	CHL	CHC-C4B	4.58	1.47	1.39
38	Y	609	CHL	OBD-CAD	4.57	1.28	1.22
38	Z	608	CHL	CHD-C1D	4.57	1.47	1.39
38	W	609	CHL	CHC-C4B	4.57	1.47	1.39
38	Y	606	CHL	O2A-CGA	4.57	1.45	1.30
38	V	601	CHL	CHC-C4B	4.57	1.47	1.39
38	Z	606	CHL	CHC-C4B	4.57	1.47	1.39
38	U	609	CHL	CHD-C1D	4.56	1.47	1.39
38	W	609	CHL	OBD-CAD	4.56	1.28	1.22
38	W	608	CHL	C3B-C2B	4.56	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	Y	601	CHL	CHC-C4B	4.56	1.47	1.39
38	U	608	CHL	C3B-C2B	4.55	1.46	1.40
38	U	607	CHL	O2A-CGA	4.55	1.45	1.30
38	Z	605	CHL	CHD-C1D	4.55	1.47	1.39
38	V	607	CHL	O2A-CGA	4.55	1.45	1.30
38	U	601	CHL	CHD-C4C	4.55	1.48	1.39
38	U	601	CHL	CHC-C4B	4.54	1.47	1.39
38	Z	606	CHL	O2A-CGA	4.54	1.45	1.30
38	X	605	CHL	O2A-CGA	4.54	1.45	1.30
38	Z	606	CHL	CHD-C4C	4.53	1.48	1.39
38	X	608	CHL	CHD-C4C	4.53	1.48	1.39
38	W	605	CHL	O2A-CGA	4.52	1.45	1.30
38	Z	607	CHL	CHB-C4A	-4.52	1.33	1.38
38	Z	609	CHL	CHC-C1C	4.52	1.48	1.39
38	W	601	CHL	CHD-C4C	4.52	1.48	1.39
38	Y	601	CHL	CHB-C1B	4.52	1.46	1.39
38	X	608	CHL	CHB-C1B	4.51	1.46	1.39
38	X	609	CHL	CHD-C1D	4.51	1.46	1.39
38	W	606	CHL	O2A-CGA	4.51	1.45	1.30
38	Z	601	CHL	CHC-C4B	4.50	1.46	1.39
38	W	601	CHL	CHB-C4A	-4.50	1.33	1.38
38	Y	607	CHL	CHC-C1C	4.50	1.48	1.39
38	W	609	CHL	CHD-C1D	4.49	1.46	1.39
38	Z	606	CHL	CHB-C1B	4.49	1.46	1.39
38	W	607	CHL	CHD-C4C	4.49	1.48	1.39
38	Y	606	CHL	CHD-C4C	4.48	1.48	1.39
38	U	608	CHL	CHC-C4B	4.48	1.46	1.39
38	W	601	CHL	CHC-C4B	4.48	1.46	1.39
38	X	606	CHL	CHD-C4C	4.48	1.48	1.39
38	X	608	CHL	CHD-C1D	4.48	1.46	1.39
38	V	601	CHL	CHD-C4C	4.48	1.48	1.39
38	Z	605	CHL	CHB-C1B	4.47	1.46	1.39
38	X	605	CHL	CHB-C1B	4.47	1.46	1.39
38	Y	605	CHL	CHB-C1B	4.47	1.46	1.39
38	X	609	CHL	C3A-C2A	-4.47	1.50	1.54
38	U	609	CHL	OBD-CAD	4.47	1.28	1.22
38	Y	608	CHL	CHD-C4C	4.47	1.47	1.39
38	U	607	CHL	C3B-C2B	4.47	1.46	1.40
38	W	608	CHL	CHC-C4B	4.46	1.46	1.39
38	Y	607	CHL	CHD-C4C	4.46	1.47	1.39
38	Y	601	CHL	CHB-C4A	-4.45	1.33	1.38
38	V	609	CHL	CHC-C1C	4.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	Y	601	CHL	CHD-C4C	4.43	1.47	1.39
38	X	601	CHL	CHD-C1D	4.43	1.46	1.39
38	X	601	CHL	CHD-C4C	4.43	1.47	1.39
38	Z	606	CHL	CHB-C4A	-4.43	1.33	1.38
38	V	607	CHL	C3B-C2B	4.43	1.46	1.40
38	W	601	CHL	CHB-C1B	4.43	1.46	1.39
38	V	606	CHL	C3B-C2B	4.43	1.46	1.40
38	U	601	CHL	CHD-C1D	4.43	1.46	1.39
38	Y	608	CHL	CHC-C1C	4.42	1.47	1.39
38	Z	605	CHL	CHD-C4C	4.41	1.47	1.39
38	W	606	CHL	C3B-C2B	4.41	1.46	1.40
38	X	608	CHL	CHB-C4A	-4.40	1.33	1.38
38	X	605	CHL	CHB-C4A	-4.39	1.33	1.38
38	Y	608	CHL	O2A-CGA	4.39	1.46	1.33
38	Z	607	CHL	CHD-C4C	4.39	1.47	1.39
38	V	608	CHL	CHC-C4B	4.39	1.46	1.39
38	Z	601	CHL	CHD-C4C	4.38	1.47	1.39
38	W	607	CHL	CHB-C1B	4.38	1.46	1.39
38	X	607	CHL	CHD-C4C	4.38	1.47	1.39
33	L	2631	LMG	O8-C28	4.37	1.46	1.33
38	Y	605	CHL	CHB-C4A	-4.36	1.33	1.38
38	U	609	CHL	C3A-C2A	-4.36	1.50	1.54
38	X	605	CHL	CHD-C1D	4.36	1.46	1.39
38	Z	607	CHL	CHB-C1B	4.36	1.46	1.39
38	Z	608	CHL	O2A-CGA	4.36	1.46	1.33
38	Z	601	CHL	CHD-C1D	4.36	1.46	1.39
38	Y	605	CHL	CHD-C1D	4.36	1.46	1.39
38	U	606	CHL	C3B-C2B	4.35	1.46	1.40
38	Y	607	CHL	CHB-C1B	4.35	1.46	1.39
38	U	601	CHL	CHB-C1B	4.35	1.46	1.39
38	Z	605	CHL	CHB-C4A	-4.35	1.33	1.38
38	W	607	CHL	CHC-C1C	4.34	1.47	1.39
38	Z	601	CHL	O2A-CGA	4.34	1.46	1.33
38	W	606	CHL	OBD-CAD	4.34	1.28	1.22
38	X	607	CHL	CHD-C1D	4.34	1.46	1.39
38	Y	601	CHL	CHD-C1D	4.34	1.46	1.39
37	5	624	NEX	C7-C6	-4.34	1.25	1.30
38	Y	609	CHL	CHC-C1C	4.34	1.47	1.39
38	X	607	CHL	CHC-C1C	4.33	1.47	1.39
29	B	851	LHG	O8-C23	4.33	1.46	1.33
38	W	601	CHL	CHD-C1D	4.33	1.46	1.39
33	J	104	LMG	O8-C28	4.33	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	U	609	CHL	CHC-C1C	4.33	1.47	1.39
38	Z	607	CHL	CHC-C1C	4.33	1.47	1.39
33	4	624	LMG	O8-C28	4.32	1.46	1.33
29	X	2630	LHG	O8-C23	4.32	1.45	1.33
38	X	601	CHL	CHB-C4A	-4.32	1.33	1.38
38	Y	605	CHL	CHD-C4C	4.32	1.47	1.39
29	Z	2630	LHG	O8-C23	4.32	1.45	1.33
38	V	605	CHL	CHC-C4B	4.31	1.46	1.39
38	V	601	CHL	CHD-C1D	4.31	1.46	1.39
38	X	606	CHL	CHC-C1C	4.31	1.47	1.39
38	V	601	CHL	CHB-C4A	-4.31	1.33	1.38
38	V	607	CHL	CHC-C4B	4.31	1.46	1.39
38	W	607	CHL	O2A-CGA	4.31	1.45	1.33
29	9	624	LHG	O8-C23	4.30	1.45	1.33
38	X	605	CHL	CHD-C4C	4.30	1.47	1.39
33	4	623	LMG	O8-C28	4.29	1.45	1.33
38	Y	607	CHL	O2A-CGA	4.29	1.45	1.33
29	Y	2630	LHG	O8-C23	4.29	1.45	1.33
33	5	627	LMG	O8-C28	4.29	1.45	1.33
38	Y	606	CHL	CHC-C1C	4.29	1.47	1.39
38	Y	608	CHL	CHD-C1D	4.28	1.46	1.39
38	X	601	CHL	CHC-C1C	4.28	1.47	1.39
38	U	606	CHL	OBD-CAD	4.28	1.27	1.22
38	Z	607	CHL	O2A-CGA	4.28	1.45	1.33
37	Z	1623	NEX	C7-C8	-4.28	1.24	1.31
38	X	609	CHL	CHC-C1C	4.27	1.47	1.39
29	X	2630	LHG	O7-C7	4.27	1.46	1.34
38	V	609	CHL	O2A-CGA	4.26	1.45	1.33
38	W	601	CHL	O2A-CGA	4.26	1.45	1.33
33	8	626	LMG	O8-C28	4.26	1.45	1.33
29	Y	2630	LHG	O7-C7	4.26	1.46	1.34
38	Z	608	CHL	CHB-C1B	4.25	1.46	1.39
29	O	2631	LHG	O8-C23	4.25	1.45	1.33
38	Z	601	CHL	CHB-C4A	-4.25	1.33	1.38
38	V	609	CHL	CHB-C4A	-4.25	1.33	1.38
38	Z	609	CHL	O2A-CGA	4.25	1.45	1.33
38	U	609	CHL	O2A-CGA	4.25	1.45	1.33
38	V	601	CHL	CHC-C1C	4.25	1.47	1.39
38	U	601	CHL	CHC-C1C	4.24	1.47	1.39
29	B	854	LHG	O8-C23	4.24	1.45	1.33
38	X	607	CHL	O2A-CGA	4.24	1.45	1.33
38	Y	601	CHL	CHC-C1C	4.23	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	V	608	CHL	O2A-CGA	4.23	1.45	1.33
29	9	623	LHG	O8-C23	4.23	1.45	1.33
38	Y	609	CHL	O2A-CGA	4.22	1.45	1.33
38	W	601	CHL	CHC-C1C	4.22	1.47	1.39
33	H	205	LMG	O7-C10	4.22	1.46	1.34
38	V	606	CHL	CHC-C1C	4.22	1.47	1.39
38	W	609	CHL	CHC-C1C	4.22	1.47	1.39
38	X	606	CHL	CHD-C1D	4.21	1.46	1.39
38	U	607	CHL	CHC-C4B	4.21	1.46	1.39
38	X	601	CHL	O2A-CGA	4.21	1.45	1.33
38	Y	609	CHL	C3A-C2A	-4.21	1.51	1.54
38	W	609	CHL	O2A-CGA	4.21	1.45	1.33
29	8	623	LHG	O8-C23	4.21	1.45	1.33
33	J	103	LMG	O8-C28	4.21	1.45	1.33
38	Z	609	CHL	C3D-C2D	4.21	1.46	1.39
38	Y	608	CHL	CHB-C1B	4.20	1.46	1.39
38	X	609	CHL	O2A-CGA	4.20	1.45	1.33
29	5	625	LHG	O7-C7	4.19	1.46	1.34
29	2	622	LHG	O7-C7	4.19	1.46	1.34
34	B	850	DGD	O1G-C1A	4.19	1.45	1.33
38	X	608	CHL	O2A-CGA	4.19	1.45	1.33
38	X	607	CHL	CHB-C1B	4.19	1.46	1.39
38	U	601	CHL	O2A-CGA	4.19	1.45	1.33
38	W	609	CHL	CHB-C4A	-4.18	1.33	1.38
38	V	601	CHL	O2A-CGA	4.18	1.45	1.33
38	V	609	CHL	C3D-C2D	4.18	1.46	1.39
38	Z	607	CHL	CHD-C1D	4.18	1.46	1.39
29	9	624	LHG	O7-C7	4.17	1.46	1.34
33	H	205	LMG	O8-C28	4.17	1.45	1.33
29	9	622	LHG	O7-C7	4.17	1.46	1.34
38	Y	606	CHL	CHD-C1D	4.17	1.46	1.39
38	X	605	CHL	CHC-C1C	4.17	1.47	1.39
33	9	625	LMG	O8-C28	4.16	1.45	1.33
38	Y	605	CHL	CHC-C1C	4.16	1.47	1.39
38	V	605	CHL	CHB-C1B	4.16	1.46	1.39
29	A	847	LHG	O8-C23	4.15	1.45	1.33
29	B	854	LHG	O7-C7	4.15	1.46	1.34
38	U	608	CHL	CHD-C4C	4.15	1.47	1.39
29	8	622	LHG	O7-C7	4.15	1.46	1.34
29	4	622	LHG	O7-C7	4.15	1.46	1.34
38	Z	601	CHL	CHC-C1C	4.15	1.47	1.39
38	Z	608	CHL	CHC-C1C	4.14	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	U	609	CHL	CHB-C4A	-4.14	1.33	1.38
33	A	860	LMG	O8-C28	4.14	1.45	1.33
33	A	860	LMG	O7-C10	4.14	1.46	1.34
38	W	609	CHL	C3D-C2D	4.14	1.46	1.39
38	X	608	CHL	C3A-C2A	-4.14	1.51	1.54
38	Z	605	CHL	CHC-C1C	4.13	1.47	1.39
38	Y	609	CHL	C3D-C2D	4.13	1.46	1.39
29	U	2630	LHG	O7-C7	4.13	1.45	1.34
38	W	608	CHL	O2A-CGA	4.13	1.45	1.33
38	Y	601	CHL	O2A-CGA	4.12	1.45	1.33
29	5	625	LHG	O8-C23	4.12	1.45	1.33
29	9	622	LHG	O8-C23	4.12	1.45	1.33
38	X	609	CHL	CHB-C4A	-4.11	1.33	1.38
38	V	605	CHL	CHD-C1D	4.11	1.46	1.39
29	A	846	LHG	O8-C23	4.11	1.45	1.33
38	U	605	CHL	CHB-C1B	4.11	1.46	1.39
29	B	851	LHG	O7-C7	4.11	1.45	1.34
38	V	607	CHL	CHD-C1D	4.11	1.46	1.39
29	a	620	LHG	O7-C7	4.10	1.45	1.34
38	X	606	CHL	CHB-C1B	4.10	1.46	1.39
38	W	608	CHL	CHD-C4C	4.10	1.47	1.39
33	J	103	LMG	O7-C10	4.10	1.45	1.34
29	6	623	LHG	O8-C23	4.10	1.45	1.33
29	2	622	LHG	O8-C23	4.09	1.45	1.33
38	X	609	CHL	C3D-C2D	4.09	1.46	1.39
37	5	624	NEX	C7-C8	-4.09	1.25	1.31
29	1	620	LHG	O7-C7	4.09	1.45	1.34
38	Z	609	CHL	CHB-C4A	-4.09	1.33	1.38
38	Y	606	CHL	CHB-C1B	4.08	1.46	1.39
33	J	104	LMG	O7-C10	4.08	1.45	1.34
29	W	2630	LHG	O7-C7	4.08	1.45	1.34
29	4	622	LHG	O8-C23	4.07	1.45	1.33
29	8	623	LHG	O7-C7	4.07	1.45	1.34
33	4	624	LMG	O7-C10	4.07	1.45	1.34
33	5	627	LMG	O7-C10	4.07	1.45	1.34
29	5	623	LHG	O8-C23	4.07	1.45	1.33
33	4	623	LMG	O7-C10	4.07	1.45	1.34
29	5	623	LHG	O7-C7	4.06	1.45	1.34
29	3	623	LHG	O8-C23	4.06	1.45	1.33
38	U	608	CHL	CHC-C1C	4.06	1.47	1.39
29	3	624	LHG	O8-C23	4.06	1.45	1.33
33	L	2631	LMG	O7-C10	4.06	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	9	625	LMG	O7-C10	4.06	1.45	1.34
29	7	622	LHG	O8-C23	4.06	1.45	1.33
38	V	608	CHL	CHB-C1B	4.05	1.46	1.39
29	Z	2630	LHG	O7-C7	4.05	1.45	1.34
38	Y	607	CHL	C3A-C2A	-4.05	1.51	1.54
38	V	607	CHL	CHD-C4C	4.03	1.47	1.39
29	3	623	LHG	O7-C7	4.03	1.45	1.34
38	W	605	CHL	CHB-C1B	4.03	1.46	1.39
38	U	609	CHL	C3D-C2D	4.03	1.46	1.39
29	3	624	LHG	O7-C7	4.03	1.45	1.34
38	W	606	CHL	CHD-C4C	4.03	1.47	1.39
29	a	620	LHG	O8-C23	4.03	1.45	1.33
37	6	624	NEX	C7-C8	-4.02	1.25	1.31
38	Y	609	CHL	CHB-C4A	-4.02	1.33	1.38
33	V	2631	LMG	O7-C10	4.02	1.45	1.34
38	W	608	CHL	CHC-C1C	4.02	1.47	1.39
33	V	2631	LMG	O8-C28	4.02	1.45	1.33
38	U	606	CHL	CHD-C4C	4.02	1.47	1.39
29	W	2630	LHG	O8-C23	4.02	1.45	1.33
29	1	620	LHG	O8-C23	4.02	1.45	1.33
38	Z	606	CHL	CHC-C1C	4.01	1.47	1.39
29	H	204	LHG	O8-C23	4.00	1.45	1.33
29	O	2631	LHG	O7-C7	4.00	1.45	1.34
29	8	622	LHG	O8-C23	4.00	1.45	1.33
38	W	607	CHL	C3D-C2D	4.00	1.46	1.39
38	U	608	CHL	CHB-C1B	4.00	1.46	1.39
29	V	2630	LHG	O7-C7	4.00	1.45	1.34
29	U	2630	LHG	O8-C23	3.99	1.45	1.33
38	U	605	CHL	CHC-C1C	3.98	1.47	1.39
38	W	605	CHL	CHC-C1C	3.97	1.47	1.39
29	6	623	LHG	O7-C7	3.97	1.45	1.34
38	U	605	CHL	CHD-C1D	3.97	1.46	1.39
38	X	608	CHL	C3D-C2D	3.96	1.46	1.39
38	W	605	CHL	CHD-C4C	3.96	1.47	1.39
38	W	608	CHL	CHB-C1B	3.96	1.46	1.39
38	V	606	CHL	CHB-C1B	3.95	1.46	1.39
29	7	622	LHG	O7-C7	3.95	1.45	1.34
38	Z	601	CHL	C3D-C2D	3.95	1.46	1.39
29	H	204	LHG	O7-C7	3.94	1.45	1.34
29	A	847	LHG	O7-C7	3.94	1.45	1.34
38	V	609	CHL	C3A-C2A	-3.93	1.51	1.54
29	A	846	LHG	O7-C7	3.93	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	U	605	CHL	CHD-C4C	3.93	1.46	1.39
38	Y	607	CHL	C3D-C2D	3.91	1.46	1.39
34	B	850	DGD	O2G-C1B	3.91	1.45	1.34
38	U	606	CHL	CHC-C1C	3.90	1.46	1.39
38	V	606	CHL	CHD-C4C	3.90	1.46	1.39
38	W	606	CHL	CHC-C1C	3.90	1.46	1.39
38	V	608	CHL	CHD-C4C	3.89	1.46	1.39
38	Z	607	CHL	C3D-C2D	3.89	1.46	1.39
38	W	605	CHL	CHD-C1D	3.88	1.45	1.39
38	X	601	CHL	C3D-C2D	3.88	1.46	1.39
29	9	623	LHG	O7-C7	3.87	1.45	1.34
33	8	626	LMG	O7-C10	3.87	1.45	1.34
29	V	2630	LHG	O8-C23	3.85	1.44	1.33
38	V	601	CHL	C3D-C2D	3.84	1.46	1.39
38	Z	609	CHL	C3A-C2A	-3.84	1.51	1.54
38	V	607	CHL	CHC-C1C	3.83	1.46	1.39
38	W	601	CHL	C3D-C2D	3.83	1.46	1.39
38	U	607	CHL	CHC-C1C	3.82	1.46	1.39
38	V	606	CHL	OBD-CAD	3.82	1.27	1.22
38	X	607	CHL	C3D-C2D	3.82	1.46	1.39
38	U	601	CHL	C3D-C2D	3.81	1.46	1.39
38	U	607	CHL	CHB-C1B	3.80	1.45	1.39
38	U	607	CHL	CHD-C1D	3.80	1.45	1.39
37	Z	1623	NEX	C7-C6	-3.80	1.26	1.30
38	V	605	CHL	CHD-C4C	3.79	1.46	1.39
38	W	606	CHL	CHB-C1B	3.79	1.45	1.39
38	Y	601	CHL	C3D-C2D	3.78	1.46	1.39
38	U	608	CHL	CHD-C1D	3.78	1.45	1.39
38	U	607	CHL	CHD-C4C	3.77	1.46	1.39
38	W	608	CHL	CHD-C1D	3.76	1.45	1.39
38	U	606	CHL	CHB-C1B	3.75	1.45	1.39
38	V	608	CHL	CHD-C1D	3.74	1.45	1.39
38	W	607	CHL	C3A-C2A	-3.72	1.51	1.54
27	Z	604	CLA	C1D-ND	3.72	1.42	1.37
38	V	605	CHL	CHC-C1C	3.70	1.46	1.39
27	Z	612	CLA	C1D-ND	3.68	1.42	1.37
27	Z	614	CLA	C1D-ND	3.66	1.42	1.37
27	Y	614	CLA	C1D-ND	3.64	1.42	1.37
38	W	608	CHL	CHA-CBD	-3.64	1.47	1.51
27	X	610	CLA	C1D-ND	3.64	1.42	1.37
27	X	611	CLA	C1D-ND	3.63	1.42	1.37
27	U	604	CLA	CAD-C3D	-3.62	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	U	607	CHL	CHA-CBD	-3.61	1.47	1.51
38	V	608	CHL	CHC-C1C	3.61	1.46	1.39
27	Y	611	CLA	C1D-ND	3.61	1.42	1.37
27	Y	613	CLA	C1D-ND	3.60	1.42	1.37
27	Z	610	CLA	C1D-ND	3.60	1.42	1.37
27	X	602	CLA	C4B-NB	3.59	1.42	1.37
27	Y	610	CLA	C4B-NB	3.59	1.42	1.37
32	8	625	LMU	O5'-C1'	3.58	1.51	1.41
27	Y	610	CLA	C1D-ND	3.58	1.42	1.37
27	8	616	CLA	C1D-ND	3.58	1.42	1.37
27	X	612	CLA	C1D-ND	3.58	1.42	1.37
38	V	606	CHL	CHA-CBD	-3.58	1.47	1.51
27	X	610	CLA	C4B-NB	3.58	1.42	1.37
27	Y	612	CLA	C1D-ND	3.57	1.42	1.37
38	V	605	CHL	CHA-CBD	-3.57	1.47	1.51
28	A	844	PQN	C11-C12	3.56	1.56	1.50
27	Y	603	CLA	C1D-ND	3.56	1.42	1.37
27	Y	604	CLA	C1D-ND	3.56	1.42	1.37
27	X	603	CLA	C1D-ND	3.55	1.42	1.37
27	X	613	CLA	C1D-ND	3.54	1.42	1.37
38	W	606	CHL	CHD-C1D	3.53	1.45	1.39
27	X	614	CLA	C1D-ND	3.53	1.42	1.37
38	V	606	CHL	CHD-C1D	3.52	1.45	1.39
27	X	604	CLA	C1D-ND	3.51	1.42	1.37
27	5	619	CLA	C1D-ND	3.50	1.42	1.37
27	a	609	CLA	C1D-ND	3.50	1.42	1.37
27	O	2002	CLA	C1D-ND	3.50	1.42	1.37
27	1	609	CLA	C1D-ND	3.50	1.42	1.37
38	W	606	CHL	CHA-CBD	-3.49	1.47	1.51
38	U	606	CHL	CHD-C1D	3.49	1.45	1.39
27	Z	603	CLA	C1D-ND	3.49	1.42	1.37
27	Y	602	CLA	C4B-NB	3.49	1.42	1.37
38	U	608	CHL	CHA-CBD	-3.48	1.47	1.51
27	Z	613	CLA	C1D-ND	3.47	1.42	1.37
32	5	629	LMU	O5B-C1B	3.47	1.50	1.41
38	U	606	CHL	CHA-CBD	-3.47	1.47	1.51
27	Y	613	CLA	C4B-NB	3.47	1.42	1.37
27	K	206	CLA	C1D-ND	3.46	1.42	1.37
27	4	616	CLA	C1D-ND	3.46	1.42	1.37
27	Y	604	CLA	C4B-NB	3.46	1.42	1.37
27	7	615	CLA	C1D-ND	3.46	1.42	1.37
27	X	613	CLA	C4B-NB	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	612	CLA	C4B-NB	3.46	1.42	1.37
38	V	608	CHL	CHA-CBD	-3.46	1.47	1.51
27	8	616	CLA	C4B-NB	3.45	1.42	1.37
27	Z	602	CLA	C4B-NB	3.45	1.42	1.37
38	V	607	CHL	CHB-C1B	3.44	1.45	1.39
27	9	612	CLA	C1D-ND	3.44	1.42	1.37
32	5	628	LMU	O5B-C1B	3.44	1.50	1.41
27	X	604	CLA	C4B-NB	3.43	1.42	1.37
27	9	601	CLA	C1D-ND	3.43	1.42	1.37
27	Z	611	CLA	C1D-ND	3.43	1.42	1.37
27	4	612	CLA	C1D-ND	3.43	1.42	1.37
27	H	202	CLA	C1D-ND	3.42	1.42	1.37
27	A	808	CLA	C1D-ND	3.42	1.42	1.37
27	F	303	CLA	C4B-NB	3.41	1.42	1.37
32	K	208	LMU	O5'-C1'	3.40	1.50	1.41
27	a	616	CLA	C1D-ND	3.40	1.42	1.37
27	9	611	CLA	C1D-ND	3.39	1.42	1.37
27	3	611	CLA	C1D-ND	3.39	1.42	1.37
27	4	614	CLA	C1D-ND	3.38	1.42	1.37
32	1	621	LMU	O5'-C1'	3.38	1.50	1.41
28	B	842	PQN	C11-C12	3.38	1.55	1.50
27	G	204	CLA	C1D-ND	3.37	1.42	1.37
27	6	612	CLA	C1D-ND	3.37	1.42	1.37
27	X	603	CLA	C4B-NB	3.37	1.42	1.37
27	3	609	CLA	C1D-ND	3.36	1.42	1.37
27	4	604	CLA	C1D-ND	3.36	1.42	1.37
27	a	614	CLA	C1D-ND	3.36	1.42	1.37
27	K	204	CLA	C1D-ND	3.36	1.42	1.37
27	Y	611	CLA	C4B-NB	3.36	1.42	1.37
27	V	604	CLA	C1D-ND	3.36	1.42	1.37
27	Y	603	CLA	C4B-NB	3.35	1.42	1.37
27	F	304	CLA	C1D-ND	3.35	1.42	1.37
27	2	611	CLA	C1D-ND	3.35	1.42	1.37
27	5	611	CLA	C1D-ND	3.35	1.42	1.37
27	1	614	CLA	C1D-ND	3.35	1.42	1.37
27	Z	613	CLA	C4B-NB	3.35	1.42	1.37
27	9	607	CLA	C1D-ND	3.35	1.42	1.37
27	6	606	CLA	C1D-ND	3.34	1.42	1.37
27	2	601	CLA	C1D-ND	3.34	1.42	1.37
27	7	616	CLA	C1D-ND	3.34	1.42	1.37
27	6	608	CLA	C1D-ND	3.34	1.42	1.37
27	Y	614	CLA	C4B-NB	3.34	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	9	613	CLA	C1D-ND	3.34	1.42	1.37
27	J	101	CLA	C1D-ND	3.33	1.42	1.37
27	X	614	CLA	C4B-NB	3.33	1.42	1.37
27	X	611	CLA	C4B-NB	3.33	1.42	1.37
27	6	604	CLA	C1D-ND	3.33	1.42	1.37
27	2	614	CLA	C1D-ND	3.33	1.42	1.37
27	A	801	CLA	C1D-ND	3.32	1.42	1.37
27	6	618	CLA	C1D-ND	3.32	1.42	1.37
27	K	203	CLA	C1D-ND	3.32	1.42	1.37
27	4	616	CLA	C4B-NB	3.32	1.42	1.37
27	Y	612	CLA	C4B-NB	3.32	1.42	1.37
27	3	607	CLA	C1D-ND	3.31	1.42	1.37
27	8	612	CLA	C1D-ND	3.31	1.42	1.37
32	A	858	LMU	O5'-C1'	3.31	1.50	1.41
27	L	307	CLA	C1D-ND	3.31	1.42	1.37
27	X	612	CLA	C4B-NB	3.30	1.42	1.37
27	6	601	CLA	C1D-ND	3.30	1.42	1.37
27	1	609	CLA	CAB-C3B	-3.30	1.44	1.50
27	H	203	CLA	C1D-ND	3.29	1.42	1.37
27	5	607	CLA	C1D-ND	3.29	1.42	1.37
27	O	2003	CLA	C1D-ND	3.29	1.42	1.37
27	5	601	CLA	C1D-ND	3.29	1.42	1.37
27	3	615	CLA	C1D-ND	3.29	1.42	1.37
27	4	601	CLA	C1D-ND	3.29	1.42	1.37
27	a	610	CLA	C1D-ND	3.29	1.42	1.37
27	2	612	CLA	C1D-ND	3.29	1.42	1.37
27	B	811	CLA	CAD-C3D	-3.29	1.45	1.50
27	4	613	CLA	C1D-ND	3.29	1.42	1.37
27	Y	602	CLA	C1D-ND	3.29	1.42	1.37
27	9	603	CLA	CAB-C3B	-3.29	1.44	1.50
27	Z	602	CLA	C1D-ND	3.28	1.42	1.37
27	4	608	CLA	C1D-ND	3.28	1.42	1.37
27	5	604	CLA	C1D-ND	3.28	1.42	1.37
27	a	611	CLA	C1D-ND	3.28	1.42	1.37
27	3	612	CLA	C1D-ND	3.28	1.42	1.37
27	9	614	CLA	C1D-ND	3.28	1.42	1.37
27	X	602	CLA	C1D-ND	3.28	1.42	1.37
27	6	614	CLA	C1D-ND	3.28	1.42	1.37
27	Z	610	CLA	C4B-NB	3.28	1.42	1.37
27	5	614	CLA	C1D-ND	3.27	1.42	1.37
27	4	618	CLA	C1D-ND	3.27	1.42	1.37
27	1	611	CLA	C1D-ND	3.27	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	611	CLA	C1D-ND	3.27	1.42	1.37
27	5	618	CLA	C1D-ND	3.27	1.42	1.37
27	9	604	CLA	C1D-ND	3.27	1.42	1.37
27	1	614	CLA	CAB-C3B	-3.26	1.44	1.50
27	9	606	CLA	C1D-ND	3.26	1.42	1.37
27	6	603	CLA	C1D-ND	3.26	1.42	1.37
27	B	821	CLA	C1D-ND	3.26	1.42	1.37
27	2	604	CLA	C1D-ND	3.26	1.42	1.37
27	4	603	CLA	C1D-ND	3.26	1.42	1.37
27	2	607	CLA	C1D-ND	3.26	1.42	1.37
27	a	603	CLA	C1D-ND	3.26	1.42	1.37
27	Z	604	CLA	C4B-NB	3.26	1.42	1.37
27	1	612	CLA	C1D-ND	3.25	1.42	1.37
27	1	604	CLA	C1D-ND	3.25	1.42	1.37
27	2	616	CLA	C1D-ND	3.25	1.42	1.37
27	a	604	CLA	C1D-ND	3.25	1.42	1.37
27	B	840	CLA	C1D-ND	3.25	1.42	1.37
27	a	607	CLA	C1D-ND	3.25	1.42	1.37
27	a	612	CLA	C1D-ND	3.25	1.42	1.37
27	5	612	CLA	C1D-ND	3.25	1.42	1.37
27	4	609	CLA	C1D-ND	3.25	1.42	1.37
27	9	609	CLA	C1D-ND	3.24	1.42	1.37
27	6	613	CLA	C4B-NB	3.24	1.42	1.37
32	1	621	LMU	O5B-C1B	3.24	1.50	1.41
27	2	606	CLA	C1D-ND	3.24	1.42	1.37
27	W	604	CLA	C1D-ND	3.24	1.42	1.37
27	a	611	CLA	CAB-C3B	-3.24	1.44	1.50
27	5	603	CLA	CAB-C3B	-3.24	1.44	1.50
27	8	603	CLA	CAB-C3B	-3.23	1.44	1.50
27	U	604	CLA	C1D-ND	3.23	1.42	1.37
27	O	2002	CLA	CAB-C3B	-3.23	1.44	1.50
27	B	839	CLA	C1D-ND	3.23	1.42	1.37
27	3	608	CLA	C4B-NB	3.23	1.42	1.37
27	1	610	CLA	C1D-ND	3.22	1.42	1.37
27	6	618	CLA	CAB-C3B	-3.22	1.44	1.50
27	J	101	CLA	C4B-NB	3.22	1.42	1.37
27	6	611	CLA	C1D-ND	3.22	1.42	1.37
27	A	817	CLA	C1D-ND	3.22	1.42	1.37
27	A	845	CLA	C1D-ND	3.22	1.42	1.37
38	V	607	CHL	CHA-CBD	-3.22	1.47	1.51
27	B	817	CLA	C1D-ND	3.22	1.42	1.37
27	1	607	CLA	C1D-ND	3.22	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	857	LMU	O5B-C1B	3.21	1.50	1.41
27	F	303	CLA	C1D-ND	3.21	1.42	1.37
27	1	616	CLA	C1D-ND	3.21	1.42	1.37
27	8	607	CLA	CAB-C3B	-3.21	1.44	1.50
27	B	816	CLA	C1D-ND	3.21	1.42	1.37
27	B	831	CLA	C1D-ND	3.21	1.42	1.37
27	2	603	CLA	C1D-ND	3.21	1.42	1.37
27	5	604	CLA	CAB-C3B	-3.21	1.44	1.50
32	5	628	LMU	O5'-C1'	3.21	1.50	1.41
27	4	606	CLA	C1D-ND	3.21	1.42	1.37
27	3	617	CLA	C1D-ND	3.21	1.42	1.37
27	5	616	CLA	C1D-ND	3.21	1.42	1.37
27	O	2001	CLA	C1D-ND	3.20	1.42	1.37
27	1	601	CLA	C1D-ND	3.20	1.42	1.37
27	4	603	CLA	C4B-NB	3.20	1.42	1.37
27	Z	612	CLA	C4B-NB	3.20	1.42	1.37
27	6	607	CLA	CAB-C3B	-3.20	1.44	1.50
27	F	301	CLA	C4B-NB	3.20	1.42	1.37
27	5	606	CLA	C1D-ND	3.20	1.42	1.37
27	2	616	CLA	CAB-C3B	-3.20	1.44	1.50
27	5	619	CLA	CAB-C3B	-3.20	1.44	1.50
27	1	603	CLA	C1D-ND	3.20	1.42	1.37
27	1	613	CLA	C1D-ND	3.20	1.42	1.37
27	5	613	CLA	C1D-ND	3.20	1.42	1.37
27	1	616	CLA	CAB-C3B	-3.20	1.44	1.50
27	6	607	CLA	C1D-ND	3.20	1.42	1.37
27	Z	611	CLA	C4B-NB	3.20	1.42	1.37
27	4	603	CLA	CAB-C3B	-3.19	1.44	1.50
27	4	607	CLA	C1D-ND	3.19	1.42	1.37
27	3	606	CLA	C1D-ND	3.19	1.42	1.37
27	K	201	CLA	C1D-ND	3.19	1.42	1.37
32	K	208	LMU	O5B-C1B	3.19	1.50	1.41
27	G	203	CLA	C1D-ND	3.19	1.42	1.37
27	7	616	CLA	C4B-NB	3.19	1.42	1.37
27	6	603	CLA	CAB-C3B	-3.19	1.44	1.50
27	6	610	CLA	C4B-NB	3.19	1.42	1.37
27	7	609	CLA	C1D-ND	3.19	1.42	1.37
27	V	613	CLA	C1D-ND	3.19	1.42	1.37
27	A	824	CLA	C1D-ND	3.19	1.42	1.37
27	5	608	CLA	C1D-ND	3.19	1.42	1.37
32	A	858	LMU	O5B-C1B	3.18	1.50	1.41
27	7	615	CLA	CAB-C3B	-3.18	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	617	CLA	C1D-ND	3.18	1.42	1.37
27	7	613	CLA	C1D-ND	3.18	1.42	1.37
27	3	607	CLA	CAB-C3B	-3.18	1.44	1.50
27	4	610	CLA	C1D-ND	3.18	1.42	1.37
27	B	811	CLA	CAB-C3B	-3.17	1.44	1.50
27	B	805	CLA	C1D-ND	3.17	1.42	1.37
27	5	618	CLA	CAB-C3B	-3.17	1.44	1.50
27	6	616	CLA	C1D-ND	3.17	1.42	1.37
27	7	612	CLA	C1D-ND	3.17	1.42	1.37
27	B	840	CLA	C4B-NB	3.17	1.42	1.37
27	4	616	CLA	CAB-C3B	-3.17	1.44	1.50
27	A	832	CLA	C1D-ND	3.17	1.42	1.37
37	Y	1623	NEX	C7-C6	-3.16	1.27	1.30
27	3	614	CLA	C1D-ND	3.16	1.42	1.37
27	5	610	CLA	C1D-ND	3.16	1.42	1.37
27	A	812	CLA	C1D-ND	3.16	1.42	1.37
27	Z	614	CLA	C4B-NB	3.16	1.42	1.37
27	1	614	CLA	C4B-NB	3.16	1.42	1.37
27	9	610	CLA	C4B-NB	3.16	1.42	1.37
27	K	201	CLA	C4B-NB	3.16	1.42	1.37
27	O	2002	CLA	C4B-NB	3.16	1.42	1.37
27	8	607	CLA	C1D-ND	3.16	1.42	1.37
27	5	616	CLA	CAB-C3B	-3.16	1.44	1.50
27	2	609	CLA	C4B-NB	3.16	1.42	1.37
27	9	611	CLA	C4B-NB	3.16	1.42	1.37
27	B	818	CLA	C1D-ND	3.16	1.42	1.37
27	9	604	CLA	CAB-C3B	-3.16	1.44	1.50
27	8	601	CLA	C1D-ND	3.15	1.42	1.37
27	7	615	CLA	C4B-NB	3.15	1.42	1.37
27	B	812	CLA	C4B-NB	3.15	1.42	1.37
27	a	613	CLA	C1D-ND	3.15	1.42	1.37
27	1	606	CLA	C1D-ND	3.15	1.42	1.37
27	8	614	CLA	C1D-ND	3.15	1.42	1.37
27	9	606	CLA	C4B-NB	3.15	1.42	1.37
27	A	823	CLA	C1D-ND	3.15	1.42	1.37
27	a	608	CLA	C4B-NB	3.15	1.42	1.37
27	A	843	CLA	C4B-NB	3.15	1.42	1.37
27	a	606	CLA	C1D-ND	3.15	1.42	1.37
27	8	609	CLA	C1D-ND	3.15	1.42	1.37
27	B	815	CLA	C1D-ND	3.15	1.42	1.37
27	3	604	CLA	C1D-ND	3.15	1.42	1.37
27	A	835	CLA	C1D-ND	3.15	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	604	CLA	C4B-NB	3.15	1.42	1.37
27	3	611	CLA	CAB-C3B	-3.15	1.44	1.50
27	O	2003	CLA	C4B-NB	3.14	1.42	1.37
27	5	603	CLA	C1D-ND	3.14	1.42	1.37
27	A	820	CLA	C1D-ND	3.14	1.42	1.37
27	5	619	CLA	C4B-NB	3.14	1.42	1.37
27	7	616	CLA	CAB-C3B	-3.14	1.44	1.50
27	A	805	CLA	C1D-ND	3.14	1.42	1.37
27	A	806	CLA	C1D-ND	3.14	1.42	1.37
27	1	604	CLA	C4B-NB	3.14	1.42	1.37
27	8	613	CLA	C4B-NB	3.14	1.42	1.37
27	8	603	CLA	C1D-ND	3.14	1.42	1.37
27	8	613	CLA	C1D-ND	3.14	1.42	1.37
27	7	604	CLA	C1D-ND	3.14	1.42	1.37
27	A	804	CLA	C1D-ND	3.14	1.42	1.37
27	1	608	CLA	C1D-ND	3.14	1.42	1.37
27	4	604	CLA	CAB-C3B	-3.14	1.44	1.50
27	3	611	CLA	C4B-NB	3.13	1.42	1.37
27	7	603	CLA	C1D-ND	3.13	1.42	1.37
27	B	826	CLA	C1D-ND	3.13	1.42	1.37
27	8	608	CLA	C1D-ND	3.13	1.42	1.37
27	5	618	CLA	C4B-NB	3.13	1.42	1.37
27	4	618	CLA	CAB-C3B	-3.13	1.44	1.50
27	A	816	CLA	C1D-ND	3.13	1.42	1.37
27	A	821	CLA	C1D-ND	3.13	1.42	1.37
27	L	306	CLA	C1D-ND	3.13	1.42	1.37
27	6	602	CLA	C1D-ND	3.13	1.42	1.37
27	a	604	CLA	C4B-NB	3.13	1.42	1.37
38	Y	608	CHL	CHA-CBD	-3.13	1.48	1.51
27	a	601	CLA	C1D-ND	3.13	1.42	1.37
27	1	601	CLA	C4B-NB	3.13	1.42	1.37
27	A	818	CLA	C1D-ND	3.12	1.42	1.37
27	B	834	CLA	C1D-ND	3.12	1.42	1.37
27	2	616	CLA	C4B-NB	3.12	1.42	1.37
27	3	613	CLA	C1D-ND	3.12	1.42	1.37
38	X	606	CHL	CHA-CBD	-3.12	1.48	1.51
27	8	606	CLA	C1D-ND	3.12	1.42	1.37
27	A	814	CLA	C1D-ND	3.12	1.42	1.37
27	9	603	CLA	C1D-ND	3.12	1.42	1.37
27	B	812	CLA	C1D-ND	3.12	1.42	1.37
27	2	603	CLA	C4B-NB	3.11	1.42	1.37
27	B	822	CLA	C1D-ND	3.11	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	613	CLA	C1D-ND	3.11	1.42	1.37
32	A	857	LMU	O5'-C1'	3.11	1.49	1.41
27	B	837	CLA	C1D-ND	3.11	1.42	1.37
27	5	603	CLA	C4B-NB	3.11	1.41	1.37
27	A	825	CLA	C1D-ND	3.11	1.41	1.37
27	B	804	CLA	C1D-ND	3.11	1.41	1.37
27	B	823	CLA	C4B-NB	3.11	1.41	1.37
27	A	828	CLA	C1D-ND	3.11	1.41	1.37
27	6	614	CLA	C4B-NB	3.10	1.41	1.37
27	B	806	CLA	C1D-ND	3.10	1.41	1.37
27	A	834	CLA	C1D-ND	3.10	1.41	1.37
27	B	830	CLA	C1D-ND	3.10	1.41	1.37
27	4	618	CLA	C4B-NB	3.10	1.41	1.37
27	5	610	CLA	C4B-NB	3.10	1.41	1.37
32	5	629	LMU	O5'-C1'	3.10	1.49	1.41
27	G	203	CLA	C4B-NB	3.10	1.41	1.37
27	a	611	CLA	C4B-NB	3.10	1.41	1.37
27	B	832	CLA	C1D-ND	3.09	1.41	1.37
27	3	613	CLA	C4B-NB	3.09	1.41	1.37
27	7	611	CLA	C1D-ND	3.09	1.41	1.37
27	1	608	CLA	C4B-NB	3.09	1.41	1.37
27	3	614	CLA	C4B-NB	3.09	1.41	1.37
27	6	613	CLA	C1D-ND	3.09	1.41	1.37
27	B	802	CLA	C1D-ND	3.09	1.41	1.37
27	8	616	CLA	CAB-C3B	-3.09	1.44	1.50
27	a	608	CLA	C1D-ND	3.09	1.41	1.37
27	A	803	CLA	C1D-ND	3.09	1.41	1.37
27	4	611	CLA	C4B-NB	3.09	1.41	1.37
27	6	617	CLA	C1D-ND	3.09	1.41	1.37
27	6	609	CLA	C1D-ND	3.09	1.41	1.37
27	B	819	CLA	C1D-ND	3.09	1.41	1.37
27	G	204	CLA	C4B-NB	3.08	1.41	1.37
27	B	835	CLA	C1D-ND	3.08	1.41	1.37
27	B	809	CLA	C1D-ND	3.08	1.41	1.37
27	L	302	CLA	C1D-ND	3.08	1.41	1.37
27	8	604	CLA	C1D-ND	3.08	1.41	1.37
27	6	611	CLA	C4B-NB	3.07	1.41	1.37
27	6	620	CLA	C4B-NB	3.07	1.41	1.37
27	A	833	CLA	C1D-ND	3.07	1.41	1.37
27	3	603	CLA	C1D-ND	3.07	1.41	1.37
27	5	609	CLA	C1D-ND	3.07	1.41	1.37
27	a	614	CLA	C4B-NB	3.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	607	CLA	C1D-ND	3.07	1.41	1.37
27	A	838	CLA	C1D-ND	3.07	1.41	1.37
27	B	827	CLA	C1D-ND	3.06	1.41	1.37
32	8	625	LMU	O5B-C1B	3.06	1.49	1.41
27	V	611	CLA	C1D-ND	3.06	1.41	1.37
27	L	304	CLA	C1D-ND	3.06	1.41	1.37
27	K	206	CLA	C4B-NB	3.06	1.41	1.37
27	2	604	CLA	C4B-NB	3.06	1.41	1.37
27	6	610	CLA	C1D-ND	3.06	1.41	1.37
27	2	609	CLA	C1D-ND	3.06	1.41	1.37
27	B	811	CLA	C1D-ND	3.06	1.41	1.37
38	Y	606	CHL	CHA-CBD	-3.06	1.48	1.51
27	A	823	CLA	C4B-NB	3.06	1.41	1.37
27	1	611	CLA	C4B-NB	3.05	1.41	1.37
27	3	610	CLA	C1D-ND	3.05	1.41	1.37
27	7	601	CLA	C1D-ND	3.05	1.41	1.37
27	B	808	CLA	C4B-NB	3.05	1.41	1.37
27	W	612	CLA	C1D-ND	3.04	1.41	1.37
27	A	842	CLA	C1D-ND	3.04	1.41	1.37
27	1	613	CLA	C4B-NB	3.04	1.41	1.37
38	Z	606	CHL	CHA-CBD	-3.04	1.48	1.51
27	7	610	CLA	C1D-ND	3.04	1.41	1.37
27	a	613	CLA	C4B-NB	3.04	1.41	1.37
27	1	610	CLA	C4B-NB	3.04	1.41	1.37
27	B	833	CLA	C4B-NB	3.04	1.41	1.37
27	3	610	CLA	C4B-NB	3.04	1.41	1.37
27	8	607	CLA	C4B-NB	3.04	1.41	1.37
27	B	810	CLA	C4B-NB	3.04	1.41	1.37
27	H	203	CLA	C4B-NB	3.04	1.41	1.37
27	2	611	CLA	C4B-NB	3.04	1.41	1.37
27	5	614	CLA	C4B-NB	3.04	1.41	1.37
27	7	604	CLA	C4B-NB	3.04	1.41	1.37
27	A	837	CLA	C1D-ND	3.04	1.41	1.37
27	a	607	CLA	C4B-NB	3.03	1.41	1.37
27	4	614	CLA	C4B-NB	3.03	1.41	1.37
27	U	610	CLA	C4B-NB	3.03	1.41	1.37
27	6	602	CLA	C4B-NB	3.03	1.41	1.37
27	A	840	CLA	C1D-ND	3.03	1.41	1.37
27	B	841	CLA	C4B-NB	3.03	1.41	1.37
27	4	602	CLA	C1D-ND	3.03	1.41	1.37
27	9	614	CLA	C4B-NB	3.03	1.41	1.37
27	A	809	CLA	C1D-ND	3.02	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	612	CLA	C4B-NB	3.02	1.41	1.37
27	4	613	CLA	C4B-NB	3.02	1.41	1.37
27	W	614	CLA	C1D-ND	3.02	1.41	1.37
27	L	302	CLA	C4B-NB	3.02	1.41	1.37
27	a	610	CLA	C4B-NB	3.02	1.41	1.37
27	A	813	CLA	C1D-ND	3.02	1.41	1.37
27	A	821	CLA	C4B-NB	3.02	1.41	1.37
27	4	602	CLA	C4B-NB	3.02	1.41	1.37
27	U	614	CLA	C1D-ND	3.02	1.41	1.37
27	9	613	CLA	C4B-NB	3.02	1.41	1.37
27	3	608	CLA	CMB-C2B	-3.01	1.44	1.50
27	4	606	CLA	C4B-NB	3.01	1.41	1.37
27	5	611	CLA	C4B-NB	3.01	1.41	1.37
27	A	826	CLA	C1D-ND	3.01	1.41	1.37
27	F	304	CLA	C4B-NB	3.01	1.41	1.37
27	B	825	CLA	C1D-ND	3.01	1.41	1.37
27	a	601	CLA	C4B-NB	3.01	1.41	1.37
27	U	612	CLA	C1D-ND	3.01	1.41	1.37
27	6	606	CLA	C4B-NB	3.00	1.41	1.37
27	9	602	CLA	C1D-ND	3.00	1.41	1.37
27	7	614	CLA	C1D-ND	3.00	1.41	1.37
27	9	610	CLA	C1D-ND	3.00	1.41	1.37
27	B	835	CLA	C4B-NB	3.00	1.41	1.37
27	6	608	CLA	C4B-NB	3.00	1.41	1.37
27	6	618	CLA	C4B-NB	2.99	1.41	1.37
27	B	819	CLA	C4B-NB	2.99	1.41	1.37
27	2	610	CLA	C4B-NB	2.99	1.41	1.37
27	B	838	CLA	C1D-ND	2.99	1.41	1.37
27	a	606	CLA	C4B-NB	2.99	1.41	1.37
27	9	601	CLA	C4B-NB	2.99	1.41	1.37
27	B	803	CLA	C1D-ND	2.99	1.41	1.37
27	A	843	CLA	C1D-ND	2.99	1.41	1.37
27	3	615	CLA	C4B-NB	2.99	1.41	1.37
27	6	603	CLA	C4B-NB	2.99	1.41	1.37
27	8	610	CLA	C1D-ND	2.99	1.41	1.37
27	B	811	CLA	C4B-NB	2.99	1.41	1.37
27	V	603	CLA	C1D-ND	2.99	1.41	1.37
27	A	829	CLA	C1D-ND	2.99	1.41	1.37
27	3	602	CLA	C1D-ND	2.99	1.41	1.37
27	A	810	CLA	C1D-ND	2.99	1.41	1.37
27	A	827	CLA	C1D-ND	2.99	1.41	1.37
27	B	837	CLA	C4B-NB	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	612	CLA	C4B-NB	2.99	1.41	1.37
27	5	612	CLA	C4B-NB	2.99	1.41	1.37
27	6	604	CLA	C4B-NB	2.99	1.41	1.37
27	A	812	CLA	C4B-NB	2.99	1.41	1.37
27	B	830	CLA	C4B-NB	2.98	1.41	1.37
27	V	610	CLA	C1D-ND	2.98	1.41	1.37
27	6	617	CLA	C4B-NB	2.98	1.41	1.37
27	L	306	CLA	C4B-NB	2.98	1.41	1.37
27	2	614	CLA	C4B-NB	2.98	1.41	1.37
27	9	604	CLA	C4B-NB	2.98	1.41	1.37
27	8	614	CLA	C4B-NB	2.98	1.41	1.37
27	1	612	CLA	C4B-NB	2.98	1.41	1.37
27	9	603	CLA	C4B-NB	2.98	1.41	1.37
27	9	609	CLA	C4B-NB	2.98	1.41	1.37
27	9	612	CLA	C4B-NB	2.98	1.41	1.37
27	4	604	CLA	C4B-NB	2.98	1.41	1.37
27	8	612	CLA	C4B-NB	2.97	1.41	1.37
35	7	619	LUT	C22-C21	-2.97	1.51	1.54
27	B	813	CLA	C1D-ND	2.97	1.41	1.37
27	A	837	CLA	C4B-NB	2.97	1.41	1.37
27	L	307	CLA	C4B-NB	2.97	1.41	1.37
27	8	602	CLA	C1D-ND	2.97	1.41	1.37
27	W	611	CLA	C1D-ND	2.97	1.41	1.37
27	7	606	CLA	C1D-ND	2.97	1.41	1.37
27	B	833	CLA	C1D-ND	2.97	1.41	1.37
27	7	612	CLA	C4B-NB	2.97	1.41	1.37
27	1	609	CLA	C4B-NB	2.97	1.41	1.37
27	8	611	CLA	C1D-ND	2.97	1.41	1.37
27	A	839	CLA	C1D-ND	2.97	1.41	1.37
27	K	203	CLA	C4B-NB	2.97	1.41	1.37
27	8	610	CLA	C4B-NB	2.97	1.41	1.37
27	8	611	CLA	C4B-NB	2.96	1.41	1.37
27	O	2001	CLA	C4B-NB	2.96	1.41	1.37
27	4	612	CLA	C4B-NB	2.96	1.41	1.37
27	7	608	CLA	C1D-ND	2.96	1.41	1.37
27	B	836	CLA	C1D-ND	2.96	1.41	1.37
27	5	616	CLA	C4B-NB	2.96	1.41	1.37
27	B	829	CLA	C1D-ND	2.96	1.41	1.37
27	6	607	CLA	C4B-NB	2.95	1.41	1.37
27	B	832	CLA	C4B-NB	2.95	1.41	1.37
27	U	611	CLA	C1D-ND	2.95	1.41	1.37
27	B	808	CLA	C1D-ND	2.95	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	L	303	CLA	C1D-ND	2.95	1.41	1.37
27	6	620	CLA	C1D-ND	2.95	1.41	1.37
27	A	811	CLA	C1D-ND	2.95	1.41	1.37
27	A	805	CLA	C4B-NB	2.95	1.41	1.37
27	Z	603	CLA	C1B-C2B	2.95	1.50	1.43
27	7	614	CLA	C4B-NB	2.95	1.41	1.37
27	A	826	CLA	C4B-NB	2.94	1.41	1.37
27	a	603	CLA	C4B-NB	2.94	1.41	1.37
27	a	609	CLA	C4B-NB	2.94	1.41	1.37
27	W	603	CLA	C1D-ND	2.94	1.41	1.37
38	U	607	CHL	CBD-CGD	-2.94	1.48	1.52
27	A	807	CLA	C1D-ND	2.94	1.41	1.37
27	1	606	CLA	C4B-NB	2.94	1.41	1.37
27	5	608	CLA	C4B-NB	2.94	1.41	1.37
27	A	816	CLA	C4B-NB	2.94	1.41	1.37
27	9	602	CLA	C4B-NB	2.94	1.41	1.37
27	U	603	CLA	C1D-ND	2.94	1.41	1.37
27	5	613	CLA	C4B-NB	2.94	1.41	1.37
27	A	854	CLA	C4B-NB	2.93	1.41	1.37
27	Z	612	CLA	C1B-C2B	2.93	1.50	1.43
27	4	601	CLA	C4B-NB	2.93	1.41	1.37
27	6	612	CLA	C4B-NB	2.93	1.41	1.37
27	A	832	CLA	C4B-NB	2.93	1.41	1.37
27	7	611	CLA	C4B-NB	2.92	1.41	1.37
27	Z	603	CLA	C4B-NB	2.92	1.41	1.37
27	X	613	CLA	C1B-C2B	2.92	1.50	1.43
27	A	801	CLA	C4B-NB	2.92	1.41	1.37
27	B	828	CLA	C1D-ND	2.92	1.41	1.37
37	X	1623	NEX	C7-C6	-2.92	1.27	1.30
27	B	815	CLA	C4B-NB	2.92	1.41	1.37
37	V	1623	NEX	C7-C8	-2.92	1.27	1.31
27	3	603	CLA	C4B-NB	2.92	1.41	1.37
27	7	610	CLA	C4B-NB	2.92	1.41	1.37
27	3	602	CLA	C4B-NB	2.92	1.41	1.37
27	B	804	CLA	C4B-NB	2.91	1.41	1.37
27	A	819	CLA	C1D-ND	2.91	1.41	1.37
35	V	1620	LUT	C22-C21	-2.91	1.51	1.54
27	B	823	CLA	C1D-ND	2.91	1.41	1.37
27	A	854	CLA	C1D-ND	2.91	1.41	1.37
27	B	807	CLA	C1D-ND	2.91	1.41	1.37
27	B	824	CLA	C4B-NB	2.91	1.41	1.37
27	W	613	CLA	C1D-ND	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	839	CLA	C4B-NB	2.91	1.41	1.37
27	B	831	CLA	C4B-NB	2.90	1.41	1.37
27	B	820	CLA	C1D-ND	2.90	1.41	1.37
27	1	603	CLA	C4B-NB	2.90	1.41	1.37
27	1	607	CLA	C4B-NB	2.90	1.41	1.37
27	a	602	CLA	C1D-ND	2.90	1.41	1.37
27	B	826	CLA	C4B-NB	2.90	1.41	1.37
27	A	822	CLA	C1D-ND	2.89	1.41	1.37
27	3	609	CLA	C4B-NB	2.89	1.41	1.37
27	U	612	CLA	C4B-NB	2.89	1.41	1.37
27	L	304	CLA	C4B-NB	2.89	1.41	1.37
27	6	609	CLA	C4B-NB	2.89	1.41	1.37
27	U	604	CLA	C4B-NB	2.89	1.41	1.37
27	B	814	CLA	C1D-ND	2.89	1.41	1.37
27	H	202	CLA	C4B-NB	2.89	1.41	1.37
27	A	831	CLA	C4B-NB	2.89	1.41	1.37
27	5	602	CLA	C4B-NB	2.89	1.41	1.37
27	B	822	CLA	C4B-NB	2.89	1.41	1.37
27	B	816	CLA	C4B-NB	2.89	1.41	1.37
27	1	616	CLA	C4B-NB	2.89	1.41	1.37
27	2	602	CLA	C4B-NB	2.89	1.41	1.37
27	A	815	CLA	C1D-ND	2.89	1.41	1.37
27	4	609	CLA	C4B-NB	2.89	1.41	1.37
27	A	808	CLA	C4B-NB	2.89	1.41	1.37
27	F	301	CLA	C1D-ND	2.89	1.41	1.37
27	7	607	CLA	C4B-NB	2.89	1.41	1.37
27	A	830	CLA	C1D-ND	2.89	1.41	1.37
27	a	616	CLA	C4B-NB	2.88	1.41	1.37
38	Z	605	CHL	CHA-CBD	-2.88	1.48	1.51
27	5	606	CLA	C4B-NB	2.88	1.41	1.37
27	1	602	CLA	C1D-ND	2.88	1.41	1.37
27	2	602	CLA	C1D-ND	2.88	1.41	1.37
27	U	613	CLA	C1D-ND	2.88	1.41	1.37
27	A	836	CLA	C4B-NB	2.88	1.41	1.37
27	2	606	CLA	C4B-NB	2.88	1.41	1.37
27	Y	613	CLA	C1B-C2B	2.88	1.49	1.43
27	5	609	CLA	C4B-NB	2.88	1.41	1.37
27	7	606	CLA	C4B-NB	2.87	1.41	1.37
27	V	614	CLA	C1D-ND	2.87	1.41	1.37
27	A	824	CLA	C4B-NB	2.87	1.41	1.37
27	2	607	CLA	C4B-NB	2.87	1.41	1.37
27	A	831	CLA	C1D-ND	2.87	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	821	CLA	C4B-NB	2.87	1.41	1.37
27	3	608	CLA	C1D-ND	2.86	1.41	1.37
27	1	602	CLA	C4B-NB	2.86	1.41	1.37
27	L	303	CLA	C4B-NB	2.86	1.41	1.37
27	V	614	CLA	CMD-C2D	-2.86	1.44	1.50
27	2	613	CLA	C4B-NB	2.86	1.41	1.37
27	U	614	CLA	C4B-NB	2.86	1.41	1.37
27	7	608	CLA	C4B-NB	2.86	1.41	1.37
27	8	604	CLA	C4B-NB	2.86	1.41	1.37
27	A	810	CLA	C4B-NB	2.86	1.41	1.37
27	B	841	CLA	C1D-ND	2.86	1.41	1.37
27	5	601	CLA	C4B-NB	2.86	1.41	1.37
27	3	617	CLA	C4B-NB	2.86	1.41	1.37
27	W	610	CLA	C4B-NB	2.86	1.41	1.37
27	A	840	CLA	C4B-NB	2.86	1.41	1.37
27	6	601	CLA	C4B-NB	2.85	1.41	1.37
27	A	841	CLA	C1D-ND	2.85	1.41	1.37
27	B	838	CLA	C4B-NB	2.85	1.41	1.37
27	2	610	CLA	C1D-ND	2.85	1.41	1.37
27	8	602	CLA	C4B-NB	2.85	1.41	1.37
27	A	842	CLA	C4B-NB	2.85	1.41	1.37
27	7	613	CLA	C4B-NB	2.85	1.41	1.37
27	A	836	CLA	C1D-ND	2.85	1.41	1.37
27	A	822	CLA	C4B-NB	2.84	1.41	1.37
27	3	607	CLA	C4B-NB	2.84	1.41	1.37
27	4	610	CLA	C4B-NB	2.84	1.41	1.37
27	8	606	CLA	C4B-NB	2.84	1.41	1.37
27	W	604	CLA	C4B-NB	2.84	1.41	1.37
27	3	604	CLA	C4B-NB	2.84	1.41	1.37
27	8	608	CLA	C4B-NB	2.84	1.41	1.37
27	7	602	CLA	C1D-ND	2.84	1.41	1.37
37	Z	1623	NEX	C1-C6	-2.84	1.49	1.54
27	8	609	CLA	C4B-NB	2.84	1.41	1.37
27	A	818	CLA	C4B-NB	2.84	1.41	1.37
27	A	834	CLA	C4B-NB	2.84	1.41	1.37
27	A	841	CLA	C4B-NB	2.84	1.41	1.37
27	V	611	CLA	C4B-NB	2.84	1.41	1.37
27	W	614	CLA	C4B-NB	2.84	1.41	1.37
27	A	833	CLA	C4B-NB	2.84	1.41	1.37
27	A	811	CLA	C4B-NB	2.83	1.41	1.37
27	Z	611	CLA	C1B-C2B	2.83	1.49	1.43
27	B	814	CLA	C4B-NB	2.83	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	602	CLA	C4B-NB	2.83	1.41	1.37
27	B	839	CLA	C4B-NB	2.83	1.41	1.37
27	4	608	CLA	C4B-NB	2.82	1.41	1.37
27	B	820	CLA	C4B-NB	2.82	1.41	1.37
27	B	829	CLA	C4B-NB	2.82	1.41	1.37
27	A	815	CLA	C4B-NB	2.82	1.41	1.37
27	Z	613	CLA	C1B-C2B	2.82	1.49	1.43
27	2	601	CLA	C4B-NB	2.82	1.41	1.37
27	B	836	CLA	C4B-NB	2.82	1.41	1.37
27	B	810	CLA	C1D-ND	2.82	1.41	1.37
27	4	607	CLA	C4B-NB	2.82	1.41	1.37
27	7	609	CLA	C4B-NB	2.81	1.41	1.37
27	9	607	CLA	C4B-NB	2.81	1.41	1.37
27	A	845	CLA	C4B-NB	2.81	1.41	1.37
38	Z	608	CHL	CHA-CBD	-2.81	1.48	1.51
27	Y	604	CLA	C1B-C2B	2.81	1.49	1.43
27	6	616	CLA	C4B-NB	2.81	1.41	1.37
27	4	601	CLA	C1B-C2B	2.81	1.49	1.43
37	U	1623	NEX	C7-C8	-2.81	1.27	1.31
27	B	818	CLA	C4B-NB	2.81	1.41	1.37
27	B	807	CLA	C4B-NB	2.80	1.41	1.37
27	V	602	CLA	CMD-C2D	-2.80	1.45	1.50
27	A	807	CLA	C4B-NB	2.80	1.41	1.37
27	W	612	CLA	C4B-NB	2.80	1.41	1.37
27	A	817	CLA	C4B-NB	2.80	1.41	1.37
27	B	813	CLA	C4B-NB	2.80	1.41	1.37
27	B	825	CLA	C4B-NB	2.80	1.41	1.37
37	W	1623	NEX	C7-C6	-2.80	1.27	1.30
27	5	602	CLA	C1D-ND	2.80	1.41	1.37
27	8	603	CLA	C4B-NB	2.79	1.41	1.37
27	A	813	CLA	C4B-NB	2.79	1.41	1.37
27	A	802	CLA	C4B-NB	2.79	1.41	1.37
27	7	602	CLA	C4B-NB	2.79	1.41	1.37
27	A	828	CLA	C4B-NB	2.79	1.41	1.37
27	U	613	CLA	C4B-NB	2.78	1.41	1.37
35	U	1620	LUT	C22-C21	-2.78	1.51	1.54
27	V	614	CLA	C4B-NB	2.77	1.41	1.37
27	V	604	CLA	C4B-NB	2.77	1.41	1.37
27	W	611	CLA	C4B-NB	2.77	1.41	1.37
27	K	204	CLA	C4B-NB	2.77	1.41	1.37
27	B	824	CLA	C1D-ND	2.77	1.41	1.37
27	X	604	CLA	C1B-C2B	2.76	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Y	614	CLA	C1B-C2B	2.76	1.49	1.43
27	2	610	CLA	CMD-C2D	-2.76	1.45	1.50
27	A	803	CLA	C4B-NB	2.76	1.41	1.37
27	B	828	CLA	CMD-C2D	-2.76	1.45	1.50
27	A	820	CLA	C4B-NB	2.76	1.41	1.37
27	5	611	CLA	C1B-C2B	2.75	1.49	1.43
27	A	835	CLA	C4B-NB	2.75	1.41	1.37
27	V	612	CLA	C1D-ND	2.75	1.41	1.37
27	V	604	CLA	CMB-C2B	-2.75	1.45	1.50
27	B	809	CLA	C4B-NB	2.75	1.41	1.37
35	5	620	LUT	C22-C21	-2.75	1.51	1.54
27	W	602	CLA	CMD-C2D	-2.75	1.45	1.50
27	3	604	CLA	C1B-C2B	2.75	1.49	1.43
38	W	605	CHL	CHA-CBD	-2.75	1.48	1.51
27	B	803	CLA	C4B-NB	2.74	1.41	1.37
37	W	1623	NEX	C7-C8	-2.74	1.27	1.31
27	B	802	CLA	C4B-NB	2.74	1.41	1.37
27	7	601	CLA	C4B-NB	2.74	1.41	1.37
27	A	829	CLA	C4B-NB	2.74	1.41	1.37
27	A	801	CLA	C1B-C2B	2.73	1.49	1.43
27	Y	603	CLA	C1B-C2B	2.73	1.49	1.43
27	A	832	CLA	CMB-C2B	-2.73	1.45	1.50
27	Z	604	CLA	C1B-C2B	2.73	1.49	1.43
35	W	1621	LUT	C22-C21	-2.73	1.51	1.54
27	X	603	CLA	C1B-C2B	2.73	1.49	1.43
27	X	611	CLA	C1B-C2B	2.73	1.49	1.43
27	A	814	CLA	C4B-NB	2.73	1.41	1.37
27	U	602	CLA	CMD-C2D	-2.73	1.45	1.50
37	Y	1623	NEX	C7-C8	-2.72	1.27	1.31
27	K	201	CLA	C1B-C2B	2.72	1.49	1.43
27	B	805	CLA	C4B-NB	2.72	1.41	1.37
27	2	613	CLA	C1B-C2B	2.72	1.49	1.43
27	3	606	CLA	C4B-NB	2.72	1.41	1.37
27	W	613	CLA	C4B-NB	2.72	1.41	1.37
35	V	1621	LUT	C22-C21	-2.72	1.51	1.54
27	U	610	CLA	C1D-ND	2.72	1.41	1.37
27	6	614	CLA	CMD-C2D	-2.72	1.45	1.50
27	A	840	CLA	CMD-C2D	-2.71	1.45	1.50
35	W	1620	LUT	C22-C21	-2.71	1.51	1.54
27	5	607	CLA	C4B-NB	2.71	1.41	1.37
27	X	614	CLA	C1B-C2B	2.71	1.49	1.43
27	B	827	CLA	C4B-NB	2.71	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	V	610	CLA	CMD-C2D	-2.71	1.45	1.50
27	5	619	CLA	C1B-C2B	2.71	1.49	1.43
27	B	828	CLA	C4B-NB	2.71	1.41	1.37
27	U	611	CLA	C4B-NB	2.70	1.41	1.37
27	8	616	CLA	C4B-C3B	2.70	1.49	1.43
27	Y	611	CLA	C1B-C2B	2.70	1.49	1.43
27	5	617	CLA	C1B-C2B	2.70	1.49	1.43
27	V	612	CLA	C4B-NB	2.70	1.41	1.37
27	A	815	CLA	C1B-C2B	2.70	1.49	1.43
27	B	806	CLA	C4B-NB	2.70	1.41	1.37
27	B	834	CLA	C4B-NB	2.70	1.41	1.37
27	H	202	CLA	C1B-C2B	2.70	1.49	1.43
27	A	802	CLA	C1D-ND	2.70	1.41	1.37
27	6	603	CLA	C1B-C2B	2.70	1.49	1.43
27	B	817	CLA	C4B-NB	2.69	1.41	1.37
27	F	301	CLA	CMD-C2D	-2.69	1.45	1.50
27	3	606	CLA	C1B-C2B	2.69	1.49	1.43
37	U	1623	NEX	C7-C6	-2.69	1.27	1.30
27	5	617	CLA	C4B-NB	2.69	1.41	1.37
27	W	613	CLA	C1B-C2B	2.69	1.49	1.43
27	Z	610	CLA	C1B-C2B	2.69	1.49	1.43
27	7	603	CLA	C4B-NB	2.68	1.41	1.37
27	A	825	CLA	C4B-NB	2.68	1.41	1.37
27	6	604	CLA	C1B-C2B	2.68	1.49	1.43
27	1	614	CLA	C4B-C3B	2.68	1.49	1.43
27	3	611	CLA	C1B-C2B	2.68	1.49	1.43
27	O	2001	CLA	C1B-C2B	2.68	1.49	1.43
27	7	616	CLA	C1B-C2B	2.68	1.49	1.43
27	8	604	CLA	C1B-C2B	2.68	1.49	1.43
27	8	601	CLA	C4B-NB	2.68	1.41	1.37
27	A	809	CLA	C4B-NB	2.68	1.41	1.37
27	8	603	CLA	C1B-C2B	2.67	1.49	1.43
37	X	1623	NEX	C7-C8	-2.67	1.27	1.31
27	8	616	CLA	C1B-C2B	2.67	1.49	1.43
27	4	609	CLA	C1B-C2B	2.67	1.49	1.43
27	9	604	CLA	C4B-C3B	2.67	1.49	1.43
35	3	618	LUT	C22-C21	-2.67	1.51	1.54
27	B	821	CLA	C3C-C4C	2.66	1.45	1.40
27	B	802	CLA	C1B-C2B	2.66	1.49	1.43
38	U	605	CHL	CHA-CBD	-2.66	1.48	1.51
27	W	603	CLA	C4B-NB	2.66	1.41	1.37
27	Z	614	CLA	C1B-C2B	2.66	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	1	617	LUT	C22-C21	-2.66	1.51	1.54
27	4	604	CLA	C1B-C2B	2.66	1.49	1.43
27	A	842	CLA	CMC-C2C	-2.66	1.45	1.50
27	X	612	CLA	C1B-C2B	2.65	1.49	1.43
27	U	603	CLA	CMD-C2D	-2.65	1.45	1.50
27	9	603	CLA	CMB-C2B	-2.65	1.45	1.50
27	O	2002	CLA	C1B-C2B	2.65	1.49	1.43
27	2	616	CLA	C1B-C2B	2.65	1.49	1.43
27	U	610	CLA	CMD-C2D	-2.65	1.45	1.50
27	W	603	CLA	CMD-C2D	-2.65	1.45	1.50
27	A	804	CLA	C1B-C2B	2.65	1.49	1.43
27	5	612	CLA	C1B-C2B	2.65	1.49	1.43
27	2	614	CLA	C1B-C2B	2.64	1.49	1.43
27	Z	602	CLA	C1B-C2B	2.64	1.49	1.43
27	Y	612	CLA	C1B-C2B	2.64	1.49	1.43
27	O	2003	CLA	C1B-C2B	2.64	1.49	1.43
27	L	307	CLA	C1B-C2B	2.64	1.49	1.43
27	a	609	CLA	C1B-C2B	2.64	1.49	1.43
27	4	612	CLA	C1B-C2B	2.64	1.49	1.43
27	2	603	CLA	CMB-C2B	-2.64	1.45	1.50
27	A	831	CLA	CMB-C2B	-2.64	1.45	1.50
27	Y	602	CLA	C1B-C2B	2.64	1.49	1.43
27	3	612	CLA	C3B-C4B	2.63	1.50	1.42
27	W	610	CLA	CMB-C2B	-2.63	1.45	1.50
27	B	815	CLA	C1B-C2B	2.63	1.49	1.43
27	4	607	CLA	C1B-C2B	2.63	1.49	1.43
27	7	616	CLA	C4B-C3B	2.63	1.49	1.43
27	9	601	CLA	C1B-C2B	2.63	1.49	1.43
27	A	830	CLA	C4B-NB	2.63	1.41	1.37
27	W	613	CLA	CMC-C2C	-2.63	1.45	1.50
35	U	1621	LUT	C22-C21	-2.63	1.51	1.54
27	4	616	CLA	C1B-C2B	2.62	1.49	1.43
27	V	602	CLA	C4B-NB	2.62	1.41	1.37
27	3	614	CLA	C1B-C2B	2.62	1.49	1.43
27	Y	610	CLA	C1B-C2B	2.62	1.49	1.43
27	8	607	CLA	C4B-C3B	2.62	1.49	1.43
27	V	612	CLA	CMB-C2B	-2.62	1.45	1.50
27	8	608	CLA	C1B-C2B	2.62	1.49	1.43
36	U	1622	XAT	O24-C25	-2.62	1.42	1.46
27	A	826	CLA	CMD-C2D	-2.62	1.45	1.50
27	9	613	CLA	C1B-C2B	2.62	1.49	1.43
27	U	604	CLA	CMB-C2B	-2.62	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	U	602	CLA	C4B-NB	2.62	1.41	1.37
27	1	609	CLA	C1B-C2B	2.62	1.49	1.43
27	B	832	CLA	C1B-C2B	2.61	1.49	1.43
27	1	602	CLA	C1B-C2B	2.61	1.49	1.43
27	4	618	CLA	C1B-C2B	2.61	1.49	1.43
27	9	612	CLA	C1B-C2B	2.61	1.49	1.43
27	2	610	CLA	C3B-C4B	2.61	1.50	1.42
27	1	612	CLA	C1B-C2B	2.61	1.49	1.43
27	5	619	CLA	C4B-C3B	2.61	1.49	1.43
27	A	804	CLA	CMD-C2D	-2.61	1.45	1.50
27	W	602	CLA	C1D-ND	2.61	1.41	1.37
27	7	615	CLA	C1B-C2B	2.61	1.49	1.43
30	A	850	BCR	C30-C25	-2.61	1.50	1.53
27	U	613	CLA	C1B-C2B	2.61	1.49	1.43
27	V	613	CLA	CMD-C2D	-2.61	1.45	1.50
27	8	610	CLA	CMD-C2D	-2.61	1.45	1.50
35	a	617	LUT	C22-C21	-2.60	1.51	1.54
27	A	804	CLA	C4B-NB	2.60	1.41	1.37
27	2	603	CLA	CMD-C2D	-2.60	1.45	1.50
27	A	840	CLA	C1B-C2B	2.60	1.49	1.43
27	1	608	CLA	C1B-C2B	2.60	1.49	1.43
27	Z	610	CLA	C3B-C4B	2.60	1.50	1.42
27	A	832	CLA	CMD-C2D	-2.60	1.45	1.50
27	6	618	CLA	C4B-C3B	2.60	1.49	1.43
27	U	614	CLA	CMD-C2D	-2.60	1.45	1.50
27	4	610	CLA	C1B-C2B	2.60	1.49	1.43
27	B	829	CLA	CMB-C2B	-2.60	1.45	1.50
27	5	604	CLA	C1B-C2B	2.60	1.49	1.43
27	A	836	CLA	CMB-C2B	-2.60	1.45	1.50
27	H	203	CLA	C1B-C2B	2.60	1.49	1.43
27	X	602	CLA	C1B-C2B	2.60	1.49	1.43
27	1	616	CLA	C4B-C3B	2.60	1.49	1.43
27	B	809	CLA	CMB-C2B	-2.59	1.45	1.50
27	6	607	CLA	C4B-C3B	2.59	1.49	1.43
36	W	1622	XAT	O24-C25	-2.59	1.42	1.46
27	6	620	CLA	C1B-C2B	2.59	1.49	1.43
27	3	615	CLA	CMB-C2B	-2.59	1.45	1.50
27	9	614	CLA	C1B-C2B	2.59	1.49	1.43
27	A	830	CLA	CMD-C2D	-2.59	1.45	1.50
27	7	608	CLA	C1B-C2B	2.59	1.49	1.43
27	3	607	CLA	C4B-C3B	2.59	1.49	1.43
27	5	617	CLA	CMB-C2B	-2.59	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	L	306	CLA	C1B-C2B	2.59	1.49	1.43
27	5	616	CLA	C1B-C2B	2.59	1.49	1.43
27	U	602	CLA	C1D-ND	2.59	1.41	1.37
27	O	2002	CLA	C4B-C3B	2.59	1.49	1.43
35	V	1621	LUT	C1-C6	-2.59	1.50	1.53
27	B	834	CLA	C1B-C2B	2.59	1.49	1.43
27	5	614	CLA	C1B-C2B	2.59	1.49	1.43
27	V	611	CLA	C1B-C2B	2.58	1.49	1.43
27	B	811	CLA	CMB-C2B	-2.58	1.45	1.50
27	U	613	CLA	CMC-C2C	-2.58	1.45	1.50
27	K	206	CLA	C1B-C2B	2.58	1.49	1.43
27	9	609	CLA	C1B-C2B	2.58	1.49	1.43
27	W	610	CLA	CMD-C2D	-2.58	1.45	1.50
27	6	612	CLA	C1B-C2B	2.58	1.49	1.43
27	4	603	CLA	C1B-C2B	2.58	1.49	1.43
27	4	608	CLA	C1B-C2B	2.58	1.49	1.43
27	7	602	CLA	CMD-C2D	-2.58	1.45	1.50
27	A	845	CLA	C1B-C2B	2.58	1.49	1.43
27	a	611	CLA	C4B-C3B	2.58	1.49	1.43
27	W	602	CLA	C4B-NB	2.58	1.41	1.37
27	9	611	CLA	C1B-C2B	2.58	1.49	1.43
27	5	603	CLA	C1B-C2B	2.57	1.49	1.43
27	A	827	CLA	C4B-NB	2.57	1.41	1.37
27	A	821	CLA	C1B-C2B	2.57	1.49	1.43
27	9	604	CLA	C1B-C2B	2.57	1.49	1.43
27	a	612	CLA	C1B-C2B	2.57	1.49	1.43
27	1	603	CLA	C1B-C2B	2.57	1.49	1.43
27	B	814	CLA	CMD-C2D	-2.57	1.45	1.50
27	U	603	CLA	C4B-NB	2.57	1.41	1.37
27	a	602	CLA	C1B-C2B	2.57	1.49	1.43
27	6	617	CLA	C1B-C2B	2.57	1.49	1.43
27	W	604	CLA	CMB-C2B	-2.57	1.45	1.50
27	7	615	CLA	C4B-C3B	2.57	1.49	1.43
27	U	610	CLA	CMB-C2B	-2.57	1.45	1.50
27	V	603	CLA	CMD-C2D	-2.56	1.45	1.50
27	B	830	CLA	CMB-C2B	-2.56	1.45	1.50
27	4	616	CLA	C4B-C3B	2.56	1.49	1.43
27	2	611	CLA	C1B-C2B	2.56	1.49	1.43
27	5	618	CLA	C4B-C3B	2.56	1.49	1.43
27	8	607	CLA	C1B-C2B	2.56	1.49	1.43
27	3	609	CLA	C1B-C2B	2.56	1.49	1.43
27	5	602	CLA	CMD-C2D	-2.56	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	V	610	CLA	CMC-C2C	-2.56	1.45	1.50
27	A	835	CLA	C1B-C2B	2.56	1.49	1.43
27	F	304	CLA	C1B-C2B	2.56	1.49	1.43
27	B	807	CLA	CMD-C2D	-2.56	1.45	1.50
27	5	604	CLA	C4B-C3B	2.56	1.49	1.43
27	X	610	CLA	C1B-C2B	2.56	1.49	1.43
27	V	614	CLA	CMB-C2B	-2.56	1.45	1.50
27	A	809	CLA	C1B-C2B	2.56	1.49	1.43
27	W	614	CLA	CMD-C2D	-2.55	1.45	1.50
27	6	614	CLA	C1B-C2B	2.55	1.49	1.43
27	5	616	CLA	C4B-C3B	2.55	1.49	1.43
27	B	822	CLA	C1B-C2B	2.55	1.49	1.43
27	K	204	CLA	C1B-C2B	2.55	1.49	1.43
27	A	810	CLA	CMD-C2D	-2.55	1.45	1.50
27	A	842	CLA	C1B-C2B	2.55	1.49	1.43
27	1	610	CLA	C3B-C4B	2.55	1.50	1.42
27	B	821	CLA	C1B-C2B	2.55	1.49	1.43
27	8	612	CLA	C1B-C2B	2.55	1.49	1.43
27	A	819	CLA	CMD-C2D	-2.55	1.45	1.50
27	B	840	CLA	C1B-C2B	2.55	1.49	1.43
27	1	616	CLA	C1B-C2B	2.55	1.49	1.43
27	A	801	CLA	CMD-C2D	-2.54	1.45	1.50
38	V	608	CHL	CBD-CGD	-2.54	1.49	1.52
27	A	806	CLA	C4B-NB	2.54	1.41	1.37
27	V	602	CLA	CMC-C2C	-2.54	1.45	1.50
27	3	610	CLA	CMD-C2D	-2.54	1.45	1.50
27	a	616	CLA	C1B-C2B	2.54	1.49	1.43
27	2	607	CLA	C1B-C2B	2.54	1.49	1.43
27	3	608	CLA	CMD-C2D	-2.54	1.45	1.50
27	V	603	CLA	CMB-C2B	-2.54	1.45	1.50
27	a	610	CLA	C3B-C4B	2.54	1.50	1.42
27	7	616	CLA	CMD-C2D	-2.54	1.45	1.50
27	A	825	CLA	C1B-C2B	2.54	1.49	1.43
27	8	601	CLA	CMD-C2D	-2.54	1.45	1.50
27	a	607	CLA	C1B-C2B	2.54	1.49	1.43
27	2	612	CLA	C1B-C2B	2.54	1.49	1.43
27	9	607	CLA	C1B-C2B	2.54	1.49	1.43
27	B	820	CLA	C1B-C2B	2.54	1.49	1.43
27	8	602	CLA	C1B-C2B	2.54	1.49	1.43
27	2	616	CLA	C4B-C3B	2.54	1.49	1.43
27	6	618	CLA	C1B-C2B	2.54	1.49	1.43
27	A	816	CLA	C1B-C2B	2.54	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	603	CLA	C1B-C2B	2.53	1.49	1.43
27	G	204	CLA	C1B-C2B	2.53	1.49	1.43
27	W	614	CLA	C1B-C2B	2.53	1.49	1.43
38	U	608	CHL	CBD-CGD	-2.53	1.49	1.52
27	6	601	CLA	C1B-C2B	2.53	1.49	1.43
27	a	601	CLA	C1B-C2B	2.53	1.49	1.43
27	G	203	CLA	C1B-C2B	2.53	1.49	1.43
38	W	608	CHL	CBD-CGD	-2.53	1.49	1.52
27	4	611	CLA	C1B-C2B	2.53	1.49	1.43
27	A	814	CLA	CMC-C2C	-2.53	1.45	1.50
27	7	602	CLA	C1B-C2B	2.53	1.49	1.43
27	8	606	CLA	C1B-C2B	2.53	1.49	1.43
27	B	824	CLA	CMD-C2D	-2.53	1.45	1.50
27	A	819	CLA	C4B-NB	2.53	1.41	1.37
27	4	618	CLA	C4B-C3B	2.53	1.49	1.43
27	B	817	CLA	CMB-C2B	-2.53	1.45	1.50
27	5	610	CLA	C3B-C4B	2.53	1.50	1.42
27	L	304	CLA	C1B-C2B	2.52	1.49	1.43
27	6	607	CLA	C1B-C2B	2.52	1.49	1.43
27	U	614	CLA	C1B-C2B	2.52	1.49	1.43
27	3	617	CLA	C1B-C2B	2.52	1.49	1.43
27	7	607	CLA	C1B-C2B	2.52	1.49	1.43
27	B	820	CLA	CMB-C2B	-2.52	1.45	1.50
27	B	811	CLA	C1B-C2B	2.52	1.49	1.43
27	V	613	CLA	C4B-NB	2.52	1.41	1.37
35	W	1621	LUT	C1-C6	-2.52	1.50	1.53
27	U	603	CLA	CMB-C2B	-2.52	1.45	1.50
27	6	606	CLA	C1B-C2B	2.52	1.49	1.43
27	2	602	CLA	C1B-C2B	2.52	1.49	1.43
27	8	601	CLA	C1B-C2B	2.52	1.49	1.43
27	7	603	CLA	C1B-C2B	2.52	1.49	1.43
27	W	603	CLA	CMB-C2B	-2.52	1.45	1.50
27	W	610	CLA	C1D-ND	2.52	1.41	1.37
27	3	607	CLA	C1B-C2B	2.52	1.49	1.43
27	8	611	CLA	C1B-C2B	2.52	1.49	1.43
27	1	604	CLA	C1B-C2B	2.51	1.49	1.43
27	3	609	CLA	CMB-C2B	-2.51	1.45	1.50
27	B	819	CLA	CMB-C2B	-2.51	1.45	1.50
27	6	610	CLA	CMD-C2D	-2.51	1.45	1.50
27	A	808	CLA	C1B-C2B	2.51	1.49	1.43
27	V	603	CLA	C4B-NB	2.51	1.41	1.37
27	5	603	CLA	CMB-C2B	-2.51	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	835	CLA	C1B-C2B	2.51	1.49	1.43
27	H	203	CLA	CMD-C2D	-2.51	1.45	1.50
27	a	608	CLA	C1B-C2B	2.50	1.49	1.43
27	7	612	CLA	C1B-C2B	2.50	1.49	1.43
27	B	836	CLA	CMD-C2D	-2.50	1.45	1.50
27	A	822	CLA	CMB-C2B	-2.50	1.45	1.50
27	Z	602	CLA	C3B-C4B	2.50	1.50	1.42
27	V	603	CLA	C1B-C2B	2.50	1.49	1.43
27	A	838	CLA	C4B-NB	2.50	1.41	1.37
27	5	606	CLA	C1B-C2B	2.50	1.49	1.43
27	U	611	CLA	C1B-C2B	2.50	1.49	1.43
27	a	606	CLA	C1B-C2B	2.50	1.49	1.43
27	A	815	CLA	CMC-C2C	-2.50	1.45	1.50
27	1	606	CLA	C1B-C2B	2.50	1.49	1.43
27	1	609	CLA	C4B-C3B	2.50	1.49	1.43
27	W	612	CLA	C1B-C2B	2.50	1.49	1.43
27	B	815	CLA	CMB-C2B	-2.50	1.45	1.50
27	5	602	CLA	C1B-C2B	2.50	1.49	1.43
27	a	604	CLA	C1B-C2B	2.50	1.49	1.43
27	A	806	CLA	C1B-C2B	2.50	1.49	1.43
27	V	611	CLA	CMD-C2D	-2.50	1.45	1.50
27	A	802	CLA	CMD-C2D	-2.50	1.45	1.50
38	V	605	CHL	CBD-CGD	-2.49	1.49	1.52
27	A	818	CLA	C1B-C2B	2.49	1.49	1.43
27	V	602	CLA	CMB-C2B	-2.49	1.45	1.50
27	A	811	CLA	C1B-C2B	2.49	1.49	1.43
28	A	844	PQN	C5-C4	2.49	1.53	1.48
27	A	842	CLA	CMD-C2D	-2.49	1.45	1.50
27	8	610	CLA	C3B-C4B	2.49	1.50	1.42
27	2	604	CLA	C1B-C2B	2.49	1.49	1.43
27	4	602	CLA	C1B-C2B	2.49	1.49	1.43
27	K	203	CLA	C1B-C2B	2.49	1.49	1.43
27	B	806	CLA	C1B-C2B	2.49	1.49	1.43
35	2	619	LUT	C22-C21	-2.49	1.51	1.54
27	A	834	CLA	C1B-C2B	2.49	1.49	1.43
27	V	611	CLA	CMC-C2C	-2.49	1.45	1.50
27	1	613	CLA	C1B-C2B	2.49	1.49	1.43
27	Y	602	CLA	C3B-C4B	2.49	1.50	1.42
27	7	601	CLA	CMD-C2D	-2.49	1.45	1.50
27	6	602	CLA	C1B-C2B	2.49	1.49	1.43
27	5	601	CLA	C1B-C2B	2.49	1.49	1.43
35	U	1621	LUT	C1-C6	-2.49	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	837	CLA	C1B-C2B	2.49	1.49	1.43
27	4	603	CLA	C4B-C3B	2.49	1.49	1.43
27	5	613	CLA	C1B-C2B	2.48	1.49	1.43
27	X	610	CLA	C3B-C4B	2.48	1.50	1.42
27	A	837	CLA	CMB-C2B	-2.48	1.45	1.50
27	A	816	CLA	CMD-C2D	-2.48	1.45	1.50
27	A	836	CLA	CMD-C2D	-2.48	1.45	1.50
27	7	611	CLA	C1B-C2B	2.48	1.49	1.43
27	B	812	CLA	CMB-C2B	-2.48	1.45	1.50
28	A	844	PQN	C10-C1	2.48	1.53	1.48
27	3	611	CLA	C4B-C3B	2.48	1.49	1.43
27	7	603	CLA	CMD-C2D	-2.48	1.45	1.50
27	U	602	CLA	CMC-C2C	-2.48	1.45	1.50
27	A	829	CLA	CMD-C2D	-2.48	1.45	1.50
27	1	611	CLA	CMB-C2B	-2.48	1.45	1.50
27	8	614	CLA	CMD-C2D	-2.48	1.45	1.50
27	A	822	CLA	CMD-C2D	-2.48	1.45	1.50
27	B	827	CLA	CMD-C2D	-2.48	1.45	1.50
27	1	607	CLA	C1B-C2B	2.48	1.48	1.43
27	W	611	CLA	C1B-C2B	2.48	1.48	1.43
27	B	839	CLA	C1B-C2B	2.48	1.48	1.43
27	B	816	CLA	C1B-C2B	2.48	1.48	1.43
27	2	606	CLA	C1B-C2B	2.48	1.48	1.43
27	B	835	CLA	CMD-C2D	-2.47	1.45	1.50
27	B	825	CLA	C1B-C2B	2.47	1.48	1.43
27	Y	610	CLA	C3B-C4B	2.47	1.49	1.42
27	B	803	CLA	C1B-C2B	2.47	1.48	1.43
27	3	603	CLA	CMD-C2D	-2.47	1.45	1.50
27	5	609	CLA	CMB-C2B	-2.47	1.45	1.50
27	9	603	CLA	C4B-C3B	2.47	1.48	1.43
27	7	610	CLA	C3B-C4B	2.47	1.49	1.42
27	4	606	CLA	C1B-C2B	2.47	1.48	1.43
27	B	820	CLA	CMD-C2D	-2.47	1.45	1.50
27	A	810	CLA	CMB-C2B	-2.47	1.45	1.50
27	A	835	CLA	CMD-C2D	-2.47	1.45	1.50
27	A	833	CLA	CMD-C2D	-2.47	1.45	1.50
27	A	820	CLA	C1B-C2B	2.47	1.48	1.43
27	1	614	CLA	C1B-C2B	2.47	1.48	1.43
27	A	823	CLA	C1B-C2B	2.47	1.48	1.43
27	5	618	CLA	C1B-C2B	2.47	1.48	1.43
27	B	836	CLA	CMB-C2B	-2.47	1.45	1.50
27	7	612	CLA	CMD-C2D	-2.47	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	614	CLA	C1B-C2B	2.47	1.48	1.43
27	8	603	CLA	C4B-C3B	2.47	1.48	1.43
27	6	620	CLA	CMD-C2D	-2.47	1.45	1.50
27	B	802	CLA	CMD-C2D	-2.47	1.45	1.50
27	B	814	CLA	C1B-C2B	2.47	1.48	1.43
27	4	614	CLA	C1B-C2B	2.46	1.48	1.43
27	Z	602	CLA	CHC-C1C	2.46	1.43	1.38
27	1	601	CLA	C1B-C2B	2.46	1.48	1.43
27	4	604	CLA	C4B-C3B	2.46	1.48	1.43
27	A	828	CLA	CMD-C2D	-2.46	1.45	1.50
27	A	839	CLA	C1B-C2B	2.46	1.48	1.43
27	B	837	CLA	CMB-C2B	-2.46	1.45	1.50
27	B	813	CLA	CMB-C2B	-2.46	1.45	1.50
27	B	841	CLA	CMD-C2D	-2.46	1.45	1.50
27	7	613	CLA	C1B-C2B	2.46	1.48	1.43
27	4	602	CLA	CMD-C2D	-2.46	1.45	1.50
27	U	612	CLA	C1B-C2B	2.46	1.48	1.43
27	5	609	CLA	CMD-C2D	-2.46	1.45	1.50
27	W	602	CLA	CMC-C2C	-2.46	1.45	1.50
27	A	812	CLA	CMD-C2D	-2.46	1.45	1.50
27	A	839	CLA	CMB-C2B	-2.46	1.45	1.50
27	a	611	CLA	CMB-C2B	-2.46	1.45	1.50
27	A	815	CLA	CMD-C2D	-2.46	1.45	1.50
27	X	602	CLA	C3B-C4B	2.46	1.49	1.42
27	V	612	CLA	CMD-C2D	-2.45	1.45	1.50
27	a	613	CLA	C1B-C2B	2.45	1.48	1.43
27	B	840	CLA	CMB-C2B	-2.45	1.45	1.50
27	8	602	CLA	CMD-C2D	-2.45	1.45	1.50
27	A	807	CLA	CMD-C2D	-2.45	1.45	1.50
27	B	808	CLA	C1B-C2B	2.45	1.48	1.43
27	2	601	CLA	C1B-C2B	2.45	1.48	1.43
27	3	613	CLA	C1B-C2B	2.45	1.48	1.43
27	8	614	CLA	C1B-C2B	2.45	1.48	1.43
27	B	828	CLA	CMB-C2B	-2.45	1.45	1.50
27	5	603	CLA	CMD-C2D	-2.45	1.45	1.50
27	B	823	CLA	CMD-C2D	-2.45	1.45	1.50
27	V	604	CLA	C1B-C2B	2.45	1.48	1.43
27	4	613	CLA	C1B-C2B	2.45	1.48	1.43
27	B	818	CLA	CMB-C2B	-2.45	1.45	1.50
27	A	842	CLA	CMB-C2B	-2.45	1.45	1.50
35	8	619	LUT	C22-C21	-2.45	1.51	1.54
27	A	806	CLA	CMD-C2D	-2.45	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	602	CLA	CMC-C2C	-2.45	1.45	1.50
27	B	818	CLA	C1B-C2B	2.45	1.48	1.43
27	B	804	CLA	CMD-C2D	-2.44	1.45	1.50
27	B	837	CLA	CMD-C2D	-2.44	1.45	1.50
27	A	827	CLA	CMD-C2D	-2.44	1.45	1.50
27	B	832	CLA	CMD-C2D	-2.44	1.45	1.50
27	8	603	CLA	CMB-C2B	-2.44	1.45	1.50
27	B	813	CLA	CMD-C2D	-2.44	1.45	1.50
27	A	812	CLA	C1B-C2B	2.44	1.48	1.43
30	A	852	BCR	C30-C25	-2.44	1.50	1.53
27	6	609	CLA	C1B-C2B	2.44	1.48	1.43
27	B	806	CLA	CMC-C2C	-2.44	1.45	1.50
38	W	607	CHL	CBD-CGD	-2.44	1.49	1.52
27	9	613	CLA	CMB-C2B	-2.44	1.45	1.50
27	Y	602	CLA	CHC-C1C	2.44	1.43	1.38
27	7	604	CLA	C1B-C2B	2.44	1.48	1.43
27	4	602	CLA	C3B-C4B	2.44	1.49	1.42
27	W	604	CLA	C1B-C2B	2.44	1.48	1.43
27	U	612	CLA	CMB-C2B	-2.44	1.45	1.50
27	B	834	CLA	CMD-C2D	-2.44	1.45	1.50
38	V	607	CHL	CBD-CGD	-2.44	1.49	1.52
27	A	824	CLA	C1B-C2B	2.44	1.48	1.43
27	5	609	CLA	C1B-C2B	2.44	1.48	1.43
27	W	612	CLA	CMB-C2B	-2.43	1.45	1.50
27	A	801	CLA	CMB-C2B	-2.43	1.45	1.50
27	a	616	CLA	CMD-C2D	-2.43	1.45	1.50
27	B	813	CLA	CMC-C2C	-2.43	1.45	1.50
27	U	602	CLA	CMB-C2B	-2.43	1.45	1.50
27	3	603	CLA	C1B-C2B	2.43	1.48	1.43
27	5	608	CLA	C1B-C2B	2.43	1.48	1.43
27	5	606	CLA	CMD-C2D	-2.43	1.45	1.50
27	7	609	CLA	C1B-C2B	2.43	1.48	1.43
27	9	602	CLA	C1B-C2B	2.43	1.48	1.43
27	W	602	CLA	CMB-C2B	-2.43	1.45	1.50
27	4	608	CLA	CMD-C2D	-2.43	1.45	1.50
27	L	302	CLA	CMB-C2B	-2.43	1.45	1.50
36	X	1622	XAT	O24-C25	-2.43	1.43	1.46
27	A	826	CLA	C3B-C4B	2.43	1.49	1.42
27	9	610	CLA	C1B-C2B	2.43	1.48	1.43
36	Y	1622	XAT	O24-C25	-2.43	1.43	1.46
27	A	831	CLA	CMD-C2D	-2.43	1.45	1.50
27	L	303	CLA	CMD-C2D	-2.43	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	V	613	CLA	C1B-C2B	2.42	1.48	1.43
27	8	611	CLA	CMD-C2D	-2.42	1.45	1.50
27	A	811	CLA	CMB-C2B	-2.42	1.45	1.50
27	A	814	CLA	CMD-C2D	-2.42	1.45	1.50
27	B	806	CLA	CMD-C2D	-2.42	1.45	1.50
27	B	838	CLA	CMD-C2D	-2.42	1.45	1.50
27	a	602	CLA	CMD-C2D	-2.42	1.45	1.50
27	1	602	CLA	CMD-C2D	-2.42	1.45	1.50
27	9	609	CLA	CMD-C2D	-2.42	1.45	1.50
27	F	303	CLA	C1B-C2B	2.42	1.48	1.43
27	A	817	CLA	C1B-C2B	2.42	1.48	1.43
27	7	613	CLA	CMD-C2D	-2.42	1.45	1.50
27	B	804	CLA	C1B-C2B	2.42	1.48	1.43
27	U	613	CLA	CMD-C2D	-2.42	1.45	1.50
27	A	821	CLA	CMD-C2D	-2.42	1.45	1.50
27	A	843	CLA	CMB-C2B	-2.42	1.45	1.50
27	A	835	CLA	CMB-C2B	-2.42	1.45	1.50
27	X	602	CLA	CHC-C1C	2.42	1.43	1.38
27	B	838	CLA	C1B-C2B	2.42	1.48	1.43
27	V	610	CLA	C4B-NB	2.42	1.41	1.37
27	2	609	CLA	CMB-C2B	-2.42	1.45	1.50
27	6	611	CLA	C1B-C2B	2.42	1.48	1.43
27	A	825	CLA	CMB-C2B	-2.42	1.45	1.50
27	A	854	CLA	C1B-C2B	2.42	1.48	1.43
27	U	604	CLA	C1B-C2B	2.42	1.48	1.43
27	3	602	CLA	CMD-C2D	-2.42	1.45	1.50
27	A	803	CLA	C1B-C2B	2.41	1.48	1.43
27	B	810	CLA	CMD-C2D	-2.41	1.45	1.50
27	B	826	CLA	CMD-C2D	-2.41	1.45	1.50
27	F	301	CLA	CMB-C2B	-2.41	1.45	1.50
27	B	819	CLA	CMD-C2D	-2.41	1.45	1.50
27	4	602	CLA	CMC-C2C	-2.41	1.45	1.50
27	B	807	CLA	C1B-C2B	2.41	1.48	1.43
27	3	614	CLA	CMD-C2D	-2.41	1.45	1.50
27	A	820	CLA	CMD-C2D	-2.41	1.45	1.50
27	B	831	CLA	C3B-C4B	2.41	1.49	1.42
27	8	613	CLA	CMB-C2B	-2.41	1.45	1.50
27	A	802	CLA	C3B-C4B	2.41	1.49	1.42
27	a	610	CLA	C1B-C2B	2.41	1.48	1.43
27	B	831	CLA	C1B-C2B	2.41	1.48	1.43
27	V	614	CLA	CMC-C2C	-2.41	1.45	1.50
27	6	603	CLA	C4B-C3B	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	606	CLA	C1B-C2B	2.41	1.48	1.43
27	V	613	CLA	CMC-C2C	-2.41	1.45	1.50
27	W	613	CLA	CMD-C2D	-2.41	1.45	1.50
27	7	611	CLA	CMC-C2C	-2.40	1.45	1.50
27	1	610	CLA	C1B-C2B	2.40	1.48	1.43
27	B	807	CLA	CMB-C2B	-2.40	1.45	1.50
27	V	610	CLA	CMB-C2B	-2.40	1.45	1.50
27	9	603	CLA	C1B-C2B	2.40	1.48	1.43
27	B	810	CLA	C3B-C4B	2.40	1.49	1.42
27	A	819	CLA	C1B-C2B	2.40	1.48	1.43
27	L	303	CLA	CMB-C2B	-2.40	1.45	1.50
27	6	613	CLA	C1B-C2B	2.40	1.48	1.43
27	3	604	CLA	CMD-C2D	-2.40	1.45	1.50
27	A	838	CLA	CMD-C2D	-2.40	1.45	1.50
27	B	821	CLA	CMD-C2D	-2.40	1.45	1.50
27	A	831	CLA	CMC-C2C	-2.40	1.45	1.50
27	A	817	CLA	CMD-C2D	-2.40	1.45	1.50
27	L	302	CLA	CMD-C2D	-2.40	1.45	1.50
27	2	606	CLA	CMB-C2B	-2.40	1.45	1.50
27	9	607	CLA	CMB-C2B	-2.40	1.45	1.50
27	A	843	CLA	CMD-C2D	-2.40	1.45	1.50
27	4	608	CLA	CMB-C2B	-2.40	1.45	1.50
27	8	609	CLA	CMD-C2D	-2.40	1.45	1.50
27	3	608	CLA	CMC-C2C	-2.40	1.45	1.50
27	7	609	CLA	CMD-C2D	-2.40	1.45	1.50
27	B	824	CLA	C1B-C2B	2.40	1.48	1.43
27	A	818	CLA	CMD-C2D	-2.40	1.45	1.50
27	B	834	CLA	CMB-C2B	-2.40	1.45	1.50
27	8	607	CLA	CMD-C2D	-2.40	1.45	1.50
27	5	603	CLA	C4B-C3B	2.39	1.48	1.43
27	9	602	CLA	CMD-C2D	-2.39	1.45	1.50
27	U	611	CLA	CMD-C2D	-2.39	1.45	1.50
27	A	830	CLA	C1B-C2B	2.39	1.48	1.43
27	3	602	CLA	C1B-C2B	2.39	1.48	1.43
27	A	822	CLA	CMC-C2C	-2.39	1.45	1.50
27	3	613	CLA	CMB-C2B	-2.39	1.45	1.50
27	U	612	CLA	CMD-C2D	-2.39	1.45	1.50
27	7	611	CLA	CMD-C2D	-2.39	1.45	1.50
27	8	609	CLA	C1B-C2B	2.39	1.48	1.43
27	2	602	CLA	CMD-C2D	-2.39	1.45	1.50
27	A	837	CLA	C1B-C2B	2.39	1.48	1.43
27	7	604	CLA	CMD-C2D	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	811	CLA	C4B-C3B	2.39	1.48	1.43
27	8	608	CLA	CMC-C2C	-2.39	1.45	1.50
27	V	603	CLA	CMC-C2C	-2.39	1.45	1.50
27	B	811	CLA	CMD-C2D	-2.39	1.45	1.50
27	1	612	CLA	CMD-C2D	-2.39	1.45	1.50
27	1	604	CLA	CMD-C2D	-2.39	1.45	1.50
27	9	610	CLA	CMC-C2C	-2.39	1.45	1.50
27	9	606	CLA	C1B-C2B	2.39	1.48	1.43
27	B	833	CLA	CMC-C2C	-2.39	1.45	1.50
27	5	614	CLA	CMD-C2D	-2.39	1.45	1.50
27	A	819	CLA	CMB-C2B	-2.39	1.45	1.50
27	K	206	CLA	CMB-C2B	-2.39	1.45	1.50
27	B	813	CLA	MG-NB	-2.39	2.01	2.05
27	6	603	CLA	CMD-C2D	-2.39	1.45	1.50
27	Z	614	CLA	C3B-C4B	2.39	1.49	1.42
27	9	610	CLA	C3B-C4B	2.39	1.49	1.42
27	F	304	CLA	CMD-C2D	-2.39	1.45	1.50
27	B	808	CLA	CMD-C2D	-2.39	1.45	1.50
27	6	601	CLA	CMD-C2D	-2.39	1.45	1.50
27	B	829	CLA	C1B-C2B	2.39	1.48	1.43
27	B	803	CLA	CMD-C2D	-2.38	1.45	1.50
27	B	833	CLA	CMD-C2D	-2.38	1.45	1.50
27	1	616	CLA	CMD-C2D	-2.38	1.45	1.50
27	7	608	CLA	CMB-C2B	-2.38	1.45	1.50
27	B	802	CLA	CMB-C2B	-2.38	1.45	1.50
27	A	845	CLA	CMB-C2B	-2.38	1.45	1.50
27	J	101	CLA	C1B-C2B	2.38	1.48	1.43
27	B	839	CLA	CMB-C2B	-2.38	1.45	1.50
27	9	603	CLA	CMD-C2D	-2.38	1.45	1.50
27	V	602	CLA	C1D-ND	2.38	1.41	1.37
27	B	836	CLA	C3B-C4B	2.38	1.49	1.42
27	A	813	CLA	C1B-C2B	2.38	1.48	1.43
27	7	614	CLA	C1B-C2B	2.38	1.48	1.43
27	7	614	CLA	CMB-C2B	-2.38	1.45	1.50
27	7	601	CLA	C1B-C2B	2.38	1.48	1.43
27	A	833	CLA	CMB-C2B	-2.38	1.45	1.50
27	L	303	CLA	C1B-C2B	2.38	1.48	1.43
27	A	824	CLA	CMD-C2D	-2.38	1.45	1.50
27	7	609	CLA	CMB-C2B	-2.38	1.45	1.50
27	Y	610	CLA	CHC-C1C	2.38	1.43	1.38
27	A	827	CLA	C1B-C2B	2.38	1.48	1.43
27	A	839	CLA	CMD-C2D	-2.38	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	822	CLA	CMD-C2D	-2.38	1.45	1.50
27	3	612	CLA	C1B-C2B	2.38	1.48	1.43
27	O	2003	CLA	CMD-C2D	-2.38	1.45	1.50
27	8	613	CLA	CMD-C2D	-2.38	1.45	1.50
27	2	604	CLA	CMD-C2D	-2.37	1.45	1.50
27	A	803	CLA	CMD-C2D	-2.37	1.45	1.50
27	3	606	CLA	CMD-C2D	-2.37	1.45	1.50
27	4	610	CLA	CMD-C2D	-2.37	1.45	1.50
27	A	805	CLA	C1B-C2B	2.37	1.48	1.43
27	B	830	CLA	CMD-C2D	-2.37	1.45	1.50
27	B	841	CLA	CMC-C2C	-2.37	1.45	1.50
27	1	611	CLA	C1B-C2B	2.37	1.48	1.43
27	B	833	CLA	C1B-C2B	2.37	1.48	1.43
27	U	604	CLA	CMD-C2D	-2.37	1.45	1.50
27	A	820	CLA	CMB-C2B	-2.37	1.45	1.50
27	B	840	CLA	CMD-C2D	-2.37	1.45	1.50
27	A	843	CLA	C3B-C4B	2.37	1.49	1.42
27	B	808	CLA	CMB-C2B	-2.37	1.45	1.50
27	8	613	CLA	C3B-C4B	2.37	1.49	1.42
27	W	612	CLA	CMD-C2D	-2.37	1.45	1.50
27	4	601	CLA	CMD-C2D	-2.37	1.45	1.50
27	9	610	CLA	CMD-C2D	-2.37	1.45	1.50
27	B	809	CLA	C1B-C2B	2.37	1.48	1.43
27	A	833	CLA	C1B-C2B	2.37	1.48	1.43
27	6	616	CLA	C1B-C2B	2.37	1.48	1.43
27	a	604	CLA	CMD-C2D	-2.37	1.45	1.50
37	V	1623	NEX	O24-C25	-2.37	1.43	1.46
27	V	613	CLA	CMB-C2B	-2.37	1.45	1.50
27	F	303	CLA	C3B-C4B	2.37	1.49	1.42
27	B	812	CLA	CMC-C2C	-2.37	1.45	1.50
27	A	822	CLA	C3B-C4B	2.37	1.49	1.42
27	B	818	CLA	CMD-C2D	-2.37	1.45	1.50
27	6	607	CLA	CMD-C2D	-2.36	1.45	1.50
27	9	602	CLA	C3B-C4B	2.36	1.49	1.42
27	8	603	CLA	CMD-C2D	-2.36	1.45	1.50
27	B	827	CLA	C1B-C2B	2.36	1.48	1.43
27	B	837	CLA	CMC-C2C	-2.36	1.45	1.50
27	4	606	CLA	CMB-C2B	-2.36	1.45	1.50
27	B	836	CLA	CMC-C2C	-2.36	1.45	1.50
27	3	603	CLA	CMC-C2C	-2.36	1.45	1.50
27	B	821	CLA	CMB-C2B	-2.36	1.45	1.50
27	K	203	CLA	CMD-C2D	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	840	CLA	CMB-C2B	-2.36	1.45	1.50
27	B	805	CLA	C1B-C2B	2.36	1.48	1.43
27	A	827	CLA	CMB-C2B	-2.36	1.45	1.50
27	6	609	CLA	CMB-C2B	-2.36	1.45	1.50
27	A	838	CLA	C1B-C2B	2.36	1.48	1.43
27	B	823	CLA	CMB-C2B	-2.36	1.45	1.50
27	A	828	CLA	C1B-C2B	2.36	1.48	1.43
38	V	606	CHL	CBD-CGD	-2.36	1.49	1.52
27	B	805	CLA	CMD-C2D	-2.36	1.45	1.50
30	4	621	BCR	C1-C6	-2.36	1.50	1.53
27	A	805	CLA	CMD-C2D	-2.36	1.45	1.50
27	O	2002	CLA	CMD-C2D	-2.36	1.45	1.50
27	1	602	CLA	CMB-C2B	-2.36	1.45	1.50
27	5	604	CLA	CMB-C2B	-2.36	1.45	1.50
27	6	601	CLA	CMB-C2B	-2.36	1.45	1.50
27	6	609	CLA	CMD-C2D	-2.35	1.45	1.50
27	8	614	CLA	CMB-C2B	-2.35	1.45	1.50
27	A	812	CLA	CMB-C2B	-2.35	1.45	1.50
27	3	612	CLA	CMD-C2D	-2.35	1.45	1.50
27	A	821	CLA	CMB-C2B	-2.35	1.45	1.50
27	B	810	CLA	CMB-C2B	-2.35	1.45	1.50
27	3	609	CLA	CMD-C2D	-2.35	1.45	1.50
27	3	610	CLA	C3B-C4B	2.35	1.49	1.42
27	A	803	CLA	CMB-C2B	-2.35	1.46	1.50
27	8	612	CLA	CMC-C2C	-2.35	1.46	1.50
36	a	618	XAT	O24-C25	-2.35	1.43	1.46
27	6	617	CLA	CMD-C2D	-2.35	1.46	1.50
27	A	807	CLA	CMB-C2B	-2.35	1.46	1.50
27	B	839	CLA	CMD-C2D	-2.35	1.46	1.50
36	V	1622	XAT	O4-C5	-2.35	1.43	1.46
27	U	614	CLA	CMB-C2B	-2.35	1.46	1.50
27	B	826	CLA	C1B-C2B	2.35	1.48	1.43
27	X	610	CLA	CHC-C1C	2.35	1.43	1.38
27	A	826	CLA	CMB-C2B	-2.35	1.46	1.50
27	A	807	CLA	CMC-C2C	-2.35	1.46	1.50
27	A	841	CLA	CMB-C2B	-2.35	1.46	1.50
27	4	609	CLA	CMD-C2D	-2.35	1.46	1.50
27	7	610	CLA	CMD-C2D	-2.35	1.46	1.50
27	1	602	CLA	CMC-C2C	-2.35	1.46	1.50
27	Z	604	CLA	C3B-C4B	2.35	1.49	1.42
27	A	811	CLA	CMD-C2D	-2.35	1.46	1.50
27	A	823	CLA	CMB-C2B	-2.35	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K	201	CLA	CMD-C2D	-2.35	1.46	1.50
27	L	304	CLA	CMD-C2D	-2.35	1.46	1.50
27	a	603	CLA	CMD-C2D	-2.35	1.46	1.50
27	2	610	CLA	C1B-C2B	2.35	1.48	1.43
27	B	825	CLA	CMD-C2D	-2.35	1.46	1.50
27	B	827	CLA	CMB-C2B	-2.35	1.46	1.50
27	4	603	CLA	CMD-C2D	-2.34	1.46	1.50
27	7	602	CLA	CMC-C2C	-2.34	1.46	1.50
27	W	603	CLA	C1B-C2B	2.34	1.48	1.43
27	A	820	CLA	CMC-C2C	-2.34	1.46	1.50
27	2	614	CLA	CMD-C2D	-2.34	1.46	1.50
27	8	608	CLA	CMD-C2D	-2.34	1.46	1.50
27	A	814	CLA	C1B-C2B	2.34	1.48	1.43
27	2	604	CLA	C3B-C4B	2.34	1.49	1.42
27	2	609	CLA	CMD-C2D	-2.34	1.46	1.50
27	W	611	CLA	CMD-C2D	-2.34	1.46	1.50
27	G	203	CLA	C3B-C4B	2.34	1.49	1.42
27	B	831	CLA	CMD-C2D	-2.34	1.46	1.50
27	9	604	CLA	CMD-C2D	-2.34	1.46	1.50
27	a	611	CLA	C1B-C2B	2.34	1.48	1.43
28	B	842	PQN	C5-C4	2.34	1.52	1.48
27	8	612	CLA	CMB-C2B	-2.34	1.46	1.50
27	A	823	CLA	CMD-C2D	-2.34	1.46	1.50
27	U	603	CLA	C1B-C2B	2.34	1.48	1.43
27	A	841	CLA	C1B-C2B	2.34	1.48	1.43
27	1	603	CLA	CMD-C2D	-2.34	1.46	1.50
27	F	301	CLA	C3B-C4B	2.34	1.49	1.42
27	A	809	CLA	CMD-C2D	-2.34	1.46	1.50
27	7	604	CLA	CMB-C2B	-2.34	1.46	1.50
27	B	829	CLA	CMD-C2D	-2.34	1.46	1.50
27	1	601	CLA	CMD-C2D	-2.34	1.46	1.50
27	6	603	CLA	CMB-C2B	-2.34	1.46	1.50
27	A	806	CLA	CMC-C2C	-2.34	1.46	1.50
27	A	806	CLA	CMB-C2B	-2.34	1.46	1.50
27	B	805	CLA	CMB-C2B	-2.34	1.46	1.50
27	6	604	CLA	CMD-C2D	-2.34	1.46	1.50
27	A	845	CLA	CMD-C2D	-2.34	1.46	1.50
27	5	618	CLA	CMB-C2B	-2.34	1.46	1.50
27	A	830	CLA	MG-NB	-2.34	2.01	2.05
27	6	602	CLA	CMC-C2C	-2.33	1.46	1.50
27	2	601	CLA	CMC-C2C	-2.33	1.46	1.50
27	A	836	CLA	C1B-C2B	2.33	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	W	1622	XAT	O4-C5	-2.33	1.43	1.46
27	A	831	CLA	C1B-C2B	2.33	1.48	1.43
27	A	854	CLA	CMD-C2D	-2.33	1.46	1.50
27	3	603	CLA	CMB-C2B	-2.33	1.46	1.50
27	a	612	CLA	CMD-C2D	-2.33	1.46	1.50
27	6	613	CLA	C3B-C4B	2.33	1.49	1.42
38	U	606	CHL	CBD-CGD	-2.33	1.49	1.52
27	5	613	CLA	CMB-C2B	-2.33	1.46	1.50
38	Y	607	CHL	CBD-CGD	-2.33	1.49	1.52
27	3	606	CLA	CMB-C2B	-2.33	1.46	1.50
27	3	617	CLA	CMD-C2D	-2.33	1.46	1.50
27	8	604	CLA	CMD-C2D	-2.33	1.46	1.50
27	A	802	CLA	CMC-C2C	-2.33	1.46	1.50
27	7	613	CLA	CMB-C2B	-2.33	1.46	1.50
27	W	614	CLA	CMB-C2B	-2.33	1.46	1.50
27	Y	611	CLA	C3B-C4B	2.33	1.49	1.42
27	A	810	CLA	C1B-C2B	2.33	1.48	1.43
27	B	836	CLA	C1B-C2B	2.33	1.48	1.43
27	B	816	CLA	CMB-C2B	-2.33	1.46	1.50
27	3	613	CLA	CMD-C2D	-2.33	1.46	1.50
27	7	612	CLA	CMB-C2B	-2.33	1.46	1.50
27	U	602	CLA	C1B-C2B	2.33	1.48	1.43
27	7	601	CLA	C3B-C4B	2.32	1.49	1.42
27	1	607	CLA	CMD-C2D	-2.32	1.46	1.50
35	6	619	LUT	C22-C21	-2.32	1.51	1.54
27	L	304	CLA	CMB-C2B	-2.32	1.46	1.50
27	A	834	CLA	CMB-C2B	-2.32	1.46	1.50
27	G	204	CLA	CMB-C2B	-2.32	1.46	1.50
27	a	601	CLA	CMD-C2D	-2.32	1.46	1.50
27	2	613	CLA	CMD-C2D	-2.32	1.46	1.50
27	Y	612	CLA	C3B-C4B	2.32	1.49	1.42
27	8	609	CLA	CMB-C2B	-2.32	1.46	1.50
27	7	603	CLA	CMB-C2B	-2.32	1.46	1.50
27	A	829	CLA	C3B-C4B	2.32	1.49	1.42
27	B	841	CLA	C1B-C2B	2.32	1.48	1.43
27	8	613	CLA	C1B-C2B	2.32	1.48	1.43
27	A	841	CLA	CMD-C2D	-2.32	1.46	1.50
27	A	816	CLA	CMB-C2B	-2.32	1.46	1.50
27	6	613	CLA	CMD-C2D	-2.32	1.46	1.50
27	a	602	CLA	CMC-C2C	-2.32	1.46	1.50
27	B	838	CLA	CMB-C2B	-2.32	1.46	1.50
27	B	822	CLA	CMB-C2B	-2.32	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	9	606	CLA	CMB-C2B	-2.32	1.46	1.50
27	6	608	CLA	C1B-C2B	2.32	1.48	1.43
27	A	829	CLA	CMC-C2C	-2.32	1.46	1.50
36	U	1622	XAT	O4-C5	-2.32	1.43	1.46
27	5	616	CLA	CMB-C2B	-2.32	1.46	1.50
27	W	604	CLA	CMD-C2D	-2.32	1.46	1.50
27	B	804	CLA	CMB-C2B	-2.31	1.46	1.50
27	H	203	CLA	CMB-C2B	-2.31	1.46	1.50
27	A	820	CLA	C3B-C4B	2.31	1.49	1.42
27	X	612	CLA	C3B-C4B	2.31	1.49	1.42
27	6	604	CLA	CMC-C2C	-2.31	1.46	1.50
27	A	801	CLA	CMC-C2C	-2.31	1.46	1.50
27	A	808	CLA	CMD-C2D	-2.31	1.46	1.50
27	W	612	CLA	CMC-C2C	-2.31	1.46	1.50
27	2	609	CLA	C3B-C4B	2.31	1.49	1.42
27	A	805	CLA	CMB-C2B	-2.31	1.46	1.50
27	B	824	CLA	CMC-C2C	-2.31	1.46	1.50
27	B	841	CLA	C3B-C4B	2.31	1.49	1.42
27	B	841	CLA	CHC-C1C	2.31	1.43	1.38
27	6	602	CLA	CMD-C2D	-2.31	1.46	1.50
27	B	809	CLA	CMD-C2D	-2.31	1.46	1.50
27	5	607	CLA	CMD-C2D	-2.31	1.46	1.50
27	B	824	CLA	CMB-C2B	-2.31	1.46	1.50
27	A	829	CLA	C1B-C2B	2.31	1.48	1.43
27	3	610	CLA	C1B-C2B	2.31	1.48	1.43
27	7	604	CLA	CMC-C2C	-2.31	1.46	1.50
27	7	614	CLA	CMD-C2D	-2.31	1.46	1.50
27	8	608	CLA	CMB-C2B	-2.31	1.46	1.50
27	Y	614	CLA	C3B-C4B	2.31	1.49	1.42
27	A	818	CLA	C3B-C4B	2.31	1.49	1.42
27	9	606	CLA	C3B-C4B	2.31	1.49	1.42
27	7	607	CLA	CMC-C2C	-2.31	1.46	1.50
27	7	606	CLA	CMD-C2D	-2.31	1.46	1.50
27	A	821	CLA	CMC-C2C	-2.30	1.46	1.50
27	B	806	CLA	CMB-C2B	-2.30	1.46	1.50
27	2	601	CLA	C3B-C4B	2.30	1.49	1.42
27	6	602	CLA	C3B-C4B	2.30	1.49	1.42
27	A	813	CLA	CMD-C2D	-2.30	1.46	1.50
27	6	610	CLA	C3B-C4B	2.30	1.49	1.42
27	L	307	CLA	CMB-C2B	-2.30	1.46	1.50
27	6	616	CLA	CMD-C2D	-2.30	1.46	1.50
27	A	830	CLA	CMB-C2B	-2.30	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	837	CLA	CMD-C2D	-2.30	1.46	1.50
27	5	617	CLA	CMD-C2D	-2.30	1.46	1.50
27	8	602	CLA	CMB-C2B	-2.30	1.46	1.50
27	2	602	CLA	CMC-C2C	-2.30	1.46	1.50
27	7	610	CLA	C1B-C2B	2.30	1.48	1.43
27	O	2001	CLA	CMD-C2D	-2.30	1.46	1.50
27	9	614	CLA	CMB-C2B	-2.30	1.46	1.50
27	Z	611	CLA	C3B-C4B	2.30	1.49	1.42
27	6	613	CLA	CMB-C2B	-2.30	1.46	1.50
27	6	616	CLA	CMB-C2B	-2.30	1.46	1.50
27	8	607	CLA	CMC-C2C	-2.30	1.46	1.50
27	X	611	CLA	C3B-C4B	2.30	1.49	1.42
27	A	825	CLA	CMD-C2D	-2.30	1.46	1.50
27	W	602	CLA	C1B-C2B	2.30	1.48	1.43
27	L	307	CLA	CMD-C2D	-2.30	1.46	1.50
27	7	612	CLA	CMC-C2C	-2.30	1.46	1.50
27	A	815	CLA	CMB-C2B	-2.30	1.46	1.50
27	A	854	CLA	CMB-C2B	-2.30	1.46	1.50
27	7	610	CLA	CMC-C2C	-2.30	1.46	1.50
27	5	610	CLA	C1B-C2B	2.30	1.48	1.43
27	a	614	CLA	C3B-C4B	2.30	1.49	1.42
27	A	807	CLA	C1B-C2B	2.30	1.48	1.43
27	2	609	CLA	C1B-C2B	2.30	1.48	1.43
27	A	825	CLA	CMC-C2C	-2.30	1.46	1.50
27	6	610	CLA	C1B-C2B	2.30	1.48	1.43
27	J	101	CLA	C3B-C4B	2.30	1.49	1.42
27	a	602	CLA	CMB-C2B	-2.30	1.46	1.50
27	A	826	CLA	C1B-C2B	2.30	1.48	1.43
27	B	830	CLA	C1B-C2B	2.30	1.48	1.43
27	A	834	CLA	CMD-C2D	-2.30	1.46	1.50
27	3	614	CLA	CMC-C2C	-2.30	1.46	1.50
27	7	603	CLA	MG-NB	-2.30	2.01	2.05
27	3	615	CLA	C1B-C2B	2.30	1.48	1.43
27	3	604	CLA	CMC-C2C	-2.30	1.46	1.50
27	B	823	CLA	C3B-C4B	2.30	1.49	1.42
27	2	603	CLA	C3B-C4B	2.30	1.49	1.42
27	G	204	CLA	CMD-C2D	-2.30	1.46	1.50
27	7	608	CLA	CMD-C2D	-2.30	1.46	1.50
27	2	603	CLA	C1B-C2B	2.30	1.48	1.43
27	B	812	CLA	C3B-C4B	2.29	1.49	1.42
27	4	604	CLA	CMC-C2C	-2.29	1.46	1.50
27	a	610	CLA	CMD-C2D	-2.29	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	X	607	CHL	CBD-CGD	-2.29	1.49	1.52
38	W	606	CHL	CBD-CGD	-2.29	1.49	1.52
27	F	303	CLA	CMB-C2B	-2.29	1.46	1.50
27	a	607	CLA	CMD-C2D	-2.29	1.46	1.50
27	A	827	CLA	CMC-C2C	-2.29	1.46	1.50
27	5	610	CLA	CMC-C2C	-2.29	1.46	1.50
27	B	808	CLA	CMC-C2C	-2.29	1.46	1.50
27	1	608	CLA	CMD-C2D	-2.29	1.46	1.50
27	3	611	CLA	CMB-C2B	-2.29	1.46	1.50
27	X	614	CLA	C3B-C4B	2.29	1.49	1.42
27	L	306	CLA	CMC-C2C	-2.29	1.46	1.50
27	B	833	CLA	C3B-C4B	2.29	1.49	1.42
27	5	617	CLA	CMC-C2C	-2.29	1.46	1.50
27	A	828	CLA	CMB-C2B	-2.29	1.46	1.50
27	1	609	CLA	CMD-C2D	-2.29	1.46	1.50
27	4	610	CLA	CMC-C2C	-2.29	1.46	1.50
27	4	613	CLA	CMB-C2B	-2.29	1.46	1.50
27	A	813	CLA	CMC-C2C	-2.29	1.46	1.50
27	a	608	CLA	CMD-C2D	-2.29	1.46	1.50
27	U	603	CLA	MG-NB	-2.29	2.01	2.05
27	K	203	CLA	CMB-C2B	-2.29	1.46	1.50
27	2	616	CLA	CMD-C2D	-2.29	1.46	1.50
27	A	813	CLA	CMB-C2B	-2.29	1.46	1.50
27	2	612	CLA	CMB-C2B	-2.29	1.46	1.50
27	3	606	CLA	CMC-C2C	-2.28	1.46	1.50
27	6	611	CLA	CMD-C2D	-2.28	1.46	1.50
27	X	603	CLA	CMB-C2B	-2.28	1.46	1.50
27	a	601	CLA	CMB-C2B	-2.28	1.46	1.50
27	2	612	CLA	CMD-C2D	-2.28	1.46	1.50
27	4	604	CLA	CMB-C2B	-2.28	1.46	1.50
27	A	805	CLA	CMC-C2C	-2.28	1.46	1.50
27	J	101	CLA	CMD-C2D	-2.28	1.46	1.50
27	a	613	CLA	CMB-C2B	-2.28	1.46	1.50
27	3	603	CLA	C3B-C4B	2.28	1.49	1.42
27	7	611	CLA	C3B-C4B	2.28	1.49	1.42
27	Z	610	CLA	CMD-C2D	-2.28	1.46	1.50
27	3	602	CLA	C3B-C4B	2.28	1.49	1.42
27	Y	604	CLA	C3B-C4B	2.28	1.49	1.42
27	6	611	CLA	CMB-C2B	-2.28	1.46	1.50
27	7	606	CLA	CMB-C2B	-2.28	1.46	1.50
27	6	616	CLA	C3B-C4B	2.28	1.49	1.42
27	Y	603	CLA	C3B-C4B	2.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	854	CLA	CMC-C2C	-2.28	1.46	1.50
27	1	601	CLA	CMB-C2B	-2.28	1.46	1.50
27	K	203	CLA	C3B-C4B	2.28	1.49	1.42
27	W	613	CLA	CMB-C2B	-2.28	1.46	1.50
27	B	815	CLA	CMD-C2D	-2.28	1.46	1.50
27	4	616	CLA	CMD-C2D	-2.28	1.46	1.50
27	V	611	CLA	CMB-C2B	-2.27	1.46	1.50
27	5	607	CLA	C1B-C2B	2.27	1.48	1.43
27	3	615	CLA	C3B-C4B	2.27	1.49	1.42
27	9	606	CLA	CMC-C2C	-2.27	1.46	1.50
32	A	858	LMU	C3B-C2B	-2.27	1.48	1.52
27	B	810	CLA	C1B-C2B	2.27	1.48	1.43
27	B	803	CLA	CMC-C2C	-2.27	1.46	1.50
27	5	610	CLA	CMD-C2D	-2.27	1.46	1.50
27	L	307	CLA	CMC-C2C	-2.27	1.46	1.50
27	3	607	CLA	CMD-C2D	-2.27	1.46	1.50
27	O	2001	CLA	CMC-C2C	-2.27	1.46	1.50
27	4	608	CLA	CMC-C2C	-2.27	1.46	1.50
27	4	614	CLA	CMB-C2B	-2.27	1.46	1.50
36	Z	1622	XAT	O24-C25	-2.27	1.43	1.46
27	V	612	CLA	C1B-C2B	2.27	1.48	1.43
27	1	614	CLA	CMD-C2D	-2.27	1.46	1.50
27	B	809	CLA	MG-NB	-2.27	2.01	2.05
27	1	604	CLA	CMB-C2B	-2.27	1.46	1.50
27	X	613	CLA	C3B-C4B	2.27	1.49	1.42
27	A	839	CLA	CMC-C2C	-2.27	1.46	1.50
27	1	613	CLA	CMB-C2B	-2.27	1.46	1.50
27	9	604	CLA	CMB-C2B	-2.27	1.46	1.50
27	1	609	CLA	CMB-C2B	-2.27	1.46	1.50
27	9	601	CLA	CMD-C2D	-2.27	1.46	1.50
27	V	612	CLA	CMC-C2C	-2.27	1.46	1.50
27	1	611	CLA	CMD-C2D	-2.27	1.46	1.50
27	8	606	CLA	CMD-C2D	-2.27	1.46	1.50
38	U	605	CHL	CBD-CGD	-2.27	1.49	1.52
30	6	622	BCR	C1-C6	-2.27	1.50	1.53
27	Y	612	CLA	CHC-C1C	2.27	1.43	1.38
27	A	832	CLA	C1B-C2B	2.27	1.48	1.43
27	2	607	CLA	CMB-C2B	-2.27	1.46	1.50
27	B	832	CLA	CMC-C2C	-2.27	1.46	1.50
27	4	607	CLA	CMD-C2D	-2.27	1.46	1.50
30	B	846	BCR	C30-C25	-2.26	1.50	1.53
27	B	833	CLA	CMB-C2B	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	L	302	CLA	C1B-C2B	2.26	1.48	1.43
27	a	614	CLA	CMD-C2D	-2.26	1.46	1.50
27	4	612	CLA	C3B-C4B	2.26	1.49	1.42
27	Y	613	CLA	C3B-C4B	2.26	1.49	1.42
27	5	602	CLA	CMB-C2B	-2.26	1.46	1.50
27	5	606	CLA	CMB-C2B	-2.26	1.46	1.50
27	F	304	CLA	C3B-C4B	2.26	1.49	1.42
27	Z	612	CLA	C3B-C4B	2.26	1.49	1.42
27	A	817	CLA	CMB-C2B	-2.26	1.46	1.50
27	W	603	CLA	MG-NB	-2.26	2.01	2.05
27	6	608	CLA	CMD-C2D	-2.26	1.46	1.50
27	B	819	CLA	C1B-C2B	2.26	1.48	1.43
27	3	613	CLA	C3B-C4B	2.26	1.49	1.42
27	B	807	CLA	CMC-C2C	-2.26	1.46	1.50
27	X	603	CLA	C3B-C4B	2.26	1.49	1.42
27	4	613	CLA	CMD-C2D	-2.26	1.46	1.50
27	5	612	CLA	CMD-C2D	-2.26	1.46	1.50
27	1	613	CLA	CMD-C2D	-2.26	1.46	1.50
27	4	611	CLA	CMB-C2B	-2.26	1.46	1.50
27	8	611	CLA	CMC-C2C	-2.26	1.46	1.50
27	A	826	CLA	CMC-C2C	-2.26	1.46	1.50
27	2	607	CLA	CMD-C2D	-2.26	1.46	1.50
27	5	616	CLA	CMC-C2C	-2.26	1.46	1.50
27	U	612	CLA	CMC-C2C	-2.26	1.46	1.50
27	B	819	CLA	C3B-C4B	2.26	1.49	1.42
36	8	620	XAT	O24-C25	-2.26	1.43	1.46
27	5	608	CLA	CMB-C2B	-2.26	1.46	1.50
27	B	827	CLA	CMC-C2C	-2.26	1.46	1.50
27	2	604	CLA	CMC-C2C	-2.26	1.46	1.50
27	B	818	CLA	CMC-C2C	-2.26	1.46	1.50
27	6	608	CLA	CMB-C2B	-2.26	1.46	1.50
27	A	809	CLA	CMC-C2C	-2.26	1.46	1.50
27	5	607	CLA	CMC-C2C	-2.26	1.46	1.50
27	U	613	CLA	CMB-C2B	-2.26	1.46	1.50
27	8	612	CLA	CMD-C2D	-2.25	1.46	1.50
27	X	604	CLA	C3B-C4B	2.25	1.49	1.42
27	K	204	CLA	CMD-C2D	-2.25	1.46	1.50
27	a	608	CLA	CMB-C2B	-2.25	1.46	1.50
27	5	609	CLA	CMC-C2C	-2.25	1.46	1.50
27	U	611	CLA	CMC-C2C	-2.25	1.46	1.50
27	7	606	CLA	MG-NB	-2.25	2.01	2.05
27	8	614	CLA	C3B-C4B	2.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	606	CLA	CMD-C2D	-2.25	1.46	1.50
27	3	604	CLA	CMB-C2B	-2.25	1.46	1.50
27	Z	603	CLA	CMD-C2D	-2.25	1.46	1.50
27	G	203	CLA	CMD-C2D	-2.25	1.46	1.50
27	a	613	CLA	CMD-C2D	-2.25	1.46	1.50
27	3	609	CLA	CMC-C2C	-2.25	1.46	1.50
27	6	617	CLA	CMC-C2C	-2.25	1.46	1.50
27	5	601	CLA	CMD-C2D	-2.25	1.46	1.50
27	4	603	CLA	CMB-C2B	-2.25	1.46	1.50
27	7	602	CLA	C3B-C4B	2.25	1.49	1.42
36	7	620	XAT	O24-C25	-2.25	1.43	1.46
27	4	614	CLA	C3B-C4B	2.25	1.49	1.42
27	A	843	CLA	CMC-C2C	-2.25	1.46	1.50
27	7	607	CLA	CMD-C2D	-2.25	1.46	1.50
27	F	303	CLA	CMD-C2D	-2.25	1.46	1.50
27	2	606	CLA	CMD-C2D	-2.25	1.46	1.50
27	B	828	CLA	C1B-C2B	2.25	1.48	1.43
27	B	829	CLA	CMC-C2C	-2.25	1.46	1.50
27	6	608	CLA	CMC-C2C	-2.25	1.46	1.50
27	8	613	CLA	CMC-C2C	-2.25	1.46	1.50
27	4	613	CLA	C3B-C4B	2.25	1.49	1.42
27	O	2001	CLA	CMB-C2B	-2.25	1.46	1.50
27	3	610	CLA	CMC-C2C	-2.25	1.46	1.50
27	6	610	CLA	CMB-C2B	-2.25	1.46	1.50
27	6	611	CLA	C3B-C4B	2.25	1.49	1.42
27	A	824	CLA	CMB-C2B	-2.25	1.46	1.50
27	a	609	CLA	CMD-C2D	-2.25	1.46	1.50
27	5	601	CLA	CMB-C2B	-2.25	1.46	1.50
30	O	2005	BCR	C30-C25	-2.25	1.50	1.53
27	A	804	CLA	CMB-C2B	-2.25	1.46	1.50
27	V	614	CLA	C1B-C2B	2.24	1.48	1.43
27	B	835	CLA	C3B-C4B	2.24	1.49	1.42
27	B	835	CLA	CMB-C2B	-2.24	1.46	1.50
27	a	604	CLA	CMB-C2B	-2.24	1.46	1.50
27	B	822	CLA	CMC-C2C	-2.24	1.46	1.50
27	4	614	CLA	CMD-C2D	-2.24	1.46	1.50
27	A	819	CLA	MG-NB	-2.24	2.01	2.05
27	A	814	CLA	CMB-C2B	-2.24	1.46	1.50
27	A	824	CLA	CMC-C2C	-2.24	1.46	1.50
27	9	611	CLA	CMB-C2B	-2.24	1.46	1.50
27	W	611	CLA	CMC-C2C	-2.24	1.46	1.50
27	A	816	CLA	CMC-C2C	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	V	604	CLA	CMD-C2D	-2.24	1.46	1.50
27	Z	613	CLA	C3B-C4B	2.24	1.49	1.42
27	2	610	CLA	CMC-C2C	-2.24	1.46	1.50
27	5	608	CLA	CMD-C2D	-2.24	1.46	1.50
27	a	616	CLA	C3B-C4B	2.24	1.49	1.42
27	B	814	CLA	CMC-C2C	-2.24	1.46	1.50
27	2	602	CLA	CMB-C2B	-2.24	1.46	1.50
27	A	819	CLA	CMC-C2C	-2.24	1.46	1.50
27	6	610	CLA	CMC-C2C	-2.24	1.46	1.50
27	B	805	CLA	C3B-C4B	2.24	1.49	1.42
27	2	613	CLA	CMB-C2B	-2.24	1.46	1.50
27	a	613	CLA	C3B-C4B	2.24	1.49	1.42
27	5	608	CLA	CMC-C2C	-2.23	1.46	1.50
27	U	611	CLA	CMB-C2B	-2.23	1.46	1.50
27	B	805	CLA	CMC-C2C	-2.23	1.46	1.50
27	L	306	CLA	CMD-C2D	-2.23	1.46	1.50
27	6	609	CLA	CMC-C2C	-2.23	1.46	1.50
27	7	608	CLA	CMC-C2C	-2.23	1.46	1.50
27	9	607	CLA	CMD-C2D	-2.23	1.46	1.50
27	W	610	CLA	CMC-C2C	-2.23	1.46	1.50
36	W	1622	XAT	C2-C1	-2.23	1.51	1.54
27	O	2002	CLA	CMB-C2B	-2.23	1.46	1.50
27	B	813	CLA	C1B-C2B	2.23	1.48	1.43
27	7	607	CLA	CMB-C2B	-2.23	1.46	1.50
30	L	308	BCR	C30-C25	-2.23	1.50	1.53
27	1	608	CLA	C3B-C4B	2.23	1.49	1.42
36	3	619	XAT	O4-C5	-2.23	1.43	1.46
27	1	606	CLA	CMB-C2B	-2.23	1.46	1.50
27	6	606	CLA	CMD-C2D	-2.23	1.46	1.50
30	A	851	BCR	C1-C6	-2.23	1.50	1.53
27	B	816	CLA	CMD-C2D	-2.23	1.46	1.50
27	4	611	CLA	CMD-C2D	-2.23	1.46	1.50
27	O	2003	CLA	CMB-C2B	-2.23	1.46	1.50
27	9	612	CLA	C3B-C4B	2.23	1.49	1.42
27	7	604	CLA	C3B-C4B	2.23	1.49	1.42
27	J	101	CLA	CMB-C2B	-2.23	1.46	1.50
27	A	828	CLA	C3B-C4B	2.23	1.49	1.42
27	X	612	CLA	CHC-C1C	2.23	1.43	1.38
27	B	826	CLA	C3B-C4B	2.23	1.49	1.42
27	1	606	CLA	CMD-C2D	-2.23	1.46	1.50
36	5	621	XAT	O24-C25	-2.23	1.43	1.46
36	9	620	XAT	O4-C5	-2.23	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	844	PQN	C2-C1	2.23	1.52	1.47
27	6	612	CLA	CMD-C2D	-2.23	1.46	1.50
27	A	808	CLA	CMC-C2C	-2.23	1.46	1.50
27	4	601	CLA	CMB-C2B	-2.23	1.46	1.50
27	7	610	CLA	CMB-C2B	-2.23	1.46	1.50
27	A	802	CLA	C1B-C2B	2.23	1.48	1.43
27	L	306	CLA	CMB-C2B	-2.23	1.46	1.50
27	V	604	CLA	CMC-C2C	-2.23	1.46	1.50
27	1	610	CLA	CMD-C2D	-2.22	1.46	1.50
37	U	1623	NEX	O24-C25	-2.22	1.43	1.46
27	4	618	CLA	CMB-C2B	-2.22	1.46	1.50
27	U	610	CLA	CMC-C2C	-2.22	1.46	1.50
27	A	810	CLA	C3B-C4B	2.22	1.49	1.42
27	5	604	CLA	CMD-C2D	-2.22	1.46	1.50
27	Y	603	CLA	CMB-C2B	-2.22	1.46	1.50
27	8	610	CLA	C1B-C2B	2.22	1.48	1.43
27	A	802	CLA	CHC-C1C	2.22	1.42	1.38
27	V	602	CLA	C1B-C2B	2.22	1.48	1.43
27	B	804	CLA	C3B-C4B	2.22	1.49	1.42
27	9	609	CLA	C3B-C4B	2.22	1.49	1.42
27	1	608	CLA	CMB-C2B	-2.22	1.46	1.50
27	7	602	CLA	CMB-C2B	-2.22	1.46	1.50
27	K	206	CLA	CMD-C2D	-2.22	1.46	1.50
27	a	614	CLA	CMB-C2B	-2.22	1.46	1.50
27	9	610	CLA	CMB-C2B	-2.22	1.46	1.50
27	6	608	CLA	C3B-C4B	2.22	1.49	1.42
27	5	608	CLA	C3B-C4B	2.22	1.49	1.42
27	B	813	CLA	C3B-C4B	2.22	1.49	1.42
36	1	618	XAT	O24-C25	-2.22	1.43	1.46
27	a	610	CLA	CMC-C2C	-2.22	1.46	1.50
27	5	602	CLA	CMC-C2C	-2.22	1.46	1.50
27	V	602	CLA	C3B-C4B	2.22	1.49	1.42
27	8	606	CLA	C3B-C4B	2.22	1.49	1.42
27	2	602	CLA	C3B-C4B	2.22	1.49	1.42
27	O	2003	CLA	CMC-C2C	-2.22	1.46	1.50
27	V	610	CLA	C1B-C2B	2.22	1.48	1.43
27	B	826	CLA	CMB-C2B	-2.22	1.46	1.50
27	a	603	CLA	CMC-C2C	-2.22	1.46	1.50
27	3	607	CLA	CMB-C2B	-2.22	1.46	1.50
27	6	614	CLA	CMB-C2B	-2.22	1.46	1.50
27	7	609	CLA	C3B-C4B	2.22	1.49	1.42
27	Z	610	CLA	CHC-C1C	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	7	619	LUT	C1-C6	-2.22	1.50	1.53
27	A	807	CLA	C3B-C4B	2.22	1.49	1.42
27	B	816	CLA	C3B-C4B	2.22	1.49	1.42
27	9	614	CLA	C3B-C4B	2.22	1.49	1.42
27	6	617	CLA	CMB-C2B	-2.21	1.46	1.50
27	A	843	CLA	C1B-C2B	2.21	1.48	1.43
27	6	604	CLA	CMB-C2B	-2.21	1.46	1.50
27	a	606	CLA	CMB-C2B	-2.21	1.46	1.50
27	V	603	CLA	MG-NB	-2.21	2.01	2.05
27	4	611	CLA	C3B-C4B	2.21	1.49	1.42
27	Z	602	CLA	CMD-C2D	-2.21	1.46	1.50
27	A	803	CLA	CMC-C2C	-2.21	1.46	1.50
27	2	611	CLA	CMD-C2D	-2.21	1.46	1.50
27	6	613	CLA	CMC-C2C	-2.21	1.46	1.50
27	A	808	CLA	CMB-C2B	-2.21	1.46	1.50
27	A	836	CLA	CMC-C2C	-2.21	1.46	1.50
27	3	614	CLA	CMB-C2B	-2.21	1.46	1.50
27	2	611	CLA	C3B-C4B	2.21	1.49	1.42
27	B	817	CLA	CMD-C2D	-2.21	1.46	1.50
27	K	204	CLA	CMC-C2C	-2.21	1.46	1.50
27	9	601	CLA	CMB-C2B	-2.21	1.46	1.50
27	6	606	CLA	C3B-C4B	2.21	1.49	1.42
27	6	613	CLA	CHC-C1C	2.21	1.42	1.38
27	5	616	CLA	CMD-C2D	-2.21	1.46	1.50
27	9	612	CLA	CMD-C2D	-2.21	1.46	1.50
27	3	613	CLA	CMC-C2C	-2.21	1.46	1.50
27	9	613	CLA	CMC-C2C	-2.21	1.46	1.50
27	L	303	CLA	C3B-C4B	2.21	1.49	1.42
27	A	818	CLA	CMC-C2C	-2.21	1.46	1.50
27	K	203	CLA	CMC-C2C	-2.21	1.46	1.50
27	9	613	CLA	CMD-C2D	-2.21	1.46	1.50
27	U	614	CLA	CMC-C2C	-2.21	1.46	1.50
27	K	204	CLA	CMB-C2B	-2.21	1.46	1.50
27	A	817	CLA	C3B-C4B	2.21	1.49	1.42
27	3	617	CLA	CMB-C2B	-2.21	1.46	1.50
27	6	612	CLA	CMB-C2B	-2.21	1.46	1.50
27	1	603	CLA	CMB-C2B	-2.21	1.46	1.50
27	4	604	CLA	CMD-C2D	-2.21	1.46	1.50
27	4	610	CLA	CMB-C2B	-2.21	1.46	1.50
37	V	1623	NEX	C7-C6	-2.21	1.28	1.30
27	A	834	CLA	CMC-C2C	-2.21	1.46	1.50
27	K	201	CLA	CMB-C2B	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	618	CLA	CMD-C2D	-2.21	1.46	1.50
27	a	608	CLA	C3B-C4B	2.21	1.49	1.42
27	1	612	CLA	C3B-C4B	2.20	1.49	1.42
27	1	614	CLA	CMB-C2B	-2.20	1.46	1.50
27	F	301	CLA	CHC-C1C	2.20	1.42	1.38
27	8	603	CLA	CMC-C2C	-2.20	1.46	1.50
27	1	613	CLA	C3B-C4B	2.20	1.49	1.42
27	3	614	CLA	C3B-C4B	2.20	1.49	1.42
27	5	607	CLA	C3B-C4B	2.20	1.49	1.42
27	a	613	CLA	CMC-C2C	-2.20	1.46	1.50
27	A	835	CLA	CMC-C2C	-2.20	1.46	1.50
27	a	616	CLA	CMB-C2B	-2.20	1.46	1.50
27	5	618	CLA	CMD-C2D	-2.20	1.46	1.50
27	8	610	CLA	CMC-C2C	-2.20	1.46	1.50
27	3	602	CLA	CMC-C2C	-2.20	1.46	1.50
27	K	204	CLA	C3B-C4B	2.20	1.49	1.42
27	W	610	CLA	C1B-C2B	2.20	1.48	1.43
27	B	828	CLA	CMC-C2C	-2.20	1.46	1.50
27	A	817	CLA	CMC-C2C	-2.20	1.46	1.50
27	5	604	CLA	CMC-C2C	-2.20	1.46	1.50
36	6	621	XAT	O4-C5	-2.20	1.43	1.46
27	B	839	CLA	CMC-C2C	-2.20	1.46	1.50
27	B	832	CLA	CMB-C2B	-2.20	1.46	1.50
27	4	613	CLA	CMC-C2C	-2.20	1.46	1.50
27	B	823	CLA	C1B-C2B	2.20	1.48	1.43
27	3	617	CLA	CMC-C2C	-2.20	1.46	1.50
27	7	615	CLA	CMB-C2B	-2.20	1.46	1.50
27	A	814	CLA	C3B-C4B	2.20	1.49	1.42
27	A	838	CLA	CMB-C2B	-2.20	1.46	1.50
27	a	606	CLA	C3B-C4B	2.20	1.49	1.42
27	6	614	CLA	C3B-C4B	2.20	1.49	1.42
27	5	613	CLA	CMD-C2D	-2.20	1.46	1.50
27	5	607	CLA	CHC-C1C	2.20	1.42	1.38
27	3	608	CLA	C1B-C2B	2.20	1.48	1.43
27	a	603	CLA	CMB-C2B	-2.20	1.46	1.50
27	6	620	CLA	C3B-C4B	2.20	1.49	1.42
27	U	603	CLA	CMC-C2C	-2.19	1.46	1.50
27	7	614	CLA	C3B-C4B	2.19	1.49	1.42
27	B	824	CLA	C3B-C4B	2.19	1.49	1.42
27	8	606	CLA	CMC-C2C	-2.19	1.46	1.50
27	F	301	CLA	C1B-C2B	2.19	1.48	1.43
27	A	845	CLA	CMC-C2C	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	9	606	CLA	CMD-C2D	-2.19	1.46	1.50
36	V	1622	XAT	C2-C1	-2.19	1.51	1.54
27	W	611	CLA	CMB-C2B	-2.19	1.46	1.50
27	Y	614	CLA	CHC-C1C	2.19	1.42	1.38
37	6	624	NEX	O24-C25	-2.19	1.43	1.46
27	9	611	CLA	C3B-C4B	2.19	1.49	1.42
27	1	603	CLA	CMC-C2C	-2.19	1.46	1.50
28	B	842	PQN	C10-C1	2.19	1.52	1.48
27	7	606	CLA	C3B-C4B	2.19	1.49	1.42
27	V	614	CLA	C3B-C4B	2.19	1.49	1.42
27	7	615	CLA	CMD-C2D	-2.19	1.46	1.50
27	9	609	CLA	CMB-C2B	-2.19	1.46	1.50
38	Y	605	CHL	CHA-CBD	-2.19	1.49	1.51
27	L	304	CLA	C3B-C4B	2.19	1.49	1.42
27	1	611	CLA	C3B-C4B	2.19	1.49	1.42
27	B	809	CLA	CMC-C2C	-2.19	1.46	1.50
27	B	810	CLA	CHC-C1C	2.19	1.42	1.38
27	B	825	CLA	CMC-C2C	-2.19	1.46	1.50
27	7	614	CLA	CMC-C2C	-2.19	1.46	1.50
27	1	604	CLA	C3B-C4B	2.19	1.49	1.42
27	a	609	CLA	CMB-C2B	-2.19	1.46	1.50
27	8	611	CLA	CMB-C2B	-2.19	1.46	1.50
27	F	304	CLA	CMC-C2C	-2.19	1.46	1.50
27	6	602	CLA	CHC-C1C	2.19	1.42	1.38
27	a	609	CLA	CMC-C2C	-2.19	1.46	1.50
27	2	616	CLA	CMB-C2B	-2.19	1.46	1.50
27	A	826	CLA	MG-NB	-2.19	2.01	2.05
27	B	815	CLA	CMC-C2C	-2.19	1.46	1.50
27	1	610	CLA	CMC-C2C	-2.19	1.46	1.50
27	4	607	CLA	CMB-C2B	-2.19	1.46	1.50
27	9	610	CLA	CHC-C1C	2.19	1.42	1.38
27	A	834	CLA	MG-NB	-2.19	2.01	2.05
36	6	621	XAT	O24-C25	-2.19	1.43	1.46
27	6	606	CLA	CMB-C2B	-2.19	1.46	1.50
27	9	607	CLA	CMC-C2C	-2.19	1.46	1.50
27	A	810	CLA	CMC-C2C	-2.18	1.46	1.50
27	B	804	CLA	CMC-C2C	-2.18	1.46	1.50
27	9	614	CLA	CMD-C2D	-2.18	1.46	1.50
27	4	616	CLA	CMB-C2B	-2.18	1.46	1.50
27	Y	603	CLA	CMD-C2D	-2.18	1.46	1.50
27	2	607	CLA	C3B-C4B	2.18	1.49	1.42
27	5	613	CLA	CMC-C2C	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X	603	CLA	CMD-C2D	-2.18	1.46	1.50
27	5	614	CLA	C3B-C4B	2.18	1.49	1.42
27	B	827	CLA	C3B-C4B	2.18	1.49	1.42
27	O	2003	CLA	C3B-C4B	2.18	1.49	1.42
27	7	601	CLA	CMC-C2C	-2.18	1.46	1.50
27	B	821	CLA	C3B-C4B	2.18	1.49	1.42
27	B	822	CLA	C3B-C4B	2.18	1.49	1.42
27	V	612	CLA	C3B-C4B	2.18	1.49	1.42
27	B	814	CLA	CMB-C2B	-2.18	1.46	1.50
27	L	302	CLA	C3B-C4B	2.18	1.49	1.42
27	2	612	CLA	C3B-C4B	2.18	1.49	1.42
27	A	809	CLA	CMB-C2B	-2.18	1.46	1.50
27	a	611	CLA	CMD-C2D	-2.18	1.46	1.50
27	2	614	CLA	CMC-C2C	-2.18	1.46	1.50
27	4	609	CLA	CMC-C2C	-2.18	1.46	1.50
27	7	613	CLA	CMC-C2C	-2.18	1.46	1.50
27	7	603	CLA	CMC-C2C	-2.18	1.46	1.50
27	Z	614	CLA	CHC-C1C	2.18	1.42	1.38
27	B	812	CLA	CMD-C2D	-2.18	1.46	1.50
27	4	602	CLA	CMB-C2B	-2.18	1.46	1.50
27	3	615	CLA	CMD-C2D	-2.18	1.46	1.50
27	8	607	CLA	CMB-C2B	-2.18	1.46	1.50
27	5	601	CLA	C3B-C4B	2.18	1.49	1.42
35	Z	1620	LUT	C22-C21	-2.17	1.52	1.54
27	O	2002	CLA	CMC-C2C	-2.17	1.46	1.50
27	2	614	CLA	CMB-C2B	-2.17	1.46	1.50
27	Y	614	CLA	CMD-C2D	-2.17	1.46	1.50
30	L	308	BCR	C1-C6	-2.17	1.51	1.53
27	A	824	CLA	C3B-C4B	2.17	1.49	1.42
27	B	832	CLA	C3B-C4B	2.17	1.49	1.42
27	B	803	CLA	CMB-C2B	-2.17	1.46	1.50
27	6	617	CLA	C3B-C4B	2.17	1.49	1.42
27	7	611	CLA	CMB-C2B	-2.17	1.46	1.50
27	8	610	CLA	CMB-C2B	-2.17	1.46	1.50
27	7	606	CLA	CMC-C2C	-2.17	1.46	1.50
27	1	614	CLA	CHC-C1C	2.17	1.42	1.38
27	2	606	CLA	C3B-C4B	2.17	1.49	1.42
27	B	812	CLA	C1B-C2B	2.17	1.48	1.43
27	5	613	CLA	C3B-C4B	2.17	1.49	1.42
27	a	612	CLA	C3B-C4B	2.17	1.49	1.42
27	6	601	CLA	CMC-C2C	-2.17	1.46	1.50
27	4	610	CLA	C3B-C4B	2.17	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1	606	CLA	C3B-C4B	2.17	1.49	1.42
27	5	619	CLA	CMD-C2D	-2.17	1.46	1.50
38	U	601	CHL	CMC-C2C	2.17	1.49	1.44
27	B	814	CLA	C3B-C4B	2.17	1.49	1.42
27	1	613	CLA	CMC-C2C	-2.17	1.46	1.50
27	A	807	CLA	MG-NB	-2.17	2.01	2.05
27	2	613	CLA	CMC-C2C	-2.17	1.46	1.50
27	1	611	CLA	CMC-C2C	-2.17	1.46	1.50
27	A	811	CLA	CMC-C2C	-2.17	1.46	1.50
27	9	611	CLA	CMD-C2D	-2.17	1.46	1.50
27	a	601	CLA	C3B-C4B	2.17	1.49	1.42
27	a	604	CLA	C3B-C4B	2.17	1.49	1.42
27	a	612	CLA	CMC-C2C	-2.17	1.46	1.50
27	W	614	CLA	CMC-C2C	-2.16	1.46	1.50
27	B	808	CLA	C3B-C4B	2.16	1.49	1.42
36	2	620	XAT	O24-C25	-2.16	1.43	1.46
27	3	608	CLA	MG-NB	-2.16	2.01	2.05
27	L	306	CLA	C3B-C4B	2.16	1.49	1.42
27	5	612	CLA	C3B-C4B	2.16	1.49	1.42
27	U	610	CLA	C1B-C2B	2.16	1.48	1.43
27	W	610	CLA	C3B-C4B	2.16	1.49	1.42
36	4	620	XAT	O24-C25	-2.16	1.43	1.46
27	A	840	CLA	CMC-C2C	-2.16	1.46	1.50
27	8	602	CLA	C3B-C4B	2.16	1.49	1.42
27	A	828	CLA	CMC-C2C	-2.16	1.46	1.50
27	A	830	CLA	CMC-C2C	-2.16	1.46	1.50
27	A	841	CLA	C3B-C4B	2.16	1.49	1.42
27	B	819	CLA	CMC-C2C	-2.16	1.46	1.50
27	V	610	CLA	C3B-C4B	2.16	1.49	1.42
27	Y	611	CLA	CHC-C1C	2.16	1.42	1.38
27	Z	614	CLA	CMD-C2D	-2.16	1.46	1.50
27	5	612	CLA	CMC-C2C	-2.16	1.46	1.50
27	Z	613	CLA	CMD-C2D	-2.16	1.46	1.50
27	B	802	CLA	CMC-C2C	-2.16	1.46	1.50
27	8	612	CLA	C3B-C4B	2.16	1.49	1.42
27	O	2001	CLA	C3B-C4B	2.16	1.49	1.42
27	H	202	CLA	CMB-C2B	-2.16	1.46	1.50
27	8	601	CLA	CMB-C2B	-2.16	1.46	1.50
27	6	612	CLA	C3B-C4B	2.16	1.49	1.42
27	A	822	CLA	C1B-C2B	2.16	1.48	1.43
27	6	607	CLA	CMC-C2C	-2.16	1.46	1.50
27	8	609	CLA	CMC-C2C	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	9	614	CLA	CMC-C2C	-2.16	1.46	1.50
27	A	810	CLA	MG-NB	-2.16	2.01	2.05
27	G	203	CLA	CHC-C1C	2.16	1.42	1.38
35	X	1621	LUT	C22-C21	-2.16	1.52	1.54
27	5	602	CLA	MG-NB	-2.15	2.01	2.05
36	5	621	XAT	O4-C5	-2.15	1.43	1.46
36	9	620	XAT	O24-C25	-2.15	1.43	1.46
27	U	612	CLA	C3B-C4B	2.15	1.49	1.42
27	8	611	CLA	C3B-C4B	2.15	1.49	1.42
27	F	303	CLA	CHC-C1C	2.15	1.42	1.38
27	8	616	CLA	CHC-C1C	2.15	1.42	1.38
27	X	614	CLA	CHC-C1C	2.15	1.42	1.38
27	B	825	CLA	C3B-C4B	2.15	1.49	1.42
36	U	1622	XAT	C2-C1	-2.15	1.51	1.54
27	B	825	CLA	CMB-C2B	-2.15	1.46	1.50
27	2	604	CLA	CMB-C2B	-2.15	1.46	1.50
27	8	604	CLA	CMB-C2B	-2.15	1.46	1.50
38	V	609	CHL	CBD-CGD	-2.15	1.49	1.52
27	3	602	CLA	CMB-C2B	-2.15	1.46	1.50
27	9	602	CLA	CMC-C2C	-2.15	1.46	1.50
27	6	604	CLA	C3B-C4B	2.15	1.49	1.42
27	4	609	CLA	CMB-C2B	-2.15	1.46	1.50
27	9	602	CLA	CMB-C2B	-2.15	1.46	1.50
27	B	807	CLA	MG-NB	-2.15	2.01	2.05
27	5	608	CLA	CHC-C1C	2.15	1.42	1.38
27	5	603	CLA	CMC-C2C	-2.15	1.46	1.50
27	5	612	CLA	CMB-C2B	-2.15	1.46	1.50
27	2	612	CLA	CMC-C2C	-2.15	1.46	1.50
27	8	613	CLA	CHC-C1C	2.15	1.42	1.38
27	A	805	CLA	C3B-C4B	2.15	1.49	1.42
27	a	614	CLA	CMC-C2C	-2.15	1.46	1.50
27	8	601	CLA	CMC-C2C	-2.15	1.46	1.50
38	X	605	CHL	CHA-CBD	-2.15	1.49	1.51
27	J	101	CLA	CHC-C1C	2.15	1.42	1.38
27	6	610	CLA	CHC-C1C	2.15	1.42	1.38
27	A	823	CLA	C3B-C4B	2.15	1.49	1.42
27	8	606	CLA	CMB-C2B	-2.15	1.46	1.50
27	2	610	CLA	CHC-C1C	2.15	1.42	1.38
27	1	601	CLA	C3B-C4B	2.15	1.49	1.42
27	B	831	CLA	CMB-C2B	-2.15	1.46	1.50
27	1	607	CLA	CMC-C2C	-2.15	1.46	1.50
27	a	607	CLA	CMC-C2C	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1	612	CLA	CMC-C2C	-2.14	1.46	1.50
27	3	615	CLA	CMC-C2C	-2.14	1.46	1.50
27	X	610	CLA	CMD-C2D	-2.14	1.46	1.50
30	G	205	BCR	C1-C6	-2.14	1.51	1.53
27	A	836	CLA	MG-NB	-2.14	2.01	2.05
27	1	616	CLA	CMB-C2B	-2.14	1.46	1.50
27	4	611	CLA	CMC-C2C	-2.14	1.46	1.50
36	7	620	XAT	O4-C5	-2.14	1.43	1.46
27	1	610	CLA	CMB-C2B	-2.14	1.46	1.50
27	1	612	CLA	CMB-C2B	-2.14	1.46	1.50
27	Y	602	CLA	CMD-C2D	-2.14	1.46	1.50
27	A	838	CLA	C3B-C4B	2.14	1.49	1.42
27	8	603	CLA	MG-NB	-2.14	2.01	2.05
27	A	854	CLA	C3B-C4B	2.14	1.49	1.42
27	a	603	CLA	C3B-C4B	2.14	1.49	1.42
27	a	604	CLA	CMC-C2C	-2.14	1.46	1.50
27	2	606	CLA	CMC-C2C	-2.14	1.46	1.50
27	6	620	CLA	CHC-C1C	2.14	1.42	1.38
27	4	606	CLA	CMD-C2D	-2.14	1.46	1.50
27	5	601	CLA	CMC-C2C	-2.14	1.46	1.50
27	3	614	CLA	CHC-C1C	2.14	1.42	1.38
27	A	829	CLA	CMB-C2B	-2.14	1.46	1.50
27	4	612	CLA	CMB-C2B	-2.14	1.46	1.50
27	5	606	CLA	MG-NB	-2.14	2.01	2.05
27	6	620	CLA	CMC-C2C	-2.14	1.46	1.50
27	a	607	CLA	CMB-C2B	-2.14	1.46	1.50
27	4	603	CLA	CMC-C2C	-2.14	1.46	1.50
27	5	611	CLA	C3B-C4B	2.14	1.49	1.42
27	8	604	CLA	C3B-C4B	2.14	1.49	1.42
27	B	841	CLA	MG-NB	-2.14	2.01	2.05
27	B	823	CLA	CHC-C1C	2.14	1.42	1.38
27	A	833	CLA	CMC-C2C	-2.14	1.46	1.50
27	5	606	CLA	CMC-C2C	-2.14	1.46	1.50
27	B	806	CLA	MG-NB	-2.14	2.01	2.05
27	7	612	CLA	C3B-C4B	2.14	1.49	1.42
27	4	606	CLA	MG-NB	-2.14	2.01	2.05
27	1	604	CLA	CMC-C2C	-2.14	1.46	1.50
27	5	611	CLA	CMD-C2D	-2.14	1.46	1.50
38	W	605	CHL	CBD-CGD	-2.14	1.49	1.52
27	B	811	CLA	CMC-C2C	-2.13	1.46	1.50
27	F	303	CLA	CMC-C2C	-2.13	1.46	1.50
27	2	603	CLA	CMC-C2C	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	618	CLA	CMB-C2B	-2.13	1.46	1.50
37	Y	1623	NEX	O24-C25	-2.13	1.43	1.46
27	7	613	CLA	C3B-C4B	2.13	1.49	1.42
27	a	610	CLA	CMB-C2B	-2.13	1.46	1.50
27	A	822	CLA	MG-NB	-2.13	2.01	2.05
27	a	602	CLA	C3B-C4B	2.13	1.49	1.42
27	a	611	CLA	CMC-C2C	-2.13	1.46	1.50
27	1	608	CLA	CMC-C2C	-2.13	1.46	1.50
27	5	602	CLA	C3B-C4B	2.13	1.49	1.42
27	1	609	CLA	CMC-C2C	-2.13	1.46	1.50
27	9	604	CLA	CMC-C2C	-2.13	1.46	1.50
27	A	814	CLA	MG-NB	-2.13	2.01	2.05
27	B	841	CLA	CMB-C2B	-2.13	1.46	1.50
27	A	808	CLA	C3B-C4B	2.13	1.48	1.42
38	X	601	CHL	CBD-CGD	-2.13	1.49	1.52
36	2	620	XAT	O4-C5	-2.13	1.43	1.46
27	3	602	CLA	CHC-C1C	2.13	1.42	1.38
27	5	603	CLA	MG-NB	-2.13	2.01	2.05
27	2	611	CLA	CMB-C2B	-2.13	1.46	1.50
27	L	304	CLA	CMC-C2C	-2.13	1.46	1.50
37	X	1623	NEX	O24-C25	-2.13	1.43	1.46
27	1	603	CLA	C3B-C4B	2.13	1.48	1.42
27	U	614	CLA	MG-NB	-2.13	2.01	2.05
27	W	614	CLA	MG-NB	-2.13	2.01	2.05
27	B	820	CLA	CMC-C2C	-2.13	1.46	1.50
27	a	612	CLA	CMB-C2B	-2.13	1.46	1.50
27	9	609	CLA	CMC-C2C	-2.13	1.46	1.50
27	9	601	CLA	C3B-C4B	2.13	1.48	1.42
27	B	820	CLA	C3B-C4B	2.13	1.48	1.42
27	A	821	CLA	C3B-C4B	2.13	1.48	1.42
27	5	610	CLA	CMB-C2B	-2.13	1.46	1.50
27	A	841	CLA	MG-NB	-2.13	2.01	2.05
27	B	803	CLA	C3B-C4B	2.12	1.48	1.42
27	A	813	CLA	C3B-C4B	2.12	1.48	1.42
27	5	611	CLA	CMB-C2B	-2.12	1.46	1.50
27	6	602	CLA	CMB-C2B	-2.12	1.46	1.50
38	Y	601	CHL	CMC-C2C	2.12	1.49	1.44
37	5	624	NEX	O24-C25	-2.12	1.43	1.46
27	F	304	CLA	CMB-C2B	-2.12	1.46	1.50
27	A	839	CLA	C3B-C4B	2.12	1.48	1.42
27	2	609	CLA	CMC-C2C	-2.12	1.46	1.50
27	1	602	CLA	MG-NB	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	614	CLA	CMC-C2C	-2.12	1.46	1.50
27	8	609	CLA	C3B-C4B	2.12	1.48	1.42
27	W	602	CLA	MG-NB	-2.12	2.01	2.05
27	2	610	CLA	CMB-C2B	-2.12	1.46	1.50
27	U	602	CLA	MG-NB	-2.12	2.01	2.05
27	a	601	CLA	CMC-C2C	-2.12	1.46	1.50
27	A	812	CLA	CMC-C2C	-2.12	1.46	1.50
27	7	601	CLA	CMB-C2B	-2.12	1.46	1.50
27	8	616	CLA	CMD-C2D	-2.12	1.46	1.50
27	3	604	CLA	C3B-C4B	2.12	1.48	1.42
27	B	840	CLA	C3B-C4B	2.12	1.48	1.42
27	W	603	CLA	CMC-C2C	-2.12	1.46	1.50
27	A	837	CLA	MG-NB	-2.12	2.01	2.05
27	W	614	CLA	C3B-C4B	2.12	1.48	1.42
27	7	609	CLA	CMC-C2C	-2.12	1.46	1.50
27	8	608	CLA	C3B-C4B	2.12	1.48	1.42
27	W	612	CLA	C3B-C4B	2.12	1.48	1.42
27	B	821	CLA	CHC-C1C	2.12	1.42	1.38
27	3	610	CLA	CHC-C1C	2.12	1.42	1.38
27	3	612	CLA	CMC-C2C	-2.12	1.46	1.50
27	U	610	CLA	C3B-C4B	2.12	1.48	1.42
27	a	606	CLA	CMC-C2C	-2.12	1.46	1.50
27	6	607	CLA	CMB-C2B	-2.12	1.46	1.50
38	V	601	CHL	CMC-C2C	2.12	1.49	1.44
27	A	838	CLA	MG-NB	-2.12	2.01	2.05
27	A	804	CLA	CMC-C2C	-2.12	1.46	1.50
27	A	828	CLA	MG-NB	-2.12	2.01	2.05
27	1	607	CLA	C3B-C4B	2.12	1.48	1.42
27	4	608	CLA	C3B-C4B	2.12	1.48	1.42
27	B	830	CLA	CMC-C2C	-2.11	1.46	1.50
27	Y	610	CLA	CMD-C2D	-2.11	1.46	1.50
27	A	812	CLA	C3B-C4B	2.11	1.48	1.42
27	B	830	CLA	C3B-C4B	2.11	1.48	1.42
27	Y	611	CLA	CMD-C2D	-2.11	1.46	1.50
27	Y	612	CLA	CMD-C2D	-2.11	1.46	1.50
27	Y	613	CLA	CMD-C2D	-2.11	1.46	1.50
27	5	607	CLA	CMB-C2B	-2.11	1.46	1.50
27	6	607	CLA	CHC-C1C	2.11	1.42	1.38
27	B	838	CLA	C3B-C4B	2.11	1.48	1.42
27	Z	604	CLA	CHC-C1C	2.11	1.42	1.38
36	8	620	XAT	O4-C5	-2.11	1.43	1.46
27	J	101	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	610	CLA	CMB-C2B	-2.11	1.46	1.50
27	A	802	CLA	CMB-C2B	-2.11	1.46	1.50
27	A	823	CLA	CMC-C2C	-2.11	1.46	1.50
27	5	606	CLA	C3B-C4B	2.11	1.48	1.42
35	2	619	LUT	C1-C6	-2.11	1.51	1.53
27	B	834	CLA	MG-NB	-2.11	2.01	2.05
27	A	833	CLA	MG-NB	-2.11	2.01	2.05
27	6	609	CLA	C3B-C4B	2.11	1.48	1.42
27	3	611	CLA	CMC-C2C	-2.11	1.46	1.50
27	5	619	CLA	CMB-C2B	-2.11	1.46	1.50
27	7	607	CLA	C3B-C4B	2.11	1.48	1.42
27	X	602	CLA	CMD-C2D	-2.11	1.46	1.50
38	Z	609	CHL	CBD-CGD	-2.11	1.49	1.52
27	5	611	CLA	CMC-C2C	-2.11	1.46	1.50
36	4	620	XAT	O4-C5	-2.11	1.43	1.46
27	W	603	CLA	C1B-NB	-2.11	1.35	1.37
27	5	614	CLA	CMC-C2C	-2.11	1.46	1.50
27	A	815	CLA	C3B-C4B	2.11	1.48	1.42
27	Y	604	CLA	CMB-C2B	-2.11	1.46	1.50
27	9	613	CLA	C3B-C4B	2.11	1.48	1.42
27	B	838	CLA	MG-NB	-2.11	2.01	2.05
27	6	614	CLA	CMC-C2C	-2.11	1.46	1.50
27	a	609	CLA	C3B-C4B	2.11	1.48	1.42
38	X	605	CHL	CMC-C2C	2.10	1.49	1.44
27	3	612	CLA	CMB-C2B	-2.10	1.46	1.50
27	4	618	CLA	CMD-C2D	-2.10	1.46	1.50
27	G	203	CLA	CMB-C2B	-2.10	1.46	1.50
27	4	612	CLA	CMD-C2D	-2.10	1.46	1.50
27	7	616	CLA	CMB-C2B	-2.10	1.46	1.50
27	3	606	CLA	MG-NB	-2.10	2.01	2.05
27	1	602	CLA	C3B-C4B	2.10	1.48	1.42
27	1	614	CLA	CMC-C2C	-2.10	1.46	1.50
27	B	824	CLA	MG-NB	-2.10	2.01	2.05
27	A	811	CLA	C3B-C4B	2.10	1.48	1.42
27	B	810	CLA	CMC-C2C	-2.10	1.46	1.50
27	B	828	CLA	MG-NB	-2.10	2.01	2.05
27	6	618	CLA	CMC-C2C	-2.10	1.46	1.50
27	2	604	CLA	CHC-C1C	2.10	1.42	1.38
27	7	603	CLA	C3B-C4B	2.10	1.48	1.42
27	U	614	CLA	C3B-C4B	2.10	1.48	1.42
27	K	203	CLA	CHC-C1C	2.10	1.42	1.38
27	X	604	CLA	CHC-C1C	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	616	CLA	CMC-C2C	-2.10	1.46	1.50
27	4	607	CLA	CMC-C2C	-2.10	1.46	1.50
27	L	307	CLA	C3B-C4B	2.10	1.48	1.42
27	A	832	CLA	C3B-C4B	2.10	1.48	1.42
27	U	611	CLA	MG-NB	-2.10	2.01	2.05
38	Y	609	CHL	CBD-CGD	-2.10	1.49	1.52
38	X	601	CHL	CMC-C2C	2.10	1.49	1.44
27	8	604	CLA	CMC-C2C	-2.10	1.46	1.50
27	9	612	CLA	CMB-C2B	-2.10	1.46	1.50
27	a	614	CLA	CHC-C1C	2.10	1.42	1.38
27	V	614	CLA	MG-NB	-2.10	2.01	2.05
27	B	838	CLA	CMC-C2C	-2.10	1.46	1.50
27	1	606	CLA	CMC-C2C	-2.10	1.46	1.50
27	A	816	CLA	C3B-C4B	2.10	1.48	1.42
30	B	845	BCR	C1-C6	-2.10	1.51	1.53
27	X	611	CLA	CHC-C1C	2.10	1.42	1.38
27	7	614	CLA	MG-NB	-2.10	2.01	2.05
30	O	2004	BCR	C1-C6	-2.10	1.51	1.53
27	a	602	CLA	MG-NB	-2.10	2.01	2.05
27	4	606	CLA	C3B-C4B	2.09	1.48	1.42
27	A	832	CLA	CMC-C2C	-2.09	1.46	1.50
27	A	819	CLA	MG-ND	-2.09	2.01	2.05
27	A	806	CLA	C3B-C4B	2.09	1.48	1.42
27	2	614	CLA	C3B-C4B	2.09	1.48	1.42
35	3	618	LUT	C1-C6	-2.09	1.51	1.53
27	H	203	CLA	C3B-C4B	2.09	1.48	1.42
27	A	829	CLA	CHC-C1C	2.09	1.42	1.38
27	A	840	CLA	MG-NB	-2.09	2.01	2.05
27	B	823	CLA	CMC-C2C	-2.09	1.46	1.50
27	H	202	CLA	CMD-C2D	-2.09	1.46	1.50
27	B	816	CLA	CMC-C2C	-2.09	1.46	1.50
27	X	602	CLA	CMC-C2C	-2.09	1.46	1.50
27	A	834	CLA	C3B-C4B	2.09	1.48	1.42
27	A	837	CLA	CMC-C2C	-2.09	1.46	1.50
28	B	842	PQN	C2-C1	2.09	1.52	1.47
27	B	817	CLA	CMC-C2C	-2.09	1.46	1.50
27	X	611	CLA	CMD-C2D	-2.09	1.46	1.50
27	3	603	CLA	MG-NB	-2.09	2.01	2.05
27	Y	610	CLA	CMB-C2B	-2.09	1.46	1.50
27	B	817	CLA	C1B-C2B	2.09	1.48	1.43
27	B	820	CLA	MG-NB	-2.09	2.01	2.05
27	B	826	CLA	CMC-C2C	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	806	CLA	C3B-C4B	2.09	1.48	1.42
27	A	843	CLA	CHC-C1C	2.09	1.42	1.38
27	X	613	CLA	CHC-C1C	2.09	1.42	1.38
27	H	202	CLA	CMC-C2C	-2.09	1.46	1.50
27	7	602	CLA	CHC-C1C	2.09	1.42	1.38
27	6	620	CLA	CMB-C2B	-2.09	1.46	1.50
27	A	842	CLA	C3B-C4B	2.09	1.48	1.42
27	B	837	CLA	C3B-C4B	2.09	1.48	1.42
27	G	204	CLA	CMC-C2C	-2.08	1.46	1.50
27	U	604	CLA	CMC-C2C	-2.08	1.46	1.50
36	1	618	XAT	O4-C5	-2.08	1.43	1.46
27	L	302	CLA	CMC-C2C	-2.08	1.46	1.50
27	3	611	CLA	CMD-C2D	-2.08	1.46	1.50
27	4	609	CLA	C3B-C4B	2.08	1.48	1.42
27	V	612	CLA	MG-NB	-2.08	2.01	2.05
27	8	601	CLA	C3B-C4B	2.08	1.48	1.42
27	9	604	CLA	CHC-C1C	2.08	1.42	1.38
27	Y	613	CLA	CHC-C1C	2.08	1.42	1.38
30	A	848	BCR	C30-C25	-2.08	1.51	1.53
35	Y	1620	LUT	C22-C21	-2.08	1.52	1.54
27	B	839	CLA	C3B-C4B	2.08	1.48	1.42
27	K	201	CLA	C3B-C4B	2.08	1.48	1.42
27	X	612	CLA	CMB-C2B	-2.08	1.46	1.50
27	U	612	CLA	MG-NB	-2.08	2.01	2.05
27	B	810	CLA	MG-NB	-2.08	2.01	2.05
38	Z	608	CHL	CMC-C2C	2.08	1.49	1.44
27	A	841	CLA	CMC-C2C	-2.08	1.46	1.50
27	X	613	CLA	CMD-C2D	-2.08	1.46	1.50
27	B	836	CLA	C1B-NB	-2.08	1.35	1.37
27	B	817	CLA	C3B-C4B	2.07	1.48	1.42
38	Z	606	CHL	CMC-C2C	2.07	1.49	1.44
35	6	619	LUT	C1-C6	-2.07	1.51	1.53
27	B	831	CLA	CMC-C2C	-2.07	1.46	1.50
27	X	604	CLA	CMD-C2D	-2.07	1.46	1.50
27	K	206	CLA	C3B-C4B	2.07	1.48	1.42
27	a	607	CLA	C3B-C4B	2.07	1.48	1.42
27	B	840	CLA	CMC-C2C	-2.07	1.46	1.50
27	a	608	CLA	CMC-C2C	-2.07	1.46	1.50
27	X	614	CLA	CMD-C2D	-2.07	1.46	1.50
27	W	604	CLA	CMC-C2C	-2.07	1.46	1.50
27	G	204	CLA	MG-NB	-2.07	2.01	2.05
27	6	618	CLA	CHC-C1C	2.07	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	616	CLA	CMB-C2B	-2.07	1.46	1.50
27	B	828	CLA	C3B-C4B	2.07	1.48	1.42
27	Y	604	CLA	CMD-C2D	-2.07	1.46	1.50
27	Y	613	CLA	CMB-C2B	-2.07	1.46	1.50
27	B	827	CLA	MG-NB	-2.07	2.01	2.05
27	9	611	CLA	CHC-C1C	2.07	1.42	1.38
38	Z	601	CHL	CBD-CGD	-2.07	1.49	1.52
27	2	603	CLA	MG-NB	-2.07	2.01	2.05
27	A	828	CLA	CHC-C1C	2.07	1.42	1.38
27	3	617	CLA	C3B-C4B	2.07	1.48	1.42
27	2	611	CLA	CMC-C2C	-2.07	1.46	1.50
27	7	601	CLA	MG-NB	-2.07	2.01	2.05
27	W	611	CLA	MG-NB	-2.07	2.01	2.05
27	6	616	CLA	CMC-C2C	-2.07	1.46	1.50
27	X	613	CLA	CMB-C2B	-2.07	1.46	1.50
27	V	602	CLA	MG-NB	-2.07	2.01	2.05
27	A	807	CLA	CHC-C1C	2.07	1.42	1.38
30	7	621	BCR	C1-C6	-2.06	1.51	1.53
27	2	607	CLA	CMC-C2C	-2.06	1.46	1.50
27	9	602	CLA	MG-NB	-2.06	2.01	2.05
27	7	614	CLA	CHC-C1C	2.06	1.42	1.38
27	1	601	CLA	CMC-C2C	-2.06	1.46	1.50
27	2	602	CLA	CHC-C1C	2.06	1.42	1.38
27	X	612	CLA	CMD-C2D	-2.06	1.46	1.50
27	2	607	CLA	CHC-C1C	2.06	1.42	1.38
27	W	610	CLA	MG-NB	-2.06	2.01	2.05
27	4	612	CLA	CMC-C2C	-2.06	1.46	1.50
27	5	614	CLA	CMB-C2B	-2.06	1.46	1.50
27	X	604	CLA	CMB-C2B	-2.06	1.46	1.50
35	Z	1621	LUT	C22-C21	-2.06	1.52	1.54
27	A	804	CLA	C3B-C4B	2.06	1.48	1.42
27	W	612	CLA	MG-NB	-2.06	2.01	2.05
27	4	614	CLA	CHC-C1C	2.06	1.42	1.38
38	Z	607	CHL	CBD-CGD	-2.06	1.49	1.52
27	A	840	CLA	C3B-C4B	2.06	1.48	1.42
27	Y	604	CLA	CHC-C1C	2.06	1.42	1.38
27	4	601	CLA	CMC-C2C	-2.06	1.46	1.50
36	9	620	XAT	C22-C21	-2.06	1.51	1.54
30	B	853	BCR	C1-C6	-2.06	1.51	1.53
38	W	609	CHL	CMC-C2C	2.06	1.49	1.44
27	B	836	CLA	MG-NB	-2.06	2.01	2.05
27	5	607	CLA	MG-NB	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	818	CLA	CMB-C2B	-2.06	1.46	1.50
27	6	611	CLA	CMC-C2C	-2.06	1.46	1.50
27	9	603	CLA	CMC-C2C	-2.06	1.46	1.50
27	2	613	CLA	C3B-C4B	2.06	1.48	1.42
27	a	606	CLA	MG-NB	-2.06	2.01	2.05
27	H	203	CLA	CMC-C2C	-2.06	1.46	1.50
27	3	607	CLA	CMC-C2C	-2.06	1.46	1.50
27	9	601	CLA	CMC-C2C	-2.05	1.46	1.50
27	V	611	CLA	C3B-C4B	2.05	1.48	1.42
38	W	601	CHL	CMC-C2C	2.05	1.49	1.44
30	B	847	BCR	C1-C6	-2.05	1.51	1.53
27	Z	612	CLA	CMD-C2D	-2.05	1.46	1.50
27	B	813	CLA	CHC-C1C	2.05	1.42	1.38
27	A	806	CLA	MG-NB	-2.05	2.01	2.05
27	B	826	CLA	MG-NB	-2.05	2.01	2.05
27	G	203	CLA	CMC-C2C	-2.05	1.46	1.50
27	B	805	CLA	MG-NB	-2.05	2.01	2.05
27	9	612	CLA	CMC-C2C	-2.05	1.46	1.50
27	A	827	CLA	C3B-C4B	2.05	1.48	1.42
27	K	206	CLA	CMC-C2C	-2.05	1.46	1.50
27	6	611	CLA	CHC-C1C	2.05	1.42	1.38
27	7	616	CLA	CHC-C1C	2.05	1.42	1.38
27	3	614	CLA	MG-NB	-2.05	2.01	2.05
27	A	810	CLA	CHC-C1C	2.05	1.42	1.38
27	4	606	CLA	CMC-C2C	-2.05	1.46	1.50
27	6	601	CLA	C3B-C4B	2.05	1.48	1.42
27	6	606	CLA	CMC-C2C	-2.05	1.46	1.50
27	X	603	CLA	CHC-C1C	2.05	1.42	1.38
27	1	607	CLA	CMB-C2B	-2.05	1.46	1.50
27	X	613	CLA	CMC-C2C	-2.05	1.46	1.50
27	2	601	CLA	CMD-C2D	-2.05	1.46	1.50
27	8	606	CLA	MG-NB	-2.04	2.01	2.05
27	G	204	CLA	C3B-C4B	2.04	1.48	1.42
27	W	602	CLA	C3B-C4B	2.04	1.48	1.42
27	Y	612	CLA	CMB-C2B	-2.04	1.46	1.50
27	B	826	CLA	CHC-C1C	2.04	1.42	1.38
27	2	607	CLA	MG-NB	-2.04	2.01	2.05
27	7	602	CLA	MG-NB	-2.04	2.01	2.05
36	5	621	XAT	C22-C21	-2.04	1.51	1.54
27	U	604	CLA	C3B-C4B	2.04	1.48	1.42
27	B	802	CLA	MG-NB	-2.04	2.01	2.05
27	5	609	CLA	C3B-C4B	2.04	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	815	CLA	MG-NB	-2.04	2.01	2.05
27	A	842	CLA	MG-NB	-2.04	2.01	2.05
27	2	602	CLA	MG-NB	-2.04	2.01	2.05
27	X	610	CLA	CMB-C2B	-2.04	1.46	1.50
27	Y	614	CLA	CMB-C2B	-2.04	1.46	1.50
27	U	611	CLA	C3B-C4B	2.04	1.48	1.42
27	7	604	CLA	CHC-C1C	2.04	1.42	1.38
38	X	609	CHL	CMC-C2C	2.04	1.49	1.44
27	2	609	CLA	CHC-C1C	2.04	1.42	1.38
30	3	621	BCR	C1-C6	-2.04	1.51	1.53
27	1	603	CLA	MG-NB	-2.04	2.01	2.05
27	X	611	CLA	CMB-C2B	-2.04	1.46	1.50
27	8	611	CLA	CHC-C1C	2.04	1.42	1.38
38	U	609	CHL	CMC-C2C	2.04	1.49	1.44
27	A	845	CLA	C3B-C4B	2.04	1.48	1.42
27	1	606	CLA	MG-NB	-2.04	2.01	2.05
27	Y	613	CLA	CMC-C2C	-2.04	1.46	1.50
27	Z	612	CLA	CHC-C1C	2.04	1.42	1.38
27	A	829	CLA	MG-NB	-2.04	2.01	2.05
27	a	616	CLA	CMC-C2C	-2.04	1.46	1.50
27	5	619	CLA	CMC-C2C	-2.04	1.46	1.50
35	X	1620	LUT	C22-C21	-2.04	1.52	1.54
27	1	601	CLA	CHC-C1C	2.04	1.42	1.38
27	A	838	CLA	CMC-C2C	-2.04	1.46	1.50
27	7	608	CLA	C3B-C4B	2.04	1.48	1.42
27	5	602	CLA	CHC-C1C	2.04	1.42	1.38
38	W	609	CHL	CBD-CGD	-2.03	1.49	1.52
38	Y	609	CHL	CMC-C2C	2.03	1.49	1.44
27	B	817	CLA	MG-NB	-2.03	2.01	2.05
35	V	1620	LUT	C1-C6	-2.03	1.51	1.53
27	4	616	CLA	CHC-C1C	2.03	1.42	1.38
27	W	604	CLA	C3B-C4B	2.03	1.48	1.42
27	B	811	CLA	MG-NB	-2.03	2.01	2.05
27	2	606	CLA	MG-NB	-2.03	2.01	2.05
30	K	207	BCR	C30-C25	-2.03	1.51	1.53
27	Z	611	CLA	CMD-C2D	-2.03	1.46	1.50
27	B	812	CLA	CHC-C1C	2.03	1.42	1.38
27	A	841	CLA	CHC-C1C	2.03	1.42	1.38
27	9	607	CLA	MG-NB	-2.03	2.01	2.05
27	A	837	CLA	C3B-C4B	2.03	1.48	1.42
33	V	2631	LMG	O1-C1	2.03	1.43	1.40
27	5	610	CLA	CHC-C1C	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	608	CLA	CHC-C1C	2.03	1.42	1.38
27	A	827	CLA	MG-NB	-2.03	2.01	2.05
36	3	619	XAT	O24-C25	-2.03	1.43	1.46
27	U	603	CLA	CAC-C3C	-2.03	1.45	1.51
27	Z	613	CLA	CMC-C2C	-2.03	1.46	1.50
27	B	833	CLA	CHC-C1C	2.03	1.42	1.38
27	6	612	CLA	CMC-C2C	-2.03	1.46	1.50
27	X	614	CLA	CMB-C2B	-2.03	1.46	1.50
27	O	2003	CLA	CHC-C1C	2.03	1.42	1.38
27	6	616	CLA	CHC-C1C	2.03	1.42	1.38
27	U	610	CLA	MG-NB	-2.03	2.01	2.05
27	2	601	CLA	CHC-C1C	2.03	1.42	1.38
27	A	804	CLA	MG-NB	-2.03	2.01	2.05
27	F	301	CLA	MG-NB	-2.03	2.01	2.05
38	Z	609	CHL	CMC-C2C	2.03	1.49	1.44
27	W	611	CLA	C3B-C4B	2.03	1.48	1.42
30	B	844	BCR	C1-C6	-2.03	1.51	1.53
27	A	839	CLA	MG-NB	-2.02	2.01	2.05
27	4	613	CLA	CHC-C1C	2.02	1.42	1.38
38	U	609	CHL	CBD-CGD	-2.02	1.50	1.52
36	X	1622	XAT	O4-C5	-2.02	1.43	1.46
27	9	611	CLA	CMC-C2C	-2.02	1.46	1.50
27	B	821	CLA	MG-NB	-2.02	2.01	2.05
36	V	1622	XAT	O24-C25	-2.02	1.43	1.46
27	9	606	CLA	CHC-C1C	2.02	1.42	1.38
36	V	1622	XAT	C22-C21	-2.02	1.51	1.54
37	Z	1623	NEX	O24-C25	-2.02	1.43	1.46
27	4	614	CLA	CMC-C2C	-2.02	1.46	1.50
27	8	616	CLA	CMC-C2C	-2.02	1.46	1.50
27	9	603	CLA	C3B-C2B	-2.02	1.36	1.44
27	a	616	CLA	CHC-C1C	2.02	1.42	1.38
27	2	611	CLA	CHC-C1C	2.02	1.42	1.38
38	Z	601	CHL	CMC-C2C	2.02	1.49	1.44
27	Y	602	CLA	CMC-C2C	-2.02	1.46	1.50
27	B	837	CLA	MG-NB	-2.02	2.01	2.05
27	8	608	CLA	MG-NB	-2.02	2.01	2.05
27	O	2001	CLA	CHC-C1C	2.02	1.42	1.38
27	4	616	CLA	CMC-C2C	-2.02	1.46	1.50
27	A	833	CLA	C3B-C4B	2.02	1.48	1.42
27	4	602	CLA	CHC-C1C	2.02	1.42	1.38
27	B	834	CLA	CMC-C2C	-2.02	1.46	1.50
27	6	618	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	608	CLA	C3B-C4B	2.02	1.48	1.42
27	H	202	CLA	C3B-C4B	2.02	1.48	1.42
27	A	835	CLA	MG-NB	-2.02	2.01	2.05
27	8	602	CLA	MG-NB	-2.01	2.01	2.05
27	V	602	CLA	MG-ND	-2.01	2.01	2.05
27	a	611	CLA	MG-NB	-2.01	2.01	2.05
30	3	621	BCR	C30-C25	-2.01	1.51	1.53
27	5	614	CLA	CHC-C1C	2.01	1.42	1.38
27	Y	603	CLA	CHC-C1C	2.01	1.42	1.38
27	4	607	CLA	C3B-C4B	2.01	1.48	1.42
27	2	601	CLA	CMB-C2B	-2.01	1.46	1.50
27	B	831	CLA	CHC-C1C	2.01	1.42	1.38
27	Z	613	CLA	CHC-C1C	2.01	1.42	1.38
27	Z	603	CLA	MG-NB	-2.01	2.01	2.05
27	B	818	CLA	C3B-C4B	2.01	1.48	1.42
27	7	615	CLA	CMC-C2C	-2.01	1.46	1.50
27	Z	603	CLA	C3B-C4B	2.01	1.48	1.42
27	B	814	CLA	CHC-C1C	2.01	1.42	1.38
27	F	301	CLA	CMC-C2C	-2.01	1.46	1.50
27	A	826	CLA	C1B-NB	-2.01	1.35	1.37
27	8	610	CLA	CHC-C1C	2.01	1.42	1.38
27	8	614	CLA	CHC-C1C	2.01	1.42	1.38
27	a	603	CLA	MG-NB	-2.01	2.01	2.05
27	1	601	CLA	MG-NB	-2.01	2.01	2.05
27	9	602	CLA	CHC-C1C	2.01	1.42	1.38
27	Z	613	CLA	CMB-C2B	-2.01	1.46	1.50
38	Y	605	CHL	CMC-C2C	2.01	1.49	1.44
27	6	606	CLA	MG-NB	-2.01	2.01	2.05
27	K	204	CLA	MG-NB	-2.01	2.01	2.05
27	B	835	CLA	CMC-C2C	-2.01	1.46	1.50
27	6	609	CLA	MG-NB	-2.01	2.01	2.05
27	F	304	CLA	CHC-C1C	2.01	1.42	1.38
27	2	616	CLA	CHC-C1C	2.01	1.42	1.38
27	A	854	CLA	CHC-C1C	2.00	1.42	1.38
38	V	606	CHL	CBD-CAD	-2.00	1.46	1.53
27	K	201	CLA	CMC-C2C	-2.00	1.46	1.50
27	Y	611	CLA	CMB-C2B	-2.00	1.46	1.50
27	A	803	CLA	C3B-C4B	2.00	1.48	1.42
27	B	803	CLA	MG-NB	-2.00	2.01	2.05
27	5	618	CLA	MG-NB	-2.00	2.01	2.05
27	8	614	CLA	MG-NB	-2.00	2.01	2.05
27	8	602	CLA	CHC-C1C	2.00	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	4	619	LUT	C22-C21	-2.00	1.52	1.54
27	3	613	CLA	CHC-C1C	2.00	1.42	1.38
27	Z	604	CLA	CMD-C2D	-2.00	1.46	1.50
27	W	603	CLA	CAC-C3C	-2.00	1.46	1.51
30	8	621	BCR	C1-C6	-2.00	1.51	1.53
27	F	303	CLA	MG-NB	-2.00	2.01	2.05

All (3890) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	W	606	CHL	O2A-CGA-O1A	-17.09	79.39	123.33
30	B	852	BCR	C32-C1-C6	-15.22	86.38	110.24
38	W	606	CHL	O2A-CGA-CBA	14.67	160.37	114.00
30	6	622	BCR	C40-C30-C25	-14.46	87.56	110.24
36	U	1622	XAT	C37-C21-C36	-14.22	86.72	107.37
36	W	1622	XAT	C37-C21-C36	-14.20	86.74	107.37
36	Y	1622	XAT	C37-C21-C36	-14.04	86.97	107.37
36	X	1622	XAT	C37-C21-C36	-14.01	87.02	107.37
36	Z	1622	XAT	C37-C21-C36	-13.84	87.26	107.37
38	W	606	CHL	O1A-CGA-CBA	-13.27	81.00	123.09
30	3	620	BCR	C7-C8-C9	12.75	145.10	126.23
36	U	1622	XAT	C37-C21-C22	-12.64	86.76	108.97
36	W	1622	XAT	C37-C21-C22	-12.63	86.76	108.97
30	3	620	BCR	C40-C30-C25	-12.38	90.83	110.24
36	Z	1622	XAT	C37-C21-C22	-12.20	87.53	108.97
36	X	1622	XAT	C37-C21-C22	-12.15	87.61	108.97
36	Y	1622	XAT	C37-C21-C22	-12.13	87.65	108.97
30	O	2005	BCR	C40-C30-C25	-11.51	92.19	110.24
30	6	622	BCR	C39-C30-C25	11.47	128.22	110.24
30	K	207	BCR	C40-C30-C25	-10.95	93.06	110.24
38	U	601	CHL	C1B-CHB-C4A	9.83	127.64	121.32
38	W	601	CHL	C1B-CHB-C4A	9.70	127.56	121.32
38	Y	601	CHL	C1B-CHB-C4A	9.70	127.56	121.32
38	Z	607	CHL	C1B-CHB-C4A	9.64	127.52	121.32
38	X	605	CHL	O2D-CGD-CBD	9.43	121.31	110.95
38	Y	605	CHL	O2D-CGD-CBD	9.39	121.26	110.95
38	X	601	CHL	C1B-CHB-C4A	9.25	127.27	121.32
30	3	620	BCR	C4-C5-C6	-9.15	110.34	122.70
38	V	601	CHL	C1B-CHB-C4A	9.08	127.17	121.32
30	3	620	BCR	C39-C30-C25	9.03	124.41	110.24
38	Z	601	CHL	C1B-CHB-C4A	8.99	127.10	121.32
38	W	605	CHL	O2D-CGD-CBD	8.92	120.75	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	U	605	CHL	O2D-CGD-CBD	8.92	120.74	110.95
30	B	852	BCR	C32-C1-C31	-8.86	83.26	108.63
38	W	607	CHL	O2D-CGD-CBD	8.81	120.63	110.95
38	V	609	CHL	O2D-CGD-CBD	8.77	120.58	110.95
38	Y	607	CHL	O2D-CGD-CBD	8.44	120.22	110.95
38	Z	609	CHL	O2D-CGD-CBD	8.39	120.16	110.95
30	O	2004	BCR	C33-C5-C6	8.37	133.62	124.48
38	U	609	CHL	O2D-CGD-CBD	8.34	120.11	110.95
38	X	607	CHL	C1B-CHB-C4A	8.33	126.68	121.32
38	Y	609	CHL	O2D-CGD-CBD	8.26	120.03	110.95
38	X	601	CHL	O2D-CGD-CBD	8.14	119.89	110.95
38	X	609	CHL	O2D-CGD-CBD	8.14	119.89	110.95
38	Y	606	CHL	O2D-CGD-CBD	8.13	119.88	110.95
38	X	606	CHL	O2D-CGD-CBD	8.12	119.87	110.95
38	W	609	CHL	O2D-CGD-CBD	8.09	119.83	110.95
38	U	607	CHL	O2D-CGD-CBD	8.08	119.82	110.95
38	Z	601	CHL	O2D-CGD-CBD	8.07	119.81	110.95
30	3	620	BCR	C30-C25-C26	-8.03	111.67	122.64
38	Z	606	CHL	O2D-CGD-CBD	7.90	119.63	110.95
38	X	607	CHL	O2D-CGD-CBD	7.88	119.60	110.95
38	V	606	CHL	OBD-CAD-C3D	-7.84	115.66	127.89
35	5	620	LUT	C8-C7-C6	-7.84	106.06	127.00
38	Z	607	CHL	O2D-CGD-CBD	7.83	119.55	110.95
38	V	601	CHL	O2D-CGD-CBD	7.79	119.51	110.95
30	O	2005	BCR	C39-C30-C25	7.76	122.41	110.24
38	X	608	CHL	O2D-CGD-CBD	7.75	119.46	110.95
38	Y	601	CHL	O2D-CGD-CBD	7.73	119.44	110.95
38	V	606	CHL	CHA-C1A-C2A	-7.71	115.20	133.31
30	3	620	BCR	C23-C24-C25	-7.71	106.40	127.00
38	Z	605	CHL	O2D-CGD-CBD	7.69	119.40	110.95
38	X	606	CHL	CHA-C1A-C2A	-7.68	115.27	133.31
38	Z	606	CHL	CHA-C1A-C2A	-7.66	115.32	133.31
38	U	606	CHL	OBD-CAD-C3D	-7.66	115.95	127.89
38	U	605	CHL	CHA-C1A-C2A	-7.64	115.38	133.31
38	Y	606	CHL	CHA-C1A-C2A	-7.63	115.39	133.31
38	W	605	CHL	CHA-C1A-C2A	-7.63	115.39	133.31
36	U	1622	XAT	C36-C21-C22	7.62	122.36	108.97
38	W	601	CHL	O2D-CGD-CBD	7.62	119.32	110.95
36	W	1622	XAT	C36-C21-C22	7.62	122.36	108.97
38	W	606	CHL	OBD-CAD-C3D	-7.59	116.05	127.89
38	U	601	CHL	O2D-CGD-CBD	7.58	119.28	110.95
30	3	620	BCR	C34-C9-C8	7.56	129.63	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	Y	1622	XAT	C36-C21-C22	7.54	122.23	108.97
36	X	1622	XAT	C36-C21-C22	7.54	122.21	108.97
38	V	608	CHL	CHA-C1A-C2A	-7.51	115.67	133.31
38	W	608	CHL	CHA-C1A-C2A	-7.51	115.68	133.31
38	V	607	CHL	CHA-C1A-C2A	-7.50	115.71	133.31
38	V	605	CHL	O2D-CGD-CBD	7.49	119.18	110.95
35	2	619	LUT	C8-C7-C6	-7.48	107.01	127.00
38	X	605	CHL	CHA-C1A-C2A	-7.48	115.74	133.31
38	U	608	CHL	CHA-C1A-C2A	-7.48	115.75	133.31
38	Y	608	CHL	CHA-C1A-C2A	-7.46	115.80	133.31
38	W	606	CHL	CHA-C1A-C2A	-7.44	115.83	133.31
38	U	606	CHL	CHA-C1A-C2A	-7.44	115.85	133.31
38	Z	605	CHL	CHA-C1A-C2A	-7.43	115.87	133.31
38	Z	608	CHL	O2D-CGD-CBD	7.39	119.07	110.95
35	W	1620	LUT	C8-C7-C6	-7.38	107.29	127.00
38	X	606	CHL	OBD-CAD-C3D	-7.38	116.39	127.89
35	U	1620	LUT	C8-C7-C6	-7.37	107.32	127.00
38	Z	608	CHL	CHA-C1A-C2A	-7.36	116.02	133.31
37	W	1623	NEX	O24-C25-C24	7.34	120.37	113.49
37	U	1623	NEX	O24-C25-C24	7.33	120.36	113.49
30	3	620	BCR	C40-C30-C39	-7.33	87.66	108.63
38	U	606	CHL	O2D-CGD-CBD	7.32	118.99	110.95
38	Y	606	CHL	OBD-CAD-C3D	-7.31	116.49	127.89
38	W	606	CHL	O2D-CGD-CBD	7.28	118.94	110.95
38	W	609	CHL	C1B-CHB-C4A	7.28	126.00	121.32
30	8	621	BCR	C8-C7-C6	-7.25	107.62	127.00
37	V	1623	NEX	O24-C25-C24	7.24	120.28	113.49
35	7	619	LUT	C8-C7-C6	-7.24	107.66	127.00
30	B	852	BCR	C31-C1-C6	7.23	121.59	110.24
38	V	605	CHL	CHA-C1A-C2A	-7.22	116.35	133.31
35	X	1620	LUT	C8-C7-C6	-7.21	107.75	127.00
35	Y	1620	LUT	C8-C7-C6	-7.20	107.77	127.00
38	Y	608	CHL	O2D-CGD-CBD	7.18	118.84	110.95
30	J	102	BCR	C28-C27-C26	-7.17	101.27	114.06
38	Z	605	CHL	OBD-CAD-C3D	-7.17	116.71	127.89
36	Z	1622	XAT	C36-C21-C22	7.16	121.56	108.97
37	X	1623	NEX	O24-C25-C24	7.16	120.20	113.49
37	Y	1623	NEX	O24-C25-C24	7.15	120.19	113.49
30	6	622	BCR	C40-C30-C39	-7.05	88.44	108.63
38	Z	606	CHL	OBD-CAD-C3D	-7.05	116.89	127.89
38	W	605	CHL	OBD-CAD-C3D	-7.01	116.96	127.89
38	X	605	CHL	OBD-CAD-C3D	-7.00	116.98	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	U	605	CHL	OBD-CAD-C3D	-6.99	116.98	127.89
38	Y	605	CHL	OBD-CAD-C3D	-6.99	116.99	127.89
36	V	1622	XAT	C38-C25-C26	-6.97	110.83	122.30
30	B	849	BCR	C23-C24-C25	-6.96	108.40	127.00
37	Z	1623	NEX	O24-C25-C24	6.96	120.01	113.49
30	3	620	BCR	C8-C9-C10	-6.96	108.07	119.01
38	V	605	CHL	OBD-CAD-C3D	-6.94	117.06	127.89
38	W	608	CHL	O2D-CGD-CBD	6.94	118.58	110.95
36	X	1622	XAT	O24-C25-C24	6.94	120.00	113.49
36	Y	1622	XAT	O24-C25-C24	6.93	119.99	113.49
38	U	608	CHL	O2D-CGD-CBD	6.93	118.56	110.95
38	V	607	CHL	OBD-CAD-C3D	-6.92	117.09	127.89
38	Y	608	CHL	OBD-CAD-C3D	-6.89	117.15	127.89
30	O	2004	BCR	C4-C5-C6	-6.88	113.40	122.70
36	W	1622	XAT	O24-C25-C24	6.88	119.94	113.49
38	V	608	CHL	OBD-CAD-C3D	-6.85	117.20	127.89
38	Z	608	CHL	OBD-CAD-C3D	-6.84	117.22	127.89
38	V	608	CHL	O2D-CGD-CBD	6.83	118.46	110.95
35	6	619	LUT	C8-C7-C6	-6.81	108.81	127.00
38	V	606	CHL	O2D-CGD-CBD	6.81	118.43	110.95
38	U	609	CHL	C1B-CHB-C4A	6.80	125.70	121.32
36	U	1622	XAT	O24-C25-C24	6.79	119.86	113.49
30	K	207	BCR	C40-C30-C39	-6.76	89.28	108.63
38	X	609	CHL	C1B-CHB-C4A	6.75	125.67	121.32
38	V	607	CHL	O2D-CGD-CBD	6.71	118.32	110.95
38	W	608	CHL	OBD-CAD-C3D	-6.68	117.47	127.89
30	2	623	BCR	C28-C27-C26	-6.67	102.17	114.06
38	U	607	CHL	OBD-CAD-C3D	-6.66	117.50	127.89
38	U	607	CHL	CHA-C1A-C2A	-6.66	117.66	133.31
38	U	608	CHL	OBD-CAD-C3D	-6.66	117.50	127.89
30	O	2005	BCR	C40-C30-C39	-6.62	89.67	108.63
30	5	622	BCR	C40-C30-C25	6.58	120.56	110.24
27	V	603	CLA	C4A-NA-C1A	6.53	109.66	106.68
38	Z	607	CHL	C4D-ND-C1D	-6.52	100.27	105.22
30	6	622	BCR	C30-C25-C26	-6.51	113.73	122.64
30	O	2004	BCR	C8-C7-C6	-6.51	109.61	127.00
30	L	301	BCR	C8-C7-C6	-6.48	109.70	127.00
36	W	1622	XAT	C38-C25-C26	-6.47	111.66	122.30
36	V	1622	XAT	O24-C25-C24	6.47	119.55	113.49
30	3	622	BCR	C3-C4-C5	-6.44	102.57	114.06
27	A	815	CLA	C4A-NA-C1A	6.44	109.62	106.68
36	U	1622	XAT	C38-C25-C26	-6.42	111.74	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	846	BCR	C23-C24-C25	-6.32	110.10	127.00
27	A	834	CLA	C4A-NA-C1A	6.32	109.56	106.68
30	3	622	BCR	C38-C26-C25	-6.30	117.61	124.48
30	4	621	BCR	C40-C30-C25	6.30	120.13	110.24
27	Z	603	CLA	C4A-NA-C1A	6.24	109.53	106.68
35	5	620	LUT	C21-C26-C27	-6.24	105.65	112.83
36	W	1622	XAT	C18-C5-C6	-6.24	112.04	122.30
30	F	305	BCR	C28-C27-C26	-6.20	103.00	114.06
36	U	1622	XAT	C18-C5-C6	-6.18	112.13	122.30
38	X	601	CHL	C4D-ND-C1D	-6.16	100.54	105.22
30	8	621	BCR	C40-C30-C25	6.15	119.89	110.24
35	Y	1620	LUT	C21-C26-C27	-6.15	105.76	112.83
36	V	1622	XAT	C18-C5-C6	-6.14	112.19	122.30
38	W	601	CHL	C4D-ND-C1D	-6.11	100.58	105.22
30	8	621	BCR	C23-C24-C25	-6.10	110.69	127.00
38	Y	601	CHL	C4D-ND-C1D	-6.09	100.60	105.22
38	V	601	CHL	C4D-ND-C1D	-6.07	100.61	105.22
38	U	601	CHL	C4D-ND-C1D	-6.07	100.62	105.22
30	A	856	BCR	C8-C7-C6	-6.06	110.81	127.00
35	X	1620	LUT	C21-C26-C27	-6.06	105.86	112.83
27	B	806	CLA	C4A-NA-C1A	6.05	109.44	106.68
36	7	620	XAT	O4-C5-C4	6.04	119.15	113.49
27	B	840	CLA	C4A-NA-C1A	6.03	109.43	106.68
27	7	603	CLA	C4A-NA-C1A	6.03	109.43	106.68
27	8	603	CLA	C4A-NA-C1A	6.03	109.43	106.68
30	O	2005	BCR	C24-C23-C22	-6.02	117.33	126.23
36	5	621	XAT	O4-C5-C4	6.02	119.13	113.49
27	A	809	CLA	C4A-NA-C1A	6.01	109.42	106.68
27	A	806	CLA	C4A-NA-C1A	6.00	109.42	106.68
37	X	1623	NEX	C11-C10-C9	-6.00	118.86	127.28
37	Y	1623	NEX	C11-C10-C9	-6.00	118.87	127.28
36	3	619	XAT	C38-C25-C26	-5.99	112.44	122.30
38	Z	601	CHL	C4D-ND-C1D	-5.96	100.69	105.22
36	Z	1622	XAT	C38-C25-C26	-5.96	112.50	122.30
30	K	207	BCR	C29-C30-C25	5.95	119.08	110.44
27	5	601	CLA	C4A-NA-C1A	5.92	109.38	106.68
27	A	814	CLA	C4A-NA-C1A	5.92	109.38	106.68
36	X	1622	XAT	C38-C25-C26	-5.92	112.56	122.30
30	B	846	BCR	C38-C26-C25	-5.91	118.04	124.48
30	6	622	BCR	C33-C5-C6	-5.90	118.05	124.48
36	Y	1622	XAT	C38-C25-C26	-5.90	112.59	122.30
30	B	849	BCR	C28-C27-C26	-5.90	103.54	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	X	607	CHL	C4D-ND-C1D	-5.88	100.75	105.22
28	A	844	PQN	C11-C12-C13	-5.87	116.71	126.83
27	4	618	CLA	C4A-NA-C1A	5.85	109.35	106.68
27	W	614	CLA	C4A-NA-C1A	5.85	109.35	106.68
37	5	624	NEX	C38-C25-C26	-5.85	112.68	122.30
27	W	603	CLA	C4A-NA-C1A	5.85	109.35	106.68
27	A	821	CLA	C4A-NA-C1A	5.84	109.34	106.68
27	A	819	CLA	C4A-NA-C1A	5.84	109.34	106.68
38	U	601	CHL	CHA-C1A-C2A	-5.84	119.60	133.31
38	X	609	CHL	C4D-ND-C1D	-5.84	100.79	105.22
37	6	624	NEX	C38-C25-C26	-5.83	112.70	122.30
30	B	852	BCR	C33-C5-C6	-5.83	118.12	124.48
30	B	849	BCR	C7-C8-C9	-5.83	117.61	126.23
27	B	837	CLA	C4A-NA-C1A	5.83	109.34	106.68
38	Y	601	CHL	CHA-C1A-C2A	-5.82	119.64	133.31
27	6	618	CLA	C4A-NA-C1A	5.82	109.33	106.68
27	K	204	CLA	C4A-NA-C1A	5.81	109.33	106.68
27	3	603	CLA	C4A-NA-C1A	5.79	109.32	106.68
27	a	603	CLA	C4A-NA-C1A	5.78	109.32	106.68
27	H	203	CLA	C4A-NA-C1A	5.77	109.31	106.68
27	B	838	CLA	C4A-NA-C1A	5.77	109.31	106.68
30	7	621	BCR	C40-C30-C25	5.77	119.29	110.24
30	a	619	BCR	C40-C30-C25	5.77	119.29	110.24
38	U	609	CHL	C4D-ND-C1D	-5.77	100.84	105.22
38	W	609	CHL	C4D-ND-C1D	-5.76	100.85	105.22
38	V	601	CHL	CHA-C1A-C2A	-5.76	119.78	133.31
36	a	618	XAT	O4-C5-C4	5.76	118.89	113.49
30	1	619	BCR	C40-C30-C25	5.76	119.27	110.24
38	W	601	CHL	CHA-C1A-C2A	-5.75	119.80	133.31
38	Z	607	CHL	CHA-C1A-C2A	-5.75	119.81	133.31
27	U	603	CLA	C4A-NA-C1A	5.74	109.30	106.68
27	8	608	CLA	C4A-NA-C1A	5.73	109.30	106.68
27	1	603	CLA	C4A-NA-C1A	5.73	109.29	106.68
36	X	1622	XAT	C18-C5-C6	-5.71	112.90	122.30
27	3	606	CLA	C4A-NA-C1A	5.71	109.28	106.68
36	Y	1622	XAT	C18-C5-C6	-5.69	112.94	122.30
30	B	852	BCR	C32-C1-C2	-5.69	87.11	108.95
27	B	824	CLA	C4A-NA-C1A	5.68	109.27	106.68
38	X	601	CHL	CHA-C1A-C2A	-5.68	119.97	133.31
36	1	618	XAT	O4-C5-C4	5.68	118.81	113.49
27	A	807	CLA	C4A-NA-C1A	5.67	109.27	106.68
30	A	849	BCR	C24-C23-C22	-5.67	117.85	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	3	619	XAT	O24-C25-C24	5.67	118.80	113.49
35	V	1620	LUT	C8-C7-C6	-5.66	111.88	127.00
27	U	614	CLA	C4A-NA-C1A	5.65	109.26	106.68
28	B	842	PQN	C11-C12-C13	-5.65	117.10	126.83
30	A	849	BCR	C28-C27-C26	-5.65	103.98	114.06
36	a	618	XAT	C18-C5-C6	-5.65	113.01	122.30
36	5	621	XAT	C18-C5-C6	-5.65	113.01	122.30
35	U	1620	LUT	C21-C26-C27	-5.64	106.34	112.83
27	U	611	CLA	C4A-NA-C1A	5.64	109.25	106.68
38	U	609	CHL	CHA-C1A-C2A	-5.64	120.06	133.31
27	B	820	CLA	C4A-NA-C1A	5.64	109.25	106.68
27	1	602	CLA	C4A-NA-C1A	5.64	109.25	106.68
36	6	621	XAT	C18-C5-C6	-5.64	113.03	122.30
27	4	603	CLA	C4A-NA-C1A	5.63	109.25	106.68
36	1	618	XAT	C18-C5-C6	-5.63	113.03	122.30
36	Z	1622	XAT	C37-C21-C26	-5.62	94.87	110.05
35	W	1620	LUT	C21-C26-C27	-5.62	106.37	112.83
27	L	306	CLA	C4A-NA-C1A	5.62	109.24	106.68
27	A	817	CLA	C4A-NA-C1A	5.61	109.24	106.68
27	a	602	CLA	C4A-NA-C1A	5.61	109.24	106.68
30	8	621	BCR	C38-C26-C25	-5.61	118.37	124.48
36	5	621	XAT	O24-C25-C24	5.61	118.75	113.49
30	1	619	BCR	C23-C24-C25	-5.60	112.04	127.00
36	7	620	XAT	C18-C5-C6	-5.60	113.09	122.30
30	K	202	BCR	C28-C27-C26	-5.59	104.09	114.06
30	3	620	BCR	C40-C30-C29	-5.59	87.50	108.95
27	A	837	CLA	C4A-NA-C1A	5.59	109.23	106.68
27	3	604	CLA	C4A-NA-C1A	5.59	109.23	106.68
38	X	608	CHL	C4D-ND-C1D	-5.58	100.98	105.22
30	4	621	BCR	C33-C5-C6	-5.58	118.40	124.48
30	a	619	BCR	C23-C24-C25	-5.58	112.10	127.00
38	W	609	CHL	CHA-C1A-C2A	-5.58	120.22	133.31
27	2	606	CLA	C4A-NA-C1A	5.57	109.22	106.68
30	B	847	BCR	C23-C24-C25	-5.56	112.15	127.00
27	2	607	CLA	C4A-NA-C1A	5.56	109.21	106.68
30	3	620	BCR	C1-C6-C5	-5.55	115.05	122.64
36	4	620	XAT	O4-C5-C4	5.55	118.69	113.49
27	4	601	CLA	C4A-NA-C1A	5.55	109.21	106.68
27	U	612	CLA	C4A-NA-C1A	5.55	109.21	106.68
36	8	620	XAT	C18-C5-C6	-5.55	113.17	122.30
30	A	850	BCR	C32-C1-C6	5.54	118.93	110.24
36	4	620	XAT	C38-C25-C26	-5.53	113.19	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	Z	606	CHL	C4D-ND-C1D	5.53	109.42	105.22
38	X	609	CHL	CHA-C1A-C2A	-5.52	120.33	133.31
27	W	602	CLA	C4A-NA-C1A	5.52	109.20	106.68
36	4	620	XAT	C18-C5-C6	-5.52	113.21	122.30
36	2	620	XAT	C38-C25-C26	-5.52	113.22	122.30
27	B	826	CLA	C4A-NA-C1A	5.52	109.20	106.68
36	U	1622	XAT	C37-C21-C26	-5.52	95.15	110.05
38	Z	601	CHL	CHA-C1A-C2A	-5.51	120.36	133.31
38	X	607	CHL	CHA-C1A-C2A	-5.51	120.36	133.31
27	U	602	CLA	C4A-NA-C1A	5.51	109.19	106.68
27	B	809	CLA	C4A-NA-C1A	5.51	109.19	106.68
27	A	838	CLA	C4A-NA-C1A	5.51	109.19	106.68
36	W	1622	XAT	C37-C21-C26	-5.50	95.19	110.05
30	B	849	BCR	C3-C4-C5	-5.50	104.26	114.06
27	A	840	CLA	C4A-NA-C1A	5.50	109.19	106.68
36	6	621	XAT	C38-C25-C26	-5.49	113.26	122.30
30	A	848	BCR	C23-C24-C25	-5.49	112.34	127.00
36	7	620	XAT	O24-C25-C24	5.49	118.63	113.49
27	B	831	CLA	C4A-NA-C1A	5.47	109.17	106.68
30	A	852	BCR	C28-C27-C26	-5.47	104.30	114.06
27	Z	611	CLA	C4A-NA-C1A	5.46	109.17	106.68
27	A	804	CLA	C4A-NA-C1A	5.46	109.17	106.68
36	Z	1622	XAT	O24-C25-C24	5.46	118.61	113.49
30	B	845	BCR	C37-C22-C21	-5.45	113.98	122.82
38	U	607	CHL	C4D-ND-C1D	5.45	109.35	105.22
27	5	602	CLA	C4A-NA-C1A	5.44	109.16	106.68
36	Z	1622	XAT	C18-C5-C6	-5.44	113.34	122.30
38	V	607	CHL	C4D-ND-C1D	5.43	109.34	105.22
27	8	607	CLA	C4A-NA-C1A	5.43	109.16	106.68
38	Z	605	CHL	C4D-ND-C1D	5.43	109.34	105.22
27	B	827	CLA	C4A-NA-C1A	5.42	109.15	106.68
27	L	307	CLA	C4A-NA-C1A	5.42	109.15	106.68
36	9	620	XAT	C38-C25-C26	-5.41	113.39	122.30
36	8	620	XAT	O24-C25-C24	5.41	118.56	113.49
27	F	303	CLA	C4A-NA-C1A	5.41	109.15	106.68
38	Y	609	CHL	C4D-ND-C1D	-5.41	101.11	105.22
30	B	848	BCR	C24-C23-C22	-5.41	118.23	126.23
30	4	621	BCR	C23-C24-C25	-5.40	112.57	127.00
27	W	611	CLA	C4A-NA-C1A	5.40	109.14	106.68
27	A	842	CLA	C4A-NA-C1A	5.39	109.14	106.68
27	3	617	CLA	C4A-NA-C1A	5.39	109.14	106.68
30	G	205	BCR	C38-C26-C25	-5.39	118.60	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	807	CLA	C4A-NA-C1A	5.39	109.14	106.68
30	4	621	BCR	C38-C26-C25	-5.38	118.61	124.48
36	X	1622	XAT	C37-C21-C26	-5.37	95.53	110.05
38	Z	608	CHL	C4D-ND-C1D	5.37	109.30	105.22
27	5	603	CLA	C4A-NA-C1A	5.37	109.13	106.68
35	7	619	LUT	C21-C26-C27	-5.37	106.65	112.83
30	K	207	BCR	C39-C30-C25	5.37	118.66	110.24
36	X	1622	XAT	O4-C5-C4	5.34	118.50	113.49
35	3	618	LUT	C8-C7-C6	-5.34	112.72	127.00
30	L	308	BCR	C3-C4-C5	-5.34	104.53	114.06
37	6	624	NEX	O24-C25-C24	5.34	118.50	113.49
27	2	602	CLA	C4A-NA-C1A	5.34	109.11	106.68
30	K	207	BCR	C30-C25-C26	-5.34	115.34	122.64
27	B	813	CLA	C4A-NA-C1A	5.34	109.11	106.68
36	Y	1622	XAT	C37-C21-C26	-5.33	95.64	110.05
30	A	852	BCR	C3-C4-C5	-5.33	104.55	114.06
36	Y	1622	XAT	O4-C5-C4	5.33	118.48	113.49
27	a	601	CLA	C4A-NA-C1A	5.33	109.11	106.68
27	2	601	CLA	C4A-NA-C1A	5.33	109.11	106.68
30	8	621	BCR	C1-C6-C5	-5.32	115.37	122.64
27	W	612	CLA	C4A-NA-C1A	5.32	109.11	106.68
27	1	601	CLA	C4A-NA-C1A	5.31	109.10	106.68
30	7	621	BCR	C33-C5-C6	-5.31	118.69	124.48
38	V	605	CHL	C4D-ND-C1D	5.31	109.25	105.22
27	U	613	CLA	C4A-NA-C1A	5.29	109.09	106.68
35	1	617	LUT	C8-C7-C6	-5.29	112.87	127.00
36	Z	1622	XAT	O4-C5-C4	5.29	118.45	113.49
30	6	622	BCR	C40-C30-C29	-5.28	88.67	108.95
27	A	810	CLA	C4A-NA-C1A	5.28	109.09	106.68
27	A	839	CLA	C4A-NA-C1A	5.28	109.09	106.68
27	G	204	CLA	C4A-NA-C1A	5.28	109.09	106.68
38	W	606	CHL	C4D-ND-C1D	5.28	109.23	105.22
35	a	617	LUT	C8-C7-C6	-5.28	112.90	127.00
35	X	1621	LUT	C7-C8-C9	-5.28	118.43	126.23
27	4	607	CLA	C4A-NA-C1A	5.27	109.08	106.68
38	V	606	CHL	C4D-ND-C1D	5.27	109.22	105.22
27	B	815	CLA	C4A-NA-C1A	5.26	109.08	106.68
30	B	852	BCR	C34-C9-C10	-5.26	114.30	122.82
35	Y	1621	LUT	C7-C8-C9	-5.25	118.47	126.23
27	A	813	CLA	C4A-NA-C1A	5.25	109.08	106.68
27	X	603	CLA	C4A-NA-C1A	5.25	109.08	106.68
36	3	619	XAT	O4-C5-C4	5.24	118.41	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	6	621	XAT	O4-C5-C18	5.24	120.90	115.05
36	2	620	XAT	C18-C5-C6	-5.23	113.69	122.30
27	B	832	CLA	C4A-NA-C1A	5.23	109.06	106.68
27	A	854	CLA	C4A-NA-C1A	5.23	109.06	106.68
27	K	203	CLA	C4A-NA-C1A	5.23	109.06	106.68
30	L	301	BCR	C28-C27-C26	-5.22	104.75	114.06
27	G	203	CLA	C4A-NA-C1A	5.22	109.06	106.68
27	V	612	CLA	C4A-NA-C1A	5.22	109.06	106.68
27	W	613	CLA	C4A-NA-C1A	5.22	109.06	106.68
27	A	835	CLA	C4A-NA-C1A	5.21	109.06	106.68
27	7	602	CLA	C4A-NA-C1A	5.21	109.06	106.68
38	V	609	CHL	C4D-ND-C1D	-5.21	101.27	105.22
30	A	850	BCR	C38-C26-C25	-5.20	118.81	124.48
35	U	1621	LUT	C7-C8-C9	-5.20	118.54	126.23
38	Y	609	CHL	CHA-C1A-C2A	-5.20	121.09	133.31
35	W	1621	LUT	C7-C8-C9	-5.20	118.55	126.23
27	5	607	CLA	C4A-NA-C1A	5.19	109.05	106.68
27	B	836	CLA	C4A-NA-C1A	5.19	109.05	106.68
38	Y	608	CHL	C4D-ND-C1D	5.18	109.15	105.22
36	3	619	XAT	C18-C5-C6	-5.17	113.79	122.30
27	A	818	CLA	C4A-NA-C1A	5.17	109.04	106.68
27	A	829	CLA	C4A-NA-C1A	5.16	109.03	106.68
27	5	613	CLA	C4A-NA-C1A	5.16	109.03	106.68
38	X	605	CHL	C4D-ND-C1D	5.15	109.13	105.22
27	L	303	CLA	C4A-NA-C1A	5.15	109.03	106.68
38	U	606	CHL	OBD-CAD-CBD	5.14	133.37	125.82
30	J	102	BCR	C20-C21-C22	-5.14	120.06	127.28
27	B	805	CLA	C4A-NA-C1A	5.14	109.02	106.68
27	A	816	CLA	C4A-NA-C1A	5.13	109.02	106.68
27	9	606	CLA	C4A-NA-C1A	5.12	109.02	106.68
27	Y	603	CLA	C4A-NA-C1A	5.12	109.02	106.68
27	Z	612	CLA	C4A-NA-C1A	5.12	109.02	106.68
38	U	606	CHL	C4D-ND-C1D	5.12	109.10	105.22
37	Z	1623	NEX	C38-C25-C26	-5.11	113.89	122.30
27	8	601	CLA	C4A-NA-C1A	5.11	109.01	106.68
27	A	826	CLA	C4A-NA-C1A	5.11	109.01	106.68
30	3	622	BCR	C20-C21-C22	-5.10	120.12	127.28
27	6	604	CLA	C4A-NA-C1A	5.10	109.01	106.68
27	5	612	CLA	C4A-NA-C1A	5.10	109.01	106.68
38	W	606	CHL	OBD-CAD-CBD	5.10	133.31	125.82
36	6	621	XAT	O24-C25-C38	5.10	120.75	115.05
30	B	846	BCR	C3-C4-C5	-5.10	104.97	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	V	611	CLA	C4A-NA-C1A	5.09	109.00	106.68
38	Y	605	CHL	C4D-ND-C1D	5.09	109.08	105.22
27	Z	613	CLA	C4A-NA-C1A	5.09	109.00	106.68
38	X	606	CHL	C4D-ND-C1D	5.08	109.08	105.22
36	9	620	XAT	C18-C5-C6	-5.08	113.94	122.30
30	5	622	BCR	C38-C26-C25	-5.08	118.94	124.48
30	3	622	BCR	C24-C23-C22	-5.08	118.72	126.23
36	1	618	XAT	C38-C25-C26	-5.08	113.95	122.30
27	B	810	CLA	C4A-NA-C1A	5.07	108.99	106.68
36	a	618	XAT	C38-C25-C26	-5.07	113.96	122.30
36	2	620	XAT	O4-C5-C4	5.06	118.24	113.49
27	K	206	CLA	C4A-NA-C1A	5.06	108.99	106.68
27	V	613	CLA	C4A-NA-C1A	5.06	108.99	106.68
35	5	620	LUT	C26-C27-C28	-5.06	116.71	124.58
30	B	852	BCR	C7-C8-C9	-5.05	118.76	126.23
27	4	609	CLA	C4A-NA-C1A	5.05	108.98	106.68
38	Y	606	CHL	C4D-ND-C1D	5.05	109.05	105.22
36	4	620	XAT	O24-C25-C38	5.05	120.69	115.05
27	B	818	CLA	C4A-NA-C1A	5.05	108.98	106.68
27	9	612	CLA	C4A-NA-C1A	5.05	108.98	106.68
30	O	2005	BCR	C20-C21-C22	-5.05	120.20	127.28
38	X	608	CHL	CHA-C1A-C2A	-5.04	121.46	133.31
27	A	820	CLA	C4A-NA-C1A	5.04	108.98	106.68
27	7	615	CLA	C4A-NA-C1A	5.04	108.98	106.68
38	V	606	CHL	OBD-CAD-CBD	5.04	133.22	125.82
30	A	849	BCR	C20-C21-C22	-5.03	120.22	127.28
27	5	618	CLA	C4A-NA-C1A	5.03	108.97	106.68
38	V	609	CHL	CHA-C1A-C2A	-5.02	121.51	133.31
38	V	608	CHL	C4D-ND-C1D	5.02	109.03	105.22
38	W	605	CHL	C4D-ND-C1D	5.02	109.03	105.22
30	3	620	BCR	C33-C5-C6	5.02	129.96	124.48
38	U	605	CHL	C4D-ND-C1D	5.01	109.02	105.22
27	9	609	CLA	C4A-NA-C1A	5.01	108.97	106.68
27	A	841	CLA	C4A-NA-C1A	5.01	108.96	106.68
27	9	602	CLA	C4A-NA-C1A	5.01	108.96	106.68
27	8	612	CLA	C4A-NA-C1A	5.01	108.96	106.68
27	6	603	CLA	C4A-NA-C1A	5.00	108.96	106.68
27	4	613	CLA	C4A-NA-C1A	5.00	108.96	106.68
30	B	801	BCR	C16-C17-C18	-5.00	120.27	127.28
27	8	602	CLA	C4A-NA-C1A	4.99	108.96	106.68
30	B	845	BCR	C24-C23-C22	-4.99	118.85	126.23
30	B	848	BCR	C29-C30-C25	4.99	117.68	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	V	608	CHL	OBD-CAD-CBD	4.99	133.14	125.82
38	W	608	CHL	C4D-ND-C1D	4.98	109.00	105.22
27	2	611	CLA	C4A-NA-C1A	4.98	108.95	106.68
27	5	609	CLA	C4A-NA-C1A	4.98	108.95	106.68
27	9	607	CLA	C4A-NA-C1A	4.98	108.95	106.68
36	8	620	XAT	C38-C25-C26	-4.97	114.11	122.30
27	9	613	CLA	C4A-NA-C1A	4.97	108.95	106.68
27	X	612	CLA	C4A-NA-C1A	4.97	108.95	106.68
27	5	617	CLA	C4A-NA-C1A	4.97	108.94	106.68
38	U	608	CHL	C4D-ND-C1D	4.97	108.99	105.22
30	O	2005	BCR	C40-C30-C29	-4.96	89.90	108.95
36	V	1622	XAT	O4-C5-C18	4.96	120.59	115.05
27	Y	612	CLA	C4A-NA-C1A	4.96	108.94	106.68
27	1	606	CLA	C4A-NA-C1A	4.96	108.94	106.68
36	7	620	XAT	C38-C25-C26	-4.96	114.15	122.30
27	A	803	CLA	C4A-NA-C1A	4.95	108.94	106.68
30	B	848	BCR	C39-C30-C25	-4.95	102.48	110.24
35	Z	1621	LUT	C7-C8-C9	-4.95	118.92	126.23
36	9	620	XAT	O4-C5-C18	4.94	120.57	115.05
27	7	612	CLA	C4A-NA-C1A	4.94	108.93	106.68
27	A	828	CLA	C4A-NA-C1A	4.94	108.93	106.68
27	O	2001	CLA	C4A-NA-C1A	4.94	108.93	106.68
27	A	825	CLA	C4A-NA-C1A	4.94	108.93	106.68
27	B	811	CLA	C4A-NA-C1A	4.94	108.93	106.68
27	B	812	CLA	C4A-NA-C1A	4.94	108.93	106.68
27	F	304	CLA	C4A-NA-C1A	4.94	108.93	106.68
27	2	613	CLA	C4A-NA-C1A	4.93	108.93	106.68
38	V	605	CHL	OBD-CAD-CBD	4.93	133.06	125.82
27	B	821	CLA	C4A-NA-C1A	4.93	108.93	106.68
27	a	606	CLA	C4A-NA-C1A	4.93	108.93	106.68
27	4	606	CLA	C4A-NA-C1A	4.93	108.93	106.68
27	7	607	CLA	C4A-NA-C1A	4.93	108.93	106.68
27	A	808	CLA	C4A-NA-C1A	4.92	108.92	106.68
27	8	613	CLA	C4A-NA-C1A	4.92	108.92	106.68
27	4	602	CLA	C4A-NA-C1A	4.92	108.92	106.68
30	7	623	BCR	C32-C1-C6	4.90	117.93	110.24
36	9	620	XAT	O24-C25-C24	4.89	118.08	113.49
36	1	618	XAT	O4-C5-C18	4.89	120.52	115.05
38	X	606	CHL	OBD-CAD-CBD	4.89	133.00	125.82
30	3	620	BCR	C11-C10-C9	4.89	134.14	127.28
36	W	1622	XAT	O4-C5-C4	4.88	118.07	113.49
35	a	617	LUT	C26-C27-C28	-4.88	116.98	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	816	CLA	C4A-NA-C1A	4.88	108.91	106.68
27	V	602	CLA	C4A-NA-C1A	4.88	108.91	106.68
30	2	623	BCR	C20-C21-C22	-4.88	120.44	127.28
27	B	841	CLA	C4A-NA-C1A	4.87	108.90	106.68
38	Y	606	CHL	OBD-CAD-CBD	4.87	132.97	125.82
30	K	207	BCR	C40-C30-C29	-4.87	90.25	108.95
27	3	614	CLA	C4A-NA-C1A	4.87	108.90	106.68
36	3	619	XAT	C6-C7-C8	-4.87	115.71	125.99
35	1	617	LUT	C26-C27-C28	-4.87	117.01	124.58
27	V	604	CLA	C4A-NA-C1A	4.86	108.90	106.68
35	Z	1620	LUT	C26-C27-C28	-4.86	117.01	124.58
27	B	834	CLA	C4A-NA-C1A	4.86	108.90	106.68
27	4	612	CLA	C4A-NA-C1A	4.86	108.90	106.68
30	8	621	BCR	C4-C5-C6	-4.86	116.14	122.70
27	6	601	CLA	C4A-NA-C1A	4.85	108.89	106.68
36	U	1622	XAT	O4-C5-C4	4.85	118.04	113.49
30	F	305	BCR	C36-C18-C17	-4.85	114.96	122.82
38	V	607	CHL	OBD-CAD-CBD	4.85	132.94	125.82
30	L	309	BCR	C16-C17-C18	-4.85	120.48	127.28
30	9	621	BCR	C20-C21-C22	-4.84	120.49	127.28
37	W	1623	NEX	C15-C14-C13	-4.84	120.49	127.28
37	U	1623	NEX	C38-C25-C26	-4.84	114.34	122.30
30	5	622	BCR	C33-C5-C6	-4.84	119.20	124.48
27	A	823	CLA	C4A-NA-C1A	4.84	108.89	106.68
27	8	606	CLA	C4A-NA-C1A	4.84	108.89	106.68
38	Z	609	CHL	CHA-C1A-C2A	-4.83	121.96	133.31
37	Y	1623	NEX	C38-C25-C26	-4.83	114.35	122.30
36	8	620	XAT	O4-C5-C4	4.83	118.02	113.49
27	6	612	CLA	C4A-NA-C1A	4.83	108.88	106.68
38	Y	607	CHL	C4D-ND-C1D	-4.83	101.56	105.22
30	B	852	BCR	C8-C9-C10	4.83	126.60	119.01
37	W	1623	NEX	C38-C25-C26	-4.83	114.36	122.30
27	5	619	CLA	C4A-NA-C1A	4.82	108.88	106.68
37	V	1623	NEX	C15-C14-C13	-4.82	120.52	127.28
27	6	607	CLA	C4A-NA-C1A	4.82	108.88	106.68
27	9	614	CLA	C4A-NA-C1A	4.82	108.88	106.68
30	5	622	BCR	C23-C24-C25	-4.81	114.14	127.00
27	7	601	CLA	C4A-NA-C1A	4.81	108.87	106.68
36	5	621	XAT	C38-C25-C26	-4.81	114.39	122.30
27	3	612	CLA	C4A-NA-C1A	4.81	108.87	106.68
36	a	618	XAT	O4-C5-C18	4.81	120.42	115.05
36	3	619	XAT	O4-C5-C18	4.80	120.41	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	619	LUT	C21-C26-C27	-4.80	107.31	112.83
30	7	621	BCR	C8-C7-C6	-4.80	114.19	127.00
27	B	839	CLA	C4A-NA-C1A	4.80	108.87	106.68
37	U	1623	NEX	C15-C14-C13	-4.79	120.55	127.28
27	A	836	CLA	C4A-NA-C1A	4.79	108.87	106.68
30	B	852	BCR	C15-C14-C13	-4.79	120.56	127.28
27	3	613	CLA	C4A-NA-C1A	4.79	108.86	106.68
38	U	607	CHL	OBD-CAD-CBD	4.79	132.85	125.82
27	1	609	CLA	C4A-NA-C1A	4.79	108.86	106.68
30	G	205	BCR	C20-C21-C22	-4.79	120.56	127.28
27	U	604	CLA	C4A-NA-C1A	4.79	108.86	106.68
30	F	305	BCR	C20-C21-C22	-4.79	120.56	127.28
30	K	202	BCR	C30-C25-C26	-4.78	116.10	122.64
27	3	609	CLA	C4A-NA-C1A	4.78	108.86	106.68
37	U	1623	NEX	C35-C34-C33	-4.77	120.58	127.28
37	X	1623	NEX	C38-C25-C26	-4.77	114.45	122.30
30	B	847	BCR	C24-C23-C22	-4.77	119.18	126.23
27	H	202	CLA	C4A-NA-C1A	4.77	108.85	106.68
27	9	604	CLA	C4A-NA-C1A	4.77	108.85	106.68
27	A	827	CLA	C4A-NA-C1A	4.77	108.85	106.68
37	W	1623	NEX	C35-C34-C33	-4.76	120.60	127.28
35	9	619	LUT	C7-C8-C9	-4.76	119.19	126.23
27	9	601	CLA	C4A-NA-C1A	4.76	108.85	106.68
27	X	613	CLA	C4A-NA-C1A	4.76	108.85	106.68
27	A	824	CLA	C4A-NA-C1A	4.75	108.85	106.68
27	Y	613	CLA	C4A-NA-C1A	4.75	108.85	106.68
27	A	845	CLA	C4A-NA-C1A	4.74	108.84	106.68
27	4	604	CLA	C4A-NA-C1A	4.74	108.84	106.68
38	U	608	CHL	OBD-CAD-CBD	4.74	132.78	125.82
27	B	803	CLA	C4A-NA-C1A	4.74	108.84	106.68
27	W	604	CLA	C4A-NA-C1A	4.74	108.84	106.68
36	V	1622	XAT	O4-C5-C4	4.74	117.93	113.49
27	A	805	CLA	C4A-NA-C1A	4.73	108.84	106.68
27	a	609	CLA	C4A-NA-C1A	4.73	108.84	106.68
38	W	608	CHL	OBD-CAD-CBD	4.73	132.77	125.82
38	W	605	CHL	OBD-CAD-CBD	4.73	132.76	125.82
27	a	612	CLA	C4A-NA-C1A	4.73	108.84	106.68
27	3	607	CLA	C4A-NA-C1A	4.73	108.84	106.68
36	a	618	XAT	O24-C25-C24	4.73	117.92	113.49
36	1	618	XAT	O24-C25-C24	4.73	117.92	113.49
38	W	607	CHL	C4D-ND-C1D	-4.72	101.63	105.22
27	7	608	CLA	C4A-NA-C1A	4.72	108.83	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	802	CLA	C4A-NA-C1A	4.72	108.83	106.68
30	B	844	BCR	C36-C18-C19	4.72	125.29	118.09
35	3	618	LUT	C26-C27-C28	-4.71	117.25	124.58
27	O	2003	CLA	C4A-NA-C1A	4.71	108.83	106.68
27	1	613	CLA	C4A-NA-C1A	4.71	108.83	106.68
38	Y	608	CHL	OBD-CAD-CBD	4.71	132.73	125.82
35	2	619	LUT	C26-C27-C28	-4.71	117.25	124.58
30	2	623	BCR	C33-C5-C6	-4.71	119.35	124.48
38	Z	609	CHL	C4D-ND-C1D	-4.71	101.65	105.22
27	2	612	CLA	C4A-NA-C1A	4.70	108.82	106.68
38	Z	605	CHL	OBD-CAD-CBD	4.69	132.71	125.82
36	9	620	XAT	O4-C5-C4	4.69	117.88	113.49
27	a	613	CLA	C4A-NA-C1A	4.68	108.82	106.68
37	X	1623	NEX	C15-C14-C13	-4.68	120.71	127.28
30	7	621	BCR	C24-C23-C22	-4.68	119.31	126.23
38	U	605	CHL	OBD-CAD-CBD	4.68	132.69	125.82
27	1	612	CLA	C4A-NA-C1A	4.68	108.81	106.68
27	A	830	CLA	C4A-NA-C1A	4.68	108.81	106.68
27	X	611	CLA	C4A-NA-C1A	4.68	108.81	106.68
30	7	623	BCR	C3-C4-C5	-4.67	105.72	114.06
30	K	202	BCR	C27-C26-C25	-4.67	116.39	122.70
27	X	614	CLA	C4A-NA-C1A	4.67	108.81	106.68
27	5	611	CLA	C4A-NA-C1A	4.67	108.81	106.68
30	K	207	BCR	C7-C8-C9	-4.66	119.34	126.23
27	2	604	CLA	C4A-NA-C1A	4.66	108.81	106.68
27	8	604	CLA	C4A-NA-C1A	4.66	108.81	106.68
27	3	608	CLA	C4A-NA-C1A	4.66	108.81	106.68
30	7	621	BCR	C38-C26-C25	-4.66	119.40	124.48
30	a	619	BCR	C3-C4-C5	-4.65	105.76	114.06
27	6	617	CLA	C4A-NA-C1A	4.65	108.80	106.68
30	A	848	BCR	C38-C26-C25	-4.65	119.41	124.48
30	K	207	BCR	C23-C24-C25	-4.64	114.60	127.00
30	2	623	BCR	C16-C17-C18	-4.64	120.77	127.28
35	V	1621	LUT	C7-C8-C9	-4.63	119.38	126.23
36	2	620	XAT	O24-C25-C24	4.63	117.83	113.49
27	6	616	CLA	C4A-NA-C1A	4.63	108.79	106.68
27	K	201	CLA	C4A-NA-C1A	4.63	108.79	106.68
27	3	615	CLA	C4A-NA-C1A	4.62	108.79	106.68
30	1	619	BCR	C3-C4-C5	-4.62	105.82	114.06
27	8	611	CLA	C4A-NA-C1A	4.62	108.78	106.68
37	Y	1623	NEX	C15-C14-C13	-4.61	120.81	127.28
30	9	621	BCR	C33-C5-C6	-4.61	119.45	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	852	BCR	C20-C21-C22	-4.61	120.81	127.28
27	5	604	CLA	C4A-NA-C1A	4.61	108.78	106.68
27	6	609	CLA	C4A-NA-C1A	4.61	108.78	106.68
27	A	833	CLA	C4A-NA-C1A	4.61	108.78	106.68
37	5	624	NEX	O24-C25-C38	4.61	120.19	115.05
27	Y	614	CLA	C4A-NA-C1A	4.61	108.78	106.68
27	2	614	CLA	C4A-NA-C1A	4.60	108.78	106.68
38	X	605	CHL	OBD-CAD-CBD	4.60	132.58	125.82
30	6	622	BCR	C30-C25-C24	4.60	128.12	115.65
27	B	829	CLA	C4A-NA-C1A	4.60	108.78	106.68
30	B	852	BCR	C1-C6-C5	-4.59	116.36	122.64
27	Z	604	CLA	C4A-NA-C1A	4.59	108.77	106.68
30	A	848	BCR	C8-C7-C6	-4.59	114.74	127.00
30	5	622	BCR	C20-C21-C22	-4.59	120.84	127.28
35	Z	1620	LUT	C8-C7-C6	-4.58	114.76	127.00
30	B	844	BCR	C7-C8-C9	-4.58	119.46	126.23
30	2	623	BCR	C7-C8-C9	-4.58	119.46	126.23
30	B	847	BCR	C33-C5-C6	-4.58	119.49	124.48
38	Y	605	CHL	OBD-CAD-CBD	4.58	132.54	125.82
28	B	842	PQN	C15-C13-C12	-4.58	110.89	121.17
27	2	616	CLA	C4A-NA-C1A	4.57	108.77	106.68
27	4	610	CLA	C4A-NA-C1A	4.57	108.77	106.68
38	Z	608	CHL	OBD-CAD-CBD	4.57	132.53	125.82
37	Z	1623	NEX	C11-C10-C9	-4.57	120.87	127.28
27	1	611	CLA	C4A-NA-C1A	4.56	108.76	106.68
27	a	614	CLA	C4A-NA-C1A	4.56	108.76	106.68
36	5	621	XAT	C6-C7-C8	-4.56	116.36	125.99
30	3	620	BCR	C37-C22-C23	4.56	125.05	118.09
27	6	606	CLA	C4A-NA-C1A	4.55	108.76	106.68
38	Z	606	CHL	OBD-CAD-CBD	4.55	132.51	125.82
27	A	801	CLA	C4A-NA-C1A	4.55	108.75	106.68
27	Y	611	CLA	C4A-NA-C1A	4.55	108.75	106.68
27	a	611	CLA	C4A-NA-C1A	4.55	108.75	106.68
30	G	205	BCR	C8-C7-C6	-4.55	114.86	127.00
37	W	1623	NEX	C11-C10-C9	-4.54	120.91	127.28
27	a	608	CLA	C4A-NA-C1A	4.54	108.75	106.68
27	Y	602	CLA	C4A-NA-C1A	4.54	108.75	106.68
27	7	613	CLA	C4A-NA-C1A	4.53	108.75	106.68
27	8	616	CLA	C4A-NA-C1A	4.53	108.75	106.68
27	7	606	CLA	C4A-NA-C1A	4.53	108.75	106.68
27	1	608	CLA	C4A-NA-C1A	4.52	108.74	106.68
27	5	608	CLA	C4A-NA-C1A	4.52	108.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	6	611	CLA	C4A-NA-C1A	4.52	108.74	106.68
37	W	1623	NEX	C27-C28-C29	-4.51	118.53	125.53
30	B	849	BCR	C4-C5-C6	-4.51	116.61	122.70
27	6	608	CLA	C4A-NA-C1A	4.51	108.74	106.68
27	2	609	CLA	C4A-NA-C1A	4.50	108.73	106.68
37	U	1623	NEX	C27-C28-C29	-4.50	118.54	125.53
27	6	602	CLA	C4A-NA-C1A	4.50	108.73	106.68
30	3	621	BCR	C23-C24-C25	-4.50	114.98	127.00
30	B	843	BCR	C7-C8-C9	-4.50	119.58	126.23
27	9	603	CLA	C4A-NA-C1A	4.49	108.73	106.68
37	Y	1623	NEX	C35-C34-C33	-4.49	120.98	127.28
36	Z	1622	XAT	O4-C5-C18	4.49	120.06	115.05
27	3	602	CLA	C4A-NA-C1A	4.48	108.72	106.68
37	U	1623	NEX	C11-C10-C9	-4.48	120.99	127.28
30	A	856	BCR	C28-C27-C26	-4.48	106.06	114.06
30	5	622	BCR	C8-C7-C6	-4.47	115.05	127.00
27	1	614	CLA	C4A-NA-C1A	4.47	108.72	106.68
29	V	2630	LHG	O7-C7-C8	4.47	121.14	111.48
37	X	1623	NEX	C35-C34-C33	-4.46	121.02	127.28
27	A	811	CLA	C4A-NA-C1A	4.46	108.72	106.68
27	a	607	CLA	C4A-NA-C1A	4.46	108.71	106.68
27	4	611	CLA	C4A-NA-C1A	4.46	108.71	106.68
27	9	611	CLA	C4A-NA-C1A	4.46	108.71	106.68
33	H	205	LMG	O7-C10-C11	4.45	121.11	111.48
30	3	622	BCR	C23-C24-C25	-4.45	115.12	127.00
27	A	843	CLA	C4A-NA-C1A	4.45	108.71	106.68
30	A	851	BCR	C28-C27-C26	-4.44	106.14	114.06
27	1	607	CLA	C4A-NA-C1A	4.43	108.70	106.68
35	V	1620	LUT	C26-C27-C28	-4.43	117.68	124.58
35	Z	1620	LUT	C21-C26-C27	-4.43	107.73	112.83
36	2	620	XAT	O4-C5-C18	4.43	120.00	115.05
27	7	611	CLA	C4A-NA-C1A	4.42	108.70	106.68
35	6	619	LUT	C26-C27-C28	-4.42	117.70	124.58
27	4	614	CLA	C4A-NA-C1A	4.41	108.69	106.68
35	4	619	LUT	C35-C34-C33	-4.41	121.09	127.28
33	J	104	LMG	O7-C10-C11	4.41	121.02	111.48
27	3	611	CLA	C4A-NA-C1A	4.41	108.69	106.68
27	5	606	CLA	C4A-NA-C1A	4.41	108.69	106.68
27	X	604	CLA	C4A-NA-C1A	4.41	108.69	106.68
30	K	202	BCR	C20-C21-C22	-4.41	121.10	127.28
35	9	619	LUT	C26-C27-C28	-4.41	117.72	124.58
36	6	621	XAT	C6-C7-C8	-4.40	116.69	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	207	BCR	C20-C21-C22	-4.40	121.11	127.28
36	X	1622	XAT	O4-C5-C18	4.39	119.96	115.05
37	V	1623	NEX	C27-C28-C29	-4.39	118.72	125.53
36	Y	1622	XAT	O4-C5-C18	4.39	119.95	115.05
27	a	616	CLA	C4A-NA-C1A	4.39	108.68	106.68
27	2	610	CLA	C4A-NA-C1A	4.39	108.68	106.68
30	3	621	BCR	C33-C5-C6	-4.39	119.70	124.48
37	6	624	NEX	O24-C25-C38	4.38	119.94	115.05
30	A	851	BCR	C7-C8-C9	-4.38	119.76	126.23
27	4	608	CLA	C4A-NA-C1A	4.37	108.67	106.68
30	B	844	BCR	C37-C22-C23	4.37	124.76	118.09
30	B	847	BCR	C38-C26-C25	-4.36	119.72	124.48
30	B	847	BCR	C8-C7-C6	-4.36	115.34	127.00
30	A	850	BCR	C16-C17-C18	-4.36	121.16	127.28
35	Z	1621	LUT	C17-C1-C6	-4.36	103.41	110.24
30	1	619	BCR	C38-C26-C25	-4.35	119.74	124.48
30	A	848	BCR	C20-C21-C22	-4.35	121.18	127.28
30	A	852	BCR	C39-C30-C25	-4.34	103.44	110.24
30	a	619	BCR	C38-C26-C25	-4.34	119.75	124.48
30	B	853	BCR	C24-C23-C22	-4.33	119.82	126.23
30	7	623	BCR	C20-C21-C22	-4.33	121.21	127.28
38	U	605	CHL	C1A-CHA-C4D	-4.33	111.76	118.98
27	Y	604	CLA	C4A-NA-C1A	4.33	108.65	106.68
30	B	843	BCR	C20-C21-C22	-4.33	121.21	127.28
27	O	2002	CLA	C4A-NA-C1A	4.32	108.65	106.68
27	X	602	CLA	C4A-NA-C1A	4.32	108.65	106.68
37	V	1623	NEX	C38-C25-C26	-4.32	115.19	122.30
27	B	804	CLA	C4A-NA-C1A	4.32	108.65	106.68
30	A	848	BCR	C16-C17-C18	-4.32	121.22	127.28
38	W	605	CHL	C1A-CHA-C4D	-4.31	111.78	118.98
30	L	308	BCR	C28-C27-C26	-4.31	106.37	114.06
27	1	616	CLA	C4A-NA-C1A	4.31	108.65	106.68
30	F	305	BCR	C38-C26-C25	-4.31	119.78	124.48
30	9	621	BCR	C16-C17-C18	-4.31	121.24	127.28
27	4	616	CLA	C4A-NA-C1A	4.31	108.64	106.68
27	6	620	CLA	C4A-NA-C1A	4.30	108.64	106.68
35	7	619	LUT	C26-C27-C28	-4.30	117.88	124.58
30	7	623	BCR	C38-C26-C25	-4.30	119.79	124.48
29	5	625	LHG	O7-C7-C8	4.30	120.78	111.48
30	L	305	BCR	C20-C21-C22	-4.30	121.25	127.28
30	B	846	BCR	C28-C27-C26	-4.30	106.40	114.06
27	A	822	CLA	C4A-NA-C1A	4.29	108.64	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	620	BCR	C8-C7-C6	4.29	138.47	127.00
30	A	851	BCR	C16-C17-C18	-4.29	121.26	127.28
35	8	619	LUT	C26-C27-C28	-4.29	117.91	124.58
30	1	619	BCR	C20-C21-C22	-4.29	121.27	127.28
38	X	601	CHL	C1-C2-C3	-4.28	119.18	126.20
30	1	619	BCR	C28-C27-C26	-4.28	106.42	114.06
35	V	1621	LUT	C8-C7-C6	-4.28	115.57	127.00
30	a	619	BCR	C28-C27-C26	-4.28	106.43	114.06
35	4	619	LUT	C26-C27-C28	-4.28	117.92	124.58
37	X	1623	NEX	C27-C28-C29	-4.28	118.89	125.53
27	5	614	CLA	C4A-NA-C1A	4.27	108.63	106.68
27	Z	602	CLA	C4A-NA-C1A	4.27	108.62	106.68
30	O	2005	BCR	C30-C25-C26	-4.26	116.81	122.64
36	3	619	XAT	O24-C25-C38	4.26	119.81	115.05
30	A	849	BCR	C36-C18-C19	4.26	124.60	118.09
27	7	609	CLA	C4A-NA-C1A	4.26	108.62	106.68
30	B	844	BCR	C15-C16-C17	-4.26	114.81	123.52
27	F	301	CLA	C4A-NA-C1A	4.25	108.62	106.68
30	L	305	BCR	C11-C10-C9	-4.25	121.32	127.28
30	a	619	BCR	C20-C21-C22	-4.25	121.32	127.28
27	6	613	CLA	C4A-NA-C1A	4.25	108.62	106.68
29	1	620	LHG	O7-C7-C8	4.24	120.66	111.48
30	4	621	BCR	C20-C21-C22	-4.24	121.33	127.28
37	5	624	NEX	O24-C25-C24	4.24	117.46	113.49
35	4	619	LUT	C21-C26-C27	-4.23	107.96	112.83
27	9	610	CLA	C4A-NA-C1A	4.22	108.61	106.68
29	a	620	LHG	O7-C7-C8	4.22	120.61	111.48
27	A	816	CLA	C1-C2-C3	-4.21	119.29	126.20
30	B	848	BCR	C8-C7-C6	-4.21	115.74	127.00
27	1	610	CLA	C3A-C2A-C1A	-4.21	101.99	106.30
37	Y	1623	NEX	C27-C28-C29	-4.21	119.00	125.53
37	5	624	NEX	C26-C27-C28	-4.20	117.12	125.99
35	6	619	LUT	C21-C26-C27	-4.19	108.01	112.83
36	4	620	XAT	O4-C5-C18	4.19	119.73	115.05
27	B	802	CLA	C4A-NA-C1A	4.18	108.59	106.68
27	B	814	CLA	C4A-NA-C1A	4.18	108.58	106.68
30	A	852	BCR	C37-C22-C23	4.17	124.47	118.09
27	A	812	CLA	C4A-NA-C1A	4.17	108.58	106.68
38	Y	607	CHL	CHA-C1A-C2A	-4.16	123.54	133.31
36	8	620	XAT	O4-C5-C18	4.15	119.69	115.05
27	3	609	CLA	O2D-CGD-CBD	4.15	118.49	111.23
27	B	808	CLA	C4A-NA-C1A	4.15	108.57	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	852	BCR	C7-C8-C9	-4.15	120.09	126.23
30	B	801	BCR	C28-C27-C26	-4.15	106.65	114.06
38	X	605	CHL	C1A-CHA-C4D	-4.15	112.06	118.98
27	8	609	CLA	C4A-NA-C1A	4.15	108.57	106.68
30	3	621	BCR	C11-C10-C9	-4.15	121.46	127.28
30	A	849	BCR	C16-C17-C18	-4.14	121.47	127.28
32	1	621	LMU	C1B-O1B-C4'	-4.14	108.17	117.98
30	3	620	BCR	C15-C16-C17	-4.14	115.05	123.52
38	Y	605	CHL	C1A-CHA-C4D	-4.13	112.08	118.98
30	A	850	BCR	C20-C21-C22	-4.13	121.48	127.28
27	A	831	CLA	C4A-NA-C1A	4.13	108.56	106.68
27	1	604	CLA	C4A-NA-C1A	4.12	108.56	106.68
35	8	619	LUT	C8-C7-C6	-4.12	116.00	127.00
27	A	826	CLA	CMB-C2B-C1B	-4.12	119.15	125.42
27	V	614	CLA	C4A-NA-C1A	4.12	108.56	106.68
38	W	601	CHL	C1-C2-C3	-4.12	119.45	126.20
30	3	620	BCR	C15-C14-C13	-4.12	121.51	127.28
30	B	843	BCR	C16-C17-C18	-4.11	121.52	127.28
35	a	617	LUT	C21-C26-C27	-4.10	108.11	112.83
35	1	617	LUT	C21-C26-C27	-4.09	108.12	112.83
27	8	614	CLA	C4A-NA-C1A	4.09	108.55	106.68
27	J	101	CLA	C4A-NA-C1A	4.09	108.54	106.68
30	J	102	BCR	C23-C24-C25	-4.09	116.08	127.00
30	7	621	BCR	C39-C30-C25	-4.09	103.83	110.24
36	a	618	XAT	O24-C25-C38	4.09	119.61	115.05
27	B	822	CLA	C4A-NA-C1A	4.09	108.54	106.68
35	5	620	LUT	C35-C15-C14	-4.09	115.16	123.52
38	Y	607	CHL	CMA-C3A-C4A	-4.08	105.81	114.61
35	4	619	LUT	C35-C15-C14	-4.08	115.17	123.52
27	B	830	CLA	C4A-NA-C1A	4.08	108.54	106.68
38	Y	609	CHL	C1B-CHB-C4A	4.08	123.95	121.32
30	B	843	BCR	C37-C22-C23	4.08	124.32	118.09
36	5	621	XAT	O4-C5-C18	4.08	119.60	115.05
30	9	621	BCR	C11-C10-C9	-4.08	121.56	127.28
30	1	619	BCR	C37-C22-C23	4.07	124.31	118.09
27	L	304	CLA	C4A-NA-C1A	4.07	108.53	106.68
27	5	616	CLA	C4A-NA-C1A	4.06	108.53	106.68
27	7	614	CLA	C4A-NA-C1A	4.06	108.53	106.68
29	9	624	LHG	O7-C7-C8	4.05	120.24	111.48
30	B	848	BCR	C16-C17-C18	-4.05	121.60	127.28
29	8	623	LHG	O7-C7-C8	4.05	120.24	111.48
27	B	819	CLA	C4A-NA-C1A	4.05	108.53	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	618	XAT	O24-C25-C38	4.05	119.57	115.05
28	A	844	PQN	C15-C13-C12	-4.04	112.09	121.17
30	6	622	BCR	C16-C17-C18	-4.04	121.61	127.28
35	9	619	LUT	C35-C34-C33	-4.04	121.61	127.28
27	Z	614	CLA	C4A-NA-C1A	4.04	108.52	106.68
38	V	605	CHL	C1A-CHA-C4D	-4.04	112.24	118.98
27	a	604	CLA	C4A-NA-C1A	4.04	108.52	106.68
30	B	847	BCR	C36-C18-C19	4.03	124.25	118.09
27	L	302	CLA	C4A-NA-C1A	4.03	108.52	106.68
30	K	207	BCR	C16-C17-C18	-4.03	121.62	127.28
30	J	102	BCR	C39-C30-C25	-4.03	103.92	110.24
30	a	619	BCR	C37-C22-C23	4.03	124.25	118.09
30	B	845	BCR	C16-C17-C18	-4.03	121.62	127.28
30	A	856	BCR	C33-C5-C6	-4.03	120.09	124.48
30	B	846	BCR	C20-C21-C22	-4.03	121.63	127.28
29	O	2631	LHG	O7-C7-C8	4.03	120.19	111.48
30	B	801	BCR	C29-C30-C25	4.02	116.28	110.44
35	8	619	LUT	C7-C8-C9	-4.02	120.28	126.23
35	Z	1621	LUT	C21-C26-C27	-4.02	108.20	112.83
27	2	603	CLA	C4A-NA-C1A	4.02	108.51	106.68
36	4	620	XAT	C6-C7-C8	-4.02	117.50	125.99
30	O	2005	BCR	C16-C17-C18	-4.02	121.64	127.28
30	B	801	BCR	C16-C15-C14	-4.02	115.30	123.52
30	5	622	BCR	C3-C4-C5	-4.02	106.89	114.06
27	V	610	CLA	C4A-NA-C1A	4.01	108.51	106.68
33	V	2631	LMG	O7-C10-C11	4.01	120.16	111.48
30	A	851	BCR	C30-C25-C26	-4.01	117.16	122.64
38	W	606	CHL	C1A-CHA-C4D	-4.01	112.29	118.98
27	3	609	CLA	O2D-CGD-O1D	-4.00	116.07	123.85
30	O	2004	BCR	C20-C21-C22	-3.99	121.68	127.28
30	A	852	BCR	C24-C23-C22	-3.99	120.33	126.23
36	6	621	XAT	O4-C5-C4	3.99	117.23	113.49
38	U	606	CHL	C1A-CHA-C4D	-3.99	112.33	118.98
36	2	620	XAT	O24-C25-C38	3.99	119.50	115.05
36	4	620	XAT	O24-C25-C24	3.99	117.23	113.49
30	B	852	BCR	C15-C16-C17	-3.98	115.37	123.52
38	W	607	CHL	CHA-C1A-C2A	-3.98	123.96	133.31
30	3	620	BCR	C10-C11-C12	-3.98	111.67	123.20
29	B	851	LHG	O7-C7-C8	3.98	120.09	111.48
30	O	2004	BCR	C1-C6-C5	-3.98	117.20	122.64
27	B	835	CLA	C4A-NA-C1A	3.98	108.49	106.68
36	1	618	XAT	C6-C7-C8	-3.97	117.59	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	7	610	CLA	C4A-NA-C1A	3.97	108.49	106.68
27	B	817	CLA	C4A-NA-C1A	3.97	108.49	106.68
30	8	621	BCR	C3-C4-C5	-3.97	106.98	114.06
30	7	623	BCR	C8-C7-C6	-3.96	116.41	127.00
30	5	622	BCR	C16-C17-C18	-3.96	121.72	127.28
27	B	818	CLA	C4-C3-C5	3.96	122.10	115.23
35	W	1621	LUT	C26-C27-C28	-3.96	118.42	124.58
30	B	847	BCR	C20-C21-C22	-3.96	121.72	127.28
27	7	604	CLA	C4A-NA-C1A	3.96	108.48	106.68
35	U	1621	LUT	C26-C27-C28	-3.95	118.43	124.58
30	B	849	BCR	C20-C21-C22	-3.95	121.73	127.28
30	L	301	BCR	C20-C21-C22	-3.95	121.73	127.28
27	6	614	CLA	C4A-NA-C1A	3.95	108.48	106.68
27	U	610	CLA	C4A-NA-C1A	3.95	108.48	106.68
36	a	618	XAT	C6-C7-C8	-3.95	117.64	125.99
35	V	1621	LUT	C17-C1-C6	-3.95	104.06	110.24
30	A	849	BCR	C27-C26-C25	-3.94	117.38	122.70
36	U	1622	XAT	O4-C5-C18	3.94	119.45	115.05
33	L	2631	LMG	O7-C10-C11	3.94	120.00	111.48
30	7	621	BCR	C20-C21-C22	-3.94	121.76	127.28
30	L	305	BCR	C37-C22-C23	3.93	124.09	118.09
38	W	607	CHL	CMA-C3A-C4A	-3.93	106.14	114.61
35	X	1620	LUT	C17-C1-C6	3.92	116.39	110.24
37	5	624	NEX	C5-C6-C1	3.91	123.58	119.70
27	3	615	CLA	CMB-C2B-C1B	-3.91	119.46	125.42
30	K	202	BCR	C16-C17-C18	-3.91	121.79	127.28
30	B	852	BCR	C37-C22-C23	3.91	124.06	118.09
36	W	1622	XAT	O4-C5-C18	3.91	119.42	115.05
30	1	619	BCR	C15-C14-C13	-3.90	121.81	127.28
30	B	846	BCR	C37-C22-C23	3.90	124.04	118.09
30	A	852	BCR	C34-C9-C10	-3.90	116.50	122.82
38	X	606	CHL	C1A-CHA-C4D	-3.89	112.48	118.98
27	A	805	CLA	O2D-CGD-O1D	-3.89	116.27	123.85
35	Y	1620	LUT	C17-C1-C6	3.89	116.35	110.24
38	U	601	CHL	C1-C2-C3	-3.89	119.82	126.20
27	1	610	CLA	C4A-NA-C1A	3.89	108.45	106.68
30	7	623	BCR	C16-C17-C18	-3.89	121.83	127.28
30	O	2005	BCR	C29-C30-C25	3.89	116.08	110.44
33	J	103	LMG	O7-C10-C11	3.89	119.89	111.48
27	B	833	CLA	C4A-NA-C1A	3.88	108.45	106.68
30	B	849	BCR	C38-C26-C25	-3.88	120.25	124.48
30	G	205	BCR	C16-C17-C18	-3.88	121.84	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	8	610	CLA	CMB-C2B-C1B	-3.88	119.51	125.42
27	8	610	CLA	C4A-NA-C1A	3.88	108.45	106.68
30	B	847	BCR	C15-C16-C17	-3.88	115.58	123.52
30	B	852	BCR	C20-C21-C22	-3.88	121.84	127.28
30	K	207	BCR	C27-C26-C25	-3.87	117.47	122.70
36	Z	1622	XAT	O24-C25-C38	3.87	119.38	115.05
38	V	601	CHL	C1-C2-C3	-3.87	119.86	126.20
30	K	202	BCR	C36-C18-C19	3.86	123.99	118.09
36	U	1622	XAT	C27-C28-C29	-3.86	119.54	125.53
27	a	610	CLA	C4A-NA-C1A	3.86	108.44	106.68
38	V	608	CHL	CBC-CAC-C3C	-3.86	107.35	112.87
30	8	621	BCR	C37-C22-C23	3.85	123.97	118.09
38	Y	606	CHL	C1A-CHA-C4D	-3.85	112.56	118.98
30	K	202	BCR	C37-C22-C23	3.85	123.96	118.09
36	W	1622	XAT	C27-C28-C29	-3.84	119.56	125.53
30	a	619	BCR	C15-C14-C13	-3.84	121.89	127.28
27	7	601	CLA	CMB-C2B-C1B	-3.84	119.57	125.42
36	V	1622	XAT	O24-C25-C38	3.84	119.34	115.05
37	V	1623	NEX	C35-C34-C33	-3.84	121.90	127.28
30	4	621	BCR	C36-C18-C19	3.84	123.95	118.09
38	W	608	CHL	C1A-CHA-C4D	-3.83	112.59	118.98
30	B	852	BCR	C35-C13-C12	-3.82	112.25	118.09
35	Z	1621	LUT	C26-C27-C28	-3.82	118.64	124.58
30	4	621	BCR	C33-C5-C4	3.82	121.74	113.60
36	2	620	XAT	C12-C13-C14	-3.82	113.00	119.01
27	W	610	CLA	C4A-NA-C1A	3.82	108.42	106.68
30	A	848	BCR	C7-C8-C9	-3.81	120.59	126.23
36	U	1622	XAT	C15-C35-C34	-3.81	115.72	123.52
38	V	606	CHL	C1C-C2C-CMC	3.81	133.67	126.80
30	B	848	BCR	C20-C21-C22	-3.81	121.93	127.28
34	B	850	DGD	C2G-O2G-C1B	-3.81	108.68	117.80
30	B	801	BCR	C36-C18-C19	3.81	123.90	118.09
30	A	851	BCR	C30-C25-C24	3.80	125.97	115.65
30	B	801	BCR	C20-C21-C22	-3.80	121.95	127.28
27	B	825	CLA	C4A-NA-C1A	3.80	108.41	106.68
30	B	848	BCR	C28-C27-C26	-3.80	107.28	114.06
30	B	844	BCR	C11-C10-C9	-3.80	121.95	127.28
30	B	848	BCR	C27-C26-C25	-3.79	117.58	122.70
36	3	619	XAT	C26-C27-C28	-3.79	117.98	125.99
38	V	606	CHL	C1A-CHA-C4D	-3.79	112.66	118.98
27	7	616	CLA	C4A-NA-C1A	3.79	108.41	106.68
36	6	621	XAT	O24-C25-C24	3.79	117.04	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	U	1623	NEX	C17-C1-C6	-3.79	107.08	110.47
30	L	301	BCR	C36-C18-C19	3.78	123.87	118.09
36	8	620	XAT	O24-C25-C38	3.78	119.28	115.05
38	U	607	CHL	CMD-C2D-C3D	3.78	132.24	124.68
36	X	1622	XAT	C27-C28-C29	-3.78	119.66	125.53
30	B	844	BCR	C20-C21-C22	-3.78	121.98	127.28
36	W	1622	XAT	C15-C35-C34	-3.78	115.79	123.52
35	V	1621	LUT	C26-C27-C28	-3.78	118.70	124.58
27	6	610	CLA	C4A-NA-C1A	3.77	108.40	106.68
27	2	610	CLA	CMB-C2B-C1B	-3.77	119.67	125.42
30	A	856	BCR	C20-C21-C22	-3.77	121.98	127.28
30	B	846	BCR	C36-C18-C19	3.77	123.85	118.09
36	Z	1622	XAT	C36-C21-C26	3.77	120.23	110.05
33	5	627	LMG	O7-C10-C11	3.77	119.64	111.48
33	9	625	LMG	O7-C10-C11	3.77	119.64	111.48
27	V	611	CLA	O2D-CGD-O1D	-3.77	116.51	123.85
38	Z	605	CHL	C1A-CHA-C4D	-3.77	112.70	118.98
38	U	608	CHL	C1A-CHA-C4D	-3.77	112.70	118.98
36	Y	1622	XAT	C27-C28-C29	-3.77	119.69	125.53
30	4	621	BCR	C7-C8-C9	-3.76	120.67	126.23
30	7	621	BCR	C7-C8-C9	-3.76	120.68	126.23
36	8	620	XAT	C35-C15-C14	-3.75	115.84	123.52
36	9	620	XAT	C6-C7-C8	-3.75	118.07	125.99
29	9	622	LHG	O7-C7-C8	3.75	119.58	111.48
30	A	856	BCR	C29-C30-C25	3.74	115.86	110.44
30	L	301	BCR	C29-C30-C25	3.74	115.86	110.44
37	U	1623	NEX	O24-C25-C38	3.72	119.21	115.05
35	Y	1620	LUT	C26-C27-C28	-3.72	118.79	124.58
38	Z	606	CHL	C1A-CHA-C4D	-3.72	112.77	118.98
30	3	622	BCR	C36-C18-C19	3.72	123.77	118.09
30	3	622	BCR	C16-C17-C18	-3.71	122.08	127.28
36	2	620	XAT	C35-C15-C14	-3.71	115.93	123.52
27	O	2001	CLA	C3A-C2A-C1A	-3.71	102.51	106.30
36	8	620	XAT	C6-C7-C8	-3.71	118.16	125.99
30	J	102	BCR	C36-C18-C19	3.71	123.75	118.09
33	8	626	LMG	O7-C10-C11	3.70	119.48	111.48
35	X	1620	LUT	C26-C27-C28	-3.70	118.82	124.58
30	L	301	BCR	C34-C9-C10	-3.70	116.83	122.82
29	H	204	LHG	O7-C7-C8	3.70	119.48	111.48
27	a	610	CLA	CMB-C2B-C1B	-3.70	119.79	125.42
36	4	620	XAT	C35-C15-C14	-3.69	115.96	123.52
37	W	1623	NEX	C17-C1-C6	-3.69	107.17	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	L	308	BCR	C11-C10-C9	-3.69	122.10	127.28
30	L	309	BCR	C20-C21-C22	-3.69	122.11	127.28
30	A	852	BCR	C27-C26-C25	-3.69	117.72	122.70
30	3	620	BCR	C39-C30-C29	3.68	123.10	108.95
38	V	608	CHL	C1A-CHA-C4D	-3.68	112.84	118.98
30	L	309	BCR	C16-C15-C14	-3.68	115.99	123.52
29	B	854	LHG	O7-C7-C8	3.68	119.44	111.48
37	Z	1623	NEX	C15-C14-C13	-3.68	122.12	127.28
37	Z	1623	NEX	C15-C35-C34	-3.67	116.00	123.52
36	7	620	XAT	O4-C5-C18	3.67	119.15	115.05
27	1	610	CLA	CMB-C2B-C1B	-3.67	119.83	125.42
30	B	853	BCR	C7-C8-C9	-3.67	120.81	126.23
37	W	1623	NEX	O24-C25-C38	3.67	119.15	115.05
36	9	620	XAT	O24-C25-C38	3.67	119.14	115.05
27	3	603	CLA	CMB-C2B-C1B	-3.67	119.84	125.42
30	B	844	BCR	C15-C14-C13	-3.66	122.14	127.28
30	B	852	BCR	C10-C11-C12	-3.66	112.58	123.20
30	L	308	BCR	C30-C25-C26	-3.66	117.63	122.64
30	A	850	BCR	C23-C24-C25	-3.66	117.22	127.00
32	A	857	LMU	C1B-O1B-C4'	-3.66	109.31	117.98
27	5	610	CLA	C4A-NA-C1A	3.65	108.34	106.68
29	9	623	LHG	O7-C7-C8	3.65	119.38	111.48
30	B	845	BCR	C37-C22-C23	3.65	123.66	118.09
29	X	2630	LHG	O7-C7-C8	3.64	119.36	111.48
37	Z	1623	NEX	C26-C27-C28	-3.64	118.29	125.99
30	4	621	BCR	C16-C17-C18	-3.64	122.17	127.28
36	X	1622	XAT	C15-C35-C34	-3.64	116.07	123.52
35	Z	1620	LUT	C7-C8-C9	-3.64	120.86	126.23
27	1	614	CLA	C2A-C3A-C4A	-3.63	102.38	106.24
30	G	205	BCR	C7-C8-C9	-3.63	120.86	126.23
36	Y	1622	XAT	C15-C35-C34	-3.63	116.09	123.52
30	B	848	BCR	C36-C18-C19	3.63	123.64	118.09
29	2	622	LHG	O7-C7-C8	3.63	119.34	111.48
30	K	207	BCR	C11-C10-C9	-3.63	122.19	127.28
37	6	624	NEX	C26-C27-C28	-3.62	118.33	125.99
30	J	102	BCR	C24-C23-C22	-3.62	120.88	126.23
30	7	623	BCR	C36-C18-C19	3.62	123.62	118.09
38	U	609	CHL	CBC-CAC-C3C	-3.62	107.69	112.87
30	B	849	BCR	C16-C17-C18	-3.62	122.20	127.28
30	a	619	BCR	C11-C10-C9	-3.62	122.20	127.28
30	4	621	BCR	C39-C30-C25	-3.62	104.57	110.24
38	X	608	CHL	C1B-CHB-C4A	3.62	123.65	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	V	606	CHL	CMD-C2D-C3D	3.61	131.90	124.68
30	6	622	BCR	C20-C21-C22	-3.61	122.21	127.28
30	1	619	BCR	C11-C10-C9	-3.61	122.22	127.28
29	Y	2630	LHG	O7-C7-C8	3.61	119.28	111.48
30	L	308	BCR	C38-C26-C25	-3.60	120.56	124.48
30	L	308	BCR	C20-C21-C22	-3.60	122.23	127.28
30	B	849	BCR	C11-C10-C9	-3.60	122.23	127.28
38	U	605	CHL	CMA-C3A-C4A	-3.60	106.86	114.61
38	Z	606	CHL	CMB-C2B-C3B	3.60	131.87	124.68
30	B	849	BCR	C36-C18-C19	3.59	123.58	118.09
36	8	620	XAT	C12-C13-C14	-3.59	113.36	119.01
30	L	308	BCR	C16-C17-C18	-3.59	122.25	127.28
30	L	308	BCR	C7-C8-C9	-3.59	120.93	126.23
30	L	305	BCR	C36-C18-C19	3.58	123.56	118.09
30	A	851	BCR	C40-C30-C25	3.58	115.86	110.24
30	1	619	BCR	C36-C18-C19	3.58	123.56	118.09
35	5	620	LUT	C28-C29-C30	-3.58	113.38	119.01
38	W	608	CHL	CBC-CAC-C3C	-3.58	107.75	112.87
30	B	845	BCR	C36-C18-C19	3.58	123.55	118.09
30	3	621	BCR	C8-C7-C6	-3.58	117.44	127.00
37	Y	1623	NEX	O24-C25-C38	3.58	119.04	115.05
36	8	620	XAT	C26-C27-C28	-3.57	118.44	125.99
37	X	1623	NEX	O24-C25-C38	3.57	119.04	115.05
30	L	305	BCR	C16-C17-C18	-3.57	122.27	127.28
30	A	856	BCR	C16-C17-C18	-3.57	122.27	127.28
38	W	605	CHL	CMA-C3A-C4A	-3.57	106.92	114.61
38	Y	608	CHL	C1A-CHA-C4D	-3.57	113.03	118.98
30	a	619	BCR	C36-C18-C19	3.57	123.54	118.09
35	V	1620	LUT	C17-C1-C6	-3.57	104.65	110.24
30	O	2004	BCR	C34-C9-C8	-3.57	112.64	118.09
30	F	305	BCR	C24-C23-C22	-3.57	120.96	126.23
38	U	608	CHL	CBC-CAC-C3C	-3.56	107.77	112.87
36	U	1622	XAT	C6-C7-C8	-3.56	118.46	125.99
33	4	623	LMG	O7-C10-C11	3.56	119.19	111.48
38	Z	608	CHL	C1A-CHA-C4D	-3.56	113.04	118.98
30	J	102	BCR	C15-C16-C17	-3.56	116.23	123.52
36	W	1622	XAT	C6-C7-C8	-3.56	118.47	125.99
27	A	822	CLA	CMB-C2B-C1B	-3.56	120.00	125.42
30	7	621	BCR	C28-C27-C26	-3.55	107.72	114.06
33	A	860	LMG	O7-C10-C11	3.55	119.17	111.48
29	W	2630	LHG	O7-C7-C8	3.55	119.15	111.48
29	3	624	LHG	O7-C7-C8	3.54	119.15	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	202	BCR	C7-C8-C9	-3.54	120.99	126.23
30	A	856	BCR	C36-C18-C19	3.54	123.50	118.09
27	B	828	CLA	C4A-NA-C1A	3.54	108.29	106.68
30	9	621	BCR	C1-C6-C5	-3.53	117.81	122.64
30	B	852	BCR	C36-C18-C19	3.53	123.49	118.09
30	6	622	BCR	C38-C26-C25	-3.53	120.63	124.48
30	3	621	BCR	C37-C22-C23	3.53	123.48	118.09
30	G	205	BCR	C24-C23-C22	-3.53	121.01	126.23
30	B	852	BCR	C33-C5-C4	3.53	121.12	113.60
30	7	621	BCR	C16-C17-C18	-3.53	122.33	127.28
27	7	610	CLA	CMB-C2B-C1B	-3.53	120.05	125.42
35	Y	1621	LUT	C26-C27-C28	-3.52	119.09	124.58
36	Y	1622	XAT	C36-C21-C26	3.52	119.56	110.05
36	4	620	XAT	C12-C13-C14	-3.52	113.47	119.01
35	X	1621	LUT	C26-C27-C28	-3.52	119.10	124.58
30	8	621	BCR	C36-C18-C19	3.52	123.46	118.09
29	U	2630	LHG	O7-C7-C8	3.51	119.08	111.48
30	B	849	BCR	C33-C5-C4	3.51	121.08	113.60
33	4	624	LMG	O7-C10-C11	3.51	119.07	111.48
36	2	620	XAT	C6-C7-C8	-3.51	118.57	125.99
30	O	2004	BCR	C24-C23-C22	-3.51	121.05	126.23
38	V	607	CHL	C1A-CHA-C4D	-3.51	113.13	118.98
36	X	1622	XAT	C36-C21-C26	3.50	119.50	110.05
27	Z	610	CLA	C4A-NA-C1A	3.50	108.28	106.68
33	V	2631	LMG	O1-C1-C2	3.49	113.58	108.27
30	L	309	BCR	C3-C4-C5	-3.49	107.83	114.06
30	8	621	BCR	C20-C21-C22	-3.49	122.38	127.28
30	O	2005	BCR	C33-C5-C6	-3.49	120.67	124.48
30	L	305	BCR	C15-C16-C17	-3.49	116.38	123.52
27	L	303	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
36	7	620	XAT	C6-C7-C8	-3.49	118.62	125.99
30	B	853	BCR	C33-C5-C6	-3.48	120.68	124.48
36	Z	1622	XAT	C15-C35-C34	-3.48	116.39	123.52
38	Z	605	CHL	C1C-C2C-CMC	3.47	133.06	126.80
30	A	852	BCR	C29-C30-C25	3.47	115.48	110.44
30	A	851	BCR	C36-C18-C19	3.47	123.39	118.09
36	5	621	XAT	C27-C28-C29	-3.47	120.15	125.53
32	A	858	LMU	C6B-C5B-C4B	-3.47	108.79	113.53
35	4	619	LUT	C30-C31-C32	-3.46	113.17	123.20
30	6	622	BCR	C24-C23-C22	-3.46	121.11	126.23
30	G	205	BCR	C23-C24-C25	-3.46	117.75	127.00
30	a	619	BCR	C15-C16-C17	-3.46	116.44	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	X	607	CHL	CMA-C3A-C4A	-3.46	107.17	114.61
35	U	1621	LUT	C17-C1-C6	-3.45	104.83	110.24
30	L	308	BCR	C39-C30-C25	-3.45	104.83	110.24
30	L	308	BCR	C33-C5-C6	-3.45	120.72	124.48
27	X	610	CLA	C4A-NA-C1A	3.45	108.25	106.68
30	A	849	BCR	C7-C8-C9	-3.45	121.13	126.23
30	K	207	BCR	C39-C30-C29	3.45	122.19	108.95
27	8	602	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
36	4	620	XAT	C26-C27-C28	-3.45	118.70	125.99
38	W	606	CHL	CMD-C2D-C3D	3.45	131.57	124.68
38	Z	607	CHL	C3D-C4D-ND	3.45	118.47	112.94
30	4	621	BCR	C37-C22-C23	3.44	123.35	118.09
27	B	841	CLA	C3B-C4B-NB	-3.44	107.46	110.53
38	Z	601	CHL	C1-C2-C3	-3.44	120.56	126.20
30	4	621	BCR	C1-C6-C5	-3.44	117.94	122.64
38	Y	605	CHL	C1C-C2C-CMC	3.44	133.00	126.80
30	1	619	BCR	C15-C16-C17	-3.44	116.49	123.52
30	B	846	BCR	C16-C17-C18	-3.43	122.46	127.28
35	Z	1621	LUT	C8-C7-C6	-3.43	117.83	127.00
38	Y	601	CHL	C1-C2-C3	-3.43	120.57	126.20
37	Y	1623	NEX	C4-C3-C2	-3.43	106.34	111.03
29	4	622	LHG	O7-C7-C8	3.43	118.90	111.48
38	X	605	CHL	C1C-C2C-CMC	3.43	132.98	126.80
38	V	608	CHL	C1C-C2C-CMC	3.43	132.98	126.80
30	A	849	BCR	C3-C4-C5	-3.42	107.95	114.06
30	B	801	BCR	C40-C30-C25	-3.42	104.88	110.24
30	A	851	BCR	C24-C23-C22	-3.42	121.18	126.23
35	W	1621	LUT	C17-C1-C6	-3.42	104.89	110.24
30	O	2004	BCR	C36-C18-C19	3.42	123.31	118.09
29	9	623	LHG	C5-O7-C7	-3.41	109.63	117.80
27	A	804	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
29	3	623	LHG	O7-C7-C8	3.41	118.86	111.48
30	2	623	BCR	C11-C10-C9	-3.41	122.50	127.28
36	3	619	XAT	C8-C9-C10	-3.41	113.65	119.01
38	U	606	CHL	CMD-C2D-C3D	3.41	131.49	124.68
27	3	610	CLA	C4A-NA-C1A	3.40	108.23	106.68
27	1	606	CLA	CBD-CHA-C1A	3.40	131.64	128.03
30	3	621	BCR	C7-C8-C9	-3.40	121.20	126.23
38	W	609	CHL	CBC-CAC-C3C	-3.39	108.01	112.87
38	Z	608	CHL	C1C-C2C-CMC	3.39	132.92	126.80
30	B	846	BCR	C7-C8-C9	-3.39	121.22	126.23
38	V	609	CHL	CBC-CAC-C3C	-3.39	108.02	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	619	BCR	C16-C17-C18	-3.39	122.53	127.28
35	6	619	LUT	C35-C15-C14	-3.38	116.60	123.52
30	B	801	BCR	C37-C22-C23	3.38	123.25	118.09
35	U	1621	LUT	C1-C6-C5	-3.38	118.01	122.64
37	6	624	NEX	C5-C6-C1	3.38	123.05	119.70
36	X	1622	XAT	C7-C8-C9	-3.38	120.28	125.53
30	B	852	BCR	C31-C1-C2	3.38	121.93	108.95
35	W	1621	LUT	C1-C6-C5	-3.38	118.02	122.64
27	A	828	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
35	3	618	LUT	C7-C8-C9	-3.38	121.24	126.23
30	B	848	BCR	C7-C8-C9	-3.38	121.24	126.23
30	A	852	BCR	C4-C5-C6	-3.37	118.14	122.70
30	a	619	BCR	C16-C17-C18	-3.37	122.55	127.28
38	W	607	CHL	C4C-C3C-C2C	-3.37	100.66	108.42
30	K	207	BCR	C36-C18-C19	3.37	123.23	118.09
36	U	1622	XAT	C24-C23-C22	-3.37	104.49	110.79
30	A	849	BCR	C11-C10-C9	-3.37	122.56	127.28
36	U	1622	XAT	C36-C21-C26	3.37	119.13	110.05
36	W	1622	XAT	C36-C21-C26	3.36	119.13	110.05
27	A	812	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
27	B	807	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
38	X	601	CHL	C3D-C4D-ND	3.36	118.33	112.94
27	A	817	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
38	U	601	CHL	C3D-C4D-ND	3.36	118.32	112.94
36	Z	1622	XAT	C31-C30-C29	-3.35	122.57	127.28
30	1	619	BCR	C7-C8-C9	-3.35	121.27	126.23
30	B	853	BCR	C37-C22-C23	3.35	123.21	118.09
30	A	851	BCR	C29-C30-C25	-3.35	105.57	110.44
30	2	623	BCR	C30-C25-C26	-3.35	118.06	122.64
36	X	1622	XAT	C6-C7-C8	-3.34	118.92	125.99
30	F	305	BCR	C8-C9-C10	-3.34	113.75	119.01
36	V	1622	XAT	C6-C7-C8	-3.34	118.92	125.99
28	A	844	PQN	C14-C13-C12	-3.34	115.04	123.63
30	A	848	BCR	C36-C18-C17	-3.34	117.40	122.82
30	B	843	BCR	C3-C4-C5	-3.34	108.10	114.06
27	1	606	CLA	C3A-C2A-C1A	-3.34	102.89	106.30
27	Y	610	CLA	C4A-NA-C1A	3.34	108.20	106.68
36	Y	1622	XAT	C7-C8-C9	-3.34	120.35	125.53
38	X	609	CHL	C1-C2-C3	-3.33	120.73	126.20
30	L	308	BCR	C38-C26-C27	3.33	120.70	113.60
36	W	1622	XAT	C24-C23-C22	-3.33	104.56	110.79
38	Y	601	CHL	C3D-C4D-ND	3.33	118.28	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	7	616	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
30	a	619	BCR	C7-C8-C9	-3.33	121.31	126.23
27	B	808	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
35	9	619	LUT	C21-C26-C27	-3.33	109.00	112.83
38	X	607	CHL	CMB-C2B-C3B	3.33	131.33	124.68
36	a	618	XAT	C12-C13-C14	-3.32	113.78	119.01
30	3	620	BCR	C36-C18-C19	3.32	123.16	118.09
38	W	605	CHL	C1C-C2C-CMC	3.32	132.79	126.80
30	A	850	BCR	C31-C1-C6	-3.32	105.04	110.24
27	B	823	CLA	C4A-NA-C1A	3.32	108.19	106.68
35	Y	1621	LUT	C17-C1-C6	-3.31	105.05	110.24
36	5	621	XAT	C8-C9-C10	-3.31	113.80	119.01
38	U	605	CHL	C1C-C2C-CMC	3.31	132.77	126.80
38	V	601	CHL	C3D-C4D-ND	3.31	118.25	112.94
27	B	833	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
30	K	202	BCR	C38-C26-C27	3.31	120.65	113.60
36	9	620	XAT	C26-C27-C28	-3.31	119.00	125.99
38	U	609	CHL	C3D-C4D-ND	3.31	118.25	112.94
38	W	601	CHL	C3D-C4D-ND	3.31	118.25	112.94
30	L	308	BCR	C8-C7-C6	-3.31	118.16	127.00
30	4	621	BCR	C28-C27-C26	-3.31	108.16	114.06
30	8	621	BCR	C33-C5-C4	3.31	120.64	113.60
38	Z	601	CHL	CBC-CAC-C3C	-3.31	108.14	112.87
36	Y	1622	XAT	C6-C7-C8	-3.30	119.01	125.99
30	5	622	BCR	C39-C30-C25	-3.30	105.06	110.24
30	6	622	BCR	C7-C8-C9	-3.30	121.35	126.23
27	B	816	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
30	G	205	BCR	C36-C18-C17	-3.30	117.47	122.82
35	X	1621	LUT	C17-C1-C6	-3.30	105.07	110.24
38	Y	607	CHL	C1-C2-C3	-3.30	120.79	126.20
27	B	826	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
27	8	614	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
30	L	308	BCR	C24-C23-C22	-3.29	121.36	126.23
35	V	1621	LUT	C21-C26-C27	-3.29	109.04	112.83
30	A	849	BCR	C15-C14-C13	-3.29	122.66	127.28
38	W	609	CHL	C3D-C4D-ND	3.29	118.22	112.94
30	L	309	BCR	C37-C22-C23	3.29	123.12	118.09
38	V	608	CHL	CMD-C2D-C3D	3.29	131.26	124.68
38	X	609	CHL	C3D-C4D-ND	3.29	118.22	112.94
36	1	618	XAT	C12-C13-C14	-3.29	113.83	119.01
38	U	607	CHL	C1A-CHA-C4D	-3.29	113.50	118.98
30	A	848	BCR	C11-C10-C9	-3.29	122.67	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	851	BCR	C16-C15-C14	-3.29	116.79	123.52
35	3	618	LUT	C21-C26-C27	-3.29	109.05	112.83
38	Y	609	CHL	CBC-CAC-C3C	-3.29	108.17	112.87
30	B	844	BCR	C16-C17-C18	-3.28	122.67	127.28
38	W	605	CHL	CMD-C2D-C3D	3.28	131.25	124.68
36	W	1622	XAT	C18-C5-C4	3.28	117.93	114.24
29	A	847	LHG	O7-C7-C8	3.28	118.58	111.48
27	A	840	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
29	8	622	LHG	O7-C7-C8	3.28	118.57	111.48
30	B	801	BCR	C19-C18-C17	-3.28	113.86	119.01
36	Z	1622	XAT	C7-C8-C9	-3.28	120.45	125.53
27	6	616	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
27	A	833	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
38	X	607	CHL	C3D-C4D-ND	3.27	118.19	112.94
27	B	812	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
36	Y	1622	XAT	C31-C30-C29	-3.27	122.70	127.28
27	3	607	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
30	2	623	BCR	C39-C30-C25	-3.26	105.12	110.24
38	U	605	CHL	CMD-C2D-C3D	3.26	131.21	124.68
27	9	610	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
30	K	202	BCR	C15-C14-C13	-3.26	122.70	127.28
27	A	805	CLA	O2D-CGD-CBD	3.26	116.94	111.23
30	O	2005	BCR	C39-C30-C29	3.26	121.48	108.95
27	4	602	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
30	O	2005	BCR	C8-C7-C6	-3.26	118.29	127.00
30	B	845	BCR	C11-C10-C9	-3.26	122.71	127.28
27	4	602	CLA	CMB-C2B-C1B	-3.26	120.46	125.42
36	U	1622	XAT	C18-C5-C4	3.26	117.90	114.24
27	4	601	CLA	O2D-CGD-O1D	-3.25	117.51	123.85
36	1	618	XAT	C26-C27-C28	-3.25	119.12	125.99
30	B	845	BCR	C34-C9-C10	-3.25	117.55	122.82
36	9	620	XAT	C38-C25-C24	3.25	117.89	114.24
27	B	805	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
36	a	618	XAT	C26-C27-C28	-3.25	119.13	125.99
36	X	1622	XAT	C31-C30-C29	-3.24	122.73	127.28
27	A	820	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
27	B	831	CLA	CMB-C2B-C1B	-3.24	120.48	125.42
27	A	854	CLA	C4-C3-C5	3.24	120.86	115.23
36	Z	1622	XAT	C6-C7-C8	-3.24	119.15	125.99
29	6	623	LHG	O7-C7-C8	3.24	118.48	111.48
27	B	837	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
30	B	853	BCR	C36-C18-C19	3.23	123.03	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	832	CLA	C4A-NA-C1A	3.23	108.15	106.68
30	A	850	BCR	C7-C8-C9	-3.23	121.45	126.23
38	W	608	CHL	C1C-C2C-CMC	3.23	132.63	126.80
27	2	601	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
30	O	2005	BCR	C36-C18-C17	-3.22	117.59	122.82
27	B	838	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
38	U	608	CHL	C1C-C2C-CMC	3.22	132.61	126.80
30	L	305	BCR	C15-C14-C13	-3.22	122.76	127.28
30	O	2005	BCR	C36-C18-C19	3.22	123.00	118.09
38	Z	601	CHL	C3D-C4D-ND	3.21	118.09	112.94
33	4	624	LMG	O8-C28-C29	3.21	121.63	111.83
35	9	619	LUT	C35-C15-C14	-3.21	116.95	123.52
38	W	607	CHL	O1D-CGD-CBD	-3.21	119.86	124.72
27	B	825	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
30	F	305	BCR	C38-C26-C27	3.21	120.43	113.60
30	4	621	BCR	C3-C4-C5	-3.21	108.34	114.06
27	L	302	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
35	5	620	LUT	C35-C34-C33	-3.21	122.78	127.28
38	Y	608	CHL	C1C-C2C-CMC	3.20	132.58	126.80
30	B	845	BCR	C33-C5-C6	-3.20	120.99	124.48
38	Y	601	CHL	C4-C3-C5	3.20	120.78	115.23
27	B	818	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
37	6	624	NEX	C31-C30-C29	-3.19	122.80	127.28
35	U	1620	LUT	C35-C15-C14	-3.19	116.98	123.52
36	V	1622	XAT	C31-C30-C29	-3.19	122.80	127.28
30	L	301	BCR	C15-C16-C17	-3.19	116.99	123.52
38	W	607	CHL	C4-C3-C5	3.19	120.76	115.23
30	9	621	BCR	C38-C26-C25	-3.19	121.00	124.48
27	9	614	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
27	A	842	CLA	C4-C3-C5	3.18	120.76	115.23
35	Y	1621	LUT	C21-C26-C27	-3.18	109.16	112.83
29	B	854	LHG	O8-C23-C24	3.18	121.54	111.83
27	5	602	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
30	K	202	BCR	C11-C10-C9	-3.18	122.82	127.28
35	W	1620	LUT	C35-C15-C14	-3.18	117.02	123.52
38	Z	606	CHL	OMC-CMC-C2C	-3.18	119.60	125.12
30	3	622	BCR	C7-C8-C9	-3.18	121.54	126.23
30	2	623	BCR	C36-C18-C17	-3.18	117.67	122.82
30	G	205	BCR	C36-C18-C19	3.18	122.94	118.09
30	A	852	BCR	C1-C6-C5	-3.18	118.30	122.64
38	V	609	CHL	C3D-C4D-ND	3.17	118.03	112.94
27	8	610	CLA	CMB-C2B-C3B	3.17	134.01	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	2	620	XAT	C20-C13-C12	3.17	122.94	118.09
27	5	607	CLA	C3B-C4B-NB	-3.17	107.70	110.53
36	2	620	XAT	C26-C27-C28	-3.17	119.29	125.99
37	5	624	NEX	C31-C30-C29	-3.17	122.83	127.28
37	V	1623	NEX	O24-C25-C38	3.17	118.59	115.05
27	8	610	CLA	C4-C3-C5	3.17	120.73	115.23
30	B	801	BCR	C24-C23-C22	-3.17	121.55	126.23
37	Z	1623	NEX	C31-C30-C29	-3.17	122.84	127.28
36	V	1622	XAT	C15-C35-C34	-3.16	117.04	123.52
30	L	301	BCR	C40-C30-C25	-3.16	105.28	110.24
37	5	624	NEX	C17-C1-C6	-3.16	107.64	110.47
27	K	203	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
36	5	621	XAT	C38-C25-C24	3.16	117.80	114.24
30	A	850	BCR	C36-C18-C19	3.16	122.92	118.09
30	5	622	BCR	C7-C8-C9	-3.16	121.56	126.23
27	B	836	CLA	CMB-C2B-C1B	-3.16	120.60	125.42
35	2	619	LUT	C35-C15-C14	-3.16	117.05	123.52
35	X	1621	LUT	C21-C26-C27	-3.16	109.19	112.83
30	L	308	BCR	C27-C26-C25	-3.16	118.44	122.70
36	U	1622	XAT	C31-C30-C29	-3.16	122.85	127.28
27	a	614	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
35	U	1620	LUT	C26-C27-C28	-3.16	119.67	124.58
38	X	606	CHL	OMC-CMC-C2C	-3.15	119.65	125.12
30	O	2004	BCR	C15-C16-C17	-3.15	117.08	123.52
38	W	607	CHL	C1-C2-C3	-3.15	121.04	126.20
29	Y	2630	LHG	O8-C23-C24	3.15	121.43	111.83
38	Y	609	CHL	C1-C2-C3	-3.15	121.04	126.20
38	U	601	CHL	C1C-CHC-C4B	3.15	127.33	116.07
38	Y	606	CHL	CMD-C2D-C3D	3.15	130.97	124.68
27	6	604	CLA	O2D-CGD-O1D	-3.15	117.73	123.85
30	3	622	BCR	C33-C5-C6	-3.14	121.05	124.48
30	O	2005	BCR	C3-C4-C5	-3.14	108.45	114.06
27	4	616	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
27	5	604	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
38	Z	609	CHL	CBC-CAC-C3C	-3.14	108.38	112.87
37	Z	1623	NEX	C27-C28-C29	-3.14	120.66	125.53
27	5	610	CLA	CMB-C2B-C1B	-3.14	120.64	125.42
30	B	849	BCR	C24-C25-C26	-3.14	114.32	121.56
36	W	1622	XAT	C31-C30-C29	-3.14	122.88	127.28
27	a	604	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
30	A	849	BCR	C15-C16-C17	-3.14	117.10	123.52
35	W	1620	LUT	C26-C27-C28	-3.13	119.70	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	623	BCR	C28-C27-C26	-3.13	108.47	114.06
27	8	604	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
30	3	620	BCR	C38-C26-C25	-3.13	121.07	124.48
30	9	621	BCR	C15-C14-C13	-3.13	122.89	127.28
27	6	610	CLA	C3B-C4B-NB	-3.13	107.74	110.53
30	6	622	BCR	C37-C22-C23	3.12	122.86	118.09
29	X	2630	LHG	O8-C23-C24	3.12	121.36	111.83
38	Y	608	CHL	CMD-C2D-C3D	3.12	130.92	124.68
38	Y	609	CHL	C3D-C4D-ND	3.12	117.95	112.94
38	W	601	CHL	C1C-CHC-C4B	3.12	127.24	116.07
36	V	1622	XAT	C27-C28-C29	-3.12	120.69	125.53
27	A	807	CLA	C3B-C4B-NB	-3.12	107.74	110.53
30	A	851	BCR	C37-C22-C23	3.12	122.85	118.09
30	6	622	BCR	C23-C24-C25	-3.12	118.67	127.00
35	V	1620	LUT	C7-C8-C9	-3.12	121.62	126.23
27	6	602	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
30	5	622	BCR	C36-C18-C19	3.11	122.84	118.09
38	Y	607	CHL	O1D-CGD-CBD	-3.11	120.00	124.72
33	A	860	LMG	O1-C1-C2	3.11	113.00	108.27
35	3	618	LUT	C17-C1-C6	-3.11	105.37	110.24
36	9	620	XAT	C35-C15-C14	-3.11	117.16	123.52
30	F	305	BCR	C16-C15-C14	-3.11	117.16	123.52
38	X	606	CHL	CMD-C2D-C3D	3.11	130.89	124.68
27	1	604	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
38	X	605	CHL	O1D-CGD-CBD	-3.10	120.02	124.72
35	8	619	LUT	C1-C6-C5	-3.10	118.39	122.64
30	K	202	BCR	C15-C16-C17	-3.10	117.17	123.52
38	Y	606	CHL	OMC-CMC-C2C	-3.10	119.73	125.12
30	9	621	BCR	C7-C8-C9	-3.10	121.64	126.23
38	U	607	CHL	O1D-CGD-CBD	-3.10	120.02	124.72
30	L	309	BCR	C38-C26-C25	-3.10	121.10	124.48
30	9	621	BCR	C28-C27-C26	-3.10	108.53	114.06
27	A	804	CLA	C1-C2-C3	-3.10	121.12	126.20
38	Y	605	CHL	O1D-CGD-CBD	-3.10	120.02	124.72
27	8	606	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
30	2	623	BCR	C38-C26-C25	-3.10	121.11	124.48
38	Y	601	CHL	C1C-CHC-C4B	3.09	127.14	116.07
38	W	607	CHL	C1B-CHB-C4A	3.09	123.31	121.32
38	U	609	CHL	C1C-CHC-C4B	3.09	127.13	116.07
30	B	847	BCR	C3-C4-C5	-3.09	108.54	114.06
27	B	840	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
37	U	1623	NEX	C11-C12-C13	-3.09	117.89	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	844	PQN	C14-C13-C15	-3.09	109.86	115.23
30	L	301	BCR	C37-C22-C23	3.09	122.81	118.09
30	7	623	BCR	C15-C14-C13	-3.09	122.95	127.28
27	8	616	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
38	X	609	CHL	C1C-CHC-C4B	3.09	127.11	116.07
30	6	622	BCR	C36-C18-C19	3.09	122.80	118.09
38	V	605	CHL	C1C-C2C-CMC	3.08	132.36	126.80
27	9	613	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
30	3	621	BCR	C20-C21-C22	-3.08	122.95	127.28
30	7	621	BCR	C11-C10-C9	-3.08	122.95	127.28
38	W	609	CHL	C1C-CHC-C4B	3.08	127.10	116.07
30	9	621	BCR	C11-C12-C13	-3.08	117.91	126.36
30	F	305	BCR	C30-C25-C26	-3.08	118.42	122.64
37	W	1623	NEX	C11-C12-C13	-3.08	117.91	126.36
36	W	1622	XAT	C38-C25-C24	3.08	117.70	114.24
38	U	609	CHL	CMA-C3A-C4A	-3.08	107.97	114.61
27	A	803	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
30	2	623	BCR	C33-C5-C4	3.08	120.16	113.60
36	4	620	XAT	C10-C11-C12	-3.08	114.29	123.20
38	Y	609	CHL	C1C-CHC-C4B	3.08	127.07	116.07
27	A	837	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
30	B	845	BCR	C3-C4-C5	-3.07	108.57	114.06
37	V	1623	NEX	C31-C30-C29	-3.07	122.97	127.28
27	J	101	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
35	1	617	LUT	C7-C8-C9	-3.07	121.70	126.23
27	5	611	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
36	7	620	XAT	C26-C27-C28	-3.07	119.51	125.99
30	A	850	BCR	C30-C25-C26	-3.07	118.45	122.64
36	U	1622	XAT	C38-C25-C24	3.07	117.68	114.24
30	9	621	BCR	C36-C18-C19	3.06	122.77	118.09
38	Z	609	CHL	C3D-C4D-ND	3.06	117.85	112.94
35	a	617	LUT	C7-C8-C9	-3.06	121.70	126.23
36	2	620	XAT	C38-C25-C24	3.06	117.68	114.24
27	B	810	CLA	C3B-C4B-NB	-3.06	107.80	110.53
27	F	301	CLA	C3B-C4B-NB	-3.06	107.80	110.53
27	A	818	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
30	L	309	BCR	C39-C30-C25	3.06	115.04	110.24
38	V	607	CHL	C1C-C2C-CMC	3.06	132.31	126.80
30	G	205	BCR	C11-C10-C9	-3.06	122.99	127.28
30	A	852	BCR	C16-C17-C18	-3.06	122.99	127.28
38	X	601	CHL	C1C-CHC-C4B	3.05	127.00	116.07
33	J	104	LMG	O8-C28-C29	3.05	121.15	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	848	BCR	C24-C23-C22	-3.05	121.72	126.23
27	A	806	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
30	3	622	BCR	C11-C10-C9	-3.05	123.00	127.28
30	7	621	BCR	C36-C18-C19	3.05	122.75	118.09
30	B	844	BCR	C4-C5-C6	-3.05	118.58	122.70
36	7	620	XAT	C12-C13-C14	-3.05	114.21	119.01
38	W	606	CHL	OMC-CMC-C2C	-3.05	119.83	125.12
37	6	624	NEX	C39-C29-C30	-3.05	117.88	122.82
27	A	808	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
35	Z	1620	LUT	C35-C15-C14	-3.05	117.29	123.52
38	Z	601	CHL	C1C-CHC-C4B	3.05	126.97	116.07
30	1	619	BCR	C33-C5-C6	-3.04	121.16	124.48
27	A	827	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
30	9	621	BCR	C33-C5-C4	3.04	120.08	113.60
30	a	619	BCR	C33-C5-C6	-3.04	121.17	124.48
27	K	206	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
27	4	607	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
27	9	602	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
38	X	608	CHL	C1C-CHC-C4B	3.04	126.95	116.07
27	3	612	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
38	U	606	CHL	OMC-CMC-C2C	-3.04	119.84	125.12
35	Z	1620	LUT	C28-C29-C30	-3.04	114.23	119.01
37	Z	1623	NEX	O24-C25-C38	3.04	118.44	115.05
38	X	608	CHL	C3D-C4D-ND	3.04	117.81	112.94
30	A	852	BCR	C31-C1-C6	-3.04	105.48	110.24
27	7	606	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
27	A	839	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
38	X	605	CHL	CMD-C2D-C3D	3.04	130.75	124.68
30	L	305	BCR	C34-C9-C8	-3.04	113.45	118.09
27	V	614	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
27	4	604	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
29	3	624	LHG	C5-O7-C7	-3.03	110.54	117.80
30	7	623	BCR	C37-C22-C23	3.03	122.72	118.09
27	2	616	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
30	7	623	BCR	C31-C1-C6	-3.03	105.49	110.24
30	1	619	BCR	C38-C26-C27	3.03	120.05	113.60
30	2	623	BCR	C1-C6-C5	-3.03	118.50	122.64
30	B	844	BCR	C19-C18-C17	-3.02	114.25	119.01
36	2	620	XAT	C10-C11-C12	-3.02	114.44	123.20
38	V	601	CHL	C1C-CHC-C4B	3.02	126.88	116.07
27	B	823	CLA	C3B-C4B-NB	-3.02	107.83	110.53
35	9	619	LUT	C30-C31-C32	-3.02	114.45	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	O	2005	BCR	C7-C8-C9	-3.02	121.77	126.23
38	X	609	CHL	C4-C3-C5	3.02	120.47	115.23
38	W	609	CHL	C4-C3-C5	3.02	120.47	115.23
27	7	601	CLA	CMB-C2B-C3B	3.02	133.65	126.55
37	Y	1623	NEX	C24-C23-C22	-3.02	105.15	110.79
27	5	619	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
37	X	1623	NEX	C24-C23-C22	-3.02	105.15	110.79
38	V	608	CHL	OMC-CMC-C2C	-3.02	119.88	125.12
30	7	621	BCR	C30-C25-C24	3.02	123.83	115.65
27	A	854	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
38	W	609	CHL	C1-C2-C3	-3.01	121.26	126.20
27	a	610	CLA	CMB-C2B-C3B	3.01	133.64	126.55
30	A	849	BCR	C38-C26-C27	3.01	120.02	113.60
36	6	621	XAT	C8-C9-C10	-3.01	114.27	119.01
35	9	619	LUT	C11-C10-C9	-3.01	123.05	127.28
38	Z	606	CHL	CMD-C2D-C3D	3.01	130.70	124.68
35	W	1621	LUT	C8-C7-C6	-3.01	118.95	127.00
27	B	835	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
35	U	1621	LUT	C8-C7-C6	-3.01	118.95	127.00
27	A	826	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
30	a	619	BCR	C38-C26-C27	3.01	120.01	113.60
27	3	604	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
27	7	614	CLA	C3B-C4B-NB	-3.00	107.85	110.53
27	A	835	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
27	6	620	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
27	2	610	CLA	CMB-C2B-C3B	3.00	133.61	126.55
27	1	610	CLA	CMB-C2B-C3B	3.00	133.61	126.55
30	B	853	BCR	C20-C21-C22	-3.00	123.07	127.28
27	B	831	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
29	5	623	LHG	O7-C7-C8	3.00	117.97	111.48
29	V	2630	LHG	O8-C23-C24	3.00	120.97	111.83
30	2	623	BCR	C3-C4-C5	-3.00	108.71	114.06
30	B	853	BCR	C16-C17-C18	-3.00	123.08	127.28
27	5	607	CLA	CHB-C4A-NA	3.00	128.72	124.40
38	V	601	CHL	C4-C3-C5	3.00	120.43	115.23
27	B	841	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
29	3	623	LHG	C5-O7-C7	-2.99	110.63	117.80
27	Y	603	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
27	B	828	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
30	4	621	BCR	C11-C10-C9	-2.99	123.08	127.28
35	a	617	LUT	C35-C15-C14	-2.99	117.40	123.52
38	V	605	CHL	OMC-CMC-C2C	-2.99	119.93	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	Y	611	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
27	A	843	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
29	A	846	LHG	O7-C7-C8	2.99	117.94	111.48
27	2	613	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
30	L	308	BCR	C36-C18-C19	2.99	122.65	118.09
38	Z	607	CHL	C1C-CHC-C4B	2.99	126.76	116.07
38	Y	609	CHL	C4-C3-C5	2.99	120.41	115.23
27	B	817	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
38	Y	605	CHL	CMD-C2D-C3D	2.99	130.65	124.68
27	9	604	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
38	X	607	CHL	C1C-CHC-C4B	2.99	126.75	116.07
36	Z	1622	XAT	C27-C28-C29	-2.98	120.90	125.53
35	1	617	LUT	C35-C15-C14	-2.98	117.41	123.52
34	B	850	DGD	O2G-C1B-C2B	2.98	117.93	111.48
36	U	1622	XAT	C7-C8-C9	-2.98	120.90	125.53
27	A	831	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
30	B	843	BCR	C2-C1-C6	2.98	114.77	110.44
30	L	308	BCR	C23-C24-C25	-2.98	119.04	127.00
27	7	604	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
38	U	607	CHL	C1C-C2C-CMC	2.98	132.17	126.80
38	Y	607	CHL	C4-C3-C5	2.98	120.40	115.23
27	2	610	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
27	Y	610	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
27	X	611	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
27	B	832	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
36	8	620	XAT	C18-C5-C4	2.98	117.58	114.24
27	X	603	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
27	8	611	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
27	7	612	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
27	A	824	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
36	1	618	XAT	C10-C11-C12	-2.97	114.59	123.20
35	Z	1620	LUT	C11-C10-C9	-2.97	123.11	127.28
27	A	826	CLA	CMB-C2B-C3B	2.97	133.54	126.55
35	W	1620	LUT	C11-C10-C9	-2.97	123.11	127.28
27	A	825	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
27	7	601	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
36	7	620	XAT	C35-C15-C14	-2.97	117.44	123.52
30	1	619	BCR	C24-C25-C26	-2.97	114.72	121.56
36	5	621	XAT	O24-C25-C38	2.97	118.36	115.05
36	3	619	XAT	C15-C35-C34	-2.97	117.45	123.52
27	A	821	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
27	9	607	CLA	O2D-CGD-O1D	-2.97	118.08	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	W	1622	XAT	C7-C8-C9	-2.97	120.93	125.53
35	7	619	LUT	C35-C15-C14	-2.96	117.45	123.52
27	6	611	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
27	X	610	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
35	X	1620	LUT	C35-C15-C14	-2.96	117.46	123.52
36	U	1622	XAT	C15-C14-C13	-2.96	123.12	127.28
27	B	803	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
36	a	618	XAT	C10-C11-C12	-2.96	114.62	123.20
38	U	608	CHL	CMD-C2D-C3D	2.96	130.60	124.68
36	a	618	XAT	C35-C15-C14	-2.96	117.47	123.52
36	7	620	XAT	C38-C25-C24	2.96	117.56	114.24
38	V	609	CHL	C4-C3-C5	2.96	120.36	115.23
36	Y	1622	XAT	O24-C25-C38	2.96	118.35	115.05
30	B	801	BCR	C37-C22-C21	-2.96	118.03	122.82
27	2	609	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
35	2	619	LUT	C28-C29-C30	-2.95	114.36	119.01
36	1	618	XAT	C35-C15-C14	-2.95	117.48	123.52
27	2	601	CLA	CHB-C4A-NA	2.95	128.66	124.40
32	5	628	LMU	C1'-C2'-C3'	2.95	116.21	110.01
27	8	601	CLA	CMB-C2B-C1B	-2.95	120.93	125.42
38	U	605	CHL	OMC-CMC-C2C	-2.95	120.00	125.12
38	W	605	CHL	OMC-CMC-C2C	-2.95	120.00	125.12
27	A	822	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
27	6	601	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
38	Z	608	CHL	OMC-CMC-C2C	-2.94	120.01	125.12
30	O	2005	BCR	C38-C26-C25	-2.94	121.27	124.48
35	Y	1620	LUT	C35-C15-C14	-2.94	117.50	123.52
30	a	619	BCR	C24-C25-C26	-2.94	114.78	121.56
36	X	1622	XAT	O24-C25-C38	2.94	118.34	115.05
36	6	621	XAT	C10-C11-C12	-2.94	114.67	123.20
27	7	608	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
30	F	305	BCR	C12-C13-C14	-2.94	114.38	119.01
27	5	610	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
35	Y	1621	LUT	C8-C7-C6	-2.94	119.15	127.00
30	7	621	BCR	C37-C22-C23	2.94	122.58	118.09
38	W	608	CHL	CMD-C2D-C3D	2.94	130.55	124.68
27	7	614	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
27	5	603	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
33	8	626	LMG	O8-C28-C29	2.94	120.78	111.83
36	7	620	XAT	O24-C25-C38	2.93	118.33	115.05
30	1	619	BCR	C30-C25-C24	2.93	123.61	115.65
30	3	622	BCR	C28-C27-C26	-2.93	108.82	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	Y	607	CHL	CMB-C2B-C3B	2.93	130.55	124.68
30	8	621	BCR	C15-C16-C17	-2.93	117.52	123.52
38	V	606	CHL	OMC-CMC-C2C	-2.93	120.03	125.12
30	B	848	BCR	C16-C15-C14	-2.93	117.52	123.52
36	W	1622	XAT	C15-C14-C13	-2.93	123.17	127.28
27	7	610	CLA	CMB-C2B-C3B	2.93	133.44	126.55
27	U	611	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
27	B	822	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
27	4	608	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
30	a	619	BCR	C39-C30-C25	-2.93	105.66	110.24
30	A	850	BCR	C1-C6-C7	2.92	123.58	115.65
38	W	606	CHL	C1C-C2C-CMC	2.92	132.07	126.80
27	A	819	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
35	Y	1621	LUT	C1-C6-C5	-2.92	118.64	122.64
27	4	611	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
36	9	620	XAT	C27-C28-C29	-2.92	121.00	125.53
27	B	817	CLA	CHB-C4A-NA	2.92	128.62	124.40
30	A	856	BCR	C3-C4-C5	-2.92	108.85	114.06
36	Z	1622	XAT	C15-C14-C13	-2.92	123.18	127.28
35	a	617	LUT	C1-C6-C5	-2.92	118.64	122.64
27	B	808	CLA	C1-C2-C3	-2.92	121.41	126.20
35	1	617	LUT	C1-C6-C5	-2.92	118.65	122.64
30	8	621	BCR	C37-C22-C21	-2.92	118.09	122.82
35	X	1621	LUT	C8-C7-C6	-2.92	119.20	127.00
30	a	619	BCR	C30-C25-C24	2.92	123.56	115.65
27	2	607	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
30	B	852	BCR	C2-C1-C6	2.92	114.67	110.44
27	5	613	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
27	5	614	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
38	U	606	CHL	C1C-C2C-CMC	2.91	132.05	126.80
38	Z	609	CHL	C1-C2-C3	-2.91	121.42	126.20
35	X	1621	LUT	C1-C6-C5	-2.91	118.66	122.64
37	5	624	NEX	C39-C29-C30	-2.91	118.10	122.82
35	U	1620	LUT	C11-C10-C9	-2.91	123.19	127.28
38	W	605	CHL	O1D-CGD-CBD	-2.91	120.31	124.72
38	Z	609	CHL	C1C-CHC-C4B	2.91	126.48	116.07
30	2	623	BCR	C36-C18-C19	2.91	122.53	118.09
30	J	102	BCR	C29-C30-C25	2.91	114.67	110.44
35	Z	1620	LUT	C3-C4-C5	-2.91	104.94	112.18
27	5	609	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
30	A	850	BCR	C11-C10-C9	-2.91	123.20	127.28
30	2	623	BCR	C23-C24-C25	-2.91	119.23	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Z	1623	NEX	C11-C12-C13	-2.91	118.39	126.36
38	Z	608	CHL	CMD-C2D-C3D	2.91	130.49	124.68
30	3	620	BCR	C35-C13-C12	-2.91	113.65	118.09
30	B	843	BCR	C16-C15-C14	-2.90	117.58	123.52
27	F	303	CLA	C3B-C4B-NB	-2.90	107.94	110.53
35	4	619	LUT	C10-C11-C12	-2.90	114.79	123.20
35	9	619	LUT	C18-C5-C6	-2.90	121.32	124.48
30	B	847	BCR	C37-C22-C21	-2.90	118.12	122.82
30	3	620	BCR	C30-C25-C24	2.90	123.51	115.65
38	Z	607	CHL	C4-C3-C5	2.90	120.26	115.23
36	3	619	XAT	C10-C11-C12	-2.90	114.80	123.20
38	U	608	CHL	CMB-C2B-C3B	2.90	130.47	124.68
36	9	620	XAT	C12-C13-C14	-2.90	114.45	119.01
37	5	624	NEX	C15-C35-C34	-2.90	117.59	123.52
30	F	305	BCR	C19-C18-C17	2.90	123.56	119.01
27	A	807	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
27	A	830	CLA	C3B-C4B-NB	-2.89	107.95	110.53
27	A	842	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
37	Z	1623	NEX	C39-C29-C30	-2.89	118.13	122.82
38	W	606	CHL	CBC-CAC-C3C	-2.89	108.73	112.87
27	6	603	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
38	Z	608	CHL	O2A-CGA-CBA	2.89	120.65	111.83
30	7	623	BCR	C11-C10-C9	-2.89	123.22	127.28
27	Y	613	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
27	9	611	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
38	X	609	CHL	CBC-CAC-C3C	-2.89	108.73	112.87
30	A	856	BCR	C37-C22-C23	2.89	122.50	118.09
30	B	848	BCR	C37-C22-C23	2.89	122.50	118.09
27	6	609	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
27	2	601	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
30	5	622	BCR	C37-C22-C23	2.89	122.50	118.09
27	X	613	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
27	1	616	CLA	CAB-C3B-C2B	2.88	131.20	123.53
27	B	834	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
30	1	619	BCR	C39-C30-C25	-2.88	105.72	110.24
30	F	305	BCR	C10-C11-C12	-2.88	114.84	123.20
30	5	622	BCR	C24-C23-C22	-2.88	121.97	126.23
38	W	608	CHL	CMB-C2B-C3B	2.88	130.44	124.68
27	L	303	CLA	CHB-C4A-NA	2.88	128.56	124.40
29	9	623	LHG	O8-C23-C24	2.88	120.62	111.83
30	B	845	BCR	C1-C6-C5	-2.88	118.70	122.64
27	6	608	CLA	O2D-CGD-O1D	-2.88	118.24	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	621	BCR	C15-C14-C13	-2.88	123.24	127.28
38	Z	605	CHL	OMC-CMC-C2C	-2.88	120.12	125.12
30	B	801	BCR	C30-C25-C26	-2.88	118.70	122.64
27	V	602	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
36	Z	1622	XAT	C26-C27-C28	-2.88	119.91	125.99
38	X	607	CHL	C4-C3-C5	2.88	120.22	115.23
37	5	624	NEX	C38-C25-C24	2.88	117.47	114.24
27	A	834	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
30	L	305	BCR	C3-C4-C5	-2.87	108.93	114.06
36	6	621	XAT	C15-C35-C34	-2.87	117.64	123.52
36	4	620	XAT	C8-C9-C10	-2.87	114.49	119.01
27	A	813	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
27	B	836	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
27	G	204	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
38	U	605	CHL	O1D-CGD-CBD	-2.87	120.37	124.72
27	6	613	CLA	C3B-C4B-NB	-2.87	107.97	110.53
30	B	845	BCR	C7-C8-C9	-2.87	121.99	126.23
30	8	621	BCR	C39-C30-C25	-2.87	105.74	110.24
38	V	609	CHL	C1C-CHC-C4B	2.87	126.33	116.07
30	L	305	BCR	C8-C9-C10	2.87	123.52	119.01
35	V	1621	LUT	C1-C6-C5	-2.87	118.72	122.64
27	B	839	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
27	B	802	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
27	B	824	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
27	B	827	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
30	A	856	BCR	C30-C25-C24	2.86	123.42	115.65
30	3	620	BCR	C33-C5-C4	2.86	119.70	113.60
27	W	602	CLA	CHB-C4A-NA	2.86	128.53	124.40
38	U	608	CHL	OMC-CMC-C2C	-2.86	120.15	125.12
38	Z	607	CHL	CBC-CAC-C3C	-2.86	108.78	112.87
35	9	619	LUT	C10-C11-C12	-2.86	114.91	123.20
27	A	809	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
27	B	804	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
27	W	611	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
36	1	618	XAT	C20-C13-C12	2.86	122.46	118.09
27	A	841	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
30	J	102	BCR	C7-C8-C9	-2.86	122.01	126.23
27	6	617	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
27	A	843	CLA	C3B-C4B-NB	-2.86	107.98	110.53
27	4	610	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
27	7	607	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
29	Z	2630	LHG	O7-C7-C8	2.85	117.66	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	U	613	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
30	9	621	BCR	C24-C23-C22	-2.85	122.02	126.23
27	B	819	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
27	A	801	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
27	B	829	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
27	Y	602	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
30	B	801	BCR	C12-C13-C14	-2.85	114.53	119.01
38	U	601	CHL	C4-C3-C5	2.85	120.17	115.23
35	Z	1621	LUT	C11-C10-C9	-2.85	123.28	127.28
36	6	621	XAT	C38-C25-C24	2.85	117.44	114.24
30	L	305	BCR	C2-C1-C6	2.85	114.57	110.44
27	B	817	CLA	C3B-C4B-NB	-2.85	107.99	110.53
27	W	602	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
38	U	606	CHL	CBC-CAC-C3C	-2.85	108.80	112.87
36	6	621	XAT	C27-C28-C29	-2.85	121.11	125.53
38	V	607	CHL	CMD-C2D-C3D	2.85	130.37	124.68
27	8	613	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
27	U	602	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
38	X	605	CHL	OMC-CMC-C2C	-2.84	120.18	125.12
27	A	823	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
27	A	802	CLA	CAA-C2A-C1A	-2.84	102.66	111.97
27	U	610	CLA	C3B-C4B-NB	-2.84	107.99	110.53
38	Z	608	CHL	CMB-C2B-C3B	2.84	130.36	124.68
27	V	610	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
38	Y	608	CHL	OMC-CMC-C2C	-2.84	120.19	125.12
38	Y	609	CHL	O2A-CGA-CBA	2.84	120.49	111.83
36	a	618	XAT	C20-C13-C12	2.84	122.42	118.09
36	5	621	XAT	C10-C11-C12	-2.84	114.98	123.20
38	Z	607	CHL	C1-C2-C3	-2.84	121.55	126.20
27	a	610	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
38	W	608	CHL	OMC-CMC-C2C	-2.84	120.19	125.12
27	A	830	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
27	F	303	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
35	X	1621	LUT	C11-C10-C9	-2.84	123.30	127.28
30	9	621	BCR	C3-C4-C5	-2.84	109.00	114.06
27	W	613	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
35	8	619	LUT	C17-C1-C6	-2.83	105.80	110.24
36	Y	1622	XAT	C15-C14-C13	-2.83	123.30	127.28
30	O	2004	BCR	C16-C17-C18	-2.83	123.31	127.28
27	A	802	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
27	X	602	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
38	Y	605	CHL	OMC-CMC-C2C	-2.83	120.20	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	L	308	BCR	C31-C1-C6	-2.83	105.80	110.24
27	8	601	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
36	8	620	XAT	C10-C11-C12	-2.83	115.00	123.20
35	Y	1621	LUT	C11-C10-C9	-2.83	123.31	127.28
27	A	816	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
27	A	836	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
36	5	621	XAT	C15-C14-C13	-2.82	123.32	127.28
37	U	1623	NEX	C24-C23-C22	-2.82	105.51	110.79
27	9	601	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
27	B	814	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
27	G	203	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
30	A	852	BCR	C10-C11-C12	-2.82	115.02	123.20
38	U	609	CHL	C4-C3-C5	2.82	120.12	115.23
27	W	610	CLA	C3B-C4B-NB	-2.82	108.01	110.53
27	1	611	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
27	9	603	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
37	W	1623	NEX	C24-C23-C22	-2.82	105.52	110.79
29	W	2630	LHG	O8-C23-C24	2.82	120.43	111.83
30	K	207	BCR	C32-C1-C6	-2.82	105.82	110.24
27	A	829	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
30	L	309	BCR	C7-C8-C9	-2.82	122.07	126.23
27	4	614	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
38	X	601	CHL	C4-C3-C5	2.82	120.12	115.23
29	U	2630	LHG	O8-C23-C24	2.82	120.42	111.83
27	Z	603	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
30	4	621	BCR	C15-C14-C13	-2.82	123.33	127.28
36	X	1622	XAT	C15-C14-C13	-2.82	123.33	127.28
27	B	815	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
27	8	609	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
27	V	611	CLA	O2D-CGD-CBD	2.81	116.15	111.23
27	2	611	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
27	X	614	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
27	A	836	CLA	C4-C3-C5	2.81	120.11	115.23
36	V	1622	XAT	C7-C8-C9	-2.81	121.17	125.53
27	3	603	CLA	CMB-C2B-C3B	2.81	133.16	126.55
27	F	304	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
30	A	850	BCR	C8-C7-C6	-2.81	119.49	127.00
38	Y	607	CHL	C1C-CHC-C4B	2.81	126.13	116.07
38	U	609	CHL	O2A-CGA-CBA	2.81	120.40	111.83
27	Y	614	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
27	1	614	CLA	O2D-CGD-O1D	-2.81	117.71	124.08
38	W	609	CHL	O2A-CGA-CBA	2.81	120.40	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	813	CLA	C1-C2-C3	-2.81	121.60	126.20
38	X	607	CHL	C1-C2-C3	-2.81	121.60	126.20
35	a	617	LUT	C28-C29-C30	-2.81	114.59	119.01
38	W	607	CHL	O2A-CGA-CBA	2.81	120.39	111.83
27	5	602	CLA	C3B-C4B-NB	-2.81	108.03	110.53
27	4	603	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
27	5	606	CLA	C3B-C4B-NB	-2.80	108.03	110.53
36	5	621	XAT	C20-C13-C12	2.80	122.37	118.09
27	B	826	CLA	C1-C2-C3	-2.80	121.60	126.20
27	3	608	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
38	X	609	CHL	O2A-CGA-CBA	2.80	120.38	111.83
30	L	308	BCR	C33-C5-C4	2.80	119.57	113.60
27	B	823	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
27	U	602	CLA	CHB-C4A-NA	2.80	128.44	124.40
27	A	832	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
38	W	607	CHL	CAC-C3C-C4C	2.80	129.77	124.73
27	B	810	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
27	1	613	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
27	A	838	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
27	1	610	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
27	2	607	CLA	C3B-C4B-NB	-2.80	108.03	110.53
27	Z	602	CLA	C3B-C4B-NB	-2.79	108.03	110.53
38	Z	607	CHL	CMB-C2B-C3B	2.79	130.26	124.68
27	5	608	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
38	Z	605	CHL	CMD-C2D-C3D	2.79	130.26	124.68
27	A	842	CLA	C1-C2-C3	-2.79	121.62	126.20
30	A	856	BCR	C33-C5-C4	2.79	119.54	113.60
27	6	610	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
30	L	301	BCR	C4-C5-C6	-2.79	118.94	122.70
27	1	616	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
27	U	603	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
30	3	620	BCR	C37-C22-C21	-2.79	118.30	122.82
27	1	601	CLA	O2D-CGD-O1D	-2.79	117.76	124.08
34	B	850	DGD	O1G-C1A-C2A	2.79	120.33	111.83
38	V	609	CHL	CMB-C2B-C3B	2.78	130.25	124.68
27	A	829	CLA	CMB-C2B-C1B	-2.78	121.18	125.42
36	3	619	XAT	C38-C25-C24	2.78	117.37	114.24
36	8	620	XAT	C35-C34-C33	-2.78	123.37	127.28
27	1	616	CLA	CMB-C2B-C3B	2.78	130.93	123.53
27	8	603	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
27	A	820	CLA	CHB-C4A-NA	2.78	128.42	124.40
30	5	622	BCR	C36-C18-C17	-2.78	118.31	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	8	608	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
27	Z	610	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
33	L	2631	LMG	O8-C28-C29	2.78	120.32	111.83
27	a	613	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
38	V	608	CHL	CMB-C2B-C3B	2.78	130.24	124.68
30	A	851	BCR	C15-C14-C13	-2.78	123.38	127.28
33	5	627	LMG	O8-C28-C29	2.78	120.31	111.83
30	7	623	BCR	C8-C9-C10	-2.78	114.64	119.01
27	X	604	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
35	V	1621	LUT	C3-C4-C5	-2.78	105.27	112.18
27	Z	614	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
27	a	616	CLA	O2D-CGD-O1D	-2.78	118.45	123.85
30	L	309	BCR	C36-C18-C19	2.77	122.33	118.09
30	B	847	BCR	C15-C14-C13	-2.77	123.39	127.28
27	A	814	CLA	C1-C2-C3	-2.77	121.65	126.20
27	H	203	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
29	B	851	LHG	O8-C23-C24	2.77	120.29	111.83
36	6	621	XAT	C26-C27-C28	-2.77	120.13	125.99
27	V	612	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
35	1	617	LUT	C28-C29-C30	-2.77	114.65	119.01
38	V	609	CHL	O1D-CGD-CBD	-2.77	120.52	124.72
36	U	1622	XAT	O24-C25-C38	2.77	118.14	115.05
30	B	846	BCR	C30-C25-C24	2.77	123.16	115.65
27	a	601	CLA	O2D-CGD-O1D	-2.77	117.80	124.08
30	L	301	BCR	C31-C1-C6	2.77	114.58	110.24
30	B	849	BCR	C15-C16-C17	-2.77	117.86	123.52
27	6	607	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
28	B	842	PQN	C14-C13-C12	-2.77	116.52	123.63
30	9	621	BCR	C36-C18-C17	-2.77	118.34	122.82
27	B	813	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
30	B	849	BCR	C15-C14-C13	-2.76	123.40	127.28
30	A	852	BCR	C8-C9-C10	2.76	123.36	119.01
38	V	609	CHL	O2A-CGA-CBA	2.76	120.26	111.83
27	3	617	CLA	CHB-C4A-NA	2.76	128.39	124.40
30	O	2004	BCR	C8-C9-C10	2.76	123.35	119.01
30	3	621	BCR	C16-C17-C18	-2.76	123.41	127.28
27	3	610	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
30	A	852	BCR	C16-C15-C14	-2.76	117.87	123.52
27	4	613	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
30	L	305	BCR	C38-C26-C25	-2.76	121.47	124.48
27	L	304	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
27	Y	604	CLA	O2D-CGD-O1D	-2.76	118.48	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	V	613	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
38	Z	607	CHL	CMA-C3A-C4A	-2.76	108.67	114.61
27	V	604	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
27	W	612	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
30	B	853	BCR	C15-C16-C17	-2.75	117.88	123.52
36	7	620	XAT	C10-C11-C12	-2.75	115.22	123.20
38	W	607	CHL	C3D-C4D-ND	2.75	117.36	112.94
37	Z	1623	NEX	C8-C7-C6	-2.75	174.41	177.66
27	2	604	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
27	B	803	CLA	CHB-C4A-NA	2.75	128.37	124.40
30	O	2005	BCR	C11-C10-C9	-2.75	123.42	127.28
36	V	1622	XAT	C38-C25-C24	2.75	117.33	114.24
27	6	602	CLA	C3B-C4B-NB	-2.75	108.07	110.53
36	V	1622	XAT	C26-C27-C28	-2.75	120.18	125.99
30	B	843	BCR	C24-C23-C22	-2.75	122.17	126.23
27	B	809	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
27	3	615	CLA	CMB-C2B-C3B	2.75	133.02	126.55
27	2	606	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
27	B	813	CLA	C3B-C4B-NB	-2.75	108.08	110.53
30	K	207	BCR	C28-C27-C26	-2.75	109.16	114.06
27	8	604	CLA	C1-C2-C3	-2.75	122.32	126.76
30	F	305	BCR	C39-C30-C25	-2.75	105.93	110.24
27	W	604	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
37	V	1623	NEX	C24-C23-C22	-2.75	105.65	110.79
36	Z	1622	XAT	C24-C23-C22	-2.75	105.65	110.79
27	U	604	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
27	U	610	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
27	B	806	CLA	O2D-CGD-O1D	-2.74	118.50	123.85
27	U	612	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
29	9	624	LHG	O8-C23-C24	2.74	120.20	111.83
27	3	602	CLA	C3B-C4B-NB	-2.74	108.08	110.53
27	3	609	CLA	CHB-C4A-NA	2.74	128.36	124.40
27	K	204	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
30	L	301	BCR	C27-C26-C25	-2.74	119.00	122.70
27	2	601	CLA	C1-C2-C3	-2.74	121.70	126.20
27	7	611	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
30	A	850	BCR	C36-C18-C17	-2.74	118.38	122.82
27	7	602	CLA	C3B-C4B-NB	-2.74	108.08	110.53
30	A	856	BCR	C11-C10-C9	-2.74	123.44	127.28
27	a	607	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
27	8	607	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
27	9	602	CLA	C3B-C4B-NB	-2.73	108.09	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	W	603	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
27	A	807	CLA	C1-C2-C3	-2.73	121.72	126.20
30	K	207	BCR	C24-C23-C22	-2.73	122.19	126.23
38	W	607	CHL	C1C-CHC-C4B	2.73	125.85	116.07
35	4	619	LUT	C7-C8-C9	-2.73	122.19	126.23
35	8	619	LUT	C35-C15-C14	-2.73	117.93	123.52
30	K	207	BCR	C38-C26-C27	2.73	119.42	113.60
27	3	615	CLA	O2D-CGD-O1D	-2.73	117.89	124.08
30	B	846	BCR	C11-C10-C9	-2.73	123.45	127.28
30	L	301	BCR	C3-C4-C5	-2.73	109.19	114.06
27	X	602	CLA	C3B-C4B-NB	-2.73	108.10	110.53
36	2	620	XAT	C27-C28-C29	-2.73	121.30	125.53
38	Y	607	CHL	O2A-CGA-CBA	2.73	120.15	111.83
38	Y	607	CHL	C1B-CHB-C4A	2.73	123.08	121.32
38	Y	608	CHL	O2A-CGA-CBA	2.72	120.14	111.83
38	Y	606	CHL	CMB-C2B-C3B	2.72	130.13	124.68
30	A	851	BCR	C33-C5-C6	-2.72	121.51	124.48
27	Z	613	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
27	6	620	CLA	C3B-C4B-NB	-2.72	108.10	110.53
38	V	606	CHL	CMB-C2B-C3B	2.72	130.12	124.68
27	A	810	CLA	C3B-C4B-NB	-2.72	108.10	110.53
36	X	1622	XAT	C32-C33-C34	-2.72	114.74	119.01
38	Y	607	CHL	C3D-C4D-ND	2.72	117.30	112.94
35	4	619	LUT	C8-C7-C6	-2.72	119.74	127.00
27	Y	612	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
30	K	207	BCR	C36-C18-C17	-2.72	118.42	122.82
27	5	619	CLA	C2A-C1A-CHA	2.72	128.58	123.87
30	A	856	BCR	C1-C6-C5	-2.71	118.93	122.64
38	W	601	CHL	C4-C3-C5	2.71	119.94	115.23
33	4	623	LMG	O8-C28-C29	2.71	120.10	111.83
27	X	612	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
27	U	611	CLA	CHB-C4A-NA	2.71	128.31	124.40
36	8	620	XAT	C28-C29-C30	-2.71	114.75	119.01
27	4	610	CLA	C1-C2-C3	-2.71	121.76	126.20
27	3	602	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
38	W	605	CHL	C1A-CHA-CBD	2.70	139.29	132.36
36	Y	1622	XAT	C32-C33-C34	-2.70	114.76	119.01
29	3	623	LHG	O8-C23-C24	2.70	120.08	111.83
27	6	607	CLA	CHB-C4A-NA	2.70	128.30	124.40
27	2	612	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
37	6	624	NEX	C17-C1-C6	-2.70	108.05	110.47
30	B	844	BCR	C24-C23-C22	-2.70	122.24	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	847	LHG	O8-C23-C24	2.70	120.07	111.83
27	B	819	CLA	C1-C2-C3	-2.70	121.77	126.20
27	a	603	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
36	Z	1622	XAT	C11-C10-C9	-2.70	123.49	127.28
38	X	609	CHL	CMA-C3A-C4A	-2.70	108.80	114.61
35	7	619	LUT	C7-C8-C9	-2.70	122.24	126.23
27	A	822	CLA	CMB-C2B-C3B	2.70	132.89	126.55
27	H	203	CLA	CHB-C4A-NA	2.70	128.29	124.40
30	9	621	BCR	C37-C22-C23	2.70	122.21	118.09
36	6	621	XAT	C15-C14-C13	-2.69	123.50	127.28
27	A	804	CLA	O2D-CGD-CBD	2.69	115.94	111.23
27	2	604	CLA	C3B-C4B-NB	-2.69	108.12	110.53
35	Z	1621	LUT	C3-C4-C5	-2.69	105.47	112.18
35	8	619	LUT	C3-C4-C5	-2.69	105.47	112.18
27	B	820	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
27	3	614	CLA	O2D-CGD-O1D	-2.69	117.97	124.08
37	Y	1623	NEX	C11-C12-C13	-2.69	118.98	126.36
27	W	610	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
36	W	1622	XAT	O24-C25-C38	2.69	118.06	115.05
27	B	820	CLA	CHB-C4A-NA	2.69	128.28	124.40
30	L	301	BCR	C23-C24-C25	-2.69	119.81	127.00
27	8	608	CLA	CHB-C4A-NA	2.69	128.28	124.40
30	7	621	BCR	C24-C25-C26	-2.69	115.36	121.56
27	A	828	CLA	C3B-C4B-NB	-2.69	108.13	110.53
35	Z	1620	LUT	C17-C1-C6	-2.69	106.03	110.24
37	X	1623	NEX	C11-C12-C13	-2.69	119.00	126.36
30	L	305	BCR	C33-C5-C6	-2.69	121.55	124.48
30	B	846	BCR	C15-C16-C17	-2.69	118.02	123.52
35	6	619	LUT	C35-C34-C33	-2.69	123.51	127.28
30	A	850	BCR	C24-C23-C22	-2.69	122.26	126.23
38	W	601	CHL	O2A-CGA-CBA	2.69	120.02	111.83
33	J	103	LMG	O8-C28-C29	2.69	120.02	111.83
38	X	606	CHL	CMB-C2B-C3B	2.68	130.05	124.68
30	4	621	BCR	C15-C16-C17	-2.68	118.03	123.52
30	2	623	BCR	C38-C26-C27	2.68	119.32	113.60
27	1	608	CLA	O2D-CGD-O1D	-2.68	117.99	124.08
38	U	605	CHL	C1A-CHA-CBD	2.68	139.23	132.36
38	U	609	CHL	CMB-C2B-C3B	2.68	130.04	124.68
27	a	608	CLA	O2D-CGD-O1D	-2.68	118.00	124.08
30	O	2004	BCR	C40-C30-C25	-2.68	106.04	110.24
36	2	620	XAT	C30-C31-C32	-2.68	115.44	123.20
38	Y	605	CHL	C1A-CHA-CBD	2.68	139.22	132.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	Z	604	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
27	6	613	CLA	O2D-CGD-O1D	-2.68	118.00	124.08
27	5	610	CLA	CMB-C2B-C3B	2.68	132.84	126.55
38	X	605	CHL	C1A-CHA-CBD	2.68	139.21	132.36
27	Z	610	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
36	U	1622	XAT	C32-C33-C34	-2.67	114.80	119.01
27	W	611	CLA	CHB-C4A-NA	2.67	128.26	124.40
27	7	602	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
27	A	841	CLA	C3B-C4B-NB	-2.67	108.14	110.53
36	Z	1622	XAT	C38-C25-C24	2.67	117.24	114.24
37	V	1623	NEX	C11-C10-C9	-2.67	123.53	127.28
38	X	605	CHL	O2D-CGD-O1D	-2.67	118.65	123.85
37	U	1623	NEX	C39-C29-C30	-2.67	118.49	122.82
27	8	612	CLA	CHB-C4A-NA	2.67	128.25	124.40
30	A	856	BCR	C15-C16-C17	-2.67	118.06	123.52
36	a	618	XAT	C8-C9-C10	-2.67	114.81	119.01
37	W	1623	NEX	C39-C29-C30	-2.67	118.49	122.82
27	4	602	CLA	CMB-C2B-C3B	2.67	132.83	126.55
27	Y	610	CLA	C3B-C4B-NB	-2.67	108.15	110.53
27	5	610	CLA	CHB-C4A-NA	2.67	128.25	124.40
27	U	612	CLA	CHB-C4A-NA	2.67	128.25	124.40
27	3	609	CLA	CBA-CAA-C2A	2.67	121.73	113.79
27	3	617	CLA	O2D-CGD-O1D	-2.67	118.03	124.08
27	B	812	CLA	C3B-C4B-NB	-2.67	108.15	110.53
27	5	618	CLA	CMB-C2B-C3B	2.67	130.62	123.53
35	1	617	LUT	C17-C1-C6	-2.67	106.06	110.24
35	V	1620	LUT	C11-C10-C9	-2.67	123.54	127.28
30	2	623	BCR	C16-C15-C14	-2.67	118.07	123.52
27	5	607	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
30	A	856	BCR	C15-C14-C13	-2.66	123.54	127.28
27	8	613	CLA	C3B-C4B-NB	-2.66	108.15	110.53
30	O	2005	BCR	C2-C1-C6	2.66	114.31	110.44
27	W	614	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
36	2	620	XAT	C32-C33-C34	-2.66	114.82	119.01
38	V	606	CHL	C3D-CAD-CBD	2.66	111.11	107.61
30	B	844	BCR	C37-C22-C21	-2.66	118.50	122.82
27	F	301	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
27	1	609	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
36	5	621	XAT	C15-C35-C34	-2.66	118.08	123.52
35	8	619	LUT	C21-C26-C27	-2.66	109.77	112.83
30	L	309	BCR	C8-C9-C10	-2.66	114.83	119.01
27	B	819	CLA	C3B-C4B-NB	-2.66	108.16	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	O	2005	BCR	C28-C29-C30	-2.66	105.02	114.43
30	L	308	BCR	C15-C14-C13	-2.66	123.55	127.28
36	1	618	XAT	C8-C9-C10	-2.66	114.83	119.01
30	A	852	BCR	C2-C1-C6	2.66	114.30	110.44
35	3	618	LUT	C11-C10-C9	-2.66	123.55	127.28
35	5	620	LUT	C30-C31-C32	-2.66	115.50	123.20
30	A	852	BCR	C37-C22-C21	-2.66	118.51	122.82
27	A	845	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
30	L	308	BCR	C1-C6-C5	-2.66	119.01	122.64
27	2	609	CLA	C3B-C4B-NB	-2.66	108.16	110.53
27	V	602	CLA	C3B-C4B-NB	-2.66	108.16	110.53
27	A	806	CLA	CAA-C2A-C3A	-2.66	105.82	113.00
27	8	612	CLA	O2D-CGD-O1D	-2.66	118.06	124.08
27	1	612	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
27	W	603	CLA	CHB-C4A-NA	2.65	128.23	124.40
27	a	612	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
27	A	838	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
38	Y	605	CHL	O2D-CGD-O1D	-2.65	118.69	123.85
38	W	607	CHL	OMC-CMC-C2C	-2.65	120.52	125.12
33	A	860	LMG	O8-C28-C29	2.65	119.92	111.83
36	3	619	XAT	C19-C9-C8	2.65	122.14	118.09
29	B	851	LHG	C5-O7-C7	-2.65	111.45	117.80
27	Z	602	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
27	2	603	CLA	O2D-CGD-O1D	-2.65	118.07	124.08
27	B	811	CLA	O2D-CGD-O1D	-2.65	118.07	124.08
30	A	856	BCR	C30-C25-C26	-2.65	119.02	122.64
27	L	303	CLA	O2D-CGD-CBD	2.65	115.86	111.23
27	1	602	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
30	2	623	BCR	C27-C26-C25	-2.65	119.13	122.70
27	4	609	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
38	X	609	CHL	CMB-C2B-C3B	2.65	129.97	124.68
27	J	101	CLA	C3B-C4B-NB	-2.64	108.17	110.53
27	6	611	CLA	C3B-C4B-NB	-2.64	108.17	110.53
27	Y	602	CLA	C3B-C4B-NB	-2.64	108.17	110.53
27	A	811	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
30	6	622	BCR	C8-C7-C6	-2.64	119.93	127.00
27	O	2001	CLA	O2D-CGD-O1D	-2.64	118.08	124.08
27	A	819	CLA	CHB-C4A-NA	2.64	128.22	124.40
27	8	611	CLA	C3B-C4B-NB	-2.64	108.17	110.53
30	A	852	BCR	C12-C13-C14	-2.64	114.85	119.01
37	X	1623	NEX	C26-C27-C28	-2.64	120.41	125.99
30	O	2004	BCR	C11-C10-C9	-2.64	123.57	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	2	602	CLA	C3B-C4B-NB	-2.64	108.17	110.53
27	5	606	CLA	O2D-CGD-O1D	-2.64	118.09	124.08
30	B	849	BCR	C30-C25-C24	2.64	122.81	115.65
27	K	203	CLA	C1-C2-C3	-2.64	121.87	126.20
38	X	606	CHL	C1B-CHB-C4A	-2.64	119.63	121.32
36	8	620	XAT	C7-C8-C9	-2.64	121.44	125.53
30	L	308	BCR	C37-C22-C23	2.64	122.11	118.09
27	A	806	CLA	CHB-C4A-NA	2.63	128.20	124.40
27	8	610	CLA	CHB-C4A-NA	2.63	128.20	124.40
38	X	608	CHL	O2A-CGA-CBA	2.63	119.86	111.83
36	W	1622	XAT	C32-C33-C34	-2.63	114.87	119.01
35	a	617	LUT	C17-C1-C6	-2.63	106.11	110.24
27	2	602	CLA	O2D-CGD-O1D	-2.63	118.11	124.08
27	A	807	CLA	CHB-C4A-NA	2.63	128.20	124.40
33	9	625	LMG	O8-C28-C29	2.63	119.86	111.83
27	U	614	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
27	V	602	CLA	CHB-C4A-NA	2.63	128.20	124.40
27	6	614	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
38	Z	609	CHL	O1D-CGD-CBD	-2.63	120.74	124.72
30	1	619	BCR	C11-C12-C13	-2.63	119.16	126.36
27	U	613	CLA	CHB-C4A-NA	2.63	128.19	124.40
38	W	609	CHL	CMA-C3A-C4A	-2.63	108.95	114.61
27	B	821	CLA	CHC-C1C-C2C	-2.63	124.19	129.94
27	B	827	CLA	CHB-C4A-NA	2.63	128.19	124.40
27	4	612	CLA	CHB-C4A-NA	2.63	128.19	124.40
27	5	601	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
27	W	612	CLA	CHB-C4A-NA	2.62	128.19	124.40
27	6	608	CLA	C3B-C4B-NB	-2.62	108.19	110.53
27	V	610	CLA	CHB-C4A-NA	2.62	128.19	124.40
27	Z	611	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
27	3	613	CLA	O2D-CGD-O1D	-2.62	118.13	124.08
38	Y	608	CHL	CMB-C2B-C3B	2.62	129.92	124.68
30	a	619	BCR	C11-C12-C13	-2.62	119.18	126.36
27	A	802	CLA	CHB-C4A-NA	2.62	128.18	124.40
27	L	306	CLA	O2D-CGD-O1D	-2.62	118.14	124.08
27	2	601	CLA	CMB-C2B-C3B	2.62	132.71	126.55
38	Y	601	CHL	CMB-C2B-C3B	2.62	129.91	124.68
38	Y	606	CHL	C1C-C2C-CMC	2.62	131.52	126.80
27	B	831	CLA	CMB-C2B-C3B	2.62	132.70	126.55
27	O	2003	CLA	O2D-CGD-O1D	-2.62	118.15	124.08
27	9	609	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
35	W	1621	LUT	C11-C10-C9	-2.61	123.61	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	W	609	CHL	CMB-C2B-C3B	2.61	129.91	124.68
38	U	607	CHL	C1A-CHA-CBD	2.61	139.05	132.36
30	A	852	BCR	C36-C18-C17	-2.61	118.58	122.82
35	4	619	LUT	C39-C29-C28	2.61	122.08	118.09
27	B	803	CLA	C3B-C4B-NB	-2.61	108.20	110.53
27	7	606	CLA	C3B-C4B-NB	-2.61	108.20	110.53
38	Z	606	CHL	O1D-CGD-CBD	-2.61	120.76	124.72
27	U	613	CLA	C1-C2-C3	-2.61	121.92	126.20
30	L	305	BCR	C30-C25-C24	2.61	122.73	115.65
27	A	802	CLA	C3B-C4B-NB	-2.61	108.20	110.53
38	X	607	CHL	O1D-CGD-CBD	-2.61	120.77	124.72
27	W	613	CLA	C1-C2-C3	-2.61	121.92	126.20
27	A	817	CLA	O2D-CGD-CBD	2.61	115.79	111.23
27	X	610	CLA	C3B-C4B-NB	-2.61	108.20	110.53
27	B	817	CLA	C4-C3-C5	2.61	119.75	115.23
30	J	102	BCR	C10-C11-C12	-2.61	115.65	123.20
30	A	851	BCR	C19-C18-C17	-2.61	114.91	119.01
27	A	814	CLA	CHB-C4A-NA	2.61	128.16	124.40
27	9	606	CLA	O2D-CGD-O1D	-2.60	118.17	124.08
38	X	606	CHL	C1C-C2C-CMC	2.60	131.50	126.80
27	a	602	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
30	O	2005	BCR	C31-C1-C6	-2.60	106.16	110.24
30	4	621	BCR	C36-C18-C17	-2.60	118.60	122.82
30	A	851	BCR	C20-C21-C22	-2.60	123.63	127.28
30	B	853	BCR	C15-C14-C13	-2.60	123.63	127.28
29	8	623	LHG	O8-C23-C24	2.60	119.77	111.83
27	5	618	CLA	CAB-C3B-C2B	2.60	130.45	123.53
38	Y	601	CHL	CBC-CAC-C3C	-2.60	109.15	112.87
27	5	619	CLA	CHB-C4A-NA	2.60	128.16	124.40
38	Z	601	CHL	O2A-CGA-CBA	2.60	119.77	111.83
35	Z	1620	LUT	C35-C34-C33	-2.60	123.63	127.28
27	1	609	CLA	CAB-C3B-C2B	2.60	130.44	123.53
27	U	603	CLA	CHB-C4A-NA	2.60	128.15	124.40
38	V	601	CHL	O2A-CGA-CBA	2.60	119.76	111.83
27	B	830	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
29	O	2631	LHG	C5-O7-C7	-2.60	111.58	117.80
27	6	606	CLA	O2D-CGD-O1D	-2.60	118.19	124.08
35	2	619	LUT	C35-C34-C33	-2.60	123.64	127.28
27	7	613	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
38	V	605	CHL	CMB-C2B-C3B	2.60	129.87	124.68
35	2	619	LUT	C7-C8-C9	-2.60	122.40	126.23
27	Y	610	CLA	C1-C2-C3	-2.59	121.95	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	V	605	CHL	C1A-CHA-CBD	2.59	139.00	132.36
36	5	621	XAT	C26-C27-C28	-2.59	120.51	125.99
27	X	610	CLA	C1-C2-C3	-2.59	121.95	126.20
27	A	815	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
27	4	612	CLA	O2D-CGD-O1D	-2.59	118.21	124.08
35	U	1621	LUT	C11-C10-C9	-2.59	123.65	127.28
38	X	606	CHL	O1D-CGD-CBD	-2.59	120.80	124.72
38	Z	608	CHL	CBC-CAC-C3C	-2.59	109.17	112.87
37	Y	1623	NEX	C26-C27-C28	-2.59	120.53	125.99
35	a	617	LUT	C3-C4-C5	-2.59	105.74	112.18
38	Y	609	CHL	O1D-CGD-CBD	-2.59	120.80	124.72
27	5	608	CLA	C3B-C4B-NB	-2.59	108.22	110.53
38	V	608	CHL	O2A-CGA-CBA	2.59	119.72	111.83
33	L	2631	LMG	C8-O7-C10	-2.59	111.61	117.80
36	3	619	XAT	C4-C3-C2	-2.58	105.96	110.79
30	O	2004	BCR	C15-C14-C13	-2.58	123.65	127.28
32	5	628	LMU	C2'-C3'-C4'	2.58	115.54	109.68
27	4	606	CLA	C3B-C4B-NB	-2.58	108.22	110.53
27	W	613	CLA	CHB-C4A-NA	2.58	128.13	124.40
38	Z	609	CHL	C4-C3-C5	2.58	119.71	115.23
27	L	307	CLA	O2D-CGD-O1D	-2.58	118.22	124.08
27	3	614	CLA	C3B-C4B-NB	-2.58	108.23	110.53
27	U	610	CLA	CHB-C4A-NA	2.58	128.12	124.40
30	A	848	BCR	C32-C1-C6	-2.58	106.20	110.24
27	K	203	CLA	C3B-C4B-NB	-2.58	108.23	110.53
27	B	824	CLA	CHB-C4A-NA	2.58	128.12	124.40
30	5	622	BCR	C24-C25-C26	-2.58	115.62	121.56
30	L	305	BCR	C37-C22-C21	-2.58	118.64	122.82
30	B	849	BCR	C2-C1-C6	2.58	114.18	110.44
27	5	601	CLA	CHB-C4A-NA	2.58	128.12	124.40
30	L	305	BCR	C11-C12-C13	-2.58	119.30	126.36
38	U	607	CHL	OMC-CMC-C2C	-2.58	120.65	125.12
27	6	616	CLA	C3B-C4B-NB	-2.58	108.23	110.53
35	3	618	LUT	C28-C29-C30	-2.57	114.96	119.01
36	a	618	XAT	C27-C28-C29	-2.57	121.53	125.53
27	5	612	CLA	O2D-CGD-O1D	-2.57	118.24	124.08
35	U	1621	LUT	C18-C5-C6	-2.57	121.68	124.48
36	V	1622	XAT	C15-C14-C13	-2.57	123.67	127.28
27	7	610	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
35	4	619	LUT	C18-C5-C6	-2.57	121.68	124.48
27	a	601	CLA	C3B-C4B-NB	-2.57	108.23	110.53
30	B	843	BCR	C11-C10-C9	-2.57	123.67	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	611	CLA	CHB-C4A-NA	2.57	128.11	124.40
30	A	849	BCR	C30-C25-C26	-2.57	119.12	122.64
38	Y	606	CHL	O1D-CGD-CBD	-2.57	120.83	124.72
27	5	616	CLA	CAB-C3B-C2B	2.57	130.36	123.53
27	A	810	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
35	V	1621	LUT	C11-C10-C9	-2.57	123.67	127.28
27	A	812	CLA	CHB-C4A-NA	2.57	128.11	124.40
27	4	606	CLA	O2D-CGD-O1D	-2.57	118.25	124.08
29	A	846	LHG	O8-C23-C24	2.57	119.66	111.83
30	L	301	BCR	C7-C8-C9	-2.57	122.44	126.23
27	4	603	CLA	CAB-C3B-C2B	2.57	130.35	123.53
35	W	1621	LUT	C18-C5-C6	-2.57	121.69	124.48
38	Z	609	CHL	O2A-CGA-CBA	2.57	119.66	111.83
35	9	619	LUT	C15-C14-C13	-2.56	123.68	127.28
30	B	853	BCR	C11-C10-C9	-2.56	123.68	127.28
38	U	605	CHL	O2D-CGD-O1D	-2.56	118.86	123.85
35	2	619	LUT	C30-C31-C32	-2.56	115.77	123.20
27	4	613	CLA	C3B-C4B-NB	-2.56	108.24	110.53
27	A	804	CLA	CHB-C4A-NA	2.56	128.10	124.40
27	V	612	CLA	CHB-C4A-NA	2.56	128.10	124.40
30	B	844	BCR	C28-C27-C26	-2.56	109.49	114.06
27	B	826	CLA	C3B-C4B-NB	-2.56	108.24	110.53
27	9	610	CLA	C1-C2-C3	-2.56	122.00	126.20
36	4	620	XAT	C38-C25-C24	2.56	117.12	114.24
36	3	619	XAT	C12-C13-C14	-2.56	114.98	119.01
35	1	617	LUT	C3-C4-C5	-2.56	105.81	112.18
27	B	808	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
27	3	606	CLA	O2D-CGD-O1D	-2.56	118.28	124.08
38	U	609	CHL	O1D-CGD-CBD	-2.56	120.84	124.72
36	1	618	XAT	C27-C28-C29	-2.56	121.56	125.53
27	A	809	CLA	CHB-C4A-NA	2.56	128.09	124.40
36	4	620	XAT	C20-C13-C12	2.56	121.99	118.09
36	X	1622	XAT	C38-C25-C24	2.56	117.11	114.24
27	Y	611	CLA	CHB-C4A-NA	2.56	128.09	124.40
27	3	607	CLA	CMB-C2B-C3B	2.56	130.32	123.53
38	Y	606	CHL	C1B-CHB-C4A	-2.56	119.68	121.32
36	2	620	XAT	C8-C9-C10	-2.56	114.99	119.01
27	B	806	CLA	CHB-C4A-NA	2.55	128.09	124.40
27	L	303	CLA	C3B-C4B-NB	-2.55	108.25	110.53
27	U	610	CLA	C1-C2-C3	-2.55	122.01	126.20
34	B	850	DGD	O6D-C5D-C6D	2.55	111.76	106.69
27	6	618	CLA	CAB-C3B-C2B	2.55	130.31	123.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	Y	1620	LUT	C38-C25-C24	-2.55	117.32	123.36
27	A	838	CLA	CHB-C4A-NA	2.55	128.08	124.40
27	5	603	CLA	CAB-C3B-C2B	2.55	130.31	123.53
30	7	623	BCR	C33-C5-C6	-2.55	121.70	124.48
27	6	607	CLA	CMB-C2B-C3B	2.55	130.31	123.53
35	4	619	LUT	C15-C14-C13	-2.55	123.70	127.28
30	7	623	BCR	C15-C16-C17	-2.55	118.30	123.52
38	U	606	CHL	C1A-CHA-CBD	2.55	138.89	132.36
27	W	610	CLA	C1-C2-C3	-2.55	122.02	126.20
38	X	608	CHL	CMB-C2B-C3B	2.55	129.77	124.68
30	A	848	BCR	C16-C15-C14	-2.55	118.31	123.52
27	7	616	CLA	O2D-CGD-CBD	2.54	115.68	111.23
27	6	603	CLA	CAB-C3B-C2B	2.54	130.29	123.53
27	6	617	CLA	CHB-C4A-NA	2.54	128.07	124.40
27	1	614	CLA	CMB-C2B-C3B	2.54	130.29	123.53
38	V	609	CHL	O2D-CGD-O1D	-2.54	118.90	123.85
35	7	619	LUT	C17-C1-C6	-2.54	106.25	110.24
27	A	815	CLA	CHB-C4A-NA	2.54	128.07	124.40
35	7	619	LUT	C1-C6-C5	-2.54	119.16	122.64
30	K	207	BCR	C15-C14-C13	-2.54	123.71	127.28
27	6	601	CLA	CHB-C4A-NA	2.54	128.07	124.40
30	A	848	BCR	C36-C18-C19	2.54	121.97	118.09
35	9	619	LUT	C20-C13-C12	2.54	121.97	118.09
38	V	607	CHL	OMC-CMC-C2C	-2.54	120.71	125.12
30	F	305	BCR	C29-C30-C25	2.54	114.13	110.44
30	B	849	BCR	C1-C6-C5	-2.54	119.17	122.64
30	B	848	BCR	C32-C1-C6	-2.54	106.26	110.24
27	A	801	CLA	C1-C2-C3	-2.54	122.04	126.20
27	3	607	CLA	CHB-C4A-NA	2.54	128.06	124.40
27	5	617	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
38	Z	607	CHL	O2A-CGA-CBA	2.54	119.57	111.83
38	X	609	CHL	O1D-CGD-CBD	-2.54	120.88	124.72
27	9	610	CLA	C3B-C4B-NB	-2.54	108.27	110.53
30	G	205	BCR	C33-C5-C6	-2.54	121.72	124.48
30	6	622	BCR	C11-C10-C9	-2.54	123.72	127.28
29	4	622	LHG	O8-C23-C24	2.54	119.57	111.83
35	V	1620	LUT	C28-C29-C30	-2.54	115.02	119.01
36	Y	1622	XAT	C24-C23-C22	-2.53	106.05	110.79
29	5	625	LHG	C5-O7-C7	-2.53	111.73	117.80
27	7	603	CLA	O2D-CGD-O1D	-2.53	118.33	124.08
27	8	606	CLA	C3B-C4B-NB	-2.53	108.27	110.53
38	W	605	CHL	O2D-CGD-O1D	-2.53	118.92	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	2	610	CLA	CHB-C4A-NA	2.53	128.05	124.40
30	J	102	BCR	C34-C9-C8	2.53	121.95	118.09
27	8	609	CLA	CHB-C4A-NA	2.53	128.05	124.40
27	W	610	CLA	CHB-C4A-NA	2.53	128.05	124.40
38	W	606	CHL	C1A-CHA-CBD	2.53	138.84	132.36
38	W	605	CHL	CMB-C2B-C3B	2.53	129.74	124.68
38	X	601	CHL	O2A-CGA-CBA	2.53	119.55	111.83
30	O	2004	BCR	C37-C22-C23	2.53	121.95	118.09
27	3	603	CLA	CHB-C4A-NA	2.53	128.05	124.40
35	3	618	LUT	C35-C15-C14	-2.53	118.35	123.52
27	4	616	CLA	CAB-C3B-C2B	2.53	130.25	123.53
38	U	601	CHL	O2A-CGA-CBA	2.53	119.54	111.83
30	L	309	BCR	C1-C6-C5	-2.53	119.18	122.64
36	X	1622	XAT	C24-C23-C22	-2.53	106.06	110.79
30	A	849	BCR	C11-C12-C13	-2.53	119.44	126.36
36	8	620	XAT	C27-C28-C29	-2.53	121.61	125.53
36	Y	1622	XAT	C38-C25-C24	2.53	117.08	114.24
38	V	608	CHL	C1A-CHA-CBD	2.53	138.83	132.36
27	G	203	CLA	C3B-C4B-NB	-2.52	108.28	110.53
36	6	621	XAT	C31-C30-C29	-2.52	123.74	127.28
38	U	607	CHL	O2A-CGA-CBA	2.52	121.97	114.00
30	B	844	BCR	C1-C6-C7	2.52	122.50	115.65
27	3	611	CLA	CAB-C3B-C2B	2.52	130.24	123.53
27	6	614	CLA	C3B-C4B-NB	-2.52	108.28	110.53
27	2	602	CLA	CHB-C4A-NA	2.52	128.04	124.40
27	4	610	CLA	CHB-C4A-NA	2.52	128.04	124.40
38	Z	607	CHL	O1D-CGD-CBD	-2.52	120.90	124.72
27	8	607	CLA	CAB-C3B-C2B	2.52	130.23	123.53
29	Z	2630	LHG	O8-C23-C24	2.52	119.52	111.83
27	B	821	CLA	O2D-CGD-O1D	-2.52	118.36	124.08
27	a	606	CLA	C3B-C4B-NB	-2.52	108.28	110.53
38	V	605	CHL	CMD-C2D-C3D	2.52	129.72	124.68
27	A	810	CLA	CHB-C4A-NA	2.52	128.03	124.40
30	A	851	BCR	C21-C20-C19	-2.52	115.90	123.20
36	W	1622	XAT	C11-C10-C9	-2.52	123.75	127.28
27	9	607	CLA	CHB-C4A-NA	2.52	128.03	124.40
27	5	618	CLA	O2D-CGD-O1D	-2.52	118.37	124.08
27	3	611	CLA	O2D-CGD-O1D	-2.52	118.37	124.08
35	X	1620	LUT	C38-C25-C24	-2.52	117.41	123.36
27	1	601	CLA	C3B-C4B-NB	-2.51	108.28	110.53
27	7	615	CLA	CBD-CHA-C1A	2.51	132.24	127.58
38	U	605	CHL	CMB-C2B-C3B	2.51	129.71	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	4	618	CLA	CAB-C3B-C2B	2.51	130.21	123.53
30	B	845	BCR	C20-C21-C22	-2.51	123.75	127.28
27	B	809	CLA	C3B-C4B-NB	-2.51	108.29	110.53
27	1	602	CLA	C3B-C4B-NB	-2.51	108.29	110.53
27	3	610	CLA	C3B-C4B-NB	-2.51	108.29	110.53
29	8	622	LHG	O8-C23-C24	2.51	119.50	111.83
30	F	305	BCR	C16-C17-C18	-2.51	123.75	127.28
27	3	607	CLA	CAB-C3B-C2B	2.51	130.21	123.53
30	L	305	BCR	C39-C30-C25	2.51	114.18	110.24
27	B	807	CLA	C1-C2-C3	-2.51	122.09	126.20
30	B	848	BCR	C30-C25-C26	-2.51	119.21	122.64
38	Y	605	CHL	CMB-C2B-C3B	2.51	129.70	124.68
30	K	207	BCR	C37-C22-C23	2.51	121.92	118.09
30	B	844	BCR	C30-C25-C26	-2.51	119.21	122.64
33	H	205	LMG	O6-C5-C4	2.51	114.22	109.70
27	1	606	CLA	C3B-C4B-NB	-2.51	108.29	110.53
38	V	609	CHL	C1B-CHB-C4A	2.51	122.94	121.32
38	U	608	CHL	C1A-CHA-CBD	2.51	138.78	132.36
30	3	620	BCR	C38-C26-C27	2.50	118.94	113.60
38	Z	608	CHL	C1B-CHB-C4A	-2.50	119.71	121.32
35	Y	1620	LUT	C28-C29-C30	-2.50	115.07	119.01
27	A	834	CLA	C3B-C4B-NB	-2.50	108.30	110.53
27	2	616	CLA	CAB-C3B-C2B	2.50	130.18	123.53
27	a	611	CLA	O2D-CGD-O1D	-2.50	118.40	124.08
27	3	612	CLA	C3B-C4B-NB	-2.50	108.30	110.53
27	O	2002	CLA	CAB-C3B-C2B	2.50	130.18	123.53
38	V	609	CHL	C1-C2-C3	-2.50	122.10	126.20
38	U	609	CHL	C1-C2-C3	-2.50	122.10	126.20
27	H	202	CLA	O2D-CGD-O1D	-2.50	118.41	124.08
30	B	845	BCR	C15-C14-C13	-2.50	123.77	127.28
35	W	1621	LUT	C3-C4-C5	-2.50	105.95	112.18
27	K	201	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
27	8	611	CLA	CHB-C4A-NA	2.50	128.01	124.40
36	Y	1622	XAT	C11-C10-C9	-2.50	123.77	127.28
27	9	612	CLA	CHB-C4A-NA	2.50	128.00	124.40
35	6	619	LUT	C1-C6-C5	-2.50	119.22	122.64
27	8	601	CLA	CMB-C2B-C3B	2.50	132.42	126.55
30	6	622	BCR	C33-C5-C4	2.50	118.92	113.60
38	W	608	CHL	C1A-CHA-CBD	2.50	138.75	132.36
30	5	622	BCR	C11-C10-C9	-2.50	123.78	127.28
33	H	205	LMG	C8-O7-C10	-2.50	111.82	117.80
27	A	814	CLA	O2D-CGD-O1D	-2.49	118.99	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	7	612	CLA	CHB-C4A-NA	2.49	128.00	124.40
27	4	618	CLA	O2D-CGD-O1D	-2.49	118.42	124.08
30	A	856	BCR	C24-C23-C22	-2.49	122.55	126.23
30	A	850	BCR	C37-C22-C23	2.49	121.90	118.09
27	2	611	CLA	CHB-C4A-NA	2.49	128.00	124.40
27	A	829	CLA	CMB-C2B-C3B	2.49	132.41	126.55
30	A	850	BCR	C8-C9-C10	-2.49	115.09	119.01
27	6	618	CLA	O2D-CGD-O1D	-2.49	118.43	124.08
27	A	812	CLA	O2D-CGD-CBD	2.49	115.58	111.23
27	A	818	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
35	U	1621	LUT	C3-C4-C5	-2.49	105.98	112.18
35	4	619	LUT	C20-C13-C12	2.49	121.89	118.09
30	B	801	BCR	C32-C1-C6	-2.49	106.34	110.24
27	W	614	CLA	C3B-C4B-NB	-2.49	108.31	110.53
27	B	815	CLA	CHB-C4A-NA	2.49	127.99	124.40
37	Z	1623	NEX	C24-C23-C22	-2.49	106.14	110.79
38	X	601	CHL	CMB-C2B-C3B	2.49	129.65	124.68
37	X	1623	NEX	C39-C29-C30	-2.49	118.79	122.82
30	L	305	BCR	C1-C6-C7	2.49	122.40	115.65
38	V	601	CHL	O2D-CGD-O1D	-2.49	119.01	123.85
27	a	614	CLA	C3B-C4B-NB	-2.49	108.31	110.53
27	Z	614	CLA	C3B-C4B-NB	-2.49	108.31	110.53
35	5	620	LUT	C1-C6-C5	-2.49	119.24	122.64
27	B	834	CLA	CHB-C4A-NA	2.48	127.99	124.40
27	a	602	CLA	C3B-C4B-NB	-2.48	108.31	110.53
30	J	102	BCR	C38-C26-C25	-2.48	121.78	124.48
30	3	622	BCR	C15-C16-C17	-2.48	118.44	123.52
38	W	601	CHL	CMB-C2B-C3B	2.48	129.64	124.68
27	2	607	CLA	CHB-C4A-NA	2.48	127.98	124.40
38	X	605	CHL	CMB-C2B-C3B	2.48	129.64	124.68
36	4	620	XAT	C35-C34-C33	-2.48	123.80	127.28
29	7	622	LHG	O7-C7-C8	2.48	116.84	111.48
27	4	603	CLA	CHB-C4A-NA	2.48	127.98	124.40
30	F	305	BCR	C27-C26-C25	-2.48	119.36	122.70
37	V	1623	NEX	C39-C29-C30	-2.48	118.80	122.82
27	6	612	CLA	O2D-CGD-O1D	-2.48	118.46	124.08
27	7	615	CLA	CAB-C3B-C2B	2.48	130.12	123.53
27	5	614	CLA	C3B-C4B-NB	-2.48	108.32	110.53
27	Z	603	CLA	CHB-C4A-NA	2.48	127.97	124.40
36	X	1622	XAT	C11-C10-C9	-2.48	123.81	127.28
30	G	205	BCR	C16-C15-C14	-2.48	118.45	123.52
36	2	620	XAT	C28-C29-C30	-2.48	115.11	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	V	1620	LUT	C38-C25-C24	-2.48	117.50	123.36
27	8	602	CLA	O2D-CGD-CBD	2.47	115.56	111.23
27	B	837	CLA	CHB-C4A-NA	2.47	127.97	124.40
27	A	827	CLA	C3B-C4B-NB	-2.47	108.32	110.53
27	X	612	CLA	C3B-C4B-NB	-2.47	108.32	110.53
38	W	606	CHL	CMB-C2B-C3B	2.47	129.62	124.68
30	B	845	BCR	C21-C20-C19	-2.47	116.04	123.20
35	3	618	LUT	C35-C34-C33	-2.47	123.81	127.28
30	J	102	BCR	C30-C25-C26	-2.47	119.26	122.64
27	8	603	CLA	CAB-C3B-C2B	2.47	130.10	123.53
37	Y	1623	NEX	C39-C29-C30	-2.47	118.81	122.82
27	A	839	CLA	C3B-C4B-NB	-2.47	108.32	110.53
27	7	604	CLA	C3B-C4B-NB	-2.47	108.32	110.53
27	A	805	CLA	CHB-C4A-NA	2.47	127.97	124.40
27	8	607	CLA	CMB-C2B-C3B	2.47	130.10	123.53
30	A	850	BCR	C15-C14-C13	-2.47	123.81	127.28
27	1	607	CLA	O2D-CGD-O1D	-2.47	118.48	124.08
28	B	842	PQN	C16-C15-C13	-2.47	107.46	113.47
36	6	621	XAT	C12-C13-C14	-2.47	115.13	119.01
38	Z	605	CHL	CMB-C2B-C3B	2.47	129.61	124.68
27	8	613	CLA	CHB-C4A-NA	2.47	127.96	124.40
27	2	614	CLA	O2D-CGD-O1D	-2.47	118.48	124.08
30	L	308	BCR	C4-C5-C6	-2.47	119.37	122.70
30	B	846	BCR	C15-C14-C13	-2.47	123.82	127.28
38	U	606	CHL	CMB-C2B-C3B	2.47	129.61	124.68
30	B	849	BCR	C37-C22-C23	2.47	121.85	118.09
38	U	609	CHL	O2D-CGD-O1D	-2.46	119.05	123.85
36	7	620	XAT	C7-C8-C9	-2.46	121.71	125.53
27	5	613	CLA	CHB-C4A-NA	2.46	127.96	124.40
38	Z	605	CHL	O1D-CGD-CBD	-2.46	120.99	124.72
27	L	306	CLA	CHB-C4A-NA	2.46	127.95	124.40
27	a	612	CLA	CHB-C4A-NA	2.46	127.95	124.40
29	5	625	LHG	O8-C23-C24	2.46	119.35	111.83
27	B	806	CLA	C3B-C4B-NB	-2.46	108.33	110.53
38	U	601	CHL	CMB-C2B-C3B	2.46	129.60	124.68
37	V	1623	NEX	C15-C35-C34	-2.46	118.48	123.52
27	A	830	CLA	CHB-C4A-NA	2.46	127.95	124.40
27	B	831	CLA	CHB-C4A-NA	2.46	127.95	124.40
36	6	621	XAT	C24-C23-C22	-2.46	106.19	110.79
37	X	1623	NEX	C31-C30-C29	-2.46	123.83	127.28
27	A	814	CLA	C3B-C4B-NB	-2.46	108.33	110.53
27	6	609	CLA	CHB-C4A-NA	2.46	127.95	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	827	CLA	C1-C2-C3	-2.46	122.17	126.20
30	7	623	BCR	C23-C24-C25	-2.46	120.43	127.00
36	U	1622	XAT	C11-C10-C9	-2.46	123.83	127.28
27	4	618	CLA	CHB-C4A-NA	2.46	127.95	124.40
35	X	1620	LUT	C28-C29-C30	-2.46	115.14	119.01
27	4	601	CLA	O2D-CGD-CBD	2.46	115.53	111.23
27	O	2002	CLA	CMB-C2B-C3B	2.46	130.06	123.53
27	7	616	CLA	CAB-C3B-C2B	2.46	130.06	123.53
27	1	612	CLA	CHB-C4A-NA	2.46	127.95	124.40
30	8	621	BCR	C16-C17-C18	-2.46	123.83	127.28
35	a	617	LUT	C30-C31-C32	-2.45	116.09	123.20
27	Z	612	CLA	CHB-C4A-NA	2.45	127.94	124.40
36	9	620	XAT	C10-C11-C12	-2.45	116.09	123.20
30	7	621	BCR	C15-C14-C13	-2.45	123.84	127.28
30	B	849	BCR	C36-C18-C17	-2.45	118.84	122.82
30	F	305	BCR	C34-C9-C8	2.45	121.83	118.09
30	G	205	BCR	C32-C1-C6	-2.45	106.40	110.24
38	Y	609	CHL	CMB-C2B-C3B	2.45	129.58	124.68
27	B	808	CLA	C3B-C4B-NB	-2.45	108.34	110.53
35	7	619	LUT	C30-C31-C32	-2.45	116.10	123.20
38	X	601	CHL	O2D-CGD-O1D	-2.45	119.08	123.85
30	7	621	BCR	C36-C18-C17	-2.45	118.85	122.82
36	1	618	XAT	C24-C23-C22	-2.45	106.21	110.79
35	U	1621	LUT	C18-C5-C4	2.45	118.93	114.42
27	A	827	CLA	CHB-C4A-NA	2.45	127.94	124.40
30	A	852	BCR	C20-C19-C18	-2.45	119.65	126.36
27	A	834	CLA	CHB-C4A-NA	2.45	127.93	124.40
27	L	304	CLA	CHB-C4A-NA	2.45	127.93	124.40
27	6	604	CLA	CHB-C4A-NA	2.45	127.93	124.40
27	9	606	CLA	CHB-C4A-NA	2.45	127.93	124.40
27	4	604	CLA	CAB-C3B-C2B	2.45	130.04	123.53
30	6	622	BCR	C16-C15-C14	-2.45	118.51	123.52
35	8	619	LUT	C38-C25-C24	-2.45	117.57	123.36
27	A	840	CLA	CAA-CBA-CGA	-2.45	106.26	113.21
36	6	621	XAT	C18-C5-C4	2.45	116.99	114.24
30	K	207	BCR	C30-C25-C24	2.45	122.29	115.65
36	V	1622	XAT	C31-C32-C33	-2.45	119.65	126.36
27	5	617	CLA	C1-C2-C3	-2.45	122.80	126.76
27	4	609	CLA	CHB-C4A-NA	2.45	127.93	124.40
30	3	621	BCR	C32-C1-C6	-2.44	106.41	110.24
27	W	614	CLA	CHB-C4A-NA	2.44	127.93	124.40
35	U	1620	LUT	C11-C12-C13	-2.44	119.66	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	8	614	CLA	C3B-C4B-NB	-2.44	108.35	110.53
27	5	619	CLA	CAB-C3B-C2B	2.44	130.03	123.53
27	Z	612	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
27	A	814	CLA	C4-C3-C5	2.44	119.47	115.23
38	Z	601	CHL	C4-C3-C5	2.44	119.47	115.23
27	A	832	CLA	C3B-C4B-NB	-2.44	108.35	110.53
36	Z	1622	XAT	C31-C32-C33	-2.44	119.67	126.36
27	A	835	CLA	CHB-C4A-NA	2.44	127.92	124.40
27	L	307	CLA	CHB-C4A-NA	2.44	127.92	124.40
27	4	614	CLA	C3B-C4B-NB	-2.44	108.35	110.53
30	3	622	BCR	C36-C18-C17	-2.44	118.86	122.82
30	L	305	BCR	C1-C6-C5	-2.44	119.30	122.64
27	2	606	CLA	CHB-C4A-NA	2.44	127.92	124.40
27	Y	612	CLA	C3B-C4B-NB	-2.44	108.35	110.53
27	6	607	CLA	CAB-C3B-C2B	2.44	130.02	123.53
27	A	817	CLA	CHB-C4A-NA	2.44	127.92	124.40
27	a	611	CLA	CMB-C2B-C3B	2.44	130.01	123.53
30	B	852	BCR	C16-C17-C18	-2.44	123.86	127.28
38	Z	609	CHL	O2D-CGD-O1D	-2.44	119.10	123.85
27	U	614	CLA	C3B-C4B-NB	-2.44	108.35	110.53
30	J	102	BCR	C27-C26-C25	-2.44	119.41	122.70
38	X	601	CHL	O1D-CGD-CBD	-2.44	121.03	124.72
27	3	602	CLA	CHB-C4A-NA	2.44	127.92	124.40
27	V	610	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
30	B	801	BCR	C21-C20-C19	-2.44	116.14	123.20
35	1	617	LUT	C30-C31-C32	-2.44	116.14	123.20
29	7	622	LHG	O8-C23-C24	2.44	119.26	111.83
35	W	1620	LUT	C11-C12-C13	-2.44	119.68	126.36
36	8	620	XAT	C32-C33-C34	-2.44	115.18	119.01
37	Z	1623	NEX	C32-C33-C34	-2.44	115.18	119.01
27	3	613	CLA	C3B-C4B-NB	-2.44	108.36	110.53
36	9	620	XAT	C20-C13-C12	2.44	121.81	118.09
36	a	618	XAT	C4-C3-C2	-2.43	106.24	110.79
27	9	612	CLA	O2D-CGD-O1D	-2.43	118.56	124.08
27	4	604	CLA	CHB-C4A-NA	2.43	127.91	124.40
38	U	601	CHL	CMA-C3A-C4A	-2.43	109.37	114.61
38	W	609	CHL	O1D-CGD-CBD	-2.43	121.03	124.72
30	B	846	BCR	C24-C25-C26	-2.43	115.95	121.56
30	B	801	BCR	C7-C8-C9	-2.43	122.64	126.23
38	U	607	CHL	CMB-C2B-C3B	2.43	129.54	124.68
30	L	309	BCR	C36-C18-C17	-2.43	118.88	122.82
27	A	818	CLA	CHB-C4A-NA	2.43	127.90	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	814	CLA	CHB-C4A-NA	2.43	127.90	124.40
27	B	822	CLA	CHB-C4A-NA	2.43	127.90	124.40
35	X	1620	LUT	C11-C10-C9	-2.43	123.88	127.28
27	B	807	CLA	O2D-CGD-CBD	2.43	115.47	111.23
27	A	838	CLA	CMB-C2B-C3B	2.43	132.25	126.55
38	Z	601	CHL	O1D-CGD-CBD	-2.43	121.05	124.72
30	L	308	BCR	C15-C16-C17	-2.42	118.56	123.52
38	W	609	CHL	O2D-CGD-O1D	-2.42	119.13	123.85
27	5	612	CLA	CHB-C4A-NA	2.42	127.90	124.40
27	1	603	CLA	O2D-CGD-O1D	-2.42	118.58	124.08
27	3	603	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
35	W	1621	LUT	C18-C5-C4	2.42	118.88	114.42
36	1	618	XAT	C4-C3-C2	-2.42	106.26	110.79
27	6	608	CLA	CHB-C4A-NA	2.42	127.90	124.40
30	4	621	BCR	C38-C26-C27	2.42	118.76	113.60
30	9	621	BCR	C23-C24-C25	-2.42	120.53	127.00
38	Y	607	CHL	OMC-CMC-C2C	-2.42	120.91	125.12
27	B	816	CLA	C3B-C4B-NB	-2.42	108.37	110.53
30	2	623	BCR	C37-C22-C23	2.42	121.78	118.09
36	a	618	XAT	C24-C23-C22	-2.42	106.26	110.79
30	B	844	BCR	C33-C5-C4	2.42	118.75	113.60
38	Z	601	CHL	O2D-CGD-O1D	-2.42	119.14	123.85
27	9	614	CLA	C3B-C4B-NB	-2.42	108.37	110.53
27	1	610	CLA	CHB-C4A-NA	2.42	127.89	124.40
37	Y	1623	NEX	C31-C30-C29	-2.42	123.89	127.28
38	X	607	CHL	O2A-CGA-CBA	2.42	119.21	111.83
27	1	603	CLA	CHB-C4A-NA	2.42	127.89	124.40
27	B	811	CLA	CAB-C3B-C2B	2.42	129.95	123.53
27	9	607	CLA	C3B-C4B-NB	-2.42	108.37	110.53
36	5	621	XAT	C12-C13-C14	-2.41	115.21	119.01
27	X	612	CLA	CHB-C4A-NA	2.41	127.88	124.40
27	O	2002	CLA	O2D-CGD-O1D	-2.41	118.60	124.08
30	6	622	BCR	C3-C4-C5	-2.41	109.75	114.06
27	6	616	CLA	CHB-C4A-NA	2.41	127.88	124.40
38	X	605	CHL	CMA-C3A-C4A	-2.41	109.41	114.61
27	8	610	CLA	C4-C3-C2	-2.41	117.43	123.63
27	3	604	CLA	CHB-C4A-NA	2.41	127.88	124.40
27	A	830	CLA	C4-C3-C5	2.41	119.42	115.23
27	8	616	CLA	CAB-C3B-C2B	2.41	129.94	123.53
27	B	829	CLA	CHB-C4A-NA	2.41	127.88	124.40
30	7	623	BCR	C38-C26-C27	2.41	118.74	113.60
30	3	620	BCR	C16-C17-C18	-2.41	123.90	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	O	2631	LHG	O8-C23-C24	2.41	119.19	111.83
27	B	825	CLA	CHB-C4A-NA	2.41	127.88	124.40
27	7	609	CLA	CHB-C4A-NA	2.41	127.88	124.40
36	1	618	XAT	C38-C25-C24	2.41	116.95	114.24
27	B	837	CLA	C1-C2-C3	-2.41	122.25	126.20
38	Y	605	CHL	CMA-C3A-C4A	-2.41	109.42	114.61
27	K	204	CLA	C3B-C4B-NB	-2.41	108.38	110.53
37	5	624	NEX	C15-C14-C13	-2.41	123.90	127.28
30	7	623	BCR	C11-C12-C13	-2.41	119.76	126.36
27	a	602	CLA	CHB-C4A-NA	2.41	127.88	124.40
37	U	1623	NEX	C31-C30-C29	-2.41	123.90	127.28
35	a	617	LUT	C35-C34-C33	-2.41	123.90	127.28
27	1	607	CLA	CHB-C4A-NA	2.41	127.87	124.40
30	3	620	BCR	C3-C4-C5	-2.41	109.76	114.06
27	4	616	CLA	CMB-C2B-C3B	2.41	129.93	123.53
27	7	603	CLA	C3B-C4B-NB	-2.41	108.38	110.53
35	X	1621	LUT	C18-C5-C4	2.40	118.84	114.42
27	V	610	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
30	F	305	BCR	C15-C16-C17	-2.40	118.60	123.52
35	U	1620	LUT	C17-C1-C6	2.40	114.01	110.24
27	8	608	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
27	9	602	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
35	Y	1620	LUT	C11-C10-C9	-2.40	123.91	127.28
27	6	606	CLA	C3B-C4B-NB	-2.40	108.39	110.53
35	6	619	LUT	C17-C1-C6	-2.40	106.47	110.24
38	Y	609	CHL	O2D-CGD-O1D	-2.40	119.17	123.85
38	Z	601	CHL	CMA-C3A-C4A	-2.40	109.44	114.61
27	5	604	CLA	CAB-C3B-C2B	2.40	129.91	123.53
37	6	624	NEX	C35-C34-C33	-2.40	123.91	127.28
30	L	301	BCR	C30-C25-C26	-2.40	119.36	122.64
30	5	622	BCR	C30-C25-C24	2.40	122.16	115.65
33	4	624	LMG	O8-C28-O10	-2.40	117.63	123.63
27	X	603	CLA	CHB-C4A-NA	2.40	127.86	124.40
35	7	619	LUT	C35-C34-C33	-2.40	123.92	127.28
30	7	623	BCR	C24-C23-C22	-2.40	122.69	126.23
36	8	620	XAT	C4-C3-C2	-2.40	106.31	110.79
37	X	1623	NEX	C4-C3-C2	-2.40	106.31	110.79
27	a	607	CLA	CHB-C4A-NA	2.40	127.86	124.40
30	A	850	BCR	C11-C12-C13	-2.40	119.79	126.36
27	B	818	CLA	CHB-C4A-NA	2.40	127.86	124.40
30	B	852	BCR	C19-C18-C17	-2.40	115.24	119.01
32	K	208	LMU	C3B-C4B-C5B	2.40	114.58	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	813	CLA	CHB-C4A-NA	2.39	127.86	124.40
38	V	601	CHL	CMB-C2B-C3B	2.39	129.47	124.68
27	A	810	CLA	CAA-CBA-CGA	-2.39	106.41	113.21
27	a	601	CLA	CHB-C4A-NA	2.39	127.85	124.40
30	7	623	BCR	C2-C1-C6	2.39	113.92	110.44
27	Z	610	CLA	CHB-C4A-NA	2.39	127.85	124.40
27	A	821	CLA	C1-C2-C3	-2.39	122.28	126.20
27	B	826	CLA	CHB-C4A-NA	2.39	127.85	124.40
27	V	603	CLA	CHB-C4A-NA	2.39	127.85	124.40
27	Z	610	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
27	A	817	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
30	J	102	BCR	C8-C9-C10	-2.39	115.25	119.01
30	7	623	BCR	C1-C6-C7	2.39	122.14	115.65
35	2	619	LUT	C11-C10-C9	-2.39	123.93	127.28
30	L	308	BCR	C2-C1-C6	2.39	113.91	110.44
27	B	805	CLA	C3B-C4B-NB	-2.39	108.40	110.53
27	a	613	CLA	CHB-C4A-NA	2.39	127.85	124.40
36	2	620	XAT	C7-C8-C9	-2.39	121.82	125.53
30	7	621	BCR	C23-C24-C25	-2.39	120.62	127.00
27	2	612	CLA	CHB-C4A-NA	2.39	127.85	124.40
27	B	835	CLA	C3B-C4B-NB	-2.39	108.40	110.53
27	a	611	CLA	CAB-C3B-C2B	2.39	129.88	123.53
27	8	616	CLA	CMB-C2B-C3B	2.39	129.88	123.53
27	A	845	CLA	CHB-C4A-NA	2.39	127.85	124.40
38	Y	601	CHL	CMA-C3A-C4A	-2.39	109.47	114.61
30	B	844	BCR	C11-C12-C13	-2.39	119.82	126.36
27	B	804	CLA	CHB-C4A-NA	2.39	127.84	124.40
27	a	603	CLA	CHB-C4A-NA	2.39	127.84	124.40
27	W	603	CLA	C1-C2-C3	-2.39	122.29	126.20
36	Y	1622	XAT	C18-C5-C4	2.39	116.92	114.24
27	Y	612	CLA	CHB-C4A-NA	2.39	127.84	124.40
36	9	620	XAT	C8-C9-C10	-2.39	115.26	119.01
27	3	613	CLA	CHB-C4A-NA	2.39	127.84	124.40
36	a	618	XAT	C38-C25-C24	2.38	116.92	114.24
27	5	601	CLA	C3B-C4B-NB	-2.38	108.40	110.53
27	B	828	CLA	C3B-C4B-NB	-2.38	108.40	110.53
36	6	621	XAT	C4-C3-C2	-2.38	106.33	110.79
38	Y	601	CHL	O2A-CGA-CBA	2.38	119.10	111.83
27	a	610	CLA	CHB-C4A-NA	2.38	127.84	124.40
27	1	613	CLA	CHB-C4A-NA	2.38	127.84	124.40
35	Z	1621	LUT	C31-C30-C29	-2.38	123.94	127.28
27	A	840	CLA	O2D-CGD-CBD	2.38	115.39	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	Z	610	CLA	CMB-C2B-C3B	2.38	132.15	126.55
27	1	602	CLA	CHB-C4A-NA	2.38	127.83	124.40
35	V	1620	LUT	C35-C15-C14	-2.38	118.65	123.52
27	8	602	CLA	C3B-C4B-NB	-2.38	108.41	110.53
36	4	620	XAT	C28-C29-C30	-2.38	115.27	119.01
27	1	601	CLA	CHB-C4A-NA	2.38	127.83	124.40
27	4	607	CLA	CHB-C4A-NA	2.38	127.83	124.40
27	5	609	CLA	CHB-C4A-NA	2.38	127.83	124.40
27	U	614	CLA	CHB-C4A-NA	2.38	127.83	124.40
38	V	607	CHL	CMB-C2B-C3B	2.38	129.43	124.68
27	6	602	CLA	CHB-C4A-NA	2.38	127.83	124.40
27	8	607	CLA	CHB-C4A-NA	2.38	127.83	124.40
30	B	846	BCR	C32-C1-C6	-2.38	106.52	110.24
27	3	617	CLA	C3B-C4B-NB	-2.38	108.41	110.53
35	1	617	LUT	C35-C34-C33	-2.38	123.95	127.28
30	K	202	BCR	C11-C12-C13	-2.38	119.85	126.36
27	6	618	CLA	CMB-C2B-C3B	2.38	129.84	123.53
38	X	601	CHL	CMA-C3A-C4A	-2.38	109.49	114.61
30	7	623	BCR	C36-C18-C17	-2.37	118.97	122.82
37	W	1623	NEX	C31-C30-C29	-2.37	123.95	127.28
27	8	601	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
27	8	614	CLA	O2D-CGD-CBD	2.37	115.38	111.23
27	B	836	CLA	CHB-C4A-NA	2.37	127.83	124.40
38	W	601	CHL	O1D-CGD-CBD	-2.37	121.12	124.72
27	7	616	CLA	CMB-C2B-C3B	2.37	129.84	123.53
36	a	618	XAT	C28-C29-C30	-2.37	115.28	119.01
27	8	602	CLA	CHB-C4A-NA	2.37	127.82	124.40
27	K	204	CLA	CHB-C4A-NA	2.37	127.82	124.40
35	Y	1621	LUT	C18-C5-C4	2.37	118.78	114.42
27	B	808	CLA	O2D-CGD-CBD	2.37	115.37	111.23
27	9	610	CLA	O2D-CGD-CBD	2.37	115.37	111.23
38	V	605	CHL	O1D-CGD-CBD	-2.37	121.13	124.72
38	X	609	CHL	O2D-CGD-O1D	-2.37	119.24	123.85
38	V	606	CHL	C1A-CHA-CBD	2.37	138.42	132.36
27	Z	613	CLA	C1-C2-C3	-2.37	122.32	126.20
29	5	623	LHG	O8-C23-C24	2.37	119.05	111.83
36	X	1622	XAT	C18-C5-C4	2.37	116.90	114.24
35	U	1621	LUT	O23-C23-C22	-2.37	105.86	110.06
27	1	609	CLA	CHB-C4A-NA	2.37	127.81	124.40
27	A	829	CLA	C3B-C4B-NB	-2.36	108.42	110.53
27	7	602	CLA	CHB-C4A-NA	2.36	127.81	124.40
27	H	203	CLA	C1-C2-C3	-2.36	122.32	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	613	CLA	C1-C2-C3	-2.36	122.32	126.20
27	7	604	CLA	CHB-C4A-NA	2.36	127.81	124.40
27	V	614	CLA	C3B-C4B-NB	-2.36	108.42	110.53
27	7	610	CLA	C1-C2-C3	-2.36	122.33	126.20
36	1	618	XAT	C28-C29-C30	-2.36	115.29	119.01
27	8	614	CLA	CHB-C4A-NA	2.36	127.81	124.40
27	Z	611	CLA	CHB-C4A-NA	2.36	127.81	124.40
30	L	305	BCR	C33-C5-C4	2.36	118.63	113.60
27	7	610	CLA	CHB-C4A-NA	2.36	127.81	124.40
27	U	603	CLA	C1-C2-C3	-2.36	122.33	126.20
27	V	604	CLA	CHB-C4A-NA	2.36	127.81	124.40
27	3	606	CLA	CHB-C4A-NA	2.36	127.81	124.40
30	A	848	BCR	C37-C22-C21	-2.36	118.99	122.82
27	8	609	CLA	C3B-C4B-NB	-2.36	108.42	110.53
27	B	835	CLA	CHB-C4A-NA	2.36	127.81	124.40
27	8	604	CLA	CHB-C4A-NA	2.36	127.81	124.40
27	B	813	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
27	W	610	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
27	F	304	CLA	CHB-C4A-NA	2.36	127.80	124.40
35	W	1620	LUT	C17-C1-C6	2.36	113.94	110.24
27	B	836	CLA	CMB-C2B-C3B	2.36	132.09	126.55
36	5	621	XAT	C19-C9-C8	2.36	121.69	118.09
27	a	609	CLA	O2D-CGD-O1D	-2.36	118.73	124.08
30	B	845	BCR	C29-C30-C25	2.36	113.86	110.44
27	9	611	CLA	CHB-C4A-NA	2.36	127.80	124.40
27	X	614	CLA	C3B-C4B-NB	-2.36	108.43	110.53
27	A	833	CLA	CHB-C4A-NA	2.35	127.80	124.40
27	A	824	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
35	W	1621	LUT	O23-C23-C22	-2.35	105.89	110.06
27	A	820	CLA	O2D-CGD-CBD	2.35	115.34	111.23
27	2	603	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
27	Y	602	CLA	CHB-C4A-NA	2.35	127.79	124.40
27	V	613	CLA	CHB-C4A-NA	2.35	127.79	124.40
27	5	604	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
30	B	801	BCR	C35-C13-C12	2.35	121.68	118.09
30	B	849	BCR	C11-C12-C13	-2.35	119.92	126.36
38	Y	607	CHL	CED-O2D-CGD	2.35	121.25	115.92
27	8	610	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
30	B	844	BCR	C1-C6-C5	-2.35	119.43	122.64
27	7	607	CLA	CHB-C4A-NA	2.35	127.79	124.40
37	6	624	NEX	C15-C14-C13	-2.35	123.98	127.28
27	A	810	CLA	O2A-CGA-O1A	-2.35	117.75	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	851	BCR	C10-C11-C12	-2.35	116.40	123.20
30	3	621	BCR	C37-C22-C21	-2.35	119.01	122.82
30	5	622	BCR	C15-C14-C13	-2.35	123.99	127.28
35	7	619	LUT	C28-C29-C30	-2.35	115.32	119.01
35	3	618	LUT	C1-C6-C5	-2.35	119.43	122.64
27	K	203	CLA	O2D-CGD-CBD	2.35	115.33	111.23
27	B	824	CLA	C3B-C4B-NB	-2.35	108.44	110.53
30	1	619	BCR	C36-C18-C17	-2.35	119.02	122.82
27	Y	603	CLA	CHB-C4A-NA	2.34	127.78	124.40
27	A	813	CLA	CMB-C2B-C1B	-2.34	121.85	125.42
27	W	602	CLA	C3B-C4B-NB	-2.34	108.44	110.53
38	Y	606	CHL	O2D-CGD-O1D	-2.34	119.28	123.85
27	B	828	CLA	CMB-C2B-C1B	-2.34	121.85	125.42
33	V	2631	LMG	O8-C28-C29	2.34	118.98	111.83
27	B	832	CLA	C3B-C4B-NB	-2.34	108.44	110.53
27	V	603	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
27	4	607	CLA	C3B-C4B-NB	-2.34	108.44	110.53
38	W	601	CHL	CBC-CAC-C3C	-2.34	109.52	112.87
27	L	302	CLA	CHB-C4A-NA	2.34	127.78	124.40
27	9	604	CLA	CAB-C3B-C2B	2.34	129.75	123.53
27	A	854	CLA	C1-C2-C3	-2.34	122.36	126.20
27	U	610	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
29	8	623	LHG	C5-O7-C7	-2.34	112.19	117.80
27	B	811	CLA	CBD-CHA-C1A	2.34	131.92	127.58
37	Z	1623	NEX	C17-C1-C6	-2.34	108.38	110.47
38	Y	601	CHL	O1D-CGD-CBD	-2.34	121.17	124.72
35	W	1621	LUT	C15-C14-C13	-2.34	124.00	127.28
27	B	822	CLA	C3B-C4B-NB	-2.34	108.44	110.53
27	6	612	CLA	CHB-C4A-NA	2.34	127.78	124.40
30	5	622	BCR	C33-C5-C4	2.34	118.58	113.60
27	4	609	CLA	C1-C2-C3	-2.34	122.37	126.20
30	A	852	BCR	C38-C26-C27	2.34	118.58	113.60
35	1	617	LUT	C18-C5-C4	2.34	118.72	114.42
30	L	301	BCR	C32-C1-C6	-2.34	106.58	110.24
35	Y	1621	LUT	C15-C35-C34	-2.34	118.74	123.52
27	A	808	CLA	CHB-C4A-NA	2.34	127.77	124.40
30	1	619	BCR	C23-C22-C21	-2.34	115.33	119.01
27	5	616	CLA	CMB-C2B-C3B	2.34	129.74	123.53
37	6	624	NEX	C15-C35-C34	-2.34	118.74	123.52
30	a	619	BCR	C36-C18-C17	-2.34	119.03	122.82
27	1	604	CLA	CHB-C4A-NA	2.34	127.77	124.40
27	B	805	CLA	CHB-C4A-NA	2.34	127.77	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	602	CLA	CHB-C4A-NA	2.34	127.77	124.40
30	a	619	BCR	C23-C22-C21	-2.34	115.34	119.01
30	B	852	BCR	C21-C20-C19	-2.33	116.44	123.20
37	U	1623	NEX	C2-C1-C6	2.33	111.48	109.21
27	a	609	CLA	CHB-C4A-NA	2.33	127.77	124.40
27	6	618	CLA	CHB-C4A-NA	2.33	127.77	124.40
27	A	835	CLA	C3B-C4B-NB	-2.33	108.45	110.53
30	J	102	BCR	C12-C13-C14	-2.33	115.34	119.01
35	9	619	LUT	C39-C29-C28	2.33	121.65	118.09
30	K	207	BCR	C15-C16-C17	-2.33	118.74	123.52
30	A	850	BCR	C38-C26-C27	2.33	118.57	113.60
30	6	622	BCR	C38-C26-C27	2.33	118.57	113.60
27	2	616	CLA	CHB-C4A-NA	2.33	127.77	124.40
38	X	608	CHL	O1D-CGD-CBD	-2.33	121.19	124.72
27	2	610	CLA	C1-C2-C3	-2.33	122.38	126.20
27	4	609	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
27	Y	610	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
27	3	612	CLA	CHB-C4A-NA	2.33	127.77	124.40
38	U	606	CHL	C3D-CAD-CBD	2.33	110.67	107.61
27	A	822	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
27	A	821	CLA	CHB-C4A-NA	2.33	127.76	124.40
27	A	829	CLA	CHB-C4A-NA	2.33	127.76	124.40
30	L	308	BCR	C29-C30-C25	2.33	113.82	110.44
27	A	819	CLA	C3B-C4B-NB	-2.33	108.45	110.53
30	B	848	BCR	C38-C26-C27	2.33	118.56	113.60
36	3	619	XAT	C24-C23-C22	-2.33	106.44	110.79
27	K	203	CLA	CAA-CBA-CGA	-2.33	106.60	113.21
30	B	852	BCR	C12-C13-C14	2.33	122.67	119.01
27	B	817	CLA	C6-C5-C3	2.33	119.14	113.47
27	2	616	CLA	CMB-C2B-C3B	2.33	129.72	123.53
27	J	101	CLA	CHB-C4A-NA	2.33	127.76	124.40
27	W	603	CLA	C3B-C4B-NB	-2.33	108.45	110.53
35	6	619	LUT	C7-C8-C9	-2.33	122.80	126.23
30	3	620	BCR	C20-C21-C22	-2.33	124.02	127.28
38	X	606	CHL	O2D-CGD-O1D	-2.32	119.32	123.85
27	4	611	CLA	C3B-C4B-NB	-2.32	108.45	110.53
38	Y	609	CHL	CMA-C3A-C4A	-2.32	109.60	114.61
27	A	811	CLA	CHB-C4A-NA	2.32	127.75	124.40
27	B	830	CLA	CHB-C4A-NA	2.32	127.75	124.40
38	Z	605	CHL	C1A-CHA-CBD	2.32	138.31	132.36
35	U	1621	LUT	C15-C14-C13	-2.32	124.02	127.28
27	U	604	CLA	CBD-CHA-C1A	2.32	131.89	127.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	2	603	CLA	CHB-C1B-NB	2.32	127.53	124.05
27	2	612	CLA	C3B-C4B-NB	-2.32	108.46	110.53
27	a	604	CLA	CHB-C4A-NA	2.32	127.75	124.40
30	O	2004	BCR	C30-C25-C26	-2.32	119.46	122.64
27	7	615	CLA	CMB-C2B-C3B	2.32	129.70	123.53
27	Y	603	CLA	C3B-C4B-NB	-2.32	108.46	110.53
27	A	822	CLA	CHB-C4A-NA	2.32	127.75	124.40
27	A	841	CLA	CHB-C4A-NA	2.32	127.75	124.40
32	K	208	LMU	O5B-C5B-C4B	2.32	113.88	109.70
27	B	812	CLA	CHB-C4A-NA	2.32	127.75	124.40
30	7	621	BCR	C32-C1-C6	-2.32	106.61	110.24
30	L	308	BCR	C11-C12-C13	-2.32	120.00	126.36
27	3	610	CLA	CHB-C4A-NA	2.32	127.75	124.40
38	V	607	CHL	C1A-CHA-CBD	2.32	138.30	132.36
36	7	620	XAT	C4-C3-C2	-2.32	106.45	110.79
36	4	620	XAT	C32-C33-C34	-2.32	115.36	119.01
30	A	849	BCR	C33-C5-C6	-2.32	121.95	124.48
27	V	610	CLA	CMB-C2B-C3B	2.32	132.00	126.55
27	A	816	CLA	CHB-C4A-NA	2.32	127.74	124.40
36	7	620	XAT	C15-C35-C34	-2.32	118.78	123.52
27	B	814	CLA	C3B-C4B-NB	-2.32	108.46	110.53
27	2	611	CLA	C3B-C4B-NB	-2.32	108.46	110.53
38	Z	608	CHL	C1A-CHA-CBD	2.32	138.29	132.36
38	Y	608	CHL	C1B-CHB-C4A	-2.32	119.83	121.32
38	Z	606	CHL	C1C-C2C-CMC	2.32	130.98	126.80
30	6	622	BCR	C1-C6-C5	-2.32	119.47	122.64
32	5	629	LMU	C1'-O5'-C5'	-2.32	109.20	113.72
27	6	611	CLA	CHB-C4A-NA	2.32	127.74	124.40
38	X	608	CHL	O2D-CGD-O1D	-2.31	119.34	123.85
27	B	831	CLA	C4-C3-C5	2.31	119.25	115.23
38	Z	609	CHL	CMB-C2B-C3B	2.31	129.31	124.68
38	U	606	CHL	O1D-CGD-CBD	-2.31	121.21	124.72
36	2	620	XAT	C35-C34-C33	-2.31	124.03	127.28
27	Y	613	CLA	C1-C2-C3	-2.31	122.41	126.20
35	8	619	LUT	C11-C10-C9	-2.31	124.03	127.28
27	a	608	CLA	CHB-C4A-NA	2.31	127.74	124.40
27	Y	614	CLA	C3B-C4B-NB	-2.31	108.47	110.53
38	W	606	CHL	C3D-CAD-CBD	2.31	110.65	107.61
27	A	839	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
33	J	104	LMG	C8-O7-C10	-2.31	112.26	117.80
36	4	620	XAT	C30-C31-C32	-2.31	116.50	123.20
27	a	610	CLA	O2A-CGA-O1A	-2.31	117.85	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	1623	NEX	C2-C1-C6	2.31	111.46	109.21
35	Z	1620	LUT	C38-C25-C24	-2.31	117.89	123.36
27	9	602	CLA	CHB-C4A-NA	2.31	127.73	124.40
32	8	625	LMU	O5'-C1'-C2'	2.31	115.12	110.37
35	6	619	LUT	C12-C13-C14	-2.31	115.38	119.01
30	3	622	BCR	C11-C12-C13	-2.31	120.03	126.36
27	4	611	CLA	CHB-C4A-NA	2.31	127.73	124.40
27	6	606	CLA	CHB-C4A-NA	2.31	127.73	124.40
35	V	1620	LUT	C35-C34-C33	-2.31	124.04	127.28
38	X	601	CHL	CBC-CAC-C3C	-2.31	109.57	112.87
27	X	603	CLA	C3B-C4B-NB	-2.31	108.47	110.53
27	a	614	CLA	O2D-CGD-CBD	2.31	115.26	111.23
35	V	1621	LUT	C15-C35-C34	-2.31	118.80	123.52
27	9	602	CLA	O2D-CGD-CBD	2.31	115.26	111.23
27	X	610	CLA	CHB-C4A-NA	2.31	127.73	124.40
30	B	843	BCR	C4-C5-C6	-2.31	119.59	122.70
27	Z	610	CLA	C1-C2-C3	-2.31	122.42	126.20
37	X	1623	NEX	C15-C35-C34	-2.30	118.80	123.52
27	B	837	CLA	C3B-C4B-NB	-2.30	108.47	110.53
27	B	808	CLA	CHB-C4A-NA	2.30	127.72	124.40
27	5	602	CLA	CHB-C4A-NA	2.30	127.72	124.40
27	5	611	CLA	CHB-C4A-NA	2.30	127.72	124.40
27	W	604	CLA	CHB-C4A-NA	2.30	127.72	124.40
36	9	620	XAT	C4-C3-C2	-2.30	106.48	110.79
27	1	616	CLA	CAB-C3B-C4B	-2.30	121.91	125.42
38	V	601	CHL	CMA-C3A-C4A	-2.30	109.65	114.61
27	O	2003	CLA	CHB-C4A-NA	2.30	127.72	124.40
36	8	620	XAT	C20-C13-C12	2.30	121.61	118.09
27	A	837	CLA	C3B-C4B-NB	-2.30	108.47	110.53
27	4	601	CLA	CHB-C4A-NA	2.30	127.72	124.40
30	9	621	BCR	C16-C15-C14	-2.30	118.81	123.52
38	Y	608	CHL	C1A-CHA-CBD	2.30	138.25	132.36
35	2	619	LUT	C17-C1-C6	-2.30	106.64	110.24
27	A	825	CLA	CHB-C4A-NA	2.30	127.72	124.40
27	1	608	CLA	CHB-C4A-NA	2.30	127.72	124.40
30	6	622	BCR	C39-C30-C29	2.30	117.78	108.95
30	L	301	BCR	C15-C14-C13	-2.30	124.05	127.28
27	5	617	CLA	CHB-C4A-NA	2.30	127.72	124.40
27	U	604	CLA	CHB-C4A-NA	2.30	127.72	124.40
27	4	603	CLA	CMB-C2B-C3B	2.30	129.64	123.53
27	6	614	CLA	CHB-C4A-NA	2.30	127.72	124.40
36	9	620	XAT	C31-C30-C29	-2.30	124.06	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Y	1623	NEX	C15-C35-C34	-2.30	118.82	123.52
27	B	816	CLA	CHB-C4A-NA	2.30	127.71	124.40
27	X	610	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
27	4	618	CLA	CMB-C2B-C3B	2.30	129.63	123.53
27	A	836	CLA	CHB-C4A-NA	2.30	127.71	124.40
36	V	1622	XAT	C35-C34-C33	-2.30	124.06	127.28
27	B	810	CLA	CHB-C4A-NA	2.30	127.71	124.40
36	8	620	XAT	C11-C10-C9	-2.29	124.06	127.28
30	2	623	BCR	C29-C30-C25	2.29	113.77	110.44
27	U	602	CLA	C3B-C4B-NB	-2.29	108.48	110.53
27	5	608	CLA	CHB-C4A-NA	2.29	127.71	124.40
27	8	614	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
27	Z	602	CLA	CHB-C4A-NA	2.29	127.71	124.40
27	7	613	CLA	CHB-C4A-NA	2.29	127.71	124.40
30	B	844	BCR	C21-C20-C19	-2.29	116.56	123.20
27	1	613	CLA	C11-C12-C13	-2.29	108.35	115.97
38	Y	601	CHL	O2D-CGD-O1D	-2.29	119.39	123.85
27	1	611	CLA	CHB-C4A-NA	2.29	127.70	124.40
30	L	309	BCR	C30-C25-C24	2.29	121.86	115.65
27	7	603	CLA	CHB-C4A-NA	2.29	127.70	124.40
35	U	1621	LUT	C15-C35-C34	-2.29	118.84	123.52
27	a	611	CLA	CHB-C4A-NA	2.29	127.70	124.40
27	9	604	CLA	CHB-C4A-NA	2.29	127.70	124.40
35	X	1621	LUT	C15-C35-C34	-2.29	118.84	123.52
38	X	606	CHL	C1A-CHA-CBD	2.29	138.22	132.36
27	F	304	CLA	C3B-C4B-NB	-2.29	108.49	110.53
27	B	841	CLA	C1-C2-C3	-2.29	122.45	126.20
35	a	617	LUT	C18-C5-C4	2.29	118.62	114.42
27	4	602	CLA	CHB-C4A-NA	2.28	127.70	124.40
27	B	820	CLA	C1-C2-C3	-2.28	123.07	126.76
38	Z	601	CHL	CMB-C2B-C3B	2.28	129.25	124.68
27	9	606	CLA	C3B-C4B-NB	-2.28	108.49	110.53
27	B	833	CLA	CHB-C4A-NA	2.28	127.69	124.40
38	X	606	CHL	C3D-CAD-CBD	2.28	110.61	107.61
27	2	614	CLA	CHB-C4A-NA	2.28	127.69	124.40
27	8	603	CLA	CHB-C4A-NA	2.28	127.69	124.40
36	W	1622	XAT	C31-C32-C33	-2.28	120.11	126.36
27	9	609	CLA	C3B-C4B-NB	-2.28	108.50	110.53
27	2	609	CLA	CHB-C4A-NA	2.28	127.69	124.40
32	5	629	LMU	C1B-O1B-C4'	-2.28	112.58	117.98
27	B	833	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
29	6	623	LHG	C5-O7-C7	-2.28	112.34	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	4	613	CLA	CHB-C4A-NA	2.28	127.69	124.40
27	7	611	CLA	CHB-C4A-NA	2.28	127.69	124.40
27	V	602	CLA	C1-C2-C3	-2.28	122.47	126.20
36	7	620	XAT	C18-C5-C4	2.28	116.80	114.24
27	a	616	CLA	C3B-C4B-NB	-2.28	108.50	110.53
27	1	611	CLA	C3B-C4B-NB	-2.28	108.50	110.53
27	U	603	CLA	C3B-C4B-NB	-2.28	108.50	110.53
27	5	616	CLA	CHB-C4A-NA	2.27	127.68	124.40
38	Z	606	CHL	C3D-CAD-CBD	2.27	110.60	107.61
27	A	835	CLA	CAC-C3C-C4C	2.27	127.75	124.79
30	B	847	BCR	C1-C6-C7	2.27	121.82	115.65
33	8	626	LMG	C8-O7-C10	-2.27	112.35	117.80
30	3	622	BCR	C15-C14-C13	-2.27	124.09	127.28
38	W	607	CHL	CMB-C2B-C3B	2.27	129.23	124.68
36	V	1622	XAT	C24-C23-C22	-2.27	106.54	110.79
27	4	602	CLA	O2D-CGD-CBD	2.27	115.20	111.23
36	X	1622	XAT	C26-C27-C28	-2.27	121.19	125.99
38	Y	608	CHL	O1D-CGD-CBD	-2.27	121.28	124.72
27	a	613	CLA	C3B-C4B-NB	-2.27	108.50	110.53
27	B	828	CLA	C1-C2-C3	-2.27	122.47	126.20
27	9	609	CLA	CHB-C4A-NA	2.27	127.68	124.40
27	3	604	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
27	6	603	CLA	CHB-C4A-NA	2.27	127.68	124.40
38	U	601	CHL	O1D-CGD-CBD	-2.27	121.28	124.72
27	6	620	CLA	CHB-C4A-NA	2.27	127.68	124.40
27	a	614	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
27	9	601	CLA	C3B-C4B-NB	-2.27	108.50	110.53
27	G	203	CLA	CHB-C4A-NA	2.27	127.67	124.40
27	B	826	CLA	O2D-CGD-CBD	2.27	115.20	111.23
27	B	832	CLA	O2D-CGD-CBD	2.27	115.19	111.23
35	X	1621	LUT	C15-C14-C13	-2.27	124.10	127.28
27	9	603	CLA	CHB-C4A-NA	2.27	127.67	124.40
38	X	608	CHL	C1-C2-C3	-2.27	122.48	126.20
35	8	619	LUT	C30-C31-C32	-2.27	116.63	123.20
38	U	601	CHL	C4C-CHD-C1D	2.27	124.18	116.07
38	Y	606	CHL	C1A-CHA-CBD	2.27	138.16	132.36
27	G	204	CLA	CHB-C4A-NA	2.27	127.67	124.40
27	K	203	CLA	CHB-C4A-NA	2.27	127.67	124.40
30	3	622	BCR	C38-C26-C27	2.26	118.42	113.60
30	L	309	BCR	C2-C3-C4	-2.26	106.30	111.28
36	Y	1622	XAT	C26-C27-C28	-2.26	121.21	125.99
30	O	2005	BCR	C15-C14-C13	-2.26	124.10	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	F	305	BCR	C32-C1-C6	-2.26	106.69	110.24
38	U	601	CHL	O2D-CGD-O1D	-2.26	119.44	123.85
30	A	850	BCR	C16-C15-C14	-2.26	118.89	123.52
35	W	1621	LUT	C15-C35-C34	-2.26	118.89	123.52
27	X	614	CLA	CHB-C4A-NA	2.26	127.67	124.40
30	B	848	BCR	C11-C10-C9	-2.26	124.11	127.28
35	3	618	LUT	C38-C25-C24	-2.26	118.01	123.36
38	W	606	CHL	O1D-CGD-CBD	-2.26	121.29	124.72
36	7	620	XAT	C32-C33-C34	-2.26	115.45	119.01
38	Z	608	CHL	O1D-CGD-CBD	-2.26	121.29	124.72
27	W	611	CLA	C3B-C4B-NB	-2.26	108.51	110.53
27	B	838	CLA	CHB-C4A-NA	2.26	127.66	124.40
27	9	614	CLA	CHB-C4A-NA	2.26	127.66	124.40
36	8	620	XAT	C24-C23-C22	-2.26	106.56	110.79
38	Z	605	CHL	C3D-CAD-CBD	2.26	110.58	107.61
36	3	619	XAT	C27-C28-C29	-2.26	122.02	125.53
27	4	610	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
27	B	816	CLA	O2D-CGD-CBD	2.26	115.18	111.23
37	5	624	NEX	C24-C23-C22	-2.26	106.56	110.79
33	4	623	LMG	O6-C5-C6	2.26	112.04	106.44
27	1	609	CLA	CMB-C2B-C3B	2.26	129.53	123.53
30	O	2005	BCR	C37-C22-C21	-2.26	119.16	122.82
27	5	604	CLA	CHB-C4A-NA	2.26	127.66	124.40
38	Y	609	CHL	C7-C6-C5	-2.26	107.25	113.26
27	5	609	CLA	C3B-C4B-NB	-2.26	108.52	110.53
27	K	206	CLA	CHB-C4A-NA	2.26	127.66	124.40
36	7	620	XAT	C28-C29-C30	-2.26	115.46	119.01
27	X	613	CLA	C6-C5-C3	2.26	118.96	113.47
30	A	849	BCR	C1-C6-C5	-2.26	119.55	122.64
36	a	618	XAT	C15-C35-C34	-2.25	118.91	123.52
27	Z	604	CLA	C3B-C4B-NB	-2.25	108.52	110.53
30	A	851	BCR	C27-C26-C25	-2.25	119.66	122.70
30	3	622	BCR	C2-C1-C6	2.25	113.71	110.44
27	4	606	CLA	CHB-C4A-NA	2.25	127.65	124.40
28	B	842	PQN	C16-C17-C18	-2.25	108.47	115.97
35	Y	1621	LUT	C31-C30-C29	-2.25	124.12	127.28
35	V	1621	LUT	C15-C14-C13	-2.25	124.12	127.28
36	U	1622	XAT	C31-C32-C33	-2.25	120.19	126.36
36	7	620	XAT	C27-C28-C29	-2.25	122.03	125.53
27	9	604	CLA	CMB-C2B-C3B	2.25	129.52	123.53
30	A	848	BCR	C33-C5-C6	-2.25	122.03	124.48
30	4	621	BCR	C24-C25-C26	-2.25	116.37	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	621	BCR	C15-C16-C17	-2.25	118.91	123.52
30	L	309	BCR	C1-C6-C7	2.25	121.76	115.65
27	B	814	CLA	C1-C2-C3	-2.25	122.51	126.20
27	B	833	CLA	C4-C3-C5	2.25	119.14	115.23
27	B	811	CLA	O1D-CGD-CBD	2.25	127.70	120.19
27	9	610	CLA	CHB-C4A-NA	2.25	127.65	124.40
27	8	613	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
27	A	820	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
27	A	837	CLA	CHB-C4A-NA	2.25	127.64	124.40
27	2	604	CLA	CHB-C4A-NA	2.25	127.64	124.40
27	Y	610	CLA	CHB-C4A-NA	2.25	127.64	124.40
29	a	620	LHG	O8-C23-C24	2.25	118.69	111.83
27	8	601	CLA	CHB-C4A-NA	2.25	127.64	124.40
27	8	606	CLA	CHB-C4A-NA	2.25	127.64	124.40
27	1	607	CLA	CAA-C2A-C3A	-2.25	111.08	116.23
27	4	602	CLA	C3B-C4B-NB	-2.25	108.53	110.53
30	L	301	BCR	C29-C28-C27	-2.24	106.34	111.28
30	6	622	BCR	C29-C30-C25	2.24	113.70	110.44
35	X	1621	LUT	C31-C30-C29	-2.24	124.13	127.28
27	7	608	CLA	CHB-C4A-NA	2.24	127.64	124.40
30	B	845	BCR	C33-C5-C4	2.24	118.38	113.60
27	Y	613	CLA	C6-C5-C3	2.24	118.93	113.47
27	X	603	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
27	B	838	CLA	C3B-C4B-NB	-2.24	108.53	110.53
27	B	809	CLA	CHB-C4A-NA	2.24	127.63	124.40
36	V	1622	XAT	C18-C5-C4	2.24	116.76	114.24
30	B	801	BCR	C27-C26-C25	-2.24	119.68	122.70
27	A	805	CLA	C3B-C4B-NB	-2.24	108.53	110.53
27	1	614	CLA	CAB-C3B-C2B	2.24	129.48	123.53
30	5	622	BCR	C32-C1-C6	-2.24	106.73	110.24
38	Y	607	CHL	CAC-C3C-C4C	2.24	129.78	124.03
30	B	848	BCR	C37-C22-C21	-2.24	119.19	122.82
27	a	616	CLA	CHB-C4A-NA	2.24	127.63	124.40
27	Y	604	CLA	C1-C2-C3	-2.24	123.14	126.76
27	B	833	CLA	CHD-C1D-ND	-2.24	121.65	124.80
27	B	833	CLA	C3B-C4B-NB	-2.24	108.53	110.53
27	a	607	CLA	C3B-C4B-NB	-2.24	108.53	110.53
27	3	609	CLA	CAC-C3C-C4C	2.24	127.70	124.79
35	X	1621	LUT	C3-C4-C5	-2.24	106.61	112.18
38	W	601	CHL	C6-C7-C8	-2.24	108.53	115.97
29	1	620	LHG	O8-C23-C24	2.24	118.65	111.83
27	Y	611	CLA	C3B-C4B-NB	-2.23	108.53	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	834	CLA	CHD-C1D-ND	-2.23	121.66	124.80
30	F	305	BCR	C8-C7-C6	-2.23	121.03	127.00
30	K	202	BCR	C30-C25-C24	2.23	121.71	115.65
27	A	822	CLA	C3B-C4B-NB	-2.23	108.54	110.53
27	1	608	CLA	C3B-C4B-NB	-2.23	108.54	110.53
30	A	852	BCR	C33-C5-C4	2.23	118.36	113.60
38	Y	605	CHL	CAC-C3C-C4C	2.23	129.77	124.03
27	U	603	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
27	X	604	CLA	CHB-C4A-NA	2.23	127.62	124.40
30	J	102	BCR	C30-C25-C24	2.23	121.70	115.65
27	A	843	CLA	C1-C2-C3	-2.23	122.54	126.20
33	H	205	LMG	O8-C28-C29	2.23	118.63	111.83
30	B	844	BCR	C29-C28-C27	-2.23	106.38	111.28
38	W	607	CHL	O2D-CGD-O1D	-2.23	119.51	123.85
30	L	301	BCR	C10-C11-C12	-2.23	116.74	123.20
27	A	822	CLA	C7-C6-C5	-2.23	107.32	113.26
27	B	802	CLA	CHB-C4A-NA	2.23	127.61	124.40
32	8	625	LMU	C1B-O1B-C4'	-2.23	112.70	117.98
27	4	601	CLA	C1-C2-C3	-2.23	122.55	126.20
27	Y	603	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
30	3	622	BCR	C1-C6-C7	2.23	121.69	115.65
27	A	821	CLA	C3B-C4B-NB	-2.23	108.54	110.53
30	O	2004	BCR	C32-C1-C6	-2.23	106.75	110.24
27	2	601	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
27	B	817	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
27	4	608	CLA	CHB-C4A-NA	2.23	127.61	124.40
27	Y	614	CLA	CHB-C4A-NA	2.23	127.61	124.40
36	1	618	XAT	C15-C35-C34	-2.23	118.97	123.52
27	3	611	CLA	CMB-C2B-C3B	2.23	129.45	123.53
27	B	834	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
35	5	620	LUT	C11-C10-C9	-2.23	124.16	127.28
38	Y	606	CHL	C3D-CAD-CBD	2.23	110.53	107.61
30	F	305	BCR	C37-C22-C21	-2.23	119.21	122.82
36	V	1622	XAT	C11-C10-C9	-2.22	124.16	127.28
32	5	628	LMU	C1B-O1B-C4'	-2.22	112.70	117.98
35	V	1620	LUT	C1-C6-C5	-2.22	119.60	122.64
27	B	813	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
36	Y	1622	XAT	C31-C32-C33	-2.22	120.26	126.36
38	Y	601	CHL	C4C-CHD-C1D	2.22	124.03	116.07
27	W	603	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
27	V	611	CLA	CHB-C4A-NA	2.22	127.61	124.40
27	7	601	CLA	C4-C3-C2	-2.22	117.92	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	X	605	CHL	CAC-C3C-C4C	2.22	129.74	124.03
36	2	620	XAT	C24-C23-C22	-2.22	106.64	110.79
35	6	619	LUT	C3-C4-C5	-2.22	106.65	112.18
30	B	846	BCR	C33-C5-C6	-2.22	122.06	124.48
36	Z	1622	XAT	C18-C5-C4	2.22	116.73	114.24
27	3	611	CLA	CHB-C4A-NA	2.22	127.60	124.40
27	Z	604	CLA	CHB-C4A-NA	2.22	127.60	124.40
37	6	624	NEX	C24-C23-C22	-2.22	106.64	110.79
27	W	611	CLA	CAA-CBA-CGA	-2.22	106.91	113.21
27	U	612	CLA	C3B-C4B-NB	-2.22	108.55	110.53
38	Z	605	CHL	CAC-C3C-C4C	2.22	129.73	124.03
27	A	832	CLA	C1-C2-C3	-2.22	123.17	126.76
38	W	608	CHL	O2A-CGA-CBA	2.22	120.52	112.14
27	B	829	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
30	F	305	BCR	C36-C18-C19	2.22	121.48	118.09
30	B	845	BCR	C15-C16-C17	-2.22	118.98	123.52
33	4	624	LMG	C8-O7-C10	-2.22	112.49	117.80
27	B	820	CLA	C3B-C4B-NB	-2.22	108.55	110.53
27	9	603	CLA	CAB-C3B-C2B	2.21	129.42	123.53
27	B	821	CLA	C3B-C4B-NB	-2.21	108.55	110.53
27	U	611	CLA	C3B-C4B-NB	-2.21	108.55	110.53
36	Y	1622	XAT	C12-C13-C14	-2.21	115.53	119.01
36	8	620	XAT	C38-C25-C24	2.21	116.73	114.24
27	A	815	CLA	C3B-C4B-NB	-2.21	108.55	110.53
27	A	833	CLA	C3B-C4B-NB	-2.21	108.55	110.53
27	K	201	CLA	CHB-C4A-NA	2.21	127.59	124.40
27	L	307	CLA	C3B-C4B-NB	-2.21	108.56	110.53
27	A	840	CLA	CHB-C4A-NA	2.21	127.59	124.40
27	5	618	CLA	CHB-C4A-NA	2.21	127.59	124.40
36	5	621	XAT	C30-C31-C32	-2.21	116.79	123.20
27	3	614	CLA	CHB-C4A-NA	2.21	127.59	124.40
30	B	845	BCR	C8-C9-C10	2.21	122.49	119.01
27	3	608	CLA	C3B-C4B-NB	-2.21	108.56	110.53
27	5	603	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
27	6	601	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
27	A	824	CLA	CHB-C4A-NA	2.21	127.59	124.40
27	B	829	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
27	6	610	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
27	a	606	CLA	CHB-C4A-NA	2.21	127.59	124.40
27	4	608	CLA	C3B-C4B-NB	-2.21	108.56	110.53
30	O	2005	BCR	C11-C12-C13	-2.21	120.31	126.36
27	A	842	CLA	CHB-C4A-NA	2.21	127.59	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	832	CLA	CHB-C4A-NA	2.21	127.59	124.40
29	V	2630	LHG	O8-C23-O10	-2.21	118.11	123.63
27	2	613	CLA	CHB-C4A-NA	2.21	127.58	124.40
36	4	620	XAT	C18-C5-C4	2.21	116.72	114.24
30	B	849	BCR	C31-C1-C6	-2.21	106.78	110.24
35	Y	1621	LUT	C15-C14-C13	-2.21	124.18	127.28
27	a	608	CLA	C3B-C4B-NB	-2.21	108.56	110.53
27	5	613	CLA	C3B-C4B-NB	-2.21	108.56	110.53
27	6	617	CLA	C3B-C4B-NB	-2.21	108.56	110.53
38	Z	607	CHL	O2D-CGD-O1D	-2.21	119.56	123.85
27	1	606	CLA	CHB-C4A-NA	2.21	127.58	124.40
29	6	623	LHG	O8-C23-C24	2.20	118.56	111.83
27	4	610	CLA	C3B-C4B-NB	-2.20	108.56	110.53
30	B	846	BCR	C2-C1-C6	2.20	113.64	110.44
30	3	621	BCR	C11-C12-C13	-2.20	120.32	126.36
36	9	620	XAT	C35-C34-C33	-2.20	124.19	127.28
38	W	601	CHL	O2D-CGD-O1D	-2.20	119.56	123.85
27	O	2001	CLA	C3B-C4B-NB	-2.20	108.56	110.53
35	Y	1621	LUT	C3-C4-C5	-2.20	106.69	112.18
30	7	623	BCR	C30-C25-C26	-2.20	119.62	122.64
30	A	850	BCR	C7-C6-C5	-2.20	116.48	121.56
35	9	619	LUT	C40-C33-C32	2.20	121.45	118.09
38	V	607	CHL	CAA-C2A-C3A	2.20	118.95	113.00
27	1	613	CLA	C3B-C4B-NB	-2.20	108.56	110.53
27	4	604	CLA	CMB-C2B-C3B	2.20	129.38	123.53
27	B	827	CLA	C3B-C4B-NB	-2.20	108.57	110.53
27	9	604	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
27	5	616	CLA	CBD-CHA-C1A	2.20	131.66	127.58
27	A	828	CLA	O2D-CGD-CBD	2.20	115.08	111.23
36	4	620	XAT	C4-C3-C2	-2.20	106.68	110.79
37	5	624	NEX	C8-C7-C6	-2.20	175.07	177.66
27	3	607	CLA	O2D-CGD-CBD	2.20	115.07	111.23
27	5	610	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
27	Z	602	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
27	1	614	CLA	CHB-C4A-NA	2.20	127.55	124.43
30	F	305	BCR	C35-C13-C12	2.20	121.44	118.09
27	1	616	CLA	CHB-C4A-NA	2.20	127.57	124.40
27	1	607	CLA	C3B-C4B-NB	-2.20	108.57	110.53
27	5	611	CLA	C3B-C4B-NB	-2.20	108.57	110.53
35	Y	1621	LUT	O23-C23-C22	-2.20	106.17	110.06
35	5	620	LUT	C12-C13-C14	-2.19	115.56	119.01
27	A	824	CLA	C4-C3-C5	2.19	119.04	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	X	608	CHL	OMC-CMC-C2C	-2.19	121.31	125.12
30	A	851	BCR	C11-C10-C9	-2.19	124.20	127.28
38	X	601	CHL	C4C-CHD-C1D	2.19	123.92	116.07
27	A	818	CLA	CMB-C2B-C3B	2.19	131.71	126.55
27	B	804	CLA	C3B-C4B-NB	-2.19	108.57	110.53
27	F	303	CLA	CHB-C4A-NA	2.19	127.56	124.40
36	5	621	XAT	C4-C3-C2	-2.19	106.69	110.79
27	1	602	CLA	C1-C2-C3	-2.19	122.61	126.20
27	7	611	CLA	C3B-C4B-NB	-2.19	108.57	110.53
27	V	614	CLA	O2A-CGA-O1A	-2.19	117.69	123.33
27	A	801	CLA	C1D-ND-C4D	-2.19	104.77	106.31
30	6	622	BCR	C15-C14-C13	-2.19	124.20	127.28
36	X	1622	XAT	C31-C32-C33	-2.19	120.35	126.36
27	a	603	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
38	Z	606	CHL	C1A-CHA-CBD	2.19	137.97	132.36
35	8	619	LUT	C35-C34-C33	-2.19	124.20	127.28
35	3	618	LUT	C30-C31-C32	-2.19	116.85	123.20
27	7	601	CLA	CHB-C4A-NA	2.19	127.56	124.40
30	L	301	BCR	C24-C23-C22	-2.19	123.00	126.23
27	B	807	CLA	C3B-C4B-NB	-2.19	108.58	110.53
27	3	613	CLA	C1-C2-C3	-2.19	122.61	126.20
27	B	822	CLA	O2D-CGD-CBD	2.19	115.06	111.23
35	9	619	LUT	C8-C7-C6	-2.19	121.15	127.00
30	2	623	BCR	C11-C12-C13	-2.19	120.36	126.36
27	A	839	CLA	CHB-C4A-NA	2.19	127.56	124.40
33	4	624	LMG	C3-C4-C5	2.19	114.20	110.23
27	A	828	CLA	CHB-C4A-NA	2.19	127.56	124.40
27	B	819	CLA	CHB-C4A-NA	2.19	127.56	124.40
27	Z	611	CLA	C3B-C4B-NB	-2.18	108.58	110.53
27	A	842	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
36	a	618	XAT	C19-C9-C8	2.18	121.42	118.09
27	W	612	CLA	C3B-C4B-NB	-2.18	108.58	110.53
27	A	833	CLA	CBA-CAA-C2A	2.18	120.29	113.79
27	8	604	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
27	1	603	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
27	A	826	CLA	C3B-C4B-NB	-2.18	108.58	110.53
27	9	601	CLA	CHB-C4A-NA	2.18	127.55	124.40
30	B	801	BCR	C24-C25-C26	2.18	126.58	121.56
35	X	1621	LUT	C18-C5-C6	-2.18	122.11	124.48
27	A	831	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
35	Z	1621	LUT	C35-C34-C33	-2.18	124.22	127.28
27	A	831	CLA	CHB-C4A-NA	2.18	127.55	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	Z	1621	LUT	O23-C23-C22	-2.18	106.19	110.06
38	Z	605	CHL	O2D-CGD-O1D	-2.18	119.61	123.85
27	8	608	CLA	C3B-C4B-NB	-2.18	108.59	110.53
38	W	601	CHL	C4C-CHD-C1D	2.18	123.86	116.07
27	6	614	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
27	5	619	CLA	CMB-C2B-C3B	2.18	129.32	123.53
38	Z	606	CHL	O2D-CGD-O1D	-2.18	119.61	123.85
33	8	626	LMG	O3-C3-C2	-2.18	105.24	110.38
38	U	601	CHL	CBC-CAC-C3C	-2.18	109.76	112.87
27	B	802	CLA	C3B-C4B-NB	-2.18	108.59	110.53
36	8	620	XAT	C30-C31-C32	-2.17	116.90	123.20
38	W	606	CHL	C1B-CHB-C4A	-2.17	119.92	121.32
30	L	301	BCR	C12-C13-C14	-2.17	115.59	119.01
38	Y	605	CHL	C3D-CAD-CBD	2.17	110.47	107.61
27	B	833	CLA	O2D-CGD-CBD	2.17	115.03	111.23
30	B	848	BCR	C12-C13-C14	-2.17	115.59	119.01
35	8	619	LUT	C28-C29-C30	-2.17	115.59	119.01
30	A	849	BCR	C16-C15-C14	-2.17	119.07	123.52
37	5	624	NEX	C16-C1-C6	-2.17	108.53	110.47
36	8	620	XAT	C8-C9-C10	-2.17	115.59	119.01
30	B	846	BCR	C38-C26-C27	2.17	118.23	113.60
36	1	618	XAT	C19-C9-C8	2.17	121.41	118.09
27	6	616	CLA	C4-C3-C5	2.17	119.00	115.23
32	5	629	LMU	C1B-C2B-C3B	2.17	114.58	110.01
27	6	609	CLA	C3B-C4B-NB	-2.17	108.59	110.53
35	1	617	LUT	C38-C25-C24	-2.17	118.22	123.36
35	Z	1620	LUT	C30-C31-C32	-2.17	116.91	123.20
27	A	811	CLA	O1D-CGD-CBD	2.17	128.80	124.52
38	X	607	CHL	CAC-C3C-C4C	2.17	129.61	124.03
38	X	607	CHL	O2D-CGD-O1D	-2.17	119.62	123.85
27	B	839	CLA	CHB-C4A-NA	2.17	127.53	124.40
30	L	305	BCR	C24-C23-C22	-2.17	123.03	126.23
27	B	807	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
27	B	825	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
27	3	606	CLA	C3B-C4B-NB	-2.17	108.59	110.53
38	Z	608	CHL	O2D-CGD-O1D	-2.17	119.63	123.85
27	6	613	CLA	CHB-C4A-NA	2.17	127.53	124.40
27	A	801	CLA	CBA-CAA-C2A	-2.17	107.35	113.79
30	B	847	BCR	C36-C18-C17	-2.17	119.31	122.82
35	Y	1621	LUT	C18-C5-C6	-2.17	122.12	124.48
27	a	614	CLA	CHB-C4A-NA	2.17	127.51	124.43
27	B	811	CLA	CHB-C4A-NA	2.16	127.52	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	845	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
30	J	102	BCR	C33-C5-C6	-2.16	122.12	124.48
27	6	601	CLA	C6-C5-C3	-2.16	108.19	113.47
35	a	617	LUT	C38-C25-C24	-2.16	118.24	123.36
36	7	620	XAT	C30-C31-C32	-2.16	116.93	123.20
27	Z	613	CLA	CHB-C4A-NA	2.16	127.52	124.40
30	4	621	BCR	C11-C12-C13	-2.16	120.43	126.36
27	7	609	CLA	CBD-CHA-C1A	2.16	131.59	127.58
36	X	1622	XAT	C12-C13-C14	-2.16	115.61	119.01
27	Y	604	CLA	CHB-C4A-NA	2.16	127.52	124.40
30	F	305	BCR	C7-C8-C9	-2.16	123.04	126.23
27	B	827	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
27	B	837	CLA	O2D-CGD-CBD	2.16	115.01	111.23
30	4	621	BCR	C4-C5-C6	-2.16	119.78	122.70
27	a	602	CLA	C1-C2-C3	-2.16	122.66	126.20
35	X	1621	LUT	O23-C23-C22	-2.16	106.23	110.06
35	V	1620	LUT	C15-C14-C13	-2.16	124.25	127.28
27	K	203	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
38	Z	608	CHL	CAC-C3C-C4C	2.16	129.58	124.03
30	B	846	BCR	C37-C22-C21	-2.16	119.32	122.82
27	B	826	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
27	X	613	CLA	CHB-C4A-NA	2.16	127.51	124.40
27	X	611	CLA	O1A-CGA-CBA	2.16	129.93	123.09
27	A	832	CLA	CHB-C4A-NA	2.16	127.51	124.40
27	a	601	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
30	J	102	BCR	C15-C14-C13	-2.16	124.25	127.28
38	X	605	CHL	C3D-CAD-CBD	2.16	110.44	107.61
27	A	831	CLA	CMB-C2B-C1B	-2.16	122.14	125.42
27	5	601	CLA	C4-C3-C5	2.16	118.97	115.23
35	6	619	LUT	C22-C23-C24	2.15	114.38	111.18
27	4	614	CLA	CHB-C4A-NA	2.15	127.51	124.40
38	U	607	CHL	O2A-CGA-O1A	-2.15	117.80	123.33
36	a	618	XAT	C32-C33-C34	-2.15	115.62	119.01
27	1	601	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
38	Z	609	CHL	C1-O2A-CGA	2.15	121.86	116.65
37	W	1623	NEX	O24-C25-C26	-2.15	57.22	58.93
27	A	838	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
27	V	613	CLA	C3B-C4B-NB	-2.15	108.61	110.53
30	6	622	BCR	C36-C18-C17	-2.15	119.33	122.82
27	A	801	CLA	CHB-C4A-NA	2.15	127.50	124.40
36	9	620	XAT	C24-C23-C22	-2.15	106.77	110.79
27	B	838	CLA	O2D-CGD-CBD	2.15	114.99	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	623	BCR	C33-C5-C4	2.15	118.18	113.60
27	A	823	CLA	C3B-C4B-NB	-2.15	108.61	110.53
27	7	601	CLA	C3B-C4B-NB	-2.15	108.61	110.53
27	X	611	CLA	C3B-C4B-NB	-2.15	108.61	110.53
27	3	602	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
27	2	601	CLA	O1D-CGD-CBD	2.15	128.76	124.52
35	4	619	LUT	C11-C10-C9	-2.15	124.26	127.28
30	4	621	BCR	C30-C25-C24	2.15	121.48	115.65
27	B	823	CLA	CHB-C4A-NA	2.15	127.50	124.40
27	7	616	CLA	CHB-C4A-NA	2.15	127.50	124.40
36	8	620	XAT	C31-C30-C29	-2.15	124.27	127.28
27	B	807	CLA	CHB-C4A-NA	2.15	127.50	124.40
27	F	301	CLA	CHB-C4A-NA	2.15	127.50	124.40
27	A	801	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
27	3	603	CLA	O1D-CGD-CBD	2.15	128.75	124.52
36	7	620	XAT	C8-C9-C10	-2.15	115.63	119.01
27	B	818	CLA	O2D-CGD-CBD	2.15	114.98	111.23
27	7	613	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
36	1	618	XAT	C32-C33-C34	-2.15	115.63	119.01
27	A	823	CLA	CHB-C4A-NA	2.15	127.50	124.40
27	A	854	CLA	C11-C10-C8	-2.15	108.83	115.97
36	6	621	XAT	C19-C9-C8	2.15	121.37	118.09
35	6	619	LUT	C11-C10-C9	-2.15	124.27	127.28
27	V	613	CLA	C1-C2-C3	-2.15	122.68	126.20
27	G	204	CLA	C3B-C4B-NB	-2.15	108.61	110.53
27	7	604	CLA	C1-C2-C3	-2.14	122.68	126.20
30	L	305	BCR	C4-C5-C6	-2.14	119.81	122.70
38	Z	606	CHL	C1B-CHB-C4A	-2.14	119.94	121.32
37	Y	1623	NEX	C18-C5-C4	-2.14	108.06	111.51
27	Y	613	CLA	CHB-C4A-NA	2.14	127.49	124.40
30	A	850	BCR	C1-C6-C5	-2.14	119.71	122.64
37	6	624	NEX	C28-C29-C30	2.14	122.38	119.01
30	3	621	BCR	C15-C16-C17	-2.14	119.13	123.52
30	L	301	BCR	C37-C22-C21	-2.14	119.34	122.82
27	B	819	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
27	3	610	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
27	A	811	CLA	C3B-C4B-NB	-2.14	108.62	110.53
27	A	843	CLA	CHB-C4A-NA	2.14	127.49	124.40
27	B	813	CLA	CHB-C4A-NA	2.14	127.49	124.40
36	Z	1622	XAT	C32-C33-C34	-2.14	115.64	119.01
30	3	622	BCR	C37-C22-C21	-2.14	119.34	122.82
38	Z	601	CHL	C4C-CHD-C1D	2.14	123.73	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	207	BCR	C2-C1-C6	2.14	113.55	110.44
27	H	202	CLA	CHB-C4A-NA	2.14	127.49	124.40
37	Z	1623	NEX	C40-C33-C32	2.14	121.36	118.09
27	Y	604	CLA	C3B-C4B-NB	-2.14	108.62	110.53
27	a	606	CLA	CBD-CHA-C1A	2.14	131.55	127.58
38	X	608	CHL	C4C-CHD-C1D	2.14	123.72	116.07
35	1	617	LUT	C11-C10-C9	-2.14	124.28	127.28
32	5	628	LMU	O5'-C1'-C2'	2.14	114.77	110.37
27	2	610	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
38	V	605	CHL	O2D-CGD-O1D	-2.14	119.69	123.85
30	F	305	BCR	C23-C24-C25	-2.14	121.29	127.00
27	B	840	CLA	CHB-C4A-NA	2.14	127.48	124.40
30	A	849	BCR	C36-C18-C17	-2.14	119.35	122.82
27	6	610	CLA	CHB-C4A-NA	2.14	127.48	124.40
38	Z	609	CHL	C11-C12-C13	-2.14	108.86	115.97
28	B	842	PQN	C11-C3-C4	-2.14	116.33	118.58
30	7	623	BCR	C7-C8-C9	-2.14	123.07	126.23
27	5	604	CLA	O2D-CGD-CBD	2.14	114.97	111.23
30	K	202	BCR	C23-C24-C25	-2.14	121.29	127.00
30	L	301	BCR	C34-C9-C8	2.14	121.35	118.09
27	8	616	CLA	O2D-CGD-CBD	2.14	114.96	111.23
38	V	601	CHL	O1D-CGD-CBD	-2.14	121.48	124.72
27	A	842	CLA	C3B-C4B-NB	-2.14	108.62	110.53
38	X	608	CHL	C4-C3-C5	2.14	118.93	115.23
27	7	613	CLA	CHD-C1D-ND	-2.13	121.80	124.80
38	W	601	CHL	CED-O2D-CGD	2.13	120.76	115.92
30	F	305	BCR	C20-C19-C18	-2.13	120.51	126.36
27	5	602	CLA	O2D-CGD-CBD	2.13	114.96	111.23
35	W	1621	LUT	C21-C26-C27	-2.13	110.37	112.83
27	9	610	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
27	B	830	CLA	CHD-C1D-ND	-2.13	121.80	124.80
30	6	622	BCR	C23-C22-C21	-2.13	115.66	119.01
38	V	609	CHL	CMA-C3A-C4A	-2.13	110.02	114.61
35	U	1621	LUT	C21-C26-C27	-2.13	110.38	112.83
27	A	808	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
27	5	601	CLA	C1-C2-C3	-2.13	122.71	126.20
38	U	608	CHL	O1D-CGD-CBD	-2.13	121.49	124.72
27	A	828	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
27	4	616	CLA	CHB-C4A-NA	2.13	127.47	124.40
27	A	836	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
27	1	613	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
27	9	602	CLA	CMB-C2B-C3B	2.13	131.56	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	X	607	CHL	C11-C12-C13	-2.13	108.89	115.97
30	J	102	BCR	C38-C26-C27	2.13	118.14	113.60
27	A	824	CLA	C1-C2-C3	-2.13	122.71	126.20
27	6	602	CLA	O2D-CGD-CBD	2.13	114.95	111.23
27	7	604	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
38	X	607	CHL	C6-C5-C3	-2.13	108.29	113.47
32	5	628	LMU	O5B-C1B-C2B	2.13	114.74	110.37
30	B	846	BCR	C19-C18-C17	-2.13	115.67	119.01
27	B	805	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
37	6	624	NEX	C35-C15-C14	-2.12	119.17	123.52
27	B	837	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
27	8	603	CLA	CMB-C2B-C3B	2.12	129.18	123.53
27	L	302	CLA	O2D-CGD-CBD	2.12	114.94	111.23
27	X	604	CLA	C3B-C4B-NB	-2.12	108.63	110.53
27	9	613	CLA	CHB-C4A-NA	2.12	127.46	124.40
27	B	818	CLA	C6-C5-C3	2.12	118.64	113.47
27	2	606	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
27	a	613	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
27	5	601	CLA	CAA-C2A-C3A	-2.12	107.27	113.00
38	X	609	CHL	CAC-C3C-C4C	2.12	129.48	124.03
27	A	819	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
36	8	620	XAT	C15-C35-C34	-2.12	119.18	123.52
27	4	613	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
38	W	608	CHL	O1D-CGD-CBD	-2.12	121.51	124.72
30	B	848	BCR	C10-C11-C12	-2.12	117.06	123.20
36	3	619	XAT	C35-C15-C14	-2.12	119.19	123.52
35	Z	1621	LUT	C27-C28-C29	-2.12	121.77	126.32
38	V	609	CHL	C4C-CHD-C1D	2.12	123.65	116.07
33	A	860	LMG	C7-O1-C1	-2.12	109.26	113.80
37	6	624	NEX	C27-C28-C29	-2.12	122.25	125.53
27	5	603	CLA	CHB-C4A-NA	2.12	127.45	124.40
27	3	612	CLA	CMB-C2B-C1B	-2.12	122.20	125.42
36	U	1622	XAT	C16-C1-C2	-2.12	105.25	108.97
38	V	607	CHL	O2D-CGD-O1D	-2.12	119.73	123.85
35	7	619	LUT	C11-C10-C9	-2.12	124.31	127.28
38	Z	607	CHL	CAC-C3C-C4C	2.12	129.47	124.03
36	W	1622	XAT	C16-C1-C2	-2.12	105.25	108.97
30	K	202	BCR	C37-C22-C21	-2.12	119.39	122.82
35	V	1621	LUT	C31-C30-C29	-2.11	124.31	127.28
27	3	610	CLA	CMB-C2B-C3B	2.11	131.52	126.55
38	U	606	CHL	C1B-CHB-C4A	-2.11	119.96	121.32
35	Z	1621	LUT	C15-C14-C13	-2.11	124.31	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	6	616	CLA	C6-C5-C3	2.11	118.62	113.47
27	L	303	CLA	CHD-C1D-ND	-2.11	121.83	124.80
37	5	624	NEX	C10-C11-C12	-2.11	117.08	123.20
30	2	623	BCR	C30-C25-C24	2.11	121.38	115.65
38	Z	607	CHL	C4C-CHD-C1D	2.11	123.63	116.07
38	W	601	CHL	CMA-C3A-C4A	-2.11	110.06	114.61
27	A	808	CLA	C3B-C4B-NB	-2.11	108.64	110.53
27	7	613	CLA	C3B-C4B-NB	-2.11	108.64	110.53
38	Y	607	CHL	C4C-CHD-C1D	2.11	123.63	116.07
27	5	613	CLA	CHD-C1D-ND	-2.11	121.83	124.80
27	6	603	CLA	CMB-C2B-C3B	2.11	129.15	123.53
30	G	205	BCR	C37-C22-C21	-2.11	119.40	122.82
36	a	618	XAT	C35-C34-C33	-2.11	124.32	127.28
36	5	621	XAT	C36-C21-C22	-2.11	105.26	108.97
27	3	608	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
27	B	821	CLA	CHB-C4A-NA	2.11	127.44	124.40
27	A	854	CLA	C6-C7-C8	-2.11	108.95	115.97
30	L	309	BCR	C29-C28-C27	-2.11	106.64	111.28
30	B	847	BCR	C11-C10-C9	-2.11	124.32	127.28
27	A	813	CLA	C3B-C4B-NB	-2.11	108.65	110.53
38	U	607	CHL	CBC-CAC-C3C	-2.11	109.86	112.87
29	3	624	LHG	O8-C23-C24	2.11	118.26	111.83
27	B	814	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
30	L	301	BCR	C16-C17-C18	-2.11	124.32	127.28
30	L	309	BCR	C23-C24-C25	-2.11	121.37	127.00
27	9	613	CLA	C3B-C4B-NB	-2.11	108.65	110.53
27	7	615	CLA	CHB-C4A-NA	2.11	127.44	124.40
30	B	853	BCR	C32-C1-C6	-2.11	106.94	110.24
35	Y	1620	LUT	C12-C13-C14	-2.11	115.70	119.01
35	Z	1621	LUT	C35-C15-C14	-2.11	119.21	123.52
27	1	602	CLA	O1D-CGD-CBD	2.11	128.67	124.52
27	7	609	CLA	C3B-C4B-NB	-2.10	108.65	110.53
27	Z	614	CLA	CHB-C4A-NA	2.10	127.44	124.40
27	L	304	CLA	C3B-C4B-NB	-2.10	108.65	110.53
30	B	843	BCR	C23-C22-C21	-2.10	115.70	119.01
38	W	606	CHL	O2D-CGD-O1D	-2.10	119.75	123.85
27	A	806	CLA	O1D-CGD-CBD	2.10	128.67	124.52
35	Z	1621	LUT	C36-C21-C26	2.10	112.73	109.55
27	5	604	CLA	CMB-C2B-C3B	2.10	129.12	123.53
30	O	2004	BCR	C36-C18-C17	-2.10	119.41	122.82
30	O	2005	BCR	C33-C5-C4	2.10	118.08	113.60
27	V	604	CLA	CHD-C1D-ND	-2.10	121.84	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	5	620	LUT	C39-C29-C28	2.10	121.30	118.09
38	W	607	CHL	C4C-CHD-C1D	2.10	123.59	116.07
27	2	610	CLA	C3B-C4B-NB	-2.10	108.66	110.53
37	U	1623	NEX	C15-C35-C34	-2.10	119.22	123.52
27	5	603	CLA	CMB-C2B-C3B	2.10	129.11	123.53
38	Y	607	CHL	O2D-CGD-O1D	-2.10	119.76	123.85
27	4	604	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
27	6	601	CLA	C3B-C4B-NB	-2.10	108.66	110.53
30	B	843	BCR	C7-C6-C5	2.10	126.39	121.56
38	Z	607	CHL	OMC-CMC-C2C	-2.10	121.48	125.12
27	6	604	CLA	C3B-C4B-NB	-2.10	108.66	110.53
30	B	845	BCR	C16-C15-C14	-2.10	119.23	123.52
30	3	621	BCR	C40-C30-C25	-2.10	106.95	110.24
33	V	2631	LMG	C8-O7-C10	-2.10	112.78	117.80
27	A	809	CLA	C3B-C4B-NB	-2.10	108.66	110.53
27	2	614	CLA	C3B-C4B-NB	-2.10	108.66	110.53
30	B	843	BCR	C20-C19-C18	-2.10	120.62	126.36
27	A	825	CLA	O1D-CGD-CBD	2.10	128.65	124.52
30	L	309	BCR	C23-C22-C21	-2.09	115.71	119.01
27	B	812	CLA	O2D-CGD-CBD	2.09	114.89	111.23
38	Y	601	CHL	CED-O2D-CGD	2.09	120.66	115.92
27	8	606	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
27	7	607	CLA	C3B-C4B-NB	-2.09	108.66	110.53
27	Y	604	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
38	U	606	CHL	O2D-CGD-O1D	-2.09	119.78	123.85
33	H	205	LMG	C3-C4-C5	2.09	114.02	110.23
36	3	619	XAT	O4-C5-C6	-2.09	57.27	58.93
35	a	617	LUT	C11-C10-C9	-2.09	124.34	127.28
27	J	101	CLA	O2D-CGD-CBD	2.09	114.89	111.23
38	U	605	CHL	CAC-C3C-C4C	2.09	129.40	124.03
27	4	614	CLA	CHD-C1D-ND	-2.09	121.86	124.80
38	Z	609	CHL	C4C-CHD-C1D	2.09	123.55	116.07
27	6	604	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
30	B	847	BCR	C7-C8-C9	-2.09	123.14	126.23
27	X	604	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
38	V	608	CHL	O1D-CGD-CBD	-2.09	121.56	124.72
27	a	602	CLA	O1D-CGD-CBD	2.09	128.63	124.52
35	2	619	LUT	C38-C25-C24	-2.09	118.42	123.36
33	H	205	LMG	C6-C5-C4	-2.09	107.90	113.02
27	A	811	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
38	V	601	CHL	C4C-CHD-C1D	2.09	123.53	116.07
27	A	840	CLA	O2A-CGA-O1A	-2.09	118.41	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	1623	NEX	C26-C27-C28	-2.09	121.58	125.99
27	1	606	CLA	C2A-C1A-CHA	2.09	125.94	122.71
37	X	1623	NEX	O24-C25-C26	-2.09	57.28	58.93
38	V	606	CHL	O1D-CGD-CBD	-2.09	121.56	124.72
35	V	1620	LUT	C15-C35-C34	-2.08	119.25	123.52
27	A	832	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
35	X	1620	LUT	C12-C13-C14	-2.08	115.73	119.01
30	A	856	BCR	C27-C26-C25	-2.08	119.89	122.70
27	B	832	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
30	O	2004	BCR	C29-C30-C25	2.08	113.46	110.44
35	V	1620	LUT	C30-C31-C32	-2.08	117.17	123.20
27	6	604	CLA	O2D-CGD-CBD	2.08	114.87	111.23
35	4	619	LUT	C40-C33-C32	2.08	121.27	118.09
38	W	605	CHL	CAC-C3C-C4C	2.08	129.38	124.03
27	A	838	CLA	C1-C2-C3	-2.08	123.40	126.76
33	J	104	LMG	O8-C28-O10	-2.08	118.42	123.63
27	B	836	CLA	C3B-C4B-NB	-2.08	108.67	110.53
35	U	1620	LUT	C28-C29-C30	-2.08	115.74	119.01
27	A	834	CLA	C4-C3-C2	-2.08	118.28	123.63
30	B	853	BCR	C21-C20-C19	-2.08	117.17	123.20
38	X	607	CHL	C4C-CHD-C1D	2.08	123.51	116.07
27	V	612	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
36	1	618	XAT	C35-C34-C33	-2.08	124.36	127.28
27	7	611	CLA	O1D-CGD-CBD	2.08	128.62	124.52
27	1	610	CLA	C2A-C1A-CHA	2.08	125.94	122.71
38	W	609	CHL	C4C-CHD-C1D	2.08	123.51	116.07
27	a	609	CLA	CAC-C3C-C4C	2.08	127.49	124.79
36	7	620	XAT	C20-C13-C12	2.08	121.26	118.09
36	3	619	XAT	C32-C33-C34	-2.08	115.74	119.01
27	5	608	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
38	Z	605	CHL	CBC-CAC-C3C	-2.08	109.90	112.87
35	Y	1620	LUT	C15-C35-C34	-2.08	119.27	123.52
27	A	805	CLA	CHD-C1D-ND	-2.08	121.88	124.80
38	X	607	CHL	CED-O2D-CGD	2.08	120.63	115.92
38	U	601	CHL	CED-O2D-CGD	2.08	120.63	115.92
27	Z	613	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
35	1	617	LUT	C8-C9-C10	-2.08	115.74	119.01
27	B	825	CLA	O1D-CGD-CBD	2.08	128.61	124.52
38	U	609	CHL	C4C-CHD-C1D	2.08	123.49	116.07
27	4	609	CLA	C3B-C4B-NB	-2.07	108.68	110.53
36	4	620	XAT	C19-C9-C8	2.07	121.26	118.09
36	a	618	XAT	C30-C31-C32	-2.07	117.19	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	618	XAT	C30-C31-C32	-2.07	117.19	123.20
27	6	616	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
30	B	853	BCR	C37-C22-C21	-2.07	119.46	122.82
27	A	819	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
36	3	619	XAT	C15-C14-C13	-2.07	124.37	127.28
38	X	609	CHL	C4C-CHD-C1D	2.07	123.49	116.07
27	B	820	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
36	4	620	XAT	C39-C29-C28	2.07	121.25	118.09
37	U	1623	NEX	C26-C27-C28	-2.07	121.61	125.99
27	A	843	CLA	CHB-C1B-NB	2.07	127.16	124.05
35	5	620	LUT	C38-C25-C24	-2.07	118.46	123.36
27	A	826	CLA	CHB-C4A-NA	2.07	127.39	124.40
30	7	621	BCR	C3-C4-C5	-2.07	110.36	114.06
27	5	614	CLA	CHB-C4A-NA	2.07	127.37	124.43
36	3	619	XAT	C30-C31-C32	-2.07	117.20	123.20
27	U	604	CLA	O1D-CGD-CBD	2.07	128.56	124.50
27	3	604	CLA	C3B-C4B-NB	-2.07	108.68	110.53
27	B	833	CLA	C4-C3-C2	-2.07	118.31	123.63
27	3	615	CLA	CHB-C4A-NA	2.07	127.39	124.40
27	Z	602	CLA	C1-C2-C3	-2.07	122.81	126.20
27	B	828	CLA	CMB-C2B-C3B	2.07	131.41	126.55
38	Y	609	CHL	C4C-CHD-C1D	2.07	123.47	116.07
29	B	854	LHG	C6-C5-C4	-2.07	106.96	111.78
35	6	619	LUT	C27-C28-C29	-2.07	121.88	126.32
27	1	609	CLA	CAC-C3C-C4C	2.07	127.48	124.79
27	G	204	CLA	O1D-CGD-CBD	2.07	128.60	124.52
27	W	604	CLA	O1D-CGD-CBD	2.07	128.60	124.52
35	X	1620	LUT	C15-C35-C34	-2.07	119.29	123.52
38	Z	607	CHL	C6-C5-C3	-2.07	108.43	113.47
30	3	620	BCR	C27-C26-C25	-2.07	119.91	122.70
27	4	614	CLA	C4-C3-C5	2.07	118.81	115.23
30	B	845	BCR	C23-C22-C21	2.07	122.26	119.01
37	W	1623	NEX	C15-C35-C34	-2.07	119.29	123.52
36	Z	1622	XAT	C35-C34-C33	-2.07	124.38	127.28
27	A	818	CLA	C3B-C4B-NB	-2.07	108.69	110.53
27	Z	603	CLA	C3B-C4B-NB	-2.07	108.69	110.53
27	V	612	CLA	C3B-C4B-NB	-2.07	108.69	110.53
30	A	851	BCR	C3-C4-C5	-2.07	110.37	114.06
27	6	608	CLA	CHD-C1D-ND	-2.07	121.90	124.80
29	1	620	LHG	C5-O7-C7	-2.07	112.85	117.80
27	B	828	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
30	J	102	BCR	C16-C17-C18	-2.06	124.38	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	Y	607	CHL	C11-C12-C13	-2.06	109.11	115.97
27	7	614	CLA	CHB-C4A-NA	2.06	127.38	124.40
27	Y	613	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
30	K	202	BCR	C32-C1-C6	-2.06	107.01	110.24
35	6	619	LUT	C30-C31-C32	-2.06	117.22	123.20
27	A	816	CLA	C3B-C4B-NB	-2.06	108.69	110.53
38	X	609	CHL	C7-C6-C5	-2.06	107.76	113.26
27	A	825	CLA	C1-C2-C3	-2.06	122.82	126.20
38	Y	608	CHL	CAC-C3C-C4C	2.06	129.33	124.03
36	5	621	XAT	C18-C5-C4	2.06	116.56	114.24
27	A	832	CLA	CHD-C1D-ND	-2.06	121.90	124.80
30	B	845	BCR	C11-C12-C13	-2.06	120.71	126.36
27	Y	614	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
27	L	302	CLA	CHD-C1D-ND	-2.06	121.90	124.80
30	B	849	BCR	C33-C5-C6	-2.06	122.24	124.48
38	U	605	CHL	C3D-CAD-CBD	2.06	110.32	107.61
35	Y	1621	LUT	C38-C25-C24	-2.06	118.49	123.36
27	3	607	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
27	9	614	CLA	O2D-CGD-CBD	2.06	114.83	111.23
30	A	849	BCR	C29-C30-C25	2.06	113.43	110.44
27	V	612	CLA	O1D-CGD-CBD	2.06	128.58	124.52
30	G	205	BCR	C28-C27-C26	-2.06	110.39	114.06
27	A	814	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
35	Y	1621	LUT	C27-C28-C29	-2.06	121.90	126.32
27	K	204	CLA	O2A-CGA-O1A	-2.06	118.04	123.33
27	9	613	CLA	CHD-C1D-ND	-2.06	121.91	124.80
36	9	620	XAT	C30-C31-C32	-2.06	117.24	123.20
27	A	818	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
27	W	613	CLA	C6-C5-C3	2.05	118.47	113.47
35	Z	1621	LUT	C38-C25-C24	-2.05	118.50	123.36
27	a	607	CLA	O2A-CGA-O1A	-2.05	118.05	123.33
30	7	621	BCR	C11-C12-C13	-2.05	120.73	126.36
38	Z	609	CHL	CAC-C3C-C4C	2.05	129.31	124.03
27	3	611	CLA	CMA-C3A-C2A	-2.05	111.52	116.23
37	V	1623	NEX	O24-C25-C26	-2.05	57.30	58.93
30	3	620	BCR	C32-C1-C6	2.05	113.46	110.24
27	2	613	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
27	B	831	CLA	C3B-C4B-NB	-2.05	108.70	110.53
27	9	611	CLA	C3B-C4B-NB	-2.05	108.70	110.53
27	4	614	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
27	5	617	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
27	A	817	CLA	CMB-C2B-C3B	2.05	131.37	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	3	609	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
35	X	1621	LUT	C27-C28-C29	-2.05	121.91	126.32
27	X	613	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
27	7	610	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
33	4	624	LMG	C7-O1-C1	-2.05	109.40	113.80
35	4	619	LUT	C28-C29-C30	-2.05	115.79	119.01
27	B	830	CLA	C3B-C4B-NB	-2.05	108.70	110.53
29	2	622	LHG	O8-C23-C24	2.05	118.08	111.83
35	W	1620	LUT	C38-C25-C24	-2.05	118.51	123.36
30	B	853	BCR	C38-C26-C25	-2.05	122.25	124.48
35	Z	1621	LUT	C15-C35-C34	-2.05	119.33	123.52
27	5	603	CLA	CBC-CAC-C3C	-2.05	106.87	112.42
27	4	610	CLA	O1D-CGD-CBD	2.05	128.56	124.52
27	O	2002	CLA	CHB-C4A-NA	2.05	127.35	124.40
27	A	831	CLA	O1D-CGD-CBD	2.05	128.56	124.52
27	A	832	CLA	O1D-CGD-CBD	2.05	128.56	124.52
38	Z	606	CHL	CED-O2D-CGD	2.05	120.56	115.92
33	J	104	LMG	O7-C10-O9	-2.05	118.92	123.70
27	V	602	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
33	J	103	LMG	C8-O7-C10	-2.05	112.90	117.80
27	6	616	CLA	O1D-CGD-CBD	2.05	128.55	124.52
37	U	1623	NEX	C30-C31-C32	-2.05	117.27	123.20
30	A	852	BCR	C19-C18-C17	2.05	122.23	119.01
35	W	1620	LUT	C28-C29-C30	-2.05	115.79	119.01
27	5	619	CLA	CHA-C1A-NA	-2.05	121.76	126.39
37	W	1623	NEX	C30-C31-C32	-2.04	117.28	123.20
27	4	616	CLA	O2D-CGD-CBD	2.04	114.80	111.23
27	U	613	CLA	C6-C5-C3	2.04	118.45	113.47
35	Y	1620	LUT	C35-C34-C33	-2.04	124.41	127.28
30	A	851	BCR	C38-C26-C27	2.04	117.95	113.60
27	V	602	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
27	B	828	CLA	CHB-C4A-NA	2.04	127.35	124.40
27	6	602	CLA	CHD-C1D-ND	-2.04	121.93	124.80
27	A	838	CLA	C3B-C4B-NB	-2.04	108.71	110.53
30	B	848	BCR	C3-C4-C5	-2.04	110.41	114.06
30	J	102	BCR	C32-C1-C6	-2.04	107.04	110.24
27	a	611	CLA	CAA-C2A-C3A	-2.04	111.55	116.23
35	U	1620	LUT	C35-C34-C33	-2.04	124.41	127.28
35	X	1621	LUT	C38-C25-C24	-2.04	118.53	123.36
37	Y	1623	NEX	C17-C1-C6	-2.04	108.64	110.47
30	L	305	BCR	C24-C25-C26	-2.04	116.85	121.56
27	3	603	CLA	O2A-CGA-O1A	-2.04	118.52	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	5	628	LMU	C1B-C2B-C3B	2.04	114.30	110.01
27	B	812	CLA	CHD-C1D-ND	-2.04	121.93	124.80
29	a	620	LHG	C5-O7-C7	-2.04	112.92	117.80
30	B	843	BCR	C15-C14-C13	-2.04	124.42	127.28
27	7	609	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
27	L	303	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
27	2	613	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
27	4	601	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
30	3	621	BCR	C15-C14-C13	-2.04	124.42	127.28
38	W	609	CHL	CAC-C3C-C4C	2.04	129.27	124.03
36	9	620	XAT	C15-C14-C13	-2.04	124.42	127.28
32	8	625	LMU	C4B-C3B-C2B	2.04	114.41	110.83
38	Y	608	CHL	O2D-CGD-O1D	-2.04	119.88	123.85
35	U	1620	LUT	C38-C25-C24	-2.04	118.54	123.36
27	8	616	CLA	CHB-C4A-NA	2.04	127.34	124.40
30	A	851	BCR	C24-C25-C26	-2.04	116.87	121.56
27	A	836	CLA	C3B-C4B-NB	-2.04	108.71	110.53
36	3	619	XAT	C28-C29-C30	-2.04	115.81	119.01
35	2	619	LUT	C1-C6-C5	-2.03	119.86	122.64
27	A	825	CLA	C3B-C4B-NB	-2.03	108.71	110.53
27	B	805	CLA	O2D-CGD-CBD	2.03	114.78	111.23
30	B	849	BCR	C37-C22-C21	-2.03	119.52	122.82
36	U	1622	XAT	C10-C11-C12	-2.03	117.31	123.20
33	4	623	LMG	C8-O7-C10	-2.03	112.93	117.80
27	X	611	CLA	O2A-CGA-O1A	-2.03	118.11	123.33
35	W	1621	LUT	C31-C30-C29	-2.03	124.43	127.28
38	Z	605	CHL	CED-O2D-CGD	2.03	120.53	115.92
38	V	607	CHL	CAC-C3C-C4C	2.03	129.25	124.03
35	6	619	LUT	C28-C29-C30	-2.03	115.81	119.01
30	L	301	BCR	C1-C6-C5	-2.03	119.86	122.64
35	V	1621	LUT	O23-C23-C22	-2.03	106.46	110.06
27	3	608	CLA	CHB-C1B-NB	2.03	127.09	124.05
27	3	610	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
36	W	1622	XAT	C10-C11-C12	-2.03	117.32	123.20
27	3	606	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
27	A	824	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
27	a	616	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
27	7	608	CLA	C3B-C4B-NB	-2.03	108.72	110.53
38	W	605	CHL	O2A-CGA-CBA	2.03	120.41	114.00
27	a	603	CLA	CHD-C1D-ND	-2.03	121.95	124.80
38	X	607	CHL	C11-C10-C8	-2.03	109.22	115.97
27	2	601	CLA	CAA-C2A-C3A	-2.03	107.52	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	621	XAT	C32-C33-C34	-2.03	115.82	119.01
30	B	845	BCR	C8-C7-C6	-2.03	121.58	127.00
27	B	841	CLA	CHB-C4A-NA	2.03	127.33	124.40
27	A	813	CLA	CMB-C2B-C3B	2.03	131.32	126.55
27	5	618	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
27	2	603	CLA	CHB-C4A-NA	2.03	127.33	124.40
35	a	617	LUT	C8-C9-C10	-2.03	115.82	119.01
30	B	849	BCR	C29-C28-C27	-2.03	106.82	111.28
30	B	843	BCR	C15-C16-C17	-2.02	119.38	123.52
30	L	301	BCR	C33-C5-C4	2.02	117.91	113.60
38	W	605	CHL	C3D-CAD-CBD	2.02	110.27	107.61
29	1	620	LHG	O7-C7-O9	-2.02	118.97	123.70
27	A	809	CLA	C1-C2-C3	-2.02	122.88	126.20
27	U	604	CLA	CHD-C1D-ND	-2.02	121.96	124.80
29	a	620	LHG	O7-C7-O9	-2.02	118.98	123.70
38	W	608	CHL	O2D-CGD-O1D	-2.02	119.91	123.85
30	8	621	BCR	C36-C18-C17	-2.02	119.54	122.82
37	U	1623	NEX	O24-C25-C26	-2.02	57.33	58.93
36	7	620	XAT	C24-C23-C22	-2.02	107.01	110.79
37	Y	1623	NEX	O24-C25-C26	-2.02	57.33	58.93
27	5	619	CLA	O2D-CGD-CBD	2.02	114.76	111.23
30	B	801	BCR	C10-C11-C12	-2.02	117.34	123.20
36	Y	1622	XAT	C10-C11-C12	-2.02	117.35	123.20
36	X	1622	XAT	C10-C11-C12	-2.02	117.35	123.20
27	3	607	CLA	CHD-C1D-ND	-2.02	121.96	124.80
27	A	820	CLA	CMB-C2B-C3B	2.02	131.30	126.55
27	9	603	CLA	CMB-C2B-C3B	2.02	128.90	123.53
37	X	1623	NEX	C17-C1-C6	-2.02	108.67	110.47
38	Z	605	CHL	C1B-CHB-C4A	-2.02	120.03	121.32
27	7	614	CLA	CHB-C1B-NB	2.02	127.08	124.05
27	B	809	CLA	CHD-C1D-ND	-2.02	121.96	124.80
27	1	616	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
30	A	849	BCR	C8-C9-C10	-2.02	115.84	119.01
27	1	603	CLA	CHD-C1D-ND	-2.02	121.96	124.80
30	B	843	BCR	C11-C12-C13	-2.02	120.83	126.36
30	K	202	BCR	C36-C18-C17	-2.02	119.55	122.82
27	H	203	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
37	X	1623	NEX	C30-C31-C32	-2.02	117.36	123.20
30	8	621	BCR	C11-C12-C13	-2.01	120.84	126.36
27	V	604	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
29	9	622	LHG	C5-O7-C7	-2.01	112.97	117.80
29	3	624	LHG	O7-C7-O9	-2.01	119.00	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	3	617	CLA	CMA-C3A-C2A	-2.01	111.61	116.23
35	8	619	LUT	C18-C5-C4	2.01	118.12	114.42
35	Y	1620	LUT	C11-C12-C13	-2.01	120.84	126.36
30	3	620	BCR	C12-C13-C14	2.01	122.18	119.01
27	5	609	CLA	C1-C2-C3	-2.01	122.90	126.20
27	B	802	CLA	CHC-C4B-NB	2.01	127.07	124.05
27	A	854	CLA	CMD-C2D-C3D	2.01	132.30	127.69
37	Y	1623	NEX	C30-C31-C32	-2.01	117.37	123.20
27	5	616	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
27	4	608	CLA	C11-C12-C13	-2.01	109.28	115.97
33	4	624	LMG	C6-C5-C4	-2.01	108.08	113.02
35	6	619	LUT	C38-C25-C24	-2.01	118.60	123.36
36	4	620	XAT	C27-C28-C29	-2.01	122.41	125.53
35	7	619	LUT	O23-C23-C22	-2.01	106.50	110.06
33	H	205	LMG	O6-C1-C2	-2.01	106.24	110.37
27	B	825	CLA	CHD-C1D-ND	-2.01	121.98	124.80
27	B	830	CLA	O1D-CGD-CBD	2.01	128.48	124.52
37	V	1623	NEX	C11-C12-C13	-2.01	120.86	126.36
35	7	619	LUT	C38-C25-C24	-2.01	118.61	123.36
27	A	801	CLA	O1D-CGD-CBD	2.01	128.48	124.52
30	A	851	BCR	C38-C26-C25	-2.01	122.29	124.48
27	A	808	CLA	CHD-C1D-ND	-2.01	121.98	124.80
27	A	802	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
38	X	608	CHL	CMA-C3A-C4A	-2.01	110.29	114.61
27	8	604	CLA	O2D-CGD-CBD	2.00	114.73	111.23
35	U	1621	LUT	C31-C30-C29	-2.00	124.47	127.28
27	6	620	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
27	6	602	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
38	Z	608	CHL	C3D-CAD-CBD	2.00	110.24	107.61
30	F	305	BCR	C30-C25-C24	2.00	121.08	115.65
30	B	801	BCR	C38-C26-C27	2.00	117.86	113.60
30	B	852	BCR	C24-C23-C22	-2.00	123.27	126.23
38	U	608	CHL	O2D-CGD-O1D	-2.00	119.95	123.85
27	B	837	CLA	CHD-C1D-ND	-2.00	121.99	124.80
27	B	839	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
35	X	1620	LUT	C11-C12-C13	-2.00	120.88	126.36

All (379) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	801	CLA	ND
27	A	802	CLA	ND

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Mol	Chain	Res	Type	Atom
27	A	803	CLA	ND
27	A	804	CLA	ND
27	A	806	CLA	ND
27	A	807	CLA	ND
27	A	809	CLA	ND
27	A	810	CLA	ND
27	A	811	CLA	ND
27	A	812	CLA	ND
27	A	813	CLA	ND
27	A	814	CLA	ND
27	A	815	CLA	ND
27	A	816	CLA	ND
27	A	819	CLA	ND
27	A	820	CLA	ND
27	A	821	CLA	ND
27	A	822	CLA	ND
27	A	823	CLA	ND
27	A	824	CLA	ND
27	A	825	CLA	ND
27	A	826	CLA	ND
27	A	827	CLA	ND
27	A	828	CLA	ND
27	A	829	CLA	ND
27	A	830	CLA	ND
27	A	831	CLA	ND
27	A	832	CLA	ND
27	A	833	CLA	ND
27	A	834	CLA	ND
27	A	836	CLA	ND
27	A	838	CLA	ND
27	A	839	CLA	ND
27	A	841	CLA	ND
27	A	842	CLA	ND
27	A	843	CLA	ND
27	A	845	CLA	ND
27	A	854	CLA	ND
27	B	802	CLA	ND
27	B	803	CLA	ND
27	B	804	CLA	ND
27	B	805	CLA	ND
27	B	806	CLA	ND
27	B	808	CLA	ND

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Mol	Chain	Res	Type	Atom
27	B	809	CLA	ND
27	B	810	CLA	ND
27	B	811	CLA	ND
27	B	812	CLA	ND
27	B	813	CLA	ND
27	B	814	CLA	ND
27	B	815	CLA	ND
27	B	816	CLA	ND
27	B	817	CLA	ND
27	B	819	CLA	ND
27	B	820	CLA	ND
27	B	821	CLA	ND
27	B	823	CLA	ND
27	B	824	CLA	ND
27	B	826	CLA	ND
27	B	827	CLA	ND
27	B	828	CLA	ND
27	B	829	CLA	ND
27	B	830	CLA	ND
27	B	831	CLA	ND
27	B	833	CLA	ND
27	B	834	CLA	ND
27	B	835	CLA	ND
27	B	836	CLA	ND
27	B	839	CLA	ND
27	B	840	CLA	ND
27	B	841	CLA	ND
27	F	301	CLA	ND
27	G	203	CLA	ND
27	G	204	CLA	ND
27	H	202	CLA	ND
27	J	101	CLA	ND
27	K	201	CLA	ND
27	K	204	CLA	ND
27	K	206	CLA	ND
27	L	302	CLA	ND
27	L	304	CLA	ND
27	L	306	CLA	ND
27	L	307	CLA	ND
27	O	2001	CLA	ND
27	O	2002	CLA	ND
27	O	2003	CLA	ND

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Mol	Chain	Res	Type	Atom
27	a	602	CLA	ND
27	a	603	CLA	ND
27	a	604	CLA	ND
27	a	606	CLA	ND
27	a	607	CLA	ND
27	a	608	CLA	ND
27	a	609	CLA	ND
27	a	610	CLA	ND
27	a	611	CLA	ND
27	a	612	CLA	ND
27	a	613	CLA	ND
27	a	614	CLA	ND
27	a	616	CLA	ND
27	1	602	CLA	ND
27	1	603	CLA	ND
27	1	604	CLA	ND
27	1	606	CLA	ND
27	1	607	CLA	ND
27	1	608	CLA	ND
27	1	609	CLA	ND
27	1	610	CLA	ND
27	1	611	CLA	ND
27	1	612	CLA	ND
27	1	613	CLA	ND
27	1	614	CLA	ND
27	1	616	CLA	ND
27	2	601	CLA	ND
27	2	602	CLA	ND
27	2	603	CLA	ND
27	2	604	CLA	ND
27	2	606	CLA	ND
27	2	607	CLA	ND
27	2	609	CLA	ND
27	2	610	CLA	ND
27	2	611	CLA	ND
27	2	612	CLA	ND
27	2	613	CLA	ND
27	2	614	CLA	ND
27	2	616	CLA	ND
27	3	602	CLA	ND
27	3	603	CLA	ND
27	3	604	CLA	ND

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Mol	Chain	Res	Type	Atom
27	3	606	CLA	ND
27	3	607	CLA	ND
27	3	608	CLA	ND
27	3	609	CLA	ND
27	3	610	CLA	ND
27	3	611	CLA	ND
27	3	612	CLA	ND
27	3	613	CLA	ND
27	3	614	CLA	ND
27	3	615	CLA	ND
27	3	617	CLA	ND
27	4	601	CLA	ND
27	4	602	CLA	ND
27	4	603	CLA	ND
27	4	604	CLA	ND
27	4	606	CLA	ND
27	4	607	CLA	ND
27	4	608	CLA	ND
27	4	609	CLA	ND
27	4	610	CLA	ND
27	4	611	CLA	ND
27	4	612	CLA	ND
27	4	613	CLA	ND
27	4	614	CLA	ND
27	4	616	CLA	ND
27	4	618	CLA	ND
27	5	601	CLA	ND
27	5	603	CLA	ND
27	5	604	CLA	ND
27	5	607	CLA	ND
27	5	608	CLA	ND
27	5	609	CLA	ND
27	5	610	CLA	ND
27	5	611	CLA	ND
27	5	612	CLA	ND
27	5	613	CLA	ND
27	5	614	CLA	ND
27	5	616	CLA	ND
27	5	617	CLA	ND
27	5	618	CLA	ND
27	5	619	CLA	ND
27	6	601	CLA	ND

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Mol	Chain	Res	Type	Atom
27	6	602	CLA	ND
27	6	603	CLA	ND
27	6	606	CLA	ND
27	6	607	CLA	ND
27	6	608	CLA	ND
27	6	609	CLA	ND
27	6	610	CLA	ND
27	6	611	CLA	ND
27	6	612	CLA	ND
27	6	613	CLA	ND
27	6	614	CLA	ND
27	6	616	CLA	ND
27	6	617	CLA	ND
27	6	618	CLA	ND
27	6	620	CLA	ND
27	7	601	CLA	ND
27	7	602	CLA	ND
27	7	603	CLA	ND
27	7	604	CLA	ND
27	7	607	CLA	ND
27	7	608	CLA	ND
27	7	609	CLA	ND
27	7	610	CLA	ND
27	7	611	CLA	ND
27	7	612	CLA	ND
27	7	613	CLA	ND
27	7	614	CLA	ND
27	7	615	CLA	ND
27	7	616	CLA	ND
27	8	601	CLA	ND
27	8	602	CLA	ND
27	8	603	CLA	ND
27	8	604	CLA	ND
27	8	606	CLA	ND
27	8	607	CLA	ND
27	8	608	CLA	ND
27	8	609	CLA	ND
27	8	610	CLA	ND
27	8	611	CLA	ND
27	8	612	CLA	ND
27	8	613	CLA	ND
27	8	614	CLA	ND

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Mol	Chain	Res	Type	Atom
27	8	616	CLA	ND
27	9	601	CLA	ND
27	9	603	CLA	ND
27	9	604	CLA	ND
27	9	606	CLA	ND
27	9	609	CLA	ND
27	9	610	CLA	ND
27	9	611	CLA	ND
27	9	612	CLA	ND
27	9	613	CLA	ND
27	9	614	CLA	ND
27	X	602	CLA	ND
27	X	603	CLA	ND
27	X	604	CLA	ND
27	X	610	CLA	ND
27	X	611	CLA	ND
27	X	612	CLA	ND
27	X	613	CLA	ND
27	X	614	CLA	ND
27	Y	602	CLA	ND
27	Y	603	CLA	ND
27	Y	604	CLA	ND
27	Y	610	CLA	ND
27	Y	611	CLA	ND
27	Y	612	CLA	ND
27	Y	613	CLA	ND
27	Y	614	CLA	ND
27	Z	602	CLA	ND
27	Z	603	CLA	ND
27	Z	604	CLA	ND
27	Z	610	CLA	ND
27	Z	611	CLA	ND
27	Z	612	CLA	ND
27	Z	613	CLA	ND
27	Z	614	CLA	ND
27	U	602	CLA	ND
27	U	603	CLA	ND
27	U	604	CLA	ND
27	U	610	CLA	ND
27	U	611	CLA	ND
27	U	612	CLA	ND
27	U	613	CLA	ND

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Mol	Chain	Res	Type	Atom
27	U	614	CLA	ND
27	V	602	CLA	ND
27	V	603	CLA	ND
27	V	604	CLA	ND
27	V	610	CLA	ND
27	V	611	CLA	ND
27	V	612	CLA	ND
27	V	613	CLA	ND
27	V	614	CLA	ND
27	W	602	CLA	ND
27	W	603	CLA	ND
27	W	604	CLA	ND
27	W	610	CLA	ND
27	W	611	CLA	ND
27	W	612	CLA	ND
27	W	613	CLA	ND
27	W	614	CLA	ND
38	X	601	CHL	NC
38	X	601	CHL	ND
38	X	601	CHL	NA
38	X	605	CHL	NC
38	X	605	CHL	ND
38	X	605	CHL	NA
38	X	606	CHL	NC
38	X	606	CHL	ND
38	X	606	CHL	NA
38	X	607	CHL	NC
38	X	607	CHL	ND
38	X	607	CHL	NA
38	X	608	CHL	NC
38	X	608	CHL	ND
38	X	608	CHL	NA
38	X	609	CHL	NC
38	X	609	CHL	ND
38	X	609	CHL	NA
38	Y	601	CHL	NC
38	Y	601	CHL	ND
38	Y	601	CHL	NA
38	Y	605	CHL	NC
38	Y	605	CHL	ND
38	Y	605	CHL	NA
38	Y	606	CHL	NC

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Mol	Chain	Res	Type	Atom
38	Y	606	CHL	ND
38	Y	606	CHL	NA
38	Y	607	CHL	NC
38	Y	607	CHL	ND
38	Y	607	CHL	NA
38	Y	608	CHL	NC
38	Y	608	CHL	ND
38	Y	608	CHL	NA
38	Y	609	CHL	NC
38	Y	609	CHL	ND
38	Y	609	CHL	NA
38	Z	601	CHL	NC
38	Z	601	CHL	ND
38	Z	601	CHL	NA
38	Z	605	CHL	NC
38	Z	605	CHL	ND
38	Z	605	CHL	NA
38	Z	606	CHL	NC
38	Z	606	CHL	ND
38	Z	606	CHL	NA
38	Z	607	CHL	NC
38	Z	607	CHL	ND
38	Z	607	CHL	NA
38	Z	608	CHL	NC
38	Z	608	CHL	ND
38	Z	608	CHL	NA
38	Z	609	CHL	NC
38	Z	609	CHL	ND
38	Z	609	CHL	NA
38	U	601	CHL	NC
38	U	601	CHL	ND
38	U	601	CHL	NA
38	U	605	CHL	NC
38	U	605	CHL	ND
38	U	605	CHL	NA
38	U	606	CHL	NC
38	U	606	CHL	ND
38	U	606	CHL	NA
38	U	607	CHL	NC
38	U	607	CHL	ND
38	U	607	CHL	NA
38	U	608	CHL	NC

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Mol	Chain	Res	Type	Atom
38	U	608	CHL	ND
38	U	608	CHL	NA
38	U	609	CHL	NC
38	U	609	CHL	ND
38	U	609	CHL	NA
38	V	601	CHL	NC
38	V	601	CHL	ND
38	V	601	CHL	NA
38	V	605	CHL	NC
38	V	605	CHL	ND
38	V	605	CHL	NA
38	V	606	CHL	NC
38	V	606	CHL	ND
38	V	606	CHL	NA
38	V	607	CHL	NC
38	V	607	CHL	ND
38	V	607	CHL	NA
38	V	608	CHL	NC
38	V	608	CHL	ND
38	V	608	CHL	NA
38	V	609	CHL	NC
38	V	609	CHL	ND
38	V	609	CHL	NA
38	W	601	CHL	NC
38	W	601	CHL	ND
38	W	601	CHL	NA
38	W	605	CHL	NC
38	W	605	CHL	ND
38	W	605	CHL	NA
38	W	606	CHL	NC
38	W	606	CHL	ND
38	W	606	CHL	NA
38	W	607	CHL	NC
38	W	607	CHL	ND
38	W	607	CHL	NA
38	W	608	CHL	NC
38	W	608	CHL	ND
38	W	608	CHL	NA
38	W	609	CHL	NC
38	W	609	CHL	ND
38	W	609	CHL	NA

All (3213) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	801	CLA	CBD-CGD-O2D-CED
27	A	801	CLA	O1D-CGD-O2D-CED
27	A	804	CLA	C1A-C2A-CAA-CBA
27	A	804	CLA	C3A-C2A-CAA-CBA
27	A	804	CLA	CHA-CBD-CGD-O1D
27	A	804	CLA	CHA-CBD-CGD-O2D
27	A	805	CLA	C3A-C2A-CAA-CBA
27	A	806	CLA	C1A-C2A-CAA-CBA
27	A	806	CLA	CAD-CBD-CGD-O1D
27	A	806	CLA	CAD-CBD-CGD-O2D
27	A	809	CLA	CHA-CBD-CGD-O1D
27	A	809	CLA	CHA-CBD-CGD-O2D
27	A	810	CLA	C1A-C2A-CAA-CBA
27	A	810	CLA	C4B-C3B-CAB-CBB
27	A	812	CLA	C1A-C2A-CAA-CBA
27	A	812	CLA	CHA-CBD-CGD-O1D
27	A	812	CLA	CHA-CBD-CGD-O2D
27	A	815	CLA	CBD-CGD-O2D-CED
27	A	816	CLA	C1A-C2A-CAA-CBA
27	A	816	CLA	C3A-C2A-CAA-CBA
27	A	819	CLA	C1A-C2A-CAA-CBA
27	A	819	CLA	C3A-C2A-CAA-CBA
27	A	820	CLA	C3A-C2A-CAA-CBA
27	A	821	CLA	C1A-C2A-CAA-CBA
27	A	821	CLA	C3A-C2A-CAA-CBA
27	A	821	CLA	C4B-C3B-CAB-CBB
27	A	823	CLA	C4B-C3B-CAB-CBB
27	A	825	CLA	C1A-C2A-CAA-CBA
27	A	825	CLA	C3A-C2A-CAA-CBA
27	A	825	CLA	C2B-C3B-CAB-CBB
27	A	825	CLA	C4B-C3B-CAB-CBB
27	A	826	CLA	CHA-CBD-CGD-O2D
27	A	833	CLA	C1A-C2A-CAA-CBA
27	A	834	CLA	C2B-C3B-CAB-CBB
27	A	834	CLA	C4B-C3B-CAB-CBB
27	A	835	CLA	CHA-CBD-CGD-O1D
27	A	835	CLA	CHA-CBD-CGD-O2D
27	A	841	CLA	C1A-C2A-CAA-CBA
27	B	802	CLA	CBD-CGD-O2D-CED
27	B	803	CLA	C3A-C2A-CAA-CBA
27	B	803	CLA	CBD-CGD-O2D-CED
27	B	805	CLA	C3A-C2A-CAA-CBA
27	B	808	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	B	808	CLA	CHA-CBD-CGD-O2D
27	B	809	CLA	C1A-C2A-CAA-CBA
27	B	810	CLA	C1A-C2A-CAA-CBA
27	B	810	CLA	CHA-CBD-CGD-O1D
27	B	810	CLA	CHA-CBD-CGD-O2D
27	B	815	CLA	CHA-CBD-CGD-O2D
27	B	818	CLA	C3A-C2A-CAA-CBA
27	B	819	CLA	C2B-C3B-CAB-CBB
27	B	819	CLA	C4B-C3B-CAB-CBB
27	B	821	CLA	C2B-C3B-CAB-CBB
27	B	821	CLA	C4B-C3B-CAB-CBB
27	B	822	CLA	C1A-C2A-CAA-CBA
27	B	827	CLA	CBD-CGD-O2D-CED
27	B	828	CLA	C14-C13-C15-C16
27	B	829	CLA	C1A-C2A-CAA-CBA
27	B	830	CLA	C1A-C2A-CAA-CBA
27	B	830	CLA	C3A-C2A-CAA-CBA
27	B	833	CLA	C4B-C3B-CAB-CBB
27	B	833	CLA	CHA-CBD-CGD-O1D
27	B	833	CLA	CHA-CBD-CGD-O2D
27	B	835	CLA	CBD-CGD-O2D-CED
27	F	301	CLA	CBD-CGD-O2D-CED
27	F	303	CLA	C1A-C2A-CAA-CBA
27	F	303	CLA	C3A-C2A-CAA-CBA
27	F	303	CLA	CBD-CGD-O2D-CED
27	G	203	CLA	CBD-CGD-O2D-CED
27	G	204	CLA	CBD-CGD-O2D-CED
27	H	203	CLA	C1A-C2A-CAA-CBA
27	J	101	CLA	C1A-C2A-CAA-CBA
27	K	201	CLA	C4B-C3B-CAB-CBB
27	K	203	CLA	C1A-C2A-CAA-CBA
27	K	203	CLA	C4B-C3B-CAB-CBB
27	K	206	CLA	C2B-C3B-CAB-CBB
27	K	206	CLA	C4B-C3B-CAB-CBB
27	O	2001	CLA	CHA-CBD-CGD-O2D
27	O	2003	CLA	C1A-C2A-CAA-CBA
27	a	601	CLA	C2B-C3B-CAB-CBB
27	a	601	CLA	C4B-C3B-CAB-CBB
27	a	606	CLA	CHA-CBD-CGD-O2D
27	a	606	CLA	CAD-CBD-CGD-O2D
27	a	607	CLA	CBD-CGD-O2D-CED
27	a	609	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	a	609	CLA	C4B-C3B-CAB-CBB
27	a	611	CLA	CAD-CBD-CGD-O2D
27	a	613	CLA	C2B-C3B-CAB-CBB
27	a	613	CLA	C4B-C3B-CAB-CBB
27	1	601	CLA	C2B-C3B-CAB-CBB
27	1	601	CLA	C4B-C3B-CAB-CBB
27	1	606	CLA	CHA-CBD-CGD-O2D
27	1	606	CLA	CAD-CBD-CGD-O2D
27	1	613	CLA	C2B-C3B-CAB-CBB
27	1	613	CLA	C4B-C3B-CAB-CBB
27	2	601	CLA	C6-C7-C8-C9
27	2	604	CLA	CBD-CGD-O2D-CED
27	2	609	CLA	C1A-C2A-CAA-CBA
27	2	610	CLA	CHA-CBD-CGD-O1D
27	2	610	CLA	CHA-CBD-CGD-O2D
27	2	611	CLA	C1A-C2A-CAA-CBA
27	2	611	CLA	C2B-C3B-CAB-CBB
27	2	611	CLA	C4B-C3B-CAB-CBB
27	3	603	CLA	CBD-CGD-O2D-CED
27	3	606	CLA	CHA-CBD-CGD-O2D
27	3	609	CLA	C3A-C2A-CAA-CBA
27	3	609	CLA	CHA-CBD-CGD-O1D
27	3	609	CLA	CHA-CBD-CGD-O2D
27	3	610	CLA	C1A-C2A-CAA-CBA
27	3	610	CLA	C3A-C2A-CAA-CBA
27	3	611	CLA	CHA-CBD-CGD-O2D
27	3	615	CLA	C1A-C2A-CAA-CBA
27	4	601	CLA	C3A-C2A-CAA-CBA
27	4	606	CLA	C1A-C2A-CAA-CBA
27	4	606	CLA	C3A-C2A-CAA-CBA
27	4	609	CLA	O1A-CGA-O2A-C1
27	4	611	CLA	C1A-C2A-CAA-CBA
27	4	611	CLA	C2B-C3B-CAB-CBB
27	4	611	CLA	C4B-C3B-CAB-CBB
27	4	612	CLA	C1A-C2A-CAA-CBA
27	4	612	CLA	C3A-C2A-CAA-CBA
27	4	613	CLA	C2B-C3B-CAB-CBB
27	4	613	CLA	C4B-C3B-CAB-CBB
27	4	616	CLA	CAD-CBD-CGD-O1D
27	4	616	CLA	CAD-CBD-CGD-O2D
27	4	618	CLA	C1A-C2A-CAA-CBA
27	4	618	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	5	601	CLA	C4B-C3B-CAB-CBB
27	5	608	CLA	C1A-C2A-CAA-CBA
27	5	608	CLA	C3A-C2A-CAA-CBA
27	5	609	CLA	C1A-C2A-CAA-CBA
27	5	609	CLA	C3A-C2A-CAA-CBA
27	5	609	CLA	C6-C7-C8-C9
27	5	611	CLA	C1A-C2A-CAA-CBA
27	5	611	CLA	C3A-C2A-CAA-CBA
27	5	611	CLA	C4B-C3B-CAB-CBB
27	5	612	CLA	C1A-C2A-CAA-CBA
27	5	612	CLA	C3A-C2A-CAA-CBA
27	5	613	CLA	C2B-C3B-CAB-CBB
27	5	613	CLA	C4B-C3B-CAB-CBB
27	5	614	CLA	C1A-C2A-CAA-CBA
27	5	614	CLA	C3A-C2A-CAA-CBA
27	5	614	CLA	C2B-C3B-CAB-CBB
27	5	614	CLA	C4B-C3B-CAB-CBB
27	5	614	CLA	CBD-CGD-O2D-CED
27	5	617	CLA	CBD-CGD-O2D-CED
27	5	619	CLA	CHA-CBD-CGD-O1D
27	5	619	CLA	CHA-CBD-CGD-O2D
27	6	601	CLA	CAD-CBD-CGD-O1D
27	6	601	CLA	CAD-CBD-CGD-O2D
27	6	604	CLA	C2B-C3B-CAB-CBB
27	6	604	CLA	C4B-C3B-CAB-CBB
27	6	609	CLA	C1A-C2A-CAA-CBA
27	6	611	CLA	C1A-C2A-CAA-CBA
27	6	611	CLA	C3A-C2A-CAA-CBA
27	6	612	CLA	C1A-C2A-CAA-CBA
27	6	612	CLA	C3A-C2A-CAA-CBA
27	6	617	CLA	C1A-C2A-CAA-CBA
27	6	617	CLA	C3A-C2A-CAA-CBA
27	6	617	CLA	CBD-CGD-O2D-CED
27	6	620	CLA	C1A-C2A-CAA-CBA
27	6	620	CLA	C3A-C2A-CAA-CBA
27	7	602	CLA	CHA-CBD-CGD-O1D
27	7	602	CLA	CHA-CBD-CGD-O2D
27	7	604	CLA	CHA-CBD-CGD-O2D
27	7	606	CLA	C1A-C2A-CAA-CBA
27	7	606	CLA	C3A-C2A-CAA-CBA
27	7	609	CLA	C1A-C2A-CAA-CBA
27	7	609	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	7	612	CLA	CBD-CGD-O2D-CED
27	7	613	CLA	C2B-C3B-CAB-CBB
27	7	613	CLA	C4B-C3B-CAB-CBB
27	7	614	CLA	C1A-C2A-CAA-CBA
27	7	614	CLA	C4B-C3B-CAB-CBB
27	7	615	CLA	CAD-CBD-CGD-O2D
27	8	607	CLA	C1A-C2A-CAA-CBA
27	8	607	CLA	C3A-C2A-CAA-CBA
27	8	607	CLA	CBD-CGD-O2D-CED
27	8	609	CLA	C1A-C2A-CAA-CBA
27	8	609	CLA	C3A-C2A-CAA-CBA
27	8	611	CLA	C1A-C2A-CAA-CBA
27	8	612	CLA	C1A-C2A-CAA-CBA
27	8	612	CLA	C3A-C2A-CAA-CBA
27	8	614	CLA	C1A-C2A-CAA-CBA
27	9	601	CLA	C2B-C3B-CAB-CBB
27	9	601	CLA	C4B-C3B-CAB-CBB
27	9	611	CLA	C1A-C2A-CAA-CBA
27	9	612	CLA	C1A-C2A-CAA-CBA
27	9	612	CLA	C3A-C2A-CAA-CBA
27	9	613	CLA	C2B-C3B-CAB-CBB
27	9	613	CLA	C4B-C3B-CAB-CBB
27	X	603	CLA	CHA-CBD-CGD-O2D
27	X	610	CLA	CBD-CGD-O2D-CED
27	X	611	CLA	C1A-C2A-CAA-CBA
27	X	611	CLA	C3A-C2A-CAA-CBA
27	X	611	CLA	C2B-C3B-CAB-CBB
27	X	611	CLA	C4B-C3B-CAB-CBB
27	X	612	CLA	CHA-CBD-CGD-O1D
27	X	612	CLA	CHA-CBD-CGD-O2D
27	X	614	CLA	CBD-CGD-O2D-CED
27	Y	603	CLA	CHA-CBD-CGD-O2D
27	Y	610	CLA	CBD-CGD-O2D-CED
27	Y	611	CLA	C1A-C2A-CAA-CBA
27	Y	611	CLA	C3A-C2A-CAA-CBA
27	Y	611	CLA	C2B-C3B-CAB-CBB
27	Y	611	CLA	C4B-C3B-CAB-CBB
27	Y	612	CLA	CHA-CBD-CGD-O2D
27	Y	614	CLA	CBD-CGD-O2D-CED
27	U	610	CLA	CBD-CGD-O2D-CED
27	U	611	CLA	C1A-C2A-CAA-CBA
27	U	611	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	U	611	CLA	C2B-C3B-CAB-CBB
27	U	611	CLA	C4B-C3B-CAB-CBB
27	U	612	CLA	CHA-CBD-CGD-O1D
27	U	612	CLA	CHA-CBD-CGD-O2D
27	U	614	CLA	CBD-CGD-O2D-CED
27	V	604	CLA	CBD-CGD-O2D-CED
27	V	611	CLA	CAD-CBD-CGD-O1D
27	V	611	CLA	CAD-CBD-CGD-O2D
27	V	614	CLA	C2B-C3B-CAB-CBB
27	V	614	CLA	C4B-C3B-CAB-CBB
27	W	610	CLA	CBD-CGD-O2D-CED
27	W	611	CLA	C1A-C2A-CAA-CBA
27	W	611	CLA	C3A-C2A-CAA-CBA
27	W	611	CLA	C2B-C3B-CAB-CBB
27	W	611	CLA	C4B-C3B-CAB-CBB
27	W	612	CLA	CHA-CBD-CGD-O1D
27	W	612	CLA	CHA-CBD-CGD-O2D
27	W	614	CLA	CBD-CGD-O2D-CED
28	A	844	PQN	C11-C12-C13-C14
29	A	846	LHG	C3-O3-P-O5
29	A	846	LHG	C4-O6-P-O3
29	A	846	LHG	C4-O6-P-O4
29	A	847	LHG	C3-O3-P-O5
29	A	847	LHG	C4-O6-P-O4
29	B	851	LHG	C3-O3-P-O4
29	B	851	LHG	C3-O3-P-O5
29	B	851	LHG	C3-O3-P-O6
29	B	854	LHG	C1-C2-C3-O3
29	B	854	LHG	C4-O6-P-O3
29	B	854	LHG	C4-O6-P-O4
29	H	204	LHG	C4-O6-P-O3
29	O	2631	LHG	C3-O3-P-O6
29	O	2631	LHG	C8-C7-O7-C5
29	2	622	LHG	C3-O3-P-O6
29	2	622	LHG	C4-O6-P-O3
29	2	622	LHG	C4-O6-P-O4
29	3	623	LHG	C4-O6-P-O3
29	3	623	LHG	C4-O6-P-O4
29	3	624	LHG	C3-O3-P-O4
29	3	624	LHG	C3-O3-P-O5
29	3	624	LHG	C3-O3-P-O6
29	4	622	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
29	4	622	LHG	C3-O3-P-O6
29	4	622	LHG	C4-O6-P-O5
29	5	623	LHG	C3-O3-P-O4
29	5	623	LHG	C3-O3-P-O6
29	5	623	LHG	C4-O6-P-O3
29	5	623	LHG	C4-O6-P-O5
29	5	623	LHG	O7-C5-C6-O8
29	5	625	LHG	C3-O3-P-O5
29	5	625	LHG	C3-O3-P-O6
29	6	623	LHG	C3-O3-P-O6
29	6	623	LHG	C4-O6-P-O3
29	6	623	LHG	C4-O6-P-O4
29	7	622	LHG	C1-C2-C3-O3
29	7	622	LHG	O2-C2-C3-O3
29	7	622	LHG	C3-O3-P-O4
29	7	622	LHG	C3-O3-P-O6
29	7	622	LHG	C4-O6-P-O3
29	7	622	LHG	C4-O6-P-O4
29	7	622	LHG	C4-O6-P-O5
29	7	622	LHG	O7-C5-C6-O8
29	8	623	LHG	C3-O3-P-O5
29	8	623	LHG	C4-O6-P-O3
29	8	623	LHG	C4-O6-P-O4
29	9	622	LHG	C3-O3-P-O5
29	9	622	LHG	C4-O6-P-O3
29	9	622	LHG	C4-O6-P-O4
29	9	623	LHG	C3-O3-P-O6
29	9	623	LHG	C4-O6-P-O3
29	9	623	LHG	C4-O6-P-O4
29	9	623	LHG	C4-O6-P-O5
29	9	623	LHG	C8-C7-O7-C5
29	9	624	LHG	O1-C1-C2-C3
29	X	2630	LHG	C3-O3-P-O4
29	X	2630	LHG	C3-O3-P-O6
29	X	2630	LHG	C4-O6-P-O3
29	X	2630	LHG	C4-O6-P-O5
29	Y	2630	LHG	C3-O3-P-O4
29	Y	2630	LHG	C3-O3-P-O6
29	Y	2630	LHG	C4-O6-P-O3
29	Y	2630	LHG	C4-O6-P-O5
29	Z	2630	LHG	C3-O3-P-O4
29	Z	2630	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
29	Z	2630	LHG	C4-O6-P-O3
29	Z	2630	LHG	C4-O6-P-O4
29	Z	2630	LHG	C4-O6-P-O5
29	U	2630	LHG	C3-O3-P-O4
29	U	2630	LHG	C3-O3-P-O6
29	U	2630	LHG	C4-O6-P-O3
29	U	2630	LHG	C4-O6-P-O5
29	V	2630	LHG	C4-O6-P-O3
29	W	2630	LHG	C3-O3-P-O4
29	W	2630	LHG	C3-O3-P-O6
29	W	2630	LHG	C4-O6-P-O3
29	W	2630	LHG	C4-O6-P-O5
30	A	849	BCR	C23-C24-C25-C26
30	A	850	BCR	C5-C6-C7-C8
30	A	851	BCR	C5-C6-C7-C8
30	A	856	BCR	C1-C6-C7-C8
30	A	856	BCR	C5-C6-C7-C8
30	B	801	BCR	C23-C24-C25-C26
30	B	844	BCR	C23-C24-C25-C26
30	B	844	BCR	C23-C24-C25-C30
30	B	845	BCR	C5-C6-C7-C8
30	B	847	BCR	C21-C22-C23-C24
30	B	848	BCR	C23-C24-C25-C26
30	B	849	BCR	C5-C6-C7-C8
30	J	102	BCR	C5-C6-C7-C8
30	K	202	BCR	C23-C24-C25-C26
30	K	202	BCR	C23-C24-C25-C30
30	L	301	BCR	C1-C6-C7-C8
30	L	301	BCR	C5-C6-C7-C8
30	O	2005	BCR	C21-C22-C23-C24
30	a	619	BCR	C23-C24-C25-C26
30	a	619	BCR	C23-C24-C25-C30
30	1	619	BCR	C23-C24-C25-C26
30	1	619	BCR	C23-C24-C25-C30
30	2	623	BCR	C5-C6-C7-C8
30	3	620	BCR	C11-C12-C13-C14
30	3	620	BCR	C11-C12-C13-C35
30	3	622	BCR	C21-C22-C23-C24
30	4	621	BCR	C5-C6-C7-C8
30	4	621	BCR	C23-C24-C25-C26
30	4	621	BCR	C23-C24-C25-C30
30	5	622	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	5	622	BCR	C23-C24-C25-C30
30	7	621	BCR	C21-C22-C23-C24
30	7	623	BCR	C1-C6-C7-C8
30	7	623	BCR	C5-C6-C7-C8
30	8	621	BCR	C1-C6-C7-C8
30	8	621	BCR	C23-C24-C25-C26
30	8	621	BCR	C23-C24-C25-C30
30	9	621	BCR	C5-C6-C7-C8
32	K	208	LMU	O5'-C1'-O1'-C1
32	5	628	LMU	O5'-C1'-O1'-C1
33	J	104	LMG	O10-C28-O8-C9
33	J	104	LMG	C29-C28-O8-C9
33	8	626	LMG	O9-C10-O7-C8
33	8	626	LMG	C11-C10-O7-C8
34	B	850	DGD	C2B-C1B-O2G-C2G
35	V	1621	LUT	C7-C8-C9-C10
37	Z	1623	NEX	O24-C26-C27-C28
37	V	1623	NEX	O24-C26-C27-C28
38	X	601	CHL	C1C-C2C-CMC-OMC
38	X	601	CHL	C3C-C2C-CMC-OMC
38	X	601	CHL	C6-C7-C8-C10
38	X	607	CHL	C1C-C2C-CMC-OMC
38	X	607	CHL	C3C-C2C-CMC-OMC
38	X	607	CHL	CBD-CGD-O2D-CED
38	X	608	CHL	C1C-C2C-CMC-OMC
38	X	608	CHL	C3C-C2C-CMC-OMC
38	X	608	CHL	CBD-CGD-O2D-CED
38	X	609	CHL	C3A-C2A-CAA-CBA
38	Y	607	CHL	C1C-C2C-CMC-OMC
38	Y	607	CHL	C3C-C2C-CMC-OMC
38	Y	607	CHL	CBD-CGD-O2D-CED
38	Y	609	CHL	C3A-C2A-CAA-CBA
38	Z	601	CHL	C1C-C2C-CMC-OMC
38	Z	601	CHL	C3C-C2C-CMC-OMC
38	Z	607	CHL	C1C-C2C-CMC-OMC
38	Z	607	CHL	C3C-C2C-CMC-OMC
38	Z	607	CHL	CHA-CBD-CGD-O1D
38	Z	609	CHL	CHA-CBD-CGD-O1D
38	U	608	CHL	CBD-CGD-O2D-CED
38	V	607	CHL	C1A-C2A-CAA-CBA
38	V	607	CHL	C3A-C2A-CAA-CBA
38	V	609	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
38	V	609	CHL	C3C-C2C-CMC-OMC
38	W	601	CHL	C6-C7-C8-C10
38	W	607	CHL	C1C-C2C-CMC-OMC
38	W	607	CHL	C3C-C2C-CMC-OMC
38	W	607	CHL	CBD-CGD-O2D-CED
38	W	608	CHL	CBD-CGD-O2D-CED
38	W	609	CHL	C3A-C2A-CAA-CBA
27	2	601	CLA	O1D-CGD-O2D-CED
38	X	607	CHL	O1D-CGD-O2D-CED
38	Y	607	CHL	O1D-CGD-O2D-CED
27	A	802	CLA	O1D-CGD-O2D-CED
27	A	811	CLA	O1D-CGD-O2D-CED
27	A	825	CLA	O1D-CGD-O2D-CED
27	B	802	CLA	O1D-CGD-O2D-CED
27	B	803	CLA	O1D-CGD-O2D-CED
27	B	835	CLA	O1D-CGD-O2D-CED
27	a	607	CLA	O1D-CGD-O2D-CED
27	2	606	CLA	O1D-CGD-O2D-CED
38	X	608	CHL	O1D-CGD-O2D-CED
27	A	802	CLA	CBD-CGD-O2D-CED
27	A	810	CLA	CBD-CGD-O2D-CED
27	A	811	CLA	CBD-CGD-O2D-CED
27	A	818	CLA	CBD-CGD-O2D-CED
27	A	825	CLA	CBD-CGD-O2D-CED
27	A	829	CLA	CBD-CGD-O2D-CED
27	B	806	CLA	CBD-CGD-O2D-CED
27	B	809	CLA	CBD-CGD-O2D-CED
27	B	810	CLA	CBD-CGD-O2D-CED
27	B	836	CLA	CBD-CGD-O2D-CED
27	K	201	CLA	CBD-CGD-O2D-CED
27	2	601	CLA	CBD-CGD-O2D-CED
27	2	606	CLA	CBD-CGD-O2D-CED
27	2	607	CLA	CBD-CGD-O2D-CED
27	2	612	CLA	CBD-CGD-O2D-CED
27	2	616	CLA	CBD-CGD-O2D-CED
27	3	604	CLA	CBD-CGD-O2D-CED
27	3	608	CLA	CBD-CGD-O2D-CED
27	5	603	CLA	CBD-CGD-O2D-CED
27	5	607	CLA	CBD-CGD-O2D-CED
27	5	608	CLA	CBD-CGD-O2D-CED
27	6	603	CLA	CBD-CGD-O2D-CED
27	6	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	7	604	CLA	CBD-CGD-O2D-CED
27	7	608	CLA	CBD-CGD-O2D-CED
27	7	613	CLA	CBD-CGD-O2D-CED
27	X	602	CLA	CBD-CGD-O2D-CED
27	Y	602	CLA	CBD-CGD-O2D-CED
27	Z	610	CLA	CBD-CGD-O2D-CED
27	V	610	CLA	CBD-CGD-O2D-CED
27	V	613	CLA	CBD-CGD-O2D-CED
38	Y	608	CHL	CBD-CGD-O2D-CED
38	Z	608	CHL	CBD-CGD-O2D-CED
38	U	607	CHL	CBD-CGD-O2D-CED
38	V	608	CHL	CBD-CGD-O2D-CED
27	A	821	CLA	O1A-CGA-O2A-C1
27	8	613	CLA	O1A-CGA-O2A-C1
27	9	604	CLA	O1A-CGA-O2A-C1
29	3	624	LHG	O10-C23-O8-C6
27	F	301	CLA	O1D-CGD-O2D-CED
32	K	208	LMU	O5B-C1B-O1B-C4'
27	A	829	CLA	O1D-CGD-O2D-CED
27	2	612	CLA	O1D-CGD-O2D-CED
38	U	607	CHL	O1D-CGD-O2D-CED
38	W	607	CHL	O1D-CGD-O2D-CED
27	8	613	CLA	CBA-CGA-O2A-C1
27	9	604	CLA	CBA-CGA-O2A-C1
29	3	624	LHG	C24-C23-O8-C6
27	A	834	CLA	CBD-CGD-O2D-CED
27	7	601	CLA	CBD-CGD-O2D-CED
27	A	822	CLA	O1A-CGA-O2A-C1
27	B	802	CLA	O1A-CGA-O2A-C1
27	4	613	CLA	O1A-CGA-O2A-C1
27	5	607	CLA	O1A-CGA-O2A-C1
27	7	604	CLA	O1A-CGA-O2A-C1
27	F	303	CLA	O1D-CGD-O2D-CED
27	G	203	CLA	O1D-CGD-O2D-CED
27	2	604	CLA	O1D-CGD-O2D-CED
27	3	603	CLA	O1D-CGD-O2D-CED
27	5	603	CLA	O1D-CGD-O2D-CED
27	5	614	CLA	O1D-CGD-O2D-CED
27	6	603	CLA	O1D-CGD-O2D-CED
27	X	614	CLA	O1D-CGD-O2D-CED
27	Y	614	CLA	O1D-CGD-O2D-CED
38	Z	608	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
38	U	608	CHL	O1D-CGD-O2D-CED
27	B	827	CLA	O1D-CGD-O2D-CED
27	G	204	CLA	O1D-CGD-O2D-CED
27	5	617	CLA	O1D-CGD-O2D-CED
27	6	617	CLA	O1D-CGD-O2D-CED
27	8	607	CLA	O1D-CGD-O2D-CED
27	X	610	CLA	O1D-CGD-O2D-CED
27	Y	610	CLA	O1D-CGD-O2D-CED
27	U	610	CLA	O1D-CGD-O2D-CED
27	W	610	CLA	O1D-CGD-O2D-CED
38	W	608	CHL	O1D-CGD-O2D-CED
27	6	607	CLA	CBD-CGD-O2D-CED
27	6	608	CLA	CBD-CGD-O2D-CED
38	Z	607	CHL	CBD-CGD-O2D-CED
29	O	2631	LHG	O9-C7-O7-C5
29	3	623	LHG	O9-C7-O7-C5
34	B	850	DGD	O1B-C1B-O2G-C2G
27	A	815	CLA	O1D-CGD-O2D-CED
27	A	804	CLA	C3-C5-C6-C7
27	B	808	CLA	C3-C5-C6-C7
27	B	809	CLA	C3-C5-C6-C7
27	B	811	CLA	C3-C5-C6-C7
27	B	816	CLA	C3-C5-C6-C7
27	B	826	CLA	C3-C5-C6-C7
27	B	839	CLA	C3-C5-C6-C7
27	a	601	CLA	C3-C5-C6-C7
27	a	603	CLA	C3-C5-C6-C7
27	1	601	CLA	C3-C5-C6-C7
27	1	603	CLA	C3-C5-C6-C7
27	1	611	CLA	C3-C5-C6-C7
27	3	607	CLA	C3-C5-C6-C7
27	4	604	CLA	C3-C5-C6-C7
27	6	602	CLA	C3-C5-C6-C7
27	7	602	CLA	C3-C5-C6-C7
27	7	613	CLA	C3-C5-C6-C7
27	Z	603	CLA	C3-C5-C6-C7
27	Z	613	CLA	C3-C5-C6-C7
28	B	842	PQN	C13-C15-C16-C17
38	X	601	CHL	C3-C5-C6-C7
38	Z	601	CHL	C3-C5-C6-C7
27	7	612	CLA	O1D-CGD-O2D-CED
27	A	821	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	A	822	CLA	CBA-CGA-O2A-C1
27	A	834	CLA	CBA-CGA-O2A-C1
27	4	609	CLA	CBA-CGA-O2A-C1
27	4	613	CLA	CBA-CGA-O2A-C1
27	A	840	CLA	CBD-CGD-O2D-CED
27	A	841	CLA	CBD-CGD-O2D-CED
27	A	854	CLA	CBD-CGD-O2D-CED
27	B	813	CLA	CBD-CGD-O2D-CED
27	B	814	CLA	CBD-CGD-O2D-CED
27	B	822	CLA	CBD-CGD-O2D-CED
27	B	840	CLA	CBD-CGD-O2D-CED
27	F	304	CLA	CBD-CGD-O2D-CED
27	K	204	CLA	CBD-CGD-O2D-CED
27	a	604	CLA	CBD-CGD-O2D-CED
27	a	613	CLA	CBD-CGD-O2D-CED
27	1	604	CLA	CBD-CGD-O2D-CED
27	1	609	CLA	CBD-CGD-O2D-CED
27	1	613	CLA	CBD-CGD-O2D-CED
27	2	610	CLA	CBD-CGD-O2D-CED
27	3	602	CLA	CBD-CGD-O2D-CED
27	4	610	CLA	CBD-CGD-O2D-CED
27	4	616	CLA	CBD-CGD-O2D-CED
27	5	602	CLA	CBD-CGD-O2D-CED
27	5	610	CLA	CBD-CGD-O2D-CED
27	6	614	CLA	CBD-CGD-O2D-CED
27	6	620	CLA	CBD-CGD-O2D-CED
27	7	607	CLA	CBD-CGD-O2D-CED
27	8	610	CLA	CBD-CGD-O2D-CED
27	9	601	CLA	CBD-CGD-O2D-CED
27	X	611	CLA	CBD-CGD-O2D-CED
27	Y	611	CLA	CBD-CGD-O2D-CED
27	Z	614	CLA	CBD-CGD-O2D-CED
27	U	602	CLA	CBD-CGD-O2D-CED
27	U	611	CLA	CBD-CGD-O2D-CED
27	W	602	CLA	CBD-CGD-O2D-CED
27	W	611	CLA	CBD-CGD-O2D-CED
38	Z	606	CHL	CBD-CGD-O2D-CED
38	V	606	CHL	CBD-CGD-O2D-CED
38	V	609	CHL	CBD-CGD-O2D-CED
29	3	623	LHG	C8-C7-O7-C5
27	5	608	CLA	O1D-CGD-O2D-CED
27	U	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	V	604	CLA	O1D-CGD-O2D-CED
27	W	614	CLA	O1D-CGD-O2D-CED
27	8	604	CLA	O1A-CGA-O2A-C1
27	B	821	CLA	O1A-CGA-O2A-C1
27	A	854	CLA	C4-C3-C5-C6
27	B	831	CLA	C4-C3-C5-C6
27	8	610	CLA	C4-C3-C5-C6
38	X	601	CHL	C4-C3-C5-C6
38	Y	601	CHL	C4-C3-C5-C6
38	U	601	CHL	C4-C3-C5-C6
38	W	601	CHL	C4-C3-C5-C6
27	A	854	CLA	C2-C3-C5-C6
38	Y	601	CHL	C2-C3-C5-C6
38	U	601	CHL	C2-C3-C5-C6
38	W	601	CHL	C2-C3-C5-C6
27	B	821	CLA	CBA-CGA-O2A-C1
38	W	601	CHL	CBD-CGD-O2D-CED
27	B	806	CLA	O1D-CGD-O2D-CED
27	B	809	CLA	O1D-CGD-O2D-CED
27	6	610	CLA	O1D-CGD-O2D-CED
27	V	613	CLA	O1D-CGD-O2D-CED
38	Y	608	CHL	O1D-CGD-O2D-CED
27	A	805	CLA	C3-C5-C6-C7
27	A	822	CLA	C2A-CAA-CBA-CGA
27	A	840	CLA	C3-C5-C6-C7
27	A	839	CLA	O1A-CGA-O2A-C1
27	A	818	CLA	C3-C5-C6-C7
27	A	821	CLA	C3-C5-C6-C7
27	A	834	CLA	C3-C5-C6-C7
27	B	806	CLA	C3-C5-C6-C7
27	4	601	CLA	C3-C5-C6-C7
27	X	613	CLA	C3-C5-C6-C7
27	Y	613	CLA	C3-C5-C6-C7
27	U	613	CLA	C3-C5-C6-C7
27	W	613	CLA	C3-C5-C6-C7
27	A	816	CLA	CBA-CGA-O2A-C1
27	A	818	CLA	CBA-CGA-O2A-C1
27	A	839	CLA	CBA-CGA-O2A-C1
27	B	802	CLA	CBA-CGA-O2A-C1
27	L	303	CLA	CBA-CGA-O2A-C1
27	3	603	CLA	CBA-CGA-O2A-C1
27	5	607	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	6	616	CLA	CBA-CGA-O2A-C1
27	7	604	CLA	CBA-CGA-O2A-C1
27	A	818	CLA	O1A-CGA-O2A-C1
27	A	832	CLA	O1A-CGA-O2A-C1
27	A	834	CLA	O1A-CGA-O2A-C1
27	L	303	CLA	O1A-CGA-O2A-C1
27	3	603	CLA	O1A-CGA-O2A-C1
27	3	610	CLA	O1A-CGA-O2A-C1
27	4	604	CLA	O1A-CGA-O2A-C1
29	9	623	LHG	O9-C7-O7-C5
33	L	2631	LMG	O9-C10-O7-C8
27	5	607	CLA	O1D-CGD-O2D-CED
27	A	806	CLA	C3-C5-C6-C7
27	B	813	CLA	C3-C5-C6-C7
27	4	613	CLA	C3-C5-C6-C7
27	5	603	CLA	C3-C5-C6-C7
27	8	601	CLA	C3-C5-C6-C7
27	V	602	CLA	C3-C5-C6-C7
27	A	807	CLA	CBD-CGD-O2D-CED
27	A	820	CLA	CBD-CGD-O2D-CED
27	K	206	CLA	CBD-CGD-O2D-CED
27	6	602	CLA	CBD-CGD-O2D-CED
27	Z	603	CLA	CBD-CGD-O2D-CED
29	B	854	LHG	O2-C2-C3-O3
29	6	623	LHG	O2-C2-C3-O3
29	9	624	LHG	O2-C2-C3-O3
27	A	818	CLA	O1D-CGD-O2D-CED
27	7	604	CLA	O1D-CGD-O2D-CED
38	V	608	CHL	O1D-CGD-O2D-CED
27	A	813	CLA	CBA-CGA-O2A-C1
27	A	830	CLA	CBA-CGA-O2A-C1
27	A	843	CLA	CBA-CGA-O2A-C1
27	B	831	CLA	CBA-CGA-O2A-C1
27	1	611	CLA	CBA-CGA-O2A-C1
27	2	613	CLA	CBA-CGA-O2A-C1
27	7	613	CLA	CBA-CGA-O2A-C1
27	8	604	CLA	CBA-CGA-O2A-C1
38	U	601	CHL	CBA-CGA-O2A-C1
27	7	613	CLA	O1A-CGA-O2A-C1
32	5	628	LMU	C4'-C5'-C6'-O6'
27	A	810	CLA	O1D-CGD-O2D-CED
27	2	616	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	3	604	CLA	O1D-CGD-O2D-CED
27	7	608	CLA	O1D-CGD-O2D-CED
32	K	208	LMU	O5B-C5B-C6B-O6B
32	5	629	LMU	O5B-C5B-C6B-O6B
33	L	2631	LMG	C11-C10-O7-C8
27	B	831	CLA	O1A-CGA-O2A-C1
27	3	608	CLA	O1D-CGD-O2D-CED
27	Z	610	CLA	O1D-CGD-O2D-CED
27	a	614	CLA	C3-C5-C6-C7
27	6	613	CLA	C3-C5-C6-C7
27	8	606	CLA	C3-C5-C6-C7
27	A	821	CLA	CBD-CGD-O2D-CED
27	B	824	CLA	CBD-CGD-O2D-CED
27	B	839	CLA	CBD-CGD-O2D-CED
27	8	614	CLA	CBD-CGD-O2D-CED
27	9	607	CLA	CBD-CGD-O2D-CED
27	B	810	CLA	O1D-CGD-O2D-CED
27	B	836	CLA	O1D-CGD-O2D-CED
27	2	607	CLA	O1D-CGD-O2D-CED
27	7	613	CLA	O1D-CGD-O2D-CED
27	X	602	CLA	O1D-CGD-O2D-CED
27	Y	602	CLA	O1D-CGD-O2D-CED
27	A	832	CLA	CBA-CGA-O2A-C1
27	3	604	CLA	CBA-CGA-O2A-C1
27	3	610	CLA	CBA-CGA-O2A-C1
27	4	604	CLA	CBA-CGA-O2A-C1
27	Y	614	CLA	CBA-CGA-O2A-C1
27	B	818	CLA	C4-C3-C5-C6
27	L	303	CLA	C4-C3-C5-C6
27	B	818	CLA	C2-C3-C5-C6
27	B	831	CLA	C2-C3-C5-C6
38	X	601	CHL	C2-C3-C5-C6
27	A	816	CLA	O1A-CGA-O2A-C1
27	A	830	CLA	O1A-CGA-O2A-C1
27	6	616	CLA	O1A-CGA-O2A-C1
32	5	629	LMU	O5'-C5'-C6'-O6'
27	A	842	CLA	CBD-CGD-O2D-CED
27	A	843	CLA	C2A-CAA-CBA-CGA
27	2	601	CLA	C2A-CAA-CBA-CGA
27	K	201	CLA	O1D-CGD-O2D-CED
27	A	813	CLA	O1A-CGA-O2A-C1
27	A	843	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
38	U	601	CHL	O1A-CGA-O2A-C1
34	B	850	DGD	O6D-C1D-O3G-C3G
32	5	628	LMU	O5'-C5'-C6'-O6'
27	V	610	CLA	O1D-CGD-O2D-CED
27	B	828	CLA	CBA-CGA-O2A-C1
38	Y	601	CHL	CBA-CGA-O2A-C1
27	A	826	CLA	CBD-CGD-O2D-CED
27	A	827	CLA	CBD-CGD-O2D-CED
27	A	832	CLA	CBD-CGD-O2D-CED
27	A	838	CLA	CBD-CGD-O2D-CED
27	B	816	CLA	CBD-CGD-O2D-CED
27	B	819	CLA	CBD-CGD-O2D-CED
27	B	832	CLA	CBD-CGD-O2D-CED
27	B	834	CLA	CBD-CGD-O2D-CED
27	a	612	CLA	CBD-CGD-O2D-CED
27	1	612	CLA	CBD-CGD-O2D-CED
27	8	601	CLA	CBD-CGD-O2D-CED
27	8	602	CLA	CBD-CGD-O2D-CED
27	9	602	CLA	CBD-CGD-O2D-CED
27	V	614	CLA	CBD-CGD-O2D-CED
38	X	601	CHL	CBD-CGD-O2D-CED
38	Y	601	CHL	CBD-CGD-O2D-CED
38	U	601	CHL	CBD-CGD-O2D-CED
27	1	611	CLA	O1A-CGA-O2A-C1
27	2	613	CLA	O1A-CGA-O2A-C1
27	A	834	CLA	O1D-CGD-O2D-CED
27	7	601	CLA	O1D-CGD-O2D-CED
27	A	823	CLA	CBD-CGD-O2D-CED
27	4	602	CLA	CBD-CGD-O2D-CED
27	A	828	CLA	C3-C5-C6-C7
32	A	858	LMU	C5'-C4'-O1B-C1B
38	Z	607	CHL	O1D-CGD-O2D-CED
32	5	629	LMU	C4B-C5B-C6B-O6B
27	B	818	CLA	O1A-CGA-O2A-C1
27	3	604	CLA	O1A-CGA-O2A-C1
27	Y	614	CLA	O1A-CGA-O2A-C1
29	9	624	LHG	C1-C2-C3-O3
27	A	801	CLA	CBA-CGA-O2A-C1
27	A	807	CLA	CBA-CGA-O2A-C1
27	A	841	CLA	CBA-CGA-O2A-C1
27	B	813	CLA	CBA-CGA-O2A-C1
27	B	818	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	2	601	CLA	CBA-CGA-O2A-C1
27	5	604	CLA	CBA-CGA-O2A-C1
27	6	604	CLA	CBA-CGA-O2A-C1
27	8	601	CLA	CBA-CGA-O2A-C1
27	8	602	CLA	CBA-CGA-O2A-C1
27	X	604	CLA	CBA-CGA-O2A-C1
27	Y	604	CLA	CBA-CGA-O2A-C1
27	U	604	CLA	CBA-CGA-O2A-C1
27	W	604	CLA	CBA-CGA-O2A-C1
29	A	846	LHG	C24-C23-O8-C6
38	X	601	CHL	CBA-CGA-O2A-C1
27	J	101	CLA	CBD-CGD-O2D-CED
27	B	810	CLA	C2A-CAA-CBA-CGA
27	B	813	CLA	O1D-CGD-O2D-CED
27	B	822	CLA	O1D-CGD-O2D-CED
27	B	840	CLA	O1D-CGD-O2D-CED
27	K	204	CLA	O1D-CGD-O2D-CED
27	6	607	CLA	O1D-CGD-O2D-CED
27	6	608	CLA	O1D-CGD-O2D-CED
27	8	610	CLA	C2-C3-C5-C6
27	B	823	CLA	CBD-CGD-O2D-CED
27	A	807	CLA	C11-C10-C8-C9
27	A	828	CLA	C6-C7-C8-C9
27	B	802	CLA	C11-C12-C13-C14
27	B	805	CLA	C6-C7-C8-C9
27	L	303	CLA	C14-C13-C15-C16
27	1	611	CLA	C11-C10-C8-C9
27	3	609	CLA	C11-C10-C8-C9
27	5	604	CLA	C6-C7-C8-C9
27	7	601	CLA	C6-C7-C8-C9
38	X	607	CHL	C6-C7-C8-C9
38	X	608	CHL	C11-C12-C13-C14
38	X	609	CHL	C11-C10-C8-C9
38	X	609	CHL	C11-C12-C13-C14
38	Y	607	CHL	C6-C7-C8-C9
38	Y	609	CHL	C11-C10-C8-C9
38	Y	609	CHL	C11-C12-C13-C14
38	Z	607	CHL	C6-C7-C8-C9
38	Z	609	CHL	C6-C7-C8-C9
38	Z	609	CHL	C14-C13-C15-C16
38	U	609	CHL	C6-C7-C8-C9
38	U	609	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
38	V	601	CHL	C14-C13-C15-C16
38	W	607	CHL	C6-C7-C8-C9
38	W	609	CHL	C11-C10-C8-C9
38	W	609	CHL	C11-C12-C13-C14
27	A	841	CLA	O1D-CGD-O2D-CED
27	B	814	CLA	O1D-CGD-O2D-CED
27	F	304	CLA	O1D-CGD-O2D-CED
27	1	609	CLA	O1D-CGD-O2D-CED
27	Z	614	CLA	O1D-CGD-O2D-CED
27	U	602	CLA	O1D-CGD-O2D-CED
27	W	602	CLA	O1D-CGD-O2D-CED
32	K	208	LMU	C2'-C1'-O1'-C1
32	5	628	LMU	C2'-C1'-O1'-C1
32	8	625	LMU	C3'-C4'-O1B-C1B
29	3	624	LHG	O2-C2-C3-O3
27	2	610	CLA	O1D-CGD-O2D-CED
38	V	606	CHL	O1D-CGD-O2D-CED
38	V	609	CHL	O1D-CGD-O2D-CED
27	5	604	CLA	O1A-CGA-O2A-C1
27	A	835	CLA	CBD-CGD-O2D-CED
27	4	616	CLA	O1D-CGD-O2D-CED
27	5	610	CLA	O1D-CGD-O2D-CED
30	B	847	BCR	C37-C22-C23-C24
30	L	305	BCR	C7-C8-C9-C34
30	O	2005	BCR	C37-C22-C23-C24
30	7	621	BCR	C37-C22-C23-C24
30	L	305	BCR	C7-C8-C9-C10
38	Z	608	CHL	C2A-CAA-CBA-CGA
38	W	607	CHL	C2A-CAA-CBA-CGA
29	7	622	LHG	C23-C24-C25-C26
27	8	601	CLA	O1A-CGA-O2A-C1
27	U	604	CLA	O1A-CGA-O2A-C1
27	W	604	CLA	O1A-CGA-O2A-C1
27	B	810	CLA	C3-C5-C6-C7
27	4	614	CLA	C3-C5-C6-C7
32	K	208	LMU	O5'-C5'-C6'-O6'
38	X	609	CHL	CBD-CGD-O2D-CED
27	B	838	CLA	CBA-CGA-O2A-C1
27	B	813	CLA	C2C-C3C-CAC-CBC
27	B	825	CLA	CBA-CGA-O2A-C1
27	B	837	CLA	CBA-CGA-O2A-C1
27	a	609	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	2	622	LHG	C24-C23-O8-C6
27	6	614	CLA	C8-C10-C11-C12
27	3	602	CLA	O1D-CGD-O2D-CED
27	4	610	CLA	O1D-CGD-O2D-CED
27	7	607	CLA	O1D-CGD-O2D-CED
27	9	601	CLA	O1D-CGD-O2D-CED
27	X	611	CLA	O1D-CGD-O2D-CED
27	Y	611	CLA	O1D-CGD-O2D-CED
38	X	601	CHL	C13-C15-C16-C17
38	Z	609	CHL	C15-C16-C17-C18
38	W	601	CHL	C10-C11-C12-C13
27	W	611	CLA	C3-C5-C6-C7
27	a	604	CLA	O1D-CGD-O2D-CED
27	1	604	CLA	O1D-CGD-O2D-CED
27	6	614	CLA	O1D-CGD-O2D-CED
27	X	604	CLA	O1A-CGA-O2A-C1
27	B	829	CLA	CBD-CGD-O2D-CED
27	a	616	CLA	CBD-CGD-O2D-CED
27	1	616	CLA	CBD-CGD-O2D-CED
27	4	607	CLA	CBD-CGD-O2D-CED
27	B	802	CLA	C12-C13-C15-C16
27	B	806	CLA	C11-C10-C8-C7
27	B	813	CLA	C6-C7-C8-C10
27	V	613	CLA	C6-C7-C8-C10
38	X	608	CHL	C11-C10-C8-C7
38	Y	601	CHL	C6-C7-C8-C10
38	U	601	CHL	C6-C7-C8-C10
38	V	601	CHL	C6-C7-C8-C10
27	8	614	CLA	CBA-CGA-O2A-C1
27	A	842	CLA	C4-C3-C5-C6
27	3	602	CLA	C10-C11-C12-C13
32	5	628	LMU	C5'-C4'-O1B-C1B
27	Y	604	CLA	O1A-CGA-O2A-C1
27	6	620	CLA	O1D-CGD-O2D-CED
27	8	610	CLA	O1D-CGD-O2D-CED
27	F	301	CLA	C3-C5-C6-C7
27	V	613	CLA	C3-C5-C6-C7
27	B	824	CLA	C10-C11-C12-C13
27	6	613	CLA	C5-C6-C7-C8
29	A	847	LHG	C23-C24-C25-C26
29	B	854	LHG	C7-C8-C9-C10
33	J	103	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	A	841	CLA	O1A-CGA-O2A-C1
27	B	813	CLA	O1A-CGA-O2A-C1
27	2	601	CLA	O1A-CGA-O2A-C1
27	6	604	CLA	O1A-CGA-O2A-C1
27	8	602	CLA	O1A-CGA-O2A-C1
29	A	846	LHG	O10-C23-O8-C6
32	5	628	LMU	O5B-C1B-O1B-C4'
27	A	831	CLA	CBD-CGD-O2D-CED
27	A	854	CLA	O1D-CGD-O2D-CED
27	U	611	CLA	O1D-CGD-O2D-CED
27	W	611	CLA	O1D-CGD-O2D-CED
27	A	807	CLA	C5-C6-C7-C8
27	A	829	CLA	C5-C6-C7-C8
27	B	802	CLA	C5-C6-C7-C8
27	B	808	CLA	C5-C6-C7-C8
27	9	609	CLA	C5-C6-C7-C8
27	X	602	CLA	C8-C10-C11-C12
27	Y	602	CLA	C8-C10-C11-C12
27	Z	604	CLA	C5-C6-C7-C8
27	Z	611	CLA	C8-C10-C11-C12
38	X	608	CHL	C15-C16-C17-C18
38	X	609	CHL	C13-C15-C16-C17
38	Z	607	CHL	C8-C10-C11-C12
38	U	601	CHL	C8-C10-C11-C12
38	W	601	CHL	C8-C10-C11-C12
27	A	809	CLA	C2A-CAA-CBA-CGA
27	A	841	CLA	C2A-CAA-CBA-CGA
27	B	831	CLA	C2A-CAA-CBA-CGA
27	B	839	CLA	C2A-CAA-CBA-CGA
27	L	302	CLA	C2A-CAA-CBA-CGA
27	a	616	CLA	C2A-CAA-CBA-CGA
27	1	616	CLA	C2A-CAA-CBA-CGA
27	3	609	CLA	C2A-CAA-CBA-CGA
27	6	616	CLA	C2A-CAA-CBA-CGA
27	8	601	CLA	C2A-CAA-CBA-CGA
27	8	604	CLA	C2A-CAA-CBA-CGA
38	Y	607	CHL	C2A-CAA-CBA-CGA
38	Y	608	CHL	C2A-CAA-CBA-CGA
38	U	607	CHL	C2A-CAA-CBA-CGA
38	W	605	CHL	C2A-CAA-CBA-CGA
27	A	842	CLA	C15-C16-C17-C18
27	B	805	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	B	827	CLA	C8-C10-C11-C12
27	B	839	CLA	C13-C15-C16-C17
27	6	601	CLA	C13-C15-C16-C17
27	6	610	CLA	C15-C16-C17-C18
27	7	610	CLA	C5-C6-C7-C8
27	8	601	CLA	C15-C16-C17-C18
27	8	610	CLA	C8-C10-C11-C12
28	A	844	PQN	C23-C25-C26-C27
38	X	608	CHL	C13-C15-C16-C17
38	Y	601	CHL	C8-C10-C11-C12
38	V	601	CHL	C13-C15-C16-C17
38	V	601	CHL	C15-C16-C17-C18
38	V	609	CHL	C8-C10-C11-C12
38	W	607	CHL	C8-C10-C11-C12
33	4	624	LMG	O6-C5-C6-O5
29	3	623	LHG	C7-C8-C9-C10
29	6	623	LHG	C23-C24-C25-C26
33	V	2631	LMG	C10-C11-C12-C13
27	A	801	CLA	O1A-CGA-O2A-C1
38	X	601	CHL	O1A-CGA-O2A-C1
33	8	626	LMG	C16-C17-C18-C19
38	Z	606	CHL	O1D-CGD-O2D-CED
32	K	208	LMU	C4B-C5B-C6B-O6B
27	A	816	CLA	C8-C10-C11-C12
27	A	820	CLA	C15-C16-C17-C18
27	A	828	CLA	C10-C11-C12-C13
27	A	831	CLA	C8-C10-C11-C12
27	A	836	CLA	C5-C6-C7-C8
27	A	842	CLA	C5-C6-C7-C8
27	B	824	CLA	C13-C15-C16-C17
27	B	826	CLA	C10-C11-C12-C13
27	B	831	CLA	C10-C11-C12-C13
27	B	834	CLA	C5-C6-C7-C8
27	B	837	CLA	C15-C16-C17-C18
27	B	839	CLA	C15-C16-C17-C18
27	3	613	CLA	C5-C6-C7-C8
27	4	601	CLA	C5-C6-C7-C8
27	4	610	CLA	C8-C10-C11-C12
27	5	602	CLA	C13-C15-C16-C17
27	6	602	CLA	C15-C16-C17-C18
27	X	602	CLA	C13-C15-C16-C17
27	X	610	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	Y	610	CLA	C8-C10-C11-C12
38	X	601	CHL	C8-C10-C11-C12
38	X	608	CHL	C5-C6-C7-C8
38	Z	601	CHL	C13-C15-C16-C17
38	V	601	CHL	C5-C6-C7-C8
38	W	607	CHL	C15-C16-C17-C18
38	W	609	CHL	C15-C16-C17-C18
27	A	811	CLA	CBA-CGA-O2A-C1
27	B	814	CLA	CBA-CGA-O2A-C1
27	B	828	CLA	O1A-CGA-O2A-C1
38	Y	601	CHL	O1A-CGA-O2A-C1
27	B	813	CLA	C4C-C3C-CAC-CBC
27	A	824	CLA	C10-C11-C12-C13
27	A	829	CLA	C8-C10-C11-C12
27	B	802	CLA	C10-C11-C12-C13
38	W	607	CHL	C13-C15-C16-C17
27	A	807	CLA	O1D-CGD-O2D-CED
27	a	613	CLA	O1D-CGD-O2D-CED
27	A	840	CLA	O1D-CGD-O2D-CED
27	K	206	CLA	O1D-CGD-O2D-CED
27	1	613	CLA	O1D-CGD-O2D-CED
27	5	602	CLA	O1D-CGD-O2D-CED
27	Z	603	CLA	O1D-CGD-O2D-CED
38	W	601	CHL	O1D-CGD-O2D-CED
27	A	828	CLA	C15-C16-C17-C18
27	B	810	CLA	C13-C15-C16-C17
27	L	303	CLA	C13-C15-C16-C17
27	6	604	CLA	C13-C15-C16-C17
27	9	613	CLA	C5-C6-C7-C8
38	X	607	CHL	C15-C16-C17-C18
38	X	608	CHL	C8-C10-C11-C12
38	Y	609	CHL	C13-C15-C16-C17
38	Z	601	CHL	C8-C10-C11-C12
27	K	203	CLA	CBD-CGD-O2D-CED
27	A	807	CLA	O1A-CGA-O2A-C1
27	a	609	CLA	O1A-CGA-O2A-C1
33	9	625	LMG	C10-C11-C12-C13
27	A	820	CLA	O1D-CGD-O2D-CED
27	A	814	CLA	C8-C10-C11-C12
27	A	816	CLA	C15-C16-C17-C18
27	A	834	CLA	C10-C11-C12-C13
27	1	613	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	4	613	CLA	C10-C11-C12-C13
27	8	613	CLA	C10-C11-C12-C13
27	9	609	CLA	C10-C11-C12-C13
27	U	602	CLA	C8-C10-C11-C12
27	V	610	CLA	C5-C6-C7-C8
27	W	602	CLA	C8-C10-C11-C12
38	Z	609	CHL	C13-C15-C16-C17
27	A	809	CLA	CBA-CGA-O2A-C1
27	A	820	CLA	CBA-CGA-O2A-C1
27	A	814	CLA	CBD-CGD-O2D-CED
27	A	817	CLA	CBD-CGD-O2D-CED
27	B	837	CLA	CBD-CGD-O2D-CED
29	B	854	LHG	C8-C7-O7-C5
29	3	624	LHG	C8-C7-O7-C5
27	B	825	CLA	O1A-CGA-O2A-C1
27	6	602	CLA	O1D-CGD-O2D-CED
27	7	601	CLA	C3-C5-C6-C7
32	5	628	LMU	C3'-C4'-O1B-C1B
27	V	610	CLA	C13-C15-C16-C17
27	A	837	CLA	CBD-CGD-O2D-CED
27	Z	610	CLA	C5-C6-C7-C8
29	B	854	LHG	O9-C7-O7-C5
29	3	624	LHG	O9-C7-O7-C5
27	A	832	CLA	C2A-CAA-CBA-CGA
27	B	828	CLA	C2A-CAA-CBA-CGA
38	X	608	CHL	C2A-CAA-CBA-CGA
27	B	805	CLA	CBA-CGA-O2A-C1
27	3	607	CLA	CBA-CGA-O2A-C1
27	5	603	CLA	CBA-CGA-O2A-C1
27	6	602	CLA	CBA-CGA-O2A-C1
27	6	614	CLA	CBA-CGA-O2A-C1
27	7	601	CLA	CBA-CGA-O2A-C1
27	8	608	CLA	CBA-CGA-O2A-C1
27	U	613	CLA	CBA-CGA-O2A-C1
27	W	613	CLA	CBA-CGA-O2A-C1
29	H	204	LHG	C24-C23-O8-C6
29	9	622	LHG	C24-C23-O8-C6
27	A	806	CLA	C8-C10-C11-C12
27	A	811	CLA	C8-C10-C11-C12
27	A	829	CLA	C10-C11-C12-C13
27	A	829	CLA	C15-C16-C17-C18
27	2	613	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	3	604	CLA	C15-C16-C17-C18
27	5	602	CLA	C8-C10-C11-C12
27	6	604	CLA	C5-C6-C7-C8
27	9	602	CLA	C8-C10-C11-C12
27	Z	610	CLA	C13-C15-C16-C17
27	V	613	CLA	C13-C15-C16-C17
28	B	842	PQN	C25-C26-C27-C28
38	Y	601	CHL	C5-C6-C7-C8
27	4	601	CLA	CBD-CGD-O2D-CED
27	Z	604	CLA	CBD-CGD-O2D-CED
27	B	816	CLA	CAA-CBA-CGA-O2A
33	4	623	LMG	C28-C29-C30-C31
27	A	811	CLA	C10-C11-C12-C13
27	A	841	CLA	C5-C6-C7-C8
27	B	833	CLA	C8-C10-C11-C12
27	3	607	CLA	C5-C6-C7-C8
27	5	613	CLA	C13-C15-C16-C17
27	Z	613	CLA	C15-C16-C17-C18
38	W	609	CHL	C13-C15-C16-C17
27	B	831	CLA	C15-C16-C17-C18
27	a	601	CLA	C5-C6-C7-C8
27	a	614	CLA	C5-C6-C7-C8
27	1	601	CLA	C5-C6-C7-C8
27	3	610	CLA	C8-C10-C11-C12
27	5	604	CLA	C10-C11-C12-C13
27	6	604	CLA	C15-C16-C17-C18
27	9	602	CLA	C5-C6-C7-C8
27	X	602	CLA	C10-C11-C12-C13
27	U	610	CLA	C5-C6-C7-C8
27	W	602	CLA	C10-C11-C12-C13
27	W	610	CLA	C5-C6-C7-C8
38	Y	601	CHL	C13-C15-C16-C17
38	U	601	CHL	C13-C15-C16-C17
38	W	607	CHL	C10-C11-C12-C13
27	B	828	CLA	C13-C15-C16-C17
27	5	609	CLA	C13-C15-C16-C17
38	Y	601	CHL	C10-C11-C12-C13
38	W	609	CHL	C8-C10-C11-C12
32	K	208	LMU	O1'-C1-C2-C3
27	5	602	CLA	C10-C11-C12-C13
27	B	824	CLA	O1D-CGD-O2D-CED
27	B	839	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	9	607	CLA	O1D-CGD-O2D-CED
27	5	617	CLA	CBA-CGA-O2A-C1
32	A	858	LMU	O5B-C5B-C6B-O6B
38	X	601	CHL	C16-C17-C18-C19
38	W	607	CHL	C16-C17-C18-C20
38	X	601	CHL	C10-C11-C12-C13
27	B	837	CLA	O1A-CGA-O2A-C1
29	a	620	LHG	C7-C8-C9-C10
27	a	609	CLA	C10-C11-C12-C13
27	5	604	CLA	C8-C10-C11-C12
30	B	852	BCR	C11-C12-C13-C35
30	O	2004	BCR	C7-C8-C9-C34
30	3	622	BCR	C37-C22-C23-C24
38	Z	605	CHL	C2A-CAA-CBA-CGA
30	B	852	BCR	C11-C12-C13-C14
30	O	2004	BCR	C7-C8-C9-C10
35	Z	1621	LUT	C7-C8-C9-C10
27	B	814	CLA	O1A-CGA-O2A-C1
27	6	602	CLA	O1A-CGA-O2A-C1
27	8	614	CLA	O1A-CGA-O2A-C1
27	A	824	CLA	C2A-CAA-CBA-CGA
27	A	833	CLA	C2A-CAA-CBA-CGA
27	A	834	CLA	C2A-CAA-CBA-CGA
27	B	809	CLA	C2A-CAA-CBA-CGA
27	4	613	CLA	C2A-CAA-CBA-CGA
27	7	603	CLA	C2A-CAA-CBA-CGA
27	8	613	CLA	C2A-CAA-CBA-CGA
27	A	806	CLA	C10-C11-C12-C13
27	a	609	CLA	C5-C6-C7-C8
27	1	613	CLA	C8-C10-C11-C12
29	6	623	LHG	O1-C1-C2-C3
29	1	620	LHG	C7-C8-C9-C10
27	B	802	CLA	C16-C17-C18-C20
27	B	816	CLA	C6-C7-C8-C10
27	5	604	CLA	C16-C17-C18-C19
27	6	601	CLA	C16-C17-C18-C20
27	V	613	CLA	C16-C17-C18-C20
28	A	844	PQN	C26-C27-C28-C30
38	X	607	CHL	C16-C17-C18-C20
38	Y	607	CHL	C16-C17-C18-C20
27	A	821	CLA	O1D-CGD-O2D-CED
27	8	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	B	805	CLA	O1A-CGA-O2A-C1
29	2	622	LHG	O10-C23-O8-C6
27	A	807	CLA	C3-C5-C6-C7
27	A	816	CLA	C3-C5-C6-C7
27	6	604	CLA	C3-C5-C6-C7
27	B	806	CLA	C5-C6-C7-C8
27	3	604	CLA	C10-C11-C12-C13
38	Y	609	CHL	C15-C16-C17-C18
27	L	303	CLA	C2-C3-C5-C6
27	A	832	CLA	O1D-CGD-O2D-CED
27	2	602	CLA	CBA-CGA-O2A-C1
27	a	610	CLA	C5-C6-C7-C8
27	6	616	CLA	C8-C10-C11-C12
29	H	204	LHG	C23-C24-C25-C26
27	7	615	CLA	CBD-CGD-O2D-CED
27	A	842	CLA	O1D-CGD-O2D-CED
38	Y	608	CHL	O2A-C1-C2-C3
27	A	807	CLA	C16-C17-C18-C20
27	B	808	CLA	C16-C17-C18-C19
27	B	816	CLA	C6-C7-C8-C9
27	B	819	CLA	C6-C7-C8-C9
27	B	819	CLA	C6-C7-C8-C10
27	5	604	CLA	C16-C17-C18-C20
27	5	613	CLA	C16-C17-C18-C19
27	5	613	CLA	C16-C17-C18-C20
27	6	601	CLA	C16-C17-C18-C19
27	Z	610	CLA	C16-C17-C18-C20
27	Z	613	CLA	C16-C17-C18-C20
38	X	608	CHL	C16-C17-C18-C19
38	Y	601	CHL	C16-C17-C18-C19
38	Y	609	CHL	C16-C17-C18-C20
38	U	601	CHL	C16-C17-C18-C19
38	V	609	CHL	C11-C12-C13-C15
38	W	601	CHL	C16-C17-C18-C20
27	A	809	CLA	O1A-CGA-O2A-C1
27	A	820	CLA	O1A-CGA-O2A-C1
27	B	837	CLA	C13-C15-C16-C17
38	Y	607	CHL	C8-C10-C11-C12
29	2	622	LHG	C11-C10-C9-C8
33	A	860	LMG	C16-C17-C18-C19
27	4	614	CLA	CBD-CGD-O2D-CED
29	B	854	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
29	5	623	LHG	C28-C29-C30-C31
33	J	104	LMG	C14-C15-C16-C17
33	9	625	LMG	C14-C15-C16-C17
33	9	625	LMG	C29-C30-C31-C32
27	a	612	CLA	O1D-CGD-O2D-CED
27	1	612	CLA	O1D-CGD-O2D-CED
38	X	601	CHL	O1D-CGD-O2D-CED
29	6	623	LHG	C7-C8-C9-C10
38	X	607	CHL	C8-C10-C11-C12
38	U	601	CHL	C10-C11-C12-C13
33	4	624	LMG	C30-C31-C32-C33
27	A	811	CLA	O1A-CGA-O2A-C1
27	5	603	CLA	O1A-CGA-O2A-C1
27	B	832	CLA	O1D-CGD-O2D-CED
27	B	829	CLA	CBA-CGA-O2A-C1
27	B	840	CLA	CBA-CGA-O2A-C1
38	W	607	CHL	CBA-CGA-O2A-C1
29	8	622	LHG	C31-C32-C33-C34
32	1	621	LMU	C7-C8-C9-C10
32	5	629	LMU	C4-C5-C6-C7
33	J	104	LMG	C16-C17-C18-C19
33	9	625	LMG	C22-C23-C24-C25
29	9	624	LHG	O1-C1-C2-O2
32	A	858	LMU	C2-C1-O1'-C1'
32	5	628	LMU	C2-C1-O1'-C1'
27	U	602	CLA	C10-C11-C12-C13
27	A	826	CLA	O1D-CGD-O2D-CED
27	B	816	CLA	O1D-CGD-O2D-CED
27	B	819	CLA	O1D-CGD-O2D-CED
27	A	806	CLA	C13-C15-C16-C17
38	X	607	CHL	C5-C6-C7-C8
27	A	815	CLA	C4B-C3B-CAB-CBB
27	A	837	CLA	C4B-C3B-CAB-CBB
27	A	841	CLA	C4B-C3B-CAB-CBB
27	B	802	CLA	C4B-C3B-CAB-CBB
27	B	807	CLA	C4B-C3B-CAB-CBB
27	B	817	CLA	C4B-C3B-CAB-CBB
27	B	823	CLA	C4B-C3B-CAB-CBB
27	B	830	CLA	C4B-C3B-CAB-CBB
27	F	301	CLA	C4B-C3B-CAB-CBB
27	H	203	CLA	C4B-C3B-CAB-CBB
27	a	604	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	1	604	CLA	C4B-C3B-CAB-CBB
27	3	617	CLA	C4B-C3B-CAB-CBB
27	5	606	CLA	C4B-C3B-CAB-CBB
27	5	617	CLA	C4B-C3B-CAB-CBB
27	6	608	CLA	C4B-C3B-CAB-CBB
27	6	614	CLA	C4B-C3B-CAB-CBB
27	8	611	CLA	C4B-C3B-CAB-CBB
27	X	603	CLA	C4B-C3B-CAB-CBB
27	X	612	CLA	C4B-C3B-CAB-CBB
27	X	614	CLA	C4B-C3B-CAB-CBB
27	Y	603	CLA	C4B-C3B-CAB-CBB
27	Y	612	CLA	C4B-C3B-CAB-CBB
27	Y	614	CLA	C4B-C3B-CAB-CBB
27	U	603	CLA	C4B-C3B-CAB-CBB
27	U	612	CLA	C4B-C3B-CAB-CBB
27	W	603	CLA	C4B-C3B-CAB-CBB
27	W	612	CLA	C4B-C3B-CAB-CBB
27	B	808	CLA	C16-C17-C18-C20
27	1	613	CLA	C16-C17-C18-C19
27	1	613	CLA	C16-C17-C18-C20
27	V	613	CLA	C16-C17-C18-C19
28	A	844	PQN	C26-C27-C28-C29
38	X	607	CHL	C16-C17-C18-C19
38	X	608	CHL	C16-C17-C18-C20
38	X	609	CHL	C16-C17-C18-C19
38	Y	609	CHL	C16-C17-C18-C19
38	Z	609	CHL	C16-C17-C18-C19
38	V	601	CHL	C16-C17-C18-C19
38	V	601	CHL	C16-C17-C18-C20
38	V	609	CHL	C11-C12-C13-C14
38	W	609	CHL	C16-C17-C18-C19
27	9	602	CLA	O1D-CGD-O2D-CED
27	V	614	CLA	O1D-CGD-O2D-CED
27	U	613	CLA	C2A-CAA-CBA-CGA
27	W	613	CLA	C2A-CAA-CBA-CGA
38	Z	607	CHL	C2A-CAA-CBA-CGA
27	B	813	CLA	C5-C6-C7-C8
27	6	610	CLA	C8-C10-C11-C12
27	8	610	CLA	C10-C11-C12-C13
38	Y	607	CHL	C13-C15-C16-C17
29	5	625	LHG	C8-C7-O7-C5
32	8	625	LMU	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
27	A	814	CLA	C11-C10-C8-C7
27	B	818	CLA	C11-C10-C8-C7
27	B	826	CLA	C11-C10-C8-C7
27	6	620	CLA	C11-C12-C13-C15
27	8	613	CLA	C11-C10-C8-C7
27	U	613	CLA	C11-C10-C8-C7
27	W	613	CLA	C11-C10-C8-C7
38	Z	601	CHL	C6-C7-C8-C10
38	V	601	CHL	C11-C12-C13-C15
29	A	846	LHG	C31-C32-C33-C34
33	5	627	LMG	C10-C11-C12-C13
27	A	807	CLA	C15-C16-C17-C18
27	A	824	CLA	C13-C15-C16-C17
27	Z	612	CLA	C10-C11-C12-C13
38	X	601	CHL	C5-C6-C7-C8
38	W	601	CHL	C15-C16-C17-C18
27	6	614	CLA	O1A-CGA-O2A-C1
27	8	608	CLA	O1A-CGA-O2A-C1
27	A	806	CLA	C3A-C2A-CAA-CBA
27	A	810	CLA	C3A-C2A-CAA-CBA
27	A	812	CLA	C3A-C2A-CAA-CBA
27	A	833	CLA	C3A-C2A-CAA-CBA
27	B	809	CLA	C3A-C2A-CAA-CBA
27	B	810	CLA	C3A-C2A-CAA-CBA
27	B	813	CLA	C3A-C2A-CAA-CBA
27	H	203	CLA	C3A-C2A-CAA-CBA
27	K	201	CLA	C3A-C2A-CAA-CBA
27	K	203	CLA	C3A-C2A-CAA-CBA
27	2	609	CLA	C3A-C2A-CAA-CBA
27	2	612	CLA	C3A-C2A-CAA-CBA
27	3	603	CLA	C3A-C2A-CAA-CBA
27	6	616	CLA	C3A-C2A-CAA-CBA
27	7	609	CLA	C3A-C2A-CAA-CBA
27	7	616	CLA	C3A-C2A-CAA-CBA
27	8	614	CLA	C3A-C2A-CAA-CBA
27	9	607	CLA	C3A-C2A-CAA-CBA
27	Z	603	CLA	C3A-C2A-CAA-CBA
27	A	838	CLA	O1D-CGD-O2D-CED
38	U	601	CHL	O1D-CGD-O2D-CED
29	5	625	LHG	C15-C16-C17-C18
33	J	104	LMG	C32-C33-C34-C35
27	A	834	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	B	806	CLA	C10-C11-C12-C13
27	B	814	CLA	C5-C6-C7-C8
27	X	610	CLA	C5-C6-C7-C8
27	Y	610	CLA	C5-C6-C7-C8
28	A	844	PQN	C18-C20-C21-C22
38	Z	601	CHL	C5-C6-C7-C8
27	A	807	CLA	C16-C17-C18-C19
27	B	802	CLA	C16-C17-C18-C19
27	Z	613	CLA	C16-C17-C18-C19
38	X	609	CHL	C16-C17-C18-C20
38	Y	607	CHL	C16-C17-C18-C19
38	Z	607	CHL	C16-C17-C18-C19
38	Z	607	CHL	C16-C17-C18-C20
38	U	601	CHL	C16-C17-C18-C20
38	W	609	CHL	C16-C17-C18-C20
27	3	607	CLA	O1A-CGA-O2A-C1
27	7	601	CLA	O1A-CGA-O2A-C1
27	U	613	CLA	O1A-CGA-O2A-C1
27	W	613	CLA	O1A-CGA-O2A-C1
27	2	611	CLA	CBD-CGD-O2D-CED
32	A	857	LMU	C5-C6-C7-C8
27	Y	614	CLA	O2A-C1-C2-C3
27	A	827	CLA	O1D-CGD-O2D-CED
27	B	834	CLA	O1D-CGD-O2D-CED
27	A	810	CLA	CBA-CGA-O2A-C1
27	a	614	CLA	CBA-CGA-O2A-C1
27	4	601	CLA	CBA-CGA-O2A-C1
33	4	623	LMG	O1-C7-C8-C9
29	Z	2630	LHG	C27-C28-C29-C30
32	5	629	LMU	C3-C4-C5-C6
38	W	601	CHL	C3-C5-C6-C7
29	3	624	LHG	C7-C8-C9-C10
27	B	832	CLA	C10-C11-C12-C13
29	B	854	LHG	C14-C15-C16-C17
29	9	623	LHG	C29-C30-C31-C32
29	9	624	LHG	C32-C33-C34-C35
27	5	617	CLA	O1A-CGA-O2A-C1
29	H	204	LHG	O10-C23-O8-C6
29	5	623	LHG	C11-C12-C13-C14
34	B	850	DGD	C3B-C4B-C5B-C6B
27	8	602	CLA	O1D-CGD-O2D-CED
29	4	622	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
34	B	850	DGD	C7B-C8B-C9B-CAB
32	5	629	LMU	C4'-C5'-C6'-O6'
27	8	601	CLA	O1D-CGD-O2D-CED
29	O	2631	LHG	C24-C25-C26-C27
33	H	205	LMG	C12-C13-C14-C15
27	Z	610	CLA	C16-C17-C18-C19
38	Y	601	CHL	C16-C17-C18-C20
27	2	602	CLA	O1A-CGA-O2A-C1
27	A	810	CLA	C2B-C3B-CAB-CBB
27	A	821	CLA	C2B-C3B-CAB-CBB
27	A	823	CLA	C2B-C3B-CAB-CBB
27	A	837	CLA	C2B-C3B-CAB-CBB
27	B	817	CLA	C2B-C3B-CAB-CBB
27	B	833	CLA	C2B-C3B-CAB-CBB
27	F	301	CLA	C2B-C3B-CAB-CBB
27	G	203	CLA	C2B-C3B-CAB-CBB
27	H	203	CLA	C2B-C3B-CAB-CBB
27	K	201	CLA	C2B-C3B-CAB-CBB
27	K	203	CLA	C2B-C3B-CAB-CBB
27	2	612	CLA	C2B-C3B-CAB-CBB
27	5	601	CLA	C2B-C3B-CAB-CBB
27	5	611	CLA	C2B-C3B-CAB-CBB
27	7	614	CLA	C2B-C3B-CAB-CBB
27	8	611	CLA	C2B-C3B-CAB-CBB
27	9	607	CLA	C2B-C3B-CAB-CBB
27	X	603	CLA	C2B-C3B-CAB-CBB
27	X	612	CLA	C2B-C3B-CAB-CBB
27	Y	603	CLA	C2B-C3B-CAB-CBB
27	Y	612	CLA	C2B-C3B-CAB-CBB
27	U	603	CLA	C2B-C3B-CAB-CBB
27	U	612	CLA	C2B-C3B-CAB-CBB
27	W	603	CLA	C2B-C3B-CAB-CBB
27	W	612	CLA	C2B-C3B-CAB-CBB
30	A	849	BCR	C1-C6-C7-C8
30	A	849	BCR	C5-C6-C7-C8
30	A	849	BCR	C23-C24-C25-C30
30	A	850	BCR	C1-C6-C7-C8
30	A	851	BCR	C1-C6-C7-C8
30	A	852	BCR	C1-C6-C7-C8
30	A	852	BCR	C5-C6-C7-C8
30	A	852	BCR	C23-C24-C25-C26
30	A	852	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
30	B	801	BCR	C23-C24-C25-C30
30	B	843	BCR	C1-C6-C7-C8
30	B	843	BCR	C5-C6-C7-C8
30	B	843	BCR	C23-C24-C25-C26
30	B	843	BCR	C23-C24-C25-C30
30	B	845	BCR	C1-C6-C7-C8
30	B	845	BCR	C23-C24-C25-C26
30	B	848	BCR	C23-C24-C25-C30
30	B	849	BCR	C1-C6-C7-C8
30	B	852	BCR	C1-C6-C7-C8
30	B	852	BCR	C5-C6-C7-C8
30	B	853	BCR	C1-C6-C7-C8
30	B	853	BCR	C5-C6-C7-C8
30	B	853	BCR	C23-C24-C25-C26
30	F	305	BCR	C1-C6-C7-C8
30	F	305	BCR	C5-C6-C7-C8
30	F	305	BCR	C23-C24-C25-C26
30	J	102	BCR	C1-C6-C7-C8
30	K	202	BCR	C1-C6-C7-C8
30	K	202	BCR	C5-C6-C7-C8
30	L	308	BCR	C23-C24-C25-C26
30	a	619	BCR	C1-C6-C7-C8
30	a	619	BCR	C5-C6-C7-C8
30	1	619	BCR	C1-C6-C7-C8
30	1	619	BCR	C5-C6-C7-C8
30	2	623	BCR	C1-C6-C7-C8
30	2	623	BCR	C23-C24-C25-C26
30	3	620	BCR	C23-C24-C25-C30
30	4	621	BCR	C1-C6-C7-C8
30	6	622	BCR	C5-C6-C7-C8
30	6	622	BCR	C23-C24-C25-C26
30	7	621	BCR	C23-C24-C25-C26
30	7	623	BCR	C23-C24-C25-C26
30	9	621	BCR	C1-C6-C7-C8
30	9	621	BCR	C23-C24-C25-C26
35	4	619	LUT	C1-C6-C7-C8
35	5	620	LUT	C1-C6-C7-C8
35	X	1620	LUT	C1-C6-C7-C8
35	Y	1620	LUT	C1-C6-C7-C8
35	U	1620	LUT	C1-C6-C7-C8
35	W	1620	LUT	C1-C6-C7-C8
29	B	851	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
29	6	623	LHG	C8-C7-O7-C5
33	A	860	LMG	C11-C10-O7-C8
33	4	624	LMG	C11-C10-O7-C8
38	Y	601	CHL	O1D-CGD-O2D-CED
27	A	836	CLA	CBA-CGA-O2A-C1
27	7	611	CLA	CBA-CGA-O2A-C1
27	8	610	CLA	CBA-CGA-O2A-C1
33	5	627	LMG	C29-C28-O8-C9
38	X	609	CHL	C15-C16-C17-C18
38	U	609	CHL	C11-C12-C13-C14
38	U	601	CHL	C3-C5-C6-C7
29	a	620	LHG	C24-C25-C26-C27
29	1	620	LHG	C24-C25-C26-C27
29	U	2630	LHG	C26-C27-C28-C29
29	W	2630	LHG	C26-C27-C28-C29
34	B	850	DGD	CEB-CFB-CGB-CHB
32	K	208	LMU	C1-C2-C3-C4
27	A	818	CLA	C2A-CAA-CBA-CGA
27	L	303	CLA	C2A-CAA-CBA-CGA
27	Z	613	CLA	C2A-CAA-CBA-CGA
38	X	607	CHL	C2A-CAA-CBA-CGA
29	H	204	LHG	C12-C13-C14-C15
29	V	2630	LHG	C11-C12-C13-C14
27	B	829	CLA	O1A-CGA-O2A-C1
27	B	840	CLA	O1A-CGA-O2A-C1
27	4	601	CLA	O1A-CGA-O2A-C1
29	9	622	LHG	O10-C23-O8-C6
38	W	607	CHL	O1A-CGA-O2A-C1
29	4	622	LHG	C27-C28-C29-C30
29	5	625	LHG	O9-C7-O7-C5
27	6	614	CLA	C4-C3-C5-C6
34	B	850	DGD	C7A-C8A-C9A-CAA
27	A	842	CLA	C2-C3-C5-C6
33	H	205	LMG	O6-C5-C6-O5
32	8	625	LMU	C5'-C4'-O1B-C1B
29	3	623	LHG	C28-C29-C30-C31
29	9	624	LHG	C24-C25-C26-C27
29	9	624	LHG	C31-C32-C33-C34
29	X	2630	LHG	C26-C27-C28-C29
29	Y	2630	LHG	C26-C27-C28-C29
29	Z	2630	LHG	C28-C29-C30-C31
33	4	624	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
27	B	841	CLA	CBA-CGA-O2A-C1
27	6	601	CLA	CBA-CGA-O2A-C1
27	6	613	CLA	CBA-CGA-O2A-C1
27	X	613	CLA	CBA-CGA-O2A-C1
27	Y	613	CLA	CBA-CGA-O2A-C1
33	4	623	LMG	C29-C28-O8-C9
38	W	601	CHL	CBA-CGA-O2A-C1
29	7	622	LHG	C26-C27-C28-C29
29	8	622	LHG	C12-C13-C14-C15
33	V	2631	LMG	C15-C16-C17-C18
29	O	2631	LHG	C25-C26-C27-C28
38	W	601	CHL	C13-C15-C16-C17
29	B	854	LHG	C33-C34-C35-C36
29	H	204	LHG	C24-C25-C26-C27
32	A	858	LMU	C6-C7-C8-C9
27	B	838	CLA	O1A-CGA-O2A-C1
27	A	843	CLA	C8-C10-C11-C12
27	4	614	CLA	CBA-CGA-O2A-C1
33	J	104	LMG	C11-C10-O7-C8
38	U	608	CHL	C2A-CAA-CBA-CGA
29	3	623	LHG	C23-C24-C25-C26
27	A	823	CLA	O1D-CGD-O2D-CED
27	B	831	CLA	C13-C15-C16-C17
27	8	602	CLA	C5-C6-C7-C8
38	Y	609	CHL	C8-C10-C11-C12
38	U	609	CHL	C8-C10-C11-C12
33	J	104	LMG	O9-C10-O7-C8
29	3	624	LHG	C9-C10-C11-C12
27	6	616	CLA	C2C-C3C-CAC-CBC
32	A	858	LMU	C5-C6-C7-C8
27	A	810	CLA	O1A-CGA-O2A-C1
27	6	616	CLA	C15-C16-C17-C18
33	9	625	LMG	C17-C18-C19-C20
30	B	849	BCR	C7-C8-C9-C10
38	Z	601	CHL	C15-C16-C17-C18
29	5	625	LHG	C30-C31-C32-C33
27	B	808	CLA	C4-C3-C5-C6
32	A	858	LMU	C1-C2-C3-C4
29	B	854	LHG	C11-C10-C9-C8
27	5	607	CLA	C15-C16-C17-C18
38	Y	607	CHL	C5-C6-C7-C8
29	U	2630	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
27	3	610	CLA	CBD-CGD-O2D-CED
29	W	2630	LHG	C17-C18-C19-C20
27	a	614	CLA	O1A-CGA-O2A-C1
27	A	802	CLA	C3-C5-C6-C7
27	3	609	CLA	C3-C5-C6-C7
27	6	604	CLA	C8-C10-C11-C12
27	6	616	CLA	C5-C6-C7-C8
27	Z	613	CLA	C10-C11-C12-C13
38	U	601	CHL	C5-C6-C7-C8
29	5	623	LHG	C10-C11-C12-C13
29	7	622	LHG	C11-C12-C13-C14
27	A	842	CLA	CBA-CGA-O2A-C1
29	A	846	LHG	C13-C14-C15-C16
29	3	624	LHG	O6-C4-C5-O7
27	5	604	CLA	C15-C16-C17-C18
27	5	613	CLA	C10-C11-C12-C13
33	J	104	LMG	C29-C30-C31-C32
33	J	104	LMG	C10-C11-C12-C13
34	B	850	DGD	O6E-C5E-C6E-O5E
27	B	832	CLA	C3-C5-C6-C7
29	9	622	LHG	O7-C5-C6-O8
29	A	846	LHG	C25-C26-C27-C28
27	B	803	CLA	CBA-CGA-O2A-C1
27	A	836	CLA	O1A-CGA-O2A-C1
29	U	2630	LHG	C16-C17-C18-C19
33	8	626	LMG	C23-C24-C25-C26
29	a	620	LHG	C32-C33-C34-C35
29	1	620	LHG	C32-C33-C34-C35
29	W	2630	LHG	C16-C17-C18-C19
29	5	623	LHG	C16-C17-C18-C19
27	4	602	CLA	O1D-CGD-O2D-CED
38	X	601	CHL	C16-C17-C18-C20
38	Z	609	CHL	C16-C17-C18-C20
38	W	601	CHL	C16-C17-C18-C19
27	6	616	CLA	C13-C15-C16-C17
29	6	623	LHG	C12-C13-C14-C15
29	6	623	LHG	C27-C28-C29-C30
29	X	2630	LHG	C16-C17-C18-C19
29	Y	2630	LHG	C16-C17-C18-C19
27	B	810	CLA	C4-C3-C5-C6
28	B	842	PQN	C14-C13-C15-C16
38	Y	601	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	A	860	LMG	C28-C29-C30-C31
27	Z	611	CLA	C2-C3-C5-C6
29	B	851	LHG	O9-C7-O7-C5
27	A	803	CLA	C2A-CAA-CBA-CGA
27	A	854	CLA	C2A-CAA-CBA-CGA
27	B	811	CLA	C2A-CAA-CBA-CGA
27	X	613	CLA	C2A-CAA-CBA-CGA
27	Y	613	CLA	C2A-CAA-CBA-CGA
27	V	613	CLA	C2A-CAA-CBA-CGA
27	A	830	CLA	CBD-CGD-O2D-CED
27	B	841	CLA	CBD-CGD-O2D-CED
27	V	611	CLA	CBD-CGD-O2D-CED
33	J	104	LMG	O6-C5-C6-O5
27	A	822	CLA	C15-C16-C17-C18
27	B	809	CLA	C10-C11-C12-C13
27	B	828	CLA	C10-C11-C12-C13
38	Y	607	CHL	C15-C16-C17-C18
32	A	858	LMU	C3'-C4'-O1B-C1B
27	A	835	CLA	O1D-CGD-O2D-CED
29	O	2631	LHG	C10-C11-C12-C13
27	B	810	CLA	C2-C1-O2A-CGA
27	5	613	CLA	C2-C1-O2A-CGA
29	6	623	LHG	O1-C1-C2-O2
27	6	613	CLA	O1A-CGA-O2A-C1
27	7	611	CLA	O1A-CGA-O2A-C1
27	8	610	CLA	O1A-CGA-O2A-C1
27	3	613	CLA	C2A-CAA-CBA-CGA
29	3	624	LHG	C11-C10-C9-C8
27	A	805	CLA	C1A-C2A-CAA-CBA
27	A	808	CLA	C1A-C2A-CAA-CBA
27	A	811	CLA	C1A-C2A-CAA-CBA
27	A	820	CLA	C1A-C2A-CAA-CBA
27	A	831	CLA	C1A-C2A-CAA-CBA
27	B	803	CLA	C1A-C2A-CAA-CBA
27	B	805	CLA	C1A-C2A-CAA-CBA
27	B	812	CLA	C1A-C2A-CAA-CBA
27	B	813	CLA	C1A-C2A-CAA-CBA
27	B	818	CLA	C1A-C2A-CAA-CBA
27	B	820	CLA	C1A-C2A-CAA-CBA
27	B	827	CLA	C1A-C2A-CAA-CBA
27	B	828	CLA	C1A-C2A-CAA-CBA
27	B	832	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	K	201	CLA	C1A-C2A-CAA-CBA
27	L	302	CLA	C1A-C2A-CAA-CBA
27	L	303	CLA	C1A-C2A-CAA-CBA
27	2	612	CLA	C1A-C2A-CAA-CBA
27	3	603	CLA	C1A-C2A-CAA-CBA
27	3	607	CLA	C1A-C2A-CAA-CBA
27	3	609	CLA	C1A-C2A-CAA-CBA
27	4	601	CLA	C1A-C2A-CAA-CBA
27	4	616	CLA	C1A-C2A-CAA-CBA
27	6	614	CLA	C1A-C2A-CAA-CBA
27	6	616	CLA	C1A-C2A-CAA-CBA
27	7	604	CLA	C1A-C2A-CAA-CBA
27	9	607	CLA	C1A-C2A-CAA-CBA
27	Z	603	CLA	C1A-C2A-CAA-CBA
27	J	101	CLA	O1D-CGD-O2D-CED
27	B	841	CLA	C10-C11-C12-C13
27	B	841	CLA	C13-C15-C16-C17
38	Z	609	CHL	C10-C11-C12-C13
29	9	623	LHG	C14-C15-C16-C17
27	X	613	CLA	O1A-CGA-O2A-C1
33	5	627	LMG	O10-C28-O8-C9
38	W	601	CHL	O1A-CGA-O2A-C1
32	K	208	LMU	C3-C4-C5-C6
27	A	830	CLA	C13-C15-C16-C17
27	5	609	CLA	C15-C16-C17-C18
29	B	854	LHG	O6-C4-C5-C6
29	3	624	LHG	O6-C4-C5-C6
29	6	623	LHG	O9-C7-O7-C5
33	4	624	LMG	O9-C10-O7-C8
27	A	801	CLA	C12-C13-C15-C16
27	A	804	CLA	C6-C7-C8-C10
27	A	809	CLA	C11-C12-C13-C15
27	A	814	CLA	C12-C13-C15-C16
27	A	822	CLA	C12-C13-C15-C16
27	A	824	CLA	C11-C10-C8-C7
27	A	826	CLA	C11-C10-C8-C7
27	A	842	CLA	C11-C12-C13-C15
27	B	805	CLA	C11-C10-C8-C7
27	B	817	CLA	C6-C7-C8-C10
27	B	817	CLA	C11-C10-C8-C7
27	B	824	CLA	C6-C7-C8-C10
27	B	824	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
27	B	827	CLA	C12-C13-C15-C16
27	B	837	CLA	C11-C12-C13-C15
27	H	203	CLA	C11-C10-C8-C7
27	4	610	CLA	C6-C7-C8-C10
27	5	604	CLA	C12-C13-C15-C16
27	5	607	CLA	C6-C7-C8-C10
27	5	607	CLA	C12-C13-C15-C16
27	5	613	CLA	C6-C7-C8-C10
27	6	616	CLA	C11-C10-C8-C7
27	6	620	CLA	C11-C10-C8-C7
27	7	602	CLA	C11-C10-C8-C7
27	8	606	CLA	C11-C12-C13-C15
27	9	609	CLA	C11-C12-C13-C15
27	9	610	CLA	C6-C7-C8-C10
27	9	613	CLA	C11-C12-C13-C15
27	X	602	CLA	C6-C7-C8-C10
27	X	613	CLA	C11-C10-C8-C7
27	X	613	CLA	C12-C13-C15-C16
27	Y	602	CLA	C6-C7-C8-C10
27	Y	613	CLA	C11-C10-C8-C7
27	Y	613	CLA	C12-C13-C15-C16
27	U	602	CLA	C6-C7-C8-C10
27	W	602	CLA	C6-C7-C8-C10
38	X	609	CHL	C11-C12-C13-C15
38	Y	609	CHL	C11-C12-C13-C15
38	Z	607	CHL	C11-C12-C13-C15
38	Z	609	CHL	C12-C13-C15-C16
38	V	609	CHL	C11-C10-C8-C7
38	W	609	CHL	C11-C12-C13-C15
38	W	609	CHL	C12-C13-C15-C16
27	B	827	CLA	C5-C6-C7-C8
27	7	602	CLA	C13-C15-C16-C17
38	U	601	CHL	C15-C16-C17-C18
27	Y	613	CLA	O1A-CGA-O2A-C1
27	B	822	CLA	C3A-C2A-CAA-CBA
27	4	611	CLA	C3A-C2A-CAA-CBA
27	8	611	CLA	C3A-C2A-CAA-CBA
27	9	606	CLA	C3A-C2A-CAA-CBA
27	B	818	CLA	C5-C6-C7-C8
27	8	601	CLA	C10-C11-C12-C13
29	3	624	LHG	C23-C24-C25-C26
33	9	625	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
27	Z	604	CLA	C4-C3-C5-C6
27	A	806	CLA	C2-C3-C5-C6
27	B	810	CLA	C2-C3-C5-C6
27	6	614	CLA	C2-C3-C5-C6
27	Z	604	CLA	C2-C3-C5-C6
27	Z	613	CLA	C2-C3-C5-C6
38	X	608	CHL	C2-C3-C5-C6
27	6	601	CLA	O1A-CGA-O2A-C1
33	4	623	LMG	O10-C28-O8-C9
33	J	103	LMG	C11-C12-C13-C14
38	X	609	CHL	O1D-CGD-O2D-CED
27	A	825	CLA	C2A-CAA-CBA-CGA
27	2	613	CLA	C2A-CAA-CBA-CGA
27	7	613	CLA	C2A-CAA-CBA-CGA
27	8	603	CLA	C2A-CAA-CBA-CGA
27	A	824	CLA	C11-C10-C8-C9
27	A	830	CLA	C6-C7-C8-C9
27	A	831	CLA	C14-C13-C15-C16
27	A	841	CLA	C11-C10-C8-C9
27	B	805	CLA	C11-C10-C8-C9
27	B	810	CLA	C11-C10-C8-C9
27	B	817	CLA	C11-C10-C8-C9
27	B	824	CLA	C6-C7-C8-C9
27	B	827	CLA	C14-C13-C15-C16
27	2	602	CLA	C14-C13-C15-C16
27	4	608	CLA	C11-C12-C13-C14
27	5	607	CLA	C14-C13-C15-C16
27	5	609	CLA	C11-C10-C8-C9
27	5	613	CLA	C6-C7-C8-C9
27	6	602	CLA	C6-C7-C8-C9
27	9	609	CLA	C11-C12-C13-C14
27	X	602	CLA	C6-C7-C8-C9
27	Y	602	CLA	C6-C7-C8-C9
27	U	613	CLA	C11-C10-C8-C9
27	W	613	CLA	C11-C10-C8-C9
28	A	844	PQN	C19-C18-C20-C21
38	U	601	CHL	C6-C7-C8-C9
32	5	629	LMU	O5B-C1B-O1B-C4'
29	X	2630	LHG	C17-C18-C19-C20
29	Y	2630	LHG	C17-C18-C19-C20
27	B	811	CLA	CBA-CGA-O2A-C1
27	3	606	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	Z	612	CLA	CBA-CGA-O2A-C1
27	Z	613	CLA	CBA-CGA-O2A-C1
27	B	823	CLA	O1D-CGD-O2D-CED
33	A	860	LMG	O9-C10-O7-C8
27	B	808	CLA	C15-C16-C17-C18
29	2	622	LHG	C4-C5-C6-O8
29	3	623	LHG	C4-C5-C6-O8
29	7	622	LHG	C4-C5-C6-O8
29	9	622	LHG	C4-C5-C6-O8
33	H	205	LMG	C7-C8-C9-O8
33	5	627	LMG	C7-C8-C9-O8
34	B	850	DGD	O1G-C1G-C2G-C3G
27	A	826	CLA	CAA-CBA-CGA-O2A
27	B	816	CLA	C5-C6-C7-C8
29	4	622	LHG	C16-C17-C18-C19
33	H	205	LMG	C29-C30-C31-C32
27	4	607	CLA	O1D-CGD-O2D-CED
27	A	804	CLA	CBA-CGA-O2A-C1
27	A	831	CLA	CBA-CGA-O2A-C1
38	Y	607	CHL	CBA-CGA-O2A-C1
27	6	604	CLA	C16-C17-C18-C19
29	7	622	LHG	C10-C11-C12-C13
27	5	613	CLA	C5-C6-C7-C8
27	B	841	CLA	O1A-CGA-O2A-C1
27	a	616	CLA	O1D-CGD-O2D-CED
38	X	609	CHL	CHA-CBD-CGD-O1D
38	X	609	CHL	CHA-CBD-CGD-O2D
38	Y	609	CHL	CHA-CBD-CGD-O1D
38	Y	609	CHL	CHA-CBD-CGD-O2D
38	Z	607	CHL	CHA-CBD-CGD-O2D
38	Z	609	CHL	CHA-CBD-CGD-O2D
38	U	609	CHL	CHA-CBD-CGD-O1D
38	U	609	CHL	CHA-CBD-CGD-O2D
38	W	609	CHL	CHA-CBD-CGD-O1D
33	L	2631	LMG	O6-C5-C6-O5
38	W	608	CHL	CBA-CGA-O2A-C1
27	A	842	CLA	O1A-CGA-O2A-C1
27	4	614	CLA	O1A-CGA-O2A-C1
27	A	806	CLA	C4-C3-C5-C6
27	Z	611	CLA	C4-C3-C5-C6
27	B	808	CLA	C2-C3-C5-C6
27	V	613	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	A	839	CLA	C5-C6-C7-C8
27	7	601	CLA	C5-C6-C7-C8
38	X	607	CHL	C13-C15-C16-C17
38	Z	607	CHL	C10-C11-C12-C13
27	B	812	CLA	C2A-CAA-CBA-CGA
32	1	621	LMU	O5B-C5B-C6B-O6B
33	8	626	LMG	O6-C5-C6-O5
27	B	803	CLA	O1A-CGA-O2A-C1
27	B	811	CLA	O1A-CGA-O2A-C1
27	Z	613	CLA	O1A-CGA-O2A-C1
27	B	833	CLA	C5-C6-C7-C8
27	5	604	CLA	C5-C6-C7-C8
27	1	616	CLA	O1D-CGD-O2D-CED
27	A	813	CLA	C2A-CAA-CBA-CGA
27	A	806	CLA	C15-C16-C17-C18
29	H	204	LHG	C25-C26-C27-C28
27	B	803	CLA	O2A-C1-C2-C3
27	A	806	CLA	C5-C6-C7-C8
33	9	625	LMG	C38-C39-C40-C41
38	Z	609	CHL	C3C-C2C-CMC-OMC
27	B	829	CLA	O1D-CGD-O2D-CED
38	W	609	CHL	C3-C5-C6-C7
29	6	623	LHG	C18-C19-C20-C21
29	6	623	LHG	C1-C2-C3-O3
29	9	624	LHG	O6-C4-C5-O7
27	A	814	CLA	CBA-CGA-O2A-C1
29	3	623	LHG	C24-C23-O8-C6
29	6	623	LHG	C24-C23-O8-C6
38	Y	608	CHL	CBA-CGA-O2A-C1
33	9	625	LMG	C13-C14-C15-C16
27	A	836	CLA	C4-C3-C5-C6
27	5	609	CLA	C16-C17-C18-C20
29	U	2630	LHG	C31-C32-C33-C34
32	8	625	LMU	C6-C7-C8-C9
27	3	606	CLA	O1A-CGA-O2A-C1
29	5	625	LHG	O7-C5-C6-O8
33	9	625	LMG	O7-C8-C9-O8
27	A	819	CLA	C11-C12-C13-C14
38	X	601	CHL	C15-C16-C17-C18
27	A	831	CLA	O1D-CGD-O2D-CED
27	Y	602	CLA	C10-C11-C12-C13
27	X	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	Y	603	CLA	CAA-CBA-CGA-O2A
32	A	857	LMU	C6-C7-C8-C9
27	a	606	CLA	CBD-CGD-O2D-CED
27	1	606	CLA	CBD-CGD-O2D-CED
32	8	625	LMU	C1-C2-C3-C4
27	A	838	CLA	CBA-CGA-O2A-C1
27	2	610	CLA	CBA-CGA-O2A-C1
27	8	606	CLA	CBA-CGA-O2A-C1
27	V	613	CLA	CBA-CGA-O2A-C1
27	W	610	CLA	CBA-CGA-O2A-C1
27	A	824	CLA	CBD-CGD-O2D-CED
28	B	842	PQN	C11-C12-C13-C14
29	3	624	LHG	C12-C13-C14-C15
34	B	850	DGD	C1A-C2A-C3A-C4A
27	6	616	CLA	C10-C11-C12-C13
27	Z	604	CLA	O1D-CGD-O2D-CED
27	5	609	CLA	C16-C17-C18-C19
27	3	604	CLA	C4-C3-C5-C6
27	V	613	CLA	C4-C3-C5-C6
38	X	608	CHL	C4-C3-C5-C6
34	B	850	DGD	CFB-CGB-CHB-CIB
27	A	805	CLA	CBA-CGA-O2A-C1
27	U	610	CLA	CBA-CGA-O2A-C1
38	V	608	CHL	CBA-CGA-O2A-C1
27	A	804	CLA	C6-C7-C8-C9
27	A	809	CLA	C11-C12-C13-C14
27	A	814	CLA	C11-C10-C8-C9
27	A	814	CLA	C14-C13-C15-C16
27	A	820	CLA	C11-C10-C8-C9
27	A	822	CLA	C14-C13-C15-C16
27	A	826	CLA	C11-C10-C8-C9
27	A	829	CLA	C14-C13-C15-C16
27	A	842	CLA	C11-C10-C8-C9
27	A	842	CLA	C11-C12-C13-C14
27	A	843	CLA	C11-C12-C13-C14
27	B	806	CLA	C11-C10-C8-C9
27	B	813	CLA	C6-C7-C8-C9
27	B	817	CLA	C6-C7-C8-C9
27	B	818	CLA	C11-C10-C8-C9
27	B	824	CLA	C14-C13-C15-C16
27	B	831	CLA	C11-C12-C13-C14
27	B	837	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	B	837	CLA	C14-C13-C15-C16
27	H	203	CLA	C11-C10-C8-C9
27	2	602	CLA	C11-C10-C8-C9
27	4	610	CLA	C6-C7-C8-C9
27	5	604	CLA	C14-C13-C15-C16
27	5	607	CLA	C6-C7-C8-C9
27	6	616	CLA	C11-C10-C8-C9
27	6	620	CLA	C11-C10-C8-C9
27	6	620	CLA	C11-C12-C13-C14
27	7	602	CLA	C11-C10-C8-C9
27	7	602	CLA	C14-C13-C15-C16
27	8	606	CLA	C11-C12-C13-C14
27	9	610	CLA	C6-C7-C8-C9
27	9	613	CLA	C11-C12-C13-C14
27	X	613	CLA	C11-C10-C8-C9
27	Y	613	CLA	C11-C10-C8-C9
27	Z	602	CLA	C6-C7-C8-C9
27	Z	613	CLA	C14-C13-C15-C16
27	U	602	CLA	C6-C7-C8-C9
27	W	602	CLA	C6-C7-C8-C9
38	Y	601	CHL	C6-C7-C8-C9
38	Z	601	CHL	C11-C10-C8-C9
38	Z	601	CHL	C11-C12-C13-C14
38	Z	607	CHL	C11-C12-C13-C14
38	V	601	CHL	C6-C7-C8-C9
38	W	601	CHL	C11-C10-C8-C9
38	W	609	CHL	C14-C13-C15-C16
27	B	808	CLA	C13-C15-C16-C17
27	B	828	CLA	C8-C10-C11-C12
27	U	613	CLA	C5-C6-C7-C8
27	Z	612	CLA	O1A-CGA-O2A-C1
27	A	832	CLA	C4B-C3B-CAB-CBB
27	A	835	CLA	C4B-C3B-CAB-CBB
27	F	304	CLA	C4B-C3B-CAB-CBB
27	G	203	CLA	C4B-C3B-CAB-CBB
27	a	608	CLA	C4B-C3B-CAB-CBB
27	1	608	CLA	C4B-C3B-CAB-CBB
27	2	604	CLA	C4B-C3B-CAB-CBB
27	2	612	CLA	C4B-C3B-CAB-CBB
27	3	614	CLA	C4B-C3B-CAB-CBB
27	4	606	CLA	C4B-C3B-CAB-CBB
27	6	611	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	6	613	CLA	C4B-C3B-CAB-CBB
27	8	609	CLA	C4B-C3B-CAB-CBB
27	8	614	CLA	C4B-C3B-CAB-CBB
27	9	606	CLA	C4B-C3B-CAB-CBB
27	9	607	CLA	C4B-C3B-CAB-CBB
27	9	611	CLA	C4B-C3B-CAB-CBB
27	9	614	CLA	C4B-C3B-CAB-CBB
27	X	610	CLA	C4B-C3B-CAB-CBB
27	X	613	CLA	C4B-C3B-CAB-CBB
27	Y	610	CLA	C4B-C3B-CAB-CBB
27	Y	613	CLA	C4B-C3B-CAB-CBB
27	U	610	CLA	C4B-C3B-CAB-CBB
27	U	614	CLA	C4B-C3B-CAB-CBB
27	V	603	CLA	C4B-C3B-CAB-CBB
27	W	610	CLA	C4B-C3B-CAB-CBB
27	W	614	CLA	C4B-C3B-CAB-CBB
27	7	611	CLA	C5-C6-C7-C8
27	W	613	CLA	C5-C6-C7-C8
27	Z	603	CLA	C16-C17-C18-C20
27	A	842	CLA	C2A-CAA-CBA-CGA
29	O	2631	LHG	C11-C10-C9-C8
29	7	622	LHG	O6-C4-C5-C6
29	A	846	LHG	C30-C31-C32-C33
29	Z	2630	LHG	C19-C20-C21-C22
27	A	807	CLA	C11-C10-C8-C7
27	A	820	CLA	C11-C10-C8-C7
27	A	828	CLA	C11-C10-C8-C7
27	A	830	CLA	C6-C7-C8-C10
27	A	831	CLA	C11-C10-C8-C7
27	A	831	CLA	C12-C13-C15-C16
27	A	841	CLA	C11-C10-C8-C7
27	A	841	CLA	C12-C13-C15-C16
27	A	842	CLA	C11-C10-C8-C7
27	A	843	CLA	C11-C12-C13-C15
27	B	810	CLA	C11-C10-C8-C7
27	B	828	CLA	C12-C13-C15-C16
27	B	831	CLA	C11-C10-C8-C7
27	B	831	CLA	C11-C12-C13-C15
27	B	837	CLA	C12-C13-C15-C16
27	B	839	CLA	C12-C13-C15-C16
27	H	203	CLA	C6-C7-C8-C10
27	2	601	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
27	2	602	CLA	C11-C10-C8-C7
27	2	602	CLA	C12-C13-C15-C16
27	3	609	CLA	C11-C10-C8-C7
27	4	608	CLA	C11-C10-C8-C7
27	4	608	CLA	C11-C12-C13-C15
27	4	610	CLA	C11-C12-C13-C15
27	5	602	CLA	C12-C13-C15-C16
27	5	604	CLA	C6-C7-C8-C10
27	5	609	CLA	C6-C7-C8-C10
27	5	609	CLA	C11-C10-C8-C7
27	6	602	CLA	C6-C7-C8-C10
27	7	602	CLA	C12-C13-C15-C16
27	Z	602	CLA	C6-C7-C8-C10
27	Z	603	CLA	C11-C10-C8-C7
27	Z	603	CLA	C11-C12-C13-C15
27	Z	613	CLA	C12-C13-C15-C16
28	A	844	PQN	C17-C18-C20-C21
38	X	601	CHL	C12-C13-C15-C16
38	X	608	CHL	C12-C13-C15-C16
38	X	609	CHL	C11-C10-C8-C7
38	Z	601	CHL	C11-C10-C8-C7
38	Z	601	CHL	C11-C12-C13-C15
27	4	601	CLA	C8-C10-C11-C12
27	7	613	CLA	C15-C16-C17-C18
27	Z	603	CLA	C15-C16-C17-C18
38	Y	601	CHL	C15-C16-C17-C18
38	Y	607	CHL	O1A-CGA-O2A-C1
27	A	841	CLA	C3A-C2A-CAA-CBA
27	B	827	CLA	C3A-C2A-CAA-CBA
27	B	827	CLA	C4-C3-C5-C6
27	B	828	CLA	C3A-C2A-CAA-CBA
27	F	301	CLA	C4-C3-C5-C6
27	6	601	CLA	C3A-C2A-CAA-CBA
27	6	609	CLA	C3A-C2A-CAA-CBA
27	9	609	CLA	C4-C3-C5-C6
27	Z	613	CLA	C4-C3-C5-C6
38	U	609	CHL	C3A-C2A-CAA-CBA
38	V	609	CHL	C3A-C2A-CAA-CBA
38	W	601	CHL	C3A-C2A-CAA-CBA
29	3	623	LHG	C9-C10-C11-C12
29	6	623	LHG	C34-C35-C36-C37
27	A	814	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	A	804	CLA	O1A-CGA-O2A-C1
27	A	831	CLA	O1A-CGA-O2A-C1
29	H	204	LHG	C31-C32-C33-C34
29	1	620	LHG	C35-C36-C37-C38
38	W	607	CHL	C16-C17-C18-C19
27	A	826	CLA	C8-C10-C11-C12
27	8	614	CLA	C5-C6-C7-C8
29	a	620	LHG	C35-C36-C37-C38
27	A	837	CLA	O1D-CGD-O2D-CED
27	B	837	CLA	O1D-CGD-O2D-CED
27	B	831	CLA	C2C-C3C-CAC-CBC
33	8	626	LMG	C33-C34-C35-C36
27	A	817	CLA	O1D-CGD-O2D-CED
27	4	614	CLA	O1D-CGD-O2D-CED
29	5	623	LHG	C4-C5-C6-O8
29	5	625	LHG	C4-C5-C6-O8
33	8	626	LMG	C7-C8-C9-O8
27	6	616	CLA	CBD-CGD-O2D-CED
27	A	825	CLA	C13-C15-C16-C17
27	A	842	CLA	C8-C10-C11-C12
27	A	814	CLA	O1A-CGA-O2A-C1
29	9	624	LHG	C27-C28-C29-C30
32	8	625	LMU	C4'-C5'-C6'-O6'
29	A	846	LHG	C32-C33-C34-C35
27	U	603	CLA	C4-C3-C5-C6
27	W	603	CLA	C4-C3-C5-C6
27	W	611	CLA	C4-C3-C5-C6
27	B	827	CLA	C2-C3-C5-C6
27	3	604	CLA	C2-C3-C5-C6
27	9	609	CLA	C2-C3-C5-C6
38	V	609	CHL	C3-C5-C6-C7
32	8	625	LMU	O5B-C5B-C6B-O6B
27	B	816	CLA	C2A-CAA-CBA-CGA
27	K	203	CLA	O1D-CGD-O2D-CED
33	5	627	LMG	C4-C5-C6-O5
29	B	854	LHG	O6-C4-C5-O7
29	O	2631	LHG	O6-C4-C5-O7
29	B	851	LHG	C11-C10-C9-C8
29	3	623	LHG	C14-C15-C16-C17
32	A	858	LMU	C4'-C5'-C6'-O6'
27	Z	614	CLA	C6-C7-C8-C9
30	B	801	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	B	846	BCR	C5-C6-C7-C8
30	F	305	BCR	C23-C24-C25-C30
30	O	2005	BCR	C5-C6-C7-C8
30	O	2005	BCR	C23-C24-C25-C26
30	2	623	BCR	C23-C24-C25-C30
30	6	622	BCR	C1-C6-C7-C8
27	A	819	CLA	CAA-CBA-CGA-O2A
27	6	610	CLA	C13-C15-C16-C17
27	6	620	CLA	C10-C11-C12-C13
32	K	208	LMU	C4-C5-C6-C7
27	K	203	CLA	C11-C10-C8-C9
27	4	604	CLA	C11-C10-C8-C9
33	4	624	LMG	C28-C29-C30-C31
29	6	623	LHG	C28-C29-C30-C31
27	4	601	CLA	O1D-CGD-O2D-CED
38	Z	609	CHL	C8-C10-C11-C12
27	4	608	CLA	CBD-CGD-O2D-CED
27	4	613	CLA	CBD-CGD-O2D-CED
38	W	608	CHL	C2A-CAA-CBA-CGA
27	A	809	CLA	C13-C15-C16-C17
29	3	623	LHG	O7-C5-C6-O8
33	A	860	LMG	O1-C7-C8-O7
33	H	205	LMG	O7-C8-C9-O8
33	8	626	LMG	O7-C8-C9-O8
27	4	604	CLA	C11-C10-C8-C7
27	A	835	CLA	C5-C6-C7-C8
27	F	301	CLA	C2-C3-C5-C6
27	W	611	CLA	C2-C3-C5-C6
29	2	622	LHG	C27-C28-C29-C30
33	J	103	LMG	C13-C14-C15-C16
33	L	2631	LMG	C13-C14-C15-C16
33	4	624	LMG	C10-C11-C12-C13
27	a	602	CLA	C3-C5-C6-C7
27	1	602	CLA	C3-C5-C6-C7
27	A	825	CLA	C6-C7-C8-C9
27	5	602	CLA	C14-C13-C15-C16
27	6	616	CLA	C11-C12-C13-C14
27	8	601	CLA	C6-C7-C8-C9
27	X	613	CLA	C14-C13-C15-C16
27	Y	613	CLA	C14-C13-C15-C16
38	X	601	CHL	C6-C7-C8-C9
38	W	601	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	2	611	CLA	O1D-CGD-O2D-CED
33	5	627	LMG	O6-C1-O1-C7
29	4	622	LHG	C30-C31-C32-C33
27	9	606	CLA	C1A-C2A-CAA-CBA
27	X	614	CLA	C1A-C2A-CAA-CBA
27	U	614	CLA	C1A-C2A-CAA-CBA
27	4	601	CLA	C2A-CAA-CBA-CGA
27	6	620	CLA	C2A-CAA-CBA-CGA
29	5	625	LHG	C10-C11-C12-C13
27	6	613	CLA	C10-C11-C12-C13
27	B	816	CLA	C2-C1-O2A-CGA
27	3	613	CLA	C2-C1-O2A-CGA
27	B	833	CLA	CBA-CGA-O2A-C1
27	U	603	CLA	CAA-CBA-CGA-O2A
27	W	603	CLA	CAA-CBA-CGA-O2A
29	8	623	LHG	C8-C7-O7-C5
27	A	829	CLA	C13-C15-C16-C17
27	X	610	CLA	CBA-CGA-O2A-C1
29	2	622	LHG	C26-C27-C28-C29
27	6	604	CLA	C16-C17-C18-C20
38	Z	601	CHL	C16-C17-C18-C20
27	B	806	CLA	C15-C16-C17-C18
27	7	601	CLA	C10-C11-C12-C13
27	X	613	CLA	C5-C6-C7-C8
27	Y	613	CLA	C5-C6-C7-C8
38	X	609	CHL	C8-C10-C11-C12
27	A	802	CLA	C11-C10-C8-C7
27	A	811	CLA	C11-C10-C8-C7
27	A	825	CLA	C6-C7-C8-C10
27	A	835	CLA	C11-C12-C13-C15
27	B	803	CLA	C6-C7-C8-C10
27	B	805	CLA	C6-C7-C8-C10
27	B	809	CLA	C12-C13-C15-C16
27	B	813	CLA	C11-C12-C13-C15
27	3	609	CLA	C6-C7-C8-C10
27	5	604	CLA	C11-C12-C13-C15
27	6	610	CLA	C6-C7-C8-C10
27	6	616	CLA	C11-C12-C13-C15
27	8	601	CLA	C6-C7-C8-C10
27	W	613	CLA	C12-C13-C15-C16
38	Y	601	CHL	C12-C13-C15-C16
38	U	601	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
38	W	607	CHL	C12-C13-C15-C16
29	8	622	LHG	C7-C8-C9-C10
32	1	621	LMU	C6-C7-C8-C9
27	2	613	CLA	C15-C16-C17-C18
30	A	849	BCR	C21-C22-C23-C24
30	6	622	BCR	C21-C22-C23-C24
35	X	1621	LUT	C7-C8-C9-C10
35	Y	1621	LUT	C7-C8-C9-C10
35	U	1621	LUT	C7-C8-C9-C10
27	5	602	CLA	CBA-CGA-O2A-C1
27	Y	610	CLA	CBA-CGA-O2A-C1
29	H	204	LHG	C14-C15-C16-C17
27	8	606	CLA	O1A-CGA-O2A-C1
38	Y	608	CHL	O1A-CGA-O2A-C1
27	A	821	CLA	C2A-CAA-CBA-CGA
27	A	830	CLA	C2A-CAA-CBA-CGA
27	B	802	CLA	C2A-CAA-CBA-CGA
27	4	609	CLA	CBD-CGD-O2D-CED
27	5	613	CLA	C2A-CAA-CBA-CGA
29	1	620	LHG	C34-C35-C36-C37
27	4	614	CLA	C4-C3-C5-C6
27	6	613	CLA	C4-C3-C5-C6
27	Y	603	CLA	C4-C3-C5-C6
38	W	607	CHL	CAA-CBA-CGA-O2A
27	A	805	CLA	O1A-CGA-O2A-C1
27	2	610	CLA	O1A-CGA-O2A-C1
29	6	623	LHG	O10-C23-O8-C6
38	V	608	CHL	O1A-CGA-O2A-C1
27	U	603	CLA	C2-C3-C5-C6
27	W	603	CLA	C2-C3-C5-C6
29	9	623	LHG	C32-C33-C34-C35
29	W	2630	LHG	C29-C30-C31-C32
29	U	2630	LHG	C29-C30-C31-C32
27	B	839	CLA	C10-C11-C12-C13
27	X	610	CLA	C13-C15-C16-C17
27	A	854	CLA	O2A-C1-C2-C3
29	B	854	LHG	C6-C5-O7-C7
27	A	838	CLA	O1A-CGA-O2A-C1
27	U	610	CLA	O1A-CGA-O2A-C1
27	V	613	CLA	O1A-CGA-O2A-C1
29	a	620	LHG	C34-C35-C36-C37
32	5	629	LMU	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	Y	610	CLA	C13-C15-C16-C17
27	W	610	CLA	O1A-CGA-O2A-C1
29	3	623	LHG	O10-C23-O8-C6
29	V	2630	LHG	C24-C25-C26-C27
29	7	622	LHG	O6-C4-C5-O7
27	X	604	CLA	O2A-C1-C2-C3
32	A	858	LMU	O5'-C1'-O1'-C1
27	3	610	CLA	O1D-CGD-O2D-CED
33	J	103	LMG	C7-C8-C9-O8
27	U	604	CLA	CAD-CBD-CGD-O2D
27	L	303	CLA	C3-C5-C6-C7
27	X	603	CLA	C4-C3-C5-C6
27	2	612	CLA	C2A-CAA-CBA-CGA
29	9	624	LHG	C28-C29-C30-C31
27	A	830	CLA	C3-C5-C6-C7
29	8	622	LHG	O7-C5-C6-O8
27	A	811	CLA	C11-C10-C8-C9
27	A	831	CLA	C11-C10-C8-C9
27	B	809	CLA	C14-C13-C15-C16
27	B	818	CLA	C6-C7-C8-C9
27	5	604	CLA	C11-C12-C13-C14
27	6	610	CLA	C6-C7-C8-C9
27	Z	603	CLA	C16-C17-C18-C19
27	5	601	CLA	CBA-CGA-O2A-C1
29	7	622	LHG	C24-C23-O8-C6
29	8	623	LHG	C11-C10-C9-C8
33	H	205	LMG	C35-C36-C37-C38
27	B	833	CLA	O1A-CGA-O2A-C1
33	H	205	LMG	C18-C19-C20-C21
32	A	858	LMU	O5'-C5'-C6'-O6'
38	W	607	CHL	C2-C1-O2A-CGA
29	Z	2630	LHG	C11-C10-C9-C8
27	B	817	CLA	C4-C3-C5-C6
27	4	601	CLA	C4-C3-C5-C6
27	6	613	CLA	C2-C3-C5-C6
27	B	803	CLA	C10-C11-C12-C13
27	7	613	CLA	C13-C15-C16-C17
27	7	615	CLA	C2A-CAA-CBA-CGA
38	Z	601	CHL	C16-C17-C18-C19
29	9	623	LHG	C7-C8-C9-C10
27	5	602	CLA	O1A-CGA-O2A-C1
27	X	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
38	Y	609	CHL	C3-C5-C6-C7
27	3	607	CLA	C2C-C3C-CAC-CBC
38	Y	601	CHL	C4C-C3C-CAC-CBC
38	Z	601	CHL	C4C-C3C-CAC-CBC
38	Z	609	CHL	C4C-C3C-CAC-CBC
38	U	601	CHL	C4C-C3C-CAC-CBC
29	3	624	LHG	C29-C30-C31-C32
27	A	842	CLA	C16-C17-C18-C20
27	3	613	CLA	CBA-CGA-O2A-C1
32	1	621	LMU	C2-C1-O1'-C1'
27	B	829	CLA	C3-C5-C6-C7
38	X	609	CHL	C3-C5-C6-C7
38	W	607	CHL	C3-C5-C6-C7
35	V	1621	LUT	C7-C8-C9-C19
32	K	208	LMU	C11-C10-C9-C8
27	A	807	CLA	C4B-C3B-CAB-CBB
27	A	824	CLA	C1A-C2A-CAA-CBA
27	B	814	CLA	C1A-C2A-CAA-CBA
27	F	303	CLA	C4B-C3B-CAB-CBB
27	H	202	CLA	C4B-C3B-CAB-CBB
27	J	101	CLA	C4B-C3B-CAB-CBB
27	a	607	CLA	C1A-C2A-CAA-CBA
27	a	608	CLA	C1A-C2A-CAA-CBA
27	2	607	CLA	C4B-C3B-CAB-CBB
27	2	616	CLA	C1A-C2A-CAA-CBA
27	4	608	CLA	C1A-C2A-CAA-CBA
27	7	616	CLA	C1A-C2A-CAA-CBA
27	9	614	CLA	C1A-C2A-CAA-CBA
27	Z	614	CLA	C4B-C3B-CAB-CBB
28	A	844	PQN	C14-C13-C15-C16
27	V	613	CLA	C10-C11-C12-C13
29	X	2630	LHG	C29-C30-C31-C32
29	Y	2630	LHG	C29-C30-C31-C32
30	B	845	BCR	C21-C22-C23-C24
35	W	1621	LUT	C7-C8-C9-C10
33	L	2631	LMG	C12-C13-C14-C15
29	5	625	LHG	C32-C33-C34-C35
27	Y	614	CLA	C2A-CAA-CBA-CGA
33	8	626	LMG	C17-C18-C19-C20
29	O	2631	LHG	O6-C4-C5-C6
29	9	624	LHG	O6-C4-C5-C6
27	Y	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	8	623	LHG	O9-C7-O7-C5
29	3	623	LHG	C11-C10-C9-C8
27	6	616	CLA	O1D-CGD-O2D-CED
27	5	604	CLA	C3-C5-C6-C7
27	A	825	CLA	C12-C13-C15-C16
27	A	828	CLA	C6-C7-C8-C10
27	B	805	CLA	C11-C12-C13-C15
27	B	806	CLA	C12-C13-C15-C16
27	B	829	CLA	C6-C7-C8-C10
27	B	839	CLA	C11-C12-C13-C15
27	L	303	CLA	C12-C13-C15-C16
27	1	611	CLA	C11-C10-C8-C7
27	4	604	CLA	C6-C7-C8-C10
27	5	607	CLA	C11-C10-C8-C7
27	5	609	CLA	C11-C12-C13-C15
27	7	602	CLA	C6-C7-C8-C10
27	X	602	CLA	C11-C12-C13-C15
27	Z	610	CLA	C11-C12-C13-C15
38	X	607	CHL	C12-C13-C15-C16
38	X	608	CHL	C11-C12-C13-C15
38	Y	609	CHL	C11-C10-C8-C7
38	U	609	CHL	C11-C10-C8-C7
38	W	607	CHL	C6-C7-C8-C10
38	W	607	CHL	C11-C12-C13-C15
38	W	609	CHL	C11-C10-C8-C7
27	2	601	CLA	C2C-C3C-CAC-CBC
27	A	801	CLA	C16-C17-C18-C20
27	4	602	CLA	C11-C12-C13-C15
29	H	204	LHG	O2-C2-C3-O3
32	1	621	LMU	C3-C4-C5-C6
27	A	825	CLA	C5-C6-C7-C8
27	L	303	CLA	C8-C10-C11-C12
33	A	860	LMG	C33-C34-C35-C36
29	5	623	LHG	C15-C16-C17-C18
27	B	829	CLA	C3A-C2A-CAA-CBA
27	2	603	CLA	CHA-CBD-CGD-O1D
27	U	613	CLA	C4-C3-C5-C6
27	W	613	CLA	C4-C3-C5-C6
27	X	603	CLA	C2-C3-C5-C6
27	2	602	CLA	C13-C15-C16-C17
27	9	609	CLA	C8-C10-C11-C12
27	5	601	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	H	204	LHG	O6-C4-C5-O7
29	A	846	LHG	C7-C8-C9-C10
27	A	802	CLA	C11-C10-C8-C9
27	A	828	CLA	C11-C10-C8-C9
27	A	829	CLA	C11-C12-C13-C14
27	A	835	CLA	C11-C12-C13-C14
27	B	803	CLA	C6-C7-C8-C9
27	B	831	CLA	C11-C10-C8-C9
27	4	604	CLA	C6-C7-C8-C9
27	4	608	CLA	C11-C10-C8-C9
27	6	604	CLA	C6-C7-C8-C9
27	W	613	CLA	C14-C13-C15-C16
28	A	844	PQN	C21-C22-C23-C24
38	X	601	CHL	C14-C13-C15-C16
38	X	608	CHL	C11-C10-C8-C9
38	Y	601	CHL	C14-C13-C15-C16
38	U	601	CHL	C14-C13-C15-C16
38	W	607	CHL	C14-C13-C15-C16
27	X	610	CLA	O1A-CGA-O2A-C1
27	Y	610	CLA	O1A-CGA-O2A-C1
38	Z	609	CHL	C5-C6-C7-C8
33	8	626	LMG	C31-C32-C33-C34
34	B	850	DGD	O6D-C5D-C6D-O5D
32	K	208	LMU	C4'-C5'-C6'-O6'
27	A	830	CLA	O1D-CGD-O2D-CED
29	8	623	LHG	C30-C31-C32-C33
27	B	825	CLA	C1-C2-C3-C4
27	O	2003	CLA	CAD-CBD-CGD-O1D
27	a	604	CLA	C1-C2-C3-C4
27	1	604	CLA	C1-C2-C3-C4
27	X	604	CLA	C1-C2-C3-C4
27	U	604	CLA	C1-C2-C3-C4
29	H	204	LHG	C30-C31-C32-C33
29	7	622	LHG	O10-C23-O8-C6
29	O	2631	LHG	O7-C5-C6-O8
33	J	103	LMG	O7-C8-C9-O8
33	4	623	LMG	O1-C7-C8-O7
33	5	627	LMG	O7-C8-C9-O8
38	Z	608	CHL	O2A-C1-C2-C3
27	A	801	CLA	C16-C17-C18-C19
33	A	860	LMG	O1-C7-C8-C9
33	9	625	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
27	B	837	CLA	C4-C3-C5-C6
27	A	836	CLA	C2-C3-C5-C6
27	Y	603	CLA	C2-C3-C5-C6
27	3	607	CLA	C8-C10-C11-C12
27	A	815	CLA	CAD-CBD-CGD-O2D
27	A	845	CLA	CAD-CBD-CGD-O2D
27	B	805	CLA	CAD-CBD-CGD-O2D
27	B	841	CLA	CAD-CBD-CGD-O2D
27	a	604	CLA	CAD-CBD-CGD-O2D
27	1	604	CLA	CAD-CBD-CGD-O2D
27	2	601	CLA	CAD-CBD-CGD-O2D
27	4	608	CLA	O1D-CGD-O2D-CED
27	3	609	CLA	C11-C12-C13-C14
27	2	610	CLA	C3-C5-C6-C7
27	a	609	CLA	C13-C15-C16-C17
29	Y	2630	LHG	C27-C28-C29-C30
29	X	2630	LHG	C27-C28-C29-C30
29	3	623	LHG	C24-C25-C26-C27
27	4	613	CLA	O1D-CGD-O2D-CED
33	5	627	LMG	O6-C5-C6-O5
29	3	624	LHG	C27-C28-C29-C30
33	8	626	LMG	C21-C22-C23-C24
27	A	807	CLA	CHA-CBD-CGD-O1D
27	A	807	CLA	CHA-CBD-CGD-O2D
27	A	808	CLA	CHA-CBD-CGD-O1D
27	A	815	CLA	CAD-CBD-CGD-O1D
27	A	821	CLA	CHA-CBD-CGD-O1D
27	A	821	CLA	CHA-CBD-CGD-O2D
27	A	825	CLA	CAD-CBD-CGD-O1D
27	A	826	CLA	CHA-CBD-CGD-O1D
27	A	845	CLA	CAD-CBD-CGD-O1D
27	B	805	CLA	CAD-CBD-CGD-O1D
27	B	813	CLA	CAD-CBD-CGD-O1D
27	B	815	CLA	CHA-CBD-CGD-O1D
27	B	841	CLA	CAD-CBD-CGD-O1D
27	K	201	CLA	CHA-CBD-CGD-O1D
27	a	604	CLA	CAD-CBD-CGD-O1D
27	a	611	CLA	CHA-CBD-CGD-O2D
27	1	604	CLA	CAD-CBD-CGD-O1D
27	1	607	CLA	CHA-CBD-CGD-O2D
27	1	607	CLA	CAD-CBD-CGD-O2D
27	1	614	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	1	614	CLA	CAD-CBD-CGD-O2D
27	2	601	CLA	CAD-CBD-CGD-O1D
27	3	613	CLA	CHA-CBD-CGD-O2D
27	3	613	CLA	CAD-CBD-CGD-O2D
27	5	612	CLA	CHA-CBD-CGD-O2D
27	5	612	CLA	CAD-CBD-CGD-O2D
27	7	604	CLA	CHA-CBD-CGD-O1D
27	8	603	CLA	CHA-CBD-CGD-O1D
27	8	603	CLA	CHA-CBD-CGD-O2D
27	8	616	CLA	CAD-CBD-CGD-O1D
27	9	614	CLA	CHA-CBD-CGD-O1D
27	X	603	CLA	CHA-CBD-CGD-O1D
27	Y	603	CLA	CHA-CBD-CGD-O1D
27	Y	612	CLA	CHA-CBD-CGD-O1D
27	U	603	CLA	CHA-CBD-CGD-O1D
27	U	603	CLA	CHA-CBD-CGD-O2D
27	U	610	CLA	CHA-CBD-CGD-O1D
27	V	602	CLA	CHA-CBD-CGD-O1D
27	V	602	CLA	CHA-CBD-CGD-O2D
27	V	604	CLA	CHA-CBD-CGD-O2D
27	V	614	CLA	CHA-CBD-CGD-O1D
27	W	603	CLA	CHA-CBD-CGD-O1D
27	W	603	CLA	CHA-CBD-CGD-O2D
27	W	610	CLA	CHA-CBD-CGD-O1D
29	B	851	LHG	C4-O6-P-O5
29	H	204	LHG	C4-O6-P-O5
29	O	2631	LHG	C3-O3-P-O5
29	2	622	LHG	C3-O3-P-O5
29	2	622	LHG	C4-O6-P-O5
29	5	623	LHG	C4-O6-P-O4
29	5	625	LHG	C4-O6-P-O5
29	6	623	LHG	C3-O3-P-O5
29	6	623	LHG	C4-O6-P-O5
29	8	623	LHG	C3-O3-P-O4
29	8	623	LHG	C3-O3-P-O6
29	9	622	LHG	C4-O6-P-O5
29	9	623	LHG	C3-O3-P-O5
29	X	2630	LHG	C4-O6-P-O4
29	Y	2630	LHG	C4-O6-P-O4
29	U	2630	LHG	C4-O6-P-O4
29	V	2630	LHG	C4-O6-P-O5
29	W	2630	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
38	V	609	CHL	CHA-CBD-CGD-O1D
38	V	609	CHL	CHA-CBD-CGD-O2D
38	W	609	CHL	CHA-CBD-CGD-O2D
27	A	835	CLA	C4C-C3C-CAC-CBC
27	5	602	CLA	C16-C17-C18-C19
27	3	610	CLA	C4-C3-C5-C6
27	Z	603	CLA	C4-C3-C5-C6
27	A	815	CLA	C2B-C3B-CAB-CBB
27	A	841	CLA	C2B-C3B-CAB-CBB
27	B	802	CLA	C2B-C3B-CAB-CBB
27	B	807	CLA	C2B-C3B-CAB-CBB
27	B	823	CLA	C2B-C3B-CAB-CBB
27	B	830	CLA	C2B-C3B-CAB-CBB
27	F	304	CLA	C2B-C3B-CAB-CBB
27	H	202	CLA	C2B-C3B-CAB-CBB
27	J	101	CLA	C2B-C3B-CAB-CBB
27	a	604	CLA	C2B-C3B-CAB-CBB
27	1	604	CLA	C2B-C3B-CAB-CBB
27	1	611	CLA	C2B-C3B-CAB-CBB
27	3	617	CLA	C2B-C3B-CAB-CBB
27	5	606	CLA	C2B-C3B-CAB-CBB
27	5	617	CLA	C2B-C3B-CAB-CBB
27	6	613	CLA	C2B-C3B-CAB-CBB
27	6	614	CLA	C2B-C3B-CAB-CBB
27	X	610	CLA	C2B-C3B-CAB-CBB
27	X	614	CLA	C2B-C3B-CAB-CBB
27	Y	610	CLA	C2B-C3B-CAB-CBB
27	Y	614	CLA	C2B-C3B-CAB-CBB
30	B	845	BCR	C23-C24-C25-C30
30	L	308	BCR	C5-C6-C7-C8
30	7	621	BCR	C23-C24-C25-C30
30	9	621	BCR	C23-C24-C25-C30
33	L	2631	LMG	C11-C12-C13-C14
27	A	801	CLA	CAA-CBA-CGA-O2A
27	B	817	CLA	C2-C3-C5-C6
27	4	601	CLA	C2-C3-C5-C6
27	U	613	CLA	C2-C3-C5-C6
27	W	613	CLA	C2-C3-C5-C6
27	A	803	CLA	C15-C16-C17-C18
27	A	831	CLA	C10-C11-C12-C13
35	Z	1621	LUT	C7-C8-C9-C19
29	6	623	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
27	8	613	CLA	C5-C6-C7-C8
27	B	818	CLA	C11-C12-C13-C15
27	B	810	CLA	CBA-CGA-O2A-C1
27	Y	613	CLA	O1D-CGD-O2D-CED
29	8	622	LHG	C28-C29-C30-C31
27	B	827	CLA	C3-C5-C6-C7
27	B	803	CLA	C15-C16-C17-C18
29	9	623	LHG	C33-C34-C35-C36
27	A	815	CLA	O1A-CGA-O2A-C1
38	V	609	CHL	C10-C11-C12-C13
27	K	203	CLA	C11-C10-C8-C7
27	B	817	CLA	C11-C12-C13-C14
33	8	626	LMG	C9-C8-O7-C10
27	A	828	CLA	C4-C3-C5-C6
27	a	613	CLA	C4-C3-C5-C6
27	1	613	CLA	C4-C3-C5-C6
34	B	850	DGD	C8A-C9A-CAA-CBA
27	4	601	CLA	C16-C17-C18-C20
38	W	608	CHL	O1A-CGA-O2A-C1
29	3	624	LHG	C30-C31-C32-C33
27	H	203	CLA	C6-C7-C8-C9
27	4	610	CLA	C11-C12-C13-C14
27	Z	603	CLA	C11-C10-C8-C9
27	Z	603	CLA	C11-C12-C13-C14
27	Z	613	CLA	C6-C7-C8-C9
27	V	613	CLA	C6-C7-C8-C9
38	X	608	CHL	C14-C13-C15-C16
27	B	841	CLA	O1D-CGD-O2D-CED
27	X	613	CLA	O1D-CGD-O2D-CED
32	5	629	LMU	C2B-C1B-O1B-C4'
27	B	802	CLA	C6-C7-C8-C10
27	V	602	CLA	C11-C10-C8-C7
38	Z	607	CHL	C11-C10-C8-C7
38	Z	609	CHL	C11-C12-C13-C15
38	U	609	CHL	C6-C7-C8-C10
33	L	2631	LMG	C16-C17-C18-C19
27	A	842	CLA	C16-C17-C18-C19
27	B	827	CLA	C2C-C3C-CAC-CBC
27	U	613	CLA	C8-C10-C11-C12
27	A	824	CLA	O1D-CGD-O2D-CED
27	4	609	CLA	O1D-CGD-O2D-CED
27	A	843	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	8	601	CLA	C4-C3-C5-C6
29	a	620	LHG	C9-C10-C11-C12
29	1	620	LHG	C9-C10-C11-C12
29	5	623	LHG	C13-C14-C15-C16
27	A	815	CLA	CBA-CGA-O2A-C1
27	a	604	CLA	CBA-CGA-O2A-C1
27	1	604	CLA	CBA-CGA-O2A-C1
27	3	609	CLA	C11-C12-C13-C15
27	5	602	CLA	C16-C17-C18-C20
29	9	623	LHG	C15-C16-C17-C18
27	a	604	CLA	O1A-CGA-O2A-C1
27	A	804	CLA	C5-C6-C7-C8
27	W	613	CLA	C8-C10-C11-C12
34	B	850	DGD	O1G-C1G-C2G-O2G
27	B	827	CLA	CAA-CBA-CGA-O2A
29	Z	2630	LHG	C26-C27-C28-C29
28	B	842	PQN	C23-C25-C26-C27
27	1	604	CLA	O1A-CGA-O2A-C1
29	6	623	LHG	C11-C10-C9-C8
27	V	611	CLA	O1D-CGD-O2D-CED
38	Y	607	CHL	CAA-CBA-CGA-O2A
27	A	814	CLA	C3-C5-C6-C7
27	a	609	CLA	C3-C5-C6-C7
29	5	625	LHG	C24-C25-C26-C27
27	7	611	CLA	O2A-C1-C2-C3
33	9	625	LMG	O7-C10-C11-C12
29	9	624	LHG	C30-C31-C32-C33
27	8	606	CLA	C15-C16-C17-C18
27	B	819	CLA	C3-C5-C6-C7
29	B	854	LHG	C15-C16-C17-C18
35	4	619	LUT	C27-C28-C29-C39
27	A	822	CLA	C2C-C3C-CAC-CBC
27	A	829	CLA	C16-C17-C18-C20
38	Z	609	CHL	C1C-C2C-CMC-OMC
29	Z	2630	LHG	C34-C35-C36-C37
29	O	2631	LHG	C24-C23-O8-C6
27	1	613	CLA	C5-C6-C7-C8
29	W	2630	LHG	C27-C28-C29-C30
27	5	614	CLA	C2A-CAA-CBA-CGA
27	8	602	CLA	C2A-CAA-CBA-CGA
38	X	605	CHL	C2A-CAA-CBA-CGA
29	U	2630	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	9	602	CLA	C4-C3-C5-C6
27	5	603	CLA	C5-C6-C7-C8
27	A	804	CLA	CBD-CGD-O2D-CED
27	Z	603	CLA	C5-C6-C7-C8
29	H	204	LHG	C10-C11-C12-C13
29	4	622	LHG	C17-C18-C19-C20
27	X	603	CLA	CAA-CBA-CGA-O1A
27	Y	603	CLA	CAA-CBA-CGA-O1A
29	3	624	LHG	C1-C2-C3-O3
32	A	857	LMU	C2-C1-O1'-C1'
27	A	854	CLA	C16-C17-C18-C19
27	4	613	CLA	C16-C17-C18-C19
29	3	623	LHG	C27-C28-C29-C30
27	A	841	CLA	C14-C13-C15-C16
27	B	802	CLA	C6-C7-C8-C9
27	B	805	CLA	C11-C12-C13-C14
27	B	806	CLA	C14-C13-C15-C16
27	7	602	CLA	C6-C7-C8-C9
38	W	607	CHL	C11-C12-C13-C14
27	X	603	CLA	CBA-CGA-O2A-C1
27	B	829	CLA	C5-C6-C7-C8
27	A	804	CLA	O1D-CGD-O2D-CED
27	B	820	CLA	C4B-C3B-CAB-CBB
27	B	841	CLA	C4B-C3B-CAB-CBB
27	7	611	CLA	C4B-C3B-CAB-CBB
27	8	613	CLA	C4B-C3B-CAB-CBB
27	V	612	CLA	C4B-C3B-CAB-CBB
27	4	603	CLA	CAA-CBA-CGA-O2A
27	A	827	CLA	CBA-CGA-O2A-C1
27	Y	603	CLA	CBA-CGA-O2A-C1
29	Z	2630	LHG	C24-C23-O8-C6
27	3	609	CLA	C4C-C3C-CAC-CBC
29	7	622	LHG	C30-C31-C32-C33
27	B	827	CLA	C2A-CAA-CBA-CGA
38	W	607	CHL	C4-C3-C5-C6
27	A	828	CLA	C2-C3-C5-C6
27	a	613	CLA	C2-C3-C5-C6
27	1	613	CLA	C2-C3-C5-C6
27	Z	603	CLA	C2-C3-C5-C6
29	Z	2630	LHG	O6-C4-C5-O7
33	J	104	LMG	C17-C18-C19-C20
27	A	825	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	X	603	CLA	O1A-CGA-O2A-C1
27	Y	603	CLA	O1A-CGA-O2A-C1
27	4	613	CLA	C16-C17-C18-C20
27	B	833	CLA	C6-C7-C8-C10
27	H	203	CLA	C12-C13-C15-C16
27	4	602	CLA	C11-C10-C8-C7
38	V	601	CHL	C11-C10-C8-C7
27	B	811	CLA	C5-C6-C7-C8
27	2	602	CLA	C15-C16-C17-C18
27	A	829	CLA	C16-C17-C18-C19
27	B	818	CLA	C11-C12-C13-C14
27	4	601	CLA	C16-C17-C18-C19
33	9	625	LMG	C30-C31-C32-C33
29	B	854	LHG	C24-C25-C26-C27
33	V	2631	LMG	C18-C19-C20-C21
29	2	622	LHG	O7-C5-C6-O8
27	A	802	CLA	C4-C3-C5-C6
27	A	837	CLA	C3A-C2A-CAA-CBA
27	A	838	CLA	C3A-C2A-CAA-CBA
27	B	816	CLA	C4-C3-C5-C6
27	B	819	CLA	C3A-C2A-CAA-CBA
27	5	617	CLA	C3A-C2A-CAA-CBA
27	V	604	CLA	C3A-C2A-CAA-CBA
38	Z	601	CHL	C3A-C2A-CAA-CBA
27	A	843	CLA	C2-C3-C5-C6
27	B	837	CLA	C2-C3-C5-C6
27	8	601	CLA	C2-C3-C5-C6
27	B	811	CLA	CAD-CBD-CGD-O1D
27	B	811	CLA	CAD-CBD-CGD-O2D
30	A	852	BCR	C11-C10-C9-C34
30	A	852	BCR	C16-C17-C18-C36
30	B	845	BCR	C11-C10-C9-C34
30	B	845	BCR	C20-C21-C22-C37
30	B	852	BCR	C11-C10-C9-C34
30	F	305	BCR	C16-C17-C18-C36
30	L	301	BCR	C11-C10-C9-C34
37	5	624	NEX	C39-C29-C30-C31
37	6	624	NEX	C39-C29-C30-C31
37	X	1623	NEX	C39-C29-C30-C31
37	Y	1623	NEX	C39-C29-C30-C31
37	Z	1623	NEX	C39-C29-C30-C31
37	U	1623	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
37	V	1623	NEX	C39-C29-C30-C31
37	W	1623	NEX	C39-C29-C30-C31
27	A	834	CLA	C8-C10-C11-C12
32	A	858	LMU	C2-C3-C4-C5
27	B	828	CLA	C5-C6-C7-C8
27	a	613	CLA	C5-C6-C7-C8
27	A	821	CLA	C2-C1-O2A-CGA
27	B	834	CLA	C2-C1-O2A-CGA
27	3	609	CLA	C2-C1-O2A-CGA
27	Z	603	CLA	C8-C10-C11-C12
27	5	616	CLA	CAA-CBA-CGA-O1A
27	X	611	CLA	CAA-CBA-CGA-O2A
27	Y	612	CLA	CAA-CBA-CGA-O1A
27	A	807	CLA	C4-C3-C5-C6
38	X	607	CHL	C4-C3-C5-C6
38	Y	607	CHL	C4-C3-C5-C6
27	A	839	CLA	C2A-CAA-CBA-CGA
27	B	835	CLA	C2A-CAA-CBA-CGA
27	9	614	CLA	C2A-CAA-CBA-CGA
27	G	204	CLA	CAA-CBA-CGA-O1A
27	4	603	CLA	CAA-CBA-CGA-O1A
27	A	808	CLA	CBA-CGA-O2A-C1
29	a	620	LHG	C4-C5-C6-O8
29	1	620	LHG	C4-C5-C6-O8
29	6	623	LHG	C4-C5-C6-O8
29	8	622	LHG	C4-C5-C6-O8
33	V	2631	LMG	C29-C30-C31-C32
32	5	629	LMU	C6-C7-C8-C9
29	B	851	LHG	C30-C31-C32-C33
29	8	622	LHG	C15-C16-C17-C18
27	X	611	CLA	CAA-CBA-CGA-O1A
27	A	834	CLA	C11-C12-C13-C14
27	B	806	CLA	C6-C7-C8-C9
27	B	826	CLA	C11-C10-C8-C9
27	B	826	CLA	C11-C12-C13-C14
27	B	829	CLA	C6-C7-C8-C9
27	a	609	CLA	C11-C12-C13-C14
27	4	602	CLA	C11-C10-C8-C9
27	7	610	CLA	C11-C10-C8-C9
27	Z	613	CLA	C11-C10-C8-C9
38	V	601	CHL	C11-C10-C8-C9
27	3	613	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	9	623	LHG	C11-C10-C9-C8
27	A	827	CLA	O1A-CGA-O2A-C1
27	5	614	CLA	CAA-CBA-CGA-O1A
27	7	615	CLA	CAA-CBA-CGA-O1A
27	7	615	CLA	CAA-CBA-CGA-O2A
33	8	626	LMG	C7-C8-O7-C10
27	B	827	CLA	C10-C11-C12-C13
27	8	608	CLA	O1D-CGD-O2D-CED
38	W	601	CHL	C1A-C2A-CAA-CBA
27	A	824	CLA	C8-C10-C11-C12
27	1	616	CLA	CAA-CBA-CGA-O1A
27	8	616	CLA	CAA-CBA-CGA-O2A
27	7	601	CLA	C4-C3-C5-C6
33	5	627	LMG	C30-C31-C32-C33
27	3	607	CLA	CBD-CGD-O2D-CED
27	B	832	CLA	CAA-CBA-CGA-O2A
27	B	816	CLA	C2-C3-C5-C6
27	9	602	CLA	C2-C3-C5-C6
27	B	824	CLA	O1A-CGA-O2A-C1
27	a	616	CLA	CAA-CBA-CGA-O1A
27	W	612	CLA	CAA-CBA-CGA-O1A
29	A	846	LHG	C23-C24-C25-C26
27	B	824	CLA	C8-C10-C11-C12
27	A	837	CLA	C1A-C2A-CAA-CBA
27	A	838	CLA	C1A-C2A-CAA-CBA
27	B	802	CLA	C1A-C2A-CAA-CBA
27	1	608	CLA	C1A-C2A-CAA-CBA
27	4	604	CLA	C1A-C2A-CAA-CBA
27	5	617	CLA	C1A-C2A-CAA-CBA
27	5	619	CLA	C1A-C2A-CAA-CBA
27	6	601	CLA	C1A-C2A-CAA-CBA
27	V	604	CLA	C1A-C2A-CAA-CBA
30	A	852	BCR	C11-C10-C9-C8
30	A	852	BCR	C16-C17-C18-C19
30	B	845	BCR	C11-C10-C9-C8
30	B	845	BCR	C20-C21-C22-C23
30	B	852	BCR	C11-C10-C9-C8
30	F	305	BCR	C16-C17-C18-C19
30	L	301	BCR	C11-C10-C9-C8
37	5	624	NEX	C28-C29-C30-C31
37	6	624	NEX	C28-C29-C30-C31
37	X	1623	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
37	Y	1623	NEX	C28-C29-C30-C31
37	Z	1623	NEX	C28-C29-C30-C31
37	U	1623	NEX	C28-C29-C30-C31
37	V	1623	NEX	C28-C29-C30-C31
37	W	1623	NEX	C28-C29-C30-C31
27	A	837	CLA	CAA-CBA-CGA-O1A
27	2	603	CLA	CAA-CBA-CGA-O1A
27	7	612	CLA	CAA-CBA-CGA-O1A
29	1	620	LHG	C26-C27-C28-C29
29	O	2631	LHG	O10-C23-O8-C6
32	K	208	LMU	C5'-C4'-O1B-C1B
29	a	620	LHG	C26-C27-C28-C29
27	A	807	CLA	C2B-C3B-CAB-CBB
27	B	818	CLA	C2B-C3B-CAB-CBB
27	B	820	CLA	C2B-C3B-CAB-CBB
27	L	307	CLA	C2B-C3B-CAB-CBB
27	a	608	CLA	C2B-C3B-CAB-CBB
27	1	608	CLA	C2B-C3B-CAB-CBB
27	2	607	CLA	C2B-C3B-CAB-CBB
27	3	614	CLA	C2B-C3B-CAB-CBB
27	4	607	CLA	C2B-C3B-CAB-CBB
27	6	608	CLA	C2B-C3B-CAB-CBB
27	6	611	CLA	C2B-C3B-CAB-CBB
27	6	617	CLA	C2B-C3B-CAB-CBB
27	8	608	CLA	C2B-C3B-CAB-CBB
27	8	609	CLA	C2B-C3B-CAB-CBB
27	8	614	CLA	C2B-C3B-CAB-CBB
27	9	614	CLA	C2B-C3B-CAB-CBB
27	X	613	CLA	C2B-C3B-CAB-CBB
27	Y	613	CLA	C2B-C3B-CAB-CBB
27	Z	614	CLA	C2B-C3B-CAB-CBB
27	U	614	CLA	C2B-C3B-CAB-CBB
27	V	603	CLA	C2B-C3B-CAB-CBB
27	V	612	CLA	C2B-C3B-CAB-CBB
27	W	614	CLA	C2B-C3B-CAB-CBB
30	L	309	BCR	C5-C6-C7-C8
30	3	620	BCR	C23-C24-C25-C26
30	6	622	BCR	C23-C24-C25-C30
30	8	621	BCR	C5-C6-C7-C8
35	2	619	LUT	C1-C6-C7-C8
35	4	619	LUT	C5-C6-C7-C8
35	X	1620	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
35	Y	1620	LUT	C5-C6-C7-C8
27	G	204	CLA	CAA-CBA-CGA-O2A
27	2	606	CLA	CAA-CBA-CGA-O2A
27	V	603	CLA	CAA-CBA-CGA-O2A
27	B	824	CLA	CBA-CGA-O2A-C1
27	A	808	CLA	O1A-CGA-O2A-C1
27	A	833	CLA	CAA-CBA-CGA-O2A
27	2	606	CLA	CAA-CBA-CGA-O1A
27	6	601	CLA	C4-C3-C5-C6
27	7	602	CLA	C4-C3-C5-C6
38	Y	609	CHL	C4-C3-C5-C6
38	V	609	CHL	C4-C3-C5-C6
29	H	204	LHG	O6-C4-C5-C6
27	A	802	CLA	C2-C3-C5-C6
27	A	825	CLA	C8-C10-C11-C12
33	V	2631	LMG	O9-C10-O7-C8
29	B	851	LHG	C23-C24-C25-C26
27	a	616	CLA	CAA-CBA-CGA-O2A
27	1	616	CLA	CAA-CBA-CGA-O2A
27	8	616	CLA	CAA-CBA-CGA-O1A
27	A	804	CLA	C11-C12-C13-C15
27	B	808	CLA	C11-C10-C8-C7
27	3	610	CLA	C11-C10-C8-C7
27	4	614	CLA	C6-C7-C8-C10
27	5	613	CLA	C12-C13-C15-C16
27	6	613	CLA	C12-C13-C15-C16
27	Z	610	CLA	C12-C13-C15-C16
27	V	610	CLA	C12-C13-C15-C16
38	X	607	CHL	C6-C7-C8-C10
38	Z	601	CHL	C12-C13-C15-C16
38	Z	607	CHL	C6-C7-C8-C10
29	3	624	LHG	C28-C29-C30-C31
27	6	602	CLA	C2A-CAA-CBA-CGA
27	6	613	CLA	C2A-CAA-CBA-CGA
27	8	616	CLA	C2A-CAA-CBA-CGA
33	H	205	LMG	C28-C29-C30-C31
29	9	624	LHG	O7-C5-C6-O8
27	5	614	CLA	CAA-CBA-CGA-O2A
27	7	612	CLA	CAA-CBA-CGA-O2A
27	Y	612	CLA	CAA-CBA-CGA-O2A
29	6	623	LHG	C30-C31-C32-C33
34	B	850	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
29	7	622	LHG	C29-C30-C31-C32
29	5	623	LHG	C14-C15-C16-C17
29	U	2630	LHG	C33-C34-C35-C36
27	L	302	CLA	CAA-CBA-CGA-O2A
27	7	603	CLA	CAA-CBA-CGA-O1A
27	V	612	CLA	CAA-CBA-CGA-O2A
27	W	612	CLA	CAA-CBA-CGA-O2A
27	B	833	CLA	C4-C3-C5-C6
27	2	610	CLA	C4-C3-C5-C6
27	5	610	CLA	C4-C3-C5-C6
38	U	609	CHL	C4-C3-C5-C6
27	8	608	CLA	CBD-CGD-O2D-CED
27	B	805	CLA	C3-C5-C6-C7
27	4	614	CLA	C2-C3-C5-C6
38	X	607	CHL	C2-C3-C5-C6
38	W	607	CHL	C2-C3-C5-C6
27	7	608	CLA	C2-C1-O2A-CGA
38	V	609	CHL	C2-C1-O2A-CGA
27	A	814	CLA	C13-C15-C16-C17
27	A	818	CLA	C8-C10-C11-C12
27	5	616	CLA	CAA-CBA-CGA-O2A
27	V	603	CLA	CAA-CBA-CGA-O1A
30	B	848	BCR	C21-C22-C23-C24
35	4	619	LUT	C27-C28-C29-C30
27	V	613	CLA	C8-C10-C11-C12
33	J	104	LMG	C28-C29-C30-C31
27	4	608	CLA	C3-C5-C6-C7
27	X	603	CLA	C3-C5-C6-C7
27	9	603	CLA	CAA-CBA-CGA-O2A
27	B	814	CLA	C11-C12-C13-C14
27	A	825	CLA	C15-C16-C17-C18
29	9	624	LHG	C10-C11-C12-C13
27	8	613	CLA	C8-C10-C11-C12
27	Z	602	CLA	C8-C10-C11-C12
27	A	833	CLA	CAA-CBA-CGA-O1A
27	1	612	CLA	CAA-CBA-CGA-O2A
38	W	606	CHL	CAA-CBA-CGA-O2A
27	A	835	CLA	C2C-C3C-CAC-CBC
29	3	624	LHG	C10-C11-C12-C13
38	X	609	CHL	C4-C3-C5-C6
38	Z	607	CHL	C4-C3-C5-C6
38	Z	609	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	A	837	CLA	CAA-CBA-CGA-O2A
27	L	302	CLA	CAA-CBA-CGA-O1A
29	3	624	LHG	C25-C26-C27-C28
38	Y	607	CHL	C2-C3-C5-C6
27	V	612	CLA	CAA-CBA-CGA-O1A
27	W	603	CLA	O1A-CGA-O2A-C1
33	8	626	LMG	O1-C7-C8-C9
27	a	612	CLA	CAA-CBA-CGA-O2A
27	4	607	CLA	CAA-CBA-CGA-O2A
29	4	622	LHG	C25-C26-C27-C28
27	U	603	CLA	O1A-CGA-O2A-C1
27	Y	603	CLA	C3-C5-C6-C7
32	K	208	LMU	C3'-C4'-O1B-C1B
27	3	607	CLA	C2A-CAA-CBA-CGA
27	A	814	CLA	C10-C11-C12-C13
27	Z	611	CLA	C10-C11-C12-C13
27	3	613	CLA	C6-C7-C8-C10
38	W	605	CHL	CAA-CBA-CGA-O2A
38	W	606	CHL	CAA-CBA-CGA-O1A
27	A	818	CLA	C4-C3-C5-C6
33	9	625	LMG	C21-C22-C23-C24
38	V	608	CHL	C2-C1-O2A-CGA
27	B	839	CLA	C4B-C3B-CAB-CBB
27	1	611	CLA	C4B-C3B-CAB-CBB
27	3	608	CLA	C4B-C3B-CAB-CBB
27	4	607	CLA	C4B-C3B-CAB-CBB
27	4	614	CLA	C4B-C3B-CAB-CBB
27	6	617	CLA	C4B-C3B-CAB-CBB
27	7	604	CLA	C4B-C3B-CAB-CBB
27	8	608	CLA	C4B-C3B-CAB-CBB
27	X	604	CLA	C4B-C3B-CAB-CBB
27	Y	604	CLA	C4B-C3B-CAB-CBB
27	B	832	CLA	O1A-CGA-O2A-C1
27	7	603	CLA	CAA-CBA-CGA-O2A
32	5	628	LMU	C2B-C1B-O1B-C4'
33	V	2631	LMG	C13-C14-C15-C16
29	Z	2630	LHG	O10-C23-O8-C6
27	5	619	CLA	CAA-CBA-CGA-O2A
38	X	601	CHL	CHA-CBD-CGD-O2D
38	U	601	CHL	CHA-CBD-CGD-O2D
38	V	601	CHL	CHA-CBD-CGD-O2D
38	W	601	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
38	W	601	CHL	CHA-CBD-CGD-O2D
27	X	613	CLA	C8-C10-C11-C12
27	Y	613	CLA	C8-C10-C11-C12
27	8	601	CLA	CAA-CBA-CGA-O2A
29	V	2630	LHG	C33-C34-C35-C36
27	5	619	CLA	CAA-CBA-CGA-O1A
27	9	603	CLA	CAA-CBA-CGA-O1A
27	9	614	CLA	CAA-CBA-CGA-O2A
29	Z	2630	LHG	O6-C4-C5-C6
27	6	617	CLA	CAA-CBA-CGA-O2A
33	V	2631	LMG	C11-C10-O7-C8
27	5	613	CLA	CBA-CGA-O2A-C1
27	A	807	CLA	C2-C3-C5-C6
38	Z	609	CHL	C2-C3-C5-C6
27	B	834	CLA	C3-C5-C6-C7
29	4	622	LHG	C15-C16-C17-C18
38	Y	607	CHL	C12-C13-C15-C16
37	V	1623	NEX	C29-C30-C31-C32
38	W	605	CHL	CAA-CBA-CGA-O1A
27	A	809	CLA	C14-C13-C15-C16
27	A	820	CLA	C11-C12-C13-C14
27	B	806	CLA	C11-C12-C13-C14
27	B	808	CLA	C6-C7-C8-C9
27	a	609	CLA	C14-C13-C15-C16
27	5	609	CLA	C11-C12-C13-C14
27	8	613	CLA	C11-C10-C8-C9
27	Z	612	CLA	C11-C12-C13-C14
38	Z	601	CHL	C6-C7-C8-C9
38	V	609	CHL	C6-C7-C8-C9
27	V	613	CLA	C15-C16-C17-C18
27	U	604	CLA	CHA-CBD-CGD-O1D
33	A	860	LMG	C8-C7-O1-C1
29	B	851	LHG	C27-C28-C29-C30
27	6	617	CLA	CAA-CBA-CGA-O1A
27	8	603	CLA	CAA-CBA-CGA-O2A
27	B	807	CLA	C2A-CAA-CBA-CGA
27	9	613	CLA	C2A-CAA-CBA-CGA
27	B	814	CLA	C2-C1-O2A-CGA
27	F	301	CLA	C2-C1-O2A-CGA
27	8	613	CLA	C2-C1-O2A-CGA
38	Y	607	CHL	C2-C1-O2A-CGA
38	Z	608	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
27	a	603	CLA	C2A-CAA-CBA-CGA
27	1	603	CLA	C2A-CAA-CBA-CGA
27	B	832	CLA	CBA-CGA-O2A-C1
27	U	603	CLA	CBA-CGA-O2A-C1
27	W	603	CLA	CBA-CGA-O2A-C1
38	X	608	CHL	CBA-CGA-O2A-C1
27	a	609	CLA	C3A-C2A-CAA-CBA
38	Y	601	CHL	C3A-C2A-CAA-CBA
38	Z	607	CHL	C3A-C2A-CAA-CBA
38	Z	609	CHL	C3A-C2A-CAA-CBA
27	4	607	CLA	CAA-CBA-CGA-O1A
27	4	616	CLA	CAA-CBA-CGA-O2A
33	4	624	LMG	C29-C30-C31-C32
27	3	610	CLA	C2-C3-C5-C6
38	U	609	CHL	C2-C3-C5-C6
27	3	607	CLA	O1D-CGD-O2D-CED
27	A	819	CLA	CAA-CBA-CGA-O1A
27	a	612	CLA	CAA-CBA-CGA-O1A
27	1	612	CLA	CAA-CBA-CGA-O1A
27	2	603	CLA	CAA-CBA-CGA-O2A
27	a	608	CLA	CAA-CBA-CGA-O2A
27	1	608	CLA	CAA-CBA-CGA-O2A
27	8	609	CLA	CAA-CBA-CGA-O2A
38	Y	606	CHL	CAA-CBA-CGA-O2A
29	9	624	LHG	C17-C18-C19-C20
27	7	602	CLA	C5-C6-C7-C8
27	B	809	CLA	O1A-CGA-O2A-C1
27	7	611	CLA	C2-C3-C5-C6
27	2	601	CLA	C4C-C3C-CAC-CBC
36	U	1622	XAT	O24-C26-C27-C28
36	W	1622	XAT	O24-C26-C27-C28
37	X	1623	NEX	O24-C26-C27-C28
37	Y	1623	NEX	O24-C26-C27-C28
37	U	1623	NEX	O24-C26-C27-C28
37	W	1623	NEX	O24-C26-C27-C28
27	9	614	CLA	CAA-CBA-CGA-O1A
29	V	2630	LHG	O6-C4-C5-O7
27	B	839	CLA	CBA-CGA-O2A-C1
27	B	823	CLA	CAA-CBA-CGA-O2A
29	O	2631	LHG	C4-C5-C6-O8
27	B	839	CLA	O1A-CGA-O2A-C1
38	X	608	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	3	610	CLA	C10-C11-C12-C13
27	a	614	CLA	CAA-CBA-CGA-O2A
27	8	603	CLA	CAA-CBA-CGA-O1A
29	9	623	LHG	C10-C11-C12-C13
27	B	806	CLA	CAA-CBA-CGA-O2A
37	U	1623	NEX	C9-C10-C11-C12
37	W	1623	NEX	C9-C10-C11-C12
27	B	832	CLA	C11-C12-C13-C14
29	8	622	LHG	C9-C10-C11-C12
27	A	841	CLA	C8-C10-C11-C12
27	4	613	CLA	C8-C10-C11-C12
27	5	611	CLA	CBD-CGD-O2D-CED
27	4	616	CLA	CAA-CBA-CGA-O1A
27	6	608	CLA	CAA-CBA-CGA-O1A
27	8	609	CLA	CAA-CBA-CGA-O1A
29	2	622	LHG	C23-C24-C25-C26
27	A	830	CLA	CAA-CBA-CGA-O2A
27	3	606	CLA	CAA-CBA-CGA-O2A
29	Z	2630	LHG	O7-C5-C6-O8
27	a	608	CLA	CAA-CBA-CGA-O1A
38	Y	606	CHL	CAA-CBA-CGA-O1A
27	A	802	CLA	C11-C12-C13-C14
27	A	804	CLA	C11-C12-C13-C14
27	A	806	CLA	C6-C7-C8-C9
27	A	825	CLA	C14-C13-C15-C16
27	B	813	CLA	C11-C12-C13-C14
27	5	607	CLA	C11-C10-C8-C9
27	8	602	CLA	C11-C10-C8-C9
27	9	610	CLA	C11-C10-C8-C9
27	X	602	CLA	C11-C12-C13-C14
27	Z	611	CLA	C11-C12-C13-C14
29	1	620	LHG	C14-C15-C16-C17
29	3	623	LHG	O8-C23-C24-C25
27	U	603	CLA	CAA-CBA-CGA-O1A
27	W	603	CLA	CAA-CBA-CGA-O1A
29	V	2630	LHG	O6-C4-C5-C6
27	1	608	CLA	CAA-CBA-CGA-O1A
27	6	608	CLA	CAA-CBA-CGA-O2A
32	8	625	LMU	O5'-C5'-C6'-O6'
29	9	622	LHG	C9-C10-C11-C12
27	A	826	CLA	C4-C3-C5-C6
34	B	850	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
27	A	807	CLA	CAA-CBA-CGA-O2A
27	9	607	CLA	CAA-CBA-CGA-O2A
27	Z	614	CLA	CBA-CGA-O2A-C1
27	A	837	CLA	C2A-CAA-CBA-CGA
27	B	806	CLA	C11-C12-C13-C15
27	B	808	CLA	C6-C7-C8-C10
27	B	814	CLA	C11-C12-C13-C15
27	a	609	CLA	C11-C12-C13-C15
27	a	609	CLA	C12-C13-C15-C16
27	2	601	CLA	C12-C13-C15-C16
27	8	601	CLA	C11-C12-C13-C15
27	Z	613	CLA	C11-C10-C8-C7
27	A	832	CLA	C2B-C3B-CAB-CBB
27	A	835	CLA	C2B-C3B-CAB-CBB
27	B	839	CLA	C2B-C3B-CAB-CBB
27	L	303	CLA	C2B-C3B-CAB-CBB
27	a	610	CLA	C2B-C3B-CAB-CBB
27	1	610	CLA	C2B-C3B-CAB-CBB
27	2	604	CLA	C2B-C3B-CAB-CBB
27	2	610	CLA	C2B-C3B-CAB-CBB
27	3	608	CLA	C2B-C3B-CAB-CBB
27	4	606	CLA	C2B-C3B-CAB-CBB
27	4	614	CLA	C2B-C3B-CAB-CBB
27	7	604	CLA	C2B-C3B-CAB-CBB
27	7	607	CLA	C2B-C3B-CAB-CBB
27	9	606	CLA	C2B-C3B-CAB-CBB
27	9	611	CLA	C2B-C3B-CAB-CBB
27	X	604	CLA	C2B-C3B-CAB-CBB
27	Y	604	CLA	C2B-C3B-CAB-CBB
27	U	610	CLA	C2B-C3B-CAB-CBB
27	W	610	CLA	C2B-C3B-CAB-CBB
30	B	846	BCR	C1-C6-C7-C8
30	B	853	BCR	C23-C24-C25-C30
30	O	2004	BCR	C23-C24-C25-C26
30	7	623	BCR	C23-C24-C25-C30
35	7	619	LUT	C1-C6-C7-C8
35	U	1620	LUT	C5-C6-C7-C8
35	W	1620	LUT	C5-C6-C7-C8
29	9	624	LHG	O8-C23-C24-C25
27	A	843	CLA	C2-C1-O2A-CGA
27	A	854	CLA	C2-C1-O2A-CGA
27	Z	612	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
38	U	609	CHL	C2-C1-O2A-CGA
29	9	624	LHG	C13-C14-C15-C16
32	1	621	LMU	C1-C2-C3-C4
27	A	834	CLA	CAA-CBA-CGA-O2A
27	8	613	CLA	C13-C15-C16-C17
27	A	826	CLA	C2-C3-C5-C6
27	B	828	CLA	C2-C3-C5-C6
27	Z	614	CLA	O1A-CGA-O2A-C1
33	V	2631	LMG	C17-C18-C19-C20
27	A	829	CLA	C2A-CAA-CBA-CGA
27	Z	604	CLA	C2A-CAA-CBA-CGA
27	W	603	CLA	C3-C5-C6-C7
27	3	609	CLA	C5-C6-C7-C8
32	1	621	LMU	C4-C5-C6-C7
27	A	804	CLA	C2C-C3C-CAC-CBC
27	A	818	CLA	CAA-CBA-CGA-O2A
27	5	608	CLA	CAA-CBA-CGA-O2A
27	W	611	CLA	CAA-CBA-CGA-O2A
27	3	612	CLA	C2A-CAA-CBA-CGA
27	B	828	CLA	C4-C3-C5-C6
27	A	843	CLA	CAA-CBA-CGA-O2A
27	W	611	CLA	C5-C6-C7-C8
29	8	623	LHG	C31-C32-C33-C34
27	U	603	CLA	C3-C5-C6-C7
27	B	823	CLA	CAA-CBA-CGA-O1A
29	B	851	LHG	C26-C27-C28-C29
29	9	624	LHG	C15-C16-C17-C18
33	9	625	LMG	C20-C21-C22-C23
29	9	622	LHG	C26-C27-C28-C29
38	W	607	CHL	CAA-CBA-CGA-O1A
33	9	625	LMG	C18-C19-C20-C21
27	A	826	CLA	C11-C12-C13-C14
27	B	839	CLA	C11-C12-C13-C14
27	3	610	CLA	C11-C10-C8-C9
27	4	614	CLA	C6-C7-C8-C9
27	6	613	CLA	C14-C13-C15-C16
27	Z	610	CLA	C11-C12-C13-C14
27	V	610	CLA	C14-C13-C15-C16
38	X	607	CHL	C14-C13-C15-C16
38	Y	607	CHL	C14-C13-C15-C16
29	9	622	LHG	C7-C8-C9-C10
29	3	623	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	A	825	CLA	O1A-CGA-O2A-C1
33	5	627	LMG	O1-C7-C8-C9
32	A	858	LMU	C4B-C5B-C6B-O6B
27	A	801	CLA	C4B-C3B-CAB-CBB
27	A	827	CLA	C1A-C2A-CAA-CBA
27	A	829	CLA	C1A-C2A-CAA-CBA
27	A	842	CLA	C4B-C3B-CAB-CBB
27	A	843	CLA	C4B-C3B-CAB-CBB
27	A	845	CLA	C1A-C2A-CAA-CBA
27	B	818	CLA	C4B-C3B-CAB-CBB
27	B	819	CLA	C1A-C2A-CAA-CBA
27	B	826	CLA	C1A-C2A-CAA-CBA
27	B	835	CLA	C4B-C3B-CAB-CBB
27	B	840	CLA	C4B-C3B-CAB-CBB
27	F	301	CLA	C1A-C2A-CAA-CBA
27	L	307	CLA	C4B-C3B-CAB-CBB
27	a	606	CLA	C1A-C2A-CAA-CBA
27	3	613	CLA	C4B-C3B-CAB-CBB
27	6	610	CLA	C4B-C3B-CAB-CBB
27	8	606	CLA	C1A-C2A-CAA-CBA
27	Z	603	CLA	C4B-C3B-CAB-CBB
27	Z	613	CLA	C4B-C3B-CAB-CBB
27	9	607	CLA	CAA-CBA-CGA-O1A
27	A	821	CLA	CAA-CBA-CGA-O2A
27	B	809	CLA	CAA-CBA-CGA-O2A
27	B	813	CLA	CAA-CBA-CGA-O2A
27	6	616	CLA	CAA-CBA-CGA-O2A
29	H	204	LHG	O7-C5-C6-O8
29	Y	2630	LHG	O7-C5-C6-O8
33	L	2631	LMG	O7-C8-C9-O8
33	8	626	LMG	C24-C25-C26-C27
30	5	622	BCR	C21-C22-C23-C24
30	7	621	BCR	C7-C8-C9-C10
35	8	619	LUT	C7-C8-C9-C10
27	A	809	CLA	C16-C17-C18-C19
27	K	204	CLA	CAA-CBA-CGA-O2A
27	Z	603	CLA	CAA-CBA-CGA-O2A
29	Z	2630	LHG	C24-C25-C26-C27
27	A	802	CLA	C2A-CAA-CBA-CGA
27	4	608	CLA	C4C-C3C-CAC-CBC
38	Z	606	CHL	CAA-CBA-CGA-O2A
27	a	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	V	2631	LMG	C11-C12-C13-C14
27	A	841	CLA	CAA-CBA-CGA-O2A
27	1	602	CLA	O1A-CGA-O2A-C1
27	8	608	CLA	C2-C3-C5-C6
27	A	803	CLA	C4-C3-C5-C6
27	A	811	CLA	C2-C1-O2A-CGA
27	A	839	CLA	C2-C1-O2A-CGA
27	B	806	CLA	C2-C1-O2A-CGA
27	a	604	CLA	C2-C1-O2A-CGA
27	1	604	CLA	C2-C1-O2A-CGA
27	4	608	CLA	C2-C1-O2A-CGA
27	6	616	CLA	C2-C1-O2A-CGA
38	X	609	CHL	C2-C1-O2A-CGA
27	A	806	CLA	C6-C7-C8-C10
27	A	814	CLA	C6-C7-C8-C10
27	A	816	CLA	C11-C12-C13-C15
27	A	818	CLA	C11-C10-C8-C7
27	B	802	CLA	C11-C12-C13-C15
27	6	604	CLA	C6-C7-C8-C10
27	Z	612	CLA	C11-C12-C13-C15
28	A	844	PQN	C22-C23-C25-C26
38	Y	607	CHL	C6-C7-C8-C10
27	B	824	CLA	C5-C6-C7-C8
27	H	203	CLA	C13-C15-C16-C17
29	O	2631	LHG	C11-C12-C13-C14
27	A	804	CLA	O2A-C1-C2-C3
27	A	826	CLA	C15-C16-C17-C18
29	5	625	LHG	C19-C20-C21-C22
27	5	606	CLA	C3A-C2A-CAA-CBA
27	A	814	CLA	C2A-CAA-CBA-CGA
27	H	203	CLA	C2A-CAA-CBA-CGA
27	a	613	CLA	C2A-CAA-CBA-CGA
27	1	613	CLA	C2A-CAA-CBA-CGA
27	5	602	CLA	C2A-CAA-CBA-CGA
27	U	604	CLA	O2A-C1-C2-C3
27	A	830	CLA	CAA-CBA-CGA-O1A
27	A	840	CLA	C4-C3-C5-C6
27	B	802	CLA	C3A-C2A-CAA-CBA
27	B	826	CLA	C3A-C2A-CAA-CBA
27	F	301	CLA	C3A-C2A-CAA-CBA
27	a	606	CLA	C3A-C2A-CAA-CBA
27	1	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	1	614	CLA	CHA-CBD-CGD-O1D
27	3	606	CLA	CHA-CBD-CGD-O1D
27	3	611	CLA	CHA-CBD-CGD-O1D
27	3	614	CLA	CHA-CBD-CGD-O1D
27	5	619	CLA	C3A-C2A-CAA-CBA
27	8	606	CLA	C3A-C2A-CAA-CBA
27	2	601	CLA	C16-C17-C18-C20
33	5	627	LMG	C13-C14-C15-C16
27	B	833	CLA	C2-C3-C5-C6
27	7	601	CLA	C2-C3-C5-C6
33	J	104	LMG	C12-C13-C14-C15
32	5	629	LMU	C1-C2-C3-C4
27	W	611	CLA	CAA-CBA-CGA-O1A
27	B	809	CLA	CBA-CGA-O2A-C1
33	9	625	LMG	C28-C29-C30-C31
27	A	813	CLA	CAA-CBA-CGA-O2A
27	B	813	CLA	CAA-CBA-CGA-O1A
33	A	860	LMG	C13-C14-C15-C16
27	V	602	CLA	C8-C10-C11-C12
27	Z	603	CLA	C2A-CAA-CBA-CGA
27	1	602	CLA	CBA-CGA-O2A-C1
27	B	808	CLA	C11-C10-C8-C9
27	3	609	CLA	C6-C7-C8-C9
27	5	613	CLA	C14-C13-C15-C16
27	Z	610	CLA	C14-C13-C15-C16
38	Z	601	CHL	C14-C13-C15-C16
38	Z	609	CHL	C11-C12-C13-C14
38	V	609	CHL	C11-C10-C8-C9
27	A	807	CLA	CAA-CBA-CGA-O1A
27	3	606	CLA	CAA-CBA-CGA-O1A
27	A	827	CLA	C10-C11-C12-C13
29	9	623	LHG	C31-C32-C33-C34
38	V	601	CHL	C3-C5-C6-C7
27	A	818	CLA	CAA-CBA-CGA-O1A
27	5	608	CLA	CAA-CBA-CGA-O1A
27	a	602	CLA	CBA-CGA-O2A-C1
27	1	614	CLA	CAD-CBD-CGD-O1D
27	2	614	CLA	CAD-CBD-CGD-O1D
27	3	615	CLA	CAD-CBD-CGD-O1D
27	7	609	CLA	CHA-CBD-CGD-O2D
27	7	615	CLA	CHA-CBD-CGD-O2D
29	5	625	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
29	3	623	LHG	O10-C23-C24-C25
27	7	602	CLA	C8-C10-C11-C12
29	a	620	LHG	O1-C1-C2-O2
29	A	847	LHG	O8-C23-C24-C25
29	7	622	LHG	O8-C23-C24-C25
27	A	834	CLA	CAA-CBA-CGA-O1A
29	X	2630	LHG	O7-C5-C6-O8
33	5	627	LMG	O1-C7-C8-O7
33	8	626	LMG	O1-C7-C8-O7
27	B	806	CLA	CAA-CBA-CGA-O1A
29	5	625	LHG	C17-C18-C19-C20
29	9	624	LHG	C4-C5-C6-O8
27	B	809	CLA	C13-C15-C16-C17
27	A	810	CLA	CAA-CBA-CGA-O2A
27	H	203	CLA	CAA-CBA-CGA-O2A
27	K	204	CLA	CAA-CBA-CGA-O1A
38	Z	606	CHL	CAA-CBA-CGA-O1A
27	5	613	CLA	C15-C16-C17-C18
37	U	1623	NEX	C29-C30-C31-C32
27	A	843	CLA	CAA-CBA-CGA-O1A
27	Z	603	CLA	CAA-CBA-CGA-O1A
27	A	825	CLA	CBA-CGA-O2A-C1
27	A	813	CLA	CAD-CBD-CGD-O2D
27	A	816	CLA	CAD-CBD-CGD-O2D
27	A	825	CLA	CAD-CBD-CGD-O2D
27	A	834	CLA	CAD-CBD-CGD-O2D
27	B	809	CLA	CAD-CBD-CGD-O2D
27	B	813	CLA	CAD-CBD-CGD-O2D
27	B	825	CLA	CAD-CBD-CGD-O2D
27	B	834	CLA	CAD-CBD-CGD-O2D
27	F	303	CLA	CAD-CBD-CGD-O2D
27	a	612	CLA	CAD-CBD-CGD-O2D
27	1	612	CLA	CAD-CBD-CGD-O2D
27	2	616	CLA	CAD-CBD-CGD-O2D
27	5	614	CLA	CAD-CBD-CGD-O2D
27	8	616	CLA	CAD-CBD-CGD-O2D
27	6	603	CLA	CAA-CBA-CGA-O2A
33	A	860	LMG	O8-C28-C29-C30
27	A	838	CLA	C2C-C3C-CAC-CBC
27	9	602	CLA	C10-C11-C12-C13
38	Z	607	CHL	C13-C15-C16-C17
27	A	802	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	B	802	CLA	C2-C1-O2A-CGA
27	B	811	CLA	C2-C1-O2A-CGA
27	B	829	CLA	C2-C1-O2A-CGA
27	A	818	CLA	C11-C12-C13-C15
27	6	613	CLA	C16-C17-C18-C20
27	5	609	CLA	C10-C11-C12-C13
27	B	817	CLA	CAA-CBA-CGA-O2A
27	B	834	CLA	CAA-CBA-CGA-O2A
27	5	607	CLA	CAA-CBA-CGA-O2A
27	8	608	CLA	CAA-CBA-CGA-O2A
27	A	839	CLA	O1D-CGD-O2D-CED
38	U	607	CHL	CAA-CBA-CGA-O2A
27	2	613	CLA	CAA-CBA-CGA-O2A
38	Y	601	CHL	C2C-C3C-CAC-CBC
27	A	810	CLA	CAA-CBA-CGA-O1A
27	A	821	CLA	CAA-CBA-CGA-O1A
27	A	841	CLA	CAA-CBA-CGA-O1A
27	B	809	CLA	CAA-CBA-CGA-O1A
27	6	616	CLA	CAA-CBA-CGA-O1A
29	7	622	LHG	O10-C23-C24-C25

There are no ring outliers.

232 monomers are involved in 515 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	812	CLA	1	0
27	A	819	CLA	1	0
35	X	1621	LUT	2	0
27	B	803	CLA	4	0
38	Z	601	CHL	7	0
27	2	603	CLA	2	0
27	B	836	CLA	1	0
36	W	1622	XAT	1	0
30	K	202	BCR	8	0
32	A	857	LMU	1	0
38	W	606	CHL	3	0
37	Z	1623	NEX	4	0
27	A	802	CLA	2	0
27	7	613	CLA	3	0
27	H	203	CLA	1	0
38	W	605	CHL	3	0
27	4	609	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	9	613	CLA	1	0
38	U	607	CHL	2	0
36	6	621	XAT	1	0
38	V	609	CHL	4	0
38	Z	608	CHL	1	0
27	B	821	CLA	2	0
27	V	611	CLA	1	0
38	U	609	CHL	7	0
38	Y	606	CHL	3	0
27	W	613	CLA	2	0
30	B	852	BCR	5	0
30	7	621	BCR	3	0
27	L	307	CLA	2	0
27	A	808	CLA	2	0
27	7	608	CLA	1	0
27	A	801	CLA	2	0
27	4	613	CLA	1	0
27	3	609	CLA	1	0
36	Y	1622	XAT	1	0
27	2	601	CLA	5	0
33	A	860	LMG	1	0
27	2	610	CLA	1	0
27	B	818	CLA	3	0
35	2	619	LUT	2	0
27	4	616	CLA	1	0
27	Y	611	CLA	3	0
30	A	856	BCR	10	0
27	B	835	CLA	1	0
27	4	608	CLA	1	0
27	A	817	CLA	1	0
37	5	624	NEX	2	0
30	3	621	BCR	9	0
33	L	2631	LMG	1	0
35	U	1620	LUT	2	0
29	9	624	LHG	1	0
27	U	604	CLA	1	0
30	a	619	BCR	2	0
36	7	620	XAT	2	0
30	7	623	BCR	7	0
38	Y	609	CHL	6	0
27	5	607	CLA	1	0
27	6	613	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	813	CLA	1	0
30	4	621	BCR	3	0
29	9	623	LHG	2	0
27	B	825	CLA	1	0
30	G	205	BCR	2	0
30	3	622	BCR	4	0
38	X	609	CHL	2	0
27	3	602	CLA	1	0
27	A	820	CLA	3	0
27	W	611	CLA	1	0
30	B	849	BCR	4	0
38	Z	607	CHL	2	0
27	3	612	CLA	1	0
27	A	841	CLA	1	0
27	B	809	CLA	1	0
27	1	611	CLA	1	0
27	A	854	CLA	7	0
38	X	601	CHL	3	0
29	Z	2630	LHG	2	0
38	Y	607	CHL	6	0
35	V	1620	LUT	2	0
27	V	602	CLA	1	0
32	K	208	LMU	1	0
27	W	604	CLA	1	0
38	X	608	CHL	5	0
27	3	608	CLA	1	0
38	Z	606	CHL	3	0
27	8	611	CLA	1	0
29	V	2630	LHG	2	0
27	6	601	CLA	1	0
30	O	2005	BCR	8	0
27	B	833	CLA	2	0
30	F	305	BCR	8	0
38	U	608	CHL	1	0
38	Z	605	CHL	1	0
30	L	301	BCR	7	0
37	Y	1623	NEX	2	0
33	5	627	LMG	1	0
33	V	2631	LMG	3	0
27	2	613	CLA	1	0
37	6	624	NEX	1	0
27	V	610	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	2	623	BCR	9	0
36	1	618	XAT	1	0
27	Z	613	CLA	2	0
35	Y	1620	LUT	3	0
38	V	601	CHL	5	0
27	A	803	CLA	5	0
35	9	619	LUT	2	0
27	B	839	CLA	1	0
30	6	622	BCR	3	0
27	A	811	CLA	1	0
27	B	808	CLA	6	0
30	B	848	BCR	8	0
27	5	603	CLA	1	0
30	B	846	BCR	4	0
27	B	834	CLA	1	0
27	A	843	CLA	1	0
27	V	613	CLA	1	0
38	U	605	CHL	3	0
29	B	851	LHG	1	0
30	J	102	BCR	10	0
38	U	601	CHL	3	0
36	Z	1622	XAT	1	0
35	3	618	LUT	3	0
27	B	830	CLA	1	0
38	V	608	CHL	12	0
27	B	802	CLA	2	0
36	3	619	XAT	1	0
29	7	622	LHG	1	0
38	W	601	CHL	3	0
35	8	619	LUT	3	0
27	U	613	CLA	2	0
27	K	204	CLA	1	0
27	B	840	CLA	3	0
27	6	618	CLA	1	0
35	a	617	LUT	4	0
27	A	825	CLA	1	0
38	X	607	CHL	4	0
27	8	606	CLA	1	0
27	a	611	CLA	1	0
30	B	843	BCR	7	0
38	W	607	CHL	7	0
35	6	619	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	U	606	CHL	2	0
30	A	852	BCR	11	0
35	7	619	LUT	2	0
27	3	606	CLA	2	0
27	A	809	CLA	2	0
34	B	850	DGD	3	0
30	A	850	BCR	5	0
27	6	616	CLA	1	0
38	X	605	CHL	1	0
27	B	832	CLA	2	0
27	W	610	CLA	1	0
29	5	625	LHG	1	0
27	B	837	CLA	1	0
35	Z	1621	LUT	1	0
38	W	609	CHL	4	0
30	B	801	BCR	9	0
27	A	829	CLA	4	0
27	8	613	CLA	2	0
30	B	847	BCR	5	0
27	4	610	CLA	2	0
36	U	1622	XAT	3	0
30	B	844	BCR	4	0
35	X	1620	LUT	3	0
37	W	1623	NEX	2	0
27	5	617	CLA	1	0
38	X	606	CHL	1	0
27	X	613	CLA	2	0
30	B	845	BCR	3	0
27	9	614	CLA	1	0
35	4	619	LUT	4	0
27	B	827	CLA	1	0
30	L	309	BCR	7	0
27	3	617	CLA	3	0
37	V	1623	NEX	1	0
27	4	614	CLA	1	0
30	L	305	BCR	6	0
38	W	608	CHL	1	0
38	Y	601	CHL	3	0
30	8	621	BCR	3	0
30	A	849	BCR	4	0
27	B	804	CLA	1	0
27	6	606	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	9	621	BCR	5	0
27	B	828	CLA	1	0
27	F	303	CLA	1	0
27	8	604	CLA	1	0
36	a	618	XAT	1	0
27	Y	613	CLA	2	0
38	V	605	CHL	4	0
27	L	303	CLA	2	0
38	Y	605	CHL	1	0
27	9	610	CLA	3	0
27	A	834	CLA	3	0
35	Z	1620	LUT	3	0
27	B	819	CLA	2	0
27	a	603	CLA	1	0
27	A	818	CLA	1	0
35	1	617	LUT	3	0
30	1	619	BCR	2	0
30	3	620	BCR	2	0
38	V	606	CHL	3	0
36	5	621	XAT	3	0
27	Y	610	CLA	1	0
27	B	826	CLA	2	0
30	5	622	BCR	3	0
28	B	842	PQN	2	0
27	5	602	CLA	1	0
30	A	851	BCR	4	0
27	B	817	CLA	1	0
27	7	601	CLA	1	0
29	3	623	LHG	1	0
27	6	611	CLA	1	0
35	W	1620	LUT	2	0
30	A	848	BCR	4	0
27	5	619	CLA	5	0
27	X	611	CLA	3	0
38	Y	608	CHL	2	0
30	O	2004	BCR	3	0
27	K	201	CLA	6	0
27	3	603	CLA	1	0
30	B	853	BCR	2	0
27	9	609	CLA	1	0
30	K	207	BCR	9	0
27	U	611	CLA	1	0

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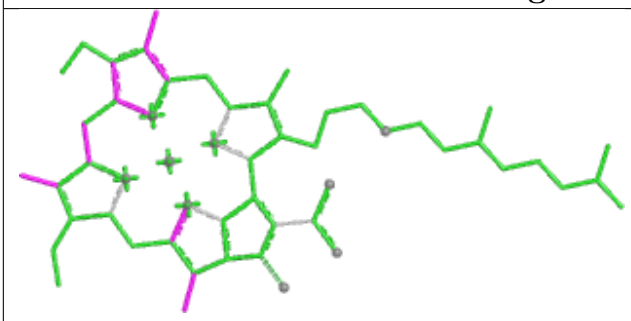
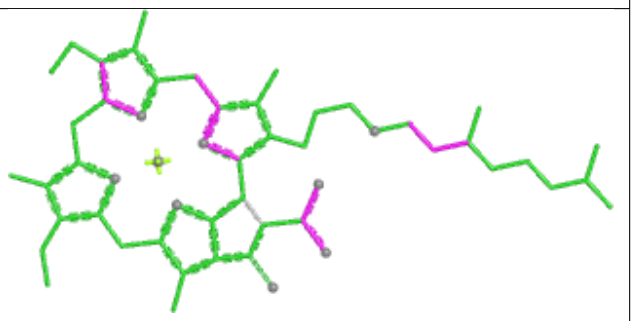
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	816	CLA	4	0
37	X	1623	NEX	2	0
38	Z	609	CHL	5	0
38	V	607	CHL	5	0
27	4	601	CLA	1	0

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

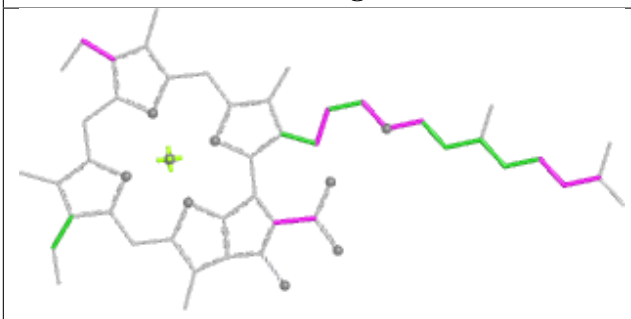
Ligand CLA 3 613



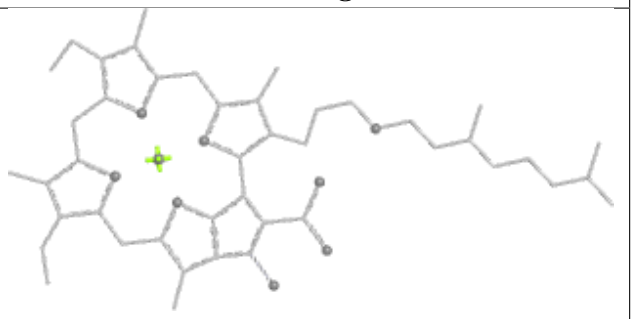
Bond lengths



Bond angles

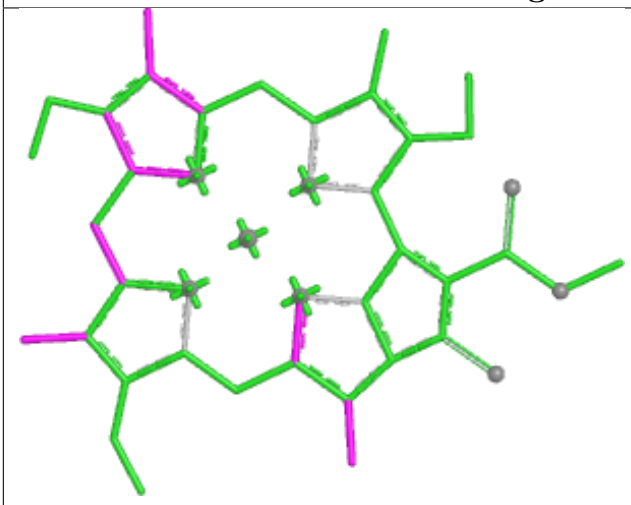


Torsions

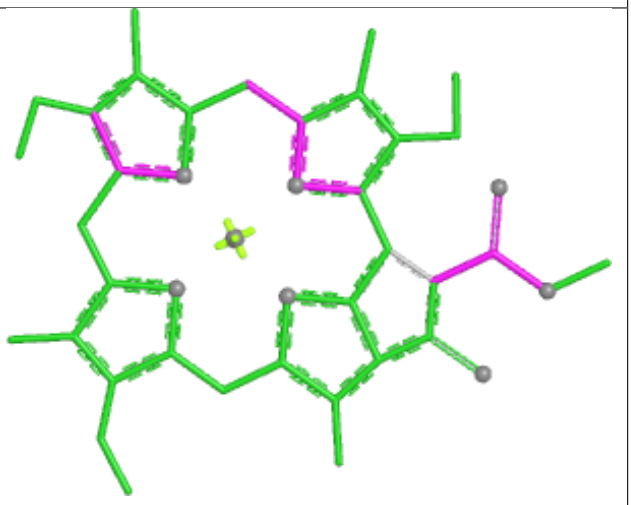


Rings

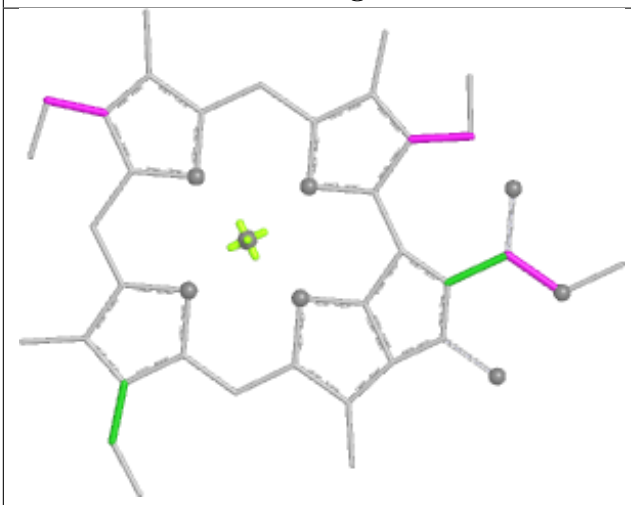
Ligand CLA J 101



Bond lengths



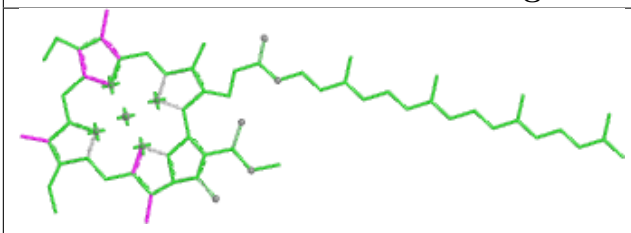
Bond angles



Torsions

Rings

Ligand CLA A 812



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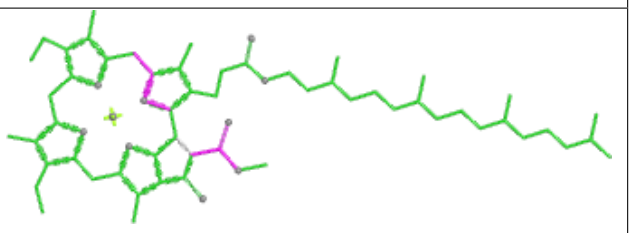

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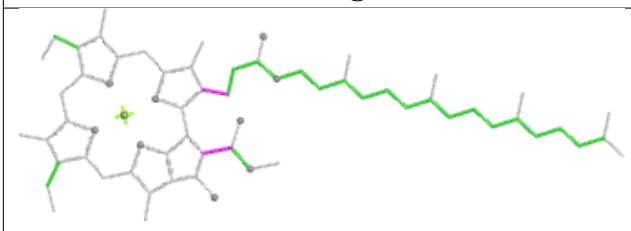
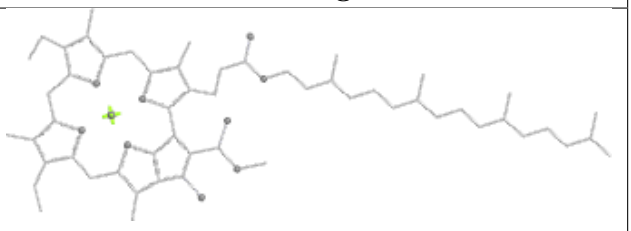
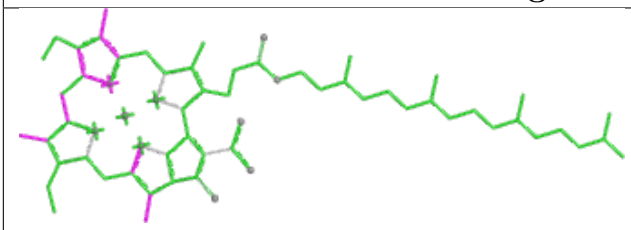
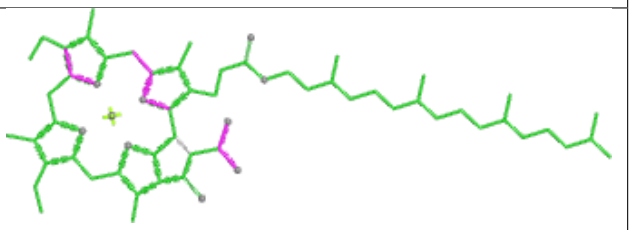
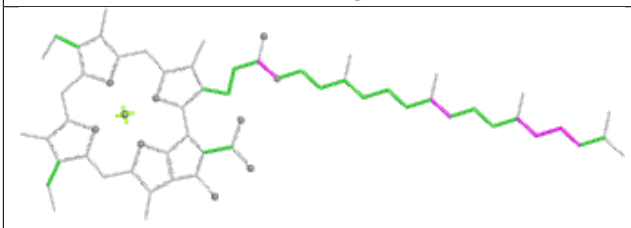
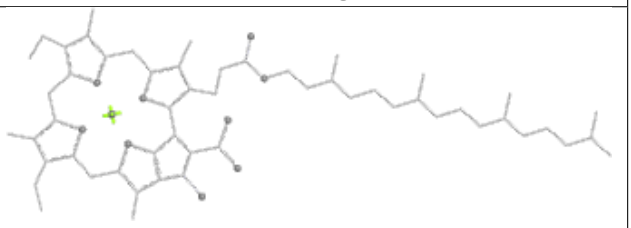
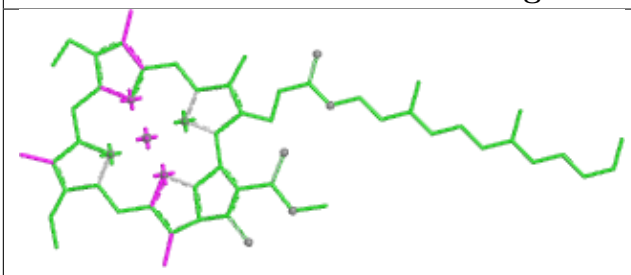
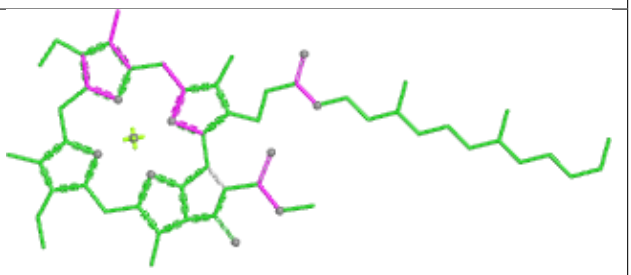
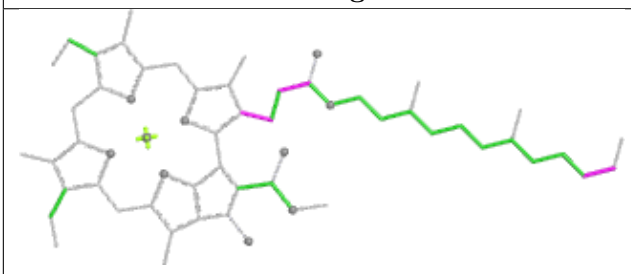
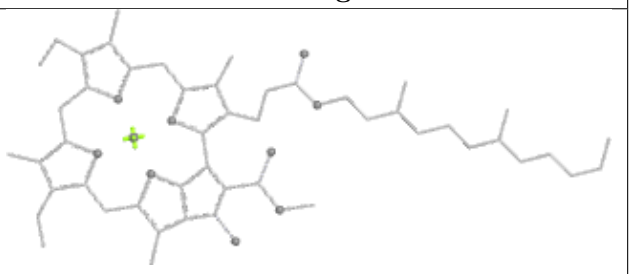


Torsions

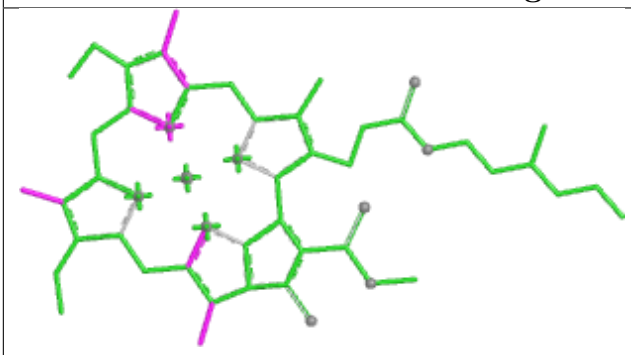


Rings

Ligand CLA 2 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 807



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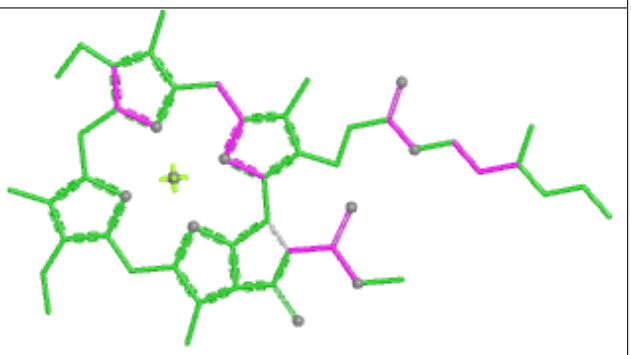

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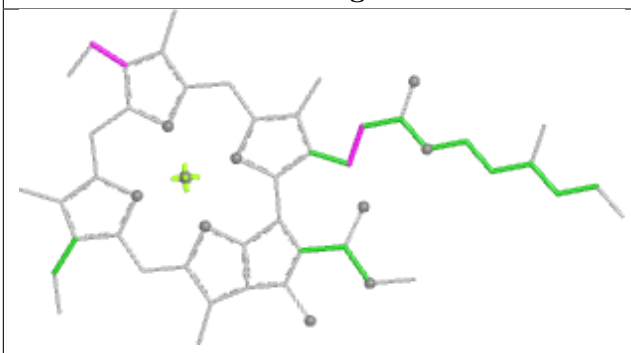
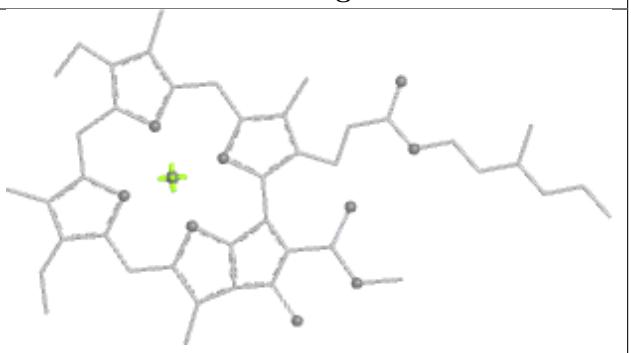
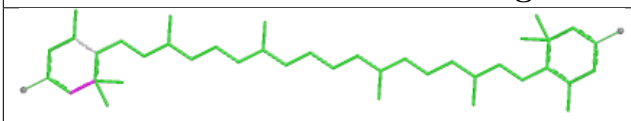


Torsions



Rings

Ligand LUT X 1621



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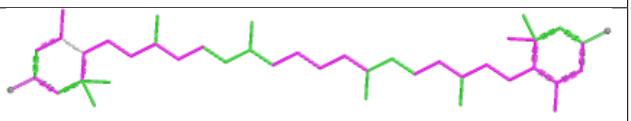

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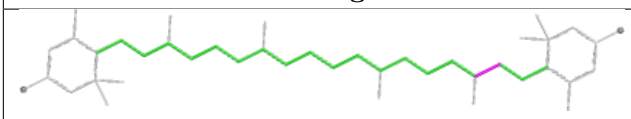

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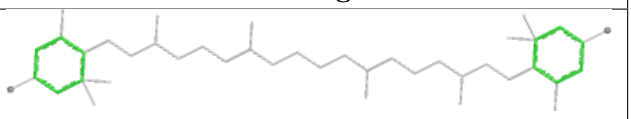
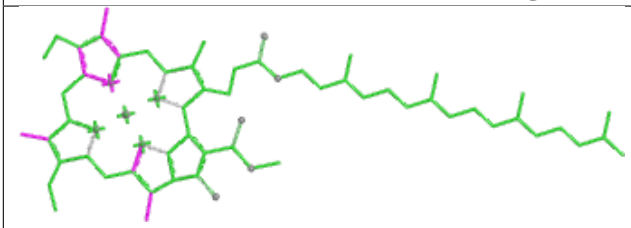


Rings

Ligand CLA B 803



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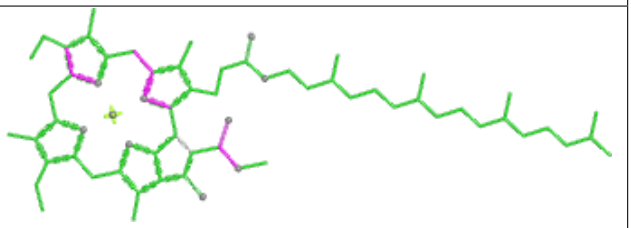
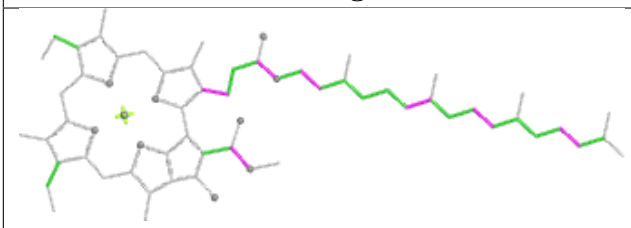
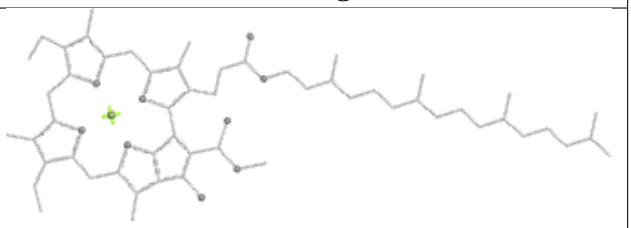


Bond angles

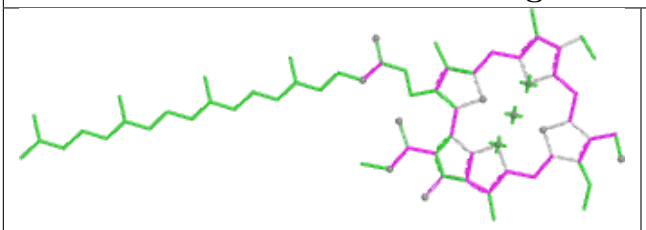


Torsions



Rings

Ligand CHL Z 601



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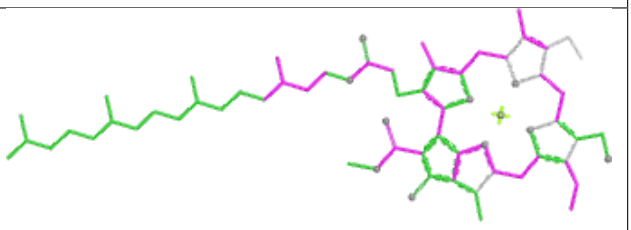

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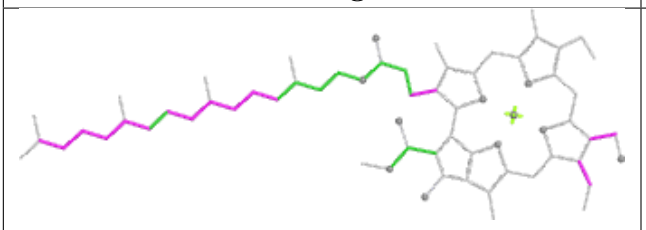

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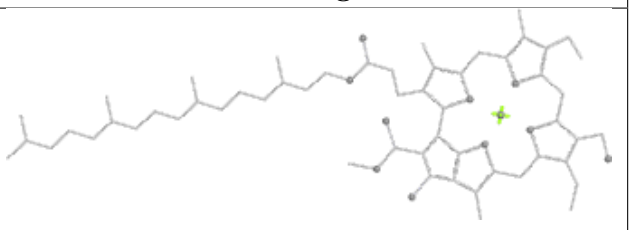

Rings

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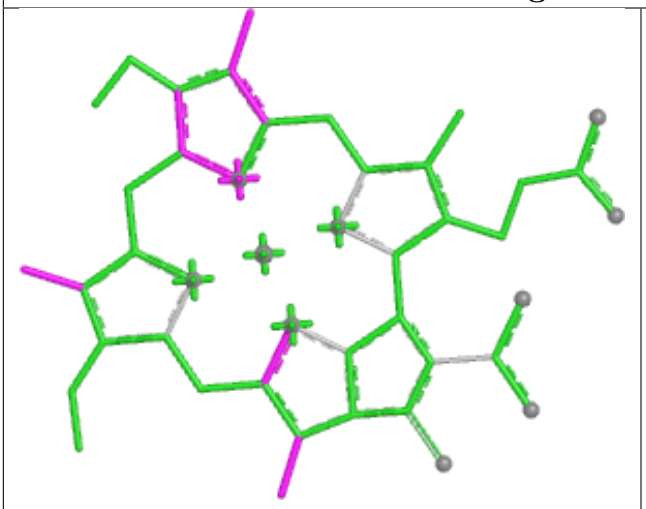

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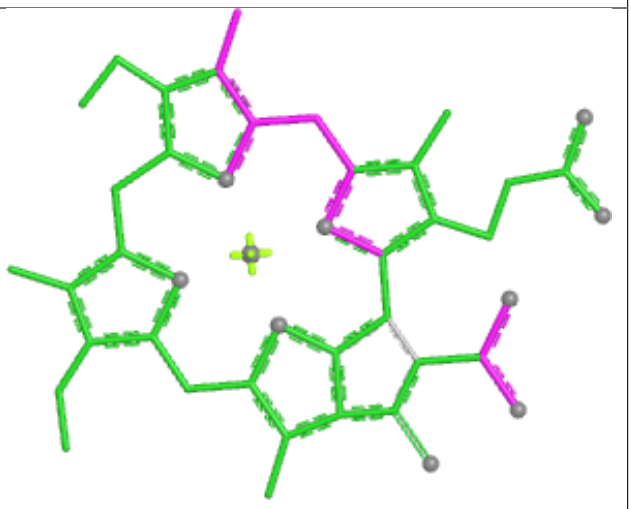

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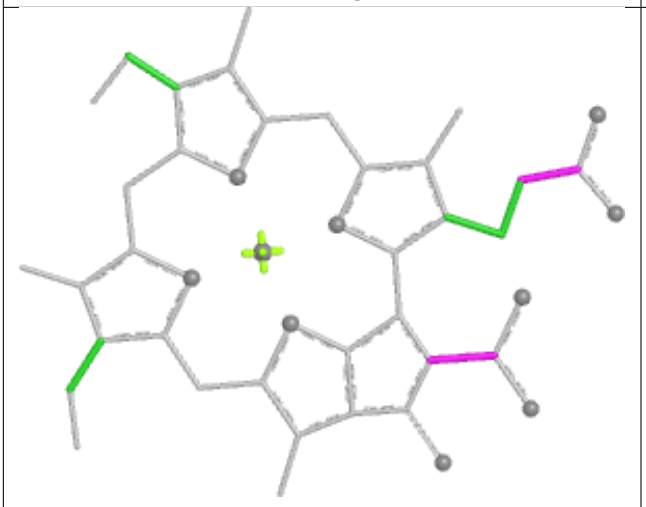

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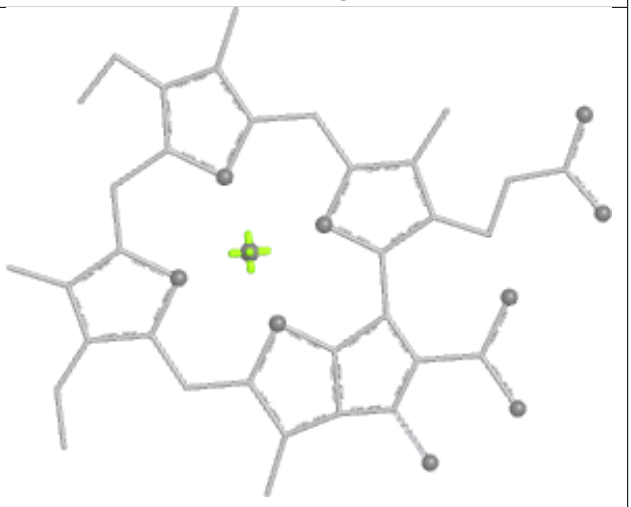
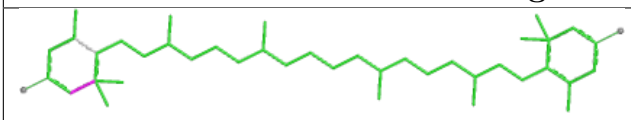


Rings

Ligand LUT 5 620



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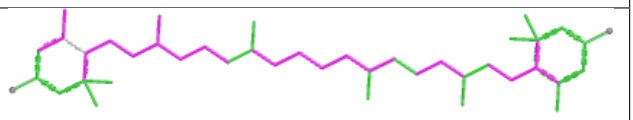
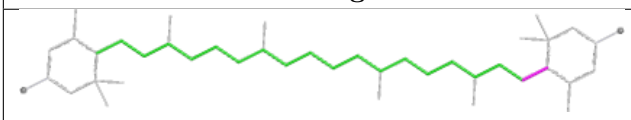


Bond angles



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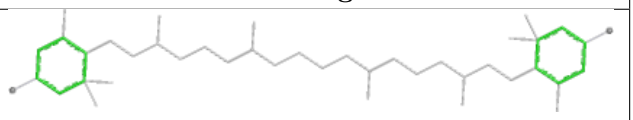
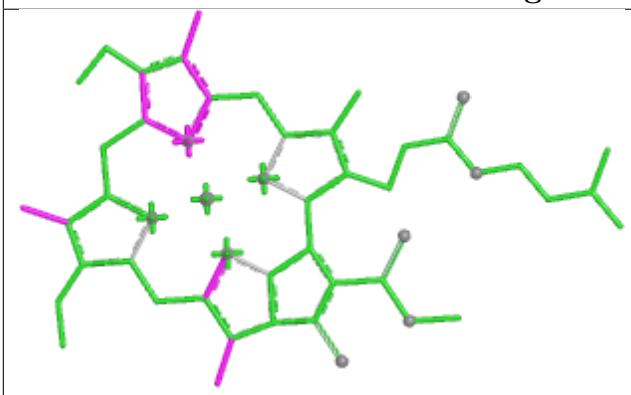
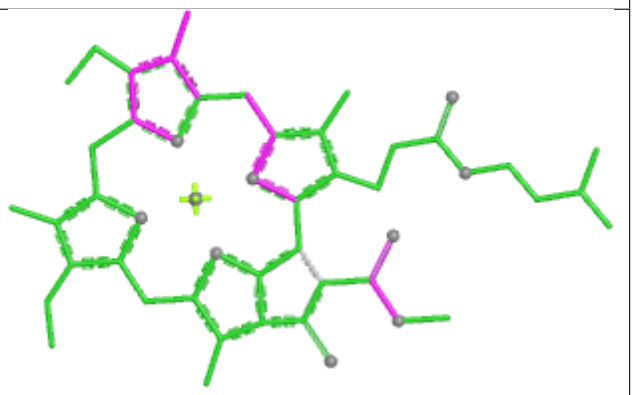


Rings

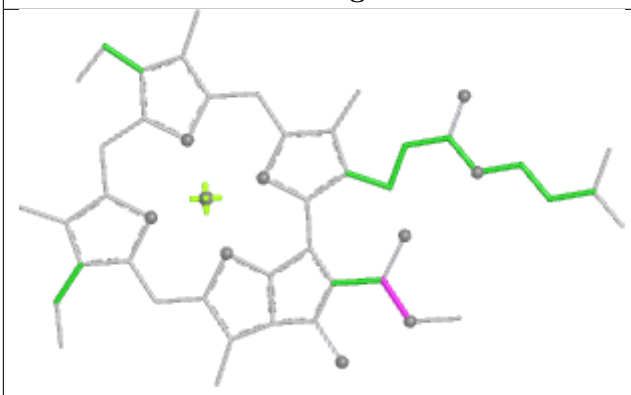
Ligand CLA B 836



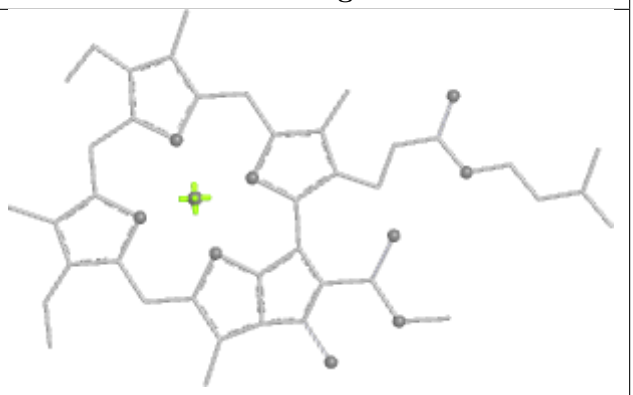
Bond lengths



Bond angles

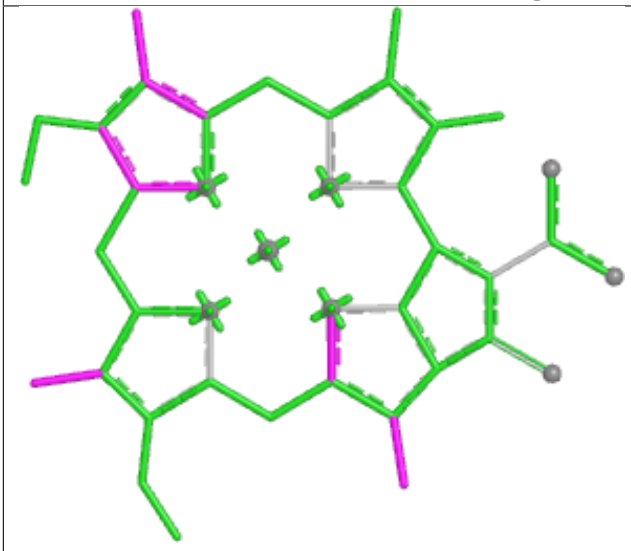


Torsions



Rings

Ligand CLA 1 607



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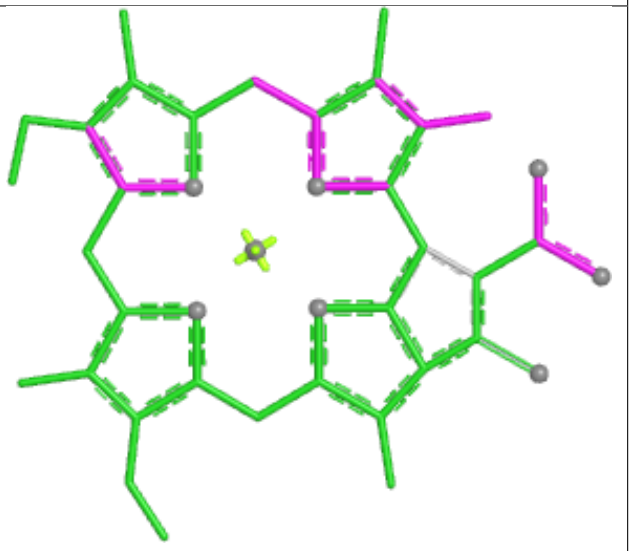
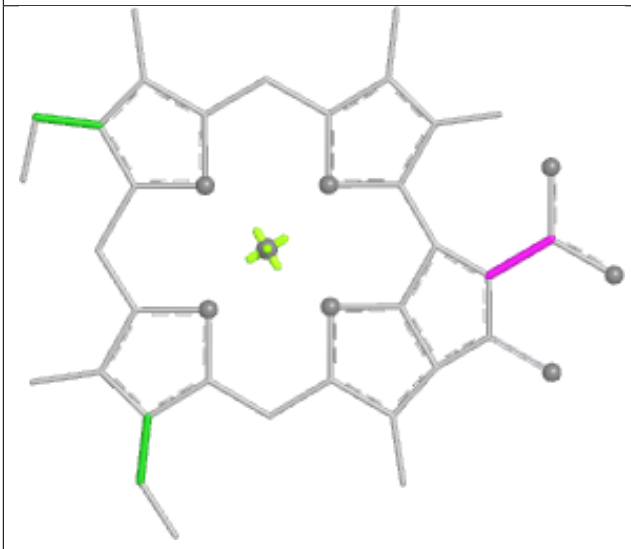
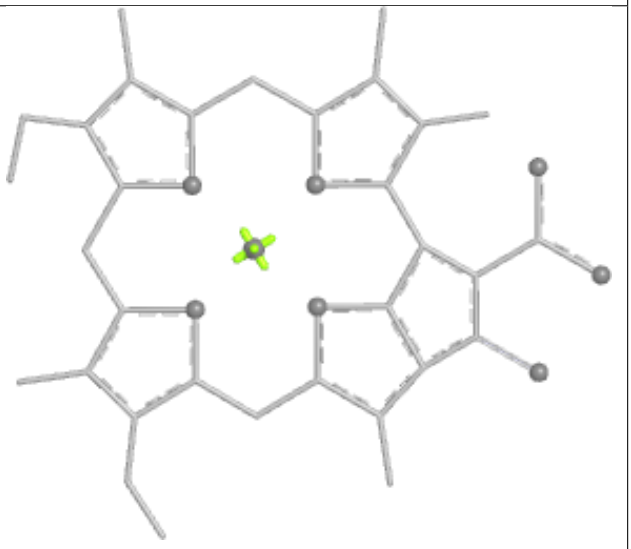


Bond angles

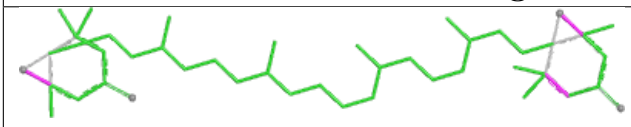


Torsions



Rings

Ligand XAT W 1622



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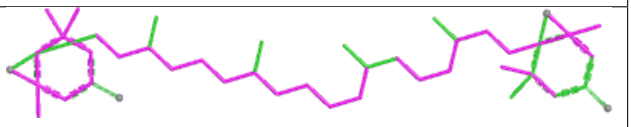
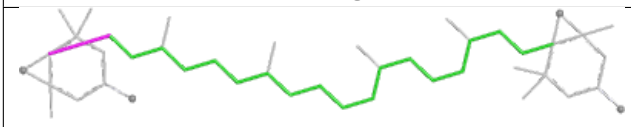
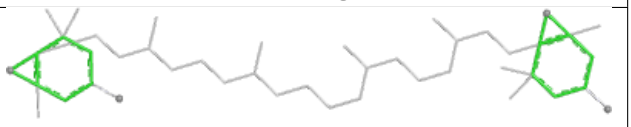


Bond angles

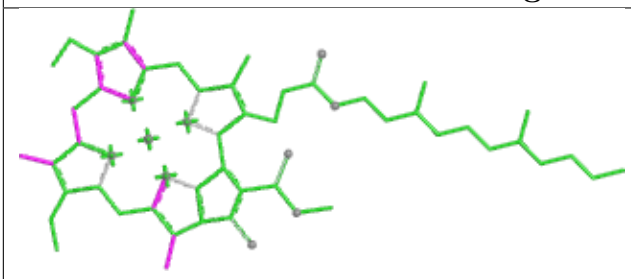


Torsions



Rings

Ligand CLA Y 602



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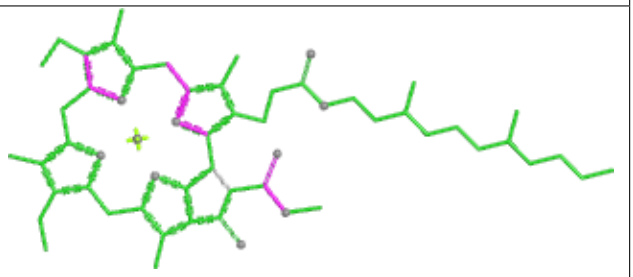
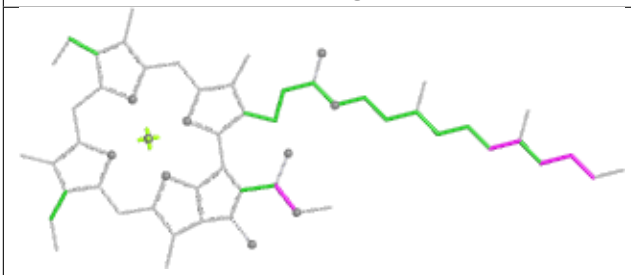
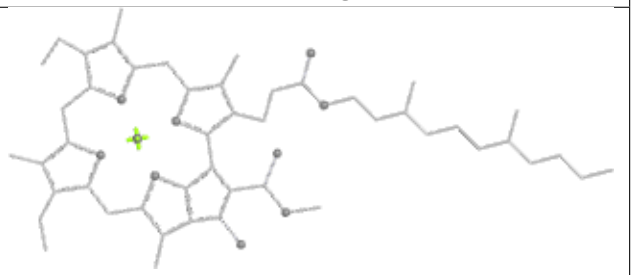


Bond angles

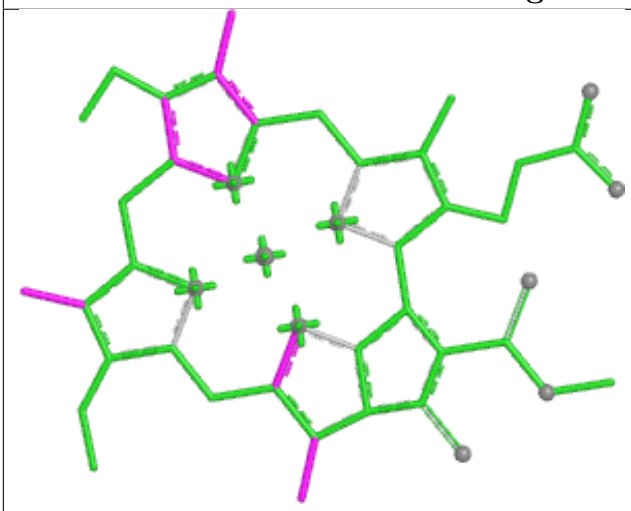


Torsions

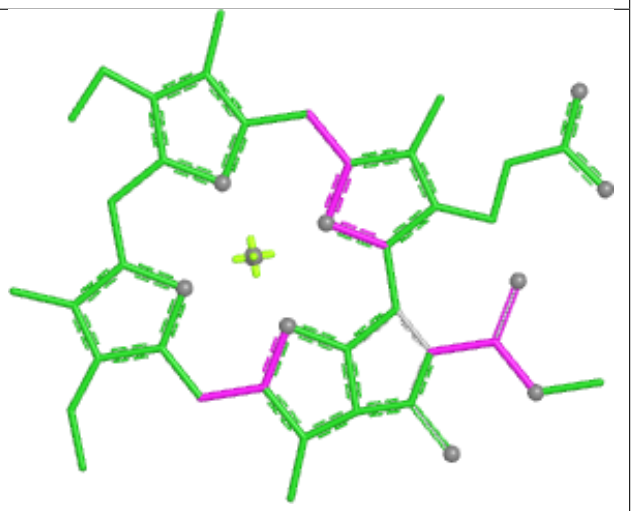


Rings

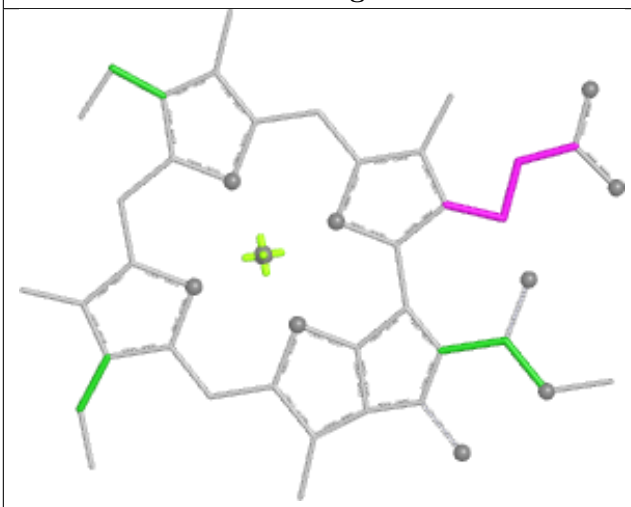
Ligand CLA L 302



Bond lengths



Bond angles



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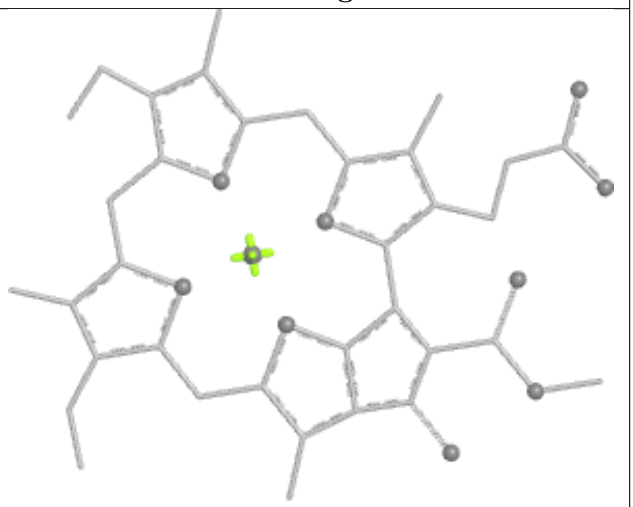
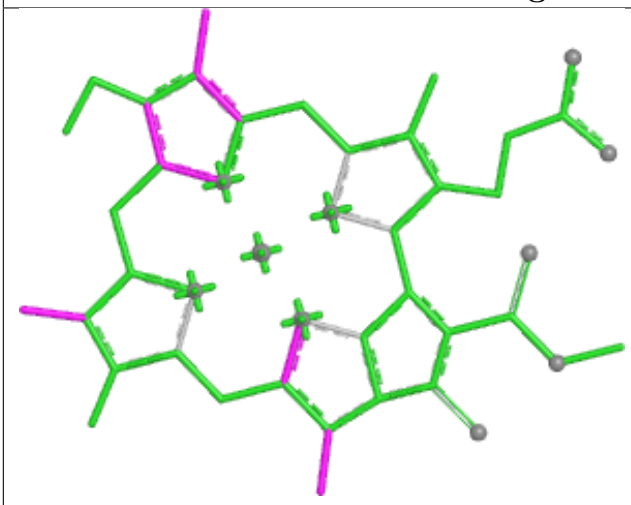


Rings

Ligand CLA 2 612



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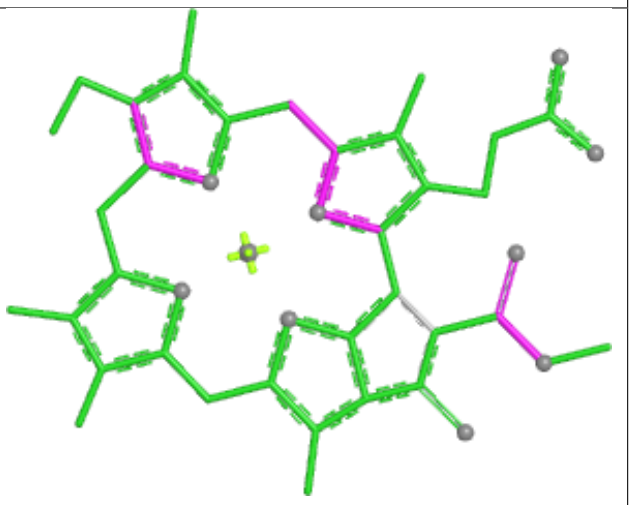

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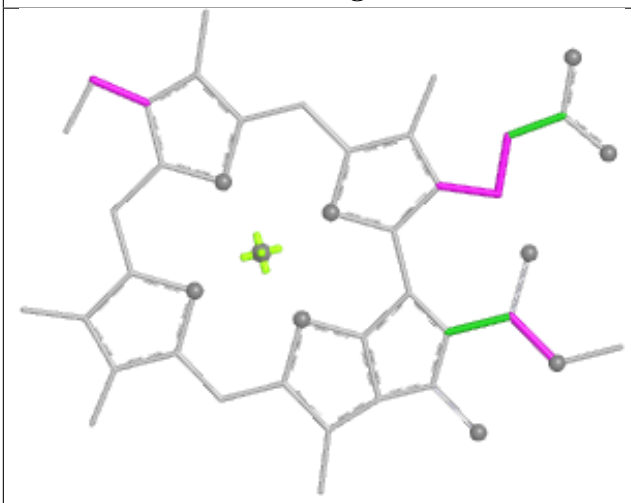
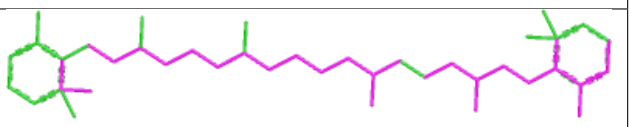


Torsions

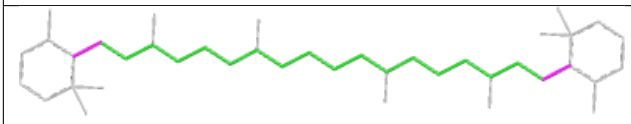
Rings

Ligand BCR K 202

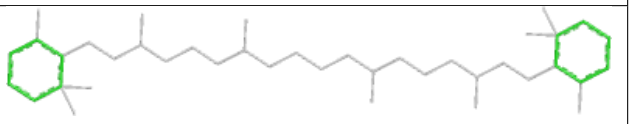
Bond lengths



Bond angles

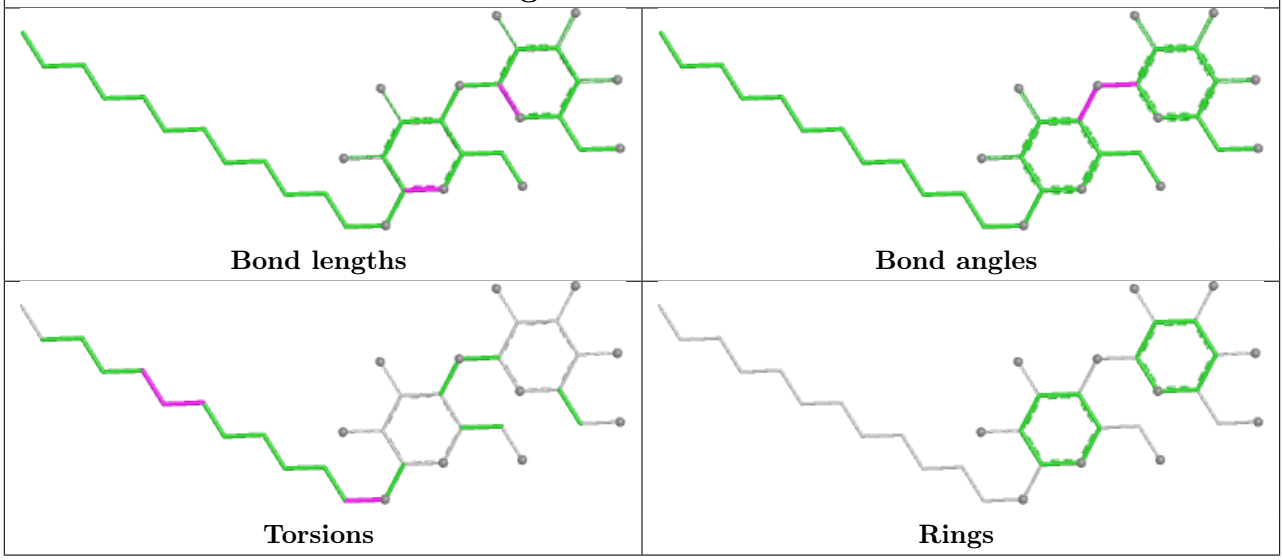


Torsions

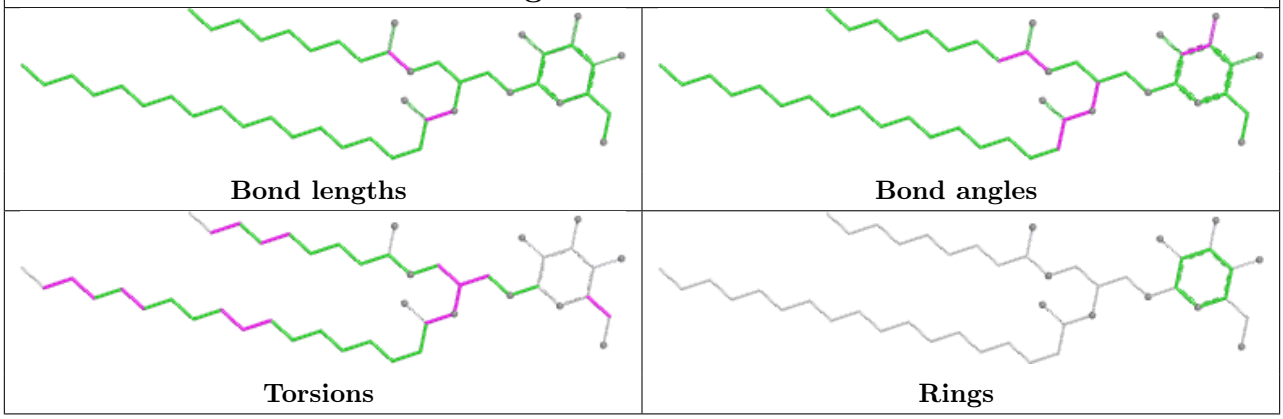


Rings

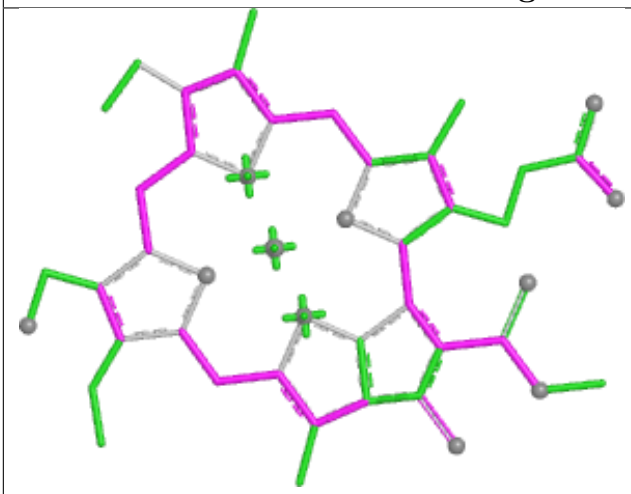
Ligand LMU A 857



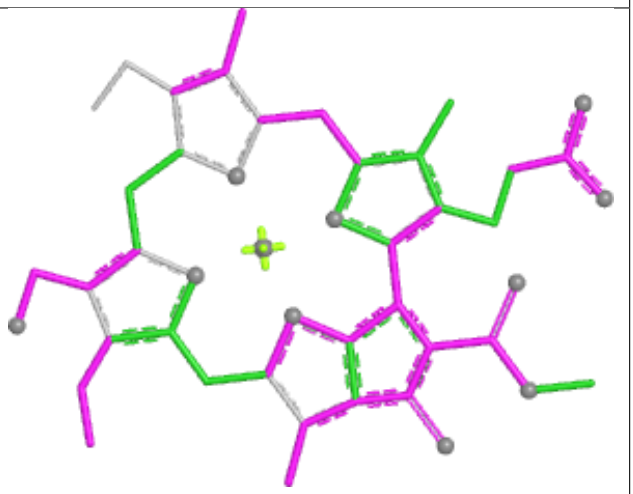
Ligand LMG 8 626



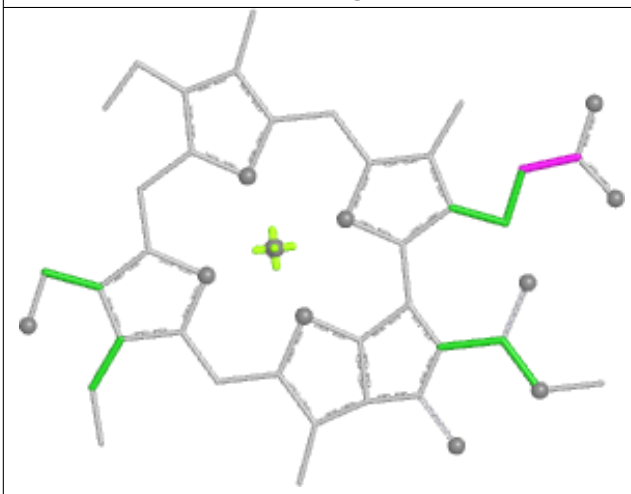
Ligand CHL W 606



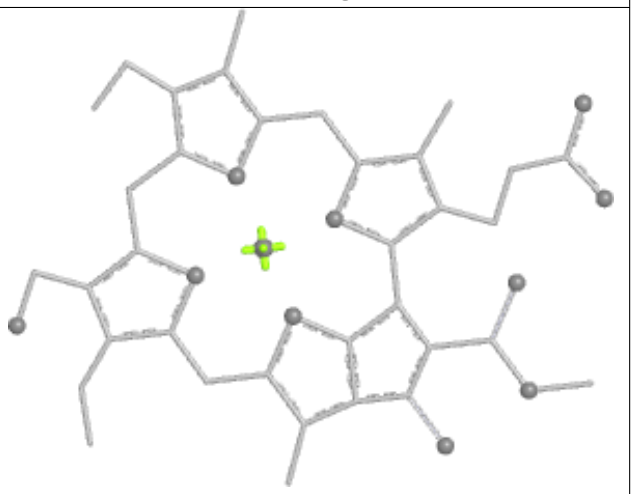
Bond lengths



Bond angles

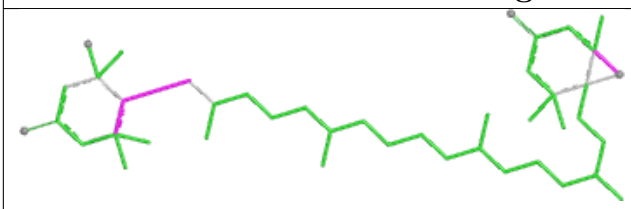


Torsions



Rings

Ligand NEX Z 1623



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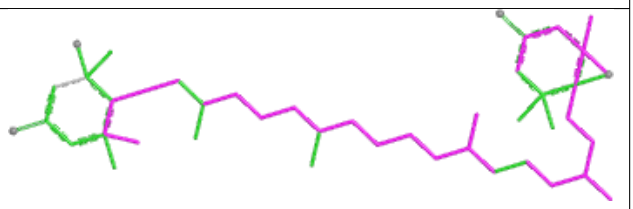
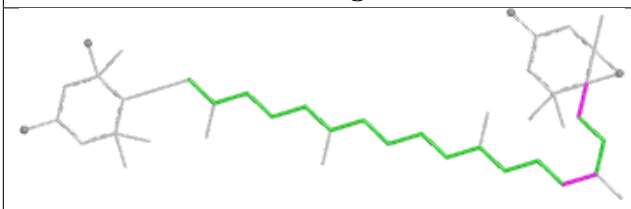
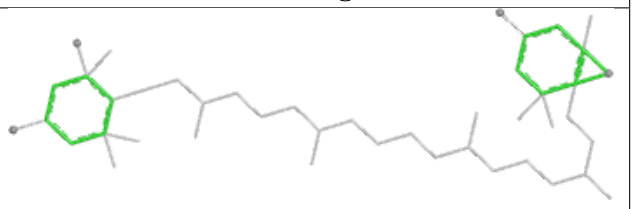


Bond angles

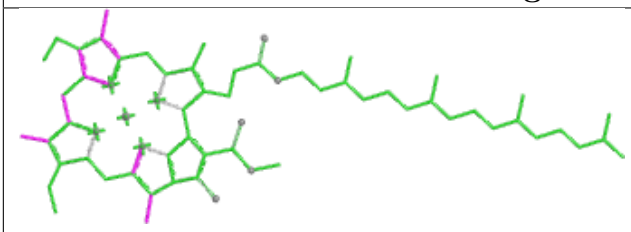


Torsions



Rings

Ligand CLA A 802



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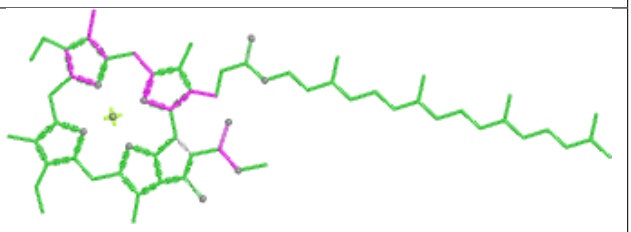
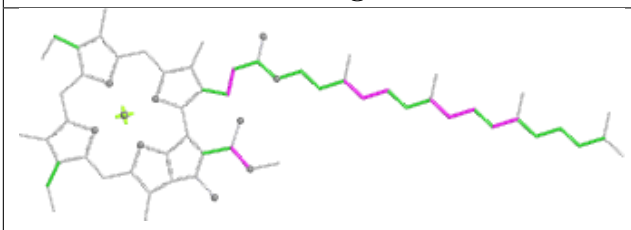


Bond angles



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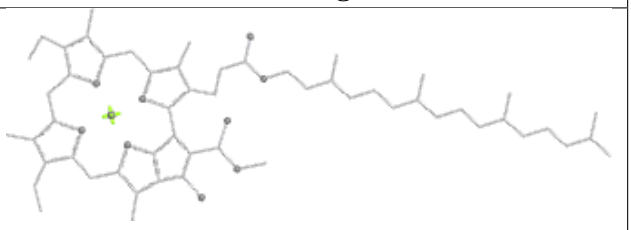
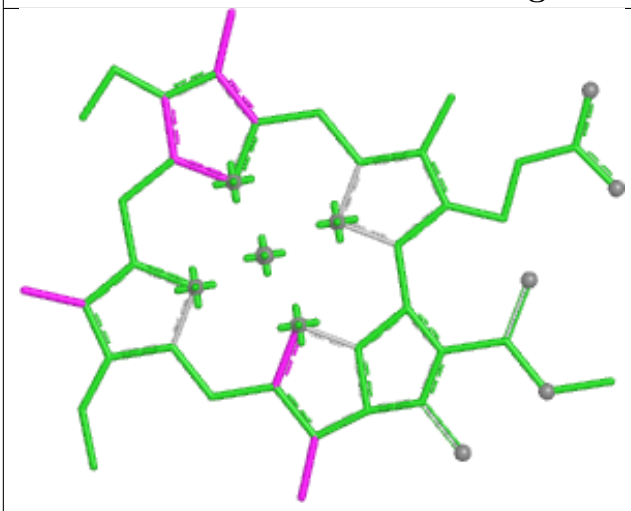


Rings

Ligand CLA 8 609



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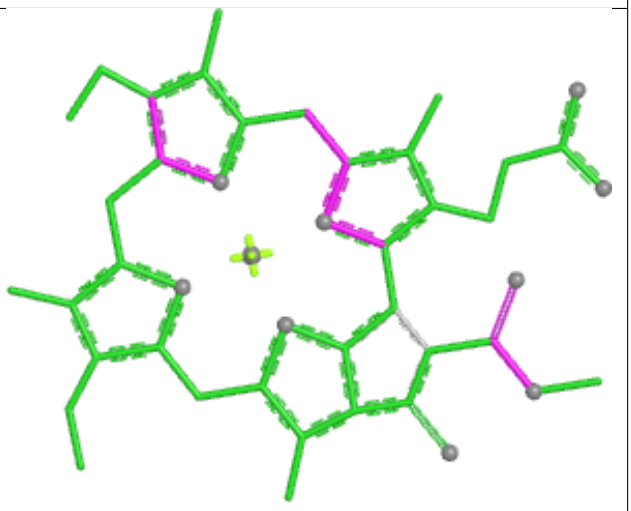
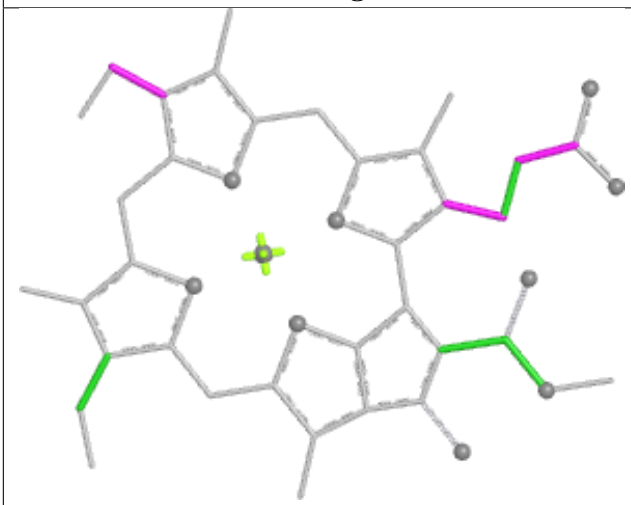


Bond angles



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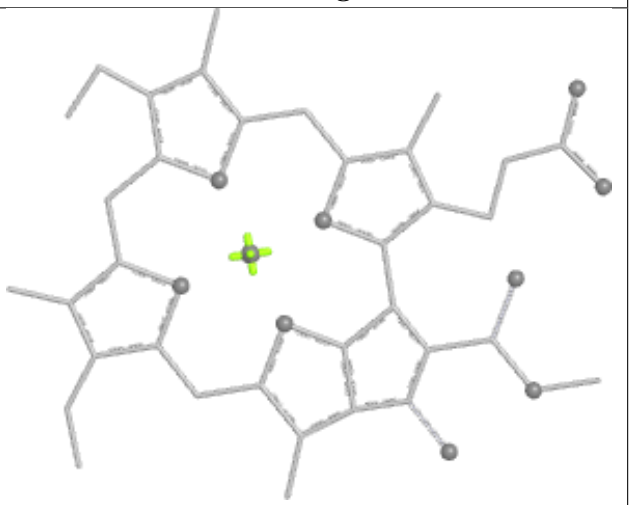
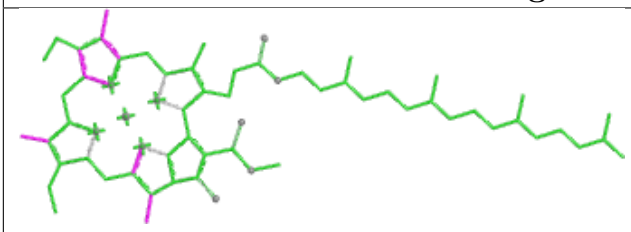
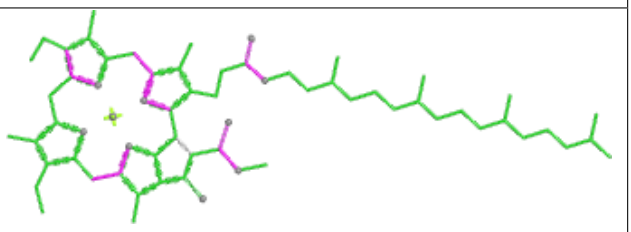
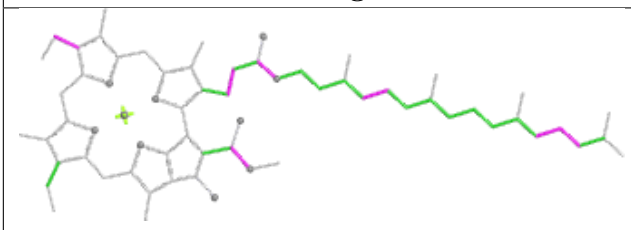
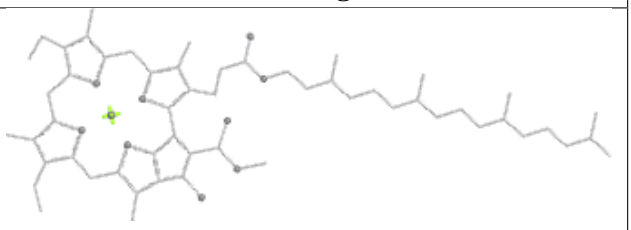
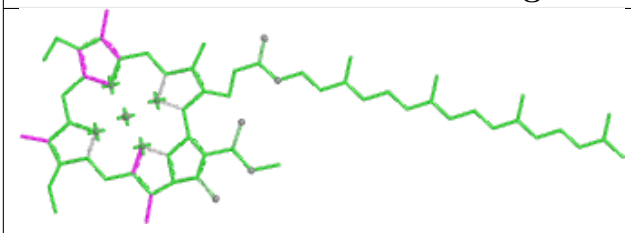
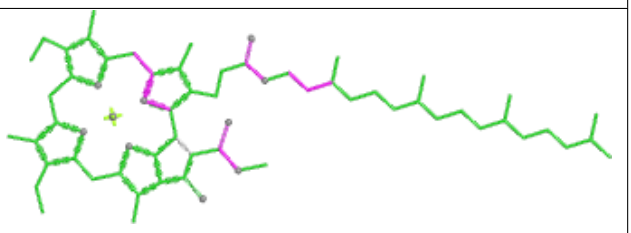
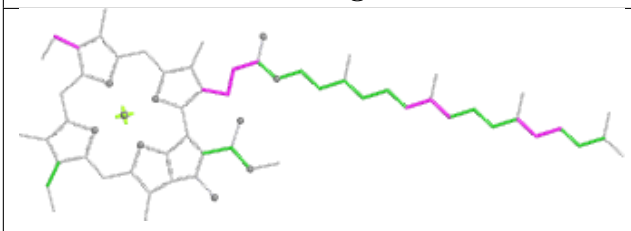
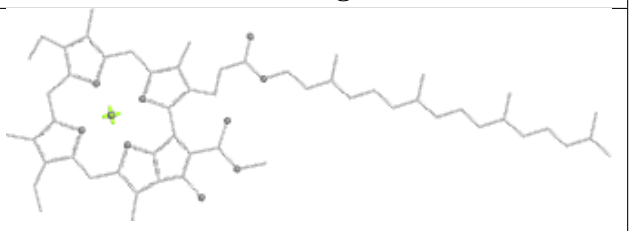
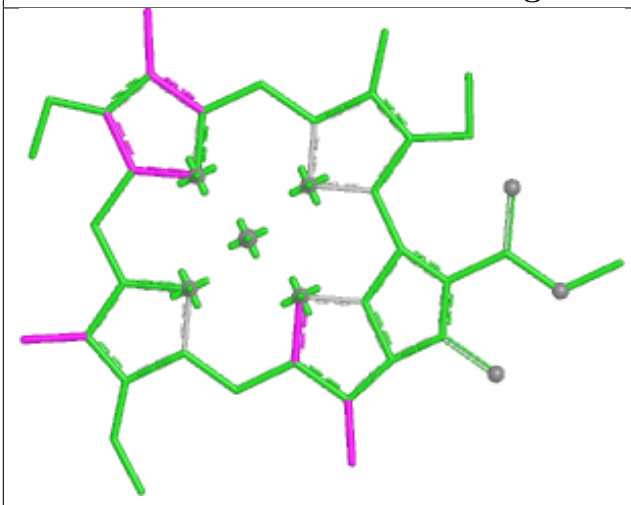


Rings

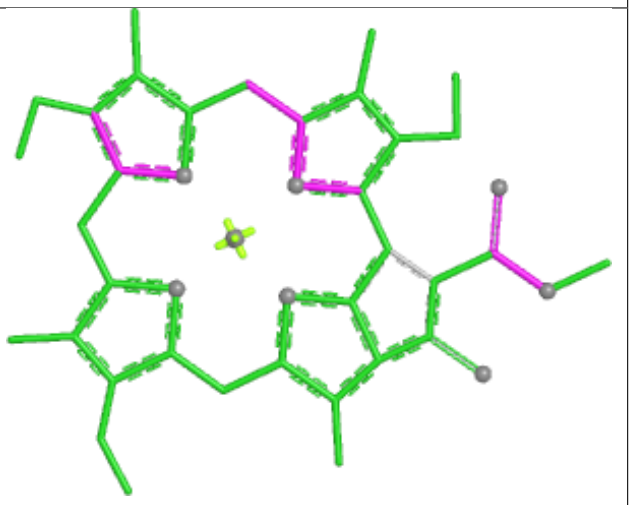
Ligand CLA 7 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

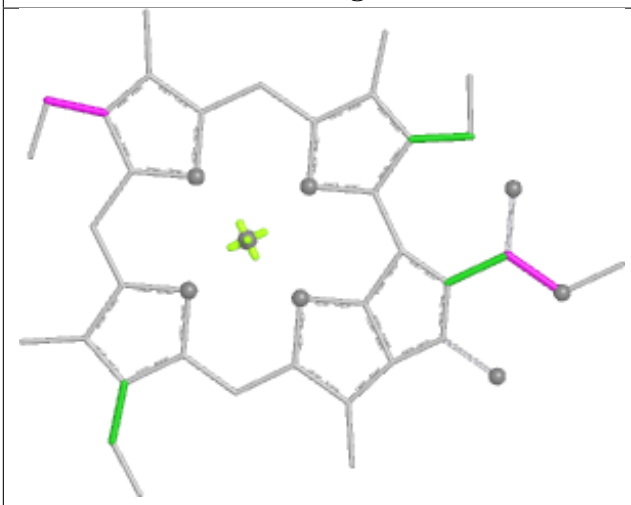
Ligand CLA A 823



Bond lengths



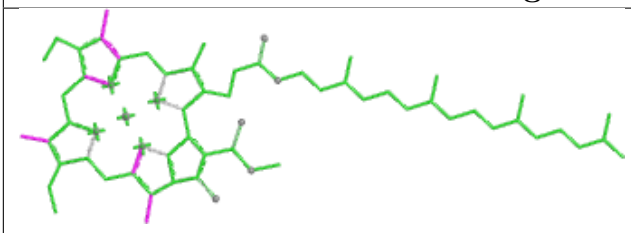
Bond angles



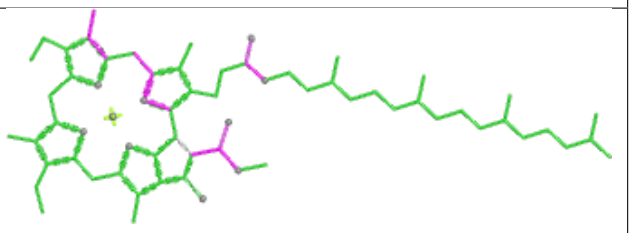
Torsions

Rings

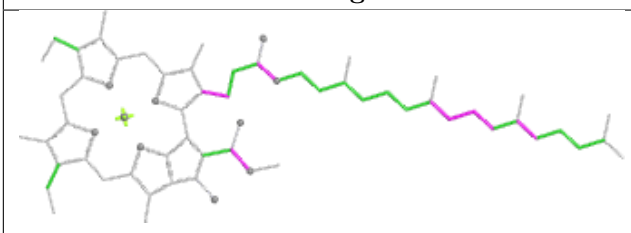
Ligand CLA A 831



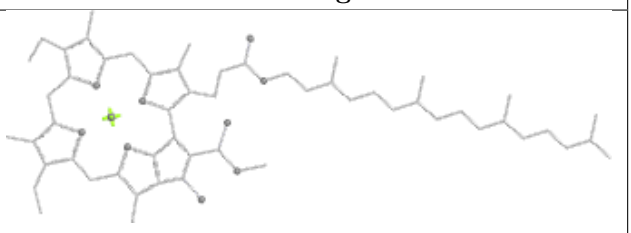
Bond lengths



Bond angles

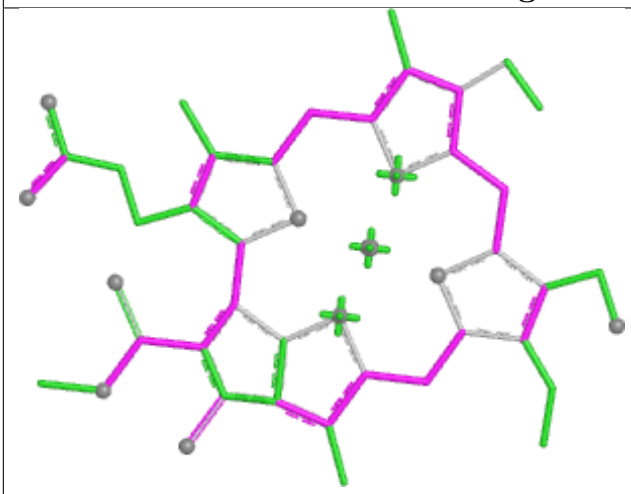


Torsions

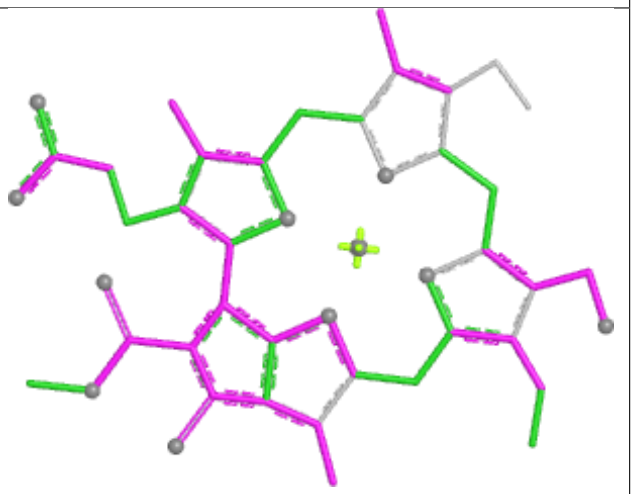


Rings

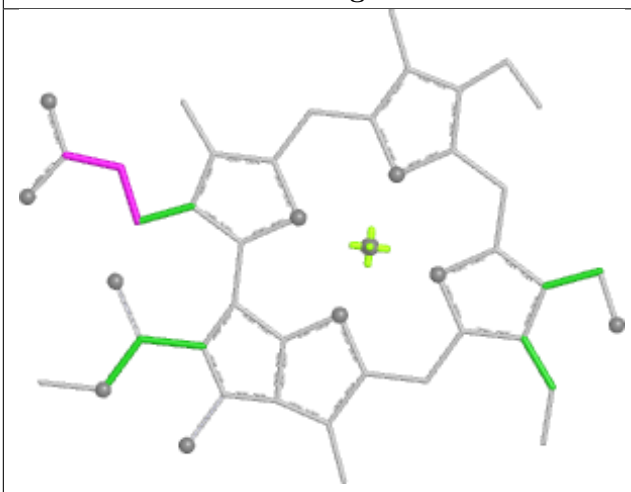
Ligand CHL W 605



Bond lengths



Bond angles



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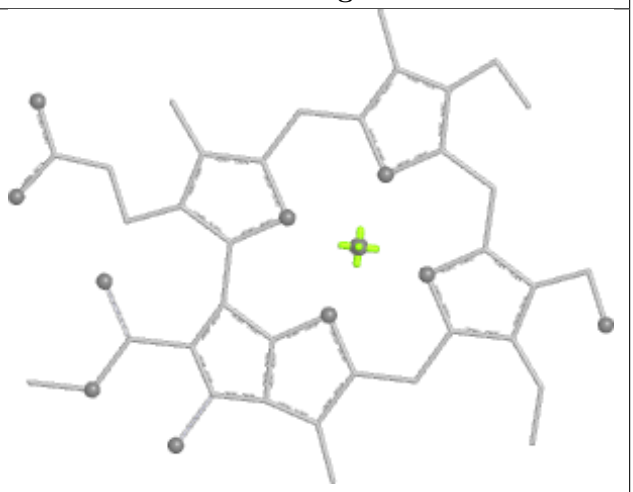
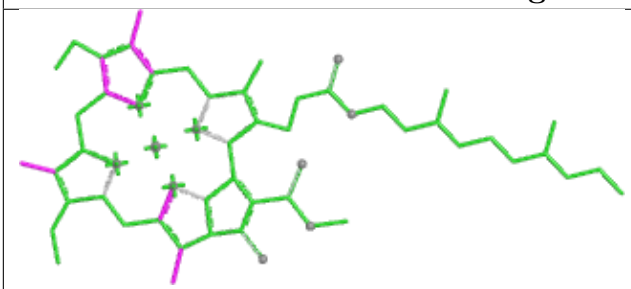


Rings

Ligand CLA 4 609



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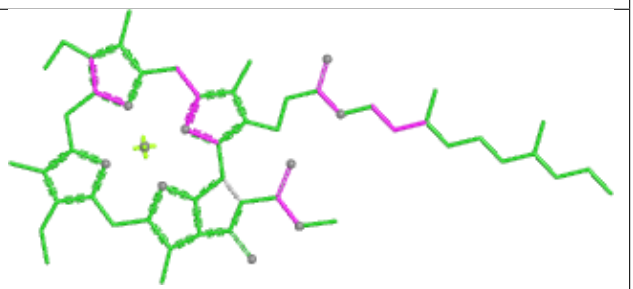
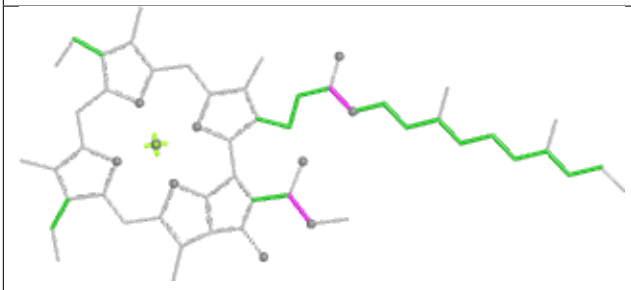


Bond angles



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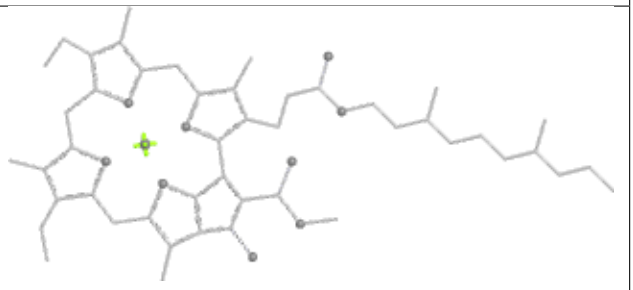
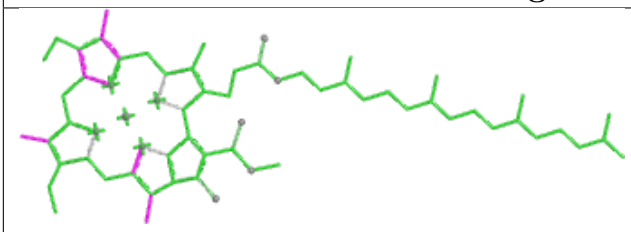


Rings

Ligand CLA 9 613



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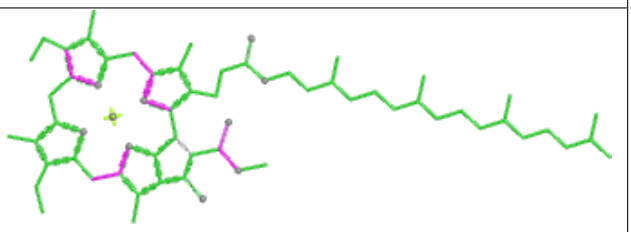
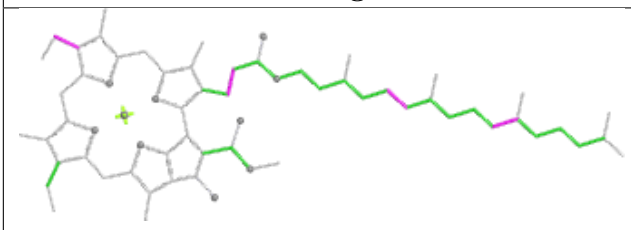
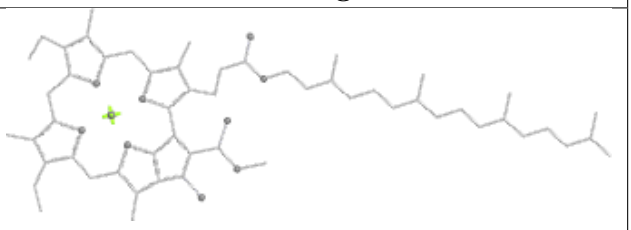


Bond angles

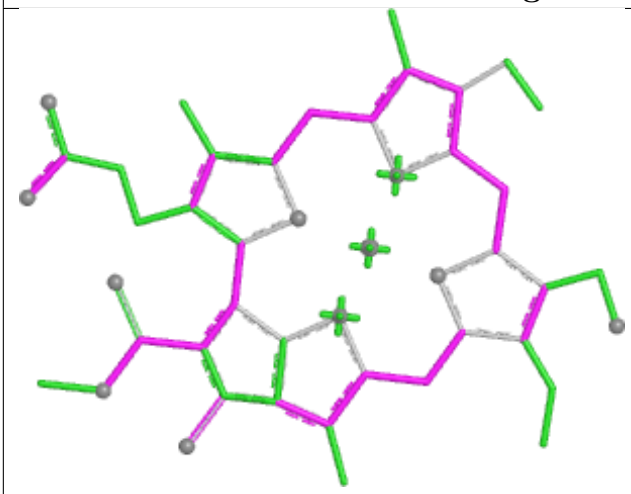


Torsions



Rings

Ligand CHL U 607



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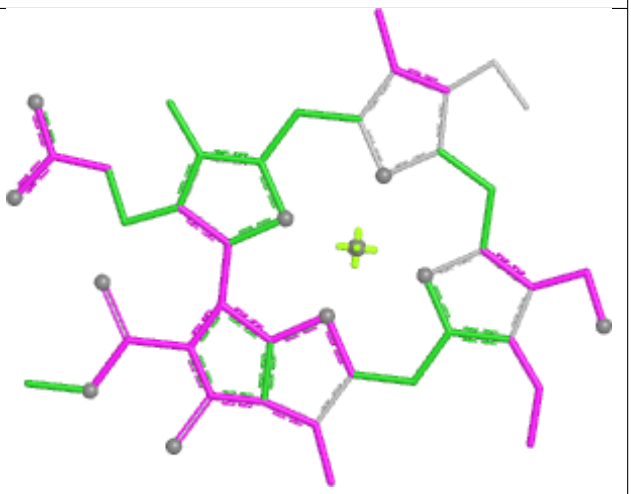
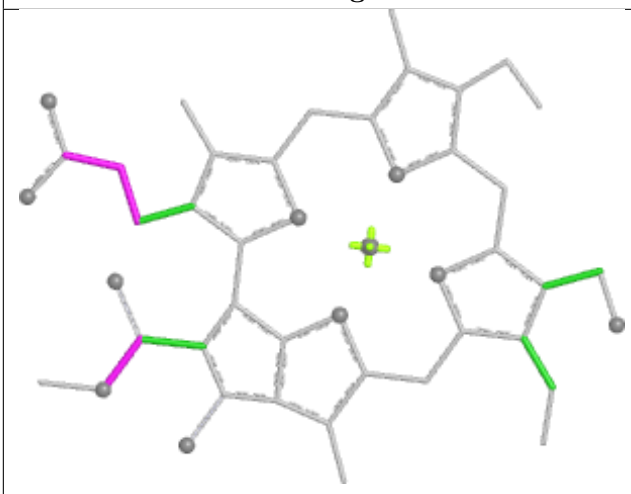


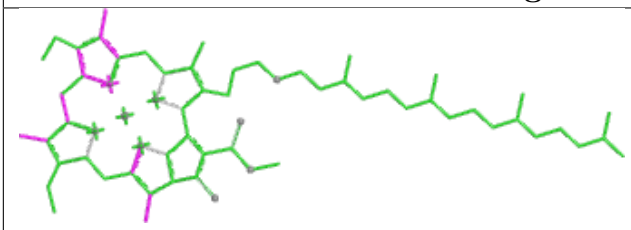
Bond angles



Torsions

Rings

Ligand CLA B 810



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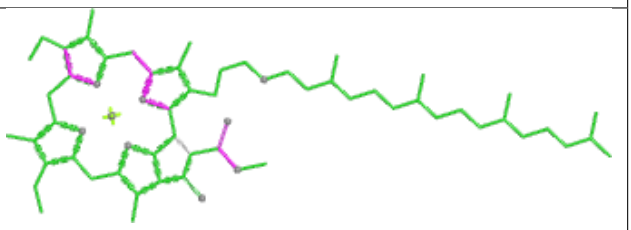
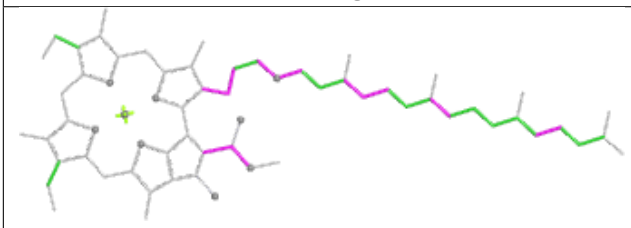


Bond angles



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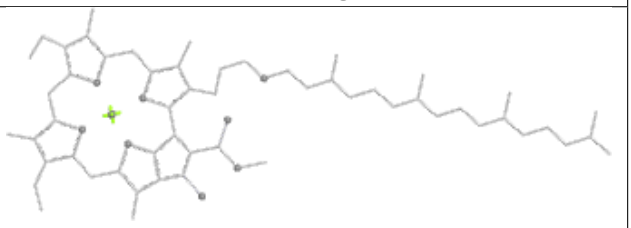
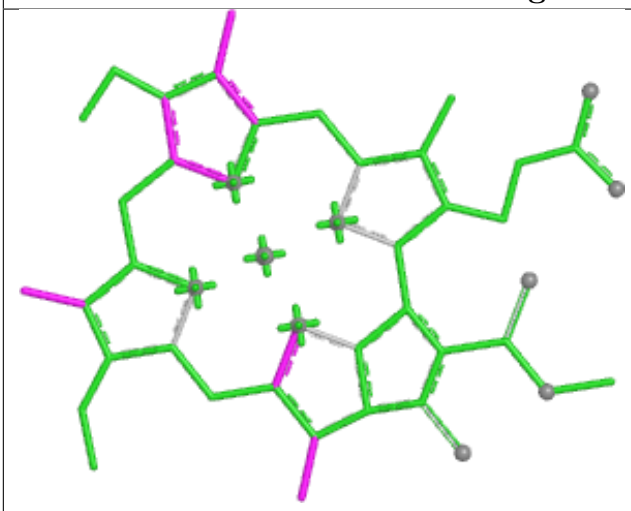


Rings

Ligand CLA 9 601



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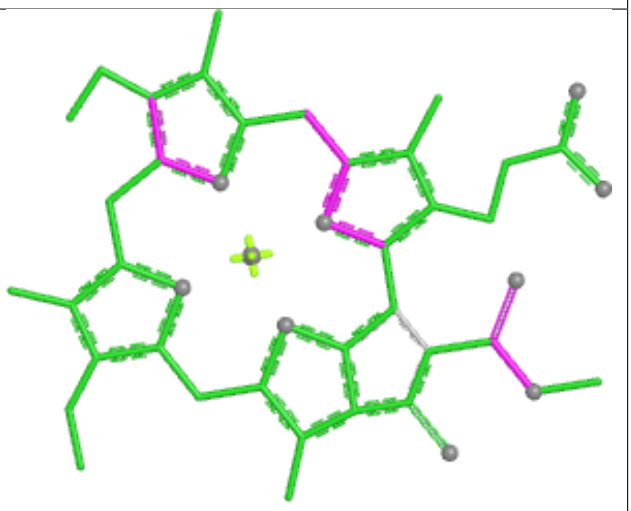
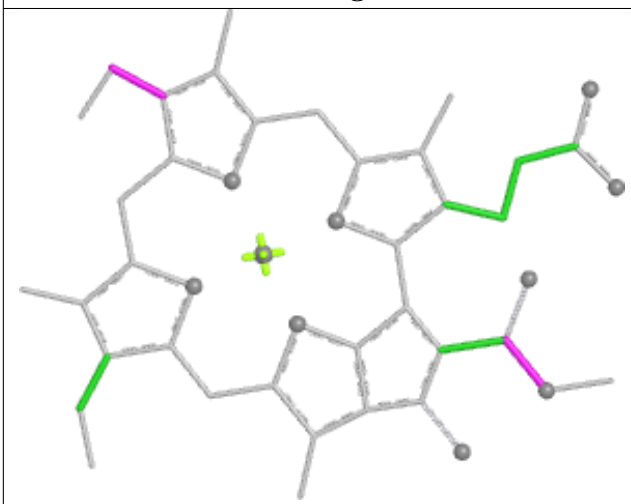


Bond angles



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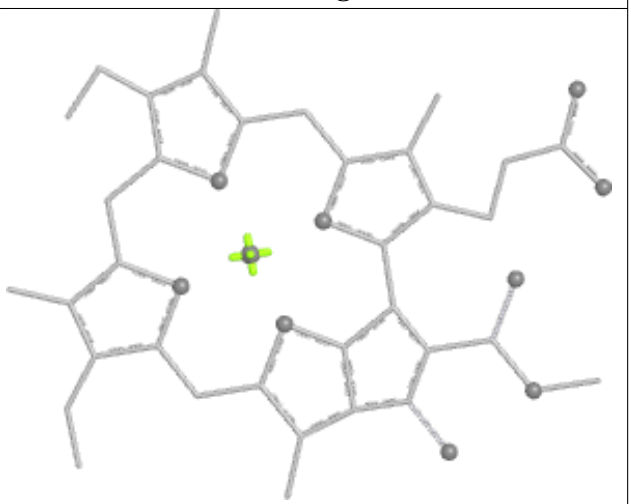
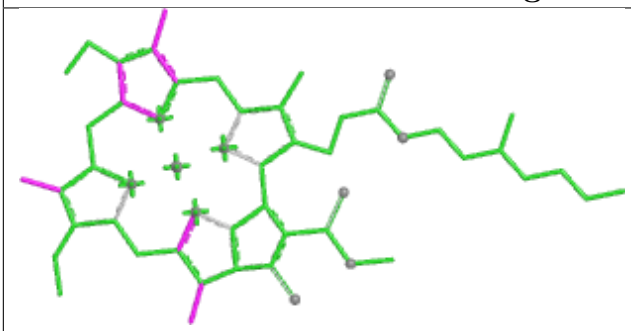


Rings

Ligand CLA A 821



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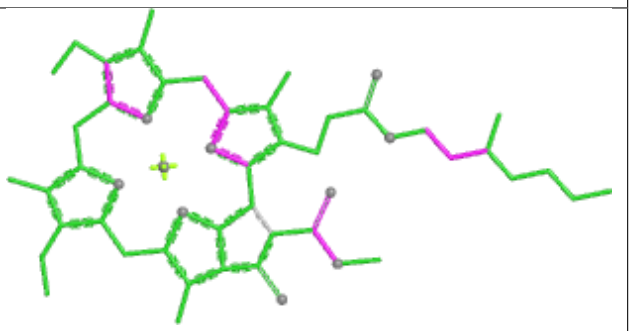
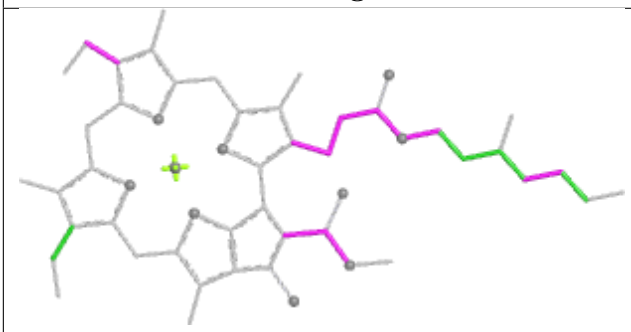


Bond angles



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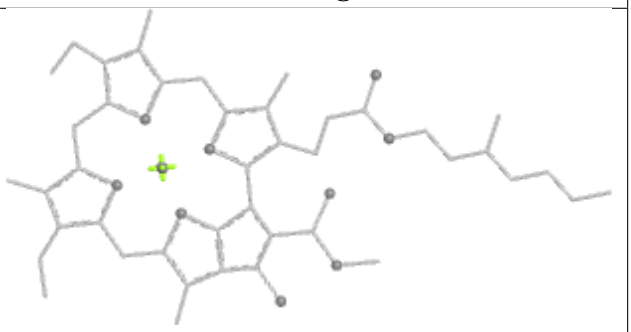
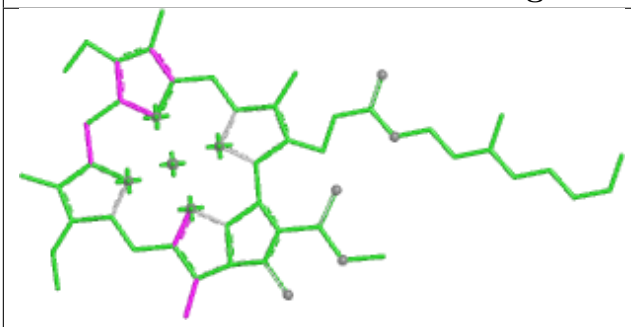


Rings

Ligand CLA Z 614



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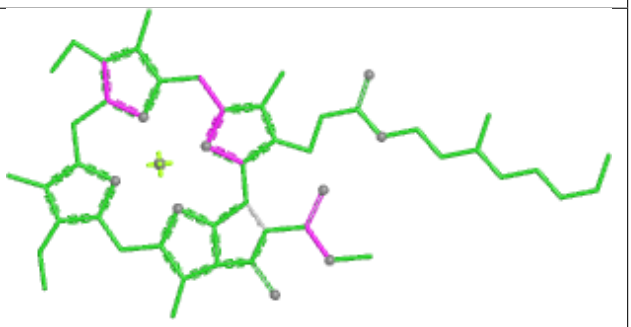
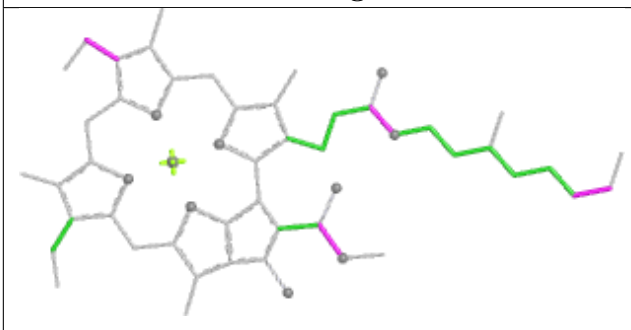
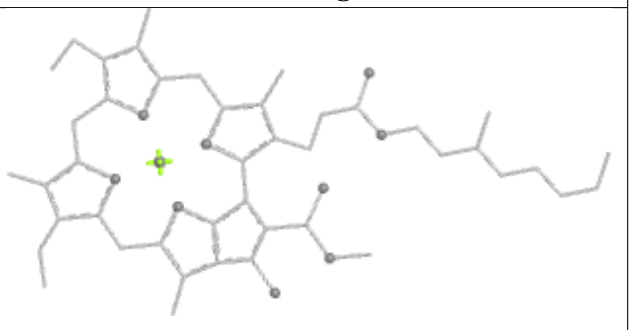


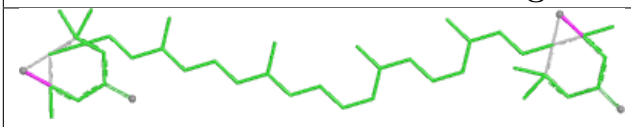
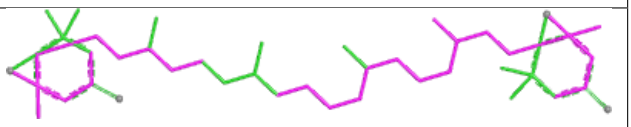
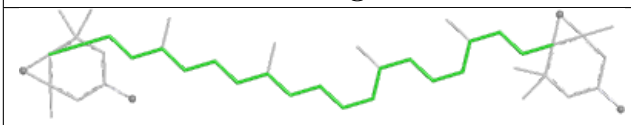
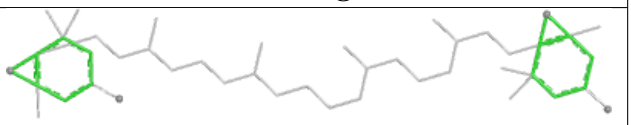
Bond angles

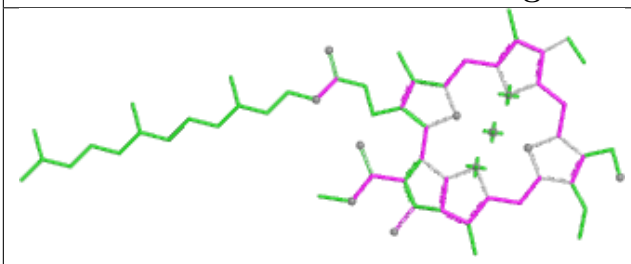
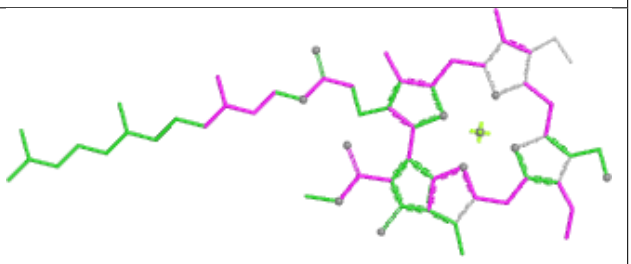
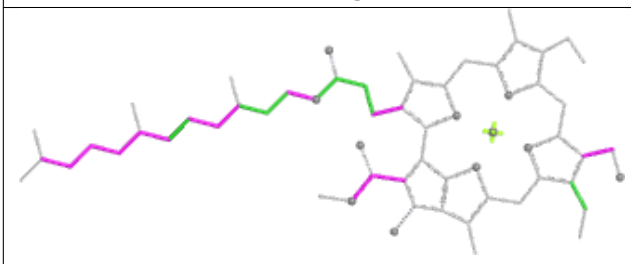
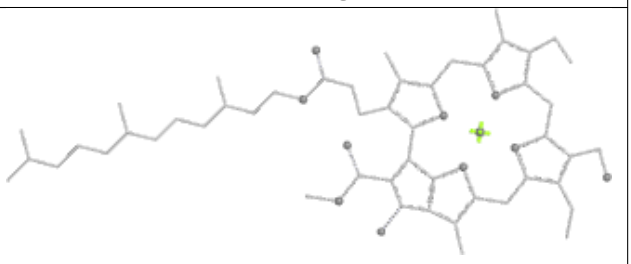


Torsions

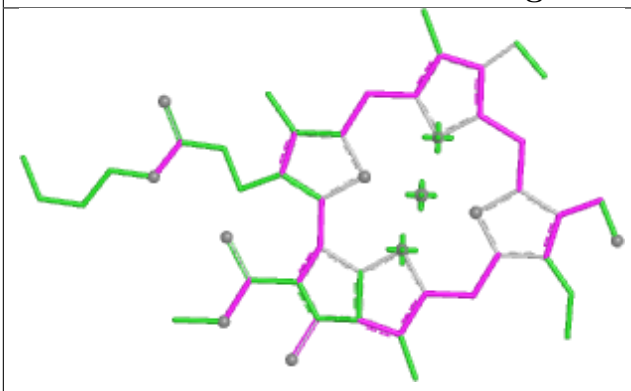


Rings

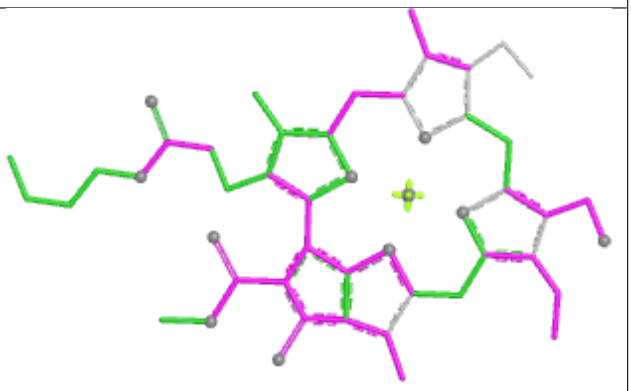
Ligand XAT 6 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL V 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

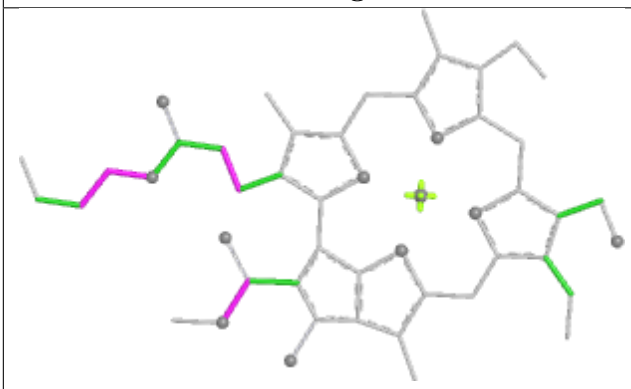
Ligand CHL Z 608



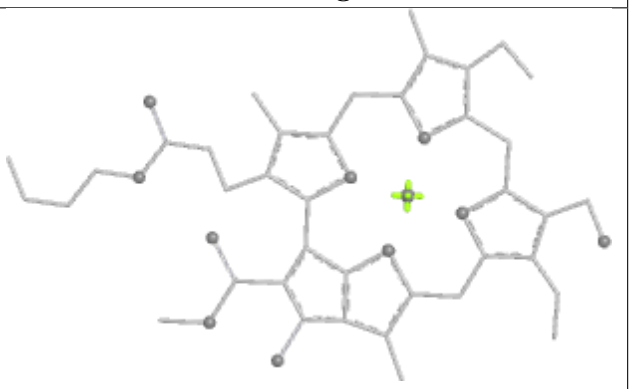
Bond lengths



Bond angles

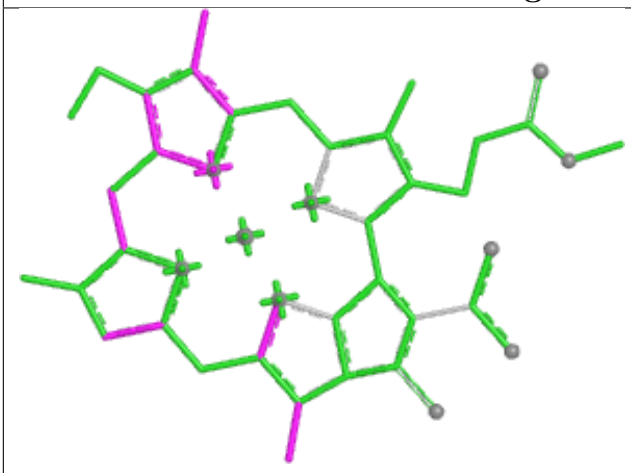


Torsions



Rings

Ligand CLA B 821



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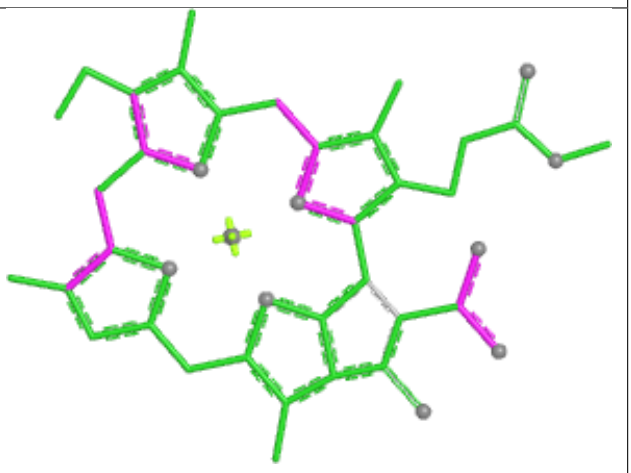
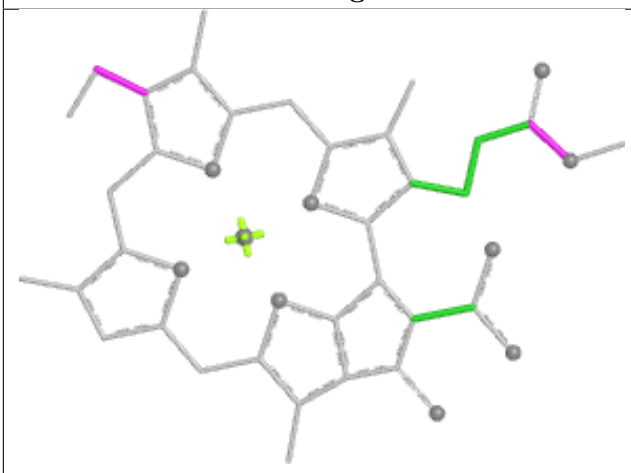


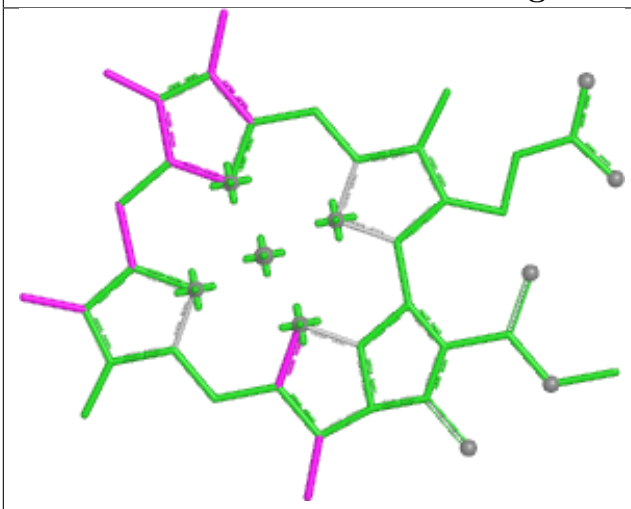
Bond angles



Torsions

Rings

Ligand CLA 8 616



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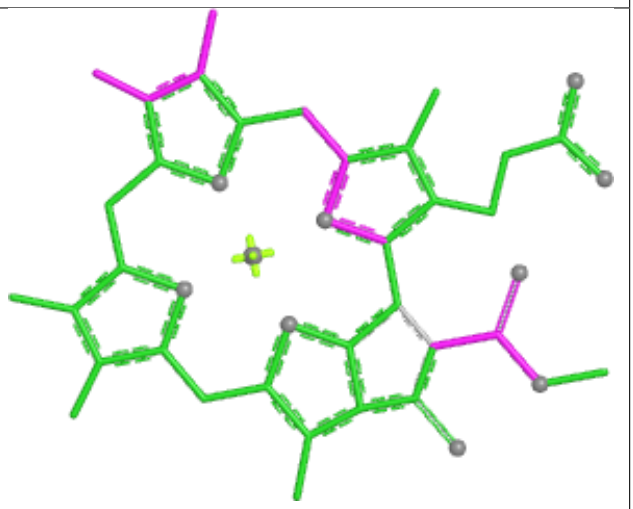
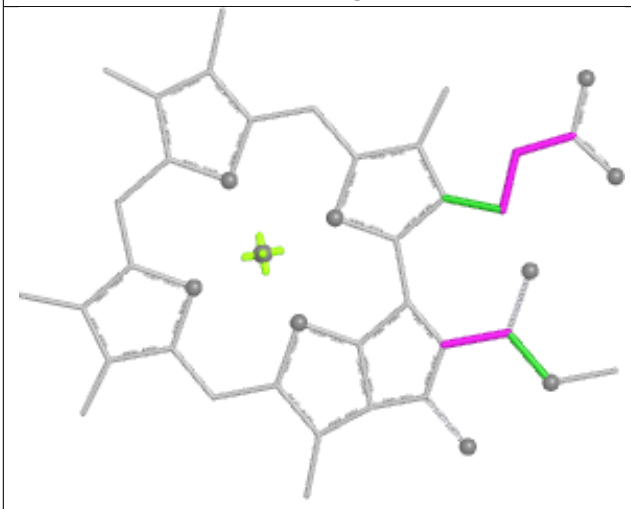


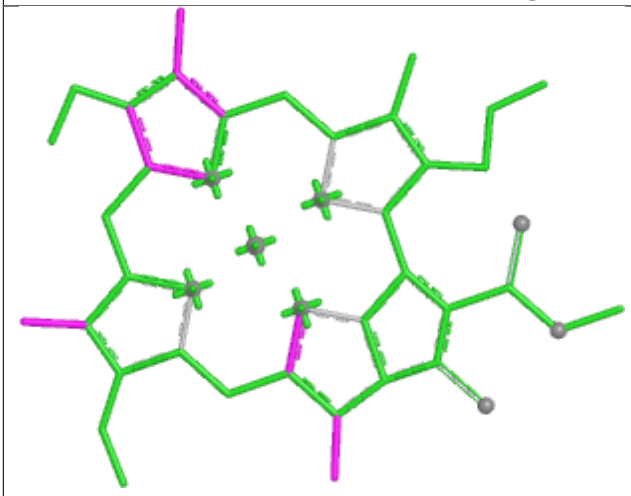
Bond angles



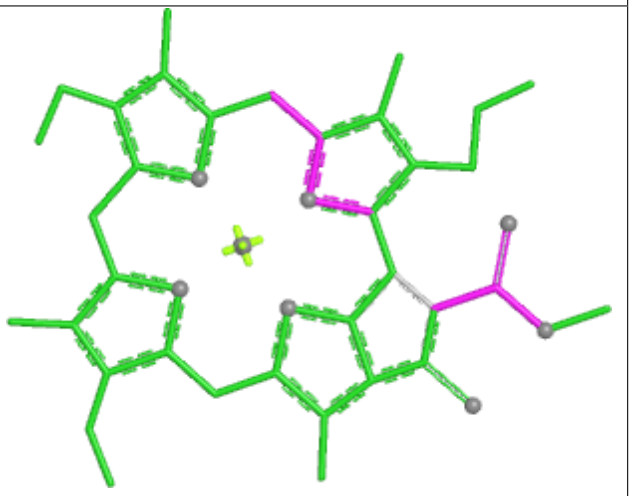
Torsions

Rings

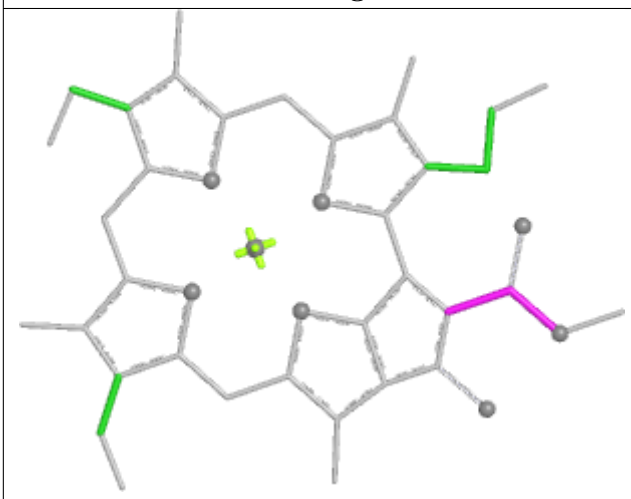
Ligand CLA V 611



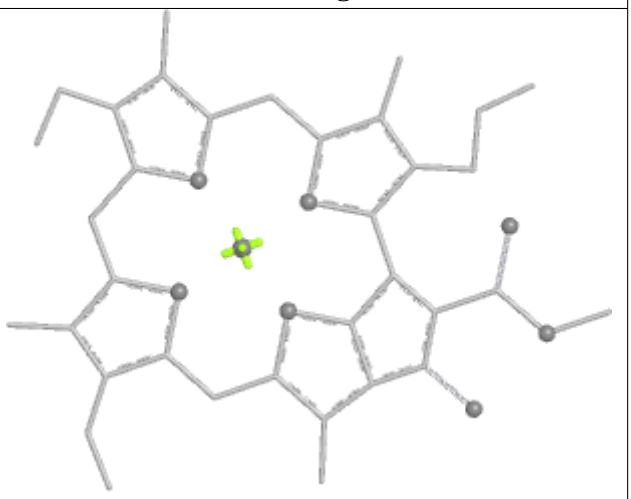
Bond lengths



Bond angles

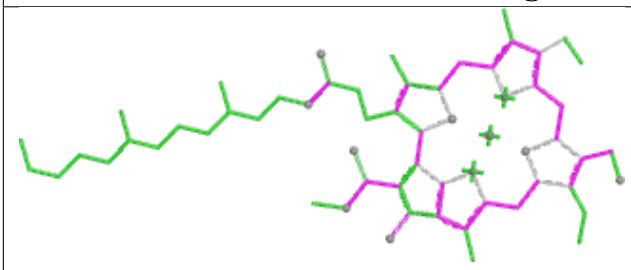


Torsions



Rings

Ligand CHL U 609



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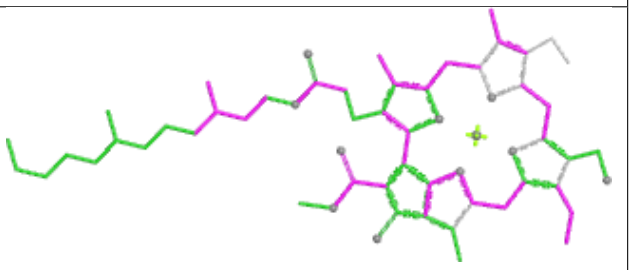

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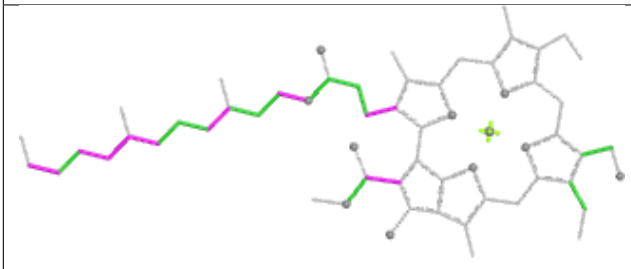

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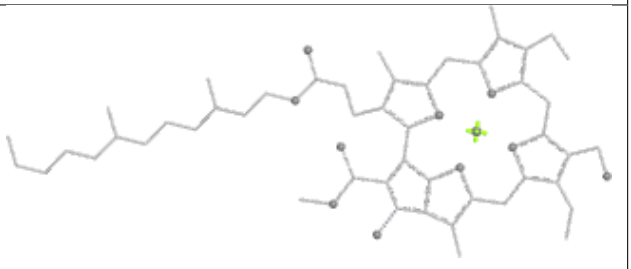
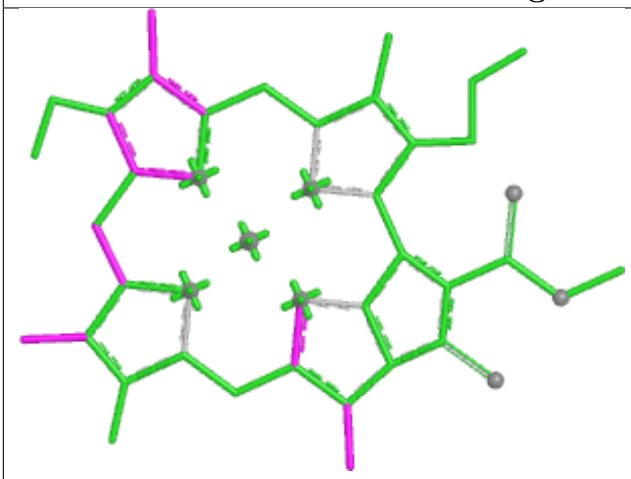


Rings

Ligand CLA 2 604



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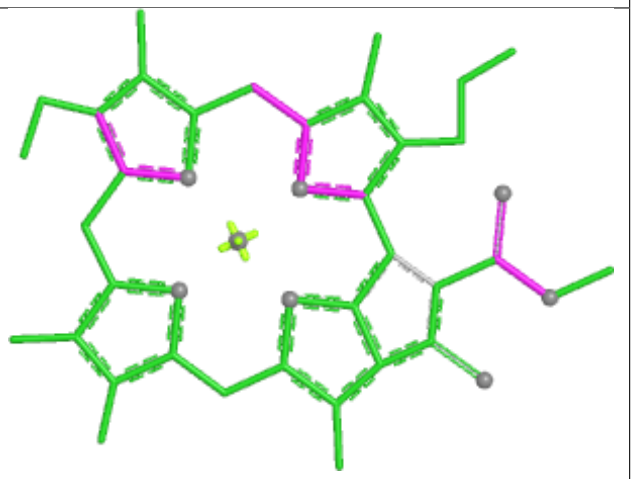
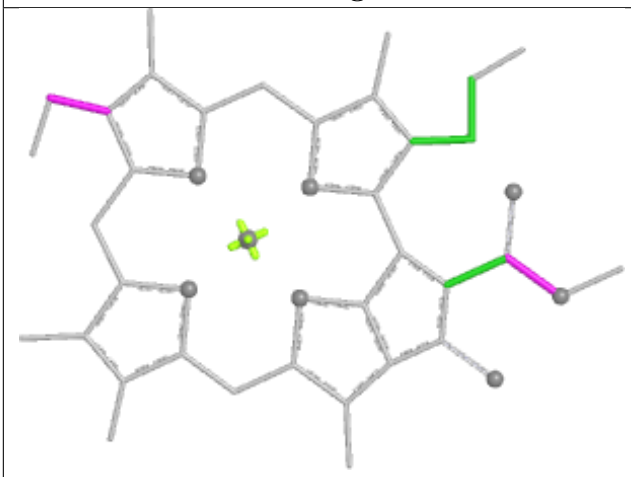


Bond angles



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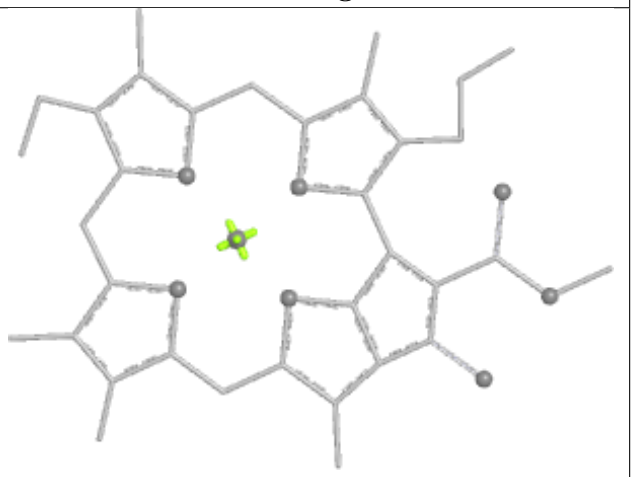
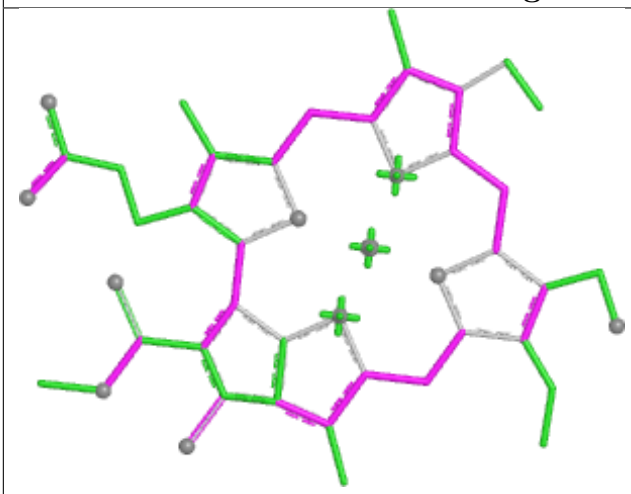


Rings

Ligand CHL Y 606



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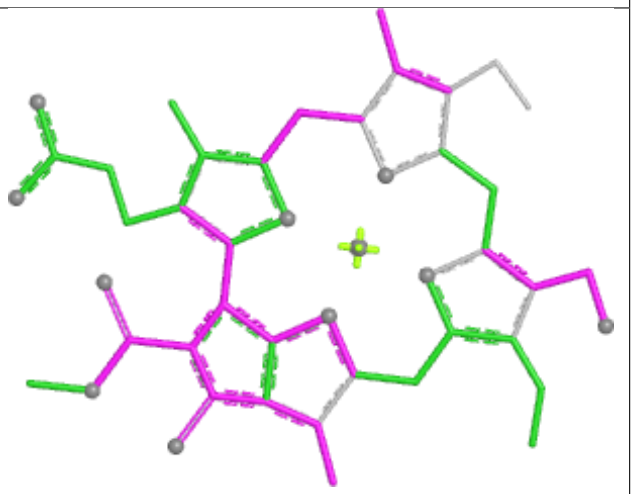
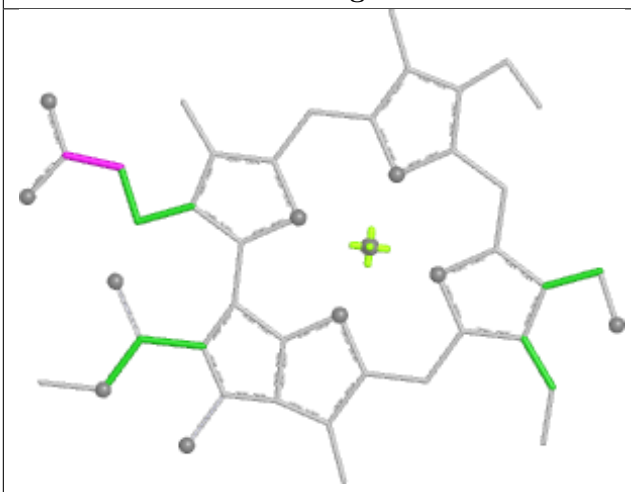


Bond angles



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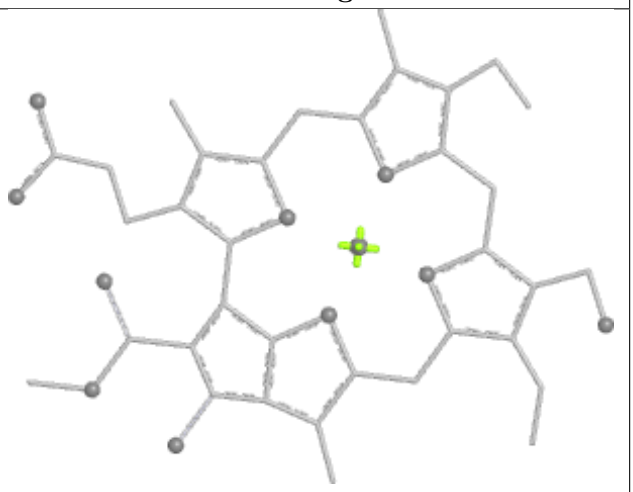
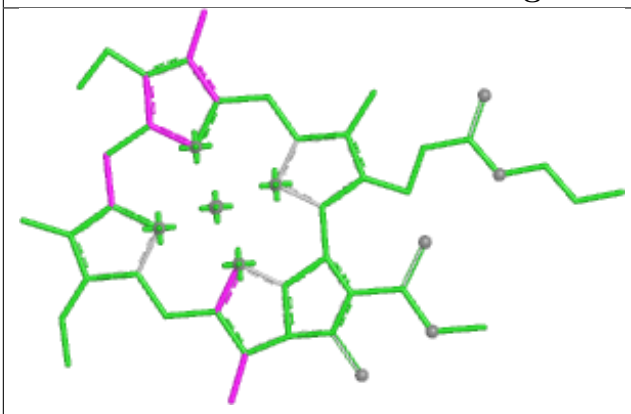


Rings

Ligand CLA Y 614



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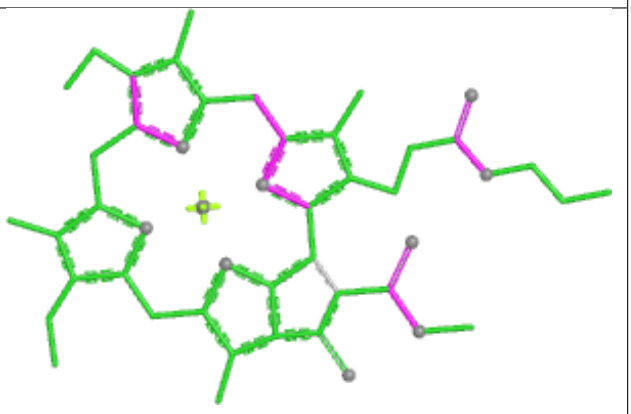
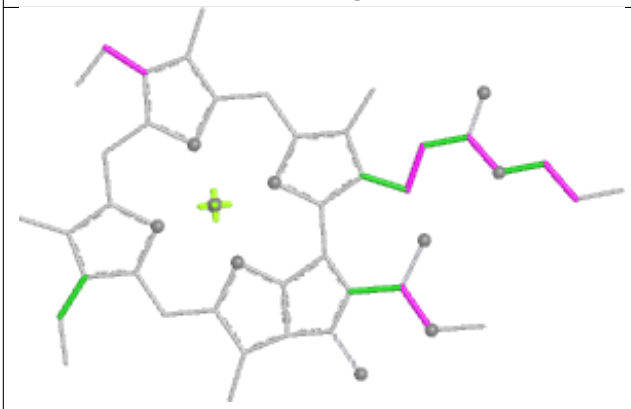


Bond angles



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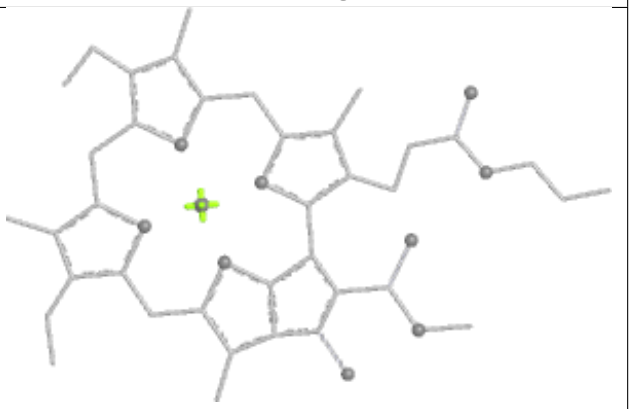
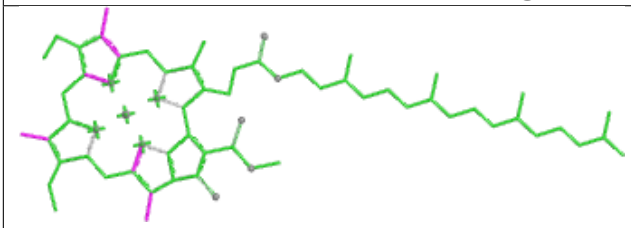


Rings

Ligand CLA W 613



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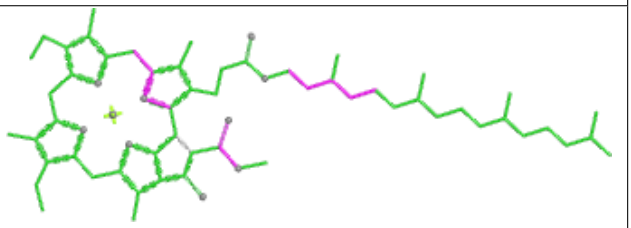
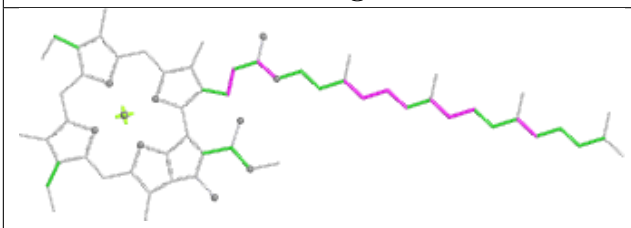


Bond angles



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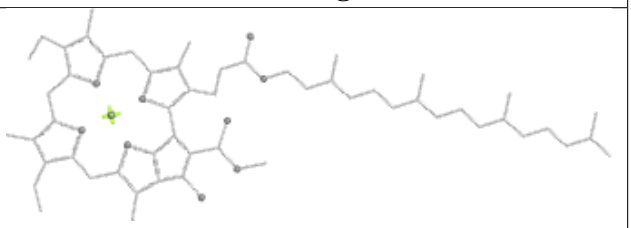
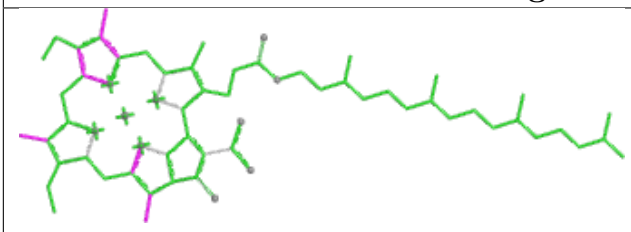


Rings

Ligand CLA a 609



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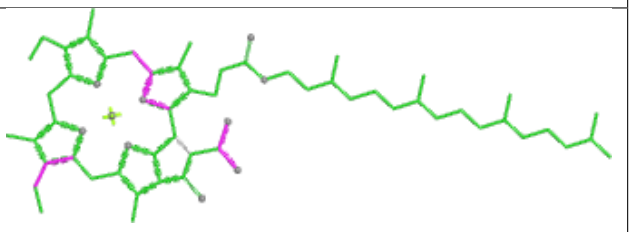

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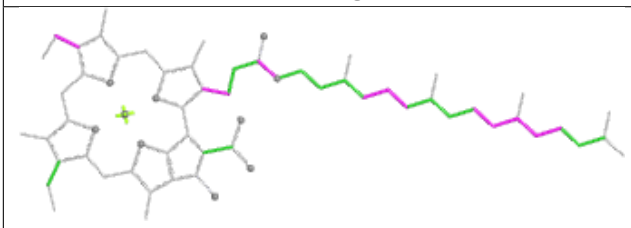

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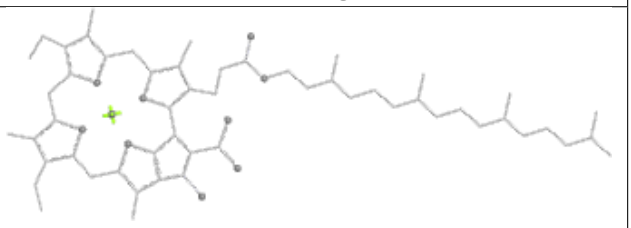
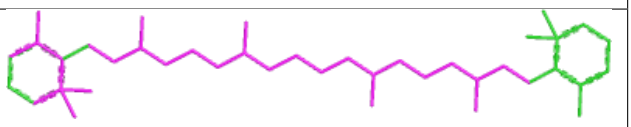


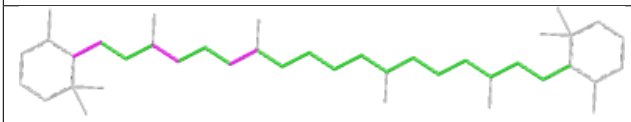
Rings

Ligand BCR B 852

Bond lengths



Bond angles



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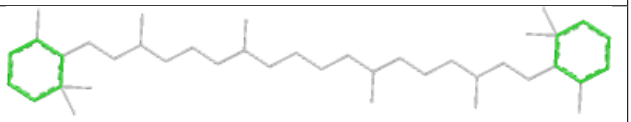
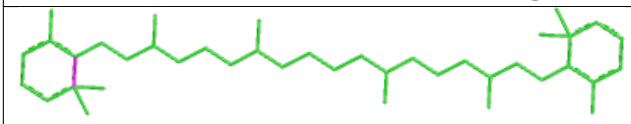


Rings

Ligand BCR 7 621



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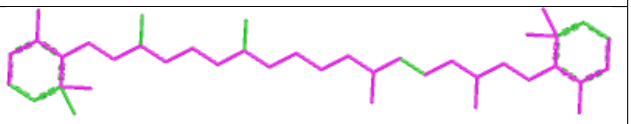
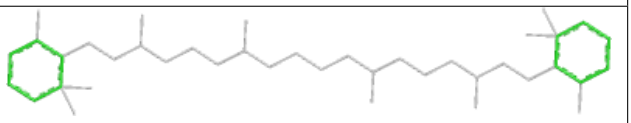


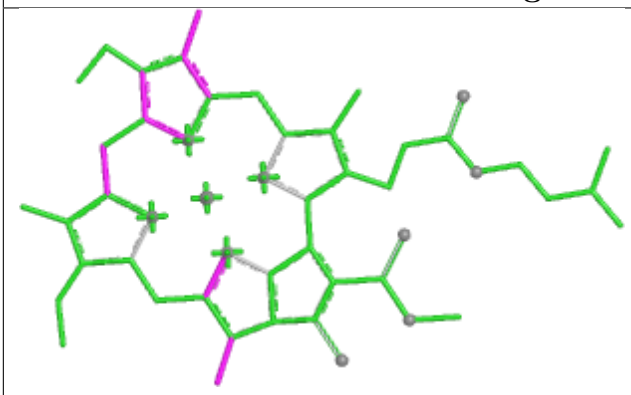
Bond angles

Torsions



Rings

Ligand CLA Y 604



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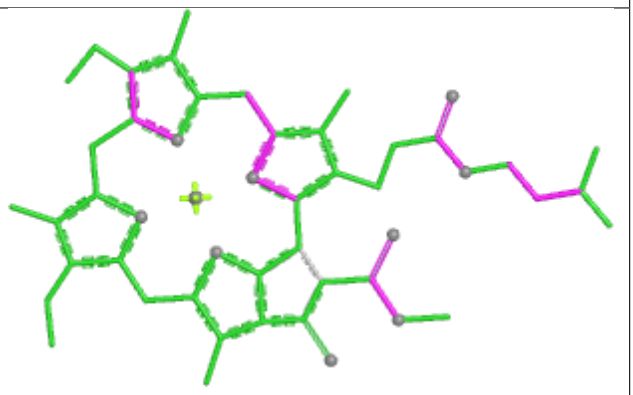
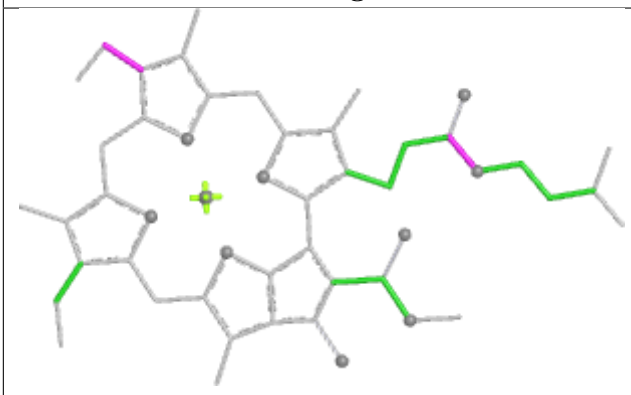


Bond angles



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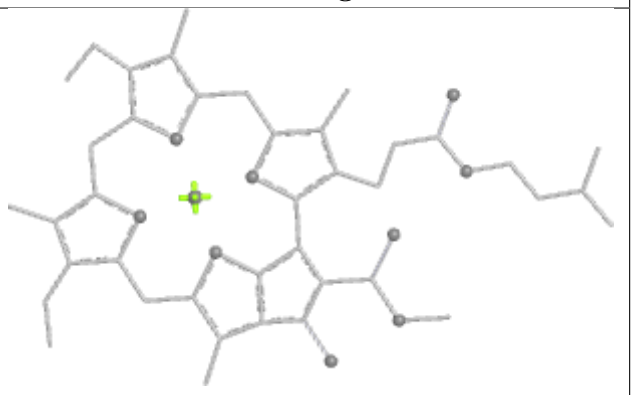
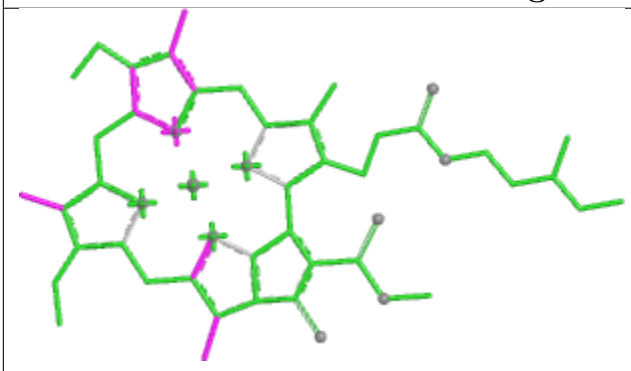


Rings

Ligand CLA 8 608



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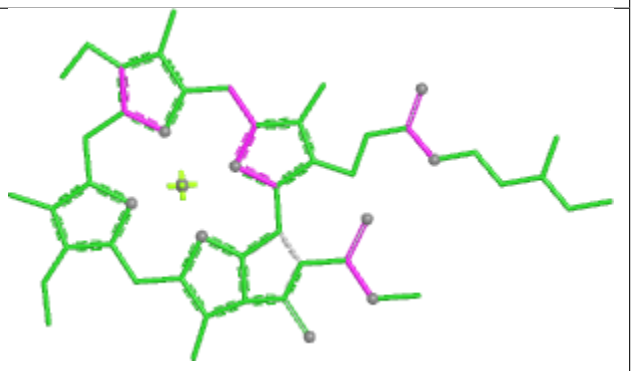
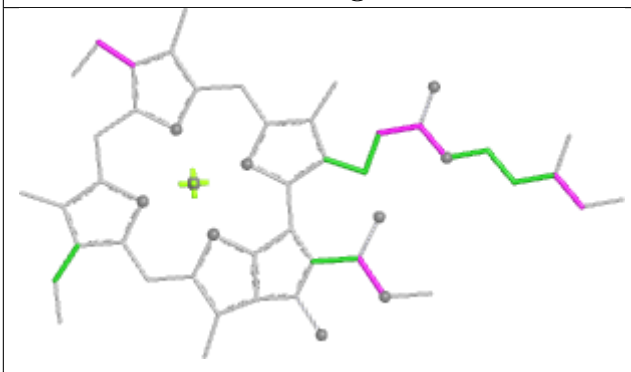


Bond angles



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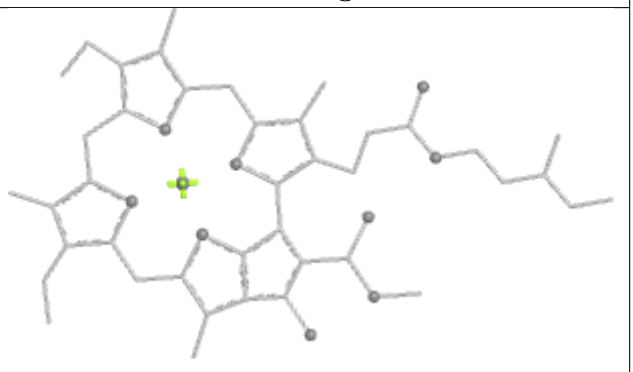
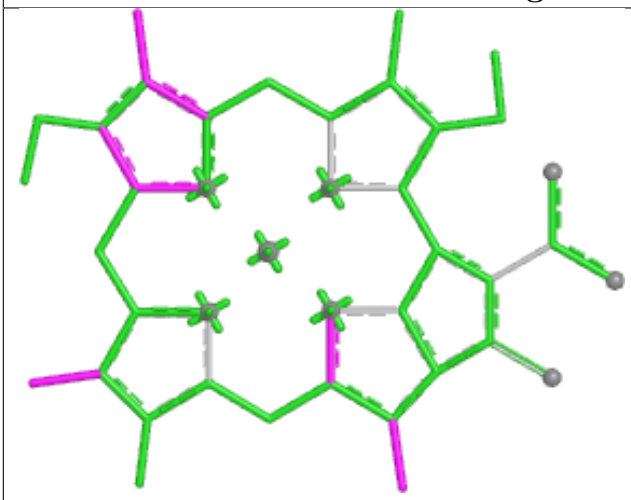


Rings

Ligand CLA L 307



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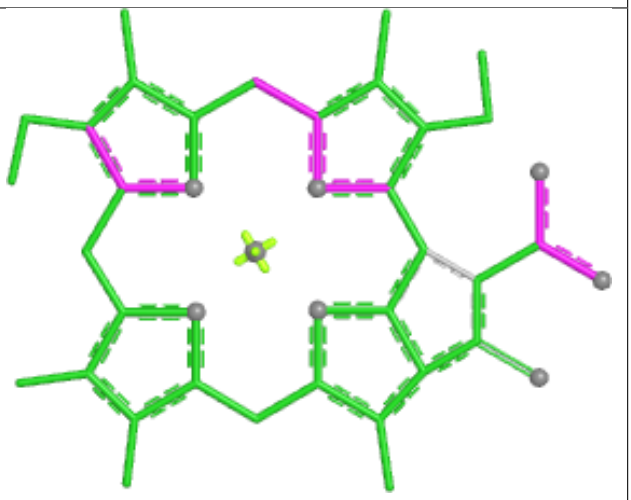

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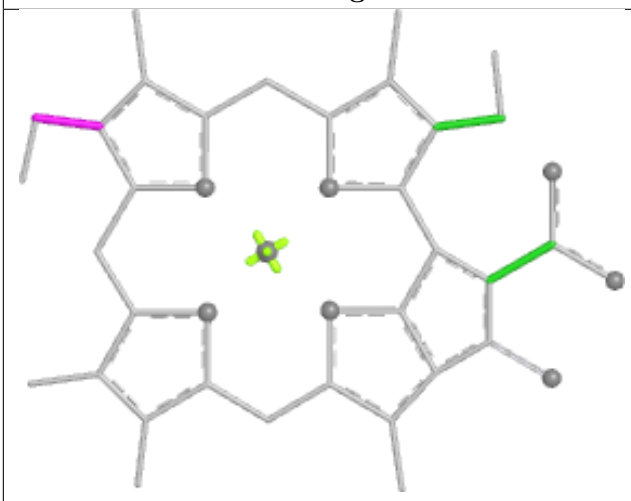

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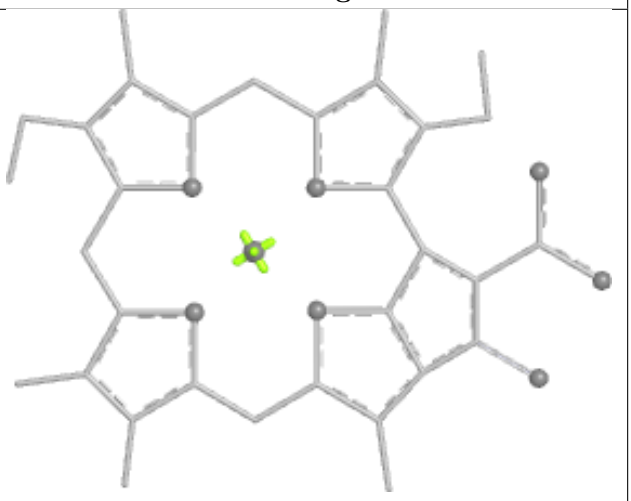
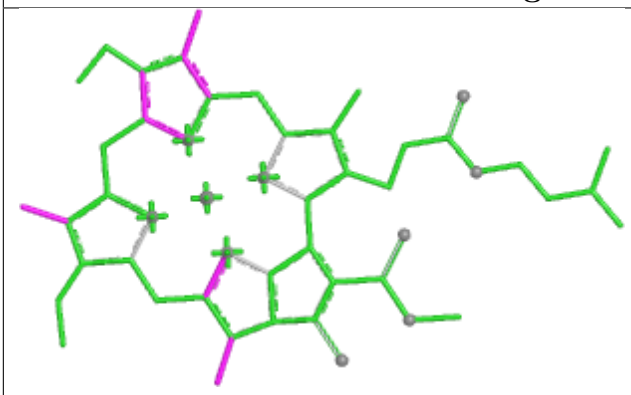


Rings

Ligand CLA A 808



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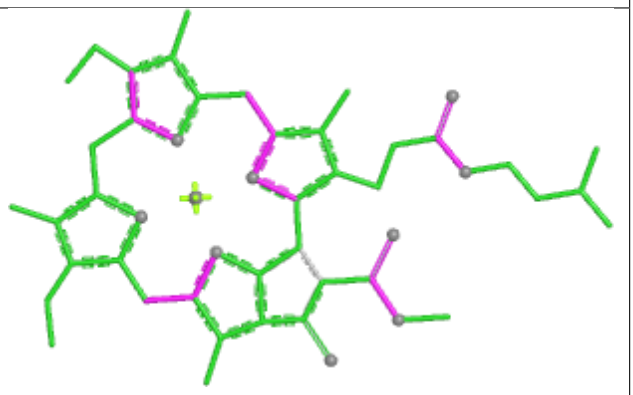
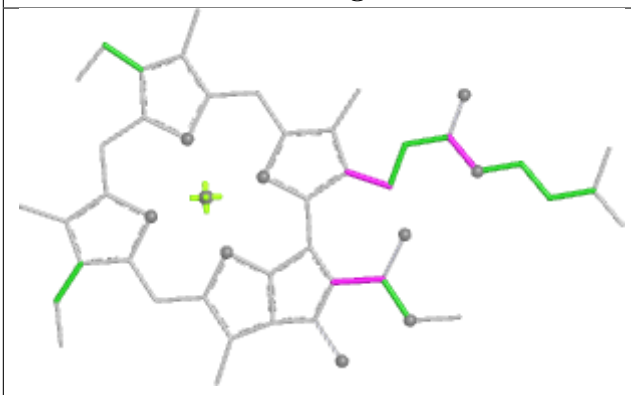


Bond angles



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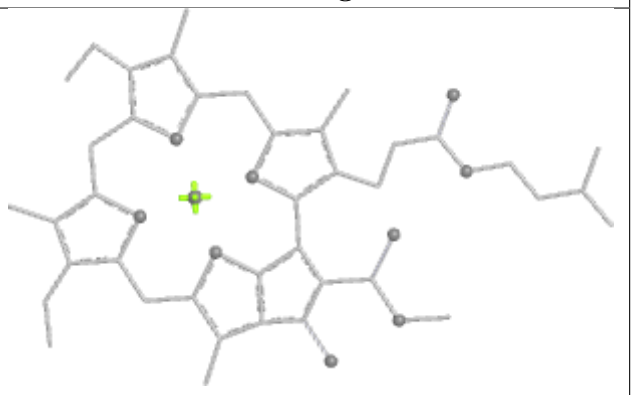
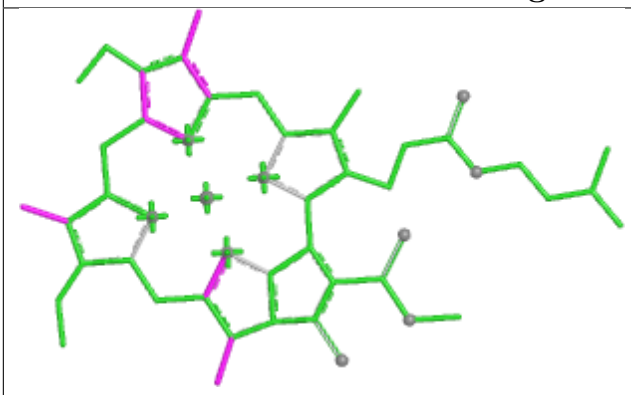


Rings

Ligand CLA 7 608



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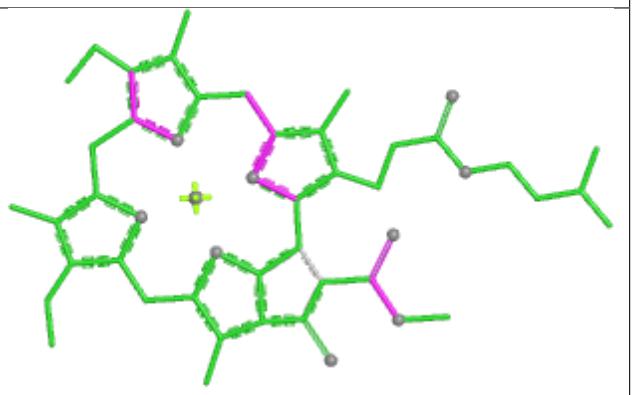
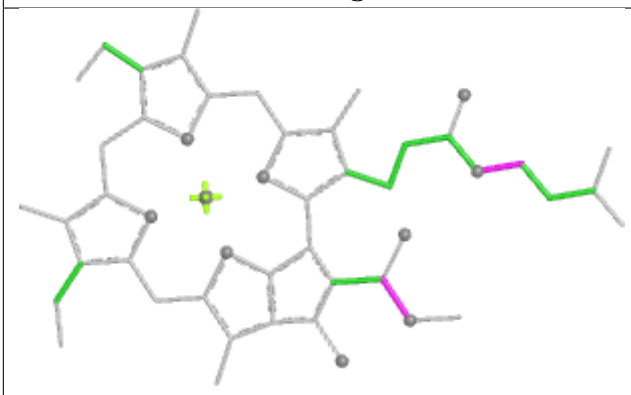


Bond angles



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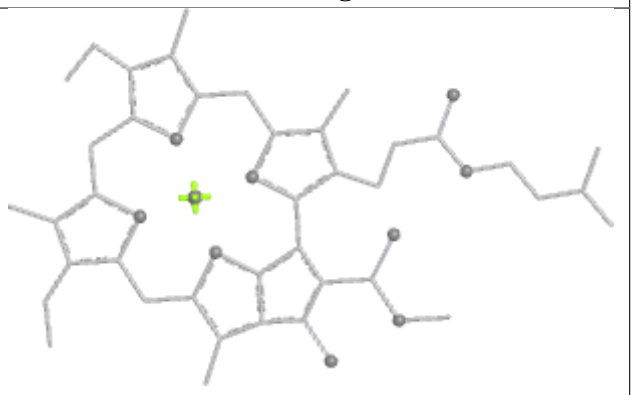
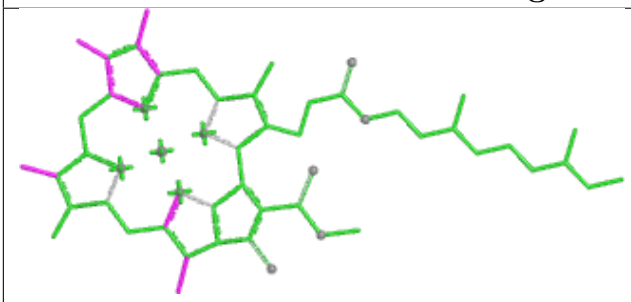


Rings

Ligand CLA 4 604



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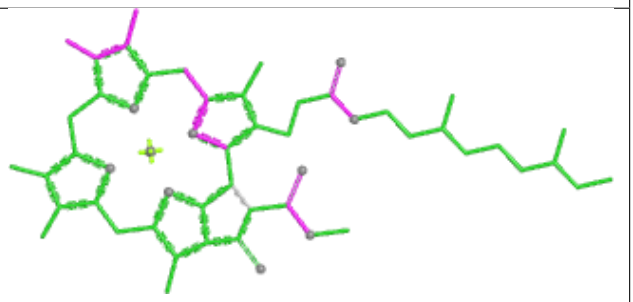
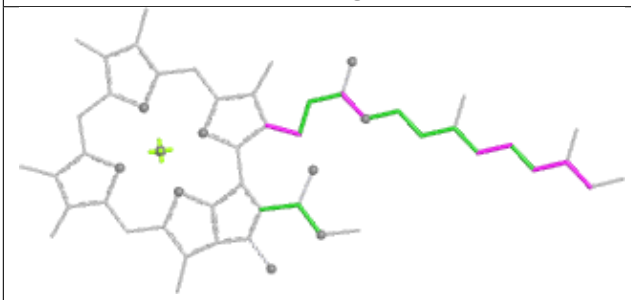
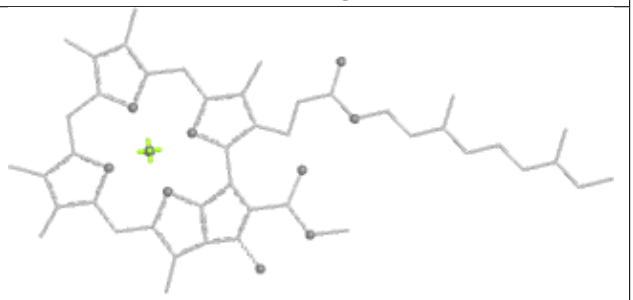


Bond angles

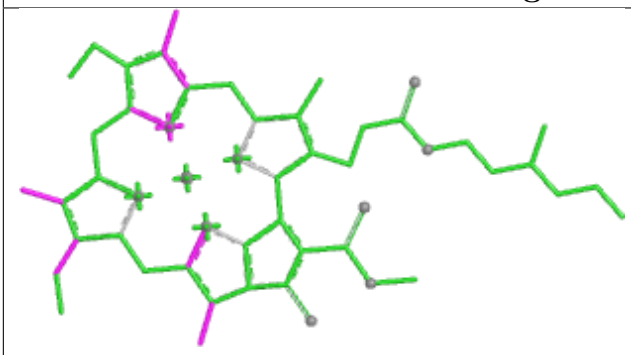


Torsions



Rings

Ligand CLA U 603



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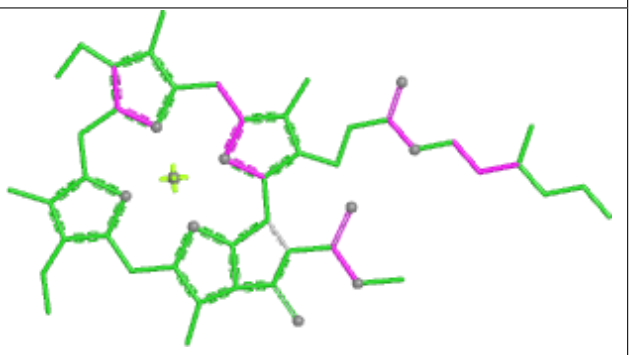

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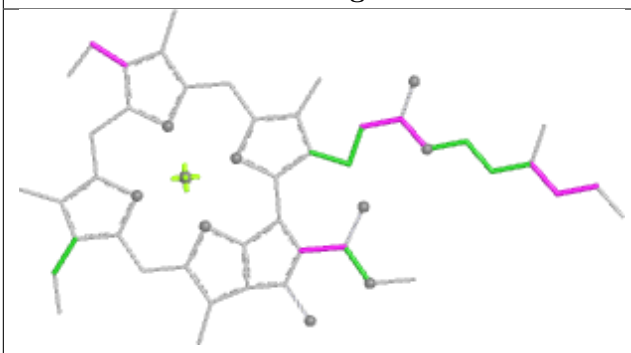

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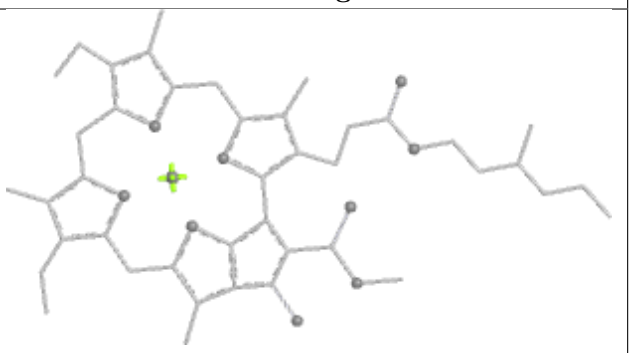
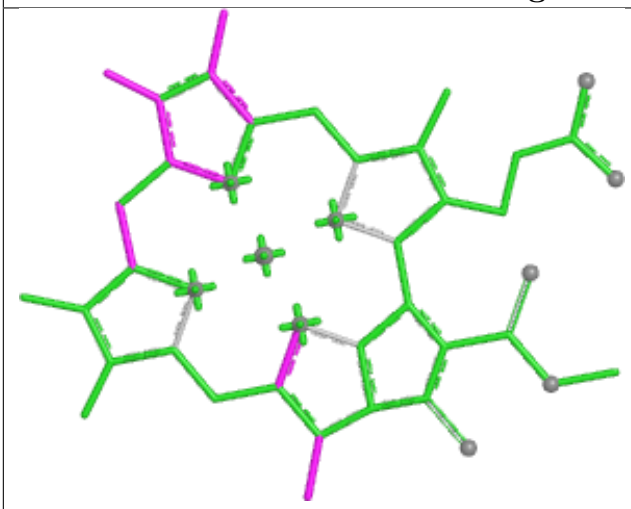


Rings

Ligand CLA 7 616



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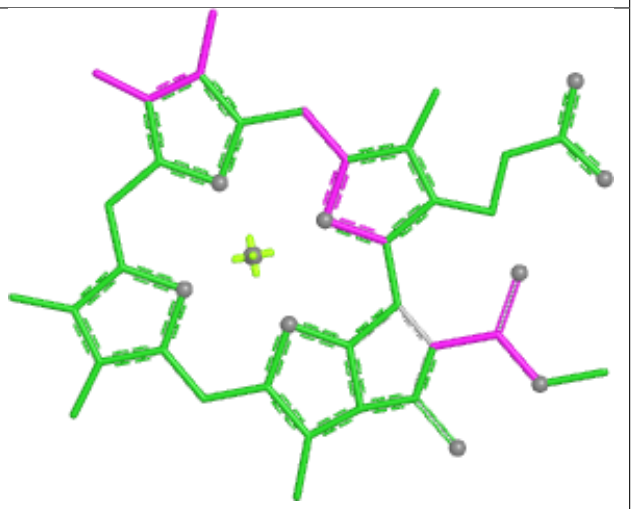

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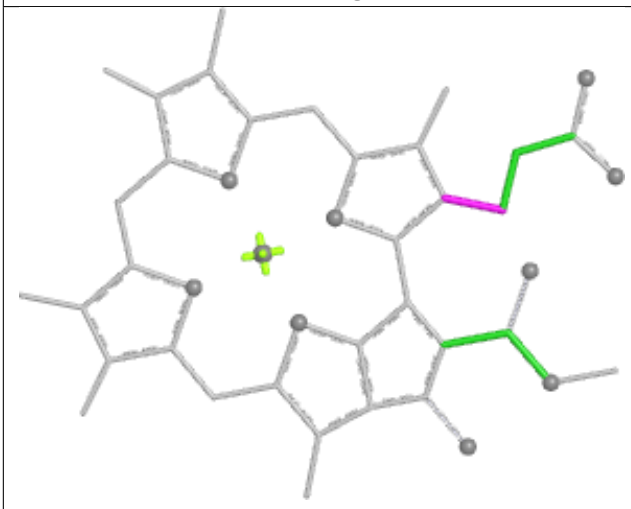
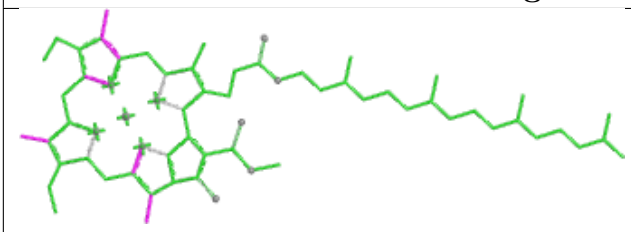


Torsions

Rings

Ligand CLA A 801



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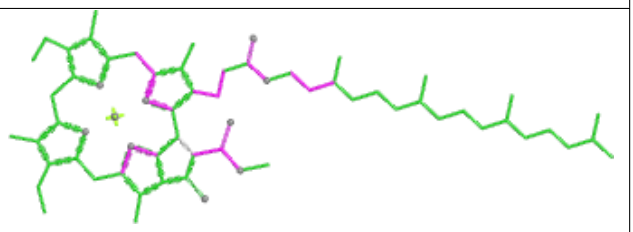

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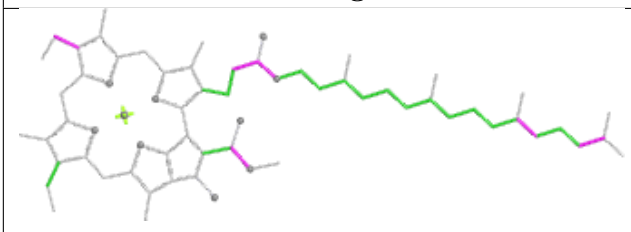

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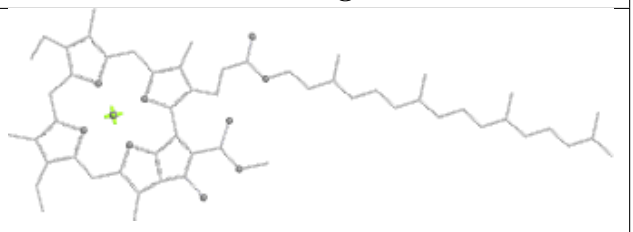
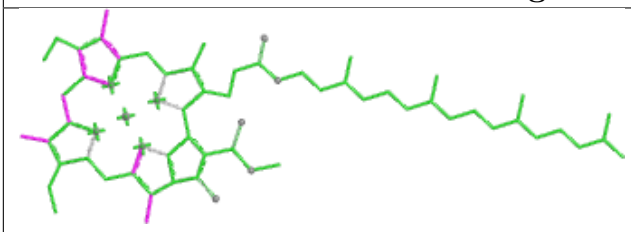


Rings

Ligand CLA 4 613



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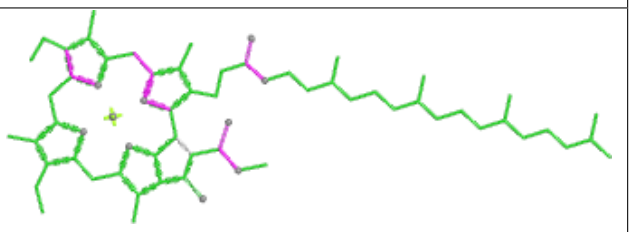

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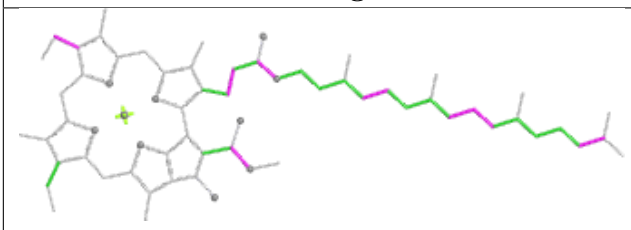

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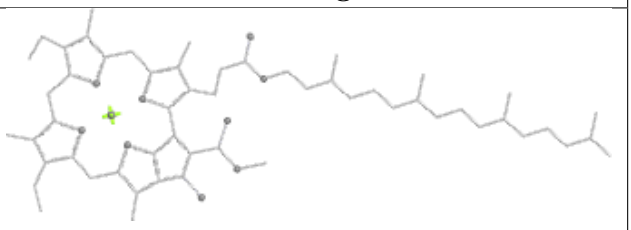

Rings

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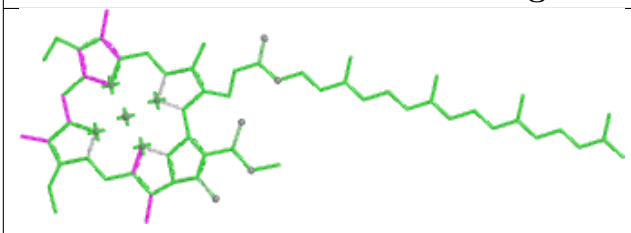

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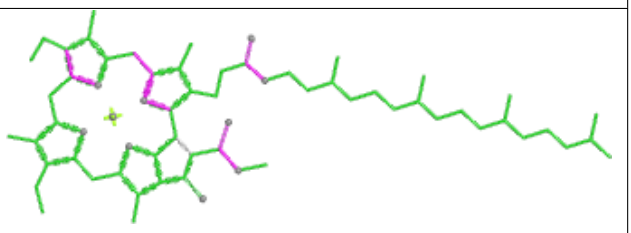

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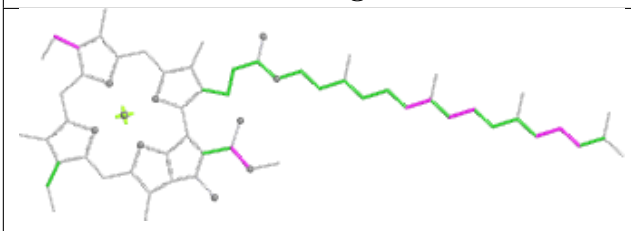

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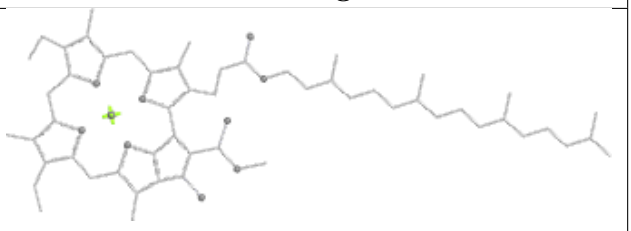

Rings

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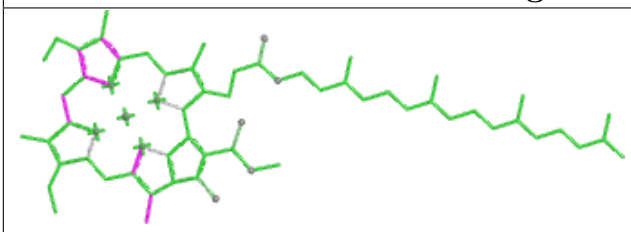

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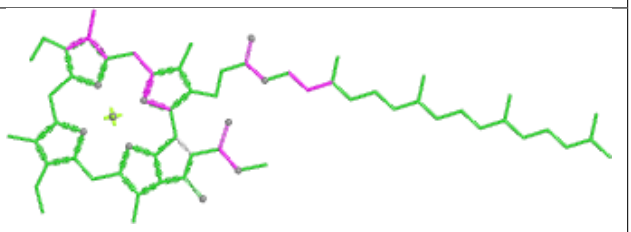

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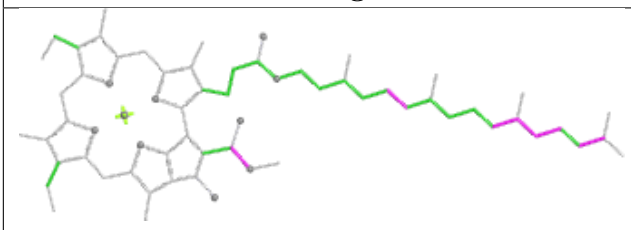

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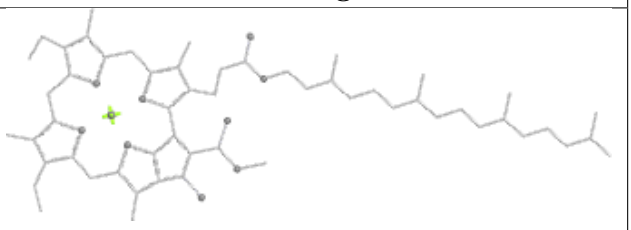
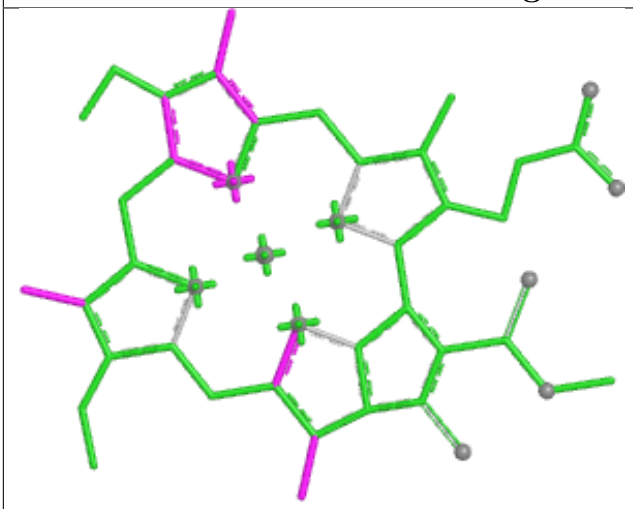


Rings

Ligand CLA G 204



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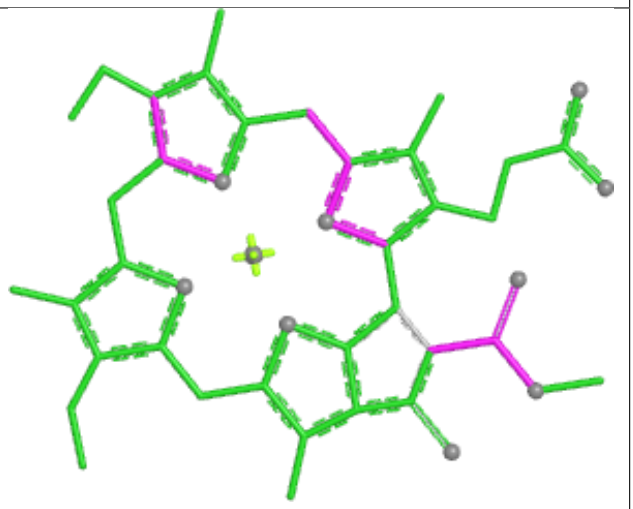

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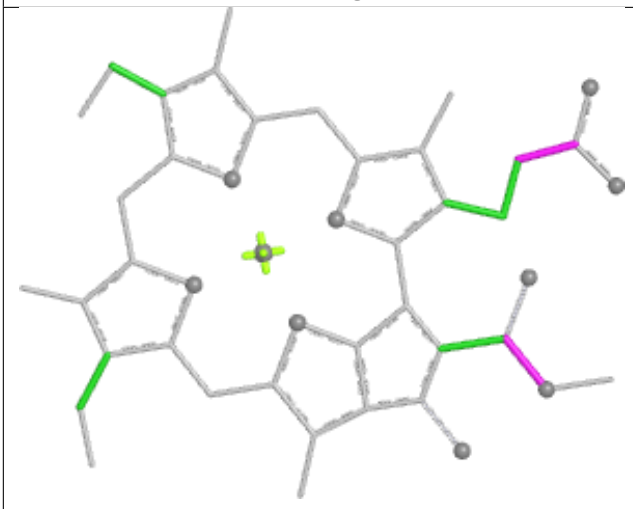
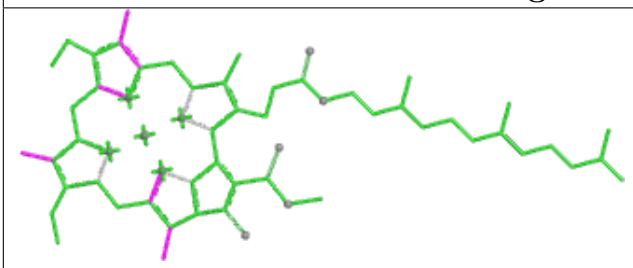


Torsions

Rings

Ligand CLA 3 609



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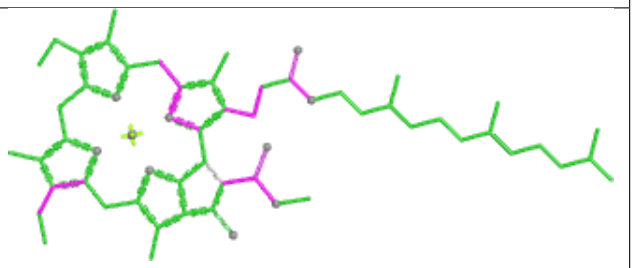

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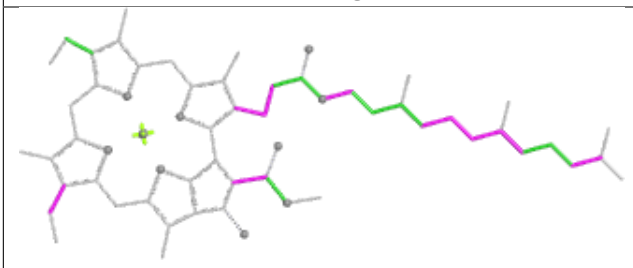

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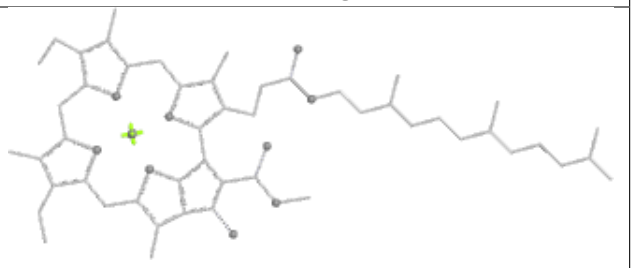
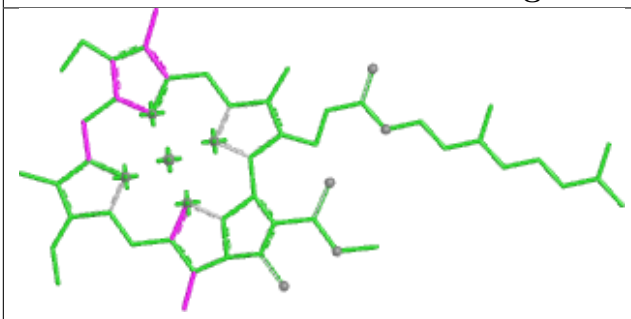


Rings

Ligand CLA Y 603



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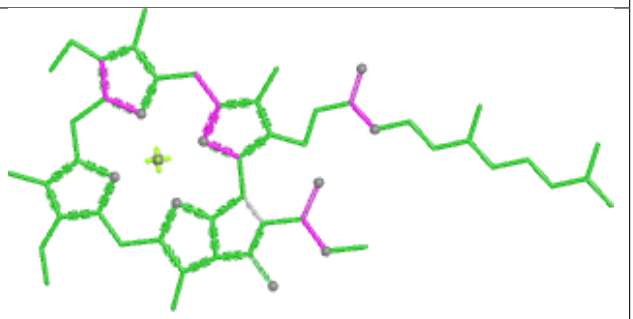

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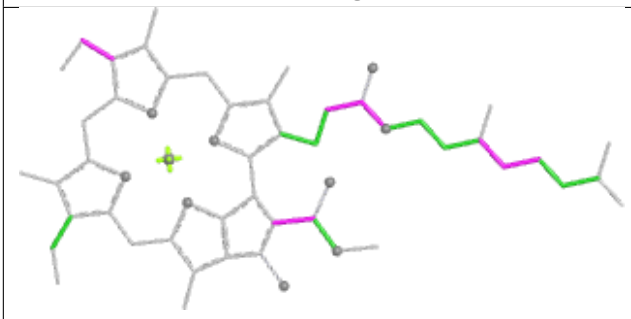

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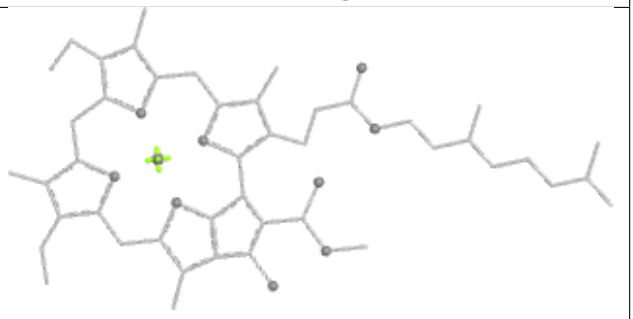
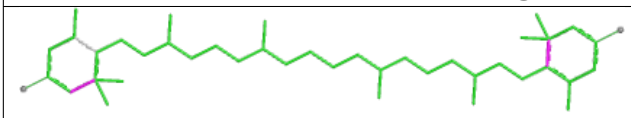


Rings

Ligand LUT V 1621



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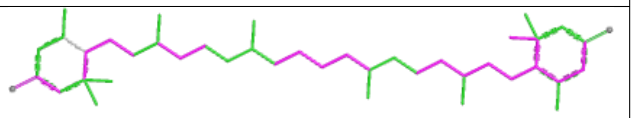

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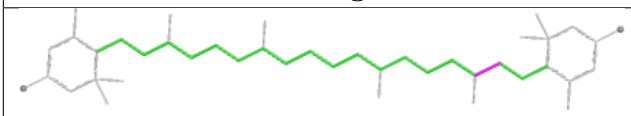

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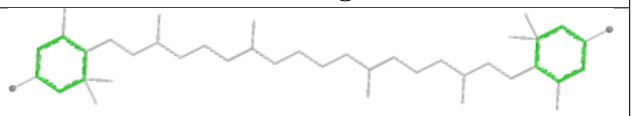
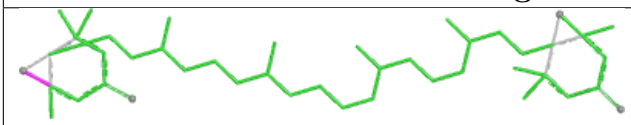


Rings

Ligand XAT Y 1622



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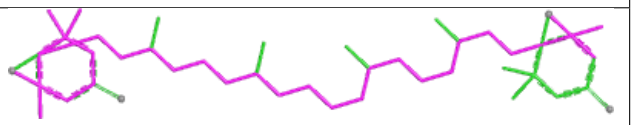
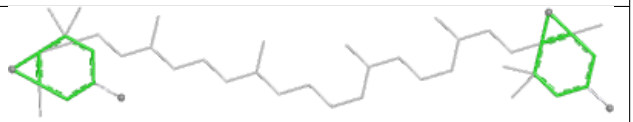


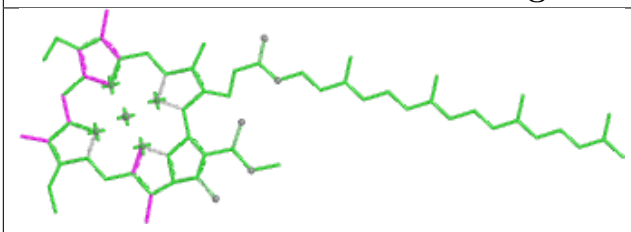
Bond angles

Torsions



Rings

Ligand CLA 2 601



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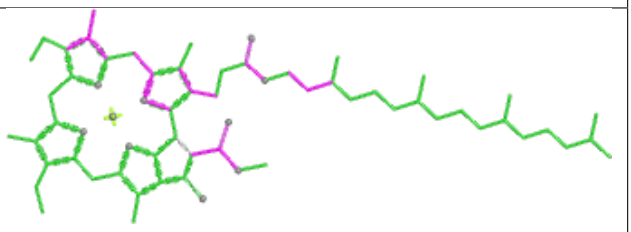
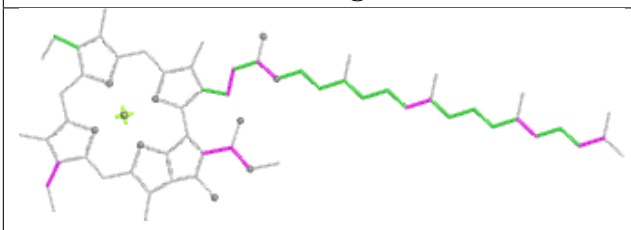


Bond angles



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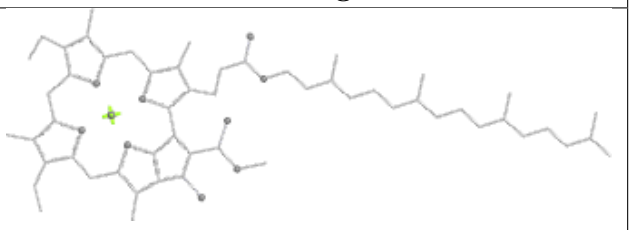
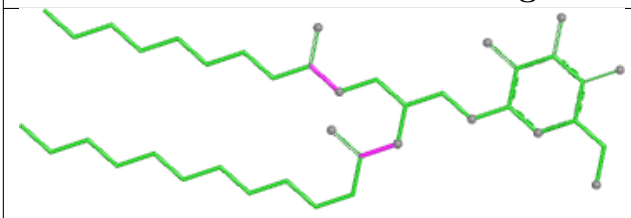


Rings

Ligand LMG A 860



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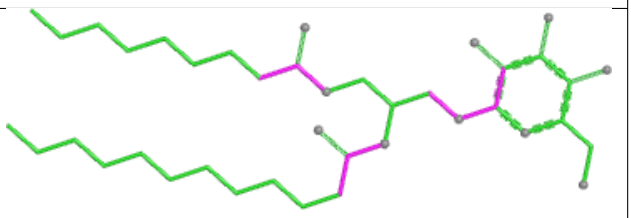
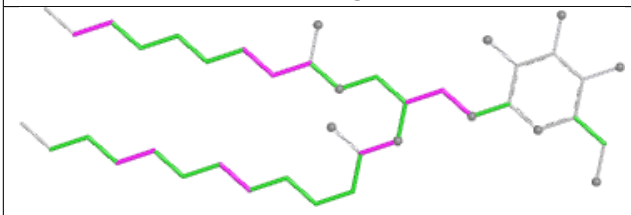


Bond angles



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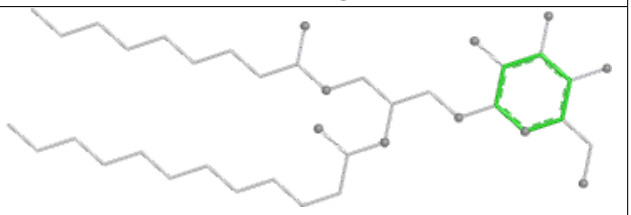
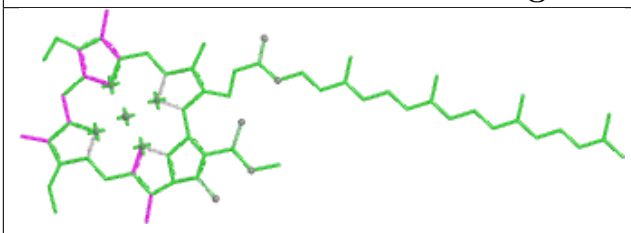


Rings

Ligand CLA 6 602



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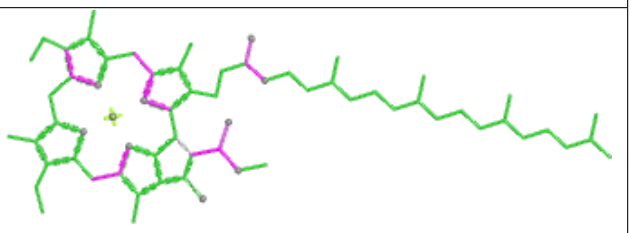

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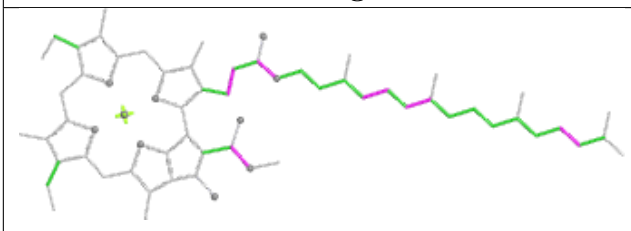
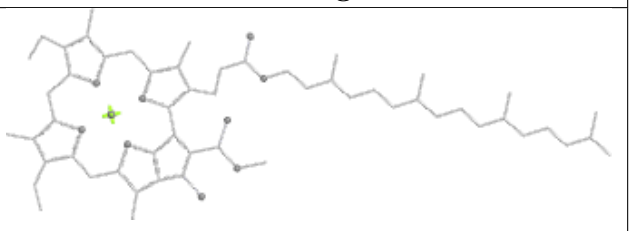
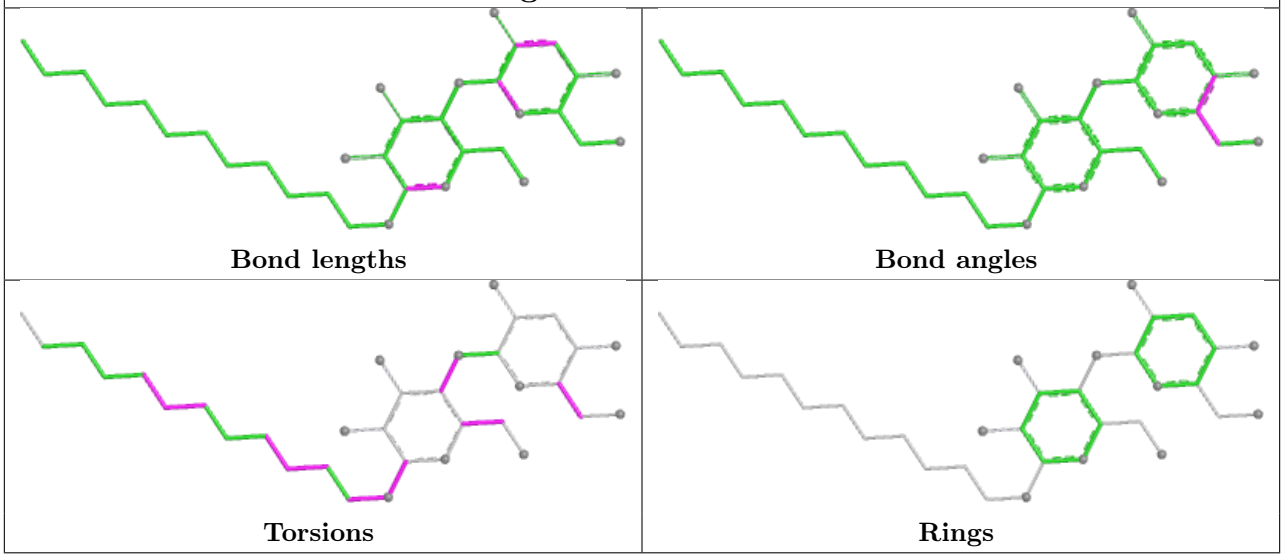


Torsions

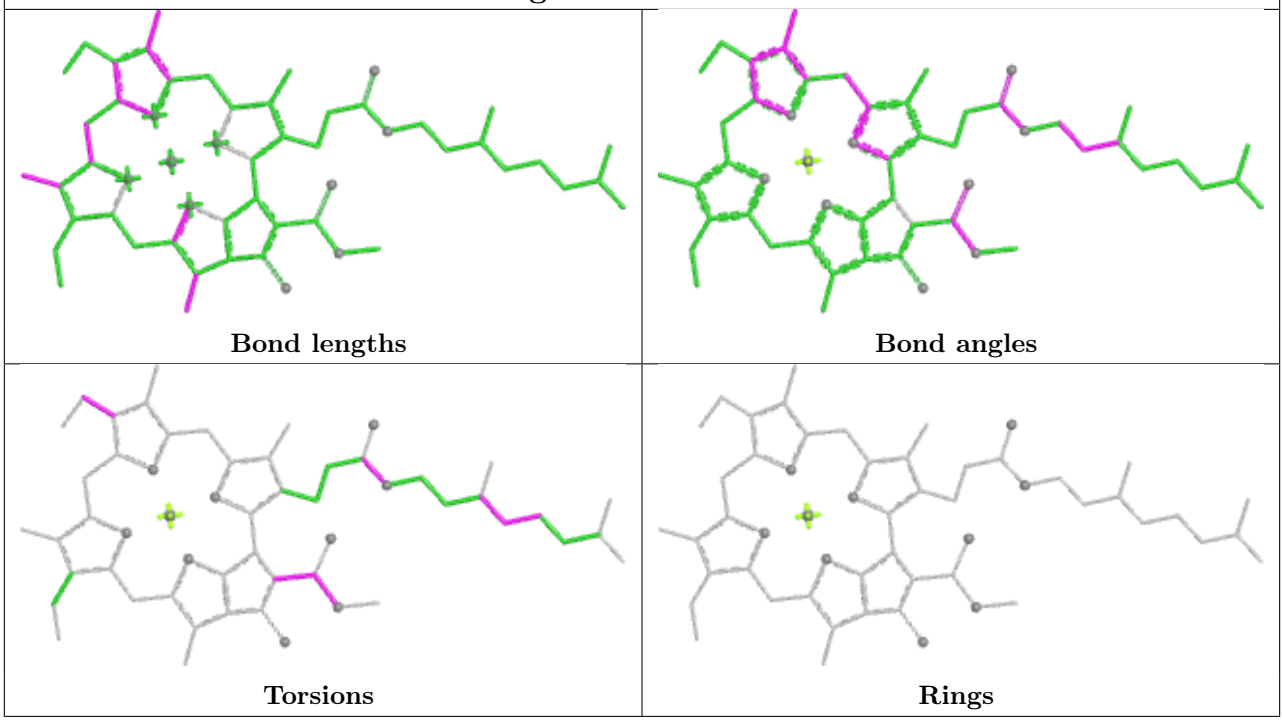


Rings

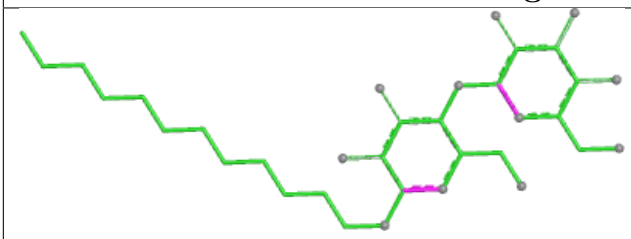
Ligand LMU A 858



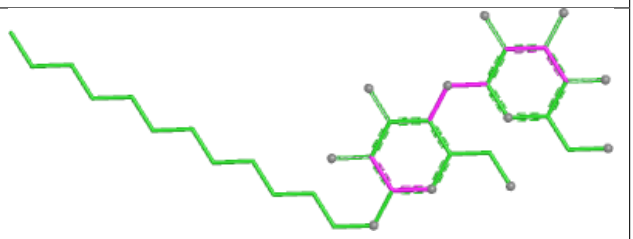
Ligand CLA 2 610



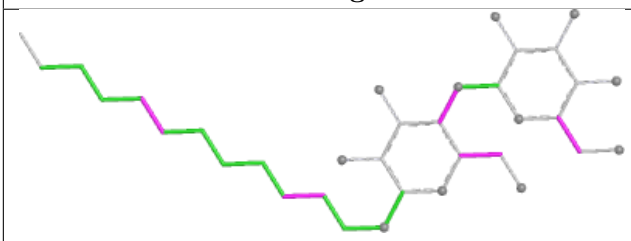
Ligand LMU 8 625



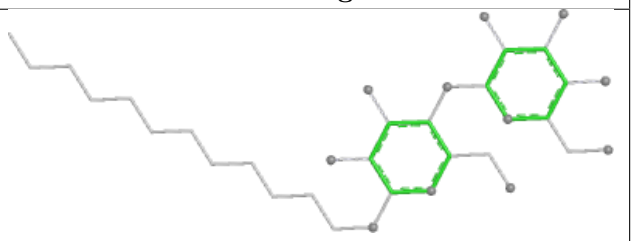
Bond lengths



Bond angles

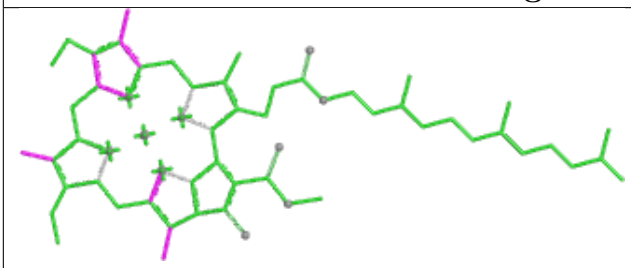


Torsions

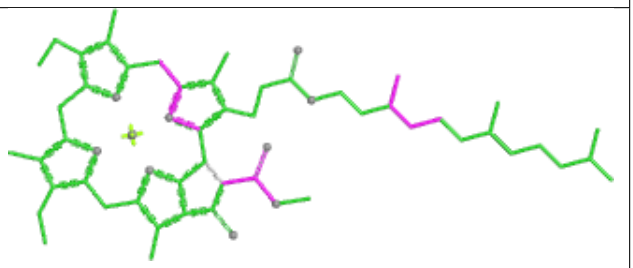


Rings

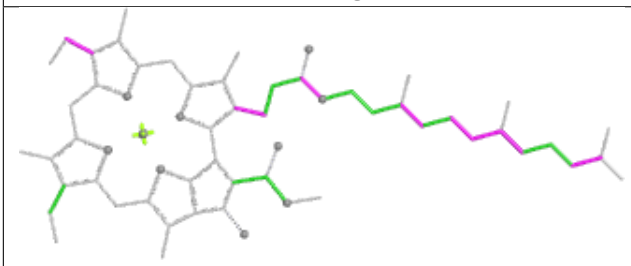
Ligand CLA B 818



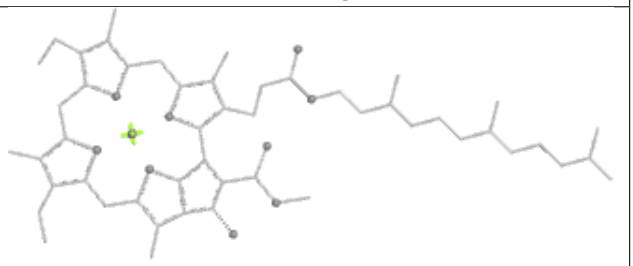
Bond lengths



Bond angles

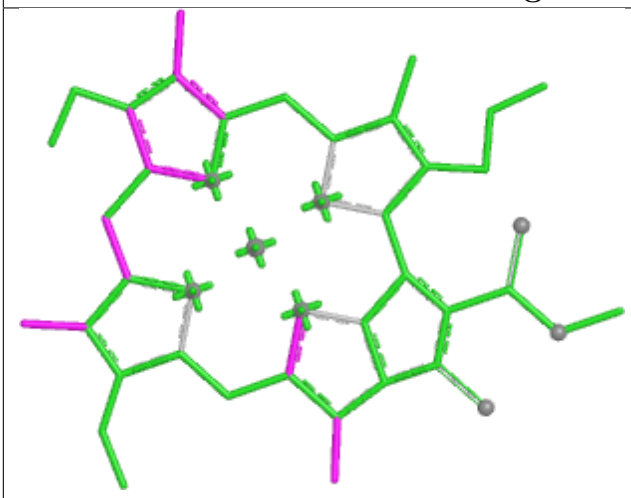


Torsions



Rings

Ligand CLA B 812



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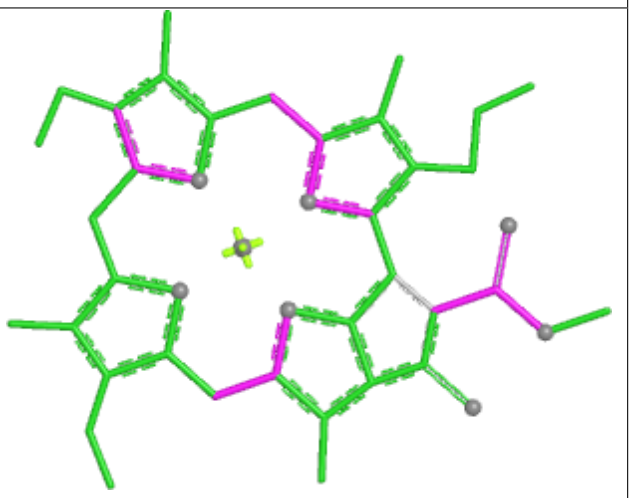
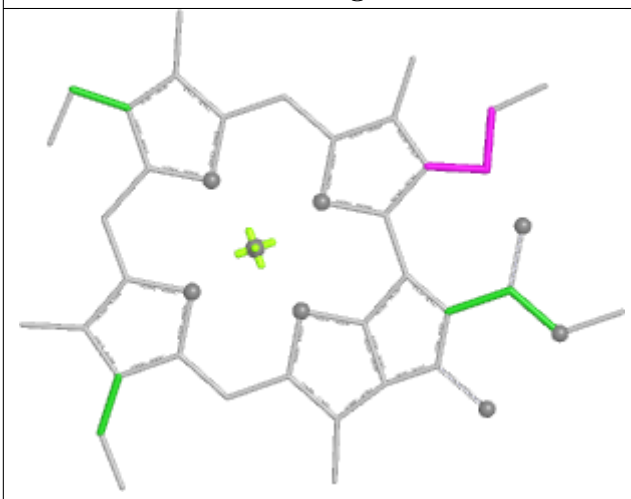
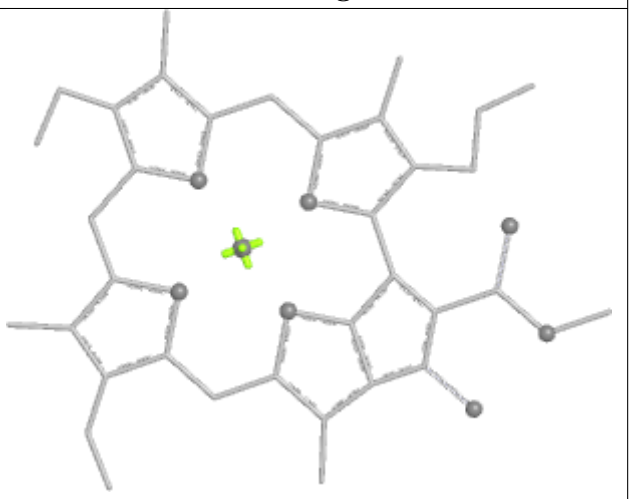


Bond angles

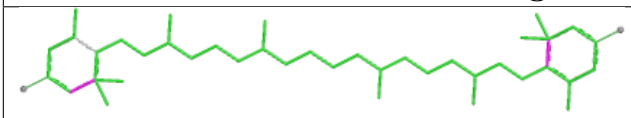


Torsions



Rings

Ligand LUT 2 619



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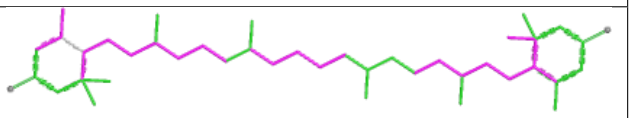
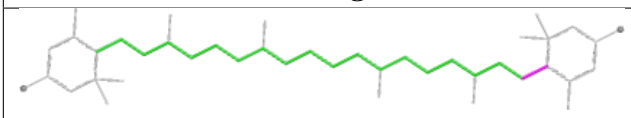


Bond angles



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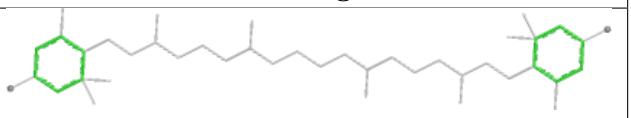
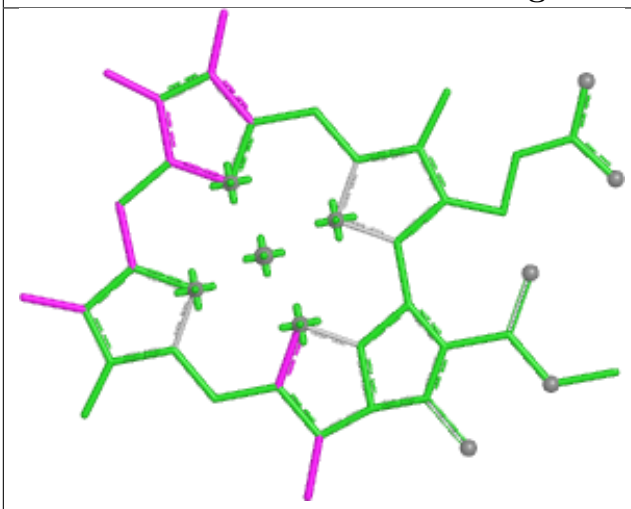


Rings

Ligand CLA 4 616



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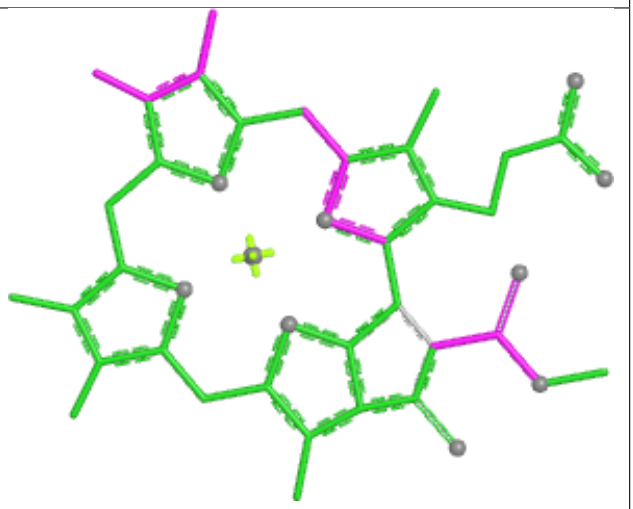
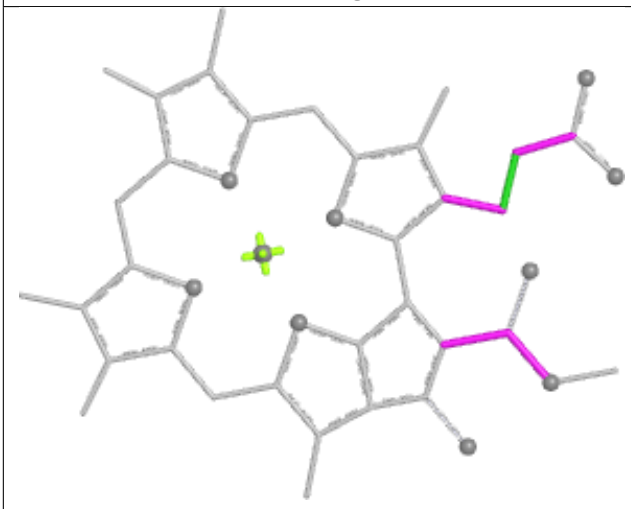


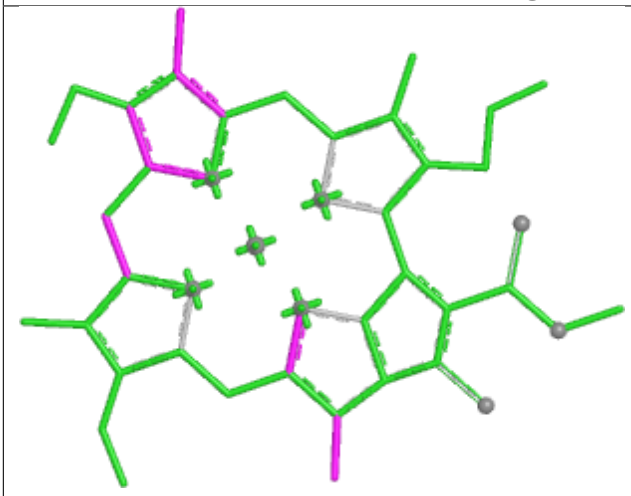
Bond angles



Torsions

Rings

Ligand CLA Y 611



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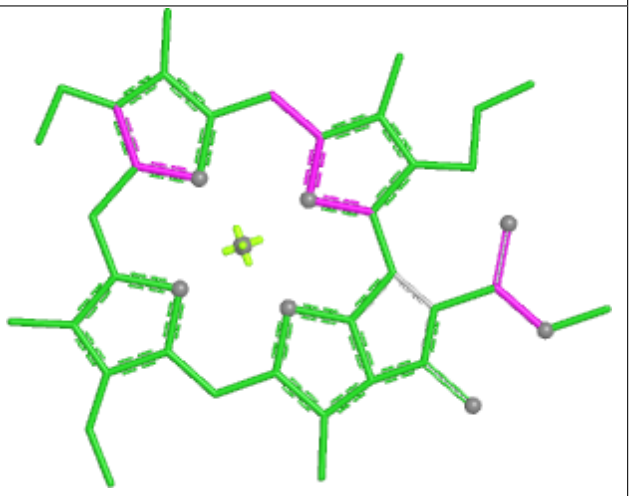
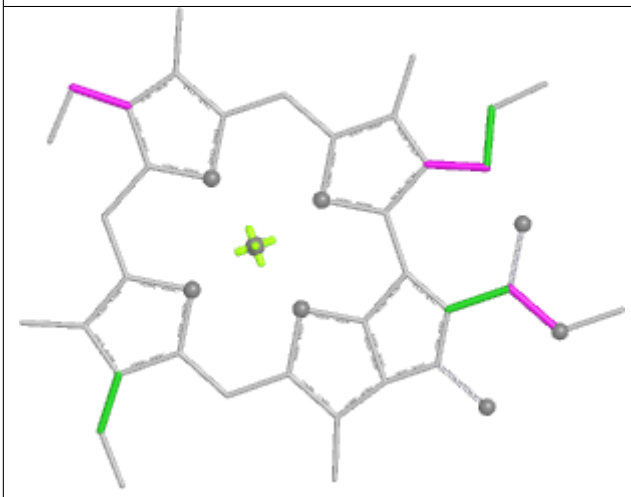


Bond angles



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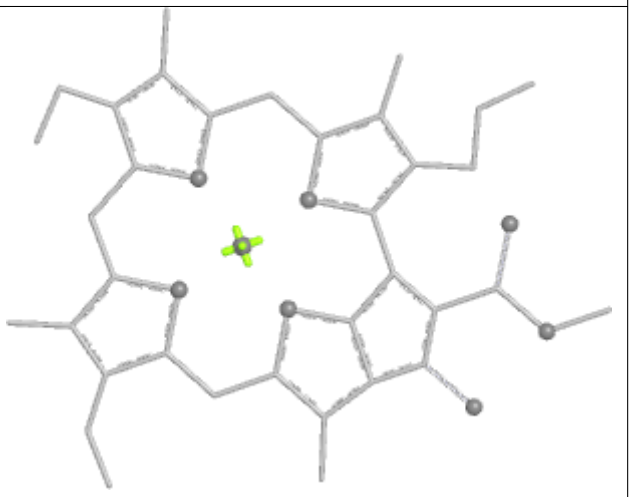
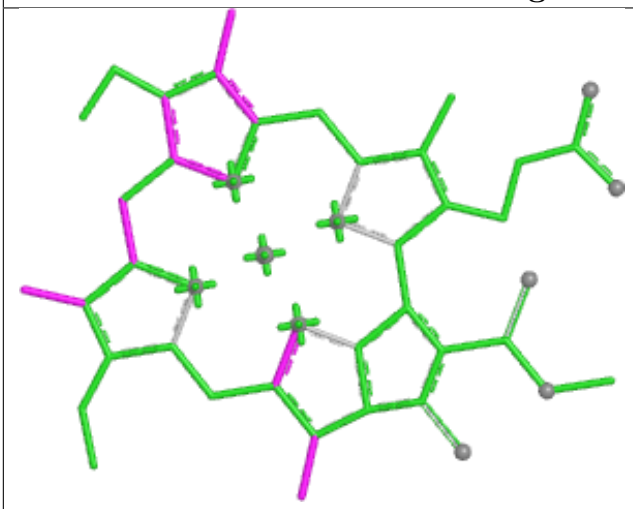


Rings

Ligand CLA 6 608



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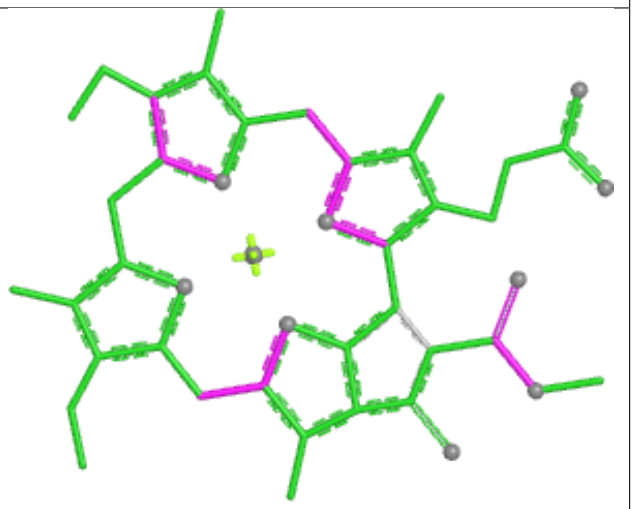
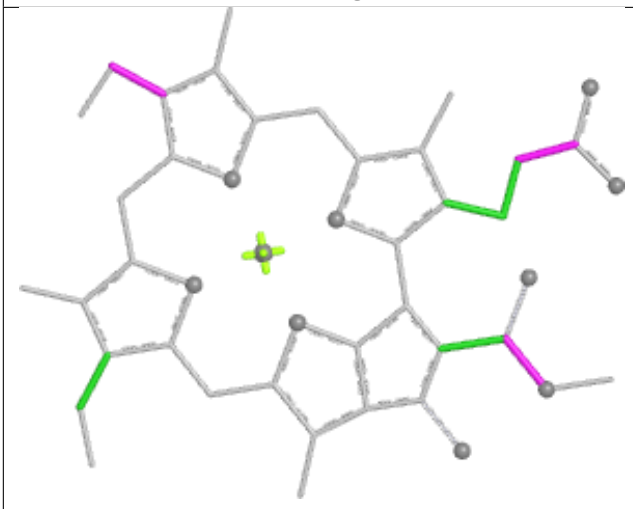


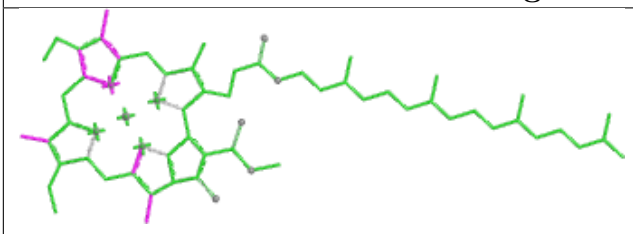
Bond angles



Torsions

Rings

Ligand CLA A 804



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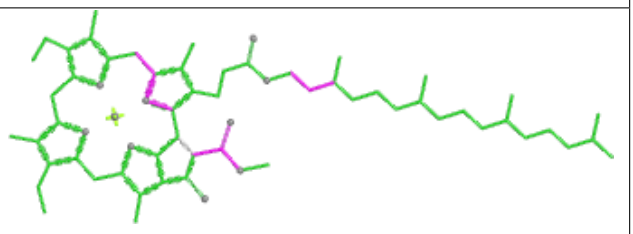
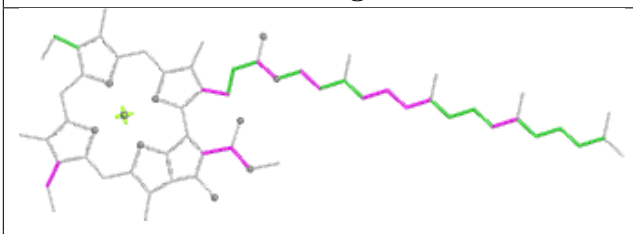
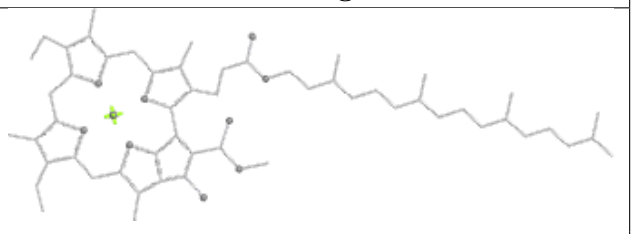


Bond angles

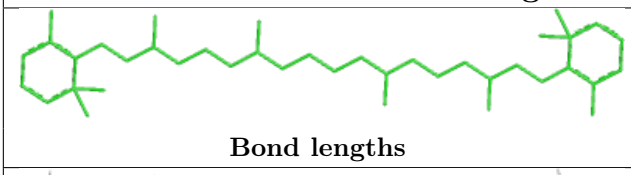


Torsions



Rings

Ligand BCR A 856



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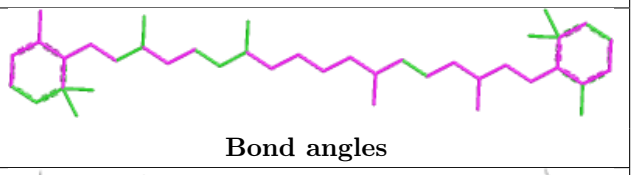
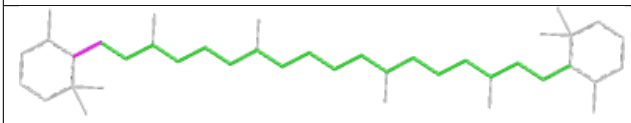


Bond angles



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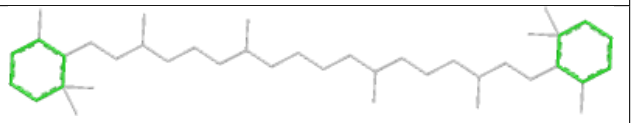
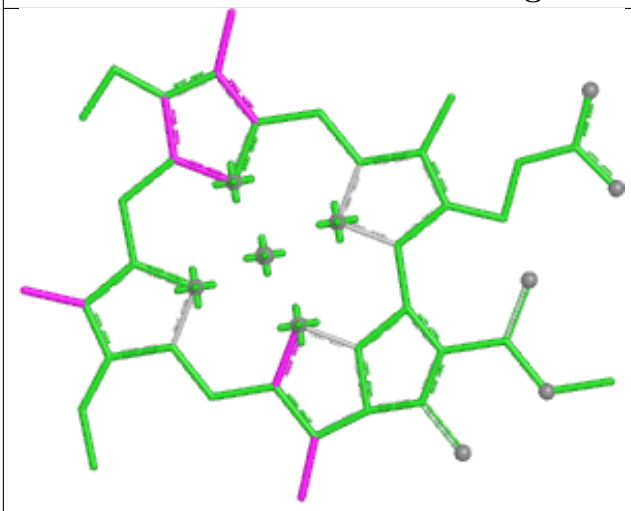


Rings

Ligand CLA B 835



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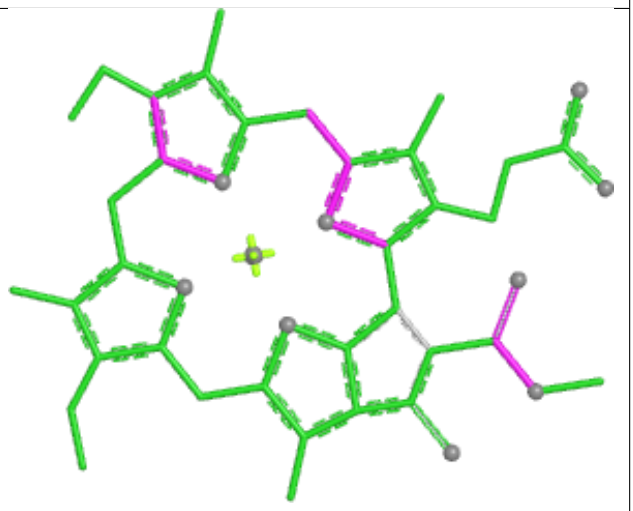
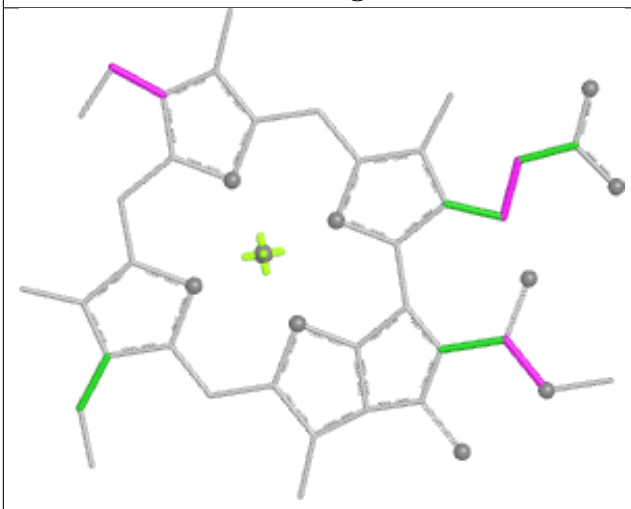


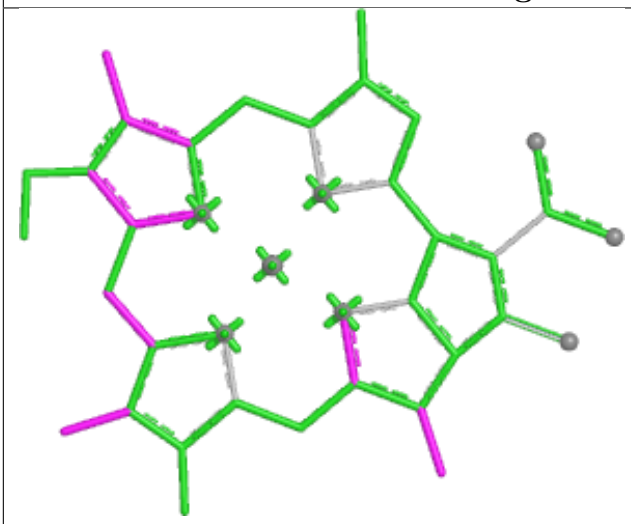
Bond angles



Torsions

Rings

Ligand CLA O 2001



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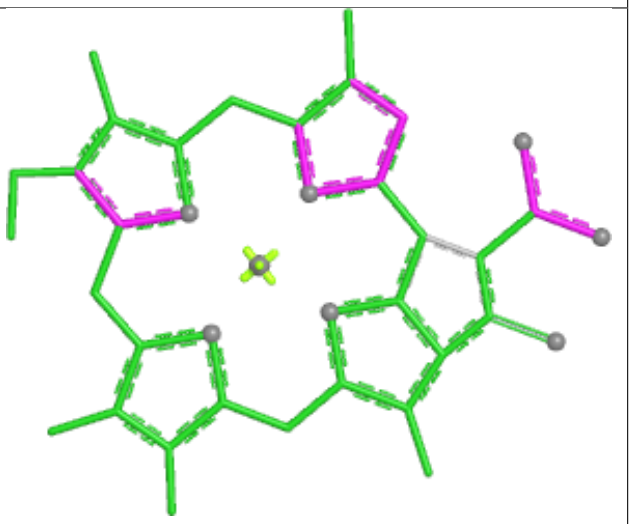
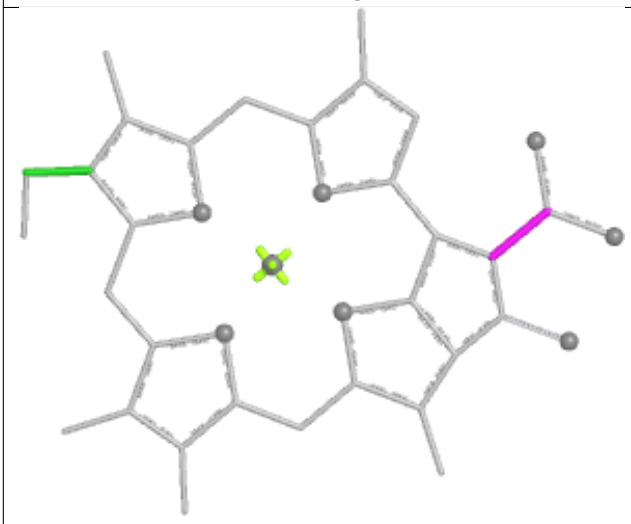
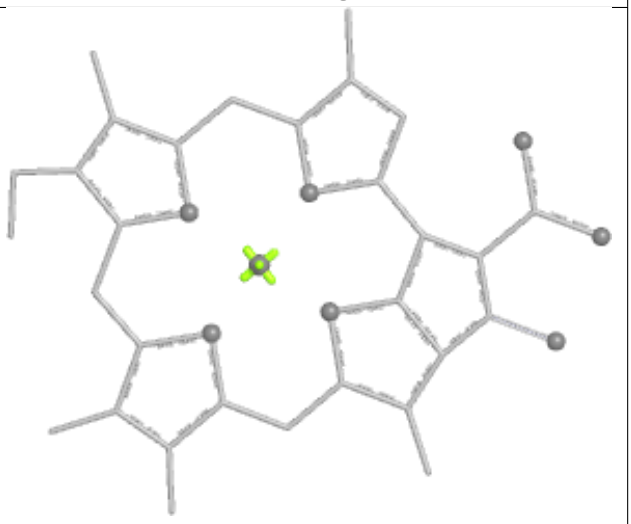


Bond angles

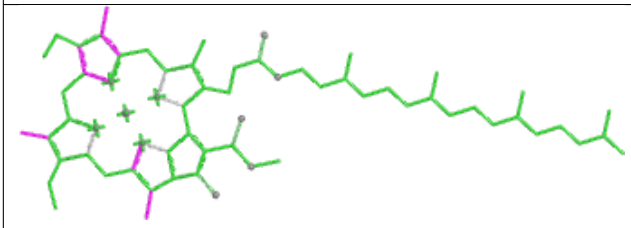


Torsions

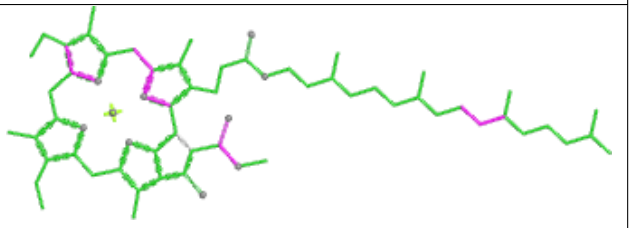


Rings

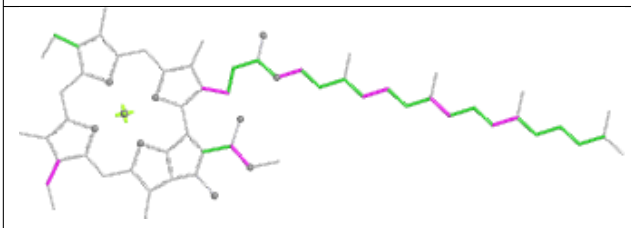
Ligand CLA 4 608



Bond lengths



Bond angles



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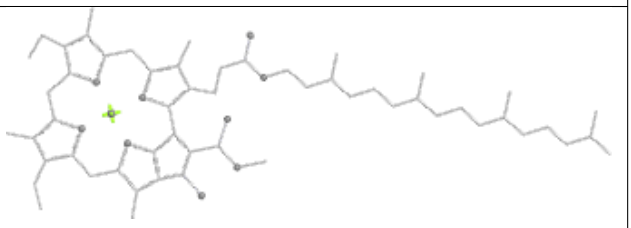
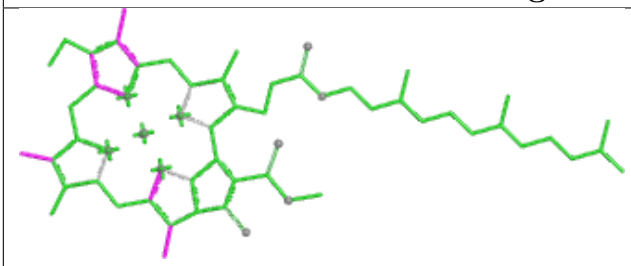
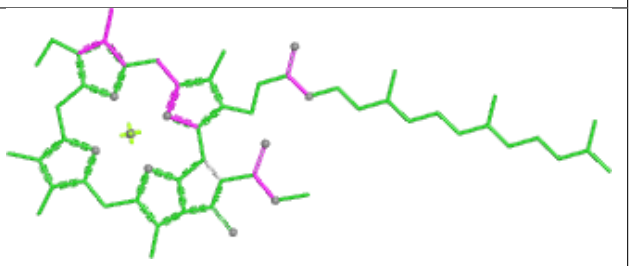


Rings

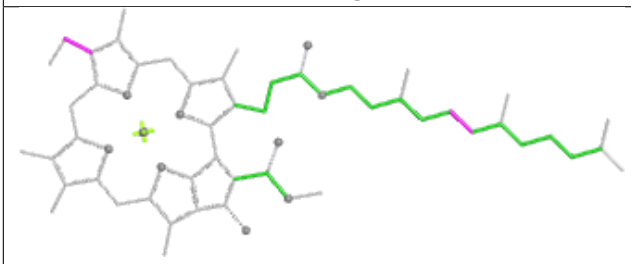
Ligand CLA a 610



Bond lengths



Bond angles



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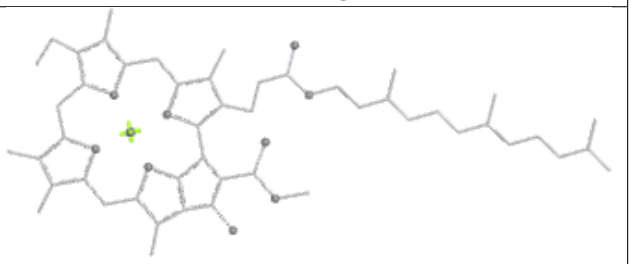
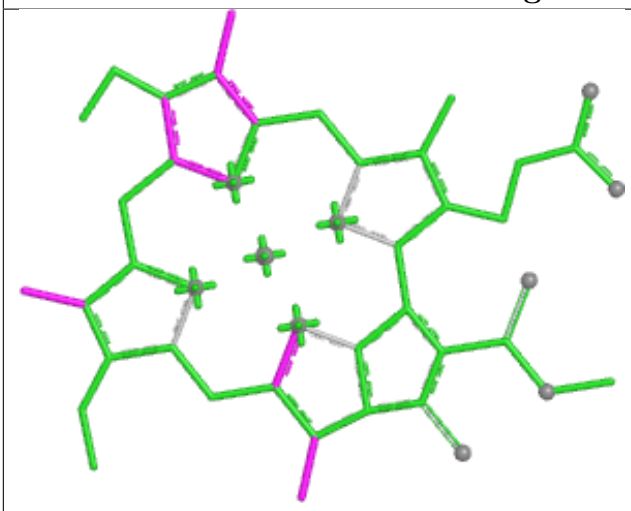
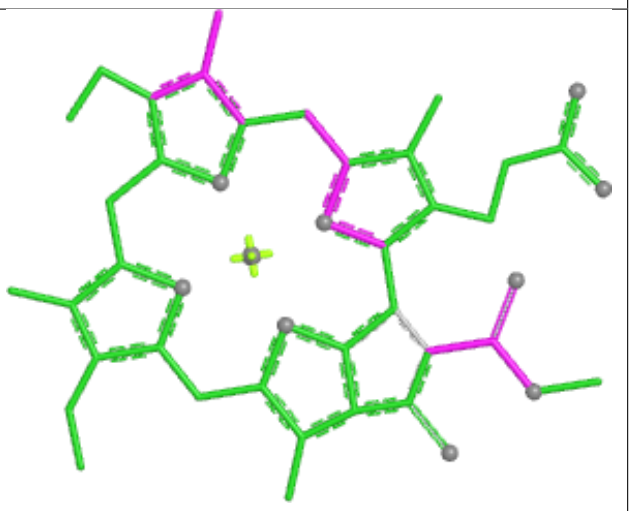


Rings

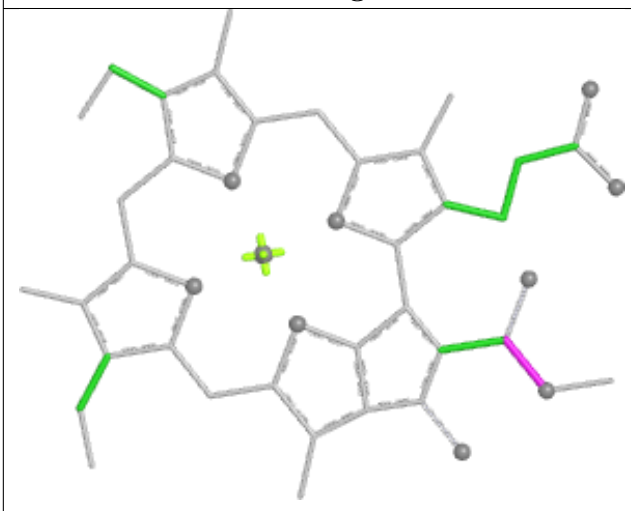
Ligand CLA A 817



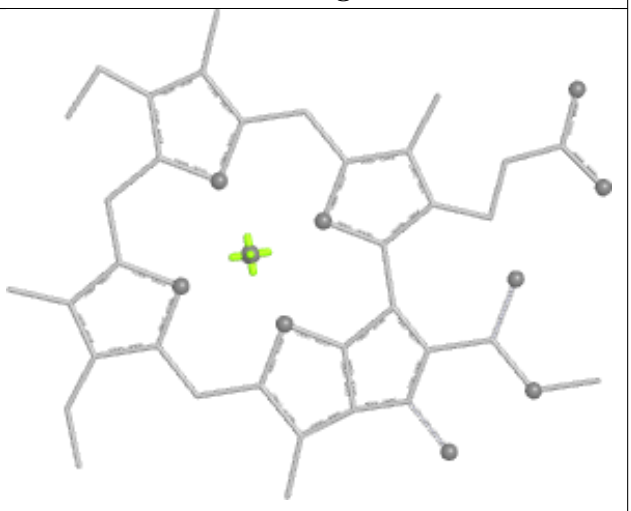
Bond lengths



Bond angles

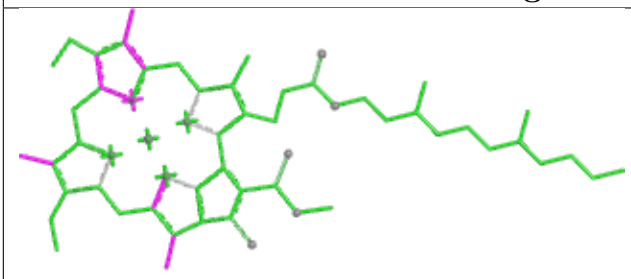


Torsions

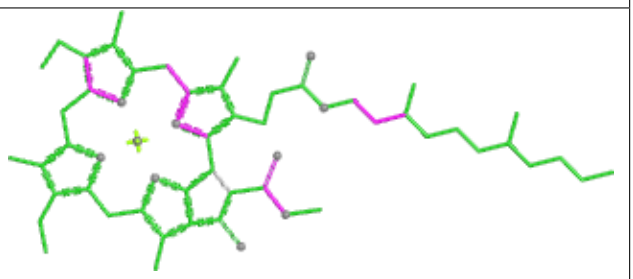


Rings

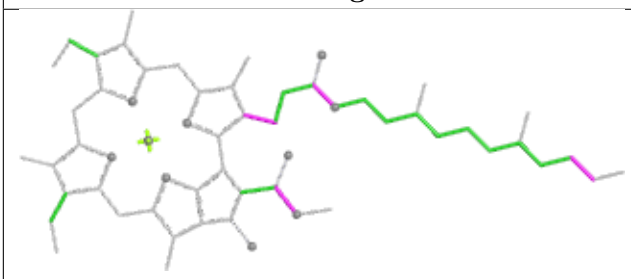
Ligand CLA A 827



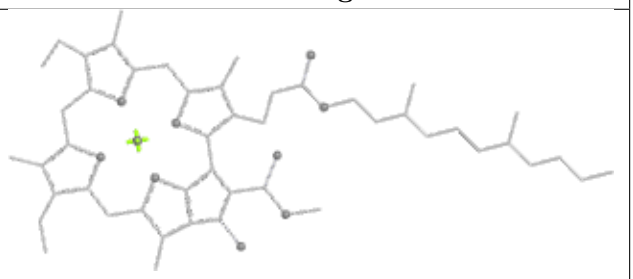
Bond lengths



Bond angles

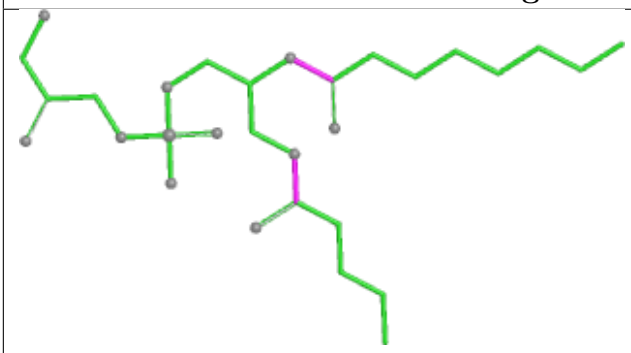


Torsions



Rings

Ligand LHG A 847



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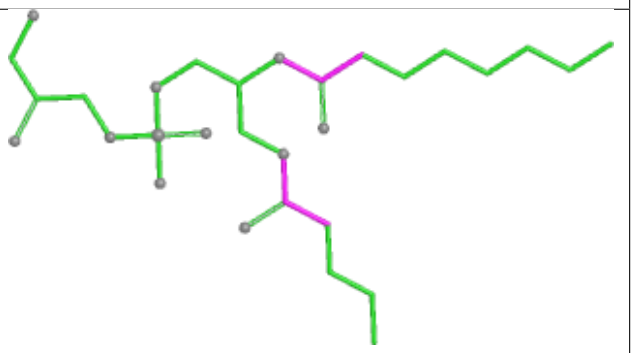
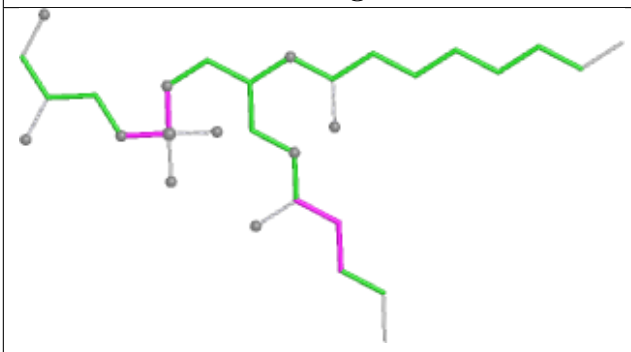
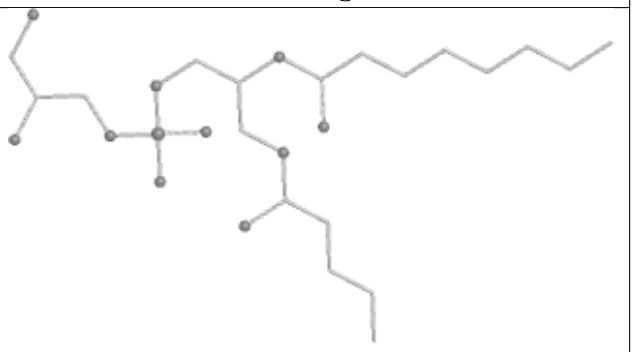


Bond angles

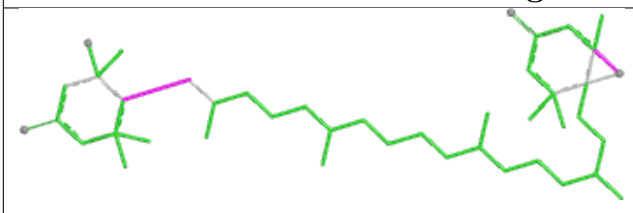


Torsions



Rings

Ligand NEX 5 624



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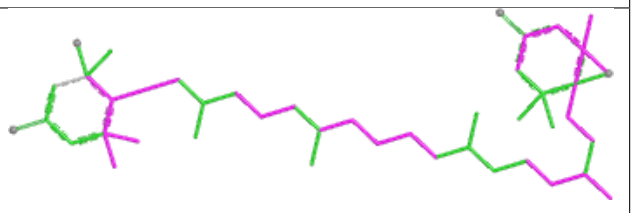
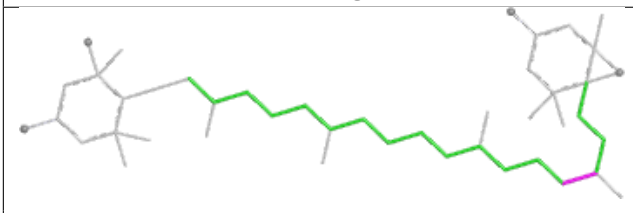


Bond angles



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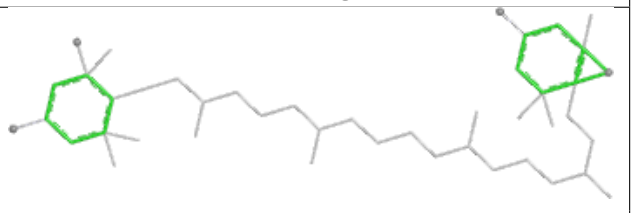
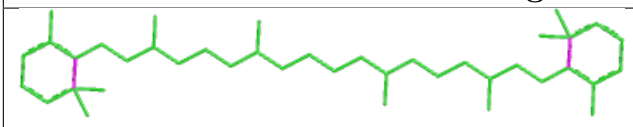


Rings

Ligand BCR 3 621



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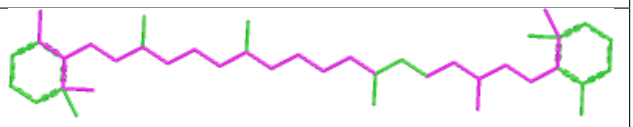
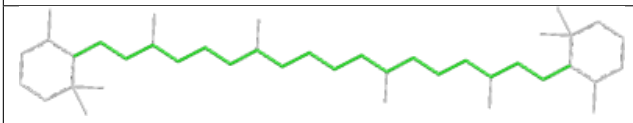


Bond angles



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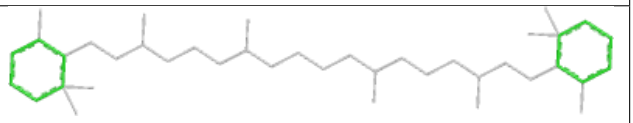
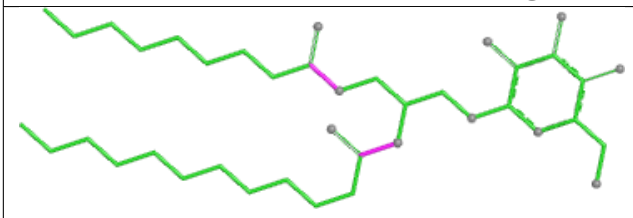


Rings

Ligand LMG J 104



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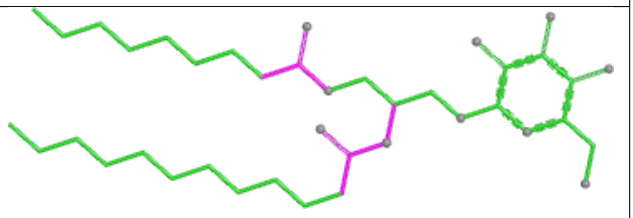
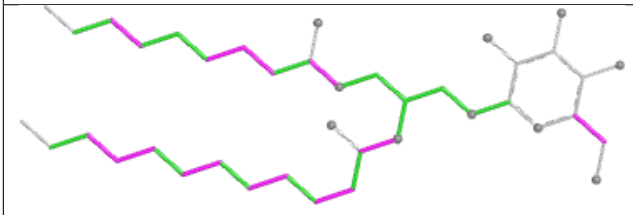


Bond angles



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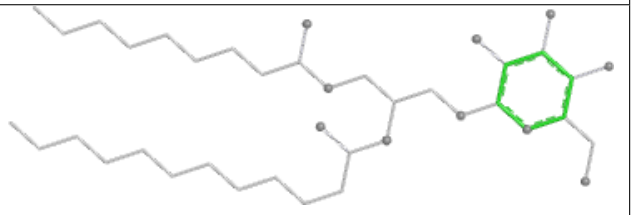
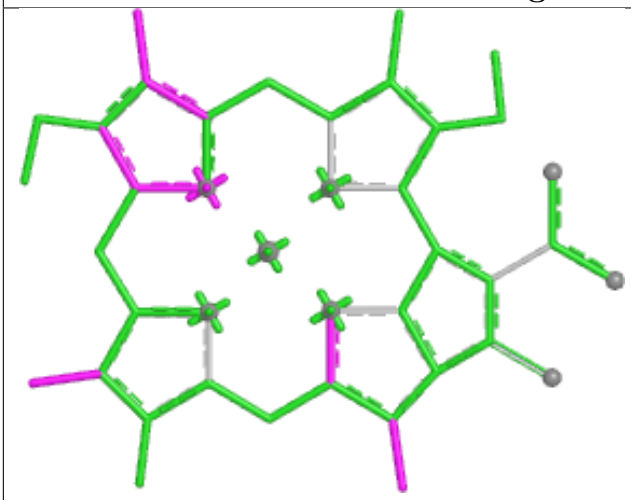


Rings

Ligand CLA 5 606



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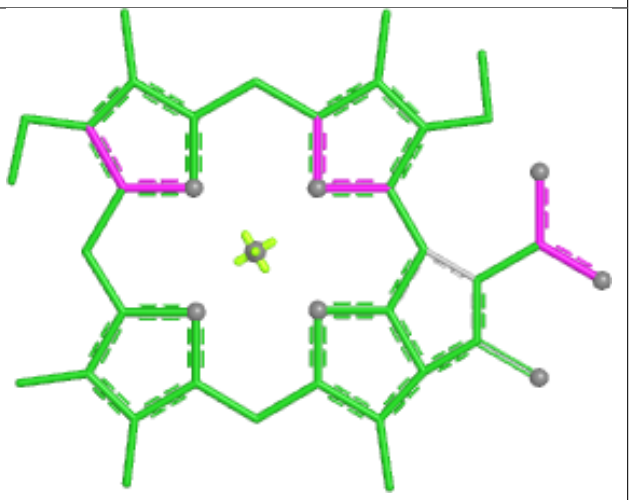
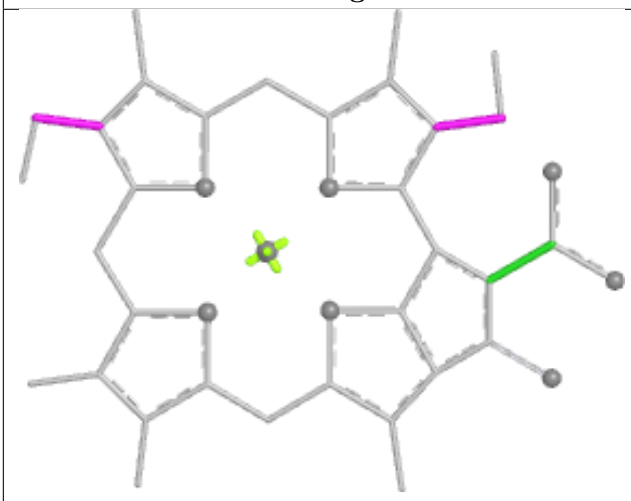
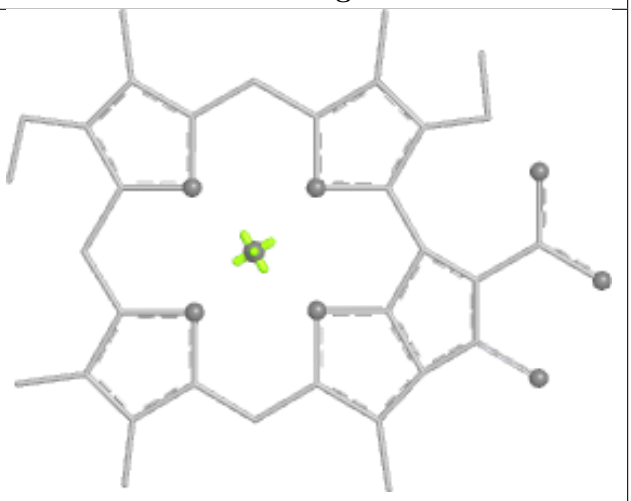


Bond angles

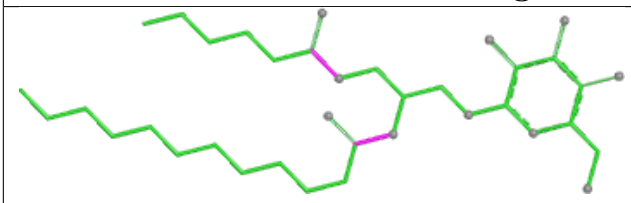


Torsions



Rings

Ligand LMG L 2631



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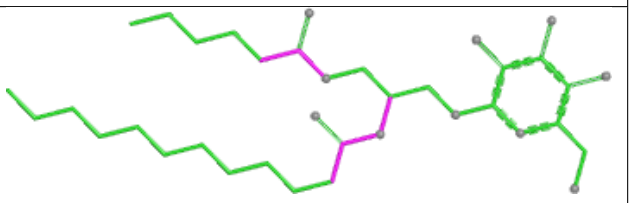
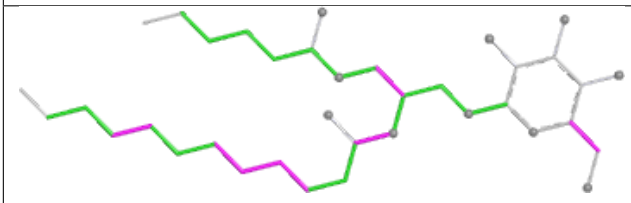


Bond angles



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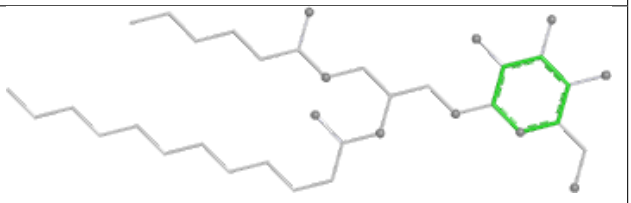
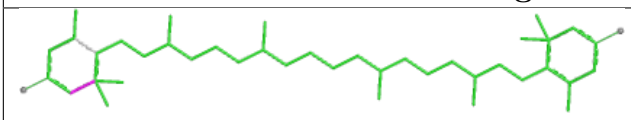


Rings

Ligand LUT U 1620



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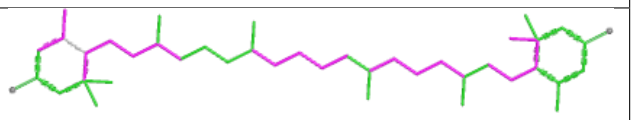
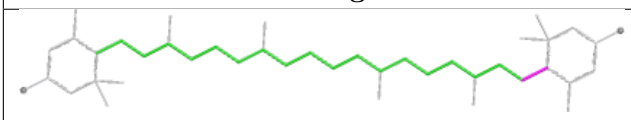
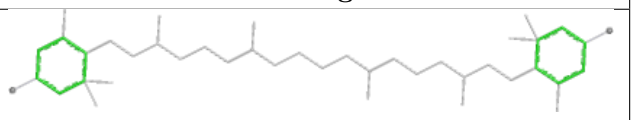


Bond angles

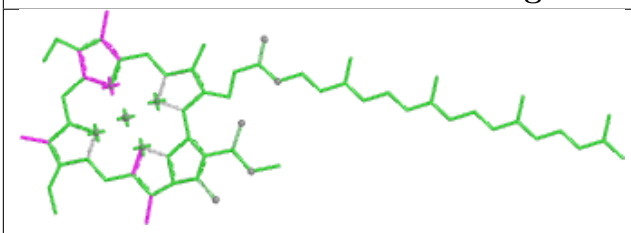


Torsions



Rings

Ligand CLA B 824



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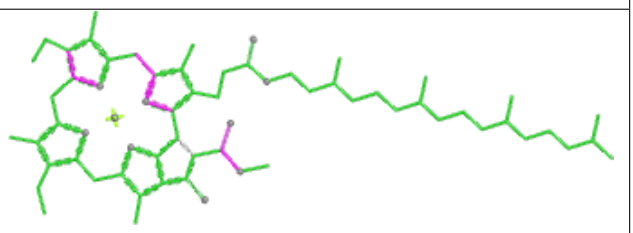
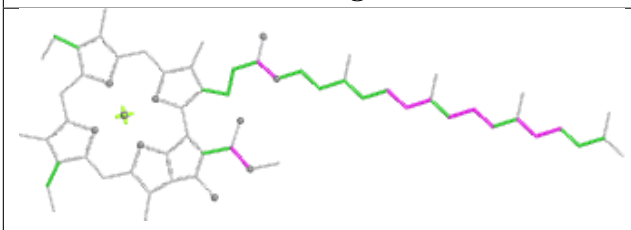


Bond angles



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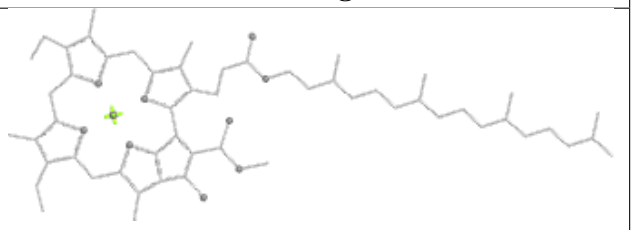
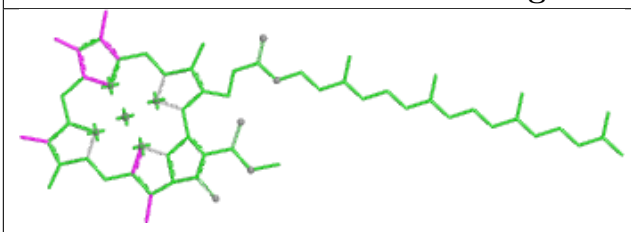


Rings

Ligand CLA 5 604



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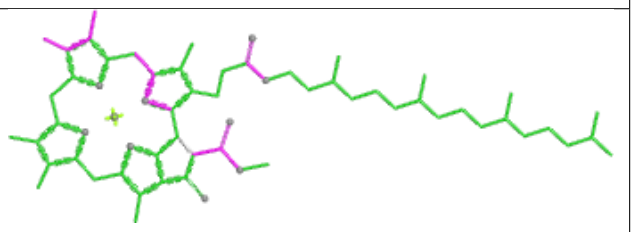
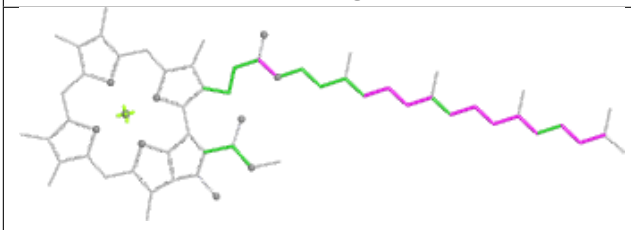


Bond angles



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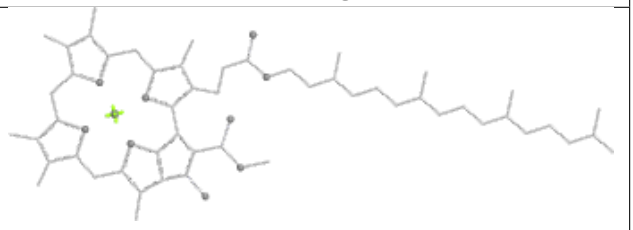
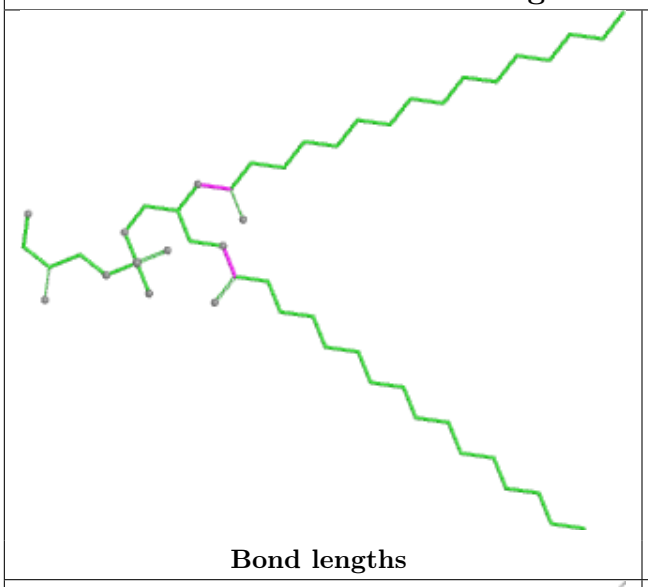


Rings

Ligand LHG 9 624



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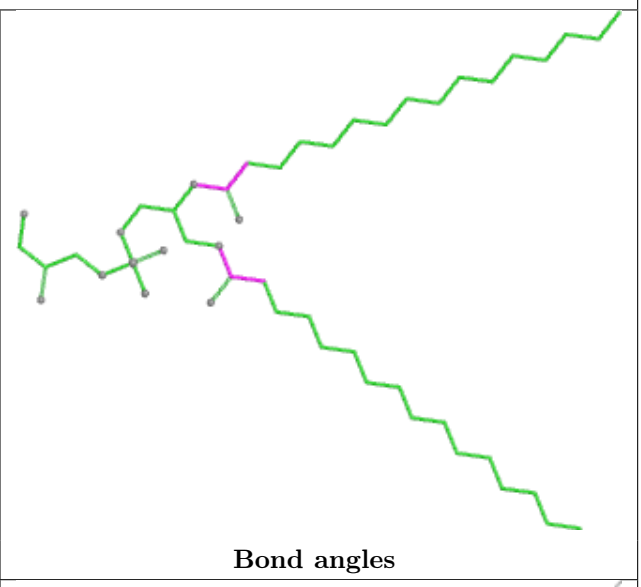
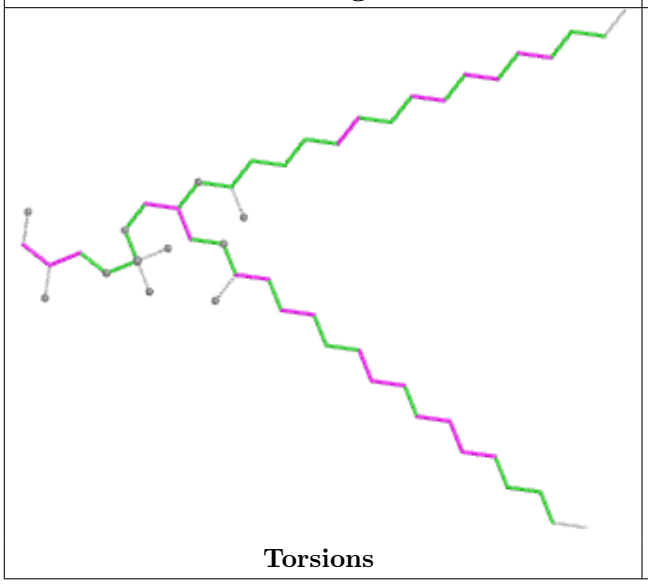


Bond angles



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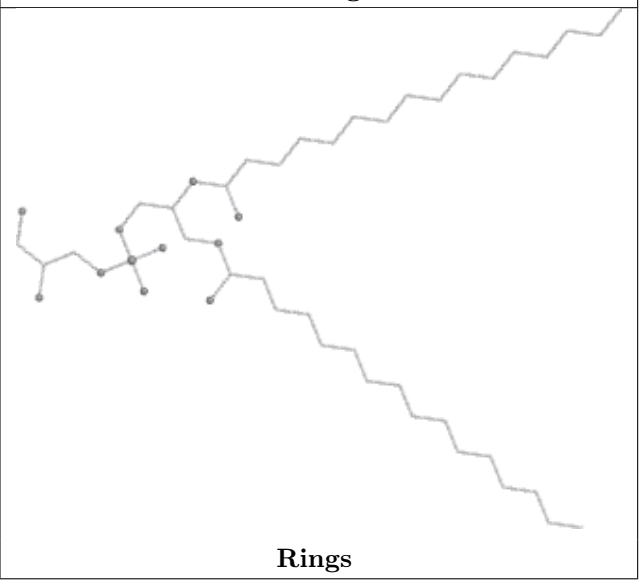
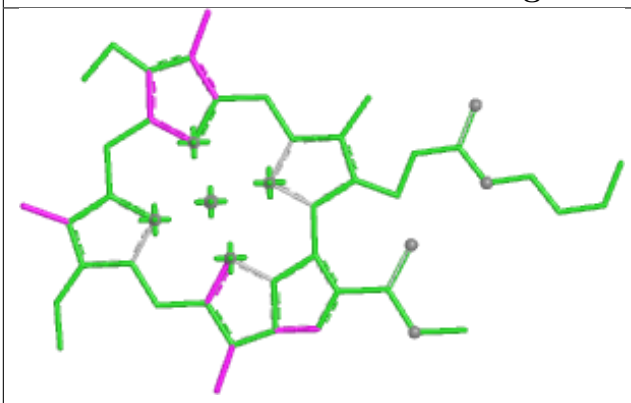


Rings

Ligand CLA U 604



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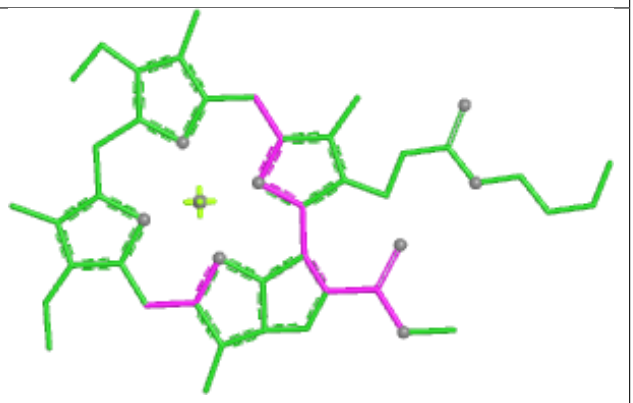
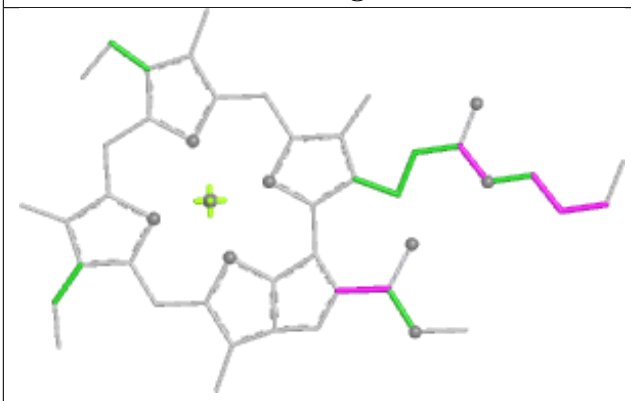


Bond angles



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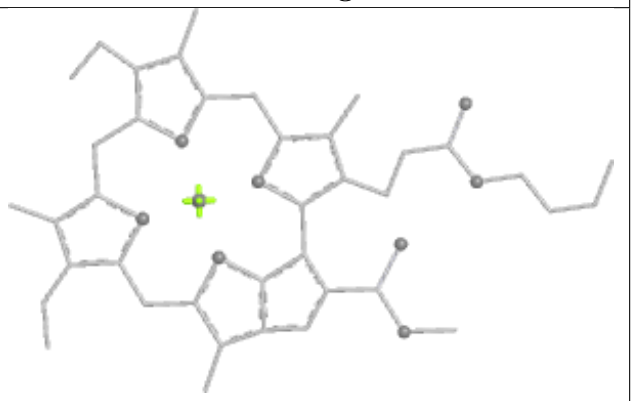
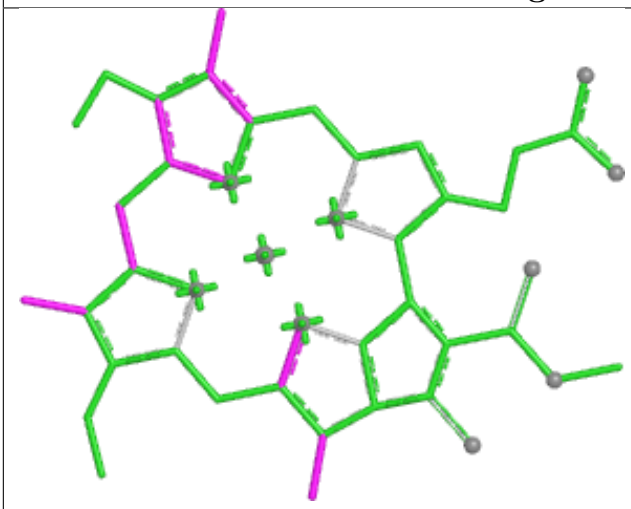


Rings

Ligand CLA 5 614



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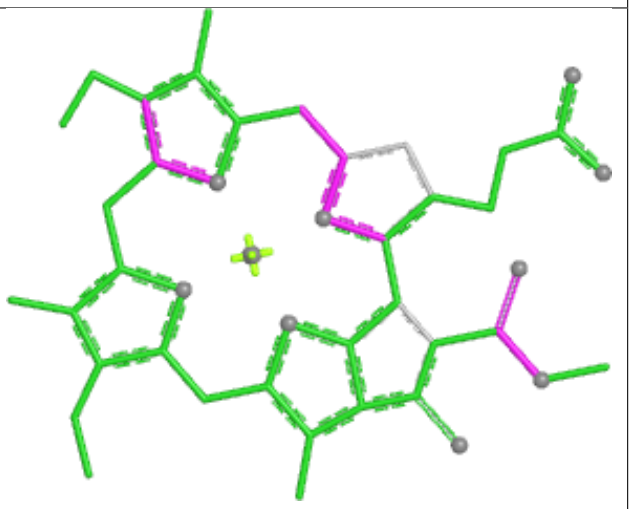
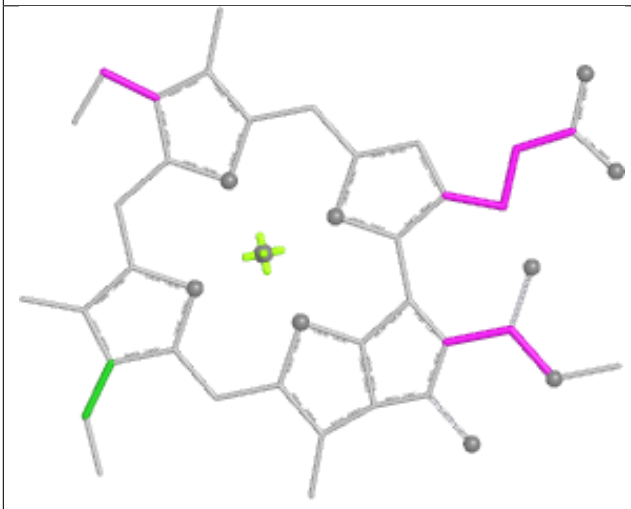


Bond angles



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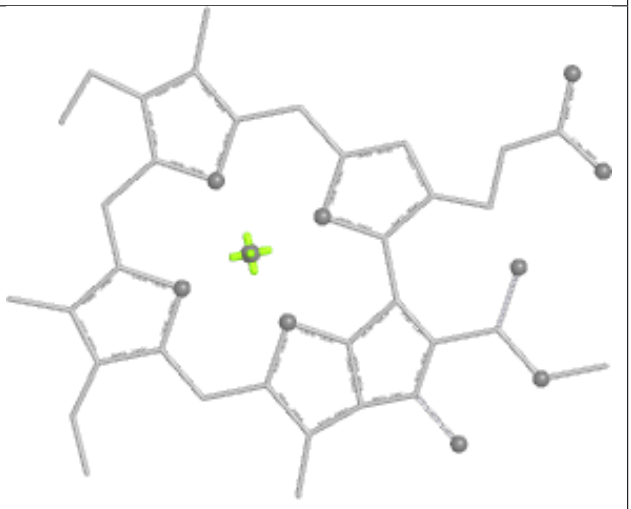
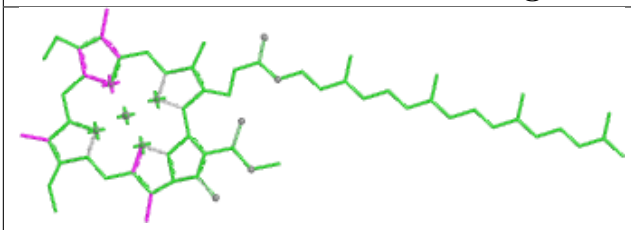
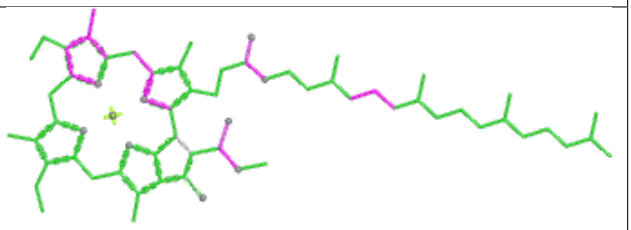


Rings

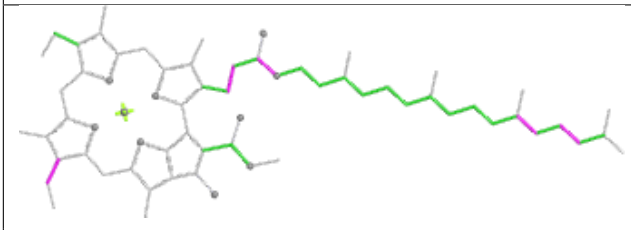
Ligand CLA A 822



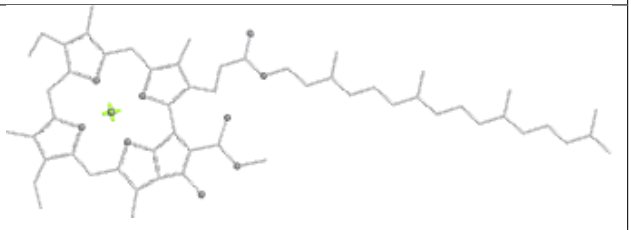
Bond lengths



Bond angles

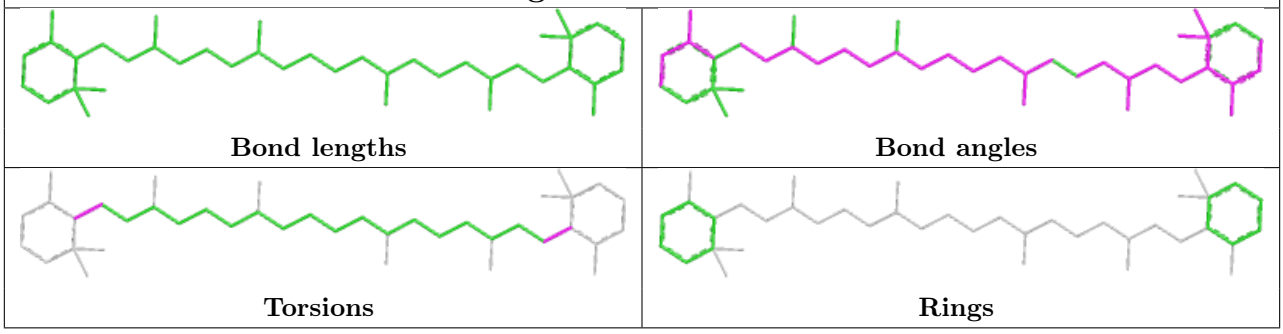


Torsions

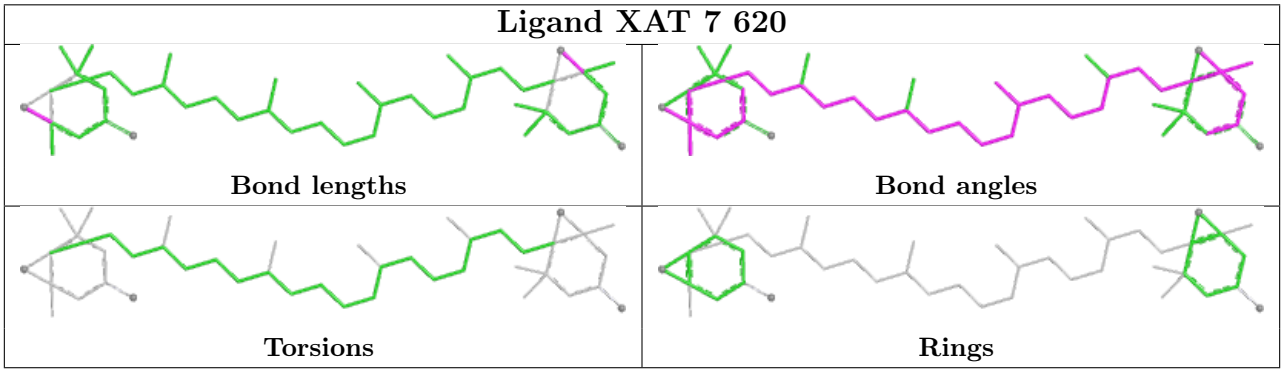


Rings

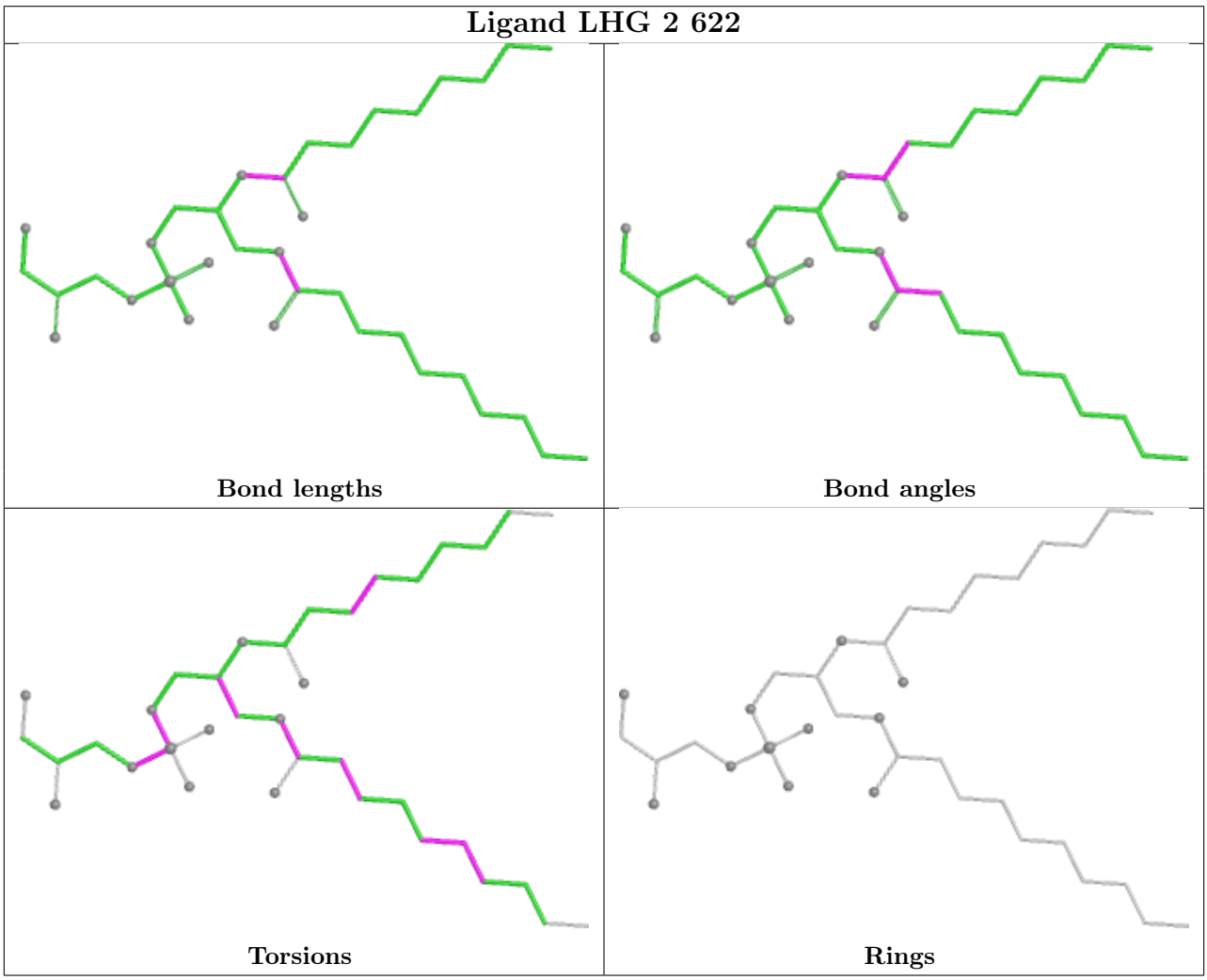
Ligand BCR a 619



Ligand XAT 7 620



Ligand LHG 2 622



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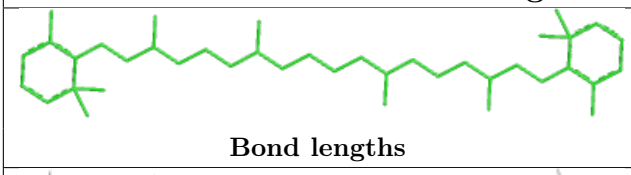
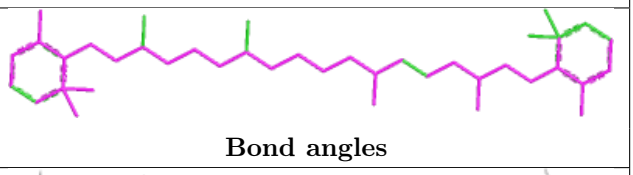
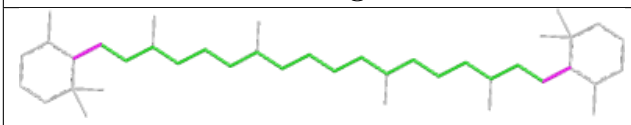


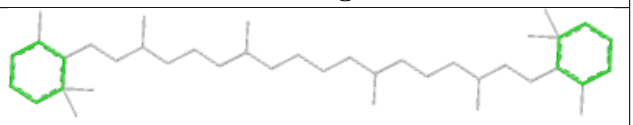
Bond lengths



Bond angles

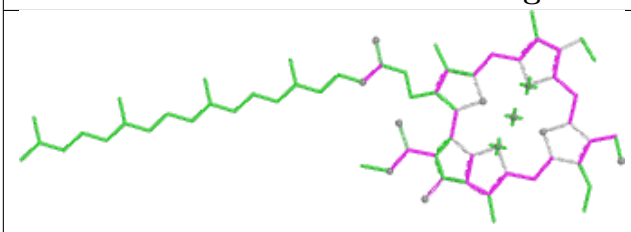


Torsions



Rings

Ligand CHL Y 609



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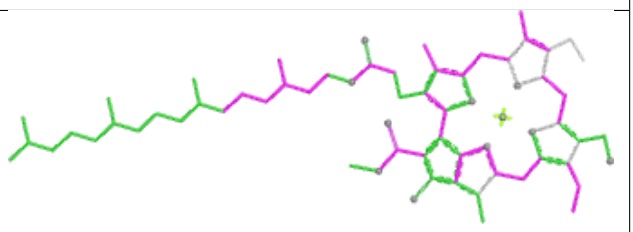
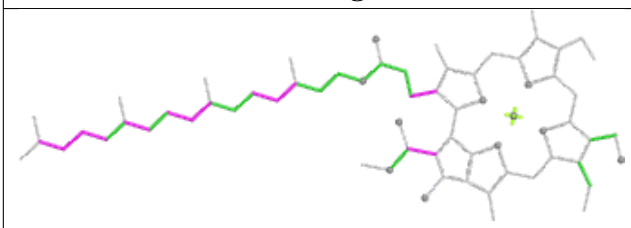


Bond angles



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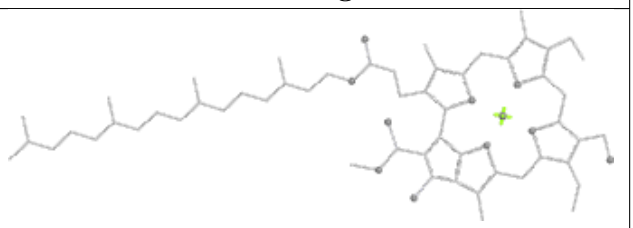
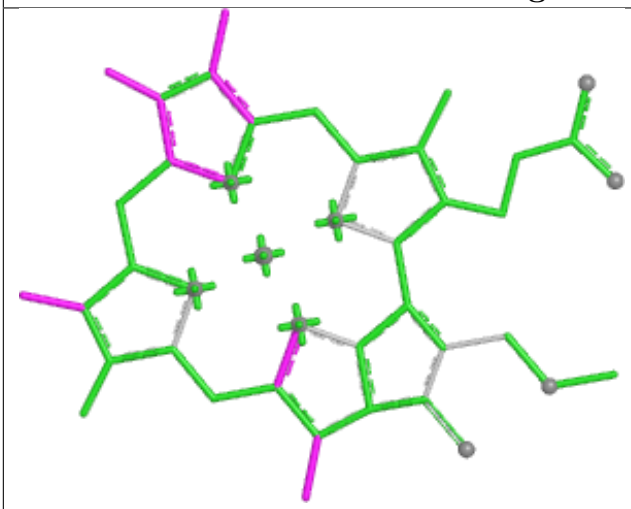


Rings

Ligand CLA 5 616



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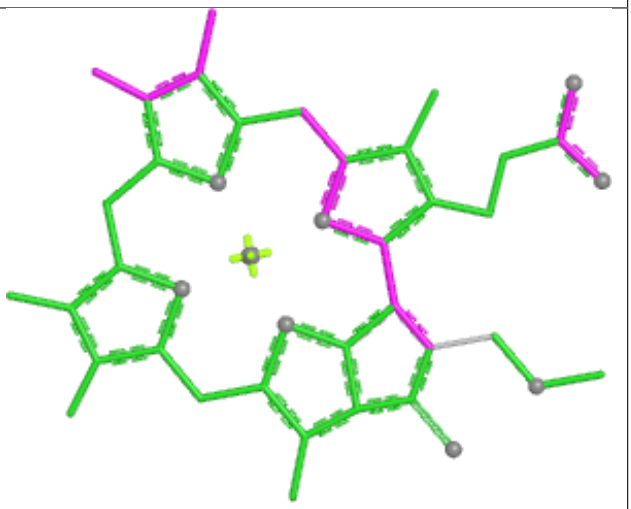
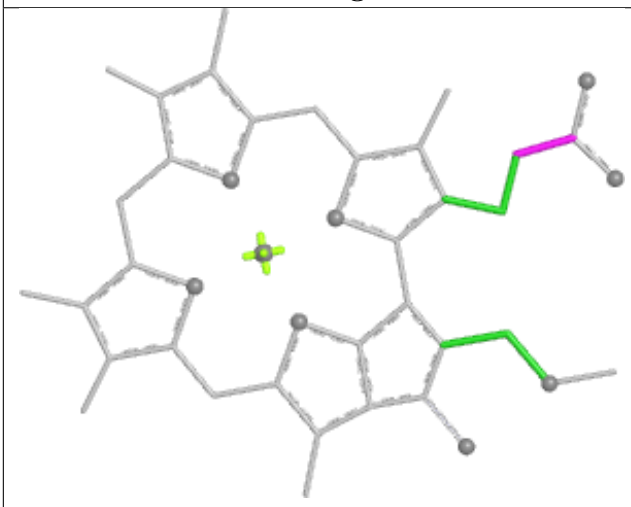


Bond angles



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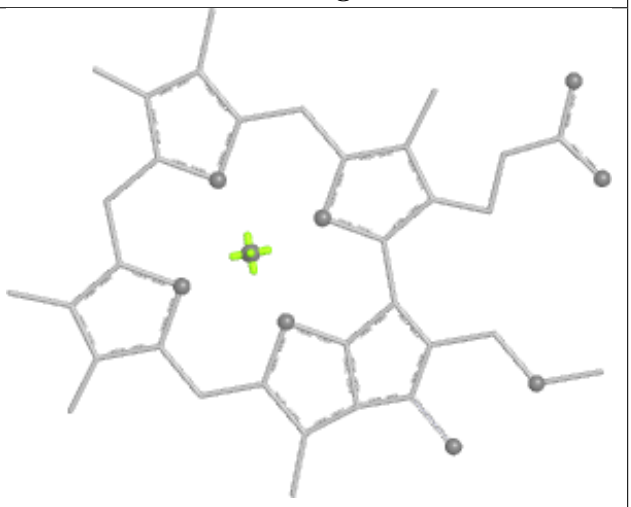
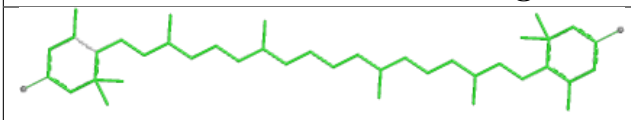


Rings

Ligand LUT Y 1621



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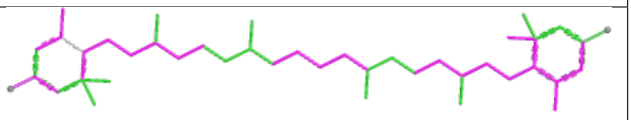
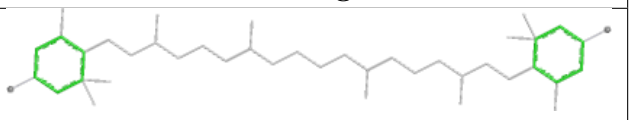


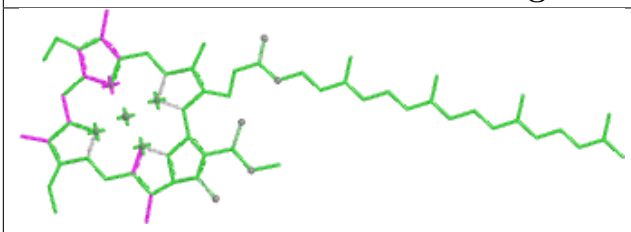
Bond angles

Torsions



Rings

Ligand CLA 5 607



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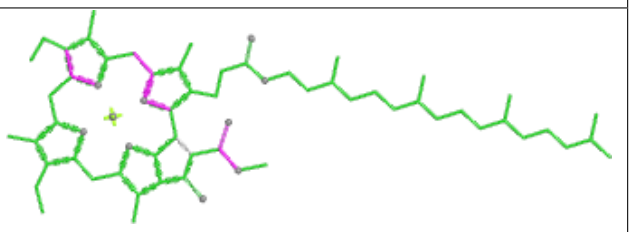
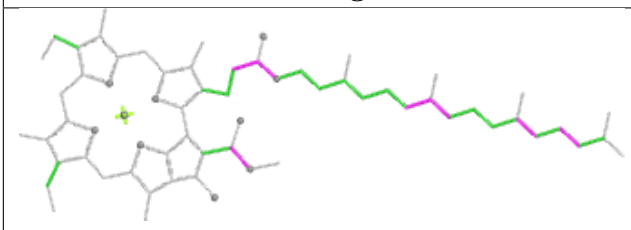


Bond angles



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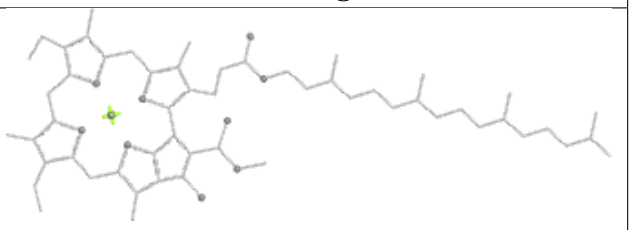
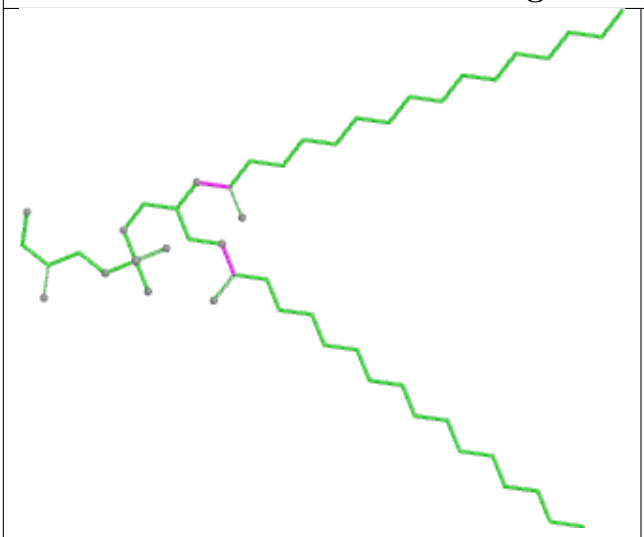


Rings

Ligand LHG 1 620



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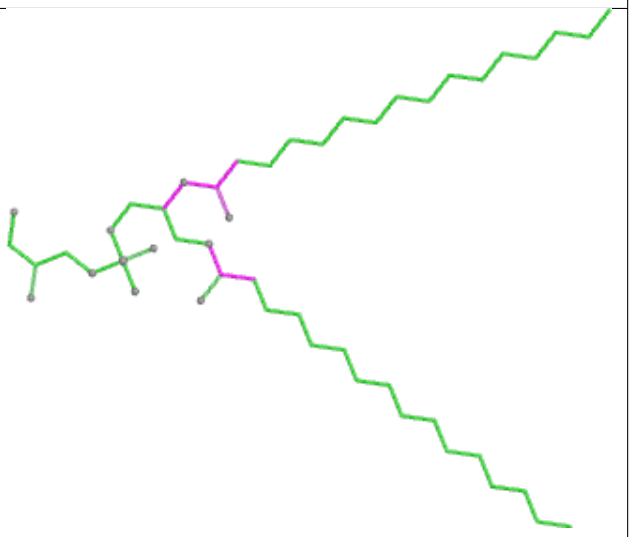

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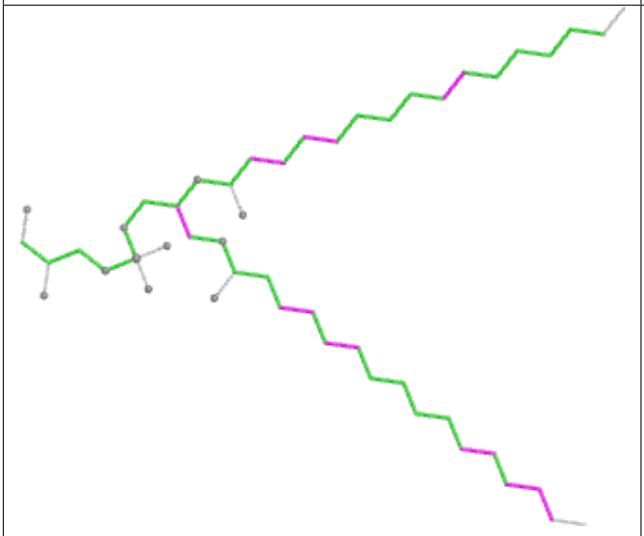

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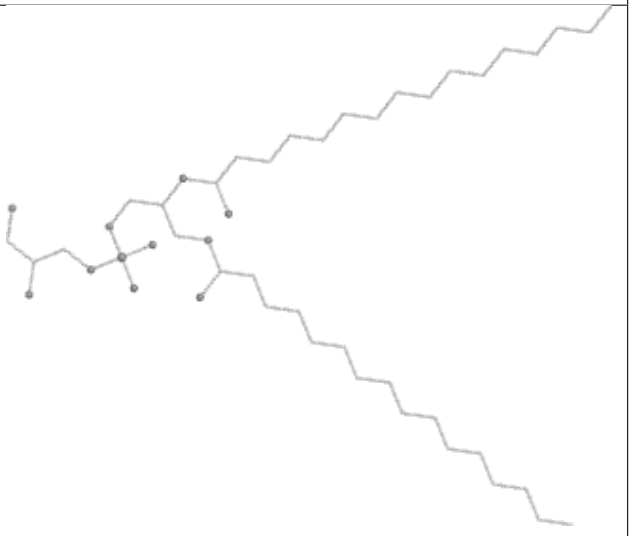
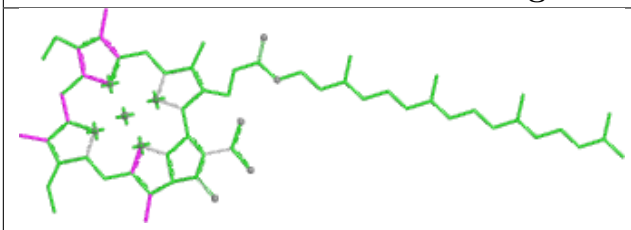


Rings

Ligand CLA 6 613



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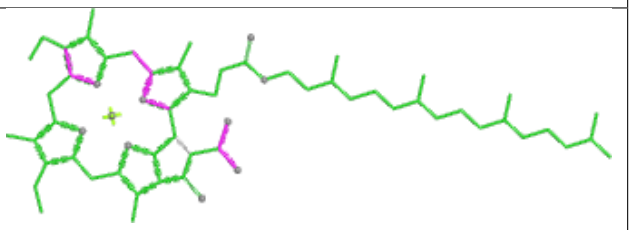
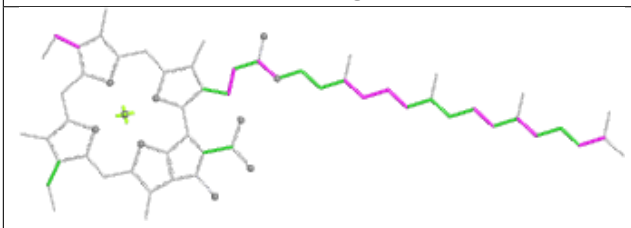
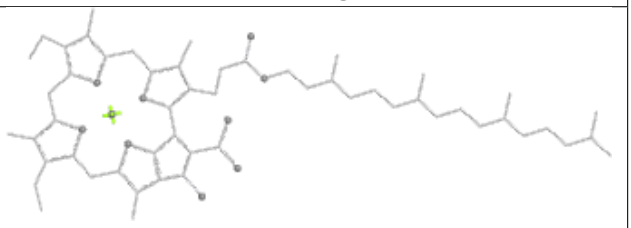


Bond angles

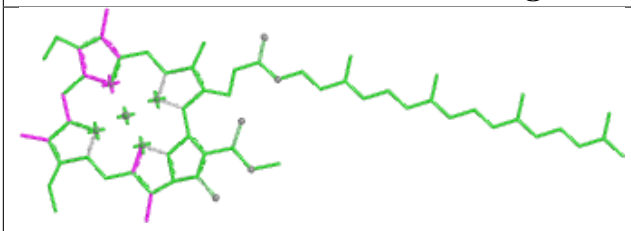


Torsions



Rings

Ligand CLA B 813



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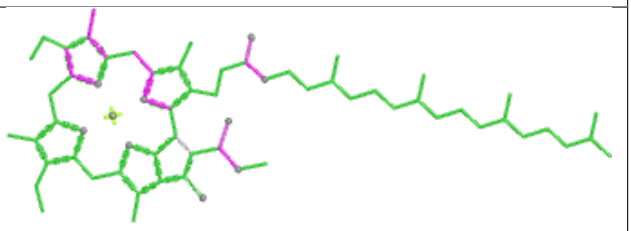
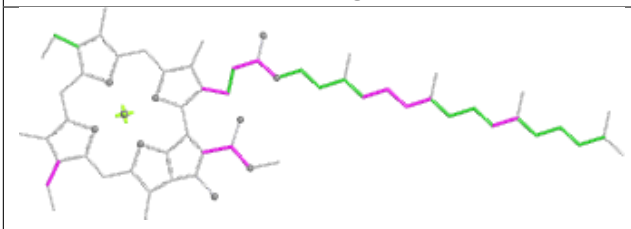
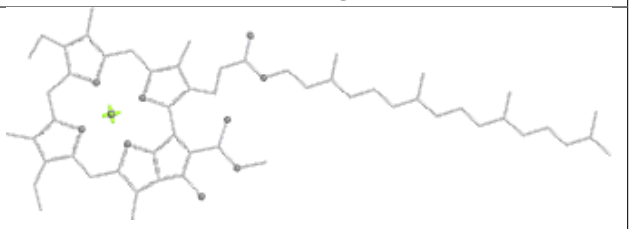


Bond angles

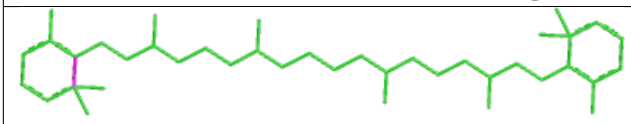


Torsions



Rings

Ligand BCR 4 621



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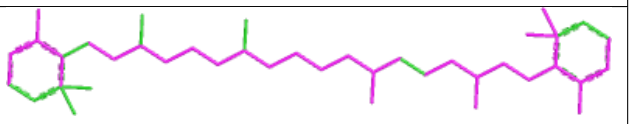

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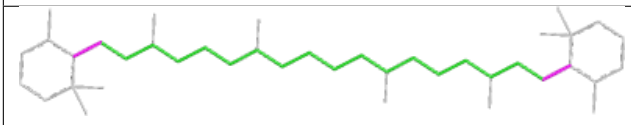

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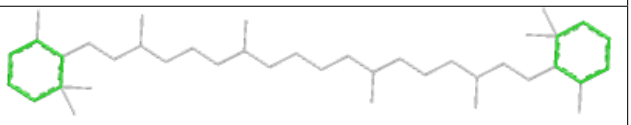
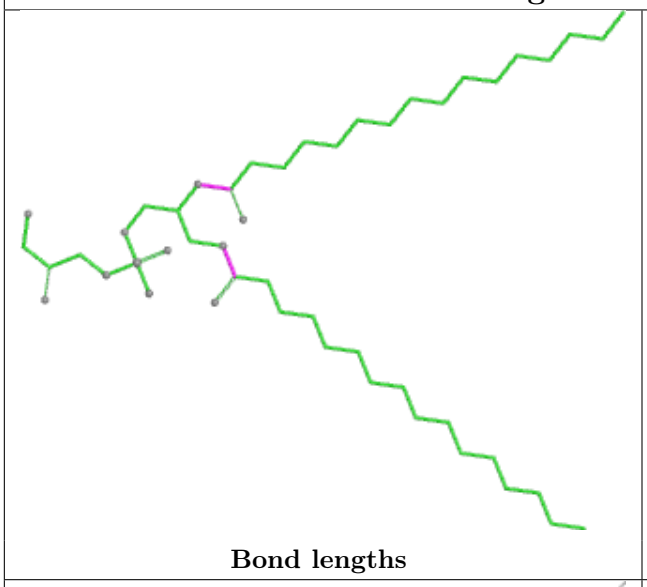


Rings

Ligand LHG 9 623



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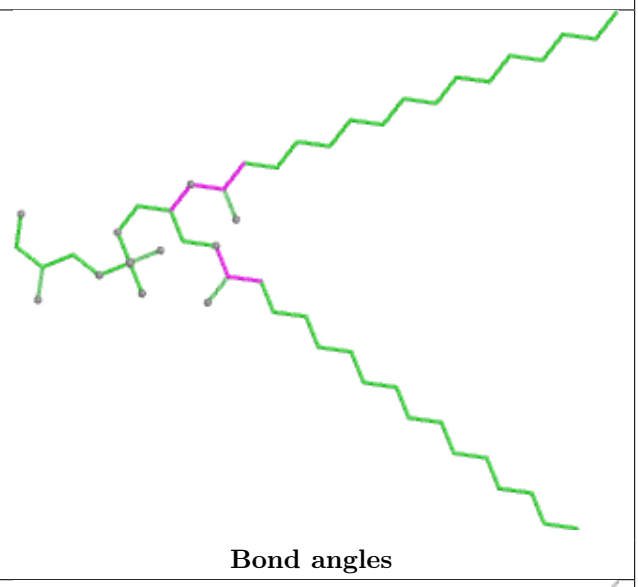

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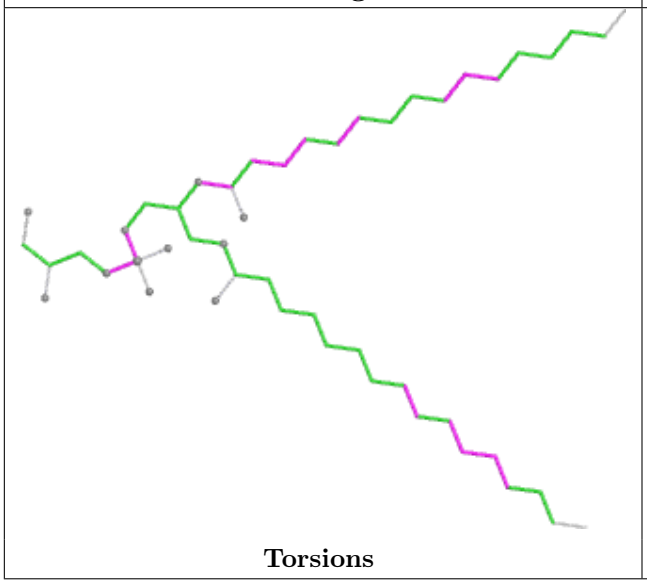

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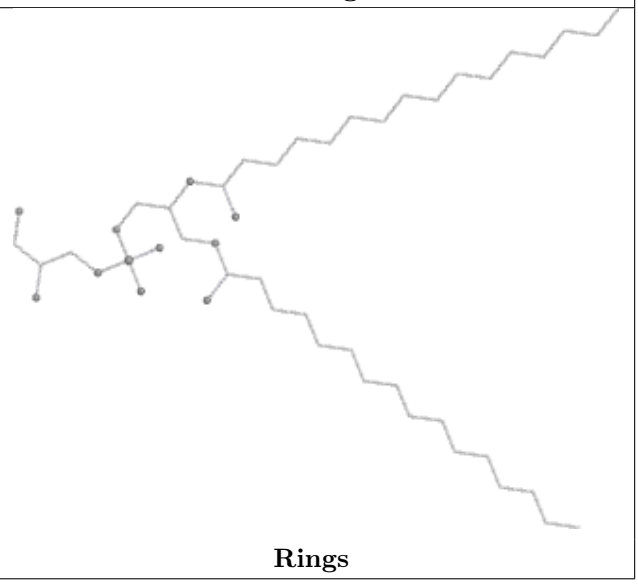
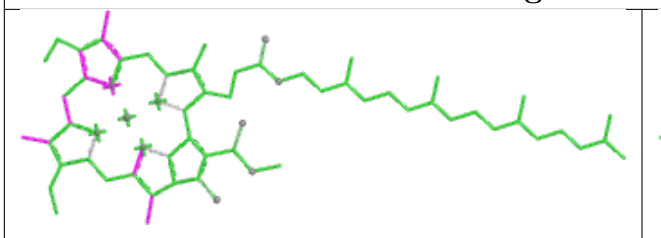


Rings

Ligand CLA A 828



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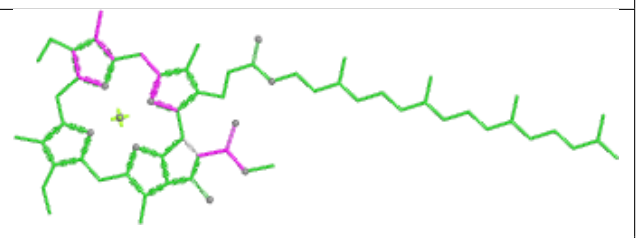
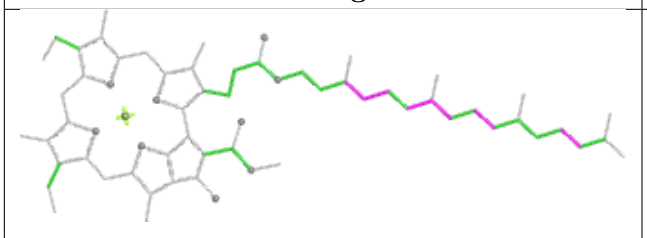


Bond angles



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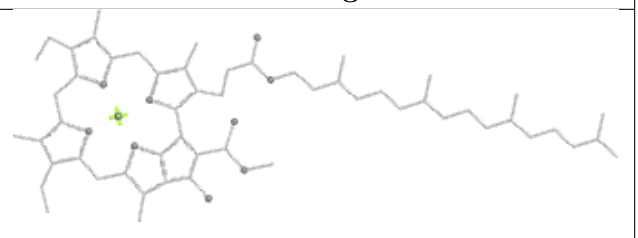
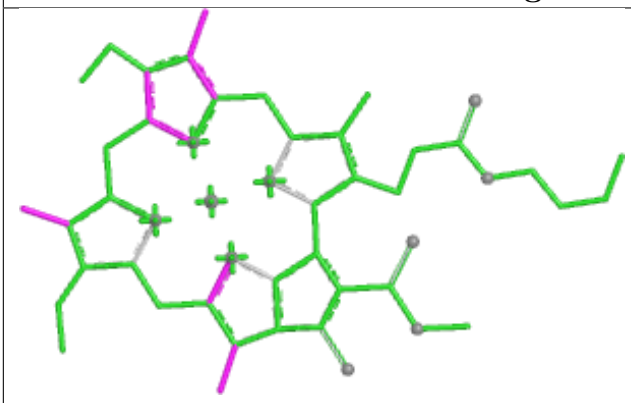


Rings

Ligand CLA B 825



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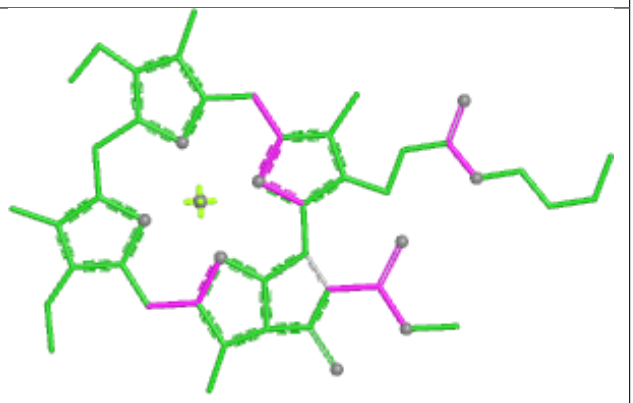
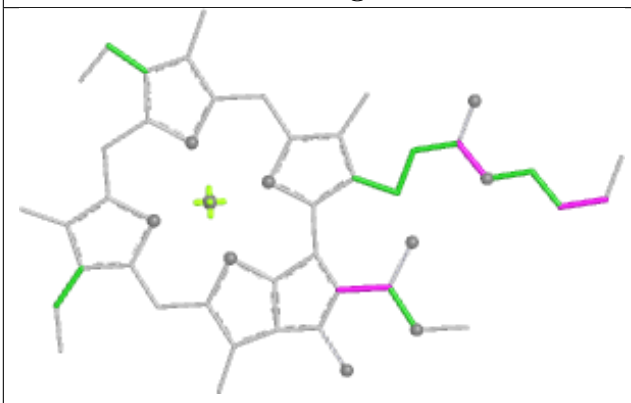


Bond angles



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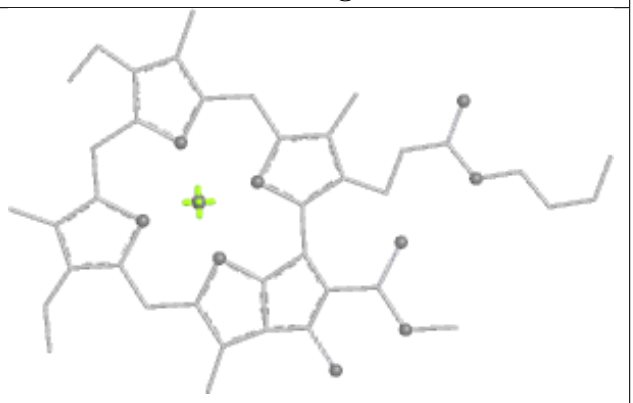
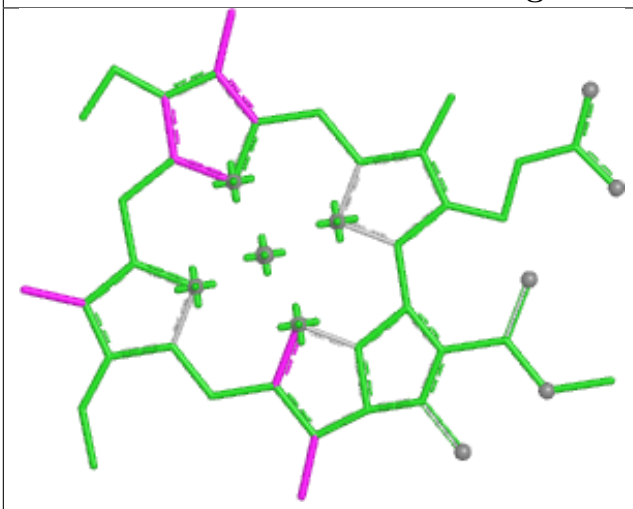
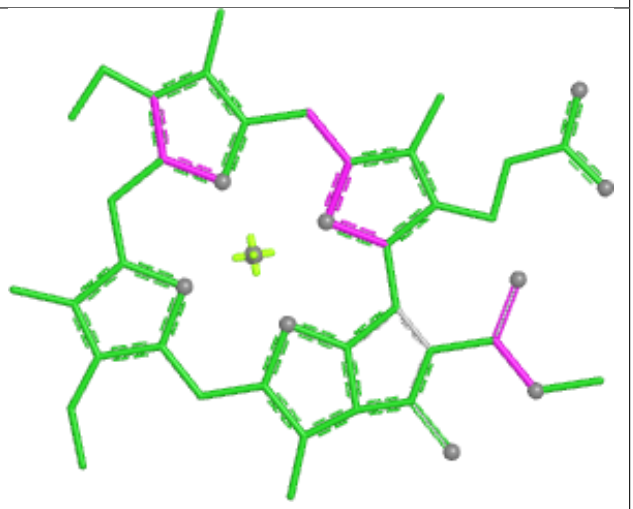


Rings

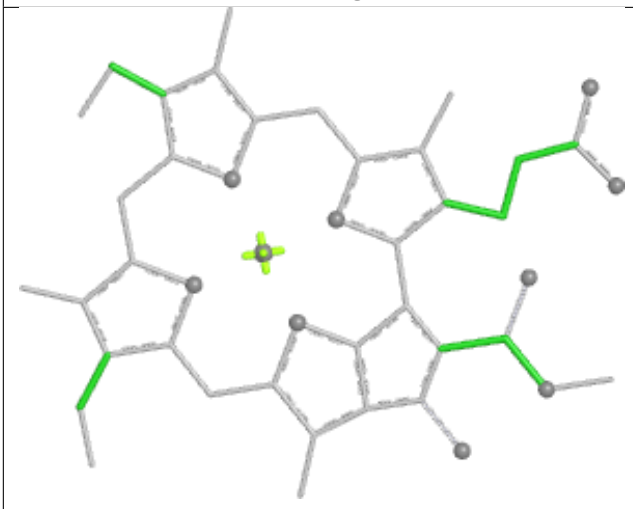
Ligand CLA L 304



Bond lengths



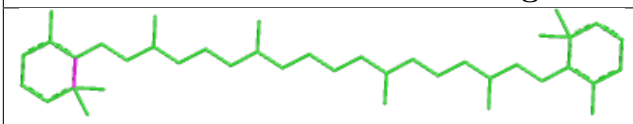
Bond angles



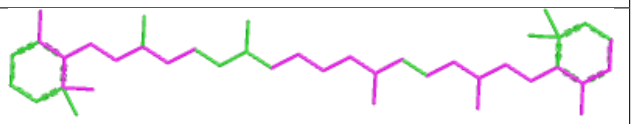
Torsions

Rings

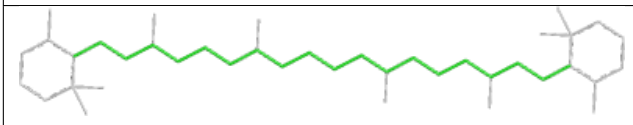
Ligand BCR G 205



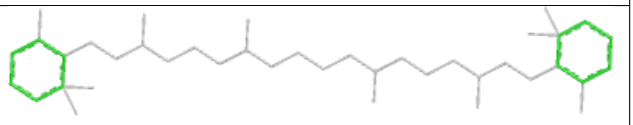
Bond lengths



Bond angles

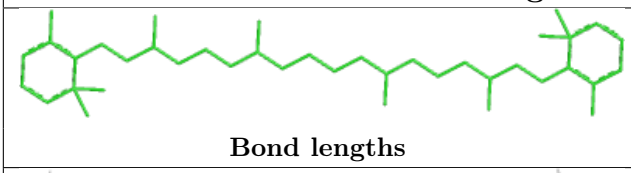


Torsions



Rings

Ligand BCR 3 622



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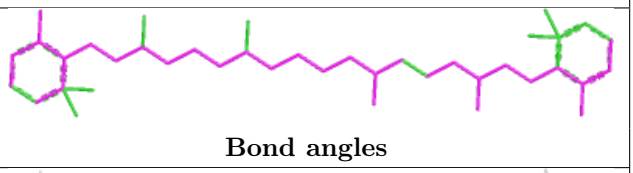
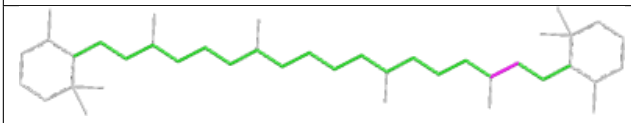
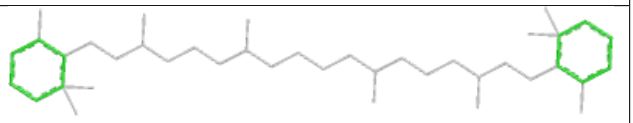


Bond angles

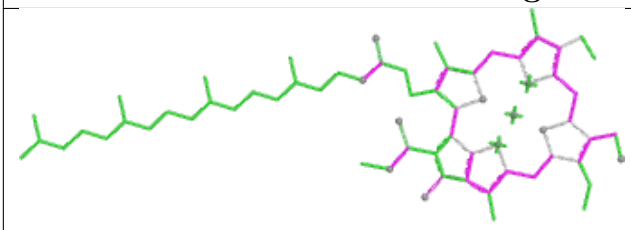


Torsions



Rings

Ligand CHL X 609



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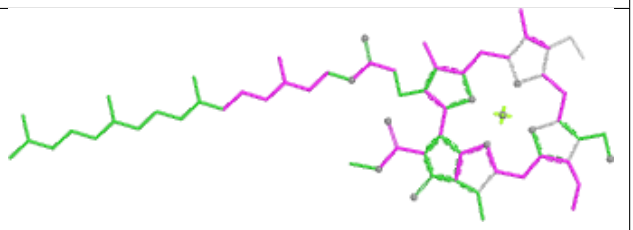
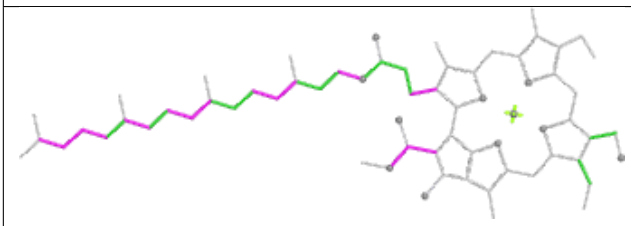
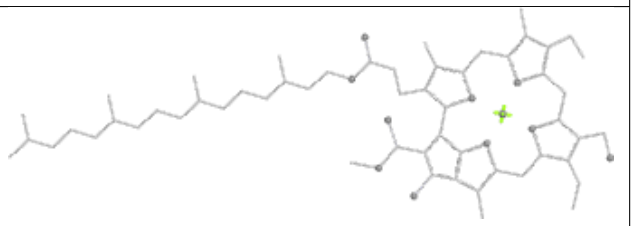


Bond angles

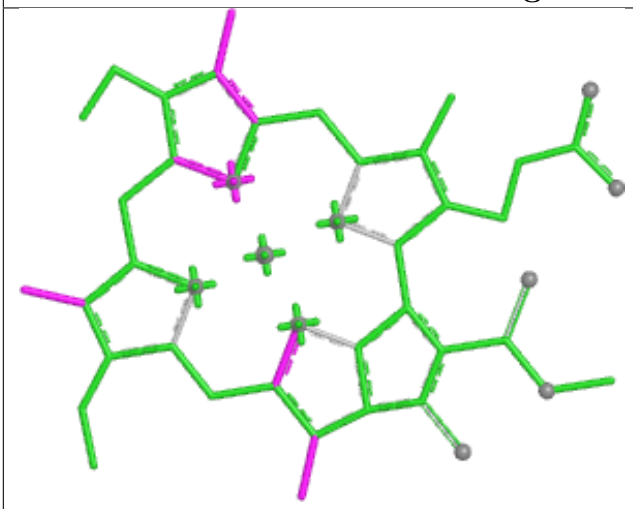


Torsions



Rings

Ligand CLA V 603



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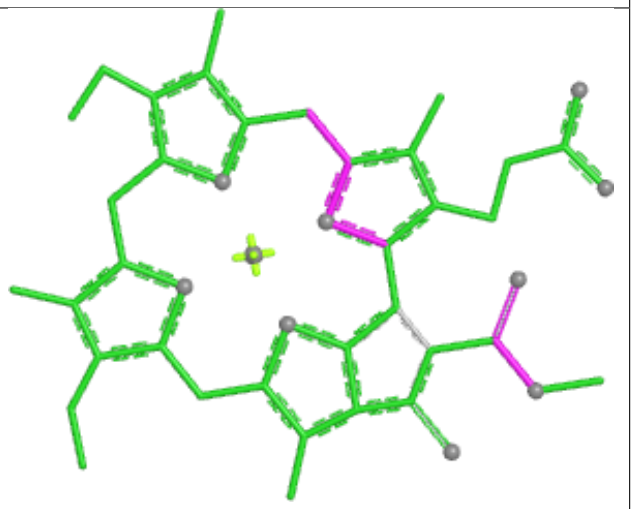
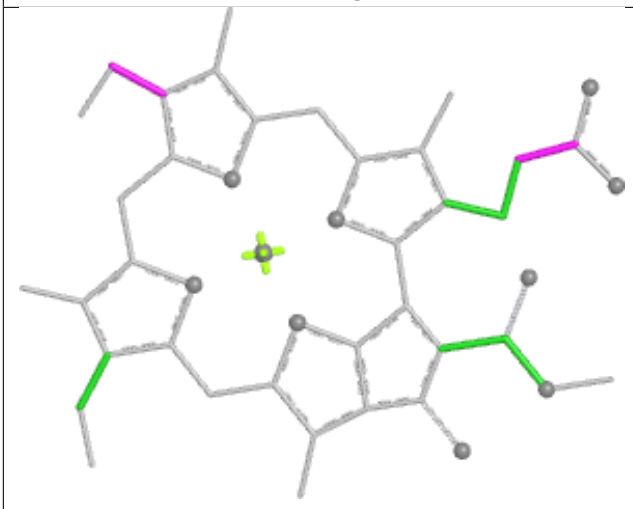


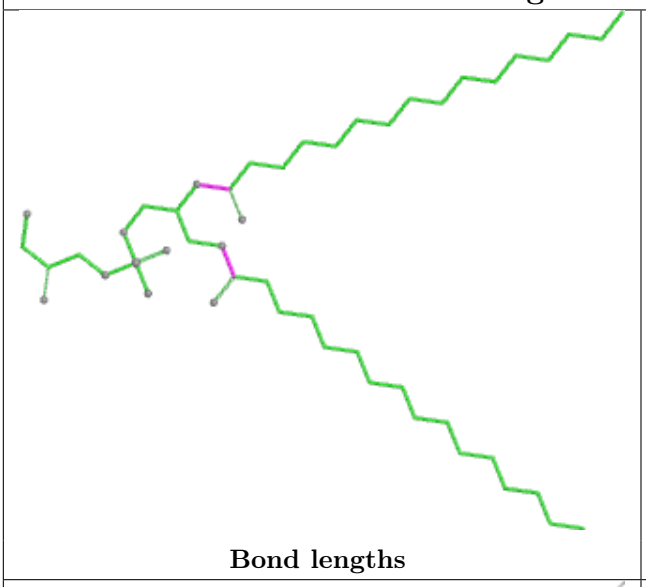
Bond angles



Torsions

Rings

Ligand LHG 4 622



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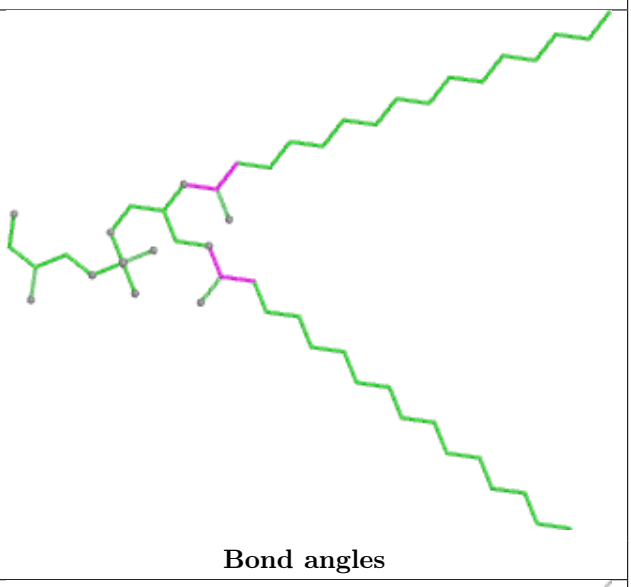
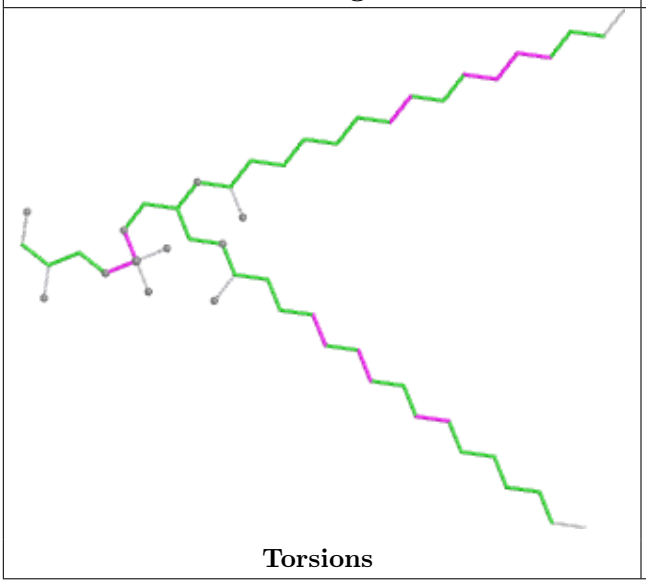
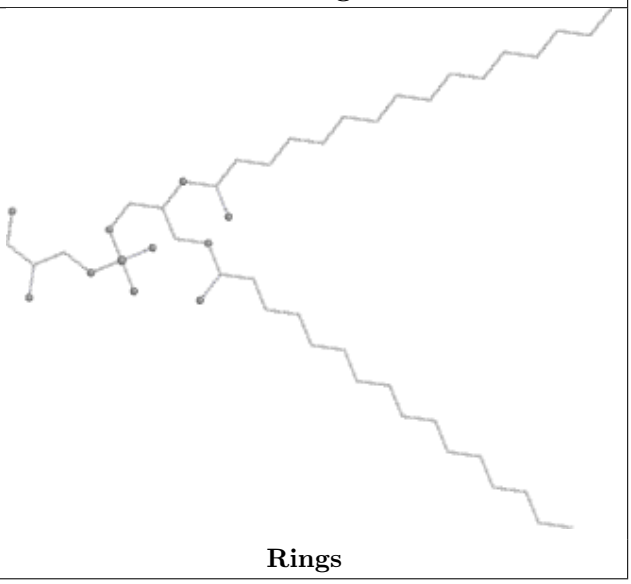


Bond angles

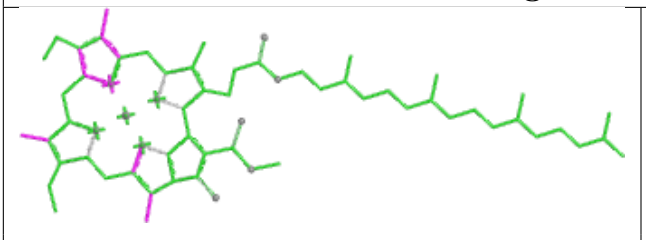


Torsions

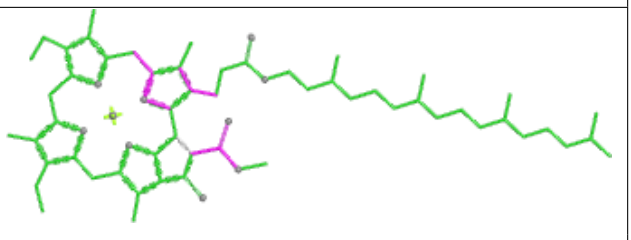


Rings

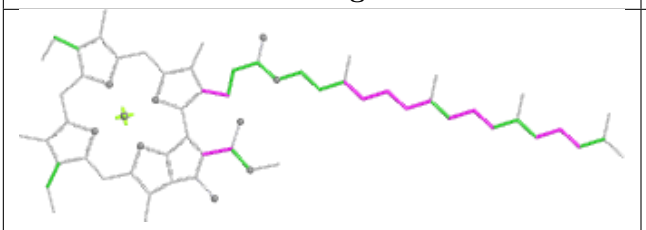
Ligand CLA A 806



Bond lengths



Bond angles



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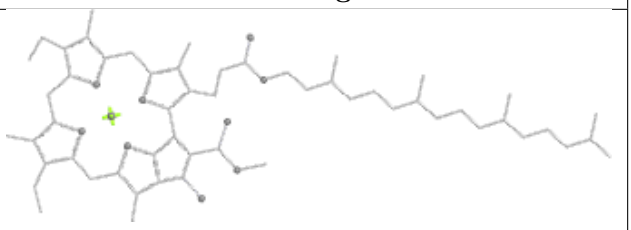
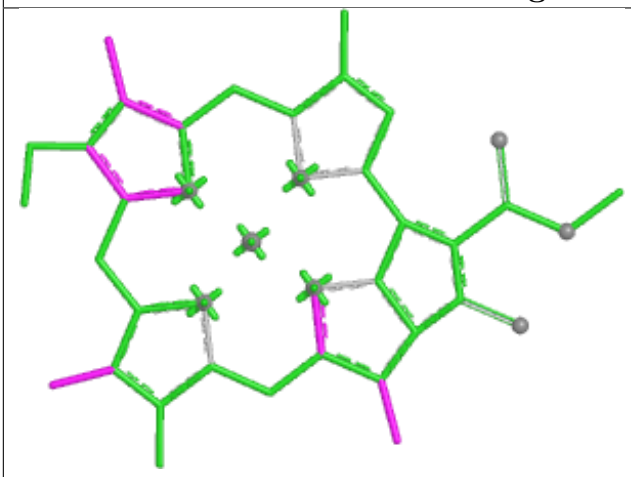


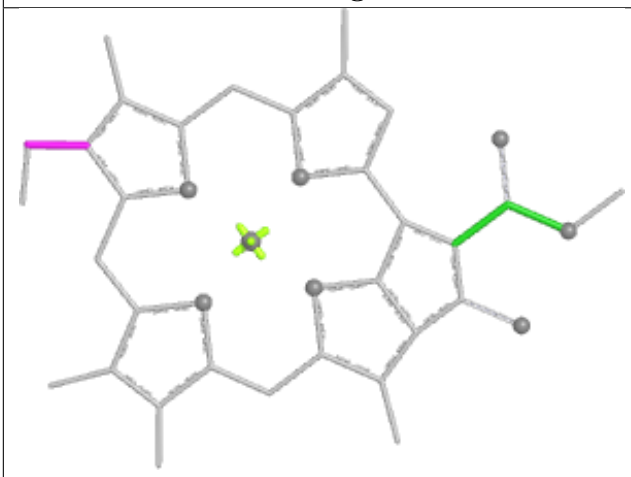
Rings

Ligand CLA 1 610

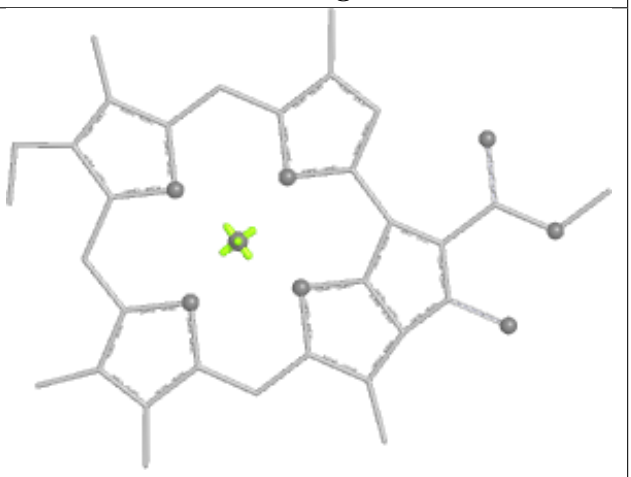


Bond lengths

Bond angles

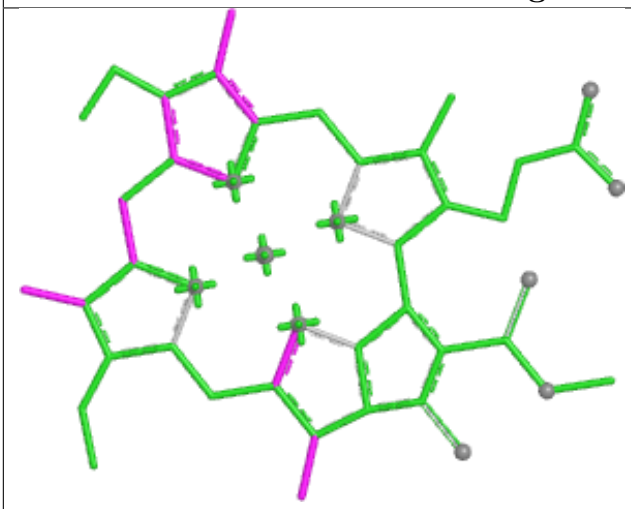


Torsions

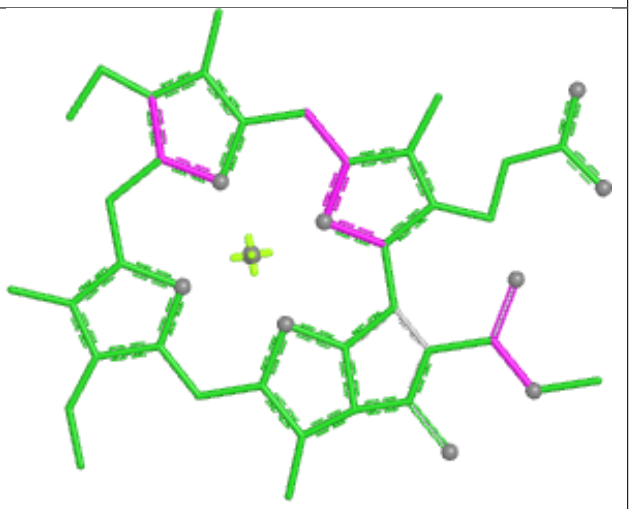


Rings

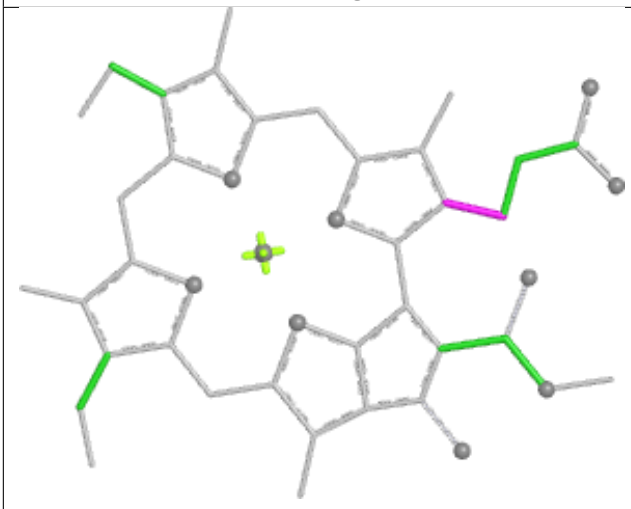
Ligand CLA 2 609



Bond lengths



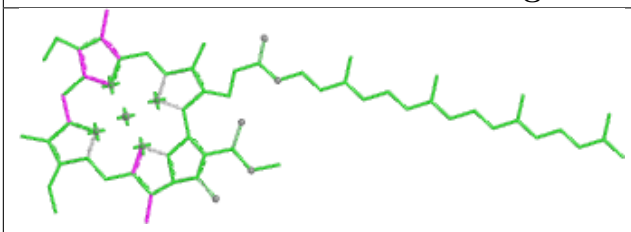
Bond angles



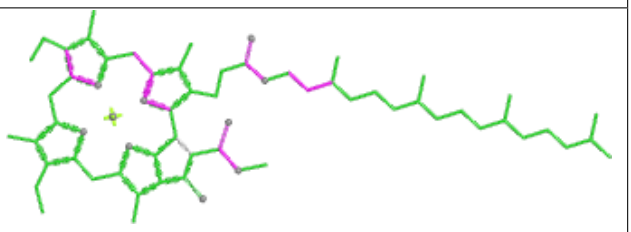
Torsions

Rings

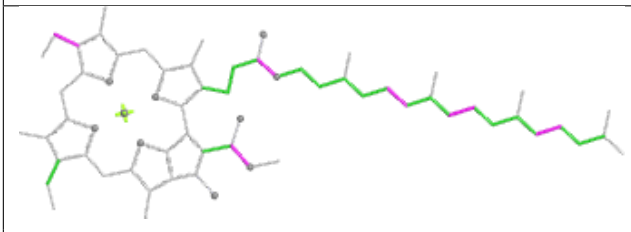
Ligand CLA X 610



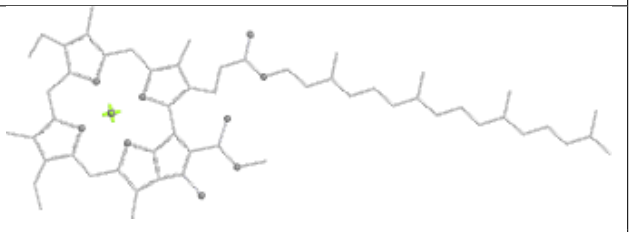
Bond lengths



Bond angles

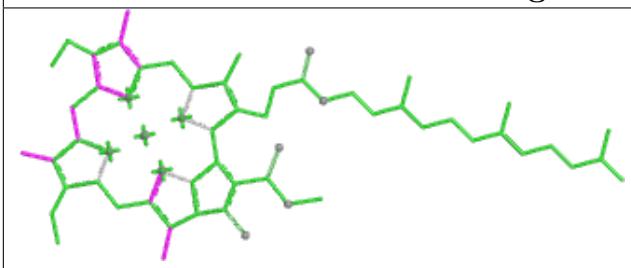


Torsions



Rings

Ligand CLA 3 602



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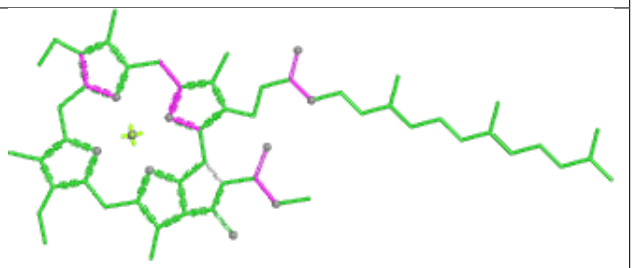
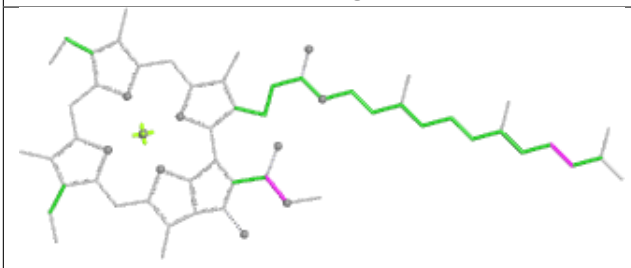


Bond angles



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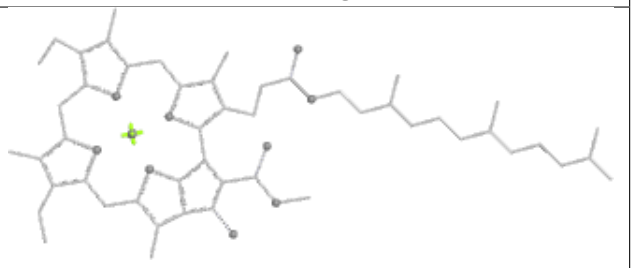
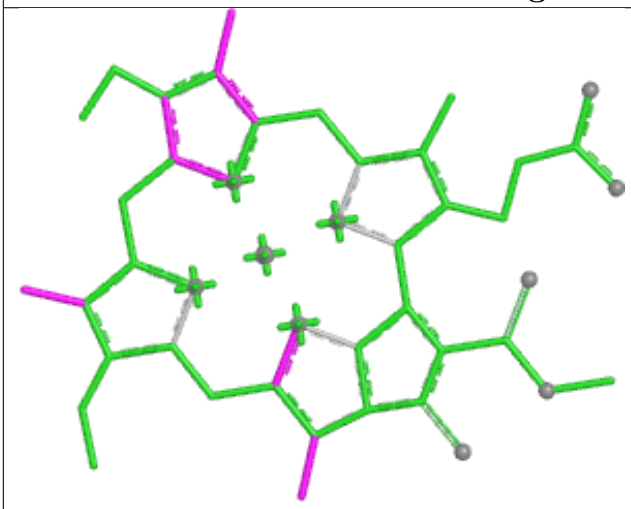


Rings

Ligand CLA 4 607



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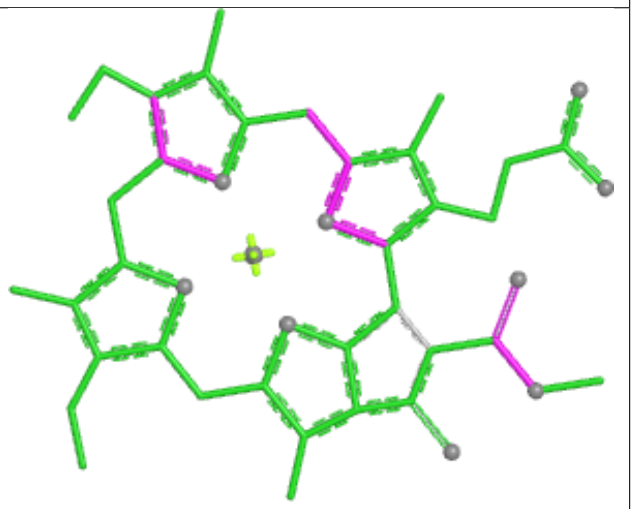
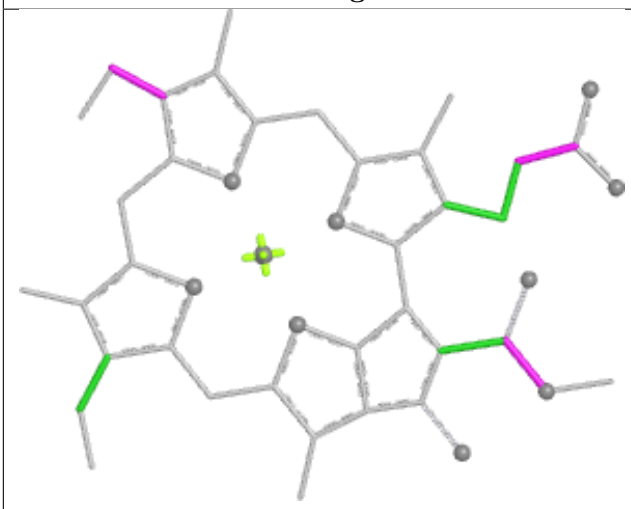


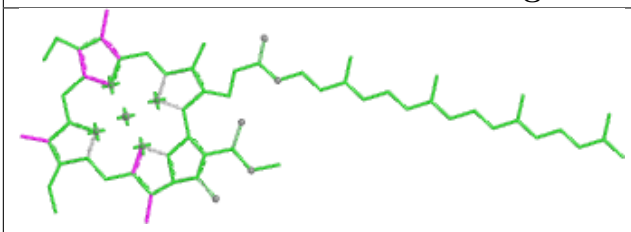
Bond angles



Torsions

Rings

Ligand CLA A 820



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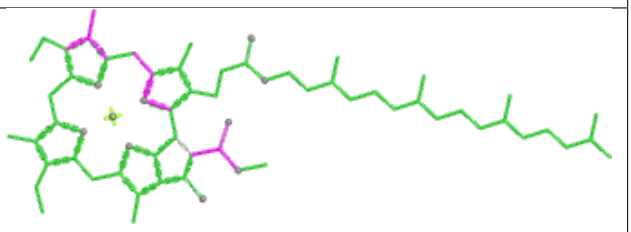
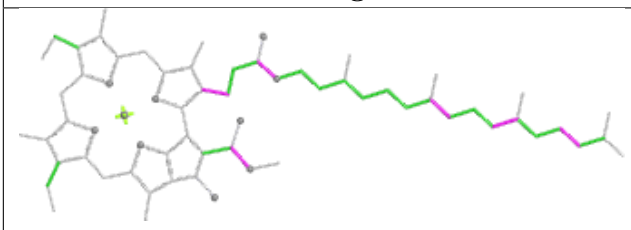
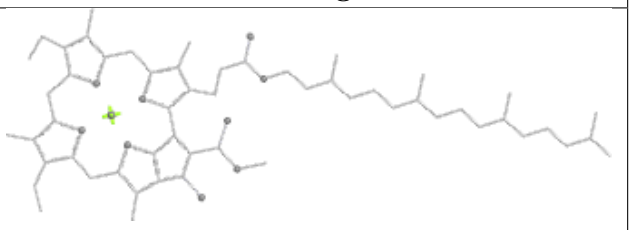


Bond angles

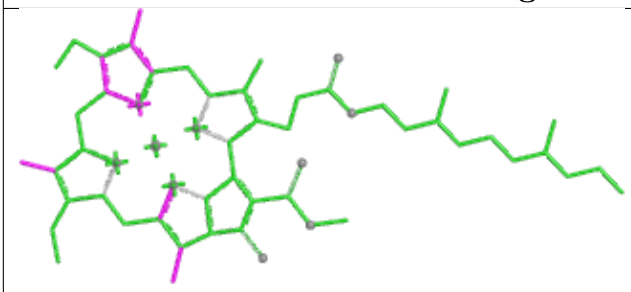


Torsions



Rings

Ligand CLA W 611



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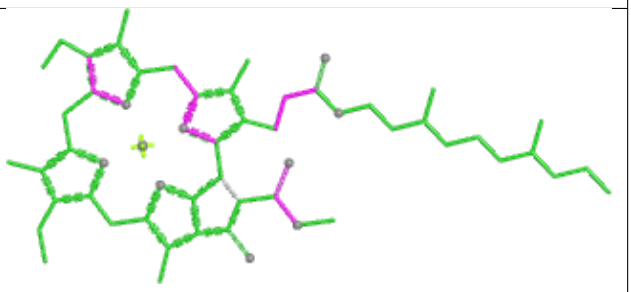
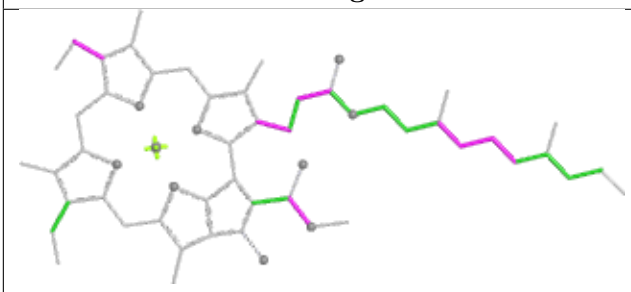
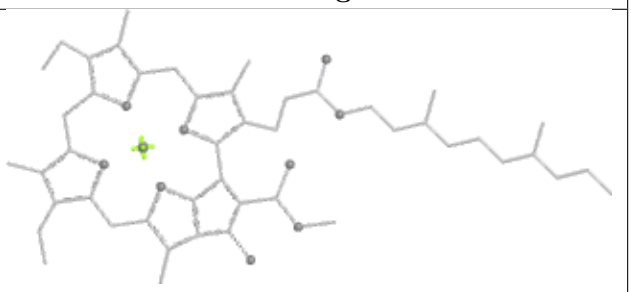


Bond angles

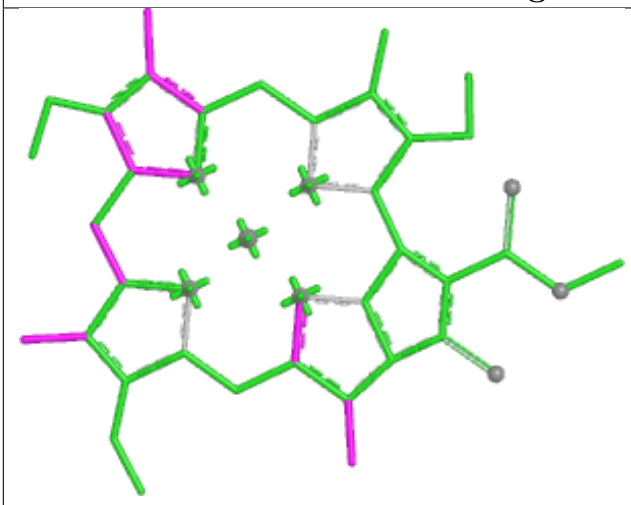


Torsions



Rings

Ligand CLA 9 611



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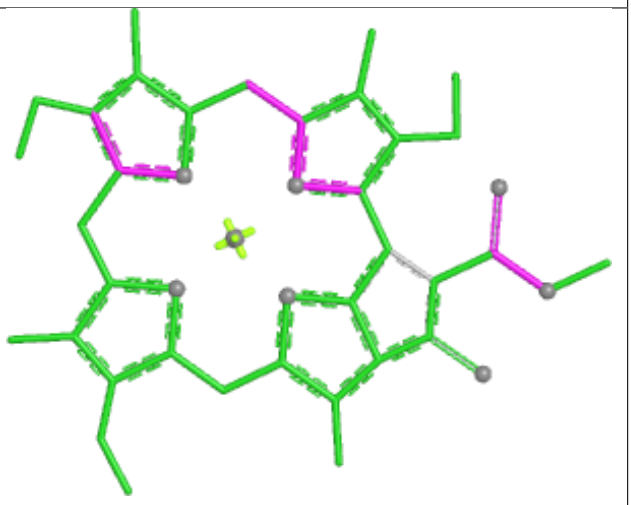
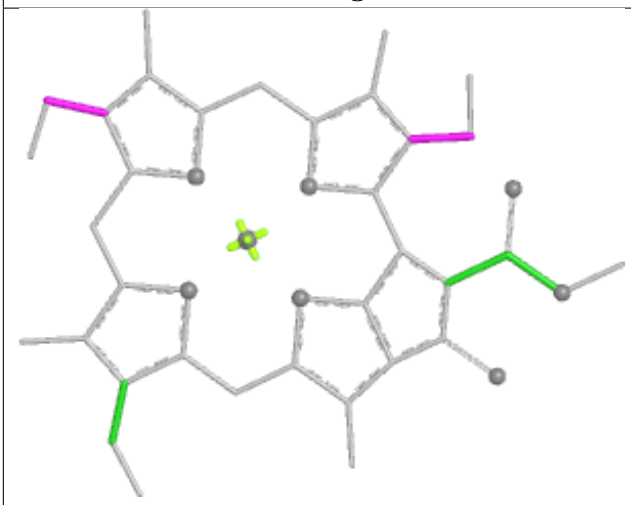


Bond angles

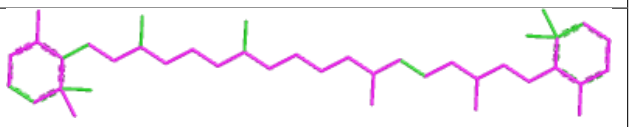


Torsions

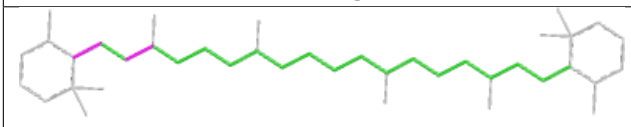
Rings

Ligand BCR B 849

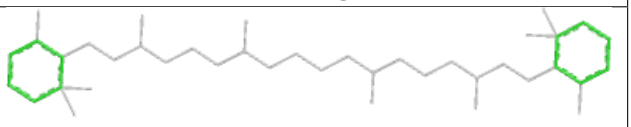
Bond lengths



Bond angles

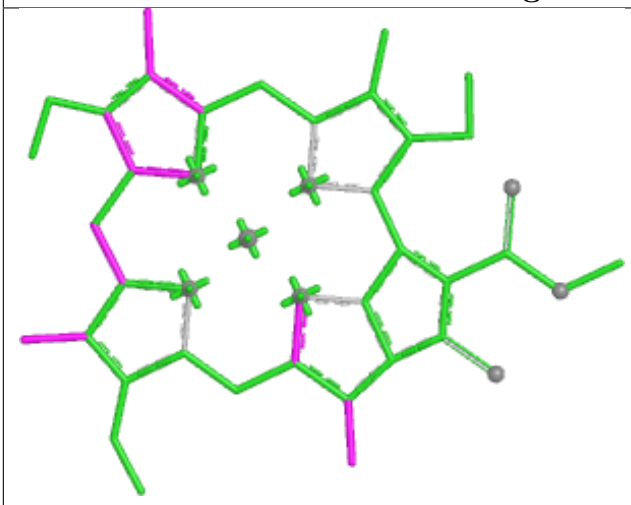


Torsions

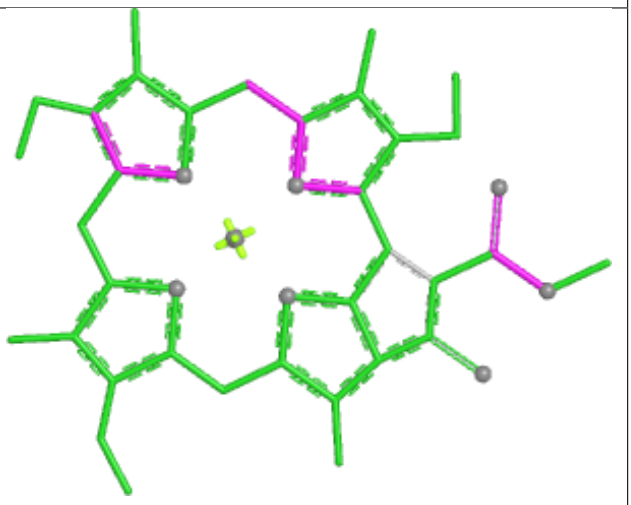


Rings

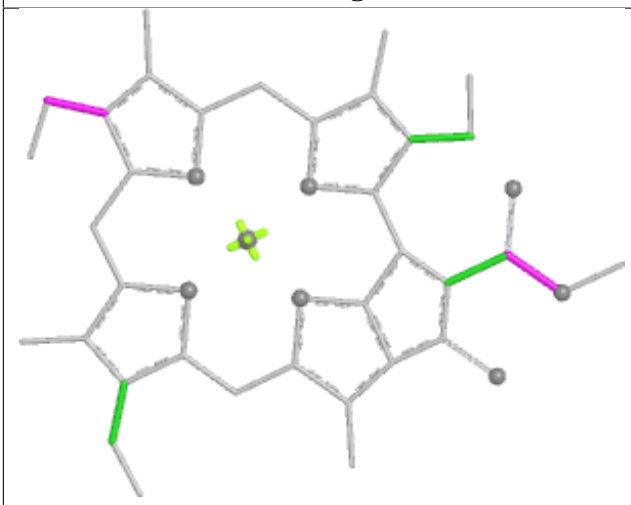
Ligand CLA G 203



Bond lengths



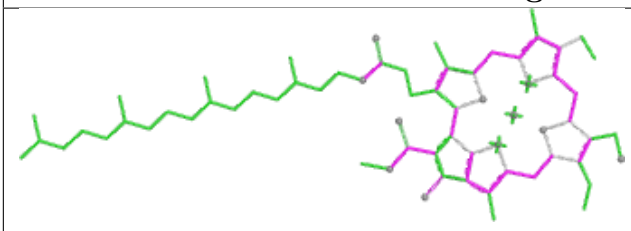
Bond angles



Torsions

Rings

Ligand CHL Z 607



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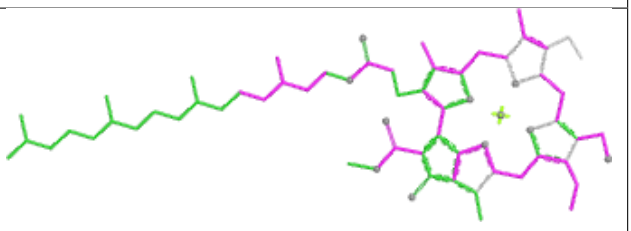
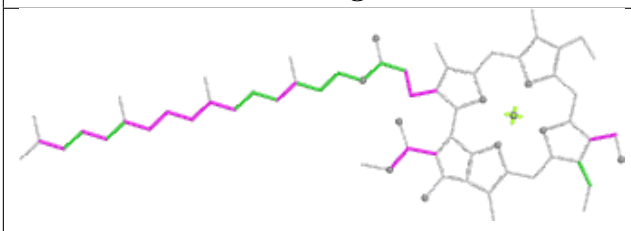
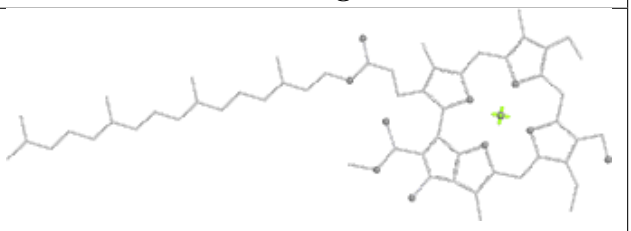


Bond angles

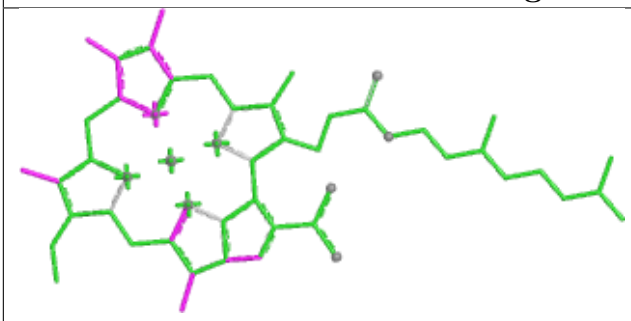


Torsions

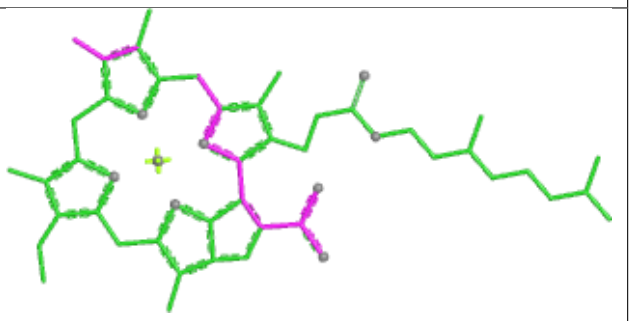


Rings

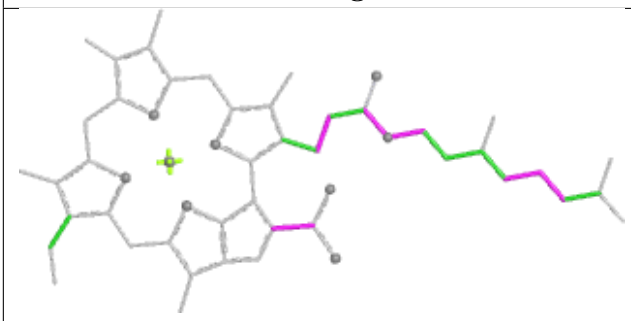
Ligand CLA B 811



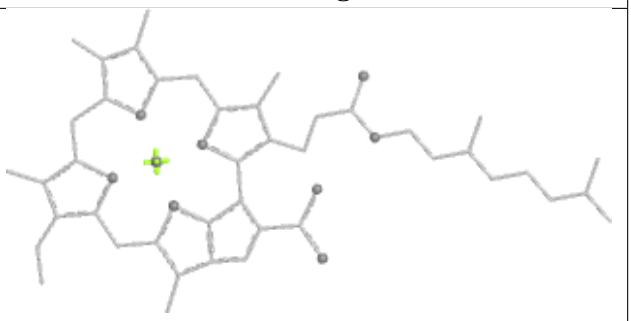
Bond lengths



Bond angles

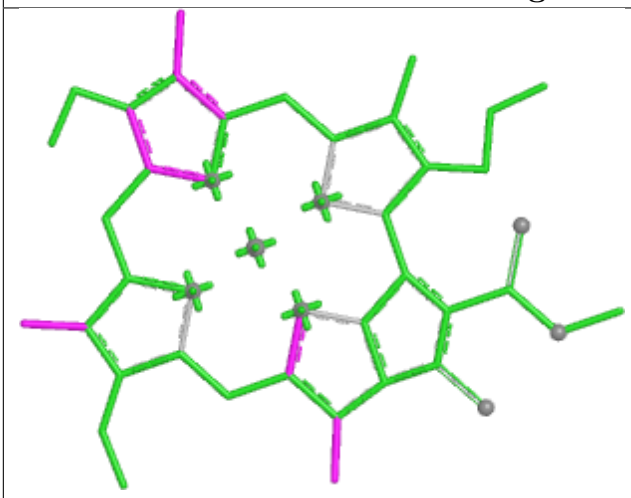


Torsions

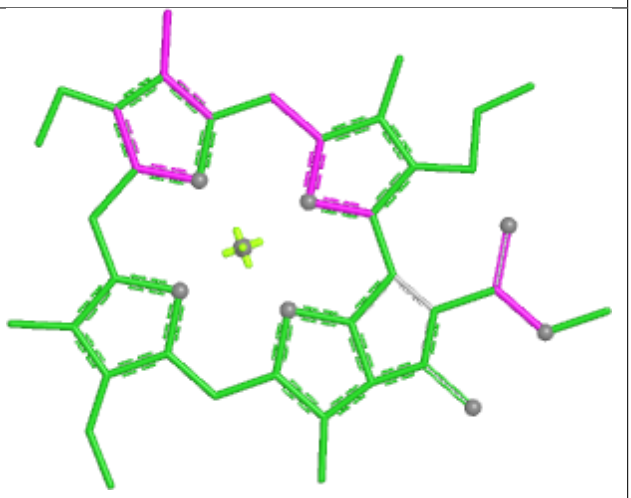


Rings

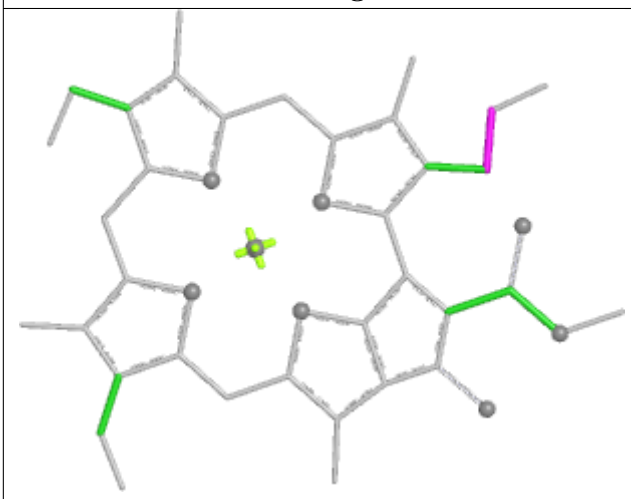
Ligand CLA 3 612



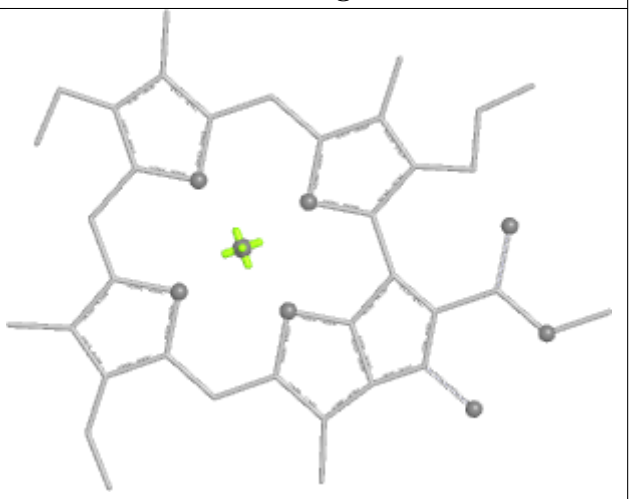
Bond lengths



Bond angles

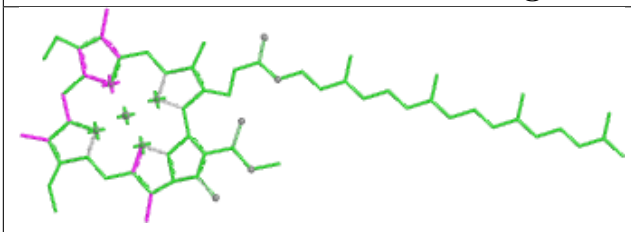


Torsions



Rings

Ligand CLA A 841



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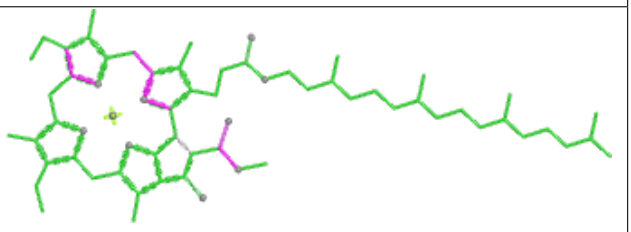
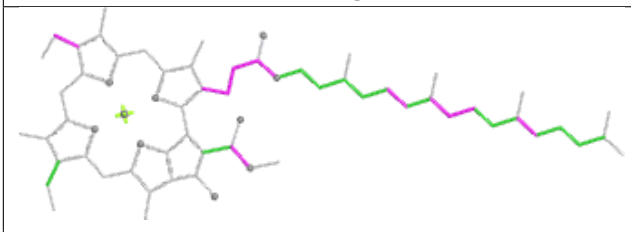
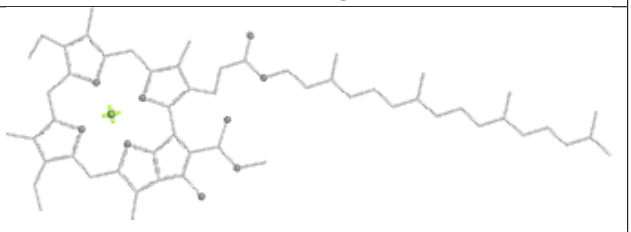


Bond angles

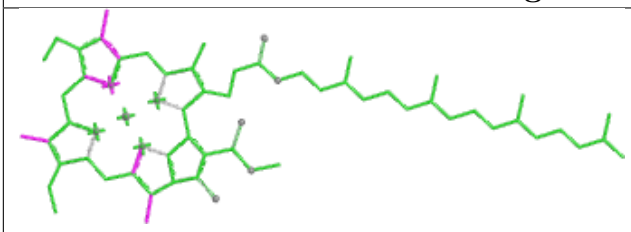


Torsions

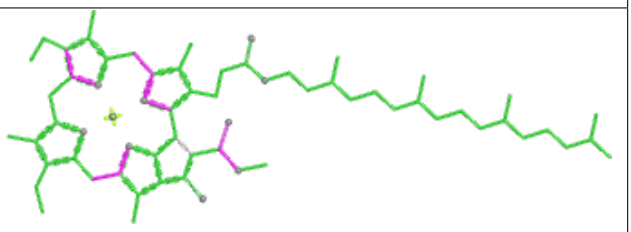


Rings

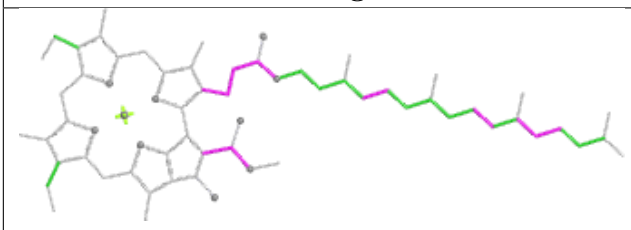
Ligand CLA B 809



Bond lengths



Bond angles



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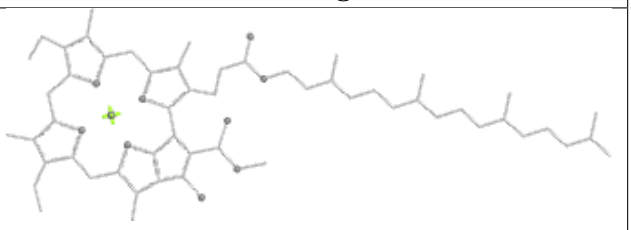
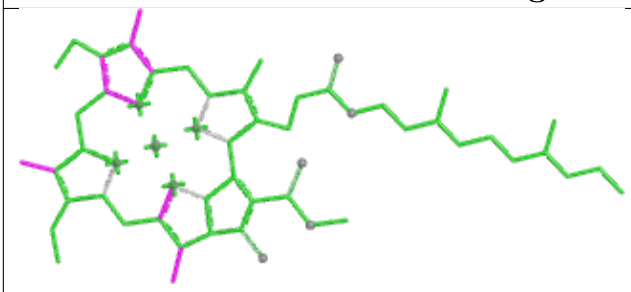


Rings

Ligand CLA 1 611



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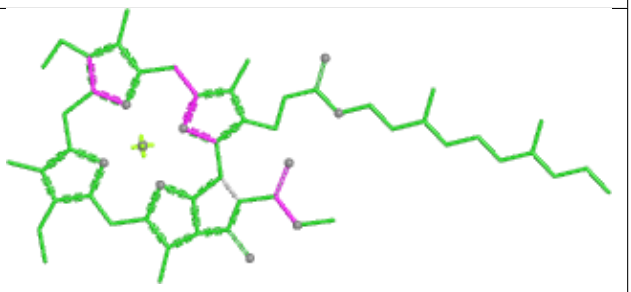
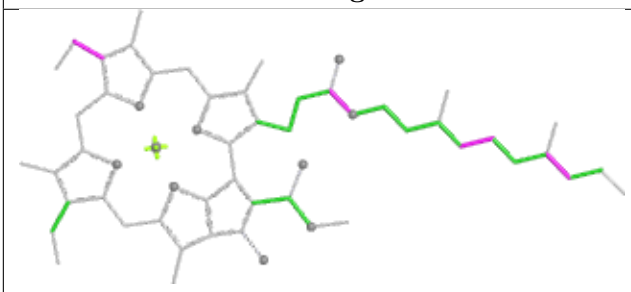


Bond angles



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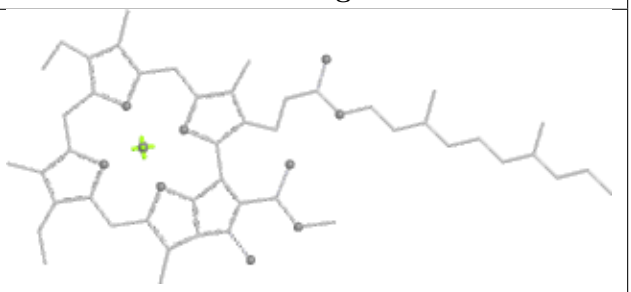
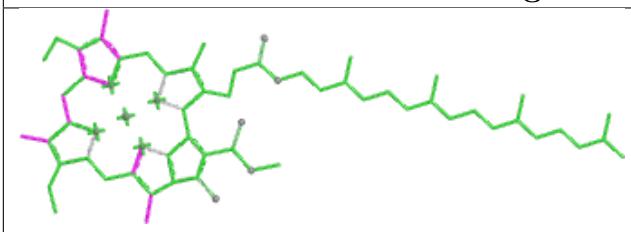
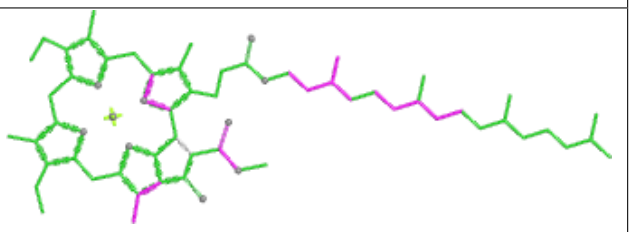
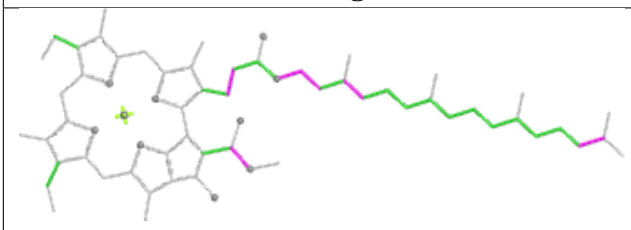
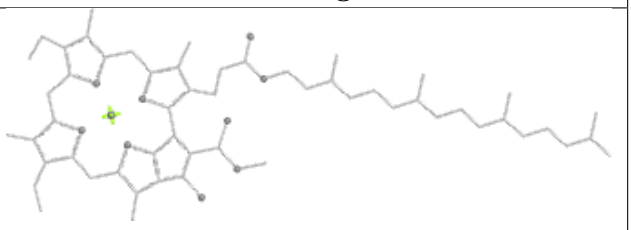
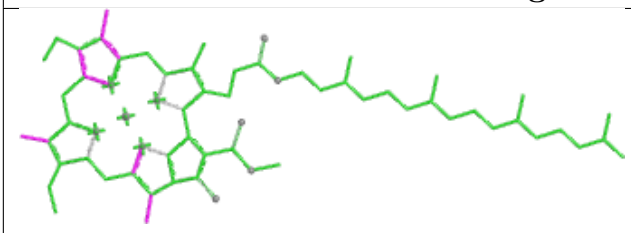
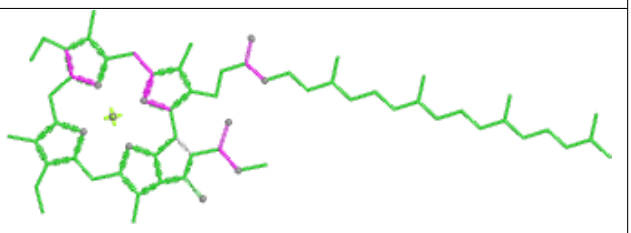
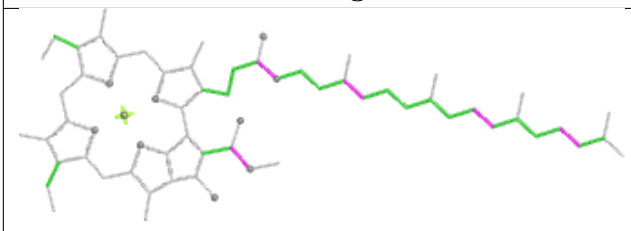
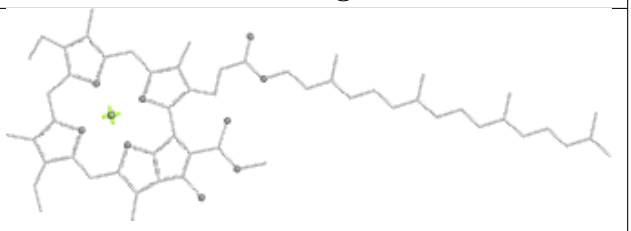
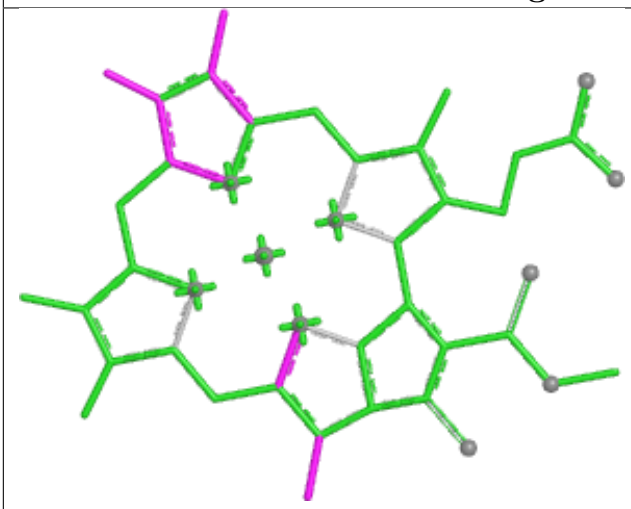


Rings

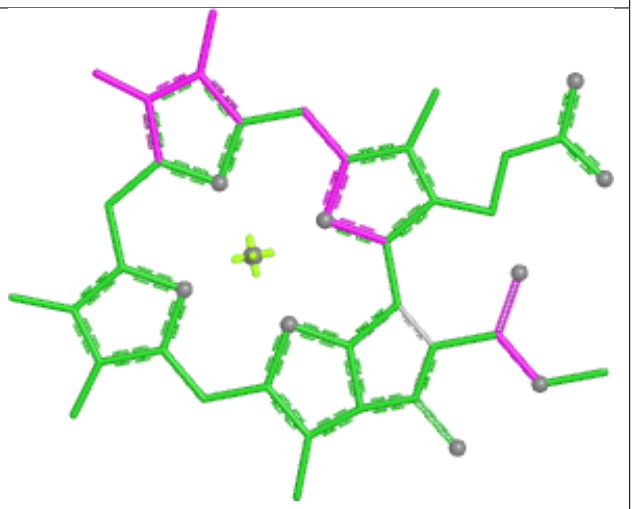
Ligand CLA A 854	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

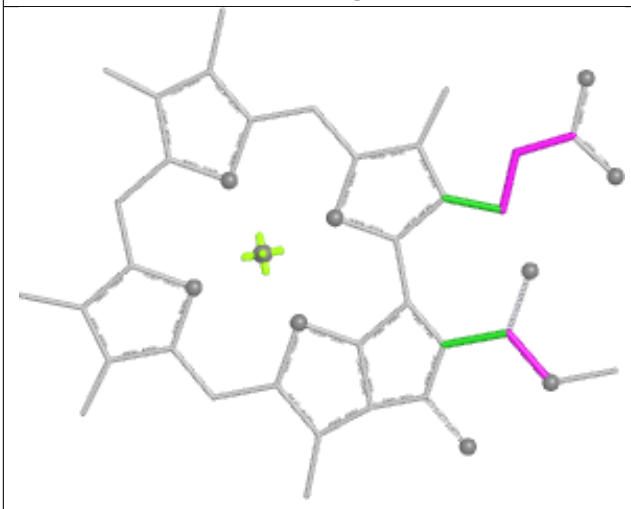
Ligand CLA 1 616



Bond lengths



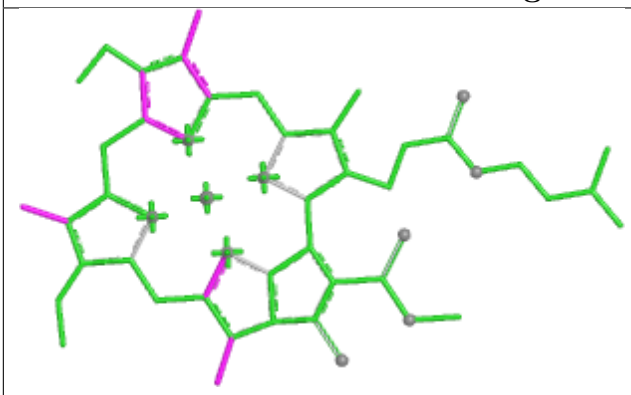
Bond angles



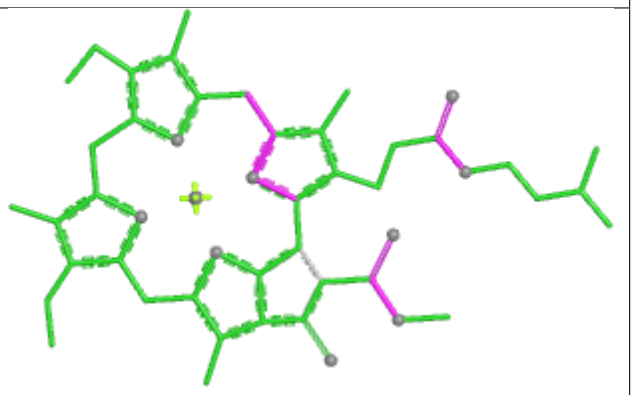
Torsions

Rings

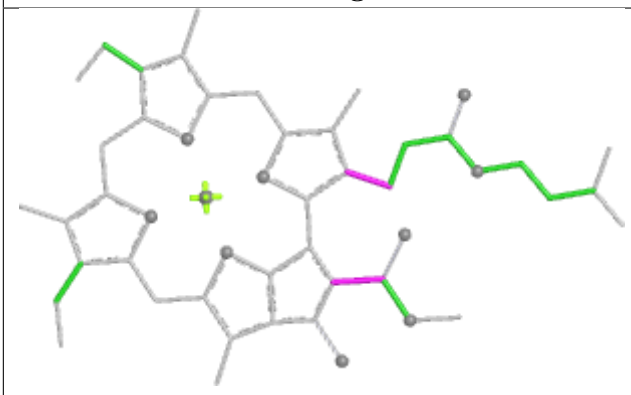
Ligand CLA A 845



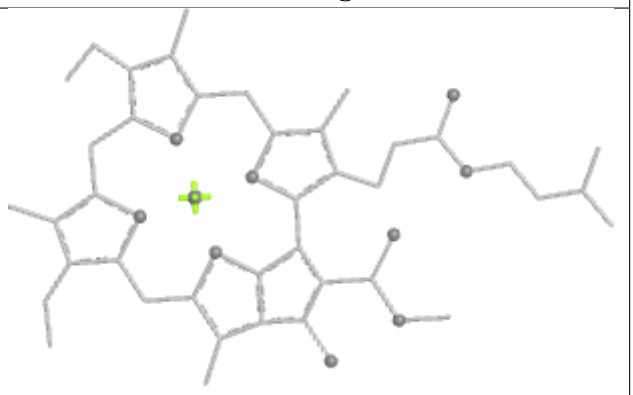
Bond lengths



Bond angles

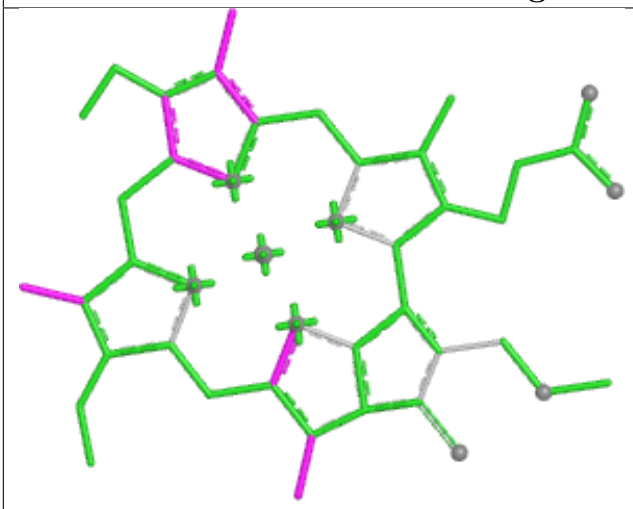


Torsions

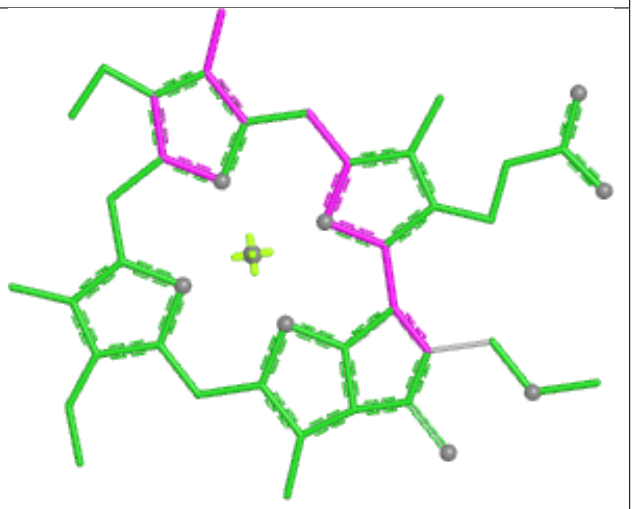


Rings

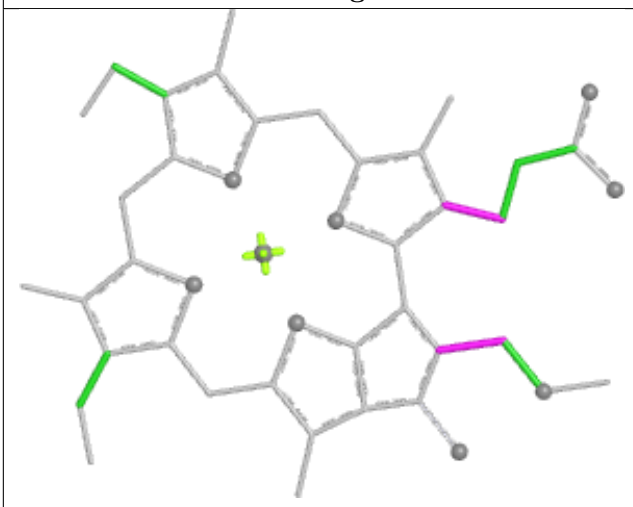
Ligand CLA 7 609



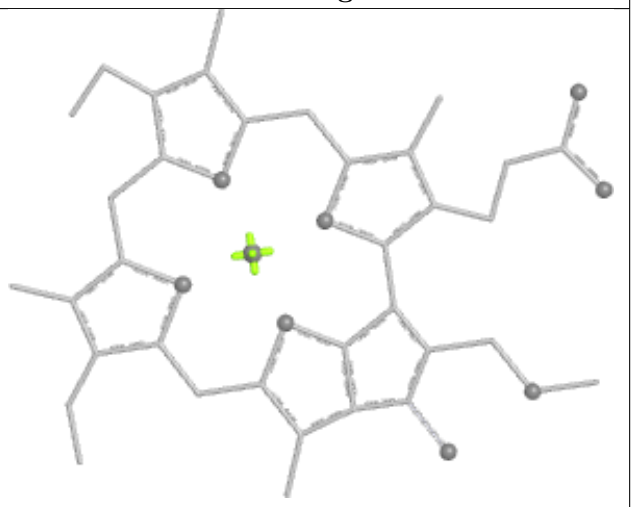
Bond lengths



Bond angles

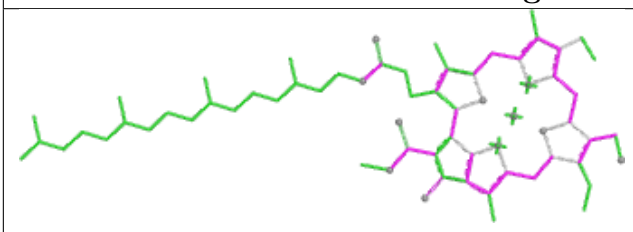


Torsions

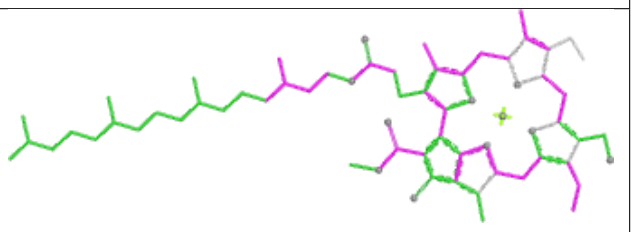


Rings

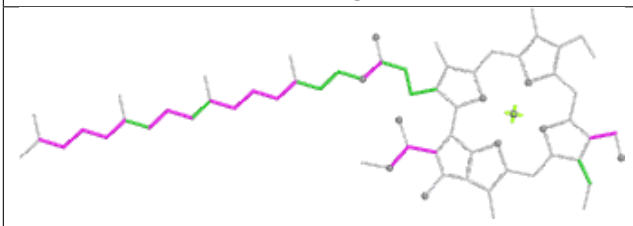
Ligand CHL X 601



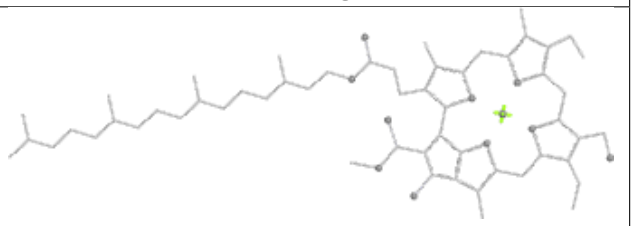
Bond lengths



Bond angles

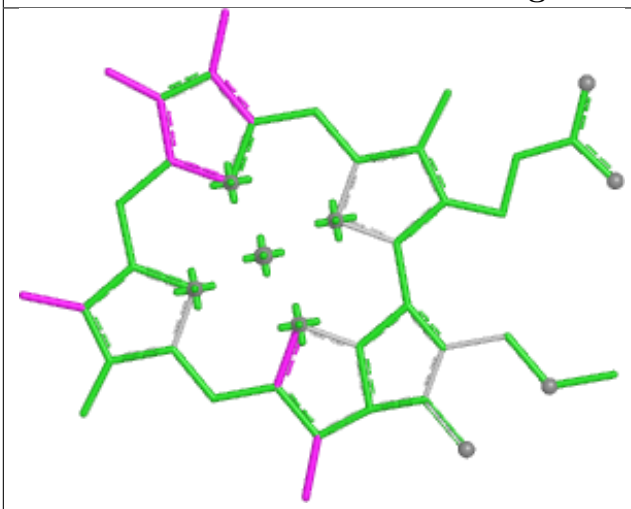


Torsions



Rings

Ligand CLA 7 615



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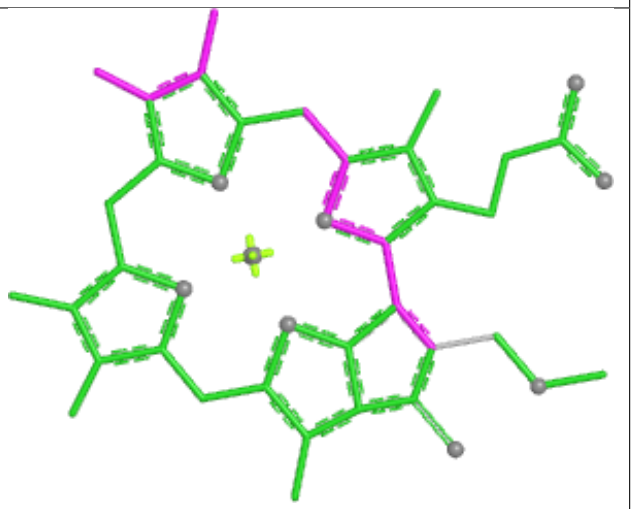
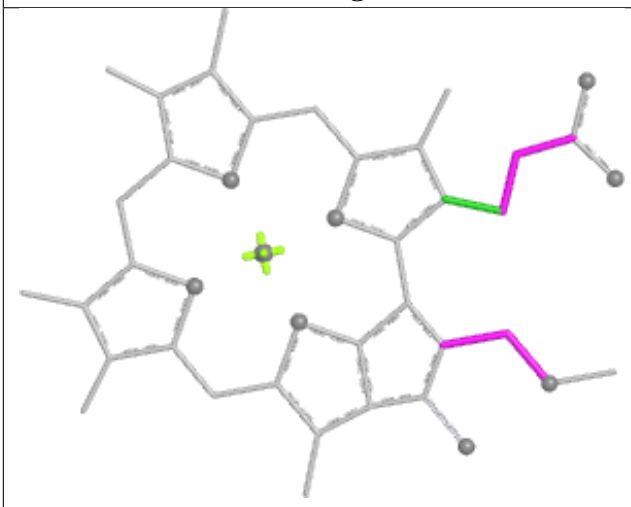
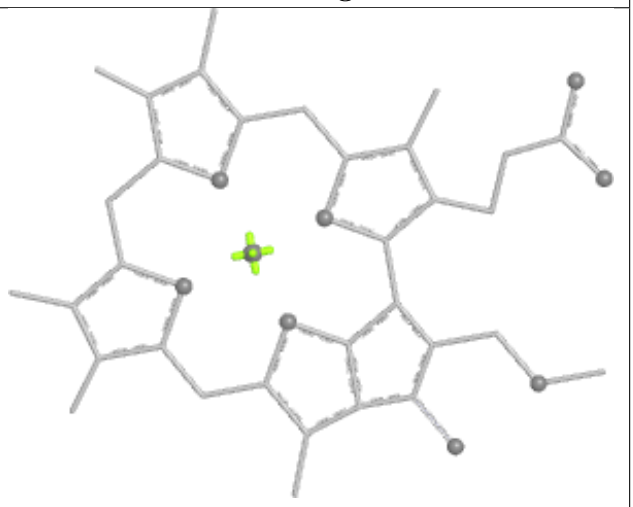


Bond angles

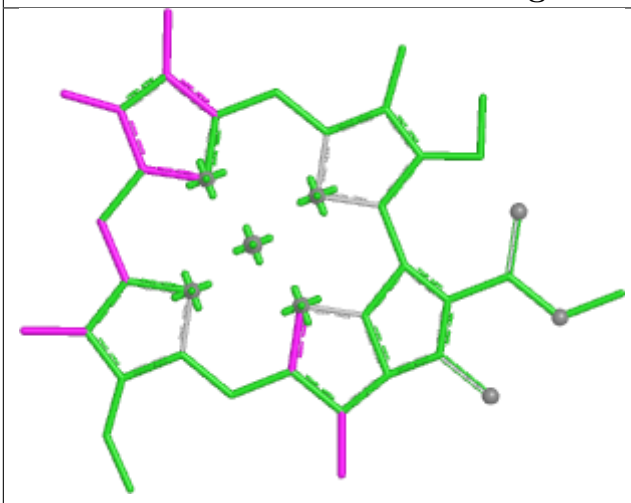


Torsions



Rings

Ligand CLA 6 607



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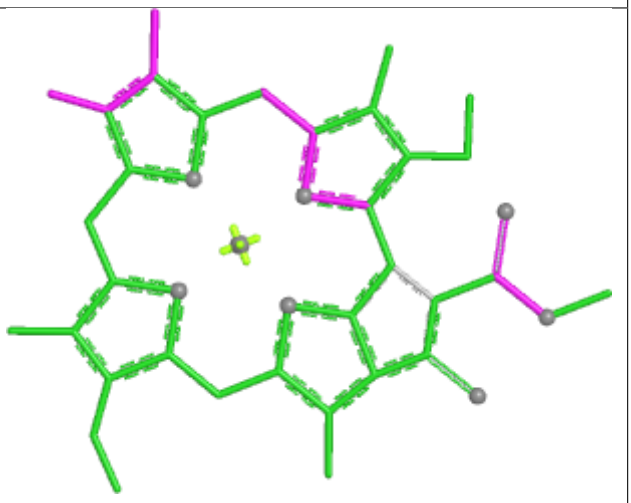
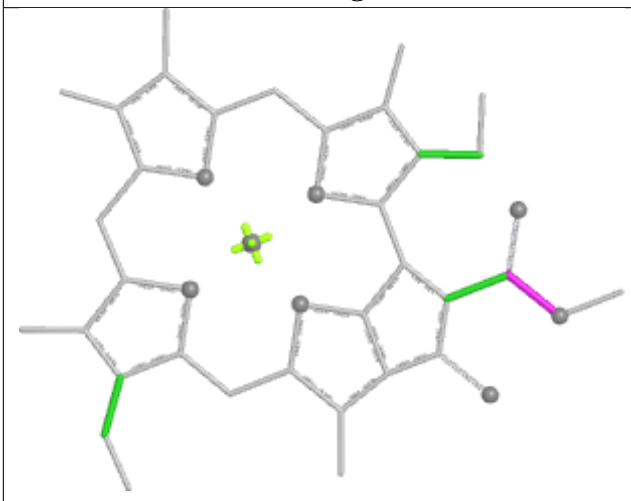


Bond angles



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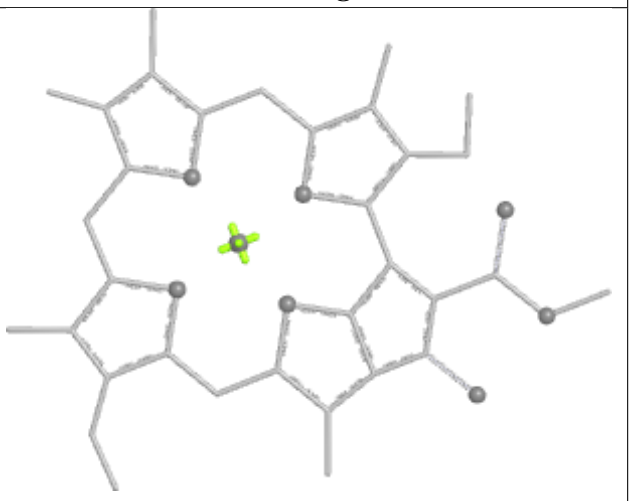
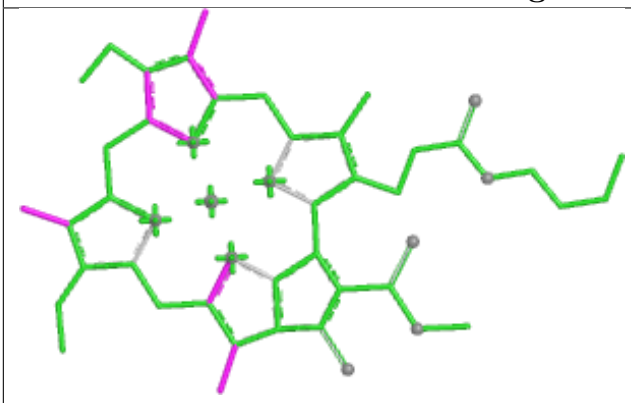


Rings

Ligand CLA 1 604



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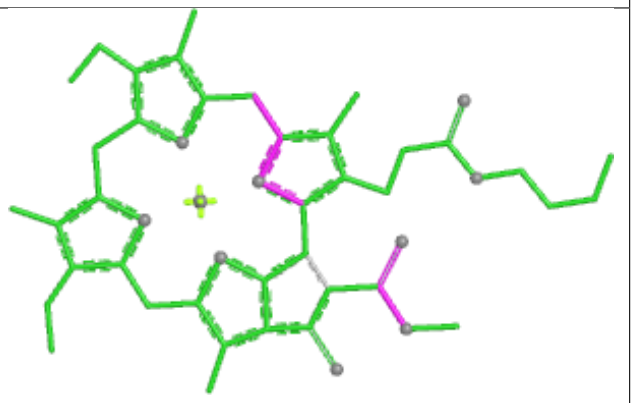
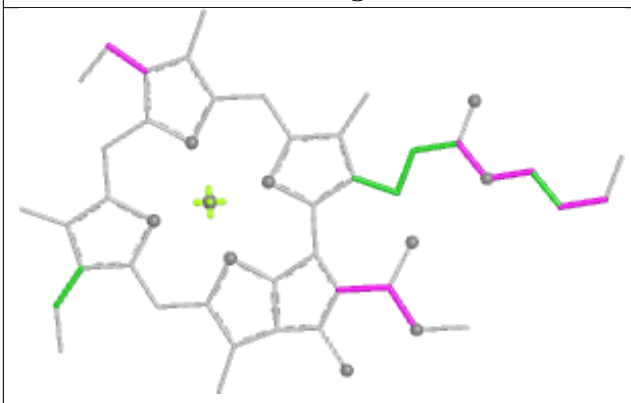
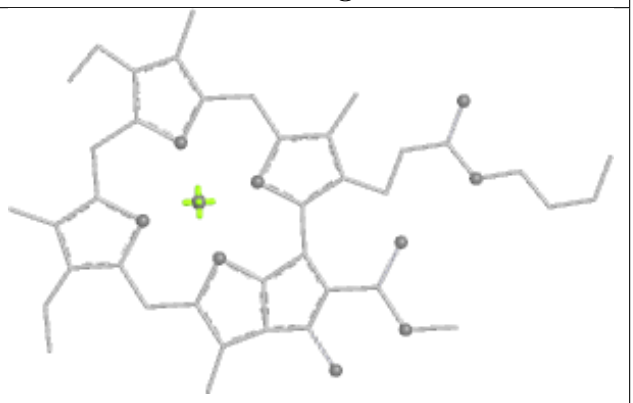


Bond angles

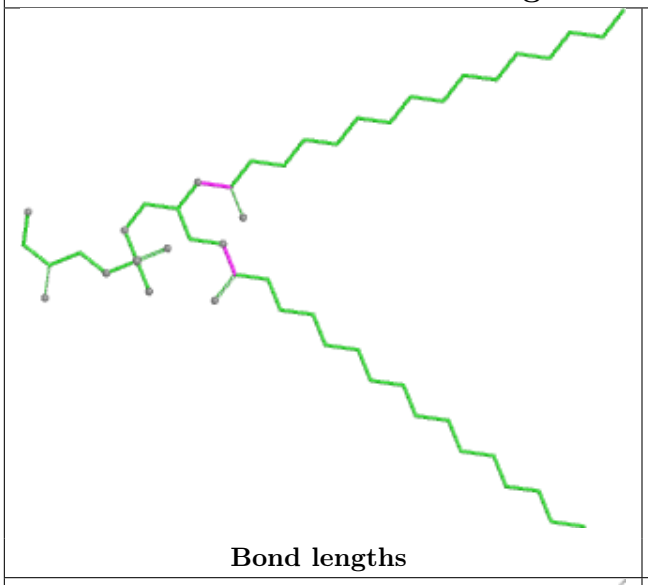


Torsions



Rings

Ligand LHG A 846



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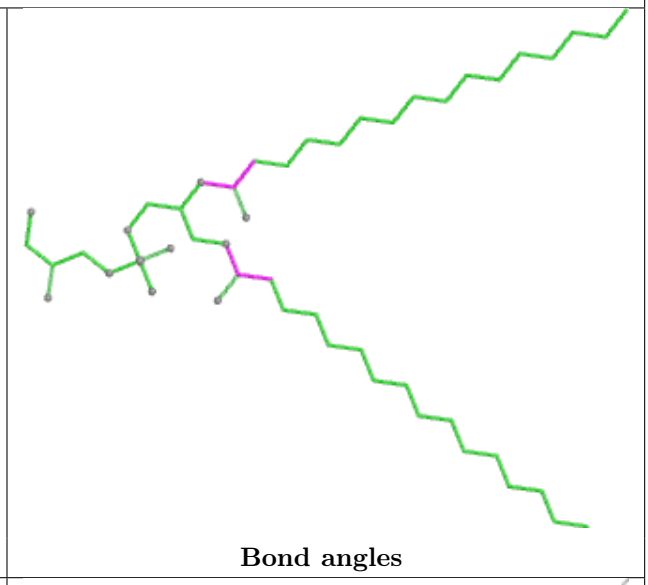
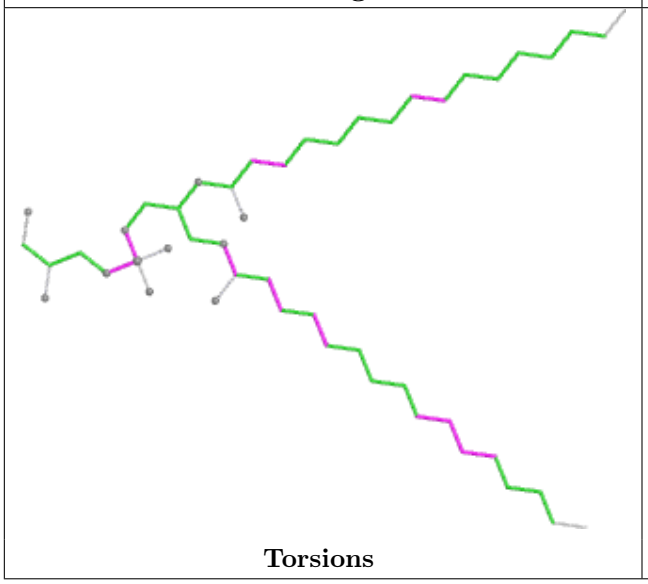


Bond angles



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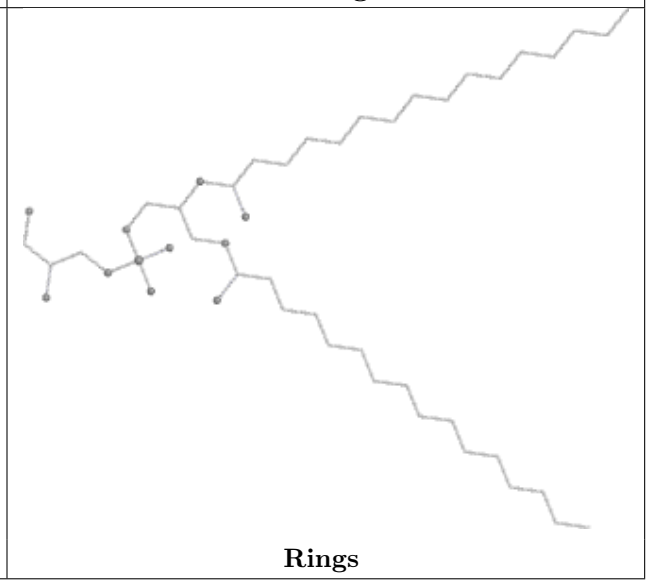
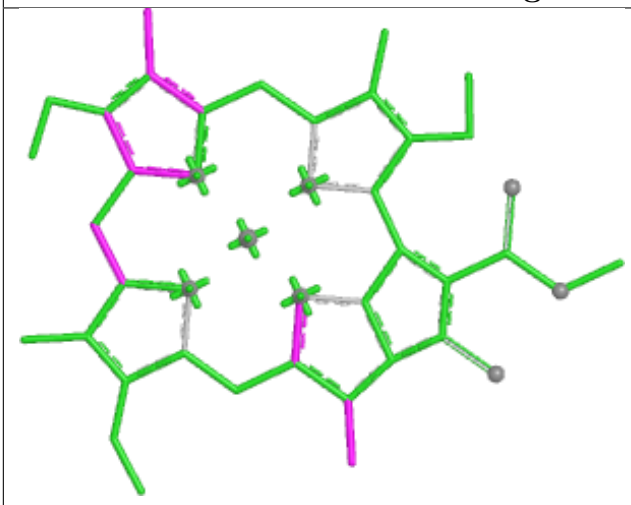


Rings

Ligand CLA X 614



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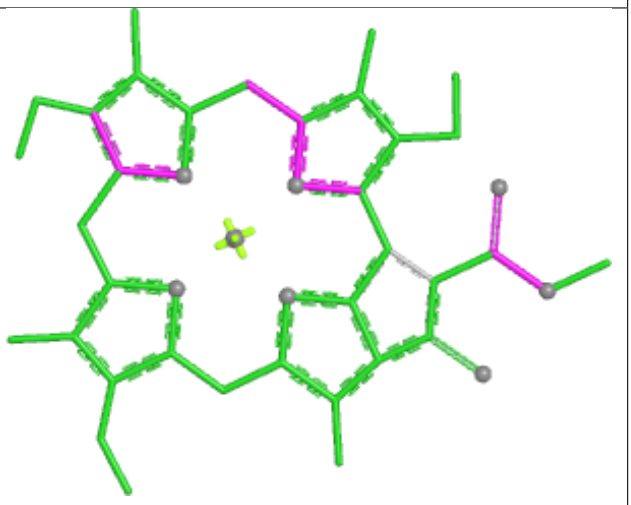
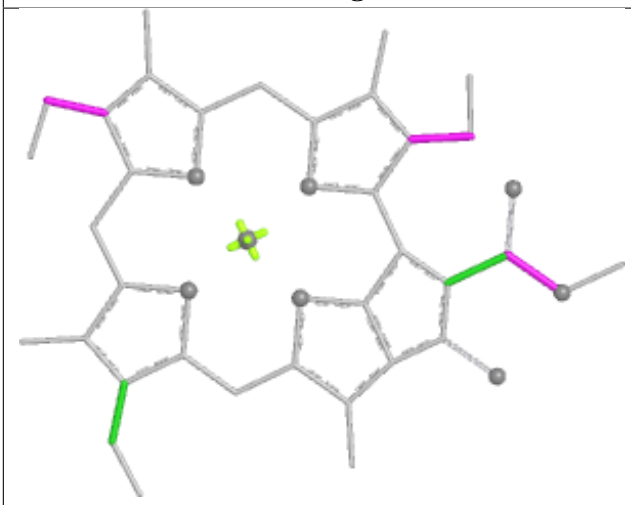


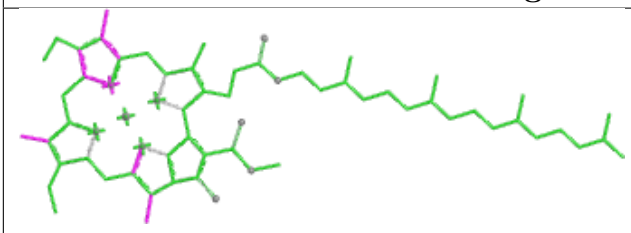
Bond angles



Torsions

Rings

Ligand CLA B 805



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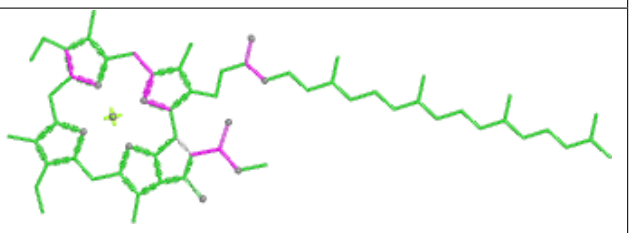
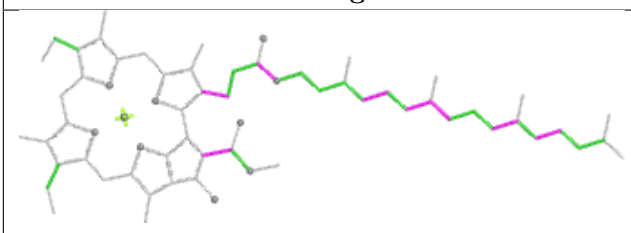


Bond angles



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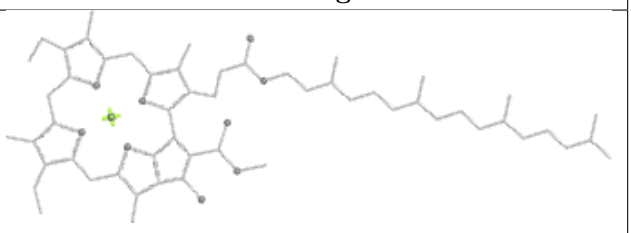
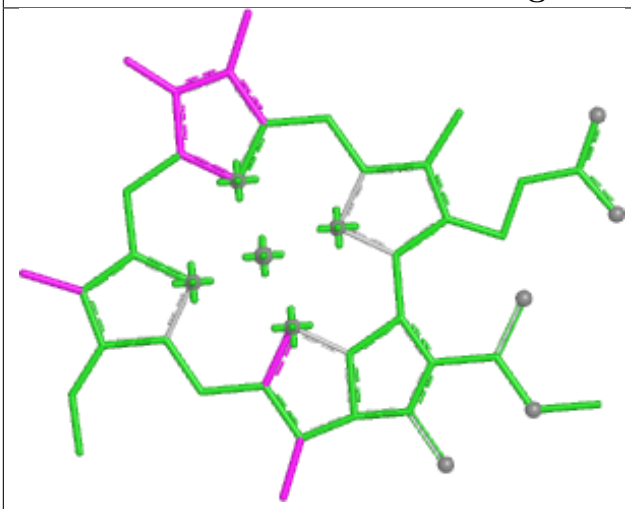


Rings

Ligand CLA 9 603



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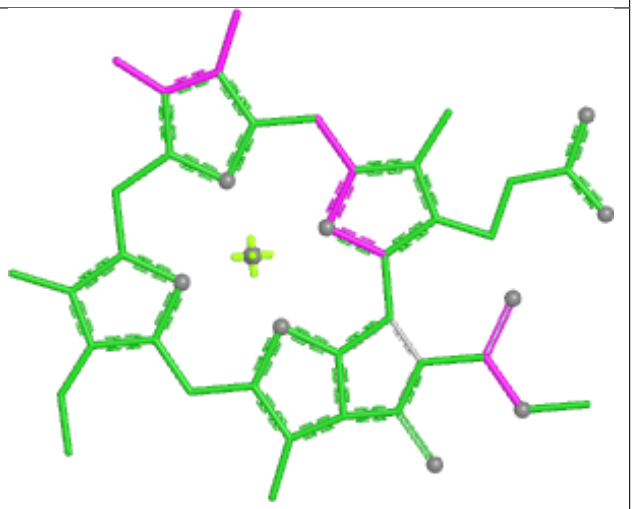
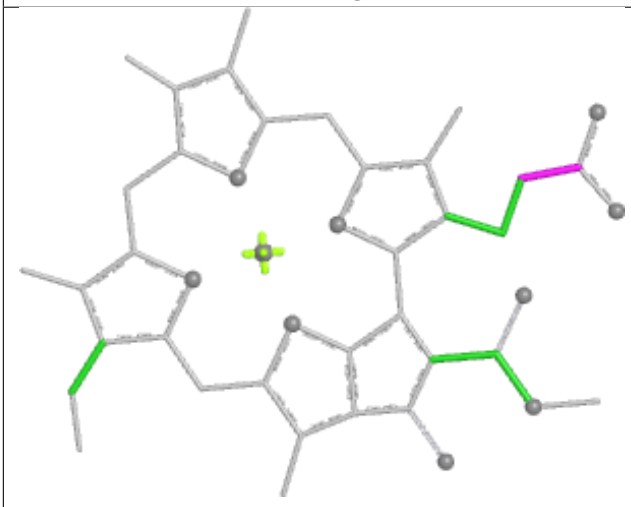


Bond angles



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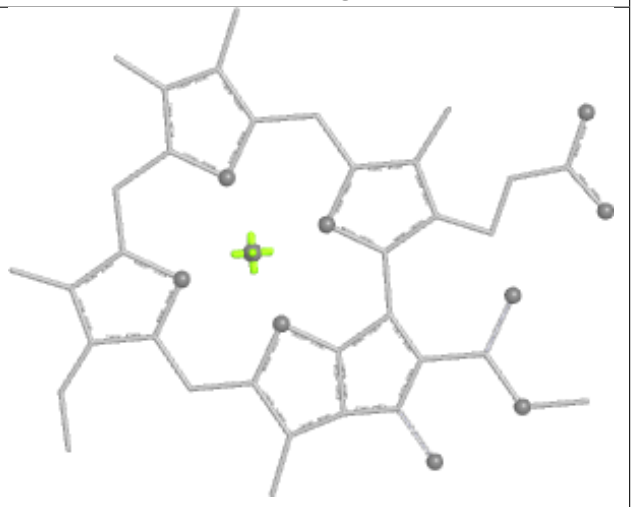
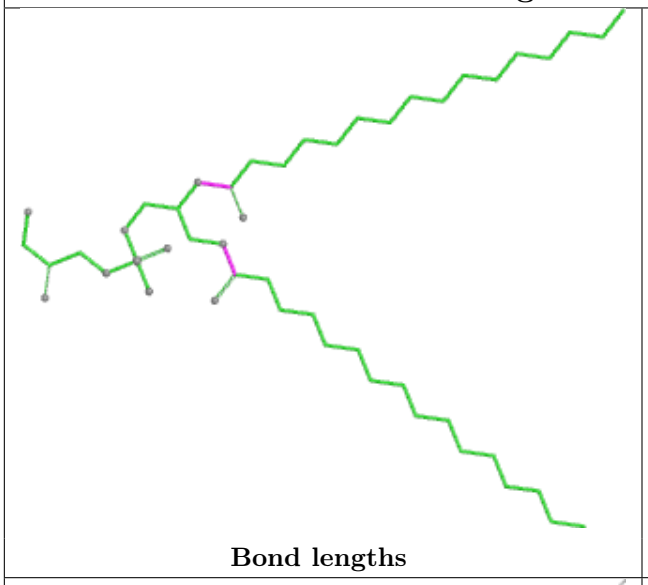


Rings

Ligand LHG Z 2630



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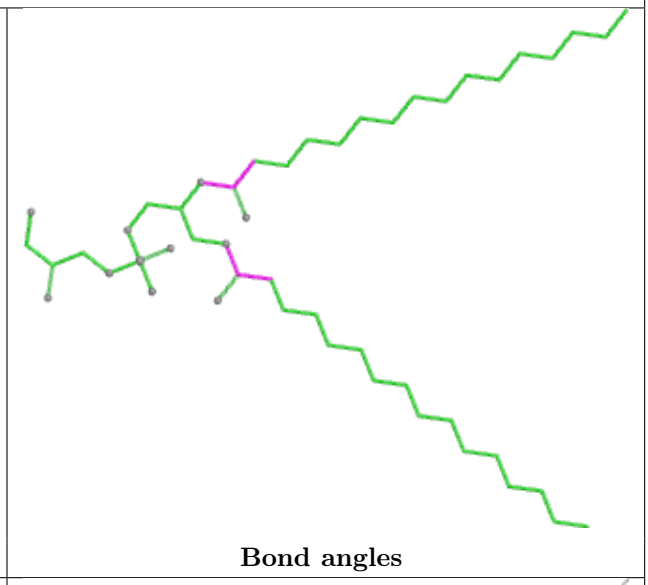
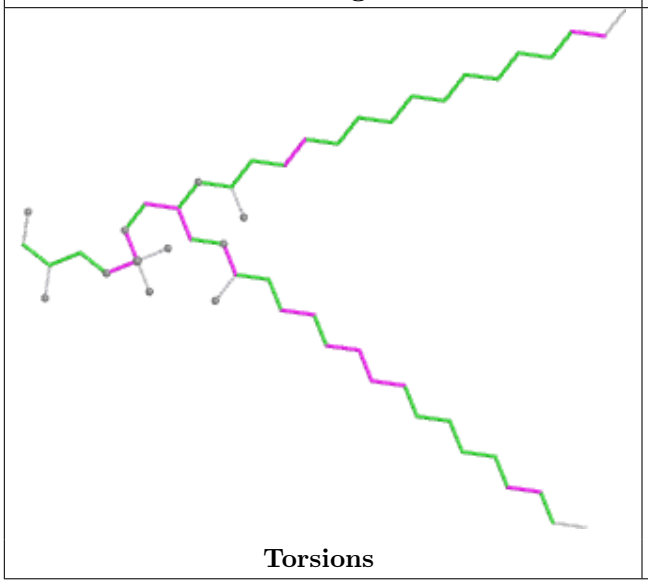


Bond angles



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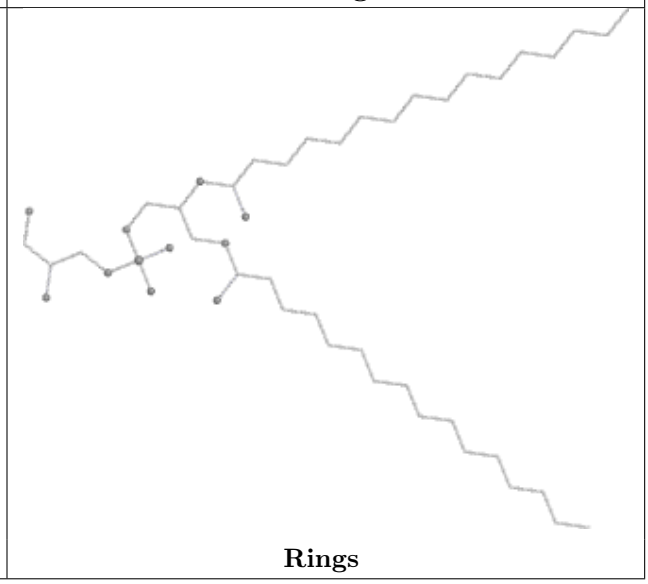
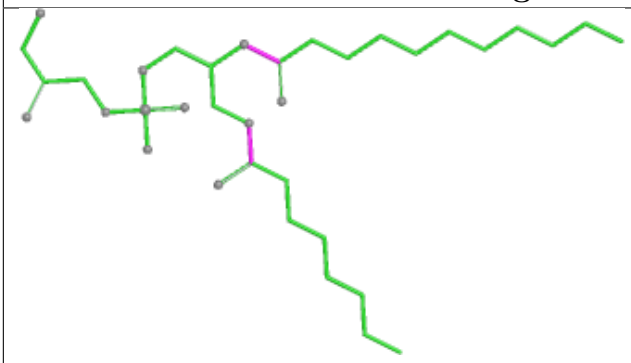


Rings

Ligand LHG O 2631



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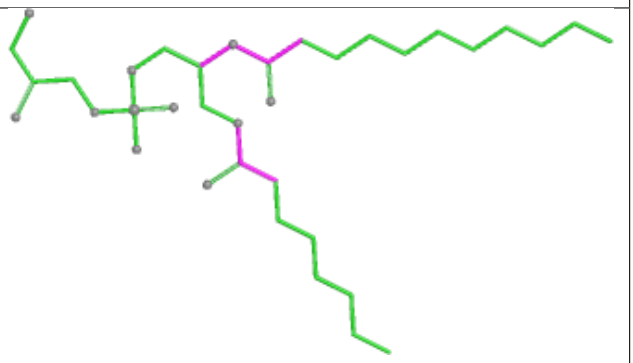
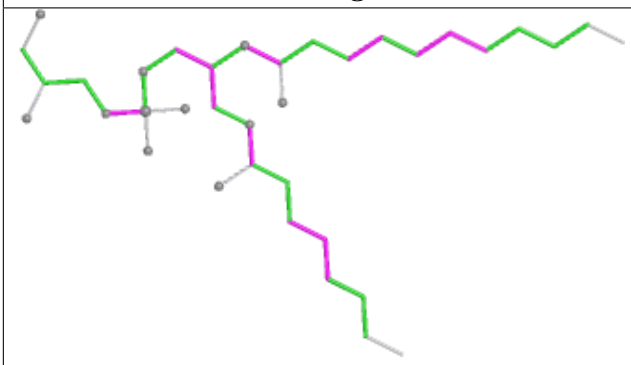


Bond angles



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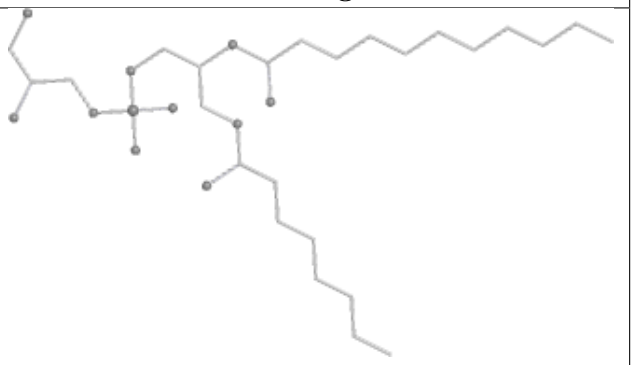
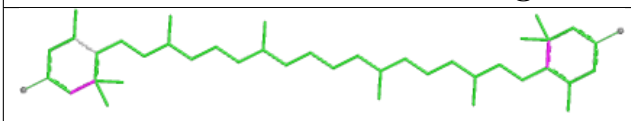


Rings

Ligand LUT U 1621



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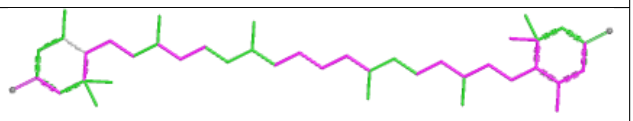
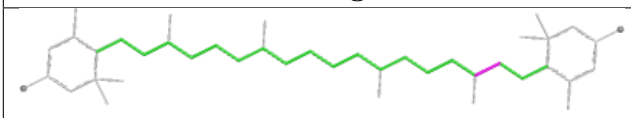


Bond angles



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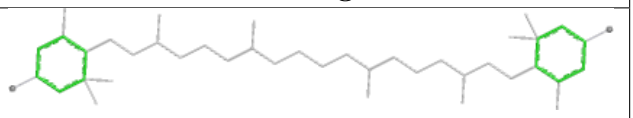
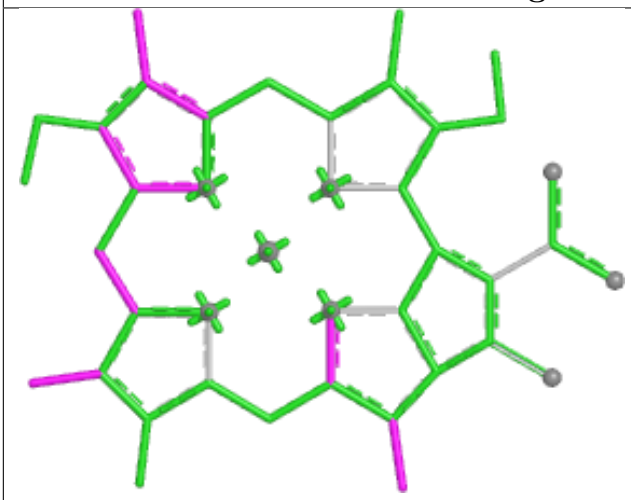


Rings

Ligand CLA 9 606



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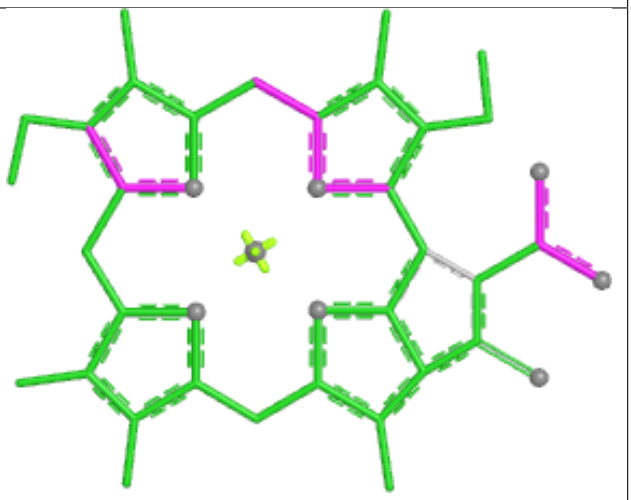

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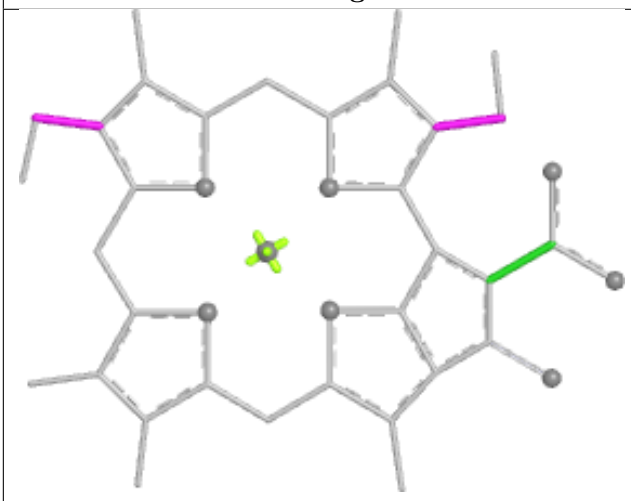

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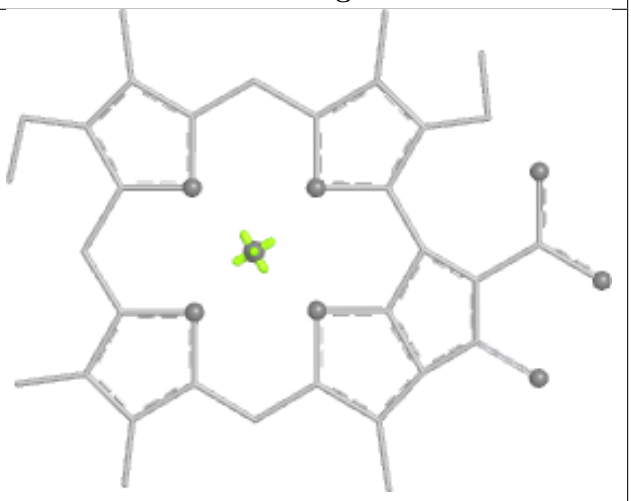
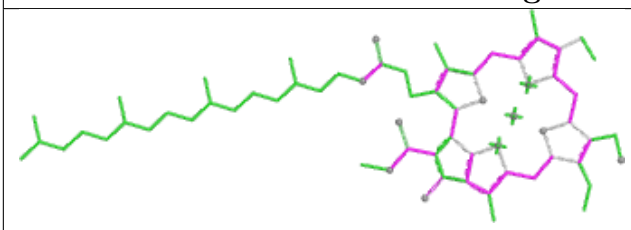


Rings

Ligand CHL Y 607



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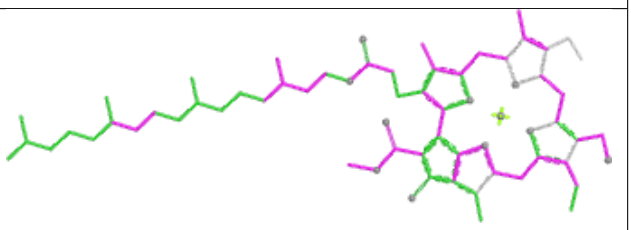
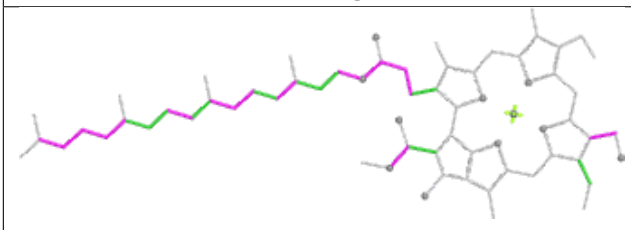
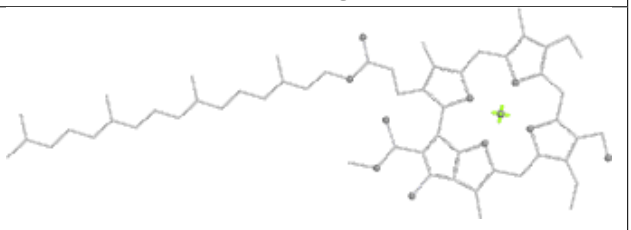


Bond angles

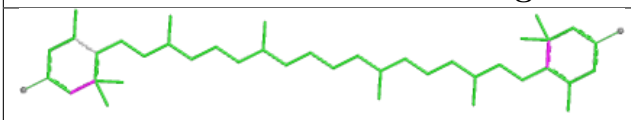


Torsions



Rings

Ligand LUT V 1620



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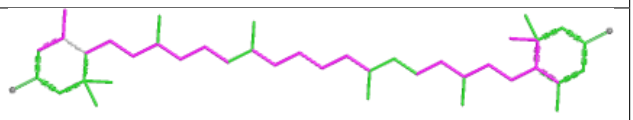
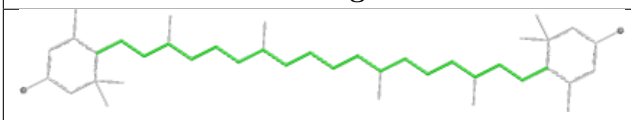


Bond angles



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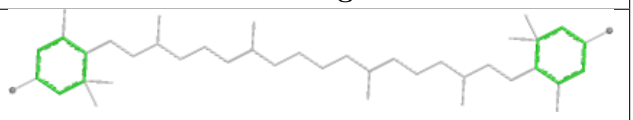
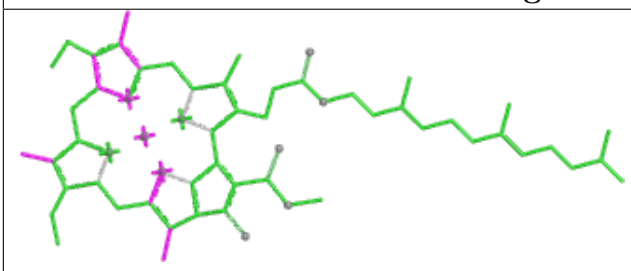


Rings

Ligand CLA V 602



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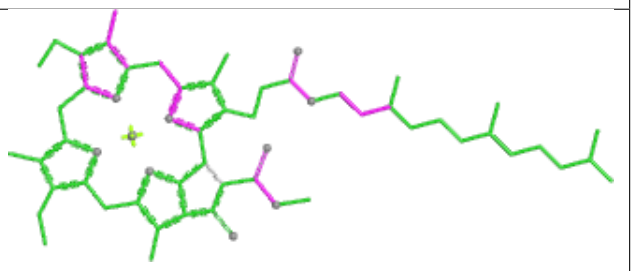
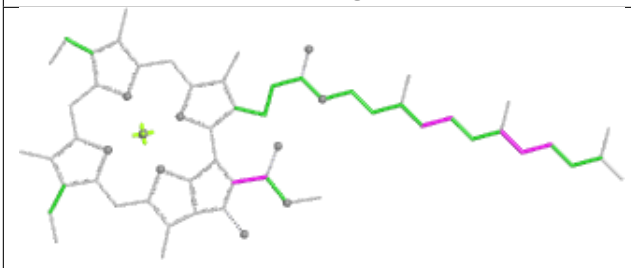
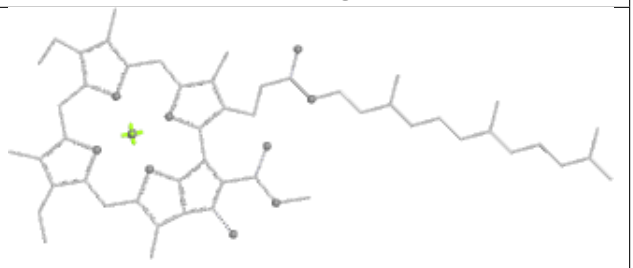


Bond angles

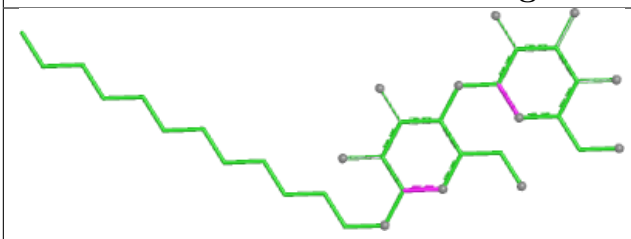


Torsions

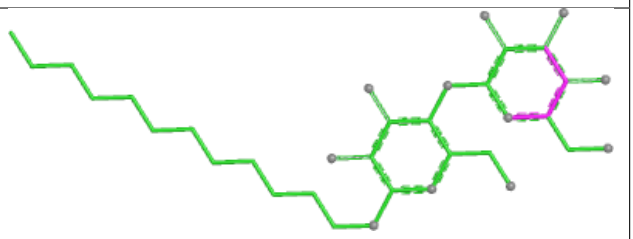


Rings

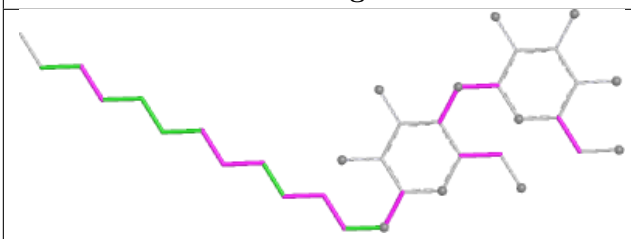
Ligand LMU K 208



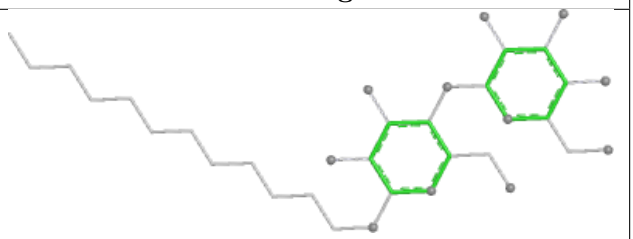
Bond lengths



Bond angles

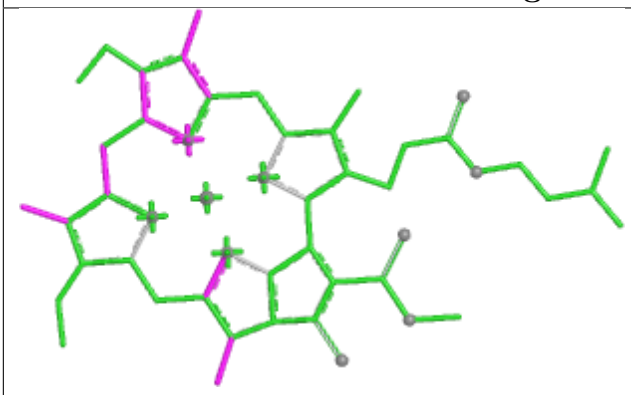


Torsions



Rings

Ligand CLA A 810



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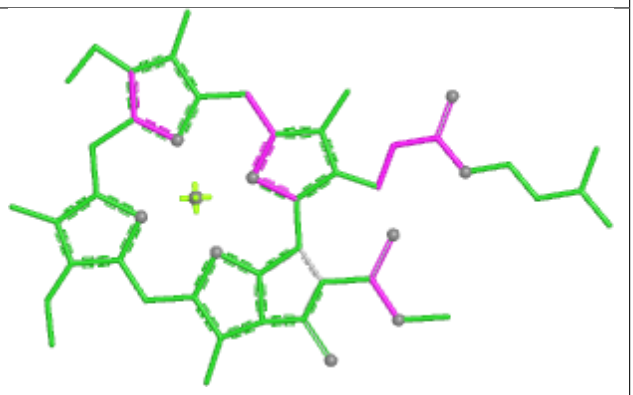

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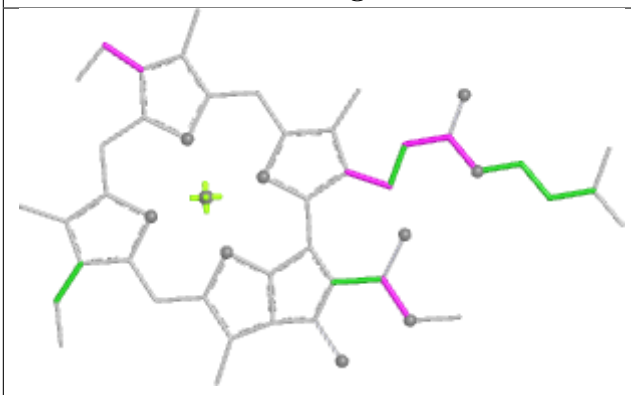

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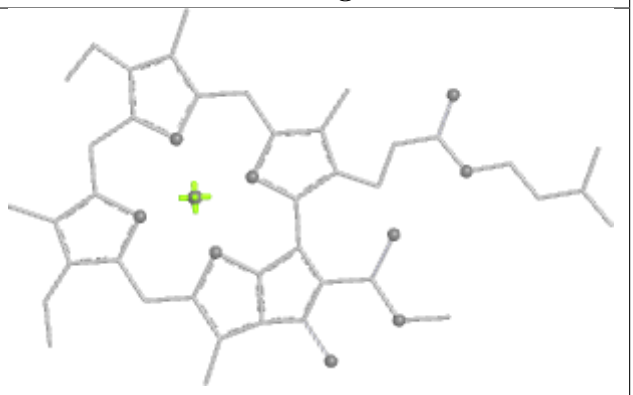
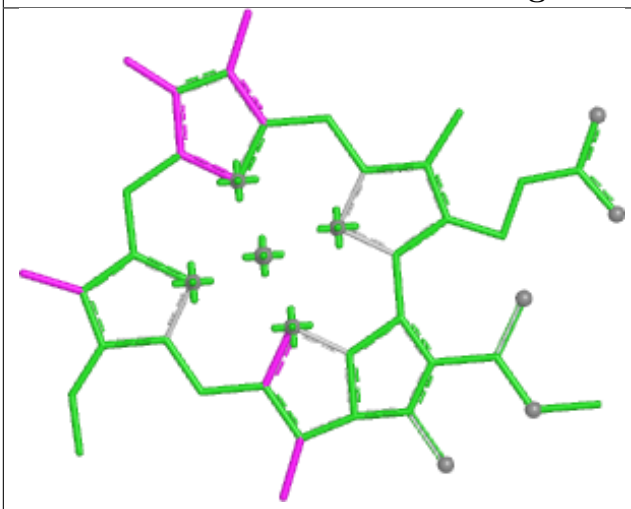


Rings

Ligand CLA 4 603



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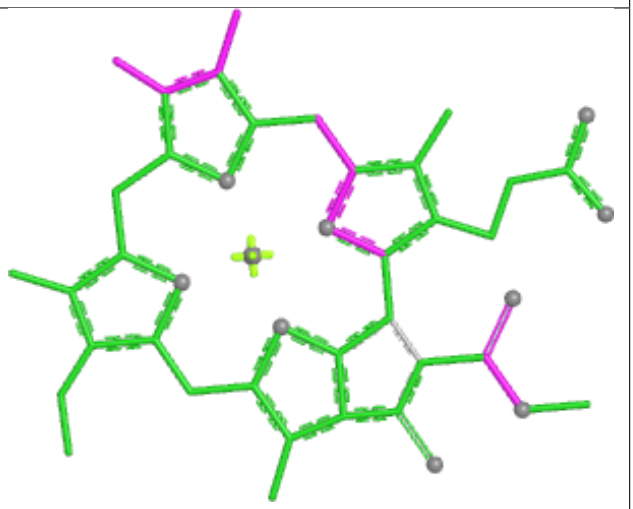
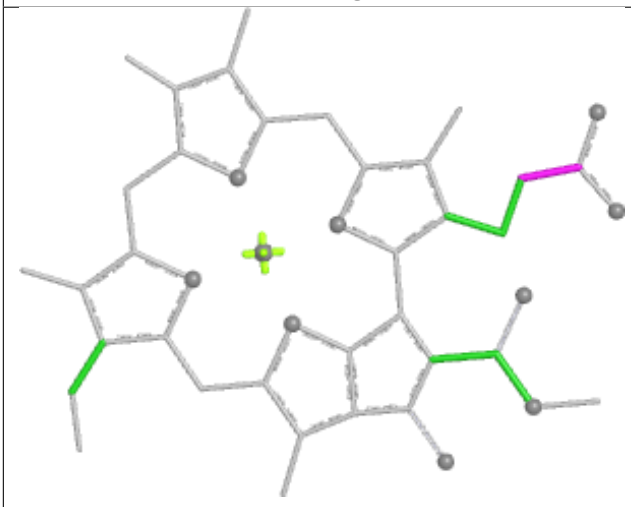


Bond angles



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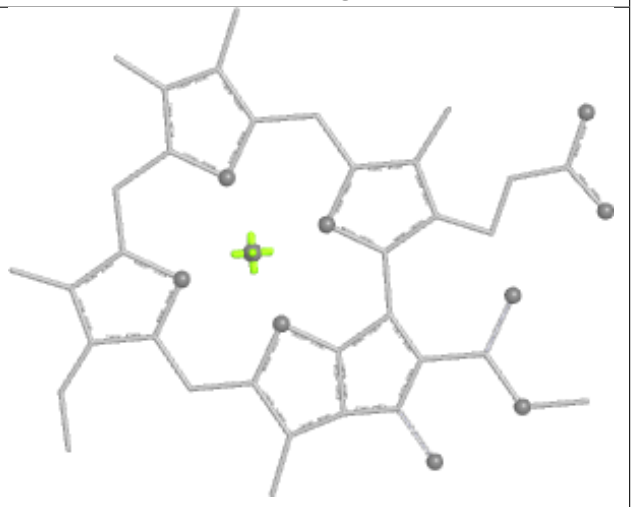
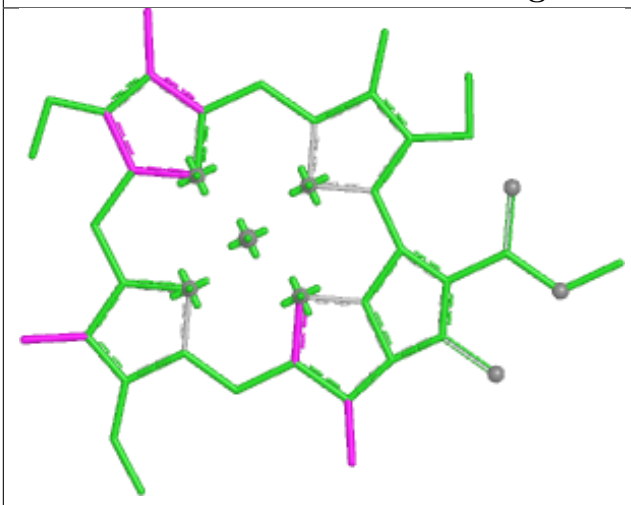


Rings

Ligand CLA 5 611



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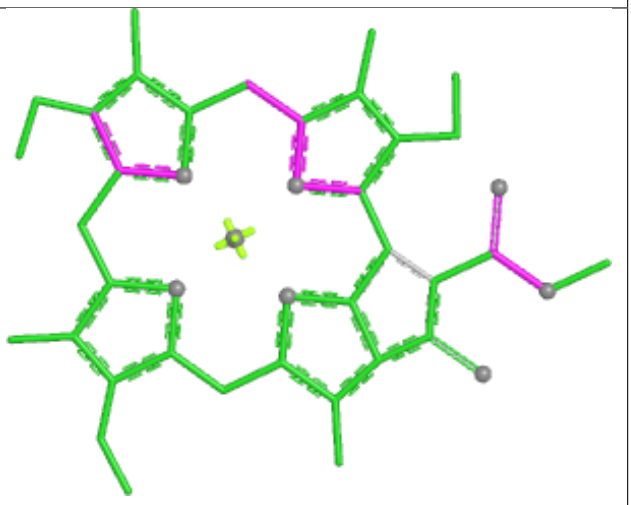
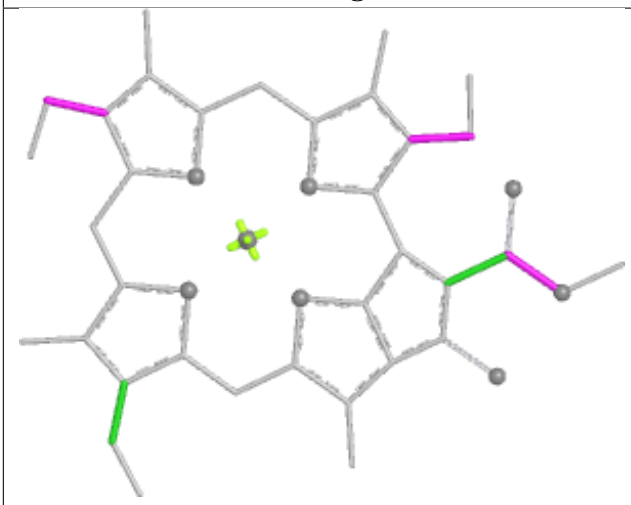


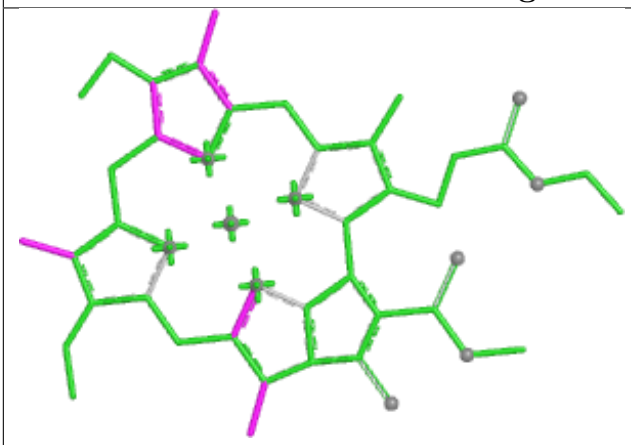
Bond angles



Torsions

Rings

Ligand CLA W 604



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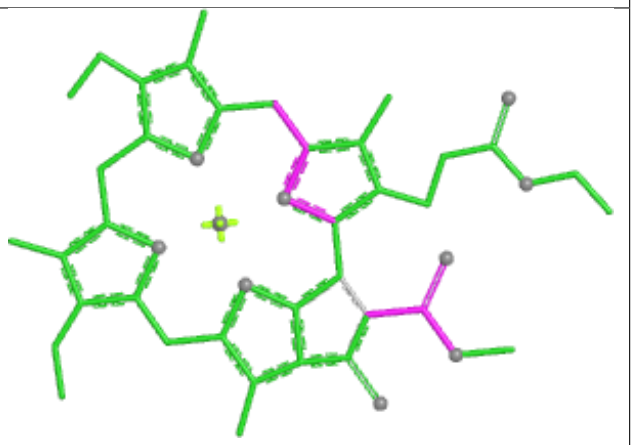
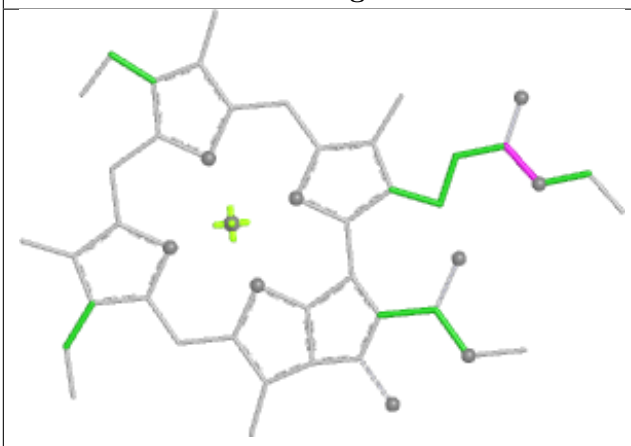


Bond angles



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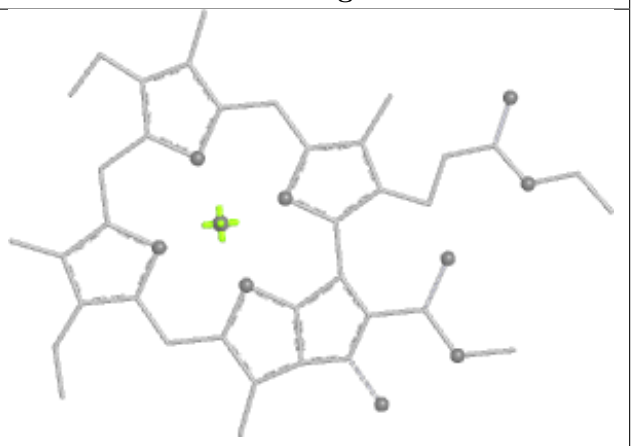
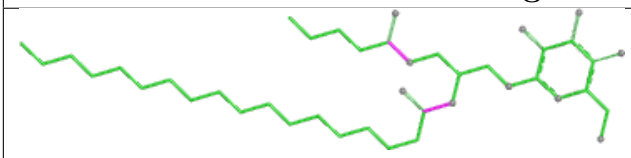


Rings

Ligand LMG J 103



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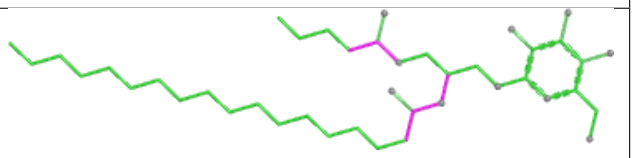
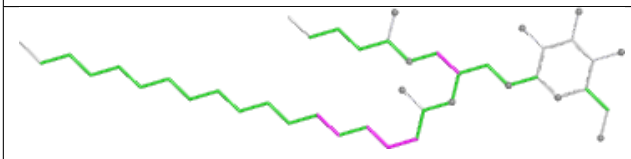


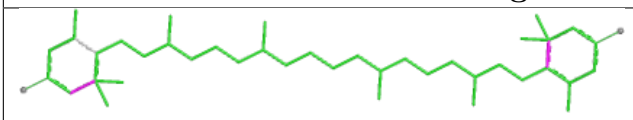
Bond angles



Torsions

Rings

Ligand LUT W 1621



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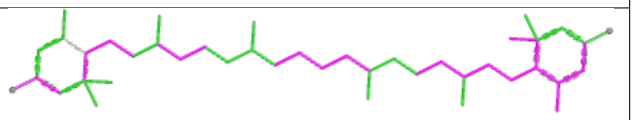
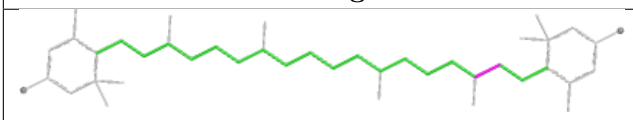


Bond angles



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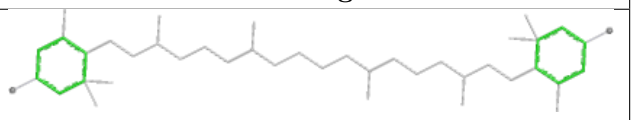
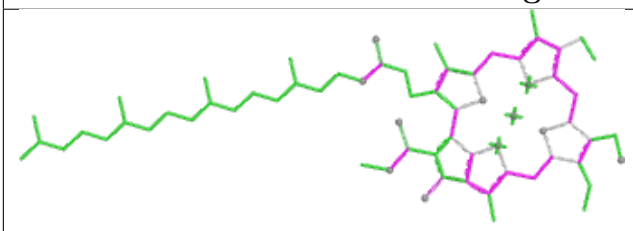
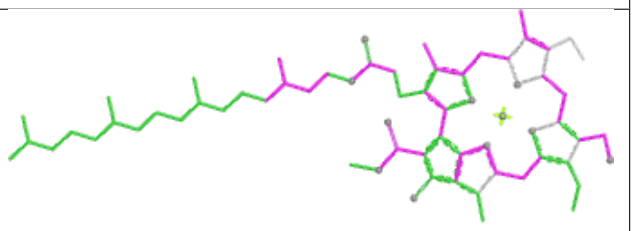


Rings

Ligand CHL X 608



Bond lengths



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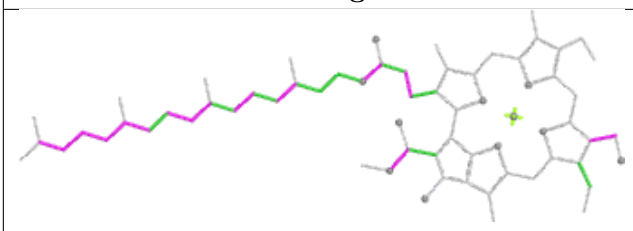

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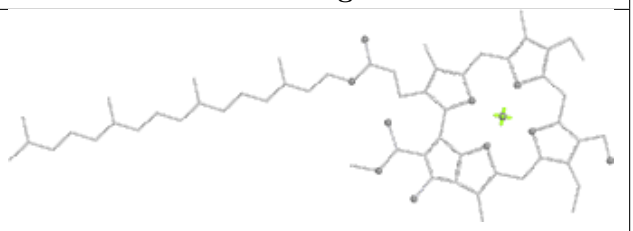
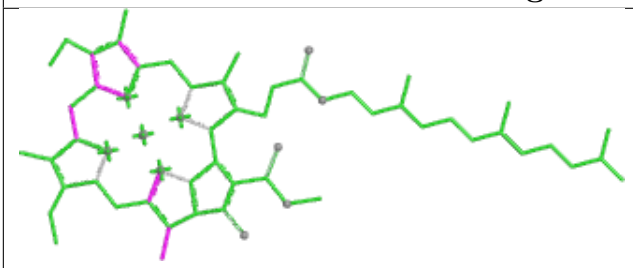


Rings

Ligand CLA Z 602



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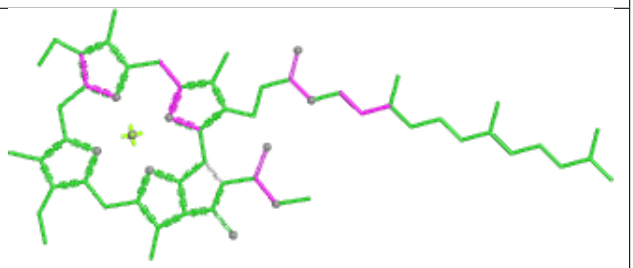
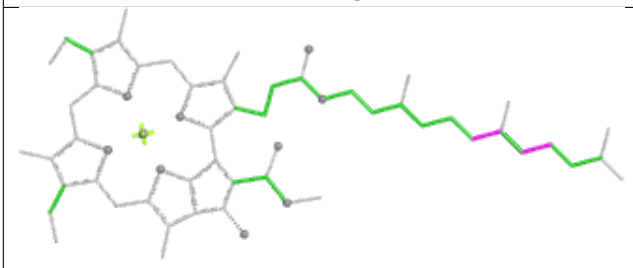


Bond angles



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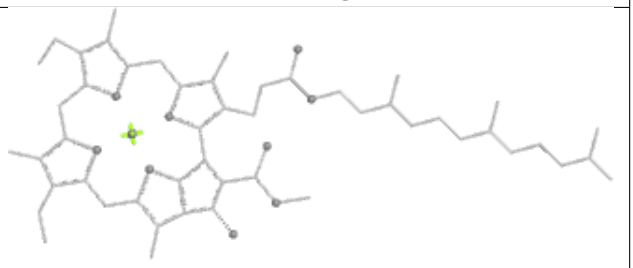
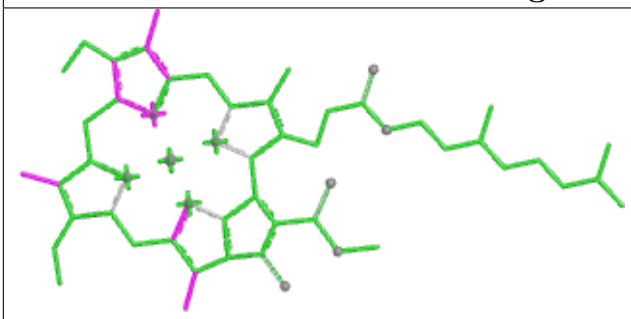


Rings

Ligand CLA 3 608



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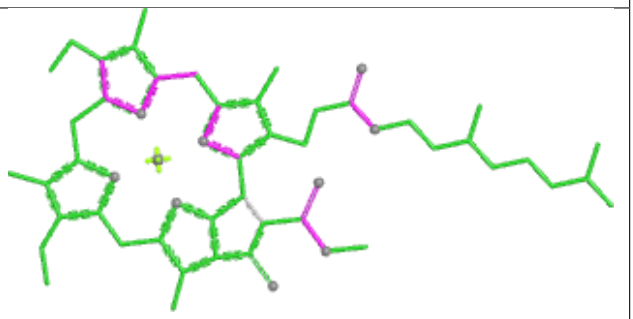
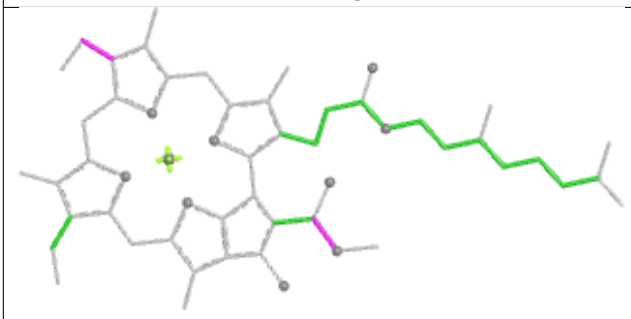


Bond angles



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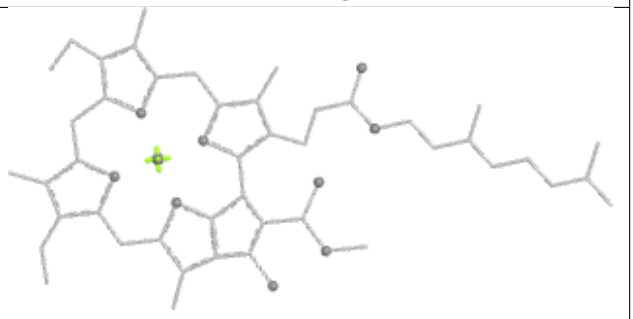
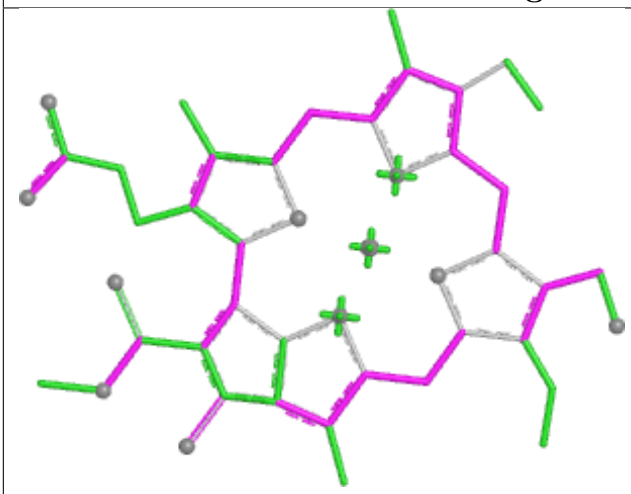


Rings

Ligand CHL Z 606



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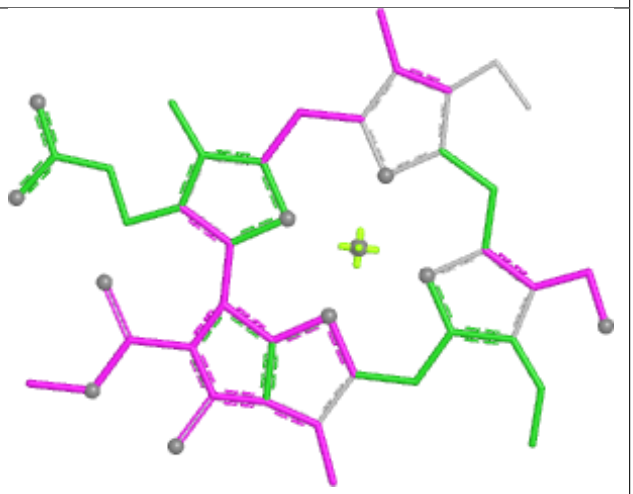

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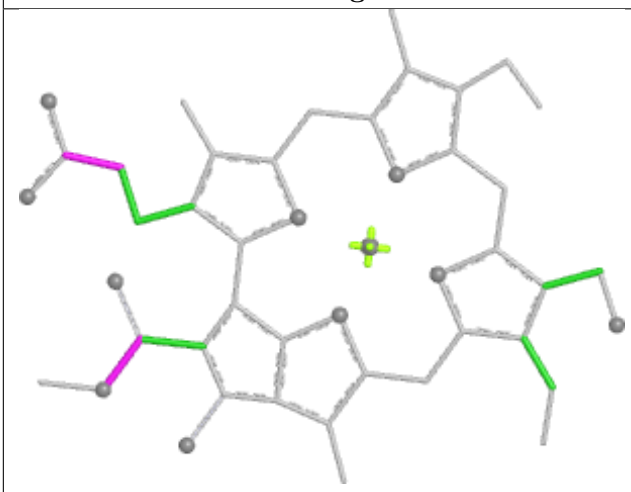

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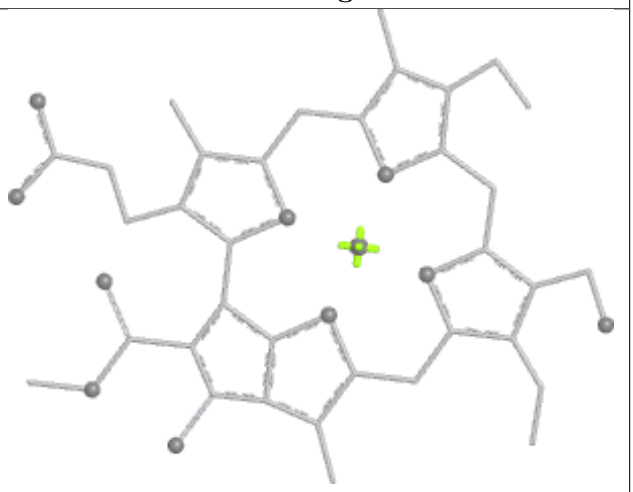
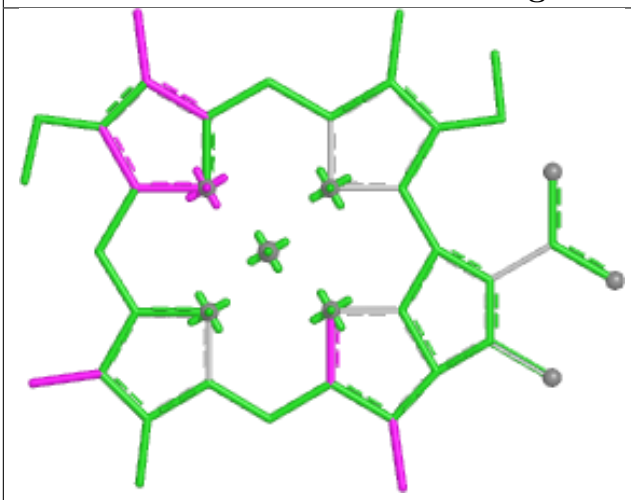


Rings

Ligand CLA 4 606



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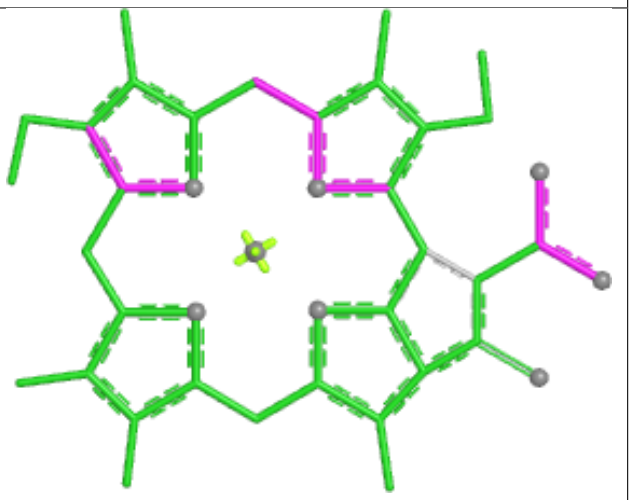

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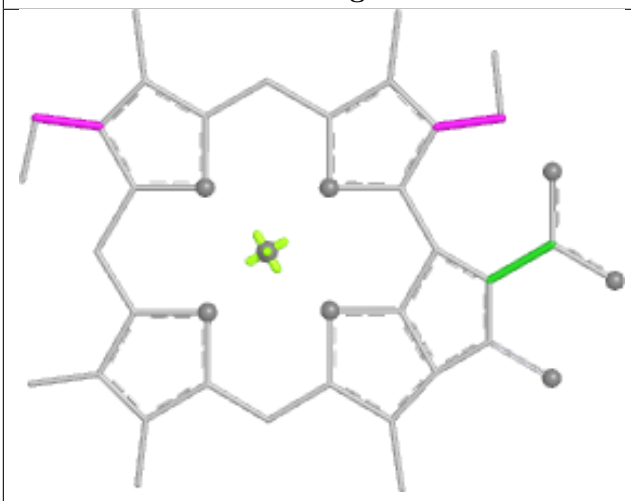
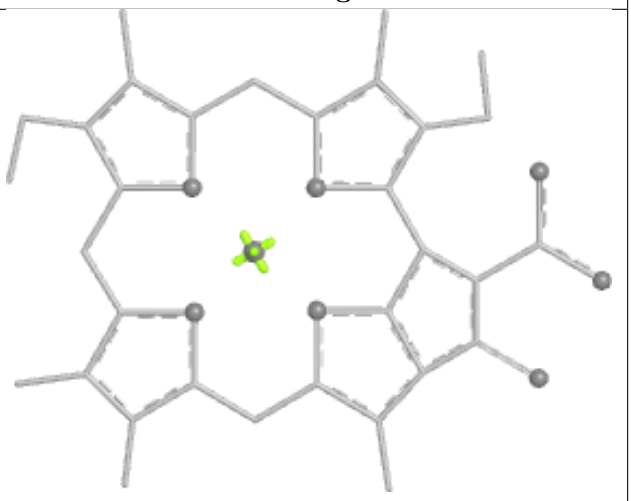
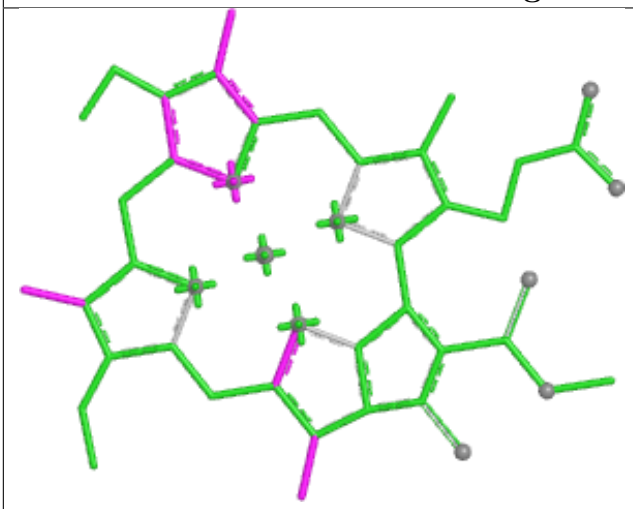


Torsions



Rings

Ligand CLA A 833



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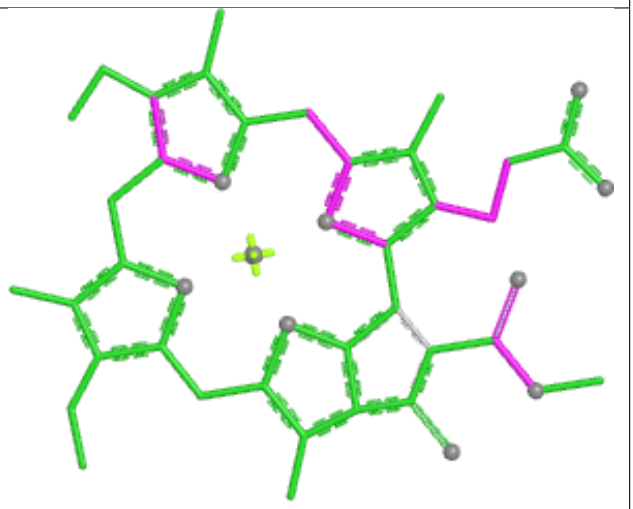
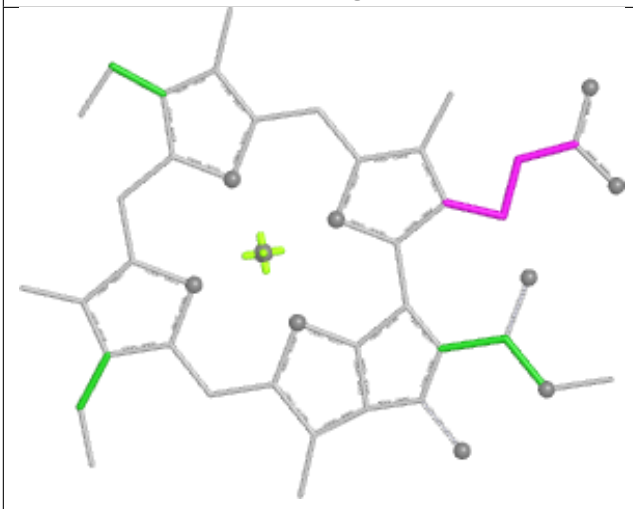


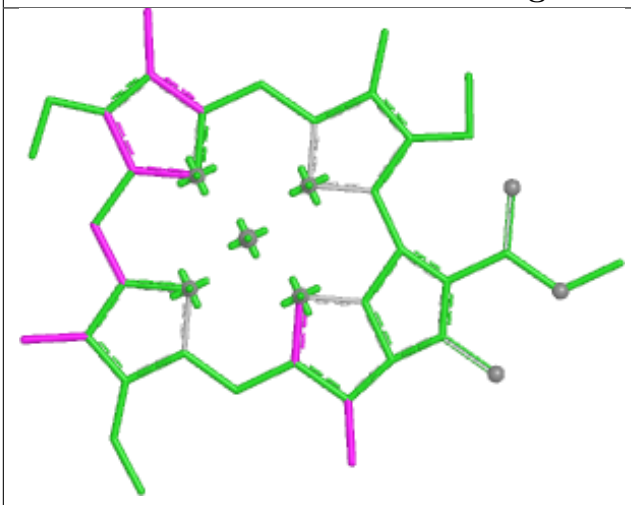
Bond angles



Torsions

Rings

Ligand CLA 8 611



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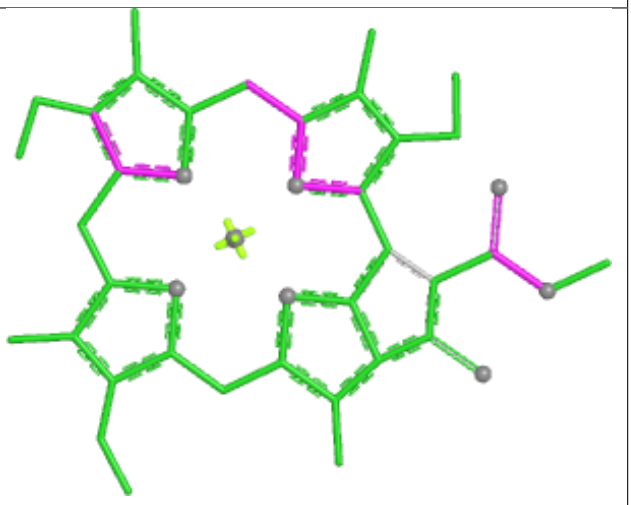
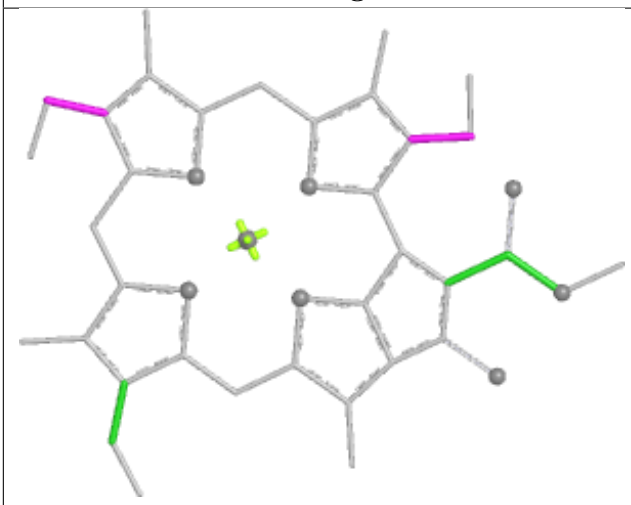


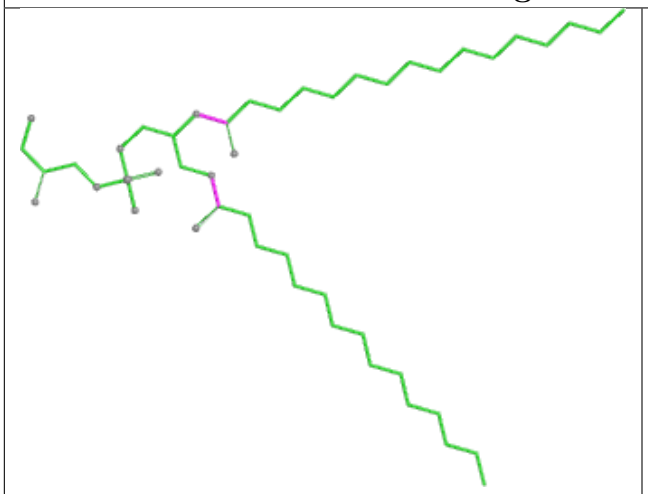
Bond angles



Torsions

Rings

Ligand LHG V 2630



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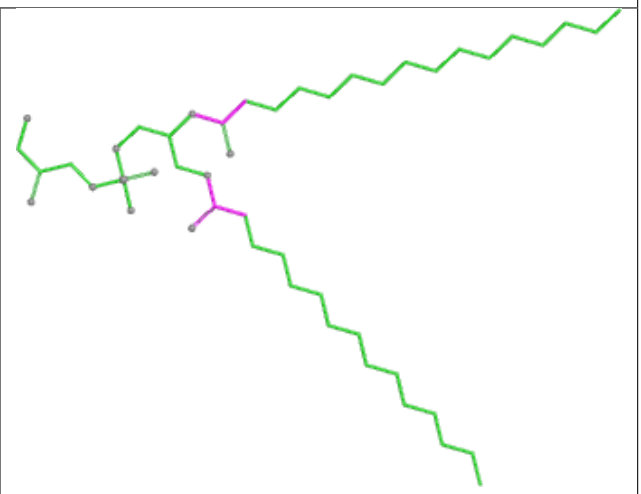
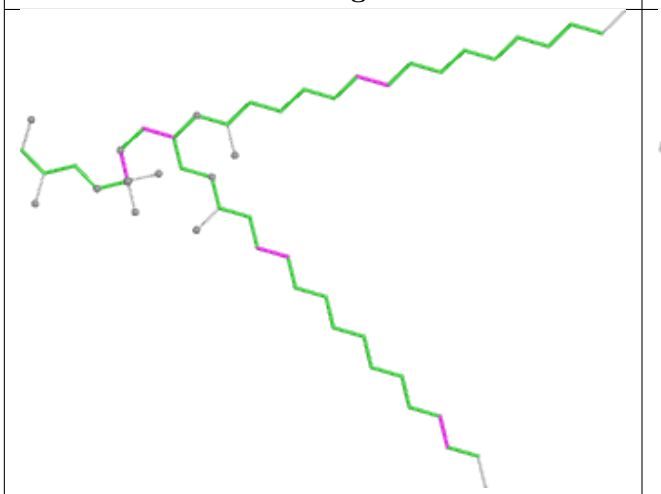
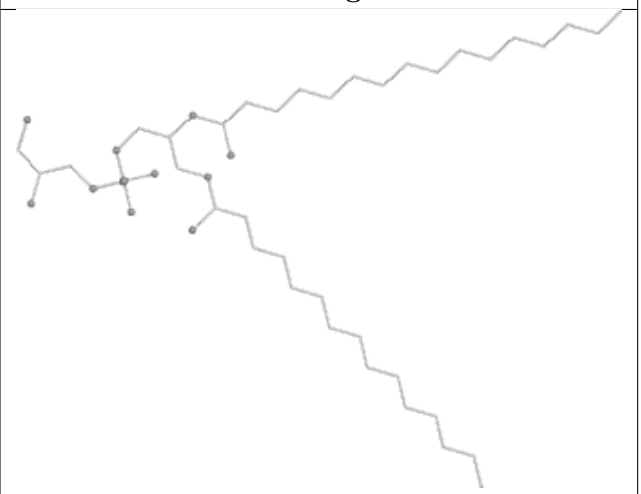


Bond angles

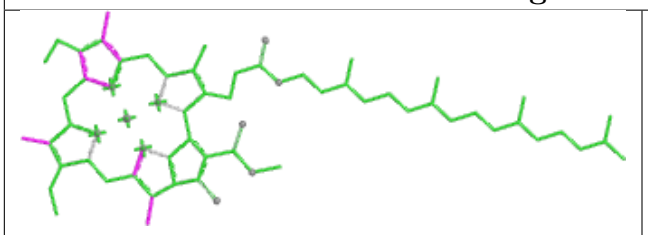


Torsions

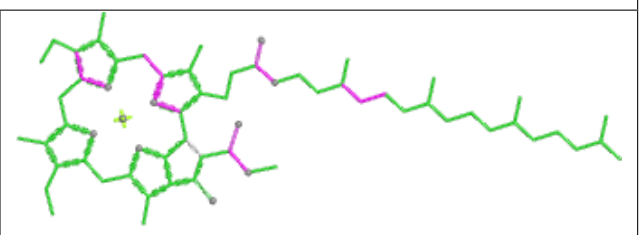


Rings

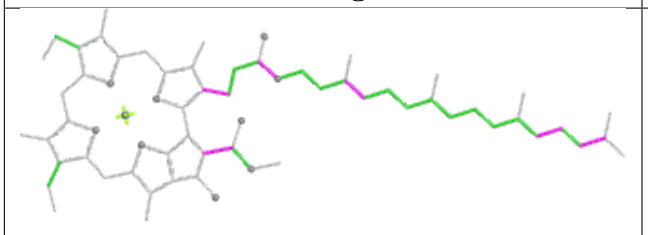
Ligand CLA 6 601



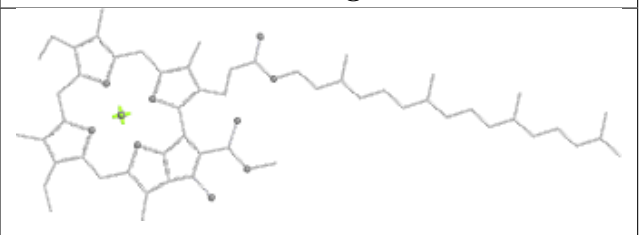
Bond lengths



Bond angles

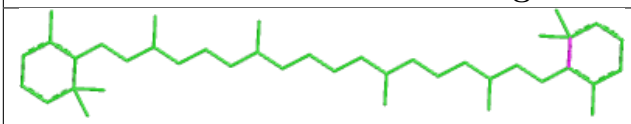


Torsions



Rings

Ligand BCR O 2005



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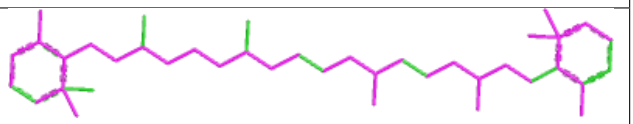

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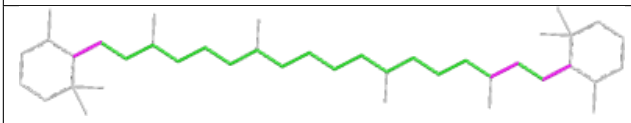

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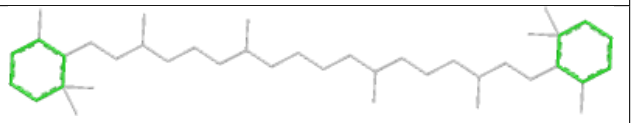
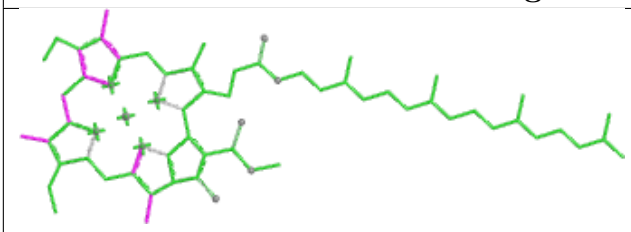


Rings

Ligand CLA B 833



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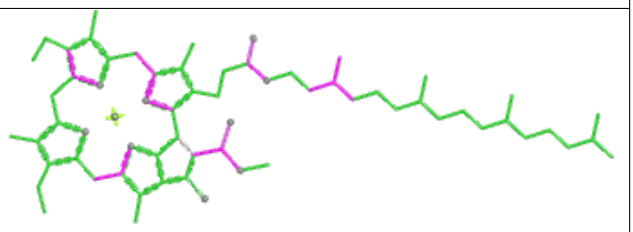
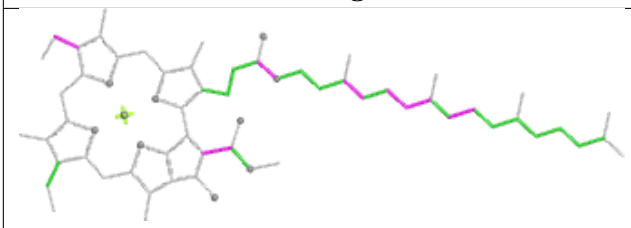
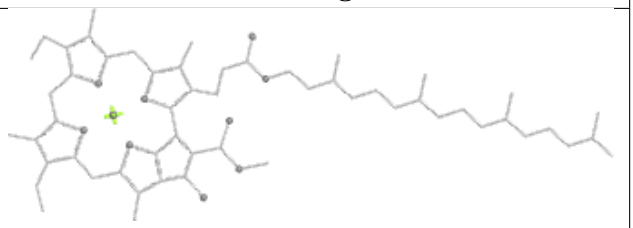


Bond angles

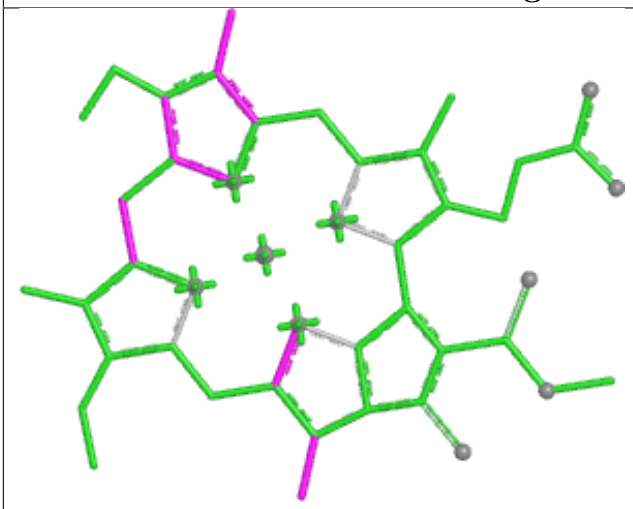


Torsions



Rings

Ligand CLA Y 612



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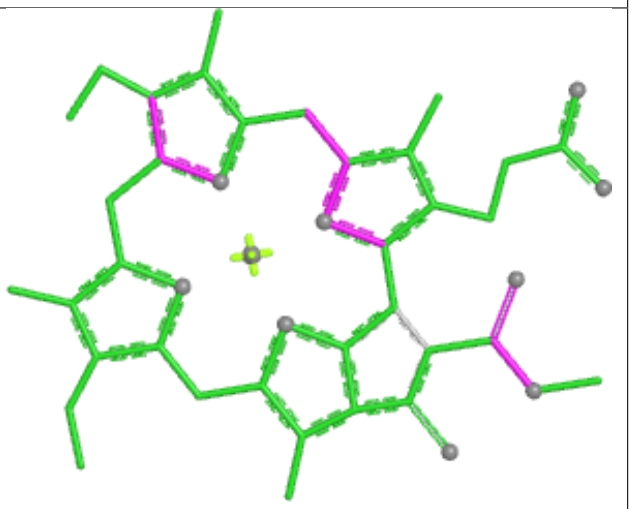
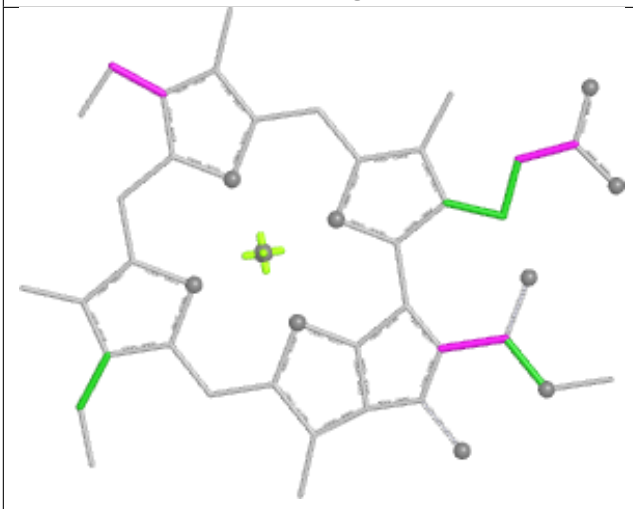


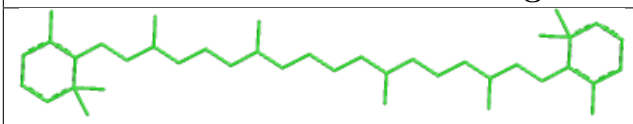
Bond angles



Torsions

Rings

Ligand BCR F 305



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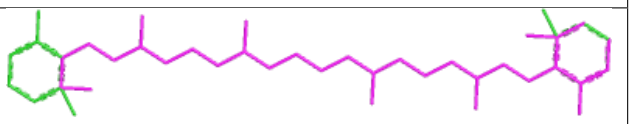
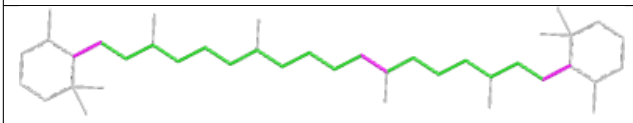
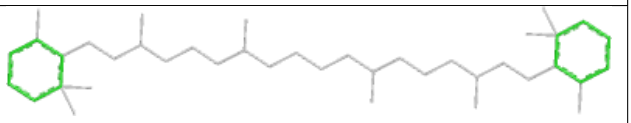


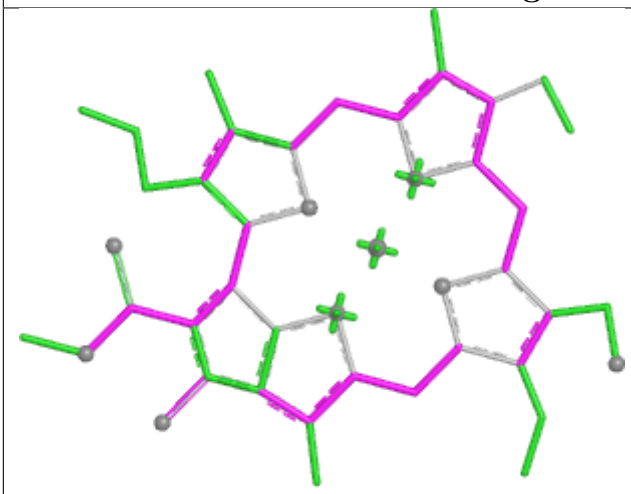
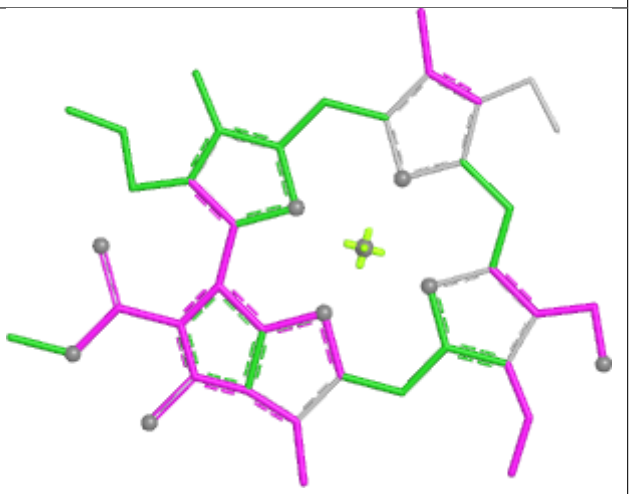
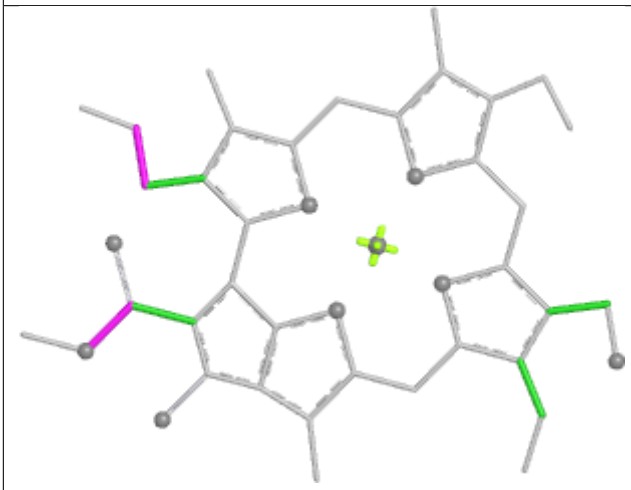
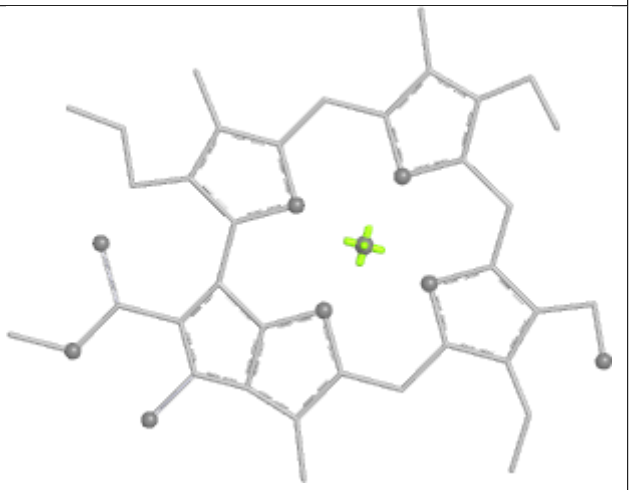
Bond angles

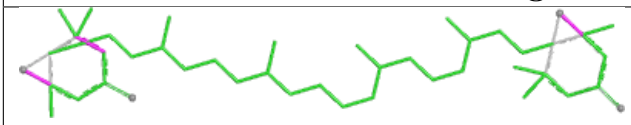
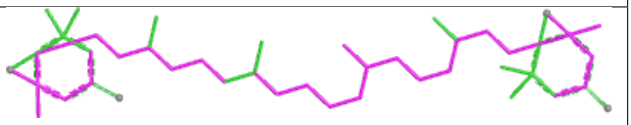
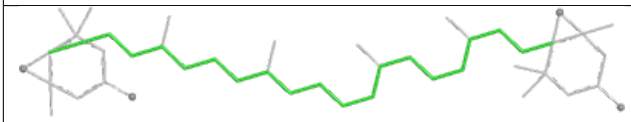
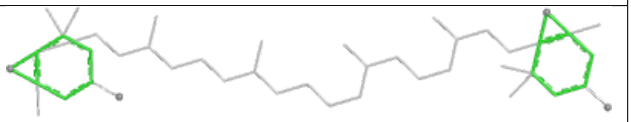


Torsions

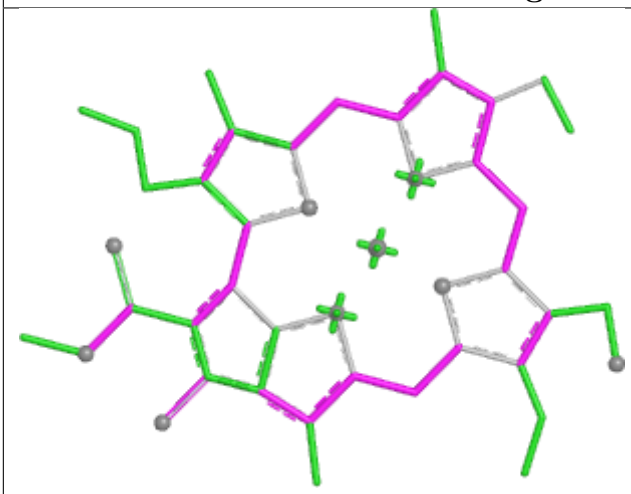


Rings

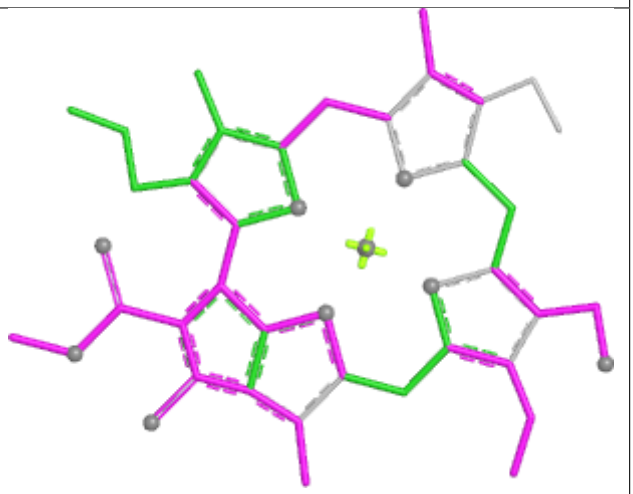
Ligand CHL U 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT 9 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

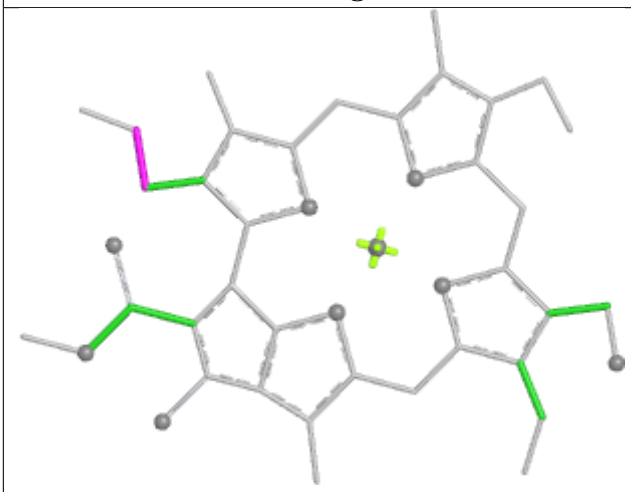
Ligand CHL Z 605



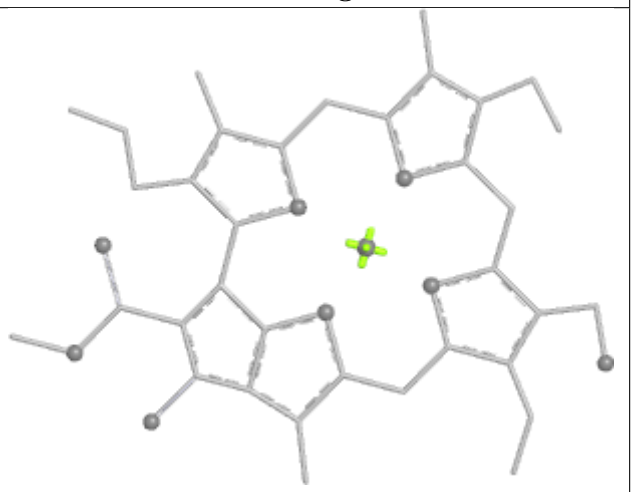
Bond lengths



Bond angles

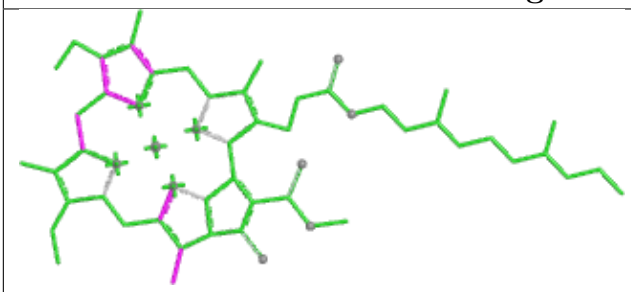


Torsions



Rings

Ligand CLA Z 604



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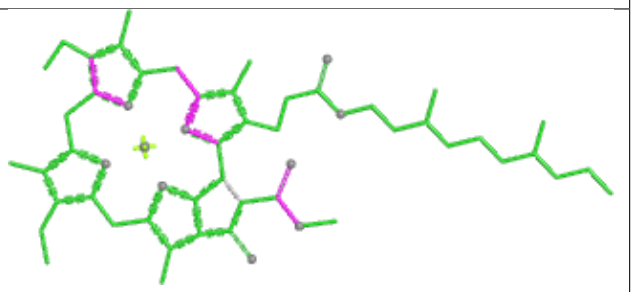
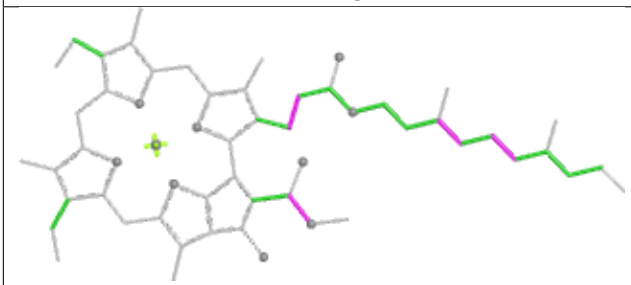
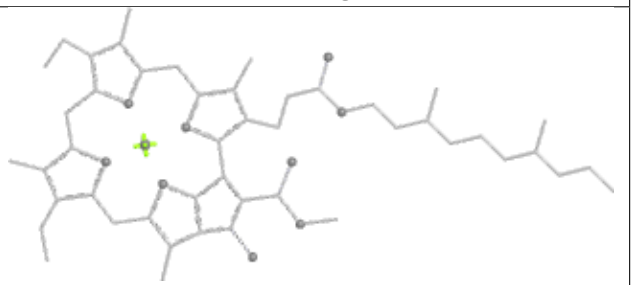


Bond angles

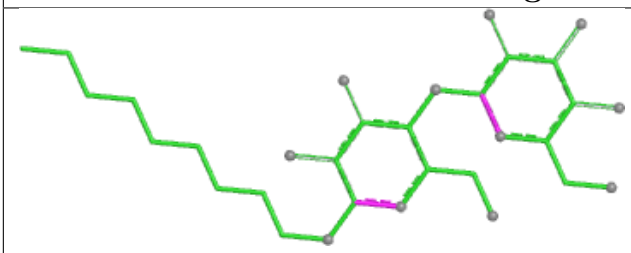


Torsions



Rings

Ligand LMU 5 629



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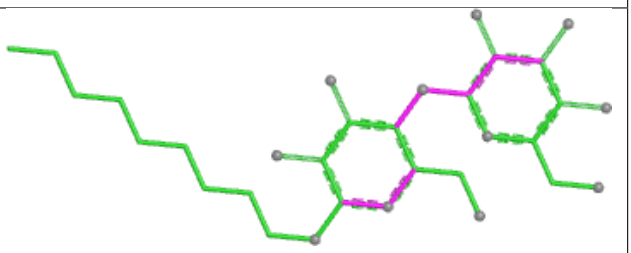
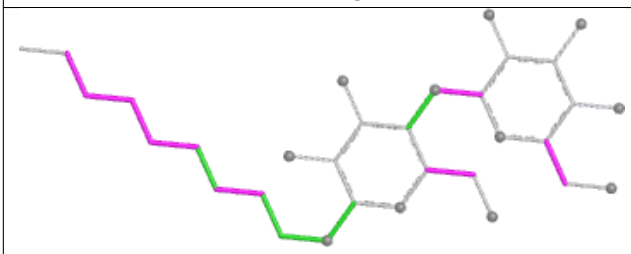


Bond angles



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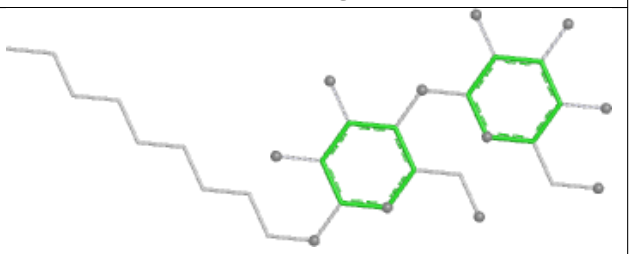
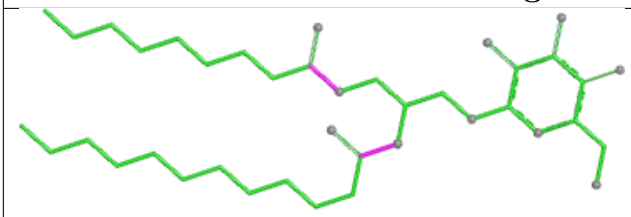


Rings

Ligand LMG 4 623



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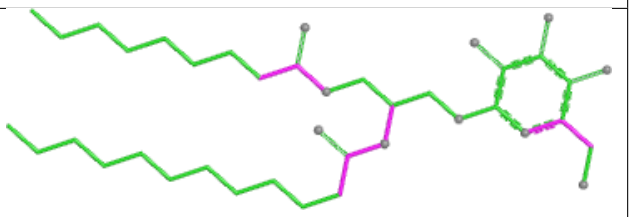
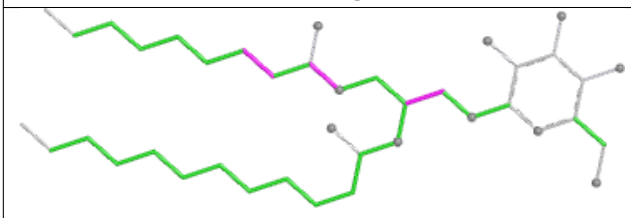
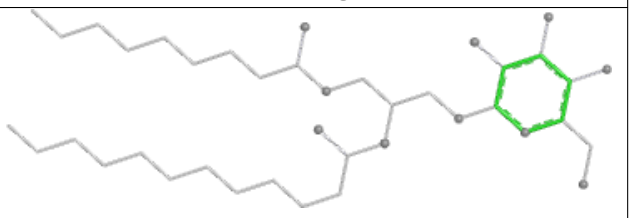


Bond angles

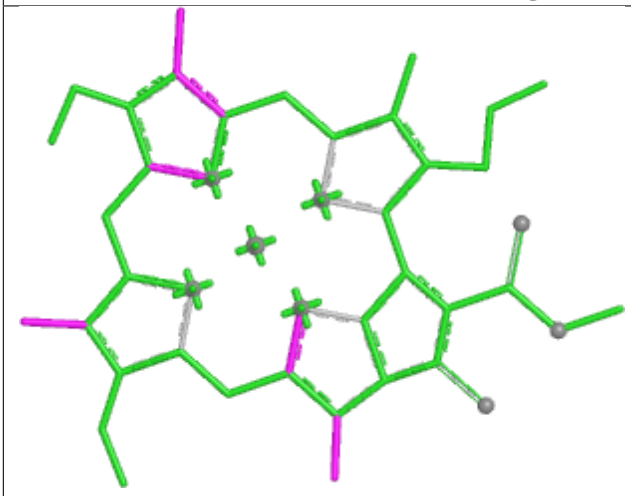


Torsions



Rings

Ligand CLA B 815



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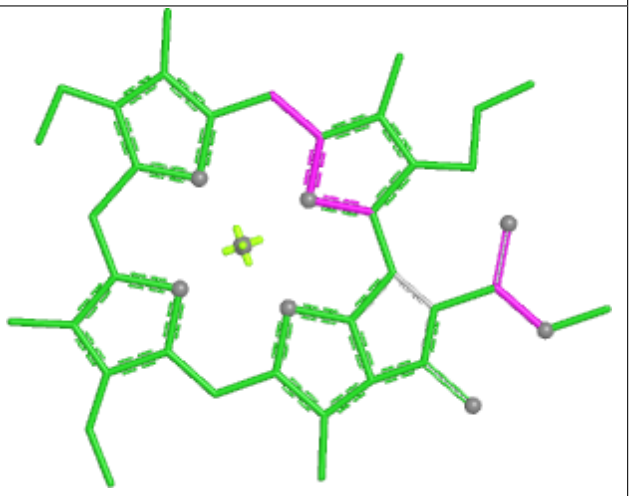
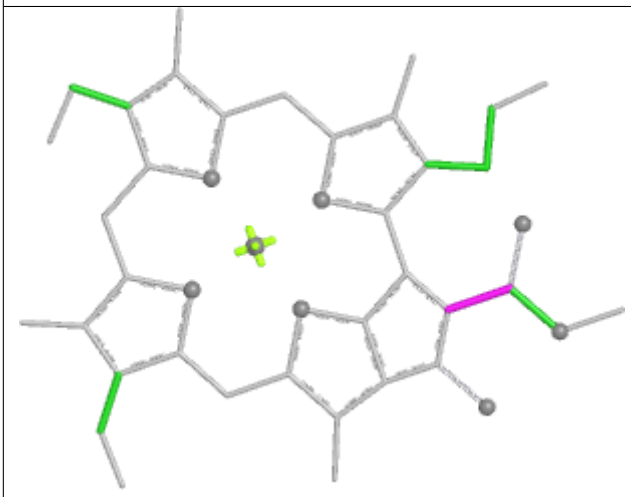
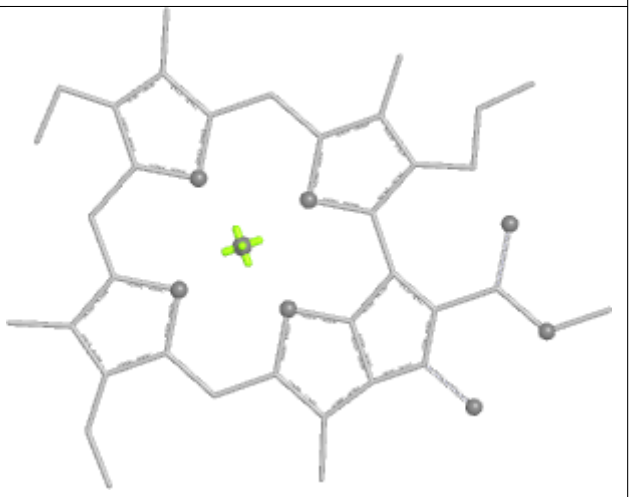


Bond angles

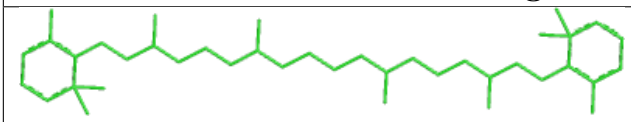


Torsions

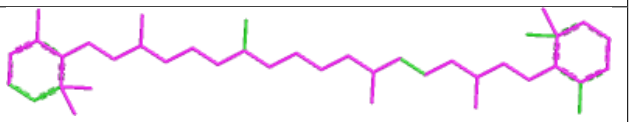


Rings

Ligand BCR L 301

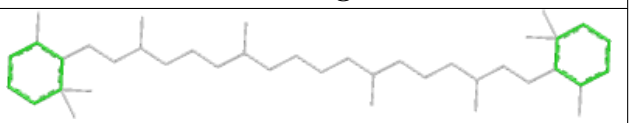


Bond lengths



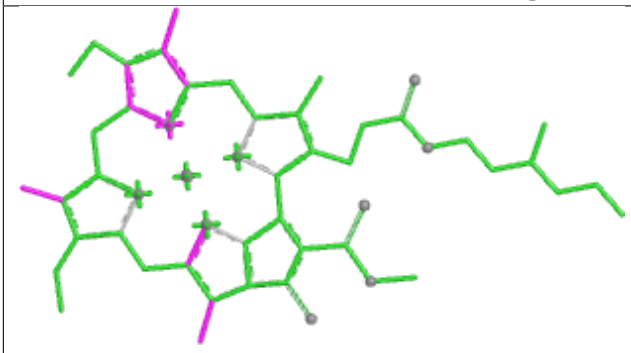
Bond angles

Torsions

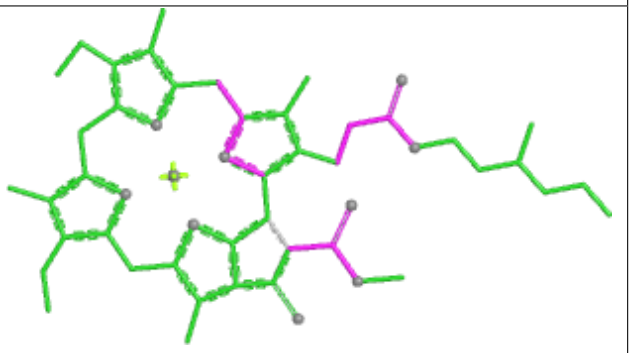


Rings

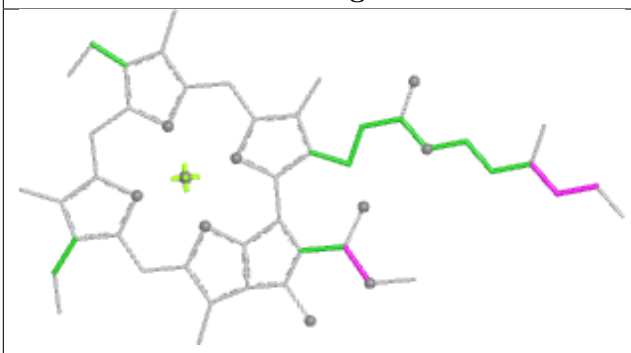
Ligand CLA A 840



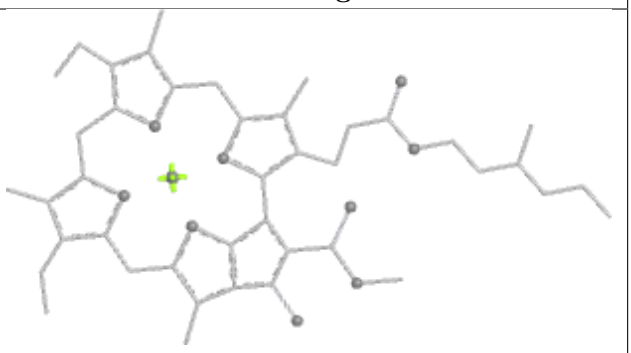
Bond lengths



Bond angles

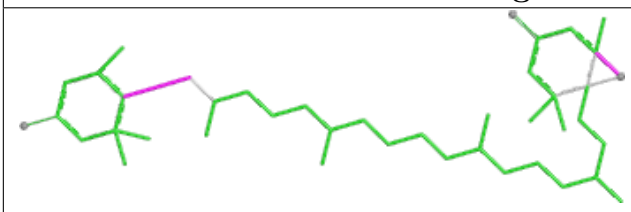


Torsions

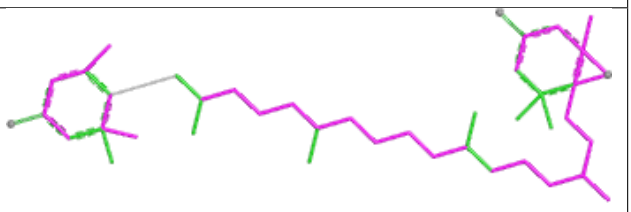


Rings

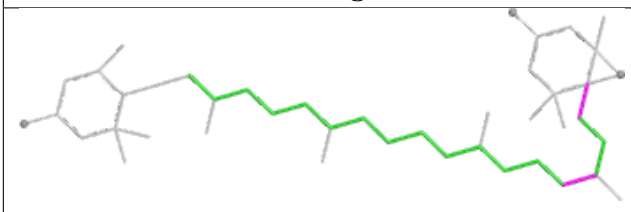
Ligand NEX Y 1623



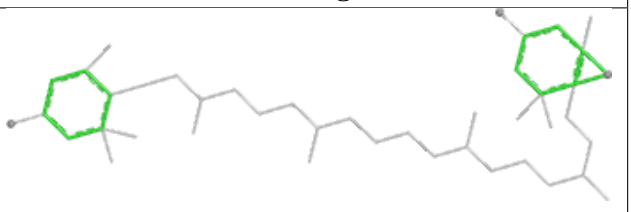
Bond lengths



Bond angles

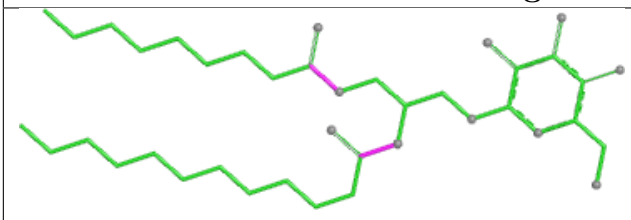


Torsions



Rings

Ligand LMG 5 627



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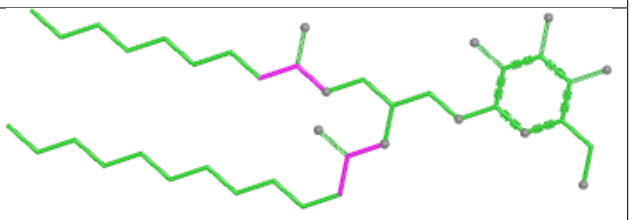

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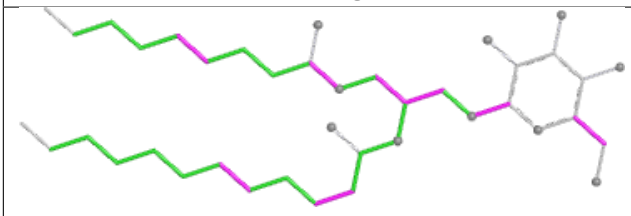

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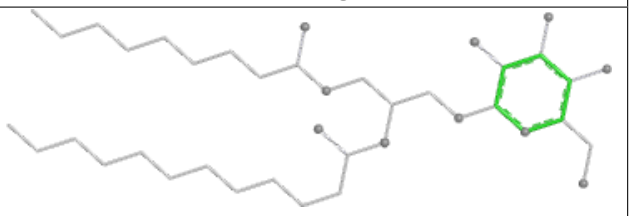
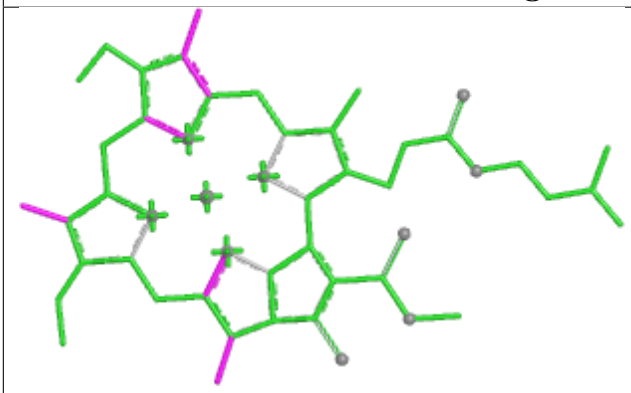


Rings

Ligand CLA V 604



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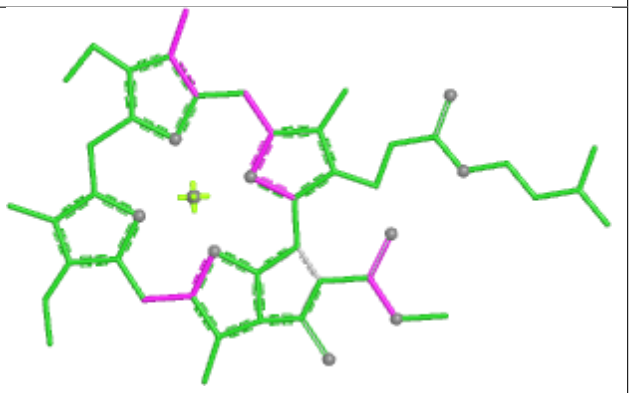

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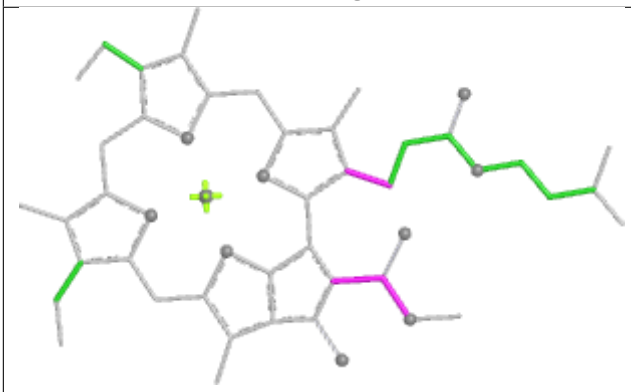

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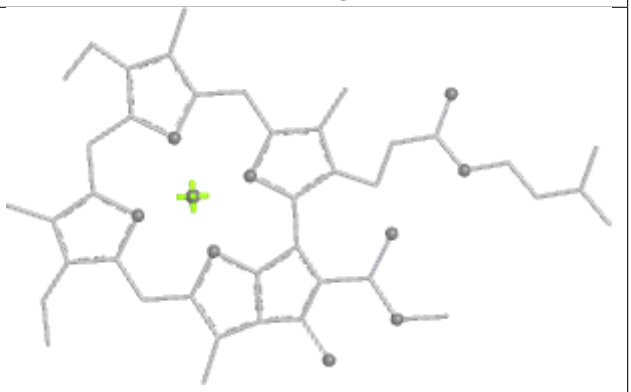
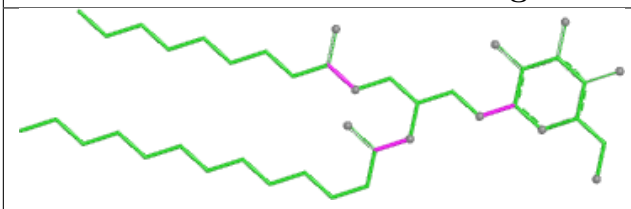


Rings

Ligand LMG V 2631



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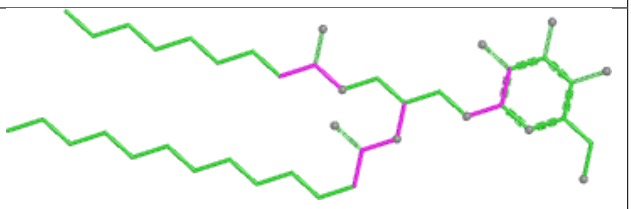

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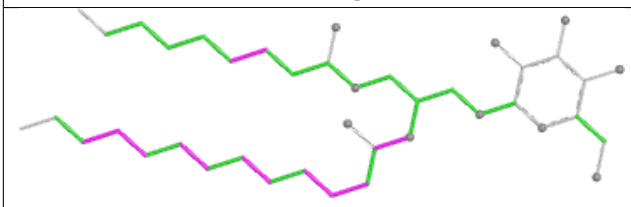

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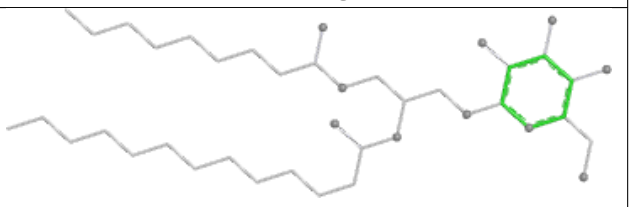
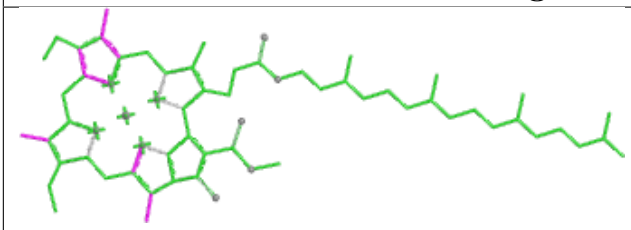


Rings

Ligand CLA 2 613



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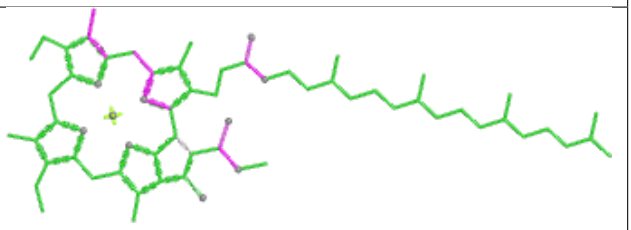

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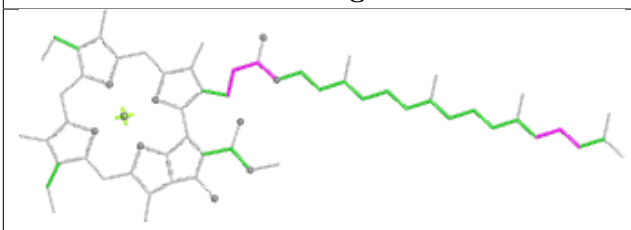

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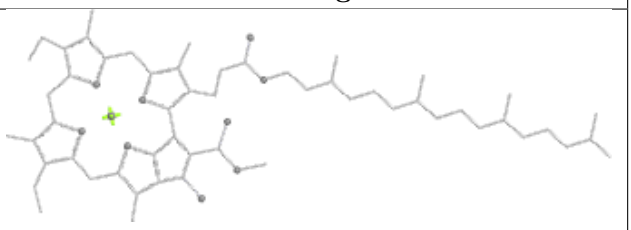
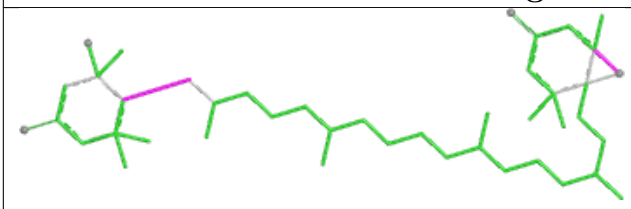


Rings

Ligand NEX 6 624



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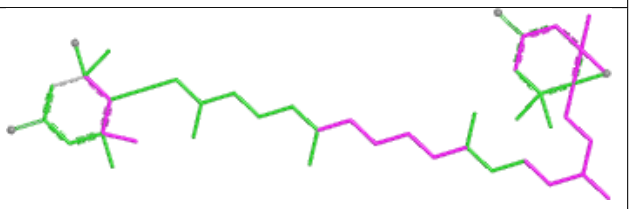
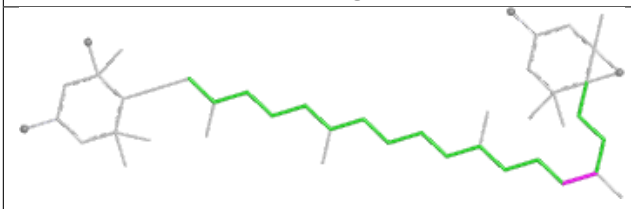


Bond angles



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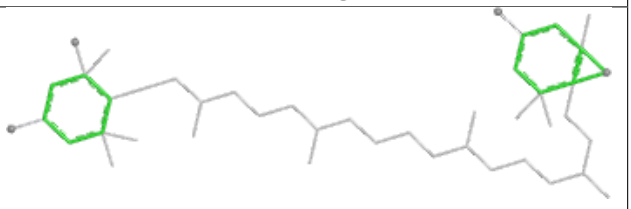
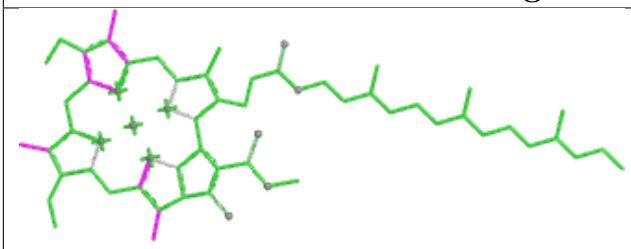
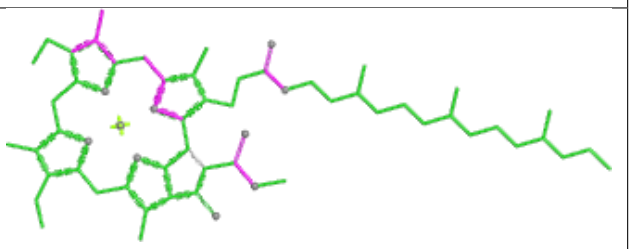
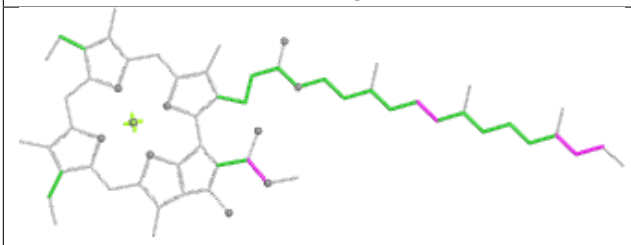
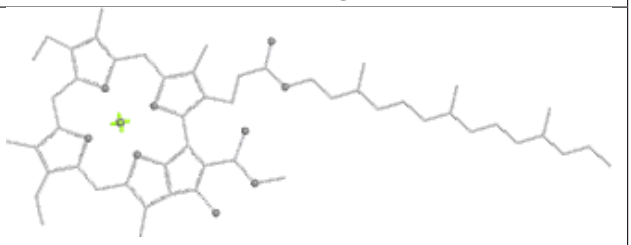
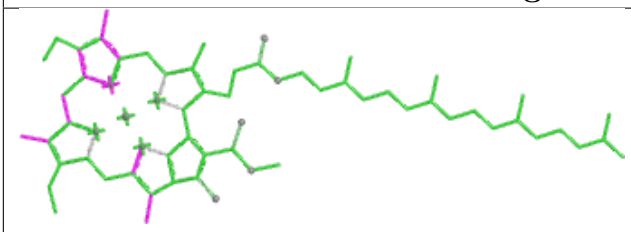
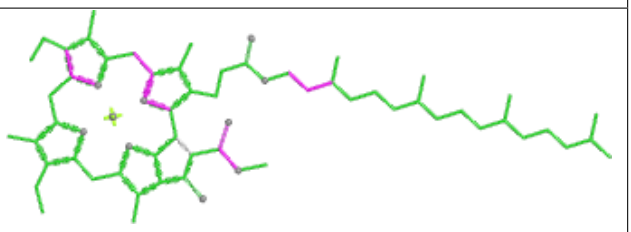
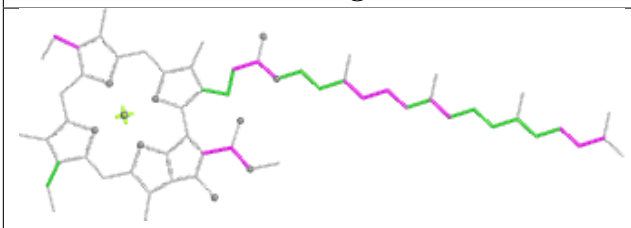
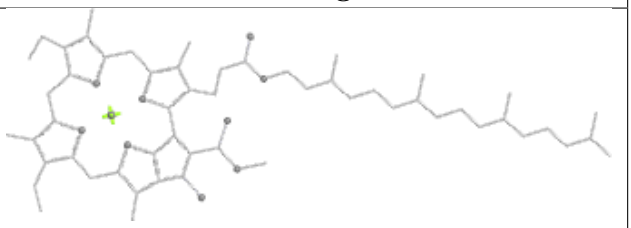
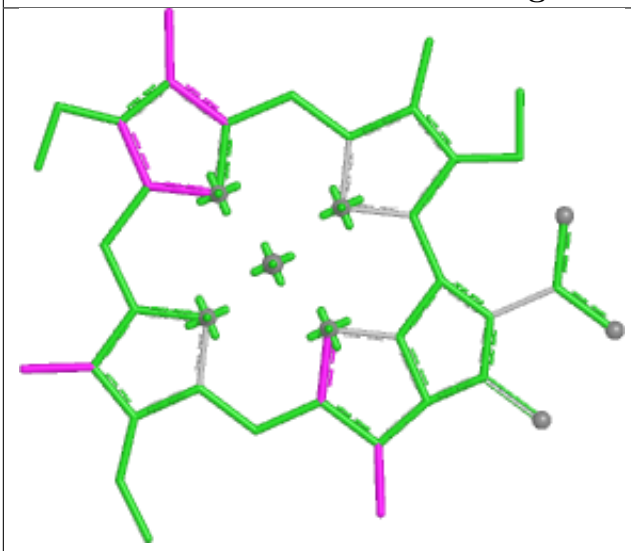


Rings

Ligand CLA V 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 612



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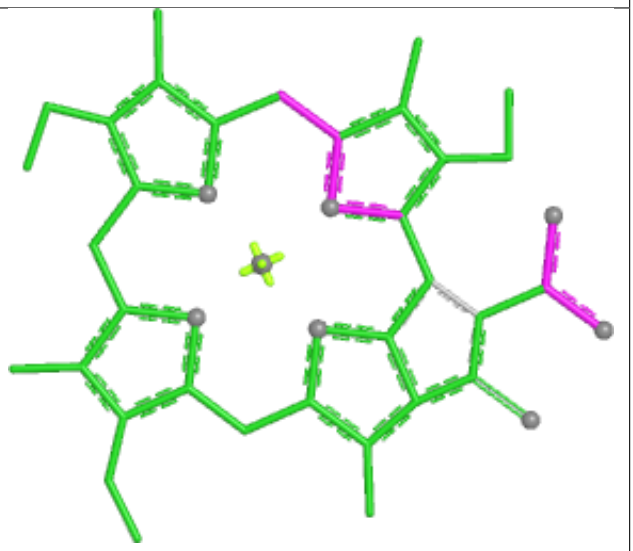
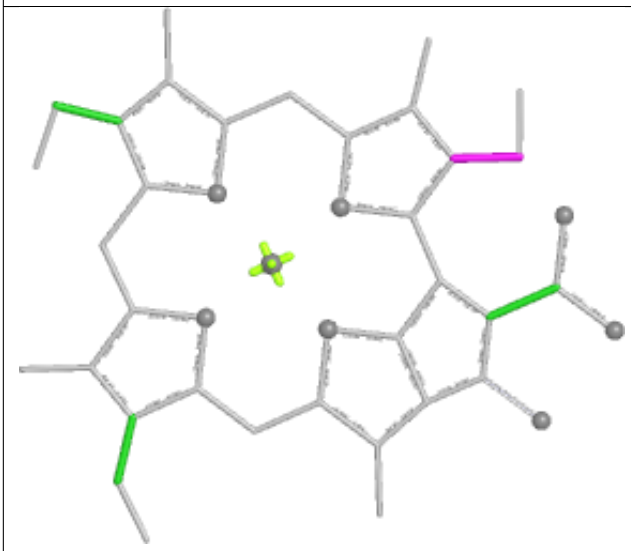


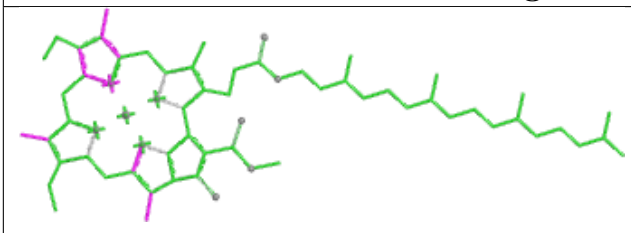
Bond angles



Torsions

Rings

Ligand CLA A 814



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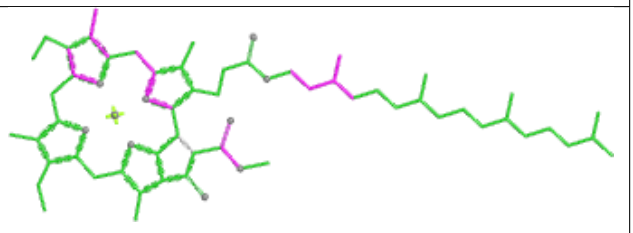
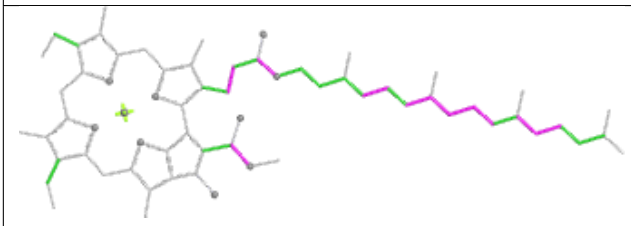
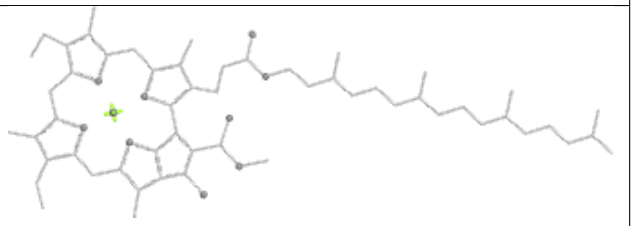


Bond angles

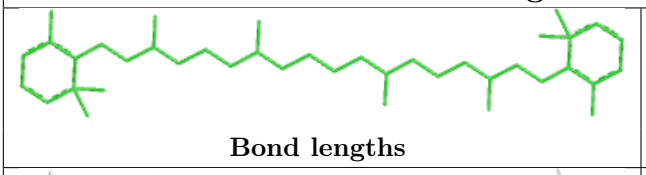


Torsions



Rings

Ligand BCR 2 623



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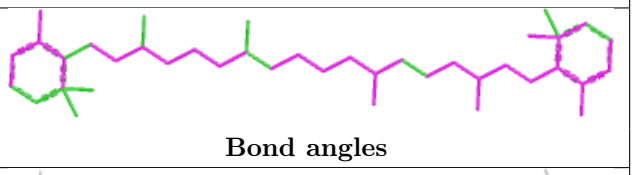
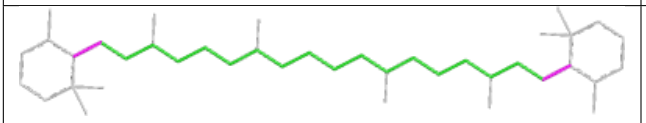


Bond angles



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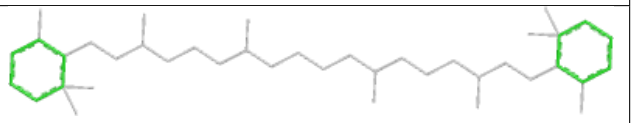
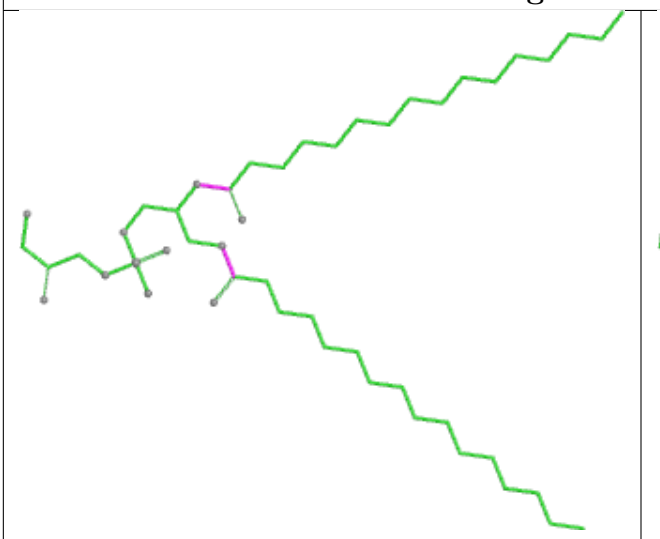


Rings

Ligand LHG 5 623



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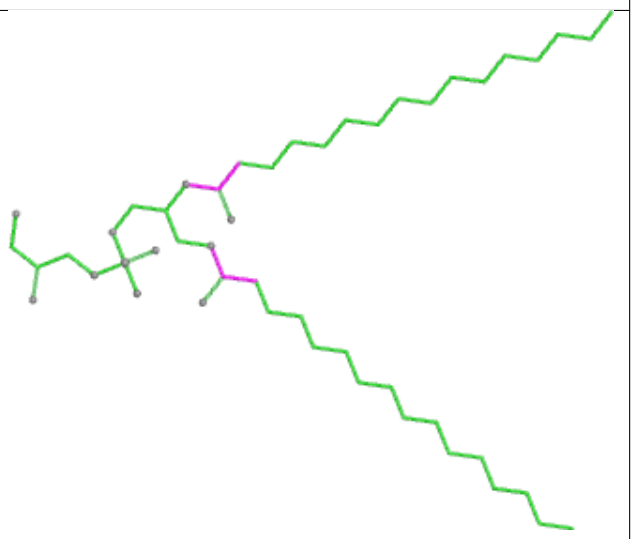
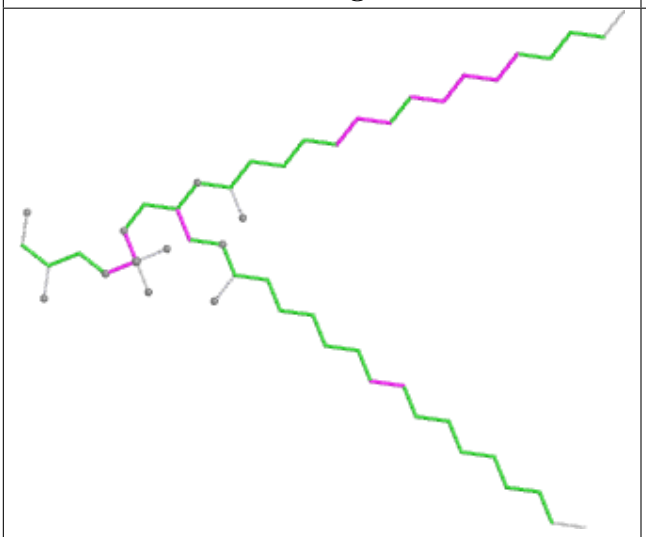


Bond angles



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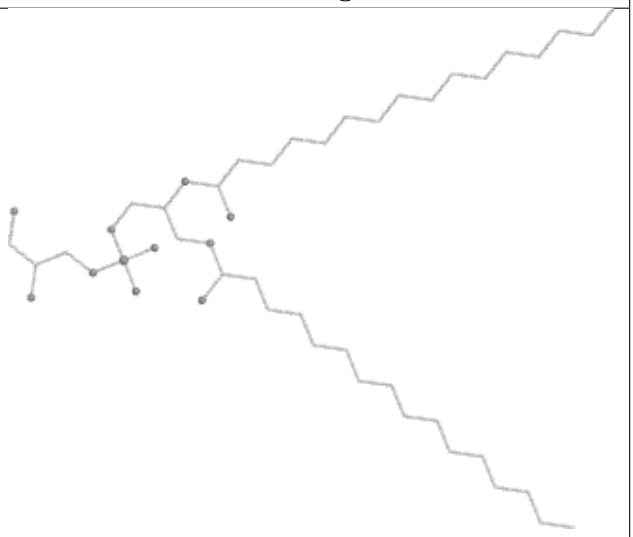
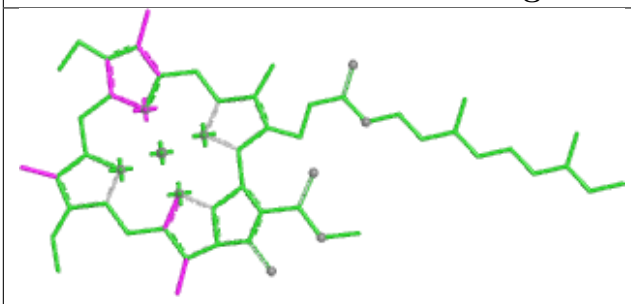


Rings

Ligand CLA U 610



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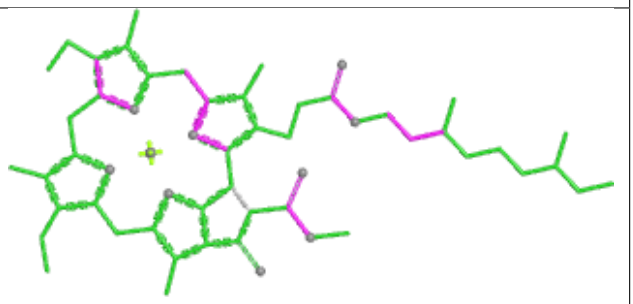
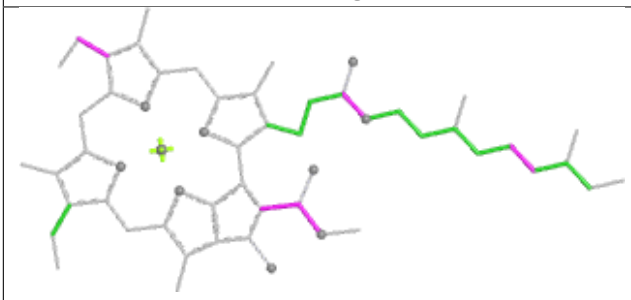
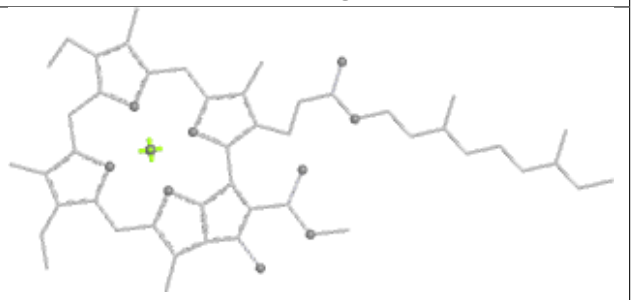


Bond angles

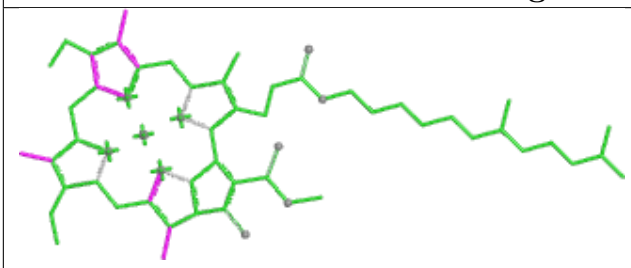


Torsions



Rings

Ligand CLA 7 611



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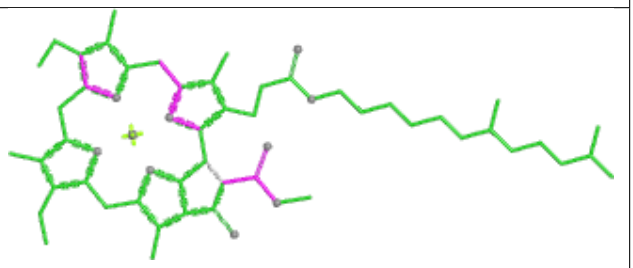
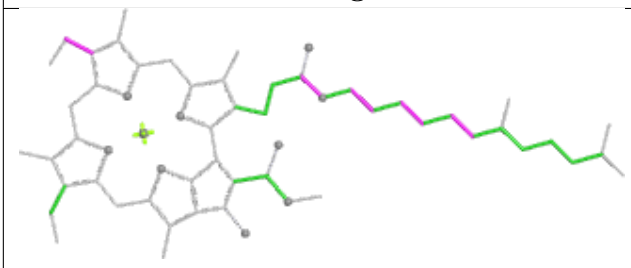
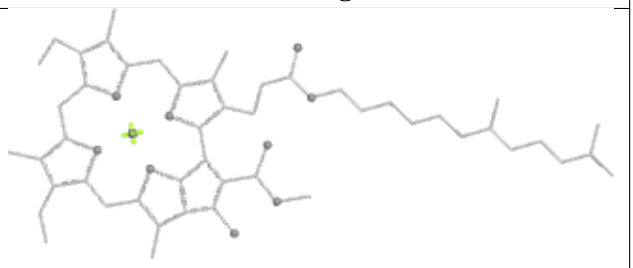


Bond angles

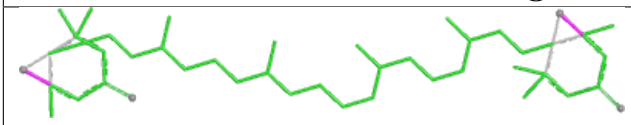


Torsions



Rings

Ligand XAT 1 618



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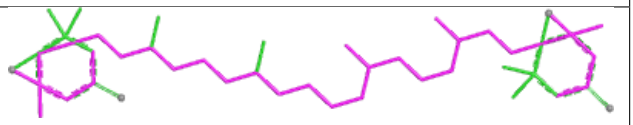

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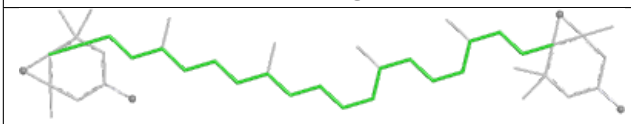

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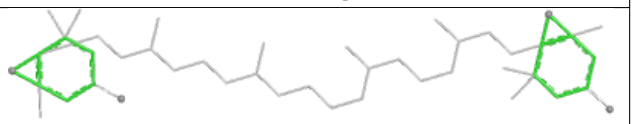
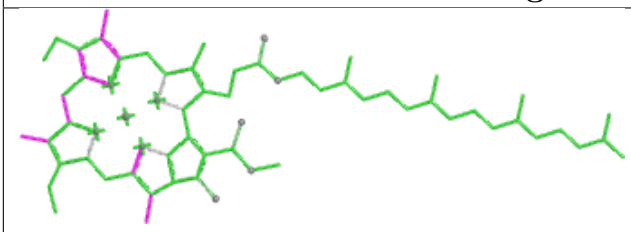


Rings

Ligand CLA Z 613



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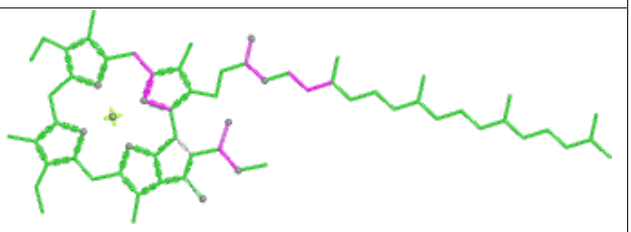
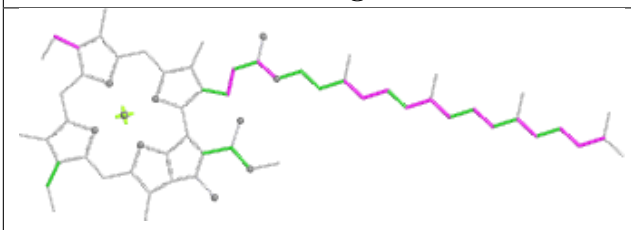


Bond angles



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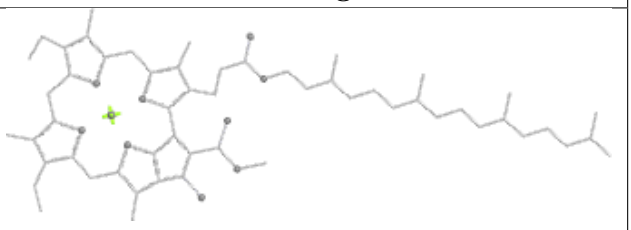
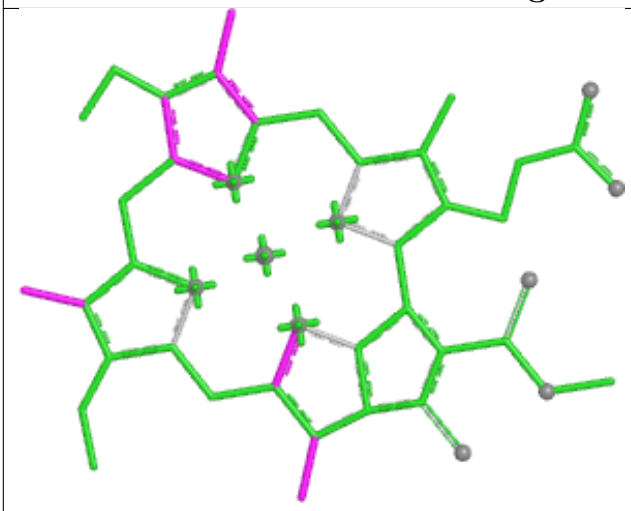


Rings

Ligand CLA 1 612



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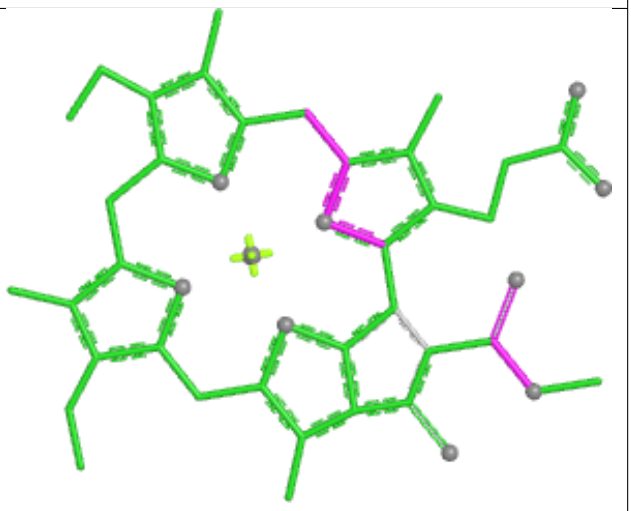
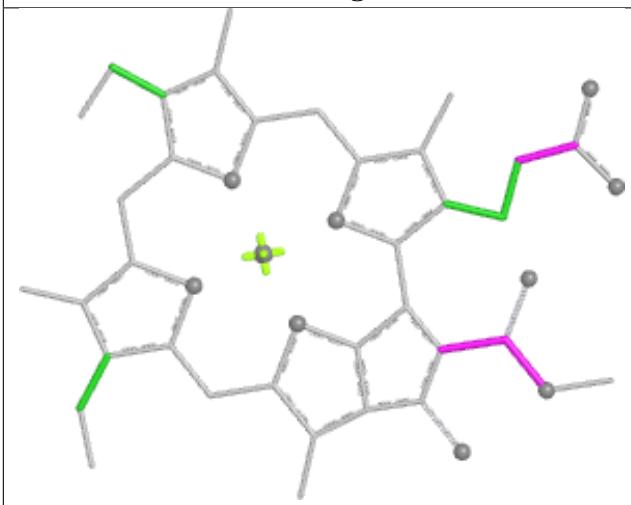


Bond angles



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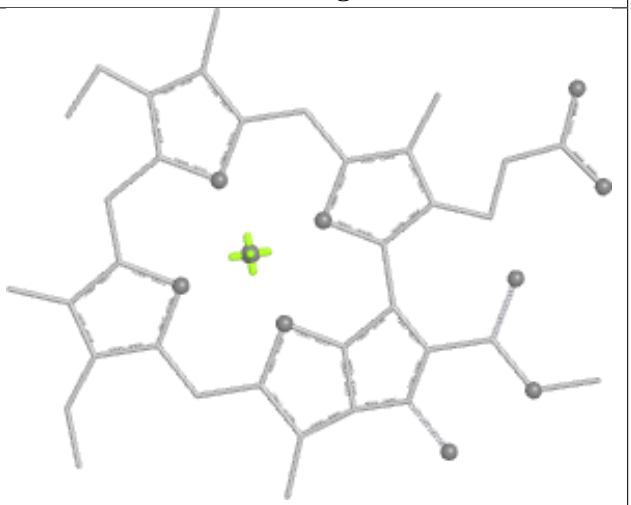
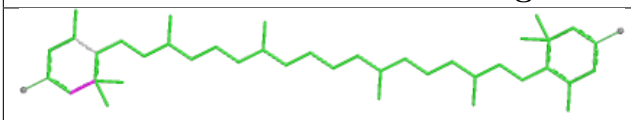


Rings

Ligand LUT Y 1620



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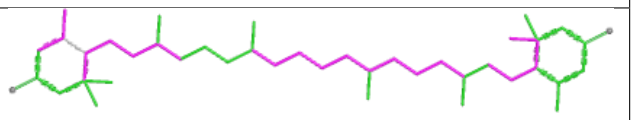
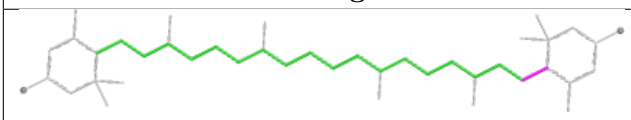


Bond angles



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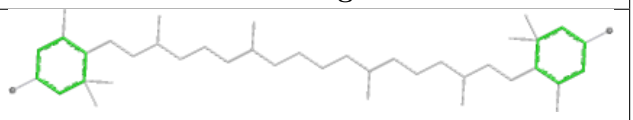
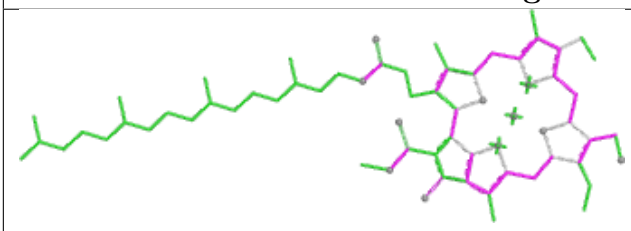


Rings

Ligand CHL V 601



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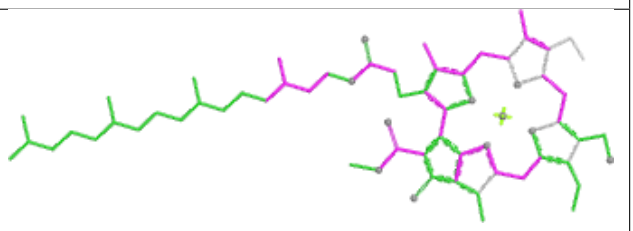
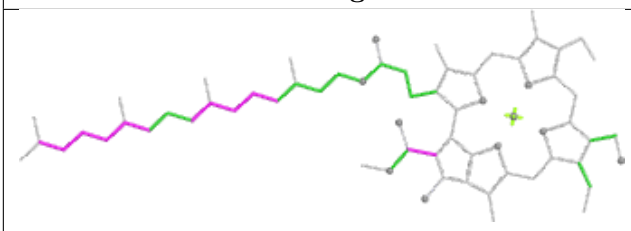


Bond angles



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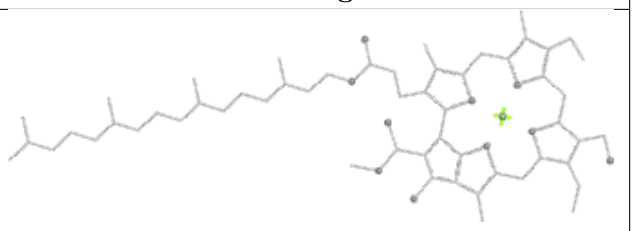
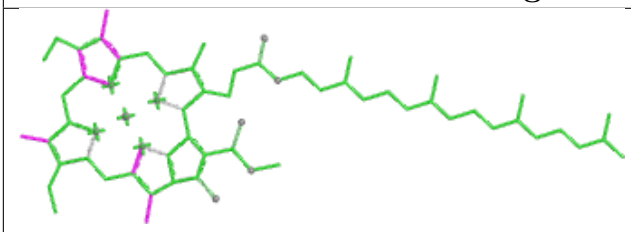


Rings

Ligand CLA A 803



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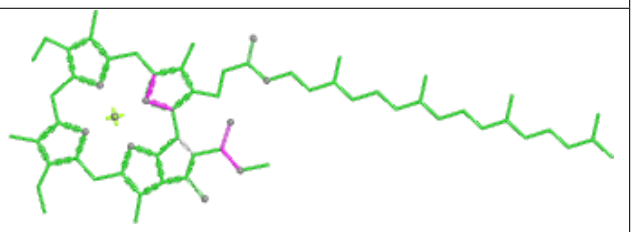

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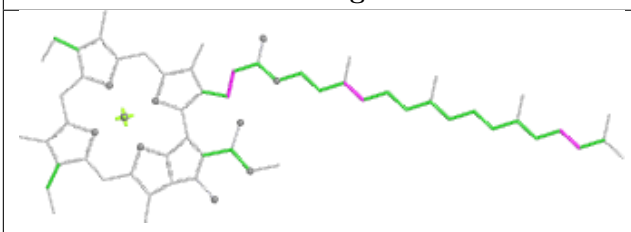

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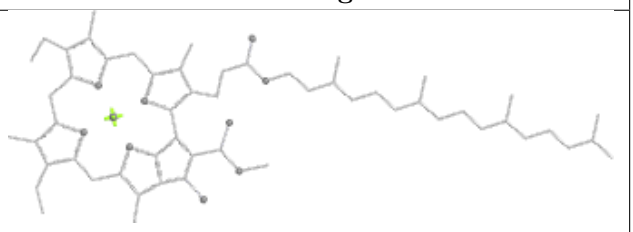
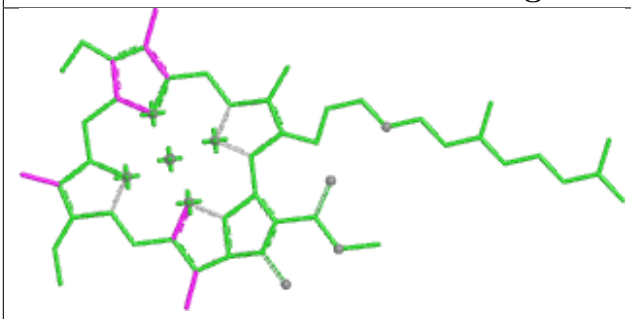


Rings

Ligand CLA B 816



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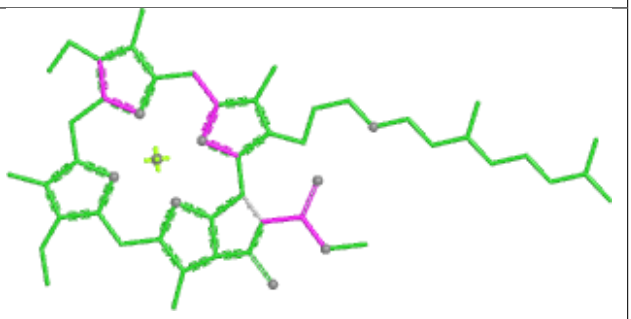

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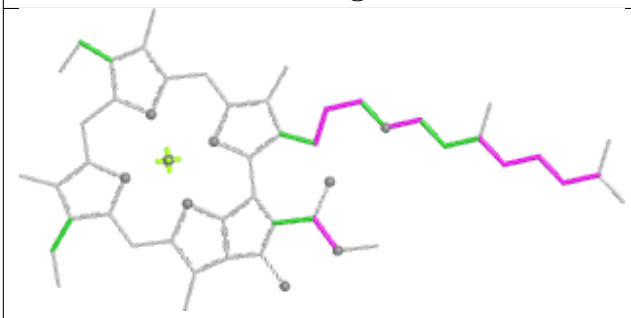

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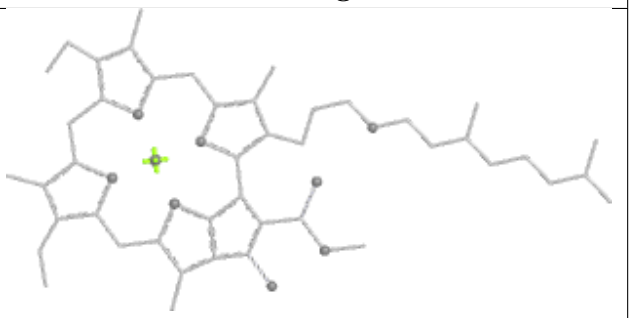
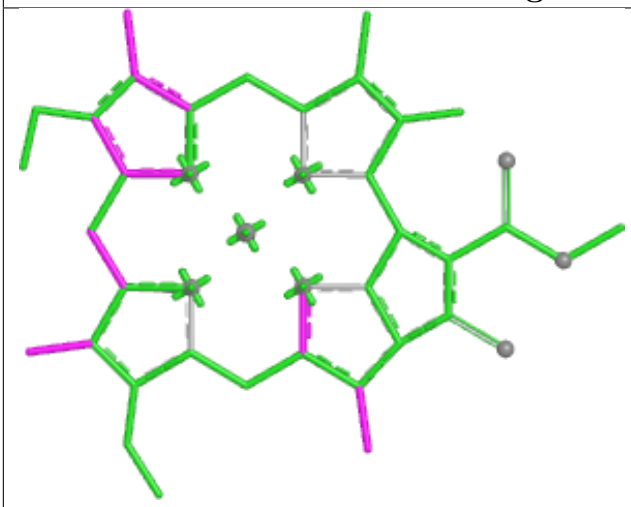


Rings

Ligand CLA F 304



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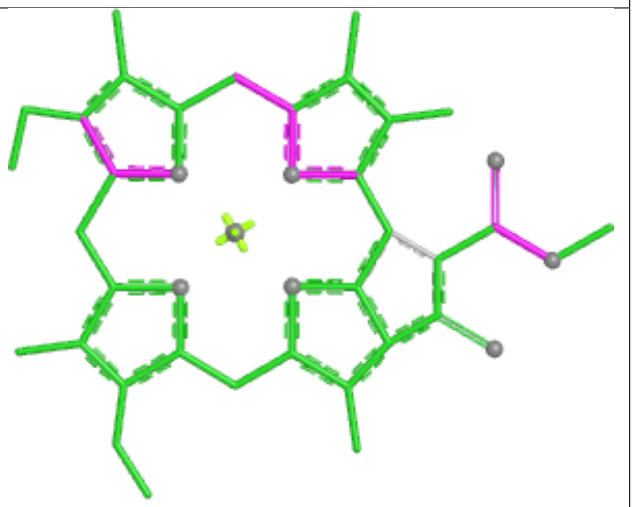
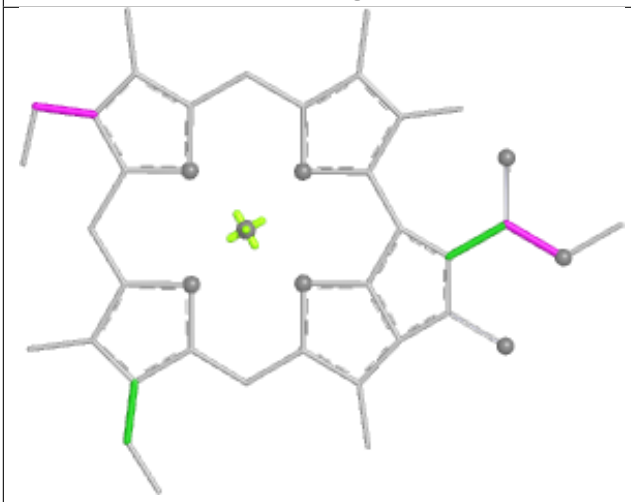
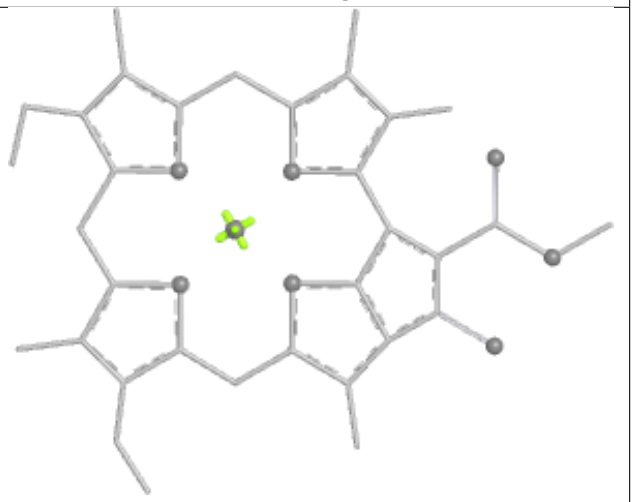


Bond angles

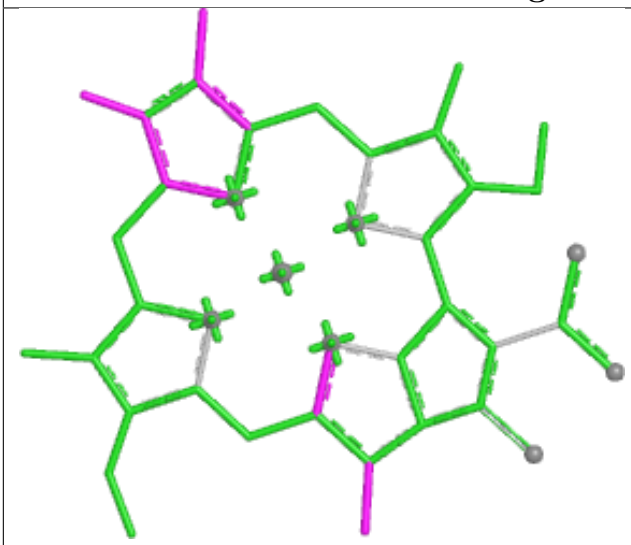


Torsions



Rings

Ligand CLA 4 618



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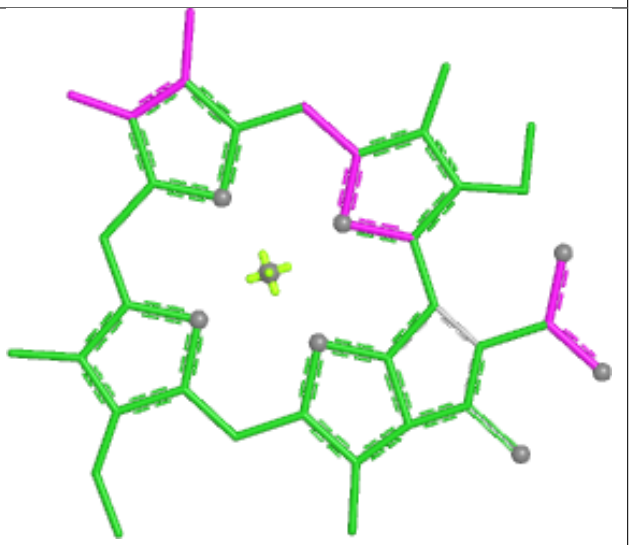
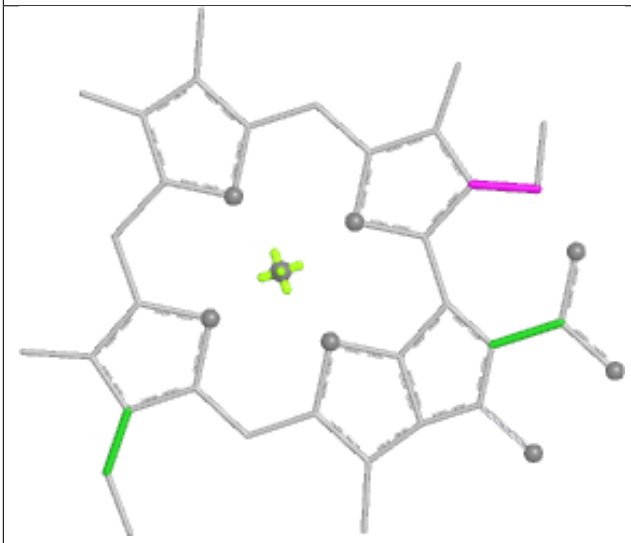


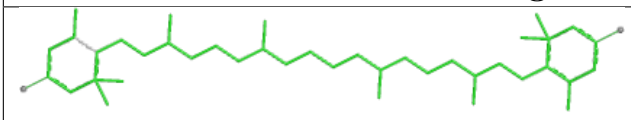
Bond angles



Torsions

Rings

Ligand LUT 9 619



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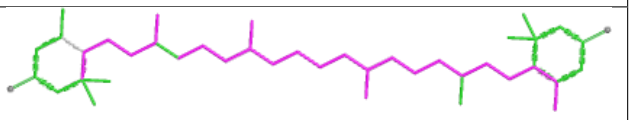
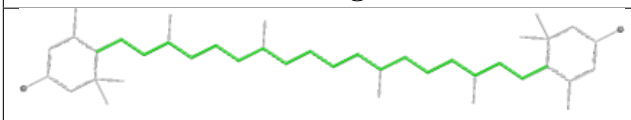


Bond angles



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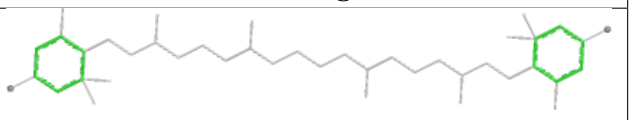
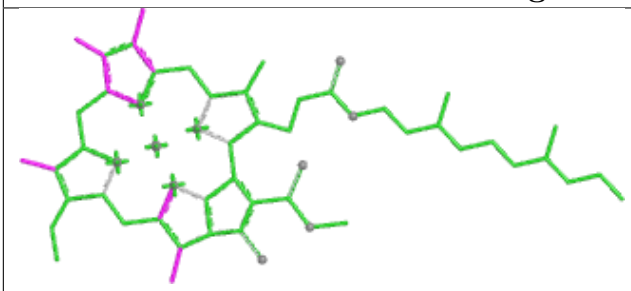


Rings

Ligand CLA 3 607



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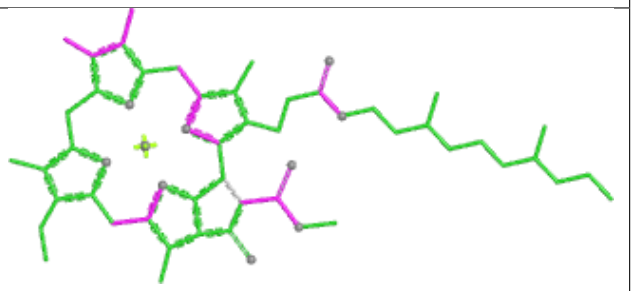
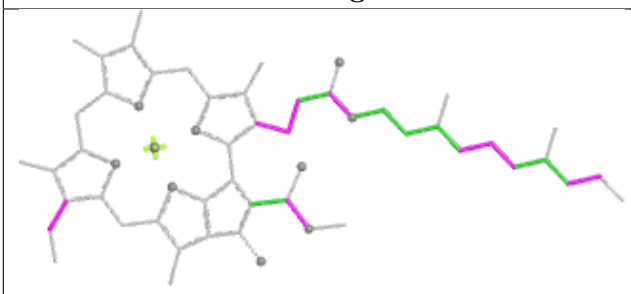


Bond angles



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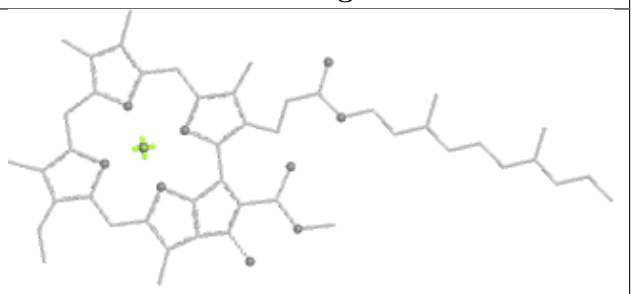
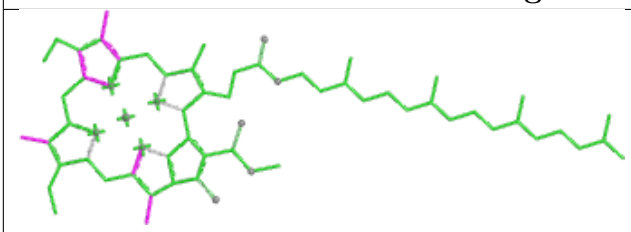
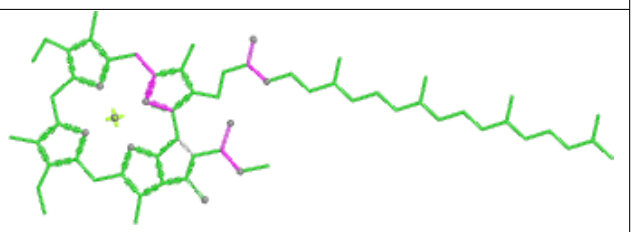


Rings

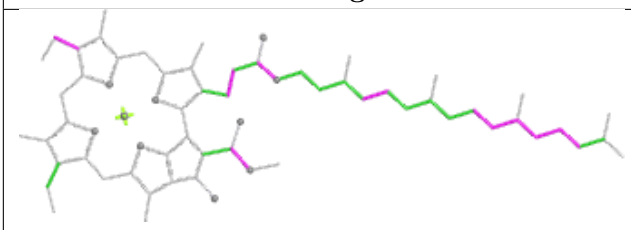
Ligand CLA B 839



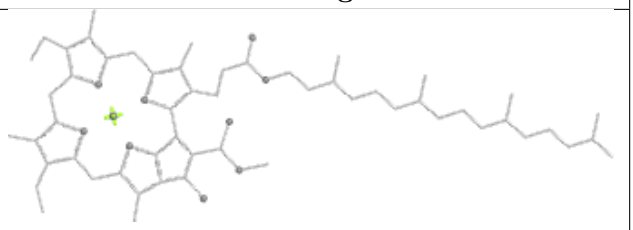
Bond lengths



Bond angles

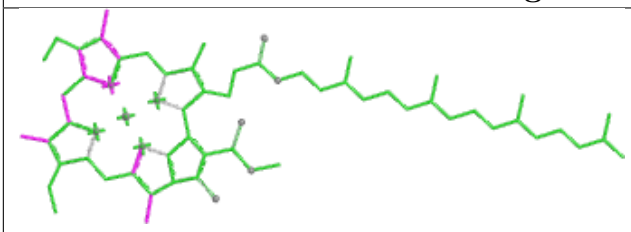


Torsions

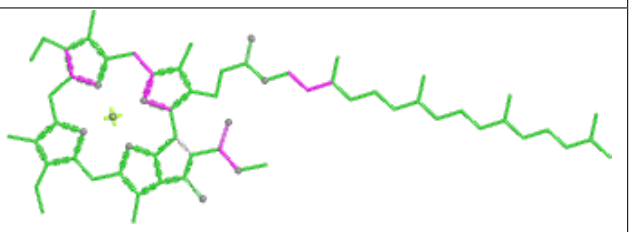


Rings

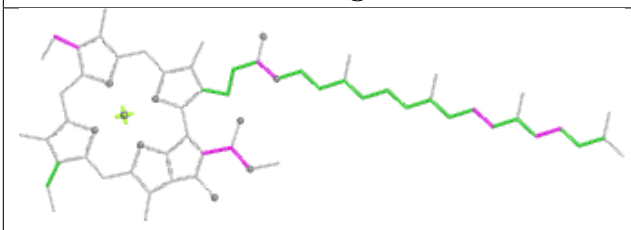
Ligand CLA B 841



Bond lengths



Bond angles



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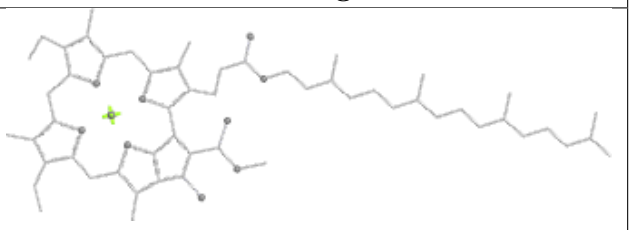


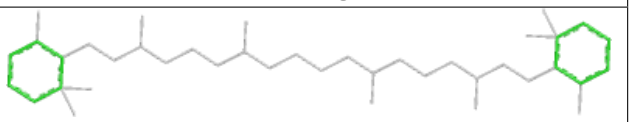
Rings

Ligand BCR 6 622

Bond lengths

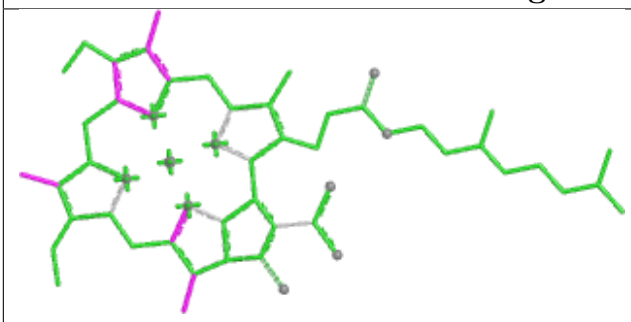
Bond angles

Torsions

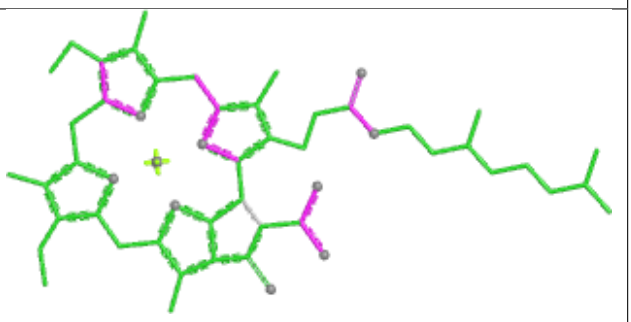


Rings

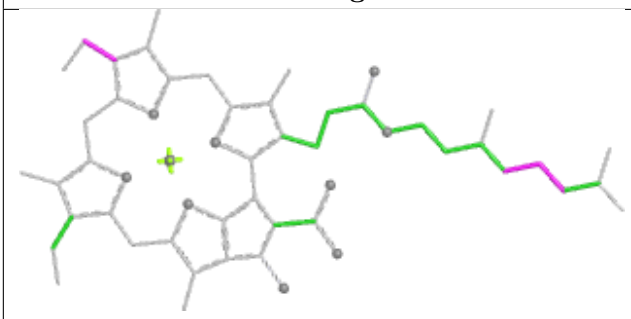
Ligand CLA a 601



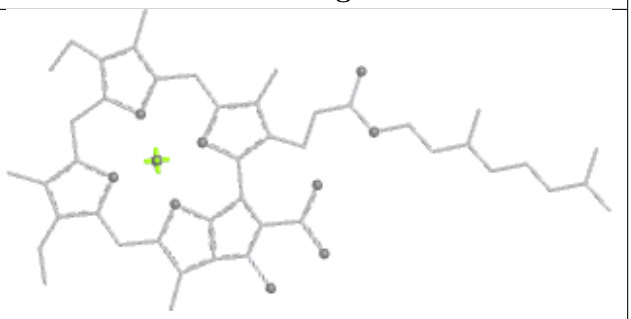
Bond lengths



Bond angles

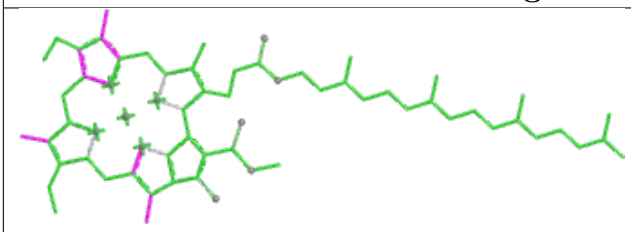


Torsions



Rings

Ligand CLA A 811



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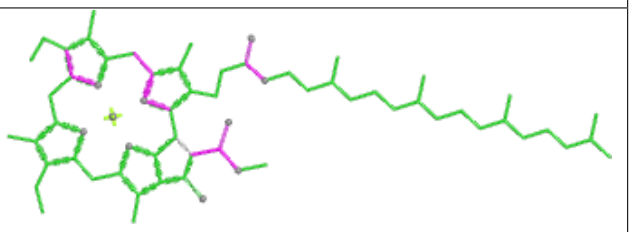
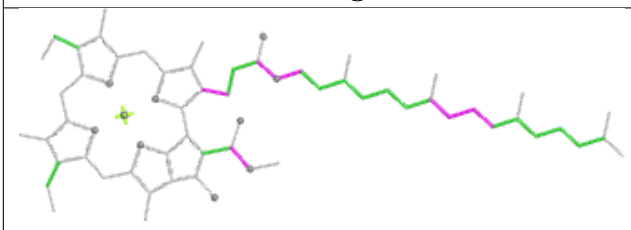


Bond angles



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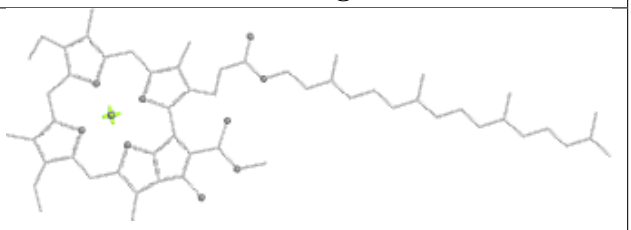
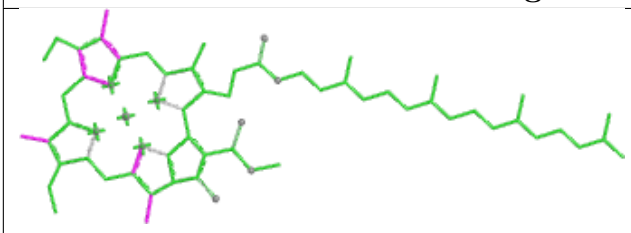


Rings

Ligand CLA B 808



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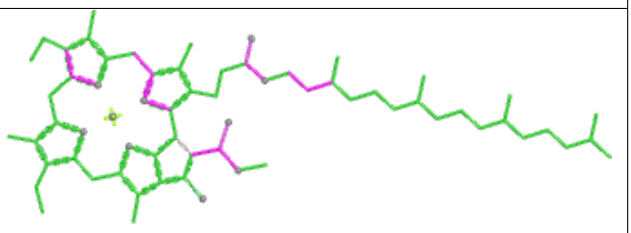
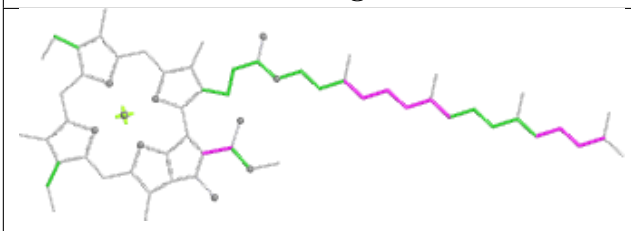
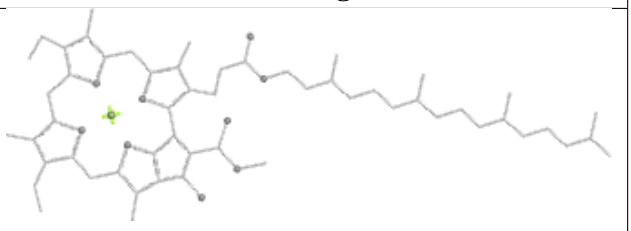


Bond angles

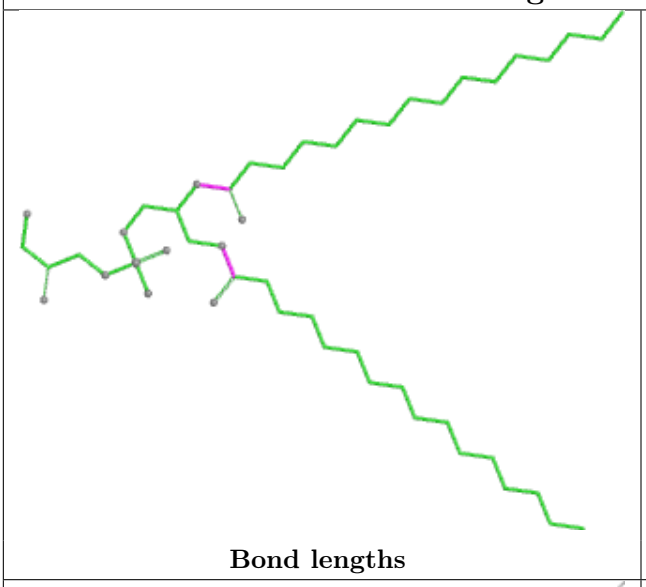


Torsions



Rings

Ligand LHG 8 622



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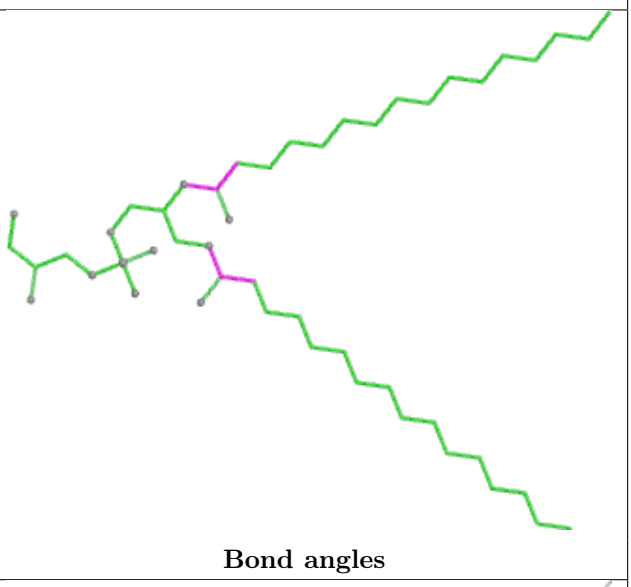
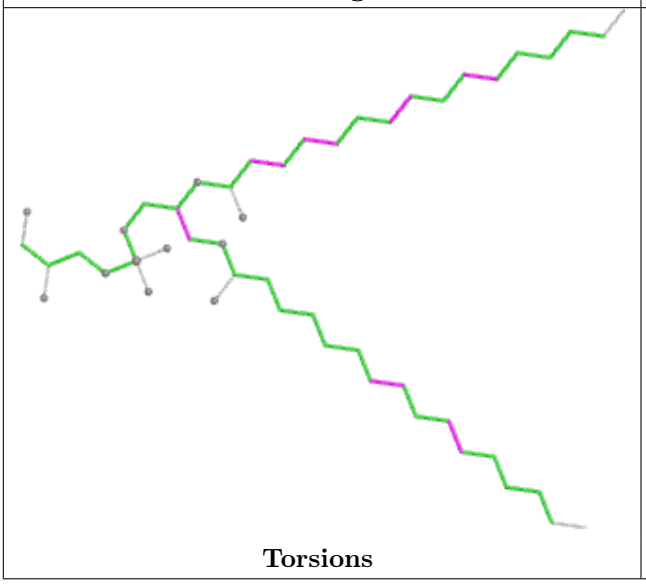


Bond angles



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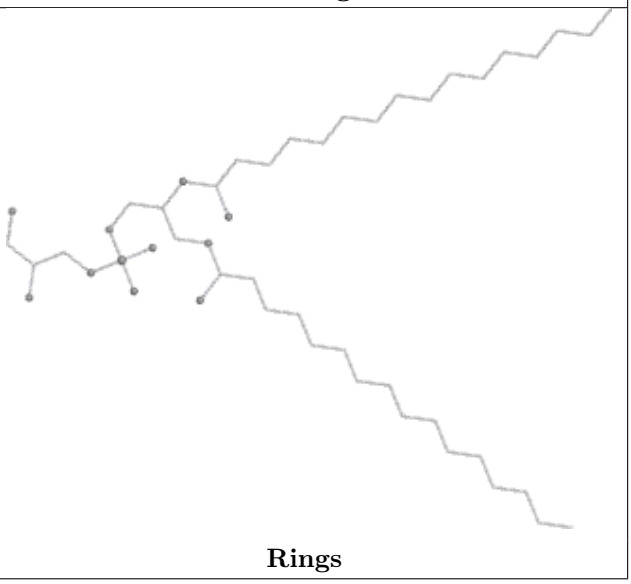
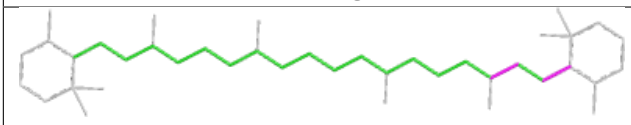


Rings

Ligand BCR B 848

Bond lengths

Bond angles



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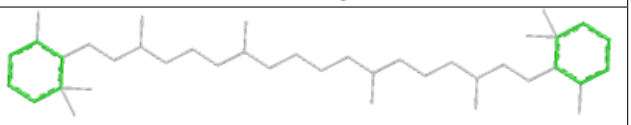
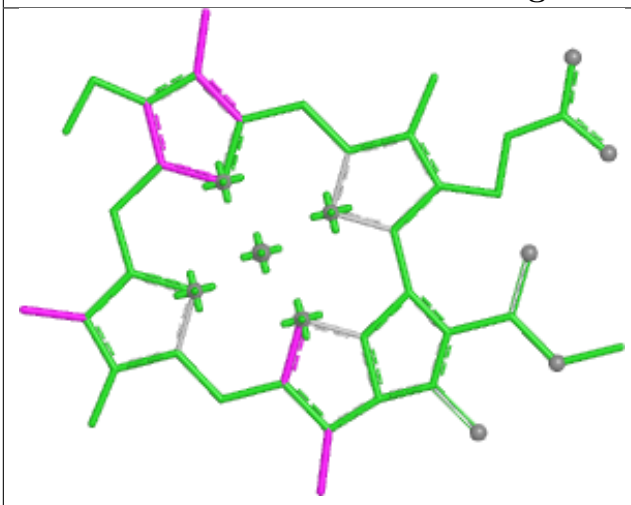


Rings

Ligand CLA 7 612



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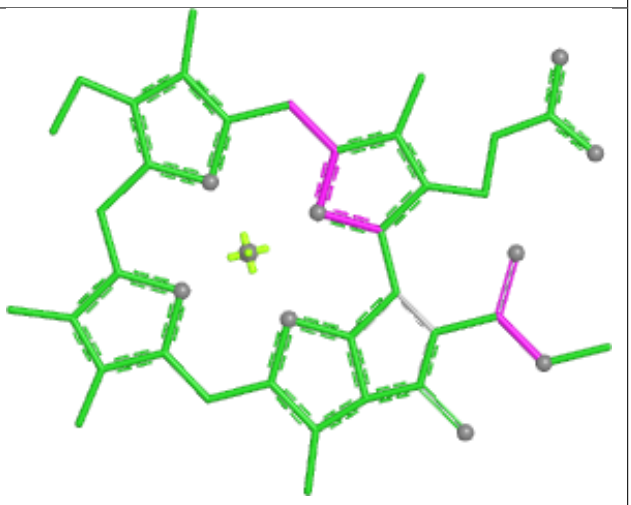

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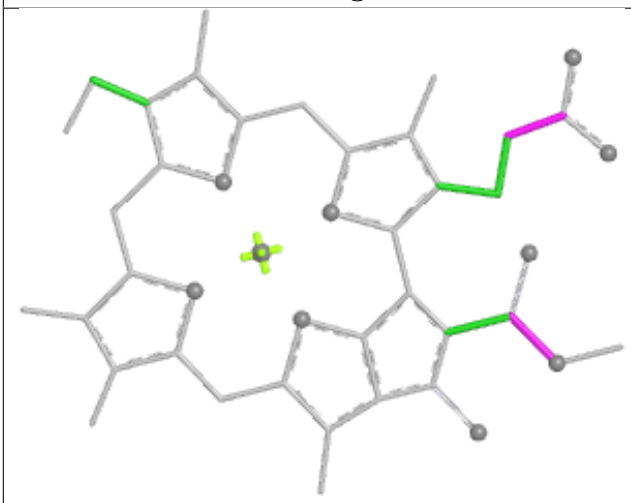
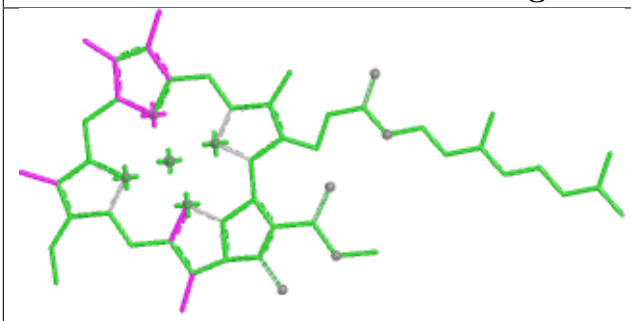


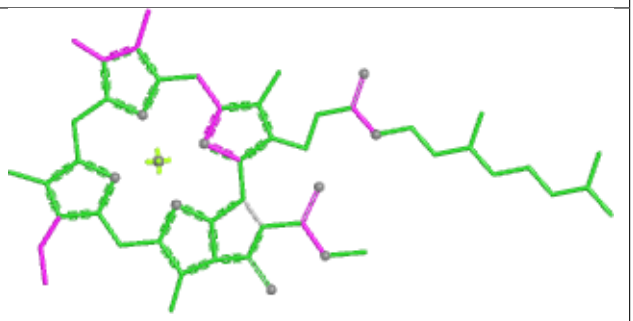
Torsions

Rings

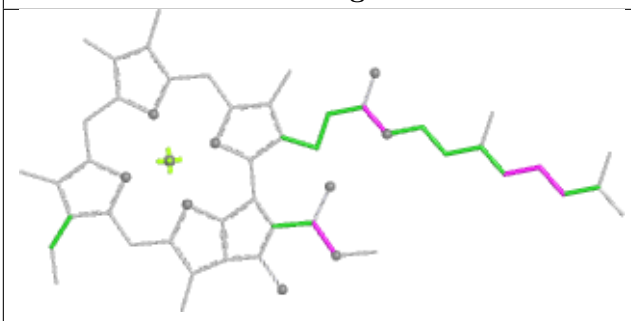
Ligand CLA 5 603



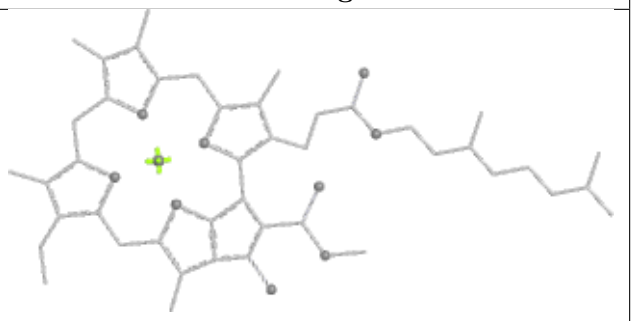
Bond lengths



Bond angles



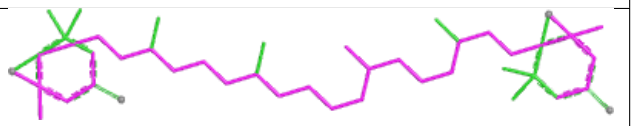
Torsions



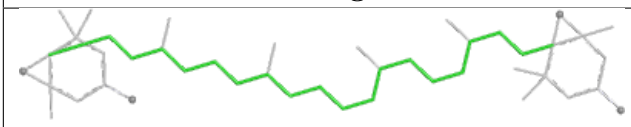
Rings

Ligand XAT 8 620

Bond lengths



Bond angles



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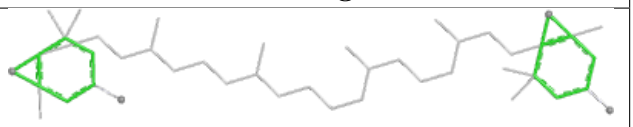
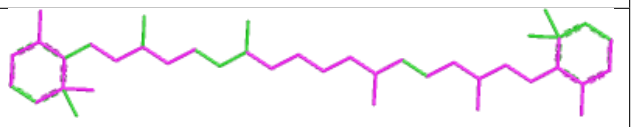


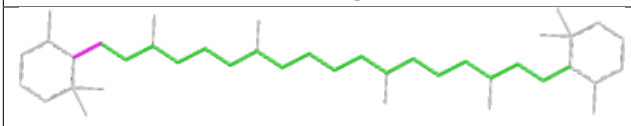
Rings

Ligand BCR B 846

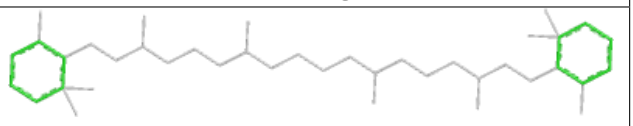
Bond lengths



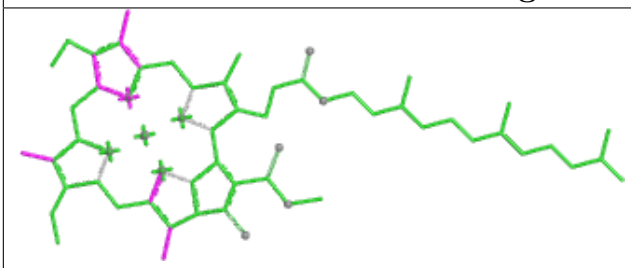
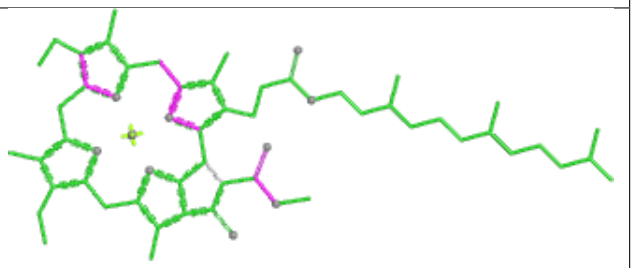
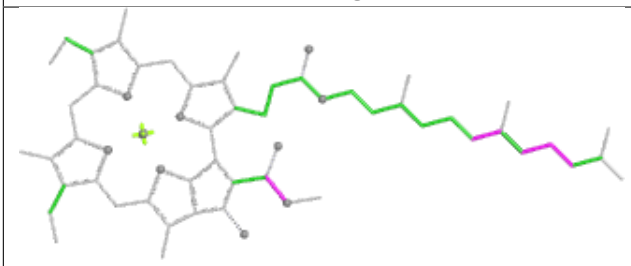
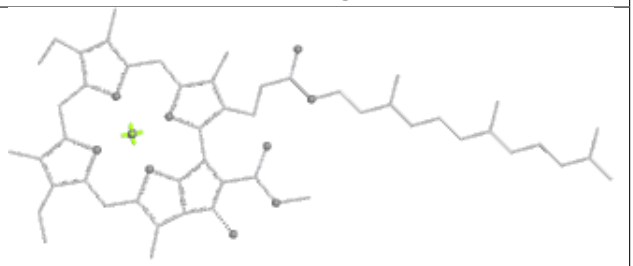
Bond angles



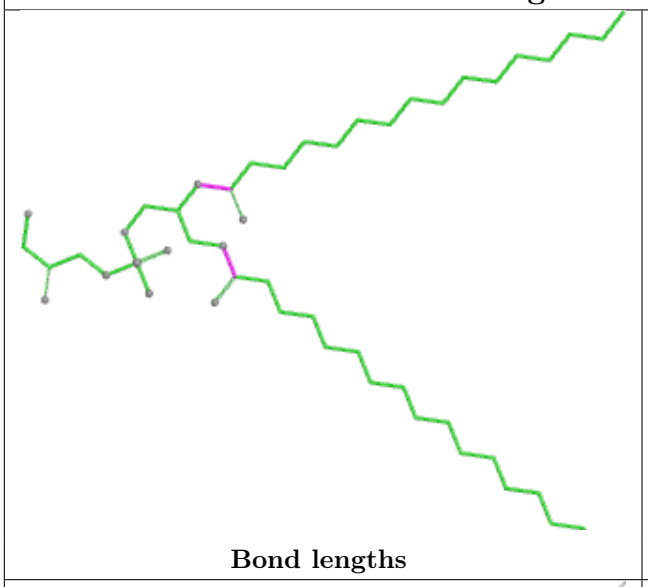
Torsions



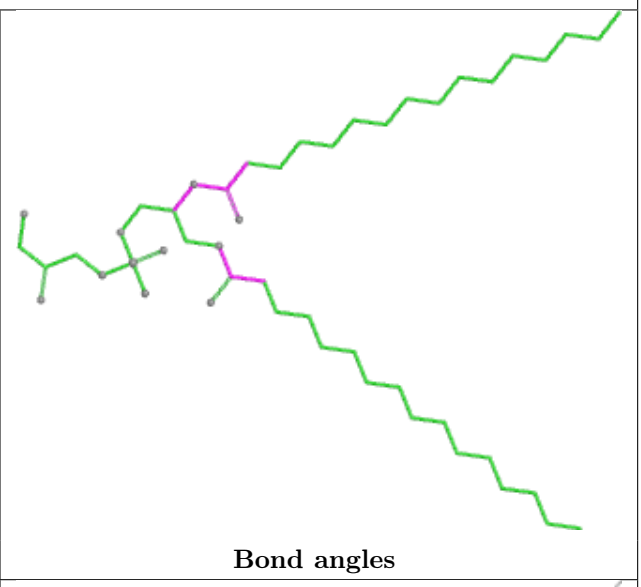
Rings

Ligand CLA W 602	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

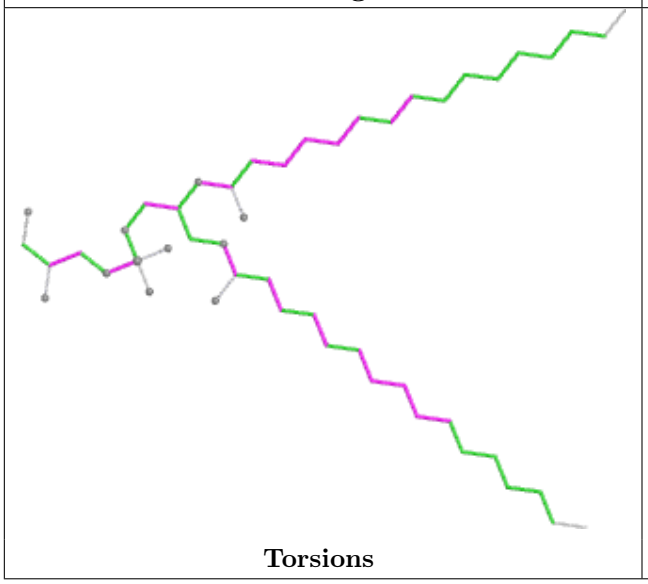
Ligand LHG 3 624



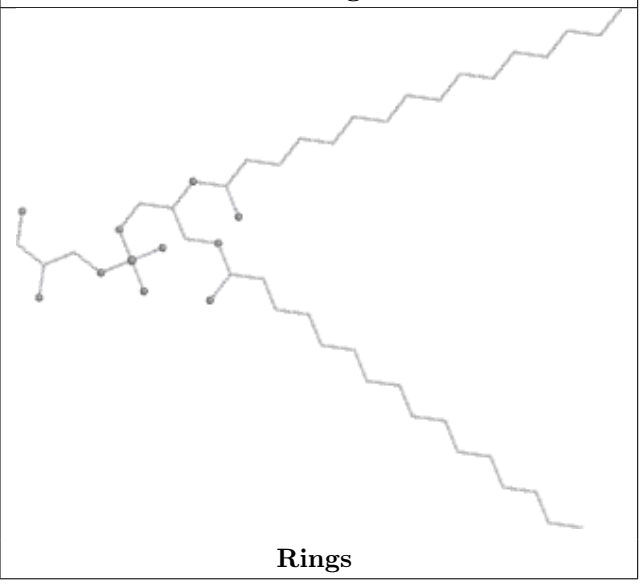
Bond lengths



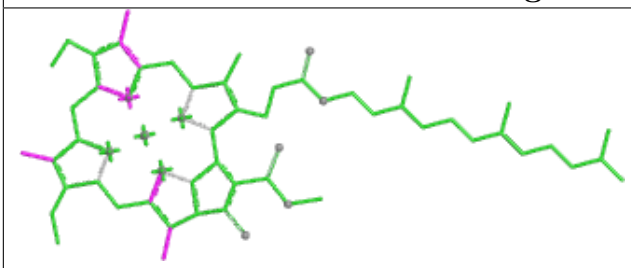
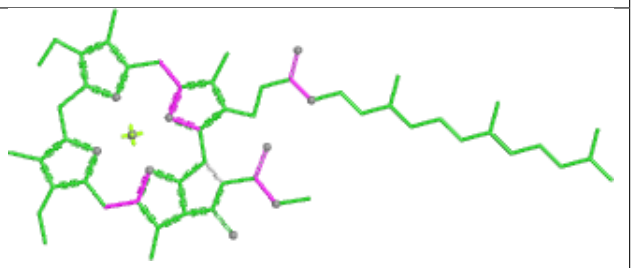
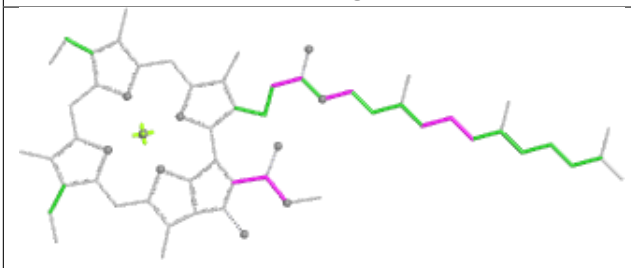
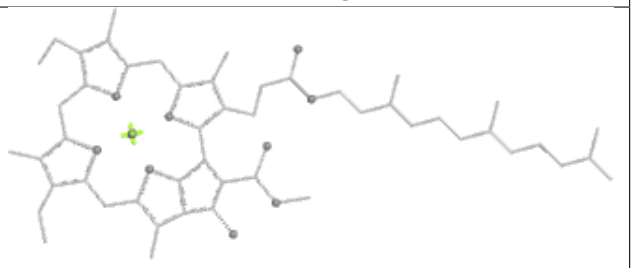
Bond angles

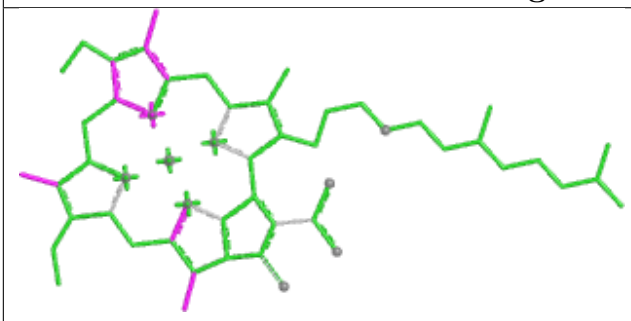
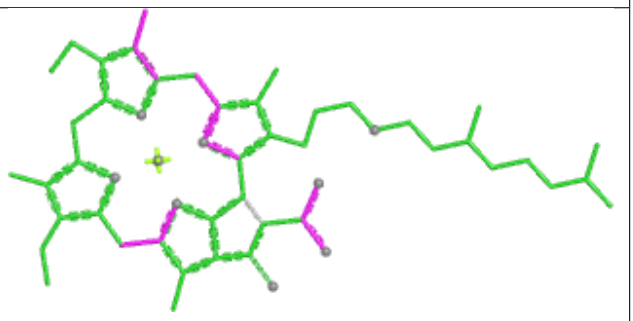
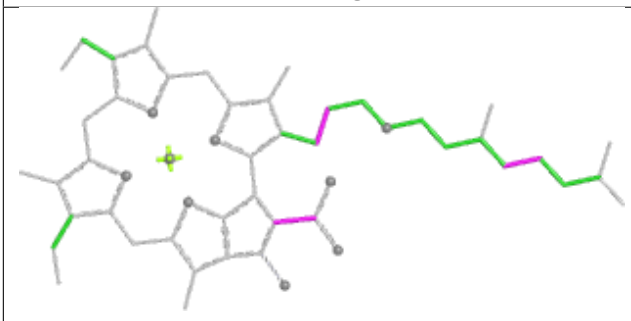
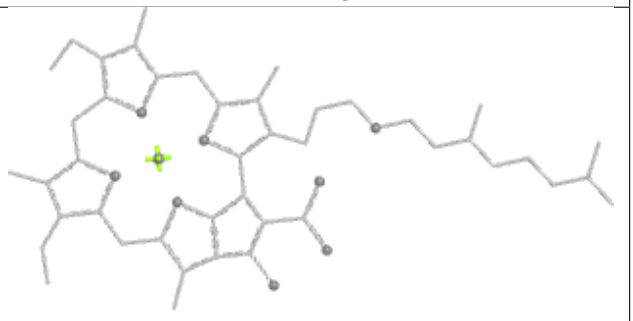


Torsions

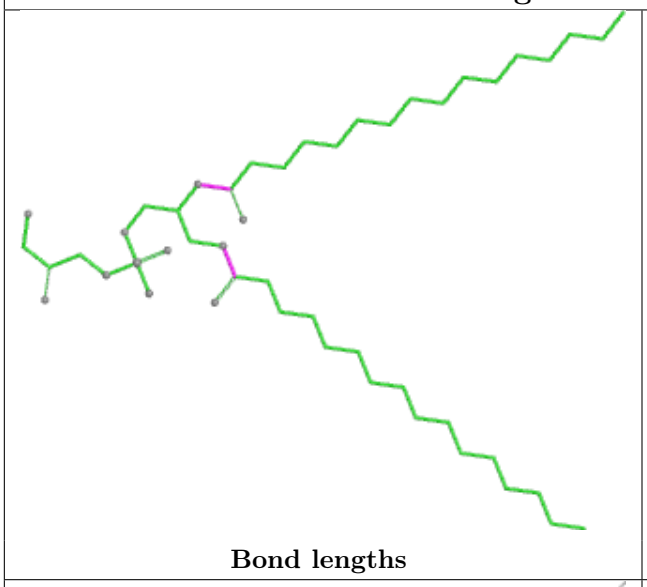


Rings

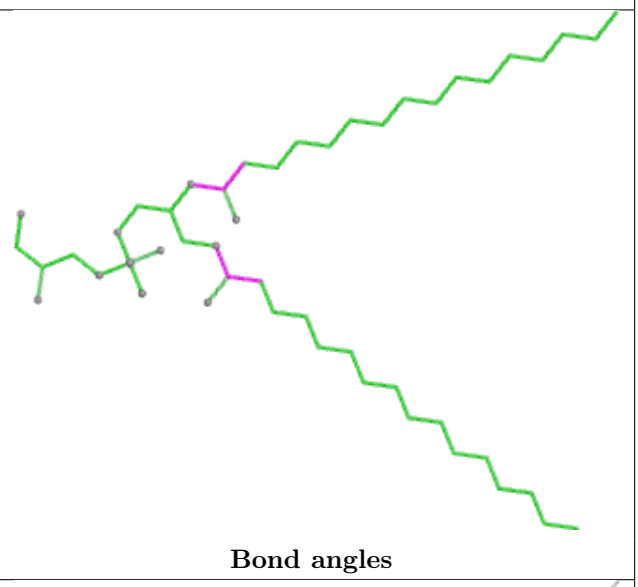
Ligand CLA B 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

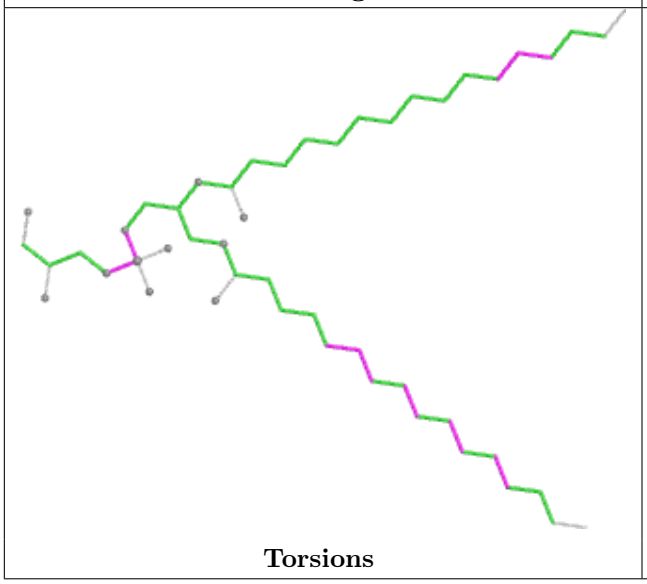
Ligand LHG U 2630



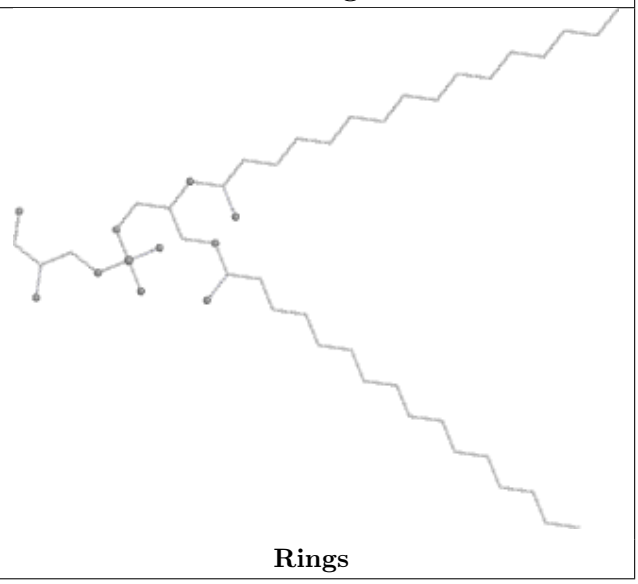
Bond lengths



Bond angles

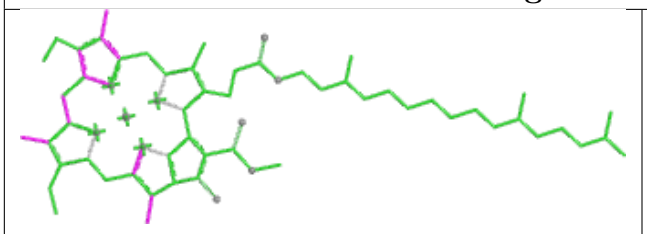


Torsions

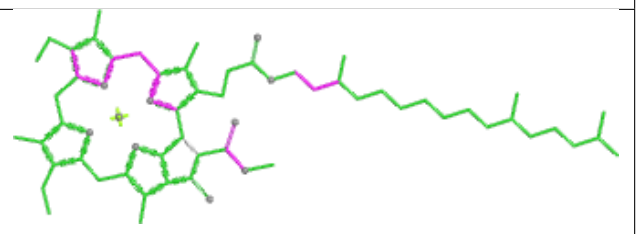


Rings

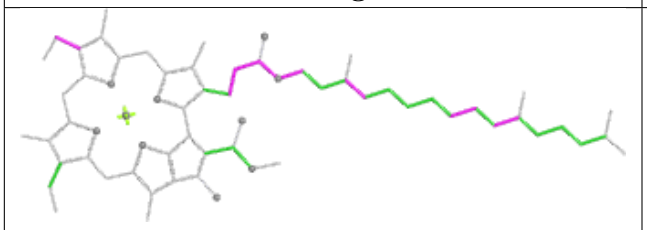
Ligand CLA A 843



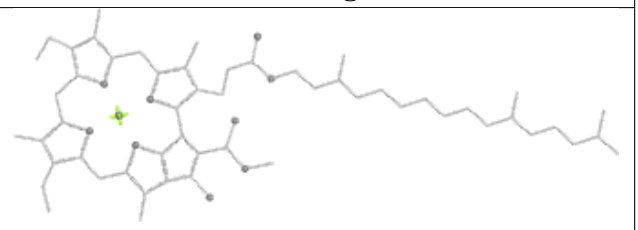
Bond lengths



Bond angles

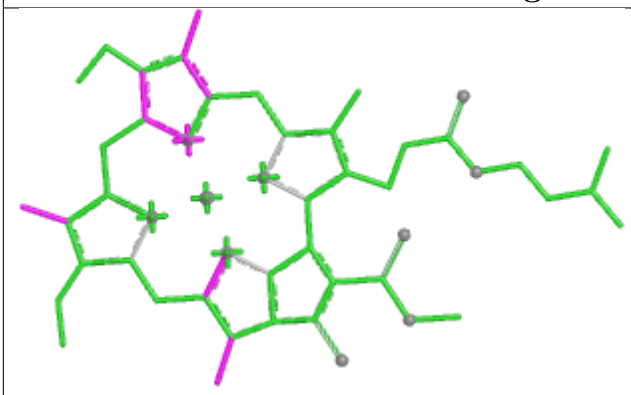


Torsions

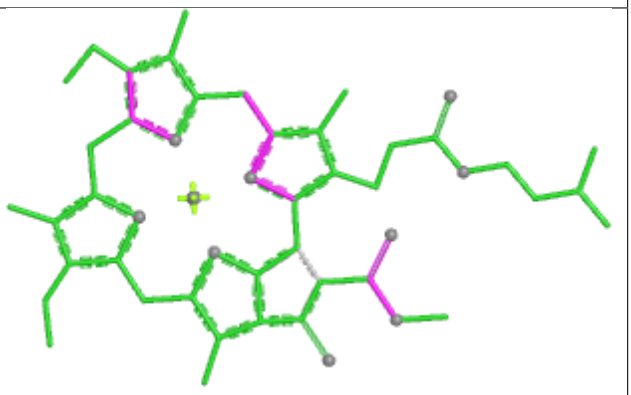


Rings

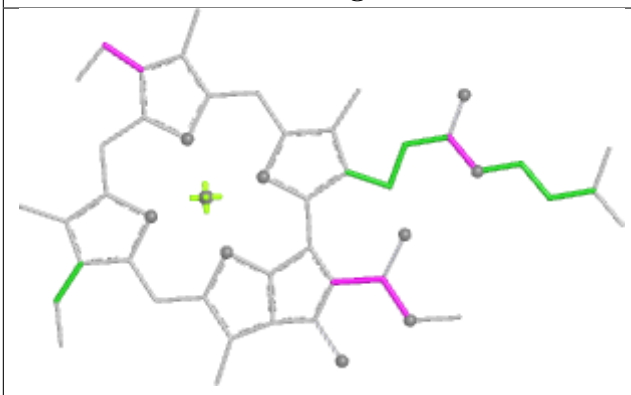
Ligand CLA A 815



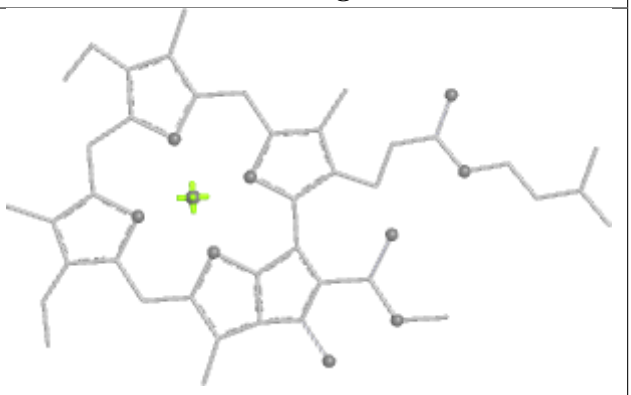
Bond lengths



Bond angles

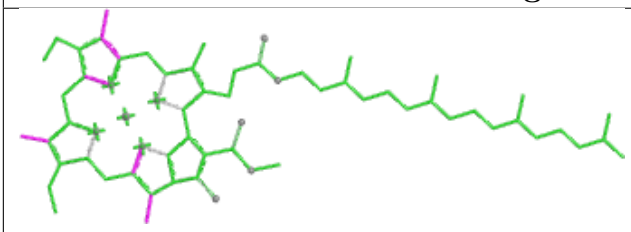


Torsions



Rings

Ligand CLA V 613



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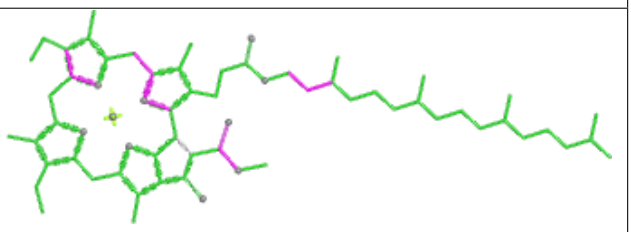
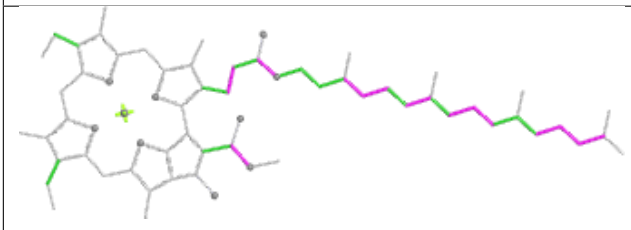
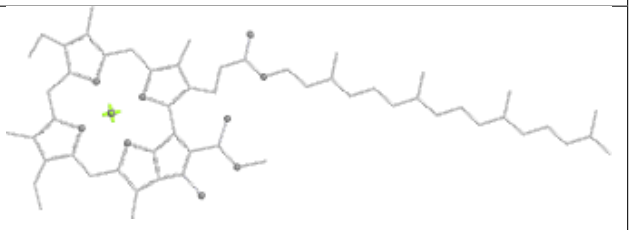


Bond angles

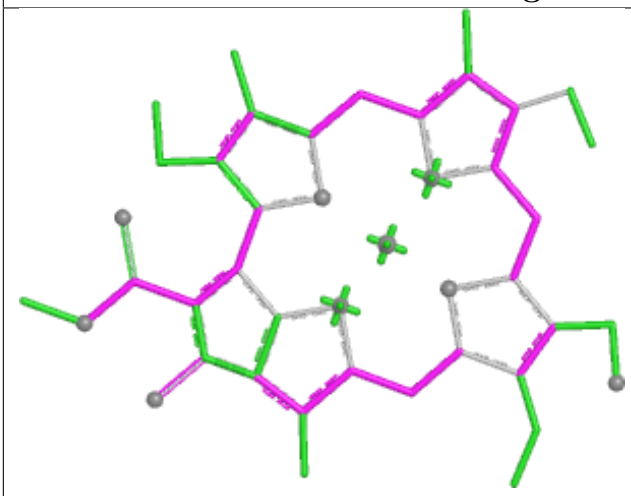


Torsions

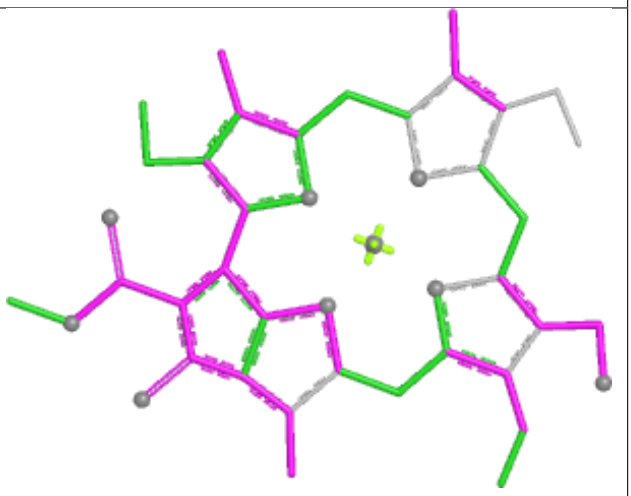


Rings

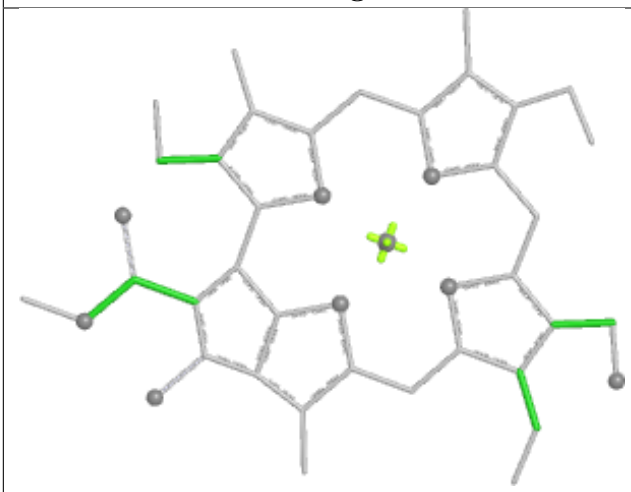
Ligand CHL U 605



Bond lengths



Bond angles



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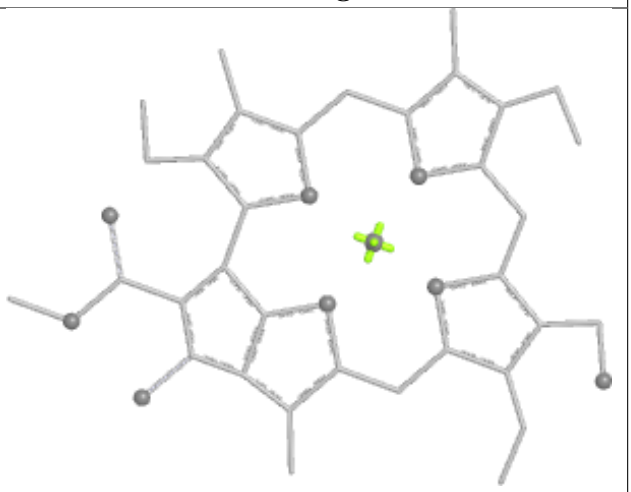
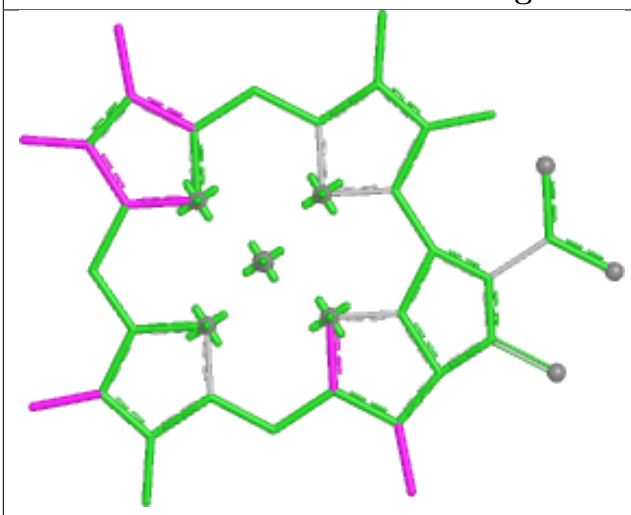


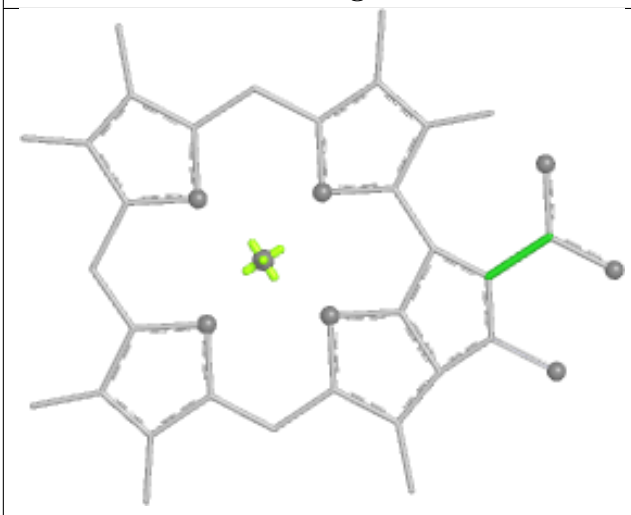
Rings

Ligand CLA O 2002



Bond lengths

Bond angles



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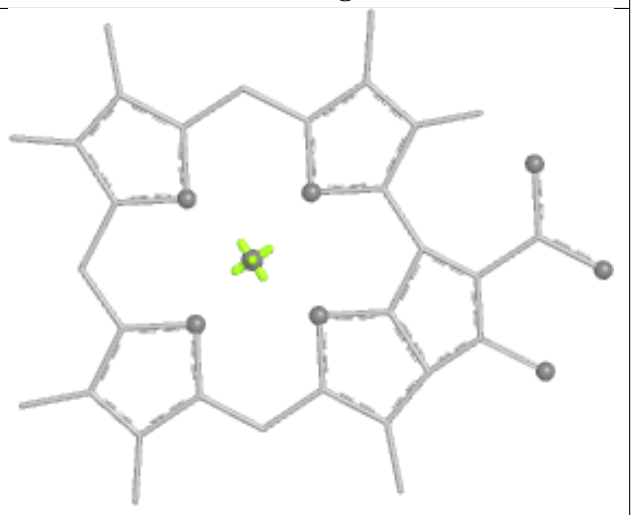
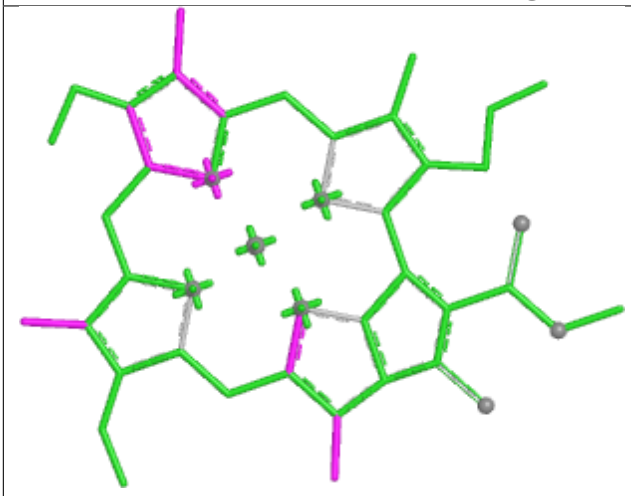
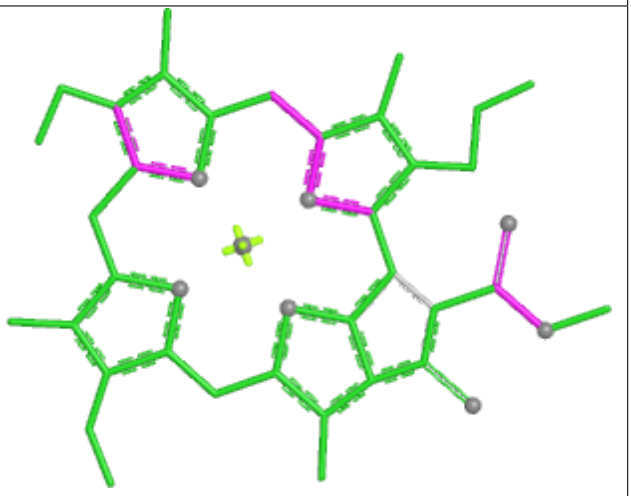


Rings

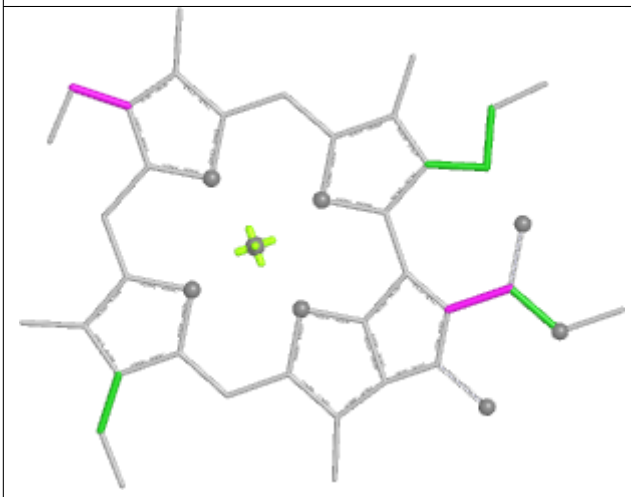
Ligand CLA U 612



Bond lengths



Bond angles



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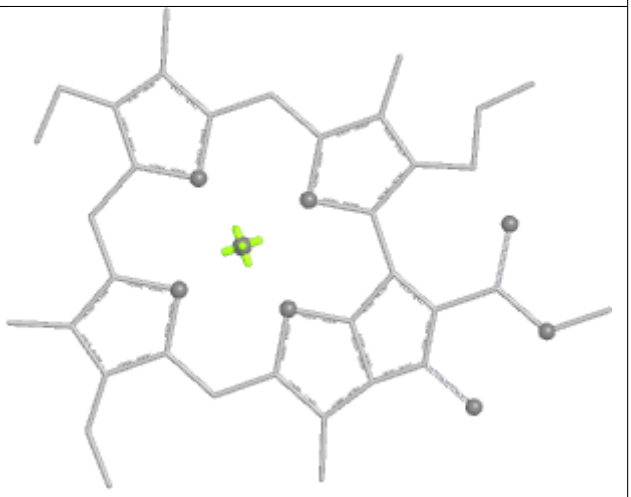
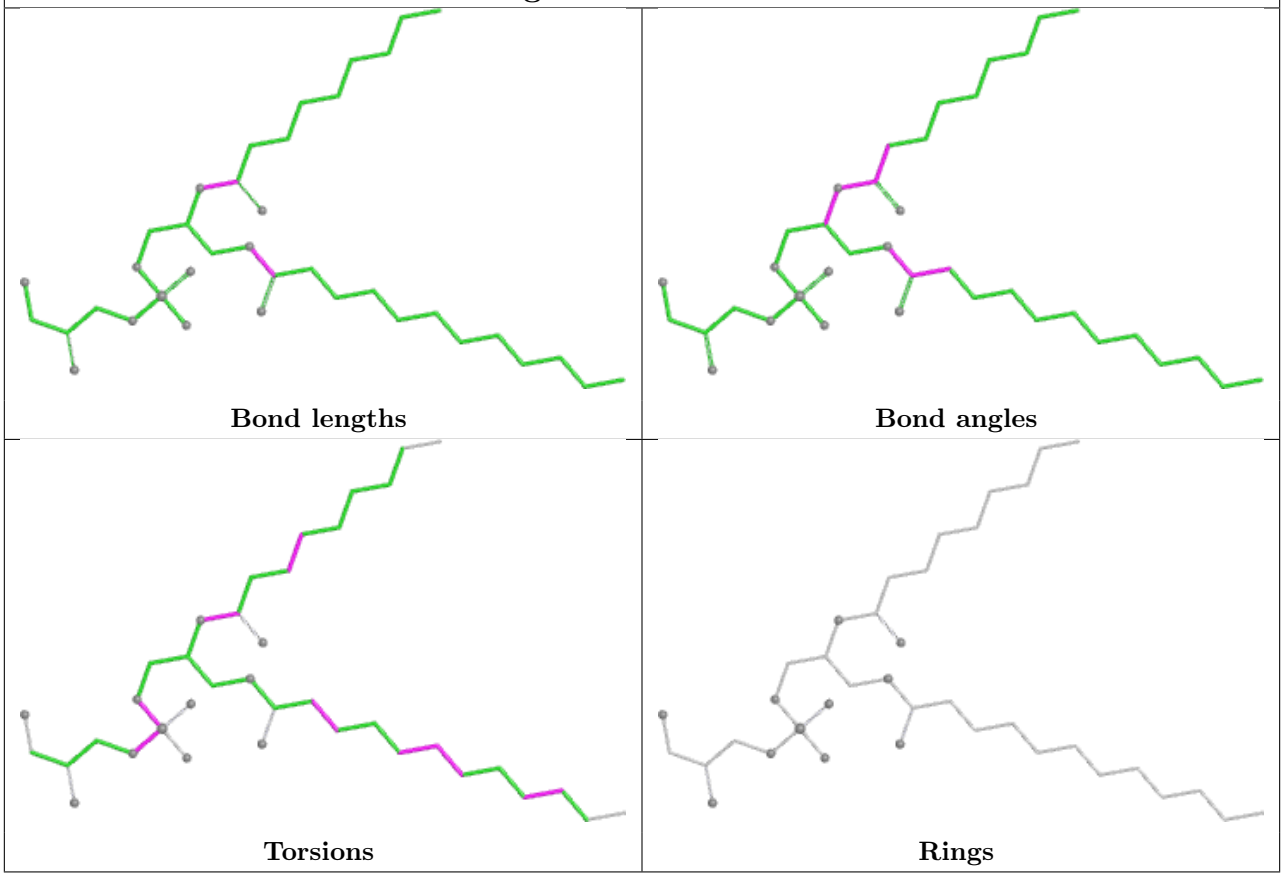
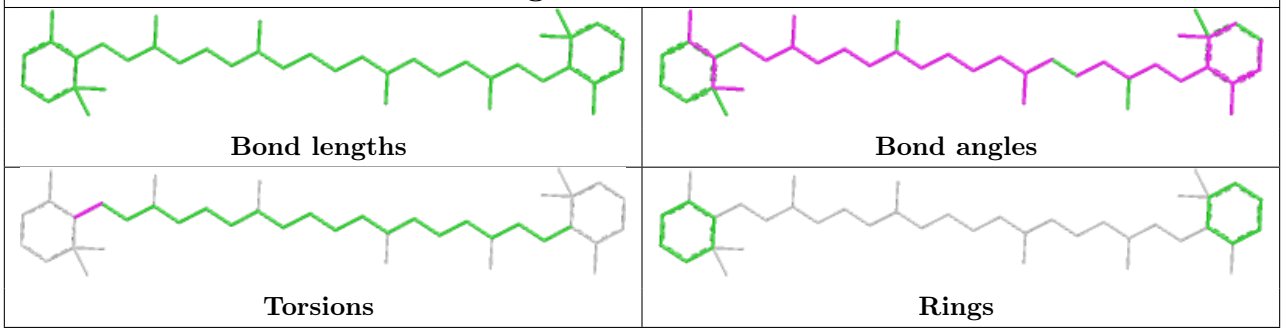


Rings

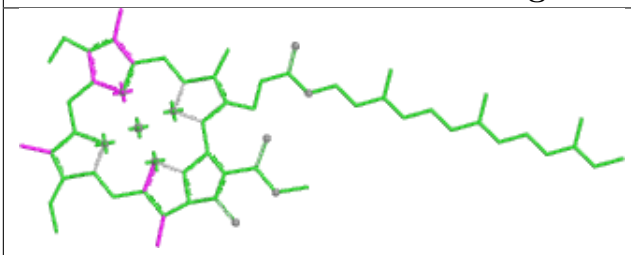
Ligand LHG B 851



Ligand BCR J 102



Ligand CLA 1 602



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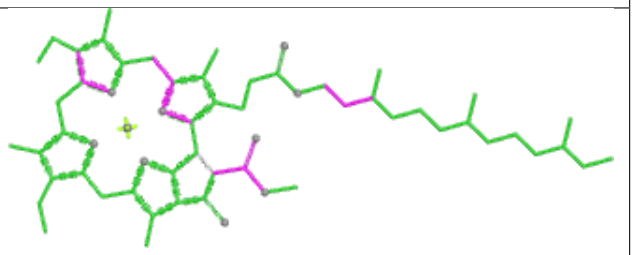
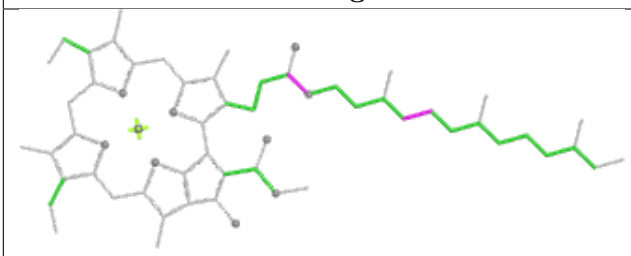


Bond angles



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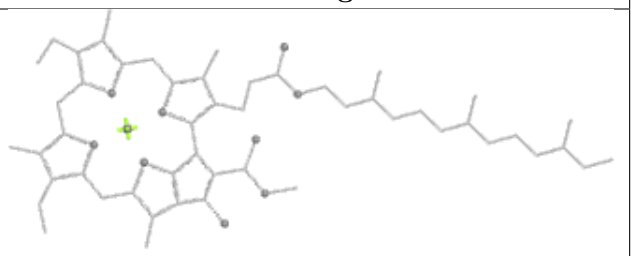
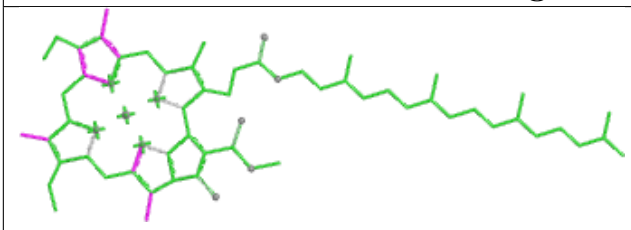


Rings

Ligand CLA 6 604



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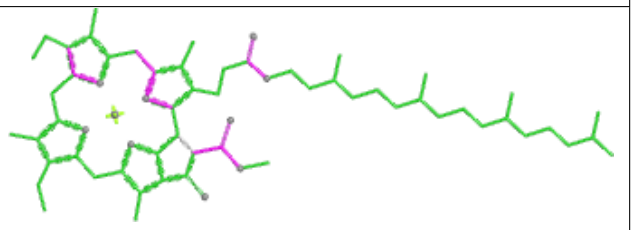

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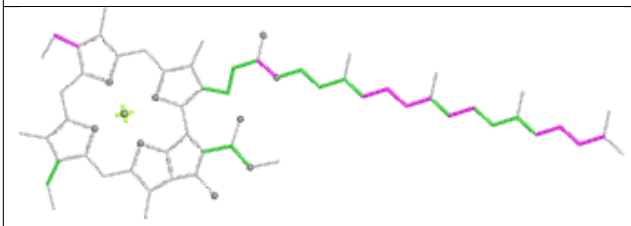

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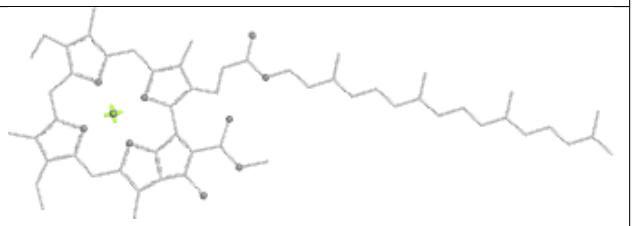
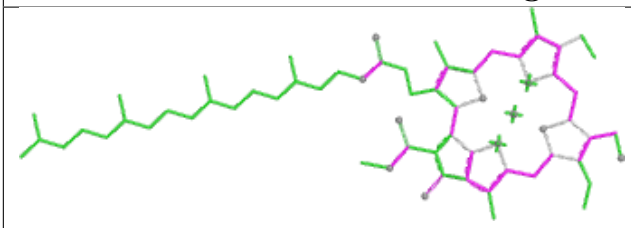


Rings

Ligand CHL U 601



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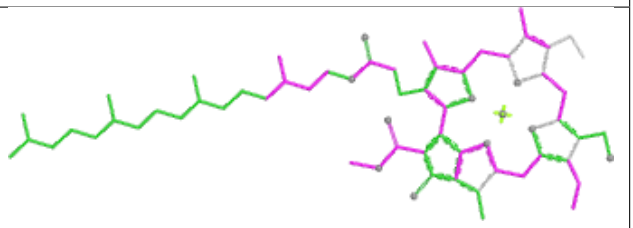

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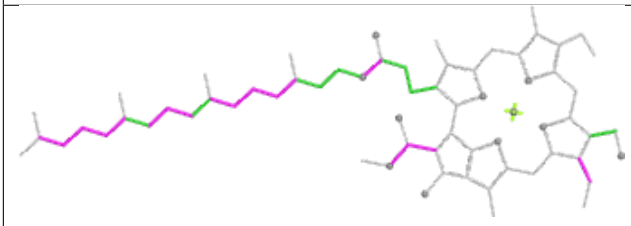

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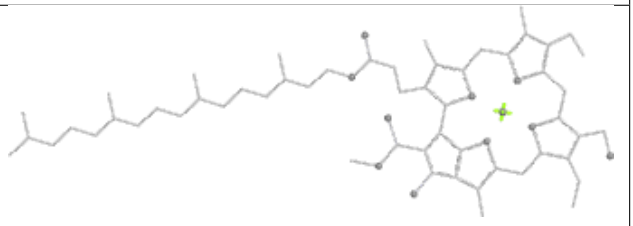
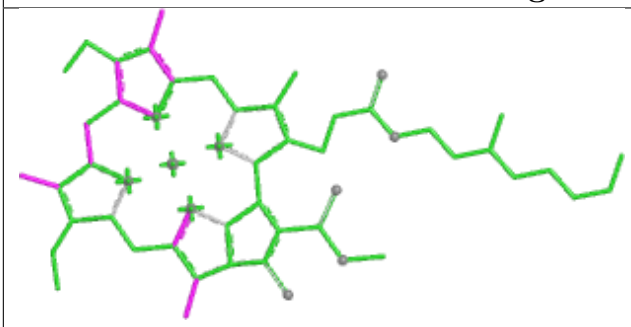


Rings

Ligand CLA 5 610



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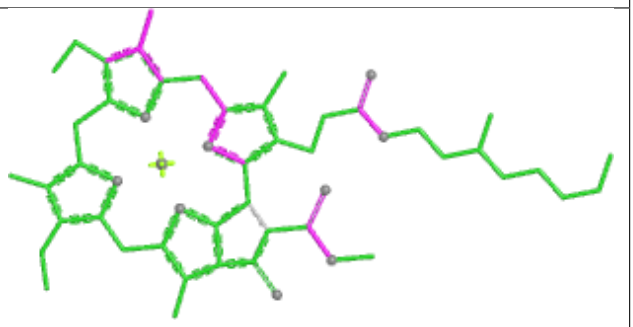
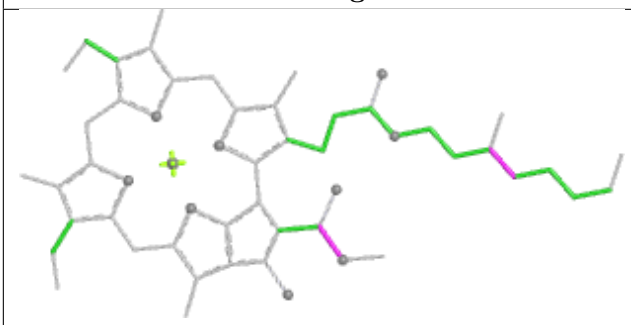


Bond angles



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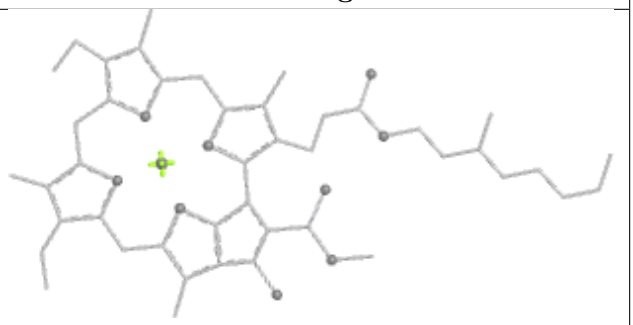
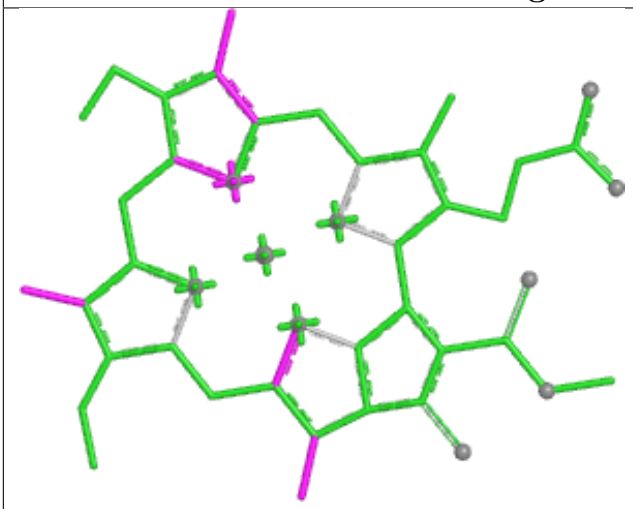


Rings

Ligand CLA 9 607



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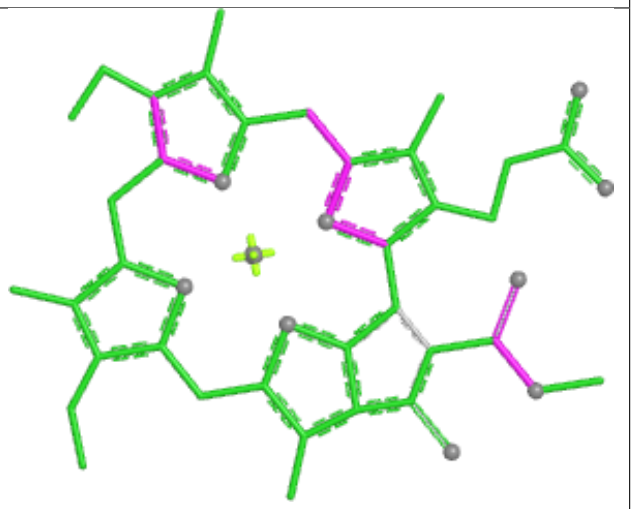

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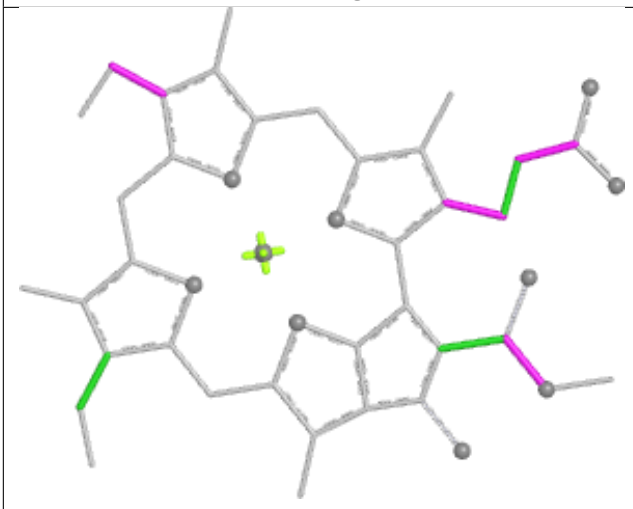
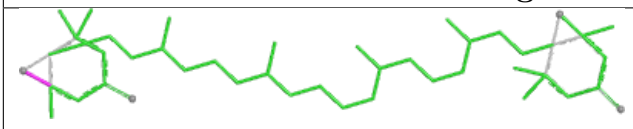


Torsions

Rings

Ligand XAT Z 1622



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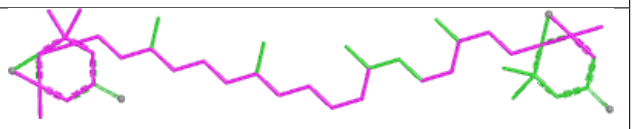
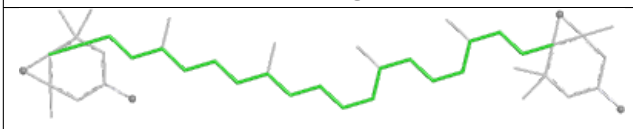
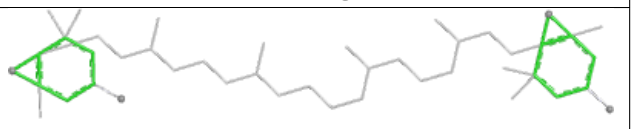


Bond angles

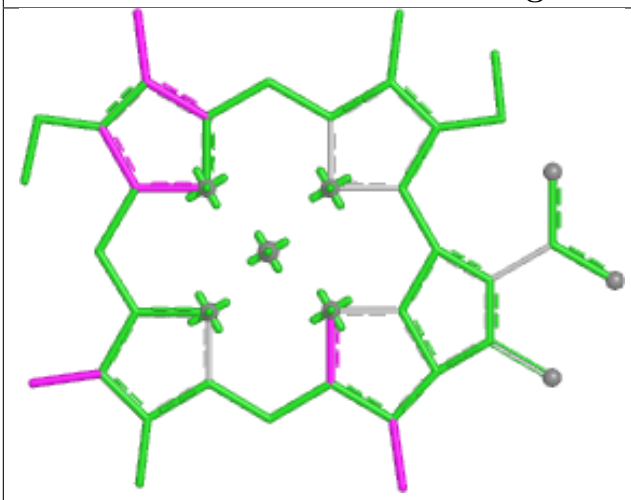


Torsions



Rings

Ligand CLA L 306



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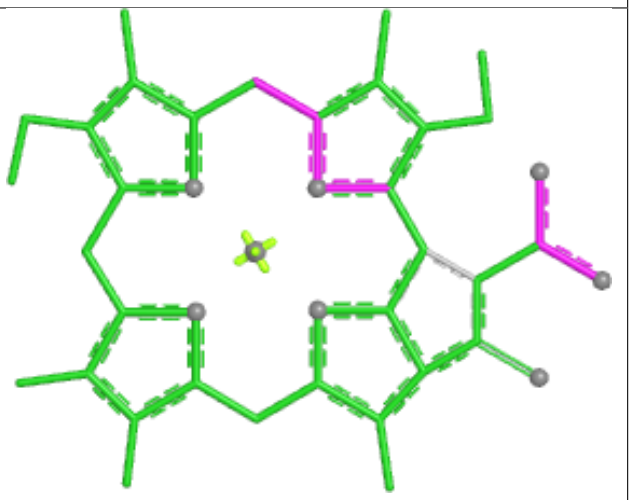
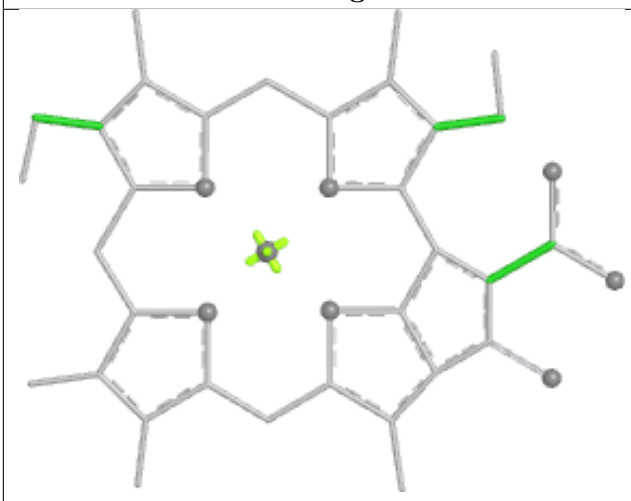


Bond angles



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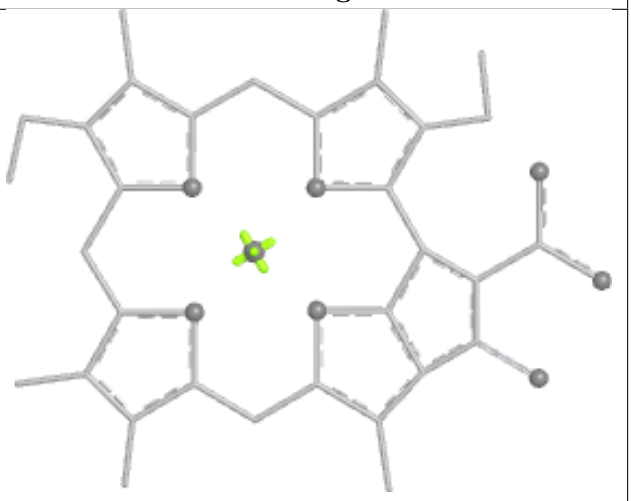
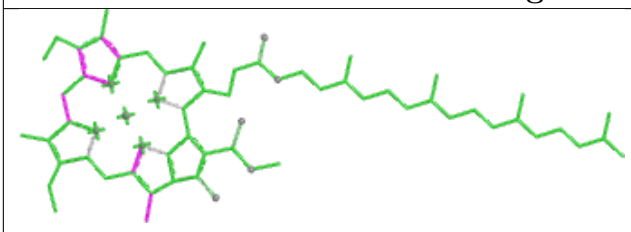


Rings

Ligand CLA Z 612



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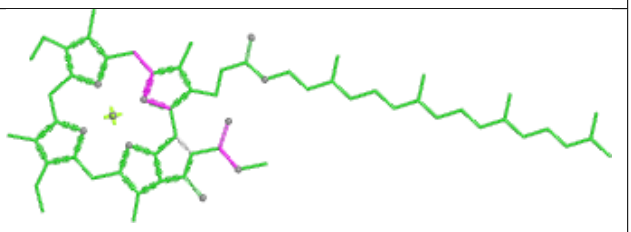
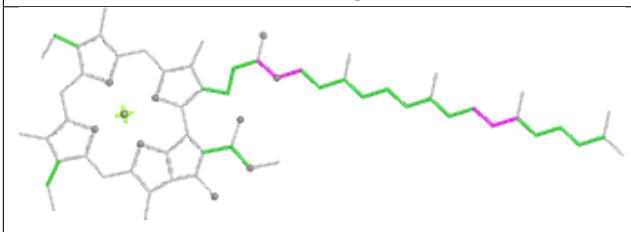


Bond angles



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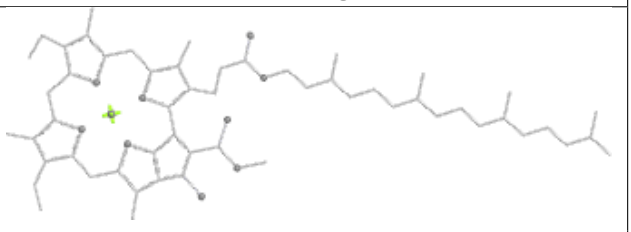
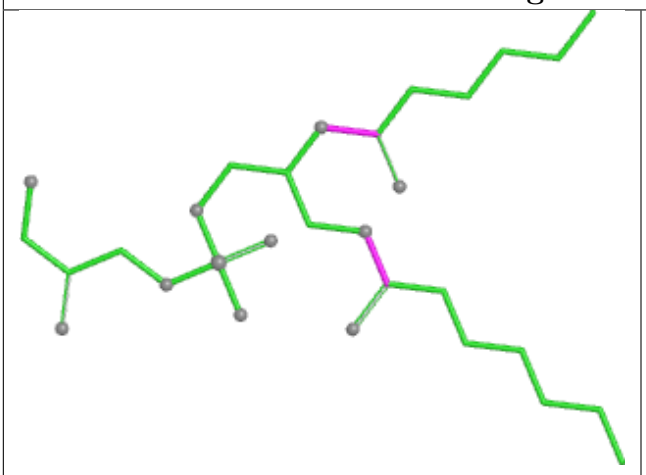


Rings

Ligand LHG 9 622



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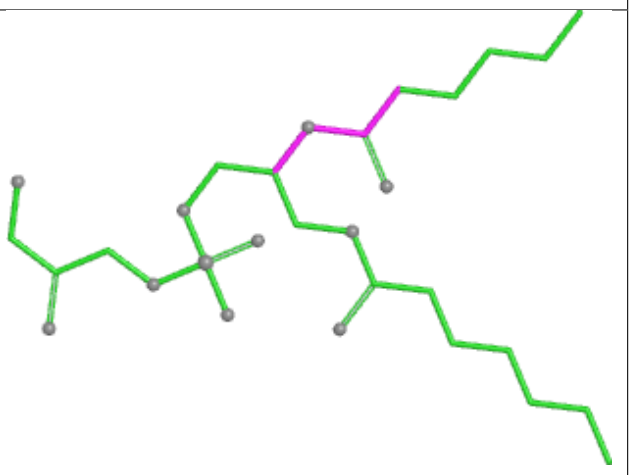
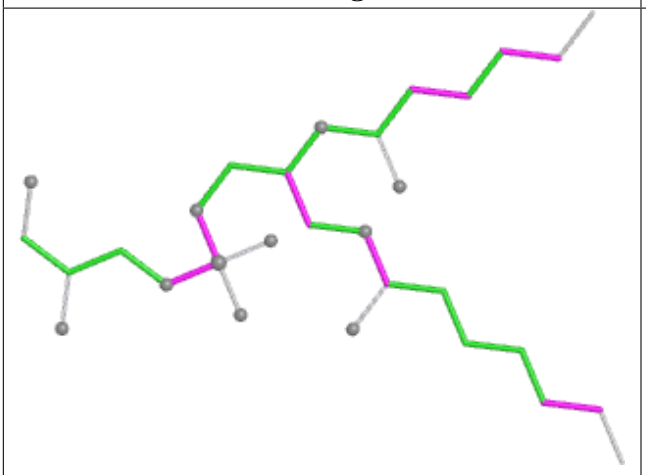
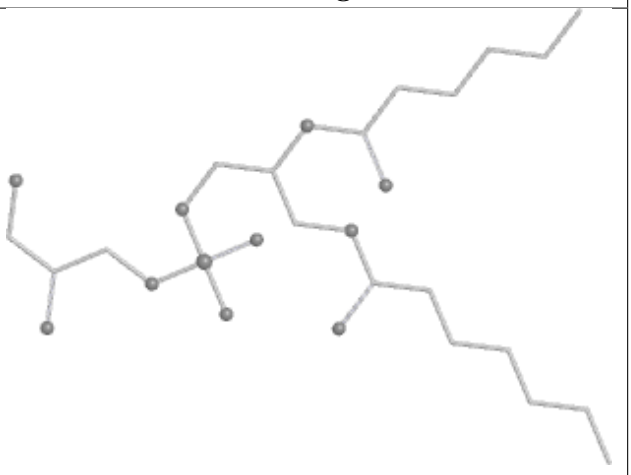


Bond angles

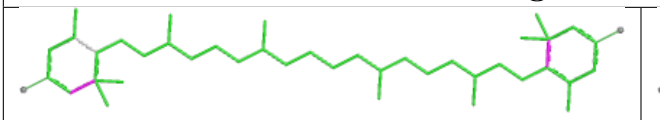


Torsions

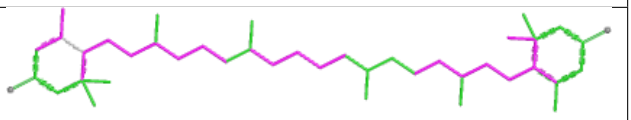


Rings

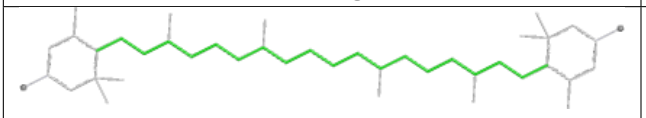
Ligand LUT 3 618



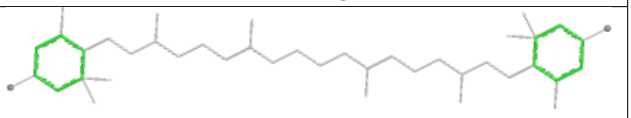
Bond lengths



Bond angles

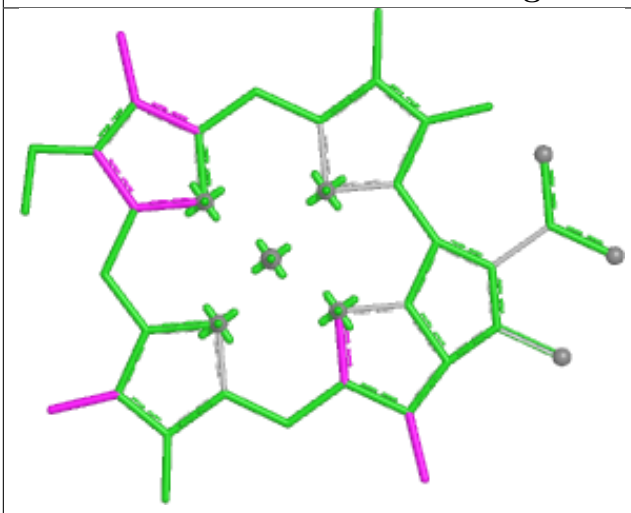


Torsions



Rings

Ligand CLA H 202



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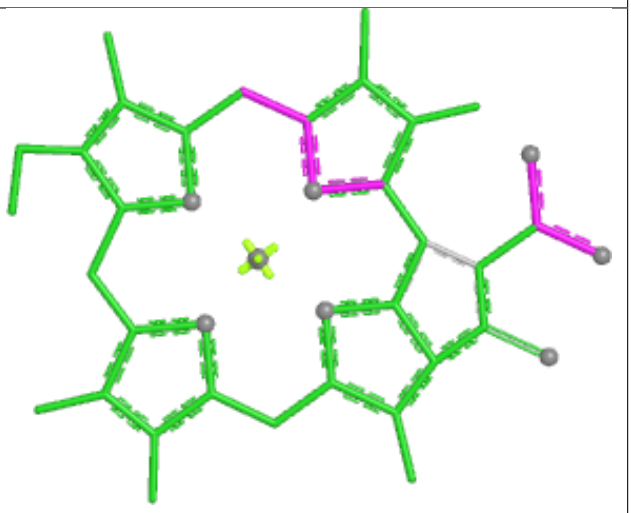
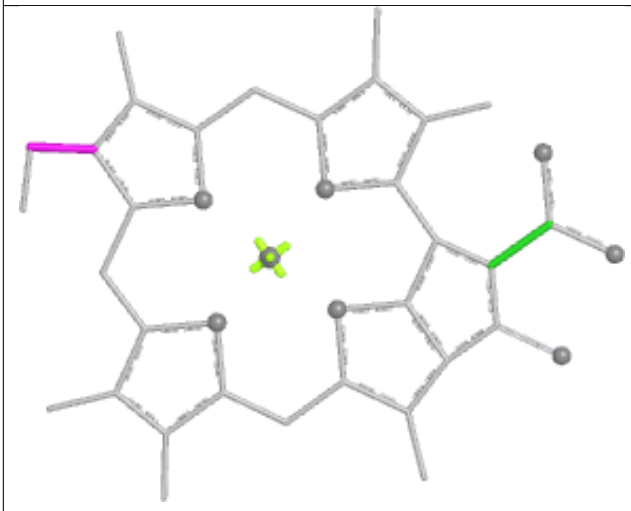
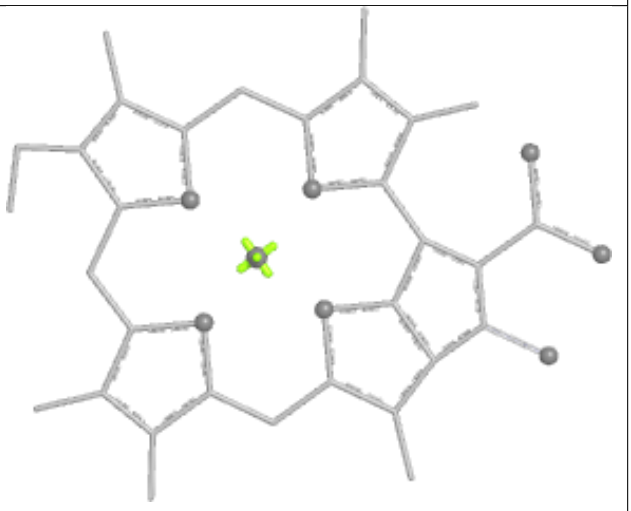


Bond angles

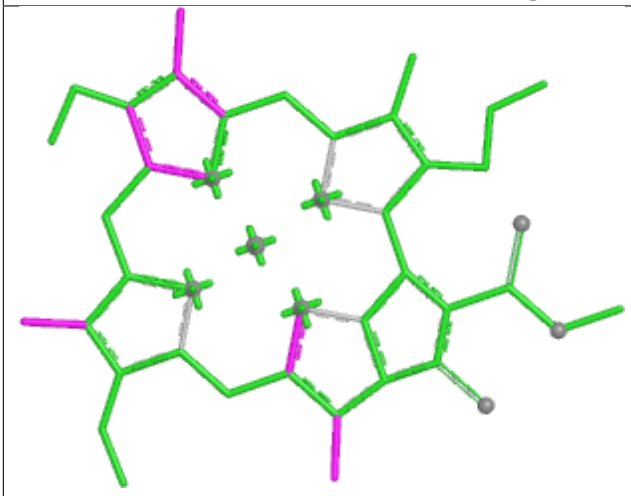


Torsions



Rings

Ligand CLA B 830



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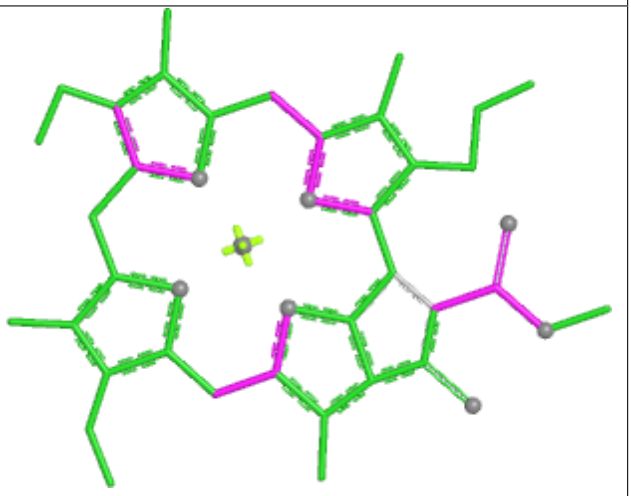
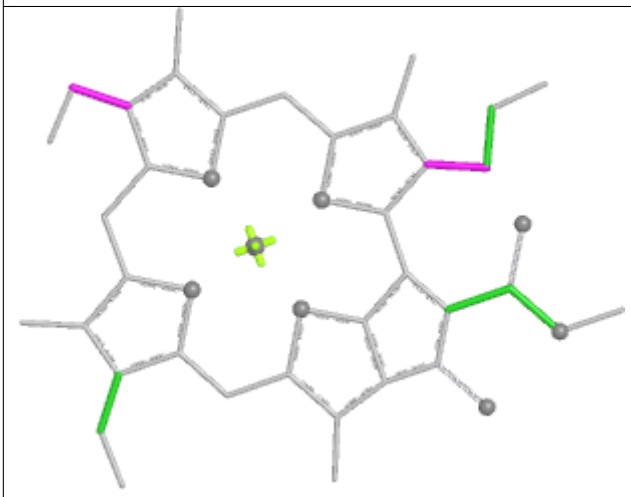
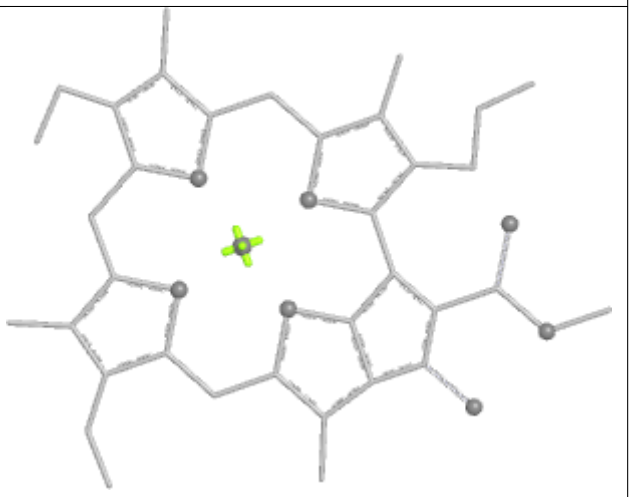


Bond angles

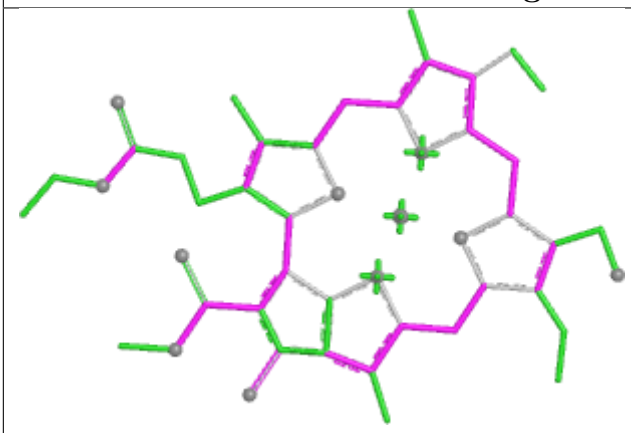


Torsions



Rings

Ligand CHL V 608



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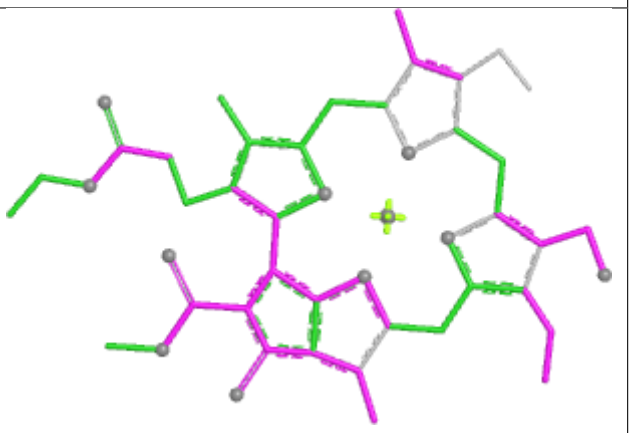
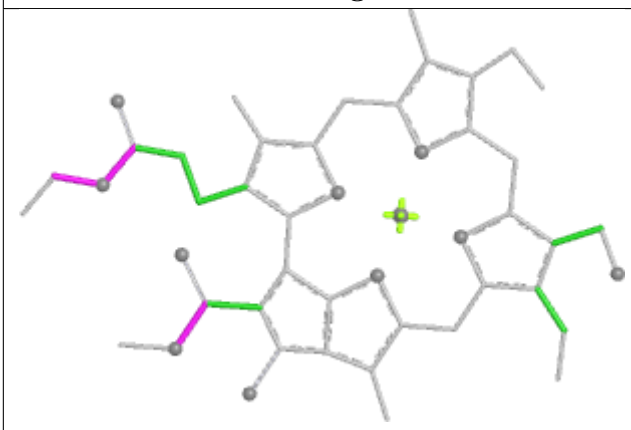


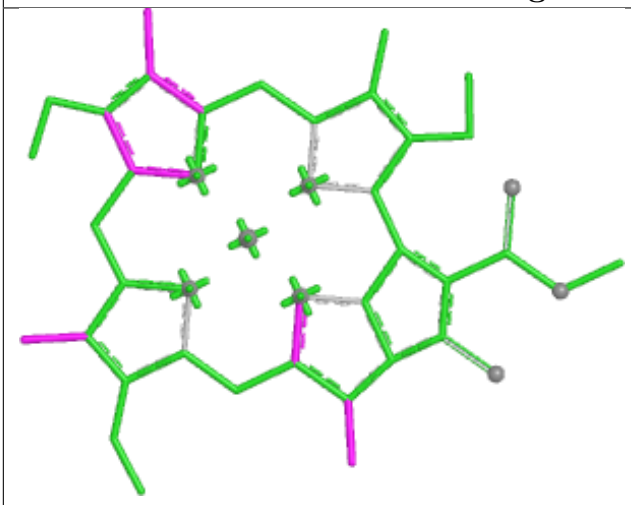
Bond angles



Torsions

Rings

Ligand CLA 4 611



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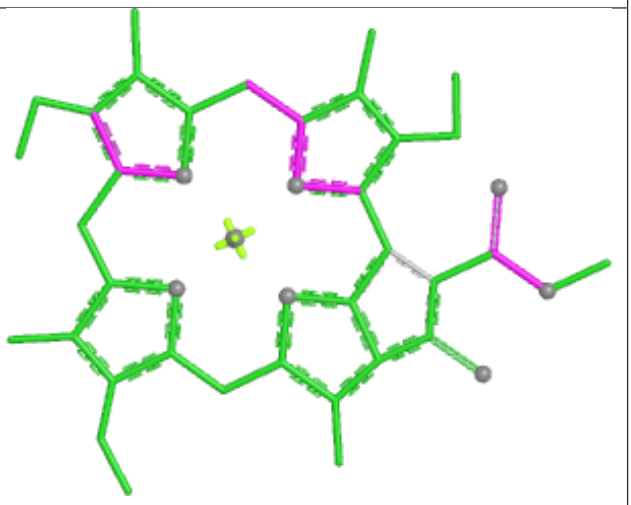
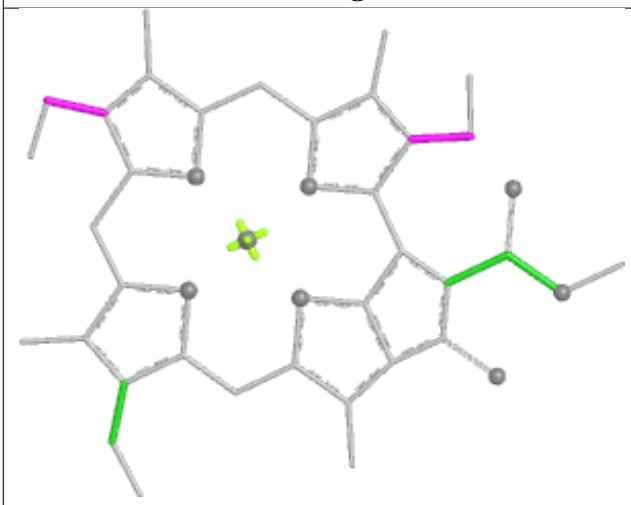


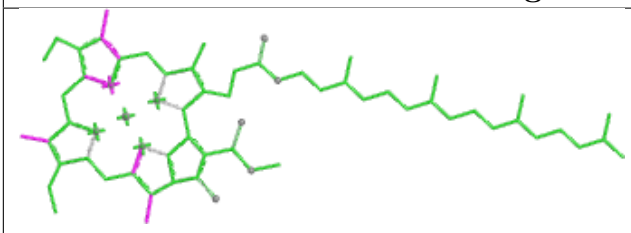
Bond angles



Torsions

Rings

Ligand CLA B 802



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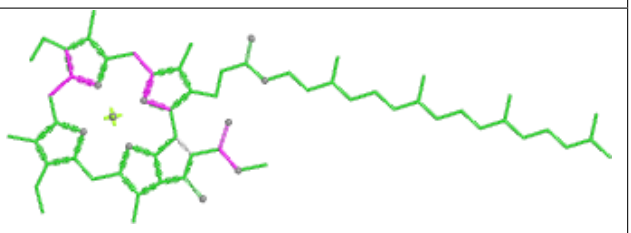
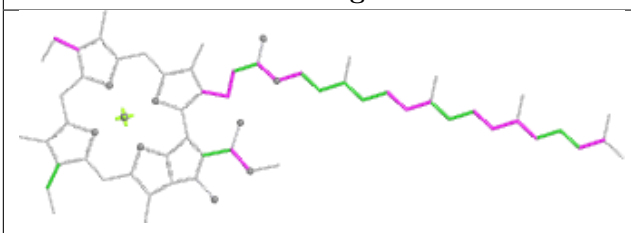


Bond angles



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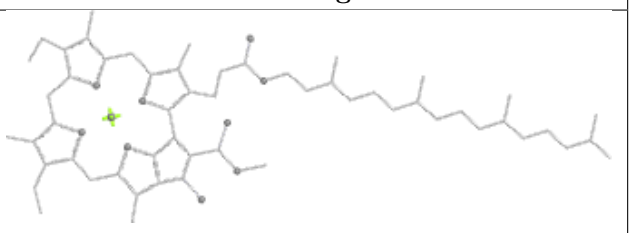
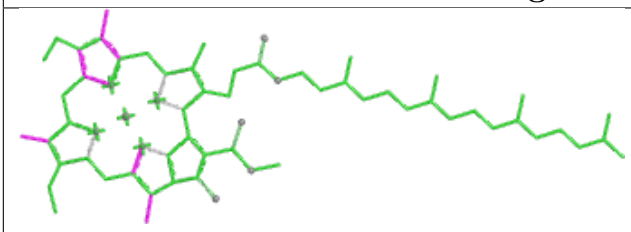


Rings

Ligand CLA 1 613



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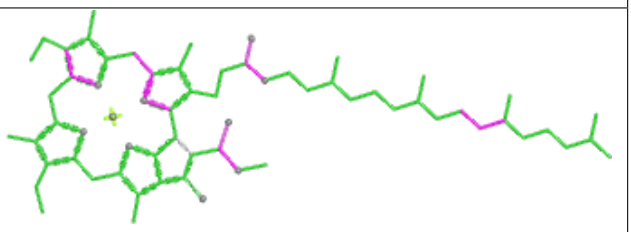

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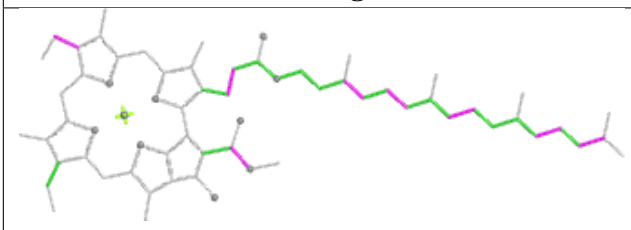

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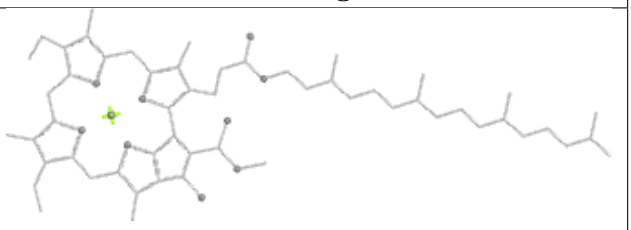
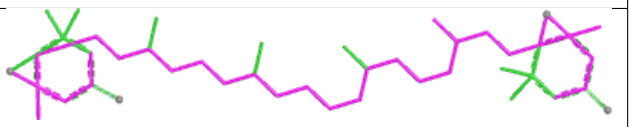


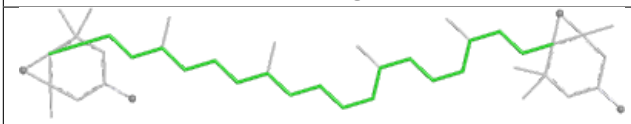
Rings

Ligand XAT 3 619

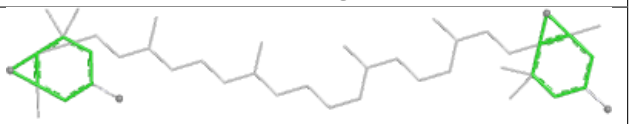
Bond lengths



Bond angles

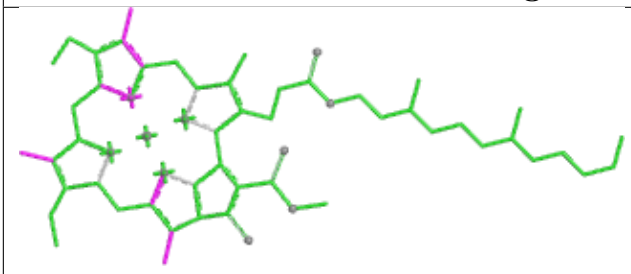


Torsions

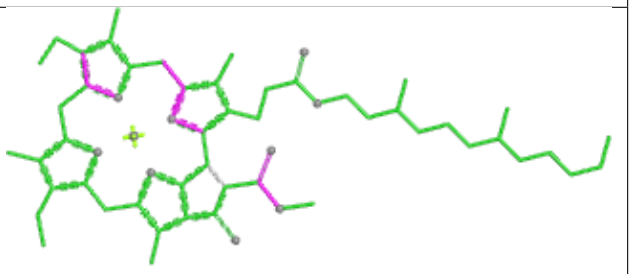


Rings

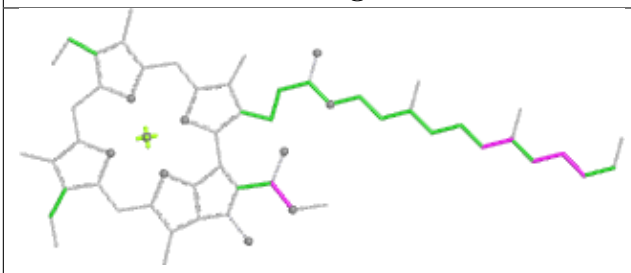
Ligand CLA U 602



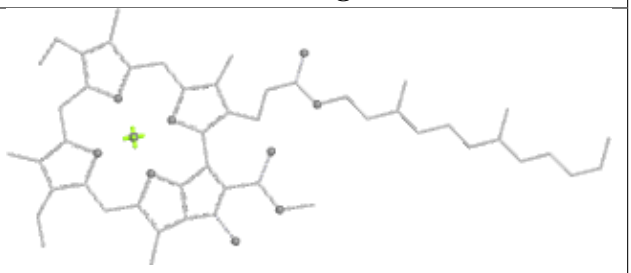
Bond lengths



Bond angles

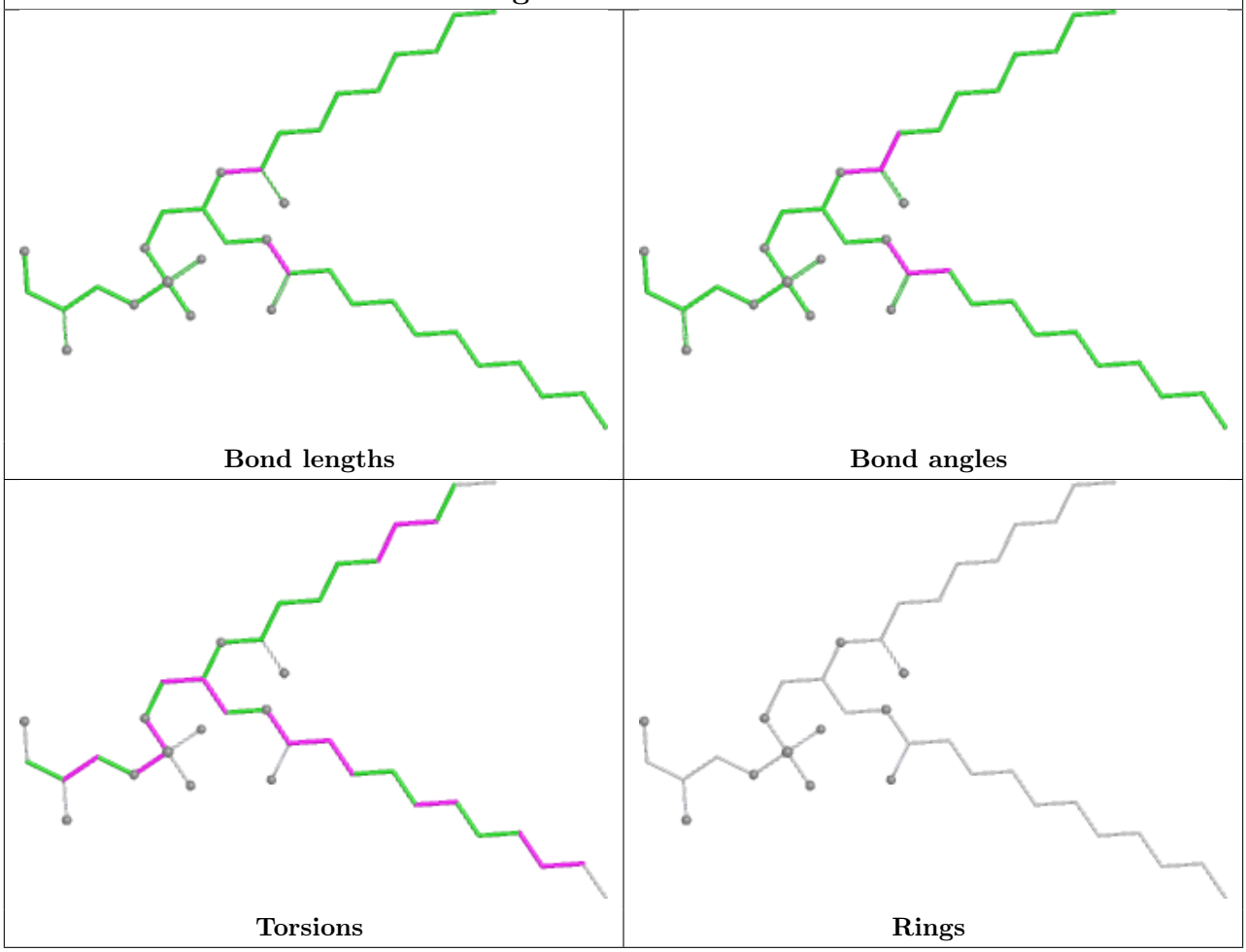


Torsions

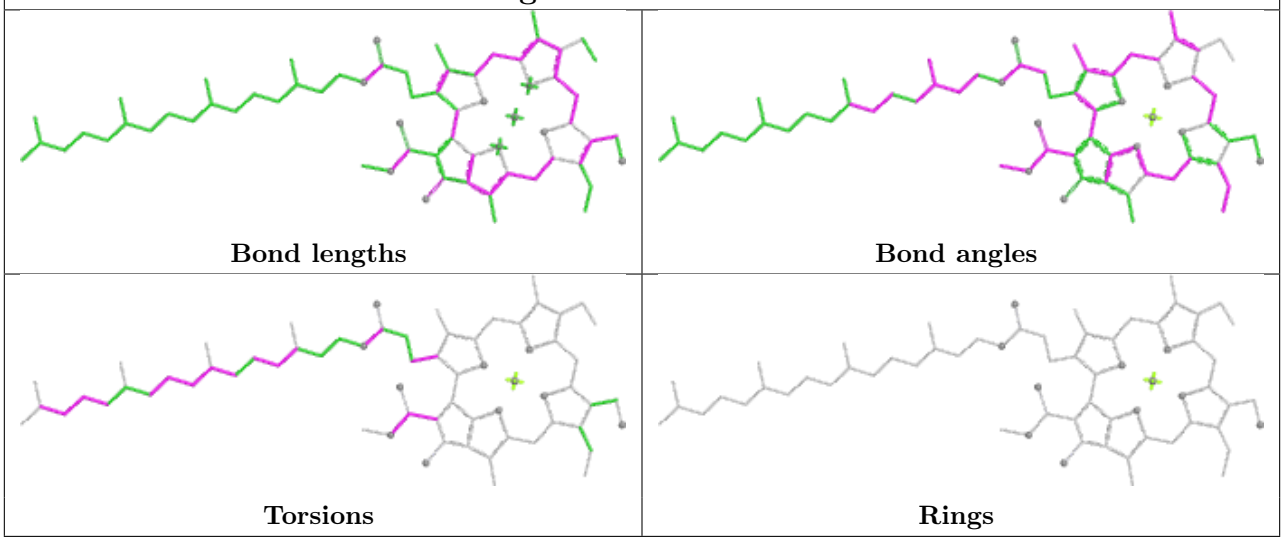


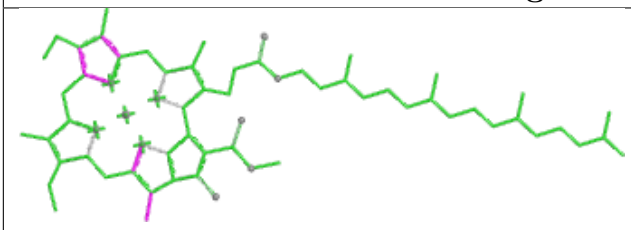
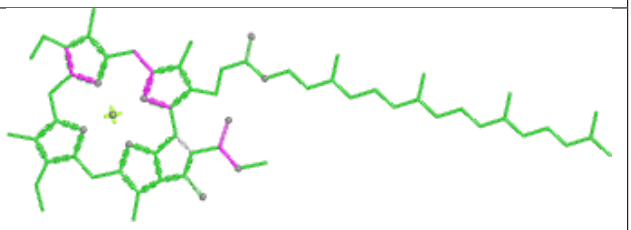
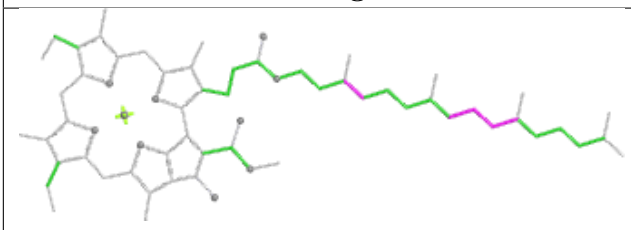
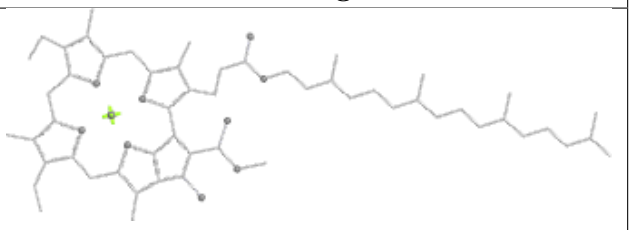
Rings

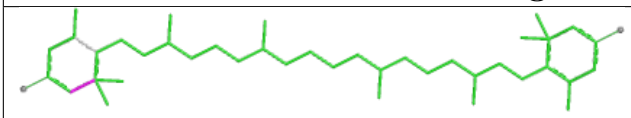
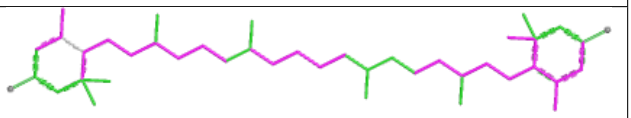
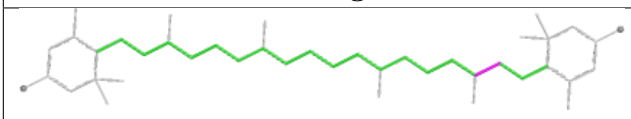
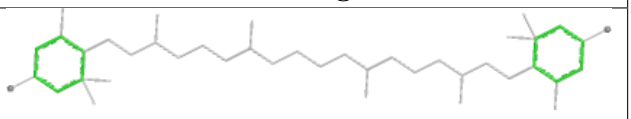
Ligand LHG 7 622



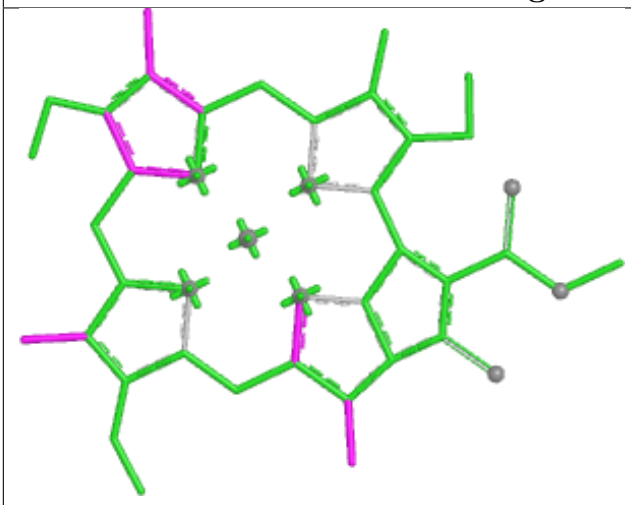
Ligand CHL W 601



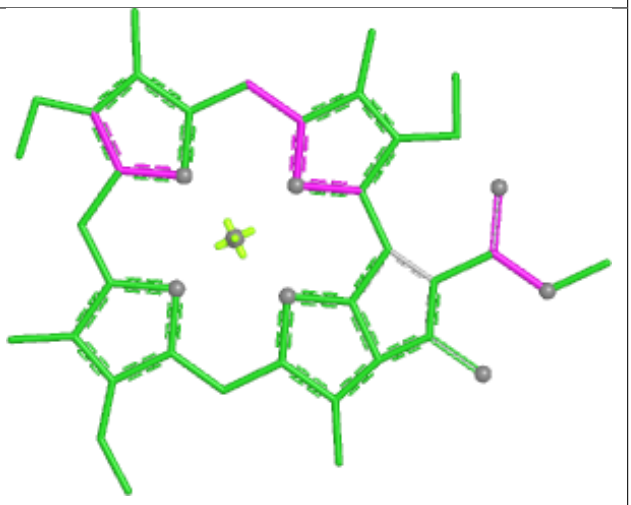
Ligand CLA Z 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 8 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

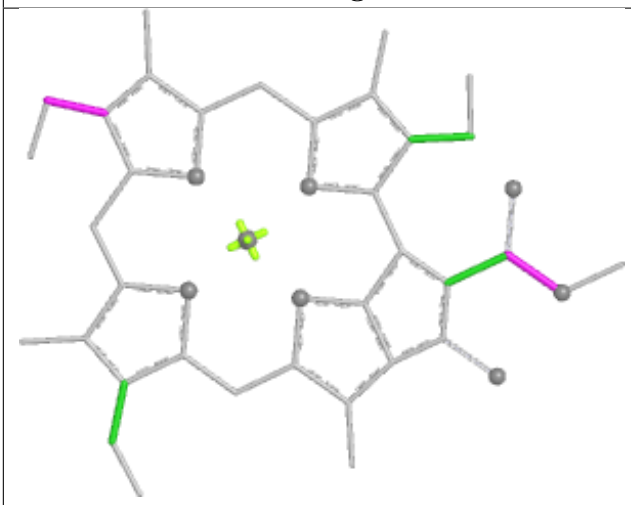
Ligand CLA 7 607



Bond lengths



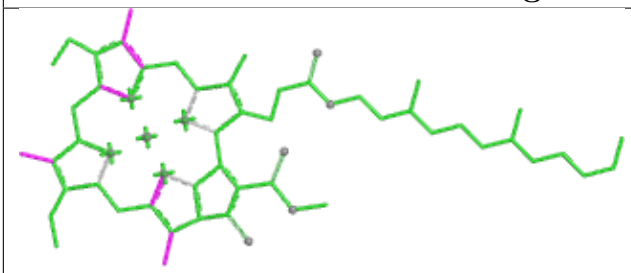
Bond angles



Torsions

Rings

Ligand CLA U 613



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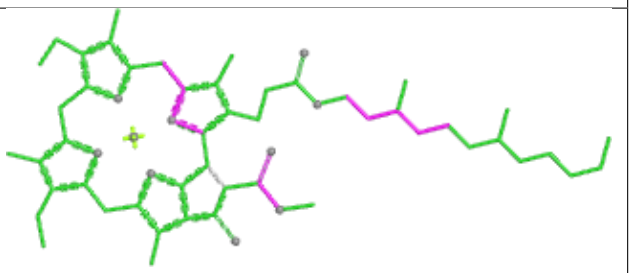
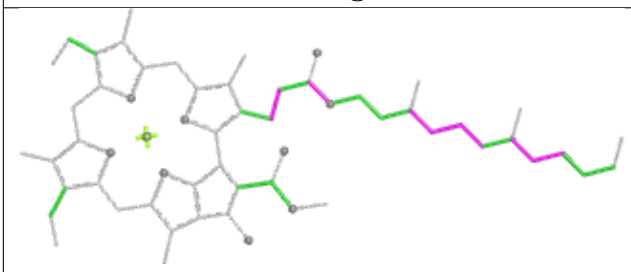
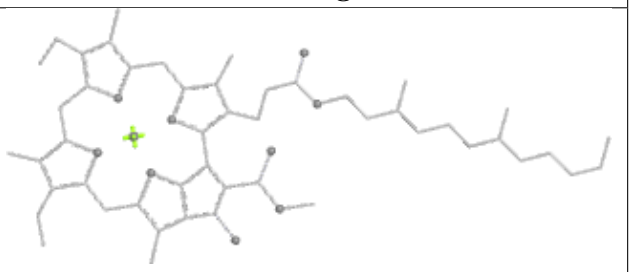


Bond angles

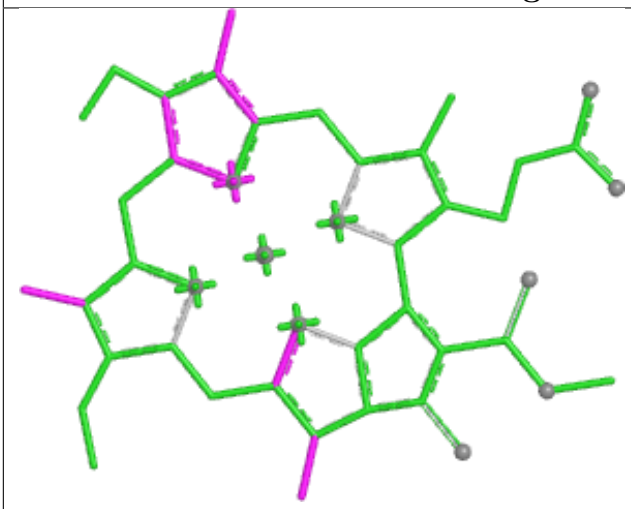


Torsions



Rings

Ligand CLA K 204



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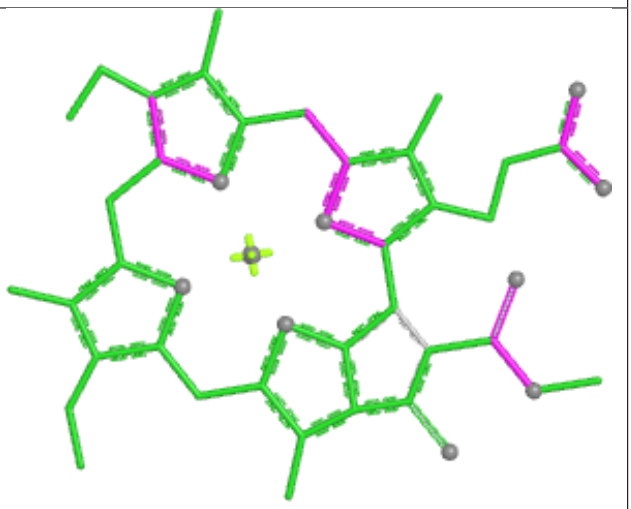
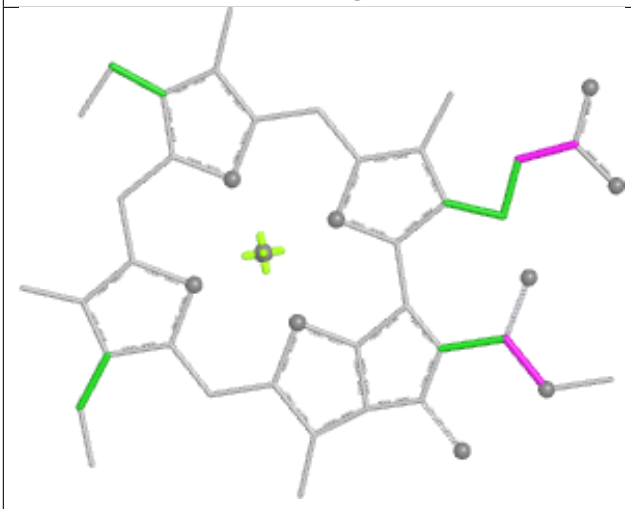


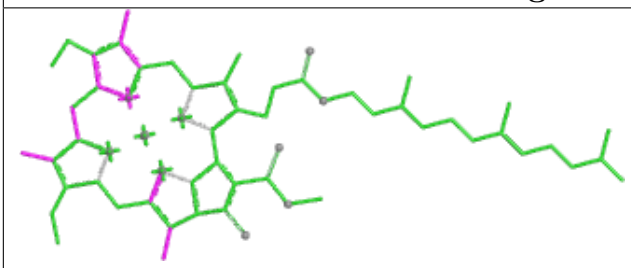
Bond angles



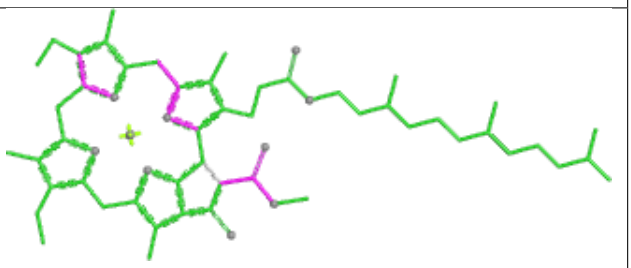
Torsions

Rings

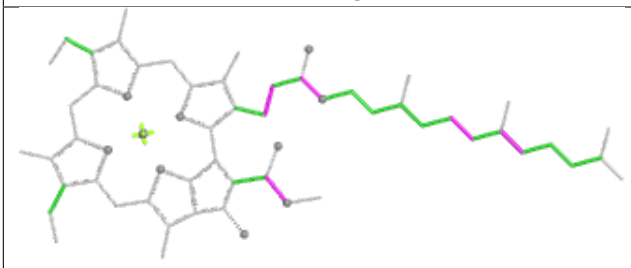
Ligand CLA 8 602



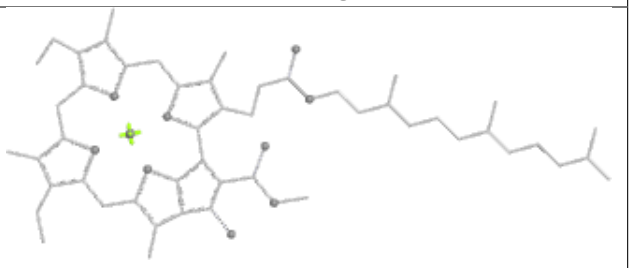
Bond lengths



Bond angles

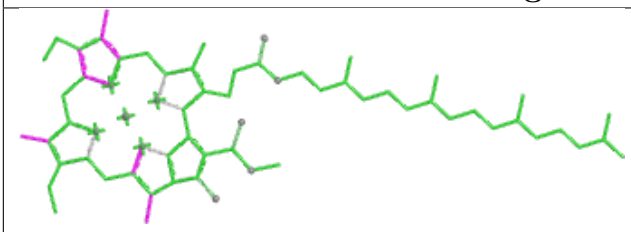


Torsions



Rings

Ligand CLA B 840



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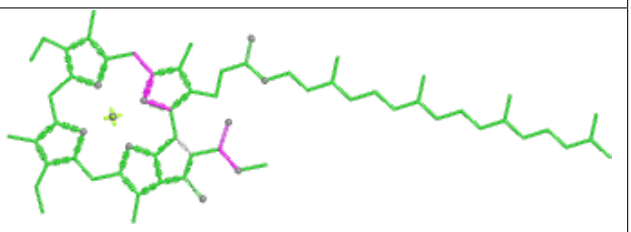
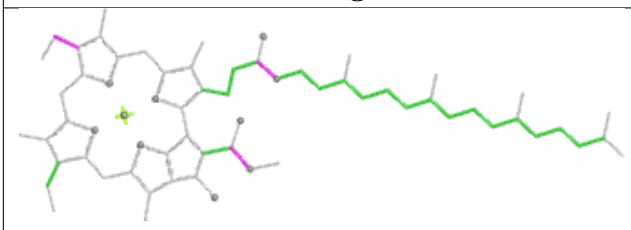


Bond angles



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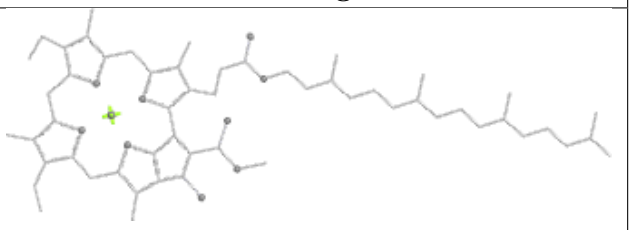
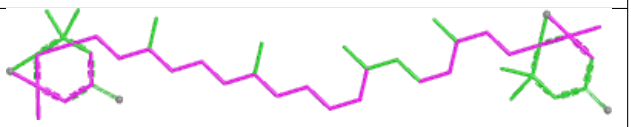


Rings

Ligand XAT V 1622

Bond lengths



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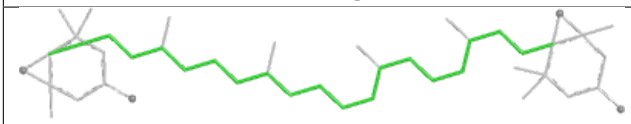

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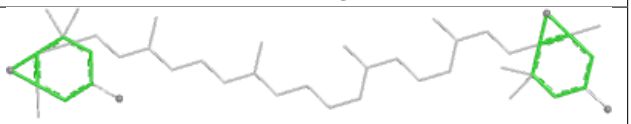
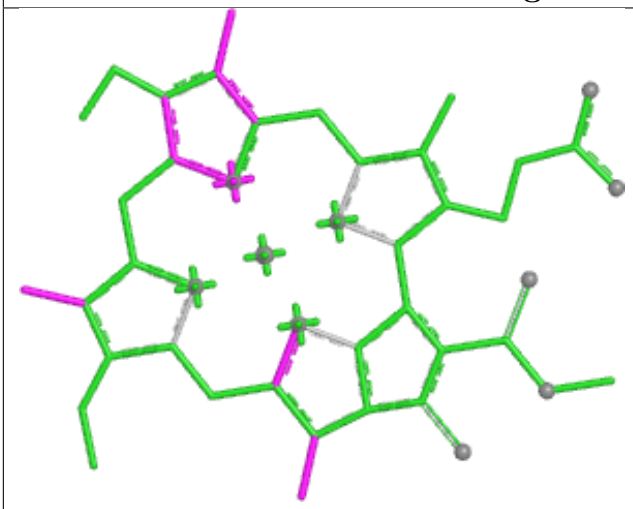


Rings

Ligand CLA V 612



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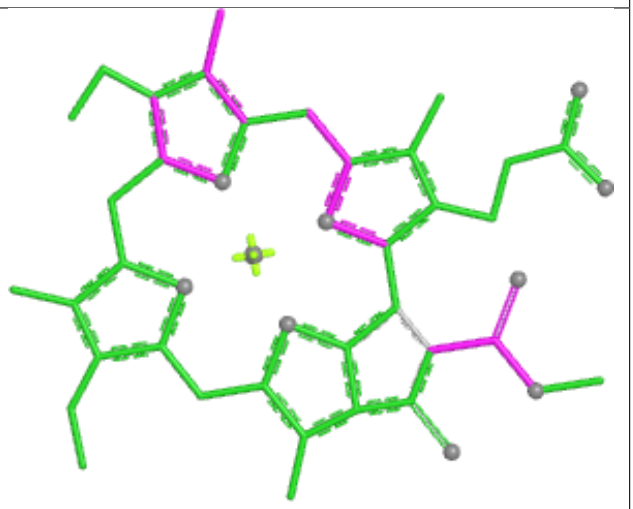
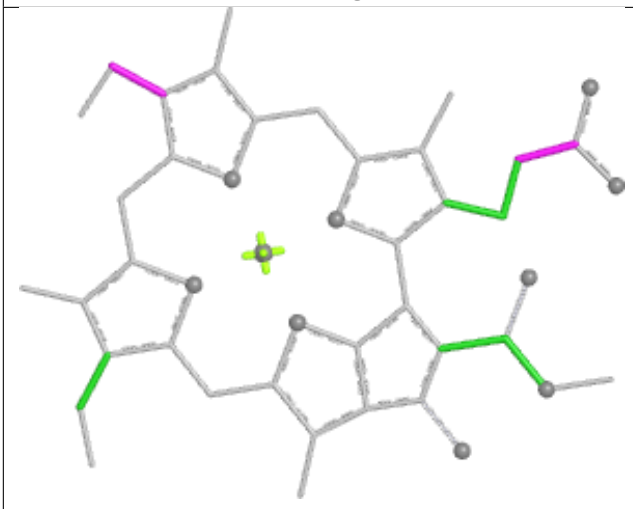


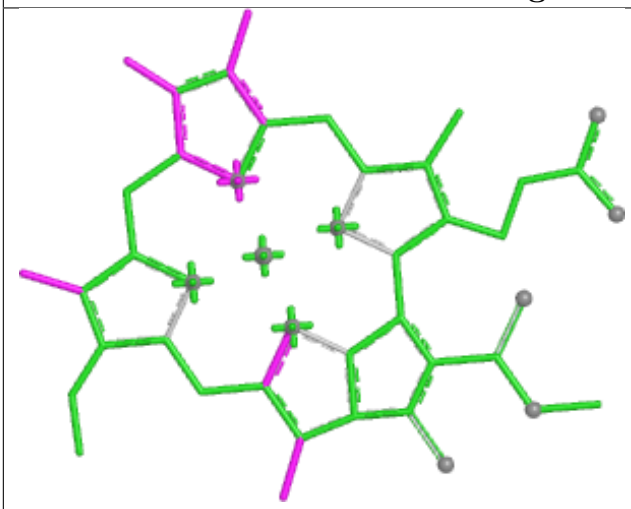
Bond angles



Torsions

Rings

Ligand CLA 8 603



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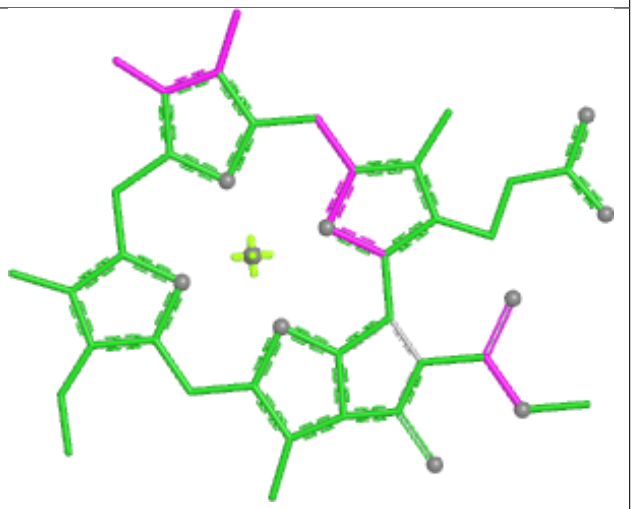

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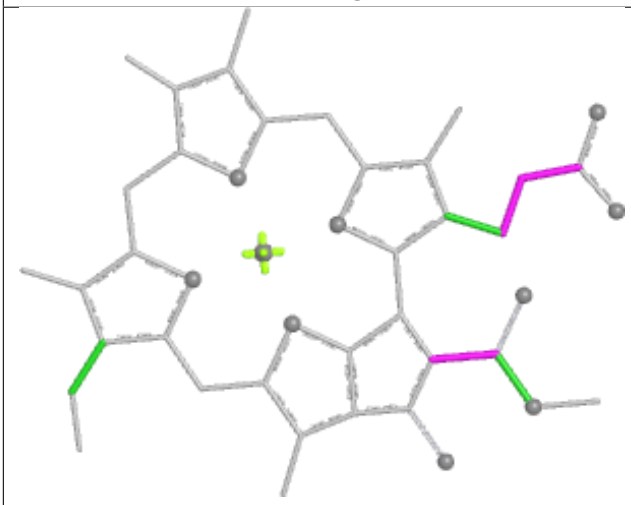

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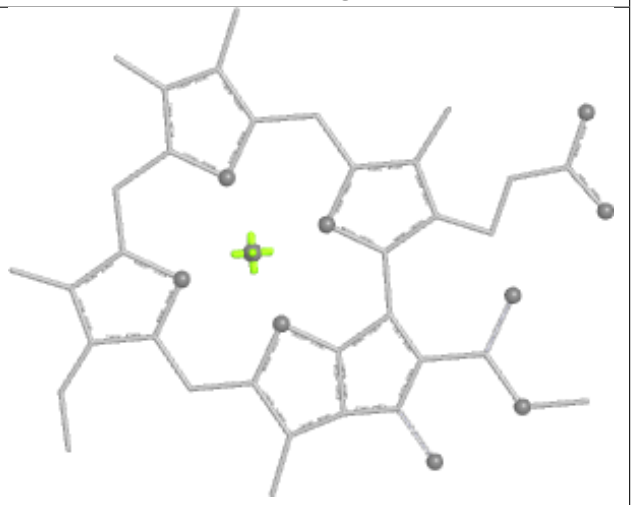
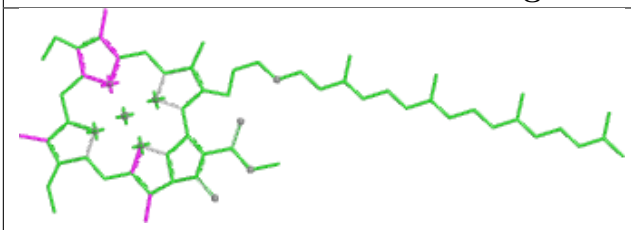


Rings

Ligand CLA A 826



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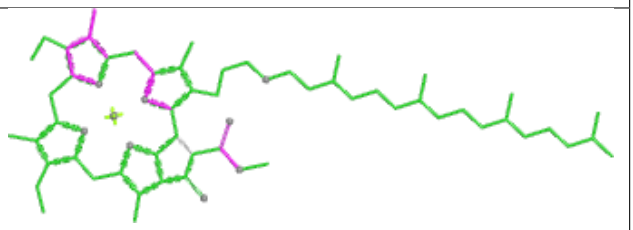

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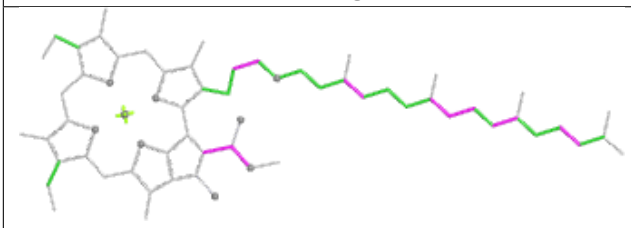

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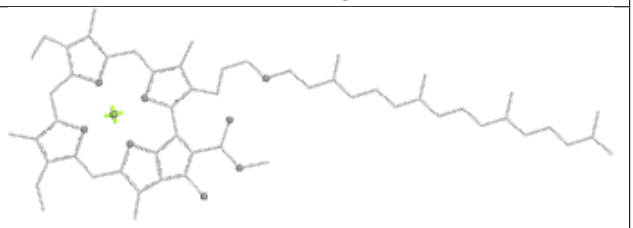
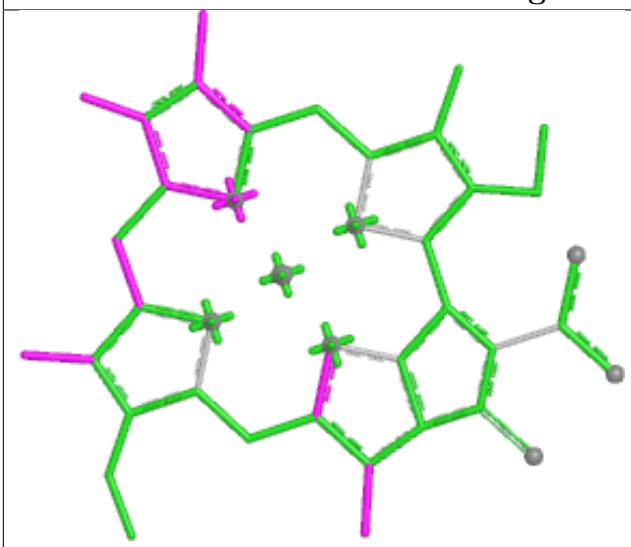


Rings

Ligand CLA 6 618



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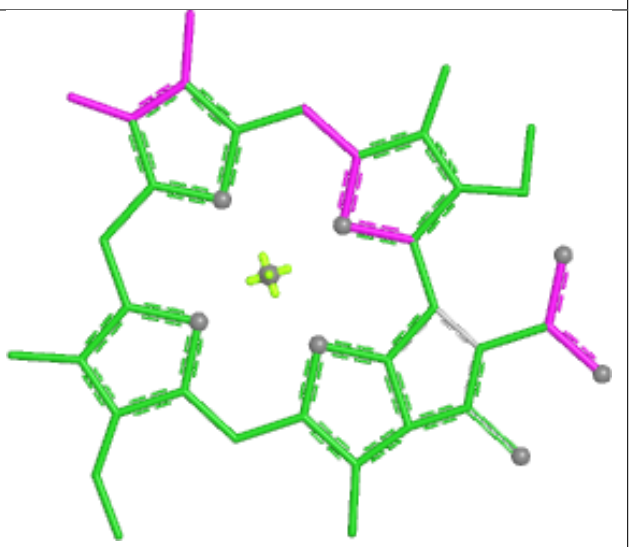
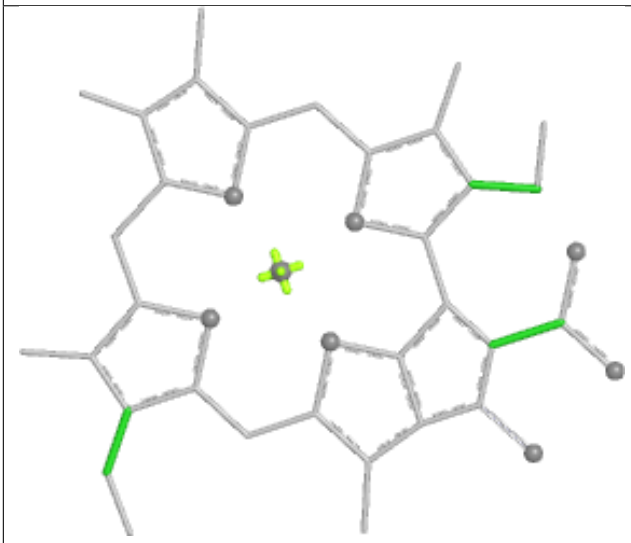


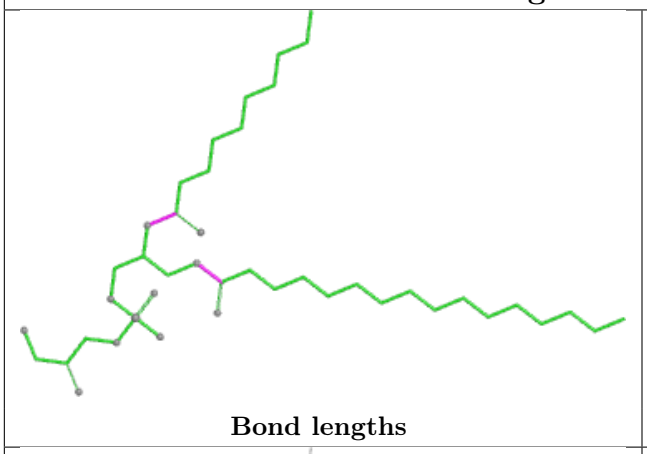
Bond angles



Torsions

Rings

Ligand LHG a 620



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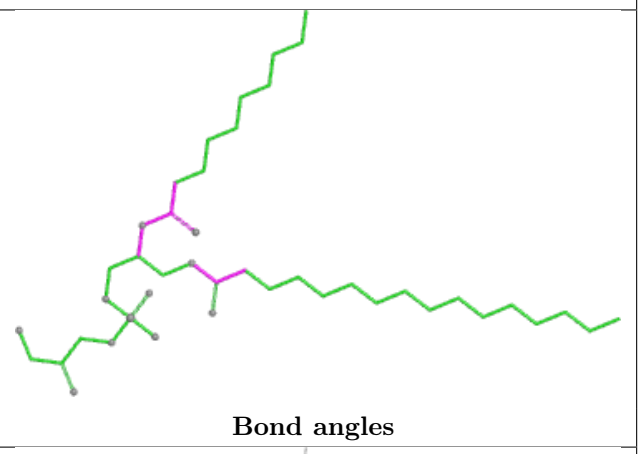

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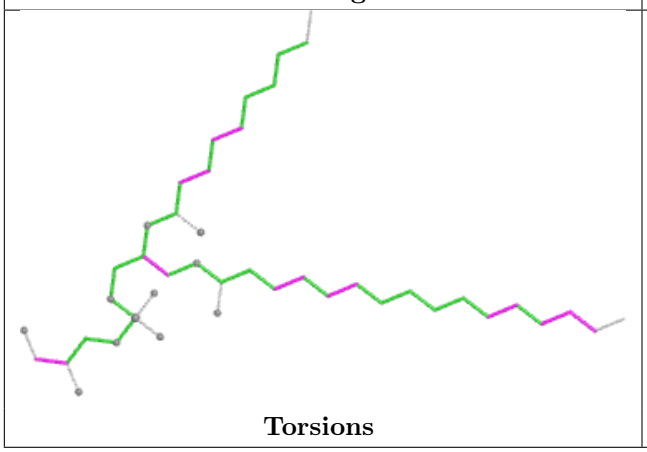

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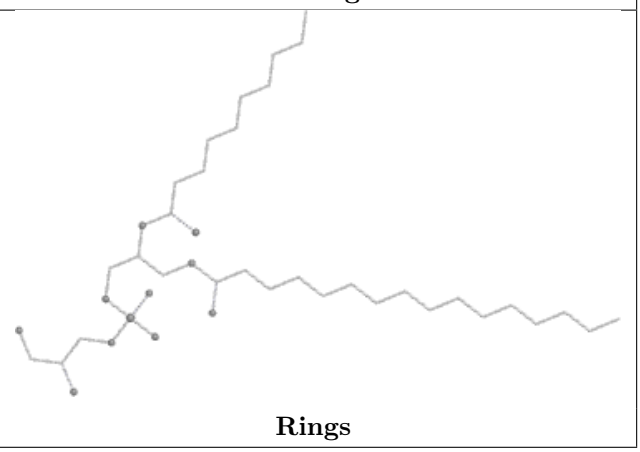

Rings

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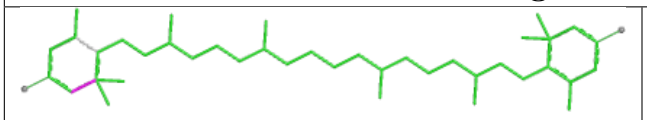

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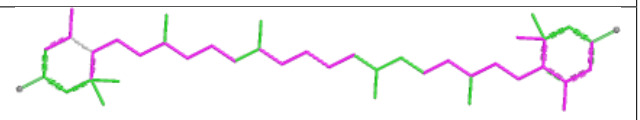
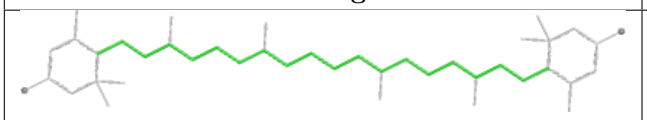


Bond angles



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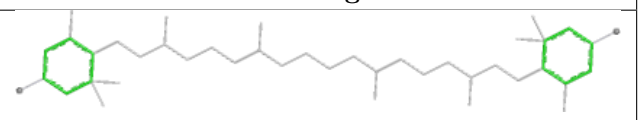
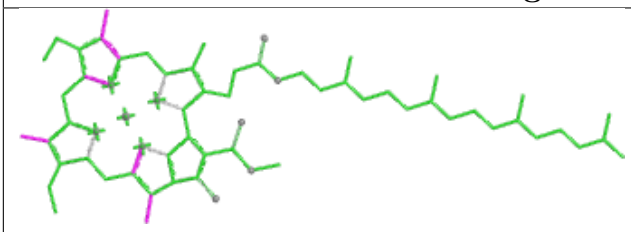


Rings

Ligand CLA A 825



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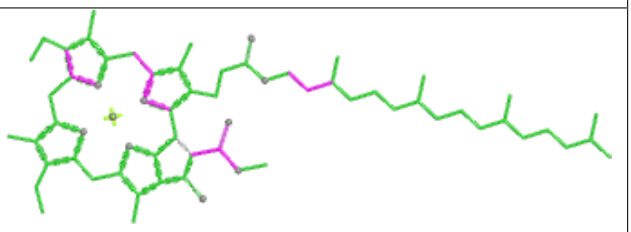

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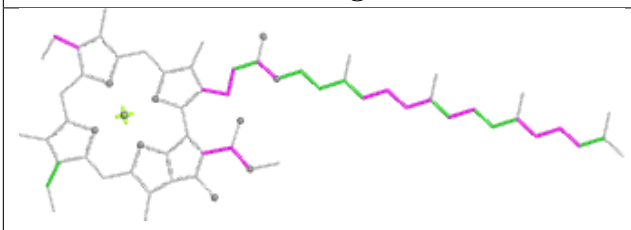

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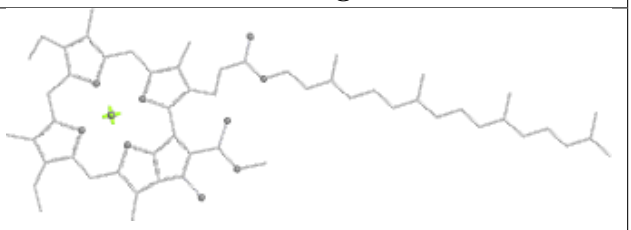
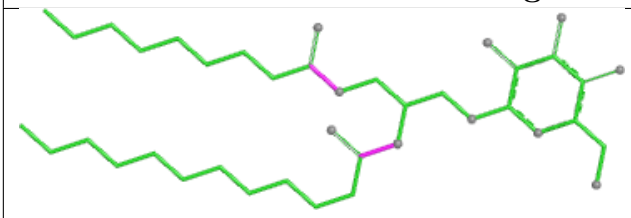


Rings

Ligand LMG 4 624



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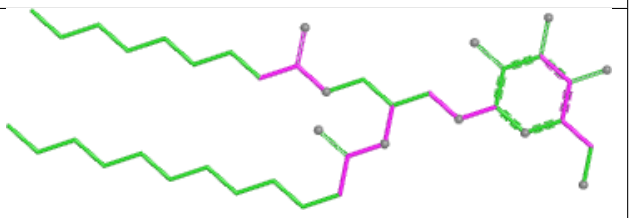

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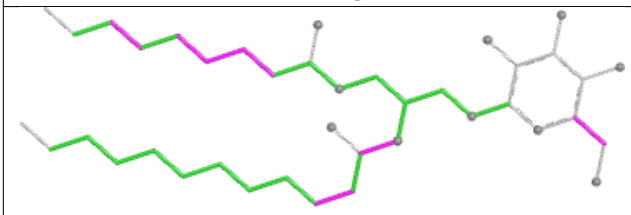

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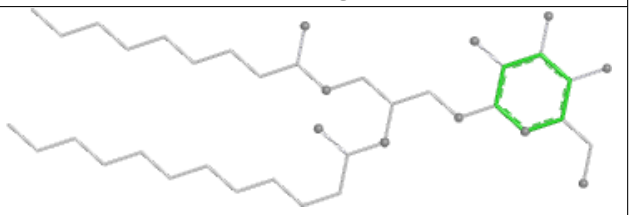
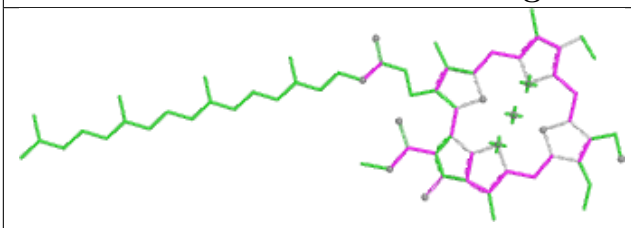


Rings

Ligand CHL X 607



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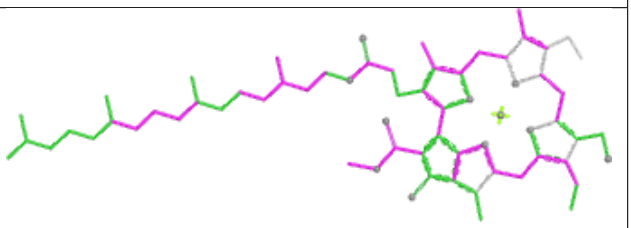
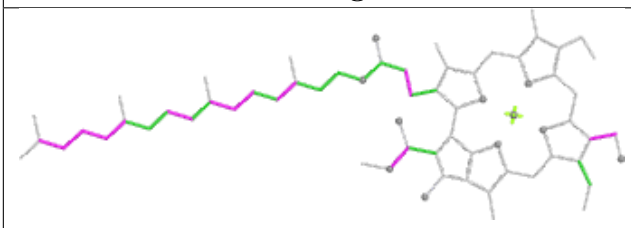


Bond angles



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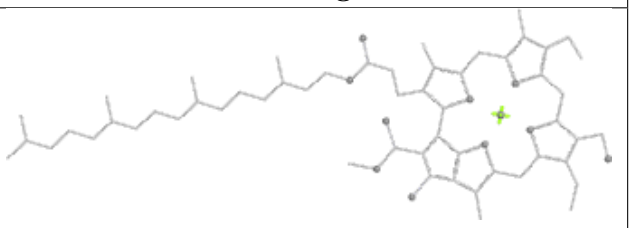
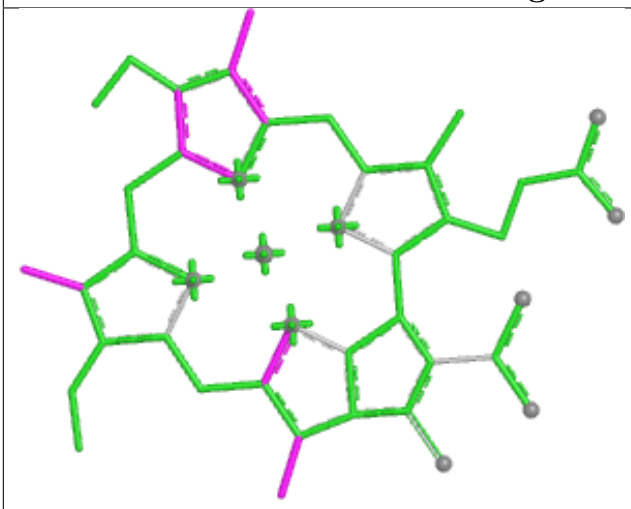


Rings

Ligand CLA 1 608



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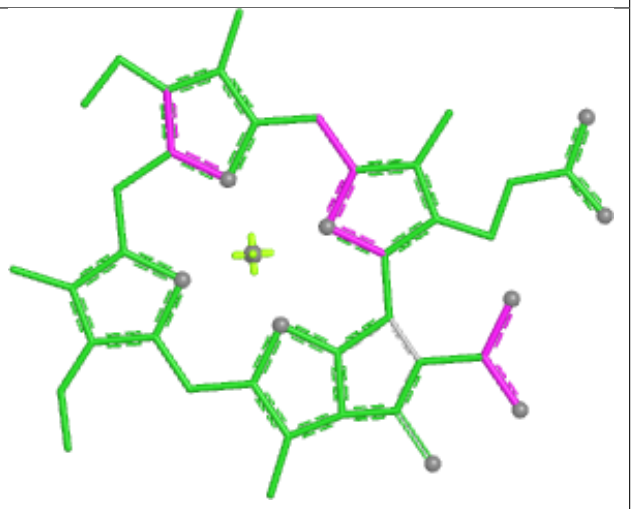
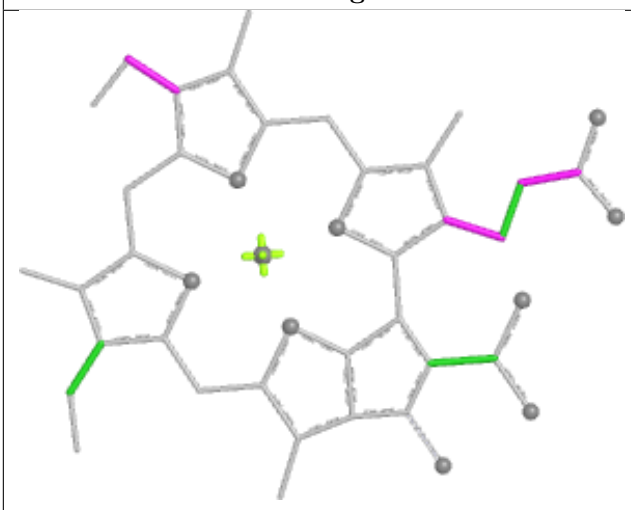
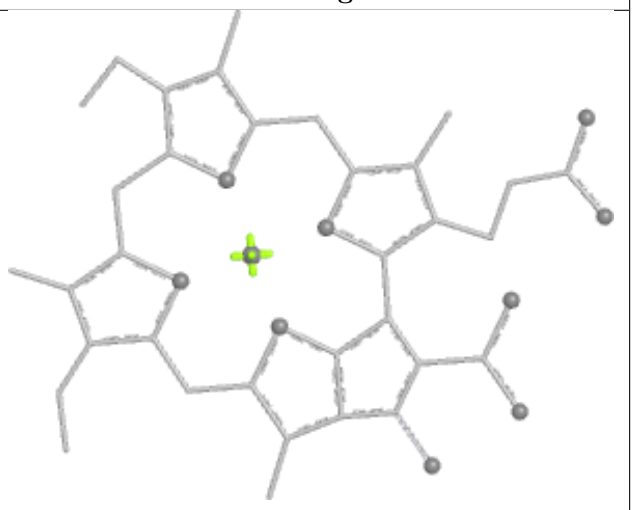


Bond angles

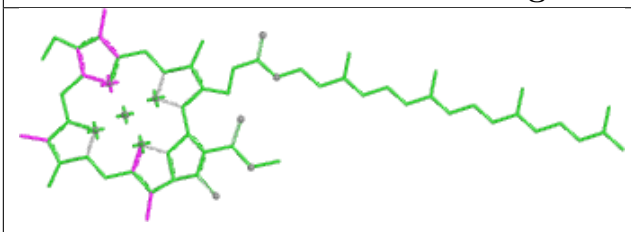


Torsions



Rings

Ligand CLA 8 606



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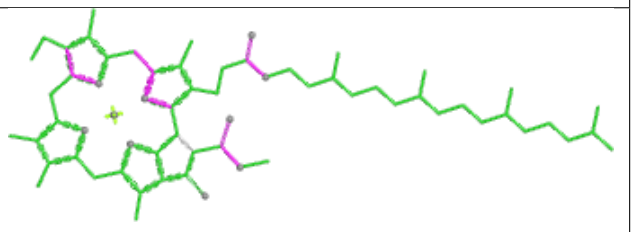
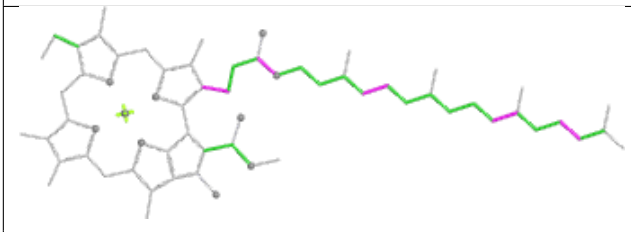


Bond angles



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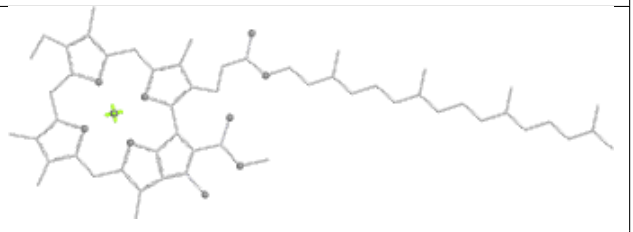
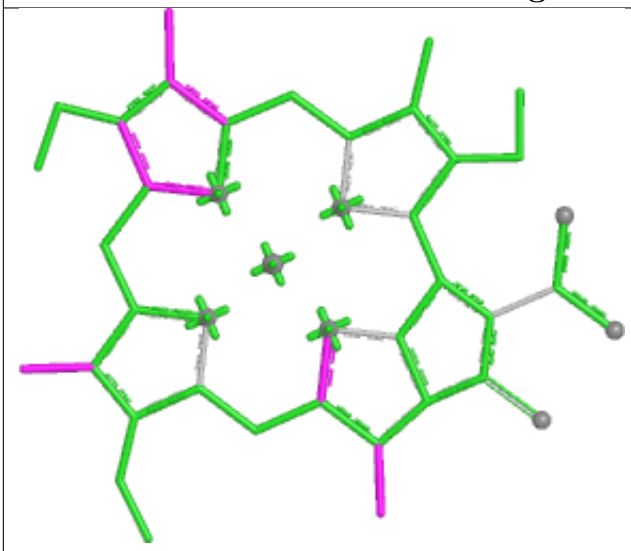


Rings

Ligand CLA 8 612



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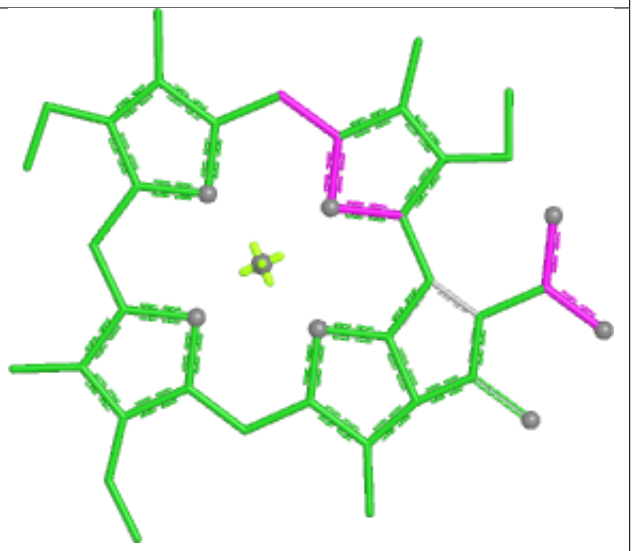
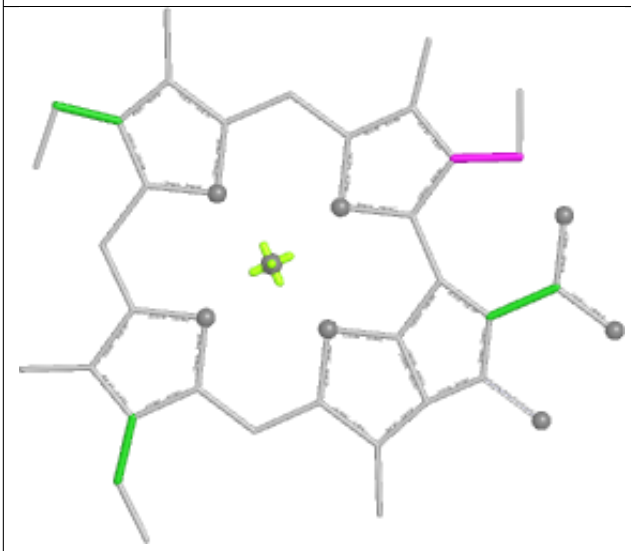


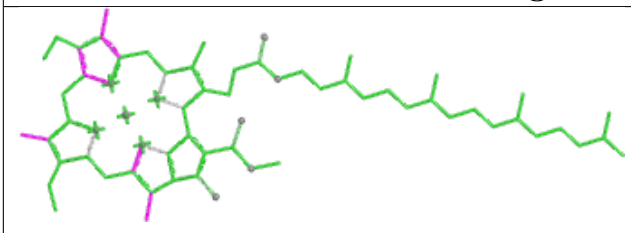
Bond angles



Torsions

Rings

Ligand CLA 8 601



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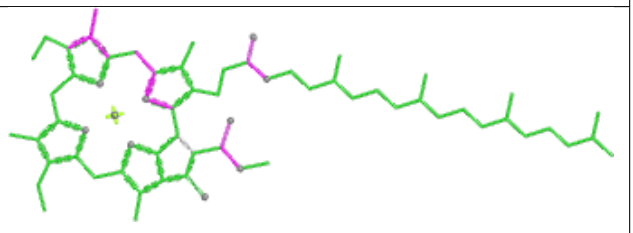
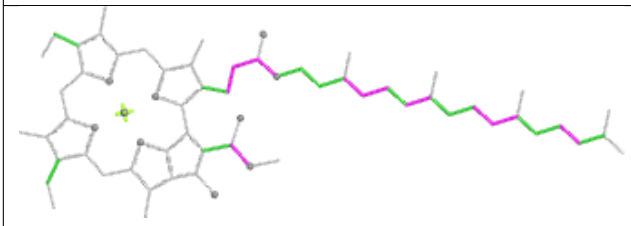
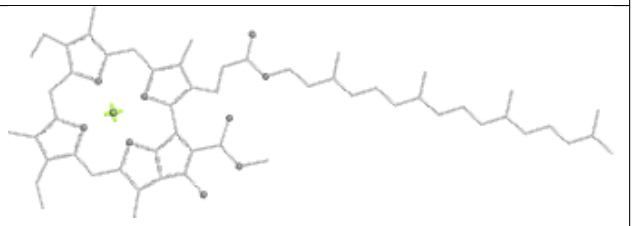


Bond angles

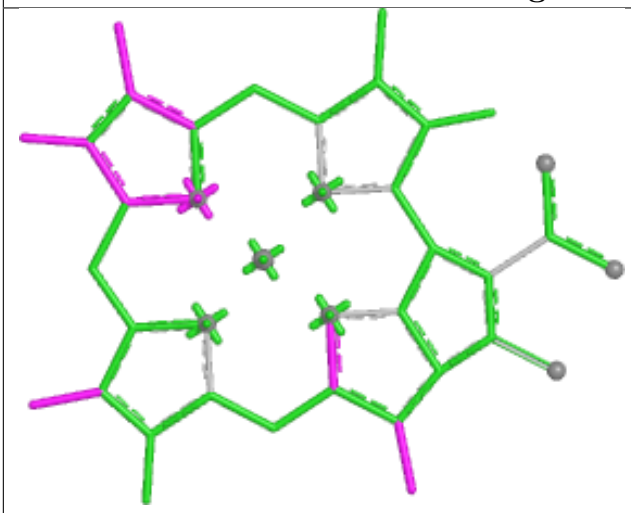


Torsions



Rings

Ligand CLA a 611



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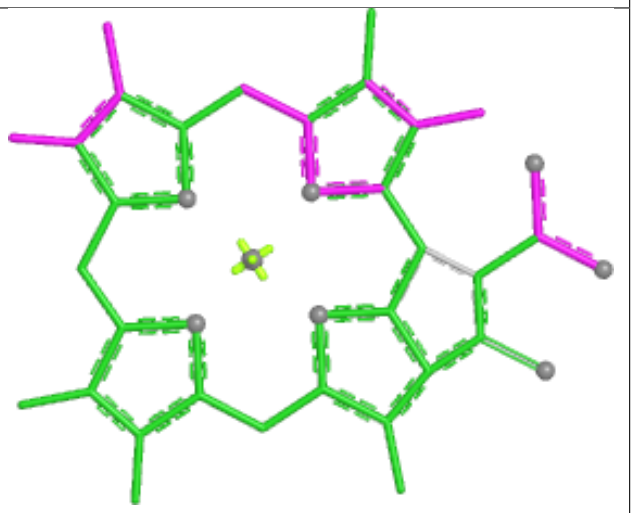
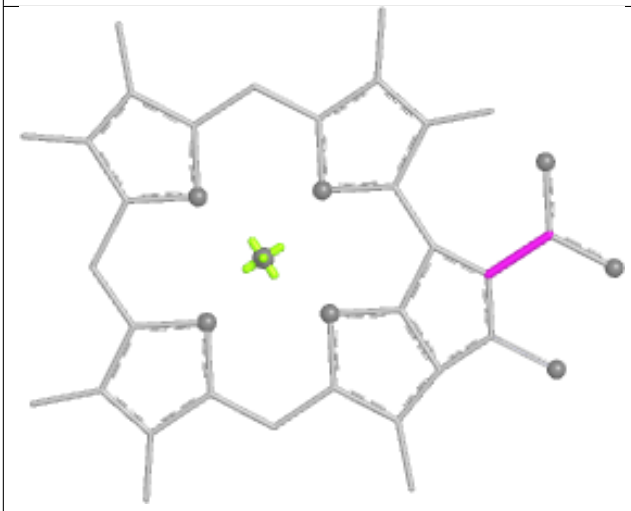
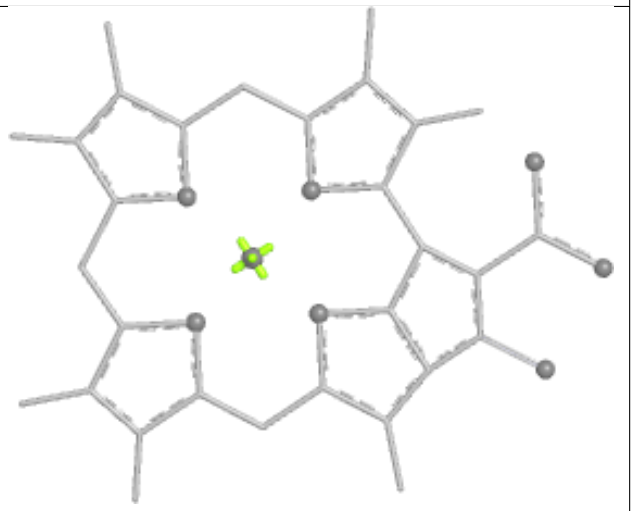


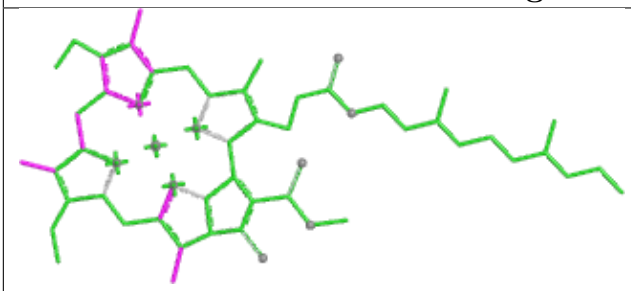
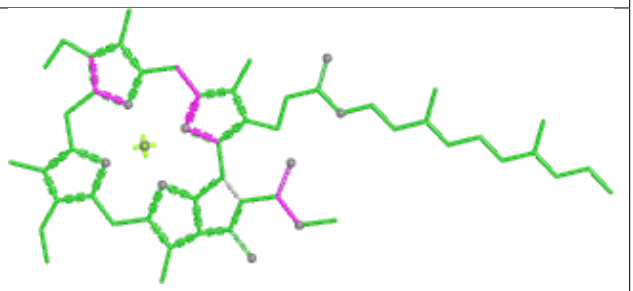
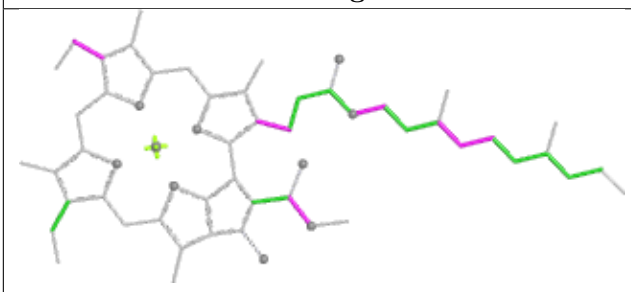
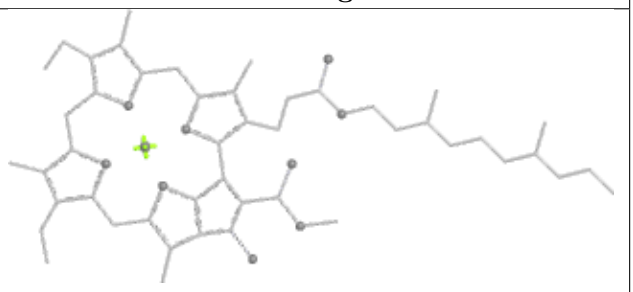
Bond angles



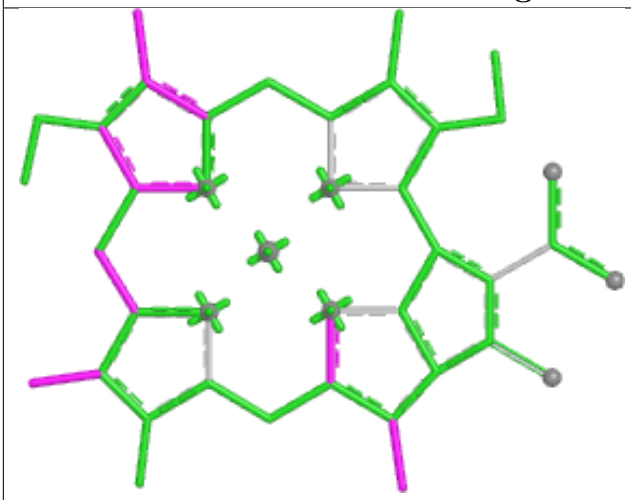
Torsions



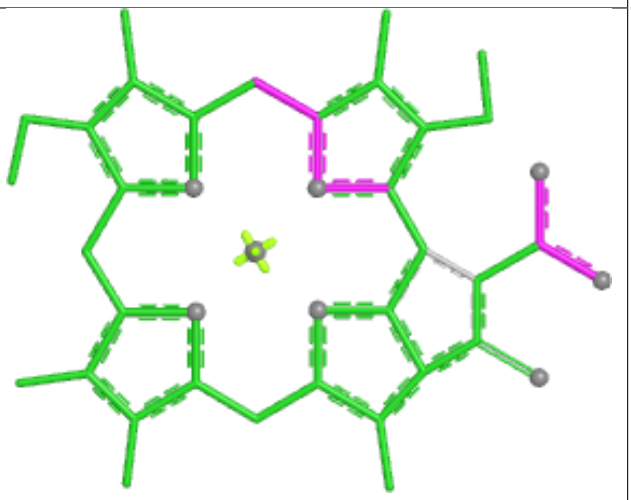
Rings

Ligand CLA F 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

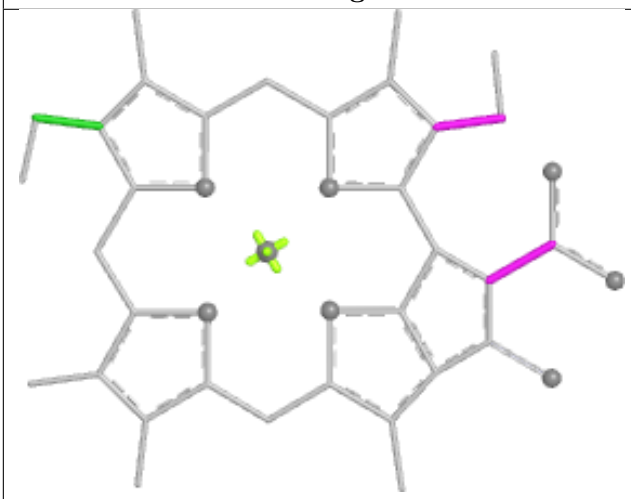
Ligand CLA O 2003



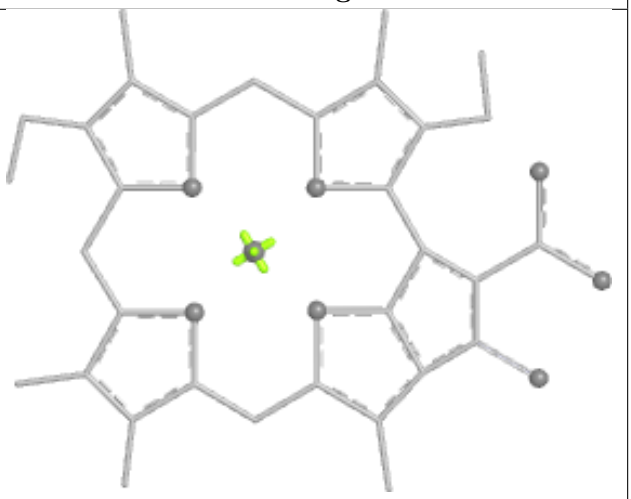
Bond lengths



Bond angles

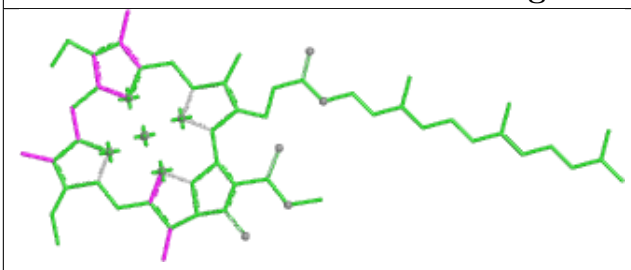


Torsions



Rings

Ligand CLA 8 610



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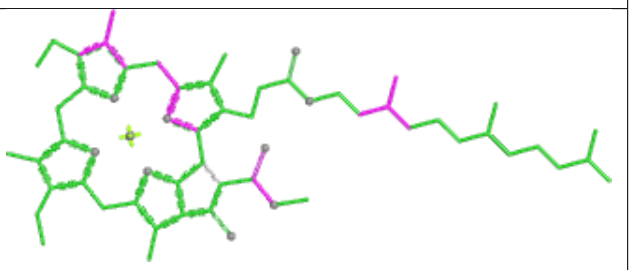
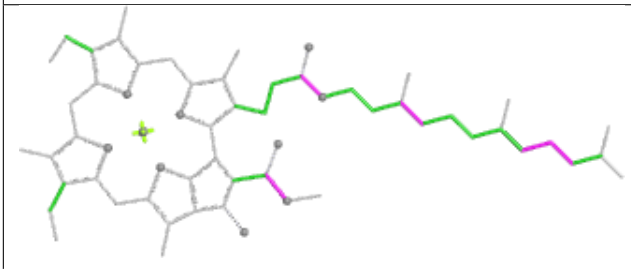


Bond angles



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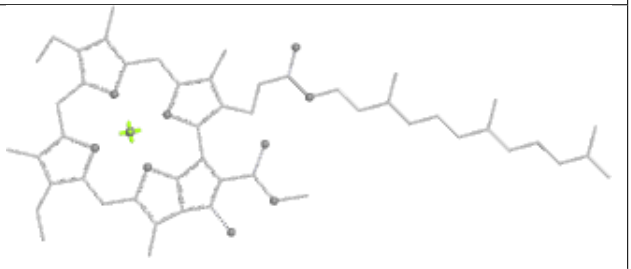
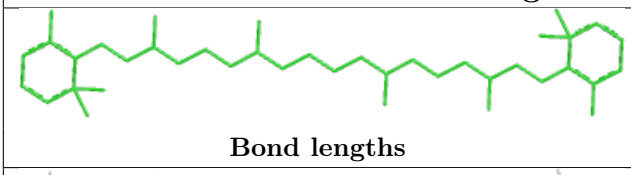


Rings

Ligand BCR B 843



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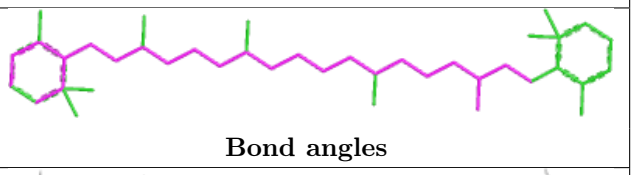
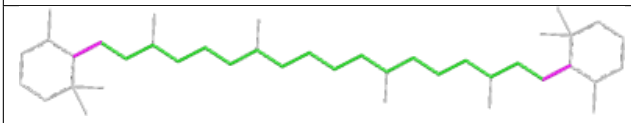


Bond angles



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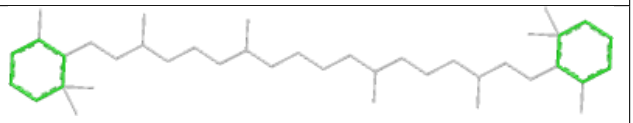
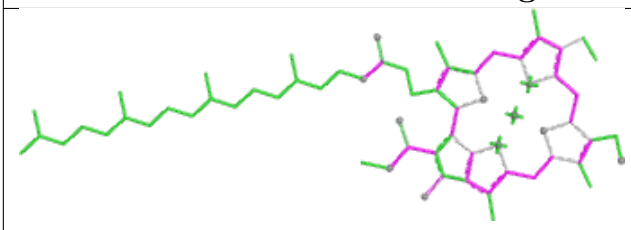


Rings

Ligand CHL W 607



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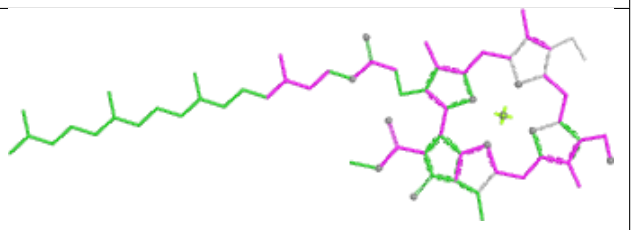
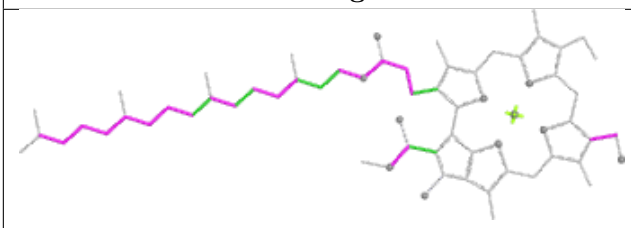


Bond angles



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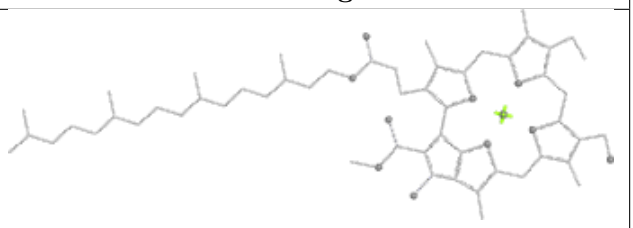
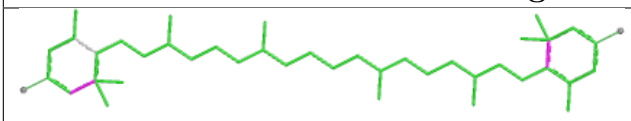


Rings

Ligand LUT 6 619



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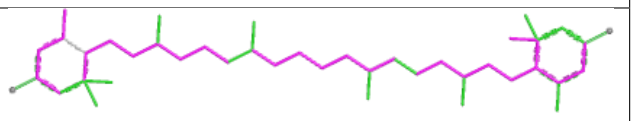
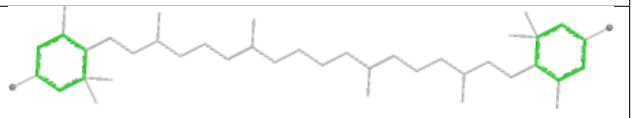


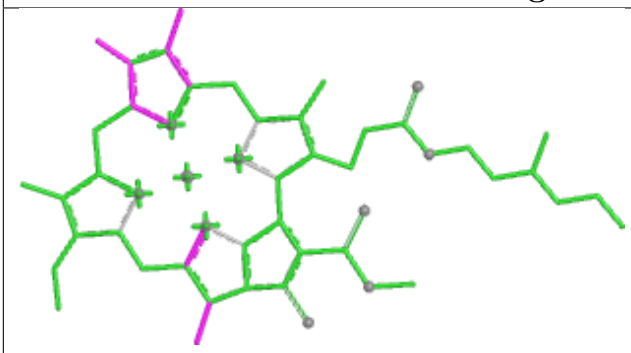
Bond angles

Torsions



Rings

Ligand CLA 6 603



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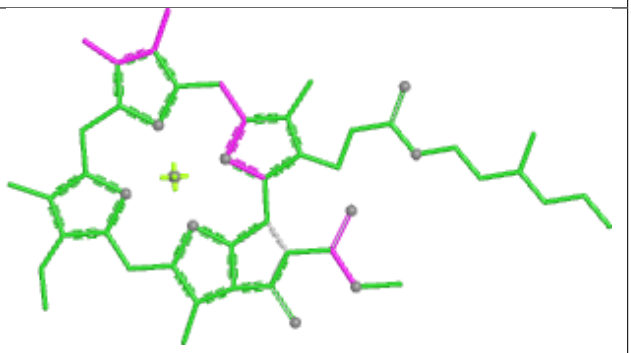
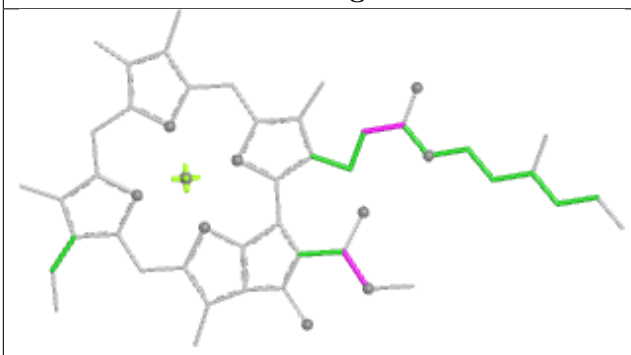
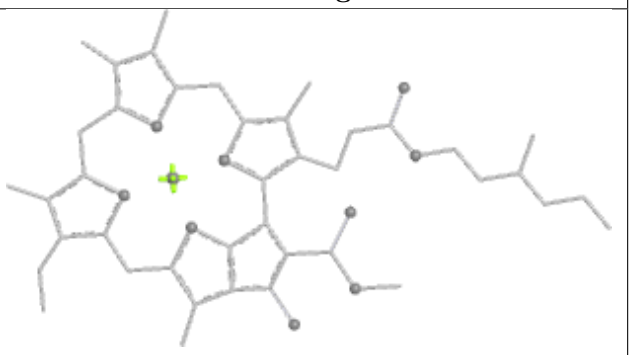


Bond angles

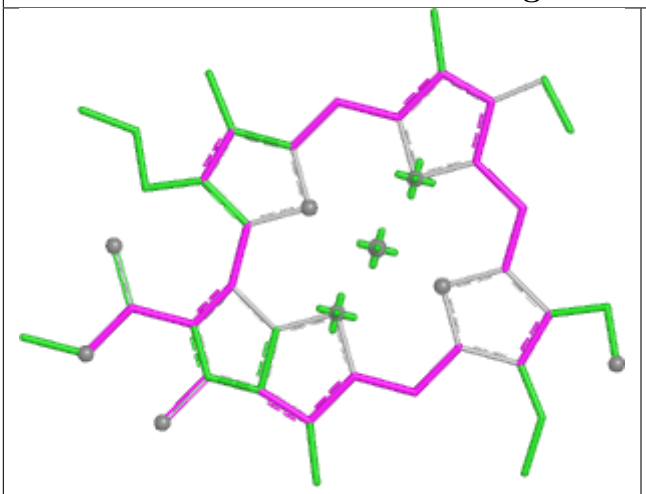


Torsions



Rings

Ligand CHL U 606



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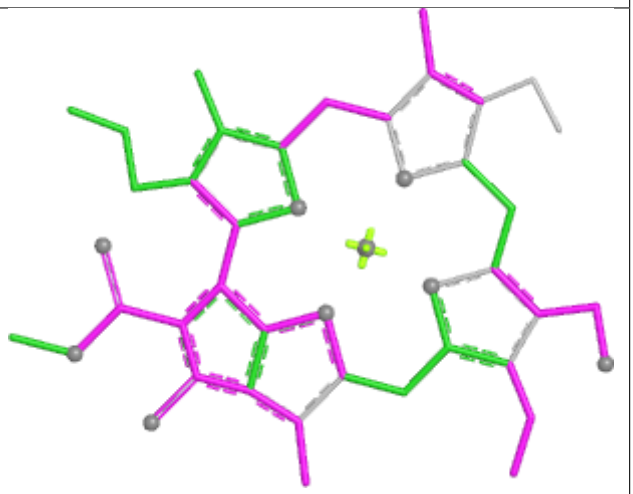
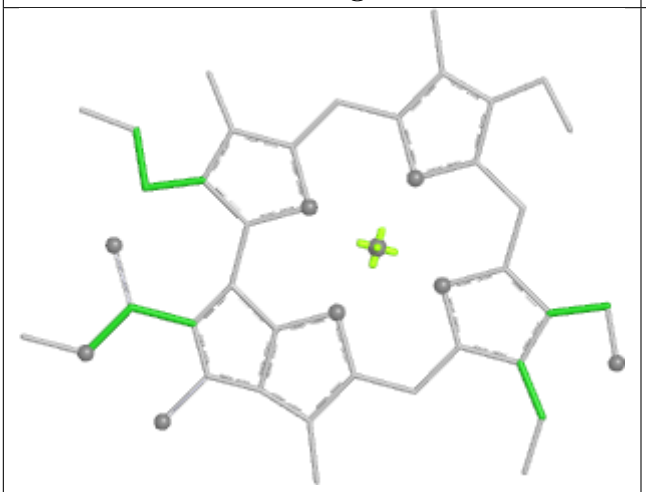
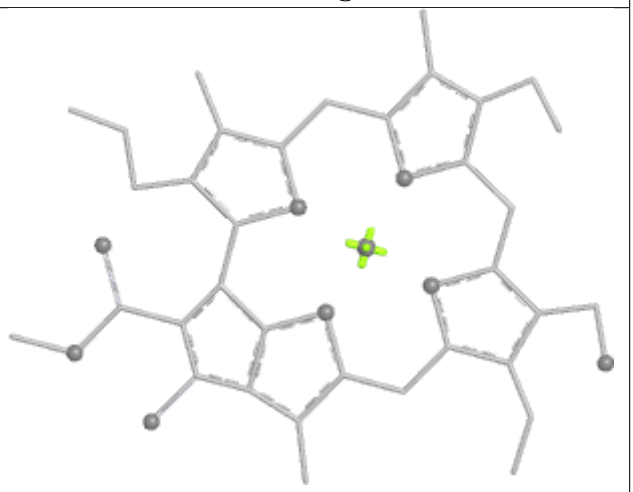


Bond angles

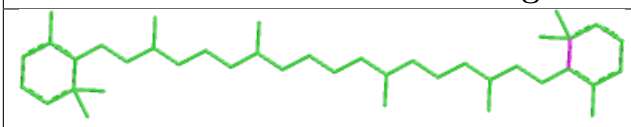


Torsions



Rings

Ligand BCR A 852



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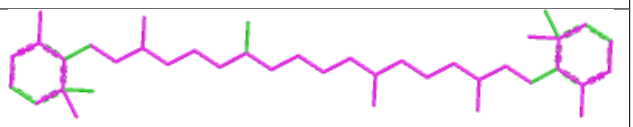
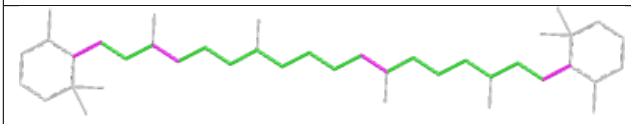


Bond angles



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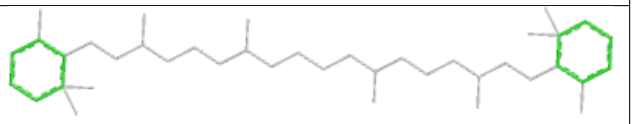
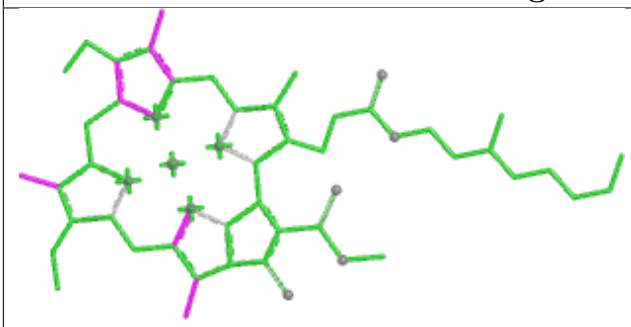


Rings

Ligand CLA a 613



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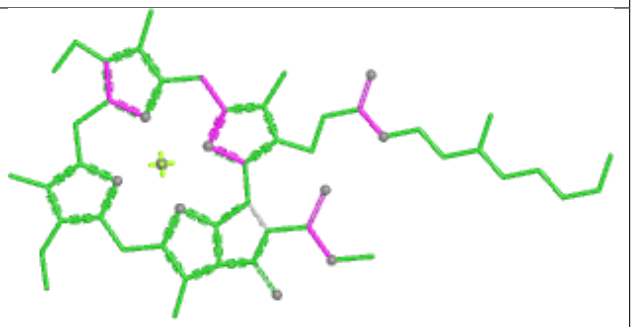
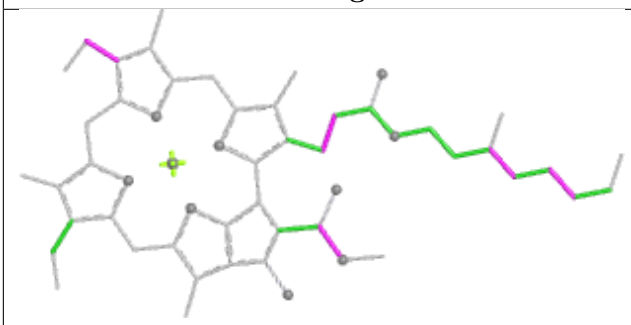
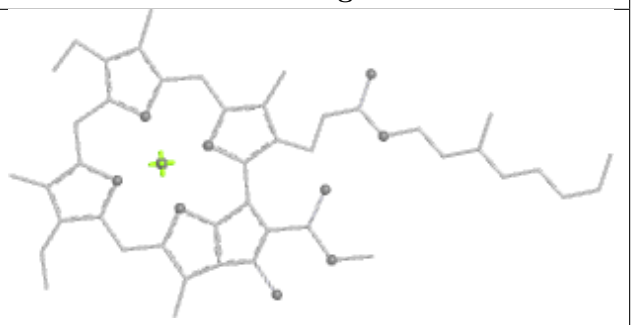


Bond angles

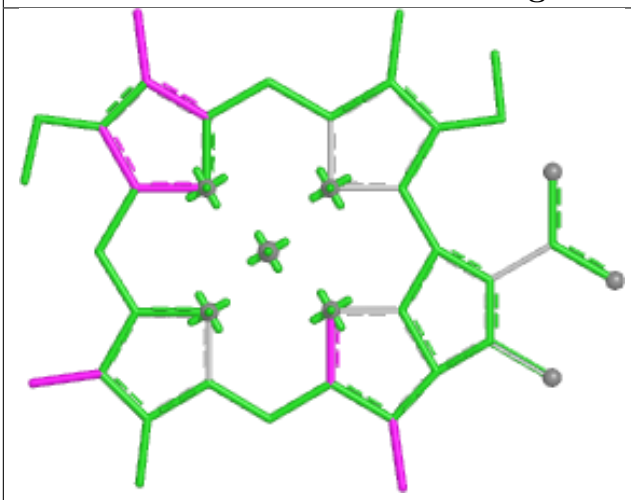


Torsions



Rings

Ligand CLA 3 615



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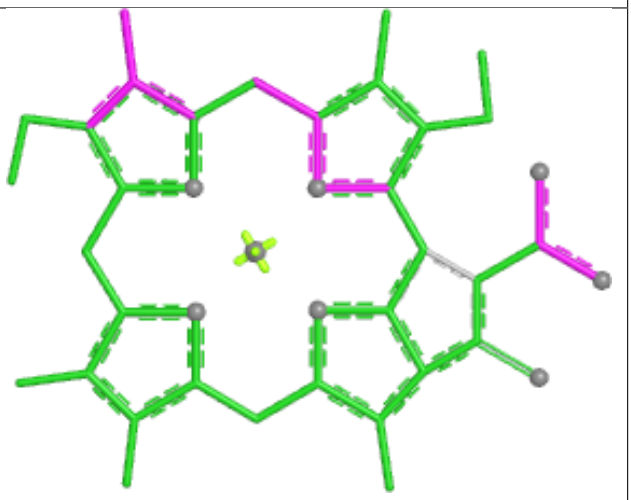
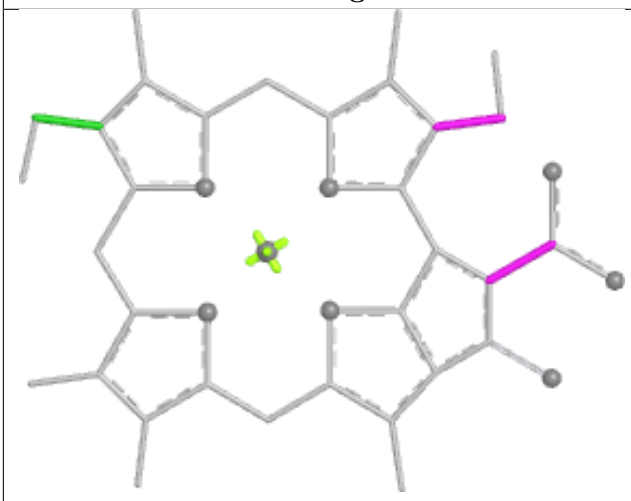
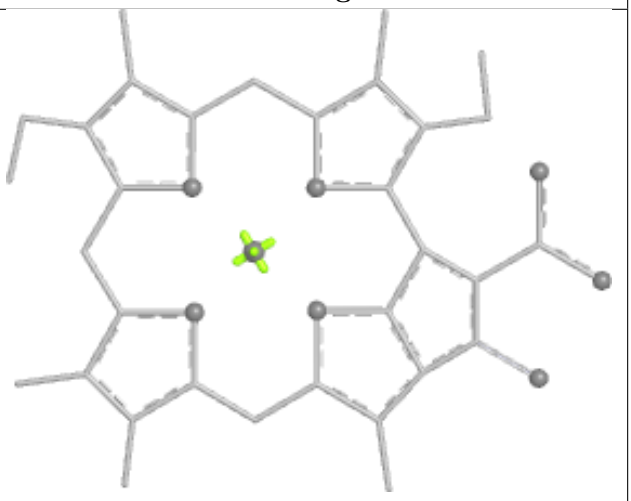


Bond angles

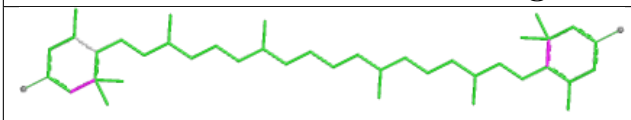


Torsions

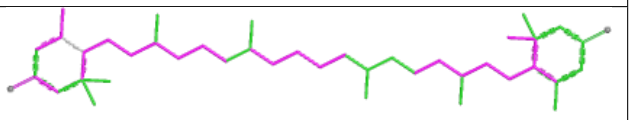


Rings

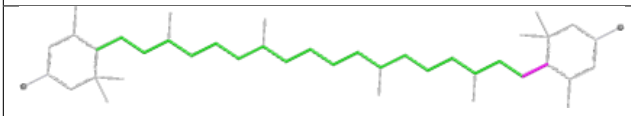
Ligand LUT 7 619



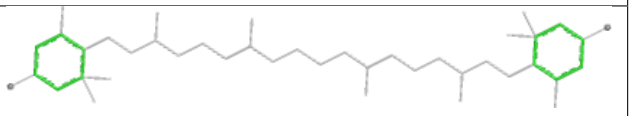
Bond lengths



Bond angles

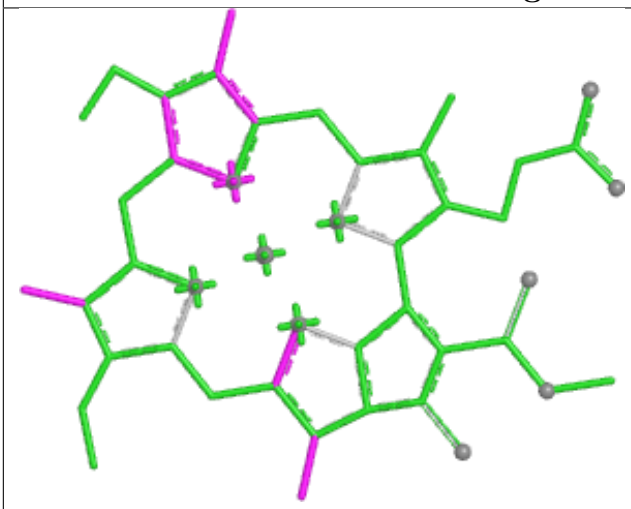


Torsions

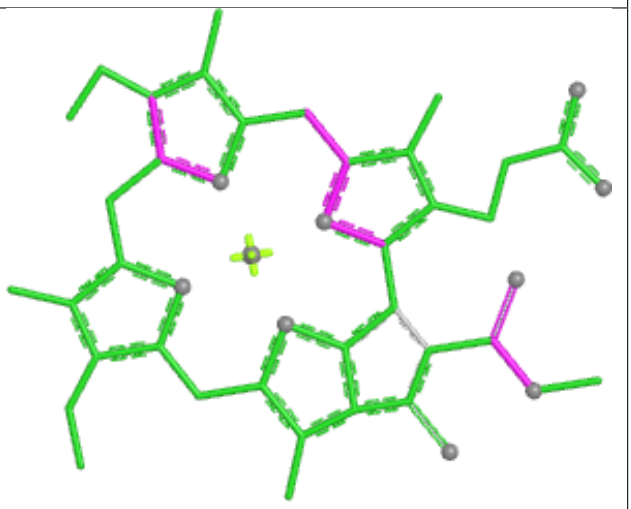


Rings

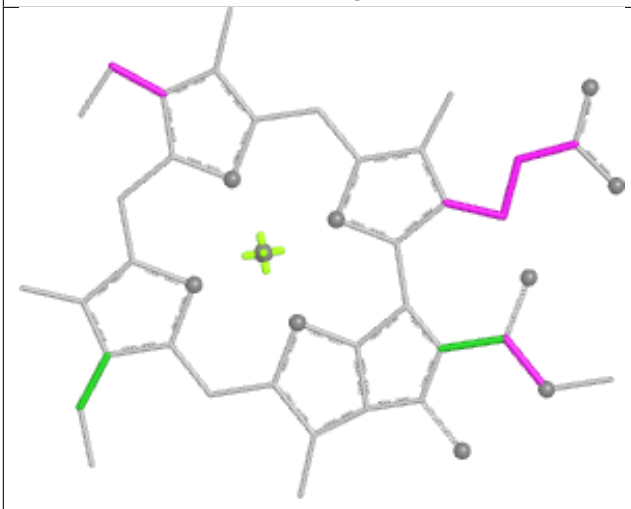
Ligand CLA A 837



Bond lengths



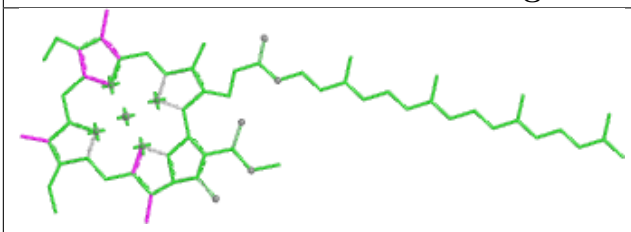
Bond angles



Torsions

Rings

Ligand CLA A 824



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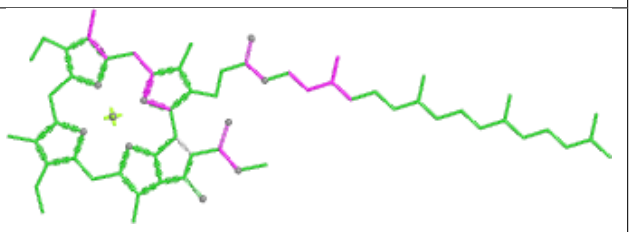
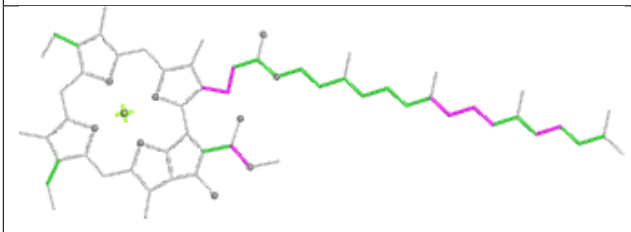
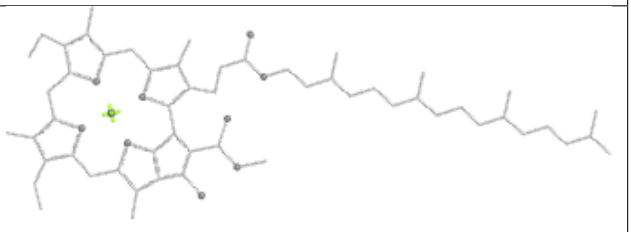


Bond angles

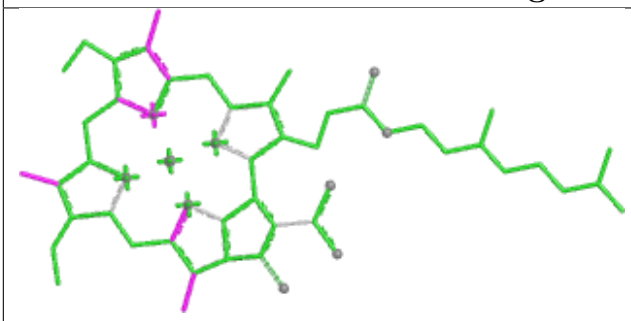


Torsions



Rings

Ligand CLA 3 606



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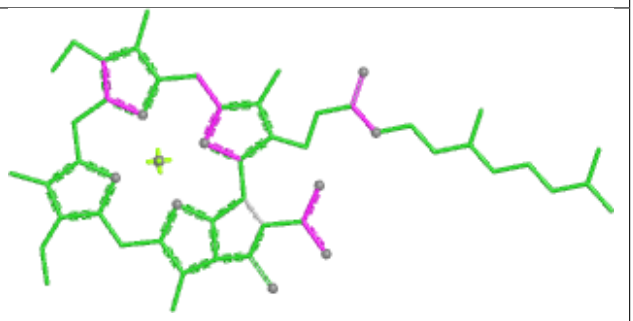
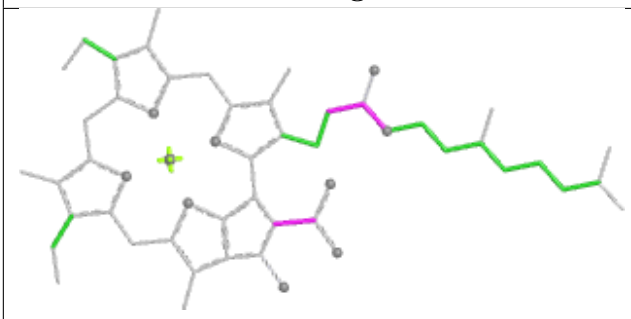
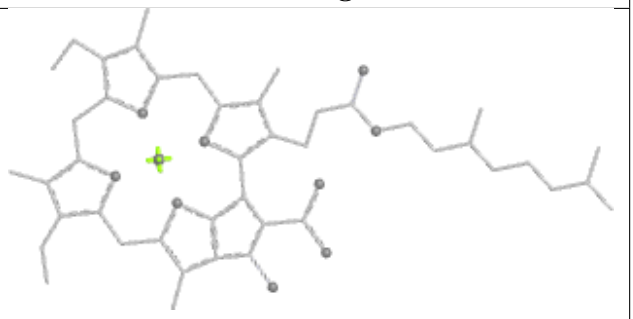


Bond angles

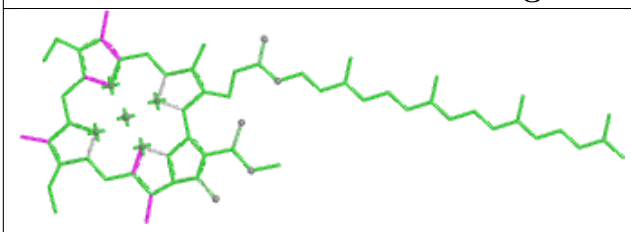


Torsions



Rings

Ligand CLA A 809



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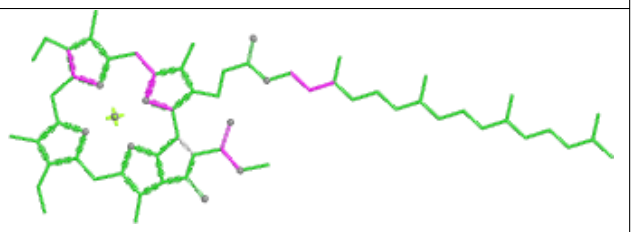
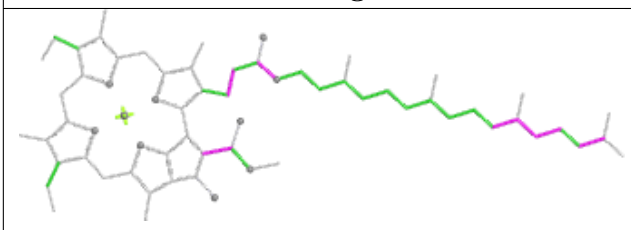


Bond angles



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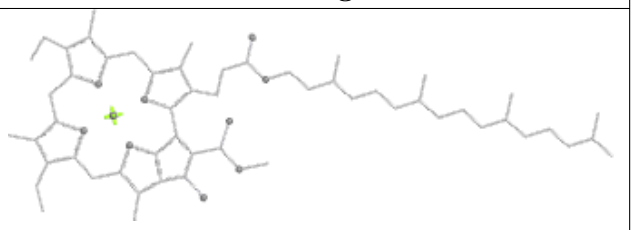
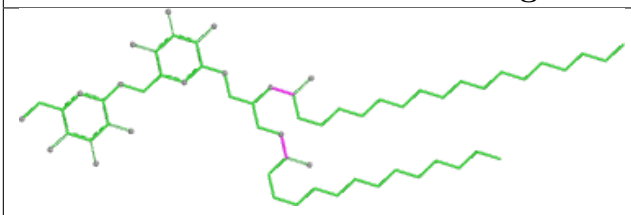


Rings

Ligand DGD B 850



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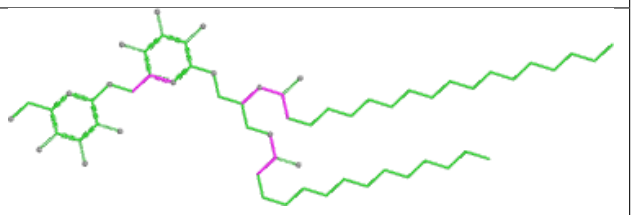
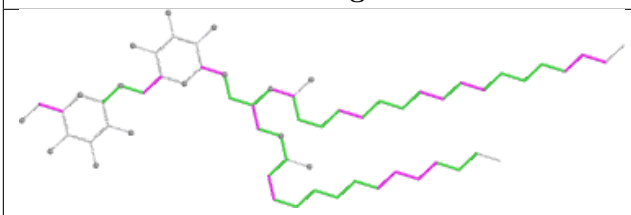


Bond angles



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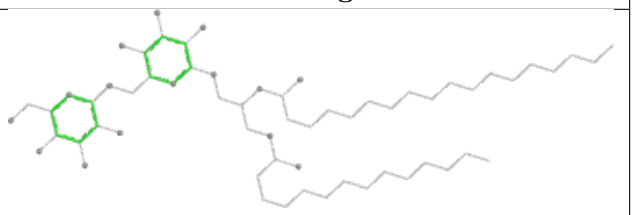
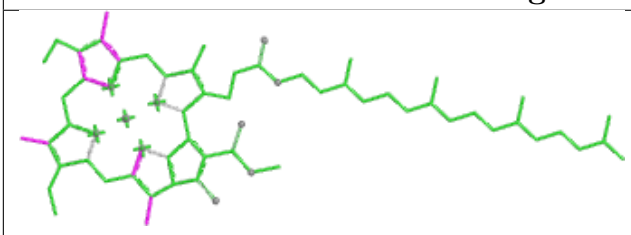


Rings

Ligand CLA 7 610



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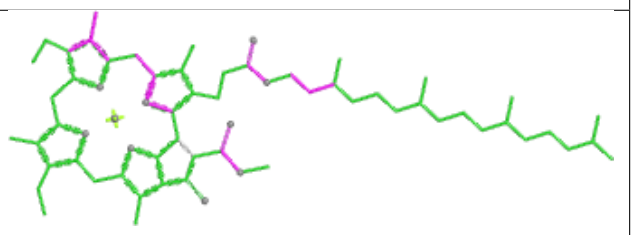
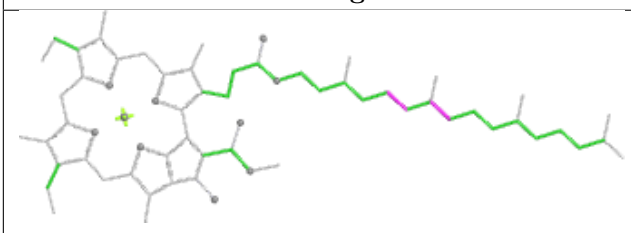


Bond angles



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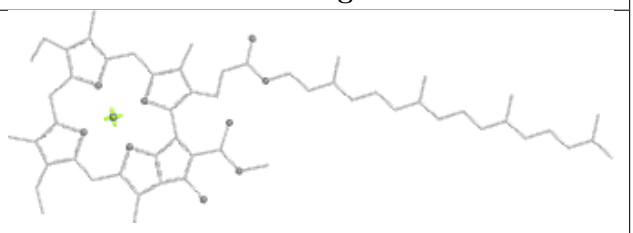
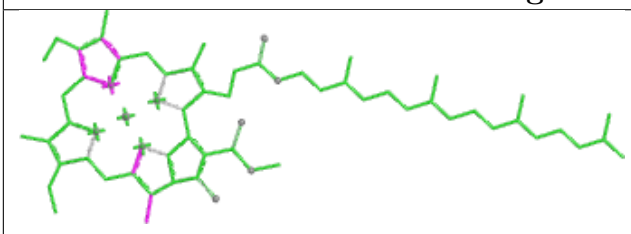


Rings

Ligand CLA Z 603



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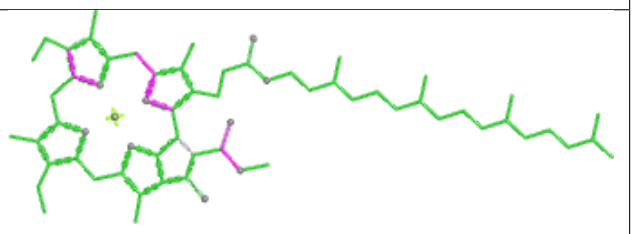
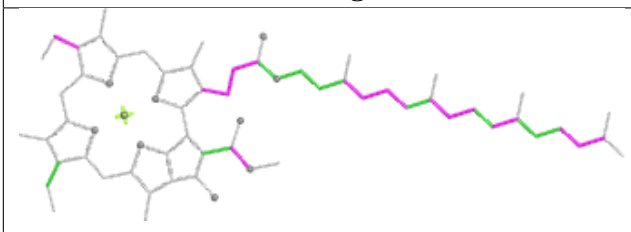


Bond angles



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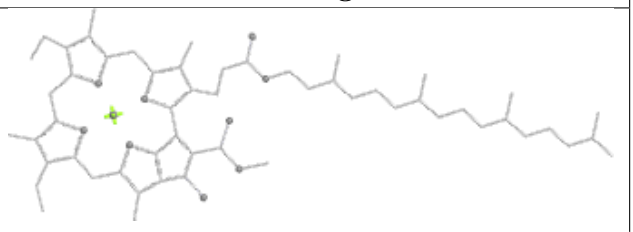
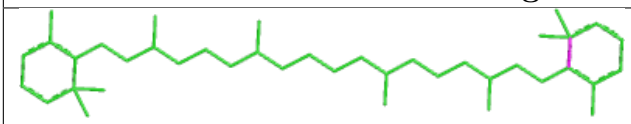


Rings

Ligand BCR A 850



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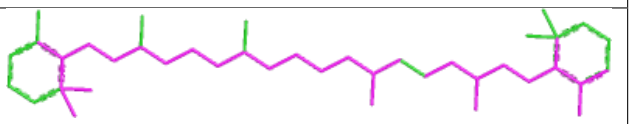
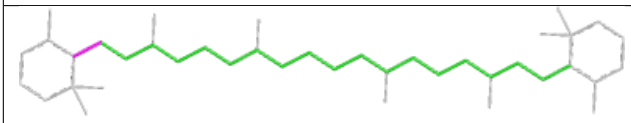
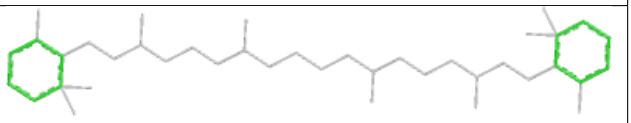


Bond angles

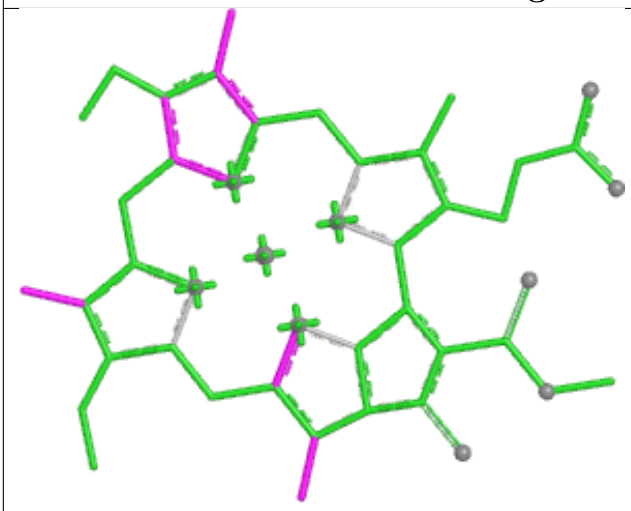


Torsions



Rings

Ligand CLA 6 617



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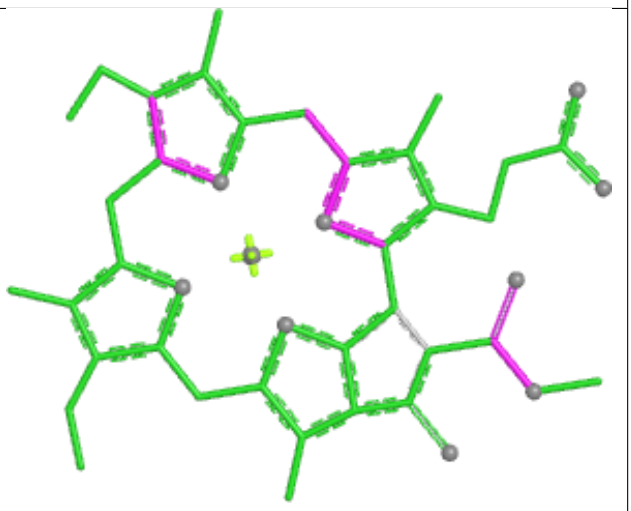
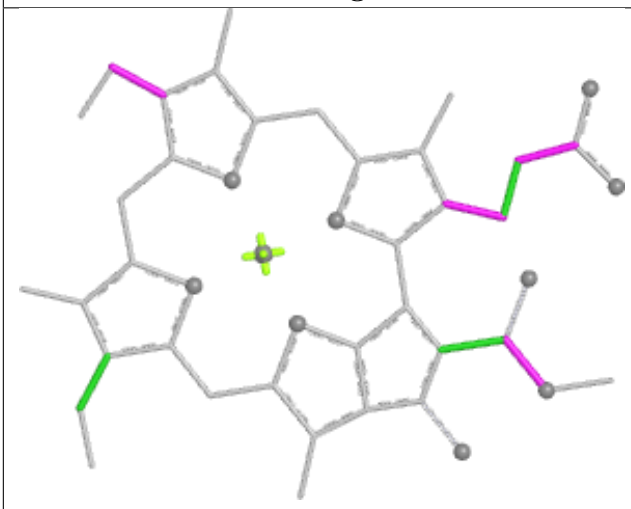


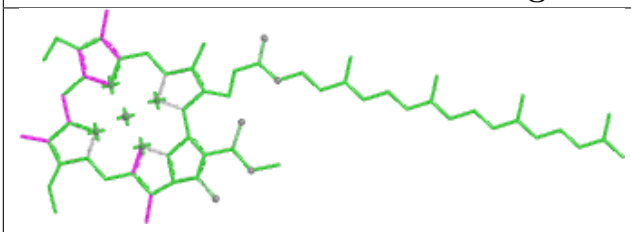
Bond angles



Torsions

Rings

Ligand CLA 6 616



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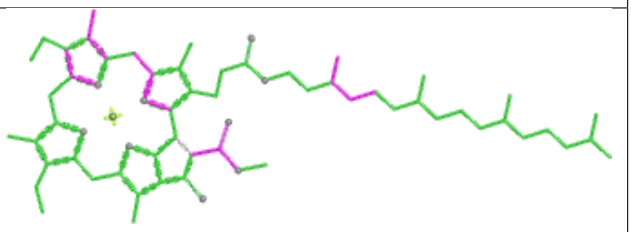

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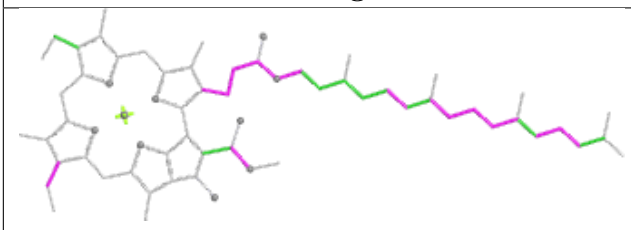

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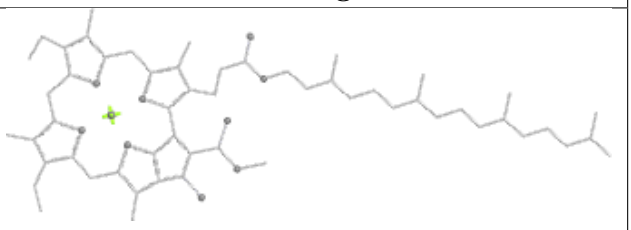
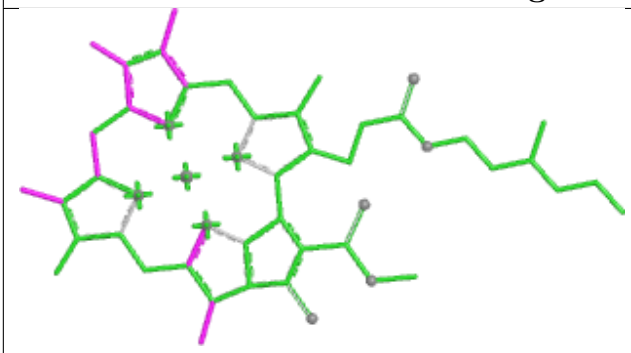


Rings

Ligand CLA 9 604



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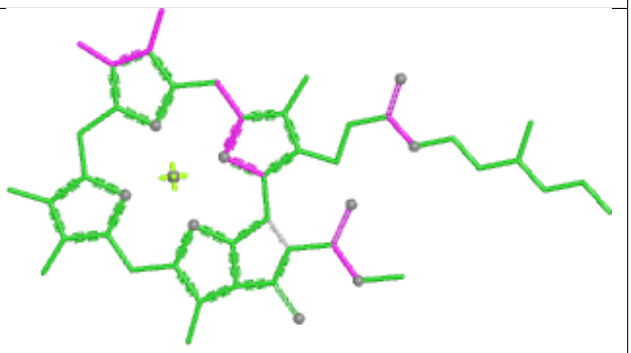
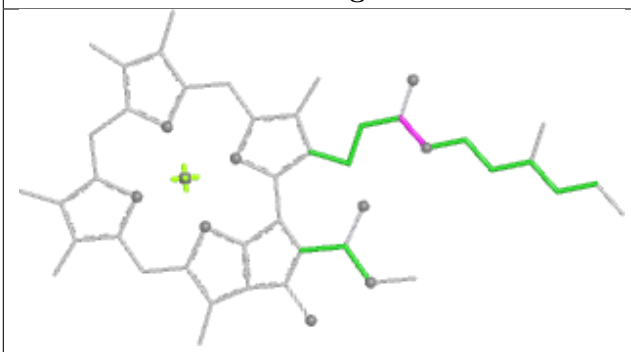
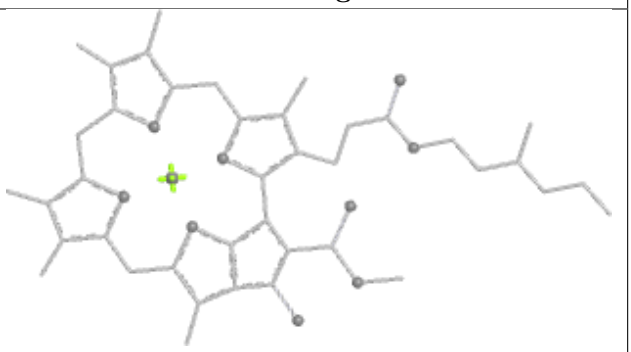


Bond angles

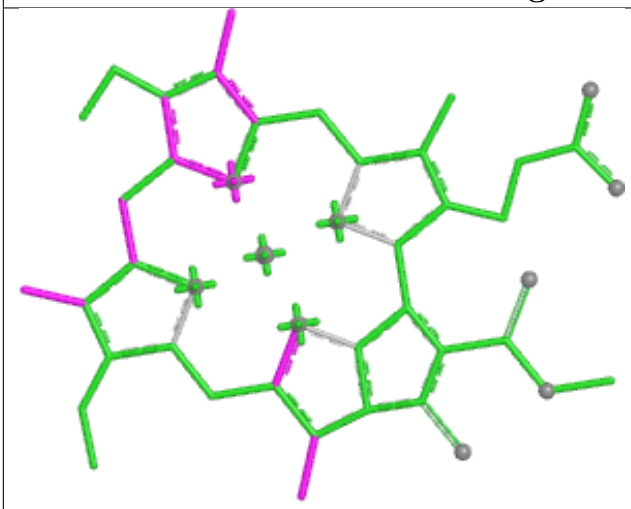


Torsions



Rings

Ligand CLA 2 607



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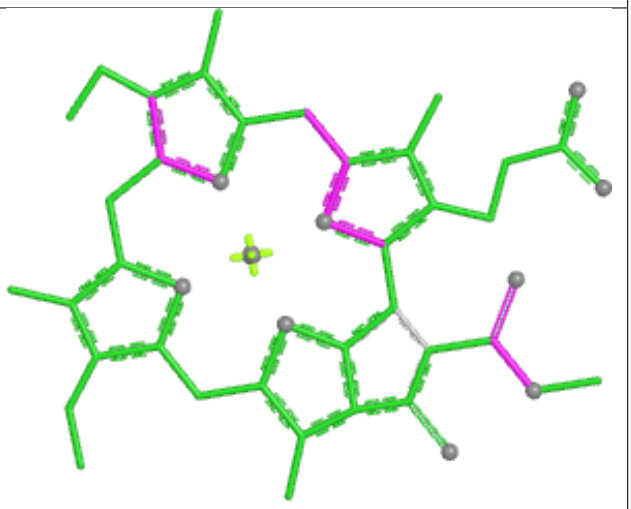
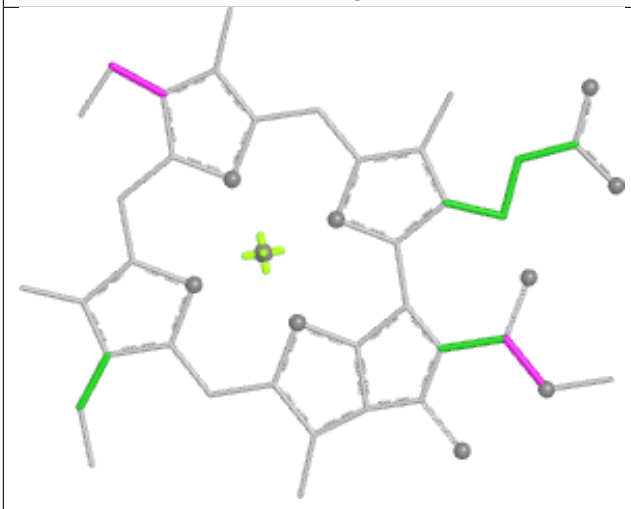


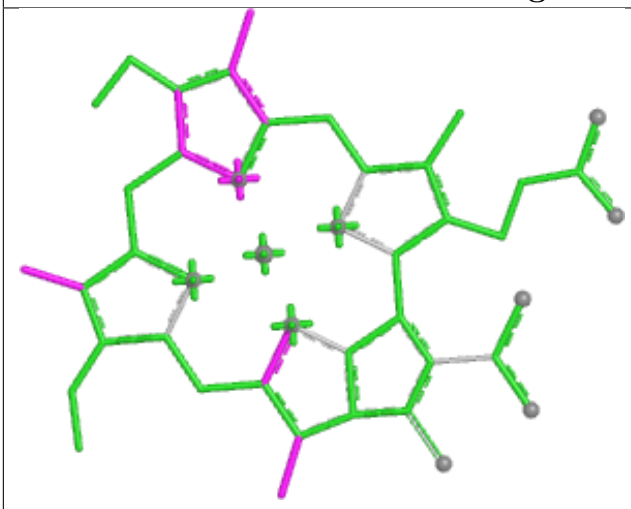
Bond angles



Torsions

Rings

Ligand CLA 7 603



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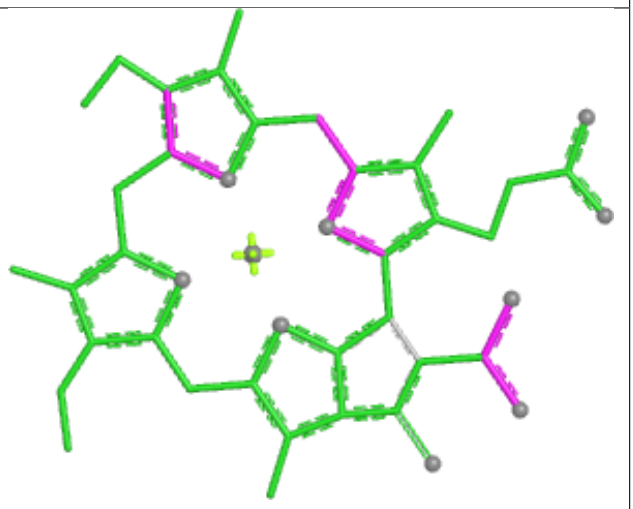
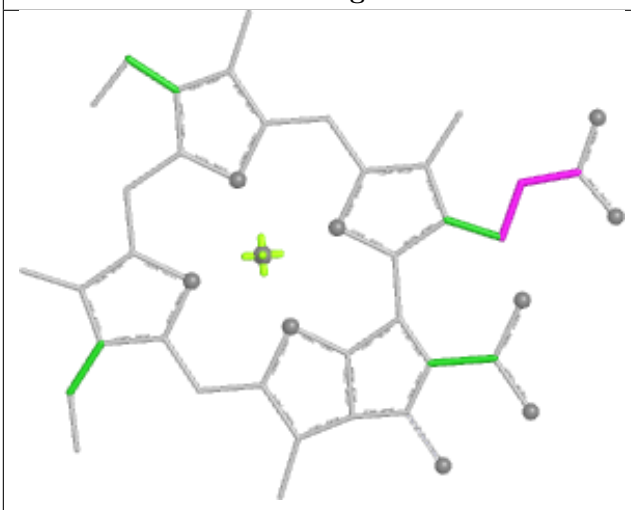
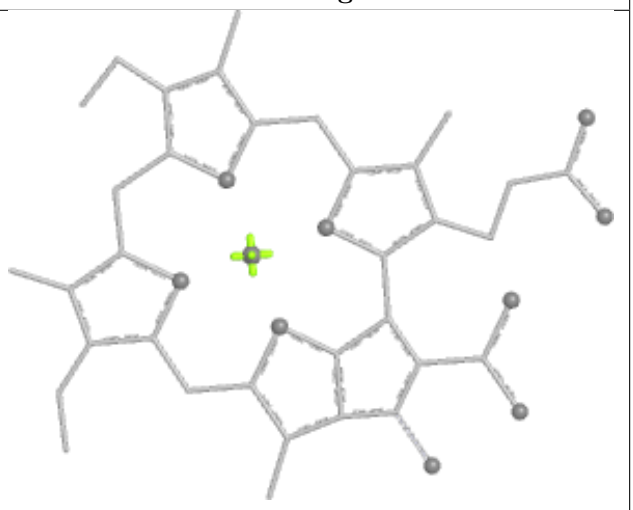


Bond angles

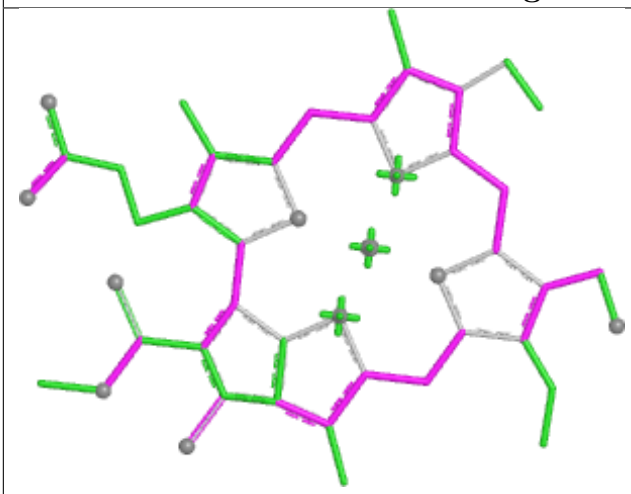


Torsions



Rings

Ligand CHL X 605



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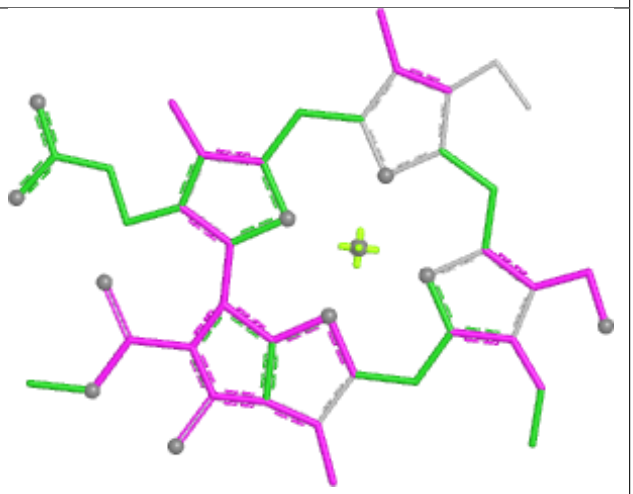
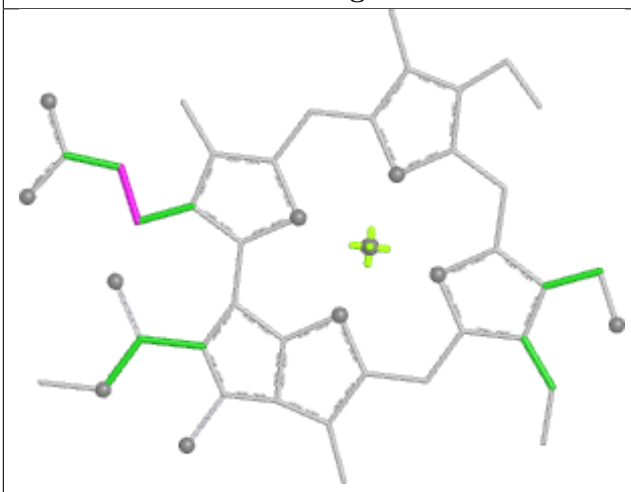
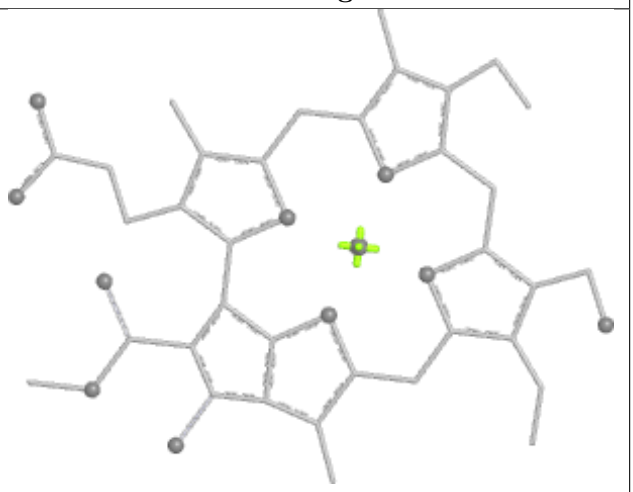


Bond angles

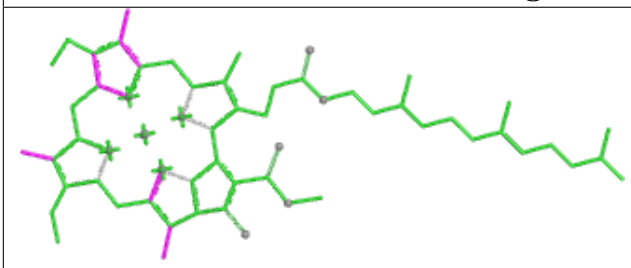


Torsions

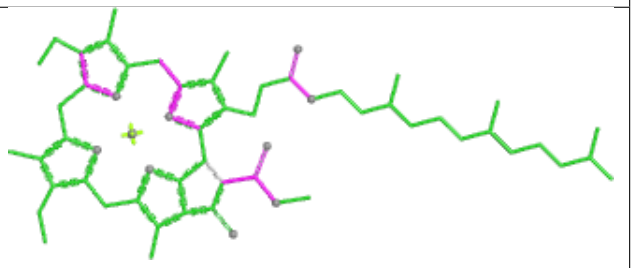


Rings

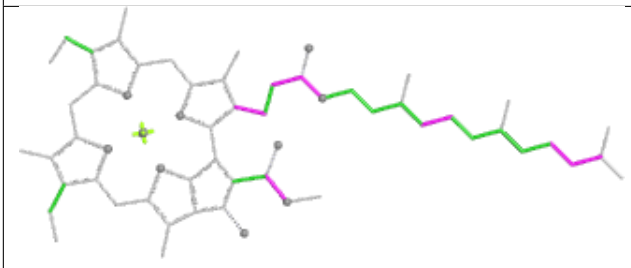
Ligand CLA B 832



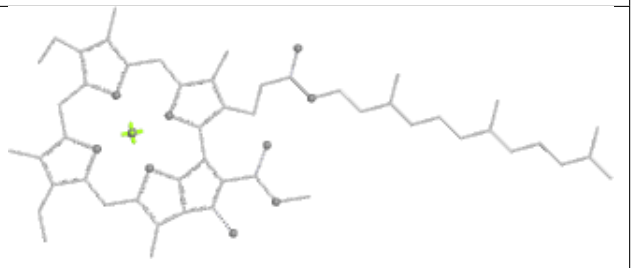
Bond lengths



Bond angles

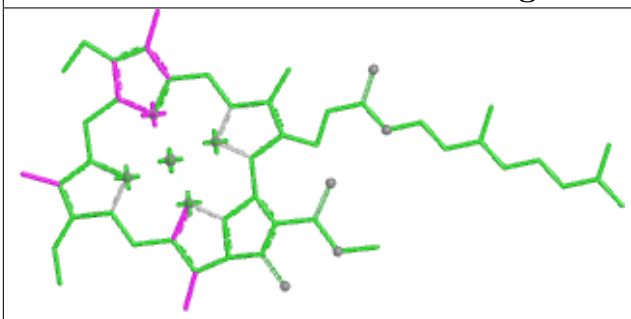


Torsions



Rings

Ligand CLA W 610



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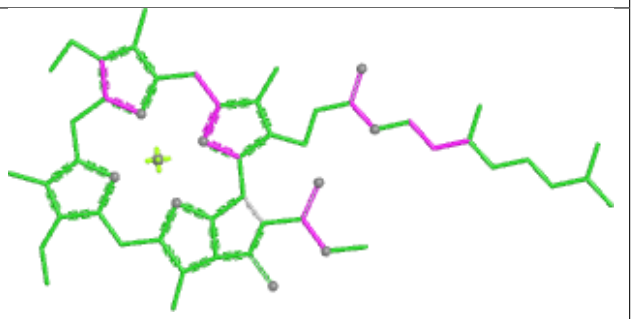
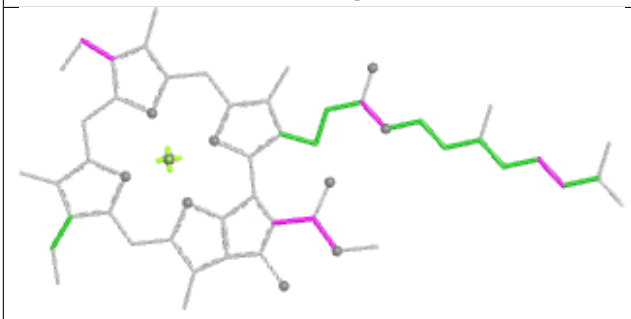
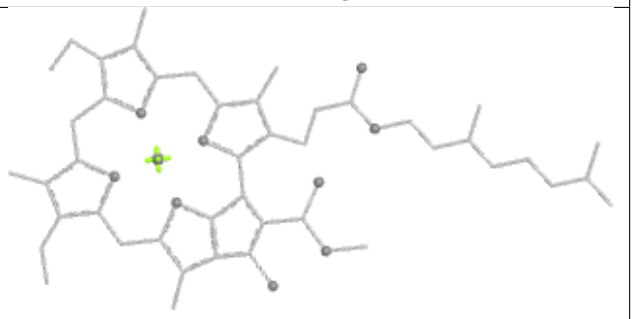


Bond angles

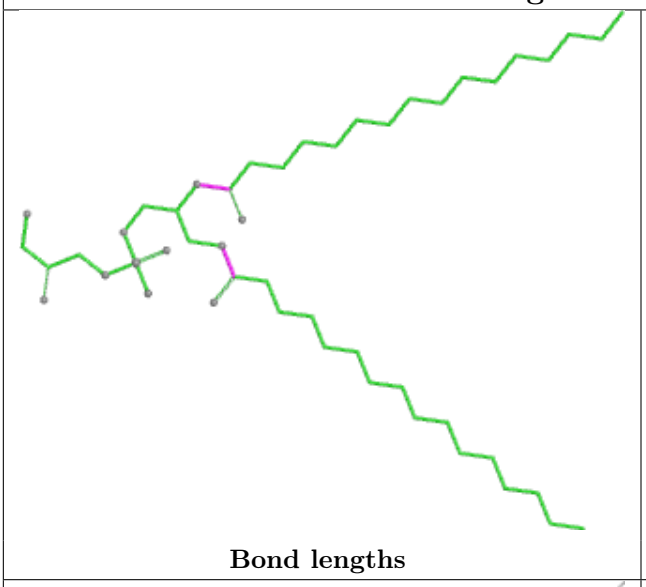


Torsions



Rings

Ligand LHG 5 625



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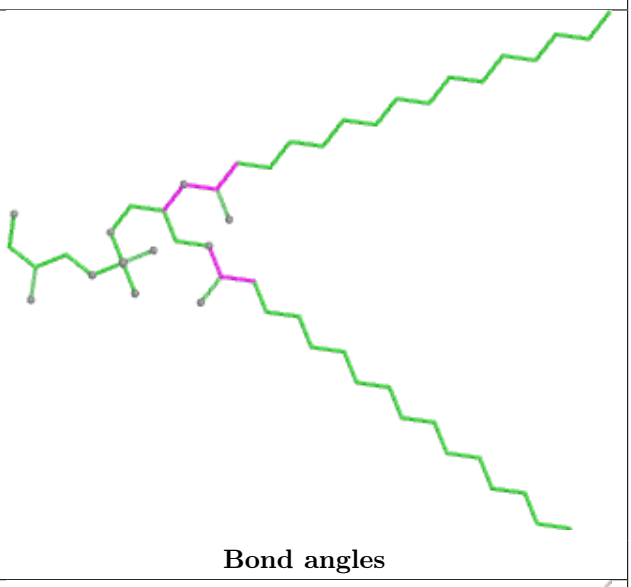
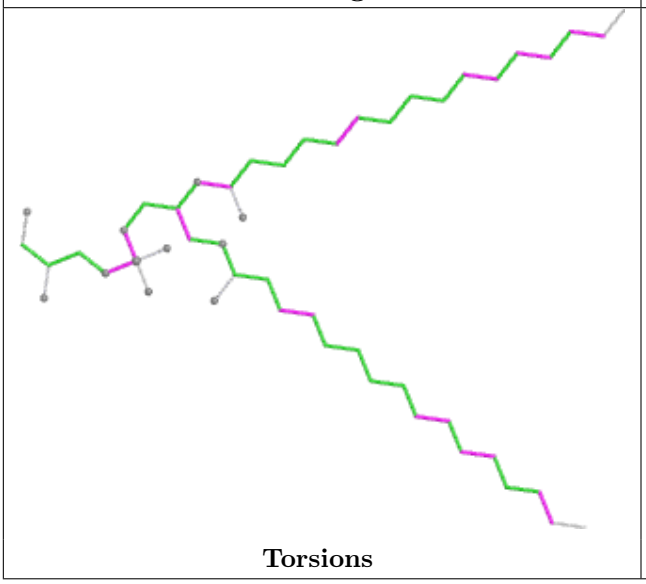


Bond angles



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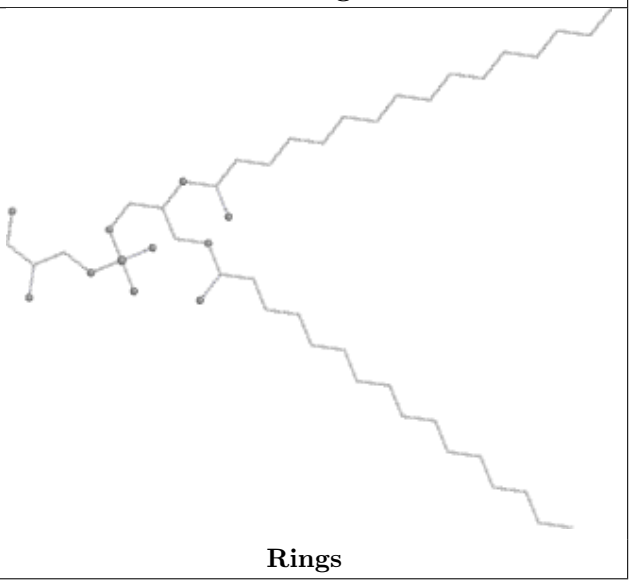
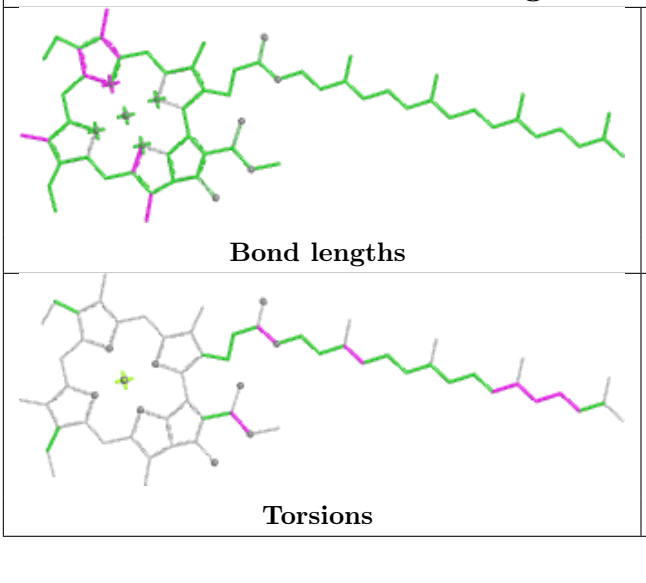


Rings

Ligand CLA B 837



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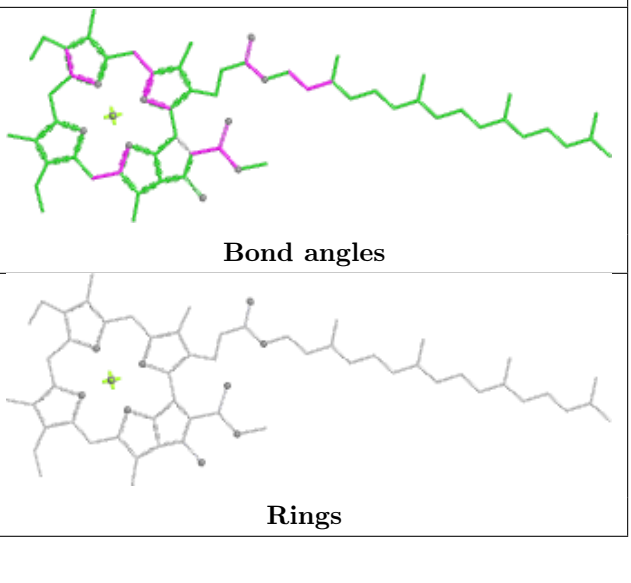
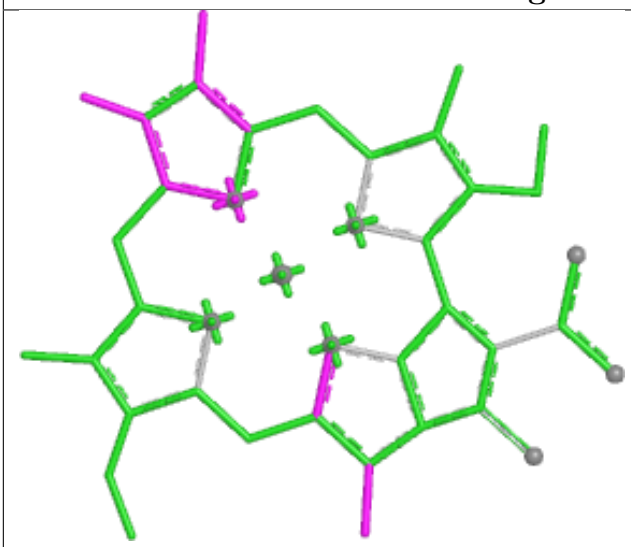


Bond angles

Torsions

Rings

Ligand CLA 5 618



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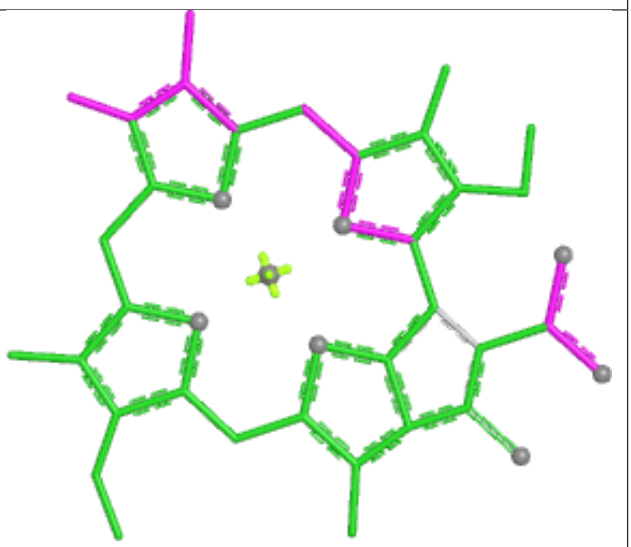
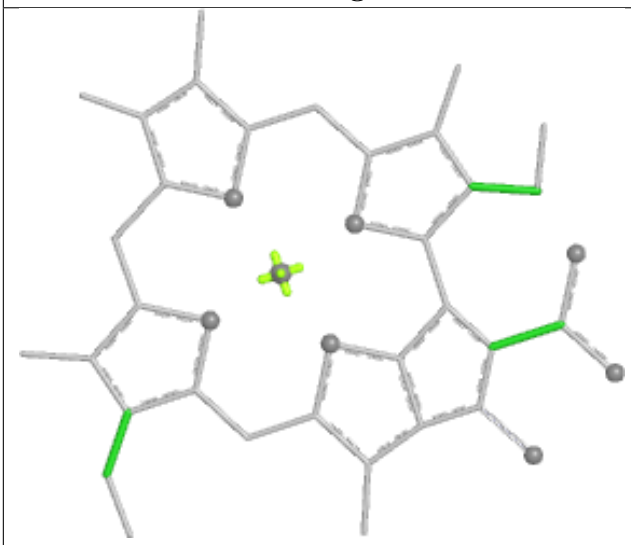


Bond angles



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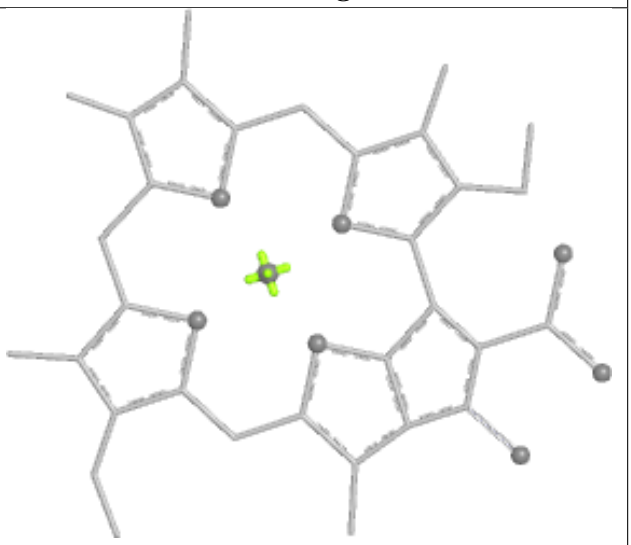
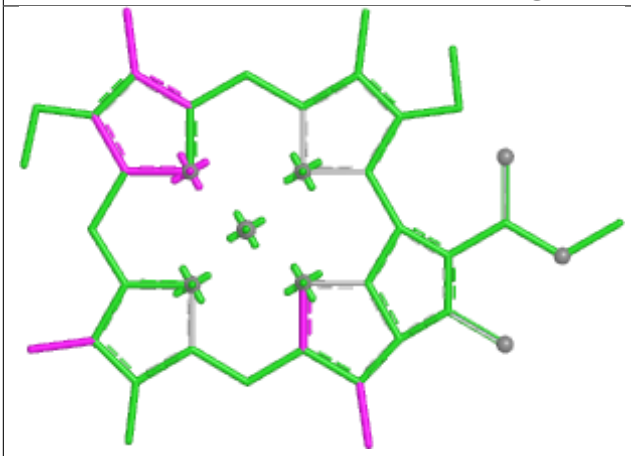


Rings

Ligand CLA 7 606



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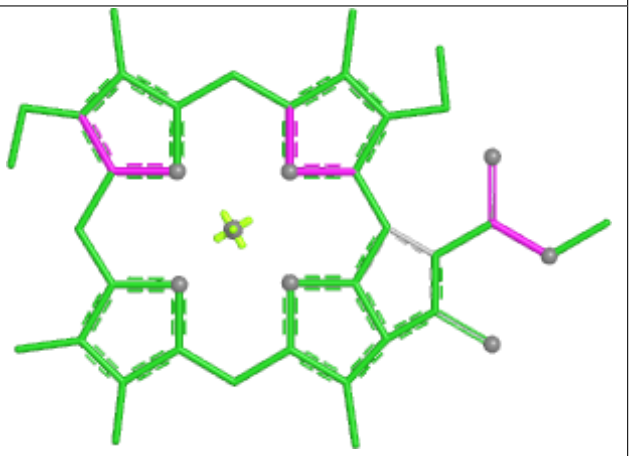
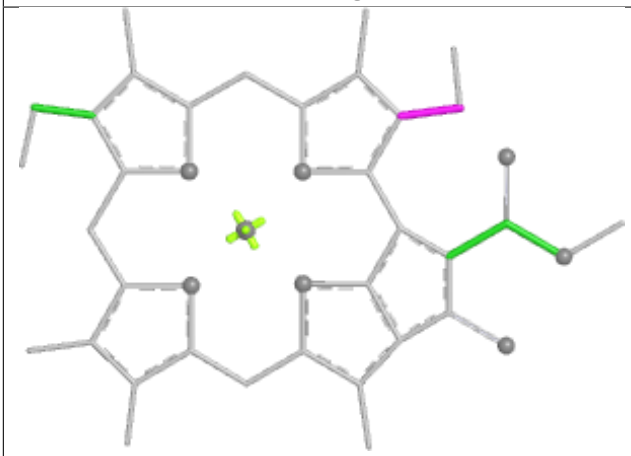
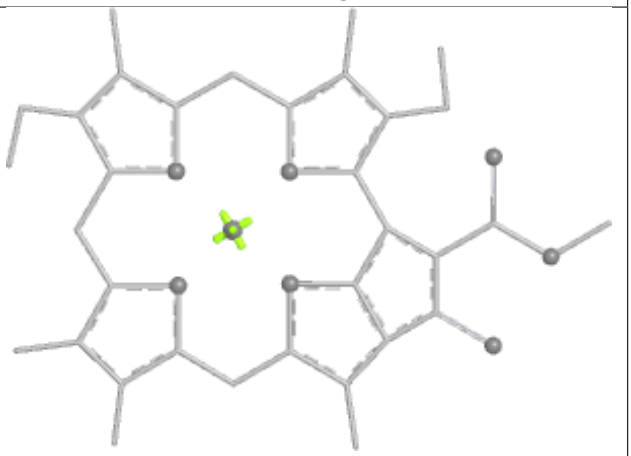


Bond angles

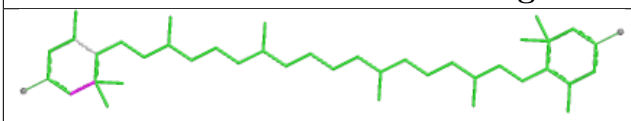


Torsions



Rings

Ligand LUT Z 1621



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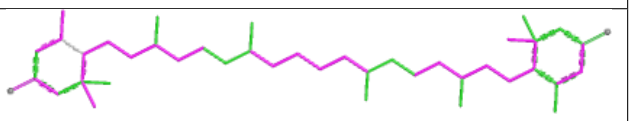

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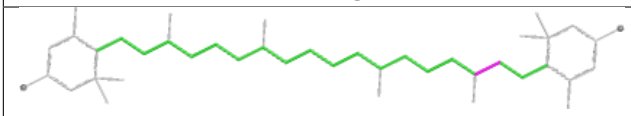

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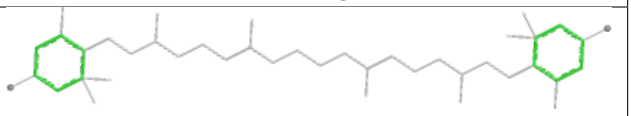
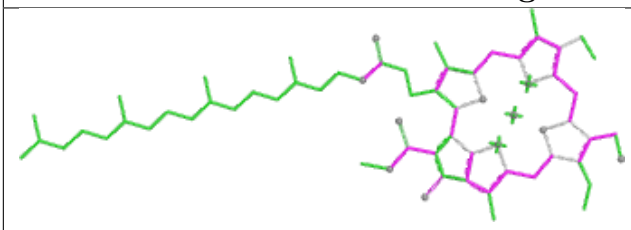


Rings

Ligand CHL W 609



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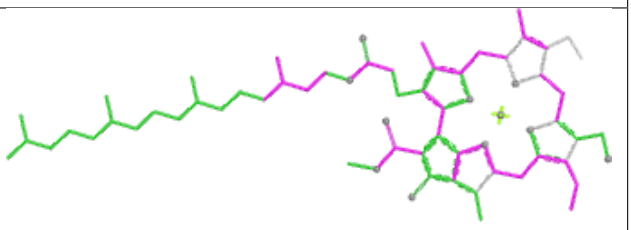
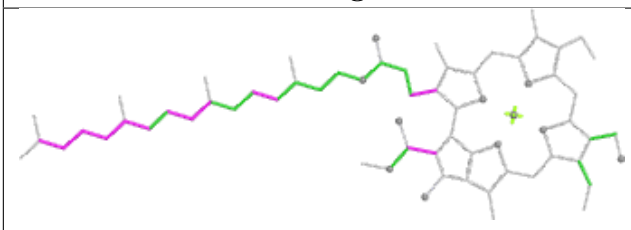


Bond angles



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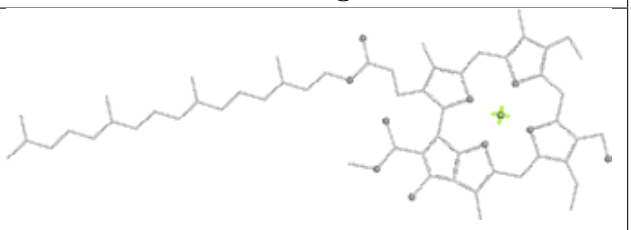
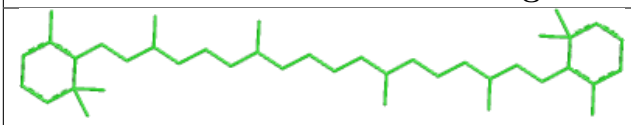


Rings

Ligand BCR B 801



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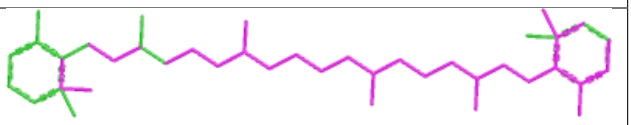
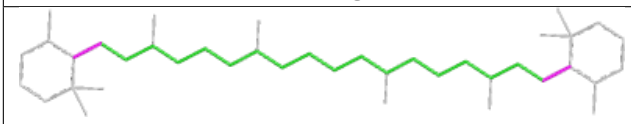


Bond angles



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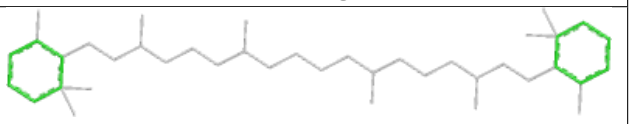
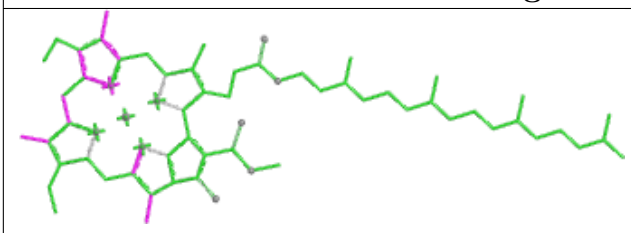


Rings

Ligand CLA A 829



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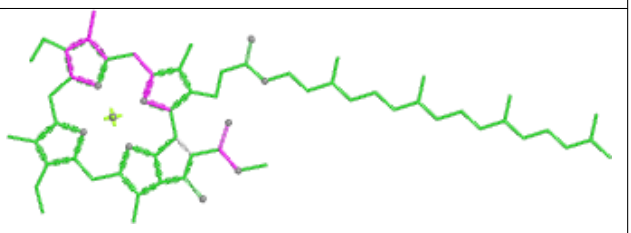

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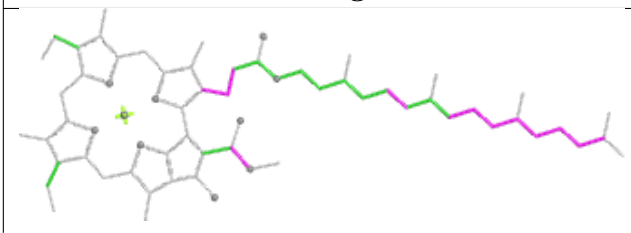

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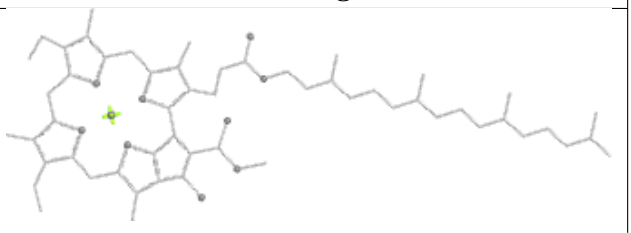
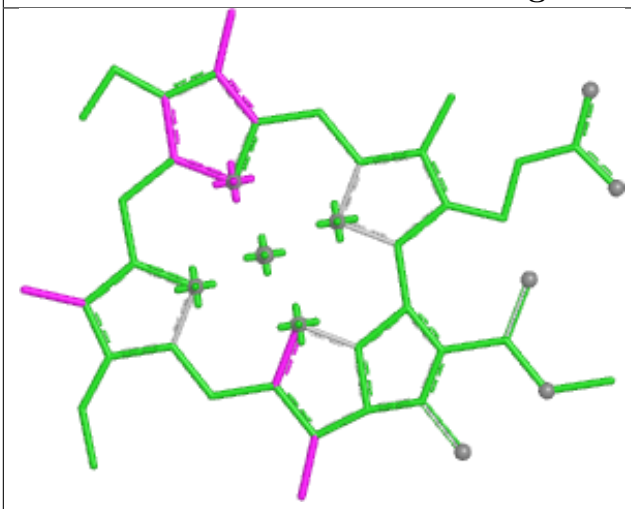


Rings

Ligand CLA 2 606



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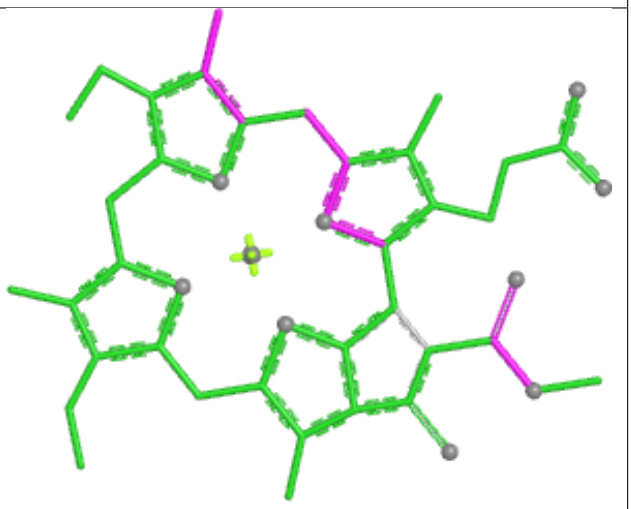
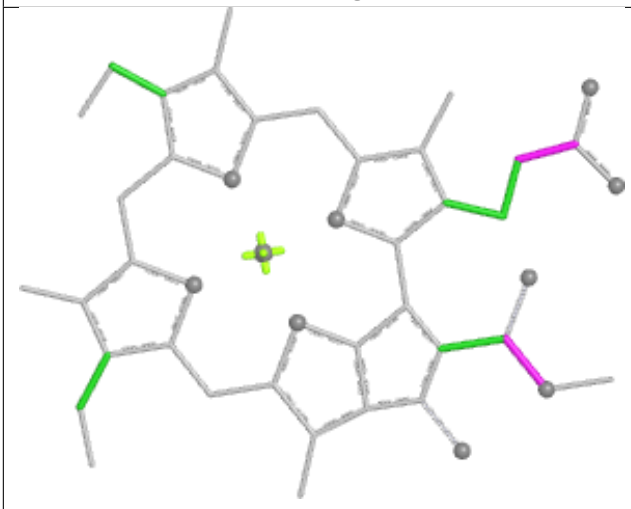


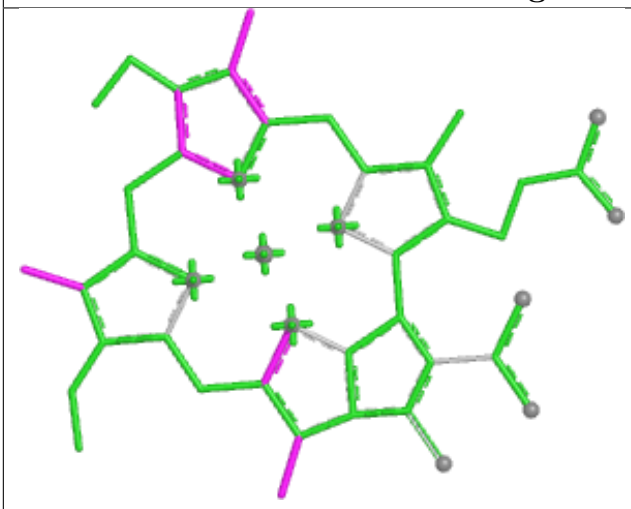
Bond angles



Torsions

Rings

Ligand CLA a 608



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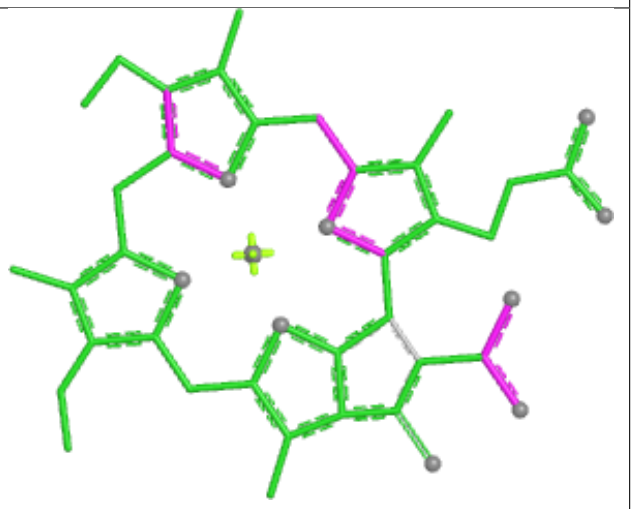
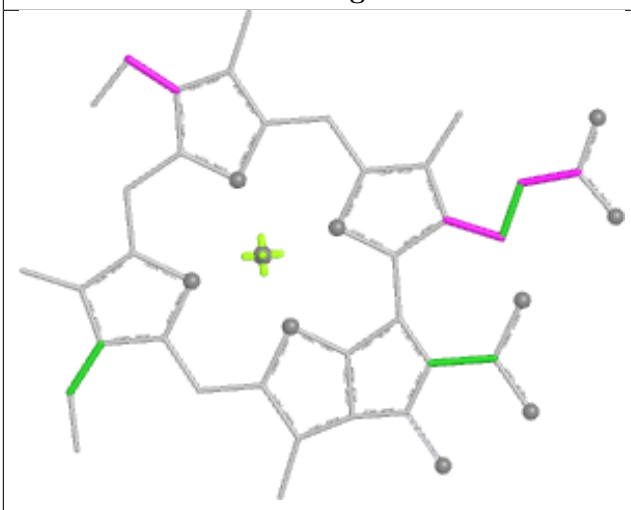


Bond angles



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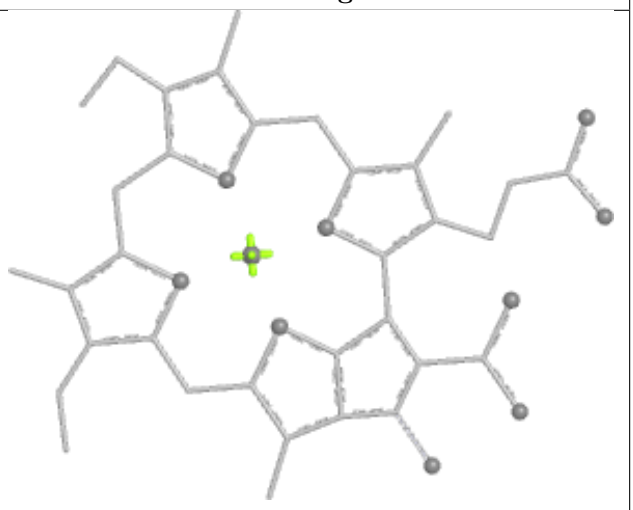
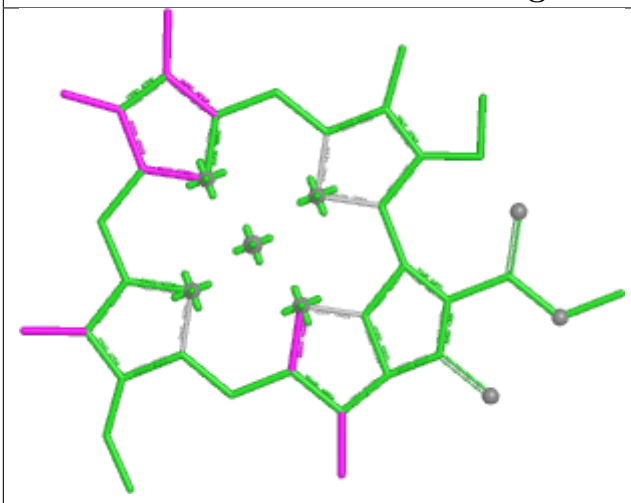
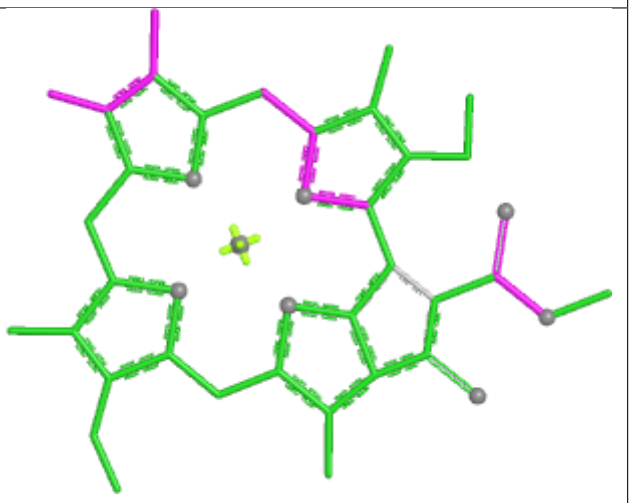


Rings

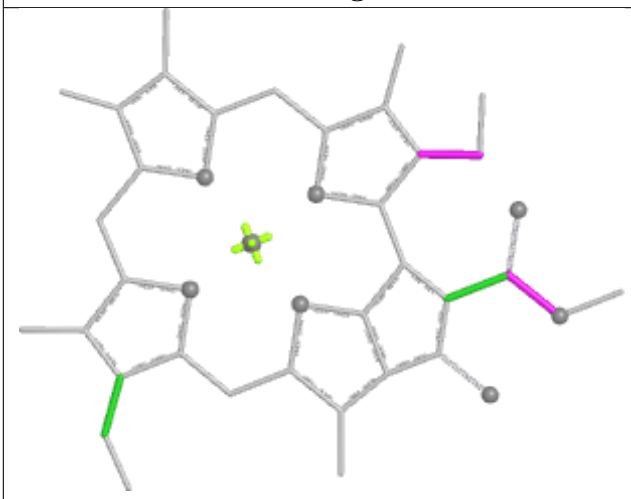
Ligand CLA 8 607



Bond lengths



Bond angles



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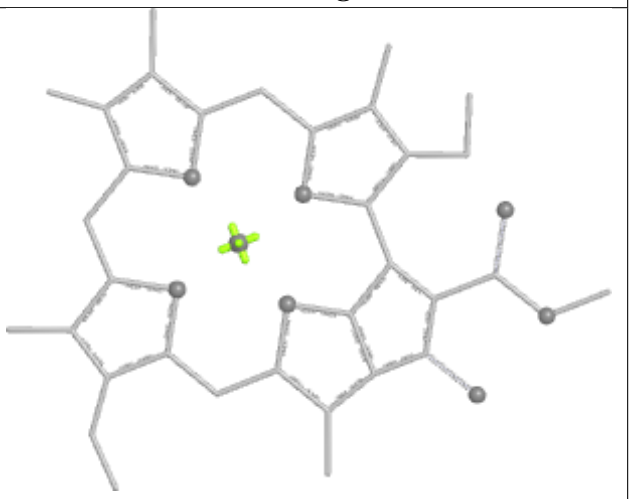
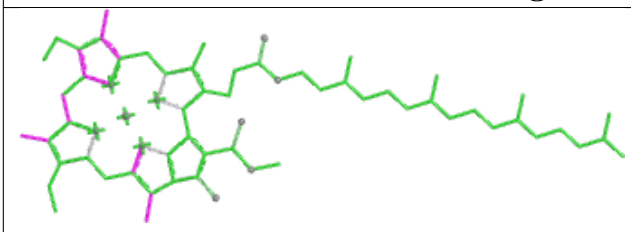
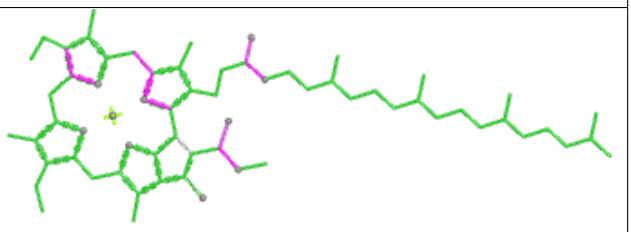


Rings

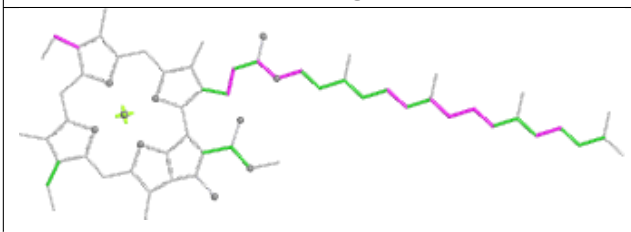
Ligand CLA 8 613



Bond lengths



Bond angles



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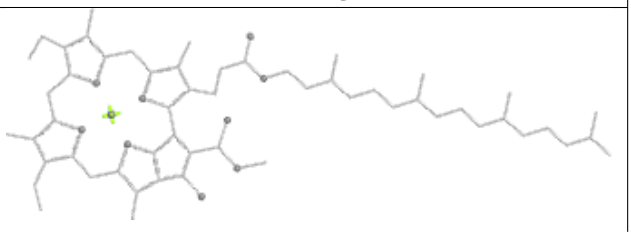
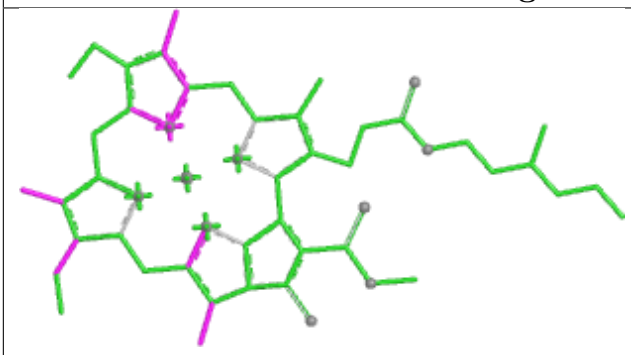
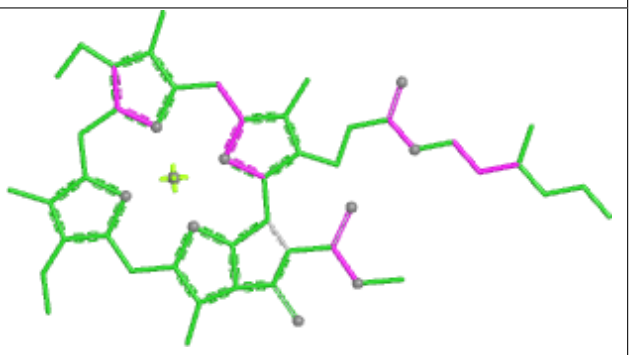


Rings

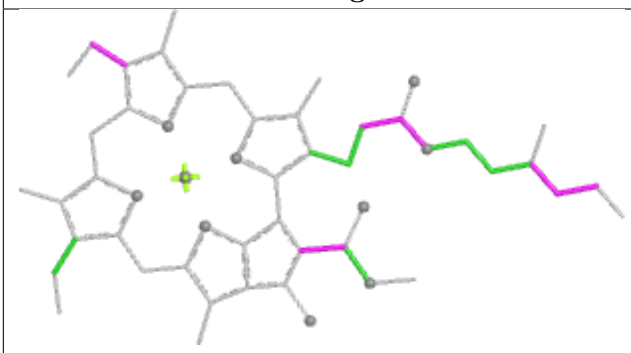
Ligand CLA W 603



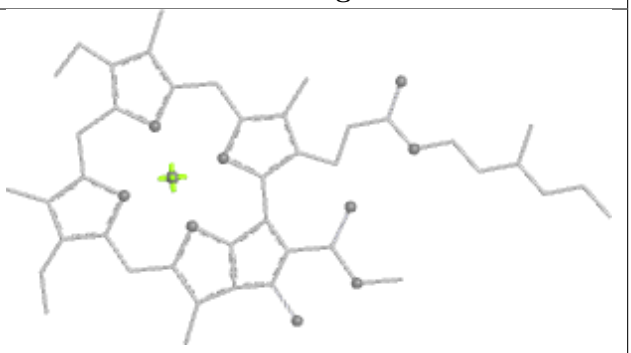
Bond lengths



Bond angles

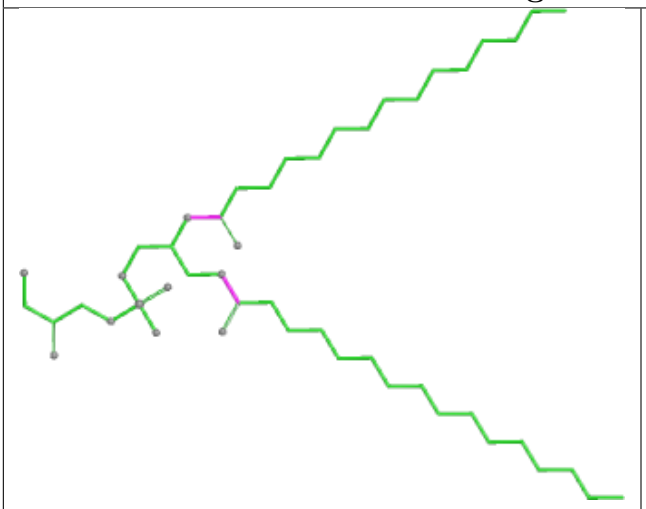


Torsions



Rings

Ligand LHG 6 623



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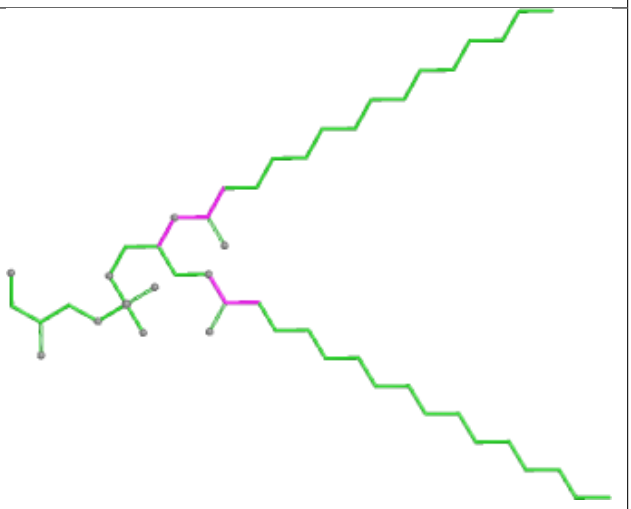
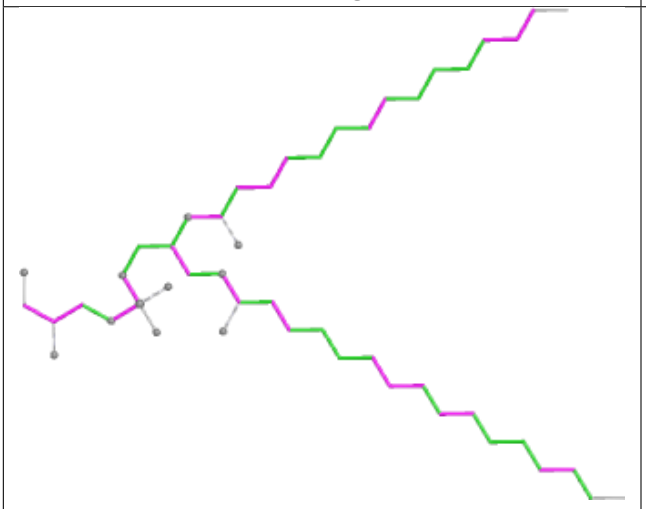


Bond angles



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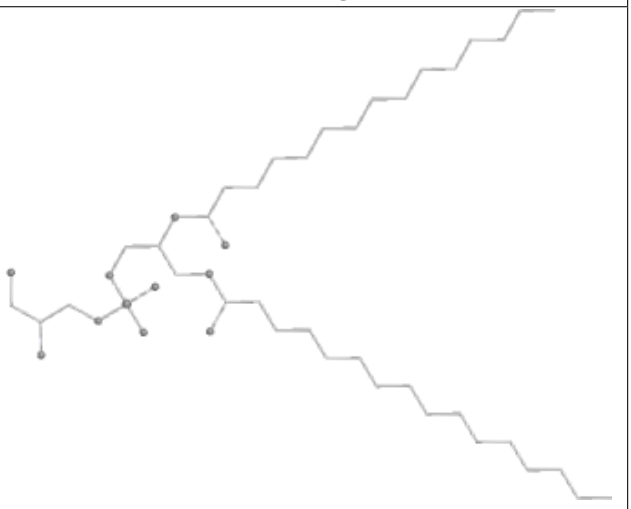
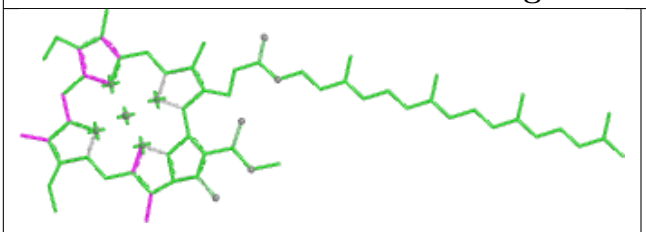


Rings

Ligand CLA X 602



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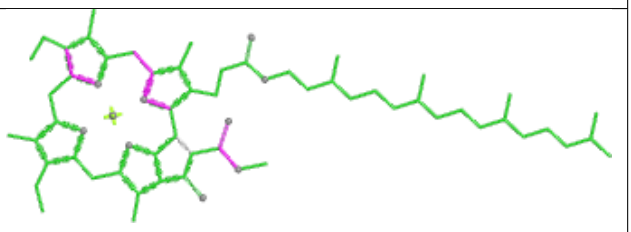
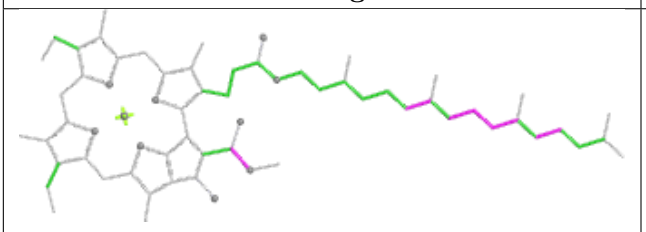
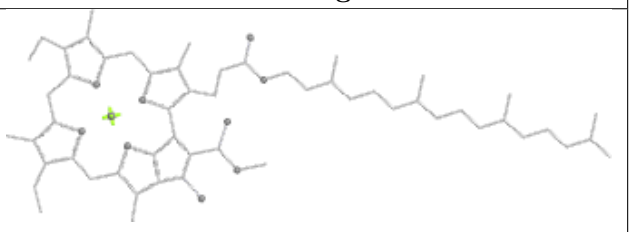


Bond angles

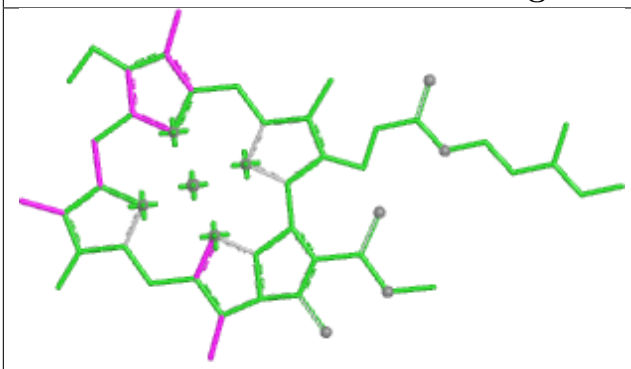


Torsions



Rings

Ligand CLA 7 604



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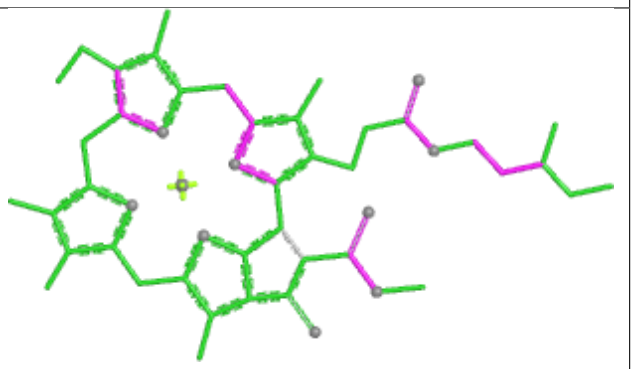
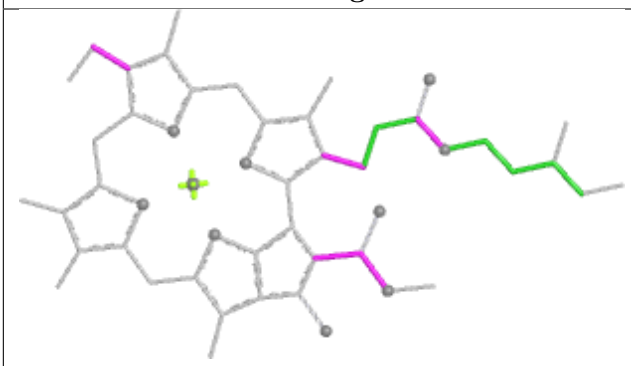


Bond angles



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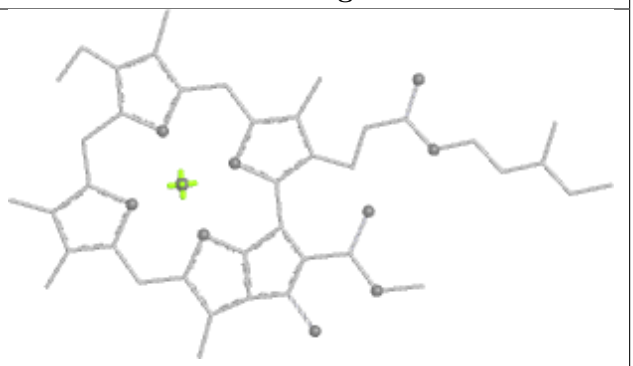
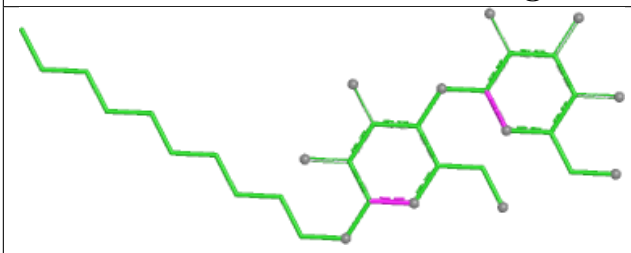


Rings

Ligand LMU 5 628



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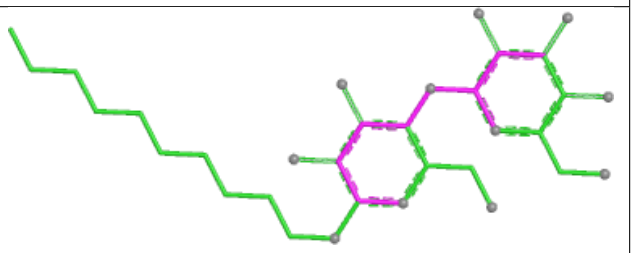

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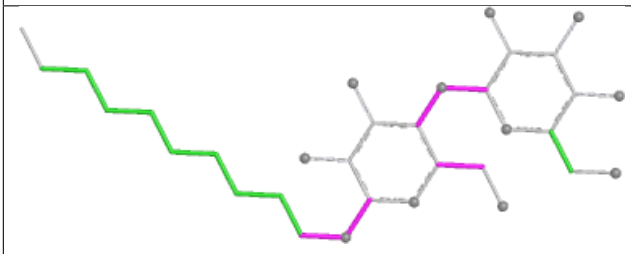

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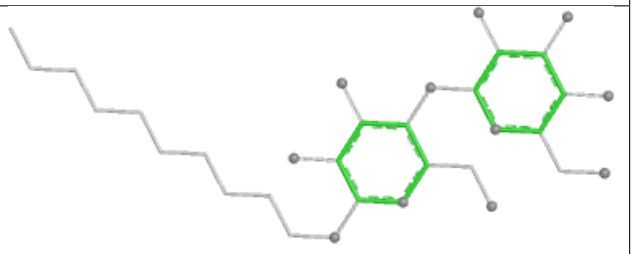
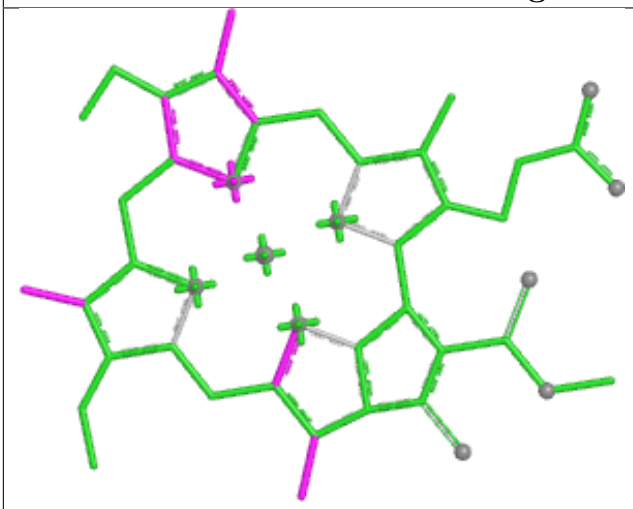


Rings

Ligand CLA 6 609



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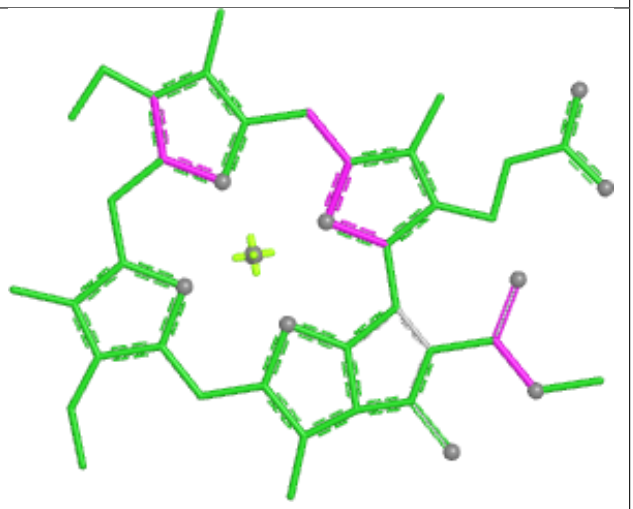

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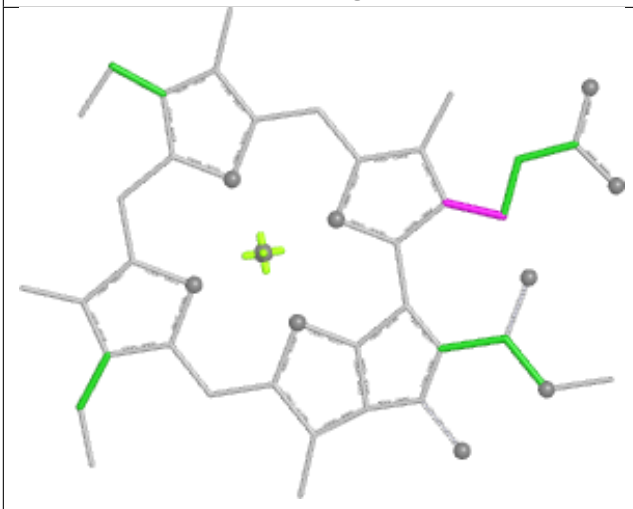
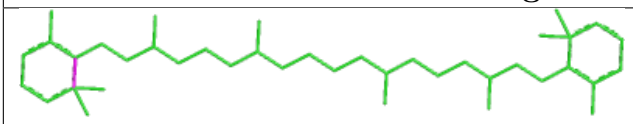


Torsions

Rings

Ligand BCR B 847



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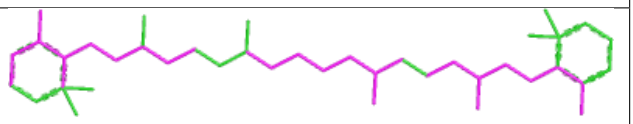

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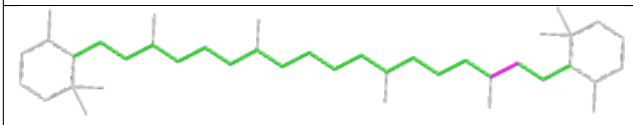
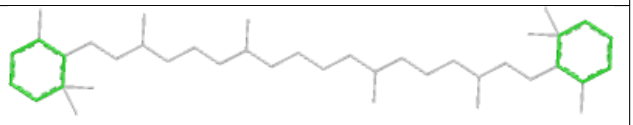
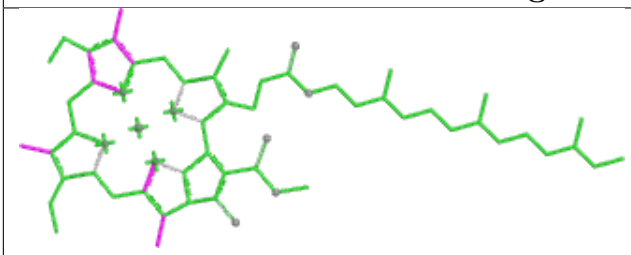
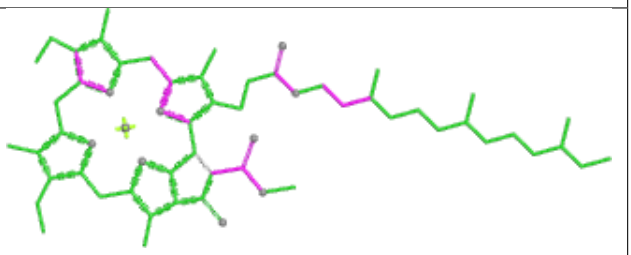
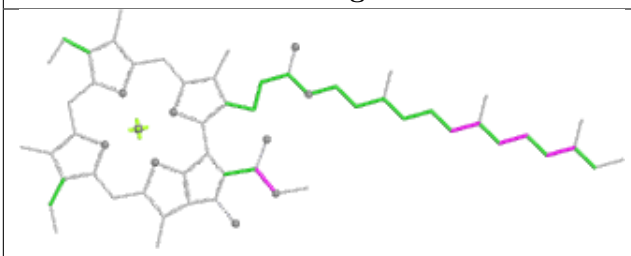
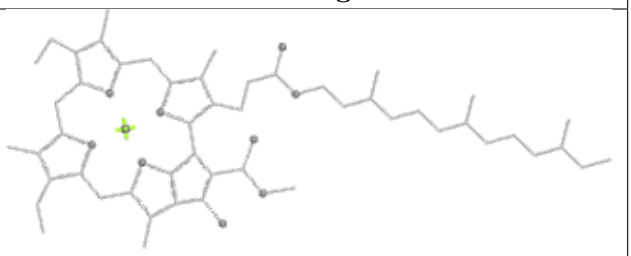
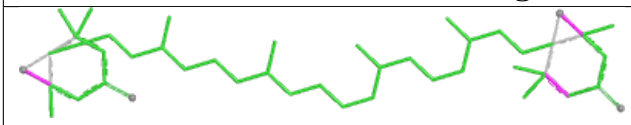
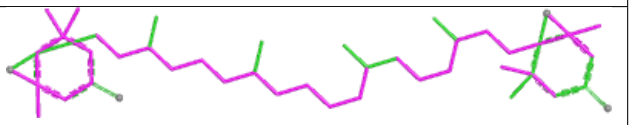
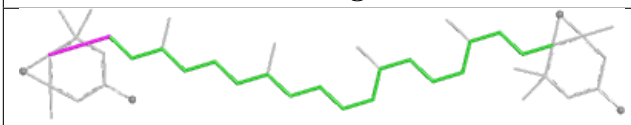
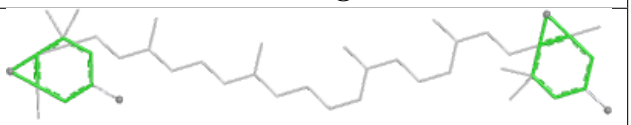


Torsions

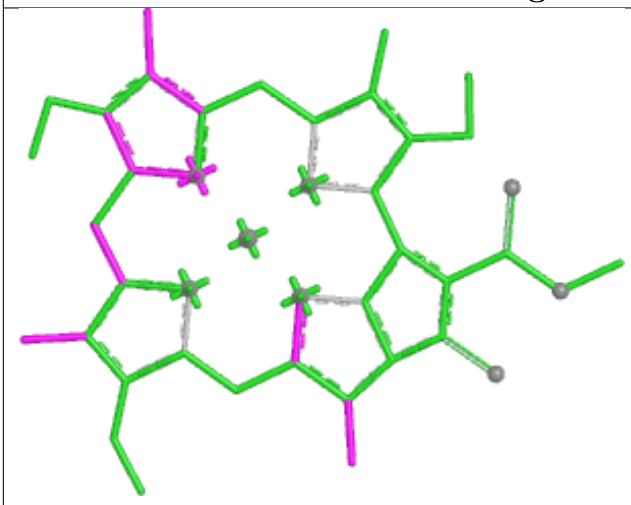


Rings

Ligand CLA 4 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT U 1622	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 614



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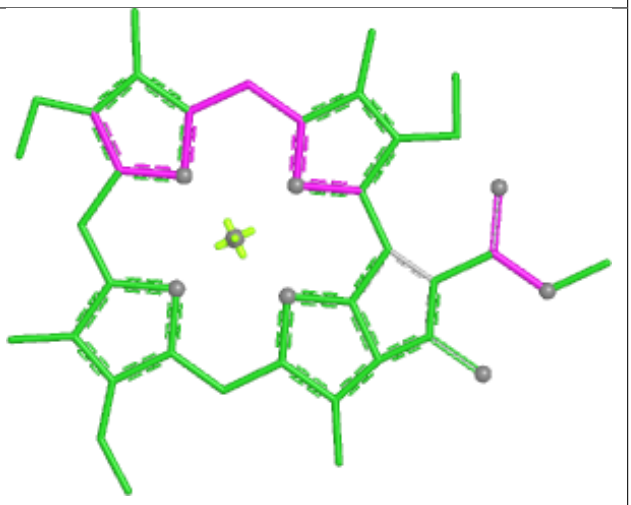
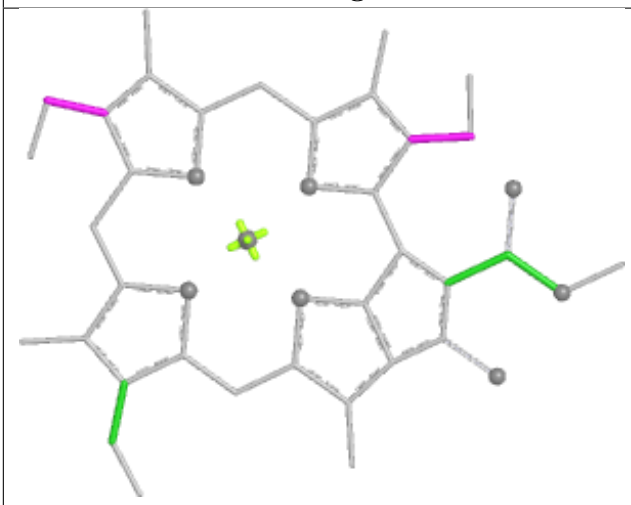


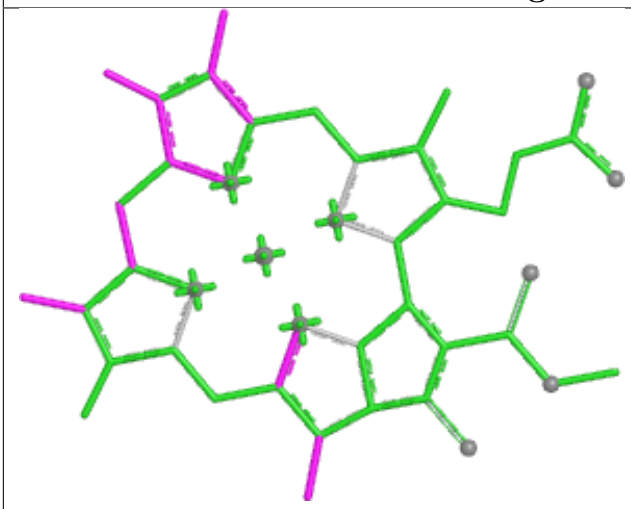
Bond angles



Torsions

Rings

Ligand CLA 2 616



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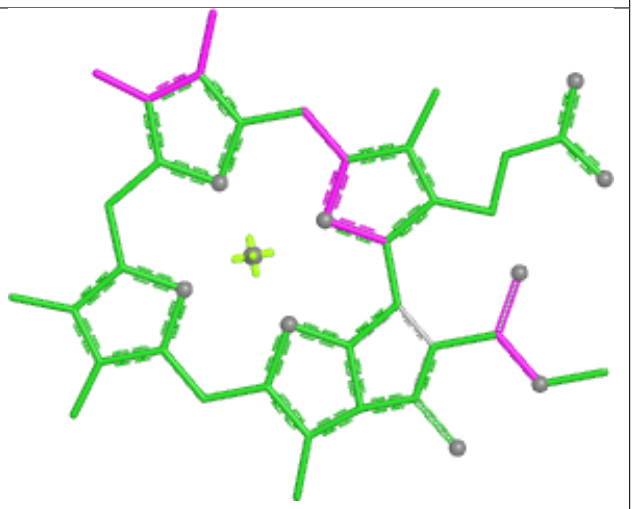

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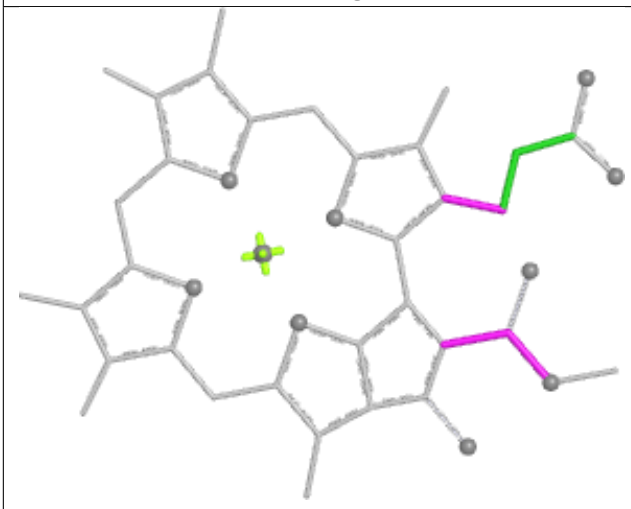
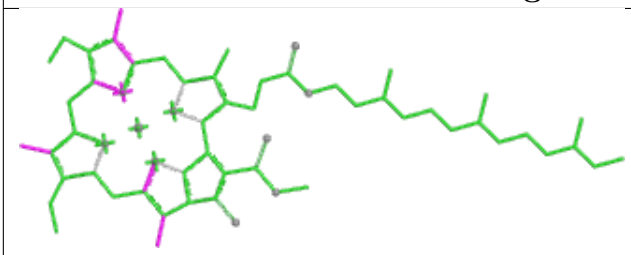


Torsions

Rings

Ligand CLA A 835



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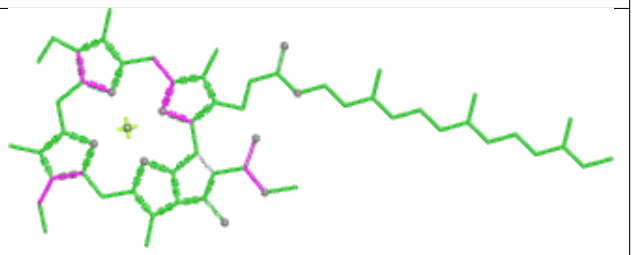
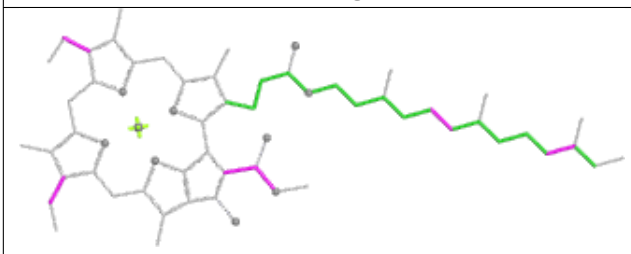


Bond angles



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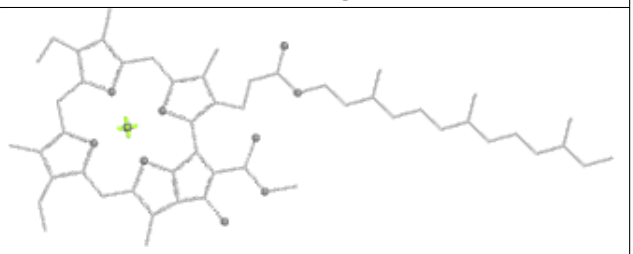
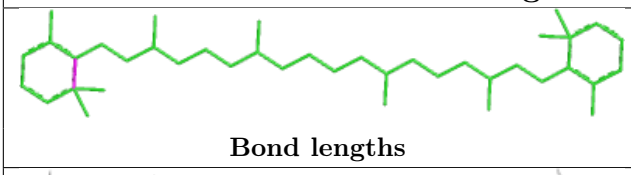
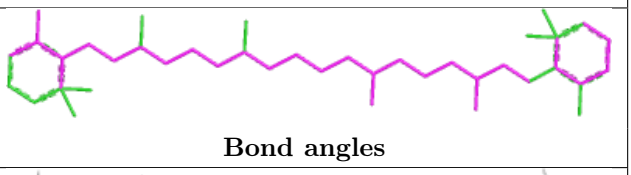


Rings

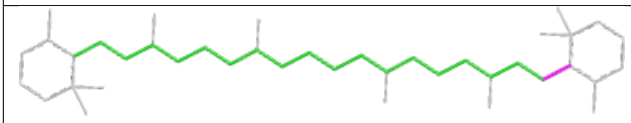
Ligand BCR B 844



Bond lengths



Bond angles



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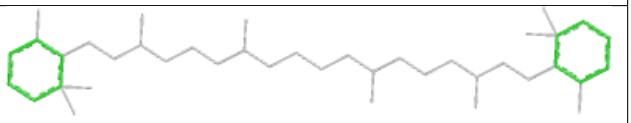
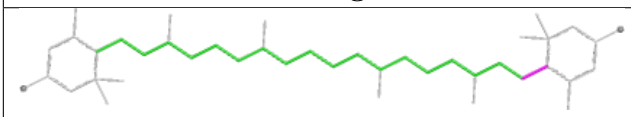


Rings

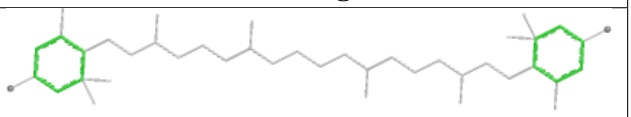
Ligand LUT X 1620

Bond lengths

Bond angles

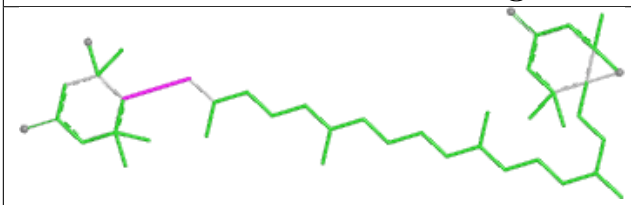


Torsions

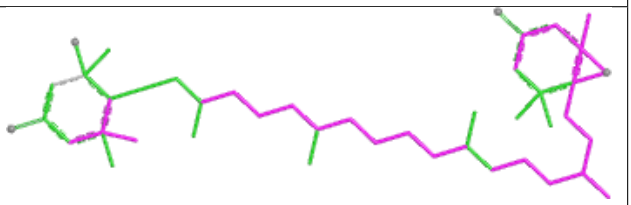


Rings

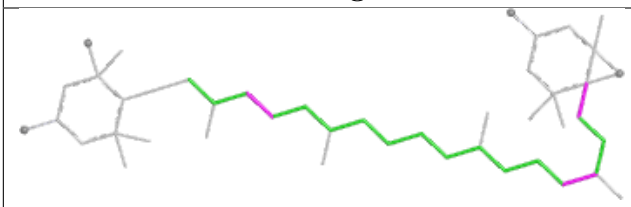
Ligand NEX W 1623



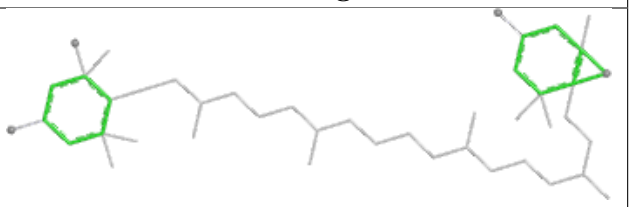
Bond lengths



Bond angles

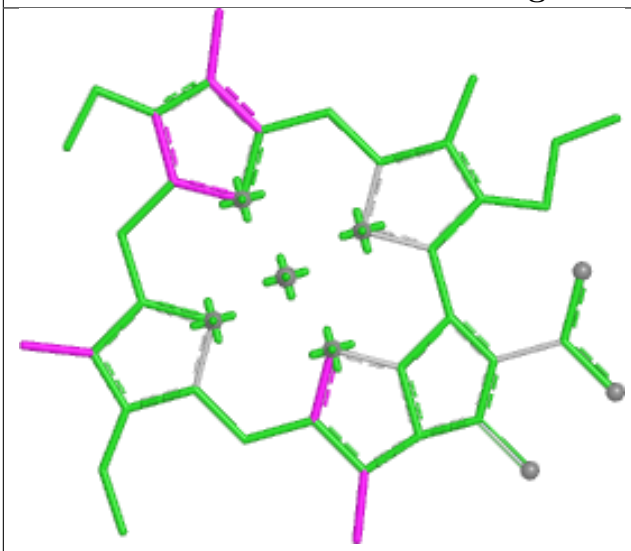


Torsions

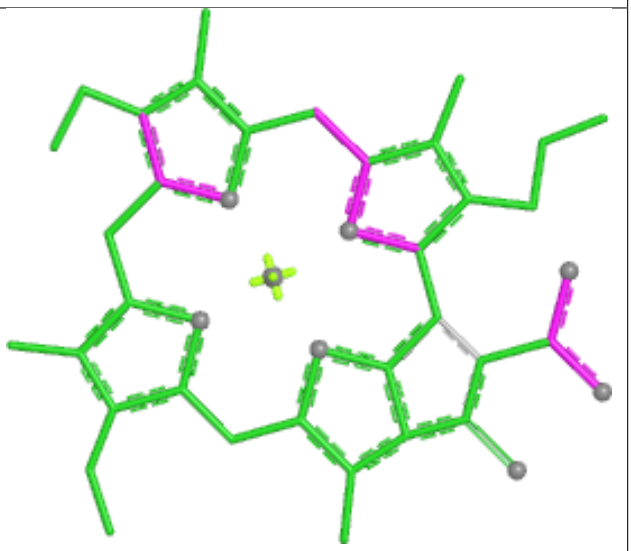


Rings

Ligand CLA 2 614



Bond lengths

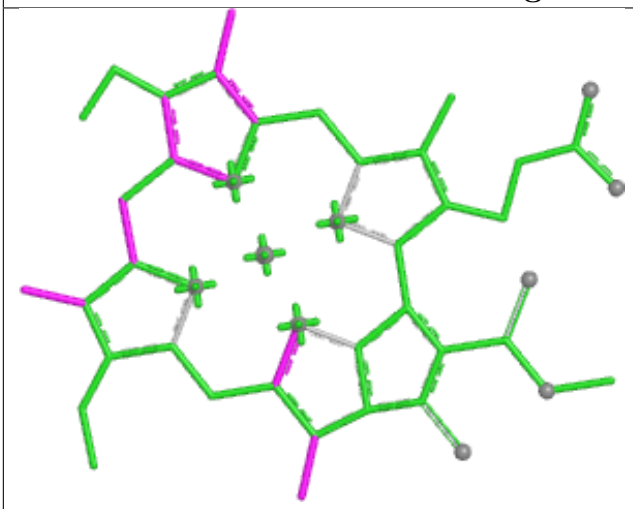


Bond angles

Torsions

Rings

Ligand CLA B 823



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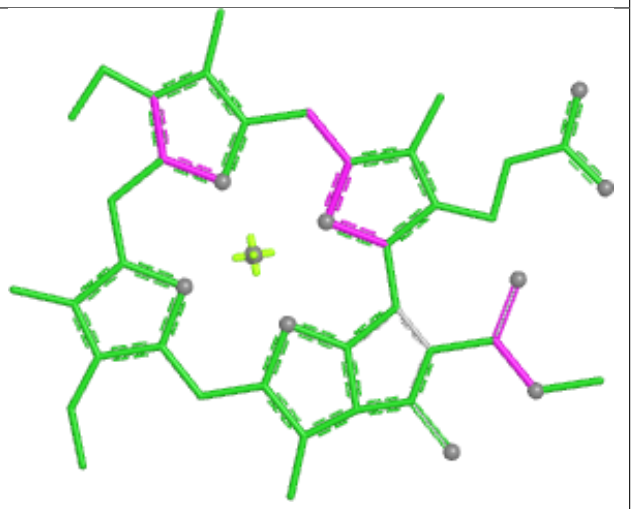
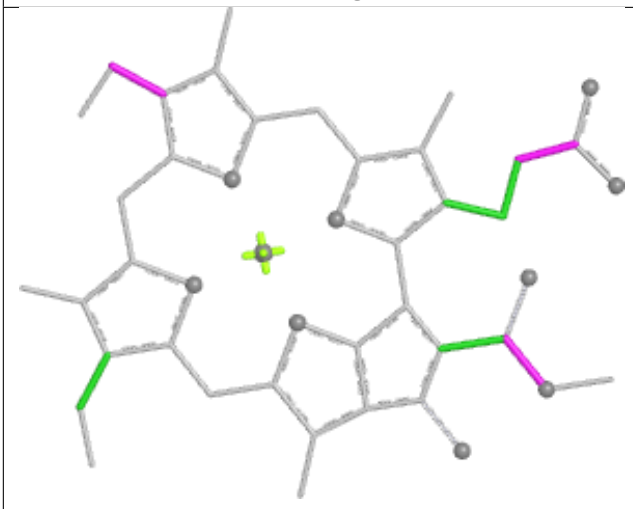


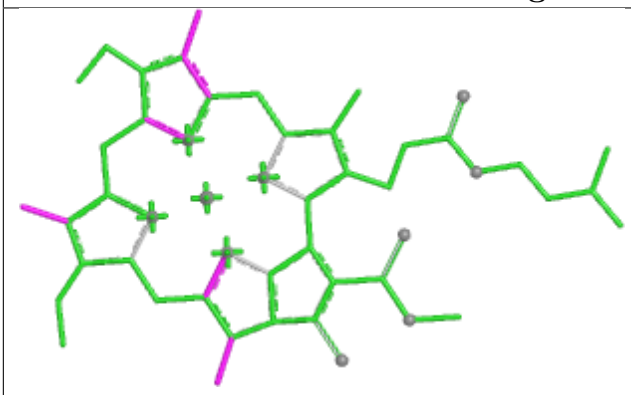
Bond angles



Torsions

Rings

Ligand CLA 5 617



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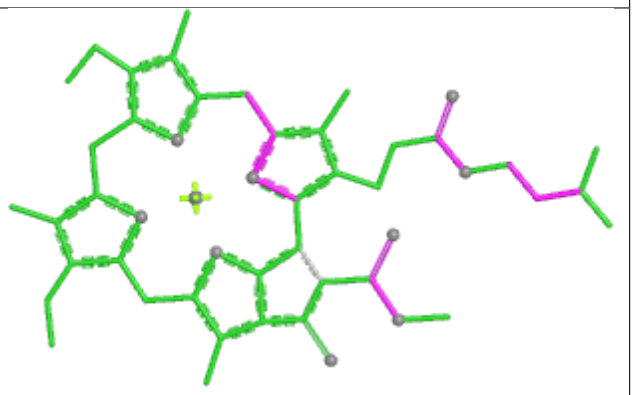

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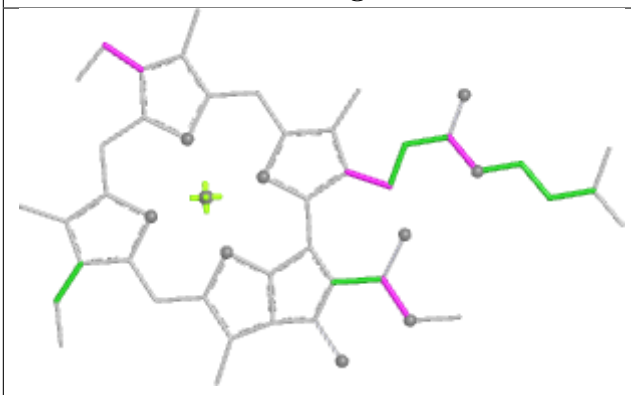
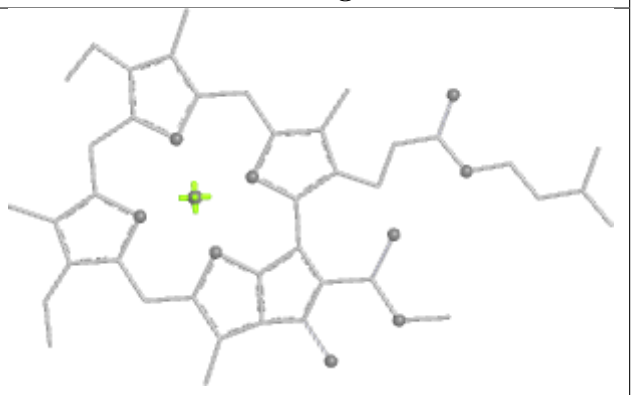
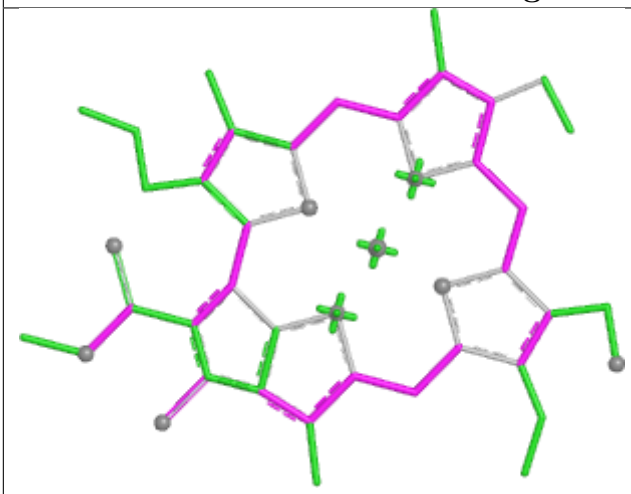


Torsions



Rings

Ligand CHL X 606



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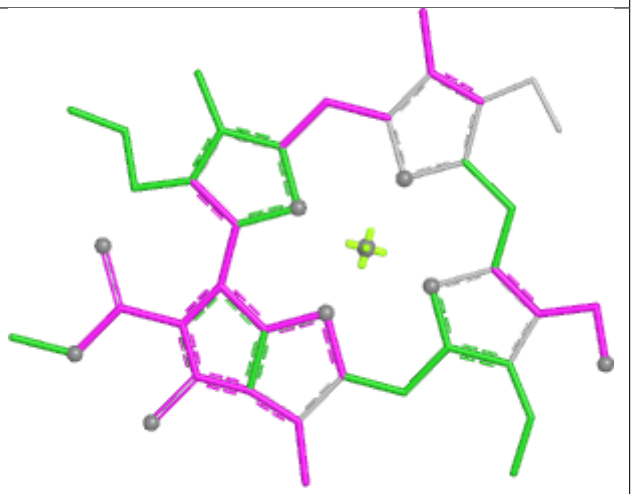
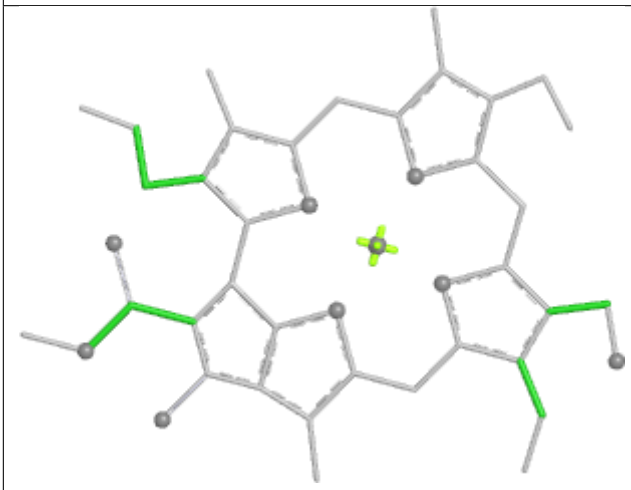
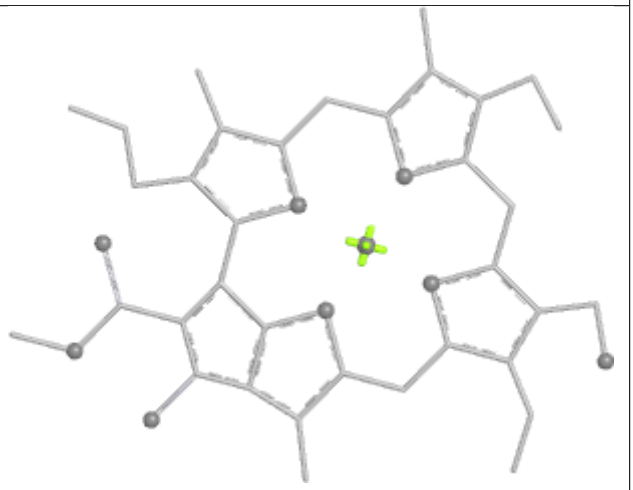


Bond angles

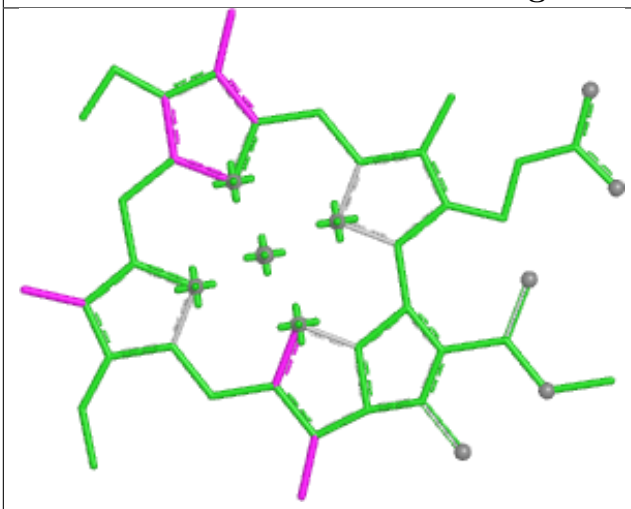


Torsions



Rings

Ligand CLA a 607



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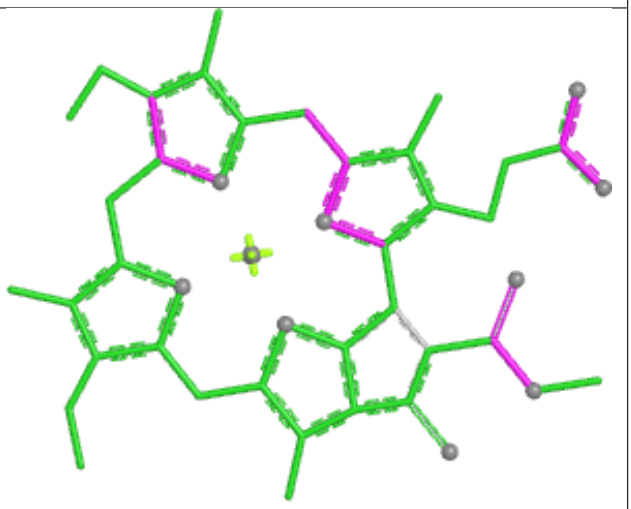

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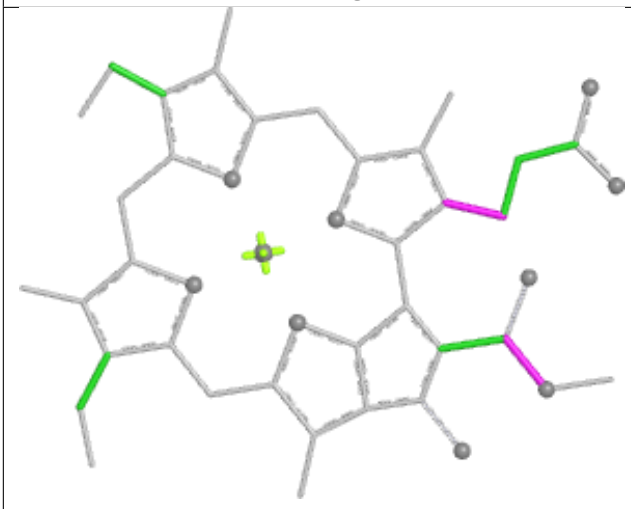
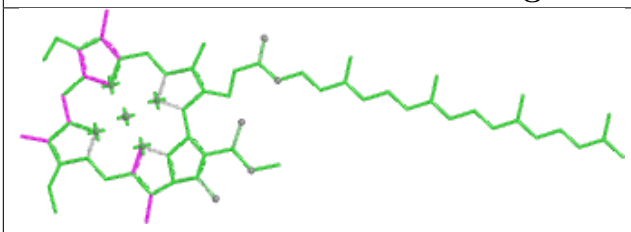


Torsions

Rings

Ligand CLA X 613



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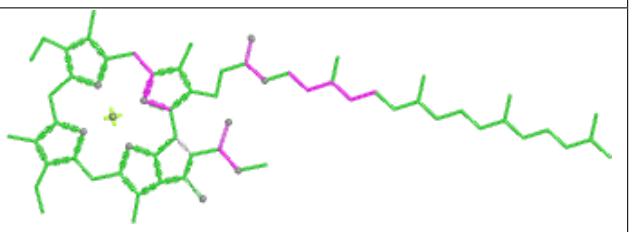
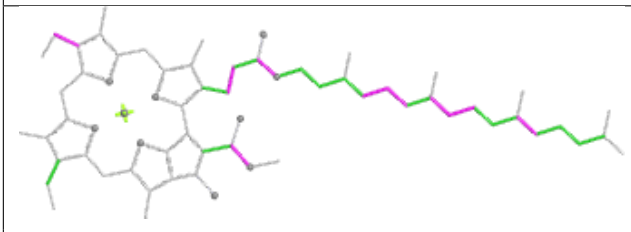


Bond angles



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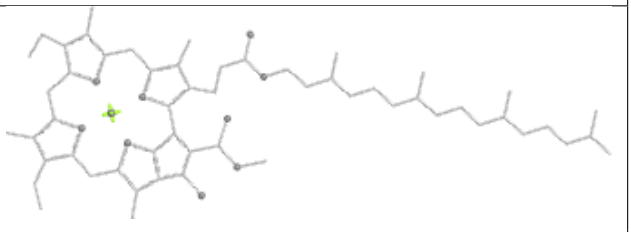
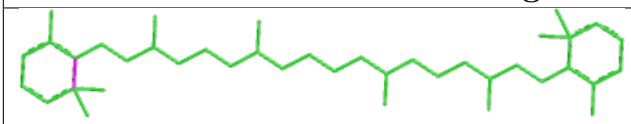
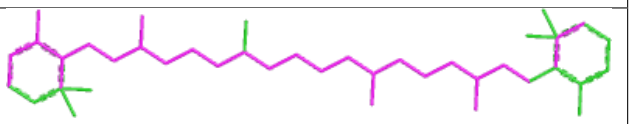
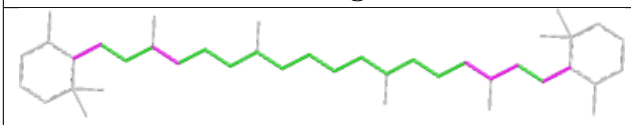
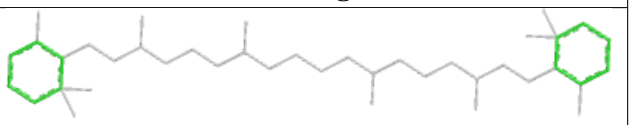


Rings

Ligand BCR B 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

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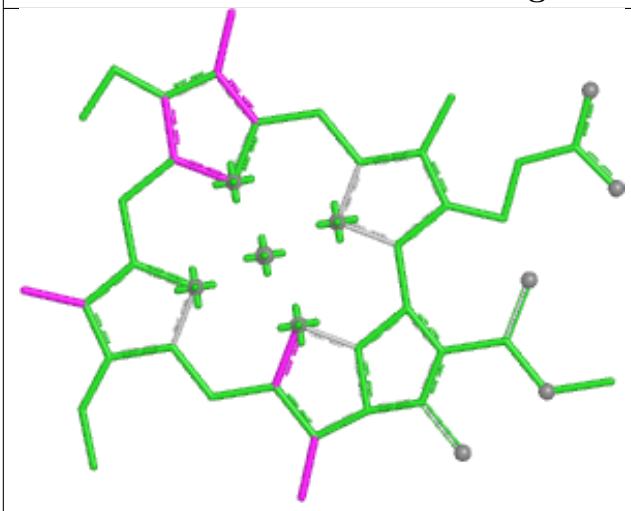
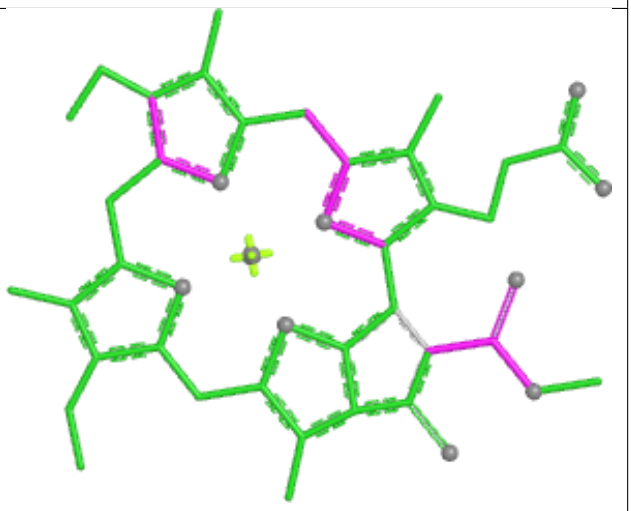
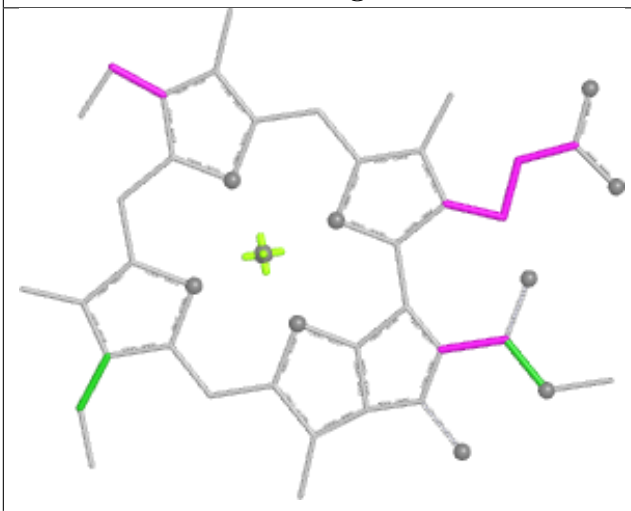
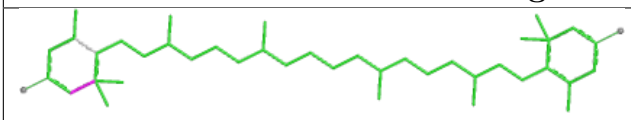
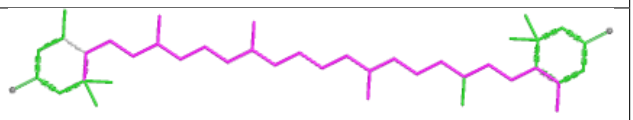
 Bond lengths	 Bond angles
 Torsions	Rings

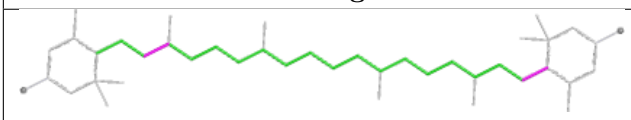
Ligand LUT 4 619



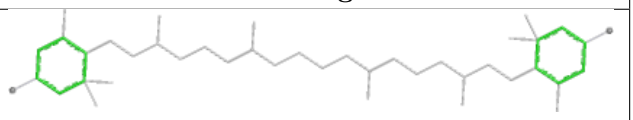
Bond lengths



Bond angles

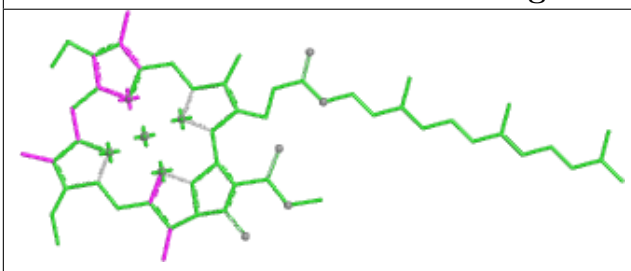


Torsions

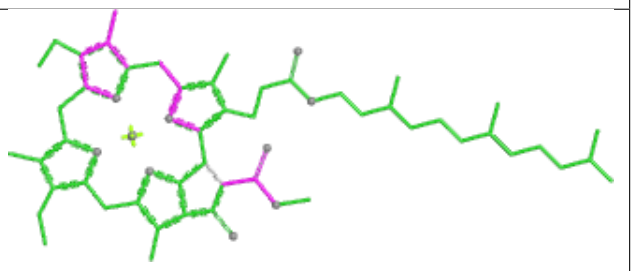


Rings

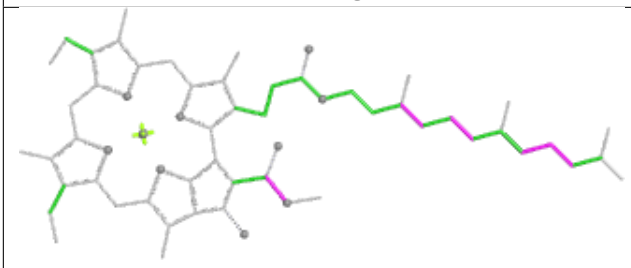
Ligand CLA 9 602



Bond lengths



Bond angles



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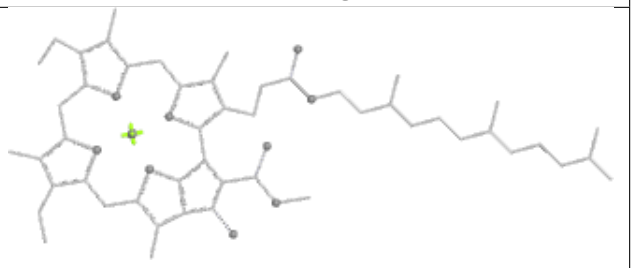
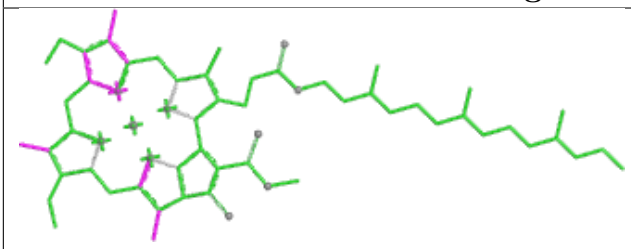


Rings

Ligand CLA B 827



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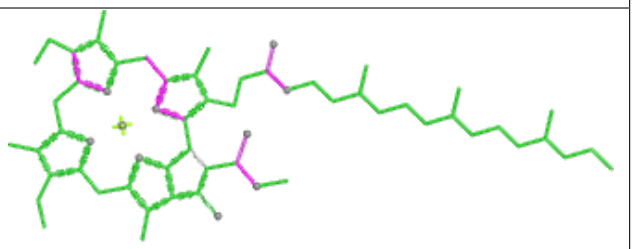
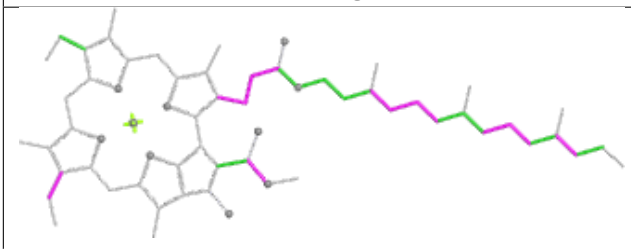


Bond angles



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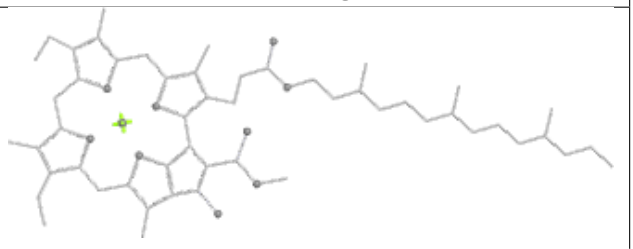
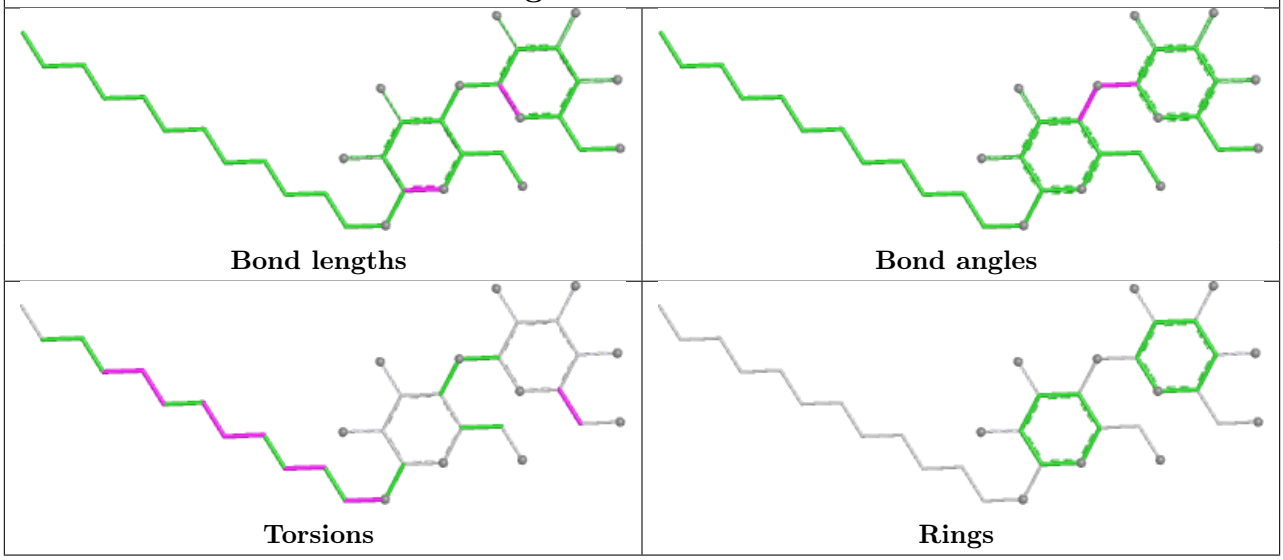
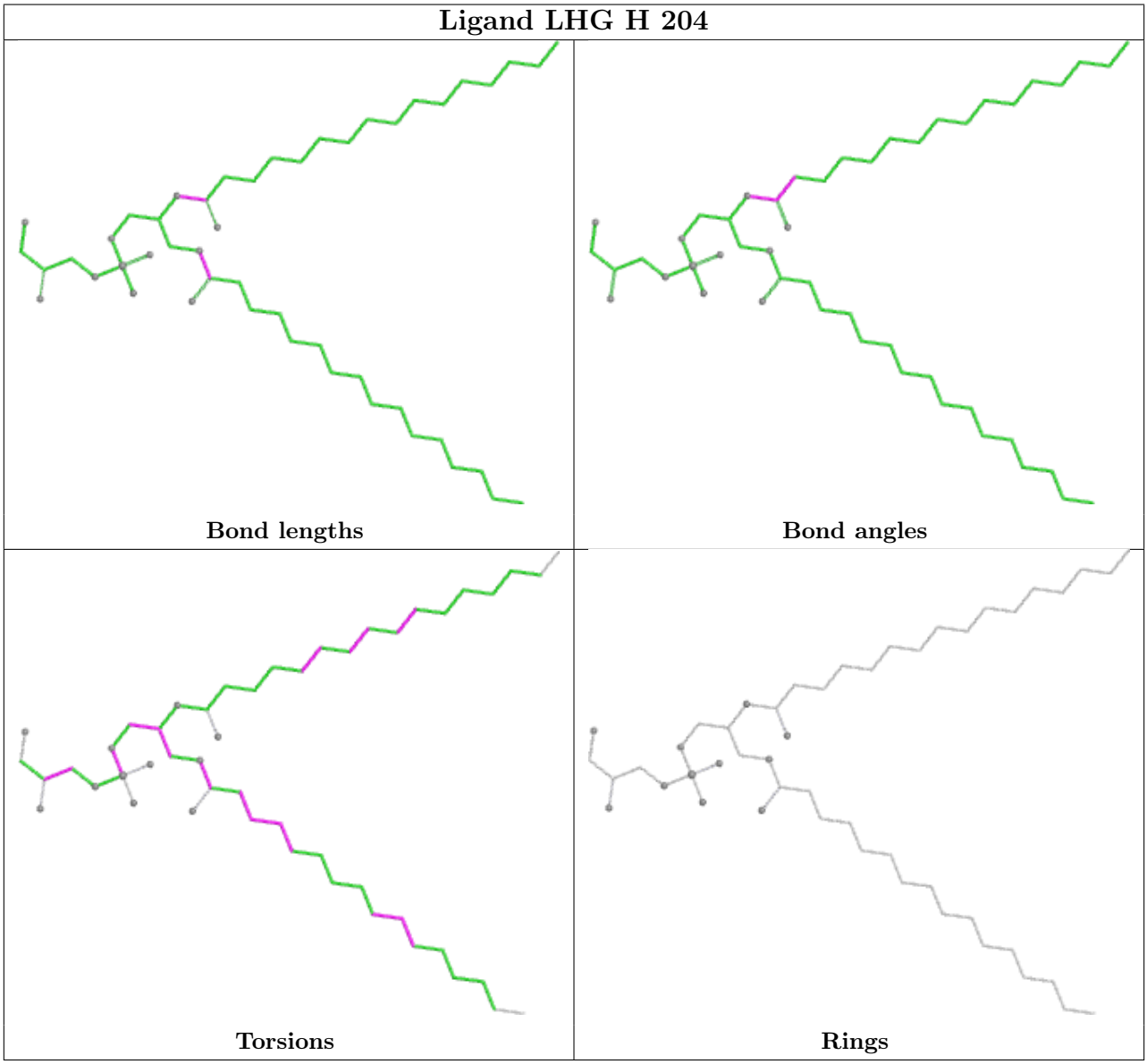


Rings

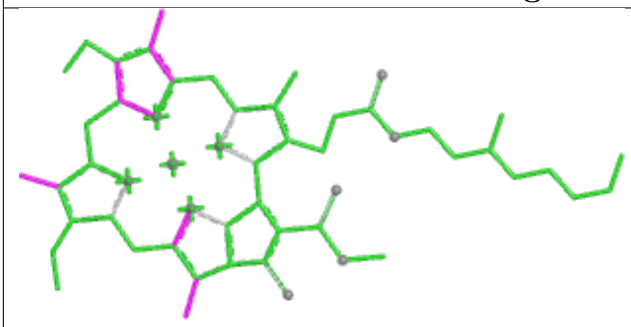
Ligand LMU 1 621



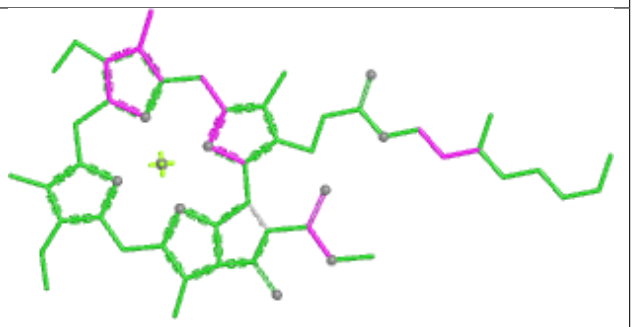
Ligand LHG H 204



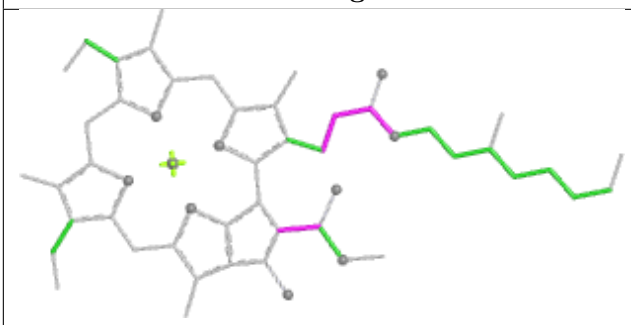
Ligand CLA A 813



Bond lengths



Bond angles



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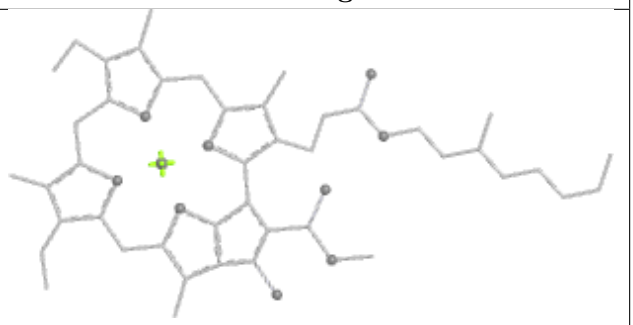
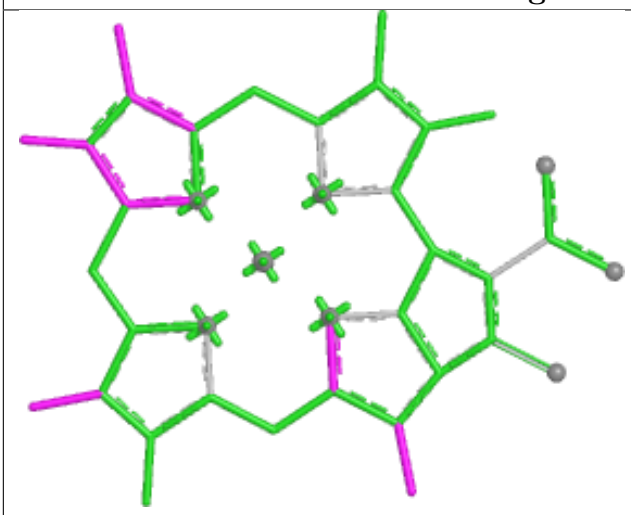


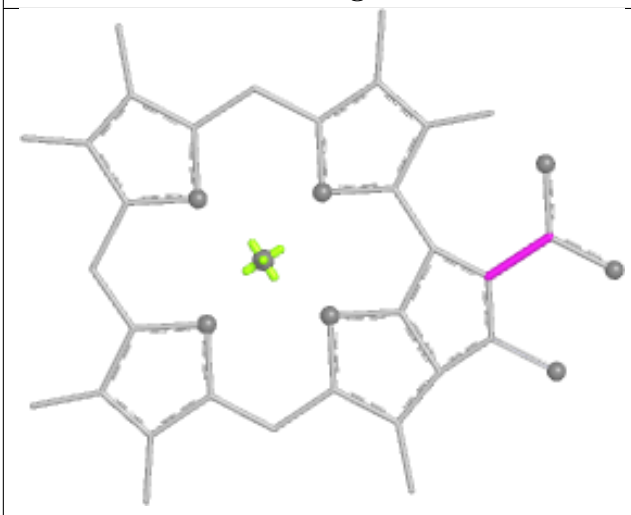
Rings

Ligand CLA 3 611

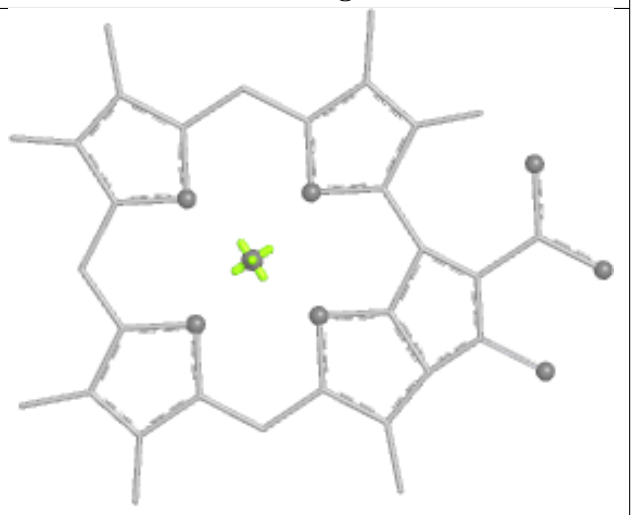


Bond lengths

Bond angles

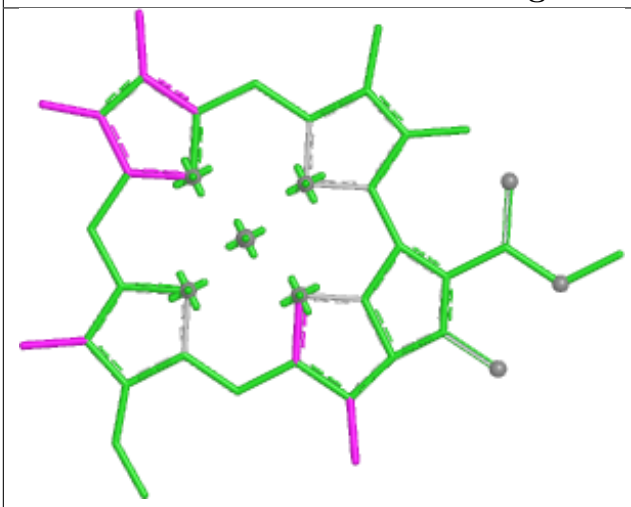


Torsions

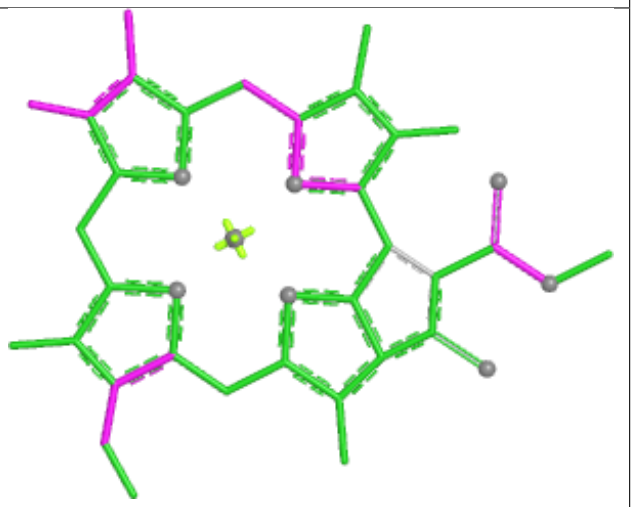


Rings

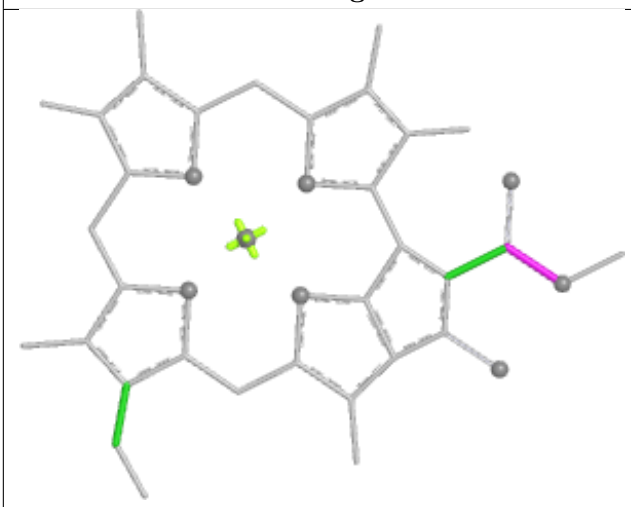
Ligand CLA 1 609



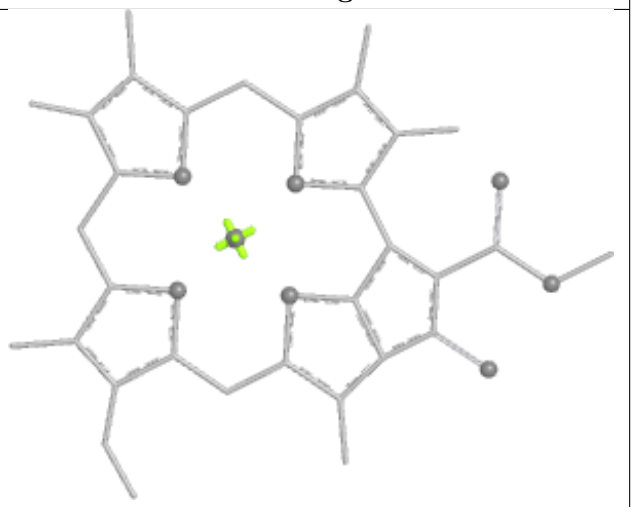
Bond lengths



Bond angles

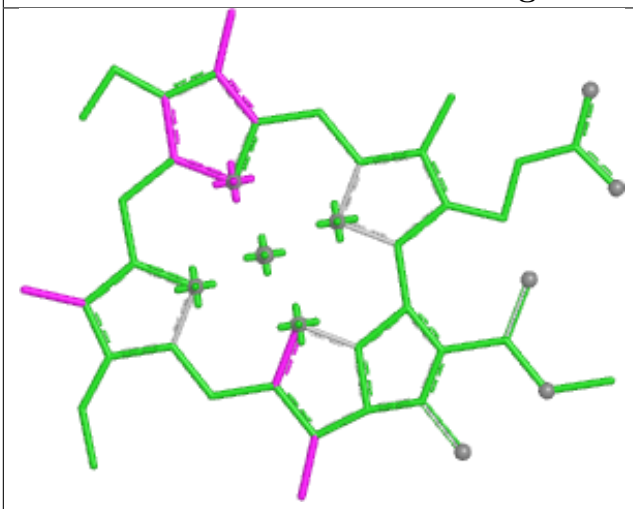


Torsions

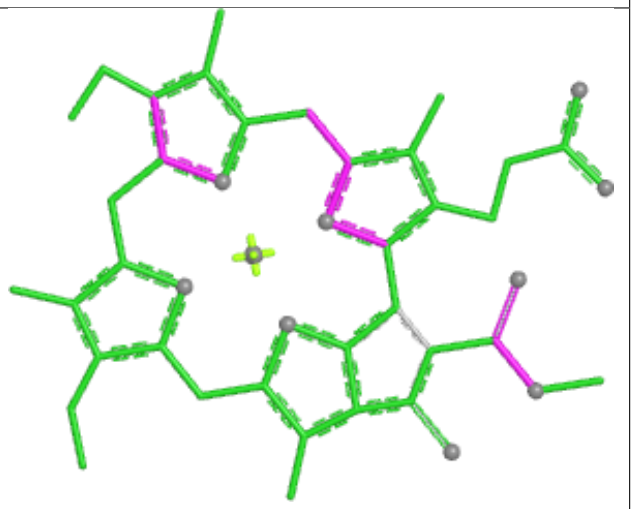


Rings

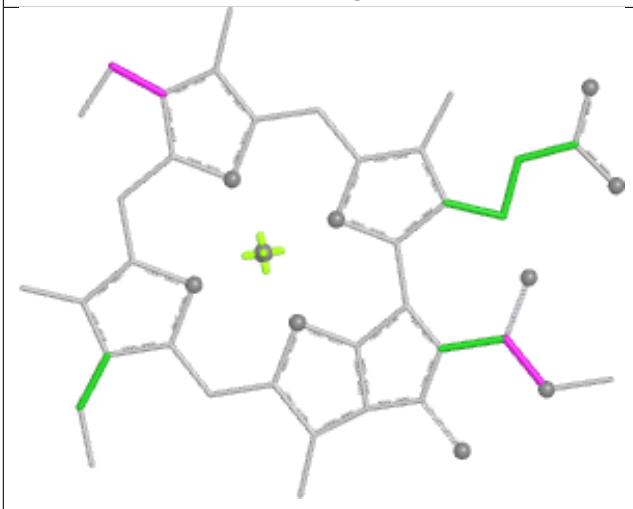
Ligand CLA W 614



Bond lengths



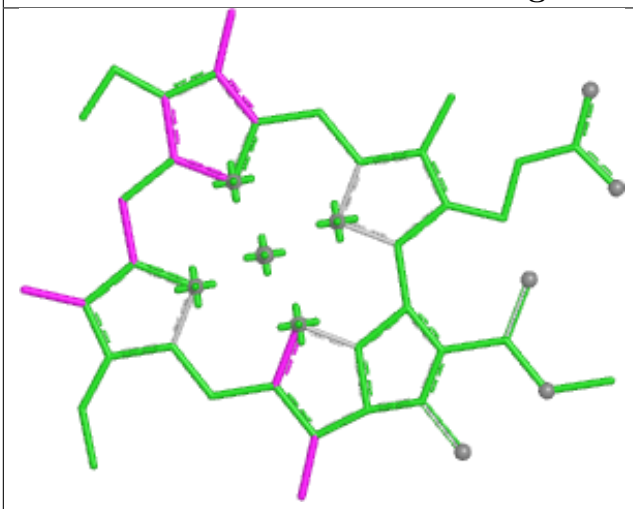
Bond angles



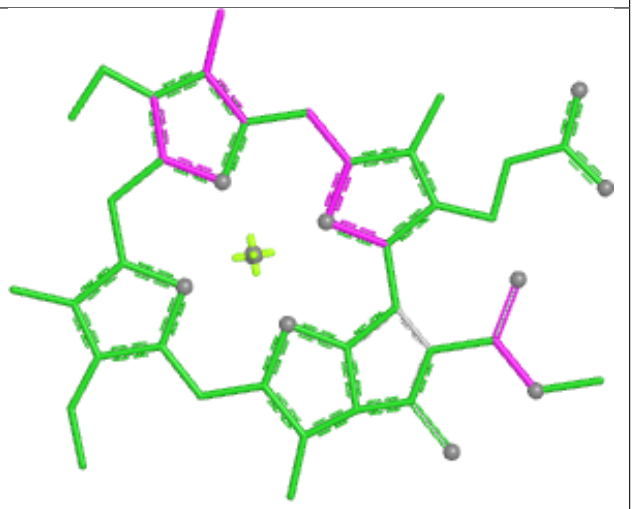
Torsions

Rings

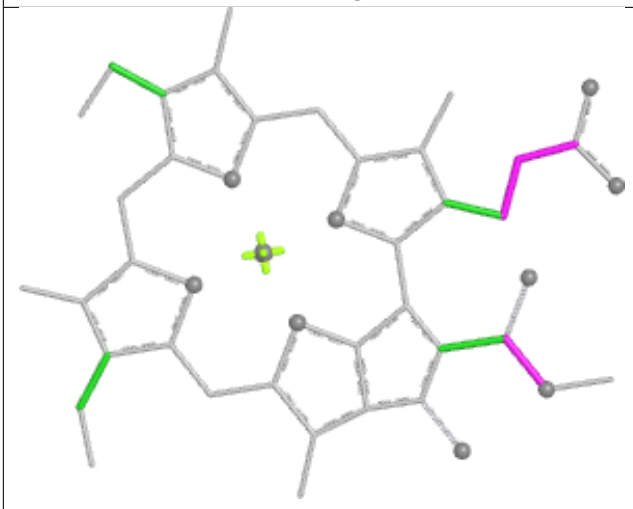
Ligand CLA a 616



Bond lengths



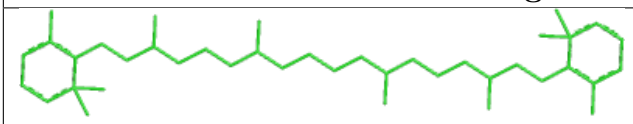
Bond angles



Torsions

Rings

Ligand BCR L 309



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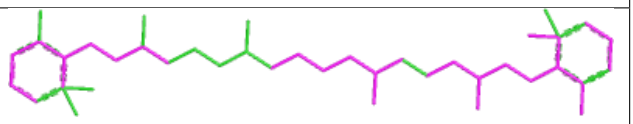
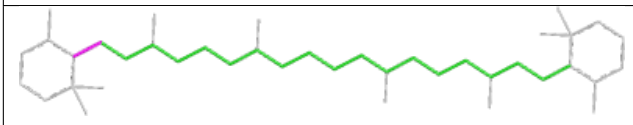
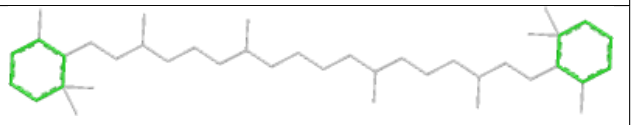


Bond angles

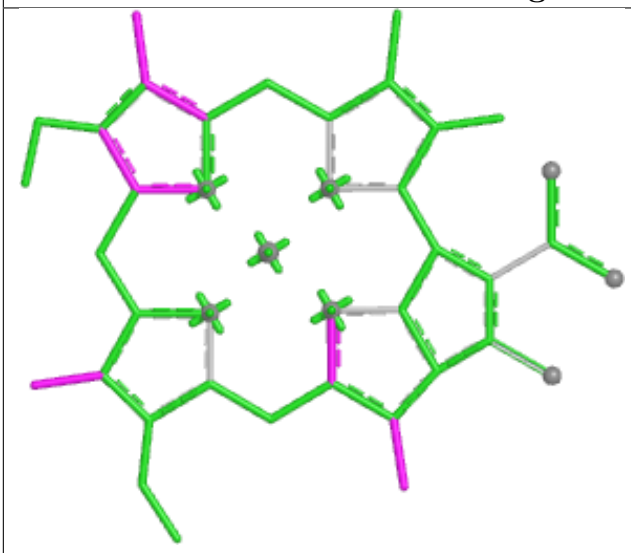


Torsions



Rings

Ligand CLA 3 617



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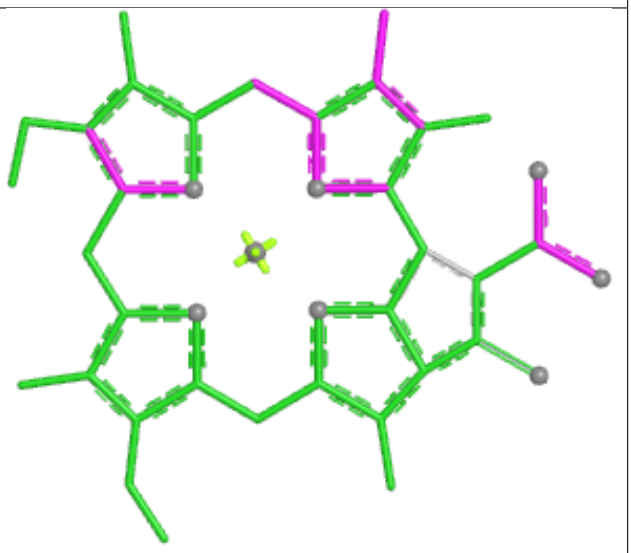
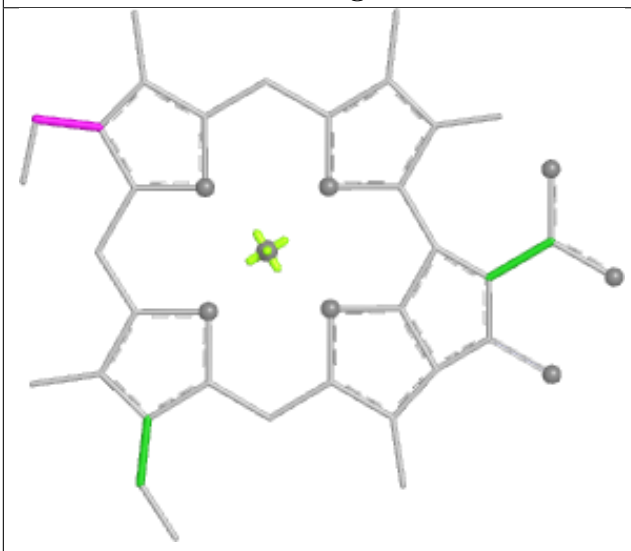
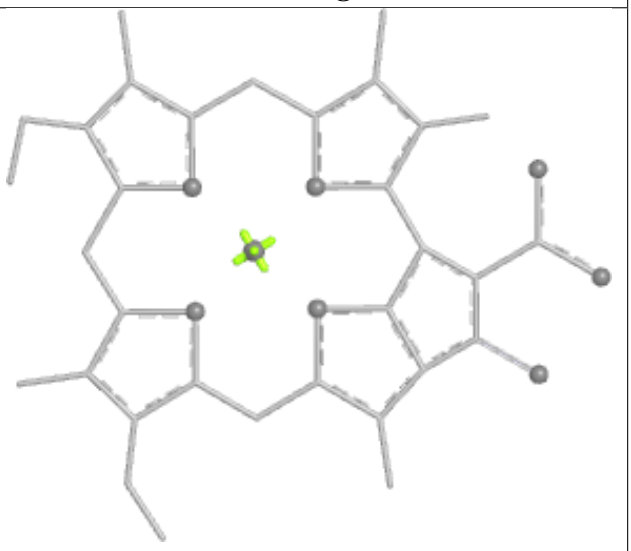


Bond angles

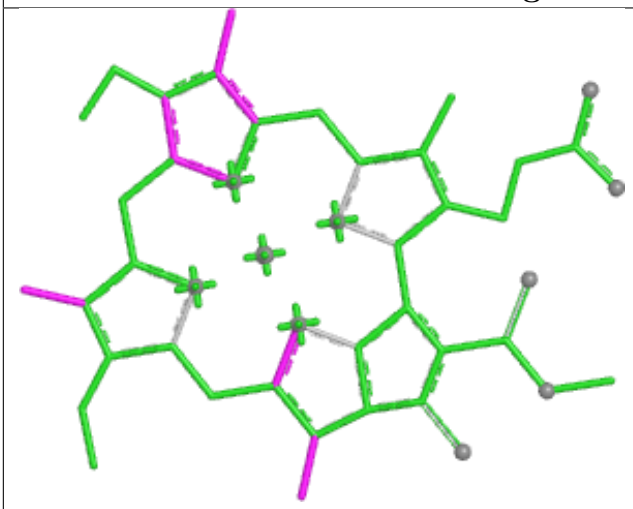


Torsions



Rings

Ligand CLA K 206



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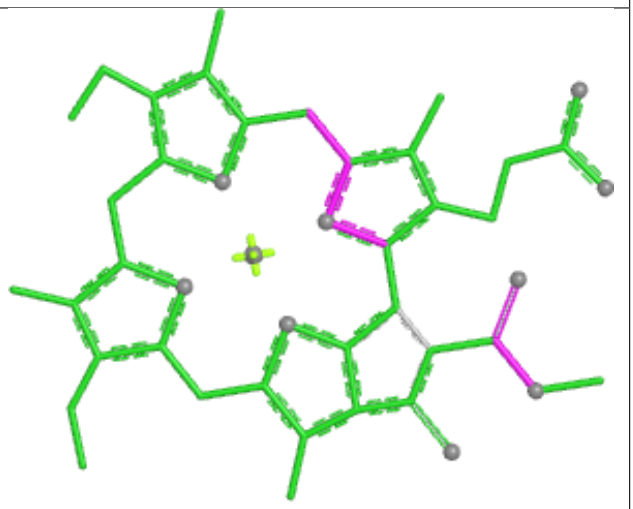
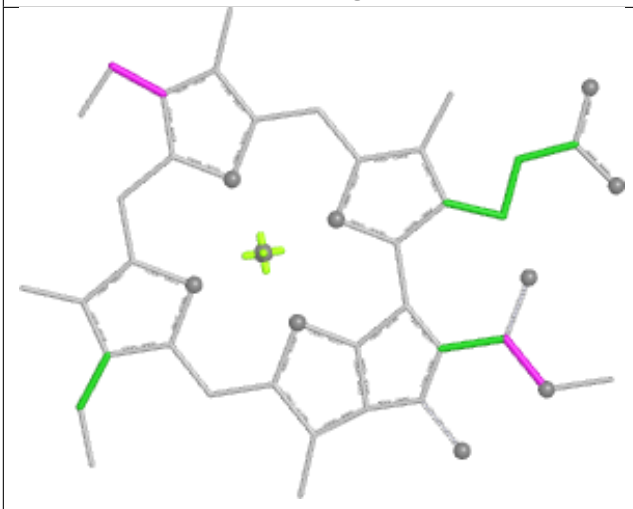


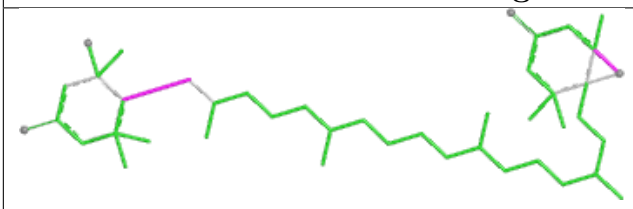
Bond angles



Torsions

Rings

Ligand NEX V 1623



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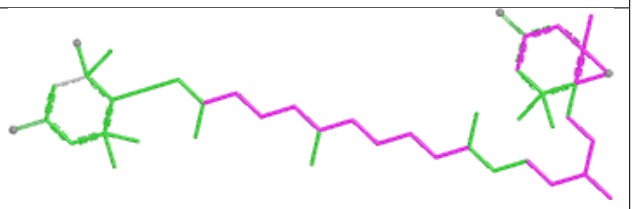

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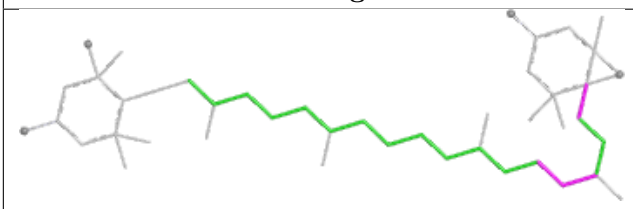

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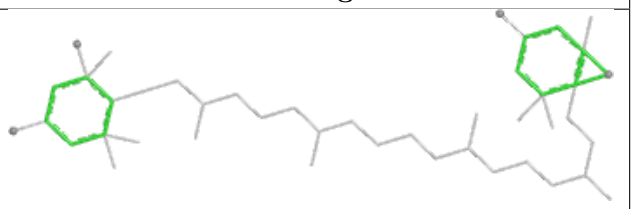
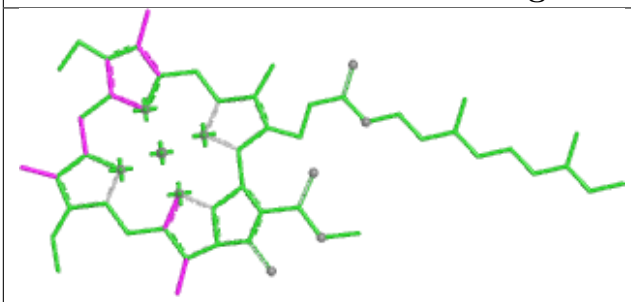


Rings

Ligand CLA 4 614



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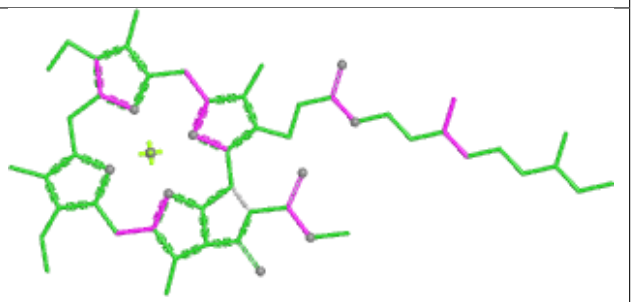

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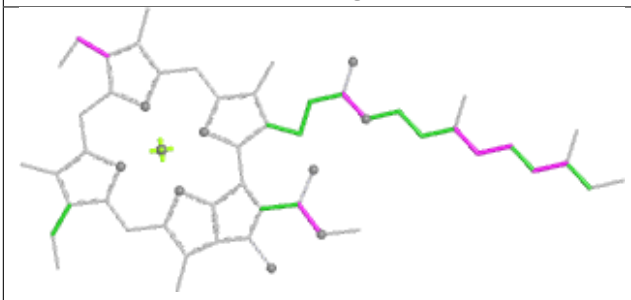

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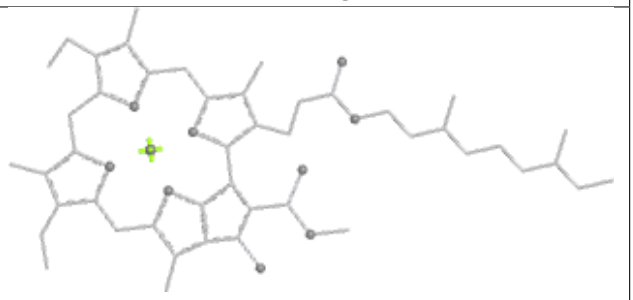
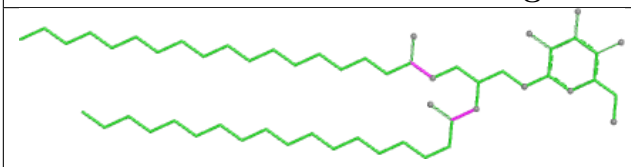


Rings

Ligand LMG 9 625



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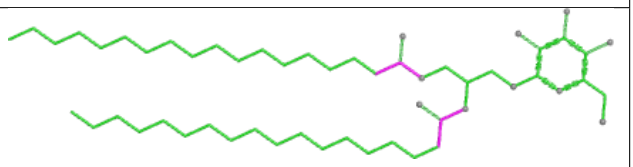

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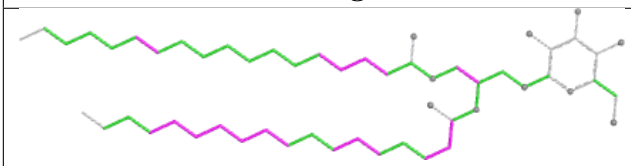

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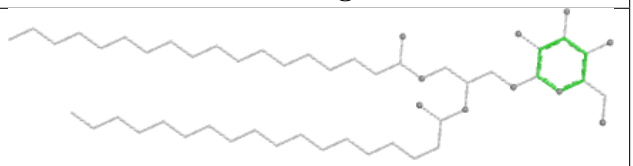
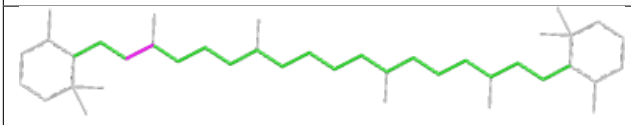


Rings

Ligand BCR L 305

Bond lengths

Bond angles



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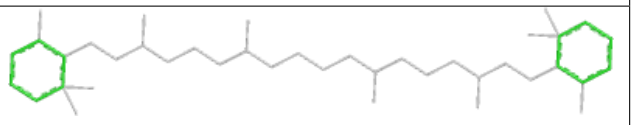
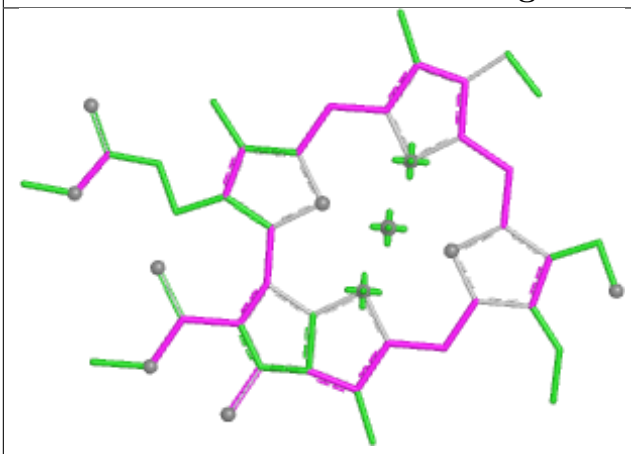


Rings

Ligand CHL W 608



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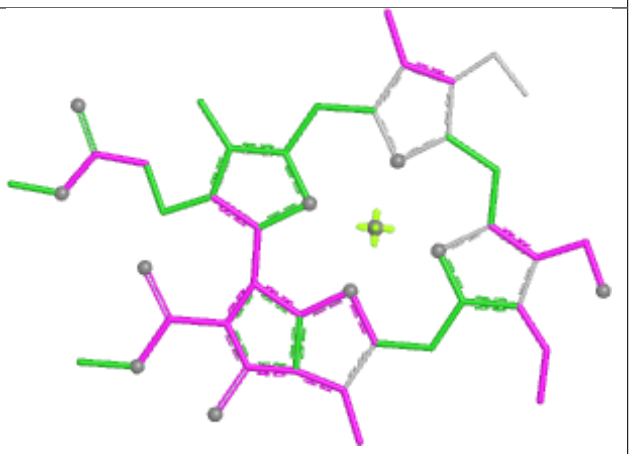
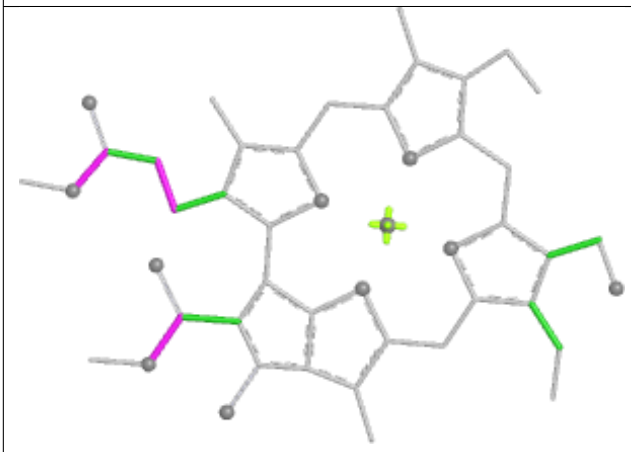


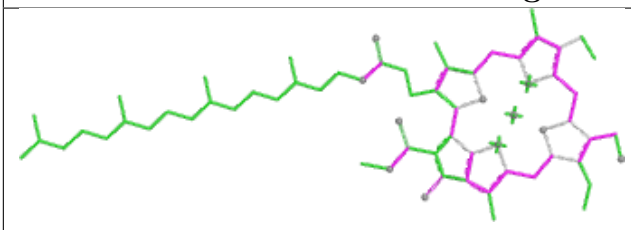
Bond angles



Torsions

Rings

Ligand CHL Y 601



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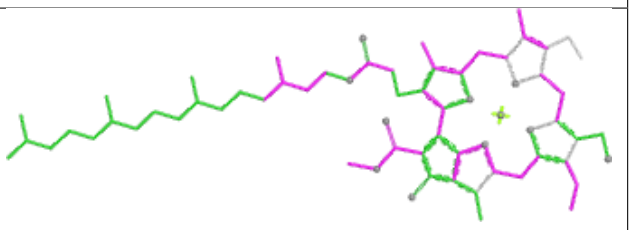
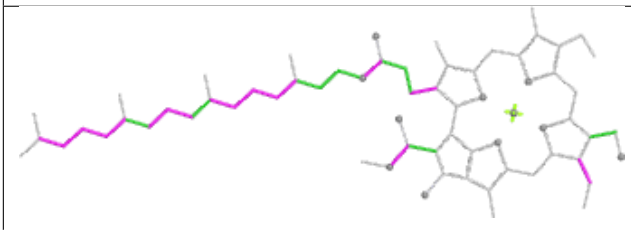
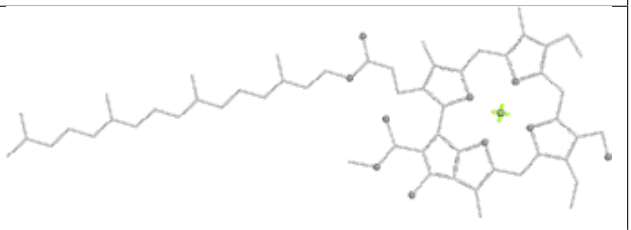


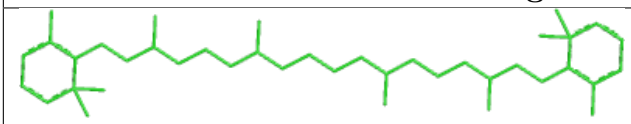
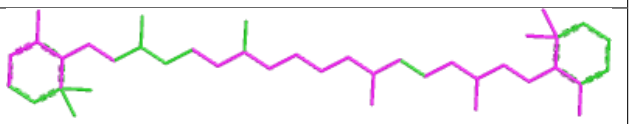
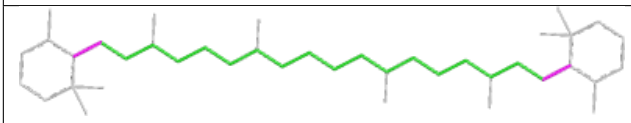
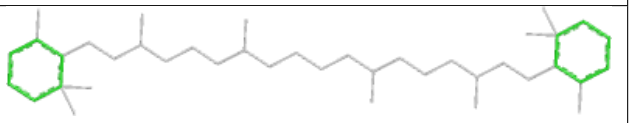
Bond angles

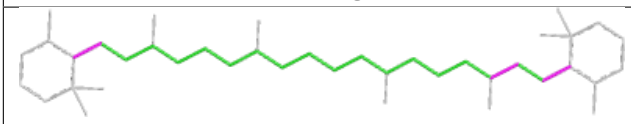
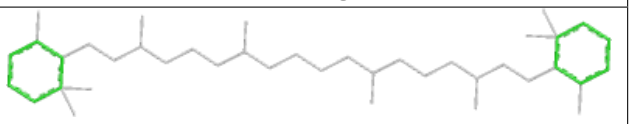


Torsions

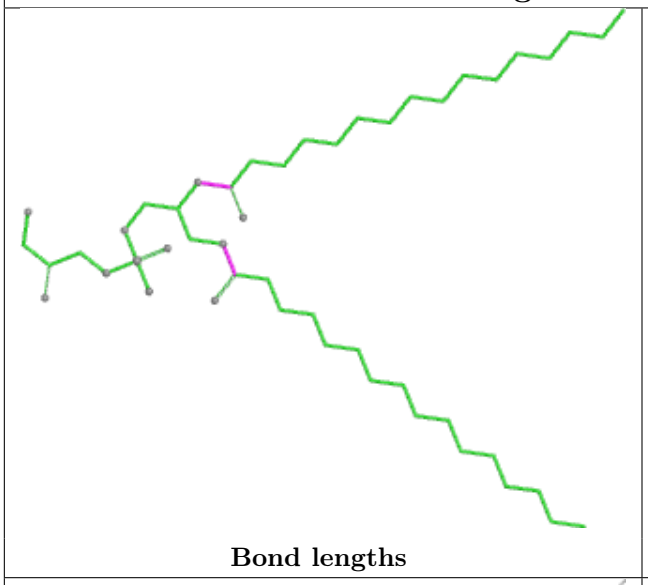


Rings

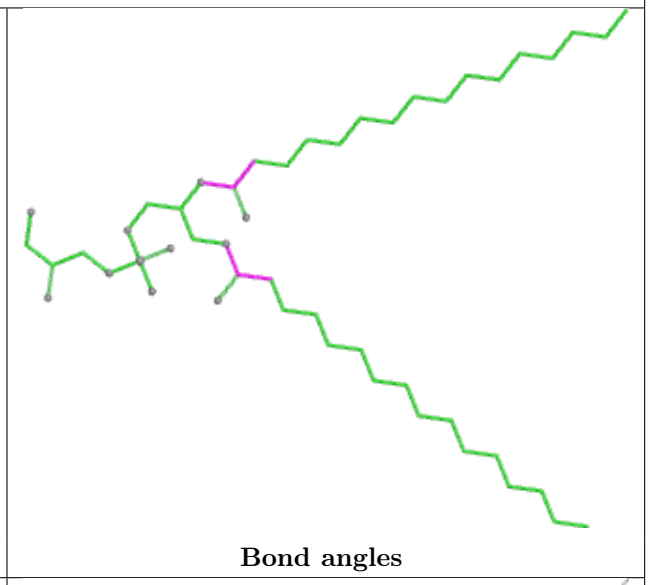
Ligand BCR 8 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 849	
Bond lengths	Bond angles
 Torsions	 Rings

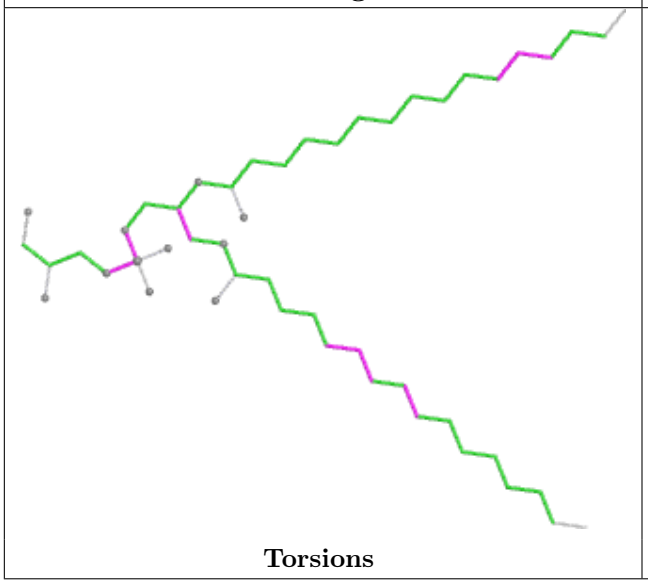
Ligand LHG X 2630



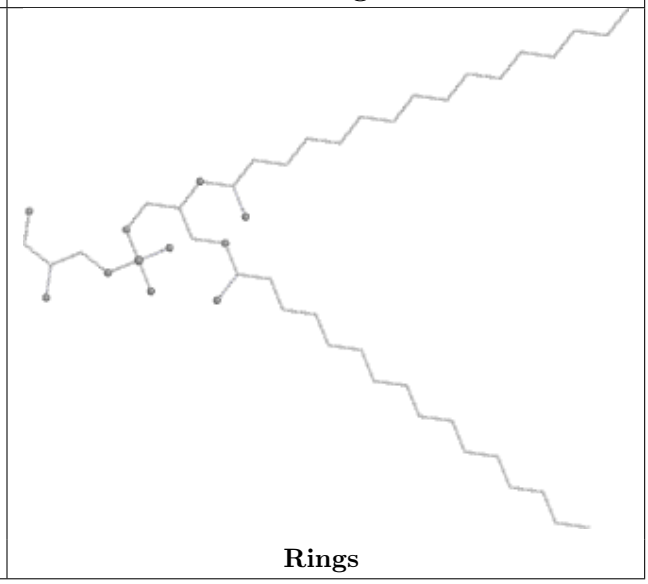
Bond lengths



Bond angles

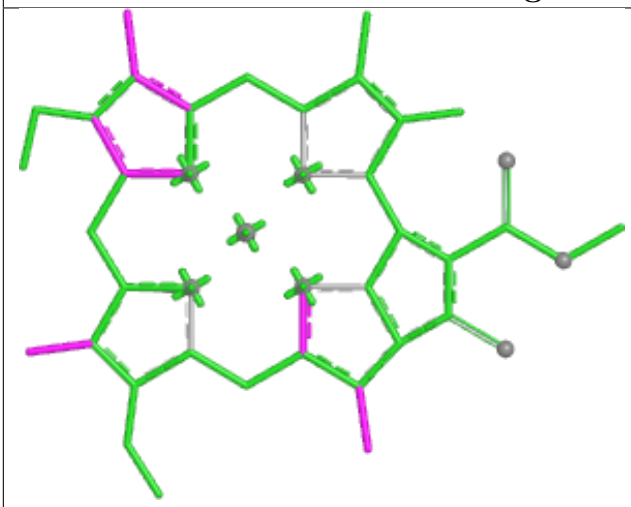


Torsions

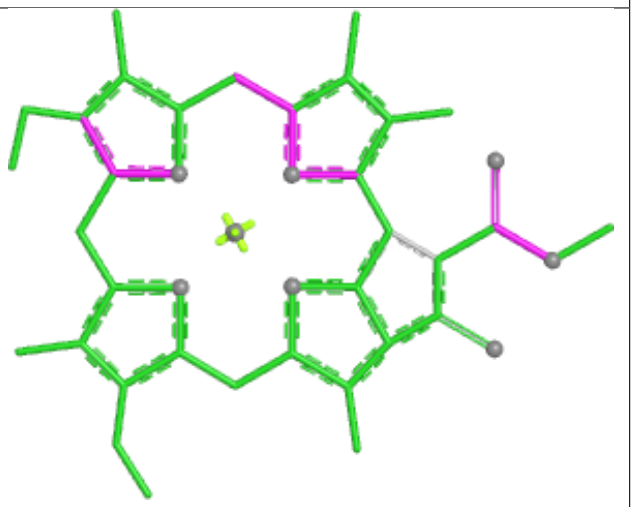


Rings

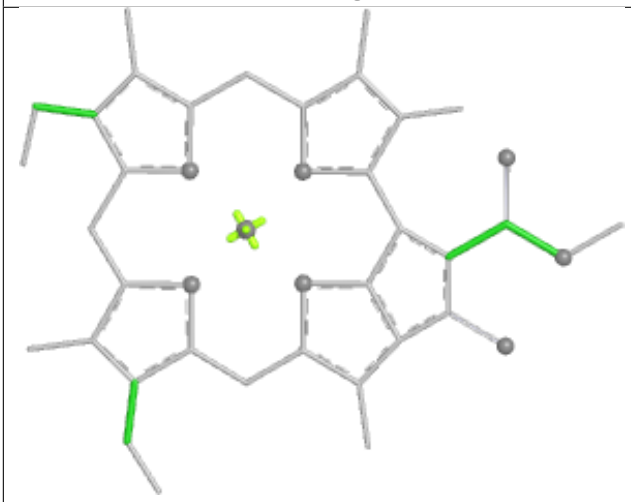
Ligand CLA B 804



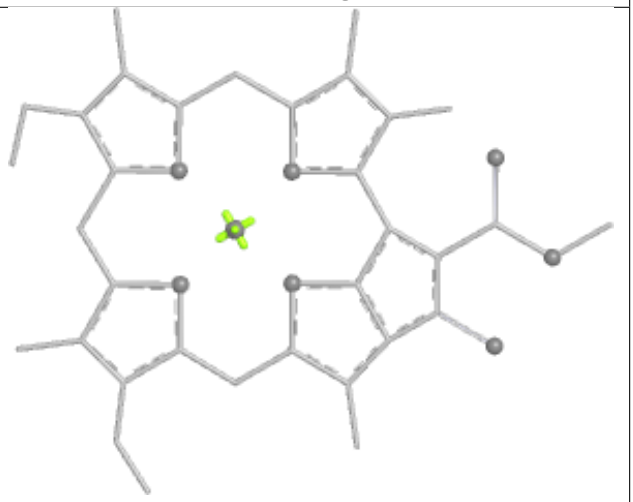
Bond lengths



Bond angles

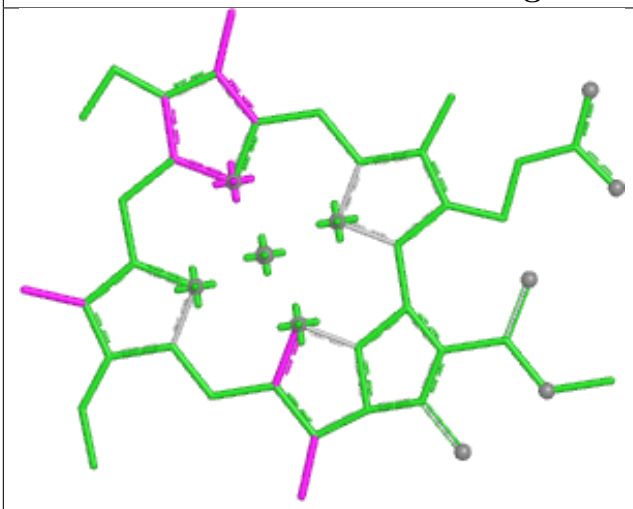


Torsions



Rings

Ligand CLA V 614



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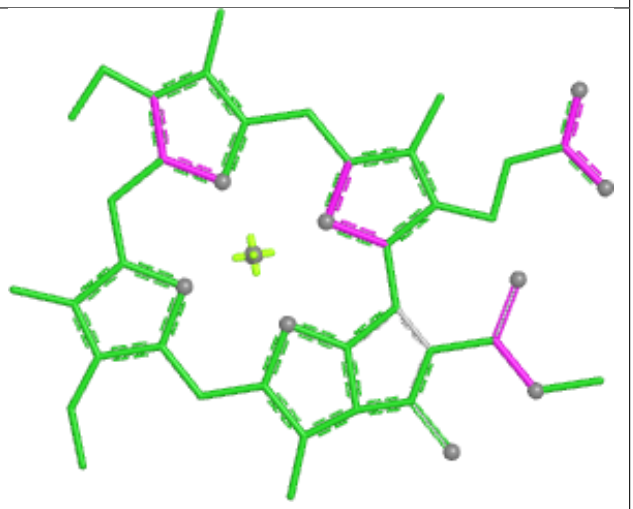
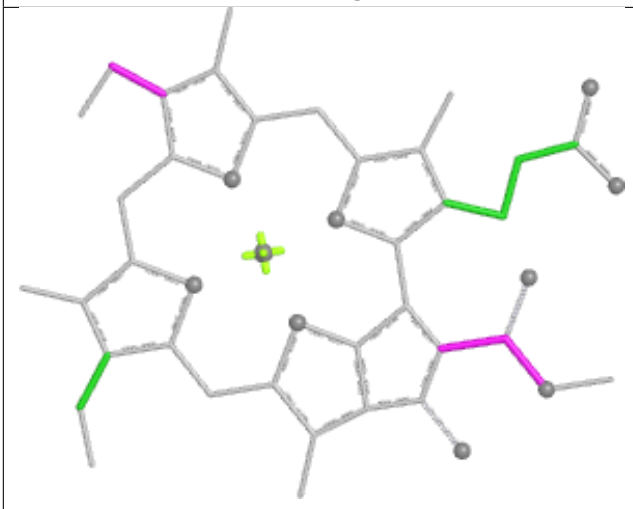


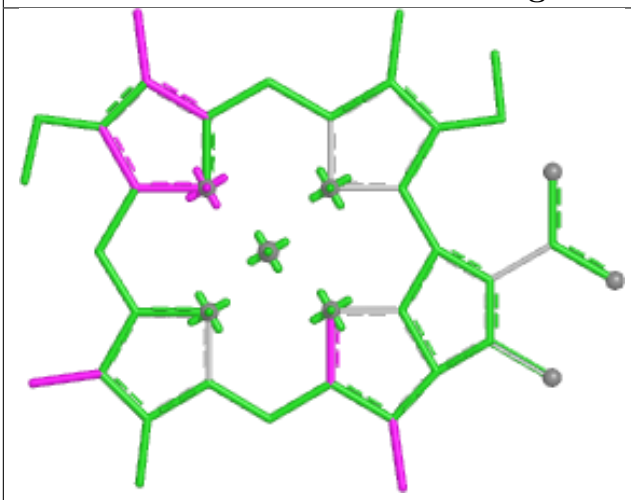
Bond angles



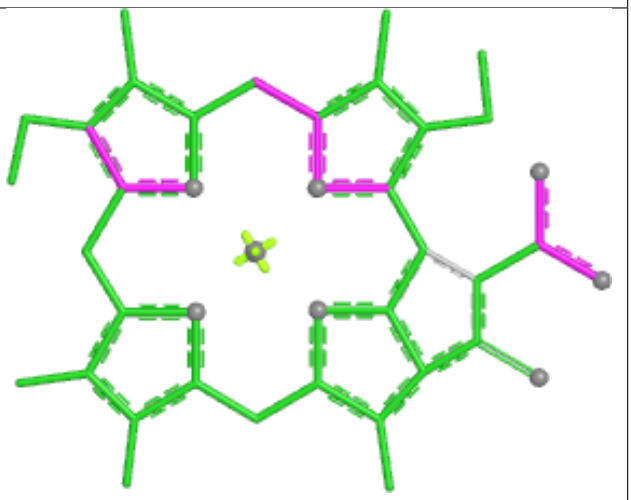
Torsions

Rings

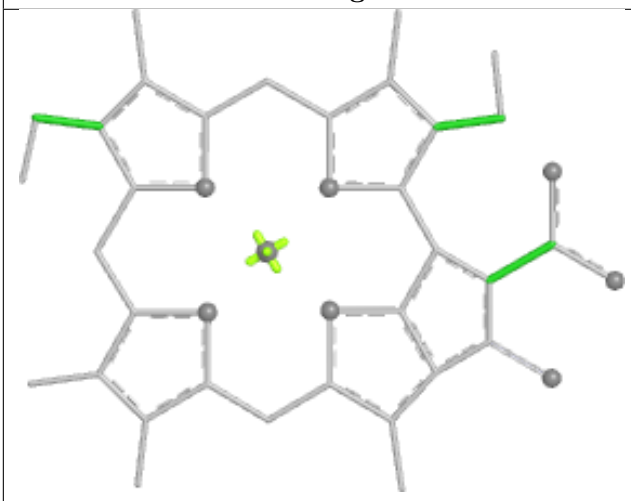
Ligand CLA 6 606



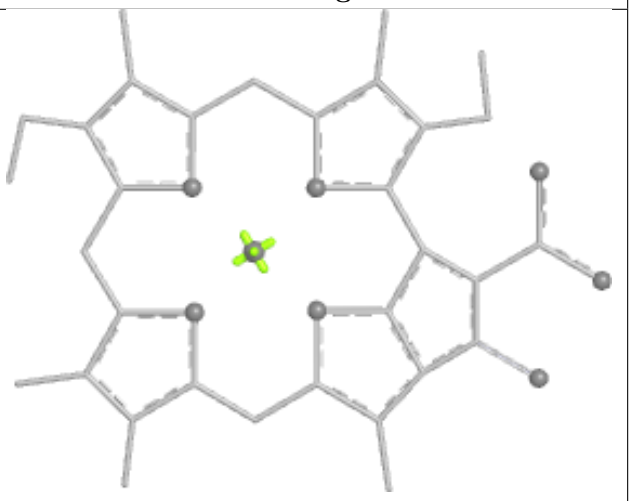
Bond lengths



Bond angles

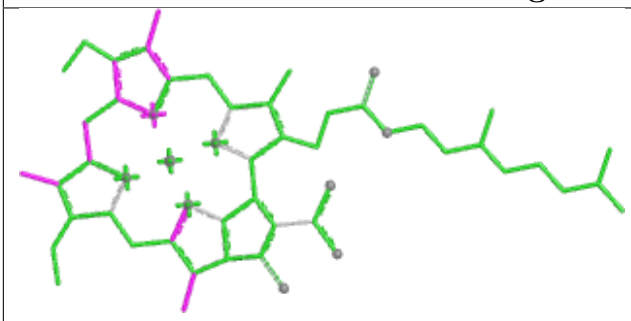


Torsions

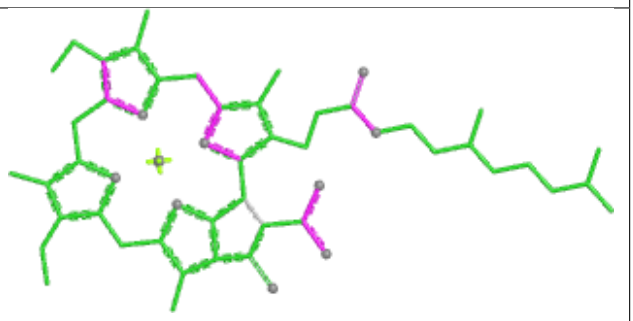


Rings

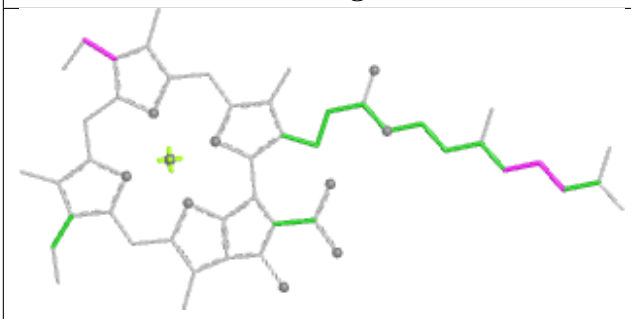
Ligand CLA 1 601



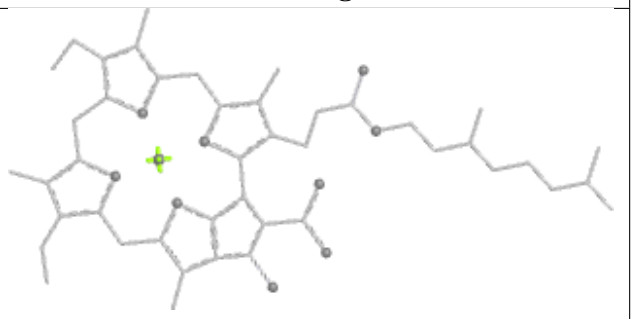
Bond lengths



Bond angles

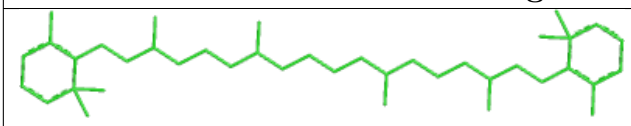


Torsions



Rings

Ligand BCR 9 621



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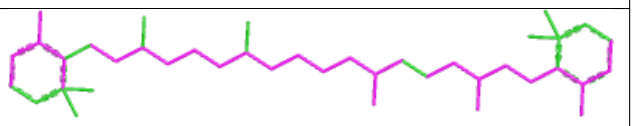
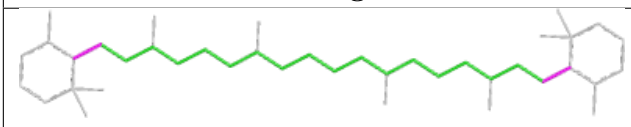
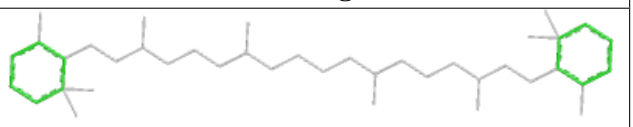


Bond angles

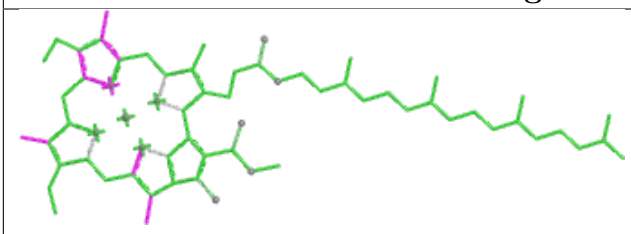


Torsions



Rings

Ligand CLA B 828



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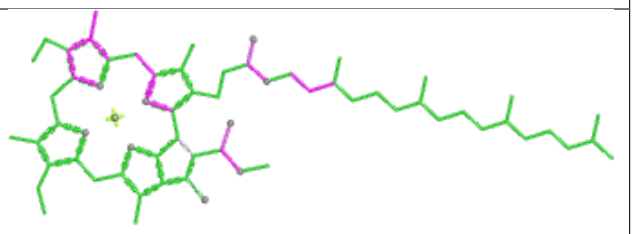
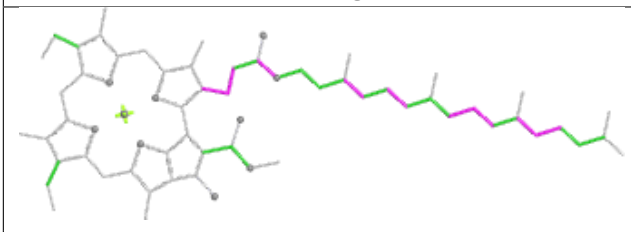


Bond angles



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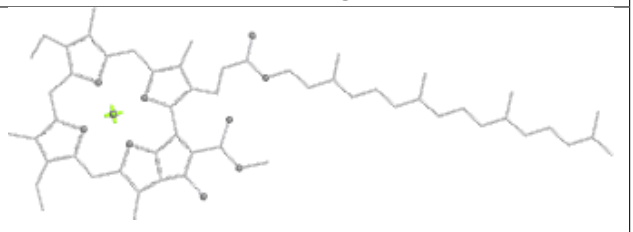
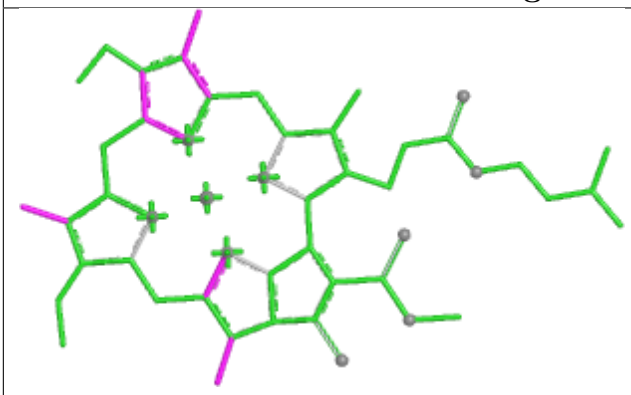


Rings

Ligand CLA A 832



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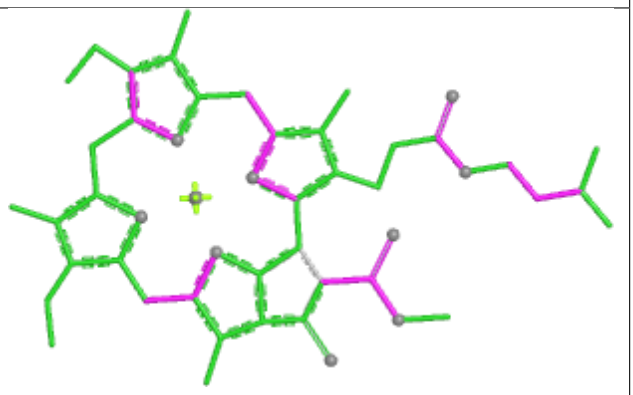
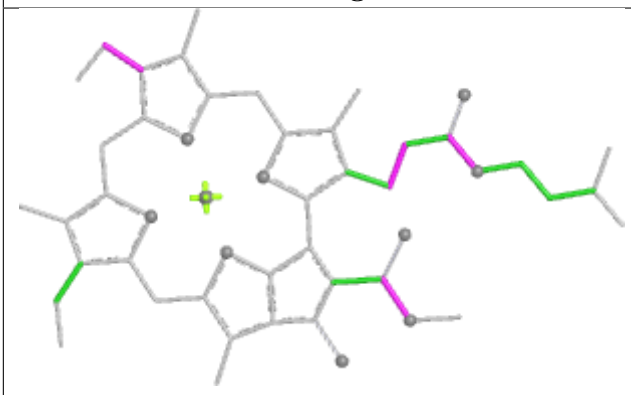


Bond angles



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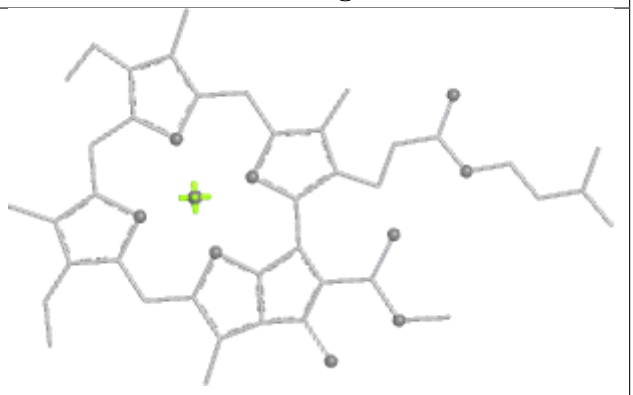
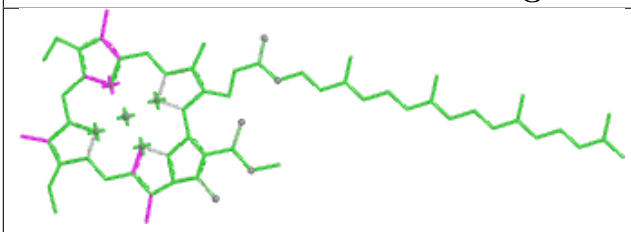


Rings

Ligand CLA A 836



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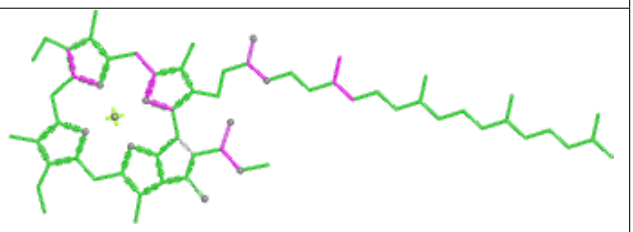
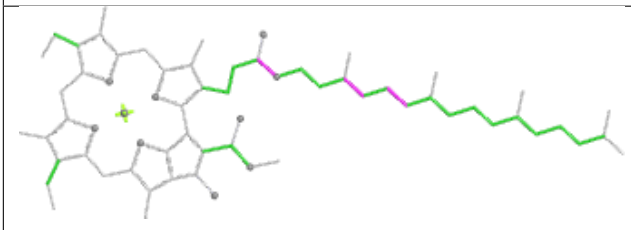


Bond angles



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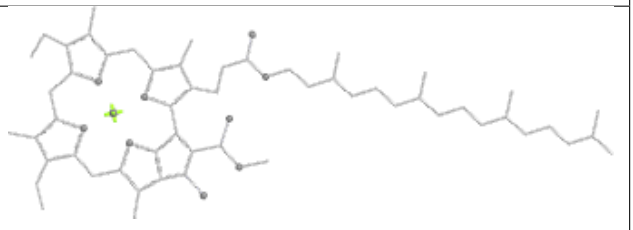
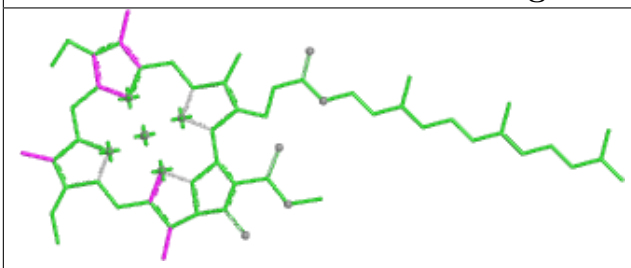
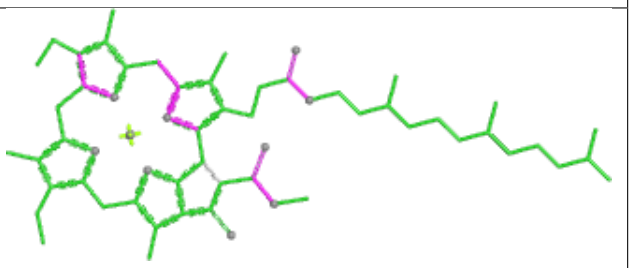
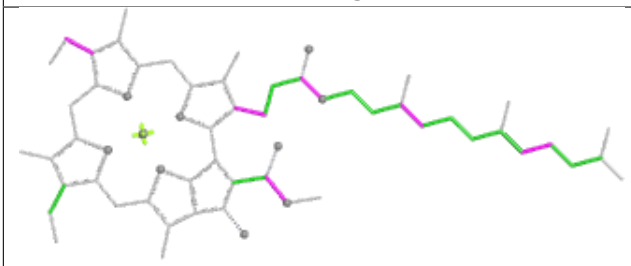
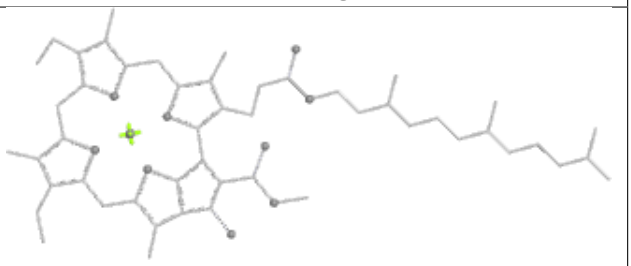


Rings

Ligand CLA 6 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

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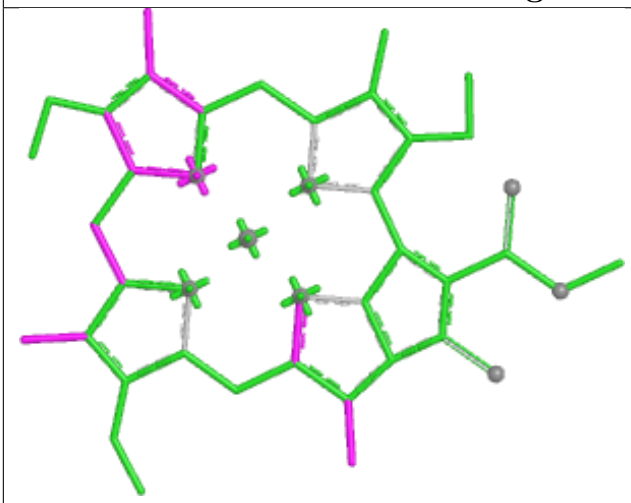
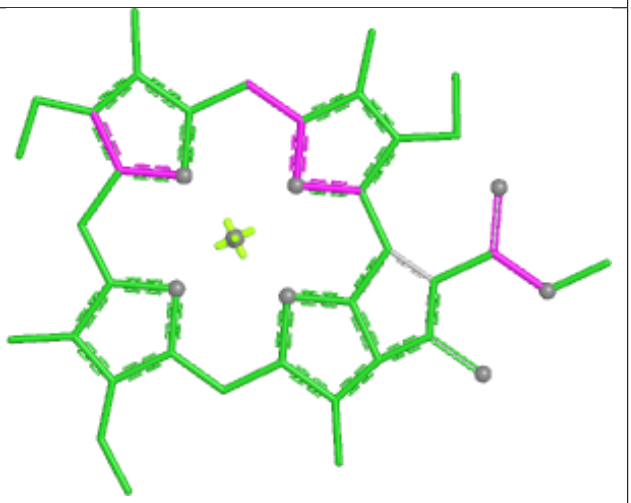
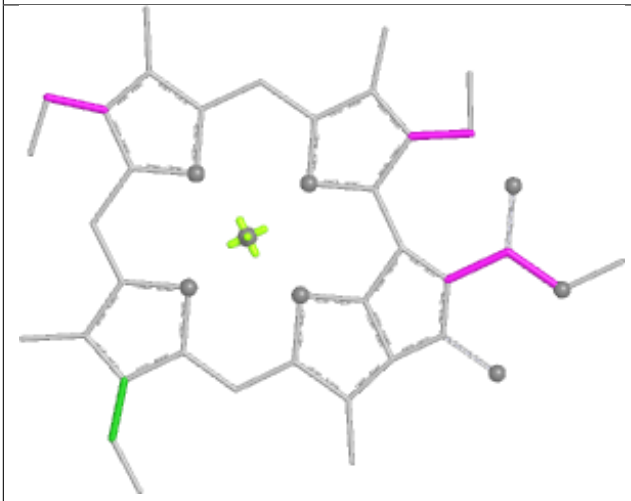
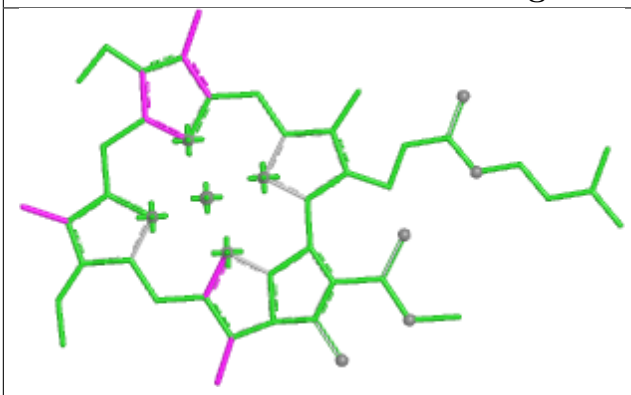
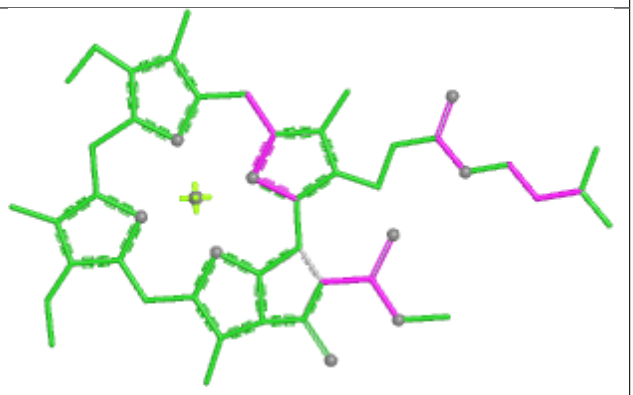
 Bond lengths	 Bond angles
 Torsions	Rings

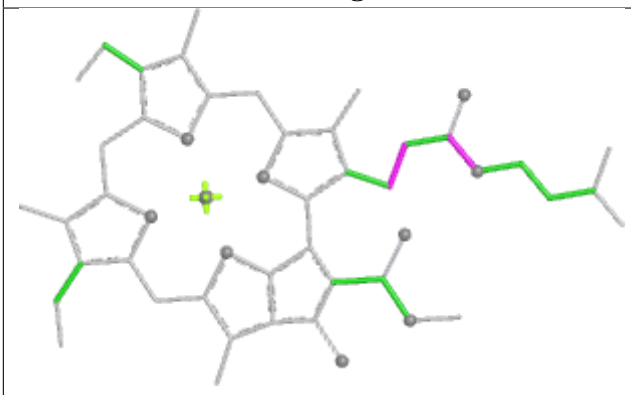
Ligand CLA 8 604



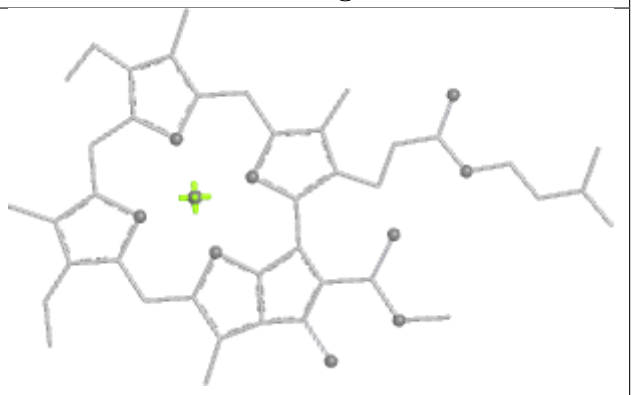
Bond lengths



Bond angles

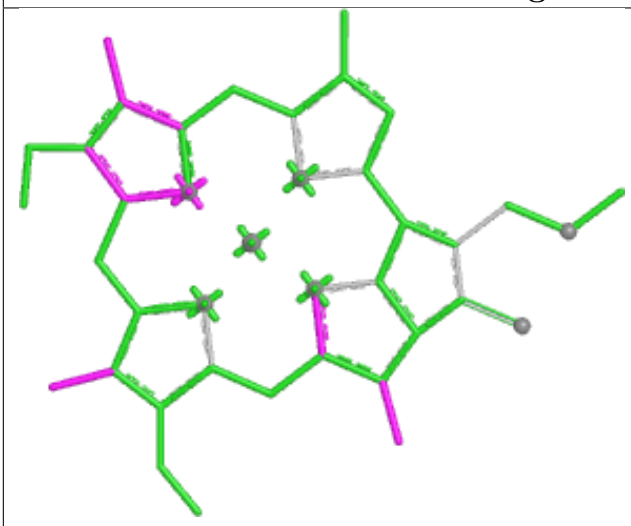


Torsions



Rings

Ligand CLA 1 606



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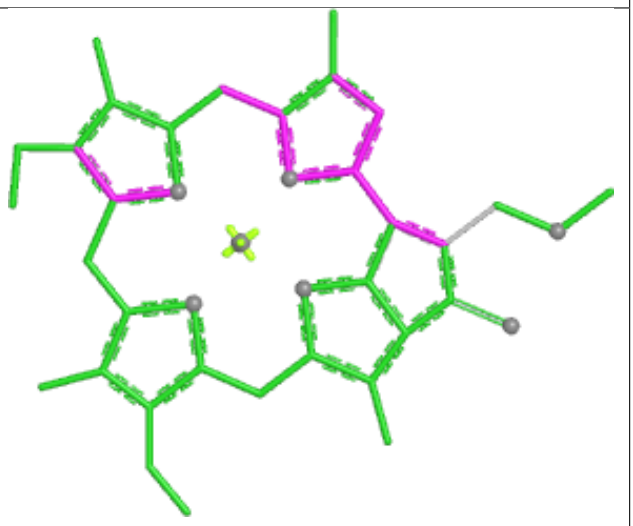

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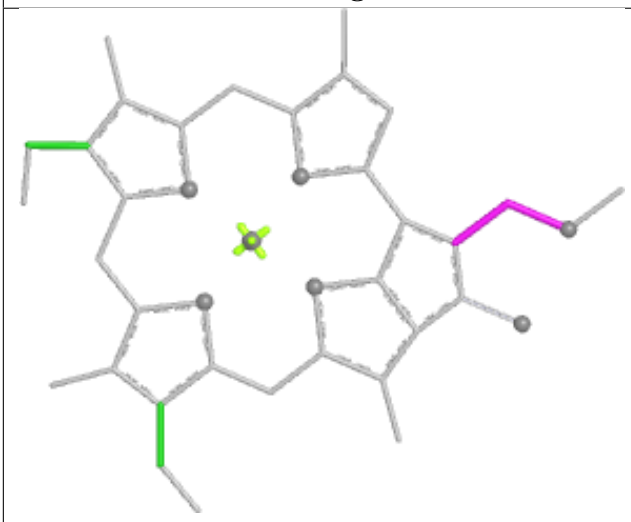
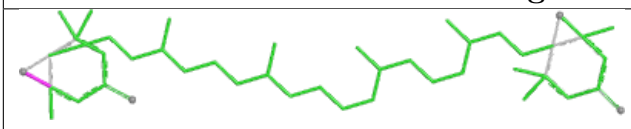


Torsions

Rings

Ligand XAT a 618



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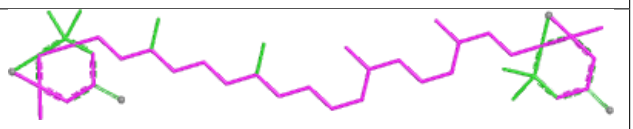

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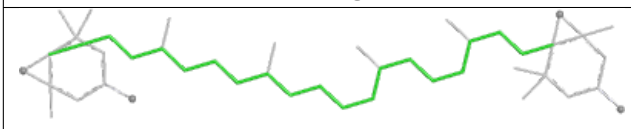
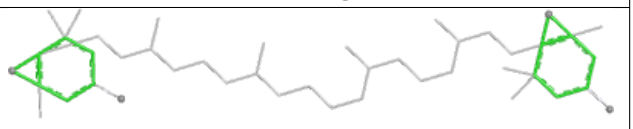
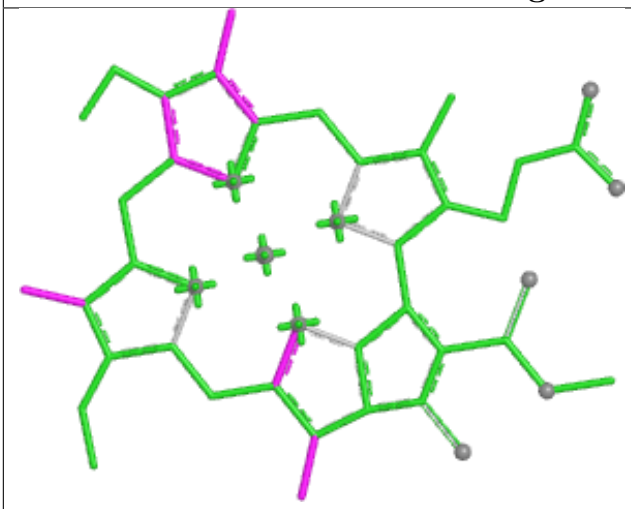


Torsions



Rings

Ligand CLA a 612



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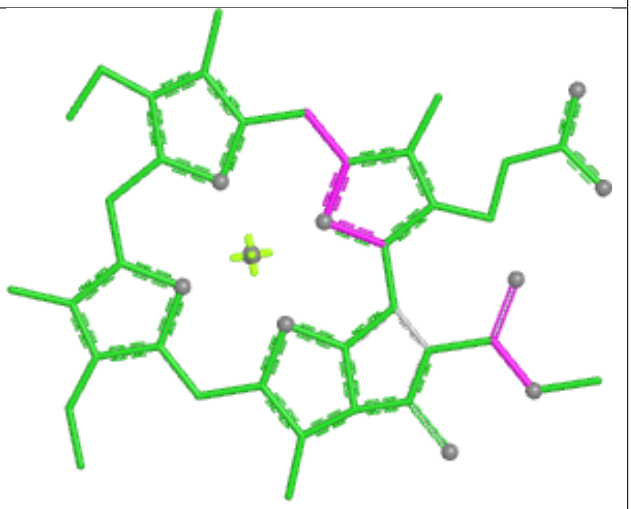
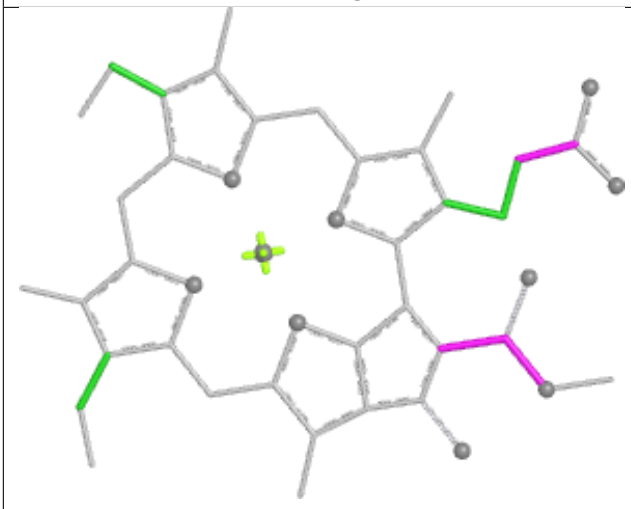


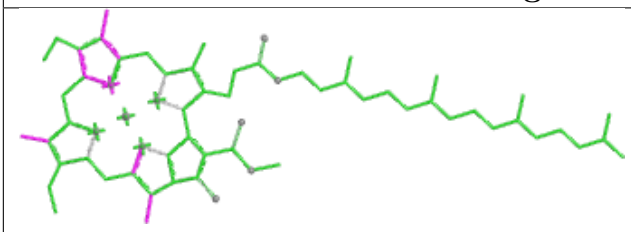
Bond angles



Torsions

Rings

Ligand CLA A 842



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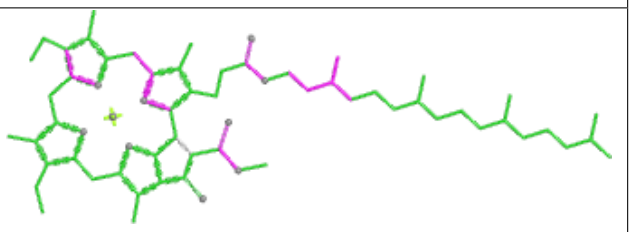
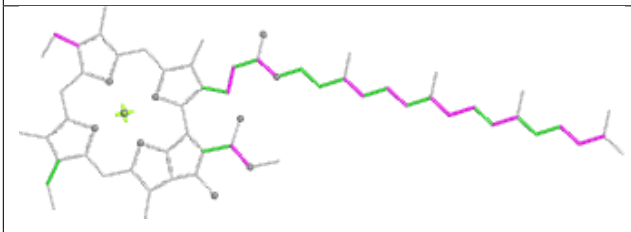


Bond angles



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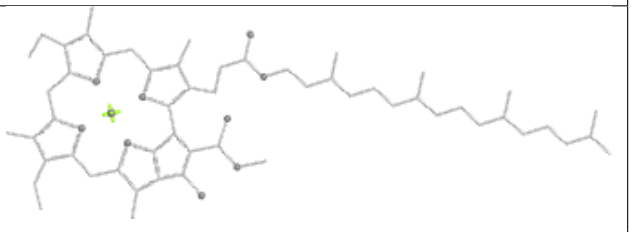
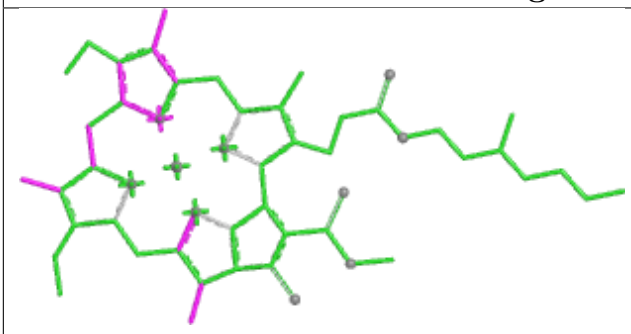


Rings

Ligand CLA 8 614



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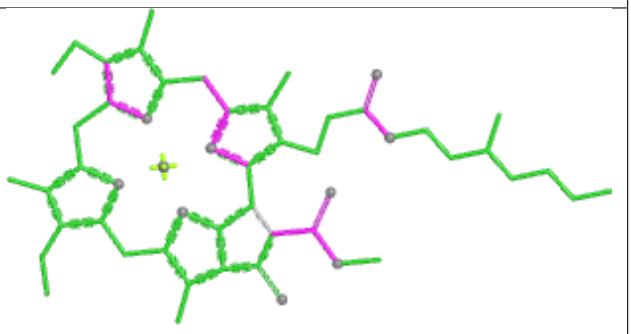
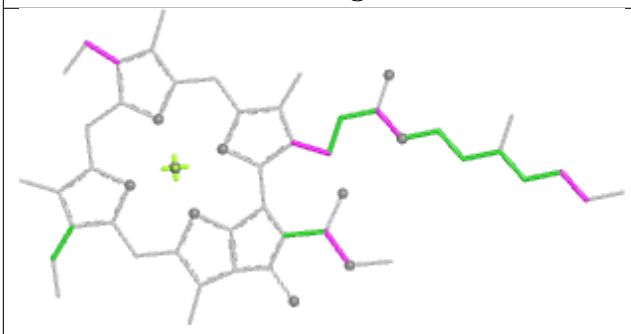


Bond angles



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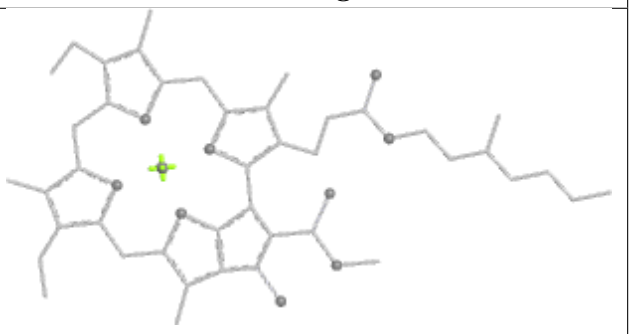
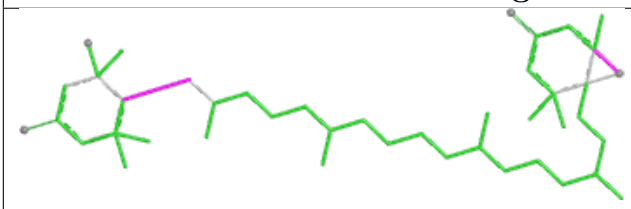
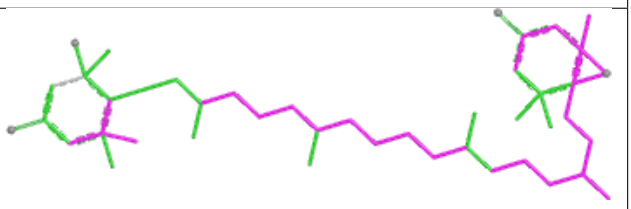


Rings

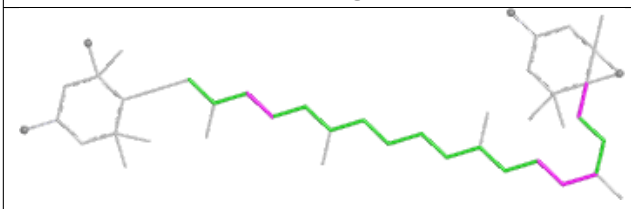
Ligand NEX U 1623



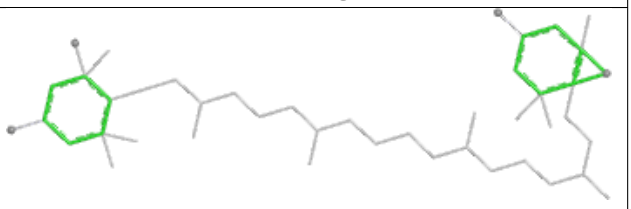
Bond lengths



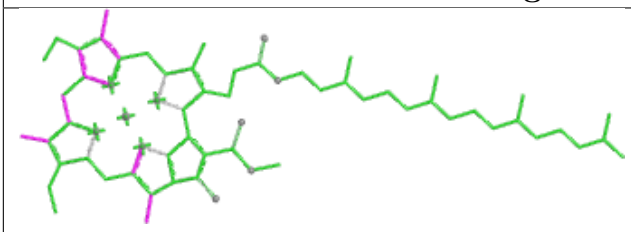
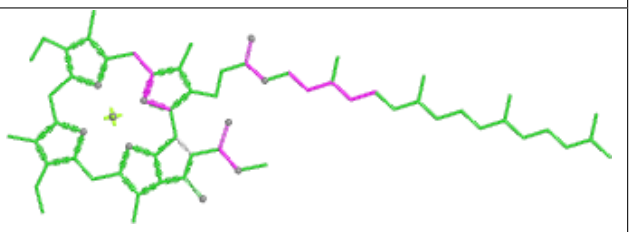
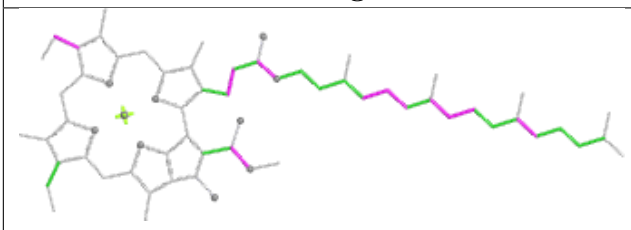
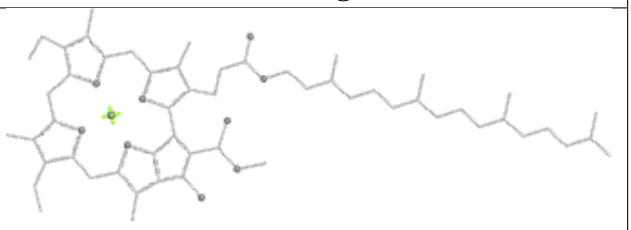
Bond angles

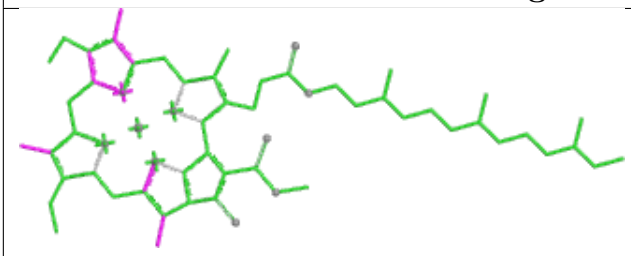
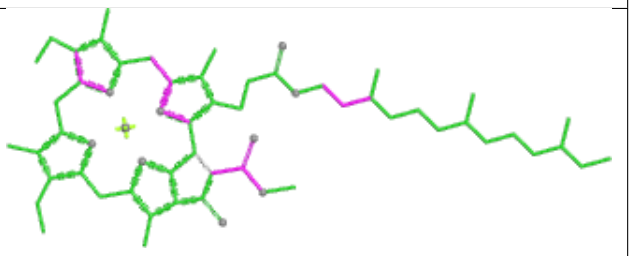
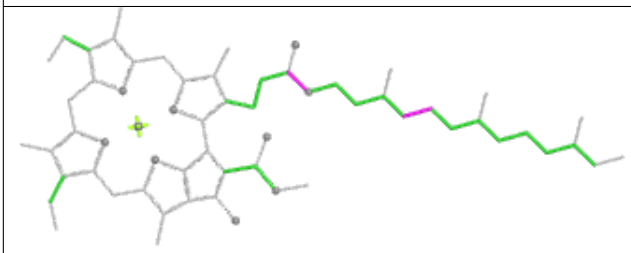
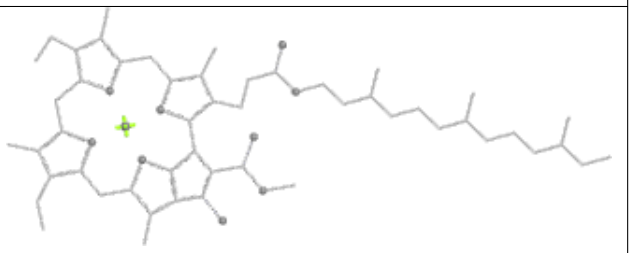


Torsions

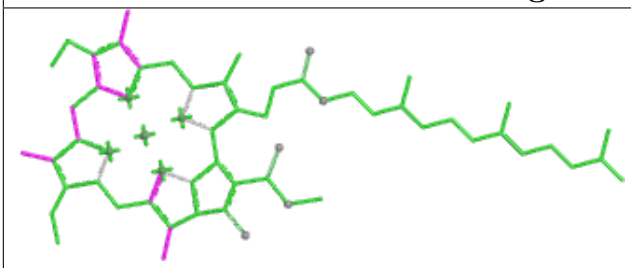


Rings

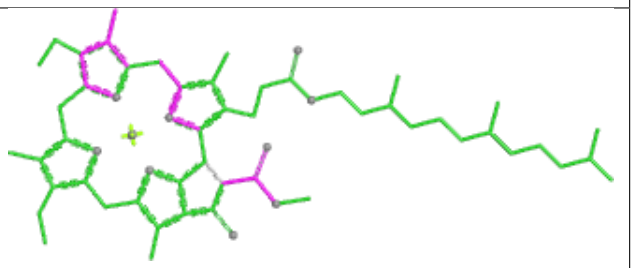
Ligand CLA Y 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

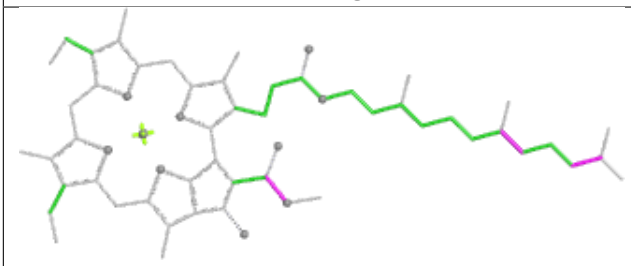
Ligand CLA 4 602



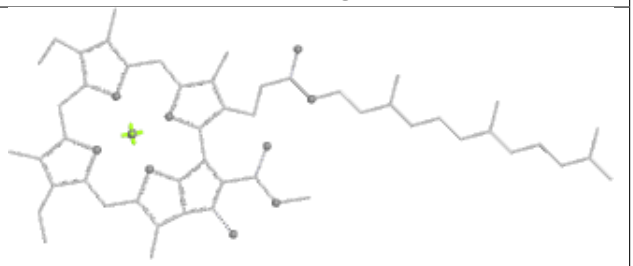
Bond lengths



Bond angles

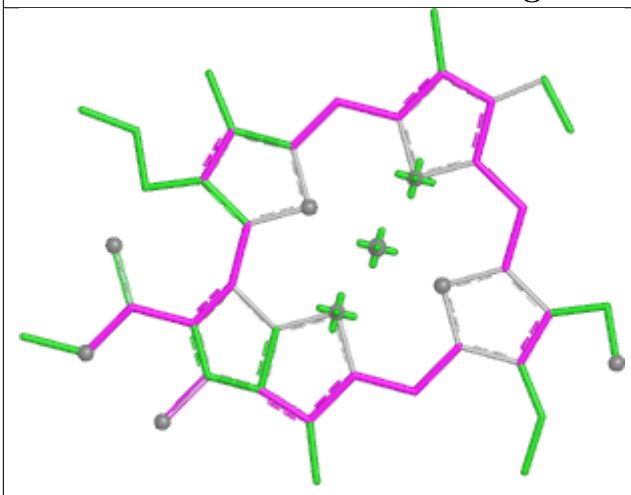


Torsions

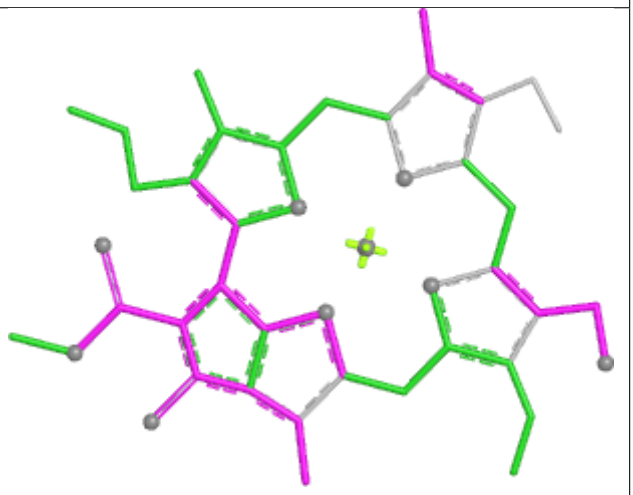


Rings

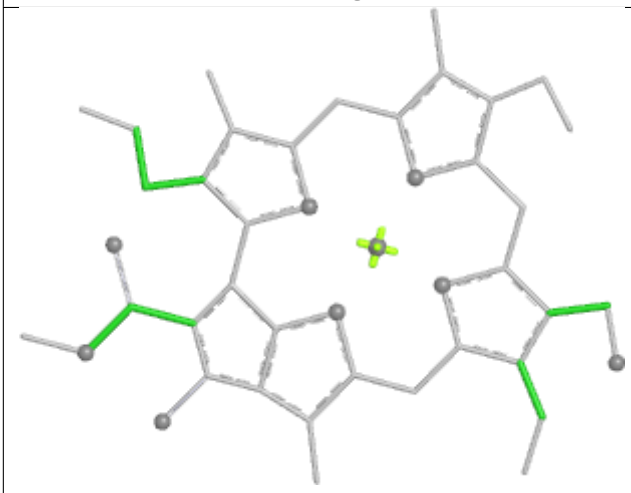
Ligand CHL V 605



Bond lengths



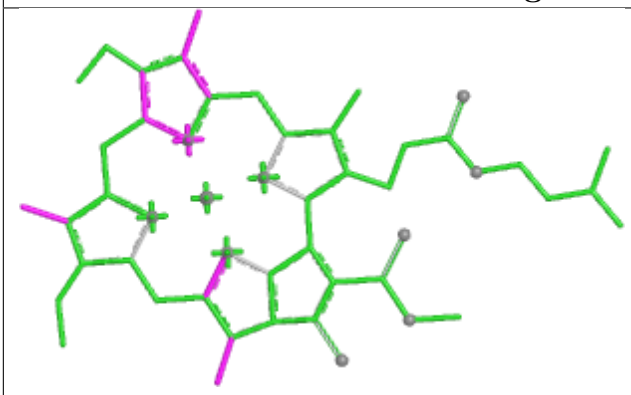
Bond angles



Torsions

Rings

Ligand CLA B 820



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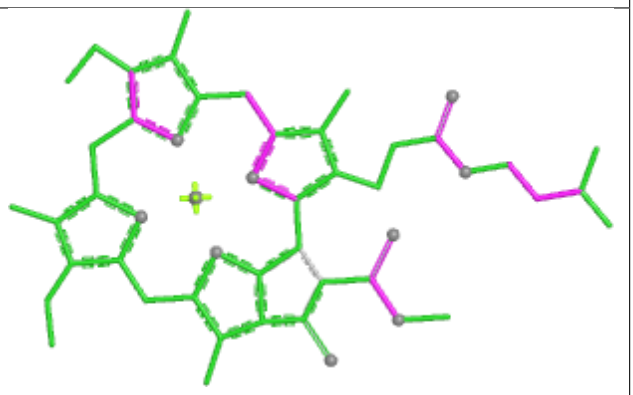
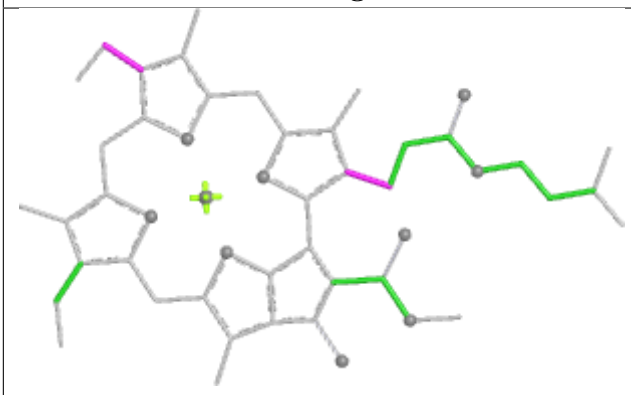
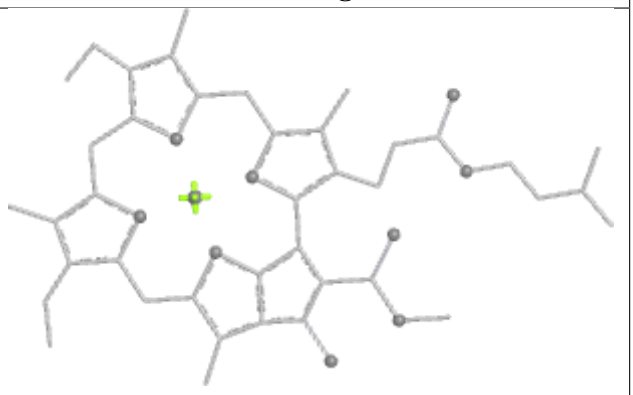


Bond angles

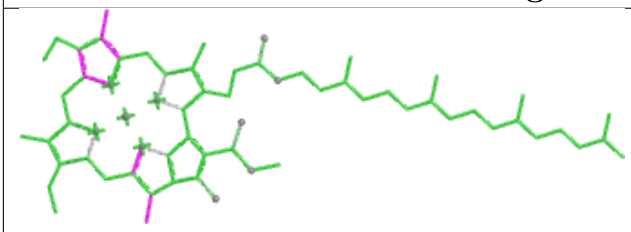


Torsions



Rings

Ligand CLA L 303



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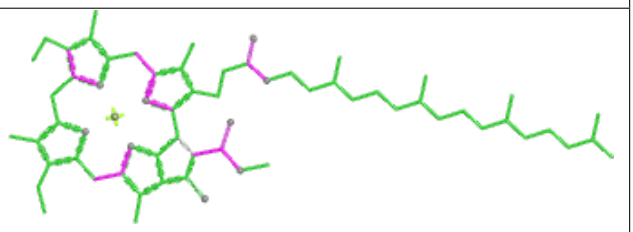
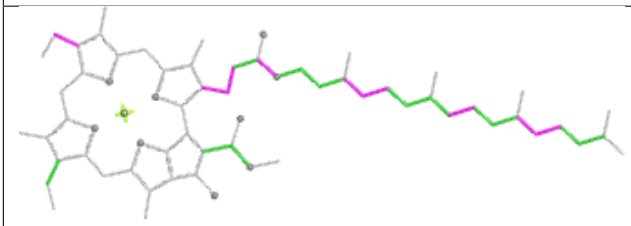


Bond angles



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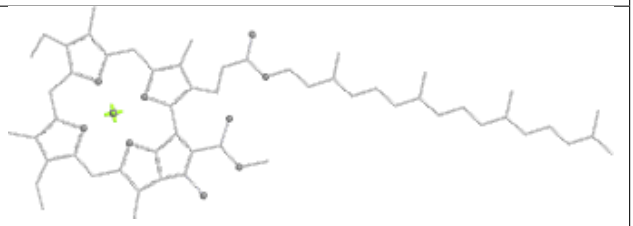
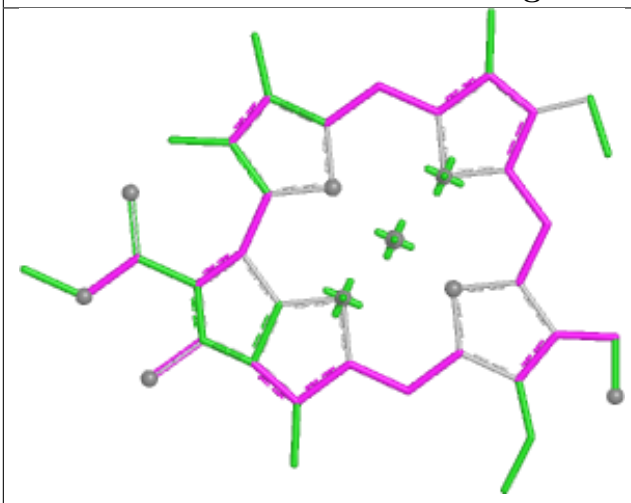


Rings

Ligand CHL Y 605



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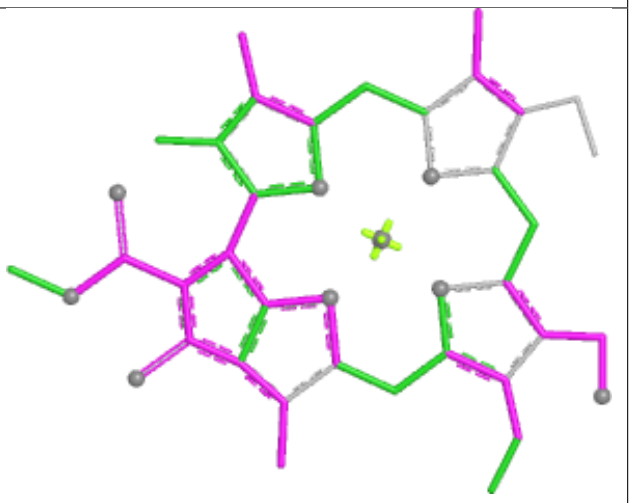
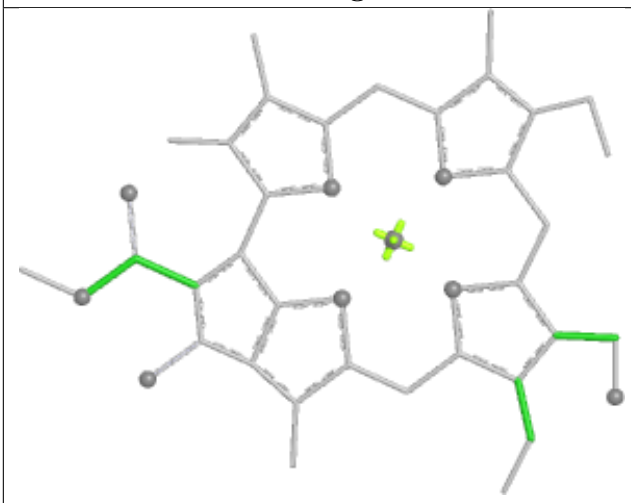
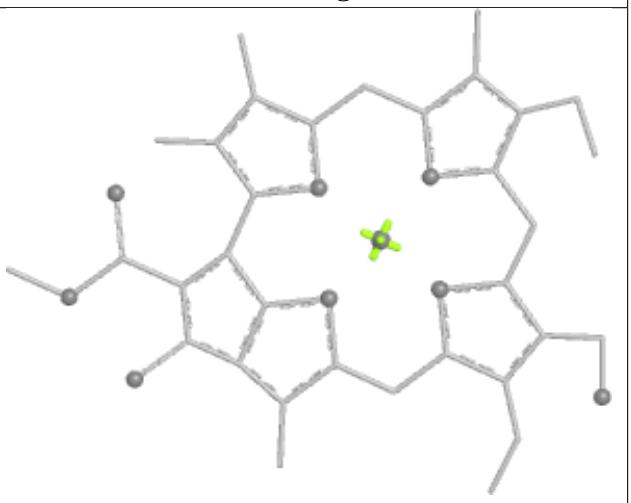


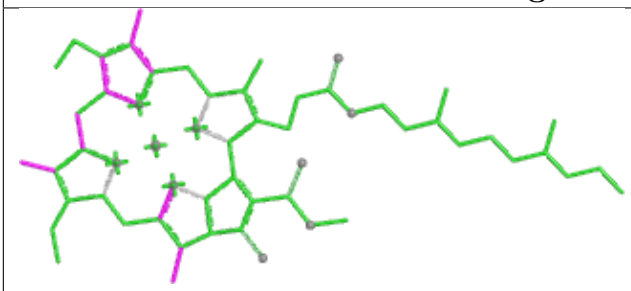
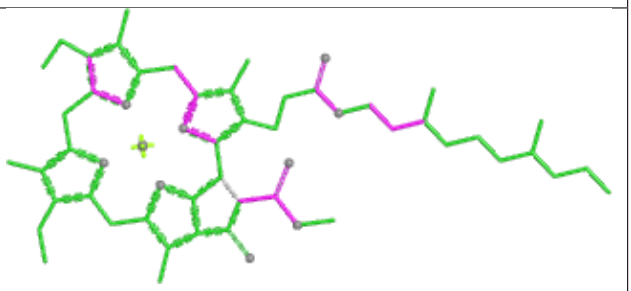
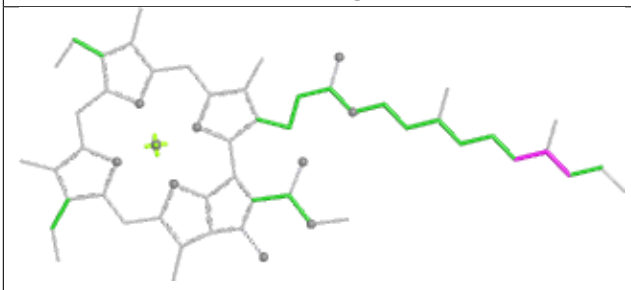
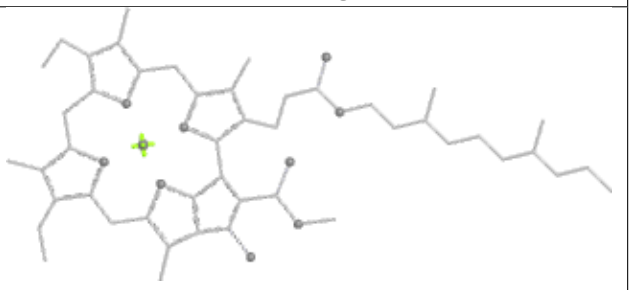
Bond angles

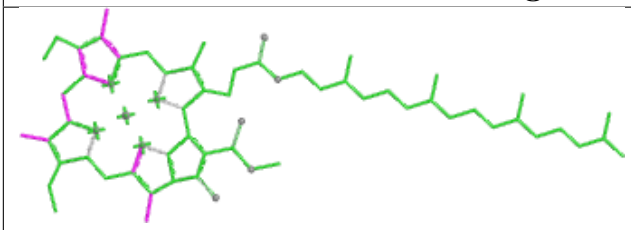
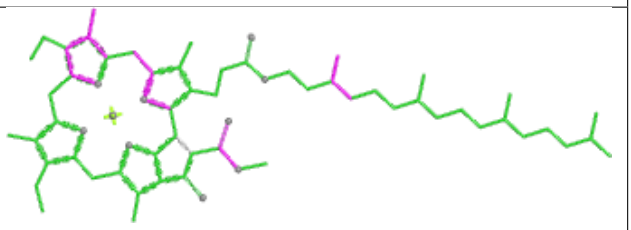
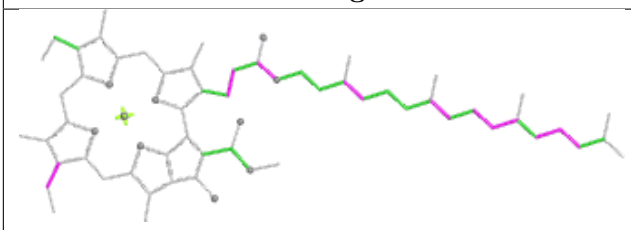
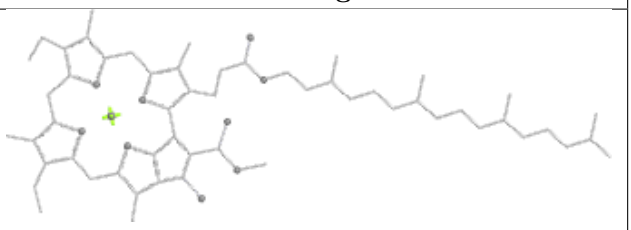


Torsions

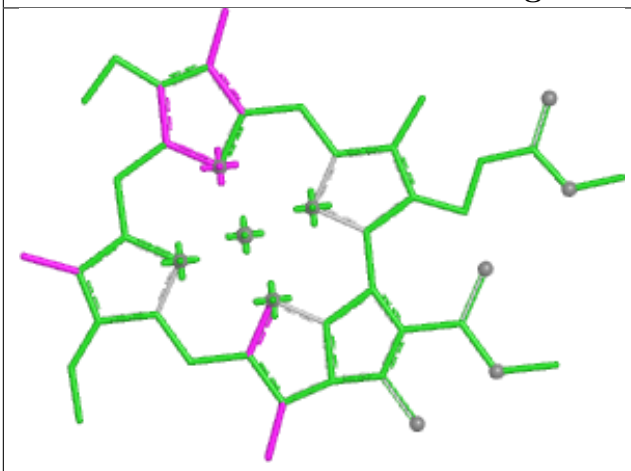


Rings

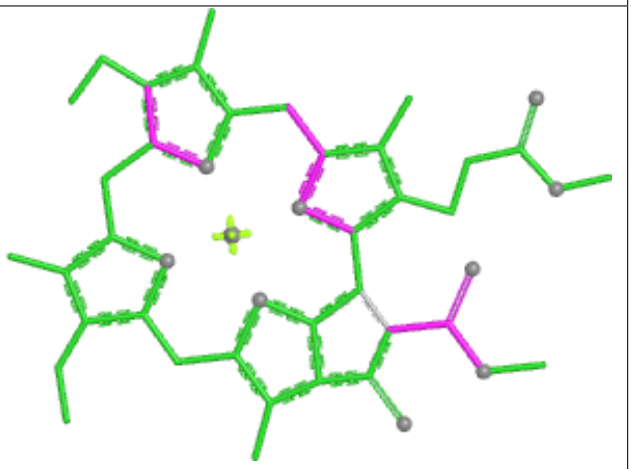
Ligand CLA 9 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

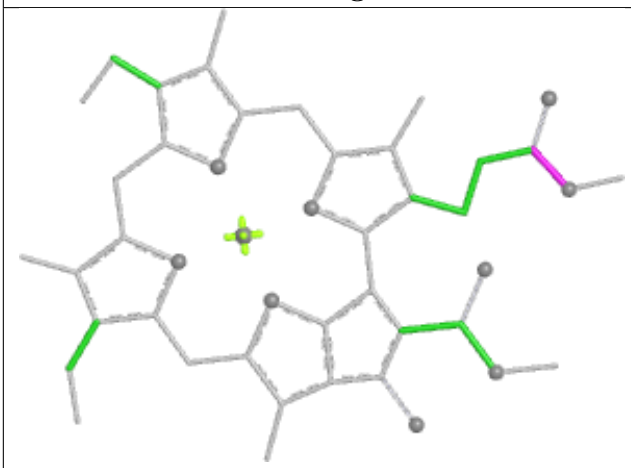
Ligand CLA B 838



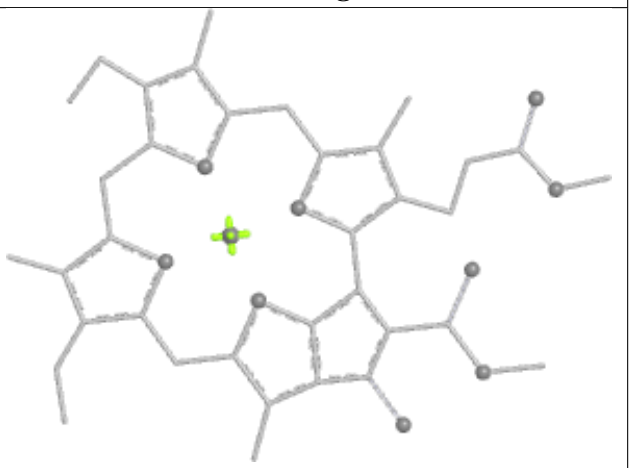
Bond lengths



Bond angles

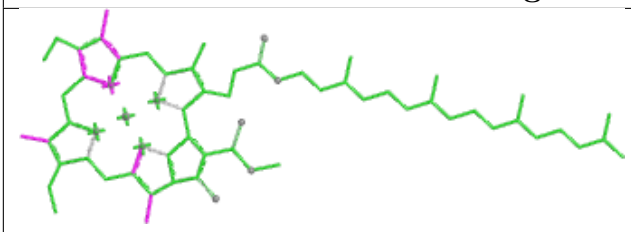


Torsions



Rings

Ligand CLA A 834



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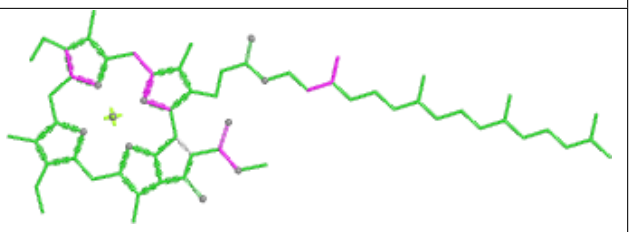
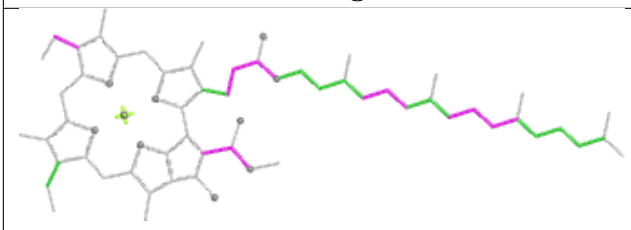
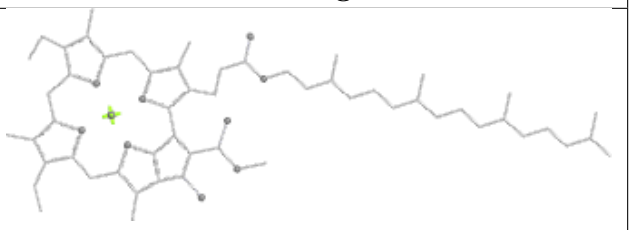


Bond angles

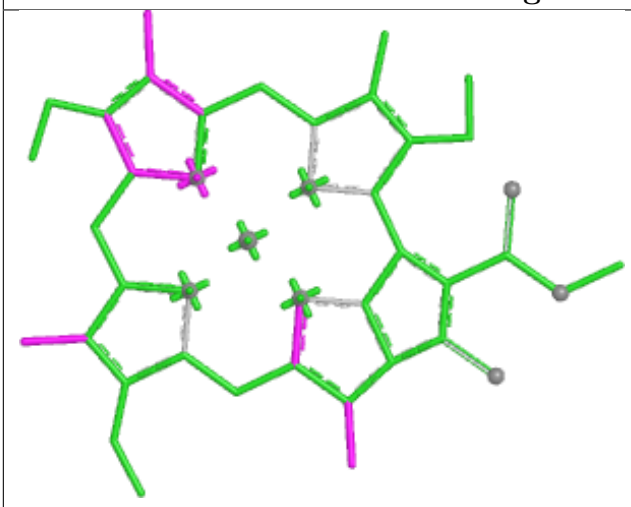


Torsions



Rings

Ligand CLA U 614



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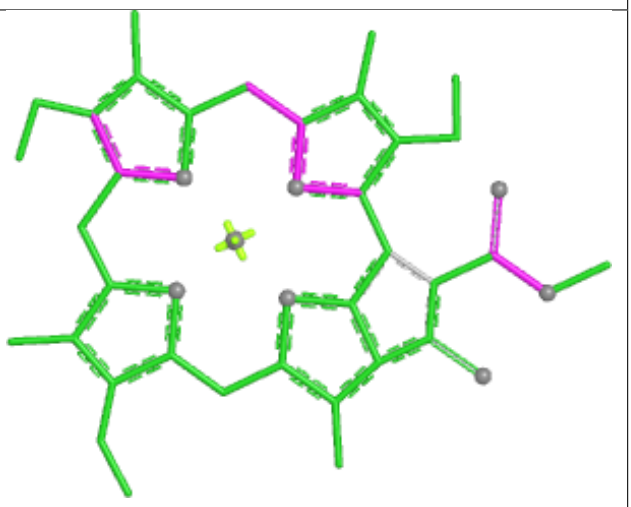
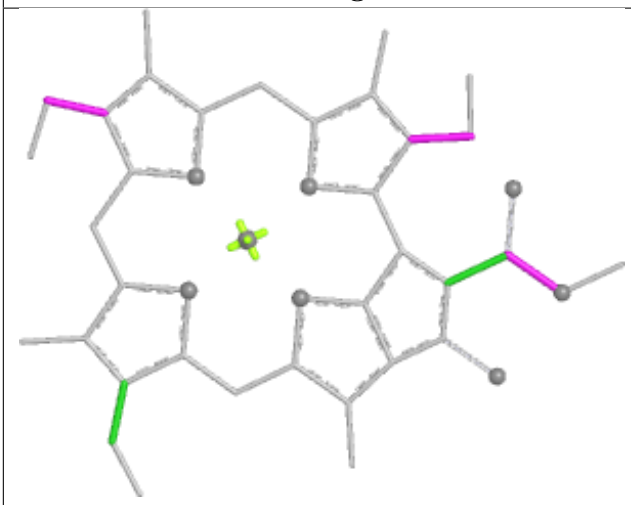


Bond angles

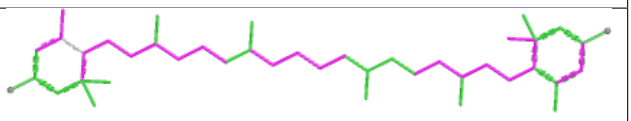


Torsions

Rings

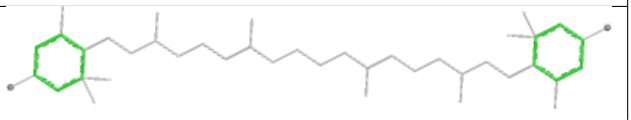
Ligand LUT Z 1620

Bond lengths



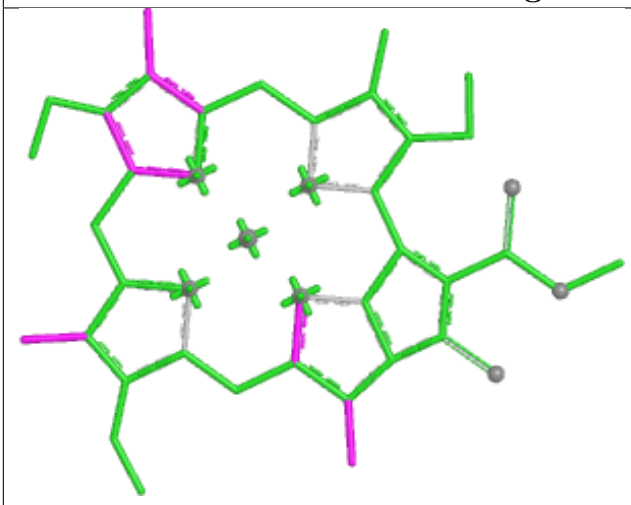
Bond angles

Torsions

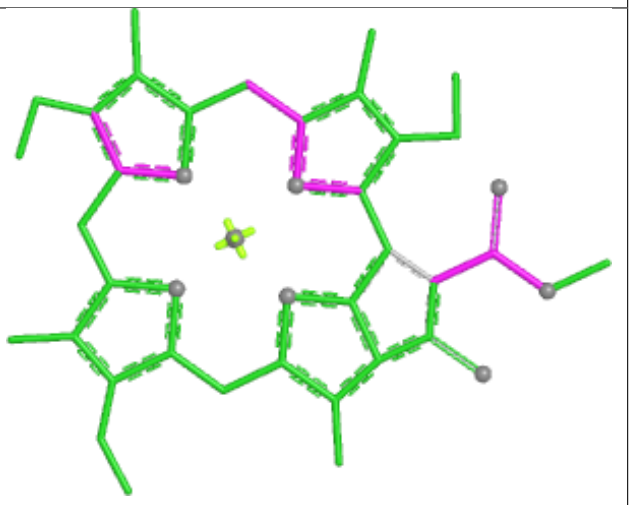


Rings

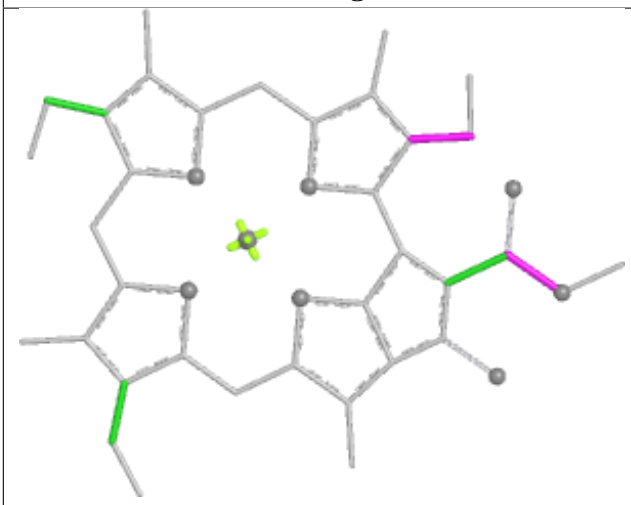
Ligand CLA B 822



Bond lengths



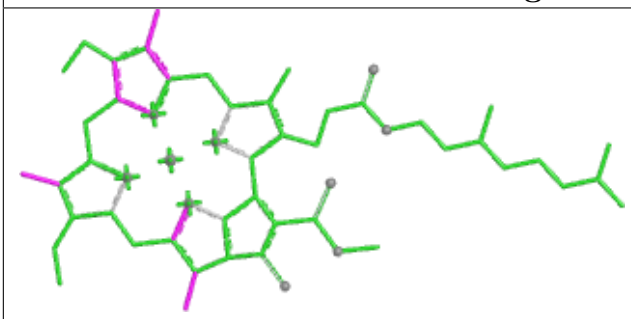
Bond angles



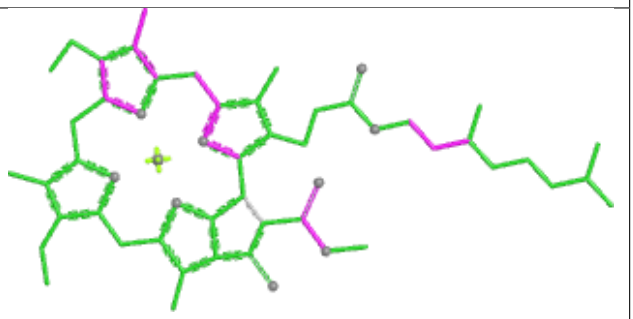
Torsions

Rings

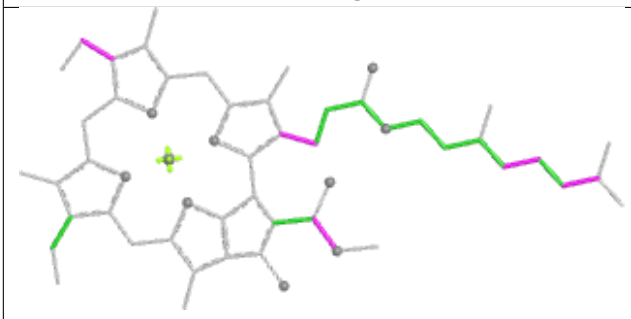
Ligand CLA B 819



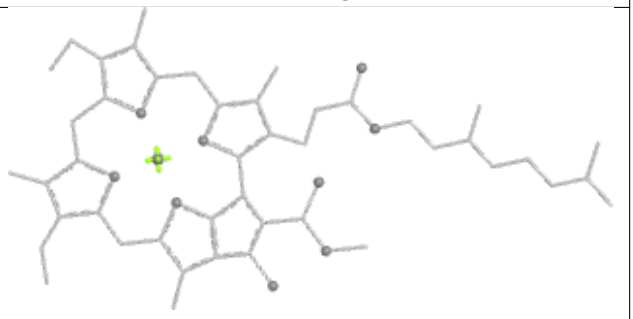
Bond lengths



Bond angles

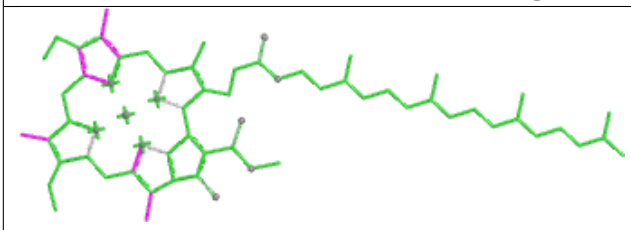


Torsions

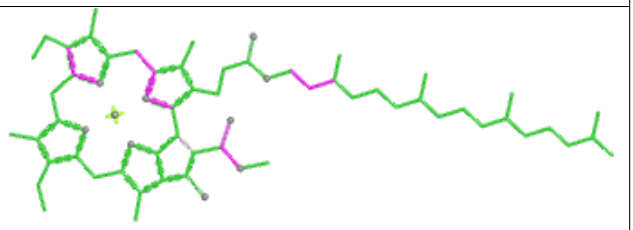


Rings

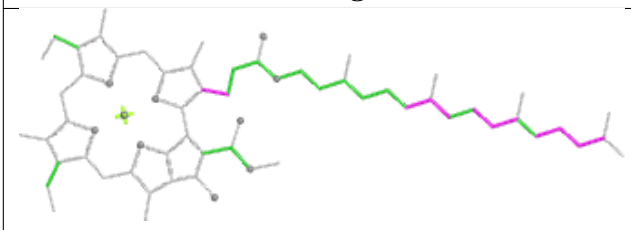
Ligand CLA 5 609



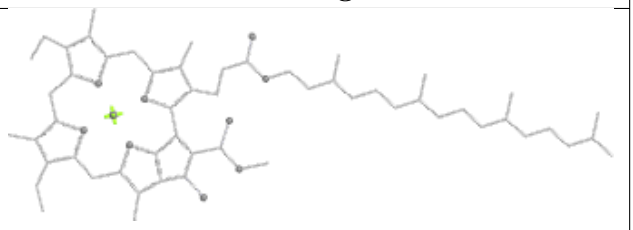
Bond lengths



Bond angles

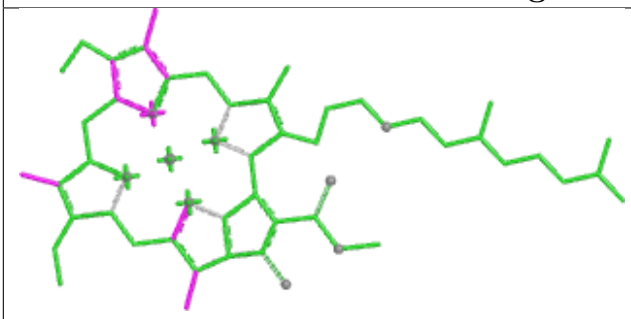


Torsions



Rings

Ligand CLA a 603



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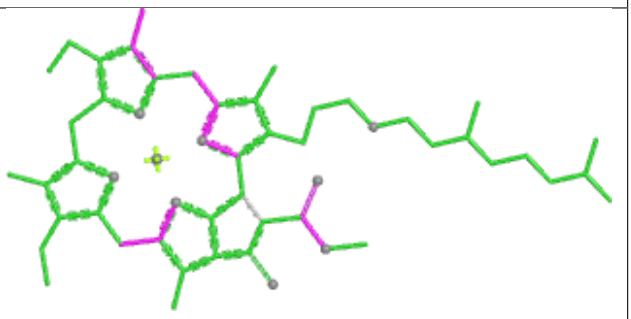

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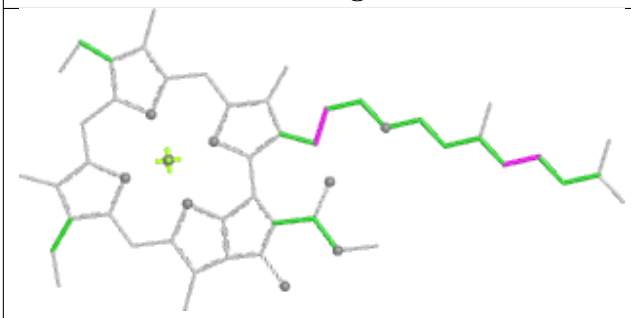
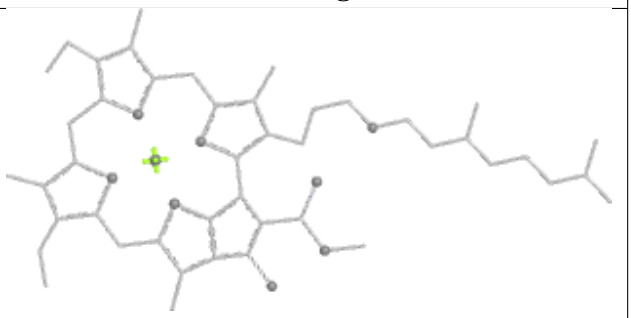
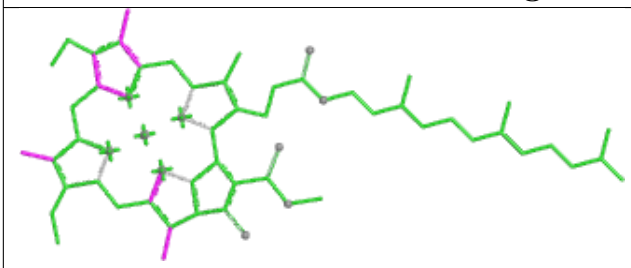


Torsions



Rings

Ligand CLA A 818



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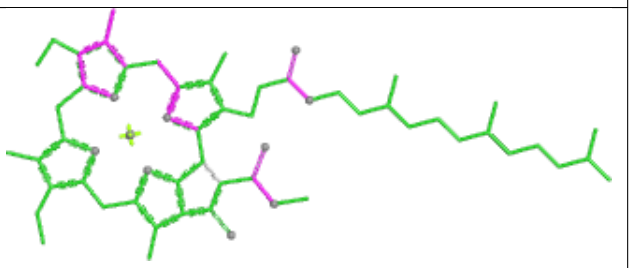

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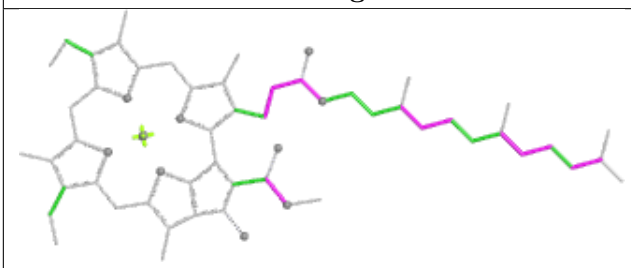

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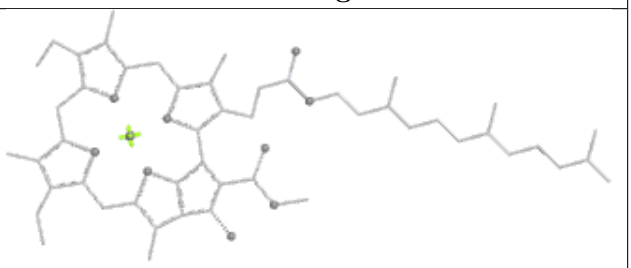
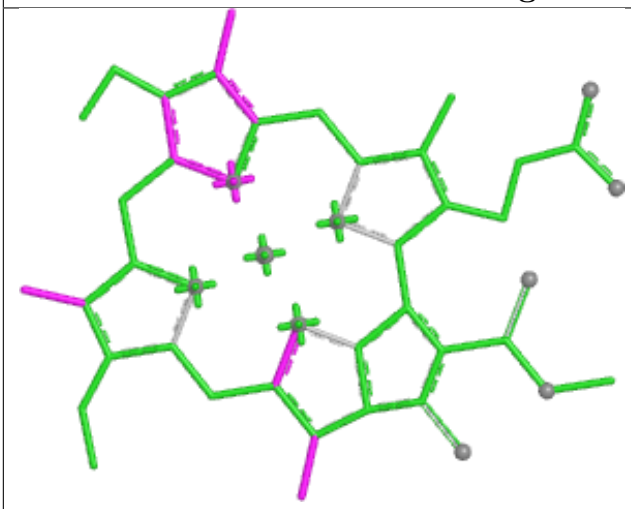


Rings

Ligand CLA W 612



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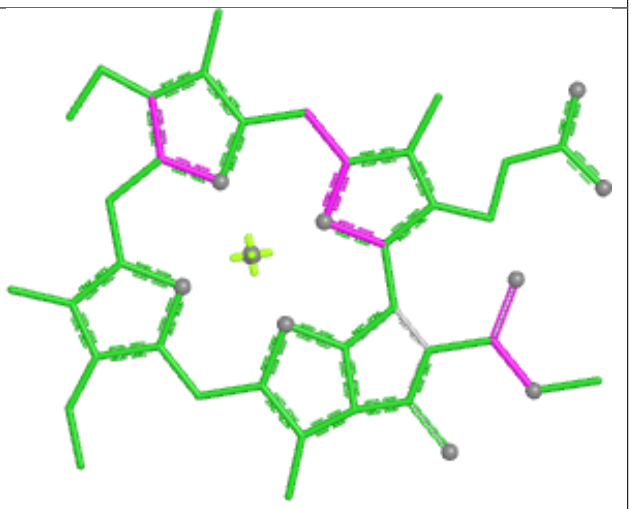

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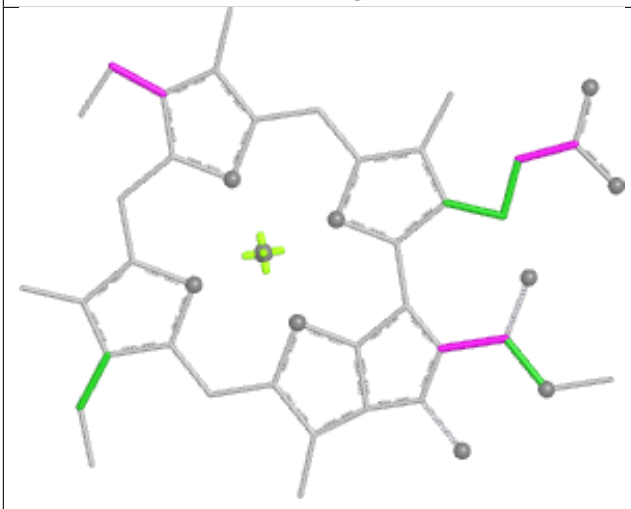
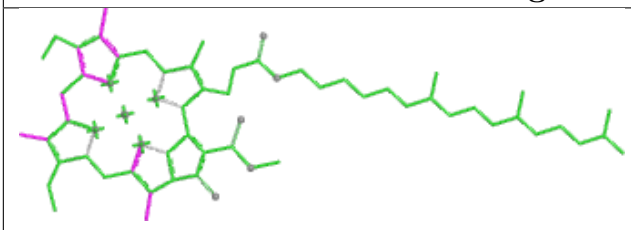


Torsions

Rings

Ligand CLA 6 620



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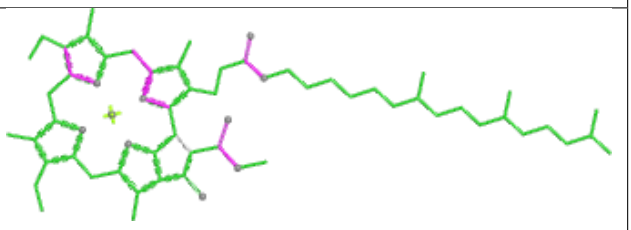

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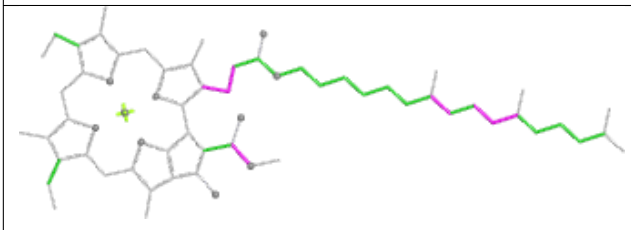

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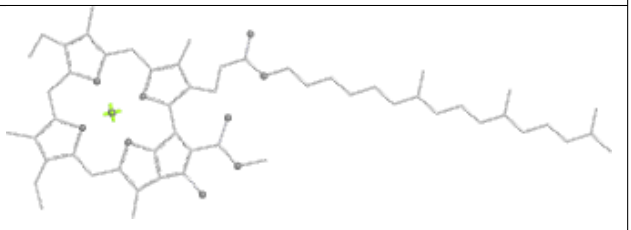
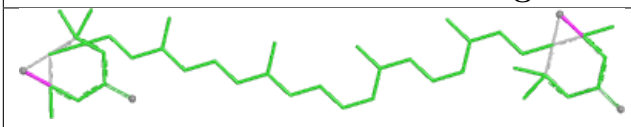
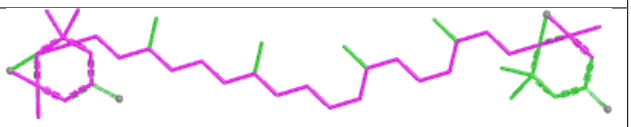
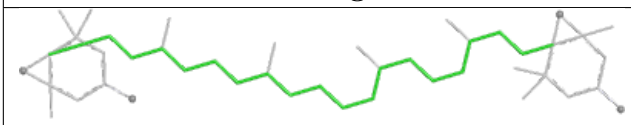
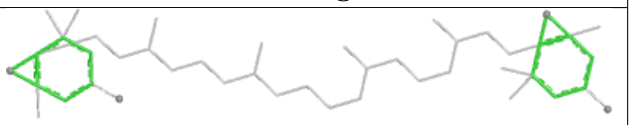


Rings

Ligand XAT X 1622	
 Bond lengths	 Bond angles
 Torsions	 Rings

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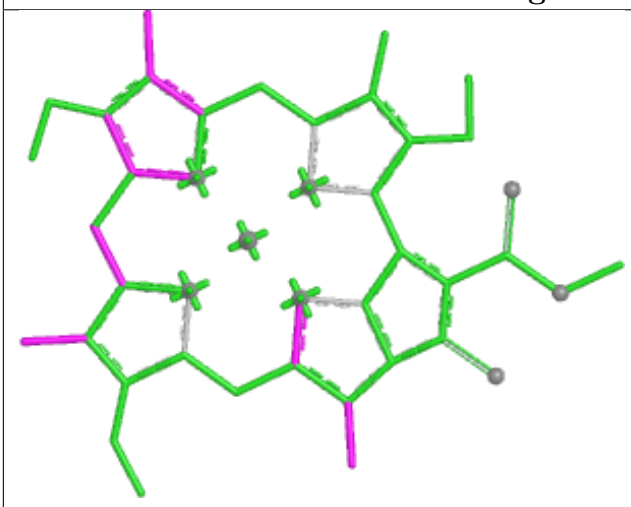
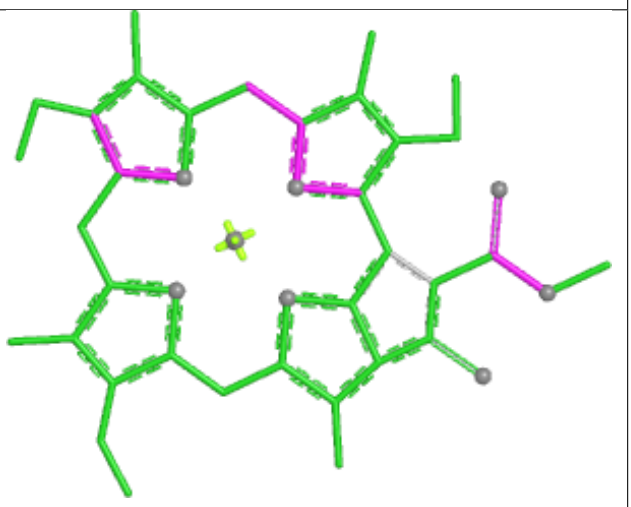
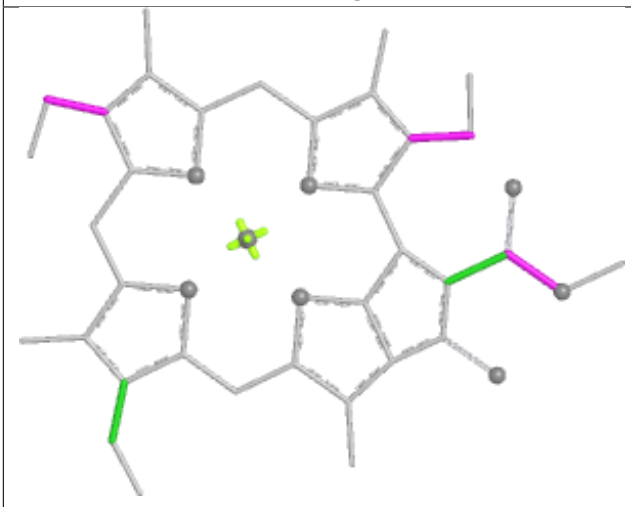
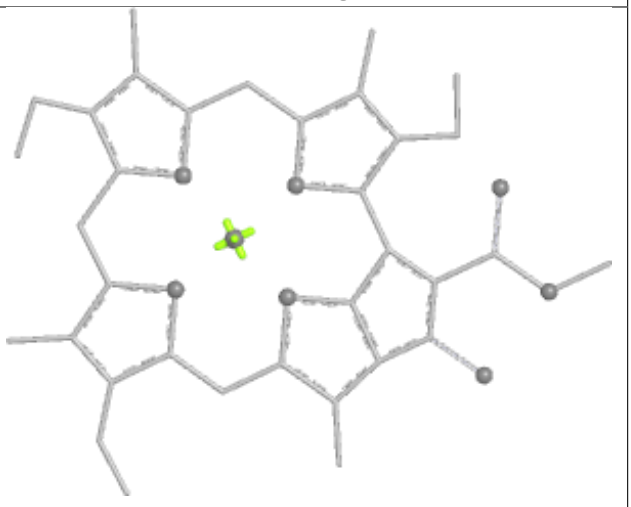
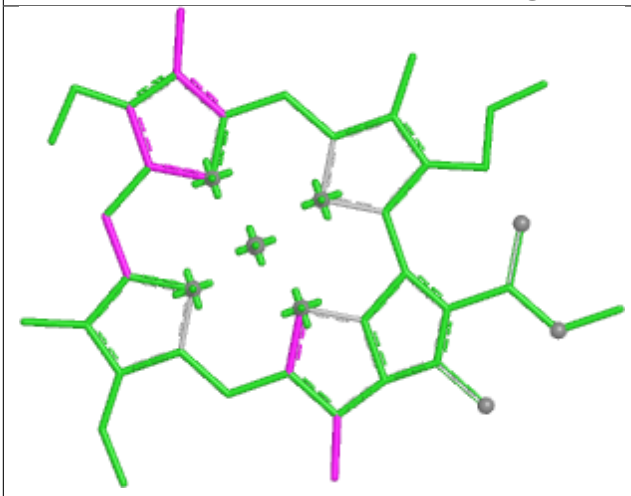
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA X 612



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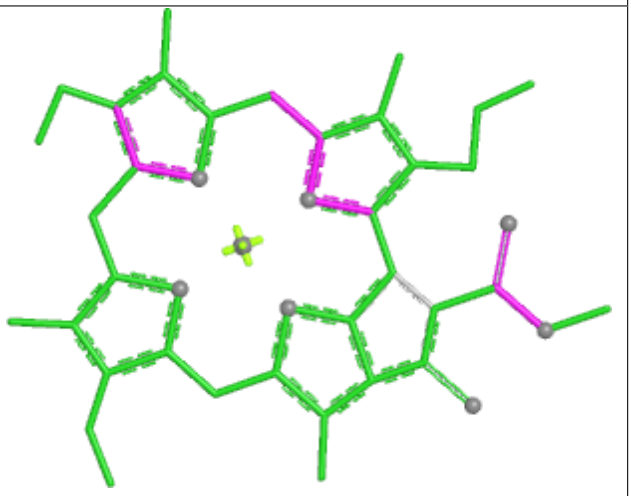

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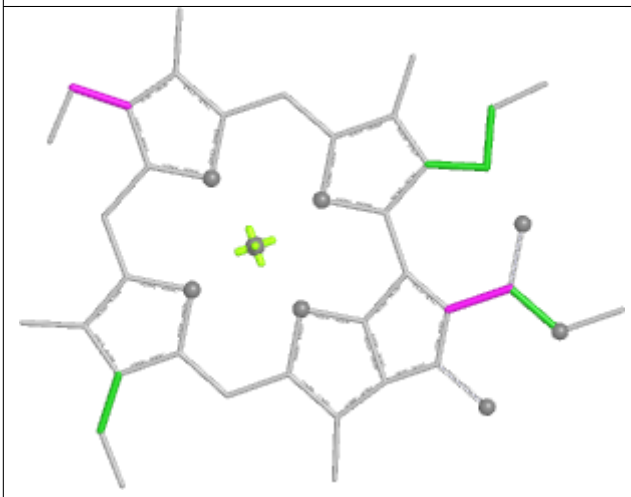

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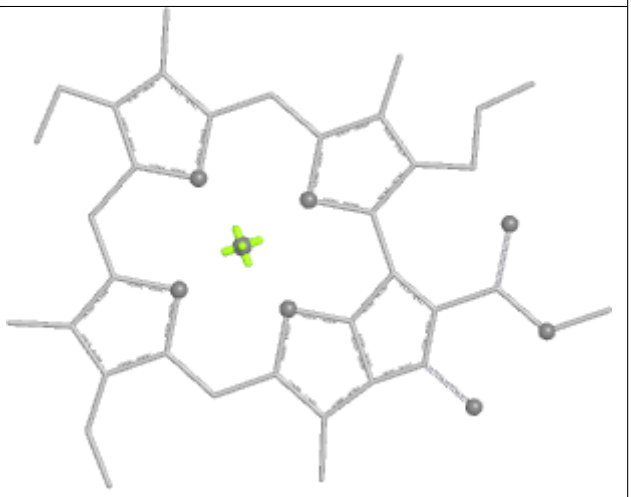
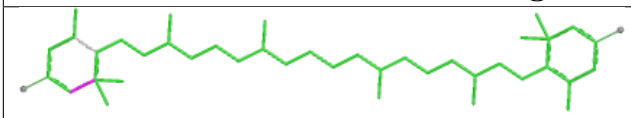


Rings

Ligand LUT 1 617



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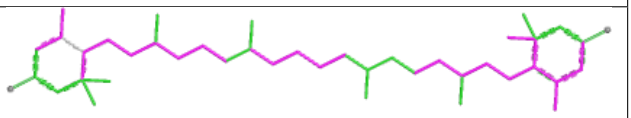

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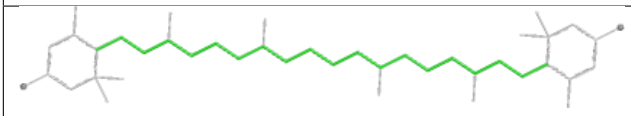

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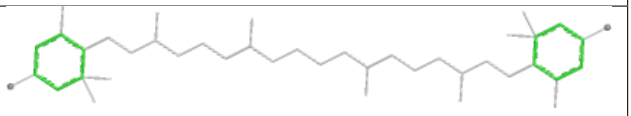
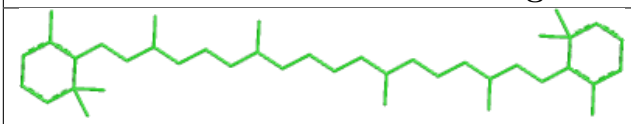


Rings

Ligand BCR 1 619



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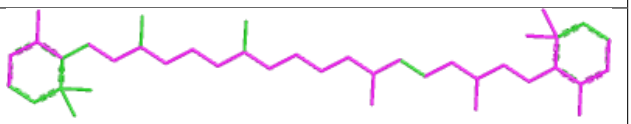

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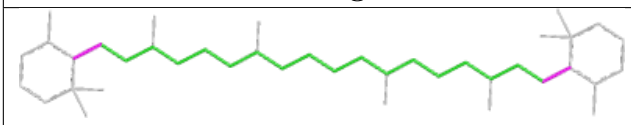

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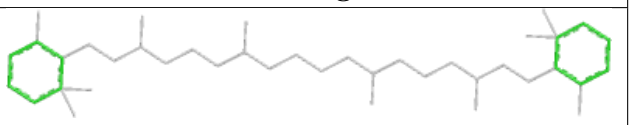
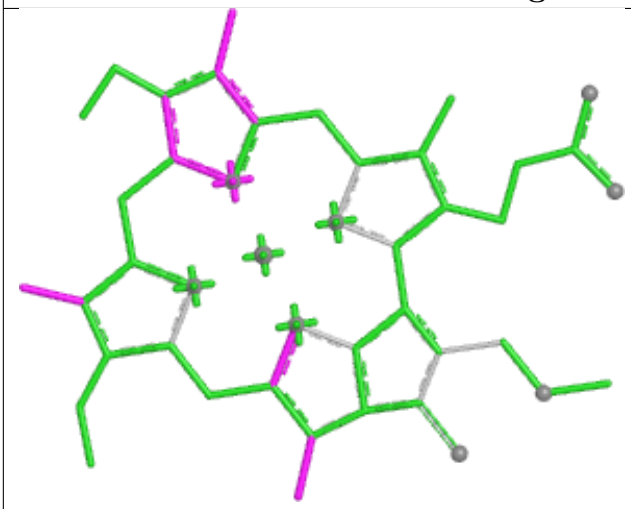


Rings

Ligand CLA a 606



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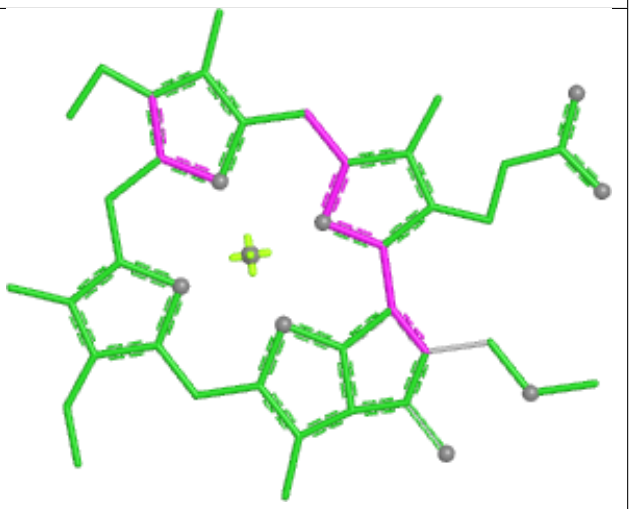
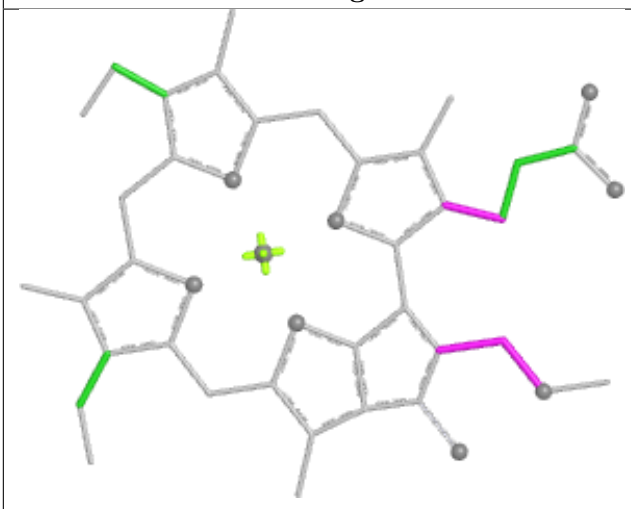


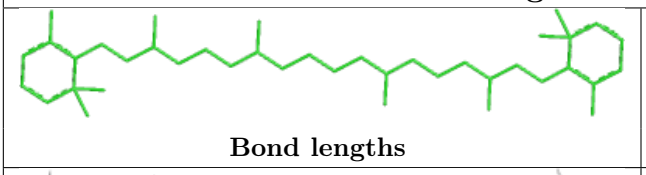
Bond angles



Torsions

Rings

Ligand BCR 3 620



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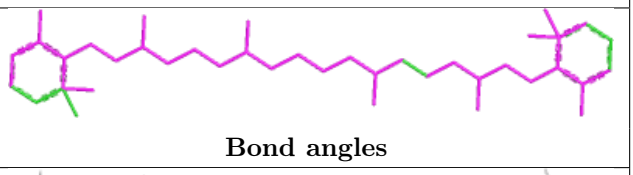

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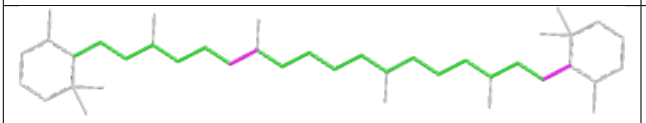
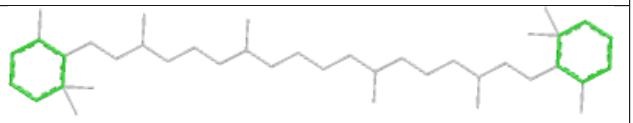
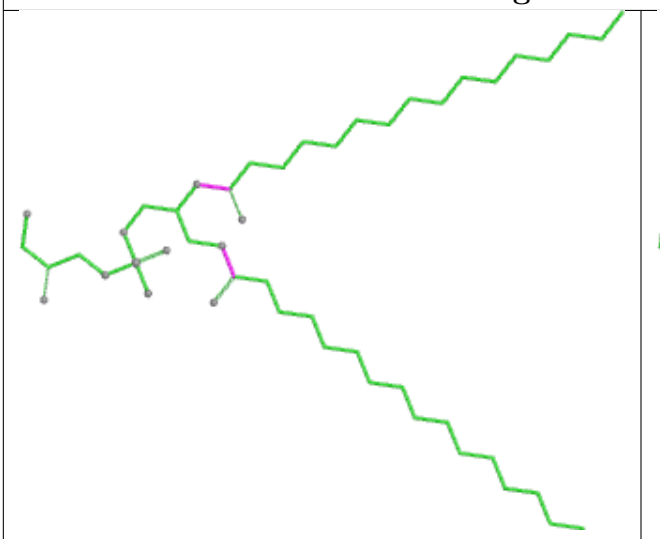


Torsions



Rings

Ligand LHG Y 2630



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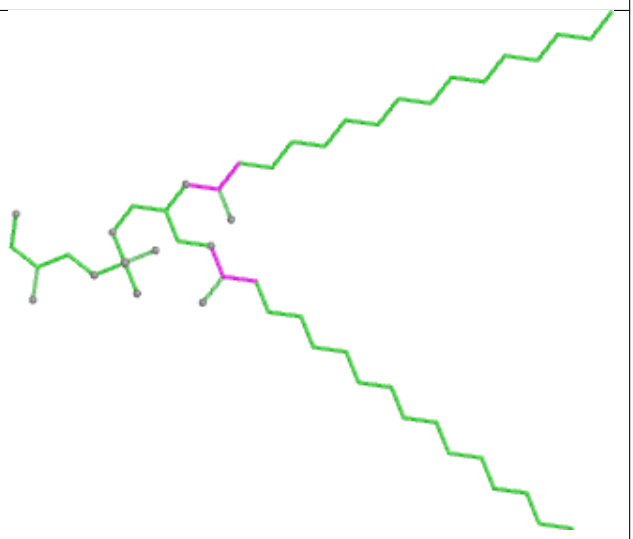
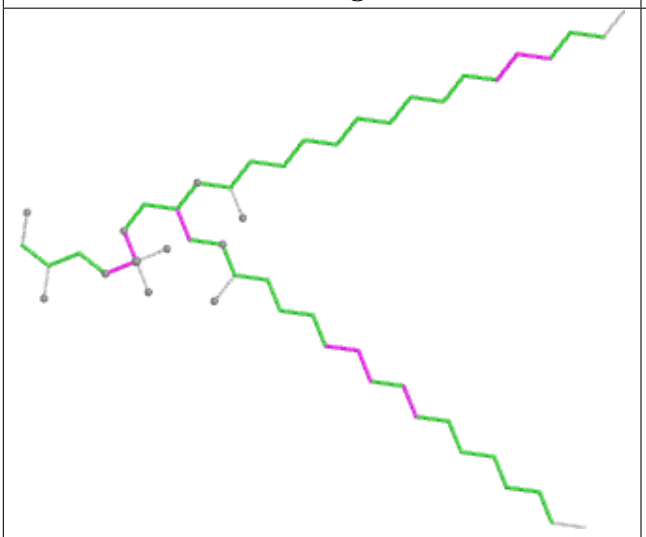
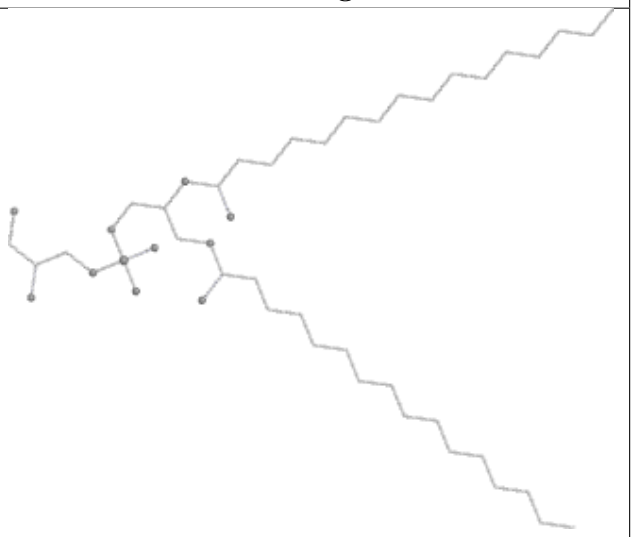


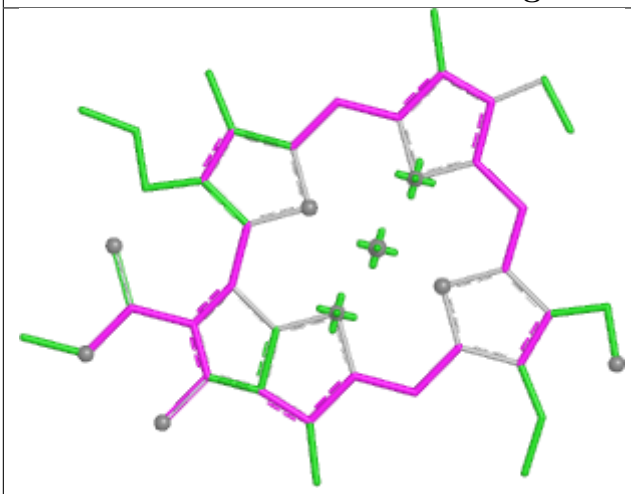
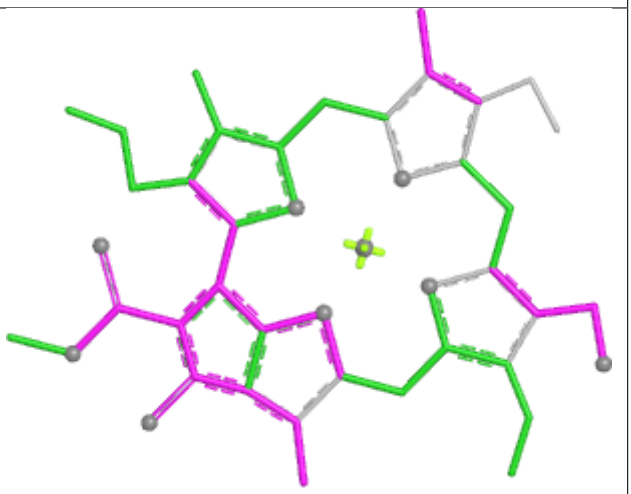
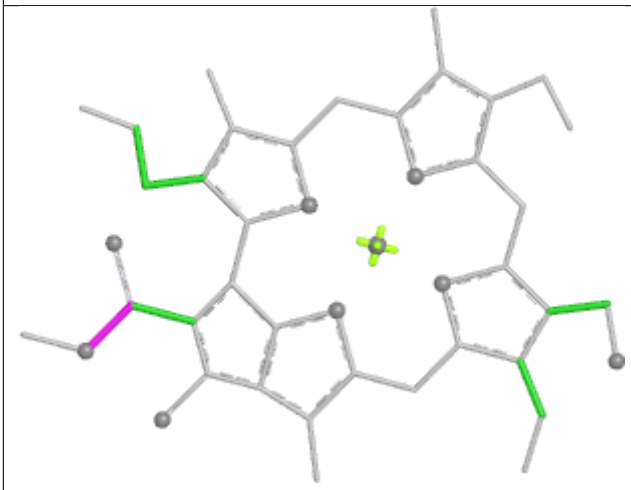
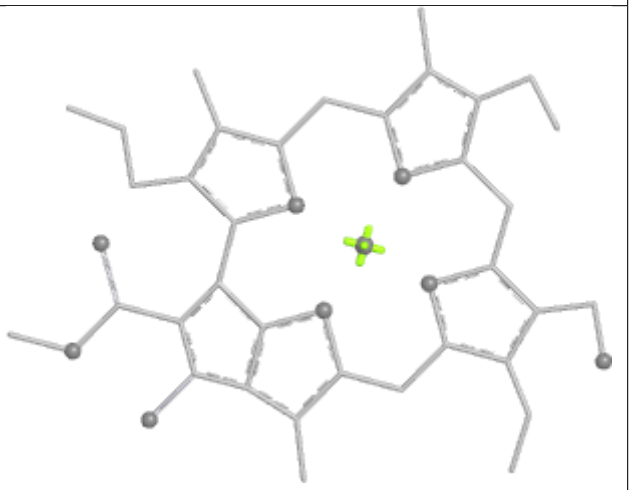
Bond angles

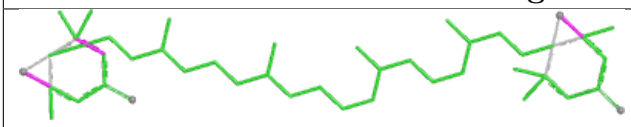
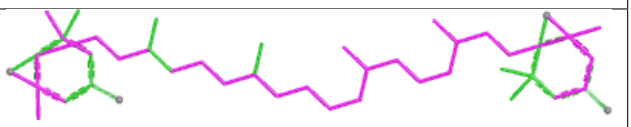
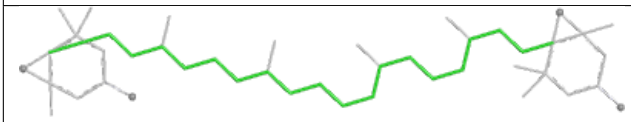
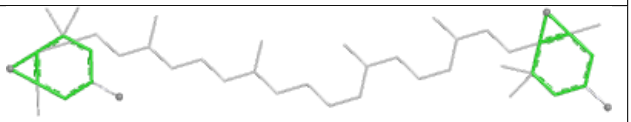


Torsions

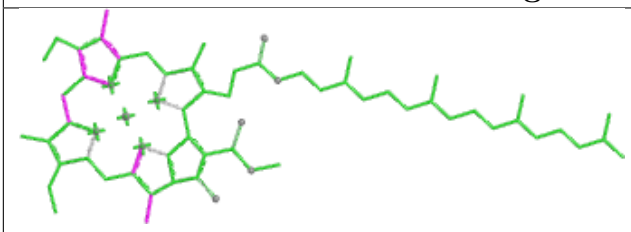


Rings

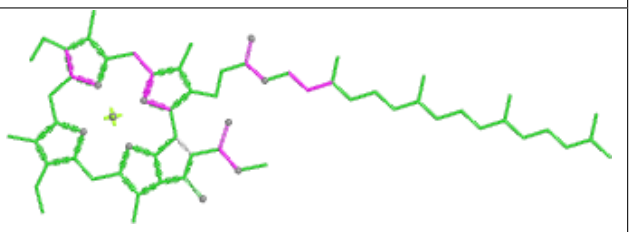
Ligand CHL V 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT 5 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

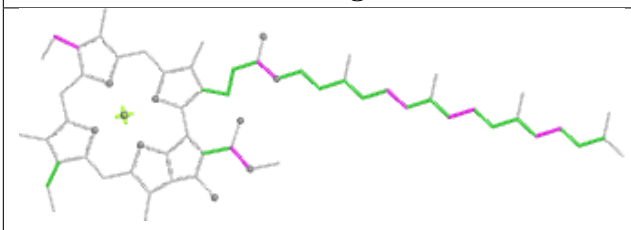
Ligand CLA Y 610



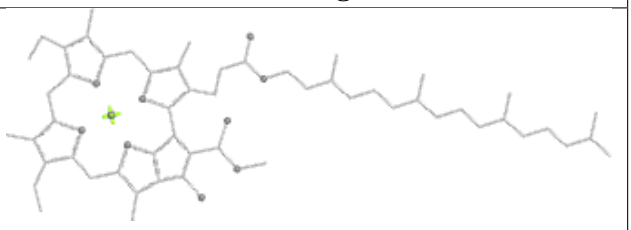
Bond lengths



Bond angles



Torsions



Rings

Ligand XAT 4 620

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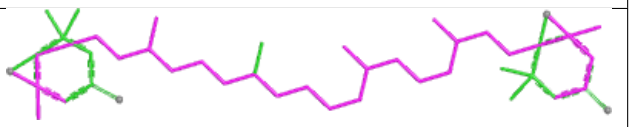

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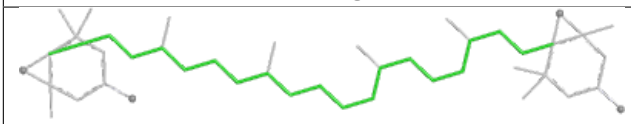

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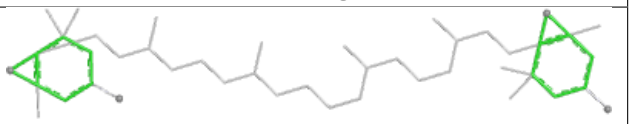
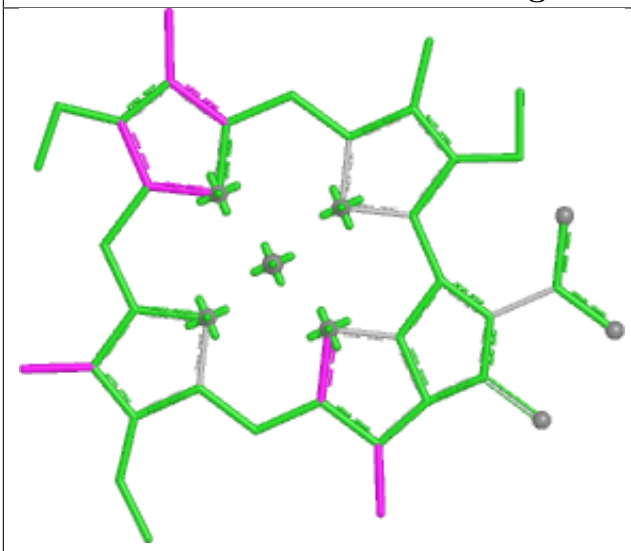
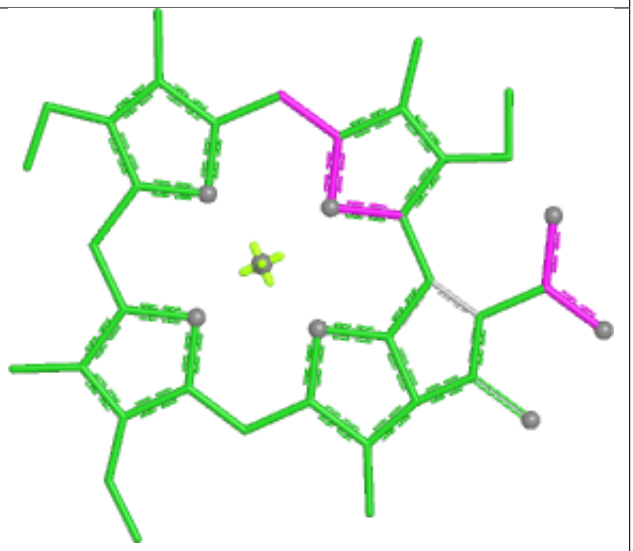


Rings

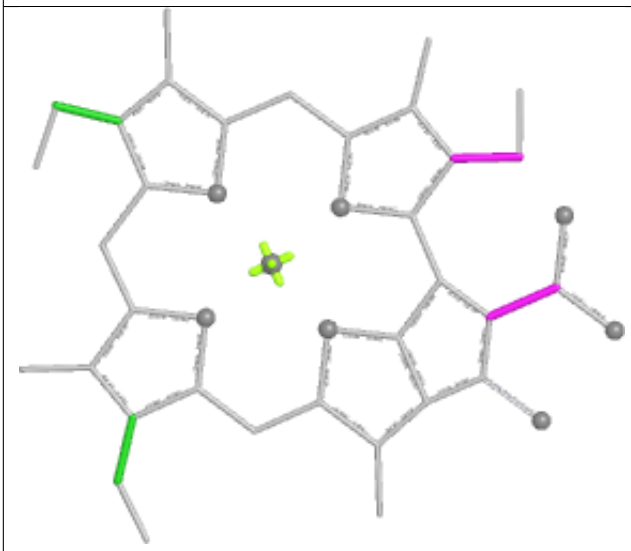
Ligand CLA 5 612



Bond lengths



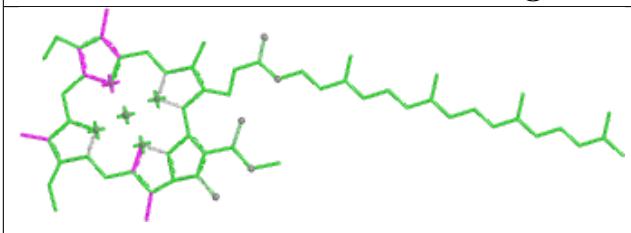
Bond angles



Torsions

Rings

Ligand CLA B 806



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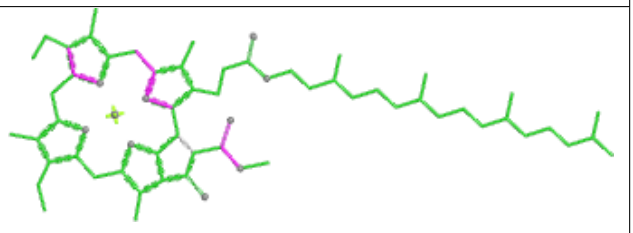
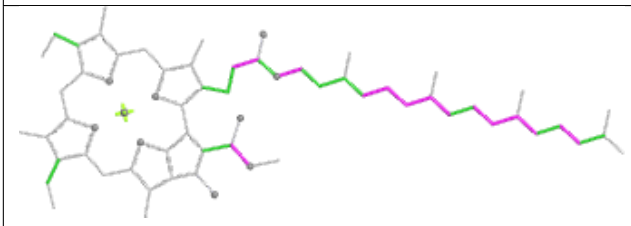
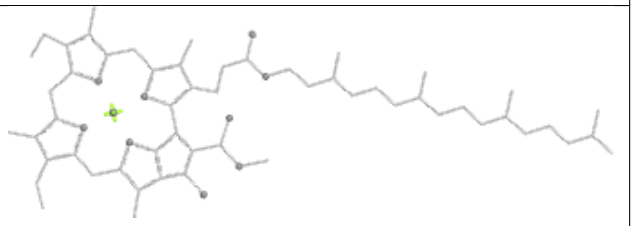


Bond angles

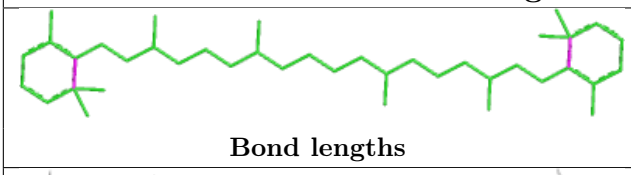


Torsions



Rings

Ligand BCR L 308



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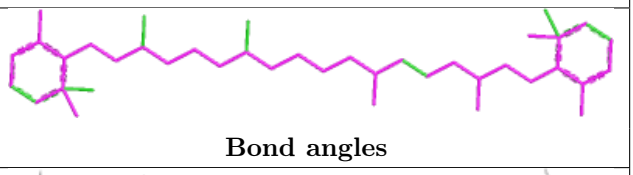
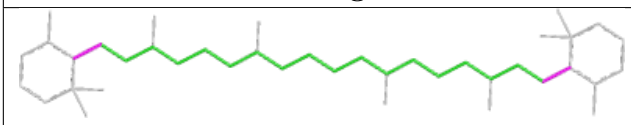


Bond angles



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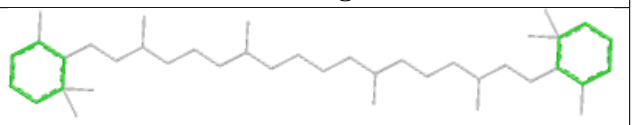
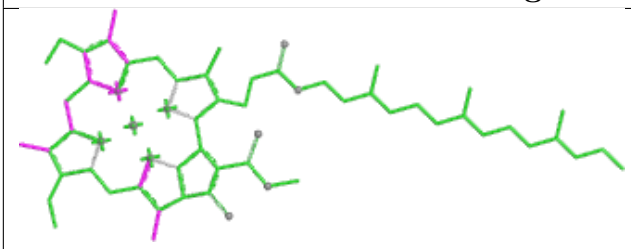
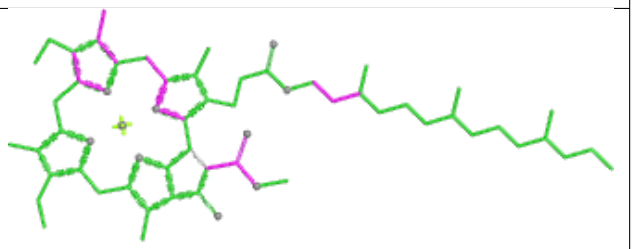


Rings

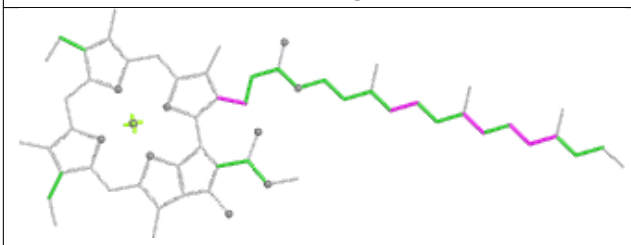
Ligand CLA B 826



Bond lengths



Bond angles



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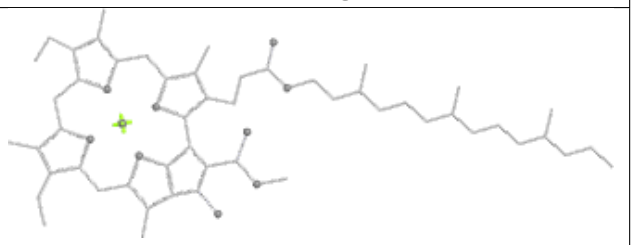
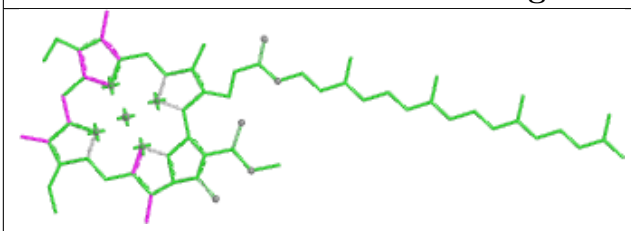


Rings

Ligand CLA 3 610



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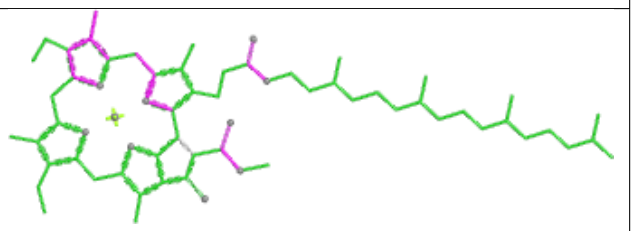
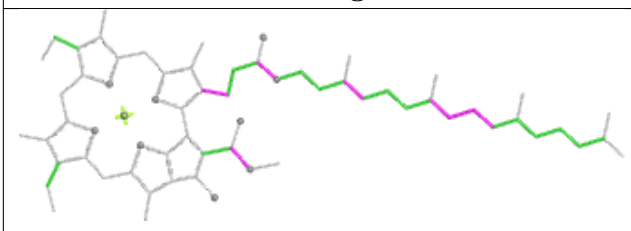


Bond angles



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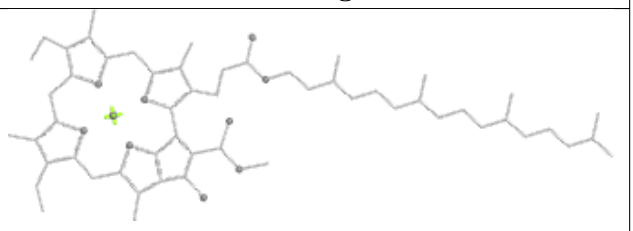
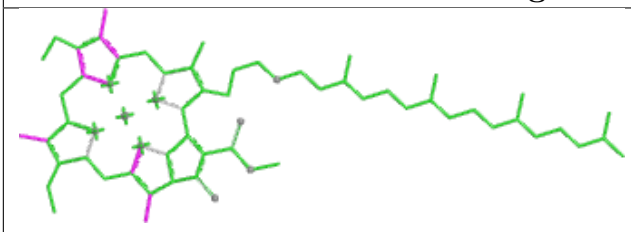


Rings

Ligand CLA 5 613



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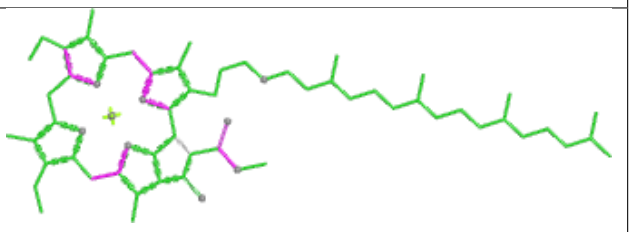
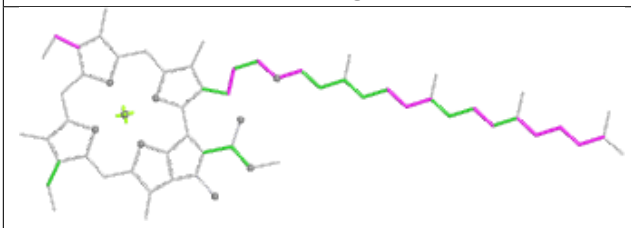


Bond angles



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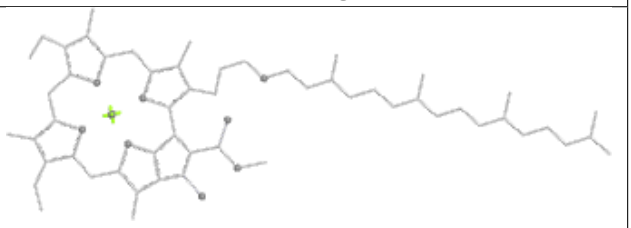
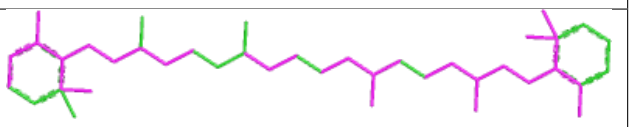


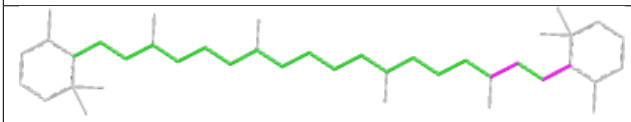
Rings

Ligand BCR 5 622

Bond lengths



Bond angles



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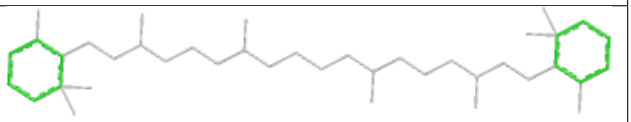
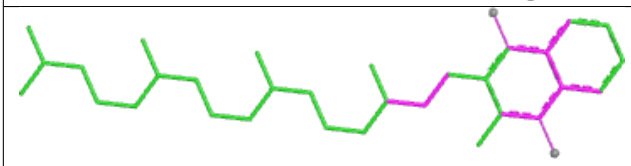
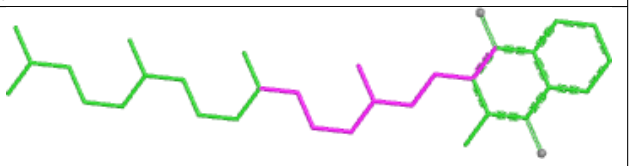


Rings

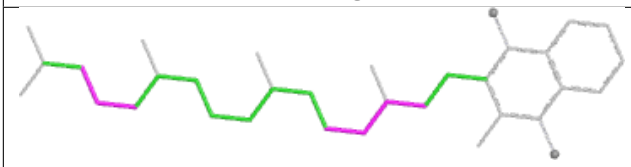
Ligand PQN B 842



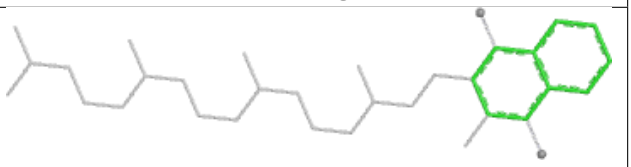
Bond lengths



Bond angles

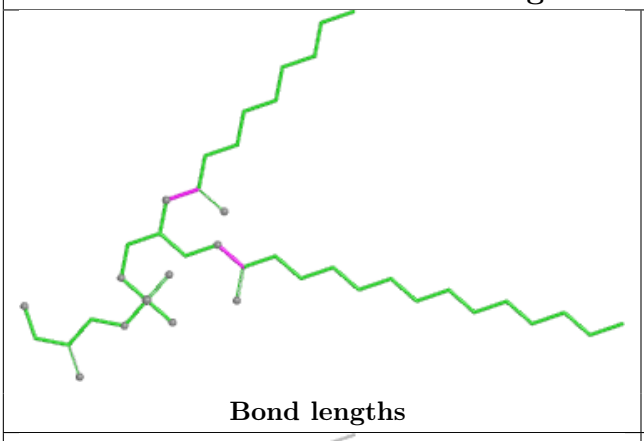


Torsions

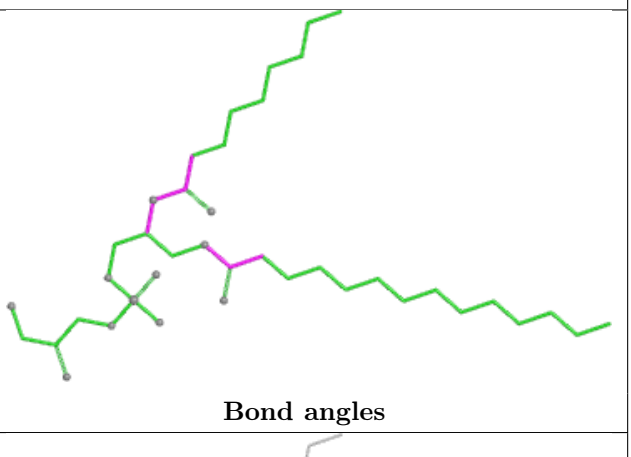


Rings

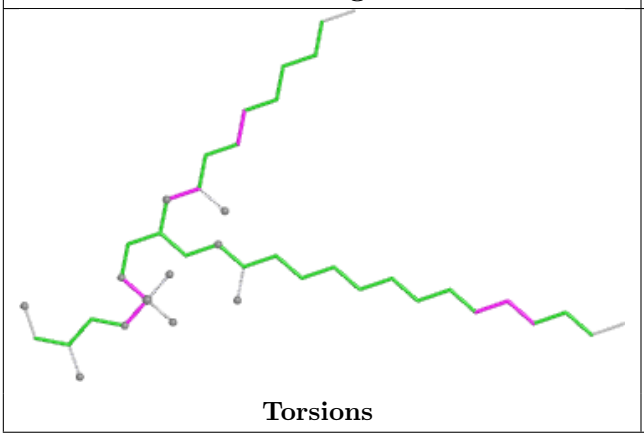
Ligand LHG 8 623



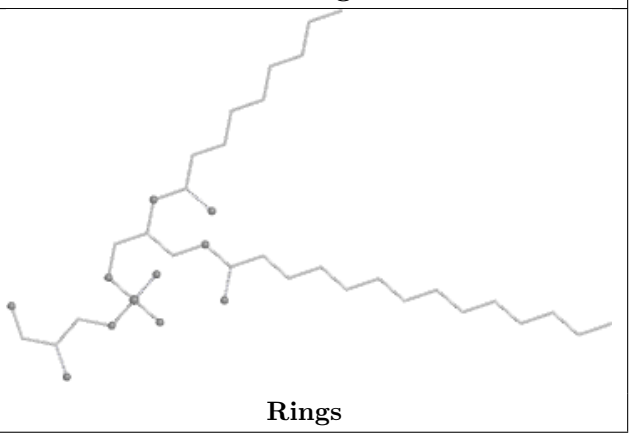
Bond lengths



Bond angles

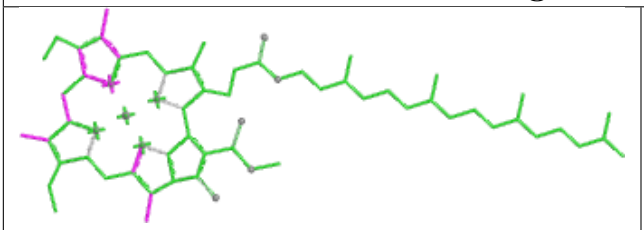


Torsions



Rings

Ligand CLA 5 602



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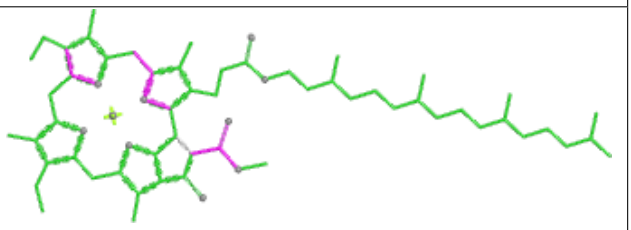
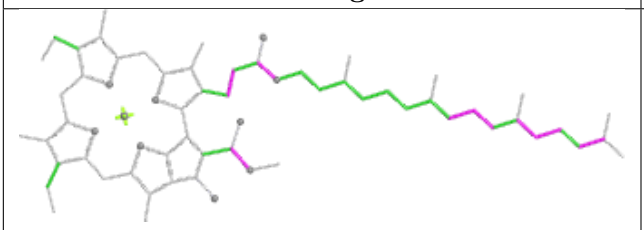
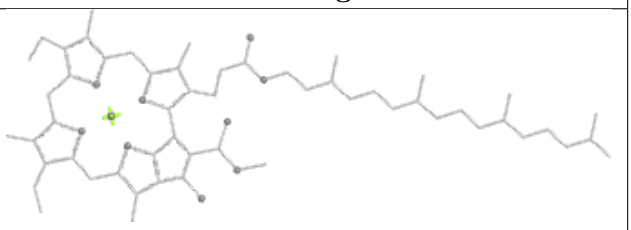


Bond angles

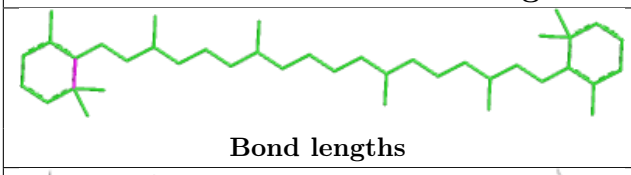


Torsions

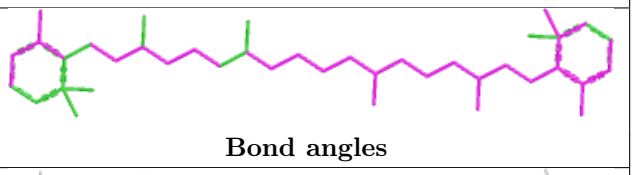


Rings

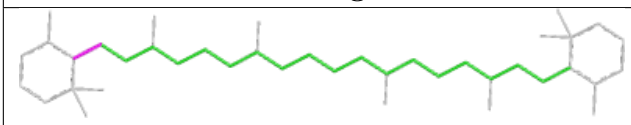
Ligand BCR A 851



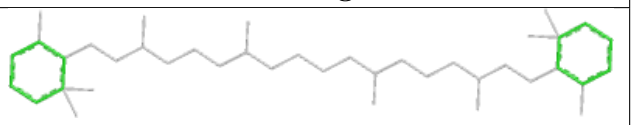
Bond lengths



Bond angles

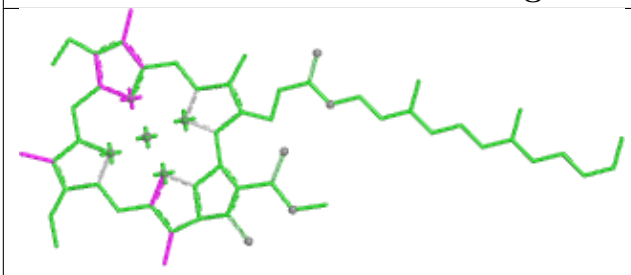


Torsions

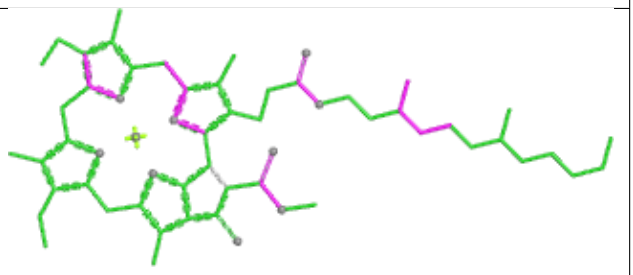


Rings

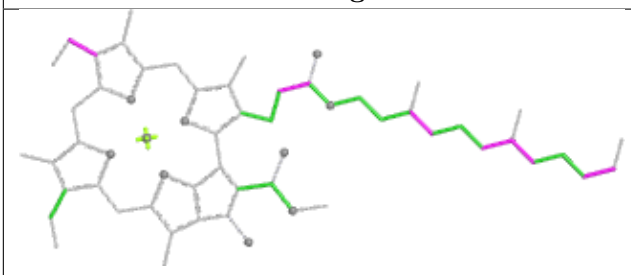
Ligand CLA B 817



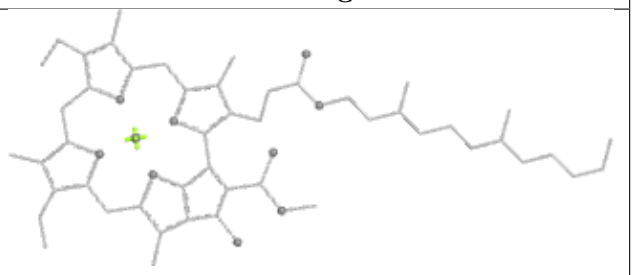
Bond lengths



Bond angles

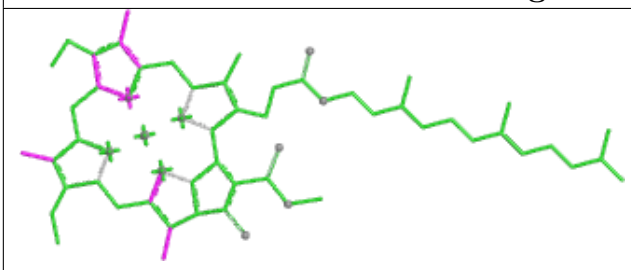


Torsions



Rings

Ligand CLA 7 601



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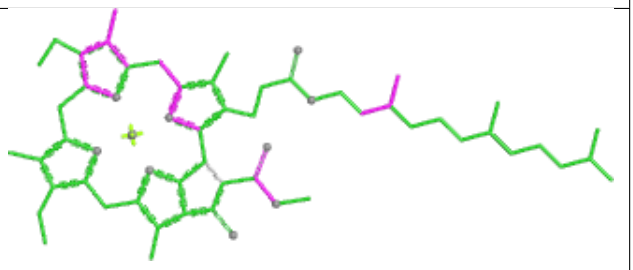

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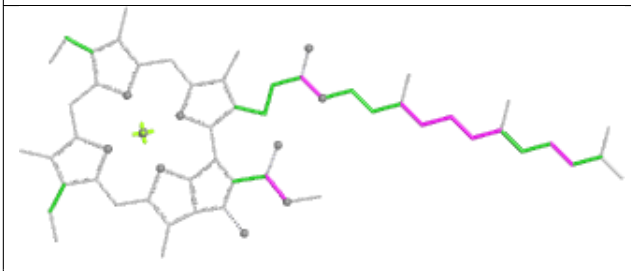

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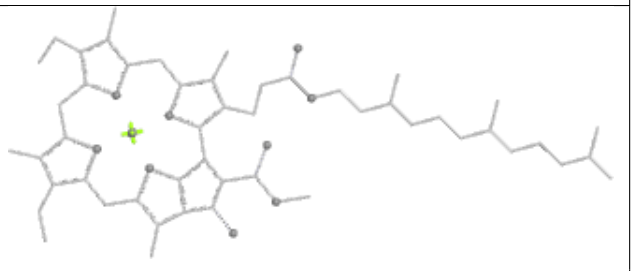
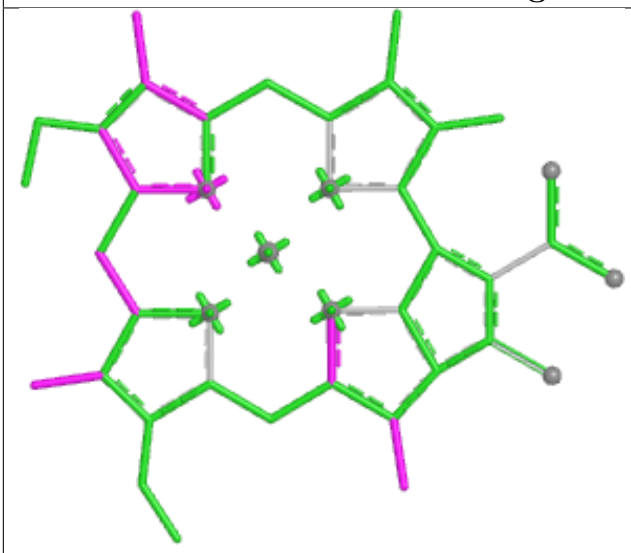


Rings

Ligand CLA 3 614



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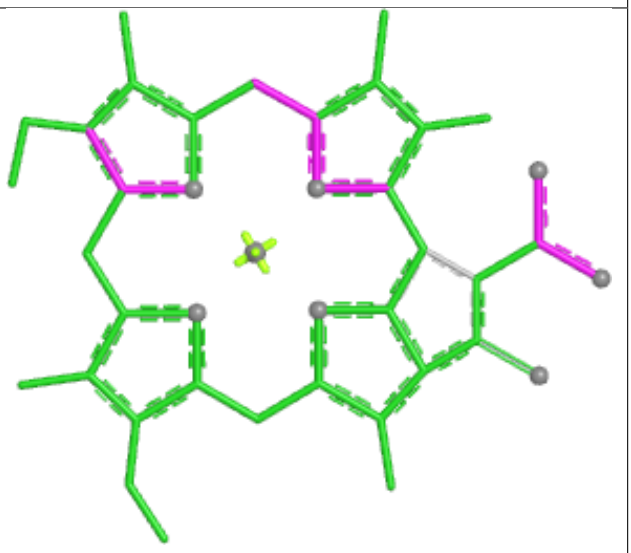

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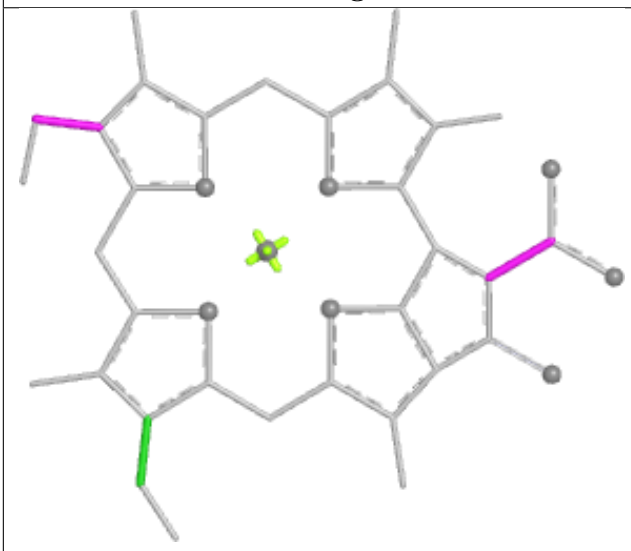

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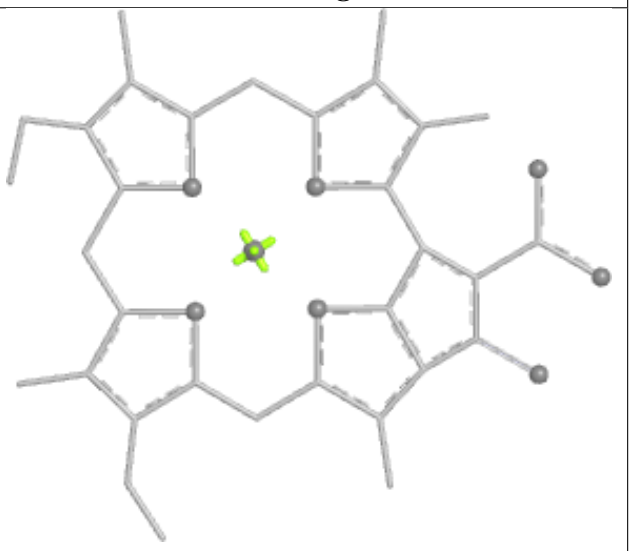
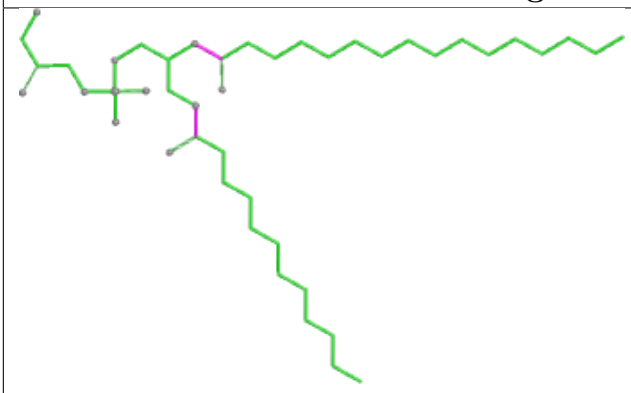


Rings

Ligand LHG 3 623



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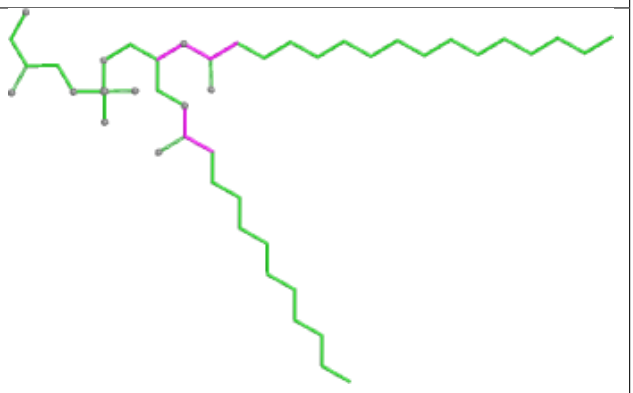
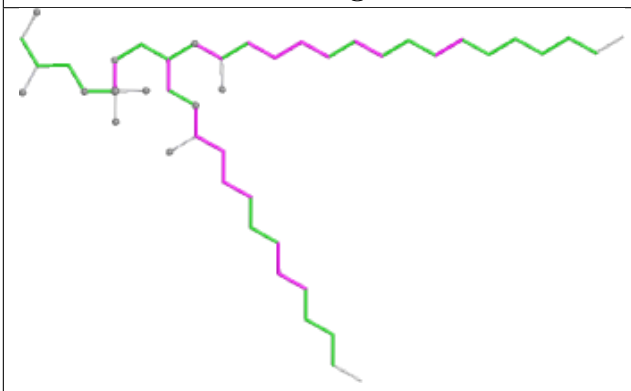


Bond angles



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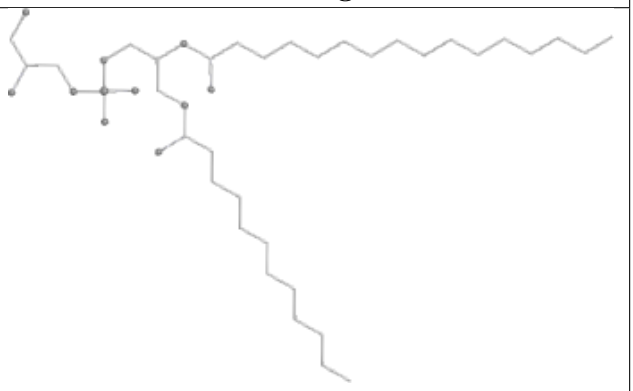
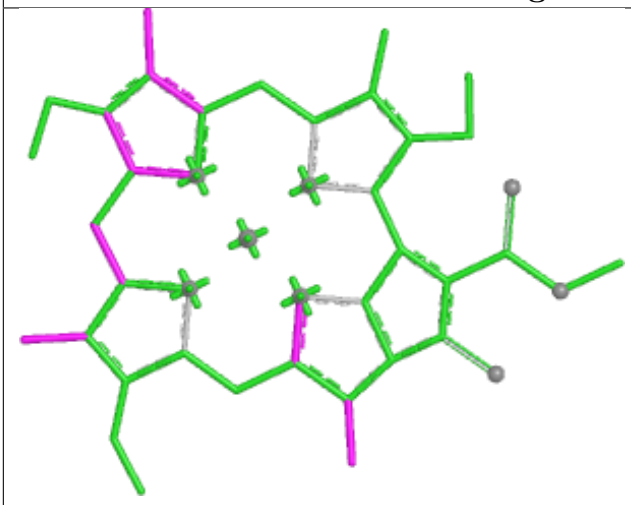


Rings

Ligand CLA 6 611



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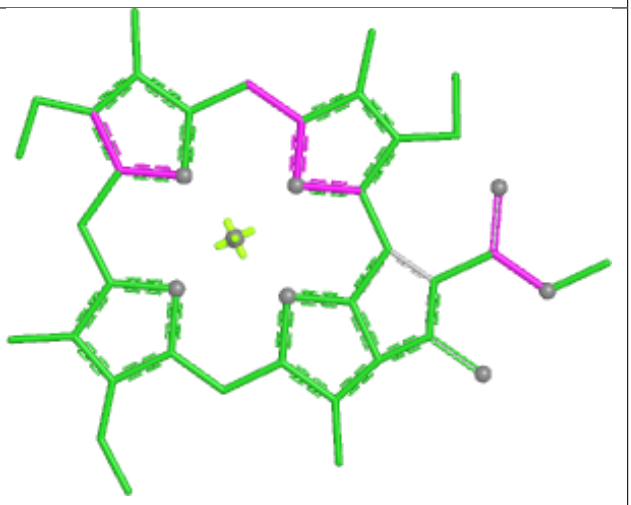

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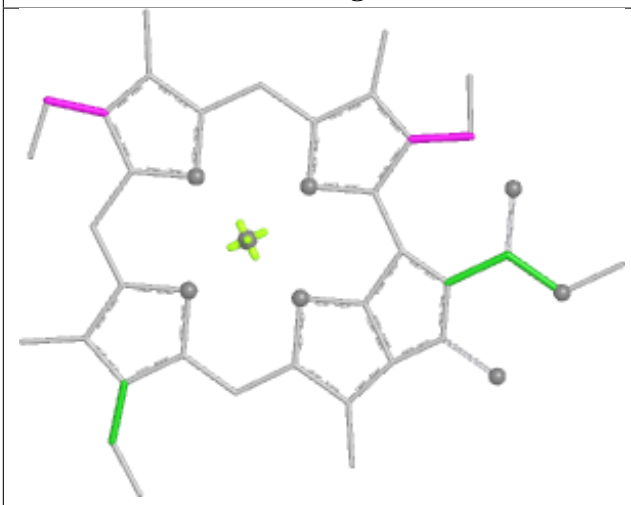
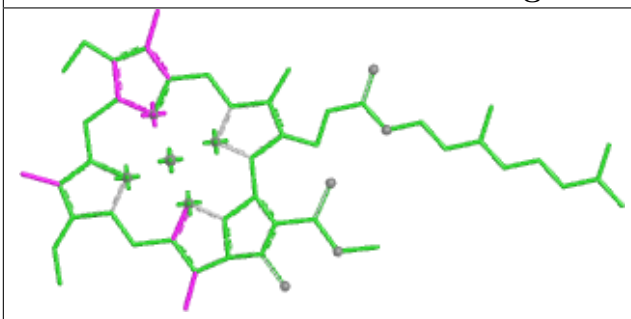


Torsions

Rings

Ligand CLA A 839



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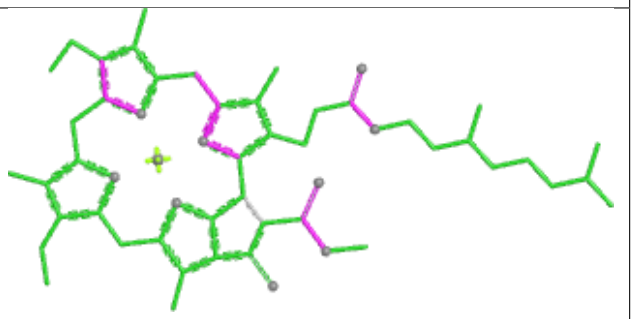

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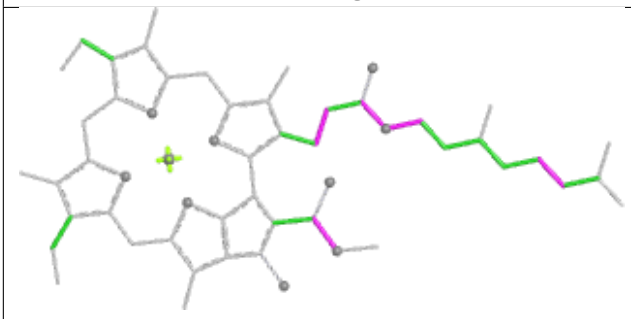

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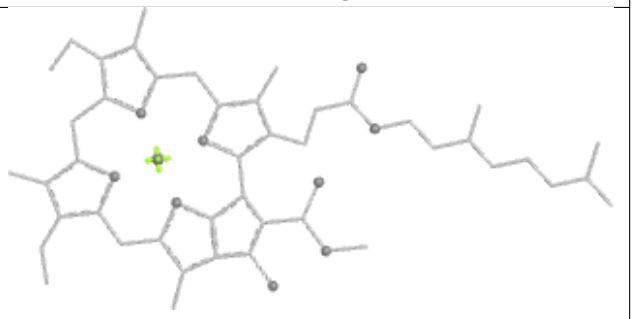
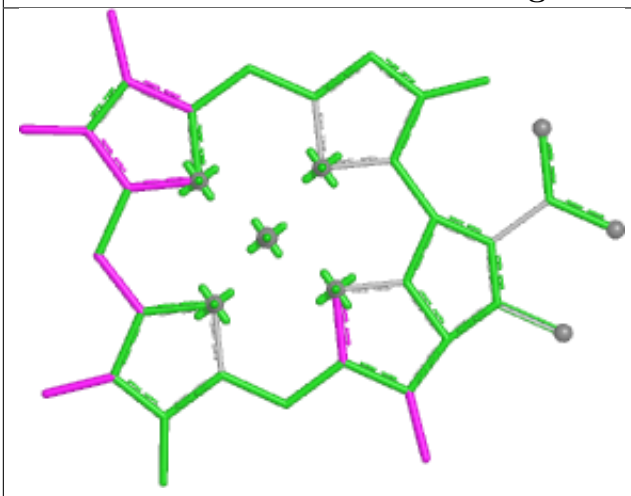


Rings

Ligand CLA 1 614



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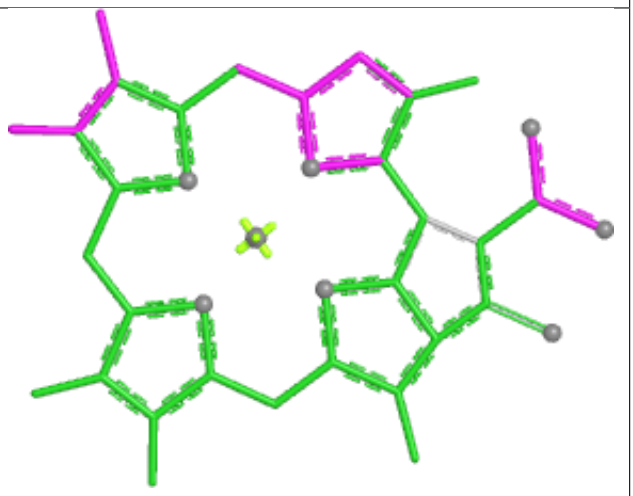
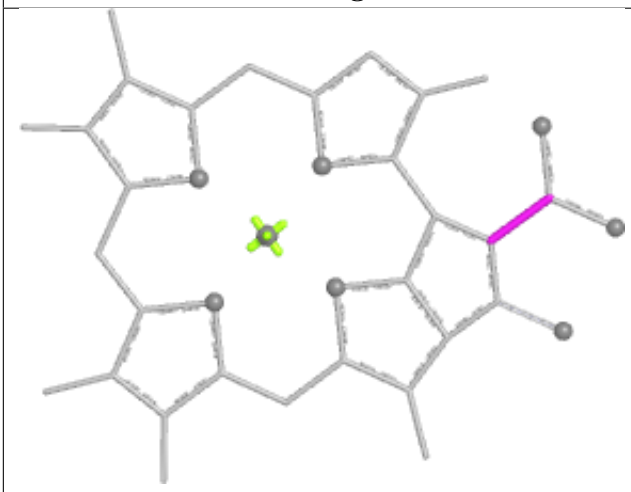


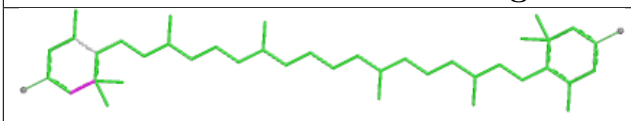
Bond angles



Torsions

Rings

Ligand LUT W 1620



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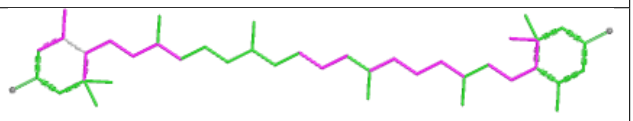
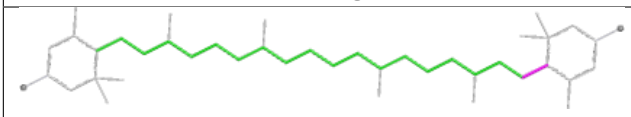


Bond angles



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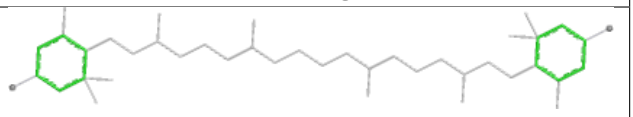
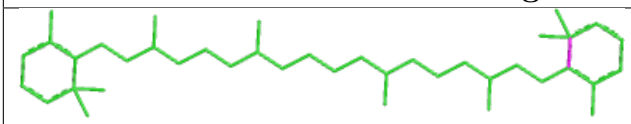


Rings

Ligand BCR A 848



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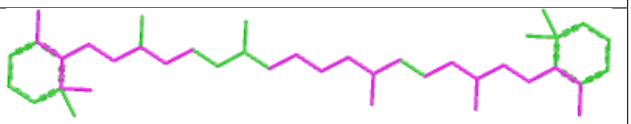
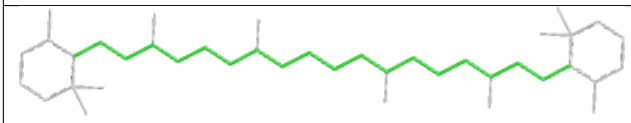


Bond angles



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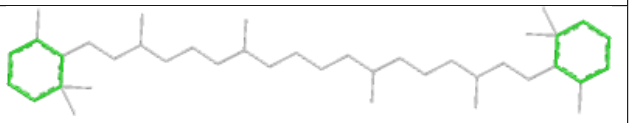
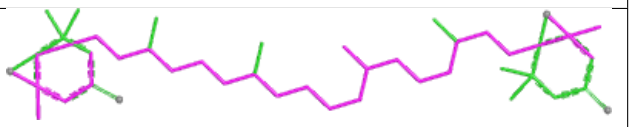


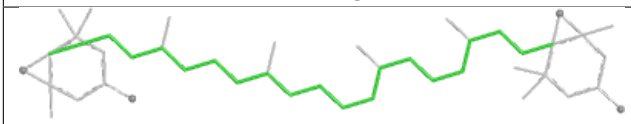
Rings

Ligand XAT 2 620

Bond lengths



Bond angles



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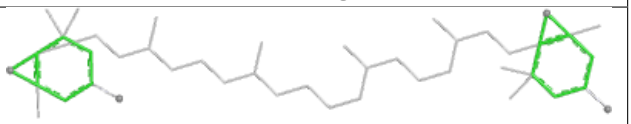
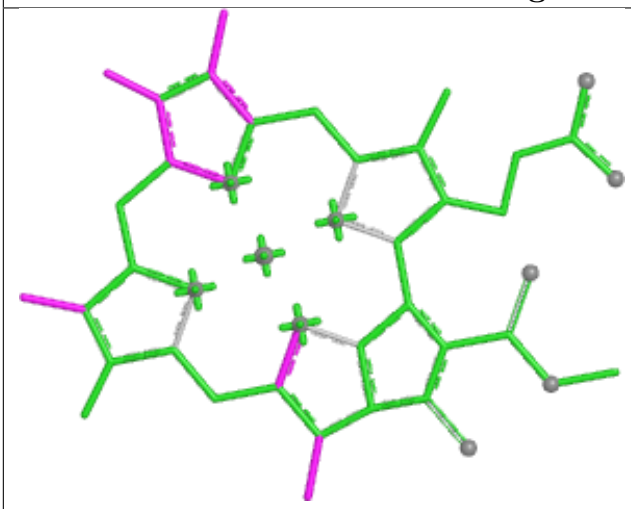


Rings

Ligand CLA 5 619



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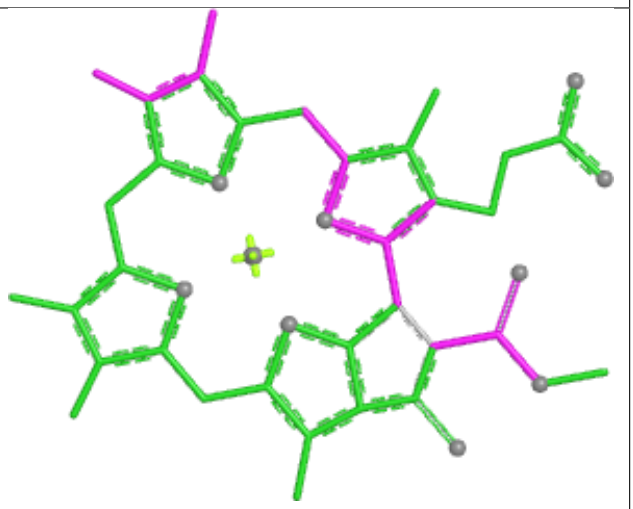

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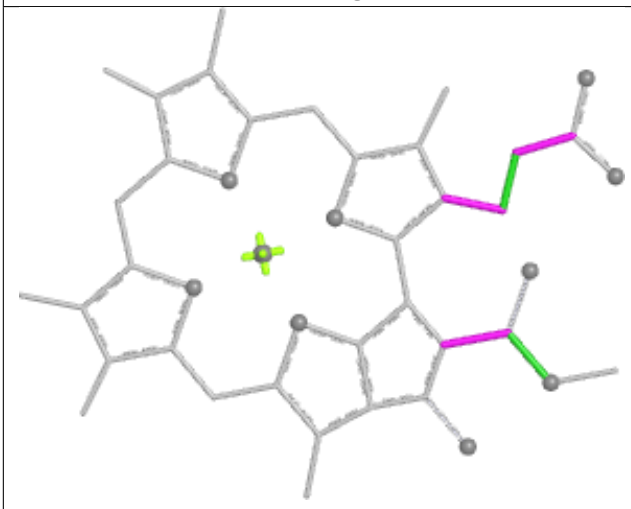
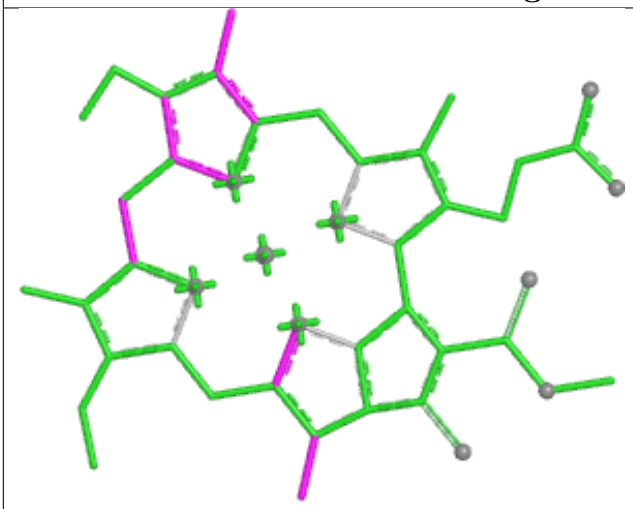


Torsions

Rings

Ligand CLA X 611



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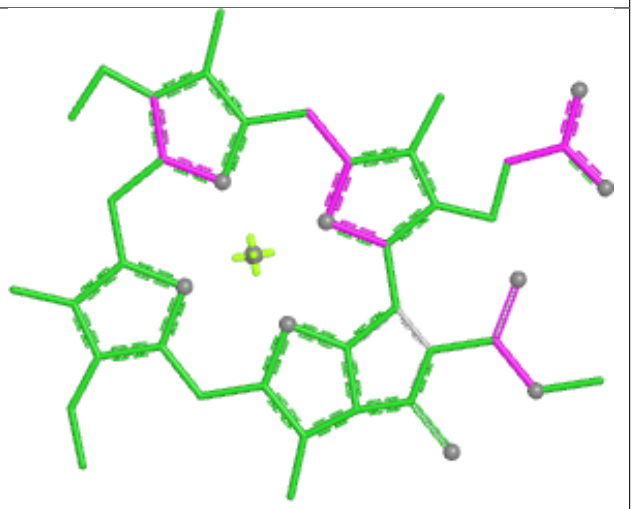

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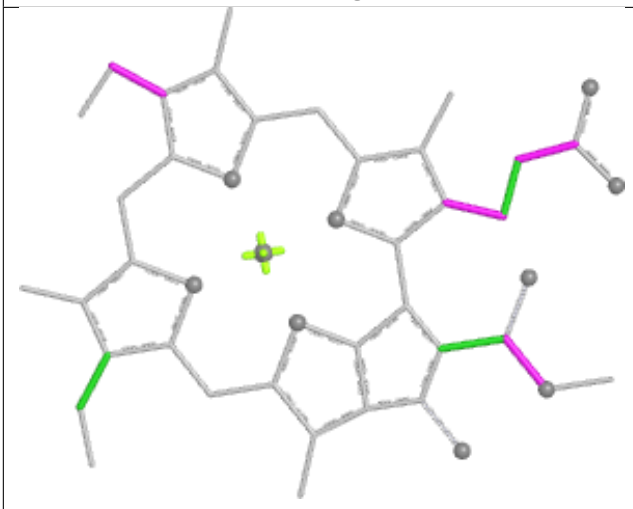
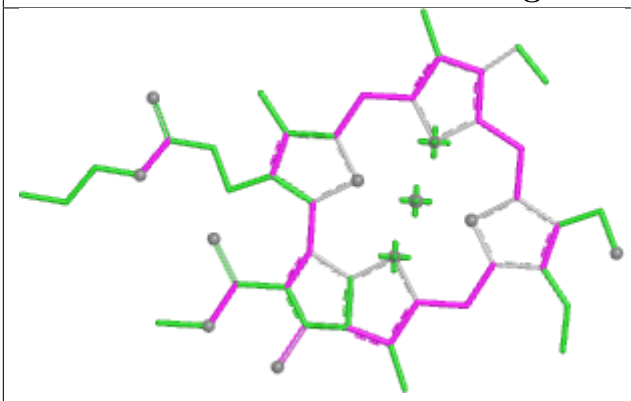


Torsions

Rings

Ligand CHL Y 608



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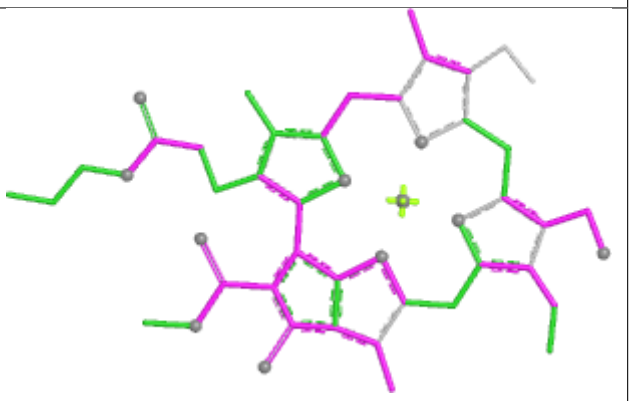
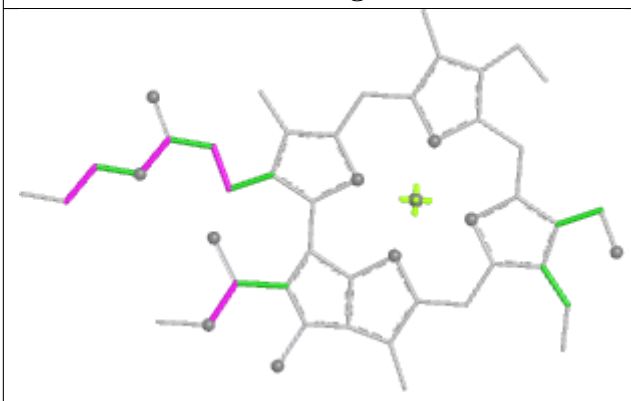


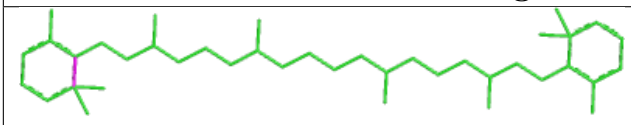
Bond angles



Torsions

Rings

Ligand BCR O 2004



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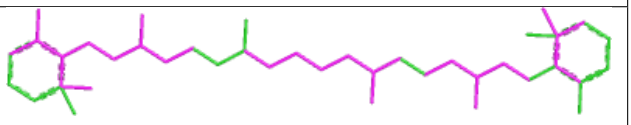
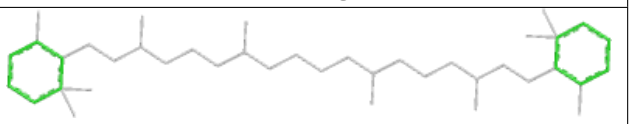


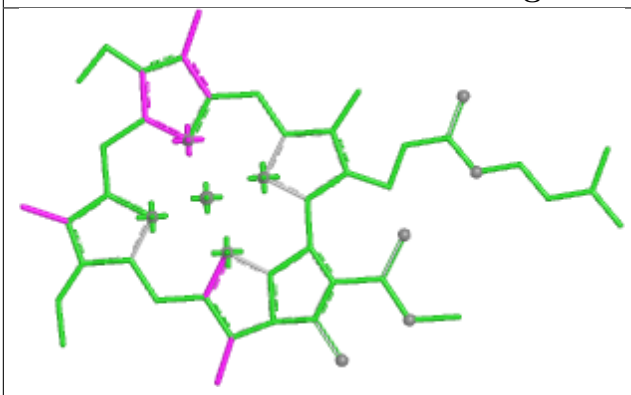
Bond angles

Torsions



Rings

Ligand CLA A 838



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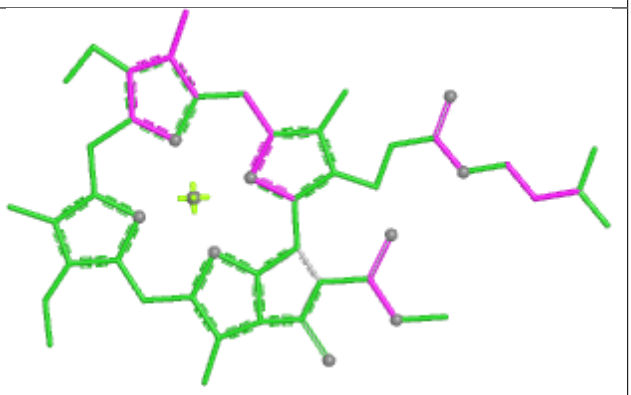
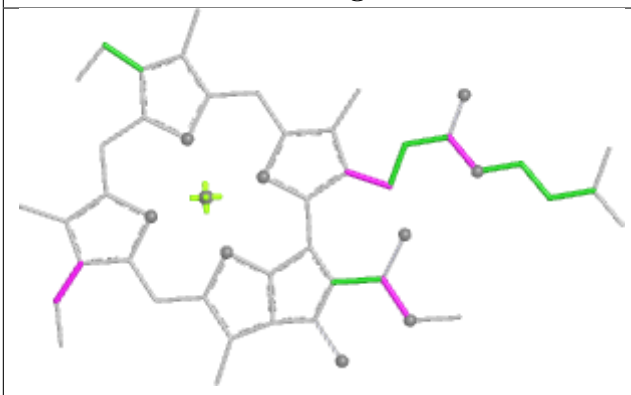


Bond angles



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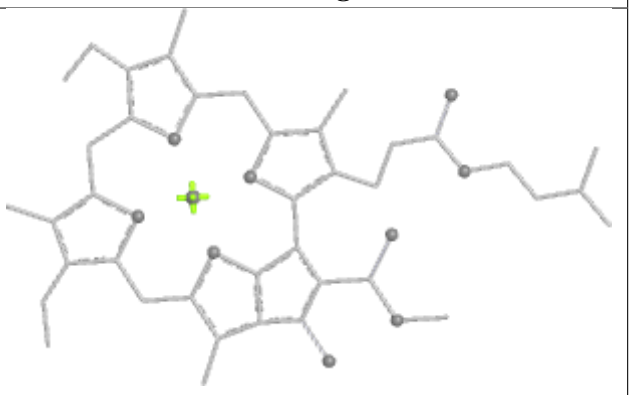
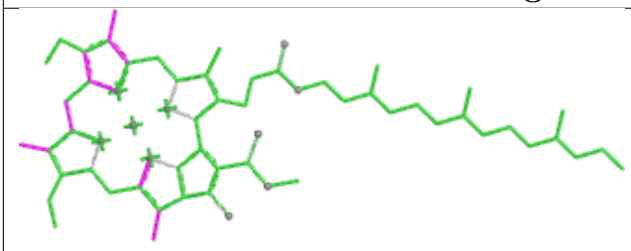


Rings

Ligand CLA B 814



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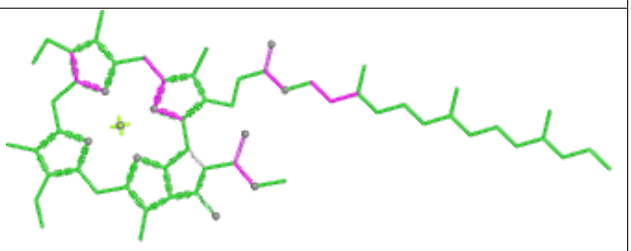
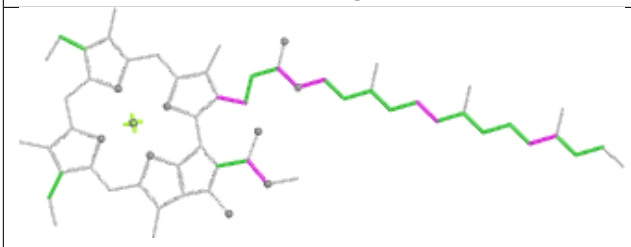
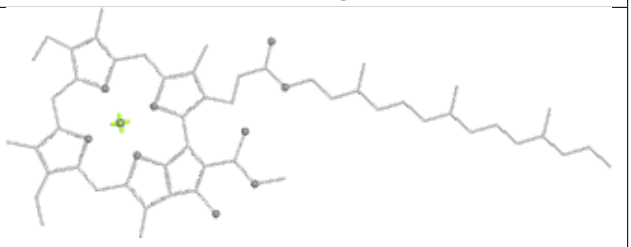


Bond angles

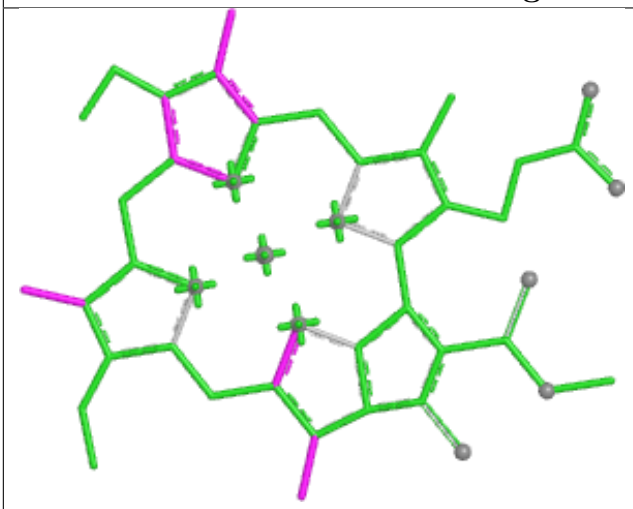


Torsions

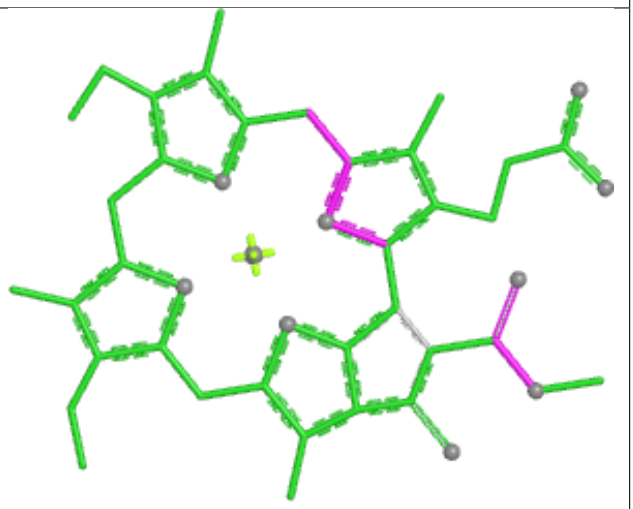


Rings

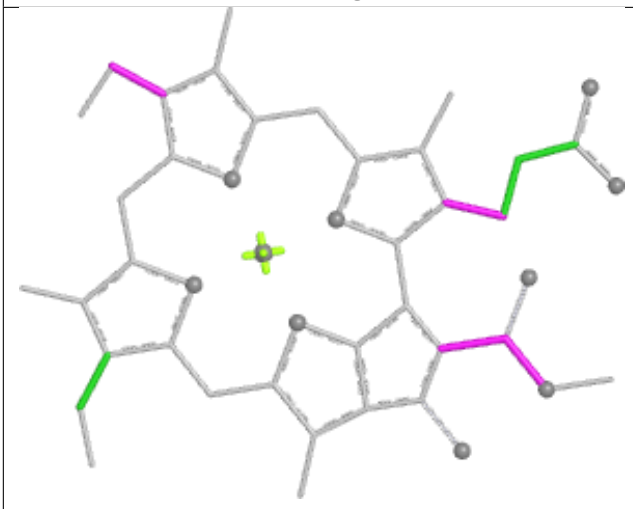
Ligand CLA K 201



Bond lengths



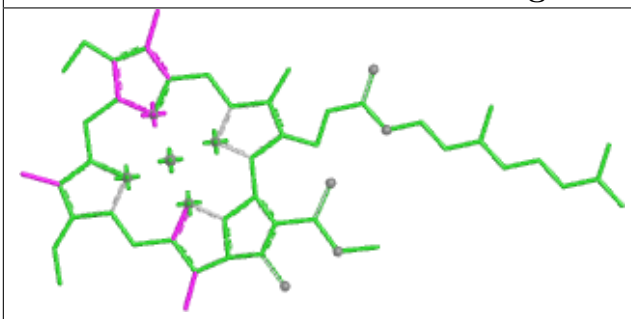
Bond angles



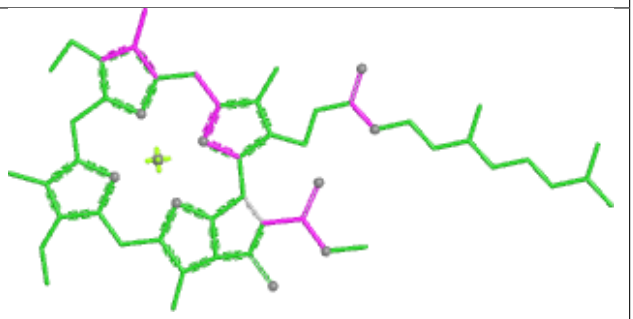
Torsions

Rings

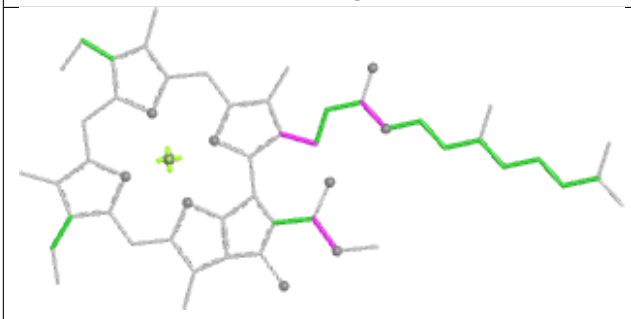
Ligand CLA 3 603



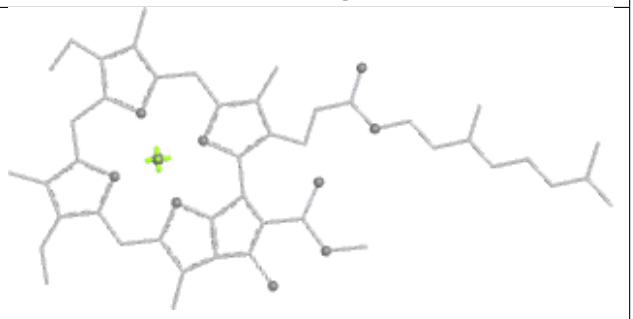
Bond lengths



Bond angles

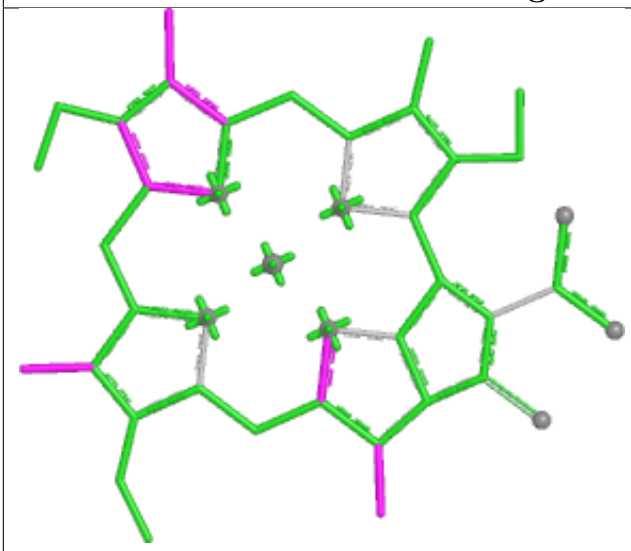


Torsions



Rings

Ligand CLA 4 612



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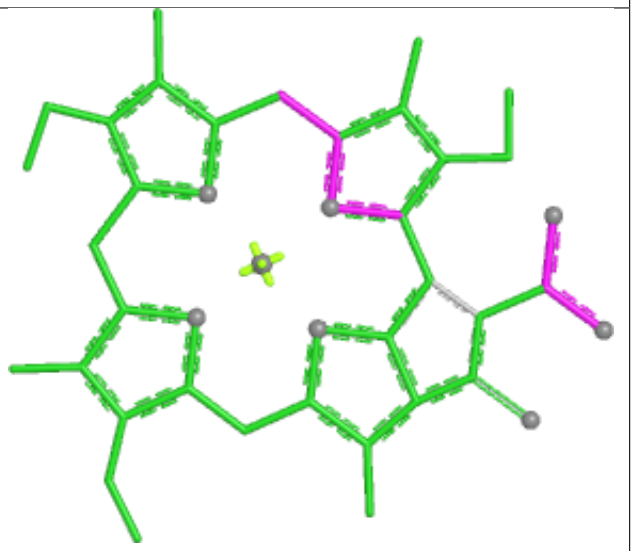
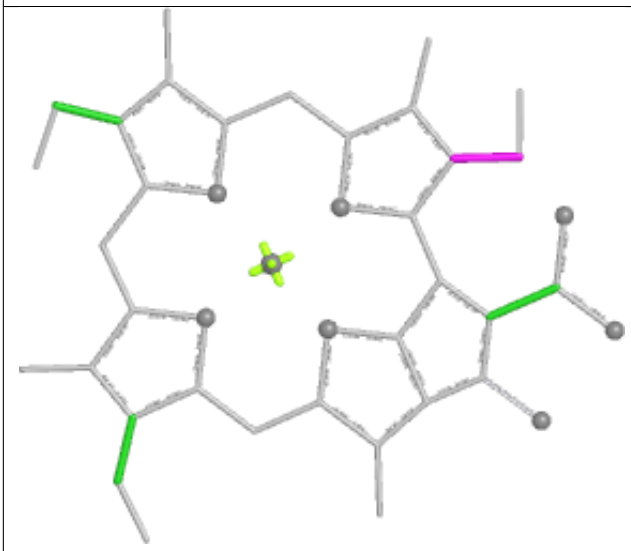


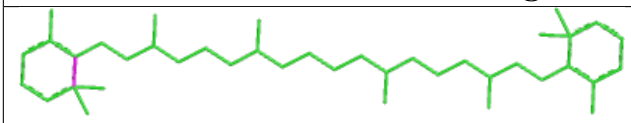
Bond angles



Torsions

Rings

Ligand BCR B 853



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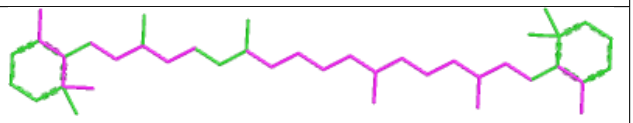
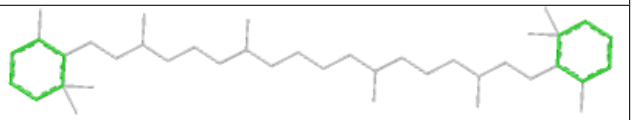


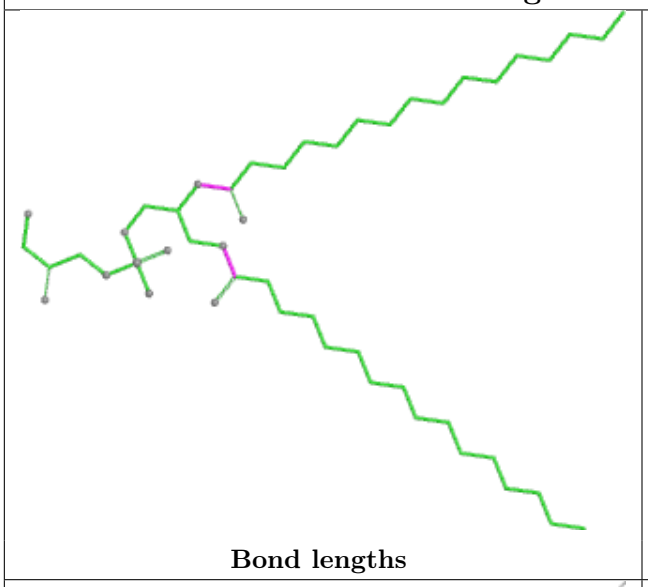
Bond angles

Torsions

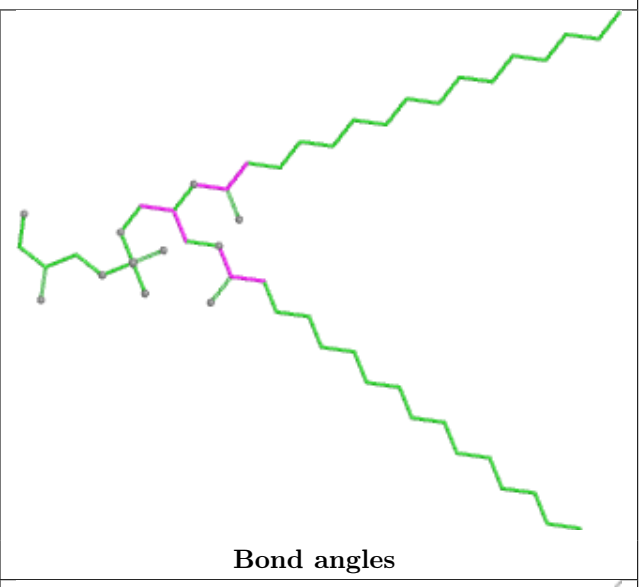


Rings

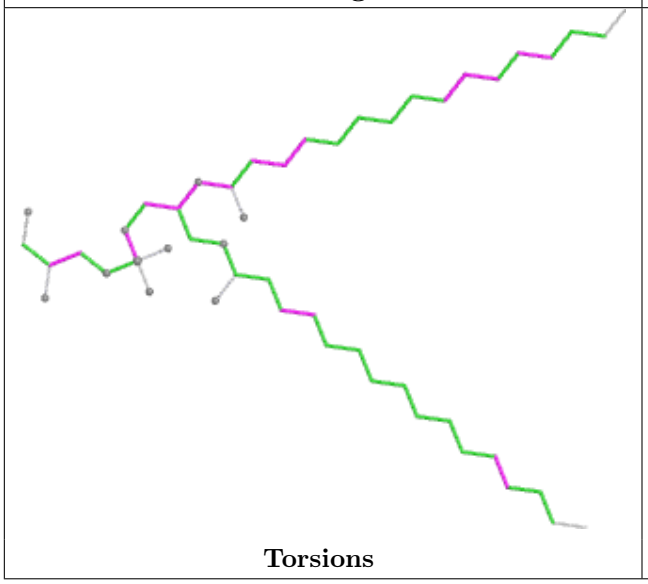
Ligand LHG B 854



Bond lengths



Bond angles



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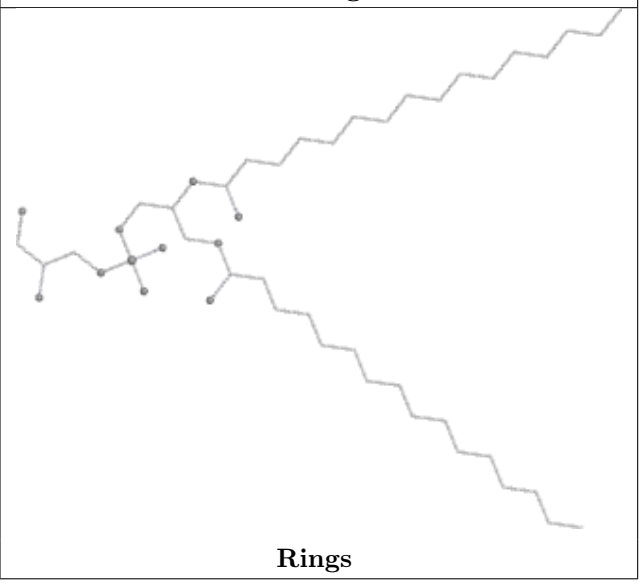
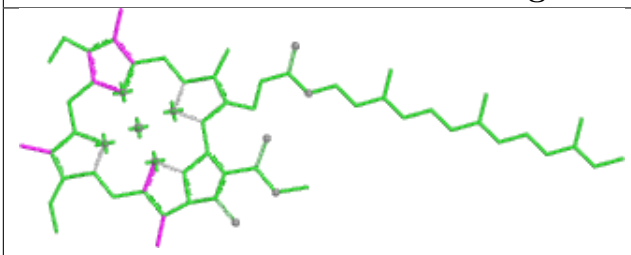
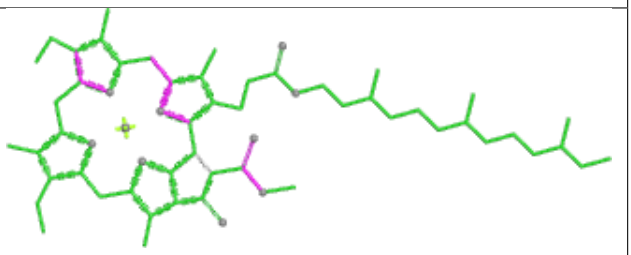
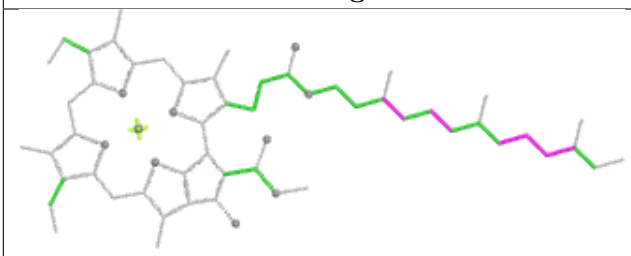
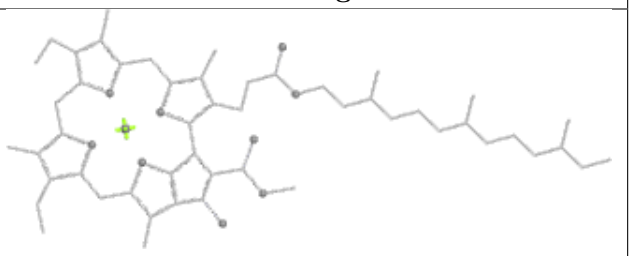
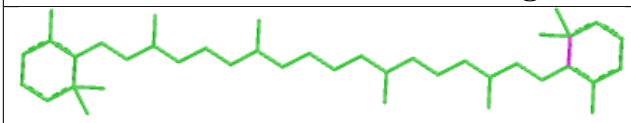
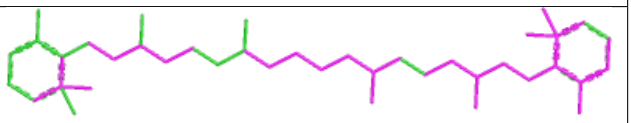
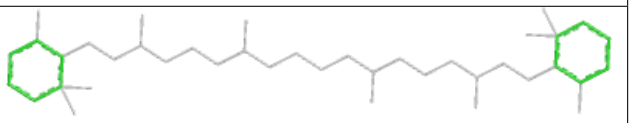
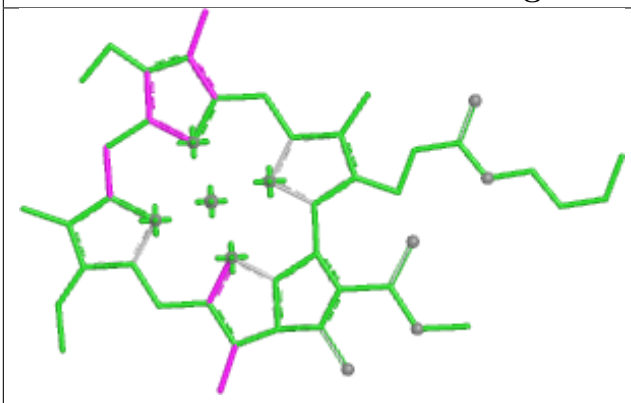


Rings

Ligand CLA 9 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR K 207	
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand CLA X 604



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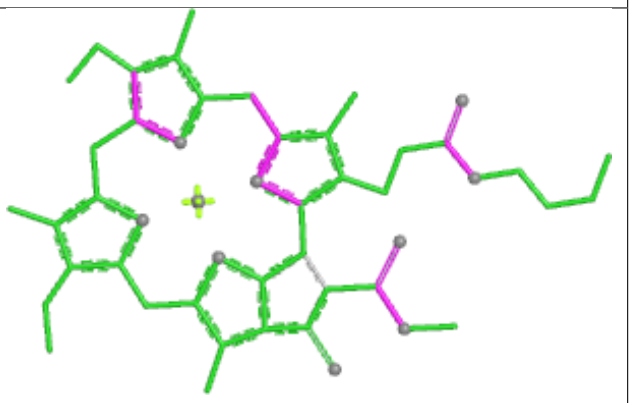
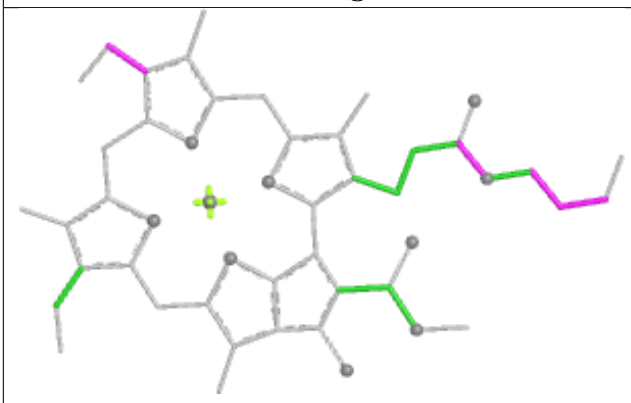
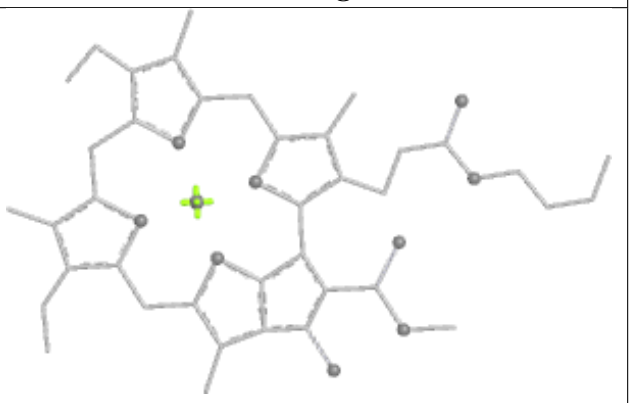


Bond angles

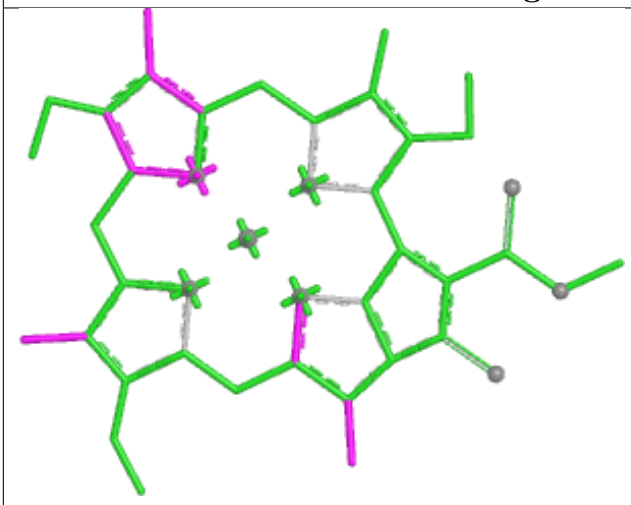


Torsions

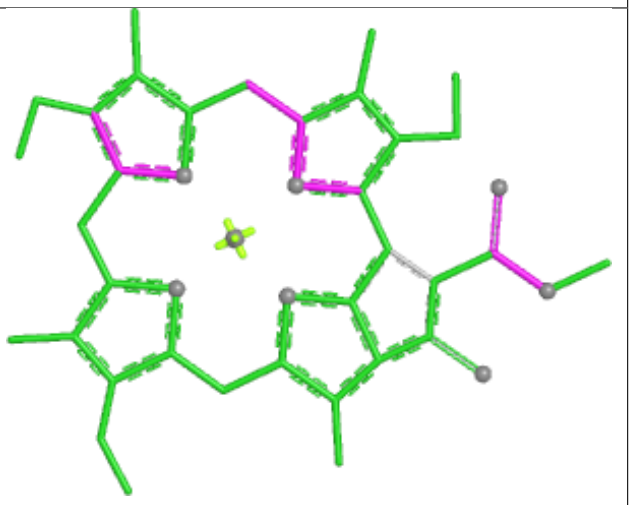


Rings

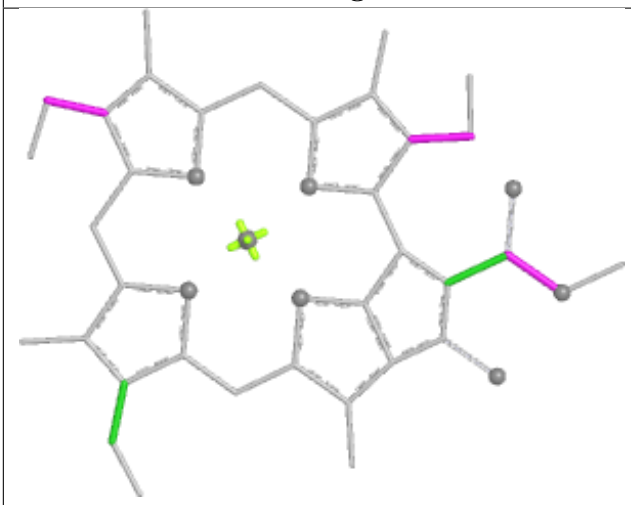
Ligand CLA U 611



Bond lengths



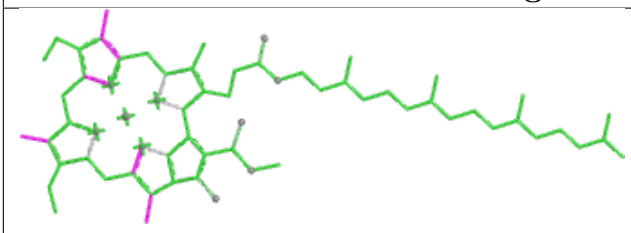
Bond angles



Torsions

Rings

Ligand CLA B 829



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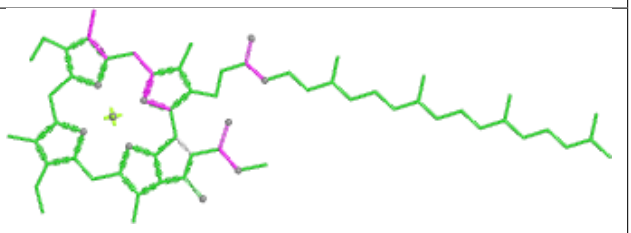
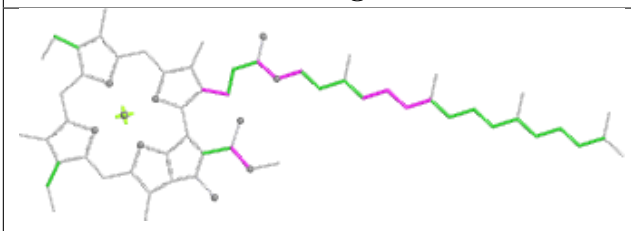
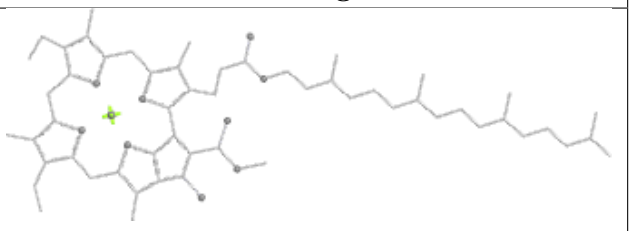


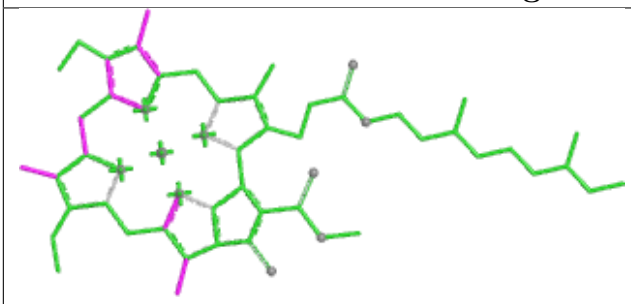
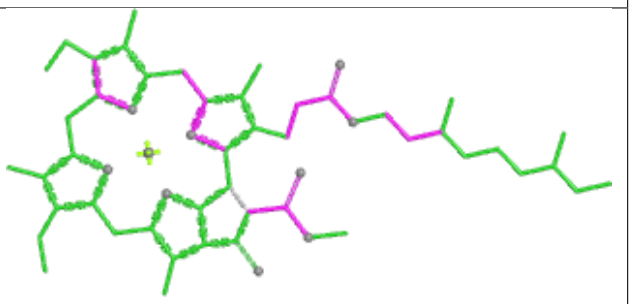
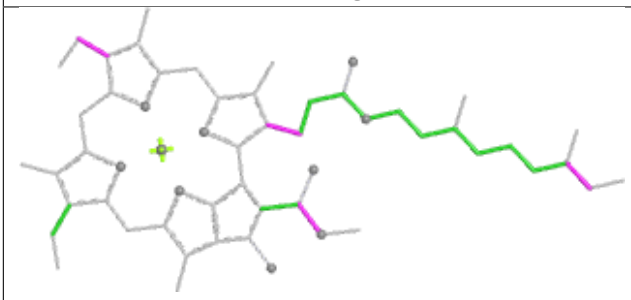
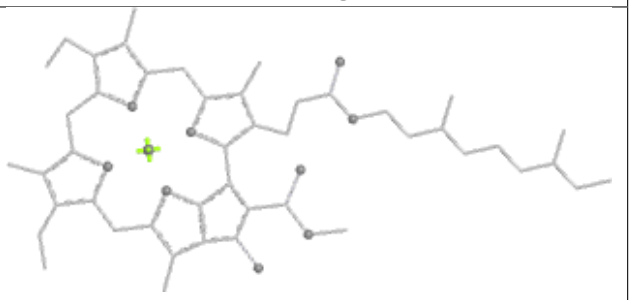
Bond angles

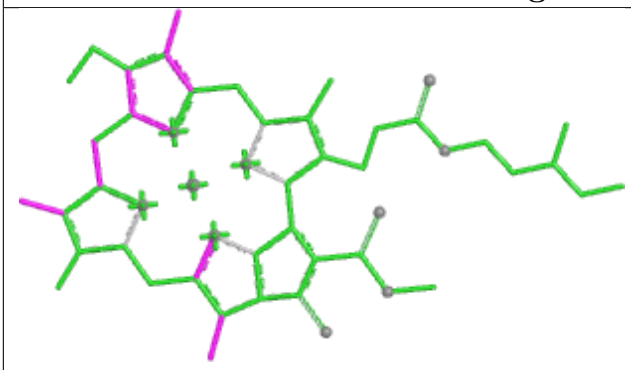
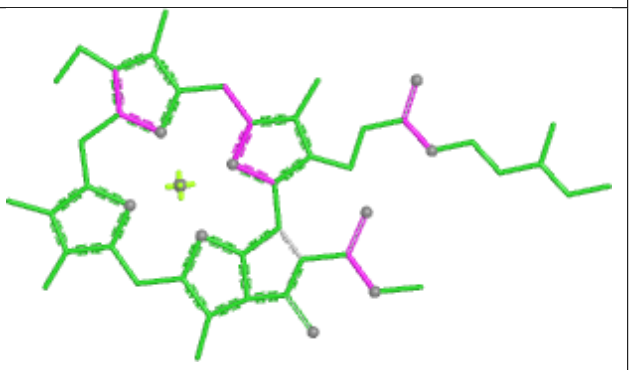
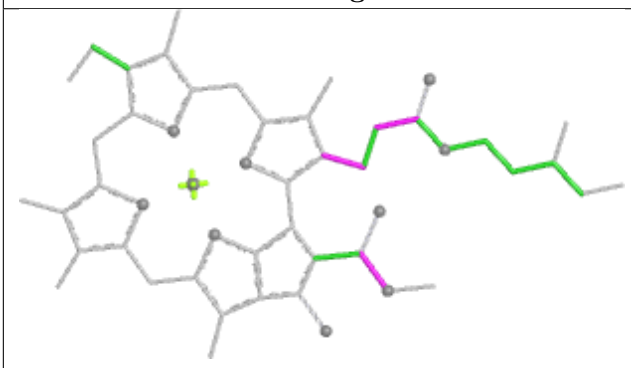
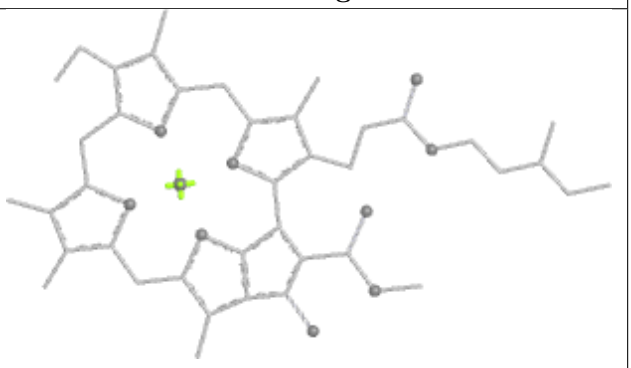


Torsions

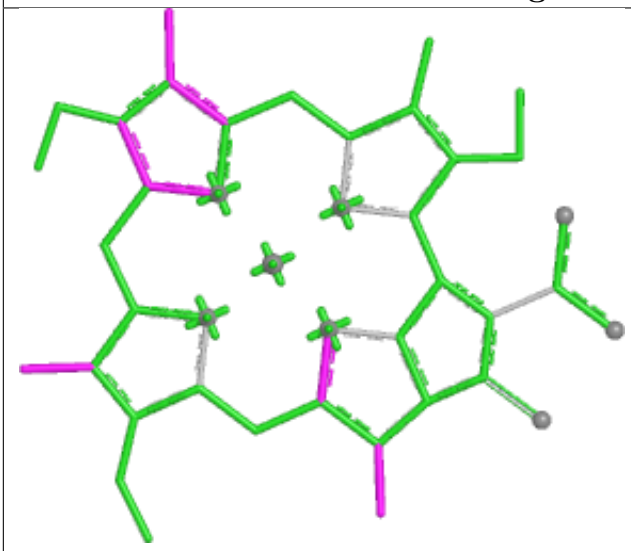


Rings

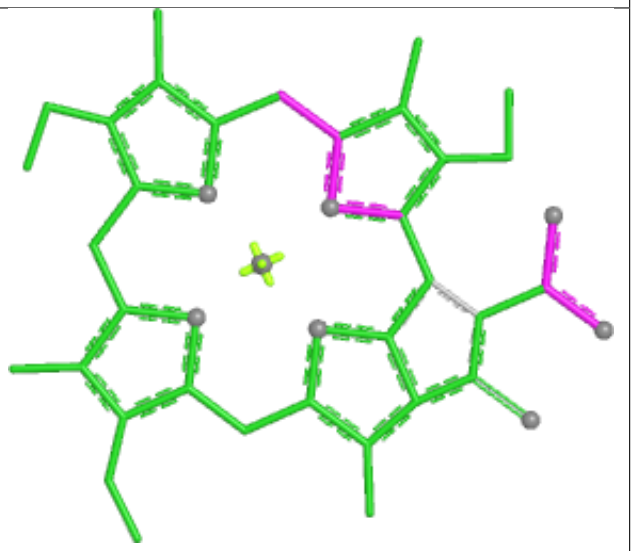
Ligand CLA K 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

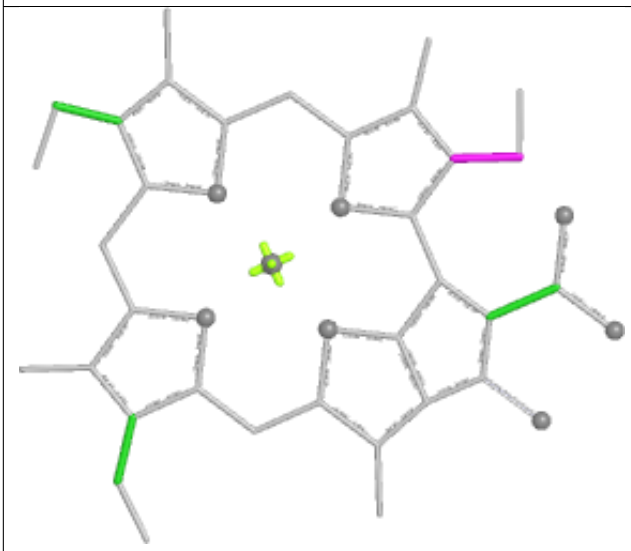
Ligand CLA 6 612



Bond lengths



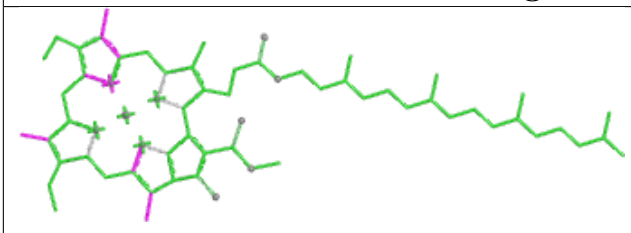
Bond angles



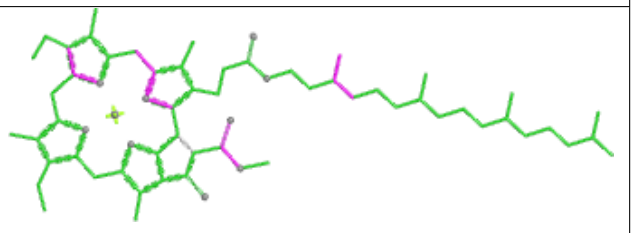
Torsions

Rings

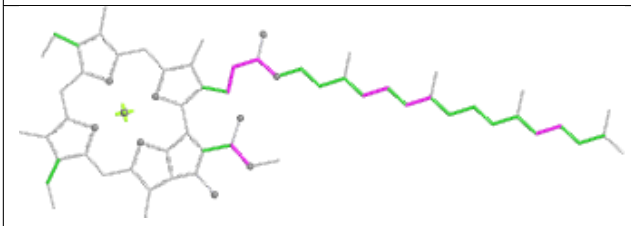
Ligand CLA A 830



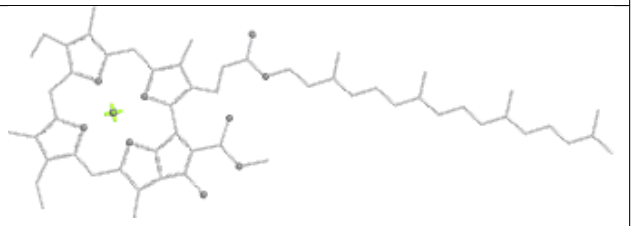
Bond lengths



Bond angles

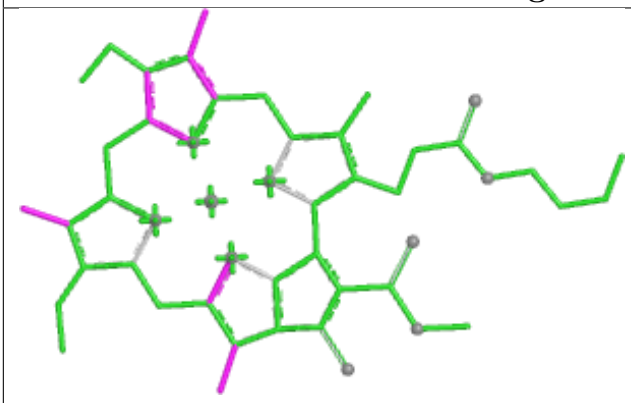


Torsions

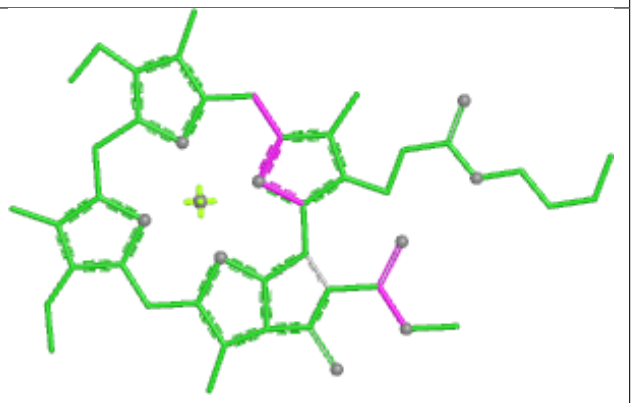


Rings

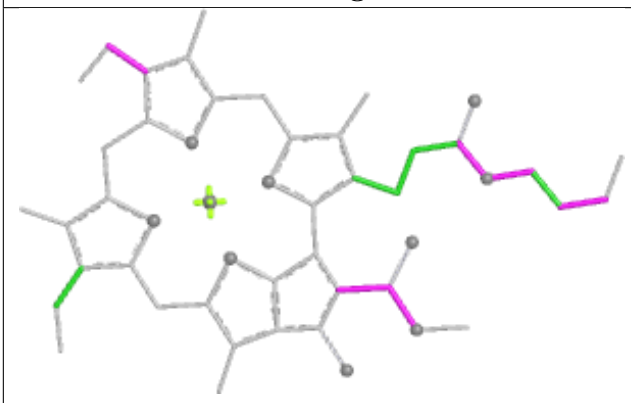
Ligand CLA a 604



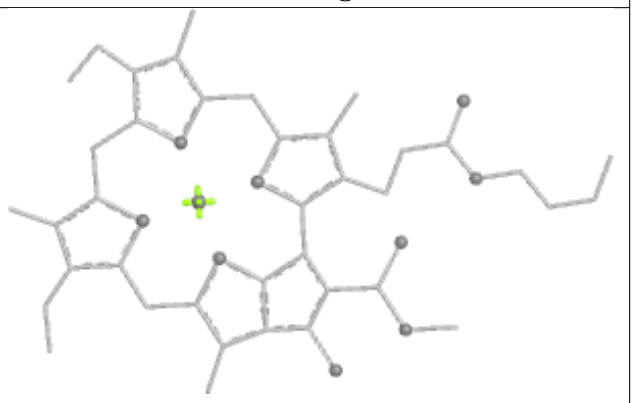
Bond lengths



Bond angles

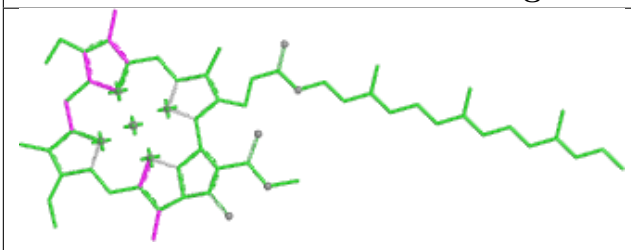


Torsions

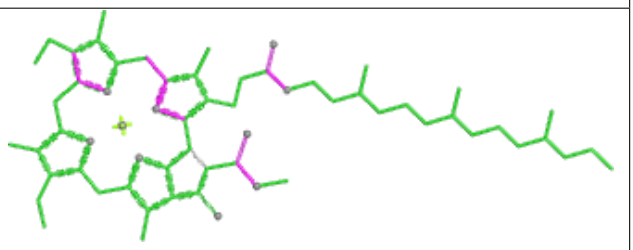


Rings

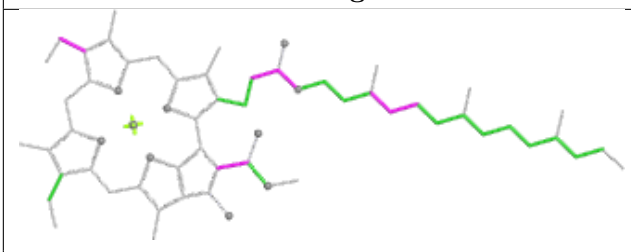
Ligand CLA X 603



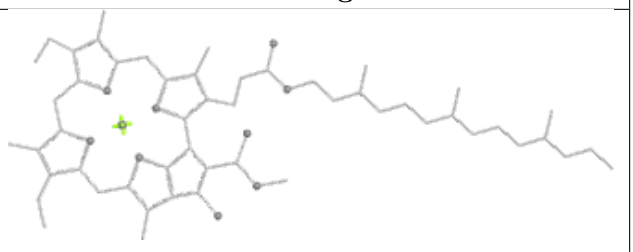
Bond lengths



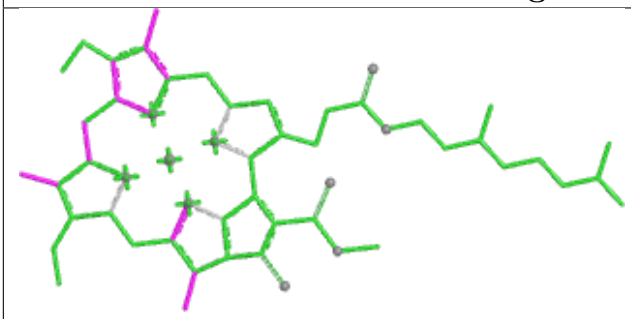
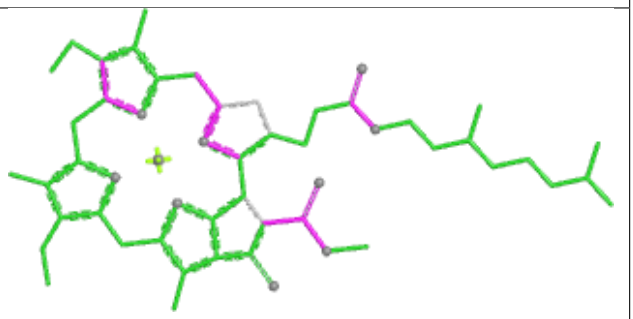
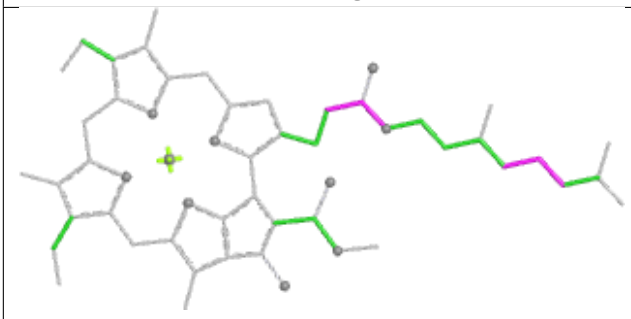
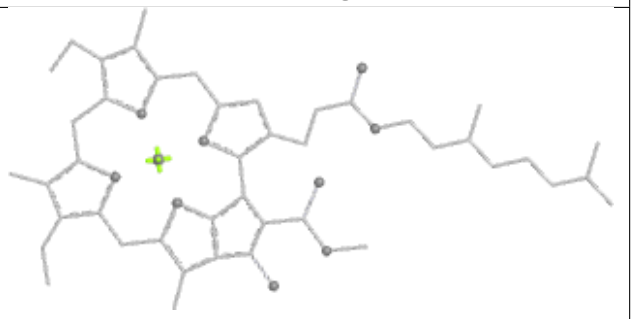
Bond angles

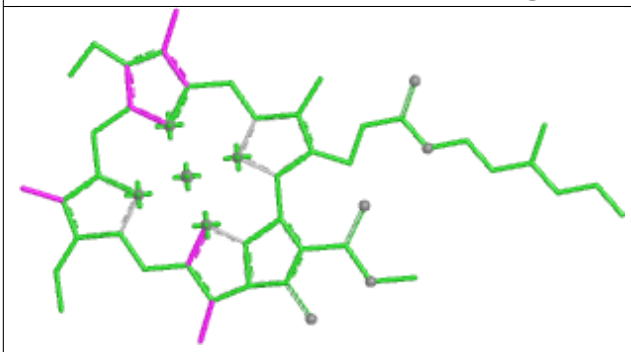
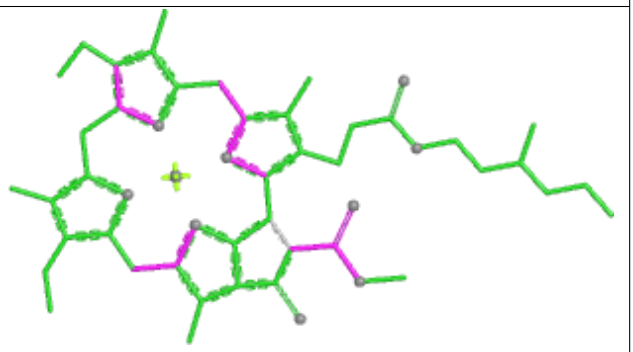
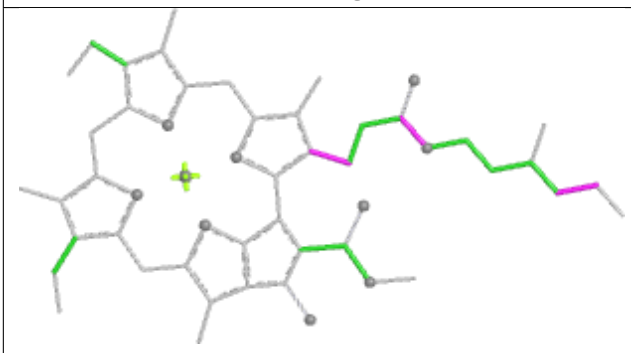
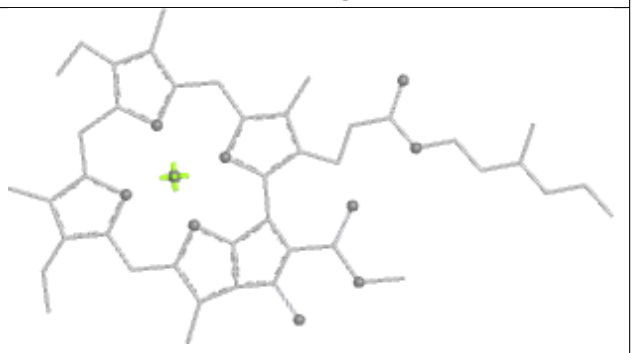


Torsions

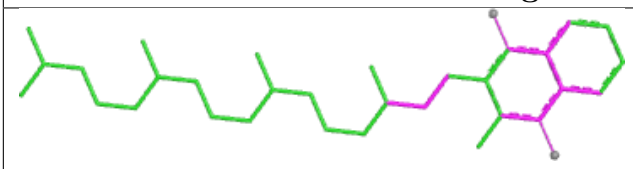


Rings

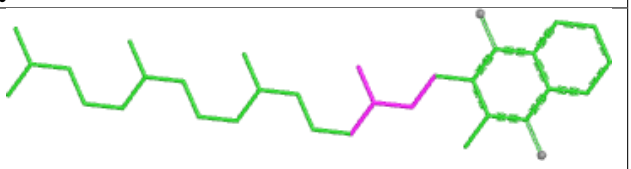
Ligand CLA a 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

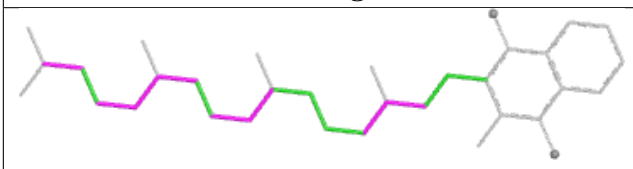
Ligand PQN A 844



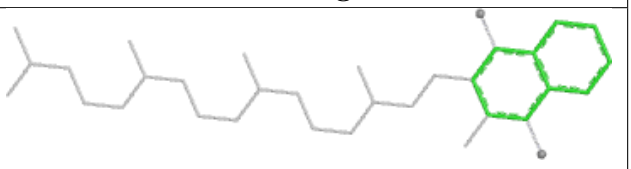
Bond lengths



Bond angles

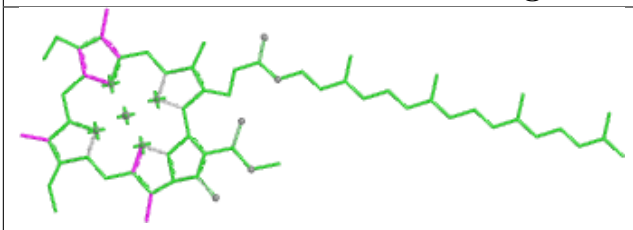


Torsions



Rings

Ligand CLA A 816



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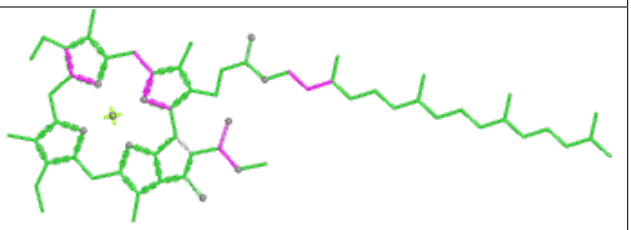
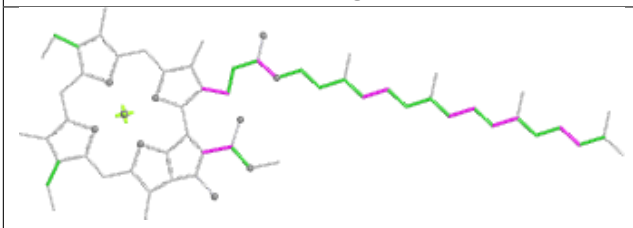
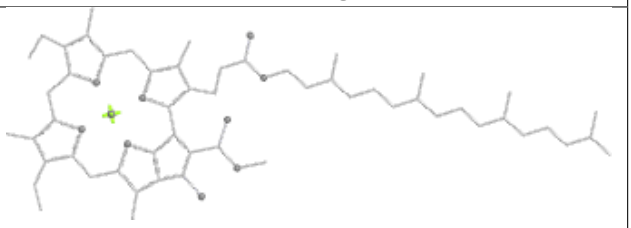


Bond angles

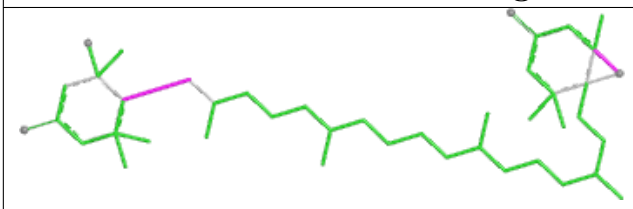


Torsions

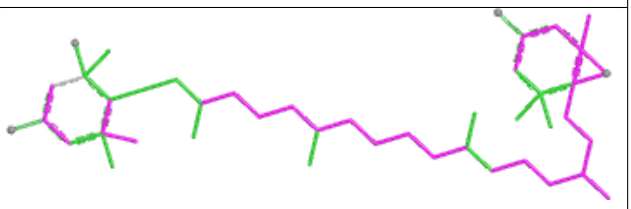


Rings

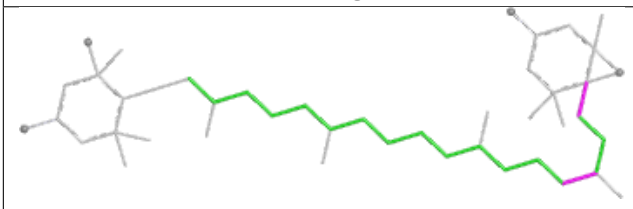
Ligand NEX X 1623



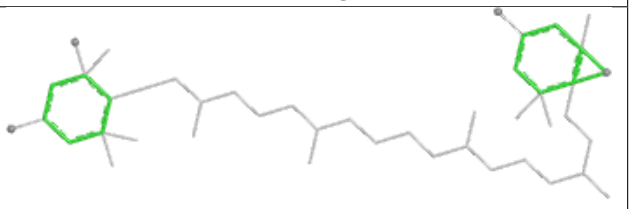
Bond lengths



Bond angles

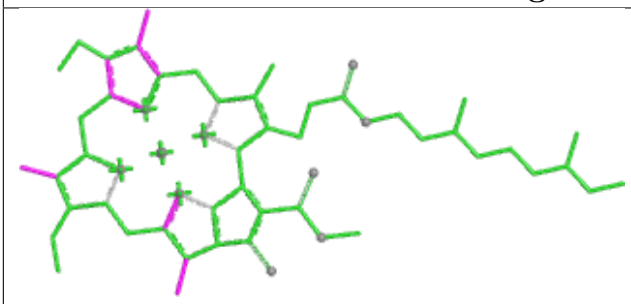


Torsions

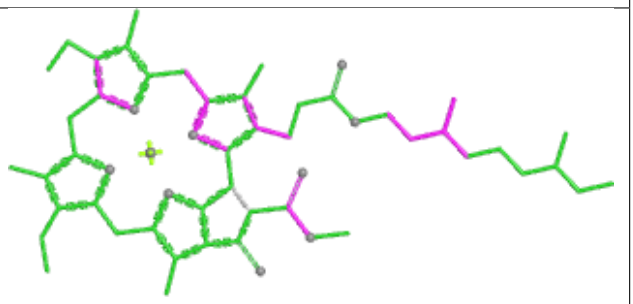


Rings

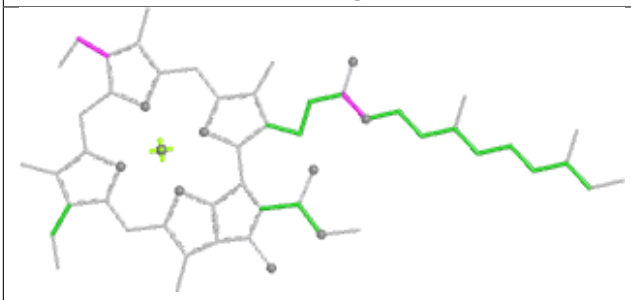
Ligand CLA 5 601



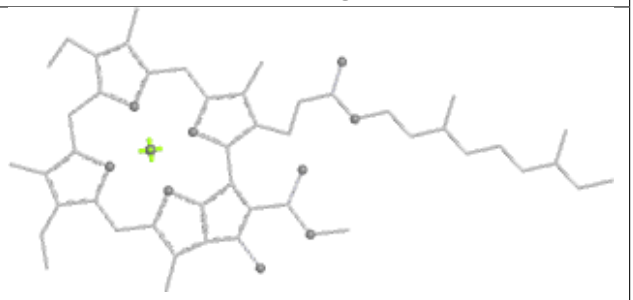
Bond lengths



Bond angles

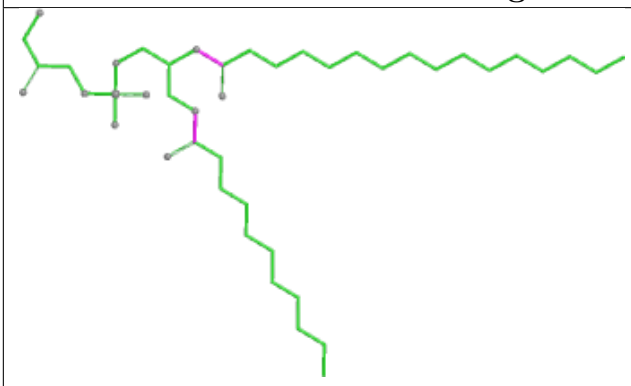


Torsions

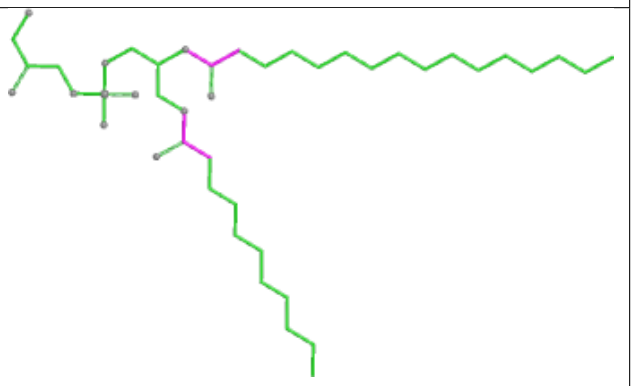


Rings

Ligand LHG W 2630

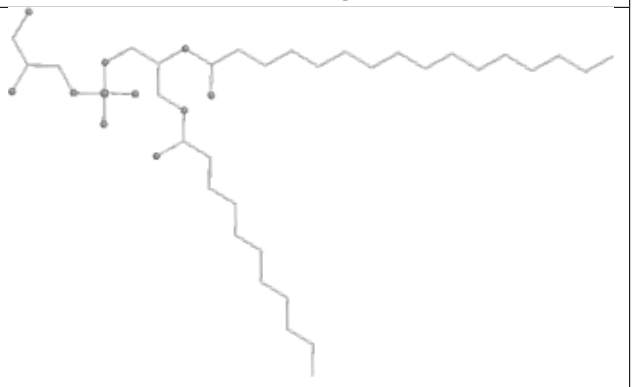


Bond lengths



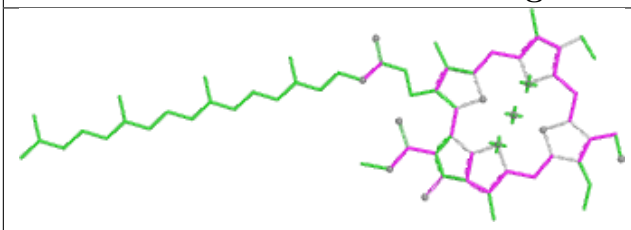
Bond angles

Torsions

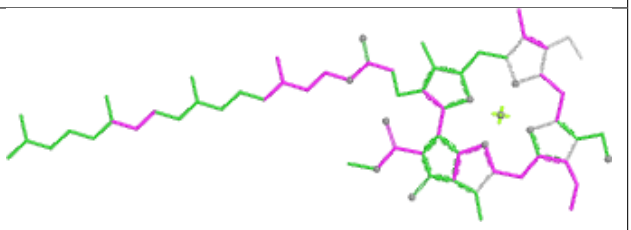


Rings

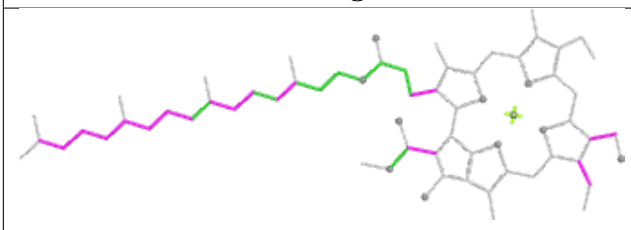
Ligand CHL Z 609



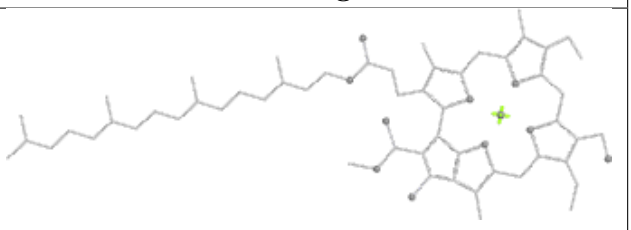
Bond lengths



Bond angles

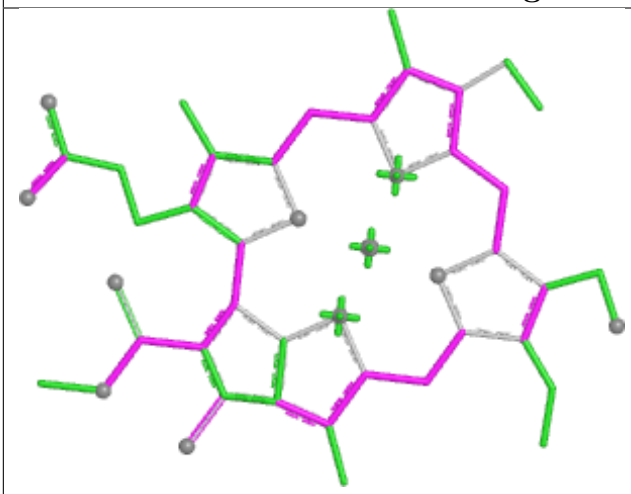


Torsions

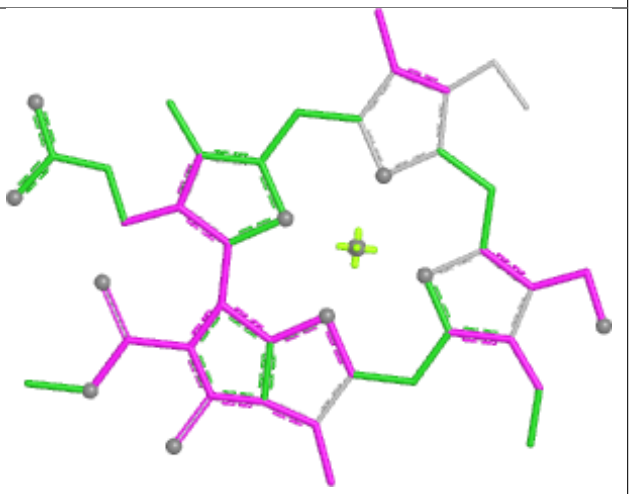


Rings

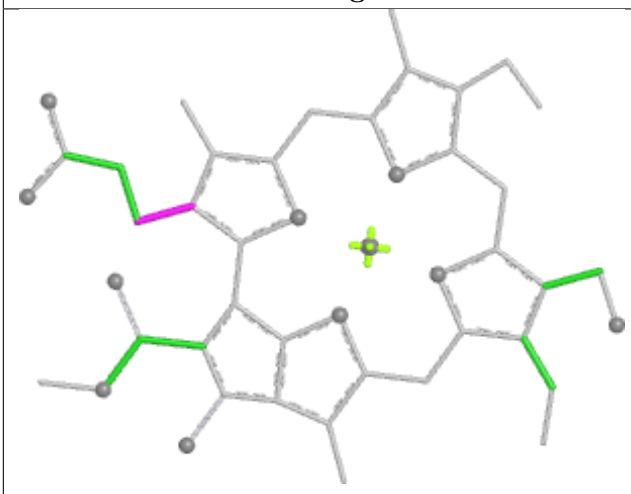
Ligand CHL V 607



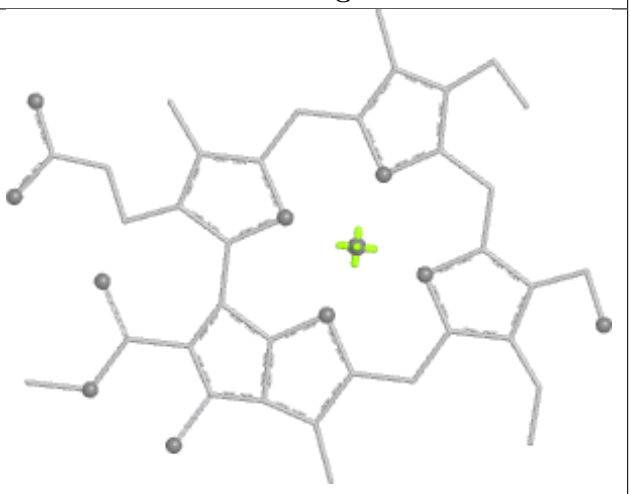
Bond lengths



Bond angles

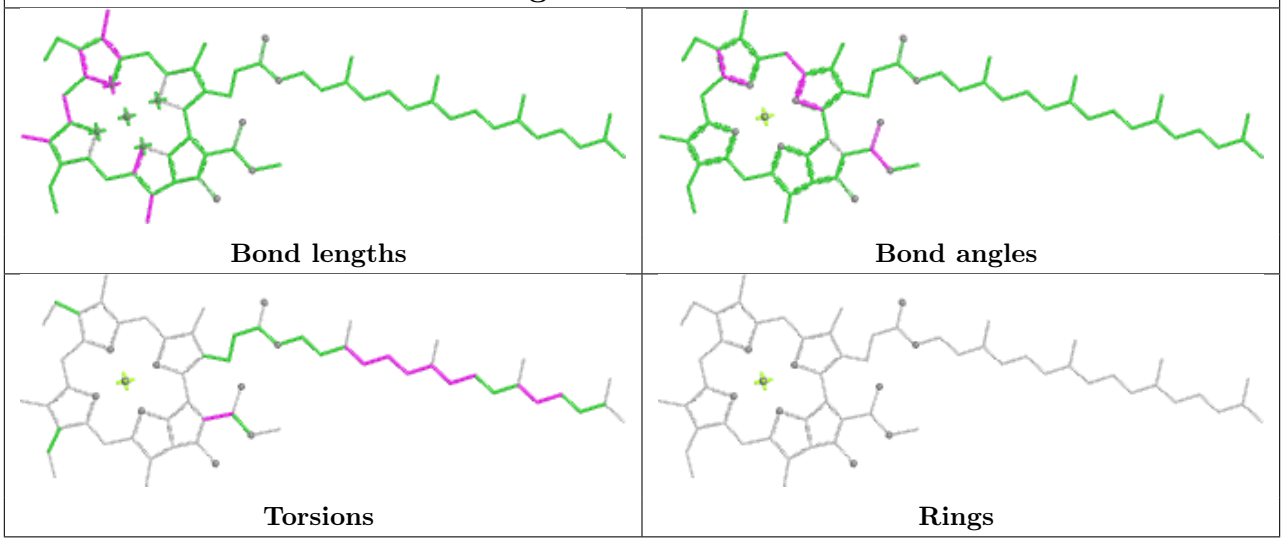


Torsions

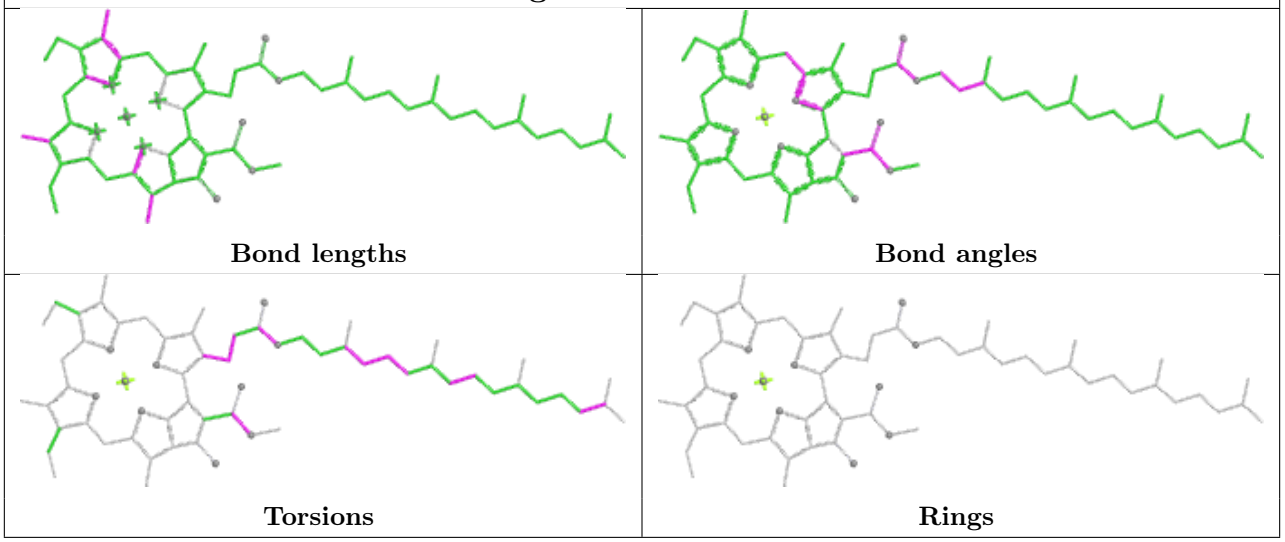


Rings

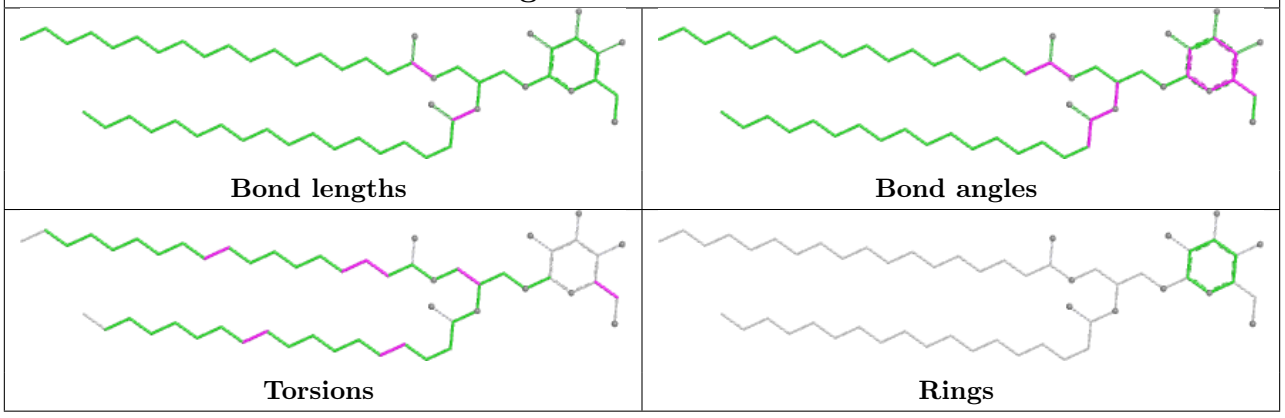
Ligand CLA 7 602



Ligand CLA 4 601



Ligand LMG H 205



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.

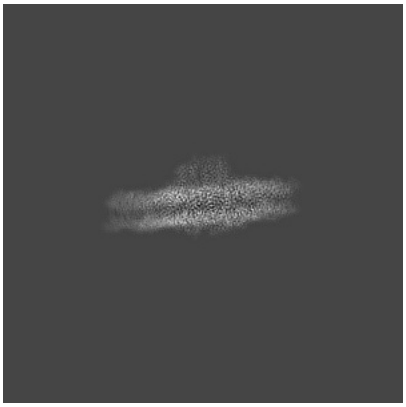
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30925. These allow visual inspection of the internal detail of the map and identification of artifacts.

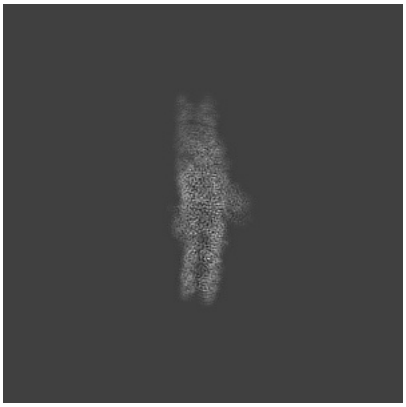
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

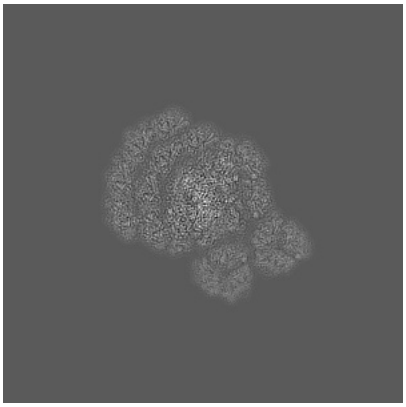
6.1.1 Primary map



X



Y

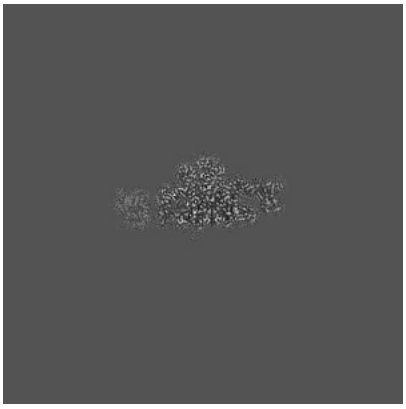


Z

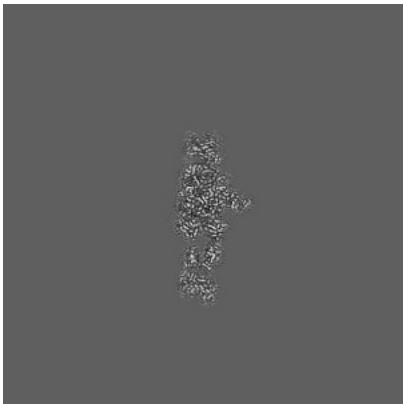
The images above show the map projected in three orthogonal directions.

6.2 Central slices

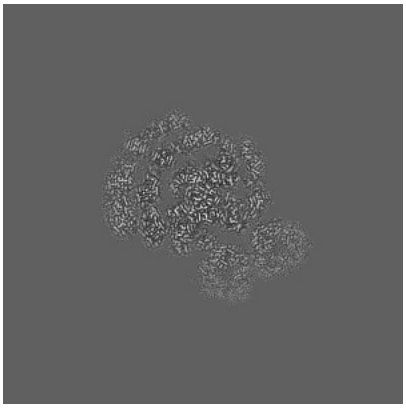
6.2.1 Primary map



X Index: 240



Y Index: 240

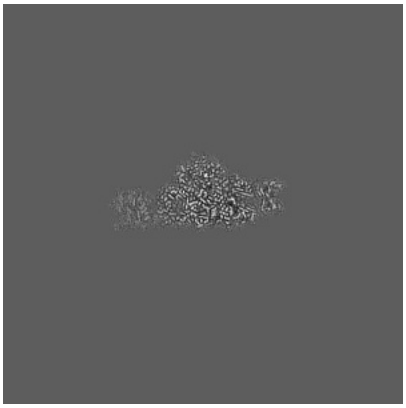


Z Index: 240

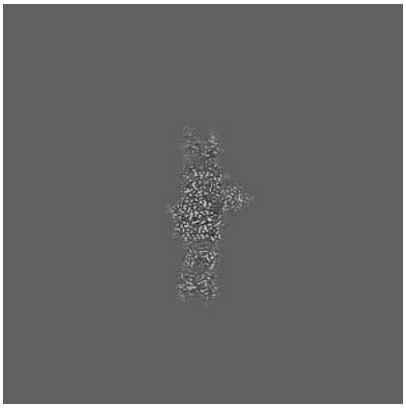
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

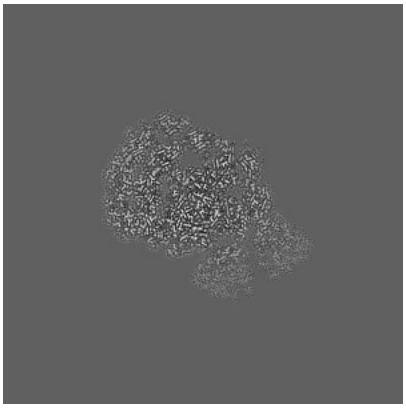
6.3.1 Primary map



X Index: 243



Y Index: 231

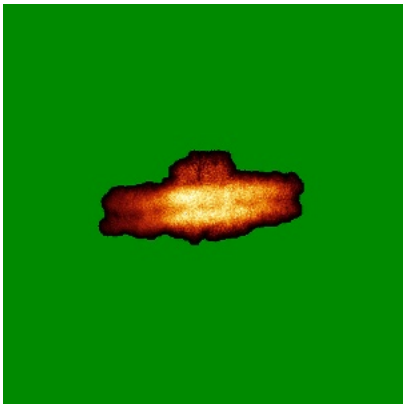


Z Index: 248

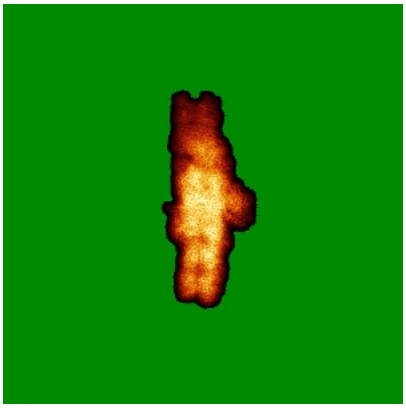
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

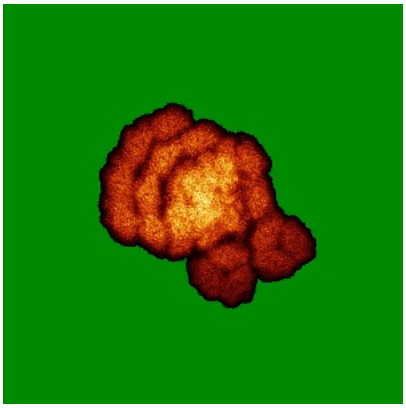
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

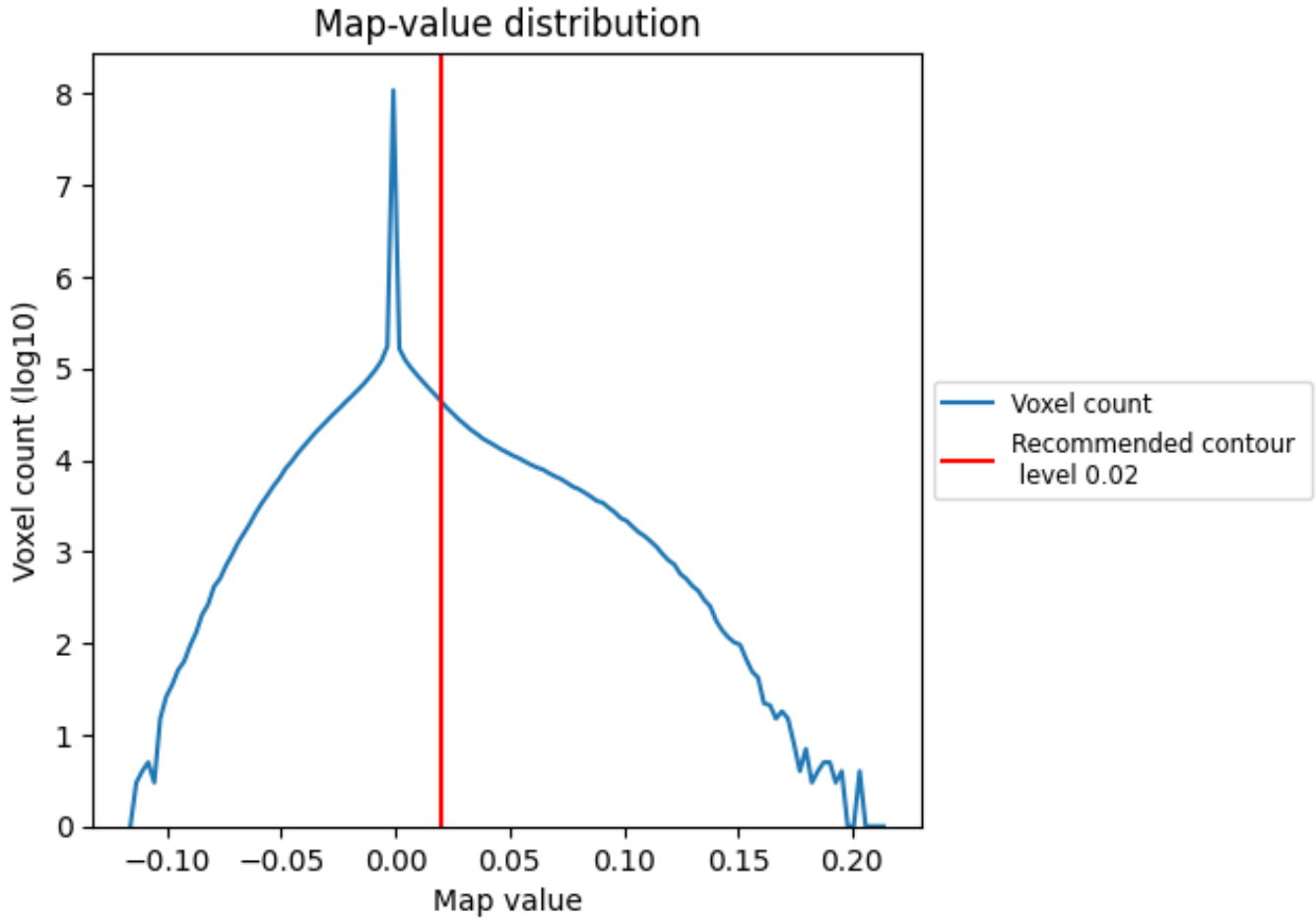
6.6 Mask visualisation (i)

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

7 Map analysis

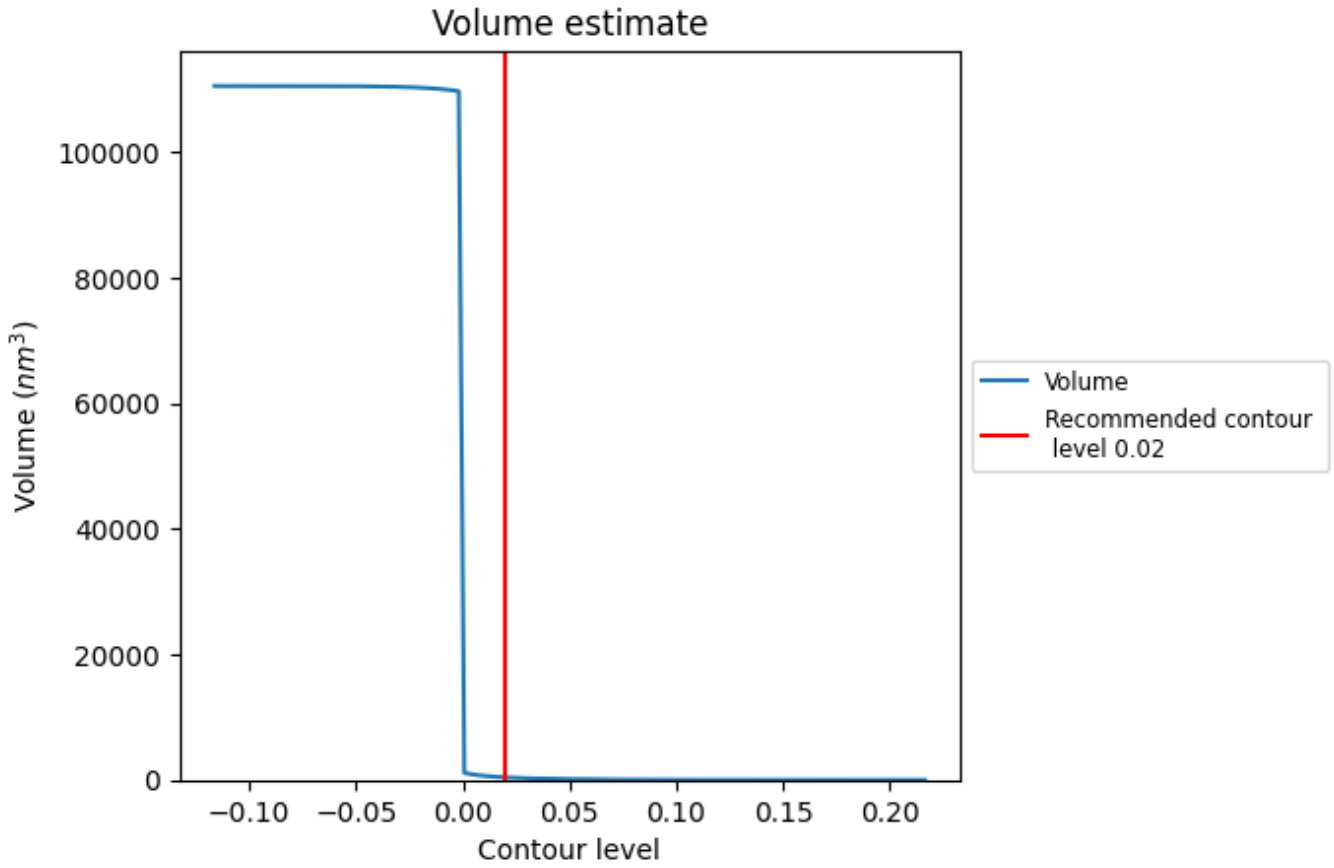
This section contains the results of statistical analysis of the map.

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.

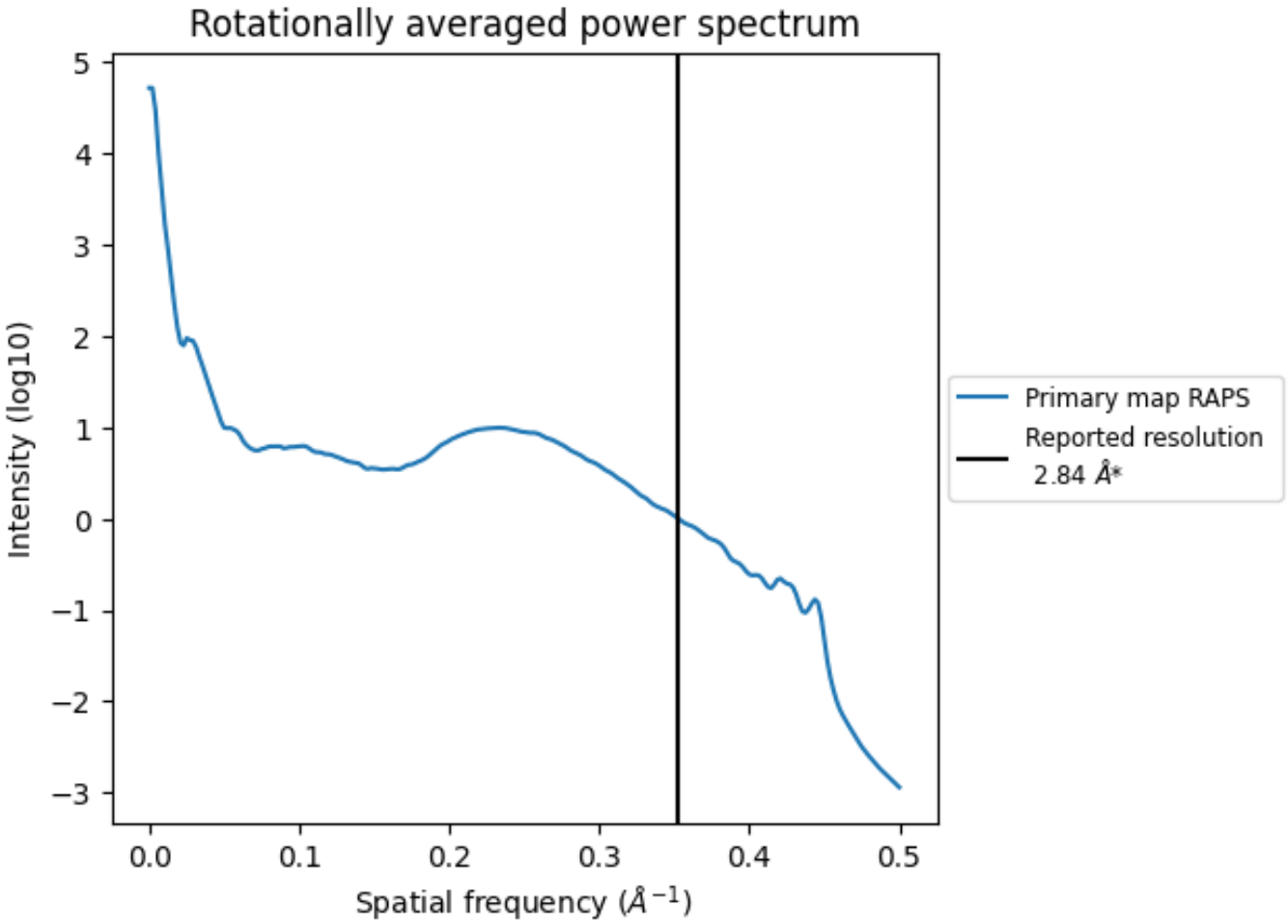
7.2 Volume estimate



The volume at the recommended contour level is 408 nm^3; this corresponds to an approximate mass of 369 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 0.352 Å^{-1}

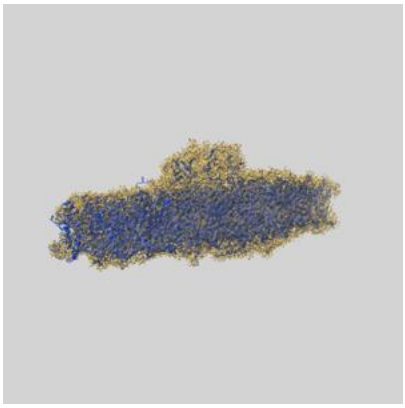
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

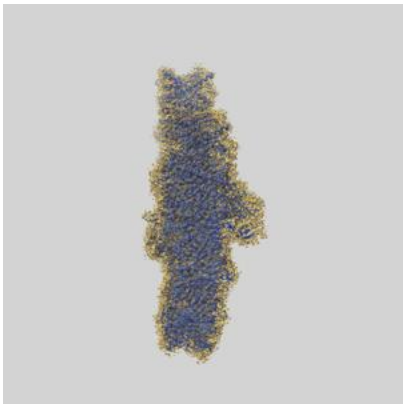
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30925 and PDB model 7DZ7. Per-residue inclusion information can be found in section 3 on page 45.

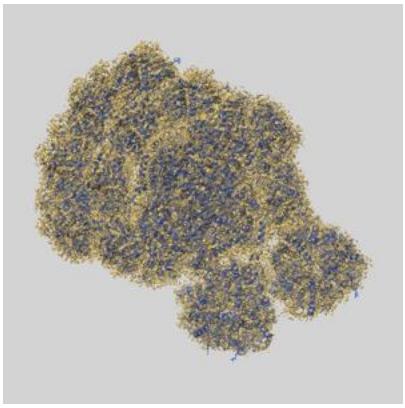
9.1 Map-model overlay



X



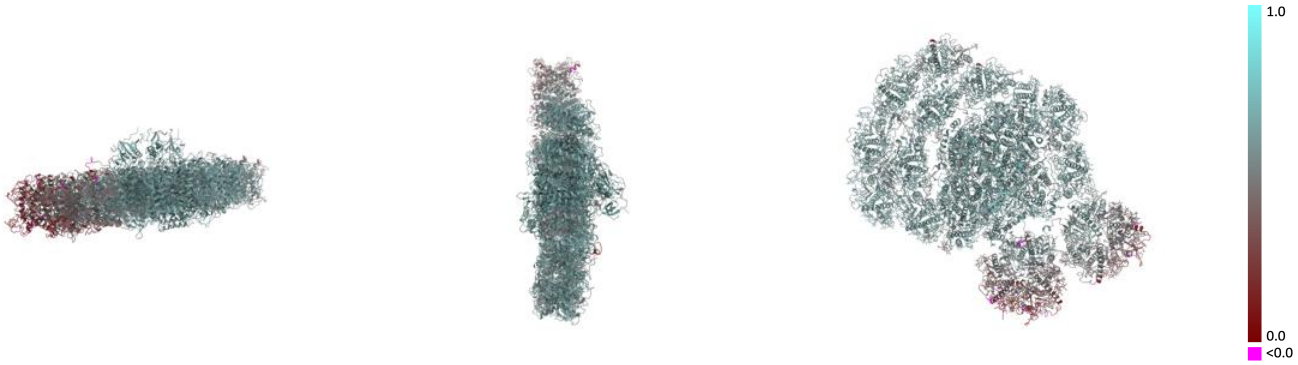
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

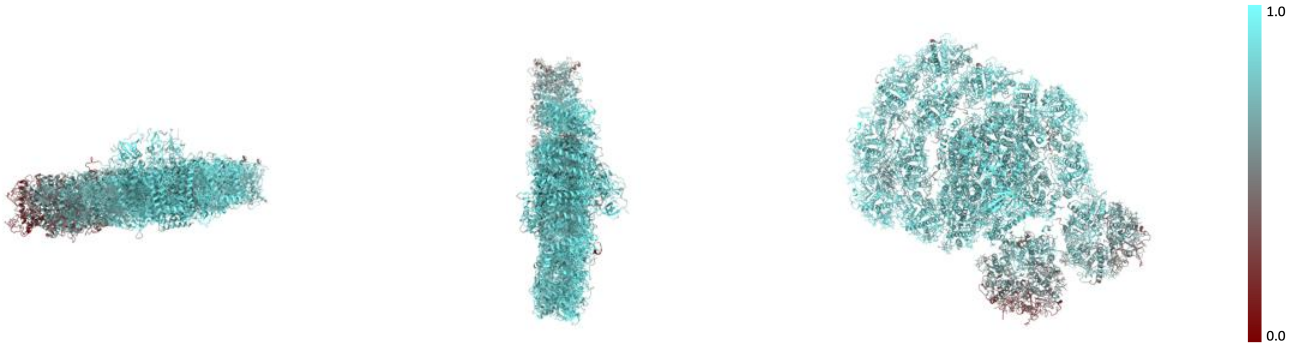
9.2 Q-score mapped to coordinate model



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.

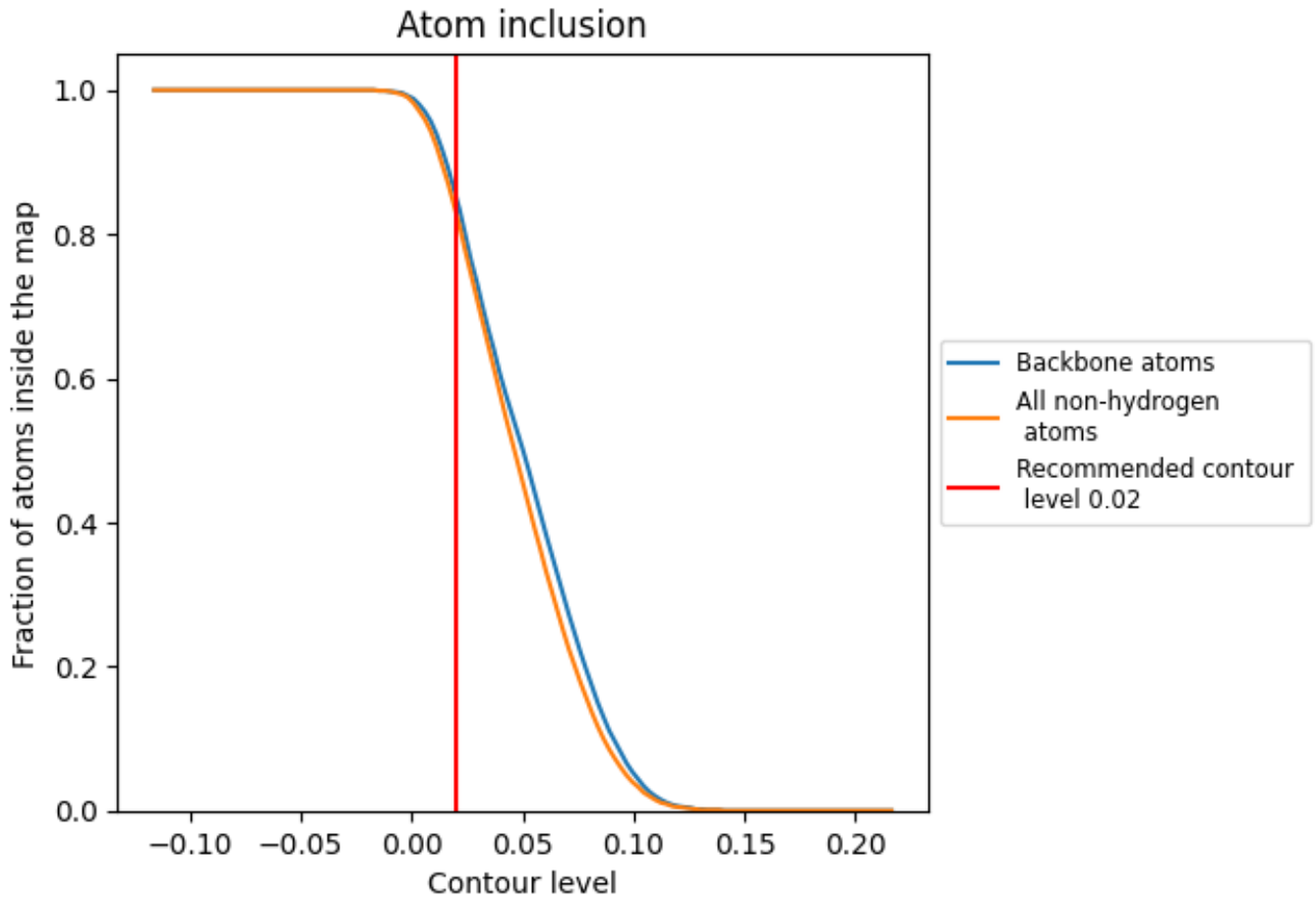
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.5670
1	0.8790	0.5940
2	0.8800	0.5990
3	0.9020	0.6140
4	0.8490	0.5800
5	0.8630	0.5940
6	0.8900	0.5990
7	0.9060	0.6200
8	0.8970	0.6110
9	0.8670	0.5870
A	0.9410	0.6400
B	0.9360	0.6400
C	0.9190	0.6060
D	0.9060	0.6130
E	0.9070	0.6130
F	0.8790	0.6120
G	0.8270	0.5770
H	0.8620	0.5940
I	0.8530	0.5910
J	0.8680	0.6090
K	0.8660	0.5900
L	0.9110	0.6180
O	0.8830	0.5910
U	0.6390	0.4250
V	0.7890	0.5490
W	0.5720	0.3910
X	0.4220	0.2990
Y	0.4770	0.3310
Z	0.7410	0.5250
a	0.8060	0.5410