Full wwPDB EM Validation Report

Mar 10, 2026 – 03:52 PM UTC

PDB ID	:	7DZ8 / pdb_00007dz8
EMDB ID	:	EMD-30926
Title	:	State transition supercomplex PSI-LHCI-LHCII from the LhcbM1 lacking mutant of Chlamydomonas reinhardtii
Authors	:	Pan, X.W.; Li, A.J.; Liu, Z.F.; Li, M.
Deposited on	:	2021-01-23
Resolution	:	3.16 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:

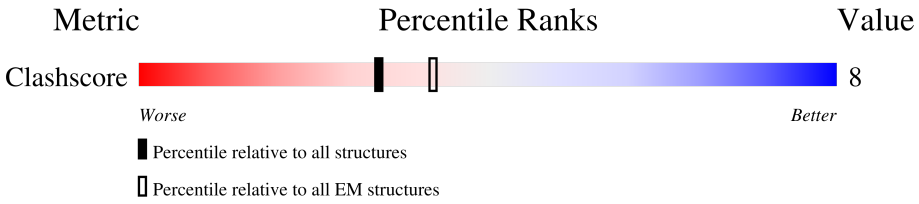
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

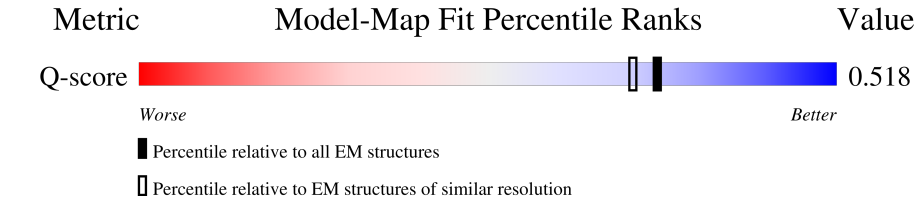
1 Overall quality at a glance

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

The reported resolution of this entry is 3.16 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	-
Q-score	-	25397	14474 (2.66 - 3.66)

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	84% 15%
2	B	735	82% 18%
3	C	81	78% 20%
4	D	196	62% 10% 27%
5	E	97	60% 5% 35%
6	F	227	65% 7% 27%

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Mol	Chain	Length	Quality of chain
7	G	126	65% 10% 25%
8	H	130	67% 10% 23%
9	I	106	29% 10% 60%
10	J	41	93% 7%
11	K	113	65% 11% 24%
12	L	196	72% 9% 19%
13	O	126	64% 13% 23%
14	1	228	66% 19% 15%
14	a	228	69% 16% 15%
15	2	246	78% 11% 12%
16	3	298	63% 11% 26%
17	4	264	70% 9% 20%
18	5	257	74% 14% 12%
19	6	257	81% 9% 11%
20	7	241	80% 8% 12%
21	8	243	80% 9% 11%
22	9	213	71% 15% 14%
23	W	249	71% 17% 12%
23	X	249	71% 18% 11%
24	U	257	66% 19% 15%
24	Y	257	73% 12% 15%
24	Z	257	70% 16% 14%
25	V	268	73% 16% 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
26	CLA	1	602	X	-	-	-
26	CLA	1	603	X	-	-	-
26	CLA	1	604	X	-	-	-
26	CLA	1	606	X	-	-	-
26	CLA	1	607	X	-	-	-
26	CLA	1	608	X	-	-	-
26	CLA	1	609	X	-	-	-
26	CLA	1	610	X	-	-	-
26	CLA	1	611	X	-	-	-
26	CLA	1	612	X	-	-	-
26	CLA	1	613	X	-	-	-
26	CLA	1	614	X	-	-	-
26	CLA	1	616	X	-	-	-
26	CLA	2	601	X	-	-	-
26	CLA	2	602	X	-	-	-
26	CLA	2	603	X	-	-	-
26	CLA	2	604	X	-	-	-
26	CLA	2	606	X	-	-	-
26	CLA	2	607	X	-	-	-
26	CLA	2	609	X	-	-	-
26	CLA	2	610	X	-	-	-
26	CLA	2	611	X	-	-	-
26	CLA	2	612	X	-	-	-
26	CLA	2	613	X	-	-	-
26	CLA	2	614	X	-	-	-
26	CLA	2	616	X	-	-	-
26	CLA	3	602	X	-	-	-
26	CLA	3	603	X	-	-	-
26	CLA	3	604	X	-	-	-
26	CLA	3	606	X	-	-	-
26	CLA	3	607	X	-	-	-
26	CLA	3	608	X	-	-	-
26	CLA	3	609	X	-	-	-
26	CLA	3	610	X	-	-	-
26	CLA	3	611	X	-	-	-
26	CLA	3	612	X	-	-	-
26	CLA	3	613	X	-	-	-
26	CLA	3	614	X	-	-	-
26	CLA	3	615	X	-	-	-
26	CLA	3	617	X	-	-	-
26	CLA	4	601	X	-	-	-
26	CLA	4	602	X	-	-	-
26	CLA	4	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	4	604	X	-	-	-
26	CLA	4	606	X	-	-	-
26	CLA	4	607	X	-	-	-
26	CLA	4	608	X	-	-	-
26	CLA	4	609	X	-	-	-
26	CLA	4	610	X	-	-	-
26	CLA	4	611	X	-	-	-
26	CLA	4	612	X	-	-	-
26	CLA	4	613	X	-	-	-
26	CLA	4	616	X	-	-	-
26	CLA	4	618	X	-	-	-
26	CLA	5	601	X	-	-	-
26	CLA	5	602	X	-	-	-
26	CLA	5	603	X	-	-	-
26	CLA	5	604	X	-	-	-
26	CLA	5	607	X	-	-	-
26	CLA	5	608	X	-	-	-
26	CLA	5	609	X	-	-	-
26	CLA	5	610	X	-	-	-
26	CLA	5	611	X	-	-	-
26	CLA	5	612	X	-	-	-
26	CLA	5	613	X	-	-	-
26	CLA	5	614	X	-	-	-
26	CLA	5	616	X	-	-	-
26	CLA	5	617	X	-	-	-
26	CLA	5	618	X	-	-	-
26	CLA	5	619	X	-	-	-
26	CLA	6	601	X	-	-	-
26	CLA	6	603	X	-	-	-
26	CLA	6	604	X	-	-	-
26	CLA	6	606	X	-	-	-
26	CLA	6	607	X	-	-	-
26	CLA	6	609	X	-	-	-
26	CLA	6	610	X	-	-	-
26	CLA	6	611	X	-	-	-
26	CLA	6	612	X	-	-	-
26	CLA	6	614	X	-	-	-
26	CLA	6	616	X	-	-	-
26	CLA	6	617	X	-	-	-
26	CLA	6	618	X	-	-	-
26	CLA	6	620	X	-	-	-
26	CLA	7	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	7	602	X	-	-	-
26	CLA	7	603	X	-	-	-
26	CLA	7	604	X	-	-	-
26	CLA	7	606	X	-	-	-
26	CLA	7	607	X	-	-	-
26	CLA	7	609	X	-	-	-
26	CLA	7	610	X	-	-	-
26	CLA	7	611	X	-	-	-
26	CLA	7	612	X	-	-	-
26	CLA	7	613	X	-	-	-
26	CLA	7	614	X	-	-	-
26	CLA	7	615	X	-	-	-
26	CLA	7	616	X	-	-	-
26	CLA	8	601	X	-	-	-
26	CLA	8	603	X	-	-	-
26	CLA	8	604	X	-	-	-
26	CLA	8	606	X	-	-	-
26	CLA	8	607	X	-	-	-
26	CLA	8	609	X	-	-	-
26	CLA	8	610	X	-	-	-
26	CLA	8	611	X	-	-	-
26	CLA	8	612	X	-	-	-
26	CLA	8	613	X	-	-	-
26	CLA	8	614	X	-	-	-
26	CLA	8	616	X	-	-	-
26	CLA	9	601	X	-	-	-
26	CLA	9	602	X	-	-	-
26	CLA	9	603	X	-	-	-
26	CLA	9	604	X	-	-	-
26	CLA	9	606	X	-	-	-
26	CLA	9	609	X	-	-	-
26	CLA	9	610	X	-	-	-
26	CLA	9	611	X	-	-	-
26	CLA	9	612	X	-	-	-
26	CLA	9	613	X	-	-	-
26	CLA	9	614	X	-	-	-
26	CLA	A	801	X	-	-	-
26	CLA	A	802	X	-	-	-
26	CLA	A	803	X	-	-	-
26	CLA	A	804	X	-	-	-
26	CLA	A	806	X	-	-	-
26	CLA	A	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	A	808	X	-	-	-
26	CLA	A	809	X	-	-	-
26	CLA	A	811	X	-	-	-
26	CLA	A	812	X	-	-	-
26	CLA	A	813	X	-	-	-
26	CLA	A	814	X	-	-	-
26	CLA	A	815	X	-	-	-
26	CLA	A	816	X	-	-	-
26	CLA	A	819	X	-	-	-
26	CLA	A	820	X	-	-	-
26	CLA	A	822	X	-	-	-
26	CLA	A	823	X	-	-	-
26	CLA	A	824	X	-	-	-
26	CLA	A	825	X	-	-	-
26	CLA	A	826	X	-	-	-
26	CLA	A	827	X	-	-	-
26	CLA	A	828	X	-	-	-
26	CLA	A	829	X	-	-	-
26	CLA	A	830	X	-	-	-
26	CLA	A	831	X	-	-	-
26	CLA	A	832	X	-	-	-
26	CLA	A	833	X	-	-	-
26	CLA	A	834	X	-	-	-
26	CLA	A	836	X	-	-	-
26	CLA	A	837	X	-	-	-
26	CLA	A	838	X	-	-	-
26	CLA	A	839	X	-	-	-
26	CLA	A	841	X	-	-	-
26	CLA	A	842	X	-	-	-
26	CLA	A	843	X	-	-	-
26	CLA	A	845	X	-	-	-
26	CLA	A	854	X	-	-	-
26	CLA	B	802	X	-	-	-
26	CLA	B	803	X	-	-	-
26	CLA	B	804	X	-	-	-
26	CLA	B	805	X	-	-	-
26	CLA	B	806	X	-	-	-
26	CLA	B	808	X	-	-	-
26	CLA	B	809	X	-	-	-
26	CLA	B	810	X	-	-	-
26	CLA	B	811	X	-	-	-
26	CLA	B	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	B	813	X	-	-	-
26	CLA	B	814	X	-	-	-
26	CLA	B	815	X	-	-	-
26	CLA	B	816	X	-	-	-
26	CLA	B	817	X	-	-	-
26	CLA	B	819	X	-	-	-
26	CLA	B	820	X	-	-	-
26	CLA	B	821	X	-	-	-
26	CLA	B	823	X	-	-	-
26	CLA	B	824	X	-	-	-
26	CLA	B	826	X	-	-	-
26	CLA	B	827	X	-	-	-
26	CLA	B	828	X	-	-	-
26	CLA	B	829	X	-	-	-
26	CLA	B	830	X	-	-	-
26	CLA	B	831	X	-	-	-
26	CLA	B	832	X	-	-	-
26	CLA	B	833	X	-	-	-
26	CLA	B	834	X	-	-	-
26	CLA	B	835	X	-	-	-
26	CLA	B	836	X	-	-	-
26	CLA	B	838	X	-	-	-
26	CLA	B	839	X	-	-	-
26	CLA	B	840	X	-	-	-
26	CLA	B	841	X	-	-	-
26	CLA	F	301	X	-	-	-
26	CLA	G	203	X	-	-	-
26	CLA	G	204	X	-	-	-
26	CLA	H	202	X	-	-	-
26	CLA	H	203	X	-	-	-
26	CLA	J	101	X	-	-	-
26	CLA	K	201	X	-	-	-
26	CLA	K	204	X	-	-	-
26	CLA	K	206	X	-	-	-
26	CLA	L	302	X	-	-	-
26	CLA	L	304	X	-	-	-
26	CLA	L	306	X	-	-	-
26	CLA	L	307	X	-	-	-
26	CLA	O	2001	X	-	-	-
26	CLA	O	2002	X	-	-	-
26	CLA	O	2003	X	-	-	-
26	CLA	U	602	X	-	-	-

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

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

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

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 69460 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
			Total	C	N	O	S		
1	A	741	5819	3805	993	999	22	0	0

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

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

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

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

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

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

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

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

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

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

- 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	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
14	a	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	216	Total	C	N	O	S	0	0
			1641	1067	279	291	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	221	Total	C	N	O	S	0	0
			1680	1091	274	310	5		
23	W	220	Total	C	N	O	S	0	0
			1671	1085	273	308	5		

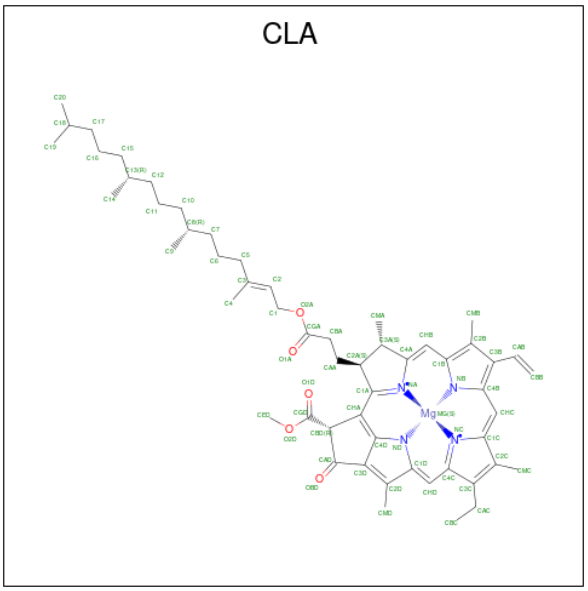
- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	219	Total	C	N	O	S	0	0
			1675	1084	272	314	5		
24	Z	221	Total	C	N	O	S	0	0
			1684	1089	274	316	5		
24	U	219	Total	C	N	O	S	0	0
			1669	1080	272	312	5		

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

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

- Molecule 26 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
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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

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Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	B	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
26	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
26	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
26	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
26	O	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
26	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
26	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
26	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	1	1	Total	C	Mg	N	O	0
			37	29	1	4	3	
26	1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
26	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
26	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
26	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			63	54	1	3	5	
26	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	2	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
26	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	3	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
26	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
26	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	5	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
26	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
26	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
26	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
26	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
26	7	1	Total	C	Mg	N	O	0
			43	33	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
26	8	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	9	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	X	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	Y	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Y	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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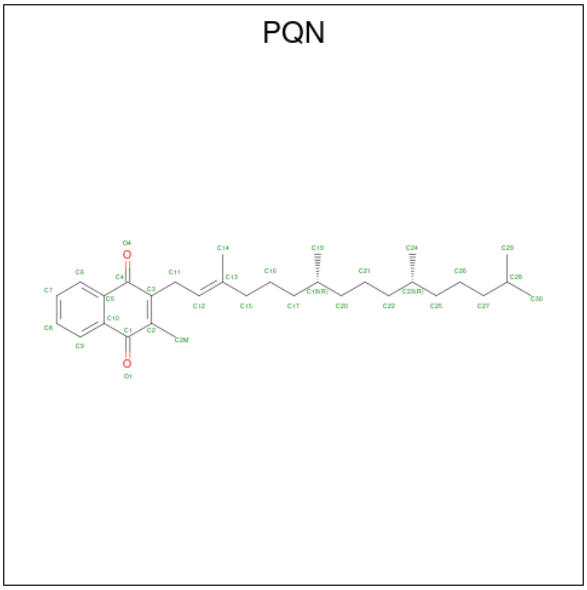
Mol	Chain	Residues	Atoms					AltConf
26	Z	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			49	40	1	4	4	
26	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			48	39	1	4	4	
26	U	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	U	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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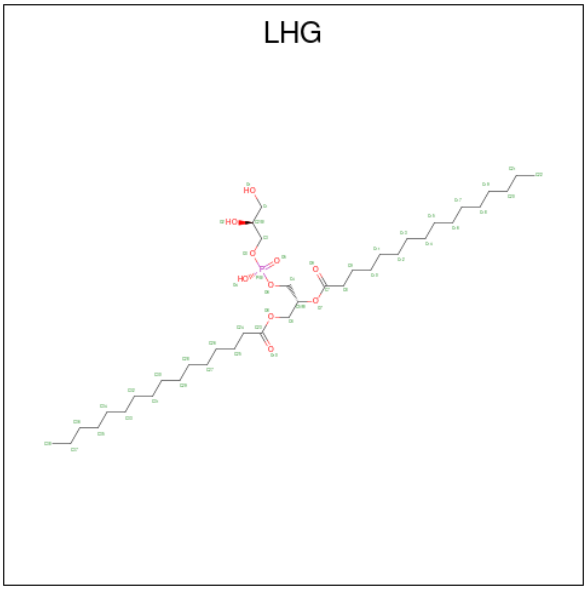
Mol	Chain	Residues	Atoms					AltConf
26	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
26	W	1	Total	C	Mg	N	O	0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

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



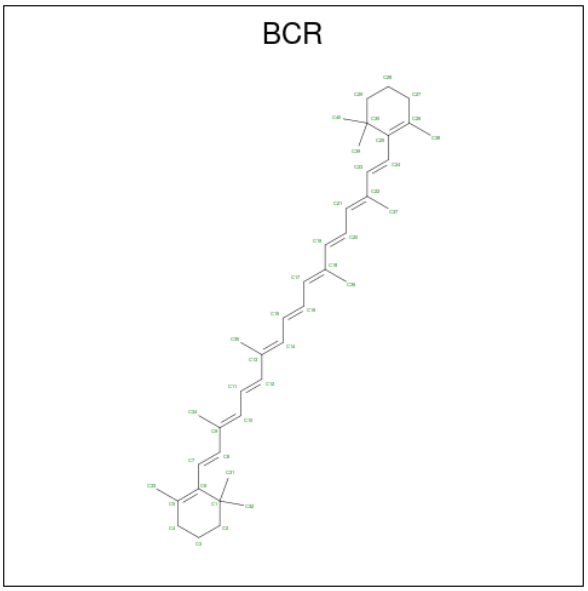
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total 49	C 38	O 10	P 1	0
28	A	1	Total 30	C 19	O 10	P 1	0
28	A	1	Total 49	C 38	O 10	P 1	0
28	B	1	Total 38	C 27	O 10	P 1	0
28	H	1	Total 49	C 38	O 10	P 1	0
28	O	1	Total 36	C 25	O 10	P 1	0
28	1	1	Total 49	C 38	O 10	P 1	0
28	a	1	Total 43	C 32	O 10	P 1	0
28	2	1	Total 36	C 25	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
28	3	1	Total	C	O	P	0
			45	34	10	1	
28	3	1	Total	C	O	P	0
			49	38	10	1	
28	4	1	Total	C	O	P	0
			49	38	10	1	
28	5	1	Total	C	O	P	0
			49	38	10	1	
28	5	1	Total	C	O	P	0
			49	38	10	1	
28	6	1	Total	C	O	P	0
			48	37	10	1	
28	7	1	Total	C	O	P	0
			37	26	10	1	
28	8	1	Total	C	O	P	0
			49	38	10	1	
28	8	1	Total	C	O	P	0
			40	29	10	1	
28	9	1	Total	C	O	P	0
			30	19	10	1	
28	9	1	Total	C	O	P	0
			49	38	10	1	
28	9	1	Total	C	O	P	0
			49	38	10	1	
28	X	1	Total	C	O	P	0
			49	38	10	1	
28	Y	1	Total	C	O	P	0
			49	38	10	1	
28	Z	1	Total	C	O	P	0
			49	38	10	1	
28	U	1	Total	C	O	P	0
			49	38	10	1	
28	V	1	Total	C	O	P	0
			36	25	10	1	
28	W	1	Total	C	O	P	0
			34	23	10	1	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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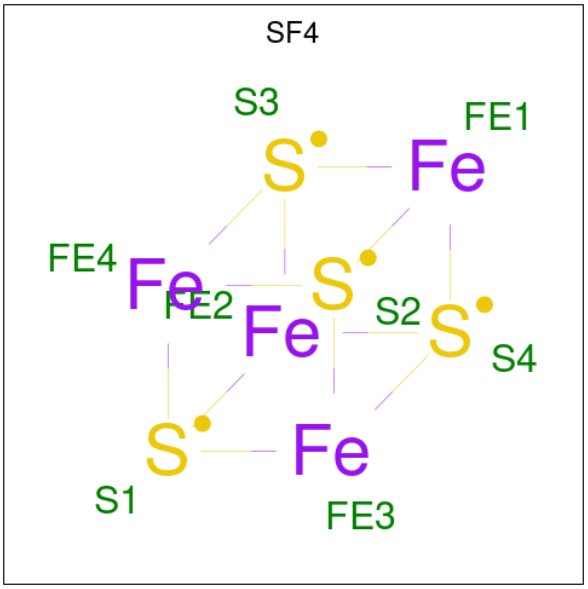
Mol	Chain	Residues	Atoms	AltConf
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	F	1	Total C 40 40	0
29	G	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	1	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	2	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	4	1	Total C 40 40	0
29	5	1	Total C 40 40	0

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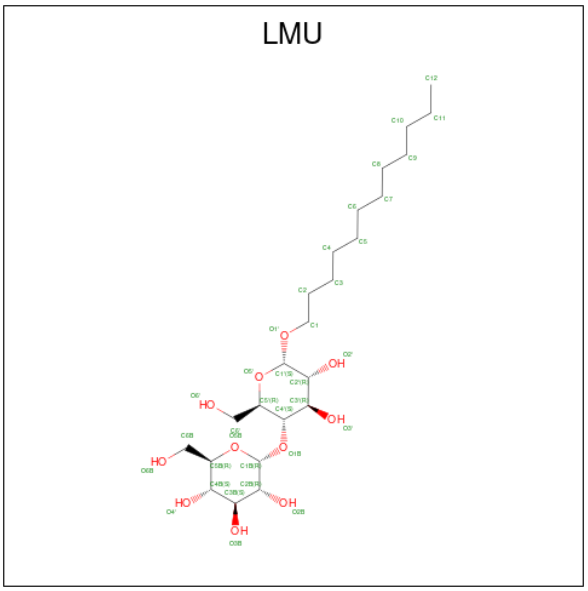
Mol	Chain	Residues	Atoms	AltConf
29	6	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	8	1	Total C 40 40	0
29	9	1	Total C 40 40	0

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



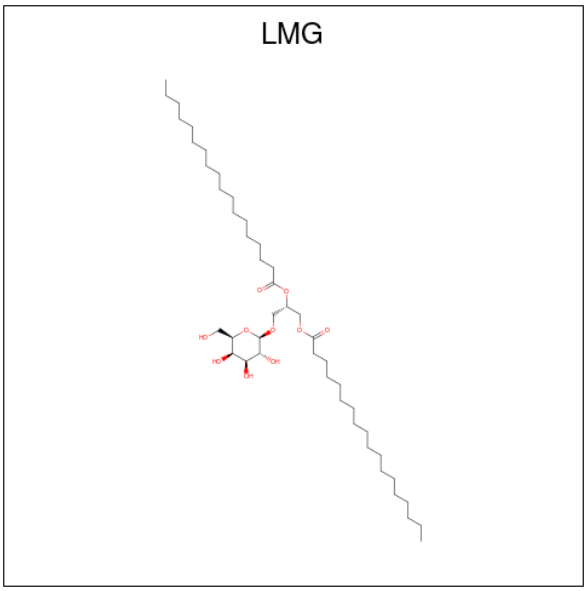
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total Fe S 8 4 4	0
30	C	1	Total Fe S 8 4 4	0
30	C	1	Total Fe S 8 4 4	0

- Molecule 31 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



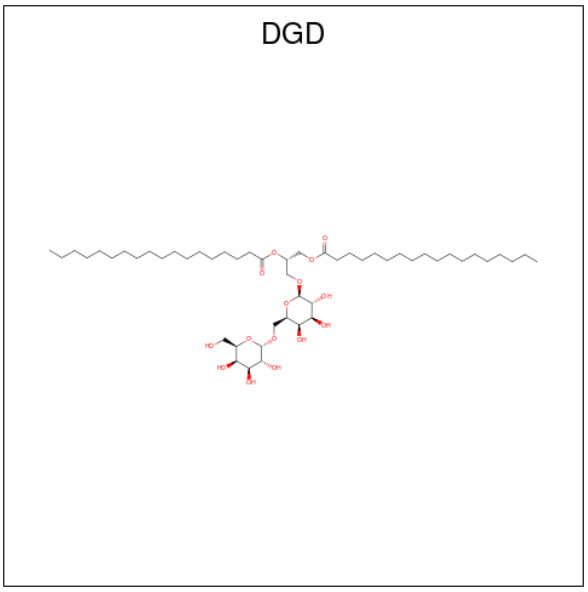
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C O 35 24 11	0
31	A	1	Total C O 34 24 10	0
31	K	1	Total C O 35 24 11	0
31	1	1	Total C O 35 24 11	0
31	5	1	Total C O 33 22 11	0
31	5	1	Total C O 32 21 11	0
31	8	1	Total C O 35 24 11	0

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



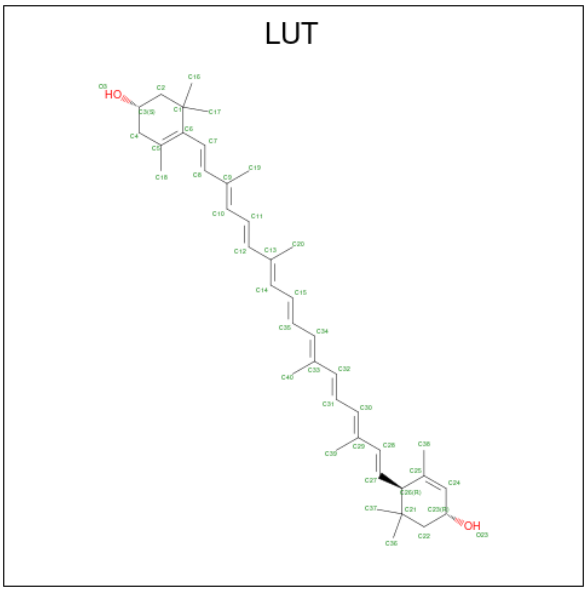
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C O 40 30 10	0
32	H	1	Total C O 55 45 10	0
32	J	1	Total C O 42 32 10	0
32	J	1	Total C O 40 30 10	0
32	L	1	Total C O 37 27 10	0
32	4	1	Total C O 40 30 10	0
32	4	1	Total C O 40 30 10	0
32	5	1	Total C O 40 30 10	0
32	8	1	Total C O 46 36 10	0
32	9	1	Total C O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

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 34 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



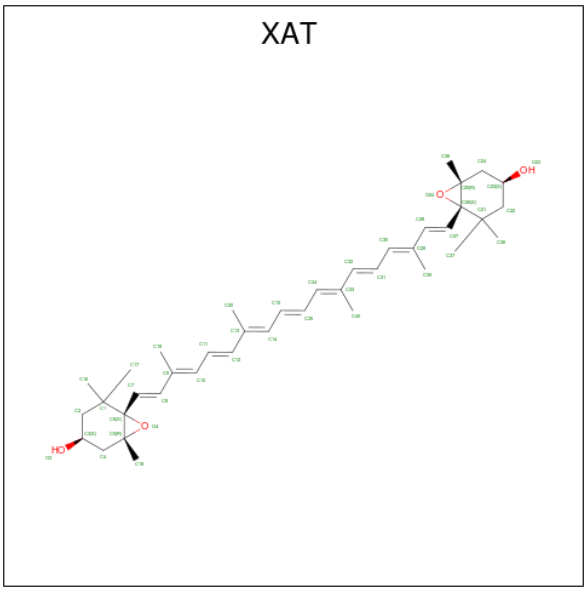
Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total	C	O	0
			42	40	2	
34	a	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
34	2	1	Total	C	O	0
			42	40	2	
34	3	1	Total	C	O	0
			42	40	2	
34	4	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	
34	6	1	Total	C	O	0
			42	40	2	
34	7	1	Total	C	O	0
			42	40	2	
34	8	1	Total	C	O	0
			42	40	2	
34	9	1	Total	C	O	0
			42	40	2	
34	X	1	Total	C	O	0
			42	40	2	
34	X	1	Total	C	O	0
			42	40	2	
34	Y	1	Total	C	O	0
			42	40	2	
34	Y	1	Total	C	O	0
			42	40	2	
34	Z	1	Total	C	O	0
			42	40	2	
34	Z	1	Total	C	O	0
			42	40	2	
34	U	1	Total	C	O	0
			42	40	2	
34	U	1	Total	C	O	0
			42	40	2	
34	V	1	Total	C	O	0
			42	40	2	
34	V	1	Total	C	O	0
			42	40	2	
34	W	1	Total	C	O	0
			42	40	2	
34	W	1	Total	C	O	0
			42	40	2	

- Molecule 35 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: $C_{40}H_{56}O_4$).



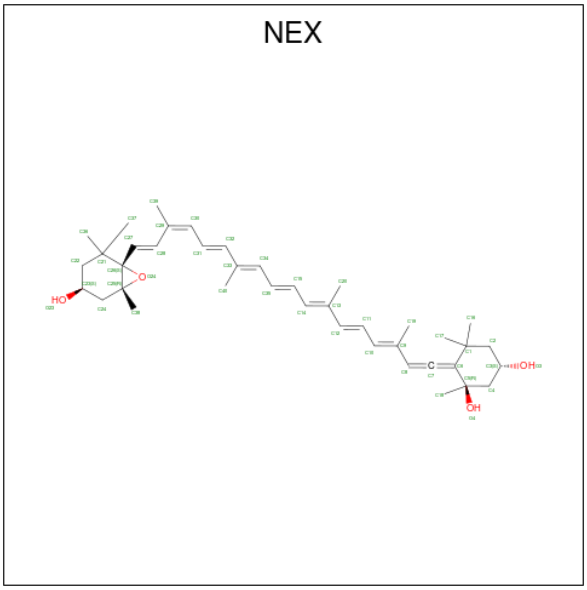
Mol	Chain	Residues	Atoms			AltConf
35	1	1	Total	C	O	0
			44	40	4	
35	a	1	Total	C	O	0
			44	40	4	
35	2	1	Total	C	O	0
			44	40	4	
35	3	1	Total	C	O	0
			44	40	4	
35	4	1	Total	C	O	0
			44	40	4	
35	5	1	Total	C	O	0
			44	40	4	
35	6	1	Total	C	O	0
			44	40	4	
35	7	1	Total	C	O	0
			44	40	4	
35	8	1	Total	C	O	0
			44	40	4	
35	9	1	Total	C	O	0
			44	40	4	
35	X	1	Total	C	O	0
			44	40	4	
35	Y	1	Total	C	O	0
			44	40	4	
35	Z	1	Total	C	O	0
			44	40	4	
35	U	1	Total	C	O	0
			44	40	4	

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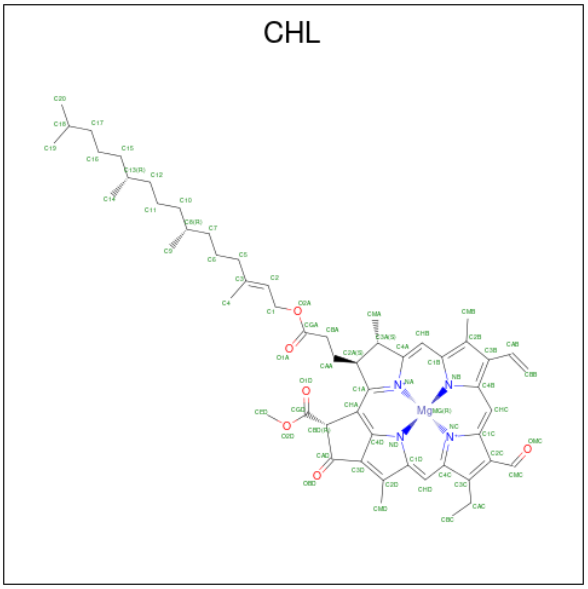
Mol	Chain	Residues	Atoms	AltConf
35	V	1	Total C O 44 40 4	0
35	W	1	Total C O 44 40 4	0

- Molecule 36 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
36	5	1	Total C O 44 40 4	0
36	6	1	Total C O 44 40 4	0
36	X	1	Total C O 44 40 4	0
36	Y	1	Total C O 44 40 4	0
36	Z	1	Total C O 44 40 4	0
36	U	1	Total C O 44 40 4	0
36	V	1	Total C O 44 40 4	0
36	W	1	Total C O 44 40 4	0

- Molecule 37 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
37	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
37	X	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
37	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
37	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
37	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
37	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	Z	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
37	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
37	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	Z	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
37	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	U	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
37	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
37	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
37	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
37	U	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
37	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
37	V	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
37	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
37	V	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
37	V	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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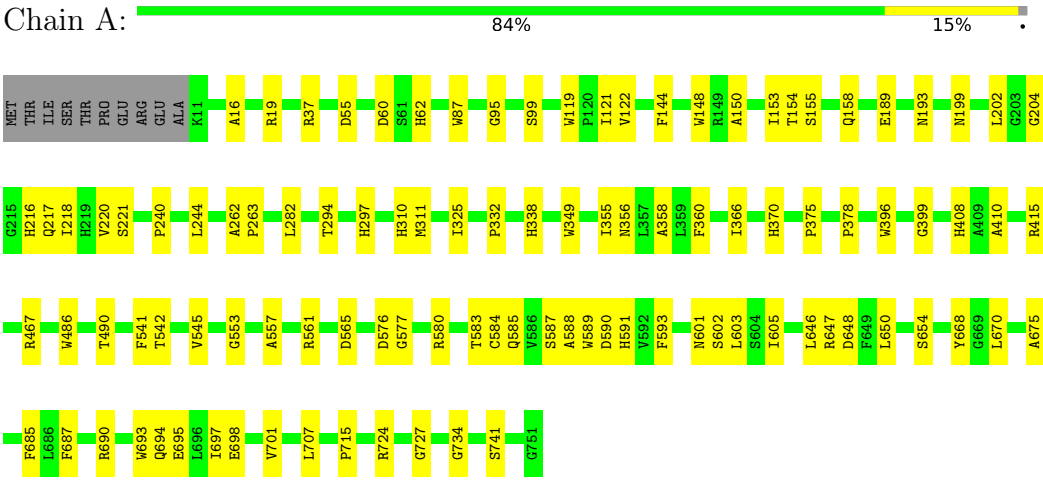
Mol	Chain	Residues	Atoms					AltConf
37	W	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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.

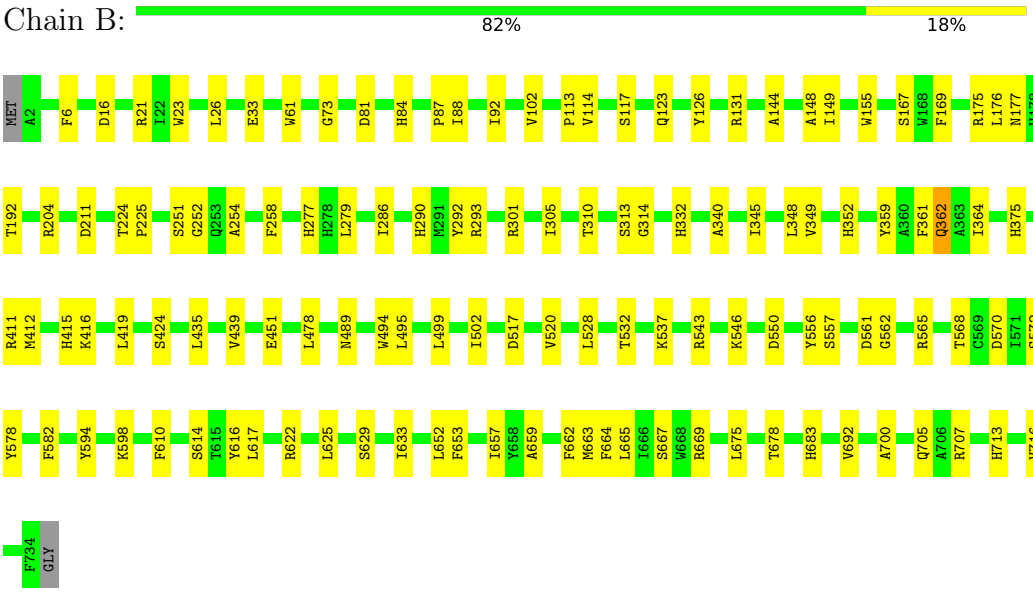
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



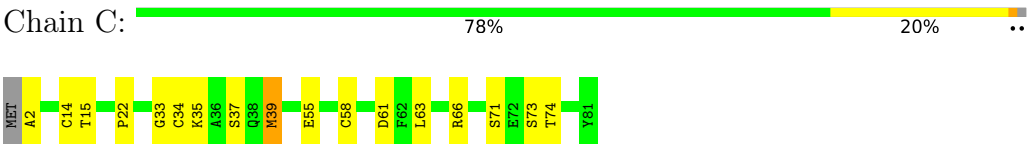
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



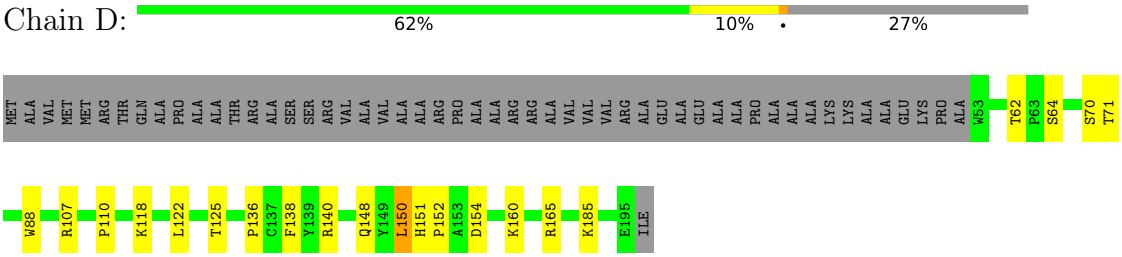
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



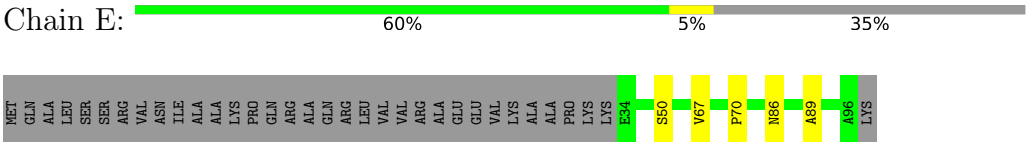
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:



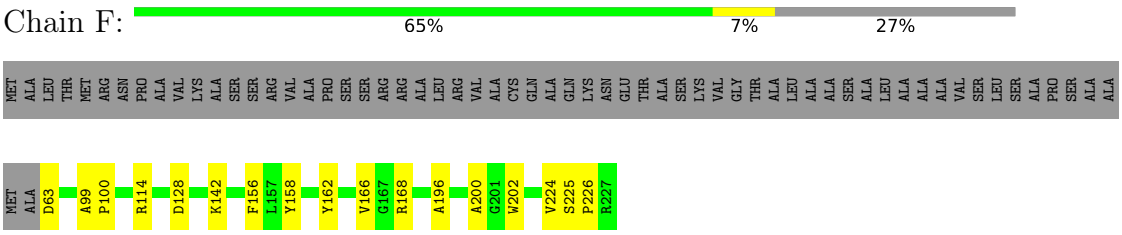
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



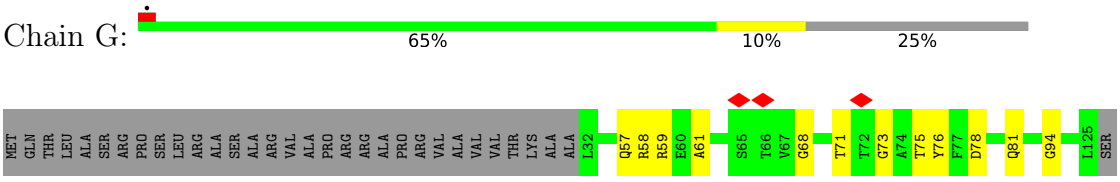
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:



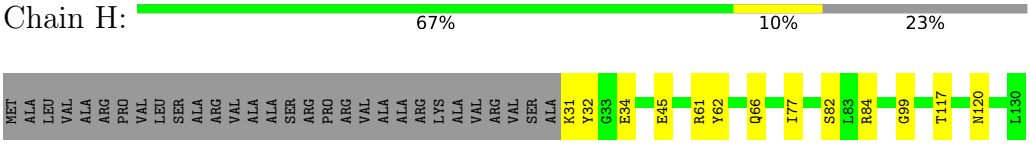
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:



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

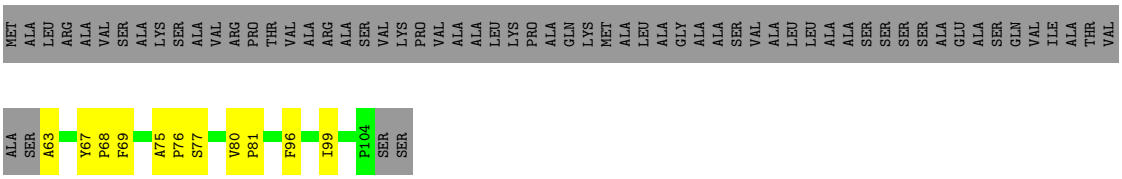
Chain H:



• Molecule 9: Photosystem I reaction center subunit VIII

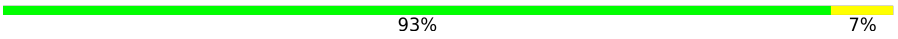
Chain I:

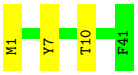




• Molecule 10: Photosystem I reaction center subunit IX

Chain J:

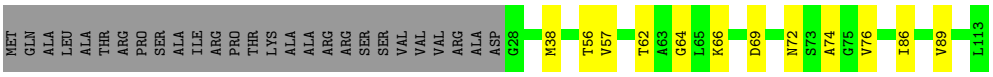




• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:

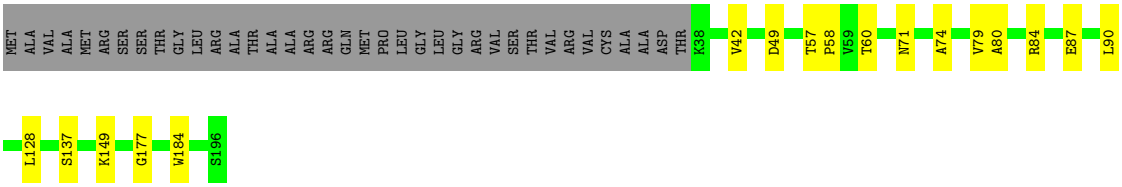




• Molecule 12: PSI subunit V

Chain L:

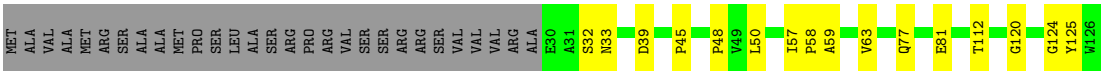




• Molecule 13: Photosystem I subunit O

Chain O:

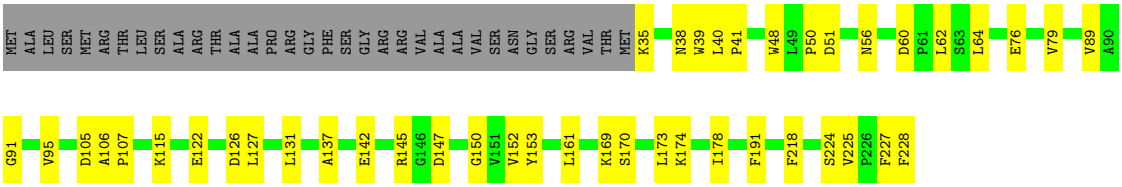




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

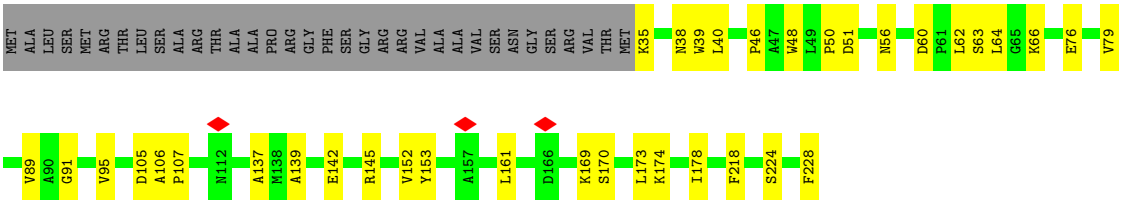




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain a:

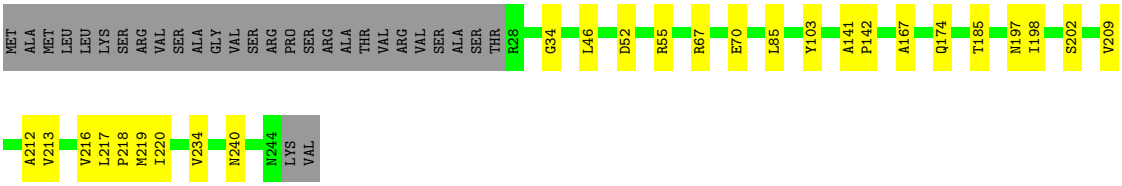




• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 2:

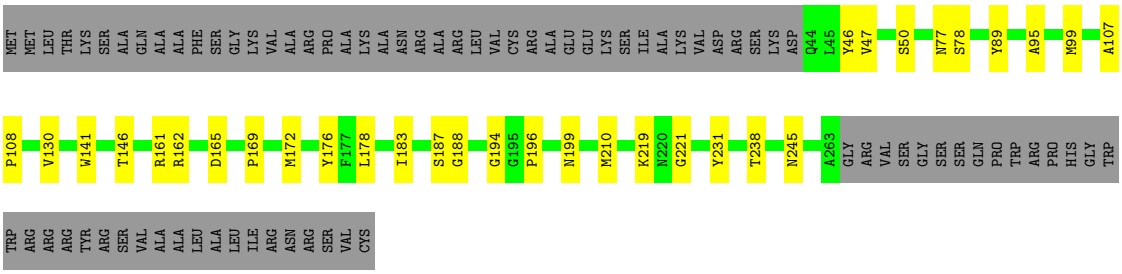




• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 3:

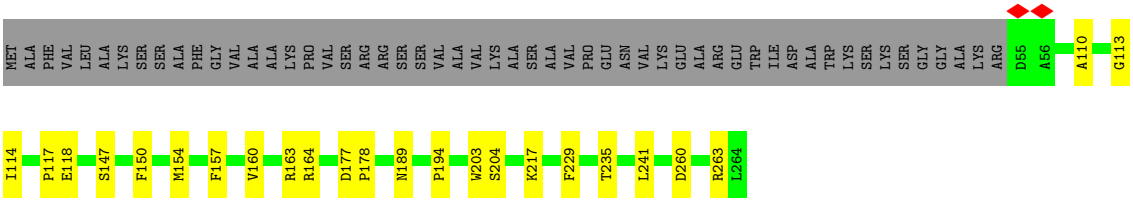




• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 4:

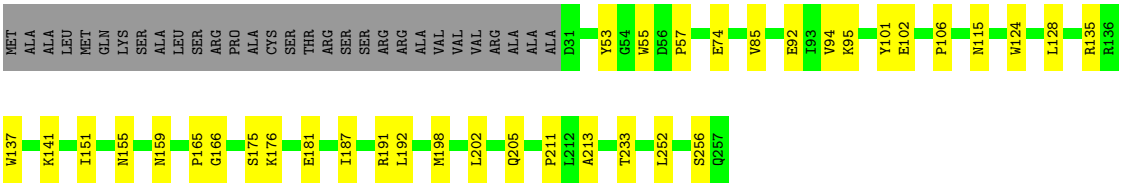




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

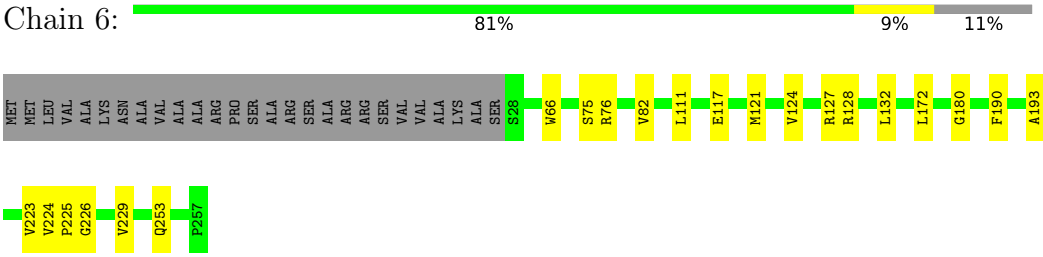
Chain 5:





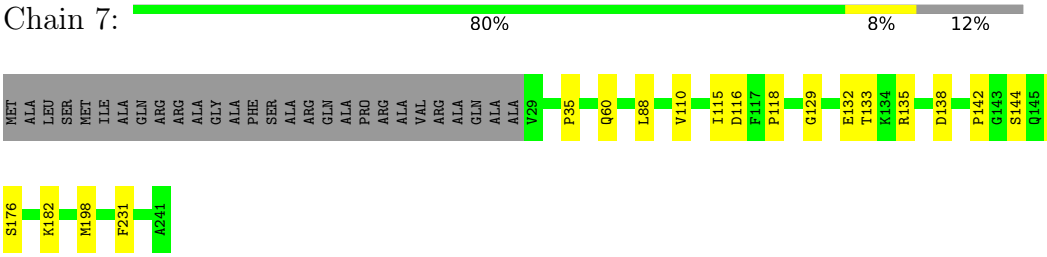
• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



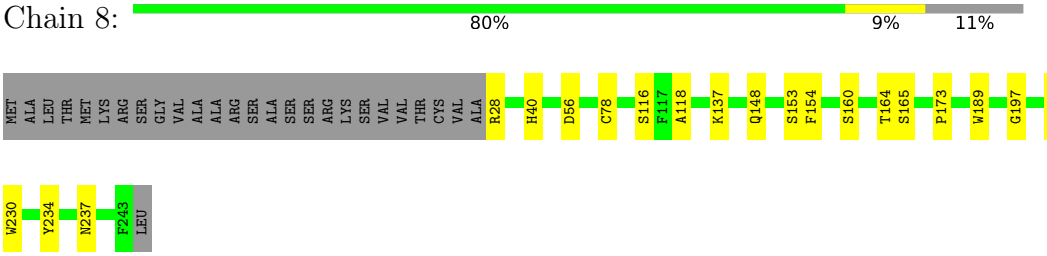
• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



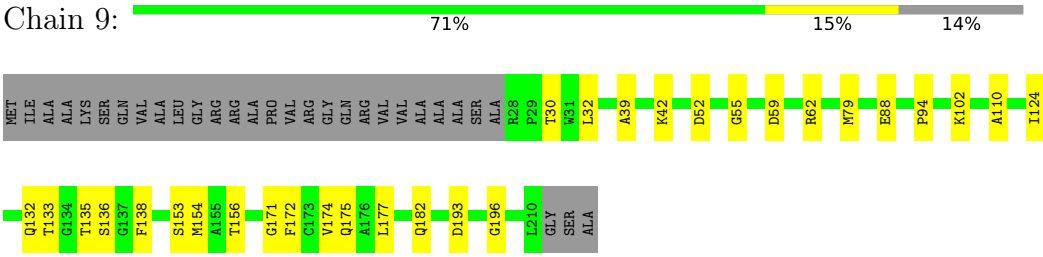
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



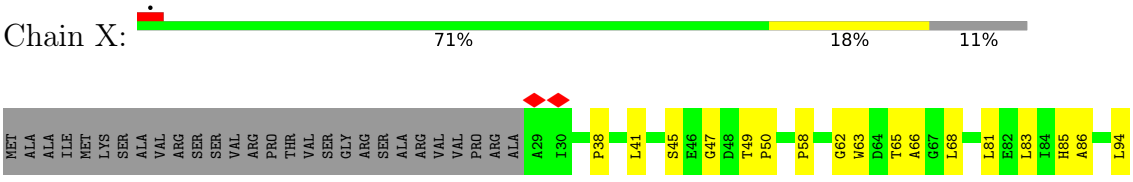
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

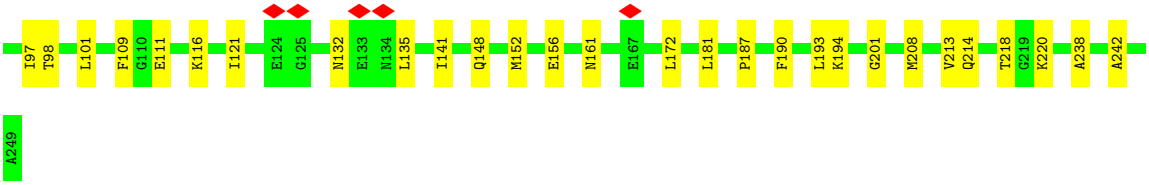
Chain 9:



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

Chain X:

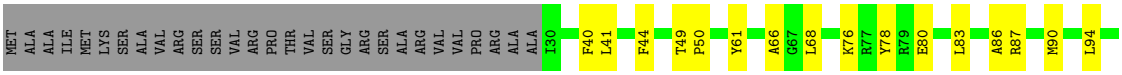


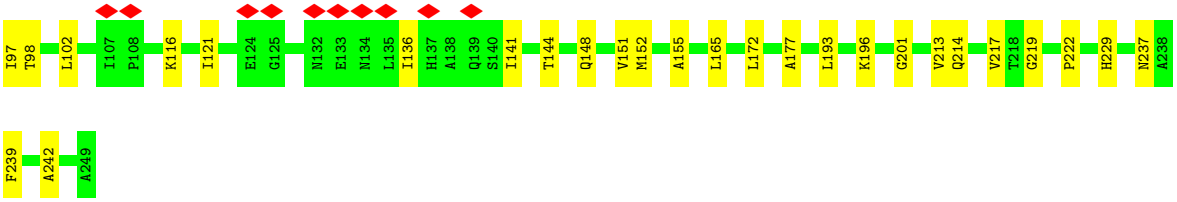


• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain W:





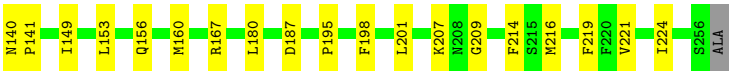


• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain Y:







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

Chain Z:







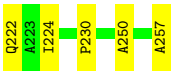
• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain U:





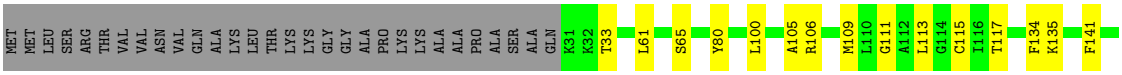


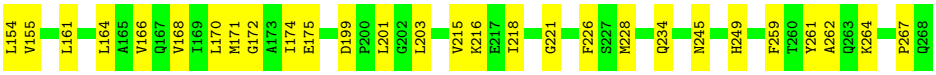


• Molecule 25: Chlorophyll a-b binding protein, chloroplastic

Chain V:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123997	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	0.116	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	360.0, 360.0, 360.0	wwPDB
Map dimensions	360, 360, 360	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: DGD, CHL, LMU, PQN, XAT, SF4, LHG, TPO, LMG, BCR, CLA, NEX, 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	0.53	0/6015	0.39	0/8201
2	B	0.52	0/6036	0.45	5/8242 (0.1%)
3	C	0.51	0/610	0.62	1/826 (0.1%)
4	D	0.44	0/1152	0.46	1/1556 (0.1%)
5	E	0.41	0/506	0.34	0/689
6	F	0.39	0/1291	0.37	0/1747
7	G	0.27	0/714	0.34	0/972
8	H	0.39	0/788	0.37	0/1059
9	I	0.52	0/329	0.46	0/456
10	J	0.45	0/349	0.33	0/478
11	K	0.38	0/587	0.42	0/795
12	L	0.47	0/1190	0.41	0/1628
13	O	0.40	0/784	0.39	0/1069
14	1	0.37	0/1490	0.46	0/2028
14	a	0.37	0/1490	0.46	0/2028
15	2	0.38	0/1730	0.43	0/2353
16	3	0.43	0/1726	0.38	0/2342
17	4	0.29	0/1686	0.34	0/2300
18	5	0.37	0/1829	0.40	0/2492
19	6	0.34	0/1833	0.38	0/2505
20	7	0.44	0/1701	0.38	0/2310
21	8	0.40	0/1692	0.37	0/2304
22	9	0.36	0/1444	0.43	0/1964
23	W	0.22	0/1721	0.54	0/2341
23	X	0.24	0/1730	0.54	0/2355
24	U	0.23	0/1717	0.55	1/2336 (0.0%)
24	Y	0.25	0/1723	0.53	0/2345
24	Z	0.23	0/1732	0.53	0/2357
25	V	0.22	0/1856	0.46	0/2518
All	All	0.41	0/47451	0.44	8/64596 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	150	LEU	N-CA-C	7.75	122.50	112.12
24	U	116	GLN	N-CA-C	6.74	118.62	111.28
2	B	495	LEU	N-CA-C	5.71	121.31	113.77
2	B	362	GLN	N-CA-C	-5.51	101.81	110.36
2	B	310	THR	CA-C-N	-5.44	114.78	120.38
2	B	310	THR	C-N-CA	-5.44	114.78	120.38
3	C	39	MET	N-CA-C	-5.42	99.45	108.07
2	B	361	PHE	CB-CA-C	5.00	119.51	111.36

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	87	0
2	B	5824	0	5579	104	0
3	C	600	0	581	15	0
4	D	1124	0	1139	16	0
5	E	496	0	491	5	0
6	F	1265	0	1301	19	0
7	G	699	0	681	11	0
8	H	776	0	765	10	0
9	I	316	0	321	9	0
10	J	337	0	336	2	0
11	K	582	0	620	10	0
12	L	1161	0	1184	15	0
13	O	758	0	740	13	0
14	1	1444	0	1396	34	0
14	a	1444	0	1396	27	0
15	2	1682	0	1665	22	0
16	3	1678	0	1637	25	0
17	4	1631	0	1587	18	0
18	5	1774	0	1746	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	6	1771	0	1770	21	0
20	7	1649	0	1589	15	0
21	8	1641	0	1618	23	0
22	9	1403	0	1381	21	0
23	W	1671	0	1604	30	0
23	X	1680	0	1622	32	0
24	U	1669	0	1603	40	0
24	Y	1675	0	1617	26	0
24	Z	1684	0	1625	29	0
25	V	1815	0	1766	50	0
26	1	666	0	522	6	0
26	2	637	0	530	4	0
26	3	724	0	628	5	0
26	4	778	0	678	7	0
26	5	878	0	758	17	0
26	6	903	0	831	11	0
26	7	756	0	635	13	0
26	8	724	0	629	8	0
26	9	595	0	491	4	0
26	A	2669	0	2693	56	0
26	B	2284	0	2237	33	0
26	F	140	0	113	6	0
26	G	87	0	64	0	0
26	H	104	0	93	0	0
26	J	42	0	31	0	0
26	K	191	0	150	3	0
26	L	235	0	184	7	0
26	O	116	0	61	0	0
26	U	400	0	342	11	0
26	V	415	0	365	11	0
26	W	426	0	377	12	0
26	X	436	0	415	16	0
26	Y	429	0	389	10	0
26	Z	427	0	386	17	0
26	a	710	0	591	8	0
27	A	33	0	46	2	0
27	B	33	0	46	3	0
28	1	49	0	74	0	0
28	2	36	0	42	0	0
28	3	94	0	137	3	0
28	4	49	0	74	0	0
28	5	98	0	148	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	6	48	0	69	0	0
28	7	37	0	44	0	0
28	8	89	0	124	0	0
28	9	128	0	178	1	0
28	A	128	0	178	0	0
28	B	38	0	46	0	0
28	H	49	0	74	0	0
28	O	36	0	42	1	0
28	U	49	0	74	1	0
28	V	36	0	42	3	0
28	W	34	0	38	1	0
28	X	49	0	74	6	0
28	Y	49	0	74	6	0
28	Z	49	0	74	9	0
28	a	43	0	59	1	0
29	1	40	0	56	2	0
29	2	40	0	56	5	0
29	3	120	0	168	19	0
29	4	40	0	56	5	0
29	5	40	0	56	2	0
29	6	40	0	56	1	0
29	7	80	0	112	8	0
29	8	40	0	56	3	0
29	9	40	0	56	7	0
29	A	240	0	336	42	0
29	B	400	0	560	44	0
29	F	40	0	56	7	0
29	G	40	0	56	4	0
29	J	40	0	56	8	0
29	K	80	0	112	8	0
29	L	160	0	224	29	0
29	O	80	0	112	9	0
29	a	40	0	56	3	0
30	A	8	0	0	0	0
30	C	16	0	0	1	0
31	1	35	0	46	0	0
31	5	65	0	76	0	0
31	8	35	0	46	0	0
31	A	69	0	90	1	0
31	K	35	0	46	0	0
32	4	80	0	100	0	0
32	5	40	0	50	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	8	46	0	65	3	0
32	9	55	0	86	2	0
32	A	40	0	50	1	0
32	H	55	0	86	0	0
32	J	82	0	107	0	0
32	L	37	0	44	0	0
32	V	55	0	86	2	0
33	B	62	0	85	1	0
34	1	42	0	56	6	0
34	2	42	0	56	7	0
34	3	42	0	56	7	0
34	4	42	0	56	3	0
34	5	42	0	56	4	0
34	6	42	0	56	5	0
34	7	42	0	56	3	0
34	8	42	0	56	6	0
34	9	42	0	56	5	0
34	U	84	0	112	8	0
34	V	84	0	112	10	0
34	W	84	0	112	8	0
34	X	84	0	112	12	0
34	Y	84	0	112	9	0
34	Z	84	0	112	10	0
34	a	42	0	56	5	0
35	1	44	0	56	3	0
35	2	44	0	56	1	0
35	3	44	0	56	2	0
35	4	44	0	56	3	0
35	5	44	0	56	2	0
35	6	44	0	56	1	0
35	7	44	0	56	1	0
35	8	44	0	56	1	0
35	9	44	0	56	0	0
35	U	44	0	56	5	0
35	V	44	0	56	6	0
35	W	44	0	56	3	0
35	X	44	0	56	3	0
35	Y	44	0	56	3	0
35	Z	44	0	56	5	0
35	a	44	0	56	3	0
36	5	44	0	56	1	0
36	6	44	0	56	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	U	44	0	56	0	0
36	V	44	0	56	11	0
36	W	44	0	56	2	0
36	X	44	0	56	2	0
36	Y	44	0	56	2	0
36	Z	44	0	56	3	0
37	U	303	0	248	14	0
37	V	309	0	253	15	0
37	W	336	0	298	9	0
37	X	353	0	342	15	0
37	Y	335	0	302	16	0
37	Z	335	0	302	14	0
All	All	69460	0	68604	1115	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 8.

All (1115) 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)
21:8:78:CYS:SG	21:8:201:MET:HE2	1.64	1.34
25:V:174:ILE:CG2	36:V:1623:NEX:H15	1.78	1.14
21:8:78:CYS:SG	21:8:201:MET:CE	2.44	1.06
18:5:192:LEU:CD1	26:5:611:CLA:HMD1	1.87	1.04
25:V:174:ILE:HG22	36:V:1623:NEX:H201	1.42	1.00
18:5:192:LEU:HD23	28:5:623:LHG:H262	1.41	0.98
14:1:225:VAL:HG11	14:1:228:PHE:CE2	2.05	0.91
18:5:192:LEU:CD2	28:5:623:LHG:H262	2.01	0.90
25:V:174:ILE:HG23	36:V:1623:NEX:H15	1.51	0.90
29:L:305:BCR:H311	29:L:305:BCR:HC8	1.52	0.89
26:B:821:CLA:C3D	29:B:843:BCR:H312	2.03	0.89
21:8:164:THR:HG22	21:8:165:SER:H	1.40	0.86
25:V:174:ILE:HG21	36:V:1623:NEX:H34	1.58	0.86
29:B:843:BCR:H362	29:G:205:BCR:H312	1.58	0.86
25:V:174:ILE:CD1	25:V:175:GLU:HG2	2.05	0.85
21:8:164:THR:HG22	21:8:165:SER:N	1.92	0.84
6:F:225:SER:OG	6:F:226:PRO:HD3	1.78	0.83
18:5:192:LEU:HD11	26:5:611:CLA:HMD1	1.58	0.83
18:5:192:LEU:HD12	26:5:611:CLA:HMD1	1.57	0.83
25:V:174:ILE:CG2	36:V:1623:NEX:H201	2.08	0.83
14:1:127:LEU:O	14:1:131:LEU:HG	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:174:ILE:HD12	25:V:175:GLU:HG2	1.63	0.81
29:3:620:BCR:H312	26:7:611:CLA:CAB	2.11	0.80
29:7:621:BCR:H312	26:8:611:CLA:HAB	1.64	0.79
18:5:192:LEU:CD1	26:5:611:CLA:CMD	2.62	0.77
29:A:852:BCR:H362	26:A:854:CLA:C4	2.15	0.77
29:L:309:BCR:H321	29:L:309:BCR:HC8	1.66	0.76
6:F:224:VAL:HG12	6:F:226:PRO:HD2	1.68	0.75
29:K:202:BCR:H331	29:K:202:BCR:HC8	1.69	0.75
34:a:617:LUT:H8	34:a:617:LUT:H161	1.69	0.75
29:L:301:BCR:H383	29:L:301:BCR:H23C	1.69	0.75
18:5:192:LEU:HD12	26:5:611:CLA:CMD	2.16	0.74
3:C:33:GLY:HA3	3:C:39:MET:HG3	1.69	0.74
24:U:157:VAL:HG23	37:U:609:CHL:HBB2	1.69	0.74
29:B:843:BCR:H383	29:B:843:BCR:H23C	1.70	0.73
29:A:856:BCR:H321	29:A:856:BCR:HC8	1.69	0.73
22:9:132:GLN:O	22:9:133:THR:HG22	1.89	0.73
14:a:62:LEU:HD22	21:8:173:PRO:HA	1.69	0.73
18:5:192:LEU:HD23	28:5:623:LHG:C26	2.17	0.73
18:5:198:MET:O	18:5:202:LEU:HD13	1.88	0.73
34:1:617:LUT:H8	34:1:617:LUT:H161	1.69	0.72
29:B:844:BCR:HC8	29:B:844:BCR:H311	1.71	0.72
34:6:619:LUT:H161	34:6:619:LUT:H8	1.70	0.72
14:1:89:VAL:HG11	34:1:617:LUT:H12	1.71	0.72
14:a:89:VAL:HG11	34:a:617:LUT:H12	1.71	0.72
34:8:619:LUT:H161	34:8:619:LUT:H8	1.72	0.72
34:3:618:LUT:H161	34:3:618:LUT:H8	1.73	0.71
15:2:174:GLN:NE2	34:2:619:LUT:O3	2.23	0.71
15:2:34:GLY:O	22:9:128:GLN:NE2	2.23	0.71
21:8:164:THR:CG2	21:8:165:SER:H	2.04	0.71
16:3:238:THR:HG21	16:3:245:ASN:HD21	1.56	0.71
14:1:41:PRO:O	21:8:148:GLN:NE2	2.23	0.71
15:2:67:ARG:NH1	15:2:70:GLU:OE1	2.24	0.71
24:Z:216:MET:HE2	34:Z:1621:LUT:H10	1.71	0.71
14:a:91:GLY:O	14:a:95:VAL:HG23	1.91	0.70
1:A:707:LEU:O	6:F:168:ARG:NH1	2.24	0.70
26:A:808:CLA:HBB2	29:J:102:BCR:H312	1.74	0.70
14:1:91:GLY:O	14:1:95:VAL:HG23	1.90	0.70
29:L:301:BCR:HC8	29:L:301:BCR:H311	1.72	0.70
20:7:132:GLU:OE1	20:7:135:ARG:NH2	2.25	0.70
26:a:601:CLA:HMD2	17:4:178:PRO:HB3	1.74	0.69
29:B:849:BCR:H23C	29:B:849:BCR:C38	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:801:BCR:H312	26:B:833:CLA:H62	1.74	0.69
3:C:35:LYS:HD3	5:E:67:VAL:HG23	1.74	0.69
1:A:325:ILE:HD13	26:A:824:CLA:HMD2	1.75	0.69
34:2:619:LUT:H42	34:2:619:LUT:H162	1.74	0.69
26:W:613:CLA:H2	26:W:614:CLA:HMD1	1.75	0.69
1:A:467:ARG:NH2	26:A:835:CLA:O1D	2.27	0.68
29:B:845:BCR:H383	29:B:845:BCR:H23C	1.75	0.68
4:D:151:HIS:HB3	4:D:152:PRO:HD3	1.75	0.68
18:5:74:GLU:HG2	18:5:187:ILE:HD11	1.74	0.68
29:L:305:BCR:H311	29:L:305:BCR:C8	2.24	0.67
25:V:174:ILE:HD11	25:V:175:GLU:HG2	1.75	0.67
1:A:561:ARG:NH1	4:D:71:THR:O	2.27	0.67
1:A:37:ARG:NH1	1:A:62:HIS:O	2.28	0.67
14:a:35:LYS:N	14:a:51:ASP:O	2.28	0.67
6:F:224:VAL:HG12	6:F:226:PRO:CD	2.24	0.67
1:A:585:GLN:HA	1:A:590:ASP:OD2	1.95	0.67
24:U:257:ALA:H	23:W:219:GLY:HA3	1.59	0.67
10:J:1:MET:N	20:7:60:GLN:OE1	2.27	0.67
26:B:821:CLA:CAD	29:B:843:BCR:H312	2.25	0.66
29:3:622:BCR:H321	29:3:622:BCR:HC8	1.77	0.66
27:B:842:PQN:H301	29:L:305:BCR:H321	1.77	0.66
23:W:148:GLN:HE22	37:W:607:CHL:HMC	1.60	0.66
2:B:169:PHE:O	2:B:175:ARG:NH2	2.28	0.66
14:1:35:LYS:N	14:1:51:ASP:O	2.28	0.66
7:G:58:ARG:NH2	7:G:94:GLY:O	2.29	0.66
29:3:622:BCR:H321	29:3:622:BCR:C8	2.25	0.65
29:7:623:BCR:H321	29:7:623:BCR:HC8	1.78	0.65
21:8:164:THR:CG2	21:8:165:SER:N	2.60	0.65
23:X:208:MET:HE2	34:X:1621:LUT:H10	1.78	0.65
29:J:102:BCR:HC8	29:J:102:BCR:H331	1.78	0.65
18:5:192:LEU:HD11	26:5:611:CLA:CMD	2.25	0.65
37:W:606:CHL:HBB2	37:W:607:CHL:HBB1	1.78	0.65
2:B:204:ARG:NH2	2:B:254:ALA:O	2.30	0.65
6:F:224:VAL:HG12	6:F:225:SER:N	2.12	0.65
26:L:302:CLA:HMB3	29:L:308:BCR:H19C	1.78	0.65
1:A:647:ARG:NH1	1:A:648:ASP:OD2	2.30	0.64
2:B:517:ASP:OD2	2:B:598:LYS:NZ	2.28	0.64
15:2:234:VAL:HG13	15:2:240:ASN:ND2	2.13	0.64
29:L:305:BCR:H392	29:L:305:BCR:H23C	1.79	0.64
29:L:309:BCR:H23C	29:L:309:BCR:H392	1.79	0.64
2:B:352:HIS:ND1	26:B:817:CLA:OBD	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:TRP:HB2	29:B:853:BCR:H312	1.78	0.63
26:A:829:CLA:H11	29:A:852:BCR:H323	1.81	0.63
36:6:624:NEX:H193	36:6:624:NEX:H161	1.78	0.63
14:1:62:LEU:HD12	35:1:618:XAT:H221	1.81	0.63
16:3:238:THR:HG21	16:3:245:ASN:ND2	2.14	0.63
29:A:852:BCR:H362	26:A:854:CLA:H42	1.81	0.62
14:a:62:LEU:HD12	35:a:618:XAT:H221	1.81	0.62
34:5:620:LUT:H161	28:5:623:LHG:H382	1.80	0.62
14:1:126:ASP:OD1	14:1:127:LEU:N	2.31	0.62
29:8:621:BCR:H331	29:8:621:BCR:HC8	1.80	0.62
29:B:852:BCR:H383	29:B:852:BCR:H23C	1.81	0.62
25:V:161:LEU:HD11	26:W:614:CLA:H2A	1.82	0.62
24:Y:49:LEU:HB2	24:Y:53:SER:HB2	1.80	0.62
26:A:829:CLA:HBC3	29:A:852:BCR:H313	1.82	0.62
29:7:621:BCR:H312	26:8:611:CLA:CAB	2.30	0.62
2:B:126:TYR:O	2:B:131:ARG:NH1	2.33	0.61
19:6:111:LEU:HD21	36:6:624:NEX:C19	2.30	0.61
23:W:144:THR:HG22	37:W:605:CHL:HAC1	1.82	0.61
14:1:115:LYS:HD2	14:1:122:GLU:OE2	2.01	0.61
15:2:46:LEU:O	15:2:67:ARG:NH2	2.32	0.61
23:X:121:ILE:HG21	23:X:141:ILE:HB	1.81	0.61
8:H:45:GLU:OE1	12:L:149:LYS:NZ	2.33	0.61
2:B:494:TRP:NE1	26:B:834:CLA:HED1	2.15	0.61
29:B:844:BCR:H311	29:B:844:BCR:C8	2.31	0.61
21:8:78:CYS:HB3	21:8:197:GLY:HA3	1.83	0.61
23:X:85:HIS:HD2	34:X:1621:LUT:H15	1.65	0.60
1:A:589:TRP:HE3	1:A:590:ASP:OD1	1.85	0.60
24:Z:124:LYS:HA	37:Z:607:CHL:HED2	1.84	0.60
16:3:141:TRP:NE1	26:3:606:CLA:OBD	2.30	0.60
21:8:234:TYR:N	26:8:613:CLA:O1A	2.34	0.60
25:V:174:ILE:HG22	36:V:1623:NEX:H15	1.81	0.60
2:B:26:LEU:CD2	29:L:305:BCR:H323	2.30	0.60
2:B:26:LEU:HD21	29:L:305:BCR:H323	1.82	0.60
24:U:128:GLN:HE22	26:U:604:CLA:HED3	1.66	0.60
28:X:2630:LHG:H101	28:X:2630:LHG:H301	1.83	0.60
24:Y:50:GLY:HA3	37:Y:601:CHL:HBB1	1.83	0.60
34:4:619:LUT:H161	34:4:619:LUT:H8	1.84	0.59
23:X:181:LEU:HD13	34:X:1620:LUT:H222	1.83	0.59
29:L:301:BCR:H312	26:L:303:CLA:C2C	2.33	0.59
2:B:489:ASN:ND2	26:B:835:CLA:OBD	2.32	0.59
14:1:41:PRO:CG	21:8:153:SER:OG	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:9:171:GLY:O	22:9:175:GLN:HB2	2.02	0.59
37:Z:607:CHL:HAA2	35:Z:1622:XAT:H41	1.85	0.59
29:3:621:BCR:H383	29:3:621:BCR:H23C	1.84	0.59
34:9:619:LUT:H8	34:9:619:LUT:H161	1.83	0.59
37:Y:601:CHL:HAC1	28:Y:2630:LHG:HC12	1.84	0.59
24:Z:49:LEU:HB2	24:Z:53:SER:HB2	1.84	0.59
24:Z:195:PRO:HA	24:Z:198:PHE:HB3	1.83	0.59
24:U:222:GLN:HE22	34:U:1620:LUT:H41	1.68	0.59
29:9:621:BCR:H333	29:9:621:BCR:H342	1.85	0.59
2:B:494:TRP:CD1	26:B:834:CLA:HED1	2.37	0.58
29:B:844:BCR:HC8	29:B:844:BCR:H321	1.84	0.58
36:5:624:NEX:H21	19:6:229:VAL:HG11	1.85	0.58
37:X:601:CHL:HED3	28:X:2630:LHG:H132	1.86	0.58
14:1:225:VAL:HG11	14:1:228:PHE:CZ	2.38	0.58
26:A:808:CLA:CBB	29:J:102:BCR:H312	2.33	0.58
36:V:1623:NEX:H181	36:V:1623:NEX:H193	1.85	0.58
29:A:850:BCR:C23	29:A:850:BCR:H383	2.34	0.58
36:X:1623:NEX:H192	36:X:1623:NEX:H171	1.86	0.58
24:Z:51:PRO:HD2	37:Z:601:CHL:HBB1	1.86	0.58
37:V:606:CHL:HMB2	37:V:609:CHL:HMC	1.86	0.57
23:W:41:LEU:HB3	23:W:44:PHE:HB2	1.86	0.57
2:B:570:ASP:OD1	2:B:707:ARG:NH2	2.36	0.57
26:3:608:CLA:HHB	29:3:622:BCR:H342	1.86	0.57
21:8:40:HIS:NE2	21:8:56:ASP:OD2	2.37	0.57
35:U:1622:XAT:H22	25:V:262:ALA:HA	1.85	0.57
13:O:63:VAL:CG2	29:O:2005:BCR:HC21	2.34	0.57
22:9:39:ALA:O	22:9:42:LYS:NZ	2.38	0.57
2:B:578:TYR:OH	2:B:665:LEU:HD23	2.04	0.57
2:B:675:LEU:O	2:B:678:THR:OG1	2.22	0.57
26:L:302:CLA:CMB	29:L:308:BCR:H19C	2.34	0.57
24:Z:94:ALA:HB1	24:Z:209:GLY:HA3	1.86	0.57
23:W:98:THR:O	23:W:102:LEU:HB2	2.05	0.57
29:B:843:BCR:HC8	29:B:843:BCR:H331	1.87	0.57
7:G:57:GLN:OE1	7:G:58:ARG:NH1	2.38	0.57
28:Z:2630:LHG:H281	28:Z:2630:LHG:HC81	1.87	0.57
29:O:2004:BCR:H383	29:O:2004:BCR:H23C	1.85	0.57
14:a:170:SER:O	14:a:174:LYS:HG3	2.04	0.57
25:V:171:MET:HA	25:V:174:ILE:CG1	2.35	0.57
19:6:76:ARG:NH2	26:6:608:CLA:OBD	2.38	0.56
23:X:49:THR:HG22	23:X:62:GLY:HA3	1.87	0.56
2:B:616:TYR:OH	2:B:622:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:132:ASN:HB2	23:X:135:LEU:HD13	1.87	0.56
29:2:623:BCR:C20	32:V:2631:LMG:H201	2.35	0.56
19:6:205:LEU:HD11	26:6:614:CLA:HMC2	1.87	0.56
1:A:121:ILE:HD13	29:A:856:BCR:H313	1.87	0.56
29:B:801:BCR:H321	6:F:156:PHE:HB2	1.86	0.56
34:3:618:LUT:H403	29:3:622:BCR:H19C	1.88	0.56
18:5:192:LEU:HD11	26:5:611:CLA:HHD	1.86	0.56
24:U:172:PRO:HG2	37:U:608:CHL:HBB2	1.87	0.56
18:5:137:TRP:NE1	26:5:619:CLA:OBD	2.36	0.56
29:9:621:BCR:H383	29:9:621:BCR:H23C	1.88	0.56
29:B:801:BCR:H312	26:B:833:CLA:C6	2.36	0.56
24:Y:214:PHE:HZ	28:Y:2630:LHG:H171	1.71	0.56
25:V:113:LEU:O	25:V:117:THR:HG23	2.05	0.56
2:B:362:GLN:C	2:B:364:ILE:H	2.13	0.56
7:G:75:THR:HG22	7:G:76:TYR:N	2.20	0.56
14:1:170:SER:O	14:1:174:LYS:HG3	2.05	0.56
26:W:610:CLA:H52	34:W:1620:LUT:H30	1.87	0.56
2:B:21:ARG:NH1	9:I:99:ILE:O	2.39	0.56
28:X:2630:LHG:H223	35:Z:1622:XAT:H8	1.88	0.56
29:A:856:BCR:H23C	29:A:856:BCR:H392	1.88	0.56
2:B:340:ALA:HB2	29:B:847:BCR:H372	1.88	0.56
3:C:2:ALA:N	3:C:71:SER:O	2.39	0.56
15:2:209:VAL:O	15:2:213:VAL:HG23	2.06	0.56
37:U:601:CHL:HHC	35:W:1622:XAT:H383	1.88	0.55
26:A:812:CLA:H192	29:A:856:BCR:H372	1.87	0.55
29:B:843:BCR:H23C	29:B:843:BCR:C38	2.37	0.55
14:1:225:VAL:CG1	14:1:228:PHE:CE2	2.84	0.55
29:4:621:BCR:H383	29:4:621:BCR:C23	2.36	0.55
12:L:74:ALA:O	12:L:84:ARG:NH2	2.40	0.55
23:X:81:LEU:HD11	26:X:603:CLA:HBD	1.88	0.55
14:a:142:GLU:OE1	14:a:145:ARG:NH2	2.37	0.55
15:2:198:ILE:N	26:2:613:CLA:O1A	2.32	0.55
34:7:619:LUT:C8	34:7:619:LUT:H181	2.37	0.55
2:B:663:MET:O	2:B:667:SER:OG	2.24	0.55
9:I:67:TYR:CE2	9:I:68:PRO:O	2.60	0.55
34:2:619:LUT:H162	34:2:619:LUT:C4	2.36	0.55
26:4:601:CLA:OBD	19:6:127:ARG:NH2	2.36	0.55
2:B:451:GLU:OE2	6:F:114:ARG:NE	2.39	0.55
4:D:118:LYS:HE3	4:D:150:LEU:HD13	1.89	0.55
29:K:202:BCR:H331	29:K:202:BCR:C8	2.31	0.54
24:Y:195:PRO:HA	24:Y:198:PHE:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:L:308:BCR:H392	29:L:308:BCR:H23C	1.89	0.54
16:3:130:VAL:HG21	35:3:619:XAT:H172	1.87	0.54
24:Y:207:LYS:HE3	28:Y:2630:LHG:HC62	1.88	0.54
25:V:168:VAL:HG23	37:V:609:CHL:HBB2	1.90	0.54
14:1:142:GLU:OE1	14:1:145:ARG:NH2	2.37	0.54
2:B:61:TRP:NE1	26:B:827:CLA:OBD	2.40	0.54
2:B:258:PHE:CE2	2:B:494:TRP:HE3	2.25	0.54
2:B:565:ARG:NH1	3:C:63:LEU:HD11	2.22	0.54
3:C:14:CYS:O	3:C:15:THR:OG1	2.25	0.54
22:9:138:PHE:HE1	29:9:621:BCR:H382	1.73	0.54
29:3:620:BCR:H331	29:3:620:BCR:C8	2.37	0.54
24:U:102:LEU:HG	34:U:1620:LUT:H35	1.89	0.54
24:U:187:ASP:OD1	24:U:187:ASP:N	2.40	0.54
1:A:150:ALA:HB2	1:A:378:PRO:HD2	1.89	0.54
29:B:849:BCR:H23C	29:B:849:BCR:H383	1.88	0.54
34:3:618:LUT:H171	34:3:618:LUT:C8	2.37	0.54
2:B:499:LEU:HA	2:B:502:ILE:HG22	1.90	0.54
1:A:577:GLY:O	1:A:583:THR:OG1	2.23	0.54
1:A:244:LEU:O	31:A:857:LMU:O2'	2.25	0.54
29:A:852:BCR:H362	26:A:854:CLA:H43	1.90	0.54
2:B:412:MET:HE1	26:B:830:CLA:C4C	2.38	0.54
14:1:38:ASN:O	14:1:39:TRP:CD1	2.61	0.54
14:a:38:ASN:O	14:a:39:TRP:CD1	2.61	0.53
29:2:623:BCR:H382	29:2:623:BCR:H23C	1.90	0.53
34:7:619:LUT:H181	34:7:619:LUT:H8	1.89	0.53
24:Y:128:GLN:HG3	24:Y:135:LEU:HG	1.90	0.53
24:Y:160:MET:HE2	36:Y:1623:NEX:H32	1.90	0.53
23:W:121:ILE:HG21	23:W:141:ILE:HB	1.90	0.53
1:A:682:SER:HB2	1:A:727:GLY:O	2.08	0.53
2:B:293:ARG:NH1	7:G:61:ALA:O	2.41	0.53
8:H:61:ARG:NH1	12:L:71:ASN:O	2.40	0.53
29:K:207:BCR:H383	29:K:207:BCR:H23C	1.90	0.53
16:3:146:THR:HG23	26:7:614:CLA:HED3	1.90	0.53
23:X:121:ILE:HG13	23:X:141:ILE:HD13	1.91	0.53
24:U:88:GLU:HA	24:U:180:LEU:HD21	1.89	0.53
37:U:609:CHL:HBB1	37:V:601:CHL:H51	1.90	0.53
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.90	0.53
10:J:7:TYR:O	10:J:10:THR:OG1	2.25	0.53
1:A:217:GLN:NE2	1:A:294:THR:OG1	2.41	0.53
8:H:62:TYR:OH	12:L:87:GLU:OE1	2.23	0.53
11:K:56:THR:OG1	11:K:57:VAL:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:669:ARG:NH1	2:B:700:ALA:O	2.42	0.53
34:6:619:LUT:C8	34:6:619:LUT:H171	2.38	0.53
2:B:167:SER:OG	7:G:78:ASP:OD1	2.25	0.53
29:2:623:BCR:H382	29:2:623:BCR:C23	2.38	0.53
26:U:610:CLA:H2	34:U:1620:LUT:H28	1.91	0.53
25:V:100:LEU:HD11	23:W:66:ALA:HA	1.91	0.53
29:1:619:BCR:H403	29:1:619:BCR:H23C	1.91	0.53
1:A:576:ASP:OD2	1:A:580:ARG:NH2	2.39	0.52
26:A:834:CLA:HAA1	29:L:301:BCR:C14	2.39	0.52
15:2:141:ALA:HB3	15:2:142:PRO:HD3	1.91	0.52
23:X:66:ALA:HA	24:Z:89:LEU:HD11	1.91	0.52
1:A:214:ALA:O	1:A:218:ILE:HG12	2.10	0.52
24:Y:129:ILE:HG21	24:Y:149:ILE:HB	1.91	0.52
1:A:589:TRP:CE3	1:A:590:ASP:OD1	2.61	0.52
13:O:63:VAL:HG21	29:O:2005:BCR:HC21	1.91	0.52
14:a:228:PHE:HB3	17:4:147:SER:HA	1.91	0.52
22:9:126:ARG:NH2	26:9:609:CLA:O1D	2.40	0.52
24:Y:45:ARG:NH1	24:Y:62:THR:O	2.42	0.52
3:C:55:GLU:HB2	3:C:63:LEU:HD13	1.92	0.52
29:a:619:BCR:H23C	29:a:619:BCR:H403	1.91	0.52
23:W:86:ALA:HB1	23:W:201:GLY:HA3	1.92	0.52
2:B:286:ILE:O	2:B:290:HIS:ND1	2.38	0.52
29:J:102:BCR:C23	29:J:102:BCR:H382	2.39	0.52
16:3:219:LYS:NZ	28:3:624:LHG:O5	2.43	0.52
19:6:111:LEU:HD21	36:6:624:NEX:H191	1.91	0.52
25:V:174:ILE:HG21	36:V:1623:NEX:C34	2.37	0.52
26:A:841:CLA:H91	26:F:303:CLA:HBC3	1.91	0.52
29:3:621:BCR:H383	29:3:621:BCR:C23	2.39	0.52
2:B:578:TYR:OH	2:B:665:LEU:CD2	2.57	0.52
6:F:224:VAL:CG1	6:F:225:SER:N	2.72	0.52
11:K:62:THR:OG1	11:K:64:GLY:O	2.26	0.52
15:2:85:LEU:HD21	34:2:619:LUT:H173	1.90	0.52
20:7:135:ARG:HH12	26:7:609:CLA:CGD	2.23	0.52
23:X:50:PRO:HG3	24:Z:85:ARG:HH21	1.75	0.52
37:V:608:CHL:HAB	36:V:1623:NEX:H202	1.92	0.52
1:A:60:ASP:OD2	1:A:415:ARG:NH1	2.43	0.52
29:B:853:BCR:H383	29:B:853:BCR:H23C	1.91	0.52
14:1:127:LEU:HG	14:1:131:LEU:HD11	1.91	0.52
26:8:604:CLA:HMA1	26:8:606:CLA:HMC2	1.92	0.52
4:D:160:LYS:O	4:D:165:ARG:NH2	2.36	0.52
29:6:622:BCR:H23C	29:6:622:BCR:H403	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:105:ALA:HB1	25:V:221:GLY:HA3	1.91	0.52
29:B:846:BCR:H331	29:B:846:BCR:C8	2.40	0.52
25:V:171:MET:HA	25:V:174:ILE:HG12	1.91	0.52
29:A:852:BCR:H382	29:A:852:BCR:H23C	1.92	0.51
2:B:345:ILE:O	2:B:349:VAL:HG23	2.09	0.51
26:B:825:CLA:HMA1	29:B:847:BCR:H14C	1.92	0.51
25:V:135:LYS:HA	37:V:607:CHL:HED2	1.92	0.51
23:W:151:VAL:HB	36:W:1623:NEX:H15	1.91	0.51
26:A:816:CLA:H201	35:3:619:XAT:H171	1.92	0.51
2:B:664:PHE:HA	27:B:842:PQN:H9	1.93	0.51
1:A:590:ASP:OD2	1:A:724:ARG:NH1	2.44	0.51
2:B:251:SER:OG	2:B:252:GLY:N	2.42	0.51
26:Z:611:CLA:HAC1	28:Z:2630:LHG:H292	1.92	0.51
2:B:723:ALA:O	2:B:727:ILE:HG12	2.11	0.51
13:O:32:SER:OG	13:O:33:ASN:N	2.41	0.51
18:5:181:GLU:N	18:5:181:GLU:OE2	2.44	0.51
26:Z:602:CLA:H2	34:Z:1621:LUT:H28	1.91	0.51
37:U:601:CHL:HED3	28:U:2630:LHG:H142	1.93	0.51
25:V:215:VAL:HA	25:V:218:ILE:HG22	1.93	0.51
26:B:821:CLA:C2D	29:B:843:BCR:H312	2.38	0.51
7:G:59:ARG:NH1	14:1:147:ASP:OD1	2.41	0.51
1:A:119:TRP:HB3	29:A:856:BCR:C32	2.41	0.51
29:8:621:BCR:H403	29:8:621:BCR:H23C	1.92	0.51
26:X:602:CLA:H72	34:X:1621:LUT:H30	1.93	0.51
24:Z:119:GLU:N	24:Z:128:GLN:OE1	2.43	0.51
24:Z:222:GLN:NE2	34:Z:1620:LUT:O3	2.37	0.51
18:5:202:LEU:HD22	26:5:613:CLA:HAC2	1.93	0.51
25:V:216:LYS:HD3	26:V:612:CLA:HBD	1.92	0.51
2:B:556:TYR:O	2:B:572:SER:OG	2.24	0.51
23:X:193:LEU:HB3	26:X:610:CLA:HHB	1.92	0.51
17:4:113:GLY:O	17:4:117:PRO:HG2	2.10	0.51
26:Z:602:CLA:H52	34:Z:1621:LUT:H30	1.92	0.51
2:B:23:TRP:CG	2:B:705:GLN:HE22	2.29	0.51
26:X:612:CLA:H2A	26:X:612:CLA:HED2	1.93	0.51
24:U:130:PHE:HZ	25:V:259:PHE:HB3	1.74	0.51
37:V:607:CHL:HHB	37:W:601:CHL:H193	1.93	0.51
26:B:803:CLA:CGA	26:B:803:CLA:H3A	2.41	0.50
29:B:845:BCR:H342	22:9:177:LEU:HD11	1.92	0.50
18:5:94:VAL:HG23	18:5:95:LYS:HG2	1.94	0.50
26:5:607:CLA:CBB	35:5:621:XAT:H193	2.42	0.50
2:B:179:HIS:CD2	26:B:813:CLA:NB	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:848:BCR:H331	29:B:848:BCR:C8	2.40	0.50
29:B:852:BCR:C23	29:B:852:BCR:C38	2.89	0.50
26:a:613:CLA:HMB3	34:a:617:LUT:H162	1.93	0.50
35:X:1622:XAT:H10	37:Y:601:CHL:H13	1.93	0.50
29:F:305:BCR:H331	29:F:305:BCR:C8	2.42	0.50
12:L:57:THR:CG2	12:L:58:PRO:HD2	2.42	0.50
26:1:613:CLA:HMB3	34:1:617:LUT:H162	1.93	0.50
26:4:607:CLA:CBB	35:4:620:XAT:H161	2.42	0.50
18:5:151:ILE:HG12	29:5:622:BCR:H321	1.93	0.50
32:5:627:LMG:O4	20:7:182:LYS:NZ	2.43	0.50
24:Y:221:VAL:HA	24:Y:224:ILE:HG22	1.94	0.50
35:Y:1622:XAT:H10	28:Z:2630:LHG:H221	1.93	0.50
26:Z:613:CLA:H91	28:Z:2630:LHG:H301	1.94	0.50
24:U:164:GLU:OE1	24:U:167:ARG:NH2	2.43	0.50
37:U:609:CHL:H62	26:V:602:CLA:H142	1.93	0.50
1:A:695:GLU:OE1	2:B:537:LYS:NZ	2.44	0.50
3:C:73:SER:OG	3:C:74:THR:N	2.45	0.50
18:5:166:GLY:N	26:5:610:CLA:OBD	2.39	0.50
24:Z:62:THR:OG1	24:Z:64:GLU:OE1	2.28	0.50
25:V:134:PHE:HA	37:V:607:CHL:HMA2	1.94	0.50
29:A:856:BCR:H311	29:A:856:BCR:C8	2.40	0.50
24:Y:201:LEU:HB3	26:Y:610:CLA:H3A	1.94	0.50
37:Z:606:CHL:HHC	37:Z:606:CHL:HBB1	1.93	0.50
29:B:844:BCR:H382	29:B:844:BCR:H23C	1.94	0.50
37:Y:607:CHL:H143	37:Z:601:CHL:H18	1.94	0.50
23:W:136:ILE:O	37:W:605:CHL:NB	2.44	0.50
29:F:305:BCR:C33	29:F:305:BCR:HC8	2.41	0.50
29:L:301:BCR:H23C	29:L:301:BCR:C38	2.39	0.50
13:O:57:ILE:HB	13:O:58:PRO:HD3	1.94	0.50
15:2:217:LEU:N	15:2:218:PRO:HD2	2.26	0.50
26:3:612:CLA:HHC	26:3:612:CLA:HBB1	1.93	0.50
24:U:221:VAL:HG21	26:U:613:CLA:HAC2	1.94	0.50
24:U:224:ILE:HD12	25:V:267:PRO:HB3	1.94	0.50
9:I:80:VAL:HB	9:I:81:PRO:HD3	1.93	0.50
29:L:309:BCR:H311	29:L:309:BCR:C8	2.40	0.50
19:6:82:VAL:HG11	34:6:619:LUT:H12	1.94	0.49
23:X:98:THR:HA	23:X:101:LEU:HB2	1.92	0.49
1:A:650:LEU:O	1:A:654:SER:OG	2.28	0.49
29:B:801:BCR:H23C	29:B:801:BCR:C38	2.42	0.49
26:B:824:CLA:O1A	26:B:824:CLA:H2A	2.12	0.49
26:K:204:CLA:HMC3	29:K:207:BCR:H332	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:135:ARG:NH2	26:6:601:CLA:OBD	2.41	0.49
18:5:202:LEU:HD11	18:5:252:LEU:CD1	2.42	0.49
24:U:45:ARG:NH2	24:U:61:LEU:O	2.45	0.49
26:V:602:CLA:H52	34:V:1621:LUT:H28	1.94	0.49
7:G:71:THR:OG1	7:G:81:GLN:OE1	2.31	0.49
35:4:620:XAT:C28	35:4:620:XAT:H381	2.42	0.49
23:X:41:LEU:HB2	23:X:45:SER:HB2	1.94	0.49
24:U:91:LEU:HD23	24:U:180:LEU:HD22	1.93	0.49
25:V:61:LEU:HB2	25:V:65:SER:HB3	1.94	0.49
13:O:45:PRO:HB2	26:Z:611:CLA:HHB	1.94	0.49
29:7:621:BCR:H23C	29:7:621:BCR:H403	1.93	0.49
35:V:1622:XAT:H22	23:W:242:ALA:HA	1.93	0.49
23:W:83:LEU:HD12	23:W:172:LEU:HD13	1.94	0.49
1:A:55:ASP:O	1:A:62:HIS:NE2	2.36	0.49
14:1:41:PRO:HG3	21:8:153:SER:OG	2.12	0.49
14:a:50:PRO:O	14:a:56:ASN:ND2	2.46	0.49
17:4:118:GLU:HB2	17:4:241:LEU:HD12	1.94	0.49
21:8:28:ARG:O	21:8:28:ARG:NH1	2.41	0.49
24:Y:216:MET:HE2	34:Y:1621:LUT:H12	1.94	0.49
24:Z:160:MET:HA	24:Z:163:VAL:HG12	1.93	0.49
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.94	0.49
2:B:582:PHE:HZ	2:B:665:LEU:HD21	1.77	0.49
14:1:76:GLU:OE2	14:1:150:GLY:HA2	2.12	0.49
2:B:561:ASP:OD2	2:B:565:ARG:NH2	2.43	0.49
20:7:129:GLY:O	20:7:133:THR:OG1	2.26	0.49
23:X:58:PRO:HG3	23:X:194:LYS:HD2	1.94	0.49
37:X:601:CHL:H51	37:Z:607:CHL:H191	1.95	0.49
12:L:57:THR:H	12:L:60:THR:HG1	1.59	0.49
26:1:611:CLA:H43	14:a:139:ALA:HB1	1.94	0.49
22:9:174:VAL:HG11	26:9:613:CLA:HAC2	1.94	0.49
26:Z:610:CLA:H52	34:Z:1620:LUT:H30	1.95	0.49
25:V:174:ILE:HD12	25:V:175:GLU:N	2.28	0.49
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.94	0.49
29:A:852:BCR:H331	29:A:852:BCR:C8	2.41	0.49
2:B:148:ALA:HB2	29:B:852:BCR:H361	1.94	0.49
29:B:848:BCR:H382	29:B:848:BCR:H23C	1.94	0.49
29:J:102:BCR:H331	29:J:102:BCR:C8	2.42	0.49
14:1:50:PRO:O	14:1:56:ASN:ND2	2.46	0.49
18:5:101:TYR:OH	18:5:205:GLN:NE2	2.37	0.49
23:X:94:LEU:HA	23:X:97:ILE:HG22	1.95	0.49
24:U:250:ALA:HB1	35:W:1622:XAT:H183	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:517:ASP:OD2	2:B:594:TYR:OH	2.30	0.48
3:C:34:CYS:SG	3:C:39:MET:HG2	2.53	0.48
6:F:162:TYR:OH	6:F:196:ALA:O	2.24	0.48
12:L:184:TRP:HB2	29:L:308:BCR:HC8	1.95	0.48
29:A:856:BCR:H392	29:A:856:BCR:C23	2.42	0.48
2:B:659:ALA:O	2:B:662:PHE:HB2	2.14	0.48
29:O:2005:BCR:H23C	29:O:2005:BCR:H383	1.95	0.48
14:a:64:LEU:HD23	21:8:160:SER:OG	2.12	0.48
18:5:55:TRP:CD1	18:5:57:PRO:HD3	2.48	0.48
28:9:622:LHG:O3	28:9:622:LHG:O1	2.28	0.48
26:A:802:CLA:CGA	26:A:802:CLA:H3A	2.42	0.48
1:A:370:HIS:ND1	26:A:819:CLA:OBD	2.47	0.48
2:B:683:HIS:NE2	2:B:692:VAL:O	2.34	0.48
36:Y:1623:NEX:H192	36:Y:1623:NEX:H181	1.95	0.48
28:Z:2630:LHG:O3	28:Z:2630:LHG:O1	2.30	0.48
1:A:87:TRP:HZ3	29:A:849:BCR:H322	1.78	0.48
29:A:848:BCR:H321	29:A:848:BCR:HC8	1.95	0.48
26:B:839:CLA:H2A	9:I:96:PHE:HE1	1.78	0.48
29:B:845:BCR:H23C	29:B:845:BCR:C38	2.43	0.48
14:a:76:GLU:OE1	14:a:152:VAL:HB	2.13	0.48
16:3:161:ARG:HD3	26:7:601:CLA:OBD	2.13	0.48
29:3:620:BCR:C31	26:7:611:CLA:CAB	2.86	0.48
29:B:846:BCR:H403	29:B:847:BCR:H272	1.95	0.48
11:K:64:GLY:O	11:K:66:LYS:N	2.46	0.48
29:K:202:BCR:HC8	29:K:202:BCR:C33	2.42	0.48
15:2:216:VAL:HB	32:9:625:LMG:H202	1.96	0.48
23:X:187:PRO:HA	23:X:190:PHE:HB3	1.94	0.48
37:X:601:CHL:H13	28:X:2630:LHG:H202	1.94	0.48
26:X:602:CLA:H142	37:Z:609:CHL:H93	1.94	0.48
24:U:210:ARG:HA	24:U:213:MET:HE3	1.96	0.48
1:A:685:PHE:HA	27:A:844:PQN:H9	1.96	0.48
18:5:192:LEU:HD21	28:5:623:LHG:H262	1.90	0.48
24:Y:156:GLN:O	24:Y:160:MET:HB2	2.13	0.48
14:1:48:TRP:NE1	14:1:60:ASP:OD2	2.45	0.48
26:4:606:CLA:H3A	29:4:621:BCR:C21	2.43	0.48
18:5:159:ASN:OD1	18:5:165:PRO:HA	2.13	0.48
36:6:624:NEX:H161	36:6:624:NEX:C19	2.44	0.48
18:5:202:LEU:CD1	18:5:252:LEU:HD12	2.44	0.48
19:6:111:LEU:HD21	36:6:624:NEX:H192	1.96	0.48
29:A:850:BCR:H313	13:O:112:THR:OG1	2.14	0.48
13:O:120:GLY:O	13:O:124:GLY:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:622:BCR:C8	29:3:622:BCR:C32	2.92	0.48
37:Y:609:CHL:HAA1	24:Z:73:THR:HG21	1.96	0.48
24:Z:91:LEU:HD23	24:Z:180:LEU:HD22	1.95	0.48
29:B:843:BCR:H331	29:B:843:BCR:C8	2.44	0.47
16:3:99:MET:HB2	34:3:618:LUT:C15	2.44	0.47
17:4:110:ALA:O	17:4:114:ILE:HG12	2.13	0.47
23:W:222:PRO:O	34:W:1620:LUT:O3	2.32	0.47
1:A:119:TRP:CG	29:A:856:BCR:H323	2.49	0.47
1:A:410:ALA:HB1	1:A:588:ALA:HB1	1.96	0.47
29:K:207:BCR:H331	29:K:207:BCR:C8	2.42	0.47
13:O:50:LEU:HD13	29:O:2005:BCR:H372	1.96	0.47
14:a:38:ASN:C	14:a:40:LEU:H	2.22	0.47
19:6:172:LEU:HG	26:6:610:CLA:HHB	1.96	0.47
25:V:164:LEU:HD13	37:V:607:CHL:HAC2	1.97	0.47
1:A:355:ILE:HD11	29:A:850:BCR:H24C	1.96	0.47
15:2:234:VAL:HG13	15:2:240:ASN:HD21	1.76	0.47
18:5:85:VAL:HG21	34:5:620:LUT:H14	1.96	0.47
18:5:175:SER:O	18:5:176:LYS:HG2	2.13	0.47
24:Y:94:ALA:HB1	24:Y:209:GLY:HA3	1.95	0.47
26:Y:603:CLA:H43	26:Z:602:CLA:H62	1.96	0.47
4:D:154:ASP:OD1	4:D:154:ASP:N	2.47	0.47
14:a:48:TRP:NE1	14:a:60:ASP:OD2	2.45	0.47
24:Y:207:LYS:CE	28:Y:2630:LHG:HC62	2.45	0.47
24:U:153:LEU:HB2	37:U:607:CHL:HBC1	1.96	0.47
23:W:80:GLU:HA	23:W:172:LEU:HD21	1.97	0.47
22:9:193:ASP:OD1	22:9:196:GLY:N	2.48	0.47
37:Y:601:CHL:H72	28:Y:2630:LHG:H212	1.97	0.47
26:U:602:CLA:H52	34:U:1621:LUT:H28	1.97	0.47
23:W:97:ILE:HG21	34:W:1620:LUT:H173	1.97	0.47
1:A:311:MET:HE1	26:A:822:CLA:C3D	2.45	0.47
29:L:305:BCR:C8	29:L:305:BCR:C31	2.90	0.47
2:B:395:PHE:O	2:B:543:ARG:NH1	2.43	0.47
8:H:31:LYS:N	8:H:34:GLU:OE1	2.48	0.47
14:a:64:LEU:HD12	35:a:618:XAT:H23	1.97	0.47
19:6:75:SER:HB3	19:6:180:GLY:HA3	1.97	0.47
20:7:198:MET:SD	26:7:602:CLA:HBB1	2.55	0.47
29:7:623:BCR:H383	29:7:623:BCR:C23	2.45	0.47
23:X:86:ALA:HB1	23:X:201:GLY:HA3	1.97	0.47
23:X:148:GLN:O	23:X:152:MET:HB2	2.14	0.47
35:Y:1622:XAT:H373	28:Z:2630:LHG:H382	1.97	0.47
24:U:61:LEU:HD11	24:U:72:ASP:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:87:ARG:HA	23:W:90:MET:HE3	1.96	0.47
2:B:375:HIS:HE2	26:B:828:CLA:C1B	2.27	0.47
29:B:852:BCR:H383	29:B:852:BCR:C23	2.45	0.47
14:1:38:ASN:C	14:1:40:LEU:H	2.22	0.47
24:Z:45:ARG:NH2	24:Z:61:LEU:O	2.48	0.47
24:U:123:PHE:HA	37:U:607:CHL:HMA2	1.96	0.47
26:V:613:CLA:H2	26:V:614:CLA:HMD1	1.97	0.47
29:A:851:BCR:C33	29:A:851:BCR:HC8	2.45	0.47
2:B:546:LYS:NZ	5:E:50:SER:O	2.42	0.47
9:I:68:PRO:O	9:I:69:PHE:HB2	2.15	0.47
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.95	0.47
2:B:359:TYR:OH	26:B:828:CLA:OBD	2.33	0.47
6:F:224:VAL:CG1	6:F:226:PRO:HD2	2.42	0.47
29:3:620:BCR:H312	26:7:611:CLA:C3B	2.45	0.47
29:A:850:BCR:C8	29:A:850:BCR:C32	2.93	0.46
2:B:279:LEU:HD21	26:B:816:CLA:HMB1	1.97	0.46
18:5:233:THR:HA	18:5:256:SER:HB3	1.97	0.46
26:9:613:CLA:HMB3	34:9:619:LUT:H162	1.98	0.46
23:X:47:GLY:N	24:Z:169:ASN:OD1	2.43	0.46
37:Y:601:CHL:HBA1	37:Y:601:CHL:H3A	1.63	0.46
24:U:230:PRO:O	34:U:1620:LUT:O3	2.31	0.46
18:5:53:TYR:N	26:5:602:CLA:OBD	2.48	0.46
24:U:160:MET:HA	24:U:163:VAL:HG22	1.96	0.46
29:A:851:BCR:H23C	29:A:851:BCR:H403	1.96	0.46
14:a:161:LEU:HD12	34:a:617:LUT:H222	1.98	0.46
34:U:1621:LUT:H15	34:U:1621:LUT:H201	1.75	0.46
1:A:217:GLN:HA	1:A:221:SER:HB2	1.96	0.46
2:B:305:ILE:HD13	26:B:822:CLA:HMD2	1.96	0.46
2:B:625:LEU:O	2:B:629:SER:OG	2.23	0.46
6:F:142:LYS:HD2	32:8:626:LMG:H202	1.97	0.46
8:H:32:TYR:OH	12:L:49:ASP:OD2	2.32	0.46
29:3:620:BCR:C8	29:3:620:BCR:C33	2.93	0.46
17:4:177:ASP:OD1	17:4:177:ASP:N	2.46	0.46
24:U:189:LEU:HD13	34:U:1620:LUT:H222	1.97	0.46
2:B:416:LYS:HA	2:B:419:LEU:HD12	1.97	0.46
17:4:229:PHE:HE1	34:4:619:LUT:H41	1.80	0.46
19:6:193:ALA:O	19:6:197:THR:OG1	2.30	0.46
19:6:253:GLN:N	26:7:615:CLA:O2A	2.48	0.46
21:8:116:SER:OG	21:8:118:ALA:O	2.31	0.46
24:Y:221:VAL:HG21	26:Y:613:CLA:HAC2	1.98	0.46
37:Y:605:CHL:HHD	37:Y:606:CHL:OBD	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:129:ILE:HG12	24:Z:149:ILE:HB	1.98	0.46
26:W:613:CLA:H162	26:W:614:CLA:HBD	1.96	0.46
32:A:860:LMG:HC1	20:7:60:GLN:HE22	1.81	0.46
12:L:79:VAL:HG12	12:L:80:ALA:N	2.31	0.46
26:a:601:CLA:OBD	17:4:163:ARG:HD3	2.16	0.46
18:5:191:ARG:HD3	26:5:602:CLA:CHD	2.46	0.46
20:7:88:LEU:HD23	26:7:604:CLA:HHD	1.98	0.46
24:Y:216:MET:HE2	34:Y:1621:LUT:H10	1.97	0.46
23:W:213:VAL:HG11	26:W:613:CLA:HAC2	1.97	0.46
25:V:109:MET:SD	26:V:610:CLA:HAB	2.56	0.46
25:V:166:VAL:HG11	37:V:605:CHL:HBC1	1.98	0.46
25:V:261:TYR:HA	25:V:264:LYS:HE2	1.98	0.46
23:W:237:ASN:HD22	23:W:237:ASN:H	1.62	0.46
1:A:144:PHE:HE2	26:A:829:CLA:HED1	1.81	0.46
29:3:620:BCR:H403	29:3:620:BCR:H23C	1.96	0.46
18:5:155:ASN:OD1	18:5:155:ASN:N	2.49	0.46
29:9:621:BCR:H342	29:9:621:BCR:C33	2.45	0.46
1:A:19:ARG:NE	16:3:78:SER:O	2.48	0.46
29:A:849:BCR:C33	29:A:849:BCR:HC8	2.45	0.46
29:A:849:BCR:H382	29:A:849:BCR:H23C	1.97	0.46
26:X:613:CLA:H2	26:X:613:CLA:H61	1.72	0.46
29:B:852:BCR:HC32	29:B:852:BCR:H322	1.69	0.46
4:D:138:PHE:CE2	4:D:151:HIS:HB2	2.50	0.46
14:1:64:LEU:HD12	35:1:618:XAT:H23	1.97	0.46
28:a:620:LHG:HC92	29:4:621:BCR:H333	1.97	0.46
17:4:150:PHE:CE2	17:4:154:MET:HG3	2.51	0.46
18:5:141:LYS:NZ	26:5:619:CLA:O1D	2.42	0.46
26:A:843:CLA:H3A	29:L:301:BCR:H322	1.98	0.45
29:3:620:BCR:C33	29:3:620:BCR:HC8	2.45	0.45
17:4:157:PHE:HA	17:4:160:VAL:HG22	1.98	0.45
20:7:171:ASP:OD2	20:7:176:SER:OG	2.28	0.45
25:V:106:ARG:HA	25:V:109:MET:HE3	1.98	0.45
1:A:121:ILE:HG13	1:A:122:VAL:HG13	1.98	0.45
26:A:841:CLA:OBD	2:B:424:SER:OG	2.26	0.45
29:O:2005:BCR:H383	29:O:2005:BCR:C23	2.46	0.45
19:6:121:MET:HA	19:6:124:VAL:HG22	1.99	0.45
26:6:606:CLA:CBB	26:6:607:CLA:HMC3	2.45	0.45
26:Y:613:CLA:H152	26:Y:613:CLA:H112	1.60	0.45
36:Z:1623:NEX:H201	36:Z:1623:NEX:H15	1.72	0.45
24:U:45:ARG:NE	24:U:68:ASP:O	2.33	0.45
37:U:608:CHL:HBD	26:U:610:CLA:HAC2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:72:ASN:O	11:K:74:ALA:N	2.47	0.45
35:2:620:XAT:C28	35:2:620:XAT:H381	2.46	0.45
34:9:619:LUT:H8	34:9:619:LUT:C16	2.46	0.45
26:U:613:CLA:H92	26:U:613:CLA:HAB	1.99	0.45
35:V:1622:XAT:H14	37:W:601:CHL:H72	1.98	0.45
1:A:396:TRP:CE3	1:A:603:LEU:HD12	2.52	0.45
2:B:92:ILE:HB	2:B:113:PRO:HB2	1.99	0.45
29:B:801:BCR:H331	29:B:801:BCR:C8	2.45	0.45
3:C:55:GLU:O	3:C:63:LEU:HD22	2.16	0.45
37:X:608:CHL:H12	34:X:1620:LUT:H383	1.98	0.45
24:Z:234:LEU:HD13	34:Z:1620:LUT:H163	1.98	0.45
34:U:1620:LUT:H201	34:U:1620:LUT:H15	1.70	0.45
2:B:575:ASP:OD1	2:B:707:ARG:NE	2.49	0.45
16:3:187:SER:OG	16:3:188:GLY:N	2.50	0.45
26:6:610:CLA:HBA2	34:6:619:LUT:O23	2.16	0.45
26:X:611:CLA:HBA2	26:X:611:CLA:H3A	1.70	0.45
24:Y:95:ARG:NH1	37:Y:608:CHL:OBD	2.50	0.45
26:Y:602:CLA:H71	26:Y:603:CLA:HHB	1.98	0.45
24:U:42:GLY:O	24:U:45:ARG:NH1	2.41	0.45
25:V:171:MET:O	25:V:174:ILE:HG13	2.15	0.45
3:C:22:PRO:C	4:D:122:LEU:HD23	2.42	0.45
26:V:602:CLA:HAB	34:V:1621:LUT:H32	1.99	0.45
9:I:63:ALA:N	15:2:202:SER:O	2.49	0.45
26:8:612:CLA:HMC3	34:8:619:LUT:H193	1.99	0.45
26:Z:613:CLA:H2	26:Z:613:CLA:H61	1.68	0.45
24:U:116:GLN:O	24:U:117:PHE:HB2	2.16	0.45
6:F:158:TYR:O	6:F:202:TRP:NE1	2.50	0.45
35:X:1622:XAT:H28	28:Y:2630:LHG:H382	1.98	0.45
37:Y:601:CHL:H143	37:Y:601:CHL:H161	1.87	0.45
24:U:222:GLN:OE1	26:U:613:CLA:ND	2.50	0.45
34:V:1620:LUT:H35	34:V:1620:LUT:H401	1.80	0.45
34:W:1621:LUT:H11	34:W:1621:LUT:H191	1.74	0.45
1:A:325:ILE:HG22	26:A:825:CLA:HED3	1.99	0.45
2:B:144:ALA:HB1	29:B:852:BCR:C21	2.46	0.45
24:Z:128:GLN:HB2	24:Z:135:LEU:HD13	1.98	0.45
1:A:204:GLY:O	1:A:208:LEU:HB2	2.17	0.45
29:B:843:BCR:HC8	29:B:843:BCR:C33	2.46	0.45
6:F:63:ASP:OD1	6:F:63:ASP:N	2.50	0.45
6:F:128:ASP:OD1	6:F:128:ASP:N	2.47	0.45
14:1:227:PHE:CD2	32:8:626:LMG:H251	2.52	0.45
15:2:197:ASN:HD21	22:9:110:ALA:HB1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:V:1622:XAT:H403	28:W:2630:LHG:H121	1.98	0.45
26:A:819:CLA:CGA	26:A:819:CLA:H3A	2.47	0.44
2:B:348:LEU:HA	26:B:825:CLA:HED1	2.00	0.44
11:K:76:VAL:HA	16:3:50:SER:HA	2.00	0.44
19:6:224:VAL:O	19:6:226:GLY:N	2.49	0.44
23:X:156:GLU:OE1	37:X:609:CHL:ND	2.50	0.44
37:X:608:CHL:H51	37:X:608:CHL:H11	1.72	0.44
26:X:613:CLA:H8	26:X:614:CLA:HMD3	1.98	0.44
24:Y:167:ARG:NH2	37:Y:609:CHL:O1D	2.50	0.44
25:V:234:GLN:HE21	25:V:245:ASN:HD22	1.65	0.44
1:A:349:TRP:HB3	26:A:806:CLA:HAC1	1.98	0.44
2:B:411:ARG:O	2:B:415:HIS:ND1	2.45	0.44
29:B:801:BCR:C10	26:F:303:CLA:HAB	2.48	0.44
4:D:138:PHE:CZ	4:D:151:HIS:HB2	2.52	0.44
14:1:106:ALA:HB3	14:1:107:PRO:HD3	2.00	0.44
17:4:189:ASN:ND2	17:4:194:PRO:O	2.49	0.44
26:X:610:CLA:HBB1	34:X:1620:LUT:H30	1.99	0.44
26:Y:613:CLA:H61	26:Y:613:CLA:H2	1.73	0.44
26:U:610:CLA:HBB1	26:U:610:CLA:H51	1.99	0.44
25:V:174:ILE:HG21	36:V:1623:NEX:H15	1.84	0.44
34:W:1620:LUT:H35	34:W:1620:LUT:H401	1.87	0.44
29:A:852:BCR:C33	29:A:852:BCR:HC8	2.46	0.44
2:B:362:GLN:C	2:B:364:ILE:N	2.75	0.44
6:F:162:TYR:O	6:F:166:VAL:HG23	2.17	0.44
7:G:71:THR:HG22	7:G:73:GLY:H	1.82	0.44
11:K:69:ASP:OD1	11:K:69:ASP:N	2.50	0.44
14:1:161:LEU:HD12	34:1:617:LUT:H222	1.98	0.44
34:1:617:LUT:C8	34:1:617:LUT:H171	2.47	0.44
26:8:612:CLA:HMC3	34:8:619:LUT:C19	2.47	0.44
25:V:171:MET:CE	25:V:174:ILE:HD11	2.47	0.44
4:D:154:ASP:OD2	4:D:165:ARG:NH1	2.49	0.44
26:3:613:CLA:HMB3	34:3:618:LUT:H162	2.00	0.44
34:Y:1620:LUT:H11	34:Y:1620:LUT:H191	1.55	0.44
24:U:110:LEU:HA	24:U:113:SER:HB2	1.98	0.44
26:A:822:CLA:H71	29:A:851:BCR:H12C	2.00	0.44
2:B:33:GLU:OE2	2:B:332:HIS:NE2	2.35	0.44
2:B:478:LEU:HD13	26:B:834:CLA:HMD3	1.98	0.44
8:H:99:GLY:O	9:I:77:SER:OG	2.32	0.44
17:4:110:ALA:HB2	35:4:620:XAT:C10	2.48	0.44
17:4:260:ASP:HB3	26:4:616:CLA:C1B	2.47	0.44
26:Z:613:CLA:H71	28:Z:2630:LHG:H172	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:170:LEU:O	25:V:174:ILE:HG23	2.17	0.44
34:V:1620:LUT:H15	34:V:1620:LUT:H201	1.82	0.44
35:V:1622:XAT:H35	35:V:1622:XAT:H401	1.81	0.44
1:A:587:SER:O	1:A:591:HIS:ND1	2.47	0.44
2:B:149:ILE:HG12	32:9:625:LMG:H262	2.00	0.44
2:B:629:SER:O	2:B:633:ILE:HG12	2.16	0.44
5:E:70:PRO:HD2	5:E:89:ALA:HA	1.99	0.44
29:L:309:BCR:H321	29:L:309:BCR:C8	2.43	0.44
14:a:106:ALA:HB3	14:a:107:PRO:HD3	2.00	0.44
22:9:172:PHE:HE1	34:9:619:LUT:C5	2.30	0.44
23:X:213:VAL:HG21	26:X:613:CLA:HAC2	1.99	0.44
34:X:1620:LUT:H11	34:X:1620:LUT:H191	1.82	0.44
3:C:61:ASP:N	5:E:86:ASN:OD1	2.51	0.44
4:D:140:ARG:N	4:D:148:GLN:O	2.49	0.44
16:3:210:MET:HE1	26:3:610:CLA:H2A	2.00	0.44
37:Z:601:CHL:H92	37:Z:601:CHL:H62	1.89	0.44
24:U:94:ALA:HB1	24:U:209:GLY:HA3	1.99	0.44
34:V:1621:LUT:H15	34:V:1621:LUT:H201	1.77	0.44
26:B:808:CLA:HHC	26:B:808:CLA:HBB1	2.00	0.44
29:B:853:BCR:H361	15:2:212:ALA:HB1	1.99	0.44
26:a:611:CLA:HHC	29:4:621:BCR:H313	1.99	0.44
34:a:617:LUT:C8	34:a:617:LUT:H171	2.47	0.44
17:4:164:ARG:NH2	26:4:609:CLA:O1D	2.40	0.44
29:7:623:BCR:HC8	29:7:623:BCR:C32	2.45	0.44
22:9:30:THR:OG1	22:9:32:LEU:O	2.36	0.44
37:X:609:CHL:H91	37:X:609:CHL:H112	1.81	0.44
25:V:172:GLY:HA2	37:V:609:CHL:HAB	2.00	0.44
23:W:94:LEU:HD21	26:W:612:CLA:HAB	2.00	0.44
1:A:119:TRP:HB3	29:A:856:BCR:H322	1.99	0.44
1:A:148:TRP:HB3	1:A:153:ILE:HG13	2.00	0.44
2:B:73:GLY:HA2	2:B:88:ILE:HB	1.99	0.44
2:B:224:THR:HB	2:B:225:PRO:HD3	2.00	0.44
2:B:565:ARG:HH11	3:C:63:LEU:HD21	1.82	0.44
2:B:572:SER:OG	2:B:573:ALA:N	2.49	0.44
14:1:169:LYS:O	14:1:173:LEU:HG	2.18	0.44
35:X:1622:XAT:H15	35:X:1622:XAT:H201	1.77	0.44
35:Z:1622:XAT:H11	35:Z:1622:XAT:H191	1.84	0.44
24:U:99:LEU:HB3	26:U:604:CLA:HBB2	2.00	0.44
35:U:1622:XAT:H181	37:V:601:CHL:H141	1.98	0.44
23:W:76:LYS:HB3	23:W:76:LYS:HE3	1.79	0.44
2:B:657:ILE:HG22	2:B:713:HIS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:75:THR:CG2	7:G:76:TYR:N	2.80	0.43
29:L:301:BCR:H352	26:L:303:CLA:HHC	1.99	0.43
21:8:207:PHE:HE1	34:8:619:LUT:H41	1.83	0.43
34:8:619:LUT:C8	34:8:619:LUT:H171	2.47	0.43
22:9:52:ASP:OD1	22:9:55:GLY:N	2.45	0.43
1:A:690:ARG:NH1	1:A:694:GLN:OE1	2.51	0.43
26:A:807:CLA:HHC	26:A:807:CLA:HBB1	2.00	0.43
29:A:849:BCR:H331	29:A:849:BCR:C8	2.47	0.43
3:C:58:CYS:HA	30:C:102:SF4:S4	2.58	0.43
6:F:224:VAL:CG1	6:F:225:SER:H	2.31	0.43
35:a:618:XAT:C28	35:a:618:XAT:H381	2.47	0.43
15:2:185:THR:HG22	26:2:613:CLA:O1D	2.18	0.43
23:W:165:LEU:HB3	23:W:177:ALA:HB3	1.99	0.43
1:A:356:ASN:O	1:A:360:PHE:HB2	2.17	0.43
1:A:408:HIS:HE1	26:A:831:CLA:NA	2.17	0.43
29:A:851:BCR:H331	29:A:851:BCR:C8	2.48	0.43
8:H:84:ARG:NH2	12:L:137:SER:OG	2.36	0.43
26:1:604:CLA:H2A	26:1:604:CLA:O1D	2.18	0.43
24:U:58:PRO:HG2	24:U:72:ASP:HB3	1.99	0.43
37:V:601:CHL:H61	37:V:601:CHL:H102	1.59	0.43
34:W:1621:LUT:H15	34:W:1621:LUT:H201	1.70	0.43
1:A:150:ALA:HB1	26:A:820:CLA:HED1	1.99	0.43
29:L:301:BCR:C38	29:L:301:BCR:C23	2.95	0.43
26:1:606:CLA:HAB	26:1:607:CLA:HMC3	2.00	0.43
35:1:618:XAT:C28	35:1:618:XAT:H381	2.47	0.43
28:3:623:LHG:H101	26:7:614:CLA:H3A	1.99	0.43
37:Z:606:CHL:HMB1	37:Z:609:CHL:HMC	2.00	0.43
26:Z:610:CLA:HMB3	26:Z:612:CLA:HAA1	2.01	0.43
1:A:486:TRP:O	1:A:490:THR:OG1	2.34	0.43
1:A:647:ARG:HA	2:B:633:ILE:HD12	2.00	0.43
1:A:668:TYR:O	1:A:741:SER:HB3	2.19	0.43
1:A:693:TRP:HZ3	26:A:802:CLA:O1D	2.02	0.43
29:G:205:BCR:H383	29:G:205:BCR:H23C	2.01	0.43
14:1:227:PHE:HB3	32:8:626:LMG:H192	1.98	0.43
14:a:152:VAL:HG13	14:a:153:TYR:CD2	2.54	0.43
23:X:161:ASN:HA	24:Y:55:ASN:HB3	1.99	0.43
24:U:51:PRO:HD2	37:U:601:CHL:HBB1	1.98	0.43
1:A:687:PHE:CD1	2:B:665:LEU:HB3	2.54	0.43
26:L:307:CLA:CBB	29:L:308:BCR:H342	2.49	0.43
20:7:144:SER:C	20:7:146:ALA:H	2.25	0.43
26:Z:603:CLA:H92	26:Z:603:CLA:H62	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:152:MET:HA	23:W:155:ALA:HB3	1.99	0.43
23:W:229:HIS:CG	26:W:613:CLA:HAA2	2.53	0.43
2:B:520:VAL:HG21	2:B:594:TYR:HB2	2.00	0.43
29:B:847:BCR:C23	29:B:847:BCR:H383	2.48	0.43
13:O:124:GLY:O	13:O:125:TYR:HB2	2.19	0.43
26:a:604:CLA:O1D	26:a:604:CLA:H2A	2.19	0.43
29:4:621:BCR:C23	29:4:621:BCR:C38	2.94	0.43
37:Y:606:CHL:HHC	37:Y:606:CHL:HBB1	2.01	0.43
24:U:153:LEU:HG	26:V:613:CLA:H201	2.00	0.43
35:U:1622:XAT:H403	28:V:2630:LHG:H121	1.99	0.43
26:V:610:CLA:H43	26:V:612:CLA:HBA1	2.00	0.43
1:A:189:GLU:O	1:A:193:ASN:ND2	2.52	0.43
2:B:211:ASP:OD1	2:B:211:ASP:N	2.50	0.43
26:B:837:CLA:CAC	29:F:305:BCR:H322	2.49	0.43
29:J:102:BCR:HC8	29:J:102:BCR:C33	2.47	0.43
14:a:169:LYS:O	14:a:173:LEU:HG	2.18	0.43
19:6:172:LEU:HD23	26:6:610:CLA:H3A	2.01	0.43
26:X:604:CLA:H2A	26:X:604:CLA:HED2	2.00	0.43
37:V:606:CHL:HAA2	36:V:1623:NEX:H403	2.01	0.43
1:A:297:HIS:HE2	26:A:820:CLA:C2B	2.32	0.43
29:A:848:BCR:H11C	29:A:848:BCR:H341	1.92	0.43
12:L:57:THR:HG23	12:L:58:PRO:HD2	2.01	0.43
16:3:89:TYR:OH	16:3:162:ARG:HG2	2.19	0.43
35:6:621:XAT:C8	35:6:621:XAT:H181	2.48	0.43
20:7:231:PHE:N	26:7:613:CLA:O1A	2.48	0.43
26:Y:610:CLA:HBB1	34:Y:1620:LUT:H30	1.99	0.43
24:U:49:LEU:HB2	24:U:53:SER:HB2	2.00	0.43
25:V:199:ASP:OD1	34:V:1620:LUT:O23	2.37	0.43
1:A:443:TRP:NE1	26:A:834:CLA:OBD	2.43	0.43
1:A:695:GLU:O	1:A:698:GLU:HG2	2.19	0.43
29:A:850:BCR:C8	29:A:850:BCR:H321	2.49	0.43
2:B:176:LEU:HD21	26:B:819:CLA:HMA3	2.01	0.43
8:H:66:GLN:HE22	26:L:302:CLA:CGD	2.32	0.43
16:3:95:ALA:HB1	16:3:221:GLY:HA3	2.01	0.43
21:8:237:ASN:ND2	26:8:613:CLA:OBD	2.52	0.43
37:Y:608:CHL:H12	34:Y:1620:LUT:H383	2.00	0.43
26:Y:613:CLA:H202	26:Y:613:CLA:H162	1.88	0.43
5:E:67:VAL:HG13	5:E:70:PRO:HB3	2.00	0.42
29:2:623:BCR:C21	32:V:2631:LMG:H201	2.48	0.42
18:5:192:LEU:HG	28:5:623:LHG:O10	2.19	0.42
29:7:623:BCR:H383	29:7:623:BCR:H23C	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:61:LEU:HD11	24:Z:72:ASP:HB2	2.01	0.42
25:V:161:LEU:HD21	26:W:614:CLA:HAA2	2.00	0.42
1:A:153:ILE:O	1:A:154:THR:OG1	2.28	0.42
1:A:670:LEU:HB3	26:A:854:CLA:H71	2.01	0.42
29:L:301:BCR:H383	29:L:301:BCR:C23	2.46	0.42
20:7:138:ASP:O	20:7:142:PRO:HA	2.19	0.42
22:9:135:THR:OG1	22:9:136:SER:N	2.52	0.42
1:A:697:ILE:O	1:A:701:VAL:HG23	2.20	0.42
26:A:829:CLA:H141	26:A:829:CLA:H161	1.91	0.42
2:B:610:PHE:O	2:B:614:SER:OG	2.26	0.42
4:D:64:SER:O	4:D:107:ARG:NE	2.44	0.42
29:O:2004:BCR:H383	29:O:2004:BCR:C23	2.49	0.42
29:3:621:BCR:C23	29:3:621:BCR:C38	2.95	0.42
18:5:202:LEU:HD11	18:5:252:LEU:HD12	1.99	0.42
35:8:620:XAT:C28	35:8:620:XAT:H381	2.49	0.42
22:9:79:MET:SD	34:9:619:LUT:H402	2.58	0.42
24:U:79:ASP:O	24:U:82:THR:OG1	2.33	0.42
35:V:1622:XAT:H391	35:V:1622:XAT:H31	1.76	0.42
1:A:338:HIS:CD2	26:A:825:CLA:ND	2.87	0.42
26:A:835:CLA:O2D	26:A:835:CLA:H2A	2.19	0.42
29:F:305:BCR:C8	29:F:305:BCR:C33	2.96	0.42
22:9:153:SER:O	22:9:156:THR:OG1	2.34	0.42
37:X:609:CHL:H143	37:X:609:CHL:H161	1.90	0.42
24:Z:214:PHE:HZ	28:Z:2630:LHG:H171	1.85	0.42
24:U:115:THR:HG23	24:U:115:THR:O	2.18	0.42
37:U:601:CHL:H101	37:U:601:CHL:H61	1.76	0.42
25:V:80:TYR:OH	28:V:2630:LHG:O5	2.34	0.42
37:V:608:CHL:H11	34:V:1620:LUT:H383	2.01	0.42
1:A:16:ALA:HA	16:3:77:ASN:HB3	2.01	0.42
26:A:818:CLA:H43	26:K:203:CLA:C3D	2.50	0.42
11:K:56:THR:HG1	11:K:57:VAL:H	1.68	0.42
14:a:137:ALA:HB1	29:a:619:BCR:C16	2.50	0.42
26:a:606:CLA:HAB	26:a:607:CLA:HMC3	2.00	0.42
15:2:103:TYR:CE1	26:2:606:CLA:HBC1	2.54	0.42
16:3:176:TYR:CZ	16:3:178:LEU:HA	2.54	0.42
29:3:620:BCR:H15C	29:3:620:BCR:H351	1.92	0.42
18:5:85:VAL:HG21	34:5:620:LUT:H12	2.01	0.42
19:6:224:VAL:HG13	19:6:225:PRO:HD2	2.02	0.42
29:7:623:BCR:H323	21:8:230:TRP:CD2	2.54	0.42
37:X:601:CHL:H61	37:Z:609:CHL:HBB1	2.00	0.42
36:X:1623:NEX:H201	36:X:1623:NEX:H15	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Y:607:CHL:H2	37:Y:607:CHL:H62	1.71	0.42
35:Y:1622:XAT:H31	35:Y:1622:XAT:H391	1.82	0.42
24:Z:218:GLY:O	24:Z:222:GLN:HB2	2.19	0.42
24:U:170:GLY:HA3	24:U:175:GLU:HA	2.02	0.42
25:V:249:HIS:CG	26:V:613:CLA:HAA2	2.54	0.42
35:V:1622:XAT:H15	35:V:1622:XAT:H201	1.74	0.42
23:W:68:LEU:HB3	23:W:78:TYR:HE2	1.84	0.42
23:W:193:LEU:HA	23:W:196:LYS:HG2	2.00	0.42
1:A:310:HIS:NE2	29:K:202:BCR:H363	2.35	0.42
1:A:590:ASP:HA	1:A:593:PHE:HB3	2.01	0.42
29:B:801:BCR:C8	29:B:801:BCR:C33	2.97	0.42
13:O:77:GLN:O	13:O:81:GLU:HG2	2.19	0.42
14:a:79:VAL:HG22	14:a:178:ILE:HD13	2.02	0.42
17:4:217:LYS:HB3	26:4:611:CLA:HMD1	2.02	0.42
18:5:211:PRO:O	34:5:620:LUT:O3	2.35	0.42
26:5:603:CLA:HBC3	35:5:621:XAT:H203	2.02	0.42
19:6:66:TRP:CZ3	19:6:132:LEU:HD13	2.55	0.42
34:7:619:LUT:H8	34:7:619:LUT:C18	2.48	0.42
21:8:189:TRP:HB3	26:8:610:CLA:H3A	2.01	0.42
22:9:94:PRO:HG3	22:9:102:LYS:HD2	2.01	0.42
26:X:602:CLA:H143	26:X:602:CLA:H112	1.81	0.42
26:X:611:CLA:HAC1	28:X:2630:LHG:H292	2.00	0.42
34:X:1621:LUT:H11	34:X:1621:LUT:H191	1.96	0.42
24:Z:210:ARG:HA	24:Z:213:MET:HE3	2.02	0.42
37:Z:606:CHL:HBA1	36:Z:1623:NEX:H403	2.01	0.42
28:Z:2630:LHG:H191	28:Z:2630:LHG:H162	1.92	0.42
25:V:228:MET:HE2	34:V:1621:LUT:H12	2.01	0.42
23:W:40:PHE:HB3	23:W:61:TYR:HB3	2.01	0.42
1:A:601:ASN:O	1:A:605:ILE:HG12	2.20	0.42
29:A:852:BCR:C8	29:A:852:BCR:C33	2.97	0.42
2:B:398:ASP:OD1	4:D:185:LYS:NZ	2.43	0.42
6:F:99:ALA:HB3	6:F:100:PRO:HD3	2.01	0.42
26:F:304:CLA:H2A	26:F:304:CLA:O2D	2.20	0.42
29:J:102:BCR:H382	29:J:102:BCR:H23C	2.02	0.42
29:a:619:BCR:H15C	29:a:619:BCR:H351	1.94	0.42
16:3:183:ILE:HA	16:3:196:PRO:HD2	2.01	0.42
19:6:223:VAL:HB	26:6:616:CLA:C1C	2.49	0.42
23:X:218:THR:HG22	23:X:220:LYS:HE2	2.02	0.42
34:X:1621:LUT:H15	34:X:1621:LUT:H201	1.92	0.42
25:V:111:GLY:O	25:V:115:CYS:N	2.53	0.42
25:V:203:LEU:HD22	26:V:610:CLA:H11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:PHE:O	1:A:545:VAL:HG23	2.20	0.42
26:A:822:CLA:OBD	26:A:824:CLA:HHD	2.20	0.42
2:B:81:ASP:OD2	2:B:84:HIS:HB3	2.19	0.42
2:B:713:HIS:CE1	26:B:840:CLA:ND	2.87	0.42
11:K:86:ILE:O	11:K:89:VAL:HG12	2.20	0.42
26:L:307:CLA:HMB2	29:L:308:BCR:H341	2.01	0.42
14:1:218:PHE:O	14:1:224:SER:HB3	2.19	0.42
16:3:231:TYR:HE1	34:3:618:LUT:C5	2.32	0.42
19:6:190:PHE:HE1	34:6:619:LUT:C5	2.33	0.42
24:Y:219:PHE:HZ	34:Y:1620:LUT:H8	1.85	0.42
24:Z:88:GLU:HA	24:Z:180:LEU:HD11	2.01	0.42
23:W:214:GLN:HA	23:W:217:VAL:HG22	2.01	0.42
26:A:803:CLA:H91	26:B:803:CLA:H101	2.02	0.42
27:A:844:PQN:H18	27:A:844:PQN:H151	1.83	0.42
26:B:837:CLA:H41	29:F:305:BCR:H321	2.02	0.42
29:B:844:BCR:C8	29:B:844:BCR:H321	2.49	0.42
14:1:137:ALA:HB1	29:1:619:BCR:C16	2.49	0.42
17:4:235:THR:HG23	17:4:263:ARG:CZ	2.50	0.42
22:9:154:MET:HG3	26:9:610:CLA:HHB	2.01	0.42
26:Z:613:CLA:H171	26:Z:614:CLA:HBD	2.01	0.42
23:W:116:LYS:HA	37:W:607:CHL:HED2	2.02	0.42
1:A:158:GLN:OE1	26:A:815:CLA:O1D	2.37	0.42
11:K:38:MET:HG3	26:K:204:CLA:HMD3	2.02	0.42
12:L:90:LEU:HD23	12:L:177:GLY:O	2.19	0.42
28:O:2631:LHG:O1	26:Z:611:CLA:HMA2	2.20	0.42
14:1:152:VAL:HG13	14:1:153:TYR:CD2	2.54	0.42
14:a:62:LEU:CD2	21:8:173:PRO:HA	2.45	0.42
26:2:613:CLA:HBB1	34:2:619:LUT:H8	2.02	0.42
29:9:621:BCR:C34	29:9:621:BCR:C5	2.98	0.42
35:U:1622:XAT:H35	35:U:1622:XAT:H401	1.89	0.42
26:W:603:CLA:H3A	26:W:603:CLA:HBA1	1.88	0.42
36:W:1623:NEX:H191	36:W:1623:NEX:H11	1.68	0.42
1:A:675:ALA:HB1	1:A:734:GLY:O	2.20	0.41
26:A:841:CLA:H121	26:F:303:CLA:CBC	2.49	0.41
2:B:557:SER:O	2:B:557:SER:OG	2.36	0.41
3:C:35:LYS:NZ	3:C:37:SER:HB3	2.35	0.41
13:O:59:ALA:HA	29:O:2005:BCR:HC42	2.02	0.41
16:3:165:ASP:O	16:3:169:PRO:HA	2.19	0.41
16:3:178:LEU:HD21	26:7:611:CLA:CBB	2.50	0.41
34:3:618:LUT:H8	34:3:618:LUT:C16	2.41	0.41
18:5:124:TRP:NE1	26:6:614:CLA:H3A	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:7:116:ASP:OD1	20:7:118:PRO:HD2	2.19	0.41
23:X:68:LEU:HD12	26:X:602:CLA:H11	2.02	0.41
24:Y:91:LEU:HD23	24:Y:180:LEU:HD22	2.02	0.41
35:U:1622:XAT:H31	35:U:1622:XAT:H391	1.77	0.41
2:B:87:PRO:O	2:B:117:SER:N	2.49	0.41
6:F:158:TYR:OH	6:F:200:ALA:O	2.36	0.41
8:H:117:THR:O	8:H:120:ASN:ND2	2.53	0.41
14:1:105:ASP:OD1	14:1:105:ASP:N	2.53	0.41
14:a:218:PHE:O	14:a:224:SER:HB3	2.19	0.41
16:3:107:ALA:HB3	16:3:108:PRO:HD3	2.02	0.41
29:8:621:BCR:H23C	29:8:621:BCR:C40	2.50	0.41
37:X:608:CHL:H143	37:X:608:CHL:H111	1.84	0.41
34:X:1621:LUT:H35	34:X:1621:LUT:H401	1.79	0.41
26:A:805:CLA:HMC1	26:A:807:CLA:OBD	2.20	0.41
26:A:809:CLA:H93	29:J:102:BCR:H343	2.02	0.41
2:B:435:LEU:O	2:B:439:VAL:HG23	2.21	0.41
2:B:653:PHE:O	2:B:657:ILE:HG13	2.20	0.41
4:D:70:SER:OG	4:D:71:THR:N	2.52	0.41
16:3:172:MET:HE1	20:7:35:PRO:HB2	2.03	0.41
19:6:128:ARG:NH2	26:6:609:CLA:O1D	2.46	0.41
37:X:601:CHL:HAC1	28:X:2630:LHG:HC11	2.03	0.41
24:U:47:LYS:HE2	24:U:57:THR:HG21	2.03	0.41
26:V:613:CLA:H91	26:V:613:CLA:H111	1.74	0.41
37:W:601:CHL:HBA1	37:W:601:CHL:H3A	1.80	0.41
35:W:1622:XAT:H11	35:W:1622:XAT:H191	1.86	0.41
29:A:856:BCR:H23C	29:A:856:BCR:H403	2.02	0.41
2:B:301:ARG:NH2	7:G:68:GLY:O	2.46	0.41
14:a:105:ASP:OD1	14:a:105:ASP:N	2.53	0.41
26:a:601:CLA:H2A	26:a:601:CLA:O2D	2.21	0.41
19:6:117:GLU:O	19:6:121:MET:HB2	2.20	0.41
22:9:59:ASP:HB3	22:9:62:ARG:HB2	2.02	0.41
29:9:621:BCR:H20C	29:9:621:BCR:H361	1.90	0.41
23:X:238:ALA:HB3	35:Z:1622:XAT:H193	2.02	0.41
36:Z:1623:NEX:H163	37:V:601:CHL:HBB2	2.01	0.41
1:A:153:ILE:HG22	1:A:155:SER:H	1.85	0.41
1:A:202:LEU:HD21	26:A:822:CLA:C3B	2.51	0.41
1:A:542:THR:HB	1:A:602:SER:HB2	2.02	0.41
26:A:803:CLA:OBD	26:B:802:CLA:HMB3	2.19	0.41
29:A:848:BCR:H20C	29:A:848:BCR:H361	1.88	0.41
26:B:808:CLA:HHC	26:B:808:CLA:CBB	2.50	0.41
4:D:125:THR:HG23	4:D:136:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:217:LEU:HA	15:2:220:ILE:HD12	2.03	0.41
15:2:219:MET:SD	22:9:124:ILE:HD13	2.60	0.41
16:3:46:TYR:OH	28:3:624:LHG:O5	2.31	0.41
24:Z:172:PRO:HG2	37:Z:608:CHL:HBB2	2.03	0.41
26:Z:610:CLA:H92	26:Z:610:CLA:H61	1.88	0.41
24:U:171:GLY:N	24:U:174:GLY:O	2.53	0.41
25:V:201:LEU:HD12	34:V:1620:LUT:H222	2.03	0.41
1:A:358:ALA:HB1	29:A:851:BCR:C9	2.51	0.41
1:A:366:ILE:HD13	26:A:827:CLA:HED3	2.02	0.41
26:A:829:CLA:O1D	26:A:830:CLA:HHB	2.21	0.41
2:B:23:TRP:CD1	2:B:705:GLN:HE22	2.37	0.41
2:B:550:ASP:OD2	3:C:66:ARG:NE	2.52	0.41
4:D:88:TRP:HB3	4:D:136:PRO:HB3	2.01	0.41
6:F:224:VAL:HG12	6:F:225:SER:H	1.84	0.41
11:K:72:ASN:C	11:K:74:ALA:H	2.29	0.41
15:2:167:ALA:HB2	34:2:619:LUT:C9	2.50	0.41
23:X:38:PRO:HB3	37:X:601:CHL:HBC1	2.02	0.41
26:X:613:CLA:H18	26:X:613:CLA:H152	1.84	0.41
24:Z:79:ASP:O	24:Z:82:THR:OG1	2.33	0.41
34:Z:1620:LUT:H35	34:Z:1620:LUT:H401	1.89	0.41
25:V:171:MET:HA	25:V:174:ILE:HG13	2.02	0.41
26:W:602:CLA:H52	34:W:1621:LUT:H30	2.02	0.41
1:A:199:ASN:HB3	26:A:821:CLA:HMD1	2.02	0.41
29:F:305:BCR:H24C	29:F:305:BCR:H371	1.86	0.41
14:a:63:SER:HB3	14:a:66:LYS:HG3	2.01	0.41
16:3:46:TYR:O	16:3:47:VAL:C	2.63	0.41
16:3:194:GLY:HA2	16:3:199:ASN:HB2	2.03	0.41
29:3:622:BCR:HC8	29:3:622:BCR:H311	2.03	0.41
26:7:613:CLA:HHD	26:7:616:CLA:OBD	2.21	0.41
34:8:619:LUT:H8	34:8:619:LUT:C16	2.41	0.41
23:X:242:ALA:HA	35:Z:1622:XAT:H42	2.03	0.41
37:X:607:CHL:H92	37:X:607:CHL:H61	1.86	0.41
24:Z:173:ALA:HB2	37:Z:608:CHL:HBB1	2.02	0.41
26:U:604:CLA:H2	37:U:606:CHL:HBD	2.02	0.41
1:A:553:GLY:O	1:A:557:ALA:HB2	2.20	0.41
26:A:837:CLA:O2D	26:A:837:CLA:H2A	2.20	0.41
2:B:653:PHE:CE2	2:B:657:ILE:HD11	2.56	0.41
8:H:77:ILE:HA	8:H:82:SER:OG	2.21	0.41
15:2:52:ASP:O	15:2:55:ARG:NH1	2.52	0.41
17:4:177:ASP:OD1	26:4:618:CLA:C4C	2.69	0.41
37:X:601:CHL:H61	37:X:601:CHL:H92	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:143:LEU:HB3	24:Z:144:VAL:H	1.77	0.41
26:Z:610:CLA:CBB	34:Z:1620:LUT:H32	2.51	0.41
24:U:102:LEU:HD23	24:U:102:LEU:HA	1.87	0.41
1:A:95:GLY:HA2	1:A:99:SER:HB3	2.03	0.41
1:A:680:ALA:HB3	26:A:802:CLA:HBB2	2.01	0.41
29:A:849:BCR:H15C	29:A:849:BCR:H351	1.93	0.41
29:A:850:BCR:H11C	29:A:850:BCR:H341	1.84	0.41
29:A:851:BCR:C33	29:A:851:BCR:C8	2.97	0.41
2:B:277:HIS:HE2	26:B:818:CLA:C2B	2.34	0.41
2:B:716:VAL:HG22	33:B:850:DGD:HBG2	2.03	0.41
26:B:808:CLA:CGA	26:B:808:CLA:C1A	2.99	0.41
27:B:842:PQN:H142	27:B:842:PQN:H112	1.92	0.41
29:F:305:BCR:H382	29:F:305:BCR:H23C	2.03	0.41
29:G:205:BCR:H383	29:G:205:BCR:C23	2.50	0.41
29:G:205:BCR:H11C	29:G:205:BCR:H341	1.91	0.41
9:I:75:ALA:N	9:I:76:PRO:HD2	2.36	0.41
29:K:202:BCR:H15C	29:K:202:BCR:H351	1.92	0.41
12:L:184:TRP:CB	29:L:308:BCR:H10C	2.51	0.41
13:O:39:ASP:OD1	13:O:39:ASP:N	2.49	0.41
14:1:79:VAL:HG22	14:1:178:ILE:HD13	2.02	0.41
26:1:601:CLA:H2A	26:1:601:CLA:O2D	2.21	0.41
17:4:203:TRP:O	17:4:204:SER:OG	2.37	0.41
18:5:74:GLU:CG	18:5:187:ILE:HD11	2.47	0.41
35:7:620:XAT:H381	35:7:620:XAT:C28	2.50	0.41
23:X:111:GLU:OE2	23:X:116:LYS:HE2	2.21	0.41
24:Y:140:ASN:HA	24:Y:141:PRO:HD3	1.94	0.41
24:Y:187:ASP:OD1	34:Y:1620:LUT:O23	2.38	0.41
26:Y:603:CLA:H11	26:Y:603:CLA:HED2	2.03	0.41
26:Z:602:CLA:HBA1	34:Z:1621:LUT:H382	2.02	0.41
37:U:608:CHL:HAA1	26:U:610:CLA:HBC1	2.03	0.41
25:V:141:PHE:HZ	23:W:239:PHE:HB3	1.86	0.41
25:V:174:ILE:HG13	25:V:175:GLU:H	1.85	0.41
23:W:49:THR:HA	23:W:50:PRO:HD3	1.90	0.41
26:W:602:CLA:HBA1	34:W:1621:LUT:H382	2.02	0.41
1:A:565:ASP:OD1	1:A:565:ASP:N	2.50	0.41
1:A:646:LEU:HD22	2:B:652:LEU:HD21	2.02	0.41
2:B:528:LEU:O	2:B:532:THR:HG22	2.21	0.41
29:B:844:BCR:H11C	29:B:844:BCR:H341	1.93	0.41
29:2:623:BCR:H20C	29:2:623:BCR:H361	1.88	0.41
18:5:128:LEU:HG	29:5:622:BCR:C15	2.51	0.41
22:9:88:GLU:OE1	22:9:182:GLN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:214:GLN:HE22	34:X:1620:LUT:H41	1.86	0.41
26:Z:610:CLA:HBB1	34:Z:1620:LUT:H32	2.03	0.41
1:A:216:HIS:CE1	26:A:815:CLA:NA	2.89	0.40
26:A:825:CLA:H62	26:A:825:CLA:H41	1.93	0.40
26:A:843:CLA:H13	12:L:128:LEU:HD21	2.02	0.40
2:B:88:ILE:HD12	2:B:114:VAL:HG21	2.03	0.40
2:B:175:ARG:HB2	26:B:813:CLA:HBC2	2.03	0.40
2:B:179:HIS:HA	2:B:183:LEU:HB3	2.03	0.40
26:1:601:CLA:OBD	21:8:137:LYS:NZ	2.42	0.40
37:X:607:CHL:H93	37:X:609:CHL:H18	2.03	0.40
25:V:226:PHE:HZ	28:V:2630:LHG:H151	1.86	0.40
1:A:332:PRO:HB2	12:L:42:VAL:HG23	2.03	0.40
1:A:584:CYS:O	2:B:669:ARG:O	2.39	0.40
13:O:48:PRO:CG	29:O:2004:BCR:H272	2.51	0.40
26:a:603:CLA:H42	21:8:154:PHE:CD2	2.56	0.40
34:4:619:LUT:H8	34:4:619:LUT:C16	2.48	0.40
26:6:602:CLA:H3A	26:6:602:CLA:CGA	2.51	0.40
36:6:624:NEX:H162	36:6:624:NEX:O3	2.21	0.40
23:X:63:TRP:HD1	23:X:65:THR:HG23	1.87	0.40
24:U:187:ASP:HB2	24:U:190:GLY:HA2	2.04	0.40
25:V:154:LEU:HB3	25:V:155:VAL:H	1.62	0.40
26:A:807:CLA:HBA1	26:A:807:CLA:H3A	1.87	0.40
29:A:850:BCR:C32	29:A:850:BCR:HC8	2.52	0.40
2:B:102:VAL:HG13	2:B:113:PRO:HG3	2.02	0.40
2:B:123:GLN:OE1	2:B:123:GLN:N	2.47	0.40
4:D:62:THR:HG23	4:D:110:PRO:HB2	2.03	0.40
18:5:106:PRO:HB2	18:5:115:ASN:HA	2.03	0.40
23:X:83:LEU:HG	23:X:172:LEU:HD11	2.03	0.40
24:Y:53:SER:O	24:Y:53:SER:OG	2.36	0.40
24:Y:153:LEU:HD13	37:Y:607:CHL:HAC2	2.03	0.40
34:V:1621:LUT:H11	34:V:1621:LUT:H191	1.80	0.40
26:W:603:CLA:HBC1	37:W:609:CHL:HBC2	2.03	0.40
1:A:220:VAL:HG22	1:A:240:PRO:HB3	2.04	0.40
1:A:262:ALA:N	1:A:263:PRO:CD	2.85	0.40
1:A:584:CYS:N	2:B:669:ARG:O	2.54	0.40
26:A:806:CLA:HBA1	26:A:806:CLA:H3A	1.95	0.40
26:A:840:CLA:H2A	26:A:840:CLA:O2D	2.21	0.40
29:A:852:BCR:H20C	29:A:852:BCR:H361	1.89	0.40
2:B:16:ASP:HB3	2:B:21:ARG:HB2	2.02	0.40
2:B:177:ASN:ND2	2:B:292:TYR:O	2.48	0.40
2:B:313:SER:O	2:B:314:GLY:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:562:GLY:O	2:B:568:THR:OG1	2.37	0.40
29:3:621:BCR:H341	29:3:621:BCR:H11C	1.88	0.40
29:3:622:BCR:H11C	29:3:622:BCR:H341	1.87	0.40
18:5:92:GLU:OE1	18:5:213:ALA:N	2.48	0.40
18:5:102:GLU:HA	26:5:607:CLA:O1D	2.21	0.40
20:7:110:VAL:HA	20:7:115:ILE:HB	2.02	0.40
29:9:621:BCR:H371	29:9:621:BCR:H24C	1.85	0.40
23:X:109:PHE:O	23:X:111:GLU:N	2.55	0.40
26:Y:602:CLA:CBB	34:Y:1621:LUT:H32	2.51	0.40
37:Y:609:CHL:HBA1	37:Z:601:CHL:H11	2.02	0.40
34:Y:1621:LUT:H11	34:Y:1621:LUT:H191	1.82	0.40
24:Z:143:LEU:HD13	24:Z:143:LEU:HA	1.98	0.40
37:U:605:CHL:HHD	37:U:606:CHL:OBD	2.21	0.40
1:A:541:PHE:HZ	26:A:803:CLA:CBB	2.35	0.40
1:A:715:PRO:HB3	26:F:301:CLA:C2C	2.51	0.40
26:A:841:CLA:H121	26:F:303:CLA:HBC1	2.02	0.40
29:A:850:BCR:H383	29:A:850:BCR:H23C	2.01	0.40
26:A:854:CLA:H11	2:B:617:LEU:HD12	2.04	0.40
2:B:6:PHE:HB2	9:I:99:ILE:HA	2.02	0.40
2:B:26:LEU:HD22	29:L:305:BCR:H323	2.01	0.40
29:B:846:BCR:H11C	29:B:846:BCR:H341	1.92	0.40
7:G:75:THR:HB	7:G:78:ASP:OD2	2.21	0.40
29:L:301:BCR:HC8	29:L:301:BCR:C31	2.44	0.40
14:1:191:PHE:HE1	34:1:617:LUT:H41	1.87	0.40
14:a:46:PRO:HB3	14:a:48:TRP:CZ2	2.57	0.40
15:2:167:ALA:CB	34:2:619:LUT:C9	3.00	0.40
26:5:619:CLA:O1A	26:5:619:CLA:CGD	2.70	0.40
26:X:610:CLA:H2	34:X:1620:LUT:H26	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	V	33	25	8,10,11	1.61	1 (12%)	10,14,16	2.14	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	V	33	25	-	3/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	33	TPO	P-O1P	3.43	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	V	33	TPO	P-OG1-CB	-5.83	107.48	123.33
25	V	33	TPO	CG2-CB-CA	-2.63	108.14	113.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	V	33	TPO	N-CA-CB-CG2
25	V	33	TPO	N-CA-CB-OG1
25	V	33	TPO	C-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

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	$\#\|Z\| > 2$
26	CLA	Y	612	24	49,53,73	1.39	7 (14%)	58,89,113	1.30	6 (10%)
26	CLA	A	808	-	54,58,73	1.30	7 (12%)	64,95,113	1.33	6 (9%)
26	CLA	4	606	-	43,48,73	1.43	8 (18%)	49,83,113	1.24	4 (8%)
29	BCR	3	620	-	41,41,41	0.78	0	56,56,56	2.41	23 (41%)
26	CLA	9	611	28	46,50,73	1.39	7 (15%)	53,85,113	1.22	2 (3%)
26	CLA	Z	602	24	62,66,73	1.22	8 (12%)	73,104,113	1.21	7 (9%)
26	CLA	B	832	-	64,68,73	1.24	8 (12%)	76,107,113	1.29	7 (9%)
34	LUT	W	1620	-	42,43,43	0.70	0	51,60,60	1.70	12 (23%)
26	CLA	A	811	-	69,73,73	1.20	7 (10%)	82,113,113	1.22	5 (6%)
31	LMU	K	208	-	36,36,36	1.14	2 (5%)	47,47,47	1.01	3 (6%)
26	CLA	3	612	16	47,51,73	1.39	8 (17%)	55,86,113	1.23	5 (9%)
26	CLA	a	601	14	57,62,73	1.27	8 (14%)	67,100,113	1.20	5 (7%)
34	LUT	Y	1621	-	42,43,43	0.87	1 (2%)	51,60,60	1.88	16 (31%)
26	CLA	X	614	-	46,50,73	1.42	7 (15%)	53,85,113	1.27	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	XAT	V	1622	-	41,47,47	0.91	1 (2%)	54,74,74	2.60	22 (40%)
26	CLA	9	602	22	64,68,73	1.22	8 (12%)	76,107,113	1.27	8 (10%)
29	BCR	6	622	-	41,41,41	0.78	1 (2%)	56,56,56	2.49	25 (44%)
37	CHL	V	607	-	40,54,74	4.15	19 (47%)	34,90,114	2.36	13 (38%)
29	BCR	B	852	-	41,41,41	0.75	1 (2%)	56,56,56	4.24	30 (53%)
36	NEX	Z	1623	-	40,46,46	1.11	3 (7%)	50,70,70	2.51	17 (34%)
26	CLA	A	823	-	46,50,73	1.37	8 (17%)	53,85,113	1.33	3 (5%)
29	BCR	B	801	-	41,41,41	0.86	0	56,56,56	2.15	17 (30%)
26	CLA	a	616	14	49,53,73	1.36	6 (12%)	58,89,113	1.37	6 (10%)
26	CLA	A	803	-	69,73,73	1.23	9 (13%)	82,113,113	1.19	4 (4%)
26	CLA	7	604	-	54,58,73	1.30	8 (14%)	63,95,113	1.22	6 (9%)
26	CLA	8	612	21	44,49,73	1.41	6 (13%)	50,84,113	1.32	3 (6%)
35	XAT	U	1622	-	41,47,47	0.94	2 (4%)	54,74,74	4.33	22 (40%)
37	CHL	X	609	23	60,74,74	3.44	20 (33%)	58,114,114	2.38	15 (25%)
29	BCR	L	309	-	41,41,41	0.73	0	56,56,56	2.43	24 (42%)
26	CLA	4	618	17	43,48,73	1.51	7 (16%)	51,83,113	1.29	4 (7%)
31	LMU	A	858	-	35,35,36	1.25	3 (8%)	44,45,47	1.00	2 (4%)
28	LHG	6	623	26	47,47,48	0.91	2 (4%)	50,53,54	0.98	3 (6%)
29	BCR	O	2004	-	41,41,41	0.85	0	56,56,56	1.97	13 (23%)
26	CLA	6	603	-	55,59,73	1.39	9 (16%)	66,96,113	1.38	5 (7%)
26	CLA	2	612	15	48,52,73	1.39	7 (14%)	57,88,113	1.27	3 (5%)
35	XAT	5	621	-	41,47,47	0.94	2 (4%)	54,74,74	2.39	19 (35%)
37	CHL	W	605	23	40,54,74	4.25	19 (47%)	34,90,114	2.84	11 (32%)
37	CHL	Y	609	24	60,74,74	3.44	20 (33%)	58,114,114	2.36	15 (25%)
26	CLA	A	807	1	69,73,73	1.21	10 (14%)	82,113,113	1.24	5 (6%)
26	CLA	Y	613	24	69,73,73	1.17	7 (10%)	82,113,113	1.18	5 (6%)
26	CLA	1	610	14	43,47,73	1.44	7 (16%)	50,81,113	1.41	8 (16%)
26	CLA	3	604	-	69,73,73	1.18	8 (11%)	82,113,113	1.17	8 (9%)
35	XAT	7	620	-	41,47,47	0.96	4 (9%)	54,74,74	2.37	19 (35%)
26	CLA	6	611	28	46,50,73	1.37	6 (13%)	53,85,113	1.28	4 (7%)
26	CLA	F	304	6	45,49,73	1.41	7 (15%)	54,84,113	1.32	5 (9%)
26	CLA	W	610	23	59,63,73	1.24	7 (11%)	70,101,113	1.24	8 (11%)
26	CLA	1	611	28	61,65,73	1.24	8 (13%)	72,103,113	1.16	6 (8%)
26	CLA	5	612	18	44,49,73	1.40	6 (13%)	50,84,113	1.26	4 (8%)
26	CLA	4	604	-	58,62,73	1.35	8 (13%)	71,100,113	1.28	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CHL	Z	601	24	60,74,74	3.42	19 (31%)	58,114,114	2.27	14 (24%)
28	LHG	U	2630	26	48,48,48	0.94	2 (4%)	51,54,54	1.10	4 (7%)
26	CLA	W	614	-	49,53,73	1.37	5 (10%)	58,89,113	1.36	4 (6%)
37	CHL	W	601	23	60,74,74	3.46	20 (33%)	58,114,114	2.20	13 (22%)
26	CLA	H	202	-	42,47,73	1.45	6 (14%)	50,82,113	1.21	3 (6%)
26	CLA	2	604	-	46,50,73	1.37	7 (15%)	54,85,113	1.31	6 (11%)
26	CLA	F	303	-	46,50,73	1.42	9 (19%)	53,85,113	1.35	4 (7%)
26	CLA	K	201	11	49,53,73	1.36	6 (12%)	58,89,113	1.22	4 (6%)
26	CLA	3	615	-	43,48,73	1.41	6 (13%)	49,83,113	1.28	4 (8%)
29	BCR	J	102	-	41,41,41	0.87	1 (2%)	56,56,56	2.43	23 (41%)
26	CLA	A	814	-	69,73,73	1.17	10 (14%)	82,113,113	1.39	10 (12%)
26	CLA	A	806	-	69,73,73	1.22	11 (15%)	82,113,113	1.37	8 (9%)
26	CLA	X	612	23	47,51,73	1.38	6 (12%)	55,86,113	1.35	5 (9%)
26	CLA	B	827	-	66,70,73	1.19	9 (13%)	78,109,113	1.31	8 (10%)
26	CLA	Y	611	28	47,51,73	1.38	6 (12%)	55,86,113	1.23	3 (5%)
36	NEX	U	1623	-	40,46,46	1.03	3 (7%)	50,70,70	2.50	19 (38%)
26	CLA	V	613	25	69,73,73	1.16	8 (11%)	82,113,113	1.16	4 (4%)
26	CLA	U	613	24	63,67,73	1.22	8 (12%)	74,105,113	1.16	5 (6%)
26	CLA	B	818	-	64,68,73	1.23	9 (14%)	76,107,113	1.33	6 (7%)
26	CLA	4	610	17	65,69,73	1.18	7 (10%)	77,108,113	1.19	6 (7%)
28	LHG	7	622	26	36,36,48	1.05	2 (5%)	39,42,54	1.03	3 (7%)
30	SF4	A	853	1,2	0,12,12	-	-	-		
34	LUT	9	619	-	42,43,43	0.87	1 (2%)	51,60,60	2.01	14 (27%)
37	CHL	V	601	25	60,74,74	3.46	19 (31%)	58,114,114	2.32	16 (27%)
37	CHL	Y	607	-	60,74,74	3.35	19 (31%)	58,114,114	2.19	13 (22%)
35	XAT	2	620	-	41,47,47	1.00	3 (7%)	54,74,74	2.43	27 (50%)
26	CLA	6	607	-	45,49,73	1.50	8 (17%)	54,84,113	1.32	5 (9%)
35	XAT	Z	1622	-	41,47,47	0.89	2 (4%)	54,74,74	2.78	21 (38%)
35	XAT	W	1622	-	41,47,47	0.93	2 (4%)	54,74,74	4.21	26 (48%)
29	BCR	B	848	-	41,41,41	0.78	0	56,56,56	2.57	14 (25%)
26	CLA	A	802	-	69,73,73	1.19	8 (11%)	82,113,113	1.37	9 (10%)
26	CLA	7	616	20	47,51,73	1.51	10 (21%)	58,87,113	1.33	5 (8%)
26	CLA	9	601	22	49,53,73	1.38	7 (14%)	58,89,113	1.29	4 (6%)
26	CLA	9	613	22	69,73,73	1.19	7 (10%)	82,113,113	1.23	5 (6%)
26	CLA	8	607	-	45,49,73	1.52	10 (22%)	54,84,113	1.30	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	W	604	-	51,55,73	1.36	7 (13%)	60,91,113	1.26	7 (11%)
26	CLA	4	614	-	60,64,73	1.24	8 (13%)	71,102,113	1.22	5 (7%)
35	XAT	6	621	-	41,47,47	0.96	3 (7%)	54,74,74	2.33	23 (42%)
26	CLA	5	604	-	67,71,73	1.29	8 (11%)	82,111,113	1.18	6 (7%)
26	CLA	6	612	19	44,49,73	1.40	7 (15%)	50,84,113	1.21	3 (6%)
37	CHL	Z	606	-	40,54,74	4.17	20 (50%)	34,90,114	3.00	15 (44%)
26	CLA	A	835	-	65,69,73	1.22	8 (12%)	77,108,113	1.25	6 (7%)
37	CHL	V	609	25	55,69,74	3.56	19 (34%)	52,108,114	2.62	15 (28%)
26	CLA	B	830	-	47,51,73	1.39	7 (14%)	55,86,113	1.31	6 (10%)
26	CLA	a	611	28	41,46,73	1.56	9 (21%)	51,81,113	1.34	7 (13%)
34	LUT	U	1621	-	42,43,43	0.73	0	51,60,60	1.63	11 (21%)
26	CLA	2	610	15	59,63,73	1.27	8 (13%)	70,101,113	1.20	7 (10%)
31	LMU	1	621	-	36,36,36	1.15	2 (5%)	47,47,47	1.01	1 (2%)
26	CLA	a	603	-	58,62,73	1.26	7 (12%)	68,99,113	1.31	3 (4%)
31	LMU	5	628	-	34,34,36	1.19	2 (5%)	45,45,47	1.16	5 (11%)
26	CLA	X	610	23	69,73,73	1.17	7 (10%)	82,113,113	1.15	7 (8%)
26	CLA	B	810	-	68,72,73	1.18	10 (14%)	80,111,113	1.39	9 (11%)
26	CLA	B	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.17	5 (6%)
26	CLA	8	608	-	55,59,73	1.31	8 (14%)	64,96,113	1.38	6 (9%)
26	CLA	W	611	28	61,65,73	1.23	7 (11%)	72,103,113	1.12	5 (6%)
29	BCR	L	305	-	41,41,41	0.85	0	56,56,56	2.53	26 (46%)
26	CLA	9	614	-	49,53,73	1.37	8 (16%)	58,89,113	1.20	4 (6%)
29	BCR	B	843	-	41,41,41	0.96	2 (4%)	56,56,56	1.96	17 (30%)
26	CLA	A	819	-	63,67,73	1.24	10 (15%)	74,105,113	1.34	6 (8%)
26	CLA	A	827	-	62,66,73	1.23	7 (11%)	73,104,113	1.16	4 (5%)
26	CLA	A	833	-	49,53,73	1.38	9 (18%)	58,89,113	1.47	9 (15%)
37	CHL	X	606	-	38,52,74	4.28	17 (44%)	31,87,114	3.00	13 (41%)
26	CLA	9	606	-	43,48,73	1.46	9 (20%)	49,83,113	1.28	4 (8%)
26	CLA	7	609	20	46,52,73	1.40	8 (17%)	57,87,113	1.21	4 (7%)
26	CLA	B	814	-	68,72,73	1.17	7 (10%)	80,111,113	1.28	5 (6%)
34	LUT	7	619	-	42,43,43	0.90	2 (4%)	51,60,60	2.10	16 (31%)
29	BCR	A	849	-	41,41,41	0.83	0	56,56,56	2.23	21 (37%)
26	CLA	a	607	-	49,53,73	1.41	9 (18%)	58,89,113	1.17	4 (6%)
37	CHL	W	606	-	40,54,74	4.08	20 (50%)	34,90,114	3.01	13 (38%)
26	CLA	A	820	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	6	610	19	69,73,73	1.19	7 (10%)	82,113,113	1.15	5 (6%)
26	CLA	Y	610	24	69,73,73	1.17	8 (11%)	82,113,113	1.12	5 (6%)
36	NEX	X	1623	-	40,46,46	1.00	3 (7%)	50,70,70	4.29	19 (38%)
26	CLA	7	606	-	45,49,73	1.42	9 (20%)	52,84,113	1.27	4 (7%)
26	CLA	B	812	-	47,51,73	1.36	7 (14%)	55,86,113	1.24	5 (9%)
26	CLA	5	614	-	48,52,73	1.39	8 (16%)	53,87,113	1.27	3 (5%)
37	CHL	Y	605	24	36,50,74	4.52	17 (47%)	29,85,114	2.53	11 (37%)
26	CLA	1	614	-	40,45,73	1.58	10 (25%)	47,79,113	1.46	6 (12%)
29	BCR	A	856	-	41,41,41	0.86	1 (2%)	56,56,56	1.99	19 (33%)
29	BCR	A	850	-	41,41,41	0.94	1 (2%)	56,56,56	2.04	13 (23%)
29	BCR	B	846	-	41,41,41	0.80	1 (2%)	56,56,56	2.38	21 (37%)
26	CLA	1	606	-	41,47,73	1.49	8 (19%)	50,80,113	1.41	5 (10%)
26	CLA	8	610	21	64,68,73	1.19	7 (10%)	76,107,113	1.29	8 (10%)
29	BCR	A	852	-	41,41,41	0.89	2 (4%)	56,56,56	2.55	27 (48%)
29	BCR	7	621	-	41,41,41	0.83	1 (2%)	56,56,56	2.31	22 (39%)
26	CLA	4	612	17	44,49,73	1.42	7 (15%)	50,84,113	1.23	3 (6%)
26	CLA	A	830	-	69,73,73	1.18	8 (11%)	82,113,113	1.21	7 (8%)
26	CLA	7	603	-	47,52,73	1.43	8 (17%)	55,88,113	1.46	3 (5%)
36	NEX	Y	1623	-	40,46,46	1.12	3 (7%)	50,70,70	2.39	17 (34%)
26	CLA	3	609	16	64,68,73	1.25	7 (10%)	76,107,113	1.24	6 (7%)
37	CHL	Y	608	-	43,57,74	4.01	19 (44%)	37,93,114	2.85	15 (40%)
26	CLA	L	307	8	43,48,73	1.41	7 (16%)	49,83,113	1.40	6 (12%)
26	CLA	1	607	-	43,48,73	1.46	9 (20%)	51,83,113	1.19	5 (9%)
32	LMG	J	104	-	40,40,55	1.02	2 (5%)	48,48,63	1.30	5 (10%)
26	CLA	4	609	17	61,65,73	1.24	5 (8%)	72,103,113	1.16	5 (6%)
26	CLA	6	620	-	68,72,73	1.16	7 (10%)	80,111,113	1.18	5 (6%)
29	BCR	B	849	-	41,41,41	0.94	2 (4%)	56,56,56	2.58	19 (33%)
26	CLA	A	831	-	69,73,73	1.20	10 (14%)	82,113,113	1.21	7 (8%)
26	CLA	6	606	-	43,48,73	1.44	7 (16%)	49,83,113	1.22	4 (8%)
37	CHL	U	609	24	54,68,74	3.53	19 (35%)	50,106,114	2.56	13 (26%)
26	CLA	7	611	28	63,67,73	1.21	7 (11%)	74,105,113	1.18	7 (9%)
29	BCR	8	621	-	41,41,41	0.75	0	56,56,56	2.83	24 (42%)
26	CLA	B	834	-	64,68,73	1.20	8 (12%)	76,107,113	1.21	6 (7%)
26	CLA	5	618	18	43,48,73	1.53	9 (20%)	51,83,113	1.32	5 (9%)
32	LMG	H	205	-	55,55,55	0.86	2 (3%)	63,63,63	1.13	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	LUT	X	1621	-	42,43,43	0.74	1 (2%)	51,60,60	1.85	15 (29%)
29	BCR	K	202	-	41,41,41	0.87	1 (2%)	56,56,56	2.29	21 (37%)
34	LUT	2	619	-	42,43,43	0.90	2 (4%)	51,60,60	2.09	15 (29%)
34	LUT	a	617	-	42,43,43	0.79	1 (2%)	51,60,60	2.04	18 (35%)
26	CLA	1	604	-	53,57,73	1.31	7 (13%)	61,93,113	1.25	4 (6%)
26	CLA	A	832	-	54,58,73	1.35	8 (14%)	64,95,113	1.43	9 (14%)
32	LMG	J	103	-	42,42,55	0.99	2 (4%)	50,50,63	1.23	7 (14%)
37	CHL	Z	609	24	60,74,74	3.44	20 (33%)	58,114,114	2.30	17 (29%)
26	CLA	4	603	17	48,52,73	1.48	9 (18%)	59,88,113	1.37	6 (10%)
26	CLA	2	602	15	59,69,73	1.32	7 (11%)	70,102,113	1.31	4 (5%)
37	CHL	W	609	23	60,74,74	3.47	20 (33%)	58,114,114	2.12	16 (27%)
28	LHG	9	624	-	48,48,48	0.94	2 (4%)	51,54,54	0.88	2 (3%)
26	CLA	G	204	7	49,53,73	1.39	8 (16%)	58,89,113	1.29	4 (6%)
34	LUT	Z	1621	-	42,43,43	0.77	0	51,60,60	1.51	9 (17%)
26	CLA	7	614	-	46,50,73	1.38	8 (17%)	53,85,113	1.27	4 (7%)
34	LUT	X	1620	-	42,43,43	0.70	0	51,60,60	1.66	11 (21%)
26	CLA	B	821	-	47,51,73	1.44	8 (17%)	54,86,113	1.29	4 (7%)
26	CLA	8	604	-	54,58,73	1.29	7 (12%)	64,95,113	1.36	9 (14%)
26	CLA	U	603	-	56,60,73	1.29	7 (12%)	65,97,113	1.36	6 (9%)
37	CHL	Y	601	24	60,74,74	3.46	20 (33%)	58,114,114	2.14	14 (24%)
26	CLA	B	808	-	69,73,73	1.18	8 (11%)	82,113,113	1.22	9 (10%)
26	CLA	B	838	-	50,54,73	1.35	8 (16%)	59,90,113	1.36	6 (10%)
26	CLA	4	611	28	46,50,73	1.35	6 (13%)	53,85,113	1.30	6 (11%)
34	LUT	5	620	-	42,43,43	0.83	1 (2%)	51,60,60	2.03	15 (29%)
26	CLA	A	816	-	69,73,73	1.18	9 (13%)	82,113,113	1.28	5 (6%)
26	CLA	B	825	-	53,57,73	1.31	7 (13%)	61,93,113	1.33	7 (11%)
26	CLA	B	826	-	66,70,73	1.21	8 (12%)	78,109,113	1.44	6 (7%)
26	CLA	a	610	14	63,67,73	1.21	7 (11%)	75,106,113	1.14	8 (10%)
26	CLA	L	302	12	49,53,73	1.42	7 (14%)	58,89,113	1.31	5 (8%)
37	CHL	V	606	-	38,52,74	4.08	18 (47%)	31,87,114	3.25	14 (45%)
26	CLA	7	615	-	44,50,73	1.53	9 (20%)	57,85,113	1.32	5 (8%)
35	XAT	8	620	-	41,47,47	0.97	3 (7%)	54,74,74	2.38	25 (46%)
26	CLA	A	825	-	69,73,73	1.18	7 (10%)	82,113,113	1.16	4 (4%)
26	CLA	3	607	16	60,64,73	1.31	8 (13%)	73,102,113	1.20	7 (9%)
26	CLA	3	617	16	43,48,73	1.41	7 (16%)	51,83,113	1.35	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CHL	W	608	-	41,55,74	4.14	19 (46%)	35,91,114	2.80	13 (37%)
26	CLA	4	601	17	69,73,73	1.15	7 (10%)	82,113,113	1.22	5 (6%)
37	CHL	U	608	-	38,52,74	4.19	18 (47%)	31,87,114	2.76	11 (35%)
29	BCR	G	205	-	41,41,41	0.80	1 (2%)	56,56,56	1.98	15 (26%)
26	CLA	3	614	-	43,48,73	1.43	8 (18%)	51,83,113	1.31	4 (7%)
26	CLA	U	614	-	46,50,73	1.38	6 (13%)	53,85,113	1.33	3 (5%)
29	BCR	a	619	-	41,41,41	0.86	0	56,56,56	2.41	22 (39%)
26	CLA	A	810	1	54,58,73	1.35	7 (12%)	64,95,113	1.36	8 (12%)
26	CLA	F	301	-	61,65,73	1.26	8 (13%)	72,103,113	1.15	4 (5%)
26	CLA	A	840	-	56,60,73	1.30	9 (16%)	65,97,113	1.39	7 (10%)
26	CLA	1	601	14	57,62,73	1.26	8 (14%)	67,100,113	1.19	5 (7%)
26	CLA	K	203	-	60,64,73	1.27	8 (13%)	71,102,113	1.36	8 (11%)
26	CLA	B	829	-	69,73,73	1.21	10 (14%)	82,113,113	1.28	7 (8%)
26	CLA	9	610	22	61,65,73	1.26	8 (13%)	72,103,113	1.24	6 (8%)
37	CHL	Z	605	24	36,50,74	4.34	18 (50%)	29,85,114	3.08	12 (41%)
29	BCR	B	847	-	41,41,41	0.91	2 (4%)	56,56,56	2.22	19 (33%)
26	CLA	Y	603	-	59,63,73	1.27	6 (10%)	70,101,113	1.38	6 (8%)
26	CLA	7	610	20	69,73,73	1.20	7 (10%)	82,113,113	1.09	5 (6%)
30	SF4	C	101	3	0,12,12	-	-	-		
26	CLA	B	802	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	7 (8%)
26	CLA	Z	610	24	69,73,73	1.15	8 (11%)	82,113,113	1.16	8 (9%)
29	BCR	B	845	-	41,41,41	0.87	1 (2%)	56,56,56	2.45	24 (42%)
37	CHL	X	607	-	60,74,74	3.38	19 (31%)	58,114,114	2.36	15 (25%)
26	CLA	9	607	-	49,53,73	1.35	7 (14%)	58,89,113	1.24	4 (6%)
26	CLA	9	604	-	54,58,73	1.40	8 (14%)	65,95,113	1.27	6 (9%)
26	CLA	B	805	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	8 (9%)
26	CLA	V	604	-	54,58,73	1.29	7 (12%)	64,95,113	1.30	6 (9%)
26	CLA	3	602	16	64,68,73	1.20	7 (10%)	76,107,113	1.18	8 (10%)
26	CLA	A	854	-	69,73,73	1.20	10 (14%)	82,113,113	1.30	8 (9%)
26	CLA	8	609	21	49,53,73	1.37	7 (14%)	58,89,113	1.31	4 (6%)
26	CLA	A	805	-	56,60,73	1.31	10 (17%)	65,97,113	1.47	8 (12%)
26	CLA	B	836	-	54,58,73	1.32	10 (18%)	64,95,113	1.46	7 (10%)
26	CLA	A	841	-	69,73,73	1.16	7 (10%)	82,113,113	1.18	5 (6%)
26	CLA	A	815	-	54,58,73	1.32	8 (14%)	64,95,113	1.32	5 (7%)
26	CLA	A	829	-	69,73,73	1.17	7 (10%)	82,113,113	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	4	602	17	64,68,73	1.23	9 (14%)	76,107,113	1.19	6 (7%)
26	CLA	A	826	-	68,72,73	1.19	10 (14%)	80,111,113	1.25	7 (8%)
26	CLA	7	608	-	54,58,73	1.31	9 (16%)	64,95,113	1.32	6 (9%)
26	CLA	5	609	18	69,73,73	1.20	7 (10%)	82,113,113	1.18	6 (7%)
26	CLA	A	801	-	69,73,73	1.19	9 (13%)	82,113,113	1.26	7 (8%)
26	CLA	7	601	20	64,68,73	1.23	8 (12%)	76,107,113	1.28	8 (10%)
37	CHL	X	605	-	40,54,74	4.36	19 (47%)	34,90,114	2.35	10 (29%)
32	LMG	4	624	-	40,40,55	1.04	2 (5%)	48,48,63	1.16	4 (8%)
26	CLA	7	613	20	69,73,73	1.18	7 (10%)	82,113,113	1.22	4 (4%)
26	CLA	6	614	-	64,68,73	1.21	7 (10%)	76,107,113	1.16	5 (6%)
26	CLA	O	2003	-	43,48,73	1.43	8 (18%)	49,83,113	1.26	3 (6%)
28	LHG	X	2630	26	48,48,48	0.92	2 (4%)	51,54,54	1.03	3 (5%)
29	BCR	L	301	-	41,41,41	0.77	0	56,56,56	2.26	25 (44%)
34	LUT	Z	1620	-	42,43,43	0.70	0	51,60,60	1.92	14 (27%)
26	CLA	1	613	-	69,73,73	1.19	9 (13%)	82,113,113	1.12	5 (6%)
26	CLA	V	610	25	66,70,73	1.17	8 (12%)	78,109,113	1.18	7 (8%)
29	BCR	7	623	-	41,41,41	0.89	1 (2%)	56,56,56	2.03	17 (30%)
26	CLA	X	604	-	53,57,73	1.33	5 (9%)	61,93,113	1.22	5 (8%)
26	CLA	8	614	-	57,61,73	1.29	9 (15%)	67,98,113	1.29	6 (8%)
26	CLA	6	608	-	49,53,73	1.37	8 (16%)	58,89,113	1.30	6 (10%)
26	CLA	A	813	-	58,62,73	1.29	9 (15%)	68,99,113	1.29	5 (7%)
37	CHL	X	608	-	57,73,74	3.40	16 (28%)	54,112,114	2.13	18 (33%)
26	CLA	B	835	-	49,53,73	1.39	8 (16%)	58,89,113	1.30	5 (8%)
26	CLA	1	609	14	44,48,73	1.49	8 (18%)	55,83,113	1.45	7 (12%)
26	CLA	6	618	19	43,48,73	1.51	8 (18%)	51,83,113	1.39	5 (9%)
29	BCR	A	851	-	41,41,41	0.82	1 (2%)	56,56,56	2.34	24 (42%)
26	CLA	B	828	-	69,73,73	1.19	7 (10%)	82,113,113	1.15	4 (4%)
37	CHL	V	608	-	42,56,74	3.99	19 (45%)	36,92,114	3.01	13 (36%)
28	LHG	Y	2630	26	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
26	CLA	a	612	14	49,53,73	1.38	8 (16%)	58,89,113	1.35	4 (6%)
26	CLA	B	815	-	47,51,73	1.37	7 (14%)	55,86,113	1.23	3 (5%)
26	CLA	W	613	23	69,73,73	1.16	7 (10%)	82,113,113	1.12	4 (4%)
35	XAT	a	618	-	41,47,47	0.89	3 (7%)	54,74,74	2.37	25 (46%)
27	PQN	A	844	-	34,34,34	3.39	10 (29%)	43,45,45	1.99	4 (9%)
28	LHG	B	851	26	37,37,48	1.05	2 (5%)	40,43,54	1.16	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	LHG	2	622	26	35,35,48	1.05	2 (5%)	38,41,54	1.18	3 (7%)
37	CHL	U	606	-	38,52,74	4.12	17 (44%)	31,87,114	3.17	12 (38%)
28	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	0.88	2 (3%)
26	CLA	5	602	18	69,73,73	1.18	8 (11%)	82,113,113	1.17	6 (7%)
26	CLA	L	306	-	43,48,73	1.42	7 (16%)	49,83,113	1.32	3 (6%)
26	CLA	2	613	15	69,73,73	1.15	6 (8%)	82,113,113	1.10	4 (4%)
26	CLA	4	607	-	49,53,73	1.38	7 (14%)	58,89,113	1.23	4 (6%)
26	CLA	6	604	-	69,73,73	1.15	6 (8%)	82,113,113	1.07	4 (4%)
26	CLA	1	603	-	56,61,73	1.27	7 (12%)	65,98,113	1.30	3 (4%)
26	CLA	O	2001	-	41,46,73	1.49	7 (17%)	47,80,113	1.38	5 (10%)
29	BCR	B	844	-	41,41,41	0.92	3 (7%)	56,56,56	2.65	26 (46%)
26	CLA	U	602	24	63,67,73	1.22	7 (11%)	74,105,113	1.18	6 (8%)
34	LUT	V	1621	-	42,43,43	0.76	0	51,60,60	2.04	16 (31%)
26	CLA	G	203	-	46,50,73	1.38	7 (15%)	53,85,113	1.34	4 (7%)
26	CLA	J	101	10	46,50,73	1.40	7 (15%)	53,85,113	1.26	4 (7%)
34	LUT	6	619	-	42,43,43	0.75	1 (2%)	51,60,60	2.18	20 (39%)
26	CLA	a	606	-	46,52,73	1.43	8 (17%)	57,87,113	1.23	2 (3%)
26	CLA	B	824	-	69,73,73	1.18	8 (11%)	82,113,113	1.16	5 (6%)
28	LHG	8	623	-	39,39,48	1.03	2 (5%)	42,45,54	1.08	2 (4%)
29	BCR	5	622	-	41,41,41	0.91	2 (4%)	56,56,56	2.32	19 (33%)
35	XAT	4	620	-	41,47,47	0.93	3 (7%)	54,74,74	2.40	23 (42%)
26	CLA	B	806	2	69,73,73	1.20	10 (14%)	82,113,113	1.37	8 (9%)
26	CLA	8	603	-	48,52,73	1.50	8 (16%)	59,88,113	1.47	5 (8%)
35	XAT	1	618	-	41,47,47	0.90	3 (7%)	54,74,74	2.37	24 (44%)
26	CLA	5	617	-	54,58,73	1.31	9 (16%)	64,95,113	1.23	5 (7%)
26	CLA	a	613	-	58,62,73	1.29	8 (13%)	68,99,113	1.20	5 (7%)
34	LUT	V	1620	-	42,43,43	0.70	0	51,60,60	1.77	12 (23%)
29	BCR	F	305	-	41,41,41	0.86	1 (2%)	56,56,56	2.31	22 (39%)
26	CLA	Y	604	-	54,58,73	1.33	7 (12%)	64,95,113	1.21	4 (6%)
36	NEX	V	1623	-	40,46,46	1.00	3 (7%)	50,70,70	2.21	19 (38%)
26	CLA	U	610	24	60,64,73	1.23	6 (10%)	71,102,113	1.27	5 (7%)
26	CLA	B	804	-	45,49,73	1.36	8 (17%)	54,84,113	1.34	4 (7%)
26	CLA	5	603	-	58,62,73	1.35	10 (17%)	71,100,113	1.33	7 (9%)
26	CLA	U	612	24	46,50,73	1.40	6 (13%)	53,85,113	1.39	4 (7%)
29	BCR	3	621	-	41,41,41	0.84	1 (2%)	56,56,56	1.87	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	4	616	17	47,51,73	1.49	8 (17%)	58,87,113	1.27	4 (6%)
26	CLA	9	612	22	44,49,73	1.41	6 (13%)	50,84,113	1.18	4 (8%)
26	CLA	2	616	-	47,51,73	1.49	8 (17%)	58,87,113	1.31	6 (10%)
26	CLA	2	609	15	49,53,73	1.40	8 (16%)	58,89,113	1.23	5 (8%)
26	CLA	A	828	-	69,73,73	1.18	8 (11%)	82,113,113	1.29	8 (9%)
26	CLA	a	602	14	65,69,73	1.23	10 (15%)	77,108,113	1.23	7 (9%)
26	CLA	A	821	-	57,61,73	1.27	7 (12%)	67,98,113	1.28	6 (8%)
26	CLA	W	612	23	49,53,73	1.39	7 (14%)	58,89,113	1.39	5 (8%)
37	CHL	X	601	23	60,74,74	3.45	20 (33%)	58,114,114	2.15	15 (25%)
26	CLA	7	612	20	48,52,73	1.40	7 (14%)	57,88,113	1.28	4 (7%)
29	BCR	3	622	-	41,41,41	0.83	1 (2%)	56,56,56	2.24	21 (37%)
26	CLA	6	601	19	69,73,73	1.14	7 (10%)	82,113,113	1.11	6 (7%)
26	CLA	B	823	-	49,53,73	1.38	8 (16%)	58,89,113	1.32	5 (8%)
26	CLA	B	803	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
26	CLA	1	612	14	49,53,73	1.37	8 (16%)	58,89,113	1.35	3 (5%)
36	NEX	5	624	-	40,46,46	1.30	3 (7%)	50,70,70	2.29	20 (40%)
29	BCR	O	2005	-	41,41,41	0.92	1 (2%)	56,56,56	3.13	22 (39%)
26	CLA	3	606	-	57,62,73	1.26	7 (12%)	67,100,113	1.32	7 (10%)
26	CLA	3	613	16	56,61,73	1.30	8 (14%)	65,98,113	1.15	5 (7%)
26	CLA	6	609	19	49,53,73	1.39	8 (16%)	58,89,113	1.27	4 (6%)
26	CLA	A	834	-	69,73,73	1.21	10 (14%)	82,113,113	1.32	10 (12%)
26	CLA	X	602	23	69,73,73	1.16	8 (11%)	82,113,113	1.18	5 (6%)
26	CLA	K	206	11	49,53,73	1.39	7 (14%)	58,89,113	1.24	4 (6%)
26	CLA	2	603	15	47,52,73	1.41	8 (17%)	55,88,113	1.26	5 (9%)
28	LHG	5	625	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
26	CLA	Z	604	-	53,57,73	1.43	8 (15%)	64,93,113	1.31	7 (10%)
32	LMG	5	627	-	40,40,55	1.03	2 (5%)	48,48,63	1.02	3 (6%)
26	CLA	A	812	-	69,73,73	1.17	7 (10%)	82,113,113	1.16	5 (6%)
26	CLA	U	611	28	46,50,73	1.40	6 (13%)	53,85,113	1.31	3 (5%)
26	CLA	1	602	14	65,69,73	1.23	9 (13%)	77,108,113	1.24	7 (9%)
26	CLA	W	602	23	64,68,73	1.22	8 (12%)	76,107,113	1.16	7 (9%)
26	CLA	K	204	-	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
34	LUT	8	619	-	42,43,43	0.86	1 (2%)	51,60,60	1.98	12 (23%)
26	CLA	3	603	-	59,63,73	1.27	9 (15%)	70,101,113	1.36	5 (7%)
26	CLA	2	611	28	46,50,73	1.37	7 (15%)	53,85,113	1.32	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	8	606	-	68,72,73	1.19	8 (11%)	81,112,113	1.11	5 (6%)
26	CLA	X	611	28	49,53,73	1.37	7 (14%)	58,89,113	1.25	4 (6%)
26	CLA	8	613	21	69,73,73	1.18	8 (11%)	82,113,113	1.13	5 (6%)
26	CLA	Z	612	24	49,53,73	1.38	7 (14%)	58,89,113	1.30	5 (8%)
28	LHG	A	847	26	29,29,48	1.17	3 (10%)	32,35,54	1.06	3 (9%)
26	CLA	V	612	25	49,53,73	1.38	7 (14%)	58,89,113	1.35	6 (10%)
26	CLA	A	836	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	7 (8%)
26	CLA	3	611	28	41,46,73	1.54	7 (17%)	51,81,113	1.29	4 (7%)
26	CLA	A	843	-	68,72,73	1.20	9 (13%)	80,111,113	1.23	8 (10%)
31	LMU	5	629	-	33,33,36	1.21	2 (6%)	44,44,47	1.28	6 (13%)
26	CLA	2	606	-	47,51,73	1.39	8 (17%)	55,86,113	1.31	6 (10%)
28	LHG	a	620	26	42,42,48	0.99	2 (4%)	45,48,54	0.84	2 (4%)
26	CLA	8	601	21	69,73,73	1.21	7 (10%)	82,113,113	1.15	4 (4%)
36	NEX	W	1623	-	40,46,46	0.98	3 (7%)	50,70,70	2.37	13 (26%)
37	CHL	U	605	24	37,51,74	4.38	17 (45%)	30,86,114	2.59	13 (43%)
26	CLA	B	817	-	63,67,73	1.23	7 (11%)	74,105,113	1.28	5 (6%)
26	CLA	2	614	-	45,50,73	1.42	8 (17%)	52,85,113	1.31	5 (9%)
26	CLA	W	603	-	56,60,73	1.29	6 (10%)	65,97,113	1.39	7 (10%)
26	CLA	X	603	-	66,70,73	1.21	7 (10%)	78,109,113	1.28	5 (6%)
26	CLA	5	601	18	60,64,73	1.25	6 (10%)	71,102,113	1.27	4 (5%)
28	LHG	3	623	-	44,44,48	0.93	2 (4%)	47,50,54	1.02	3 (6%)
34	LUT	Y	1620	-	42,43,43	0.76	0	51,60,60	3.19	19 (37%)
26	CLA	L	303	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	8 (9%)
26	CLA	B	841	28	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
26	CLA	5	606	-	43,48,73	1.45	7 (16%)	49,83,113	1.27	4 (8%)
26	CLA	8	611	28	46,50,73	1.39	6 (13%)	53,85,113	1.26	3 (5%)
37	CHL	U	607	-	40,54,74	4.17	19 (47%)	34,90,114	2.55	12 (35%)
26	CLA	2	607	-	47,52,73	1.38	8 (17%)	55,88,113	1.34	5 (9%)
29	BCR	A	848	-	41,41,41	1.05	3 (7%)	56,56,56	2.25	16 (28%)
26	CLA	7	602	20	69,73,73	1.21	9 (13%)	82,113,113	1.20	7 (8%)
32	LMG	A	860	-	40,40,55	1.01	2 (5%)	48,48,63	1.10	4 (8%)
32	LMG	V	2631	-	55,55,55	0.88	2 (3%)	63,63,63	1.12	5 (7%)
26	CLA	5	616	18	44,50,73	1.53	10 (22%)	57,85,113	1.30	5 (8%)
26	CLA	4	608	-	69,73,73	1.16	6 (8%)	82,113,113	1.16	6 (7%)
26	CLA	Y	614	-	52,56,73	1.32	7 (13%)	61,92,113	1.25	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	A	845	28	54,58,73	1.32	9 (16%)	64,95,113	1.35	6 (9%)
26	CLA	B	840	-	69,73,73	1.23	8 (11%)	82,113,113	1.24	4 (4%)
26	CLA	A	838	-	54,58,73	1.33	10 (18%)	64,95,113	1.34	5 (7%)
26	CLA	6	617	-	49,53,73	1.36	7 (14%)	58,89,113	1.26	5 (8%)
34	LUT	4	619	-	42,43,43	0.80	1 (2%)	51,60,60	2.14	17 (33%)
26	CLA	8	616	21	47,51,73	1.50	7 (14%)	58,87,113	1.35	7 (12%)
26	CLA	8	602	21	64,68,73	1.24	8 (12%)	76,107,113	1.30	8 (10%)
26	CLA	B	809	2	69,73,73	1.20	8 (11%)	82,113,113	1.26	5 (6%)
26	CLA	H	203	-	69,73,73	1.16	7 (10%)	82,113,113	1.21	4 (4%)
26	CLA	a	608	-	47,52,73	1.40	7 (14%)	55,88,113	1.27	5 (9%)
28	LHG	V	2630	26	35,35,48	1.07	2 (5%)	38,41,54	1.09	2 (5%)
26	CLA	a	609	14	67,72,73	1.18	6 (8%)	79,112,113	1.15	4 (5%)
26	CLA	6	602	19	69,73,73	1.18	8 (11%)	82,113,113	1.16	6 (7%)
26	CLA	Y	602	24	62,66,73	1.22	7 (11%)	73,104,113	1.22	7 (9%)
26	CLA	B	822	-	46,50,73	1.37	8 (17%)	53,85,113	1.25	3 (5%)
32	LMG	9	625	-	55,55,55	0.89	2 (3%)	63,63,63	1.04	6 (9%)
26	CLA	B	816	-	58,62,73	1.24	8 (13%)	68,99,113	1.28	6 (8%)
26	CLA	5	613	18	68,72,73	1.14	8 (11%)	80,111,113	1.25	7 (8%)
26	CLA	A	822	-	69,73,73	1.21	10 (14%)	82,113,113	1.24	8 (9%)
26	CLA	V	602	25	64,68,73	1.19	7 (10%)	76,107,113	1.21	6 (7%)
28	LHG	4	622	26	48,48,48	0.91	2 (4%)	51,54,54	0.83	2 (3%)
37	CHL	Z	608	-	43,57,74	4.06	20 (46%)	37,93,114	2.41	12 (32%)
26	CLA	9	609	22	65,69,73	1.21	7 (10%)	77,108,113	1.19	4 (5%)
26	CLA	5	619	-	47,51,73	1.53	8 (17%)	58,87,113	1.40	7 (12%)
26	CLA	U	604	-	52,56,73	1.45	9 (17%)	61,91,113	1.34	8 (13%)
26	CLA	B	837	-	69,73,73	1.19	9 (13%)	82,113,113	1.29	7 (8%)
29	BCR	2	623	-	41,41,41	0.88	1 (2%)	56,56,56	2.38	22 (39%)
26	CLA	1	608	-	47,52,73	1.40	8 (17%)	55,88,113	1.26	5 (9%)
33	DGD	B	850	-	63,63,67	0.84	2 (3%)	77,77,81	1.25	7 (9%)
26	CLA	a	614	-	58,62,73	1.27	8 (13%)	65,99,113	1.27	4 (6%)
26	CLA	1	616	14	47,51,73	1.49	7 (14%)	58,87,113	1.41	7 (12%)
26	CLA	a	604	-	53,57,73	1.30	7 (13%)	61,93,113	1.24	4 (6%)
28	LHG	H	204	-	48,48,48	0.93	2 (4%)	51,54,54	0.95	2 (3%)
28	LHG	Z	2630	26	48,48,48	0.93	2 (4%)	51,54,54	0.97	2 (3%)
35	XAT	X	1622	-	41,47,47	0.89	1 (2%)	54,74,74	2.52	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	L	304	-	49,53,73	1.36	6 (12%)	58,89,113	1.27	5 (8%)
26	CLA	3	610	16	69,73,73	1.18	7 (10%)	82,113,113	1.13	6 (7%)
29	BCR	4	621	-	41,41,41	0.86	1 (2%)	56,56,56	2.05	17 (30%)
28	LHG	W	2630	26	33,33,48	1.14	2 (6%)	36,39,54	1.19	3 (8%)
29	BCR	K	207	-	41,41,41	0.84	1 (2%)	56,56,56	2.80	22 (39%)
26	CLA	A	818	-	64,68,73	1.21	9 (14%)	76,107,113	1.25	6 (7%)
32	LMG	8	626	-	46,46,55	0.97	3 (6%)	54,54,63	1.11	4 (7%)
35	XAT	Y	1622	-	41,47,47	0.90	2 (4%)	54,74,74	2.66	22 (40%)
28	LHG	9	622	26	29,29,48	1.18	2 (6%)	32,35,54	1.04	1 (3%)
26	CLA	3	608	-	59,63,73	1.28	9 (15%)	70,101,113	1.16	3 (4%)
26	CLA	Z	613	24	69,73,73	1.18	7 (10%)	82,113,113	1.18	5 (6%)
26	CLA	4	613	17	69,73,73	1.20	9 (13%)	82,113,113	1.26	7 (8%)
26	CLA	A	809	1	69,73,73	1.19	9 (13%)	82,113,113	1.29	7 (8%)
35	XAT	9	620	-	41,47,47	0.95	3 (7%)	54,74,74	2.40	19 (35%)
26	CLA	A	842	-	69,73,73	1.22	9 (13%)	82,113,113	1.33	10 (12%)
37	CHL	U	601	24	60,74,74	3.49	19 (31%)	58,114,114	1.94	13 (22%)
36	NEX	6	624	-	40,46,46	1.25	5 (12%)	50,70,70	2.50	18 (36%)
26	CLA	2	601	15	69,73,73	1.14	9 (13%)	82,113,113	1.32	7 (8%)
26	CLA	B	813	-	69,73,73	1.21	10 (14%)	82,113,113	1.19	6 (7%)
26	CLA	B	819	-	59,63,73	1.27	7 (11%)	70,101,113	1.19	8 (11%)
26	CLA	5	611	28	46,50,73	1.37	6 (13%)	53,85,113	1.23	4 (7%)
26	CLA	B	833	-	69,73,73	1.16	7 (10%)	82,113,113	1.13	6 (7%)
35	XAT	3	619	-	41,47,47	0.94	3 (7%)	54,74,74	2.51	20 (37%)
26	CLA	Z	603	-	59,63,73	1.26	7 (11%)	70,101,113	1.40	8 (11%)
28	LHG	3	624	26	48,48,48	0.91	2 (4%)	51,54,54	0.98	3 (5%)
26	CLA	6	613	-	67,72,73	1.21	8 (11%)	79,112,113	1.19	8 (10%)
31	LMU	8	625	-	36,36,36	1.10	2 (5%)	47,47,47	1.25	3 (6%)
29	BCR	B	853	-	41,41,41	0.84	2 (4%)	56,56,56	1.82	14 (25%)
26	CLA	B	820	-	54,58,73	1.31	9 (16%)	64,95,113	1.35	5 (7%)
27	PQN	B	842	-	34,34,34	3.42	8 (23%)	43,45,45	1.94	7 (16%)
26	CLA	A	804	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
37	CHL	W	607	-	59,73,74	3.31	19 (32%)	59,113,114	1.90	16 (27%)
26	CLA	A	837	1	49,53,73	1.42	9 (18%)	58,89,113	1.46	4 (6%)
26	CLA	Z	611	28	46,50,73	1.46	8 (17%)	56,85,113	1.37	6 (10%)
26	CLA	B	807	-	56,60,73	1.35	10 (17%)	65,97,113	1.37	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	LUT	3	618	-	42,43,43	0.82	1 (2%)	51,60,60	2.11	13 (25%)
26	CLA	X	613	23	69,73,73	1.16	7 (10%)	82,113,113	1.12	4 (4%)
26	CLA	A	824	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
26	CLA	9	603	22	48,52,73	1.51	11 (22%)	59,88,113	1.36	4 (6%)
26	CLA	B	839	-	69,73,73	1.18	9 (13%)	82,113,113	1.14	6 (7%)
32	LMG	4	623	-	40,40,55	1.08	2 (5%)	48,48,63	1.16	5 (10%)
37	CHL	Z	607	-	60,74,74	3.42	19 (31%)	58,114,114	2.07	12 (20%)
30	SF4	C	102	3	0,12,12	-	-	-		
28	LHG	1	620	26	48,48,48	0.93	2 (4%)	51,54,54	0.80	2 (3%)
29	BCR	L	308	-	41,41,41	0.82	0	56,56,56	2.36	23 (41%)
26	CLA	B	811	-	56,60,73	1.46	10 (17%)	70,97,113	1.32	8 (11%)
26	CLA	A	839	-	59,63,73	1.29	8 (13%)	70,101,113	1.30	6 (8%)
32	LMG	L	2631	-	37,37,55	1.08	2 (5%)	45,45,63	1.19	4 (8%)
34	LUT	W	1621	-	42,43,43	0.64	0	51,60,60	1.84	14 (27%)
26	CLA	A	817	-	49,53,73	1.40	8 (16%)	58,89,113	1.37	6 (10%)
26	CLA	5	607	-	69,73,73	1.17	8 (11%)	82,113,113	1.19	5 (6%)
28	LHG	O	2631	-	35,35,48	1.07	2 (5%)	38,41,54	1.13	3 (7%)
28	LHG	A	861	-	48,48,48	0.94	2 (4%)	51,54,54	1.01	2 (3%)
29	BCR	9	621	-	41,41,41	0.72	0	56,56,56	2.94	18 (32%)
26	CLA	O	2002	-	41,46,73	1.56	8 (19%)	51,81,113	1.34	7 (13%)
26	CLA	V	603	-	49,53,73	1.37	6 (12%)	58,89,113	1.45	4 (6%)
37	CHL	Y	606	-	40,54,74	4.07	19 (47%)	34,90,114	2.92	14 (41%)
26	CLA	V	611	28	47,51,73	1.39	7 (14%)	55,86,113	1.22	3 (5%)
37	CHL	V	605	25	38,52,74	4.27	18 (47%)	31,87,114	2.80	13 (41%)
31	LMU	A	857	-	36,36,36	1.09	2 (5%)	47,47,47	1.38	8 (17%)
26	CLA	5	610	18	58,62,73	1.26	8 (13%)	68,99,113	1.20	5 (7%)
28	LHG	8	622	26	48,48,48	0.91	2 (4%)	51,54,54	0.87	2 (3%)
34	LUT	U	1620	-	42,43,43	0.70	0	51,60,60	1.71	11 (21%)
26	CLA	6	616	19	69,73,73	1.17	9 (13%)	82,113,113	1.28	9 (10%)
28	LHG	5	623	26	48,48,48	0.93	2 (4%)	51,54,54	0.88	2 (3%)
28	LHG	9	623	-	48,48,48	0.91	2 (4%)	51,54,54	0.97	2 (3%)
34	LUT	1	617	-	42,43,43	0.78	1 (2%)	51,60,60	2.04	18 (35%)
29	BCR	1	619	-	41,41,41	0.85	0	56,56,56	2.41	22 (39%)
26	CLA	Z	614	-	52,56,73	1.34	6 (11%)	61,92,113	1.25	4 (6%)
26	CLA	V	614	-	49,53,73	1.36	7 (14%)	58,89,113	1.30	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	5	608	-	54,58,73	1.33	7 (12%)	63,95,113	1.18	4 (6%)
26	CLA	7	607	-	46,50,73	1.37	7 (15%)	53,85,113	1.19	3 (5%)

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
26	CLA	Y	612	24	1/1/11/20	6/15/91/115	-
26	CLA	A	808	-	1/1/12/20	1/21/97/115	-
26	CLA	4	606	-	1/1/10/20	4/8/84/115	-
29	BCR	3	620	-	-	4/29/63/63	0/2/2/2
26	CLA	9	611	28	1/1/10/20	3/12/88/115	-
26	CLA	Z	602	24	1/1/13/20	7/31/107/115	-
26	CLA	B	832	-	1/1/14/20	12/33/109/115	-
34	LUT	W	1620	-	-	6/29/67/67	0/2/2/2
26	CLA	A	811	-	1/1/15/20	11/39/115/115	-
31	LMU	K	208	-	-	10/21/61/61	0/2/2/2
26	CLA	3	612	16	1/1/10/20	4/13/89/115	-
26	CLA	a	601	14	-	4/25/101/115	-
34	LUT	Y	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	X	614	-	1/1/10/20	4/12/88/115	-
35	XAT	V	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	9	602	22	1/1/14/20	6/33/109/115	-
29	BCR	6	622	-	-	2/29/63/63	0/2/2/2
37	CHL	V	607	-	3/3/16/26	8/15/113/137	-
29	BCR	B	852	-	-	6/29/63/63	0/2/2/2
36	NEX	Z	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	A	823	-	1/1/10/20	3/12/88/115	-
29	BCR	B	801	-	-	2/29/63/63	0/2/2/2
26	CLA	a	616	14	1/1/11/20	5/15/91/115	-
26	CLA	A	803	-	1/1/15/20	8/39/115/115	-
26	CLA	7	604	-	1/1/12/20	7/21/97/115	-
26	CLA	8	612	21	1/1/10/20	2/10/86/115	-
37	CHL	X	609	23	3/3/20/26	22/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	XAT	U	1622	-	-	4/31/93/93	0/4/4/4
29	BCR	L	309	-	-	3/29/63/63	0/2/2/2
26	CLA	4	618	17	1/1/10/20	2/8/84/115	-
31	LMU	A	858	-	-	10/21/57/61	0/2/2/2
28	LHG	6	623	26	-	19/52/52/53	-
29	BCR	O	2004	-	-	2/29/63/63	0/2/2/2
26	CLA	6	603	-	1/1/12/20	6/22/98/115	-
26	CLA	2	612	15	1/1/11/20	7/13/89/115	-
35	XAT	5	621	-	-	0/31/93/93	0/4/4/4
37	CHL	W	605	23	3/3/16/26	8/15/113/137	-
37	CHL	Y	609	24	3/3/20/26	16/39/137/137	-
26	CLA	A	807	1	1/1/15/20	19/39/115/115	-
26	CLA	Y	613	24	-	14/39/115/115	-
26	CLA	1	610	14	1/1/9/20	3/8/80/115	-
26	CLA	3	604	-	1/1/15/20	6/39/115/115	-
35	XAT	7	620	-	-	0/31/93/93	0/4/4/4
26	CLA	6	611	28	1/1/10/20	3/12/88/115	-
26	CLA	W	610	23	1/1/13/20	6/27/103/115	-
26	CLA	F	304	6	-	4/10/86/115	-
26	CLA	1	611	28	1/1/13/20	5/30/106/115	-
26	CLA	5	612	18	1/1/10/20	2/10/86/115	-
26	CLA	4	604	-	1/1/13/20	7/25/101/115	-
37	CHL	Z	601	24	3/3/20/26	18/39/137/137	-
28	LHG	U	2630	26	-	20/53/53/53	-
26	CLA	W	614	-	1/1/11/20	7/15/91/115	-
37	CHL	W	601	23	3/3/20/26	21/39/137/137	-
26	CLA	H	202	-	1/1/10/20	4/6/82/115	-
26	CLA	2	604	-	1/1/10/20	3/11/87/115	-
26	CLA	3	615	-	1/1/10/20	3/8/84/115	-
26	CLA	K	201	11	1/1/11/20	6/15/91/115	-
26	CLA	F	303	-	-	6/12/88/115	-
29	BCR	J	102	-	-	2/29/63/63	0/2/2/2
26	CLA	A	814	-	1/1/15/20	17/39/115/115	-
26	CLA	A	806	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	X	612	23	1/1/10/20	8/13/89/115	-
26	CLA	B	827	-	1/1/14/20	11/36/112/115	-
26	CLA	Y	611	28	1/1/10/20	8/13/89/115	-
36	NEX	U	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	V	613	25	1/1/15/20	18/39/115/115	-
26	CLA	U	613	24	1/1/13/20	11/32/108/115	-
26	CLA	B	818	-	-	11/33/109/115	-
26	CLA	4	610	17	1/1/14/20	7/35/111/115	-
28	LHG	7	622	26	-	18/41/41/53	-
30	SF4	A	853	1,2	-	-	0/6/5/5
34	LUT	9	619	-	-	4/29/67/67	0/2/2/2
37	CHL	V	601	25	3/3/20/26	9/39/137/137	-
37	CHL	Y	607	-	3/3/20/26	19/39/137/137	-
35	XAT	2	620	-	-	0/31/93/93	0/4/4/4
26	CLA	6	607	-	1/1/10/20	0/10/86/115	-
35	XAT	Z	1622	-	-	4/31/93/93	0/4/4/4
35	XAT	W	1622	-	-	1/31/93/93	0/4/4/4
29	BCR	B	848	-	-	4/29/63/63	0/2/2/2
26	CLA	A	802	-	1/1/15/20	11/39/115/115	-
26	CLA	7	616	20	1/1/11/20	6/11/87/115	-
26	CLA	9	601	22	1/1/11/20	6/15/91/115	-
26	CLA	9	613	22	1/1/15/20	12/39/115/115	-
26	CLA	8	607	-	1/1/10/20	2/10/86/115	-
26	CLA	W	604	-	1/1/11/20	4/18/94/115	-
26	CLA	4	614	-	-	10/29/105/115	-
35	XAT	6	621	-	-	0/31/93/93	0/4/4/4
26	CLA	5	604	-	1/1/15/20	10/35/111/115	-
26	CLA	6	612	19	1/1/10/20	4/10/86/115	-
37	CHL	Z	606	-	3/3/16/26	7/15/113/137	-
26	CLA	A	835	-	-	12/35/111/115	-
37	CHL	V	609	25	3/3/19/26	14/33/131/137	-
26	CLA	B	830	-	1/1/10/20	4/13/89/115	-
26	CLA	a	611	28	1/1/10/20	0/4/80/115	-
34	LUT	U	1621	-	-	5/29/67/67	0/2/2/2
26	CLA	2	610	15	1/1/13/20	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMU	1	621	-	-	7/21/61/61	0/2/2/2
26	CLA	a	603	-	1/1/12/20	9/25/101/115	-
31	LMU	5	628	-	-	10/19/59/61	0/2/2/2
26	CLA	X	610	23	1/1/15/20	12/39/115/115	-
26	CLA	B	810	-	1/1/14/20	18/37/113/115	-
26	CLA	B	831	-	1/1/15/20	12/39/115/115	-
26	CLA	8	608	-	-	7/23/99/115	-
26	CLA	W	611	28	1/1/13/20	9/30/106/115	-
29	BCR	L	305	-	-	2/29/63/63	0/2/2/2
26	CLA	9	614	-	1/1/11/20	5/15/91/115	-
29	BCR	B	843	-	-	4/29/63/63	0/2/2/2
26	CLA	A	819	-	1/1/13/20	5/32/108/115	-
26	CLA	A	827	-	1/1/13/20	5/31/107/115	-
26	CLA	A	833	-	1/1/11/20	5/15/91/115	-
37	CHL	X	606	-	3/3/15/26	4/13/111/137	-
26	CLA	9	606	-	1/1/10/20	3/8/84/115	-
26	CLA	7	609	20	1/1/10/20	6/12/88/115	-
26	CLA	B	814	-	1/1/14/20	13/38/114/115	-
34	LUT	7	619	-	-	2/29/67/67	0/2/2/2
29	BCR	A	849	-	-	5/29/63/63	0/2/2/2
26	CLA	a	607	-	1/1/11/20	6/15/91/115	-
37	CHL	W	606	-	3/3/16/26	1/15/113/137	-
26	CLA	A	820	-	1/1/15/20	7/39/115/115	-
26	CLA	6	610	19	1/1/15/20	11/39/115/115	-
26	CLA	Y	610	24	1/1/15/20	10/39/115/115	-
36	NEX	X	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	7	606	-	1/1/10/20	2/10/86/115	-
26	CLA	B	812	-	1/1/10/20	4/13/89/115	-
26	CLA	5	614	-	1/1/10/20	8/15/87/115	-
37	CHL	Y	605	24	3/3/15/26	2/10/108/137	-
26	CLA	1	614	-	1/1/9/20	0/4/76/115	-
29	BCR	A	856	-	-	2/29/63/63	0/2/2/2
29	BCR	A	850	-	-	2/29/63/63	0/2/2/2
29	BCR	B	846	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	1	606	-	1/1/8/20	3/7/79/115	-
26	CLA	8	610	21	1/1/14/20	9/33/109/115	-
29	BCR	A	852	-	-	8/29/63/63	0/2/2/2
29	BCR	7	621	-	-	2/29/63/63	0/2/2/2
26	CLA	4	612	17	1/1/10/20	3/10/86/115	-
26	CLA	A	830	-	1/1/15/20	13/39/115/115	-
26	CLA	7	603	-	1/1/11/20	6/13/89/115	-
37	CHL	Y	608	-	3/3/16/26	6/19/117/137	-
26	CLA	3	609	16	1/1/14/20	14/33/109/115	-
36	NEX	Y	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	L	307	8	1/1/10/20	2/8/84/115	-
26	CLA	1	607	-	1/1/10/20	4/8/84/115	-
32	LMG	J	104	-	-	12/35/55/70	0/1/1/1
26	CLA	4	609	17	1/1/13/20	4/30/106/115	-
26	CLA	6	620	-	1/1/14/20	11/37/113/115	-
29	BCR	B	849	-	-	5/29/63/63	0/2/2/2
26	CLA	A	831	-	1/1/15/20	17/39/115/115	-
26	CLA	6	606	-	1/1/10/20	2/8/84/115	-
37	CHL	U	609	24	3/3/18/26	14/32/130/137	-
26	CLA	7	611	28	1/1/13/20	4/31/107/115	-
29	BCR	8	621	-	-	2/29/63/63	0/2/2/2
26	CLA	B	834	-	1/1/14/20	4/33/109/115	-
26	CLA	5	618	18	1/1/10/20	3/8/84/115	-
32	LMG	H	205	-	-	14/50/70/70	0/1/1/1
34	LUT	X	1621	-	-	3/29/67/67	0/2/2/2
29	BCR	K	202	-	-	4/29/63/63	0/2/2/2
34	LUT	2	619	-	-	2/29/67/67	0/2/2/2
34	LUT	a	617	-	-	4/29/67/67	0/2/2/2
26	CLA	1	604	-	1/1/11/20	6/20/96/115	-
26	CLA	A	832	-	1/1/12/20	11/21/97/115	-
32	LMG	J	103	-	-	10/37/57/70	0/1/1/1
37	CHL	Z	609	24	3/3/20/26	17/39/137/137	-
26	CLA	4	603	17	1/1/11/20	4/13/89/115	-
26	CLA	2	602	15	1/1/15/20	17/49/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CHL	W	609	23	3/3/20/26	12/39/137/137	-
28	LHG	9	624	-	-	17/53/53/53	-
26	CLA	G	204	7	1/1/11/20	7/15/91/115	-
34	LUT	Z	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	7	614	-	1/1/10/20	3/12/88/115	-
34	LUT	X	1620	-	-	4/29/67/67	0/2/2/2
26	CLA	B	821	-	1/1/11/20	6/13/89/115	-
26	CLA	8	604	-	1/1/12/20	5/21/97/115	-
26	CLA	U	603	-	1/1/12/20	9/24/100/115	-
37	CHL	Y	601	24	3/3/20/26	19/39/137/137	-
26	CLA	B	808	-	1/1/15/20	13/39/115/115	-
26	CLA	B	838	-	1/1/11/20	2/17/93/115	-
26	CLA	4	611	28	1/1/10/20	6/12/88/115	-
34	LUT	5	620	-	-	0/29/67/67	0/2/2/2
26	CLA	A	816	-	1/1/15/20	14/39/115/115	-
26	CLA	B	825	-	-	3/20/96/115	-
26	CLA	B	826	-	1/1/14/20	11/36/112/115	-
26	CLA	a	610	14	1/1/14/20	8/31/107/115	-
26	CLA	L	302	12	1/1/11/20	6/15/91/115	-
37	CHL	V	606	-	3/3/15/26	5/13/111/137	-
26	CLA	7	615	-	1/1/10/20	6/8/84/115	-
35	XAT	8	620	-	-	0/31/93/93	0/4/4/4
26	CLA	A	825	-	1/1/15/20	16/39/115/115	-
26	CLA	3	607	16	1/1/13/20	6/28/104/115	-
26	CLA	3	617	16	1/1/10/20	0/8/84/115	-
37	CHL	W	608	-	3/3/16/26	9/17/115/137	-
26	CLA	4	601	17	1/1/15/20	15/39/115/115	-
37	CHL	U	608	-	3/3/15/26	5/13/111/137	-
29	BCR	G	205	-	-	2/29/63/63	0/2/2/2
26	CLA	3	614	-	1/1/10/20	2/8/84/115	-
26	CLA	U	614	-	1/1/10/20	5/12/88/115	-
29	BCR	a	619	-	-	2/29/63/63	0/2/2/2
26	CLA	A	810	1	-	7/21/97/115	-
26	CLA	F	301	-	1/1/13/20	13/30/106/115	-
26	CLA	A	840	-	-	7/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	9	610	22	1/1/13/20	5/30/106/115	-
26	CLA	K	203	-	-	10/29/105/115	-
26	CLA	B	829	-	1/1/15/20	9/39/115/115	-
26	CLA	1	601	14	-	4/25/101/115	-
37	CHL	Z	605	24	3/3/15/26	4/10/108/137	-
29	BCR	B	847	-	-	2/29/63/63	0/2/2/2
26	CLA	Y	603	-	1/1/13/20	12/27/103/115	-
26	CLA	7	610	20	1/1/15/20	7/39/115/115	-
30	SF4	C	101	3	-	-	0/6/5/5
26	CLA	B	802	-	1/1/15/20	17/39/115/115	-
26	CLA	Z	610	24	1/1/15/20	9/39/115/115	-
29	BCR	B	845	-	-	9/29/63/63	0/2/2/2
37	CHL	X	607	-	3/3/20/26	23/39/137/137	-
26	CLA	9	607	-	-	9/15/91/115	-
26	CLA	9	604	-	1/1/12/20	8/20/96/115	-
26	CLA	B	805	-	1/1/15/20	9/39/115/115	-
26	CLA	V	604	-	1/1/12/20	7/21/97/115	-
26	CLA	3	602	16	1/1/14/20	4/33/109/115	-
26	CLA	A	854	-	1/1/15/20	7/39/115/115	-
26	CLA	8	609	21	1/1/11/20	2/15/91/115	-
26	CLA	A	805	-	-	6/24/100/115	-
26	CLA	B	836	-	1/1/12/20	5/21/97/115	-
26	CLA	A	841	-	1/1/15/20	15/39/115/115	-
26	CLA	A	815	-	1/1/12/20	11/21/97/115	-
26	CLA	A	829	-	1/1/15/20	10/39/115/115	-
26	CLA	4	602	17	1/1/14/20	8/33/109/115	-
26	CLA	A	826	-	1/1/14/20	8/37/113/115	-
26	CLA	7	608	-	-	4/21/97/115	-
26	CLA	5	609	18	1/1/15/20	12/39/115/115	-
26	CLA	A	801	-	1/1/15/20	10/39/115/115	-
26	CLA	7	601	20	1/1/14/20	6/33/109/115	-
37	CHL	X	605	-	3/3/16/26	9/15/113/137	-
32	LMG	4	624	-	-	5/35/55/70	0/1/1/1
26	CLA	7	613	20	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	6	614	-	1/1/14/20	8/33/109/115	-
26	CLA	O	2003	-	1/1/10/20	5/8/84/115	-
28	LHG	X	2630	26	-	12/53/53/53	-
29	BCR	L	301	-	-	4/29/63/63	0/2/2/2
34	LUT	Z	1620	-	-	5/29/67/67	0/2/2/2
26	CLA	1	613	-	1/1/15/20	15/39/115/115	-
26	CLA	V	610	25	1/1/14/20	9/36/112/115	-
29	BCR	7	623	-	-	3/29/63/63	0/2/2/2
26	CLA	X	604	-	1/1/11/20	11/20/96/115	-
26	CLA	8	614	-	1/1/12/20	6/25/101/115	-
26	CLA	A	813	-	1/1/12/20	7/26/102/115	-
26	CLA	6	608	-	-	8/15/91/115	-
37	CHL	X	608	-	3/3/19/26	21/39/133/137	-
26	CLA	B	835	-	1/1/11/20	2/15/91/115	-
26	CLA	1	609	14	1/1/10/20	2/8/84/115	-
26	CLA	6	618	19	1/1/10/20	1/8/84/115	-
29	BCR	A	851	-	-	2/29/63/63	0/2/2/2
26	CLA	B	828	-	1/1/15/20	14/39/115/115	-
37	CHL	V	608	-	3/3/16/26	4/18/116/137	-
28	LHG	Y	2630	26	-	12/53/53/53	-
26	CLA	a	612	14	1/1/11/20	4/15/91/115	-
26	CLA	B	815	-	1/1/10/20	2/13/89/115	-
26	CLA	W	613	23	1/1/15/20	20/39/115/115	-
35	XAT	a	618	-	-	0/31/93/93	0/4/4/4
27	PQN	A	844	-	-	7/23/43/43	0/2/2/2
28	LHG	B	851	26	-	13/42/42/53	-
28	LHG	2	622	26	-	9/40/40/53	-
37	CHL	U	606	-	3/3/15/26	6/13/111/137	-
28	LHG	A	846	-	-	15/53/53/53	-
26	CLA	5	602	18	1/1/15/20	8/39/115/115	-
26	CLA	L	306	-	1/1/10/20	1/8/84/115	-
26	CLA	2	613	15	1/1/15/20	9/39/115/115	-
26	CLA	4	607	-	1/1/11/20	5/15/91/115	-
26	CLA	6	604	-	1/1/15/20	14/39/115/115	-
26	CLA	1	603	-	1/1/12/20	7/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	O	2001	-	1/1/9/20	2/6/78/115	-
29	BCR	B	844	-	-	2/29/63/63	0/2/2/2
26	CLA	U	602	24	1/1/13/20	17/32/108/115	-
34	LUT	V	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	G	203	-	1/1/10/20	4/12/88/115	-
26	CLA	J	101	10	1/1/10/20	5/12/88/115	-
34	LUT	6	619	-	-	4/29/67/67	0/2/2/2
26	CLA	a	606	-	1/1/10/20	8/12/88/115	-
26	CLA	B	824	-	1/1/15/20	13/39/115/115	-
28	LHG	8	623	-	-	10/44/44/53	-
29	BCR	5	622	-	-	1/29/63/63	0/2/2/2
35	XAT	4	620	-	-	2/31/93/93	0/4/4/4
26	CLA	B	806	2	1/1/15/20	18/39/115/115	-
26	CLA	8	603	-	1/1/11/20	5/13/89/115	-
35	XAT	1	618	-	-	0/31/93/93	0/4/4/4
26	CLA	5	617	-	1/1/12/20	10/21/97/115	-
26	CLA	a	613	-	1/1/12/20	7/26/102/115	-
34	LUT	V	1620	-	-	4/29/67/67	0/2/2/2
29	BCR	F	305	-	-	6/29/63/63	0/2/2/2
26	CLA	Y	604	-	1/1/12/20	8/21/97/115	-
36	NEX	V	1623	-	-	7/27/83/83	0/3/3/3
26	CLA	U	610	24	1/1/13/20	4/29/105/115	-
26	CLA	B	804	-	1/1/10/20	2/10/86/115	-
26	CLA	5	603	-	1/1/13/20	5/25/101/115	-
26	CLA	U	612	24	1/1/10/20	4/12/88/115	-
29	BCR	3	621	-	-	0/29/63/63	0/2/2/2
26	CLA	4	616	17	1/1/11/20	4/11/87/115	-
26	CLA	9	612	22	1/1/10/20	2/10/86/115	-
26	CLA	2	616	-	1/1/11/20	2/11/87/115	-
26	CLA	2	609	15	1/1/11/20	3/15/91/115	-
26	CLA	A	828	-	1/1/15/20	16/39/115/115	-
26	CLA	a	602	14	1/1/14/20	4/35/111/115	-
26	CLA	A	821	-	-	13/25/101/115	-
26	CLA	W	612	23	1/1/11/20	7/15/91/115	-
37	CHL	X	601	23	3/3/20/26	14/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	7	612	20	1/1/11/20	4/13/89/115	-
29	BCR	3	622	-	-	2/29/63/63	0/2/2/2
26	CLA	6	601	19	1/1/15/20	16/39/115/115	-
26	CLA	B	823	-	1/1/11/20	5/15/91/115	-
26	CLA	B	803	-	1/1/15/20	11/39/115/115	-
26	CLA	1	612	14	1/1/11/20	4/15/91/115	-
36	NEX	5	624	-	-	2/27/83/83	0/3/3/3
29	BCR	O	2005	-	-	2/29/63/63	0/2/2/2
26	CLA	3	606	-	1/1/13/20	3/25/101/115	-
26	CLA	3	613	16	1/1/12/20	8/23/99/115	-
26	CLA	6	609	19	1/1/11/20	7/15/91/115	-
26	CLA	A	834	-	1/1/15/20	12/39/115/115	-
26	CLA	X	602	23	1/1/15/20	9/39/115/115	-
26	CLA	K	206	11	1/1/11/20	6/15/91/115	-
26	CLA	2	603	15	1/1/11/20	7/13/89/115	-
28	LHG	5	625	-	-	12/53/53/53	-
26	CLA	Z	604	-	1/1/11/20	4/21/93/115	-
32	LMG	5	627	-	-	7/35/55/70	0/1/1/1
26	CLA	A	812	-	1/1/15/20	9/39/115/115	-
26	CLA	U	611	28	1/1/10/20	2/12/88/115	-
26	CLA	1	602	14	1/1/14/20	4/35/111/115	-
26	CLA	W	602	23	1/1/14/20	12/33/109/115	-
26	CLA	K	204	-	1/1/11/20	5/15/91/115	-
34	LUT	8	619	-	-	4/29/67/67	0/2/2/2
26	CLA	3	603	-	1/1/13/20	10/27/103/115	-
26	CLA	2	611	28	1/1/10/20	2/12/88/115	-
26	CLA	8	606	-	1/1/15/20	5/37/113/115	-
26	CLA	X	611	28	1/1/11/20	4/15/91/115	-
26	CLA	8	613	21	1/1/15/20	14/39/115/115	-
26	CLA	Z	612	24	1/1/11/20	7/15/91/115	-
28	LHG	A	847	26	-	6/34/34/53	-
26	CLA	V	612	25	1/1/11/20	6/15/91/115	-
26	CLA	A	836	-	1/1/15/20	9/39/115/115	-
26	CLA	3	611	28	1/1/10/20	2/4/80/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	843	-	1/1/14/20	13/37/113/115	-
31	LMU	5	629	-	-	11/18/58/61	0/2/2/2
26	CLA	2	606	-	1/1/10/20	2/13/89/115	-
28	LHG	a	620	26	-	7/47/47/53	-
26	CLA	8	601	21	1/1/15/20	15/39/115/115	-
36	NEX	W	1623	-	-	6/27/83/83	0/3/3/3
37	CHL	U	605	24	3/3/15/26	2/12/110/137	-
26	CLA	B	817	-	1/1/13/20	8/32/108/115	-
26	CLA	2	614	-	1/1/10/20	0/11/87/115	-
26	CLA	W	603	-	1/1/12/20	9/24/100/115	-
26	CLA	X	603	-	1/1/14/20	15/36/112/115	-
26	CLA	5	601	18	1/1/13/20	3/29/105/115	-
28	LHG	3	623	-	-	15/49/49/53	-
34	LUT	Y	1620	-	-	5/29/67/67	0/2/2/2
26	CLA	L	303	-	-	12/39/115/115	-
26	CLA	B	841	28	1/1/15/20	13/39/115/115	-
26	CLA	5	606	-	-	3/8/84/115	-
26	CLA	8	611	28	1/1/10/20	6/12/88/115	-
37	CHL	U	607	-	3/3/16/26	8/15/113/137	-
26	CLA	2	607	-	1/1/11/20	2/13/89/115	-
29	BCR	A	848	-	-	3/29/63/63	0/2/2/2
26	CLA	7	602	20	1/1/15/20	9/39/115/115	-
32	LMG	A	860	-	-	9/35/55/70	0/1/1/1
32	LMG	V	2631	-	-	12/50/70/70	0/1/1/1
26	CLA	5	616	18	1/1/10/20	3/8/84/115	-
26	CLA	4	608	-	1/1/15/20	11/39/115/115	-
26	CLA	Y	614	-	1/1/11/20	10/19/95/115	-
26	CLA	A	845	28	1/1/12/20	6/21/97/115	-
26	CLA	B	840	-	1/1/15/20	8/39/115/115	-
26	CLA	A	838	-	1/1/12/20	7/21/97/115	-
26	CLA	6	617	-	1/1/11/20	9/15/91/115	-
34	LUT	4	619	-	-	4/29/67/67	0/2/2/2
26	CLA	8	616	21	1/1/11/20	4/11/87/115	-
26	CLA	8	602	21	-	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	809	2	1/1/15/20	11/39/115/115	-
26	CLA	H	203	-	1/1/15/20	17/39/115/115	-
26	CLA	a	608	-	1/1/11/20	4/13/89/115	-
28	LHG	V	2630	26	-	5/40/40/53	-
26	CLA	a	609	14	1/1/15/20	14/37/113/115	-
26	CLA	Y	602	24	1/1/13/20	12/31/107/115	-
26	CLA	6	602	19	-	8/39/115/115	-
26	CLA	B	822	-	-	4/12/88/115	-
32	LMG	9	625	-	-	12/50/70/70	0/1/1/1
26	CLA	B	816	-	1/1/12/20	9/25/101/115	-
26	CLA	5	613	18	1/1/14/20	16/37/113/115	-
26	CLA	A	822	-	1/1/15/20	6/39/115/115	-
26	CLA	V	602	25	1/1/14/20	6/33/109/115	-
28	LHG	4	622	26	-	6/53/53/53	-
37	CHL	Z	608	-	3/3/16/26	5/19/117/137	-
26	CLA	9	609	22	1/1/14/20	3/35/111/115	-
26	CLA	5	619	-	1/1/11/20	9/11/87/115	-
26	CLA	U	604	-	1/1/10/20	7/20/92/115	-
26	CLA	B	837	-	-	10/39/115/115	-
29	BCR	2	623	-	-	4/29/63/63	0/2/2/2
26	CLA	1	608	-	1/1/11/20	4/13/89/115	-
33	DGD	B	850	-	-	15/51/91/95	0/2/2/2
26	CLA	a	614	-	1/1/12/20	5/27/99/115	-
26	CLA	1	616	14	1/1/11/20	5/11/87/115	-
26	CLA	a	604	-	1/1/11/20	6/20/96/115	-
28	LHG	H	204	-	-	14/53/53/53	-
28	LHG	Z	2630	26	-	18/53/53/53	-
35	XAT	X	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	L	304	-	1/1/11/20	2/15/91/115	-
26	CLA	3	610	16	1/1/15/20	12/39/115/115	-
29	BCR	4	621	-	-	2/29/63/63	0/2/2/2
28	LHG	W	2630	26	-	11/38/38/53	-
29	BCR	K	207	-	-	1/29/63/63	0/2/2/2
26	CLA	A	818	-	-	14/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	8	626	-	-	15/41/61/70	0/1/1/1
35	XAT	Y	1622	-	-	2/31/93/93	0/4/4/4
28	LHG	9	622	26	-	10/34/34/53	-
26	CLA	3	608	-	1/1/13/20	9/27/103/115	-
26	CLA	Z	613	24	1/1/15/20	8/39/115/115	-
26	CLA	4	613	17	1/1/15/20	13/39/115/115	-
26	CLA	A	809	1	1/1/15/20	11/39/115/115	-
35	XAT	9	620	-	-	0/31/93/93	0/4/4/4
26	CLA	A	842	-	1/1/15/20	18/39/115/115	-
37	CHL	U	601	24	3/3/20/26	20/39/137/137	-
36	NEX	6	624	-	-	3/27/83/83	0/3/3/3
26	CLA	2	601	15	1/1/15/20	8/39/115/115	-
26	CLA	B	813	-	1/1/15/20	19/39/115/115	-
26	CLA	B	819	-	1/1/13/20	8/27/103/115	-
26	CLA	5	611	28	1/1/10/20	2/12/88/115	-
26	CLA	B	833	-	1/1/15/20	13/39/115/115	-
35	XAT	3	619	-	-	0/31/93/93	0/4/4/4
26	CLA	Z	603	-	1/1/13/20	10/27/103/115	-
28	LHG	3	624	26	-	13/53/53/53	-
26	CLA	6	613	-	-	13/37/113/115	-
31	LMU	8	625	-	-	12/21/61/61	0/2/2/2
29	BCR	B	853	-	-	4/29/63/63	0/2/2/2
26	CLA	B	820	-	1/1/12/20	3/21/97/115	-
27	PQN	B	842	-	-	7/23/43/43	0/2/2/2
26	CLA	A	804	-	1/1/15/20	15/39/115/115	-
37	CHL	W	607	-	3/3/20/26	20/37/135/137	-
26	CLA	A	837	1	1/1/11/20	7/15/91/115	-
26	CLA	Z	611	28	1/1/10/20	4/11/87/115	-
26	CLA	B	807	-	-	4/24/100/115	-
34	LUT	3	618	-	-	4/29/67/67	0/2/2/2
26	CLA	X	613	23	1/1/15/20	12/39/115/115	-
26	CLA	A	824	-	1/1/15/20	9/39/115/115	-
26	CLA	9	603	22	1/1/11/20	5/13/89/115	-
26	CLA	B	839	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	4	623	-	-	7/35/55/70	0/1/1/1
37	CHL	Z	607	-	3/3/20/26	20/39/137/137	-
30	SF4	C	102	3	-	-	0/6/5/5
28	LHG	1	620	26	-	9/53/53/53	-
29	BCR	L	308	-	-	6/29/63/63	0/2/2/2
26	CLA	B	811	-	1/1/12/20	11/23/95/115	-
26	CLA	A	839	-	1/1/13/20	9/27/103/115	-
32	LMG	L	2631	-	-	4/32/52/70	0/1/1/1
34	LUT	W	1621	-	-	5/29/67/67	0/2/2/2
26	CLA	A	817	-	-	2/15/91/115	-
26	CLA	5	607	-	1/1/15/20	13/39/115/115	-
28	LHG	O	2631	-	-	12/40/40/53	-
28	LHG	A	861	-	-	19/53/53/53	-
29	BCR	9	621	-	-	4/29/63/63	0/2/2/2
26	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
26	CLA	V	603	-	1/1/11/20	6/15/91/115	-
37	CHL	Y	606	-	3/3/16/26	8/15/113/137	-
26	CLA	V	611	28	1/1/10/20	6/13/89/115	-
37	CHL	V	605	25	3/3/15/26	4/13/111/137	-
31	LMU	A	857	-	-	9/21/61/61	0/2/2/2
26	CLA	5	610	18	1/1/12/20	5/26/102/115	-
28	LHG	8	622	26	-	11/53/53/53	-
34	LUT	U	1620	-	-	7/29/67/67	0/2/2/2
26	CLA	6	616	19	1/1/15/20	16/39/115/115	-
28	LHG	5	623	26	-	15/53/53/53	-
28	LHG	9	623	-	-	20/53/53/53	-
34	LUT	1	617	-	-	4/29/67/67	0/2/2/2
29	BCR	1	619	-	-	2/29/63/63	0/2/2/2
26	CLA	Z	614	-	1/1/11/20	8/19/95/115	-
26	CLA	V	614	-	1/1/11/20	5/15/91/115	-
26	CLA	5	608	-	1/1/12/20	6/21/97/115	-
26	CLA	7	607	-	1/1/10/20	1/12/88/115	-

All (3223) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	605	CHL	C2C-C3C	11.23	1.47	1.36
37	Y	605	CHL	C2C-C3C	11.17	1.47	1.36
37	X	609	CHL	C2C-C3C	10.97	1.47	1.36
37	U	605	CHL	C2C-C3C	10.95	1.47	1.36
37	Y	609	CHL	C2C-C3C	10.95	1.47	1.36
37	W	609	CHL	C2C-C3C	10.93	1.46	1.36
37	U	609	CHL	C2C-C3C	10.91	1.46	1.36
37	W	601	CHL	C2C-C3C	10.90	1.46	1.36
37	U	601	CHL	C2C-C3C	10.87	1.46	1.36
37	Z	609	CHL	C2C-C3C	10.78	1.46	1.36
37	W	605	CHL	C2C-C3C	10.78	1.46	1.36
37	Z	608	CHL	C2C-C3C	10.76	1.46	1.36
37	W	608	CHL	C2C-C3C	10.76	1.46	1.36
37	V	601	CHL	C2C-C3C	10.75	1.46	1.36
37	Y	601	CHL	C2C-C3C	10.72	1.46	1.36
37	V	609	CHL	C2C-C3C	10.71	1.46	1.36
37	U	608	CHL	C2C-C3C	10.69	1.46	1.36
37	W	609	CHL	C1D-C2D	10.67	1.51	1.39
37	X	609	CHL	C1D-C2D	10.65	1.51	1.39
37	V	605	CHL	C2C-C3C	10.60	1.46	1.36
37	Y	605	CHL	C1D-C2D	10.56	1.51	1.39
37	Z	606	CHL	C2C-C3C	10.47	1.46	1.36
37	Z	601	CHL	C2C-C3C	10.46	1.46	1.36
37	X	601	CHL	C2C-C3C	10.44	1.46	1.36
37	U	607	CHL	C2C-C3C	10.42	1.46	1.36
37	X	608	CHL	C2C-C3C	10.42	1.46	1.36
37	X	605	CHL	C1D-C2D	10.41	1.51	1.39
37	Z	605	CHL	C2C-C3C	10.38	1.46	1.36
37	Y	608	CHL	C2C-C3C	10.36	1.46	1.36
37	V	607	CHL	C2C-C3C	10.32	1.46	1.36
37	Z	609	CHL	C1D-C2D	10.31	1.51	1.39
37	V	609	CHL	C1D-C2D	10.29	1.51	1.39
37	V	605	CHL	C1D-C2D	10.26	1.51	1.39
37	U	601	CHL	C1D-C2D	10.23	1.51	1.39
37	W	608	CHL	C1D-C2D	10.22	1.51	1.39
37	V	608	CHL	C2C-C3C	10.19	1.46	1.36
37	X	606	CHL	C2C-C3C	10.18	1.46	1.36
37	Y	609	CHL	C1D-C2D	10.16	1.51	1.39
37	Y	601	CHL	C1D-C2D	10.16	1.51	1.39
37	U	605	CHL	C1D-C2D	10.13	1.51	1.39
37	W	605	CHL	C1D-C2D	10.11	1.51	1.39
37	Z	607	CHL	C2C-C3C	10.08	1.46	1.36
37	U	606	CHL	C2C-C3C	10.07	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Z	605	CHL	C1D-C2D	10.06	1.51	1.39
37	U	609	CHL	C1D-C2D	10.03	1.51	1.39
37	V	601	CHL	C1D-C2D	10.01	1.51	1.39
37	W	601	CHL	C1D-C2D	10.00	1.50	1.39
37	W	606	CHL	C2C-C3C	9.98	1.46	1.36
37	Y	607	CHL	C2C-C3C	9.96	1.46	1.36
37	Z	606	CHL	C1D-C2D	9.96	1.50	1.39
37	Z	608	CHL	C1D-C2D	9.96	1.50	1.39
27	B	842	PQN	C12-C13	9.95	1.56	1.33
37	X	601	CHL	C1A-CHA	9.92	1.51	1.40
37	U	608	CHL	C1D-C2D	9.89	1.50	1.39
37	V	606	CHL	C2C-C3C	9.85	1.45	1.36
37	X	608	CHL	C1D-C2D	9.85	1.50	1.39
37	Z	601	CHL	C1D-C2D	9.82	1.50	1.39
37	W	607	CHL	C1D-C2D	9.82	1.50	1.39
37	X	601	CHL	C1D-C2D	9.81	1.50	1.39
37	X	607	CHL	C2C-C3C	9.79	1.45	1.36
37	W	606	CHL	C1A-CHA	9.71	1.51	1.40
37	X	607	CHL	C1D-C2D	9.69	1.50	1.39
37	X	606	CHL	C1D-C2D	9.67	1.50	1.39
27	A	844	PQN	C12-C13	9.65	1.55	1.33
37	Y	608	CHL	C1D-C2D	9.65	1.50	1.39
37	U	607	CHL	C1D-C2D	9.61	1.50	1.39
37	Y	606	CHL	C1D-C2D	9.60	1.50	1.39
37	V	608	CHL	C1D-C2D	9.58	1.50	1.39
37	U	606	CHL	C1D-C2D	9.57	1.50	1.39
37	Y	606	CHL	C2C-C3C	9.56	1.45	1.36
37	W	606	CHL	C1D-C2D	9.56	1.50	1.39
37	W	607	CHL	C1A-CHA	9.51	1.50	1.40
37	Z	607	CHL	C1D-C2D	9.38	1.50	1.39
37	X	607	CHL	C1A-CHA	9.37	1.50	1.40
37	Y	607	CHL	C1D-C2D	9.15	1.50	1.39
37	V	607	CHL	C1D-C2D	9.15	1.50	1.39
37	V	607	CHL	C1A-CHA	9.07	1.50	1.40
37	Y	607	CHL	C1A-CHA	8.99	1.50	1.40
37	U	601	CHL	C1B-C2B	8.99	1.49	1.39
37	X	606	CHL	C3B-C4B	8.97	1.50	1.41
37	V	606	CHL	C1D-C2D	8.94	1.49	1.39
37	Z	607	CHL	C1A-CHA	8.94	1.50	1.40
37	V	606	CHL	C1A-CHA	8.94	1.50	1.40
37	W	605	CHL	C1A-CHA	8.93	1.50	1.40
37	X	608	CHL	C3B-C4B	8.93	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	U	607	CHL	C1A-CHA	8.93	1.50	1.40
37	X	601	CHL	C1B-C2B	8.82	1.49	1.39
37	U	601	CHL	C1A-CHA	8.82	1.50	1.40
37	X	608	CHL	C1A-CHA	8.78	1.50	1.40
37	Z	606	CHL	C3B-C4B	8.73	1.49	1.41
37	Y	606	CHL	C3B-C4B	8.63	1.49	1.41
37	Y	601	CHL	C1A-CHA	8.63	1.49	1.40
37	Z	608	CHL	C1A-CHA	8.60	1.49	1.40
37	Y	608	CHL	C1A-CHA	8.58	1.49	1.40
37	U	605	CHL	C1B-C2B	8.57	1.49	1.39
37	Z	601	CHL	C1A-CHA	8.57	1.49	1.40
37	Y	607	CHL	C1B-C2B	8.55	1.49	1.39
37	Y	605	CHL	C1B-C2B	8.54	1.49	1.39
37	Z	605	CHL	C1B-C2B	8.51	1.49	1.39
37	X	605	CHL	C1B-C2B	8.51	1.49	1.39
37	Z	607	CHL	C1B-C2B	8.49	1.49	1.39
37	W	605	CHL	C1B-C2B	8.48	1.49	1.39
37	W	607	CHL	C1B-C2B	8.46	1.49	1.39
37	V	605	CHL	C1B-C2B	8.45	1.49	1.39
37	Y	609	CHL	C1A-CHA	8.44	1.49	1.40
37	Z	609	CHL	C1A-CHA	8.43	1.49	1.40
37	U	609	CHL	C1B-C2B	8.40	1.49	1.39
37	V	609	CHL	C1B-C2B	8.39	1.49	1.39
37	Y	605	CHL	C1A-CHA	8.38	1.49	1.40
37	Z	608	CHL	C1B-C2B	8.36	1.49	1.39
37	W	608	CHL	C1B-C2B	8.35	1.49	1.39
37	V	601	CHL	C3B-C4B	8.33	1.49	1.41
37	X	607	CHL	C1B-C2B	8.33	1.49	1.39
37	Z	601	CHL	C3B-C4B	8.28	1.49	1.41
37	Z	601	CHL	C1B-C2B	8.27	1.49	1.39
37	V	607	CHL	C1B-C2B	8.23	1.48	1.39
37	U	606	CHL	C1A-CHA	8.22	1.49	1.40
37	W	601	CHL	C3B-C4B	8.20	1.49	1.41
37	W	608	CHL	C1A-CHA	8.17	1.49	1.40
37	Z	605	CHL	C1A-CHA	8.16	1.49	1.40
37	W	601	CHL	C1B-C2B	8.16	1.48	1.39
37	V	605	CHL	C1A-CHA	8.15	1.49	1.40
37	X	605	CHL	C1A-CHA	8.14	1.49	1.40
37	Y	601	CHL	C1B-C2B	8.14	1.48	1.39
37	V	608	CHL	C1A-CHA	8.13	1.49	1.40
37	U	608	CHL	C1B-C2B	8.11	1.48	1.39
37	X	606	CHL	C1B-C2B	8.10	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	V	601	CHL	C1B-C2B	8.09	1.48	1.39
37	X	605	CHL	C3B-C4B	8.08	1.49	1.41
37	U	606	CHL	C1B-C2B	8.05	1.48	1.39
37	X	609	CHL	C1A-CHA	8.05	1.49	1.40
37	U	608	CHL	C1A-CHA	8.04	1.49	1.40
37	Z	607	CHL	C3B-C4B	8.04	1.49	1.41
37	V	608	CHL	C1B-C2B	8.02	1.48	1.39
37	U	607	CHL	C1B-C2B	8.01	1.48	1.39
37	Y	608	CHL	C1B-C2B	7.99	1.48	1.39
37	W	606	CHL	C1B-C2B	7.98	1.48	1.39
37	Y	608	CHL	C3B-C4B	7.98	1.49	1.41
37	Y	601	CHL	C3B-C4B	7.97	1.49	1.41
37	W	601	CHL	C1A-CHA	7.97	1.49	1.40
37	W	607	CHL	C3B-C4B	7.96	1.49	1.41
37	X	609	CHL	C1B-C2B	7.96	1.48	1.39
37	U	605	CHL	C1A-CHA	7.93	1.49	1.40
37	Y	605	CHL	C3B-C4B	7.90	1.49	1.41
37	X	608	CHL	C1B-C2B	7.90	1.48	1.39
37	W	609	CHL	C1A-CHA	7.87	1.48	1.40
37	W	605	CHL	C3B-C4B	7.85	1.49	1.41
37	V	601	CHL	C1A-CHA	7.85	1.48	1.40
37	X	606	CHL	C1A-CHA	7.85	1.48	1.40
27	B	842	PQN	O4-C4	7.84	1.39	1.23
27	A	844	PQN	O4-C4	7.83	1.39	1.23
37	U	609	CHL	C1A-CHA	7.80	1.48	1.40
37	Y	609	CHL	C1B-C2B	7.78	1.48	1.39
37	W	609	CHL	C3B-C4B	7.77	1.49	1.41
37	X	607	CHL	C3B-C4B	7.74	1.48	1.41
37	W	609	CHL	C1B-C2B	7.71	1.48	1.39
37	W	608	CHL	C3B-C4B	7.70	1.48	1.41
37	V	609	CHL	C1A-CHA	7.69	1.48	1.40
37	U	607	CHL	C3B-C4B	7.68	1.48	1.41
27	A	844	PQN	O1-C1	7.66	1.39	1.23
37	U	601	CHL	C3B-C4B	7.65	1.48	1.41
37	U	605	CHL	C3B-C4B	7.65	1.48	1.41
37	Z	609	CHL	C1B-C2B	7.62	1.48	1.39
37	Z	608	CHL	C3B-C4B	7.60	1.48	1.41
27	B	842	PQN	O1-C1	7.54	1.39	1.23
37	Y	607	CHL	C3B-C4B	7.53	1.48	1.41
37	Y	606	CHL	C1A-CHA	7.48	1.48	1.40
37	V	608	CHL	C3B-C4B	7.47	1.48	1.41
37	V	607	CHL	C3B-C4B	7.45	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	V	605	CHL	C3B-C4B	7.43	1.48	1.41
37	Z	605	CHL	C3B-C4B	7.41	1.48	1.41
37	Z	606	CHL	C1B-C2B	7.38	1.47	1.39
37	X	601	CHL	C3B-C4B	7.35	1.48	1.41
37	Y	609	CHL	C3B-C4B	7.34	1.48	1.41
37	U	606	CHL	C3B-C4B	7.33	1.48	1.41
37	Y	606	CHL	C1B-C2B	7.24	1.47	1.39
37	V	606	CHL	C1B-C2B	7.23	1.47	1.39
37	V	609	CHL	C3B-C4B	7.21	1.48	1.41
37	V	606	CHL	C3B-C4B	7.21	1.48	1.41
37	X	609	CHL	C3B-C4B	7.20	1.48	1.41
37	Z	606	CHL	C1A-CHA	7.16	1.48	1.40
37	U	608	CHL	C3B-C4B	7.13	1.48	1.41
37	Z	609	CHL	C3B-C4B	7.10	1.48	1.41
27	B	842	PQN	C10-C5	-7.07	1.29	1.40
27	A	844	PQN	C9-C10	6.91	1.50	1.39
37	W	606	CHL	C3B-C4B	6.84	1.48	1.41
27	A	844	PQN	C6-C5	6.82	1.50	1.39
27	B	842	PQN	C9-C10	6.81	1.50	1.39
27	A	844	PQN	C10-C5	-6.77	1.29	1.40
27	B	842	PQN	C6-C5	6.76	1.50	1.39
37	U	609	CHL	C3B-C4B	6.09	1.47	1.41
37	Z	606	CHL	C3D-C4D	-5.71	1.32	1.41
37	U	608	CHL	C3D-C4D	-5.68	1.32	1.41
37	U	609	CHL	C3D-C4D	-5.67	1.32	1.41
37	V	608	CHL	C3D-C4D	-5.61	1.33	1.41
37	W	609	CHL	C3D-C4D	-5.59	1.33	1.41
37	X	605	CHL	C3B-C2B	5.59	1.47	1.40
37	V	609	CHL	C3D-C4D	-5.55	1.33	1.41
37	Y	606	CHL	C3D-C4D	-5.55	1.33	1.41
37	V	606	CHL	C3A-C2A	-5.54	1.49	1.54
37	W	601	CHL	C3D-C4D	-5.53	1.33	1.41
37	X	605	CHL	CHC-C4B	5.52	1.48	1.39
37	X	606	CHL	C3D-C4D	-5.51	1.33	1.41
37	U	606	CHL	C3D-C4D	-5.51	1.33	1.41
37	X	609	CHL	C3D-C4D	-5.51	1.33	1.41
37	U	605	CHL	C3D-C4D	-5.50	1.33	1.41
37	Y	605	CHL	C3B-C2B	5.49	1.47	1.40
37	V	605	CHL	C3D-C4D	-5.47	1.33	1.41
26	2	602	CLA	C1B-C2B	5.47	1.49	1.34
37	Z	607	CHL	C3D-C4D	-5.47	1.33	1.41
37	Z	608	CHL	C3D-C4D	-5.47	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	V	606	CHL	C3D-C4D	-5.44	1.33	1.41
37	V	601	CHL	C3D-C4D	-5.43	1.33	1.41
37	X	606	CHL	CHC-C4B	5.40	1.48	1.39
37	Y	609	CHL	C3A-C2A	-5.39	1.50	1.54
37	X	605	CHL	C3D-C4D	-5.39	1.33	1.41
37	Y	605	CHL	C3D-C4D	-5.38	1.33	1.41
37	Y	609	CHL	C3D-C4D	-5.37	1.33	1.41
37	Z	605	CHL	C3D-C4D	-5.36	1.33	1.41
37	Z	609	CHL	C3D-C4D	-5.36	1.33	1.41
37	Y	601	CHL	C3D-C4D	-5.33	1.33	1.41
37	U	605	CHL	C3B-C2B	5.33	1.47	1.40
37	Y	605	CHL	CHB-C1B	5.27	1.48	1.39
37	Z	606	CHL	C3A-C2A	-5.27	1.50	1.54
37	V	607	CHL	C3D-C4D	-5.26	1.33	1.41
37	Z	601	CHL	C3D-C4D	-5.26	1.33	1.41
37	Z	609	CHL	C3A-C2A	-5.25	1.50	1.54
37	Y	608	CHL	C3D-C4D	-5.25	1.33	1.41
37	Z	605	CHL	C2A-C3A	-5.25	1.50	1.54
37	W	607	CHL	C3D-C4D	-5.24	1.33	1.41
37	X	605	CHL	CHB-C1B	5.23	1.48	1.39
37	W	607	CHL	CHC-C4B	5.23	1.48	1.39
37	U	605	CHL	CHB-C1B	5.22	1.48	1.39
37	U	607	CHL	C3D-C4D	-5.22	1.33	1.41
37	W	608	CHL	C3D-C4D	-5.22	1.33	1.41
37	Y	605	CHL	CHC-C4B	5.18	1.48	1.39
37	U	605	CHL	CHC-C4B	5.18	1.48	1.39
37	W	607	CHL	C3B-C2B	5.18	1.47	1.40
37	V	605	CHL	C3B-C2B	5.17	1.47	1.40
37	Y	606	CHL	CHC-C4B	5.16	1.48	1.39
37	Y	608	CHL	O2D-CGD	5.15	1.45	1.33
37	W	605	CHL	C3D-C4D	-5.14	1.33	1.41
37	W	605	CHL	O2D-CGD	5.13	1.45	1.33
37	Y	605	CHL	OBD-CAD	5.13	1.29	1.22
37	X	601	CHL	C3D-C4D	-5.12	1.33	1.41
37	W	606	CHL	O2D-CGD	5.12	1.45	1.33
37	X	605	CHL	O2D-CGD	5.12	1.45	1.33
37	Z	606	CHL	O2D-CGD	5.12	1.45	1.33
37	X	608	CHL	CHC-C4B	5.12	1.47	1.39
37	Y	606	CHL	O2D-CGD	5.12	1.45	1.33
37	X	601	CHL	OBD-CAD	5.11	1.29	1.22
37	U	608	CHL	C3A-C2A	-5.11	1.50	1.54
37	V	608	CHL	C3A-C2A	-5.11	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	607	CHL	C3D-C4D	-5.11	1.33	1.41
37	U	601	CHL	C3D-C4D	-5.11	1.33	1.41
37	X	605	CHL	OBD-CAD	5.11	1.29	1.22
37	Y	607	CHL	O2D-CGD	5.11	1.45	1.33
37	W	605	CHL	OBD-CAD	5.10	1.29	1.22
37	W	601	CHL	O2D-CGD	5.10	1.45	1.33
37	Z	605	CHL	O2D-CGD	5.10	1.45	1.33
37	U	607	CHL	CHC-C4B	5.10	1.47	1.39
37	X	601	CHL	O2D-CGD	5.10	1.45	1.33
37	U	601	CHL	O2D-CGD	5.09	1.45	1.33
37	U	605	CHL	O2D-CGD	5.09	1.45	1.33
37	X	606	CHL	C3B-C2B	5.09	1.47	1.40
37	U	606	CHL	C3A-C2A	-5.09	1.50	1.54
37	W	601	CHL	C3B-C2B	5.09	1.47	1.40
37	Y	609	CHL	O2D-CGD	5.08	1.45	1.33
37	Z	609	CHL	CHB-C4A	-5.08	1.32	1.38
37	W	607	CHL	O2D-CGD	5.08	1.45	1.33
37	X	609	CHL	O2D-CGD	5.08	1.45	1.33
37	U	609	CHL	O2D-CGD	5.07	1.45	1.33
37	V	601	CHL	O2D-CGD	5.07	1.45	1.33
37	W	606	CHL	C3D-C4D	-5.07	1.33	1.41
37	X	608	CHL	O2D-CGD	5.07	1.45	1.33
37	Y	605	CHL	O2D-CGD	5.06	1.45	1.33
37	V	605	CHL	O2D-CGD	5.06	1.45	1.33
37	W	607	CHL	OBD-CAD	5.06	1.28	1.22
37	U	606	CHL	O2D-CGD	5.05	1.45	1.33
37	X	606	CHL	O2D-CGD	5.05	1.45	1.33
37	Y	601	CHL	O2D-CGD	5.05	1.45	1.33
37	Z	606	CHL	CHC-C4B	5.05	1.47	1.39
37	Z	601	CHL	O2D-CGD	5.04	1.45	1.33
37	Z	609	CHL	O2D-CGD	5.04	1.45	1.33
37	W	601	CHL	CHC-C4B	5.04	1.47	1.39
37	V	607	CHL	O2D-CGD	5.04	1.45	1.33
37	Z	608	CHL	O2D-CGD	5.04	1.45	1.33
37	V	601	CHL	CHC-C4B	5.03	1.47	1.39
37	V	601	CHL	C3A-C2A	-5.03	1.50	1.54
37	V	609	CHL	O2D-CGD	5.02	1.45	1.33
37	Z	607	CHL	O2D-CGD	5.02	1.45	1.33
37	W	608	CHL	O2D-CGD	5.02	1.45	1.33
37	Z	609	CHL	OBD-CAD	5.01	1.28	1.22
37	X	607	CHL	C3D-C4D	-5.01	1.33	1.41
37	V	605	CHL	CHB-C1B	5.01	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Z	601	CHL	OBD-CAD	5.01	1.28	1.22
37	X	607	CHL	O2D-CGD	5.01	1.45	1.33
37	V	606	CHL	O2D-CGD	5.00	1.45	1.33
37	U	607	CHL	O2D-CGD	5.00	1.45	1.33
37	U	601	CHL	OBD-CAD	4.99	1.28	1.22
37	V	605	CHL	OBD-CAD	4.99	1.28	1.22
37	W	606	CHL	OBD-CAD	4.99	1.28	1.22
37	W	605	CHL	C3B-C2B	4.99	1.47	1.40
37	X	609	CHL	OBD-CAD	4.98	1.28	1.22
37	U	607	CHL	CHB-C4A	-4.98	1.32	1.38
37	V	607	CHL	C3B-C2B	4.98	1.47	1.40
37	V	608	CHL	O2D-CGD	4.97	1.45	1.33
37	W	609	CHL	O2D-CGD	4.97	1.45	1.33
37	Y	601	CHL	C3B-C2B	4.97	1.47	1.40
37	U	607	CHL	OBD-CAD	4.97	1.28	1.22
37	X	606	CHL	C3A-C2A	-4.97	1.50	1.54
37	X	605	CHL	CHD-C4C	4.96	1.48	1.39
37	Y	606	CHL	C3A-C2A	-4.96	1.50	1.54
37	X	607	CHL	OBD-CAD	4.96	1.28	1.22
37	V	607	CHL	CHC-C4B	4.96	1.47	1.39
37	V	609	CHL	C3A-C2A	-4.96	1.50	1.54
37	U	608	CHL	O2D-CGD	4.95	1.45	1.33
37	Y	607	CHL	OBD-CAD	4.95	1.28	1.22
37	U	605	CHL	OBD-CAD	4.95	1.28	1.22
37	Y	601	CHL	CHC-C4B	4.95	1.47	1.39
37	Z	605	CHL	C3B-C2B	4.94	1.47	1.40
37	V	605	CHL	CHC-C4B	4.94	1.47	1.39
37	Z	605	CHL	OBD-CAD	4.93	1.28	1.22
37	Z	608	CHL	CHC-C4B	4.93	1.47	1.39
37	X	607	CHL	C3A-C2A	-4.93	1.50	1.54
37	U	609	CHL	OBD-CAD	4.93	1.28	1.22
37	X	605	CHL	CHD-C1D	4.92	1.47	1.39
37	Z	608	CHL	C3B-C2B	4.91	1.47	1.40
37	Y	601	CHL	OBD-CAD	4.91	1.28	1.22
37	Y	609	CHL	CHB-C4A	-4.91	1.32	1.38
37	W	601	CHL	OBD-CAD	4.90	1.28	1.22
37	U	607	CHL	C3B-C2B	4.90	1.47	1.40
36	5	624	NEX	C7-C6	-4.90	1.24	1.30
37	Y	608	CHL	OBD-CAD	4.89	1.28	1.22
37	Z	607	CHL	OBD-CAD	4.89	1.28	1.22
37	Z	607	CHL	C3B-C2B	4.88	1.47	1.40
37	U	605	CHL	CHD-C1D	4.87	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	V	607	CHL	OBD-CAD	4.87	1.28	1.22
37	W	609	CHL	CHD-C1D	4.87	1.47	1.39
37	Y	607	CHL	C3B-C2B	4.87	1.47	1.40
37	W	607	CHL	CHB-C1B	4.87	1.47	1.39
37	W	605	CHL	CHC-C4B	4.87	1.47	1.39
37	Z	607	CHL	CHC-C4B	4.86	1.47	1.39
37	X	605	CHL	CHC-C1C	4.86	1.48	1.39
37	V	601	CHL	C3B-C2B	4.86	1.46	1.40
37	Y	608	CHL	C3A-C2A	-4.86	1.50	1.54
37	V	608	CHL	CHC-C4B	4.85	1.47	1.39
37	W	609	CHL	OBD-CAD	4.85	1.28	1.22
37	Y	605	CHL	CHD-C1D	4.84	1.47	1.39
37	V	609	CHL	OBD-CAD	4.84	1.28	1.22
37	W	609	CHL	C3B-C2B	4.84	1.46	1.40
37	V	609	CHL	C3B-C2B	4.84	1.46	1.40
37	U	601	CHL	CHD-C1D	4.83	1.47	1.39
37	W	608	CHL	C3B-C2B	4.83	1.46	1.40
37	W	608	CHL	OBD-CAD	4.82	1.28	1.22
37	U	605	CHL	CHC-C1C	4.81	1.48	1.39
37	Z	609	CHL	CHD-C1D	4.81	1.47	1.39
37	Z	607	CHL	C3A-C2A	-4.80	1.50	1.54
37	Y	605	CHL	CHC-C1C	4.80	1.48	1.39
37	V	608	CHL	C3B-C2B	4.80	1.46	1.40
37	Z	609	CHL	C3B-C2B	4.80	1.46	1.40
37	V	606	CHL	CHB-C4A	-4.79	1.32	1.38
37	V	601	CHL	OBD-CAD	4.79	1.28	1.22
37	X	606	CHL	OBD-CAD	4.79	1.28	1.22
37	X	606	CHL	CHB-C1B	4.79	1.47	1.39
37	W	607	CHL	CHC-C1C	4.78	1.48	1.39
37	Y	608	CHL	CHC-C4B	4.78	1.47	1.39
37	Y	606	CHL	CHB-C4A	-4.77	1.32	1.38
37	U	605	CHL	CHD-C4C	4.77	1.48	1.39
37	Z	606	CHL	CHB-C4A	-4.77	1.32	1.38
37	X	607	CHL	C3B-C2B	4.77	1.46	1.40
37	U	601	CHL	C3B-C2B	4.76	1.46	1.40
37	X	609	CHL	CHB-C1B	4.76	1.47	1.39
37	X	609	CHL	C3B-C2B	4.75	1.46	1.40
37	X	609	CHL	CHD-C1D	4.75	1.47	1.39
37	W	609	CHL	CHD-C4C	4.74	1.48	1.39
37	Z	601	CHL	CHC-C4B	4.74	1.47	1.39
37	X	608	CHL	C3B-C2B	4.74	1.46	1.40
37	U	601	CHL	CHC-C4B	4.73	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	607	CHL	C3A-C2A	-4.72	1.50	1.54
37	U	601	CHL	CHB-C1B	4.72	1.47	1.39
37	W	607	CHL	CHD-C1D	4.72	1.47	1.39
37	U	609	CHL	C3A-C2A	-4.72	1.50	1.54
37	Z	605	CHL	CHC-C4B	4.71	1.47	1.39
37	W	607	CHL	C2C-C3C	4.70	1.46	1.37
37	Z	608	CHL	OBD-CAD	4.70	1.28	1.22
37	Y	601	CHL	CHB-C4A	-4.70	1.33	1.38
37	W	606	CHL	C3A-C2A	-4.69	1.50	1.54
37	W	608	CHL	CHC-C4B	4.69	1.47	1.39
37	V	607	CHL	CHB-C4A	-4.69	1.33	1.38
37	V	606	CHL	CHC-C4B	4.69	1.47	1.39
37	U	601	CHL	CHD-C4C	4.68	1.48	1.39
37	Z	608	CHL	CHB-C1B	4.68	1.47	1.39
37	U	607	CHL	CHC-C1C	4.68	1.48	1.39
37	X	609	CHL	CHD-C4C	4.68	1.48	1.39
37	U	608	CHL	CHC-C4B	4.67	1.47	1.39
37	W	601	CHL	CHB-C1B	4.67	1.47	1.39
37	U	606	CHL	OBD-CAD	4.66	1.28	1.22
37	W	607	CHL	CHD-C4C	4.66	1.48	1.39
37	Y	605	CHL	CHD-C4C	4.65	1.48	1.39
37	W	609	CHL	CHB-C4A	-4.65	1.33	1.38
37	W	609	CHL	CHB-C1B	4.65	1.47	1.39
37	Y	601	CHL	CHC-C1C	4.64	1.48	1.39
37	X	607	CHL	CHC-C4B	4.64	1.47	1.39
37	Y	609	CHL	CHD-C1D	4.64	1.47	1.39
37	W	608	CHL	CHD-C4C	4.62	1.48	1.39
37	Y	608	CHL	C3B-C2B	4.62	1.46	1.40
37	Z	609	CHL	CHD-C4C	4.62	1.48	1.39
37	W	609	CHL	CHC-C4B	4.62	1.47	1.39
37	X	609	CHL	C3A-C2A	-4.62	1.50	1.54
37	Z	605	CHL	CHB-C1B	4.61	1.47	1.39
37	U	606	CHL	CHC-C4B	4.61	1.47	1.39
37	Y	608	CHL	CHB-C4A	-4.60	1.33	1.38
37	Z	606	CHL	CHC-C1C	4.59	1.48	1.39
37	U	608	CHL	CHB-C4A	-4.59	1.33	1.38
37	Z	607	CHL	CHB-C1B	4.58	1.47	1.39
37	X	606	CHL	CHC-C1C	4.58	1.48	1.39
37	V	606	CHL	C3B-C2B	4.57	1.46	1.40
37	Y	609	CHL	CHD-C4C	4.57	1.48	1.39
37	U	609	CHL	CHB-C1B	4.57	1.47	1.39
37	Y	606	CHL	CHB-C1B	4.57	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	U	609	CHL	CHD-C1D	4.57	1.47	1.39
37	X	601	CHL	CHB-C1B	4.56	1.47	1.39
37	W	608	CHL	CHD-C1D	4.56	1.47	1.39
37	V	605	CHL	CHC-C1C	4.56	1.48	1.39
37	X	608	CHL	CHB-C1B	4.56	1.47	1.39
37	Y	609	CHL	OBD-CAD	4.56	1.28	1.22
37	W	601	CHL	CHC-C1C	4.56	1.48	1.39
37	V	607	CHL	CHC-C1C	4.55	1.48	1.39
37	U	608	CHL	OBD-CAD	4.55	1.28	1.22
37	U	608	CHL	C3B-C2B	4.55	1.46	1.40
37	V	609	CHL	CHD-C1D	4.55	1.47	1.39
37	V	605	CHL	CHD-C1D	4.55	1.47	1.39
37	V	608	CHL	CHB-C1B	4.54	1.47	1.39
37	W	605	CHL	O2A-CGA	4.54	1.45	1.30
37	X	608	CHL	CHC-C1C	4.54	1.48	1.39
37	W	601	CHL	CHD-C1D	4.53	1.47	1.39
37	V	607	CHL	CHB-C1B	4.53	1.47	1.39
37	V	607	CHL	O2A-CGA	4.53	1.45	1.30
37	Y	606	CHL	O2A-CGA	4.53	1.45	1.30
37	V	601	CHL	CHC-C1C	4.53	1.48	1.39
37	X	605	CHL	O2A-CGA	4.53	1.45	1.30
37	W	608	CHL	CHB-C1B	4.53	1.47	1.39
37	W	601	CHL	CHD-C4C	4.53	1.48	1.39
37	U	609	CHL	CHD-C4C	4.52	1.48	1.39
37	Z	606	CHL	CHB-C1B	4.52	1.46	1.39
37	V	609	CHL	CHB-C1B	4.52	1.46	1.39
37	U	608	CHL	CHC-C1C	4.52	1.48	1.39
37	V	606	CHL	OBD-CAD	4.51	1.28	1.22
37	W	605	CHL	CHB-C1B	4.51	1.46	1.39
37	V	608	CHL	OBD-CAD	4.51	1.28	1.22
37	Z	601	CHL	C3A-C2A	-4.50	1.50	1.54
37	Y	609	CHL	C3B-C2B	4.50	1.46	1.40
37	Y	606	CHL	CHC-C1C	4.50	1.48	1.39
37	Z	608	CHL	CHC-C1C	4.49	1.48	1.39
37	X	609	CHL	CHC-C4B	4.49	1.46	1.39
37	Z	601	CHL	CHB-C1B	4.49	1.46	1.39
37	W	606	CHL	O2A-CGA	4.49	1.45	1.30
37	U	606	CHL	CHB-C1B	4.49	1.46	1.39
37	X	608	CHL	CHD-C1D	4.48	1.46	1.39
37	X	601	CHL	CHC-C4B	4.48	1.46	1.39
37	V	601	CHL	CHD-C4C	4.48	1.48	1.39
37	V	609	CHL	CHD-C4C	4.48	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	601	CHL	C3B-C2B	4.47	1.46	1.40
37	Z	608	CHL	C3A-C2A	-4.47	1.50	1.54
37	V	601	CHL	CHB-C4A	-4.46	1.33	1.38
37	V	609	CHL	CHC-C4B	4.46	1.46	1.39
37	U	607	CHL	O2A-CGA	4.46	1.45	1.30
37	V	601	CHL	CHB-C1B	4.46	1.46	1.39
37	W	606	CHL	CHB-C1B	4.46	1.46	1.39
37	Y	607	CHL	CHB-C4A	-4.46	1.33	1.38
37	Z	608	CHL	CHD-C4C	4.46	1.47	1.39
37	V	601	CHL	CHD-C1D	4.46	1.46	1.39
37	Z	606	CHL	C3B-C2B	4.45	1.46	1.40
37	X	606	CHL	CHD-C4C	4.45	1.47	1.39
37	V	609	CHL	CHB-C4A	-4.45	1.33	1.38
37	Z	606	CHL	O2A-CGA	4.44	1.45	1.30
37	Y	607	CHL	CHB-C1B	4.44	1.46	1.39
37	U	608	CHL	CHB-C1B	4.44	1.46	1.39
37	Y	601	CHL	CHD-C4C	4.44	1.47	1.39
37	X	608	CHL	CHD-C4C	4.43	1.47	1.39
37	Z	606	CHL	CHD-C4C	4.43	1.47	1.39
37	U	606	CHL	CHB-C4A	-4.43	1.33	1.38
37	W	609	CHL	CHC-C1C	4.43	1.47	1.39
37	U	606	CHL	C3B-C2B	4.43	1.46	1.40
37	Z	607	CHL	CHB-C4A	-4.42	1.33	1.38
28	A	861	LHG	O8-C23	4.42	1.46	1.33
37	X	608	CHL	CHB-C4A	-4.42	1.33	1.38
37	Y	601	CHL	CHD-C1D	4.41	1.46	1.39
37	V	605	CHL	CHD-C4C	4.41	1.47	1.39
37	W	605	CHL	CHD-C4C	4.41	1.47	1.39
37	W	605	CHL	CHB-C4A	-4.40	1.33	1.38
37	Y	608	CHL	CHC-C1C	4.40	1.47	1.39
37	X	606	CHL	CHB-C4A	-4.40	1.33	1.38
37	W	608	CHL	CHB-C4A	-4.39	1.33	1.38
37	Z	606	CHL	OBD-CAD	4.39	1.28	1.22
37	Z	601	CHL	CHB-C4A	-4.38	1.33	1.38
37	V	608	CHL	CHB-C4A	-4.38	1.33	1.38
37	U	609	CHL	C3B-C2B	4.38	1.46	1.40
37	W	608	CHL	C3A-C2A	-4.38	1.50	1.54
37	V	608	CHL	CHC-C1C	4.38	1.47	1.39
37	W	605	CHL	CHD-C1D	4.38	1.46	1.39
37	W	601	CHL	O2A-CGA	4.38	1.46	1.33
37	U	608	CHL	CHD-C4C	4.37	1.47	1.39
37	Z	601	CHL	C3B-C2B	4.37	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	V	609	CHL	O2A-CGA	4.36	1.46	1.33
37	X	601	CHL	C3A-C2A	-4.36	1.50	1.54
37	Z	601	CHL	CHD-C4C	4.36	1.47	1.39
37	U	609	CHL	CHB-C4A	-4.36	1.33	1.38
37	Z	607	CHL	CHC-C1C	4.35	1.47	1.39
28	8	623	LHG	O8-C23	4.35	1.46	1.33
37	X	606	CHL	CHD-C1D	4.35	1.46	1.39
37	Z	608	CHL	CHD-C1D	4.34	1.46	1.39
37	Z	601	CHL	CHC-C1C	4.34	1.47	1.39
37	Y	608	CHL	CHD-C4C	4.33	1.47	1.39
37	U	606	CHL	CHC-C1C	4.33	1.47	1.39
37	Z	605	CHL	CHD-C1D	4.33	1.46	1.39
37	X	607	CHL	CHB-C4A	-4.33	1.33	1.38
37	Z	606	CHL	CHD-C1D	4.32	1.46	1.39
37	W	609	CHL	O2A-CGA	4.32	1.45	1.33
37	X	601	CHL	CHD-C1D	4.32	1.46	1.39
37	Y	601	CHL	CHB-C1B	4.32	1.46	1.39
37	U	607	CHL	CHD-C4C	4.32	1.47	1.39
37	Y	605	CHL	C3D-C2D	4.31	1.47	1.39
37	Y	606	CHL	C3B-C2B	4.31	1.46	1.40
37	Z	609	CHL	CHC-C4B	4.31	1.46	1.39
37	V	607	CHL	CHD-C1D	4.31	1.46	1.39
28	W	2630	LHG	O8-C23	4.31	1.45	1.33
37	Y	608	CHL	CHB-C1B	4.31	1.46	1.39
37	Y	601	CHL	O2A-CGA	4.30	1.45	1.33
32	L	2631	LMG	O8-C28	4.30	1.45	1.33
37	V	608	CHL	CHD-C4C	4.30	1.47	1.39
37	Y	601	CHL	C3A-C2A	-4.29	1.51	1.54
37	X	605	CHL	C3D-C2D	4.29	1.47	1.39
28	U	2630	LHG	O8-C23	4.29	1.45	1.33
37	X	601	CHL	CHD-C4C	4.29	1.47	1.39
37	U	605	CHL	C3D-C2D	4.29	1.47	1.39
37	Y	607	CHL	CHC-C4B	4.29	1.46	1.39
37	Z	601	CHL	O2A-CGA	4.29	1.45	1.33
37	Z	605	CHL	CHC-C1C	4.28	1.47	1.39
37	W	608	CHL	CHC-C1C	4.28	1.47	1.39
37	V	601	CHL	O2A-CGA	4.28	1.45	1.33
37	Z	605	CHL	CHD-C4C	4.28	1.47	1.39
37	X	607	CHL	CHB-C1B	4.27	1.46	1.39
37	Z	608	CHL	O2A-CGA	4.27	1.45	1.33
37	U	606	CHL	CHD-C4C	4.26	1.47	1.39
28	5	623	LHG	O7-C7	4.26	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	608	CHL	O2A-CGA	4.26	1.45	1.33
37	W	606	CHL	CHD-C1D	4.26	1.46	1.39
37	V	606	CHL	CHC-C1C	4.26	1.47	1.39
37	X	609	CHL	O2A-CGA	4.25	1.45	1.33
28	9	622	LHG	O7-C7	4.25	1.46	1.34
37	Y	608	CHL	O2A-CGA	4.25	1.45	1.33
32	4	623	LMG	O8-C28	4.25	1.45	1.33
37	U	609	CHL	O2A-CGA	4.25	1.45	1.33
37	V	608	CHL	O2A-CGA	4.25	1.45	1.33
37	U	601	CHL	CHC-C1C	4.24	1.47	1.39
37	Y	609	CHL	CHC-C4B	4.24	1.46	1.39
28	9	624	LHG	O8-C23	4.24	1.45	1.33
37	U	608	CHL	CHD-C1D	4.24	1.46	1.39
37	Y	606	CHL	CHD-C4C	4.24	1.47	1.39
32	4	624	LMG	O8-C28	4.24	1.45	1.33
37	W	609	CHL	C3A-C2A	-4.23	1.51	1.54
37	Y	609	CHL	O2A-CGA	4.23	1.45	1.33
36	5	624	NEX	C7-C8	-4.22	1.25	1.31
37	Z	601	CHL	CHD-C1D	4.22	1.46	1.39
37	X	607	CHL	CHC-C1C	4.22	1.47	1.39
37	Z	609	CHL	CHC-C1C	4.22	1.47	1.39
28	V	2630	LHG	O8-C23	4.21	1.45	1.33
37	W	605	CHL	CHC-C1C	4.21	1.47	1.39
32	4	623	LMG	O7-C10	4.21	1.46	1.34
37	Z	609	CHL	CHB-C1B	4.21	1.46	1.39
37	U	607	CHL	CHB-C1B	4.21	1.46	1.39
37	Z	607	CHL	O2A-CGA	4.20	1.45	1.33
37	X	607	CHL	O2A-CGA	4.20	1.45	1.33
37	W	607	CHL	CHB-C4A	-4.20	1.33	1.38
32	5	627	LMG	O8-C28	4.20	1.45	1.33
37	U	601	CHL	O2A-CGA	4.20	1.45	1.33
37	Z	605	CHL	CHB-C4A	-4.20	1.33	1.38
37	W	605	CHL	C3A-C2A	-4.20	1.51	1.54
32	9	625	LMG	O8-C28	4.19	1.45	1.33
37	W	606	CHL	CHD-C4C	4.19	1.47	1.39
28	W	2630	LHG	O7-C7	4.19	1.46	1.34
37	W	606	CHL	CHB-C4A	-4.19	1.33	1.38
37	V	607	CHL	CHD-C4C	4.19	1.47	1.39
37	X	601	CHL	O2A-CGA	4.18	1.45	1.33
28	O	2631	LHG	O8-C23	4.17	1.45	1.33
28	H	204	LHG	O8-C23	4.17	1.45	1.33
28	Z	2630	LHG	O8-C23	4.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	847	LHG	O8-C23	4.17	1.45	1.33
28	X	2630	LHG	O8-C23	4.17	1.45	1.33
37	Y	606	CHL	OBD-CAD	4.17	1.27	1.22
37	Z	607	CHL	CHD-C1D	4.16	1.46	1.39
37	Z	609	CHL	O2A-CGA	4.16	1.45	1.33
37	V	605	CHL	C3A-C2A	-4.16	1.51	1.54
37	U	606	CHL	CHD-C1D	4.16	1.46	1.39
37	V	606	CHL	CHB-C1B	4.16	1.46	1.39
37	W	607	CHL	O2A-CGA	4.16	1.45	1.33
32	8	626	LMG	O8-C28	4.16	1.45	1.33
37	U	607	CHL	CHD-C1D	4.15	1.46	1.39
37	W	601	CHL	CHB-C4A	-4.15	1.33	1.38
28	9	623	LHG	O8-C23	4.15	1.45	1.33
28	2	622	LHG	O7-C7	4.14	1.46	1.34
28	9	624	LHG	O7-C7	4.14	1.46	1.34
37	Y	607	CHL	CHC-C1C	4.13	1.47	1.39
28	B	851	LHG	O8-C23	4.13	1.45	1.33
37	Y	607	CHL	O2A-CGA	4.13	1.45	1.33
37	X	601	CHL	CHB-C4A	-4.12	1.33	1.38
28	3	624	LHG	O8-C23	4.12	1.45	1.33
37	Z	608	CHL	CHB-C4A	-4.12	1.33	1.38
37	Y	606	CHL	CHD-C1D	4.11	1.46	1.39
32	J	103	LMG	O8-C28	4.11	1.45	1.33
37	Z	607	CHL	CHD-C4C	4.11	1.47	1.39
28	U	2630	LHG	O7-C7	4.11	1.45	1.34
37	W	608	CHL	O2A-CGA	4.10	1.45	1.33
37	X	609	CHL	CHC-C1C	4.10	1.47	1.39
37	V	609	CHL	CHC-C1C	4.09	1.47	1.39
37	Y	609	CHL	CHB-C1B	4.09	1.46	1.39
37	V	606	CHL	CHD-C1D	4.09	1.46	1.39
37	U	601	CHL	C3D-C2D	4.09	1.46	1.39
37	Y	608	CHL	CHD-C1D	4.09	1.46	1.39
37	X	607	CHL	CHD-C4C	4.09	1.47	1.39
37	X	601	CHL	CHC-C1C	4.08	1.47	1.39
37	X	609	CHL	CHB-C4A	-4.08	1.33	1.38
37	X	608	CHL	C3A-C2A	-4.08	1.51	1.54
37	W	606	CHL	CHC-C4B	4.08	1.46	1.39
28	Y	2630	LHG	O8-C23	4.07	1.45	1.33
37	X	606	CHL	C3D-C2D	4.07	1.46	1.39
32	V	2631	LMG	O8-C28	4.06	1.45	1.33
37	V	605	CHL	C3D-C2D	4.06	1.46	1.39
32	J	104	LMG	O8-C28	4.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	851	LHG	O7-C7	4.06	1.45	1.34
37	V	606	CHL	CHD-C4C	4.05	1.47	1.39
37	Y	607	CHL	CHD-C4C	4.05	1.47	1.39
28	5	625	LHG	O8-C23	4.05	1.45	1.33
37	Y	609	CHL	C3D-C2D	4.05	1.46	1.39
37	X	607	CHL	CHD-C1D	4.05	1.46	1.39
33	B	850	DGD	O1G-C1A	4.04	1.45	1.33
28	Y	2630	LHG	O7-C7	4.04	1.45	1.34
37	W	606	CHL	C3B-C2B	4.04	1.45	1.40
28	X	2630	LHG	O7-C7	4.03	1.45	1.34
28	6	623	LHG	O8-C23	4.03	1.45	1.33
32	4	624	LMG	O7-C10	4.03	1.45	1.34
28	5	623	LHG	O8-C23	4.02	1.45	1.33
28	4	622	LHG	O8-C23	4.01	1.45	1.33
28	H	204	LHG	O7-C7	4.01	1.45	1.34
28	a	620	LHG	O7-C7	4.01	1.45	1.34
28	8	623	LHG	O7-C7	4.01	1.45	1.34
28	8	622	LHG	O7-C7	4.01	1.45	1.34
28	4	622	LHG	O7-C7	4.00	1.45	1.34
32	H	205	LMG	O7-C10	4.00	1.45	1.34
28	1	620	LHG	O7-C7	4.00	1.45	1.34
32	A	860	LMG	O8-C28	4.00	1.45	1.33
28	A	861	LHG	O7-C7	4.00	1.45	1.34
37	U	609	CHL	CHC-C4B	3.99	1.46	1.39
32	V	2631	LMG	O7-C10	3.98	1.45	1.34
28	Z	2630	LHG	O7-C7	3.98	1.45	1.34
28	9	622	LHG	O8-C23	3.98	1.45	1.33
37	V	605	CHL	CHB-C4A	-3.98	1.33	1.38
37	Y	609	CHL	CHC-C1C	3.98	1.47	1.39
37	U	601	CHL	CHB-C4A	-3.98	1.33	1.38
28	a	620	LHG	O8-C23	3.98	1.44	1.33
28	1	620	LHG	O8-C23	3.98	1.44	1.33
37	X	609	CHL	C3D-C2D	3.98	1.46	1.39
28	V	2630	LHG	O7-C7	3.97	1.45	1.34
28	O	2631	LHG	O7-C7	3.97	1.45	1.34
28	A	846	LHG	O8-C23	3.97	1.44	1.33
32	9	625	LMG	O7-C10	3.96	1.45	1.34
28	5	625	LHG	O7-C7	3.96	1.45	1.34
32	A	860	LMG	O7-C10	3.95	1.45	1.34
28	3	624	LHG	O7-C7	3.95	1.45	1.34
32	H	205	LMG	O8-C28	3.95	1.44	1.33
37	W	608	CHL	C3D-C2D	3.95	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	V	608	CHL	CHD-C1D	3.95	1.46	1.39
28	7	622	LHG	O8-C23	3.94	1.44	1.33
28	3	623	LHG	O8-C23	3.94	1.44	1.33
32	J	103	LMG	O7-C10	3.93	1.45	1.34
32	5	627	LMG	O7-C10	3.93	1.45	1.34
37	Y	607	CHL	CHD-C1D	3.92	1.46	1.39
28	6	623	LHG	O7-C7	3.92	1.45	1.34
32	J	104	LMG	O7-C10	3.91	1.45	1.34
37	U	601	CHL	C3A-C2A	-3.91	1.51	1.54
37	W	605	CHL	C3D-C2D	3.90	1.46	1.39
28	A	846	LHG	O7-C7	3.89	1.45	1.34
28	9	623	LHG	O7-C7	3.89	1.45	1.34
37	U	605	CHL	CHB-C4A	-3.89	1.33	1.38
32	8	626	LMG	O7-C10	3.89	1.45	1.34
28	2	622	LHG	O8-C23	3.87	1.44	1.33
37	W	609	CHL	C3D-C2D	3.87	1.46	1.39
37	Y	607	CHL	C3D-C2D	3.86	1.46	1.39
28	8	622	LHG	O8-C23	3.86	1.44	1.33
28	7	622	LHG	O7-C7	3.85	1.45	1.34
37	V	601	CHL	C3D-C2D	3.84	1.46	1.39
37	U	609	CHL	C3D-C2D	3.84	1.46	1.39
37	W	601	CHL	C3D-C2D	3.84	1.46	1.39
28	3	623	LHG	O7-C7	3.82	1.45	1.34
37	Y	606	CHL	C3D-C2D	3.81	1.46	1.39
37	Z	609	CHL	C3D-C2D	3.81	1.46	1.39
37	U	607	CHL	C3A-C2A	-3.80	1.51	1.54
37	V	607	CHL	C3A-C2A	-3.79	1.51	1.54
32	L	2631	LMG	O7-C10	3.79	1.45	1.34
26	Z	604	CLA	CAD-C3D	-3.78	1.44	1.50
37	W	606	CHL	CHC-C1C	3.78	1.46	1.39
37	V	607	CHL	C3D-C2D	3.78	1.46	1.39
37	V	609	CHL	C3D-C2D	3.76	1.46	1.39
37	Y	601	CHL	C3D-C2D	3.75	1.46	1.39
37	W	601	CHL	C3A-C2A	-3.74	1.51	1.54
26	X	604	CLA	C1D-ND	3.74	1.42	1.37
37	Y	605	CHL	CHB-C4A	-3.74	1.34	1.38
37	W	607	CHL	C3D-C2D	3.72	1.46	1.39
37	U	609	CHL	CHC-C1C	3.72	1.46	1.39
33	B	850	DGD	O2G-C1B	3.71	1.44	1.34
37	X	601	CHL	C3D-C2D	3.70	1.46	1.39
37	Z	601	CHL	C3D-C2D	3.70	1.46	1.39
37	Z	605	CHL	C3D-C2D	3.68	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z	614	CLA	C1D-ND	3.67	1.42	1.37
28	A	847	LHG	O7-C7	3.66	1.44	1.34
37	X	605	CHL	CHB-C4A	-3.65	1.34	1.38
26	V	611	CLA	C1D-ND	3.64	1.42	1.37
37	U	606	CHL	C3D-C2D	3.64	1.45	1.39
26	X	603	CLA	C1D-ND	3.63	1.42	1.37
37	Z	606	CHL	C3D-C2D	3.63	1.45	1.39
37	U	607	CHL	C3D-C2D	3.62	1.45	1.39
37	X	607	CHL	C3D-C2D	3.62	1.45	1.39
36	6	624	NEX	C7-C6	-3.62	1.26	1.30
26	U	604	CLA	CAD-C3D	-3.62	1.45	1.50
26	U	610	CLA	C1D-ND	3.62	1.42	1.37
37	W	607	CHL	C3A-C2A	-3.61	1.51	1.54
26	X	610	CLA	C1D-ND	3.61	1.42	1.37
26	U	612	CLA	C1D-ND	3.60	1.42	1.37
26	Y	611	CLA	C1D-ND	3.60	1.42	1.37
26	Y	614	CLA	C1D-ND	3.60	1.42	1.37
36	6	624	NEX	C7-C8	-3.60	1.26	1.31
26	X	612	CLA	C1D-ND	3.60	1.42	1.37
37	Y	608	CHL	C3D-C2D	3.59	1.45	1.39
26	X	614	CLA	C1D-ND	3.59	1.42	1.37
26	8	616	CLA	C1D-ND	3.59	1.42	1.37
26	U	611	CLA	C1D-ND	3.59	1.42	1.37
26	W	604	CLA	C1D-ND	3.58	1.42	1.37
31	5	629	LMU	O5B-C1B	3.57	1.51	1.41
37	U	608	CHL	C3D-C2D	3.57	1.45	1.39
26	U	614	CLA	C1D-ND	3.56	1.42	1.37
36	Y	1623	NEX	C7-C8	-3.55	1.26	1.31
26	Y	603	CLA	C1D-ND	3.55	1.42	1.37
26	9	603	CLA	CAB-C3B	-3.54	1.43	1.50
26	W	612	CLA	C1D-ND	3.54	1.42	1.37
37	W	606	CHL	C3D-C2D	3.53	1.45	1.39
26	V	610	CLA	C1D-ND	3.52	1.42	1.37
26	Y	612	CLA	C1D-ND	3.52	1.42	1.37
37	Y	605	CHL	C2A-C3A	-3.51	1.51	1.54
36	Z	1623	NEX	C7-C6	-3.50	1.26	1.30
37	Z	607	CHL	C3D-C2D	3.50	1.45	1.39
26	Y	604	CLA	C1D-ND	3.50	1.42	1.37
26	W	611	CLA	C1D-ND	3.48	1.42	1.37
26	Z	612	CLA	C1D-ND	3.48	1.42	1.37
26	U	603	CLA	C1D-ND	3.48	1.42	1.37
37	V	606	CHL	C3D-C2D	3.47	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	101	CLA	C1D-ND	3.47	1.42	1.37
26	Y	602	CLA	C1D-ND	3.46	1.42	1.37
37	Z	608	CHL	C3D-C2D	3.46	1.45	1.39
26	Z	604	CLA	C1D-ND	3.45	1.42	1.37
26	X	604	CLA	C4B-NB	3.44	1.42	1.37
26	3	612	CLA	C4B-NB	3.43	1.42	1.37
26	5	611	CLA	C1D-ND	3.43	1.42	1.37
37	U	605	CHL	C3A-C2A	-3.42	1.51	1.54
26	9	612	CLA	C1D-ND	3.42	1.42	1.37
26	V	602	CLA	C1D-ND	3.42	1.42	1.37
26	W	610	CLA	C1D-ND	3.42	1.42	1.37
26	Y	604	CLA	C4B-NB	3.42	1.42	1.37
26	Y	610	CLA	C4B-NB	3.42	1.42	1.37
36	Y	1623	NEX	C7-C6	-3.42	1.26	1.30
26	V	603	CLA	C1D-ND	3.42	1.42	1.37
26	V	614	CLA	C1D-ND	3.42	1.42	1.37
26	W	602	CLA	C1D-ND	3.40	1.42	1.37
26	X	611	CLA	C1D-ND	3.40	1.42	1.37
26	9	611	CLA	C1D-ND	3.40	1.42	1.37
37	V	608	CHL	C3D-C2D	3.40	1.45	1.39
31	K	208	LMU	O5B-C1B	3.39	1.50	1.41
26	X	610	CLA	C4B-NB	3.39	1.42	1.37
26	Z	603	CLA	C1D-ND	3.39	1.42	1.37
26	U	602	CLA	C1D-ND	3.38	1.42	1.37
31	5	628	LMU	O5B-C1B	3.38	1.50	1.41
26	V	612	CLA	C1D-ND	3.38	1.42	1.37
26	B	811	CLA	CAD-C3D	-3.38	1.45	1.50
37	X	605	CHL	C3A-C2A	-3.37	1.51	1.54
26	1	614	CLA	C1D-ND	3.36	1.42	1.37
26	L	302	CLA	CMB-C2B	-3.36	1.43	1.50
26	U	613	CLA	C4B-NB	3.36	1.42	1.37
26	6	608	CLA	C1D-ND	3.35	1.42	1.37
26	9	610	CLA	C4B-NB	3.35	1.42	1.37
26	U	613	CLA	C1D-ND	3.35	1.42	1.37
26	8	616	CLA	CAB-C3B	-3.35	1.43	1.50
26	V	604	CLA	C1D-ND	3.35	1.42	1.37
26	W	604	CLA	C4B-NB	3.35	1.42	1.37
26	9	614	CLA	C4B-NB	3.35	1.42	1.37
26	U	604	CLA	C1D-ND	3.35	1.42	1.37
26	5	604	CLA	C1D-ND	3.34	1.42	1.37
26	Y	612	CLA	C4B-NB	3.34	1.42	1.37
26	W	614	CLA	C1D-ND	3.34	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	609	CLA	C1D-ND	3.34	1.42	1.37
26	4	611	CLA	C1D-ND	3.33	1.42	1.37
26	5	601	CLA	C1D-ND	3.33	1.42	1.37
26	4	602	CLA	C4B-NB	3.33	1.42	1.37
26	1	607	CLA	C4B-NB	3.32	1.42	1.37
36	Z	1623	NEX	C7-C8	-3.32	1.26	1.31
26	X	602	CLA	C1D-ND	3.32	1.42	1.37
26	4	612	CLA	C1D-ND	3.32	1.42	1.37
26	6	618	CLA	C1D-ND	3.32	1.42	1.37
26	O	2002	CLA	CAB-C3B	-3.31	1.44	1.50
26	1	616	CLA	C1D-ND	3.31	1.42	1.37
26	4	604	CLA	C1D-ND	3.31	1.42	1.37
26	8	607	CLA	CAB-C3B	-3.31	1.44	1.50
26	W	603	CLA	C1D-ND	3.30	1.42	1.37
26	7	615	CLA	CAB-C3B	-3.30	1.44	1.50
26	5	616	CLA	CAB-C3B	-3.30	1.44	1.50
26	a	614	CLA	C1D-ND	3.30	1.42	1.37
26	6	607	CLA	CAB-C3B	-3.30	1.44	1.50
26	W	613	CLA	C4B-NB	3.29	1.42	1.37
26	2	602	CLA	C4B-C3B	3.29	1.48	1.38
26	5	603	CLA	CAB-C3B	-3.29	1.44	1.50
26	4	603	CLA	CAB-C3B	-3.29	1.44	1.50
26	Y	613	CLA	C1D-ND	3.29	1.42	1.37
26	X	603	CLA	C4B-NB	3.28	1.42	1.37
26	3	609	CLA	C1D-ND	3.28	1.42	1.37
26	Z	610	CLA	C4B-NB	3.28	1.42	1.37
26	6	612	CLA	C1D-ND	3.28	1.42	1.37
26	9	601	CLA	C1D-ND	3.28	1.42	1.37
26	U	604	CLA	C4B-NB	3.28	1.42	1.37
26	Z	613	CLA	C1D-ND	3.28	1.42	1.37
26	V	611	CLA	C4B-NB	3.28	1.42	1.37
31	A	858	LMU	O5B-C1B	3.28	1.50	1.41
26	1	604	CLA	C1D-ND	3.28	1.42	1.37
26	2	612	CLA	C1D-ND	3.28	1.42	1.37
26	3	607	CLA	CAB-C3B	-3.27	1.44	1.50
26	8	603	CLA	CAB-C3B	-3.27	1.44	1.50
26	a	604	CLA	C1D-ND	3.27	1.42	1.37
26	2	616	CLA	CAB-C3B	-3.27	1.44	1.50
26	7	616	CLA	CAB-C3B	-3.27	1.44	1.50
31	A	858	LMU	O5'-C1'	3.27	1.50	1.41
26	4	618	CLA	CAB-C3B	-3.26	1.44	1.50
26	5	614	CLA	C1D-ND	3.26	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	619	CLA	CAB-C3B	-3.26	1.44	1.50
26	Y	610	CLA	C1D-ND	3.26	1.42	1.37
26	4	613	CLA	C4B-NB	3.26	1.42	1.37
26	4	604	CLA	CAB-C3B	-3.26	1.44	1.50
26	1	608	CLA	C1D-ND	3.26	1.42	1.37
26	9	614	CLA	C1D-ND	3.26	1.42	1.37
26	6	604	CLA	C1D-ND	3.25	1.42	1.37
26	a	608	CLA	C1D-ND	3.25	1.42	1.37
26	Z	604	CLA	C4B-NB	3.25	1.42	1.37
26	1	606	CLA	C1D-ND	3.25	1.42	1.37
26	U	611	CLA	C4B-NB	3.25	1.42	1.37
31	1	621	LMU	O5'-C1'	3.25	1.50	1.41
26	6	603	CLA	CAB-C3B	-3.24	1.44	1.50
26	F	304	CLA	C1D-ND	3.24	1.42	1.37
31	8	625	LMU	O5B-C1B	3.24	1.50	1.41
26	a	607	CLA	C4B-NB	3.24	1.42	1.37
26	3	612	CLA	C1D-ND	3.24	1.42	1.37
26	X	613	CLA	C1D-ND	3.24	1.42	1.37
26	V	613	CLA	C1D-ND	3.24	1.42	1.37
26	5	610	CLA	C4B-NB	3.24	1.42	1.37
26	W	602	CLA	C4B-NB	3.23	1.42	1.37
26	9	611	CLA	C4B-NB	3.23	1.42	1.37
26	W	614	CLA	C4B-NB	3.23	1.42	1.37
26	2	602	CLA	C4D-ND	-3.23	1.32	1.37
26	4	608	CLA	C1D-ND	3.22	1.42	1.37
26	4	610	CLA	C1D-ND	3.22	1.42	1.37
26	6	610	CLA	C4B-NB	3.22	1.42	1.37
26	B	811	CLA	CAB-C3B	-3.22	1.44	1.50
27	B	842	PQN	C11-C12	3.22	1.55	1.50
31	8	625	LMU	O5'-C1'	3.22	1.50	1.41
26	K	206	CLA	C1D-ND	3.22	1.42	1.37
26	9	612	CLA	C4B-NB	3.22	1.42	1.37
26	5	619	CLA	C1D-ND	3.22	1.42	1.37
26	a	616	CLA	C1D-ND	3.21	1.42	1.37
26	5	604	CLA	CAB-C3B	-3.21	1.44	1.50
26	6	611	CLA	C1D-ND	3.21	1.42	1.37
26	3	611	CLA	C1D-ND	3.21	1.42	1.37
26	B	829	CLA	CMB-C2B	-3.20	1.44	1.50
26	9	604	CLA	CAB-C3B	-3.20	1.44	1.50
26	1	616	CLA	CAB-C3B	-3.20	1.44	1.50
26	4	614	CLA	C1D-ND	3.20	1.42	1.37
31	A	857	LMU	O5B-C1B	3.20	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	611	CLA	C4B-NB	3.20	1.42	1.37
26	1	610	CLA	C1D-ND	3.19	1.42	1.37
26	9	613	CLA	C1D-ND	3.19	1.42	1.37
26	a	611	CLA	CAB-C3B	-3.19	1.44	1.50
26	B	830	CLA	C4B-NB	3.19	1.42	1.37
26	Z	612	CLA	C4B-NB	3.18	1.42	1.37
31	1	621	LMU	O5B-C1B	3.18	1.50	1.41
26	A	837	CLA	CMB-C2B	-3.18	1.44	1.50
26	H	202	CLA	C1D-ND	3.18	1.42	1.37
26	a	601	CLA	C1D-ND	3.18	1.42	1.37
26	4	618	CLA	C4B-NB	3.18	1.42	1.37
26	5	618	CLA	CAB-C3B	-3.18	1.44	1.50
26	4	616	CLA	CAB-C3B	-3.18	1.44	1.50
31	K	208	LMU	O5'-C1'	3.17	1.50	1.41
26	K	206	CLA	C4B-NB	3.17	1.42	1.37
26	5	618	CLA	C1D-ND	3.17	1.42	1.37
26	Z	611	CLA	CAB-C3B	-3.17	1.44	1.50
26	X	613	CLA	C4B-NB	3.17	1.42	1.37
26	Y	613	CLA	C4B-NB	3.17	1.42	1.37
26	5	612	CLA	C1D-ND	3.17	1.42	1.37
26	1	609	CLA	CAB-C3B	-3.17	1.44	1.50
26	W	611	CLA	C4B-NB	3.16	1.42	1.37
26	X	614	CLA	C4B-NB	3.16	1.42	1.37
26	6	618	CLA	CAB-C3B	-3.16	1.44	1.50
26	V	612	CLA	C4B-NB	3.16	1.42	1.37
31	5	628	LMU	O5'-C1'	3.16	1.50	1.41
26	6	613	CLA	C4B-NB	3.16	1.42	1.37
26	Z	614	CLA	C4B-NB	3.16	1.42	1.37
26	3	611	CLA	CAB-C3B	-3.15	1.44	1.50
26	1	613	CLA	C1D-ND	3.15	1.42	1.37
26	7	615	CLA	C1D-ND	3.15	1.42	1.37
31	5	629	LMU	O5'-C1'	3.15	1.49	1.41
26	F	304	CLA	C4B-NB	3.15	1.42	1.37
26	6	614	CLA	C1D-ND	3.15	1.42	1.37
26	Z	613	CLA	C4B-NB	3.15	1.42	1.37
26	K	201	CLA	C1D-ND	3.14	1.42	1.37
26	6	606	CLA	C1D-ND	3.14	1.42	1.37
26	4	607	CLA	C1D-ND	3.14	1.42	1.37
26	W	610	CLA	C4B-NB	3.14	1.42	1.37
26	7	603	CLA	C1D-ND	3.14	1.42	1.37
26	3	610	CLA	C4B-NB	3.14	1.42	1.37
26	2	616	CLA	C1D-ND	3.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	X	602	CLA	C4B-NB	3.13	1.42	1.37
26	a	606	CLA	C4B-NB	3.13	1.42	1.37
26	4	618	CLA	C1D-ND	3.13	1.42	1.37
26	4	607	CLA	C4B-NB	3.13	1.42	1.37
26	a	606	CLA	C1D-ND	3.13	1.42	1.37
26	1	611	CLA	C1D-ND	3.13	1.42	1.37
26	4	616	CLA	C4B-NB	3.13	1.42	1.37
26	U	614	CLA	C4B-NB	3.13	1.42	1.37
26	a	613	CLA	C1D-ND	3.12	1.42	1.37
26	2	604	CLA	C1D-ND	3.12	1.42	1.37
26	Z	602	CLA	C1D-ND	3.12	1.42	1.37
26	5	609	CLA	C1D-ND	3.12	1.42	1.37
31	A	857	LMU	O5'-C1'	3.12	1.49	1.41
26	G	204	CLA	C1D-ND	3.12	1.42	1.37
26	B	830	CLA	C1D-ND	3.12	1.42	1.37
26	a	611	CLA	C1D-ND	3.12	1.42	1.37
26	V	614	CLA	C4B-NB	3.12	1.42	1.37
26	7	610	CLA	C4B-NB	3.11	1.42	1.37
26	5	608	CLA	C1D-ND	3.11	1.41	1.37
26	6	607	CLA	C4B-NB	3.11	1.41	1.37
26	2	611	CLA	C1D-ND	3.11	1.41	1.37
26	3	614	CLA	C1D-ND	3.11	1.41	1.37
26	Z	610	CLA	C1D-ND	3.11	1.41	1.37
26	1	606	CLA	C4B-NB	3.11	1.41	1.37
26	G	203	CLA	C1D-ND	3.11	1.41	1.37
26	X	611	CLA	C4B-NB	3.11	1.41	1.37
26	W	613	CLA	C1D-ND	3.10	1.41	1.37
26	8	606	CLA	C1D-ND	3.10	1.41	1.37
26	9	609	CLA	C1D-ND	3.10	1.41	1.37
26	V	603	CLA	C4B-NB	3.10	1.41	1.37
26	G	204	CLA	C4B-NB	3.10	1.41	1.37
29	O	2005	BCR	C30-C25	-3.10	1.49	1.53
26	A	822	CLA	C1D-ND	3.10	1.41	1.37
26	1	601	CLA	C1D-ND	3.10	1.41	1.37
26	6	603	CLA	C1D-ND	3.10	1.41	1.37
26	U	612	CLA	C4B-NB	3.10	1.41	1.37
26	O	2003	CLA	C1D-ND	3.10	1.41	1.37
26	Y	614	CLA	C4B-NB	3.09	1.41	1.37
26	8	601	CLA	C1D-ND	3.09	1.41	1.37
26	X	612	CLA	C4B-NB	3.09	1.41	1.37
26	K	203	CLA	C1D-ND	3.09	1.41	1.37
26	a	610	CLA	C1D-ND	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	610	CLA	C1D-ND	3.09	1.41	1.37
26	8	604	CLA	C1D-ND	3.09	1.41	1.37
26	8	607	CLA	C4B-NB	3.09	1.41	1.37
26	U	602	CLA	C4B-NB	3.08	1.41	1.37
26	2	614	CLA	C1D-ND	3.08	1.41	1.37
26	a	607	CLA	C1D-ND	3.08	1.41	1.37
26	1	614	CLA	CAB-C3B	-3.08	1.44	1.50
26	V	604	CLA	C4B-NB	3.08	1.41	1.37
26	H	203	CLA	C1D-ND	3.07	1.41	1.37
26	1	607	CLA	C1D-ND	3.07	1.41	1.37
26	5	619	CLA	C4B-NB	3.07	1.41	1.37
26	2	609	CLA	C4B-NB	3.07	1.41	1.37
26	6	617	CLA	C1D-ND	3.07	1.41	1.37
29	4	621	BCR	C30-C25	-3.06	1.49	1.53
26	O	2002	CLA	C1D-ND	3.06	1.41	1.37
26	6	613	CLA	C1D-ND	3.06	1.41	1.37
26	A	817	CLA	C1D-ND	3.06	1.41	1.37
26	B	840	CLA	C1D-ND	3.06	1.41	1.37
26	3	614	CLA	C4B-NB	3.06	1.41	1.37
29	K	207	BCR	C30-C25	-3.06	1.49	1.53
26	Z	611	CLA	C4B-NB	3.06	1.41	1.37
26	5	603	CLA	C4B-NB	3.06	1.41	1.37
26	2	603	CLA	C4B-NB	3.06	1.41	1.37
26	8	603	CLA	C1D-ND	3.06	1.41	1.37
26	7	612	CLA	C1D-ND	3.05	1.41	1.37
26	7	616	CLA	C1D-ND	3.05	1.41	1.37
26	5	604	CLA	C4B-NB	3.05	1.41	1.37
26	4	613	CLA	C1D-ND	3.04	1.41	1.37
26	Y	603	CLA	C4B-NB	3.04	1.41	1.37
26	B	822	CLA	C1D-ND	3.04	1.41	1.37
26	U	603	CLA	C4B-NB	3.04	1.41	1.37
26	a	609	CLA	C1D-ND	3.04	1.41	1.37
26	L	304	CLA	C1D-ND	3.04	1.41	1.37
26	O	2001	CLA	C4B-NB	3.04	1.41	1.37
26	F	303	CLA	C4B-NB	3.04	1.41	1.37
26	8	611	CLA	C1D-ND	3.04	1.41	1.37
26	a	612	CLA	C4B-NB	3.03	1.41	1.37
26	2	609	CLA	C1D-ND	3.03	1.41	1.37
26	a	616	CLA	C4B-NB	3.03	1.41	1.37
26	9	604	CLA	C1D-ND	3.03	1.41	1.37
26	W	603	CLA	C4B-NB	3.03	1.41	1.37
26	A	801	CLA	C1D-ND	3.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	618	CLA	C4B-NB	3.03	1.41	1.37
26	1	603	CLA	C1D-ND	3.02	1.41	1.37
27	A	844	PQN	C11-C12	3.02	1.55	1.50
26	9	604	CLA	C4B-NB	3.02	1.41	1.37
26	4	616	CLA	C1D-ND	3.02	1.41	1.37
26	6	620	CLA	C1D-ND	3.02	1.41	1.37
26	4	612	CLA	C4B-NB	3.01	1.41	1.37
26	9	601	CLA	C4B-NB	3.01	1.41	1.37
26	3	611	CLA	C4B-NB	3.01	1.41	1.37
26	5	606	CLA	C4B-NB	3.01	1.41	1.37
26	5	612	CLA	C4B-NB	3.01	1.41	1.37
26	3	607	CLA	C1D-ND	3.01	1.41	1.37
26	4	610	CLA	C4B-NB	3.01	1.41	1.37
26	7	602	CLA	C4B-NB	3.01	1.41	1.37
26	Z	602	CLA	C4B-NB	3.01	1.41	1.37
26	O	2002	CLA	C4B-NB	3.00	1.41	1.37
26	1	609	CLA	C1D-ND	3.00	1.41	1.37
26	2	606	CLA	C1D-ND	3.00	1.41	1.37
26	8	609	CLA	C1D-ND	3.00	1.41	1.37
26	8	614	CLA	CMD-C2D	-3.00	1.44	1.50
26	B	808	CLA	C4B-NB	3.00	1.41	1.37
26	2	616	CLA	C4B-NB	3.00	1.41	1.37
26	2	614	CLA	C4B-NB	3.00	1.41	1.37
26	1	608	CLA	C4B-NB	2.99	1.41	1.37
26	B	807	CLA	CMD-C2D	-2.99	1.44	1.50
26	1	604	CLA	C4B-NB	2.99	1.41	1.37
26	L	307	CLA	C1D-ND	2.99	1.41	1.37
26	a	611	CLA	C4B-NB	2.99	1.41	1.37
26	Y	602	CLA	C4B-NB	2.99	1.41	1.37
26	2	610	CLA	C4B-NB	2.98	1.41	1.37
26	4	606	CLA	C1D-ND	2.98	1.41	1.37
26	5	610	CLA	C1D-ND	2.98	1.41	1.37
26	Z	611	CLA	C1D-ND	2.98	1.41	1.37
26	6	608	CLA	C4B-NB	2.98	1.41	1.37
26	F	303	CLA	C1D-ND	2.98	1.41	1.37
26	B	831	CLA	C1D-ND	2.98	1.41	1.37
26	4	614	CLA	C4B-NB	2.98	1.41	1.37
26	8	607	CLA	C1D-ND	2.98	1.41	1.37
26	a	603	CLA	C1D-ND	2.98	1.41	1.37
26	7	615	CLA	C4B-NB	2.98	1.41	1.37
26	6	616	CLA	C1D-ND	2.97	1.41	1.37
26	V	613	CLA	C4B-NB	2.97	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	613	CLA	C4B-NB	2.97	1.41	1.37
26	1	611	CLA	C4B-NB	2.97	1.41	1.37
26	A	803	CLA	CMB-C2B	-2.97	1.44	1.50
26	B	821	CLA	C1D-ND	2.97	1.41	1.37
26	1	612	CLA	C4B-NB	2.97	1.41	1.37
26	1	616	CLA	C4B-NB	2.96	1.41	1.37
26	6	609	CLA	C1D-ND	2.96	1.41	1.37
26	a	602	CLA	C1D-ND	2.96	1.41	1.37
26	8	601	CLA	C4B-NB	2.96	1.41	1.37
26	8	610	CLA	C1D-ND	2.96	1.41	1.37
26	V	602	CLA	C4B-NB	2.96	1.41	1.37
37	X	608	CHL	C3D-C2D	2.96	1.46	1.37
26	3	604	CLA	C1D-ND	2.96	1.41	1.37
26	A	811	CLA	C1D-ND	2.96	1.41	1.37
26	a	608	CLA	C4B-NB	2.96	1.41	1.37
26	Z	603	CLA	C4B-NB	2.96	1.41	1.37
26	B	809	CLA	C1D-ND	2.95	1.41	1.37
26	J	101	CLA	C4B-NB	2.95	1.41	1.37
26	A	843	CLA	CMB-C2B	-2.95	1.44	1.50
26	V	610	CLA	C4B-NB	2.95	1.41	1.37
26	1	616	CLA	C4B-C3B	2.95	1.50	1.43
26	3	615	CLA	C1D-ND	2.95	1.41	1.37
26	4	609	CLA	C1B-C2B	2.95	1.50	1.43
26	a	604	CLA	C4B-NB	2.95	1.41	1.37
26	A	812	CLA	C1D-ND	2.95	1.41	1.37
26	3	617	CLA	C1D-ND	2.95	1.41	1.37
26	A	811	CLA	CMB-C2B	-2.95	1.44	1.50
26	2	611	CLA	C4B-NB	2.94	1.41	1.37
26	5	609	CLA	CMB-C2B	-2.94	1.44	1.50
26	6	602	CLA	C4B-NB	2.94	1.41	1.37
26	A	837	CLA	C1D-ND	2.94	1.41	1.37
26	B	841	CLA	C1D-ND	2.94	1.41	1.37
26	6	607	CLA	C1D-ND	2.94	1.41	1.37
29	B	849	BCR	C30-C25	-2.94	1.50	1.53
26	3	602	CLA	C1D-ND	2.94	1.41	1.37
26	B	823	CLA	C1D-ND	2.94	1.41	1.37
26	L	306	CLA	C1D-ND	2.93	1.41	1.37
26	2	603	CLA	C1D-ND	2.93	1.41	1.37
26	7	613	CLA	C1D-ND	2.93	1.41	1.37
26	A	822	CLA	CMC-C2C	-2.93	1.44	1.50
26	1	603	CLA	C4B-NB	2.93	1.41	1.37
26	6	609	CLA	C4B-NB	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L	302	CLA	C4B-NB	2.93	1.41	1.37
26	8	603	CLA	C4B-NB	2.93	1.41	1.37
26	7	609	CLA	C4B-NB	2.93	1.41	1.37
26	A	826	CLA	CMD-C2D	-2.93	1.44	1.50
26	A	831	CLA	CMB-C2B	-2.93	1.44	1.50
26	A	842	CLA	CMB-C2B	-2.93	1.44	1.50
26	a	603	CLA	C4B-NB	2.92	1.41	1.37
26	B	817	CLA	CMB-C2B	-2.92	1.44	1.50
26	4	603	CLA	C1D-ND	2.92	1.41	1.37
26	9	606	CLA	C4B-NB	2.92	1.41	1.37
26	2	604	CLA	C4B-NB	2.92	1.41	1.37
26	B	821	CLA	C4B-NB	2.92	1.41	1.37
26	5	602	CLA	C4B-NB	2.92	1.41	1.37
34	8	619	LUT	C22-C21	-2.92	1.51	1.54
26	4	609	CLA	C4B-NB	2.92	1.41	1.37
26	5	606	CLA	C1D-ND	2.92	1.41	1.37
26	W	612	CLA	C4B-NB	2.92	1.41	1.37
26	6	614	CLA	CMD-C2D	-2.92	1.44	1.50
26	A	842	CLA	CMC-C2C	-2.91	1.44	1.50
26	B	808	CLA	C1D-ND	2.91	1.41	1.37
26	B	819	CLA	C4B-NB	2.91	1.41	1.37
26	6	601	CLA	C1D-ND	2.91	1.41	1.37
26	B	824	CLA	CMD-C2D	-2.91	1.44	1.50
26	A	810	CLA	CMD-C2D	-2.91	1.44	1.50
26	B	820	CLA	C4B-NB	2.91	1.41	1.37
26	6	611	CLA	C4B-NB	2.91	1.41	1.37
26	A	824	CLA	C1D-ND	2.91	1.41	1.37
26	8	613	CLA	C4B-NB	2.91	1.41	1.37
26	6	618	CLA	C4B-NB	2.91	1.41	1.37
26	5	611	CLA	C4B-NB	2.90	1.41	1.37
26	9	606	CLA	C1D-ND	2.90	1.41	1.37
26	B	806	CLA	CMC-C2C	-2.90	1.44	1.50
26	7	616	CLA	CMD-C2D	-2.90	1.44	1.50
26	A	823	CLA	C1D-ND	2.90	1.41	1.37
26	B	803	CLA	CMD-C2D	-2.90	1.44	1.50
26	A	832	CLA	CMB-C2B	-2.90	1.44	1.50
26	O	2001	CLA	C1D-ND	2.90	1.41	1.37
34	7	619	LUT	C22-C21	-2.90	1.51	1.54
26	H	202	CLA	C4B-NB	2.90	1.41	1.37
26	B	818	CLA	C1D-ND	2.89	1.41	1.37
26	8	612	CLA	C1D-ND	2.89	1.41	1.37
26	a	609	CLA	C4B-NB	2.89	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	204	CLA	C1D-ND	2.89	1.41	1.37
26	a	612	CLA	C1D-ND	2.89	1.41	1.37
26	B	829	CLA	C4B-NB	2.89	1.41	1.37
26	6	603	CLA	C4B-NB	2.89	1.41	1.37
26	B	819	CLA	C1D-ND	2.89	1.41	1.37
29	B	849	BCR	C1-C6	-2.89	1.50	1.53
26	4	603	CLA	C4B-NB	2.89	1.41	1.37
26	7	602	CLA	CMD-C2D	-2.89	1.44	1.50
26	7	601	CLA	C1D-ND	2.89	1.41	1.37
26	9	603	CLA	C4B-NB	2.89	1.41	1.37
26	A	832	CLA	CMD-C2D	-2.89	1.44	1.50
26	4	602	CLA	C1D-ND	2.89	1.41	1.37
26	8	616	CLA	C4B-NB	2.88	1.41	1.37
34	9	619	LUT	C22-C21	-2.88	1.51	1.54
26	4	601	CLA	C1D-ND	2.88	1.41	1.37
26	A	854	CLA	CMC-C2C	-2.88	1.44	1.50
26	5	617	CLA	C1D-ND	2.88	1.41	1.37
29	A	850	BCR	C30-C25	-2.88	1.50	1.53
26	B	835	CLA	C1D-ND	2.88	1.41	1.37
26	1	602	CLA	C1D-ND	2.88	1.41	1.37
26	B	840	CLA	CMB-C2B	-2.87	1.44	1.50
26	B	841	CLA	C4B-NB	2.87	1.41	1.37
26	B	811	CLA	CMB-C2B	-2.87	1.44	1.50
26	B	811	CLA	C4B-NB	2.87	1.41	1.37
26	A	821	CLA	C1D-ND	2.87	1.41	1.37
26	7	606	CLA	C1D-ND	2.87	1.41	1.37
26	A	838	CLA	C1D-ND	2.86	1.41	1.37
26	B	836	CLA	CMD-C2D	-2.86	1.44	1.50
26	6	613	CLA	CMB-C2B	-2.86	1.44	1.50
26	1	612	CLA	C1D-ND	2.86	1.41	1.37
26	6	602	CLA	C1D-ND	2.86	1.41	1.37
26	3	608	CLA	C4B-NB	2.86	1.41	1.37
26	B	839	CLA	CMB-C2B	-2.86	1.44	1.50
26	B	815	CLA	C1D-ND	2.86	1.41	1.37
26	3	607	CLA	C4B-NB	2.86	1.41	1.37
26	G	203	CLA	C4B-NB	2.86	1.41	1.37
26	K	201	CLA	C1B-C2B	2.86	1.49	1.43
26	B	840	CLA	C4B-NB	2.85	1.41	1.37
26	4	608	CLA	C4B-NB	2.85	1.41	1.37
26	B	838	CLA	C1D-ND	2.85	1.41	1.37
26	2	612	CLA	C4B-NB	2.85	1.41	1.37
26	7	607	CLA	C4B-NB	2.85	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	602	CLA	C4B-NB	2.85	1.41	1.37
26	Z	603	CLA	C1B-C2B	2.85	1.49	1.43
26	B	828	CLA	C1D-ND	2.85	1.41	1.37
26	F	301	CLA	C4B-NB	2.85	1.41	1.37
34	2	619	LUT	C1-C6	-2.85	1.50	1.53
26	L	302	CLA	C1D-ND	2.85	1.41	1.37
26	5	614	CLA	C4B-NB	2.85	1.41	1.37
26	9	607	CLA	C1D-ND	2.85	1.41	1.37
26	Z	613	CLA	C1B-C2B	2.84	1.49	1.43
26	6	614	CLA	C4B-NB	2.84	1.41	1.37
26	A	810	CLA	C1D-ND	2.84	1.41	1.37
26	3	603	CLA	CMD-C2D	-2.84	1.44	1.50
26	A	804	CLA	C1D-ND	2.84	1.41	1.37
26	7	609	CLA	C1D-ND	2.84	1.41	1.37
26	8	604	CLA	C4B-NB	2.83	1.41	1.37
26	4	606	CLA	C4B-NB	2.83	1.41	1.37
26	8	602	CLA	C4B-NB	2.83	1.41	1.37
26	B	812	CLA	C4B-NB	2.83	1.41	1.37
26	A	804	CLA	CMD-C2D	-2.83	1.45	1.50
26	A	842	CLA	CMD-C2D	-2.83	1.45	1.50
26	8	602	CLA	C1D-ND	2.83	1.41	1.37
26	U	610	CLA	C1B-C2B	2.83	1.49	1.43
26	A	828	CLA	CMD-C2D	-2.83	1.45	1.50
26	B	818	CLA	CMB-C2B	-2.83	1.45	1.50
36	U	1623	NEX	C7-C6	-2.83	1.27	1.30
26	A	817	CLA	CMD-C2D	-2.83	1.45	1.50
26	B	826	CLA	CMD-C2D	-2.83	1.45	1.50
26	8	612	CLA	C4B-NB	2.83	1.41	1.37
26	A	833	CLA	C1D-ND	2.82	1.41	1.37
26	8	610	CLA	C4B-NB	2.82	1.41	1.37
26	A	805	CLA	C1D-ND	2.82	1.41	1.37
26	2	613	CLA	C1D-ND	2.82	1.41	1.37
26	A	825	CLA	CMB-C2B	-2.82	1.45	1.50
26	8	613	CLA	C1D-ND	2.82	1.41	1.37
26	B	837	CLA	C4B-NB	2.81	1.41	1.37
26	5	616	CLA	C4B-NB	2.81	1.41	1.37
26	a	610	CLA	C4B-NB	2.81	1.41	1.37
26	B	825	CLA	CMD-C2D	-2.81	1.45	1.50
26	9	602	CLA	C4B-NB	2.81	1.41	1.37
26	2	610	CLA	C1D-ND	2.81	1.41	1.37
26	6	606	CLA	C4B-NB	2.81	1.41	1.37
26	8	606	CLA	C4B-NB	2.81	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	612	CLA	C4B-NB	2.81	1.41	1.37
26	1	609	CLA	C1B-C2B	2.80	1.49	1.43
26	4	604	CLA	C4B-NB	2.80	1.41	1.37
26	A	845	CLA	C4B-NB	2.80	1.41	1.37
26	5	603	CLA	C1D-ND	2.80	1.41	1.37
26	7	616	CLA	C4B-NB	2.80	1.41	1.37
26	B	818	CLA	CMD-C2D	-2.80	1.45	1.50
26	a	609	CLA	C1B-C2B	2.80	1.49	1.43
26	H	203	CLA	C4B-NB	2.80	1.41	1.37
36	W	1623	NEX	C7-C8	-2.80	1.27	1.31
26	a	602	CLA	C4B-NB	2.80	1.41	1.37
26	6	617	CLA	C4B-NB	2.80	1.41	1.37
26	9	602	CLA	C1D-ND	2.80	1.41	1.37
36	6	624	NEX	C1-C6	-2.79	1.49	1.54
26	A	816	CLA	C1D-ND	2.79	1.41	1.37
26	B	806	CLA	C1D-ND	2.79	1.41	1.37
26	A	838	CLA	CMD-C2D	-2.79	1.45	1.50
26	2	601	CLA	C1D-ND	2.79	1.41	1.37
26	8	611	CLA	C4B-NB	2.79	1.41	1.37
26	8	614	CLA	C1D-ND	2.79	1.41	1.37
26	B	821	CLA	C3C-C4C	2.79	1.46	1.40
26	A	809	CLA	C1D-ND	2.79	1.41	1.37
26	A	827	CLA	C1D-ND	2.79	1.41	1.37
26	U	610	CLA	C4B-NB	2.79	1.41	1.37
26	B	832	CLA	C1D-ND	2.79	1.41	1.37
26	2	606	CLA	C4B-NB	2.79	1.41	1.37
26	7	608	CLA	C4B-NB	2.79	1.41	1.37
26	8	602	CLA	CMC-C2C	-2.79	1.45	1.50
26	W	603	CLA	C1B-C2B	2.79	1.49	1.43
26	B	809	CLA	CMB-C2B	-2.79	1.45	1.50
26	5	613	CLA	C4B-NB	2.79	1.41	1.37
26	7	611	CLA	CMD-C2D	-2.79	1.45	1.50
26	5	601	CLA	C4B-NB	2.78	1.41	1.37
26	1	609	CLA	C4B-NB	2.78	1.41	1.37
26	9	603	CLA	CMB-C2B	-2.78	1.45	1.50
26	A	819	CLA	CMD-C2D	-2.78	1.45	1.50
26	9	613	CLA	C4B-NB	2.78	1.41	1.37
26	A	839	CLA	CMB-C2B	-2.77	1.45	1.50
26	A	830	CLA	CMD-C2D	-2.77	1.45	1.50
26	9	610	CLA	C1D-ND	2.77	1.41	1.37
26	A	808	CLA	C1D-ND	2.77	1.41	1.37
26	A	834	CLA	C1D-ND	2.77	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	607	CLA	C1D-ND	2.77	1.41	1.37
26	8	608	CLA	C1D-ND	2.77	1.41	1.37
26	A	828	CLA	C1D-ND	2.77	1.41	1.37
26	1	610	CLA	C4B-NB	2.77	1.41	1.37
26	B	822	CLA	C4B-NB	2.77	1.41	1.37
26	8	609	CLA	C4B-NB	2.77	1.41	1.37
26	3	617	CLA	C4B-NB	2.77	1.41	1.37
26	K	201	CLA	C4B-NB	2.77	1.41	1.37
26	B	828	CLA	CMB-C2B	-2.77	1.45	1.50
26	F	301	CLA	C1D-ND	2.77	1.41	1.37
26	3	609	CLA	CMD-C2D	-2.76	1.45	1.50
26	7	604	CLA	C4B-NB	2.76	1.41	1.37
26	A	803	CLA	CMD-C2D	-2.76	1.45	1.50
26	4	616	CLA	C1B-C2B	2.76	1.49	1.43
26	9	611	CLA	C1B-C2B	2.76	1.49	1.43
26	B	835	CLA	CMD-C2D	-2.76	1.45	1.50
26	A	807	CLA	C1D-ND	2.76	1.41	1.37
34	5	620	LUT	C22-C21	-2.76	1.51	1.54
26	B	807	CLA	CMB-C2B	-2.76	1.45	1.50
26	3	609	CLA	CMB-C2B	-2.76	1.45	1.50
26	4	601	CLA	C4B-NB	2.76	1.41	1.37
36	V	1623	NEX	C7-C8	-2.76	1.27	1.31
26	U	603	CLA	C1B-C2B	2.75	1.49	1.43
26	X	603	CLA	C1B-C2B	2.75	1.49	1.43
26	5	616	CLA	C1D-ND	2.75	1.41	1.37
26	B	831	CLA	C4B-NB	2.75	1.41	1.37
26	A	811	CLA	C4B-NB	2.75	1.41	1.37
26	5	612	CLA	C1B-C2B	2.75	1.49	1.43
26	A	806	CLA	CMD-C2D	-2.75	1.45	1.50
26	B	820	CLA	C1D-ND	2.75	1.41	1.37
26	A	818	CLA	CMD-C2D	-2.75	1.45	1.50
26	1	602	CLA	CMD-C2D	-2.75	1.45	1.50
26	X	613	CLA	C1B-C2B	2.75	1.49	1.43
26	3	613	CLA	C1D-ND	2.75	1.41	1.37
26	6	620	CLA	C4B-NB	2.75	1.41	1.37
26	A	825	CLA	C1D-ND	2.75	1.41	1.37
26	2	613	CLA	C4B-NB	2.75	1.41	1.37
26	A	813	CLA	CMD-C2D	-2.75	1.45	1.50
26	B	839	CLA	CMD-C2D	-2.75	1.45	1.50
26	B	827	CLA	C1D-ND	2.74	1.41	1.37
26	A	802	CLA	CMC-C2C	-2.74	1.45	1.50
26	B	837	CLA	C1D-ND	2.74	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	842	CLA	C4B-NB	2.74	1.41	1.37
26	3	606	CLA	C1D-ND	2.74	1.41	1.37
26	A	813	CLA	CMB-C2B	-2.74	1.45	1.50
26	2	609	CLA	CMB-C2B	-2.74	1.45	1.50
26	A	812	CLA	C4B-NB	2.74	1.41	1.37
26	5	617	CLA	CMB-C2B	-2.74	1.45	1.50
26	A	832	CLA	C4B-NB	2.74	1.41	1.37
26	A	831	CLA	C1D-ND	2.74	1.41	1.37
26	a	601	CLA	C4B-NB	2.74	1.41	1.37
26	1	602	CLA	CMC-C2C	-2.74	1.45	1.50
26	5	607	CLA	C4B-NB	2.74	1.41	1.37
26	Y	613	CLA	C1B-C2B	2.74	1.49	1.43
26	A	819	CLA	CMB-C2B	-2.74	1.45	1.50
26	2	613	CLA	C1B-C2B	2.74	1.49	1.43
26	6	602	CLA	CMC-C2C	-2.74	1.45	1.50
26	7	601	CLA	CMD-C2D	-2.74	1.45	1.50
26	A	806	CLA	C1D-ND	2.73	1.41	1.37
26	A	843	CLA	C4B-NB	2.73	1.41	1.37
26	B	812	CLA	C1D-ND	2.73	1.41	1.37
26	2	607	CLA	C4B-NB	2.73	1.41	1.37
29	B	843	BCR	C30-C25	-2.73	1.50	1.53
26	K	203	CLA	C4B-NB	2.73	1.41	1.37
26	8	602	CLA	CMD-C2D	-2.73	1.45	1.50
26	A	821	CLA	C4B-NB	2.73	1.41	1.37
26	B	815	CLA	CMB-C2B	-2.73	1.45	1.50
26	B	825	CLA	C1D-ND	2.73	1.41	1.37
26	3	603	CLA	C1D-ND	2.73	1.41	1.37
26	L	304	CLA	C1B-C2B	2.73	1.49	1.43
26	B	820	CLA	CMD-C2D	-2.73	1.45	1.50
26	6	609	CLA	CMB-C2B	-2.73	1.45	1.50
26	A	839	CLA	C1D-ND	2.73	1.41	1.37
26	a	602	CLA	CMD-C2D	-2.73	1.45	1.50
26	B	825	CLA	C4B-NB	2.73	1.41	1.37
26	3	609	CLA	C4B-NB	2.73	1.41	1.37
26	5	609	CLA	C4B-NB	2.72	1.41	1.37
26	4	603	CLA	C1B-C2B	2.72	1.49	1.43
26	7	611	CLA	C1D-ND	2.72	1.41	1.37
26	3	611	CLA	C1B-C2B	2.72	1.49	1.43
26	A	806	CLA	CMC-C2C	-2.72	1.45	1.50
36	X	1623	NEX	C7-C6	-2.72	1.27	1.30
26	X	611	CLA	C1B-C2B	2.72	1.49	1.43
26	B	834	CLA	C1D-ND	2.72	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	614	CLA	C1D-ND	2.72	1.41	1.37
26	B	816	CLA	C1D-ND	2.72	1.41	1.37
26	5	602	CLA	C1D-ND	2.72	1.41	1.37
26	A	845	CLA	CMD-C2D	-2.72	1.45	1.50
26	A	840	CLA	CMD-C2D	-2.72	1.45	1.50
26	5	613	CLA	C1D-ND	2.72	1.41	1.37
26	6	611	CLA	C1B-C2B	2.72	1.49	1.43
26	A	817	CLA	C4B-NB	2.72	1.41	1.37
26	A	843	CLA	CMD-C2D	-2.72	1.45	1.50
26	A	815	CLA	CMC-C2C	-2.72	1.45	1.50
26	3	613	CLA	CMB-C2B	-2.71	1.45	1.50
26	B	814	CLA	CMD-C2D	-2.71	1.45	1.50
26	4	606	CLA	C1B-C2B	2.71	1.49	1.43
26	B	808	CLA	CMC-C2C	-2.71	1.45	1.50
26	B	838	CLA	C4B-NB	2.71	1.41	1.37
26	B	808	CLA	CMB-C2B	-2.71	1.45	1.50
26	7	610	CLA	CMC-C2C	-2.71	1.45	1.50
26	1	601	CLA	C4B-NB	2.71	1.41	1.37
26	O	2001	CLA	CMD-C2D	-2.71	1.45	1.50
26	B	812	CLA	CMD-C2D	-2.71	1.45	1.50
26	A	801	CLA	CMB-C2B	-2.71	1.45	1.50
34	2	619	LUT	C22-C21	-2.71	1.51	1.54
26	A	835	CLA	CMD-C2D	-2.71	1.45	1.50
26	2	602	CLA	CMC-C2C	-2.71	1.45	1.50
26	a	610	CLA	CMD-C2D	-2.71	1.45	1.50
26	3	608	CLA	C1D-ND	2.70	1.41	1.37
26	B	837	CLA	CMB-C2B	-2.70	1.45	1.50
26	B	828	CLA	CMD-C2D	-2.70	1.45	1.50
26	F	303	CLA	CMB-C2B	-2.70	1.45	1.50
26	8	613	CLA	CMD-C2D	-2.70	1.45	1.50
26	U	611	CLA	C1B-C2B	2.70	1.49	1.43
26	A	814	CLA	C4B-NB	2.70	1.41	1.37
26	7	602	CLA	C1D-ND	2.70	1.41	1.37
26	9	603	CLA	C1D-ND	2.70	1.41	1.37
26	B	833	CLA	CMD-C2D	-2.70	1.45	1.50
26	9	607	CLA	C4B-NB	2.70	1.41	1.37
26	8	614	CLA	C4B-NB	2.70	1.41	1.37
26	A	824	CLA	CMB-C2B	-2.70	1.45	1.50
26	F	301	CLA	CMD-C2D	-2.70	1.45	1.50
36	X	1623	NEX	C7-C8	-2.70	1.27	1.31
26	A	805	CLA	CMD-C2D	-2.70	1.45	1.50
26	3	610	CLA	C1D-ND	2.69	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	806	CLA	CMB-C2B	-2.69	1.45	1.50
26	5	607	CLA	C1D-ND	2.69	1.41	1.37
26	A	838	CLA	CMB-C2B	-2.69	1.45	1.50
26	K	203	CLA	CMD-C2D	-2.69	1.45	1.50
26	A	829	CLA	C1D-ND	2.69	1.41	1.37
26	B	833	CLA	C1D-ND	2.69	1.41	1.37
26	7	606	CLA	C4B-NB	2.69	1.41	1.37
26	7	608	CLA	C1D-ND	2.69	1.41	1.37
26	B	829	CLA	C1D-ND	2.69	1.41	1.37
26	B	813	CLA	CMD-C2D	-2.69	1.45	1.50
26	7	611	CLA	CMC-C2C	-2.69	1.45	1.50
34	4	619	LUT	C22-C21	-2.69	1.51	1.54
34	3	618	LUT	C22-C21	-2.69	1.51	1.54
26	B	809	CLA	CMC-C2C	-2.69	1.45	1.50
26	V	603	CLA	C1B-C2B	2.69	1.49	1.43
26	B	805	CLA	C1D-ND	2.69	1.41	1.37
26	7	607	CLA	C1D-ND	2.69	1.41	1.37
26	2	612	CLA	C1B-C2B	2.69	1.49	1.43
26	5	617	CLA	CMD-C2D	-2.69	1.45	1.50
26	a	614	CLA	C4B-NB	2.69	1.41	1.37
26	3	613	CLA	CMD-C2D	-2.69	1.45	1.50
26	8	601	CLA	CMB-C2B	-2.69	1.45	1.50
26	B	814	CLA	C4B-NB	2.69	1.41	1.37
26	B	832	CLA	CMB-C2B	-2.68	1.45	1.50
34	Y	1621	LUT	C1-C6	-2.68	1.50	1.53
26	B	816	CLA	C4B-NB	2.68	1.41	1.37
26	3	608	CLA	CMB-C2B	-2.68	1.45	1.50
26	A	845	CLA	C1D-ND	2.68	1.41	1.37
26	A	802	CLA	CMD-C2D	-2.68	1.45	1.50
26	3	606	CLA	CMB-C2B	-2.68	1.45	1.50
26	6	606	CLA	C1B-C2B	2.68	1.49	1.43
26	O	2001	CLA	C1B-C2B	2.68	1.49	1.43
26	B	840	CLA	CMD-C2D	-2.68	1.45	1.50
26	9	612	CLA	C1B-C2B	2.68	1.49	1.43
26	A	815	CLA	C1D-ND	2.68	1.41	1.37
26	B	813	CLA	CMB-C2B	-2.68	1.45	1.50
26	9	603	CLA	CMD-C2D	-2.68	1.45	1.50
26	B	807	CLA	C1D-ND	2.68	1.41	1.37
26	5	601	CLA	C1B-C2B	2.68	1.49	1.43
26	A	809	CLA	CMB-C2B	-2.68	1.45	1.50
26	A	807	CLA	C4B-NB	2.68	1.41	1.37
26	4	611	CLA	C4B-NB	2.68	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	601	CLA	C4B-NB	2.68	1.41	1.37
26	6	618	CLA	C1B-C2B	2.68	1.49	1.43
26	B	833	CLA	C4B-NB	2.68	1.41	1.37
26	a	613	CLA	CMD-C2D	-2.67	1.45	1.50
26	8	601	CLA	CMD-C2D	-2.67	1.45	1.50
26	4	610	CLA	C1B-C2B	2.67	1.49	1.43
26	9	613	CLA	C1B-C2B	2.67	1.49	1.43
26	Z	613	CLA	CMD-C2D	-2.67	1.45	1.50
26	7	604	CLA	C1D-ND	2.67	1.41	1.37
26	7	603	CLA	CMD-C2D	-2.67	1.45	1.50
26	L	306	CLA	C4B-NB	2.67	1.41	1.37
26	6	616	CLA	C4B-NB	2.67	1.41	1.37
26	1	610	CLA	CMD-C2D	-2.67	1.45	1.50
26	U	612	CLA	C1B-C2B	2.67	1.49	1.43
26	a	602	CLA	CMC-C2C	-2.67	1.45	1.50
26	A	836	CLA	CMD-C2D	-2.67	1.45	1.50
26	7	612	CLA	C4B-NB	2.67	1.41	1.37
26	B	832	CLA	C4B-NB	2.67	1.41	1.37
26	2	610	CLA	CMD-C2D	-2.67	1.45	1.50
26	A	831	CLA	C4B-NB	2.67	1.41	1.37
26	A	814	CLA	C1D-ND	2.67	1.41	1.37
26	8	612	CLA	C1B-C2B	2.67	1.49	1.43
26	A	813	CLA	C1D-ND	2.67	1.41	1.37
26	9	602	CLA	CMD-C2D	-2.67	1.45	1.50
26	U	613	CLA	C1B-C2B	2.67	1.49	1.43
26	A	835	CLA	CMB-C2B	-2.66	1.45	1.50
26	a	613	CLA	CMB-C2B	-2.66	1.45	1.50
26	Y	614	CLA	C1B-C2B	2.66	1.49	1.43
26	7	603	CLA	CMB-C2B	-2.66	1.45	1.50
26	B	813	CLA	C4B-NB	2.66	1.41	1.37
26	8	603	CLA	CMD-C2D	-2.66	1.45	1.50
26	A	818	CLA	C1D-ND	2.66	1.41	1.37
26	A	833	CLA	C4B-NB	2.66	1.41	1.37
26	A	815	CLA	C4B-NB	2.66	1.41	1.37
26	9	609	CLA	C4B-NB	2.66	1.41	1.37
26	K	204	CLA	CMD-C2D	-2.66	1.45	1.50
26	V	612	CLA	C1B-C2B	2.66	1.49	1.43
26	1	614	CLA	C4B-NB	2.66	1.41	1.37
26	A	807	CLA	CMB-C2B	-2.66	1.45	1.50
26	5	603	CLA	CMB-C2B	-2.66	1.45	1.50
26	Y	603	CLA	C1B-C2B	2.66	1.49	1.43
26	A	823	CLA	C4B-NB	2.66	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	613	CLA	CMD-C2D	-2.66	1.45	1.50
29	7	621	BCR	C1-C6	-2.65	1.50	1.53
26	A	822	CLA	CMD-C2D	-2.65	1.45	1.50
26	A	816	CLA	CMC-C2C	-2.65	1.45	1.50
26	B	835	CLA	CMB-C2B	-2.65	1.45	1.50
26	5	616	CLA	C1B-C2B	2.65	1.49	1.43
26	B	810	CLA	CMB-C2B	-2.65	1.45	1.50
26	8	616	CLA	C1B-C2B	2.65	1.49	1.43
26	3	615	CLA	C4B-NB	2.65	1.41	1.37
26	L	303	CLA	CMB-C2B	-2.65	1.45	1.50
26	9	601	CLA	C1B-C2B	2.65	1.49	1.43
26	X	610	CLA	C3B-C4B	2.65	1.50	1.42
26	5	608	CLA	C4B-NB	2.65	1.41	1.37
26	a	603	CLA	C1B-C2B	2.65	1.49	1.43
26	4	614	CLA	C1B-C2B	2.65	1.49	1.43
26	W	614	CLA	C1B-C2B	2.65	1.49	1.43
26	A	829	CLA	C4B-NB	2.65	1.41	1.37
26	2	614	CLA	CMD-C2D	-2.64	1.45	1.50
26	A	829	CLA	CMC-C2C	-2.64	1.45	1.50
26	1	612	CLA	C1B-C2B	2.64	1.49	1.43
26	A	837	CLA	C4B-NB	2.64	1.41	1.37
26	a	612	CLA	C1B-C2B	2.64	1.49	1.43
26	B	814	CLA	C1D-ND	2.64	1.41	1.37
26	5	607	CLA	CMB-C2B	-2.64	1.45	1.50
26	1	603	CLA	C1B-C2B	2.64	1.49	1.43
26	3	604	CLA	C4B-NB	2.64	1.41	1.37
26	A	819	CLA	CMC-C2C	-2.64	1.45	1.50
26	1	608	CLA	C1B-C2B	2.64	1.49	1.43
26	B	829	CLA	CMD-C2D	-2.64	1.45	1.50
26	W	613	CLA	C1B-C2B	2.64	1.49	1.43
26	B	838	CLA	CMD-C2D	-2.64	1.45	1.50
26	2	611	CLA	C1B-C2B	2.64	1.49	1.43
26	W	612	CLA	C1B-C2B	2.64	1.49	1.43
26	B	806	CLA	CMD-C2D	-2.64	1.45	1.50
26	A	818	CLA	C4B-NB	2.64	1.41	1.37
26	A	840	CLA	C1D-ND	2.64	1.41	1.37
26	A	807	CLA	CMC-C2C	-2.63	1.45	1.50
26	6	603	CLA	CMD-C2D	-2.63	1.45	1.50
26	3	610	CLA	C3B-C4B	2.63	1.50	1.42
26	B	824	CLA	C4B-NB	2.63	1.41	1.37
26	A	834	CLA	CMD-C2D	-2.63	1.45	1.50
26	A	854	CLA	CMB-C2B	-2.63	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	613	CLA	CMD-C2D	-2.63	1.45	1.50
26	L	304	CLA	C4B-NB	2.63	1.41	1.37
26	4	612	CLA	C1B-C2B	2.63	1.49	1.43
26	3	612	CLA	C3B-C4B	2.63	1.50	1.42
26	L	307	CLA	C1B-C2B	2.63	1.49	1.43
26	U	614	CLA	C1B-C2B	2.63	1.49	1.43
26	A	819	CLA	MG-NB	-2.63	2.00	2.05
26	A	836	CLA	CMB-C2B	-2.63	1.45	1.50
26	a	608	CLA	C1B-C2B	2.63	1.49	1.43
26	8	608	CLA	CMC-C2C	-2.63	1.45	1.50
26	B	834	CLA	CMD-C2D	-2.63	1.45	1.50
26	A	813	CLA	C4B-NB	2.62	1.41	1.37
26	B	826	CLA	C4B-NB	2.62	1.41	1.37
26	B	813	CLA	CMC-C2C	-2.62	1.45	1.50
26	A	820	CLA	C1D-ND	2.62	1.41	1.37
26	9	602	CLA	CMC-C2C	-2.62	1.45	1.50
26	B	834	CLA	CMB-C2B	-2.62	1.45	1.50
26	B	841	CLA	CMC-C2C	-2.62	1.45	1.50
26	B	824	CLA	CMC-C2C	-2.62	1.45	1.50
26	6	603	CLA	C1B-C2B	2.62	1.49	1.43
26	A	815	CLA	CMD-C2D	-2.62	1.45	1.50
26	8	608	CLA	CMD-C2D	-2.62	1.45	1.50
26	A	823	CLA	C1B-C2B	2.62	1.49	1.43
26	B	830	CLA	CMB-C2B	-2.62	1.45	1.50
26	L	306	CLA	CMC-C2C	-2.62	1.45	1.50
26	8	612	CLA	CMD-C2D	-2.62	1.45	1.50
26	6	612	CLA	C1B-C2B	2.62	1.49	1.43
26	7	613	CLA	C4B-NB	2.62	1.41	1.37
26	U	602	CLA	C1B-C2B	2.62	1.49	1.43
26	O	2002	CLA	CMD-C2D	-2.62	1.45	1.50
26	V	613	CLA	C1B-C2B	2.62	1.49	1.43
26	6	610	CLA	CMD-C2D	-2.61	1.45	1.50
26	5	611	CLA	C1B-C2B	2.61	1.49	1.43
26	A	804	CLA	C1B-C2B	2.61	1.49	1.43
26	G	204	CLA	CMB-C2B	-2.61	1.45	1.50
26	B	826	CLA	C1D-ND	2.61	1.41	1.37
26	B	835	CLA	C4B-NB	2.61	1.41	1.37
26	Y	612	CLA	C1B-C2B	2.61	1.49	1.43
26	7	610	CLA	CMB-C2B	-2.61	1.45	1.50
26	7	616	CLA	C1B-C2B	2.61	1.49	1.43
26	O	2003	CLA	C4B-NB	2.61	1.41	1.37
26	7	613	CLA	C1B-C2B	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	827	CLA	CMD-C2D	-2.61	1.45	1.50
26	Z	614	CLA	C1B-C2B	2.61	1.49	1.43
26	X	614	CLA	C1B-C2B	2.61	1.49	1.43
26	B	811	CLA	CMC-C2C	-2.61	1.45	1.50
26	B	805	CLA	CMB-C2B	-2.61	1.45	1.50
26	B	815	CLA	CMD-C2D	-2.61	1.45	1.50
26	A	820	CLA	CMD-C2D	-2.61	1.45	1.50
26	A	834	CLA	C4B-NB	2.61	1.41	1.37
26	3	602	CLA	C4B-NB	2.61	1.41	1.37
26	7	608	CLA	CMD-C2D	-2.61	1.45	1.50
26	A	835	CLA	C1D-ND	2.61	1.41	1.37
26	A	854	CLA	C4B-NB	2.61	1.41	1.37
26	Y	611	CLA	C1B-C2B	2.61	1.49	1.43
26	A	809	CLA	CMD-C2D	-2.61	1.45	1.50
26	5	604	CLA	C4B-C3B	2.61	1.49	1.43
26	A	812	CLA	CMB-C2B	-2.61	1.45	1.50
26	B	807	CLA	CMC-C2C	-2.61	1.45	1.50
26	4	608	CLA	C1B-C2B	2.60	1.49	1.43
26	B	832	CLA	CMD-C2D	-2.60	1.45	1.50
26	4	613	CLA	CMB-C2B	-2.60	1.45	1.50
26	7	614	CLA	CMD-C2D	-2.60	1.45	1.50
26	A	803	CLA	CMC-C2C	-2.60	1.45	1.50
26	7	612	CLA	CMD-C2D	-2.60	1.45	1.50
26	V	602	CLA	C1B-C2B	2.60	1.49	1.43
26	A	832	CLA	C1D-ND	2.60	1.41	1.37
26	B	810	CLA	C1D-ND	2.60	1.41	1.37
26	A	811	CLA	CMC-C2C	-2.60	1.45	1.50
26	7	611	CLA	C4B-NB	2.60	1.41	1.37
26	A	824	CLA	CMC-C2C	-2.60	1.45	1.50
26	O	2002	CLA	C4B-C3B	2.60	1.49	1.43
26	5	608	CLA	C1B-C2B	2.60	1.49	1.43
26	V	611	CLA	C1B-C2B	2.60	1.49	1.43
26	9	604	CLA	C4B-C3B	2.60	1.49	1.43
26	A	834	CLA	CMC-C2C	-2.60	1.45	1.50
26	7	604	CLA	CMD-C2D	-2.60	1.45	1.50
26	3	608	CLA	CMD-C2D	-2.60	1.45	1.50
26	U	604	CLA	CMB-C2B	-2.60	1.45	1.50
26	7	609	CLA	CMD-C2D	-2.60	1.45	1.50
26	8	610	CLA	CMD-C2D	-2.59	1.45	1.50
26	A	840	CLA	C4B-NB	2.59	1.41	1.37
26	6	604	CLA	C4B-NB	2.59	1.41	1.37
26	1	613	CLA	CMB-C2B	-2.59	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	817	CLA	CMB-C2B	-2.59	1.45	1.50
26	A	805	CLA	C4B-NB	2.59	1.41	1.37
26	B	829	CLA	CMC-C2C	-2.59	1.45	1.50
26	B	804	CLA	C1D-ND	2.59	1.41	1.37
26	8	613	CLA	CMC-C2C	-2.59	1.45	1.50
26	8	608	CLA	C4B-NB	2.59	1.41	1.37
26	6	607	CLA	CMC-C2C	-2.59	1.45	1.50
26	B	811	CLA	CMD-C2D	-2.59	1.45	1.50
26	B	833	CLA	CMC-C2C	-2.59	1.45	1.50
26	A	826	CLA	C4B-NB	2.58	1.41	1.37
26	B	839	CLA	C1D-ND	2.58	1.41	1.37
26	A	841	CLA	CMC-C2C	-2.58	1.45	1.50
26	J	101	CLA	C1B-C2B	2.58	1.49	1.43
26	B	807	CLA	C4B-NB	2.58	1.41	1.37
26	A	816	CLA	CMD-C2D	-2.58	1.45	1.50
26	5	617	CLA	C1B-C2B	2.58	1.49	1.43
26	Y	602	CLA	C1B-C2B	2.58	1.49	1.43
26	A	825	CLA	CMD-C2D	-2.58	1.45	1.50
26	A	833	CLA	CMD-C2D	-2.58	1.45	1.50
26	7	610	CLA	C1D-ND	2.58	1.41	1.37
26	B	803	CLA	CMC-C2C	-2.58	1.45	1.50
26	F	301	CLA	CMB-C2B	-2.58	1.45	1.50
26	A	808	CLA	CMD-C2D	-2.58	1.45	1.50
26	A	803	CLA	C1D-ND	2.58	1.41	1.37
26	A	821	CLA	CMD-C2D	-2.58	1.45	1.50
26	A	845	CLA	CMB-C2B	-2.58	1.45	1.50
26	3	609	CLA	CMC-C2C	-2.58	1.45	1.50
26	B	836	CLA	C1D-ND	2.57	1.41	1.37
26	K	206	CLA	CMB-C2B	-2.57	1.45	1.50
26	9	610	CLA	CMB-C2B	-2.57	1.45	1.50
26	7	607	CLA	CMB-C2B	-2.57	1.45	1.50
26	A	839	CLA	C4B-NB	2.57	1.41	1.37
26	7	613	CLA	CMD-C2D	-2.57	1.45	1.50
26	8	613	CLA	CMB-C2B	-2.57	1.45	1.50
26	4	618	CLA	C4B-C3B	2.57	1.49	1.43
26	a	612	CLA	CMD-C2D	-2.57	1.45	1.50
34	1	617	LUT	C22-C21	-2.57	1.51	1.54
34	7	619	LUT	C1-C6	-2.57	1.50	1.53
26	A	808	CLA	CMC-C2C	-2.57	1.45	1.50
26	3	604	CLA	CMB-C2B	-2.57	1.45	1.50
26	1	601	CLA	CMD-C2D	-2.57	1.45	1.50
26	9	613	CLA	CMB-C2B	-2.57	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	808	CLA	C4B-NB	2.57	1.41	1.37
26	X	612	CLA	C1B-C2B	2.57	1.49	1.43
26	B	840	CLA	CMC-C2C	-2.57	1.45	1.50
26	A	832	CLA	CMC-C2C	-2.57	1.45	1.50
26	A	839	CLA	CMC-C2C	-2.57	1.45	1.50
26	2	609	CLA	CMC-C2C	-2.56	1.45	1.50
26	B	817	CLA	CMD-C2D	-2.56	1.45	1.50
26	B	811	CLA	C1D-ND	2.56	1.41	1.37
26	A	805	CLA	CMC-C2C	-2.56	1.45	1.50
26	B	819	CLA	CMB-C2B	-2.56	1.45	1.50
26	A	801	CLA	CMD-C2D	-2.56	1.45	1.50
26	1	612	CLA	CMD-C2D	-2.56	1.45	1.50
26	X	614	CLA	CMD-C2D	-2.56	1.45	1.50
26	B	826	CLA	CMC-C2C	-2.56	1.45	1.50
26	H	202	CLA	CMB-C2B	-2.56	1.45	1.50
26	L	307	CLA	CMC-C2C	-2.56	1.45	1.50
26	A	806	CLA	MG-NB	-2.56	2.00	2.05
26	L	303	CLA	C1D-ND	2.56	1.41	1.37
26	B	813	CLA	C1D-ND	2.56	1.41	1.37
26	B	828	CLA	CMC-C2C	-2.56	1.45	1.50
26	O	2003	CLA	C1B-C2B	2.56	1.49	1.43
34	a	617	LUT	C22-C21	-2.56	1.51	1.54
26	F	304	CLA	CMD-C2D	-2.56	1.45	1.50
26	7	608	CLA	CMB-C2B	-2.56	1.45	1.50
26	X	604	CLA	C1B-C2B	2.56	1.49	1.43
26	5	610	CLA	CMC-C2C	-2.55	1.45	1.50
26	B	809	CLA	C4B-NB	2.55	1.41	1.37
26	5	608	CLA	CMD-C2D	-2.55	1.45	1.50
26	5	604	CLA	CMB-C2B	-2.55	1.45	1.50
26	a	611	CLA	C4B-C3B	2.55	1.49	1.43
26	A	842	CLA	C1D-ND	2.55	1.41	1.37
26	B	804	CLA	C4B-NB	2.55	1.41	1.37
26	W	610	CLA	C1B-C2B	2.55	1.49	1.43
26	B	814	CLA	CMC-C2C	-2.55	1.45	1.50
26	7	602	CLA	CMC-C2C	-2.55	1.45	1.50
26	2	616	CLA	C1B-C2B	2.55	1.49	1.43
26	7	615	CLA	C4B-C3B	2.55	1.49	1.43
26	W	611	CLA	C1B-C2B	2.55	1.49	1.43
26	A	813	CLA	CMC-C2C	-2.55	1.45	1.50
26	9	609	CLA	C1B-C2B	2.55	1.49	1.43
26	4	601	CLA	CMB-C2B	-2.55	1.45	1.50
34	6	619	LUT	C22-C21	-2.55	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	203	CLA	C1B-C2B	2.55	1.49	1.43
26	5	614	CLA	C1B-C2B	2.55	1.49	1.43
26	L	303	CLA	CMD-C2D	-2.55	1.45	1.50
26	3	610	CLA	CMC-C2C	-2.55	1.45	1.50
26	B	812	CLA	CMB-C2B	-2.54	1.45	1.50
26	K	204	CLA	CMC-C2C	-2.54	1.45	1.50
26	A	811	CLA	CMD-C2D	-2.54	1.45	1.50
26	A	826	CLA	CMB-C2B	-2.54	1.45	1.50
26	A	831	CLA	CMC-C2C	-2.54	1.45	1.50
26	A	833	CLA	CMB-C2B	-2.54	1.45	1.50
26	3	614	CLA	CMD-C2D	-2.54	1.45	1.50
26	7	609	CLA	CMB-C2B	-2.54	1.45	1.50
26	8	611	CLA	CMD-C2D	-2.54	1.45	1.50
26	B	826	CLA	C1B-C2B	2.54	1.49	1.43
29	B	846	BCR	C30-C25	-2.54	1.50	1.53
26	2	603	CLA	CMD-C2D	-2.54	1.45	1.50
26	8	611	CLA	CMB-C2B	-2.54	1.45	1.50
26	6	607	CLA	C4B-C3B	2.54	1.49	1.43
26	W	602	CLA	C1B-C2B	2.54	1.49	1.43
26	A	816	CLA	CMB-C2B	-2.54	1.45	1.50
26	A	825	CLA	C1B-C2B	2.54	1.49	1.43
26	4	618	CLA	C1B-C2B	2.54	1.49	1.43
26	B	820	CLA	C1B-C2B	2.54	1.49	1.43
26	B	822	CLA	C1B-C2B	2.54	1.49	1.43
26	A	818	CLA	CMB-C2B	-2.54	1.45	1.50
26	9	610	CLA	CMD-C2D	-2.53	1.45	1.50
26	A	854	CLA	C1D-ND	2.53	1.41	1.37
26	B	802	CLA	C4B-NB	2.53	1.41	1.37
26	a	601	CLA	CMD-C2D	-2.53	1.45	1.50
26	7	612	CLA	C1B-C2B	2.53	1.49	1.43
37	Z	607	CHL	CBD-CGD	-2.53	1.49	1.52
26	7	604	CLA	CMC-C2C	-2.53	1.45	1.50
26	7	614	CLA	C4B-NB	2.53	1.41	1.37
26	4	602	CLA	CMD-C2D	-2.53	1.45	1.50
26	5	618	CLA	C4B-C3B	2.53	1.49	1.43
26	3	603	CLA	C4B-NB	2.53	1.41	1.37
26	B	816	CLA	CMB-C2B	-2.53	1.45	1.50
26	4	613	CLA	CMD-C2D	-2.53	1.45	1.50
26	4	614	CLA	CMD-C2D	-2.53	1.45	1.50
26	B	837	CLA	CMD-C2D	-2.53	1.45	1.50
26	4	603	CLA	CMD-C2D	-2.53	1.45	1.50
26	4	604	CLA	C1B-C2B	2.53	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	821	CLA	CMB-C2B	-2.53	1.45	1.50
26	9	609	CLA	CMD-C2D	-2.53	1.45	1.50
36	U	1623	NEX	C7-C8	-2.53	1.27	1.31
26	4	602	CLA	C3B-C4B	2.53	1.50	1.42
26	5	603	CLA	C1B-C2B	2.53	1.49	1.43
26	B	810	CLA	CMD-C2D	-2.53	1.45	1.50
26	Y	604	CLA	CMB-C2B	-2.53	1.45	1.50
26	6	614	CLA	C1B-C2B	2.53	1.49	1.43
26	B	810	CLA	C4B-NB	2.53	1.41	1.37
29	B	847	BCR	C30-C25	-2.53	1.50	1.53
26	7	602	CLA	CMB-C2B	-2.53	1.45	1.50
26	8	603	CLA	CMB-C2B	-2.53	1.45	1.50
26	9	614	CLA	C1B-C2B	2.52	1.49	1.43
26	L	307	CLA	C4B-NB	2.52	1.41	1.37
36	V	1623	NEX	C7-C6	-2.52	1.27	1.30
26	3	604	CLA	CMC-C2C	-2.52	1.45	1.50
26	K	206	CLA	C1B-C2B	2.52	1.49	1.43
26	A	820	CLA	C4B-NB	2.52	1.41	1.37
26	B	803	CLA	C1D-ND	2.52	1.41	1.37
26	A	801	CLA	CMC-C2C	-2.52	1.45	1.50
26	A	807	CLA	CMD-C2D	-2.52	1.45	1.50
26	A	805	CLA	CMB-C2B	-2.52	1.45	1.50
26	8	616	CLA	C4B-C3B	2.52	1.49	1.43
26	9	604	CLA	CMD-C2D	-2.52	1.45	1.50
26	3	604	CLA	CMD-C2D	-2.52	1.45	1.50
26	3	610	CLA	CMB-C2B	-2.52	1.45	1.50
26	Y	610	CLA	C3B-C4B	2.52	1.50	1.42
26	8	607	CLA	CMD-C2D	-2.52	1.45	1.50
26	3	607	CLA	C1B-C2B	2.52	1.49	1.43
26	B	805	CLA	CMD-C2D	-2.52	1.45	1.50
26	7	601	CLA	MG-NB	-2.52	2.00	2.05
26	8	607	CLA	C4B-C3B	2.52	1.49	1.43
26	Z	611	CLA	CMD-C2D	-2.52	1.45	1.50
26	B	817	CLA	C4B-NB	2.51	1.41	1.37
26	A	801	CLA	C1B-C2B	2.51	1.49	1.43
26	7	616	CLA	C4B-C3B	2.51	1.49	1.43
26	2	601	CLA	MG-NB	-2.51	2.00	2.05
26	9	604	CLA	CMB-C2B	-2.51	1.45	1.50
26	7	604	CLA	CMB-C2B	-2.51	1.45	1.50
26	H	203	CLA	C1B-C2B	2.51	1.49	1.43
26	5	603	CLA	CMD-C2D	-2.51	1.45	1.50
26	A	827	CLA	CMD-C2D	-2.51	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	817	CLA	C1D-ND	2.51	1.41	1.37
26	2	606	CLA	C1B-C2B	2.51	1.49	1.43
26	7	603	CLA	C4B-NB	2.51	1.41	1.37
26	3	602	CLA	CMC-C2C	-2.51	1.45	1.50
26	5	604	CLA	CMD-C2D	-2.51	1.45	1.50
26	B	815	CLA	C4B-NB	2.51	1.41	1.37
26	7	601	CLA	CMB-C2B	-2.51	1.45	1.50
26	7	613	CLA	CMC-C2C	-2.51	1.45	1.50
26	A	836	CLA	MG-NB	-2.51	2.00	2.05
26	4	602	CLA	CMC-C2C	-2.51	1.45	1.50
26	9	606	CLA	CMD-C2D	-2.51	1.45	1.50
26	3	615	CLA	CMC-C2C	-2.50	1.45	1.50
26	A	819	CLA	C1D-ND	2.50	1.41	1.37
26	A	827	CLA	C4B-NB	2.50	1.41	1.37
26	a	613	CLA	C4B-NB	2.50	1.41	1.37
26	B	839	CLA	CMC-C2C	-2.50	1.45	1.50
26	A	829	CLA	CMD-C2D	-2.50	1.45	1.50
26	A	814	CLA	CMC-C2C	-2.50	1.45	1.50
26	L	304	CLA	CMD-C2D	-2.50	1.45	1.50
26	B	823	CLA	CMD-C2D	-2.50	1.45	1.50
26	5	602	CLA	CMC-C2C	-2.50	1.45	1.50
26	2	603	CLA	C1B-C2B	2.50	1.49	1.43
26	Z	602	CLA	C1B-C2B	2.50	1.49	1.43
26	A	828	CLA	MG-NB	-2.50	2.00	2.05
26	B	824	CLA	CMB-C2B	-2.50	1.45	1.50
26	A	816	CLA	C1B-C2B	2.50	1.49	1.43
26	Z	612	CLA	C1B-C2B	2.50	1.49	1.43
26	A	817	CLA	C1B-C2B	2.50	1.49	1.43
26	3	603	CLA	C1B-C2B	2.50	1.49	1.43
26	3	610	CLA	CMD-C2D	-2.50	1.45	1.50
26	2	606	CLA	CMD-C2D	-2.50	1.45	1.50
26	6	617	CLA	CMD-C2D	-2.50	1.45	1.50
26	A	821	CLA	CMC-C2C	-2.50	1.45	1.50
26	B	827	CLA	CMB-C2B	-2.50	1.45	1.50
26	6	620	CLA	CMB-C2B	-2.50	1.45	1.50
26	K	204	CLA	C4B-NB	2.50	1.41	1.37
26	B	804	CLA	CMD-C2D	-2.50	1.45	1.50
29	B	847	BCR	C1-C6	-2.50	1.50	1.53
26	A	841	CLA	C1D-ND	2.50	1.41	1.37
26	4	602	CLA	CMB-C2B	-2.50	1.45	1.50
26	A	810	CLA	C4B-NB	2.49	1.41	1.37
26	B	831	CLA	CMD-C2D	-2.49	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	609	CLA	CMD-C2D	-2.49	1.45	1.50
26	B	831	CLA	C1B-C2B	2.49	1.49	1.43
26	A	824	CLA	C4B-NB	2.49	1.41	1.37
26	a	602	CLA	C1B-C2B	2.49	1.49	1.43
26	5	604	CLA	C1B-C2B	2.49	1.49	1.43
26	8	614	CLA	C1B-C2B	2.49	1.49	1.43
26	A	834	CLA	CMB-C2B	-2.49	1.45	1.50
26	B	802	CLA	CMD-C2D	-2.49	1.45	1.50
26	5	616	CLA	CMD-C2D	-2.49	1.45	1.50
26	8	609	CLA	CMD-C2D	-2.49	1.45	1.50
26	5	617	CLA	C4B-NB	2.49	1.41	1.37
26	3	615	CLA	C1B-C2B	2.49	1.49	1.43
26	7	610	CLA	CMD-C2D	-2.49	1.45	1.50
26	1	606	CLA	C1B-C2B	2.49	1.49	1.43
26	K	203	CLA	CMB-C2B	-2.49	1.45	1.50
26	2	609	CLA	CMD-C2D	-2.49	1.45	1.50
26	A	836	CLA	C1D-ND	2.48	1.41	1.37
26	H	202	CLA	C1B-C2B	2.48	1.49	1.43
26	1	610	CLA	C1B-C2B	2.48	1.49	1.43
26	A	814	CLA	CMB-C2B	-2.48	1.45	1.50
26	B	836	CLA	CMC-C2C	-2.48	1.45	1.50
26	A	821	CLA	C1B-C2B	2.48	1.49	1.43
26	A	841	CLA	CMD-C2D	-2.48	1.45	1.50
26	B	828	CLA	C4B-NB	2.48	1.41	1.37
26	1	613	CLA	C4B-NB	2.48	1.41	1.37
26	B	820	CLA	CMB-C2B	-2.48	1.45	1.50
26	A	820	CLA	CMB-C2B	-2.48	1.45	1.50
26	A	843	CLA	C1D-ND	2.48	1.41	1.37
26	a	612	CLA	CMB-C2B	-2.48	1.45	1.50
26	5	618	CLA	C1B-C2B	2.48	1.48	1.43
26	5	602	CLA	C1B-C2B	2.48	1.48	1.43
26	A	835	CLA	C4B-NB	2.48	1.41	1.37
26	A	826	CLA	CMC-C2C	-2.48	1.45	1.50
26	1	609	CLA	CMD-C2D	-2.48	1.45	1.50
26	9	610	CLA	C3B-C4B	2.48	1.50	1.42
26	6	604	CLA	CMB-C2B	-2.48	1.45	1.50
26	A	827	CLA	CMB-C2B	-2.48	1.45	1.50
26	O	2001	CLA	CMC-C2C	-2.48	1.45	1.50
26	5	618	CLA	CMD-C2D	-2.48	1.45	1.50
26	8	606	CLA	CMC-C2C	-2.48	1.45	1.50
26	a	616	CLA	C3B-C4B	2.48	1.49	1.42
26	4	611	CLA	C1B-C2B	2.48	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	610	CLA	CMC-C2C	-2.48	1.45	1.50
26	A	831	CLA	CMD-C2D	-2.48	1.45	1.50
26	F	303	CLA	CMD-C2D	-2.47	1.45	1.50
26	1	604	CLA	CMB-C2B	-2.47	1.45	1.50
26	2	610	CLA	CMC-C2C	-2.47	1.45	1.50
26	7	607	CLA	CMD-C2D	-2.47	1.45	1.50
26	5	610	CLA	C3B-C4B	2.47	1.49	1.42
26	B	817	CLA	CMC-C2C	-2.47	1.45	1.50
26	4	607	CLA	CMB-C2B	-2.47	1.45	1.50
35	7	620	XAT	O24-C25	-2.47	1.43	1.46
26	B	836	CLA	CMB-C2B	-2.47	1.45	1.50
26	7	602	CLA	CHC-C1C	2.47	1.43	1.38
26	A	817	CLA	CMC-C2C	-2.47	1.45	1.50
26	L	307	CLA	CMD-C2D	-2.47	1.45	1.50
26	7	613	CLA	CMB-C2B	-2.47	1.45	1.50
26	5	619	CLA	C1B-C2B	2.47	1.48	1.43
26	B	818	CLA	C4B-NB	2.47	1.41	1.37
26	4	609	CLA	CMD-C2D	-2.47	1.45	1.50
35	8	620	XAT	O24-C25	-2.47	1.43	1.46
26	4	604	CLA	C4B-C3B	2.47	1.48	1.43
26	B	818	CLA	CMC-C2C	-2.47	1.45	1.50
26	1	606	CLA	CMB-C2B	-2.47	1.45	1.50
26	8	611	CLA	C1B-C2B	2.47	1.48	1.43
26	A	812	CLA	CMD-C2D	-2.47	1.45	1.50
26	A	815	CLA	CMB-C2B	-2.47	1.45	1.50
26	2	616	CLA	C4B-C3B	2.47	1.48	1.43
26	A	816	CLA	C4B-NB	2.47	1.41	1.37
26	4	613	CLA	C1B-C2B	2.47	1.48	1.43
26	5	619	CLA	CMD-C2D	-2.47	1.45	1.50
26	6	617	CLA	CMB-C2B	-2.47	1.45	1.50
26	H	203	CLA	CMD-C2D	-2.46	1.45	1.50
26	4	610	CLA	CMD-C2D	-2.46	1.45	1.50
26	V	613	CLA	CMD-C2D	-2.46	1.45	1.50
26	7	607	CLA	C1B-C2B	2.46	1.48	1.43
26	9	606	CLA	C1B-C2B	2.46	1.48	1.43
26	B	827	CLA	C4B-NB	2.46	1.41	1.37
29	A	848	BCR	C30-C25	-2.46	1.50	1.53
26	A	802	CLA	C1D-ND	2.46	1.41	1.37
26	a	607	CLA	CMD-C2D	-2.46	1.45	1.50
26	A	834	CLA	MG-NB	-2.46	2.00	2.05
26	B	802	CLA	CMC-C2C	-2.46	1.45	1.50
26	B	837	CLA	CMC-C2C	-2.46	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	839	CLA	CMD-C2D	-2.46	1.45	1.50
26	B	810	CLA	CMC-C2C	-2.46	1.45	1.50
26	9	612	CLA	C3B-C4B	2.46	1.49	1.42
26	3	617	CLA	CMB-C2B	-2.46	1.45	1.50
26	8	610	CLA	CMC-C2C	-2.46	1.45	1.50
26	B	836	CLA	C1B-NB	-2.46	1.34	1.37
26	8	603	CLA	C1B-C2B	2.46	1.48	1.43
26	4	616	CLA	C4B-C3B	2.46	1.48	1.43
26	6	616	CLA	CMB-C2B	-2.46	1.45	1.50
26	B	819	CLA	CMD-C2D	-2.46	1.45	1.50
26	1	607	CLA	CMD-C2D	-2.46	1.45	1.50
26	A	822	CLA	CMB-C2B	-2.46	1.45	1.50
26	a	604	CLA	CMB-C2B	-2.45	1.45	1.50
26	K	204	CLA	C1B-C2B	2.45	1.48	1.43
26	3	611	CLA	C4B-C3B	2.45	1.48	1.43
26	6	620	CLA	CMD-C2D	-2.45	1.45	1.50
26	B	838	CLA	CMC-C2C	-2.45	1.45	1.50
26	7	616	CLA	CMC-C2C	-2.45	1.45	1.50
26	a	603	CLA	CMD-C2D	-2.45	1.45	1.50
26	5	616	CLA	CMB-C2B	-2.45	1.45	1.50
26	6	603	CLA	C4B-C3B	2.45	1.48	1.43
26	B	806	CLA	CMB-C2B	-2.45	1.45	1.50
26	8	606	CLA	C1B-C2B	2.45	1.48	1.43
35	U	1622	XAT	O24-C25	-2.45	1.43	1.46
26	6	620	CLA	C1B-C2B	2.45	1.48	1.43
26	B	809	CLA	CMD-C2D	-2.45	1.45	1.50
26	2	610	CLA	CMB-C2B	-2.45	1.45	1.50
26	Y	604	CLA	C1B-C2B	2.45	1.48	1.43
26	5	607	CLA	MG-NB	-2.45	2.00	2.05
26	1	602	CLA	C1B-C2B	2.45	1.48	1.43
26	2	604	CLA	C3B-C4B	2.45	1.49	1.42
26	A	837	CLA	CMD-C2D	-2.45	1.45	1.50
26	8	609	CLA	CMB-C2B	-2.45	1.45	1.50
26	1	614	CLA	C1B-C2B	2.44	1.48	1.43
26	B	805	CLA	CMC-C2C	-2.44	1.45	1.50
26	a	606	CLA	C1B-C2B	2.44	1.48	1.43
26	5	609	CLA	CMD-C2D	-2.44	1.45	1.50
26	5	619	CLA	CMB-C2B	-2.44	1.45	1.50
26	K	203	CLA	C1B-C2B	2.44	1.48	1.43
26	2	610	CLA	C3B-C4B	2.44	1.49	1.42
26	B	834	CLA	C4B-NB	2.44	1.41	1.37
26	4	601	CLA	CMD-C2D	-2.44	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	608	CLA	CMB-C2B	-2.44	1.45	1.50
26	5	613	CLA	C1B-C2B	2.44	1.48	1.43
26	8	607	CLA	C1B-C2B	2.44	1.48	1.43
26	W	610	CLA	C3B-C4B	2.44	1.49	1.42
26	F	304	CLA	CMC-C2C	-2.44	1.45	1.50
26	1	612	CLA	CMB-C2B	-2.44	1.45	1.50
26	1	608	CLA	CMD-C2D	-2.44	1.45	1.50
26	a	606	CLA	CMB-C2B	-2.44	1.45	1.50
26	9	609	CLA	CMB-C2B	-2.44	1.45	1.50
26	1	614	CLA	C4B-C3B	2.44	1.48	1.43
26	7	602	CLA	C3B-C4B	2.44	1.49	1.42
26	a	601	CLA	CMC-C2C	-2.44	1.45	1.50
26	9	613	CLA	CMD-C2D	-2.44	1.45	1.50
26	F	304	CLA	C1B-C2B	2.44	1.48	1.43
26	B	819	CLA	CMC-C2C	-2.43	1.45	1.50
26	F	304	CLA	CMB-C2B	-2.43	1.45	1.50
26	K	204	CLA	CMB-C2B	-2.43	1.45	1.50
26	6	620	CLA	CMC-C2C	-2.43	1.45	1.50
26	5	606	CLA	CMB-C2B	-2.43	1.45	1.50
26	A	826	CLA	C1D-ND	2.43	1.41	1.37
26	A	821	CLA	CMB-C2B	-2.43	1.45	1.50
26	B	823	CLA	CMB-C2B	-2.43	1.45	1.50
35	8	620	XAT	C22-C21	-2.43	1.50	1.54
26	a	608	CLA	CMD-C2D	-2.43	1.45	1.50
26	B	802	CLA	C1B-C2B	2.43	1.48	1.43
26	1	603	CLA	CMD-C2D	-2.43	1.45	1.50
26	4	612	CLA	CMD-C2D	-2.43	1.45	1.50
26	5	619	CLA	C4B-C3B	2.43	1.48	1.43
26	a	614	CLA	C1B-C2B	2.43	1.48	1.43
35	6	621	XAT	O24-C25	-2.43	1.43	1.46
26	A	828	CLA	CMB-C2B	-2.43	1.45	1.50
26	7	615	CLA	CMB-C2B	-2.43	1.45	1.50
26	4	616	CLA	CMD-C2D	-2.43	1.45	1.50
26	B	802	CLA	CMB-C2B	-2.43	1.45	1.50
26	9	603	CLA	C1B-C2B	2.43	1.48	1.43
26	Z	604	CLA	CMB-C2B	-2.43	1.45	1.50
26	B	808	CLA	CMD-C2D	-2.43	1.45	1.50
26	a	602	CLA	CMB-C2B	-2.43	1.45	1.50
26	7	606	CLA	CMD-C2D	-2.43	1.45	1.50
26	B	825	CLA	C1B-C2B	2.43	1.48	1.43
26	A	830	CLA	MG-NB	-2.43	2.01	2.05
26	5	601	CLA	CMD-C2D	-2.43	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	813	CLA	MG-NB	-2.42	2.01	2.05
26	A	830	CLA	C4B-NB	2.42	1.41	1.37
26	9	607	CLA	C1B-C2B	2.42	1.48	1.43
26	2	611	CLA	CMD-C2D	-2.42	1.45	1.50
26	W	604	CLA	CMB-C2B	-2.42	1.45	1.50
26	a	610	CLA	C1B-C2B	2.42	1.48	1.43
26	2	603	CLA	CMB-C2B	-2.42	1.45	1.50
26	3	617	CLA	C1B-C2B	2.42	1.48	1.43
26	B	802	CLA	C1D-ND	2.42	1.41	1.37
26	1	602	CLA	CMB-C2B	-2.42	1.45	1.50
26	U	613	CLA	C3B-C4B	2.42	1.49	1.42
26	H	203	CLA	CMB-C2B	-2.42	1.45	1.50
26	A	823	CLA	CMD-C2D	-2.42	1.45	1.50
26	A	839	CLA	MG-NB	-2.42	2.01	2.05
26	B	836	CLA	C4B-NB	2.42	1.41	1.37
26	3	607	CLA	C4B-C3B	2.42	1.48	1.43
26	1	604	CLA	CMD-C2D	-2.42	1.45	1.50
26	Z	611	CLA	CMB-C2B	-2.42	1.45	1.50
26	8	612	CLA	CMC-C2C	-2.42	1.45	1.50
26	A	819	CLA	MG-ND	-2.42	2.01	2.05
26	B	806	CLA	C1B-C2B	2.42	1.48	1.43
26	A	829	CLA	CMB-C2B	-2.42	1.45	1.50
26	A	810	CLA	CMC-C2C	-2.41	1.45	1.50
26	a	606	CLA	CMC-C2C	-2.41	1.45	1.50
26	a	616	CLA	CMD-C2D	-2.41	1.45	1.50
26	A	825	CLA	CMC-C2C	-2.41	1.45	1.50
26	a	604	CLA	CMD-C2D	-2.41	1.45	1.50
26	B	812	CLA	CMC-C2C	-2.41	1.45	1.50
26	A	841	CLA	CMB-C2B	-2.41	1.45	1.50
26	8	614	CLA	CMB-C2B	-2.41	1.45	1.50
26	A	830	CLA	CMB-C2B	-2.41	1.45	1.50
26	B	814	CLA	CMB-C2B	-2.41	1.45	1.50
26	B	835	CLA	C1B-C2B	2.41	1.48	1.43
26	7	612	CLA	CMC-C2C	-2.41	1.45	1.50
26	3	606	CLA	C4B-NB	2.41	1.41	1.37
26	a	609	CLA	CMB-C2B	-2.41	1.45	1.50
26	6	602	CLA	C3B-C4B	2.41	1.49	1.42
26	B	807	CLA	MG-NB	-2.41	2.01	2.05
26	B	832	CLA	CMC-C2C	-2.41	1.45	1.50
26	6	607	CLA	C1B-C2B	2.41	1.48	1.43
26	B	804	CLA	CMB-C2B	-2.41	1.45	1.50
26	5	606	CLA	C1B-C2B	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	601	CLA	C4B-NB	2.41	1.41	1.37
26	A	837	CLA	CMC-C2C	-2.41	1.45	1.50
26	8	610	CLA	C3B-C4B	2.41	1.49	1.42
26	B	822	CLA	CMD-C2D	-2.41	1.45	1.50
26	2	607	CLA	CMB-C2B	-2.41	1.45	1.50
37	U	607	CHL	CBD-CGD	-2.41	1.49	1.52
26	A	809	CLA	C4B-NB	2.40	1.41	1.37
26	7	608	CLA	C1B-C2B	2.40	1.48	1.43
26	1	601	CLA	CMC-C2C	-2.40	1.45	1.50
26	X	602	CLA	C1B-C2B	2.40	1.48	1.43
26	A	842	CLA	MG-NB	-2.40	2.01	2.05
26	3	603	CLA	MG-NB	-2.40	2.01	2.05
26	A	840	CLA	CMB-C2B	-2.40	1.45	1.50
26	3	617	CLA	CMD-C2D	-2.40	1.45	1.50
26	A	845	CLA	CMC-C2C	-2.40	1.45	1.50
26	2	614	CLA	CMB-C2B	-2.40	1.45	1.50
26	3	615	CLA	CMB-C2B	-2.40	1.45	1.50
26	B	812	CLA	C1B-C2B	2.40	1.48	1.43
26	B	834	CLA	C1B-C2B	2.40	1.48	1.43
26	7	610	CLA	C3B-C4B	2.40	1.49	1.42
26	9	609	CLA	CMC-C2C	-2.40	1.45	1.50
26	1	611	CLA	C1B-C2B	2.40	1.48	1.43
26	2	604	CLA	CMC-C2C	-2.40	1.45	1.50
26	B	833	CLA	C1B-C2B	2.40	1.48	1.43
26	B	825	CLA	CMC-C2C	-2.40	1.45	1.50
26	1	606	CLA	CMC-C2C	-2.40	1.45	1.50
26	6	613	CLA	CMC-C2C	-2.40	1.45	1.50
26	6	604	CLA	C1B-C2B	2.40	1.48	1.43
26	A	829	CLA	C3B-C4B	2.39	1.49	1.42
26	A	841	CLA	C1B-C2B	2.39	1.48	1.43
26	B	824	CLA	C1D-ND	2.39	1.41	1.37
26	A	835	CLA	CMC-C2C	-2.39	1.45	1.50
29	B	845	BCR	C1-C6	-2.39	1.50	1.53
26	A	825	CLA	C4B-NB	2.39	1.41	1.37
26	4	603	CLA	CMC-C2C	-2.39	1.45	1.50
26	A	843	CLA	MG-NB	-2.39	2.01	2.05
26	7	611	CLA	CMB-C2B	-2.39	1.45	1.50
26	B	811	CLA	C1B-C2B	2.39	1.48	1.43
26	6	618	CLA	C4B-C3B	2.39	1.48	1.43
26	U	604	CLA	C3B-C4B	2.39	1.49	1.42
26	B	804	CLA	C1B-C2B	2.39	1.48	1.43
26	1	609	CLA	CMB-C2B	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	614	CLA	C1B-C2B	2.39	1.48	1.43
26	4	610	CLA	C3B-C4B	2.39	1.49	1.42
26	3	612	CLA	CMD-C2D	-2.39	1.45	1.50
26	9	602	CLA	C1B-C2B	2.39	1.48	1.43
26	a	609	CLA	CMC-C2C	-2.39	1.45	1.50
26	6	602	CLA	CMD-C2D	-2.39	1.45	1.50
26	B	814	CLA	C1B-C2B	2.39	1.48	1.43
26	G	203	CLA	CMD-C2D	-2.38	1.45	1.50
26	A	804	CLA	CMC-C2C	-2.38	1.45	1.50
26	A	822	CLA	C4B-NB	2.38	1.41	1.37
26	a	614	CLA	CMB-C2B	-2.38	1.45	1.50
26	A	826	CLA	MG-NB	-2.38	2.01	2.05
29	3	622	BCR	C30-C25	-2.38	1.50	1.53
26	6	617	CLA	C1B-C2B	2.38	1.48	1.43
26	8	602	CLA	C3B-C4B	2.38	1.49	1.42
26	B	804	CLA	CMC-C2C	-2.38	1.45	1.50
26	8	602	CLA	CMB-C2B	-2.38	1.45	1.50
26	7	606	CLA	CMB-C2B	-2.38	1.45	1.50
26	7	611	CLA	C1B-C2B	2.38	1.48	1.43
26	6	610	CLA	C3B-C4B	2.38	1.49	1.42
26	8	603	CLA	C4B-C3B	2.38	1.48	1.43
26	A	840	CLA	CMC-C2C	-2.38	1.45	1.50
26	6	616	CLA	C1B-C2B	2.38	1.48	1.43
26	7	603	CLA	C1B-C2B	2.38	1.48	1.43
26	Z	614	CLA	C3B-C4B	2.38	1.49	1.42
26	B	832	CLA	C1B-C2B	2.38	1.48	1.43
26	Z	602	CLA	C3B-C4B	2.38	1.49	1.42
26	V	614	CLA	C1B-C2B	2.38	1.48	1.43
26	B	827	CLA	CMC-C2C	-2.38	1.45	1.50
26	B	839	CLA	MG-NB	-2.38	2.01	2.05
26	1	613	CLA	CMC-C2C	-2.38	1.45	1.50
26	A	820	CLA	CMC-C2C	-2.38	1.45	1.50
26	B	815	CLA	CMC-C2C	-2.38	1.45	1.50
26	5	602	CLA	CMD-C2D	-2.38	1.45	1.50
26	1	616	CLA	C1B-C2B	2.38	1.48	1.43
26	V	604	CLA	C1B-C2B	2.38	1.48	1.43
26	5	602	CLA	CMB-C2B	-2.37	1.45	1.50
26	G	204	CLA	CMD-C2D	-2.37	1.45	1.50
26	Y	602	CLA	C3B-C4B	2.37	1.49	1.42
26	B	803	CLA	C4B-NB	2.37	1.41	1.37
26	A	824	CLA	CMD-C2D	-2.37	1.45	1.50
26	2	614	CLA	C1B-C2B	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L	302	CLA	CMC-C2C	-2.37	1.45	1.50
26	O	2003	CLA	CMD-C2D	-2.37	1.45	1.50
26	6	610	CLA	CMC-C2C	-2.37	1.45	1.50
26	A	808	CLA	C1B-C2B	2.37	1.48	1.43
26	B	831	CLA	CMC-C2C	-2.37	1.45	1.50
26	6	604	CLA	CMC-C2C	-2.37	1.45	1.50
26	A	833	CLA	CMC-C2C	-2.37	1.45	1.50
26	1	616	CLA	CMD-C2D	-2.37	1.45	1.50
26	L	303	CLA	C4B-NB	2.37	1.41	1.37
26	6	602	CLA	C1B-C2B	2.37	1.48	1.43
29	A	848	BCR	C1-C6	-2.37	1.50	1.53
26	B	818	CLA	MG-NB	-2.37	2.01	2.05
26	5	606	CLA	CMC-C2C	-2.37	1.45	1.50
26	A	801	CLA	C4B-NB	2.37	1.41	1.37
26	A	812	CLA	CMC-C2C	-2.37	1.45	1.50
26	3	608	CLA	CMC-C2C	-2.37	1.45	1.50
26	6	607	CLA	CMB-C2B	-2.36	1.45	1.50
26	B	823	CLA	C4B-NB	2.36	1.41	1.37
26	5	614	CLA	CMD-C2D	-2.36	1.45	1.50
26	9	606	CLA	CMB-C2B	-2.36	1.45	1.50
26	Z	603	CLA	CMD-C2D	-2.36	1.45	1.50
26	9	610	CLA	CMC-C2C	-2.36	1.45	1.50
26	Y	610	CLA	C1B-C2B	2.36	1.48	1.43
26	3	606	CLA	C1B-C2B	2.36	1.48	1.43
26	5	609	CLA	CMC-C2C	-2.36	1.45	1.50
26	6	612	CLA	CMC-C2C	-2.36	1.45	1.50
26	8	604	CLA	C1B-C2B	2.36	1.48	1.43
26	3	606	CLA	MG-NB	-2.36	2.01	2.05
26	X	614	CLA	C3B-C4B	2.36	1.49	1.42
26	7	603	CLA	CMC-C2C	-2.36	1.45	1.50
26	B	822	CLA	CMB-C2B	-2.36	1.45	1.50
26	2	607	CLA	CMD-C2D	-2.36	1.45	1.50
26	6	601	CLA	CMB-C2B	-2.36	1.45	1.50
26	a	604	CLA	C1B-C2B	2.36	1.48	1.43
26	a	616	CLA	C1B-C2B	2.36	1.48	1.43
26	4	607	CLA	C1B-C2B	2.36	1.48	1.43
29	5	622	BCR	C30-C25	-2.36	1.50	1.53
26	Z	611	CLA	C1B-C2B	2.36	1.48	1.43
26	3	606	CLA	CMC-C2C	-2.36	1.45	1.50
26	3	615	CLA	CMD-C2D	-2.36	1.45	1.50
26	8	608	CLA	MG-NB	-2.36	2.01	2.05
26	B	838	CLA	C1B-C2B	2.36	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	612	CLA	C1B-C2B	2.36	1.48	1.43
26	2	601	CLA	CMD-C2D	-2.36	1.45	1.50
26	L	306	CLA	C1B-C2B	2.36	1.48	1.43
35	2	620	XAT	O24-C25	-2.35	1.43	1.46
26	1	614	CLA	CMB-C2B	-2.35	1.45	1.50
26	3	603	CLA	CMB-C2B	-2.35	1.45	1.50
26	B	830	CLA	C1B-C2B	2.35	1.48	1.43
26	W	604	CLA	C1B-C2B	2.35	1.48	1.43
26	3	607	CLA	CMD-C2D	-2.35	1.45	1.50
26	3	607	CLA	CMB-C2B	-2.35	1.45	1.50
26	A	803	CLA	C4B-NB	2.35	1.41	1.37
26	L	306	CLA	CMD-C2D	-2.35	1.46	1.50
26	K	203	CLA	MG-NB	-2.35	2.01	2.05
26	B	833	CLA	CMB-C2B	-2.35	1.46	1.50
26	4	616	CLA	CMC-C2C	-2.35	1.46	1.50
26	9	613	CLA	CMC-C2C	-2.35	1.46	1.50
26	6	601	CLA	C1B-C2B	2.35	1.48	1.43
26	Z	610	CLA	C3B-C4B	2.35	1.49	1.42
26	9	606	CLA	CMC-C2C	-2.35	1.46	1.50
26	B	836	CLA	MG-NB	-2.35	2.01	2.05
26	7	601	CLA	C4B-NB	2.35	1.40	1.37
26	B	831	CLA	CMB-C2B	-2.35	1.46	1.50
26	9	607	CLA	CMB-C2B	-2.35	1.46	1.50
26	A	802	CLA	CMB-C2B	-2.35	1.46	1.50
26	2	606	CLA	CMC-C2C	-2.35	1.46	1.50
31	A	858	LMU	C3B-C2B	-2.35	1.48	1.52
26	2	613	CLA	CMB-C2B	-2.35	1.46	1.50
26	A	823	CLA	CMB-C2B	-2.35	1.46	1.50
26	F	301	CLA	CMC-C2C	-2.34	1.46	1.50
26	A	814	CLA	CMD-C2D	-2.34	1.46	1.50
29	B	853	BCR	C1-C6	-2.34	1.50	1.53
26	L	304	CLA	CMC-C2C	-2.34	1.46	1.50
26	5	604	CLA	CMC-C2C	-2.34	1.46	1.50
26	5	607	CLA	CMC-C2C	-2.34	1.46	1.50
26	6	604	CLA	CMD-C2D	-2.34	1.46	1.50
26	B	841	CLA	C1B-C2B	2.34	1.48	1.43
26	A	833	CLA	C1B-NB	-2.34	1.34	1.37
26	Z	602	CLA	CMC-C2C	-2.34	1.46	1.50
26	4	606	CLA	CMB-C2B	-2.34	1.46	1.50
26	B	840	CLA	MG-NB	-2.34	2.01	2.05
26	9	604	CLA	CMC-C2C	-2.34	1.46	1.50
26	W	602	CLA	C3B-C4B	2.34	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	204	CLA	C1B-C2B	2.34	1.48	1.43
26	8	609	CLA	C1B-C2B	2.34	1.48	1.43
26	V	610	CLA	C1B-C2B	2.34	1.48	1.43
26	O	2001	CLA	CMB-C2B	-2.34	1.46	1.50
26	6	609	CLA	CMD-C2D	-2.34	1.46	1.50
26	5	612	CLA	C3B-C4B	2.34	1.49	1.42
37	V	606	CHL	CBD-CGD	-2.34	1.49	1.52
26	5	608	CLA	CMB-C2B	-2.34	1.46	1.50
35	3	619	XAT	O4-C5	-2.34	1.43	1.46
26	4	601	CLA	C1B-C2B	2.34	1.48	1.43
26	B	805	CLA	MG-NB	-2.34	2.01	2.05
26	A	809	CLA	MG-NB	-2.34	2.01	2.05
26	3	606	CLA	CMD-C2D	-2.33	1.46	1.50
26	9	602	CLA	CMB-C2B	-2.33	1.46	1.50
26	B	803	CLA	C1B-C2B	2.33	1.48	1.43
26	A	802	CLA	C3B-C4B	2.33	1.49	1.42
26	B	816	CLA	CMD-C2D	-2.33	1.46	1.50
26	a	602	CLA	C3B-C4B	2.33	1.49	1.42
26	H	202	CLA	CMD-C2D	-2.33	1.46	1.50
26	X	610	CLA	CHC-C1C	2.33	1.43	1.38
26	A	854	CLA	CMD-C2D	-2.33	1.46	1.50
26	O	2002	CLA	CMC-C2C	-2.33	1.46	1.50
26	1	607	CLA	C3B-C4B	2.33	1.49	1.42
26	F	303	CLA	C1B-C2B	2.33	1.48	1.43
26	a	607	CLA	CMB-C2B	-2.33	1.46	1.50
26	B	820	CLA	CMC-C2C	-2.33	1.46	1.50
26	6	613	CLA	CMD-C2D	-2.33	1.46	1.50
26	A	826	CLA	MG-ND	-2.33	2.01	2.05
26	B	803	CLA	CMB-C2B	-2.33	1.46	1.50
26	8	606	CLA	CMB-C2B	-2.33	1.46	1.50
26	A	840	CLA	MG-NB	-2.33	2.01	2.05
26	B	830	CLA	CMD-C2D	-2.33	1.46	1.50
26	K	206	CLA	CMC-C2C	-2.33	1.46	1.50
26	A	840	CLA	C1B-C2B	2.33	1.48	1.43
26	9	603	CLA	CMC-C2C	-2.33	1.46	1.50
26	4	603	CLA	C4B-C3B	2.33	1.48	1.43
26	3	602	CLA	CMD-C2D	-2.33	1.46	1.50
26	5	606	CLA	CMD-C2D	-2.33	1.46	1.50
26	U	611	CLA	C3B-C4B	2.33	1.49	1.42
26	a	611	CLA	C1B-C2B	2.33	1.48	1.43
37	Y	607	CHL	CBD-CGD	-2.33	1.49	1.52
26	A	841	CLA	MG-NB	-2.33	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	845	CLA	C3B-C4B	2.33	1.49	1.42
26	A	802	CLA	C4B-NB	2.32	1.40	1.37
26	7	606	CLA	MG-NB	-2.32	2.01	2.05
26	A	808	CLA	CMB-C2B	-2.32	1.46	1.50
26	5	616	CLA	C4B-C3B	2.32	1.48	1.43
26	a	613	CLA	CMC-C2C	-2.32	1.46	1.50
26	4	606	CLA	CMD-C2D	-2.32	1.46	1.50
26	K	204	CLA	MG-NB	-2.32	2.01	2.05
26	B	819	CLA	C3B-C4B	2.32	1.49	1.42
26	a	613	CLA	C1B-C2B	2.32	1.48	1.43
26	V	611	CLA	C3B-C4B	2.32	1.49	1.42
26	A	818	CLA	CMC-C2C	-2.32	1.46	1.50
26	V	614	CLA	C3B-C4B	2.32	1.49	1.42
26	K	201	CLA	CMD-C2D	-2.32	1.46	1.50
26	A	824	CLA	C1B-C2B	2.32	1.48	1.43
26	A	827	CLA	C1B-C2B	2.32	1.48	1.43
26	A	838	CLA	C1B-C2B	2.32	1.48	1.43
26	4	613	CLA	C3B-C4B	2.32	1.49	1.42
26	A	830	CLA	C1D-ND	2.32	1.40	1.37
26	A	837	CLA	C1B-C2B	2.32	1.48	1.43
26	1	604	CLA	C1B-C2B	2.32	1.48	1.43
26	V	602	CLA	C3B-C4B	2.32	1.49	1.42
26	A	804	CLA	C4B-NB	2.32	1.40	1.37
26	a	607	CLA	C3B-C4B	2.32	1.49	1.42
26	5	608	CLA	CMC-C2C	-2.32	1.46	1.50
26	5	614	CLA	CMB-C2B	-2.32	1.46	1.50
26	A	814	CLA	C1B-C2B	2.32	1.48	1.43
26	U	614	CLA	C3B-C4B	2.32	1.49	1.42
26	O	2003	CLA	CMB-C2B	-2.31	1.46	1.50
37	U	608	CHL	CBD-CGD	-2.31	1.49	1.52
26	3	614	CLA	CMB-C2B	-2.31	1.46	1.50
26	A	803	CLA	MG-ND	-2.31	2.01	2.05
26	B	837	CLA	MG-NB	-2.31	2.01	2.05
26	5	603	CLA	C4B-C3B	2.31	1.48	1.43
26	A	813	CLA	MG-NB	-2.31	2.01	2.05
35	6	621	XAT	O4-C5	-2.31	1.43	1.46
26	U	613	CLA	CMC-C2C	-2.31	1.46	1.50
26	O	2002	CLA	C1B-C2B	2.31	1.48	1.43
26	7	614	CLA	CMC-C2C	-2.31	1.46	1.50
26	A	836	CLA	C4B-NB	2.31	1.40	1.37
26	2	601	CLA	CMC-C2C	-2.31	1.46	1.50
26	B	805	CLA	C4B-NB	2.31	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	853	BCR	C30-C25	-2.31	1.50	1.53
26	A	810	CLA	CMB-C2B	-2.31	1.46	1.50
26	2	604	CLA	CMD-C2D	-2.31	1.46	1.50
26	3	614	CLA	C1B-C2B	2.31	1.48	1.43
26	7	606	CLA	C1B-C2B	2.31	1.48	1.43
26	B	802	CLA	MG-NB	-2.31	2.01	2.05
26	A	841	CLA	C4B-NB	2.31	1.40	1.37
26	B	821	CLA	C1B-C2B	2.31	1.48	1.43
26	1	609	CLA	CMC-C2C	-2.31	1.46	1.50
26	A	834	CLA	C1B-C2B	2.31	1.48	1.43
26	4	607	CLA	CMD-C2D	-2.31	1.46	1.50
26	a	601	CLA	C1B-C2B	2.31	1.48	1.43
26	A	806	CLA	C4B-NB	2.31	1.40	1.37
26	4	608	CLA	CMB-C2B	-2.31	1.46	1.50
35	4	620	XAT	O24-C25	-2.31	1.43	1.46
26	5	613	CLA	CMB-C2B	-2.31	1.46	1.50
26	6	603	CLA	CMC-C2C	-2.31	1.46	1.50
26	8	611	CLA	CMC-C2C	-2.31	1.46	1.50
35	5	621	XAT	O24-C25	-2.31	1.43	1.46
26	1	601	CLA	C1B-C2B	2.30	1.48	1.43
35	9	620	XAT	O24-C25	-2.30	1.43	1.46
36	V	1623	NEX	O24-C25	-2.30	1.43	1.46
26	2	610	CLA	CHC-C1C	2.30	1.43	1.38
26	7	601	CLA	CMC-C2C	-2.30	1.46	1.50
26	B	808	CLA	C1B-C2B	2.30	1.48	1.43
26	8	604	CLA	CMC-C2C	-2.30	1.46	1.50
26	9	604	CLA	C1B-C2B	2.30	1.48	1.43
26	B	838	CLA	CMB-C2B	-2.30	1.46	1.50
26	3	611	CLA	CMD-C2D	-2.30	1.46	1.50
29	B	844	BCR	C1-C6	-2.30	1.50	1.53
26	6	608	CLA	C1B-C2B	2.30	1.48	1.43
26	1	614	CLA	CMD-C2D	-2.30	1.46	1.50
26	9	601	CLA	CMD-C2D	-2.30	1.46	1.50
26	A	812	CLA	C1B-C2B	2.30	1.48	1.43
26	2	602	CLA	CMD-C2D	-2.30	1.46	1.50
26	8	602	CLA	C1B-C2B	2.30	1.48	1.43
26	B	828	CLA	MG-NB	-2.30	2.01	2.05
26	7	615	CLA	C1B-C2B	2.30	1.48	1.43
26	8	610	CLA	C1B-C2B	2.30	1.48	1.43
26	U	610	CLA	C3B-C4B	2.30	1.49	1.42
26	F	303	CLA	CMC-C2C	-2.30	1.46	1.50
26	B	817	CLA	MG-NB	-2.30	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	606	CLA	C3B-C4B	2.30	1.49	1.42
26	Z	612	CLA	C3B-C4B	2.30	1.49	1.42
35	5	621	XAT	O4-C5	-2.30	1.43	1.46
26	1	613	CLA	C1B-C2B	2.30	1.48	1.43
26	H	203	CLA	CMC-C2C	-2.30	1.46	1.50
26	a	606	CLA	CMD-C2D	-2.30	1.46	1.50
26	1	602	CLA	C3B-C4B	2.30	1.49	1.42
26	A	835	CLA	MG-NB	-2.30	2.01	2.05
26	X	602	CLA	C3B-C4B	2.30	1.49	1.42
26	Z	602	CLA	CHC-C1C	2.30	1.43	1.38
26	W	604	CLA	C3B-C4B	2.30	1.49	1.42
26	8	614	CLA	CMC-C2C	-2.30	1.46	1.50
26	A	825	CLA	MG-NB	-2.30	2.01	2.05
26	1	610	CLA	CMC-C2C	-2.29	1.46	1.50
26	Y	610	CLA	CMB-C2B	-2.29	1.46	1.50
26	B	826	CLA	MG-NB	-2.29	2.01	2.05
26	B	841	CLA	CMD-C2D	-2.29	1.46	1.50
26	B	823	CLA	C1B-C2B	2.29	1.48	1.43
26	U	612	CLA	C3B-C4B	2.29	1.49	1.42
26	7	603	CLA	MG-NB	-2.29	2.01	2.05
27	A	844	PQN	C10-C1	2.29	1.52	1.48
26	a	611	CLA	CMD-C2D	-2.29	1.46	1.50
26	a	614	CLA	CMD-C2D	-2.29	1.46	1.50
26	A	811	CLA	C1B-C2B	2.29	1.48	1.43
26	8	613	CLA	C1B-C2B	2.29	1.48	1.43
26	2	607	CLA	MG-NB	-2.29	2.01	2.05
26	A	829	CLA	MG-NB	-2.29	2.01	2.05
26	Z	604	CLA	C1B-C2B	2.29	1.48	1.43
26	2	616	CLA	CMD-C2D	-2.29	1.46	1.50
26	9	601	CLA	CMB-C2B	-2.29	1.46	1.50
26	Y	611	CLA	CMD-C2D	-2.29	1.46	1.50
26	3	610	CLA	CHC-C1C	2.29	1.43	1.38
26	9	611	CLA	CMD-C2D	-2.29	1.46	1.50
26	3	602	CLA	C1B-C2B	2.29	1.48	1.43
26	8	601	CLA	CMC-C2C	-2.29	1.46	1.50
26	B	841	CLA	CMB-C2B	-2.29	1.46	1.50
26	1	606	CLA	CMD-C2D	-2.29	1.46	1.50
26	3	613	CLA	C1B-C2B	2.29	1.48	1.43
26	B	816	CLA	MG-NB	-2.29	2.01	2.05
26	a	607	CLA	C1B-C2B	2.28	1.48	1.43
26	6	610	CLA	CMB-C2B	-2.28	1.46	1.50
26	Y	611	CLA	C3B-C4B	2.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	206	CLA	CMD-C2D	-2.28	1.46	1.50
26	5	613	CLA	CMC-C2C	-2.28	1.46	1.50
26	A	818	CLA	C1B-C2B	2.28	1.48	1.43
26	4	609	CLA	CMC-C2C	-2.28	1.46	1.50
26	7	614	CLA	MG-NB	-2.28	2.01	2.05
26	B	836	CLA	C1B-C2B	2.28	1.48	1.43
26	Z	611	CLA	C4B-C3B	2.28	1.48	1.43
26	B	815	CLA	C1B-C2B	2.28	1.48	1.43
26	A	807	CLA	C3B-C4B	2.28	1.49	1.42
26	W	603	CLA	CMD-C2D	-2.28	1.46	1.50
26	Y	612	CLA	C3B-C4B	2.28	1.49	1.42
26	2	614	CLA	CMC-C2C	-2.28	1.46	1.50
26	A	838	CLA	C4B-NB	2.28	1.40	1.37
26	a	610	CLA	CMC-C2C	-2.28	1.46	1.50
26	5	610	CLA	CMB-C2B	-2.28	1.46	1.50
26	6	614	CLA	CMC-C2C	-2.28	1.46	1.50
26	B	805	CLA	C1B-NB	-2.28	1.34	1.37
26	5	607	CLA	CMD-C2D	-2.28	1.46	1.50
26	1	601	CLA	CMB-C2B	-2.28	1.46	1.50
26	4	603	CLA	CMB-C2B	-2.28	1.46	1.50
26	1	611	CLA	CMD-C2D	-2.28	1.46	1.50
26	8	612	CLA	CMB-C2B	-2.28	1.46	1.50
26	9	614	CLA	C3B-C4B	2.28	1.49	1.42
26	A	838	CLA	MG-NB	-2.28	2.01	2.05
26	A	838	CLA	CMC-C2C	-2.28	1.46	1.50
26	6	608	CLA	CMC-C2C	-2.27	1.46	1.50
26	2	601	CLA	CMB-C2B	-2.27	1.46	1.50
26	B	812	CLA	C3B-C4B	2.27	1.49	1.42
26	4	612	CLA	C3B-C4B	2.27	1.49	1.42
26	B	811	CLA	C4B-C3B	2.27	1.48	1.43
26	L	302	CLA	MG-NB	-2.27	2.01	2.05
26	A	830	CLA	C1B-C2B	2.27	1.48	1.43
26	8	607	CLA	CMB-C2B	-2.27	1.46	1.50
26	5	612	CLA	CMD-C2D	-2.27	1.46	1.50
26	9	607	CLA	CMC-C2C	-2.27	1.46	1.50
26	W	613	CLA	CMD-C2D	-2.27	1.46	1.50
26	A	804	CLA	MG-NB	-2.27	2.01	2.05
26	F	301	CLA	C1B-C2B	2.27	1.48	1.43
26	B	824	CLA	C1B-C2B	2.27	1.48	1.43
26	Z	610	CLA	CMC-C2C	-2.27	1.46	1.50
26	A	843	CLA	C3B-C4B	2.27	1.49	1.42
26	X	612	CLA	C3B-C4B	2.27	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	W	1623	NEX	O24-C25	-2.27	1.43	1.46
26	B	823	CLA	CMC-C2C	-2.27	1.46	1.50
26	A	815	CLA	MG-NB	-2.27	2.01	2.05
26	L	302	CLA	CMD-C2D	-2.27	1.46	1.50
26	W	611	CLA	C3B-C4B	2.27	1.49	1.42
26	1	609	CLA	C4B-C3B	2.27	1.48	1.43
26	4	604	CLA	CMC-C2C	-2.26	1.46	1.50
26	a	614	CLA	MG-NB	-2.26	2.01	2.05
26	5	613	CLA	CMD-C2D	-2.26	1.46	1.50
26	A	806	CLA	C1B-NB	-2.26	1.34	1.37
26	1	602	CLA	MG-NB	-2.26	2.01	2.05
26	J	101	CLA	CMB-C2B	-2.26	1.46	1.50
26	4	606	CLA	CMC-C2C	-2.26	1.46	1.50
36	6	624	NEX	O24-C25	-2.26	1.43	1.46
26	A	803	CLA	MG-NB	-2.26	2.01	2.05
26	6	606	CLA	CMD-C2D	-2.26	1.46	1.50
26	6	611	CLA	CMC-C2C	-2.26	1.46	1.50
26	8	606	CLA	CMD-C2D	-2.26	1.46	1.50
26	A	837	CLA	MG-NB	-2.26	2.01	2.05
26	7	604	CLA	C1B-C2B	2.26	1.48	1.43
26	B	824	CLA	MG-ND	-2.26	2.01	2.05
26	8	610	CLA	CMB-C2B	-2.26	1.46	1.50
26	B	825	CLA	CMB-C2B	-2.26	1.46	1.50
26	B	829	CLA	C1B-NB	-2.26	1.34	1.37
26	7	608	CLA	CMC-C2C	-2.26	1.46	1.50
26	W	612	CLA	CMD-C2D	-2.26	1.46	1.50
26	A	802	CLA	MG-ND	-2.26	2.01	2.05
26	2	606	CLA	CMB-C2B	-2.26	1.46	1.50
26	8	609	CLA	CMC-C2C	-2.26	1.46	1.50
27	A	844	PQN	C5-C4	2.26	1.52	1.48
26	6	601	CLA	CMD-C2D	-2.26	1.46	1.50
26	6	606	CLA	CMB-C2B	-2.26	1.46	1.50
26	6	607	CLA	CMD-C2D	-2.26	1.46	1.50
26	6	618	CLA	CMD-C2D	-2.26	1.46	1.50
26	B	823	CLA	MG-NB	-2.25	2.01	2.05
26	W	614	CLA	C3B-C4B	2.25	1.49	1.42
26	A	809	CLA	CMC-C2C	-2.25	1.46	1.50
26	Z	613	CLA	CMB-C2B	-2.25	1.46	1.50
26	Z	604	CLA	C3B-C4B	2.25	1.49	1.42
37	Y	609	CHL	CBD-CGD	-2.25	1.49	1.52
26	8	604	CLA	C3B-C4B	2.25	1.49	1.42
26	6	608	CLA	CMD-C2D	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	602	CLA	MG-NB	-2.25	2.01	2.05
26	6	612	CLA	CMB-C2B	-2.25	1.46	1.50
26	7	606	CLA	CMC-C2C	-2.25	1.46	1.50
26	B	817	CLA	MG-ND	-2.25	2.01	2.05
26	4	616	CLA	CMB-C2B	-2.25	1.46	1.50
26	B	830	CLA	CMC-C2C	-2.25	1.46	1.50
26	a	612	CLA	CMC-C2C	-2.25	1.46	1.50
26	5	610	CLA	CMD-C2D	-2.25	1.46	1.50
26	A	822	CLA	C3B-C4B	2.25	1.49	1.42
26	8	601	CLA	C3B-C4B	2.25	1.49	1.42
26	X	611	CLA	C3B-C4B	2.25	1.49	1.42
26	B	806	CLA	MG-NB	-2.25	2.01	2.05
26	2	604	CLA	C1B-C2B	2.25	1.48	1.43
26	1	610	CLA	C3B-C4B	2.25	1.49	1.42
26	B	838	CLA	MG-NB	-2.25	2.01	2.05
26	2	609	CLA	C3B-C4B	2.25	1.49	1.42
26	6	606	CLA	CMC-C2C	-2.25	1.46	1.50
26	6	614	CLA	CMB-C2B	-2.25	1.46	1.50
26	3	612	CLA	CMC-C2C	-2.25	1.46	1.50
26	9	602	CLA	C3B-C4B	2.25	1.49	1.42
26	6	609	CLA	C1B-C2B	2.25	1.48	1.43
26	6	602	CLA	CMB-C2B	-2.25	1.46	1.50
26	9	601	CLA	CMC-C2C	-2.24	1.46	1.50
26	Y	613	CLA	CMD-C2D	-2.24	1.46	1.50
26	1	607	CLA	CMB-C2B	-2.24	1.46	1.50
26	2	612	CLA	CMD-C2D	-2.24	1.46	1.50
26	8	604	CLA	CMD-C2D	-2.24	1.46	1.50
29	2	623	BCR	C30-C25	-2.24	1.50	1.53
26	1	612	CLA	CMC-C2C	-2.24	1.46	1.50
26	Z	614	CLA	CMD-C2D	-2.24	1.46	1.50
26	5	618	CLA	CMB-C2B	-2.24	1.46	1.50
26	A	807	CLA	MG-NB	-2.24	2.01	2.05
26	A	830	CLA	CMC-C2C	-2.24	1.46	1.50
37	X	609	CHL	CMC-C2C	2.24	1.49	1.44
26	A	809	CLA	C1B-NB	-2.24	1.34	1.37
26	6	613	CLA	C3B-C4B	2.24	1.49	1.42
26	B	834	CLA	CMC-C2C	-2.24	1.46	1.50
26	9	607	CLA	CMD-C2D	-2.24	1.46	1.50
26	Y	613	CLA	CMC-C2C	-2.24	1.46	1.50
26	B	826	CLA	CMB-C2B	-2.24	1.46	1.50
26	7	608	CLA	MG-NB	-2.24	2.01	2.05
26	1	611	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	826	CLA	C3B-C4B	2.24	1.49	1.42
26	1	607	CLA	C1B-C2B	2.23	1.48	1.43
26	O	2003	CLA	CMC-C2C	-2.23	1.46	1.50
26	7	607	CLA	CMC-C2C	-2.23	1.46	1.50
26	Y	614	CLA	C3B-C4B	2.23	1.49	1.42
29	G	205	BCR	C1-C6	-2.23	1.50	1.53
26	B	810	CLA	MG-NB	-2.23	2.01	2.05
26	B	810	CLA	C1B-NB	-2.23	1.34	1.37
26	A	827	CLA	CMC-C2C	-2.23	1.46	1.50
26	a	603	CLA	CMC-C2C	-2.23	1.46	1.50
26	8	607	CLA	CMC-C2C	-2.23	1.46	1.50
26	X	604	CLA	C3B-C4B	2.23	1.49	1.42
26	U	604	CLA	C1B-C2B	2.23	1.48	1.43
26	3	604	CLA	C1B-C2B	2.23	1.48	1.43
26	A	836	CLA	CMC-C2C	-2.23	1.46	1.50
26	A	843	CLA	CMC-C2C	-2.23	1.46	1.50
26	V	603	CLA	CMD-C2D	-2.23	1.46	1.50
26	4	602	CLA	CHC-C1C	2.23	1.43	1.38
26	X	603	CLA	C3B-C4B	2.23	1.49	1.42
26	6	603	CLA	CMB-C2B	-2.23	1.46	1.50
26	B	809	CLA	MG-NB	-2.23	2.01	2.05
26	A	810	CLA	C1B-C2B	2.23	1.48	1.43
26	O	2002	CLA	CMB-C2B	-2.23	1.46	1.50
26	F	304	CLA	C3B-C4B	2.23	1.49	1.42
26	V	610	CLA	C3B-C4B	2.23	1.49	1.42
26	A	804	CLA	CMB-C2B	-2.23	1.46	1.50
36	W	1623	NEX	C7-C6	-2.23	1.28	1.30
37	V	605	CHL	CBD-CGD	-2.23	1.49	1.52
26	X	613	CLA	CMB-C2B	-2.23	1.46	1.50
26	3	614	CLA	CMC-C2C	-2.23	1.46	1.50
26	6	611	CLA	CMB-C2B	-2.23	1.46	1.50
26	a	606	CLA	C3B-C4B	2.23	1.49	1.42
26	2	612	CLA	CMB-C2B	-2.23	1.46	1.50
26	B	836	CLA	C3B-C4B	2.22	1.49	1.42
26	A	827	CLA	MG-NB	-2.22	2.01	2.05
26	4	604	CLA	CMB-C2B	-2.22	1.46	1.50
26	V	612	CLA	CMD-C2D	-2.22	1.46	1.50
26	A	826	CLA	C1B-NB	-2.22	1.34	1.37
37	V	607	CHL	CBD-CGD	-2.22	1.49	1.52
26	A	814	CLA	MG-NB	-2.22	2.01	2.05
26	3	608	CLA	MG-NB	-2.22	2.01	2.05
29	K	202	BCR	C30-C25	-2.22	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	845	CLA	C1B-C2B	2.22	1.48	1.43
26	8	608	CLA	C1B-C2B	2.22	1.48	1.43
26	B	821	CLA	CMD-C2D	-2.22	1.46	1.50
26	2	612	CLA	C3B-C4B	2.22	1.49	1.42
35	W	1622	XAT	O24-C25	-2.22	1.43	1.46
26	Y	614	CLA	CMD-C2D	-2.22	1.46	1.50
26	7	601	CLA	MG-ND	-2.22	2.01	2.05
26	5	617	CLA	CMC-C2C	-2.22	1.46	1.50
26	1	611	CLA	CMB-C2B	-2.22	1.46	1.50
26	G	203	CLA	CMB-C2B	-2.22	1.46	1.50
29	F	305	BCR	C30-C25	-2.22	1.50	1.53
26	U	603	CLA	CMD-C2D	-2.22	1.46	1.50
37	Y	609	CHL	CMC-C2C	2.22	1.49	1.44
26	A	828	CLA	CMC-C2C	-2.22	1.46	1.50
26	U	602	CLA	C3B-C4B	2.22	1.49	1.42
26	B	828	CLA	C1B-C2B	2.22	1.48	1.43
37	W	609	CHL	CBD-CGD	-2.22	1.49	1.52
26	A	831	CLA	MG-NB	-2.22	2.01	2.05
26	7	614	CLA	CMB-C2B	-2.22	1.46	1.50
26	V	602	CLA	CMC-C2C	-2.22	1.46	1.50
26	8	603	CLA	CMC-C2C	-2.21	1.46	1.50
26	Z	610	CLA	CMB-C2B	-2.21	1.46	1.50
26	A	822	CLA	MG-NB	-2.21	2.01	2.05
26	A	832	CLA	MG-NB	-2.21	2.01	2.05
26	A	815	CLA	C1B-C2B	2.21	1.48	1.43
26	6	616	CLA	CMD-C2D	-2.21	1.46	1.50
26	U	602	CLA	CMB-C2B	-2.21	1.46	1.50
35	Y	1622	XAT	O4-C5	-2.21	1.43	1.46
26	6	608	CLA	C3B-C4B	2.21	1.49	1.42
26	6	618	CLA	CMB-C2B	-2.21	1.46	1.50
26	a	610	CLA	C3B-C4B	2.21	1.49	1.42
26	B	822	CLA	CMC-C2C	-2.21	1.46	1.50
26	B	807	CLA	MG-ND	-2.21	2.01	2.05
26	Y	602	CLA	CMC-C2C	-2.21	1.46	1.50
26	G	203	CLA	CMC-C2C	-2.21	1.46	1.50
26	2	603	CLA	CMC-C2C	-2.21	1.46	1.50
26	6	601	CLA	CMC-C2C	-2.21	1.46	1.50
26	a	601	CLA	CMB-C2B	-2.21	1.46	1.50
26	7	609	CLA	C1B-C2B	2.21	1.48	1.43
26	B	838	CLA	C3B-C4B	2.21	1.49	1.42
26	Y	603	CLA	CMB-C2B	-2.21	1.46	1.50
26	A	807	CLA	C1B-NB	-2.21	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	614	CLA	MG-NB	-2.21	2.01	2.05
26	1	604	CLA	CMC-C2C	-2.21	1.46	1.50
26	a	611	CLA	CMB-C2B	-2.21	1.46	1.50
37	Z	601	CHL	CMC-C2C	2.21	1.49	1.44
26	V	604	CLA	C3B-C4B	2.21	1.49	1.42
29	J	102	BCR	C30-C25	-2.21	1.51	1.53
26	V	604	CLA	CMB-C2B	-2.21	1.46	1.50
26	6	617	CLA	C3B-C4B	2.21	1.49	1.42
26	B	840	CLA	C1B-C2B	2.20	1.48	1.43
26	4	608	CLA	CMC-C2C	-2.20	1.46	1.50
26	L	306	CLA	CMB-C2B	-2.20	1.46	1.50
26	a	607	CLA	CMC-C2C	-2.20	1.46	1.50
26	3	603	CLA	CMC-C2C	-2.20	1.46	1.50
26	A	835	CLA	C1B-C2B	2.20	1.48	1.43
26	B	809	CLA	C1B-C2B	2.20	1.48	1.43
26	6	610	CLA	C1B-C2B	2.20	1.48	1.43
26	A	805	CLA	MG-NB	-2.20	2.01	2.05
26	Z	610	CLA	CHC-C1C	2.20	1.42	1.38
26	3	603	CLA	MG-ND	-2.20	2.01	2.05
26	B	816	CLA	C1B-C2B	2.20	1.48	1.43
26	X	602	CLA	CMC-C2C	-2.20	1.46	1.50
37	W	606	CHL	CMC-C2C	2.20	1.49	1.44
26	V	613	CLA	CMC-C2C	-2.20	1.46	1.50
26	V	612	CLA	C3B-C4B	2.20	1.49	1.42
26	B	834	CLA	MG-NB	-2.20	2.01	2.05
26	6	618	CLA	CMC-C2C	-2.20	1.46	1.50
26	9	614	CLA	CMB-C2B	-2.20	1.46	1.50
35	6	621	XAT	C22-C21	-2.20	1.51	1.54
26	7	606	CLA	C3B-C4B	2.20	1.49	1.42
26	Z	602	CLA	CMD-C2D	-2.20	1.46	1.50
26	B	835	CLA	MG-NB	-2.20	2.01	2.05
29	A	856	BCR	C1-C6	-2.20	1.51	1.53
26	3	602	CLA	C3B-C4B	2.20	1.49	1.42
26	A	823	CLA	MG-NB	-2.20	2.01	2.05
37	U	601	CHL	CMC-C2C	2.20	1.49	1.44
26	1	603	CLA	CMC-C2C	-2.20	1.46	1.50
26	3	608	CLA	C1B-C2B	2.20	1.48	1.43
26	a	613	CLA	MG-NB	-2.20	2.01	2.05
35	9	620	XAT	O4-C5	-2.20	1.43	1.46
26	V	603	CLA	CMB-C2B	-2.20	1.46	1.50
26	G	203	CLA	C3B-C4B	2.20	1.49	1.42
35	8	620	XAT	O4-C5	-2.19	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	3	621	BCR	C1-C6	-2.19	1.51	1.53
26	B	839	CLA	CHC-C4B	-2.19	1.34	1.39
35	2	620	XAT	C22-C21	-2.19	1.51	1.54
26	a	610	CLA	CMB-C2B	-2.19	1.46	1.50
26	V	611	CLA	CMD-C2D	-2.19	1.46	1.50
26	A	836	CLA	C1B-C2B	2.19	1.48	1.43
26	9	603	CLA	MG-NB	-2.19	2.01	2.05
26	4	612	CLA	CMC-C2C	-2.19	1.46	1.50
26	X	613	CLA	C3B-C4B	2.19	1.49	1.42
26	A	834	CLA	MG-ND	-2.19	2.01	2.05
26	5	610	CLA	C1B-C2B	2.19	1.48	1.43
26	7	612	CLA	C3B-C4B	2.19	1.49	1.42
26	A	803	CLA	C1B-C2B	2.19	1.48	1.43
35	3	619	XAT	C22-C21	-2.19	1.51	1.54
26	6	613	CLA	C1B-C2B	2.19	1.48	1.43
26	8	614	CLA	MG-NB	-2.19	2.01	2.05
26	2	616	CLA	CMB-C2B	-2.19	1.46	1.50
26	5	616	CLA	CMC-C2C	-2.19	1.46	1.50
26	W	602	CLA	CMC-C2C	-2.19	1.46	1.50
26	A	824	CLA	MG-NB	-2.19	2.01	2.05
26	8	606	CLA	C3B-C4B	2.19	1.49	1.42
26	7	615	CLA	CMD-C2D	-2.19	1.46	1.50
35	2	620	XAT	O4-C5	-2.19	1.43	1.46
26	V	614	CLA	CMD-C2D	-2.19	1.46	1.50
26	A	814	CLA	C1B-NB	-2.19	1.35	1.37
29	B	843	BCR	C1-C6	-2.19	1.51	1.53
37	W	605	CHL	CMC-C2C	2.19	1.49	1.44
26	A	819	CLA	C1B-C2B	2.19	1.48	1.43
26	Y	610	CLA	CHC-C1C	2.19	1.42	1.38
29	A	848	BCR	C19-C18	2.19	1.50	1.46
26	2	601	CLA	MG-ND	-2.19	2.01	2.05
26	U	602	CLA	CMD-C2D	-2.19	1.46	1.50
26	9	610	CLA	CHC-C1C	2.18	1.42	1.38
26	4	611	CLA	CMD-C2D	-2.18	1.46	1.50
26	A	828	CLA	MG-ND	-2.18	2.01	2.05
37	V	601	CHL	CMC-C2C	2.18	1.49	1.44
26	3	614	CLA	C3B-C4B	2.18	1.49	1.42
26	8	604	CLA	CMB-C2B	-2.18	1.46	1.50
26	2	610	CLA	MG-NB	-2.18	2.01	2.05
26	1	610	CLA	CMB-C2B	-2.18	1.46	1.50
26	X	613	CLA	CMD-C2D	-2.18	1.46	1.50
26	V	604	CLA	CMD-C2D	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	611	CLA	C3B-C4B	2.18	1.49	1.42
26	Y	613	CLA	C3B-C4B	2.18	1.49	1.42
26	V	613	CLA	C3B-C4B	2.18	1.49	1.42
26	A	806	CLA	MG-ND	-2.18	2.01	2.05
26	L	304	CLA	CMB-C2B	-2.18	1.46	1.50
26	6	616	CLA	CMC-C2C	-2.18	1.46	1.50
26	G	204	CLA	CMC-C2C	-2.18	1.46	1.50
35	Z	1622	XAT	O4-C5	-2.18	1.43	1.46
26	6	612	CLA	CMD-C2D	-2.18	1.46	1.50
26	Z	603	CLA	CMB-C2B	-2.18	1.46	1.50
26	B	808	CLA	CAC-C3C	-2.18	1.45	1.51
26	7	612	CLA	CMB-C2B	-2.18	1.46	1.50
26	6	609	CLA	MG-NB	-2.18	2.01	2.05
26	9	603	CLA	C4B-C3B	2.17	1.48	1.43
26	B	827	CLA	MG-NB	-2.17	2.01	2.05
26	1	613	CLA	MG-NB	-2.17	2.01	2.05
26	Z	612	CLA	CMC-C2C	-2.17	1.46	1.50
26	4	601	CLA	CMC-C2C	-2.17	1.46	1.50
26	Y	610	CLA	CMC-C2C	-2.17	1.46	1.50
26	5	609	CLA	C1B-C2B	2.17	1.48	1.43
26	3	609	CLA	MG-NB	-2.17	2.01	2.05
26	2	611	CLA	CMB-C2B	-2.17	1.46	1.50
37	X	601	CHL	CMC-C2C	2.17	1.49	1.44
26	A	809	CLA	C1B-C2B	2.17	1.48	1.43
26	5	619	CLA	CMC-C2C	-2.17	1.46	1.50
26	9	606	CLA	MG-NB	-2.17	2.01	2.05
26	X	604	CLA	CMB-C2B	-2.17	1.46	1.50
26	B	821	CLA	C3B-C4B	2.17	1.49	1.42
26	9	612	CLA	CMD-C2D	-2.17	1.46	1.50
26	B	824	CLA	MG-NB	-2.17	2.01	2.05
26	B	841	CLA	C3B-C4B	2.17	1.49	1.42
26	B	836	CLA	MG-ND	-2.17	2.01	2.05
26	B	818	CLA	MG-ND	-2.17	2.01	2.05
26	W	602	CLA	CMD-C2D	-2.17	1.46	1.50
26	W	613	CLA	CMC-C2C	-2.17	1.46	1.50
26	6	608	CLA	CMB-C2B	-2.17	1.46	1.50
26	Z	610	CLA	C1B-C2B	2.17	1.48	1.43
26	3	602	CLA	CMB-C2B	-2.17	1.46	1.50
35	7	620	XAT	O4-C5	-2.17	1.43	1.46
26	5	607	CLA	MG-ND	-2.17	2.01	2.05
26	2	606	CLA	MG-NB	-2.16	2.01	2.05
36	5	624	NEX	O24-C25	-2.16	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W	613	CLA	CMB-C2B	-2.16	1.46	1.50
26	a	601	CLA	MG-NB	-2.16	2.01	2.05
26	A	830	CLA	MG-ND	-2.16	2.01	2.05
26	U	602	CLA	CMC-C2C	-2.16	1.46	1.50
26	B	808	CLA	C3B-C4B	2.16	1.49	1.42
26	A	842	CLA	C3B-C4B	2.16	1.49	1.42
26	5	601	CLA	CMB-C2B	-2.16	1.46	1.50
27	B	842	PQN	C5-C4	2.16	1.52	1.48
29	B	844	BCR	C16-C15	-2.16	1.30	1.36
26	9	606	CLA	C3B-C4B	2.16	1.49	1.42
26	a	604	CLA	CMC-C2C	-2.16	1.46	1.50
26	a	607	CLA	CHC-C1C	2.16	1.42	1.38
26	X	610	CLA	C1B-C2B	2.16	1.48	1.43
26	X	611	CLA	CMD-C2D	-2.16	1.46	1.50
35	4	620	XAT	O4-C5	-2.16	1.43	1.46
26	4	613	CLA	CMC-C2C	-2.16	1.46	1.50
26	V	614	CLA	CHC-C1C	2.16	1.42	1.38
26	A	832	CLA	C1B-NB	-2.16	1.35	1.37
26	L	303	CLA	MG-NB	-2.16	2.01	2.05
26	5	608	CLA	MG-NB	-2.16	2.01	2.05
26	2	602	CLA	CMB-C2B	-2.16	1.45	1.50
37	X	607	CHL	CBD-CGD	-2.16	1.49	1.52
26	B	829	CLA	CAC-C3C	-2.16	1.45	1.51
26	a	601	CLA	C3B-C4B	2.15	1.49	1.42
26	6	611	CLA	CMD-C2D	-2.15	1.46	1.50
26	X	610	CLA	CMB-C2B	-2.15	1.46	1.50
26	K	206	CLA	C3B-C4B	2.15	1.49	1.42
26	L	306	CLA	C3B-C4B	2.15	1.49	1.42
26	1	607	CLA	CMC-C2C	-2.15	1.46	1.50
26	Y	612	CLA	CMC-C2C	-2.15	1.46	1.50
26	A	820	CLA	MG-NB	-2.15	2.01	2.05
37	Y	608	CHL	CMC-C2C	2.15	1.49	1.44
26	W	603	CLA	C3B-C4B	2.15	1.49	1.42
26	A	801	CLA	MG-NB	-2.15	2.01	2.05
26	A	826	CLA	C1B-C2B	2.15	1.48	1.43
26	B	810	CLA	C1B-C2B	2.15	1.48	1.43
26	A	819	CLA	CHC-C4B	-2.15	1.34	1.39
26	1	603	CLA	CMB-C2B	-2.15	1.46	1.50
26	4	607	CLA	C3B-C4B	2.15	1.49	1.42
26	A	823	CLA	CMC-C2C	-2.15	1.46	1.50
26	Y	602	CLA	CMD-C2D	-2.15	1.46	1.50
26	4	608	CLA	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	611	CLA	CMC-C2C	-2.15	1.46	1.50
26	B	804	CLA	MG-NB	-2.15	2.01	2.05
26	B	818	CLA	C1B-C2B	2.15	1.48	1.43
26	L	307	CLA	CMB-C2B	-2.15	1.46	1.50
26	A	831	CLA	C1B-C2B	2.15	1.48	1.43
26	F	303	CLA	MG-NB	-2.15	2.01	2.05
26	6	616	CLA	MG-NB	-2.15	2.01	2.05
26	6	614	CLA	C3B-C4B	2.15	1.49	1.42
26	5	603	CLA	CMC-C2C	-2.14	1.46	1.50
26	5	612	CLA	CMC-C2C	-2.14	1.46	1.50
26	A	828	CLA	C4B-NB	2.14	1.40	1.37
26	5	611	CLA	CMB-C2B	-2.14	1.46	1.50
35	1	618	XAT	O24-C25	-2.14	1.43	1.46
37	Y	601	CHL	CMC-C2C	2.14	1.49	1.44
26	Y	613	CLA	CMB-C2B	-2.14	1.46	1.50
26	V	612	CLA	CMB-C2B	-2.14	1.46	1.50
26	9	611	CLA	C3B-C4B	2.14	1.49	1.42
29	A	852	BCR	C30-C25	-2.14	1.51	1.53
26	B	816	CLA	CMC-C2C	-2.14	1.46	1.50
26	Z	611	CLA	CMC-C2C	-2.14	1.46	1.50
26	W	612	CLA	CMC-C2C	-2.14	1.46	1.50
35	X	1622	XAT	O4-C5	-2.14	1.43	1.46
26	1	606	CLA	MG-NB	-2.14	2.01	2.05
26	A	831	CLA	C1B-NB	-2.14	1.35	1.37
26	9	610	CLA	C1B-C2B	2.14	1.48	1.43
26	W	614	CLA	CMD-C2D	-2.14	1.46	1.50
26	A	804	CLA	MG-ND	-2.14	2.01	2.05
26	9	601	CLA	C3B-C4B	2.14	1.49	1.42
26	Z	614	CLA	CMB-C2B	-2.14	1.46	1.50
26	5	606	CLA	C3B-C4B	2.14	1.49	1.42
26	B	830	CLA	C3B-C4B	2.14	1.49	1.42
26	1	601	CLA	C3B-C4B	2.14	1.49	1.42
26	5	602	CLA	MG-NB	-2.14	2.01	2.05
26	B	832	CLA	MG-NB	-2.14	2.01	2.05
26	A	839	CLA	C1B-C2B	2.14	1.48	1.43
26	A	838	CLA	CHC-C4B	-2.14	1.34	1.39
26	5	602	CLA	C3B-C4B	2.14	1.49	1.42
26	A	838	CLA	C1B-NB	-2.14	1.35	1.37
26	Y	602	CLA	CHC-C1C	2.14	1.42	1.38
26	W	613	CLA	C3B-C4B	2.14	1.49	1.42
26	6	612	CLA	C3B-C4B	2.14	1.49	1.42
26	B	835	CLA	CMC-C2C	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	617	CLA	CMC-C2C	-2.14	1.46	1.50
26	J	101	CLA	C3B-C4B	2.14	1.49	1.42
26	B	813	CLA	C1B-C2B	2.13	1.48	1.43
26	7	601	CLA	C1B-C2B	2.13	1.48	1.43
26	G	204	CLA	C3B-C4B	2.13	1.49	1.42
26	Y	604	CLA	C3B-C4B	2.13	1.49	1.42
26	8	606	CLA	MG-NB	-2.13	2.01	2.05
35	4	620	XAT	C22-C21	-2.13	1.51	1.54
26	a	603	CLA	C3B-C4B	2.13	1.49	1.42
26	3	613	CLA	MG-NB	-2.13	2.01	2.05
26	X	603	CLA	CMB-C2B	-2.13	1.46	1.50
37	W	607	CHL	CBD-CGD	-2.13	1.49	1.52
26	V	612	CLA	CMC-C2C	-2.13	1.46	1.50
26	W	604	CLA	CMD-C2D	-2.13	1.46	1.50
26	B	837	CLA	CAC-C3C	-2.13	1.45	1.51
26	7	611	CLA	MG-NB	-2.13	2.01	2.05
26	U	610	CLA	CMC-C2C	-2.13	1.46	1.50
26	U	613	CLA	CMD-C2D	-2.13	1.46	1.50
26	A	808	CLA	C3B-C4B	2.13	1.48	1.42
26	A	814	CLA	C3B-C4B	2.13	1.48	1.42
26	5	609	CLA	MG-NB	-2.13	2.01	2.05
26	W	602	CLA	CMB-C2B	-2.13	1.46	1.50
26	A	807	CLA	MG-ND	-2.13	2.01	2.05
26	U	603	CLA	CMB-C2B	-2.13	1.46	1.50
26	2	609	CLA	C1B-C2B	2.13	1.48	1.43
26	1	608	CLA	CMB-C2B	-2.13	1.46	1.50
37	V	609	CHL	CMC-C2C	2.13	1.49	1.44
26	a	604	CLA	C3B-C4B	2.13	1.48	1.42
26	B	827	CLA	C1B-C2B	2.13	1.48	1.43
26	B	831	CLA	C3B-C4B	2.13	1.48	1.42
26	a	612	CLA	C3B-C4B	2.13	1.48	1.42
26	A	816	CLA	MG-NB	-2.13	2.01	2.05
26	A	822	CLA	MG-ND	-2.13	2.01	2.05
26	V	611	CLA	CMB-C2B	-2.13	1.46	1.50
26	F	303	CLA	CAC-C3C	-2.13	1.45	1.51
26	7	616	CLA	CHC-C1C	2.12	1.42	1.38
26	U	614	CLA	CHC-C1C	2.12	1.42	1.38
26	B	839	CLA	C4B-NB	2.12	1.40	1.37
26	B	810	CLA	C3B-C4B	2.12	1.48	1.42
26	A	817	CLA	MG-NB	-2.12	2.01	2.05
26	2	614	CLA	C3B-C4B	2.12	1.48	1.42
26	W	612	CLA	CMB-C2B	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	618	CLA	CMC-C2C	-2.12	1.46	1.50
26	X	613	CLA	CMC-C2C	-2.12	1.46	1.50
37	W	601	CHL	CMC-C2C	2.12	1.49	1.44
26	3	617	CLA	CMC-C2C	-2.12	1.46	1.50
26	7	604	CLA	C3B-C4B	2.12	1.48	1.42
26	B	839	CLA	MG-ND	-2.12	2.01	2.05
26	6	606	CLA	C3B-C4B	2.12	1.48	1.42
26	A	837	CLA	C1B-NB	-2.12	1.35	1.37
26	1	607	CLA	CHC-C1C	2.12	1.42	1.38
26	5	607	CLA	C1B-C2B	2.12	1.48	1.43
26	5	614	CLA	CMC-C2C	-2.12	1.46	1.50
26	6	616	CLA	C3B-C4B	2.12	1.48	1.42
26	6	603	CLA	MG-NB	-2.12	2.01	2.05
26	3	609	CLA	C1B-C2B	2.12	1.48	1.43
26	B	807	CLA	C1B-C2B	2.12	1.48	1.43
26	1	604	CLA	C3B-C4B	2.12	1.48	1.42
26	7	610	CLA	CHC-C1C	2.12	1.42	1.38
26	U	614	CLA	CMD-C2D	-2.12	1.46	1.50
26	5	617	CLA	CAC-C3C	-2.12	1.45	1.51
36	U	1623	NEX	O24-C25	-2.12	1.43	1.46
26	B	802	CLA	MG-ND	-2.12	2.01	2.05
26	7	616	CLA	MG-NB	-2.12	2.01	2.05
26	B	818	CLA	CHC-C4B	-2.12	1.34	1.39
26	B	831	CLA	MG-NB	-2.12	2.01	2.05
26	5	610	CLA	CHC-C1C	2.12	1.42	1.38
26	X	602	CLA	CHC-C1C	2.12	1.42	1.38
26	4	607	CLA	CMC-C2C	-2.12	1.46	1.50
35	9	620	XAT	C22-C21	-2.12	1.51	1.54
26	3	604	CLA	MG-NB	-2.12	2.01	2.05
26	3	612	CLA	CHC-C1C	2.12	1.42	1.38
26	4	618	CLA	CMD-C2D	-2.12	1.46	1.50
26	B	837	CLA	C1B-C2B	2.12	1.48	1.43
29	6	622	BCR	C1-C6	-2.12	1.51	1.53
29	7	623	BCR	C1-C6	-2.12	1.51	1.53
26	2	612	CLA	CMC-C2C	-2.12	1.46	1.50
26	B	813	CLA	C1B-NB	-2.12	1.35	1.37
26	K	201	CLA	CMB-C2B	-2.12	1.46	1.50
26	Y	603	CLA	CMD-C2D	-2.12	1.46	1.50
26	4	606	CLA	C3B-C4B	2.12	1.48	1.42
26	A	854	CLA	MG-ND	-2.12	2.01	2.05
28	A	847	LHG	O7-C5	-2.11	1.41	1.46
26	3	612	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	613	CLA	C3B-C4B	2.11	1.48	1.42
26	a	603	CLA	CMB-C2B	-2.11	1.46	1.50
26	V	610	CLA	CMC-C2C	-2.11	1.46	1.50
26	U	604	CLA	CHC-C1C	2.11	1.42	1.38
29	A	852	BCR	C1-C6	-2.11	1.51	1.53
26	7	609	CLA	C3B-C4B	2.11	1.48	1.42
26	B	841	CLA	MG-NB	-2.11	2.01	2.05
26	a	606	CLA	MG-NB	-2.11	2.01	2.05
26	8	613	CLA	MG-NB	-2.11	2.01	2.05
26	a	608	CLA	CMB-C2B	-2.11	1.46	1.50
26	A	811	CLA	MG-NB	-2.11	2.01	2.05
26	B	832	CLA	C3B-C4B	2.11	1.48	1.42
26	A	840	CLA	MG-ND	-2.11	2.01	2.05
26	B	825	CLA	C3B-C4B	2.11	1.48	1.42
26	3	604	CLA	C3B-C4B	2.11	1.48	1.42
26	H	203	CLA	C3B-C4B	2.11	1.48	1.42
26	5	617	CLA	MG-NB	-2.11	2.01	2.05
26	X	612	CLA	CMC-C2C	-2.11	1.46	1.50
26	B	829	CLA	MG-NB	-2.11	2.01	2.05
26	A	828	CLA	C1B-C2B	2.11	1.48	1.43
26	4	606	CLA	MG-NB	-2.11	2.01	2.05
26	9	613	CLA	CHC-C4B	-2.11	1.34	1.39
26	V	614	CLA	CMB-C2B	-2.11	1.46	1.50
26	W	612	CLA	C3B-C4B	2.11	1.48	1.42
26	U	613	CLA	CMB-C2B	-2.11	1.46	1.50
26	W	602	CLA	CHC-C1C	2.11	1.42	1.38
26	8	601	CLA	MG-NB	-2.11	2.01	2.05
26	A	833	CLA	C1B-C2B	2.11	1.48	1.43
26	2	601	CLA	C1B-C2B	2.11	1.48	1.43
26	U	603	CLA	C3B-C4B	2.11	1.48	1.42
26	4	613	CLA	MG-NB	-2.11	2.01	2.05
35	7	620	XAT	C22-C21	-2.11	1.51	1.54
26	Y	611	CLA	CMB-C2B	-2.11	1.46	1.50
26	A	854	CLA	C3B-C4B	2.11	1.48	1.42
26	3	613	CLA	CMC-C2C	-2.10	1.46	1.50
26	A	820	CLA	C1B-C2B	2.10	1.48	1.43
26	A	833	CLA	MG-NB	-2.10	2.01	2.05
35	V	1622	XAT	O4-C5	-2.10	1.43	1.46
26	A	818	CLA	C3B-C4B	2.10	1.48	1.42
26	1	603	CLA	C3B-C4B	2.10	1.48	1.42
26	K	203	CLA	CMC-C2C	-2.10	1.46	1.50
26	2	607	CLA	C1B-C2B	2.10	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	101	CLA	CMD-C2D	-2.10	1.46	1.50
26	a	608	CLA	CMC-C2C	-2.10	1.46	1.50
26	Y	604	CLA	CMC-C2C	-2.10	1.46	1.50
26	1	601	CLA	MG-NB	-2.10	2.01	2.05
26	9	609	CLA	MG-NB	-2.10	2.01	2.05
37	X	601	CHL	CBD-CGD	-2.10	1.49	1.52
26	A	801	CLA	CHC-C4B	-2.10	1.34	1.39
26	A	806	CLA	CAC-C3C	-2.10	1.45	1.51
26	A	810	CLA	C3B-C4B	2.10	1.48	1.42
26	B	813	CLA	MG-ND	-2.10	2.01	2.05
26	2	611	CLA	CMC-C2C	-2.10	1.46	1.50
26	A	833	CLA	C3B-C4B	2.10	1.48	1.42
26	Y	603	CLA	C3B-C4B	2.10	1.48	1.42
26	Z	610	CLA	CMD-C2D	-2.10	1.46	1.50
26	8	609	CLA	C3B-C4B	2.10	1.48	1.42
26	7	602	CLA	MG-NB	-2.10	2.01	2.05
26	V	602	CLA	CMD-C2D	-2.10	1.46	1.50
26	A	805	CLA	C3B-C4B	2.10	1.48	1.42
26	8	616	CLA	CHC-C1C	2.10	1.42	1.38
26	W	604	CLA	CHC-C1C	2.10	1.42	1.38
26	A	836	CLA	MG-ND	-2.10	2.01	2.05
26	J	101	CLA	CMC-C2C	-2.10	1.46	1.50
26	A	854	CLA	MG-NB	-2.10	2.01	2.05
26	7	615	CLA	CMC-C2C	-2.10	1.46	1.50
26	B	806	CLA	MG-ND	-2.10	2.01	2.05
26	1	612	CLA	MG-NB	-2.10	2.01	2.05
26	B	839	CLA	C1B-C2B	2.10	1.48	1.43
26	9	603	CLA	CHC-C4B	-2.10	1.34	1.39
26	1	612	CLA	C3B-C4B	2.09	1.48	1.42
37	Z	609	CHL	CMC-C2C	2.09	1.49	1.44
26	2	607	CLA	C3B-C4B	2.09	1.48	1.42
26	B	806	CLA	C4B-NB	2.09	1.40	1.37
37	Y	606	CHL	CBD-CGD	-2.09	1.49	1.52
37	W	601	CHL	CBD-CGD	-2.09	1.49	1.52
26	5	603	CLA	MG-NB	-2.09	2.01	2.05
26	V	603	CLA	C3B-C4B	2.09	1.48	1.42
26	A	824	CLA	CHC-C4B	-2.09	1.34	1.39
26	L	303	CLA	C1B-C2B	2.09	1.48	1.43
26	A	842	CLA	MG-ND	-2.09	2.01	2.05
26	5	616	CLA	MG-NB	-2.09	2.01	2.05
26	X	602	CLA	CMD-C2D	-2.09	1.46	1.50
26	Z	603	CLA	C3B-C4B	2.09	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	818	CLA	MG-NB	-2.09	2.01	2.05
26	6	609	CLA	CMC-C2C	-2.09	1.46	1.50
26	W	610	CLA	CHC-C1C	2.09	1.42	1.38
26	2	601	CLA	C3B-C4B	2.09	1.48	1.42
26	K	203	CLA	MG-ND	-2.09	2.01	2.05
26	L	307	CLA	MG-NB	-2.09	2.01	2.05
26	X	614	CLA	CMB-C2B	-2.09	1.46	1.50
26	4	613	CLA	CHC-C1C	2.09	1.42	1.38
26	4	614	CLA	CMC-C2C	-2.09	1.46	1.50
26	X	610	CLA	CMC-C2C	-2.09	1.46	1.50
26	U	610	CLA	CMD-C2D	-2.09	1.46	1.50
26	F	301	CLA	C3B-C4B	2.09	1.48	1.42
26	a	611	CLA	CMC-C2C	-2.09	1.46	1.50
26	9	611	CLA	CMB-C2B	-2.09	1.46	1.50
26	W	611	CLA	CHC-C1C	2.09	1.42	1.38
26	Y	610	CLA	CMD-C2D	-2.09	1.46	1.50
26	1	608	CLA	C3B-C4B	2.08	1.48	1.42
26	B	834	CLA	MG-ND	-2.08	2.01	2.05
26	Z	613	CLA	CMC-C2C	-2.08	1.46	1.50
26	B	815	CLA	MG-NB	-2.08	2.01	2.05
26	5	613	CLA	MG-NB	-2.08	2.01	2.05
26	9	614	CLA	CMD-C2D	-2.08	1.46	1.50
26	U	604	CLA	CMD-C2D	-2.08	1.46	1.50
26	B	810	CLA	MG-ND	-2.08	2.01	2.05
26	U	611	CLA	CMB-C2B	-2.08	1.46	1.50
26	A	843	CLA	MG-ND	-2.08	2.01	2.05
26	4	604	CLA	CMD-C2D	-2.08	1.46	1.50
26	5	611	CLA	CMD-C2D	-2.08	1.46	1.50
26	7	606	CLA	MG-ND	-2.08	2.01	2.05
26	8	602	CLA	MG-NB	-2.08	2.01	2.05
26	Y	612	CLA	CMD-C2D	-2.08	1.46	1.50
26	V	613	CLA	CMB-C2B	-2.08	1.46	1.50
35	a	618	XAT	O24-C25	-2.08	1.43	1.46
26	B	823	CLA	MG-ND	-2.08	2.01	2.05
26	a	608	CLA	C3B-C4B	2.08	1.48	1.42
26	B	806	CLA	CAC-C3C	-2.08	1.45	1.51
26	3	614	CLA	MG-NB	-2.08	2.01	2.05
26	X	602	CLA	CMB-C2B	-2.08	1.46	1.50
26	V	610	CLA	CMD-C2D	-2.08	1.46	1.50
26	B	820	CLA	MG-NB	-2.08	2.01	2.05
26	F	301	CLA	MG-NB	-2.08	2.01	2.05
26	A	842	CLA	C1B-NB	-2.08	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	620	CLA	C3B-C4B	2.08	1.48	1.42
26	B	821	CLA	CMC-C2C	-2.08	1.45	1.50
26	B	807	CLA	C1B-NB	-2.08	1.35	1.37
26	B	833	CLA	MG-NB	-2.08	2.01	2.05
26	2	609	CLA	MG-NB	-2.07	2.01	2.05
26	A	820	CLA	C3B-C4B	2.07	1.48	1.42
26	2	604	CLA	CMB-C2B	-2.07	1.46	1.50
26	2	611	CLA	C3B-C4B	2.07	1.48	1.42
26	A	854	CLA	C1B-C2B	2.07	1.48	1.43
35	U	1622	XAT	O4-C5	-2.07	1.43	1.46
26	A	834	CLA	C1B-NB	-2.07	1.35	1.37
35	a	618	XAT	C22-C21	-2.07	1.51	1.54
26	Z	604	CLA	CMD-C2D	-2.07	1.46	1.50
26	B	829	CLA	C3B-C4B	2.07	1.48	1.42
26	7	613	CLA	CHC-C4B	-2.07	1.34	1.39
26	1	607	CLA	MG-NB	-2.07	2.01	2.05
26	2	616	CLA	CMC-C2C	-2.07	1.46	1.50
26	B	813	CLA	C3B-C4B	2.07	1.48	1.42
26	A	845	CLA	MG-NB	-2.07	2.01	2.05
26	A	816	CLA	CHC-C4B	-2.07	1.34	1.39
26	9	614	CLA	CMC-C2C	-2.07	1.46	1.50
26	A	835	CLA	MG-ND	-2.07	2.01	2.05
26	9	602	CLA	MG-NB	-2.07	2.01	2.05
26	9	603	CLA	C3B-C2B	-2.07	1.36	1.44
26	F	303	CLA	C3B-C4B	2.07	1.48	1.42
26	B	820	CLA	MG-ND	-2.07	2.01	2.05
26	a	614	CLA	C3B-C4B	2.07	1.48	1.42
35	Z	1622	XAT	O24-C25	-2.07	1.43	1.46
26	4	618	CLA	CMB-C2B	-2.07	1.46	1.50
26	A	839	CLA	MG-ND	-2.07	2.01	2.05
26	G	204	CLA	MG-NB	-2.07	2.01	2.05
26	2	607	CLA	CMC-C2C	-2.06	1.46	1.50
26	2	614	CLA	MG-NB	-2.06	2.01	2.05
26	B	827	CLA	C3B-C4B	2.06	1.48	1.42
26	7	609	CLA	CMC-C2C	-2.06	1.46	1.50
37	X	605	CHL	CMC-C2C	2.06	1.49	1.44
26	6	601	CLA	C3B-C4B	2.06	1.48	1.42
26	Y	604	CLA	CMD-C2D	-2.06	1.46	1.50
26	B	803	CLA	MG-ND	-2.06	2.01	2.05
26	A	815	CLA	C3B-C4B	2.06	1.48	1.42
26	1	608	CLA	CMC-C2C	-2.06	1.46	1.50
26	B	820	CLA	C3B-C4B	2.06	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	837	CLA	CHC-C4B	-2.06	1.34	1.39
26	B	835	CLA	MG-ND	-2.06	2.01	2.05
26	2	606	CLA	MG-ND	-2.06	2.01	2.05
35	1	618	XAT	O4-C5	-2.06	1.43	1.46
26	V	604	CLA	CMC-C2C	-2.06	1.46	1.50
26	A	816	CLA	CAC-C3C	-2.06	1.45	1.51
37	W	608	CHL	CMC-C2C	2.06	1.49	1.44
26	A	845	CLA	C1B-NB	-2.06	1.35	1.37
26	3	617	CLA	MG-NB	-2.06	2.01	2.05
26	7	604	CLA	MG-NB	-2.06	2.01	2.05
26	V	602	CLA	CHC-C1C	2.06	1.42	1.38
37	W	609	CHL	CMC-C2C	2.06	1.49	1.44
26	B	827	CLA	CAC-C3C	-2.06	1.45	1.51
26	Z	604	CLA	CMC-C2C	-2.06	1.46	1.50
26	4	614	CLA	MG-NB	-2.06	2.01	2.05
26	8	607	CLA	CHC-C1C	2.06	1.42	1.38
26	X	612	CLA	CMB-C2B	-2.06	1.46	1.50
26	a	612	CLA	MG-NB	-2.06	2.01	2.05
26	Z	612	CLA	CMB-C2B	-2.06	1.46	1.50
26	6	602	CLA	MG-NB	-2.06	2.01	2.05
26	L	303	CLA	CMC-C2C	-2.05	1.46	1.50
26	X	611	CLA	CMB-C2B	-2.05	1.46	1.50
26	B	809	CLA	CAC-C3C	-2.05	1.45	1.51
26	4	614	CLA	CMB-C2B	-2.05	1.46	1.50
37	Z	609	CHL	CBD-CGD	-2.05	1.49	1.52
35	1	618	XAT	C22-C21	-2.05	1.51	1.54
26	A	832	CLA	MG-ND	-2.05	2.01	2.05
26	4	602	CLA	C1B-C2B	2.05	1.47	1.43
34	X	1621	LUT	C22-C21	-2.05	1.52	1.54
26	W	611	CLA	CMD-C2D	-2.05	1.46	1.50
26	a	611	CLA	MG-NB	-2.05	2.01	2.05
26	B	806	CLA	CHC-C4B	-2.05	1.34	1.39
29	B	852	BCR	C30-C25	-2.05	1.51	1.53
35	W	1622	XAT	O4-C5	-2.05	1.43	1.46
26	a	613	CLA	C3B-C4B	2.05	1.48	1.42
26	1	616	CLA	CHC-C1C	2.05	1.42	1.38
26	O	2003	CLA	C3B-C4B	2.05	1.48	1.42
26	8	616	CLA	CMB-C2B	-2.05	1.46	1.50
26	A	803	CLA	CAC-C3C	-2.05	1.45	1.51
36	X	1623	NEX	O24-C25	-2.05	1.43	1.46
26	B	811	CLA	MG-NB	-2.05	2.01	2.05
26	K	201	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	614	CLA	CHC-C1C	2.05	1.42	1.38
35	Y	1622	XAT	O24-C25	-2.05	1.43	1.46
26	X	614	CLA	CHC-C1C	2.05	1.42	1.38
26	A	843	CLA	C1B-NB	-2.05	1.35	1.37
36	Z	1623	NEX	O24-C25	-2.05	1.43	1.46
37	W	606	CHL	CBD-CGD	-2.05	1.49	1.52
26	A	809	CLA	MG-ND	-2.05	2.01	2.05
26	3	603	CLA	CHC-C4B	-2.05	1.34	1.39
26	a	607	CLA	MG-NB	-2.04	2.01	2.05
26	4	610	CLA	CMB-C2B	-2.04	1.46	1.50
35	3	619	XAT	O24-C25	-2.04	1.43	1.46
26	B	805	CLA	MG-ND	-2.04	2.01	2.05
35	7	620	XAT	C2-C1	-2.04	1.51	1.54
26	A	821	CLA	C3B-C4B	2.04	1.48	1.42
26	A	802	CLA	CAC-C3C	-2.04	1.45	1.51
26	A	813	CLA	C3B-C4B	2.04	1.48	1.42
37	X	609	CHL	CBD-CGD	-2.04	1.49	1.52
26	A	813	CLA	MG-ND	-2.04	2.01	2.05
26	1	611	CLA	CMC-C2C	-2.04	1.46	1.50
26	8	613	CLA	C3B-C4B	2.04	1.48	1.42
26	U	612	CLA	CMD-C2D	-2.04	1.46	1.50
26	A	819	CLA	C4B-NB	2.04	1.40	1.37
26	7	616	CLA	CMB-C2B	-2.04	1.46	1.50
37	U	609	CHL	CMC-C2C	2.04	1.49	1.44
26	A	822	CLA	C1B-C2B	2.04	1.47	1.43
26	3	608	CLA	C1B-NB	-2.04	1.35	1.37
26	W	610	CLA	CMB-C2B	-2.04	1.46	1.50
26	4	602	CLA	MG-NB	-2.04	2.01	2.05
26	O	2003	CLA	MG-NB	-2.04	2.01	2.05
26	9	606	CLA	MG-ND	-2.04	2.01	2.05
26	5	617	CLA	CHC-C4B	-2.04	1.34	1.39
26	2	602	CLA	CAC-C3C	-2.04	1.45	1.51
26	B	803	CLA	MG-NB	-2.04	2.01	2.05
26	X	603	CLA	CMD-C2D	-2.04	1.46	1.50
26	A	838	CLA	MG-ND	-2.04	2.01	2.05
26	4	601	CLA	MG-NB	-2.04	2.01	2.05
26	1	602	CLA	C1B-NB	-2.04	1.35	1.37
26	B	807	CLA	CHC-C4B	-2.04	1.34	1.39
26	4	612	CLA	CMB-C2B	-2.04	1.46	1.50
37	V	608	CHL	CBD-CGD	-2.04	1.49	1.52
26	1	613	CLA	C3B-C4B	2.04	1.48	1.42
26	A	814	CLA	MG-ND	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	840	CLA	MG-ND	-2.04	2.01	2.05
26	L	302	CLA	C3B-C4B	2.04	1.48	1.42
26	7	603	CLA	MG-ND	-2.04	2.01	2.05
26	A	831	CLA	C3B-C4B	2.03	1.48	1.42
26	9	611	CLA	CMC-C2C	-2.03	1.46	1.50
26	B	819	CLA	MG-NB	-2.03	2.01	2.05
37	Z	608	CHL	CBD-CGD	-2.03	1.49	1.52
26	6	613	CLA	MG-NB	-2.03	2.01	2.05
26	4	614	CLA	C3B-C4B	2.03	1.48	1.42
26	A	806	CLA	C3B-C4B	2.03	1.48	1.42
26	5	613	CLA	C3B-C4B	2.03	1.48	1.42
26	A	801	CLA	CAC-C3C	-2.03	1.45	1.51
26	B	822	CLA	C3B-C4B	2.03	1.48	1.42
26	5	614	CLA	C3B-C4B	2.03	1.48	1.42
26	4	611	CLA	CMB-C2B	-2.03	1.46	1.50
26	A	822	CLA	CHC-C1C	2.03	1.42	1.38
26	4	603	CLA	MG-NB	-2.03	2.01	2.05
37	Z	608	CHL	CMC-C2C	2.03	1.49	1.44
26	A	819	CLA	C1B-NB	-2.03	1.35	1.37
26	2	603	CLA	CHC-C4B	-2.03	1.34	1.39
26	Z	613	CLA	MG-NB	-2.03	2.01	2.05
26	A	818	CLA	CHC-C4B	-2.03	1.34	1.39
26	B	829	CLA	CHC-C4B	-2.03	1.34	1.39
26	A	831	CLA	CHC-C4B	-2.03	1.34	1.39
26	X	611	CLA	CMC-C2C	-2.03	1.46	1.50
26	8	614	CLA	C3B-C4B	2.03	1.48	1.42
37	Z	606	CHL	CMC-C2C	2.03	1.49	1.44
26	A	817	CLA	C3B-C4B	2.03	1.48	1.42
29	A	851	BCR	C1-C6	-2.03	1.51	1.53
26	a	614	CLA	CHC-C1C	2.03	1.42	1.38
26	B	814	CLA	MG-NB	-2.03	2.01	2.05
26	3	608	CLA	MG-ND	-2.03	2.01	2.05
26	A	840	CLA	CHC-C4B	-2.03	1.34	1.39
26	O	2001	CLA	MG-NB	-2.02	2.01	2.05
26	1	611	CLA	MG-NB	-2.02	2.01	2.05
26	W	610	CLA	CMC-C2C	-2.02	1.46	1.50
26	5	616	CLA	O2A-CGA	2.02	1.37	1.30
26	A	823	CLA	C3B-C4B	2.02	1.48	1.42
26	B	837	CLA	C3B-C4B	2.02	1.48	1.42
37	Y	601	CHL	CBD-CGD	-2.02	1.50	1.52
26	9	607	CLA	MG-NB	-2.02	2.01	2.05
26	A	805	CLA	C1B-C2B	2.02	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	607	CLA	CMC-C2C	-2.02	1.46	1.50
26	5	601	CLA	C3B-C4B	2.02	1.48	1.42
36	Y	1623	NEX	O24-C25	-2.02	1.43	1.46
26	a	616	CLA	CHC-C1C	2.02	1.42	1.38
26	A	812	CLA	CHC-C4B	-2.02	1.34	1.39
26	W	611	CLA	CMB-C2B	-2.02	1.46	1.50
29	B	844	BCR	C30-C25	-2.02	1.51	1.53
26	2	613	CLA	CMC-C2C	-2.02	1.46	1.50
26	B	816	CLA	C3B-C4B	2.02	1.48	1.42
26	2	603	CLA	C3B-C4B	2.02	1.48	1.42
26	a	602	CLA	MG-ND	-2.02	2.01	2.05
26	A	820	CLA	CAC-C3C	-2.02	1.45	1.51
26	X	603	CLA	CMC-C2C	-2.02	1.46	1.50
26	6	608	CLA	CHC-C1C	2.02	1.42	1.38
26	Z	603	CLA	CMC-C2C	-2.02	1.46	1.50
26	A	834	CLA	C3B-C4B	2.02	1.48	1.42
26	V	610	CLA	CMB-C2B	-2.02	1.46	1.50
26	5	614	CLA	MG-NB	-2.02	2.01	2.05
26	a	602	CLA	C1B-NB	-2.02	1.35	1.37
26	7	608	CLA	CAC-C3C	-2.02	1.45	1.51
26	A	806	CLA	C1B-C2B	2.02	1.47	1.43
26	7	608	CLA	MG-ND	-2.02	2.01	2.05
35	a	618	XAT	O4-C5	-2.02	1.43	1.46
26	3	611	CLA	CMB-C2B	-2.02	1.46	1.50
26	V	611	CLA	CMC-C2C	-2.02	1.46	1.50
26	B	822	CLA	MG-NB	-2.02	2.01	2.05
26	5	618	CLA	MG-NB	-2.02	2.01	2.05
26	U	604	CLA	MG-NB	-2.02	2.01	2.05
26	Z	612	CLA	CMD-C2D	-2.02	1.46	1.50
32	8	626	LMG	O1-C1	2.01	1.43	1.40
26	7	614	CLA	C3B-C4B	2.01	1.48	1.42
26	U	612	CLA	CMB-C2B	-2.01	1.46	1.50
26	V	610	CLA	CHC-C1C	2.01	1.42	1.38
37	Z	605	CHL	CBD-CGD	-2.01	1.50	1.52
26	9	612	CLA	CMC-C2C	-2.01	1.46	1.50
26	6	609	CLA	C3B-C4B	2.01	1.48	1.42
26	W	603	CLA	CMC-C2C	-2.01	1.46	1.50
26	U	613	CLA	CHC-C1C	2.01	1.42	1.38
26	B	826	CLA	C3B-C4B	2.01	1.48	1.42
26	8	614	CLA	MG-ND	-2.01	2.01	2.05
26	A	813	CLA	C1B-C2B	2.01	1.47	1.43
26	Y	614	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	607	CLA	MG-NB	-2.01	2.01	2.05
26	1	614	CLA	CMC-C2C	-2.01	1.46	1.50
26	A	805	CLA	MG-ND	-2.01	2.01	2.05
26	7	609	CLA	MG-NB	-2.01	2.01	2.05
29	5	622	BCR	C23-C22	2.01	1.50	1.46
37	Z	606	CHL	CBD-CGD	-2.01	1.50	1.52
26	B	804	CLA	C3B-C4B	2.01	1.48	1.42
26	U	603	CLA	CMC-C2C	-2.01	1.46	1.50
27	A	844	PQN	C3-C2	-2.01	1.31	1.35
26	8	608	CLA	MG-ND	-2.01	2.01	2.05
26	5	603	CLA	CAC-C3C	-2.01	1.46	1.51
26	1	614	CLA	CHC-C1C	2.01	1.42	1.38
26	B	803	CLA	C3B-C4B	2.01	1.48	1.42
26	7	602	CLA	MG-ND	-2.00	2.01	2.05
26	A	805	CLA	CAC-C3C	-2.00	1.46	1.51
26	U	611	CLA	CMD-C2D	-2.00	1.46	1.50
36	6	624	NEX	C22-C21	-2.00	1.51	1.54
26	Y	614	CLA	CHC-C1C	2.00	1.42	1.38
26	1	613	CLA	C1B-NB	-2.00	1.35	1.37
26	A	807	CLA	CAC-C3C	-2.00	1.46	1.51
26	Y	612	CLA	CHC-C1C	2.00	1.42	1.38
26	H	202	CLA	CMC-C2C	-2.00	1.46	1.50
26	A	854	CLA	C4-C3	-2.00	1.45	1.50
26	6	616	CLA	MG-ND	-2.00	2.01	2.05
26	L	303	CLA	C3B-C4B	2.00	1.48	1.42
26	1	608	CLA	MG-NB	-2.00	2.01	2.05
26	V	613	CLA	CHC-C1C	2.00	1.42	1.38
26	7	607	CLA	C3B-C4B	2.00	1.48	1.42
26	Z	602	CLA	CMB-C2B	-2.00	1.46	1.50
26	7	615	CLA	MG-NB	-2.00	2.01	2.05

All (3934) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	X	1623	NEX	C17-C1-C6	-20.23	92.37	110.47
35	U	1622	XAT	C37-C21-C36	-17.67	81.69	107.37
35	W	1622	XAT	C37-C21-C36	-17.66	81.72	107.37
29	B	852	BCR	C32-C1-C6	-16.83	83.85	110.24
35	U	1622	XAT	C37-C21-C22	-15.27	82.13	108.97
35	W	1622	XAT	C37-C21-C22	-14.62	83.27	108.97
29	O	2005	BCR	C40-C30-C25	-11.50	92.21	110.24
29	B	848	BCR	C24-C23-C22	-11.07	109.86	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	606	CHL	C1B-CHB-C4A	10.68	128.19	121.32
36	X	1623	NEX	C16-C1-C6	10.55	119.91	110.47
29	K	207	BCR	C40-C30-C25	-10.36	93.99	110.24
37	U	606	CHL	C1B-CHB-C4A	10.31	127.96	121.32
37	V	606	CHL	C1B-CHB-C4A	10.30	127.95	121.32
29	B	852	BCR	C8-C9-C10	10.15	134.98	119.01
29	9	621	BCR	C24-C23-C22	-10.15	111.22	126.23
37	X	609	CHL	O2D-CGD-CBD	10.14	122.09	110.95
29	8	621	BCR	C33-C5-C6	9.88	135.26	124.48
37	X	607	CHL	C1B-CHB-C4A	9.79	127.62	121.32
37	Y	609	CHL	O2D-CGD-CBD	9.71	121.61	110.95
37	V	608	CHL	C1B-CHB-C4A	9.64	127.53	121.32
37	U	609	CHL	O2D-CGD-CBD	9.49	121.37	110.95
29	B	852	BCR	C32-C1-C31	-9.29	82.04	108.63
34	Y	1620	LUT	C15-C35-C34	-9.26	104.57	123.52
36	X	1623	NEX	C17-C1-C16	-9.19	82.31	108.63
37	W	608	CHL	C1B-CHB-C4A	9.18	127.23	121.32
37	Z	609	CHL	O2D-CGD-CBD	9.12	120.97	110.95
37	Z	606	CHL	C1B-CHB-C4A	9.10	127.18	121.32
37	V	609	CHL	C1B-CHB-C4A	8.98	127.10	121.32
37	V	606	CHL	O2D-CGD-CBD	8.96	120.80	110.95
37	Y	605	CHL	O2D-CGD-CBD	8.90	120.72	110.95
37	V	609	CHL	O2D-CGD-CBD	8.87	120.69	110.95
37	Y	608	CHL	C1B-CHB-C4A	8.85	127.02	121.32
37	Z	605	CHL	C1B-CHB-C4A	8.81	126.99	121.32
37	X	606	CHL	O2D-CGD-CBD	8.80	120.61	110.95
37	U	605	CHL	O2D-CGD-CBD	8.78	120.59	110.95
37	V	601	CHL	C1B-CHB-C4A	8.76	126.96	121.32
37	V	605	CHL	O2D-CGD-CBD	8.66	120.46	110.95
37	W	605	CHL	O2D-CGD-CBD	8.57	120.36	110.95
37	W	601	CHL	O2D-CGD-CBD	8.56	120.35	110.95
37	U	609	CHL	C1B-CHB-C4A	8.53	126.81	121.32
37	Y	606	CHL	C1B-CHB-C4A	8.41	126.73	121.32
27	A	844	PQN	C11-C12-C13	-8.31	112.52	126.83
29	B	852	BCR	C34-C9-C10	-8.26	109.43	122.82
37	Y	607	CHL	C1B-CHB-C4A	8.25	126.63	121.32
36	W	1623	NEX	O24-C25-C24	8.23	121.20	113.49
37	Z	605	CHL	O2D-CGD-CBD	8.17	119.92	110.95
35	U	1622	XAT	C36-C21-C22	8.12	123.24	108.97
34	9	619	LUT	C8-C7-C6	-8.02	105.58	127.00
37	Z	606	CHL	O2D-CGD-CBD	7.98	119.72	110.95
29	J	102	BCR	C28-C27-C26	-7.93	99.91	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	4	619	LUT	C8-C7-C6	-7.93	105.81	127.00
37	X	605	CHL	O2D-CGD-CBD	7.91	119.64	110.95
37	V	608	CHL	O2D-CGD-CBD	7.90	119.63	110.95
37	Z	601	CHL	O2D-CGD-CBD	7.87	119.59	110.95
35	W	1622	XAT	C36-C21-C22	7.82	122.71	108.97
37	U	606	CHL	O2D-CGD-CBD	7.82	119.53	110.95
37	V	601	CHL	O2D-CGD-CBD	7.77	119.48	110.95
37	W	609	CHL	O2D-CGD-CBD	7.73	119.44	110.95
37	Y	601	CHL	O2D-CGD-CBD	7.69	119.39	110.95
37	U	608	CHL	O2D-CGD-CBD	7.68	119.39	110.95
34	Y	1620	LUT	C11-C10-C9	-7.65	116.55	127.28
37	U	601	CHL	O2D-CGD-CBD	7.62	119.32	110.95
37	Y	606	CHL	O2D-CGD-CBD	7.61	119.31	110.95
35	Z	1622	XAT	C15-C14-C13	-7.51	116.74	127.28
34	Y	1620	LUT	C20-C13-C14	-7.48	110.70	122.82
37	Y	608	CHL	O2D-CGD-CBD	7.47	119.15	110.95
37	Z	601	CHL	C1B-CHB-C4A	7.32	126.03	121.32
29	B	849	BCR	C39-C30-C25	-7.31	98.79	110.24
37	X	601	CHL	C1B-CHB-C4A	7.29	126.01	121.32
29	O	2005	BCR	C24-C23-C22	-7.25	115.51	126.23
29	A	852	BCR	C24-C23-C22	-7.22	115.55	126.23
37	U	607	CHL	O2D-CGD-CBD	7.20	118.86	110.95
26	2	602	CLA	CMB-C2B-C3B	7.19	128.11	116.53
37	Z	608	CHL	O2D-CGD-CBD	7.17	118.83	110.95
27	B	842	PQN	C11-C12-C13	-7.16	114.50	126.83
37	W	605	CHL	C1B-CHB-C4A	7.12	125.91	121.32
26	B	826	CLA	C4A-NA-C1A	7.11	109.92	106.68
36	Z	1623	NEX	O24-C25-C24	7.08	120.13	113.49
29	B	852	BCR	C31-C1-C6	7.07	121.33	110.24
36	Y	1623	NEX	O24-C25-C24	7.06	120.11	113.49
35	Y	1622	XAT	C15-C14-C13	-7.05	117.39	127.28
29	A	850	BCR	C8-C7-C6	-7.02	108.26	127.00
29	5	622	BCR	C23-C24-C25	-7.00	108.31	127.00
36	X	1623	NEX	C2-C1-C6	6.99	116.01	109.21
37	Y	609	CHL	C1B-CHB-C4A	6.99	125.82	121.32
37	W	608	CHL	O2D-CGD-CBD	6.99	118.63	110.95
34	7	619	LUT	C8-C7-C6	-6.98	108.36	127.00
36	6	624	NEX	C8-C7-C6	-6.97	169.43	177.66
29	B	852	BCR	C7-C8-C9	-6.96	115.94	126.23
37	X	606	CHL	C1B-CHB-C4A	6.94	125.78	121.32
27	A	844	PQN	C14-C13-C15	-6.92	103.22	115.23
37	W	606	CHL	O2D-CGD-CBD	6.89	118.52	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Y	1620	LUT	C15-C14-C13	6.89	136.94	127.28
37	Z	607	CHL	O2D-CGD-CBD	6.88	118.51	110.95
36	U	1623	NEX	O24-C25-C24	6.86	119.92	113.49
37	X	607	CHL	O2D-CGD-CBD	6.84	118.46	110.95
29	B	844	BCR	C27-C26-C25	-6.83	113.48	122.70
37	W	607	CHL	O2D-CGD-CBD	6.82	118.44	110.95
35	5	621	XAT	O24-C25-C24	6.81	119.87	113.49
37	X	601	CHL	O2D-CGD-CBD	6.80	118.42	110.95
26	A	837	CLA	C4A-NA-C1A	6.79	109.78	106.68
26	B	810	CLA	C4A-NA-C1A	6.78	109.77	106.68
29	A	848	BCR	C38-C26-C25	-6.76	117.11	124.48
29	3	622	BCR	C38-C26-C25	-6.71	117.16	124.48
29	7	623	BCR	C8-C7-C6	-6.64	109.27	127.00
26	7	613	CLA	C4A-NA-C1A	6.61	109.69	106.68
37	Y	608	CHL	C4D-ND-C1D	-6.60	100.21	105.22
29	L	301	BCR	C8-C7-C6	-6.60	109.36	127.00
37	V	608	CHL	C4D-ND-C1D	-6.60	100.21	105.22
26	8	603	CLA	C4A-NA-C1A	6.60	109.69	106.68
34	Y	1620	LUT	C12-C13-C14	6.59	129.38	119.01
29	B	848	BCR	C23-C22-C21	-6.59	108.65	119.01
29	2	623	BCR	C28-C27-C26	-6.59	102.31	114.06
34	8	619	LUT	C8-C7-C6	-6.57	109.44	127.00
36	5	624	NEX	C38-C25-C26	-6.57	111.49	122.30
26	Z	603	CLA	C4A-NA-C1A	6.56	109.67	106.68
26	3	603	CLA	C4A-NA-C1A	6.56	109.67	106.68
26	K	204	CLA	C4A-NA-C1A	6.54	109.66	106.68
29	A	848	BCR	C8-C7-C6	-6.54	109.54	127.00
29	8	621	BCR	C40-C30-C25	6.52	120.47	110.24
29	O	2005	BCR	C39-C30-C25	6.49	120.43	110.24
26	1	603	CLA	C4A-NA-C1A	6.49	109.64	106.68
29	A	851	BCR	C40-C30-C25	6.47	120.38	110.24
29	L	305	BCR	C34-C9-C8	-6.44	108.24	118.09
29	B	846	BCR	C23-C24-C25	-6.44	109.79	127.00
26	a	603	CLA	C4A-NA-C1A	6.44	109.61	106.68
35	U	1622	XAT	O24-C25-C24	6.43	119.52	113.49
29	3	620	BCR	C3-C4-C5	-6.42	102.61	114.06
37	X	608	CHL	C4D-ND-C1D	-6.41	100.35	105.22
37	X	609	CHL	C1B-CHB-C4A	6.41	125.45	121.32
26	B	809	CLA	C4A-NA-C1A	6.40	109.60	106.68
26	V	603	CLA	C4A-NA-C1A	6.40	109.60	106.68
26	5	603	CLA	C4A-NA-C1A	6.39	109.59	106.68
37	Z	605	CHL	C4D-ND-C1D	-6.39	100.37	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	4	620	XAT	O4-C5-C4	6.38	119.47	113.49
37	Y	601	CHL	C1B-CHB-C4A	6.38	125.43	121.32
37	W	605	CHL	C4D-ND-C1D	-6.38	100.38	105.22
36	X	1623	NEX	O24-C25-C24	6.36	119.45	113.49
37	X	607	CHL	C4D-ND-C1D	-6.36	100.39	105.22
35	Z	1622	XAT	O24-C25-C24	6.35	119.45	113.49
26	A	819	CLA	C4A-NA-C1A	6.33	109.57	106.68
37	U	608	CHL	C4D-ND-C1D	-6.33	100.42	105.22
26	B	806	CLA	C4A-NA-C1A	6.32	109.56	106.68
29	B	846	BCR	C38-C26-C25	-6.32	117.59	124.48
34	Y	1620	LUT	C35-C15-C14	6.31	136.42	123.52
26	7	603	CLA	C4A-NA-C1A	6.30	109.55	106.68
37	V	609	CHL	C4D-ND-C1D	-6.30	100.44	105.22
26	A	814	CLA	C4A-NA-C1A	6.30	109.55	106.68
29	8	621	BCR	C38-C26-C25	-6.29	117.62	124.48
37	U	608	CHL	C1B-CHB-C4A	6.26	125.35	121.32
26	W	603	CLA	C4A-NA-C1A	6.26	109.53	106.68
37	W	601	CHL	C1B-CHB-C4A	6.25	125.35	121.32
37	Y	607	CHL	O2D-CGD-CBD	6.25	117.82	110.95
37	Z	606	CHL	C4D-ND-C1D	-6.25	100.47	105.22
29	9	621	BCR	C28-C27-C26	-6.25	102.91	114.06
37	U	606	CHL	C4D-ND-C1D	-6.25	100.48	105.22
37	Z	601	CHL	C4D-ND-C1D	-6.24	100.48	105.22
26	A	815	CLA	C4A-NA-C1A	6.24	109.53	106.68
34	3	618	LUT	C8-C7-C6	-6.24	110.34	127.00
37	Y	607	CHL	C4D-ND-C1D	-6.23	100.49	105.22
26	A	823	CLA	C4A-NA-C1A	6.22	109.52	106.68
29	A	852	BCR	C28-C27-C26	-6.21	102.98	114.06
29	B	845	BCR	C33-C5-C6	-6.20	117.72	124.48
29	K	202	BCR	C28-C27-C26	-6.18	103.03	114.06
29	A	848	BCR	C23-C24-C25	-6.18	110.49	127.00
26	A	828	CLA	C4A-NA-C1A	6.18	109.50	106.68
26	A	816	CLA	C4A-NA-C1A	6.17	109.50	106.68
37	W	608	CHL	C4D-ND-C1D	-6.17	100.53	105.22
37	V	601	CHL	C4D-ND-C1D	-6.17	100.54	105.22
29	A	856	BCR	C8-C7-C6	-6.17	110.52	127.00
29	K	207	BCR	C40-C30-C39	-6.16	90.99	108.63
37	V	607	CHL	O2D-CGD-CBD	6.16	117.71	110.95
29	8	621	BCR	C4-C5-C6	-6.15	114.39	122.70
26	B	837	CLA	C4A-NA-C1A	6.14	109.48	106.68
37	Y	606	CHL	C4D-ND-C1D	-6.12	100.58	105.22
29	4	621	BCR	C23-C24-C25	-6.11	110.67	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	O	2004	BCR	C8-C7-C6	-6.11	110.67	127.00
26	X	603	CLA	C4A-NA-C1A	6.10	109.46	106.68
36	V	1623	NEX	O24-C25-C24	6.10	119.21	113.49
35	3	619	XAT	C18-C5-C6	-6.10	112.27	122.30
35	3	619	XAT	C38-C25-C26	-6.09	112.27	122.30
26	A	809	CLA	C4A-NA-C1A	6.09	109.46	106.68
26	A	802	CLA	C4A-NA-C1A	6.08	109.45	106.68
36	W	1623	NEX	C11-C10-C9	-6.07	118.76	127.28
26	A	834	CLA	C4A-NA-C1A	6.06	109.44	106.68
29	F	305	BCR	C28-C27-C26	-6.06	103.25	114.06
35	7	620	XAT	O4-C5-C4	6.05	119.17	113.49
26	6	603	CLA	C4A-NA-C1A	6.05	109.44	106.68
26	2	601	CLA	C4A-NA-C1A	6.05	109.44	106.68
37	Z	609	CHL	C1B-CHB-C4A	6.05	125.21	121.32
26	A	821	CLA	C4A-NA-C1A	6.04	109.44	106.68
36	6	624	NEX	C38-C25-C26	-6.04	112.37	122.30
29	6	622	BCR	C40-C30-C25	6.02	119.69	110.24
26	3	606	CLA	C4A-NA-C1A	6.01	109.42	106.68
29	B	849	BCR	C20-C21-C22	-5.99	118.87	127.28
26	W	614	CLA	C4A-NA-C1A	5.98	109.41	106.68
26	B	820	CLA	C4A-NA-C1A	5.98	109.41	106.68
37	Z	606	CHL	CHA-C1A-C2A	-5.97	119.30	133.31
35	7	620	XAT	C18-C5-C6	-5.96	112.49	122.30
37	V	609	CHL	CHA-C1A-C2A	-5.93	119.38	133.31
37	Y	601	CHL	C4D-ND-C1D	-5.92	100.73	105.22
26	Z	613	CLA	C4A-NA-C1A	5.92	109.38	106.68
37	Z	608	CHL	C4D-ND-C1D	-5.90	100.74	105.22
26	B	824	CLA	C4A-NA-C1A	5.90	109.37	106.68
36	U	1623	NEX	C20-C13-C12	5.89	127.09	118.09
29	3	620	BCR	C40-C30-C25	5.89	119.48	110.24
36	W	1623	NEX	C15-C14-C13	-5.88	119.03	127.28
29	L	309	BCR	C39-C30-C25	5.88	119.47	110.24
26	Y	603	CLA	C4A-NA-C1A	5.88	109.36	106.68
26	B	811	CLA	C4A-NA-C1A	5.88	109.36	106.68
37	X	609	CHL	CHA-C1A-C2A	-5.87	119.53	133.31
35	4	620	XAT	O24-C25-C38	5.86	121.60	115.05
26	L	303	CLA	C4A-NA-C1A	5.86	109.35	106.68
35	X	1622	XAT	O24-C25-C24	5.85	118.98	113.49
34	2	619	LUT	C21-C26-C27	-5.85	106.10	112.83
29	O	2005	BCR	C40-C30-C39	-5.85	91.89	108.63
26	6	618	CLA	C4A-NA-C1A	5.85	109.35	106.68
37	Z	607	CHL	C1B-CHB-C4A	5.84	125.08	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	619	BCR	C33-C5-C6	-5.82	118.13	124.48
29	L	305	BCR	C33-C5-C6	-5.82	118.13	124.48
26	U	612	CLA	C4A-NA-C1A	5.81	109.33	106.68
29	6	622	BCR	C33-C5-C6	-5.81	118.14	124.48
26	1	612	CLA	C4A-NA-C1A	5.81	109.33	106.68
29	a	619	BCR	C33-C5-C6	-5.80	118.16	124.48
35	6	621	XAT	C38-C25-C26	-5.79	112.77	122.30
37	U	607	CHL	C4D-ND-C1D	-5.79	100.83	105.22
35	3	619	XAT	O24-C25-C24	5.79	118.91	113.49
35	U	1622	XAT	C15-C14-C13	-5.78	119.17	127.28
26	U	603	CLA	C4A-NA-C1A	5.78	109.31	106.68
29	7	621	BCR	C23-C24-C25	-5.78	111.57	127.00
29	K	207	BCR	C39-C30-C25	5.77	119.30	110.24
26	B	836	CLA	C4A-NA-C1A	5.77	109.31	106.68
37	W	606	CHL	C4D-ND-C1D	-5.76	100.84	105.22
26	a	612	CLA	C4A-NA-C1A	5.76	109.31	106.68
35	a	618	XAT	O4-C5-C4	5.76	118.89	113.49
29	F	305	BCR	C36-C18-C17	-5.76	113.48	122.82
29	9	621	BCR	C23-C22-C21	-5.76	109.96	119.01
29	B	852	BCR	C32-C1-C2	-5.75	86.85	108.95
29	9	621	BCR	C27-C26-C25	-5.75	114.93	122.70
26	5	601	CLA	C4A-NA-C1A	5.75	109.30	106.68
37	X	609	CHL	C4D-ND-C1D	-5.75	100.86	105.22
26	B	841	CLA	C4A-NA-C1A	5.74	109.30	106.68
29	5	622	BCR	C8-C7-C6	-5.73	111.68	127.00
26	a	609	CLA	C4A-NA-C1A	5.72	109.29	106.68
26	B	838	CLA	C4A-NA-C1A	5.72	109.29	106.68
37	Y	606	CHL	CHA-C1A-C2A	-5.71	119.89	133.31
34	a	617	LUT	C8-C7-C6	-5.71	111.74	127.00
26	L	307	CLA	C4A-NA-C1A	5.71	109.28	106.68
29	B	845	BCR	C37-C22-C21	-5.71	113.57	122.82
26	B	813	CLA	C4A-NA-C1A	5.71	109.28	106.68
29	B	801	BCR	C16-C17-C18	-5.71	119.28	127.28
26	4	603	CLA	C4A-NA-C1A	5.70	109.28	106.68
37	X	606	CHL	C4D-ND-C1D	-5.70	100.89	105.22
26	5	613	CLA	C4A-NA-C1A	5.70	109.28	106.68
26	A	839	CLA	C4A-NA-C1A	5.69	109.28	106.68
26	B	840	CLA	C4A-NA-C1A	5.69	109.28	106.68
37	V	608	CHL	CHA-C1A-C2A	-5.69	119.95	133.31
26	B	827	CLA	C4A-NA-C1A	5.68	109.27	106.68
37	Z	607	CHL	C4D-ND-C1D	-5.68	100.91	105.22
29	8	621	BCR	C23-C24-C25	-5.67	111.84	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	W	1622	XAT	C38-C25-C26	-5.67	112.98	122.30
29	B	847	BCR	C38-C26-C25	-5.66	118.30	124.48
29	B	846	BCR	C28-C27-C26	-5.66	103.96	114.06
37	X	608	CHL	C1B-CHB-C4A	5.66	124.97	121.32
29	9	621	BCR	C33-C5-C6	-5.66	118.31	124.48
37	U	609	CHL	C4D-ND-C1D	-5.66	100.93	105.22
26	A	806	CLA	C4A-NA-C1A	5.65	109.26	106.68
26	A	824	CLA	C4A-NA-C1A	5.65	109.26	106.68
34	1	617	LUT	C8-C7-C6	-5.65	111.91	127.00
35	X	1622	XAT	O4-C5-C4	5.65	118.78	113.49
35	1	618	XAT	O4-C5-C4	5.65	118.78	113.49
26	B	831	CLA	C4A-NA-C1A	5.64	109.25	106.68
26	6	620	CLA	C4A-NA-C1A	5.64	109.25	106.68
37	U	609	CHL	CHA-C1A-C2A	-5.64	120.06	133.31
26	B	803	CLA	C4A-NA-C1A	5.64	109.25	106.68
37	U	606	CHL	CHA-C1A-C2A	-5.63	120.08	133.31
29	a	619	BCR	C40-C30-C25	5.63	119.07	110.24
35	8	620	XAT	C18-C5-C6	-5.62	113.05	122.30
29	a	619	BCR	C8-C7-C6	-5.62	111.98	127.00
29	1	619	BCR	C8-C7-C6	-5.62	111.99	127.00
29	1	619	BCR	C40-C30-C25	5.62	119.06	110.24
26	B	814	CLA	C4A-NA-C1A	5.62	109.24	106.68
35	W	1622	XAT	O24-C25-C24	5.62	118.75	113.49
26	B	807	CLA	C4A-NA-C1A	5.61	109.24	106.68
29	J	102	BCR	C20-C21-C22	-5.60	119.42	127.28
37	Y	609	CHL	C4D-ND-C1D	-5.60	100.97	105.22
37	X	601	CHL	C4D-ND-C1D	-5.59	100.97	105.22
35	9	620	XAT	C18-C5-C6	-5.59	113.09	122.30
26	1	609	CLA	C4A-NA-C1A	5.59	109.23	106.68
26	V	613	CLA	C4A-NA-C1A	5.58	109.22	106.68
29	9	621	BCR	C7-C8-C9	5.58	134.48	126.23
35	9	620	XAT	O24-C25-C24	5.57	118.71	113.49
26	A	805	CLA	C4A-NA-C1A	5.56	109.22	106.68
29	6	622	BCR	C38-C26-C25	-5.56	118.42	124.48
29	B	852	BCR	C20-C21-C22	-5.55	119.50	127.28
35	7	620	XAT	O24-C25-C24	5.55	118.69	113.49
35	V	1622	XAT	C18-C5-C6	-5.55	113.17	122.30
36	U	1623	NEX	C35-C34-C33	-5.55	119.50	127.28
29	L	308	BCR	C7-C8-C9	-5.54	118.03	126.23
26	1	602	CLA	C4A-NA-C1A	5.54	109.20	106.68
26	A	835	CLA	C4A-NA-C1A	5.53	109.20	106.68
29	L	305	BCR	C11-C10-C9	-5.53	119.53	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	609	CLA	C4A-NA-C1A	5.50	109.19	106.68
29	3	620	BCR	C38-C26-C25	-5.50	118.48	124.48
26	8	608	CLA	C4A-NA-C1A	5.50	109.19	106.68
35	Y	1622	XAT	O4-C5-C4	5.50	118.64	113.49
26	A	829	CLA	C4A-NA-C1A	5.49	109.18	106.68
29	B	848	BCR	C8-C7-C6	-5.49	112.34	127.00
26	A	811	CLA	C4A-NA-C1A	5.48	109.18	106.68
35	V	1622	XAT	C38-C25-C26	-5.48	113.28	122.30
37	V	601	CHL	CHA-C1A-C2A	-5.48	120.44	133.31
26	F	303	CLA	C4A-NA-C1A	5.48	109.18	106.68
35	Y	1622	XAT	O24-C25-C24	5.48	118.63	113.49
35	5	621	XAT	C18-C5-C6	-5.48	113.28	122.30
37	W	608	CHL	CHA-C1A-C2A	-5.48	120.45	133.31
26	2	611	CLA	C4A-NA-C1A	5.47	109.18	106.68
26	A	804	CLA	C4A-NA-C1A	5.46	109.17	106.68
34	6	619	LUT	C8-C7-C6	-5.45	112.43	127.00
35	X	1622	XAT	C38-C25-C26	-5.45	113.34	122.30
26	9	609	CLA	C4A-NA-C1A	5.44	109.16	106.68
26	G	203	CLA	C4A-NA-C1A	5.44	109.16	106.68
37	V	607	CHL	C4D-ND-C1D	-5.44	101.09	105.22
29	G	205	BCR	C8-C7-C6	-5.43	112.49	127.00
26	8	612	CLA	C4A-NA-C1A	5.43	109.16	106.68
29	A	852	BCR	C37-C22-C23	5.42	126.37	118.09
29	A	849	BCR	C28-C27-C26	-5.42	104.39	114.06
35	V	1622	XAT	O4-C5-C18	5.42	121.10	115.05
26	A	817	CLA	C4A-NA-C1A	5.41	109.15	106.68
26	B	804	CLA	C4A-NA-C1A	5.41	109.15	106.68
26	5	602	CLA	C4A-NA-C1A	5.41	109.15	106.68
29	7	621	BCR	C8-C7-C6	-5.41	112.55	127.00
26	A	854	CLA	C4A-NA-C1A	5.41	109.15	106.68
37	W	601	CHL	C4D-ND-C1D	-5.40	101.12	105.22
34	W	1621	LUT	C15-C14-C13	-5.40	119.70	127.28
26	7	608	CLA	C4A-NA-C1A	5.40	109.14	106.68
26	Y	613	CLA	C4A-NA-C1A	5.40	109.14	106.68
36	X	1623	NEX	C15-C14-C13	-5.39	119.71	127.28
35	U	1622	XAT	C38-C25-C26	-5.39	113.43	122.30
35	V	1622	XAT	O4-C5-C4	5.38	118.53	113.49
26	K	201	CLA	C4A-NA-C1A	5.38	109.13	106.68
35	a	618	XAT	C38-C25-C26	-5.38	113.45	122.30
26	U	611	CLA	C4A-NA-C1A	5.38	109.13	106.68
26	a	602	CLA	C4A-NA-C1A	5.37	109.13	106.68
37	W	609	CHL	CHA-C1A-C2A	-5.37	120.70	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	611	CLA	C4A-NA-C1A	5.37	109.13	106.68
37	V	606	CHL	C4D-ND-C1D	-5.36	101.15	105.22
37	V	605	CHL	C1B-CHB-C4A	5.36	124.77	121.32
26	B	833	CLA	C4A-NA-C1A	5.35	109.12	106.68
37	Z	609	CHL	C4D-ND-C1D	-5.35	101.16	105.22
35	1	618	XAT	C38-C25-C26	-5.35	113.49	122.30
35	3	619	XAT	O4-C5-C18	5.35	121.03	115.05
26	L	304	CLA	C4A-NA-C1A	5.35	109.12	106.68
26	A	801	CLA	C4A-NA-C1A	5.34	109.12	106.68
26	B	805	CLA	C4A-NA-C1A	5.34	109.11	106.68
37	V	605	CHL	C4D-ND-C1D	-5.34	101.17	105.22
26	a	601	CLA	C4A-NA-C1A	5.33	109.11	106.68
26	a	616	CLA	C4A-NA-C1A	5.33	109.11	106.68
26	A	807	CLA	C4A-NA-C1A	5.32	109.11	106.68
29	O	2004	BCR	C3-C4-C5	-5.32	104.57	114.06
37	Y	608	CHL	CHA-C1A-C2A	-5.31	120.83	133.31
34	9	619	LUT	C21-C26-C27	-5.31	106.72	112.83
36	Z	1623	NEX	C15-C14-C13	-5.31	119.83	127.28
36	6	624	NEX	O24-C25-C24	5.31	118.46	113.49
26	A	813	CLA	C4A-NA-C1A	5.30	109.10	106.68
26	2	606	CLA	C4A-NA-C1A	5.30	109.10	106.68
29	F	305	BCR	C38-C26-C25	-5.30	118.70	124.48
26	A	838	CLA	C4A-NA-C1A	5.29	109.09	106.68
35	5	621	XAT	O4-C5-C18	5.28	120.95	115.05
37	V	605	CHL	CHA-C1A-C2A	-5.28	120.91	133.31
37	W	609	CHL	C4D-ND-C1D	-5.28	101.21	105.22
37	W	609	CHL	C1B-CHB-C4A	5.27	124.72	121.32
26	9	613	CLA	C4A-NA-C1A	5.27	109.08	106.68
29	K	207	BCR	C30-C25-C26	-5.27	115.43	122.64
35	9	620	XAT	O4-C5-C4	5.27	118.43	113.49
29	A	852	BCR	C3-C4-C5	-5.27	104.66	114.06
26	A	842	CLA	C4A-NA-C1A	5.27	109.08	106.68
26	K	203	CLA	C4A-NA-C1A	5.26	109.08	106.68
29	K	207	BCR	C40-C30-C29	-5.26	88.75	108.95
26	9	601	CLA	C4A-NA-C1A	5.26	109.08	106.68
35	U	1622	XAT	C18-C5-C6	-5.26	113.65	122.30
35	Z	1622	XAT	C6-C7-C8	-5.25	114.90	125.99
29	L	309	BCR	C38-C26-C25	-5.25	118.76	124.48
26	V	612	CLA	C4A-NA-C1A	5.24	109.07	106.68
37	Y	609	CHL	CHA-C1A-C2A	-5.24	121.01	133.31
29	6	622	BCR	C23-C24-C25	-5.24	113.01	127.00
29	L	308	BCR	C28-C27-C26	-5.23	104.73	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	W	1622	XAT	O4-C5-C4	5.22	118.39	113.49
29	A	849	BCR	C20-C21-C22	-5.21	119.97	127.28
26	U	610	CLA	C4A-NA-C1A	5.21	109.06	106.68
34	3	618	LUT	C18-C5-C6	-5.21	118.80	124.48
37	Z	609	CHL	CHA-C1A-C2A	-5.21	121.08	133.31
26	A	830	CLA	C4A-NA-C1A	5.21	109.05	106.68
26	A	836	CLA	C4A-NA-C1A	5.21	109.05	106.68
29	B	844	BCR	C16-C17-C18	-5.20	119.98	127.28
26	2	613	CLA	C4A-NA-C1A	5.20	109.05	106.68
29	4	621	BCR	C33-C5-C6	-5.20	118.81	124.48
29	2	623	BCR	C33-C5-C6	-5.19	118.82	124.48
34	5	620	LUT	C21-C26-C27	-5.19	106.85	112.83
35	U	1622	XAT	O4-C5-C18	5.19	120.84	115.05
29	B	852	BCR	C15-C16-C17	-5.19	112.91	123.52
37	X	606	CHL	CHA-C1A-C2A	-5.18	121.14	133.31
26	A	803	CLA	C4A-NA-C1A	5.18	109.04	106.68
26	B	832	CLA	C4A-NA-C1A	5.18	109.04	106.68
29	O	2005	BCR	C8-C7-C6	-5.18	113.17	127.00
37	W	605	CHL	CHA-C1A-C2A	-5.18	121.16	133.31
26	9	611	CLA	C4A-NA-C1A	5.17	109.04	106.68
26	B	816	CLA	C4A-NA-C1A	5.17	109.04	106.68
35	Z	1622	XAT	O4-C5-C4	5.16	118.33	113.49
26	5	619	CLA	C4A-NA-C1A	5.15	109.03	106.68
35	2	620	XAT	C18-C5-C6	-5.14	113.83	122.30
29	B	849	BCR	C33-C5-C6	-5.14	118.88	124.48
26	9	606	CLA	C4A-NA-C1A	5.14	109.02	106.68
26	1	601	CLA	C4A-NA-C1A	5.14	109.02	106.68
37	Z	601	CHL	CHA-C1A-C2A	-5.14	121.25	133.31
35	8	620	XAT	O4-C5-C4	5.13	118.30	113.49
35	U	1622	XAT	C31-C30-C29	-5.13	120.08	127.28
35	Z	1622	XAT	C38-C25-C26	-5.12	113.87	122.30
26	1	616	CLA	C4A-NA-C1A	5.12	109.02	106.68
37	W	601	CHL	CHA-C1A-C2A	-5.11	121.30	133.31
26	4	608	CLA	C4A-NA-C1A	5.11	109.01	106.68
34	Y	1621	LUT	C7-C8-C9	-5.10	118.69	126.23
36	X	1623	NEX	C17-C1-C2	-5.10	84.90	109.06
26	5	616	CLA	C4A-NA-C1A	5.10	109.00	106.68
37	U	608	CHL	CHA-C1A-C2A	-5.10	121.34	133.31
26	6	602	CLA	C4A-NA-C1A	5.09	109.00	106.68
26	W	613	CLA	C4A-NA-C1A	5.09	109.00	106.68
35	Y	1622	XAT	C38-C25-C26	-5.09	113.92	122.30
29	B	847	BCR	C23-C24-C25	-5.08	113.42	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	9	602	CLA	C4A-NA-C1A	5.08	109.00	106.68
29	K	202	BCR	C30-C25-C26	-5.08	115.69	122.64
29	O	2005	BCR	C40-C30-C29	-5.08	89.45	108.95
29	B	849	BCR	C27-C26-C25	-5.08	115.84	122.70
37	Y	607	CHL	CHA-C1A-C2A	-5.08	121.39	133.31
36	Z	1623	NEX	C2-C1-C6	5.07	114.14	109.21
29	A	850	BCR	C23-C24-C25	-5.07	113.45	127.00
34	7	619	LUT	C18-C5-C6	5.07	130.01	124.48
29	O	2005	BCR	C20-C21-C22	-5.07	120.17	127.28
29	7	621	BCR	C40-C30-C25	5.07	118.19	110.24
26	4	614	CLA	C4A-NA-C1A	5.07	108.99	106.68
26	4	604	CLA	C4A-NA-C1A	5.06	108.99	106.68
26	A	841	CLA	C4A-NA-C1A	5.05	108.98	106.68
29	9	621	BCR	C34-C9-C8	5.05	125.81	118.09
36	6	624	NEX	O24-C25-C38	5.05	120.70	115.05
26	3	617	CLA	C4A-NA-C1A	5.05	108.98	106.68
35	2	620	XAT	C38-C25-C26	-5.04	114.01	122.30
26	W	612	CLA	C4A-NA-C1A	5.03	108.98	106.68
26	a	608	CLA	C4A-NA-C1A	5.03	108.97	106.68
35	W	1622	XAT	C18-C5-C6	-5.03	114.03	122.30
29	2	623	BCR	C7-C8-C9	-5.03	118.80	126.23
37	U	601	CHL	C4D-ND-C1D	-5.03	101.41	105.22
35	9	620	XAT	C38-C25-C26	-5.02	114.04	122.30
26	A	810	CLA	C4A-NA-C1A	5.02	108.97	106.68
35	6	621	XAT	O4-C5-C4	5.01	118.19	113.49
26	1	608	CLA	C4A-NA-C1A	5.01	108.97	106.68
26	V	604	CLA	C4A-NA-C1A	5.01	108.97	106.68
26	2	614	CLA	C4A-NA-C1A	5.01	108.96	106.68
26	A	833	CLA	C4A-NA-C1A	5.00	108.96	106.68
34	V	1621	LUT	C11-C10-C9	-5.00	120.27	127.28
26	A	825	CLA	C4A-NA-C1A	5.00	108.96	106.68
36	Z	1623	NEX	C17-C1-C6	-5.00	106.00	110.47
35	6	621	XAT	O24-C25-C24	4.99	118.17	113.49
29	5	622	BCR	C3-C4-C5	-4.99	105.16	114.06
26	8	602	CLA	C4A-NA-C1A	4.99	108.95	106.68
37	X	605	CHL	C4D-ND-C1D	-4.98	101.44	105.22
29	B	852	BCR	C15-C14-C13	-4.98	120.29	127.28
26	6	609	CLA	C4A-NA-C1A	4.98	108.95	106.68
35	a	618	XAT	O24-C25-C38	4.98	120.61	115.05
29	K	202	BCR	C20-C21-C22	-4.97	120.30	127.28
29	B	847	BCR	C24-C23-C22	-4.97	118.88	126.23
29	2	623	BCR	C8-C7-C6	-4.97	113.71	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	826	CLA	C4A-NA-C1A	4.97	108.95	106.68
37	V	606	CHL	CHA-C1A-C2A	-4.97	121.64	133.31
34	W	1621	LUT	C11-C10-C9	-4.96	120.31	127.28
26	U	614	CLA	C4A-NA-C1A	4.96	108.94	106.68
35	1	618	XAT	O24-C25-C38	4.95	120.58	115.05
26	3	611	CLA	C4A-NA-C1A	4.95	108.94	106.68
35	4	620	XAT	C18-C5-C6	-4.95	114.15	122.30
35	V	1622	XAT	C31-C30-C29	-4.95	120.34	127.28
36	U	1623	NEX	C38-C25-C26	-4.95	114.16	122.30
26	8	606	CLA	C4A-NA-C1A	4.94	108.94	106.68
36	V	1623	NEX	C15-C14-C13	-4.94	120.34	127.28
34	Y	1620	LUT	C11-C12-C13	-4.94	112.81	126.36
35	V	1622	XAT	O24-C25-C38	4.94	120.57	115.05
26	6	616	CLA	C4A-NA-C1A	4.94	108.93	106.68
27	B	842	PQN	C14-C13-C15	-4.93	106.66	115.23
26	7	611	CLA	C4A-NA-C1A	4.93	108.93	106.68
29	B	844	BCR	C20-C21-C22	-4.93	120.36	127.28
27	B	842	PQN	C15-C13-C12	-4.93	110.11	121.17
26	F	304	CLA	C4A-NA-C1A	4.92	108.92	106.68
26	6	606	CLA	C4A-NA-C1A	4.92	108.92	106.68
26	9	603	CLA	C4A-NA-C1A	4.92	108.92	106.68
35	8	620	XAT	O24-C25-C38	4.92	120.55	115.05
36	Y	1623	NEX	C38-C25-C26	-4.92	114.21	122.30
34	Y	1620	LUT	C7-C8-C9	-4.91	118.96	126.23
26	A	840	CLA	C4A-NA-C1A	4.91	108.92	106.68
26	8	611	CLA	C4A-NA-C1A	4.91	108.92	106.68
34	2	619	LUT	C1-C6-C5	-4.91	115.93	122.64
26	4	613	CLA	C4A-NA-C1A	4.91	108.92	106.68
26	A	818	CLA	C4A-NA-C1A	4.89	108.91	106.68
26	O	2003	CLA	C4A-NA-C1A	4.89	108.91	106.68
35	W	1622	XAT	C37-C21-C26	-4.88	96.86	110.05
26	B	817	CLA	C4A-NA-C1A	4.88	108.91	106.68
26	A	820	CLA	C4A-NA-C1A	4.88	108.90	106.68
35	V	1622	XAT	C15-C14-C13	-4.88	120.44	127.28
26	A	808	CLA	C4A-NA-C1A	4.87	108.90	106.68
34	2	619	LUT	C8-C7-C6	-4.86	114.01	127.00
29	G	205	BCR	C20-C21-C22	-4.86	120.46	127.28
26	7	615	CLA	C4A-NA-C1A	4.86	108.90	106.68
36	V	1623	NEX	C38-C25-C26	-4.86	114.31	122.30
37	W	607	CHL	C4D-ND-C1D	-4.84	101.54	105.22
37	Z	608	CHL	CHA-C1A-C2A	-4.84	121.94	133.31
29	F	305	BCR	C20-C21-C22	-4.84	120.49	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	839	CLA	C4A-NA-C1A	4.84	108.89	106.68
26	1	606	CLA	C4A-NA-C1A	4.84	108.89	106.68
37	U	605	CHL	C4D-ND-C1D	-4.83	101.55	105.22
34	U	1620	LUT	C15-C14-C13	-4.83	120.50	127.28
36	6	624	NEX	C5-C6-C1	4.83	124.49	119.70
26	A	827	CLA	C4A-NA-C1A	4.83	108.88	106.68
26	B	835	CLA	C4A-NA-C1A	4.83	108.88	106.68
36	6	624	NEX	C2-C1-C6	4.83	113.91	109.21
36	X	1623	NEX	C38-C25-C26	-4.83	114.36	122.30
35	U	1622	XAT	O4-C5-C4	4.83	118.01	113.49
35	V	1622	XAT	O24-C25-C24	4.82	118.01	113.49
35	5	621	XAT	O4-C5-C4	4.82	118.01	113.49
35	U	1622	XAT	C27-C28-C29	-4.82	118.05	125.53
34	X	1621	LUT	C35-C34-C33	-4.82	120.52	127.28
26	B	812	CLA	C4A-NA-C1A	4.82	108.88	106.68
29	B	849	BCR	C23-C24-C25	-4.82	114.13	127.00
37	X	608	CHL	CHA-C1A-C2A	-4.81	122.01	133.31
29	L	308	BCR	C3-C4-C5	-4.81	105.48	114.06
29	B	848	BCR	C28-C27-C26	-4.81	105.48	114.06
36	Z	1623	NEX	C27-C28-C29	-4.81	118.07	125.53
26	3	613	CLA	C4A-NA-C1A	4.81	108.87	106.68
29	A	849	BCR	C24-C23-C22	-4.81	119.12	126.23
34	4	619	LUT	C26-C27-C28	-4.81	117.10	124.58
29	2	623	BCR	C20-C21-C22	-4.81	120.54	127.28
26	8	607	CLA	C4A-NA-C1A	4.80	108.87	106.68
29	K	202	BCR	C36-C18-C19	4.80	125.43	118.09
29	B	849	BCR	C38-C26-C25	4.80	129.72	124.48
26	H	203	CLA	C4A-NA-C1A	4.80	108.87	106.68
26	7	601	CLA	C4A-NA-C1A	4.80	108.87	106.68
29	5	622	BCR	C38-C26-C25	-4.79	119.25	124.48
26	2	616	CLA	C4A-NA-C1A	4.79	108.87	106.68
29	1	619	BCR	C23-C24-C25	-4.79	114.21	127.00
26	3	609	CLA	C4A-NA-C1A	4.79	108.86	106.68
37	Z	607	CHL	CHA-C1A-C2A	-4.79	122.07	133.31
36	5	624	NEX	O24-C25-C38	4.79	120.40	115.05
26	A	831	CLA	C4A-NA-C1A	4.78	108.86	106.68
26	2	607	CLA	C4A-NA-C1A	4.78	108.86	106.68
35	X	1622	XAT	C18-C5-C6	-4.78	114.43	122.30
36	Y	1623	NEX	C27-C28-C29	-4.78	118.11	125.53
26	4	606	CLA	C4A-NA-C1A	4.78	108.86	106.68
35	7	620	XAT	C38-C25-C26	-4.78	114.44	122.30
29	a	619	BCR	C23-C24-C25	-4.77	114.25	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	J	102	BCR	C36-C18-C19	4.77	125.38	118.09
35	3	619	XAT	O4-C5-C4	4.77	117.96	113.49
26	3	608	CLA	C4A-NA-C1A	4.77	108.85	106.68
29	K	207	BCR	C29-C30-C25	4.76	117.36	110.44
26	3	614	CLA	C4A-NA-C1A	4.76	108.85	106.68
26	5	606	CLA	C4A-NA-C1A	4.76	108.85	106.68
37	Y	601	CHL	CHA-C1A-C2A	-4.76	122.13	133.31
34	V	1621	LUT	C15-C14-C13	-4.76	120.61	127.28
26	Z	611	CLA	C4A-NA-C1A	4.75	108.85	106.68
35	W	1622	XAT	O4-C5-C18	4.75	120.36	115.05
26	9	610	CLA	C4A-NA-C1A	4.75	108.85	106.68
29	B	853	BCR	C24-C23-C22	-4.74	119.22	126.23
26	V	611	CLA	C4A-NA-C1A	4.74	108.84	106.68
36	Z	1623	NEX	C38-C25-C26	-4.74	114.50	122.30
29	B	849	BCR	C7-C8-C9	-4.74	119.23	126.23
35	Y	1622	XAT	C18-C5-C6	-4.73	114.52	122.30
26	A	812	CLA	C4A-NA-C1A	4.72	108.83	106.68
37	X	607	CHL	CHA-C1A-C2A	-4.72	122.22	133.31
26	B	808	CLA	C4A-NA-C1A	4.72	108.83	106.68
35	a	618	XAT	C18-C5-C6	-4.72	114.54	122.30
29	L	309	BCR	C23-C24-C25	-4.72	114.39	127.00
29	G	205	BCR	C16-C17-C18	-4.71	120.67	127.28
27	B	842	PQN	C14-C13-C12	-4.71	111.52	123.63
26	8	616	CLA	C4A-NA-C1A	4.71	108.83	106.68
29	7	623	BCR	C38-C26-C25	-4.71	119.35	124.48
35	1	618	XAT	C18-C5-C6	-4.71	114.56	122.30
36	X	1623	NEX	C27-C28-C29	-4.70	118.23	125.53
36	Y	1623	NEX	C35-C34-C33	-4.70	120.68	127.28
29	B	801	BCR	C20-C21-C22	-4.70	120.68	127.28
26	G	204	CLA	C4A-NA-C1A	4.70	108.82	106.68
26	5	609	CLA	C4A-NA-C1A	4.69	108.82	106.68
36	5	624	NEX	C26-C27-C28	-4.68	116.10	125.99
26	B	802	CLA	C4A-NA-C1A	4.67	108.81	106.68
29	3	621	BCR	C8-C7-C6	-4.67	114.52	127.00
26	8	601	CLA	C4A-NA-C1A	4.67	108.81	106.68
36	W	1623	NEX	C38-C25-C26	-4.67	114.61	122.30
26	2	612	CLA	C4A-NA-C1A	4.67	108.81	106.68
26	4	602	CLA	C4A-NA-C1A	4.67	108.81	106.68
29	A	851	BCR	C37-C22-C23	4.66	125.21	118.09
26	7	612	CLA	C4A-NA-C1A	4.66	108.81	106.68
29	L	309	BCR	C7-C8-C9	-4.66	119.34	126.23
35	U	1622	XAT	C37-C21-C26	-4.66	97.47	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	X	1622	XAT	C15-C14-C13	-4.66	120.74	127.28
26	3	607	CLA	C4A-NA-C1A	4.66	108.80	106.68
26	Z	602	CLA	C4A-NA-C1A	4.66	108.80	106.68
29	2	623	BCR	C38-C26-C25	-4.66	119.40	124.48
35	Y	1622	XAT	C6-C7-C8	-4.65	116.15	125.99
26	5	607	CLA	C4A-NA-C1A	4.65	108.80	106.68
26	X	613	CLA	C4A-NA-C1A	4.65	108.80	106.68
29	7	623	BCR	C20-C21-C22	-4.65	120.75	127.28
26	a	614	CLA	C4A-NA-C1A	4.65	108.80	106.68
26	8	609	CLA	C4A-NA-C1A	4.65	108.80	106.68
35	2	620	XAT	O4-C5-C18	4.65	120.24	115.05
26	6	617	CLA	C4A-NA-C1A	4.64	108.80	106.68
29	6	622	BCR	C8-C7-C6	-4.64	114.61	127.00
26	3	604	CLA	C4A-NA-C1A	4.64	108.79	106.68
26	8	614	CLA	C4A-NA-C1A	4.64	108.79	106.68
26	5	617	CLA	C4A-NA-C1A	4.63	108.79	106.68
26	7	616	CLA	C4A-NA-C1A	4.63	108.79	106.68
34	5	620	LUT	C26-C27-C28	-4.63	117.37	124.58
26	5	604	CLA	C4A-NA-C1A	4.63	108.79	106.68
37	X	605	CHL	CHA-C1A-C2A	-4.63	122.44	133.31
26	6	607	CLA	C4A-NA-C1A	4.63	108.79	106.68
29	B	846	BCR	C3-C4-C5	-4.63	105.81	114.06
26	X	602	CLA	C4A-NA-C1A	4.62	108.79	106.68
26	a	606	CLA	C4A-NA-C1A	4.62	108.79	106.68
34	U	1621	LUT	C15-C14-C13	-4.61	120.81	127.28
26	O	2001	CLA	C4A-NA-C1A	4.61	108.78	106.68
26	1	614	CLA	C4A-NA-C1A	4.61	108.78	106.68
26	5	612	CLA	C4A-NA-C1A	4.61	108.78	106.68
37	U	605	CHL	CHA-C1A-C2A	-4.60	122.50	133.31
34	V	1621	LUT	C7-C8-C9	-4.60	119.43	126.23
26	L	306	CLA	C4A-NA-C1A	4.60	108.78	106.68
26	3	615	CLA	C4A-NA-C1A	4.60	108.78	106.68
35	Y	1622	XAT	O24-C25-C38	4.60	120.19	115.05
35	Z	1622	XAT	C18-C5-C6	-4.60	114.73	122.30
29	O	2005	BCR	C29-C30-C25	4.60	117.12	110.44
26	B	822	CLA	C4A-NA-C1A	4.60	108.78	106.68
26	9	607	CLA	C4A-NA-C1A	4.60	108.78	106.68
35	6	621	XAT	C18-C5-C6	-4.59	114.74	122.30
35	W	1622	XAT	C11-C10-C9	-4.59	120.84	127.28
26	8	604	CLA	C4A-NA-C1A	4.59	108.77	106.68
35	2	620	XAT	O24-C25-C38	4.59	120.17	115.05
35	5	621	XAT	C38-C25-C26	-4.57	114.78	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	828	CLA	C4A-NA-C1A	4.57	108.77	106.68
26	8	613	CLA	C4A-NA-C1A	4.57	108.77	106.68
36	Y	1623	NEX	C15-C14-C13	-4.57	120.87	127.28
34	Z	1620	LUT	C11-C10-C9	-4.57	120.87	127.28
26	A	832	CLA	C4A-NA-C1A	4.57	108.76	106.68
34	Z	1620	LUT	C26-C27-C28	-4.57	117.47	124.58
26	4	616	CLA	C4A-NA-C1A	4.57	108.76	106.68
34	6	619	LUT	C18-C5-C6	-4.56	119.51	124.48
37	Y	605	CHL	C4D-ND-C1D	-4.56	101.76	105.22
29	B	844	BCR	C15-C16-C17	-4.56	114.19	123.52
26	X	612	CLA	C4A-NA-C1A	4.56	108.76	106.68
34	V	1620	LUT	C11-C10-C9	-4.55	120.89	127.28
34	Z	1620	LUT	C7-C8-C9	-4.55	119.50	126.23
29	J	102	BCR	C15-C16-C17	-4.55	114.21	123.52
29	a	619	BCR	C20-C21-C22	-4.55	120.90	127.28
26	A	843	CLA	C4A-NA-C1A	4.55	108.75	106.68
29	B	801	BCR	C28-C27-C26	-4.55	105.95	114.06
26	B	834	CLA	C4A-NA-C1A	4.55	108.75	106.68
26	X	611	CLA	C4A-NA-C1A	4.55	108.75	106.68
29	B	847	BCR	C33-C5-C6	-4.55	119.52	124.48
35	X	1622	XAT	O24-C25-C38	4.54	120.13	115.05
26	4	618	CLA	C4A-NA-C1A	4.54	108.75	106.68
34	6	619	LUT	C16-C1-C6	4.54	117.36	110.24
26	6	613	CLA	C4A-NA-C1A	4.53	108.75	106.68
26	9	604	CLA	C4A-NA-C1A	4.53	108.75	106.68
26	K	206	CLA	C4A-NA-C1A	4.53	108.75	106.68
26	7	606	CLA	C4A-NA-C1A	4.53	108.75	106.68
29	7	621	BCR	C28-C27-C26	-4.53	105.98	114.06
37	Z	608	CHL	C1B-CHB-C4A	4.53	124.24	121.32
29	B	843	BCR	C16-C17-C18	-4.53	120.93	127.28
26	B	823	CLA	C4A-NA-C1A	4.53	108.74	106.68
35	U	1622	XAT	C6-C7-C8	-4.53	116.42	125.99
37	W	606	CHL	CHA-C1A-C2A	-4.53	122.68	133.31
26	B	821	CLA	C4A-NA-C1A	4.52	108.74	106.68
35	3	619	XAT	C6-C7-C8	-4.52	116.43	125.99
29	K	207	BCR	C20-C21-C22	-4.51	120.95	127.28
26	F	301	CLA	C4A-NA-C1A	4.51	108.74	106.68
26	4	610	CLA	C4A-NA-C1A	4.51	108.74	106.68
35	9	620	XAT	C26-C27-C28	-4.51	116.46	125.99
26	4	601	CLA	C4A-NA-C1A	4.50	108.73	106.68
26	X	614	CLA	C4A-NA-C1A	4.50	108.73	106.68
29	B	801	BCR	C37-C22-C23	4.50	124.97	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5	622	BCR	C33-C5-C6	-4.50	119.57	124.48
35	2	620	XAT	O24-C25-C24	4.50	117.71	113.49
35	Z	1622	XAT	C26-C27-C28	-4.50	116.48	125.99
26	Y	604	CLA	C4A-NA-C1A	4.50	108.73	106.68
29	A	850	BCR	C20-C21-C22	-4.49	120.98	127.28
34	W	1620	LUT	C11-C10-C9	-4.49	120.98	127.28
26	J	101	CLA	C4A-NA-C1A	4.49	108.73	106.68
29	1	619	BCR	C20-C21-C22	-4.48	120.99	127.28
34	X	1620	LUT	C7-C8-C9	-4.48	119.61	126.23
26	Z	614	CLA	C4A-NA-C1A	4.47	108.72	106.68
34	7	619	LUT	C21-C26-C27	-4.47	107.69	112.83
29	O	2005	BCR	C30-C25-C26	-4.47	116.53	122.64
26	6	608	CLA	C4A-NA-C1A	4.47	108.72	106.68
26	A	845	CLA	CMB-C2B-C1B	-4.47	118.61	125.42
35	1	618	XAT	O24-C25-C24	4.47	117.68	113.49
29	O	2004	BCR	C20-C21-C22	-4.47	121.01	127.28
26	B	818	CLA	C4A-NA-C1A	4.46	108.72	106.68
26	5	610	CLA	C4A-NA-C1A	4.46	108.72	106.68
26	5	611	CLA	C4A-NA-C1A	4.46	108.72	106.68
29	B	844	BCR	C38-C26-C25	4.46	129.35	124.48
29	B	845	BCR	C29-C30-C25	4.45	116.91	110.44
35	5	621	XAT	C6-C7-C8	-4.44	116.60	125.99
37	U	607	CHL	C1B-CHB-C4A	4.44	124.18	121.32
26	6	610	CLA	C4A-NA-C1A	4.44	108.71	106.68
35	Z	1622	XAT	O24-C25-C38	4.44	120.01	115.05
29	B	843	BCR	C20-C21-C22	-4.44	121.05	127.28
35	X	1622	XAT	O4-C5-C18	4.44	120.01	115.05
34	3	618	LUT	C19-C9-C8	-4.44	111.31	118.09
29	B	843	BCR	C37-C22-C23	4.44	124.87	118.09
26	4	611	CLA	C4A-NA-C1A	4.43	108.70	106.68
29	B	845	BCR	C24-C23-C22	-4.43	119.68	126.23
35	a	618	XAT	O24-C25-C24	4.43	117.64	113.49
29	K	207	BCR	C7-C8-C9	-4.43	119.68	126.23
26	B	836	CLA	CMB-C2B-C1B	-4.43	118.68	125.42
26	7	610	CLA	C4A-NA-C1A	4.42	108.70	106.68
29	B	847	BCR	C8-C7-C6	-4.41	115.20	127.00
37	U	607	CHL	CHA-C1A-C2A	-4.41	122.95	133.31
29	B	843	BCR	C7-C8-C9	-4.41	119.71	126.23
35	8	620	XAT	C38-C25-C26	-4.41	115.04	122.30
26	5	608	CLA	C4A-NA-C1A	4.41	108.69	106.68
26	V	614	CLA	C4A-NA-C1A	4.41	108.69	106.68
29	6	622	BCR	C28-C27-C26	-4.41	106.20	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	U	601	CHL	CHA-C1A-C2A	-4.40	122.97	133.31
29	B	847	BCR	C3-C4-C5	-4.40	106.21	114.06
29	3	621	BCR	C33-C5-C6	-4.40	119.69	124.48
29	B	852	BCR	C23-C24-C25	-4.40	115.26	127.00
35	Z	1622	XAT	O4-C5-C18	4.39	119.96	115.05
36	U	1623	NEX	O24-C25-C38	4.39	119.96	115.05
26	2	609	CLA	C4A-NA-C1A	4.39	108.68	106.68
29	L	309	BCR	C16-C17-C18	-4.38	121.14	127.28
36	Z	1623	NEX	C31-C30-C29	-4.38	121.14	127.28
29	L	308	BCR	C30-C25-C24	4.37	127.50	115.65
26	L	302	CLA	C4A-NA-C1A	4.37	108.67	106.68
36	X	1623	NEX	O24-C25-C38	4.37	119.93	115.05
35	W	1622	XAT	C15-C14-C13	-4.36	121.16	127.28
26	H	202	CLA	C4A-NA-C1A	4.36	108.67	106.68
35	4	620	XAT	C6-C7-C8	-4.36	116.78	125.99
26	7	602	CLA	C4A-NA-C1A	4.36	108.67	106.68
29	B	844	BCR	C7-C8-C9	-4.35	119.79	126.23
26	B	830	CLA	C4A-NA-C1A	4.35	108.67	106.68
26	U	604	CLA	C4A-NA-C1A	4.35	108.66	106.68
29	B	852	BCR	C19-C18-C17	-4.34	112.17	119.01
26	7	604	CLA	C4A-NA-C1A	4.34	108.66	106.68
29	9	621	BCR	C38-C26-C25	4.33	129.21	124.48
29	3	622	BCR	C16-C17-C18	-4.33	121.20	127.28
29	7	621	BCR	C20-C21-C22	-4.33	121.20	127.28
36	U	1623	NEX	C27-C28-C29	-4.33	118.81	125.53
32	H	205	LMG	O7-C10-C11	4.33	120.85	111.48
29	B	852	BCR	C35-C13-C12	-4.32	111.48	118.09
32	J	103	LMG	O7-C10-C11	4.32	120.83	111.48
34	X	1620	LUT	C26-C27-C28	-4.32	117.86	124.58
29	B	848	BCR	C37-C22-C23	4.31	124.68	118.09
37	X	608	CHL	C3D-C4D-ND	4.31	118.95	110.42
36	5	624	NEX	O24-C25-C24	4.31	117.53	113.49
34	5	620	LUT	C35-C15-C14	-4.31	114.70	123.52
29	L	301	BCR	C34-C9-C10	-4.31	115.84	122.82
34	V	1621	LUT	C31-C30-C29	-4.31	121.24	127.28
26	A	829	CLA	CMB-C2B-C1B	-4.31	118.86	125.42
37	V	607	CHL	CHA-C1A-C2A	-4.31	123.20	133.31
26	Y	614	CLA	C4A-NA-C1A	4.30	108.64	106.68
29	L	301	BCR	C28-C27-C26	-4.30	106.38	114.06
36	5	624	NEX	C8-C7-C6	-4.30	172.59	177.66
29	B	846	BCR	C20-C21-C22	-4.30	121.25	127.28
26	5	618	CLA	C4A-NA-C1A	4.30	108.64	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	7	607	CLA	C4A-NA-C1A	4.30	108.64	106.68
26	5	614	CLA	C4A-NA-C1A	4.30	108.64	106.68
34	X	1621	LUT	C26-C27-C28	-4.30	117.89	124.58
29	8	621	BCR	C20-C21-C22	-4.29	121.26	127.28
29	L	301	BCR	C20-C21-C22	-4.29	121.27	127.28
37	X	608	CHL	O2D-CGD-CBD	4.28	118.43	111.43
28	2	622	LHG	O7-C7-C8	4.28	120.75	111.48
35	V	1622	XAT	C35-C34-C33	-4.28	121.27	127.28
26	3	602	CLA	C4A-NA-C1A	4.28	108.63	106.68
34	V	1620	LUT	C35-C34-C33	-4.27	121.29	127.28
36	Y	1623	NEX	C16-C1-C6	-4.27	106.65	110.47
35	V	1622	XAT	C11-C10-C9	-4.27	121.29	127.28
29	B	853	BCR	C37-C22-C23	4.27	124.61	118.09
29	B	852	BCR	C10-C11-C12	-4.26	110.85	123.20
37	W	606	CHL	CBC-CAC-C3C	-4.26	106.77	112.87
26	V	602	CLA	C4A-NA-C1A	4.26	108.62	106.68
36	V	1623	NEX	C27-C28-C29	-4.26	118.92	125.53
34	a	617	LUT	C18-C5-C6	-4.26	119.83	124.48
35	Z	1622	XAT	C35-C34-C33	-4.26	121.31	127.28
29	A	851	BCR	C3-C4-C5	-4.26	106.47	114.06
29	B	844	BCR	C19-C18-C17	-4.26	112.31	119.01
35	Y	1622	XAT	O4-C5-C18	4.25	119.80	115.05
29	B	849	BCR	C1-C6-C5	-4.25	116.83	122.64
26	A	826	CLA	CMB-C2B-C1B	-4.24	118.96	125.42
35	9	620	XAT	C6-C7-C8	-4.24	117.03	125.99
27	A	844	PQN	C15-C13-C12	-4.24	111.66	121.17
34	1	617	LUT	C18-C5-C6	-4.23	119.87	124.48
26	4	607	CLA	C4A-NA-C1A	4.23	108.61	106.68
26	O	2001	CLA	C3A-C2A-C1A	-4.22	101.99	106.30
35	W	1622	XAT	O24-C25-C38	4.21	119.75	115.05
27	A	844	PQN	C14-C13-C12	-4.21	112.82	123.63
35	9	620	XAT	O4-C5-C18	4.20	119.75	115.05
29	L	305	BCR	C3-C4-C5	-4.20	106.56	114.06
29	9	621	BCR	C16-C17-C18	-4.19	121.40	127.28
34	8	619	LUT	C18-C5-C6	-4.19	119.91	124.48
26	W	610	CLA	C4A-NA-C1A	4.19	108.59	106.68
29	3	622	BCR	C3-C4-C5	-4.19	106.59	114.06
29	B	847	BCR	C15-C16-C17	-4.18	114.96	123.52
29	3	620	BCR	C23-C24-C25	-4.18	115.83	127.00
35	Z	1622	XAT	C35-C15-C14	-4.18	114.97	123.52
32	8	626	LMG	O7-C10-C11	4.18	120.52	111.48
37	U	607	CHL	CMA-C3A-C4A	-4.18	105.61	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Y	1620	LUT	C35-C34-C33	4.18	133.13	127.28
29	L	305	BCR	C33-C5-C4	4.17	122.49	113.60
29	9	621	BCR	C20-C21-C22	-4.17	121.43	127.28
29	A	848	BCR	C20-C21-C22	-4.17	121.43	127.28
26	1	604	CLA	C4A-NA-C1A	4.17	108.58	106.68
35	2	620	XAT	C35-C15-C14	-4.16	115.00	123.52
29	B	845	BCR	C34-C9-C10	-4.16	116.07	122.82
34	1	617	LUT	C26-C27-C28	-4.15	118.11	124.58
29	O	2005	BCR	C16-C17-C18	-4.15	121.45	127.28
26	2	610	CLA	C4A-NA-C1A	4.15	108.57	106.68
35	4	620	XAT	C38-C25-C26	-4.14	115.48	122.30
29	A	851	BCR	C16-C17-C18	-4.14	121.47	127.28
26	6	604	CLA	C4A-NA-C1A	4.14	108.57	106.68
33	B	850	DGD	O2G-C1B-C2B	4.14	120.43	111.48
26	2	603	CLA	C4A-NA-C1A	4.13	108.56	106.68
35	U	1622	XAT	C35-C34-C33	-4.13	121.48	127.28
26	a	613	CLA	C4A-NA-C1A	4.13	108.56	106.68
29	A	851	BCR	C30-C25-C24	4.13	126.85	115.65
29	L	309	BCR	C4-C5-C6	-4.13	117.12	122.70
36	5	624	NEX	C5-C6-C1	4.13	123.79	119.70
29	B	845	BCR	C3-C4-C5	-4.12	106.71	114.06
36	W	1623	NEX	C27-C28-C29	-4.12	119.14	125.53
35	Y	1622	XAT	C31-C30-C29	-4.12	121.50	127.28
34	a	617	LUT	C26-C27-C28	-4.12	118.17	124.58
26	a	604	CLA	C4A-NA-C1A	4.11	108.56	106.68
34	6	619	LUT	C26-C27-C28	-4.11	118.18	124.58
26	Z	604	CLA	C4A-NA-C1A	4.11	108.55	106.68
29	3	622	BCR	C20-C21-C22	-4.11	121.52	127.28
29	3	620	BCR	C28-C27-C26	-4.10	106.74	114.06
29	9	621	BCR	C8-C9-C10	-4.10	112.56	119.01
34	V	1620	LUT	C26-C27-C28	-4.10	118.20	124.58
29	A	851	BCR	C20-C21-C22	-4.10	121.53	127.28
36	X	1623	NEX	C35-C34-C33	-4.10	121.53	127.28
29	L	309	BCR	C20-C21-C22	-4.09	121.54	127.28
36	Z	1623	NEX	C5-C6-C1	4.09	123.75	119.70
26	6	612	CLA	C4A-NA-C1A	4.08	108.54	106.68
37	V	607	CHL	CMA-C3A-C4A	-4.08	105.82	114.61
26	B	815	CLA	C4A-NA-C1A	4.07	108.54	106.68
26	W	604	CLA	C4A-NA-C1A	4.07	108.54	106.68
29	B	848	BCR	C38-C26-C25	4.07	128.93	124.48
29	K	207	BCR	C24-C23-C22	-4.07	120.21	126.23
28	O	2631	LHG	O7-C7-C8	4.07	120.29	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	X	601	CHL	CHA-C1A-C2A	-4.07	123.75	133.31
29	O	2004	BCR	C24-C23-C22	-4.07	120.22	126.23
35	8	620	XAT	O4-C5-C18	4.06	119.59	115.05
29	K	202	BCR	C27-C26-C25	-4.06	117.21	122.70
29	B	844	BCR	C30-C25-C26	-4.06	117.09	122.64
26	1	613	CLA	C4A-NA-C1A	4.06	108.53	106.68
26	B	829	CLA	CMB-C2B-C1B	-4.05	119.25	125.42
26	B	829	CLA	C4A-NA-C1A	4.04	108.52	106.68
26	Y	602	CLA	C4A-NA-C1A	4.04	108.52	106.68
29	B	844	BCR	C37-C22-C23	4.04	124.26	118.09
29	3	622	BCR	C23-C24-C25	-4.03	116.22	127.00
26	a	611	CLA	C4A-NA-C1A	4.03	108.52	106.68
34	U	1621	LUT	C11-C10-C9	-4.03	121.62	127.28
29	J	102	BCR	C39-C30-C25	-4.03	103.93	110.24
29	L	308	BCR	C37-C22-C23	4.03	124.24	118.09
32	V	2631	LMG	O7-C10-C11	4.03	120.19	111.48
26	1	610	CLA	C3A-C2A-C1A	-4.03	102.18	106.30
28	U	2630	LHG	O7-C7-C8	4.02	120.19	111.48
35	2	620	XAT	O4-C5-C4	4.02	117.26	113.49
29	A	849	BCR	C27-C26-C25	-4.02	117.27	122.70
26	9	614	CLA	C4A-NA-C1A	4.02	108.51	106.68
29	B	848	BCR	C16-C17-C18	-4.01	121.65	127.28
34	2	619	LUT	C26-C27-C28	-4.01	118.34	124.58
34	W	1621	LUT	C35-C34-C33	-4.01	121.66	127.28
32	H	205	LMG	C8-O7-C10	-4.00	108.21	117.80
34	2	619	LUT	C11-C10-C9	-4.00	121.67	127.28
28	W	2630	LHG	O7-C7-C8	3.99	120.12	111.48
29	B	849	BCR	C37-C22-C23	-3.99	111.99	118.09
35	X	1622	XAT	C6-C7-C8	-3.99	117.55	125.99
26	4	613	CLA	C1-O2A-CGA	3.99	126.31	116.65
26	1	611	CLA	C4A-NA-C1A	3.99	108.50	106.68
29	B	845	BCR	C36-C18-C19	3.99	124.18	118.09
31	5	629	LMU	O5B-C1B-C2B	3.98	118.55	110.37
29	3	622	BCR	C7-C8-C9	-3.98	120.35	126.23
26	3	612	CLA	C4A-NA-C1A	3.98	108.50	106.68
29	L	301	BCR	C15-C16-C17	-3.98	115.38	123.52
29	F	305	BCR	C30-C25-C26	-3.98	117.20	122.64
29	B	844	BCR	C36-C18-C19	3.97	124.16	118.09
35	3	619	XAT	C26-C27-C28	-3.97	117.59	125.99
29	G	205	BCR	C38-C26-C25	-3.97	120.15	124.48
26	B	825	CLA	C4A-NA-C1A	3.97	108.49	106.68
33	B	850	DGD	O6D-C5D-C6D	3.97	114.56	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	305	BCR	C20-C21-C22	-3.96	121.72	127.28
26	6	601	CLA	C4A-NA-C1A	3.96	108.49	106.68
36	V	1623	NEX	C17-C1-C6	-3.96	106.93	110.47
29	3	620	BCR	C20-C21-C22	-3.95	121.73	127.28
29	B	844	BCR	C15-C14-C13	-3.95	121.73	127.28
35	W	1622	XAT	C6-C7-C8	-3.95	117.64	125.99
34	5	620	LUT	C8-C7-C6	-3.94	116.48	127.00
29	1	619	BCR	C38-C26-C25	-3.94	120.19	124.48
26	B	818	CLA	C4-C3-C5	3.93	122.06	115.23
26	7	614	CLA	C4A-NA-C1A	3.93	108.47	106.68
29	9	621	BCR	C37-C22-C23	3.93	124.09	118.09
26	U	602	CLA	C4A-NA-C1A	3.93	108.47	106.68
34	3	618	LUT	C11-C10-C9	-3.92	121.78	127.28
29	J	102	BCR	C23-C24-C25	-3.92	116.53	127.00
29	a	619	BCR	C38-C26-C25	-3.92	120.21	124.48
26	3	610	CLA	C4A-NA-C1A	3.92	108.47	106.68
26	Y	612	CLA	C4A-NA-C1A	3.92	108.47	106.68
26	8	610	CLA	C4A-NA-C1A	3.91	108.46	106.68
26	O	2002	CLA	C4A-NA-C1A	3.91	108.46	106.68
26	7	602	CLA	C3B-C4B-NB	-3.90	107.05	110.53
29	L	308	BCR	C20-C19-C18	-3.90	115.67	126.36
29	L	308	BCR	C23-C22-C21	-3.90	112.88	119.01
34	X	1620	LUT	C11-C10-C9	-3.89	121.82	127.28
29	A	849	BCR	C36-C18-C19	3.89	124.03	118.09
34	Y	1620	LUT	C26-C27-C28	-3.89	118.53	124.58
29	B	846	BCR	C37-C22-C23	3.89	124.02	118.09
29	B	847	BCR	C20-C21-C22	-3.89	121.83	127.28
32	J	104	LMG	O7-C10-C11	3.88	119.88	111.48
36	Y	1623	NEX	O24-C25-C38	3.88	119.39	115.05
26	A	836	CLA	C4-C3-C5	3.88	121.96	115.23
35	Z	1622	XAT	C31-C30-C29	-3.88	121.84	127.28
29	5	622	BCR	C20-C21-C22	-3.87	121.85	127.28
31	A	857	LMU	C1'-C2'-C3'	3.87	118.15	110.01
29	A	856	BCR	C20-C21-C22	-3.87	121.85	127.28
37	V	609	CHL	CBC-CAC-C3C	-3.87	107.33	112.87
29	3	621	BCR	C20-C21-C22	-3.87	121.85	127.28
34	8	619	LUT	C26-C27-C28	-3.87	118.56	124.58
29	B	852	BCR	C11-C10-C9	3.86	132.70	127.28
35	5	621	XAT	C27-C28-C29	-3.86	119.54	125.53
36	6	624	NEX	C16-C1-C6	-3.86	107.02	110.47
35	8	620	XAT	C26-C27-C28	-3.86	117.84	125.99
29	4	621	BCR	C3-C4-C5	-3.85	107.18	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	U	1622	XAT	O24-C25-C38	3.85	119.35	115.05
34	Y	1621	LUT	C1-C6-C5	-3.85	117.37	122.64
29	B	853	BCR	C7-C8-C9	-3.85	120.54	126.23
29	4	621	BCR	C38-C26-C25	-3.85	120.28	124.48
26	W	602	CLA	C4A-NA-C1A	3.85	108.44	106.68
29	7	621	BCR	C38-C26-C25	-3.85	120.29	124.48
34	U	1620	LUT	C26-C27-C28	-3.84	118.60	124.58
29	3	622	BCR	C16-C15-C14	-3.84	115.67	123.52
37	Z	609	CHL	CBC-CAC-C3C	-3.84	107.38	112.87
35	7	620	XAT	C6-C7-C8	-3.84	117.88	125.99
29	B	847	BCR	C36-C18-C19	3.83	123.94	118.09
35	X	1622	XAT	C11-C10-C9	-3.83	121.91	127.28
35	6	621	XAT	O4-C5-C18	3.83	119.33	115.05
28	X	2630	LHG	O7-C7-C8	3.82	119.74	111.48
26	6	614	CLA	C4A-NA-C1A	3.81	108.42	106.68
34	3	618	LUT	C18-C5-C4	3.81	121.42	114.42
35	1	618	XAT	O4-C5-C18	3.81	119.30	115.05
34	Y	1621	LUT	C15-C14-C13	-3.81	121.94	127.28
29	O	2005	BCR	C38-C26-C25	-3.81	120.33	124.48
34	7	619	LUT	C19-C9-C8	-3.80	112.28	118.09
29	A	848	BCR	C36-C18-C17	-3.80	116.66	122.82
29	L	305	BCR	C32-C1-C6	-3.80	104.29	110.24
34	1	617	LUT	C21-C26-C27	-3.79	108.47	112.83
29	4	621	BCR	C20-C21-C22	-3.79	121.97	127.28
34	Y	1621	LUT	C35-C34-C33	-3.79	121.97	127.28
26	Z	612	CLA	C4A-NA-C1A	3.79	108.41	106.68
34	a	617	LUT	C21-C26-C27	-3.78	108.47	112.83
29	B	852	BCR	C36-C18-C19	3.78	123.87	118.09
26	4	612	CLA	C4A-NA-C1A	3.78	108.40	106.68
29	A	850	BCR	C16-C17-C18	-3.78	121.98	127.28
26	3	610	CLA	C3B-C4B-NB	-3.78	107.16	110.53
29	2	623	BCR	C16-C17-C18	-3.77	121.98	127.28
29	9	621	BCR	C3-C4-C5	-3.77	107.33	114.06
36	W	1623	NEX	C35-C34-C33	-3.77	122.00	127.28
29	B	852	BCR	C37-C22-C23	3.76	123.84	118.09
26	1	610	CLA	C4A-NA-C1A	3.76	108.39	106.68
29	B	853	BCR	C33-C5-C6	-3.76	120.38	124.48
35	Z	1622	XAT	C11-C10-C9	-3.76	122.01	127.28
29	B	801	BCR	C16-C15-C14	-3.76	115.83	123.52
35	6	621	XAT	O24-C25-C38	3.75	119.24	115.05
29	K	202	BCR	C37-C22-C23	3.75	123.81	118.09
31	1	621	LMU	C1B-O1B-C4'	-3.75	109.10	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	625	LMU	C1'-C2'-C3'	3.74	117.89	110.01
35	Y	1622	XAT	C26-C27-C28	-3.74	118.08	125.99
36	Y	1623	NEX	C11-C10-C9	-3.74	122.03	127.28
32	5	627	LMG	O7-C10-C11	3.74	119.57	111.48
29	B	849	BCR	C16-C17-C18	-3.74	122.04	127.28
28	B	851	LHG	O7-C7-C8	3.74	119.56	111.48
29	B	845	BCR	C7-C8-C9	-3.73	120.71	126.23
29	B	845	BCR	C37-C22-C23	3.73	123.79	118.09
35	a	618	XAT	O4-C5-C18	3.73	119.22	115.05
34	X	1620	LUT	C15-C14-C13	-3.73	122.05	127.28
26	B	826	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
34	8	619	LUT	C19-C9-C8	-3.72	112.40	118.09
29	1	619	BCR	C28-C27-C26	-3.72	107.42	114.06
29	L	308	BCR	C30-C25-C26	-3.72	117.56	122.64
29	L	308	BCR	C16-C17-C18	-3.72	122.07	127.28
34	W	1620	LUT	C35-C34-C33	-3.72	122.07	127.28
29	K	207	BCR	C39-C30-C29	3.71	123.21	108.95
36	6	624	NEX	C26-C27-C28	-3.71	118.14	125.99
29	B	844	BCR	C21-C20-C19	-3.71	112.45	123.20
29	a	619	BCR	C28-C27-C26	-3.71	107.44	114.06
29	A	849	BCR	C3-C4-C5	-3.71	107.44	114.06
29	B	846	BCR	C30-C25-C24	3.71	125.70	115.65
34	Z	1620	LUT	C15-C14-C13	-3.70	122.09	127.28
29	3	620	BCR	C11-C10-C9	-3.70	122.09	127.28
29	B	846	BCR	C8-C7-C6	-3.70	117.12	127.00
29	B	801	BCR	C33-C5-C6	-3.70	120.45	124.48
29	A	852	BCR	C38-C26-C25	-3.70	120.45	124.48
34	8	619	LUT	C16-C1-C6	3.70	116.04	110.24
37	Z	601	CHL	C1-C2-C3	-3.69	120.14	126.20
29	8	621	BCR	C8-C7-C6	-3.69	117.13	127.00
29	2	623	BCR	C11-C10-C9	-3.69	122.10	127.28
29	3	621	BCR	C23-C24-C25	-3.69	117.14	127.00
26	8	610	CLA	CMB-C2B-C1B	-3.69	119.80	125.42
35	2	620	XAT	C6-C7-C8	-3.69	118.20	125.99
36	Z	1623	NEX	O24-C25-C38	3.69	119.17	115.05
29	7	621	BCR	C33-C5-C6	-3.69	120.46	124.48
35	2	620	XAT	C27-C28-C29	-3.68	119.82	125.53
26	B	825	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
35	U	1622	XAT	C15-C35-C34	-3.68	116.00	123.52
26	a	610	CLA	C4A-NA-C1A	3.67	108.36	106.68
29	B	801	BCR	C24-C23-C22	-3.67	120.80	126.23
36	V	1623	NEX	O24-C25-C38	3.67	119.15	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	U	1623	NEX	C31-C30-C29	-3.67	122.13	127.28
28	A	861	LHG	O7-C7-C8	3.67	119.42	111.48
29	F	305	BCR	C16-C15-C14	-3.67	116.01	123.52
36	U	1623	NEX	C15-C14-C13	-3.66	122.14	127.28
26	1	607	CLA	C4A-NA-C1A	3.66	108.35	106.68
26	A	822	CLA	C4A-NA-C1A	3.66	108.35	106.68
26	2	604	CLA	C4A-NA-C1A	3.66	108.35	106.68
36	V	1623	NEX	C15-C35-C34	-3.66	116.04	123.52
28	9	622	LHG	O7-C7-C8	3.66	119.39	111.48
34	Y	1621	LUT	C11-C10-C9	-3.65	122.15	127.28
29	A	856	BCR	C33-C5-C6	-3.65	120.50	124.48
26	A	854	CLA	CMB-C2B-C1B	-3.65	119.86	125.42
29	3	620	BCR	C24-C23-C22	-3.65	120.84	126.23
26	Y	611	CLA	C4A-NA-C1A	3.65	108.34	106.68
28	Z	2630	LHG	O7-C7-C8	3.64	119.37	111.48
29	5	622	BCR	C37-C22-C21	-3.64	116.92	122.82
29	L	301	BCR	C36-C18-C19	3.64	123.64	118.09
29	8	621	BCR	C36-C18-C19	3.64	123.64	118.09
29	3	620	BCR	C16-C17-C18	-3.64	122.18	127.28
35	8	620	XAT	C6-C7-C8	-3.63	118.31	125.99
34	V	1620	LUT	C15-C14-C13	-3.63	122.18	127.28
29	K	207	BCR	C11-C10-C9	-3.63	122.19	127.28
34	5	620	LUT	C7-C8-C9	-3.63	120.86	126.23
28	9	623	LHG	O7-C7-C8	3.63	119.33	111.48
26	Y	610	CLA	C4A-NA-C1A	3.63	108.33	106.68
35	V	1622	XAT	C27-C28-C29	-3.63	119.90	125.53
28	H	204	LHG	O7-C7-C8	3.62	119.30	111.48
35	Z	1622	XAT	C4-C3-C2	-3.61	104.03	110.79
29	F	305	BCR	C36-C18-C19	3.61	123.61	118.09
29	7	623	BCR	C36-C18-C19	3.61	123.61	118.09
28	V	2630	LHG	O7-C7-C8	3.61	119.29	111.48
28	3	624	LHG	O7-C7-C8	3.61	119.29	111.48
29	7	623	BCR	C28-C27-C26	-3.61	107.62	114.06
34	U	1621	LUT	C35-C34-C33	-3.60	122.23	127.28
35	W	1622	XAT	C35-C34-C33	-3.60	122.23	127.28
35	6	621	XAT	C6-C7-C8	-3.60	118.39	125.99
29	A	856	BCR	C36-C18-C19	3.59	123.58	118.09
26	2	610	CLA	C3B-C4B-NB	-3.59	107.32	110.53
29	1	619	BCR	C37-C22-C23	3.59	123.57	118.09
37	V	607	CHL	C1B-CHB-C4A	3.59	123.63	121.32
29	A	852	BCR	C7-C8-C9	-3.59	120.92	126.23
29	6	622	BCR	C20-C21-C22	-3.59	122.25	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	X	1622	XAT	C4-C3-C2	-3.58	104.09	110.79
29	B	853	BCR	C20-C21-C22	-3.58	122.26	127.28
29	7	623	BCR	C16-C17-C18	-3.58	122.26	127.28
34	4	619	LUT	C21-C26-C27	-3.58	108.72	112.83
29	A	852	BCR	C36-C18-C17	-3.57	117.03	122.82
35	X	1622	XAT	C35-C34-C33	-3.57	122.27	127.28
28	5	625	LHG	O7-C7-C8	3.57	119.21	111.48
29	3	621	BCR	C37-C22-C23	3.57	123.54	118.09
29	9	621	BCR	C1-C6-C5	-3.57	117.76	122.64
35	3	619	XAT	O24-C25-C38	3.57	119.03	115.05
29	3	622	BCR	C11-C10-C9	-3.56	122.28	127.28
28	9	624	LHG	O7-C7-C8	3.56	119.19	111.48
29	K	202	BCR	C16-C17-C18	-3.56	122.29	127.28
37	V	605	CHL	CBC-CAC-C3C	-3.56	107.78	112.87
29	G	205	BCR	C16-C15-C14	-3.55	116.25	123.52
29	3	620	BCR	C7-C8-C9	-3.55	120.98	126.23
37	Z	606	CHL	C1C-CHC-C4B	3.55	128.76	116.07
36	Y	1623	NEX	C5-C6-C1	3.54	123.21	119.70
31	8	625	LMU	C2'-C3'-C4'	3.54	117.71	109.68
26	1	606	CLA	C3A-C2A-C1A	-3.54	102.68	106.30
37	W	607	CHL	CHA-C1A-C2A	-3.54	125.01	133.31
35	X	1622	XAT	C26-C27-C28	-3.53	118.53	125.99
29	B	849	BCR	C3-C4-C5	-3.53	107.76	114.06
29	A	849	BCR	C38-C26-C27	3.53	121.12	113.60
29	B	844	BCR	C24-C23-C22	-3.53	121.02	126.23
26	A	845	CLA	C4A-NA-C1A	3.52	108.29	106.68
26	X	604	CLA	C4A-NA-C1A	3.52	108.29	106.68
29	a	619	BCR	C37-C22-C23	3.52	123.47	118.09
29	4	621	BCR	C16-C17-C18	-3.52	122.34	127.28
31	A	858	LMU	C6B-C5B-C4B	-3.52	108.72	113.53
29	A	852	BCR	C31-C1-C6	-3.52	104.73	110.24
32	4	624	LMG	O7-C10-C11	3.52	119.09	111.48
29	A	852	BCR	C34-C9-C10	-3.51	117.13	122.82
29	A	849	BCR	C16-C17-C18	-3.51	122.36	127.28
28	6	623	LHG	O7-C7-C8	3.51	119.07	111.48
29	A	851	BCR	C23-C22-C21	-3.50	113.50	119.01
29	J	102	BCR	C24-C23-C22	-3.50	121.05	126.23
29	O	2005	BCR	C3-C4-C5	-3.50	107.81	114.06
26	a	607	CLA	C4A-NA-C1A	3.50	108.28	106.68
37	Z	606	CHL	C3D-C4D-ND	3.50	118.56	112.94
26	8	604	CLA	C1-C2-C3	-3.50	121.10	126.76
35	1	618	XAT	C6-C7-C8	-3.50	118.59	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	801	BCR	C29-C30-C25	3.50	115.52	110.44
29	L	309	BCR	C2-C1-C6	3.50	115.52	110.44
29	L	301	BCR	C4-C5-C6	-3.50	117.98	122.70
35	a	618	XAT	C6-C7-C8	-3.50	118.60	125.99
36	V	1623	NEX	C2-C1-C6	3.50	112.61	109.21
29	L	301	BCR	C40-C30-C25	-3.50	104.76	110.24
35	9	620	XAT	C35-C15-C14	-3.49	116.37	123.52
37	X	606	CHL	OMC-CMC-C2C	-3.49	119.05	125.12
32	L	2631	LMG	C8-O7-C10	-3.49	109.44	117.80
29	B	801	BCR	C21-C20-C19	-3.49	113.08	123.20
34	W	1620	LUT	C7-C8-C9	-3.49	121.07	126.23
29	J	102	BCR	C7-C8-C9	-3.49	121.07	126.23
26	4	613	CLA	O2A-CGA-O1A	-3.49	114.91	123.63
37	Y	609	CHL	O1D-CGD-CBD	-3.49	119.44	124.72
29	B	852	BCR	C2-C1-C6	3.49	115.50	110.44
29	O	2005	BCR	C39-C30-C29	3.48	122.33	108.95
26	7	609	CLA	C4A-NA-C1A	3.48	108.27	106.68
29	L	309	BCR	C8-C9-C10	-3.48	113.53	119.01
29	6	622	BCR	C16-C17-C18	-3.48	122.39	127.28
35	6	621	XAT	C38-C25-C24	3.48	118.15	114.24
29	2	623	BCR	C39-C30-C25	-3.48	104.78	110.24
29	A	856	BCR	C16-C17-C18	-3.48	122.40	127.28
34	9	619	LUT	C26-C27-C28	-3.48	119.17	124.58
29	A	856	BCR	C37-C22-C23	3.48	123.40	118.09
34	5	620	LUT	C17-C1-C6	-3.47	104.80	110.24
28	Y	2630	LHG	O7-C7-C8	3.47	118.99	111.48
26	W	610	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
29	F	305	BCR	C24-C23-C22	-3.46	121.12	126.23
29	B	846	BCR	C24-C25-C26	-3.45	113.60	121.56
29	7	621	BCR	C37-C22-C23	3.45	123.36	118.09
29	A	849	BCR	C11-C10-C9	-3.45	122.44	127.28
26	V	610	CLA	C4A-NA-C1A	3.45	108.25	106.68
29	A	850	BCR	C38-C26-C25	-3.45	120.72	124.48
26	A	829	CLA	CMB-C2B-C3B	3.45	134.66	126.55
35	4	620	XAT	C35-C15-C14	-3.45	116.46	123.52
29	8	621	BCR	C37-C22-C23	3.45	123.36	118.09
29	L	308	BCR	C21-C20-C19	-3.45	113.21	123.20
26	B	810	CLA	CAA-C2A-C3A	-3.45	103.68	113.00
29	B	844	BCR	C28-C27-C26	-3.45	107.91	114.06
37	V	609	CHL	C3D-C4D-ND	3.45	118.47	112.94
29	B	852	BCR	C8-C7-C6	-3.44	117.80	127.00
26	Z	604	CLA	CMB-C2B-C1B	-3.44	120.17	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	7	619	LUT	C26-C27-C28	-3.44	119.22	124.58
29	A	851	BCR	C28-C27-C26	-3.44	107.92	114.06
26	5	613	CLA	C4-C3-C5	3.44	121.20	115.23
29	L	308	BCR	C38-C26-C25	-3.44	120.73	124.48
34	Z	1620	LUT	C30-C31-C32	-3.43	113.25	123.20
34	U	1621	LUT	C26-C27-C28	-3.43	119.23	124.58
34	3	618	LUT	C26-C27-C28	-3.43	119.24	124.58
34	5	620	LUT	C3-C4-C5	-3.43	103.63	112.18
26	Z	610	CLA	C4A-NA-C1A	3.43	108.25	106.68
34	U	1620	LUT	C7-C8-C9	-3.43	121.16	126.23
29	O	2005	BCR	C36-C18-C17	-3.43	117.26	122.82
34	Z	1620	LUT	C35-C34-C33	-3.43	122.47	127.28
29	5	622	BCR	C37-C22-C23	3.43	123.33	118.09
29	K	202	BCR	C15-C16-C17	-3.43	116.50	123.52
35	Y	1622	XAT	C27-C28-C29	-3.43	120.21	125.53
26	A	840	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
35	Y	1622	XAT	C4-C3-C2	-3.43	104.38	110.79
34	X	1621	LUT	C30-C31-C32	-3.42	113.28	123.20
26	A	804	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
29	K	202	BCR	C7-C8-C9	-3.42	121.17	126.23
34	Z	1621	LUT	C26-C27-C28	-3.42	119.26	124.58
29	O	2005	BCR	C31-C1-C6	-3.42	104.88	110.24
26	A	802	CLA	CMB-C2B-C1B	-3.42	120.22	125.42
29	A	848	BCR	C16-C17-C18	-3.41	122.49	127.28
26	U	604	CLA	CMB-C2B-C1B	-3.41	120.22	125.42
26	8	610	CLA	C4-C3-C5	3.41	121.15	115.23
29	A	851	BCR	C7-C8-C9	-3.41	121.19	126.23
29	G	205	BCR	C11-C10-C9	-3.41	122.50	127.28
34	V	1620	LUT	C7-C8-C9	-3.41	121.19	126.23
37	X	609	CHL	C3D-C4D-ND	3.41	118.40	112.94
26	Y	602	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
35	1	618	XAT	C26-C27-C28	-3.41	118.79	125.99
29	G	205	BCR	C36-C18-C19	3.40	123.28	118.09
29	B	846	BCR	C11-C10-C9	-3.40	122.51	127.28
26	1	602	CLA	CMB-C2B-C1B	-3.40	120.25	125.42
36	Z	1623	NEX	C15-C35-C34	-3.40	116.57	123.52
35	8	620	XAT	O24-C25-C24	3.40	116.67	113.49
28	8	623	LHG	O7-C7-C8	3.39	118.82	111.48
29	8	621	BCR	C15-C16-C17	-3.39	116.58	123.52
26	U	613	CLA	C4A-NA-C1A	3.39	108.23	106.68
29	3	621	BCR	C11-C10-C9	-3.39	122.52	127.28
35	U	1622	XAT	C11-C10-C9	-3.39	122.52	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	852	BCR	C35-C13-C14	3.39	128.31	122.82
35	3	619	XAT	C38-C25-C24	3.39	118.05	114.24
37	Y	609	CHL	C1C-CHC-C4B	3.39	128.20	116.07
34	6	619	LUT	C18-C5-C4	3.39	120.65	114.42
29	L	305	BCR	C37-C22-C21	-3.39	117.33	122.82
26	W	611	CLA	C4A-NA-C1A	3.39	108.22	106.68
29	A	851	BCR	C24-C25-C26	-3.39	113.75	121.56
35	2	620	XAT	C12-C13-C14	-3.39	113.68	119.01
26	A	814	CLA	C4-C3-C5	3.39	121.10	115.23
34	X	1621	LUT	C35-C15-C14	-3.38	116.59	123.52
29	F	305	BCR	C38-C26-C27	3.38	120.81	113.60
26	1	614	CLA	C2A-C3A-C4A	-3.38	102.65	106.24
35	W	1622	XAT	C26-C27-C28	-3.38	118.84	125.99
29	G	205	BCR	C7-C8-C9	-3.38	121.23	126.23
29	B	849	BCR	C30-C25-C26	-3.38	118.02	122.64
26	A	854	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
29	1	619	BCR	C36-C18-C17	-3.38	117.35	122.82
26	9	612	CLA	C4A-NA-C1A	3.38	108.22	106.68
29	A	850	BCR	C33-C5-C6	-3.38	120.80	124.48
36	U	1623	NEX	C20-C13-C14	-3.37	117.35	122.82
26	B	819	CLA	C4A-NA-C1A	3.37	108.22	106.68
29	B	845	BCR	C16-C17-C18	-3.37	122.55	127.28
35	5	621	XAT	C8-C9-C10	-3.37	113.71	119.01
29	B	844	BCR	C11-C10-C9	-3.37	122.55	127.28
34	W	1621	LUT	C26-C27-C28	-3.37	119.34	124.58
35	7	620	XAT	O24-C25-C38	3.37	118.81	115.05
37	X	601	CHL	CBC-CAC-C3C	-3.37	108.05	112.87
26	2	607	CLA	C3B-C4B-NB	-3.37	107.53	110.53
28	7	622	LHG	O7-C7-C8	3.36	118.75	111.48
26	a	602	CLA	CMB-C2B-C1B	-3.36	120.30	125.42
35	a	618	XAT	C26-C27-C28	-3.36	118.89	125.99
26	1	604	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
29	B	845	BCR	C8-C9-C10	3.36	124.29	119.01
26	B	826	CLA	C1-C2-C3	-3.36	120.69	126.20
35	7	620	XAT	O4-C5-C18	3.36	118.80	115.05
35	Y	1622	XAT	C35-C15-C14	-3.36	116.65	123.52
26	a	604	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
34	Y	1620	LUT	C30-C31-C32	-3.35	113.48	123.20
29	5	622	BCR	C36-C18-C19	3.35	123.21	118.09
26	A	805	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
35	X	1622	XAT	C31-C30-C29	-3.35	122.58	127.28
35	W	1622	XAT	C31-C30-C29	-3.35	122.58	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	5	620	LUT	C28-C29-C30	-3.35	113.74	119.01
37	Y	606	CHL	C1C-CHC-C4B	3.35	128.05	116.07
37	V	601	CHL	C3D-C4D-ND	3.35	118.31	112.94
37	X	606	CHL	C1C-CHC-C4B	3.35	128.04	116.07
29	4	621	BCR	C11-C10-C9	-3.34	122.59	127.28
37	Y	607	CHL	C1C-CHC-C4B	3.34	128.03	116.07
35	X	1622	XAT	C10-C11-C12	-3.34	113.52	123.20
26	8	602	CLA	CMB-C2B-C1B	-3.34	120.33	125.42
29	5	622	BCR	C36-C18-C17	-3.34	117.41	122.82
34	W	1620	LUT	C21-C26-C27	-3.34	108.99	112.83
29	O	2005	BCR	C23-C24-C25	-3.34	118.09	127.00
29	L	305	BCR	C15-C14-C13	-3.33	122.61	127.28
37	Z	605	CHL	C3D-C4D-ND	3.33	118.28	112.94
29	a	619	BCR	C36-C18-C17	-3.33	117.42	122.82
34	6	619	LUT	C21-C26-C27	-3.33	109.00	112.83
29	O	2004	BCR	C16-C17-C18	-3.33	122.61	127.28
26	X	610	CLA	C4A-NA-C1A	3.33	108.20	106.68
37	W	608	CHL	C3D-C4D-ND	3.32	118.27	112.94
26	A	822	CLA	CMB-C2B-C1B	-3.32	120.36	125.42
36	Z	1623	NEX	C11-C10-C9	-3.32	122.62	127.28
34	a	617	LUT	C16-C1-C6	3.32	115.45	110.24
29	3	622	BCR	C28-C27-C26	-3.32	108.14	114.06
29	B	852	BCR	C37-C22-C21	-3.32	117.44	122.82
26	A	820	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
34	1	617	LUT	C16-C1-C6	3.32	115.45	110.24
34	W	1620	LUT	C26-C27-C28	-3.32	119.42	124.58
34	3	618	LUT	C16-C1-C6	3.32	115.44	110.24
31	5	629	LMU	C1B-C2B-C3B	3.31	116.98	110.01
29	A	850	BCR	C11-C10-C9	-3.31	122.63	127.28
35	7	620	XAT	C27-C28-C29	-3.31	120.40	125.53
35	2	620	XAT	C10-C11-C12	-3.31	113.62	123.20
28	5	623	LHG	O7-C7-C8	3.30	118.62	111.48
34	V	1621	LUT	C35-C34-C33	-3.30	122.65	127.28
29	6	622	BCR	C36-C18-C19	3.30	123.12	118.09
29	L	309	BCR	C36-C18-C17	-3.30	117.48	122.82
26	9	613	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
35	4	620	XAT	C27-C28-C29	-3.29	120.42	125.53
35	Y	1622	XAT	C35-C34-C33	-3.29	122.66	127.28
34	X	1621	LUT	C10-C11-C12	-3.29	113.67	123.20
35	W	1622	XAT	C27-C28-C29	-3.29	120.42	125.53
37	Y	606	CHL	C3D-C4D-ND	3.29	118.21	112.94
35	U	1622	XAT	C31-C32-C33	-3.29	117.35	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	860	LMG	O1-C1-C2	3.28	113.26	108.27
32	4	623	LMG	O7-C10-C11	3.28	118.58	111.48
37	W	609	CHL	C3D-C4D-ND	3.28	118.20	112.94
34	6	619	LUT	C19-C9-C8	-3.28	113.08	118.09
29	3	622	BCR	C37-C22-C23	3.28	123.09	118.09
29	B	849	BCR	C36-C18-C19	3.28	123.09	118.09
37	Z	601	CHL	C1C-CHC-C4B	3.27	127.79	116.07
37	U	609	CHL	C3D-C4D-ND	3.27	118.19	112.94
26	A	826	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
37	X	606	CHL	CBC-CAC-C3C	-3.26	108.20	112.87
29	3	620	BCR	C39-C30-C25	-3.26	105.12	110.24
27	B	842	PQN	C11-C3-C4	-3.26	115.14	118.58
35	6	621	XAT	C27-C28-C29	-3.26	120.48	125.53
34	W	1621	LUT	C31-C30-C29	-3.25	122.72	127.28
29	1	619	BCR	C30-C25-C24	3.25	124.47	115.65
29	L	305	BCR	C16-C17-C18	-3.25	122.72	127.28
35	6	621	XAT	C26-C27-C28	-3.25	119.12	125.99
26	U	610	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
37	U	608	CHL	C3D-C4D-ND	3.25	118.15	112.94
29	a	619	BCR	C30-C25-C24	3.25	124.46	115.65
36	5	624	NEX	C38-C25-C24	3.25	117.89	114.24
34	Y	1620	LUT	C32-C33-C34	-3.24	113.91	119.01
29	K	207	BCR	C36-C18-C19	3.24	123.04	118.09
29	B	846	BCR	C7-C8-C9	-3.24	121.44	126.23
26	2	604	CLA	CMB-C2B-C1B	-3.24	120.49	125.42
34	U	1620	LUT	C21-C26-C27	-3.24	109.11	112.83
29	B	846	BCR	C36-C18-C19	3.24	123.03	118.09
37	U	609	CHL	C1C-CHC-C4B	3.24	127.65	116.07
29	J	102	BCR	C38-C26-C25	-3.23	120.95	124.48
34	Z	1621	LUT	C10-C11-C12	-3.23	113.84	123.20
26	A	817	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
26	9	610	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
35	1	618	XAT	C35-C15-C14	-3.23	116.92	123.52
36	U	1623	NEX	C16-C1-C6	3.23	113.36	110.47
37	X	609	CHL	O1D-CGD-CBD	-3.23	119.83	124.72
37	Z	607	CHL	C1C-CHC-C4B	3.22	127.60	116.07
29	L	308	BCR	C2-C1-C6	3.22	115.12	110.44
37	Y	608	CHL	C1C-CHC-C4B	3.22	127.60	116.07
26	5	607	CLA	C3B-C4B-NB	-3.22	107.66	110.53
29	A	852	BCR	C2-C1-C6	3.22	115.11	110.44
29	O	2004	BCR	C36-C18-C17	-3.22	117.60	122.82
29	3	620	BCR	C37-C22-C23	3.22	123.00	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	621	BCR	C36-C18-C19	3.22	123.00	118.09
26	B	838	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
26	A	832	CLA	CAA-C2A-C1A	-3.21	101.44	111.97
26	Y	611	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
29	a	619	BCR	C24-C25-C26	-3.21	114.16	121.56
37	V	601	CHL	C1C-CHC-C4B	3.21	127.56	116.07
37	U	608	CHL	C1C-CHC-C4B	3.21	127.56	116.07
37	V	609	CHL	C1C-CHC-C4B	3.21	127.56	116.07
35	a	618	XAT	C35-C15-C14	-3.21	116.95	123.52
26	B	827	CLA	CHB-C4A-NA	3.21	129.03	124.40
37	U	601	CHL	CBC-CAC-C3C	-3.21	108.28	112.87
29	1	619	BCR	C24-C25-C26	-3.21	114.17	121.56
37	Y	608	CHL	CBC-CAC-C3C	-3.21	108.28	112.87
37	X	606	CHL	C3D-C4D-ND	3.20	118.08	112.94
37	W	608	CHL	C1C-CHC-C4B	3.20	127.53	116.07
37	W	605	CHL	C3D-C4D-ND	3.20	118.07	112.94
29	B	852	BCR	C33-C5-C6	-3.20	120.99	124.48
26	B	807	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
35	7	620	XAT	C26-C27-C28	-3.20	119.23	125.99
29	B	845	BCR	C33-C5-C4	3.20	120.42	113.60
26	B	810	CLA	CHB-C4A-NA	3.20	129.02	124.40
35	5	621	XAT	C10-C11-C12	-3.20	113.94	123.20
26	B	836	CLA	CMB-C2B-C3B	3.20	134.06	126.55
26	A	809	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
37	U	606	CHL	C3D-C4D-ND	3.19	118.06	112.94
37	X	608	CHL	C1C-CHC-C4B	3.19	127.48	116.07
37	X	609	CHL	C1C-CHC-C4B	3.19	127.47	116.07
29	A	850	BCR	C36-C18-C19	3.19	122.95	118.09
29	L	309	BCR	C15-C14-C13	-3.18	122.81	127.28
29	K	202	BCR	C15-C14-C13	-3.18	122.82	127.28
29	B	848	BCR	C27-C26-C25	-3.18	118.41	122.70
26	A	840	CLA	O2D-CGD-CBD	3.18	116.79	111.23
26	A	845	CLA	CMB-C2B-C3B	3.18	134.03	126.55
35	W	1622	XAT	C36-C21-C26	3.18	118.63	110.05
26	8	602	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
29	8	621	BCR	C1-C6-C5	-3.18	118.29	122.64
26	X	612	CLA	CAA-C2A-C3A	-3.18	104.41	113.00
35	8	620	XAT	C10-C11-C12	-3.18	113.99	123.20
37	W	605	CHL	C1C-CHC-C4B	3.18	127.44	116.07
29	A	856	BCR	C11-C10-C9	-3.18	122.82	127.28
37	U	601	CHL	C1-C2-C3	-3.18	120.99	126.20
29	K	207	BCR	C23-C24-C25	-3.18	118.52	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	V	608	CHL	C1C-CHC-C4B	3.17	127.43	116.07
34	V	1621	LUT	C26-C27-C28	-3.17	119.64	124.58
29	L	305	BCR	C8-C9-C10	3.17	124.00	119.01
37	Z	605	CHL	C1C-CHC-C4B	3.17	127.41	116.07
26	V	602	CLA	CMB-C2B-C1B	-3.17	120.59	125.42
36	5	624	NEX	C39-C29-C30	-3.17	117.68	122.82
26	A	832	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
26	B	837	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
37	Y	609	CHL	C3D-C4D-ND	3.17	118.02	112.94
26	1	616	CLA	CMB-C2B-C3B	3.17	131.95	123.53
32	L	2631	LMG	O7-C10-C11	3.17	118.33	111.48
36	U	1623	NEX	C11-C12-C13	3.17	135.05	126.36
26	A	813	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
37	V	605	CHL	C3D-C4D-ND	3.17	118.02	112.94
36	Y	1623	NEX	C24-C23-C22	-3.16	104.87	110.79
26	U	614	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
37	X	605	CHL	C3D-C4D-ND	3.16	118.01	112.94
28	5	625	LHG	C5-O7-C7	-3.16	110.24	117.80
26	5	610	CLA	C3B-C4B-NB	-3.16	107.71	110.53
29	2	623	BCR	C23-C24-C25	-3.16	118.57	127.00
37	Z	601	CHL	C4-C3-C5	3.16	120.70	115.23
37	V	608	CHL	C3D-C4D-ND	3.15	118.00	112.94
36	W	1623	NEX	C31-C30-C29	-3.15	122.86	127.28
29	A	849	BCR	C7-C8-C9	-3.15	121.58	126.23
26	Y	614	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
37	V	606	CHL	O1D-CGD-CBD	-3.15	119.95	124.72
29	6	622	BCR	C7-C8-C9	-3.15	121.58	126.23
35	V	1622	XAT	C6-C7-C8	-3.15	119.34	125.99
37	W	601	CHL	C1C-CHC-C4B	3.15	127.33	116.07
37	V	606	CHL	CMB-C2B-C3B	3.15	130.97	124.68
26	B	827	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
26	A	833	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
34	W	1620	LUT	C15-C14-C13	-3.14	122.87	127.28
26	A	830	CLA	C3B-C4B-NB	-3.14	107.72	110.53
29	J	102	BCR	C10-C11-C12	-3.14	114.10	123.20
37	W	607	CHL	C4C-C3C-C2C	-3.14	101.19	108.42
37	W	601	CHL	C3D-C4D-ND	3.14	117.97	112.94
29	A	851	BCR	C36-C18-C19	3.14	122.88	118.09
35	V	1622	XAT	C31-C32-C33	-3.14	117.76	126.36
37	Z	605	CHL	CAA-C2A-C3A	-3.13	109.04	116.23
32	A	860	LMG	O7-C10-C11	3.13	118.25	111.48
29	B	843	BCR	C11-C10-C9	-3.13	122.89	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	849	BCR	C30-C25-C26	-3.13	118.36	122.64
37	X	607	CHL	C1C-CHC-C4B	3.13	127.26	116.07
29	6	622	BCR	C11-C10-C9	-3.13	122.89	127.28
28	8	622	LHG	O7-C7-C8	3.13	118.24	111.48
37	Y	608	CHL	C3D-C4D-ND	3.12	117.95	112.94
29	L	301	BCR	C23-C24-C25	-3.12	118.65	127.00
26	9	602	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
35	Y	1622	XAT	C24-C23-C22	-3.12	104.96	110.79
28	9	623	LHG	C5-O7-C7	-3.12	110.33	117.80
26	7	601	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
35	V	1622	XAT	C26-C27-C28	-3.12	119.40	125.99
35	7	620	XAT	C35-C15-C14	-3.12	117.14	123.52
37	Y	601	CHL	C1C-CHC-C4B	3.12	127.23	116.07
26	V	612	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
29	L	305	BCR	C37-C22-C23	3.12	122.85	118.09
35	9	620	XAT	O24-C25-C38	3.12	118.53	115.05
37	U	609	CHL	O1D-CGD-CBD	-3.12	120.00	124.72
26	5	619	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
29	5	622	BCR	C24-C25-C26	-3.12	114.38	121.56
35	4	620	XAT	O24-C25-C24	3.12	116.41	113.49
26	B	820	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
28	A	847	LHG	O7-C7-C8	3.12	118.22	111.48
26	B	810	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
34	Z	1621	LUT	C35-C34-C33	-3.11	122.91	127.28
29	B	852	BCR	C40-C30-C25	-3.11	105.36	110.24
29	6	622	BCR	C39-C30-C25	-3.11	105.36	110.24
26	X	610	CLA	C3B-C4B-NB	-3.11	107.75	110.53
29	L	309	BCR	C3-C4-C5	-3.11	108.51	114.06
29	A	848	BCR	C24-C23-C22	-3.11	121.64	126.23
26	Z	614	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
26	W	612	CLA	CAA-C2A-C3A	-3.11	104.60	113.00
34	V	1621	LUT	C7-C6-C5	3.11	128.71	121.56
26	L	302	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
34	U	1620	LUT	C18-C5-C6	-3.10	121.10	124.48
29	O	2005	BCR	C2-C1-C6	3.10	114.94	110.44
35	4	620	XAT	C8-C9-C10	-3.10	114.13	119.01
26	6	602	CLA	C3B-C4B-NB	-3.10	107.76	110.53
29	L	301	BCR	C7-C8-C9	-3.10	121.65	126.23
29	6	622	BCR	C37-C22-C23	3.10	122.82	118.09
35	3	619	XAT	C10-C11-C12	-3.10	114.23	123.20
37	W	606	CHL	C1C-CHC-C4B	3.10	127.15	116.07
29	B	801	BCR	C40-C30-C25	3.10	115.10	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Y	1620	LUT	C18-C5-C6	-3.09	121.11	124.48
26	7	610	CLA	C3B-C4B-NB	-3.09	107.77	110.53
26	2	601	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
37	Z	601	CHL	C3D-C4D-ND	3.09	117.89	112.94
26	Y	603	CLA	CAA-C2A-C3A	-3.09	104.66	113.00
26	B	840	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
36	W	1623	NEX	C11-C12-C13	-3.09	117.90	126.36
29	A	848	BCR	C37-C22-C21	-3.08	117.82	122.82
26	B	815	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
29	K	202	BCR	C11-C10-C9	-3.08	122.96	127.28
29	O	2004	BCR	C31-C1-C6	-3.08	105.42	110.24
35	6	621	XAT	C10-C11-C12	-3.08	114.29	123.20
34	6	619	LUT	C35-C15-C14	-3.07	117.23	123.52
26	1	609	CLA	CAB-C3B-C2B	3.07	131.70	123.53
26	B	812	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
34	8	619	LUT	C18-C5-C4	3.07	120.06	114.42
26	A	814	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
26	a	614	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
29	B	848	BCR	C20-C21-C22	-3.07	122.98	127.28
29	J	102	BCR	C19-C18-C17	-3.07	114.19	119.01
26	4	614	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
29	2	623	BCR	C32-C1-C6	-3.06	105.44	110.24
37	U	605	CHL	C3D-C4D-ND	3.06	117.85	112.94
29	A	852	BCR	C15-C16-C17	-3.06	117.25	123.52
34	X	1621	LUT	C16-C1-C6	-3.06	105.44	110.24
26	A	838	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
35	X	1622	XAT	C27-C28-C29	-3.06	120.78	125.53
26	8	606	CLA	C3B-C4B-NB	-3.06	107.80	110.53
35	9	620	XAT	C10-C11-C12	-3.06	114.34	123.20
29	a	619	BCR	C7-C8-C9	-3.06	121.71	126.23
29	O	2005	BCR	C7-C8-C9	-3.06	121.71	126.23
37	Y	601	CHL	C3D-C4D-ND	3.06	117.84	112.94
37	W	609	CHL	C1C-CHC-C4B	3.05	127.00	116.07
29	a	619	BCR	C16-C17-C18	-3.05	123.00	127.28
26	7	616	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
26	6	620	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
26	A	816	CLA	C1-C2-C3	-3.05	121.20	126.20
28	3	623	LHG	O7-C7-C8	3.05	118.07	111.48
37	Z	609	CHL	O1D-CGD-CBD	-3.05	120.10	124.72
26	8	616	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
26	A	808	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
26	A	826	CLA	CMB-C2B-C3B	3.04	133.70	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	848	BCR	C24-C25-C26	-3.04	114.56	121.56
26	V	614	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
37	Z	609	CHL	C3D-C4D-ND	3.04	117.81	112.94
37	Z	609	CHL	C1C-CHC-C4B	3.03	126.93	116.07
29	L	309	BCR	C36-C18-C19	3.03	122.72	118.09
37	X	607	CHL	CAA-C2A-C3A	-3.03	104.80	113.00
35	8	620	XAT	C18-C5-C4	3.03	117.65	114.24
28	3	623	LHG	C5-O7-C7	-3.03	110.54	117.80
29	3	620	BCR	C30-C25-C24	3.03	123.87	115.65
26	U	602	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
26	Y	603	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
29	3	622	BCR	C24-C23-C22	-3.03	121.75	126.23
26	2	602	CLA	C4A-NA-C1A	3.03	109.49	106.28
26	K	203	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
29	1	619	BCR	C7-C8-C9	-3.02	121.76	126.23
29	4	621	BCR	C7-C8-C9	-3.02	121.76	126.23
29	L	305	BCR	C34-C9-C10	3.02	127.71	122.82
29	B	853	BCR	C16-C17-C18	-3.02	123.04	127.28
37	Z	608	CHL	C1C-CHC-C4B	3.02	126.88	116.07
35	1	618	XAT	C10-C11-C12	-3.02	114.45	123.20
26	B	808	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
26	Y	603	CLA	CHB-C4A-NA	3.02	128.75	124.40
35	W	1622	XAT	C4-C3-C2	-3.02	105.15	110.79
29	A	849	BCR	C33-C5-C6	-3.02	121.19	124.48
26	A	812	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
26	O	2002	CLA	CMB-C2B-C3B	3.01	131.54	123.53
35	a	618	XAT	C10-C11-C12	-3.01	114.46	123.20
26	A	837	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
26	5	602	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
32	J	104	LMG	C6-C5-C4	-3.01	105.62	113.02
26	W	602	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
29	B	849	BCR	C33-C5-C4	3.01	120.02	113.60
29	B	843	BCR	C15-C14-C13	-3.01	123.05	127.28
35	2	620	XAT	C28-C29-C30	-3.01	114.27	119.01
34	4	619	LUT	C16-C1-C6	3.01	114.97	110.24
29	B	843	BCR	C16-C15-C14	-3.01	117.36	123.52
28	4	622	LHG	O7-C7-C8	3.01	117.99	111.48
26	A	839	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
37	V	606	CHL	C1C-CHC-C4B	3.01	126.84	116.07
35	V	1622	XAT	C24-C23-C22	-3.01	105.16	110.79
36	Y	1623	NEX	C2-C1-C6	3.01	112.14	109.21
29	A	848	BCR	C30-C25-C24	3.01	123.81	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	2	620	XAT	C32-C33-C34	-3.01	114.28	119.01
26	X	604	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
26	a	610	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
29	A	851	BCR	C2-C1-C6	3.01	114.81	110.44
26	B	818	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
29	G	205	BCR	C24-C23-C22	-3.01	121.79	126.23
29	1	619	BCR	C16-C17-C18	-3.00	123.06	127.28
26	9	613	CLA	C1-C2-C3	-3.00	121.28	126.20
31	A	857	LMU	C2'-C3'-C4'	3.00	116.50	109.68
37	Y	607	CHL	C3D-C4D-ND	3.00	117.75	112.94
37	V	605	CHL	C1C-CHC-C4B	3.00	126.81	116.07
26	X	603	CLA	CHB-C4A-NA	3.00	128.73	124.40
26	2	613	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
36	6	624	NEX	C39-C29-C30	-3.00	117.95	122.82
37	X	601	CHL	C1C-CHC-C4B	3.00	126.80	116.07
26	Z	603	CLA	CHB-C4A-NA	3.00	128.73	124.40
26	9	614	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
37	U	606	CHL	C1C-CHC-C4B	3.00	126.79	116.07
26	W	612	CLA	CHB-C4A-NA	2.99	128.72	124.40
26	B	803	CLA	CHB-C4A-NA	2.99	128.72	124.40
26	X	610	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
26	8	604	CLA	CMB-C2B-C1B	-2.99	120.86	125.42
34	6	619	LUT	C11-C10-C9	-2.99	123.08	127.28
26	A	854	CLA	CMB-C2B-C3B	2.99	133.58	126.55
26	B	805	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
26	Z	603	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
26	8	603	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
37	W	601	CHL	C4-C3-C5	2.99	120.41	115.23
26	B	841	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
26	A	825	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
26	2	611	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
29	L	305	BCR	C36-C18-C19	2.98	122.64	118.09
36	6	624	NEX	C15-C35-C34	-2.98	117.42	123.52
26	1	616	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
26	6	603	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
26	2	616	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
29	L	308	BCR	C4-C5-C6	-2.98	118.68	122.70
26	6	610	CLA	C3B-C4B-NB	-2.98	107.87	110.53
26	B	841	CLA	C3B-C4B-NB	-2.97	107.88	110.53
29	3	622	BCR	C8-C7-C6	-2.97	119.06	127.00
26	9	601	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
34	5	620	LUT	C35-C34-C33	-2.97	123.11	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	J	104	LMG	O8-C28-C29	2.97	120.89	111.83
26	8	610	CLA	CMB-C2B-C3B	2.97	133.53	126.55
26	8	614	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
37	X	609	CHL	O2D-CGD-O1D	-2.96	118.08	123.85
26	Y	610	CLA	C3B-C4B-NB	-2.96	107.89	110.53
26	4	601	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
37	X	607	CHL	C3D-C4D-ND	2.96	117.69	112.94
35	4	620	XAT	C18-C5-C4	2.96	117.56	114.24
26	A	824	CLA	C4-C3-C5	2.96	120.36	115.23
35	W	1622	XAT	C10-C11-C12	-2.96	114.63	123.20
37	U	601	CHL	C1C-CHC-C4B	2.96	126.65	116.07
35	5	621	XAT	O24-C25-C38	2.96	118.35	115.05
26	Z	611	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
26	A	810	CLA	CHB-C4A-NA	2.96	128.67	124.40
26	8	613	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
35	1	618	XAT	C27-C28-C29	-2.95	120.95	125.53
29	G	205	BCR	C36-C18-C17	-2.95	118.03	122.82
26	6	602	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
26	9	610	CLA	C3B-C4B-NB	-2.95	107.90	110.53
34	3	618	LUT	C21-C26-C27	-2.95	109.44	112.83
28	U	2630	LHG	O8-C23-C24	2.95	120.83	111.83
31	A	857	LMU	C1B-O1B-C4'	-2.95	110.99	117.98
26	B	819	CLA	C3B-C4B-NB	-2.95	107.90	110.53
37	V	609	CHL	CMA-C3A-C4A	-2.95	108.26	114.61
29	5	622	BCR	C30-C25-C24	2.95	123.64	115.65
29	J	102	BCR	C29-C30-C25	2.95	114.72	110.44
34	2	619	LUT	C7-C8-C9	-2.94	121.88	126.23
26	2	601	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
29	O	2004	BCR	C2-C1-C6	2.94	114.71	110.44
26	3	609	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
29	B	843	BCR	C15-C16-C17	-2.94	117.50	123.52
29	A	852	BCR	C23-C22-C21	-2.94	114.38	119.01
26	6	607	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
37	Y	605	CHL	C3D-C4D-ND	2.94	117.65	112.94
29	8	621	BCR	C37-C22-C21	-2.94	118.05	122.82
26	B	834	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
26	U	603	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
29	A	852	BCR	C20-C21-C22	-2.94	123.16	127.28
26	a	616	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
26	W	604	CLA	CMB-C2B-C1B	-2.93	120.95	125.42
26	A	813	CLA	C3B-C4B-NB	-2.93	107.91	110.53
26	4	602	CLA	C3B-C4B-NB	-2.93	107.91	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	5	620	LUT	C11-C10-C9	-2.93	123.16	127.28
26	H	203	CLA	CAA-C2A-C3A	-2.93	105.07	113.00
26	1	610	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
37	Z	609	CHL	CMB-C2B-C3B	2.93	130.55	124.68
26	G	203	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
28	A	861	LHG	O8-C23-C24	2.93	120.78	111.83
29	O	2005	BCR	C33-C5-C6	-2.93	121.28	124.48
34	V	1620	LUT	C30-C31-C32	-2.93	114.71	123.20
28	8	623	LHG	O8-C23-C24	2.93	120.77	111.83
37	U	601	CHL	C3D-C4D-ND	2.93	117.64	112.94
36	W	1623	NEX	O24-C25-C38	2.93	118.32	115.05
29	K	207	BCR	C8-C7-C6	-2.93	119.18	127.00
29	O	2004	BCR	C36-C18-C19	2.93	122.56	118.09
26	B	810	CLA	C1-C2-C3	-2.93	121.40	126.20
33	B	850	DGD	O1G-C1A-C2A	2.93	120.76	111.83
36	X	1623	NEX	C16-C1-C2	2.92	122.91	109.06
29	B	844	BCR	C33-C5-C6	-2.92	121.30	124.48
29	8	621	BCR	C8-C9-C10	-2.92	114.42	119.01
29	O	2004	BCR	C7-C8-C9	-2.92	121.92	126.23
26	7	615	CLA	CMB-C2B-C3B	2.92	131.29	123.53
26	B	814	CLA	CHB-C4A-NA	2.92	128.61	124.40
32	4	623	LMG	O8-C28-C29	2.92	120.73	111.83
37	V	607	CHL	C1C-CHC-C4B	2.92	126.50	116.07
26	V	604	CLA	CMB-C2B-C1B	-2.92	120.98	125.42
26	8	604	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
35	Y	1622	XAT	C11-C10-C9	-2.92	123.19	127.28
37	U	607	CHL	C1C-CHC-C4B	2.92	126.50	116.07
35	2	620	XAT	C30-C31-C32	-2.92	114.75	123.20
26	W	603	CLA	CHB-C4A-NA	2.92	128.61	124.40
29	B	843	BCR	C36-C18-C19	2.91	122.54	118.09
29	B	845	BCR	C15-C16-C17	-2.91	117.56	123.52
29	B	852	BCR	C31-C1-C2	2.91	120.14	108.95
26	B	822	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
37	W	609	CHL	O2A-CGA-CBA	2.91	120.72	111.83
29	7	623	BCR	C11-C10-C9	-2.91	123.19	127.28
26	B	816	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
29	3	621	BCR	C7-C8-C9	-2.91	121.92	126.23
37	V	608	CHL	CBC-CAC-C3C	-2.91	108.70	112.87
26	V	603	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
26	7	607	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
29	B	845	BCR	C1-C6-C5	-2.91	118.66	122.64
29	5	622	BCR	C16-C17-C18	-2.91	123.20	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	H	203	CLA	CHB-C4A-NA	2.91	128.60	124.40
26	B	823	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
34	Y	1620	LUT	C10-C11-C12	2.91	131.62	123.20
34	9	619	LUT	C8-C9-C10	2.91	123.58	119.01
26	8	608	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
37	Z	608	CHL	C3D-C4D-ND	2.90	117.60	112.94
34	W	1620	LUT	C35-C15-C14	-2.90	117.58	123.52
26	5	604	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
29	B	847	BCR	C11-C10-C9	-2.90	123.21	127.28
29	B	853	BCR	C36-C18-C19	2.90	122.52	118.09
26	8	611	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
35	3	619	XAT	C8-C9-C10	-2.90	114.44	119.01
29	K	207	BCR	C16-C17-C18	-2.90	123.21	127.28
26	A	835	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
35	a	618	XAT	C27-C28-C29	-2.90	121.03	125.53
26	Y	612	CLA	CHB-C4A-NA	2.90	128.58	124.40
32	J	103	LMG	O8-C28-C29	2.90	120.67	111.83
26	A	802	CLA	CHB-C4A-NA	2.89	128.58	124.40
26	9	610	CLA	O2D-CGD-CBD	2.89	116.29	111.23
26	A	841	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
26	A	818	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
26	6	601	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
37	X	601	CHL	O2A-CGA-CBA	2.89	120.65	111.83
35	4	620	XAT	C10-C11-C12	-2.89	114.82	123.20
29	B	846	BCR	C38-C26-C27	2.89	119.76	113.60
29	A	851	BCR	C40-C30-C29	-2.89	97.86	108.95
29	L	309	BCR	C16-C15-C14	-2.89	117.61	123.52
26	5	609	CLA	C1-C2-C3	-2.89	121.47	126.20
29	F	305	BCR	C12-C13-C14	-2.89	114.47	119.01
26	A	843	CLA	C3B-C4B-NB	-2.89	107.95	110.53
26	Z	612	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
29	F	305	BCR	C16-C17-C18	-2.89	123.23	127.28
26	A	842	CLA	CMB-C2B-C1B	-2.88	121.03	125.42
28	a	620	LHG	O8-C23-C24	2.88	120.63	111.83
26	A	807	CLA	C3B-C4B-NB	-2.88	107.96	110.53
29	F	305	BCR	C7-C8-C9	-2.88	121.97	126.23
35	U	1622	XAT	C36-C21-C26	2.88	117.83	110.05
26	B	803	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
29	L	308	BCR	C24-C25-C26	-2.88	114.92	121.56
26	5	613	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
37	W	609	CHL	CMB-C2B-C3B	2.88	130.44	124.68
26	A	809	CLA	C1-C2-C3	-2.88	121.48	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	607	CHL	C1C-CHC-C4B	2.88	126.36	116.07
26	B	806	CLA	CHB-C4A-NA	2.87	128.55	124.40
35	9	620	XAT	C38-C25-C24	2.87	117.47	114.24
26	4	602	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
37	X	601	CHL	C1-C2-C3	-2.87	121.49	126.20
34	8	619	LUT	C21-C26-C27	-2.87	109.52	112.83
26	1	606	CLA	CBD-CHA-C1A	2.87	131.07	128.03
29	6	622	BCR	C30-C25-C24	2.87	123.44	115.65
29	7	623	BCR	C23-C24-C25	-2.87	119.33	127.00
28	V	2630	LHG	O8-C23-C24	2.87	120.59	111.83
29	L	301	BCR	C29-C30-C25	2.87	114.61	110.44
29	3	620	BCR	C8-C7-C6	-2.87	119.33	127.00
26	B	806	CLA	C1-C2-C3	-2.87	121.50	126.20
34	5	620	LUT	C30-C31-C32	-2.87	114.89	123.20
29	a	619	BCR	C11-C10-C9	-2.87	123.26	127.28
26	A	808	CLA	C1-C2-C3	-2.87	122.12	126.76
37	V	608	CHL	O2A-CGA-CBA	2.87	120.57	111.83
26	B	817	CLA	CHB-C4A-NA	2.86	128.53	124.40
29	K	202	BCR	C33-C5-C6	2.86	127.61	124.48
26	X	602	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
26	A	840	CLA	CAA-CBA-CGA	-2.86	105.08	113.21
29	B	845	BCR	C20-C21-C22	-2.86	123.26	127.28
34	4	619	LUT	C19-C9-C8	-2.86	113.72	118.09
26	8	601	CLA	C3B-C4B-NB	-2.86	107.97	110.53
28	B	851	LHG	O8-C23-C24	2.86	120.56	111.83
26	6	616	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
26	4	613	CLA	C3B-C4B-NB	-2.86	107.98	110.53
26	H	203	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
28	1	620	LHG	O8-C23-C24	2.86	120.55	111.83
37	U	607	CHL	C3D-C4D-ND	2.86	117.52	112.94
26	X	603	CLA	CAA-C2A-C3A	-2.86	105.28	113.00
26	6	620	CLA	CHB-C4A-NA	2.86	128.52	124.40
34	W	1621	LUT	C15-C35-C34	-2.86	117.68	123.52
26	Y	613	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
26	W	614	CLA	CHB-C4A-NA	2.85	128.52	124.40
29	1	619	BCR	C11-C10-C9	-2.85	123.28	127.28
32	9	625	LMG	O8-C28-C29	2.85	120.54	111.83
37	X	605	CHL	C1C-CHC-C4B	2.85	126.28	116.07
28	W	2630	LHG	O8-C23-C24	2.85	120.53	111.83
35	4	620	XAT	C12-C13-C14	-2.85	114.52	119.01
29	B	853	BCR	C15-C16-C17	-2.85	117.68	123.52
26	7	611	CLA	O2D-CGD-O1D	-2.85	118.30	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	611	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
37	Y	601	CHL	C1-C2-C3	-2.85	121.53	126.20
34	Y	1620	LUT	C40-C33-C32	2.85	122.44	118.09
35	7	620	XAT	C10-C11-C12	-2.85	114.96	123.20
29	A	851	BCR	C24-C23-C22	-2.84	122.03	126.23
29	A	852	BCR	C10-C11-C12	-2.84	114.96	123.20
37	W	601	CHL	O1D-CGD-CBD	-2.84	120.41	124.72
26	A	803	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
26	B	832	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
26	A	831	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
26	A	807	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
26	V	613	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
29	A	849	BCR	C38-C26-C25	-2.84	121.39	124.48
37	X	608	CHL	CAD-C3D-C4D	2.84	114.65	110.21
29	3	621	BCR	C32-C1-C6	-2.84	105.79	110.24
32	J	103	LMG	C8-O7-C10	-2.84	111.00	117.80
26	A	833	CLA	CMB-C2B-C1B	-2.84	121.10	125.42
26	A	822	CLA	CMB-C2B-C3B	2.84	133.22	126.55
36	5	624	NEX	C17-C1-C6	-2.84	107.93	110.47
26	3	604	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
29	L	309	BCR	C10-C11-C12	-2.83	114.99	123.20
32	8	626	LMG	O8-C28-C29	2.83	120.48	111.83
37	V	609	CHL	C1-O2A-CGA	2.83	123.51	116.65
26	5	610	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
29	B	843	BCR	C24-C23-C22	-2.83	122.05	126.23
35	U	1622	XAT	C4-C3-C2	-2.83	105.50	110.79
34	8	619	LUT	C11-C10-C9	-2.83	123.31	127.28
37	Z	607	CHL	C3D-C4D-ND	2.83	117.48	112.94
33	B	850	DGD	C2G-O2G-C1B	-2.83	111.02	117.80
26	9	607	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
34	4	619	LUT	C8-C9-C10	2.83	123.46	119.01
29	B	846	BCR	C15-C16-C17	-2.83	117.73	123.52
35	8	620	XAT	C35-C34-C33	-2.83	123.31	127.28
29	L	309	BCR	C37-C22-C23	2.83	122.41	118.09
34	4	619	LUT	C10-C11-C12	-2.83	115.01	123.20
29	L	308	BCR	C33-C5-C4	2.83	119.62	113.60
26	B	823	CLA	C3B-C4B-NB	-2.83	108.01	110.53
26	A	819	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
26	L	303	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
26	B	829	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
26	8	607	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
29	8	621	BCR	C15-C14-C13	-2.83	123.32	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	7	602	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
26	3	612	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
26	4	603	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
34	2	619	LUT	C28-C29-C30	-2.82	114.57	119.01
29	B	847	BCR	C7-C8-C9	-2.82	122.06	126.23
34	7	619	LUT	C8-C9-C10	2.82	123.44	119.01
26	6	613	CLA	C1-C2-C3	-2.82	121.58	126.20
35	8	620	XAT	C35-C15-C14	-2.82	117.75	123.52
34	4	619	LUT	C18-C5-C6	-2.82	121.41	124.48
26	4	604	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
28	H	204	LHG	O8-C23-C24	2.82	120.43	111.83
26	K	206	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
26	a	608	CLA	O2D-CGD-O1D	-2.82	117.69	124.08
34	V	1621	LUT	C27-C28-C29	-2.82	120.27	126.32
29	A	849	BCR	C15-C14-C13	-2.81	123.33	127.28
26	A	818	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
26	9	611	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
26	6	614	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
26	A	834	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
36	X	1623	NEX	C39-C29-C30	-2.81	118.26	122.82
26	A	802	CLA	CMB-C2B-C3B	2.81	133.16	126.55
29	A	856	BCR	C38-C26-C25	-2.81	121.42	124.48
26	V	604	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
29	2	623	BCR	C30-C25-C26	-2.81	118.80	122.64
26	6	604	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
29	3	620	BCR	C15-C14-C13	-2.81	123.34	127.28
35	4	620	XAT	C26-C27-C28	-2.81	120.05	125.99
26	A	845	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
26	4	608	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
29	G	205	BCR	C37-C22-C23	2.81	122.38	118.09
26	a	613	CLA	CMB-C2B-C1B	-2.81	121.15	125.42
26	2	609	CLA	C3B-C4B-NB	-2.81	108.03	110.53
26	B	802	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
34	X	1621	LUT	C15-C14-C13	-2.80	123.34	127.28
26	8	609	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
29	B	852	BCR	C24-C23-C22	-2.80	122.09	126.23
26	9	604	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
37	U	601	CHL	C4-C3-C5	2.80	120.09	115.23
26	7	606	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
26	L	304	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
34	4	619	LUT	C35-C15-C14	-2.80	117.79	123.52
26	B	833	CLA	O2D-CGD-O1D	-2.80	118.40	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	820	CLA	O2D-CGD-CBD	2.80	116.12	111.23
29	3	621	BCR	C40-C30-C25	-2.80	105.85	110.24
26	Z	610	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
26	1	608	CLA	O2D-CGD-O1D	-2.80	117.73	124.08
29	L	305	BCR	C30-C25-C26	-2.80	118.81	122.64
35	8	620	XAT	C27-C28-C29	-2.80	121.19	125.53
29	7	621	BCR	C15-C16-C17	-2.80	117.80	123.52
37	V	605	CHL	O1D-CGD-CBD	-2.80	120.48	124.72
26	6	608	CLA	C3B-C4B-NB	-2.79	108.03	110.53
26	Z	602	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
26	U	603	CLA	CHB-C4A-NA	2.79	128.43	124.40
26	J	101	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
26	7	608	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
26	V	602	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
26	Y	612	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
37	W	601	CHL	O2A-CGA-CBA	2.79	120.34	111.83
37	Y	609	CHL	O2A-CGA-CBA	2.79	120.34	111.83
36	Y	1623	NEX	C4-C3-C2	-2.79	105.57	110.79
26	B	827	CLA	CMA-C3A-C4A	-2.79	104.28	111.77
26	a	603	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
26	B	805	CLA	CMB-C2B-C1B	-2.79	121.17	125.42
35	X	1622	XAT	C24-C23-C22	-2.79	105.58	110.79
26	4	616	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
26	A	814	CLA	CMB-C2B-C1B	-2.79	121.18	125.42
26	W	604	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
29	7	621	BCR	C30-C25-C24	2.79	123.21	115.65
26	1	611	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
26	A	802	CLA	CAA-C2A-C1A	-2.79	102.85	111.97
26	U	610	CLA	CHB-C4A-NA	2.78	128.42	124.40
35	5	621	XAT	C15-C35-C34	-2.78	117.82	123.52
34	9	619	LUT	C19-C9-C8	-2.78	113.83	118.09
26	A	836	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
29	A	850	BCR	C24-C23-C22	-2.78	122.12	126.23
37	V	606	CHL	CBC-CAC-C3C	-2.78	108.89	112.87
36	X	1623	NEX	C28-C29-C30	2.78	123.38	119.01
26	F	304	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
34	Y	1621	LUT	C16-C1-C6	-2.78	105.88	110.24
26	B	826	CLA	CHB-C4A-NA	2.78	128.41	124.40
26	U	612	CLA	CHB-C4A-NA	2.78	128.41	124.40
29	B	852	BCR	C29-C30-C25	2.78	114.47	110.44
26	2	604	CLA	CMB-C2B-C3B	2.78	133.08	126.55
26	A	805	CLA	CHB-C4A-NA	2.78	128.41	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	804	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
26	2	604	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
26	4	610	CLA	CHB-C4A-NA	2.78	128.41	124.40
26	1	607	CLA	C3B-C4B-NB	-2.77	108.05	110.53
26	A	806	CLA	CAA-C2A-C1A	-2.77	102.90	111.97
37	Y	605	CHL	O2D-CGD-O1D	-2.77	118.46	123.85
29	4	621	BCR	C40-C30-C25	-2.77	105.90	110.24
29	K	202	BCR	C37-C22-C21	-2.77	118.33	122.82
36	Z	1623	NEX	C26-C27-C28	-2.77	120.14	125.99
26	V	610	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
37	Y	605	CHL	C1C-CHC-C4B	2.77	125.97	116.07
26	B	824	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
29	1	619	BCR	C36-C18-C19	2.77	122.31	118.09
26	7	603	CLA	O2D-CGD-O1D	-2.77	117.81	124.08
29	6	622	BCR	C38-C26-C27	2.76	119.49	113.60
29	B	845	BCR	C8-C7-C6	-2.76	119.61	127.00
26	4	613	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
29	7	623	BCR	C36-C18-C17	-2.76	118.34	122.82
26	8	606	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
31	A	857	LMU	O5B-C5B-C4B	2.76	114.67	109.70
34	4	619	LUT	C12-C13-C14	-2.76	114.67	119.01
34	U	1620	LUT	C11-C10-C9	-2.76	123.41	127.28
26	U	612	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
26	1	613	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
36	V	1623	NEX	C24-C23-C22	-2.76	105.63	110.79
37	Z	609	CHL	O2A-CGA-CBA	2.76	120.25	111.83
26	Y	604	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
32	V	2631	LMG	O1-C1-C2	2.76	112.46	108.27
29	L	301	BCR	C10-C11-C12	-2.76	115.21	123.20
37	Y	609	CHL	CMA-C3A-C4A	-2.76	108.67	114.61
26	5	603	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
36	5	624	NEX	C31-C30-C29	-2.76	123.41	127.28
26	9	602	CLA	C1-C2-C3	-2.76	121.68	126.20
26	B	816	CLA	C3B-C4B-NB	-2.75	108.07	110.53
26	V	611	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
35	W	1622	XAT	C7-C8-C9	-2.75	121.26	125.53
29	B	845	BCR	C11-C10-C9	-2.75	123.42	127.28
36	X	1623	NEX	C11-C10-C9	-2.75	123.42	127.28
29	B	801	BCR	C39-C30-C25	-2.75	105.93	110.24
26	V	612	CLA	CHB-C4A-NA	2.75	128.37	124.40
26	W	613	CLA	CHB-C4A-NA	2.75	128.37	124.40
26	X	611	CLA	O2D-CGD-O1D	-2.75	118.50	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	816	CLA	C1-C2-C3	-2.75	121.69	126.20
26	A	828	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
26	V	602	CLA	CMB-C2B-C3B	2.75	133.01	126.55
36	5	624	NEX	C15-C35-C34	-2.75	117.90	123.52
26	A	804	CLA	C1-C2-C3	-2.75	121.70	126.20
26	B	821	CLA	CHC-C1C-C2C	-2.75	123.93	129.94
29	L	308	BCR	C33-C5-C6	-2.75	121.49	124.48
37	W	607	CHL	CMA-C3A-C4A	-2.75	108.69	114.61
35	3	619	XAT	C27-C28-C29	-2.75	121.27	125.53
26	V	603	CLA	CHB-C4A-NA	2.74	128.36	124.40
37	V	607	CHL	C3D-C4D-ND	2.74	117.34	112.94
26	B	837	CLA	C3B-C4B-NB	-2.74	108.08	110.53
26	6	608	CLA	CHB-C4A-NA	2.74	128.36	124.40
26	1	614	CLA	CAB-C3B-C2B	2.74	130.82	123.53
34	V	1621	LUT	C15-C35-C34	-2.74	117.91	123.52
26	3	607	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
26	3	609	CLA	CHB-C4A-NA	2.74	128.36	124.40
34	6	619	LUT	C22-C23-C24	2.74	115.25	111.18
26	B	817	CLA	C3B-C4B-NB	-2.74	108.08	110.53
34	W	1621	LUT	C36-C21-C26	2.74	113.70	109.55
37	W	605	CHL	O1D-CGD-CBD	-2.74	120.57	124.72
37	X	606	CHL	O2D-CGD-O1D	-2.74	118.52	123.85
36	V	1623	NEX	C39-C29-C30	-2.74	118.38	122.82
32	4	624	LMG	O8-C28-C29	2.74	120.18	111.83
34	W	1621	LUT	C27-C28-C29	-2.74	120.44	126.32
26	W	603	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
26	5	608	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
37	U	607	CHL	CMB-C2B-C3B	2.74	130.15	124.68
37	X	608	CHL	O2A-CGA-CBA	2.74	120.18	111.83
34	8	619	LUT	C8-C9-C10	2.73	123.31	119.01
26	A	827	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
26	7	606	CLA	C3B-C4B-NB	-2.73	108.09	110.53
29	A	852	BCR	C21-C20-C19	-2.73	115.28	123.20
35	9	620	XAT	C8-C9-C10	-2.73	114.71	119.01
36	X	1623	NEX	C11-C12-C13	-2.73	118.87	126.36
29	L	301	BCR	C3-C4-C5	-2.73	109.19	114.06
31	5	628	LMU	C1B-O1B-C4'	-2.73	111.51	117.98
26	5	606	CLA	C3B-C4B-NB	-2.73	108.09	110.53
26	A	806	CLA	CMB-C2B-C1B	-2.73	121.26	125.42
29	2	623	BCR	C3-C4-C5	-2.73	109.19	114.06
26	X	614	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
35	Z	1622	XAT	C11-C12-C13	-2.73	118.89	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1	617	LUT	C11-C10-C9	-2.73	123.45	127.28
29	a	619	BCR	C36-C18-C19	2.72	122.25	118.09
29	L	305	BCR	C30-C25-C24	2.72	123.04	115.65
36	W	1623	NEX	C15-C35-C34	-2.72	117.94	123.52
26	O	2001	CLA	O2D-CGD-O1D	-2.72	117.90	124.08
26	4	611	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
37	Z	601	CHL	CBC-CAC-C3C	-2.72	108.98	112.87
26	Z	611	CLA	CAB-C3B-C2B	2.72	130.76	123.53
37	Z	609	CHL	C1-C2-C3	-2.72	121.74	126.20
37	W	607	CHL	OMC-CMC-C2C	-2.72	120.40	125.12
29	8	621	BCR	C28-C27-C26	-2.72	109.21	114.06
26	A	828	CLA	C3B-C4B-NB	-2.72	108.11	110.53
35	3	619	XAT	C4-C3-C2	-2.72	105.71	110.79
26	8	612	CLA	CHB-C4A-NA	2.71	128.32	124.40
26	X	602	CLA	CHB-C4A-NA	2.71	128.32	124.40
26	1	614	CLA	O2D-CGD-O1D	-2.71	117.93	124.08
29	7	621	BCR	C32-C1-C6	-2.71	105.99	110.24
35	4	620	XAT	C35-C34-C33	-2.71	123.47	127.28
37	V	609	CHL	O2D-CGD-O1D	-2.71	118.57	123.85
34	7	619	LUT	C16-C1-C6	-2.71	105.99	110.24
37	W	606	CHL	C3D-C4D-ND	2.71	117.29	112.94
34	1	617	LUT	C35-C15-C14	-2.71	117.97	123.52
26	5	611	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
26	B	829	CLA	CMB-C2B-C3B	2.71	132.92	126.55
37	Y	606	CHL	OMC-CMC-C2C	-2.71	120.42	125.12
37	U	607	CHL	OMC-CMC-C2C	-2.71	120.42	125.12
37	Y	607	CHL	O2A-CGA-CBA	2.71	120.09	111.83
26	A	842	CLA	C1-C2-C3	-2.71	121.76	126.20
26	U	614	CLA	CHB-C4A-NA	2.71	128.31	124.40
26	W	613	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
26	L	307	CLA	O2D-CGD-O1D	-2.71	117.94	124.08
37	Y	608	CHL	O2A-CGA-CBA	2.71	120.09	111.83
26	F	301	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
26	F	303	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
26	A	833	CLA	CAA-C2A-C3A	-2.71	105.69	113.00
26	1	609	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
36	6	624	NEX	C24-C23-C22	-2.70	105.73	110.79
29	7	621	BCR	C16-C17-C18	-2.70	123.48	127.28
26	L	304	CLA	CHB-C4A-NA	2.70	128.30	124.40
26	W	614	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
26	5	602	CLA	C3B-C4B-NB	-2.70	108.12	110.53
36	Y	1623	NEX	C39-C29-C30	-2.70	118.44	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	G	205	BCR	C28-C27-C26	-2.70	109.24	114.06
26	X	612	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
26	U	604	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
26	3	617	CLA	O2D-CGD-O1D	-2.70	117.95	124.08
26	5	617	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
36	6	624	NEX	C10-C11-C12	-2.70	115.37	123.20
29	B	848	BCR	C16-C15-C14	-2.70	117.99	123.52
26	A	805	CLA	CMB-C2B-C1B	-2.70	121.31	125.42
37	X	607	CHL	O2A-CGA-CBA	2.70	120.07	111.83
26	A	843	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
32	V	2631	LMG	O8-C28-C29	2.70	120.06	111.83
29	7	621	BCR	C38-C26-C27	2.70	119.35	113.60
34	a	617	LUT	C35-C15-C14	-2.70	118.00	123.52
26	7	601	CLA	CMB-C2B-C3B	2.70	132.90	126.55
28	A	847	LHG	C5-O7-C7	-2.70	111.34	117.80
26	a	612	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
29	6	622	BCR	C3-C4-C5	-2.70	109.25	114.06
26	1	601	CLA	O2D-CGD-O1D	-2.69	117.97	124.08
29	B	848	BCR	C32-C1-C6	-2.69	106.02	110.24
35	6	621	XAT	C4-C3-C2	-2.69	105.75	110.79
26	A	832	CLA	C3B-C4B-NB	-2.69	108.13	110.53
29	8	621	BCR	C3-C4-C5	-2.69	109.25	114.06
29	2	623	BCR	C36-C18-C17	-2.69	118.45	122.82
29	A	849	BCR	C15-C16-C17	-2.69	118.01	123.52
29	A	852	BCR	C38-C26-C27	2.69	119.33	113.60
26	9	609	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
34	5	620	LUT	C18-C5-C6	-2.69	121.55	124.48
37	X	601	CHL	C3D-C4D-ND	2.69	117.25	112.94
26	3	612	CLA	C3B-C4B-NB	-2.69	108.13	110.53
26	6	617	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
29	2	623	BCR	C38-C26-C27	2.69	119.33	113.60
37	Z	608	CHL	O2A-CGA-CBA	2.69	120.03	111.83
26	5	614	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
26	3	611	CLA	O2D-CGD-O1D	-2.69	117.98	124.08
34	V	1620	LUT	C35-C15-C14	-2.69	118.02	123.52
26	B	836	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
35	7	620	XAT	C28-C29-C30	-2.68	114.79	119.01
37	W	601	CHL	C1-C2-C3	-2.68	121.80	126.20
26	6	610	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
26	A	831	CLA	CMB-C2B-C1B	-2.68	121.33	125.42
26	X	612	CLA	CHB-C4A-NA	2.68	128.27	124.40
26	A	807	CLA	CHB-C4A-NA	2.68	128.27	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	611	CLA	CHB-C4A-NA	2.68	128.27	124.40
26	V	614	CLA	CHB-C4A-NA	2.68	128.27	124.40
26	L	302	CLA	CMB-C2B-C1B	-2.68	121.33	125.42
29	B	843	BCR	C30-C25-C26	-2.68	118.97	122.64
29	L	301	BCR	C37-C22-C23	2.68	122.18	118.09
37	Y	606	CHL	CBC-CAC-C3C	-2.68	109.04	112.87
37	X	606	CHL	CMA-C3A-C4A	-2.68	108.84	114.61
26	A	842	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
37	U	609	CHL	O2D-CGD-O1D	-2.68	118.63	123.85
26	A	810	CLA	CAA-C2A-C3A	-2.68	105.76	113.00
26	A	806	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
26	a	607	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
28	O	2631	LHG	C5-O7-C7	-2.68	111.39	117.80
26	a	606	CLA	C3B-C4B-NB	-2.68	108.14	110.53
26	3	603	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
37	X	609	CHL	O2A-CGA-CBA	2.68	120.00	111.83
26	1	601	CLA	C3B-C4B-NB	-2.67	108.14	110.53
35	7	620	XAT	C18-C5-C4	2.67	117.24	114.24
29	A	849	BCR	C1-C6-C5	-2.67	118.98	122.64
34	8	619	LUT	C35-C15-C14	-2.67	118.05	123.52
26	6	613	CLA	O2D-CGD-O1D	-2.67	118.02	124.08
29	8	621	BCR	C38-C26-C27	2.67	119.29	113.60
29	4	621	BCR	C8-C7-C6	-2.67	119.87	127.00
26	6	608	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
37	Y	601	CHL	O2A-CGA-CBA	2.67	119.97	111.83
29	B	848	BCR	C29-C30-C25	2.67	114.31	110.44
31	5	628	LMU	C1'-C2'-C3'	2.67	115.62	110.01
29	K	202	BCR	C33-C5-C4	-2.67	107.91	113.60
26	a	607	CLA	C3B-C4B-NB	-2.67	108.15	110.53
26	5	619	CLA	CHB-C4A-NA	2.67	128.25	124.40
36	Z	1623	NEX	C24-C23-C22	-2.67	105.80	110.79
26	8	616	CLA	O1D-CGD-CBD	2.67	129.78	124.52
37	V	606	CHL	C3D-C4D-ND	2.67	117.22	112.94
26	1	612	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
33	B	850	DGD	C1D-O6D-C5D	-2.67	108.52	113.72
26	L	303	CLA	CHB-C4A-NA	2.66	128.25	124.40
29	a	619	BCR	C38-C26-C27	2.66	119.28	113.60
26	8	607	CLA	CMB-C2B-C3B	2.66	130.61	123.53
32	9	625	LMG	O7-C10-C11	2.66	117.24	111.48
26	6	616	CLA	C3B-C4B-NB	-2.66	108.15	110.53
26	V	604	CLA	CHB-C4A-NA	2.66	128.24	124.40
37	W	609	CHL	O1D-CGD-CBD	-2.66	120.69	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	621	BCR	C11-C10-C9	-2.66	123.55	127.28
26	2	602	CLA	O2D-CGD-O1D	-2.66	118.04	124.08
32	L	2631	LMG	O8-C28-C29	2.66	119.95	111.83
26	B	807	CLA	C1-C2-C3	-2.66	121.84	126.20
26	5	618	CLA	CMB-C2B-C3B	2.66	130.60	123.53
29	1	619	BCR	C38-C26-C27	2.66	119.27	113.60
26	7	614	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
26	5	610	CLA	CHB-C4A-NA	2.66	128.24	124.40
35	9	620	XAT	C12-C13-C14	-2.66	114.83	119.01
28	B	851	LHG	C5-O7-C7	-2.66	111.43	117.80
26	2	612	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
26	1	606	CLA	C3B-C4B-NB	-2.66	108.16	110.53
26	A	829	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
26	3	613	CLA	O2D-CGD-O1D	-2.66	118.05	124.08
34	2	619	LUT	C15-C35-C34	-2.66	118.08	123.52
26	W	610	CLA	C1-C2-C3	-2.66	121.84	126.20
29	F	305	BCR	C11-C10-C9	-2.66	123.55	127.28
37	U	605	CHL	O2D-CGD-O1D	-2.66	118.68	123.85
26	4	618	CLA	O2D-CGD-O1D	-2.65	118.06	124.08
29	8	621	BCR	C11-C10-C9	-2.65	123.56	127.28
29	3	620	BCR	C36-C18-C17	-2.65	118.52	122.82
29	L	308	BCR	C1-C6-C5	-2.65	119.01	122.64
26	a	601	CLA	O2D-CGD-O1D	-2.65	118.06	124.08
26	A	805	CLA	O2D-CGD-CBD	2.65	115.87	111.23
29	O	2004	BCR	C33-C5-C6	-2.65	121.59	124.48
26	U	613	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
34	9	619	LUT	C16-C1-C6	2.65	114.40	110.24
26	A	819	CLA	CHB-C4A-NA	2.65	128.22	124.40
37	X	608	CHL	C4D-CHA-CBD	-2.65	106.47	109.18
37	U	605	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
34	Z	1620	LUT	C15-C35-C34	-2.65	118.10	123.52
26	Y	610	CLA	CHB-C4A-NA	2.65	128.22	124.40
37	W	607	CHL	O2A-CGA-CBA	2.65	119.91	111.83
26	a	613	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
28	A	846	LHG	O7-C7-C8	2.65	117.21	111.48
29	L	309	BCR	C11-C10-C9	-2.65	123.57	127.28
26	X	602	CLA	CMB-C2B-C1B	-2.65	121.39	125.42
35	6	621	XAT	C28-C29-C30	-2.65	114.85	119.01
26	3	617	CLA	CHB-C4A-NA	2.65	128.22	124.40
26	8	604	CLA	CMB-C2B-C3B	2.65	132.77	126.55
35	Z	1622	XAT	C18-C5-C4	2.64	117.21	114.24
26	A	806	CLA	CHB-C4A-NA	2.64	128.22	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	830	CLA	CHD-C1D-ND	-2.64	121.08	124.80
26	L	306	CLA	O2D-CGD-O1D	-2.64	118.08	124.08
29	B	853	BCR	C11-C10-C9	-2.64	123.57	127.28
26	Z	603	CLA	CAA-C2A-C3A	-2.64	105.86	113.00
26	B	838	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
26	a	602	CLA	CMB-C2B-C3B	2.64	132.76	126.55
34	V	1621	LUT	C1-C6-C5	-2.64	119.03	122.64
29	4	621	BCR	C37-C22-C23	2.64	122.12	118.09
26	A	811	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
26	A	832	CLA	CHB-C4A-NA	2.64	128.21	124.40
34	X	1620	LUT	C18-C5-C6	-2.64	121.60	124.48
26	B	817	CLA	C4-C3-C5	2.64	119.81	115.23
35	5	621	XAT	C30-C31-C32	-2.64	115.55	123.20
34	X	1621	LUT	C7-C8-C9	-2.64	122.33	126.23
26	1	602	CLA	CMB-C2B-C3B	2.64	132.76	126.55
29	L	309	BCR	C34-C9-C8	2.64	122.12	118.09
26	8	602	CLA	CMB-C2B-C3B	2.64	132.75	126.55
26	A	823	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
26	2	601	CLA	C3B-C4B-NB	-2.64	108.17	110.53
26	A	809	CLA	CHB-C4A-NA	2.64	128.21	124.40
26	A	833	CLA	CHB-C4A-NA	2.64	128.21	124.40
26	A	824	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
26	B	831	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
37	V	606	CHL	C1C-C2C-CMC	2.64	131.55	126.80
34	a	617	LUT	C11-C10-C9	-2.63	123.58	127.28
34	V	1620	LUT	C18-C5-C6	-2.63	121.61	124.48
26	7	608	CLA	C3B-C4B-NB	-2.63	108.18	110.53
36	6	624	NEX	C19-C9-C10	2.63	127.08	122.82
37	V	609	CHL	O1D-CGD-CBD	-2.63	120.73	124.72
29	A	852	BCR	C1-C6-C5	-2.63	119.04	122.64
29	B	852	BCR	C1-C6-C5	-2.63	119.04	122.64
26	1	611	CLA	C3B-C4B-NB	-2.63	108.18	110.53
34	9	619	LUT	C35-C15-C14	-2.63	118.14	123.52
37	U	601	CHL	O2A-CGA-CBA	2.63	119.86	111.83
26	B	819	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
26	B	828	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
37	Z	606	CHL	O1D-CGD-CBD	-2.63	120.74	124.72
31	5	629	LMU	C1'-O5'-C5'	-2.63	108.59	113.72
26	7	615	CLA	CAB-C3B-C2B	2.63	130.52	123.53
29	7	621	BCR	C7-C8-C9	-2.63	122.35	126.23
37	V	601	CHL	O2A-CGA-CBA	2.63	119.84	111.83
29	L	305	BCR	C7-C6-C5	-2.62	115.51	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	4	620	XAT	C32-C33-C34	-2.62	114.88	119.01
35	4	620	XAT	C24-C23-C22	-2.62	105.88	110.79
32	4	623	LMG	O1-C1-C2	2.62	112.26	108.27
26	1	603	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	1	613	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
26	B	804	CLA	CHB-C4A-NA	2.62	128.18	124.40
26	4	616	CLA	CAB-C3B-C2B	2.62	130.50	123.53
26	8	612	CLA	O2D-CGD-O1D	-2.62	118.13	124.08
26	B	826	CLA	O2D-CGD-CBD	2.62	115.81	111.23
26	3	610	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
29	7	623	BCR	C24-C23-C22	-2.62	122.36	126.23
26	2	610	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
26	1	616	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
26	9	602	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
34	V	1621	LUT	C11-C12-C13	-2.62	119.19	126.36
29	B	844	BCR	C16-C15-C14	-2.62	118.17	123.52
37	U	607	CHL	O1D-CGD-CBD	-2.61	120.76	124.72
26	A	835	CLA	C3B-C4B-NB	-2.61	108.20	110.53
26	5	619	CLA	C2A-C1A-CHA	2.61	128.40	123.87
29	K	202	BCR	C38-C26-C27	2.61	119.17	113.60
29	J	102	BCR	C8-C9-C10	-2.61	114.90	119.01
29	O	2004	BCR	C11-C10-C9	-2.61	123.61	127.28
26	5	607	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
29	O	2005	BCR	C16-C15-C14	-2.61	118.17	123.52
26	5	601	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
29	G	205	BCR	C32-C1-C6	-2.61	106.15	110.24
34	1	617	LUT	C10-C11-C12	-2.61	115.64	123.20
26	O	2002	CLA	CAB-C3B-C2B	2.61	130.47	123.53
26	K	204	CLA	CHB-C4A-NA	2.61	128.17	124.40
26	B	809	CLA	C3B-C4B-NB	-2.61	108.20	110.53
34	Z	1621	LUT	C30-C31-C32	-2.61	115.64	123.20
26	a	616	CLA	CMB-C2B-C1B	-2.61	121.45	125.42
26	7	613	CLA	CHB-C4A-NA	2.61	128.16	124.40
36	X	1623	NEX	C24-C23-C22	-2.61	105.92	110.79
26	B	813	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
26	5	617	CLA	C1-C2-C3	-2.61	122.55	126.76
29	3	622	BCR	C33-C5-C6	-2.60	121.64	124.48
26	3	614	CLA	C3B-C4B-NB	-2.60	108.21	110.53
34	Z	1620	LUT	C35-C15-C14	-2.60	118.19	123.52
26	Z	612	CLA	CHB-C4A-NA	2.60	128.16	124.40
29	K	202	BCR	C24-C23-C22	-2.60	122.39	126.23
37	Z	605	CHL	CBC-CAC-C3C	-2.60	109.15	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	1	618	XAT	C12-C13-C14	-2.60	114.92	119.01
29	L	305	BCR	C15-C16-C17	-2.60	118.19	123.52
26	B	809	CLA	CHB-C4A-NA	2.60	128.16	124.40
36	5	624	NEX	C24-C23-C22	-2.60	105.92	110.79
26	7	601	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
34	1	617	LUT	C28-C29-C30	-2.60	114.92	119.01
26	3	606	CLA	C1-C2-C3	-2.60	121.94	126.20
29	O	2005	BCR	C36-C18-C19	2.60	122.06	118.09
34	U	1620	LUT	C15-C35-C34	-2.60	118.20	123.52
26	a	603	CLA	CHB-C4A-NA	2.60	128.15	124.40
29	5	622	BCR	C32-C1-C6	-2.60	106.17	110.24
34	a	617	LUT	C28-C29-C30	-2.60	114.92	119.01
36	6	624	NEX	C27-C28-C29	-2.60	121.50	125.53
26	4	607	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
26	9	604	CLA	CMB-C2B-C3B	2.60	130.43	123.53
26	2	601	CLA	CMB-C2B-C3B	2.60	132.65	126.55
28	A	847	LHG	O8-C23-C24	2.59	119.75	111.83
35	a	618	XAT	C12-C13-C14	-2.59	114.93	119.01
35	9	620	XAT	C28-C29-C30	-2.59	114.93	119.01
26	8	601	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
35	9	620	XAT	C35-C34-C33	-2.59	123.64	127.28
26	4	613	CLA	O2A-CGA-CBA	2.59	119.74	111.83
34	Z	1621	LUT	C15-C14-C13	-2.59	123.64	127.28
37	X	605	CHL	CBC-CAC-C3C	-2.59	109.16	112.87
26	A	830	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
26	B	809	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
29	3	620	BCR	C36-C18-C19	2.59	122.05	118.09
37	Y	605	CHL	O1D-CGD-CBD	-2.59	120.79	124.72
34	Z	1620	LUT	C39-C29-C28	2.59	122.05	118.09
26	A	810	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
26	a	601	CLA	C3B-C4B-NB	-2.59	108.22	110.53
29	A	856	BCR	C7-C8-C9	-2.59	122.40	126.23
36	6	624	NEX	C28-C29-C30	2.59	123.08	119.01
37	Z	605	CHL	O1D-CGD-CBD	-2.59	120.80	124.72
26	Z	610	CLA	C3B-C4B-NB	-2.59	108.22	110.53
34	Y	1621	LUT	C26-C27-C28	-2.59	120.55	124.58
26	A	839	CLA	C3B-C4B-NB	-2.59	108.22	110.53
26	9	607	CLA	C3B-C4B-NB	-2.59	108.22	110.53
29	B	844	BCR	C40-C30-C25	-2.59	106.19	110.24
34	6	619	LUT	C10-C11-C12	-2.59	115.71	123.20
29	B	847	BCR	C15-C14-C13	-2.59	123.65	127.28
26	V	602	CLA	C1-C2-C3	-2.59	121.96	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O	2003	CLA	O2D-CGD-O1D	-2.58	118.22	124.08
35	V	1622	XAT	C38-C25-C24	2.58	117.14	114.24
37	V	608	CHL	CMB-C2B-C3B	2.58	129.85	124.68
29	7	623	BCR	C32-C1-C6	2.58	114.29	110.24
29	B	849	BCR	C23-C22-C21	2.58	123.07	119.01
26	9	614	CLA	C3B-C4B-NB	-2.58	108.22	110.53
26	a	610	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
29	A	851	BCR	C31-C1-C6	-2.58	106.19	110.24
26	7	612	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
36	X	1623	NEX	C26-C27-C28	-2.58	120.54	125.99
29	B	853	BCR	C15-C14-C13	-2.58	123.66	127.28
29	B	843	BCR	C11-C12-C13	-2.58	119.30	126.36
29	8	621	BCR	C39-C30-C25	-2.58	106.20	110.24
26	8	608	CLA	C3B-C4B-NB	-2.57	108.23	110.53
37	W	607	CHL	C3D-C4D-ND	2.57	117.07	112.94
34	3	618	LUT	C8-C9-C10	2.57	123.06	119.01
37	W	607	CHL	CAC-C3C-C4C	2.57	129.36	124.73
32	8	626	LMG	C8-O7-C10	-2.57	111.64	117.80
34	a	617	LUT	C10-C11-C12	-2.57	115.75	123.20
26	8	616	CLA	CHB-C4A-NA	2.57	128.11	124.40
26	8	610	CLA	CHB-C4A-NA	2.57	128.11	124.40
26	B	813	CLA	C3B-C4B-NB	-2.57	108.24	110.53
26	A	835	CLA	CHB-C4A-NA	2.57	128.10	124.40
34	a	617	LUT	C35-C34-C33	-2.57	123.68	127.28
29	L	308	BCR	C38-C26-C27	2.57	119.07	113.60
29	B	801	BCR	C24-C25-C26	2.57	127.47	121.56
26	3	608	CLA	O2D-CGD-O1D	-2.57	118.86	123.85
26	W	612	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
29	B	849	BCR	C16-C15-C14	-2.56	118.27	123.52
35	2	620	XAT	C20-C13-C12	2.56	122.00	118.09
35	8	620	XAT	C12-C13-C14	-2.56	114.98	119.01
26	K	203	CLA	CAA-CBA-CGA	-2.56	105.93	113.21
26	3	606	CLA	CHB-C4A-NA	2.56	128.10	124.40
26	a	616	CLA	C3B-C4B-NB	-2.56	108.24	110.53
26	K	203	CLA	C3B-C4B-NB	-2.56	108.24	110.53
31	A	857	LMU	C4B-C3B-C2B	2.56	115.33	110.83
34	4	619	LUT	C18-C5-C4	2.56	119.13	114.42
28	O	2631	LHG	O8-C23-C24	2.56	119.64	111.83
29	A	852	BCR	C8-C9-C10	2.56	123.03	119.01
28	3	623	LHG	O8-C23-C24	2.56	119.64	111.83
35	3	619	XAT	C28-C29-C30	-2.56	114.99	119.01
32	J	104	LMG	O1-C1-C2	2.56	112.16	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	604	CLA	CMB-C2B-C3B	2.56	130.33	123.53
29	4	621	BCR	C11-C12-C13	-2.56	119.35	126.36
29	B	846	BCR	C2-C1-C6	2.56	114.15	110.44
26	2	616	CLA	CAB-C3B-C2B	2.56	130.32	123.53
34	a	617	LUT	C1-C6-C5	-2.56	119.14	122.64
26	U	613	CLA	CAC-C3C-C4C	2.55	128.11	124.79
26	Z	602	CLA	CHB-C4A-NA	2.55	128.09	124.40
26	B	814	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
26	2	614	CLA	O2D-CGD-O1D	-2.55	118.28	124.08
26	Z	614	CLA	CHB-C4A-NA	2.55	128.09	124.40
35	7	620	XAT	C30-C31-C32	-2.55	115.80	123.20
26	A	822	CLA	C7-C6-C5	-2.55	106.46	113.26
26	5	618	CLA	CAB-C3B-C2B	2.55	130.31	123.53
26	Z	604	CLA	CMB-C2B-C3B	2.55	132.55	126.55
26	7	613	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
26	W	610	CLA	CHB-C4A-NA	2.55	128.08	124.40
37	X	606	CHL	O1D-CGD-CBD	-2.55	120.86	124.72
26	B	820	CLA	CHB-C4A-NA	2.55	128.08	124.40
37	V	609	CHL	CMB-C2B-C3B	2.55	129.78	124.68
26	A	842	CLA	C3B-C4B-NB	-2.55	108.26	110.53
26	U	610	CLA	C1-C2-C3	-2.55	122.02	126.20
29	L	309	BCR	C40-C30-C25	-2.55	106.25	110.24
35	5	621	XAT	C12-C13-C14	-2.55	115.00	119.01
35	8	620	XAT	C4-C3-C2	-2.54	106.03	110.79
26	A	842	CLA	C4-C3-C5	2.54	119.64	115.23
26	A	837	CLA	CHB-C4A-NA	2.54	128.07	124.40
26	A	801	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
26	G	204	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
26	3	602	CLA	CHB-C4A-NA	2.54	128.07	124.40
29	B	844	BCR	C3-C4-C5	-2.54	109.53	114.06
37	Y	606	CHL	CAC-C3C-C4C	2.54	130.56	124.03
37	Z	601	CHL	O2A-CGA-CBA	2.54	119.58	111.83
26	A	816	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
34	1	617	LUT	C35-C34-C33	-2.54	123.72	127.28
35	8	620	XAT	C24-C23-C22	-2.54	106.05	110.79
26	Z	613	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
26	L	303	CLA	C3B-C4B-NB	-2.54	108.27	110.53
26	4	603	CLA	CAB-C3B-C2B	2.53	130.27	123.53
26	A	832	CLA	C1-C2-C3	-2.53	122.66	126.76
31	K	208	LMU	C3B-C4B-C5B	2.53	114.83	110.23
37	U	605	CHL	C1C-CHC-C4B	2.53	125.13	116.07
37	X	608	CHL	C1-C2-C3	-2.53	122.05	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	2	623	BCR	C37-C22-C23	2.53	121.95	118.09
26	1	609	CLA	CAB-C3B-C4B	-2.53	121.56	125.42
26	7	610	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	8	608	CLA	CHB-C4A-NA	2.53	128.05	124.40
37	Z	609	CHL	O2D-CGD-O1D	-2.53	118.92	123.85
28	6	623	LHG	C5-O7-C7	-2.53	111.74	117.80
26	4	606	CLA	O2D-CGD-O1D	-2.53	118.34	124.08
26	A	801	CLA	CBA-CAA-C2A	-2.53	106.27	113.79
26	B	812	CLA	C3B-C4B-NB	-2.53	108.27	110.53
26	V	610	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	A	838	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	1	602	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
26	2	616	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	X	613	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
26	W	611	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
26	A	840	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
26	4	603	CLA	CHB-C4A-NA	2.53	128.04	124.40
35	a	618	XAT	C30-C31-C32	-2.53	115.88	123.20
37	Y	609	CHL	O2D-CGD-O1D	-2.53	118.93	123.85
26	8	610	CLA	C4-C3-C2	-2.52	117.14	123.63
26	7	604	CLA	O2D-CGD-O1D	-2.52	118.93	123.85
26	A	843	CLA	C1-C2-C3	-2.52	122.06	126.20
26	4	618	CLA	CMB-C2B-C3B	2.52	130.24	123.53
35	7	620	XAT	C38-C25-C24	2.52	117.08	114.24
26	a	601	CLA	CHB-C4A-NA	2.52	128.04	124.40
26	7	602	CLA	CHB-C4A-NA	2.52	128.04	124.40
29	A	852	BCR	C4-C5-C6	-2.52	119.30	122.70
26	a	602	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
34	X	1620	LUT	C31-C30-C29	-2.52	123.74	127.28
26	5	606	CLA	O2D-CGD-O1D	-2.52	118.36	124.08
26	2	613	CLA	CHB-C4A-NA	2.52	128.04	124.40
26	3	610	CLA	CHB-C4A-NA	2.52	128.04	124.40
31	A	857	LMU	C3B-C4B-C5B	2.52	114.80	110.23
26	6	601	CLA	CHB-C4A-NA	2.52	128.04	124.40
26	6	611	CLA	CHB-C4A-NA	2.52	128.04	124.40
35	1	618	XAT	C30-C31-C32	-2.52	115.90	123.20
36	U	1623	NEX	C39-C29-C30	-2.52	118.73	122.82
26	K	201	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
26	1	612	CLA	CHB-C4A-NA	2.52	128.03	124.40
29	L	305	BCR	C1-C6-C7	2.52	122.48	115.65
26	A	821	CLA	CHB-C4A-NA	2.52	128.03	124.40
26	Z	604	CLA	CBD-CHA-C1A	2.52	132.25	127.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	9	603	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
26	A	843	CLA	CMB-C2B-C1B	-2.52	121.59	125.42
37	Z	606	CHL	CMB-C2B-C3B	2.52	129.71	124.68
34	W	1620	LUT	C27-C28-C29	-2.52	120.91	126.32
29	B	801	BCR	C36-C18-C19	2.52	121.93	118.09
26	W	611	CLA	CHB-C4A-NA	2.52	128.03	124.40
29	A	850	BCR	C36-C18-C17	-2.52	118.74	122.82
29	A	856	BCR	C36-C18-C17	-2.52	118.74	122.82
26	7	604	CLA	CHB-C4A-NA	2.51	128.03	124.40
37	Y	601	CHL	C4-C3-C5	2.51	119.59	115.23
26	7	616	CLA	CMB-C2B-C3B	2.51	130.21	123.53
37	V	601	CHL	C1-C2-C3	-2.51	122.08	126.20
26	5	612	CLA	O2D-CGD-O1D	-2.51	118.38	124.08
26	B	825	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
37	X	608	CHL	C4-C3-C5	2.51	119.59	115.23
32	9	625	LMG	O1-C1-C2	2.51	112.09	108.27
26	B	811	CLA	O2D-CGD-O1D	-2.51	118.38	124.08
26	6	618	CLA	CHB-C4A-NA	2.51	128.02	124.40
26	X	610	CLA	CHB-C4A-NA	2.51	128.02	124.40
26	6	601	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
26	a	611	CLA	CAB-C3B-C2B	2.51	130.21	123.53
36	U	1623	NEX	C11-C10-C9	-2.51	123.76	127.28
35	2	620	XAT	C26-C27-C28	-2.51	120.69	125.99
26	B	818	CLA	CHB-C4A-NA	2.51	128.02	124.40
26	Z	611	CLA	CMB-C2B-C3B	2.51	130.20	123.53
26	A	802	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
34	6	619	LUT	C3-C4-C5	-2.51	105.94	112.18
29	3	621	BCR	C15-C16-C17	-2.51	118.39	123.52
26	5	616	CLA	CAB-C3B-C2B	2.51	130.19	123.53
37	V	607	CHL	CMB-C2B-C3B	2.51	129.69	124.68
29	6	622	BCR	C32-C1-C6	-2.50	106.31	110.24
26	B	817	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
26	B	835	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
26	7	603	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	1	603	CLA	O2D-CGD-O1D	-2.50	118.40	124.08
37	X	609	CHL	CMB-C2B-C3B	2.50	129.68	124.68
26	2	607	CLA	O2D-CGD-O1D	-2.50	118.40	124.08
26	B	806	CLA	C5-C3-C2	2.50	126.78	121.17
26	7	616	CLA	CAB-C3B-C2B	2.50	130.18	123.53
37	W	609	CHL	C4-C3-C5	2.50	119.57	115.23
29	A	849	BCR	C11-C12-C13	-2.50	119.50	126.36
26	Y	614	CLA	CHB-C4A-NA	2.50	128.01	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	606	CLA	O2D-CGD-O1D	-2.50	118.41	124.08
26	G	203	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	K	204	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
26	1	604	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	A	817	CLA	O2D-CGD-CBD	2.50	115.60	111.23
29	A	852	BCR	C12-C13-C14	-2.50	115.08	119.01
29	7	621	BCR	C24-C25-C26	-2.50	115.80	121.56
37	W	601	CHL	CMB-C2B-C3B	2.50	129.68	124.68
26	Z	610	CLA	CHB-C4A-NA	2.50	128.00	124.40
26	B	811	CLA	CHB-C4A-NA	2.50	128.00	124.40
29	L	305	BCR	C38-C26-C25	-2.50	121.76	124.48
26	B	832	CLA	C5-C3-C2	2.50	126.77	121.17
26	U	613	CLA	CHB-C4A-NA	2.50	128.00	124.40
37	Y	601	CHL	CMB-C2B-C3B	2.50	129.67	124.68
29	A	850	BCR	C16-C15-C14	-2.49	118.41	123.52
37	Z	607	CHL	CED-O2D-CGD	2.49	121.57	115.92
34	X	1621	LUT	C18-C5-C6	-2.49	121.76	124.48
26	2	604	CLA	C3B-C4B-NB	-2.49	108.31	110.53
34	V	1621	LUT	C1-C2-C3	2.49	119.06	113.59
26	U	603	CLA	C2A-C1A-CHA	2.49	128.19	123.87
37	W	605	CHL	CMB-C2B-C3B	2.49	129.66	124.68
26	a	612	CLA	CHB-C4A-NA	2.49	128.00	124.40
26	8	603	CLA	CAB-C3B-C2B	2.49	130.15	123.53
26	4	612	CLA	O2D-CGD-O1D	-2.49	118.43	124.08
37	U	609	CHL	C4-C3-C5	2.49	119.55	115.23
29	B	801	BCR	C23-C22-C21	-2.49	115.09	119.01
35	a	618	XAT	C8-C9-C10	-2.49	115.09	119.01
34	1	617	LUT	C1-C6-C5	-2.49	119.23	122.64
29	3	620	BCR	C15-C16-C17	-2.49	118.43	123.52
26	A	822	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
26	B	819	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
29	G	205	BCR	C23-C24-C25	-2.49	120.36	127.00
26	V	614	CLA	C3B-C4B-NB	-2.49	108.31	110.53
26	B	826	CLA	C3B-C4B-NB	-2.48	108.31	110.53
37	V	601	CHL	CBC-CAC-C3C	-2.48	109.32	112.87
35	X	1622	XAT	C15-C35-C34	-2.48	118.44	123.52
26	1	601	CLA	CHB-C4A-NA	2.48	127.98	124.40
34	6	619	LUT	C12-C13-C14	-2.48	115.10	119.01
26	3	606	CLA	O2D-CGD-O1D	-2.48	118.45	124.08
26	6	603	CLA	CAB-C3B-C2B	2.48	130.13	123.53
29	F	305	BCR	C19-C18-C17	2.48	122.91	119.01
26	2	611	CLA	CHB-C4A-NA	2.48	127.98	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	604	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
34	X	1620	LUT	C15-C35-C34	-2.48	118.44	123.52
26	A	819	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
35	2	620	XAT	C37-C21-C36	-2.48	103.77	107.37
26	6	616	CLA	CHB-C4A-NA	2.48	127.98	124.40
37	X	609	CHL	C4-C3-C5	2.48	119.53	115.23
26	5	612	CLA	CHB-C4A-NA	2.48	127.98	124.40
26	B	808	CLA	C1D-ND-C4D	-2.48	104.57	106.31
26	A	834	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
32	V	2631	LMG	C8-O7-C10	-2.48	111.86	117.80
26	9	609	CLA	CHB-C4A-NA	2.48	127.98	124.40
29	7	621	BCR	C36-C18-C17	-2.48	118.80	122.82
26	B	831	CLA	CHB-C4A-NA	2.48	127.98	124.40
26	a	611	CLA	O2D-CGD-O1D	-2.48	118.46	124.08
26	a	604	CLA	CHB-C4A-NA	2.48	127.98	124.40
26	a	609	CLA	CHB-C4A-NA	2.48	127.98	124.40
29	B	843	BCR	C23-C22-C21	-2.48	115.11	119.01
35	2	620	XAT	C35-C34-C33	-2.48	123.80	127.28
26	3	607	CLA	CAB-C3B-C2B	2.48	130.12	123.53
26	8	614	CLA	C1-C2-C3	-2.48	122.14	126.20
29	L	301	BCR	C29-C28-C27	-2.48	105.83	111.28
26	6	609	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
26	6	606	CLA	CHB-C4A-NA	2.48	127.97	124.40
26	5	619	CLA	CAB-C3B-C2B	2.47	130.11	123.53
26	X	603	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
26	A	803	CLA	CMB-C2B-C1B	-2.47	121.65	125.42
37	Z	607	CHL	CAA-C2A-C3A	-2.47	106.31	113.00
35	1	618	XAT	C4-C3-C2	-2.47	106.16	110.79
26	6	612	CLA	O2D-CGD-O1D	-2.47	118.47	124.08
35	a	618	XAT	C35-C34-C33	-2.47	123.81	127.28
34	Y	1621	LUT	C27-C28-C29	-2.47	121.01	126.32
26	7	608	CLA	CHB-C4A-NA	2.47	127.97	124.40
34	7	619	LUT	C15-C35-C34	-2.47	118.46	123.52
26	Y	610	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
26	Y	611	CLA	CHB-C4A-NA	2.47	127.97	124.40
37	V	605	CHL	O2D-CGD-O1D	-2.47	119.04	123.85
36	Z	1623	NEX	C30-C31-C32	-2.47	116.05	123.20
26	5	619	CLA	CMB-C2B-C3B	2.47	130.09	123.53
29	K	202	BCR	C19-C18-C17	-2.47	115.13	119.01
26	3	615	CLA	O2D-CGD-O1D	-2.47	118.48	124.08
26	8	607	CLA	CAB-C3B-C2B	2.47	130.09	123.53
29	A	848	BCR	C19-C18-C17	2.47	122.89	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O	2002	CLA	O2D-CGD-O1D	-2.47	118.48	124.08
26	6	618	CLA	O2D-CGD-O1D	-2.47	118.49	124.08
26	4	606	CLA	C3B-C4B-NB	-2.47	108.33	110.53
36	6	624	NEX	C31-C30-C29	-2.46	123.82	127.28
26	4	611	CLA	CHB-C4A-NA	2.46	127.96	124.40
26	7	604	CLA	C3B-C4B-NB	-2.46	108.33	110.53
26	A	802	CLA	CAA-C2A-C3A	-2.46	106.34	113.00
37	X	605	CHL	O1D-CGD-CBD	-2.46	120.99	124.72
26	A	815	CLA	CHB-C4A-NA	2.46	127.95	124.40
26	3	607	CLA	CHB-C4A-NA	2.46	127.95	124.40
26	5	617	CLA	CHB-C4A-NA	2.46	127.95	124.40
34	8	619	LUT	C38-C25-C24	-2.46	117.53	123.36
26	a	611	CLA	CMB-C2B-C3B	2.46	130.08	123.53
26	4	604	CLA	CHB-C4A-NA	2.46	127.95	124.40
35	1	618	XAT	C35-C34-C33	-2.46	123.83	127.28
35	U	1622	XAT	C10-C11-C12	-2.46	116.07	123.20
29	L	305	BCR	C4-C5-C6	-2.46	119.38	122.70
26	B	832	CLA	CHB-C4A-NA	2.46	127.95	124.40
26	A	822	CLA	C3B-C4B-NB	-2.46	108.33	110.53
26	3	603	CLA	CHB-C4A-NA	2.46	127.95	124.40
34	Y	1621	LUT	C7-C6-C5	2.46	127.22	121.56
35	a	618	XAT	C28-C29-C30	-2.46	115.14	119.01
26	3	604	CLA	CMB-C2B-C1B	-2.46	121.68	125.42
26	A	845	CLA	C1-C2-C3	-2.46	122.78	126.76
37	Y	608	CHL	CMB-C2B-C3B	2.46	129.59	124.68
26	5	606	CLA	CHB-C4A-NA	2.46	127.95	124.40
34	9	619	LUT	C10-C11-C12	-2.46	116.08	123.20
35	1	618	XAT	C28-C29-C30	-2.46	115.14	119.01
26	7	614	CLA	C3B-C4B-NB	-2.46	108.34	110.53
37	W	605	CHL	O2D-CGD-O1D	-2.45	119.07	123.85
26	9	606	CLA	CHB-C4A-NA	2.45	127.94	124.40
36	6	624	NEX	C15-C14-C13	-2.45	123.84	127.28
26	5	604	CLA	CMB-C2B-C3B	2.45	130.05	123.53
37	U	606	CHL	CBC-CAC-C3C	-2.45	109.36	112.87
37	Z	607	CHL	O2A-CGA-CBA	2.45	119.31	111.83
26	U	602	CLA	C1-C2-C3	-2.45	122.18	126.20
26	4	608	CLA	CHB-C4A-NA	2.45	127.94	124.40
34	Y	1621	LUT	C30-C31-C32	-2.45	116.09	123.20
29	3	622	BCR	C36-C18-C17	-2.45	118.84	122.82
37	V	607	CHL	CBC-CAC-C3C	-2.45	109.36	112.87
34	7	619	LUT	C35-C15-C14	-2.45	118.50	123.52
26	J	101	CLA	C3B-C4B-NB	-2.45	108.34	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	Z	1622	XAT	C19-C9-C8	2.45	121.83	118.09
26	6	618	CLA	CAB-C3B-C2B	2.45	130.04	123.53
29	F	305	BCR	C8-C9-C10	-2.45	115.16	119.01
26	B	811	CLA	CBD-CHA-C1A	2.45	132.12	127.58
26	A	834	CLA	C3B-C4B-NB	-2.45	108.34	110.53
26	B	832	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
29	B	843	BCR	C24-C25-C26	2.45	127.19	121.56
26	A	824	CLA	CHB-C4A-NA	2.45	127.93	124.40
26	L	307	CLA	CHB-C4A-NA	2.45	127.93	124.40
26	X	611	CLA	CHB-C4A-NA	2.45	127.93	124.40
37	X	607	CHL	CAC-C3C-C4C	2.45	130.32	124.03
37	U	606	CHL	O1D-CGD-CBD	-2.45	121.01	124.72
37	Y	609	CHL	C4-C3-C5	2.45	119.47	115.23
37	V	608	CHL	O1D-CGD-CBD	-2.45	121.02	124.72
26	1	609	CLA	CHB-C4A-NA	2.44	127.93	124.40
26	8	608	CLA	O2A-CGA-O1A	-2.44	117.51	123.63
37	V	606	CHL	CAA-C2A-C3A	-2.44	106.39	113.00
26	2	606	CLA	CHB-C4A-NA	2.44	127.93	124.40
26	5	613	CLA	C3B-C4B-NB	-2.44	108.35	110.53
26	9	603	CLA	CAB-C3B-C2B	2.44	130.02	123.53
37	Y	609	CHL	C1-C2-C3	-2.44	122.19	126.20
35	1	618	XAT	C8-C9-C10	-2.44	115.17	119.01
34	W	1620	LUT	C18-C5-C6	-2.44	121.82	124.48
32	9	625	LMG	C8-O7-C10	-2.44	111.95	117.80
37	W	609	CHL	CMD-C2D-C3D	-2.44	119.80	124.68
26	Z	604	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
35	a	618	XAT	C4-C3-C2	-2.44	106.23	110.79
35	V	1622	XAT	C7-C8-C9	-2.44	121.74	125.53
26	A	804	CLA	CHB-C4A-NA	2.44	127.92	124.40
26	9	607	CLA	CHB-C4A-NA	2.44	127.92	124.40
26	Z	602	CLA	C3B-C4B-NB	-2.44	108.35	110.53
26	B	806	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
26	2	603	CLA	O2D-CGD-O1D	-2.44	118.55	124.08
37	Y	607	CHL	CMB-C2B-C3B	2.44	129.56	124.68
37	Y	605	CHL	CAA-C2A-C3A	-2.44	110.64	116.23
29	B	852	BCR	C1-C6-C7	2.44	122.26	115.65
37	Z	601	CHL	O1D-CGD-CBD	-2.44	121.03	124.72
26	A	817	CLA	CHB-C4A-NA	2.44	127.92	124.40
26	8	613	CLA	C3B-C4B-NB	-2.44	108.36	110.53
37	X	605	CHL	CMB-C2B-C3B	2.44	129.55	124.68
26	9	612	CLA	O2D-CGD-O1D	-2.44	118.56	124.08
26	B	839	CLA	O2D-CGD-O1D	-2.44	119.11	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Y	608	CHL	CMA-C3A-C4A	-2.43	109.36	114.61
34	4	619	LUT	C28-C29-C30	-2.43	115.18	119.01
29	A	856	BCR	C30-C25-C24	2.43	122.25	115.65
26	A	812	CLA	CHB-C4A-NA	2.43	127.91	124.40
37	U	609	CHL	O2A-CGA-CBA	2.43	119.25	111.83
26	4	618	CLA	CAB-C3B-C2B	2.43	130.00	123.53
28	A	846	LHG	O8-C23-C24	2.43	119.25	111.83
34	6	619	LUT	C35-C34-C33	-2.43	123.87	127.28
26	1	607	CLA	O2D-CGD-O1D	-2.43	118.57	124.08
29	5	622	BCR	C11-C10-C9	-2.43	123.87	127.28
26	A	843	CLA	CAA-CBA-CGA	-2.43	106.31	113.21
28	3	624	LHG	C5-O7-C7	-2.43	111.98	117.80
26	7	616	CLA	CHB-C4A-NA	2.43	127.91	124.40
26	X	614	CLA	CHB-C4A-NA	2.43	127.91	124.40
37	U	608	CHL	O1D-CGD-CBD	-2.43	121.04	124.72
26	A	815	CLA	C3B-C4B-NB	-2.43	108.36	110.53
28	5	623	LHG	O8-C23-C24	2.43	119.24	111.83
29	6	622	BCR	C30-C25-C26	-2.43	119.32	122.64
26	B	837	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
35	6	621	XAT	C8-C9-C10	-2.43	115.19	119.01
34	W	1621	LUT	C11-C12-C13	-2.42	119.71	126.36
26	Z	611	CLA	O2D-CGD-CBD	2.42	115.47	111.23
26	6	614	CLA	O2A-CGA-O1A	-2.42	117.56	123.63
26	Y	613	CLA	CHB-C4A-NA	2.42	127.90	124.40
26	B	808	CLA	O2A-CGA-O1A	-2.42	117.56	123.63
26	5	618	CLA	O2D-CGD-O1D	-2.42	118.58	124.08
29	L	305	BCR	C11-C12-C13	-2.42	119.72	126.36
34	7	619	LUT	C1-C6-C5	-2.42	119.33	122.64
37	W	607	CHL	O1D-CGD-CBD	-2.42	121.05	124.72
26	4	604	CLA	CAB-C3B-C2B	2.42	129.97	123.53
29	L	308	BCR	C15-C14-C13	-2.42	123.88	127.28
26	9	606	CLA	O2D-CGD-O1D	-2.42	118.58	124.08
26	1	602	CLA	CHB-C4A-NA	2.42	127.89	124.40
34	V	1621	LUT	C18-C5-C6	2.42	127.13	124.48
26	A	805	CLA	C3B-C4B-NB	-2.42	108.37	110.53
26	A	815	CLA	C1-C2-C3	-2.42	122.85	126.76
29	6	622	BCR	C37-C22-C21	-2.42	118.90	122.82
35	Z	1622	XAT	C40-C33-C32	2.42	121.78	118.09
26	A	806	CLA	O1D-CGD-CBD	2.42	129.29	124.52
37	U	608	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
34	a	617	LUT	C18-C5-C4	2.42	118.87	114.42
26	F	304	CLA	CHB-C4A-NA	2.42	127.89	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	8	602	CLA	CHB-C4A-NA	2.42	127.89	124.40
29	L	305	BCR	C24-C23-C22	-2.42	122.66	126.23
29	6	622	BCR	C1-C6-C7	2.42	122.21	115.65
26	1	608	CLA	CHB-C4A-NA	2.42	127.89	124.40
26	U	611	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
28	5	625	LHG	O8-C23-C24	2.42	119.20	111.83
26	V	613	CLA	CHB-C4A-NA	2.42	127.89	124.40
29	B	844	BCR	C37-C22-C21	-2.42	118.90	122.82
26	F	301	CLA	C3B-C4B-NB	-2.42	108.37	110.53
26	B	827	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
26	5	607	CLA	CHB-C4A-NA	2.41	127.88	124.40
28	6	623	LHG	O8-C23-C24	2.41	119.20	111.83
29	K	202	BCR	C11-C12-C13	-2.41	119.75	126.36
26	B	810	CLA	C11-C10-C8	-2.41	107.94	115.97
29	4	621	BCR	C15-C14-C13	-2.41	123.89	127.28
37	V	601	CHL	CMB-C2B-C3B	2.41	129.50	124.68
37	Z	605	CHL	CMB-C2B-C3B	2.41	129.50	124.68
29	F	305	BCR	C10-C11-C12	-2.41	116.21	123.20
26	Y	612	CLA	CAA-C2A-C3A	-2.41	106.48	113.00
35	2	620	XAT	C18-C5-C4	2.41	116.95	114.24
26	B	802	CLA	C3B-C4B-NB	-2.41	108.38	110.53
37	Z	608	CHL	CBC-CAC-C3C	-2.41	109.42	112.87
26	A	841	CLA	C3B-C4B-NB	-2.41	108.38	110.53
34	3	618	LUT	C38-C25-C24	-2.41	117.66	123.36
26	A	828	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
37	Y	606	CHL	O1D-CGD-CBD	-2.41	121.07	124.72
26	5	604	CLA	CAB-C3B-C2B	2.41	129.93	123.53
26	B	819	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
35	X	1622	XAT	C7-C8-C9	-2.41	121.79	125.53
26	L	303	CLA	C4-C3-C5	2.41	119.41	115.23
26	2	606	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
26	4	601	CLA	CHB-C4A-NA	2.41	127.87	124.40
26	A	814	CLA	CHB-C4A-NA	2.41	127.87	124.40
37	Y	601	CHL	C4C-CHD-C1D	2.41	124.68	116.07
29	B	801	BCR	C8-C7-C6	-2.41	120.57	127.00
29	A	856	BCR	C40-C30-C25	2.41	114.02	110.24
26	6	610	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
37	Y	607	CHL	CED-O2D-CGD	2.41	121.37	115.92
36	U	1623	NEX	C31-C32-C33	-2.41	119.77	126.36
37	V	601	CHL	O1D-CGD-CBD	-2.40	121.08	124.72
35	8	620	XAT	C7-C8-C9	-2.40	121.80	125.53
26	B	830	CLA	CHB-C4A-NA	2.40	127.87	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	614	CLA	CMB-C2B-C3B	2.40	129.92	123.53
37	Y	605	CHL	CMB-C2B-C3B	2.40	129.49	124.68
37	Z	607	CHL	CAC-C3C-C4C	2.40	130.21	124.03
29	3	621	BCR	C36-C18-C19	2.40	121.76	118.09
31	5	629	LMU	C6'-C5'-C4'	-2.40	106.62	113.38
26	6	607	CLA	CMB-C2B-C3B	2.40	129.92	123.53
26	B	822	CLA	CHB-C4A-NA	2.40	127.87	124.40
26	1	610	CLA	CHB-C4A-NA	2.40	127.87	124.40
32	A	860	LMG	C7-O1-C1	-2.40	108.64	113.80
29	3	620	BCR	C24-C25-C26	-2.40	116.02	121.56
26	4	612	CLA	CHB-C4A-NA	2.40	127.86	124.40
26	Y	602	CLA	CHB-C4A-NA	2.40	127.86	124.40
29	O	2005	BCR	C28-C29-C30	-2.40	105.93	114.43
34	U	1621	LUT	C21-C26-C27	-2.40	110.06	112.83
26	B	835	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
26	8	603	CLA	CHB-C4A-NA	2.40	127.86	124.40
26	L	307	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
26	K	203	CLA	CAA-C2A-C1A	2.40	119.84	111.97
37	Y	609	CHL	CMB-C2B-C3B	2.40	129.48	124.68
37	V	601	CHL	CMA-C3A-C4A	-2.40	109.44	114.61
35	V	1622	XAT	C15-C35-C34	-2.40	118.61	123.52
34	7	619	LUT	C12-C13-C14	-2.40	115.24	119.01
26	B	834	CLA	CHB-C4A-NA	2.40	127.86	124.40
26	a	608	CLA	CHB-C4A-NA	2.40	127.86	124.40
27	B	842	PQN	C26-C25-C23	-2.40	108.00	115.97
31	K	208	LMU	C1'-C2'-C3'	2.40	115.05	110.01
26	A	806	CLA	C3B-C4B-NB	-2.40	108.39	110.53
29	6	622	BCR	C33-C5-C4	2.40	118.70	113.60
26	7	604	CLA	O2A-CGA-O1A	-2.40	117.64	123.63
26	3	611	CLA	CAB-C3B-C2B	2.40	129.90	123.53
34	U	1621	LUT	C30-C31-C32	-2.39	116.26	123.20
29	3	622	BCR	C38-C26-C27	2.39	118.70	113.60
29	3	620	BCR	C11-C12-C13	-2.39	119.80	126.36
26	a	609	CLA	O2D-CGD-O1D	-2.39	118.65	124.08
37	W	607	CHL	C4-C3-C5	2.39	119.38	115.23
37	U	605	CHL	C4C-CHD-C1D	2.39	124.63	116.07
37	Z	608	CHL	CMB-C2B-C3B	2.39	129.46	124.68
26	2	612	CLA	CHB-C4A-NA	2.39	127.85	124.40
26	K	201	CLA	CHB-C4A-NA	2.39	127.85	124.40
26	A	822	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
34	4	619	LUT	C30-C31-C32	-2.39	116.28	123.20
26	A	813	CLA	C1-C2-C3	-2.39	122.28	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	602	CLA	CHB-C4A-NA	2.39	127.85	124.40
26	8	614	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
26	B	836	CLA	CHB-C4A-NA	2.39	127.85	124.40
29	L	309	BCR	C33-C5-C6	2.39	127.09	124.48
34	4	619	LUT	C1-C6-C5	-2.39	119.37	122.64
26	9	606	CLA	C3B-C4B-NB	-2.39	108.40	110.53
26	a	611	CLA	CAA-C2A-C3A	-2.39	110.76	116.23
37	Z	609	CHL	CMA-C3A-C4A	-2.39	109.47	114.61
29	A	851	BCR	C8-C7-C6	-2.39	120.62	127.00
26	A	810	CLA	C3B-C4B-NB	-2.39	108.40	110.53
26	B	830	CLA	CAC-C3C-C4C	2.39	127.89	124.79
26	7	612	CLA	CHB-C4A-NA	2.39	127.84	124.40
26	8	611	CLA	CHB-C4A-NA	2.39	127.84	124.40
26	A	832	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
36	5	624	NEX	C28-C29-C30	2.39	122.76	119.01
26	6	606	CLA	C3B-C4B-NB	-2.38	108.40	110.53
26	a	602	CLA	CHB-C4A-NA	2.38	127.84	124.40
32	A	860	LMG	O8-C28-C29	2.38	119.11	111.83
34	X	1621	LUT	C20-C13-C12	2.38	121.73	118.09
26	4	610	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
29	J	102	BCR	C3-C4-C5	-2.38	109.81	114.06
26	6	610	CLA	CHB-C4A-NA	2.38	127.84	124.40
26	2	616	CLA	CMB-C2B-C3B	2.38	129.87	123.53
35	9	620	XAT	C18-C5-C4	2.38	116.92	114.24
37	Y	608	CHL	C1C-C2C-CMC	2.38	131.10	126.80
26	5	609	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
26	3	607	CLA	CMB-C2B-C3B	2.38	129.86	123.53
37	X	608	CHL	OMC-CMC-C2C	-2.38	120.98	125.12
26	3	614	CLA	O2D-CGD-O1D	-2.38	118.68	124.08
37	Y	608	CHL	O1D-CGD-CBD	-2.38	121.11	124.72
32	J	104	LMG	C8-O7-C10	-2.38	112.10	117.80
37	W	606	CHL	CAC-C3C-C4C	2.38	130.15	124.03
26	W	603	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
35	7	620	XAT	C8-C9-C10	-2.38	115.27	119.01
29	A	849	BCR	C37-C22-C21	-2.38	118.96	122.82
29	A	851	BCR	C30-C25-C26	-2.38	119.39	122.64
28	X	2630	LHG	O8-C23-C24	2.38	119.09	111.83
34	Z	1620	LUT	C16-C1-C6	-2.38	106.51	110.24
29	4	621	BCR	C36-C18-C19	2.38	121.72	118.09
34	X	1621	LUT	C19-C9-C8	2.38	121.72	118.09
34	1	617	LUT	C18-C5-C4	2.38	118.79	114.42
26	5	613	CLA	CHB-C4A-NA	2.38	127.83	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	820	CLA	CHB-C4A-NA	2.38	127.83	124.40
26	B	823	CLA	CHB-C4A-NA	2.38	127.83	124.40
35	Y	1622	XAT	C30-C31-C32	-2.38	116.31	123.20
34	5	620	LUT	C39-C29-C28	2.38	121.72	118.09
37	W	601	CHL	O2D-CGD-O1D	-2.38	119.22	123.85
35	4	620	XAT	C4-C3-C2	-2.38	106.35	110.79
26	B	841	CLA	CHB-C4A-NA	2.38	127.83	124.40
26	A	815	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
37	W	609	CHL	C1-C2-C3	-2.37	122.31	126.20
37	W	606	CHL	CED-O2D-CGD	2.37	121.30	115.92
26	H	202	CLA	CHB-C4A-NA	2.37	127.83	124.40
29	B	847	BCR	C36-C18-C17	-2.37	118.97	122.82
26	A	842	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
26	V	611	CLA	CHB-C4A-NA	2.37	127.83	124.40
29	9	621	BCR	C36-C18-C17	-2.37	118.97	122.82
35	4	620	XAT	O4-C5-C18	2.37	117.70	115.05
26	A	820	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
29	B	846	BCR	C16-C17-C18	-2.37	123.95	127.28
29	L	309	BCR	C37-C22-C21	-2.37	118.97	122.82
37	Z	608	CHL	O1D-CGD-CBD	-2.37	121.13	124.72
26	L	306	CLA	CHB-C4A-NA	2.37	127.82	124.40
26	4	609	CLA	CHB-C4A-NA	2.37	127.82	124.40
32	J	103	LMG	O6-C5-C6	2.37	112.31	106.44
26	B	838	CLA	C3B-C4B-NB	-2.37	108.42	110.53
26	Y	604	CLA	CHB-C4A-NA	2.37	127.82	124.40
35	Z	1622	XAT	C24-C23-C22	-2.37	106.36	110.79
36	U	1623	NEX	C24-C23-C22	-2.37	106.36	110.79
26	a	610	CLA	CHB-C4A-NA	2.37	127.82	124.40
26	2	603	CLA	CHB-C4A-NA	2.37	127.82	124.40
26	B	834	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
26	B	810	CLA	C3B-C4B-NB	-2.37	108.42	110.53
34	2	619	LUT	C35-C15-C14	-2.37	118.68	123.52
29	A	856	BCR	C15-C14-C13	-2.37	123.96	127.28
37	V	607	CHL	OMC-CMC-C2C	-2.37	121.01	125.12
26	A	822	CLA	CHB-C4A-NA	2.37	127.81	124.40
26	a	611	CLA	CMA-C3A-C2A	-2.37	110.80	116.23
37	V	605	CHL	CMB-C2B-C3B	2.37	129.41	124.68
37	V	605	CHL	CMA-C3A-C4A	-2.37	109.51	114.61
26	B	814	CLA	O2A-CGA-O1A	-2.36	117.71	123.63
26	L	303	CLA	O2D-CGD-CBD	2.36	115.36	111.23
29	B	847	BCR	C37-C22-C21	-2.36	118.99	122.82
37	U	607	CHL	CBC-CAC-C3C	-2.36	109.49	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	9	613	CLA	CHB-C4A-NA	2.36	127.81	124.40
34	V	1621	LUT	C16-C1-C6	-2.36	106.54	110.24
35	3	619	XAT	C15-C35-C34	-2.36	118.69	123.52
34	6	619	LUT	C31-C30-C29	-2.36	123.97	127.28
29	B	853	BCR	C37-C22-C21	-2.36	118.99	122.82
29	3	620	BCR	C23-C22-C21	-2.36	115.30	119.01
26	8	609	CLA	CHB-C4A-NA	2.36	127.80	124.40
36	5	624	NEX	C27-C28-C29	-2.36	121.87	125.53
26	4	601	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
37	V	606	CHL	O2D-CGD-O1D	-2.36	119.26	123.85
37	U	605	CHL	CMA-C3A-C4A	-2.36	109.53	114.61
26	V	603	CLA	CAA-C2A-C3A	-2.36	106.63	113.00
35	V	1622	XAT	C4-C3-C2	-2.36	106.38	110.79
29	J	102	BCR	C30-C25-C24	2.36	122.05	115.65
26	5	602	CLA	CHB-C4A-NA	2.36	127.80	124.40
26	2	614	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
26	6	617	CLA	CHB-C4A-NA	2.36	127.80	124.40
26	U	604	CLA	CMB-C2B-C3B	2.36	132.09	126.55
37	X	606	CHL	CMB-C2B-C3B	2.35	129.39	124.68
26	B	816	CLA	CHB-C4A-NA	2.35	127.80	124.40
26	X	613	CLA	CHB-C4A-NA	2.35	127.80	124.40
26	3	602	CLA	C1-C2-C3	-2.35	122.34	126.20
35	2	620	XAT	C38-C25-C24	2.35	116.88	114.24
29	A	851	BCR	C15-C16-C17	-2.35	118.71	123.52
26	6	613	CLA	C3B-C4B-NB	-2.35	108.43	110.53
29	L	301	BCR	C31-C1-C6	2.35	113.93	110.24
29	B	853	BCR	C32-C1-C6	-2.35	106.56	110.24
32	5	627	LMG	O8-C28-C29	2.35	119.00	111.83
29	B	844	BCR	C29-C30-C25	2.35	113.85	110.44
26	5	603	CLA	CAB-C3B-C2B	2.35	129.78	123.53
26	7	608	CLA	CAA-CBA-CGA	-2.35	106.54	113.21
34	W	1620	LUT	C30-C31-C32	-2.35	116.39	123.20
26	A	805	CLA	CMB-C2B-C3B	2.35	132.08	126.55
29	3	620	BCR	C38-C26-C27	2.35	118.61	113.60
26	8	607	CLA	CHB-C4A-NA	2.35	127.79	124.40
37	Z	605	CHL	O2D-CGD-O1D	-2.35	119.28	123.85
34	W	1621	LUT	C36-C21-C22	-2.35	105.03	109.41
26	1	611	CLA	C5-C3-C2	2.35	126.44	121.17
36	W	1623	NEX	C39-C29-C30	-2.35	119.01	122.82
26	A	843	CLA	CHB-C1B-NB	2.35	127.57	124.05
37	W	609	CHL	CMA-C3A-C4A	-2.35	109.55	114.61
29	J	102	BCR	C30-C25-C26	-2.35	119.43	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	5	628	LMU	C2'-C3'-C4'	2.35	115.01	109.68
36	V	1623	NEX	C26-C27-C28	-2.35	121.03	125.99
26	A	834	CLA	CHB-C4A-NA	2.35	127.79	124.40
29	4	621	BCR	C36-C18-C17	-2.35	119.02	122.82
37	U	601	CHL	C1B-CHB-C4A	2.35	122.83	121.32
26	B	831	CLA	C3B-C4B-NB	-2.35	108.44	110.53
26	6	607	CLA	CAB-C3B-C2B	2.35	129.77	123.53
26	A	825	CLA	CHB-C4A-NA	2.35	127.78	124.40
26	3	612	CLA	CHB-C4A-NA	2.35	127.78	124.40
31	8	625	LMU	O5'-C1'-C2'	2.34	115.19	110.37
29	3	622	BCR	C37-C22-C21	-2.34	119.02	122.82
26	1	601	CLA	O2A-CGA-O1A	-2.34	117.76	123.63
26	K	203	CLA	CHB-C4A-NA	2.34	127.78	124.40
26	A	808	CLA	CMB-C2B-C1B	-2.34	121.85	125.42
26	5	616	CLA	CBD-CHA-C1A	2.34	131.93	127.58
26	8	613	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
26	9	602	CLA	O2D-CGD-CBD	2.34	115.33	111.23
29	6	622	BCR	C15-C14-C13	-2.34	123.99	127.28
26	2	607	CLA	CHB-C4A-NA	2.34	127.78	124.40
29	7	623	BCR	C38-C26-C27	2.34	118.59	113.60
26	4	610	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
32	V	2631	LMG	C7-O1-C1	-2.34	108.78	113.80
26	5	603	CLA	CHB-C4A-NA	2.34	127.78	124.40
29	L	301	BCR	C33-C5-C4	2.34	118.58	113.60
32	9	625	LMG	C1-O6-C5	-2.34	109.15	113.72
37	Y	605	CHL	CBC-CAC-C3C	-2.34	109.52	112.87
34	Y	1620	LUT	C38-C25-C24	-2.34	117.83	123.36
34	Z	1621	LUT	C19-C9-C8	2.34	121.66	118.09
26	2	609	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
26	A	808	CLA	CHB-C4A-NA	2.34	127.77	124.40
26	B	824	CLA	CHB-C4A-NA	2.34	127.77	124.40
29	B	852	BCR	C3-C4-C5	-2.34	109.89	114.06
26	U	604	CLA	CHB-C1B-NB	2.34	127.55	124.05
29	B	853	BCR	C1-C6-C5	-2.34	119.44	122.64
26	B	814	CLA	C1-C2-C3	-2.34	122.37	126.20
26	A	821	CLA	O2D-CGD-O1D	-2.33	119.30	123.85
29	K	207	BCR	C32-C1-C6	-2.33	106.58	110.24
26	B	811	CLA	CAB-C3B-C2B	2.33	129.74	123.53
26	9	604	CLA	CAB-C3B-C2B	2.33	129.74	123.53
26	K	203	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
35	8	620	XAT	C38-C25-C24	2.33	116.86	114.24
26	W	604	CLA	CHB-C4A-NA	2.33	127.77	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	821	CLA	O2D-CGD-O1D	-2.33	118.79	124.08
37	U	605	CHL	CMB-C2B-C3B	2.33	129.34	124.68
37	W	608	CHL	CMB-C2B-C3B	2.33	129.34	124.68
26	3	609	CLA	CBA-CAA-C2A	2.33	120.73	113.79
26	6	616	CLA	CBC-CAC-C3C	2.33	118.74	112.42
29	L	308	BCR	C31-C1-C6	-2.33	106.59	110.24
26	G	203	CLA	C3B-C4B-NB	-2.33	108.45	110.53
37	Y	607	CHL	CAA-C2A-C3A	-2.33	106.70	113.00
29	A	849	BCR	C37-C22-C23	2.33	121.65	118.09
26	4	613	CLA	CHB-C4A-NA	2.33	127.76	124.40
32	H	205	LMG	O8-C28-C29	2.33	118.94	111.83
26	X	614	CLA	C3B-C4B-NB	-2.33	108.45	110.53
26	W	611	CLA	C3B-C4B-NB	-2.33	108.45	110.53
34	9	619	LUT	C18-C5-C6	-2.33	121.94	124.48
34	Z	1620	LUT	C18-C5-C6	-2.33	121.94	124.48
29	A	850	BCR	C31-C1-C6	-2.33	106.59	110.24
31	K	208	LMU	O5'-C1'-C2'	2.33	115.15	110.37
37	U	608	CHL	CMB-C2B-C3B	2.33	129.33	124.68
26	F	301	CLA	CHB-C4A-NA	2.33	127.76	124.40
34	Y	1621	LUT	C1-C2-C3	2.33	118.70	113.59
26	V	604	CLA	CMB-C2B-C3B	2.33	132.02	126.55
26	5	609	CLA	CHB-C4A-NA	2.32	127.75	124.40
37	X	607	CHL	O1D-CGD-CBD	-2.32	121.20	124.72
26	A	823	CLA	CHB-C4A-NA	2.32	127.75	124.40
26	B	807	CLA	O2D-CGD-CBD	2.32	115.29	111.23
26	X	603	CLA	C2A-C1A-CHA	2.32	127.90	123.87
26	8	602	CLA	C1-C2-C3	-2.32	122.39	126.20
26	6	607	CLA	CHB-C4A-NA	2.32	127.75	124.40
29	6	622	BCR	C15-C16-C17	-2.32	118.77	123.52
26	a	608	CLA	C3B-C4B-NB	-2.32	108.46	110.53
37	X	607	CHL	C4-C3-C5	2.32	119.26	115.23
26	6	613	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
26	W	603	CLA	C2A-C1A-CHA	2.32	127.90	123.87
37	Z	609	CHL	C4-C3-C5	2.32	119.26	115.23
26	B	815	CLA	CHB-C4A-NA	2.32	127.75	124.40
26	9	601	CLA	CHB-C4A-NA	2.32	127.75	124.40
26	3	608	CLA	C3B-C4B-NB	-2.32	108.46	110.53
37	Z	605	CHL	C4C-CHD-C1D	2.32	124.37	116.07
29	a	619	BCR	C32-C1-C6	-2.32	106.60	110.24
28	Z	2630	LHG	O8-C23-C24	2.32	118.91	111.83
34	a	617	LUT	C8-C9-C10	2.32	122.65	119.01
35	3	619	XAT	C24-C23-C22	-2.32	106.46	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	851	BCR	C11-C10-C9	-2.32	124.03	127.28
34	V	1621	LUT	C30-C31-C32	-2.32	116.49	123.20
29	4	621	BCR	C15-C16-C17	-2.32	118.78	123.52
34	X	1621	LUT	C39-C29-C28	2.32	121.63	118.09
34	a	617	LUT	C19-C9-C8	-2.32	114.55	118.09
28	U	2630	LHG	C5-O7-C7	-2.32	112.25	117.80
29	a	619	BCR	C11-C12-C13	-2.31	120.02	126.36
29	B	845	BCR	C15-C14-C13	-2.31	124.03	127.28
26	X	610	CLA	CHB-C1B-NB	2.31	127.52	124.05
28	9	624	LHG	O8-C23-C24	2.31	118.89	111.83
26	A	836	CLA	CHB-C4A-NA	2.31	127.74	124.40
26	K	206	CLA	CHB-C4A-NA	2.31	127.74	124.40
26	2	610	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
34	X	1620	LUT	C35-C34-C33	-2.31	124.03	127.28
26	B	805	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
26	B	807	CLA	C3B-C4B-NB	-2.31	108.47	110.53
37	Y	601	CHL	O1D-CGD-CBD	-2.31	121.22	124.72
26	A	820	CLA	C7-C6-C5	-2.31	107.10	113.26
26	6	603	CLA	CMB-C2B-C3B	2.31	129.67	123.53
29	J	102	BCR	C38-C26-C27	2.31	118.52	113.60
26	O	2002	CLA	CAA-C2A-C3A	-2.31	110.93	116.23
26	3	604	CLA	CHB-C4A-NA	2.31	127.73	124.40
26	A	837	CLA	O2D-CGD-CBD	2.31	115.27	111.23
29	1	619	BCR	C32-C1-C6	-2.31	106.62	110.24
26	6	614	CLA	C3B-C4B-NB	-2.31	108.47	110.53
26	B	837	CLA	O2D-CGD-CBD	2.31	115.27	111.23
29	6	622	BCR	C36-C18-C17	-2.31	119.08	122.82
26	B	830	CLA	CHD-C1D-C2D	2.31	130.29	125.49
34	Y	1620	LUT	C8-C9-C10	2.31	122.64	119.01
26	2	610	CLA	CHB-C1B-NB	2.31	127.51	124.05
34	5	620	LUT	C11-C12-C13	-2.31	120.04	126.36
26	6	604	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
37	V	608	CHL	O2D-CGD-O1D	-2.31	119.36	123.85
31	5	629	LMU	C1B-O1B-C4'	-2.31	112.51	117.98
37	V	609	CHL	C4-C3-C5	2.31	119.23	115.23
29	L	305	BCR	C39-C30-C25	2.30	113.86	110.24
26	8	614	CLA	C3B-C4B-NB	-2.30	108.47	110.53
37	U	605	CHL	CBC-CAC-C3C	-2.30	109.57	112.87
26	a	601	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
26	A	804	CLA	O2D-CGD-CBD	2.30	115.26	111.23
26	B	827	CLA	C3B-C4B-NB	-2.30	108.47	110.53
26	4	614	CLA	O2A-CGA-O1A	-2.30	117.87	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	X	605	CHL	O2D-CGD-O1D	-2.30	119.37	123.85
26	4	609	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
37	V	606	CHL	CAC-C3C-C4C	2.30	129.94	124.03
26	3	602	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
26	3	617	CLA	C3B-C4B-NB	-2.30	108.48	110.53
26	5	610	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
26	8	613	CLA	CHB-C4A-NA	2.30	127.72	124.40
28	3	624	LHG	O8-C23-C24	2.30	118.84	111.83
37	X	607	CHL	CMB-C2B-C3B	2.30	129.28	124.68
26	4	614	CLA	C3B-C4B-NB	-2.30	108.48	110.53
35	Y	1622	XAT	C40-C33-C32	2.30	121.60	118.09
29	7	621	BCR	C15-C14-C13	-2.30	124.06	127.28
26	9	604	CLA	CHB-C4A-NA	2.30	127.72	124.40
29	9	621	BCR	C29-C28-C27	-2.30	106.22	111.28
26	V	610	CLA	C1-C2-C3	-2.30	122.43	126.20
36	5	624	NEX	C2-C1-C6	2.30	111.44	109.21
37	Z	601	CHL	O2D-CGD-O1D	-2.30	119.38	123.85
26	W	602	CLA	C1-C2-C3	-2.30	122.44	126.20
37	X	601	CHL	C4-C3-C5	2.30	119.21	115.23
37	U	601	CHL	O1D-CGD-CBD	-2.30	121.24	124.72
26	A	834	CLA	C4-C3-C2	-2.30	117.73	123.63
26	B	833	CLA	CHB-C4A-NA	2.30	127.71	124.40
29	F	305	BCR	C8-C7-C6	-2.29	120.87	127.00
35	1	618	XAT	C37-C21-C22	2.29	113.00	108.97
29	B	849	BCR	C11-C12-C13	-2.29	120.07	126.36
26	5	601	CLA	CHB-C4A-NA	2.29	127.71	124.40
34	Y	1621	LUT	C38-C25-C24	-2.29	117.93	123.36
29	A	852	BCR	C8-C7-C6	-2.29	120.87	127.00
29	3	621	BCR	C16-C17-C18	-2.29	124.06	127.28
29	B	845	BCR	C28-C27-C26	-2.29	109.97	114.06
26	4	610	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
37	U	609	CHL	CMA-C3A-C4A	-2.29	109.67	114.61
29	A	851	BCR	C15-C14-C13	-2.29	124.06	127.28
35	8	620	XAT	C31-C30-C29	-2.29	124.06	127.28
26	A	811	CLA	O1D-CGD-CBD	2.29	129.04	124.52
26	B	802	CLA	CHB-C4A-NA	2.29	127.71	124.40
26	7	607	CLA	CHB-C4A-NA	2.29	127.71	124.40
26	7	615	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
37	Y	601	CHL	O2D-CGD-O1D	-2.29	119.39	123.85
34	X	1621	LUT	C11-C10-C9	-2.29	124.06	127.28
26	A	811	CLA	CHB-C4A-NA	2.29	127.71	124.40
36	Y	1623	NEX	C28-C29-C30	2.29	122.61	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	Y	1623	NEX	C26-C27-C28	-2.29	121.15	125.99
26	a	616	CLA	CMB-C2B-C3B	2.29	131.94	126.55
35	8	620	XAT	C8-C9-C10	-2.29	115.41	119.01
26	a	613	CLA	CMB-C2B-C3B	2.29	131.94	126.55
37	X	609	CHL	CMA-C3A-C4A	-2.29	109.68	114.61
26	7	606	CLA	CHB-C4A-NA	2.29	127.70	124.40
35	W	1622	XAT	C35-C15-C14	-2.29	118.84	123.52
26	A	845	CLA	O1D-CGD-CBD	2.29	129.03	124.52
28	8	622	LHG	O8-C23-C24	2.29	118.81	111.83
26	B	832	CLA	C3B-C4B-NB	-2.29	108.49	110.53
29	B	844	BCR	C11-C12-C13	-2.29	120.09	126.36
26	B	825	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
34	V	1620	LUT	C39-C29-C28	2.29	121.58	118.09
26	2	611	CLA	C3B-C4B-NB	-2.29	108.49	110.53
26	1	609	CLA	CMA-C3A-C2A	-2.29	110.99	116.23
26	B	825	CLA	CHB-C4A-NA	2.29	127.70	124.40
26	B	833	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
26	J	101	CLA	CHB-C4A-NA	2.28	127.70	124.40
34	2	619	LUT	C15-C14-C13	-2.28	124.07	127.28
36	5	624	NEX	C15-C14-C13	-2.28	124.07	127.28
26	B	806	CLA	C9-C8-C10	-2.28	103.13	111.27
26	a	616	CLA	CHB-C4A-NA	2.28	127.70	124.40
26	Z	613	CLA	CHB-C4A-NA	2.28	127.70	124.40
37	W	605	CHL	CBC-CAC-C3C	-2.28	109.60	112.87
35	7	620	XAT	C32-C33-C34	-2.28	115.42	119.01
37	Y	607	CHL	C1-C2-C3	-2.28	122.46	126.20
29	3	622	BCR	C30-C25-C26	-2.28	119.52	122.64
26	8	603	CLA	CMB-C2B-C3B	2.28	129.60	123.53
29	1	619	BCR	C11-C12-C13	-2.28	120.11	126.36
37	X	606	CHL	CAC-C3C-C4C	2.28	129.89	124.03
26	2	609	CLA	CHB-C4A-NA	2.28	127.69	124.40
29	7	621	BCR	C37-C22-C21	-2.28	119.12	122.82
26	B	802	CLA	CBA-CAA-C2A	-2.28	107.01	113.79
26	W	603	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
29	7	623	BCR	C37-C22-C23	2.28	121.57	118.09
34	6	619	LUT	C17-C1-C6	-2.28	106.67	110.24
26	A	818	CLA	CHB-C4A-NA	2.28	127.69	124.40
26	W	602	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
26	7	611	CLA	CHB-C4A-NA	2.28	127.69	124.40
35	7	620	XAT	C7-C8-C9	-2.28	122.00	125.53
26	3	602	CLA	C3B-C4B-NB	-2.28	108.50	110.53
29	4	621	BCR	C33-C5-C4	2.28	118.45	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1	617	LUT	C19-C9-C8	-2.28	114.61	118.09
26	B	805	CLA	C3B-C4B-NB	-2.28	108.50	110.53
26	A	812	CLA	O1D-CGD-CBD	2.27	129.00	124.52
26	8	616	CLA	CMB-C2B-C3B	2.27	129.58	123.53
26	A	835	CLA	O2D-CGD-CBD	2.27	115.21	111.23
37	X	607	CHL	C6-C5-C3	-2.27	107.93	113.47
35	Y	1622	XAT	C10-C11-C12	-2.27	116.61	123.20
26	4	604	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
26	8	614	CLA	CHB-C4A-NA	2.27	127.68	124.40
26	V	610	CLA	C3B-C4B-NB	-2.27	108.50	110.53
26	A	819	CLA	CMB-C2B-C3B	2.27	131.90	126.55
29	L	301	BCR	C15-C14-C13	-2.27	124.09	127.28
26	O	2002	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
26	B	818	CLA	CHC-C4B-NB	2.27	127.46	124.05
34	Z	1620	LUT	C38-C25-C24	-2.27	117.98	123.36
31	A	857	LMU	O5'-C1'-C2'	2.27	115.04	110.37
29	A	851	BCR	C33-C5-C6	-2.27	122.01	124.48
29	a	619	BCR	C1-C6-C7	2.27	121.81	115.65
37	U	606	CHL	CMB-C2B-C3B	2.27	129.22	124.68
29	B	845	BCR	C23-C22-C21	2.27	122.58	119.01
29	L	301	BCR	C8-C9-C10	2.27	122.58	119.01
26	3	613	CLA	C3B-C4B-NB	-2.27	108.50	110.53
37	U	609	CHL	C1-C2-C3	-2.27	122.48	126.20
26	3	614	CLA	CHB-C4A-NA	2.27	127.68	124.40
37	Z	607	CHL	O1D-CGD-CBD	-2.27	121.28	124.72
29	1	619	BCR	C1-C6-C7	2.27	121.81	115.65
34	Y	1621	LUT	C31-C30-C29	-2.27	124.10	127.28
32	9	625	LMG	C12-C11-C10	-2.27	105.38	113.69
26	O	2001	CLA	C3B-C4B-NB	-2.27	108.50	110.53
37	U	605	CHL	OMC-CMC-C2C	-2.27	121.18	125.12
26	8	602	CLA	C3B-C4B-NB	-2.27	108.51	110.53
26	8	604	CLA	CHB-C4A-NA	2.27	127.67	124.40
37	U	601	CHL	O2D-CGD-O1D	-2.27	119.44	123.85
26	6	601	CLA	O2D-CGD-CBD	2.27	115.19	111.23
26	4	607	CLA	C3B-C4B-NB	-2.27	108.51	110.53
32	4	623	LMG	O6-C5-C6	2.26	112.05	106.44
37	V	601	CHL	O2D-CGD-O1D	-2.26	119.44	123.85
35	a	618	XAT	C37-C21-C22	2.26	112.95	108.97
29	3	620	BCR	C30-C25-C26	-2.26	119.54	122.64
29	L	301	BCR	C34-C9-C8	2.26	121.55	118.09
26	8	610	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
29	8	621	BCR	C11-C12-C13	-2.26	120.16	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	813	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
34	U	1621	LUT	C18-C5-C6	-2.26	122.02	124.48
37	U	606	CHL	O2D-CGD-O1D	-2.26	119.45	123.85
26	6	613	CLA	CHB-C4A-NA	2.26	127.66	124.40
26	9	610	CLA	CHB-C4A-NA	2.26	127.66	124.40
34	V	1620	LUT	C38-C25-C24	-2.26	118.02	123.36
34	W	1620	LUT	C39-C29-C28	2.26	121.53	118.09
29	8	621	BCR	C32-C1-C6	-2.26	106.71	110.24
26	X	602	CLA	CMB-C2B-C3B	2.26	131.85	126.55
26	7	610	CLA	O2D-CGD-O1D	-2.26	119.46	123.85
26	U	604	CLA	CHB-C4A-NA	2.25	127.65	124.40
36	Z	1623	NEX	C35-C34-C33	-2.25	124.12	127.28
31	5	628	LMU	O5'-C1'-C2'	2.25	115.00	110.37
26	A	830	CLA	CHB-C4A-NA	2.25	127.65	124.40
26	6	609	CLA	CHB-C4A-NA	2.25	127.65	124.40
29	J	102	BCR	C32-C1-C6	-2.25	106.71	110.24
26	1	608	CLA	C3B-C4B-NB	-2.25	108.52	110.53
29	3	621	BCR	C37-C22-C21	-2.25	119.17	122.82
36	5	624	NEX	C35-C34-C33	-2.25	124.12	127.28
29	B	843	BCR	C32-C1-C6	-2.25	106.71	110.24
26	1	613	CLA	CMB-C2B-C3B	2.25	131.85	126.55
29	A	851	BCR	C16-C15-C14	-2.25	118.91	123.52
28	2	622	LHG	O8-C23-C24	2.25	118.70	111.83
26	Z	614	CLA	C3B-C4B-NB	-2.25	108.52	110.53
26	B	837	CLA	CHB-C4A-NA	2.25	127.65	124.40
34	1	617	LUT	C8-C9-C10	2.25	122.55	119.01
36	V	1623	NEX	C28-C29-C30	2.25	122.55	119.01
26	A	833	CLA	CMB-C2B-C3B	2.25	131.84	126.55
37	Y	605	CHL	C4C-CHD-C1D	2.25	124.12	116.07
26	6	616	CLA	C4-C3-C5	2.25	119.13	115.23
37	U	605	CHL	CAC-C3C-C4C	2.25	129.81	124.03
37	Y	606	CHL	CMB-C2B-C3B	2.25	129.18	124.68
37	V	601	CHL	C4C-CHD-C1D	2.25	124.11	116.07
35	4	620	XAT	C30-C31-C32	-2.25	116.68	123.20
26	A	831	CLA	CAA-CBA-CGA	-2.25	106.82	113.21
29	A	849	BCR	C36-C18-C17	-2.25	119.17	122.82
26	A	821	CLA	O1D-CGD-CBD	2.25	128.95	124.52
34	2	619	LUT	C19-C9-C8	-2.25	114.66	118.09
37	W	607	CHL	C1-C2-C3	-2.25	122.52	126.20
26	5	618	CLA	CHB-C4A-NA	2.25	127.64	124.40
29	J	102	BCR	C37-C22-C21	-2.25	119.18	122.82
26	A	811	CLA	C1-C2-C3	-2.25	122.52	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	5	620	LUT	C18-C5-C4	2.25	118.55	114.42
29	7	621	BCR	C39-C30-C25	-2.25	106.72	110.24
26	2	606	CLA	CAC-C3C-C4C	2.25	127.71	124.79
26	B	820	CLA	C3B-C4B-NB	-2.24	108.53	110.53
26	1	616	CLA	CHB-C4A-NA	2.24	127.64	124.40
26	2	604	CLA	CHB-C4A-NA	2.24	127.64	124.40
26	B	839	CLA	CAC-C3C-C4C	2.24	127.71	124.79
26	L	303	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
26	4	611	CLA	C3B-C4B-NB	-2.24	108.53	110.53
34	Y	1620	LUT	C16-C1-C6	-2.24	106.73	110.24
26	X	610	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
26	Y	602	CLA	O2D-CGD-CBD	2.24	115.14	111.23
26	8	616	CLA	CAB-C3B-C2B	2.24	129.48	123.53
34	Y	1621	LUT	C17-C1-C6	-2.24	106.73	110.24
37	Z	607	CHL	CMB-C2B-C3B	2.24	129.15	124.68
26	A	819	CLA	C3B-C4B-NB	-2.24	108.53	110.53
26	7	609	CLA	C3B-C4B-NB	-2.24	108.53	110.53
26	Z	612	CLA	C3B-C4B-NB	-2.24	108.53	110.53
26	B	807	CLA	CHB-C4A-NA	2.24	127.63	124.40
35	a	618	XAT	C32-C33-C34	-2.24	115.49	119.01
26	B	808	CLA	CHB-C4A-NA	2.24	127.63	124.40
33	B	850	DGD	O2G-C1B-O1B	-2.24	118.48	123.70
36	U	1623	NEX	C2-C1-C6	-2.24	107.04	109.21
26	A	810	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
26	U	613	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
29	J	102	BCR	C34-C9-C8	2.24	121.50	118.09
35	6	621	XAT	C18-C5-C4	2.24	116.75	114.24
26	B	805	CLA	CMB-C2B-C3B	2.24	131.81	126.55
35	8	620	XAT	C28-C29-C30	-2.24	115.49	119.01
26	V	613	CLA	C3B-C4B-NB	-2.23	108.53	110.53
26	B	818	CLA	C6-C5-C3	2.23	118.91	113.47
29	A	849	BCR	C29-C30-C25	2.23	113.68	110.44
35	Z	1622	XAT	C30-C31-C32	-2.23	116.73	123.20
37	W	605	CHL	C4C-CHD-C1D	2.23	124.06	116.07
26	A	834	CLA	C1-O2A-CGA	-2.23	111.25	116.65
26	4	608	CLA	C3B-C4B-NB	-2.23	108.54	110.53
26	2	606	CLA	O1D-CGD-CBD	2.23	128.92	124.52
37	Z	608	CHL	C4C-CHD-C1D	2.23	124.06	116.07
26	Z	604	CLA	C1-C2-C3	-2.23	123.15	126.76
29	3	621	BCR	C15-C14-C13	-2.23	124.15	127.28
37	W	606	CHL	O1D-CGD-CBD	-2.23	121.34	124.72
26	6	603	CLA	CHB-C4A-NA	2.23	127.62	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	308	BCR	C29-C30-C25	2.23	113.68	110.44
36	V	1623	NEX	C19-C9-C8	2.23	123.89	118.94
34	U	1620	LUT	C39-C29-C28	2.23	121.50	118.09
32	4	624	LMG	O1-C1-C2	2.23	111.66	108.27
26	B	830	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
26	A	816	CLA	CHB-C4A-NA	2.23	127.62	124.40
29	1	619	BCR	C15-C14-C13	-2.23	124.15	127.28
26	7	601	CLA	O1D-CGD-CBD	2.23	128.92	124.52
29	B	844	BCR	C8-C7-C6	-2.23	121.04	127.00
26	A	802	CLA	C3A-C2A-C1A	2.23	104.68	101.34
32	4	624	LMG	O8-C28-O10	-2.23	118.05	123.63
35	5	621	XAT	C24-C23-C22	-2.23	106.62	110.79
26	3	604	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
29	B	848	BCR	C21-C20-C19	-2.23	116.74	123.20
29	B	845	BCR	C16-C15-C14	-2.23	118.96	123.52
26	4	601	CLA	C1-C2-C3	-2.23	122.55	126.20
31	A	858	LMU	O5B-C1B-C2B	2.23	115.10	111.20
29	L	309	BCR	C11-C12-C13	-2.23	120.26	126.36
37	Y	607	CHL	CAC-C3C-C4C	2.23	129.75	124.03
34	7	619	LUT	C18-C5-C4	-2.23	110.33	114.42
26	3	615	CLA	C3B-C4B-NB	-2.23	108.54	110.53
26	A	841	CLA	CHB-C4A-NA	2.23	127.61	124.40
36	Z	1623	NEX	C40-C33-C32	2.23	121.49	118.09
27	B	842	PQN	C24-C23-C22	-2.22	103.34	111.27
26	B	808	CLA	C1-C2-C3	-2.22	122.55	126.20
26	Y	602	CLA	C1-C2-C3	-2.22	122.55	126.20
36	U	1623	NEX	C10-C11-C12	2.22	129.64	123.20
26	W	604	CLA	CMB-C2B-C3B	2.22	131.78	126.55
26	1	616	CLA	CAB-C3B-C2B	2.22	129.44	123.53
26	5	603	CLA	C4-C3-C5	2.22	119.09	115.23
26	B	838	CLA	CMB-C2B-C3B	2.22	131.78	126.55
26	9	602	CLA	CMB-C2B-C3B	2.22	131.78	126.55
26	A	841	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
35	2	620	XAT	C8-C9-C10	-2.22	115.51	119.01
35	6	621	XAT	C35-C34-C33	-2.22	124.16	127.28
26	A	842	CLA	CHB-C4A-NA	2.22	127.61	124.40
26	3	609	CLA	C3B-C4B-NB	-2.22	108.55	110.53
35	6	621	XAT	C12-C13-C14	-2.22	115.52	119.01
29	2	623	BCR	C11-C12-C13	-2.22	120.28	126.36
32	L	2631	LMG	O1-C1-C2	2.22	111.64	108.27
35	4	620	XAT	C28-C29-C30	-2.22	115.52	119.01
37	X	601	CHL	CMA-C3A-C4A	-2.22	109.83	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	805	CLA	CHB-C4A-NA	2.22	127.60	124.40
36	U	1623	NEX	O24-C25-C26	-2.22	57.17	58.93
26	A	814	CLA	CAA-C2A-C3A	-2.22	107.01	113.00
26	a	614	CLA	O2D-CGD-CBD	2.22	115.11	111.23
26	6	616	CLA	C1-O2A-CGA	-2.22	111.28	116.65
37	X	608	CHL	CMB-C2B-C3B	2.22	129.11	124.68
26	Z	613	CLA	CHC-C4B-NB	2.22	127.37	124.05
26	7	608	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
26	6	618	CLA	CMB-C2B-C3B	2.21	129.42	123.53
29	a	619	BCR	C15-C14-C13	-2.21	124.17	127.28
37	Z	606	CHL	O2D-CGD-O1D	-2.21	119.54	123.85
26	4	611	CLA	CMB-C2B-C3B	2.21	131.76	126.55
37	W	606	CHL	C1C-C2C-CMC	2.21	130.79	126.80
35	8	620	XAT	C32-C33-C34	-2.21	115.53	119.01
37	X	609	CHL	CMD-C2D-C3D	-2.21	120.26	124.68
26	3	607	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
34	a	617	LUT	C15-C35-C34	-2.21	119.00	123.52
26	Z	612	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
26	5	601	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
34	2	619	LUT	C27-C28-C29	-2.21	121.57	126.32
34	Z	1620	LUT	C28-C29-C30	-2.21	115.54	119.01
26	A	842	CLA	CMB-C2B-C3B	2.21	131.74	126.55
26	6	602	CLA	CHB-C4A-NA	2.21	127.59	124.40
26	X	604	CLA	CHB-C4A-NA	2.21	127.59	124.40
26	B	839	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
26	Z	603	CLA	CBC-CAC-C3C	-2.21	106.44	112.42
26	1	602	CLA	O1D-CGD-CBD	2.21	128.87	124.52
26	A	838	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
26	A	829	CLA	CHB-C4A-NA	2.21	127.58	124.40
26	7	609	CLA	CBD-CHA-C1A	2.20	131.67	127.58
26	7	609	CLA	CHB-C4A-NA	2.20	127.58	124.40
29	K	207	BCR	C15-C16-C17	-2.20	119.01	123.52
26	a	611	CLA	CHB-C4A-NA	2.20	127.58	124.40
28	B	851	LHG	O8-C23-O10	-2.20	118.12	123.63
29	A	852	BCR	C37-C22-C21	-2.20	119.25	122.82
26	O	2002	CLA	CMA-C3A-C2A	-2.20	111.18	116.23
37	X	605	CHL	C4C-CHD-C1D	2.20	123.95	116.07
29	B	846	BCR	C19-C18-C17	-2.20	115.55	119.01
36	U	1623	NEX	C12-C13-C14	-2.20	115.55	119.01
29	L	301	BCR	C36-C18-C17	-2.20	119.25	122.82
26	A	828	CLA	CMB-C2B-C3B	2.20	131.72	126.55
26	Y	603	CLA	C2A-C1A-CHA	2.20	127.69	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	810	CLA	CHD-C1D-ND	-2.20	121.71	124.80
26	5	604	CLA	CHB-C4A-NA	2.20	127.57	124.40
34	3	618	LUT	C15-C35-C34	-2.20	119.02	123.52
29	A	852	BCR	C19-C18-C17	2.20	122.47	119.01
26	5	608	CLA	C3B-C4B-NB	-2.20	108.57	110.53
26	8	606	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
26	B	812	CLA	CHB-C4A-NA	2.20	127.57	124.40
37	X	601	CHL	CED-O2D-CGD	2.20	120.90	115.92
26	6	609	CLA	C3B-C4B-NB	-2.20	108.57	110.53
35	8	620	XAT	C15-C35-C34	-2.20	119.02	123.52
34	1	617	LUT	C15-C35-C34	-2.20	119.02	123.52
37	U	608	CHL	O2D-CGD-O1D	-2.20	119.57	123.85
26	B	808	CLA	C3B-C4B-NB	-2.20	108.57	110.53
28	a	620	LHG	O7-C7-C8	2.20	116.23	111.48
29	L	301	BCR	C27-C26-C25	-2.20	119.74	122.70
35	2	620	XAT	C7-C8-C9	-2.20	122.12	125.53
26	B	819	CLA	CHB-C4A-NA	2.20	127.57	124.40
26	6	611	CLA	C3B-C4B-NB	-2.20	108.57	110.53
35	4	620	XAT	C19-C9-C8	2.20	121.44	118.09
26	A	834	CLA	CAA-CBA-CGA	-2.20	106.97	113.21
26	4	611	CLA	CMB-C2B-C1B	-2.20	122.08	125.42
26	A	814	CLA	CMB-C2B-C3B	2.20	131.71	126.55
26	B	831	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
29	J	102	BCR	C27-C26-C25	-2.19	119.74	122.70
26	A	833	CLA	O2D-CGD-CBD	2.19	115.07	111.23
37	W	608	CHL	C4C-CHD-C1D	2.19	123.92	116.07
26	5	619	CLA	O2D-CGD-CBD	2.19	115.06	111.23
35	1	618	XAT	C32-C33-C34	-2.19	115.56	119.01
37	V	607	CHL	CED-O2D-CGD	2.19	120.89	115.92
35	6	621	XAT	C35-C15-C14	-2.19	119.03	123.52
26	B	839	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
26	6	620	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
26	9	610	CLA	C4-C3-C5	2.19	119.03	115.23
26	5	614	CLA	C3B-C4B-NB	-2.19	108.57	110.53
26	6	604	CLA	CHB-C4A-NA	2.19	127.56	124.40
26	8	601	CLA	CHB-C4A-NA	2.19	127.56	124.40
26	A	827	CLA	C3B-C4B-NB	-2.19	108.57	110.53
26	7	612	CLA	C3B-C4B-NB	-2.19	108.57	110.53
26	8	604	CLA	C3B-C4B-NB	-2.19	108.57	110.53
26	Z	610	CLA	CHB-C1B-NB	2.19	127.33	124.05
29	B	846	BCR	C15-C14-C13	-2.19	124.21	127.28
29	2	623	BCR	C16-C15-C14	-2.19	119.04	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	602	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
26	A	832	CLA	O2D-CGD-CBD	2.19	115.06	111.23
26	9	602	CLA	C3B-C4B-NB	-2.19	108.58	110.53
26	5	611	CLA	CHB-C4A-NA	2.19	127.56	124.40
26	W	602	CLA	CHB-C4A-NA	2.19	127.56	124.40
29	9	621	BCR	C33-C5-C4	2.19	118.26	113.60
26	A	840	CLA	CHB-C4A-NA	2.19	127.56	124.40
29	6	622	BCR	C24-C25-C26	-2.19	116.52	121.56
35	Y	1622	XAT	C18-C5-C4	2.19	116.70	114.24
26	F	303	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
29	B	844	BCR	C39-C30-C25	2.19	113.67	110.24
34	Z	1621	LUT	C18-C5-C6	-2.18	122.10	124.48
26	A	812	CLA	CHD-C1D-ND	-2.18	121.73	124.80
26	K	204	CLA	C3B-C4B-NB	-2.18	108.58	110.53
34	V	1621	LUT	C38-C25-C24	-2.18	118.19	123.36
26	B	811	CLA	O1D-CGD-CBD	2.18	127.48	120.19
26	B	804	CLA	C3B-C4B-NB	-2.18	108.58	110.53
28	1	620	LHG	O7-C7-C8	2.18	116.20	111.48
34	U	1621	LUT	C27-C28-C29	-2.18	121.63	126.32
29	7	623	BCR	C37-C22-C21	-2.18	119.28	122.82
26	5	608	CLA	CHB-C4A-NA	2.18	127.55	124.40
37	Y	607	CHL	O1D-CGD-CBD	-2.18	121.41	124.72
34	8	619	LUT	C36-C21-C26	2.18	112.85	109.55
26	8	610	CLA	C6-C5-C3	2.18	118.78	113.47
29	B	801	BCR	C30-C25-C26	-2.18	119.66	122.64
26	A	814	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
26	5	617	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
26	A	854	CLA	O1D-CGD-CBD	2.18	128.82	124.52
26	B	809	CLA	O1D-CGD-CBD	2.18	128.82	124.52
26	Y	613	CLA	CAC-C3C-C4C	2.18	127.62	124.79
35	2	620	XAT	C4-C3-C2	-2.18	106.72	110.79
26	A	818	CLA	CMB-C2B-C3B	2.18	131.67	126.55
26	9	603	CLA	CMB-C2B-C3B	2.18	129.32	123.53
26	a	610	CLA	C1-C2-C3	-2.18	122.63	126.20
26	8	609	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
37	U	601	CHL	C4C-CHD-C1D	2.18	123.86	116.07
29	3	622	BCR	C33-C5-C4	2.18	118.24	113.60
26	A	829	CLA	C3B-C4B-NB	-2.18	108.59	110.53
26	6	601	CLA	C3B-C4B-NB	-2.17	108.59	110.53
26	B	819	CLA	CMB-C2B-C3B	2.17	131.66	126.55
37	Y	606	CHL	O2D-CGD-O1D	-2.17	119.62	123.85
36	Z	1623	NEX	C11-C12-C13	-2.17	120.40	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	611	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
37	X	607	CHL	C1-C2-C3	-2.17	122.64	126.20
26	U	604	CLA	CBD-CHA-C1A	2.17	131.61	127.58
26	K	203	CLA	C1-C2-C3	-2.17	122.64	126.20
26	B	838	CLA	CHB-C4A-NA	2.17	127.53	124.40
37	X	609	CHL	C1-C2-C3	-2.17	122.64	126.20
35	8	620	XAT	C30-C31-C32	-2.17	116.91	123.20
26	O	2003	CLA	CHB-C4A-NA	2.17	127.53	124.40
26	Z	603	CLA	C2A-C1A-CHA	2.17	127.63	123.87
35	4	620	XAT	C37-C21-C36	-2.17	104.22	107.37
34	9	619	LUT	C17-C1-C6	-2.17	106.84	110.24
29	F	305	BCR	C35-C13-C12	2.17	121.40	118.09
26	B	825	CLA	CMB-C2B-C3B	2.17	131.65	126.55
26	L	302	CLA	CHB-C4A-NA	2.17	127.53	124.40
35	W	1622	XAT	C30-C31-C32	-2.17	116.92	123.20
36	X	1623	NEX	O24-C25-C26	-2.17	57.21	58.93
35	W	1622	XAT	O4-C5-C6	-2.17	57.21	58.93
26	3	606	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
26	A	829	CLA	C4-C3-C5	2.17	118.99	115.23
34	9	619	LUT	C30-C31-C32	-2.17	116.93	123.20
26	A	828	CLA	CHB-C4A-NA	2.16	127.52	124.40
29	7	623	BCR	C15-C14-C13	-2.16	124.24	127.28
37	X	608	CHL	CAC-C3C-C4C	2.16	129.59	124.03
26	6	613	CLA	CHD-C1D-ND	-2.16	121.76	124.80
26	A	813	CLA	CHB-C4A-NA	2.16	127.52	124.40
26	3	615	CLA	CHB-C4A-NA	2.16	127.52	124.40
26	A	825	CLA	O1D-CGD-CBD	2.16	128.78	124.52
29	3	621	BCR	C4-C5-C6	2.16	125.63	122.70
29	L	301	BCR	C1-C6-C5	-2.16	119.68	122.64
26	1	611	CLA	CHB-C4A-NA	2.16	127.52	124.40
26	H	202	CLA	O2D-CGD-O1D	-2.16	119.17	124.08
32	4	623	LMG	C6-C5-C4	-2.16	107.71	113.02
37	Y	608	CHL	C4C-CHD-C1D	2.16	123.80	116.07
37	W	608	CHL	CMA-C3A-C4A	-2.16	109.95	114.61
34	W	1621	LUT	C38-C25-C24	-2.16	118.25	123.36
37	W	608	CHL	CAC-C3C-C4C	2.16	129.59	124.03
26	A	842	CLA	CHB-C1B-NB	2.16	127.29	124.05
29	B	844	BCR	C2-C1-C6	-2.16	107.30	110.44
26	B	829	CLA	CHC-C1C-NC	2.16	127.56	124.31
26	3	613	CLA	CHB-C4A-NA	2.16	127.52	124.40
37	W	606	CHL	CAA-C2A-C3A	-2.16	107.16	113.00
26	U	602	CLA	CHB-C4A-NA	2.16	127.52	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	W	610	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
26	A	828	CLA	CAA-CBA-CGA	-2.16	107.08	113.21
26	a	602	CLA	O1D-CGD-CBD	2.16	128.77	124.52
35	3	619	XAT	C35-C15-C14	-2.16	119.10	123.52
37	Z	609	CHL	CMD-C2D-C3D	-2.16	120.37	124.68
26	B	805	CLA	O1D-CGD-CBD	2.16	128.77	124.52
34	W	1620	LUT	C11-C12-C13	-2.16	120.45	126.36
26	4	616	CLA	CMB-C2B-C3B	2.16	129.26	123.53
26	A	806	CLA	CMB-C2B-C3B	2.16	131.62	126.55
29	7	621	BCR	C24-C23-C22	-2.16	123.05	126.23
29	A	856	BCR	C16-C15-C14	-2.16	119.11	123.52
26	8	606	CLA	CHB-C4A-NA	2.16	127.51	124.40
26	6	608	CLA	CHD-C1D-ND	-2.15	121.77	124.80
26	3	602	CLA	O1D-CGD-CBD	2.15	128.77	124.52
26	6	616	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
36	5	624	NEX	C35-C15-C14	-2.15	119.11	123.52
28	Y	2630	LHG	C26-C25-C24	-2.15	105.21	113.13
29	B	852	BCR	C27-C26-C25	-2.15	119.79	122.70
35	3	619	XAT	C12-C13-C14	-2.15	115.62	119.01
29	K	207	BCR	C11-C12-C13	-2.15	120.46	126.36
26	A	820	CLA	C3B-C4B-NB	-2.15	108.61	110.53
26	3	606	CLA	C3B-C4B-NB	-2.15	108.61	110.53
37	W	607	CHL	C4C-CHD-C1D	2.15	123.77	116.07
36	V	1623	NEX	C30-C31-C32	-2.15	116.97	123.20
29	A	848	BCR	C28-C27-C26	-2.15	110.22	114.06
34	3	618	LUT	C15-C14-C13	-2.15	124.26	127.28
26	7	611	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
29	B	843	BCR	C20-C19-C18	-2.15	120.47	126.36
26	F	303	CLA	CHB-C4A-NA	2.15	127.50	124.40
36	V	1623	NEX	O24-C25-C26	-2.15	57.23	58.93
29	A	850	BCR	C7-C8-C9	-2.15	123.05	126.23
26	X	613	CLA	CAC-C3C-C4C	2.15	127.59	124.79
26	U	602	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
26	B	803	CLA	CMB-C2B-C3B	2.15	131.60	126.55
26	B	824	CLA	C3B-C4B-NB	-2.15	108.61	110.53
26	1	610	CLA	C3B-C4B-NB	-2.15	108.61	110.53
26	Z	603	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
34	Z	1621	LUT	C38-C25-C24	-2.15	118.28	123.36
29	B	846	BCR	C21-C20-C19	-2.15	116.97	123.20
26	1	607	CLA	CHB-C4A-NA	2.15	127.50	124.40
26	2	610	CLA	CHB-C4A-NA	2.15	127.50	124.40
35	3	619	XAT	C18-C5-C4	2.15	116.65	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	2	623	BCR	C36-C18-C19	2.15	121.37	118.09
29	F	305	BCR	C23-C24-C25	-2.15	121.27	127.00
26	X	604	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
29	9	621	BCR	C15-C14-C13	-2.15	124.27	127.28
28	U	2630	LHG	C6-C5-C4	-2.15	106.78	111.78
26	F	304	CLA	CMA-C3A-C2A	-2.14	111.31	116.23
29	A	852	BCR	C27-C26-C25	-2.14	119.81	122.70
26	3	602	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
26	Z	604	CLA	CHB-C4A-NA	2.14	127.49	124.40
26	B	840	CLA	C1-C2-C3	-2.14	122.69	126.20
29	B	846	BCR	C37-C22-C21	-2.14	119.34	122.82
37	W	608	CHL	O2D-CGD-O1D	-2.14	119.68	123.85
26	Z	602	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
26	7	601	CLA	C3B-C4B-NB	-2.14	108.62	110.53
26	A	817	CLA	CAC-C3C-C4C	2.14	127.57	124.79
37	Z	601	CHL	C4C-CHD-C1D	2.14	123.72	116.07
26	Z	610	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
35	9	620	XAT	C4-C3-C2	-2.14	106.79	110.79
26	B	840	CLA	CHB-C4A-NA	2.14	127.49	124.40
26	A	834	CLA	CMB-C2B-C3B	2.14	131.58	126.55
34	W	1621	LUT	C37-C21-C26	-2.14	106.31	109.55
35	6	621	XAT	C15-C35-C34	-2.14	119.14	123.52
26	A	836	CLA	O1D-CGD-CBD	2.14	128.74	124.52
26	B	824	CLA	O1D-CGD-CBD	2.14	128.74	124.52
35	5	621	XAT	C19-C9-C8	2.14	121.35	118.09
29	L	308	BCR	C20-C21-C22	2.14	130.28	127.28
26	B	811	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
26	A	833	CLA	CBA-CAA-C2A	2.14	120.15	113.79
36	Y	1623	NEX	C30-C31-C32	-2.14	117.01	123.20
29	A	852	BCR	C16-C17-C18	-2.14	124.28	127.28
26	4	609	CLA	C1-C2-C3	-2.14	122.70	126.20
34	6	619	LUT	C15-C35-C34	-2.14	119.15	123.52
26	A	801	CLA	CHB-C4A-NA	2.14	127.48	124.40
26	G	204	CLA	C3B-C4B-NB	-2.14	108.62	110.53
28	4	622	LHG	O8-C23-C24	2.14	118.35	111.83
29	1	619	BCR	C24-C23-C22	-2.14	123.08	126.23
29	A	852	BCR	C16-C15-C14	-2.14	119.15	123.52
26	Y	613	CLA	C1-C2-C3	-2.14	122.70	126.20
35	6	621	XAT	C24-C23-C22	-2.13	106.80	110.79
34	U	1621	LUT	C38-C25-C24	-2.13	118.31	123.36
35	Y	1622	XAT	C7-C8-C9	-2.13	122.22	125.53
26	9	612	CLA	CHB-C4A-NA	2.13	127.48	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	L	307	CLA	CMB-C2B-C3B	2.13	131.57	126.55
26	A	821	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
26	B	803	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
34	W	1621	LUT	C31-C32-C33	-2.13	120.51	126.36
29	5	622	BCR	C15-C14-C13	-2.13	124.29	127.28
31	5	628	LMU	O5B-C5B-C4B	2.13	113.54	109.70
26	6	602	CLA	O2D-CGD-CBD	2.13	114.96	111.23
26	2	614	CLA	CHB-C4A-NA	2.13	127.48	124.40
26	B	828	CLA	CHB-C4A-NA	2.13	127.48	124.40
29	7	623	BCR	C30-C25-C26	-2.13	119.72	122.64
26	A	814	CLA	C6-C5-C3	2.13	118.66	113.47
26	U	604	CLA	C3B-C4B-NB	-2.13	108.63	110.53
29	K	202	BCR	C16-C15-C14	-2.13	119.16	123.52
29	F	305	BCR	C30-C25-C24	2.13	121.43	115.65
26	5	609	CLA	C3B-C4B-NB	-2.13	108.63	110.53
26	5	609	CLA	CHD-C1D-ND	-2.13	121.81	124.80
26	4	602	CLA	CHB-C1B-NB	2.13	127.24	124.05
26	3	604	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
26	W	610	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
34	7	619	LUT	C27-C28-C29	-2.13	121.75	126.32
35	V	1622	XAT	C11-C12-C13	-2.13	120.53	126.36
29	A	856	BCR	C30-C25-C26	-2.13	119.73	122.64
26	3	611	CLA	CMB-C2B-C3B	2.13	129.19	123.53
29	A	848	BCR	C27-C26-C25	2.13	125.58	122.70
29	K	207	BCR	C28-C29-C30	-2.13	106.90	114.43
26	L	303	CLA	CHD-C1D-ND	-2.13	121.81	124.80
26	B	829	CLA	CAA-CBA-CGA	-2.13	107.17	113.21
26	2	614	CLA	C3B-C4B-NB	-2.13	108.63	110.53
26	A	818	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
26	A	803	CLA	CMB-C2B-C3B	2.12	131.55	126.55
34	7	619	LUT	C38-C25-C24	-2.12	118.33	123.36
26	8	616	CLA	O2A-CGA-O1A	-2.12	117.87	123.33
34	Z	1621	LUT	C35-C15-C14	-2.12	119.17	123.52
26	Z	611	CLA	CHB-C4A-NA	2.12	127.46	124.40
26	4	603	CLA	CMB-C2B-C3B	2.12	129.17	123.53
37	V	609	CHL	CMD-C2D-C3D	-2.12	120.44	124.68
26	7	602	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
34	U	1620	LUT	C31-C30-C29	-2.12	124.30	127.28
34	Z	1620	LUT	C10-C11-C12	-2.12	117.05	123.20
26	a	610	CLA	C3B-C4B-NB	-2.12	108.64	110.53
26	2	601	CLA	CHB-C4A-NA	2.12	127.46	124.40
34	9	619	LUT	C28-C29-C30	-2.12	115.67	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	U	606	CHL	CAC-C3C-C4C	2.12	129.48	124.03
37	X	601	CHL	CAA-C2A-C3A	-2.12	107.27	113.00
26	V	610	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
26	A	809	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
35	1	618	XAT	O24-C25-C26	-2.12	57.25	58.93
26	B	806	CLA	C6-C5-C3	2.12	118.63	113.47
26	B	813	CLA	O1D-CGD-CBD	2.12	128.69	124.52
26	5	611	CLA	C3B-C4B-NB	-2.12	108.64	110.53
37	Z	606	CHL	C1C-C2C-CMC	2.12	130.62	126.80
34	Y	1620	LUT	C39-C29-C28	2.12	121.32	118.09
32	5	627	LMG	C8-O7-C10	-2.12	112.73	117.80
26	B	821	CLA	CHB-C4A-NA	2.12	127.45	124.40
29	B	849	BCR	C15-C14-C13	-2.12	124.31	127.28
29	B	845	BCR	C21-C20-C19	-2.12	117.07	123.20
34	2	619	LUT	C30-C31-C32	-2.12	117.07	123.20
26	7	602	CLA	C1-C2-C3	-2.12	122.73	126.20
26	8	604	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
26	A	836	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
26	7	615	CLA	CBD-CHA-C1A	2.11	131.50	127.58
26	3	612	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
37	W	607	CHL	C6-C5-C3	-2.11	108.32	113.47
37	Z	608	CHL	CMD-C2D-C3D	-2.11	120.46	124.68
29	B	847	BCR	C1-C6-C7	2.11	121.38	115.65
37	Y	608	CHL	O2D-CGD-O1D	-2.11	119.74	123.85
26	A	801	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
26	B	803	CLA	C3B-C4B-NB	-2.11	108.64	110.53
34	X	1620	LUT	C38-C25-C24	-2.11	118.36	123.36
29	K	202	BCR	C23-C24-C25	-2.11	121.36	127.00
26	W	603	CLA	CMB-C2B-C3B	2.11	131.51	126.55
35	W	1622	XAT	C15-C35-C34	-2.11	119.20	123.52
26	9	604	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
35	U	1622	XAT	O4-C5-C6	-2.11	57.26	58.93
35	Y	1622	XAT	O4-C5-C6	-2.11	57.26	58.93
26	B	828	CLA	C3B-C4B-NB	-2.11	108.65	110.53
26	X	612	CLA	C2A-C1A-CHA	2.11	127.53	123.87
34	V	1620	LUT	C21-C26-C27	-2.11	110.40	112.83
26	A	833	CLA	CHD-C1D-ND	-2.11	121.84	124.80
36	Y	1623	NEX	O24-C25-C26	-2.11	57.26	58.93
35	6	621	XAT	C37-C21-C26	-2.11	104.36	110.05
26	A	809	CLA	O2D-CGD-CBD	2.11	114.91	111.23
26	4	607	CLA	CHB-C4A-NA	2.11	127.44	124.40
29	B	846	BCR	C32-C1-C6	-2.10	106.94	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	W	612	CLA	C2A-C1A-CHA	2.10	127.52	123.87
26	8	608	CLA	CMB-C2B-C1B	-2.10	122.21	125.42
26	Y	614	CLA	C3B-C4B-NB	-2.10	108.65	110.53
26	3	609	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
26	B	820	CLA	C1-C2-C3	-2.10	123.36	126.76
35	5	621	XAT	C4-C3-C2	-2.10	106.86	110.79
26	9	602	CLA	CHB-C4A-NA	2.10	127.44	124.40
35	a	618	XAT	O24-C25-C26	-2.10	57.26	58.93
26	B	834	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
29	7	623	BCR	C11-C12-C13	-2.10	120.60	126.36
34	Y	1621	LUT	C21-C26-C27	-2.10	110.41	112.83
26	V	604	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
26	B	827	CLA	CMB-C2B-C3B	2.10	131.49	126.55
29	B	847	BCR	C40-C30-C25	-2.10	106.95	110.24
26	U	603	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
37	X	601	CHL	O1D-CGD-CBD	-2.10	121.54	124.72
34	4	619	LUT	C38-C25-C24	-2.10	118.39	123.36
26	A	854	CLA	C11-C10-C8	-2.10	108.98	115.97
37	Y	606	CHL	CMA-C3A-C4A	-2.10	110.08	114.61
26	A	831	CLA	CHB-C4A-NA	2.10	127.43	124.40
26	B	835	CLA	CHB-C4A-NA	2.10	127.43	124.40
26	1	613	CLA	CHB-C4A-NA	2.10	127.43	124.40
35	2	620	XAT	O4-C5-C6	-2.10	57.26	58.93
26	B	827	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
28	X	2630	LHG	C5-O7-C7	-2.10	112.77	117.80
34	U	1620	LUT	C30-C31-C32	-2.10	117.12	123.20
35	6	621	XAT	C15-C14-C13	-2.10	124.33	127.28
26	2	602	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
26	A	821	CLA	C3B-C4B-NB	-2.10	108.66	110.53
26	4	609	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
34	4	619	LUT	C36-C21-C26	2.10	112.72	109.55
26	B	806	CLA	CMC-C2C-C1C	-2.10	121.76	125.03
29	B	845	BCR	C30-C25-C26	-2.10	119.77	122.64
35	9	620	XAT	C24-C23-C22	-2.10	106.87	110.79
37	Z	605	CHL	OMC-CMC-C2C	-2.09	121.48	125.12
37	Y	609	CHL	CAA-C2A-C3A	-2.09	107.34	113.00
29	A	856	BCR	C15-C16-C17	-2.09	119.24	123.52
34	X	1620	LUT	C39-C29-C28	2.09	121.28	118.09
28	7	622	LHG	O8-C23-C24	2.09	118.21	111.83
26	a	607	CLA	CHB-C4A-NA	2.09	127.42	124.40
37	V	607	CHL	C4C-CHD-C1D	2.09	123.55	116.07
29	A	848	BCR	C23-C22-C21	2.09	122.30	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	X	611	CLA	C3B-C4B-NB	-2.09	108.66	110.53
26	A	836	CLA	C1-C2-C3	-2.09	122.77	126.20
26	A	805	CLA	C4-C3-C2	-2.09	118.26	123.63
26	O	2001	CLA	CHB-C4A-NA	2.09	127.42	124.40
26	4	606	CLA	CHB-C4A-NA	2.09	127.42	124.40
26	7	611	CLA	O1D-CGD-CBD	2.09	128.64	124.52
29	a	619	BCR	C24-C23-C22	-2.09	123.14	126.23
37	Z	601	CHL	C1C-C2C-CMC	2.09	130.57	126.80
37	X	609	CHL	CAC-C3C-C4C	2.09	129.40	124.03
26	U	603	CLA	CHA-C1A-NA	-2.09	121.66	126.39
26	A	840	CLA	CMB-C2B-C3B	2.09	131.46	126.55
26	5	607	CLA	O2D-CGD-CBD	2.09	114.88	111.23
37	U	606	CHL	C4C-CHD-C1D	2.09	123.54	116.07
36	V	1623	NEX	C40-C33-C32	2.09	121.28	118.09
26	1	609	CLA	CMB-C2B-C3B	2.09	129.08	123.53
26	B	836	CLA	O1D-CGD-CBD	2.09	128.64	124.52
26	A	854	CLA	CMD-C2D-C3D	2.09	132.48	127.69
37	Y	601	CHL	C1C-C2C-CMC	2.09	130.56	126.80
29	J	102	BCR	C7-C6-C5	2.09	126.36	121.56
32	H	205	LMG	O7-C10-O9	-2.09	118.83	123.70
34	X	1621	LUT	C38-C25-C24	-2.09	118.42	123.36
34	4	619	LUT	C17-C1-C6	-2.09	106.97	110.24
26	A	817	CLA	C3B-C4B-NB	-2.09	108.67	110.53
29	B	801	BCR	C7-C8-C9	-2.09	123.15	126.23
34	1	617	LUT	C12-C13-C14	-2.08	115.73	119.01
29	J	102	BCR	C2-C1-C6	2.08	113.47	110.44
26	A	843	CLA	C11-C12-C13	-2.08	109.04	115.97
35	9	620	XAT	C7-C8-C9	-2.08	122.30	125.53
34	6	619	LUT	C36-C21-C26	2.08	112.70	109.55
26	4	603	CLA	O2A-CGA-O1A	-2.08	117.97	123.33
26	2	601	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
26	W	604	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
29	5	622	BCR	C15-C16-C17	-2.08	119.25	123.52
26	B	810	CLA	O2D-CGD-CBD	2.08	114.87	111.23
26	B	832	CLA	C6-C5-C3	2.08	118.54	113.47
37	V	609	CHL	C4C-CHD-C1D	2.08	123.52	116.07
26	Y	610	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
29	K	202	BCR	C36-C18-C17	-2.08	119.44	122.82
26	4	608	CLA	CAC-C3C-C4C	2.08	127.50	124.79
29	B	849	BCR	C36-C18-C17	-2.08	119.44	122.82
37	W	608	CHL	O2A-CGA-CBA	2.08	120.00	112.14
26	A	826	CLA	CHB-C4A-NA	2.08	127.40	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	828	CLA	CAA-C2A-C1A	-2.08	105.16	111.97
37	V	607	CHL	CAC-C3C-C4C	2.08	129.38	124.03
26	Y	603	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
26	V	612	CLA	CAA-C2A-C3A	-2.08	107.38	113.00
26	Y	614	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
36	6	624	NEX	C17-C1-C6	-2.08	108.61	110.47
26	B	841	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
29	8	621	BCR	C24-C25-C26	-2.08	116.77	121.56
26	B	834	CLA	O2D-CGD-CBD	2.08	114.86	111.23
26	1	607	CLA	CAA-C2A-C3A	-2.08	111.46	116.23
28	7	622	LHG	P-O6-C4	-2.08	109.44	121.35
26	3	610	CLA	CHB-C1B-NB	2.08	127.17	124.05
32	H	205	LMG	O5-C6-C5	-2.08	104.26	111.33
26	5	616	CLA	O2A-CGA-O1A	-2.08	117.99	123.33
26	A	810	CLA	CHA-C1A-NA	-2.08	121.69	126.39
29	2	623	BCR	C30-C25-C24	2.08	121.29	115.65
26	B	811	CLA	C4-C3-C2	-2.08	118.29	123.63
26	7	613	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
29	A	851	BCR	C10-C11-C12	-2.08	117.18	123.20
34	U	1620	LUT	C27-C28-C29	-2.08	121.86	126.32
26	U	612	CLA	C3B-C4B-NB	-2.08	108.68	110.53
26	U	610	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
37	Y	606	CHL	CED-O2D-CGD	2.08	120.63	115.92
37	X	608	CHL	C4C-CHD-C1D	2.08	123.50	116.07
26	a	613	CLA	CHB-C4A-NA	2.08	127.40	124.40
35	X	1622	XAT	C18-C5-C4	2.08	116.57	114.24
26	A	839	CLA	O2D-CGD-CBD	2.08	114.86	111.23
29	5	622	BCR	C7-C8-C9	-2.08	123.17	126.23
37	X	608	CHL	CMA-C3A-C4A	-2.08	110.14	114.61
32	H	205	LMG	C9-C8-C7	-2.07	106.95	111.78
26	A	804	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
26	B	836	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
26	1	610	CLA	CMB-C2B-C3B	2.07	131.43	126.55
26	8	602	CLA	O2D-CGD-CBD	2.07	114.85	111.23
34	2	619	LUT	C11-C12-C13	-2.07	120.68	126.36
26	A	839	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
29	A	856	BCR	C1-C6-C5	-2.07	119.80	122.64
26	B	829	CLA	O1D-CGD-CBD	2.07	128.60	124.52
34	X	1621	LUT	C28-C29-C30	-2.07	115.75	119.01
36	5	624	NEX	C10-C11-C12	-2.07	117.20	123.20
26	7	610	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
26	a	610	CLA	CMB-C2B-C3B	2.07	131.42	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	9	601	CLA	C3B-C4B-NB	-2.07	108.68	110.53
32	8	626	LMG	O7-C10-O9	-2.07	118.86	123.70
34	a	617	LUT	C12-C13-C14	-2.07	115.75	119.01
34	7	619	LUT	C11-C10-C9	-2.07	124.38	127.28
26	X	604	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
26	B	813	CLA	CHB-C4A-NA	2.07	127.39	124.40
26	3	606	CLA	CHC-C4B-NB	2.07	127.15	124.05
37	Z	606	CHL	CAC-C3C-C4C	2.07	129.35	124.03
26	7	611	CLA	C3B-C4B-NB	-2.07	108.68	110.53
35	4	620	XAT	C36-C21-C26	2.07	115.63	110.05
26	V	612	CLA	O2D-CGD-CBD	2.07	114.84	111.23
26	A	838	CLA	O1D-CGD-CBD	2.07	128.60	124.52
26	B	833	CLA	CHD-C1D-ND	-2.07	121.89	124.80
34	V	1620	LUT	C11-C12-C13	-2.07	120.69	126.36
26	1	604	CLA	O1D-CGD-CBD	2.07	128.59	124.52
34	6	619	LUT	C38-C25-C24	-2.07	118.47	123.36
29	F	305	BCR	C29-C30-C25	2.07	113.44	110.44
26	5	602	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
26	B	808	CLA	C11-C10-C8	-2.07	109.10	115.97
26	W	602	CLA	O2D-CGD-CBD	2.07	114.84	111.23
26	A	826	CLA	O1D-CGD-CBD	2.07	128.59	124.52
34	W	1621	LUT	C7-C8-C9	-2.07	123.18	126.23
26	B	825	CLA	O1D-CGD-CBD	2.07	128.59	124.52
26	X	610	CLA	CHB-C1B-C2B	-2.06	121.43	127.43
37	U	609	CHL	C4C-CHD-C1D	2.06	123.45	116.07
37	X	601	CHL	C4C-CHD-C1D	2.06	123.45	116.07
26	W	604	CLA	CHB-C1B-NB	2.06	127.14	124.05
26	A	801	CLA	C2A-C1A-CHA	2.06	127.45	123.87
29	L	309	BCR	C15-C16-C17	-2.06	119.30	123.52
26	W	611	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
28	W	2630	LHG	C5-O7-C7	-2.06	112.86	117.80
37	W	601	CHL	C4C-CHD-C1D	2.06	123.45	116.07
26	6	617	CLA	O1D-CGD-CBD	2.06	128.59	124.52
26	A	816	CLA	O1D-CGD-CBD	2.06	128.59	124.52
26	9	609	CLA	CHD-C1D-ND	-2.06	121.90	124.80
36	V	1623	NEX	C31-C30-C29	-2.06	124.39	127.28
37	Z	606	CHL	C4C-CHD-C1D	2.06	123.44	116.07
26	Z	610	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
26	5	616	CLA	CHB-C4A-NA	2.06	127.37	124.40
37	V	608	CHL	OBD-CAD-C3D	-2.06	124.68	127.89
26	a	610	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
31	A	857	LMU	C1B-C2B-C3B	2.06	114.34	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	620	CLA	C3B-C4B-NB	-2.06	108.69	110.53
26	B	837	CLA	CHD-C1D-ND	-2.06	121.90	124.80
32	J	103	LMG	O8-C28-O10	-2.06	118.48	123.63
31	5	629	LMU	O5'-C5'-C6'	2.06	111.54	106.44
37	U	607	CHL	C4C-CHD-C1D	2.06	123.44	116.07
29	A	851	BCR	C39-C30-C25	-2.06	107.01	110.24
37	V	605	CHL	OMC-CMC-C2C	-2.06	121.55	125.12
26	5	612	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
26	9	614	CLA	CHB-C4A-NA	2.06	127.37	124.40
35	Z	1622	XAT	C39-C29-C28	2.06	121.23	118.09
26	B	819	CLA	CHB-C1B-NB	2.06	127.14	124.05
26	1	614	CLA	CHC-C4B-NB	2.06	127.14	124.05
35	5	621	XAT	C38-C25-C24	2.06	116.55	114.24
26	W	610	CLA	O2D-CGD-CBD	2.06	114.83	111.23
26	7	604	CLA	O1D-CGD-CBD	2.06	128.57	124.52
26	6	614	CLA	CHB-C4A-NA	2.06	127.37	124.40
26	A	831	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
26	L	307	CLA	C3B-C4B-NB	-2.06	108.69	110.53
26	B	802	CLA	O1D-CGD-CBD	2.06	128.57	124.52
26	V	610	CLA	CAA-CBA-CGA	-2.06	107.37	113.21
29	3	622	BCR	C30-C25-C24	2.06	121.22	115.65
35	a	618	XAT	C20-C13-C12	2.05	121.23	118.09
37	Z	609	CHL	CAC-C3C-C4C	2.05	129.31	124.03
26	Z	610	CLA	O2D-CGD-CBD	2.05	114.82	111.23
29	L	301	BCR	C37-C22-C21	-2.05	119.49	122.82
26	B	812	CLA	O2D-CGD-CBD	2.05	114.82	111.23
26	Y	602	CLA	CMB-C2B-C3B	2.05	131.38	126.55
26	4	610	CLA	CMB-C2B-C3B	2.05	131.38	126.55
26	B	802	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
26	A	801	CLA	CHC-C4B-NB	2.05	127.13	124.05
26	B	839	CLA	CHB-C4A-NA	2.05	127.36	124.40
26	6	613	CLA	CHB-C1B-NB	2.05	127.13	124.05
37	Y	608	CHL	CED-O2D-CGD	2.05	120.57	115.92
26	A	808	CLA	CMB-C2B-C3B	2.05	131.38	126.55
26	a	602	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
26	A	831	CLA	O1D-CGD-CBD	2.05	128.56	124.52
26	A	839	CLA	CHB-C1B-NB	2.05	127.13	124.05
35	1	618	XAT	C20-C13-C12	2.05	121.22	118.09
35	X	1622	XAT	C31-C32-C33	-2.05	120.74	126.36
26	4	602	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
26	2	609	CLA	O2A-CGA-O1A	-2.05	118.06	123.33
26	A	827	CLA	CHB-C4A-NA	2.05	127.36	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	U	1621	LUT	C11-C12-C13	-2.05	120.74	126.36
26	A	830	CLA	C7-C6-C5	-2.05	107.80	113.26
35	a	618	XAT	C38-C25-C24	2.05	116.54	114.24
26	4	608	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
37	Z	609	CHL	C4C-CHD-C1D	2.05	123.40	116.07
35	V	1622	XAT	O4-C5-C6	-2.05	57.31	58.93
26	W	613	CLA	O2D-CGD-CBD	2.05	114.81	111.23
26	A	809	CLA	C3B-C4B-NB	-2.05	108.70	110.53
26	B	823	CLA	O2A-CGA-O1A	-2.05	118.07	123.33
26	3	602	CLA	CMB-C2B-C3B	2.05	131.37	126.55
34	Y	1621	LUT	C18-C5-C4	2.05	118.19	114.42
29	L	305	BCR	C36-C18-C17	-2.05	119.50	122.82
26	7	601	CLA	CHB-C4A-NA	2.05	127.35	124.40
32	J	103	LMG	C7-O1-C1	-2.05	109.41	113.80
26	3	613	CLA	C1-C2-C3	-2.05	122.84	126.20
37	V	601	CHL	C4-C3-C5	2.05	118.78	115.23
37	Y	605	CHL	CAC-C3C-C4C	2.05	129.29	124.03
35	1	618	XAT	C38-C25-C24	2.04	116.54	114.24
26	F	304	CLA	CHD-C1D-ND	-2.04	121.92	124.80
36	W	1623	NEX	C2-C1-C6	2.04	111.20	109.21
26	a	609	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
37	W	606	CHL	C4C-CHD-C1D	2.04	123.38	116.07
26	A	835	CLA	C7-C6-C5	-2.04	107.82	113.26
26	L	304	CLA	O2A-CGA-O1A	-2.04	118.08	123.33
34	6	619	LUT	C27-C28-C29	-2.04	121.93	126.32
26	W	602	CLA	C3B-C4B-NB	-2.04	108.71	110.53
29	B	853	BCR	C21-C20-C19	-2.04	117.28	123.20
34	U	1621	LUT	C15-C35-C34	-2.04	119.34	123.52
26	A	832	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
37	X	608	CHL	CMD-C2D-C3D	-2.04	121.09	124.94
26	A	830	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
26	9	612	CLA	C3B-C4B-NB	-2.04	108.71	110.53
37	V	608	CHL	C4C-CHD-C1D	2.04	123.37	116.07
35	2	620	XAT	C11-C10-C9	-2.04	124.42	127.28
37	X	608	CHL	O2D-CGD-O1D	-2.04	119.88	123.85
37	W	609	CHL	O2D-CGD-O1D	-2.04	119.88	123.85
34	7	619	LUT	C30-C31-C32	-2.04	117.29	123.20
29	K	207	BCR	C27-C26-C25	-2.04	119.95	122.70
37	Z	606	CHL	CMD-C2D-C3D	-2.04	120.61	124.68
29	A	848	BCR	C1-C6-C5	-2.04	119.85	122.64
35	5	621	XAT	C35-C15-C14	-2.04	119.34	123.52
26	L	302	CLA	O2D-CGD-CBD	2.04	114.80	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	3	618	LUT	C1-C6-C5	-2.04	119.85	122.64
26	6	617	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
37	W	609	CHL	CAC-C3C-C4C	2.04	129.27	124.03
26	1	602	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
29	F	305	BCR	C27-C26-C25	-2.04	119.95	122.70
29	A	852	BCR	C29-C30-C25	2.04	113.40	110.44
26	1	608	CLA	O2A-CGA-O1A	-2.04	118.09	123.33
29	A	848	BCR	C11-C12-C13	-2.04	120.78	126.36
26	B	816	CLA	C6-C5-C3	2.04	118.43	113.47
26	B	810	CLA	C2A-C1A-CHA	2.04	127.40	123.87
26	a	604	CLA	O1D-CGD-CBD	2.04	128.53	124.52
29	L	308	BCR	C15-C16-C17	-2.04	119.35	123.52
26	A	804	CLA	C3B-C4B-NB	-2.04	108.71	110.53
26	1	610	CLA	C2A-C1A-CHA	2.04	125.87	122.71
35	2	620	XAT	C19-C9-C8	2.04	121.20	118.09
35	7	620	XAT	O4-C5-C6	-2.03	57.32	58.93
26	A	824	CLA	CHD-C1D-ND	-2.03	121.94	124.80
26	Z	613	CLA	C3B-C4B-NB	-2.03	108.71	110.53
26	6	602	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
26	1	610	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
26	1	616	CLA	C3B-C4B-NB	-2.03	108.22	110.33
26	a	608	CLA	O2A-CGA-O1A	-2.03	118.10	123.33
34	1	617	LUT	C27-C28-C29	-2.03	121.95	126.32
28	2	622	LHG	C6-C5-C4	-2.03	107.04	111.78
26	B	833	CLA	C3B-C4B-NB	-2.03	108.72	110.53
26	Z	602	CLA	C1-C2-C3	-2.03	122.87	126.20
33	B	850	DGD	C1D-C2D-C3D	2.03	114.28	110.01
26	7	602	CLA	O1D-CGD-CBD	2.03	128.53	124.52
26	A	802	CLA	C3B-C4B-NB	-2.03	108.72	110.53
26	A	826	CLA	C3B-C4B-NB	-2.03	108.72	110.53
26	6	612	CLA	CHB-C4A-NA	2.03	127.33	124.40
26	5	603	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
26	3	607	CLA	CHD-C1D-ND	-2.03	121.94	124.80
26	5	613	CLA	CHD-C1D-ND	-2.03	121.94	124.80
34	a	617	LUT	C27-C28-C29	-2.03	121.95	126.32
34	2	619	LUT	C22-C23-C24	2.03	114.20	111.18
35	6	621	XAT	C7-C8-C9	-2.03	122.38	125.53
36	V	1623	NEX	C38-C25-C24	2.03	116.52	114.24
37	W	607	CHL	CMB-C2B-C3B	2.03	128.74	124.68
26	U	602	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
37	Y	609	CHL	CAC-C3C-C4C	2.03	129.25	124.03
29	L	309	BCR	C12-C13-C14	-2.03	115.82	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	3	621	BCR	C39-C30-C25	2.03	113.42	110.24
26	5	613	CLA	C4-C3-C2	-2.03	118.42	123.63
35	8	620	XAT	C31-C32-C33	-2.03	120.80	126.36
29	K	207	BCR	C16-C15-C14	-2.03	119.37	123.52
35	2	620	XAT	C39-C29-C28	2.03	121.19	118.09
26	7	611	CLA	CHC-C4B-NB	2.03	127.09	124.05
37	V	605	CHL	C4C-CHD-C1D	2.03	123.32	116.07
26	2	603	CLA	CAC-C3C-C4C	2.03	127.43	124.79
29	3	621	BCR	C11-C12-C13	-2.03	120.81	126.36
26	3	610	CLA	O1D-CGD-CBD	2.03	128.51	124.52
26	A	807	CLA	CHB-C1B-NB	2.03	127.09	124.05
29	3	622	BCR	C4-C5-C6	-2.03	119.97	122.70
29	B	847	BCR	C30-C25-C24	2.03	121.15	115.65
26	2	610	CLA	C4-C3-C5	2.03	118.74	115.23
26	K	201	CLA	O2A-CGA-O1A	-2.03	118.12	123.33
37	U	608	CHL	C4C-CHD-C1D	2.03	123.31	116.07
37	X	607	CHL	C4C-CHD-C1D	2.03	123.31	116.07
29	8	621	BCR	C30-C25-C24	2.03	121.14	115.65
26	A	834	CLA	O1D-CGD-CBD	2.02	128.51	124.52
35	5	621	XAT	O4-C5-C6	-2.02	57.32	58.93
36	V	1623	NEX	C10-C11-C12	-2.02	117.33	123.20
26	A	854	CLA	C1-C2-C3	-2.02	122.88	126.20
34	9	619	LUT	C12-C13-C14	-2.02	115.83	119.01
26	4	614	CLA	CHB-C4A-NA	2.02	127.32	124.40
29	B	844	BCR	C1-C6-C7	2.02	121.14	115.65
26	3	603	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
26	A	814	CLA	O1D-CGD-CBD	2.02	128.51	124.52
35	X	1622	XAT	O24-C25-C26	-2.02	57.33	58.93
35	1	618	XAT	O4-C5-C6	-2.02	57.33	58.93
26	1	606	CLA	CHB-C4A-NA	2.02	127.32	124.40
29	O	2004	BCR	C38-C26-C25	-2.02	122.28	124.48
34	9	619	LUT	C38-C25-C24	-2.02	118.58	123.36
26	2	613	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
29	A	856	BCR	C11-C12-C13	-2.02	120.82	126.36
26	7	614	CLA	CHC-C4B-NB	2.02	127.08	124.05
26	Y	604	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
26	3	603	CLA	CAC-C3C-C4C	2.02	127.42	124.79
29	3	622	BCR	C1-C6-C7	2.02	121.13	115.65
29	B	845	BCR	C32-C1-C6	-2.02	107.08	110.24
34	a	617	LUT	C30-C31-C32	-2.02	117.35	123.20
26	3	604	CLA	C3B-C4B-NB	-2.02	108.73	110.53
29	B	848	BCR	C37-C22-C21	2.02	126.09	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	616	CLA	C1-C2-C3	-2.02	122.89	126.20
26	Z	603	CLA	O2D-CGD-CBD	2.02	114.76	111.23
26	a	614	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
29	L	301	BCR	C32-C1-C6	-2.02	107.08	110.24
37	V	606	CHL	C4C-CHD-C1D	2.02	123.29	116.07
26	2	607	CLA	O2A-CGA-O1A	-2.02	118.14	123.33
37	Z	606	CHL	CED-O2D-CGD	2.02	120.49	115.92
35	a	618	XAT	C37-C21-C36	-2.02	104.44	107.37
26	8	604	CLA	CHD-C1D-ND	-2.02	121.97	124.80
26	3	604	CLA	CMB-C2B-C3B	2.02	131.29	126.55
29	2	623	BCR	C33-C5-C4	2.02	117.89	113.60
36	W	1623	NEX	O24-C25-C26	-2.02	57.33	58.93
26	6	608	CLA	O2A-CGA-O1A	-2.01	118.15	123.33
26	2	603	CLA	O2A-CGA-O1A	-2.01	118.15	123.33
26	Y	612	CLA	CHA-C1A-NA	-2.01	121.83	126.39
26	V	612	CLA	O2A-CGA-O1A	-2.01	118.15	123.33
36	5	624	NEX	C16-C1-C6	-2.01	108.67	110.47
26	2	616	CLA	O1D-CGD-CBD	2.01	128.49	124.52
26	B	808	CLA	C16-C15-C13	-2.01	109.28	115.97
35	1	618	XAT	C24-C23-C22	-2.01	107.03	110.79
26	K	206	CLA	C3B-C4B-NB	-2.01	108.73	110.53
37	V	601	CHL	C1C-C2C-CMC	2.01	130.43	126.80
26	Z	602	CLA	CMB-C2B-C3B	2.01	131.28	126.55
26	7	601	CLA	C4-C3-C2	-2.01	118.46	123.63
26	a	612	CLA	C3B-C4B-NB	-2.01	108.73	110.53
26	5	603	CLA	C1-C2-C3	-2.01	122.90	126.20
29	L	305	BCR	C27-C26-C25	2.01	125.42	122.70
29	A	856	BCR	C39-C30-C29	-2.01	101.23	108.95
26	2	606	CLA	C3B-C4B-NB	-2.01	108.74	110.53
29	G	205	BCR	C11-C12-C13	-2.01	120.85	126.36
29	a	619	BCR	C7-C6-C5	-2.01	116.93	121.56
26	G	204	CLA	O2A-CGA-O1A	-2.01	118.17	123.33
29	B	847	BCR	C30-C25-C26	-2.01	119.89	122.64
26	Y	612	CLA	C2A-C1A-CHA	2.01	127.35	123.87
35	a	618	XAT	O4-C5-C6	-2.01	57.34	58.93
26	W	610	CLA	CMB-C2B-C3B	2.01	131.27	126.55
26	5	602	CLA	O2D-CGD-CBD	2.01	114.74	111.23
35	3	619	XAT	C35-C34-C33	-2.01	124.46	127.28
35	V	1622	XAT	O24-C25-C26	-2.01	57.34	58.93
29	2	623	BCR	C29-C30-C25	2.01	113.35	110.44
35	a	618	XAT	C24-C23-C22	-2.01	107.04	110.79
37	W	608	CHL	O1D-CGD-CBD	-2.01	121.68	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1	617	LUT	C30-C31-C32	-2.01	117.39	123.20
32	J	103	LMG	O7-C10-O9	-2.01	119.01	123.70
26	A	830	CLA	O1D-CGD-CBD	2.01	128.47	124.52
37	W	609	CHL	C4C-CHD-C1D	2.01	123.24	116.07
26	B	835	CLA	O2A-CGA-O1A	-2.01	118.17	123.33
29	5	622	BCR	C33-C5-C4	2.00	117.87	113.60
29	B	843	BCR	C36-C18-C17	-2.00	119.57	122.82
26	L	304	CLA	O1D-CGD-CBD	2.00	128.47	124.52
26	A	820	CLA	CMB-C2B-C3B	2.00	131.26	126.55
29	8	621	BCR	C34-C9-C8	2.00	121.15	118.09
29	1	619	BCR	C7-C6-C5	-2.00	116.94	121.56
26	9	613	CLA	O2D-CGD-CBD	2.00	114.73	111.23
29	K	207	BCR	C29-C28-C27	2.00	115.68	111.28
35	W	1622	XAT	C39-C29-C28	2.00	121.15	118.09
26	W	614	CLA	C3B-C4B-NB	-2.00	108.74	110.53
29	B	847	BCR	C32-C1-C6	-2.00	107.10	110.24
28	Y	2630	LHG	O8-C23-C24	2.00	117.94	111.83
34	X	1620	LUT	C21-C26-C27	-2.00	110.52	112.83
26	4	602	CLA	CHB-C4A-NA	2.00	127.29	124.40
37	Z	606	CHL	CMA-C3A-C4A	-2.00	110.30	114.61

All (378) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	A	801	CLA	ND
26	A	802	CLA	ND
26	A	803	CLA	ND
26	A	804	CLA	ND
26	A	806	CLA	ND
26	A	807	CLA	ND
26	A	808	CLA	ND
26	A	809	CLA	ND
26	A	811	CLA	ND
26	A	812	CLA	ND
26	A	813	CLA	ND
26	A	814	CLA	ND
26	A	815	CLA	ND
26	A	816	CLA	ND
26	A	819	CLA	ND
26	A	820	CLA	ND
26	A	822	CLA	ND
26	A	823	CLA	ND

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Mol	Chain	Res	Type	Atom
26	A	824	CLA	ND
26	A	825	CLA	ND
26	A	826	CLA	ND
26	A	827	CLA	ND
26	A	828	CLA	ND
26	A	829	CLA	ND
26	A	830	CLA	ND
26	A	831	CLA	ND
26	A	832	CLA	ND
26	A	833	CLA	ND
26	A	834	CLA	ND
26	A	836	CLA	ND
26	A	837	CLA	ND
26	A	838	CLA	ND
26	A	839	CLA	ND
26	A	841	CLA	ND
26	A	842	CLA	ND
26	A	843	CLA	ND
26	A	845	CLA	ND
26	A	854	CLA	ND
26	B	802	CLA	ND
26	B	803	CLA	ND
26	B	804	CLA	ND
26	B	805	CLA	ND
26	B	806	CLA	ND
26	B	808	CLA	ND
26	B	809	CLA	ND
26	B	810	CLA	ND
26	B	811	CLA	ND
26	B	812	CLA	ND
26	B	813	CLA	ND
26	B	814	CLA	ND
26	B	815	CLA	ND
26	B	816	CLA	ND
26	B	817	CLA	ND
26	B	819	CLA	ND
26	B	820	CLA	ND
26	B	821	CLA	ND
26	B	823	CLA	ND
26	B	824	CLA	ND
26	B	826	CLA	ND
26	B	827	CLA	ND

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Mol	Chain	Res	Type	Atom
26	B	828	CLA	ND
26	B	829	CLA	ND
26	B	830	CLA	ND
26	B	831	CLA	ND
26	B	832	CLA	ND
26	B	833	CLA	ND
26	B	834	CLA	ND
26	B	835	CLA	ND
26	B	836	CLA	ND
26	B	838	CLA	ND
26	B	839	CLA	ND
26	B	840	CLA	ND
26	B	841	CLA	ND
26	F	301	CLA	ND
26	G	203	CLA	ND
26	G	204	CLA	ND
26	H	202	CLA	ND
26	H	203	CLA	ND
26	J	101	CLA	ND
26	K	201	CLA	ND
26	K	204	CLA	ND
26	K	206	CLA	ND
26	L	302	CLA	ND
26	L	304	CLA	ND
26	L	306	CLA	ND
26	L	307	CLA	ND
26	O	2001	CLA	ND
26	O	2002	CLA	ND
26	O	2003	CLA	ND
26	1	602	CLA	ND
26	1	603	CLA	ND
26	1	604	CLA	ND
26	1	606	CLA	ND
26	1	607	CLA	ND
26	1	608	CLA	ND
26	1	609	CLA	ND
26	1	610	CLA	ND
26	1	611	CLA	ND
26	1	612	CLA	ND
26	1	613	CLA	ND
26	1	614	CLA	ND
26	1	616	CLA	ND

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Mol	Chain	Res	Type	Atom
26	a	602	CLA	ND
26	a	603	CLA	ND
26	a	604	CLA	ND
26	a	606	CLA	ND
26	a	607	CLA	ND
26	a	608	CLA	ND
26	a	609	CLA	ND
26	a	610	CLA	ND
26	a	611	CLA	ND
26	a	612	CLA	ND
26	a	613	CLA	ND
26	a	614	CLA	ND
26	a	616	CLA	ND
26	2	601	CLA	ND
26	2	602	CLA	ND
26	2	603	CLA	ND
26	2	604	CLA	ND
26	2	606	CLA	ND
26	2	607	CLA	ND
26	2	609	CLA	ND
26	2	610	CLA	ND
26	2	611	CLA	ND
26	2	612	CLA	ND
26	2	613	CLA	ND
26	2	614	CLA	ND
26	2	616	CLA	ND
26	3	602	CLA	ND
26	3	603	CLA	ND
26	3	604	CLA	ND
26	3	606	CLA	ND
26	3	607	CLA	ND
26	3	608	CLA	ND
26	3	609	CLA	ND
26	3	610	CLA	ND
26	3	611	CLA	ND
26	3	612	CLA	ND
26	3	613	CLA	ND
26	3	614	CLA	ND
26	3	615	CLA	ND
26	3	617	CLA	ND
26	4	601	CLA	ND
26	4	602	CLA	ND

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Mol	Chain	Res	Type	Atom
26	4	603	CLA	ND
26	4	604	CLA	ND
26	4	606	CLA	ND
26	4	607	CLA	ND
26	4	608	CLA	ND
26	4	609	CLA	ND
26	4	610	CLA	ND
26	4	611	CLA	ND
26	4	612	CLA	ND
26	4	613	CLA	ND
26	4	616	CLA	ND
26	4	618	CLA	ND
26	5	601	CLA	ND
26	5	602	CLA	ND
26	5	603	CLA	ND
26	5	604	CLA	ND
26	5	607	CLA	ND
26	5	608	CLA	ND
26	5	609	CLA	ND
26	5	610	CLA	ND
26	5	611	CLA	ND
26	5	612	CLA	ND
26	5	613	CLA	ND
26	5	614	CLA	ND
26	5	616	CLA	ND
26	5	617	CLA	ND
26	5	618	CLA	ND
26	5	619	CLA	ND
26	6	601	CLA	ND
26	6	603	CLA	ND
26	6	604	CLA	ND
26	6	606	CLA	ND
26	6	607	CLA	ND
26	6	609	CLA	ND
26	6	610	CLA	ND
26	6	611	CLA	ND
26	6	612	CLA	ND
26	6	614	CLA	ND
26	6	616	CLA	ND
26	6	617	CLA	ND
26	6	618	CLA	ND
26	6	620	CLA	ND

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Mol	Chain	Res	Type	Atom
26	7	601	CLA	ND
26	7	602	CLA	ND
26	7	603	CLA	ND
26	7	604	CLA	ND
26	7	606	CLA	ND
26	7	607	CLA	ND
26	7	609	CLA	ND
26	7	610	CLA	ND
26	7	611	CLA	ND
26	7	612	CLA	ND
26	7	613	CLA	ND
26	7	614	CLA	ND
26	7	615	CLA	ND
26	7	616	CLA	ND
26	8	601	CLA	ND
26	8	603	CLA	ND
26	8	604	CLA	ND
26	8	606	CLA	ND
26	8	607	CLA	ND
26	8	609	CLA	ND
26	8	610	CLA	ND
26	8	611	CLA	ND
26	8	612	CLA	ND
26	8	613	CLA	ND
26	8	614	CLA	ND
26	8	616	CLA	ND
26	9	601	CLA	ND
26	9	602	CLA	ND
26	9	603	CLA	ND
26	9	604	CLA	ND
26	9	606	CLA	ND
26	9	609	CLA	ND
26	9	610	CLA	ND
26	9	611	CLA	ND
26	9	612	CLA	ND
26	9	613	CLA	ND
26	9	614	CLA	ND
26	X	602	CLA	ND
26	X	603	CLA	ND
26	X	604	CLA	ND
26	X	610	CLA	ND
26	X	611	CLA	ND

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Mol	Chain	Res	Type	Atom
26	X	612	CLA	ND
26	X	613	CLA	ND
26	X	614	CLA	ND
26	Y	602	CLA	ND
26	Y	603	CLA	ND
26	Y	604	CLA	ND
26	Y	610	CLA	ND
26	Y	611	CLA	ND
26	Y	612	CLA	ND
26	Y	614	CLA	ND
26	Z	602	CLA	ND
26	Z	603	CLA	ND
26	Z	604	CLA	ND
26	Z	610	CLA	ND
26	Z	611	CLA	ND
26	Z	612	CLA	ND
26	Z	613	CLA	ND
26	Z	614	CLA	ND
26	U	602	CLA	ND
26	U	603	CLA	ND
26	U	604	CLA	ND
26	U	610	CLA	ND
26	U	611	CLA	ND
26	U	612	CLA	ND
26	U	613	CLA	ND
26	U	614	CLA	ND
26	V	602	CLA	ND
26	V	603	CLA	ND
26	V	604	CLA	ND
26	V	610	CLA	ND
26	V	611	CLA	ND
26	V	612	CLA	ND
26	V	613	CLA	ND
26	V	614	CLA	ND
26	W	602	CLA	ND
26	W	603	CLA	ND
26	W	604	CLA	ND
26	W	610	CLA	ND
26	W	611	CLA	ND
26	W	612	CLA	ND
26	W	613	CLA	ND
26	W	614	CLA	ND

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

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

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

All (3468) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	801	CLA	CBD-CGD-O2D-CED
26	A	801	CLA	O1D-CGD-O2D-CED
26	A	804	CLA	C1A-C2A-CAA-CBA
26	A	804	CLA	C3A-C2A-CAA-CBA
26	A	804	CLA	CHA-CBD-CGD-O1D
26	A	804	CLA	CHA-CBD-CGD-O2D
26	A	805	CLA	C3A-C2A-CAA-CBA
26	A	809	CLA	CHA-CBD-CGD-O1D
26	A	809	CLA	CHA-CBD-CGD-O2D
26	A	810	CLA	C2B-C3B-CAB-CBB
26	A	810	CLA	C4B-C3B-CAB-CBB
26	A	810	CLA	CBD-CGD-O2D-CED
26	A	812	CLA	C1A-C2A-CAA-CBA
26	A	815	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	A	816	CLA	C1A-C2A-CAA-CBA
26	A	816	CLA	C3A-C2A-CAA-CBA
26	A	819	CLA	C1A-C2A-CAA-CBA
26	A	819	CLA	C3A-C2A-CAA-CBA
26	A	820	CLA	C3A-C2A-CAA-CBA
26	A	821	CLA	C1A-C2A-CAA-CBA
26	A	821	CLA	C3A-C2A-CAA-CBA
26	A	821	CLA	CAD-CBD-CGD-O2D
26	A	823	CLA	C1A-C2A-CAA-CBA
26	A	825	CLA	C1A-C2A-CAA-CBA
26	A	825	CLA	C3A-C2A-CAA-CBA
26	A	825	CLA	C4B-C3B-CAB-CBB
26	A	828	CLA	CAD-CBD-CGD-O1D
26	A	828	CLA	CAD-CBD-CGD-O2D
26	A	829	CLA	CBD-CGD-O2D-CED
26	A	832	CLA	C1A-C2A-CAA-CBA
26	A	832	CLA	C3A-C2A-CAA-CBA
26	A	832	CLA	CHA-CBD-CGD-O1D
26	A	832	CLA	CHA-CBD-CGD-O2D
26	A	834	CLA	C2B-C3B-CAB-CBB
26	A	834	CLA	C4B-C3B-CAB-CBB
26	A	836	CLA	C2-C3-C5-C6
26	A	836	CLA	C4-C3-C5-C6
26	A	841	CLA	C1A-C2A-CAA-CBA
26	A	841	CLA	C3A-C2A-CAA-CBA
26	A	845	CLA	C1A-C2A-CAA-CBA
26	B	802	CLA	CBD-CGD-O2D-CED
26	B	802	CLA	C11-C12-C13-C14
26	B	803	CLA	C3A-C2A-CAA-CBA
26	B	803	CLA	CBD-CGD-O2D-CED
26	B	805	CLA	C3A-C2A-CAA-CBA
26	B	806	CLA	CBD-CGD-O2D-CED
26	B	807	CLA	C2B-C3B-CAB-CBB
26	B	807	CLA	C4B-C3B-CAB-CBB
26	B	808	CLA	CHA-CBD-CGD-O1D
26	B	808	CLA	CHA-CBD-CGD-O2D
26	B	809	CLA	C1A-C2A-CAA-CBA
26	B	809	CLA	CBD-CGD-O2D-CED
26	B	810	CLA	C1A-C2A-CAA-CBA
26	B	810	CLA	CHA-CBD-CGD-O1D
26	B	810	CLA	CHA-CBD-CGD-O2D
26	B	813	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	B	813	CLA	C3A-C2A-CAA-CBA
26	B	813	CLA	CAD-CBD-CGD-O2D
26	B	814	CLA	CBD-CGD-O2D-CED
26	B	815	CLA	C1A-C2A-CAA-CBA
26	B	817	CLA	C2B-C3B-CAB-CBB
26	B	817	CLA	C4B-C3B-CAB-CBB
26	B	818	CLA	C3A-C2A-CAA-CBA
26	B	819	CLA	C2B-C3B-CAB-CBB
26	B	819	CLA	C4B-C3B-CAB-CBB
26	B	820	CLA	C2B-C3B-CAB-CBB
26	B	820	CLA	C4B-C3B-CAB-CBB
26	B	822	CLA	C1A-C2A-CAA-CBA
26	B	822	CLA	CBD-CGD-O2D-CED
26	B	826	CLA	C11-C12-C13-C14
26	B	828	CLA	C14-C13-C15-C16
26	B	830	CLA	C1A-C2A-CAA-CBA
26	B	830	CLA	C3A-C2A-CAA-CBA
26	B	830	CLA	C4B-C3B-CAB-CBB
26	B	833	CLA	C2B-C3B-CAB-CBB
26	B	833	CLA	C4B-C3B-CAB-CBB
26	B	833	CLA	CHA-CBD-CGD-O1D
26	B	833	CLA	CHA-CBD-CGD-O2D
26	B	835	CLA	CBD-CGD-O2D-CED
26	B	841	CLA	C1A-C2A-CAA-CBA
26	B	841	CLA	C3A-C2A-CAA-CBA
26	F	301	CLA	CBD-CGD-O2D-CED
26	F	303	CLA	C1A-C2A-CAA-CBA
26	F	303	CLA	C3A-C2A-CAA-CBA
26	G	203	CLA	C2B-C3B-CAB-CBB
26	G	203	CLA	C4B-C3B-CAB-CBB
26	G	203	CLA	CBD-CGD-O2D-CED
26	G	204	CLA	CBD-CGD-O2D-CED
26	K	201	CLA	C2B-C3B-CAB-CBB
26	K	201	CLA	C4B-C3B-CAB-CBB
26	K	203	CLA	C1A-C2A-CAA-CBA
26	K	206	CLA	C1A-C2A-CAA-CBA
26	K	206	CLA	C3A-C2A-CAA-CBA
26	K	206	CLA	C2B-C3B-CAB-CBB
26	K	206	CLA	C4B-C3B-CAB-CBB
26	K	206	CLA	CBD-CGD-O2D-CED
26	L	303	CLA	C4-C3-C5-C6
26	O	2001	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	O	2003	CLA	C4B-C3B-CAB-CBB
26	O	2003	CLA	CHA-CBD-CGD-O2D
26	1	601	CLA	C4B-C3B-CAB-CBB
26	1	603	CLA	C4B-C3B-CAB-CBB
26	1	604	CLA	CAD-CBD-CGD-O1D
26	1	604	CLA	CAD-CBD-CGD-O2D
26	a	601	CLA	C4B-C3B-CAB-CBB
26	a	603	CLA	C4B-C3B-CAB-CBB
26	a	604	CLA	CAD-CBD-CGD-O1D
26	a	604	CLA	CAD-CBD-CGD-O2D
26	a	607	CLA	CBD-CGD-O2D-CED
26	a	609	CLA	C1A-C2A-CAA-CBA
26	a	609	CLA	C3A-C2A-CAA-CBA
26	2	601	CLA	CBD-CGD-O2D-CED
26	2	602	CLA	NA-C4A-CHB-C1B
26	2	602	CLA	C1B-C2B-C3B-C4B
26	2	602	CLA	CMB-C2B-C3B-C4B
26	2	602	CLA	C2B-C3B-CAB-CBB
26	2	604	CLA	CBD-CGD-O2D-CED
26	2	610	CLA	C2B-C3B-CAB-CBB
26	2	610	CLA	C4B-C3B-CAB-CBB
26	2	611	CLA	C2B-C3B-CAB-CBB
26	2	611	CLA	C4B-C3B-CAB-CBB
26	2	612	CLA	C2B-C3B-CAB-CBB
26	2	612	CLA	C4B-C3B-CAB-CBB
26	2	613	CLA	C2B-C3B-CAB-CBB
26	2	613	CLA	C4B-C3B-CAB-CBB
26	3	604	CLA	CBD-CGD-O2D-CED
26	3	608	CLA	C4B-C3B-CAB-CBB
26	3	609	CLA	C3A-C2A-CAA-CBA
26	3	609	CLA	C2B-C3B-CAB-CBB
26	3	609	CLA	C4B-C3B-CAB-CBB
26	3	609	CLA	CHA-CBD-CGD-O1D
26	3	609	CLA	CHA-CBD-CGD-O2D
26	3	610	CLA	C1A-C2A-CAA-CBA
26	3	610	CLA	C3A-C2A-CAA-CBA
26	3	610	CLA	C2B-C3B-CAB-CBB
26	3	610	CLA	C4B-C3B-CAB-CBB
26	3	611	CLA	CAD-CBD-CGD-O2D
26	3	613	CLA	CHA-CBD-CGD-O2D
26	3	614	CLA	C2B-C3B-CAB-CBB
26	3	614	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	3	615	CLA	C1A-C2A-CAA-CBA
26	3	615	CLA	CAD-CBD-CGD-O2D
26	4	601	CLA	C1A-C2A-CAA-CBA
26	4	606	CLA	C1A-C2A-CAA-CBA
26	4	606	CLA	C3A-C2A-CAA-CBA
26	4	611	CLA	C2B-C3B-CAB-CBB
26	4	611	CLA	C4B-C3B-CAB-CBB
26	4	612	CLA	C1A-C2A-CAA-CBA
26	4	613	CLA	CBA-CGA-O2A-C1
26	4	613	CLA	O1A-CGA-O2A-C1
26	4	614	CLA	C2B-C3B-CAB-CBB
26	4	614	CLA	C4B-C3B-CAB-CBB
26	4	614	CLA	CAD-CBD-CGD-O1D
26	4	614	CLA	CAD-CBD-CGD-O2D
26	4	614	CLA	CBD-CGD-O2D-CED
26	4	618	CLA	C1A-C2A-CAA-CBA
26	5	601	CLA	C2B-C3B-CAB-CBB
26	5	601	CLA	C4B-C3B-CAB-CBB
26	5	606	CLA	C2B-C3B-CAB-CBB
26	5	606	CLA	C4B-C3B-CAB-CBB
26	5	607	CLA	CBD-CGD-O2D-CED
26	5	608	CLA	C1A-C2A-CAA-CBA
26	5	608	CLA	C3A-C2A-CAA-CBA
26	5	608	CLA	CBD-CGD-O2D-CED
26	5	609	CLA	C1A-C2A-CAA-CBA
26	5	609	CLA	C3A-C2A-CAA-CBA
26	5	610	CLA	C4B-C3B-CAB-CBB
26	5	611	CLA	C4B-C3B-CAB-CBB
26	5	612	CLA	C1A-C2A-CAA-CBA
26	5	613	CLA	C2B-C3B-CAB-CBB
26	5	613	CLA	C4B-C3B-CAB-CBB
26	5	614	CLA	C1A-C2A-CAA-CBA
26	5	614	CLA	C3A-C2A-CAA-CBA
26	5	614	CLA	C2B-C3B-CAB-CBB
26	5	614	CLA	C4B-C3B-CAB-CBB
26	5	614	CLA	CBD-CGD-O2D-CED
26	5	617	CLA	C1A-C2A-CAA-CBA
26	5	617	CLA	CAD-CBD-CGD-O1D
26	5	617	CLA	CAD-CBD-CGD-O2D
26	5	617	CLA	CBD-CGD-O2D-CED
26	5	618	CLA	C1A-C2A-CAA-CBA
26	5	618	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	5	619	CLA	CHA-CBD-CGD-O1D
26	5	619	CLA	CHA-CBD-CGD-O2D
26	6	608	CLA	CBD-CGD-O2D-CED
26	6	609	CLA	C1A-C2A-CAA-CBA
26	6	611	CLA	C4B-C3B-CAB-CBB
26	6	612	CLA	C1A-C2A-CAA-CBA
26	6	612	CLA	C3A-C2A-CAA-CBA
26	6	613	CLA	CAD-CBD-CGD-O2D
26	6	614	CLA	CBD-CGD-O2D-CED
26	6	617	CLA	C1A-C2A-CAA-CBA
26	6	617	CLA	C3A-C2A-CAA-CBA
26	7	601	CLA	CAD-CBD-CGD-O1D
26	7	601	CLA	CAD-CBD-CGD-O2D
26	7	604	CLA	CHA-CBD-CGD-O1D
26	7	604	CLA	CHA-CBD-CGD-O2D
26	7	608	CLA	CBD-CGD-O2D-CED
26	7	609	CLA	C1A-C2A-CAA-CBA
26	7	609	CLA	C3A-C2A-CAA-CBA
26	7	609	CLA	CAD-CBD-CGD-O2D
26	7	612	CLA	CBD-CGD-O2D-CED
26	7	613	CLA	C2B-C3B-CAB-CBB
26	7	613	CLA	C4B-C3B-CAB-CBB
26	7	614	CLA	C1A-C2A-CAA-CBA
26	7	614	CLA	C2B-C3B-CAB-CBB
26	7	614	CLA	C4B-C3B-CAB-CBB
26	7	615	CLA	CAD-CBD-CGD-O2D
26	7	616	CLA	C1A-C2A-CAA-CBA
26	8	606	CLA	CBD-CGD-O2D-CED
26	8	607	CLA	CBD-CGD-O2D-CED
26	8	608	CLA	C4B-C3B-CAB-CBB
26	8	609	CLA	C3A-C2A-CAA-CBA
26	8	611	CLA	C1A-C2A-CAA-CBA
26	8	612	CLA	C1A-C2A-CAA-CBA
26	8	612	CLA	C3A-C2A-CAA-CBA
26	8	613	CLA	C4B-C3B-CAB-CBB
26	8	614	CLA	C1A-C2A-CAA-CBA
26	9	603	CLA	CHA-CBD-CGD-O1D
26	9	603	CLA	CHA-CBD-CGD-O2D
26	9	604	CLA	O1A-CGA-O2A-C1
26	9	604	CLA	CHA-CBD-CGD-O1D
26	9	604	CLA	CHA-CBD-CGD-O2D
26	9	606	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	9	606	CLA	C3A-C2A-CAA-CBA
26	9	607	CLA	C1A-C2A-CAA-CBA
26	9	607	CLA	C3A-C2A-CAA-CBA
26	9	610	CLA	C4B-C3B-CAB-CBB
26	9	611	CLA	C4B-C3B-CAB-CBB
26	9	612	CLA	C1A-C2A-CAA-CBA
26	9	613	CLA	C2B-C3B-CAB-CBB
26	9	613	CLA	C4B-C3B-CAB-CBB
26	X	602	CLA	CBD-CGD-O2D-CED
26	X	603	CLA	C1A-C2A-CAA-CBA
26	X	603	CLA	C3A-C2A-CAA-CBA
26	X	603	CLA	C4B-C3B-CAB-CBB
26	X	603	CLA	CHA-CBD-CGD-O1D
26	X	603	CLA	CHA-CBD-CGD-O2D
26	X	604	CLA	C1A-C2A-CAA-CBA
26	X	604	CLA	C3A-C2A-CAA-CBA
26	X	611	CLA	C2B-C3B-CAB-CBB
26	X	611	CLA	C4B-C3B-CAB-CBB
26	X	611	CLA	CAD-CBD-CGD-O1D
26	X	611	CLA	CAD-CBD-CGD-O2D
26	X	612	CLA	C2B-C3B-CAB-CBB
26	X	612	CLA	C4B-C3B-CAB-CBB
26	X	614	CLA	C1A-C2A-CAA-CBA
26	X	614	CLA	C2B-C3B-CAB-CBB
26	X	614	CLA	C4B-C3B-CAB-CBB
26	Y	603	CLA	C4B-C3B-CAB-CBB
26	Y	604	CLA	C1A-C2A-CAA-CBA
26	Y	604	CLA	C3A-C2A-CAA-CBA
26	Y	604	CLA	CBD-CGD-O2D-CED
26	Y	611	CLA	C2B-C3B-CAB-CBB
26	Y	611	CLA	C4B-C3B-CAB-CBB
26	Y	614	CLA	C2B-C3B-CAB-CBB
26	Y	614	CLA	C4B-C3B-CAB-CBB
26	Z	603	CLA	C2B-C3B-CAB-CBB
26	Z	603	CLA	C4B-C3B-CAB-CBB
26	Z	610	CLA	C4B-C3B-CAB-CBB
26	Z	610	CLA	C4-C3-C5-C6
26	Z	612	CLA	C2B-C3B-CAB-CBB
26	Z	612	CLA	C4B-C3B-CAB-CBB
26	U	603	CLA	C2B-C3B-CAB-CBB
26	U	603	CLA	C4B-C3B-CAB-CBB
26	U	611	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	U	612	CLA	C2B-C3B-CAB-CBB
26	U	612	CLA	C4B-C3B-CAB-CBB
26	U	614	CLA	C1A-C2A-CAA-CBA
26	V	611	CLA	C1A-C2A-CAA-CBA
26	V	611	CLA	C4B-C3B-CAB-CBB
26	V	612	CLA	C2B-C3B-CAB-CBB
26	V	612	CLA	C4B-C3B-CAB-CBB
26	V	614	CLA	C2B-C3B-CAB-CBB
26	V	614	CLA	C4B-C3B-CAB-CBB
26	V	614	CLA	CBD-CGD-O2D-CED
26	W	602	CLA	CHA-CBD-CGD-O1D
26	W	602	CLA	CHA-CBD-CGD-O2D
26	W	611	CLA	C1A-C2A-CAA-CBA
26	W	612	CLA	C2B-C3B-CAB-CBB
26	W	612	CLA	C4B-C3B-CAB-CBB
26	W	612	CLA	CHA-CBD-CGD-O2D
26	W	613	CLA	C2B-C3B-CAB-CBB
26	W	613	CLA	C4B-C3B-CAB-CBB
26	W	614	CLA	CBD-CGD-O2D-CED
27	B	842	PQN	C11-C12-C13-C14
28	A	846	LHG	C3-O3-P-O5
28	A	846	LHG	C3-O3-P-O6
28	A	847	LHG	C3-O3-P-O6
28	A	847	LHG	C4-O6-P-O3
28	A	847	LHG	C4-O6-P-O5
28	A	847	LHG	O6-C4-C5-O7
28	A	861	LHG	C3-O3-P-O4
28	A	861	LHG	C3-O3-P-O6
28	A	861	LHG	C4-O6-P-O3
28	A	861	LHG	C4-O6-P-O4
28	B	851	LHG	C3-O3-P-O4
28	B	851	LHG	C3-O3-P-O5
28	B	851	LHG	C3-O3-P-O6
28	H	204	LHG	C4-O6-P-O3
28	H	204	LHG	C4-O6-P-O4
28	H	204	LHG	O7-C5-C6-O8
28	O	2631	LHG	C3-O3-P-O6
28	1	620	LHG	O1-C1-C2-C3
28	1	620	LHG	C3-O3-P-O4
28	1	620	LHG	C3-O3-P-O6
28	a	620	LHG	O1-C1-C2-C3
28	a	620	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
28	a	620	LHG	C3-O3-P-O6
28	2	622	LHG	C3-O3-P-O6
28	2	622	LHG	C4-O6-P-O3
28	2	622	LHG	C4-O6-P-O4
28	2	622	LHG	C4-O6-P-O5
28	3	623	LHG	C3-O3-P-O4
28	3	623	LHG	C3-O3-P-O6
28	3	623	LHG	C4-O6-P-O5
28	3	624	LHG	C3-O3-P-O5
28	3	624	LHG	C3-O3-P-O6
28	5	623	LHG	C3-O3-P-O4
28	5	623	LHG	C3-O3-P-O6
28	5	623	LHG	C4-O6-P-O3
28	5	623	LHG	C4-O6-P-O4
28	5	623	LHG	C4-O6-P-O5
28	5	623	LHG	O7-C5-C6-O8
28	5	625	LHG	C3-O3-P-O5
28	6	623	LHG	C1-C2-C3-O3
28	6	623	LHG	C3-O3-P-O4
28	6	623	LHG	C3-O3-P-O6
28	6	623	LHG	C4-O6-P-O4
28	6	623	LHG	C4-O6-P-O5
28	7	622	LHG	C3-O3-P-O4
28	7	622	LHG	C3-O3-P-O6
28	8	622	LHG	C4-O6-P-O4
28	8	623	LHG	C4-O6-P-O3
28	8	623	LHG	C4-O6-P-O4
28	9	622	LHG	C3-O3-P-O5
28	9	622	LHG	C3-O3-P-O6
28	9	622	LHG	C4-O6-P-O3
28	9	622	LHG	O7-C5-C6-O8
28	9	623	LHG	C3-O3-P-O6
28	9	623	LHG	C4-O6-P-O3
28	9	623	LHG	C8-C7-O7-C5
28	9	624	LHG	C4-O6-P-O3
28	9	624	LHG	C4-O6-P-O4
28	9	624	LHG	C4-O6-P-O5
28	X	2630	LHG	C4-O6-P-O3
28	X	2630	LHG	C4-O6-P-O4
28	X	2630	LHG	C4-O6-P-O5
28	Y	2630	LHG	C3-O3-P-O5
28	Y	2630	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
28	Z	2630	LHG	O1-C1-C2-C3
28	Z	2630	LHG	C4-O6-P-O3
28	Z	2630	LHG	C4-O6-P-O4
28	U	2630	LHG	C4-O6-P-O3
28	U	2630	LHG	C4-O6-P-O4
28	U	2630	LHG	C4-O6-P-O5
28	V	2630	LHG	C3-O3-P-O5
28	V	2630	LHG	C4-O6-P-O5
28	W	2630	LHG	C3-O3-P-O4
28	W	2630	LHG	C3-O3-P-O5
28	W	2630	LHG	C3-O3-P-O6
28	W	2630	LHG	C4-O6-P-O3
28	W	2630	LHG	C4-O6-P-O5
29	A	849	BCR	C23-C24-C25-C26
29	A	856	BCR	C1-C6-C7-C8
29	A	856	BCR	C5-C6-C7-C8
29	B	801	BCR	C23-C24-C25-C26
29	B	843	BCR	C1-C6-C7-C8
29	B	843	BCR	C5-C6-C7-C8
29	B	843	BCR	C23-C24-C25-C26
29	B	844	BCR	C23-C24-C25-C26
29	B	844	BCR	C23-C24-C25-C30
29	B	847	BCR	C21-C22-C23-C24
29	B	848	BCR	C21-C22-C23-C24
29	B	848	BCR	C23-C24-C25-C26
29	B	848	BCR	C23-C24-C25-C30
29	B	852	BCR	C7-C8-C9-C10
29	B	853	BCR	C5-C6-C7-C8
29	J	102	BCR	C5-C6-C7-C8
29	K	202	BCR	C23-C24-C25-C26
29	K	202	BCR	C23-C24-C25-C30
29	L	301	BCR	C1-C6-C7-C8
29	L	308	BCR	C5-C6-C7-C8
29	L	308	BCR	C7-C8-C9-C10
29	L	308	BCR	C17-C18-C19-C20
29	L	309	BCR	C23-C24-C25-C26
29	L	309	BCR	C23-C24-C25-C30
29	O	2005	BCR	C21-C22-C23-C24
29	O	2005	BCR	C37-C22-C23-C24
29	1	619	BCR	C23-C24-C25-C26
29	1	619	BCR	C23-C24-C25-C30
29	a	619	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
29	a	619	BCR	C23-C24-C25-C30
29	2	623	BCR	C7-C8-C9-C10
29	3	620	BCR	C21-C22-C23-C24
29	3	620	BCR	C23-C24-C25-C26
29	6	622	BCR	C23-C24-C25-C26
29	6	622	BCR	C23-C24-C25-C30
29	7	621	BCR	C23-C24-C25-C26
29	7	621	BCR	C23-C24-C25-C30
29	7	623	BCR	C1-C6-C7-C8
29	8	621	BCR	C23-C24-C25-C26
29	8	621	BCR	C23-C24-C25-C30
29	9	621	BCR	C21-C22-C23-C24
29	9	621	BCR	C23-C24-C25-C26
29	9	621	BCR	C23-C24-C25-C30
31	A	858	LMU	C2-C1-O1'-C1'
31	K	208	LMU	O5'-C1'-O1'-C1
31	5	628	LMU	C2'-C1'-O1'-C1
31	5	628	LMU	C2-C1-O1'-C1'
32	H	205	LMG	C11-C10-O7-C8
32	L	2631	LMG	C11-C10-O7-C8
32	8	626	LMG	O6-C1-O1-C7
32	8	626	LMG	O9-C10-O7-C8
32	9	625	LMG	O7-C8-C9-O8
33	B	850	DGD	O1B-C1B-O2G-C2G
34	1	617	LUT	C1-C6-C7-C8
34	1	617	LUT	C5-C6-C7-C8
34	a	617	LUT	C1-C6-C7-C8
34	a	617	LUT	C5-C6-C7-C8
34	3	618	LUT	C1-C6-C7-C8
34	3	618	LUT	C5-C6-C7-C8
34	4	619	LUT	C1-C6-C7-C8
34	6	619	LUT	C5-C6-C7-C8
34	8	619	LUT	C1-C6-C7-C8
34	8	619	LUT	C5-C6-C7-C8
34	Y	1620	LUT	C13-C14-C15-C35
34	Y	1621	LUT	C7-C8-C9-C10
34	Y	1621	LUT	C7-C8-C9-C19
34	V	1621	LUT	C7-C8-C9-C10
34	V	1621	LUT	C7-C8-C9-C19
34	W	1621	LUT	C7-C8-C9-C10
35	4	620	XAT	C25-C26-C27-C28
35	X	1622	XAT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
35	U	1622	XAT	C11-C12-C13-C14
36	X	1623	NEX	C7-C8-C9-C10
36	V	1623	NEX	C11-C12-C13-C14
36	V	1623	NEX	C11-C12-C13-C20
36	W	1623	NEX	C31-C32-C33-C34
36	W	1623	NEX	C31-C32-C33-C40
37	X	605	CHL	C1C-C2C-CMC-OMC
37	X	606	CHL	C1C-C2C-CMC-OMC
37	X	606	CHL	C3C-C2C-CMC-OMC
37	X	607	CHL	C1C-C2C-CMC-OMC
37	X	607	CHL	C3C-C2C-CMC-OMC
37	X	608	CHL	C1C-C2C-CMC-OMC
37	X	608	CHL	C3C-C2C-CMC-OMC
37	X	608	CHL	CBD-CGD-O2D-CED
37	X	609	CHL	C1A-C2A-CAA-CBA
37	X	609	CHL	C1C-C2C-CMC-OMC
37	X	609	CHL	C3C-C2C-CMC-OMC
37	X	609	CHL	C4C-C3C-CAC-CBC
37	Y	605	CHL	C1C-C2C-CMC-OMC
37	Y	605	CHL	C3C-C2C-CMC-OMC
37	Y	606	CHL	C1C-C2C-CMC-OMC
37	Y	606	CHL	C3C-C2C-CMC-OMC
37	Y	607	CHL	CHA-CBD-CGD-O1D
37	Y	609	CHL	C1A-C2A-CAA-CBA
37	Z	605	CHL	C1C-C2C-CMC-OMC
37	Z	605	CHL	C3C-C2C-CMC-OMC
37	Z	606	CHL	C3A-C2A-CAA-CBA
37	Z	607	CHL	C1C-C2C-CMC-OMC
37	Z	607	CHL	C3C-C2C-CMC-OMC
37	Z	608	CHL	CBD-CGD-O2D-CED
37	Z	609	CHL	C1C-C2C-CMC-OMC
37	Z	609	CHL	C3C-C2C-CMC-OMC
37	U	601	CHL	C1C-C2C-CMC-OMC
37	U	601	CHL	C3C-C2C-CMC-OMC
37	U	605	CHL	C1C-C2C-CMC-OMC
37	U	605	CHL	C3C-C2C-CMC-OMC
37	U	606	CHL	C1C-C2C-CMC-OMC
37	U	606	CHL	C3C-C2C-CMC-OMC
37	U	607	CHL	C3A-C2A-CAA-CBA
37	U	607	CHL	C1C-C2C-CMC-OMC
37	U	607	CHL	C3C-C2C-CMC-OMC
37	U	608	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	U	608	CHL	C3A-C2A-CAA-CBA
37	U	609	CHL	C1A-C2A-CAA-CBA
37	U	609	CHL	C1C-C2C-CMC-OMC
37	U	609	CHL	C3C-C2C-CMC-OMC
37	U	609	CHL	C4C-C3C-CAC-CBC
37	V	605	CHL	C1C-C2C-CMC-OMC
37	V	605	CHL	C3C-C2C-CMC-OMC
37	V	607	CHL	C3A-C2A-CAA-CBA
37	V	607	CHL	C1C-C2C-CMC-OMC
37	V	607	CHL	C3C-C2C-CMC-OMC
37	V	608	CHL	C1C-C2C-CMC-OMC
37	V	608	CHL	C3C-C2C-CMC-OMC
37	V	609	CHL	C1A-C2A-CAA-CBA
37	V	609	CHL	C1C-C2C-CMC-OMC
37	V	609	CHL	C3C-C2C-CMC-OMC
37	W	605	CHL	C1A-C2A-CAA-CBA
37	W	605	CHL	C1C-C2C-CMC-OMC
37	W	605	CHL	C3C-C2C-CMC-OMC
37	W	607	CHL	C1C-C2C-CMC-OMC
37	W	607	CHL	C3C-C2C-CMC-OMC
37	W	608	CHL	C1C-C2C-CMC-OMC
37	W	608	CHL	C3C-C2C-CMC-OMC
37	W	608	CHL	CBD-CGD-O2D-CED
26	A	829	CLA	O1D-CGD-O2D-CED
26	G	203	CLA	O1D-CGD-O2D-CED
26	G	204	CLA	O1D-CGD-O2D-CED
26	1	616	CLA	O1D-CGD-O2D-CED
26	a	607	CLA	O1D-CGD-O2D-CED
26	a	616	CLA	O1D-CGD-O2D-CED
26	3	603	CLA	O1D-CGD-O2D-CED
26	6	604	CLA	O1D-CGD-O2D-CED
26	7	604	CLA	O1D-CGD-O2D-CED
37	X	607	CHL	O1D-CGD-O2D-CED
37	W	608	CHL	O1D-CGD-O2D-CED
37	W	609	CHL	O1D-CGD-O2D-CED
31	K	208	LMU	O5B-C1B-O1B-C4'
26	A	834	CLA	O1D-CGD-O2D-CED
26	B	802	CLA	O1D-CGD-O2D-CED
26	B	803	CLA	O1D-CGD-O2D-CED
26	B	835	CLA	O1D-CGD-O2D-CED
26	F	301	CLA	O1D-CGD-O2D-CED
26	K	201	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	5	614	CLA	O1D-CGD-O2D-CED
26	5	617	CLA	O1D-CGD-O2D-CED
26	6	610	CLA	O1D-CGD-O2D-CED
37	X	608	CHL	O1D-CGD-O2D-CED
37	W	607	CHL	O1D-CGD-O2D-CED
26	A	802	CLA	CBD-CGD-O2D-CED
26	A	811	CLA	CBD-CGD-O2D-CED
26	A	831	CLA	CBD-CGD-O2D-CED
26	A	832	CLA	CBD-CGD-O2D-CED
26	A	834	CLA	CBD-CGD-O2D-CED
26	A	835	CLA	CBD-CGD-O2D-CED
26	A	845	CLA	CBD-CGD-O2D-CED
26	A	854	CLA	CBD-CGD-O2D-CED
26	B	810	CLA	CBD-CGD-O2D-CED
26	B	816	CLA	CBD-CGD-O2D-CED
26	B	839	CLA	CBD-CGD-O2D-CED
26	B	840	CLA	CBD-CGD-O2D-CED
26	K	201	CLA	CBD-CGD-O2D-CED
26	K	204	CLA	CBD-CGD-O2D-CED
26	1	604	CLA	CBD-CGD-O2D-CED
26	1	616	CLA	CBD-CGD-O2D-CED
26	a	604	CLA	CBD-CGD-O2D-CED
26	a	616	CLA	CBD-CGD-O2D-CED
26	2	606	CLA	CBD-CGD-O2D-CED
26	2	612	CLA	CBD-CGD-O2D-CED
26	3	603	CLA	CBD-CGD-O2D-CED
26	3	610	CLA	CBD-CGD-O2D-CED
26	4	608	CLA	CBD-CGD-O2D-CED
26	5	603	CLA	CBD-CGD-O2D-CED
26	6	604	CLA	CBD-CGD-O2D-CED
26	6	610	CLA	CBD-CGD-O2D-CED
26	6	617	CLA	CBD-CGD-O2D-CED
26	7	604	CLA	CBD-CGD-O2D-CED
26	X	612	CLA	CBD-CGD-O2D-CED
26	Y	614	CLA	CBD-CGD-O2D-CED
26	Z	612	CLA	CBD-CGD-O2D-CED
26	U	602	CLA	CBD-CGD-O2D-CED
26	U	603	CLA	CBD-CGD-O2D-CED
26	U	614	CLA	CBD-CGD-O2D-CED
26	V	603	CLA	CBD-CGD-O2D-CED
26	V	604	CLA	CBD-CGD-O2D-CED
26	V	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	W	603	CLA	CBD-CGD-O2D-CED
37	X	607	CHL	CBD-CGD-O2D-CED
37	Y	608	CHL	CBD-CGD-O2D-CED
37	Z	607	CHL	CBD-CGD-O2D-CED
37	U	606	CHL	CBD-CGD-O2D-CED
37	U	607	CHL	CBD-CGD-O2D-CED
37	U	608	CHL	CBD-CGD-O2D-CED
37	V	607	CHL	CBD-CGD-O2D-CED
37	V	608	CHL	CBD-CGD-O2D-CED
37	W	607	CHL	CBD-CGD-O2D-CED
37	W	609	CHL	CBD-CGD-O2D-CED
26	A	839	CLA	O1A-CGA-O2A-C1
26	A	835	CLA	C4C-C3C-CAC-CBC
26	A	811	CLA	O1D-CGD-O2D-CED
26	2	606	CLA	O1D-CGD-O2D-CED
26	6	617	CLA	O1D-CGD-O2D-CED
26	Z	612	CLA	O1D-CGD-O2D-CED
37	U	607	CHL	O1D-CGD-O2D-CED
26	A	839	CLA	CBA-CGA-O2A-C1
26	8	604	CLA	CBA-CGA-O2A-C1
26	A	818	CLA	O1A-CGA-O2A-C1
26	A	821	CLA	O1A-CGA-O2A-C1
26	B	831	CLA	O1A-CGA-O2A-C1
26	L	303	CLA	O1A-CGA-O2A-C1
26	2	613	CLA	O1A-CGA-O2A-C1
26	5	603	CLA	O1A-CGA-O2A-C1
26	5	607	CLA	O1A-CGA-O2A-C1
26	6	616	CLA	O1A-CGA-O2A-C1
26	8	604	CLA	O1A-CGA-O2A-C1
26	8	613	CLA	O1A-CGA-O2A-C1
26	Z	603	CLA	O1A-CGA-O2A-C1
26	A	815	CLA	O1D-CGD-O2D-CED
26	B	806	CLA	O1D-CGD-O2D-CED
26	B	814	CLA	O1D-CGD-O2D-CED
26	K	206	CLA	O1D-CGD-O2D-CED
26	2	601	CLA	O1D-CGD-O2D-CED
26	2	604	CLA	O1D-CGD-O2D-CED
26	3	604	CLA	O1D-CGD-O2D-CED
26	V	613	CLA	O1D-CGD-O2D-CED
26	V	614	CLA	O1D-CGD-O2D-CED
37	Z	608	CHL	O1D-CGD-O2D-CED
26	B	822	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	4	614	CLA	O1D-CGD-O2D-CED
26	5	607	CLA	O1D-CGD-O2D-CED
26	6	614	CLA	O1D-CGD-O2D-CED
26	7	608	CLA	O1D-CGD-O2D-CED
26	7	612	CLA	O1D-CGD-O2D-CED
26	X	602	CLA	O1D-CGD-O2D-CED
26	Y	604	CLA	O1D-CGD-O2D-CED
26	W	614	CLA	O1D-CGD-O2D-CED
26	B	829	CLA	CBD-CGD-O2D-CED
26	Y	613	CLA	CBD-CGD-O2D-CED
26	A	822	CLA	O1A-CGA-O2A-C1
26	4	609	CLA	O1A-CGA-O2A-C1
28	9	623	LHG	O9-C7-O7-C5
32	H	205	LMG	O9-C10-O7-C8
26	B	821	CLA	O1A-CGA-O2A-C1
26	A	818	CLA	C3-C5-C6-C7
26	B	806	CLA	C3-C5-C6-C7
26	B	808	CLA	C3-C5-C6-C7
26	B	811	CLA	C3-C5-C6-C7
26	B	817	CLA	C3-C5-C6-C7
26	B	829	CLA	C3-C5-C6-C7
26	B	834	CLA	C3-C5-C6-C7
26	B	839	CLA	C3-C5-C6-C7
26	F	301	CLA	C3-C5-C6-C7
26	1	611	CLA	C3-C5-C6-C7
26	1	613	CLA	C3-C5-C6-C7
26	a	609	CLA	C3-C5-C6-C7
26	a	613	CLA	C3-C5-C6-C7
26	2	610	CLA	C3-C5-C6-C7
26	3	603	CLA	C3-C5-C6-C7
26	3	607	CLA	C3-C5-C6-C7
26	4	601	CLA	C3-C5-C6-C7
26	5	603	CLA	C3-C5-C6-C7
26	6	601	CLA	C3-C5-C6-C7
26	6	604	CLA	C3-C5-C6-C7
26	7	613	CLA	C3-C5-C6-C7
26	8	601	CLA	C3-C5-C6-C7
26	8	606	CLA	C3-C5-C6-C7
26	Z	603	CLA	C3-C5-C6-C7
27	A	844	PQN	C13-C15-C16-C17
37	Y	601	CHL	C3-C5-C6-C7
37	Z	601	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
37	W	601	CHL	C3-C5-C6-C7
26	B	813	CLA	C4C-C3C-CAC-CBC
26	A	834	CLA	CBA-CGA-O2A-C1
26	1	611	CLA	CBA-CGA-O2A-C1
26	3	603	CLA	CBA-CGA-O2A-C1
26	4	601	CLA	CBA-CGA-O2A-C1
26	4	604	CLA	CBA-CGA-O2A-C1
26	5	603	CLA	CBA-CGA-O2A-C1
26	8	613	CLA	CBA-CGA-O2A-C1
26	9	604	CLA	CBA-CGA-O2A-C1
28	A	846	LHG	C24-C23-O8-C6
32	H	205	LMG	O6-C5-C6-O5
26	A	816	CLA	CBD-CGD-O2D-CED
26	A	818	CLA	CBD-CGD-O2D-CED
26	A	827	CLA	CBD-CGD-O2D-CED
26	A	838	CLA	CBD-CGD-O2D-CED
26	B	813	CLA	CBD-CGD-O2D-CED
26	F	303	CLA	CBD-CGD-O2D-CED
26	F	304	CLA	CBD-CGD-O2D-CED
26	H	203	CLA	CBD-CGD-O2D-CED
26	3	608	CLA	CBD-CGD-O2D-CED
26	4	603	CLA	CBD-CGD-O2D-CED
26	4	604	CLA	CBD-CGD-O2D-CED
26	4	607	CLA	CBD-CGD-O2D-CED
26	4	616	CLA	CBD-CGD-O2D-CED
26	5	610	CLA	CBD-CGD-O2D-CED
26	6	602	CLA	CBD-CGD-O2D-CED
26	6	616	CLA	CBD-CGD-O2D-CED
26	6	620	CLA	CBD-CGD-O2D-CED
26	7	602	CLA	CBD-CGD-O2D-CED
26	8	602	CLA	CBD-CGD-O2D-CED
26	8	616	CLA	CBD-CGD-O2D-CED
26	9	604	CLA	CBD-CGD-O2D-CED
26	Y	603	CLA	CBD-CGD-O2D-CED
26	Y	612	CLA	CBD-CGD-O2D-CED
26	Z	614	CLA	CBD-CGD-O2D-CED
26	U	610	CLA	CBD-CGD-O2D-CED
26	V	611	CLA	CBD-CGD-O2D-CED
26	W	604	CLA	CBD-CGD-O2D-CED
26	W	610	CLA	CBD-CGD-O2D-CED
37	X	605	CHL	CBD-CGD-O2D-CED
32	8	626	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
33	B	850	DGD	C2B-C1B-O2G-C2G
26	A	810	CLA	O1D-CGD-O2D-CED
26	B	809	CLA	O1D-CGD-O2D-CED
26	2	612	CLA	O1D-CGD-O2D-CED
26	5	608	CLA	O1D-CGD-O2D-CED
26	8	606	CLA	O1D-CGD-O2D-CED
26	8	607	CLA	O1D-CGD-O2D-CED
26	X	612	CLA	O1D-CGD-O2D-CED
37	Z	607	CHL	O1D-CGD-O2D-CED
37	V	608	CHL	O1D-CGD-O2D-CED
26	Y	614	CLA	O1A-CGA-O2A-C1
26	6	608	CLA	O1D-CGD-O2D-CED
26	A	818	CLA	C4-C3-C5-C6
26	A	842	CLA	C4-C3-C5-C6
26	B	818	CLA	C4-C3-C5-C6
37	Z	601	CHL	C4-C3-C5-C6
26	A	842	CLA	C2-C3-C5-C6
26	L	303	CLA	C2-C3-C5-C6
26	Z	610	CLA	C2-C3-C5-C6
37	Z	601	CHL	C2-C3-C5-C6
26	A	854	CLA	O1D-CGD-O2D-CED
26	K	204	CLA	O1D-CGD-O2D-CED
26	1	604	CLA	O1D-CGD-O2D-CED
26	a	604	CLA	O1D-CGD-O2D-CED
26	V	604	CLA	O1D-CGD-O2D-CED
26	A	805	CLA	C3-C5-C6-C7
26	A	809	CLA	C2A-CAA-CBA-CGA
26	B	824	CLA	C2A-CAA-CBA-CGA
26	3	609	CLA	C2A-CAA-CBA-CGA
37	Z	606	CHL	C2A-CAA-CBA-CGA
26	Y	603	CLA	O1A-CGA-O2A-C1
28	3	624	LHG	O10-C23-O8-C6
26	A	854	CLA	C3-C5-C6-C7
26	B	809	CLA	C3-C5-C6-C7
26	B	816	CLA	C3-C5-C6-C7
26	1	603	CLA	C3-C5-C6-C7
26	a	603	CLA	C3-C5-C6-C7
26	2	601	CLA	C3-C5-C6-C7
26	4	602	CLA	C3-C5-C6-C7
37	X	601	CHL	C3-C5-C6-C7
26	A	818	CLA	CBA-CGA-O2A-C1
26	A	821	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	A	822	CLA	CBA-CGA-O2A-C1
26	B	802	CLA	CBA-CGA-O2A-C1
26	B	831	CLA	CBA-CGA-O2A-C1
26	L	303	CLA	CBA-CGA-O2A-C1
26	2	602	CLA	CBA-CGA-O2A-C1
26	2	613	CLA	CBA-CGA-O2A-C1
26	3	610	CLA	CBA-CGA-O2A-C1
26	4	609	CLA	CBA-CGA-O2A-C1
26	4	614	CLA	CBA-CGA-O2A-C1
26	5	607	CLA	CBA-CGA-O2A-C1
26	6	616	CLA	CBA-CGA-O2A-C1
26	7	604	CLA	CBA-CGA-O2A-C1
26	Y	614	CLA	CBA-CGA-O2A-C1
26	Z	603	CLA	CBA-CGA-O2A-C1
28	3	624	LHG	C24-C23-O8-C6
37	U	601	CHL	CBA-CGA-O2A-C1
27	A	844	PQN	C11-C12-C13-C14
31	8	625	LMU	O5'-C5'-C6'-O6'
35	Z	1622	XAT	C13-C14-C15-C35
36	X	1623	NEX	C9-C10-C11-C12
26	A	843	CLA	O1A-CGA-O2A-C1
26	1	611	CLA	O1A-CGA-O2A-C1
26	3	603	CLA	O1A-CGA-O2A-C1
26	3	610	CLA	O1A-CGA-O2A-C1
26	4	604	CLA	O1A-CGA-O2A-C1
26	4	614	CLA	O1A-CGA-O2A-C1
26	7	613	CLA	O1A-CGA-O2A-C1
28	A	846	LHG	O10-C23-O8-C6
32	J	104	LMG	O10-C28-O8-C9
32	4	623	LMG	O10-C28-O8-C9
26	A	835	CLA	C2C-C3C-CAC-CBC
32	L	2631	LMG	O9-C10-O7-C8
26	V	603	CLA	O1D-CGD-O2D-CED
37	U	606	CHL	O1D-CGD-O2D-CED
37	U	608	CHL	O1D-CGD-O2D-CED
27	A	844	PQN	C15-C16-C17-C18
26	B	821	CLA	CBA-CGA-O2A-C1
31	K	208	LMU	O5'-C5'-C6'-O6'
26	B	813	CLA	C2C-C3C-CAC-CBC
26	A	845	CLA	O1D-CGD-O2D-CED
26	B	840	CLA	O1D-CGD-O2D-CED
26	B	813	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	B	826	CLA	C3-C5-C6-C7
26	1	601	CLA	C3-C5-C6-C7
26	a	601	CLA	C3-C5-C6-C7
26	A	825	CLA	CBD-CGD-O2D-CED
26	B	824	CLA	CBD-CGD-O2D-CED
26	1	610	CLA	CBD-CGD-O2D-CED
26	a	610	CLA	CBD-CGD-O2D-CED
26	4	602	CLA	CBD-CGD-O2D-CED
26	8	604	CLA	CBD-CGD-O2D-CED
26	9	601	CLA	CBD-CGD-O2D-CED
26	X	604	CLA	CBD-CGD-O2D-CED
26	Y	611	CLA	CBD-CGD-O2D-CED
28	5	625	LHG	O2-C2-C3-O3
28	6	623	LHG	O2-C2-C3-O3
28	7	622	LHG	O2-C2-C3-O3
28	W	2630	LHG	O2-C2-C3-O3
26	3	610	CLA	O1D-CGD-O2D-CED
26	5	603	CLA	O1D-CGD-O2D-CED
26	U	614	CLA	O1D-CGD-O2D-CED
26	W	603	CLA	O1D-CGD-O2D-CED
37	Y	608	CHL	O1D-CGD-O2D-CED
26	A	805	CLA	CBA-CGA-O2A-C1
26	A	816	CLA	CBA-CGA-O2A-C1
26	A	843	CLA	CBA-CGA-O2A-C1
37	Y	601	CHL	CBA-CGA-O2A-C1
26	A	834	CLA	O1A-CGA-O2A-C1
26	2	602	CLA	O1A-CGA-O2A-C1
26	4	601	CLA	O1A-CGA-O2A-C1
37	U	601	CHL	O1A-CGA-O2A-C1
26	A	802	CLA	O1D-CGD-O2D-CED
26	A	831	CLA	O1D-CGD-O2D-CED
26	B	810	CLA	O1D-CGD-O2D-CED
26	B	816	CLA	O1D-CGD-O2D-CED
26	4	608	CLA	O1D-CGD-O2D-CED
37	V	607	CHL	O1D-CGD-O2D-CED
26	A	837	CLA	CBD-CGD-O2D-CED
26	5	602	CLA	CBD-CGD-O2D-CED
26	7	613	CLA	CBD-CGD-O2D-CED
28	3	623	LHG	C8-C7-O7-C5
31	5	629	LMU	O5B-C1B-O1B-C4'
26	7	604	CLA	O1A-CGA-O2A-C1
37	Y	601	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	H	205	LMG	C4-C5-C6-O5
26	A	807	CLA	C3-C5-C6-C7
26	A	828	CLA	C3-C5-C6-C7
26	Z	613	CLA	C3-C5-C6-C7
26	V	613	CLA	C3-C5-C6-C7
26	J	101	CLA	CBD-CGD-O2D-CED
26	4	611	CLA	CBD-CGD-O2D-CED
26	4	613	CLA	CBD-CGD-O2D-CED
26	9	614	CLA	CBD-CGD-O2D-CED
26	U	612	CLA	CBD-CGD-O2D-CED
26	U	603	CLA	O1D-CGD-O2D-CED
26	7	613	CLA	CBA-CGA-O2A-C1
26	Y	603	CLA	CBA-CGA-O2A-C1
32	J	104	LMG	C29-C28-O8-C9
32	4	623	LMG	C29-C28-O8-C9
26	B	817	CLA	C4-C3-C5-C6
26	B	818	CLA	C2-C3-C5-C6
31	A	857	LMU	O5B-C5B-C6B-O6B
26	A	807	CLA	CBD-CGD-O2D-CED
26	8	601	CLA	CBD-CGD-O2D-CED
26	U	604	CLA	CBD-CGD-O2D-CED
26	B	831	CLA	C2A-CAA-CBA-CGA
26	A	835	CLA	O1D-CGD-O2D-CED
26	A	805	CLA	O1A-CGA-O2A-C1
26	A	816	CLA	O1A-CGA-O2A-C1
26	B	802	CLA	O1A-CGA-O2A-C1
31	5	628	LMU	O5'-C1'-O1'-C1
31	8	625	LMU	O5'-C1'-O1'-C1
26	B	839	CLA	O1D-CGD-O2D-CED
26	Y	614	CLA	O1D-CGD-O2D-CED
26	A	830	CLA	CBA-CGA-O2A-C1
26	B	825	CLA	CBA-CGA-O2A-C1
26	B	837	CLA	CBA-CGA-O2A-C1
26	6	614	CLA	CBA-CGA-O2A-C1
26	9	613	CLA	CBA-CGA-O2A-C1
26	A	812	CLA	CBD-CGD-O2D-CED
26	A	839	CLA	CBD-CGD-O2D-CED
26	B	836	CLA	CBD-CGD-O2D-CED
26	K	203	CLA	CBD-CGD-O2D-CED
26	5	604	CLA	CBD-CGD-O2D-CED
26	7	606	CLA	CBD-CGD-O2D-CED
26	9	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	V	612	CLA	CBD-CGD-O2D-CED
37	X	609	CHL	CBD-CGD-O2D-CED
37	Z	609	CHL	CBD-CGD-O2D-CED
37	V	606	CHL	CBD-CGD-O2D-CED
26	6	616	CLA	C2C-C3C-CAC-CBC
31	K	208	LMU	C4'-C5'-C6'-O6'
31	5	629	LMU	O5B-C5B-C6B-O6B
28	1	620	LHG	C14-C15-C16-C17
26	8	614	CLA	CBD-CGD-O2D-CED
26	Z	603	CLA	CBD-CGD-O2D-CED
37	Z	606	CHL	CBD-CGD-O2D-CED
26	6	613	CLA	C3-C5-C6-C7
26	Y	613	CLA	O1D-CGD-O2D-CED
31	8	625	LMU	C4'-C5'-C6'-O6'
26	A	830	CLA	O1A-CGA-O2A-C1
26	B	837	CLA	O1A-CGA-O2A-C1
26	6	614	CLA	O1A-CGA-O2A-C1
28	X	2630	LHG	C1-C2-C3-O3
26	A	801	CLA	CBA-CGA-O2A-C1
26	A	814	CLA	CBA-CGA-O2A-C1
26	B	805	CLA	CBA-CGA-O2A-C1
26	B	811	CLA	CBA-CGA-O2A-C1
26	B	813	CLA	CBA-CGA-O2A-C1
26	B	814	CLA	CBA-CGA-O2A-C1
26	B	818	CLA	CBA-CGA-O2A-C1
26	B	840	CLA	CBA-CGA-O2A-C1
26	5	604	CLA	CBA-CGA-O2A-C1
26	X	613	CLA	CBA-CGA-O2A-C1
26	U	602	CLA	CBA-CGA-O2A-C1
26	U	613	CLA	CBA-CGA-O2A-C1
26	W	613	CLA	CBA-CGA-O2A-C1
28	Y	2630	LHG	C24-C23-O8-C6
37	X	601	CHL	CBA-CGA-O2A-C1
37	X	608	CHL	CBA-CGA-O2A-C1
37	Z	601	CHL	CBA-CGA-O2A-C1
26	A	821	CLA	CBD-CGD-O2D-CED
26	A	818	CLA	O1D-CGD-O2D-CED
26	A	832	CLA	O1D-CGD-O2D-CED
26	B	829	CLA	O1D-CGD-O2D-CED
26	F	303	CLA	O1D-CGD-O2D-CED
26	4	603	CLA	O1D-CGD-O2D-CED
26	4	616	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	6	616	CLA	O1D-CGD-O2D-CED
26	U	602	CLA	O1D-CGD-O2D-CED
31	5	629	LMU	C4B-C5B-C6B-O6B
31	A	858	LMU	C5'-C4'-O1B-C1B
37	X	601	CHL	O1A-CGA-O2A-C1
26	5	613	CLA	C4-C3-C5-C6
26	8	610	CLA	C4-C3-C5-C6
26	B	817	CLA	C2-C3-C5-C6
26	5	613	CLA	C2-C3-C5-C6
26	8	610	CLA	C2-C3-C5-C6
26	B	814	CLA	C3-C5-C6-C7
26	A	841	CLA	CBD-CGD-O2D-CED
26	A	807	CLA	C11-C10-C8-C9
26	A	828	CLA	C6-C7-C8-C9
26	A	829	CLA	C14-C13-C15-C16
26	B	841	CLA	C11-C10-C8-C9
26	5	609	CLA	C6-C7-C8-C9
27	B	842	PQN	C19-C18-C20-C21
37	X	607	CHL	C6-C7-C8-C9
37	X	608	CHL	C6-C7-C8-C9
37	X	609	CHL	C14-C13-C15-C16
37	Z	601	CHL	C6-C7-C8-C9
37	Z	609	CHL	C6-C7-C8-C9
37	W	601	CHL	C6-C7-C8-C9
31	A	857	LMU	C4B-C5B-C6B-O6B
26	B	813	CLA	O1D-CGD-O2D-CED
31	8	625	LMU	C2'-C1'-O1'-C1
28	8	622	LHG	O2-C2-C3-O3
28	X	2630	LHG	O2-C2-C3-O3
28	U	2630	LHG	O2-C2-C3-O3
26	H	203	CLA	O1D-CGD-O2D-CED
26	8	616	CLA	O1D-CGD-O2D-CED
37	X	605	CHL	O1D-CGD-O2D-CED
26	B	814	CLA	O1A-CGA-O2A-C1
26	B	818	CLA	O1A-CGA-O2A-C1
26	5	604	CLA	O1A-CGA-O2A-C1
26	W	613	CLA	O1A-CGA-O2A-C1
26	U	610	CLA	O1D-CGD-O2D-CED
29	B	847	BCR	C37-C22-C23-C24
29	B	848	BCR	C37-C22-C23-C24
29	B	849	BCR	C37-C22-C23-C24
29	B	852	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
29	B	852	BCR	C11-C12-C13-C35
29	L	305	BCR	C7-C8-C9-C34
29	L	308	BCR	C7-C8-C9-C34
29	L	308	BCR	C36-C18-C19-C20
29	9	621	BCR	C37-C22-C23-C24
34	1	617	LUT	C7-C8-C9-C19
34	a	617	LUT	C7-C8-C9-C19
34	3	618	LUT	C7-C8-C9-C19
34	4	619	LUT	C7-C8-C9-C19
34	6	619	LUT	C7-C8-C9-C19
34	7	619	LUT	C7-C8-C9-C19
34	9	619	LUT	C7-C8-C9-C19
34	X	1620	LUT	C7-C8-C9-C19
34	Z	1620	LUT	C7-C8-C9-C19
34	U	1620	LUT	C31-C32-C33-C40
34	V	1620	LUT	C7-C8-C9-C19
34	W	1620	LUT	C7-C8-C9-C19
35	X	1622	XAT	C11-C12-C13-C20
35	Z	1622	XAT	C11-C12-C13-C20
35	U	1622	XAT	C11-C12-C13-C20
29	L	305	BCR	C7-C8-C9-C10
34	4	619	LUT	C7-C8-C9-C10
34	6	619	LUT	C7-C8-C9-C10
34	7	619	LUT	C7-C8-C9-C10
34	9	619	LUT	C7-C8-C9-C10
34	X	1620	LUT	C7-C8-C9-C10
34	Z	1620	LUT	C11-C12-C13-C14
34	V	1620	LUT	C7-C8-C9-C10
34	W	1620	LUT	C7-C8-C9-C10
26	B	839	CLA	C2A-CAA-CBA-CGA
37	X	601	CHL	C2A-CAA-CBA-CGA
26	A	814	CLA	O1A-CGA-O2A-C1
37	Z	601	CHL	O1A-CGA-O2A-C1
32	V	2631	LMG	O6-C5-C6-O5
26	2	613	CLA	C15-C16-C17-C18
26	A	830	CLA	CBD-CGD-O2D-CED
26	1	609	CLA	CBD-CGD-O2D-CED
26	W	613	CLA	CBD-CGD-O2D-CED
28	7	622	LHG	O7-C5-C6-O8
26	A	810	CLA	CBA-CGA-O2A-C1
26	A	832	CLA	CBA-CGA-O2A-C1
26	B	828	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	5	602	CLA	CBA-CGA-O2A-C1
26	8	601	CLA	CBA-CGA-O2A-C1
26	W	610	CLA	C5-C6-C7-C8
27	A	844	PQN	C23-C25-C26-C27
37	X	601	CHL	C5-C6-C7-C8
37	X	607	CHL	C13-C15-C16-C17
28	Y	2630	LHG	O10-C23-O8-C6
26	F	304	CLA	O1D-CGD-O2D-CED
26	3	608	CLA	O1D-CGD-O2D-CED
26	9	604	CLA	O1D-CGD-O2D-CED
26	Y	603	CLA	O1D-CGD-O2D-CED
26	Z	614	CLA	O1D-CGD-O2D-CED
26	W	610	CLA	O1D-CGD-O2D-CED
26	A	828	CLA	C10-C11-C12-C13
26	B	814	CLA	C10-C11-C12-C13
26	B	824	CLA	C10-C11-C12-C13
26	B	833	CLA	C15-C16-C17-C18
26	5	613	CLA	C13-C15-C16-C17
26	8	601	CLA	C15-C16-C17-C18
26	8	610	CLA	C8-C10-C11-C12
26	Z	610	CLA	C8-C10-C11-C12
37	U	601	CHL	C8-C10-C11-C12
26	3	609	CLA	C3-C5-C6-C7
26	Y	613	CLA	C3-C5-C6-C7
26	A	827	CLA	O1D-CGD-O2D-CED
26	B	804	CLA	CBD-CGD-O2D-CED
26	L	304	CLA	CBD-CGD-O2D-CED
26	B	839	CLA	C11-C10-C8-C7
26	H	203	CLA	C12-C13-C15-C16
26	A	816	CLA	O1D-CGD-O2D-CED
37	U	601	CHL	C4-C3-C5-C6
26	B	833	CLA	C8-C10-C11-C12
26	a	609	CLA	C5-C6-C7-C8
26	5	602	CLA	C8-C10-C11-C12
37	V	601	CHL	C13-C15-C16-C17
28	6	623	LHG	C23-C24-C25-C26
28	3	623	LHG	O9-C7-O7-C5
26	6	602	CLA	O1D-CGD-O2D-CED
26	V	602	CLA	C10-C11-C12-C13
26	W	602	CLA	C10-C11-C12-C13
26	Y	612	CLA	O1D-CGD-O2D-CED
31	5	629	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
28	5	623	LHG	C7-C8-C9-C10
28	X	2630	LHG	C7-C8-C9-C10
28	V	2630	LHG	C23-C24-C25-C26
32	4	624	LMG	C28-C29-C30-C31
26	A	832	CLA	O1A-CGA-O2A-C1
26	B	813	CLA	O1A-CGA-O2A-C1
26	B	840	CLA	O1A-CGA-O2A-C1
26	X	613	CLA	O1A-CGA-O2A-C1
26	U	613	CLA	O1A-CGA-O2A-C1
26	3	609	CLA	CBD-CGD-O2D-CED
26	V	611	CLA	O1D-CGD-O2D-CED
26	A	824	CLA	C10-C11-C12-C13
26	A	828	CLA	C13-C15-C16-C17
26	A	836	CLA	C5-C6-C7-C8
26	B	828	CLA	C5-C6-C7-C8
26	B	839	CLA	C13-C15-C16-C17
26	B	839	CLA	C15-C16-C17-C18
26	3	603	CLA	C5-C6-C7-C8
26	3	604	CLA	C15-C16-C17-C18
26	6	601	CLA	C13-C15-C16-C17
37	X	607	CHL	C8-C10-C11-C12
37	Z	601	CHL	C5-C6-C7-C8
37	W	609	CHL	C15-C16-C17-C18
26	A	821	CLA	C2A-CAA-CBA-CGA
26	A	833	CLA	C2A-CAA-CBA-CGA
26	A	834	CLA	C2A-CAA-CBA-CGA
26	A	843	CLA	C2A-CAA-CBA-CGA
26	B	809	CLA	C2A-CAA-CBA-CGA
26	4	601	CLA	C2A-CAA-CBA-CGA
26	6	617	CLA	C2A-CAA-CBA-CGA
26	8	601	CLA	C2A-CAA-CBA-CGA
37	X	607	CHL	C2A-CAA-CBA-CGA
37	X	608	CHL	C2A-CAA-CBA-CGA
37	Y	607	CHL	C2A-CAA-CBA-CGA
37	Y	608	CHL	C2A-CAA-CBA-CGA
37	Z	607	CHL	C2A-CAA-CBA-CGA
37	W	605	CHL	C2A-CAA-CBA-CGA
37	W	606	CHL	C2A-CAA-CBA-CGA
37	W	607	CHL	C2A-CAA-CBA-CGA
26	4	604	CLA	O1D-CGD-O2D-CED
26	4	607	CLA	O1D-CGD-O2D-CED
26	7	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	A	802	CLA	C15-C16-C17-C18
26	A	814	CLA	C8-C10-C11-C12
26	A	825	CLA	C10-C11-C12-C13
26	A	829	CLA	C10-C11-C12-C13
26	A	834	CLA	C10-C11-C12-C13
26	B	813	CLA	C5-C6-C7-C8
26	1	613	CLA	C8-C10-C11-C12
26	4	601	CLA	C5-C6-C7-C8
26	6	613	CLA	C5-C6-C7-C8
26	6	616	CLA	C13-C15-C16-C17
26	7	613	CLA	C15-C16-C17-C18
26	Y	603	CLA	C5-C6-C7-C8
27	B	842	PQN	C25-C26-C27-C28
37	X	608	CHL	C13-C15-C16-C17
37	Z	601	CHL	C13-C15-C16-C17
37	U	601	CHL	C13-C15-C16-C17
37	V	601	CHL	C15-C16-C17-C18
28	a	620	LHG	C23-C24-C25-C26
28	5	625	LHG	C7-C8-C9-C10
26	5	610	CLA	O1D-CGD-O2D-CED
26	A	801	CLA	O1A-CGA-O2A-C1
26	U	602	CLA	O1A-CGA-O2A-C1
26	A	814	CLA	CBD-CGD-O2D-CED
26	Y	602	CLA	CBD-CGD-O2D-CED
28	Y	2630	LHG	C24-C25-C26-C27
26	6	620	CLA	O1D-CGD-O2D-CED
26	A	829	CLA	C5-C6-C7-C8
26	A	831	CLA	C10-C11-C12-C13
26	A	841	CLA	C5-C6-C7-C8
26	A	842	CLA	C5-C6-C7-C8
26	B	808	CLA	C5-C6-C7-C8
26	B	816	CLA	C5-C6-C7-C8
26	B	824	CLA	C13-C15-C16-C17
26	B	834	CLA	C8-C10-C11-C12
26	3	607	CLA	C5-C6-C7-C8
26	4	613	CLA	C10-C11-C12-C13
26	5	602	CLA	C10-C11-C12-C13
26	6	601	CLA	C15-C16-C17-C18
26	6	602	CLA	C15-C16-C17-C18
26	6	616	CLA	C8-C10-C11-C12
26	8	610	CLA	C10-C11-C12-C13
26	9	602	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	V	613	CLA	C13-C15-C16-C17
27	B	842	PQN	C15-C16-C17-C18
37	X	608	CHL	C15-C16-C17-C18
37	Y	601	CHL	C5-C6-C7-C8
37	Y	607	CHL	C5-C6-C7-C8
37	Z	607	CHL	C5-C6-C7-C8
37	W	601	CHL	C13-C15-C16-C17
37	W	601	CHL	C15-C16-C17-C18
37	W	609	CHL	C13-C15-C16-C17
26	W	604	CLA	O1D-CGD-O2D-CED
26	B	805	CLA	O1A-CGA-O2A-C1
26	B	811	CLA	O1A-CGA-O2A-C1
26	B	825	CLA	O1A-CGA-O2A-C1
26	9	613	CLA	O1A-CGA-O2A-C1
28	1	620	LHG	C23-C24-C25-C26
28	3	623	LHG	C7-C8-C9-C10
28	7	622	LHG	C23-C24-C25-C26
26	A	820	CLA	C15-C16-C17-C18
37	X	607	CHL	C5-C6-C7-C8
37	Y	607	CHL	C15-C16-C17-C18
37	Y	609	CHL	C8-C10-C11-C12
37	Z	609	CHL	C8-C10-C11-C12
37	V	609	CHL	C8-C10-C11-C12
37	W	609	CHL	C8-C10-C11-C12
26	3	613	CLA	CAA-CBA-CGA-O2A
26	1	610	CLA	O1D-CGD-O2D-CED
26	a	610	CLA	O1D-CGD-O2D-CED
26	8	602	CLA	O1D-CGD-O2D-CED
26	9	601	CLA	O1D-CGD-O2D-CED
26	X	604	CLA	O1D-CGD-O2D-CED
26	A	843	CLA	C10-C11-C12-C13
26	B	809	CLA	C13-C15-C16-C17
26	B	810	CLA	C13-C15-C16-C17
26	L	303	CLA	C8-C10-C11-C12
26	4	601	CLA	C8-C10-C11-C12
26	B	832	CLA	CBD-CGD-O2D-CED
26	5	602	CLA	O1A-CGA-O2A-C1
26	8	601	CLA	O1A-CGA-O2A-C1
37	X	608	CHL	O1A-CGA-O2A-C1
26	A	818	CLA	C2-C3-C5-C6
26	A	837	CLA	O1D-CGD-O2D-CED
26	A	838	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	4	602	CLA	O1D-CGD-O2D-CED
26	A	824	CLA	C13-C15-C16-C17
26	A	831	CLA	C5-C6-C7-C8
26	4	608	CLA	C5-C6-C7-C8
26	5	602	CLA	C13-C15-C16-C17
26	Y	613	CLA	C10-C11-C12-C13
37	X	601	CHL	C8-C10-C11-C12
26	A	811	CLA	CBA-CGA-O2A-C1
26	A	835	CLA	CBA-CGA-O2A-C1
26	5	617	CLA	CBA-CGA-O2A-C1
26	Y	614	CLA	O2A-C1-C2-C3
37	Y	608	CHL	O2A-C1-C2-C3
37	Z	608	CHL	O2A-C1-C2-C3
26	a	603	CLA	CBD-CGD-O2D-CED
28	A	861	LHG	C8-C7-O7-C5
26	A	810	CLA	O1A-CGA-O2A-C1
26	A	854	CLA	C5-C6-C7-C8
26	A	834	CLA	C3-C5-C6-C7
26	9	610	CLA	C8-C10-C11-C12
37	U	606	CHL	C2A-CAA-CBA-CGA
26	B	824	CLA	O1D-CGD-O2D-CED
26	A	816	CLA	C8-C10-C11-C12
26	A	825	CLA	C13-C15-C16-C17
28	A	861	LHG	O9-C7-O7-C5
28	7	622	LHG	C1-C2-C3-O3
26	A	822	CLA	C2A-CAA-CBA-CGA
26	A	854	CLA	C2A-CAA-CBA-CGA
26	B	827	CLA	C2A-CAA-CBA-CGA
26	Z	603	CLA	C2A-CAA-CBA-CGA
26	U	602	CLA	C2A-CAA-CBA-CGA
26	A	825	CLA	O1D-CGD-O2D-CED
26	8	604	CLA	O1D-CGD-O2D-CED
26	A	807	CLA	CBA-CGA-O2A-C1
26	A	820	CLA	CBA-CGA-O2A-C1
26	1	602	CLA	CBA-CGA-O2A-C1
28	9	624	LHG	C24-C23-O8-C6
37	Z	609	CHL	CBA-CGA-O2A-C1
26	A	829	CLA	C13-C15-C16-C17
26	A	829	CLA	C15-C16-C17-C18
26	B	818	CLA	C8-C10-C11-C12
26	1	601	CLA	C5-C6-C7-C8
26	a	601	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	3	609	CLA	C8-C10-C11-C12
26	X	602	CLA	C10-C11-C12-C13
26	W	613	CLA	C5-C6-C7-C8
37	X	609	CHL	C13-C15-C16-C17
37	Z	607	CHL	C13-C15-C16-C17
37	V	601	CHL	C5-C6-C7-C8
37	W	609	CHL	C10-C11-C12-C13
26	B	823	CLA	CBD-CGD-O2D-CED
26	Y	611	CLA	O1D-CGD-O2D-CED
26	A	806	CLA	C5-C6-C7-C8
26	V	613	CLA	C8-C10-C11-C12
37	Y	607	CHL	C13-C15-C16-C17
26	A	806	CLA	C8-C10-C11-C12
26	A	807	CLA	C5-C6-C7-C8
26	B	831	CLA	C15-C16-C17-C18
26	4	608	CLA	C10-C11-C12-C13
26	6	620	CLA	C10-C11-C12-C13
26	7	601	CLA	C8-C10-C11-C12
26	8	602	CLA	C10-C11-C12-C13
37	U	609	CHL	C8-C10-C11-C12
26	4	611	CLA	O1D-CGD-O2D-CED
26	7	613	CLA	O1D-CGD-O2D-CED
26	a	602	CLA	CBA-CGA-O2A-C1
26	B	826	CLA	C13-C15-C16-C17
37	V	605	CHL	C2A-CAA-CBA-CGA
37	V	606	CHL	C2A-CAA-CBA-CGA
28	6	623	LHG	C7-C8-C9-C10
26	B	828	CLA	C13-C15-C16-C17
26	6	604	CLA	C5-C6-C7-C8
26	Z	610	CLA	C5-C6-C7-C8
37	U	601	CHL	C5-C6-C7-C8
26	L	303	CLA	C3-C5-C6-C7
28	O	2631	LHG	C8-C7-O7-C5
28	5	625	LHG	C8-C7-O7-C5
31	K	208	LMU	O5B-C5B-C6B-O6B
26	5	602	CLA	O1D-CGD-O2D-CED
26	9	614	CLA	O1D-CGD-O2D-CED
26	U	612	CLA	O1D-CGD-O2D-CED
28	O	2631	LHG	O9-C7-O7-C5
26	Z	614	CLA	O2A-C1-C2-C3
31	K	208	LMU	C2'-C1'-O1'-C1
32	J	104	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
28	3	623	LHG	C23-C24-C25-C26
26	B	816	CLA	CAA-CBA-CGA-O2A
26	J	101	CLA	O1D-CGD-O2D-CED
26	A	841	CLA	CBA-CGA-O2A-C1
28	7	622	LHG	C24-C23-O8-C6
26	B	828	CLA	O1A-CGA-O2A-C1
26	B	809	CLA	C15-C16-C17-C18
26	B	833	CLA	C13-C15-C16-C17
37	X	609	CHL	C5-C6-C7-C8
29	2	623	BCR	C7-C8-C9-C34
34	2	619	LUT	C7-C8-C9-C19
34	8	619	LUT	C7-C8-C9-C19
34	Z	1620	LUT	C11-C12-C13-C20
34	U	1620	LUT	C7-C8-C9-C19
34	W	1620	LUT	C27-C28-C29-C39
34	W	1621	LUT	C7-C8-C9-C19
35	Y	1622	XAT	C11-C12-C13-C20
35	U	1622	XAT	C31-C32-C33-C40
36	Z	1623	NEX	C31-C32-C33-C40
29	B	849	BCR	C21-C22-C23-C24
29	B	852	BCR	C11-C12-C13-C14
34	1	617	LUT	C7-C8-C9-C10
34	a	617	LUT	C7-C8-C9-C10
34	2	619	LUT	C7-C8-C9-C10
34	3	618	LUT	C7-C8-C9-C10
34	8	619	LUT	C7-C8-C9-C10
34	Z	1620	LUT	C7-C8-C9-C10
34	U	1620	LUT	C7-C8-C9-C10
28	Y	2630	LHG	C11-C10-C9-C8
26	A	818	CLA	C2A-CAA-CBA-CGA
26	A	832	CLA	C2A-CAA-CBA-CGA
26	A	841	CLA	C2A-CAA-CBA-CGA
26	B	811	CLA	C2A-CAA-CBA-CGA
26	6	616	CLA	C2A-CAA-CBA-CGA
26	9	613	CLA	C2A-CAA-CBA-CGA
26	Y	610	CLA	C2A-CAA-CBA-CGA
26	Y	614	CLA	C2A-CAA-CBA-CGA
37	X	605	CHL	C2A-CAA-CBA-CGA
37	Z	608	CHL	C2A-CAA-CBA-CGA
37	V	607	CHL	C2A-CAA-CBA-CGA
37	W	608	CHL	CBA-CGA-O2A-C1
26	5	613	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	6	610	CLA	C8-C10-C11-C12
28	W	2630	LHG	O1-C1-C2-C3
31	8	625	LMU	C3'-C4'-O1B-C1B
36	V	1623	NEX	C9-C10-C11-C12
26	B	808	CLA	C16-C17-C18-C20
37	X	608	CHL	C16-C17-C18-C20
37	Y	607	CHL	C16-C17-C18-C19
37	Z	607	CHL	C16-C17-C18-C19
37	Z	609	CHL	C16-C17-C18-C20
37	U	601	CHL	C16-C17-C18-C19
37	W	609	CHL	C16-C17-C18-C19
26	A	807	CLA	O1D-CGD-O2D-CED
26	4	613	CLA	O1D-CGD-O2D-CED
26	8	601	CLA	O1D-CGD-O2D-CED
26	A	811	CLA	O1A-CGA-O2A-C1
26	A	820	CLA	O1A-CGA-O2A-C1
26	A	835	CLA	O1A-CGA-O2A-C1
26	5	617	CLA	O1A-CGA-O2A-C1
26	A	802	CLA	C3-C5-C6-C7
26	X	613	CLA	C3-C5-C6-C7
28	5	625	LHG	O9-C7-O7-C5
28	3	624	LHG	O6-C4-C5-O7
32	J	104	LMG	O6-C1-O1-C7
26	B	827	CLA	C10-C11-C12-C13
26	U	604	CLA	O1D-CGD-O2D-CED
26	A	804	CLA	CBA-CGA-O2A-C1
26	A	842	CLA	CBA-CGA-O2A-C1
26	6	602	CLA	CBA-CGA-O2A-C1
26	V	604	CLA	CBA-CGA-O2A-C1
26	B	837	CLA	C13-C15-C16-C17
26	3	610	CLA	C8-C10-C11-C12
37	X	609	CHL	C15-C16-C17-C18
37	Z	605	CHL	CBD-CGD-O2D-CED
26	A	842	CLA	C16-C17-C18-C20
26	B	808	CLA	C16-C17-C18-C19
26	3	603	CLA	C6-C7-C8-C9
26	5	613	CLA	C16-C17-C18-C20
26	6	604	CLA	C16-C17-C18-C19
37	X	601	CHL	C16-C17-C18-C19
37	X	609	CHL	C16-C17-C18-C19
37	Y	601	CHL	C16-C17-C18-C19
37	Y	609	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
37	Z	601	CHL	C16-C17-C18-C19
37	V	609	CHL	C11-C12-C13-C14
37	W	607	CHL	C16-C17-C18-C20
26	A	812	CLA	O1D-CGD-O2D-CED
32	4	624	LMG	O6-C5-C6-O5
32	9	625	LMG	C19-C20-C21-C22
26	5	604	CLA	O1D-CGD-O2D-CED
26	A	829	CLA	C8-C10-C11-C12
37	Z	601	CHL	C15-C16-C17-C18
28	5	623	LHG	C11-C12-C13-C14
28	7	622	LHG	C11-C12-C13-C14
28	8	622	LHG	C15-C16-C17-C18
31	8	625	LMU	C5'-C4'-O1B-C1B
26	B	841	CLA	CBA-CGA-O2A-C1
28	H	204	LHG	C24-C23-O8-C6
28	9	624	LHG	C30-C31-C32-C33
28	1	620	LHG	O1-C1-C2-O2
28	a	620	LHG	O1-C1-C2-O2
28	Z	2630	LHG	O1-C1-C2-O2
31	K	208	LMU	C2-C1-O1'-C1'
28	6	623	LHG	C27-C28-C29-C30
26	K	203	CLA	O1D-CGD-O2D-CED
26	9	607	CLA	O1D-CGD-O2D-CED
26	V	612	CLA	O1D-CGD-O2D-CED
26	A	812	CLA	C4B-C3B-CAB-CBB
26	A	821	CLA	C4B-C3B-CAB-CBB
26	A	835	CLA	C4B-C3B-CAB-CBB
26	A	837	CLA	C4B-C3B-CAB-CBB
26	A	841	CLA	C4B-C3B-CAB-CBB
26	B	802	CLA	C4B-C3B-CAB-CBB
26	B	837	CLA	C4B-C3B-CAB-CBB
26	F	303	CLA	C4B-C3B-CAB-CBB
26	F	304	CLA	C4B-C3B-CAB-CBB
26	H	202	CLA	C4B-C3B-CAB-CBB
26	1	607	CLA	C4B-C3B-CAB-CBB
26	a	607	CLA	C4B-C3B-CAB-CBB
26	a	609	CLA	C4B-C3B-CAB-CBB
26	2	609	CLA	C4B-C3B-CAB-CBB
26	5	617	CLA	C4B-C3B-CAB-CBB
26	6	608	CLA	C4B-C3B-CAB-CBB
26	6	614	CLA	C4B-C3B-CAB-CBB
26	6	620	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	8	601	CLA	C4B-C3B-CAB-CBB
26	9	601	CLA	C4B-C3B-CAB-CBB
26	9	607	CLA	C4B-C3B-CAB-CBB
26	9	614	CLA	C4B-C3B-CAB-CBB
26	Y	612	CLA	C4B-C3B-CAB-CBB
26	V	603	CLA	C4B-C3B-CAB-CBB
26	V	613	CLA	C4B-C3B-CAB-CBB
26	W	611	CLA	C4B-C3B-CAB-CBB
26	A	831	CLA	C16-C17-C18-C20
26	3	603	CLA	C6-C7-C8-C10
26	5	613	CLA	C16-C17-C18-C19
26	Y	603	CLA	C6-C7-C8-C9
26	Y	603	CLA	C6-C7-C8-C10
26	W	602	CLA	C11-C12-C13-C14
37	X	608	CHL	C16-C17-C18-C19
37	X	609	CHL	C16-C17-C18-C20
37	Y	601	CHL	C16-C17-C18-C20
37	Y	607	CHL	C16-C17-C18-C20
37	Z	607	CHL	C16-C17-C18-C20
37	Z	609	CHL	C16-C17-C18-C19
37	W	609	CHL	C16-C17-C18-C20
26	7	606	CLA	O1D-CGD-O2D-CED
26	5	616	CLA	C2A-CAA-CBA-CGA
26	7	613	CLA	C2A-CAA-CBA-CGA
26	8	613	CLA	C2A-CAA-CBA-CGA
26	9	614	CLA	C2A-CAA-CBA-CGA
37	U	607	CHL	C2A-CAA-CBA-CGA
26	B	802	CLA	C5-C6-C7-C8
37	X	607	CHL	C10-C11-C12-C13
28	3	624	LHG	C8-C7-O7-C5
26	A	807	CLA	C11-C10-C8-C7
26	B	833	CLA	C6-C7-C8-C10
26	a	609	CLA	C12-C13-C15-C16
26	8	613	CLA	C11-C10-C8-C7
26	V	613	CLA	C6-C7-C8-C10
37	X	608	CHL	C6-C7-C8-C10
37	U	601	CHL	C6-C7-C8-C10
37	V	601	CHL	C11-C12-C13-C15
32	V	2631	LMG	C10-C11-C12-C13
32	H	205	LMG	C31-C32-C33-C34
26	1	602	CLA	O1A-CGA-O2A-C1
26	a	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	A	812	CLA	C3A-C2A-CAA-CBA
26	A	833	CLA	C3A-C2A-CAA-CBA
26	A	845	CLA	C3A-C2A-CAA-CBA
26	B	809	CLA	C3A-C2A-CAA-CBA
26	B	815	CLA	C3A-C2A-CAA-CBA
26	B	826	CLA	C3A-C2A-CAA-CBA
26	K	201	CLA	C3A-C2A-CAA-CBA
26	K	203	CLA	C3A-C2A-CAA-CBA
26	a	606	CLA	C3A-C2A-CAA-CBA
26	2	612	CLA	C3A-C2A-CAA-CBA
26	3	603	CLA	C3A-C2A-CAA-CBA
26	4	601	CLA	C3A-C2A-CAA-CBA
26	5	617	CLA	C3A-C2A-CAA-CBA
26	6	616	CLA	C3A-C2A-CAA-CBA
26	6	620	CLA	C3A-C2A-CAA-CBA
26	7	616	CLA	C3A-C2A-CAA-CBA
26	8	614	CLA	C3A-C2A-CAA-CBA
26	8	616	CLA	C3A-C2A-CAA-CBA
26	Y	603	CLA	C3A-C2A-CAA-CBA
26	Y	611	CLA	C3A-C2A-CAA-CBA
26	Z	603	CLA	C3A-C2A-CAA-CBA
37	X	607	CHL	C3A-C2A-CAA-CBA
37	Z	607	CHL	C3A-C2A-CAA-CBA
28	6	623	LHG	C28-C29-C30-C31
32	8	626	LMG	C17-C18-C19-C20
26	A	842	CLA	C15-C16-C17-C18
26	B	831	CLA	C13-C15-C16-C17
37	V	606	CHL	O1D-CGD-O2D-CED
28	5	625	LHG	C27-C28-C29-C30
26	A	831	CLA	C16-C17-C18-C19
26	W	602	CLA	C11-C12-C13-C15
37	X	607	CHL	C16-C17-C18-C19
37	Y	609	CHL	C16-C17-C18-C20
37	V	601	CHL	C16-C17-C18-C20
37	V	609	CHL	C11-C12-C13-C15
26	A	807	CLA	O1A-CGA-O2A-C1
26	1	613	CLA	CBD-CGD-O2D-CED
26	a	613	CLA	CBD-CGD-O2D-CED
26	2	613	CLA	CBD-CGD-O2D-CED
31	8	625	LMU	C4-C5-C6-C7
28	5	625	LHG	C1-C2-C3-O3
37	X	609	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	J	103	LMG	C7-C8-C9-O8
28	8	622	LHG	C9-C10-C11-C12
28	Z	2630	LHG	C10-C11-C12-C13
31	A	857	LMU	C6-C7-C8-C9
32	9	625	LMG	C12-C13-C14-C15
26	4	613	CLA	C3-C5-C6-C7
26	2	610	CLA	C5-C6-C7-C8
28	A	861	LHG	C17-C18-C19-C20
28	7	622	LHG	C10-C11-C12-C13
28	8	622	LHG	C29-C30-C31-C32
28	9	624	LHG	C28-C29-C30-C31
28	U	2630	LHG	C27-C28-C29-C30
31	5	628	LMU	C6-C7-C8-C9
26	A	841	CLA	O1A-CGA-O2A-C1
37	Z	609	CHL	O1A-CGA-O2A-C1
31	A	857	LMU	C11-C10-C9-C8
31	A	858	LMU	C1-C2-C3-C4
26	B	836	CLA	O1D-CGD-O2D-CED
37	Z	606	CHL	O1D-CGD-O2D-CED
26	4	601	CLA	C16-C17-C18-C20
26	6	604	CLA	C16-C17-C18-C20
37	U	601	CHL	C16-C17-C18-C20
37	W	607	CHL	C16-C17-C18-C19
26	A	821	CLA	C2B-C3B-CAB-CBB
26	A	825	CLA	C2B-C3B-CAB-CBB
26	A	837	CLA	C2B-C3B-CAB-CBB
26	B	830	CLA	C2B-C3B-CAB-CBB
26	F	303	CLA	C2B-C3B-CAB-CBB
26	H	202	CLA	C2B-C3B-CAB-CBB
26	J	101	CLA	C2B-C3B-CAB-CBB
26	O	2003	CLA	C2B-C3B-CAB-CBB
26	1	601	CLA	C2B-C3B-CAB-CBB
26	1	603	CLA	C2B-C3B-CAB-CBB
26	1	607	CLA	C2B-C3B-CAB-CBB
26	a	601	CLA	C2B-C3B-CAB-CBB
26	a	603	CLA	C2B-C3B-CAB-CBB
26	a	607	CLA	C2B-C3B-CAB-CBB
26	a	609	CLA	C2B-C3B-CAB-CBB
26	2	609	CLA	C2B-C3B-CAB-CBB
26	3	608	CLA	C2B-C3B-CAB-CBB
26	5	610	CLA	C2B-C3B-CAB-CBB
26	5	611	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	6	611	CLA	C2B-C3B-CAB-CBB
26	6	620	CLA	C2B-C3B-CAB-CBB
26	8	601	CLA	C2B-C3B-CAB-CBB
26	8	608	CLA	C2B-C3B-CAB-CBB
26	8	613	CLA	C2B-C3B-CAB-CBB
26	9	607	CLA	C2B-C3B-CAB-CBB
26	9	610	CLA	C2B-C3B-CAB-CBB
26	9	611	CLA	C2B-C3B-CAB-CBB
26	X	603	CLA	C2B-C3B-CAB-CBB
26	Z	610	CLA	C2B-C3B-CAB-CBB
26	U	611	CLA	C2B-C3B-CAB-CBB
26	V	611	CLA	C2B-C3B-CAB-CBB
29	A	848	BCR	C1-C6-C7-C8
29	A	849	BCR	C1-C6-C7-C8
29	A	849	BCR	C5-C6-C7-C8
29	A	849	BCR	C23-C24-C25-C30
29	A	850	BCR	C1-C6-C7-C8
29	A	851	BCR	C5-C6-C7-C8
29	A	852	BCR	C5-C6-C7-C8
29	A	852	BCR	C23-C24-C25-C26
29	B	801	BCR	C23-C24-C25-C30
29	B	843	BCR	C23-C24-C25-C30
29	B	845	BCR	C1-C6-C7-C8
29	B	845	BCR	C5-C6-C7-C8
29	B	845	BCR	C23-C24-C25-C26
29	B	849	BCR	C1-C6-C7-C8
29	B	849	BCR	C5-C6-C7-C8
29	B	853	BCR	C1-C6-C7-C8
29	B	853	BCR	C23-C24-C25-C26
29	B	853	BCR	C23-C24-C25-C30
29	F	305	BCR	C5-C6-C7-C8
29	F	305	BCR	C23-C24-C25-C26
29	F	305	BCR	C23-C24-C25-C30
29	G	205	BCR	C23-C24-C25-C26
29	J	102	BCR	C1-C6-C7-C8
29	L	301	BCR	C5-C6-C7-C8
29	L	308	BCR	C1-C6-C7-C8
29	O	2004	BCR	C23-C24-C25-C26
29	2	623	BCR	C23-C24-C25-C26
29	3	620	BCR	C23-C24-C25-C30
29	3	622	BCR	C5-C6-C7-C8
29	4	621	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	5	622	BCR	C23-C24-C25-C30
29	7	623	BCR	C5-C6-C7-C8
34	6	619	LUT	C1-C6-C7-C8
34	9	619	LUT	C1-C6-C7-C8
34	U	1620	LUT	C1-C6-C7-C8
34	U	1620	LUT	C5-C6-C7-C8
34	U	1621	LUT	C1-C6-C7-C8
34	U	1621	LUT	C5-C6-C7-C8
34	V	1620	LUT	C1-C6-C7-C8
34	V	1620	LUT	C5-C6-C7-C8
34	W	1621	LUT	C1-C6-C7-C8
28	Y	2630	LHG	C18-C19-C20-C21
26	A	836	CLA	CBD-CGD-O2D-CED
28	B	851	LHG	C8-C7-O7-C5
28	6	623	LHG	C8-C7-O7-C5
32	A	860	LMG	C11-C10-O7-C8
31	A	858	LMU	C4'-C5'-C6'-O6'
26	A	813	CLA	CBA-CGA-O2A-C1
32	J	103	LMG	C29-C28-O8-C9
26	A	830	CLA	C13-C15-C16-C17
26	7	602	CLA	C13-C15-C16-C17
37	Y	601	CHL	C8-C10-C11-C12
26	A	804	CLA	C3-C5-C6-C7
26	A	839	CLA	O1D-CGD-O2D-CED
37	Z	609	CHL	O1D-CGD-O2D-CED
26	A	814	CLA	C2A-CAA-CBA-CGA
26	B	828	CLA	C2A-CAA-CBA-CGA
26	2	602	CLA	C2A-CAA-CBA-CGA
26	W	613	CLA	C2A-CAA-CBA-CGA
37	W	608	CHL	C2A-CAA-CBA-CGA
28	B	851	LHG	C23-C24-C25-C26
26	A	804	CLA	O1A-CGA-O2A-C1
26	A	842	CLA	O1A-CGA-O2A-C1
26	6	602	CLA	O1A-CGA-O2A-C1
26	V	604	CLA	O1A-CGA-O2A-C1
28	7	622	LHG	O10-C23-O8-C6
28	9	624	LHG	O10-C23-O8-C6
31	1	621	LMU	C4'-C5'-C6'-O6'
28	3	624	LHG	O9-C7-O7-C5
26	X	612	CLA	C2A-CAA-CBA-CGA
26	4	604	CLA	C11-C10-C8-C7
26	A	814	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	1	613	CLA	C4-C3-C5-C6
26	a	613	CLA	C4-C3-C5-C6
26	3	604	CLA	C4-C3-C5-C6
26	6	613	CLA	C4-C3-C5-C6
26	8	614	CLA	O1D-CGD-O2D-CED
32	H	205	LMG	C33-C34-C35-C36
26	B	805	CLA	C10-C11-C12-C13
26	A	814	CLA	C2-C3-C5-C6
37	U	601	CHL	C2-C3-C5-C6
26	3	602	CLA	C11-C12-C13-C14
28	5	623	LHG	C28-C29-C30-C31
28	5	625	LHG	C16-C17-C18-C19
26	A	815	CLA	CBA-CGA-O2A-C1
26	8	602	CLA	CBA-CGA-O2A-C1
26	W	603	CLA	CBA-CGA-O2A-C1
28	9	622	LHG	C24-C23-O8-C6
26	A	836	CLA	C11-C10-C8-C9
28	9	623	LHG	C25-C26-C27-C28
26	A	834	CLA	C5-C6-C7-C8
26	B	841	CLA	C13-C15-C16-C17
28	H	204	LHG	C10-C11-C12-C13
32	L	2631	LMG	C12-C13-C14-C15
32	9	625	LMG	C35-C36-C37-C38
26	a	609	CLA	C13-C15-C16-C17
26	2	601	CLA	C15-C16-C17-C18
26	B	841	CLA	O1A-CGA-O2A-C1
32	4	623	LMG	C31-C32-C33-C34
28	5	623	LHG	C16-C17-C18-C19
26	B	833	CLA	CBA-CGA-O2A-C1
37	U	609	CHL	CBA-CGA-O2A-C1
31	A	858	LMU	C3'-C4'-O1B-C1B
26	A	842	CLA	C16-C17-C18-C19
26	1	613	CLA	C16-C17-C18-C19
37	X	601	CHL	C16-C17-C18-C20
28	8	623	LHG	C8-C7-O7-C5
32	J	104	LMG	C11-C10-O7-C8
32	4	624	LMG	C11-C10-O7-C8
32	9	625	LMG	C11-C10-O7-C8
28	H	204	LHG	O10-C23-O8-C6
31	5	628	LMU	C3'-C4'-O1B-C1B
26	A	807	CLA	C15-C16-C17-C18
26	a	609	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	B	842	PQN	C20-C21-C22-C23
28	H	204	LHG	C32-C33-C34-C35
26	B	818	CLA	C5-C6-C7-C8
34	U	1621	LUT	C7-C8-C9-C19
26	A	806	CLA	C3-C5-C6-C7
34	U	1620	LUT	C31-C32-C33-C34
35	U	1622	XAT	C31-C32-C33-C34
32	8	626	LMG	C18-C19-C20-C21
26	A	825	CLA	C2A-CAA-CBA-CGA
26	4	613	CLA	C2A-CAA-CBA-CGA
26	B	831	CLA	C16-C17-C18-C20
26	B	832	CLA	C11-C12-C13-C14
26	B	832	CLA	C11-C12-C13-C15
26	1	613	CLA	C16-C17-C18-C20
26	3	602	CLA	C11-C12-C13-C15
26	4	601	CLA	C16-C17-C18-C19
26	9	602	CLA	C11-C12-C13-C14
37	Z	601	CHL	C16-C17-C18-C20
37	V	601	CHL	C16-C17-C18-C19
26	B	819	CLA	CBD-CGD-O2D-CED
26	7	616	CLA	CBD-CGD-O2D-CED
26	1	613	CLA	C2-C3-C5-C6
26	a	613	CLA	C2-C3-C5-C6
26	3	604	CLA	C2-C3-C5-C6
28	9	623	LHG	C34-C35-C36-C37
26	A	806	CLA	C10-C11-C12-C13
26	Z	603	CLA	O1D-CGD-O2D-CED
28	4	622	LHG	C10-C11-C12-C13
26	A	801	CLA	C3-C5-C6-C7
33	B	850	DGD	O6E-C5E-C6E-O5E
26	8	613	CLA	C5-C6-C7-C8
26	8	613	CLA	C10-C11-C12-C13
28	5	623	LHG	C12-C13-C14-C15
26	3	607	CLA	CBA-CGA-O2A-C1
28	6	623	LHG	O9-C7-O7-C5
28	a	620	LHG	C28-C29-C30-C31
28	5	623	LHG	C11-C10-C9-C8
26	3	612	CLA	CBD-CGD-O2D-CED
26	A	825	CLA	C15-C16-C17-C18
37	X	601	CHL	C15-C16-C17-C18
37	W	601	CHL	C8-C10-C11-C12
26	U	604	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	B	831	CLA	C16-C17-C18-C19
37	X	607	CHL	C16-C17-C18-C20
28	1	620	LHG	C28-C29-C30-C31
31	K	208	LMU	C4-C5-C6-C7
26	A	813	CLA	O1A-CGA-O2A-C1
26	A	815	CLA	O1A-CGA-O2A-C1
26	A	821	CLA	O1D-CGD-O2D-CED
26	B	838	CLA	CBA-CGA-O2A-C1
31	8	625	LMU	C11-C10-C9-C8
31	8	625	LMU	C1-C2-C3-C4
32	5	627	LMG	C28-C29-C30-C31
26	A	824	CLA	C8-C10-C11-C12
26	A	828	CLA	C15-C16-C17-C18
26	B	828	CLA	C10-C11-C12-C13
26	B	829	CLA	C10-C11-C12-C13
26	6	604	CLA	C8-C10-C11-C12
26	9	609	CLA	C5-C6-C7-C8
37	X	608	CHL	C8-C10-C11-C12
37	V	601	CHL	C3-C5-C6-C7
31	A	857	LMU	C3'-C4'-O1B-C1B
28	3	624	LHG	C32-C33-C34-C35
31	K	208	LMU	C3-C4-C5-C6
32	A	860	LMG	C16-C17-C18-C19
26	6	603	CLA	CBA-CGA-O2A-C1
37	X	609	CHL	CBA-CGA-O2A-C1
28	A	861	LHG	C33-C34-C35-C36
28	9	623	LHG	C16-C17-C18-C19
26	B	810	CLA	C5-C6-C7-C8
26	5	609	CLA	C13-C15-C16-C17
28	A	846	LHG	C13-C14-C15-C16
26	B	837	CLA	CBD-CGD-O2D-CED
28	A	846	LHG	C29-C30-C31-C32
26	B	811	CLA	C2-C1-O2A-CGA
26	A	807	CLA	C16-C17-C18-C19
28	U	2630	LHG	C9-C10-C11-C12
26	A	826	CLA	C4-C3-C5-C6
26	U	613	CLA	C3-C5-C6-C7
26	6	613	CLA	C2-C3-C5-C6
37	Y	607	CHL	C2-C3-C5-C6
28	B	851	LHG	O9-C7-O7-C5
32	A	860	LMG	O9-C10-O7-C8
32	J	104	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
31	5	628	LMU	C5'-C4'-O1B-C1B
28	W	2630	LHG	C1-C2-C3-O3
26	3	609	CLA	C5-C6-C7-C8
26	A	803	CLA	C2A-CAA-CBA-CGA
26	A	837	CLA	C2A-CAA-CBA-CGA
26	H	203	CLA	C2A-CAA-CBA-CGA
26	2	613	CLA	C2A-CAA-CBA-CGA
26	5	602	CLA	C2A-CAA-CBA-CGA
26	X	603	CLA	C2A-CAA-CBA-CGA
26	W	602	CLA	C2A-CAA-CBA-CGA
26	L	302	CLA	CBD-CGD-O2D-CED
28	A	846	LHG	C31-C32-C33-C34
31	5	628	LMU	C5-C6-C7-C8
26	B	804	CLA	O1D-CGD-O2D-CED
26	B	806	CLA	C5-C6-C7-C8
37	U	601	CHL	C10-C11-C12-C13
26	A	804	CLA	C2C-C3C-CAC-CBC
26	L	304	CLA	O1D-CGD-O2D-CED
32	8	626	LMG	C14-C15-C16-C17
26	B	816	CLA	C2-C1-O2A-CGA
26	8	602	CLA	O1A-CGA-O2A-C1
26	5	613	CLA	C3-C5-C6-C7
26	9	610	CLA	C3-C5-C6-C7
26	B	810	CLA	C2A-CAA-CBA-CGA
26	5	613	CLA	C2A-CAA-CBA-CGA
26	A	805	CLA	C1A-C2A-CAA-CBA
26	A	808	CLA	C1A-C2A-CAA-CBA
26	A	811	CLA	C1A-C2A-CAA-CBA
26	A	815	CLA	C1A-C2A-CAA-CBA
26	A	820	CLA	C1A-C2A-CAA-CBA
26	A	831	CLA	C1A-C2A-CAA-CBA
26	A	833	CLA	C1A-C2A-CAA-CBA
26	B	803	CLA	C1A-C2A-CAA-CBA
26	B	805	CLA	C1A-C2A-CAA-CBA
26	B	812	CLA	C1A-C2A-CAA-CBA
26	B	818	CLA	C1A-C2A-CAA-CBA
26	B	820	CLA	C1A-C2A-CAA-CBA
26	B	826	CLA	C1A-C2A-CAA-CBA
26	B	828	CLA	C1A-C2A-CAA-CBA
26	B	829	CLA	C1A-C2A-CAA-CBA
26	H	203	CLA	C1A-C2A-CAA-CBA
26	K	201	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	1	616	CLA	C1A-C2A-CAA-CBA
26	a	606	CLA	C1A-C2A-CAA-CBA
26	a	616	CLA	C1A-C2A-CAA-CBA
26	2	612	CLA	C1A-C2A-CAA-CBA
26	3	603	CLA	C1A-C2A-CAA-CBA
26	3	607	CLA	C1A-C2A-CAA-CBA
26	3	609	CLA	C1A-C2A-CAA-CBA
26	5	619	CLA	C1A-C2A-CAA-CBA
26	6	614	CLA	C1A-C2A-CAA-CBA
26	6	616	CLA	C1A-C2A-CAA-CBA
26	6	620	CLA	C1A-C2A-CAA-CBA
26	7	604	CLA	C1A-C2A-CAA-CBA
26	8	604	CLA	C1A-C2A-CAA-CBA
26	8	609	CLA	C1A-C2A-CAA-CBA
26	8	616	CLA	C1A-C2A-CAA-CBA
26	X	610	CLA	C1A-C2A-CAA-CBA
26	Y	603	CLA	C1A-C2A-CAA-CBA
26	Y	610	CLA	C1A-C2A-CAA-CBA
26	Y	611	CLA	C1A-C2A-CAA-CBA
26	Y	614	CLA	C1A-C2A-CAA-CBA
26	Z	603	CLA	C1A-C2A-CAA-CBA
26	Z	614	CLA	C1A-C2A-CAA-CBA
26	U	602	CLA	C1A-C2A-CAA-CBA
26	V	602	CLA	C1A-C2A-CAA-CBA
26	V	610	CLA	C1A-C2A-CAA-CBA
26	V	614	CLA	C1A-C2A-CAA-CBA
26	W	602	CLA	C1A-C2A-CAA-CBA
26	W	610	CLA	C1A-C2A-CAA-CBA
26	B	806	CLA	C8-C10-C11-C12
37	Z	609	CHL	C13-C15-C16-C17
31	A	858	LMU	C6-C7-C8-C9
32	J	103	LMG	O10-C28-O8-C9
32	9	625	LMG	C22-C23-C24-C25
26	Y	610	CLA	C5-C6-C7-C8
28	3	623	LHG	O6-C4-C5-C6
28	3	624	LHG	O6-C4-C5-C6
28	Z	2630	LHG	O6-C4-C5-C6
28	U	2630	LHG	O6-C4-C5-C6
28	8	623	LHG	O9-C7-O7-C5
32	4	624	LMG	O9-C10-O7-C8
32	9	625	LMG	O9-C10-O7-C8
32	V	2631	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
26	A	804	CLA	C11-C12-C13-C15
26	A	804	CLA	C12-C13-C15-C16
26	A	809	CLA	C12-C13-C15-C16
26	A	811	CLA	C11-C10-C8-C7
26	A	814	CLA	C12-C13-C15-C16
26	A	826	CLA	C11-C10-C8-C7
26	B	802	CLA	C11-C12-C13-C15
26	B	806	CLA	C11-C12-C13-C15
26	B	818	CLA	C11-C10-C8-C7
26	B	824	CLA	C12-C13-C15-C16
26	a	610	CLA	C11-C10-C8-C7
26	4	602	CLA	C6-C7-C8-C10
26	4	610	CLA	C11-C12-C13-C15
26	5	604	CLA	C11-C12-C13-C15
26	5	609	CLA	C6-C7-C8-C10
26	8	602	CLA	C11-C10-C8-C7
26	8	606	CLA	C11-C12-C13-C15
26	X	603	CLA	C12-C13-C15-C16
26	Y	610	CLA	C11-C12-C13-C15
26	Y	613	CLA	C11-C12-C13-C15
26	U	613	CLA	C6-C7-C8-C10
26	U	613	CLA	C11-C10-C8-C7
26	V	610	CLA	C11-C10-C8-C7
26	W	613	CLA	C12-C13-C15-C16
37	X	601	CHL	C11-C10-C8-C7
37	V	601	CHL	C6-C7-C8-C10
37	W	607	CHL	C11-C12-C13-C15
26	B	811	CLA	C6-C7-C8-C10
26	8	602	CLA	C11-C12-C13-C15
26	1	613	CLA	C10-C11-C12-C13
26	A	840	CLA	C2C-C3C-CAC-CBC
26	3	607	CLA	O1A-CGA-O2A-C1
26	W	603	CLA	O1A-CGA-O2A-C1
26	B	822	CLA	C3A-C2A-CAA-CBA
26	4	611	CLA	C3A-C2A-CAA-CBA
26	4	612	CLA	C3A-C2A-CAA-CBA
26	4	618	CLA	C3A-C2A-CAA-CBA
26	5	612	CLA	C3A-C2A-CAA-CBA
26	8	611	CLA	C3A-C2A-CAA-CBA
26	9	611	CLA	C3A-C2A-CAA-CBA
26	9	612	CLA	C3A-C2A-CAA-CBA
31	A	857	LMU	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
28	Z	2630	LHG	C25-C26-C27-C28
26	A	854	CLA	C10-C11-C12-C13
26	V	602	CLA	C8-C10-C11-C12
28	O	2631	LHG	C7-C8-C9-C10
33	B	850	DGD	C1B-C2B-C3B-C4B
26	B	808	CLA	C4-C3-C5-C6
26	F	301	CLA	C4-C3-C5-C6
26	9	609	CLA	C4-C3-C5-C6
26	V	613	CLA	C4-C3-C5-C6
37	Z	607	CHL	C4-C3-C5-C6
26	B	808	CLA	C2-C3-C5-C6
26	K	203	CLA	C2-C3-C5-C6
26	B	817	CLA	C10-C11-C12-C13
26	B	802	CLA	C10-C11-C12-C13
26	L	303	CLA	C10-C11-C12-C13
26	X	610	CLA	C5-C6-C7-C8
37	X	609	CHL	C8-C10-C11-C12
37	W	607	CHL	C15-C16-C17-C18
26	A	842	CLA	C2A-CAA-CBA-CGA
26	B	807	CLA	C2A-CAA-CBA-CGA
26	8	602	CLA	C2A-CAA-CBA-CGA
26	X	602	CLA	C2A-CAA-CBA-CGA
26	X	613	CLA	C2A-CAA-CBA-CGA
26	Y	602	CLA	C2A-CAA-CBA-CGA
26	Y	613	CLA	C2A-CAA-CBA-CGA
26	V	613	CLA	C2A-CAA-CBA-CGA
26	A	802	CLA	C14-C13-C15-C16
26	A	804	CLA	C11-C12-C13-C14
26	A	809	CLA	C14-C13-C15-C16
26	A	816	CLA	C11-C10-C8-C9
26	A	820	CLA	C11-C10-C8-C9
26	A	842	CLA	C11-C10-C8-C9
26	A	842	CLA	C11-C12-C13-C14
26	B	810	CLA	C11-C10-C8-C9
26	B	824	CLA	C11-C10-C8-C9
26	B	824	CLA	C14-C13-C15-C16
26	B	826	CLA	C6-C7-C8-C9
26	B	831	CLA	C11-C12-C13-C14
26	B	834	CLA	C11-C10-C8-C9
26	a	609	CLA	C14-C13-C15-C16
26	2	602	CLA	C11-C10-C8-C9
26	2	602	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	4	610	CLA	C6-C7-C8-C9
26	4	610	CLA	C11-C12-C13-C14
26	5	607	CLA	C14-C13-C15-C16
26	8	602	CLA	C11-C10-C8-C9
26	X	602	CLA	C6-C7-C8-C9
26	X	603	CLA	C14-C13-C15-C16
26	X	613	CLA	C11-C10-C8-C9
26	V	613	CLA	C14-C13-C15-C16
26	W	613	CLA	C14-C13-C15-C16
37	X	601	CHL	C11-C10-C8-C9
37	X	607	CHL	C14-C13-C15-C16
37	Z	601	CHL	C11-C10-C8-C9
37	Z	607	CHL	C6-C7-C8-C9
28	A	846	LHG	C7-C8-C9-C10
26	A	825	CLA	CBA-CGA-O2A-C1
26	B	839	CLA	CBA-CGA-O2A-C1
26	7	610	CLA	CBA-CGA-O2A-C1
28	9	622	LHG	O10-C23-O8-C6
28	U	2630	LHG	C17-C18-C19-C20
31	5	629	LMU	C2-C3-C4-C5
26	1	609	CLA	O1D-CGD-O2D-CED
28	9	623	LHG	C26-C27-C28-C29
26	B	803	CLA	C10-C11-C12-C13
28	H	204	LHG	C4-C5-C6-O8
32	5	627	LMG	C7-C8-C9-O8
32	8	626	LMG	O1-C7-C8-C9
32	8	626	LMG	C7-C8-C9-O8
37	X	606	CHL	C2A-CAA-CBA-CGA
26	A	830	CLA	O1D-CGD-O2D-CED
28	9	623	LHG	C17-C18-C19-C20
31	5	629	LMU	C3-C4-C5-C6
26	A	816	CLA	C10-C11-C12-C13
37	U	609	CHL	C2C-C3C-CAC-CBC
28	X	2630	LHG	C28-C29-C30-C31
26	A	841	CLA	O1D-CGD-O2D-CED
26	8	614	CLA	CBA-CGA-O2A-C1
28	2	622	LHG	C24-C23-O8-C6
28	A	861	LHG	C7-C8-C9-C10
28	2	622	LHG	C23-C24-C25-C26
32	J	104	LMG	O6-C5-C6-O5
26	A	801	CLA	C16-C17-C18-C19
26	B	811	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	5	625	LHG	C24-C25-C26-C27
26	U	610	CLA	C5-C6-C7-C8
37	Y	607	CHL	CHA-CBD-CGD-O2D
26	B	839	CLA	C10-C11-C12-C13
26	B	833	CLA	O1A-CGA-O2A-C1
26	6	603	CLA	O1A-CGA-O2A-C1
37	U	609	CHL	O1A-CGA-O2A-C1
26	B	814	CLA	C4-C3-C5-C6
26	K	203	CLA	C4-C3-C5-C6
37	Y	607	CHL	C4-C3-C5-C6
37	W	601	CHL	C4-C3-C5-C6
26	A	826	CLA	C2-C3-C5-C6
26	B	810	CLA	C2-C3-C5-C6
26	B	814	CLA	C2-C3-C5-C6
26	F	301	CLA	C2-C3-C5-C6
26	9	609	CLA	C2-C3-C5-C6
26	V	613	CLA	C2-C3-C5-C6
37	Z	607	CHL	C2-C3-C5-C6
26	B	805	CLA	C13-C15-C16-C17
26	6	616	CLA	C10-C11-C12-C13
26	8	613	CLA	C15-C16-C17-C18
31	5	628	LMU	O5'-C5'-C6'-O6'
26	B	812	CLA	C2A-CAA-CBA-CGA
28	A	846	LHG	C25-C26-C27-C28
34	U	1621	LUT	C7-C8-C9-C10
34	W	1620	LUT	C27-C28-C29-C30
35	Z	1622	XAT	C11-C12-C13-C14
26	A	825	CLA	O1A-CGA-O2A-C1
37	X	609	CHL	O1A-CGA-O2A-C1
28	B	851	LHG	C27-C28-C29-C30
28	Z	2630	LHG	C11-C12-C13-C14
26	L	302	CLA	C2A-CAA-CBA-CGA
26	V	610	CLA	C8-C10-C11-C12
26	W	613	CLA	O1D-CGD-O2D-CED
26	A	836	CLA	CBA-CGA-O2A-C1
26	B	806	CLA	CBA-CGA-O2A-C1
26	F	301	CLA	CBA-CGA-O2A-C1
26	a	614	CLA	CBA-CGA-O2A-C1
26	8	608	CLA	CBA-CGA-O2A-C1
26	Z	604	CLA	CBA-CGA-O2A-C1
26	B	803	CLA	O2A-C1-C2-C3
28	3	623	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	A	834	CLA	C8-C10-C11-C12
26	A	843	CLA	C11-C10-C8-C7
32	V	2631	LMG	C32-C33-C34-C35
34	Z	1621	LUT	C29-C30-C31-C32
36	Z	1623	NEX	C9-C10-C11-C12
37	X	605	CHL	C3C-C2C-CMC-OMC
26	3	609	CLA	O1D-CGD-O2D-CED
26	K	203	CLA	CBA-CGA-O2A-C1
26	X	603	CLA	CBA-CGA-O2A-C1
37	Y	609	CHL	CBA-CGA-O2A-C1
26	B	814	CLA	C16-C17-C18-C19
28	6	623	LHG	C34-C35-C36-C37
32	V	2631	LMG	C22-C23-C24-C25
26	U	602	CLA	C4-C3-C5-C6
26	B	816	CLA	C2-C3-C5-C6
26	W	613	CLA	C2-C3-C5-C6
26	U	602	CLA	C11-C12-C13-C14
26	A	807	CLA	C16-C17-C18-C20
26	8	602	CLA	C11-C12-C13-C14
31	5	629	LMU	C4-C5-C6-C7
28	A	861	LHG	C35-C36-C37-C38
28	B	851	LHG	C29-C30-C31-C32
32	8	626	LMG	C22-C23-C24-C25
26	7	611	CLA	CBA-CGA-O2A-C1
37	W	601	CHL	CBA-CGA-O2A-C1
26	3	613	CLA	C2A-CAA-CBA-CGA
28	4	622	LHG	C14-C15-C16-C17
31	5	629	LMU	C6-C7-C8-C9
37	X	601	CHL	CAA-CBA-CGA-O2A
26	U	613	CLA	C2A-CAA-CBA-CGA
26	W	614	CLA	C2A-CAA-CBA-CGA
26	6	616	CLA	C3-C5-C6-C7
26	1	606	CLA	CBD-CGD-O2D-CED
26	a	606	CLA	CBD-CGD-O2D-CED
26	7	615	CLA	CBD-CGD-O2D-CED
32	J	104	LMG	C17-C18-C19-C20
26	A	819	CLA	C11-C12-C13-C14
26	A	816	CLA	C15-C16-C17-C18
26	3	602	CLA	C10-C11-C12-C13
28	A	861	LHG	C15-C16-C17-C18
32	9	625	LMG	C24-C25-C26-C27
31	A	858	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
26	7	610	CLA	O1A-CGA-O2A-C1
28	3	624	LHG	C9-C10-C11-C12
32	H	205	LMG	C16-C17-C18-C19
26	2	601	CLA	CBA-CGA-O2A-C1
37	U	601	CHL	C15-C16-C17-C18
26	A	812	CLA	C15-C16-C17-C18
26	A	816	CLA	C13-C15-C16-C17
26	A	830	CLA	C8-C10-C11-C12
26	8	613	CLA	C8-C10-C11-C12
26	A	814	CLA	O1D-CGD-O2D-CED
26	a	603	CLA	O1D-CGD-O2D-CED
26	4	604	CLA	C11-C10-C8-C9
26	4	610	CLA	C14-C13-C15-C16
26	B	810	CLA	C4-C3-C5-C6
26	W	613	CLA	C4-C3-C5-C6
26	B	803	CLA	CBA-CGA-O2A-C1
37	Y	608	CHL	CBA-CGA-O2A-C1
26	W	613	CLA	C8-C10-C11-C12
32	A	860	LMG	C15-C16-C17-C18
32	8	626	LMG	C21-C22-C23-C24
28	8	623	LHG	O1-C1-C2-O2
31	A	857	LMU	C2-C1-O1'-C1'
31	8	625	LMU	C2-C1-O1'-C1'
26	A	804	CLA	C14-C13-C15-C16
26	A	806	CLA	C6-C7-C8-C9
26	A	811	CLA	C11-C10-C8-C9
26	A	814	CLA	C14-C13-C15-C16
26	A	826	CLA	C11-C10-C8-C9
26	A	830	CLA	C6-C7-C8-C9
26	A	841	CLA	C11-C10-C8-C9
26	A	842	CLA	C14-C13-C15-C16
26	B	818	CLA	C11-C10-C8-C9
26	a	610	CLA	C11-C10-C8-C9
26	3	610	CLA	C11-C10-C8-C9
26	5	604	CLA	C11-C12-C13-C14
26	5	609	CLA	C11-C12-C13-C14
26	6	613	CLA	C6-C7-C8-C9
26	6	616	CLA	C11-C12-C13-C14
26	6	620	CLA	C11-C12-C13-C14
26	8	606	CLA	C11-C12-C13-C14
26	Y	610	CLA	C11-C12-C13-C14
26	Z	613	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
26	U	613	CLA	C6-C7-C8-C9
26	U	613	CLA	C11-C10-C8-C9
26	V	602	CLA	C6-C7-C8-C9
26	V	610	CLA	C11-C10-C8-C9
26	W	613	CLA	C11-C10-C8-C9
37	Y	601	CHL	C6-C7-C8-C9
37	U	609	CHL	C11-C10-C8-C9
37	W	601	CHL	C11-C12-C13-C14
37	W	607	CHL	C6-C7-C8-C9
37	W	607	CHL	C11-C12-C13-C14
37	Z	605	CHL	O1D-CGD-O2D-CED
26	A	801	CLA	C8-C10-C11-C12
37	Y	609	CHL	C15-C16-C17-C18
37	Z	607	CHL	C10-C11-C12-C13
37	W	601	CHL	C5-C6-C7-C8
37	W	607	CHL	C8-C10-C11-C12
26	J	101	CLA	C4B-C3B-CAB-CBB
26	1	608	CLA	C4B-C3B-CAB-CBB
26	a	608	CLA	C4B-C3B-CAB-CBB
26	a	614	CLA	C4B-C3B-CAB-CBB
26	2	603	CLA	C4B-C3B-CAB-CBB
26	3	606	CLA	C4B-C3B-CAB-CBB
26	4	602	CLA	C4B-C3B-CAB-CBB
26	4	606	CLA	C4B-C3B-CAB-CBB
26	4	609	CLA	C4B-C3B-CAB-CBB
26	6	604	CLA	C4B-C3B-CAB-CBB
26	6	606	CLA	C4B-C3B-CAB-CBB
26	6	610	CLA	C4B-C3B-CAB-CBB
26	7	603	CLA	C4B-C3B-CAB-CBB
26	7	608	CLA	C4B-C3B-CAB-CBB
26	7	610	CLA	C4B-C3B-CAB-CBB
26	8	611	CLA	C4B-C3B-CAB-CBB
26	X	610	CLA	C4B-C3B-CAB-CBB
26	X	613	CLA	C4B-C3B-CAB-CBB
26	Y	604	CLA	C4B-C3B-CAB-CBB
26	Z	613	CLA	C4B-C3B-CAB-CBB
26	Z	614	CLA	C4B-C3B-CAB-CBB
26	U	613	CLA	C4B-C3B-CAB-CBB
26	V	610	CLA	C4B-C3B-CAB-CBB
31	1	621	LMU	C4-C5-C6-C7
31	A	858	LMU	C2-C3-C4-C5
27	B	842	PQN	C23-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	2	616	CLA	CBD-CGD-O2D-CED
26	A	827	CLA	C10-C11-C12-C13
26	Z	612	CLA	C2A-CAA-CBA-CGA
37	Y	606	CHL	C2A-CAA-CBA-CGA
26	6	616	CLA	C15-C16-C17-C18
31	1	621	LMU	C3-C4-C5-C6
31	1	621	LMU	C6-C7-C8-C9
32	V	2631	LMG	C15-C16-C17-C18
28	9	623	LHG	C7-C8-C9-C10
28	5	623	LHG	O6-C4-C5-C6
37	W	608	CHL	O1A-CGA-O2A-C1
26	A	802	CLA	C12-C13-C15-C16
26	A	806	CLA	C6-C7-C8-C10
26	A	820	CLA	C11-C10-C8-C7
26	A	830	CLA	C6-C7-C8-C10
26	A	831	CLA	C12-C13-C15-C16
26	A	842	CLA	C11-C10-C8-C7
26	A	842	CLA	C11-C12-C13-C15
26	B	806	CLA	C12-C13-C15-C16
26	B	810	CLA	C11-C10-C8-C7
26	B	824	CLA	C11-C10-C8-C7
26	B	826	CLA	C6-C7-C8-C10
26	B	826	CLA	C11-C12-C13-C15
26	B	828	CLA	C12-C13-C15-C16
26	B	831	CLA	C11-C12-C13-C15
26	B	834	CLA	C11-C10-C8-C7
26	2	602	CLA	C11-C10-C8-C7
26	2	602	CLA	C12-C13-C15-C16
26	3	610	CLA	C11-C10-C8-C7
26	4	610	CLA	C6-C7-C8-C10
26	5	607	CLA	C12-C13-C15-C16
26	5	609	CLA	C11-C12-C13-C15
26	6	616	CLA	C11-C12-C13-C15
26	6	620	CLA	C11-C12-C13-C15
26	X	602	CLA	C6-C7-C8-C10
26	X	610	CLA	C12-C13-C15-C16
26	X	613	CLA	C11-C10-C8-C7
26	Z	613	CLA	C11-C10-C8-C7
26	V	602	CLA	C6-C7-C8-C10
26	V	613	CLA	C12-C13-C15-C16
26	W	613	CLA	C11-C10-C8-C7
37	X	607	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
37	W	601	CHL	C11-C12-C13-C15
28	H	204	LHG	C7-C8-C9-C10
26	B	839	CLA	O1A-CGA-O2A-C1
26	a	614	CLA	O1A-CGA-O2A-C1
26	8	614	CLA	O1A-CGA-O2A-C1
32	J	104	LMG	C18-C19-C20-C21
26	H	203	CLA	C3A-C2A-CAA-CBA
26	6	609	CLA	C3A-C2A-CAA-CBA
26	9	602	CLA	C4-C3-C5-C6
26	V	611	CLA	C3A-C2A-CAA-CBA
26	W	611	CLA	C3A-C2A-CAA-CBA
37	Y	601	CHL	C3A-C2A-CAA-CBA
37	W	601	CHL	C3A-C2A-CAA-CBA
37	W	608	CHL	C3A-C2A-CAA-CBA
37	Y	609	CHL	C10-C11-C12-C13
26	B	832	CLA	O1D-CGD-O2D-CED
26	7	613	CLA	C10-C11-C12-C13
37	X	607	CHL	C15-C16-C17-C18
26	6	604	CLA	CBA-CGA-O2A-C1
34	Z	1620	LUT	C9-C10-C11-C12
34	V	1621	LUT	C29-C30-C31-C32
34	W	1621	LUT	C29-C30-C31-C32
36	U	1623	NEX	C29-C30-C31-C32
26	7	602	CLA	C3-C5-C6-C7
29	3	620	BCR	C37-C22-C23-C24
26	1	603	CLA	CBA-CGA-O2A-C1
26	a	603	CLA	CBA-CGA-O2A-C1
26	B	806	CLA	O1A-CGA-O2A-C1
26	F	301	CLA	O1A-CGA-O2A-C1
26	8	608	CLA	O1A-CGA-O2A-C1
37	W	601	CHL	O1A-CGA-O2A-C1
26	X	603	CLA	CBD-CGD-O2D-CED
28	O	2631	LHG	C4-C5-C6-O8
28	5	623	LHG	C4-C5-C6-O8
28	7	622	LHG	C4-C5-C6-O8
28	9	622	LHG	C4-C5-C6-O8
33	B	850	DGD	O1G-C1G-C2G-C3G
26	U	602	CLA	C3-C5-C6-C7
37	Z	607	CHL	C15-C16-C17-C18
37	U	609	CHL	C11-C12-C13-C14
37	X	607	CHL	C1A-C2A-CAA-CBA
37	Z	606	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	Z	607	CHL	C1A-C2A-CAA-CBA
37	Y	601	CHL	C13-C15-C16-C17
26	A	843	CLA	C8-C10-C11-C12
33	B	850	DGD	C9B-CAB-CBB-CCB
26	A	824	CLA	C4-C3-C5-C6
26	A	843	CLA	C4-C3-C5-C6
26	B	816	CLA	C4-C3-C5-C6
26	X	613	CLA	C4-C3-C5-C6
37	Y	601	CHL	C4-C3-C5-C6
26	H	203	CLA	CBA-CGA-O2A-C1
26	X	613	CLA	C2-C3-C5-C6
26	A	836	CLA	O1A-CGA-O2A-C1
37	Y	607	CHL	C10-C11-C12-C13
26	B	816	CLA	C2A-CAA-CBA-CGA
26	B	823	CLA	O1D-CGD-O2D-CED
26	Z	610	CLA	CBD-CGD-O2D-CED
28	7	622	LHG	C9-C10-C11-C12
26	5	609	CLA	C16-C17-C18-C20
28	5	623	LHG	O6-C4-C5-O7
26	B	821	CLA	C2B-C3B-CAB-CBB
26	F	304	CLA	C2B-C3B-CAB-CBB
26	X	610	CLA	C2B-C3B-CAB-CBB
26	Y	603	CLA	C2B-C3B-CAB-CBB
29	A	852	BCR	C23-C24-C25-C30
29	F	305	BCR	C1-C6-C7-C8
29	K	202	BCR	C5-C6-C7-C8
29	7	623	BCR	C23-C24-C25-C26
34	X	1620	LUT	C1-C6-C7-C8
34	W	1621	LUT	C5-C6-C7-C8
26	W	603	CLA	CAA-CBA-CGA-O2A
26	A	804	CLA	C10-C11-C12-C13
26	6	604	CLA	C15-C16-C17-C18
26	A	806	CLA	C13-C15-C16-C17
26	6	610	CLA	C15-C16-C17-C18
26	B	841	CLA	CBD-CGD-O2D-CED
28	9	624	LHG	C17-C18-C19-C20
32	5	627	LMG	C30-C31-C32-C33
37	W	607	CHL	CAA-CBA-CGA-O2A
26	A	829	CLA	C2A-CAA-CBA-CGA
26	L	302	CLA	O1D-CGD-O2D-CED
28	O	2631	LHG	O7-C5-C6-O8
32	5	627	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
37	W	605	CHL	CBD-CGD-O2D-CED
26	Y	602	CLA	C3-C5-C6-C7
26	2	602	CLA	NC-C1C-CHC-C4B
26	A	807	CLA	C4-C3-C5-C6
26	A	822	CLA	C4-C3-C5-C6
28	7	622	LHG	C26-C27-C28-C29
26	A	807	CLA	C2-C3-C5-C6
26	9	602	CLA	C2-C3-C5-C6
28	8	623	LHG	C32-C33-C34-C35
33	B	850	DGD	C7B-C8B-C9B-CAB
26	6	613	CLA	CBA-CGA-O2A-C1
26	Z	604	CLA	O1A-CGA-O2A-C1
26	3	608	CLA	C3-C5-C6-C7
26	4	602	CLA	C6-C7-C8-C9
26	W	613	CLA	C6-C7-C8-C9
26	A	843	CLA	C13-C15-C16-C17
31	A	857	LMU	C7-C8-C9-C10
26	A	836	CLA	O1D-CGD-O2D-CED
26	9	602	CLA	C11-C12-C13-C15
26	2	613	CLA	O1D-CGD-O2D-CED
26	B	837	CLA	C10-C11-C12-C13
28	Z	2630	LHG	C14-C15-C16-C17
26	J	101	CLA	C1A-C2A-CAA-CBA
26	L	306	CLA	C1A-C2A-CAA-CBA
26	4	611	CLA	C1A-C2A-CAA-CBA
26	7	616	CLA	O1D-CGD-O2D-CED
31	A	858	LMU	C5-C6-C7-C8
26	3	612	CLA	O1D-CGD-O2D-CED
26	A	831	CLA	CBA-CGA-O2A-C1
26	B	826	CLA	CBA-CGA-O2A-C1
34	X	1621	LUT	C29-C30-C31-C32
35	Y	1622	XAT	C13-C14-C15-C35
26	A	822	CLA	C2-C3-C5-C6
26	A	811	CLA	C13-C15-C16-C17
26	B	819	CLA	O1D-CGD-O2D-CED
26	B	839	CLA	C8-C10-C11-C12
26	3	604	CLA	C8-C10-C11-C12
26	8	601	CLA	C8-C10-C11-C12
26	A	803	CLA	CBD-CGD-O2D-CED
26	K	203	CLA	O1A-CGA-O2A-C1
37	Y	608	CHL	O1A-CGA-O2A-C1
37	Y	609	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	A	860	LMG	C29-C28-O8-C9
28	6	623	LHG	C14-C15-C16-C17
28	3	624	LHG	C11-C10-C9-C8
28	A	847	LHG	O6-C4-C5-C6
28	6	623	LHG	O6-C4-C5-C6
26	4	613	CLA	C16-C17-C18-C20
26	5	609	CLA	C16-C17-C18-C19
31	1	621	LMU	O5'-C5'-C6'-O6'
37	X	608	CHL	C10-C11-C12-C13
35	W	1622	XAT	C11-C12-C13-C20
28	O	2631	LHG	C26-C27-C28-C29
26	A	809	CLA	C11-C12-C13-C15
26	A	828	CLA	C11-C10-C8-C7
26	A	841	CLA	C11-C10-C8-C7
26	A	842	CLA	C12-C13-C15-C16
26	B	802	CLA	C6-C7-C8-C10
26	B	805	CLA	C11-C12-C13-C15
26	B	808	CLA	C12-C13-C15-C16
26	4	608	CLA	C11-C10-C8-C7
26	5	604	CLA	C11-C10-C8-C7
26	6	601	CLA	C6-C7-C8-C10
26	X	610	CLA	C11-C12-C13-C15
26	X	613	CLA	C6-C7-C8-C10
26	Y	613	CLA	C11-C10-C8-C7
26	Z	602	CLA	C11-C10-C8-C7
26	U	602	CLA	C6-C7-C8-C10
26	W	613	CLA	C6-C7-C8-C10
37	X	607	CHL	C11-C12-C13-C15
37	X	608	CHL	C12-C13-C15-C16
37	X	609	CHL	C11-C12-C13-C15
37	Y	601	CHL	C11-C12-C13-C15
37	Z	607	CHL	C12-C13-C15-C16
37	U	601	CHL	C12-C13-C15-C16
37	X	608	CHL	C5-C6-C7-C8
36	Z	1623	NEX	C31-C32-C33-C34
26	Y	602	CLA	O1D-CGD-O2D-CED
28	8	623	LHG	C24-C23-O8-C6
26	B	826	CLA	O1A-CGA-O2A-C1
26	7	611	CLA	O1A-CGA-O2A-C1
26	X	603	CLA	O1A-CGA-O2A-C1
28	2	622	LHG	O10-C23-O8-C6
32	J	103	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
32	J	103	LMG	C21-C22-C23-C24
26	1	613	CLA	O1D-CGD-O2D-CED
26	A	842	CLA	C8-C10-C11-C12
26	5	604	CLA	C5-C6-C7-C8
26	4	604	CLA	C2A-CAA-CBA-CGA
26	6	613	CLA	C2A-CAA-CBA-CGA
26	7	603	CLA	C2A-CAA-CBA-CGA
26	Z	613	CLA	C2A-CAA-CBA-CGA
26	V	602	CLA	C2A-CAA-CBA-CGA
26	a	613	CLA	O1D-CGD-O2D-CED
26	B	803	CLA	O1A-CGA-O2A-C1
26	6	613	CLA	O1A-CGA-O2A-C1
26	A	843	CLA	C2-C3-C5-C6
26	A	843	CLA	O2A-C1-C2-C3
28	9	624	LHG	C34-C35-C36-C37
36	W	1623	NEX	C13-C14-C15-C35
32	V	2631	LMG	C33-C34-C35-C36
26	A	801	CLA	C16-C17-C18-C20
26	H	203	CLA	O1A-CGA-O2A-C1
26	2	601	CLA	O1A-CGA-O2A-C1
26	6	604	CLA	O1A-CGA-O2A-C1
26	B	810	CLA	C3-C5-C6-C7
26	B	832	CLA	C3-C5-C6-C7
37	Y	607	CHL	C3-C5-C6-C7
28	9	623	LHG	C35-C36-C37-C38
28	A	846	LHG	O6-C4-C5-O7
28	6	623	LHG	O6-C4-C5-O7
26	6	620	CLA	O2A-C1-C2-C3
26	X	604	CLA	O2A-C1-C2-C3
28	4	622	LHG	C30-C31-C32-C33
32	9	625	LMG	O6-C1-O1-C7
32	9	625	LMG	C7-C8-C9-O8
37	X	608	CHL	CAD-CBD-CGD-O2D
26	A	831	CLA	O1A-CGA-O2A-C1
26	B	810	CLA	C15-C16-C17-C18
26	B	827	CLA	C8-C10-C11-C12
26	B	828	CLA	C4-C3-C5-C6
37	W	601	CHL	C2-C3-C5-C6
36	V	1623	NEX	C7-C8-C9-C19
26	2	602	CLA	C13-C15-C16-C17
28	H	204	LHG	C15-C16-C17-C18
32	A	860	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
32	J	103	LMG	O1-C7-C8-O7
32	J	103	LMG	O7-C8-C9-O8
32	J	104	LMG	O7-C8-C9-O8
33	B	850	DGD	O1G-C1G-C2G-O2G
33	B	850	DGD	O2G-C2G-C3G-O3G
26	A	826	CLA	C8-C10-C11-C12
26	A	854	CLA	C15-C16-C17-C18
26	2	601	CLA	C8-C10-C11-C12
26	A	809	CLA	C11-C12-C13-C14
26	A	828	CLA	C11-C10-C8-C9
26	B	805	CLA	C11-C12-C13-C14
26	B	806	CLA	C14-C13-C15-C16
26	6	601	CLA	C6-C7-C8-C9
26	8	610	CLA	C6-C7-C8-C9
26	X	613	CLA	C6-C7-C8-C9
26	Z	602	CLA	C11-C10-C8-C9
26	U	602	CLA	C6-C7-C8-C9
37	Y	609	CHL	C14-C13-C15-C16
37	Z	607	CHL	C14-C13-C15-C16
26	V	613	CLA	C16-C17-C18-C19
32	8	626	LMG	C20-C21-C22-C23
28	9	623	LHG	C12-C13-C14-C15
31	8	625	LMU	C6-C7-C8-C9
31	A	857	LMU	C4-C5-C6-C7
26	5	607	CLA	C10-C11-C12-C13
37	Y	609	CHL	C5-C6-C7-C8
26	A	803	CLA	C13-C15-C16-C17
26	B	819	CLA	CBA-CGA-O2A-C1
26	B	829	CLA	CBA-CGA-O2A-C1
26	A	830	CLA	C5-C6-C7-C8
26	2	613	CLA	C13-C15-C16-C17
31	8	625	LMU	C2-C3-C4-C5
26	A	828	CLA	C4-C3-C5-C6
26	B	827	CLA	C4-C3-C5-C6
26	B	828	CLA	C2-C3-C5-C6
26	B	803	CLA	C5-C6-C7-C8
37	W	607	CHL	C5-C6-C7-C8
28	9	623	LHG	C30-C31-C32-C33
37	Y	609	CHL	C4C-C3C-CAC-CBC
37	Z	609	CHL	C4C-C3C-CAC-CBC
37	V	609	CHL	C4C-C3C-CAC-CBC
37	W	608	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
37	W	609	CHL	C4C-C3C-CAC-CBC
26	V	613	CLA	C16-C17-C18-C20
32	4	623	LMG	C10-C11-C12-C13
37	V	609	CHL	C3-C5-C6-C7
28	Z	2630	LHG	C15-C16-C17-C18
26	A	813	CLA	C4B-C3B-CAB-CBB
26	A	838	CLA	C1A-C2A-CAA-CBA
26	A	839	CLA	C4B-C3B-CAB-CBB
26	A	842	CLA	C4B-C3B-CAB-CBB
26	B	812	CLA	C4B-C3B-CAB-CBB
26	B	821	CLA	C4B-C3B-CAB-CBB
26	B	840	CLA	C4B-C3B-CAB-CBB
26	F	301	CLA	C4B-C3B-CAB-CBB
26	G	204	CLA	C4B-C3B-CAB-CBB
26	L	302	CLA	C1A-C2A-CAA-CBA
26	1	611	CLA	C4B-C3B-CAB-CBB
26	2	607	CLA	C4B-C3B-CAB-CBB
26	3	613	CLA	C4B-C3B-CAB-CBB
26	4	610	CLA	C1A-C2A-CAA-CBA
26	4	613	CLA	C4B-C3B-CAB-CBB
26	6	610	CLA	C1A-C2A-CAA-CBA
26	6	613	CLA	C4B-C3B-CAB-CBB
26	X	602	CLA	C1A-C2A-CAA-CBA
26	Y	610	CLA	C4B-C3B-CAB-CBB
26	Z	604	CLA	C1A-C2A-CAA-CBA
26	Z	610	CLA	C1A-C2A-CAA-CBA
26	X	603	CLA	O1D-CGD-O2D-CED
37	Y	606	CHL	O1D-CGD-O2D-CED
33	B	850	DGD	CAB-CBB-CCB-CDB
26	B	832	CLA	CAA-CBA-CGA-O2A
29	B	849	BCR	C7-C8-C9-C10
28	O	2631	LHG	C10-C11-C12-C13
28	U	2630	LHG	C26-C27-C28-C29
28	A	846	LHG	C30-C31-C32-C33
26	6	610	CLA	C2A-CAA-CBA-CGA
26	V	604	CLA	C2A-CAA-CBA-CGA
26	Z	610	CLA	O1D-CGD-O2D-CED
28	9	623	LHG	O6-C4-C5-C6
26	8	608	CLA	CBD-CGD-O2D-CED
28	7	622	LHG	O9-C7-O7-C5
28	X	2630	LHG	C27-C28-C29-C30
26	A	802	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
26	A	807	CLA	C6-C7-C8-C10
26	A	818	CLA	C11-C10-C8-C7
26	A	828	CLA	C6-C7-C8-C10
26	B	808	CLA	C11-C10-C8-C7
26	B	813	CLA	C11-C10-C8-C7
26	B	813	CLA	C11-C12-C13-C15
26	B	814	CLA	C11-C12-C13-C15
26	K	203	CLA	C6-C7-C8-C10
26	1	613	CLA	C11-C10-C8-C7
26	5	613	CLA	C11-C10-C8-C7
26	6	610	CLA	C6-C7-C8-C10
26	X	610	CLA	C11-C10-C8-C7
26	Y	602	CLA	C6-C7-C8-C10
26	V	610	CLA	C11-C12-C13-C15
37	Y	607	CHL	C12-C13-C15-C16
37	Z	601	CHL	C6-C7-C8-C10
37	Z	601	CHL	C11-C10-C8-C7
37	Z	601	CHL	C11-C12-C13-C15
37	W	601	CHL	C12-C13-C15-C16
37	W	607	CHL	C12-C13-C15-C16
32	L	2631	LMG	C13-C14-C15-C16
26	4	613	CLA	C16-C17-C18-C19
37	W	605	CHL	O1D-CGD-O2D-CED
26	6	611	CLA	C3A-C2A-CAA-CBA
26	7	601	CLA	CBA-CGA-O2A-C1
37	Y	606	CHL	CBD-CGD-O2D-CED
31	5	628	LMU	C7-C8-C9-C10
28	Z	2630	LHG	C32-C33-C34-C35
32	A	860	LMG	O10-C28-O8-C9
28	Y	2630	LHG	C2-C3-O3-P
26	5	619	CLA	C3A-C2A-CAA-CBA
26	7	603	CLA	CHA-CBD-CGD-O1D
26	W	611	CLA	C4-C3-C5-C6
26	B	829	CLA	O1A-CGA-O2A-C1
28	A	861	LHG	O6-C4-C5-O7
28	3	623	LHG	O6-C4-C5-O7
28	7	622	LHG	O6-C4-C5-O7
28	Z	2630	LHG	O6-C4-C5-O7
28	U	2630	LHG	O6-C4-C5-O7
28	7	622	LHG	C8-C7-O7-C5
26	A	831	CLA	C14-C13-C15-C16
26	A	841	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	B	806	CLA	C11-C12-C13-C14
26	B	808	CLA	C14-C13-C15-C16
26	B	839	CLA	C11-C10-C8-C9
26	5	604	CLA	C6-C7-C8-C9
26	Y	613	CLA	C11-C10-C8-C9
37	X	607	CHL	C11-C12-C13-C14
37	X	608	CHL	C14-C13-C15-C16
37	Y	601	CHL	C11-C12-C13-C14
37	U	601	CHL	C14-C13-C15-C16
26	U	602	CLA	C10-C11-C12-C13
28	6	623	LHG	C12-C13-C14-C15
26	a	610	CLA	C5-C6-C7-C8
26	5	613	CLA	C15-C16-C17-C18
36	U	1623	NEX	C33-C34-C35-C15
26	A	811	CLA	C8-C10-C11-C12
26	7	610	CLA	C15-C16-C17-C18
26	7	613	CLA	C13-C15-C16-C17
26	8	601	CLA	C13-C15-C16-C17
37	W	609	CHL	C5-C6-C7-C8
26	B	825	CLA	C1-C2-C3-C4
26	O	2003	CLA	CAD-CBD-CGD-O1D
26	1	604	CLA	C1-C2-C3-C4
26	a	604	CLA	C1-C2-C3-C4
26	3	615	CLA	CAD-CBD-CGD-O1D
26	4	612	CLA	CAD-CBD-CGD-O1D
26	7	609	CLA	CHA-CBD-CGD-O2D
26	7	615	CLA	CHA-CBD-CGD-O2D
26	X	604	CLA	C1-C2-C3-C4
26	U	604	CLA	C1-C2-C3-C4
28	O	2631	LHG	C27-C28-C29-C30
26	7	601	CLA	O1A-CGA-O2A-C1
28	8	623	LHG	O10-C23-O8-C6
28	U	2630	LHG	O7-C5-C6-O8
32	H	205	LMG	O7-C8-C9-O8
32	5	627	LMG	O1-C7-C8-O7
32	8	626	LMG	O1-C7-C8-O7
32	A	860	LMG	O1-C7-C8-C9
32	J	103	LMG	O1-C7-C8-C9
37	Z	609	CHL	C4-C3-C5-C6
26	A	824	CLA	C2-C3-C5-C6
26	B	827	CLA	C2-C3-C5-C6
26	A	806	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	A	814	CLA	CAD-CBD-CGD-O2D
26	A	816	CLA	CAD-CBD-CGD-O2D
26	A	825	CLA	CAD-CBD-CGD-O2D
26	A	845	CLA	CAD-CBD-CGD-O2D
26	6	601	CLA	CAD-CBD-CGD-O2D
26	Y	602	CLA	CAD-CBD-CGD-O2D
26	Y	611	CLA	CAD-CBD-CGD-O2D
26	Z	611	CLA	CAD-CBD-CGD-O2D
26	Z	612	CLA	CAD-CBD-CGD-O2D
26	U	602	CLA	CAD-CBD-CGD-O2D
26	U	603	CLA	CAD-CBD-CGD-O2D
28	A	861	LHG	C28-C29-C30-C31
26	V	613	CLA	CBA-CGA-O2A-C1
31	A	858	LMU	O5'-C1'-O1'-C1
26	A	831	CLA	C3-C5-C6-C7
26	W	602	CLA	C3-C5-C6-C7
26	7	615	CLA	C2A-CAA-CBA-CGA
26	8	603	CLA	C2A-CAA-CBA-CGA
26	B	819	CLA	O1A-CGA-O2A-C1
26	B	838	CLA	O1A-CGA-O2A-C1
26	1	603	CLA	C2A-CAA-CBA-CGA
26	a	603	CLA	C2A-CAA-CBA-CGA
31	K	208	LMU	C6-C7-C8-C9
32	9	625	LMG	O7-C10-C11-C12
26	V	613	CLA	O1A-CGA-O2A-C1
26	A	806	CLA	CAD-CBD-CGD-O1D
26	A	807	CLA	CHA-CBD-CGD-O1D
26	A	807	CLA	CHA-CBD-CGD-O2D
26	A	814	CLA	CAD-CBD-CGD-O1D
26	A	815	CLA	CAD-CBD-CGD-O1D
26	A	816	CLA	CAD-CBD-CGD-O1D
26	A	821	CLA	CAD-CBD-CGD-O1D
26	A	823	CLA	CHA-CBD-CGD-O1D
26	A	823	CLA	CHA-CBD-CGD-O2D
26	A	825	CLA	CAD-CBD-CGD-O1D
26	A	831	CLA	CAD-CBD-CGD-O1D
26	A	840	CLA	CHA-CBD-CGD-O1D
26	A	840	CLA	CHA-CBD-CGD-O2D
26	A	845	CLA	CAD-CBD-CGD-O1D
26	B	813	CLA	CAD-CBD-CGD-O1D
26	B	821	CLA	CHA-CBD-CGD-O2D
26	B	821	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	B	824	CLA	CHA-CBD-CGD-O1D
26	B	824	CLA	CHA-CBD-CGD-O2D
26	B	829	CLA	CHA-CBD-CGD-O1D
26	B	841	CLA	CAD-CBD-CGD-O1D
26	H	202	CLA	CHA-CBD-CGD-O2D
26	L	307	CLA	CHA-CBD-CGD-O2D
26	O	2001	CLA	CAD-CBD-CGD-O2D
26	1	607	CLA	CHA-CBD-CGD-O2D
26	1	607	CLA	CAD-CBD-CGD-O2D
26	1	610	CLA	CHA-CBD-CGD-O1D
26	a	609	CLA	CHA-CBD-CGD-O2D
26	a	609	CLA	CAD-CBD-CGD-O2D
26	a	610	CLA	CHA-CBD-CGD-O1D
26	2	603	CLA	CHA-CBD-CGD-O2D
26	3	602	CLA	CHA-CBD-CGD-O2D
26	3	613	CLA	CAD-CBD-CGD-O2D
26	6	601	CLA	CAD-CBD-CGD-O1D
26	6	603	CLA	CHA-CBD-CGD-O1D
26	6	603	CLA	CHA-CBD-CGD-O2D
26	6	612	CLA	CHA-CBD-CGD-O2D
26	6	612	CLA	CAD-CBD-CGD-O2D
26	6	613	CLA	CHA-CBD-CGD-O2D
26	8	603	CLA	CHA-CBD-CGD-O1D
26	8	603	CLA	CHA-CBD-CGD-O2D
26	X	614	CLA	CHA-CBD-CGD-O1D
26	Y	602	CLA	CAD-CBD-CGD-O1D
26	Y	611	CLA	CAD-CBD-CGD-O1D
26	Y	614	CLA	CHA-CBD-CGD-O1D
26	Z	611	CLA	CAD-CBD-CGD-O1D
26	Z	612	CLA	CAD-CBD-CGD-O1D
26	U	602	CLA	CAD-CBD-CGD-O1D
26	U	603	CLA	CAD-CBD-CGD-O1D
26	W	612	CLA	CHA-CBD-CGD-O1D
28	A	846	LHG	C4-O6-P-O5
28	A	847	LHG	C3-O3-P-O5
28	B	851	LHG	C4-O6-P-O5
28	O	2631	LHG	C3-O3-P-O5
28	O	2631	LHG	C4-O6-P-O5
28	2	622	LHG	C3-O3-P-O5
28	3	623	LHG	C4-O6-P-O3
28	3	623	LHG	C4-O6-P-O4
28	3	624	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
28	5	625	LHG	C4-O6-P-O5
28	6	623	LHG	C4-O6-P-O3
28	8	622	LHG	C3-O3-P-O5
28	9	622	LHG	C4-O6-P-O5
28	9	623	LHG	C3-O3-P-O5
28	9	623	LHG	C4-O6-P-O5
28	Z	2630	LHG	C3-O3-P-O5
28	U	2630	LHG	C3-O3-P-O6
28	V	2630	LHG	C4-O6-P-O3
28	V	2630	LHG	C4-O6-P-O4
28	W	2630	LHG	C4-O6-P-O4
35	X	1622	XAT	C9-C10-C11-C12
37	X	605	CHL	CHA-CBD-CGD-O1D
37	X	605	CHL	CHA-CBD-CGD-O2D
37	V	606	CHL	CHA-CBD-CGD-O2D
37	V	609	CHL	CHA-CBD-CGD-O1D
37	V	609	CHL	CHA-CBD-CGD-O2D
28	4	622	LHG	C25-C26-C27-C28
26	A	803	CLA	C4-C3-C5-C6
26	A	812	CLA	C2B-C3B-CAB-CBB
26	A	839	CLA	C2B-C3B-CAB-CBB
26	A	841	CLA	C2B-C3B-CAB-CBB
26	A	842	CLA	C2B-C3B-CAB-CBB
26	B	802	CLA	C2B-C3B-CAB-CBB
26	B	837	CLA	C2B-C3B-CAB-CBB
26	4	602	CLA	C2B-C3B-CAB-CBB
26	4	613	CLA	C2B-C3B-CAB-CBB
26	5	617	CLA	C2B-C3B-CAB-CBB
26	6	604	CLA	C2B-C3B-CAB-CBB
26	6	614	CLA	C2B-C3B-CAB-CBB
26	7	610	CLA	C2B-C3B-CAB-CBB
26	9	614	CLA	C2B-C3B-CAB-CBB
26	Y	610	CLA	C2B-C3B-CAB-CBB
26	Y	612	CLA	C2B-C3B-CAB-CBB
26	Z	613	CLA	C2B-C3B-CAB-CBB
26	Z	614	CLA	C2B-C3B-CAB-CBB
26	V	603	CLA	C2B-C3B-CAB-CBB
26	V	613	CLA	C2B-C3B-CAB-CBB
26	W	611	CLA	C2B-C3B-CAB-CBB
29	A	852	BCR	C1-C6-C7-C8
29	B	845	BCR	C23-C24-C25-C30
29	L	309	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	O	2004	BCR	C23-C24-C25-C30
29	4	621	BCR	C1-C6-C7-C8
34	4	619	LUT	C5-C6-C7-C8
34	Y	1620	LUT	C1-C6-C7-C8
26	A	828	CLA	C2-C3-C5-C6
28	Z	2630	LHG	C18-C19-C20-C21
26	a	603	CLA	C6-C7-C8-C10
26	5	607	CLA	C13-C15-C16-C17
26	4	610	CLA	C12-C13-C15-C16
28	A	861	LHG	C6-C5-O7-C7
28	8	623	LHG	C6-C5-O7-C7
32	8	626	LMG	C9-C8-O7-C10
36	U	1623	NEX	C10-C11-C12-C13
26	A	819	CLA	CAA-CBA-CGA-O2A
26	B	827	CLA	CAA-CBA-CGA-O2A
26	B	832	CLA	C5-C6-C7-C8
27	A	844	PQN	C18-C20-C21-C22
26	W	611	CLA	C2-C3-C5-C6
26	1	603	CLA	C6-C7-C8-C10
33	B	850	DGD	C2A-C3A-C4A-C5A
28	7	622	LHG	O6-C4-C5-C6
26	A	838	CLA	CBA-CGA-O2A-C1
26	B	828	CLA	C8-C10-C11-C12
26	B	802	CLA	C6-C7-C8-C9
26	B	810	CLA	C6-C7-C8-C9
26	B	833	CLA	C6-C7-C8-C9
26	H	203	CLA	C11-C10-C8-C9
26	K	203	CLA	C6-C7-C8-C9
26	5	604	CLA	C11-C10-C8-C9
26	5	613	CLA	C11-C10-C8-C9
26	9	613	CLA	C11-C12-C13-C14
26	X	610	CLA	C14-C13-C15-C16
37	X	609	CHL	C11-C12-C13-C14
26	B	839	CLA	C12-C13-C15-C16
26	H	203	CLA	C11-C10-C8-C7
37	Z	609	CHL	C6-C7-C8-C10
37	W	601	CHL	C6-C7-C8-C10
28	U	2630	LHG	C1-C2-C3-O3
26	A	803	CLA	O1D-CGD-O2D-CED
26	2	616	CLA	O1D-CGD-O2D-CED
32	H	205	LMG	C30-C31-C32-C33
26	8	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	8	610	CLA	O1A-CGA-O2A-C1
26	U	602	CLA	C2-C3-C5-C6
37	Y	601	CHL	C2-C3-C5-C6
26	A	841	CLA	C3-C5-C6-C7
31	5	629	LMU	C1-C2-C3-C4
32	V	2631	LMG	C16-C17-C18-C19
26	H	203	CLA	C15-C16-C17-C18
26	A	804	CLA	C4C-C3C-CAC-CBC
28	Z	2630	LHG	O7-C5-C6-O8
26	7	602	CLA	C16-C17-C18-C20
32	V	2631	LMG	C11-C10-O7-C8
28	U	2630	LHG	C7-C8-C9-C10
26	B	811	CLA	C4-C3-C5-C6
37	V	609	CHL	C4-C3-C5-C6
28	Z	2630	LHG	C4-C5-C6-O8
31	1	621	LMU	O1'-C1-C2-C3
26	B	841	CLA	O1D-CGD-O2D-CED
28	H	204	LHG	C26-C27-C28-C29
29	A	849	BCR	C21-C22-C23-C24
26	B	837	CLA	O1D-CGD-O2D-CED
26	B	833	CLA	C5-C6-C7-C8
26	A	802	CLA	C2A-CAA-CBA-CGA
26	A	839	CLA	C2A-CAA-CBA-CGA
26	1	613	CLA	C2A-CAA-CBA-CGA
26	a	613	CLA	C2A-CAA-CBA-CGA
26	8	611	CLA	O1D-CGD-O2D-CED
34	U	1621	LUT	C29-C30-C31-C32
32	4	623	LMG	C29-C30-C31-C32
26	8	602	CLA	C4-C3-C5-C6
28	9	624	LHG	C15-C16-C17-C18
32	V	2631	LMG	O9-C10-O7-C8
31	1	621	LMU	C2-C1-O1'-C1'
28	4	622	LHG	C29-C30-C31-C32
26	5	614	CLA	CAA-CBA-CGA-O2A
26	A	814	CLA	C11-C10-C8-C9
26	A	824	CLA	C11-C10-C8-C9
26	B	813	CLA	C11-C10-C8-C9
26	B	813	CLA	C11-C12-C13-C14
26	Y	602	CLA	C6-C7-C8-C9
26	V	610	CLA	C11-C12-C13-C14
26	V	613	CLA	C6-C7-C8-C9
37	Y	607	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
37	W	607	CHL	C14-C13-C15-C16
26	X	604	CLA	CBA-CGA-O2A-C1
26	B	837	CLA	C5-C6-C7-C8
26	A	838	CLA	O1A-CGA-O2A-C1
26	A	832	CLA	C4B-C3B-CAB-CBB
26	L	303	CLA	C4B-C3B-CAB-CBB
26	5	607	CLA	C4B-C3B-CAB-CBB
26	5	608	CLA	C4B-C3B-CAB-CBB
26	6	609	CLA	C4B-C3B-CAB-CBB
26	6	617	CLA	C4B-C3B-CAB-CBB
26	Z	602	CLA	C4B-C3B-CAB-CBB
26	U	614	CLA	C4B-C3B-CAB-CBB
26	W	602	CLA	C4B-C3B-CAB-CBB
26	W	614	CLA	C4B-C3B-CAB-CBB
37	X	601	CHL	CAA-CBA-CGA-O1A
26	A	818	CLA	C8-C10-C11-C12
26	B	832	CLA	C10-C11-C12-C13
26	4	601	CLA	C4-C3-C5-C6
26	A	803	CLA	C2-C3-C5-C6
26	8	602	CLA	C2-C3-C5-C6
37	Z	609	CHL	C2-C3-C5-C6
37	V	609	CHL	C2-C3-C5-C6
28	8	622	LHG	C12-C13-C14-C15
26	X	604	CLA	O1A-CGA-O2A-C1
36	Y	1623	NEX	C33-C34-C35-C15
26	1	603	CLA	C6-C7-C8-C9
26	a	603	CLA	C6-C7-C8-C9
26	7	602	CLA	C16-C17-C18-C19
26	B	802	CLA	C12-C13-C15-C16
26	B	831	CLA	C12-C13-C15-C16
26	B	841	CLA	C11-C10-C8-C7
26	5	613	CLA	C6-C7-C8-C10
26	7	613	CLA	C11-C10-C8-C7
26	9	613	CLA	C11-C12-C13-C15
26	X	603	CLA	C6-C7-C8-C10
37	X	609	CHL	C10-C11-C12-C13
28	A	861	LHG	O2-C2-C3-O3
26	A	819	CLA	C10-C11-C12-C13
28	U	2630	LHG	C11-C10-C9-C8
31	5	629	LMU	C4'-C5'-C6'-O6'
28	5	625	LHG	C15-C16-C17-C18
26	6	601	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	9	624	LHG	O7-C5-C6-O8
26	A	815	CLA	C3A-C2A-CAA-CBA
26	A	838	CLA	C3A-C2A-CAA-CBA
26	B	810	CLA	C3A-C2A-CAA-CBA
26	B	827	CLA	C3A-C2A-CAA-CBA
26	B	828	CLA	C3A-C2A-CAA-CBA
26	B	836	CLA	C3A-C2A-CAA-CBA
26	3	612	CLA	C3A-C2A-CAA-CBA
26	6	608	CLA	C3A-C2A-CAA-CBA
37	X	606	CHL	C3A-C2A-CAA-CBA
27	A	844	PQN	C12-C13-C15-C16
28	9	623	LHG	C31-C32-C33-C34
26	1	612	CLA	CAA-CBA-CGA-O1A
26	B	811	CLA	CAD-CBD-CGD-O1D
26	B	811	CLA	CAD-CBD-CGD-O2D
26	2	602	CLA	C4B-C3B-CAB-CBB
29	A	852	BCR	C11-C10-C9-C34
29	A	852	BCR	C16-C17-C18-C36
29	B	845	BCR	C11-C10-C9-C34
29	B	845	BCR	C20-C21-C22-C37
29	F	305	BCR	C16-C17-C18-C36
29	L	301	BCR	C11-C10-C9-C34
34	Y	1620	LUT	C20-C13-C14-C15
36	5	624	NEX	C39-C29-C30-C31
36	6	624	NEX	C39-C29-C30-C31
36	X	1623	NEX	C39-C29-C30-C31
36	Y	1623	NEX	C39-C29-C30-C31
36	Z	1623	NEX	C39-C29-C30-C31
36	U	1623	NEX	C39-C29-C30-C31
36	V	1623	NEX	C39-C29-C30-C31
36	W	1623	NEX	C39-C29-C30-C31
28	4	622	LHG	C13-C14-C15-C16
26	B	802	CLA	C13-C15-C16-C17
37	U	601	CHL	C3-C5-C6-C7
26	A	814	CLA	C16-C17-C18-C19
36	Y	1623	NEX	C31-C32-C33-C40
26	a	612	CLA	CAA-CBA-CGA-O1A
26	V	612	CLA	CAA-CBA-CGA-O1A
28	5	625	LHG	C17-C18-C19-C20
26	A	828	CLA	O1A-CGA-O2A-C1
37	Z	607	CHL	C8-C10-C11-C12
26	5	619	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	V	1622	XAT	C31-C32-C33-C34
36	6	624	NEX	C11-C12-C13-C14
33	B	850	DGD	C4B-C5B-C6B-C7B
26	A	836	CLA	C10-C11-C12-C13
26	A	813	CLA	C2A-CAA-CBA-CGA
26	A	838	CLA	C2A-CAA-CBA-CGA
26	a	606	CLA	C2A-CAA-CBA-CGA
26	3	607	CLA	C2A-CAA-CBA-CGA
26	9	604	CLA	C3-C5-C6-C7
26	5	614	CLA	CAA-CBA-CGA-O1A
33	B	850	DGD	C1G-C2G-C3G-O3G
37	V	609	CHL	C10-C11-C12-C13
26	4	607	CLA	CAA-CBA-CGA-O1A
26	6	617	CLA	CAA-CBA-CGA-O1A
26	7	615	CLA	CAA-CBA-CGA-O2A
26	A	826	CLA	C14-C13-C15-C16
26	A	834	CLA	C11-C12-C13-C14
26	B	831	CLA	C14-C13-C15-C16
26	H	203	CLA	C14-C13-C15-C16
26	L	303	CLA	C14-C13-C15-C16
26	1	613	CLA	C11-C12-C13-C14
26	5	609	CLA	C11-C10-C8-C9
26	5	613	CLA	C6-C7-C8-C9
26	6	601	CLA	C11-C10-C8-C9
26	6	604	CLA	C11-C10-C8-C9
26	X	602	CLA	C11-C12-C13-C14
26	X	603	CLA	C6-C7-C8-C9
26	Y	613	CLA	C14-C13-C15-C16
37	X	601	CHL	C6-C7-C8-C9
37	Y	607	CHL	C6-C7-C8-C9
37	W	601	CHL	C11-C10-C8-C9
28	B	851	LHG	C11-C10-C9-C8
26	7	612	CLA	CAA-CBA-CGA-O1A
26	V	612	CLA	CAA-CBA-CGA-O2A
32	8	626	LMG	C7-C8-O7-C10
31	5	628	LMU	O5B-C1B-O1B-C4'
37	X	605	CHL	C1A-C2A-CAA-CBA
37	Z	609	CHL	C1A-C2A-CAA-CBA
37	V	605	CHL	C1A-C2A-CAA-CBA
37	V	606	CHL	C1A-C2A-CAA-CBA
37	W	601	CHL	C1A-C2A-CAA-CBA
37	W	607	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	7	612	CLA	CAA-CBA-CGA-O2A
26	Y	612	CLA	CAA-CBA-CGA-O1A
28	Y	2630	LHG	C12-C13-C14-C15
26	8	611	CLA	CBD-CGD-O2D-CED
37	U	608	CHL	C2A-CAA-CBA-CGA
26	a	607	CLA	CAA-CBA-CGA-O2A
37	Y	606	CHL	CAA-CBA-CGA-O2A
26	2	612	CLA	C2A-CAA-CBA-CGA
26	9	602	CLA	C2A-CAA-CBA-CGA
37	Y	601	CHL	C2A-CAA-CBA-CGA
26	B	814	CLA	C1A-C2A-CAA-CBA
26	B	827	CLA	C1A-C2A-CAA-CBA
26	B	832	CLA	C1A-C2A-CAA-CBA
26	B	836	CLA	C1A-C2A-CAA-CBA
26	L	303	CLA	C1A-C2A-CAA-CBA
26	2	601	CLA	C1A-C2A-CAA-CBA
26	3	612	CLA	C1A-C2A-CAA-CBA
26	8	610	CLA	C1A-C2A-CAA-CBA
26	Y	602	CLA	C1A-C2A-CAA-CBA
26	Z	602	CLA	C1A-C2A-CAA-CBA
26	Z	611	CLA	C1A-C2A-CAA-CBA
26	U	604	CLA	C1A-C2A-CAA-CBA
26	U	610	CLA	C1A-C2A-CAA-CBA
26	V	604	CLA	C1A-C2A-CAA-CBA
26	W	604	CLA	C1A-C2A-CAA-CBA
29	A	852	BCR	C11-C10-C9-C8
29	A	852	BCR	C16-C17-C18-C19
29	B	845	BCR	C11-C10-C9-C8
29	B	845	BCR	C20-C21-C22-C23
29	B	852	BCR	C11-C10-C9-C8
29	F	305	BCR	C16-C17-C18-C19
29	L	301	BCR	C11-C10-C9-C8
34	Y	1620	LUT	C12-C13-C14-C15
36	5	624	NEX	C28-C29-C30-C31
36	6	624	NEX	C28-C29-C30-C31
36	X	1623	NEX	C28-C29-C30-C31
36	Y	1623	NEX	C28-C29-C30-C31
36	Z	1623	NEX	C28-C29-C30-C31
36	U	1623	NEX	C28-C29-C30-C31
36	V	1623	NEX	C28-C29-C30-C31
36	W	1623	NEX	C28-C29-C30-C31
26	3	609	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	A	828	CLA	CBA-CGA-O2A-C1
26	Y	604	CLA	CBA-CGA-O2A-C1
32	H	205	LMG	C13-C14-C15-C16
26	6	601	CLA	C16-C17-C18-C20
26	A	837	CLA	CAA-CBA-CGA-O1A
26	6	617	CLA	CAA-CBA-CGA-O2A
28	U	2630	LHG	C30-C31-C32-C33
26	B	818	CLA	C3-C5-C6-C7
37	W	607	CHL	C10-C11-C12-C13
26	A	813	CLA	C2B-C3B-CAB-CBB
26	A	815	CLA	C2B-C3B-CAB-CBB
26	A	832	CLA	C2B-C3B-CAB-CBB
26	A	835	CLA	C2B-C3B-CAB-CBB
26	B	812	CLA	C2B-C3B-CAB-CBB
26	B	840	CLA	C2B-C3B-CAB-CBB
26	F	301	CLA	C2B-C3B-CAB-CBB
26	G	204	CLA	C2B-C3B-CAB-CBB
26	K	204	CLA	C2B-C3B-CAB-CBB
26	1	611	CLA	C2B-C3B-CAB-CBB
26	2	603	CLA	C2B-C3B-CAB-CBB
26	2	607	CLA	C2B-C3B-CAB-CBB
26	3	606	CLA	C2B-C3B-CAB-CBB
26	3	613	CLA	C2B-C3B-CAB-CBB
26	4	606	CLA	C2B-C3B-CAB-CBB
26	5	607	CLA	C2B-C3B-CAB-CBB
26	6	608	CLA	C2B-C3B-CAB-CBB
26	6	613	CLA	C2B-C3B-CAB-CBB
26	7	603	CLA	C2B-C3B-CAB-CBB
26	7	608	CLA	C2B-C3B-CAB-CBB
26	9	601	CLA	C2B-C3B-CAB-CBB
26	X	613	CLA	C2B-C3B-CAB-CBB
26	Y	613	CLA	C2B-C3B-CAB-CBB
26	W	602	CLA	C2B-C3B-CAB-CBB
29	A	848	BCR	C5-C6-C7-C8
29	A	851	BCR	C1-C6-C7-C8
29	2	623	BCR	C23-C24-C25-C30
29	3	622	BCR	C1-C6-C7-C8
34	9	619	LUT	C5-C6-C7-C8
34	X	1620	LUT	C5-C6-C7-C8
34	X	1621	LUT	C1-C6-C7-C8
34	Y	1620	LUT	C5-C6-C7-C8
34	Z	1621	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	8	623	LHG	C30-C31-C32-C33
26	7	611	CLA	C3-C5-C6-C7
26	B	819	CLA	C6-C7-C8-C10
26	a	607	CLA	CAA-CBA-CGA-O1A
26	A	825	CLA	C4-C3-C5-C6
26	A	827	CLA	C4-C3-C5-C6
37	U	609	CHL	C4-C3-C5-C6
26	4	601	CLA	C2-C3-C5-C6
28	W	2630	LHG	C26-C27-C28-C29
28	H	204	LHG	C23-C24-C25-C26
26	2	603	CLA	C2C-C3C-CAC-CBC
37	X	607	CHL	CBA-CGA-O2A-C1
26	7	611	CLA	O2A-C1-C2-C3
26	U	604	CLA	O2A-C1-C2-C3
26	1	612	CLA	CAA-CBA-CGA-O2A
26	a	612	CLA	CAA-CBA-CGA-O2A
26	4	603	CLA	CAA-CBA-CGA-O2A
37	Y	606	CHL	CAA-CBA-CGA-O1A
28	9	624	LHG	C16-C17-C18-C19
26	A	814	CLA	C11-C10-C8-C7
26	A	824	CLA	C11-C10-C8-C7
26	A	831	CLA	C11-C12-C13-C15
26	A	841	CLA	C12-C13-C15-C16
26	6	601	CLA	C11-C10-C8-C7
26	7	613	CLA	C11-C12-C13-C15
26	A	839	CLA	C6-C7-C8-C10
26	1	602	CLA	C2A-CAA-CBA-CGA
26	a	602	CLA	C2A-CAA-CBA-CGA
26	Z	602	CLA	C2A-CAA-CBA-CGA
28	W	2630	LHG	O7-C5-C6-O8
26	7	609	CLA	CAA-CBA-CGA-O2A
28	Z	2630	LHG	C12-C13-C14-C15
26	A	802	CLA	C5-C6-C7-C8
26	B	817	CLA	CBA-CGA-O2A-C1
26	A	801	CLA	CAA-CBA-CGA-O2A
26	2	603	CLA	CAA-CBA-CGA-O1A
26	4	607	CLA	CAA-CBA-CGA-O2A
28	8	622	LHG	C1-C2-C3-O3
26	V	610	CLA	C13-C15-C16-C17
26	A	835	CLA	C12-C13-C15-C16
35	V	1622	XAT	C31-C32-C33-C40
26	L	302	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	5	616	CLA	CAA-CBA-CGA-O2A
26	W	603	CLA	C4-C3-C5-C6
37	X	607	CHL	C4-C3-C5-C6
37	Y	609	CHL	C4-C3-C5-C6
27	B	842	PQN	C12-C13-C15-C16
37	U	609	CHL	C2-C3-C5-C6
26	8	601	CLA	C10-C11-C12-C13
37	X	609	CHL	C2C-C3C-CAC-CBC
26	7	609	CLA	CAA-CBA-CGA-O1A
26	2	602	CLA	C16-C17-C18-C19
28	B	851	LHG	C24-C25-C26-C27
32	H	205	LMG	C28-C29-C30-C31
26	Y	604	CLA	O1A-CGA-O2A-C1
26	5	607	CLA	C3-C5-C6-C7
28	8	622	LHG	C18-C19-C20-C21
26	1	608	CLA	CAA-CBA-CGA-O2A
26	a	608	CLA	CAA-CBA-CGA-O2A
26	W	614	CLA	CAA-CBA-CGA-O2A
26	A	843	CLA	C14-C13-C15-C16
26	B	802	CLA	C11-C10-C8-C9
26	B	827	CLA	C14-C13-C15-C16
26	5	607	CLA	C6-C7-C8-C9
26	8	601	CLA	C11-C12-C13-C14
34	Y	1621	LUT	C29-C30-C31-C32
35	Z	1622	XAT	C33-C34-C35-C15
26	8	608	CLA	O1D-CGD-O2D-CED
26	B	810	CLA	C16-C17-C18-C19
26	L	302	CLA	CAA-CBA-CGA-O1A
26	4	603	CLA	CAA-CBA-CGA-O1A
26	7	615	CLA	CAA-CBA-CGA-O1A
26	Y	612	CLA	CAA-CBA-CGA-O2A
28	9	624	LHG	C31-C32-C33-C34
32	A	860	LMG	C11-C12-C13-C14
32	H	205	LMG	O6-C1-O1-C7
28	U	2630	LHG	C23-C24-C25-C26
26	3	608	CLA	C4-C3-C5-C6
37	W	609	CHL	C4-C3-C5-C6
26	3	608	CLA	C2-C3-C5-C6
26	4	601	CLA	C13-C15-C16-C17
26	5	610	CLA	C5-C6-C7-C8
26	7	603	CLA	CAA-CBA-CGA-O2A
28	A	861	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	5	627	LMG	C12-C13-C14-C15
28	3	623	LHG	C4-C5-C6-O8
28	9	624	LHG	C4-C5-C6-O8
28	U	2630	LHG	C4-C5-C6-O8
32	5	627	LMG	O1-C7-C8-C9
26	G	204	CLA	CAA-CBA-CGA-O2A
26	9	603	CLA	CAA-CBA-CGA-O2A
26	W	612	CLA	CAA-CBA-CGA-O1A
26	W	612	CLA	CAA-CBA-CGA-O2A
26	U	604	CLA	CAD-CBD-CGD-O1D
37	X	608	CHL	CAD-CBD-CGD-O1D
26	A	807	CLA	C2A-CAA-CBA-CGA
26	G	204	CLA	C2A-CAA-CBA-CGA
37	Y	609	CHL	C2C-C3C-CAC-CBC
26	8	613	CLA	C16-C17-C18-C20
26	A	840	CLA	C4C-C3C-CAC-CBC
26	2	603	CLA	CAA-CBA-CGA-O2A
26	7	603	CLA	CAA-CBA-CGA-O1A
26	3	608	CLA	C5-C6-C7-C8
28	9	623	LHG	O6-C4-C5-O7
28	X	2630	LHG	O6-C4-C5-O7
26	7	602	CLA	C4-C3-C5-C6
26	Y	610	CLA	C4-C3-C5-C6
28	6	623	LHG	C17-C18-C19-C20
26	1	616	CLA	CAA-CBA-CGA-O2A
26	a	616	CLA	CAA-CBA-CGA-O2A
26	5	619	CLA	CBD-CGD-O2D-CED
26	A	817	CLA	C4B-C3B-CAB-CBB
26	A	827	CLA	C4B-C3B-CAB-CBB
26	H	203	CLA	C4B-C3B-CAB-CBB
26	K	204	CLA	C4B-C3B-CAB-CBB
26	4	601	CLA	C4B-C3B-CAB-CBB
26	X	604	CLA	C4B-C3B-CAB-CBB
26	Y	602	CLA	C4B-C3B-CAB-CBB
26	Y	613	CLA	C4B-C3B-CAB-CBB
26	B	817	CLA	O1A-CGA-O2A-C1
26	a	610	CLA	O1A-CGA-O2A-C1
37	X	607	CHL	O1A-CGA-O2A-C1
32	J	103	LMG	C22-C23-C24-C25
37	Z	606	CHL	CAA-CBA-CGA-O1A
28	9	623	LHG	C11-C12-C13-C14
26	A	833	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	A	837	CLA	CAA-CBA-CGA-O2A
26	5	616	CLA	CAA-CBA-CGA-O1A
26	V	603	CLA	CAA-CBA-CGA-O2A
26	A	818	CLA	C11-C12-C13-C15
26	2	602	CLA	C16-C17-C18-C20
26	6	601	CLA	C16-C17-C18-C19
26	Y	613	CLA	C16-C17-C18-C20
29	B	852	BCR	C11-C10-C9-C34
37	Y	601	CHL	CHA-CBD-CGD-O1D
37	Y	601	CHL	CHA-CBD-CGD-O2D
37	Z	601	CHL	CHA-CBD-CGD-O1D
37	Z	601	CHL	CHA-CBD-CGD-O2D
37	U	601	CHL	CHA-CBD-CGD-O1D
37	U	601	CHL	CHA-CBD-CGD-O2D
37	U	609	CHL	CHA-CBD-CGD-O1D
37	U	609	CHL	CHA-CBD-CGD-O2D
37	W	601	CHL	CHA-CBD-CGD-O1D
37	W	601	CHL	CHA-CBD-CGD-O2D
28	3	623	LHG	C24-C25-C26-C27
26	8	603	CLA	CAA-CBA-CGA-O2A
26	9	601	CLA	CAA-CBA-CGA-O2A
37	Z	606	CHL	CAA-CBA-CGA-O2A
37	W	605	CHL	CAA-CBA-CGA-O2A
26	B	809	CLA	O1A-CGA-O2A-C1
28	A	861	LHG	O6-C4-C5-C6
28	X	2630	LHG	O6-C4-C5-C6
26	B	829	CLA	C4-C3-C5-C6
32	8	626	LMG	O7-C8-C9-O8
26	1	608	CLA	CAA-CBA-CGA-O1A
26	a	608	CLA	CAA-CBA-CGA-O1A
26	W	614	CLA	CAA-CBA-CGA-O1A
37	W	607	CHL	CAA-CBA-CGA-O1A
26	W	603	CLA	C2-C3-C5-C6
26	A	826	CLA	C15-C16-C17-C18
26	a	602	CLA	C10-C11-C12-C13
26	A	843	CLA	C12-C13-C15-C16
26	B	802	CLA	C11-C10-C8-C7
26	5	607	CLA	C6-C7-C8-C10
26	6	602	CLA	C11-C12-C13-C15
28	O	2631	LHG	C11-C12-C13-C14
28	a	620	LHG	C27-C28-C29-C30
26	1	602	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	B	850	DGD	C4A-C5A-C6A-C7A
28	1	620	LHG	C27-C28-C29-C30
26	V	603	CLA	CAA-CBA-CGA-O1A
26	W	603	CLA	CAA-CBA-CGA-O1A
26	B	814	CLA	C11-C12-C13-C14
26	F	301	CLA	C6-C7-C8-C9
26	1	613	CLA	C11-C10-C8-C9
26	a	609	CLA	C11-C12-C13-C14
26	7	610	CLA	C14-C13-C15-C16
26	9	613	CLA	C11-C10-C8-C9
26	X	610	CLA	C11-C10-C8-C9
26	W	613	CLA	C11-C12-C13-C14
37	Y	601	CHL	C11-C10-C8-C9
37	Y	607	CHL	C11-C10-C8-C9
37	W	601	CHL	C14-C13-C15-C16
26	Z	604	CLA	CHA-CBD-CGD-O2D
32	9	625	LMG	C8-C7-O1-C1
26	7	602	CLA	C2A-CAA-CBA-CGA
26	B	806	CLA	C2-C1-O2A-CGA
26	9	604	CLA	C2-C1-O2A-CGA
26	6	601	CLA	CBA-CGA-O2A-C1
26	A	803	CLA	C3A-C2A-CAA-CBA
26	4	602	CLA	C4-C3-C5-C6
26	X	612	CLA	C3A-C2A-CAA-CBA
26	U	603	CLA	C3A-C2A-CAA-CBA
26	V	604	CLA	C3A-C2A-CAA-CBA
37	W	607	CHL	C4-C3-C5-C6
26	8	603	CLA	CAA-CBA-CGA-O1A
26	9	603	CLA	CAA-CBA-CGA-O1A
26	A	833	CLA	CAA-CBA-CGA-O1A
37	W	605	CHL	CAA-CBA-CGA-O1A
26	U	603	CLA	CAA-CBA-CGA-O2A
28	Y	2630	LHG	C16-C17-C18-C19
26	6	620	CLA	C3-C5-C6-C7
37	Y	607	CHL	C3C-C2C-CMC-OMC
37	Z	608	CHL	C3C-C2C-CMC-OMC
26	4	608	CLA	C4C-C3C-CAC-CBC
31	5	629	LMU	C2B-C1B-O1B-C4'
28	9	623	LHG	C14-C15-C16-C17
26	G	204	CLA	CAA-CBA-CGA-O1A
26	B	811	CLA	C2-C3-C5-C6
26	a	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	B	833	CLA	C10-C11-C12-C13
26	1	606	CLA	CAD-CBD-CGD-O2D
26	a	606	CLA	CAD-CBD-CGD-O2D
36	Y	1623	NEX	O24-C26-C27-C28
36	Z	1623	NEX	O24-C26-C27-C28
36	U	1623	NEX	O24-C26-C27-C28
36	W	1623	NEX	O24-C26-C27-C28
26	1	616	CLA	CAA-CBA-CGA-O1A
26	a	616	CLA	CAA-CBA-CGA-O1A
26	5	619	CLA	CAA-CBA-CGA-O2A
32	H	205	LMG	C7-C8-C9-O8
32	J	104	LMG	C7-C8-C9-O8
26	Y	602	CLA	C5-C6-C7-C8
26	B	819	CLA	C6-C7-C8-C9
26	5	613	CLA	C2-C1-O2A-CGA
26	9	601	CLA	CAA-CBA-CGA-O1A
28	B	851	LHG	C11-C12-C13-C14
26	A	802	CLA	C4-C3-C5-C6
26	7	613	CLA	C4-C3-C5-C6
26	A	824	CLA	C2A-CAA-CBA-CGA
26	A	830	CLA	C2A-CAA-CBA-CGA
26	9	607	CLA	CAA-CBA-CGA-O1A
28	Y	2630	LHG	C14-C15-C16-C17
36	X	1623	NEX	C7-C8-C9-C19
26	A	839	CLA	C6-C7-C8-C9
26	B	810	CLA	C16-C17-C18-C20
26	A	807	CLA	CAA-CBA-CGA-O2A
32	J	104	LMG	C31-C32-C33-C34
26	A	802	CLA	C11-C10-C8-C9
26	A	818	CLA	C11-C10-C8-C9
26	6	610	CLA	C6-C7-C8-C9
26	6	610	CLA	C11-C12-C13-C14
26	X	610	CLA	C11-C12-C13-C14
26	Y	613	CLA	C11-C12-C13-C14
37	Z	601	CHL	C11-C12-C13-C14
37	U	601	CHL	C6-C7-C8-C9
37	V	601	CHL	C6-C7-C8-C9
26	B	806	CLA	CAA-CBA-CGA-O2A
28	9	624	LHG	O9-C7-O7-C5
26	5	601	CLA	C3-C5-C6-C7
28	9	624	LHG	C14-C15-C16-C17
32	H	205	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	Z	2630	LHG	C11-C10-C9-C8
37	V	609	CHL	O1D-CGD-O2D-CED
28	8	622	LHG	O8-C23-C24-C25
28	U	2630	LHG	O7-C7-C8-C9
37	Y	609	CHL	C2-C3-C5-C6
26	9	607	CLA	CAA-CBA-CGA-O2A
26	5	619	CLA	C2A-CAA-CBA-CGA
26	A	801	CLA	C12-C13-C15-C16
26	A	829	CLA	C12-C13-C15-C16
26	B	827	CLA	C12-C13-C15-C16
26	B	840	CLA	C11-C10-C8-C7
26	1	613	CLA	C11-C12-C13-C15
26	a	609	CLA	C11-C12-C13-C15
26	5	609	CLA	C11-C10-C8-C7
26	7	610	CLA	C12-C13-C15-C16
26	8	601	CLA	C11-C12-C13-C15
26	Y	613	CLA	C12-C13-C15-C16
37	X	609	CHL	C12-C13-C15-C16
37	W	601	CHL	C11-C10-C8-C7
26	B	841	CLA	C3-C5-C6-C7
26	A	809	CLA	C2B-C3B-CAB-CBB
26	A	817	CLA	C2B-C3B-CAB-CBB
26	B	836	CLA	C2B-C3B-CAB-CBB
26	H	203	CLA	C2B-C3B-CAB-CBB
26	L	303	CLA	C2B-C3B-CAB-CBB
26	1	608	CLA	C2B-C3B-CAB-CBB
26	a	608	CLA	C2B-C3B-CAB-CBB
26	a	614	CLA	C2B-C3B-CAB-CBB
26	4	601	CLA	C2B-C3B-CAB-CBB
26	4	608	CLA	C2B-C3B-CAB-CBB
26	4	609	CLA	C2B-C3B-CAB-CBB
26	5	608	CLA	C2B-C3B-CAB-CBB
26	6	606	CLA	C2B-C3B-CAB-CBB
26	6	609	CLA	C2B-C3B-CAB-CBB
26	6	610	CLA	C2B-C3B-CAB-CBB
26	6	617	CLA	C2B-C3B-CAB-CBB
26	8	611	CLA	C2B-C3B-CAB-CBB
26	X	604	CLA	C2B-C3B-CAB-CBB
26	Y	602	CLA	C2B-C3B-CAB-CBB
26	Y	604	CLA	C2B-C3B-CAB-CBB
26	Z	602	CLA	C2B-C3B-CAB-CBB
26	U	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	U	613	CLA	C2B-C3B-CAB-CBB
26	U	614	CLA	C2B-C3B-CAB-CBB
26	V	610	CLA	C2B-C3B-CAB-CBB
26	W	614	CLA	C2B-C3B-CAB-CBB
29	A	850	BCR	C5-C6-C7-C8
29	G	205	BCR	C23-C24-C25-C30
29	K	202	BCR	C1-C6-C7-C8
34	X	1621	LUT	C5-C6-C7-C8
34	Z	1621	LUT	C5-C6-C7-C8
34	W	1620	LUT	C1-C6-C7-C8
34	W	1620	LUT	C5-C6-C7-C8
26	A	805	CLA	C2-C1-O2A-CGA
26	A	814	CLA	C2-C1-O2A-CGA
26	B	814	CLA	C2-C1-O2A-CGA
26	8	601	CLA	C2-C1-O2A-CGA
37	W	609	CHL	C2-C1-O2A-CGA
26	4	614	CLA	C5-C6-C7-C8
26	A	830	CLA	CAA-CBA-CGA-O2A
26	A	814	CLA	C13-C15-C16-C17
28	H	204	LHG	C11-C12-C13-C14
28	B	851	LHG	C24-C23-O8-C6
26	A	835	CLA	CAA-CBA-CGA-O2A
26	A	811	CLA	C2-C3-C5-C6
26	B	806	CLA	C2-C3-C5-C6
26	9	603	CLA	C2A-CAA-CBA-CGA
26	9	607	CLA	C2A-CAA-CBA-CGA
32	V	2631	LMG	C39-C40-C41-C42
26	B	823	CLA	CAA-CBA-CGA-O2A
26	A	806	CLA	CAA-CBA-CGA-O2A
26	A	821	CLA	CAA-CBA-CGA-O2A
28	7	622	LHG	C29-C30-C31-C32
26	a	606	CLA	CAA-CBA-CGA-O2A
26	5	619	CLA	CAA-CBA-CGA-O1A
37	Z	609	CHL	C10-C11-C12-C13
26	A	840	CLA	CAA-CBA-CGA-O2A
26	H	203	CLA	CAA-CBA-CGA-O2A
26	4	613	CLA	CAA-CBA-CGA-O2A
26	W	613	CLA	C10-C11-C12-C13
37	X	609	CHL	C4-C3-C5-C6
26	Z	613	CLA	CAA-CBA-CGA-O2A
26	4	608	CLA	C13-C15-C16-C17
26	A	825	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	6	609	CLA	CAA-CBA-CGA-O2A
26	3	608	CLA	C2A-CAA-CBA-CGA
26	6	602	CLA	C2A-CAA-CBA-CGA
26	W	612	CLA	C2A-CAA-CBA-CGA
26	6	608	CLA	CAA-CBA-CGA-O1A
26	7	601	CLA	C6-C7-C8-C9
26	8	613	CLA	C11-C10-C8-C9
28	3	623	LHG	C11-C10-C9-C8
32	4	624	LMG	C29-C30-C31-C32
26	8	613	CLA	C16-C17-C18-C19
26	a	612	CLA	O1D-CGD-O2D-CED
26	A	830	CLA	C10-C11-C12-C13
26	L	303	CLA	C13-C15-C16-C17
26	A	803	CLA	C1A-C2A-CAA-CBA
26	A	809	CLA	C4B-C3B-CAB-CBB
26	A	815	CLA	C4B-C3B-CAB-CBB
26	A	824	CLA	C4B-C3B-CAB-CBB
26	B	823	CLA	C4B-C3B-CAB-CBB
26	F	301	CLA	C1A-C2A-CAA-CBA
26	1	606	CLA	C4B-C3B-CAB-CBB
26	a	606	CLA	C4B-C3B-CAB-CBB
26	2	604	CLA	C1A-C2A-CAA-CBA
26	4	608	CLA	C4B-C3B-CAB-CBB
26	5	609	CLA	C4B-C3B-CAB-CBB
26	6	608	CLA	C1A-C2A-CAA-CBA
26	7	602	CLA	C4B-C3B-CAB-CBB
26	X	612	CLA	C1A-C2A-CAA-CBA
26	U	602	CLA	C4B-C3B-CAB-CBB
26	U	603	CLA	C1A-C2A-CAA-CBA
26	W	610	CLA	C4B-C3B-CAB-CBB
26	6	608	CLA	CAA-CBA-CGA-O2A
26	1	612	CLA	O1D-CGD-O2D-CED
26	Z	602	CLA	C3-C5-C6-C7
26	B	806	CLA	C4-C3-C5-C6
26	B	831	CLA	C4-C3-C5-C6
26	6	614	CLA	C4-C3-C5-C6
26	A	818	CLA	CAA-CBA-CGA-O2A
26	B	813	CLA	CAA-CBA-CGA-O2A
26	B	841	CLA	CAA-CBA-CGA-O2A
26	9	613	CLA	CAA-CBA-CGA-O2A
28	X	2630	LHG	O7-C5-C6-O8
29	A	848	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
29	B	845	BCR	C21-C22-C23-C24
34	U	1620	LUT	C33-C34-C35-C15
26	B	803	CLA	C15-C16-C17-C18
26	7	616	CLA	CAA-CBA-CGA-O2A
37	V	607	CHL	CAA-CBA-CGA-O2A
26	A	813	CLA	CAA-CBA-CGA-O2A
26	W	602	CLA	CAA-CBA-CGA-O2A
26	6	601	CLA	O1A-CGA-O2A-C1
26	B	806	CLA	C2A-CAA-CBA-CGA
28	H	204	LHG	C17-C18-C19-C20
28	A	861	LHG	C10-C11-C12-C13
28	A	846	LHG	O6-C4-C5-C6
28	9	622	LHG	O8-C23-C24-C25
28	X	2630	LHG	C19-C20-C21-C22
26	A	811	CLA	C4-C3-C5-C6
26	A	815	CLA	C2-C1-O2A-CGA
26	A	828	CLA	C2-C1-O2A-CGA
26	B	826	CLA	C2-C1-O2A-CGA
26	B	828	CLA	C2-C1-O2A-CGA
26	B	840	CLA	C2-C1-O2A-CGA
26	H	203	CLA	C2-C1-O2A-CGA
26	8	610	CLA	C2-C1-O2A-CGA
26	8	613	CLA	C2-C1-O2A-CGA
26	9	610	CLA	C2-C1-O2A-CGA
37	X	608	CHL	C2-C1-O2A-CGA
26	A	812	CLA	C11-C12-C13-C15
26	A	816	CLA	C6-C7-C8-C10
26	B	803	CLA	C6-C7-C8-C10
26	B	813	CLA	C6-C7-C8-C10
26	3	609	CLA	C6-C7-C8-C10
26	4	614	CLA	C6-C7-C8-C10
26	9	613	CLA	C11-C10-C8-C7
26	X	610	CLA	C6-C7-C8-C10
26	Y	610	CLA	C12-C13-C15-C16
26	W	613	CLA	C11-C12-C13-C15
37	Y	609	CHL	C11-C12-C13-C15
28	A	846	LHG	C11-C12-C13-C14
26	4	616	CLA	CAA-CBA-CGA-O2A
33	B	850	DGD	C2B-C3B-C4B-C5B
26	6	604	CLA	C13-C15-C16-C17
26	7	607	CLA	C3A-C2A-CAA-CBA
26	B	809	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	A	835	CLA	CAA-CBA-CGA-O1A
26	B	837	CLA	C2A-CAA-CBA-CGA
26	W	610	CLA	C2A-CAA-CBA-CGA
26	1	604	CLA	O2A-C1-C2-C3
26	a	604	CLA	O2A-C1-C2-C3
26	A	843	CLA	C6-C7-C8-C10
28	1	620	LHG	C17-C18-C19-C20
26	A	807	CLA	CAA-CBA-CGA-O1A
28	Y	2630	LHG	C5-C4-O6-P
26	A	810	CLA	C3A-C2A-CAA-CBA
26	A	828	CLA	C3A-C2A-CAA-CBA
26	F	301	CLA	C3A-C2A-CAA-CBA
26	H	202	CLA	CHA-CBD-CGD-O1D
26	K	204	CLA	C3A-C2A-CAA-CBA
26	L	307	CLA	CHA-CBD-CGD-O1D
26	O	2003	CLA	CHA-CBD-CGD-O1D
26	2	602	CLA	CHA-CBD-CGD-O1D
26	2	603	CLA	CHA-CBD-CGD-O1D
26	3	606	CLA	CHA-CBD-CGD-O1D
26	3	611	CLA	CHA-CBD-CGD-O1D
26	3	613	CLA	CHA-CBD-CGD-O1D
26	5	618	CLA	CHA-CBD-CGD-O1D
26	Y	610	CLA	C3A-C2A-CAA-CBA
26	Z	611	CLA	C3A-C2A-CAA-CBA
37	X	609	CHL	C3A-C2A-CAA-CBA
26	A	831	CLA	C8-C10-C11-C12
26	A	831	CLA	C13-C15-C16-C17
26	B	808	CLA	C15-C16-C17-C18
26	a	606	CLA	CAA-CBA-CGA-O1A
37	Z	607	CHL	CAA-CBA-CGA-O2A
26	B	823	CLA	CAA-CBA-CGA-O1A
26	B	813	CLA	C2A-CAA-CBA-CGA
26	Z	614	CLA	CBA-CGA-O2A-C1
26	6	609	CLA	CAA-CBA-CGA-O1A
26	A	812	CLA	C11-C12-C13-C14
26	B	808	CLA	C11-C10-C8-C9
26	4	608	CLA	C11-C10-C8-C9
26	6	602	CLA	C11-C12-C13-C14
26	7	613	CLA	C11-C10-C8-C9
26	X	610	CLA	C6-C7-C8-C9
26	W	611	CLA	CAA-CBA-CGA-O2A
26	A	840	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
28	U	2630	LHG	O9-C7-C8-C9
28	3	624	LHG	C23-C24-C25-C26
26	W	611	CLA	C5-C6-C7-C8
26	A	830	CLA	CAA-CBA-CGA-O1A
26	H	203	CLA	CAA-CBA-CGA-O1A
26	Z	613	CLA	CAA-CBA-CGA-O1A
26	3	613	CLA	CAD-CBD-CGD-O1D
26	5	606	CLA	CAD-CBD-CGD-O1D
26	6	618	CLA	CAD-CBD-CGD-O1D
26	9	606	CLA	CAD-CBD-CGD-O1D
35	4	620	XAT	C21-C26-C27-C28
36	V	1623	NEX	C7-C8-C9-C10
26	U	613	CLA	O1D-CGD-O2D-CED
37	U	607	CHL	CAA-CBA-CGA-O2A
26	A	806	CLA	CAA-CBA-CGA-O1A
26	4	613	CLA	CAA-CBA-CGA-O1A
26	3	610	CLA	C13-C15-C16-C17
26	B	827	CLA	O1A-CGA-O2A-C1
26	B	832	CLA	O1A-CGA-O2A-C1
26	W	604	CLA	O1A-CGA-O2A-C1
37	X	605	CHL	CAA-CBA-CGA-O2A
26	A	809	CLA	C8-C10-C11-C12
26	A	809	CLA	C13-C15-C16-C17
26	B	806	CLA	C10-C11-C12-C13
26	4	608	CLA	C8-C10-C11-C12
29	K	207	BCR	C7-C8-C9-C10
26	B	832	CLA	CBA-CGA-O2A-C1
26	A	821	CLA	CAA-CBA-CGA-O1A
26	9	613	CLA	CAA-CBA-CGA-O1A
28	8	622	LHG	O10-C23-C24-C25
26	B	824	CLA	C5-C6-C7-C8
26	6	613	CLA	C10-C11-C12-C13
32	4	623	LMG	C8-C7-O1-C1
32	V	2631	LMG	C8-C7-O1-C1
26	B	807	CLA	O1A-CGA-O2A-C1
26	a	613	CLA	O1A-CGA-O2A-C1
26	2	609	CLA	CAA-CBA-CGA-O2A
26	B	806	CLA	CAA-CBA-CGA-O1A
26	6	601	CLA	CAA-CBA-CGA-O2A
26	A	804	CLA	C2A-CAA-CBA-CGA
26	7	616	CLA	CAA-CBA-CGA-O1A
26	B	832	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	W	602	CLA	CAA-CBA-CGA-O1A
26	6	601	CLA	C8-C10-C11-C12
26	9	613	CLA	C15-C16-C17-C18
28	2	622	LHG	O8-C23-C24-C25
32	J	103	LMG	O7-C10-C11-C12
37	X	607	CHL	C2-C3-C5-C6
26	1	612	CLA	CBD-CGD-O2D-CED
26	A	813	CLA	CAA-CBA-CGA-O1A
28	9	622	LHG	O10-C23-C24-C25
26	Z	614	CLA	O1A-CGA-O2A-C1
26	A	815	CLA	CAD-CBD-CGD-O2D
26	A	826	CLA	CAD-CBD-CGD-O2D
26	A	831	CLA	CAD-CBD-CGD-O2D
26	B	809	CLA	CAD-CBD-CGD-O2D
26	4	607	CLA	CAD-CBD-CGD-O2D
26	6	609	CLA	CAD-CBD-CGD-O2D
26	X	604	CLA	CAD-CBD-CGD-O2D
26	X	612	CLA	CAD-CBD-CGD-O2D
26	Y	603	CLA	CAD-CBD-CGD-O2D
26	W	603	CLA	CAD-CBD-CGD-O2D
37	Y	606	CHL	CAD-CBD-CGD-O2D
37	U	606	CHL	CAD-CBD-CGD-O2D
26	1	613	CLA	O1A-CGA-O2A-C1
26	A	835	CLA	C2-C1-O2A-CGA
26	B	805	CLA	C2-C1-O2A-CGA
26	F	301	CLA	C2-C1-O2A-CGA
37	V	607	CHL	CAA-CBA-CGA-O1A
37	Y	601	CHL	C1A-C2A-CAA-CBA
37	Y	607	CHL	C1A-C2A-CAA-CBA
26	6	603	CLA	C2A-CAA-CBA-CGA
37	U	607	CHL	CAA-CBA-CGA-O1A
32	4	623	LMG	C28-C29-C30-C31
27	A	844	PQN	C16-C17-C18-C20
26	a	614	CLA	CAA-CBA-CGA-O2A
26	6	603	CLA	CAA-CBA-CGA-O2A
26	8	608	CLA	CAA-CBA-CGA-O2A
26	X	602	CLA	CAA-CBA-CGA-O2A
37	Y	607	CHL	CAA-CBA-CGA-O2A
26	A	840	CLA	CBD-CGD-O2D-CED
26	a	612	CLA	CBD-CGD-O2D-CED
26	4	616	CLA	CAA-CBA-CGA-O1A
28	9	624	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
26	B	841	CLA	CAA-CBA-CGA-O1A
28	A	861	LHG	C18-C19-C20-C21
37	Y	609	CHL	C13-C15-C16-C17
26	A	822	CLA	CAA-CBA-CGA-O2A
26	B	802	CLA	CAA-CBA-CGA-O2A
26	6	616	CLA	CAA-CBA-CGA-O2A
26	B	824	CLA	C8-C10-C11-C12
26	A	818	CLA	CAA-CBA-CGA-O1A
26	W	611	CLA	CAA-CBA-CGA-O1A
28	A	846	LHG	C27-C28-C29-C30

There are no ring outliers.

290 monomers are involved in 664 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	808	CLA	2	0
26	4	606	CLA	1	0
29	3	620	BCR	8	0
26	Z	602	CLA	4	0
34	W	1620	LUT	4	0
26	3	612	CLA	1	0
26	a	601	CLA	3	0
34	Y	1621	LUT	4	0
26	X	614	CLA	1	0
35	V	1622	XAT	6	0
29	6	622	BCR	1	0
37	V	607	CHL	4	0
29	B	852	BCR	6	0
36	Z	1623	NEX	3	0
29	B	801	BCR	7	0
26	A	803	CLA	3	0
26	7	604	CLA	1	0
26	8	612	CLA	2	0
35	U	1622	XAT	5	0
37	X	609	CHL	4	0
29	L	309	BCR	4	0
26	4	618	CLA	1	0
29	O	2004	BCR	3	0
35	5	621	XAT	2	0
37	W	605	CHL	2	0
37	Y	609	CHL	3	0
26	A	807	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Y	613	CLA	4	0
35	7	620	XAT	1	0
26	F	304	CLA	1	0
26	W	610	CLA	1	0
26	1	611	CLA	1	0
37	Z	601	CHL	4	0
28	U	2630	LHG	1	0
26	W	614	CLA	4	0
37	W	601	CHL	3	0
26	F	303	CLA	4	0
29	J	102	BCR	8	0
26	A	806	CLA	2	0
26	X	612	CLA	1	0
26	B	827	CLA	1	0
26	V	613	CLA	4	0
26	U	613	CLA	3	0
26	B	818	CLA	1	0
34	9	619	LUT	5	0
37	V	601	CHL	4	0
37	Y	607	CHL	3	0
35	2	620	XAT	1	0
26	6	607	CLA	1	0
35	Z	1622	XAT	5	0
35	W	1622	XAT	3	0
29	B	848	BCR	2	0
26	A	802	CLA	3	0
26	7	616	CLA	1	0
26	9	613	CLA	2	0
35	6	621	XAT	1	0
37	Z	606	CHL	3	0
26	A	835	CLA	2	0
37	V	609	CHL	3	0
26	B	830	CLA	1	0
26	a	611	CLA	1	0
34	U	1621	LUT	2	0
26	a	603	CLA	1	0
26	X	610	CLA	3	0
29	L	305	BCR	8	0
29	B	843	BCR	9	0
26	A	819	CLA	2	0
26	A	827	CLA	1	0
26	7	609	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	7	619	LUT	3	0
29	A	849	BCR	5	0
26	a	607	CLA	1	0
37	W	606	CHL	1	0
26	A	820	CLA	2	0
26	6	610	CLA	3	0
26	Y	610	CLA	2	0
36	X	1623	NEX	2	0
37	Y	605	CHL	1	0
29	A	856	BCR	10	0
29	A	850	BCR	8	0
29	B	846	BCR	3	0
26	1	606	CLA	1	0
26	8	610	CLA	1	0
29	A	852	BCR	10	0
29	7	621	BCR	3	0
26	A	830	CLA	1	0
36	Y	1623	NEX	2	0
37	Y	608	CHL	2	0
26	L	307	CLA	2	0
26	1	607	CLA	1	0
26	4	609	CLA	1	0
29	B	849	BCR	2	0
26	A	831	CLA	1	0
26	6	606	CLA	1	0
37	U	609	CHL	3	0
26	7	611	CLA	4	0
29	8	621	BCR	3	0
26	B	834	CLA	3	0
34	X	1621	LUT	6	0
29	K	202	BCR	5	0
34	2	619	LUT	7	0
34	a	617	LUT	5	0
26	1	604	CLA	1	0
37	Z	609	CHL	3	0
37	W	609	CHL	1	0
34	Z	1621	LUT	4	0
26	7	614	CLA	2	0
34	X	1620	LUT	6	0
26	B	821	CLA	3	0
26	8	604	CLA	1	0
37	Y	601	CHL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	808	CLA	3	0
26	4	611	CLA	1	0
34	5	620	LUT	4	0
26	A	816	CLA	1	0
26	B	825	CLA	2	0
26	L	302	CLA	3	0
37	V	606	CHL	2	0
26	7	615	CLA	1	0
35	8	620	XAT	1	0
26	A	825	CLA	3	0
26	4	601	CLA	1	0
37	U	608	CHL	3	0
29	G	205	BCR	4	0
29	a	619	BCR	3	0
26	F	301	CLA	1	0
26	A	840	CLA	1	0
26	1	601	CLA	2	0
26	K	203	CLA	1	0
26	9	610	CLA	1	0
29	B	847	BCR	4	0
26	Y	603	CLA	3	0
26	B	802	CLA	1	0
26	Z	610	CLA	5	0
29	B	845	BCR	3	0
37	X	607	CHL	2	0
26	A	854	CLA	5	0
26	A	805	CLA	1	0
26	A	841	CLA	4	0
26	A	815	CLA	2	0
26	A	829	CLA	5	0
26	7	601	CLA	1	0
26	7	613	CLA	2	0
26	6	614	CLA	2	0
28	X	2630	LHG	6	0
29	L	301	BCR	10	0
34	Z	1620	LUT	6	0
26	1	613	CLA	1	0
26	V	610	CLA	3	0
29	7	623	BCR	5	0
26	X	604	CLA	1	0
26	6	608	CLA	1	0
37	X	608	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	835	CLA	1	0
29	A	851	BCR	6	0
26	B	828	CLA	2	0
37	V	608	CHL	2	0
28	Y	2630	LHG	6	0
26	W	613	CLA	4	0
35	a	618	XAT	3	0
27	A	844	PQN	2	0
37	U	606	CHL	2	0
26	5	602	CLA	2	0
26	2	613	CLA	3	0
26	4	607	CLA	1	0
29	B	844	BCR	6	0
26	U	602	CLA	1	0
34	V	1621	LUT	5	0
34	6	619	LUT	5	0
26	a	606	CLA	1	0
26	B	824	CLA	1	0
29	5	622	BCR	2	0
35	4	620	XAT	3	0
35	1	618	XAT	3	0
26	a	613	CLA	1	0
34	V	1620	LUT	5	0
29	F	305	BCR	7	0
36	V	1623	NEX	11	0
26	U	610	CLA	4	0
26	5	603	CLA	1	0
29	3	621	BCR	4	0
26	4	616	CLA	1	0
26	A	821	CLA	1	0
26	W	612	CLA	1	0
37	X	601	CHL	7	0
29	3	622	BCR	7	0
26	6	601	CLA	1	0
26	B	803	CLA	2	0
36	5	624	NEX	1	0
29	O	2005	BCR	6	0
26	3	606	CLA	1	0
26	3	613	CLA	1	0
26	6	609	CLA	1	0
26	A	834	CLA	2	0
26	X	602	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	5	627	LMG	1	0
26	A	812	CLA	1	0
26	W	602	CLA	2	0
26	K	204	CLA	2	0
34	8	619	LUT	6	0
26	8	606	CLA	1	0
26	X	611	CLA	2	0
26	8	613	CLA	2	0
26	Z	612	CLA	1	0
26	V	612	CLA	2	0
26	A	843	CLA	2	0
26	2	606	CLA	1	0
28	a	620	LHG	1	0
36	W	1623	NEX	2	0
37	U	605	CHL	1	0
26	B	817	CLA	1	0
26	W	603	CLA	2	0
26	X	603	CLA	1	0
28	3	623	LHG	1	0
34	Y	1620	LUT	5	0
26	L	303	CLA	2	0
26	8	611	CLA	2	0
37	U	607	CHL	2	0
29	A	848	BCR	3	0
26	7	602	CLA	1	0
32	A	860	LMG	1	0
32	V	2631	LMG	2	0
26	B	840	CLA	1	0
34	4	619	LUT	3	0
28	V	2630	LHG	3	0
26	6	602	CLA	1	0
26	Y	602	CLA	2	0
26	B	822	CLA	1	0
32	9	625	LMG	2	0
26	B	816	CLA	1	0
26	5	613	CLA	1	0
26	A	822	CLA	4	0
26	V	602	CLA	3	0
37	Z	608	CHL	2	0
26	9	609	CLA	1	0
26	5	619	CLA	3	0
26	U	604	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	837	CLA	2	0
29	2	623	BCR	5	0
33	B	850	DGD	1	0
26	a	604	CLA	1	0
28	Z	2630	LHG	9	0
35	X	1622	XAT	3	0
26	3	610	CLA	1	0
29	4	621	BCR	5	0
28	W	2630	LHG	1	0
29	K	207	BCR	3	0
26	A	818	CLA	1	0
32	8	626	LMG	3	0
35	Y	1622	XAT	3	0
28	9	622	LHG	1	0
26	3	608	CLA	1	0
26	Z	613	CLA	4	0
26	A	809	CLA	1	0
37	U	601	CHL	4	0
36	6	624	NEX	6	0
26	B	813	CLA	2	0
26	B	819	CLA	1	0
26	5	611	CLA	7	0
26	B	833	CLA	2	0
35	3	619	XAT	2	0
26	Z	603	CLA	1	0
28	3	624	LHG	2	0
29	B	853	BCR	3	0
27	B	842	PQN	3	0
37	W	607	CHL	3	0
26	A	837	CLA	1	0
26	Z	611	CLA	3	0
34	3	618	LUT	7	0
26	X	613	CLA	4	0
26	A	824	CLA	2	0
26	B	839	CLA	1	0
37	Z	607	CHL	3	0
30	C	102	SF4	1	0
29	L	308	BCR	7	0
34	W	1621	LUT	4	0
26	5	607	CLA	2	0
28	O	2631	LHG	1	0
29	9	621	BCR	7	0

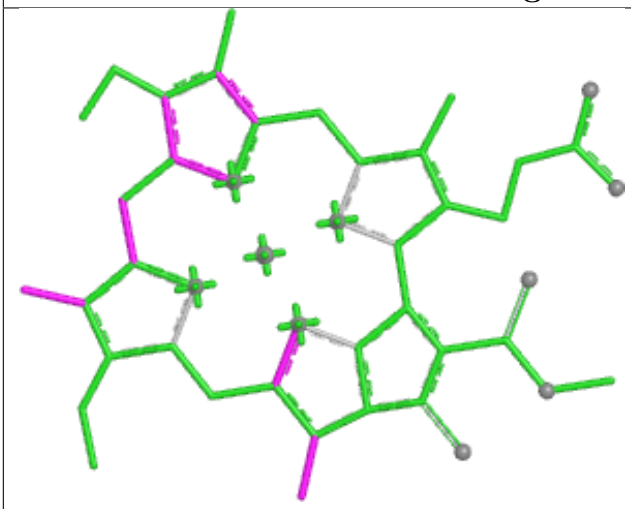
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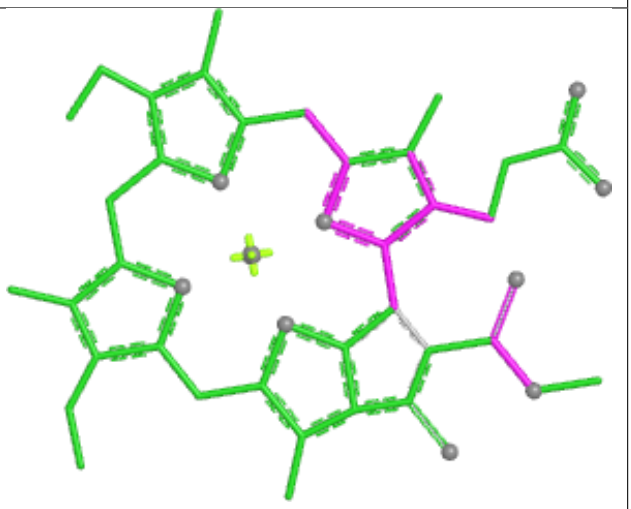
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	Y	606	CHL	2	0
37	V	605	CHL	1	0
31	A	857	LMU	1	0
26	5	610	CLA	1	0
34	U	1620	LUT	6	0
26	6	616	CLA	1	0
28	5	623	LHG	6	0
34	1	617	LUT	6	0
29	1	619	BCR	2	0
26	Z	614	CLA	1	0
26	V	614	CLA	1	0

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.

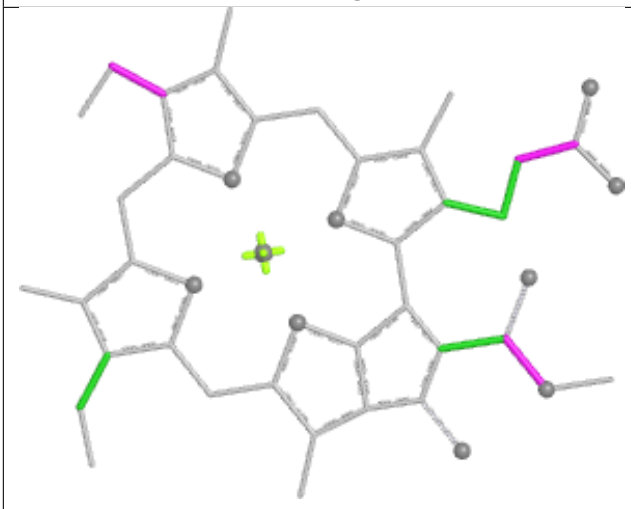
Ligand CLA Y 612



Bond lengths



Bond angles

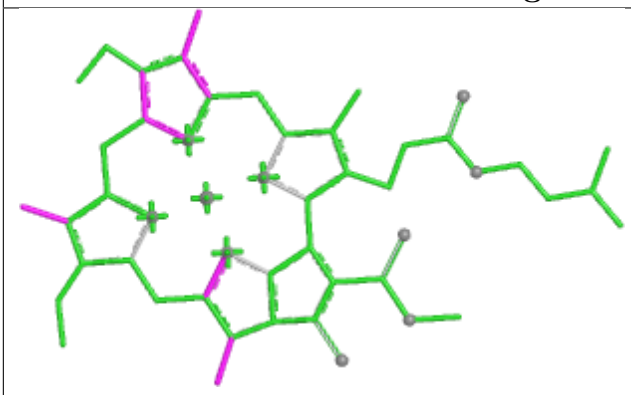


Torsions

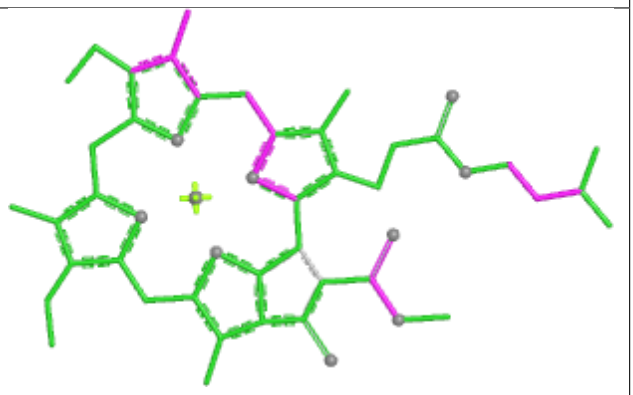


Rings

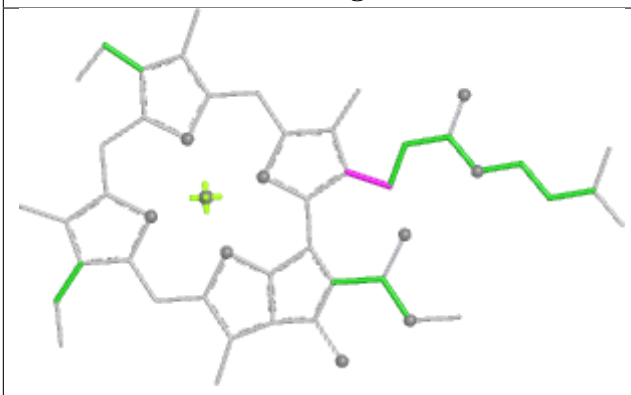
Ligand CLA A 808



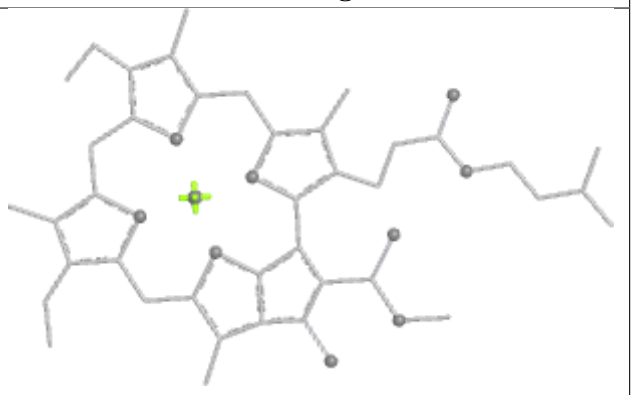
Bond lengths



Bond angles

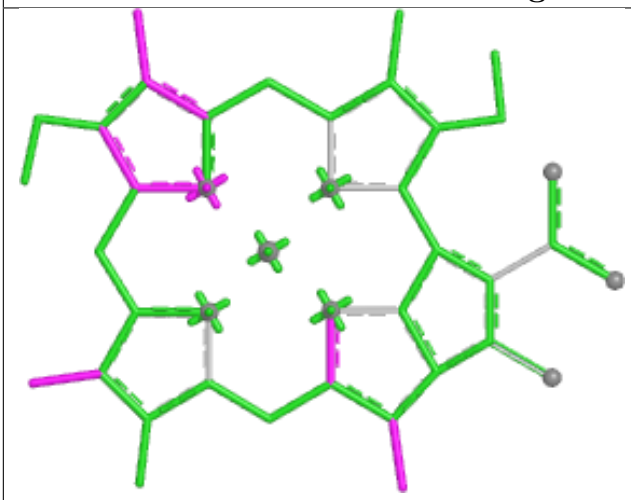


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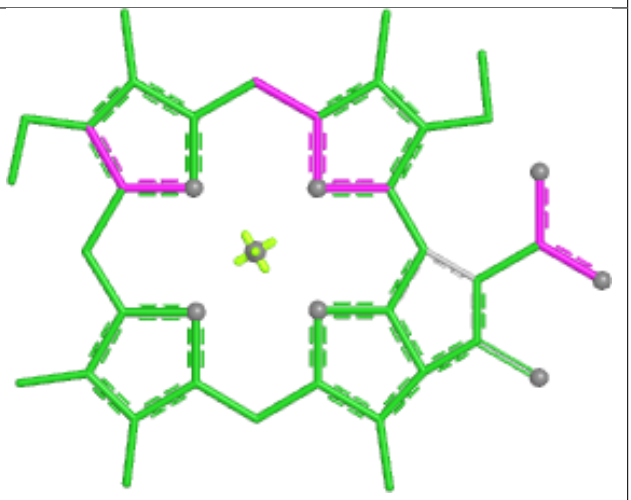


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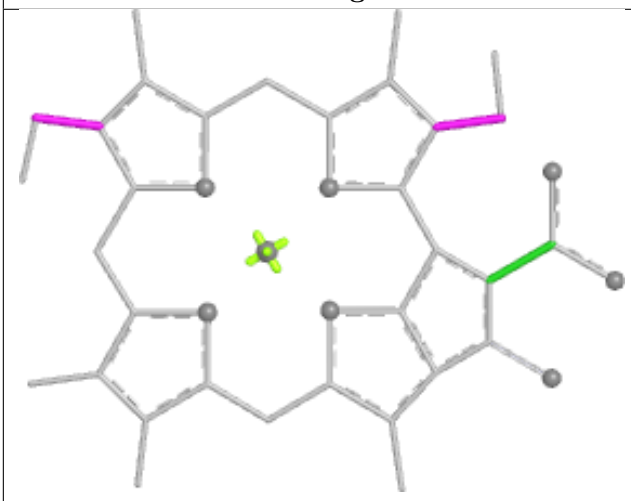
Ligand CLA 4 606



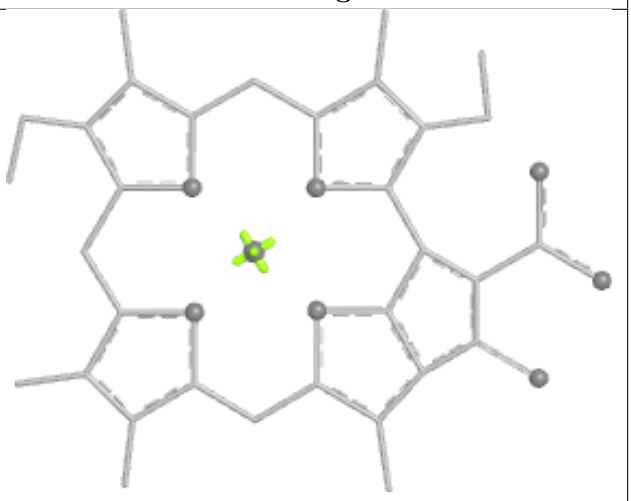
Bond lengths



Bond angles

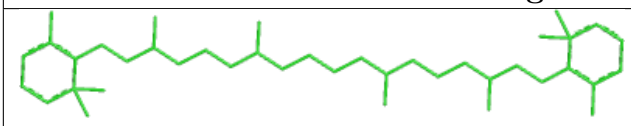


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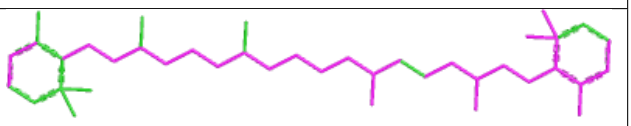


Rings

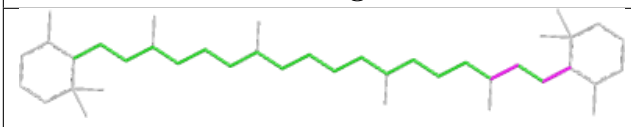
Ligand BCR 3 620



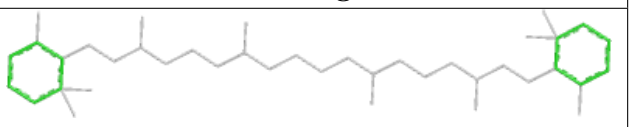
Bond lengths



Bond angles

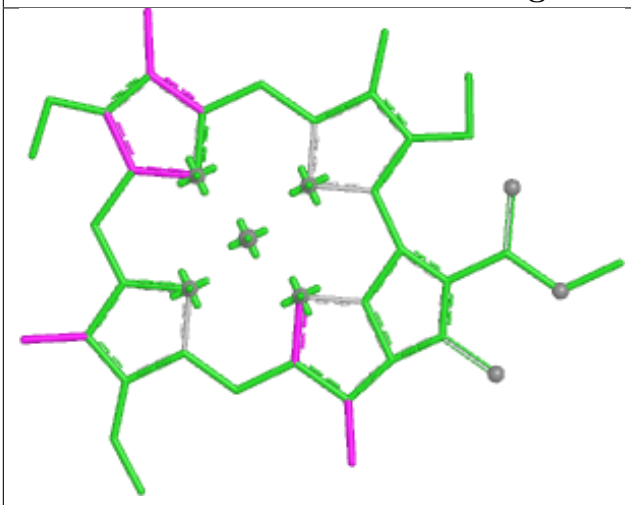


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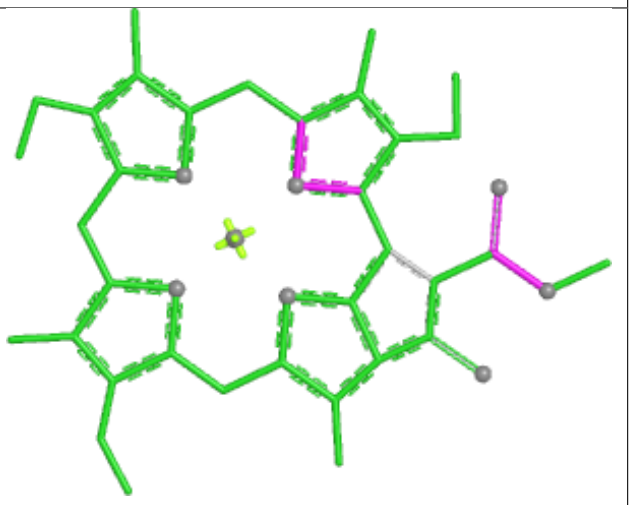


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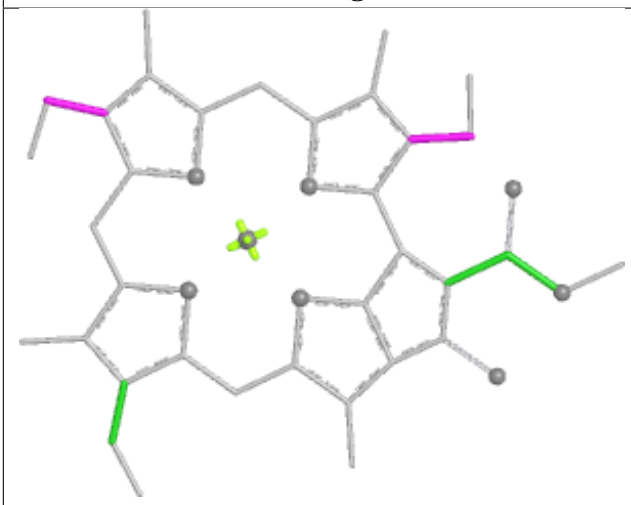
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Bond lengths



Bond angles

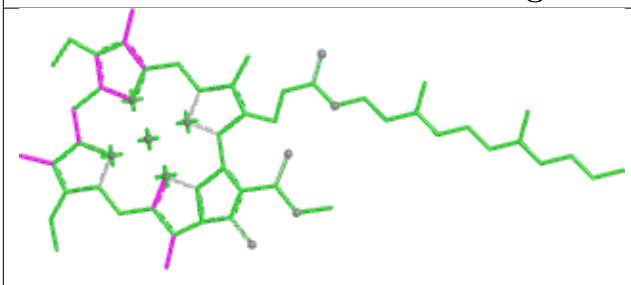


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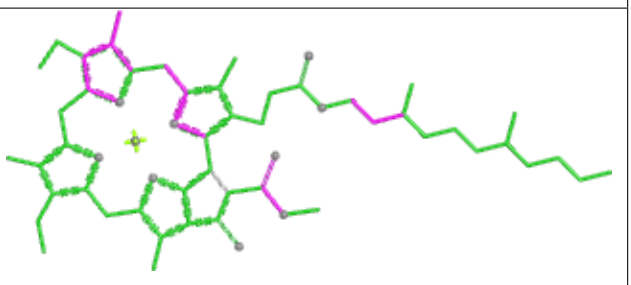


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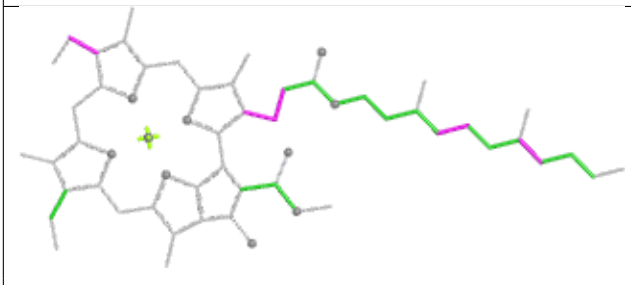
Ligand CLA Z 602



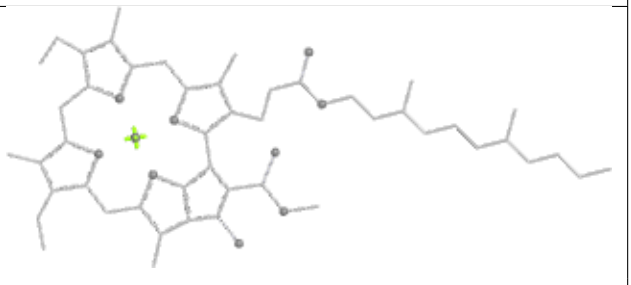
Bond lengths



Bond angles

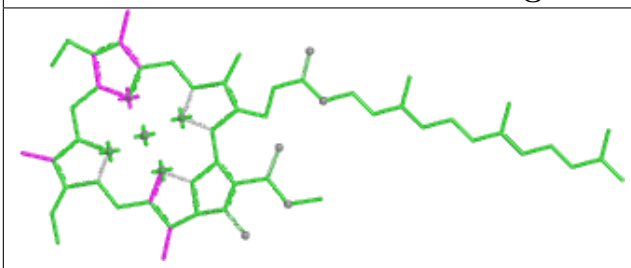


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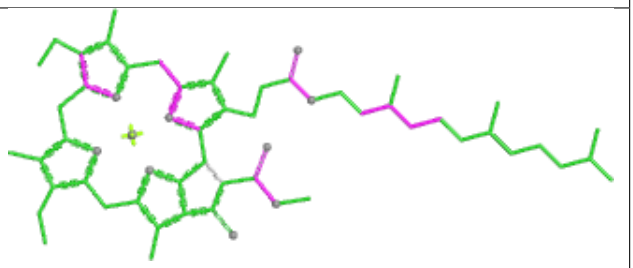


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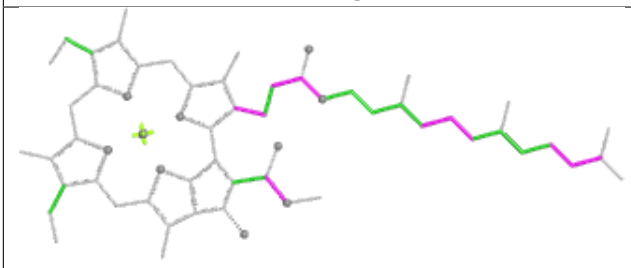
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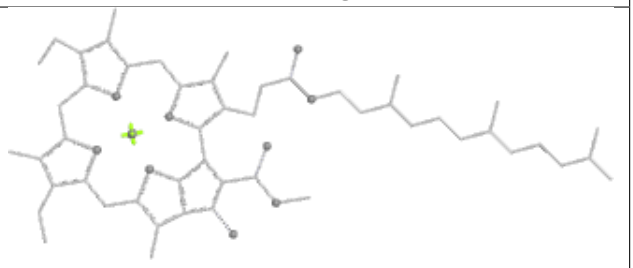
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Bond angles

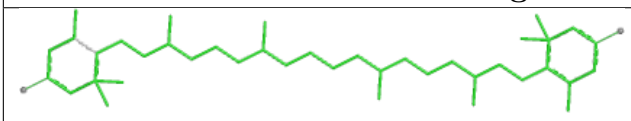


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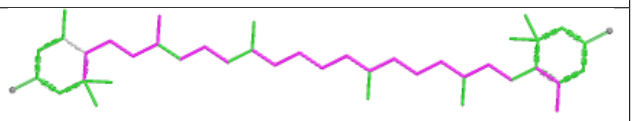


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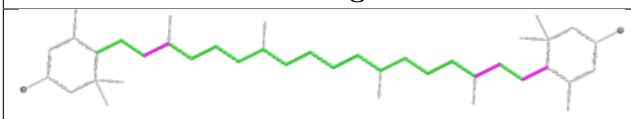
Ligand LUT W 1620



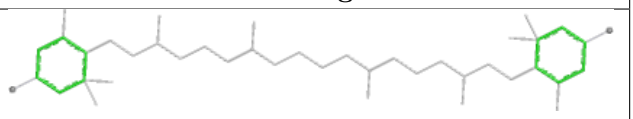
Bond lengths



Bond angles

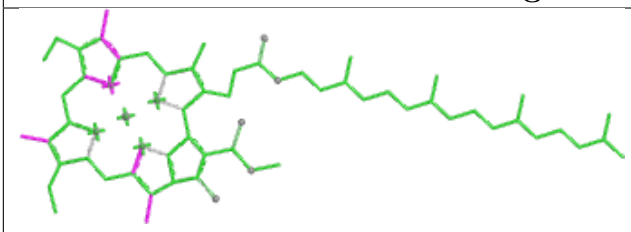


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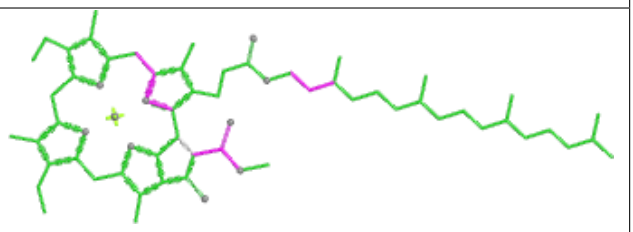


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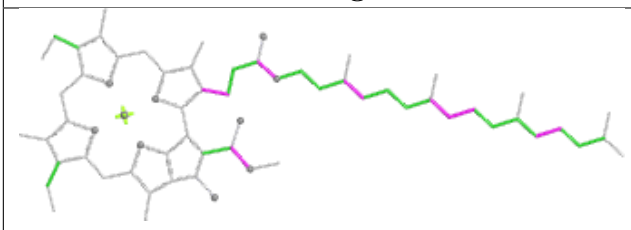
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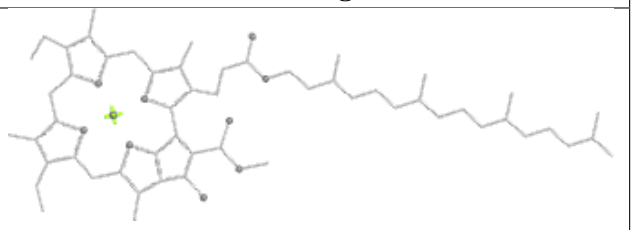
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Bond angles

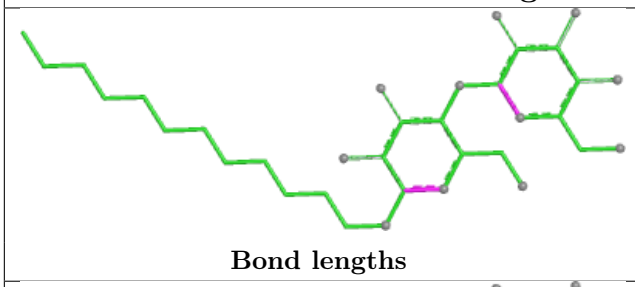


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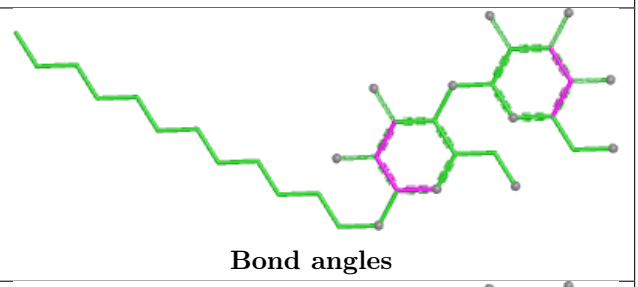


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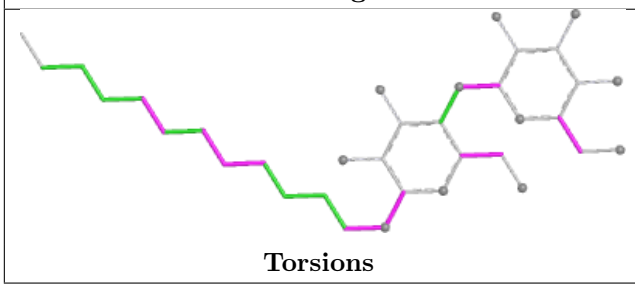
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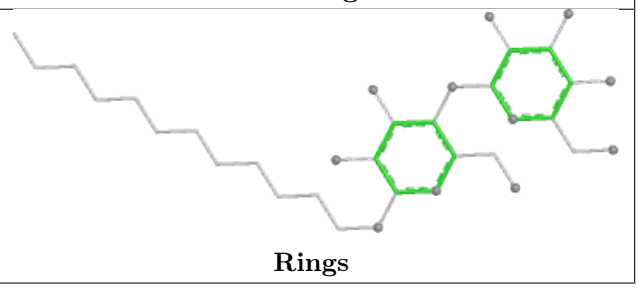
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Bond angles

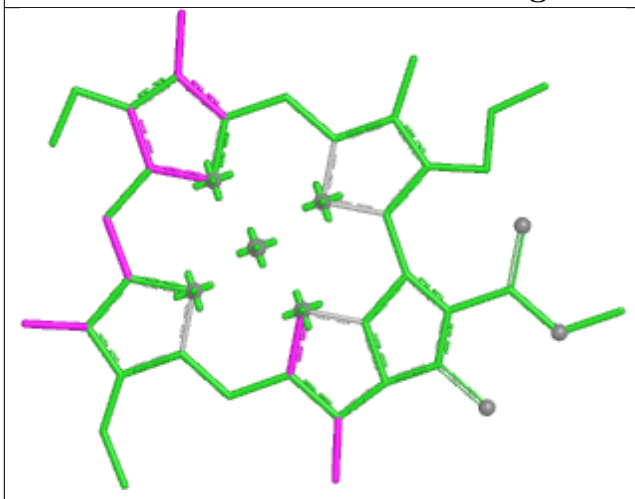


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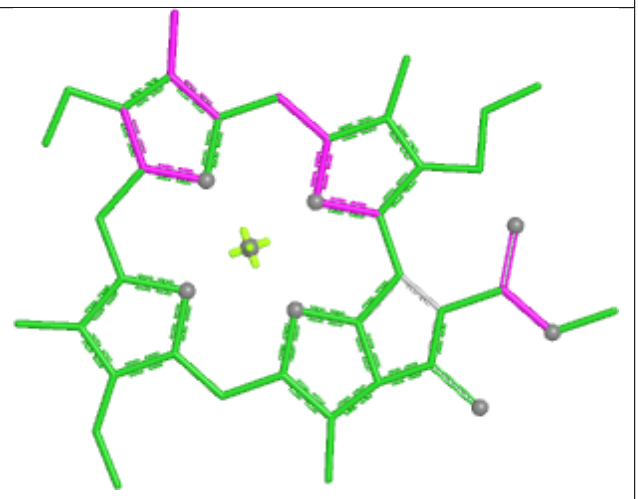


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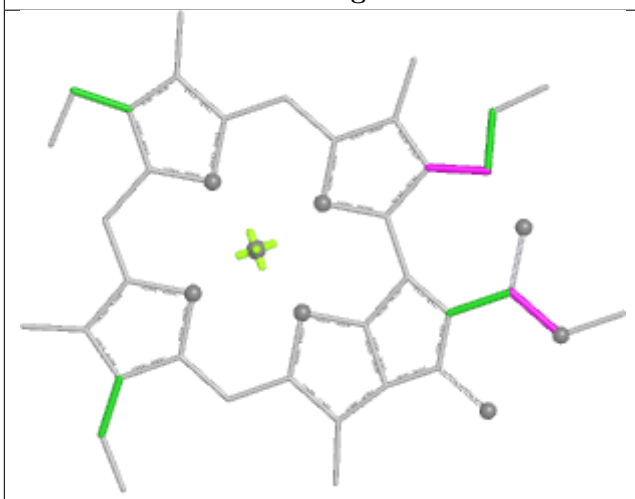
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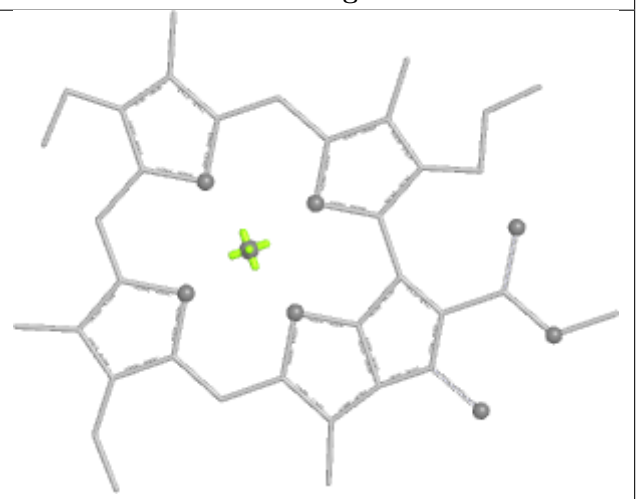
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Bond angles

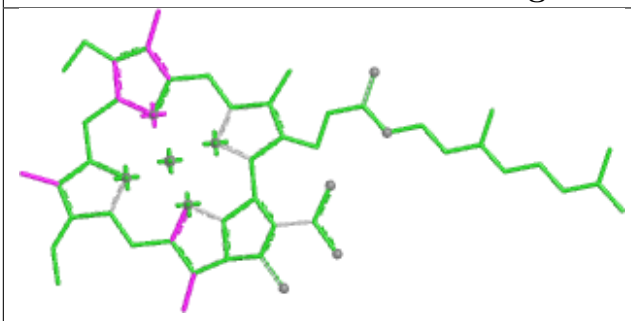


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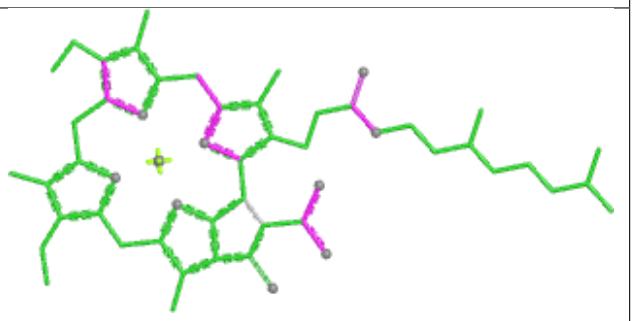


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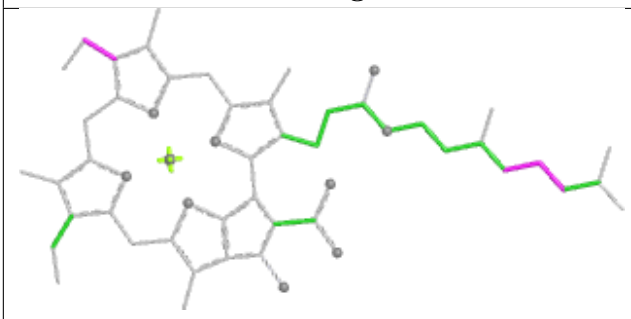
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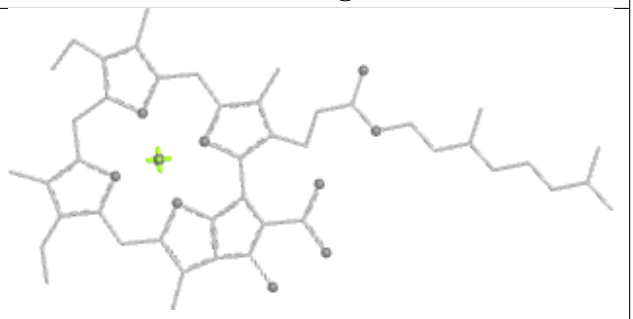
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Bond angles

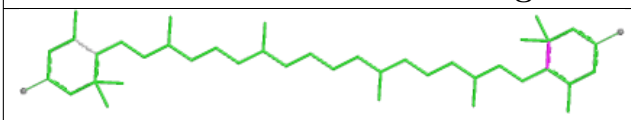


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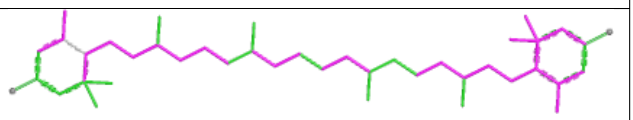


Rings

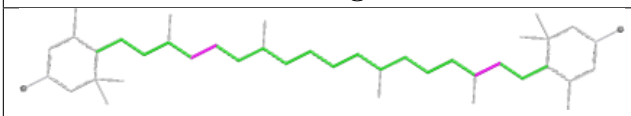
Ligand LUT Y 1621



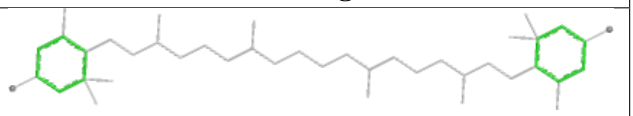
Bond lengths



Bond angles

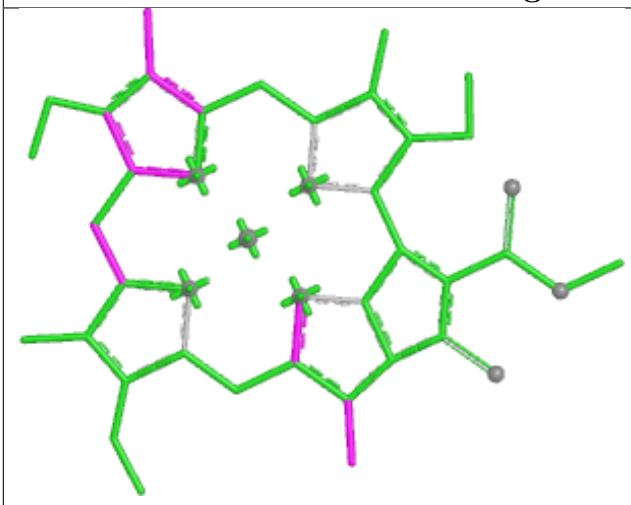


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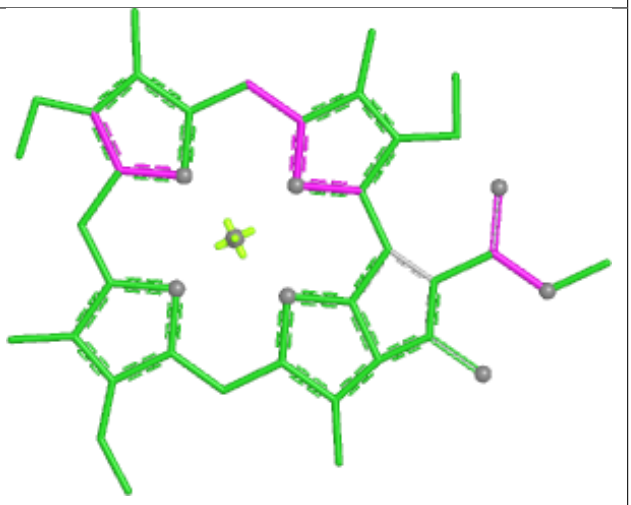


Rings

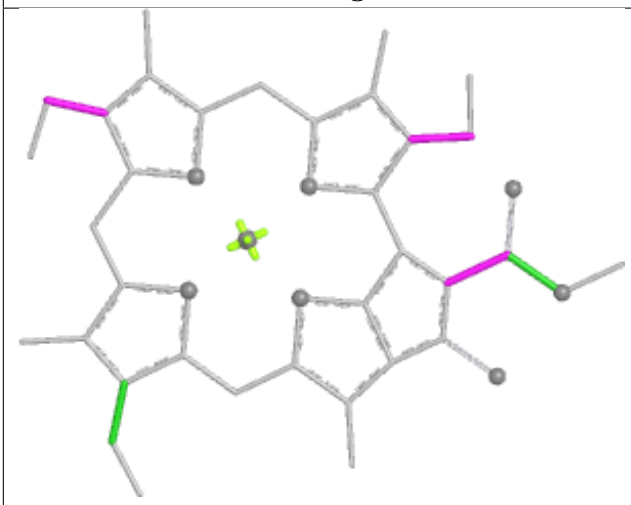
Ligand CLA X 614



Bond lengths



Bond angles

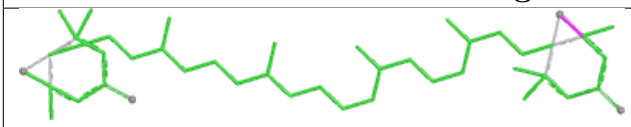


Torsions

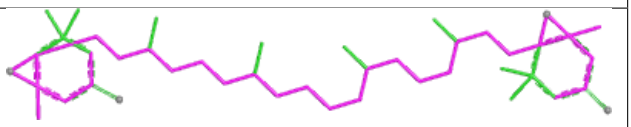


Rings

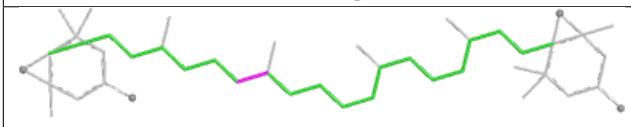
Ligand XAT V 1622



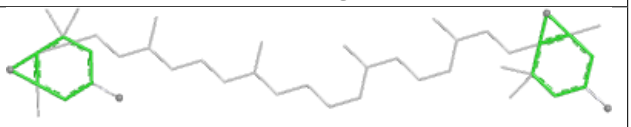
Bond lengths



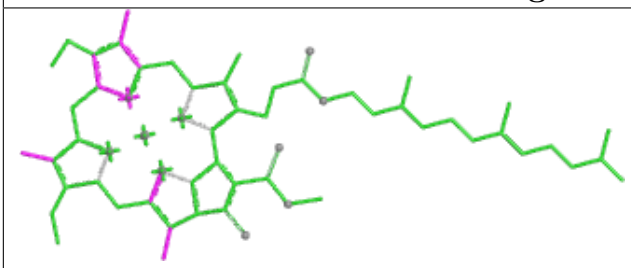
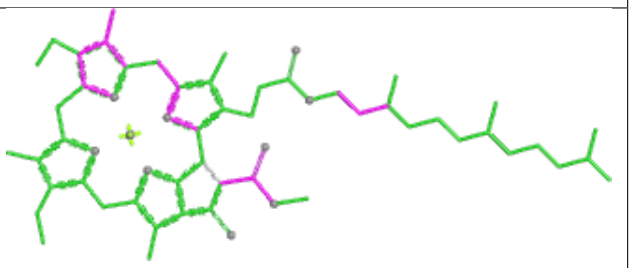
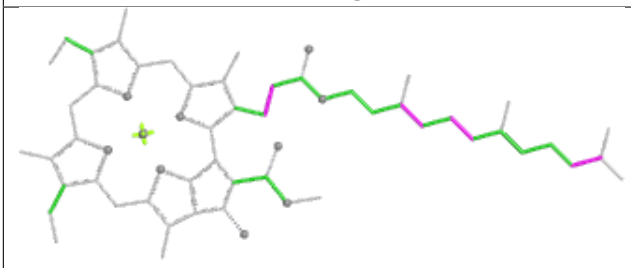
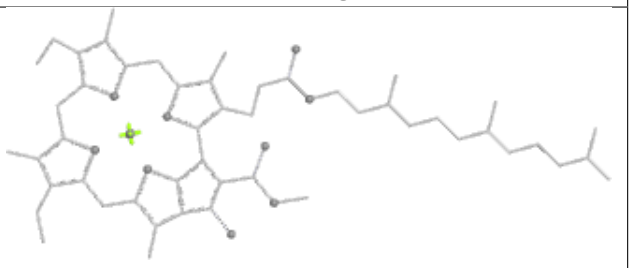
Bond angles

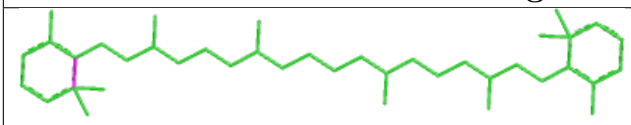
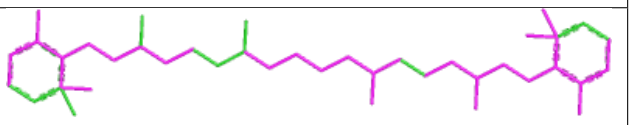
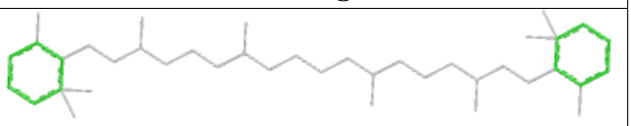


Torsions

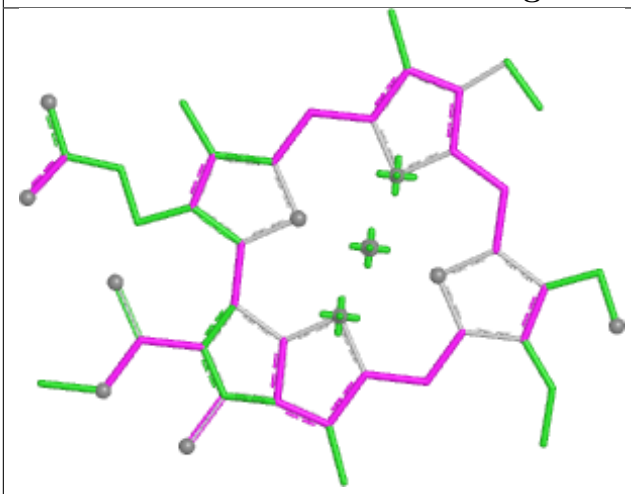


Rings

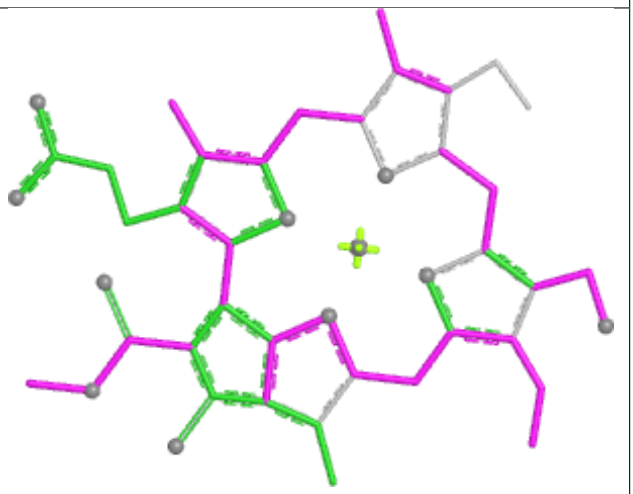
Ligand CLA 9 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 6 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

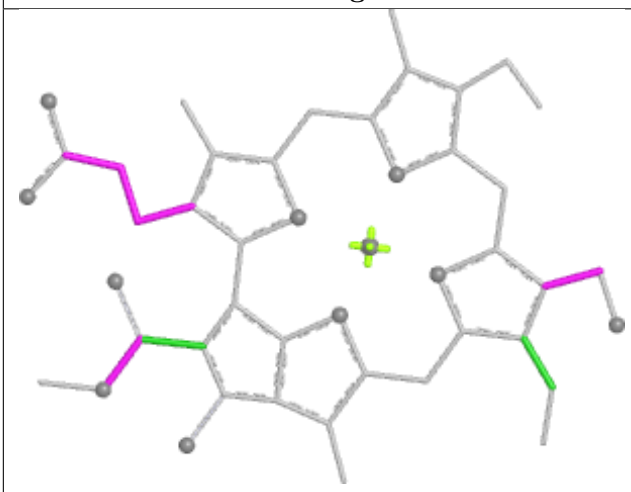
Ligand CHL V 607



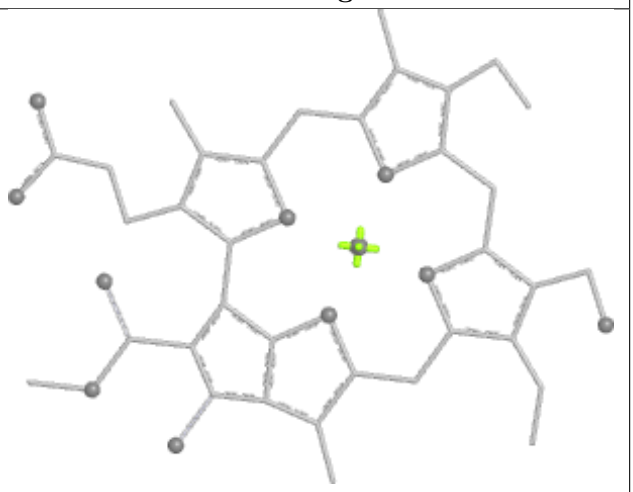
Bond lengths



Bond angles



Torsions



Rings

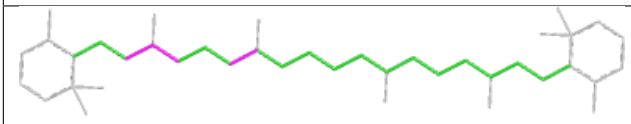
Ligand BCR B 852



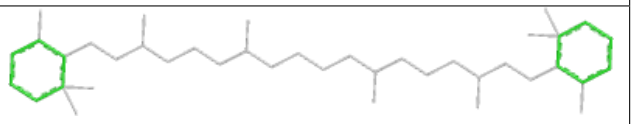
Bond lengths



Bond angles

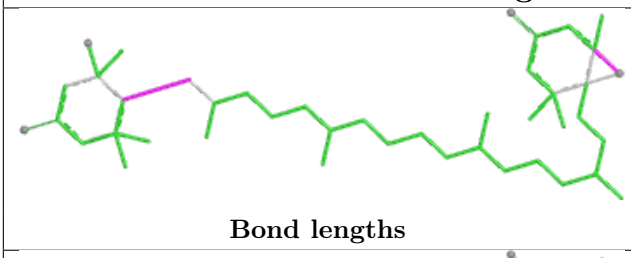


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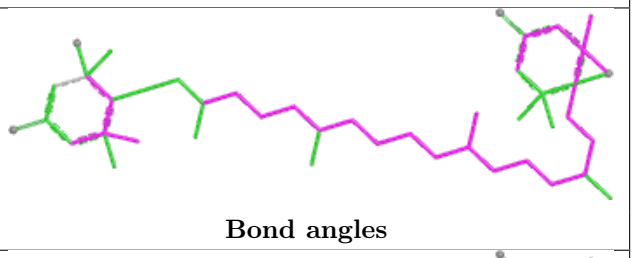


Rings

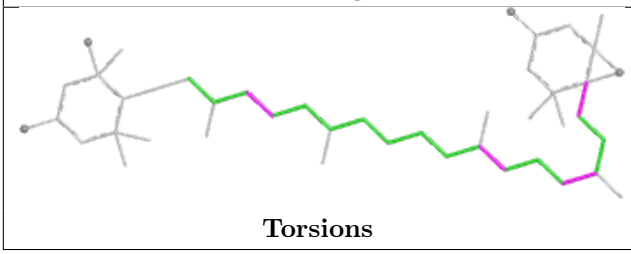
Ligand NEX Z 1623



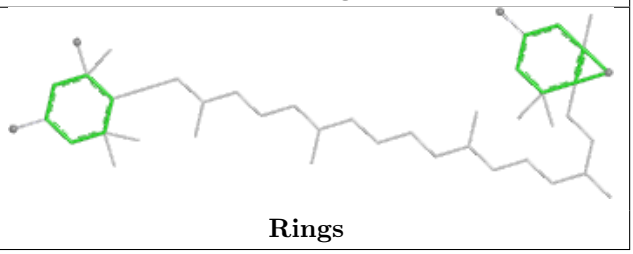
Bond lengths



Bond angles

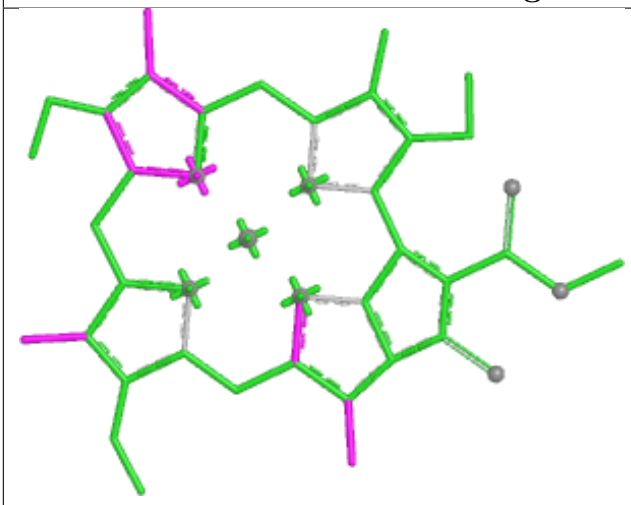


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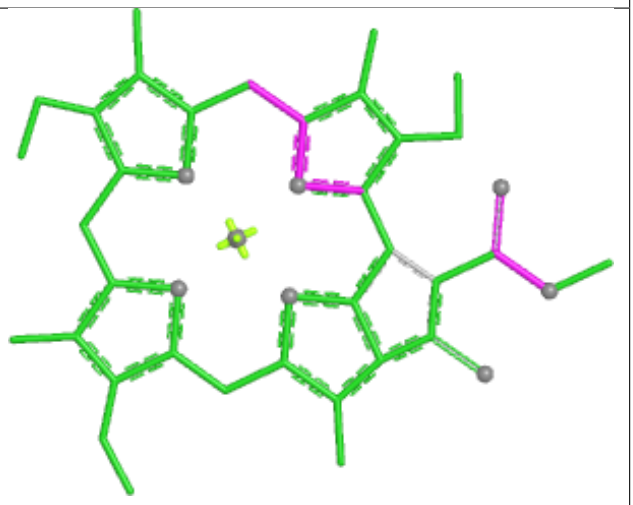


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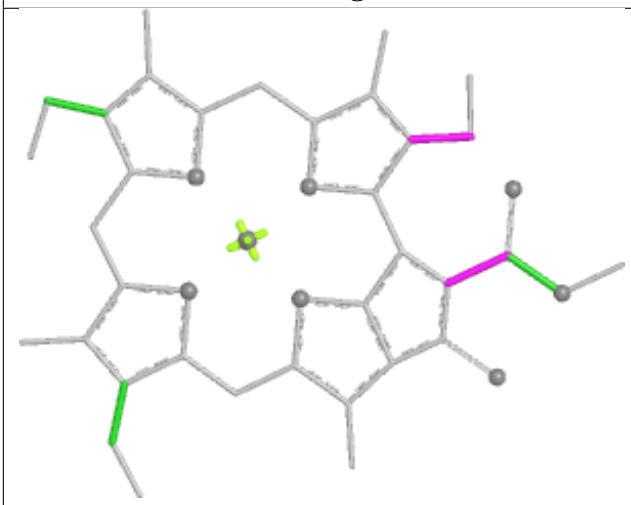
Ligand CLA A 823



Bond lengths



Bond angles

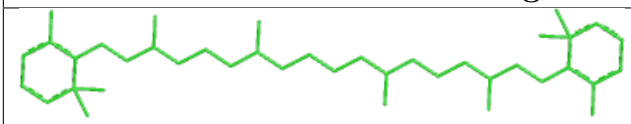


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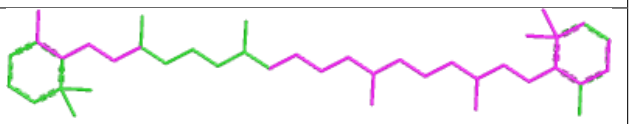


Rings

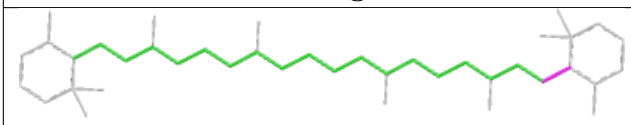
Ligand BCR B 801



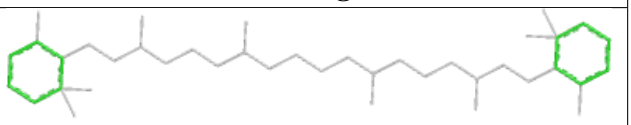
Bond lengths



Bond angles

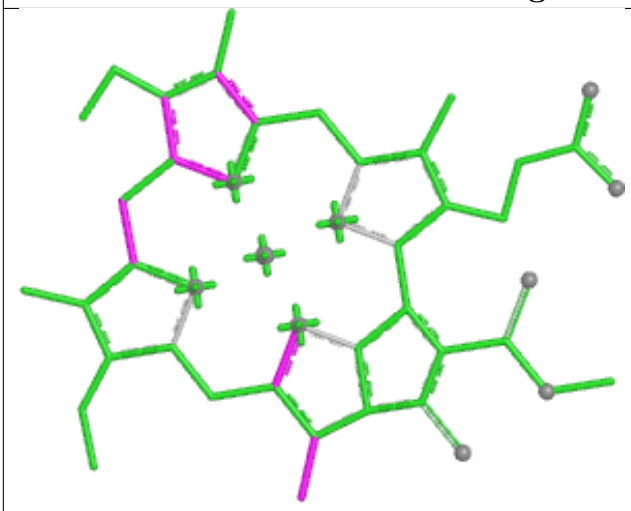


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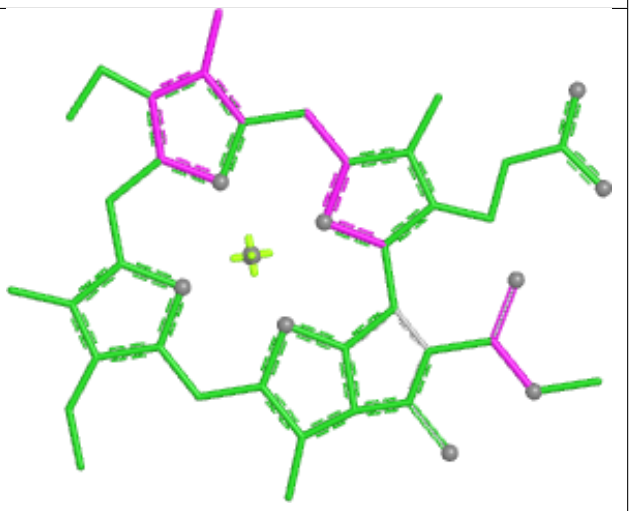


Rings

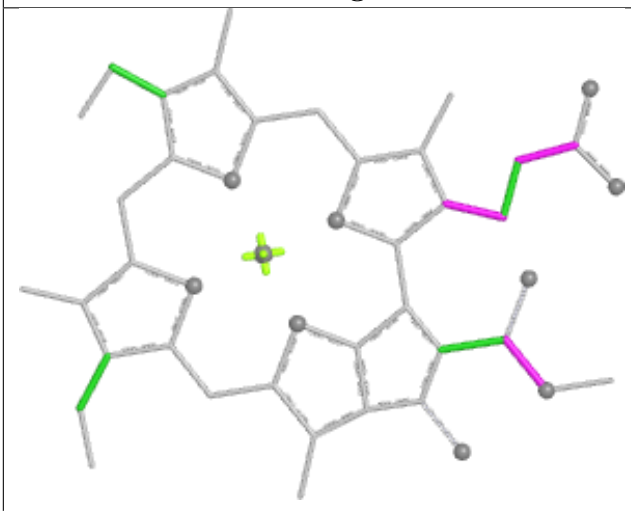
Ligand CLA a 616



Bond lengths



Bond angles

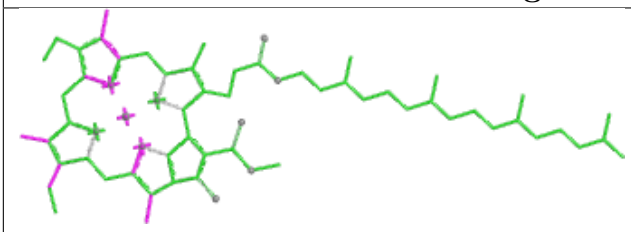


Torsions

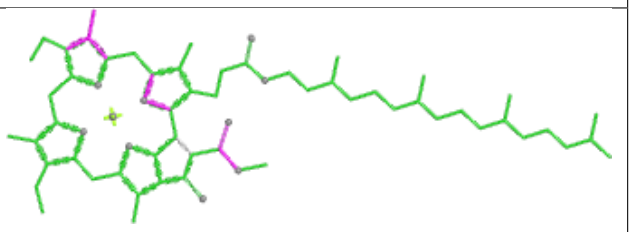


Rings

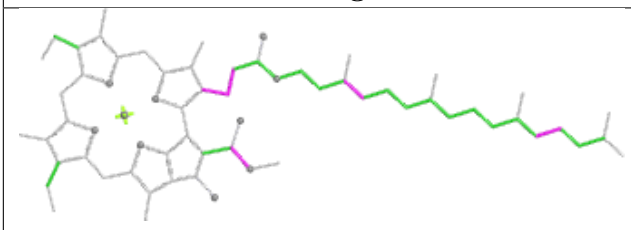
Ligand CLA A 803



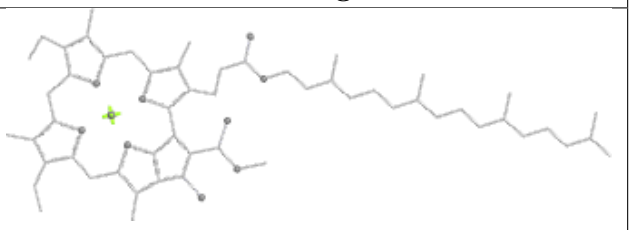
Bond lengths



Bond angles

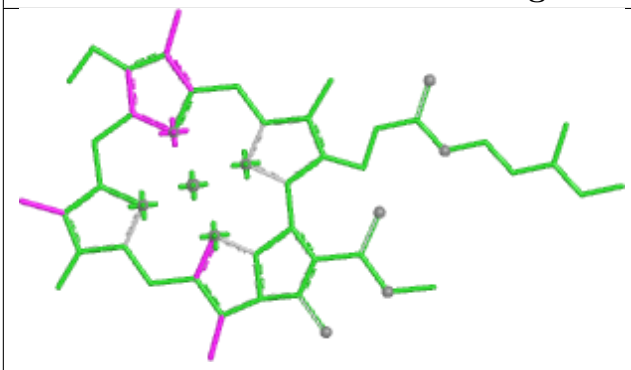


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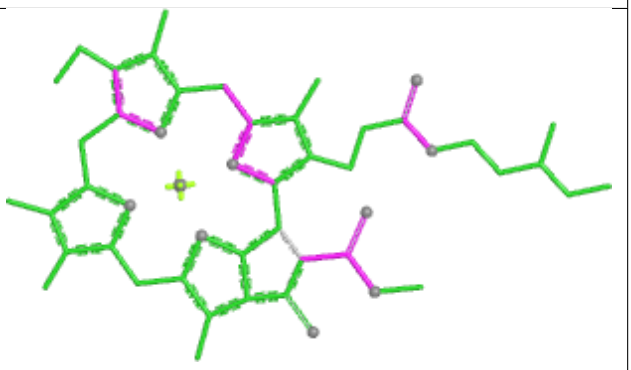


Rings

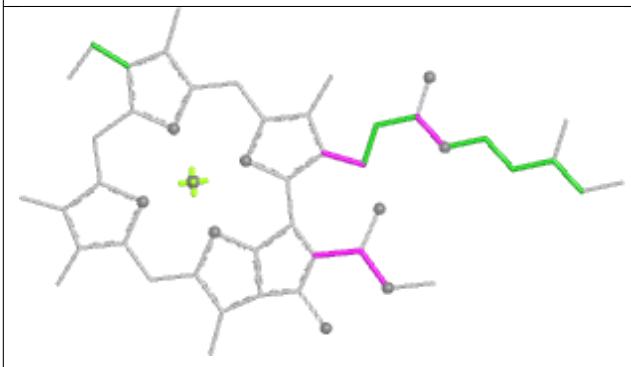
Ligand CLA 7 604



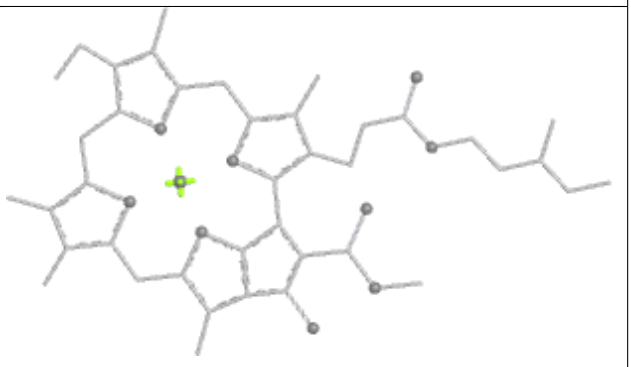
Bond lengths



Bond angles

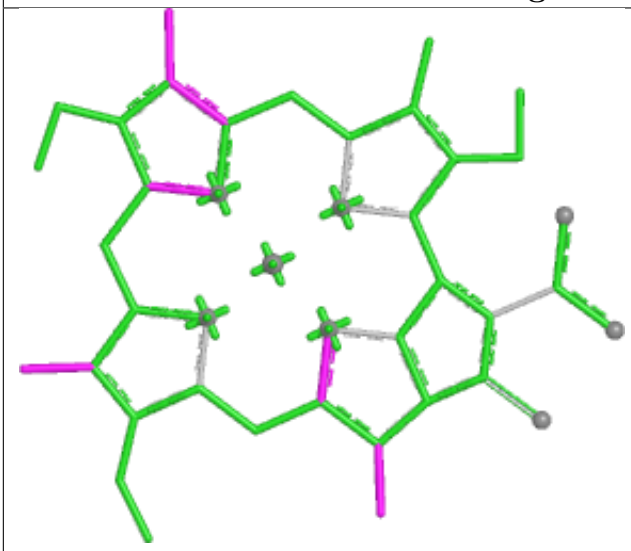


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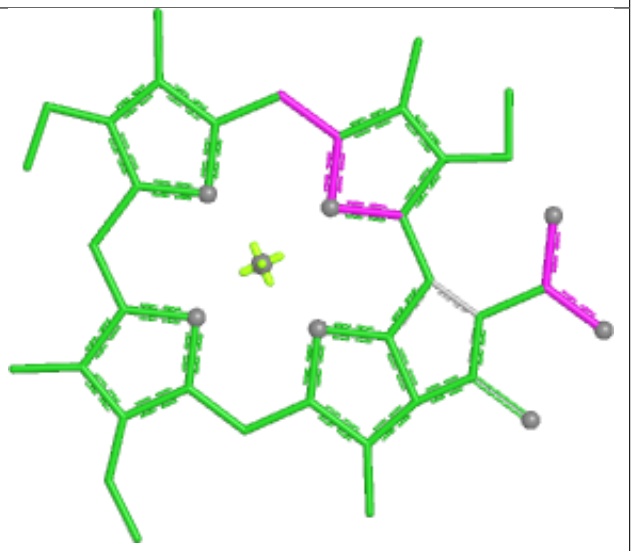


Rings

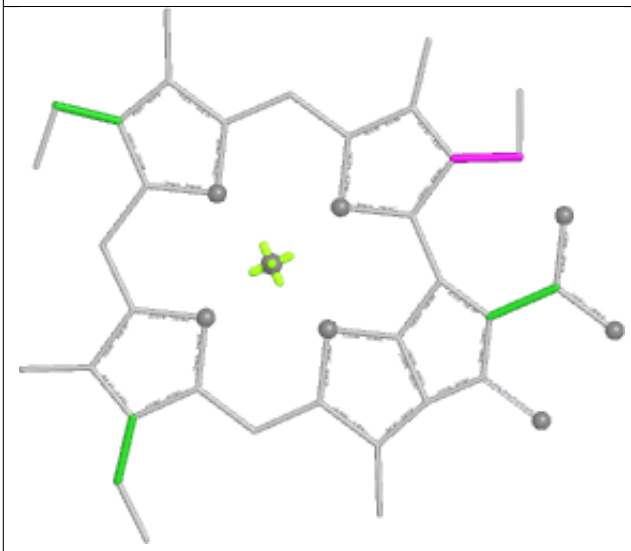
Ligand CLA 8 612



Bond lengths



Bond angles

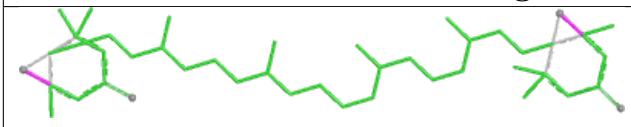


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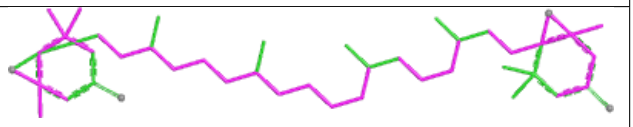


Rings

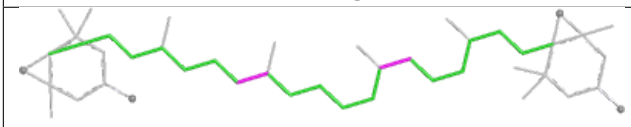
Ligand XAT U 1622



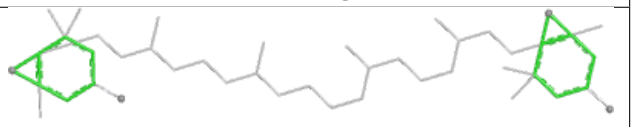
Bond lengths



Bond angles

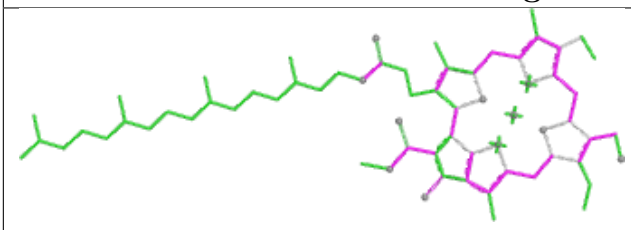


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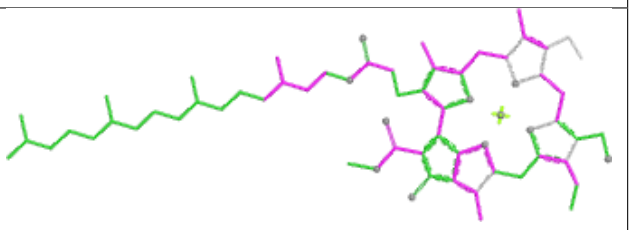


Rings

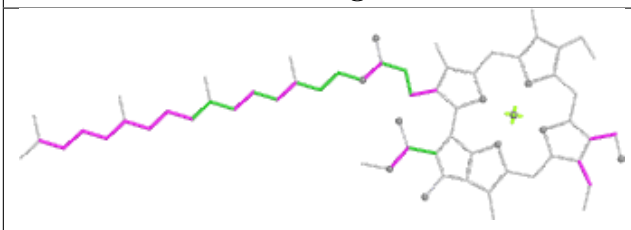
Ligand CHL X 609



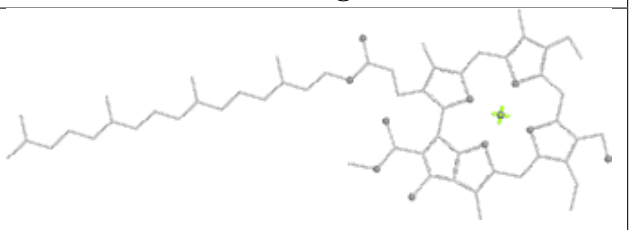
Bond lengths



Bond angles

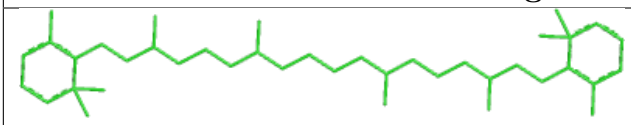


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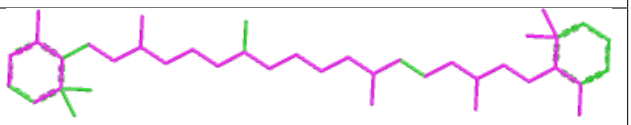


Rings

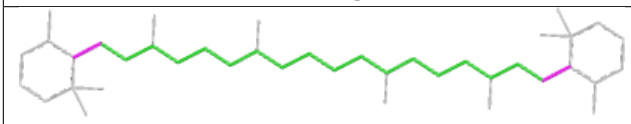
Ligand BCR L 309



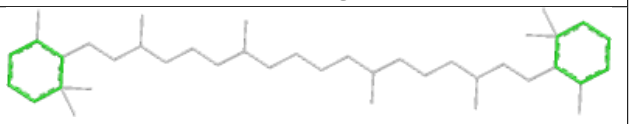
Bond lengths



Bond angles

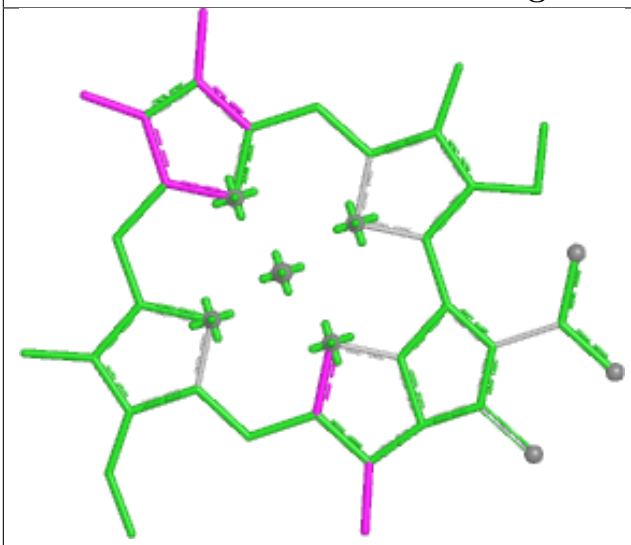


Torsions

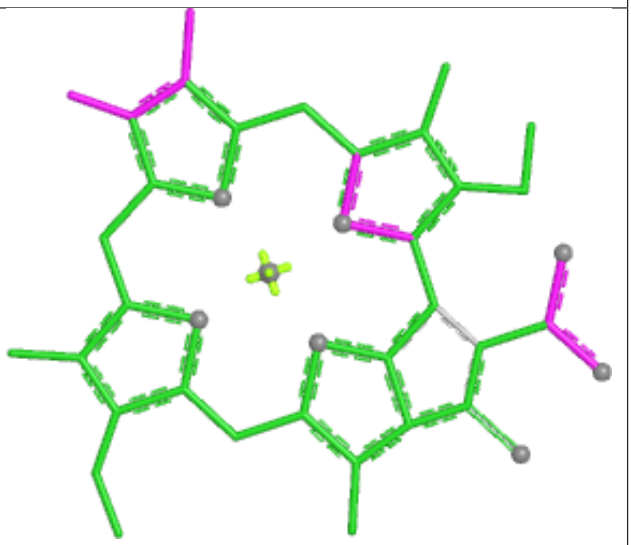


Rings

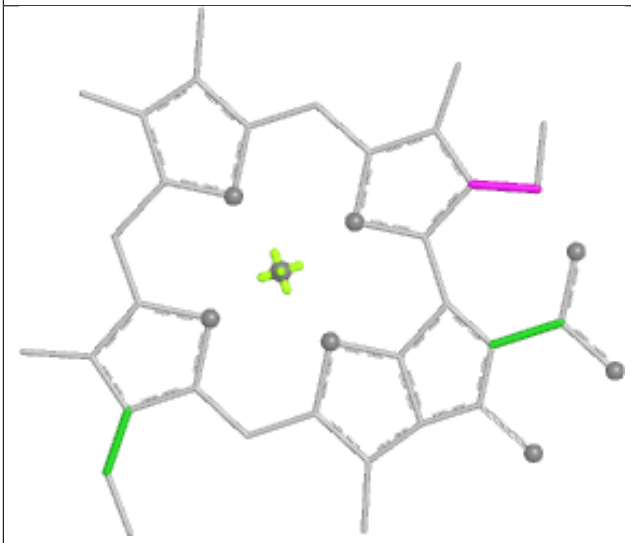
Ligand CLA 4 618



Bond lengths



Bond angles

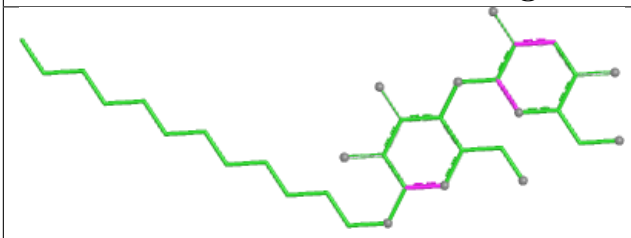


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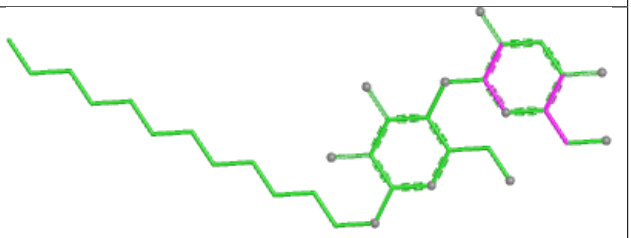


Rings

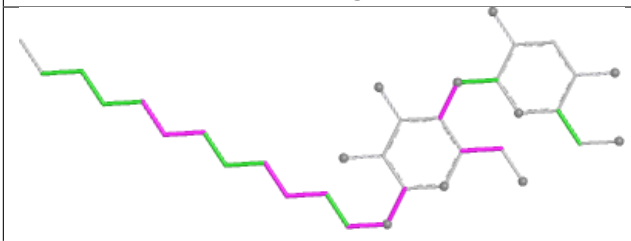
Ligand LMU A 858



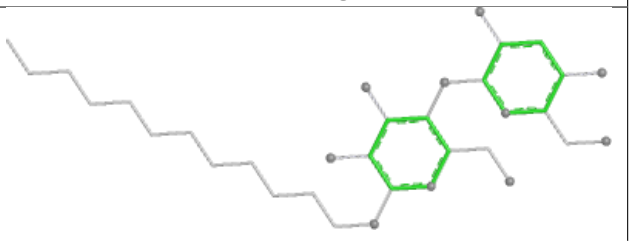
Bond lengths



Bond angles

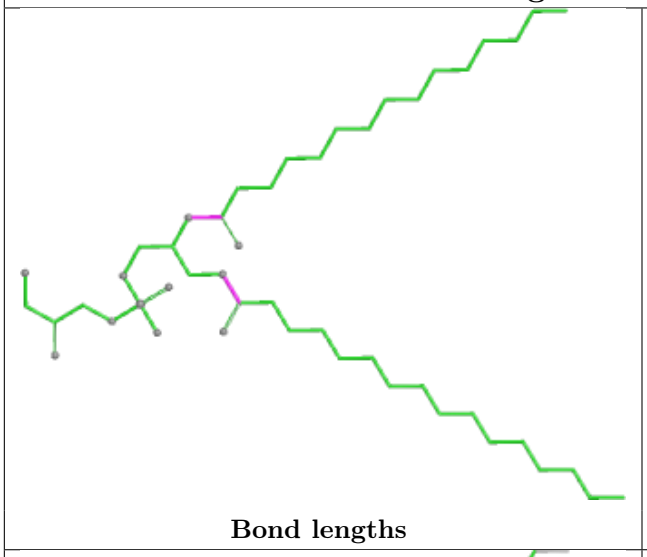


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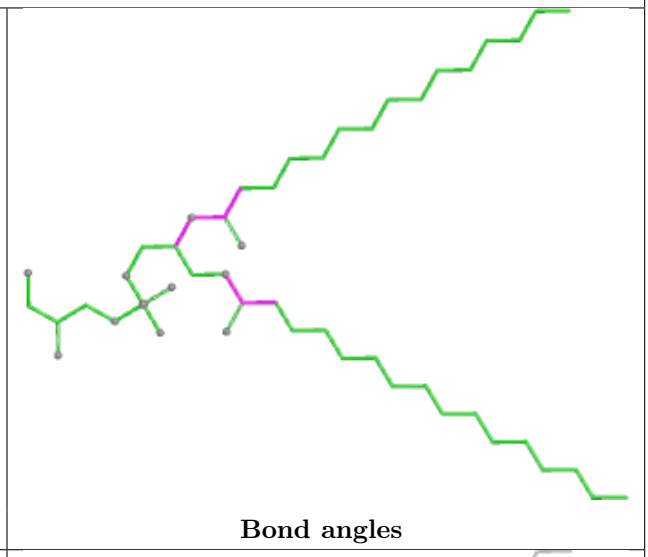


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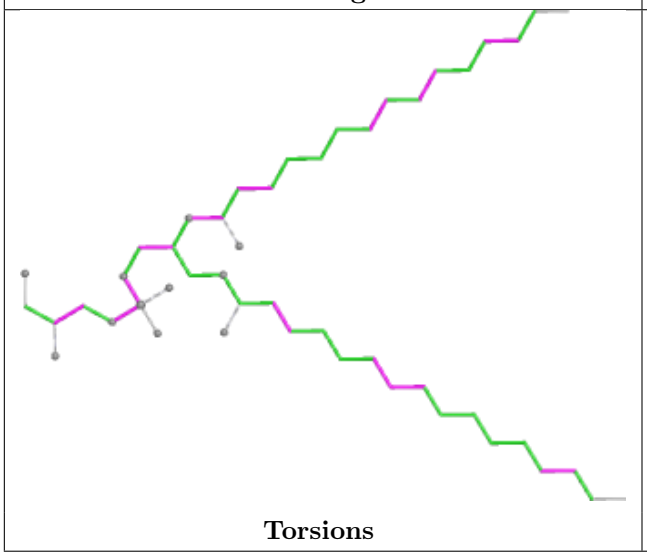
Ligand LHG 6 623



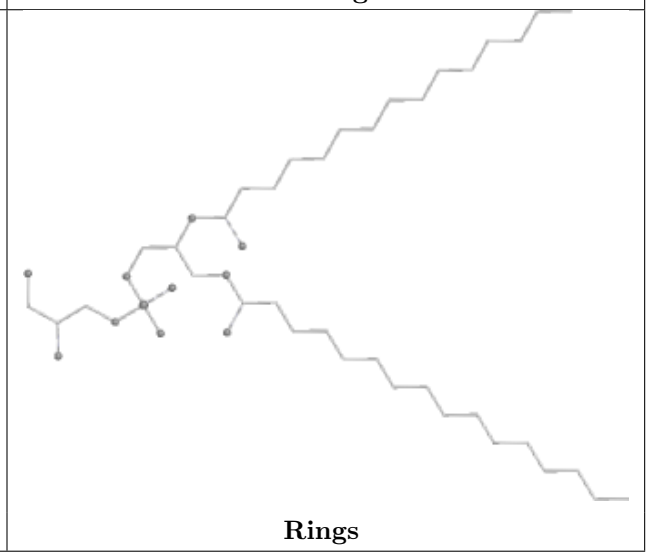
Bond lengths



Bond angles

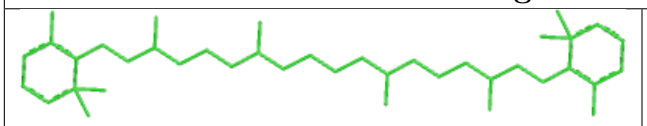


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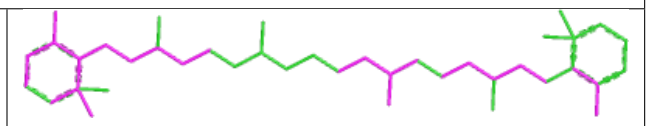


Rings

Ligand BCR O 2004



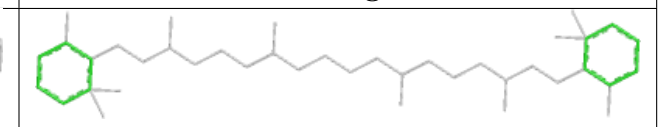
Bond lengths



Bond angles

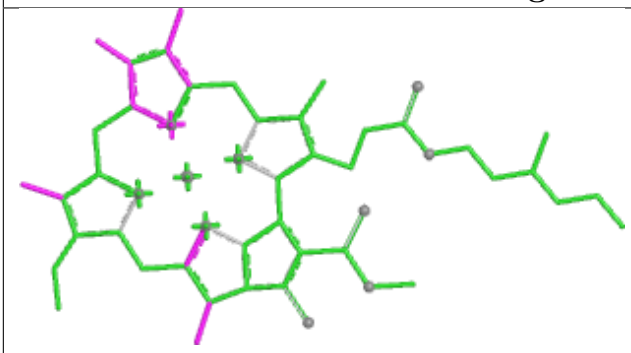


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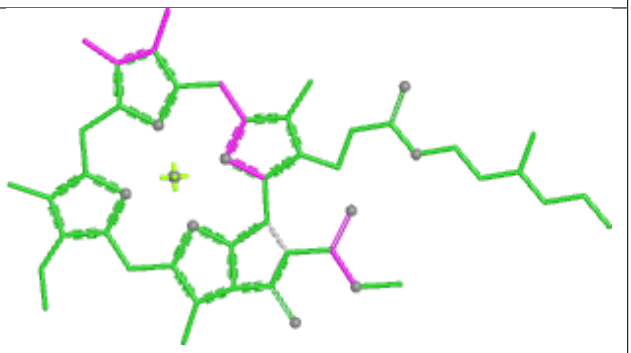


Rings

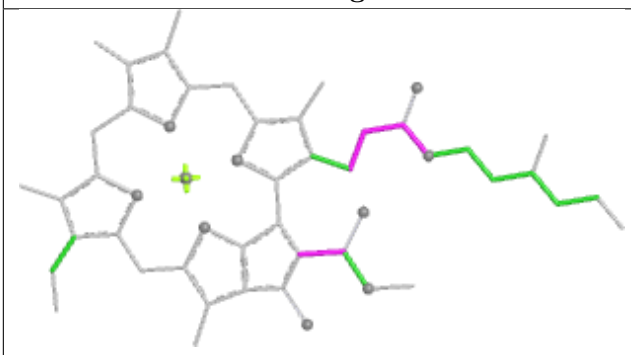
Ligand CLA 6 603



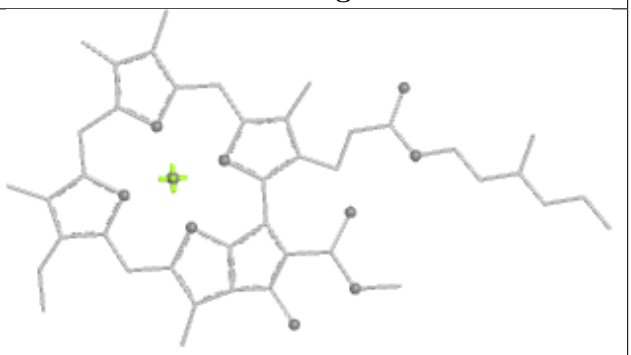
Bond lengths



Bond angles

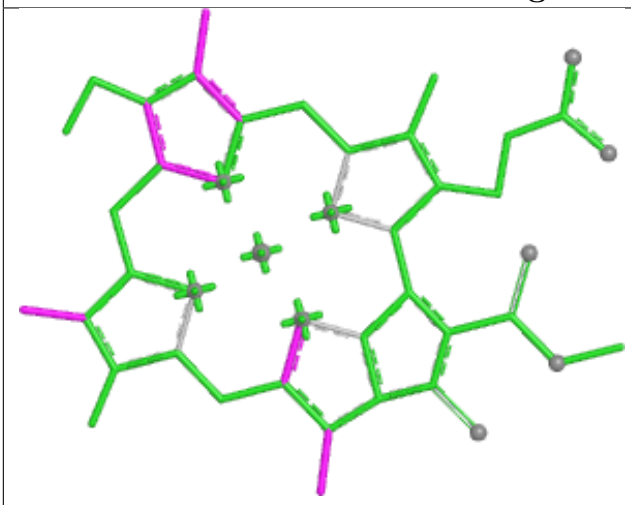


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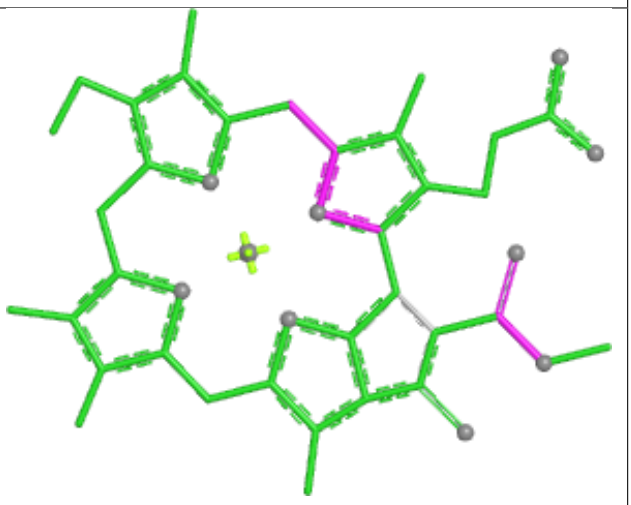


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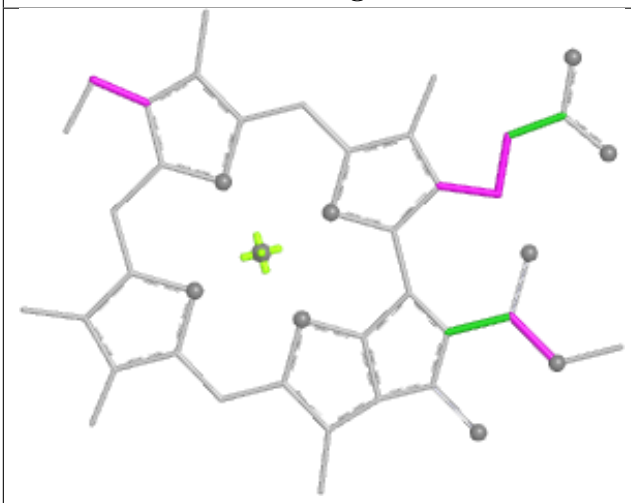
Ligand CLA 2 612



Bond lengths



Bond angles

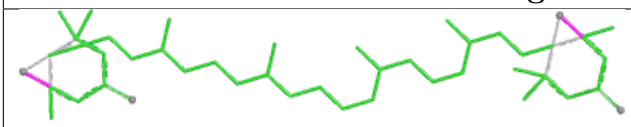


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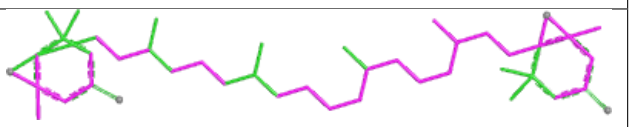


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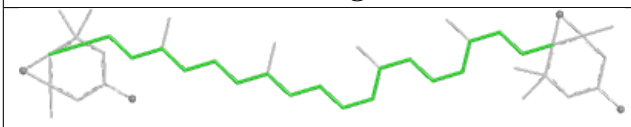
Ligand XAT 5 621



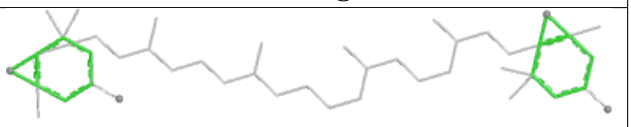
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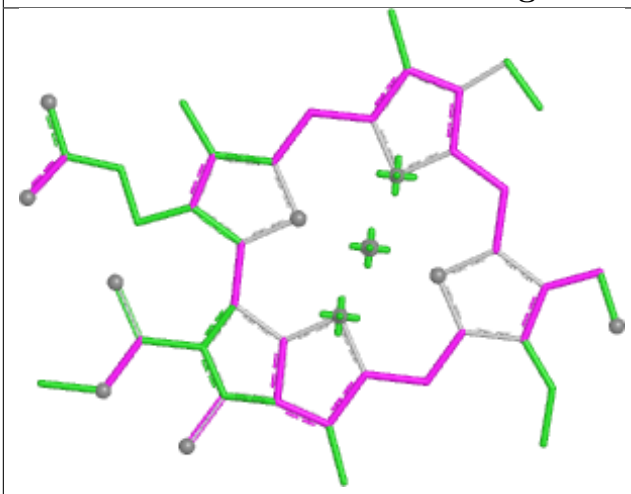


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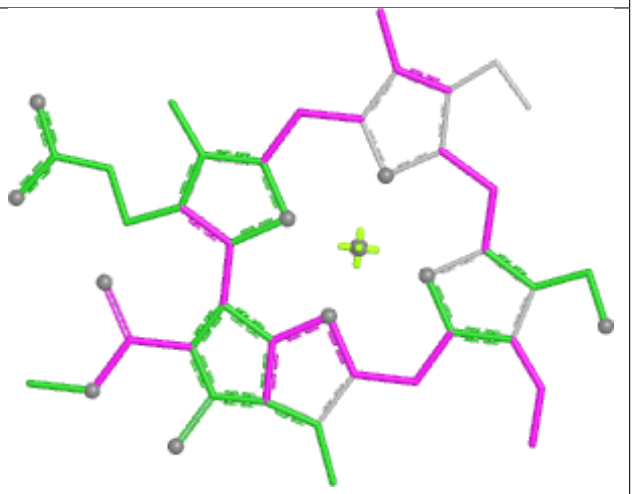


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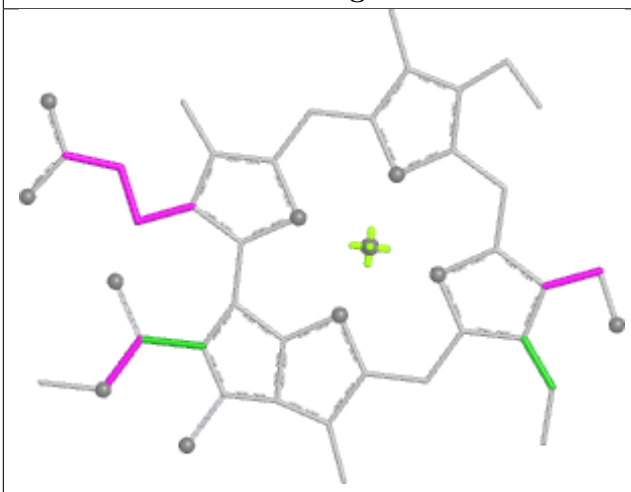
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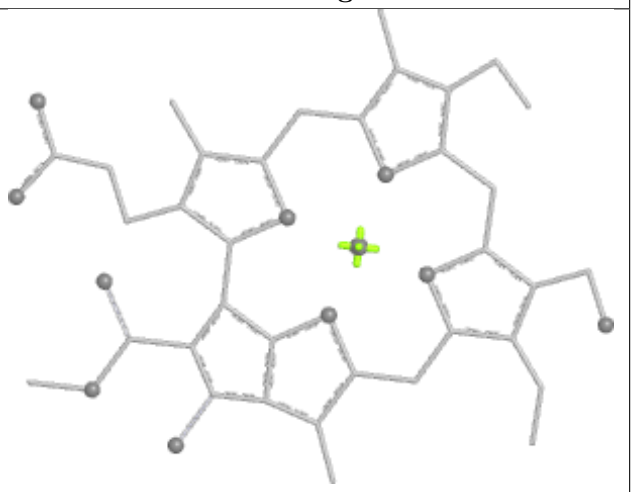
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Bond angles

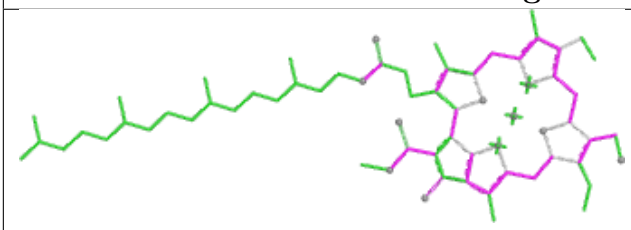


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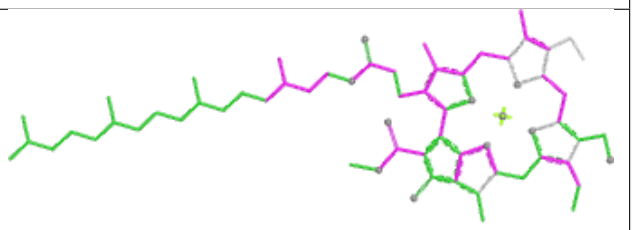


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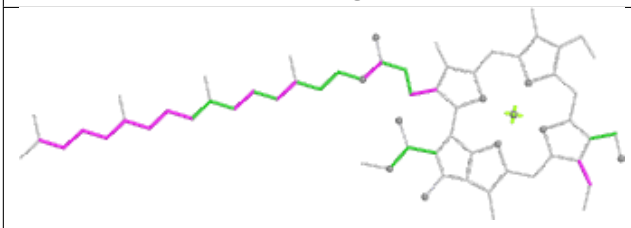
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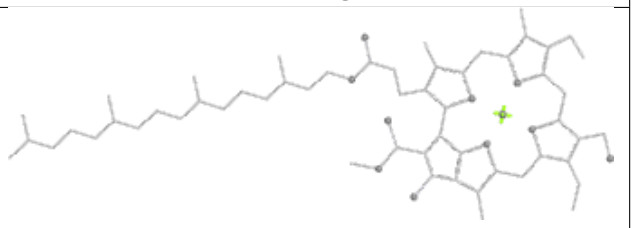
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Bond angles

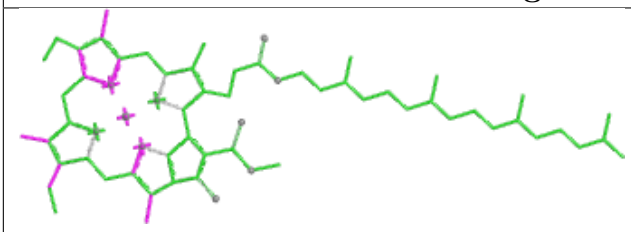


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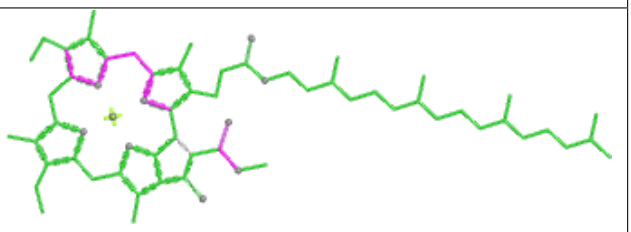


Rings

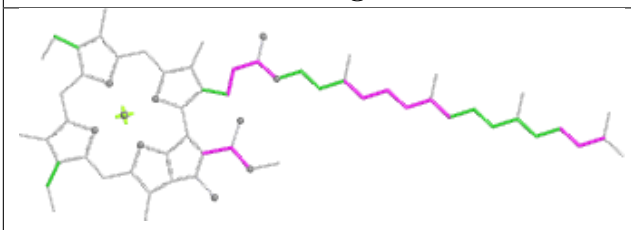
Ligand CLA A 807



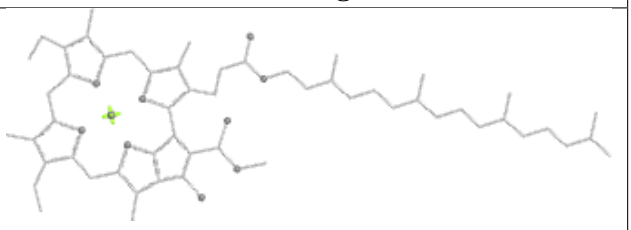
Bond lengths



Bond angles

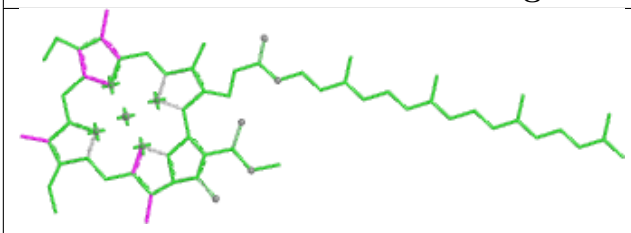


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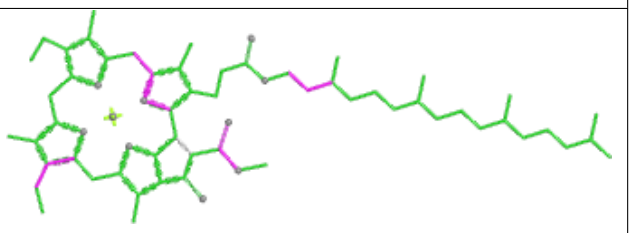


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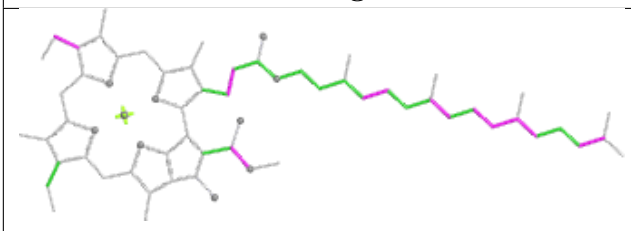
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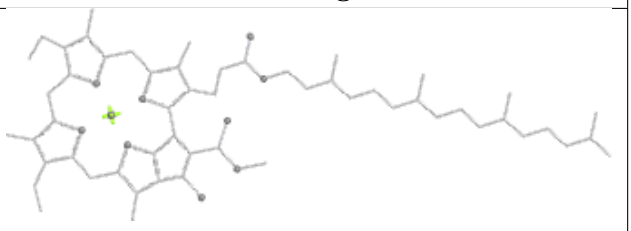
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Bond angles

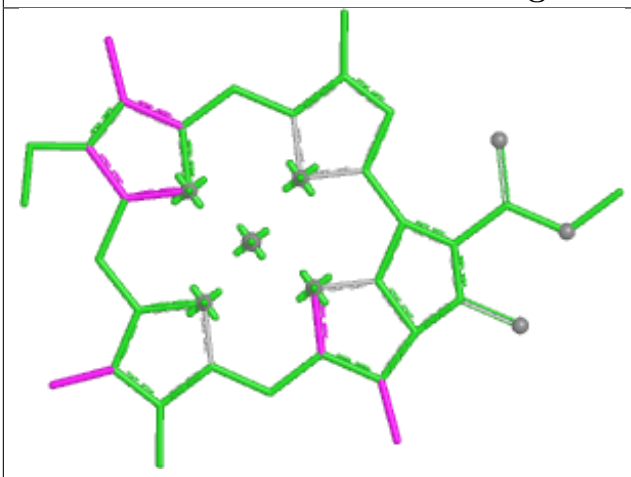


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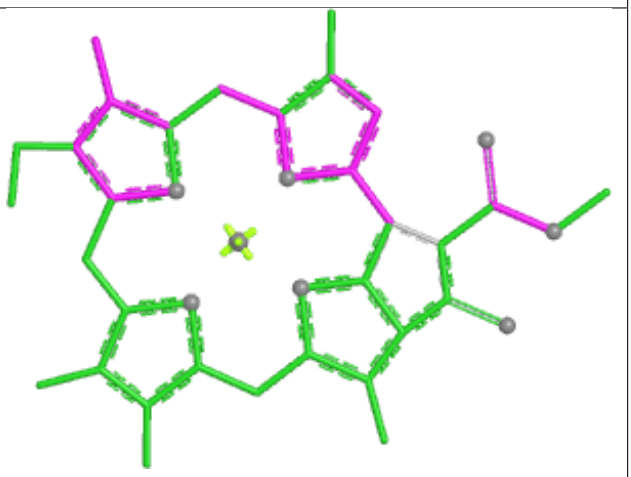


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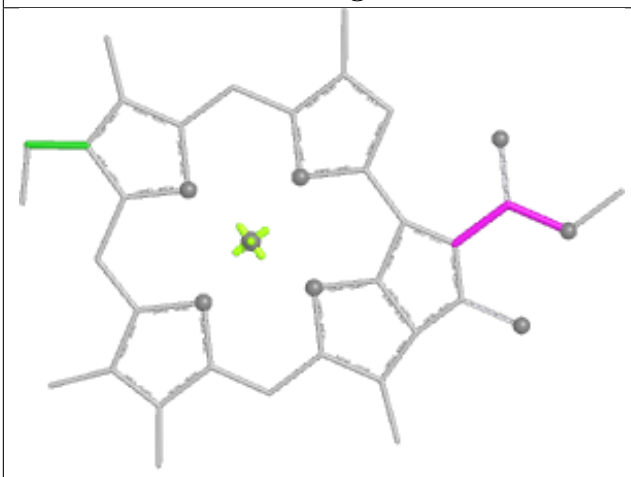
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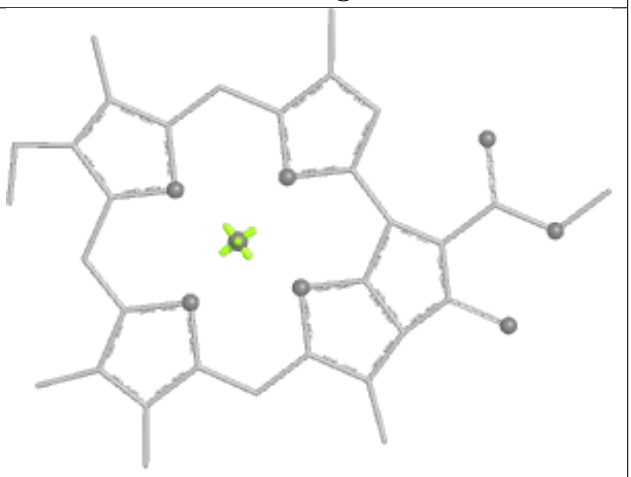
Bond lengths



Bond angles

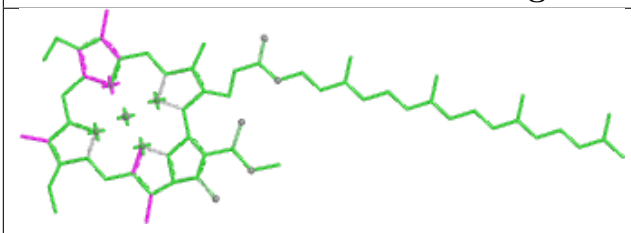


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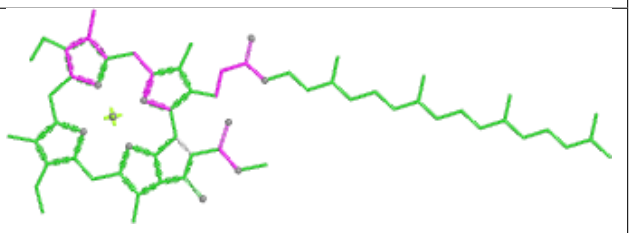


Rings

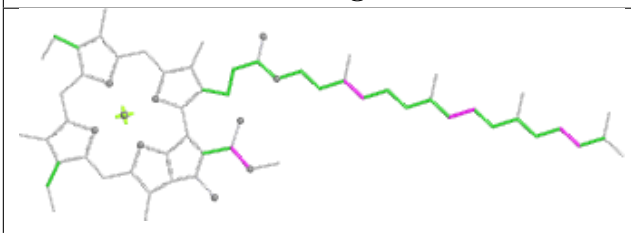
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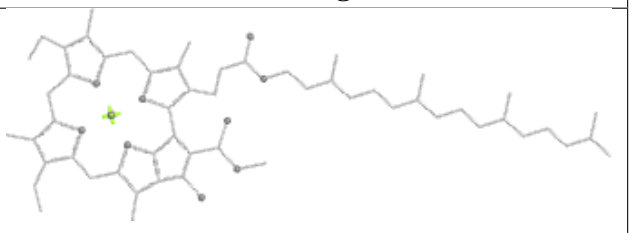
Bond lengths



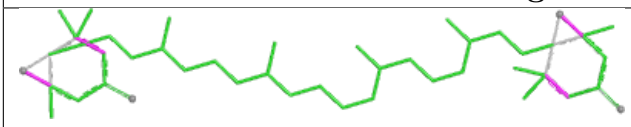
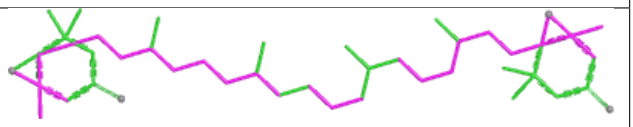
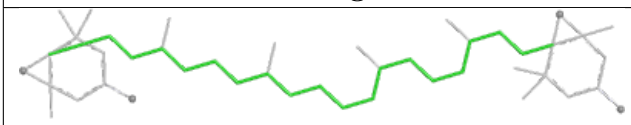
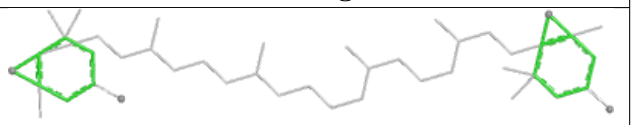
Bond angles

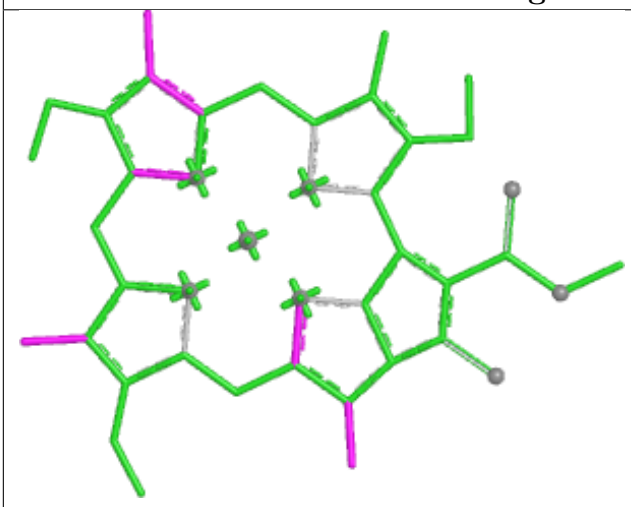
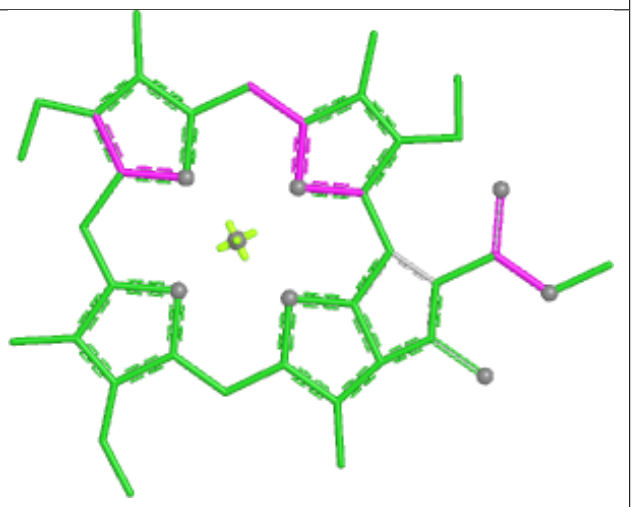
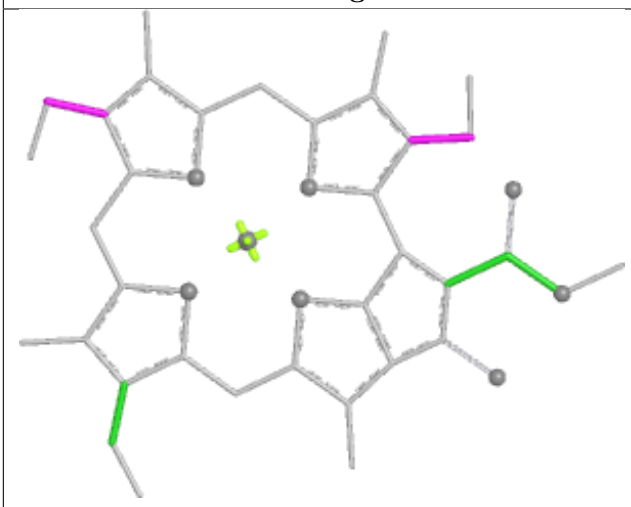


Torsions

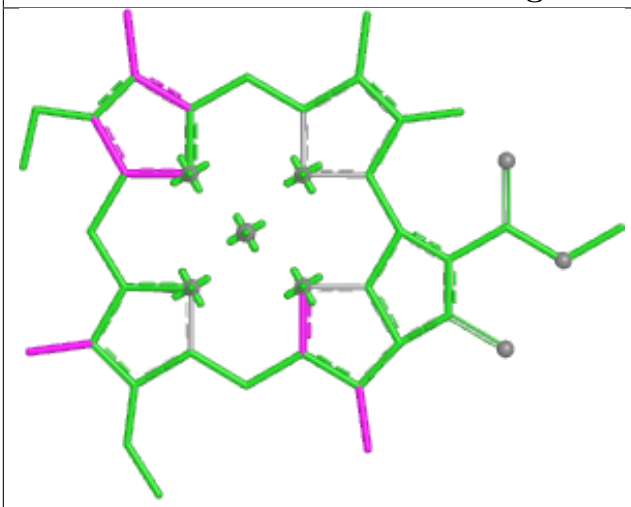


Rings

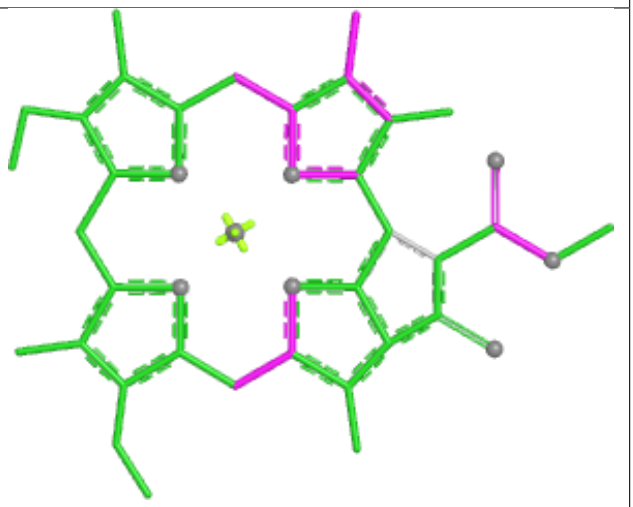
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 6 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

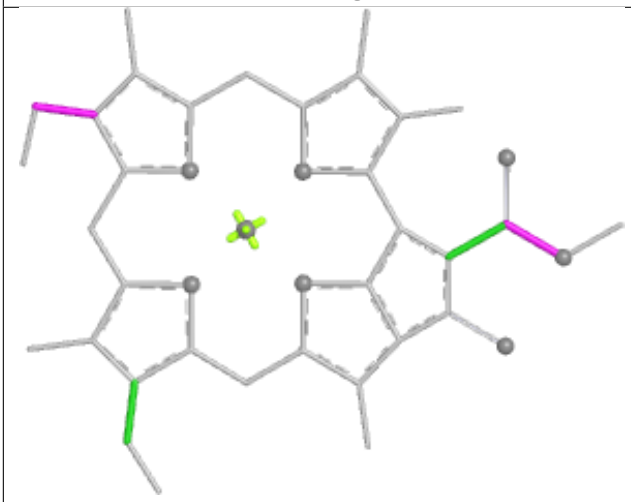
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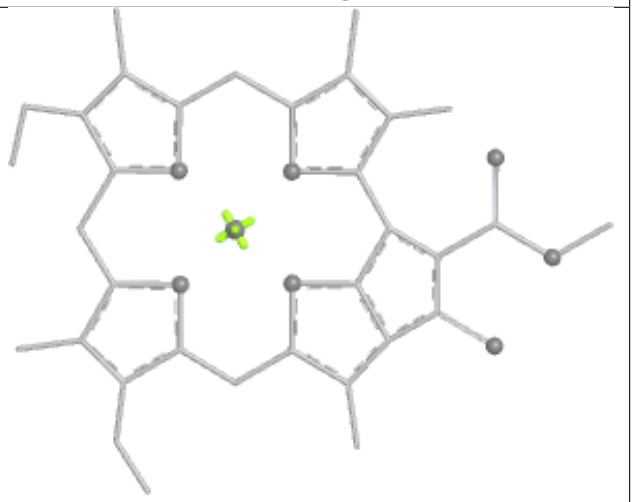
Bond lengths



Bond angles

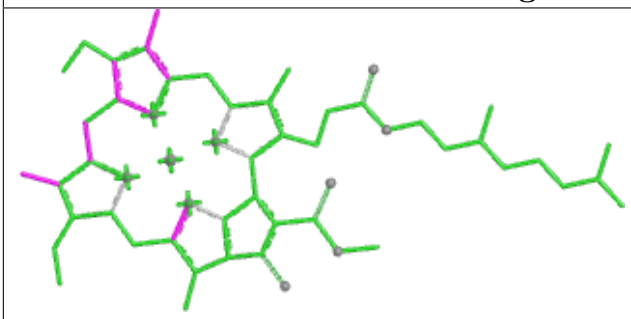


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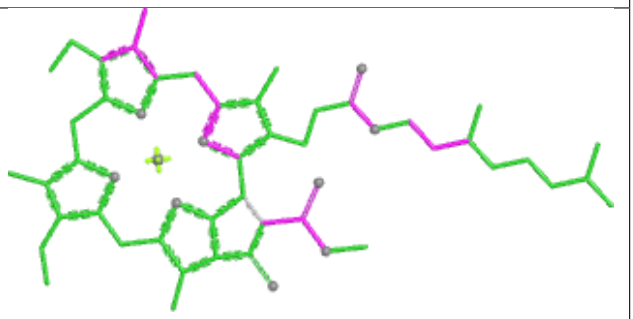


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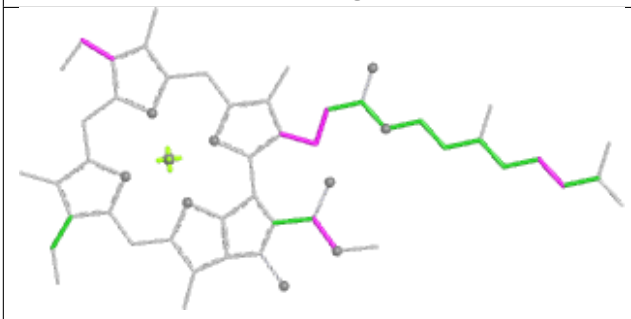
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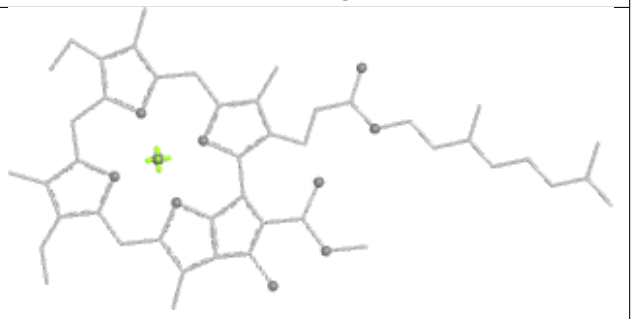
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Bond angles

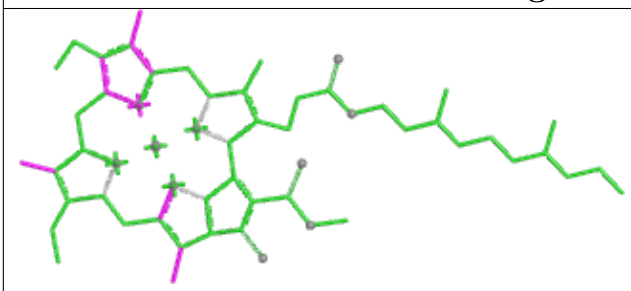


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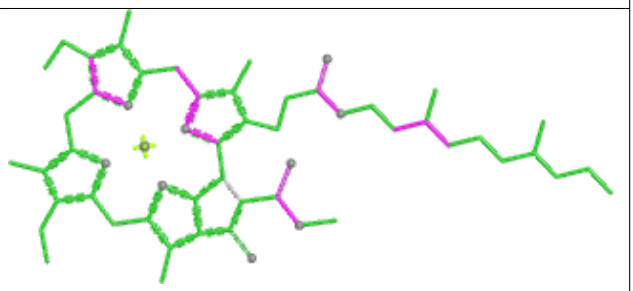


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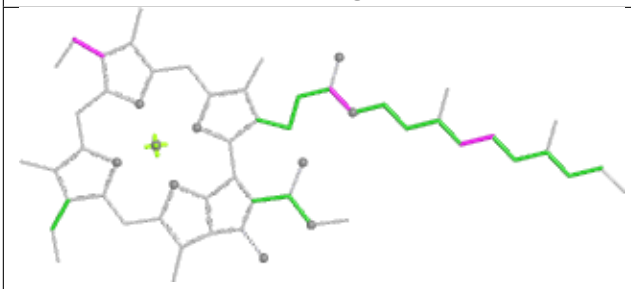
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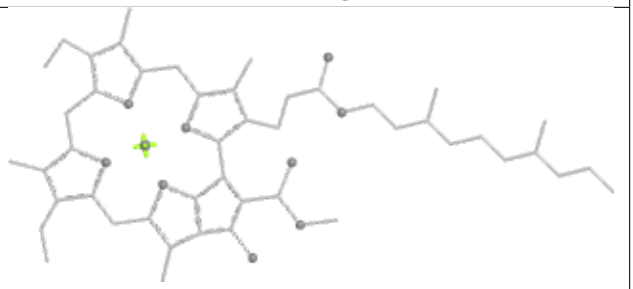
Bond lengths



Bond angles

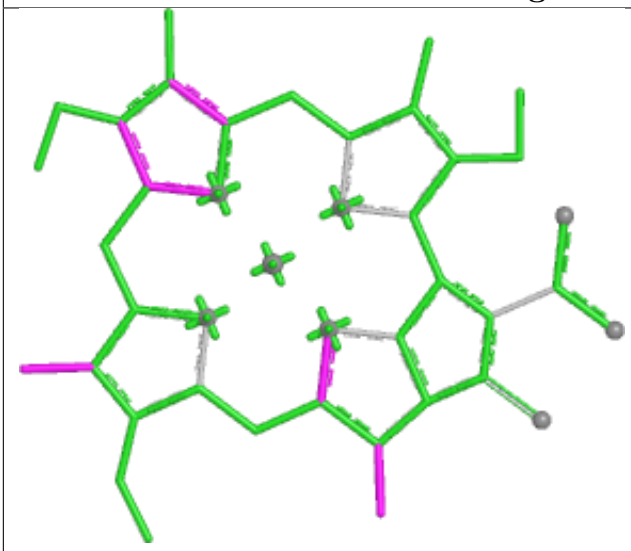


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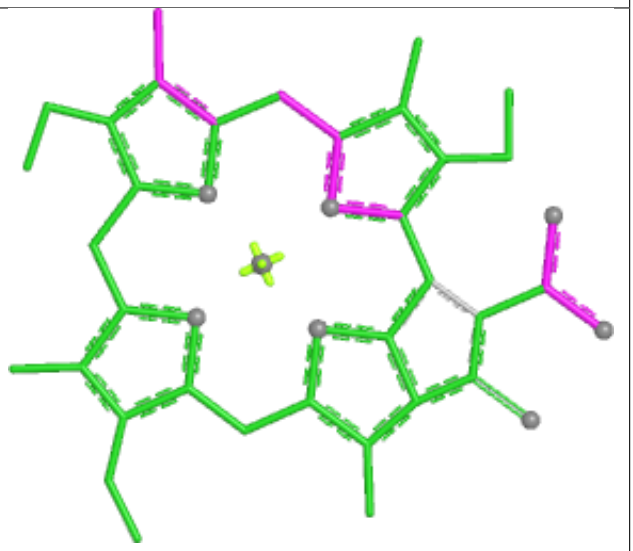


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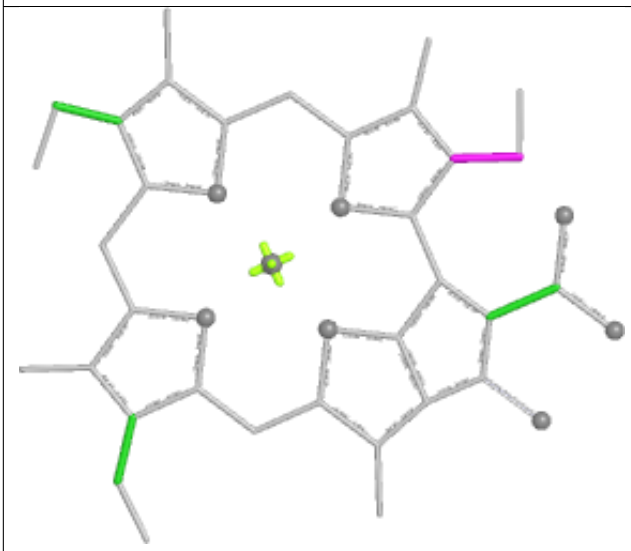
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Bond lengths



Bond angles

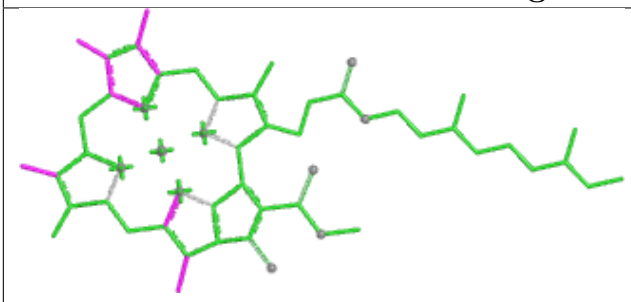


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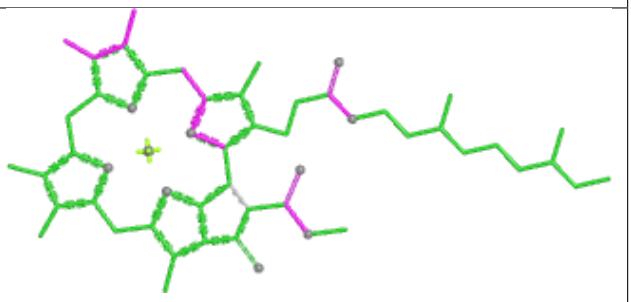


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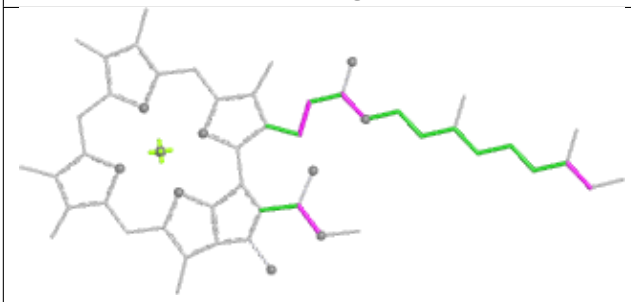
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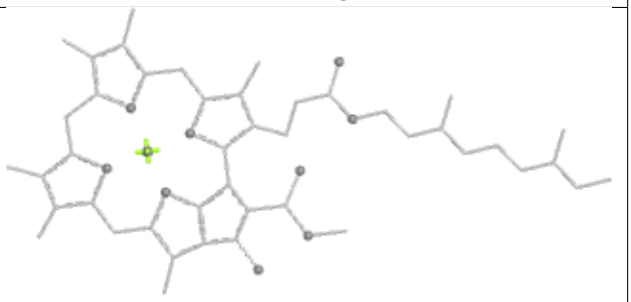
Bond lengths



Bond angles

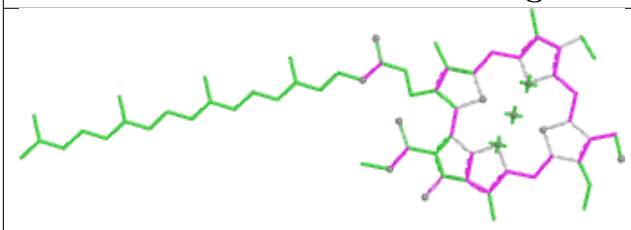


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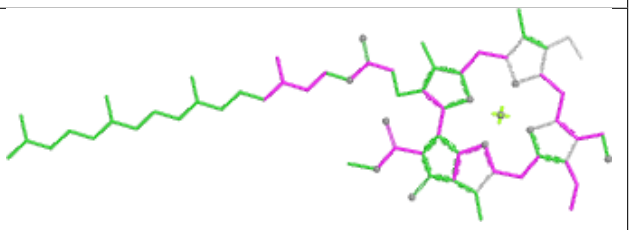


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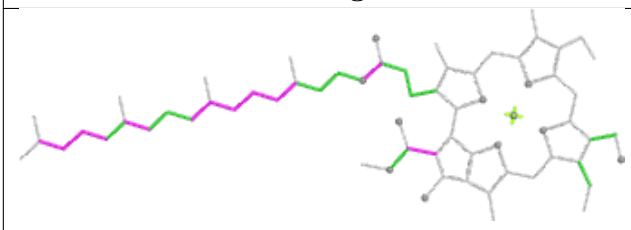
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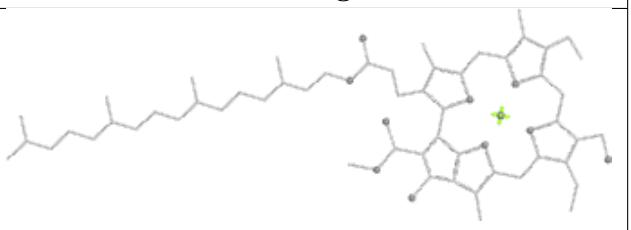
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Bond angles

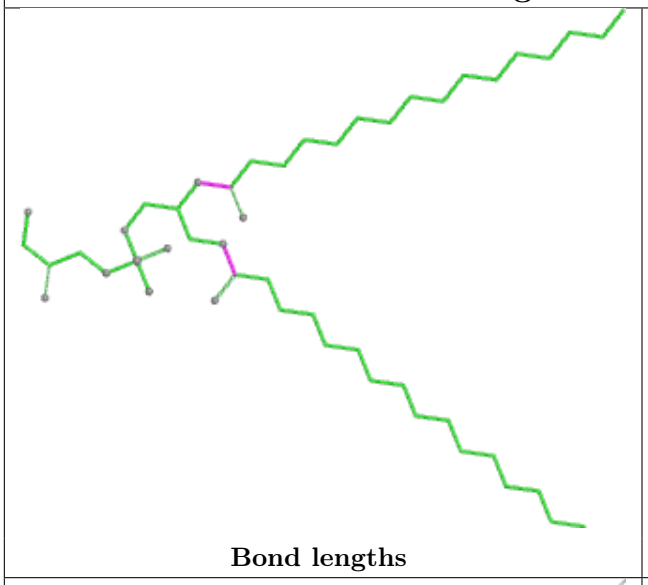


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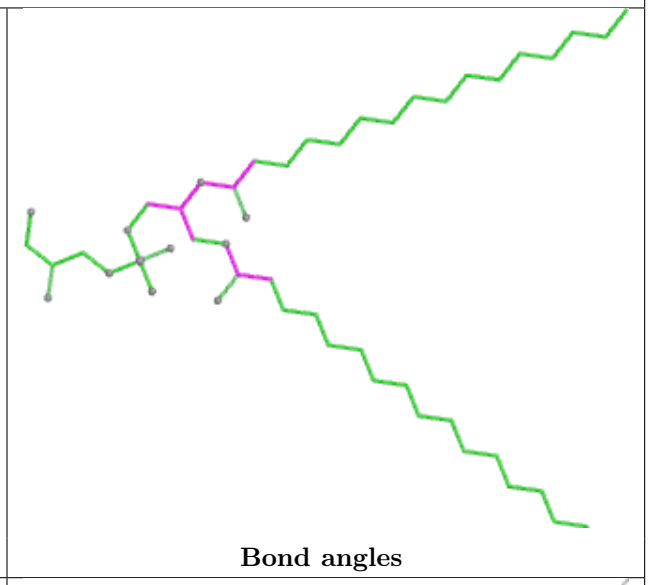


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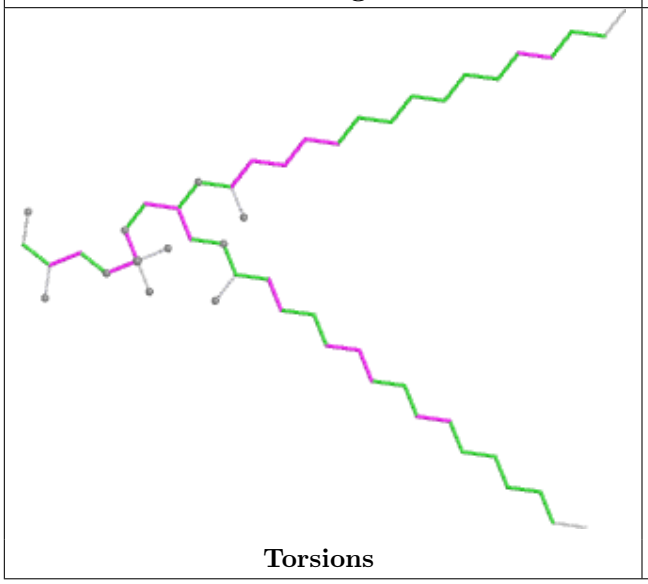
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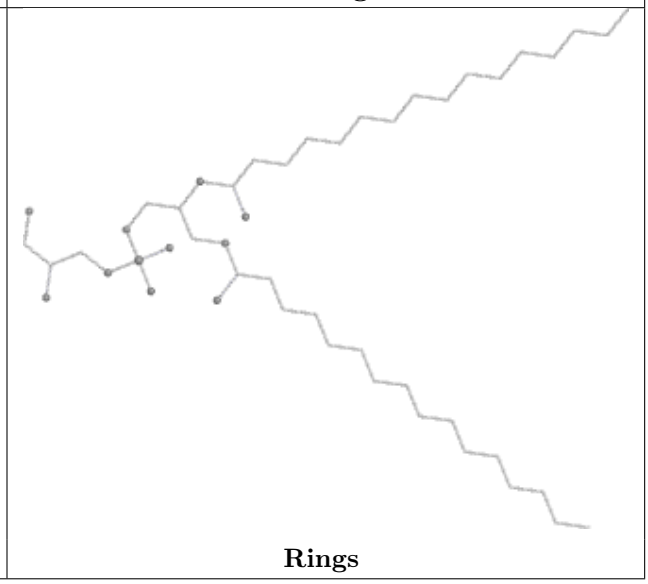
Bond lengths



Bond angles

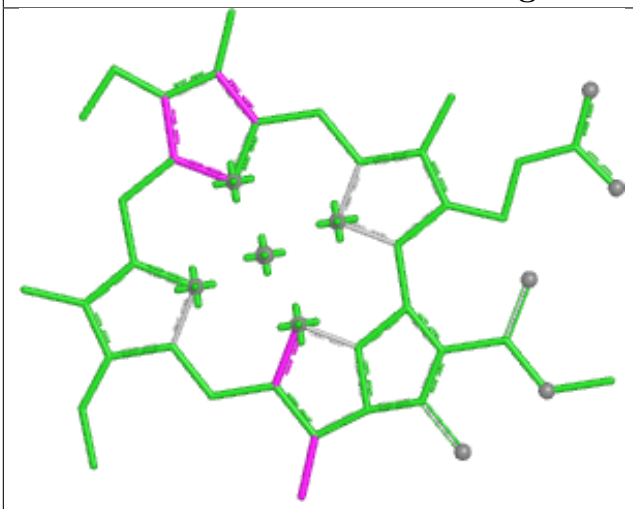


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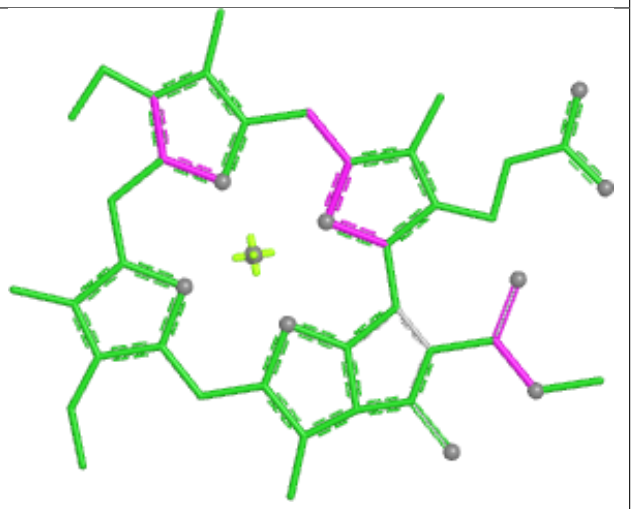


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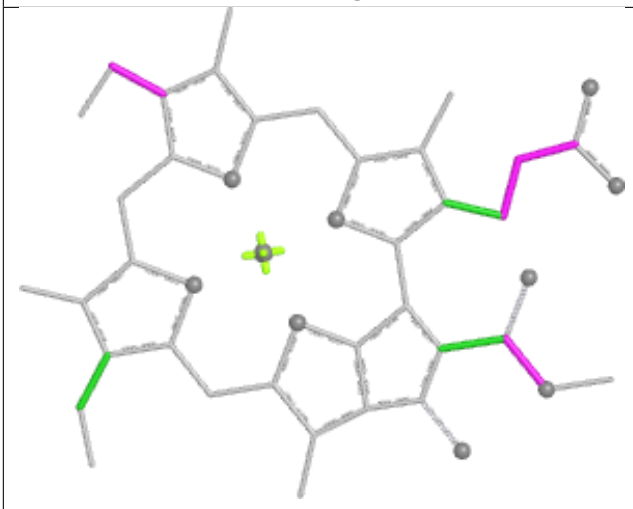
Ligand CLA W 614



Bond lengths



Bond angles

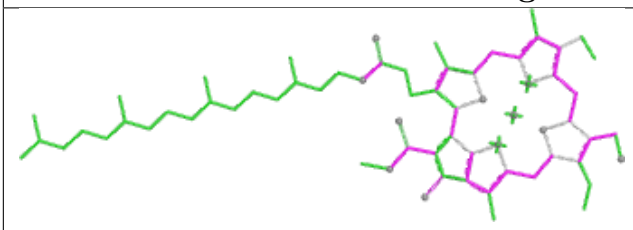


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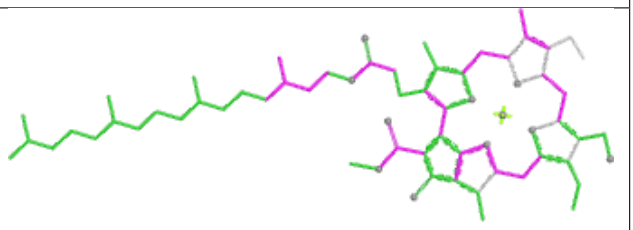


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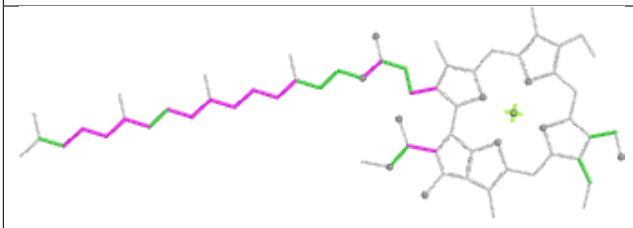
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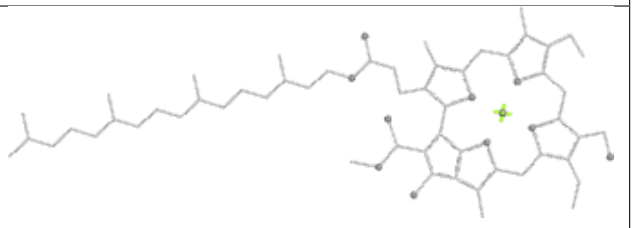
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Bond angles

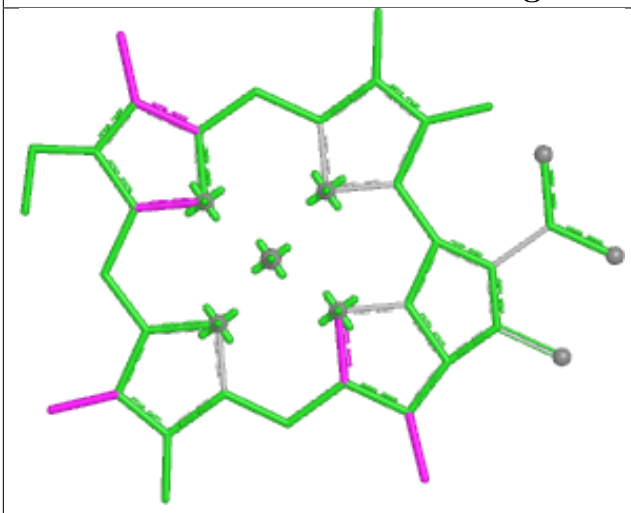


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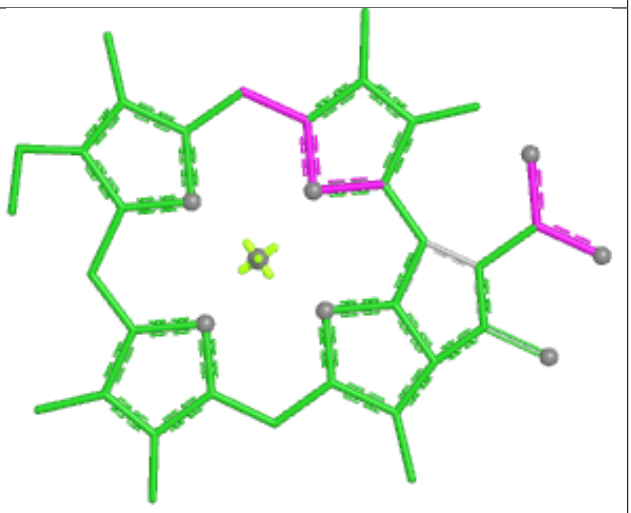


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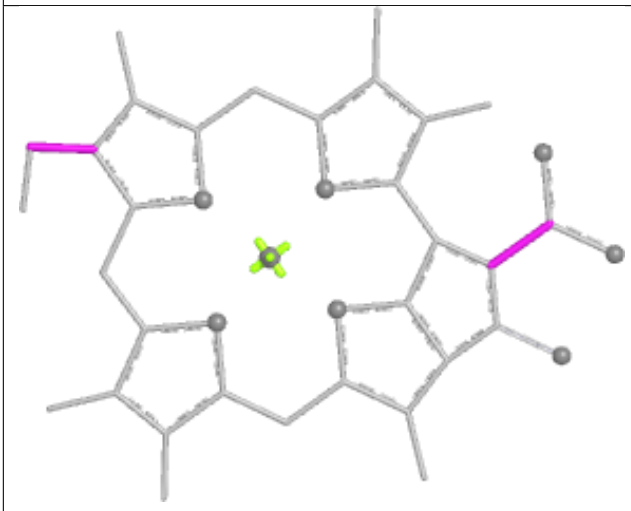
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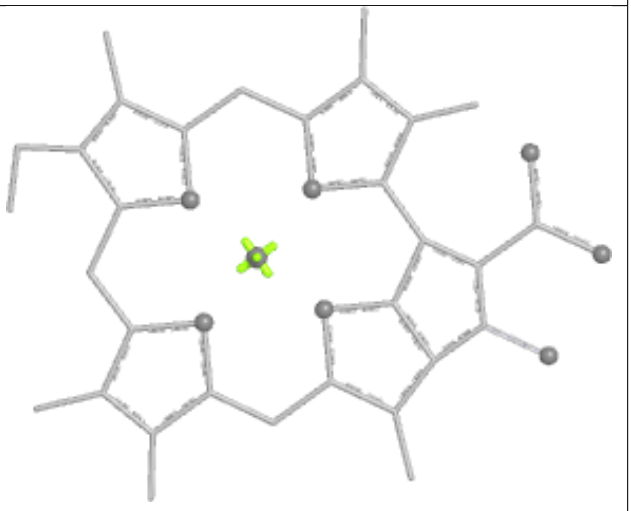
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Bond angles

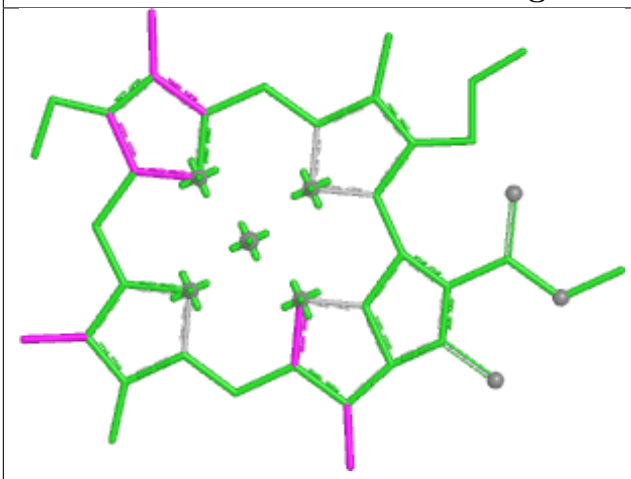


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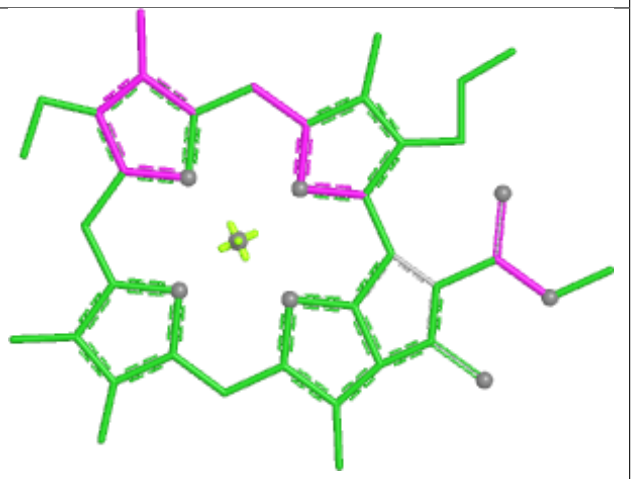


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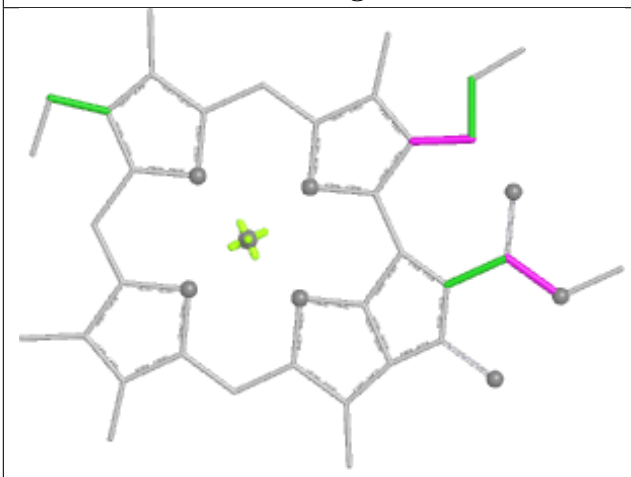
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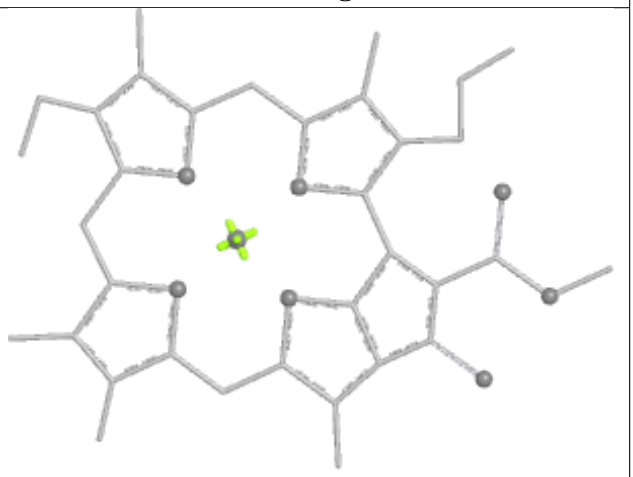
Bond lengths



Bond angles

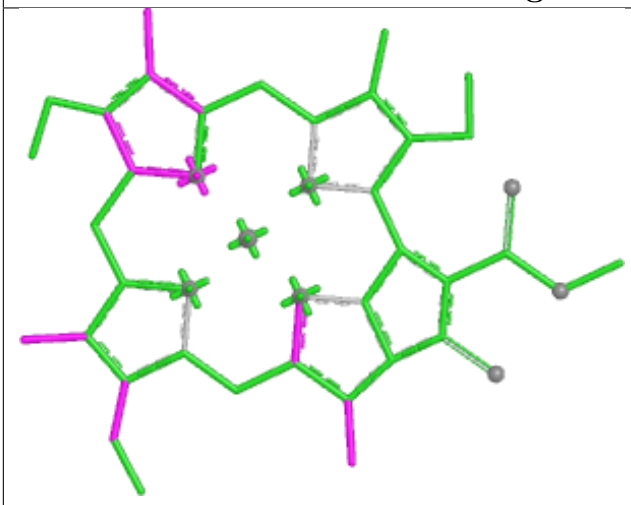


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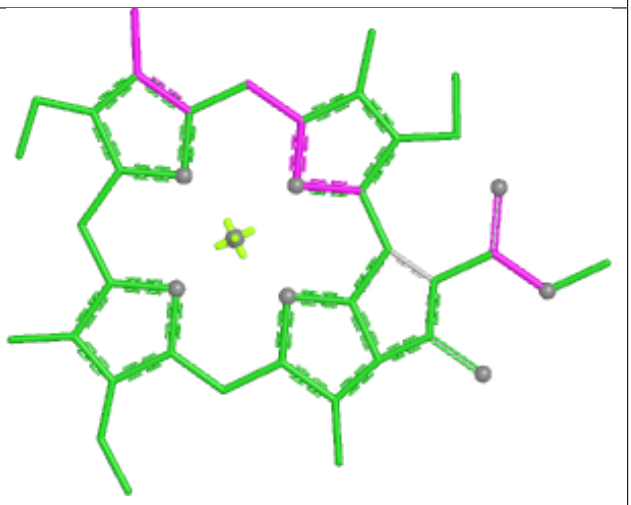


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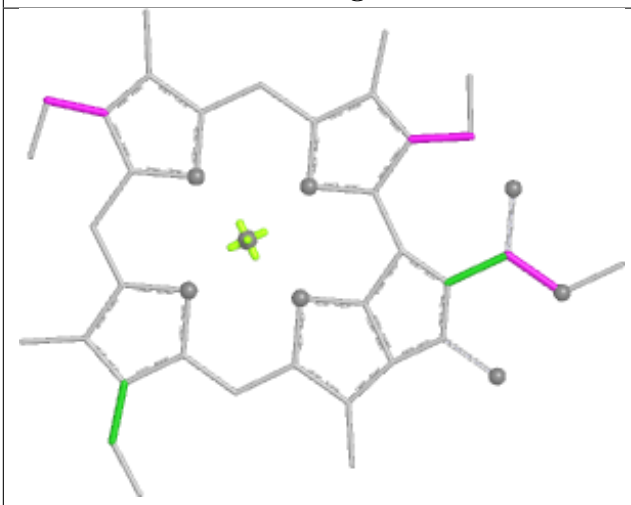
Ligand CLA F 303



Bond lengths



Bond angles

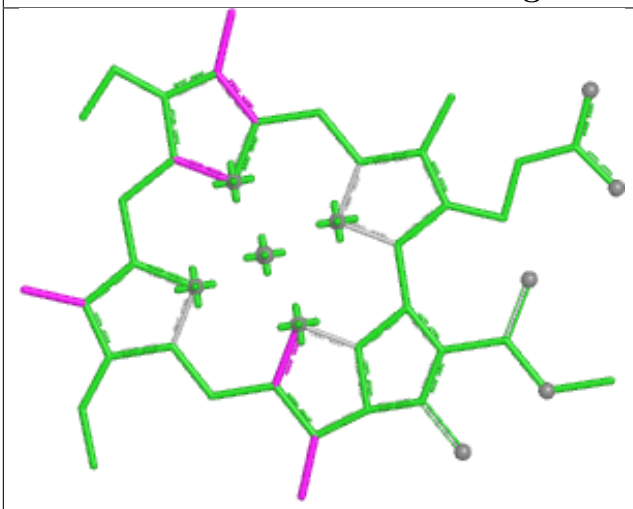


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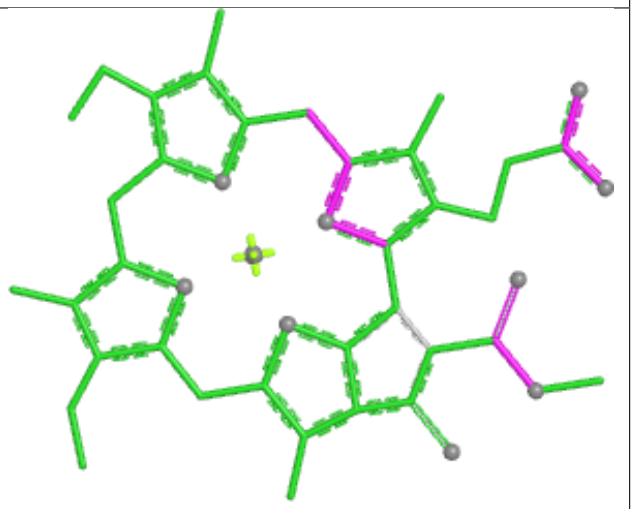


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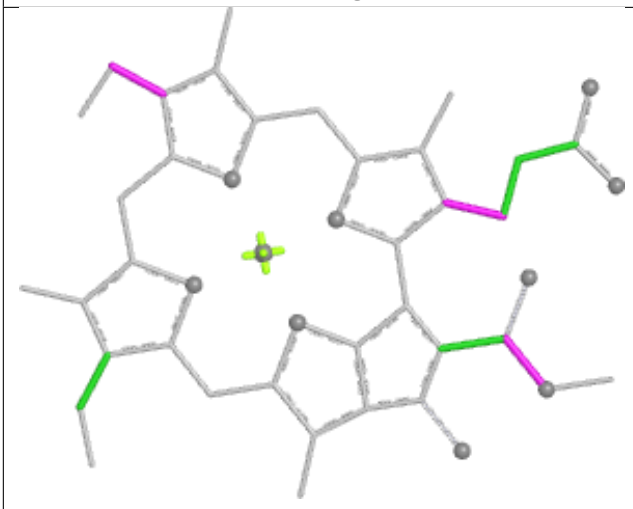
Ligand CLA K 201



Bond lengths



Bond angles

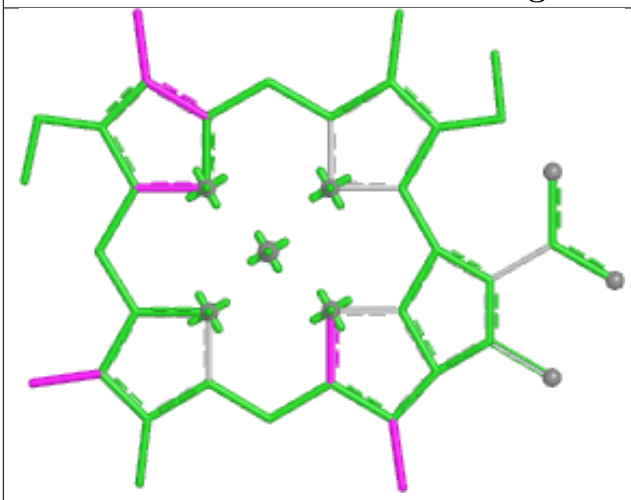


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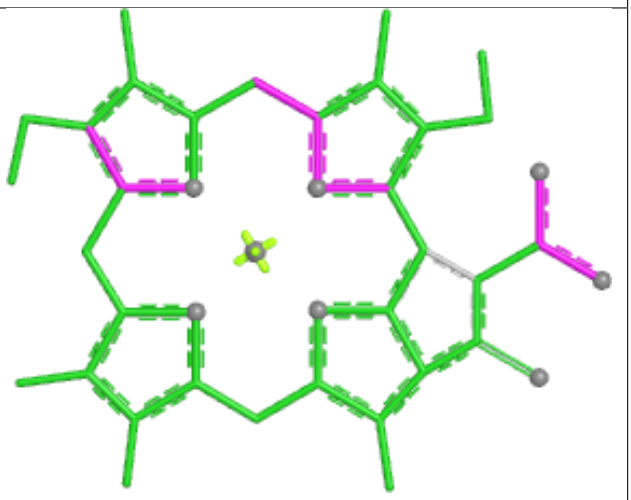


Rings

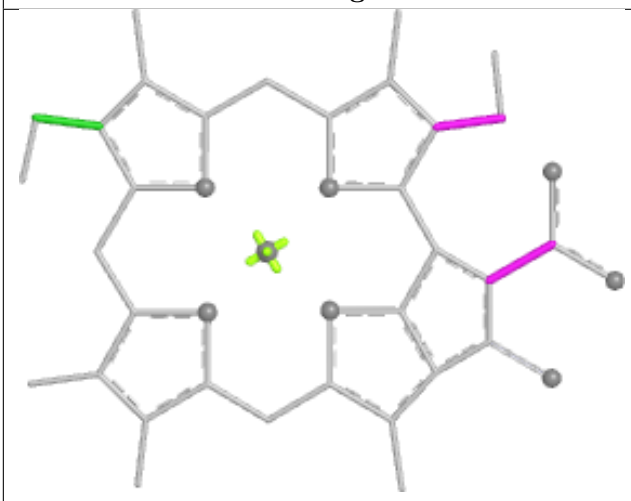
Ligand CLA 3 615



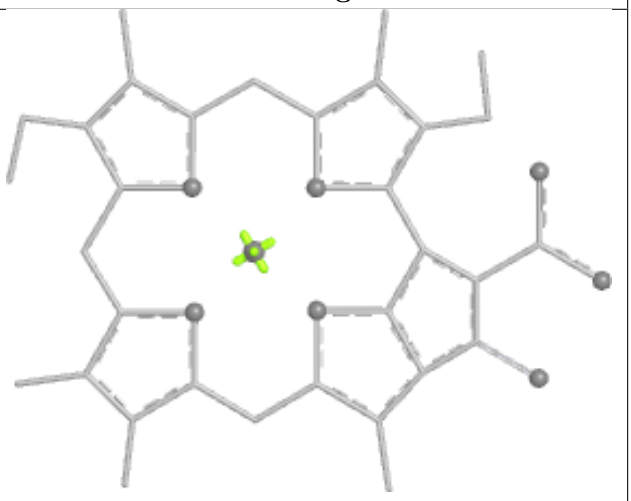
Bond lengths



Bond angles

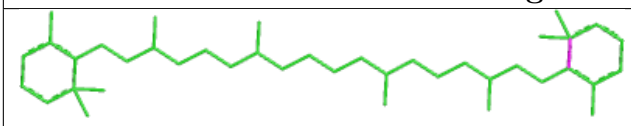


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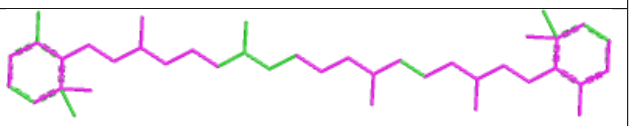


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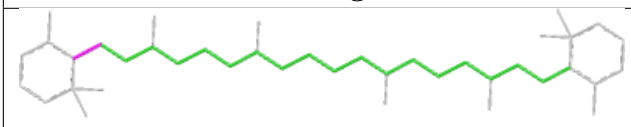
Ligand BCR J 102



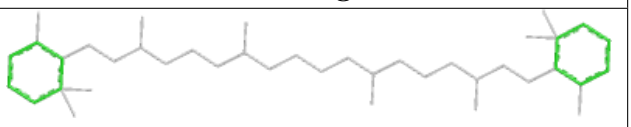
Bond lengths



Bond angles

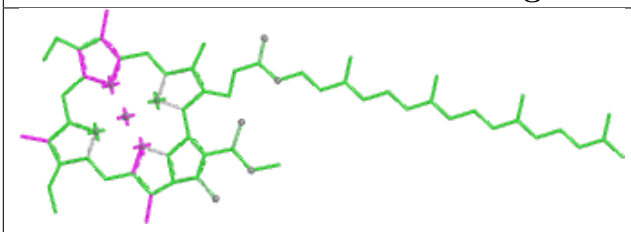


Torsions

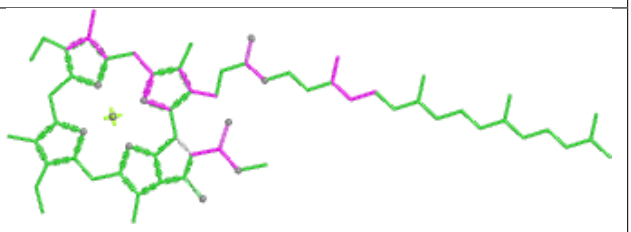


Rings

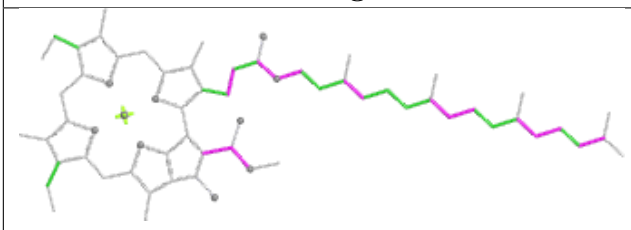
Ligand CLA A 814



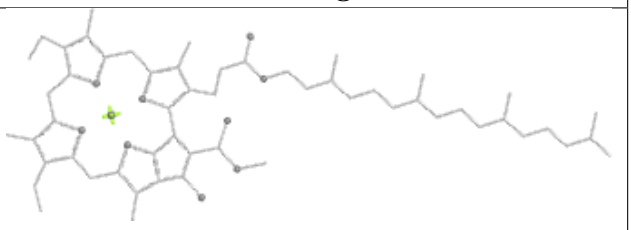
Bond lengths



Bond angles

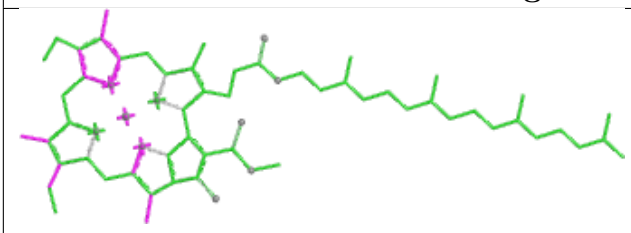


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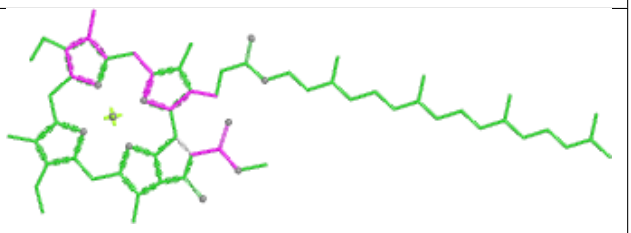


Rings

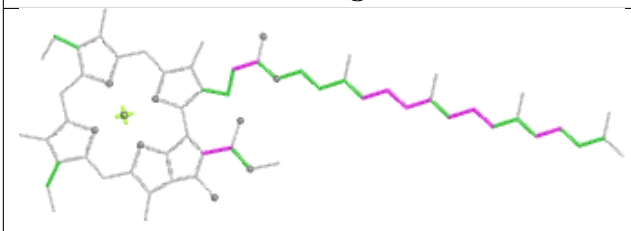
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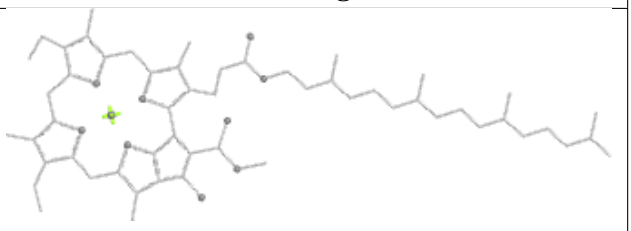
Bond lengths



Bond angles

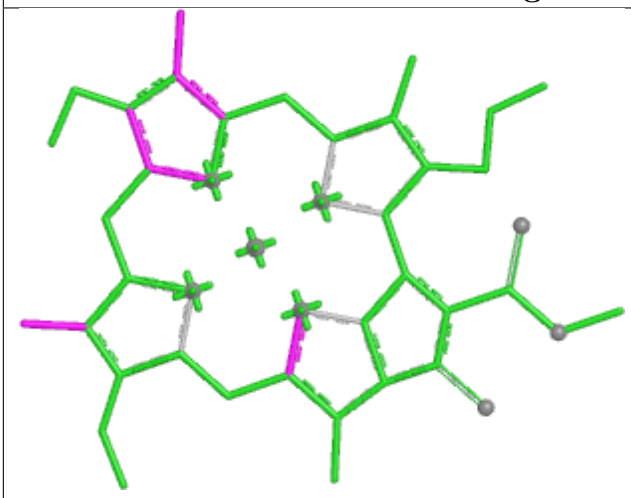


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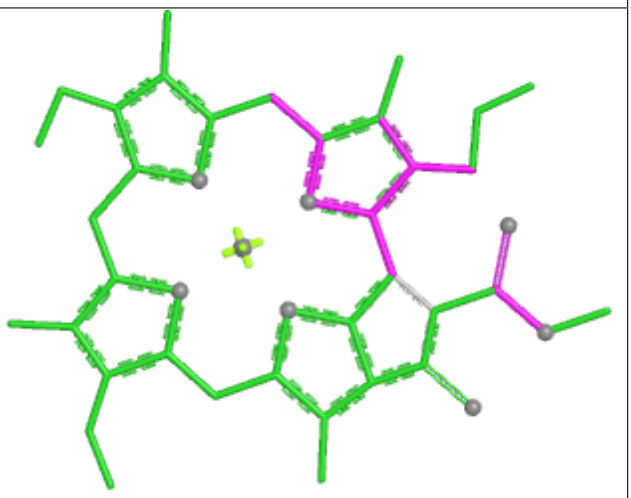


Rings

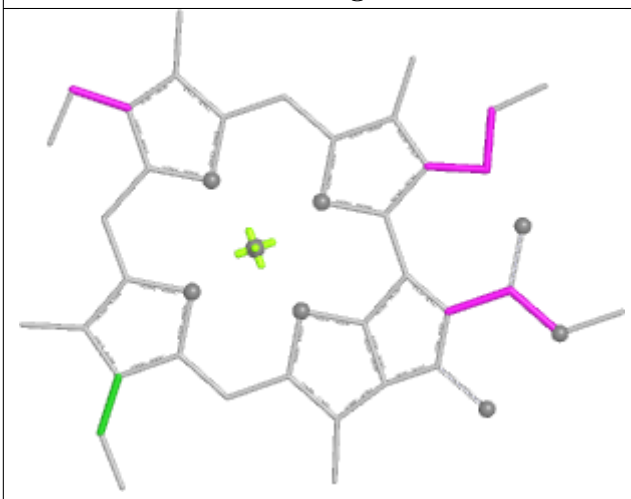
Ligand CLA X 612



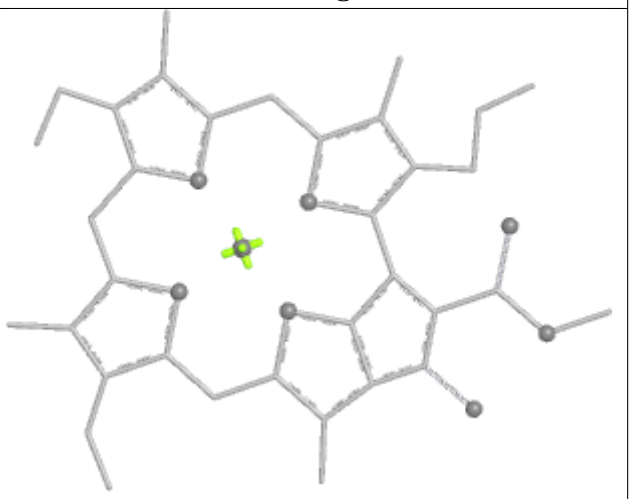
Bond lengths



Bond angles

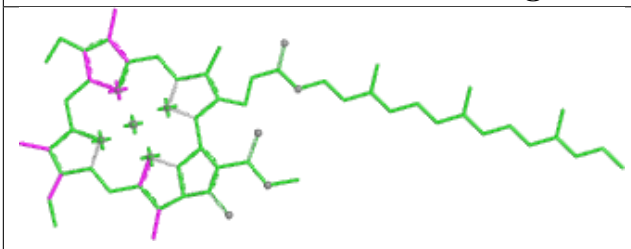


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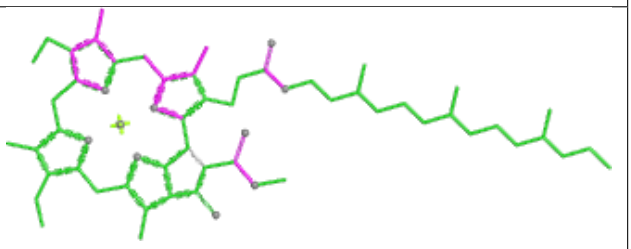


Rings

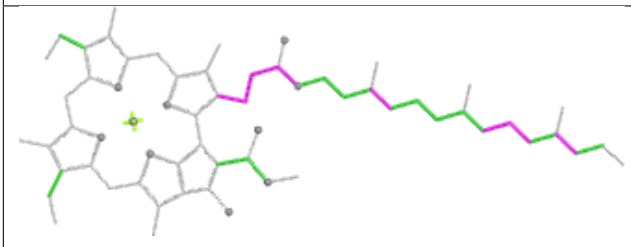
Ligand CLA B 827



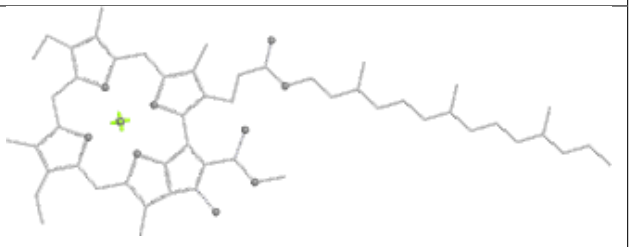
Bond lengths



Bond angles

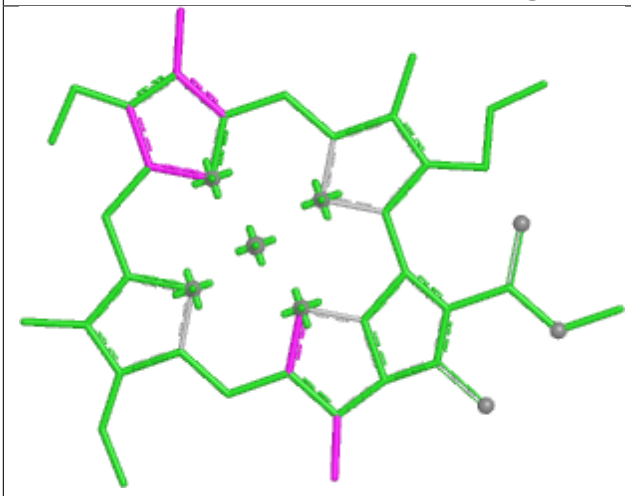


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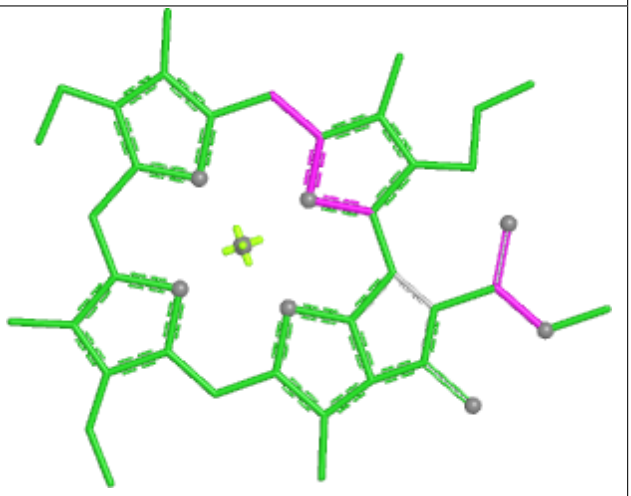


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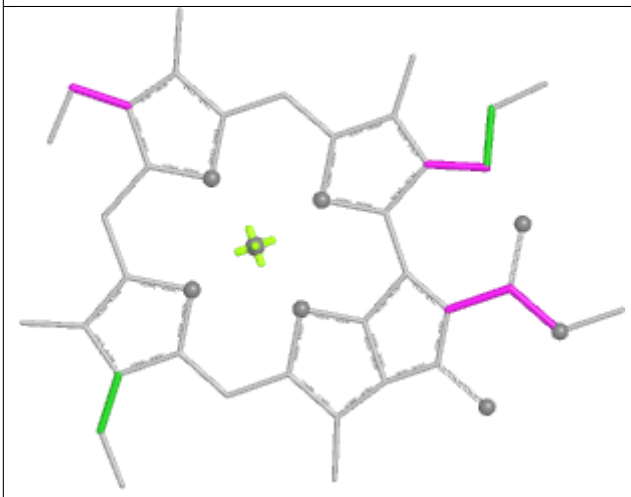
Ligand CLA Y 611



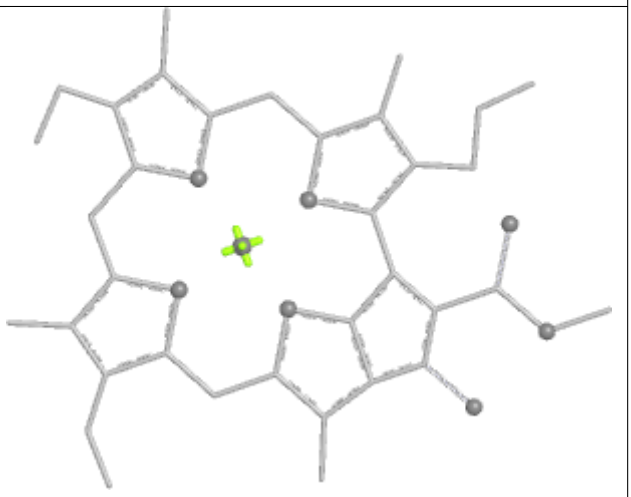
Bond lengths



Bond angles

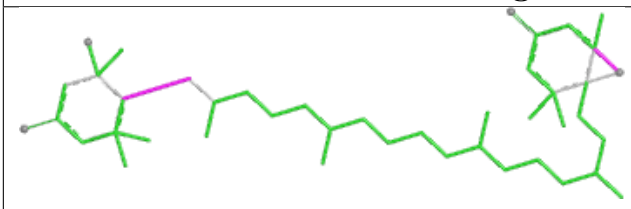


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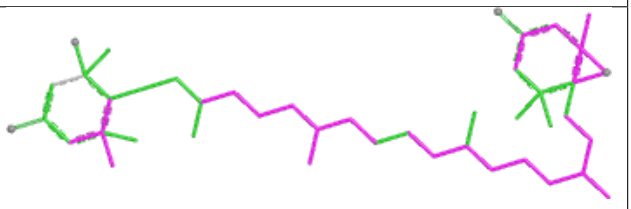


Rings

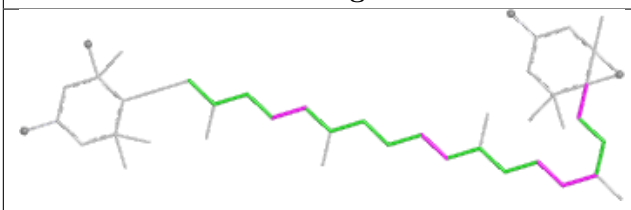
Ligand NEX U 1623



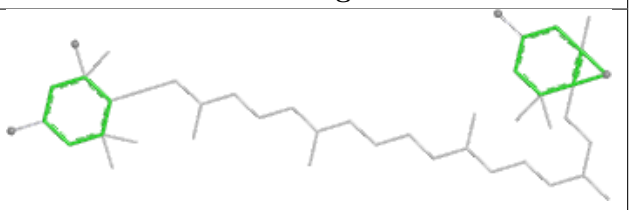
Bond lengths



Bond angles

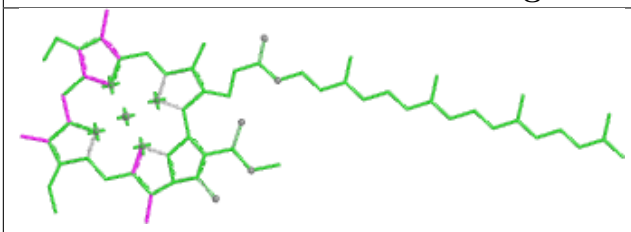


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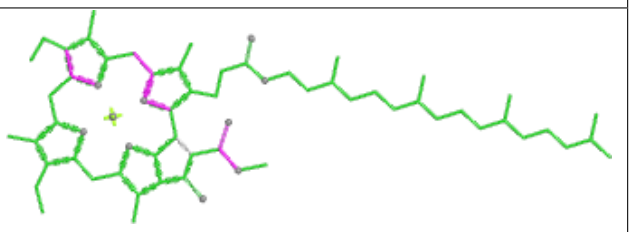


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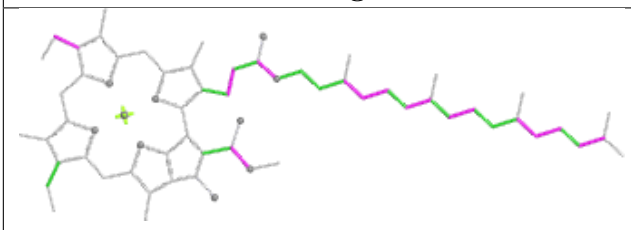
Ligand CLA V 613



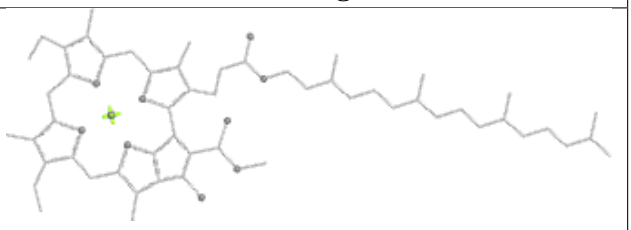
Bond lengths



Bond angles

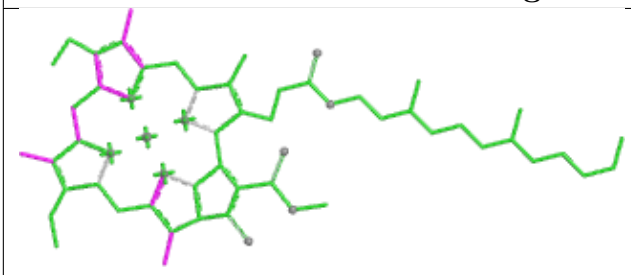


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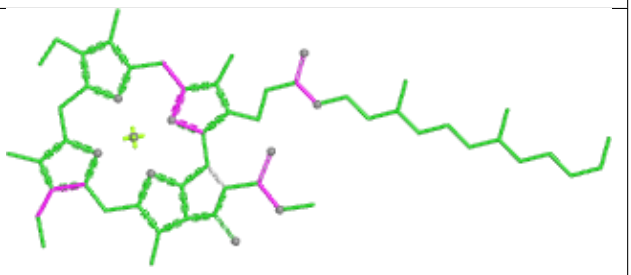


Rings

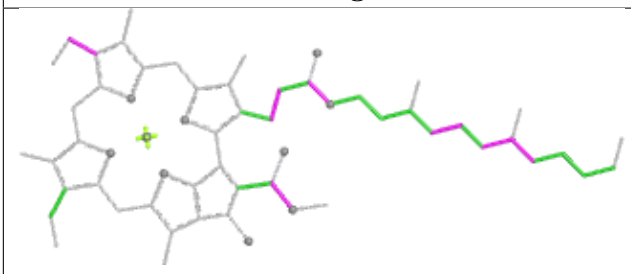
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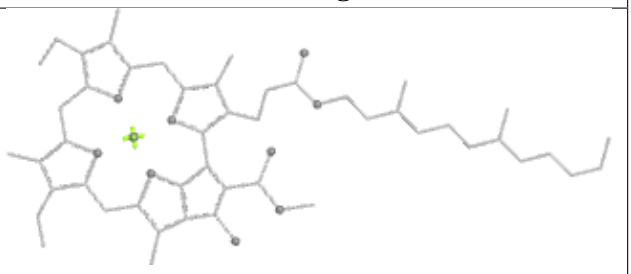
Bond lengths



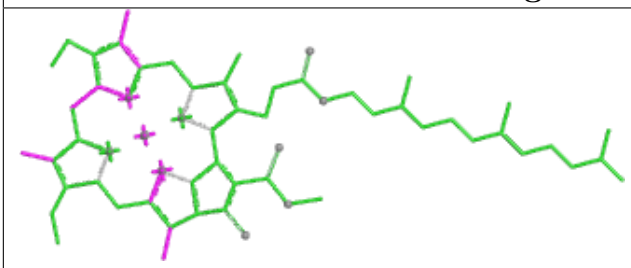
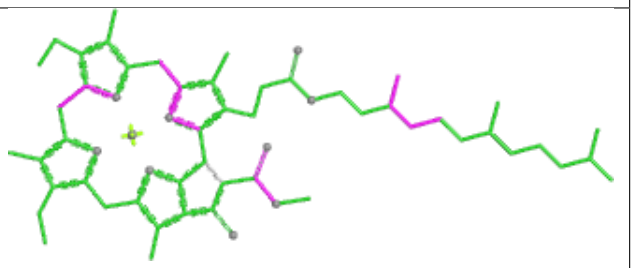
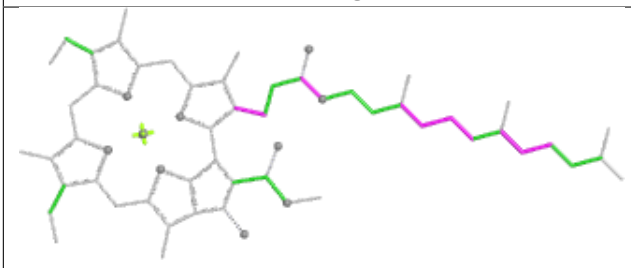
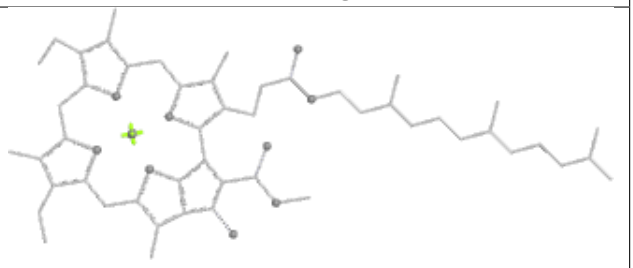
Bond angles

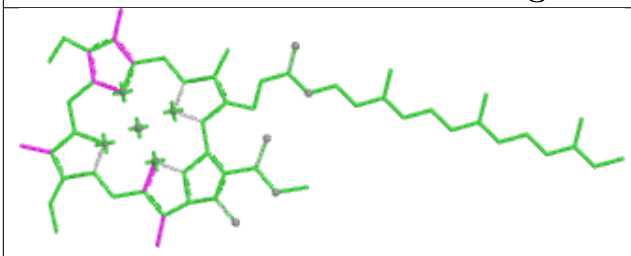
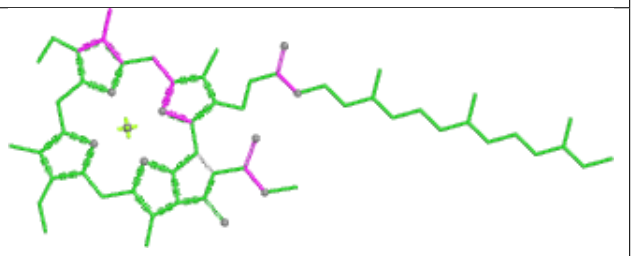
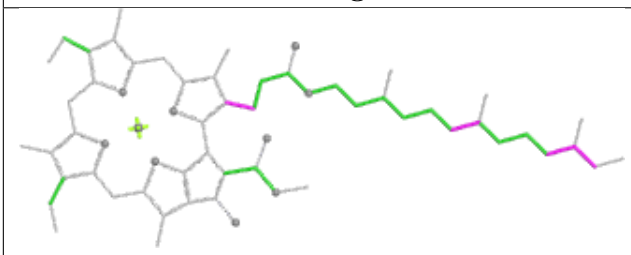
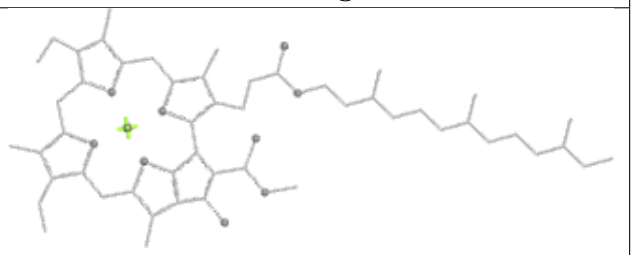


Torsions

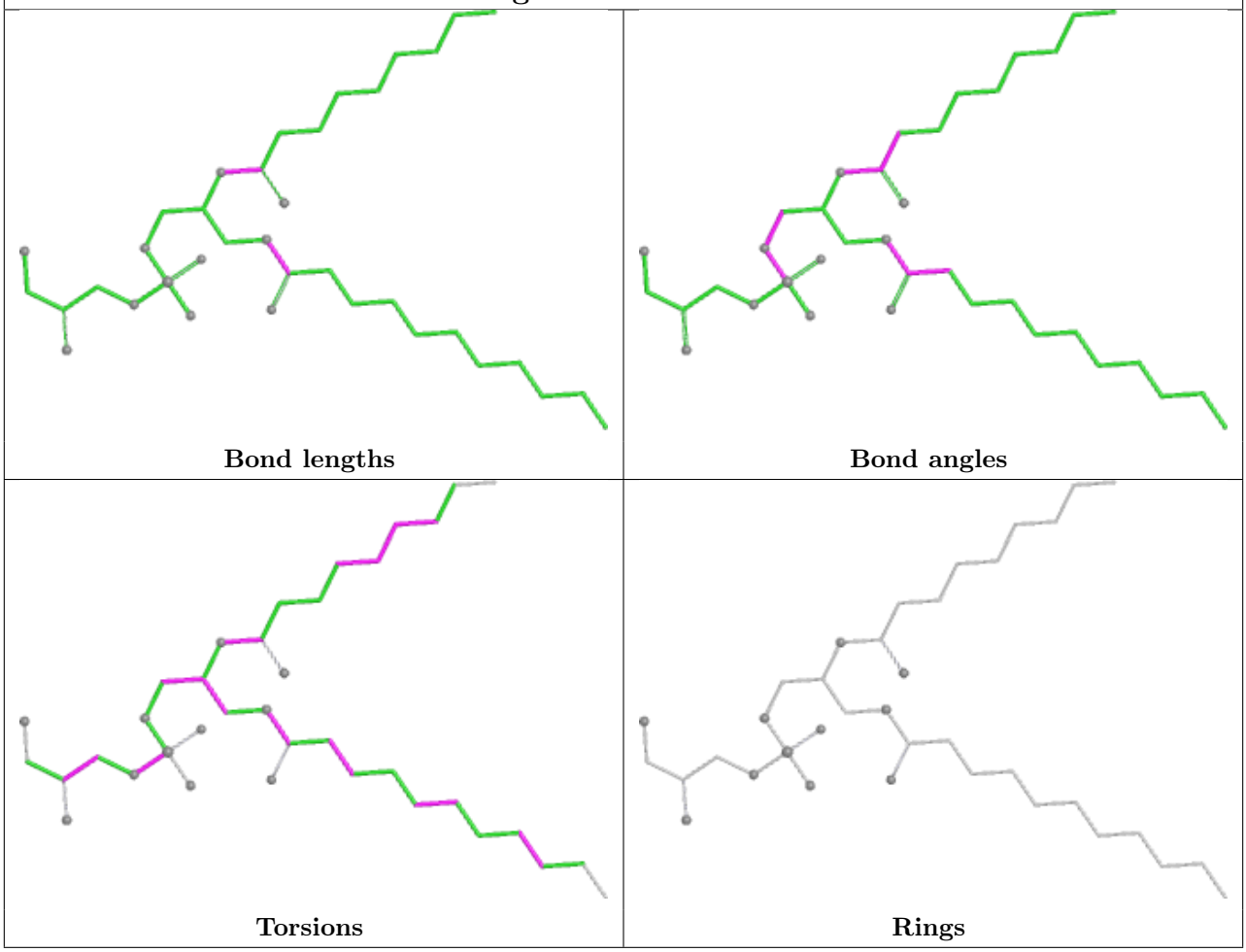


Rings

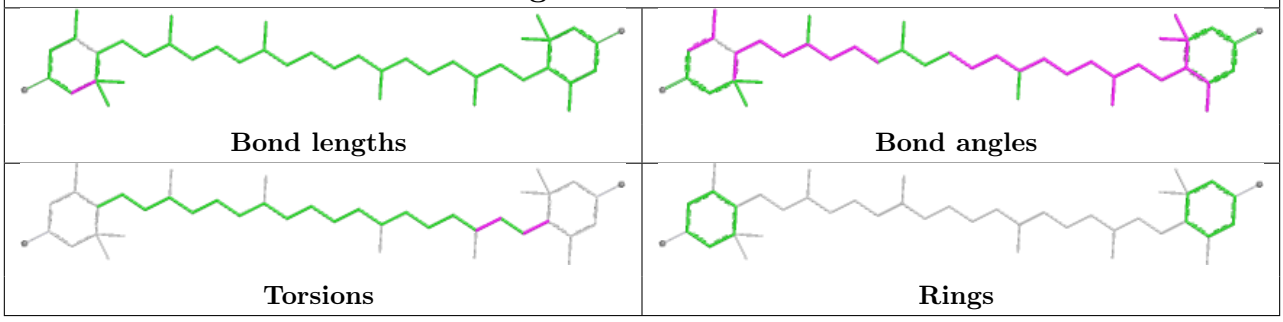
Ligand CLA B 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

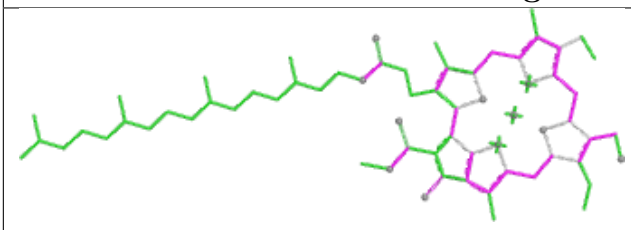
Ligand LHG 7 622



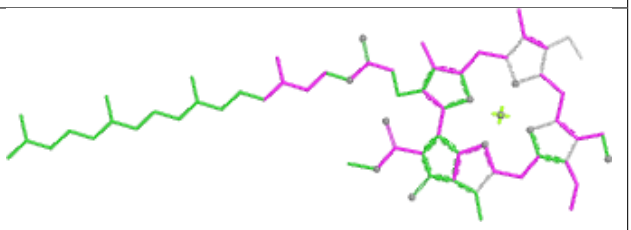
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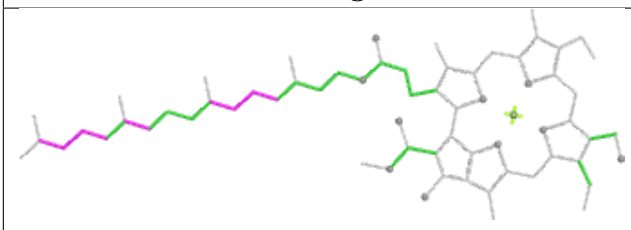
Ligand CHL V 601



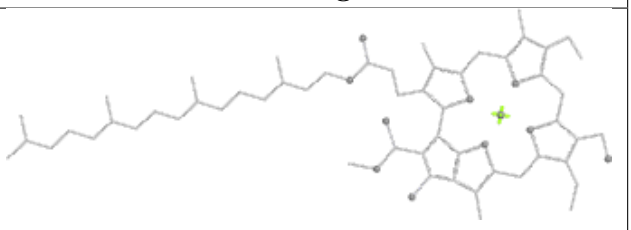
Bond lengths



Bond angles

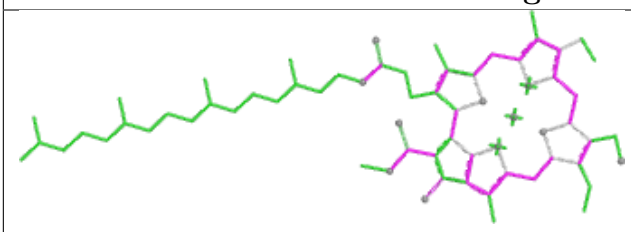


Torsions

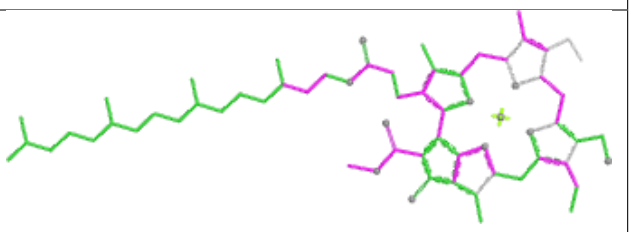


Rings

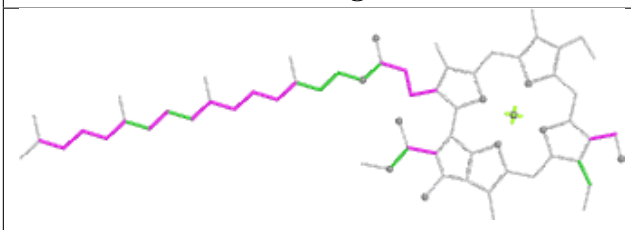
Ligand CHL Y 607



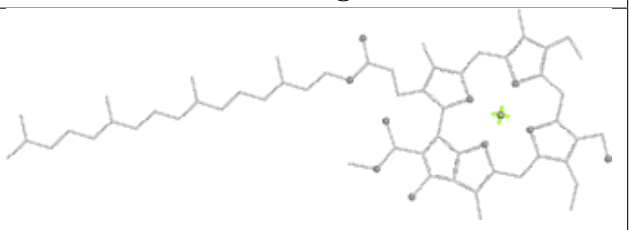
Bond lengths



Bond angles

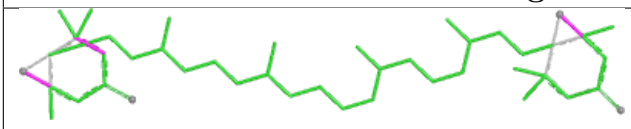


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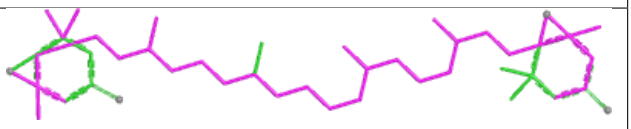


Rings

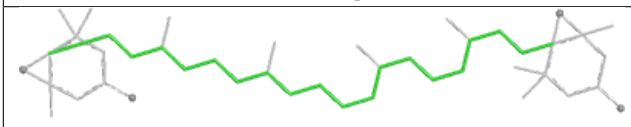
Ligand XAT 2 620



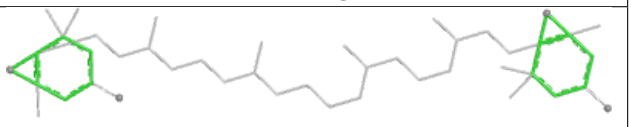
Bond lengths



Bond angles

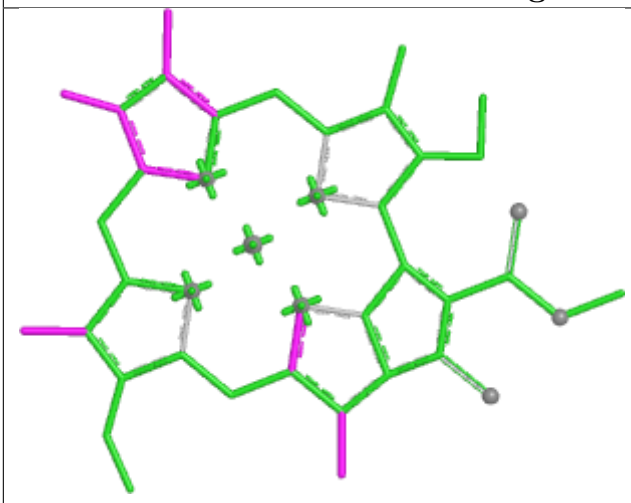


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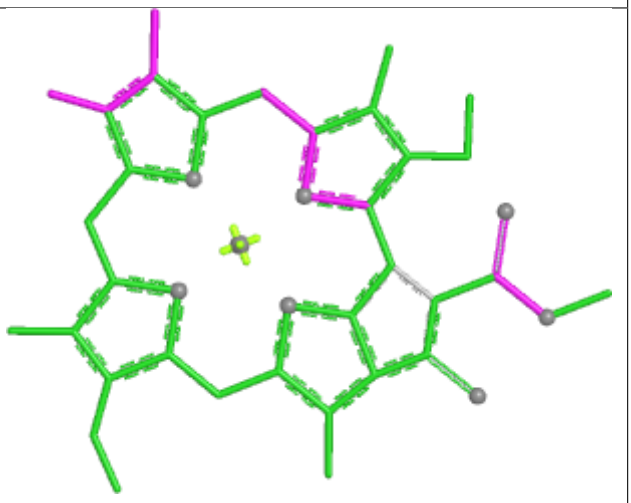


Rings

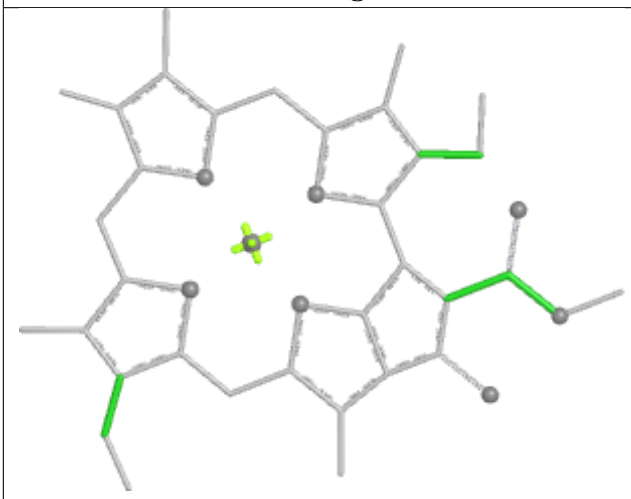
Ligand CLA 6 607



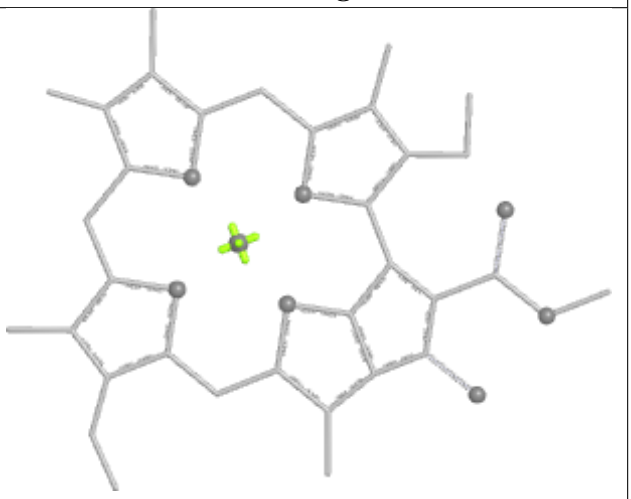
Bond lengths



Bond angles

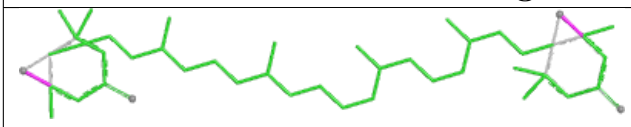


Torsions

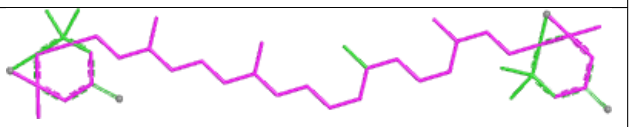


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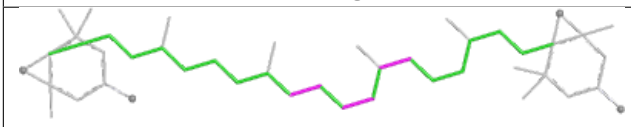
Ligand XAT Z 1622



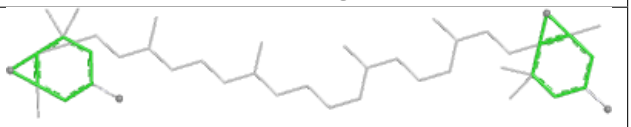
Bond lengths



Bond angles

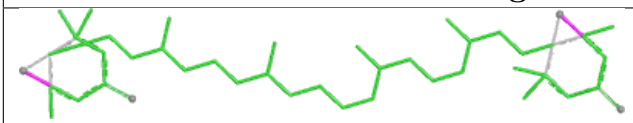


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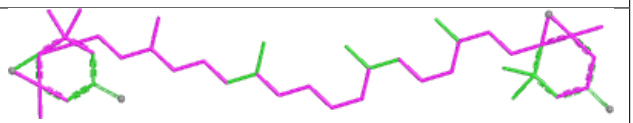


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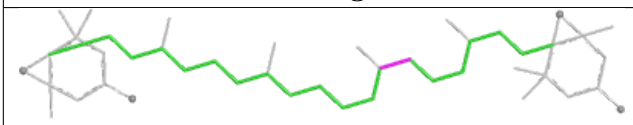
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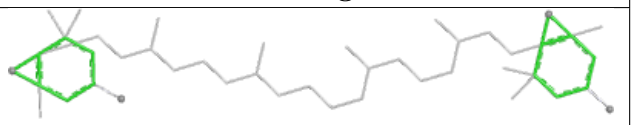
Bond lengths



Bond angles

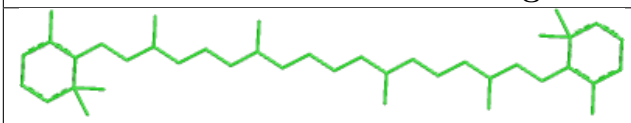


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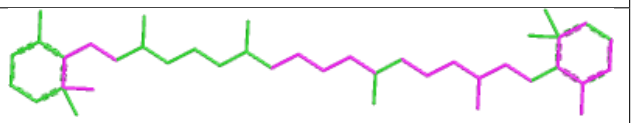


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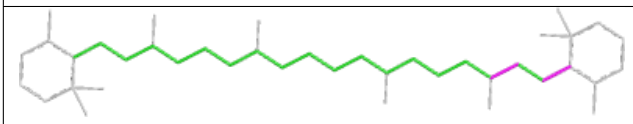
Ligand BCR B 848



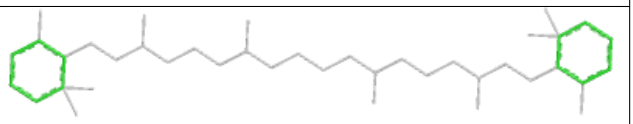
Bond lengths



Bond angles

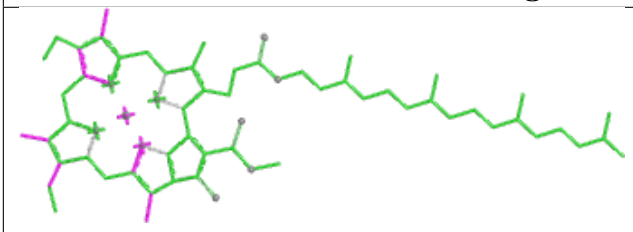


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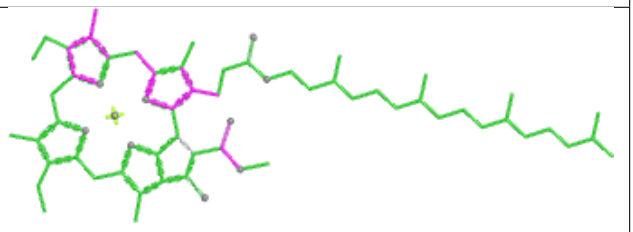


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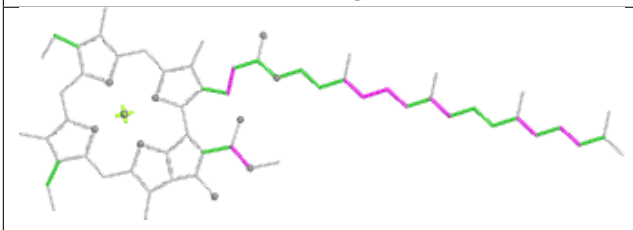
Ligand CLA A 802



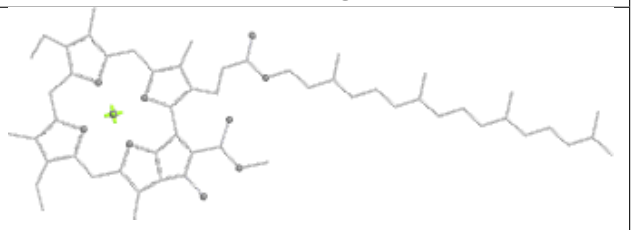
Bond lengths



Bond angles

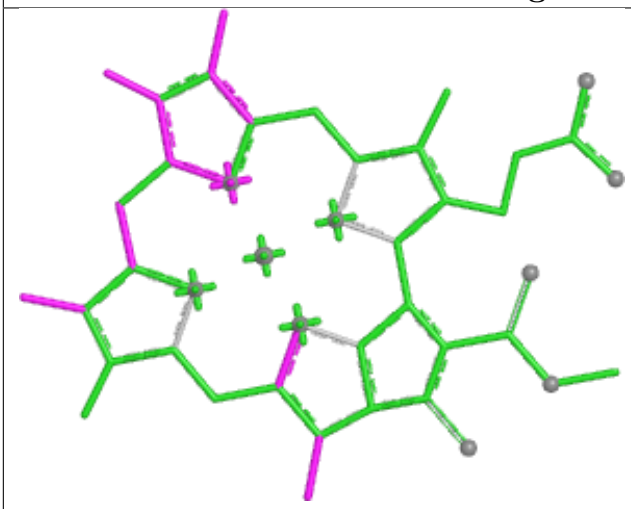


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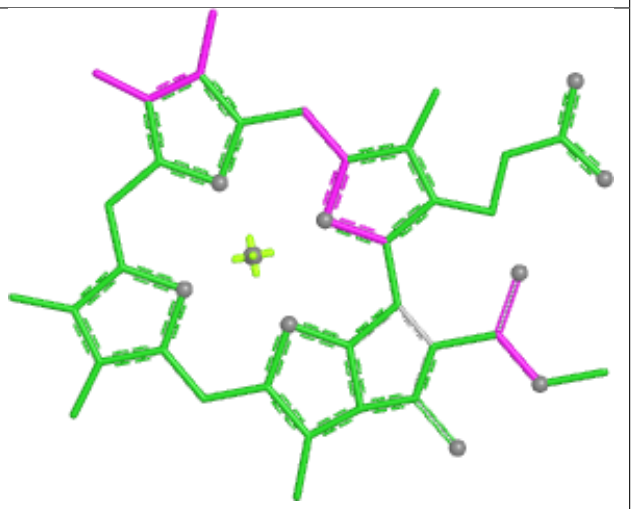


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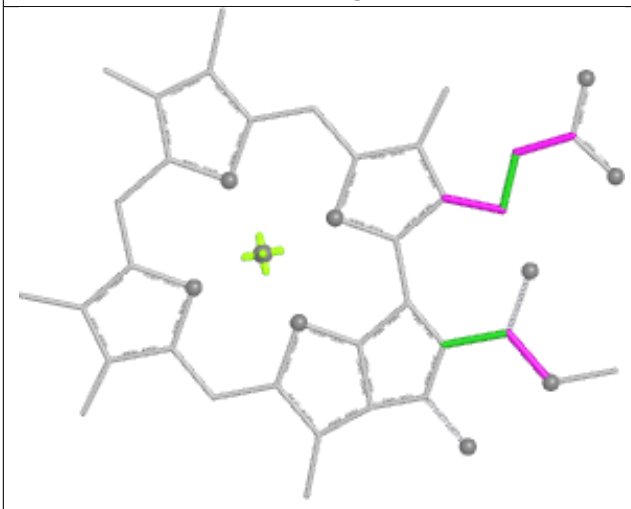
Ligand CLA 7 616



Bond lengths



Bond angles

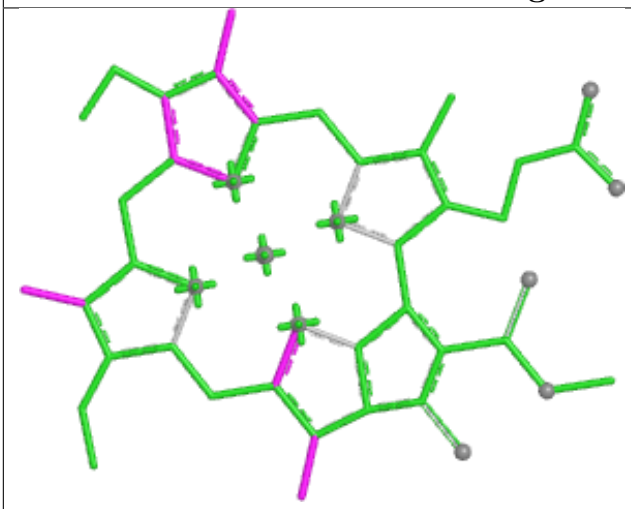


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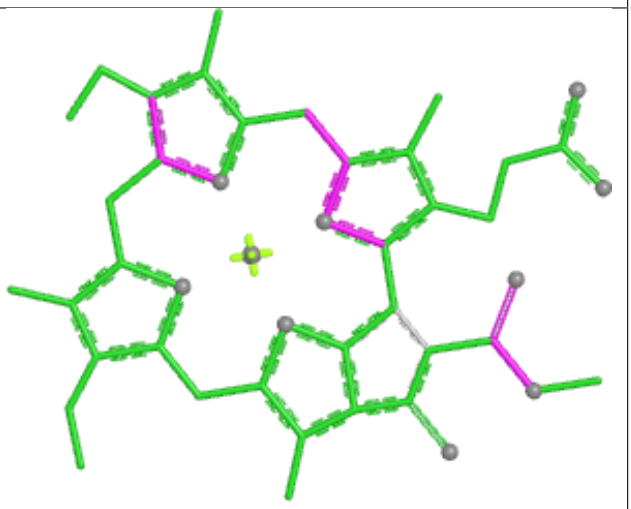


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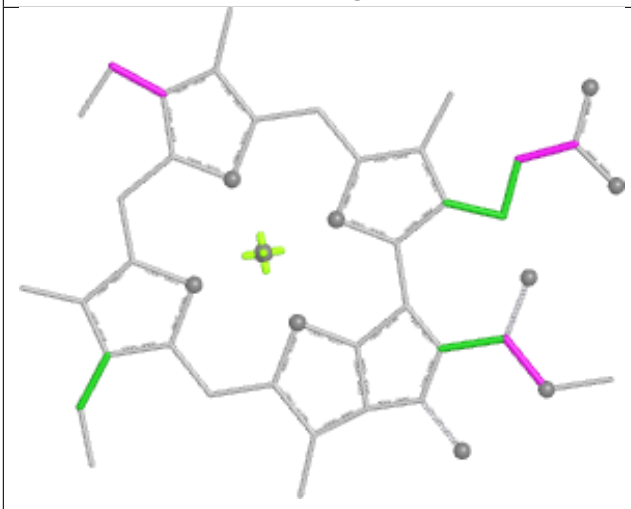
Ligand CLA 9 601



Bond lengths



Bond angles

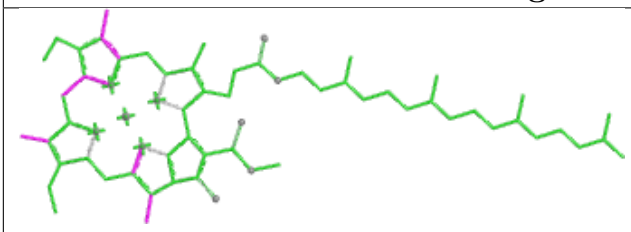


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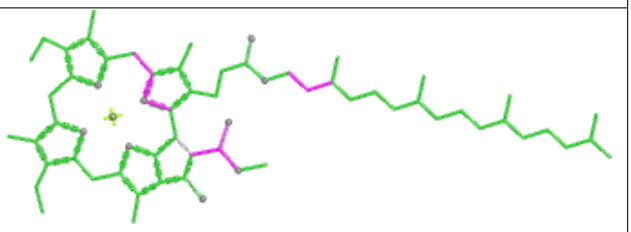


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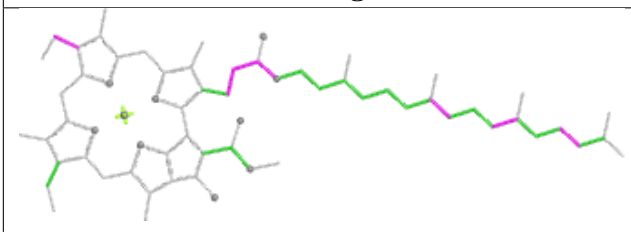
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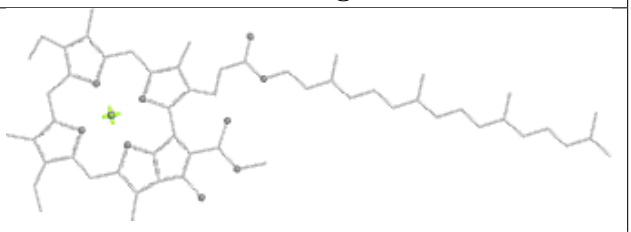
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Bond angles

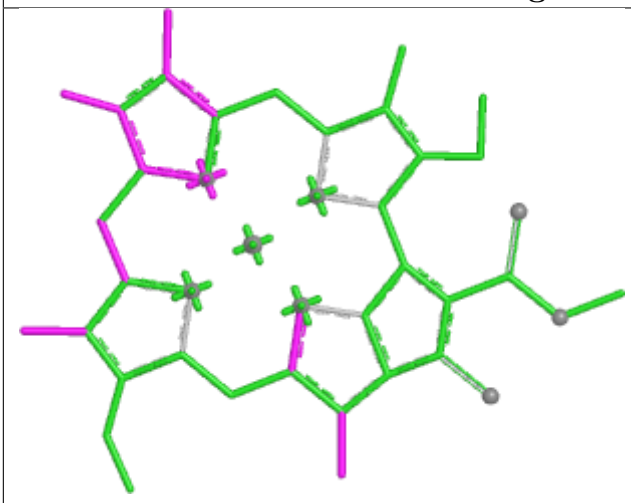


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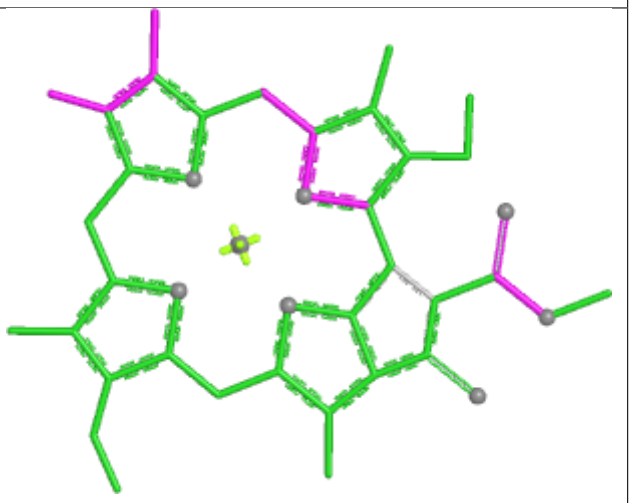


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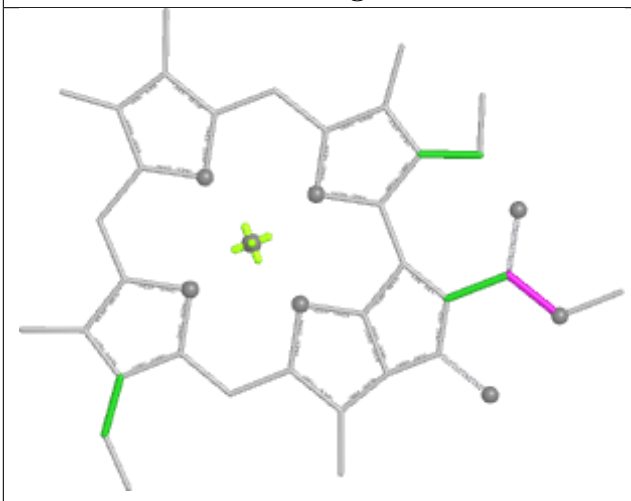
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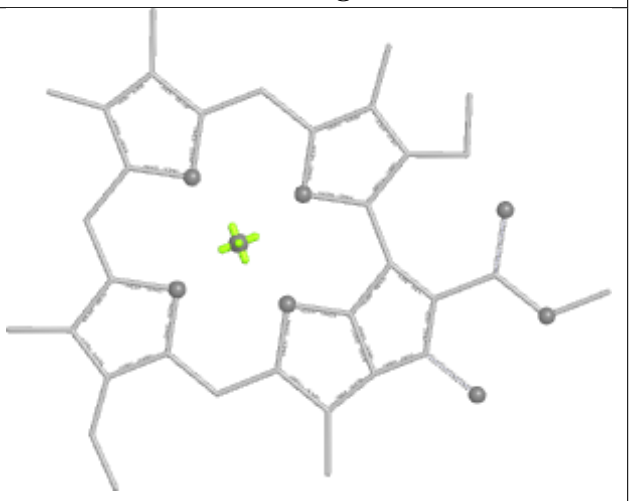
Bond lengths



Bond angles

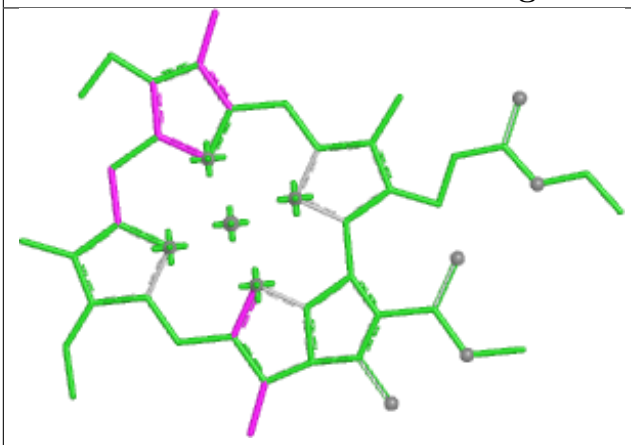


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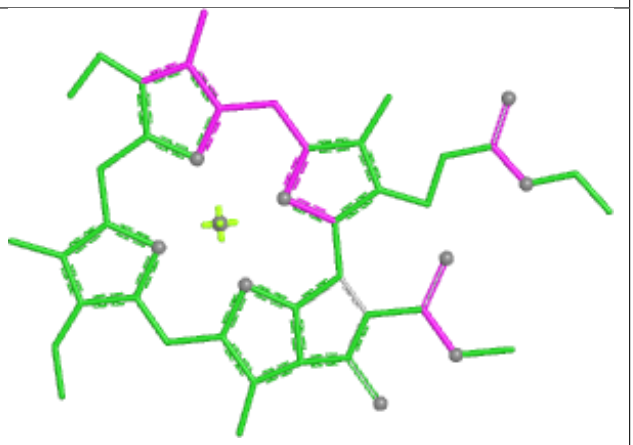


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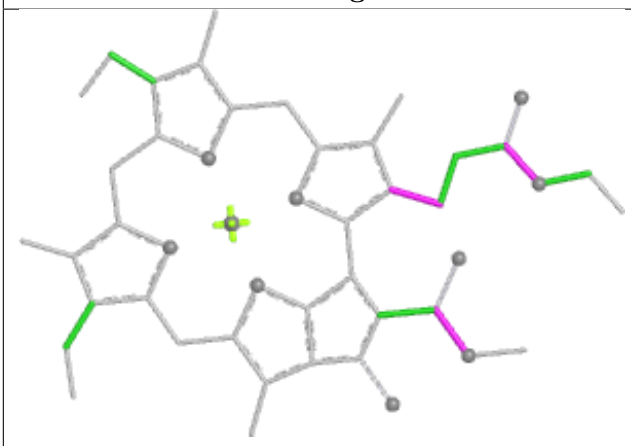
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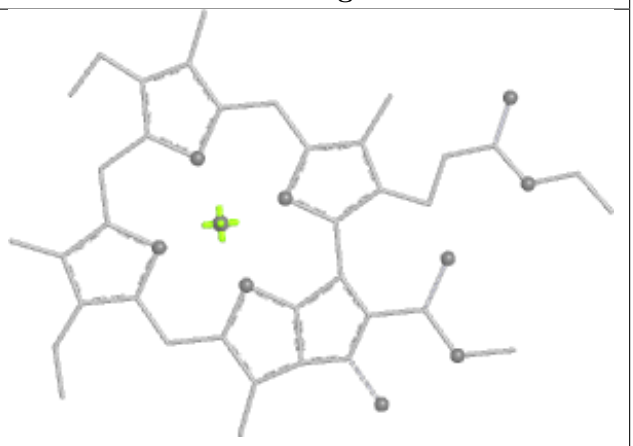
Bond lengths



Bond angles

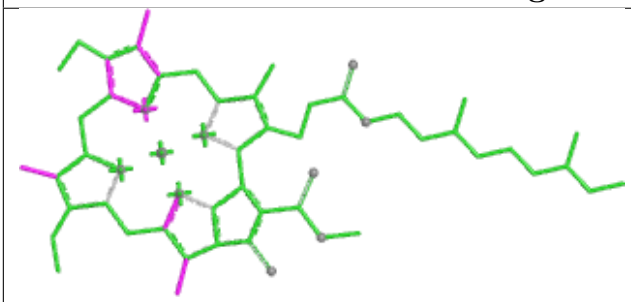


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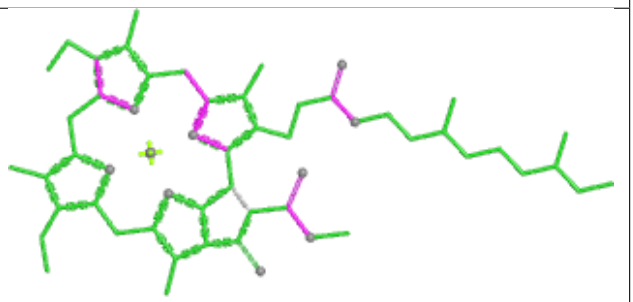


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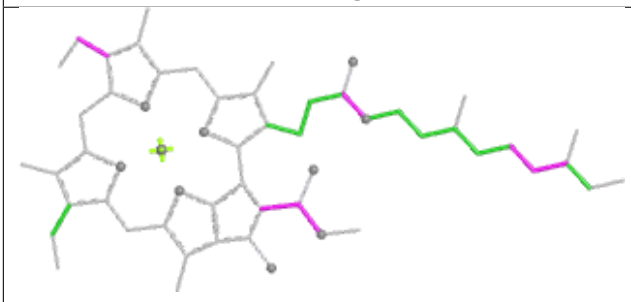
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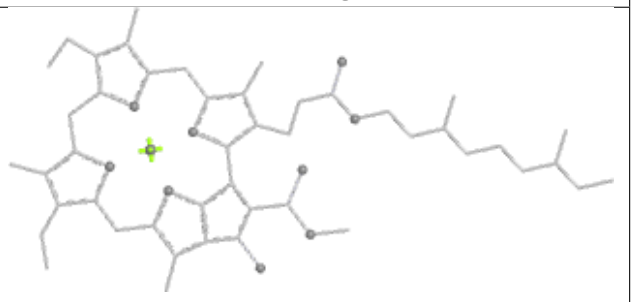
Bond lengths



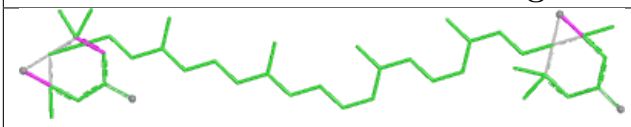
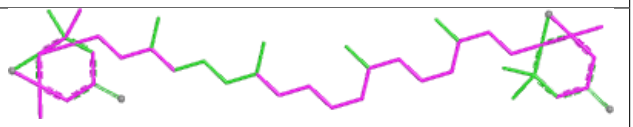
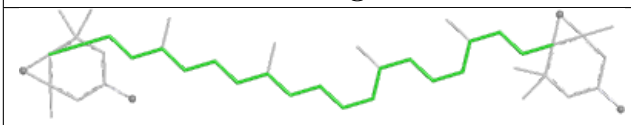
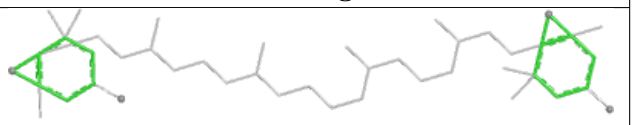
Bond angles

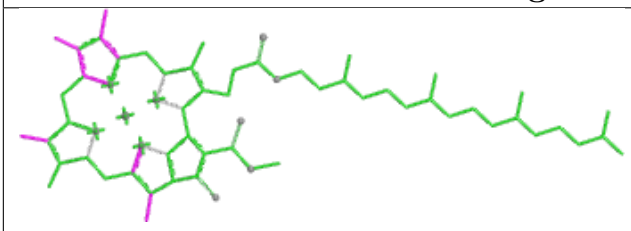
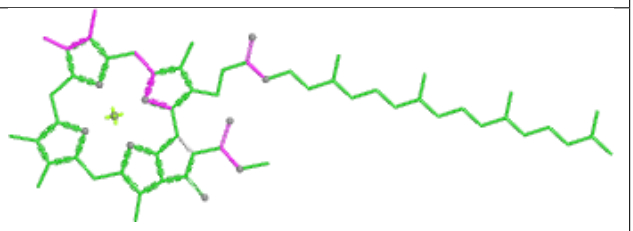
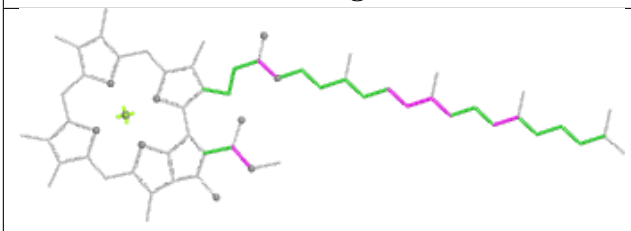
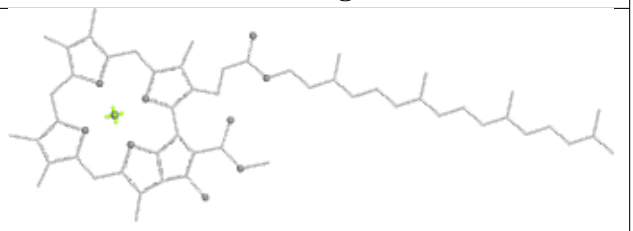


Torsions

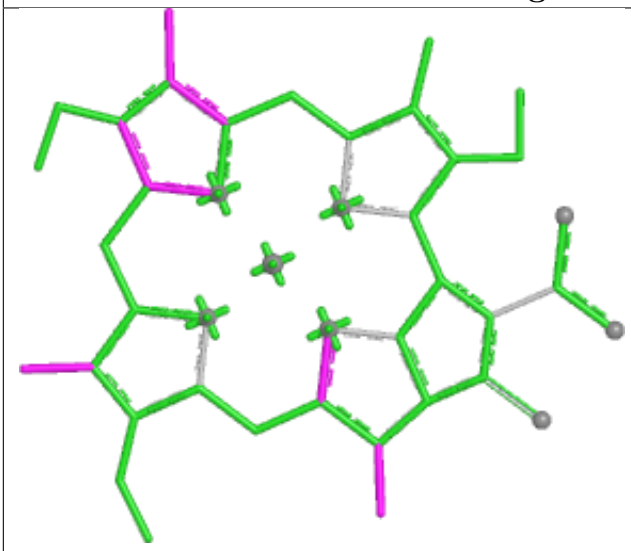


Rings

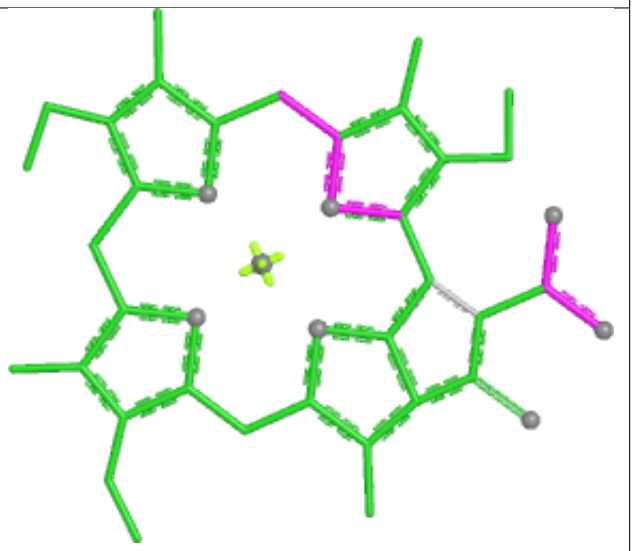
Ligand XAT 6 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

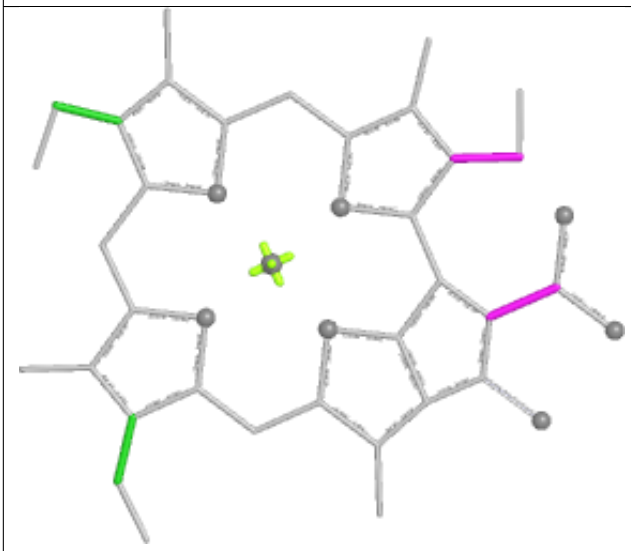
Ligand CLA 6 612



Bond lengths



Bond angles

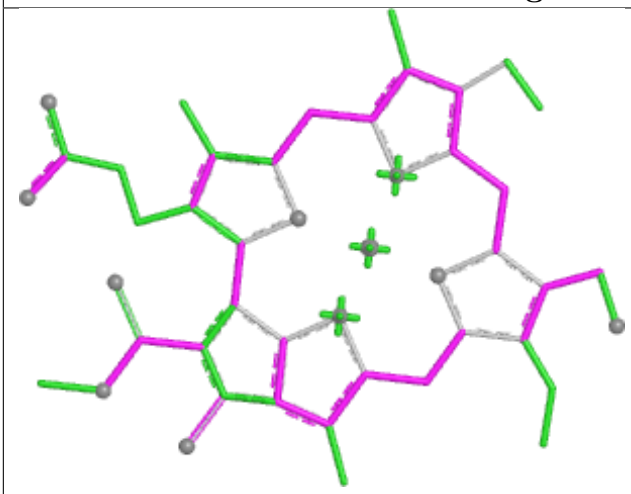


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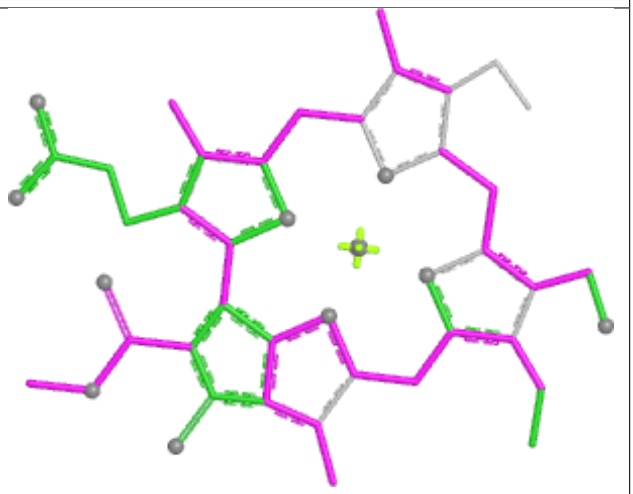


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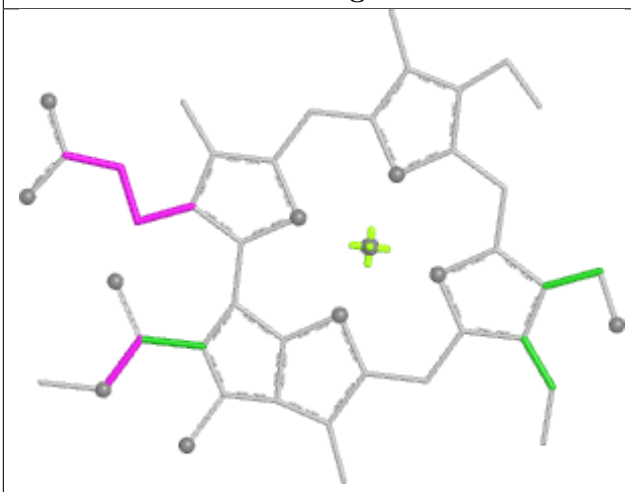
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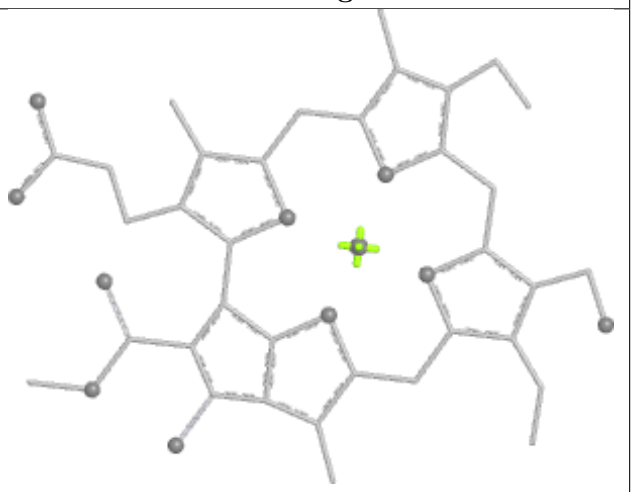
Bond lengths



Bond angles

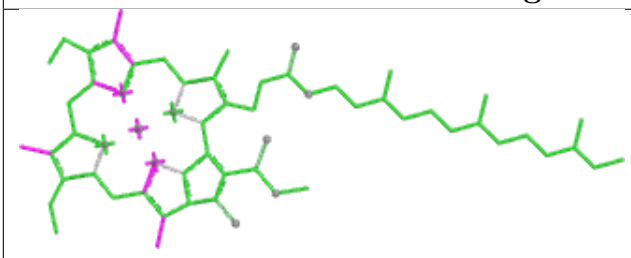


Torsions

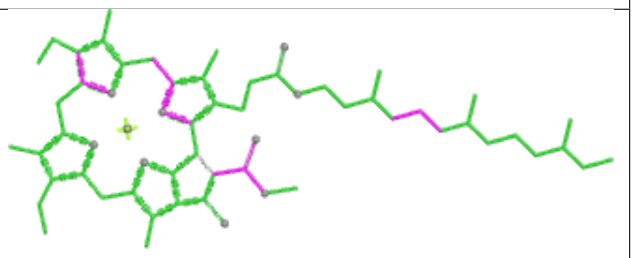


Rings

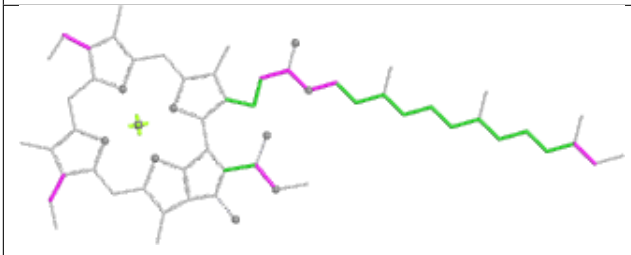
Ligand CLA A 835



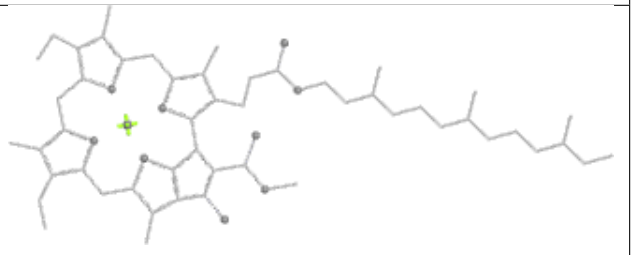
Bond lengths



Bond angles

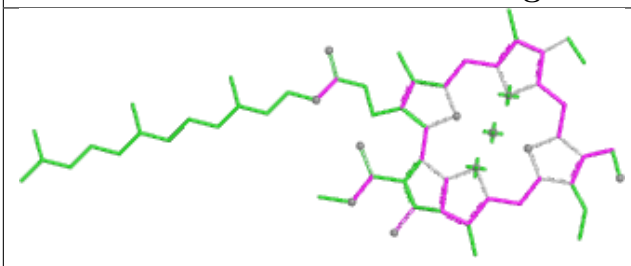


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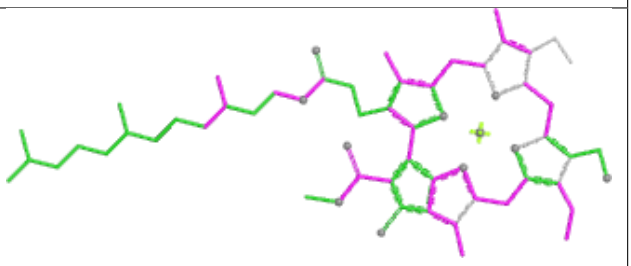


Rings

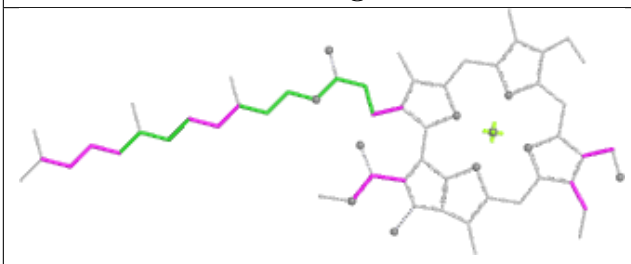
Ligand CHL V 609



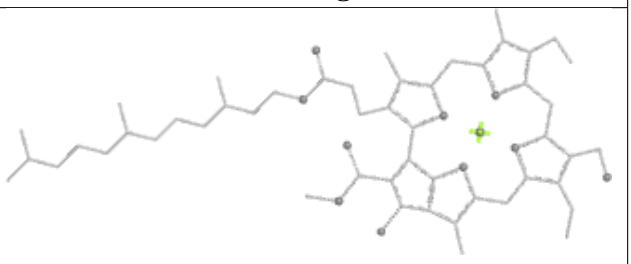
Bond lengths



Bond angles

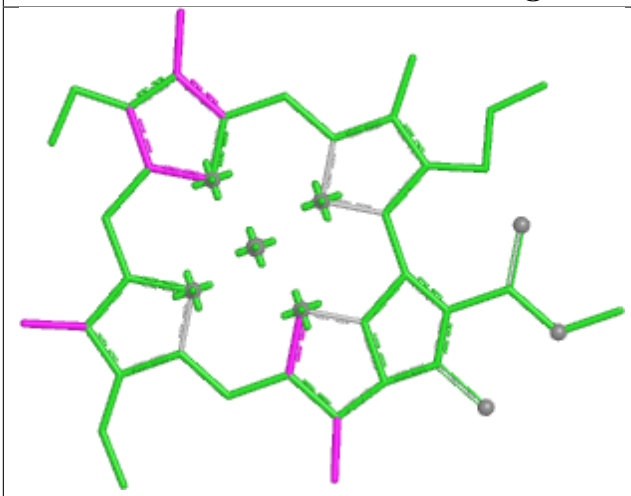


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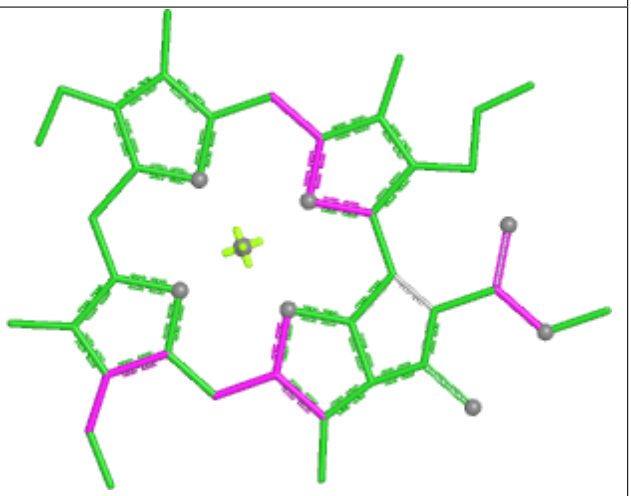


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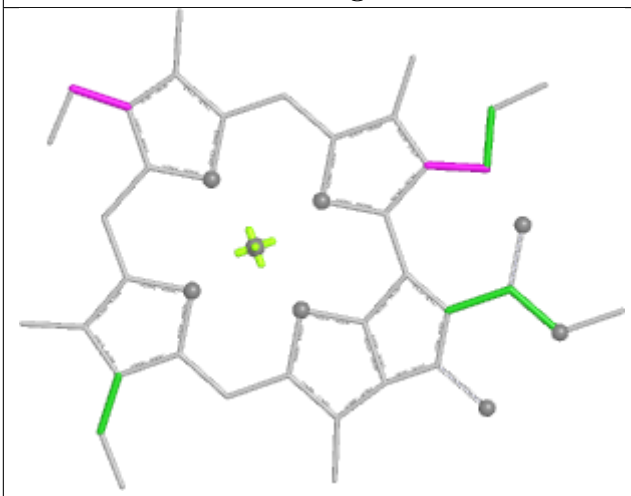
Ligand CLA B 830



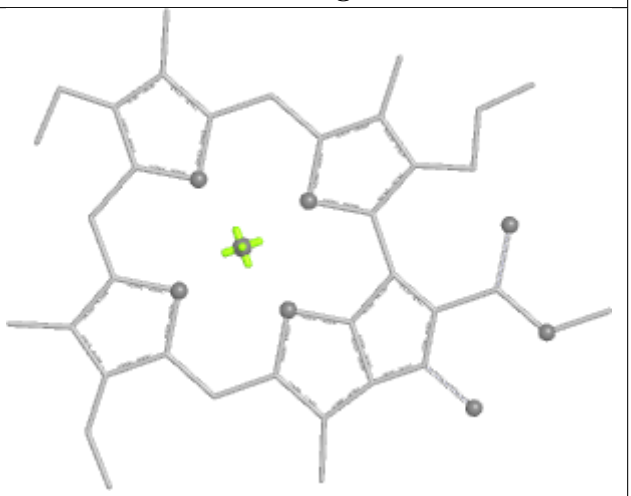
Bond lengths



Bond angles

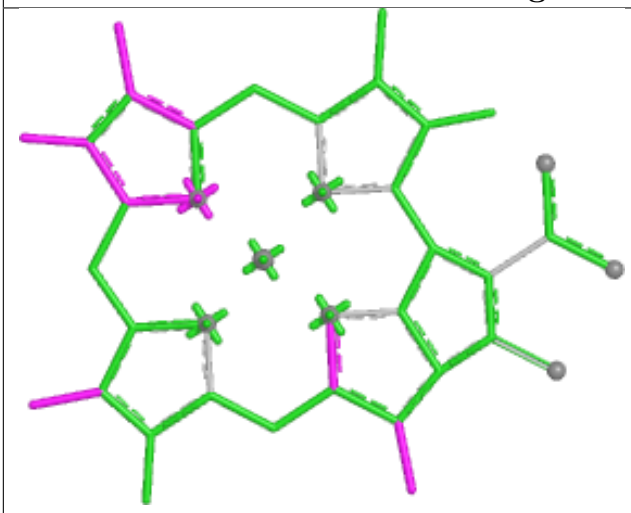


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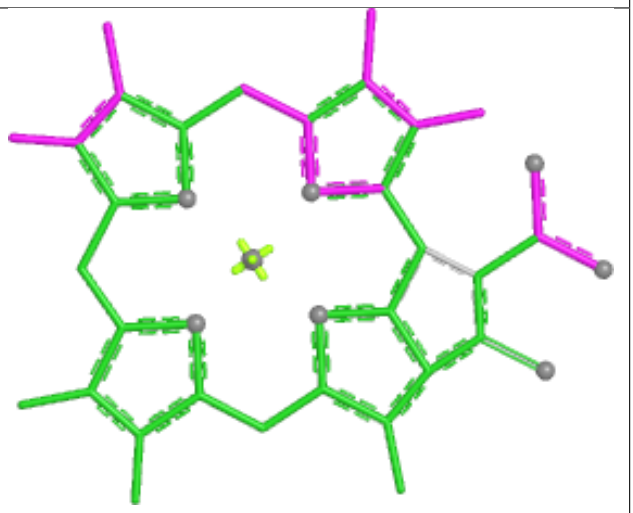


Rings

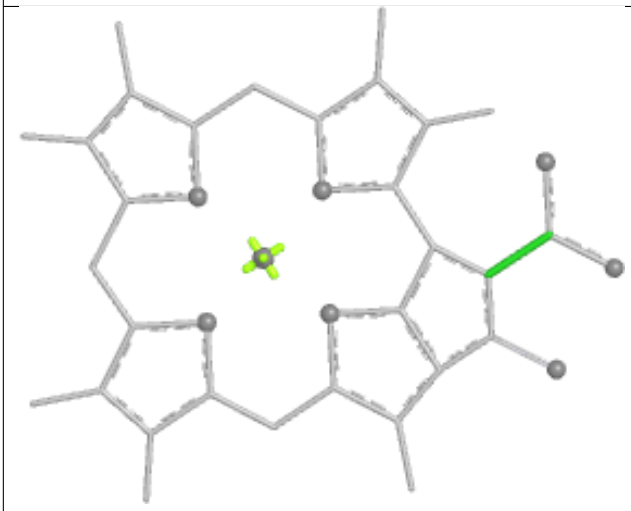
Ligand CLA a 611



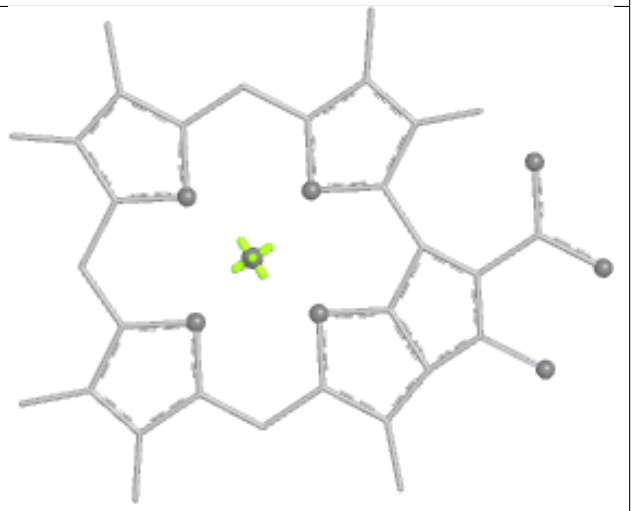
Bond lengths



Bond angles

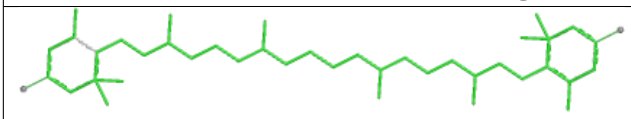


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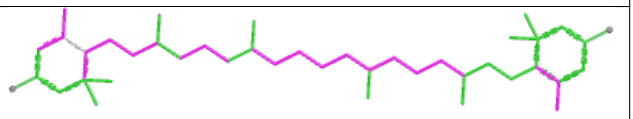


Rings

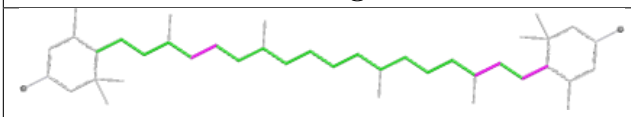
Ligand LUT U 1621



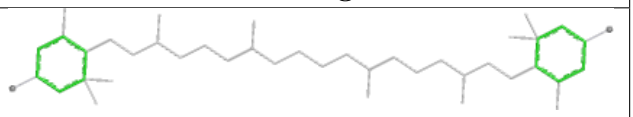
Bond lengths



Bond angles

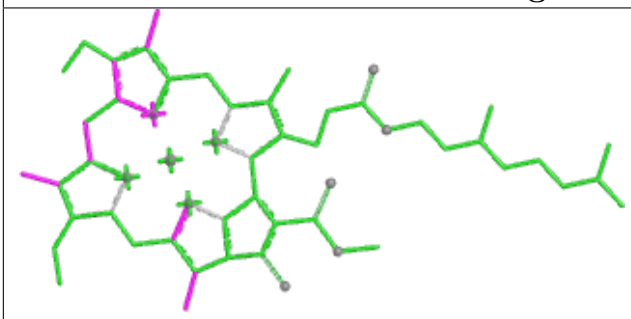


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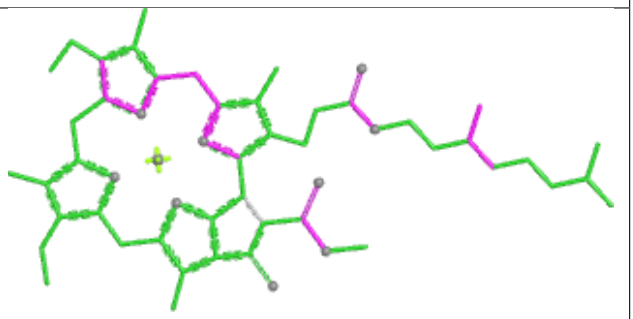


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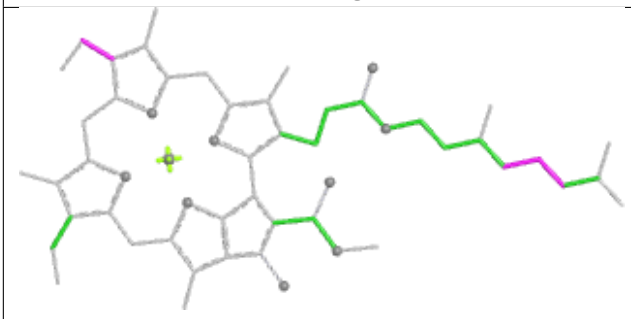
Ligand CLA 2 610



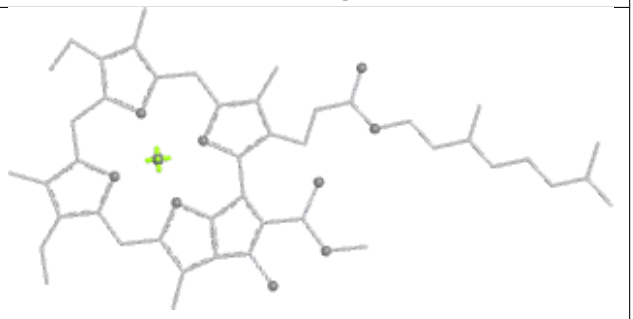
Bond lengths



Bond angles

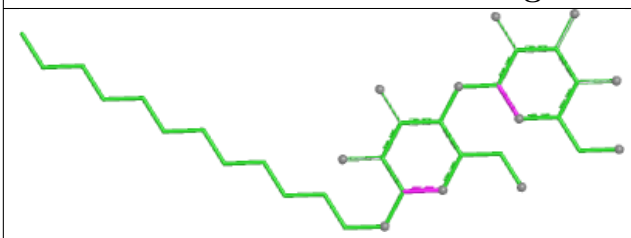


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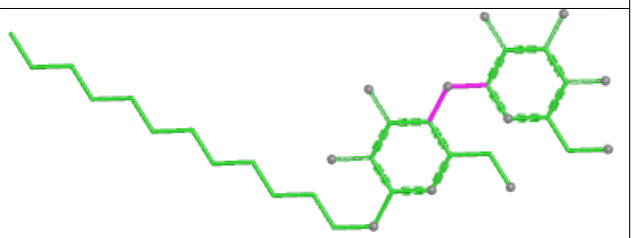


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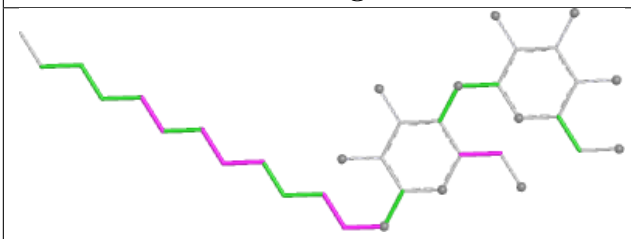
Ligand LMU 1 621



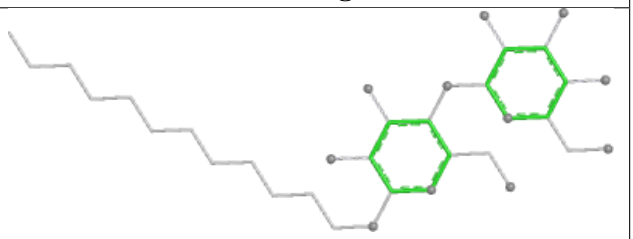
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Bond angles

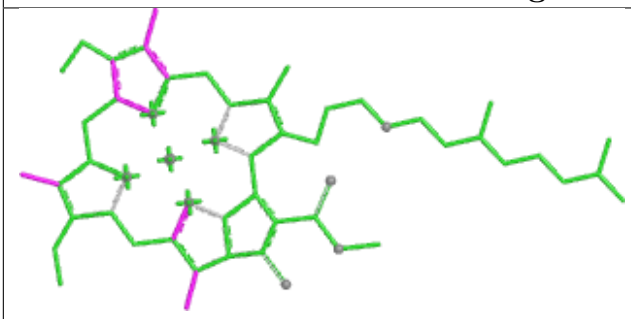


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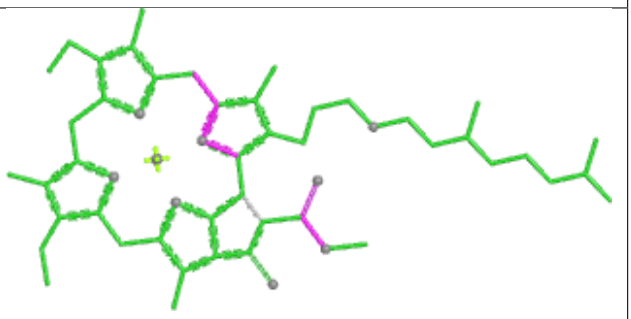


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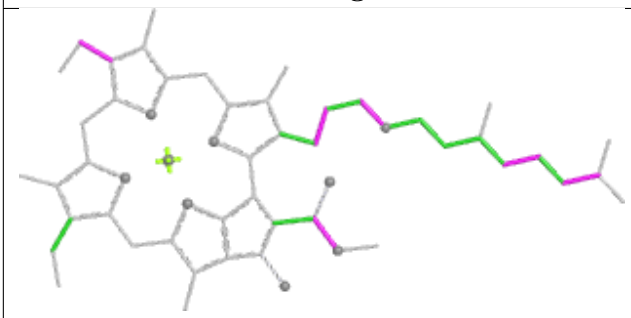
Ligand CLA a 603



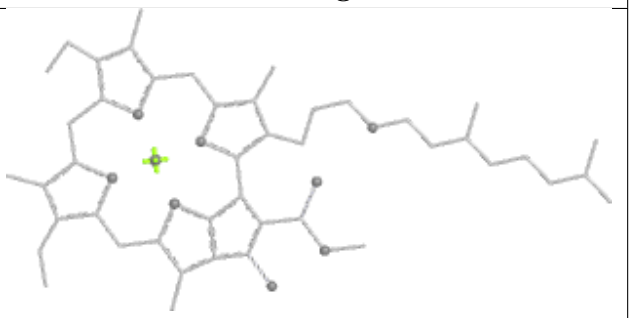
Bond lengths



Bond angles

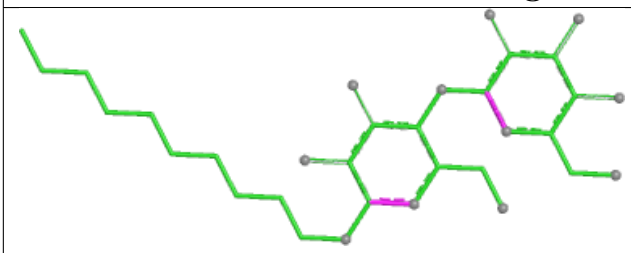


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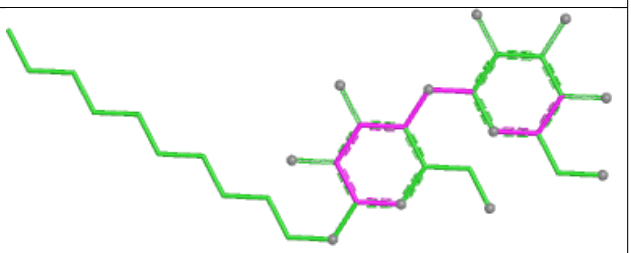


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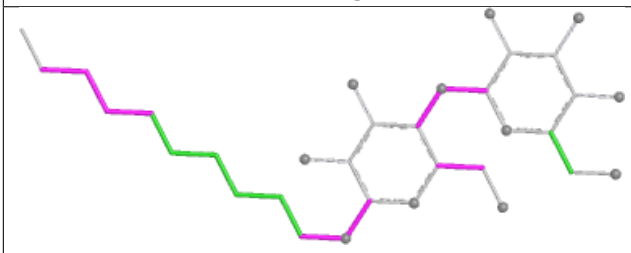
Ligand LMU 5 628



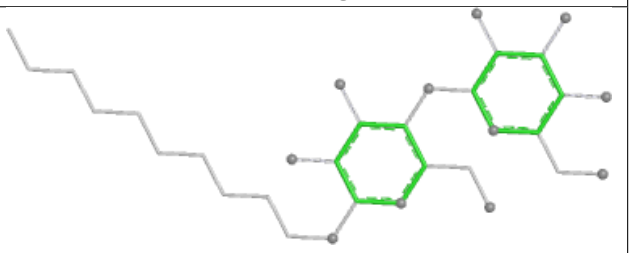
Bond lengths



Bond angles

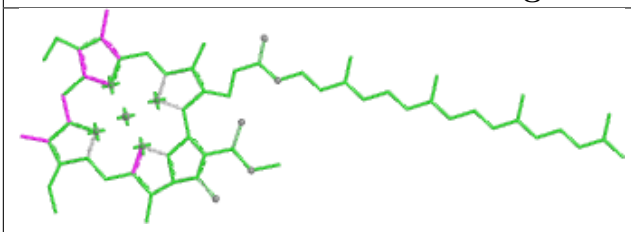


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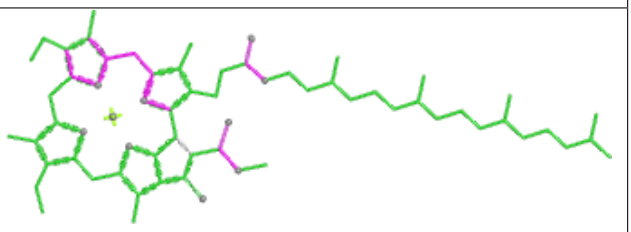


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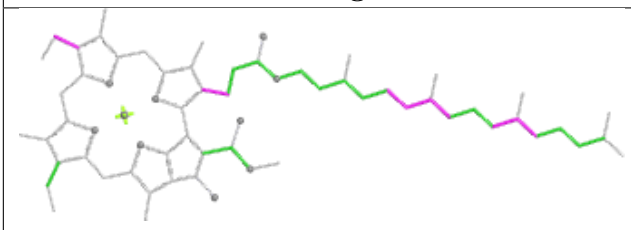
Ligand CLA X 610



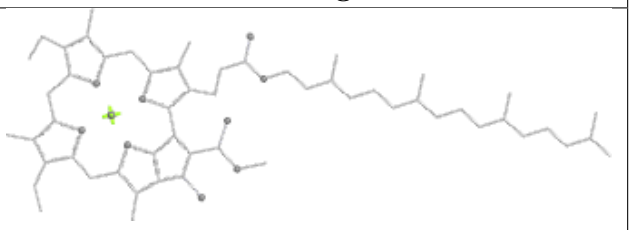
Bond lengths



Bond angles

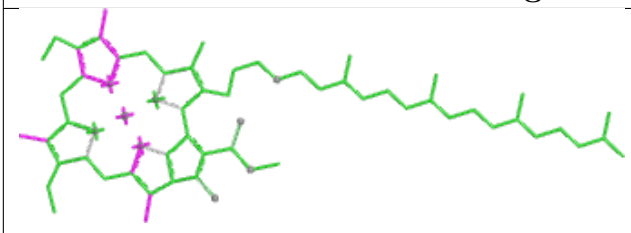


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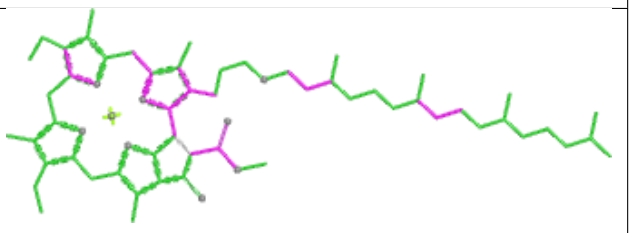


Rings

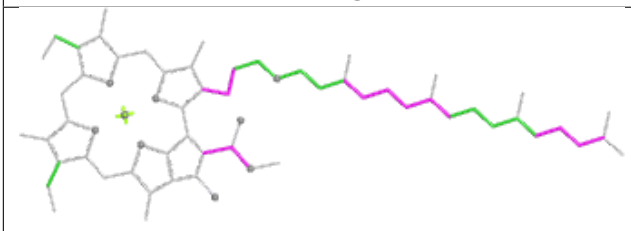
Ligand CLA B 810



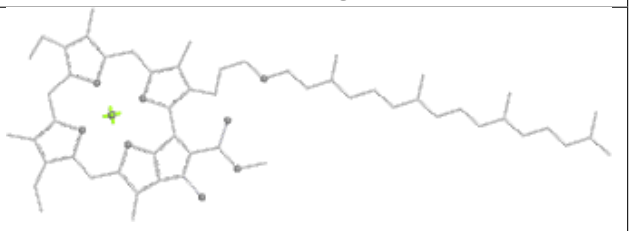
Bond lengths



Bond angles

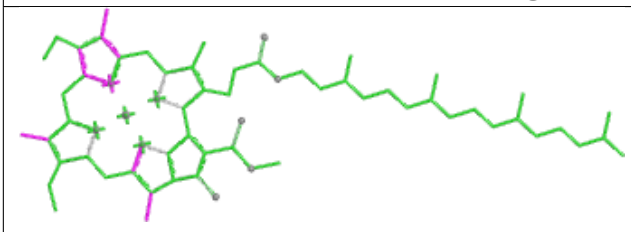


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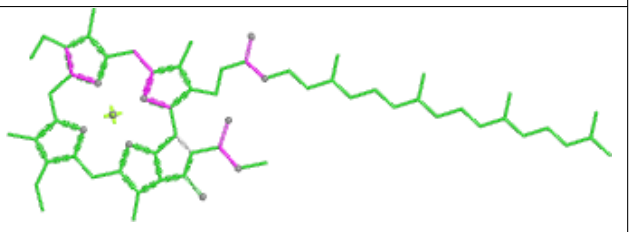


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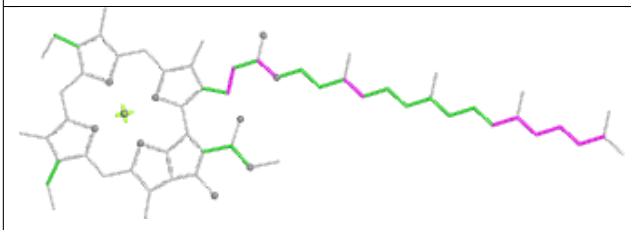
Ligand CLA B 831



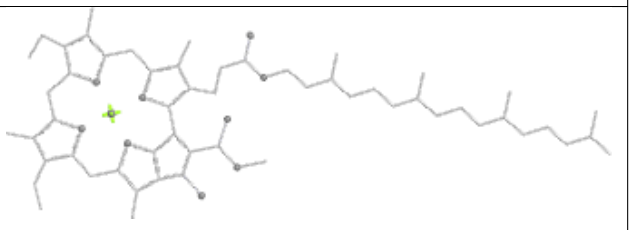
Bond lengths



Bond angles

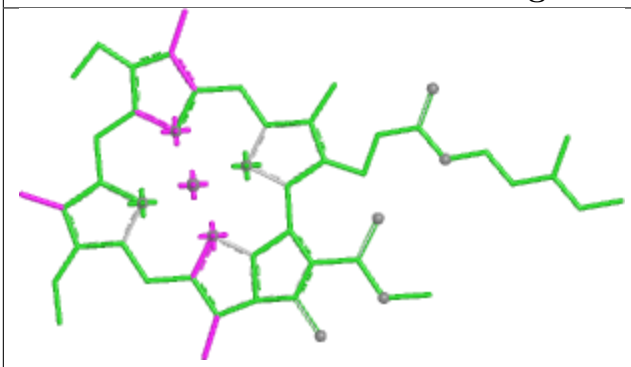


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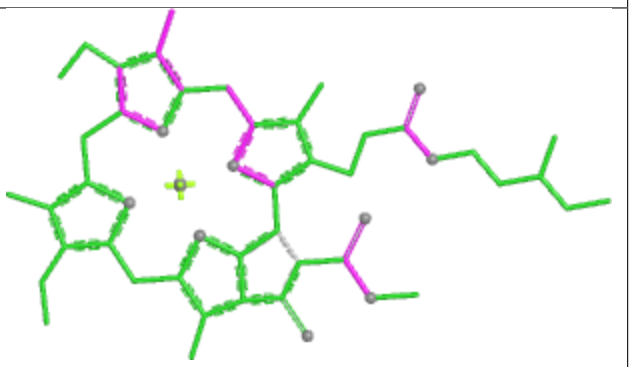


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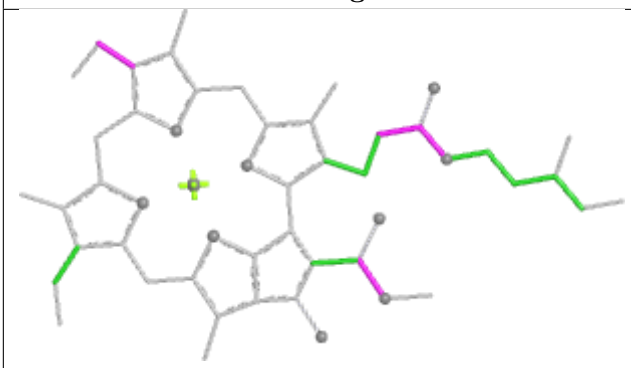
Ligand CLA 8 608



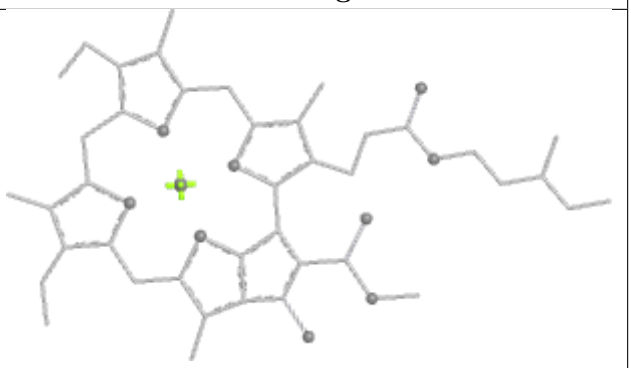
Bond lengths



Bond angles

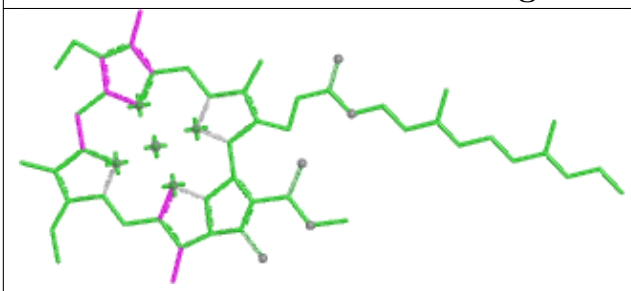


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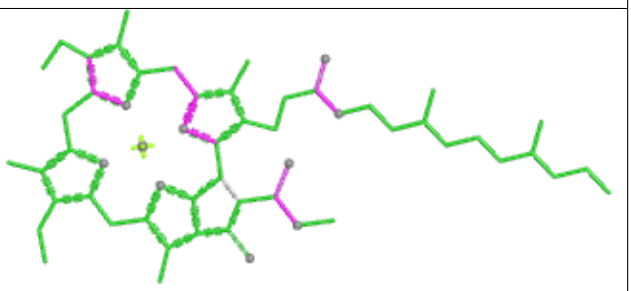


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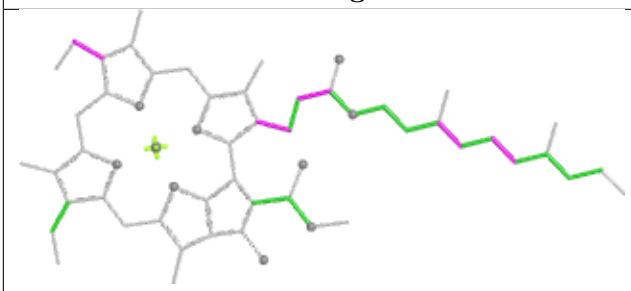
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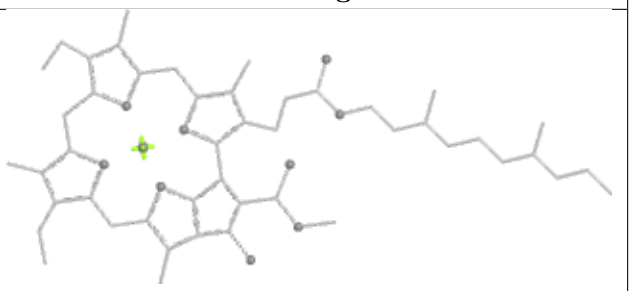
Bond lengths



Bond angles

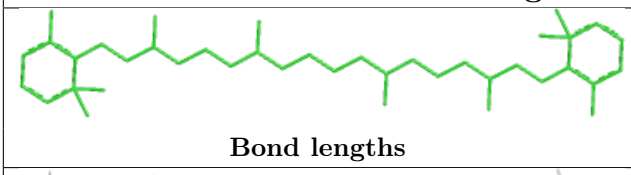


Torsions

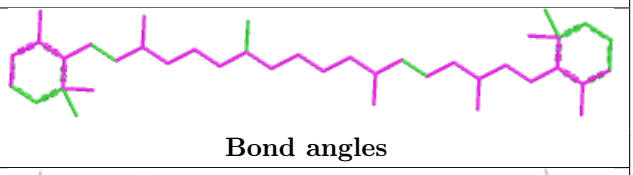


Rings

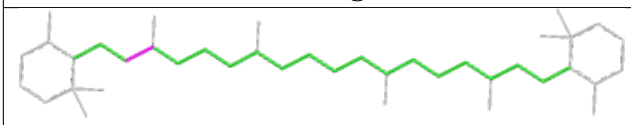
Ligand BCR L 305



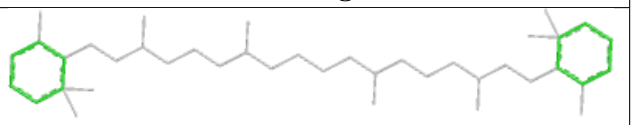
Bond lengths



Bond angles

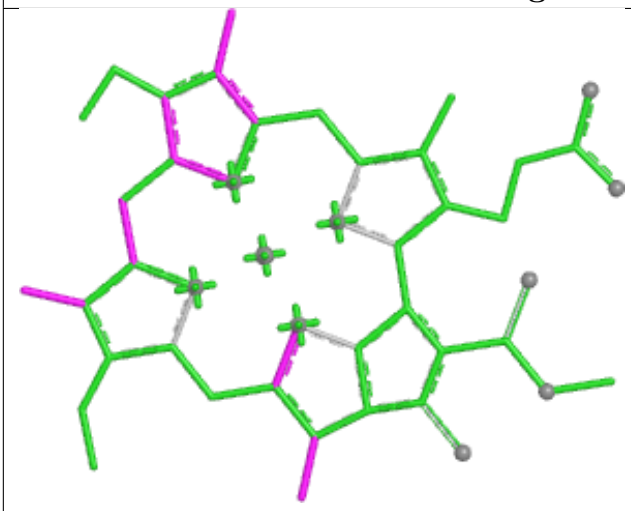


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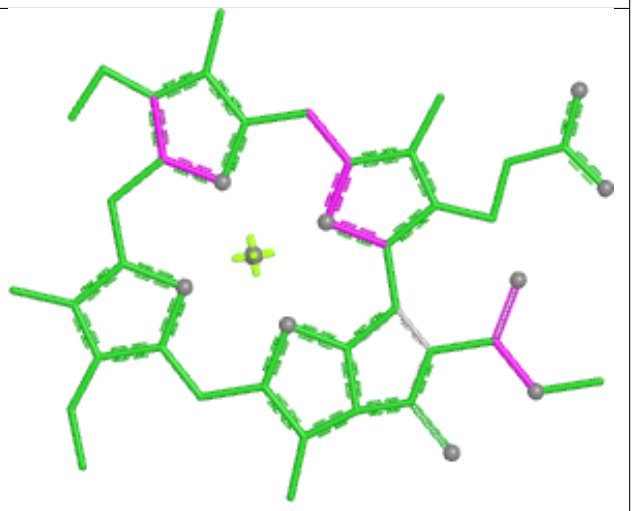


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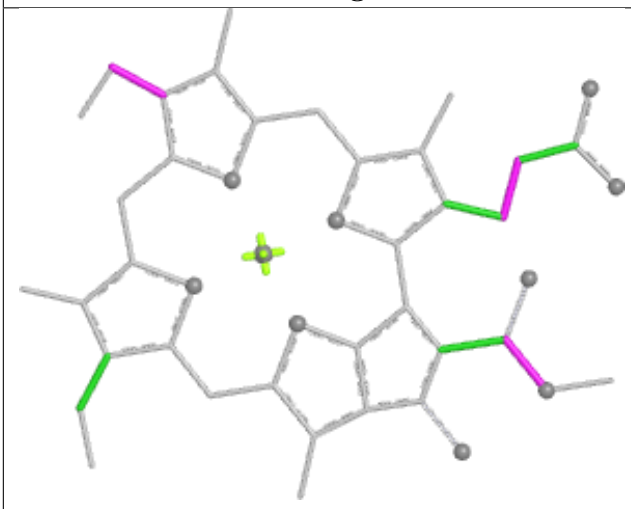
Ligand CLA 9 614



Bond lengths



Bond angles

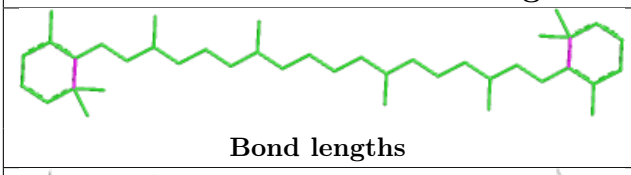


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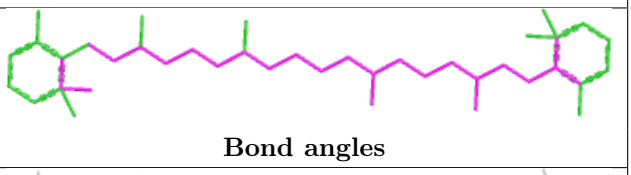


Rings

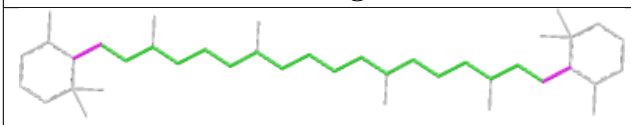
Ligand BCR B 843



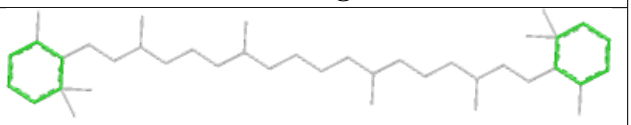
Bond lengths



Bond angles

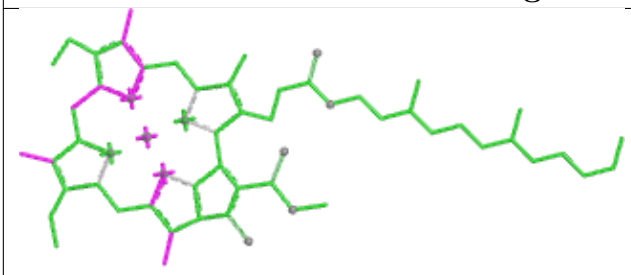


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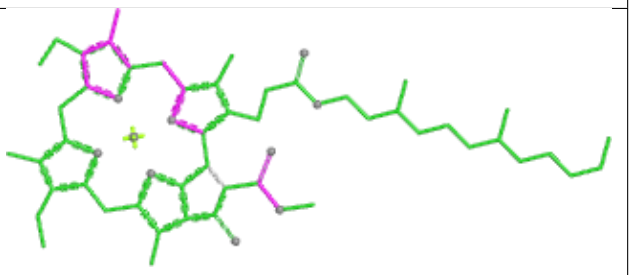


Rings

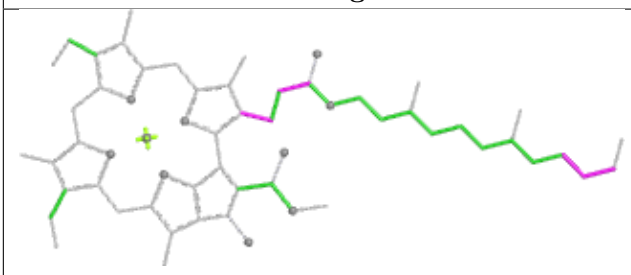
Ligand CLA A 819



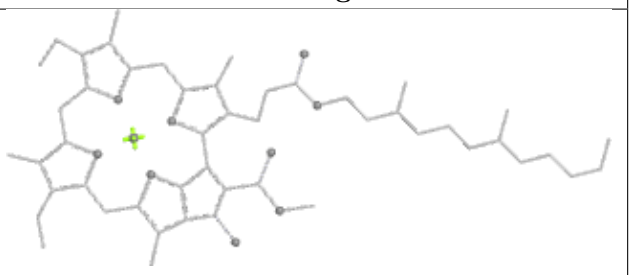
Bond lengths



Bond angles

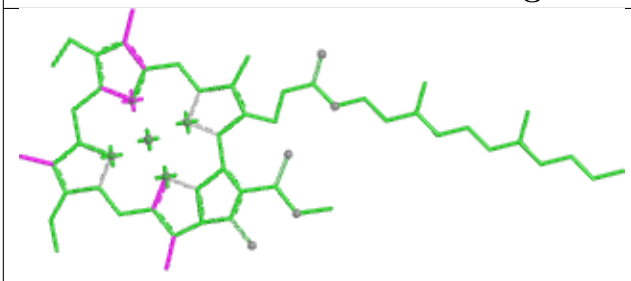


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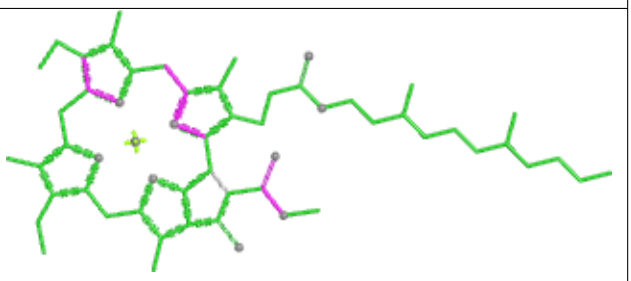


Rings

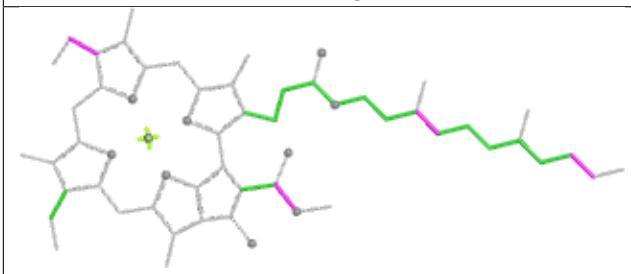
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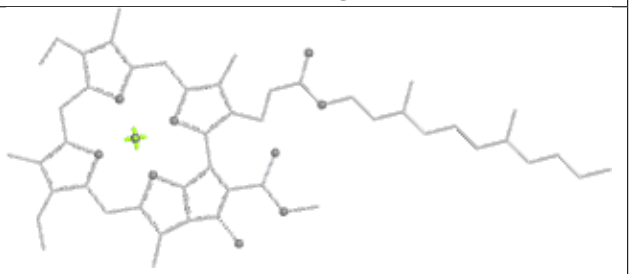
Bond lengths



Bond angles

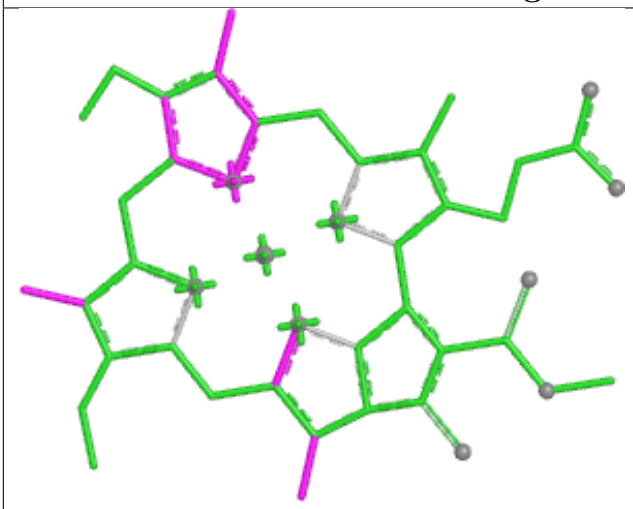


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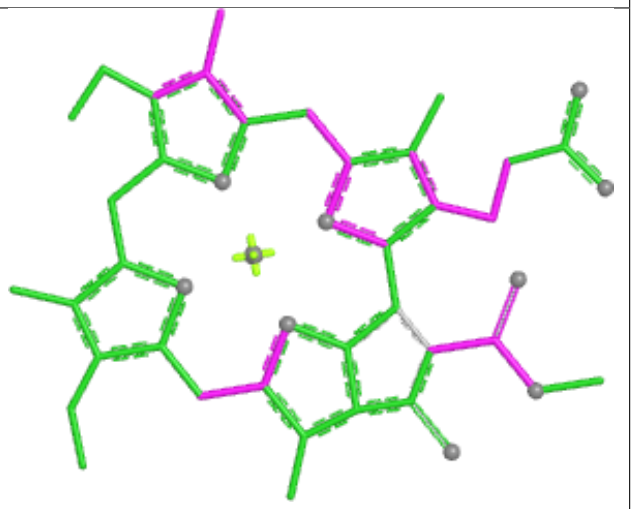


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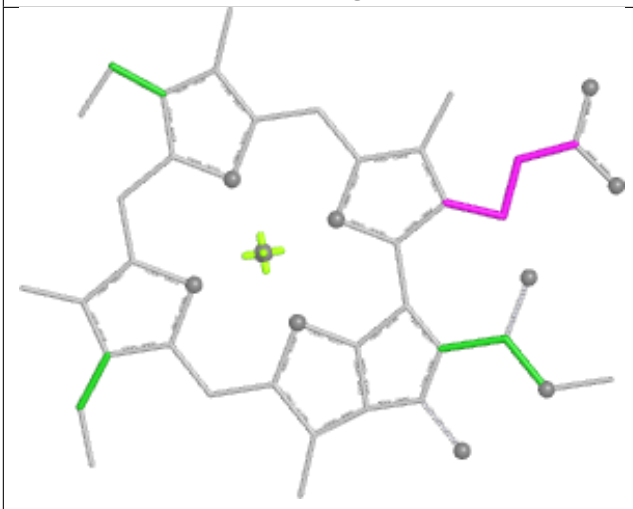
Ligand CLA A 833



Bond lengths



Bond angles

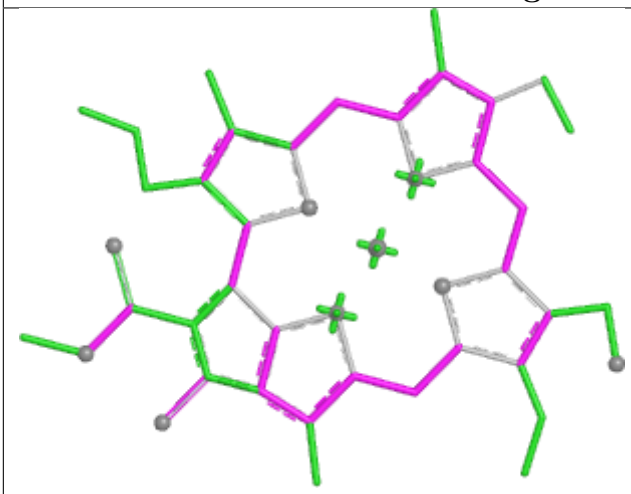


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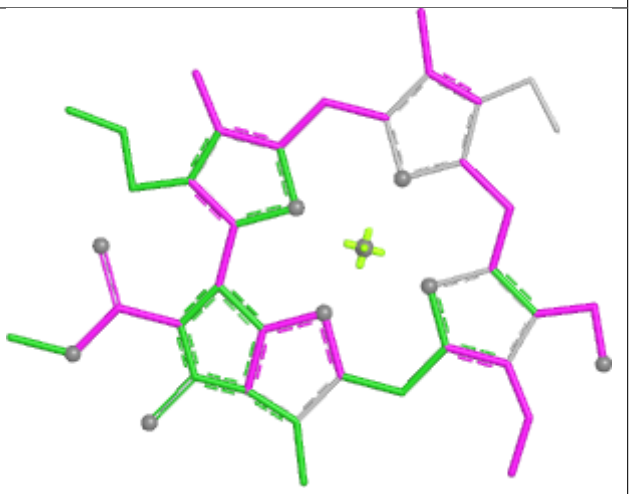


Rings

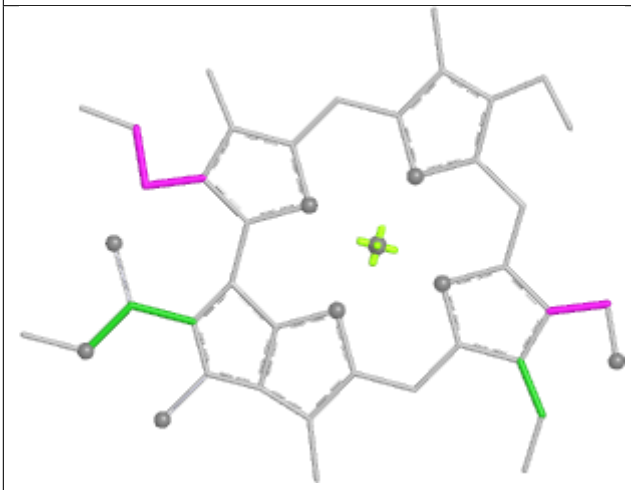
Ligand CHL X 606



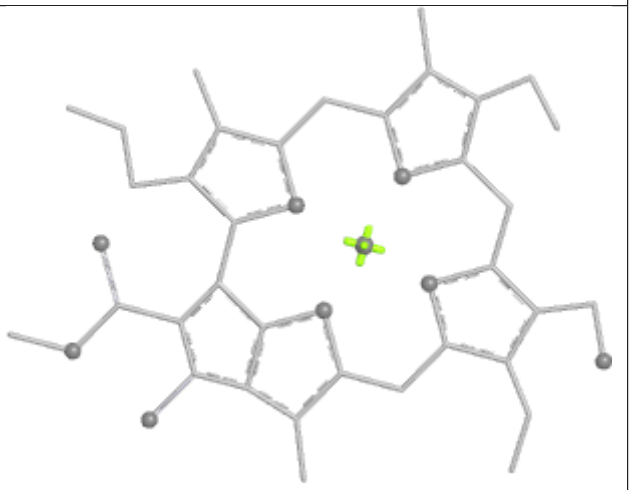
Bond lengths



Bond angles

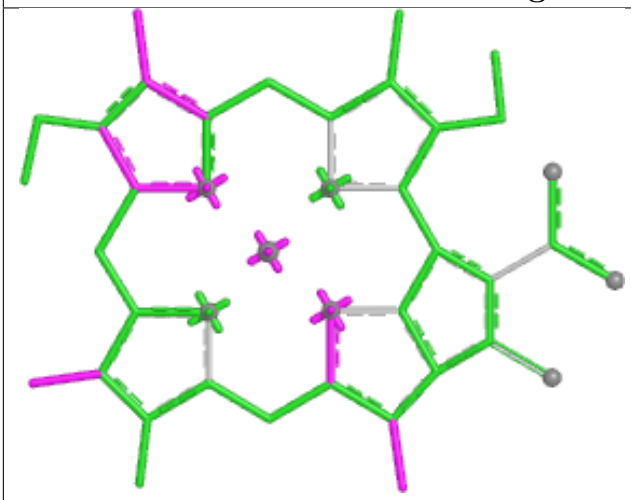


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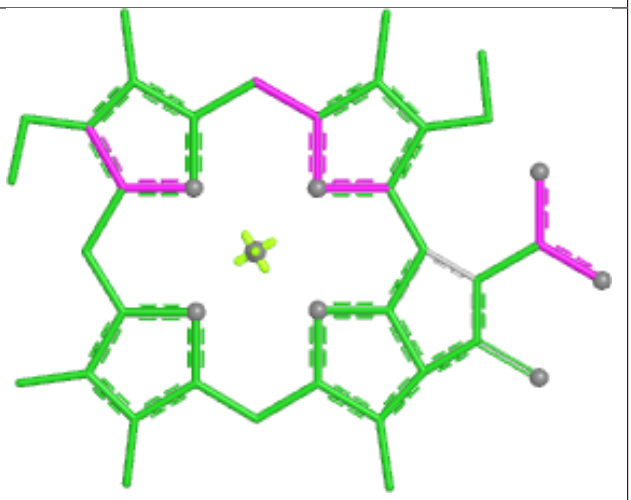


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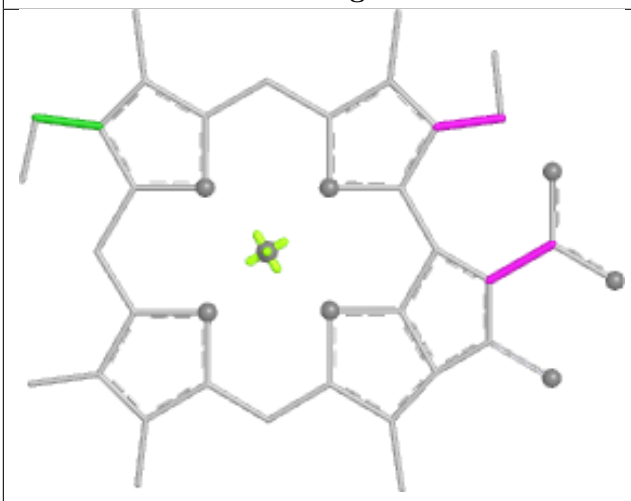
Ligand CLA 9 606



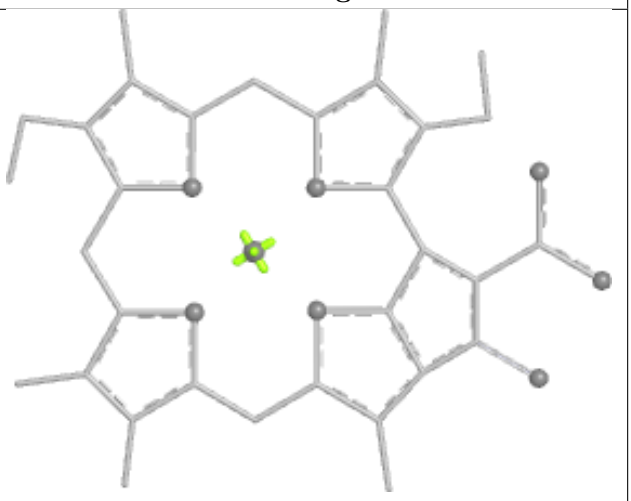
Bond lengths



Bond angles

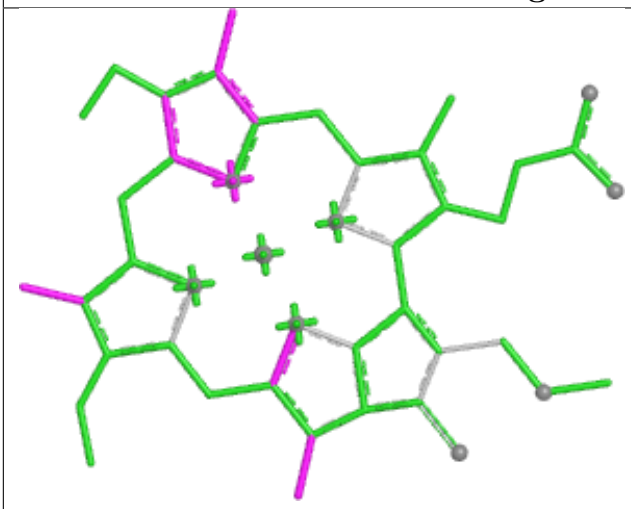


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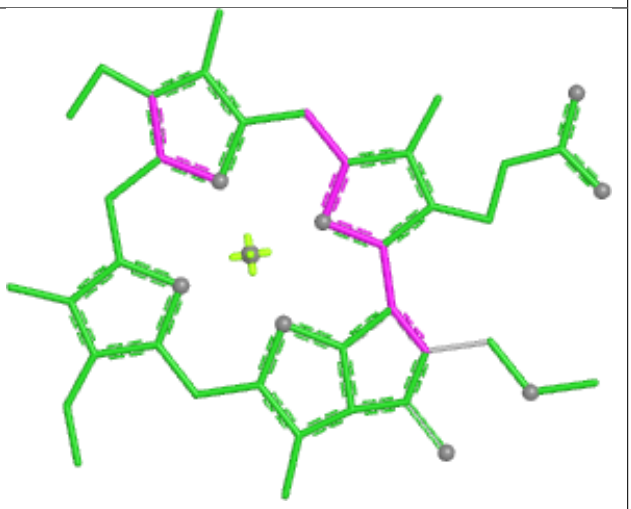


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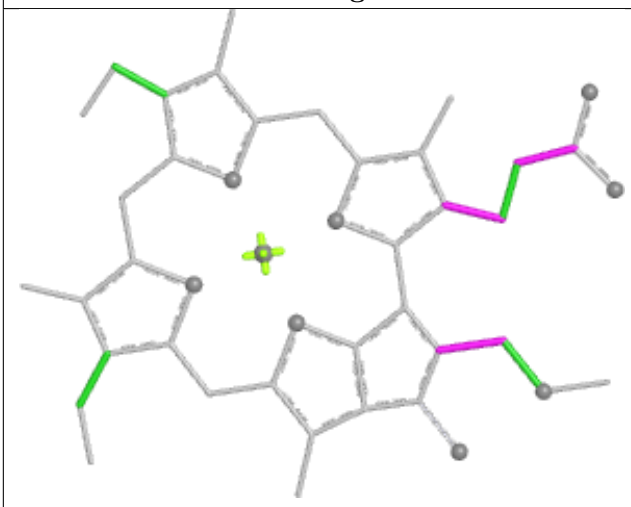
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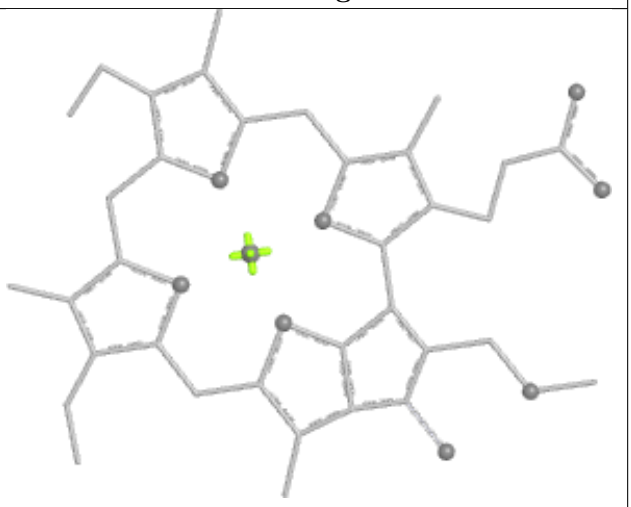
Bond lengths



Bond angles

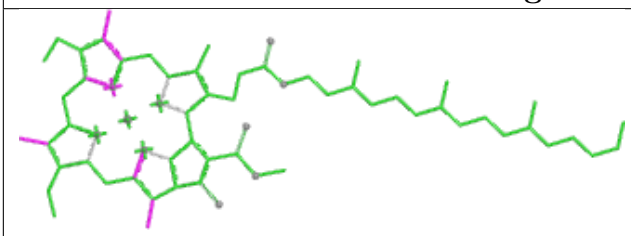


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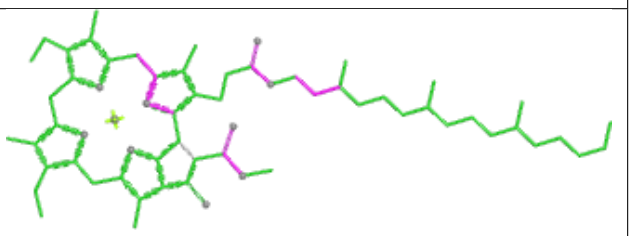


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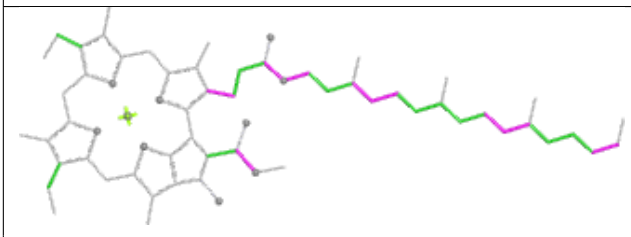
Ligand CLA B 814



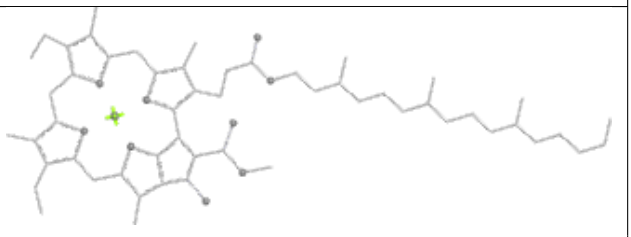
Bond lengths



Bond angles

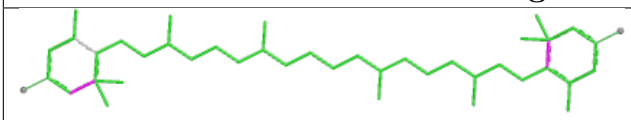


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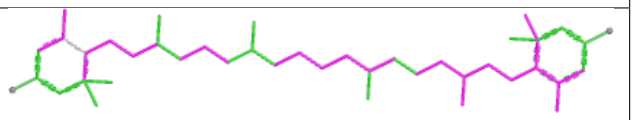


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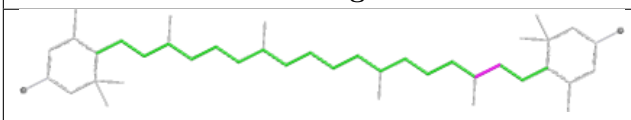
Ligand LUT 7 619



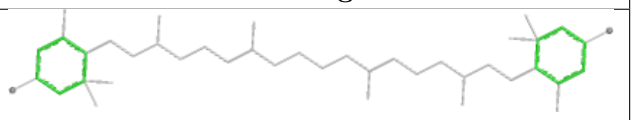
Bond lengths



Bond angles



Torsions

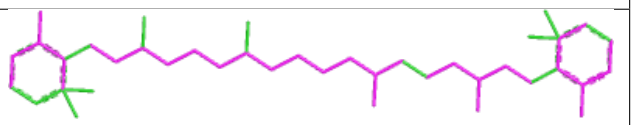


Rings

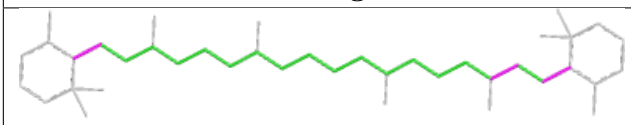
Ligand BCR A 849



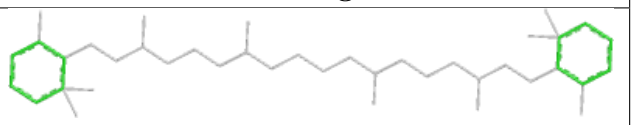
Bond lengths



Bond angles

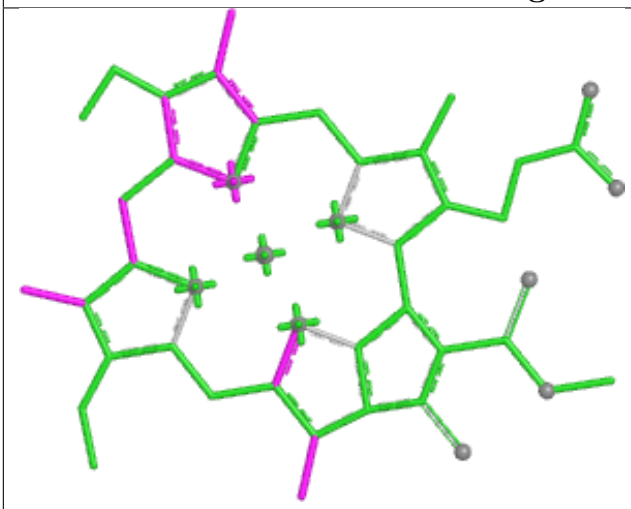


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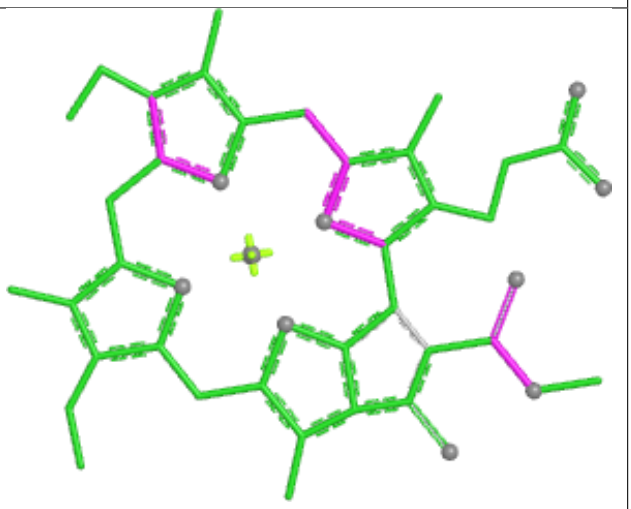


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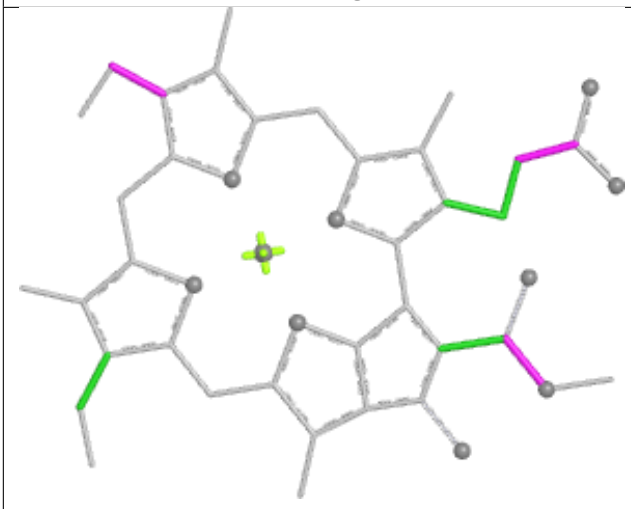
Ligand CLA a 607



Bond lengths



Bond angles

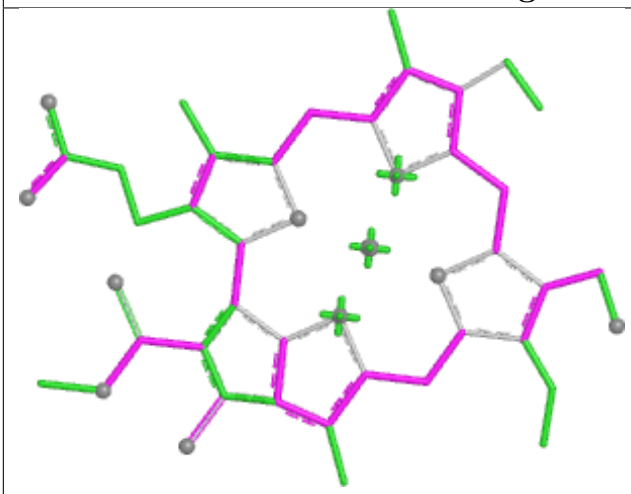


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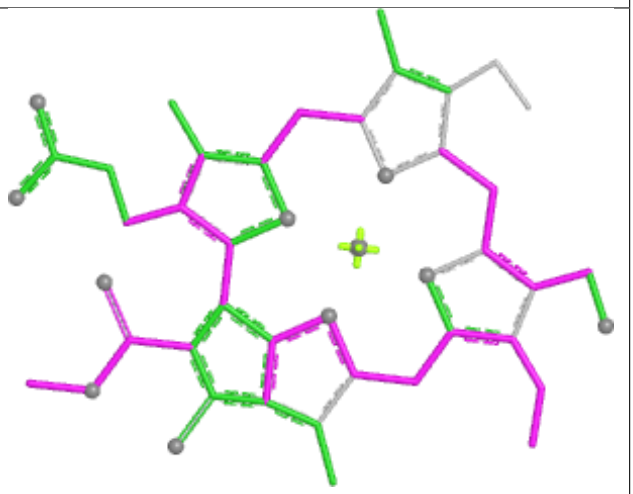


Rings

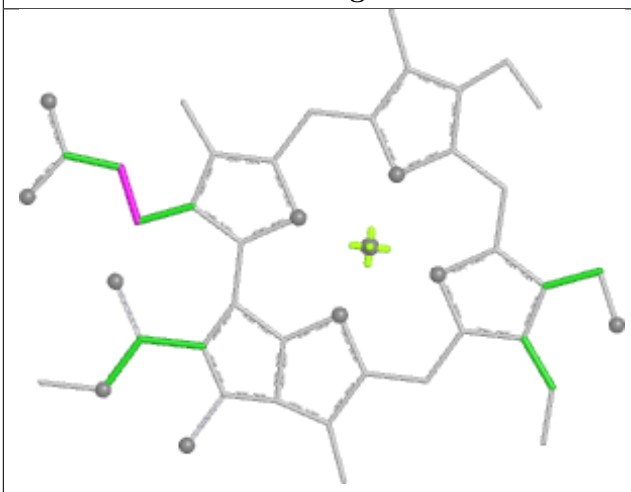
Ligand CHL W 606



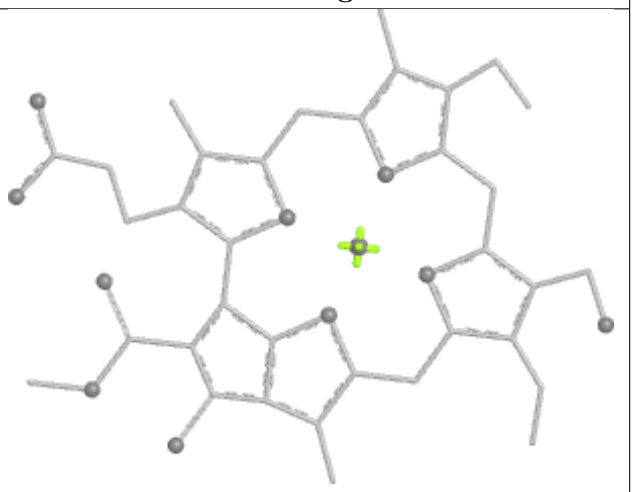
Bond lengths



Bond angles

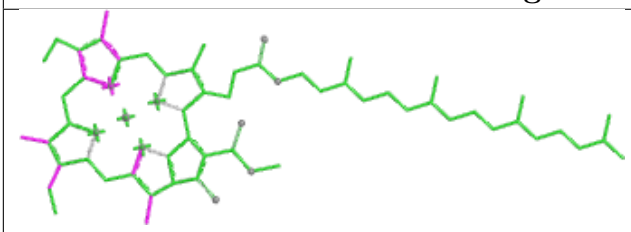


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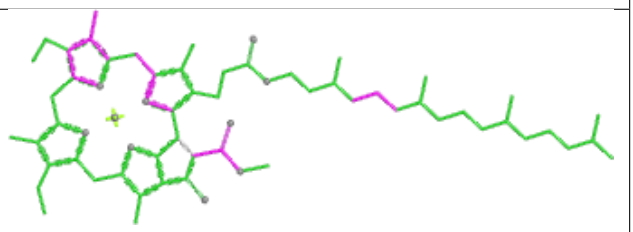


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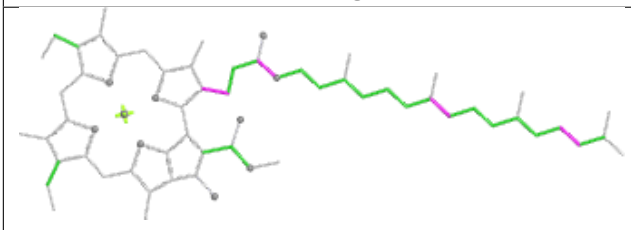
Ligand CLA A 820



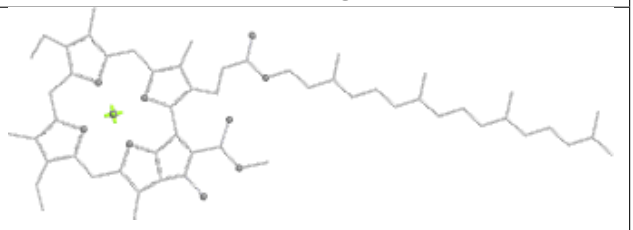
Bond lengths



Bond angles

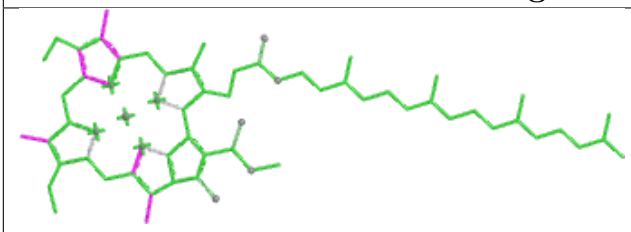


Torsions

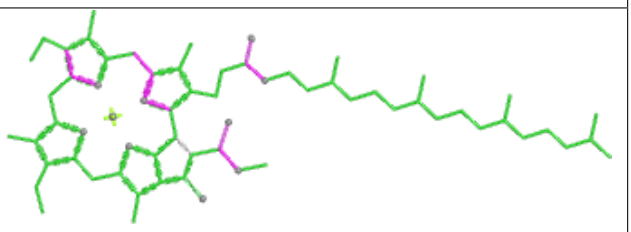


Rings

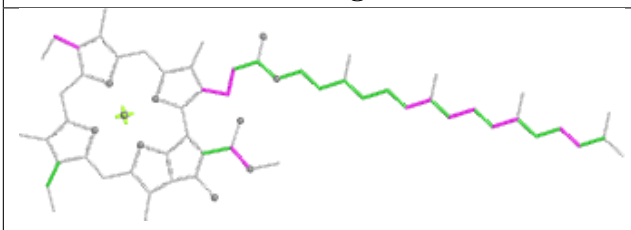
Ligand CLA 6 610



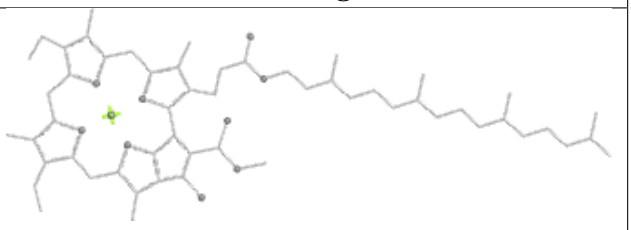
Bond lengths



Bond angles

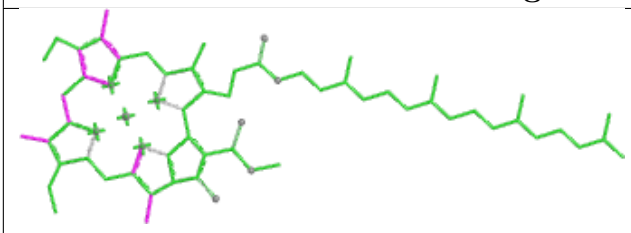


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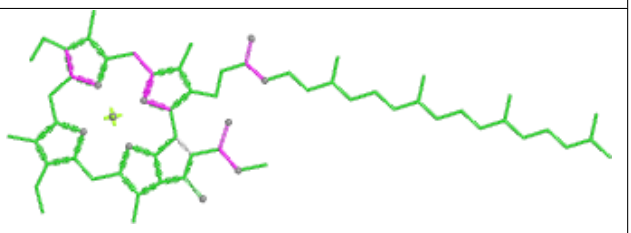


Rings

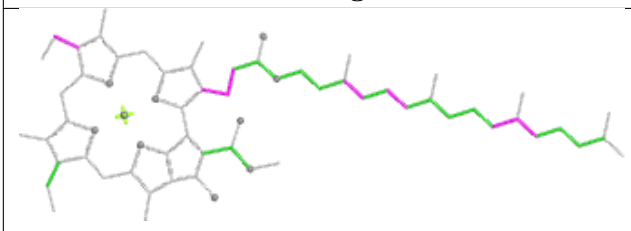
Ligand CLA Y 610



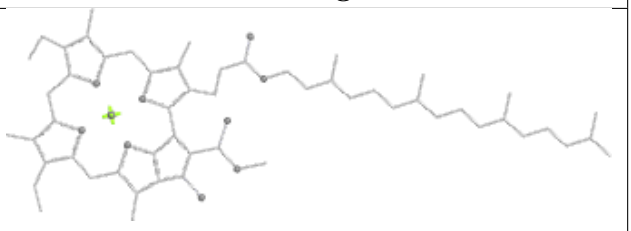
Bond lengths



Bond angles

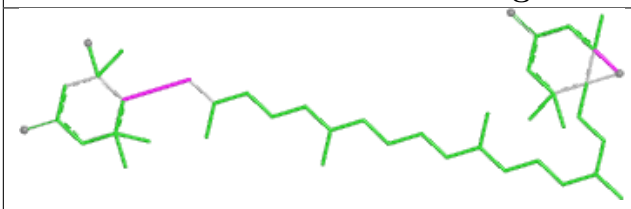


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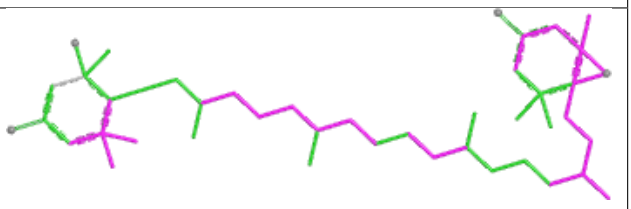


Rings

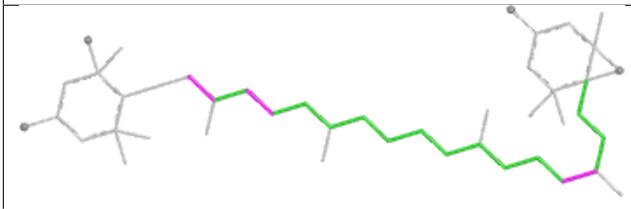
Ligand NEX X 1623



Bond lengths



Bond angles

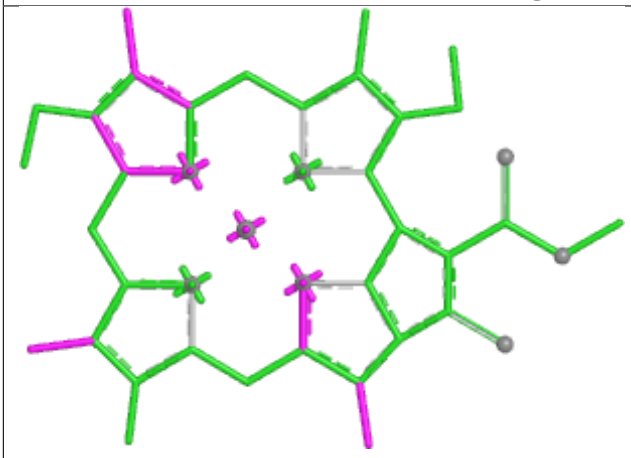


Torsions

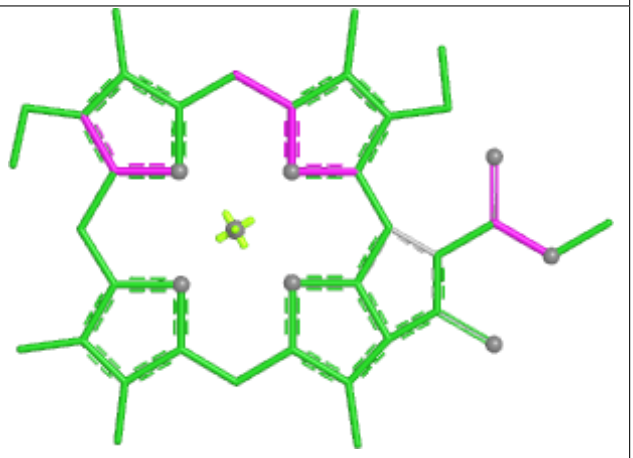


Rings

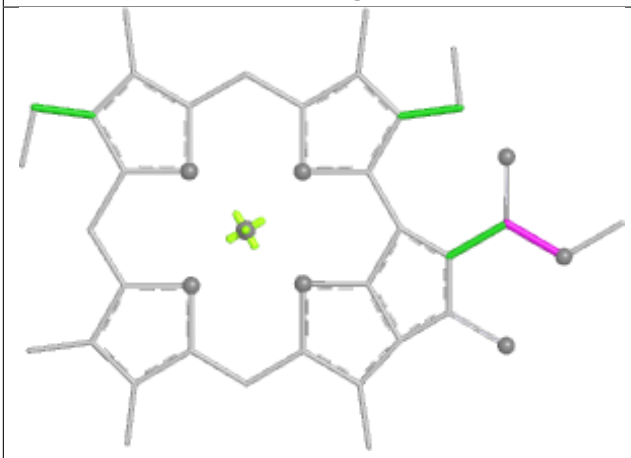
Ligand CLA 7 606



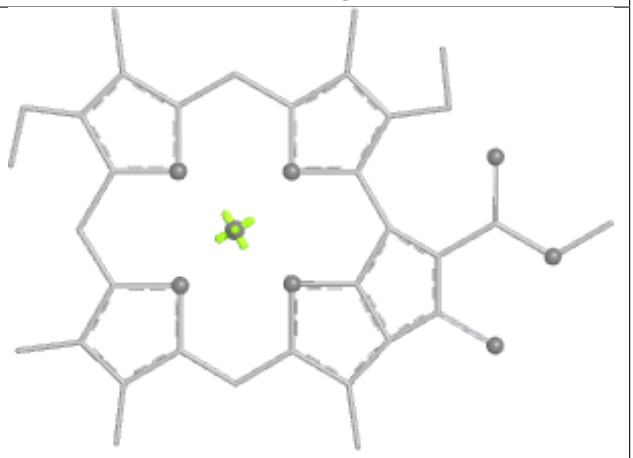
Bond lengths



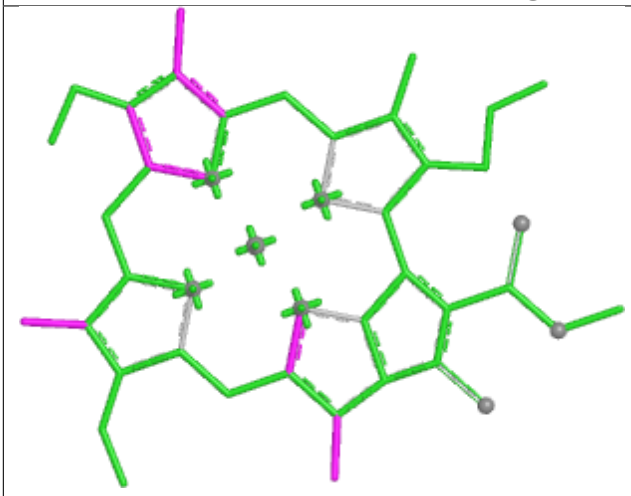
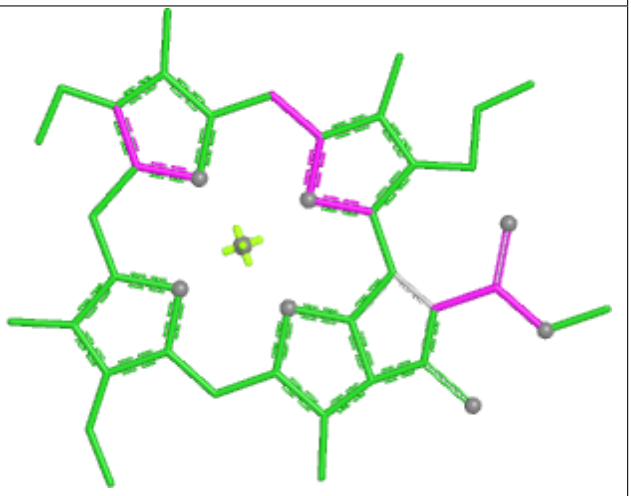
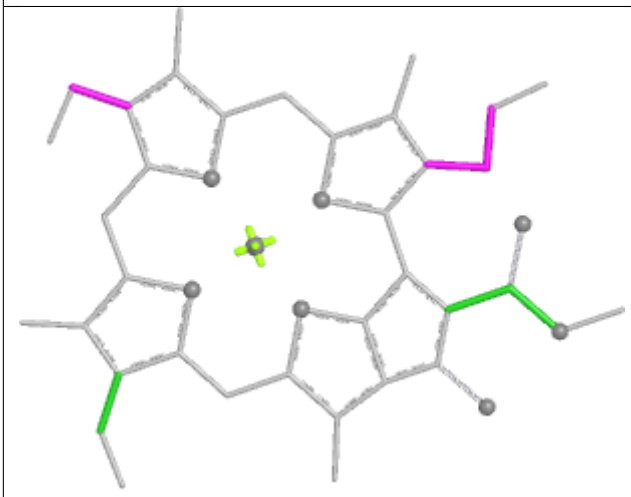
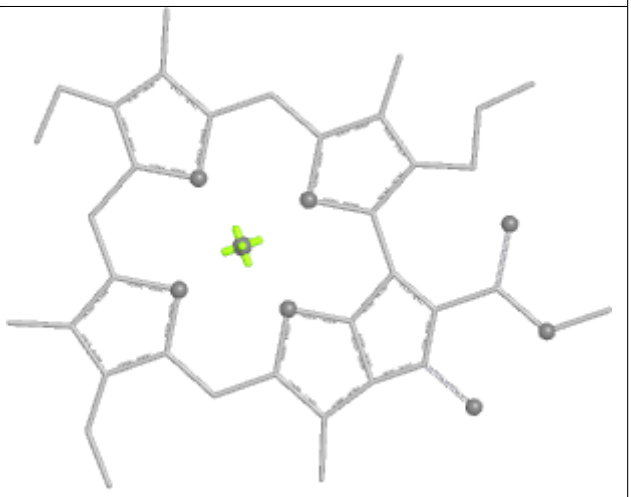
Bond angles



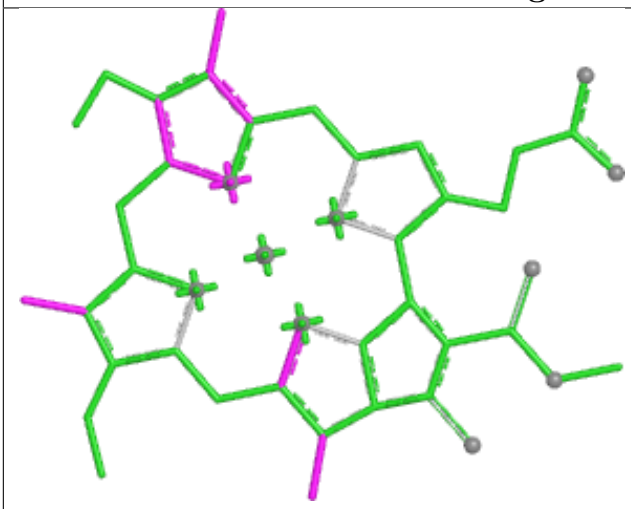
Torsions



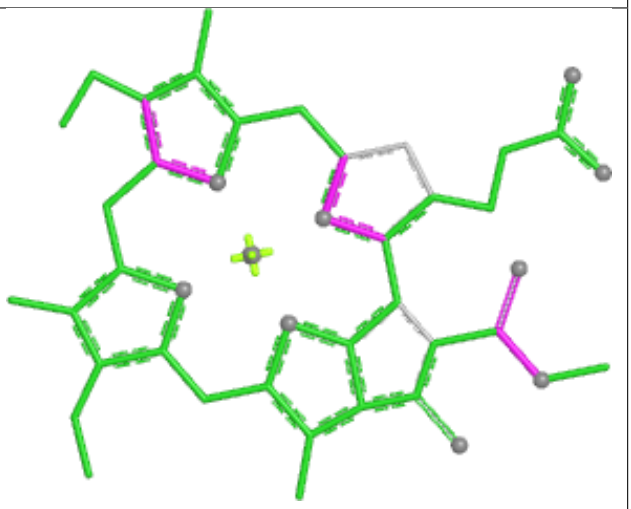
Rings

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

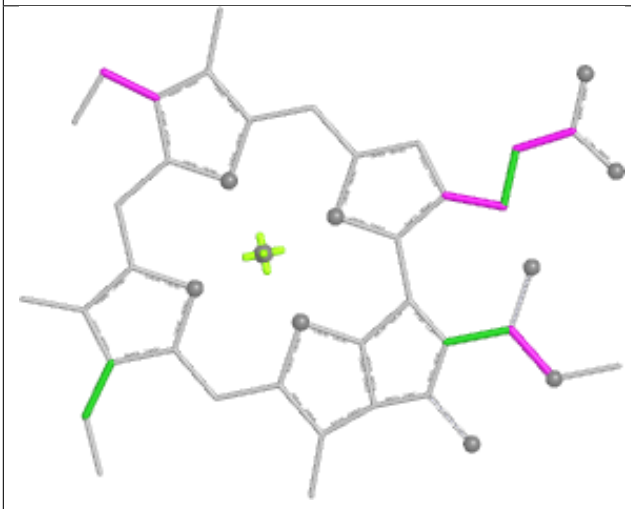
Ligand CLA 5 614



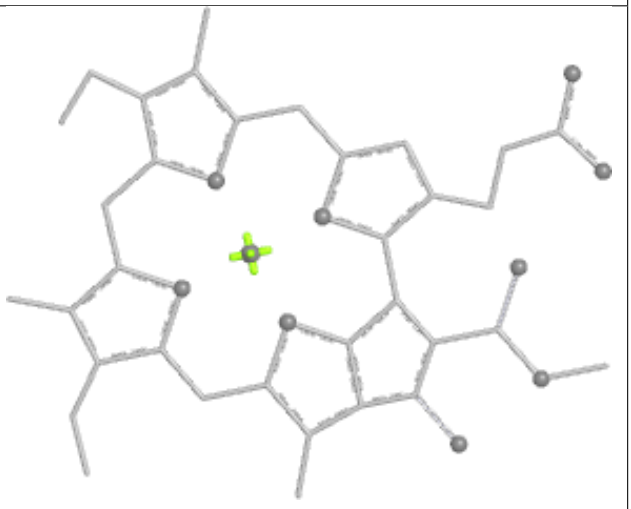
Bond lengths



Bond angles

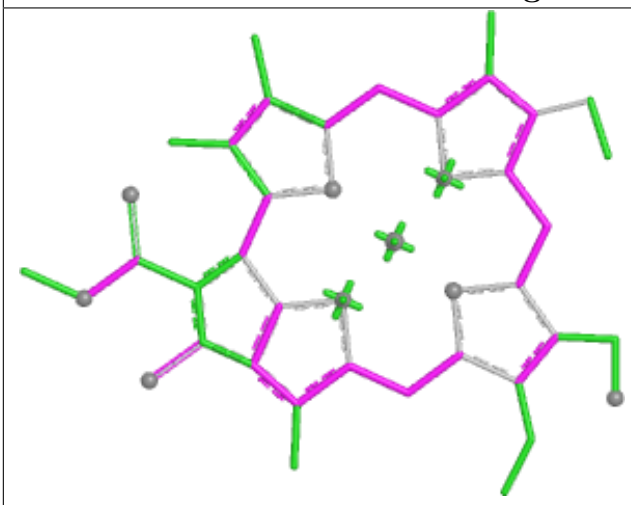


Torsions

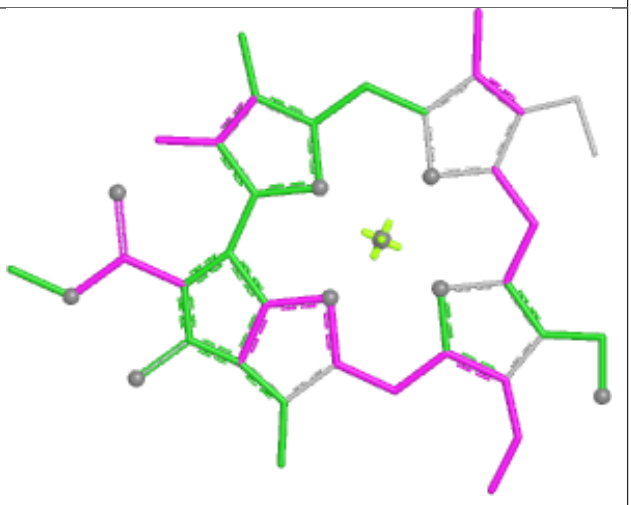


Rings

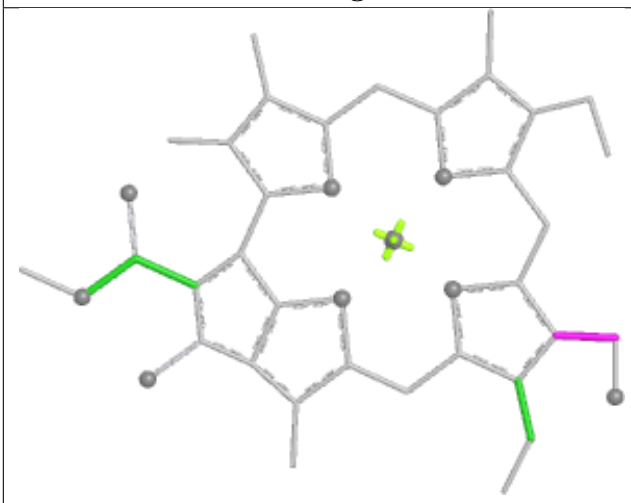
Ligand CHL Y 605



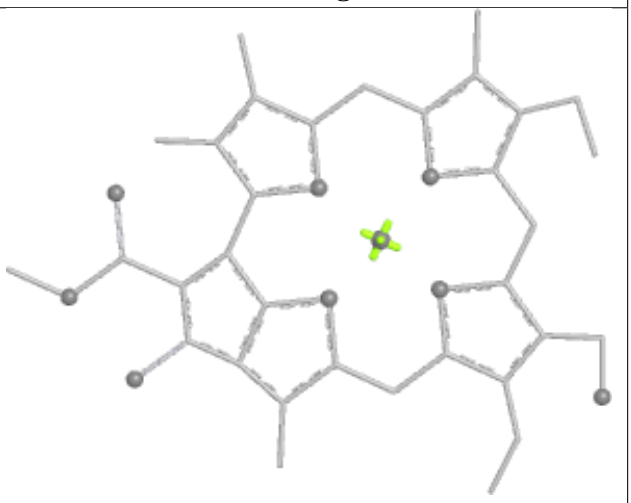
Bond lengths



Bond angles

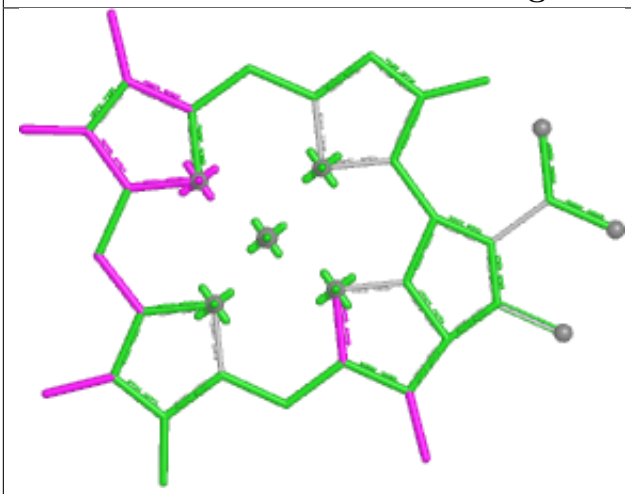


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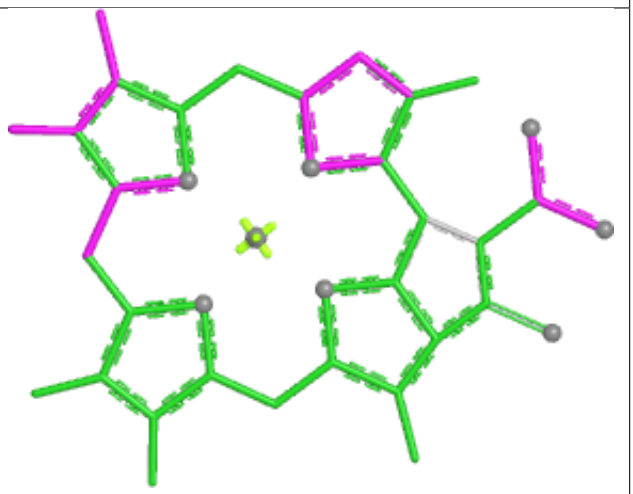


Rings

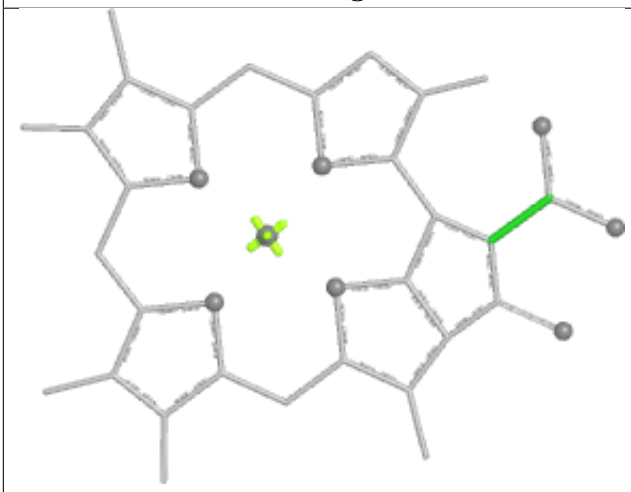
Ligand CLA 1 614



Bond lengths



Bond angles

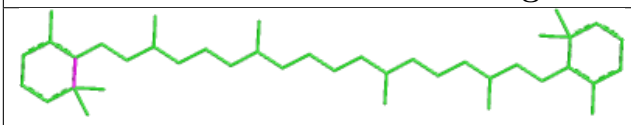


Torsions

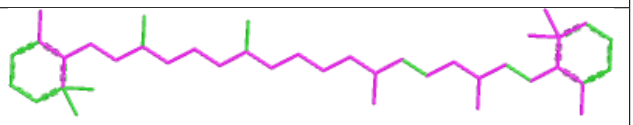


Rings

Ligand BCR A 856



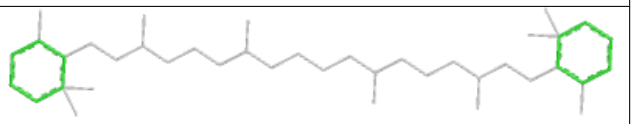
Bond lengths



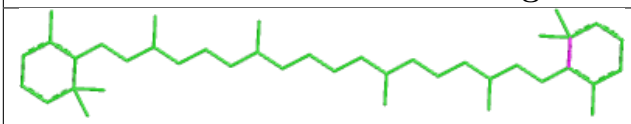
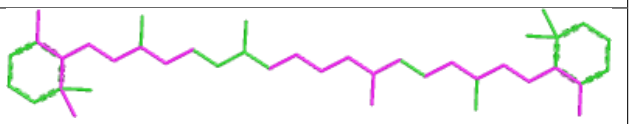
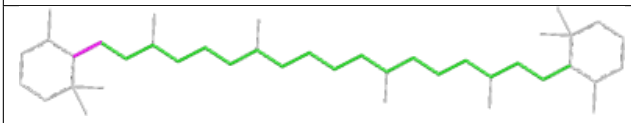
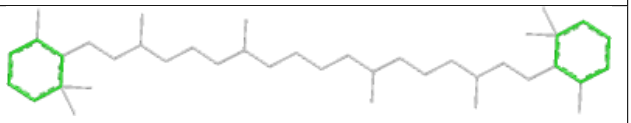
Bond angles

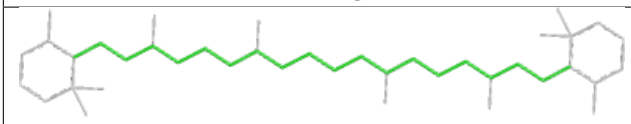
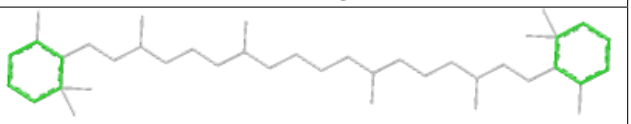


Torsions

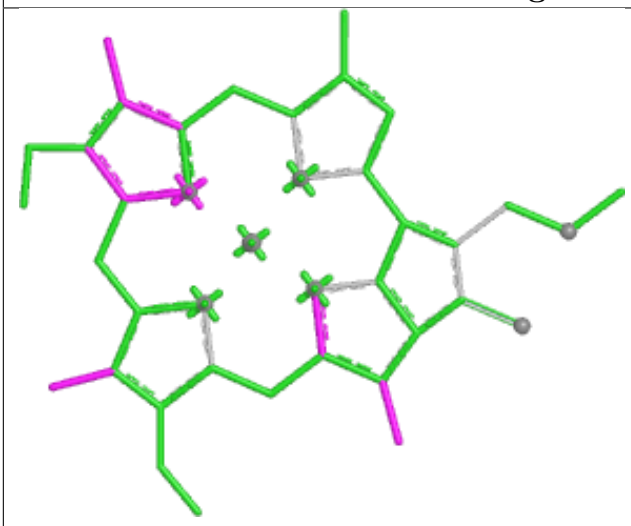


Rings

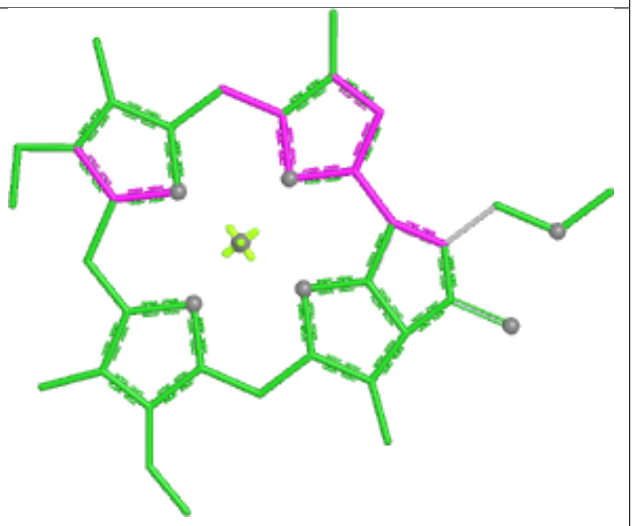
Ligand BCR A 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

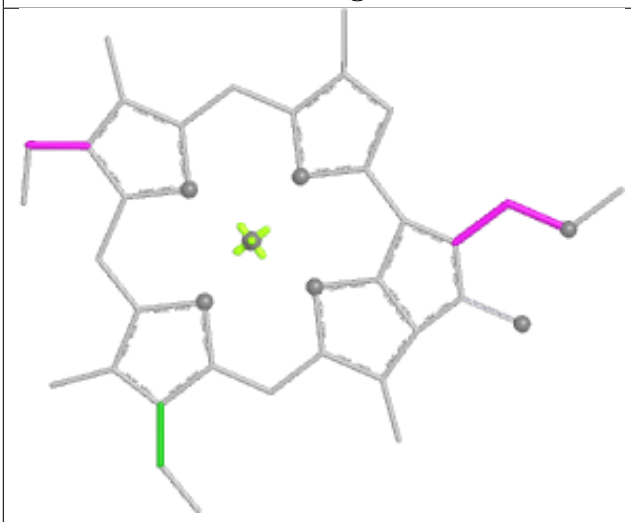
Ligand CLA 1 606



Bond lengths



Bond angles

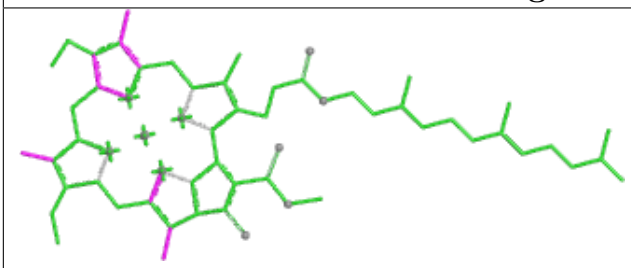


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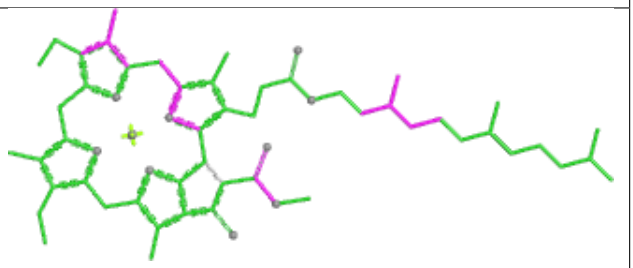


Rings

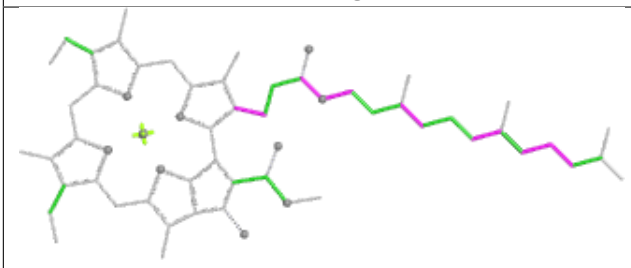
Ligand CLA 8 610



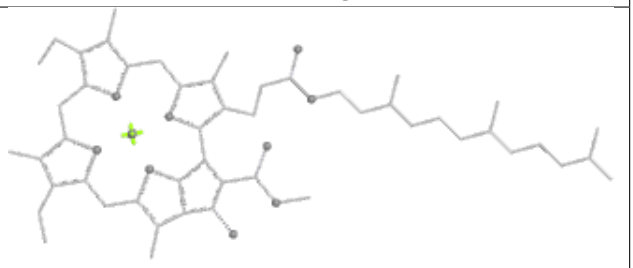
Bond lengths



Bond angles

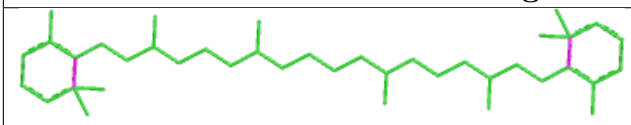


Torsions

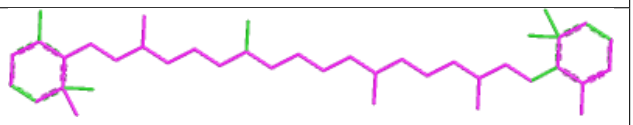


Rings

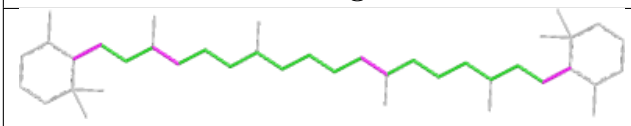
Ligand BCR A 852



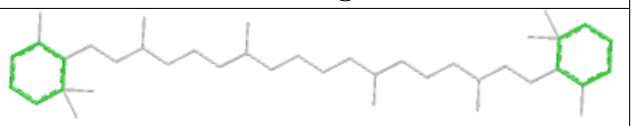
Bond lengths



Bond angles



Torsions

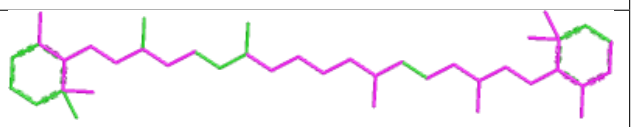


Rings

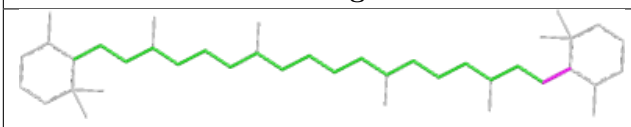
Ligand BCR 7 621



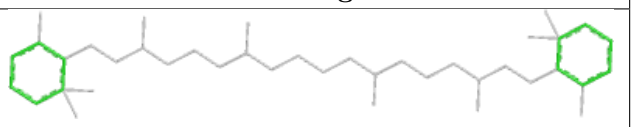
Bond lengths



Bond angles

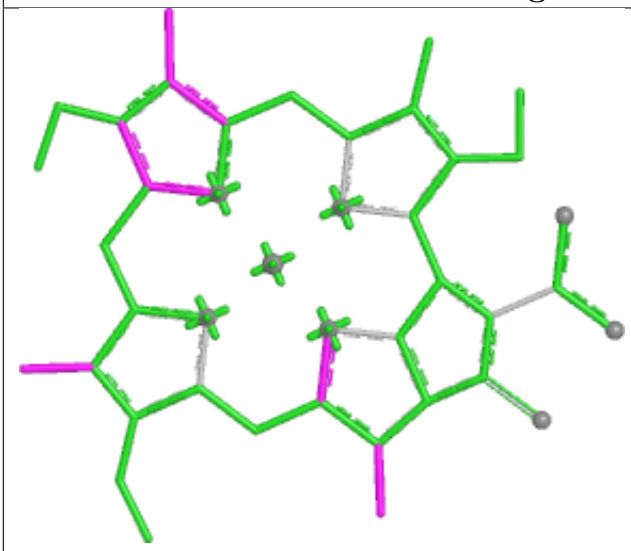


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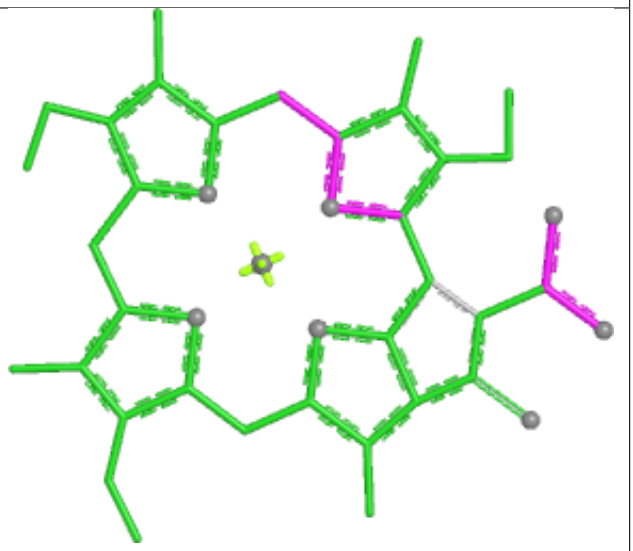


Rings

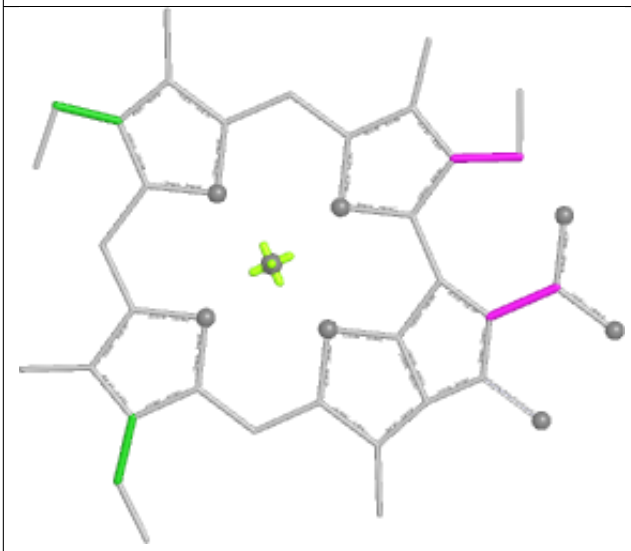
Ligand CLA 4 612



Bond lengths



Bond angles

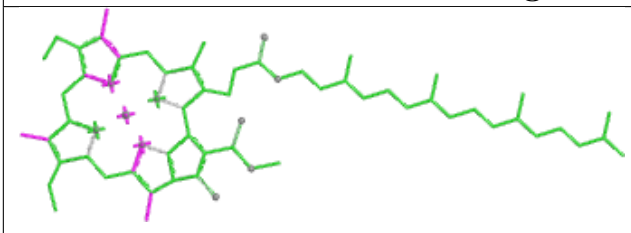


Torsions

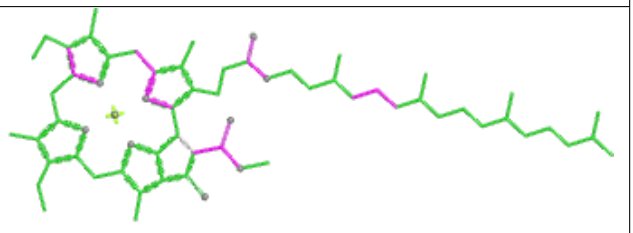


Rings

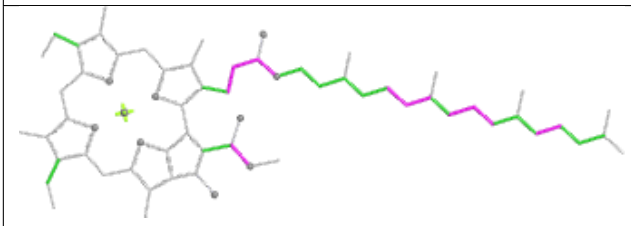
Ligand CLA A 830



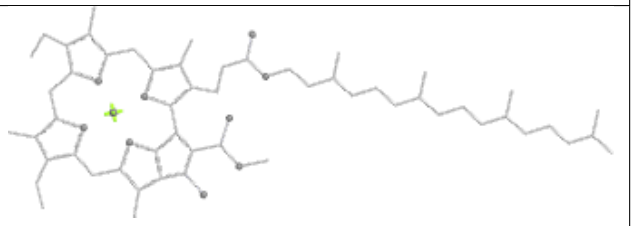
Bond lengths



Bond angles

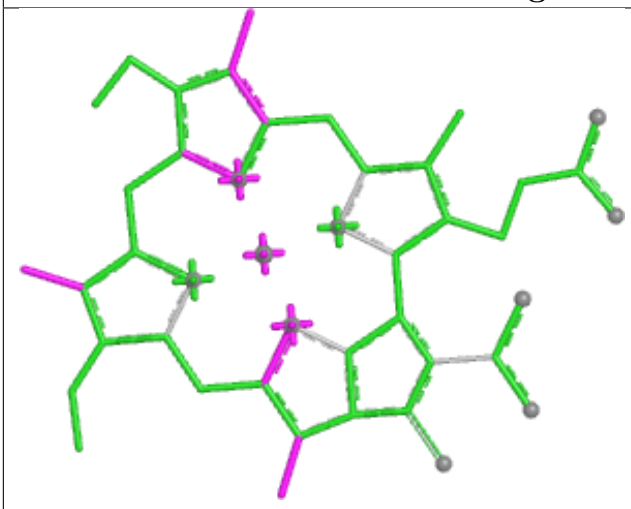


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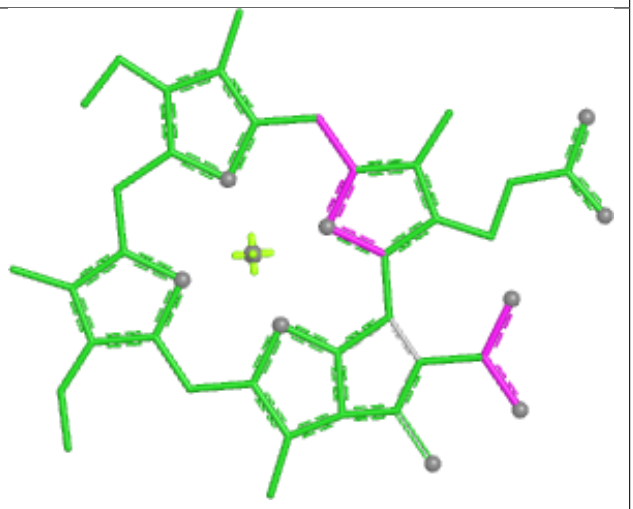


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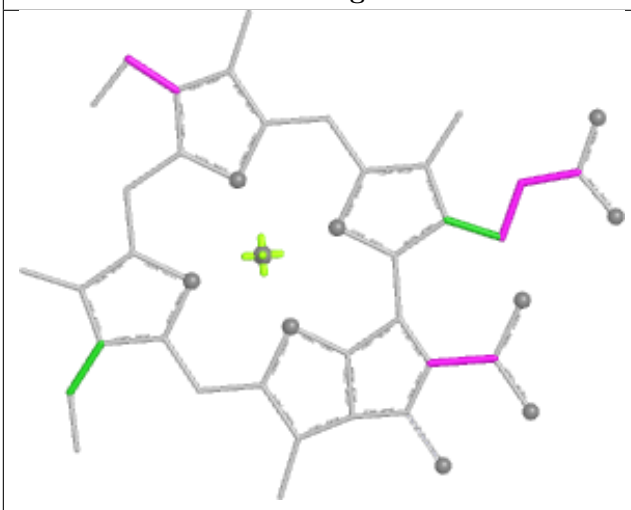
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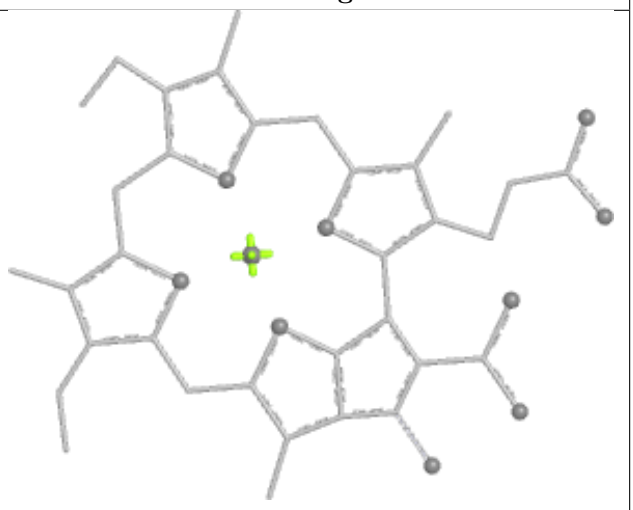
Bond lengths



Bond angles

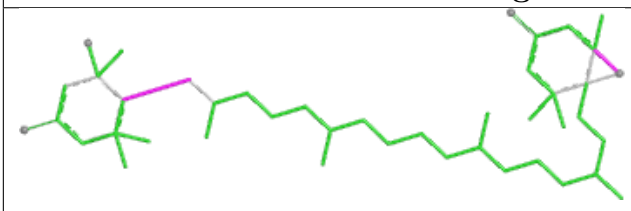


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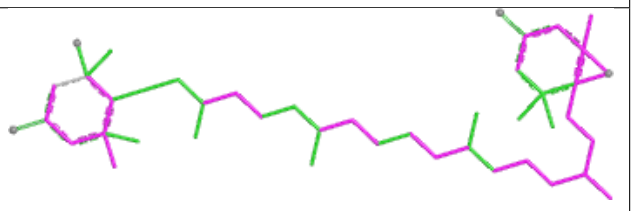


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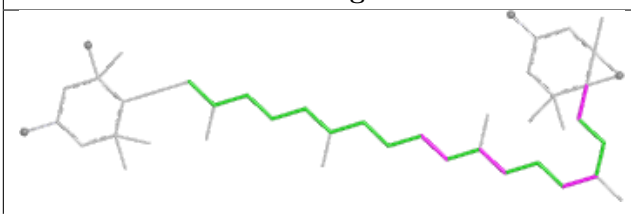
Ligand NEX Y 1623



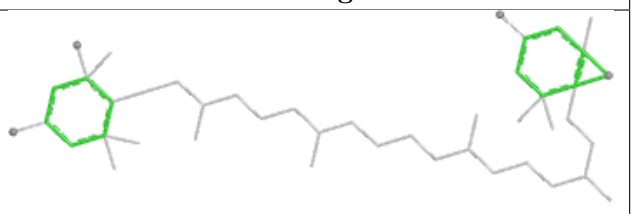
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Bond angles

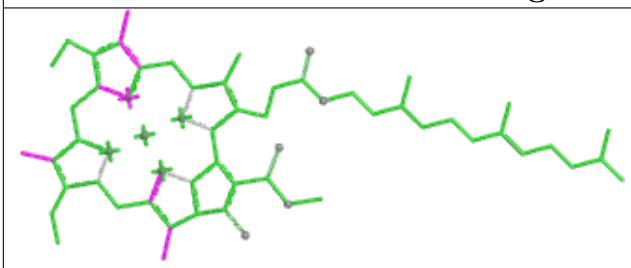


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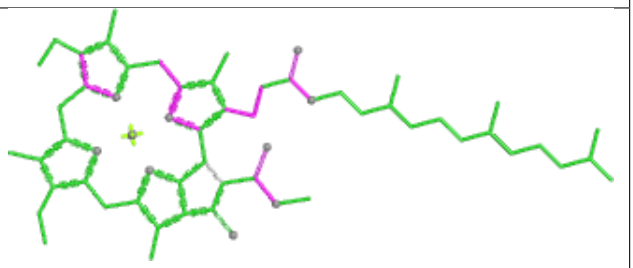


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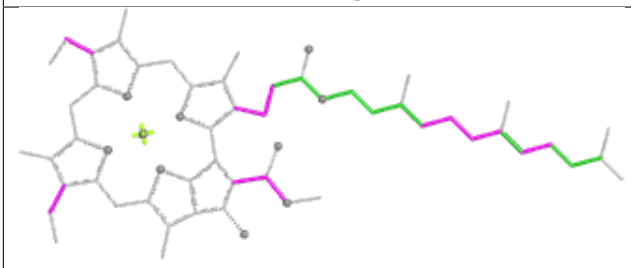
Ligand CLA 3 609



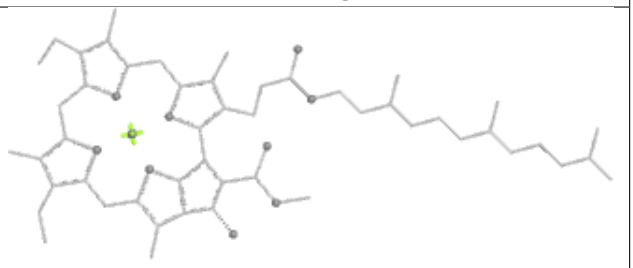
Bond lengths



Bond angles

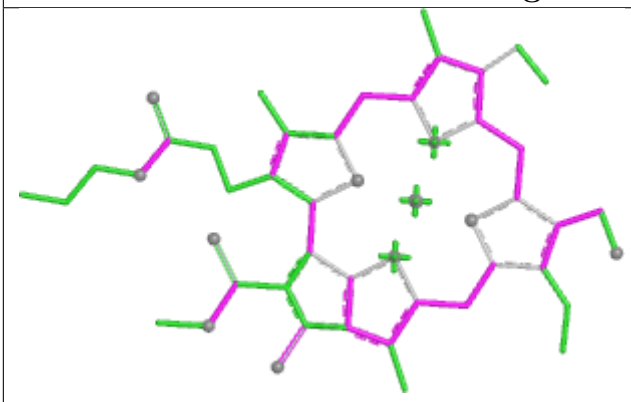


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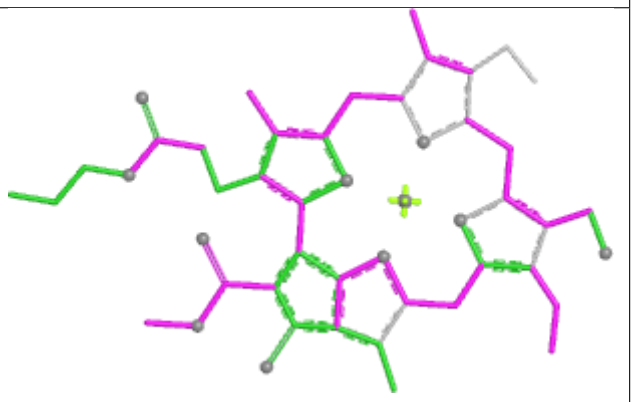


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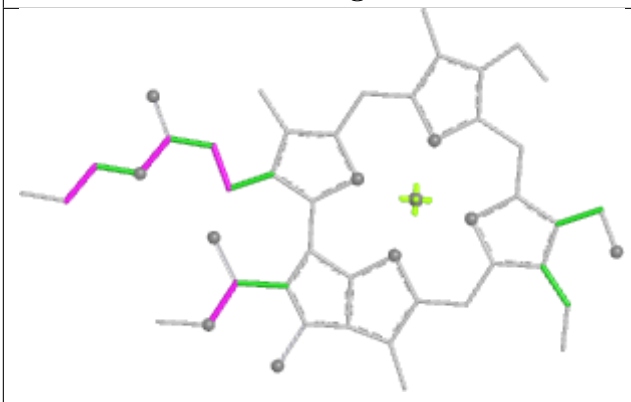
Ligand CHL Y 608



Bond lengths



Bond angles

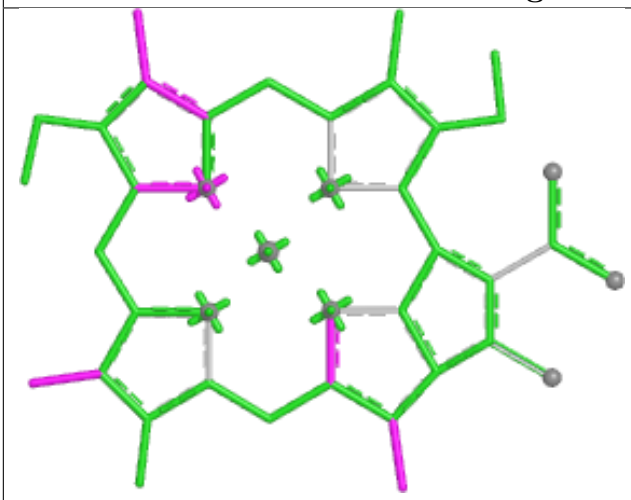


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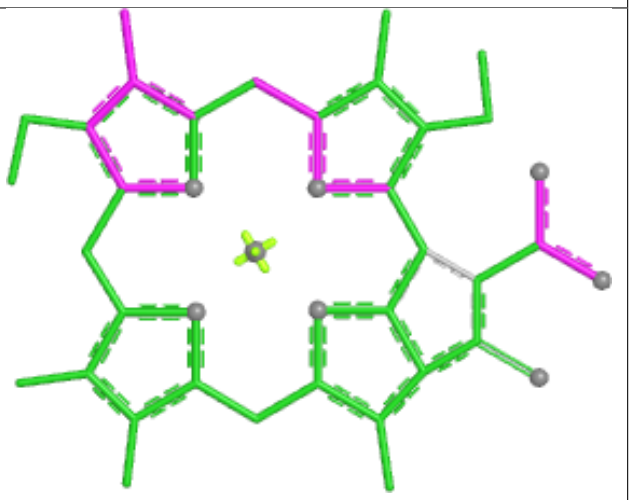


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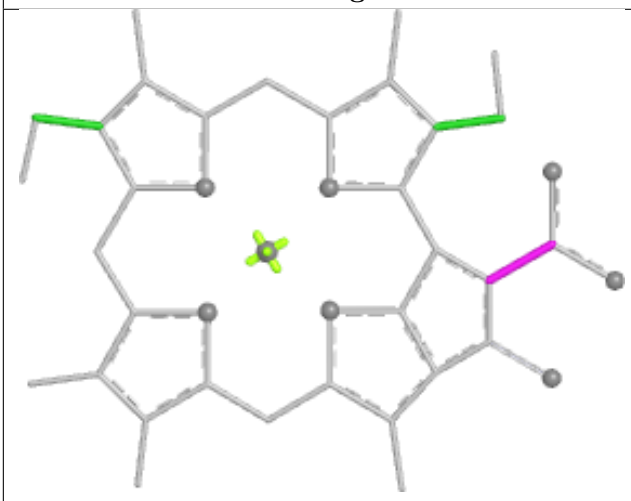
Ligand CLA L 307



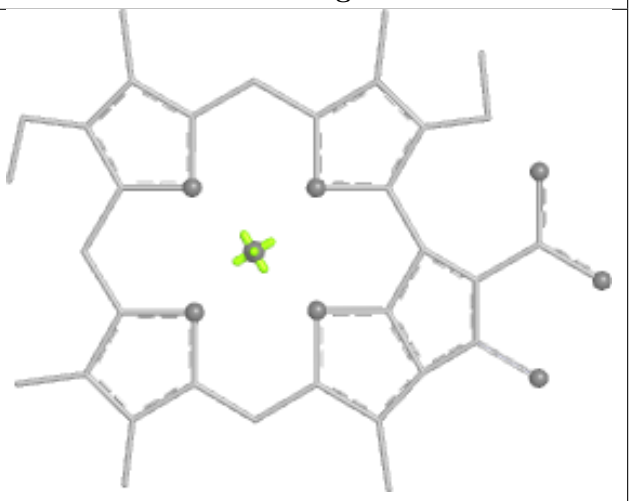
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Bond angles

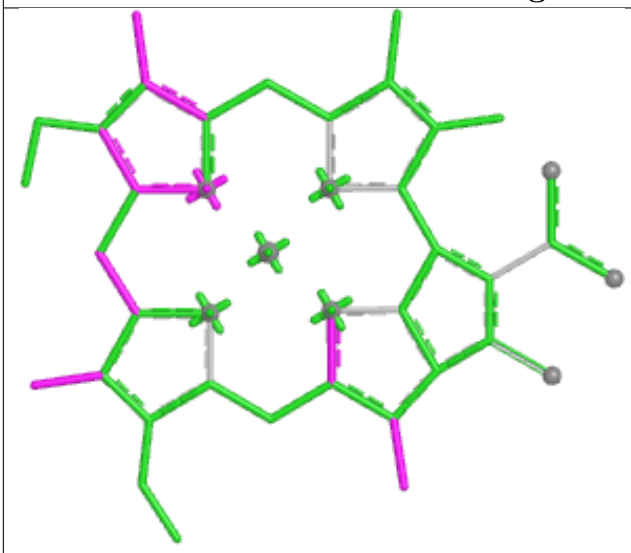


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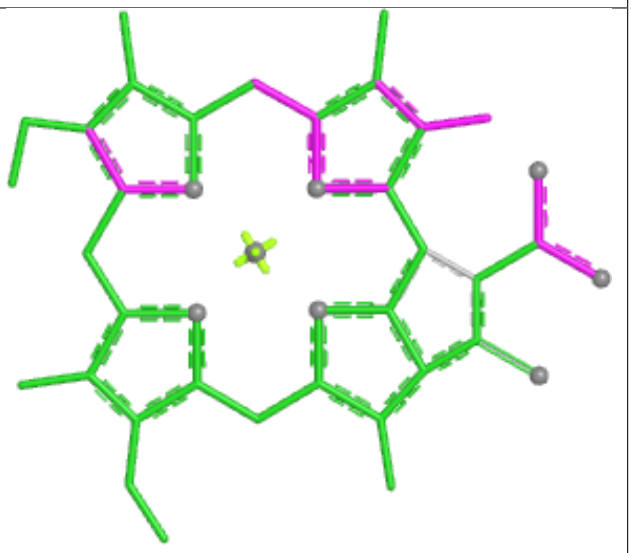


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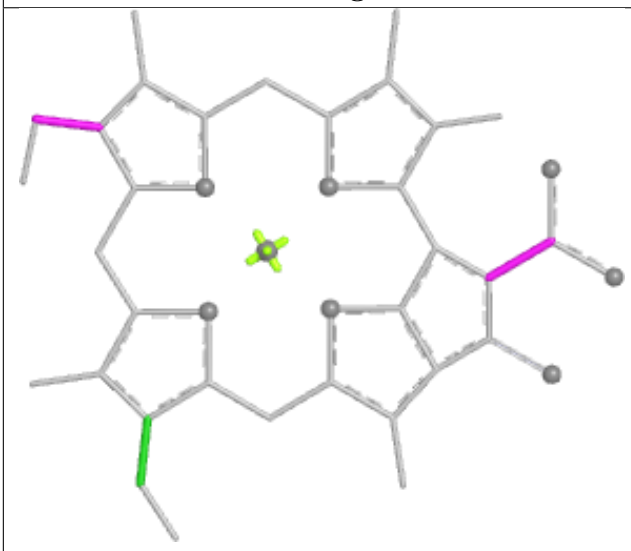
Ligand CLA 1 607



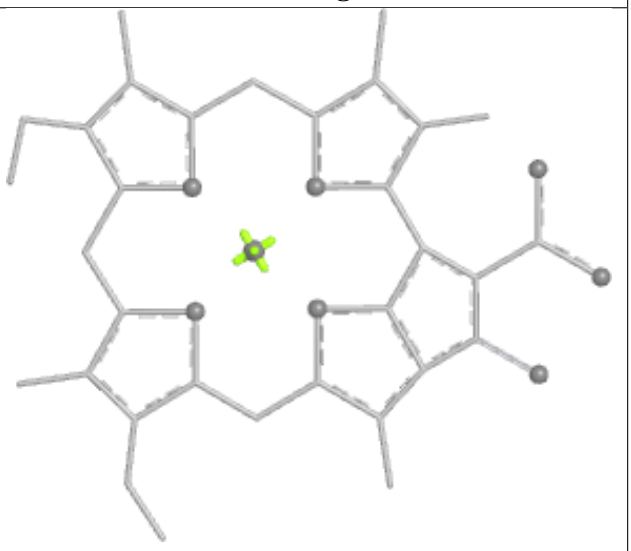
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Bond angles

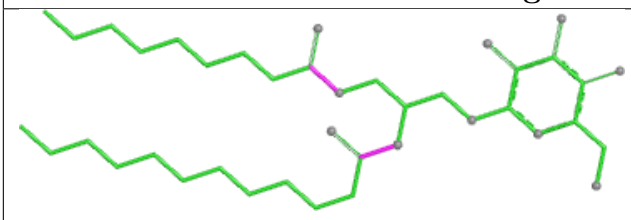


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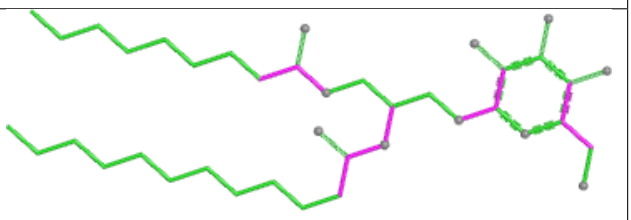


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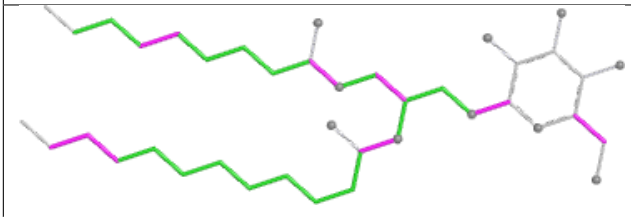
Ligand LMG J 104



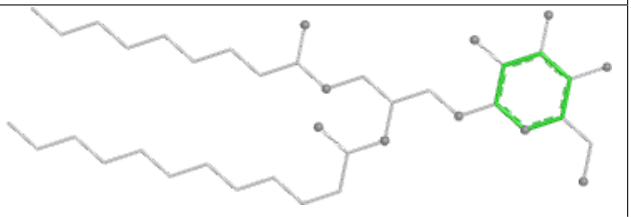
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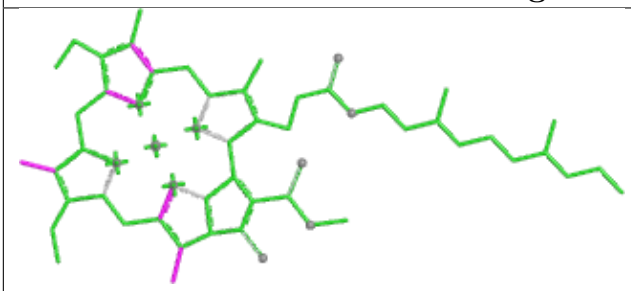


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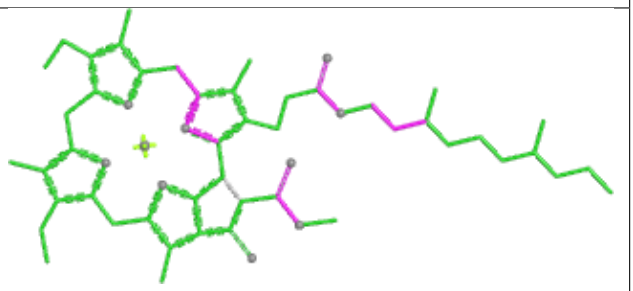


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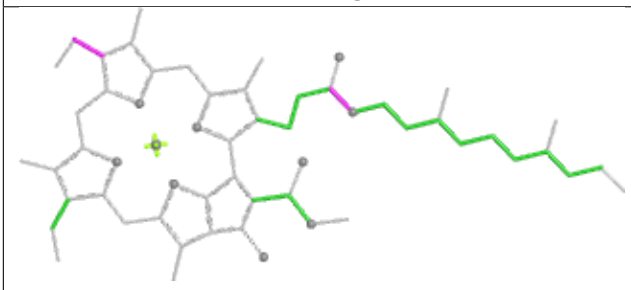
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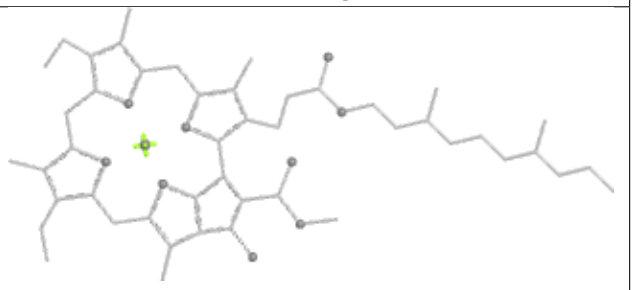
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Bond angles

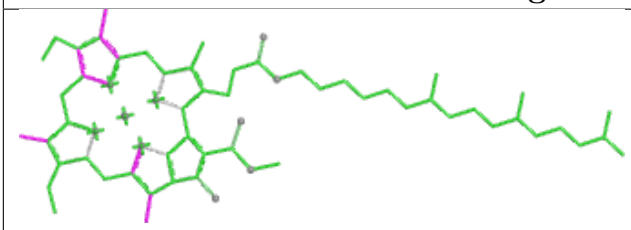


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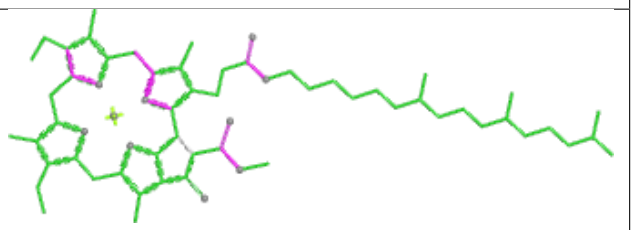


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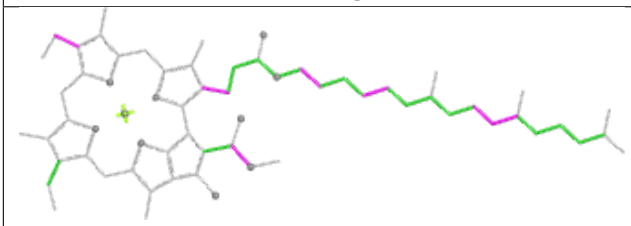
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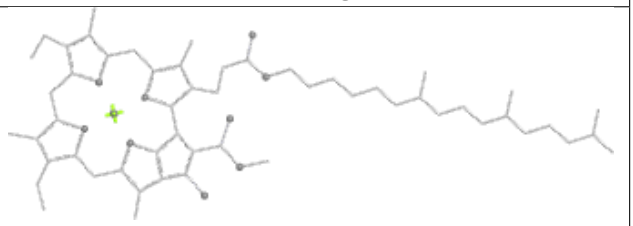
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Bond angles

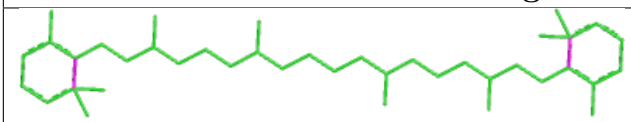


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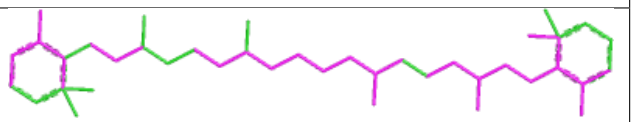


Rings

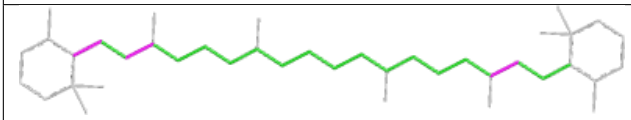
Ligand BCR B 849



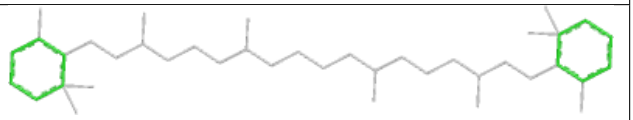
Bond lengths



Bond angles

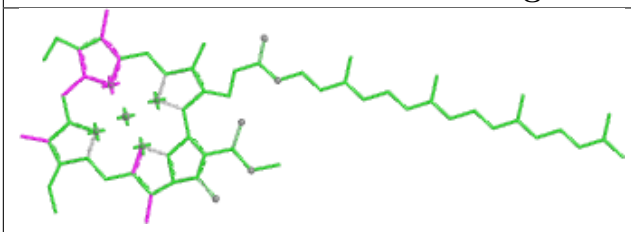


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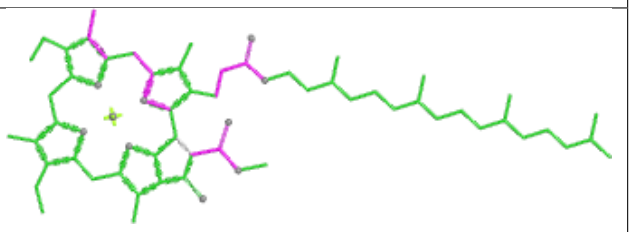


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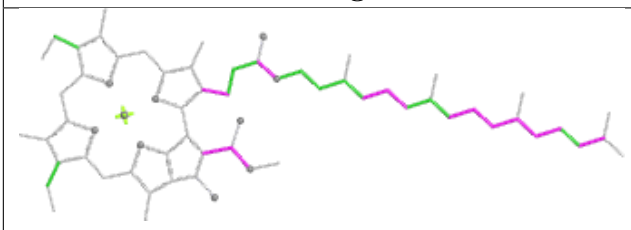
Ligand CLA A 831



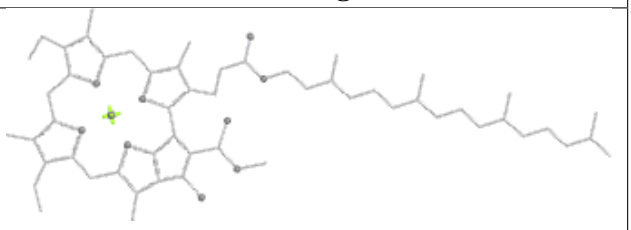
Bond lengths



Bond angles

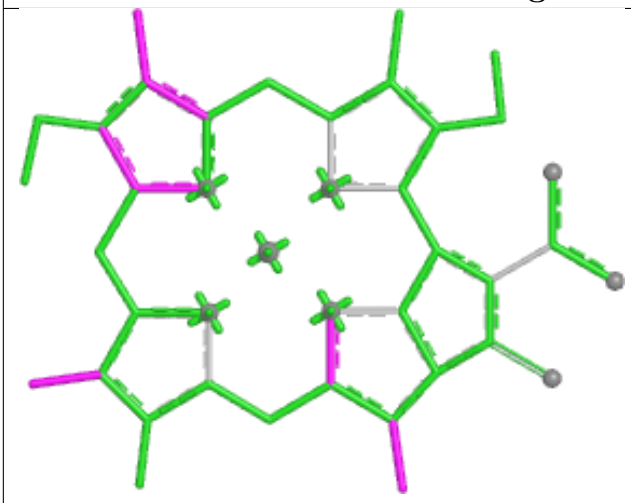


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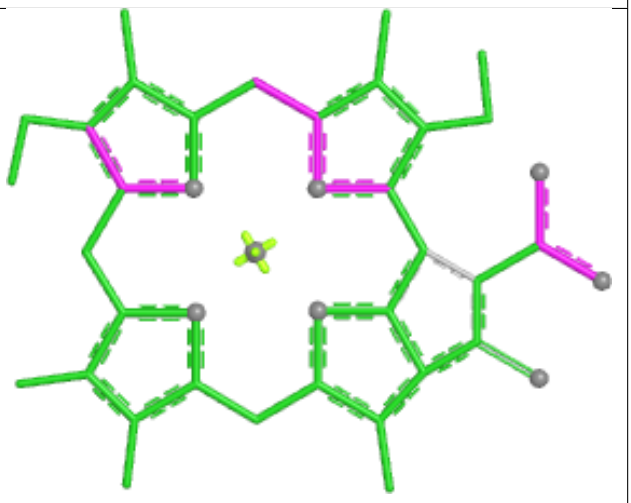


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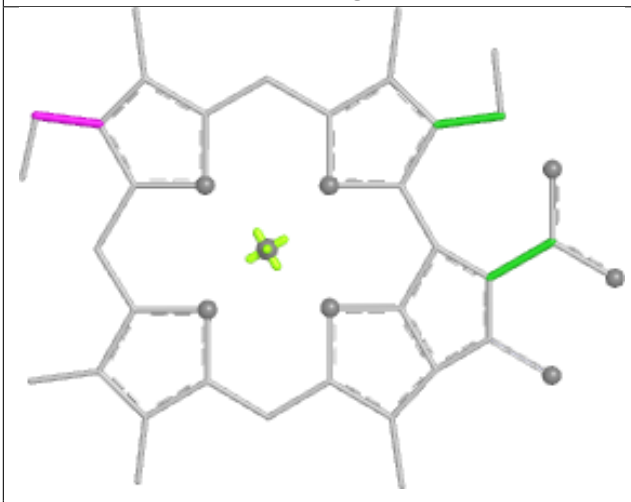
Ligand CLA 6 606



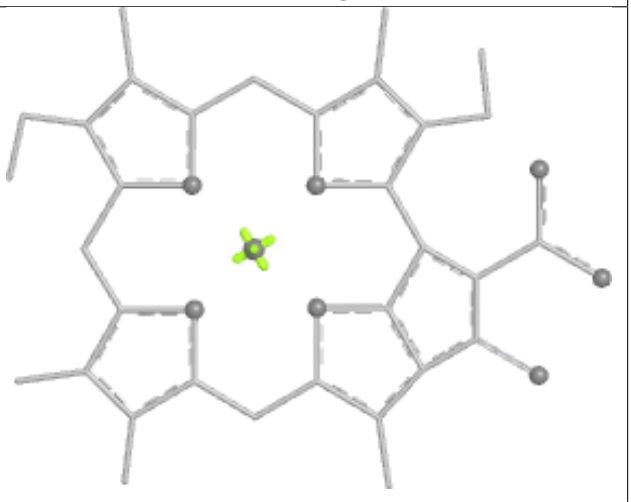
Bond lengths



Bond angles

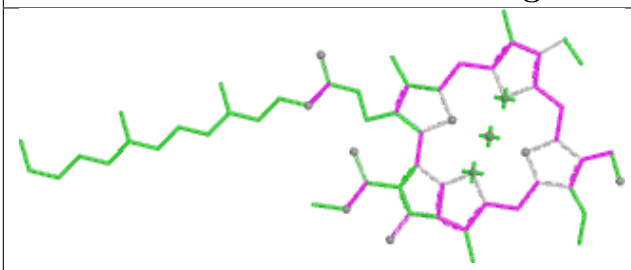


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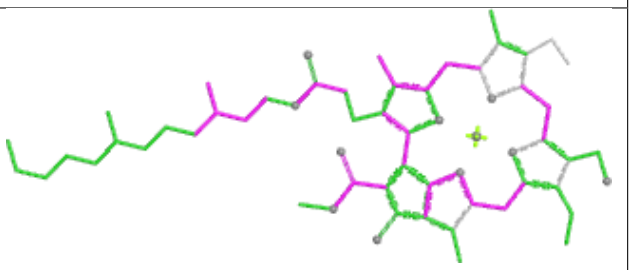


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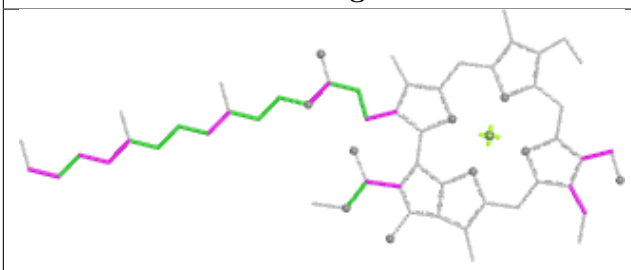
Ligand CHL U 609



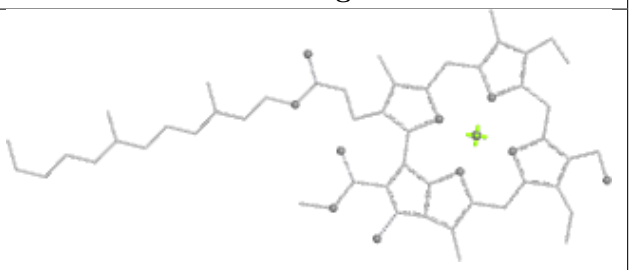
Bond lengths



Bond angles

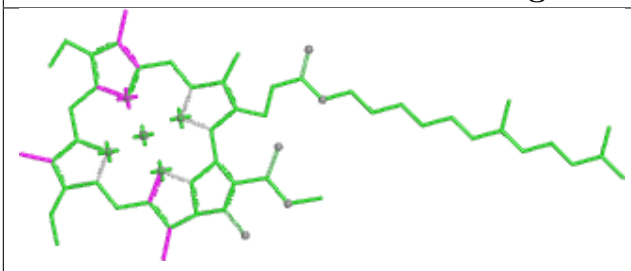


Torsions

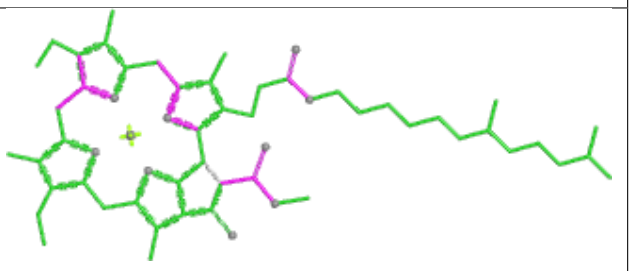


Rings

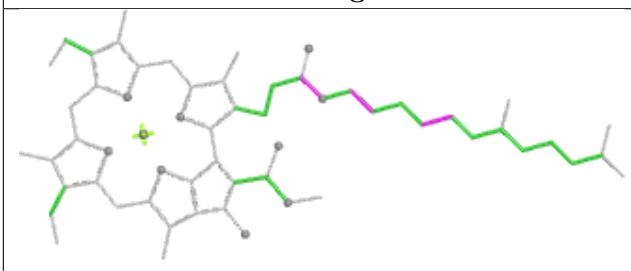
Ligand CLA 7 611



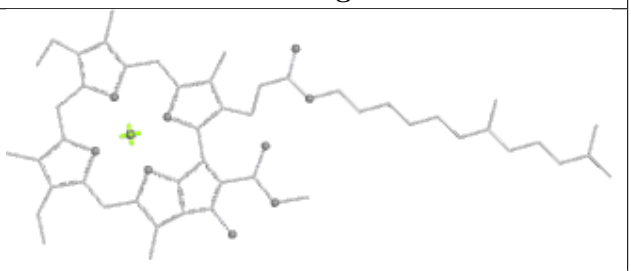
Bond lengths



Bond angles



Torsions

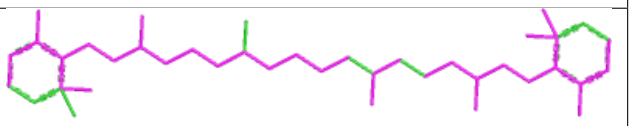


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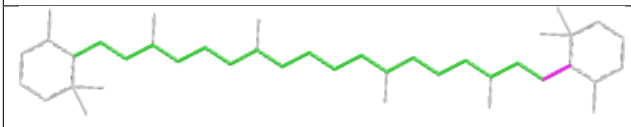
Ligand BCR 8 621



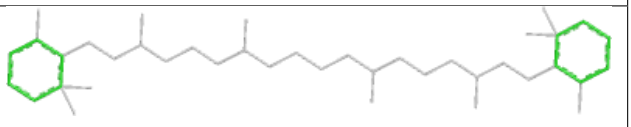
Bond lengths



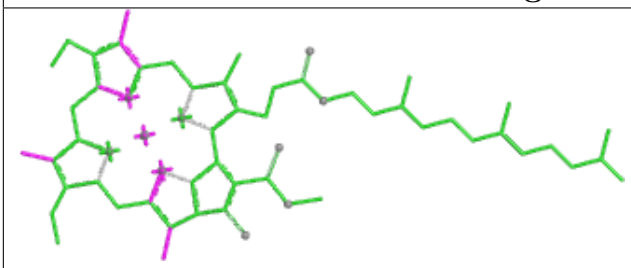
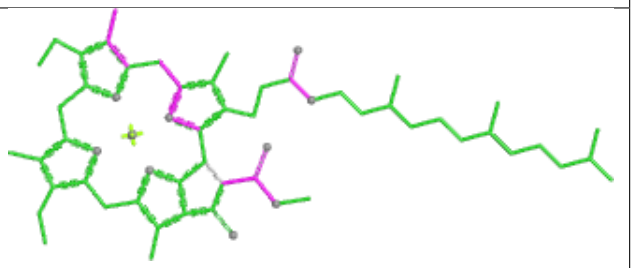
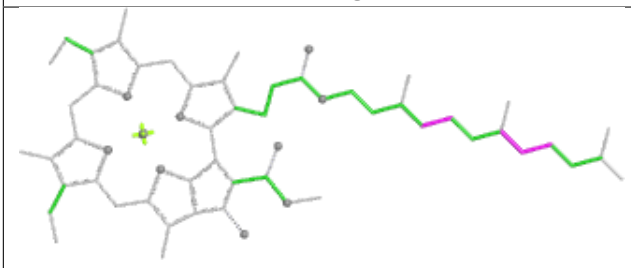
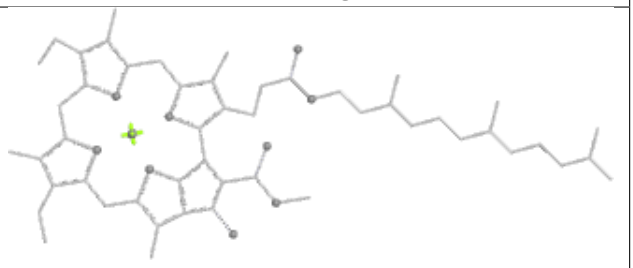
Bond angles



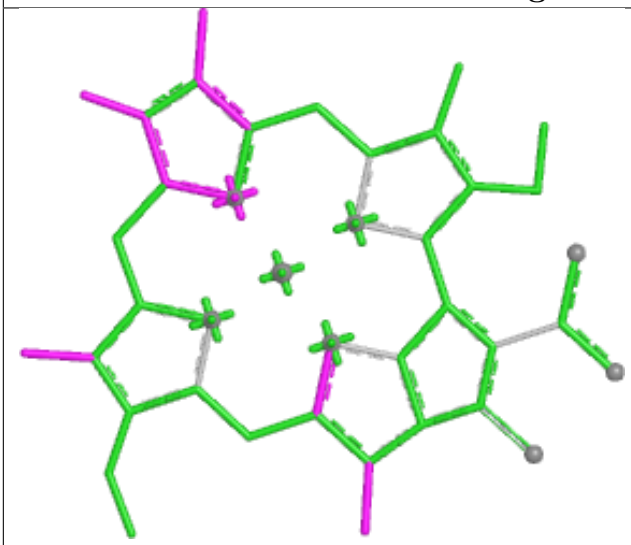
Torsions



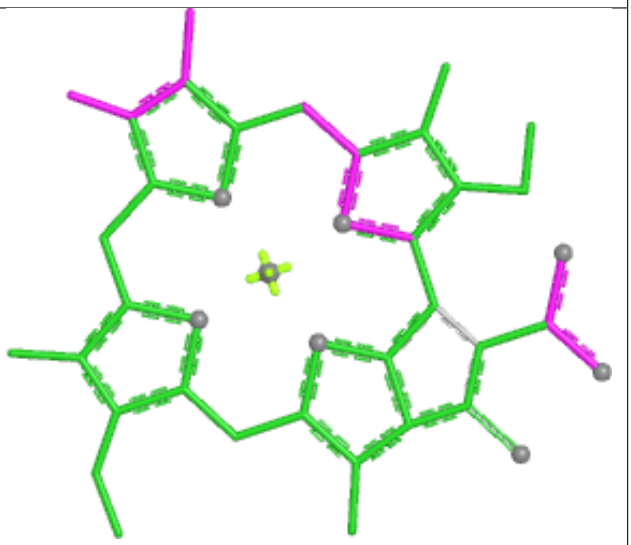
Rings

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

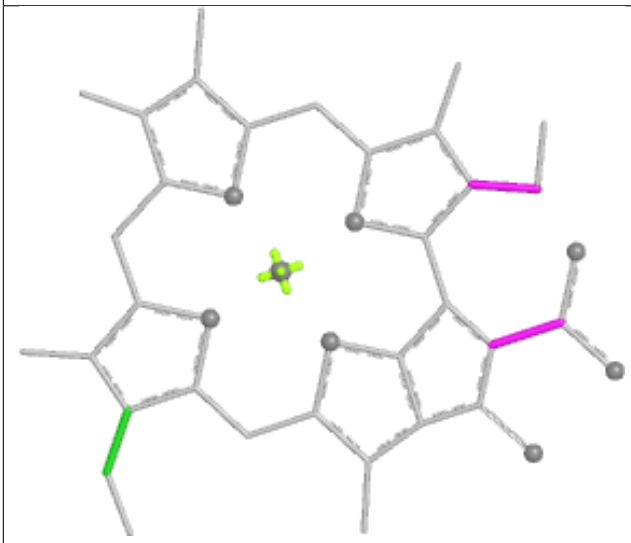
Ligand CLA 5 618



Bond lengths



Bond angles

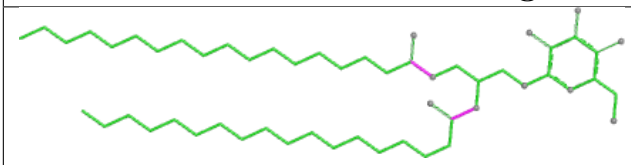


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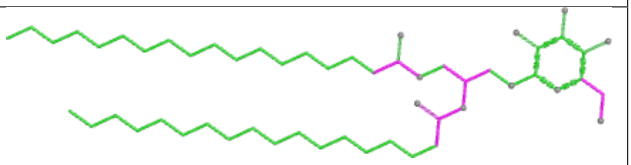


Rings

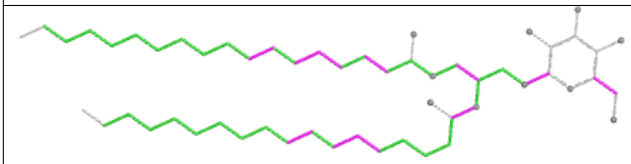
Ligand LMG H 205



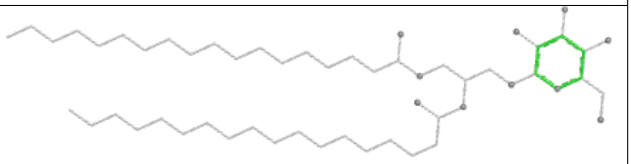
Bond lengths



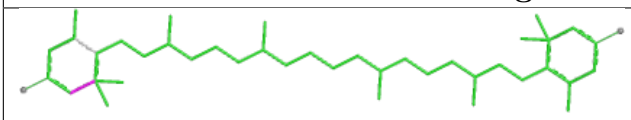
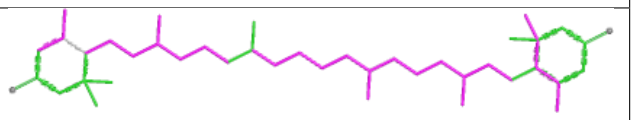
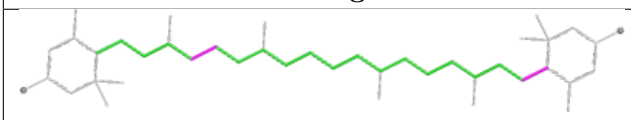
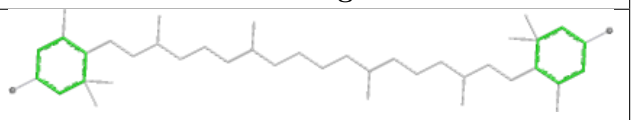
Bond angles

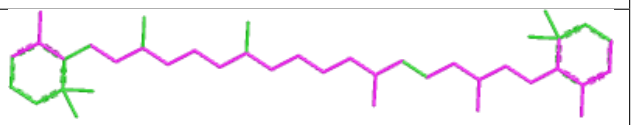
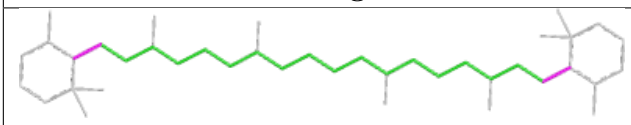
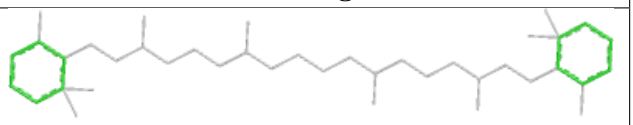


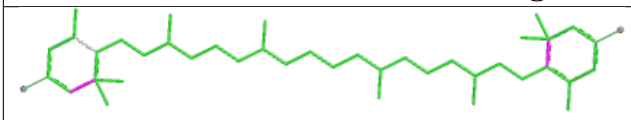
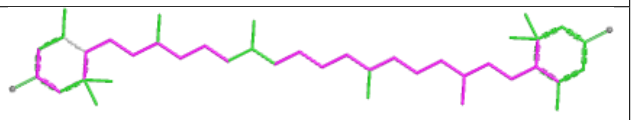
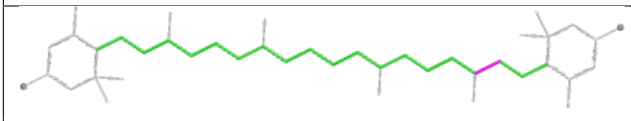
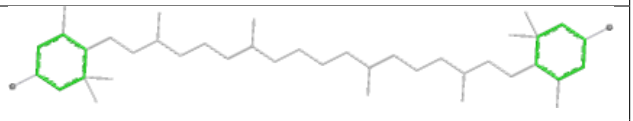
Torsions

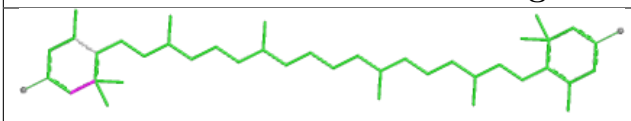
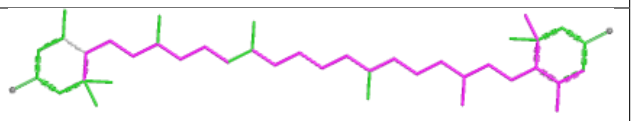
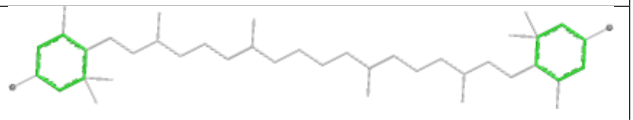


Rings

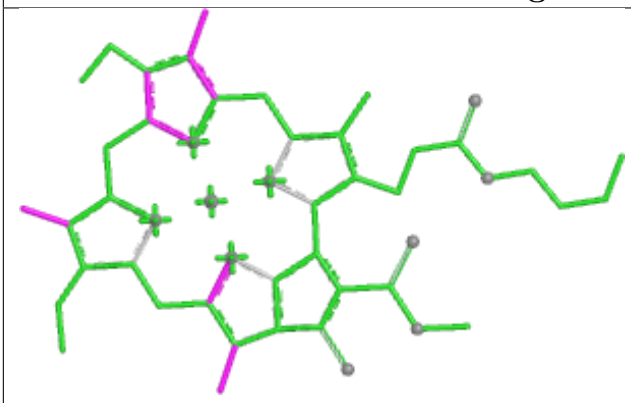
Ligand LUT X 1621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR K 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

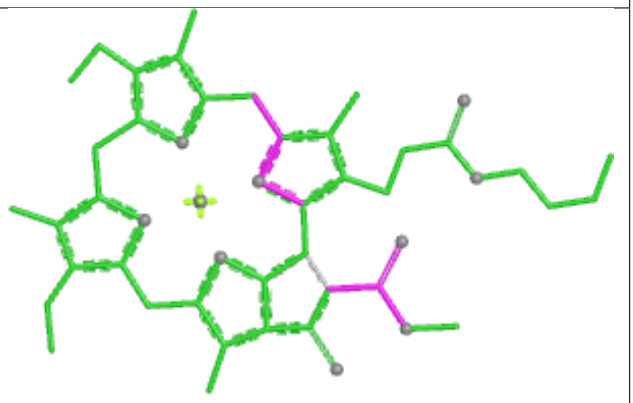
Ligand LUT 2 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT a 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

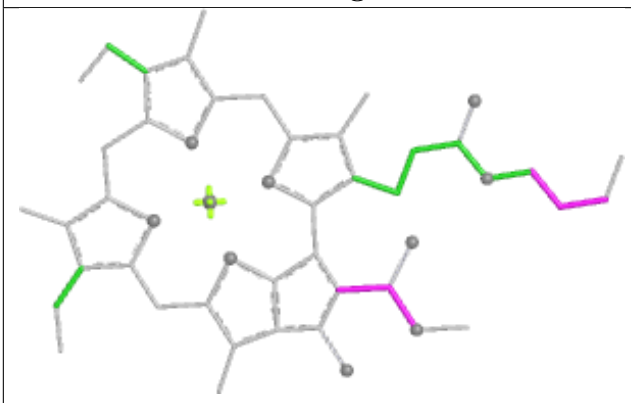
Ligand CLA 1 604



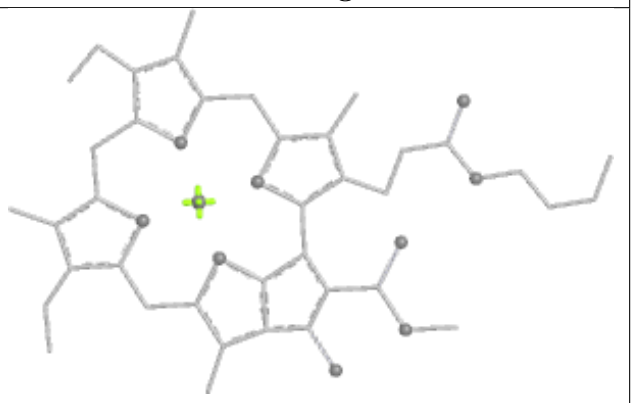
Bond lengths



Bond angles

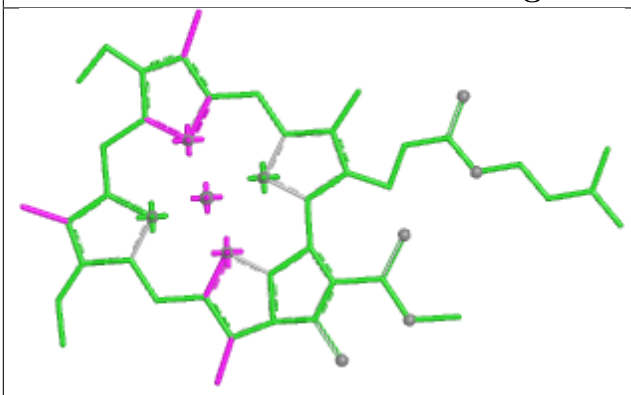


Torsions

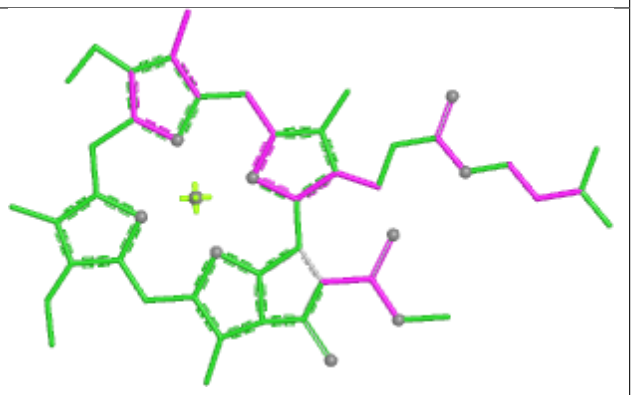


Rings

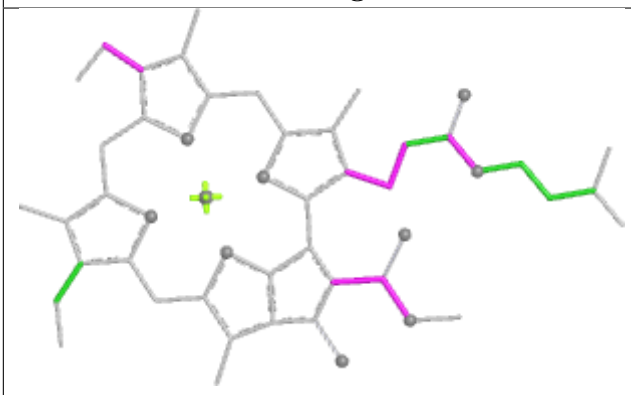
Ligand CLA A 832



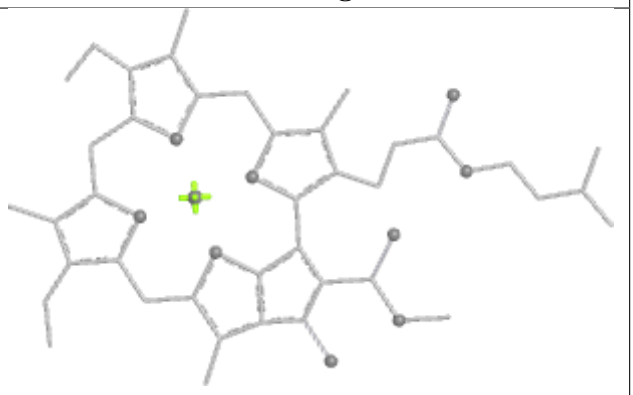
Bond lengths



Bond angles

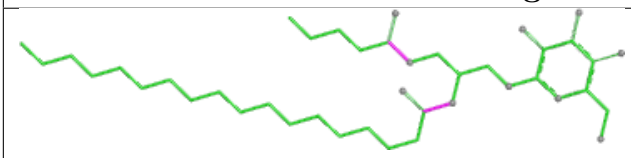


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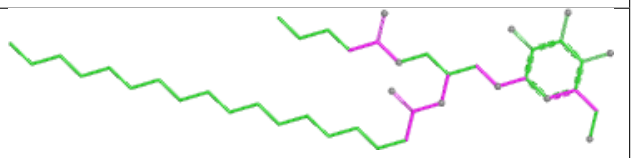


Rings

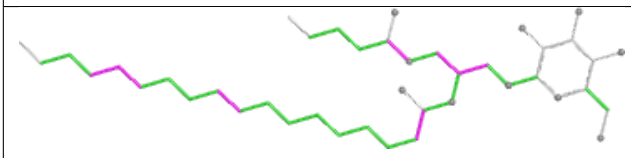
Ligand LMG J 103



Bond lengths



Bond angles

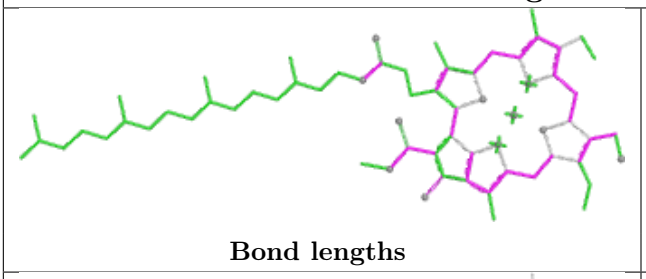


Torsions

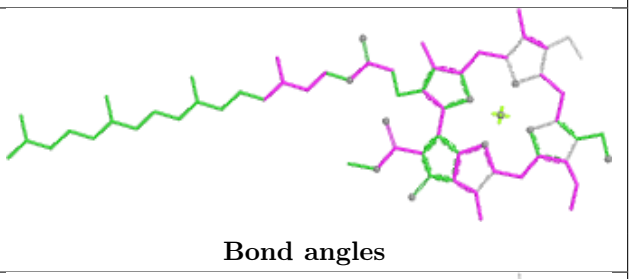


Rings

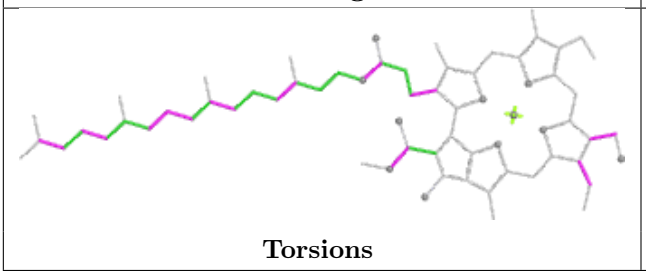
Ligand CHL Z 609



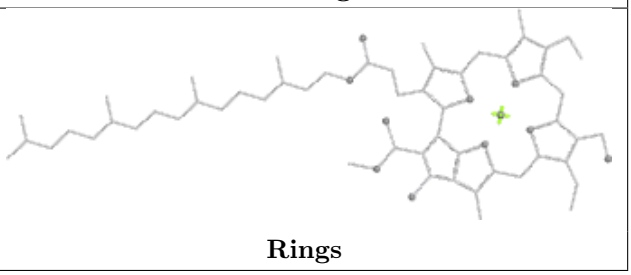
Bond lengths



Bond angles

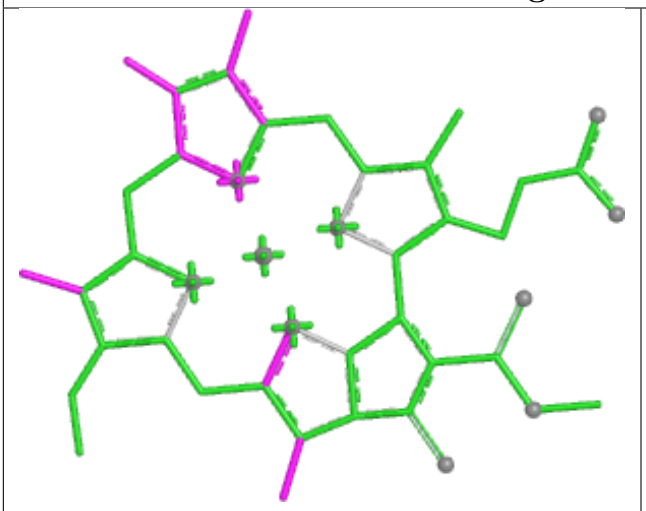


Torsions

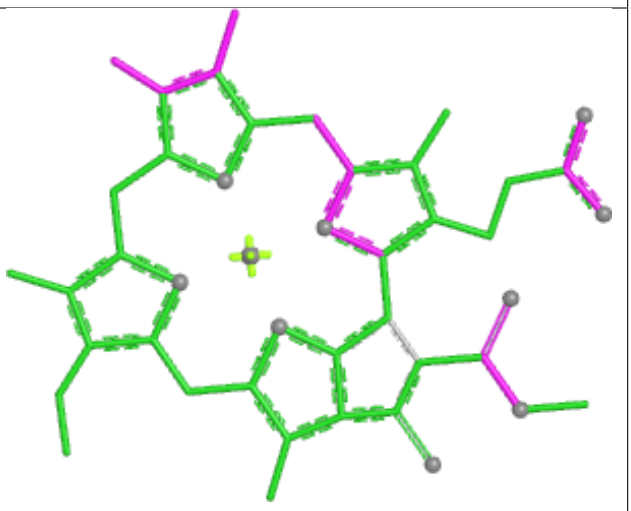


Rings

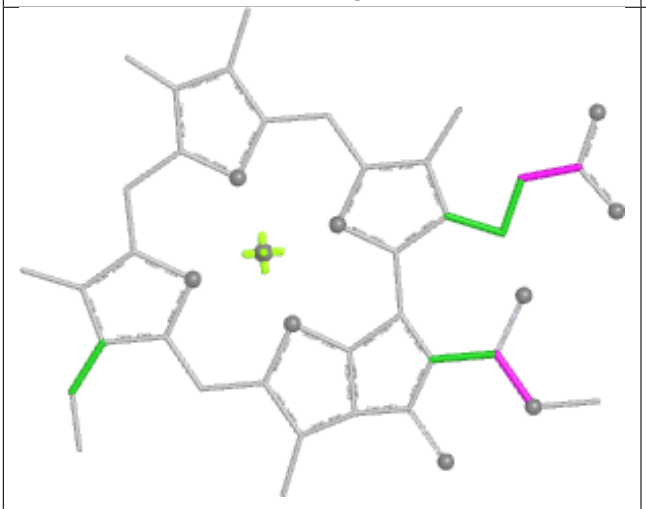
Ligand CLA 4 603



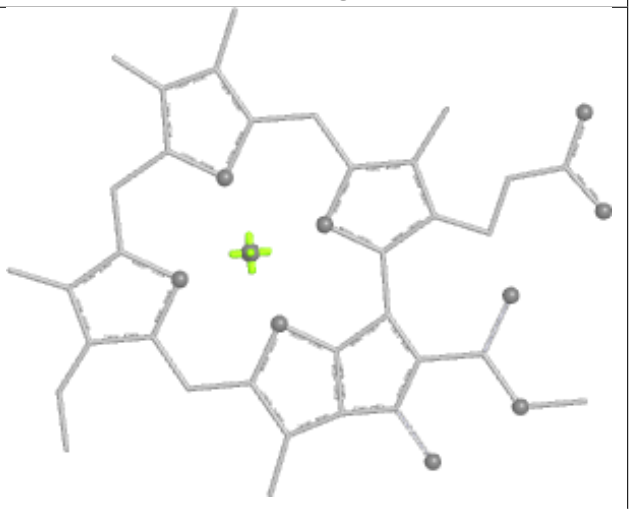
Bond lengths



Bond angles

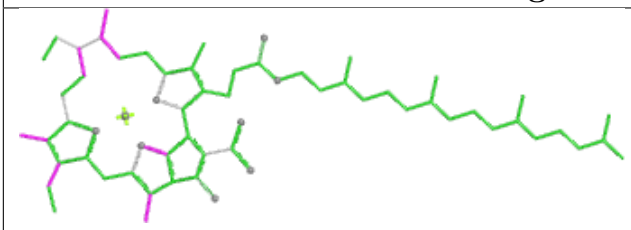


Torsions

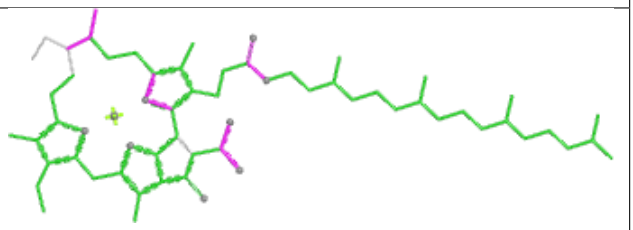


Rings

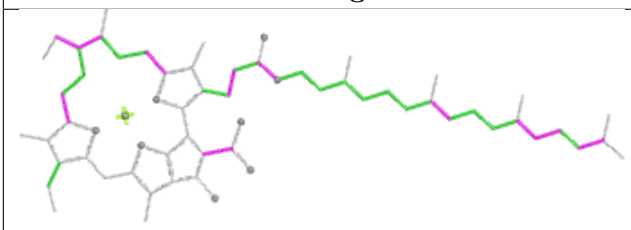
Ligand CLA 2 602



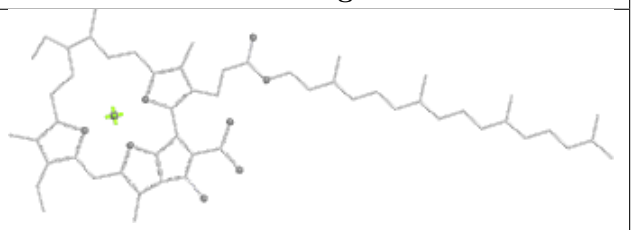
Bond lengths



Bond angles

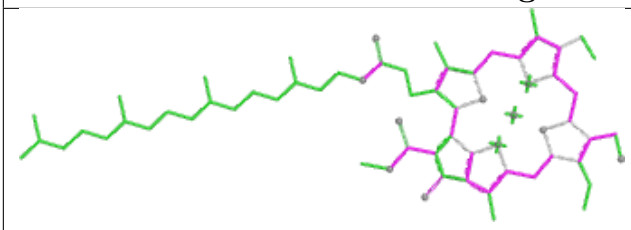


Torsions

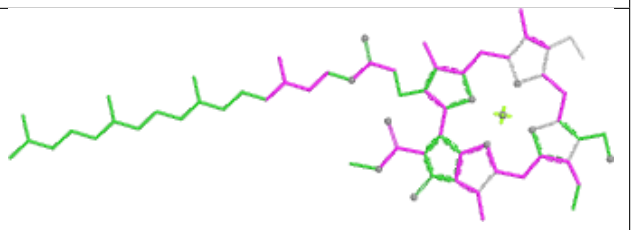


Rings

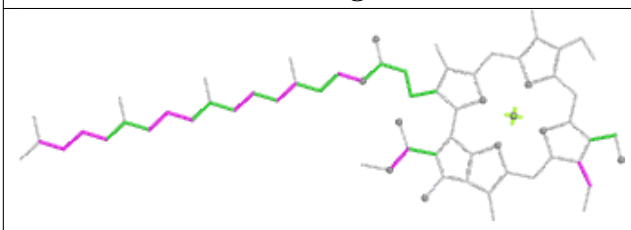
Ligand CHL W 609



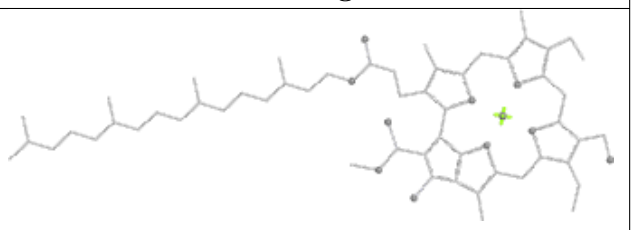
Bond lengths



Bond angles

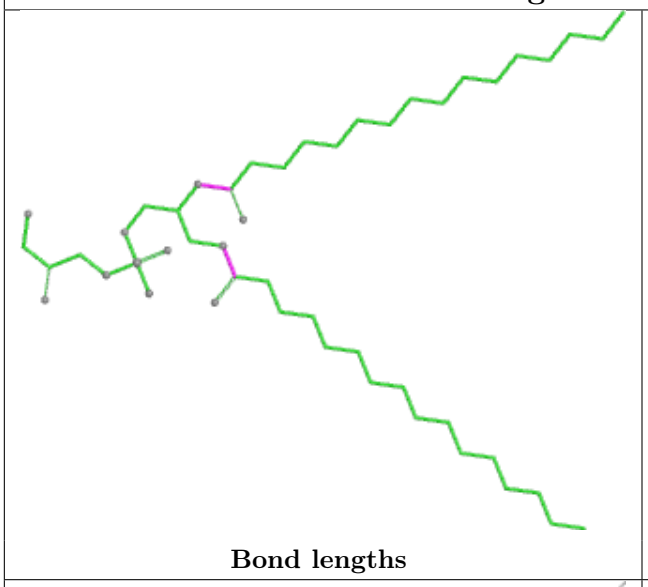


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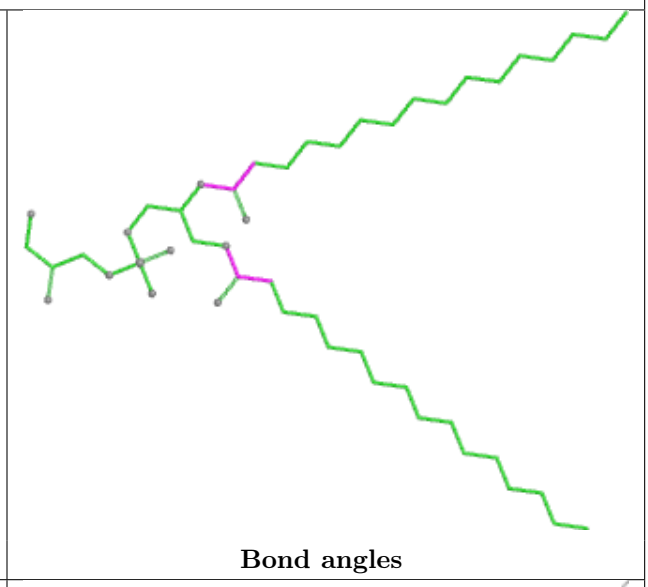


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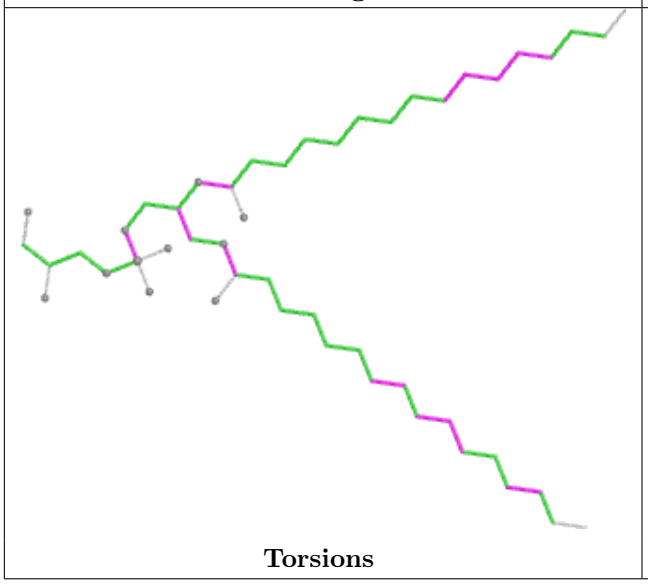
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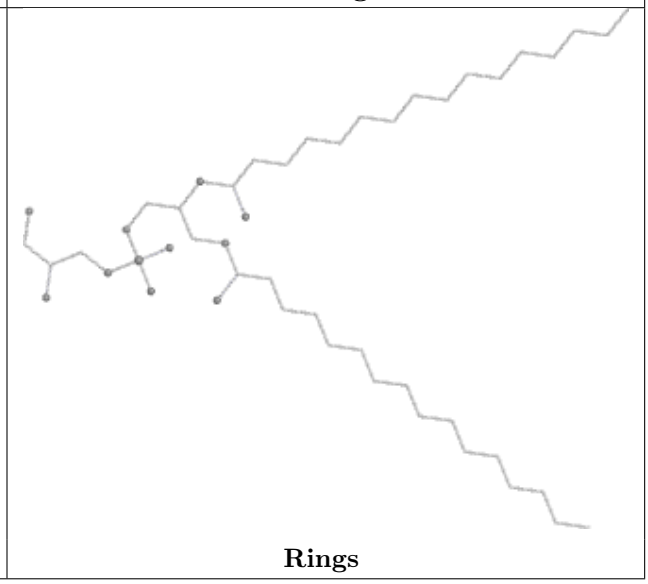
Bond lengths



Bond angles

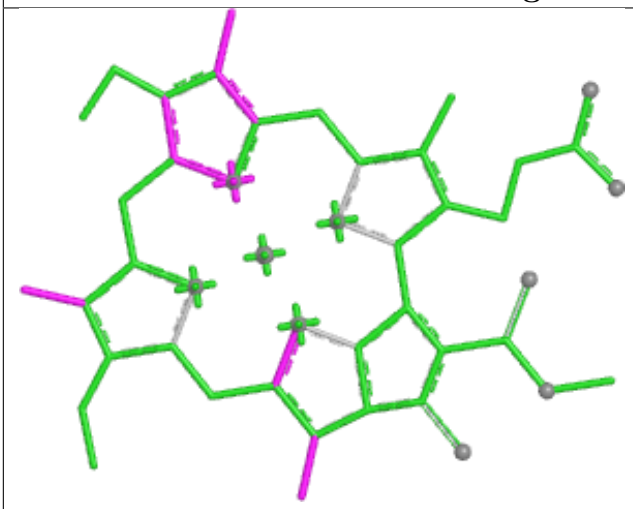


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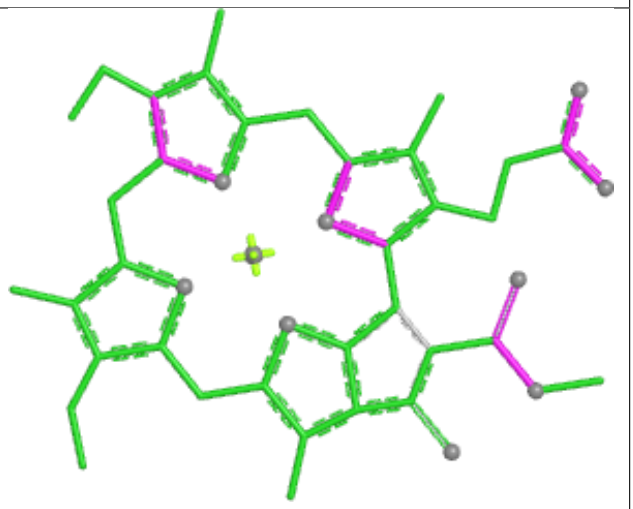


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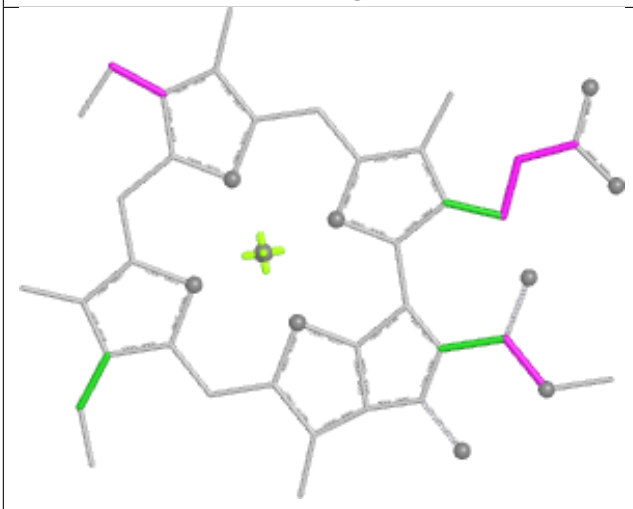
Ligand CLA G 204



Bond lengths



Bond angles

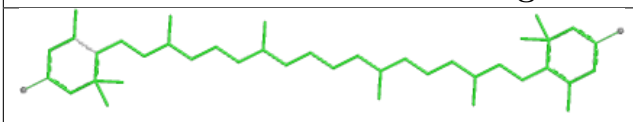


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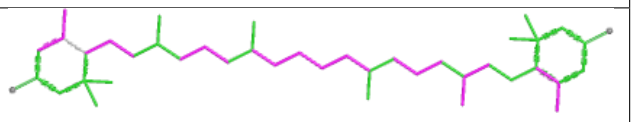


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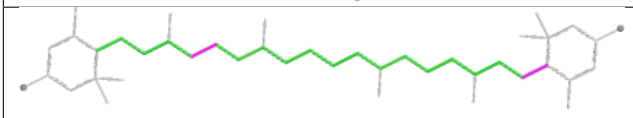
Ligand LUT Z 1621



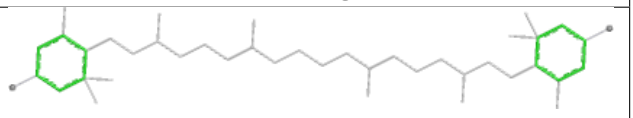
Bond lengths



Bond angles

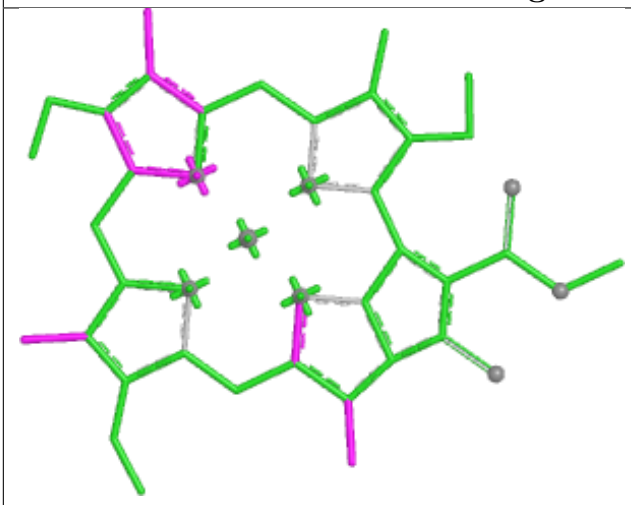


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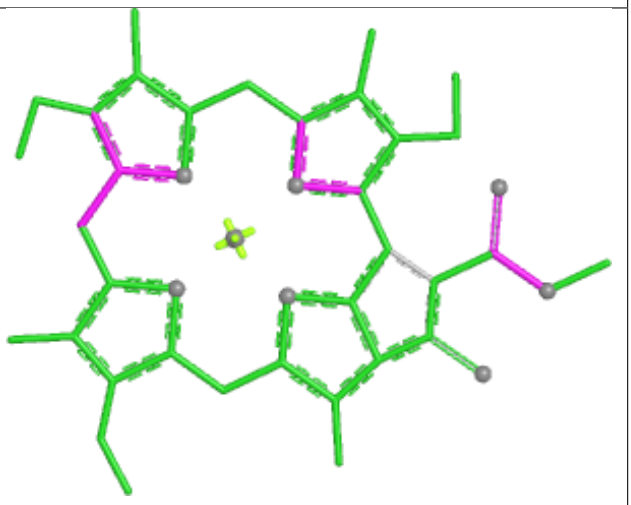


Rings

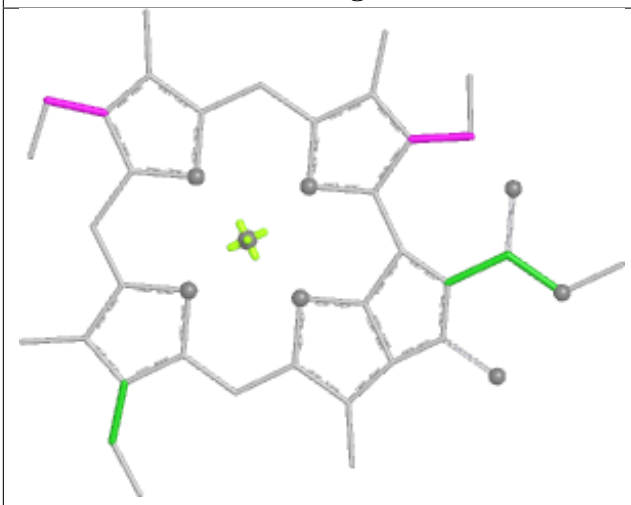
Ligand CLA 7 614



Bond lengths



Bond angles



Torsions

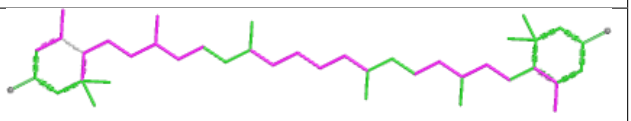


Rings

Ligand LUT X 1620



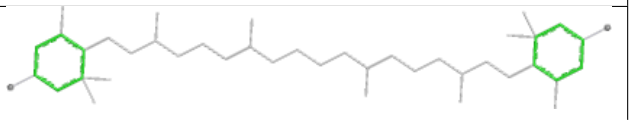
Bond lengths



Bond angles

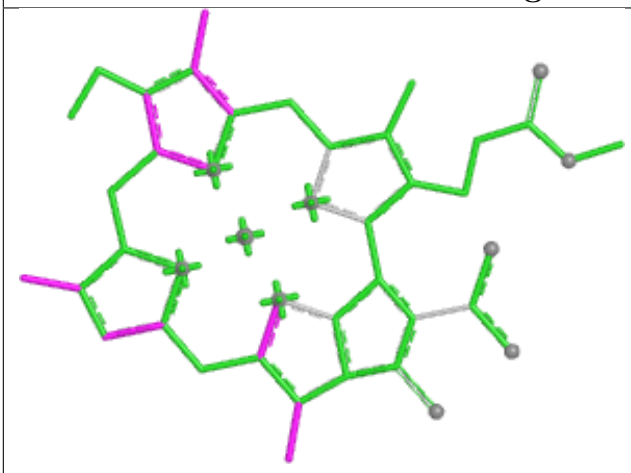


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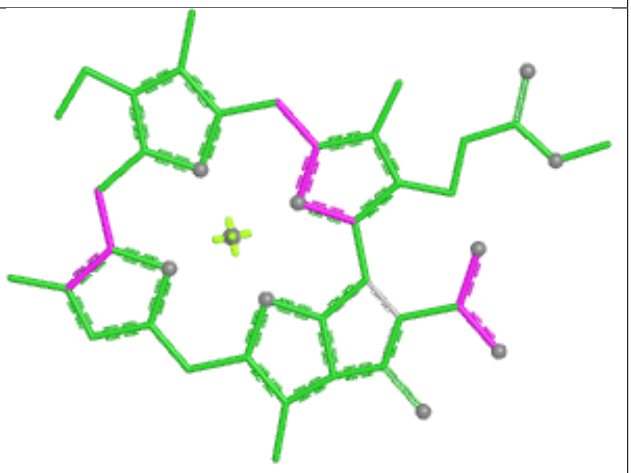


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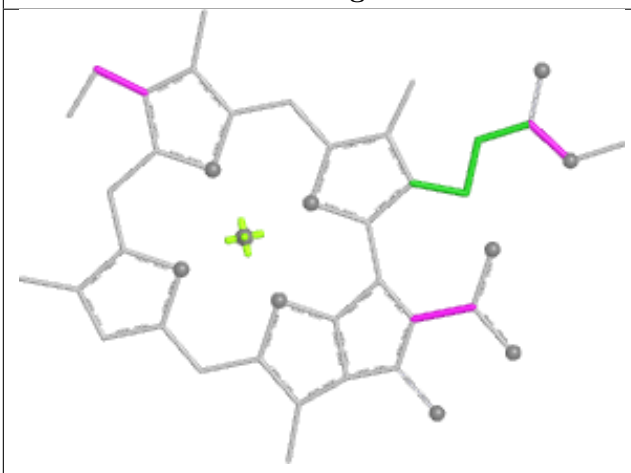
Ligand CLA B 821



Bond lengths



Bond angles

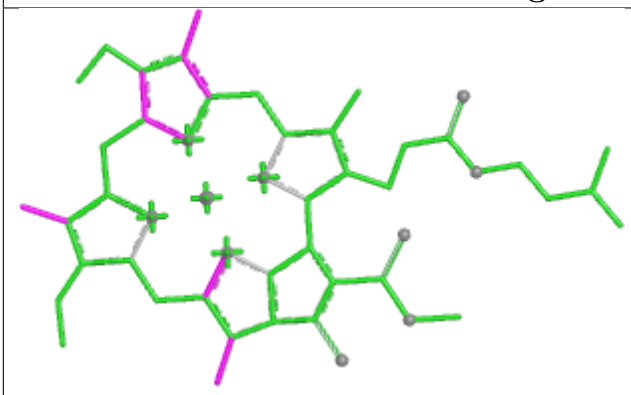


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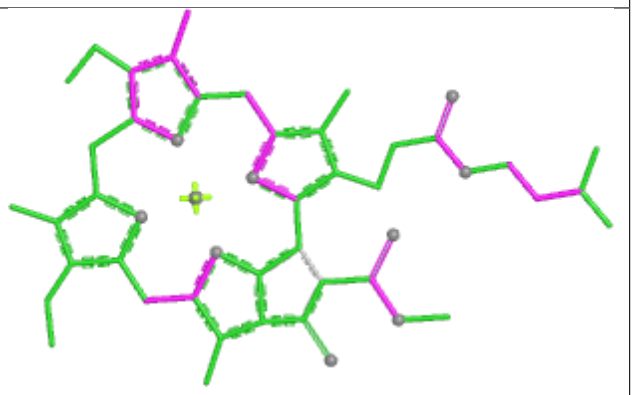


Rings

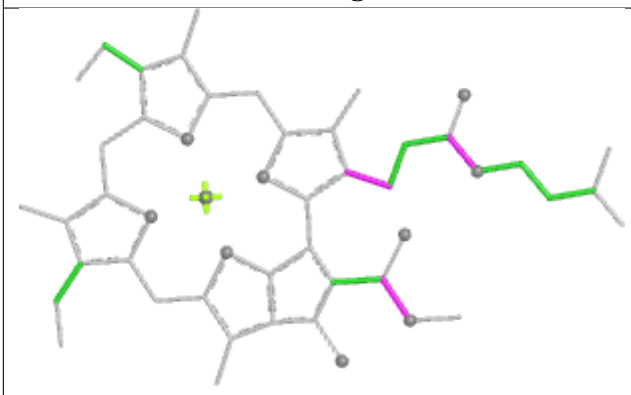
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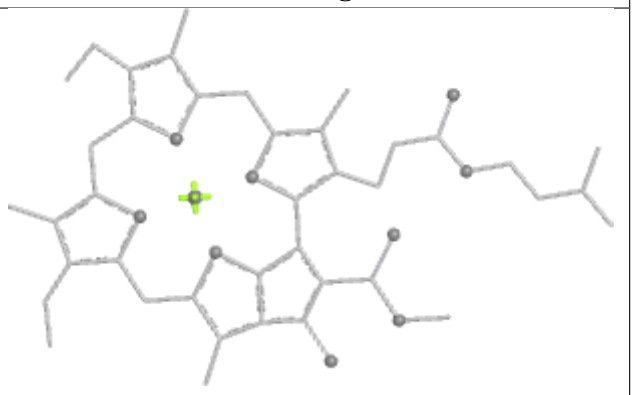
Bond lengths



Bond angles

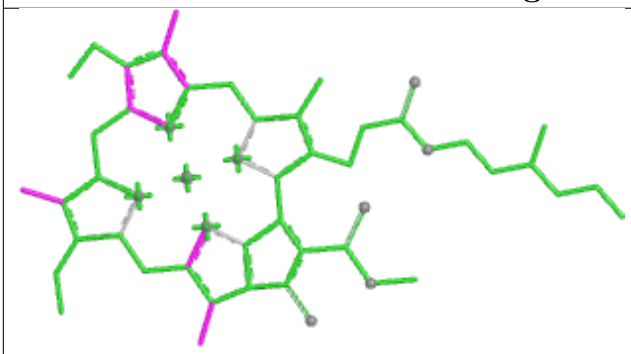


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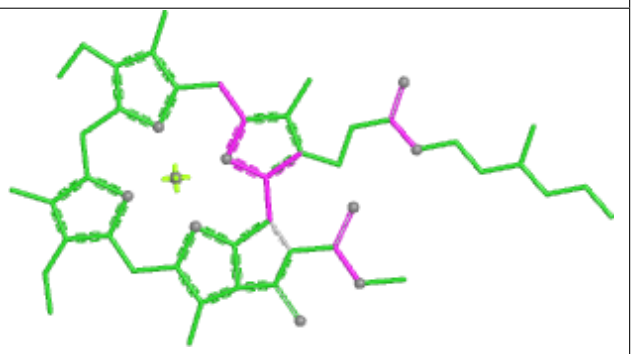


Rings

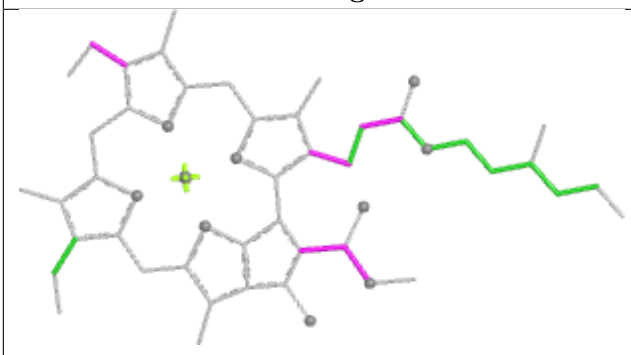
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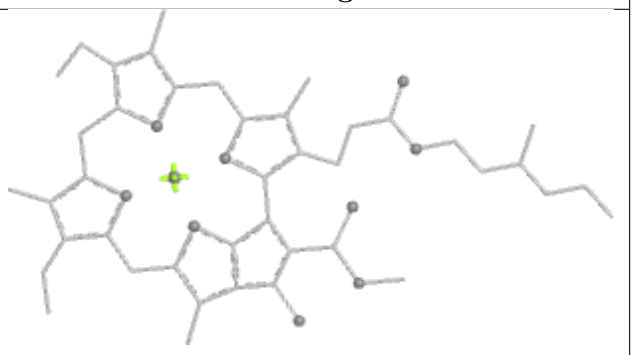
Bond lengths



Bond angles

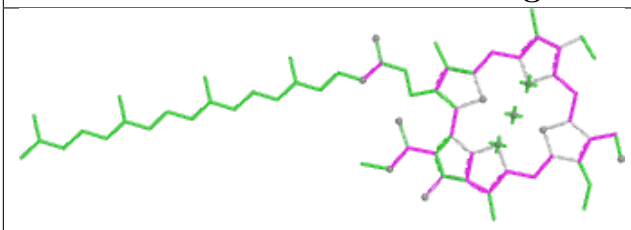


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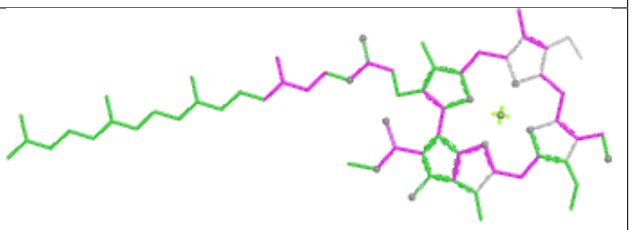


Rings

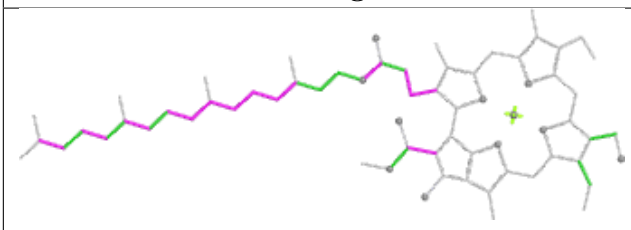
Ligand CHL Y 601



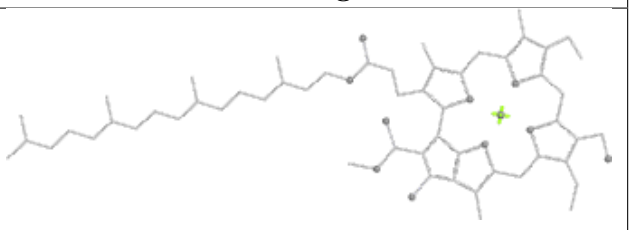
Bond lengths



Bond angles

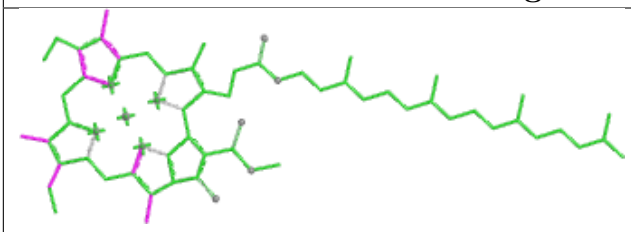


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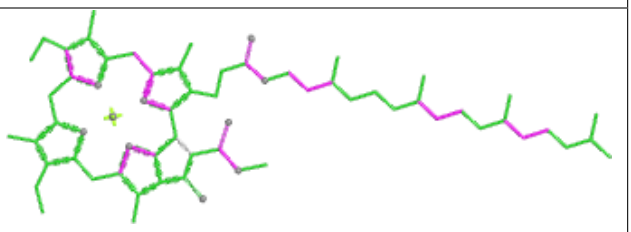


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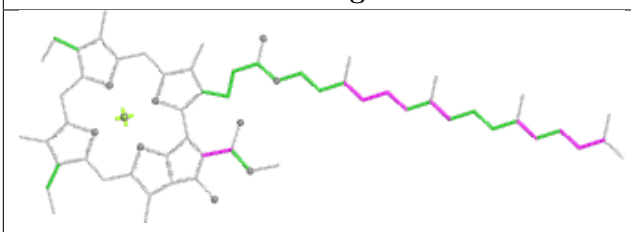
Ligand CLA B 808



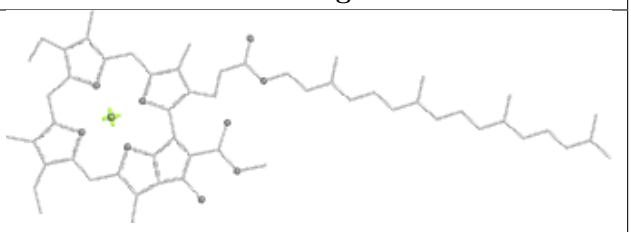
Bond lengths



Bond angles

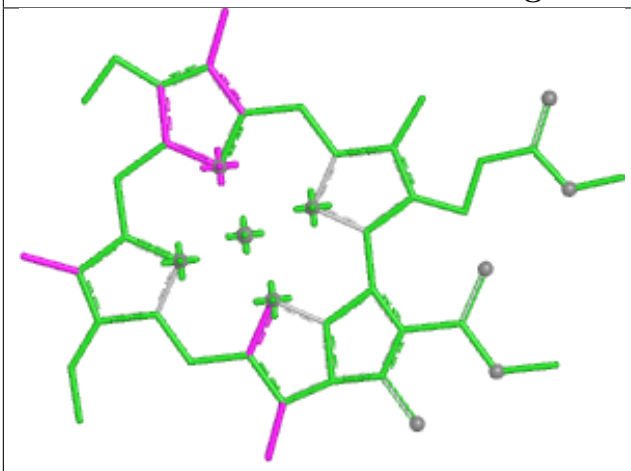


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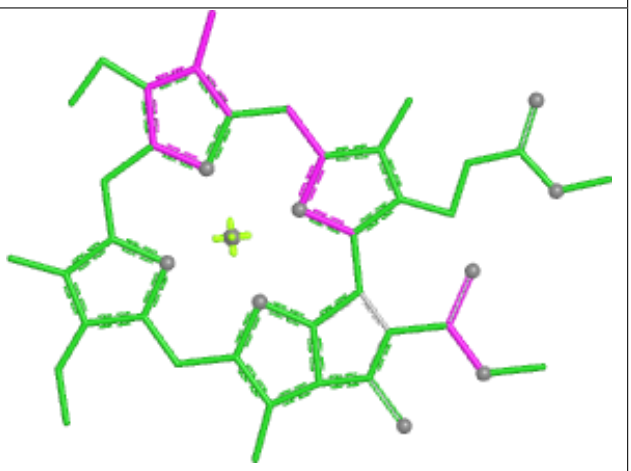


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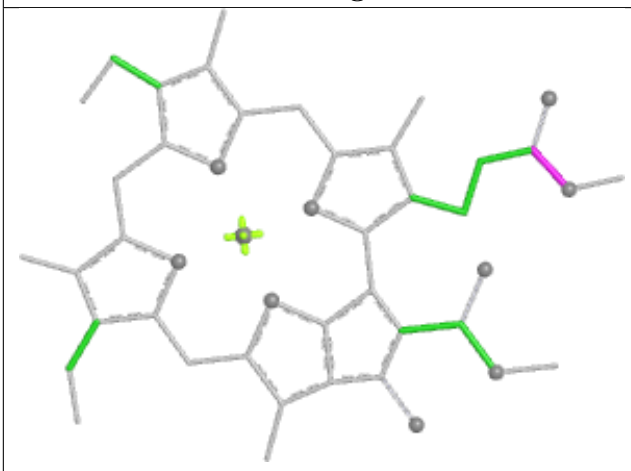
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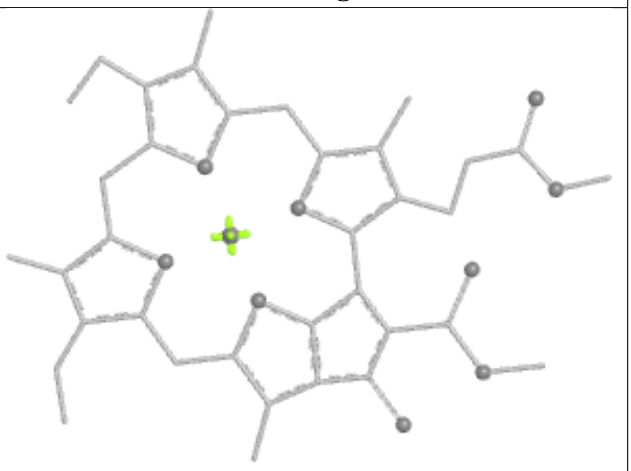
Bond lengths



Bond angles

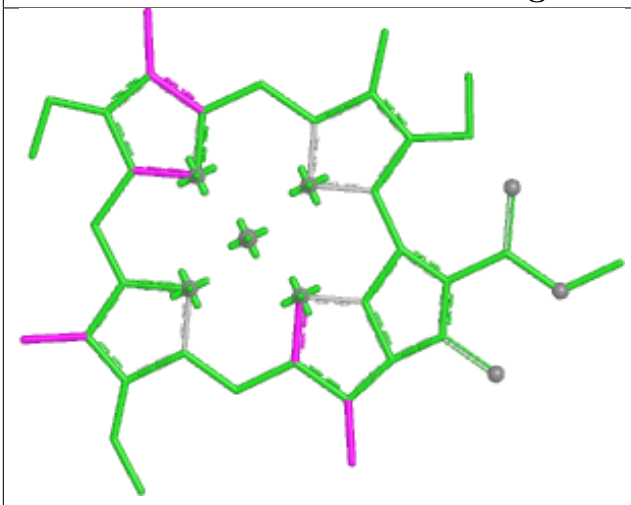


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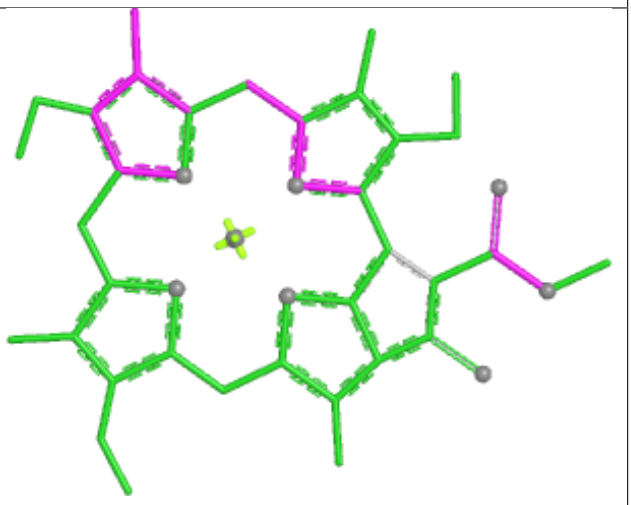


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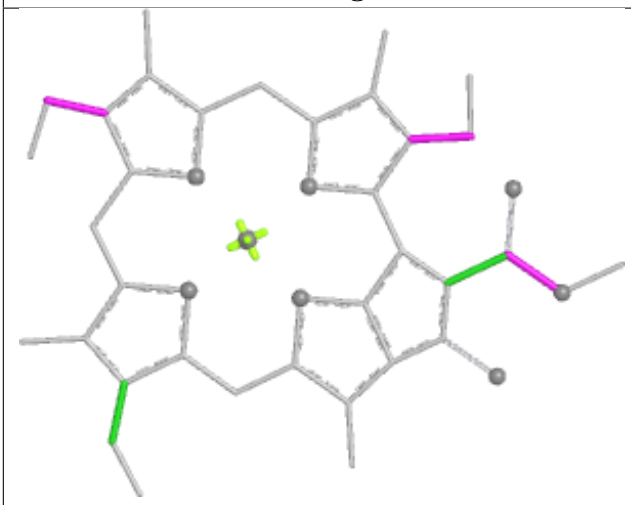
Ligand CLA 4 611



Bond lengths



Bond angles



Torsions

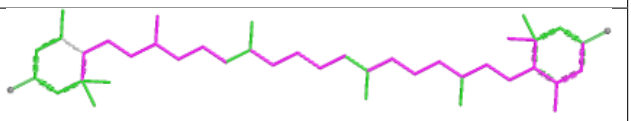


Rings

Ligand LUT 5 620



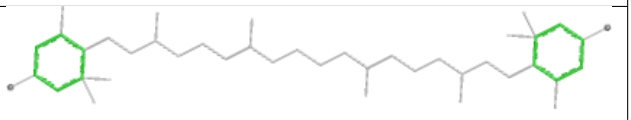
Bond lengths



Bond angles

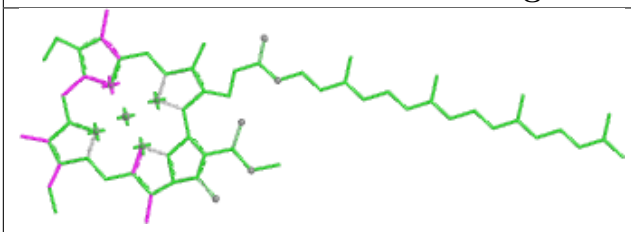


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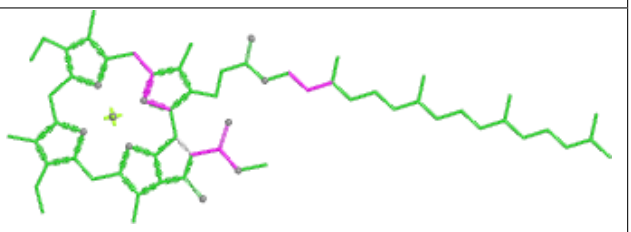


Rings

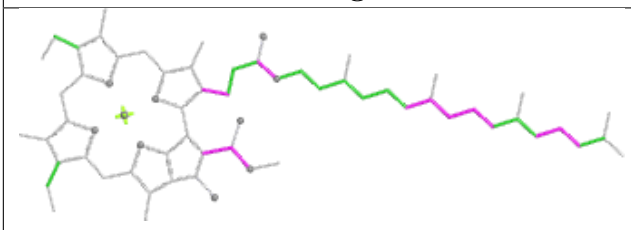
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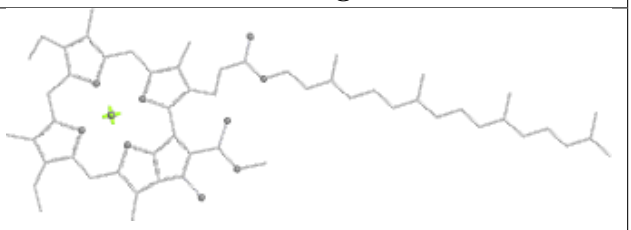
Bond lengths



Bond angles

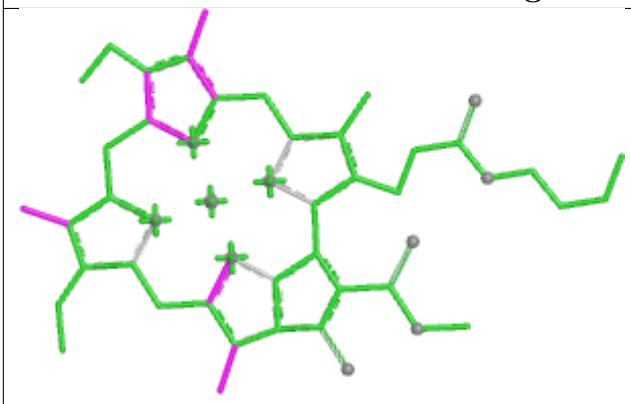


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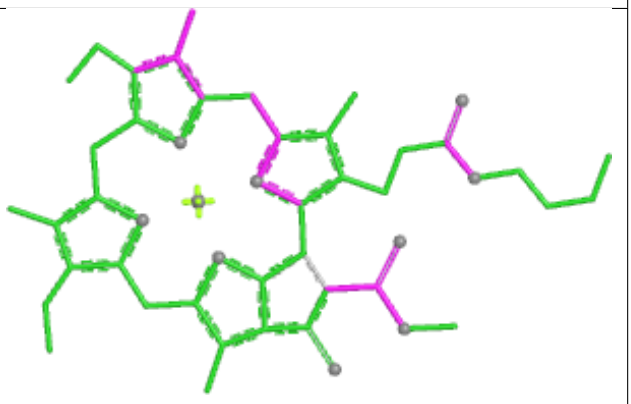


Rings

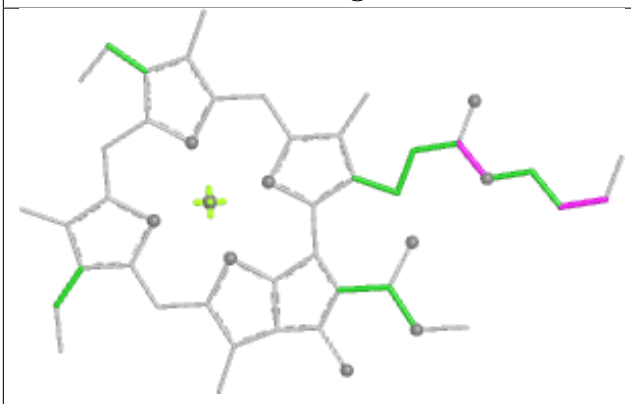
Ligand CLA B 825



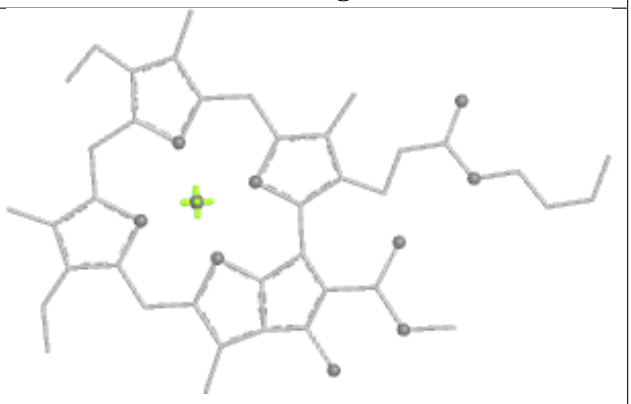
Bond lengths



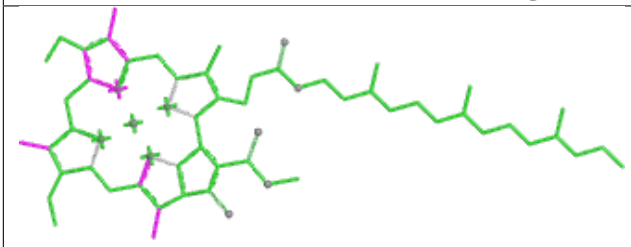
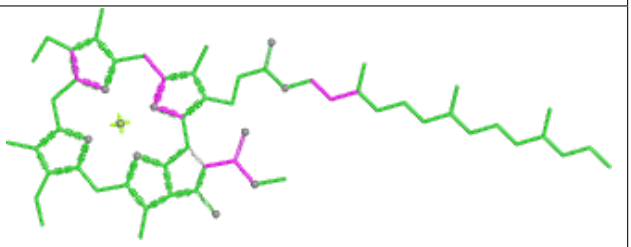
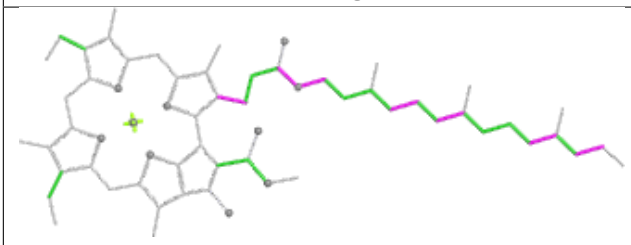
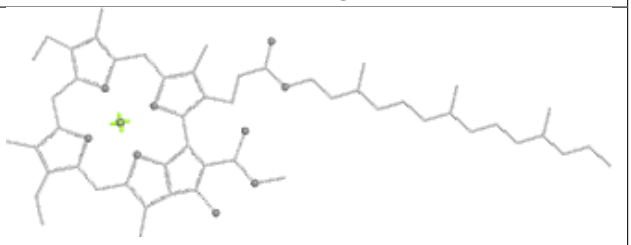
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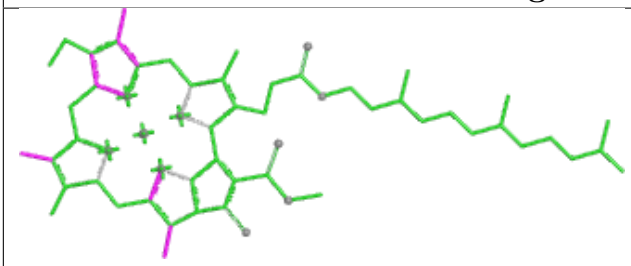
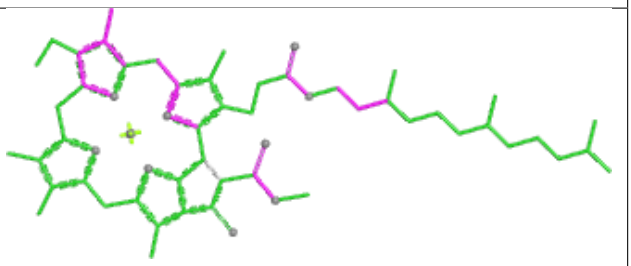
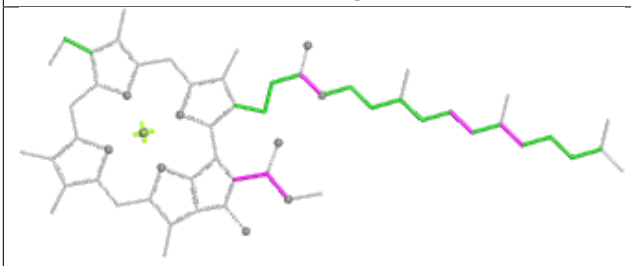
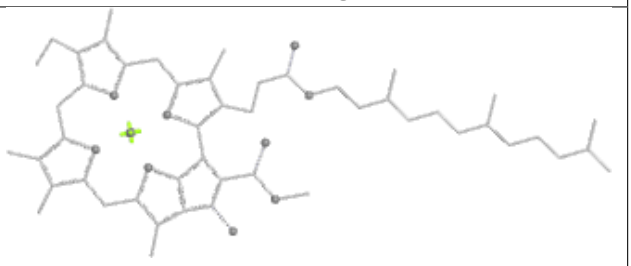


Torsions

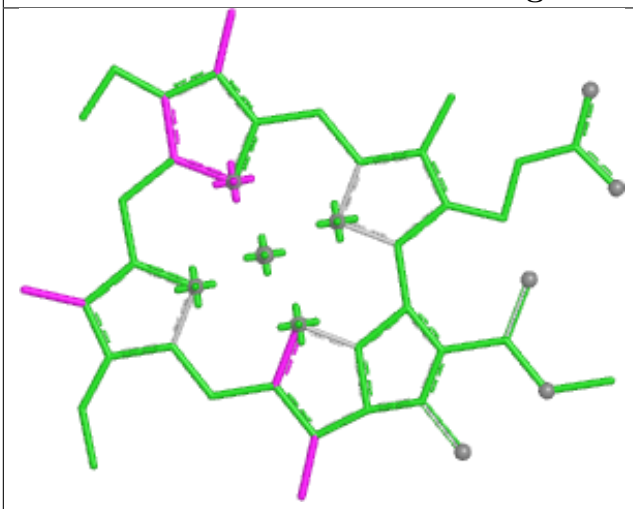


Rings

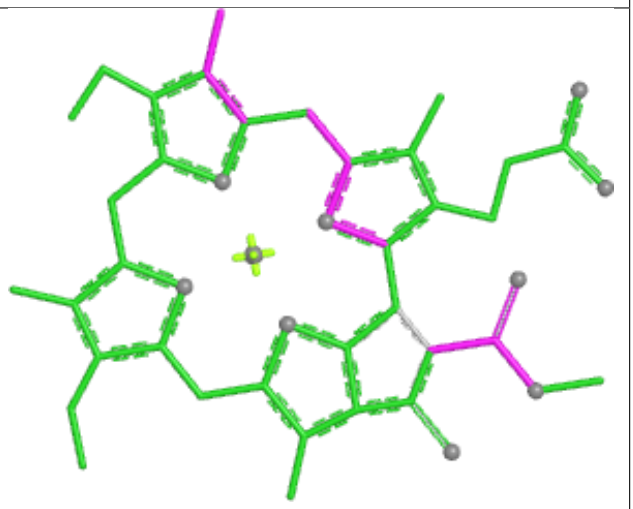
Ligand CLA B 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

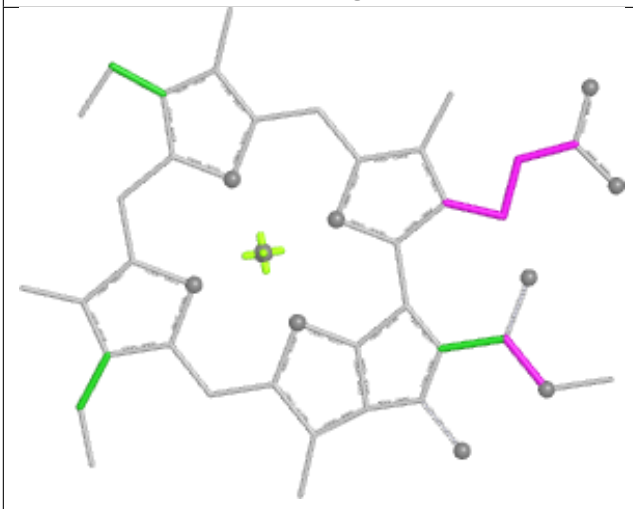
Ligand CLA L 302



Bond lengths



Bond angles

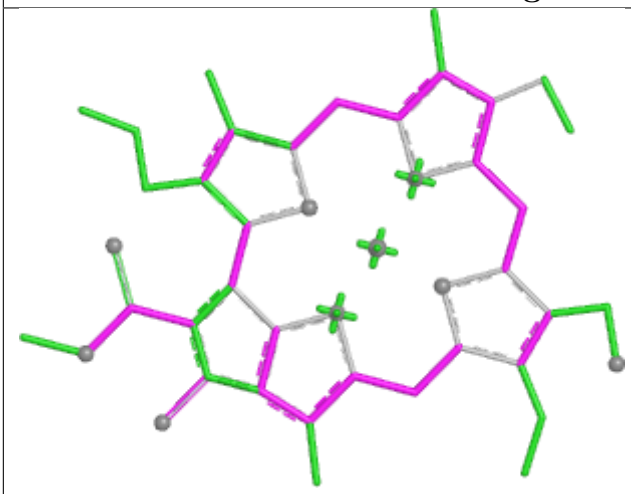


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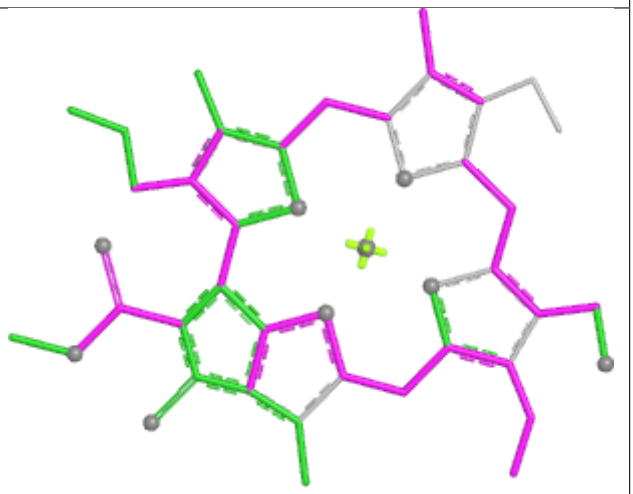


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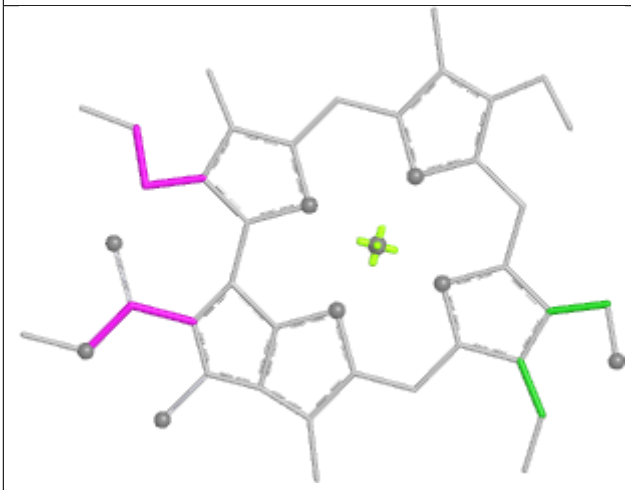
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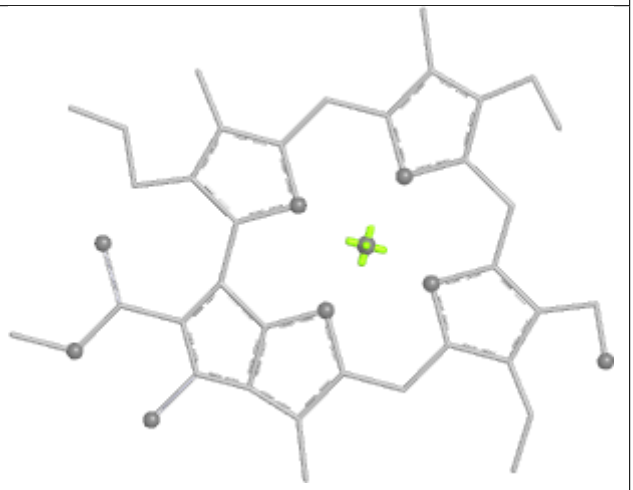
Bond lengths



Bond angles

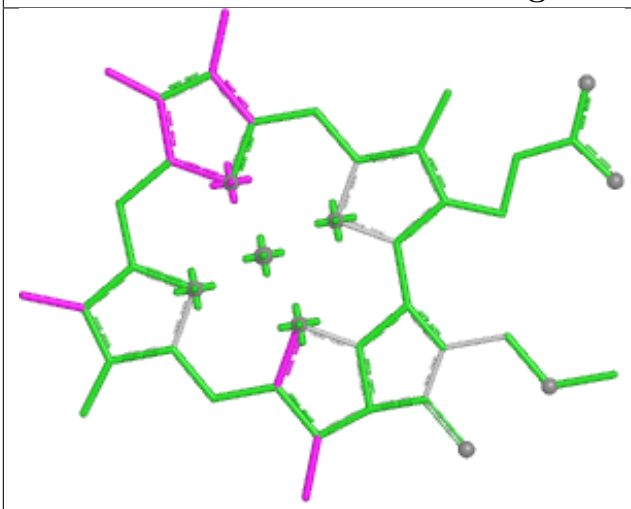


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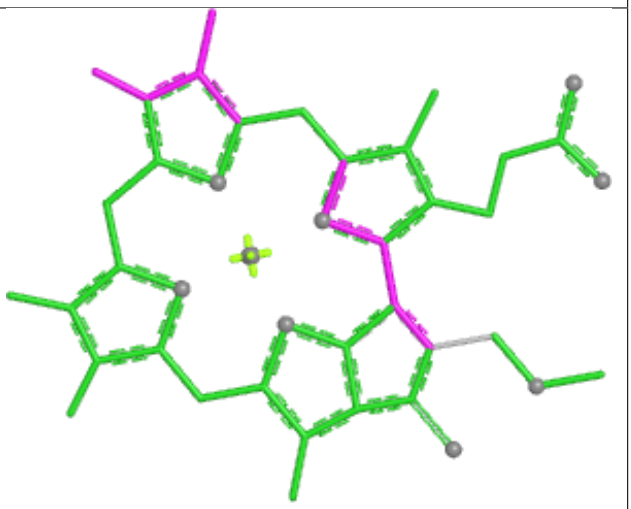


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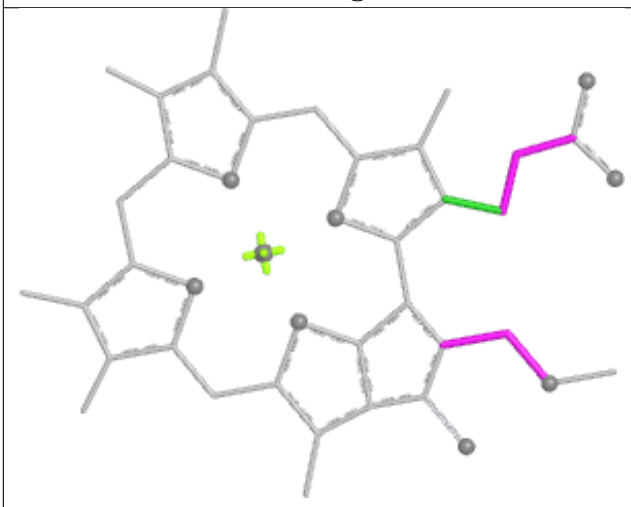
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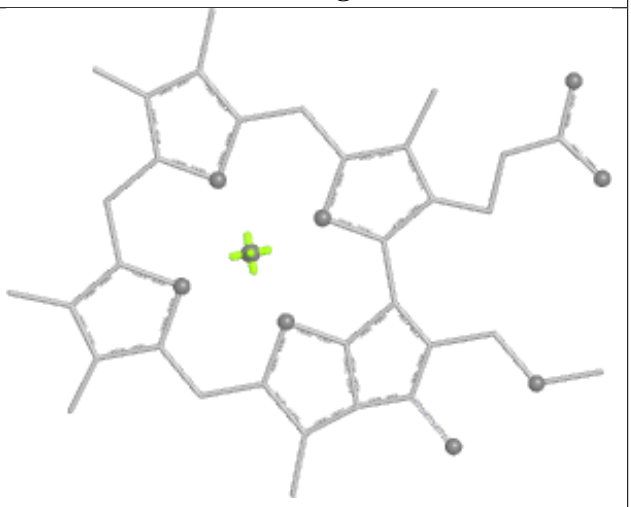
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Bond angles

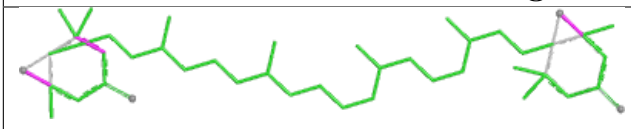


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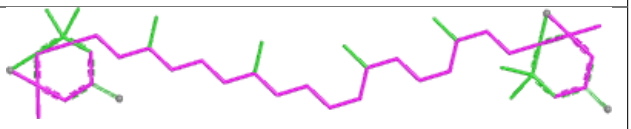


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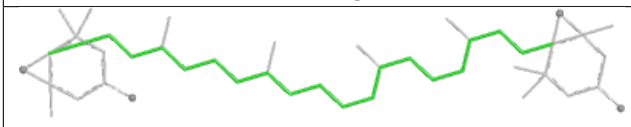
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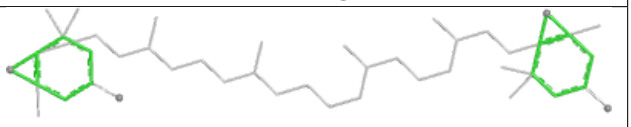
Bond lengths



Bond angles

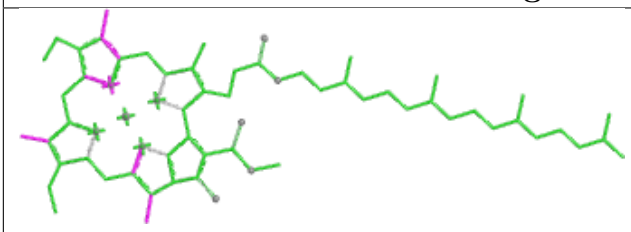


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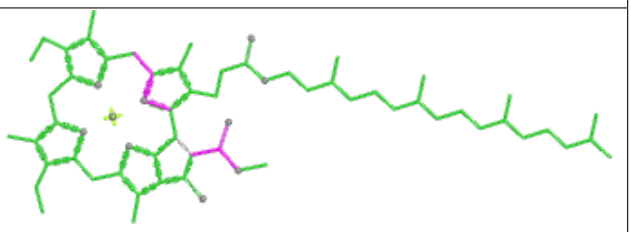


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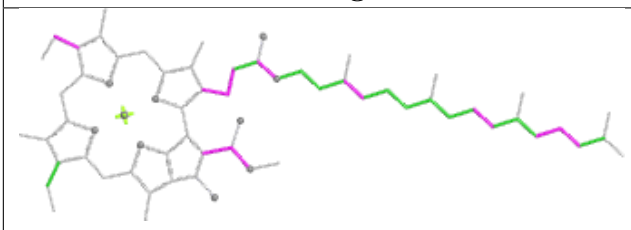
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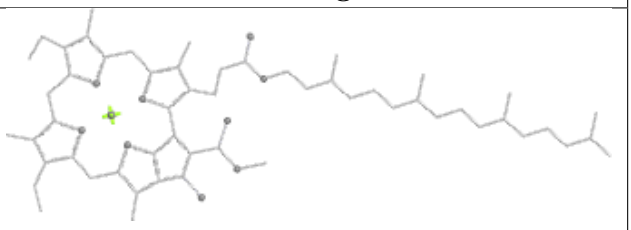
Bond lengths



Bond angles

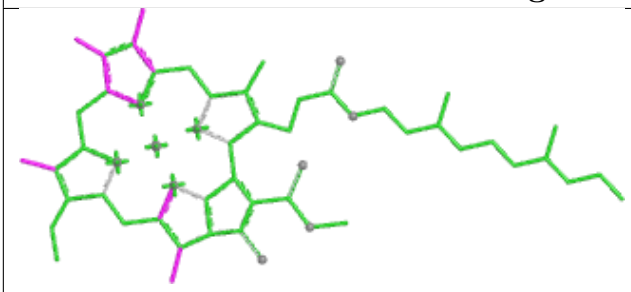


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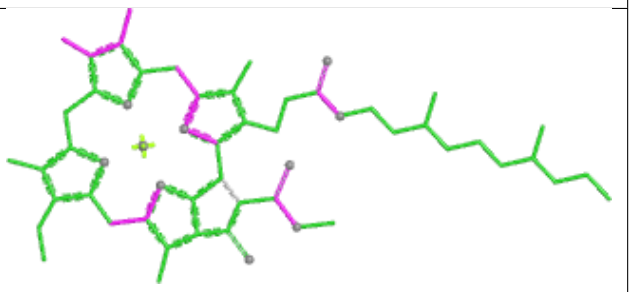


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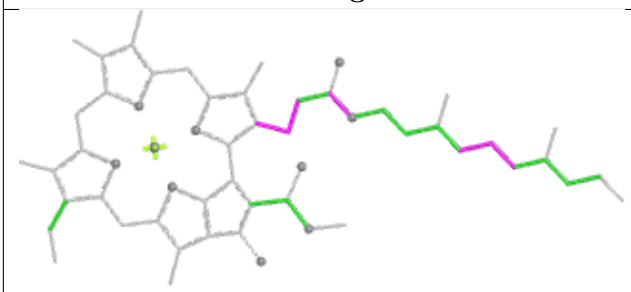
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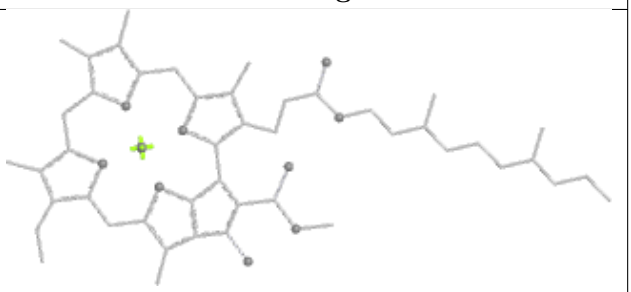
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Bond angles

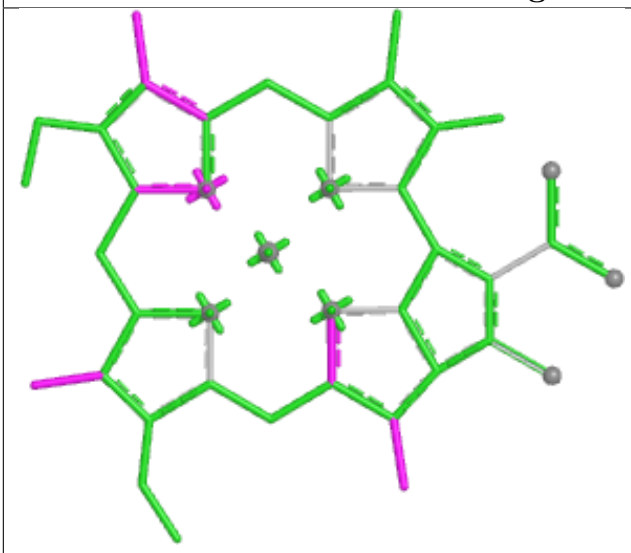


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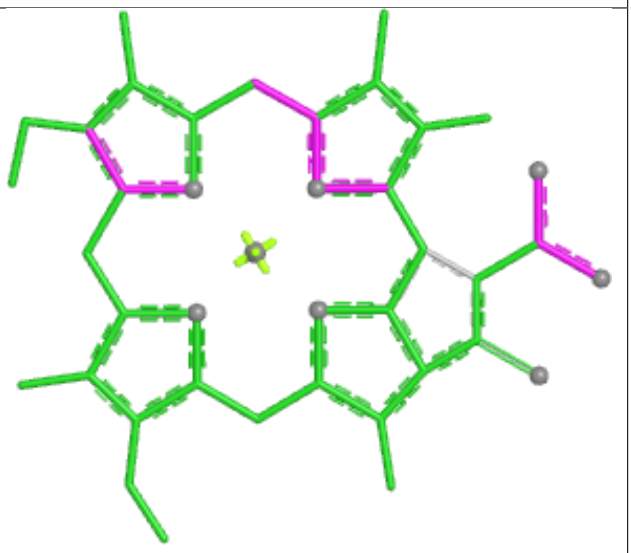


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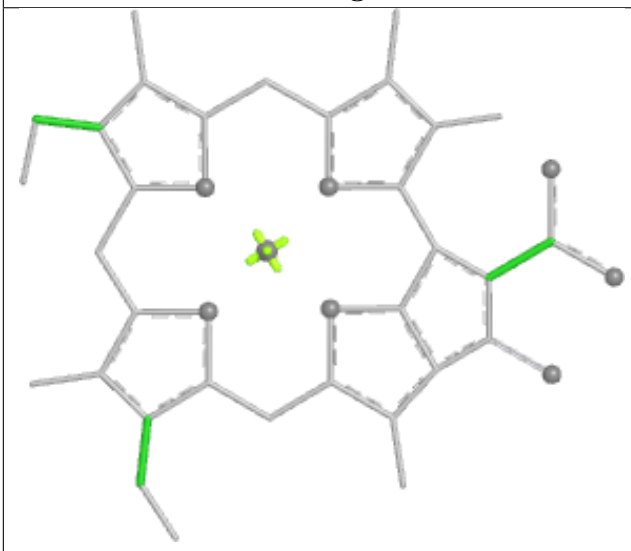
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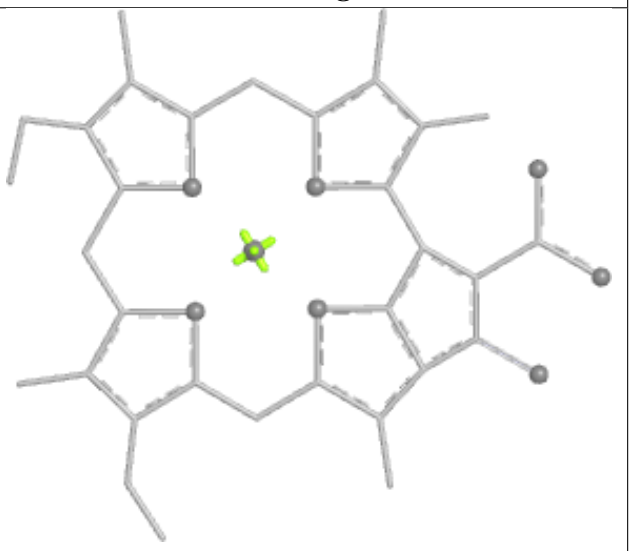
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Bond angles

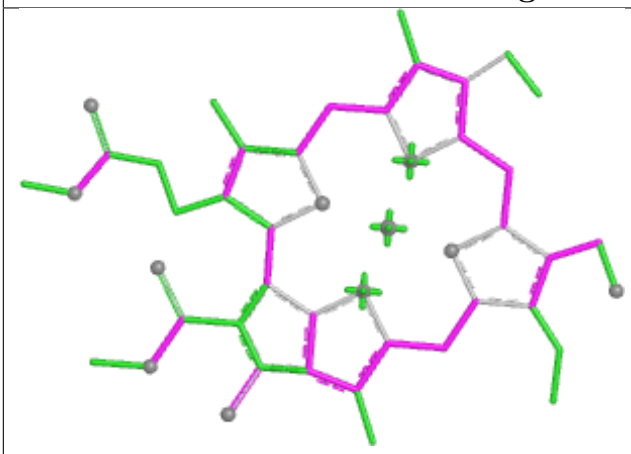


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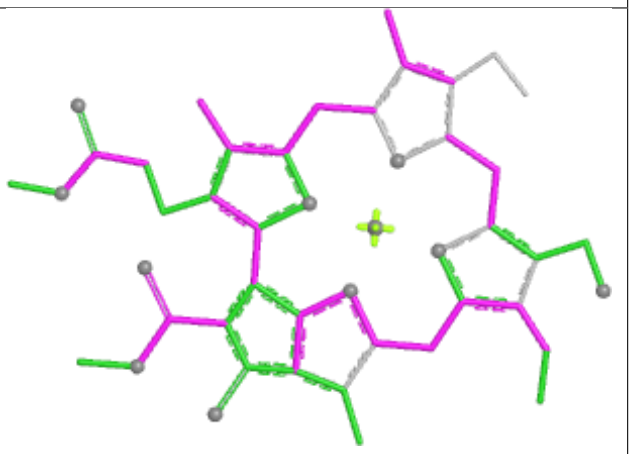


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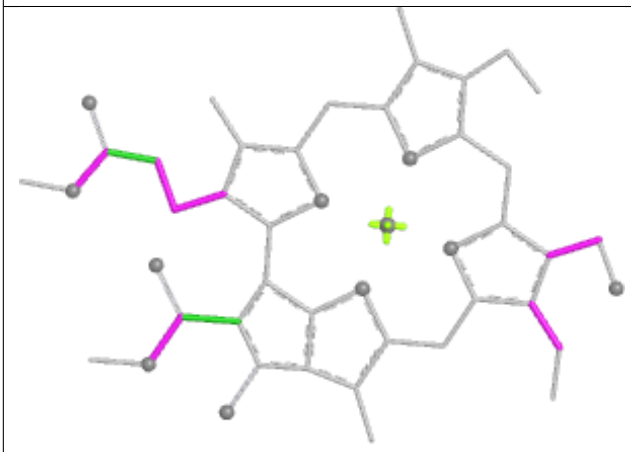
Ligand CHL W 608



Bond lengths



Bond angles

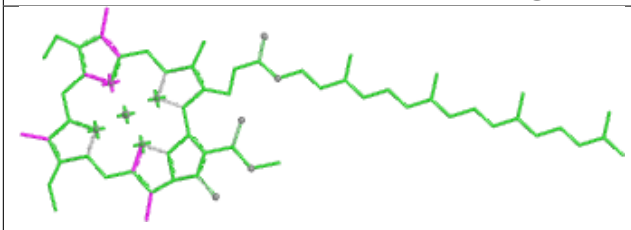


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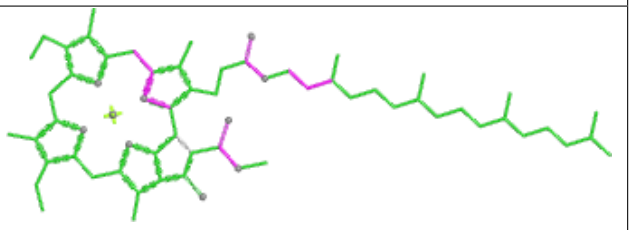


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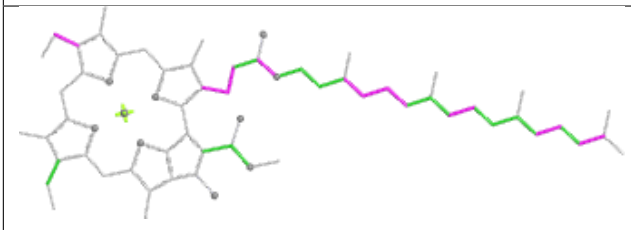
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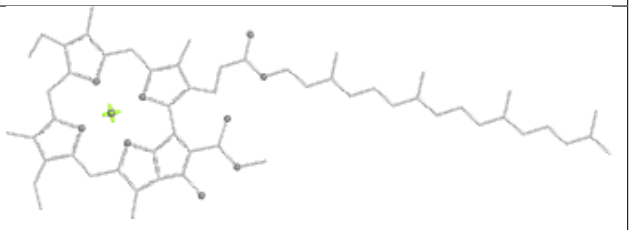
Bond lengths



Bond angles

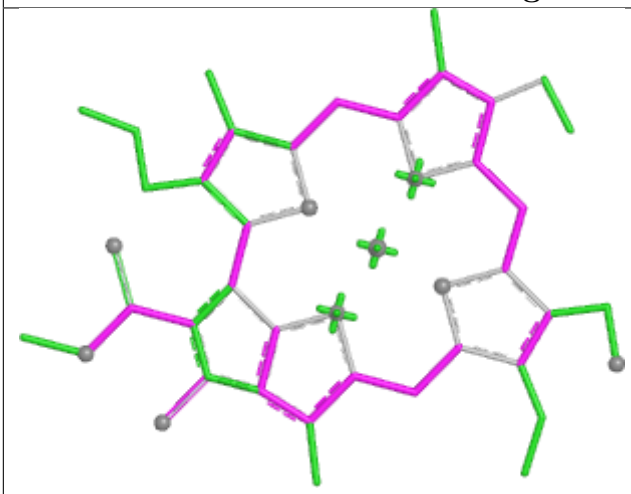


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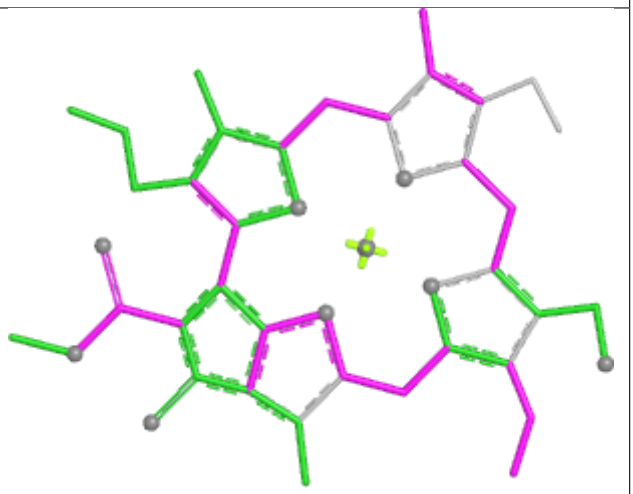


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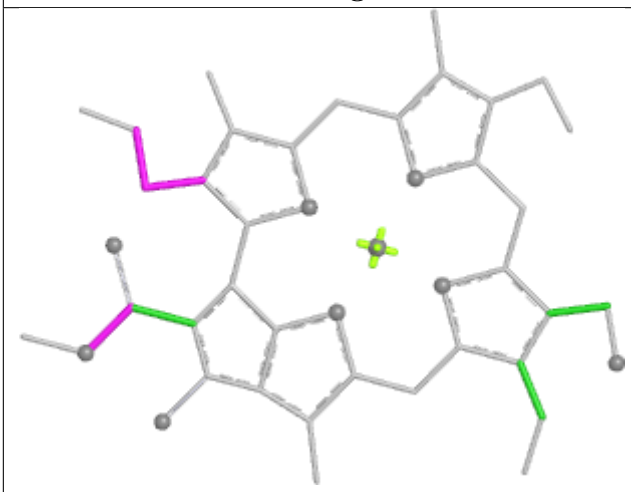
Ligand CHL U 608



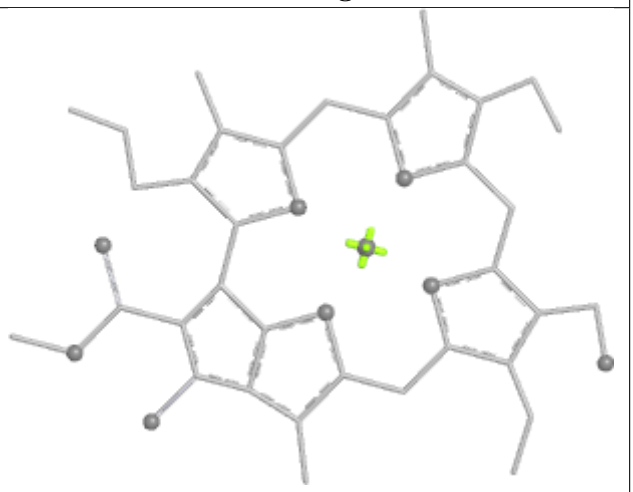
Bond lengths



Bond angles

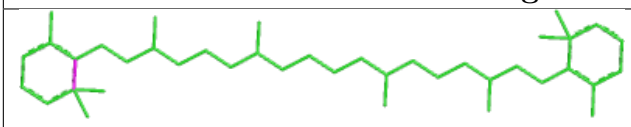


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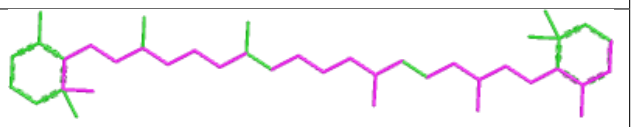


Rings

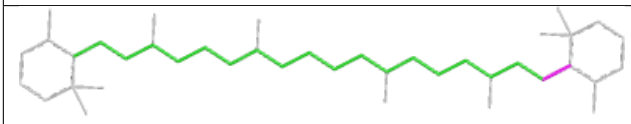
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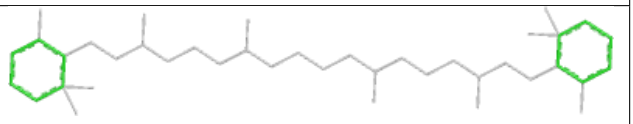
Bond lengths



Bond angles

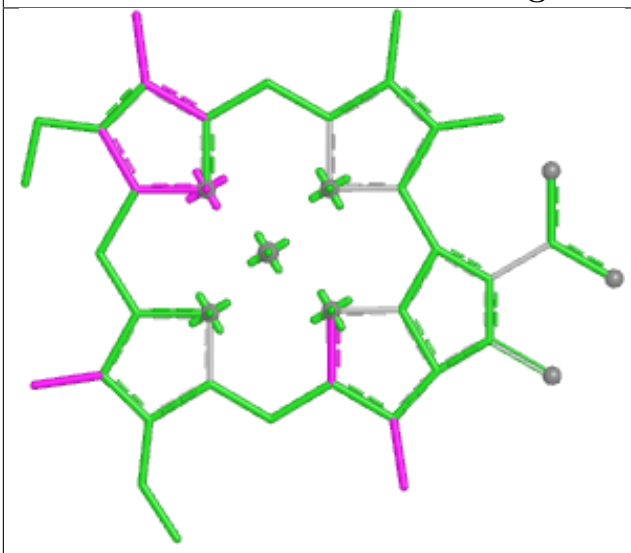


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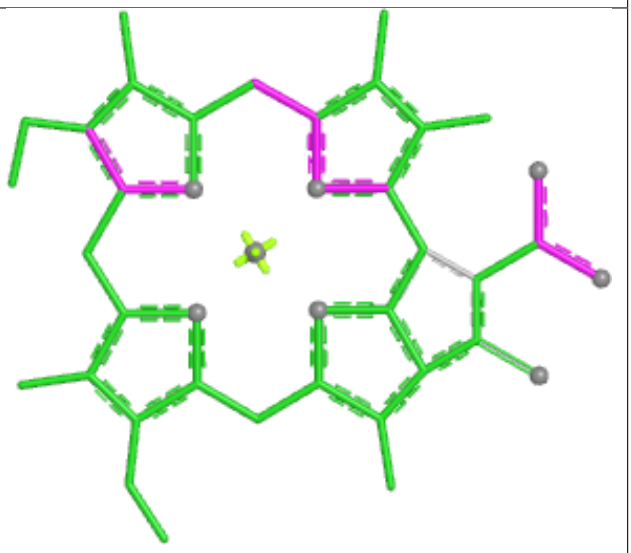


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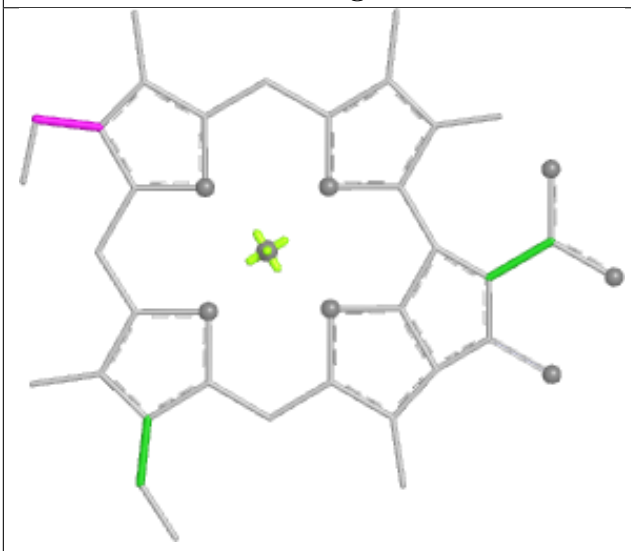
Ligand CLA 3 614



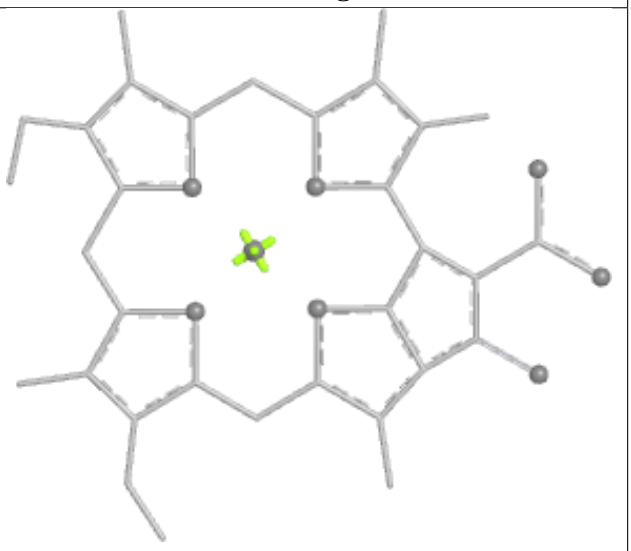
Bond lengths



Bond angles

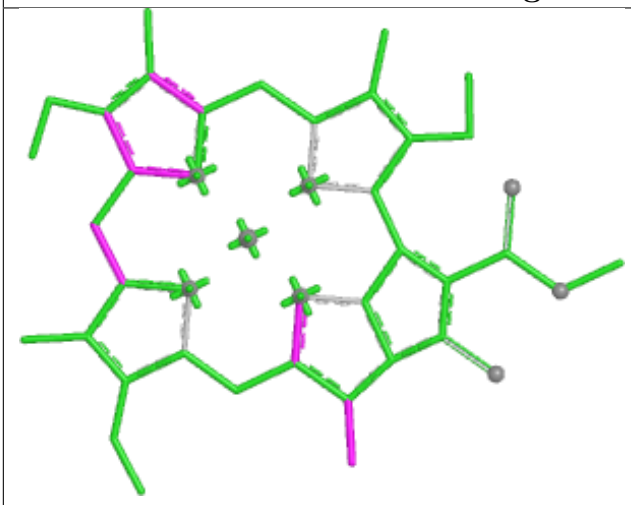


Torsions

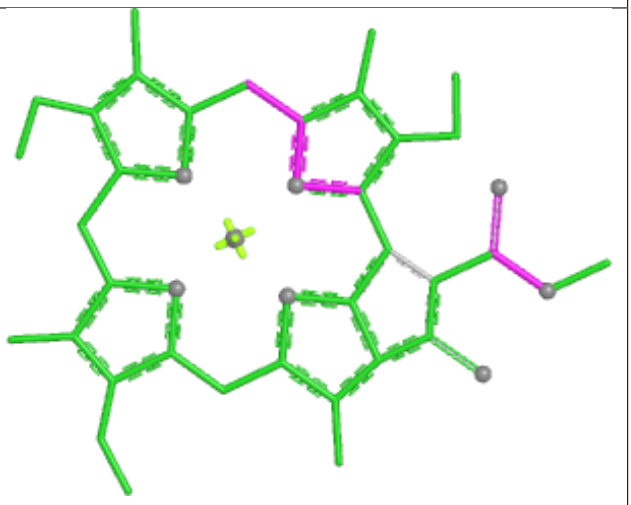


Rings

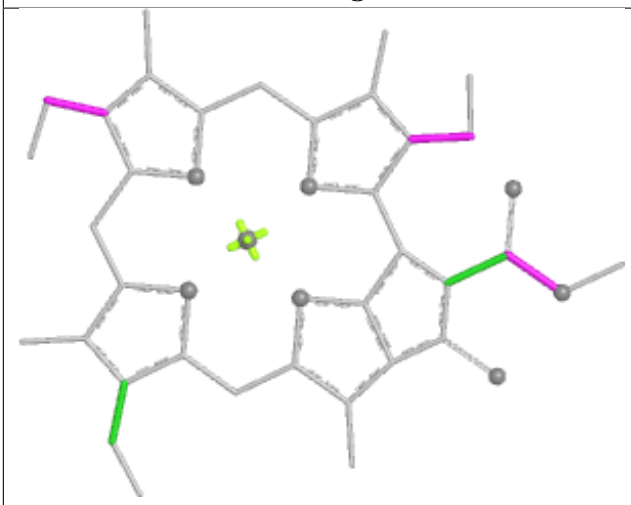
Ligand CLA U 614



Bond lengths



Bond angles



Torsions

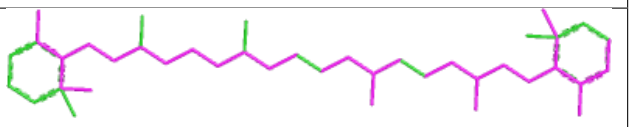


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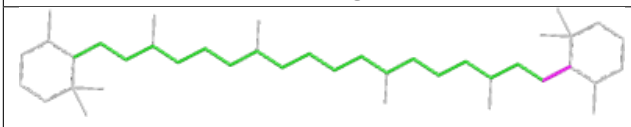
Ligand BCR a 619



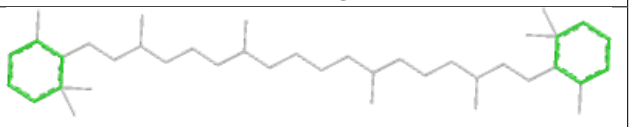
Bond lengths



Bond angles

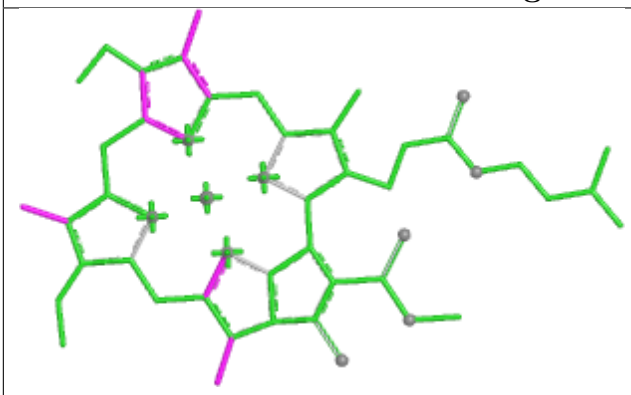


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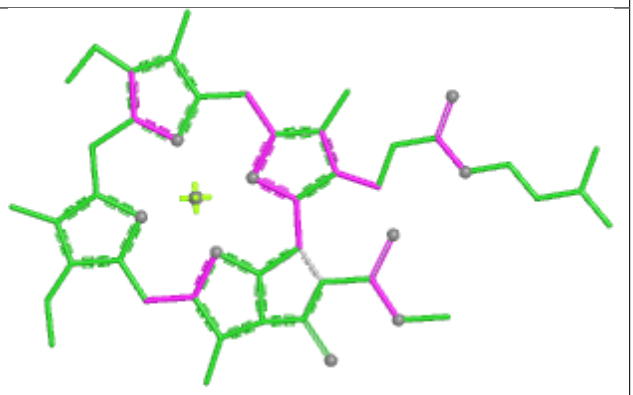


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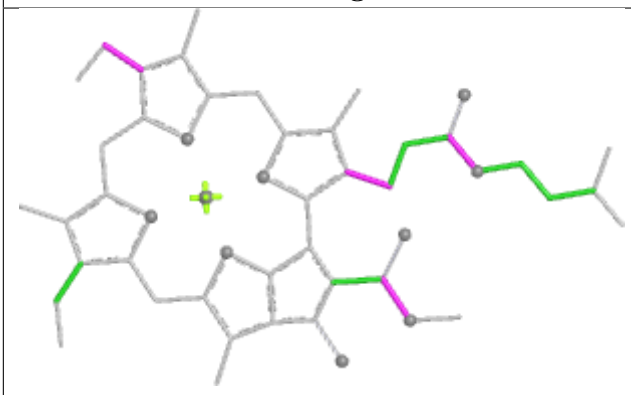
Ligand CLA A 810



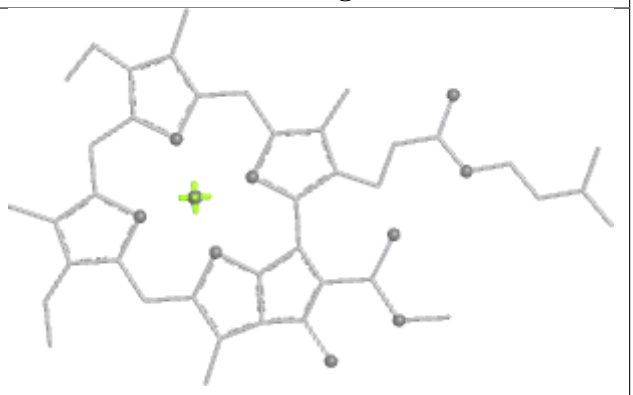
Bond lengths



Bond angles

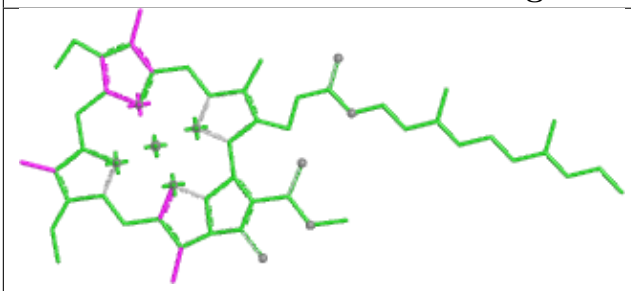


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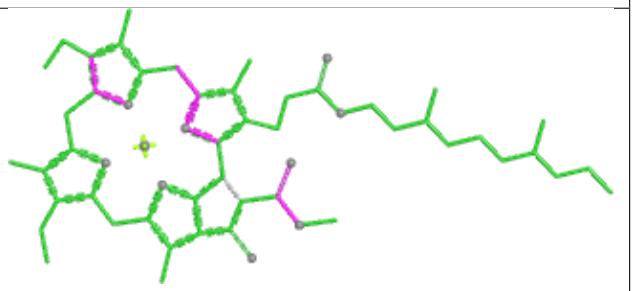


Rings

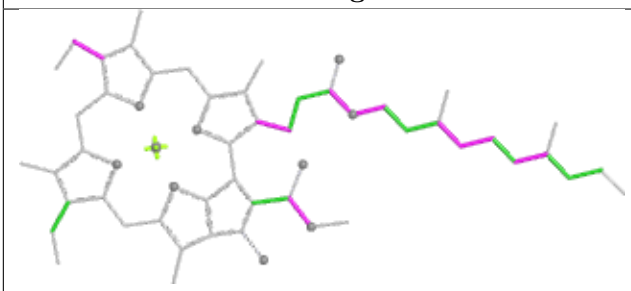
Ligand CLA F 301



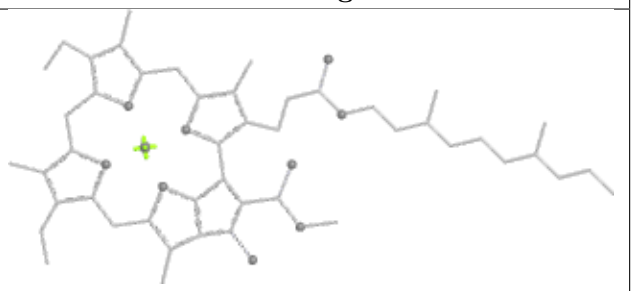
Bond lengths



Bond angles

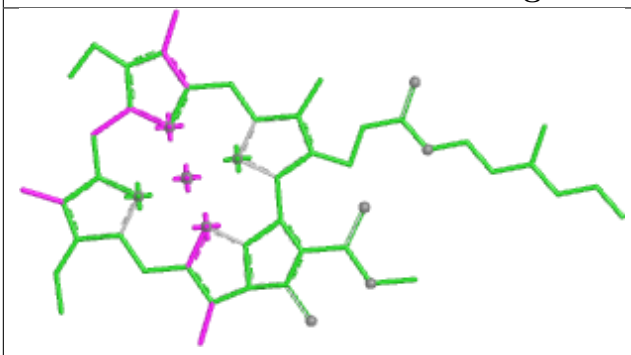


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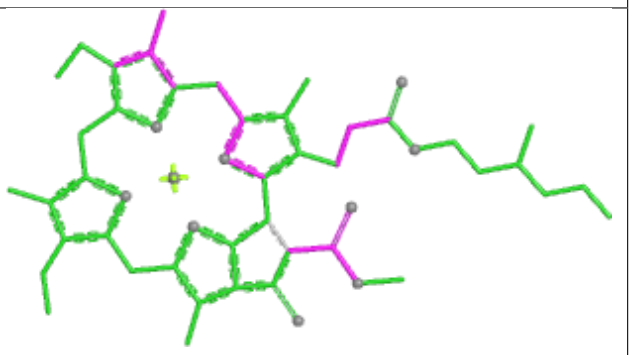


Rings

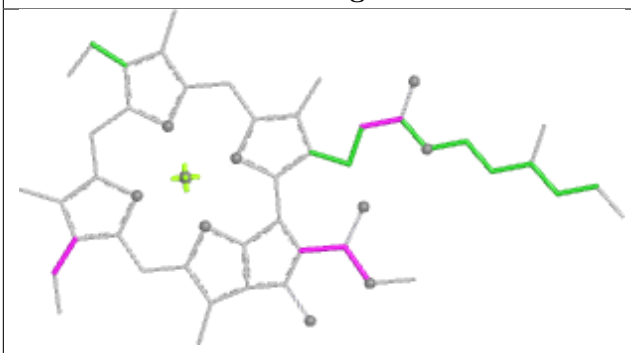
Ligand CLA A 840



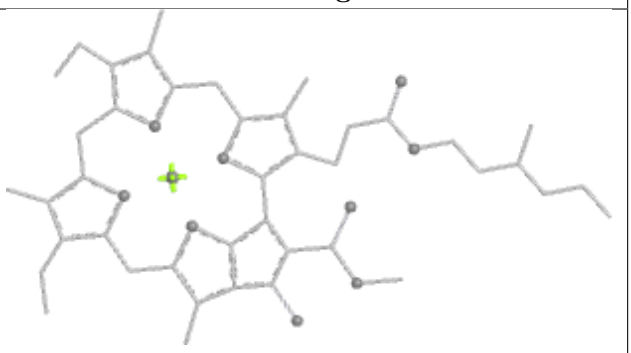
Bond lengths



Bond angles

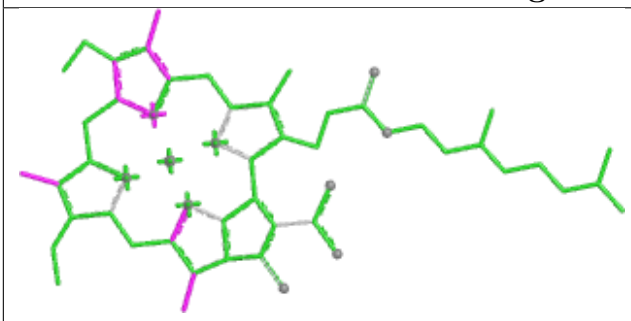


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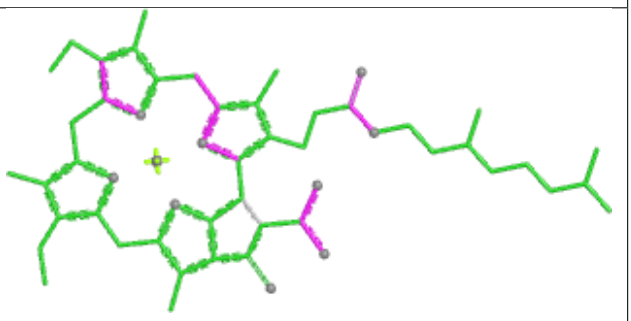


Rings

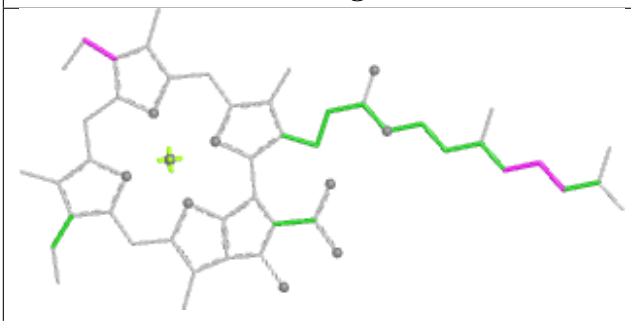
Ligand CLA 1 601



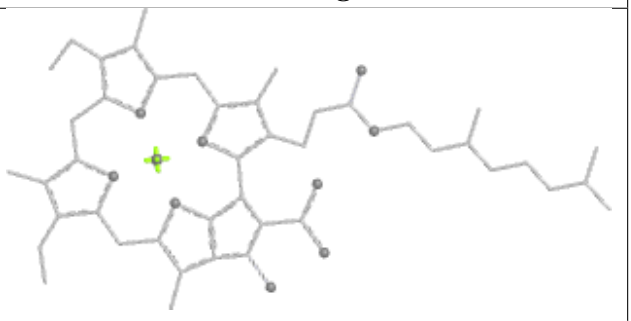
Bond lengths



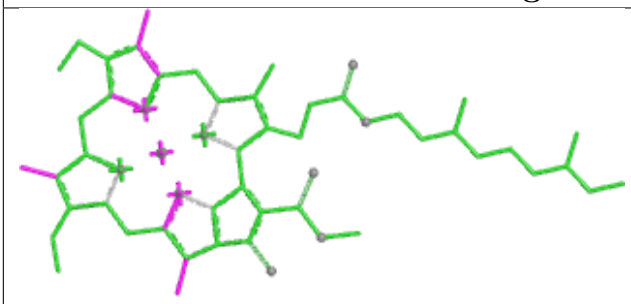
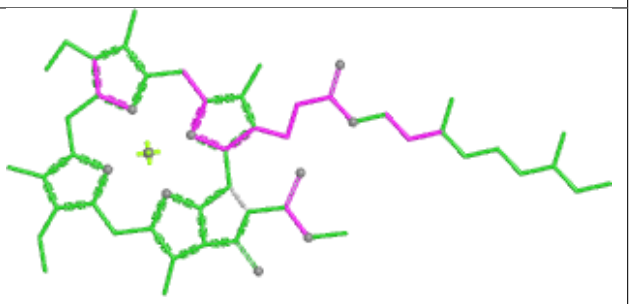
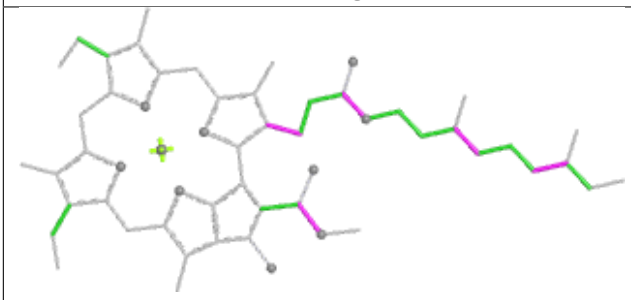
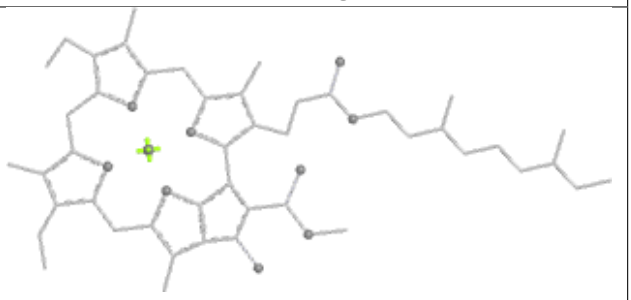
Bond angles

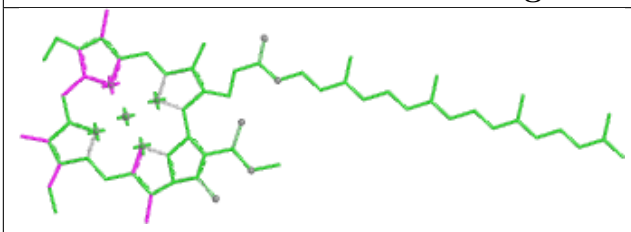
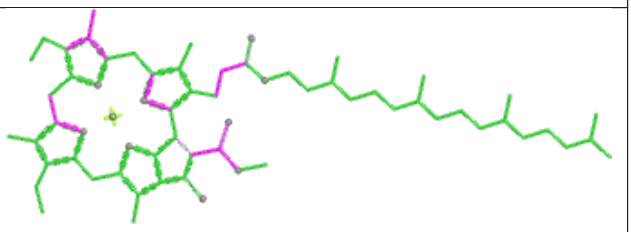
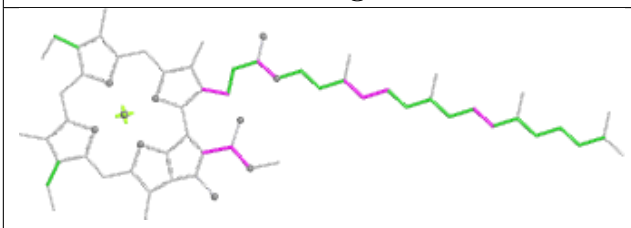
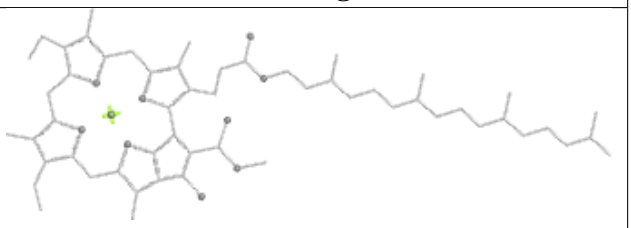


Torsions

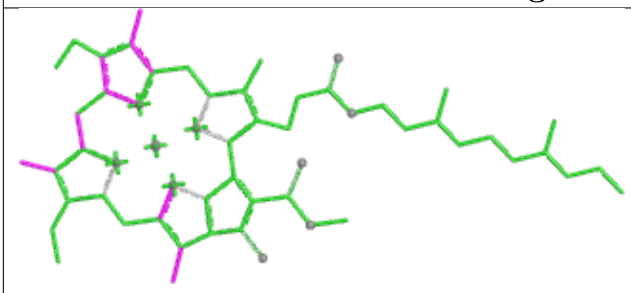


Rings

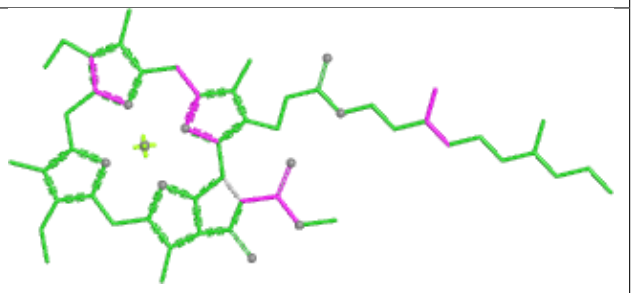
Ligand CLA K 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

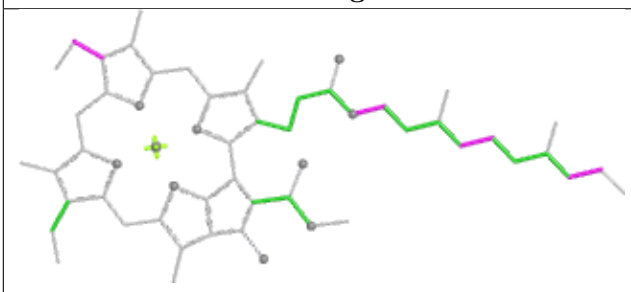
Ligand CLA 9 610



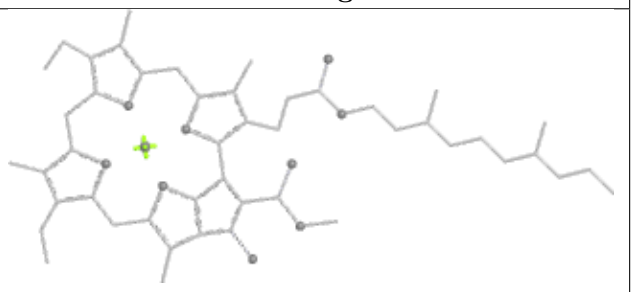
Bond lengths



Bond angles

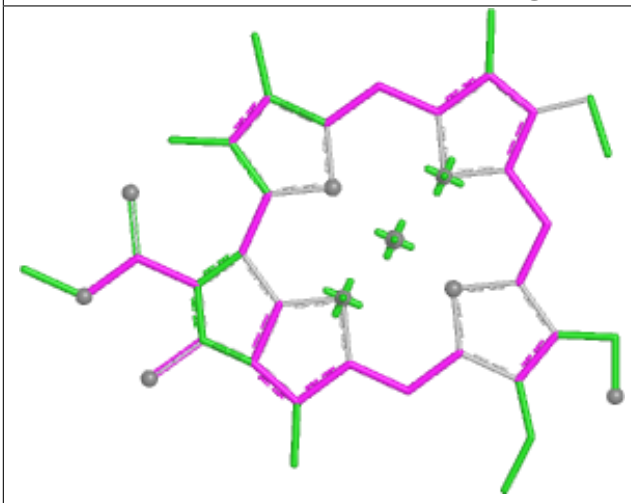


Torsions



Rings

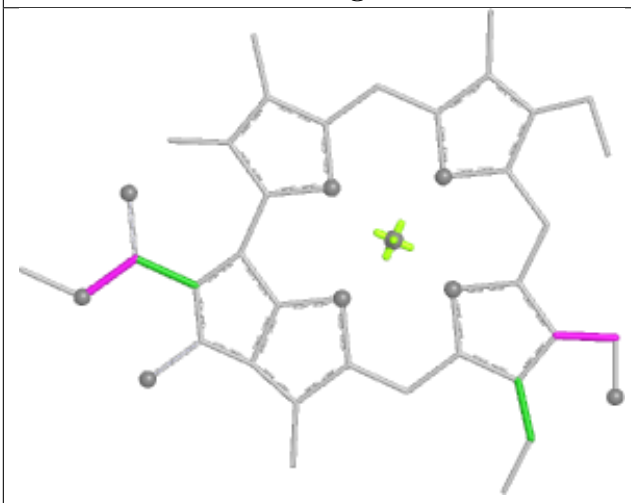
Ligand CHL Z 605



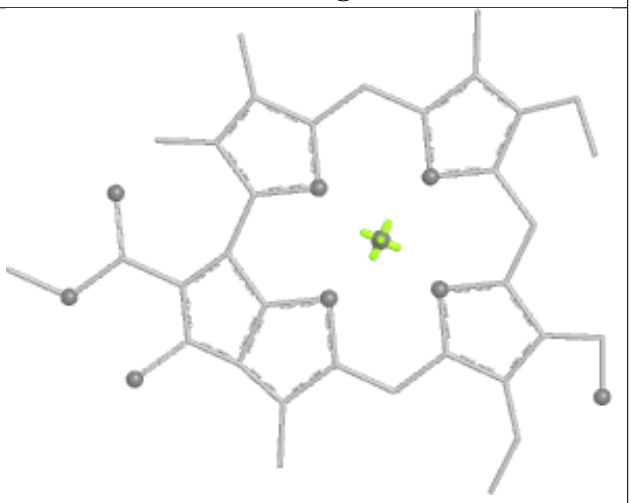
Bond lengths



Bond angles

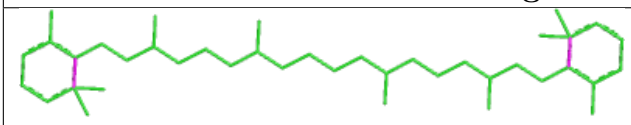


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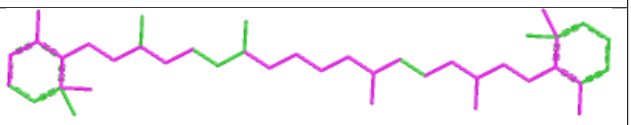


Rings

Ligand BCR B 847



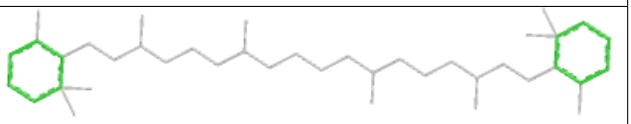
Bond lengths



Bond angles

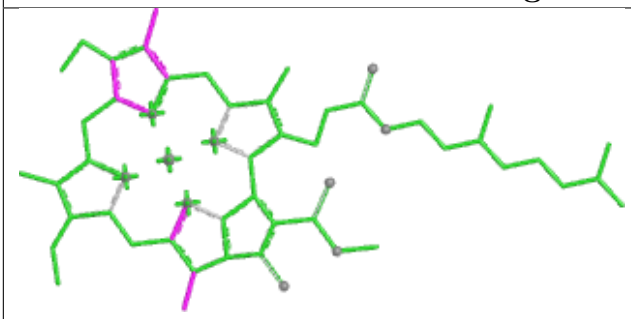


Torsions

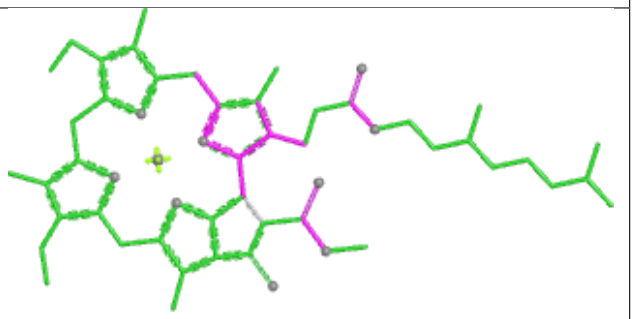


Rings

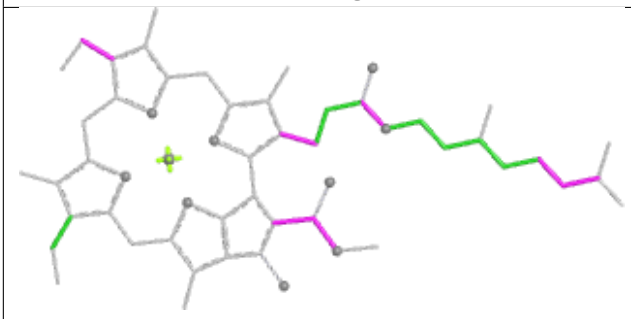
Ligand CLA Y 603



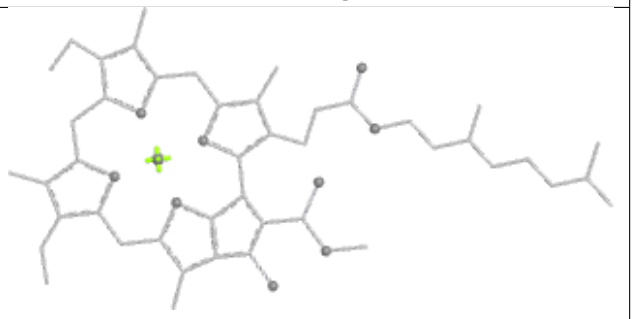
Bond lengths



Bond angles

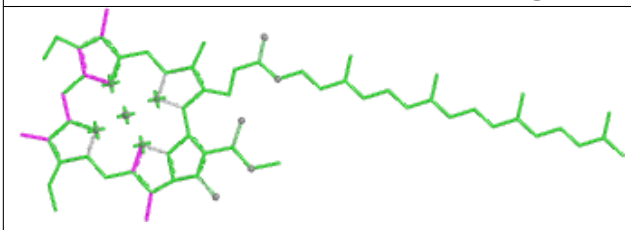


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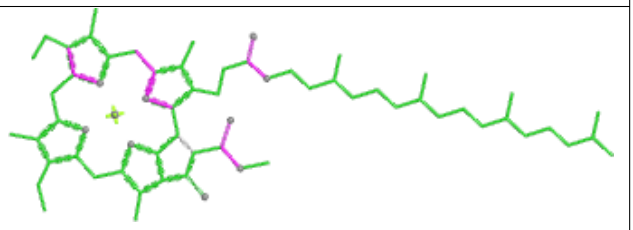


Rings

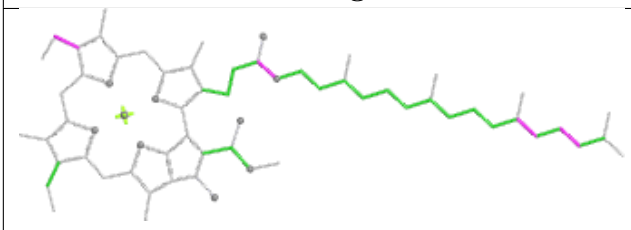
Ligand CLA 7 610



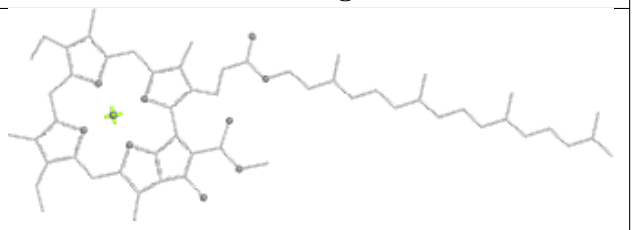
Bond lengths



Bond angles

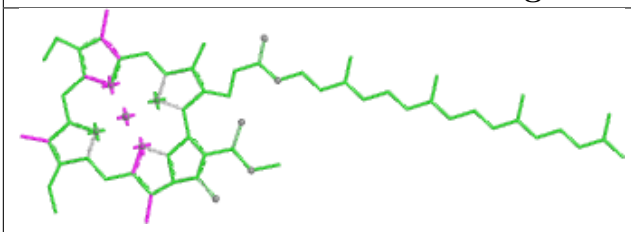


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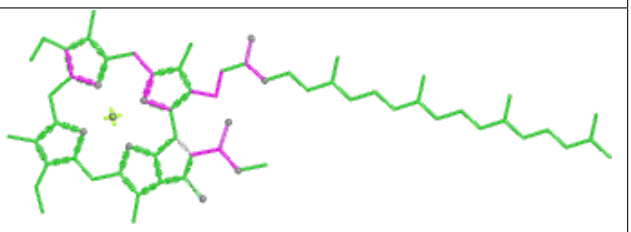


Rings

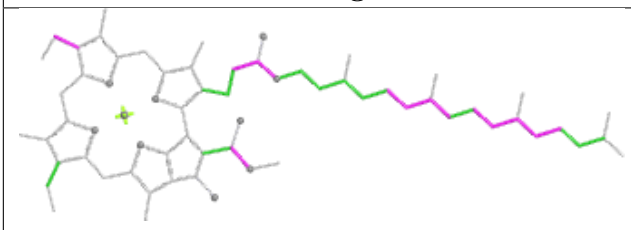
Ligand CLA B 802



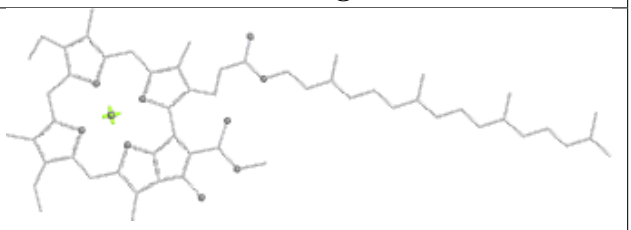
Bond lengths



Bond angles

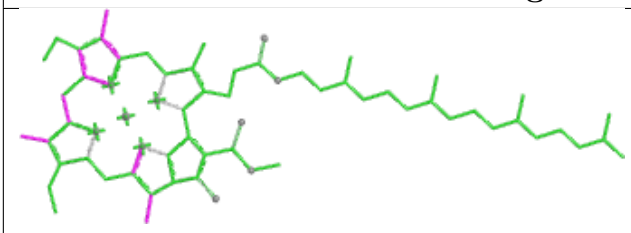


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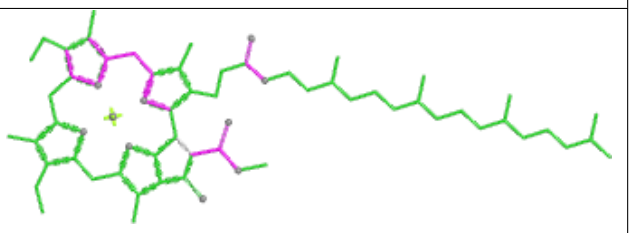


Rings

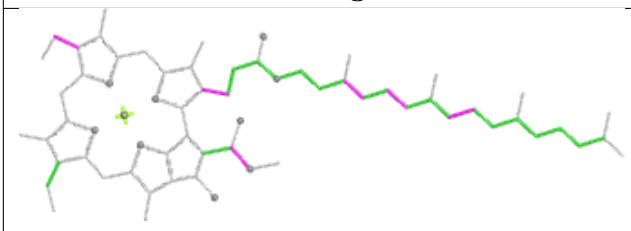
Ligand CLA Z 610



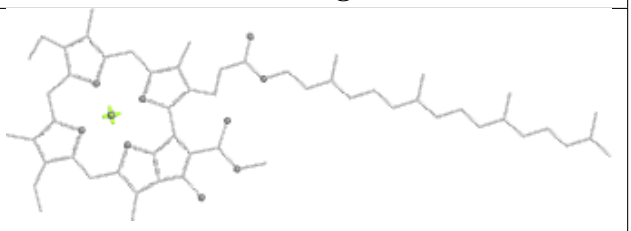
Bond lengths



Bond angles

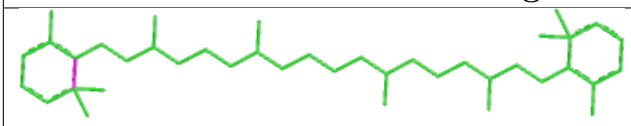


Torsions

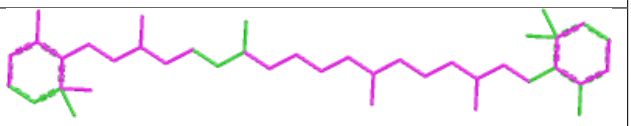


Rings

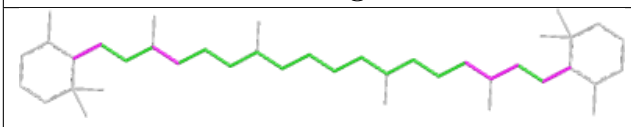
Ligand BCR B 845



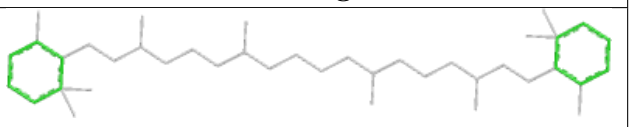
Bond lengths



Bond angles

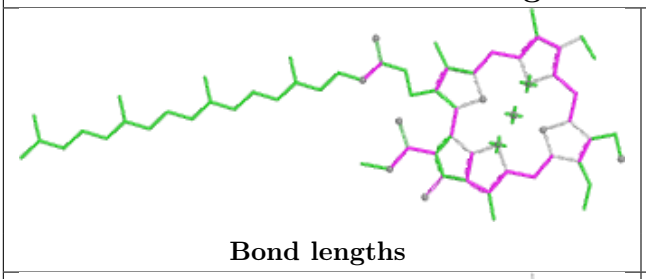


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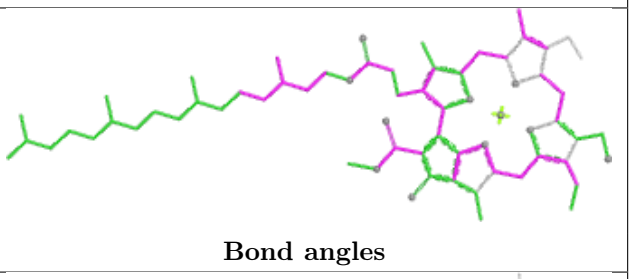


Rings

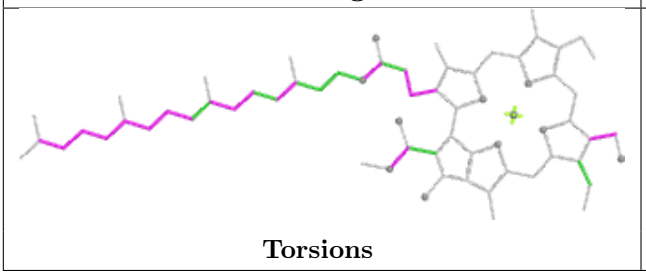
Ligand CHL X 607



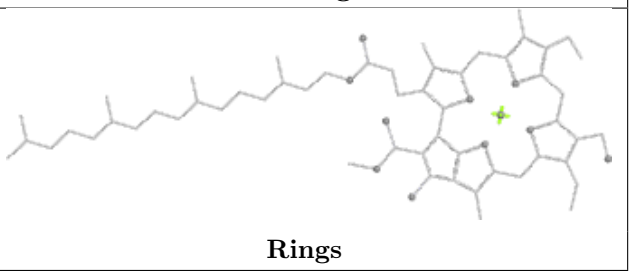
Bond lengths



Bond angles

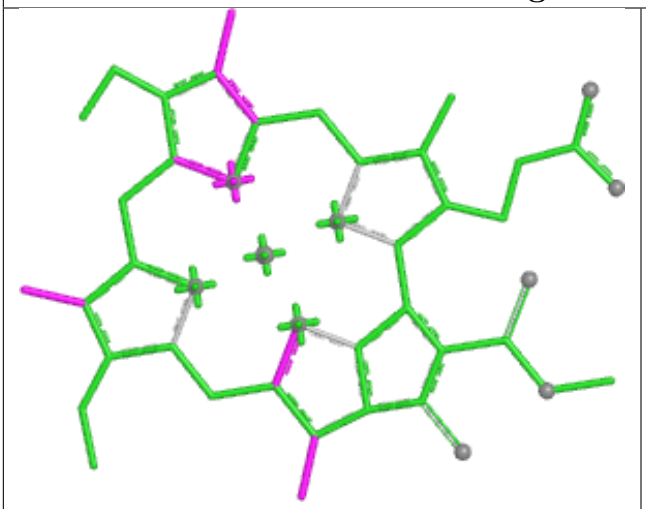


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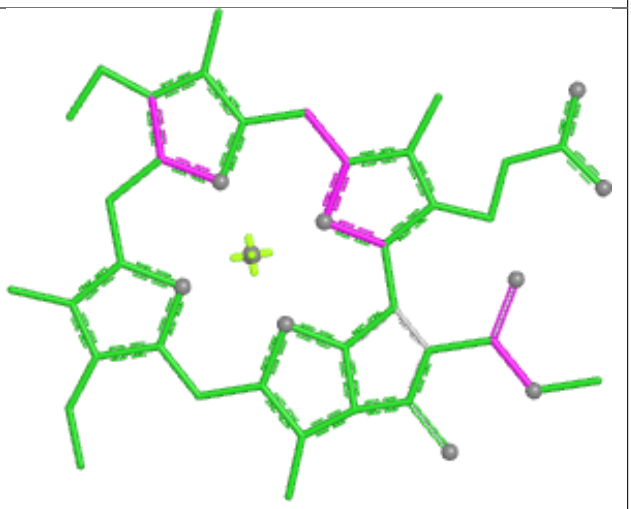


Rings

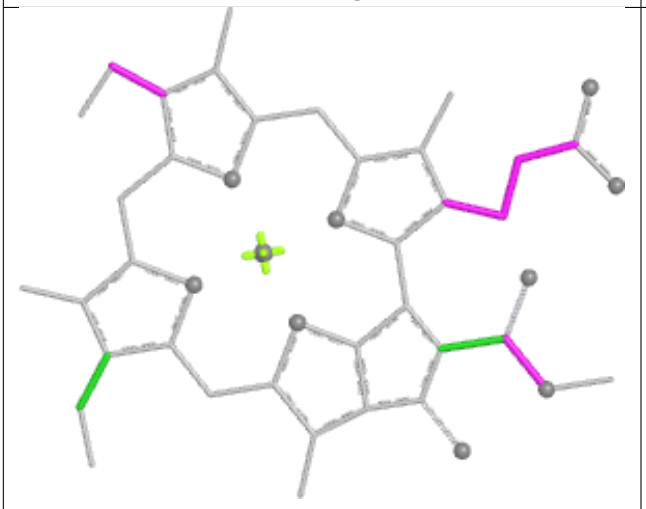
Ligand CLA 9 607



Bond lengths



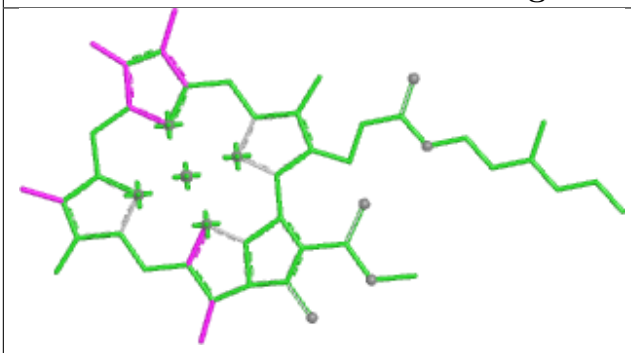
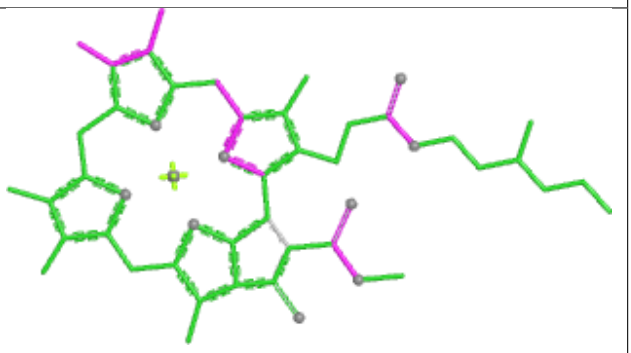
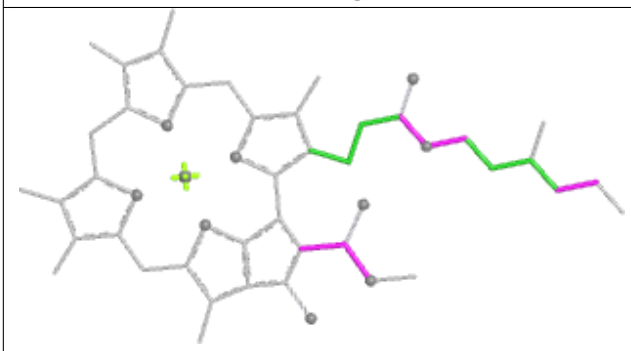
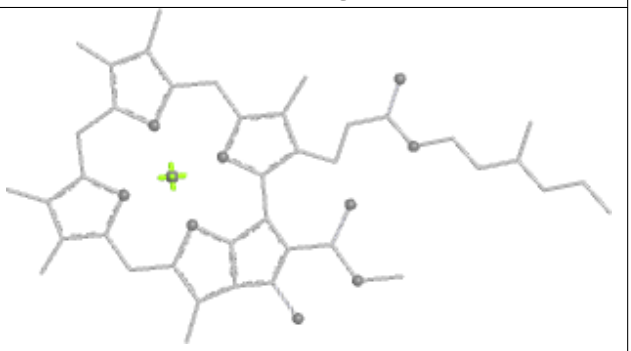
Bond angles

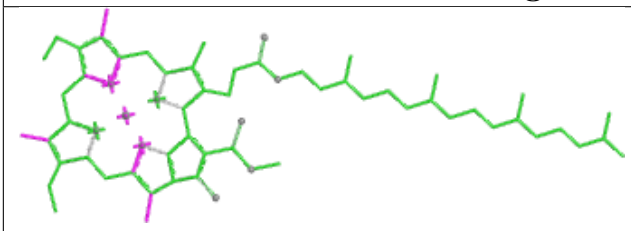
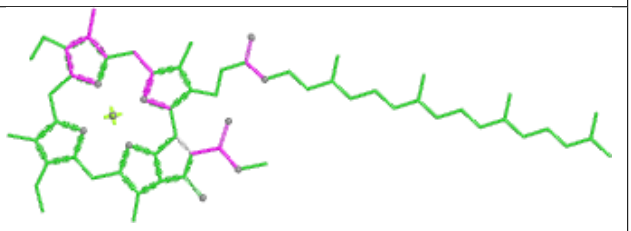
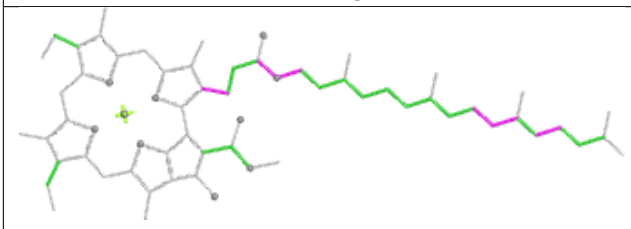
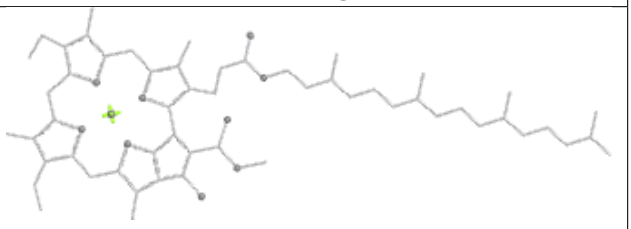


Torsions

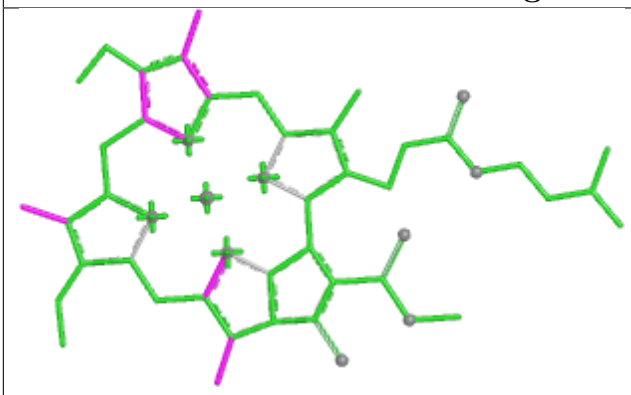


Rings

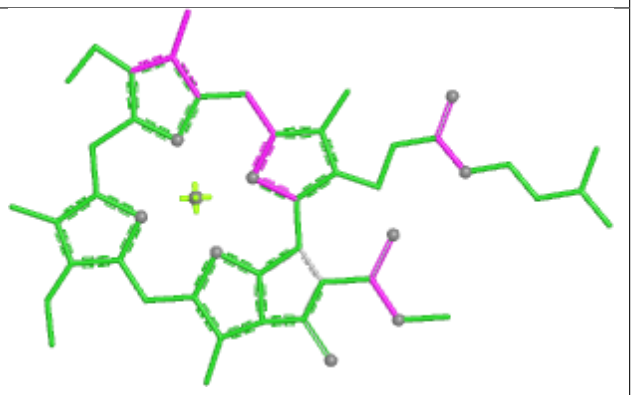
Ligand CLA 9 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

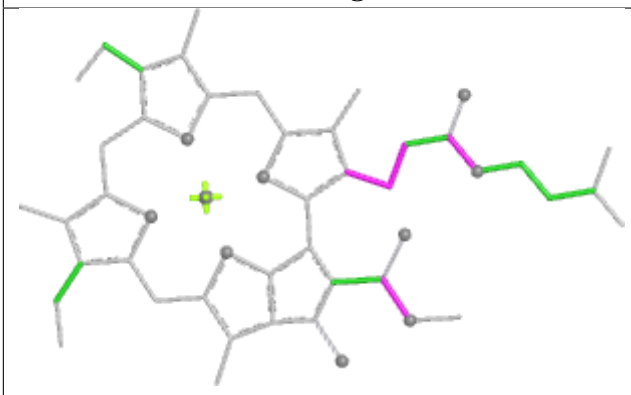
Ligand CLA V 604



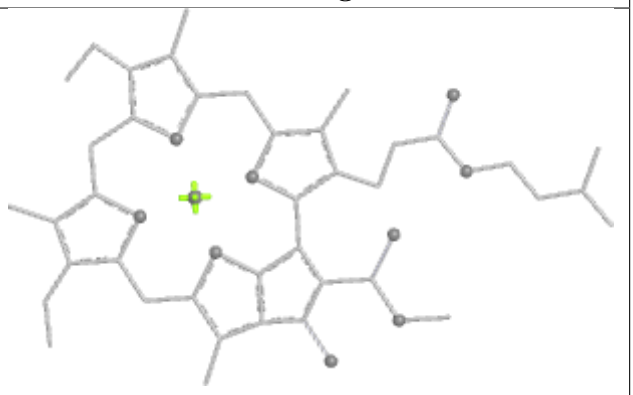
Bond lengths



Bond angles

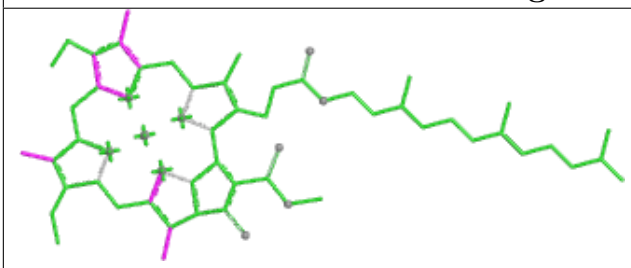


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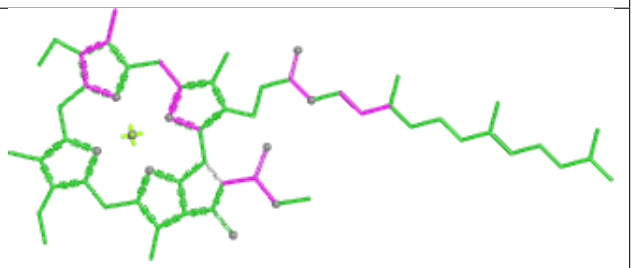


Rings

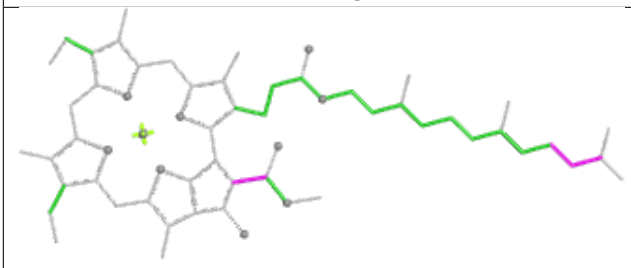
Ligand CLA 3 602



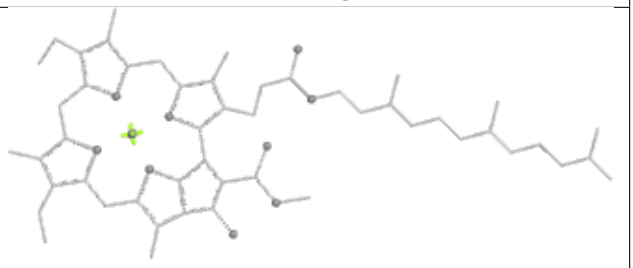
Bond lengths



Bond angles

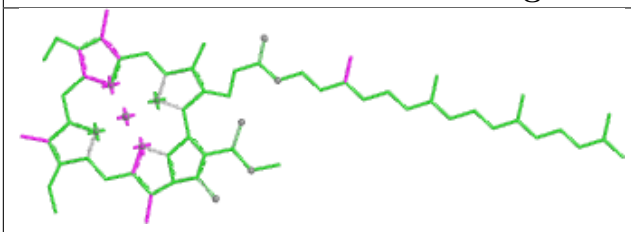


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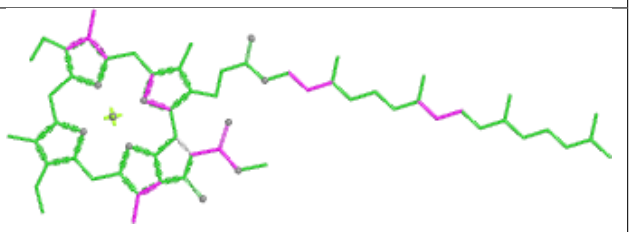


Rings

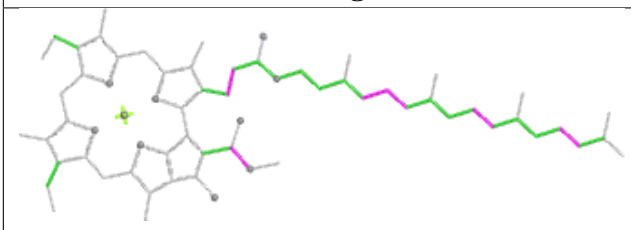
Ligand CLA A 854



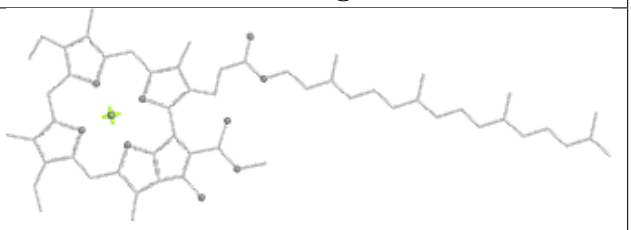
Bond lengths



Bond angles

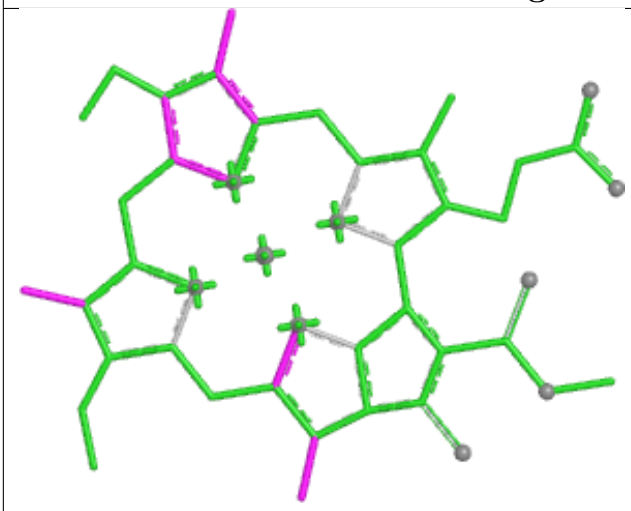


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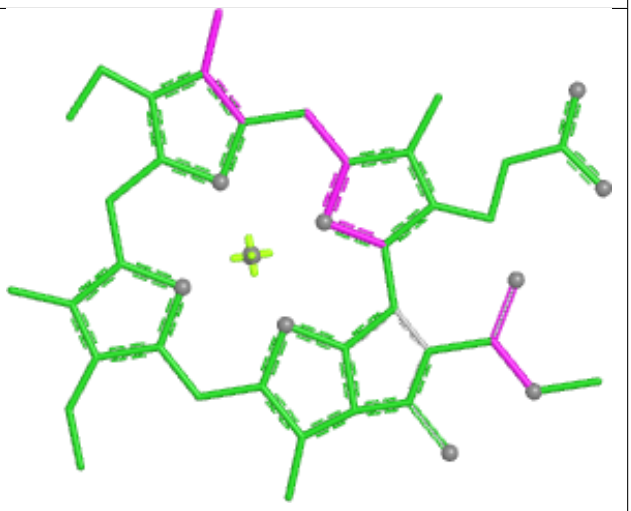


Rings

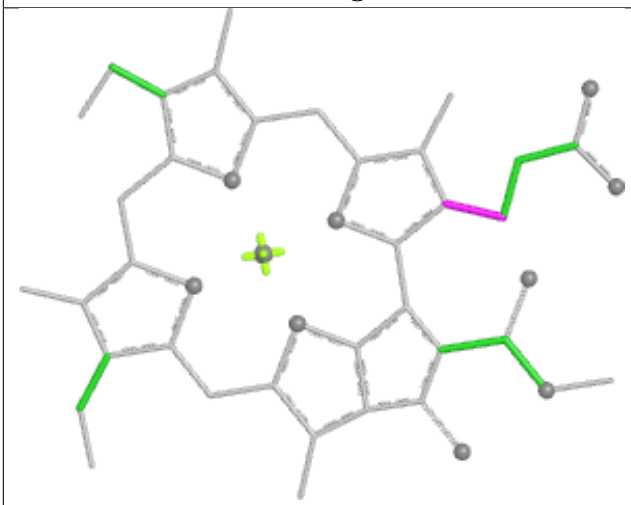
Ligand CLA 8 609



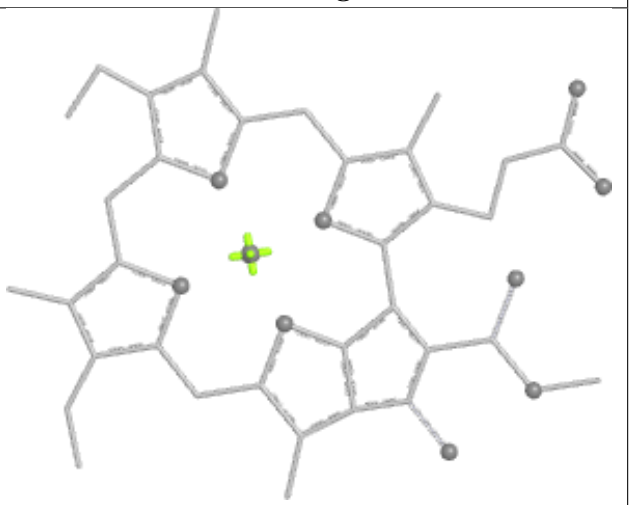
Bond lengths



Bond angles

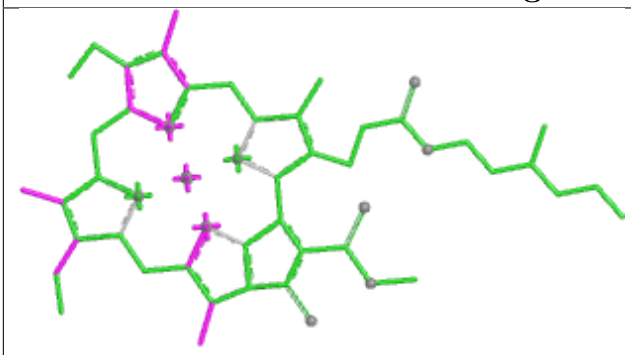


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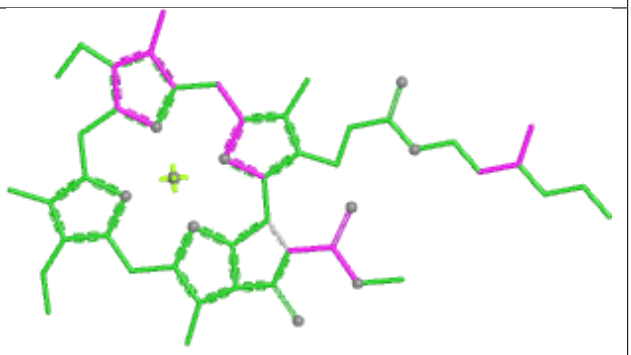


Rings

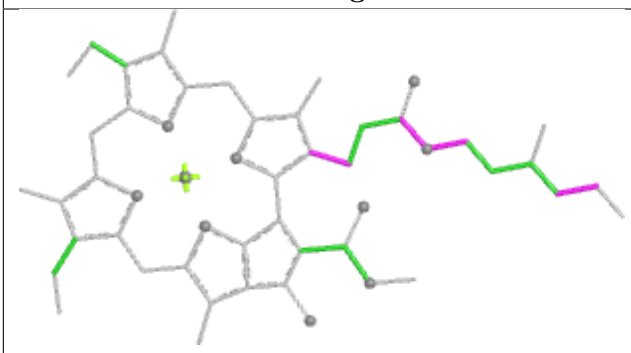
Ligand CLA A 805



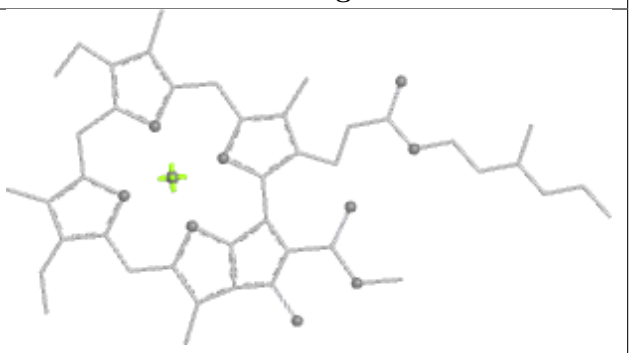
Bond lengths



Bond angles

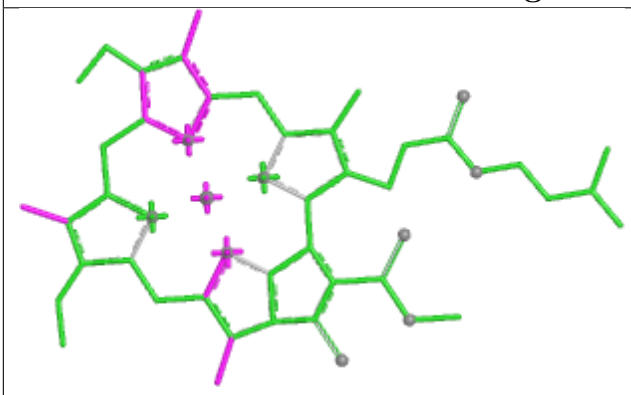


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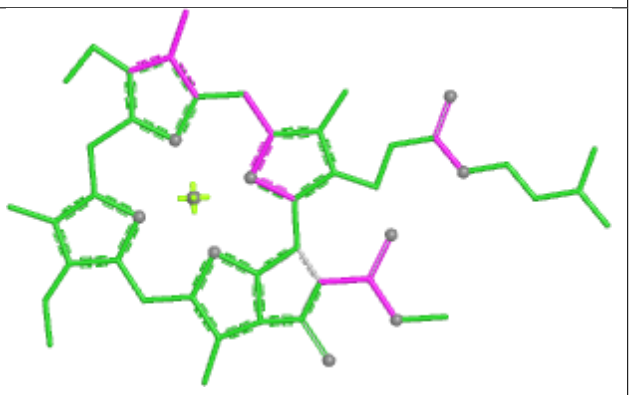


Rings

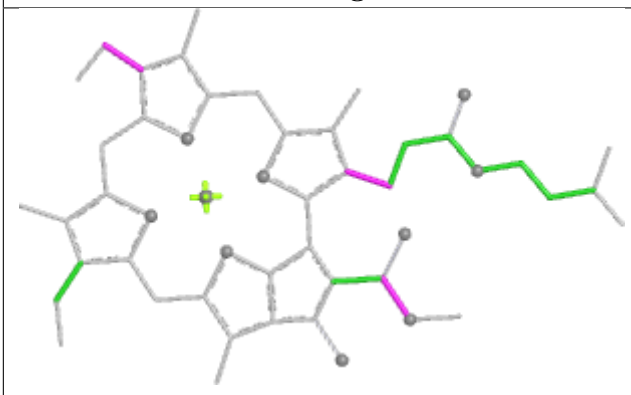
Ligand CLA B 836



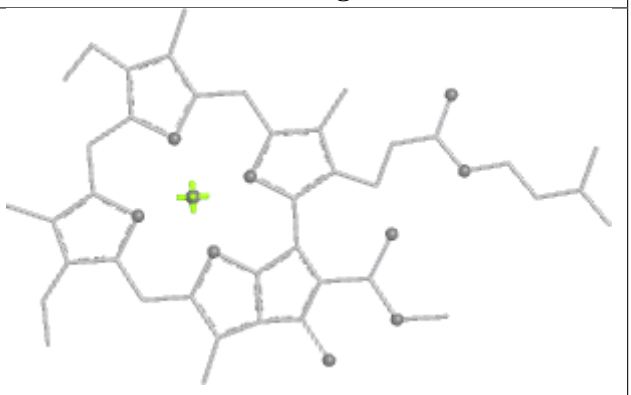
Bond lengths



Bond angles

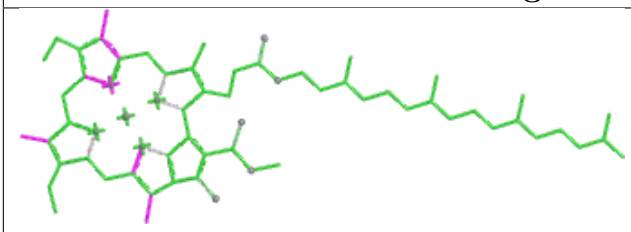


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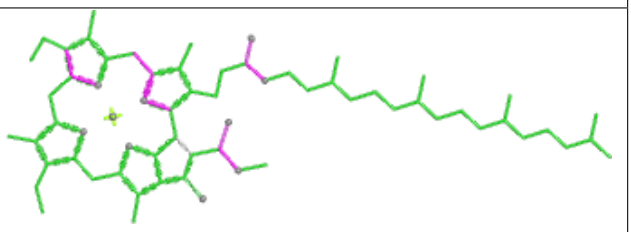


Rings

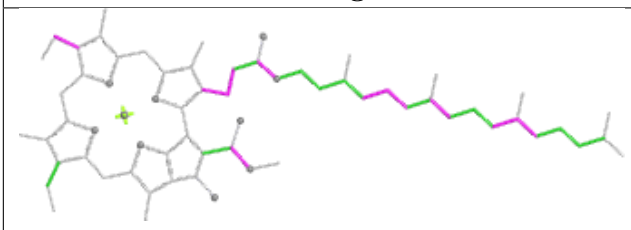
Ligand CLA A 841



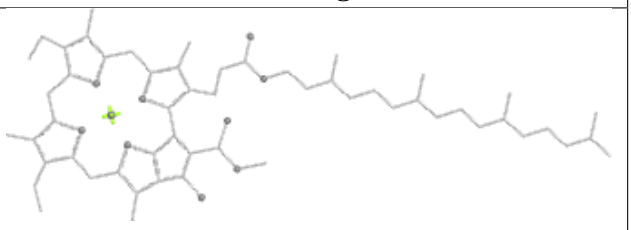
Bond lengths



Bond angles

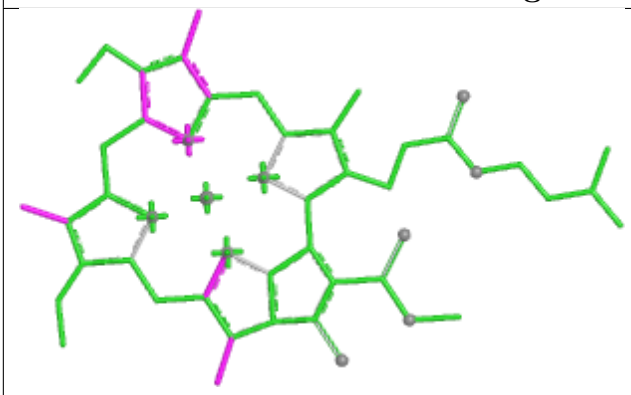


Torsions

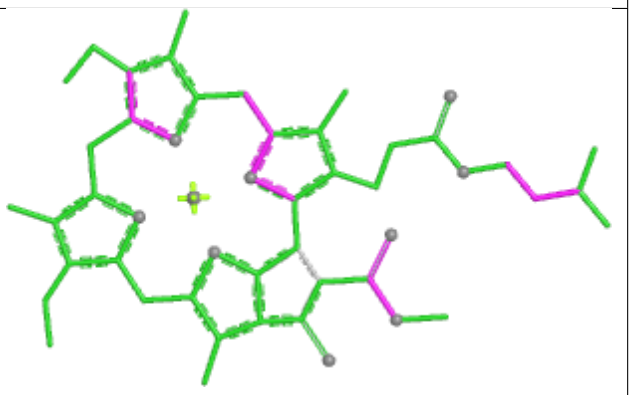


Rings

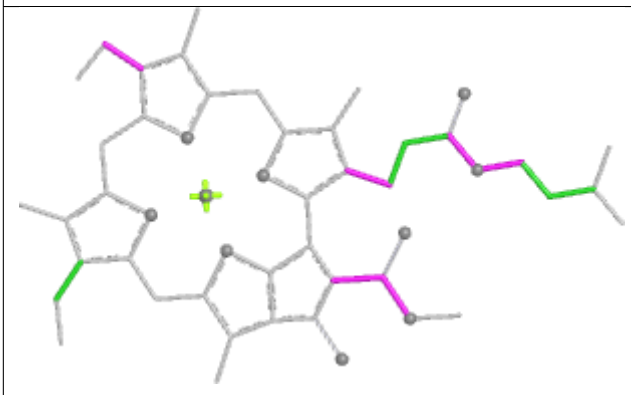
Ligand CLA A 815



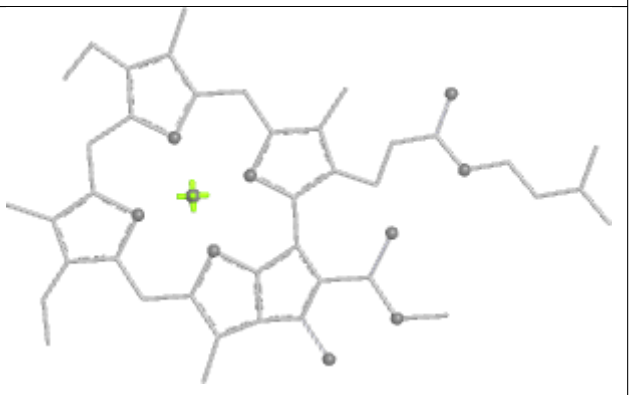
Bond lengths



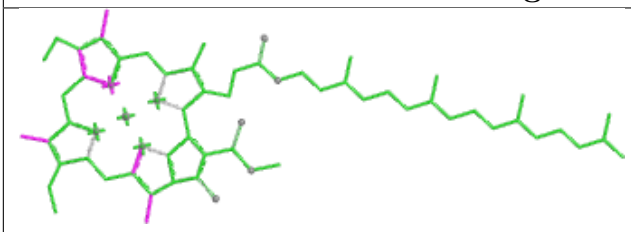
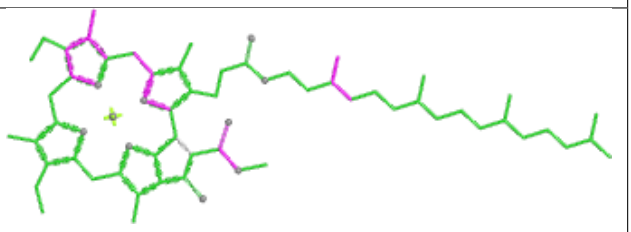
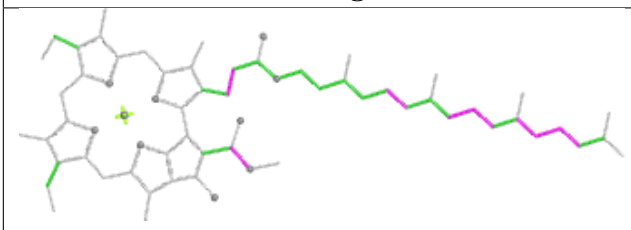
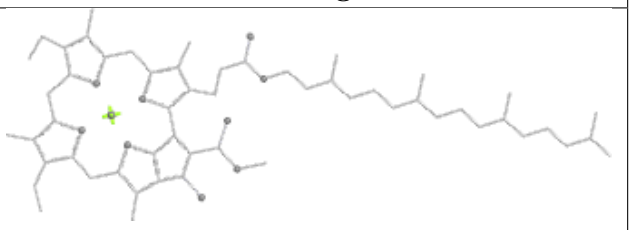
Bond angles

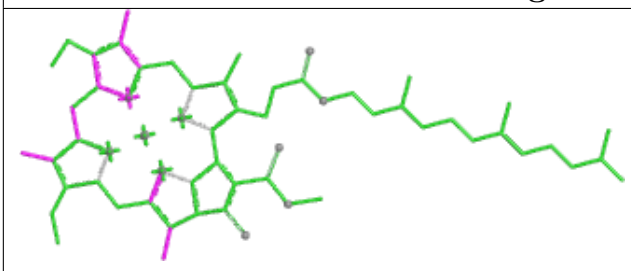
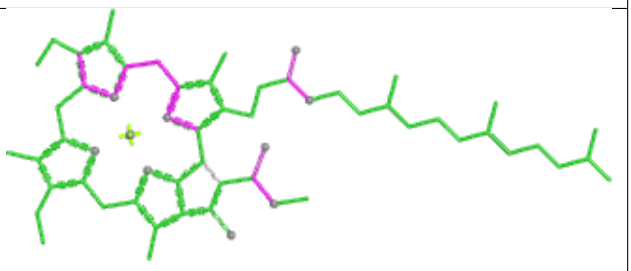
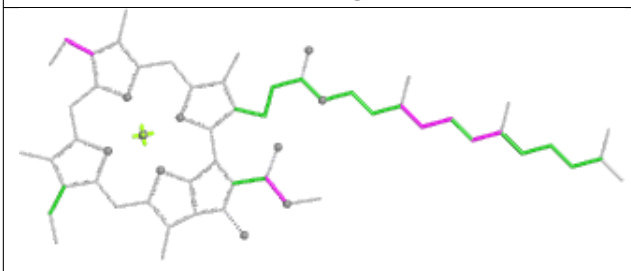
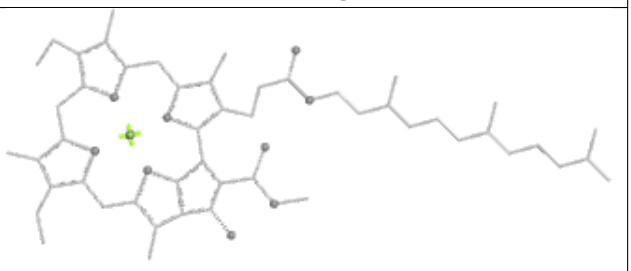


Torsions

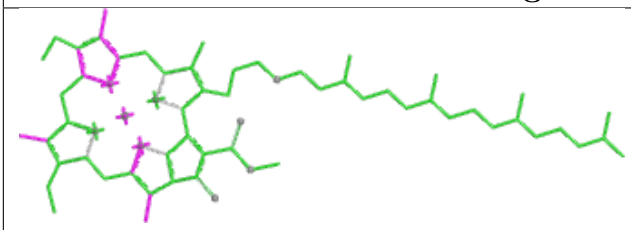


Rings

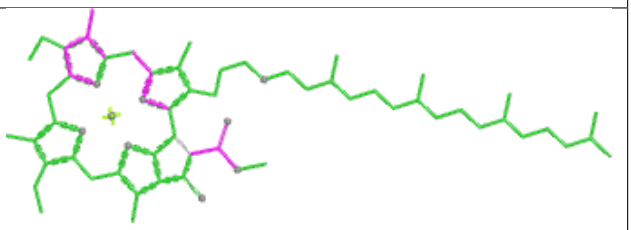
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

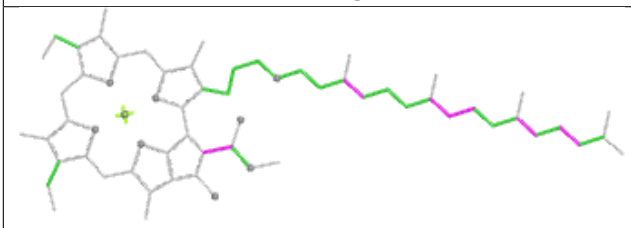
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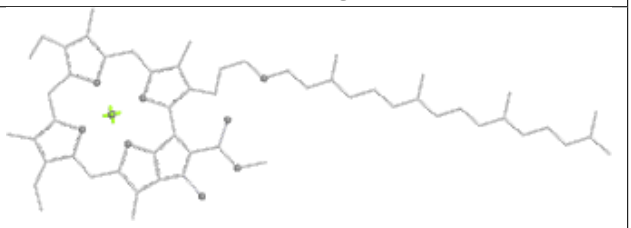
Bond lengths



Bond angles

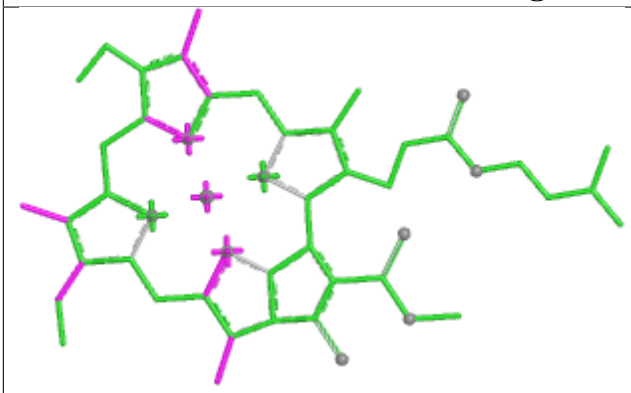


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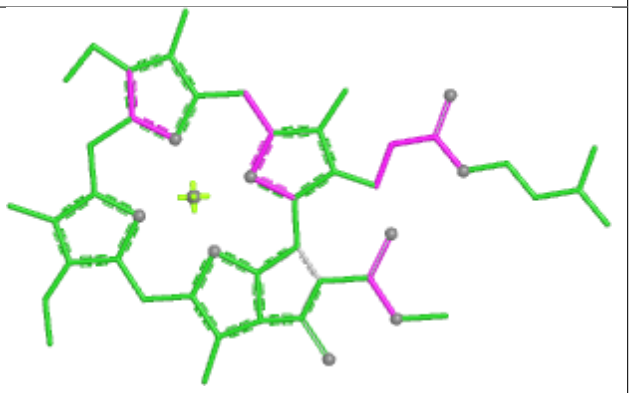


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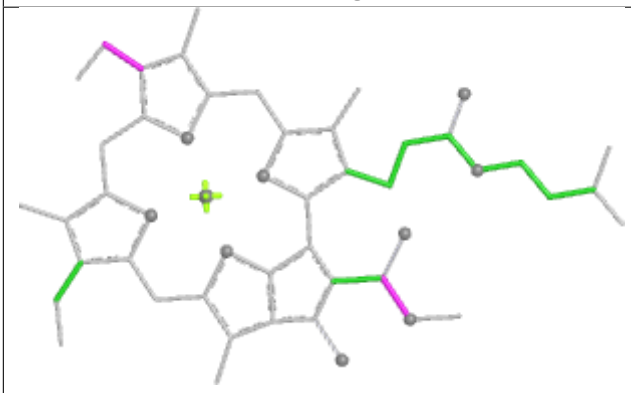
Ligand CLA 7 608



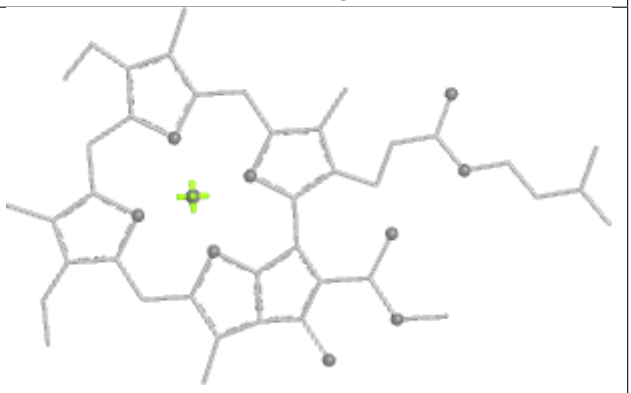
Bond lengths



Bond angles

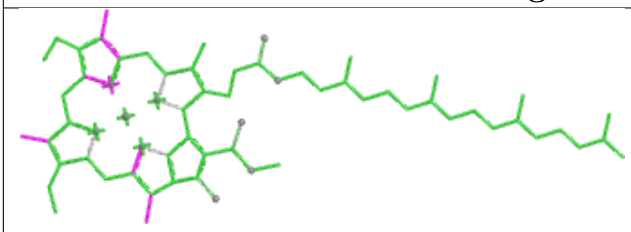


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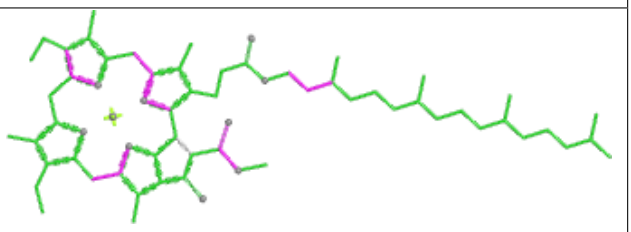


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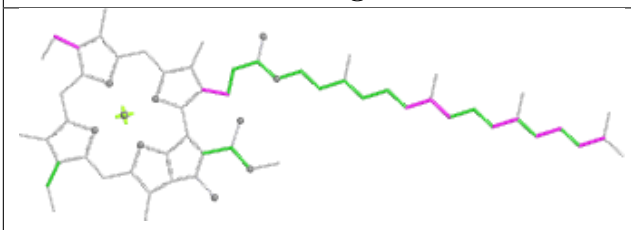
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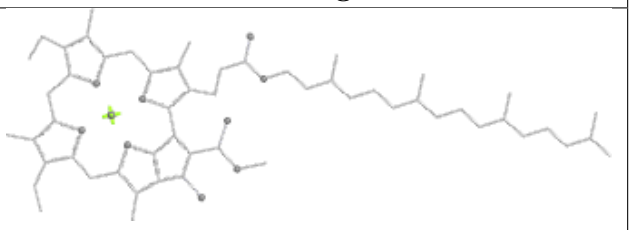
Bond lengths



Bond angles

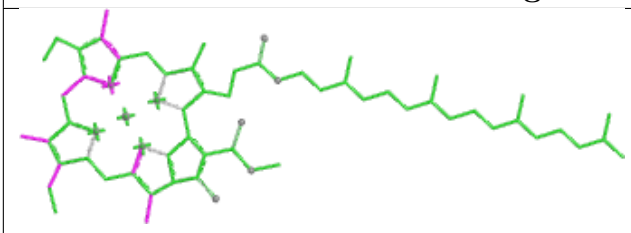


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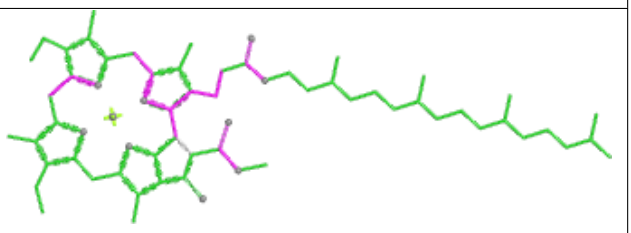


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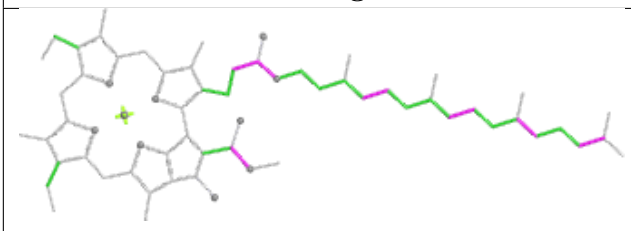
Ligand CLA A 801



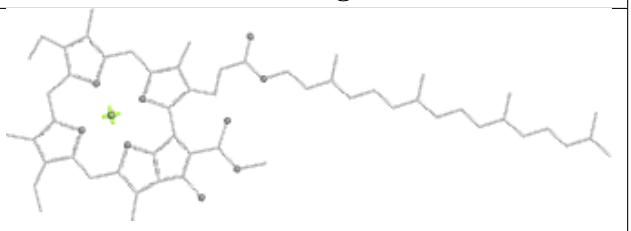
Bond lengths



Bond angles

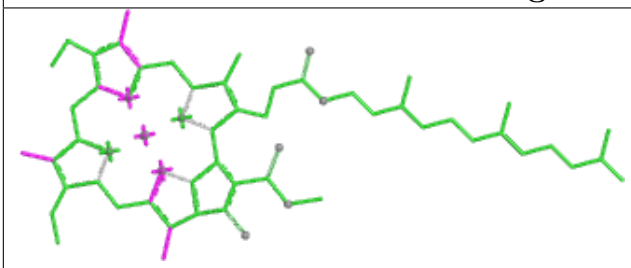


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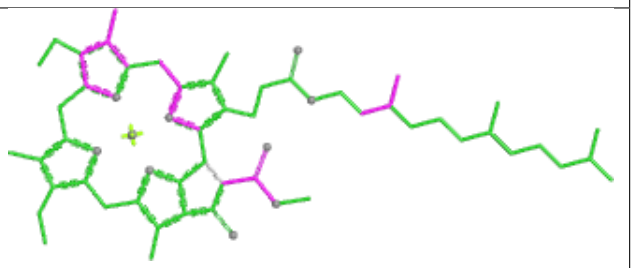


Rings

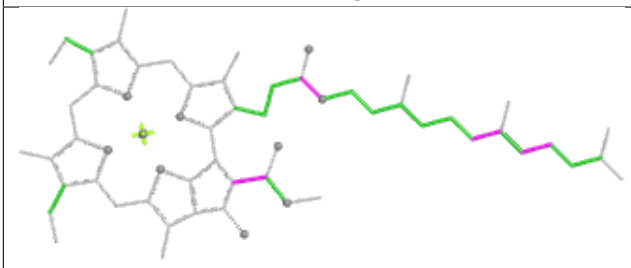
Ligand CLA 7 601



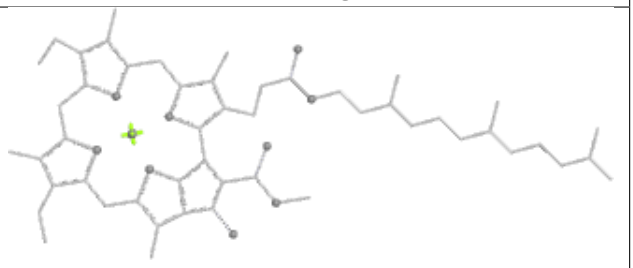
Bond lengths



Bond angles

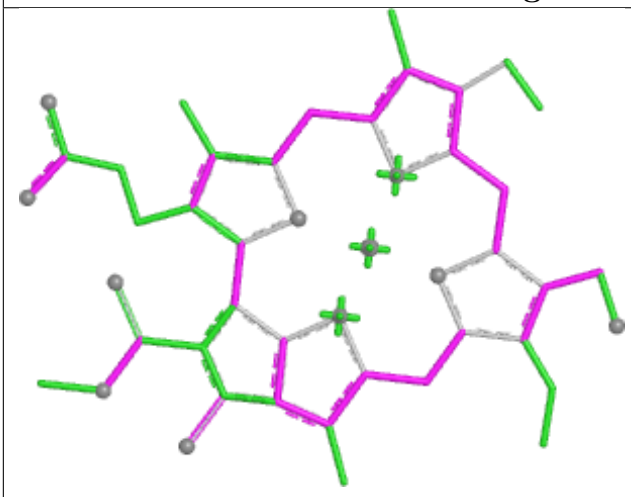


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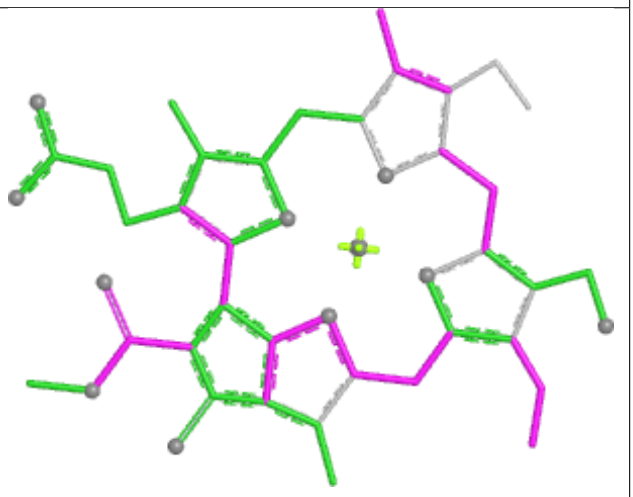


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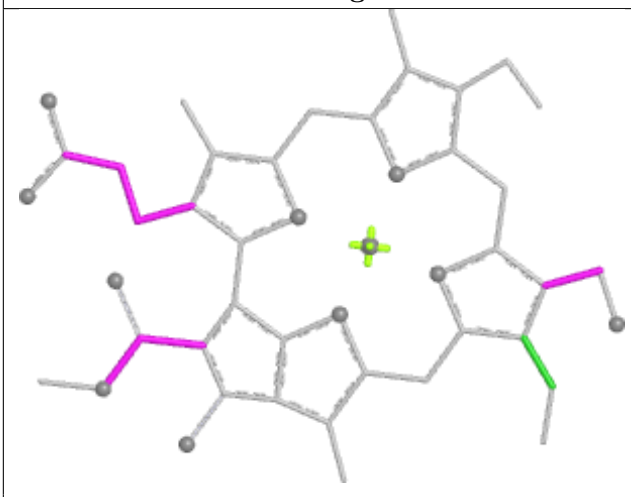
Ligand CHL X 605



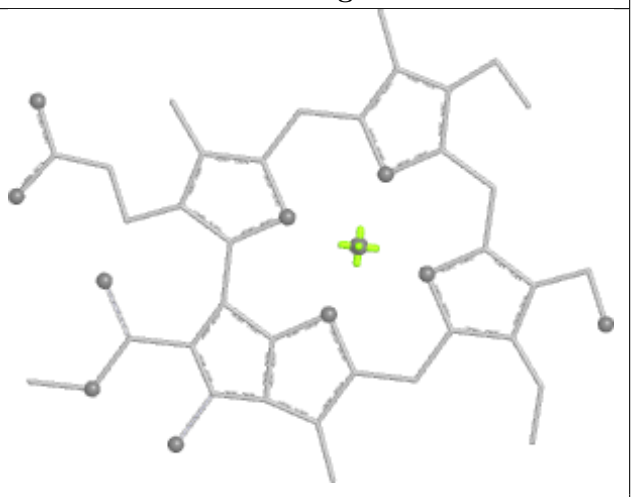
Bond lengths



Bond angles

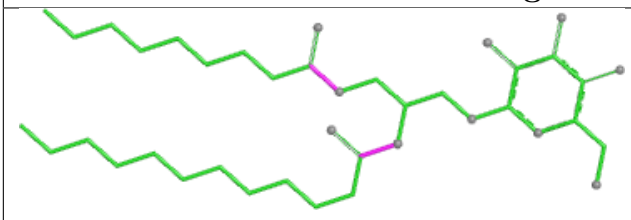


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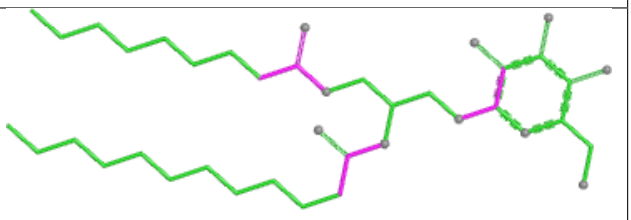


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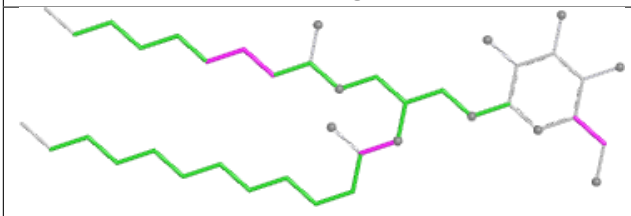
Ligand LMG 4 624



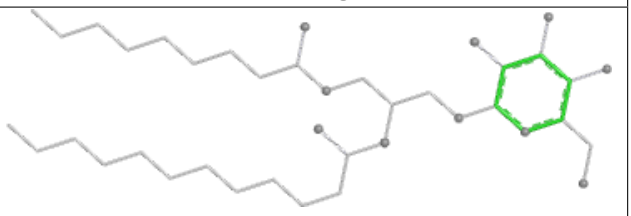
Bond lengths



Bond angles

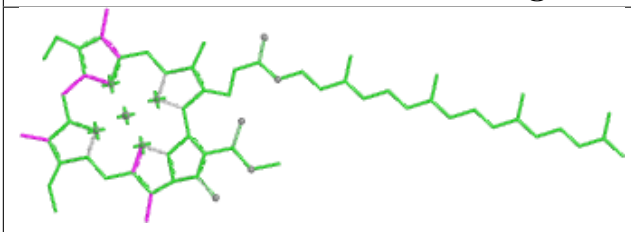


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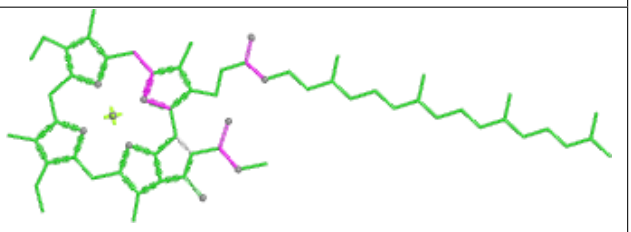


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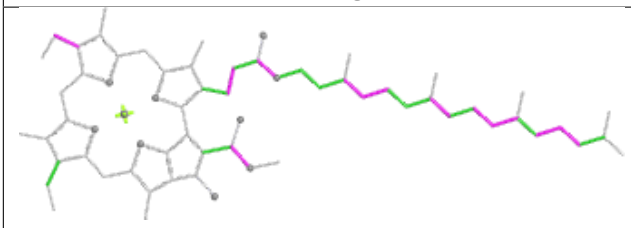
Ligand CLA 7 613



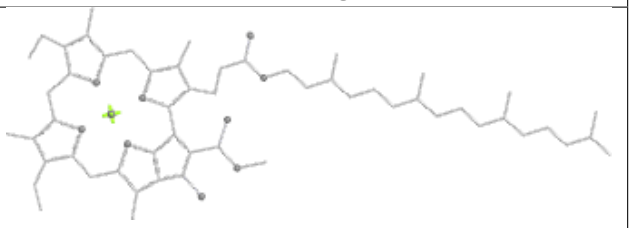
Bond lengths



Bond angles

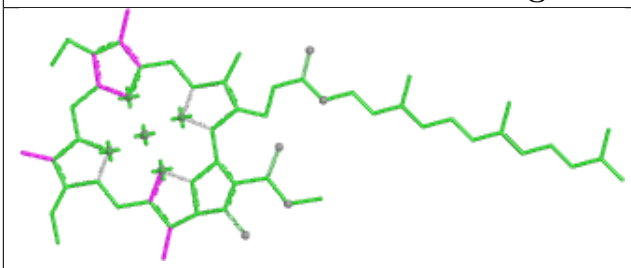


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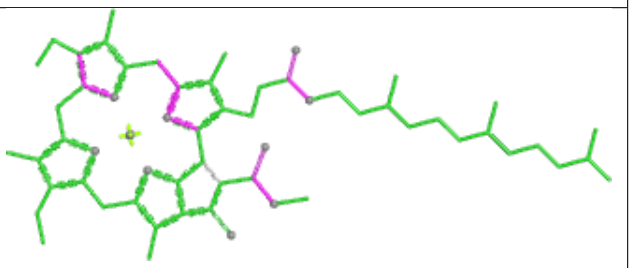


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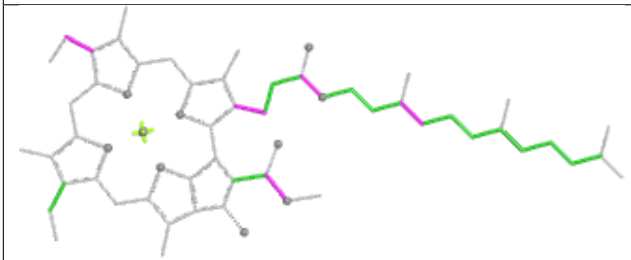
Ligand CLA 6 614



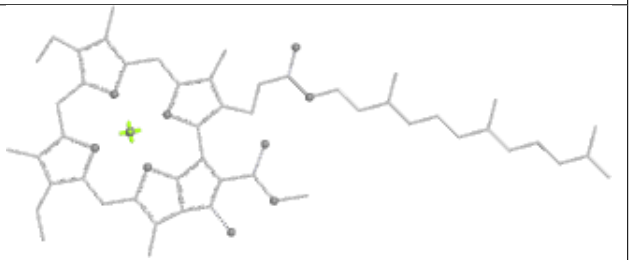
Bond lengths



Bond angles

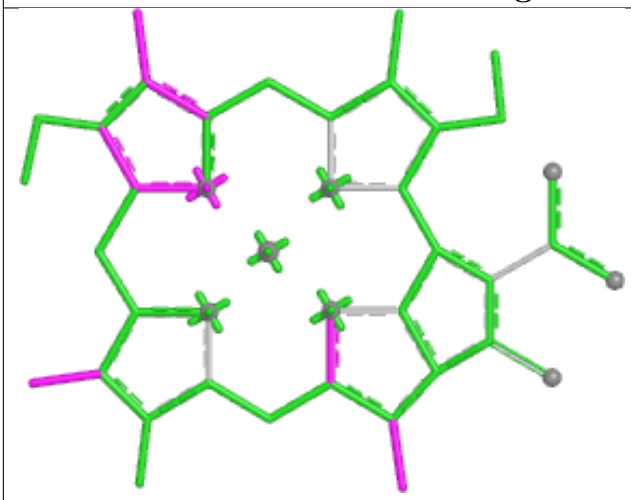


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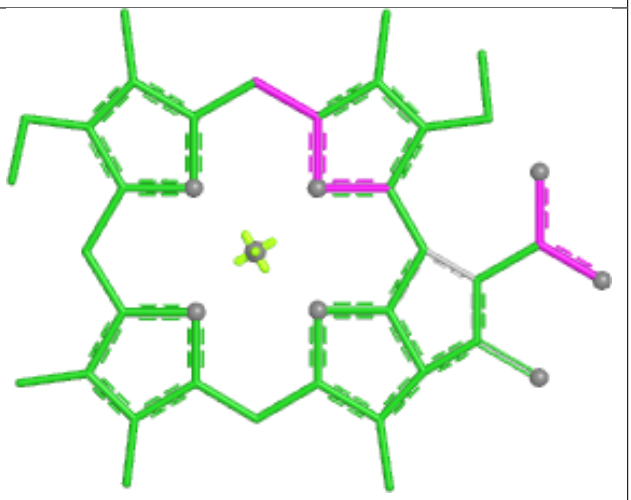


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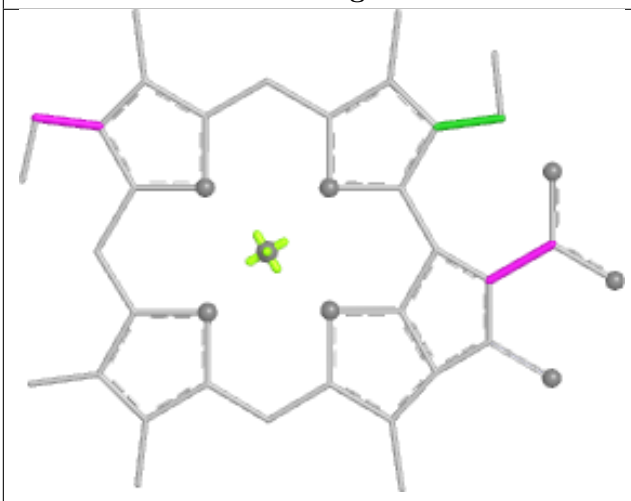
Ligand CLA O 2003



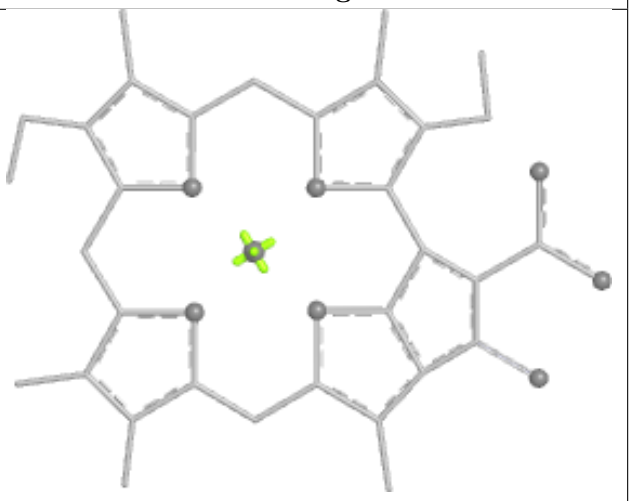
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Bond angles

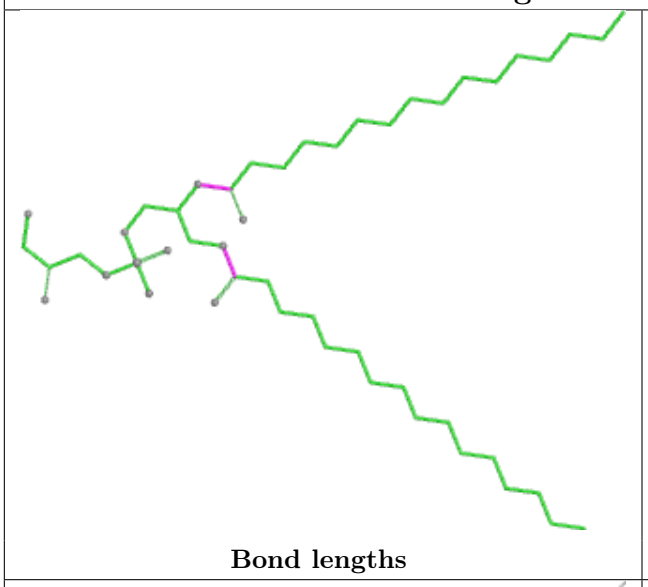


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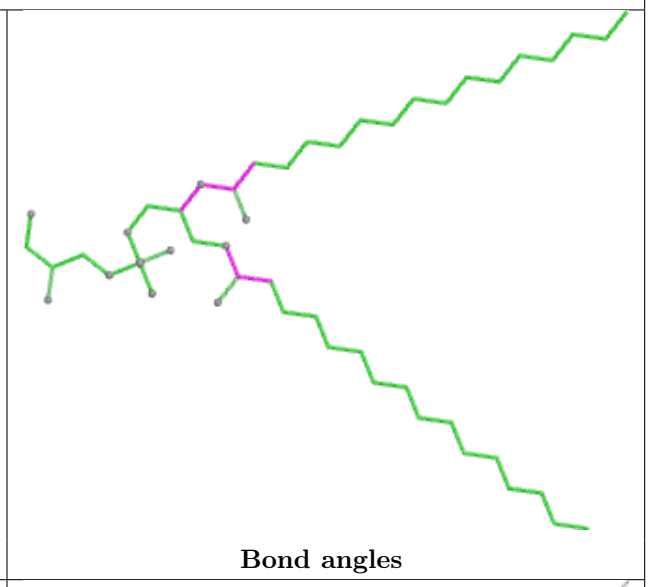


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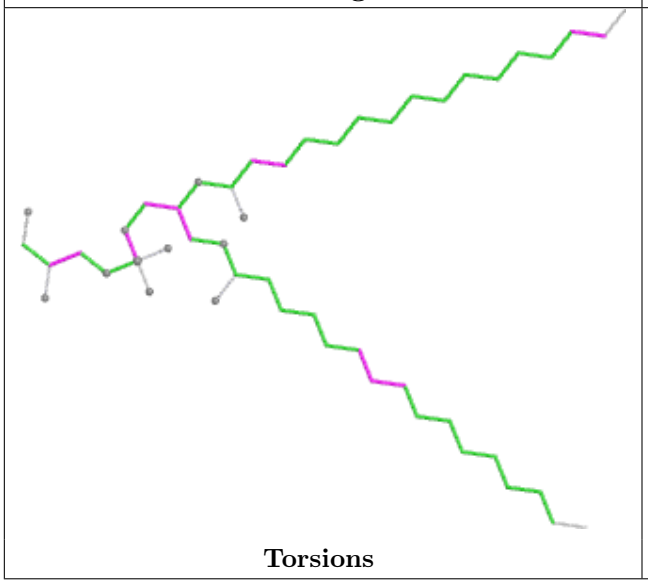
Ligand LHG X 2630



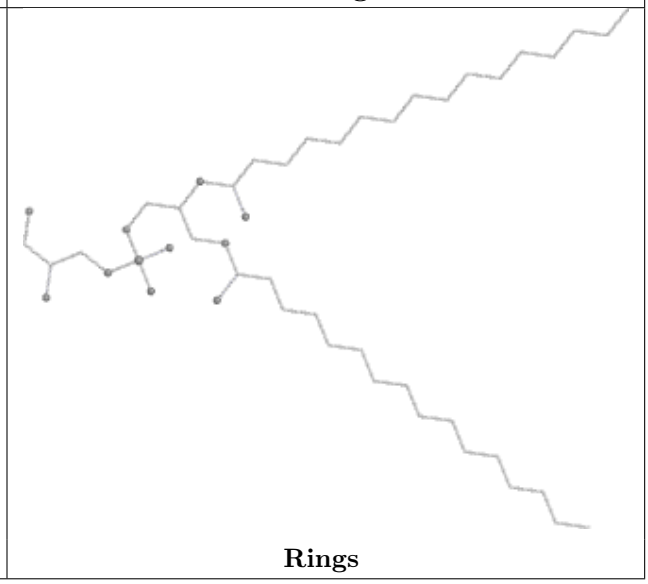
Bond lengths



Bond angles



Torsions

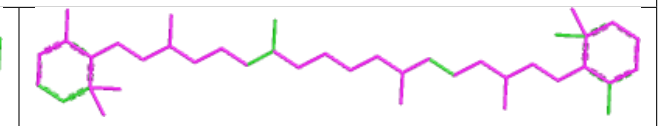


Rings

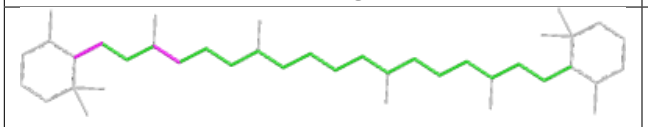
Ligand BCR L 301



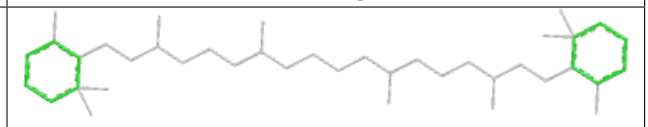
Bond lengths



Bond angles

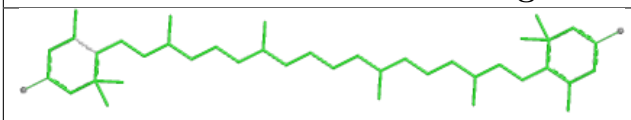


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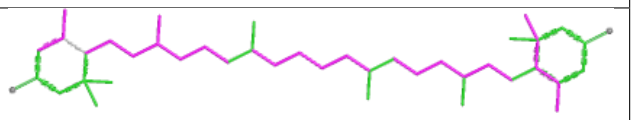


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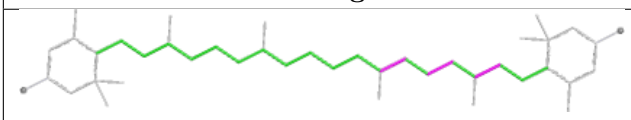
Ligand LUT Z 1620



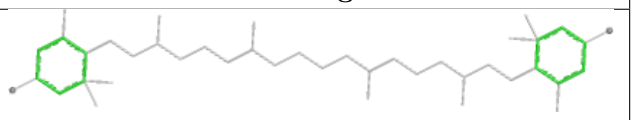
Bond lengths



Bond angles

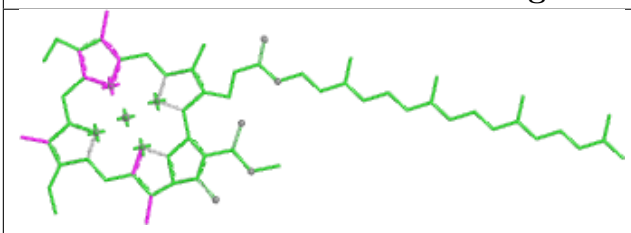


Torsions

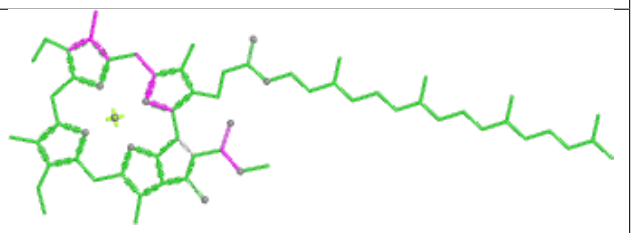


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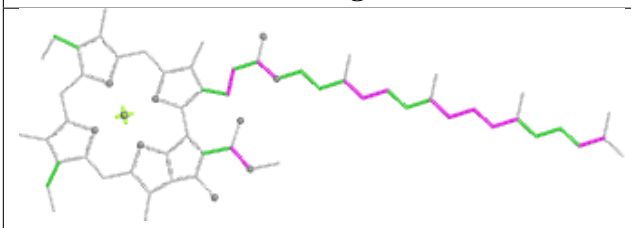
Ligand CLA 1 613



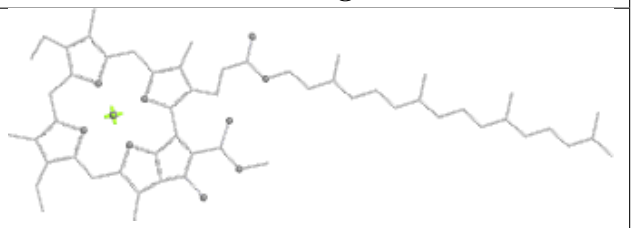
Bond lengths



Bond angles

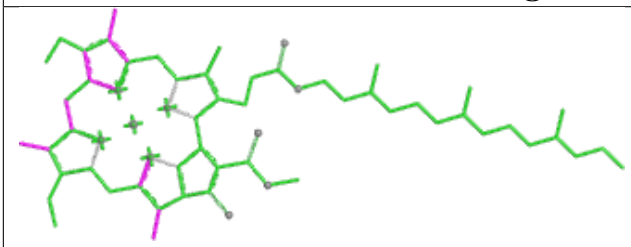


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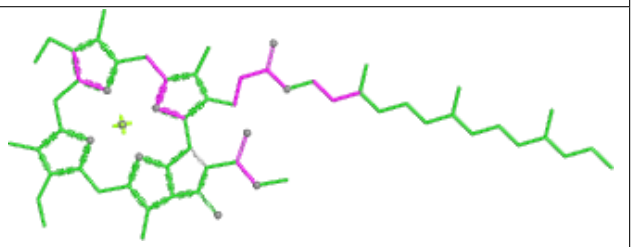


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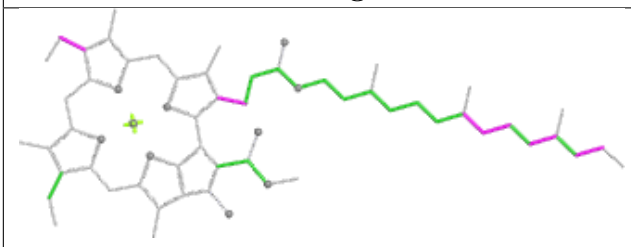
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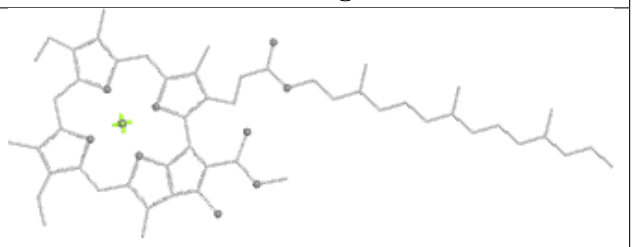
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Bond angles

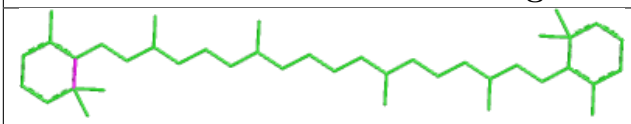


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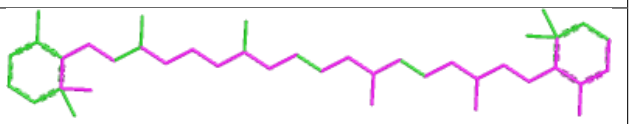


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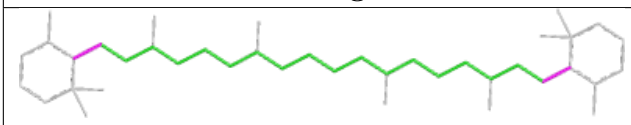
Ligand BCR 7 623



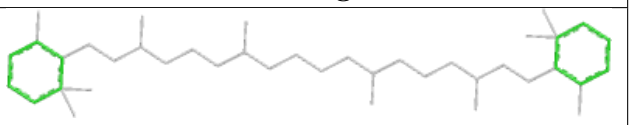
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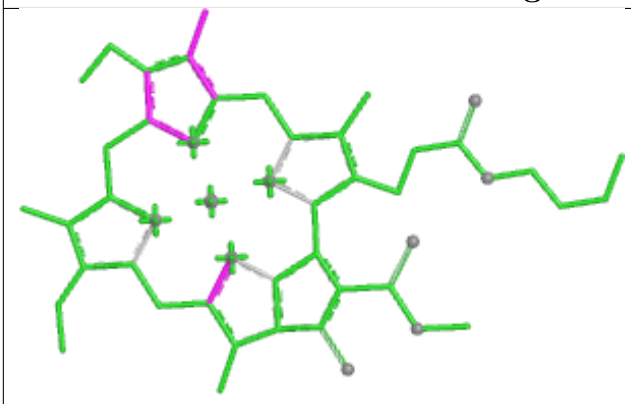


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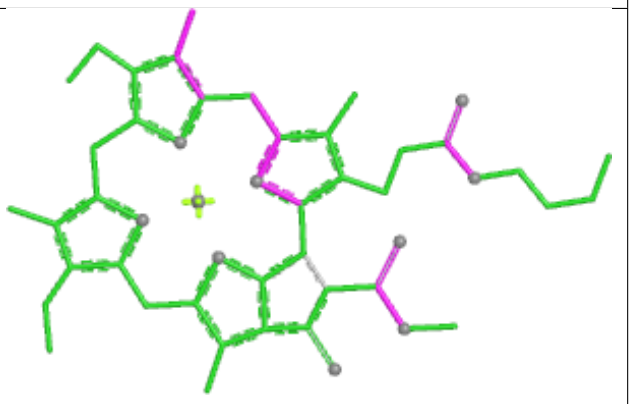


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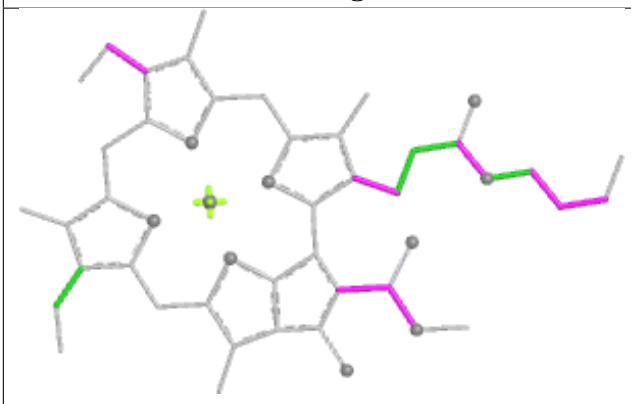
Ligand CLA X 604



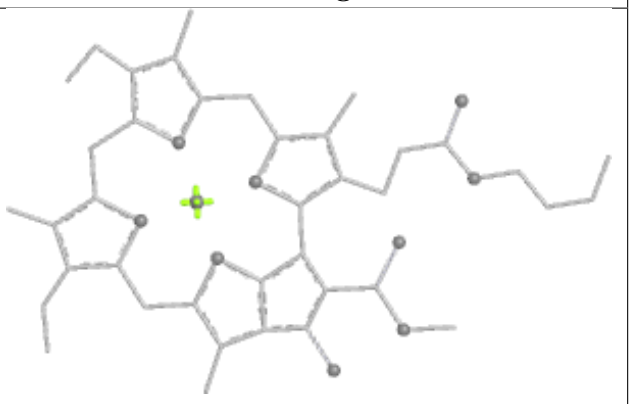
Bond lengths



Bond angles

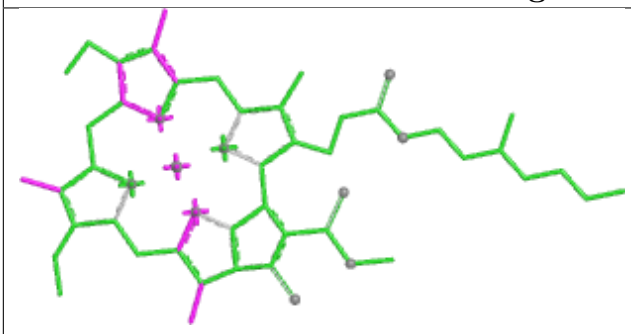


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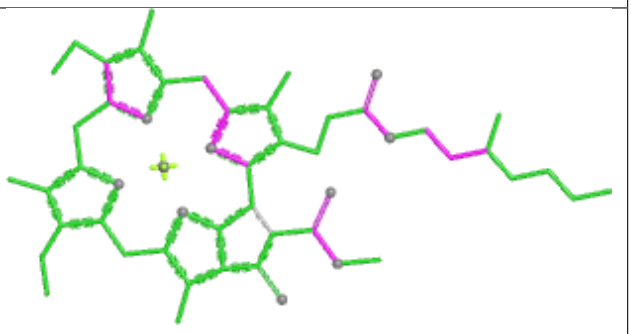


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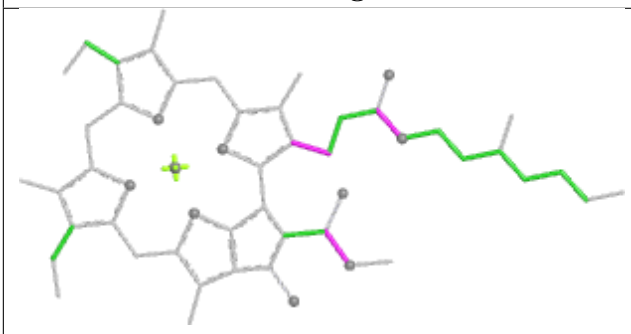
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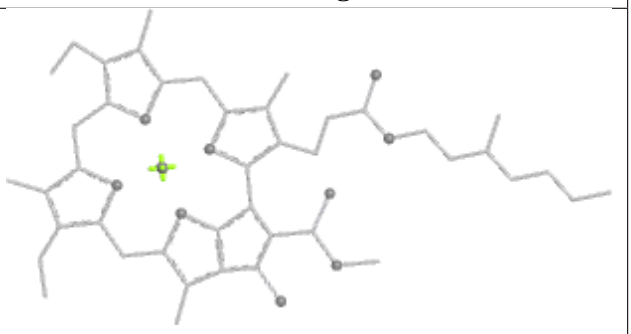
Bond lengths



Bond angles

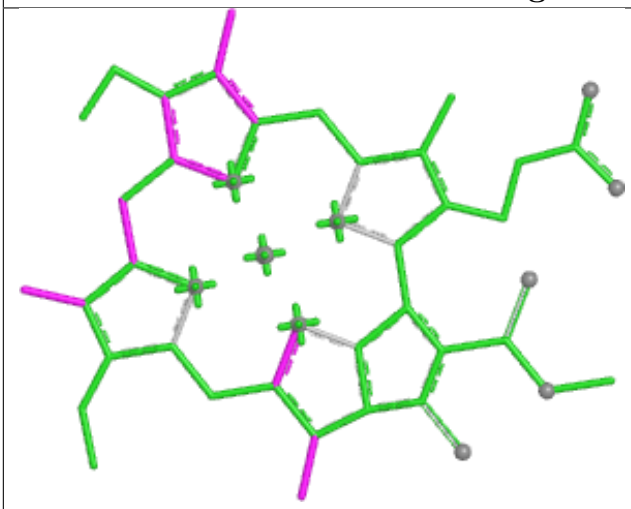


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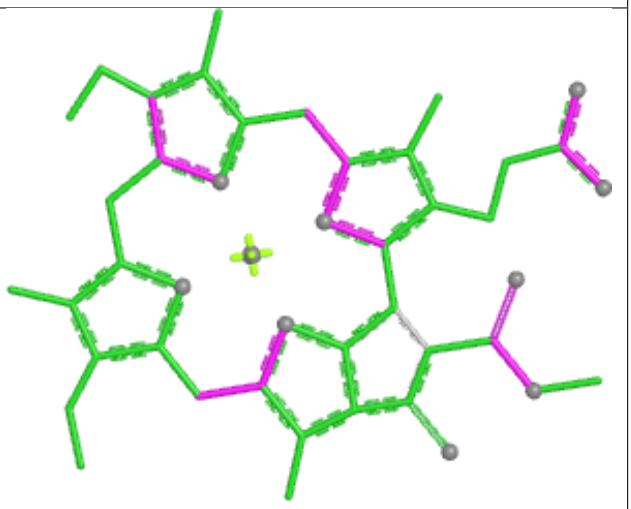


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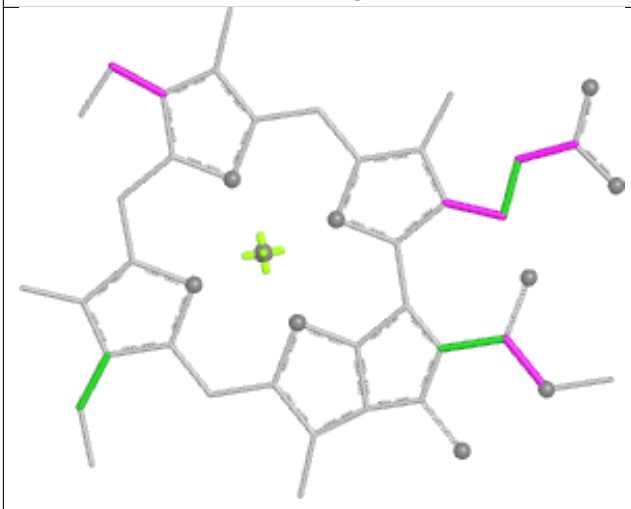
Ligand CLA 6 608



Bond lengths



Bond angles

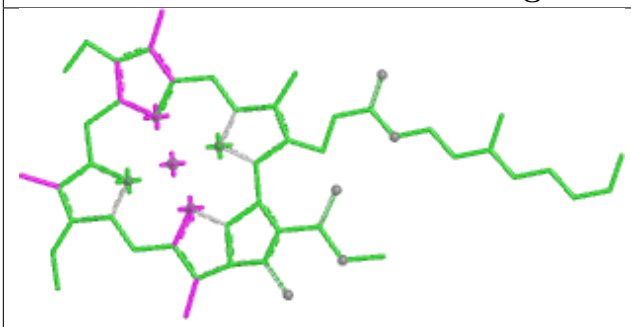


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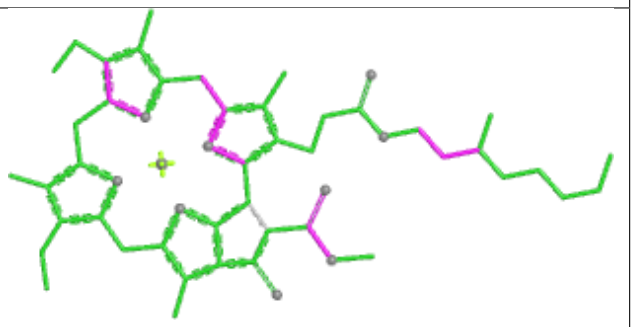


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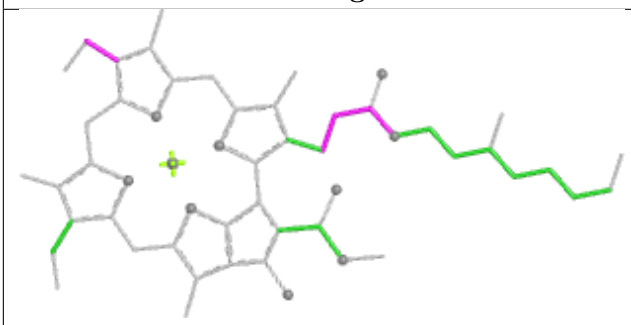
Ligand CLA A 813



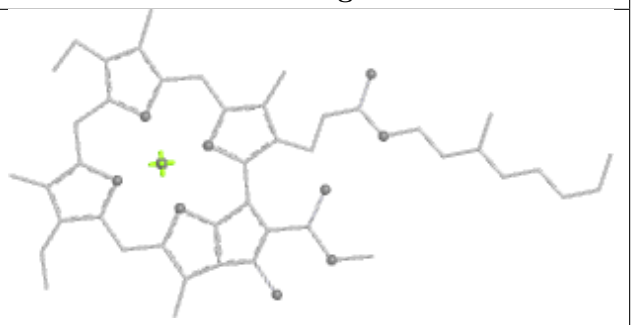
Bond lengths



Bond angles

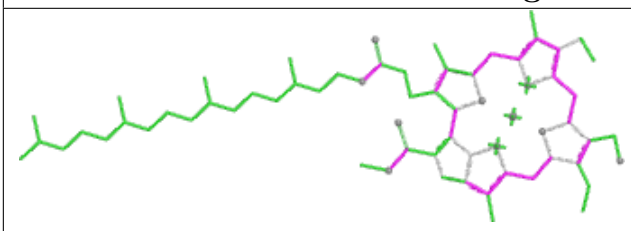


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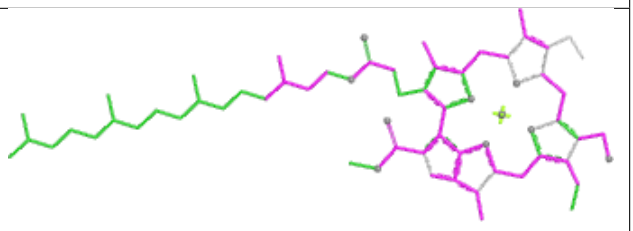


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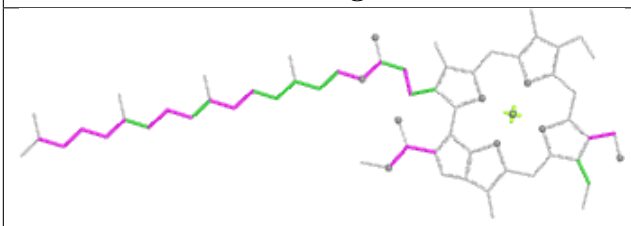
Ligand CHL X 608



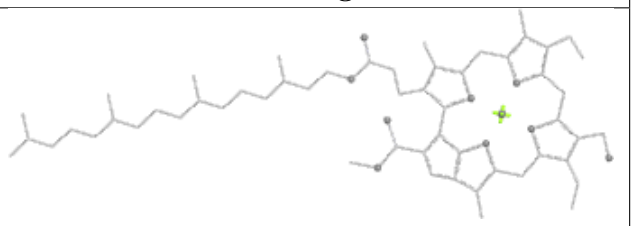
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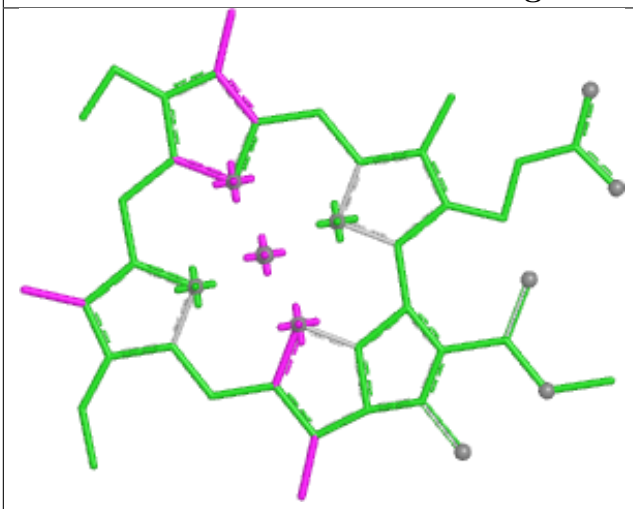


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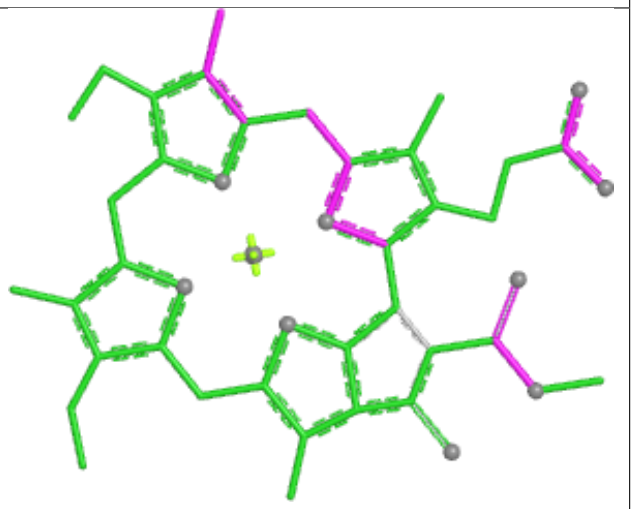


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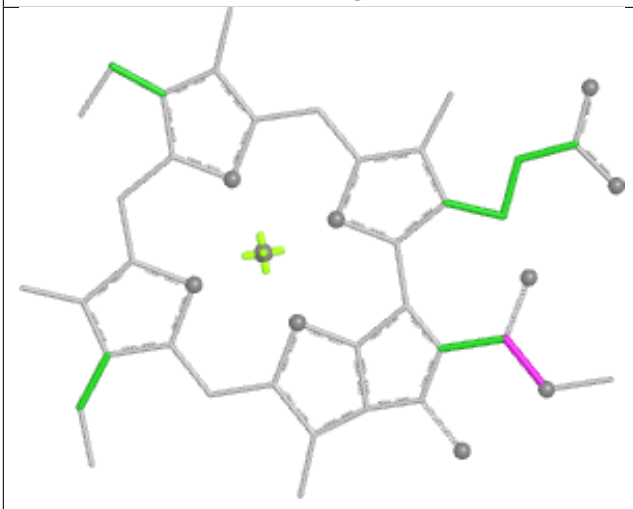
Ligand CLA B 835



Bond lengths



Bond angles

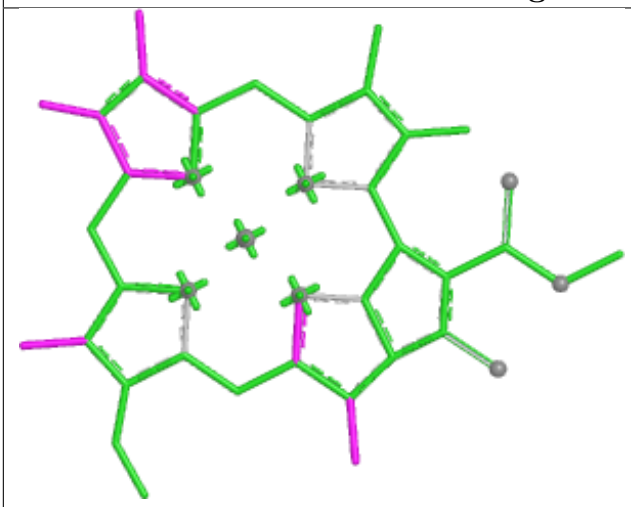


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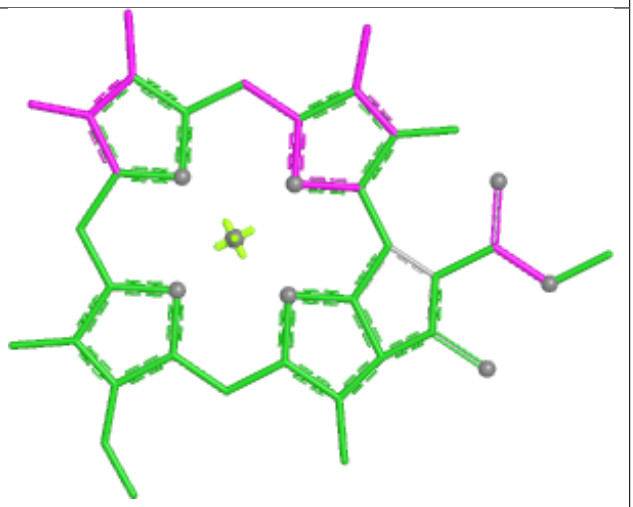


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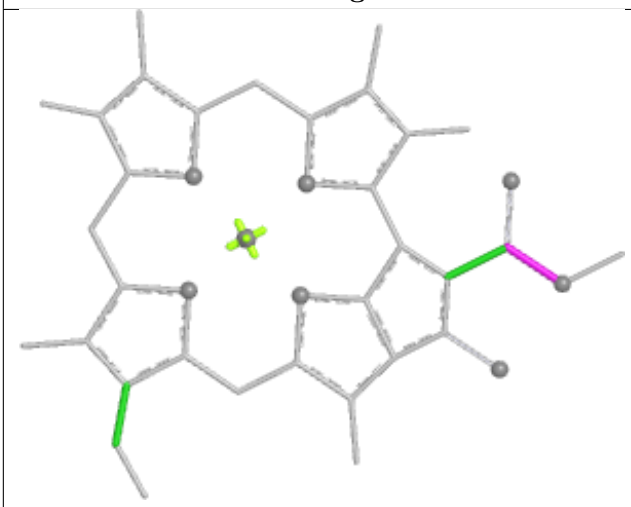
Ligand CLA 1 609



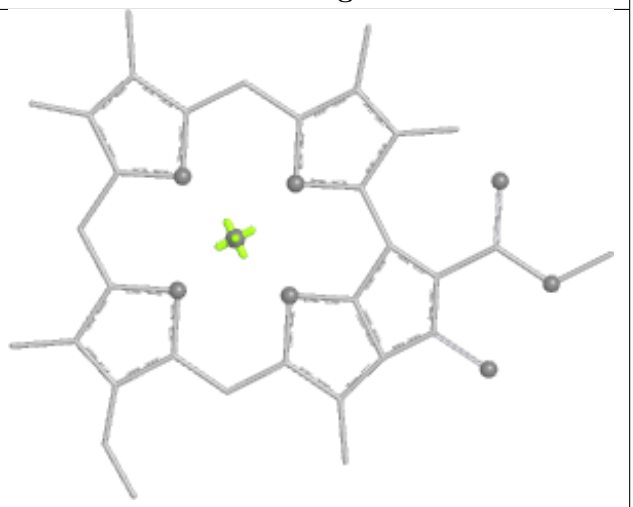
Bond lengths



Bond angles

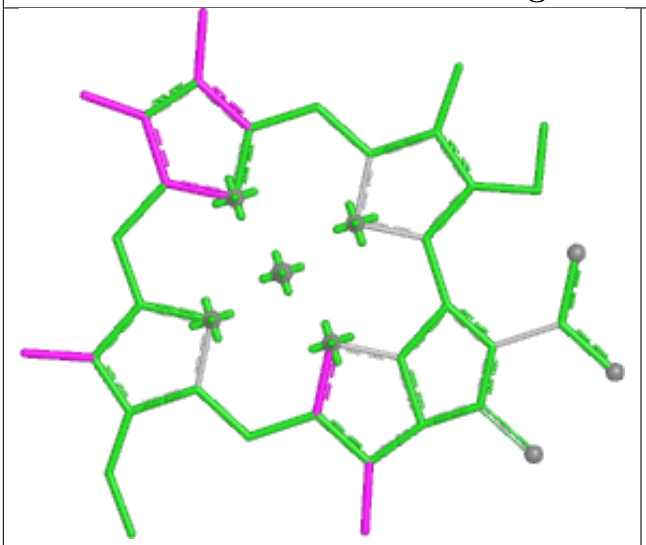


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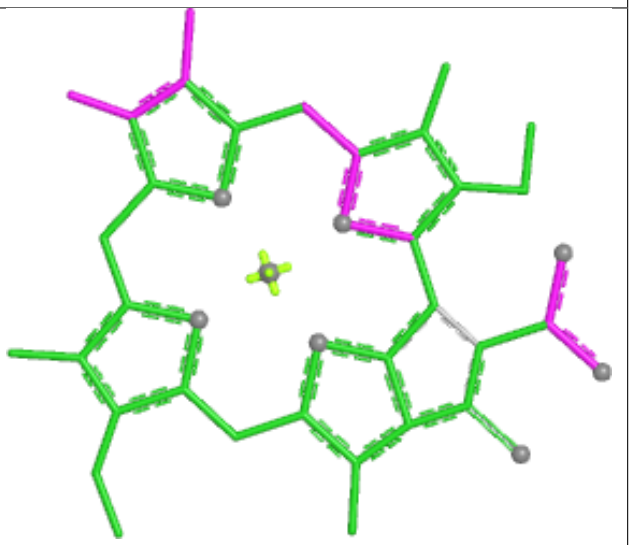


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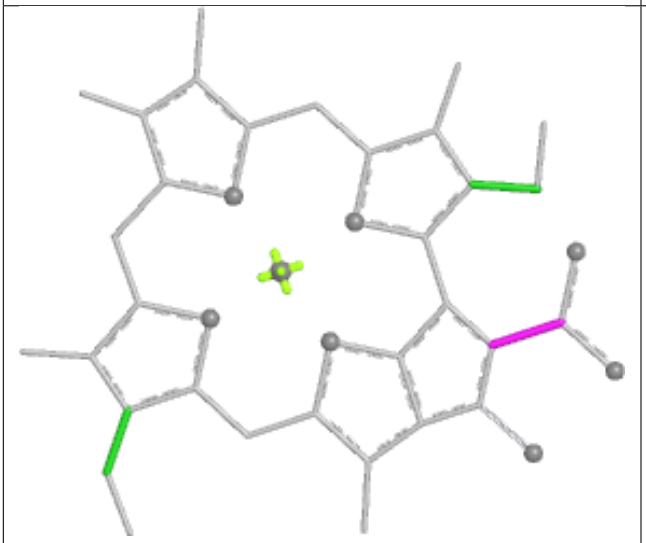
Ligand CLA 6 618



Bond lengths



Bond angles

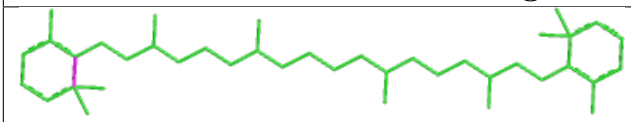


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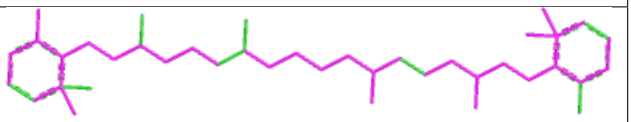


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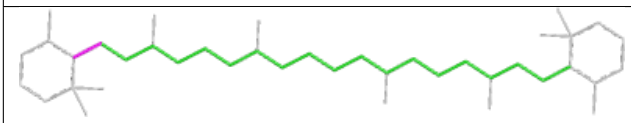
Ligand BCR A 851



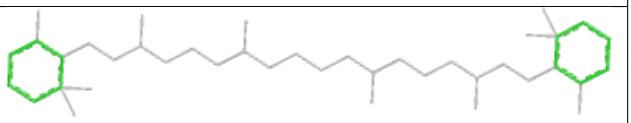
Bond lengths



Bond angles

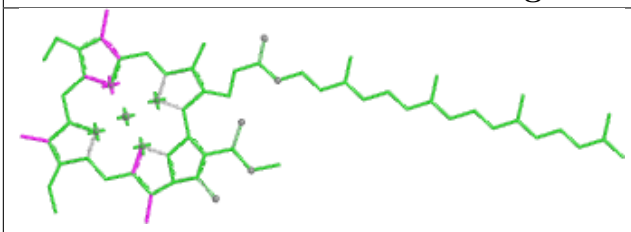


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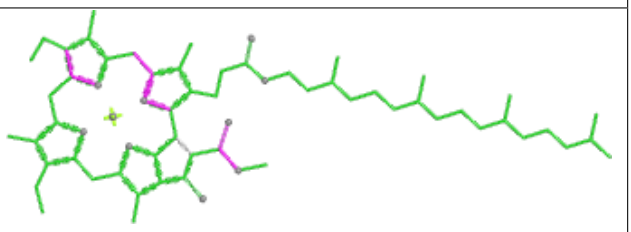


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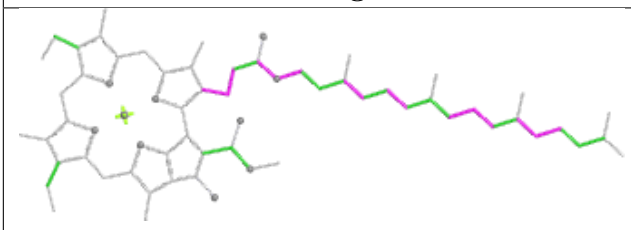
Ligand CLA B 828



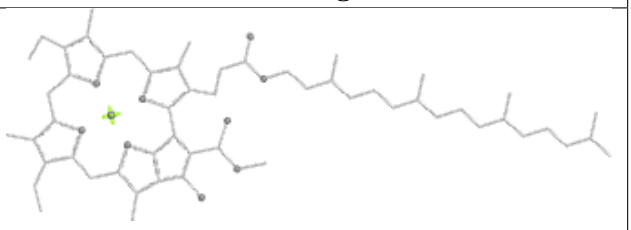
Bond lengths



Bond angles

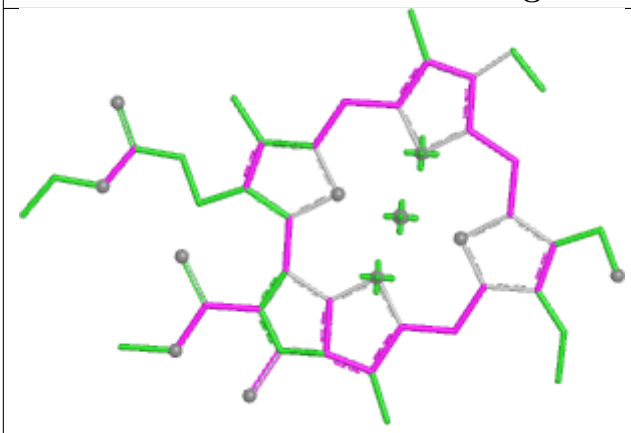


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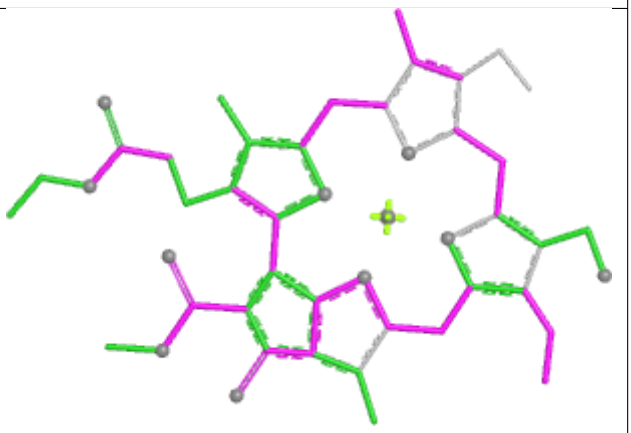


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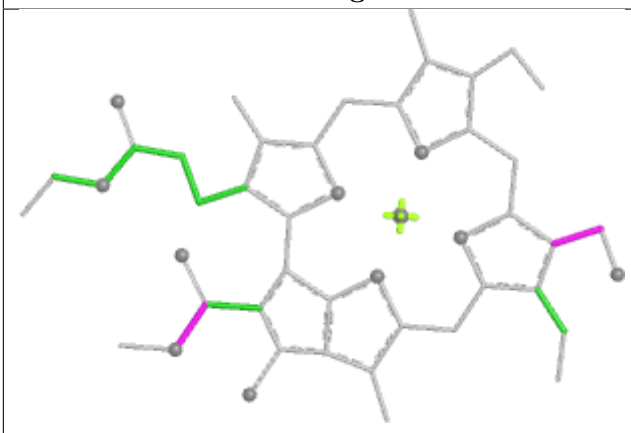
Ligand CHL V 608



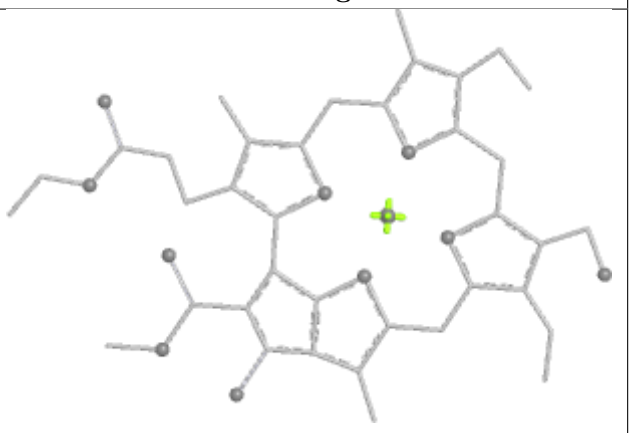
Bond lengths



Bond angles

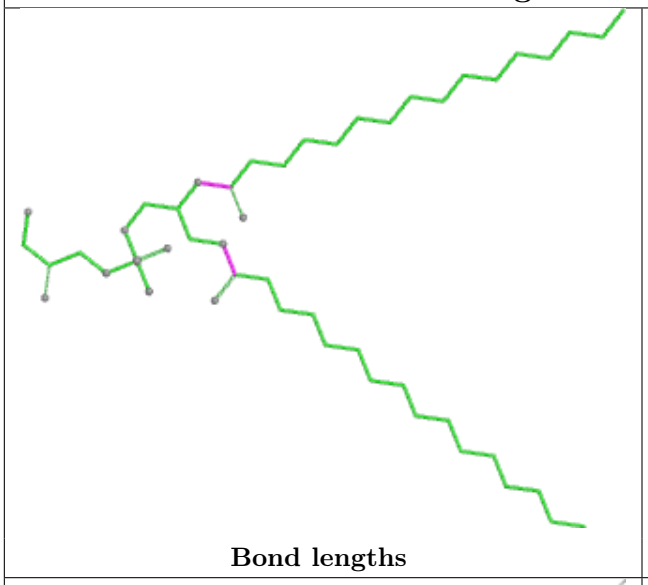


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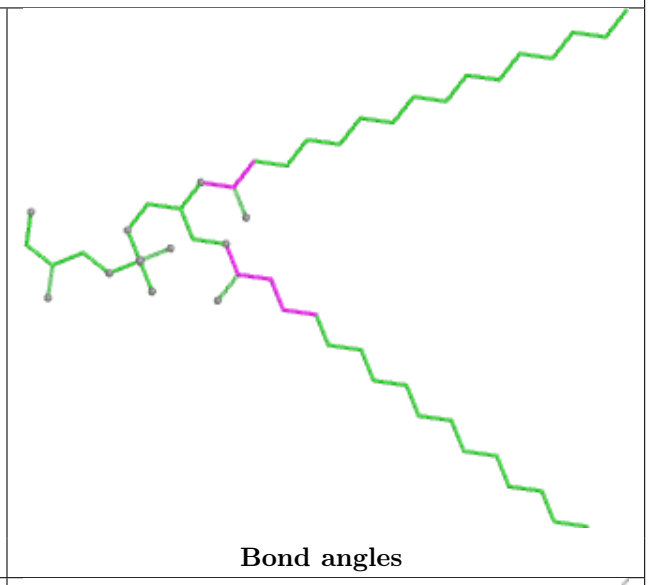


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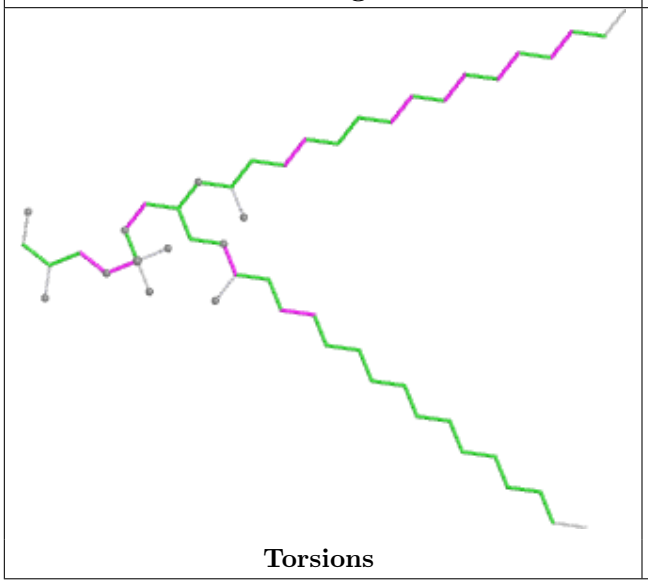
Ligand LHG Y 2630



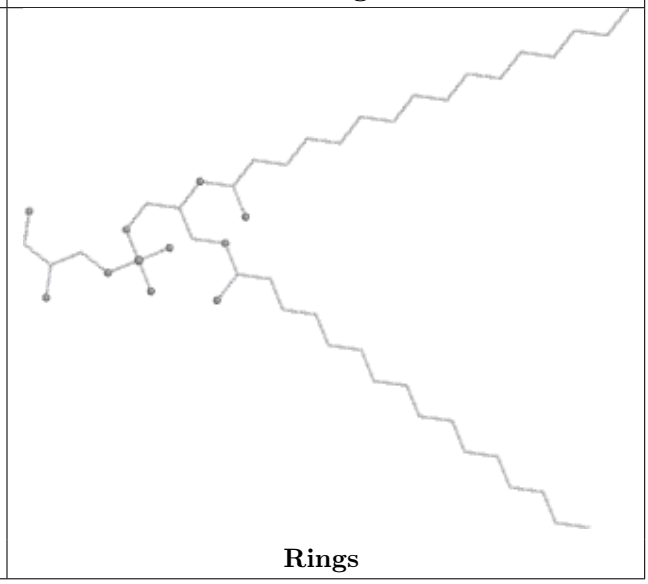
Bond lengths



Bond angles

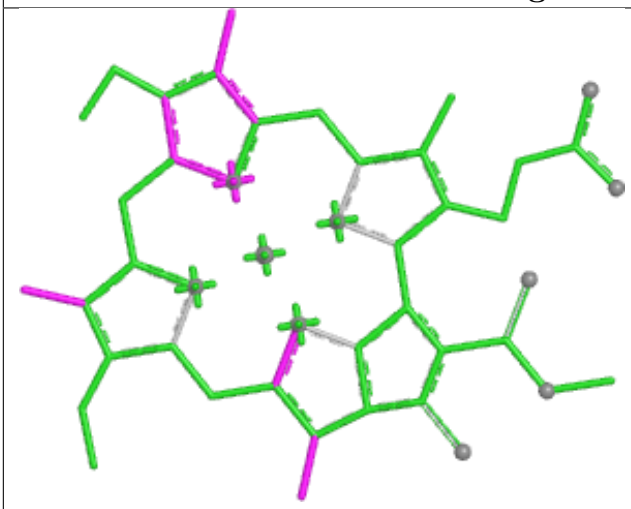


Torsions

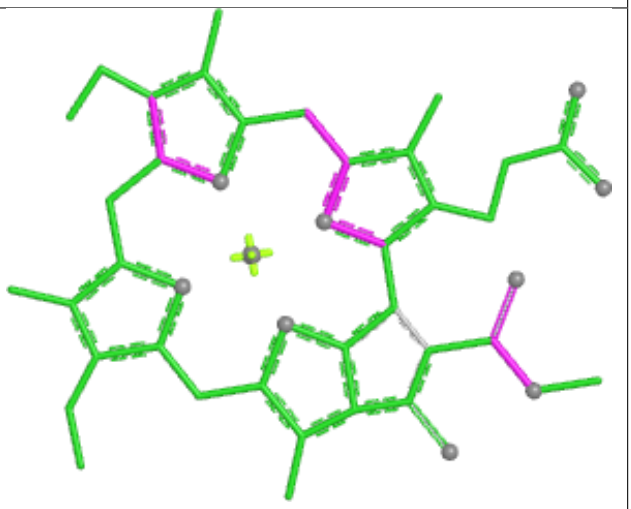


Rings

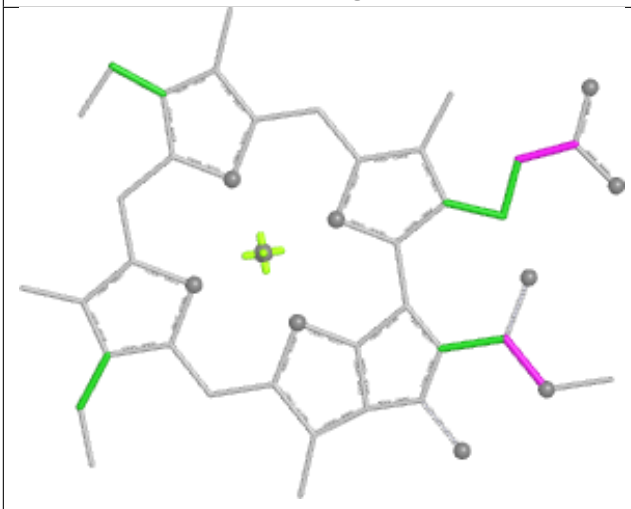
Ligand CLA a 612



Bond lengths



Bond angles

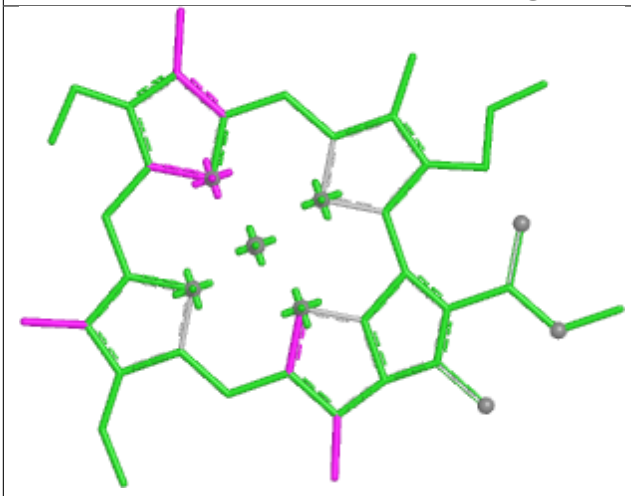


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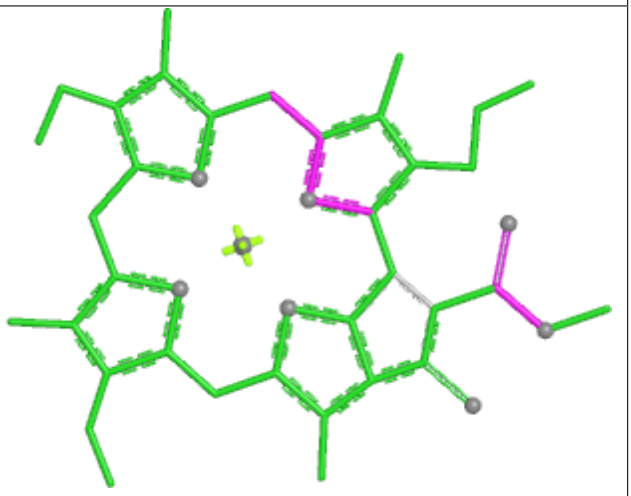


Rings

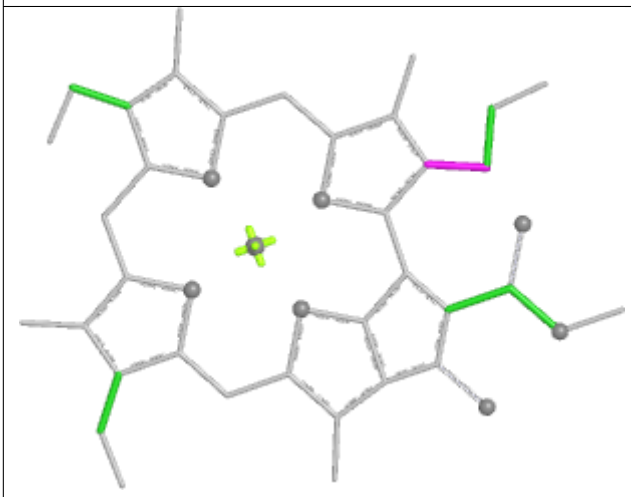
Ligand CLA B 815



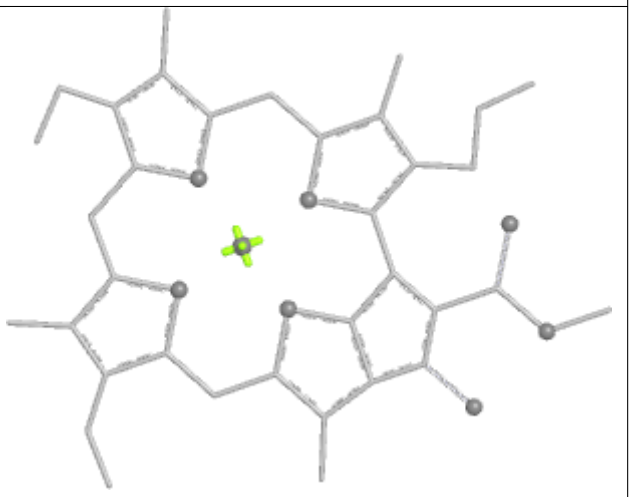
Bond lengths



Bond angles

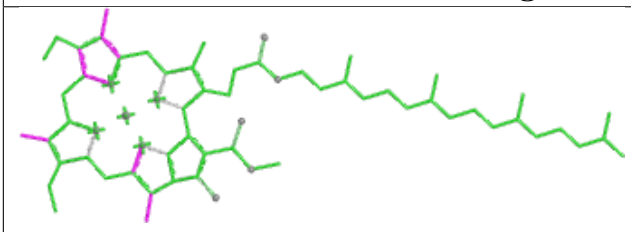


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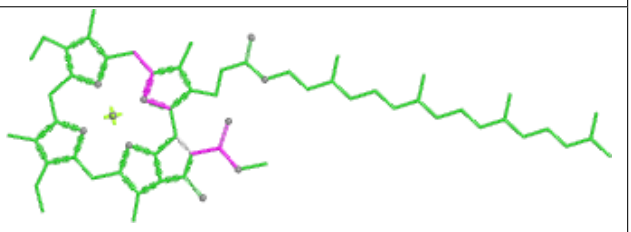


Rings

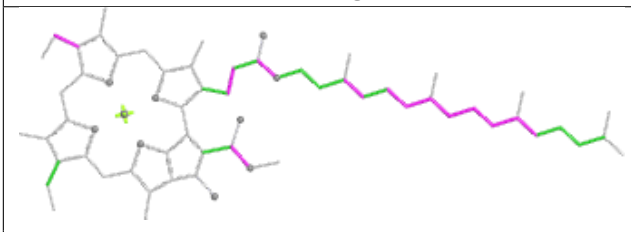
Ligand CLA W 613



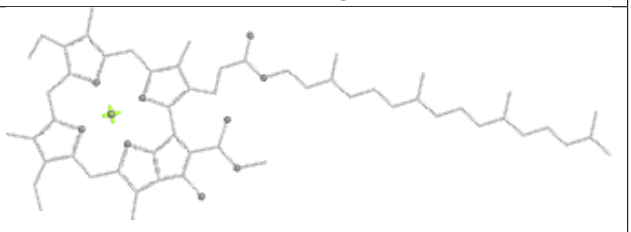
Bond lengths



Bond angles

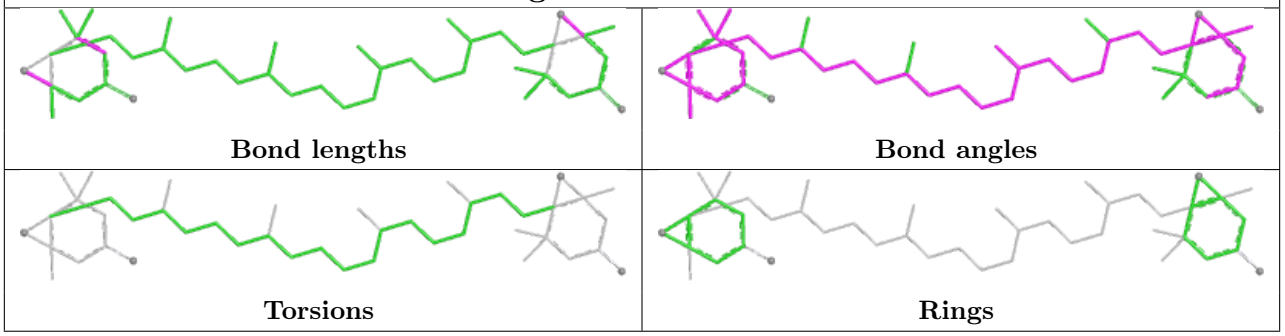


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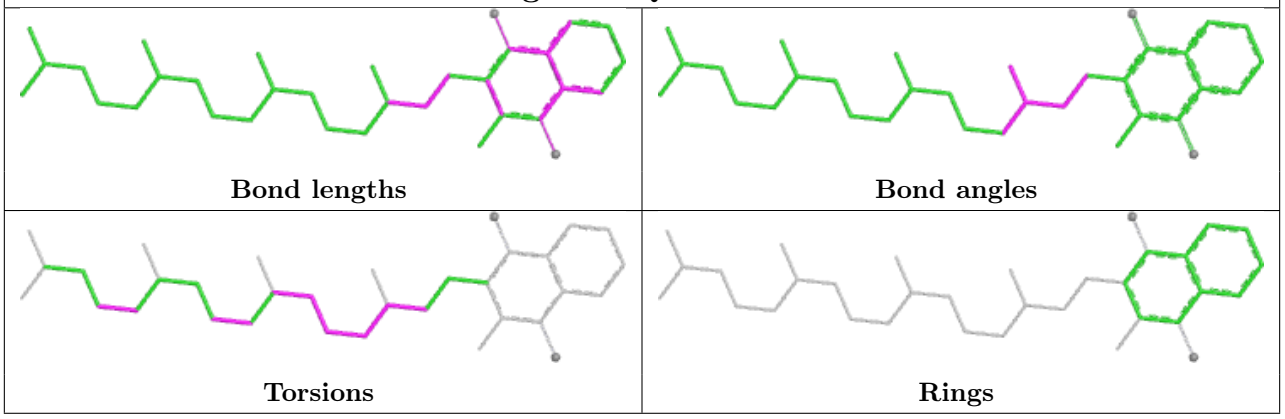


Rings

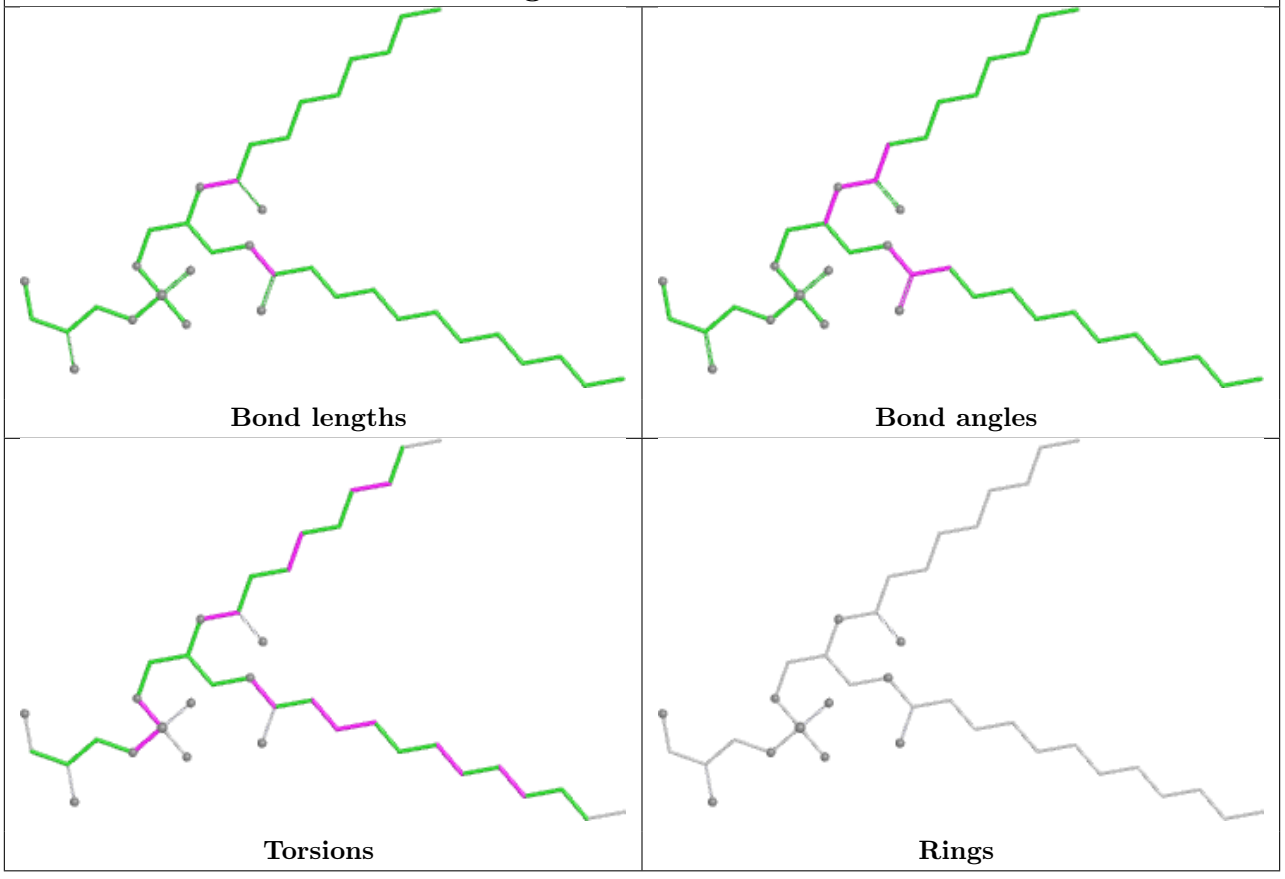
Ligand XAT a 618



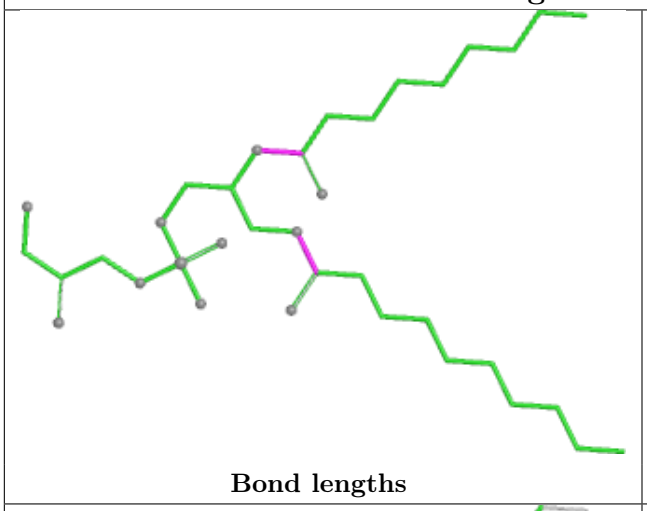
Ligand PQN A 844



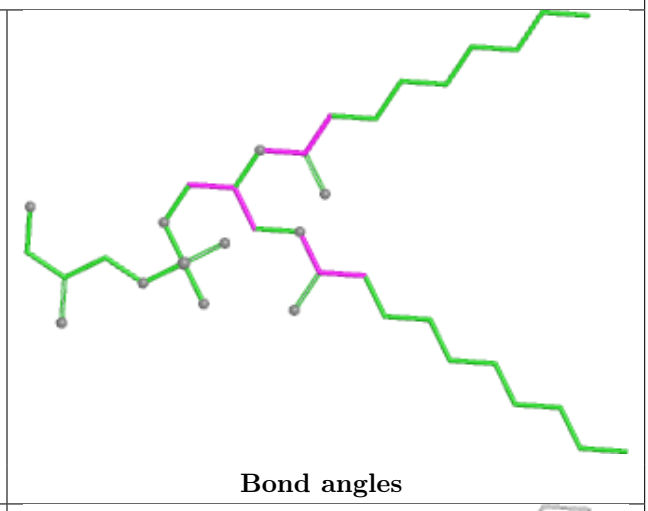
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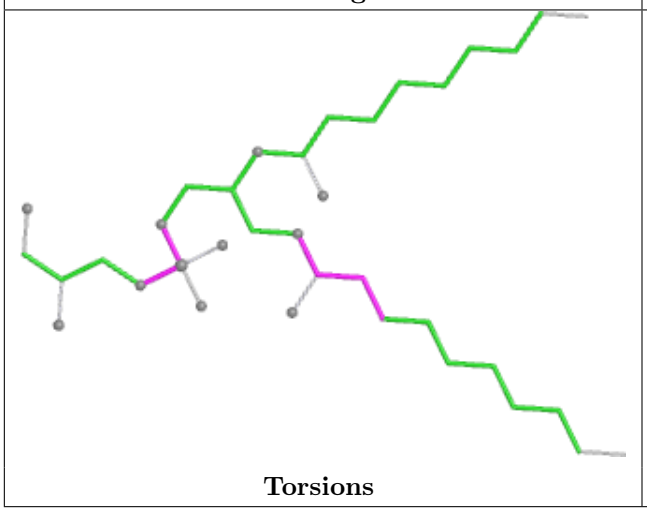
Ligand LHG 2 622



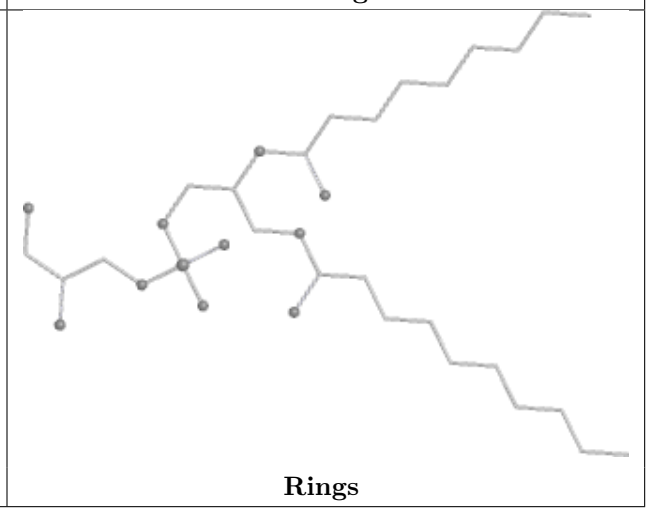
Bond lengths



Bond angles

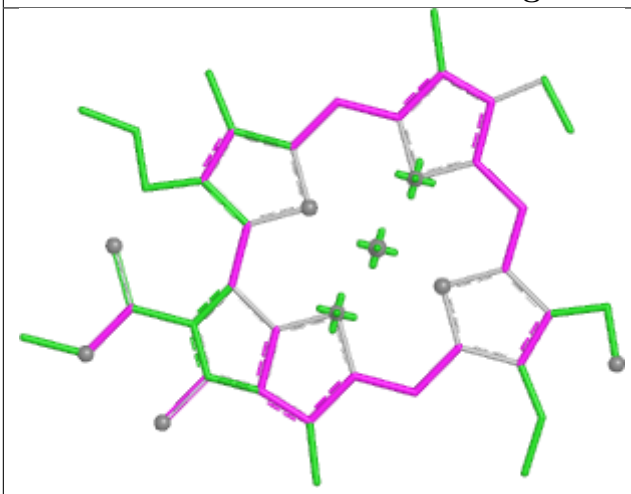


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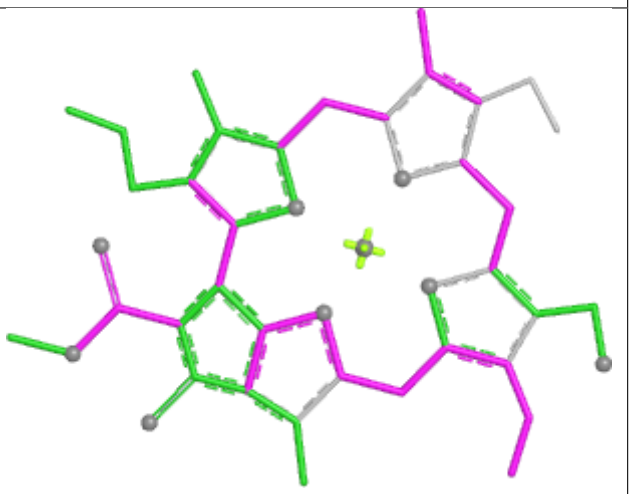


Rings

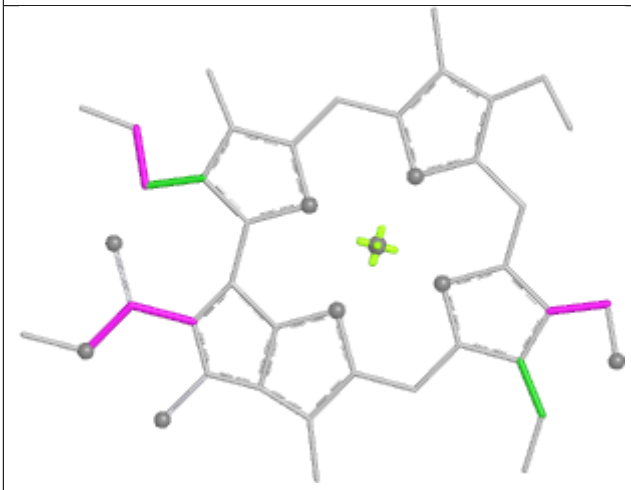
Ligand CHL U 606



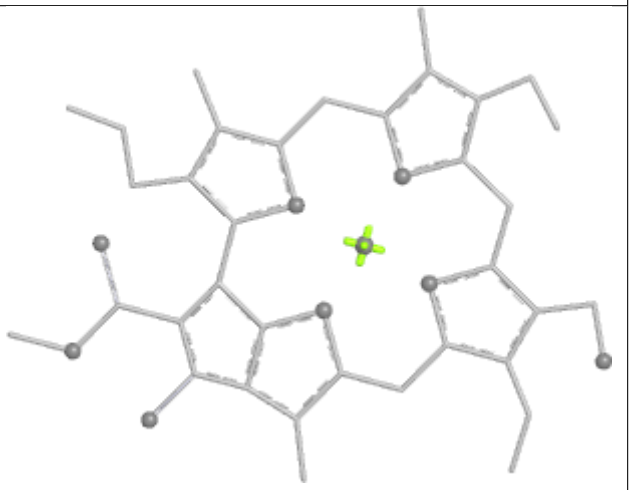
Bond lengths



Bond angles

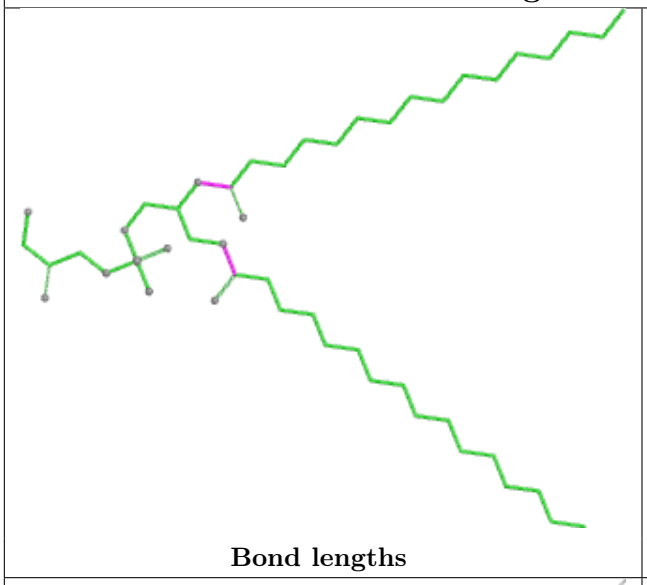


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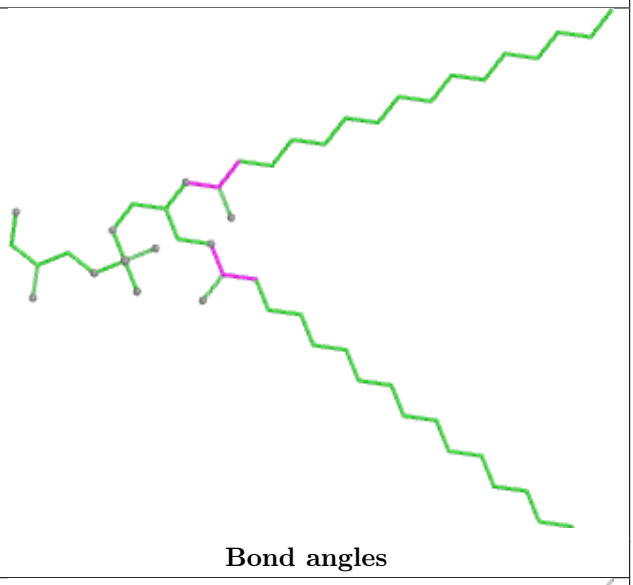


Rings

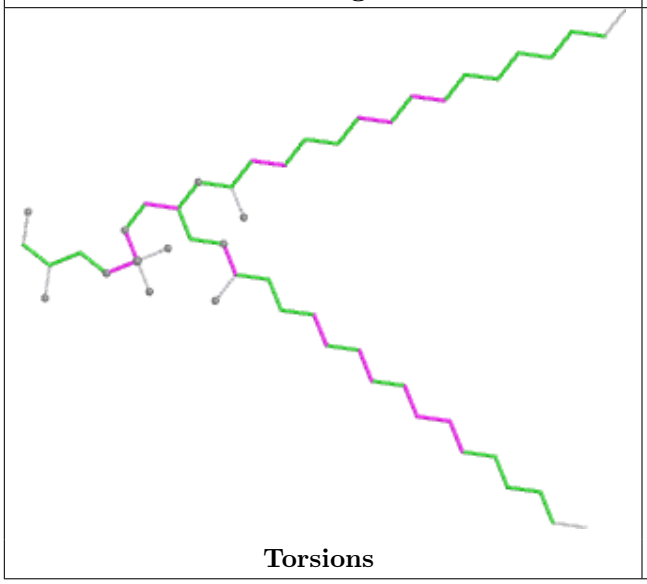
Ligand LHG A 846



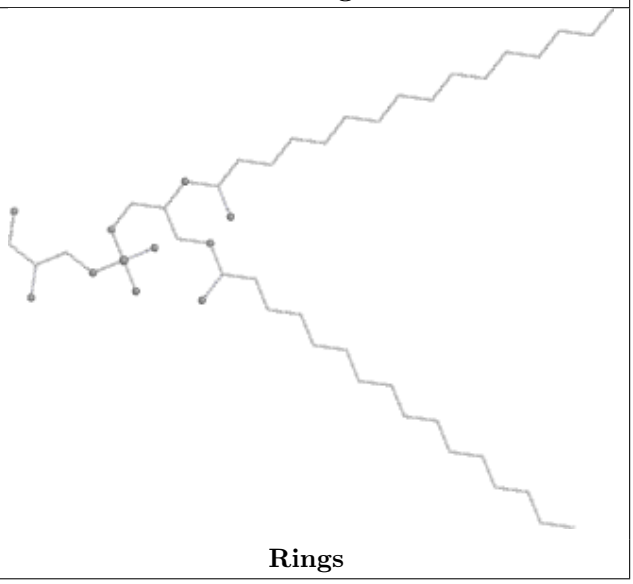
Bond lengths



Bond angles

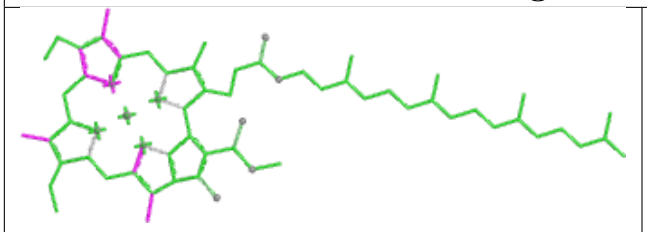


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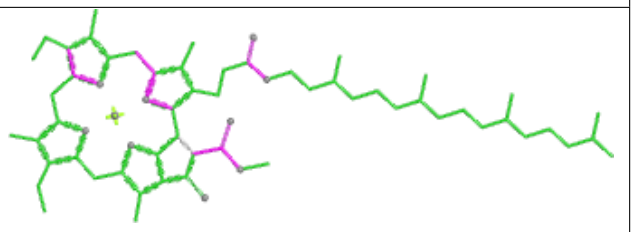


Rings

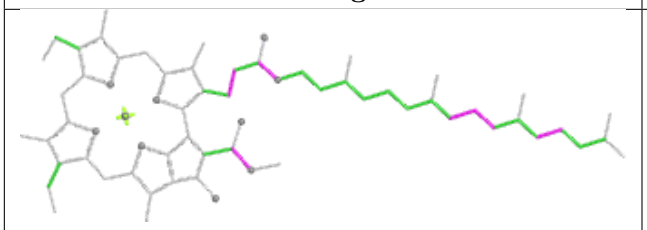
Ligand CLA 5 602



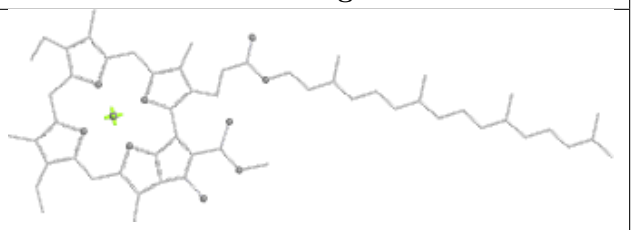
Bond lengths



Bond angles

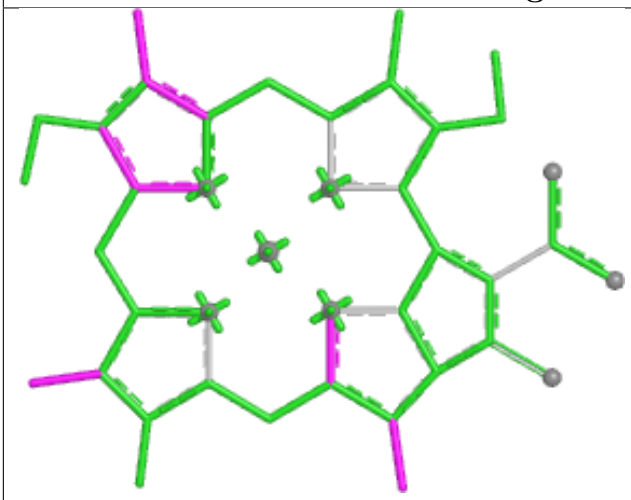


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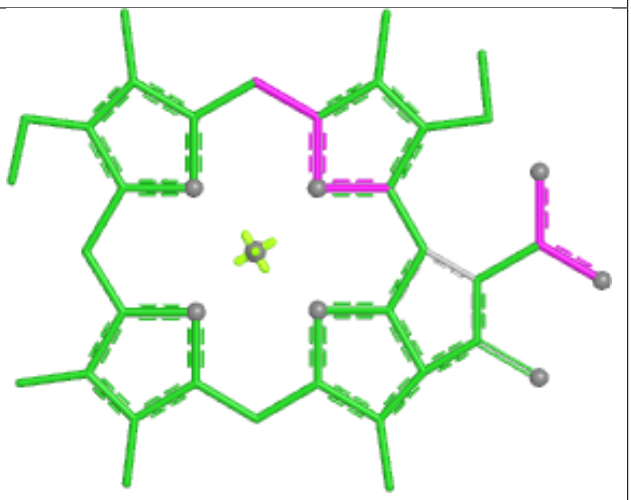


Rings

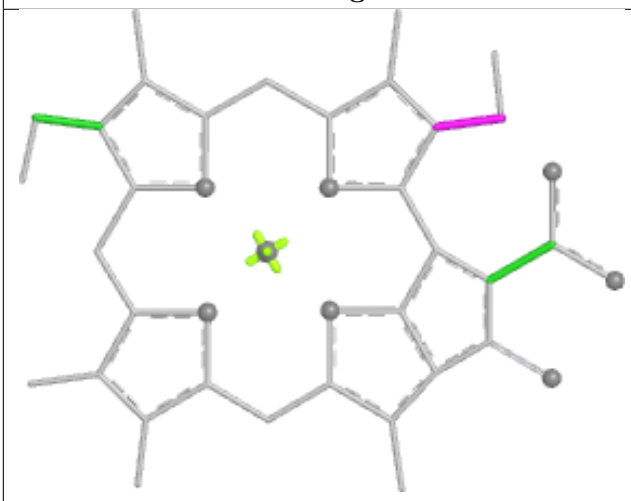
Ligand CLA L 306



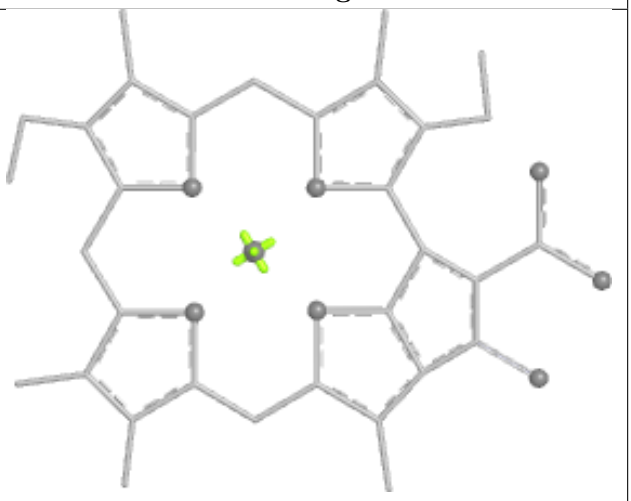
Bond lengths



Bond angles

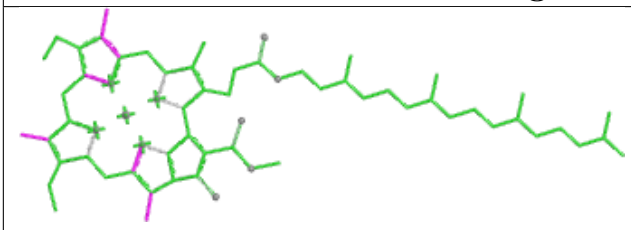


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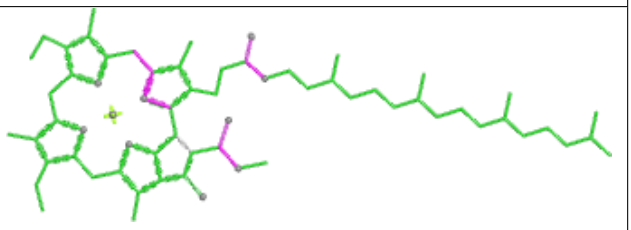


Rings

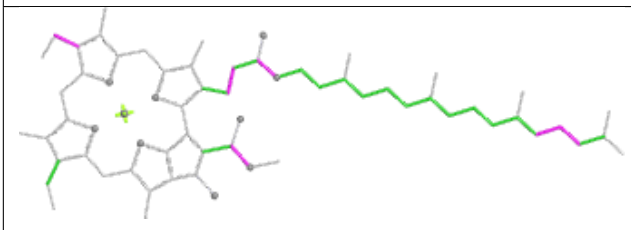
Ligand CLA 2 613



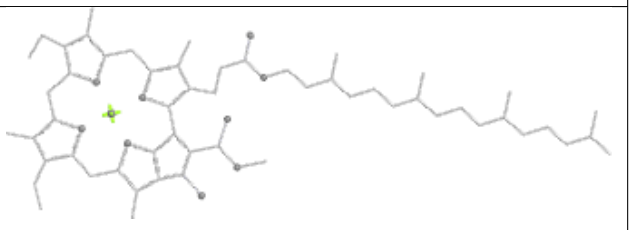
Bond lengths



Bond angles

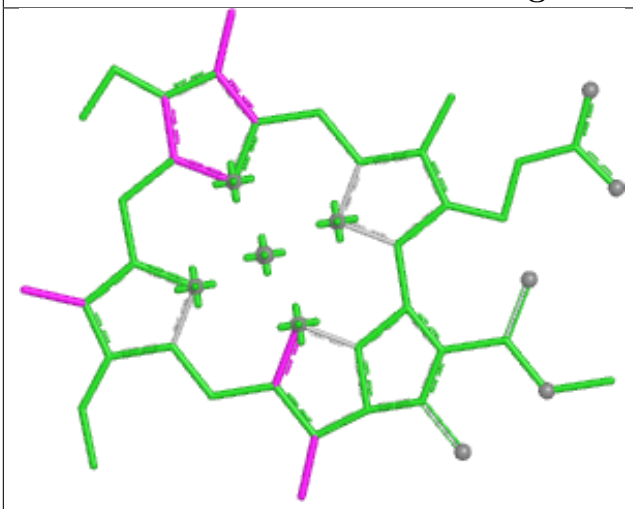


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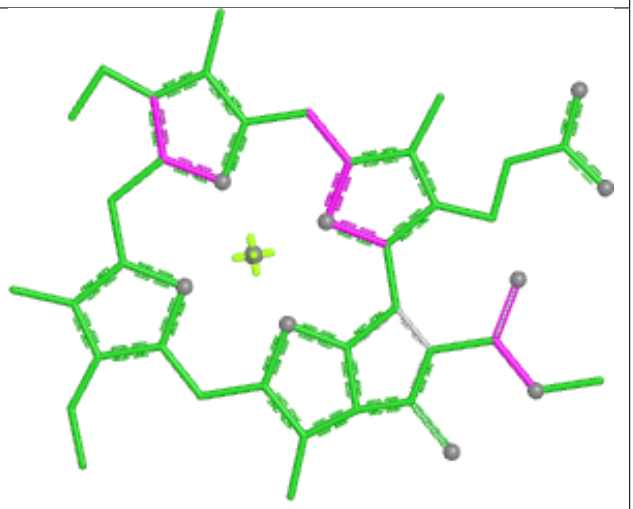


Rings

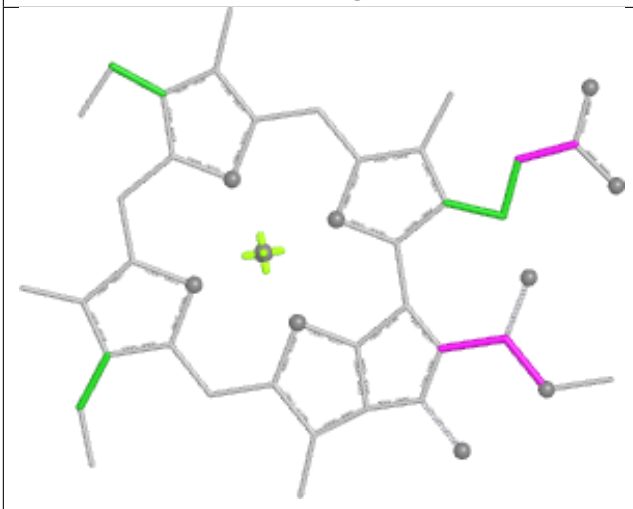
Ligand CLA 4 607



Bond lengths



Bond angles

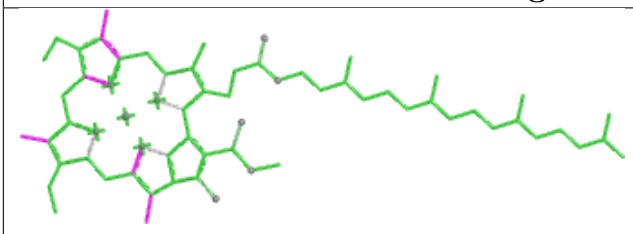


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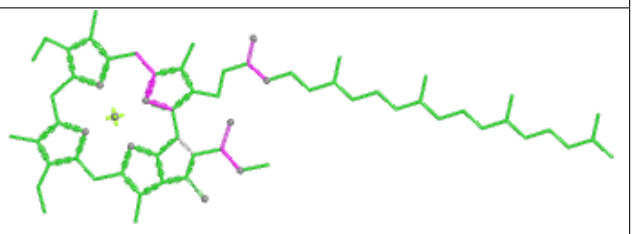


Rings

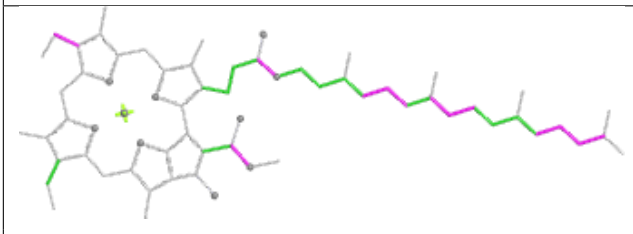
Ligand CLA 6 604



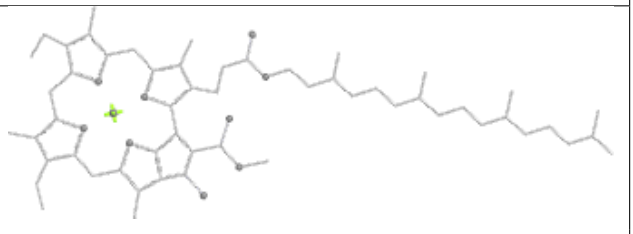
Bond lengths



Bond angles

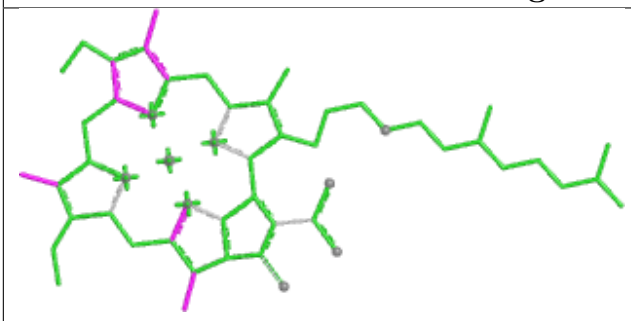


Torsions

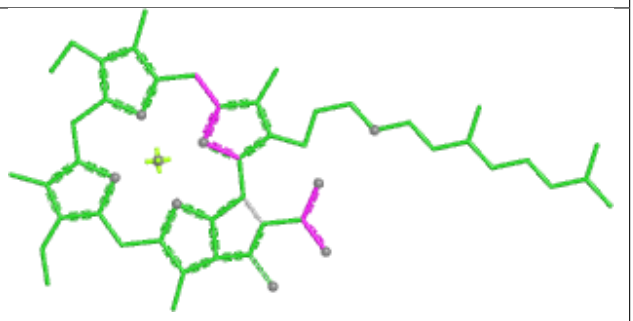


Rings

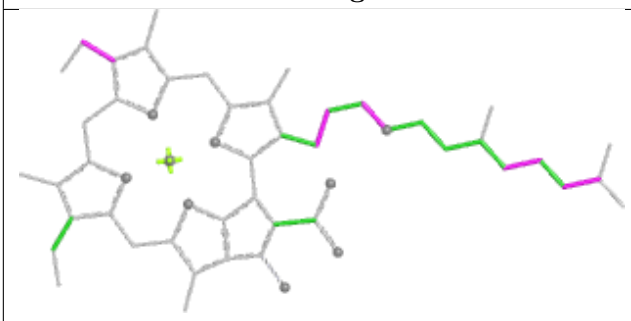
Ligand CLA 1 603



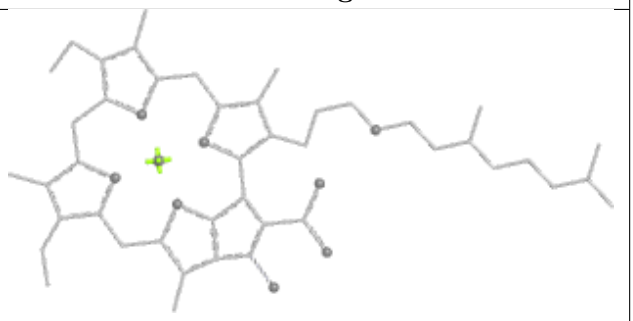
Bond lengths



Bond angles

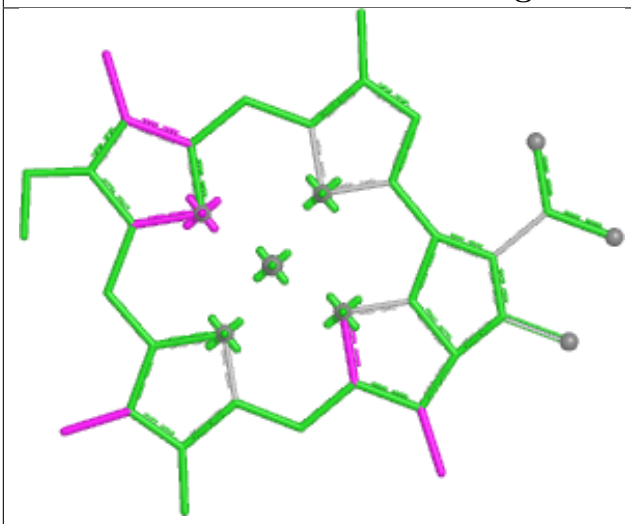


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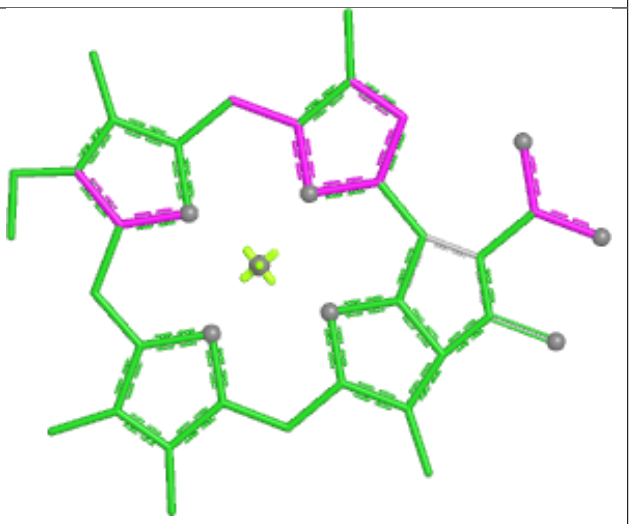


Rings

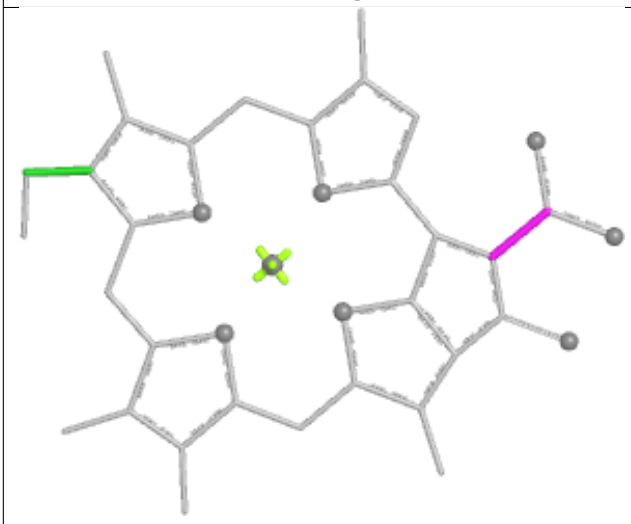
Ligand CLA O 2001



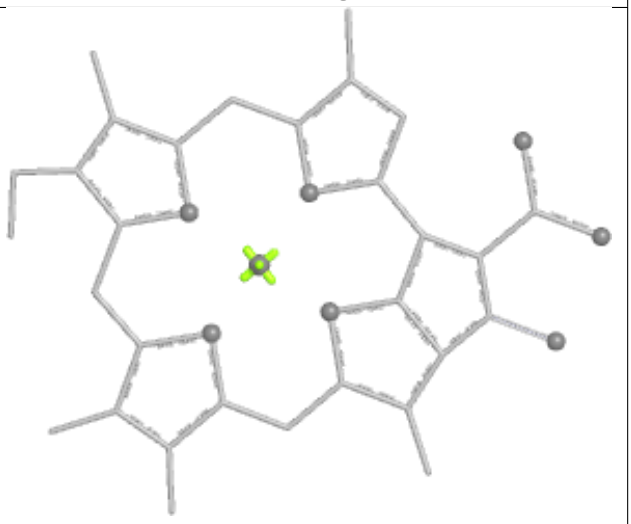
Bond lengths



Bond angles

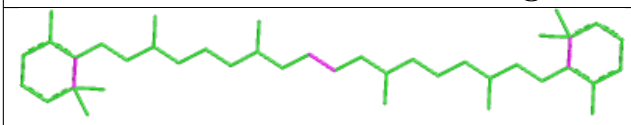


Torsions

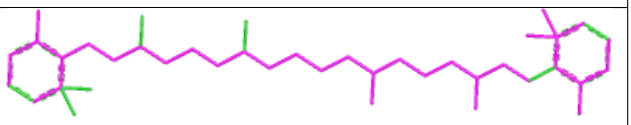


Rings

Ligand BCR B 844



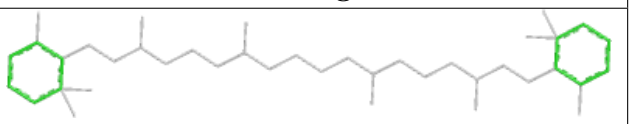
Bond lengths



Bond angles

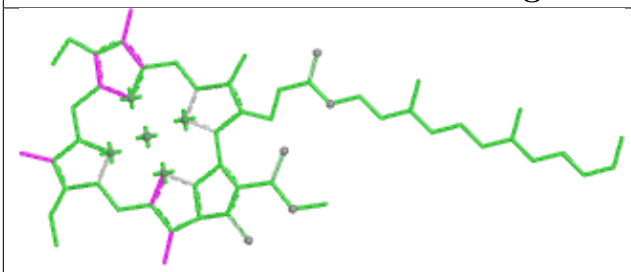


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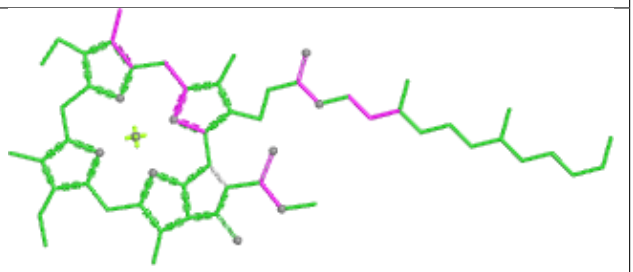


Rings

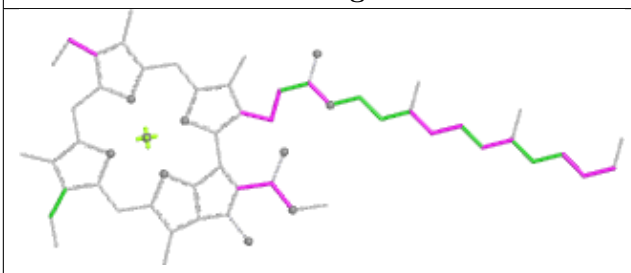
Ligand CLA U 602



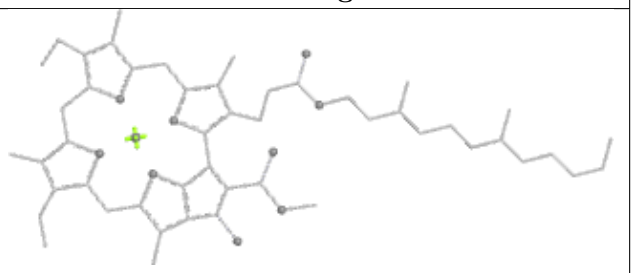
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Bond angles

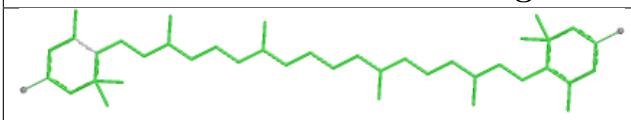


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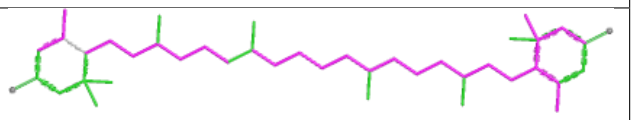


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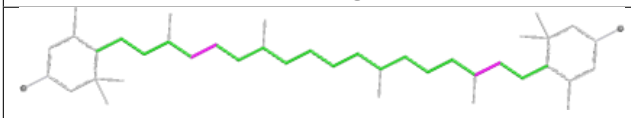
Ligand LUT V 1621



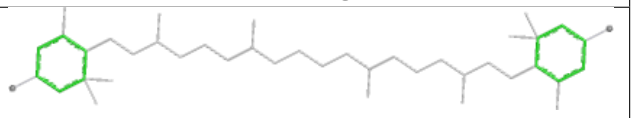
Bond lengths



Bond angles

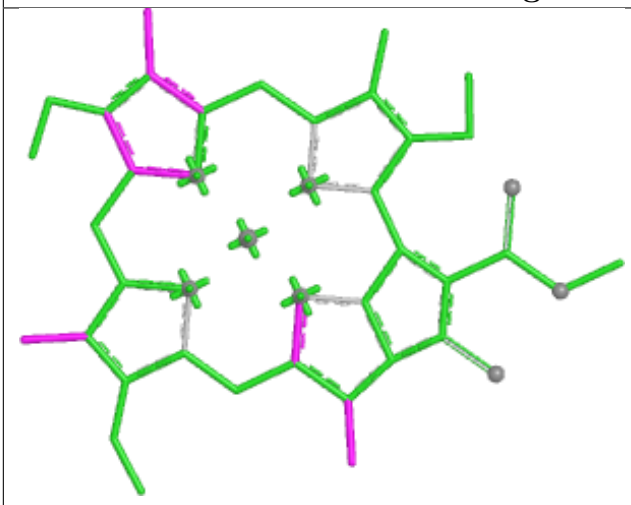


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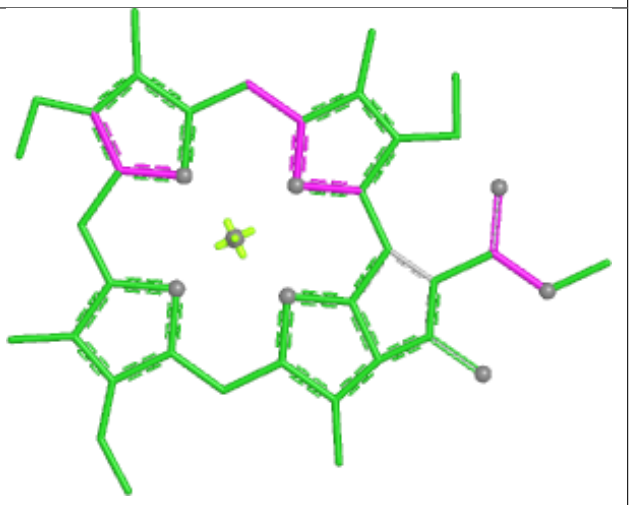


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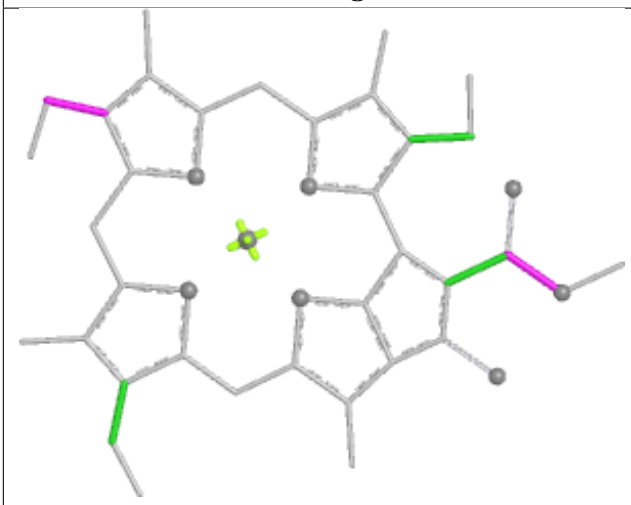
Ligand CLA G 203



Bond lengths



Bond angles

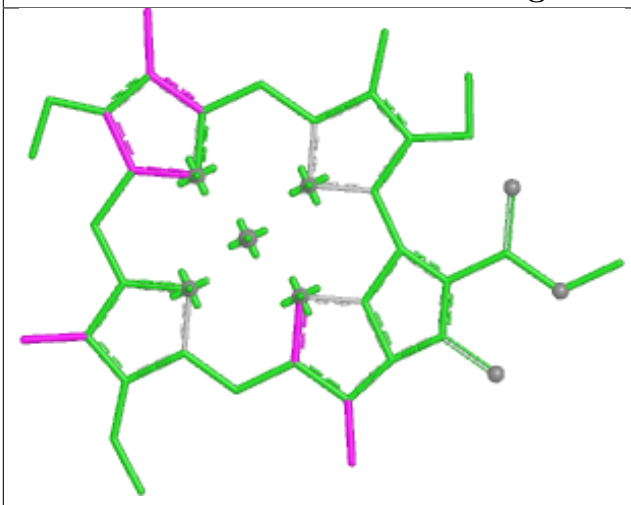


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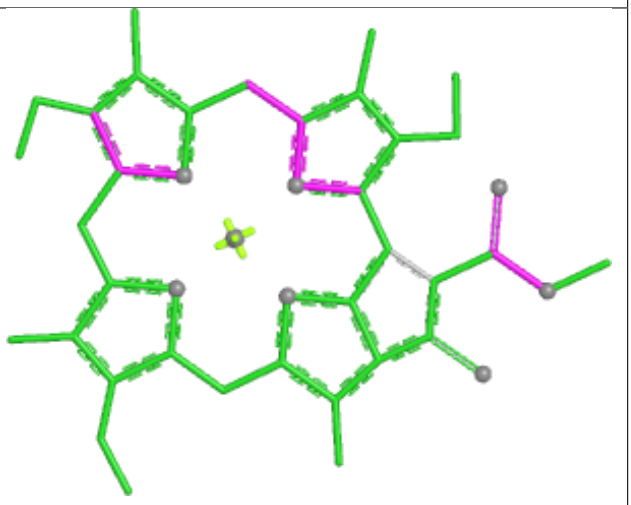


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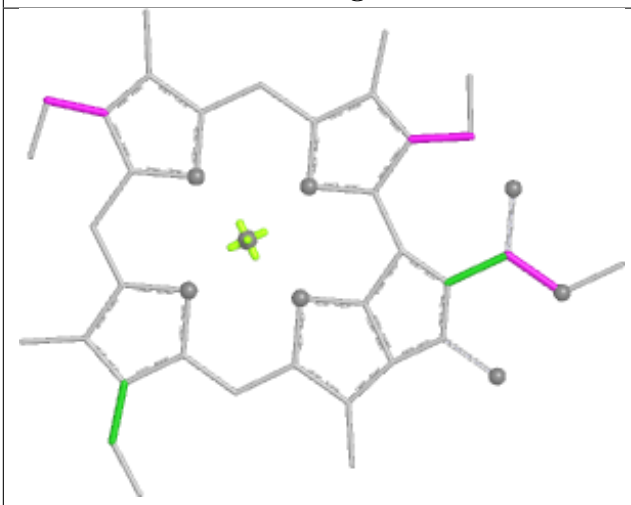
Ligand CLA J 101



Bond lengths



Bond angles



Torsions

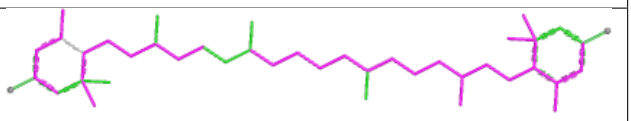


Rings

Ligand LUT 6 619



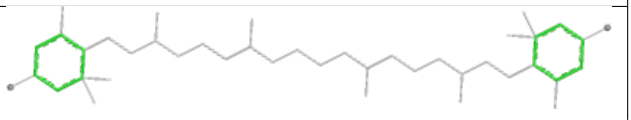
Bond lengths



Bond angles

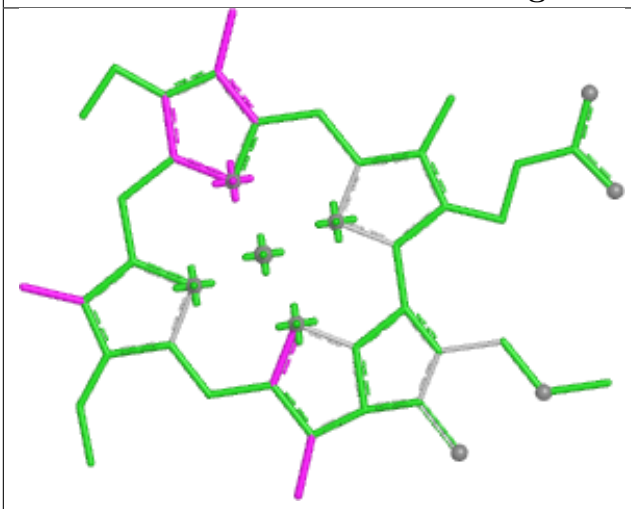


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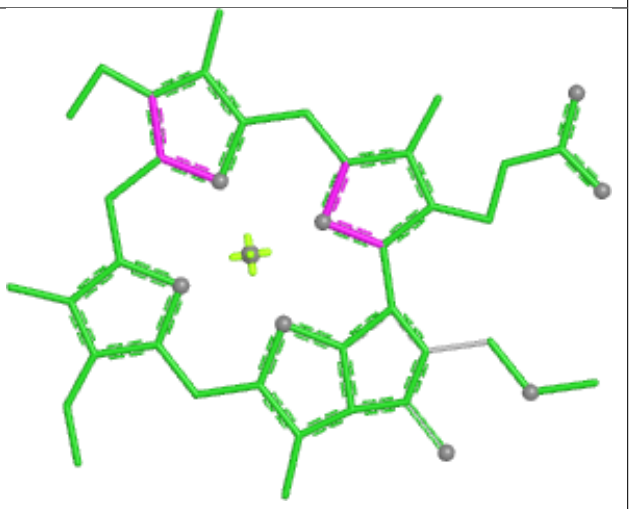


Rings

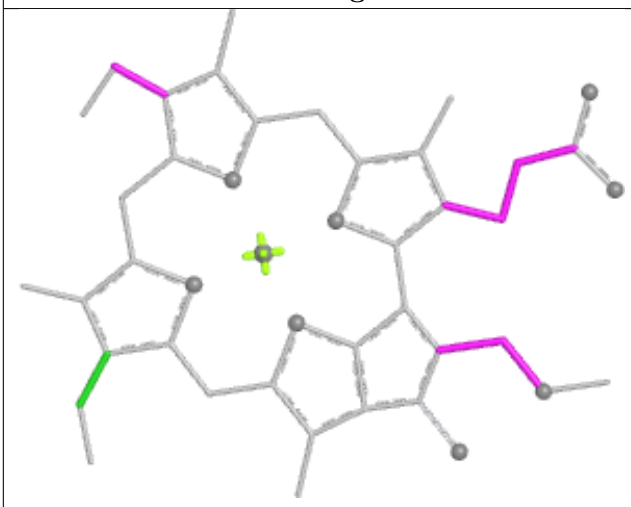
Ligand CLA a 606



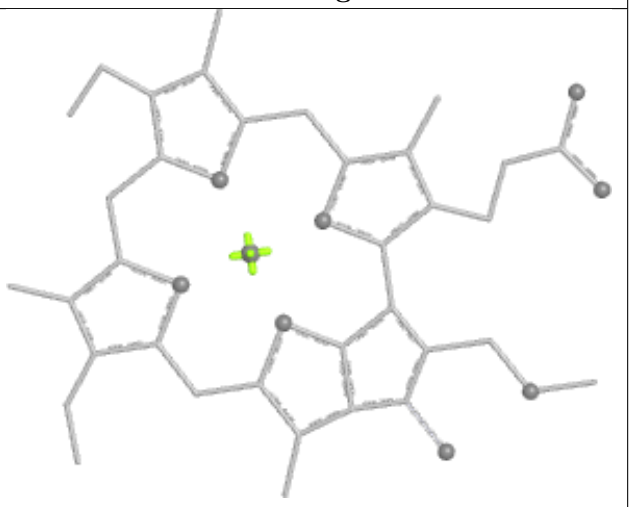
Bond lengths



Bond angles

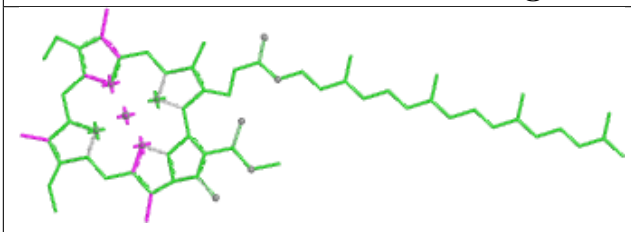


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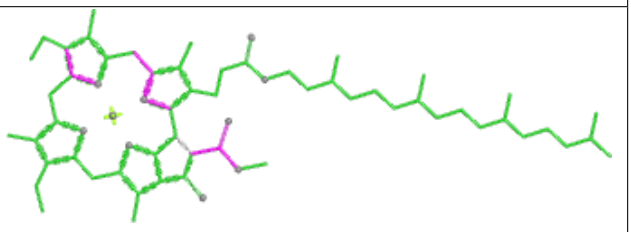


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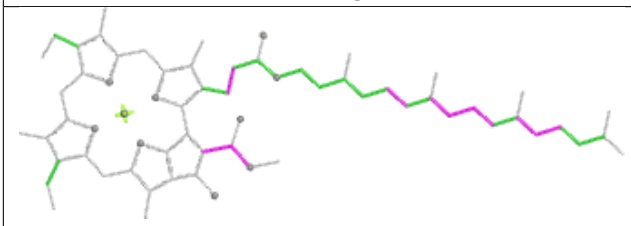
Ligand CLA B 824



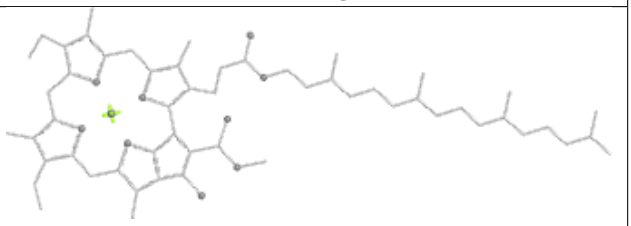
Bond lengths



Bond angles

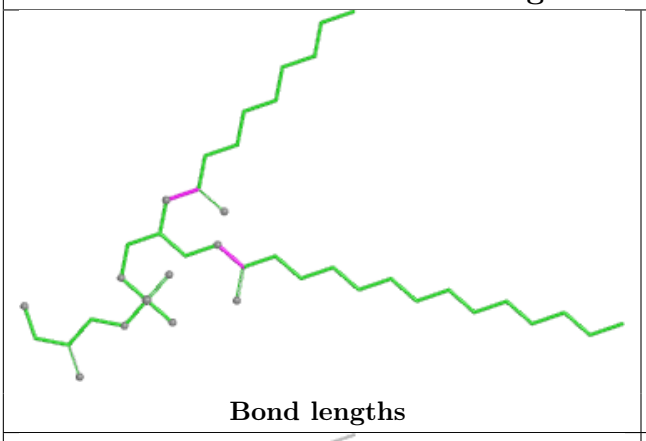


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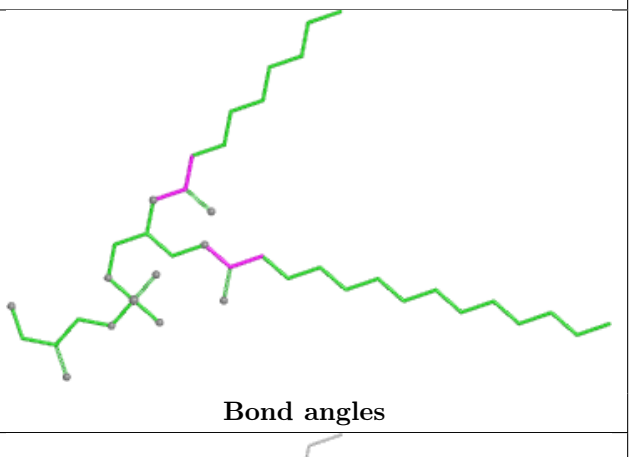


Rings

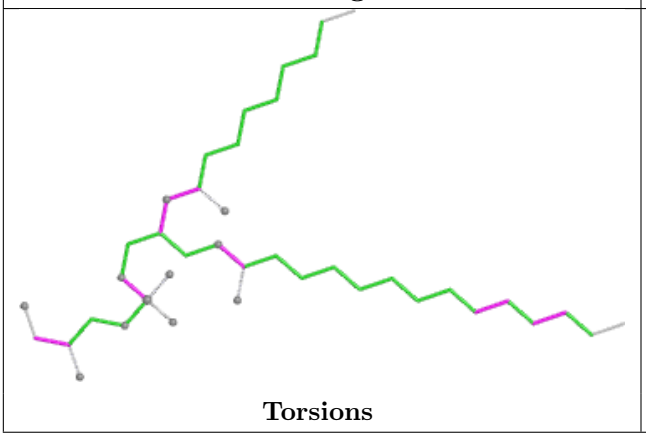
Ligand LHG 8 623



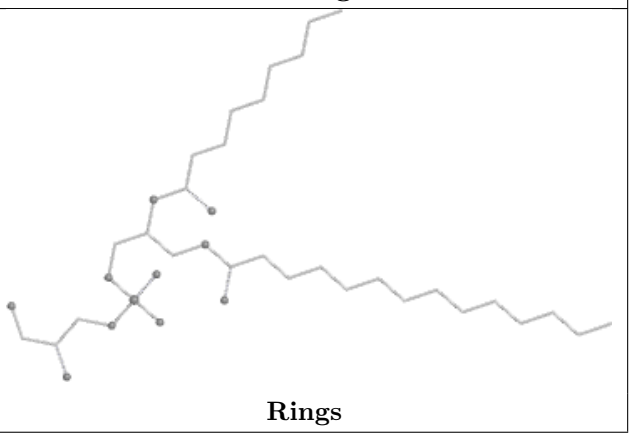
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Bond angles

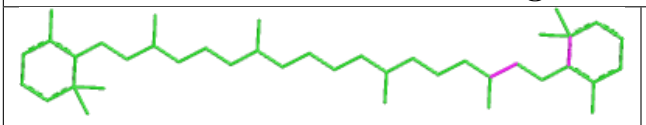


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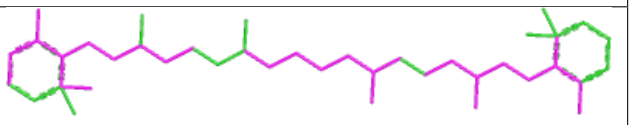


Rings

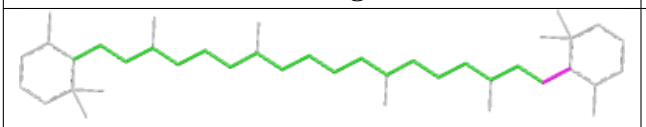
Ligand BCR 5 622



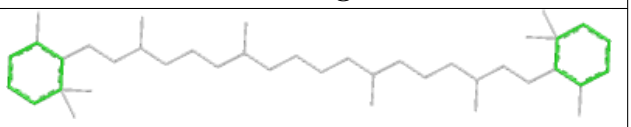
Bond lengths



Bond angles

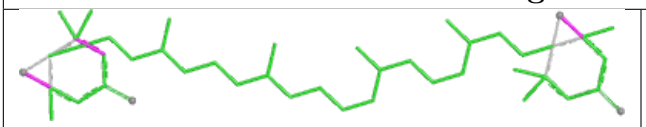


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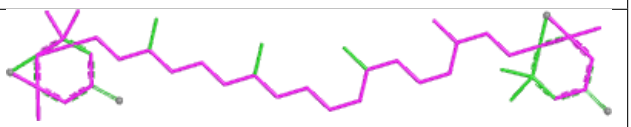


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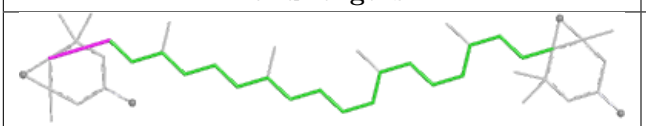
Ligand XAT 4 620



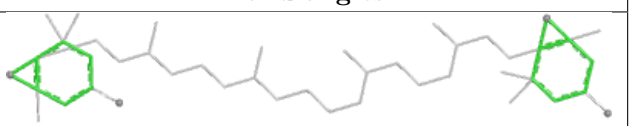
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Bond angles

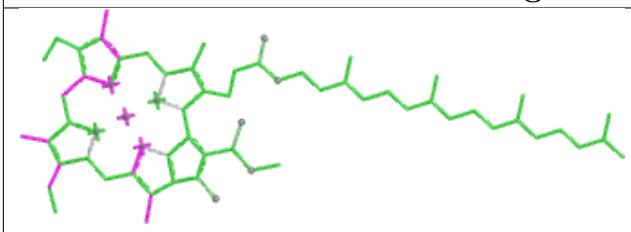


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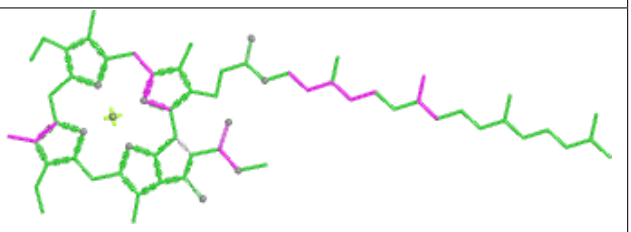


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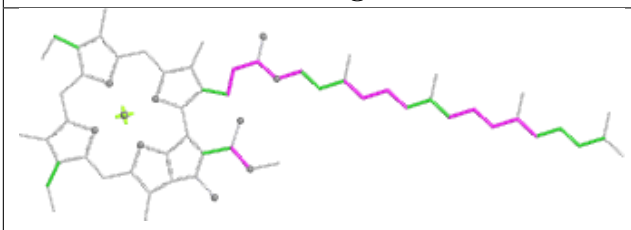
Ligand CLA B 806



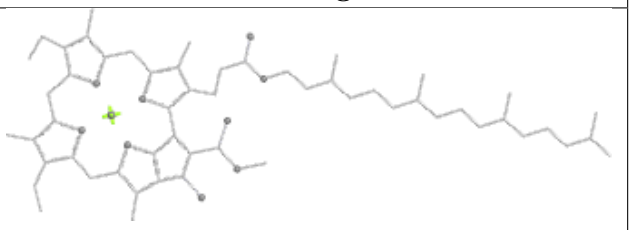
Bond lengths



Bond angles

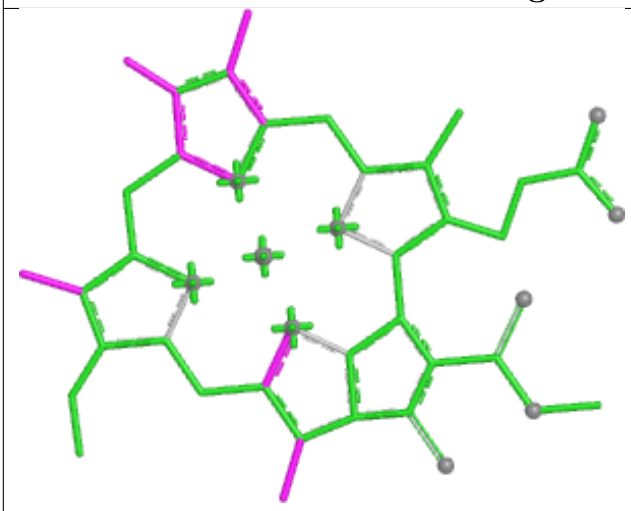


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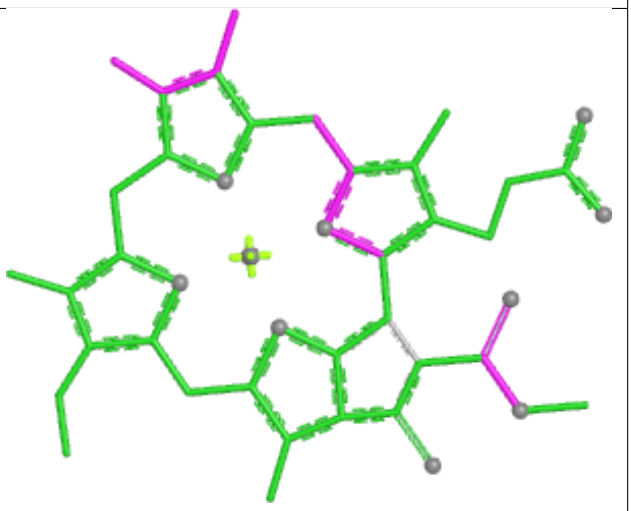


Rings

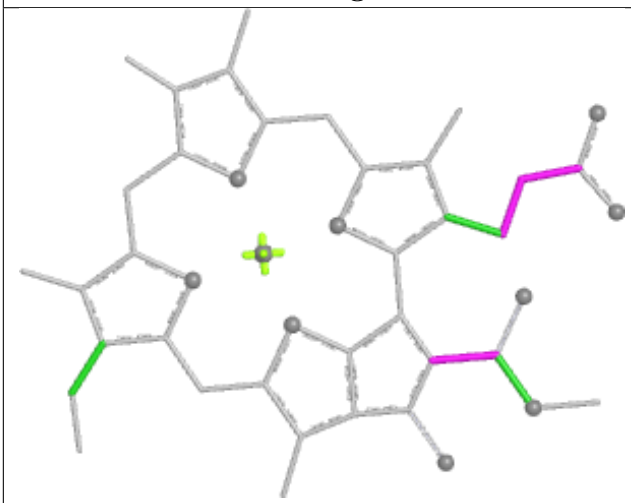
Ligand CLA 8 603



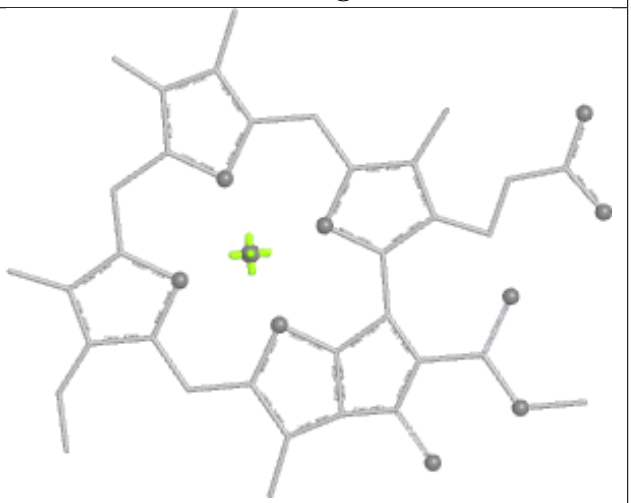
Bond lengths



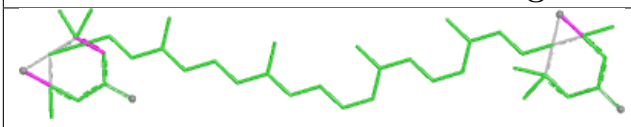
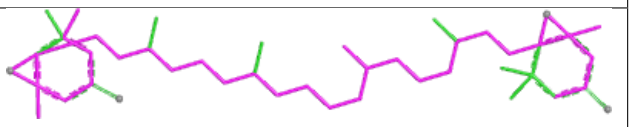
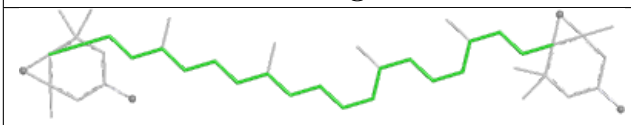
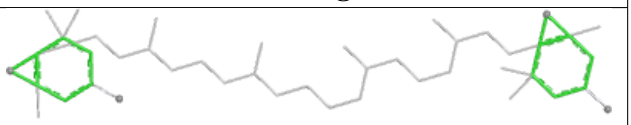
Bond angles

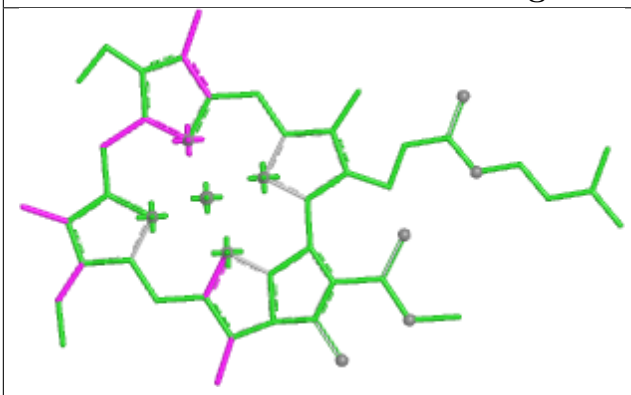
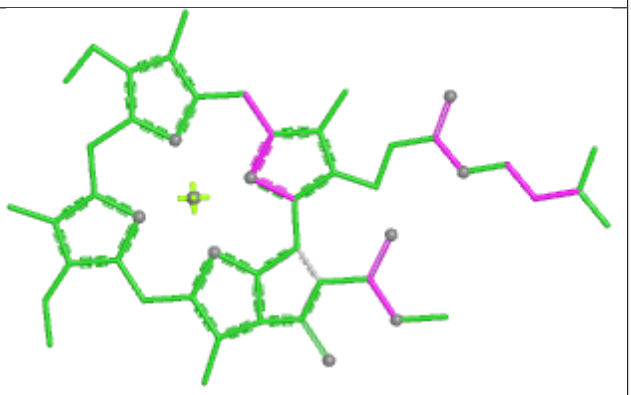
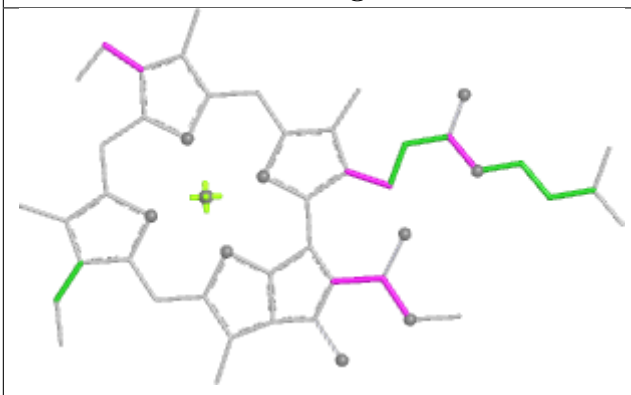
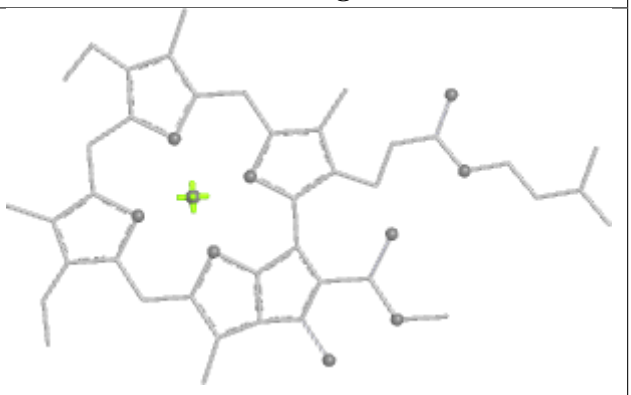


Torsions

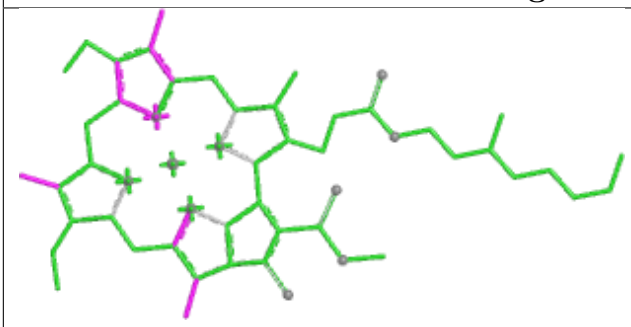


Rings

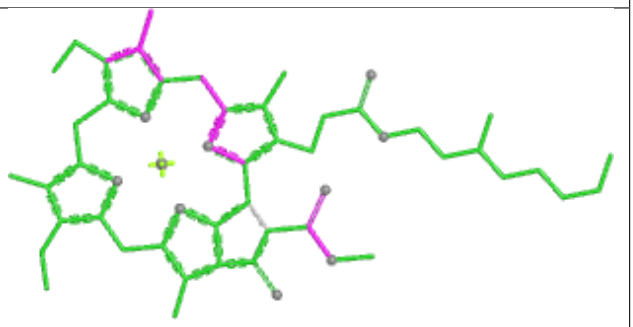
Ligand XAT 1 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

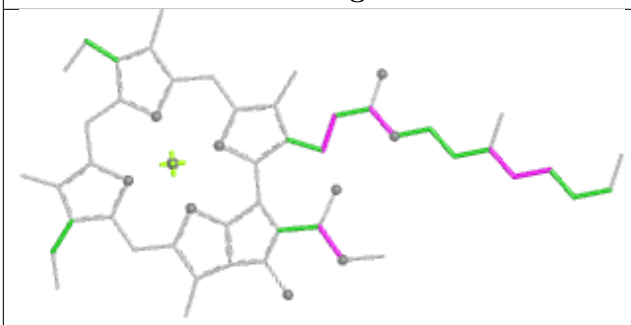
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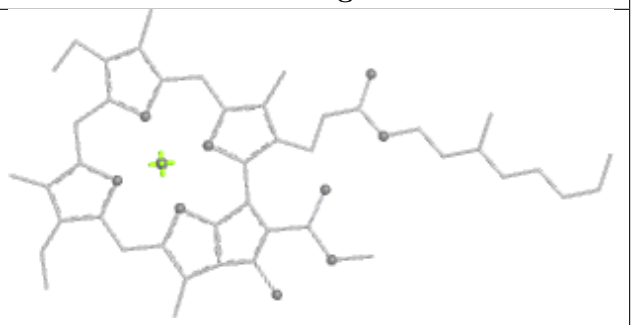
Bond lengths



Bond angles



Torsions

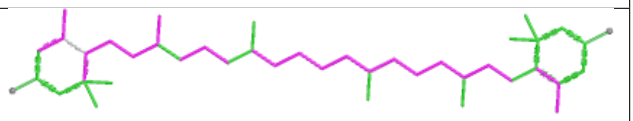


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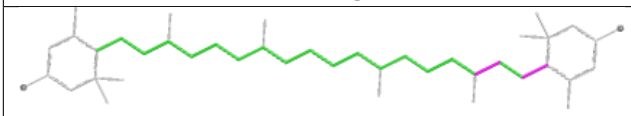
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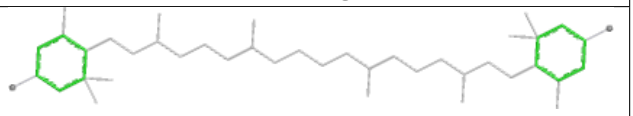
Bond lengths



Bond angles

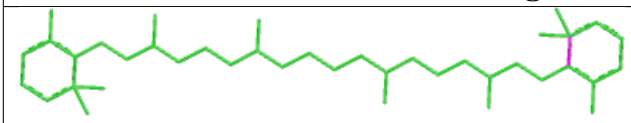


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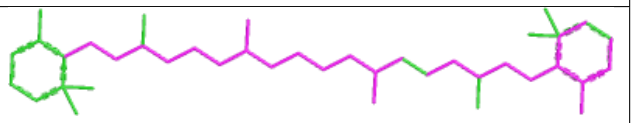


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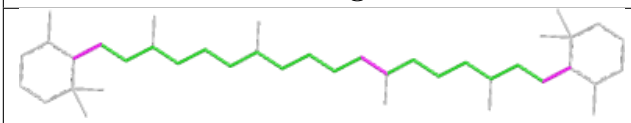
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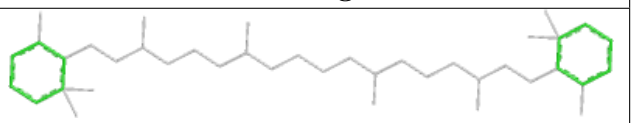
Bond lengths



Bond angles

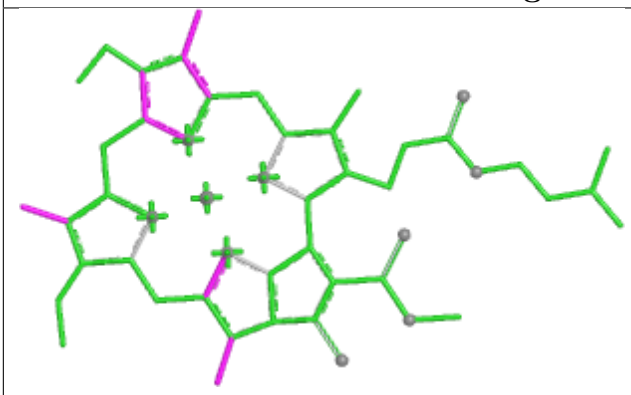


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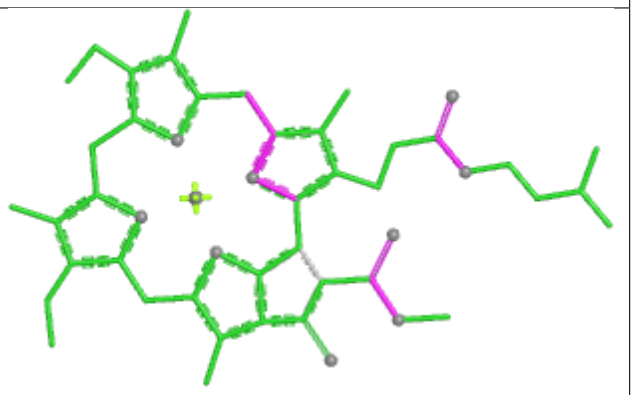


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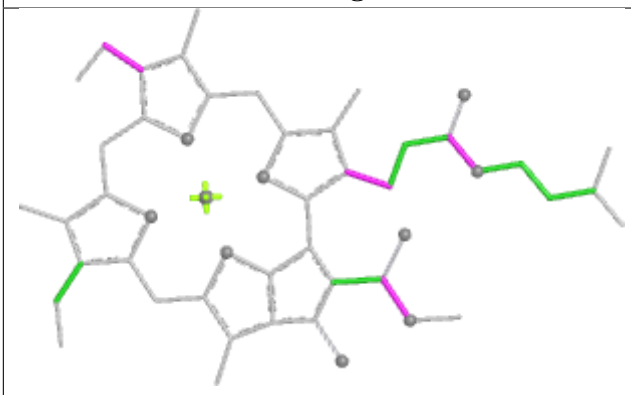
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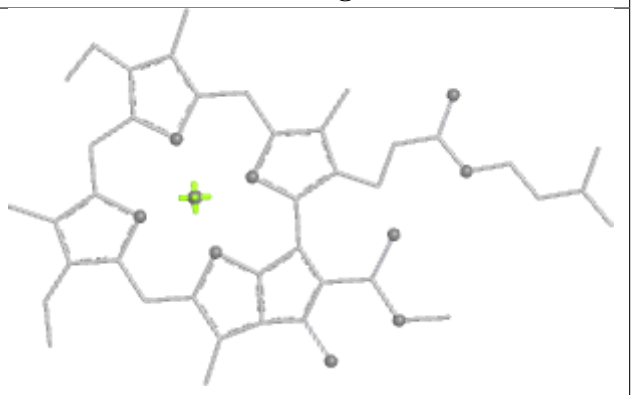
Bond lengths



Bond angles



Torsions

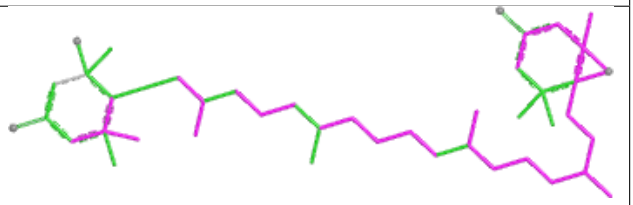


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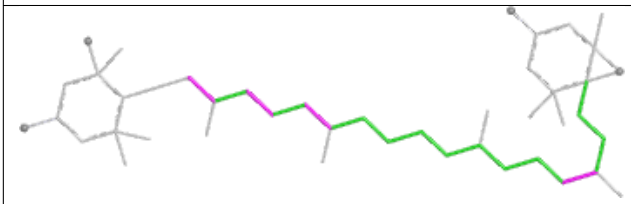
Ligand NEX V 1623



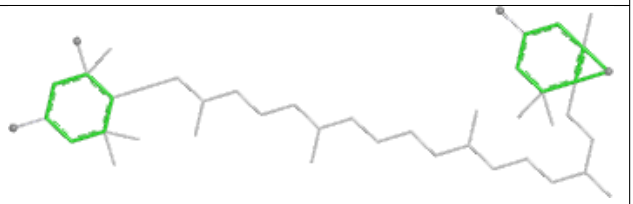
Bond lengths



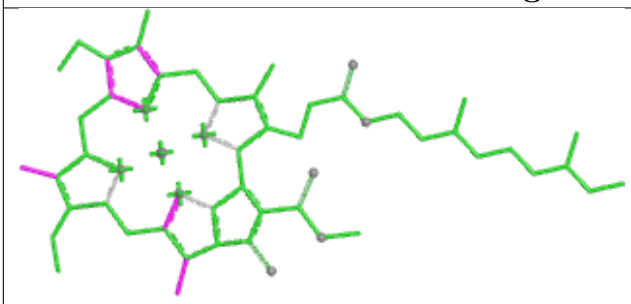
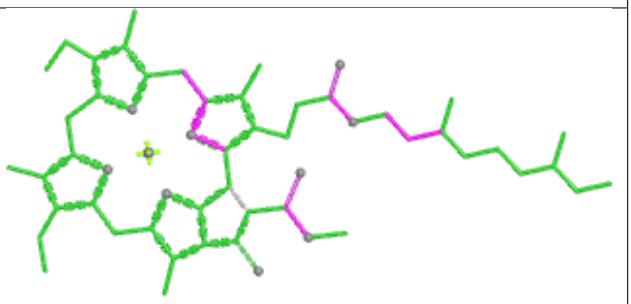
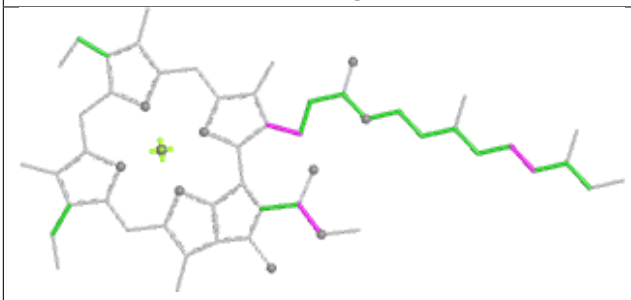
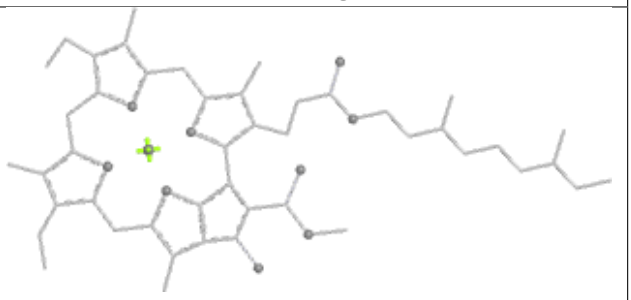
Bond angles



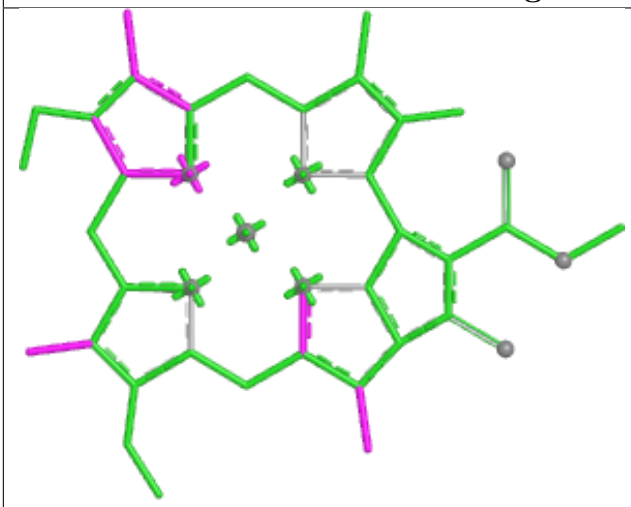
Torsions



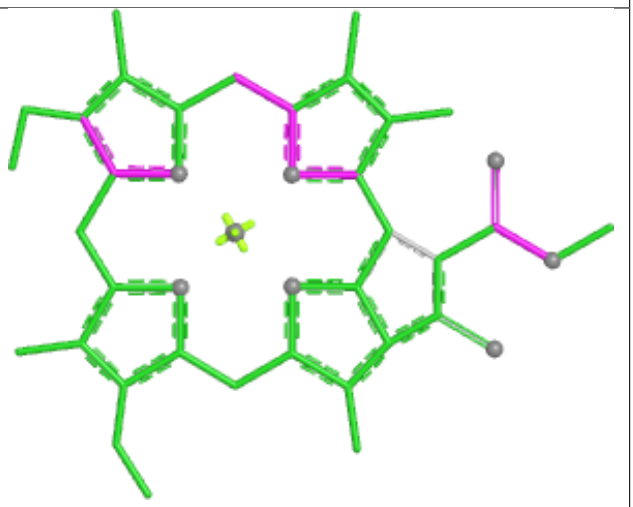
Rings

Ligand CLA U 610	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

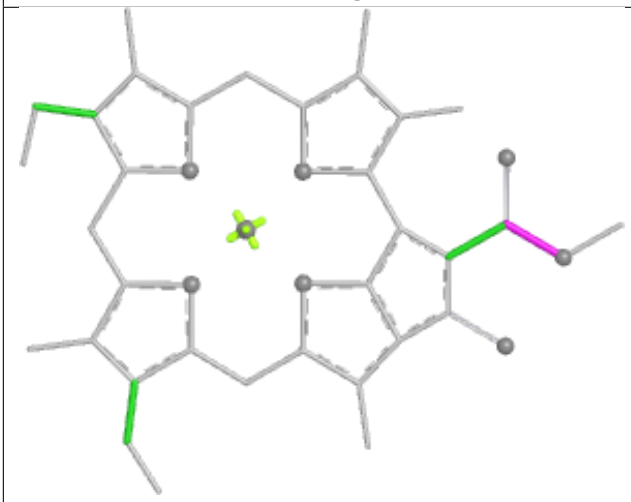
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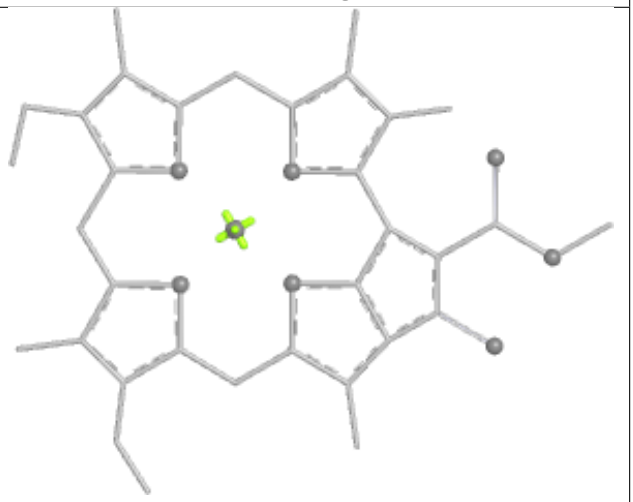
Bond lengths



Bond angles

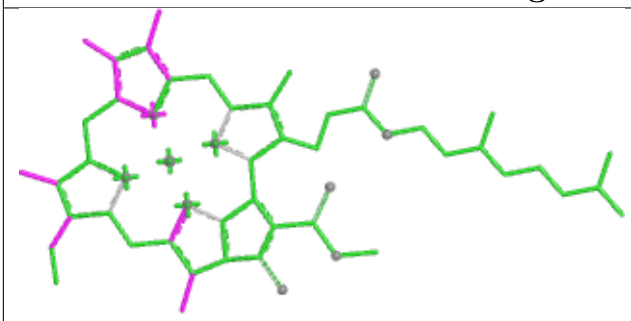


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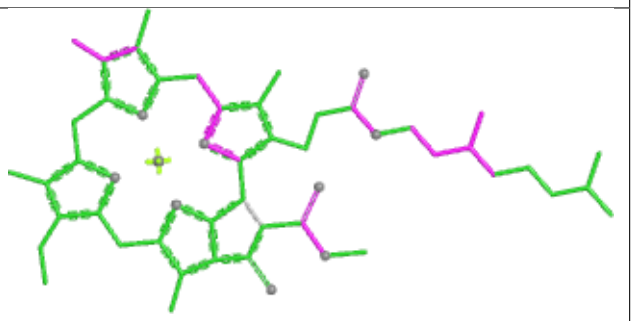


Rings

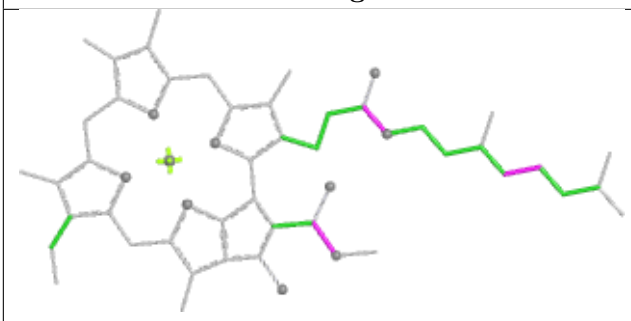
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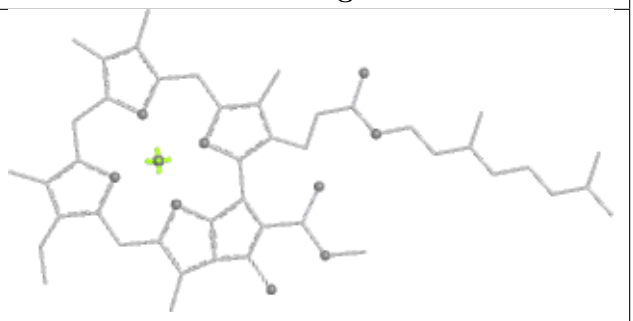
Bond lengths



Bond angles

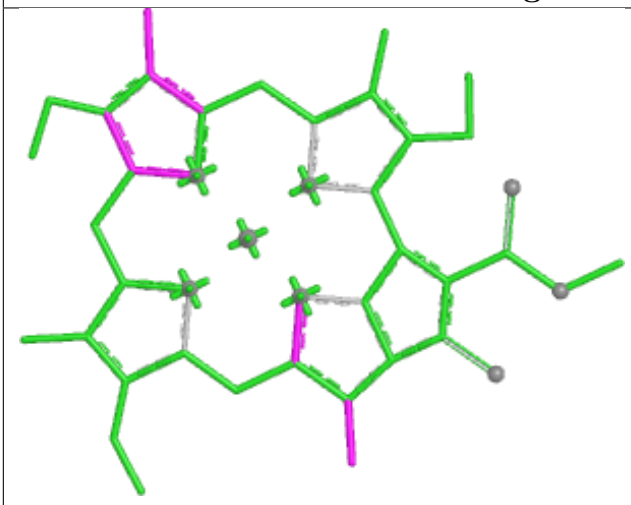


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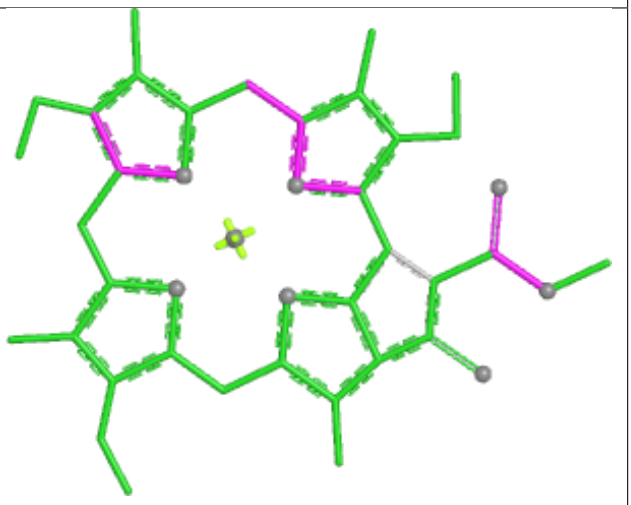


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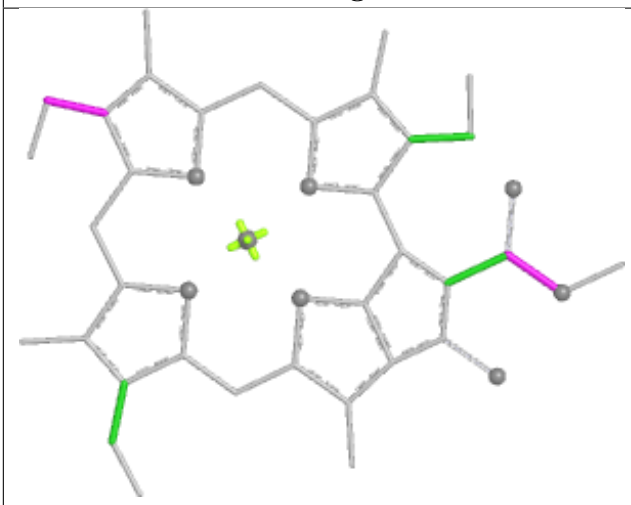
Ligand CLA U 612



Bond lengths



Bond angles



Torsions

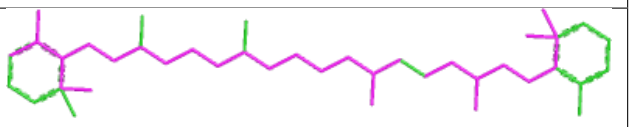


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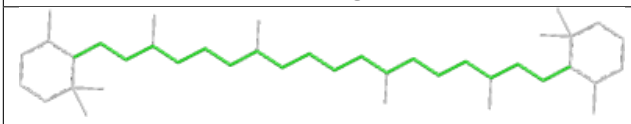
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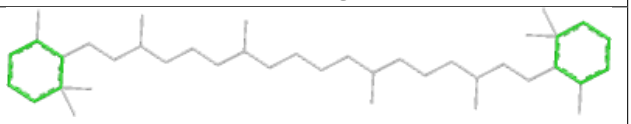
Bond lengths



Bond angles

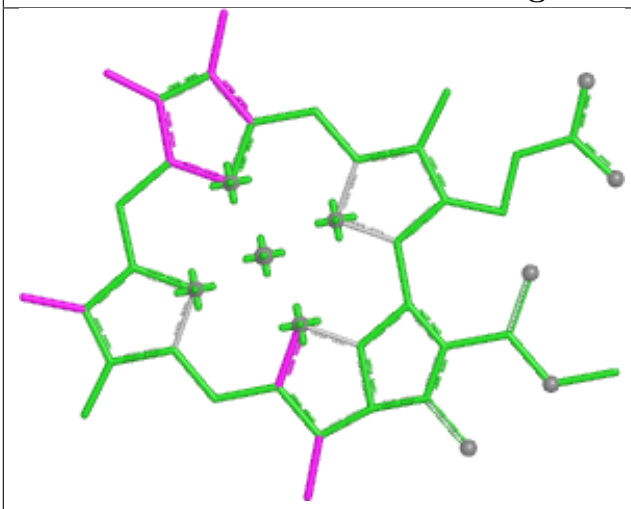


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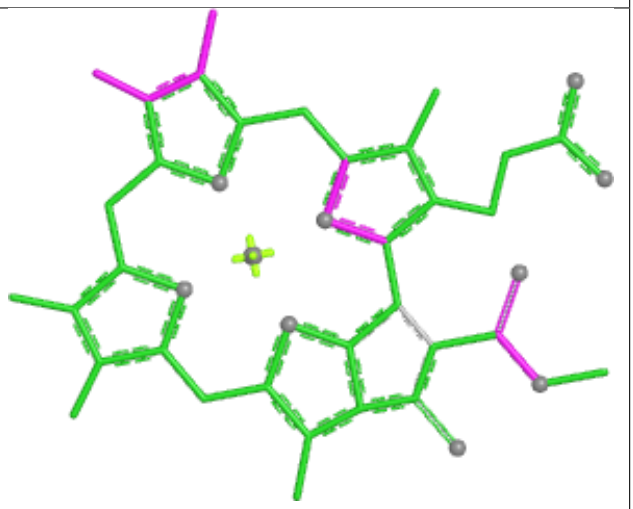


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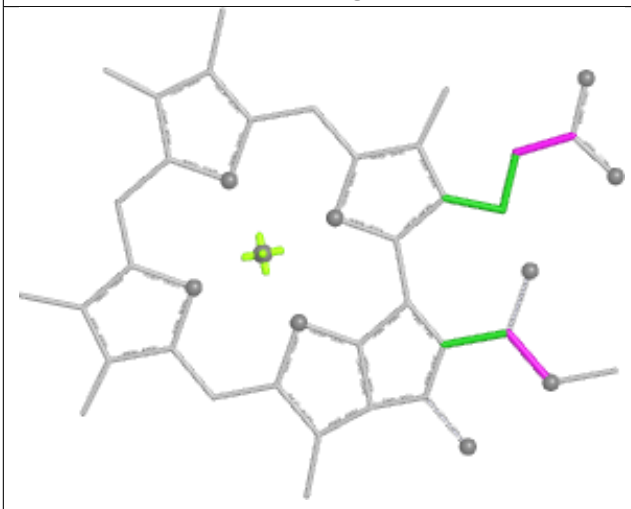
Ligand CLA 4 616



Bond lengths



Bond angles

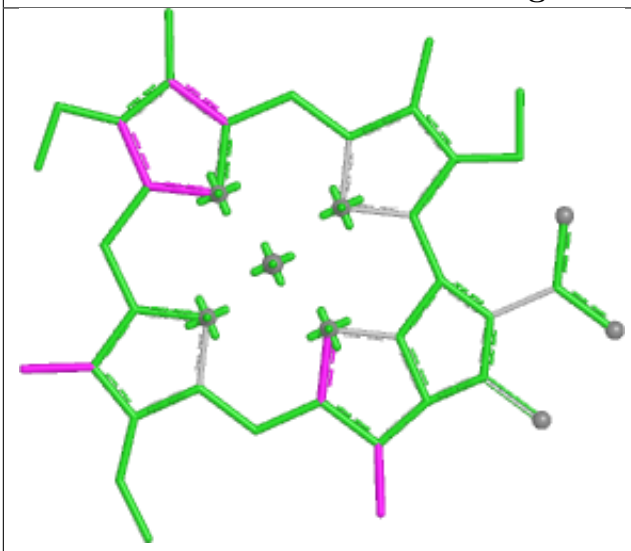


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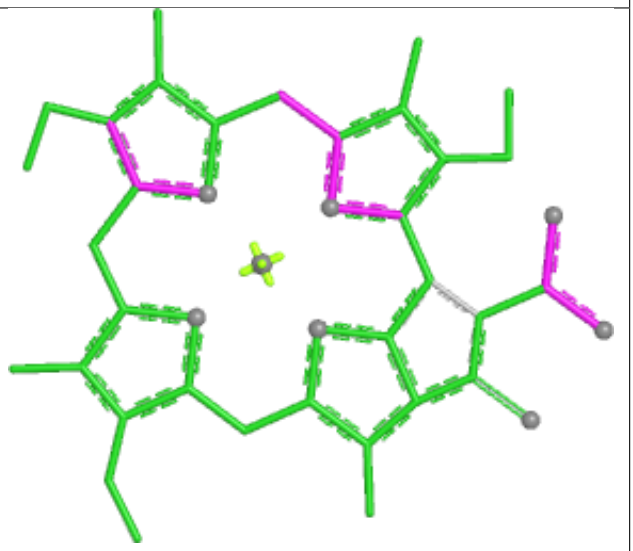


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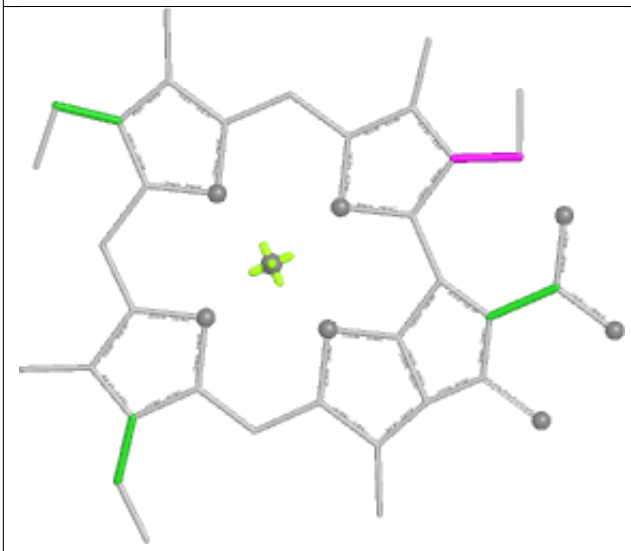
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Bond lengths



Bond angles

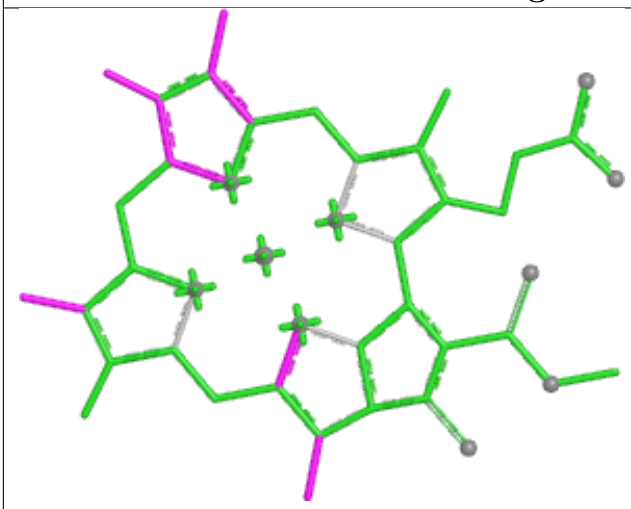


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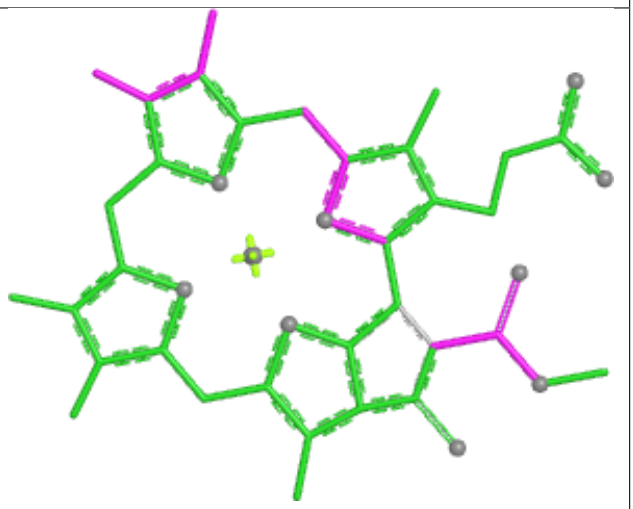


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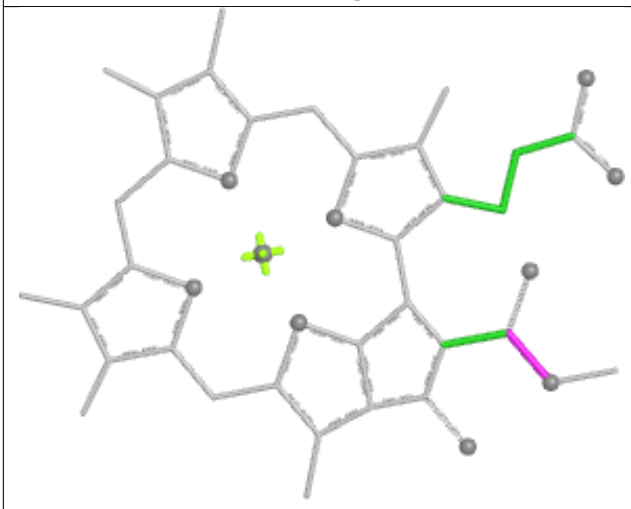
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Bond lengths



Bond angles

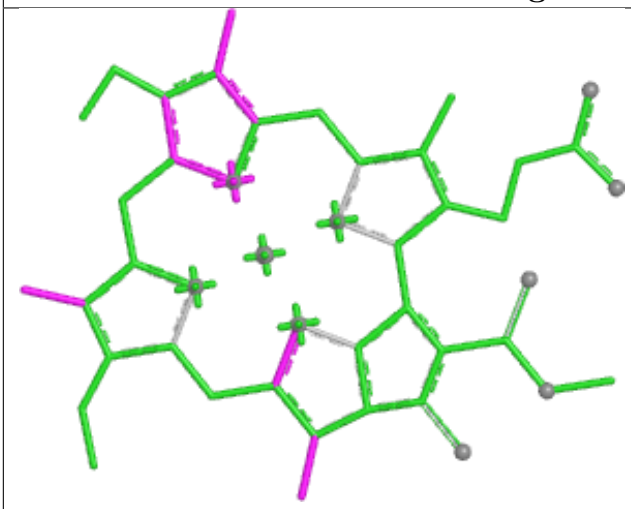


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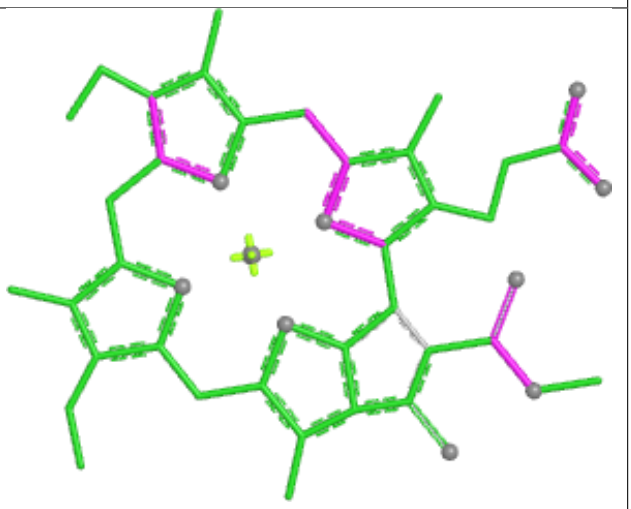


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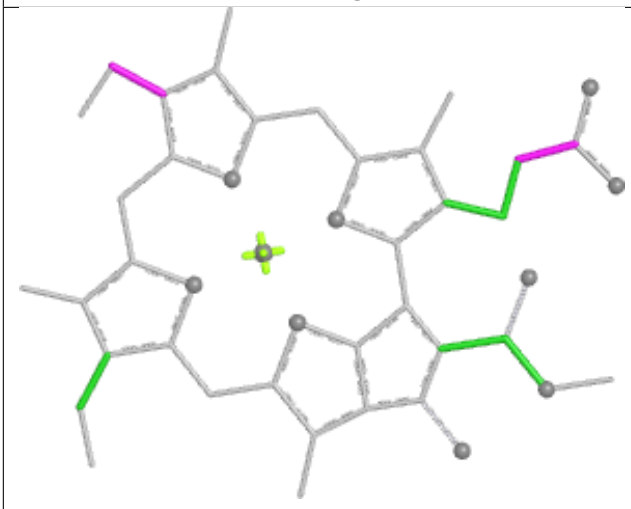
Ligand CLA 2 609



Bond lengths



Bond angles

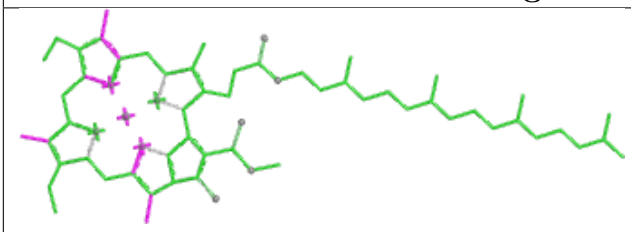


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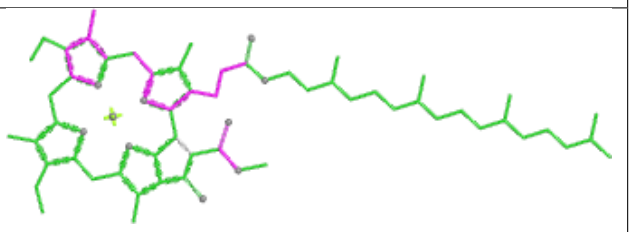


Rings

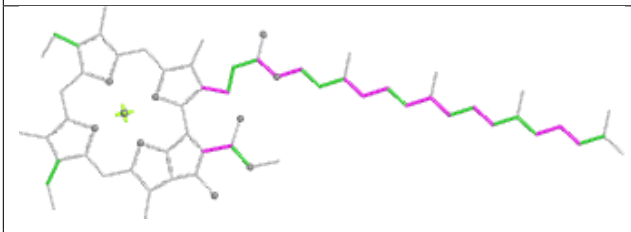
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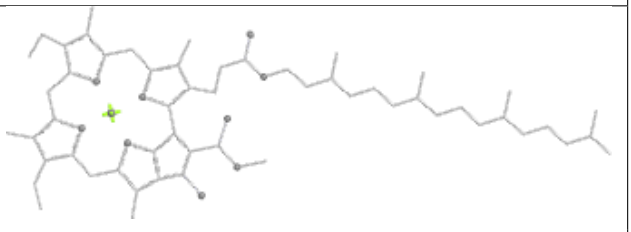
Bond lengths



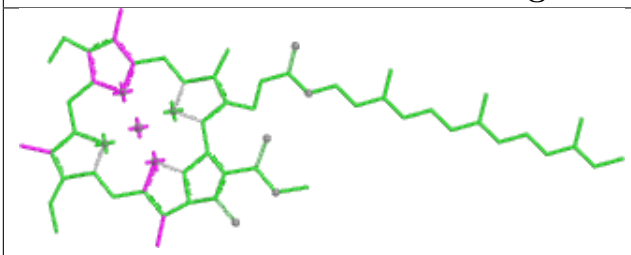
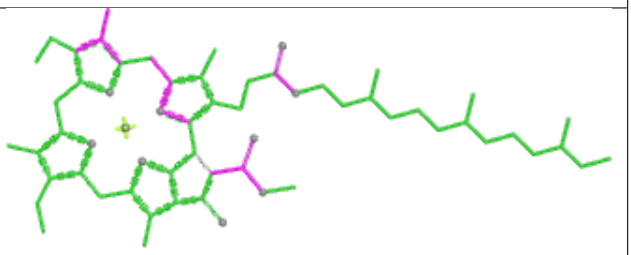
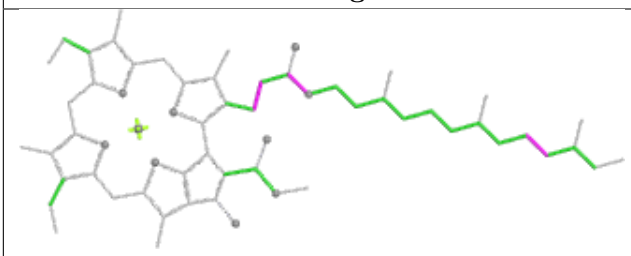
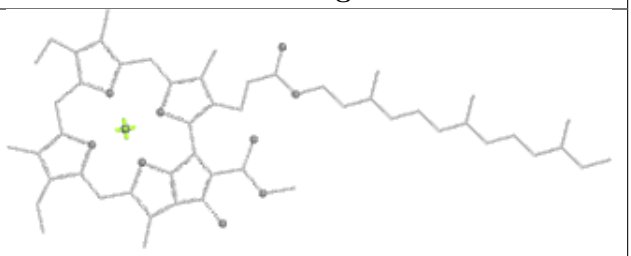
Bond angles

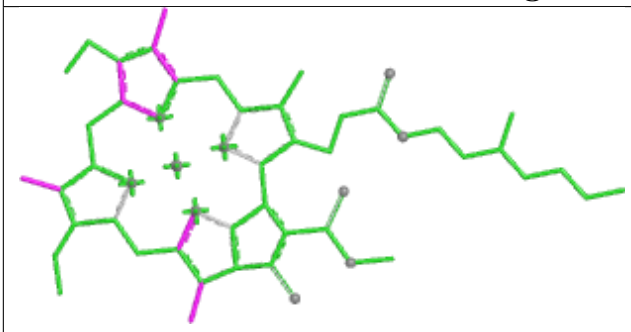
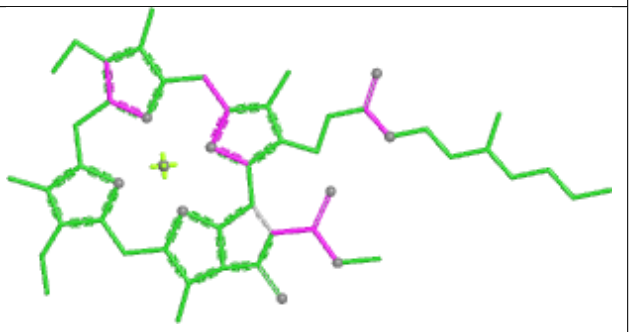
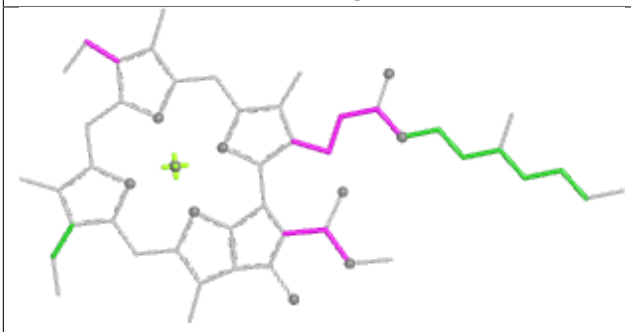
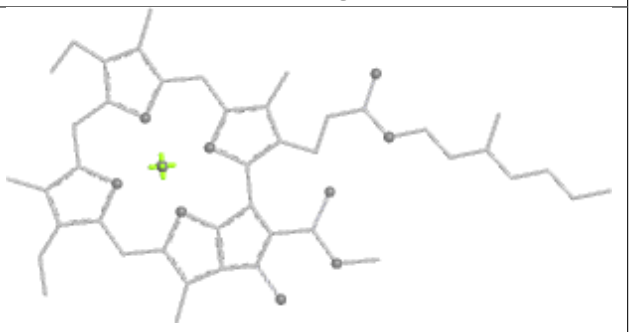


Torsions

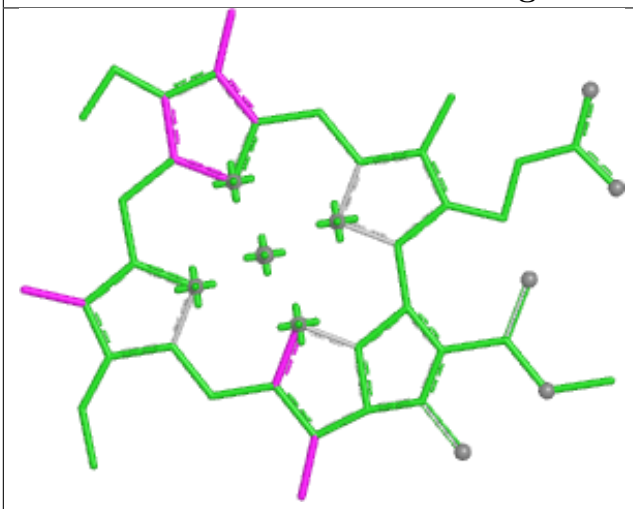


Rings

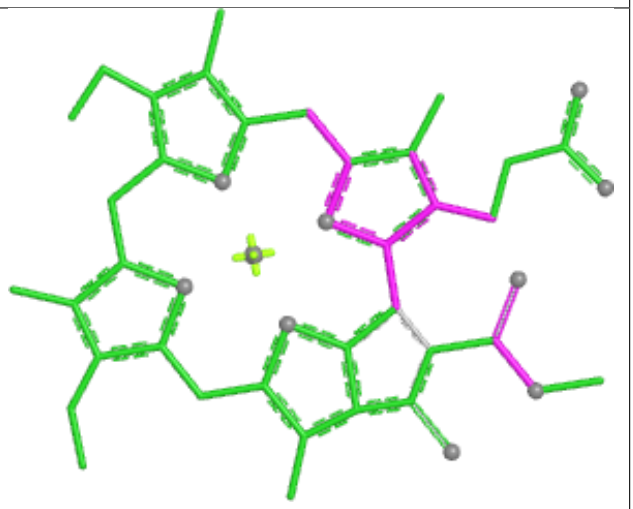
Ligand CLA a 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 821	
	
Bond lengths	Bond angles
	
Torsions	Rings

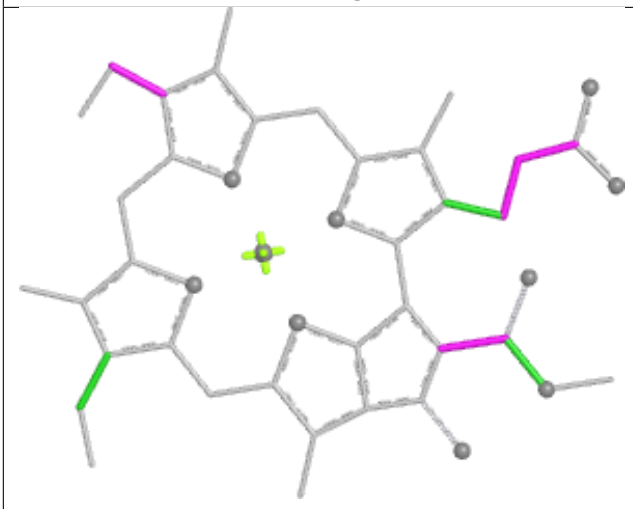
Ligand CLA W 612



Bond lengths



Bond angles

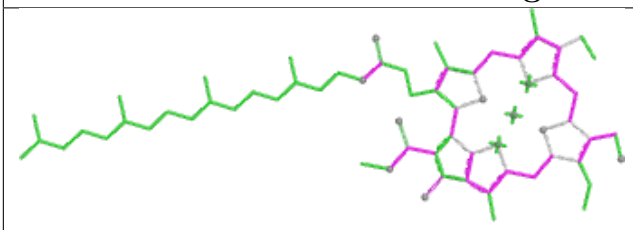


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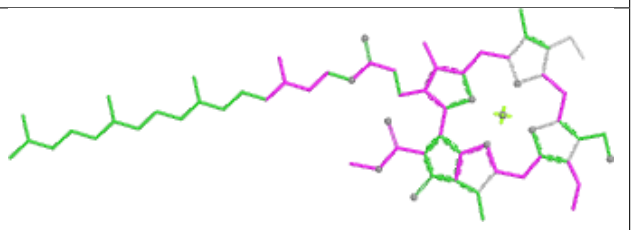


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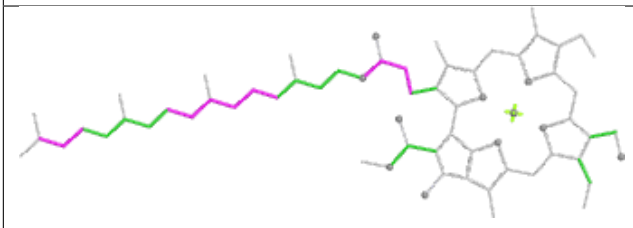
Ligand CHL X 601



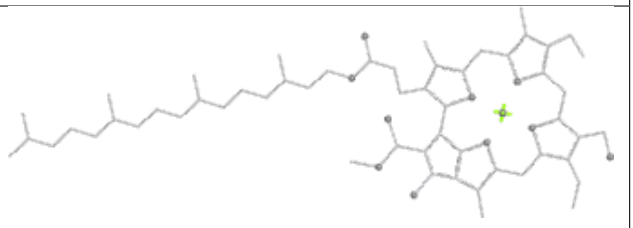
Bond lengths



Bond angles

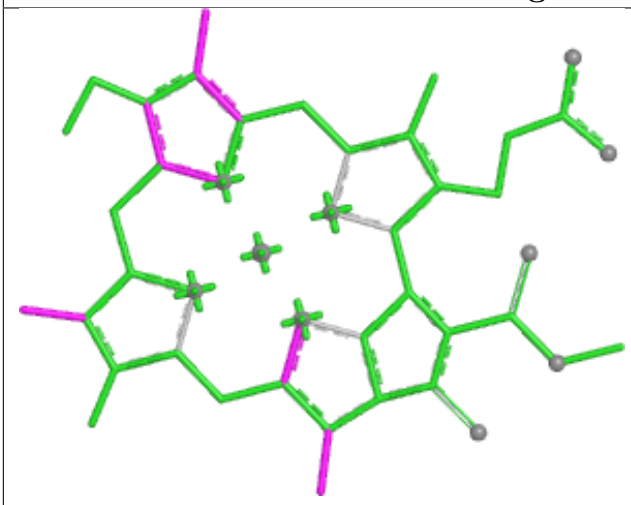


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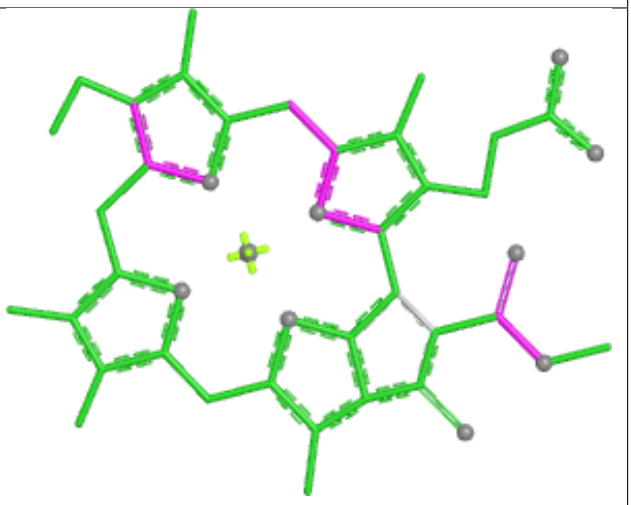


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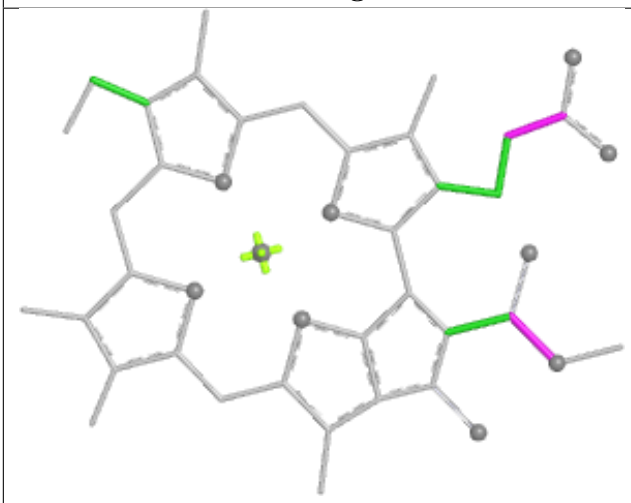
Ligand CLA 7 612



Bond lengths



Bond angles



Torsions

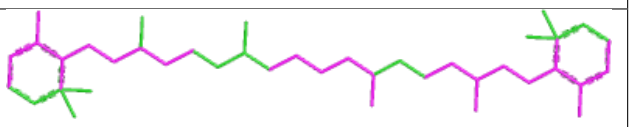


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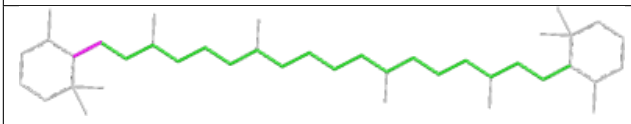
Ligand BCR 3 622



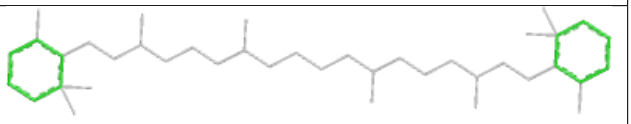
Bond lengths



Bond angles

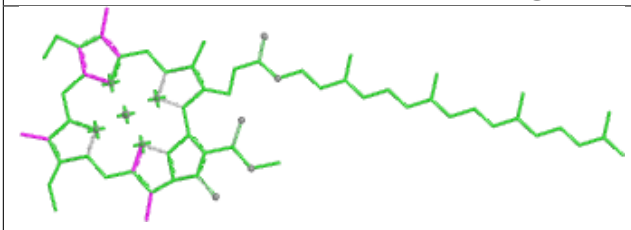


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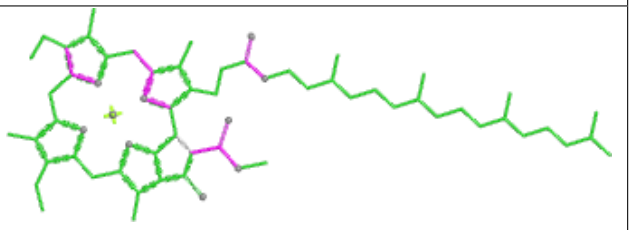


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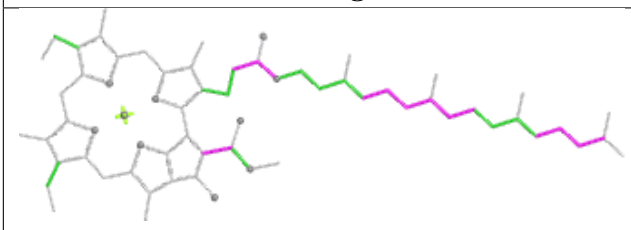
Ligand CLA 6 601



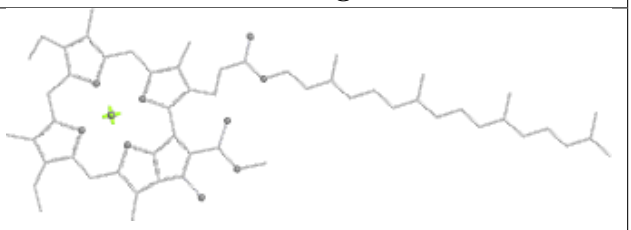
Bond lengths



Bond angles

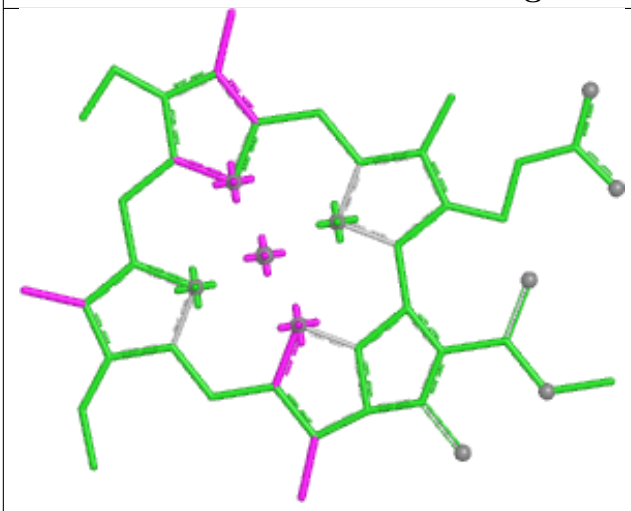


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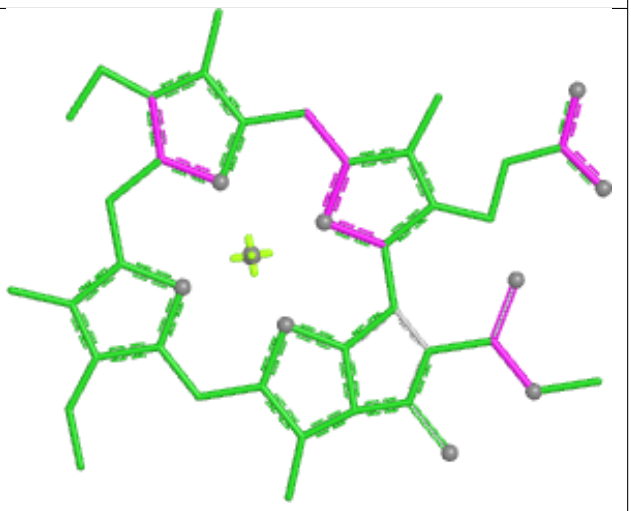


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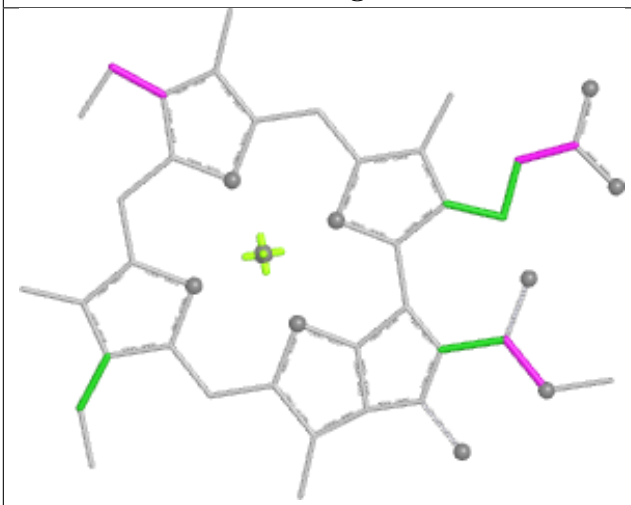
Ligand CLA B 823



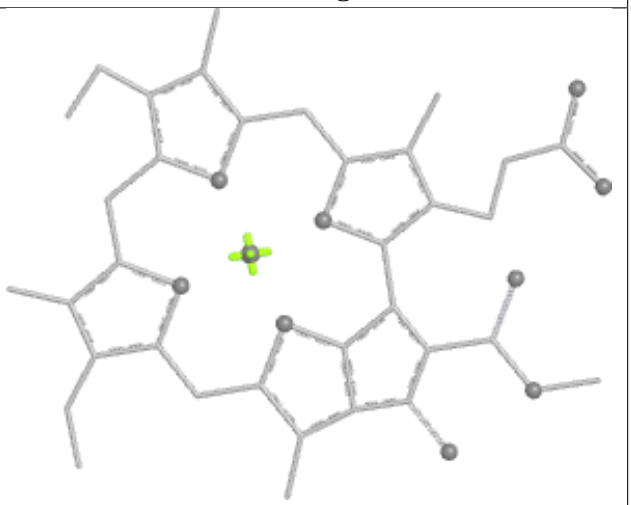
Bond lengths



Bond angles

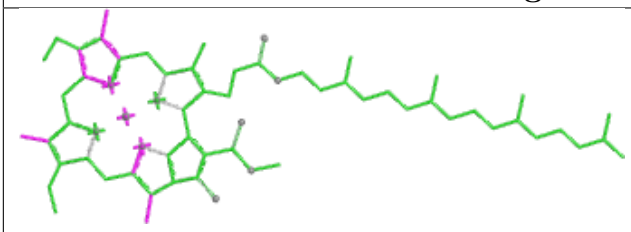


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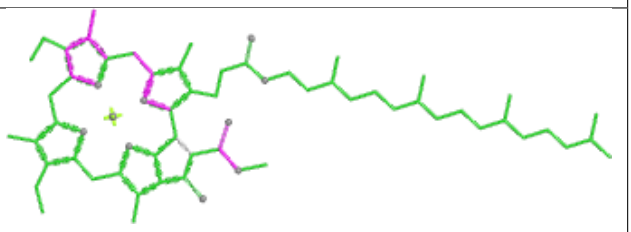


Rings

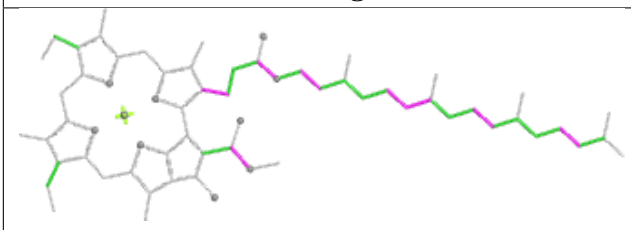
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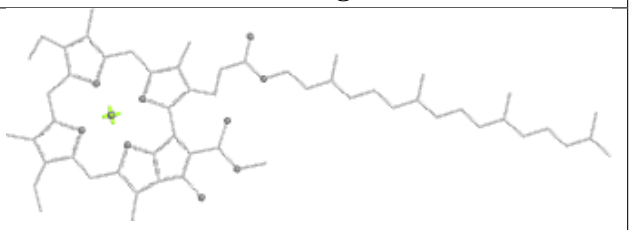
Bond lengths



Bond angles

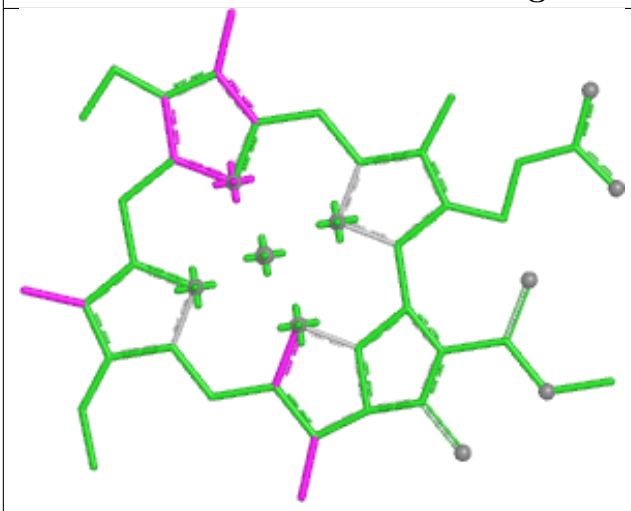


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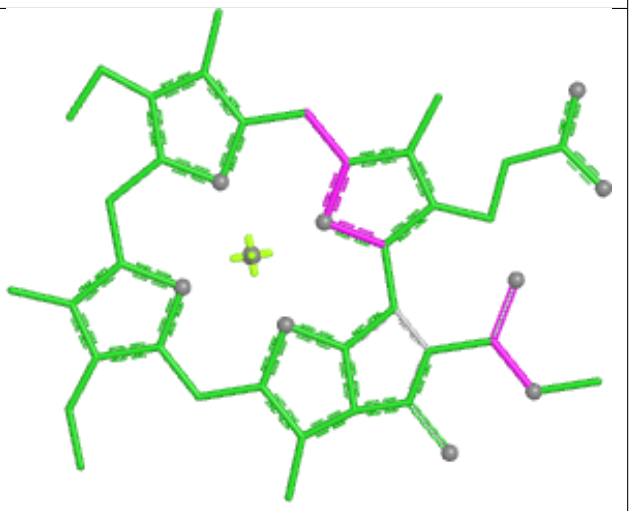


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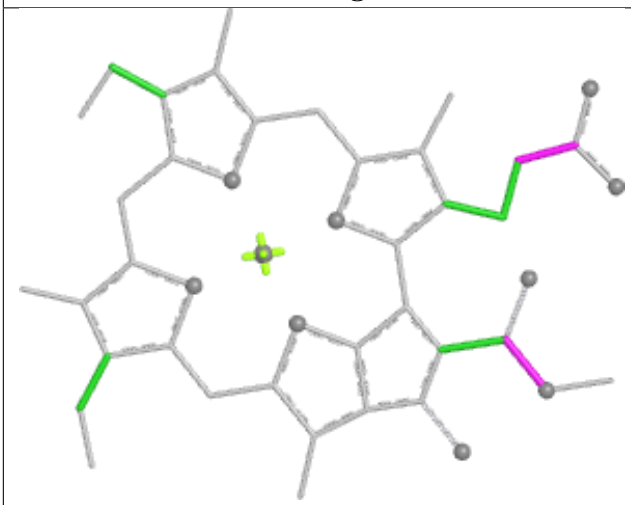
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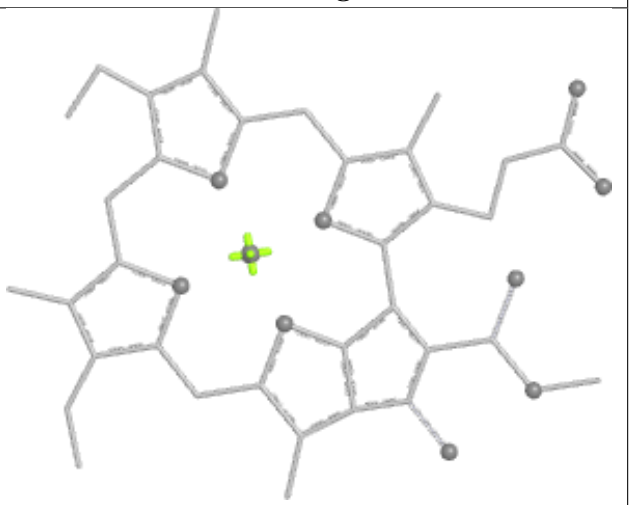
Bond lengths



Bond angles

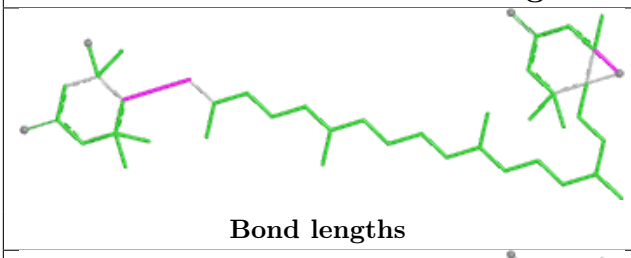


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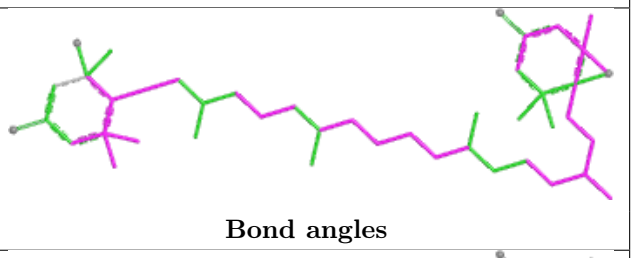


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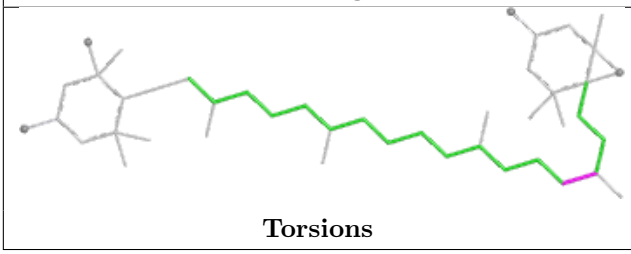
Ligand NEX 5 624



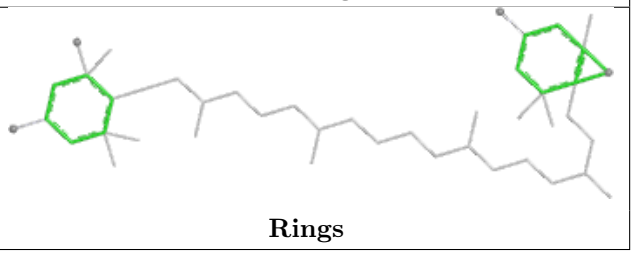
Bond lengths



Bond angles



Torsions

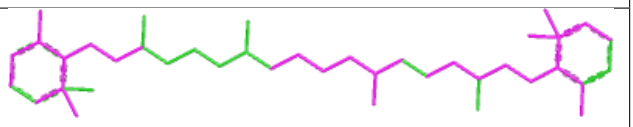


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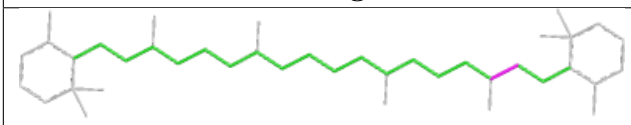
Ligand BCR O 2005



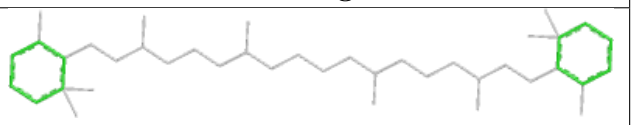
Bond lengths



Bond angles

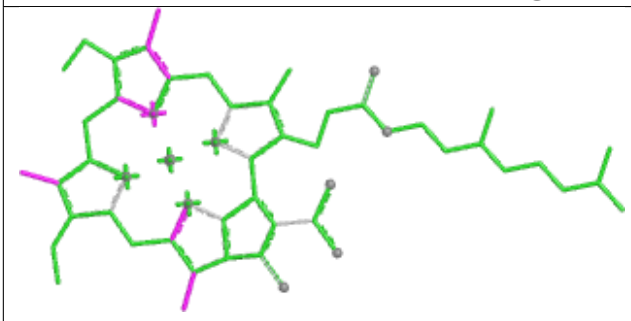


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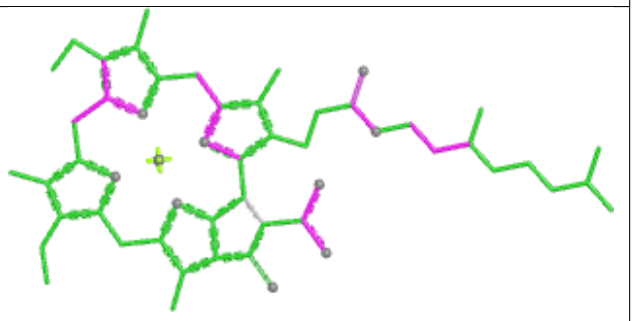


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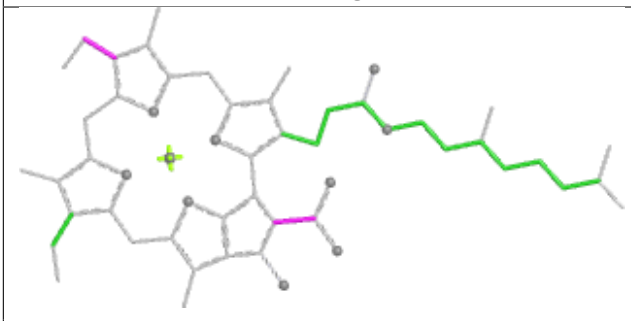
Ligand CLA 3 606



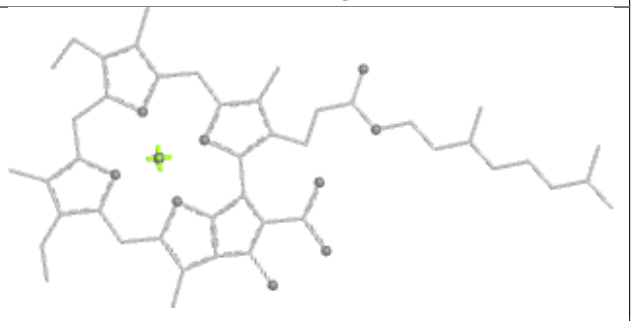
Bond lengths



Bond angles

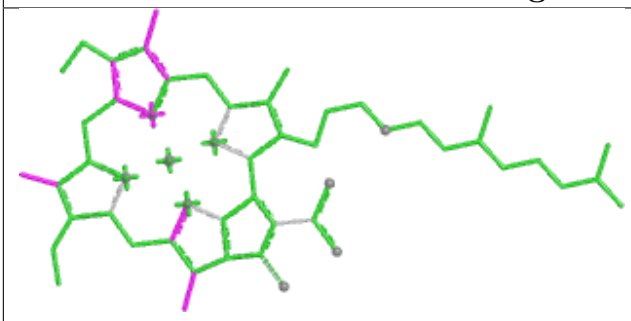


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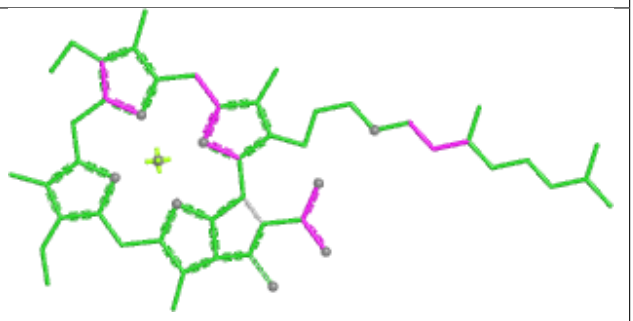


Rings

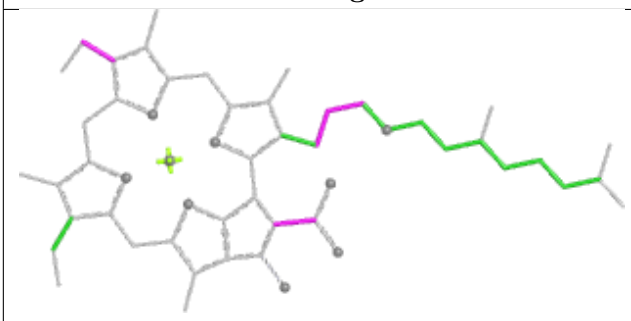
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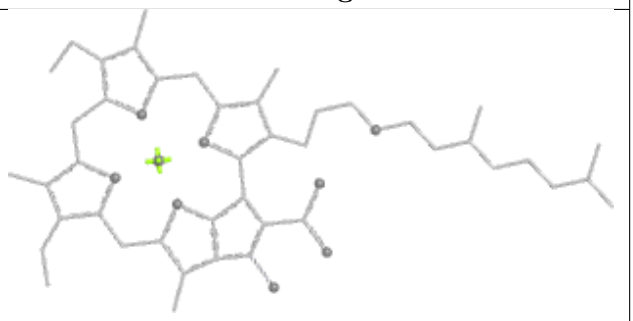
Bond lengths



Bond angles

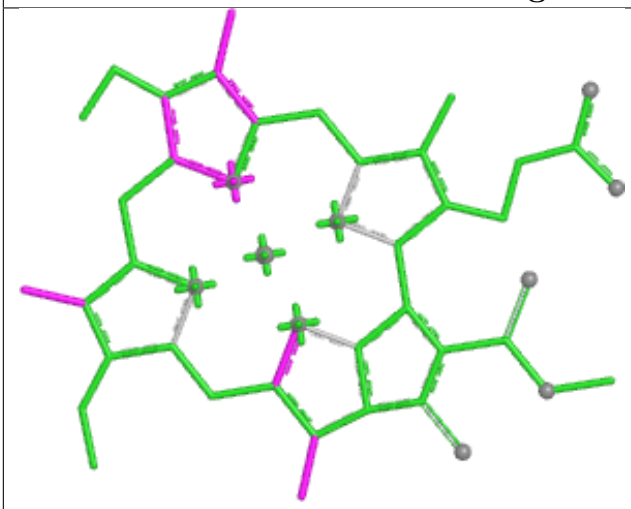


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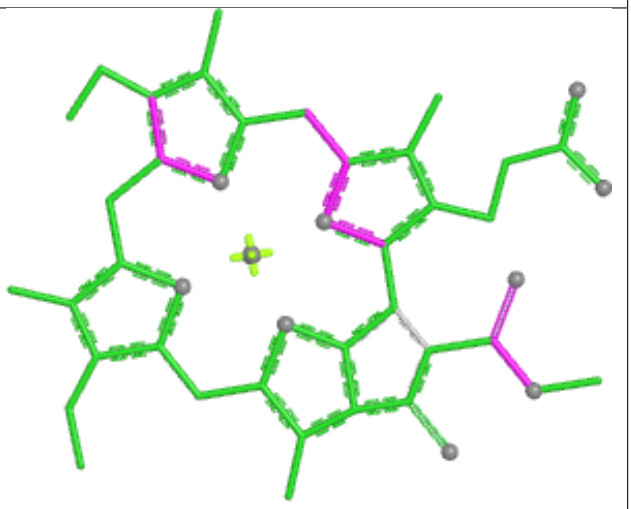


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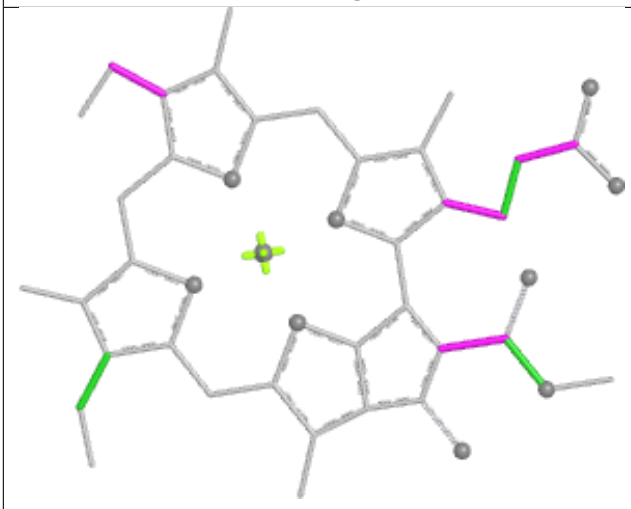
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Bond lengths



Bond angles

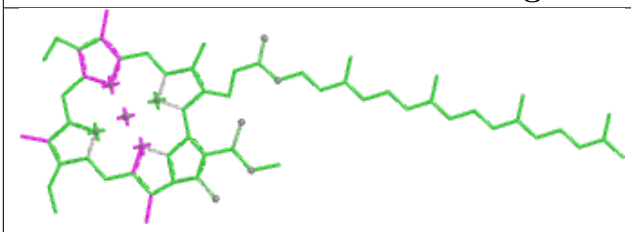


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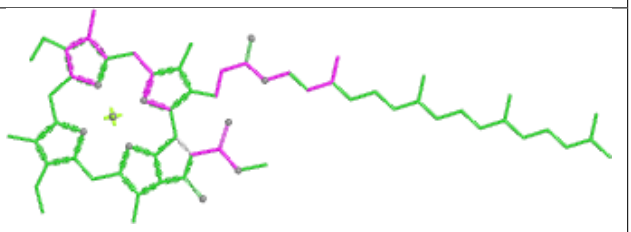


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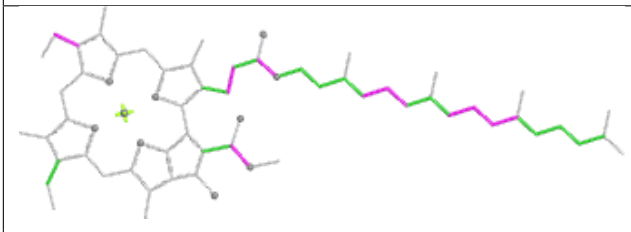
Ligand CLA A 834



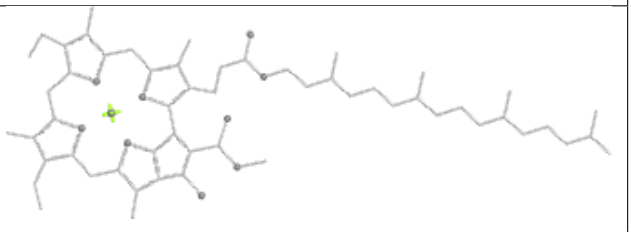
Bond lengths



Bond angles

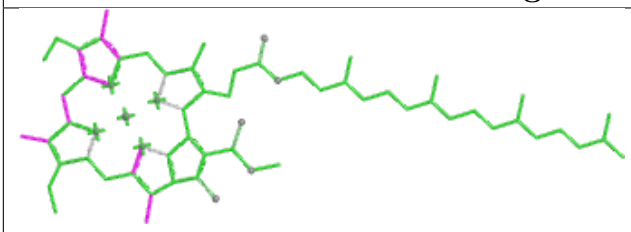


Torsions

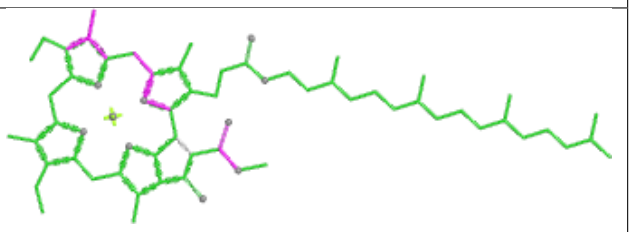


Rings

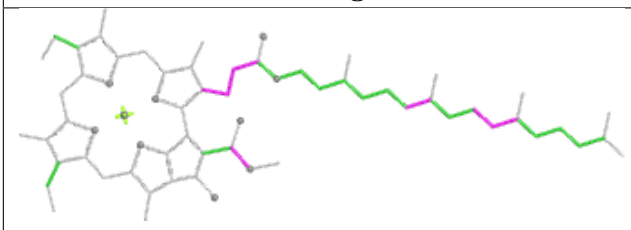
Ligand CLA X 602



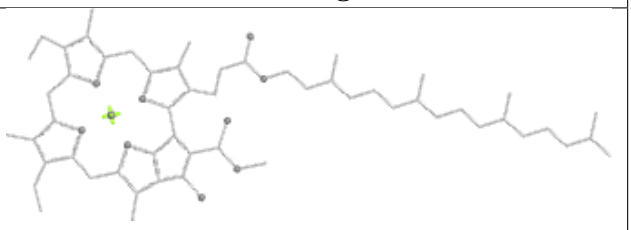
Bond lengths



Bond angles

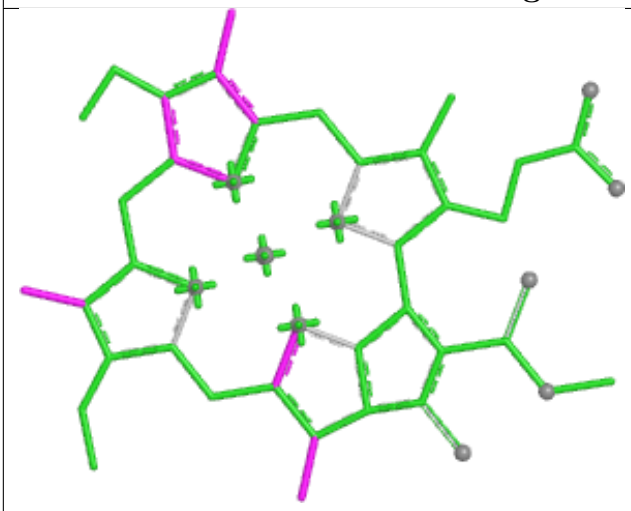


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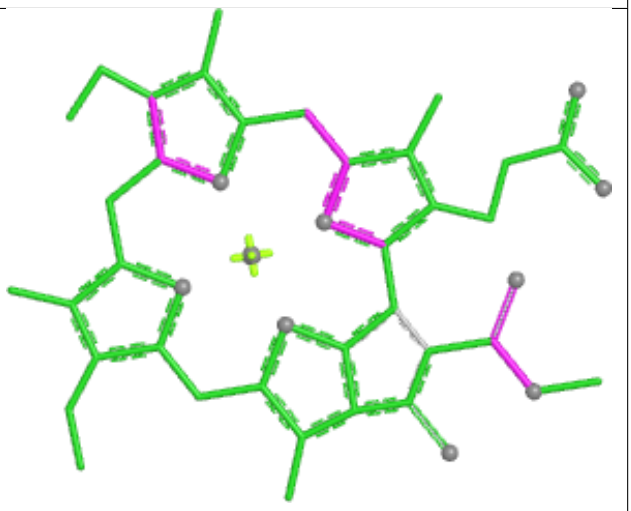


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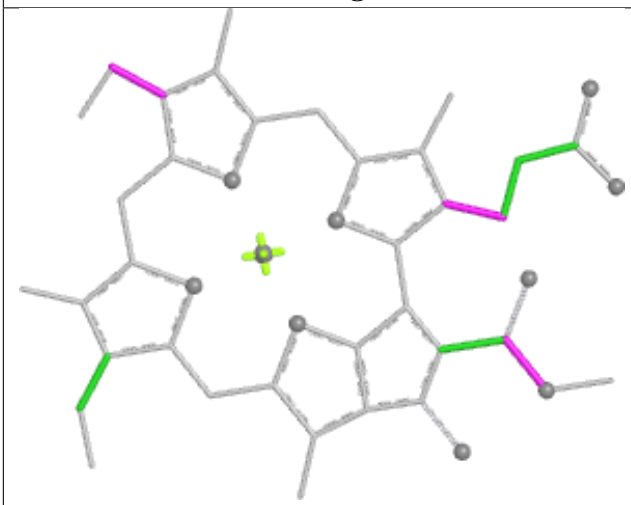
Ligand CLA K 206



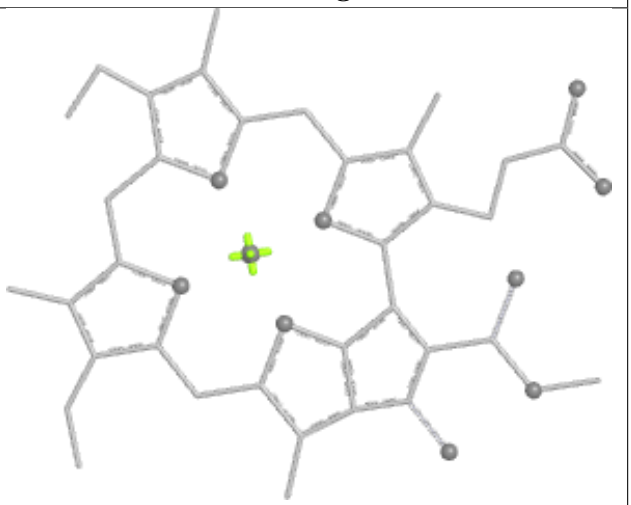
Bond lengths



Bond angles

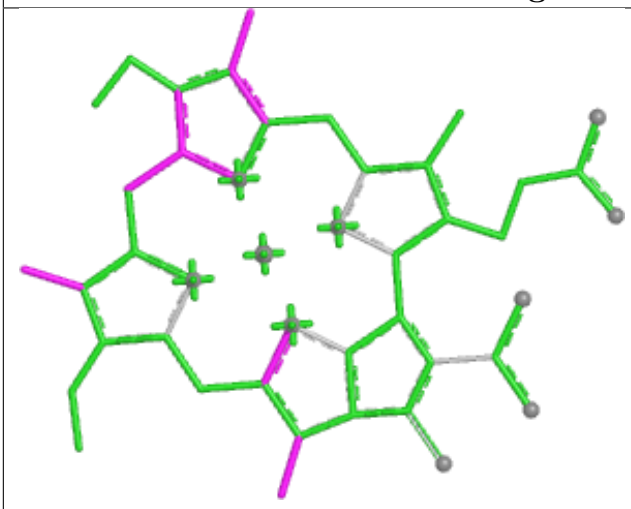


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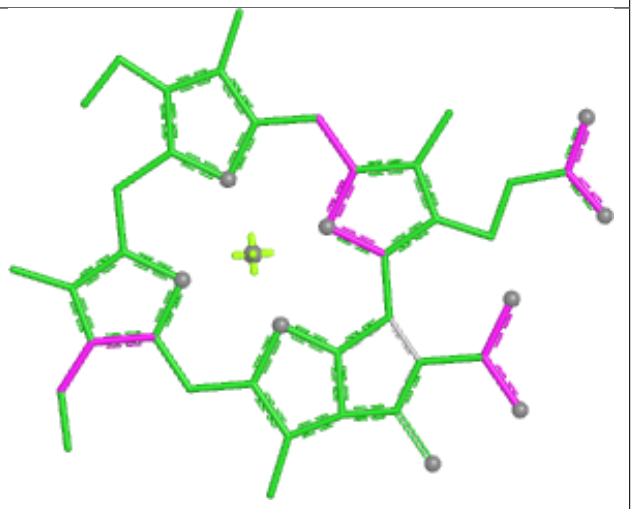


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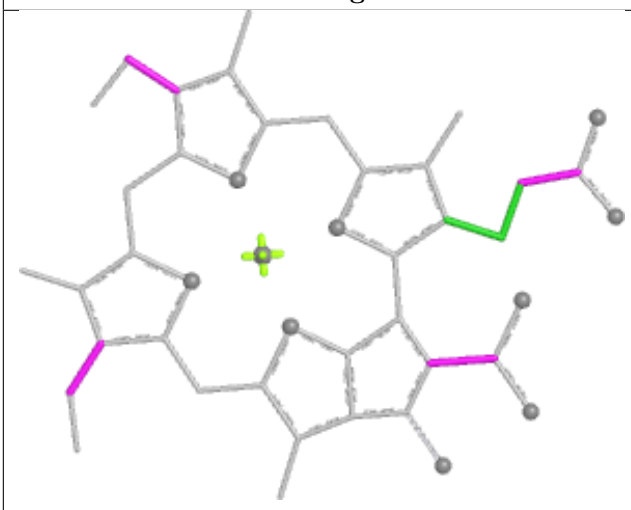
Ligand CLA 2 603



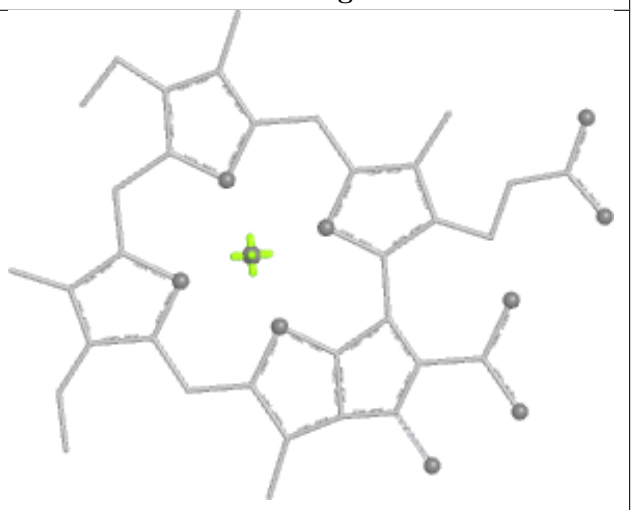
Bond lengths



Bond angles

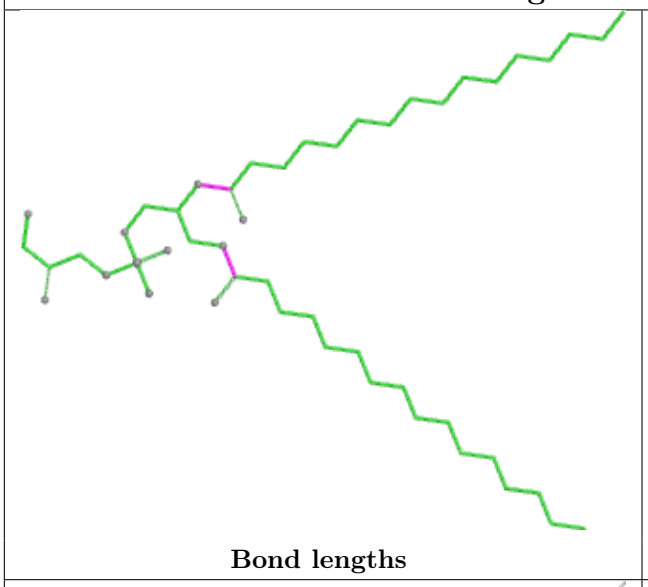


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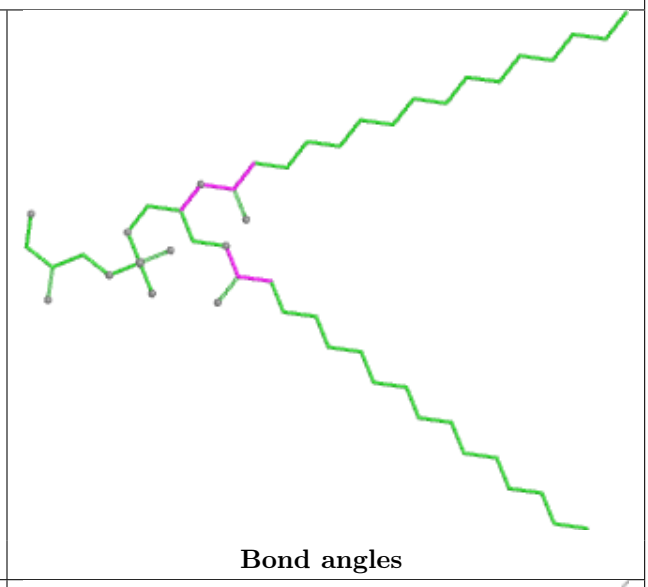


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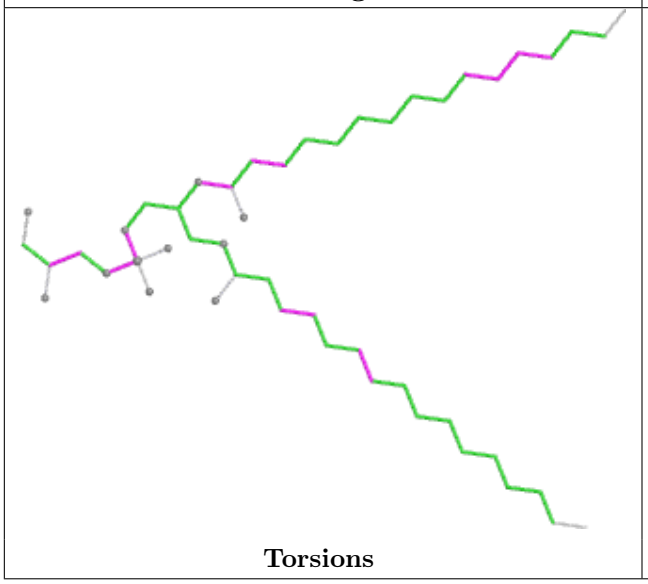
Ligand LHG 5 625



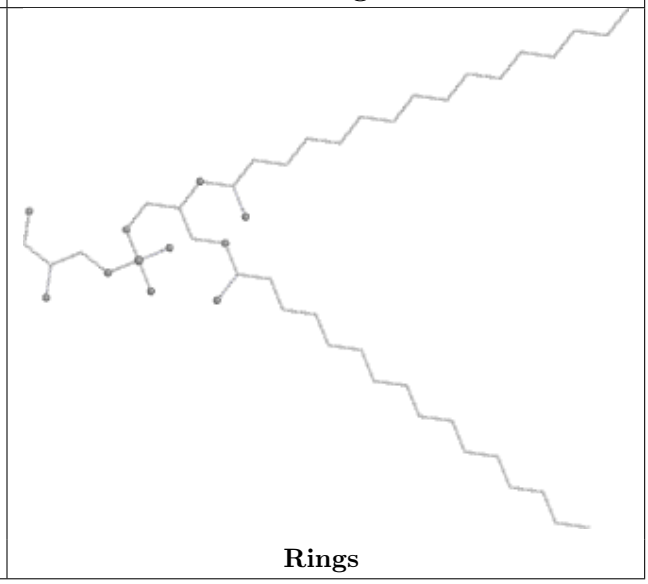
Bond lengths



Bond angles

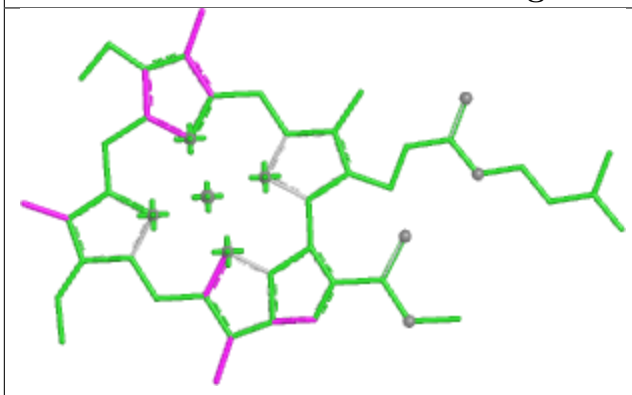


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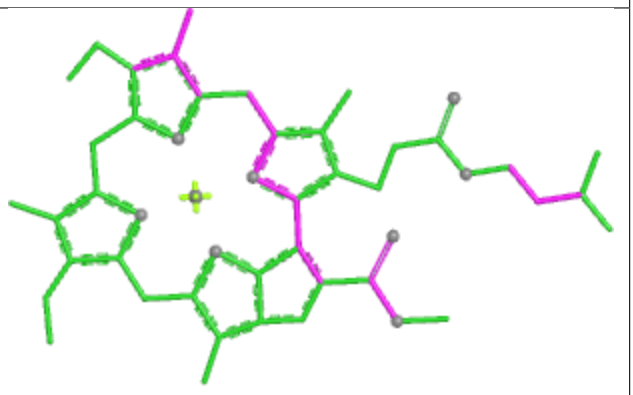


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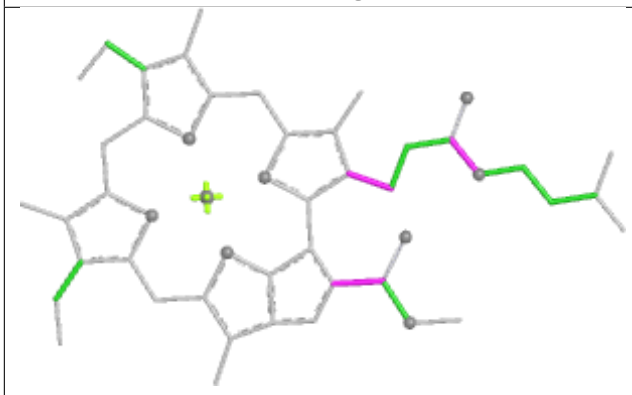
Ligand CLA Z 604



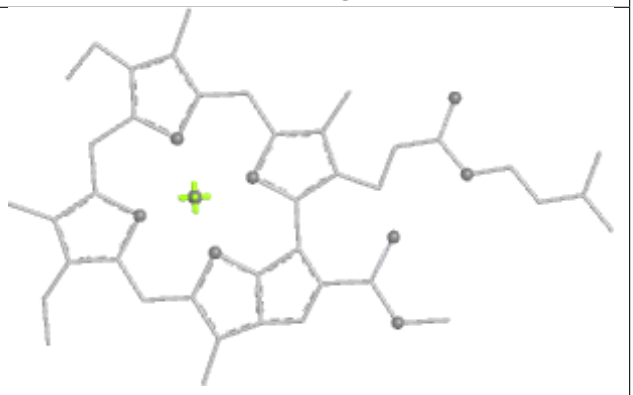
Bond lengths



Bond angles

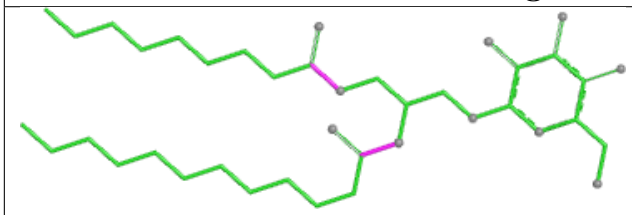


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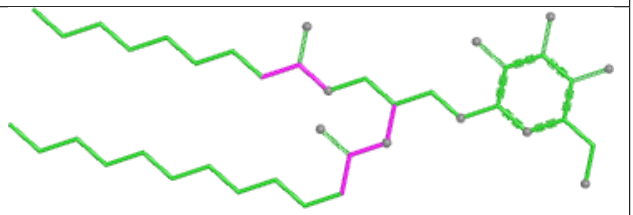


Rings

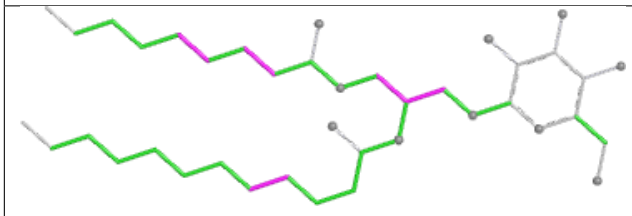
Ligand LMG 5 627



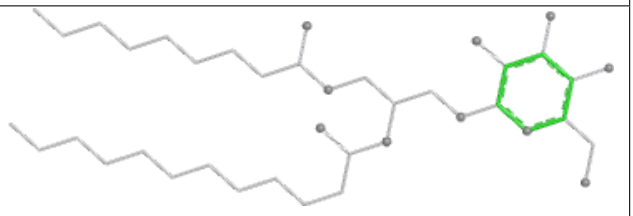
Bond lengths



Bond angles

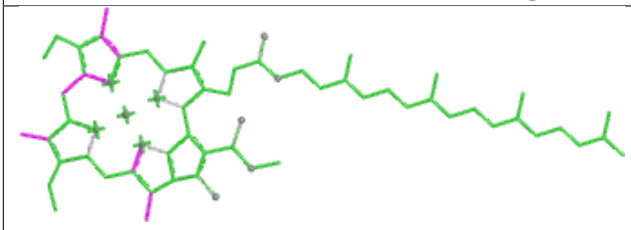


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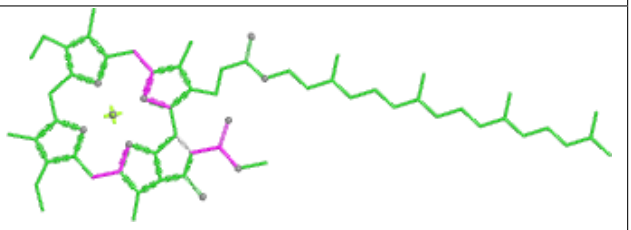


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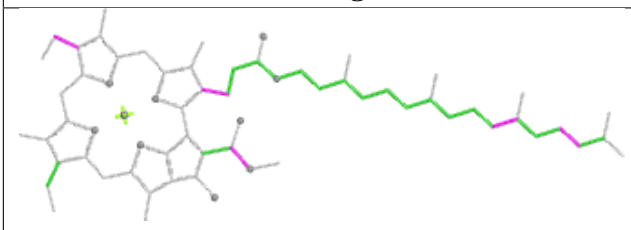
Ligand CLA A 812



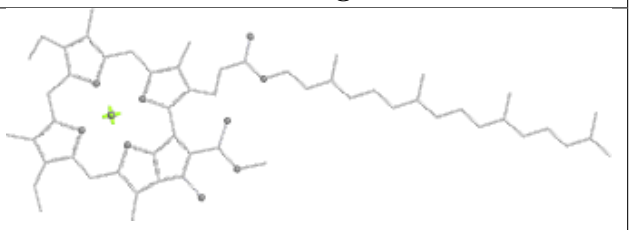
Bond lengths



Bond angles

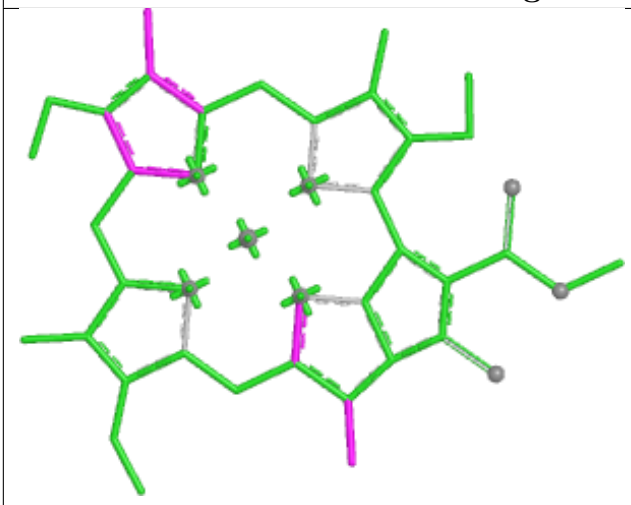


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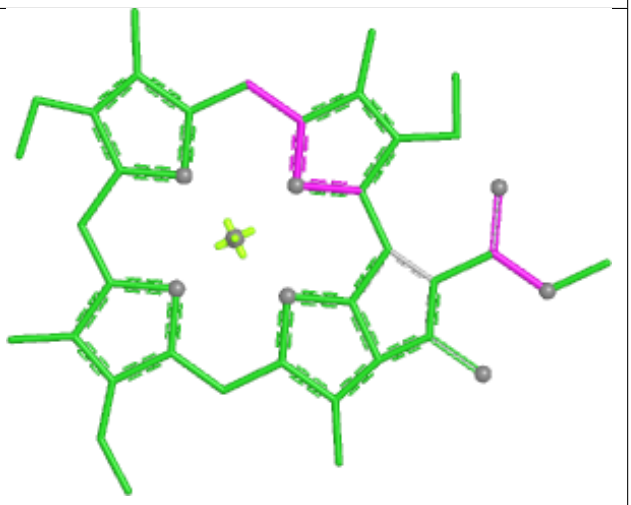


Rings

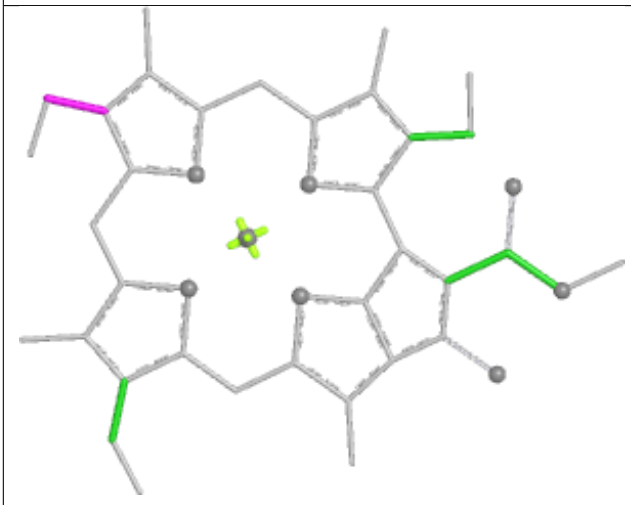
Ligand CLA U 611



Bond lengths



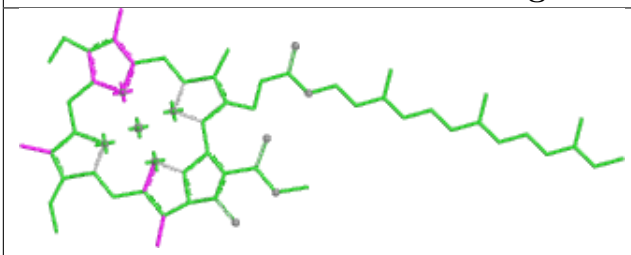
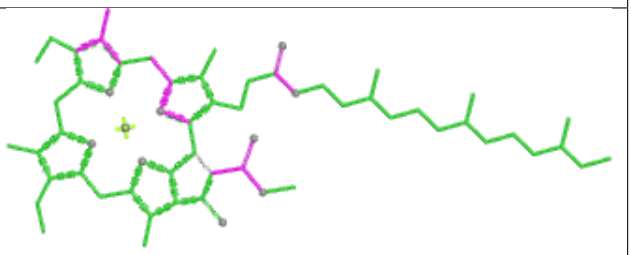
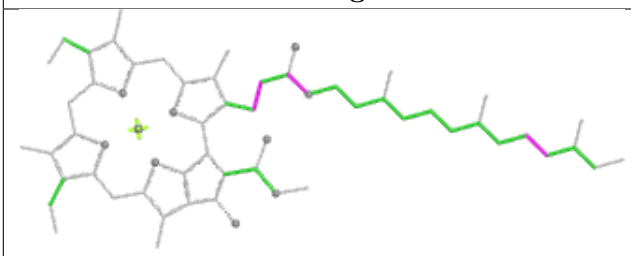
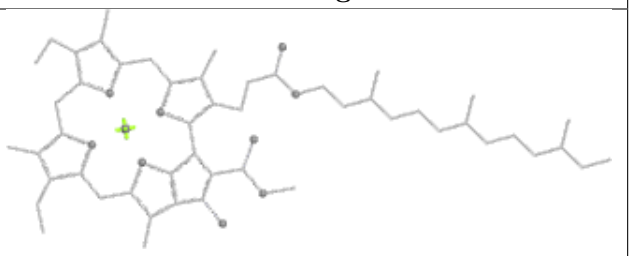
Bond angles

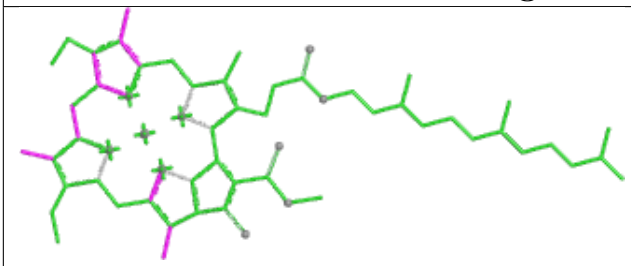
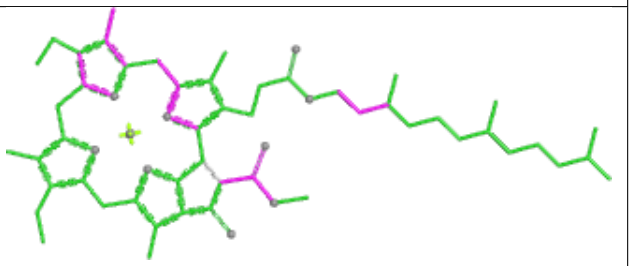
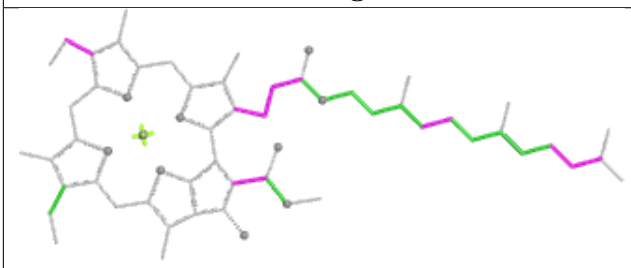
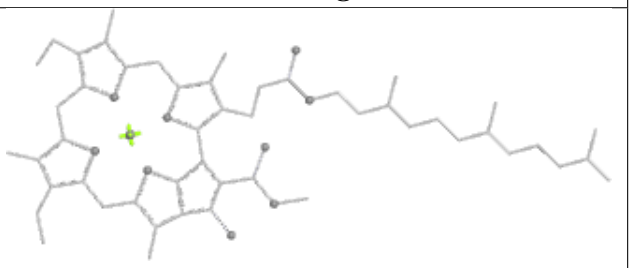


Torsions

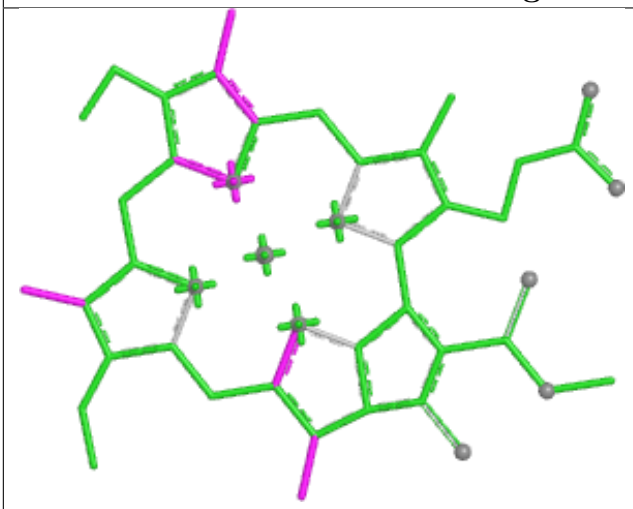


Rings

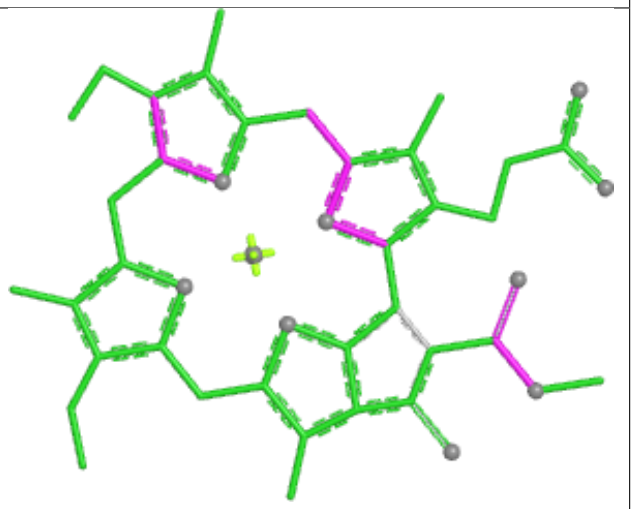
Ligand CLA 1 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA W 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

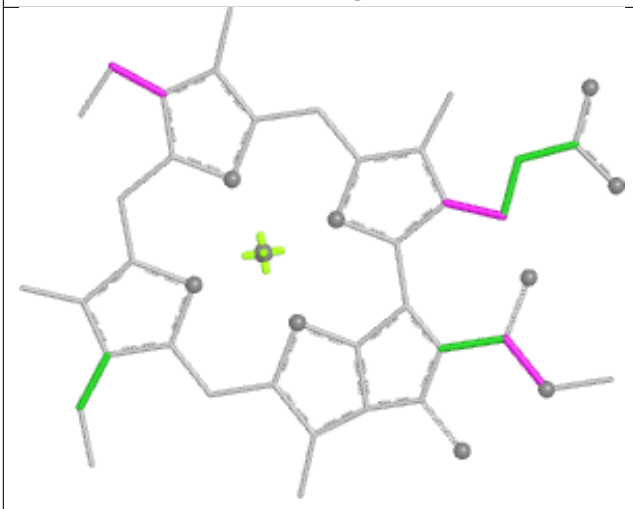
Ligand CLA K 204



Bond lengths



Bond angles

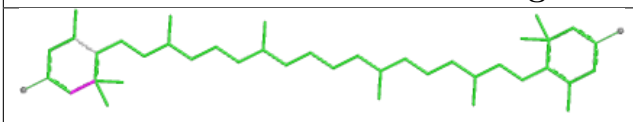


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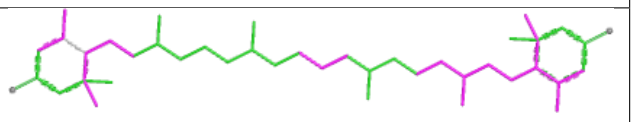


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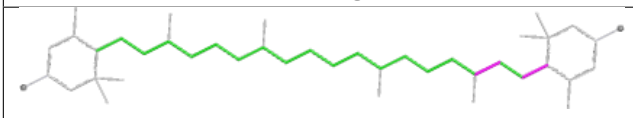
Ligand LUT 8 619



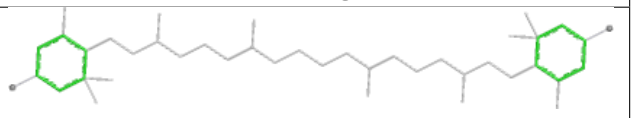
Bond lengths



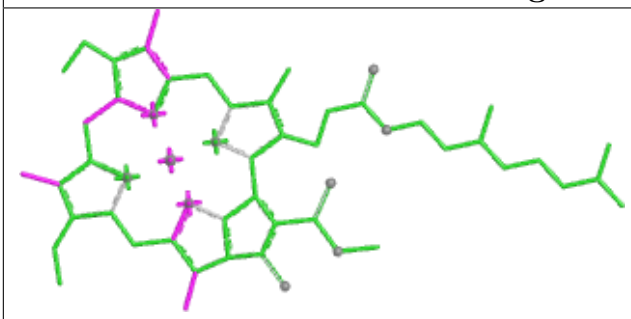
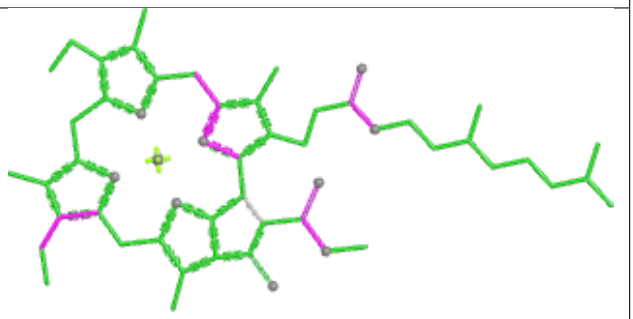
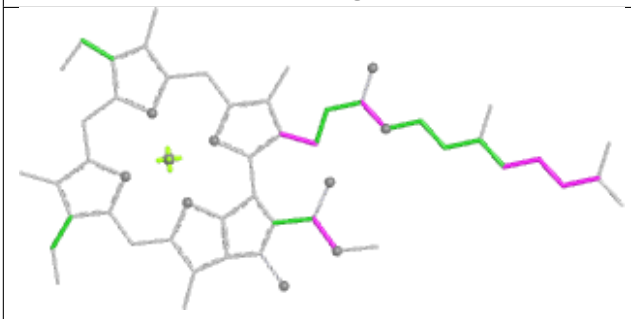
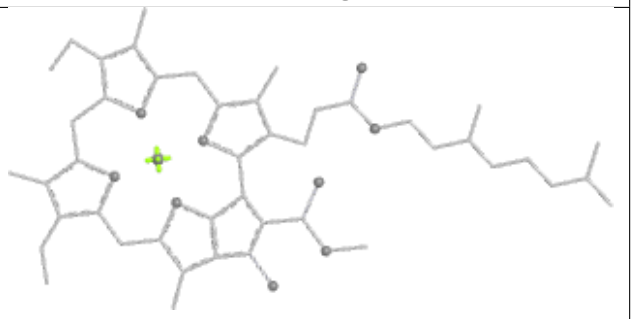
Bond angles



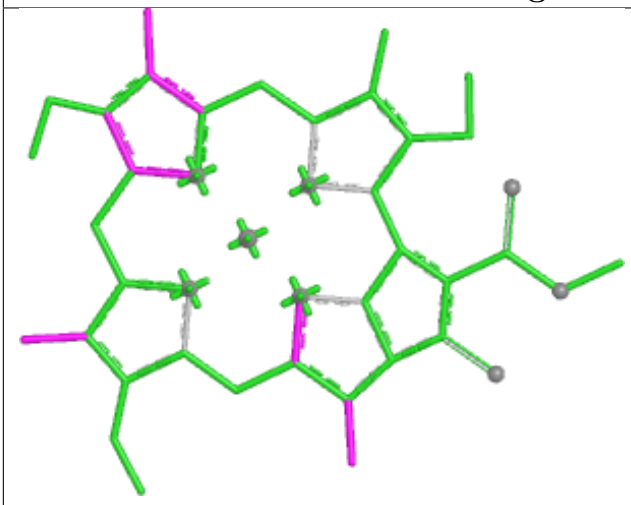
Torsions



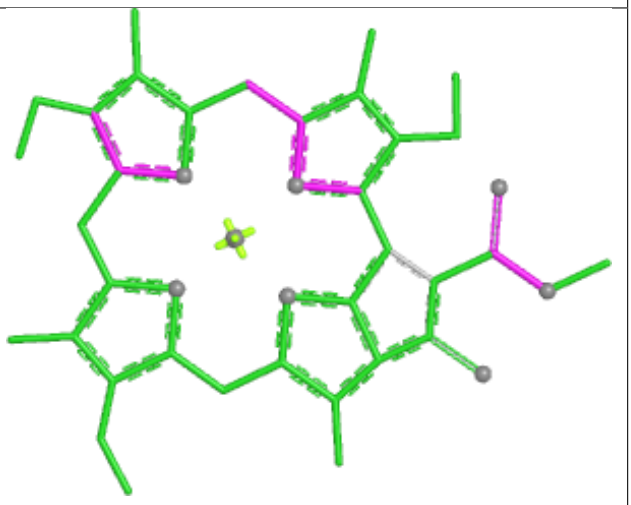
Rings

Ligand CLA 3 603	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 2 611



Bond lengths



Bond angles

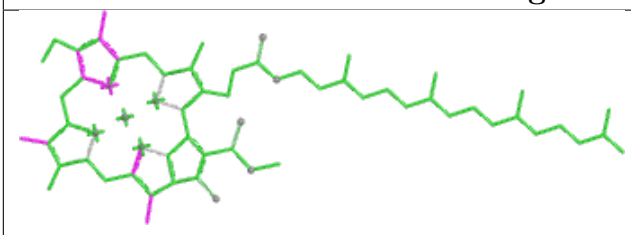


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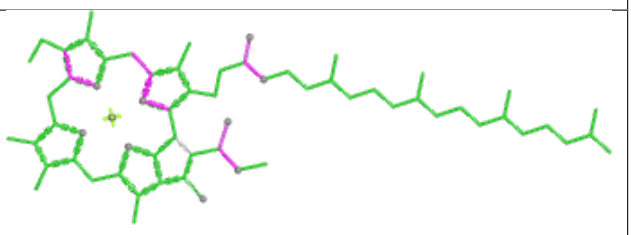


Rings

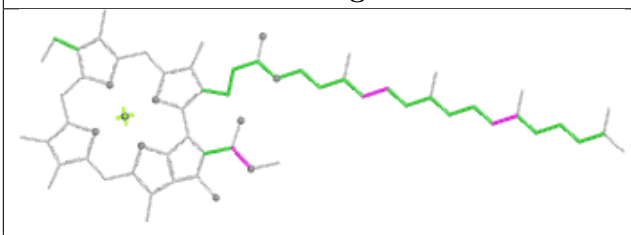
Ligand CLA 8 606



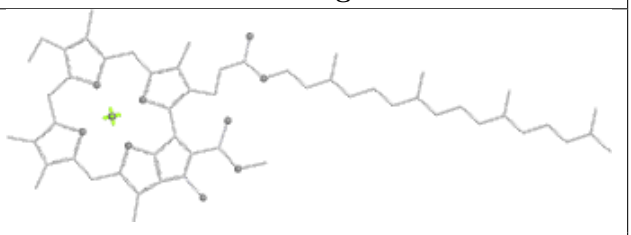
Bond lengths



Bond angles

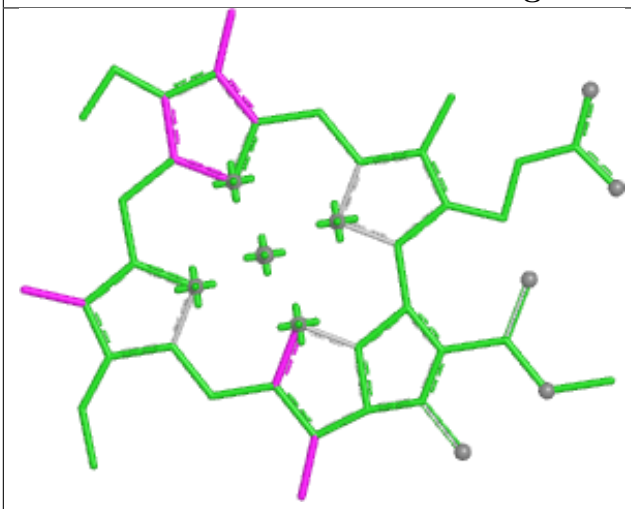


Torsions

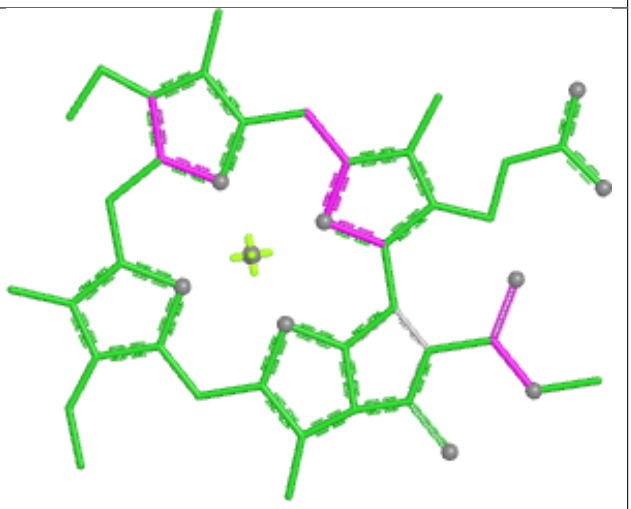


Rings

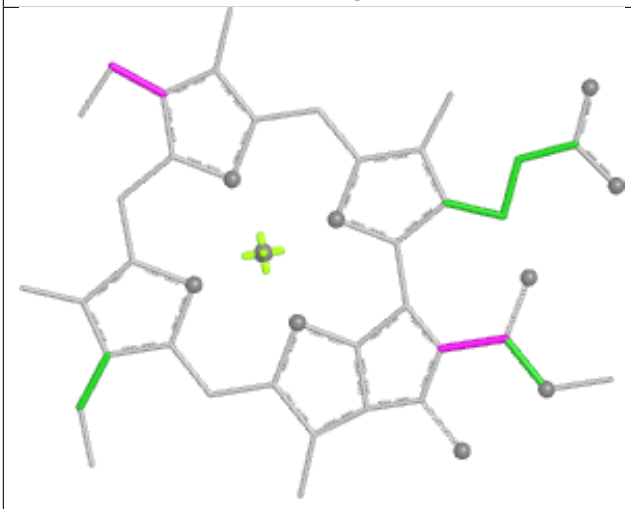
Ligand CLA X 611



Bond lengths



Bond angles

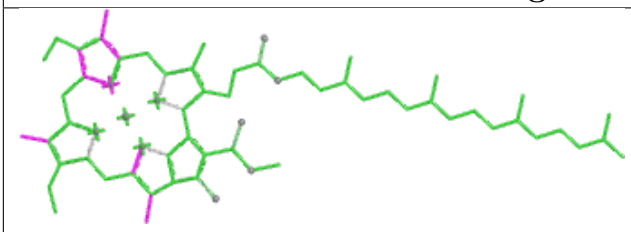


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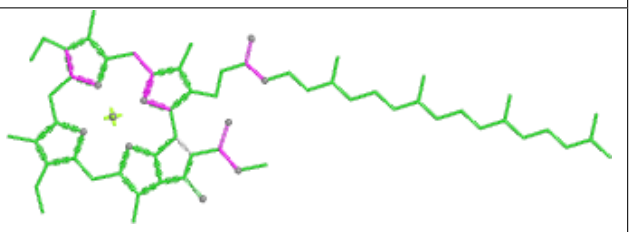


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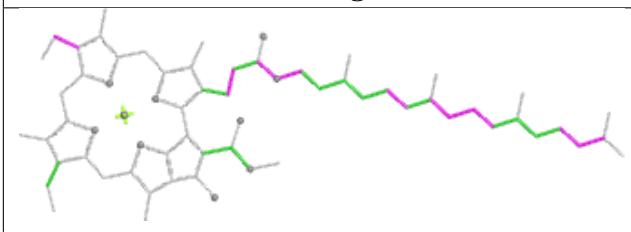
Ligand CLA 8 613



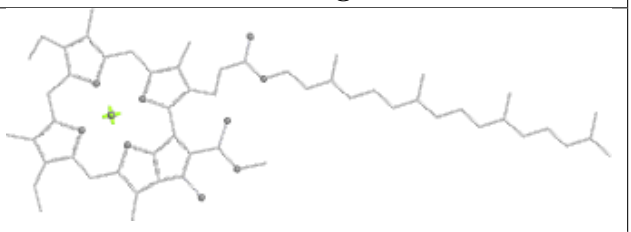
Bond lengths



Bond angles

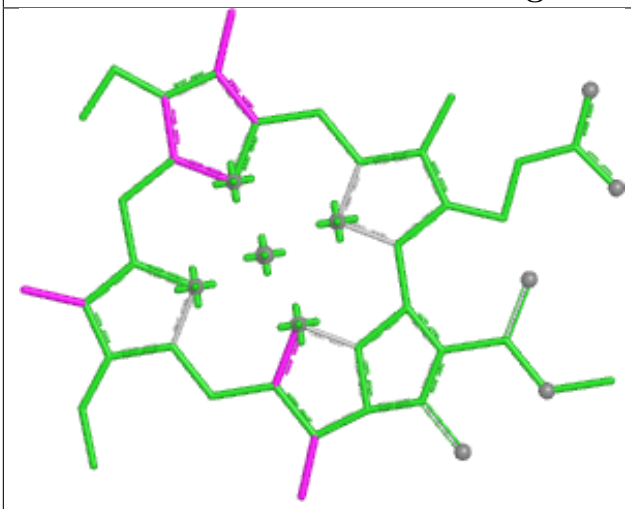


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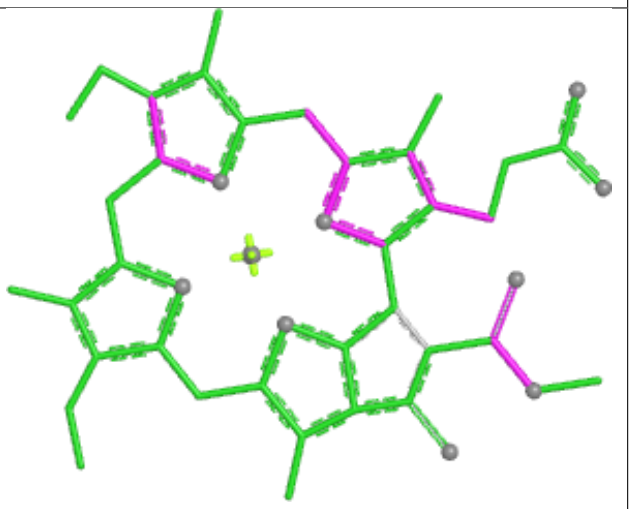


Rings

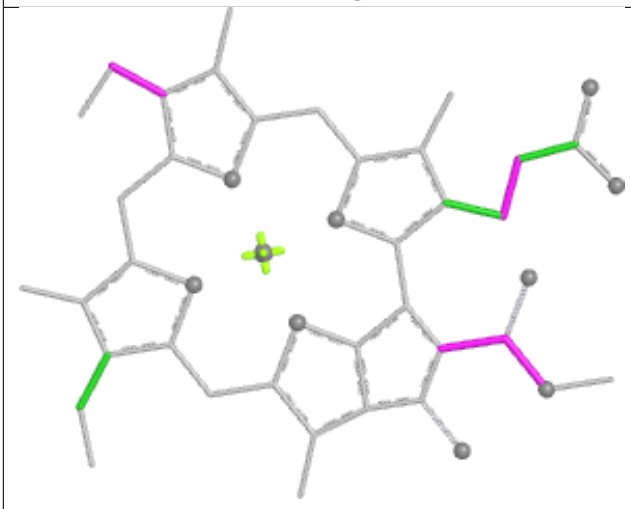
Ligand CLA Z 612



Bond lengths



Bond angles

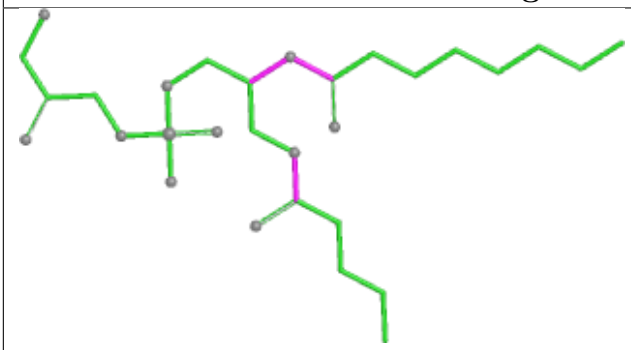


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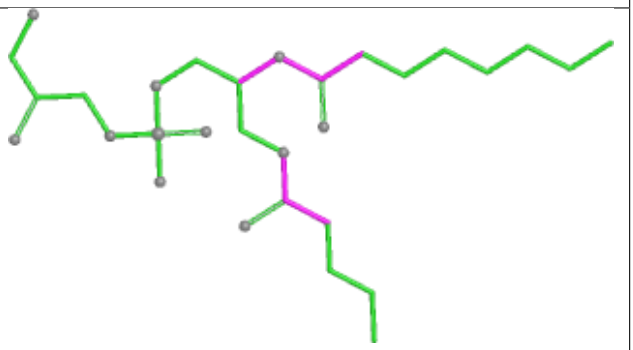


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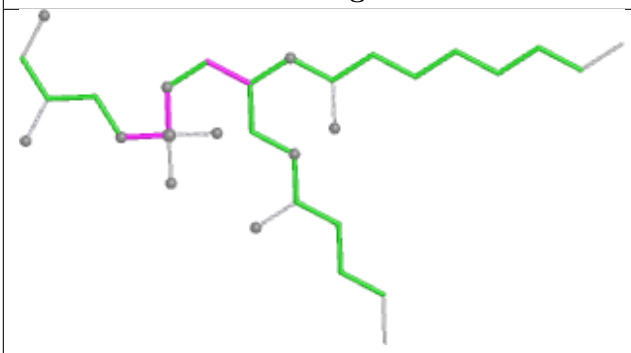
Ligand LHG A 847



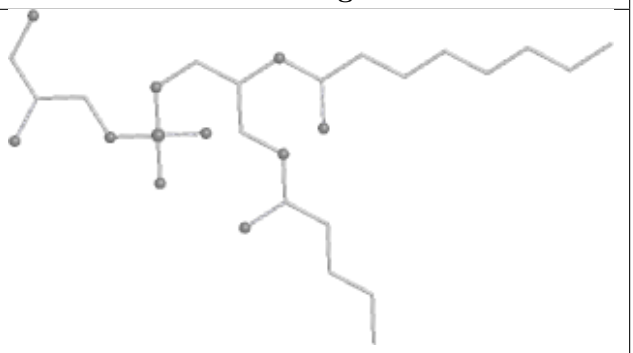
Bond lengths



Bond angles

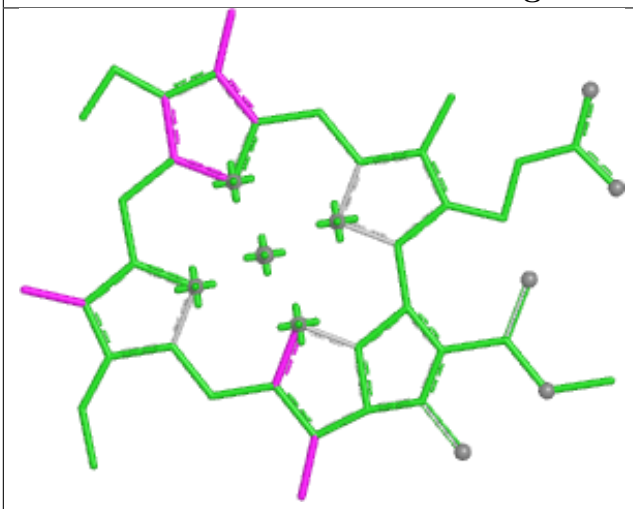


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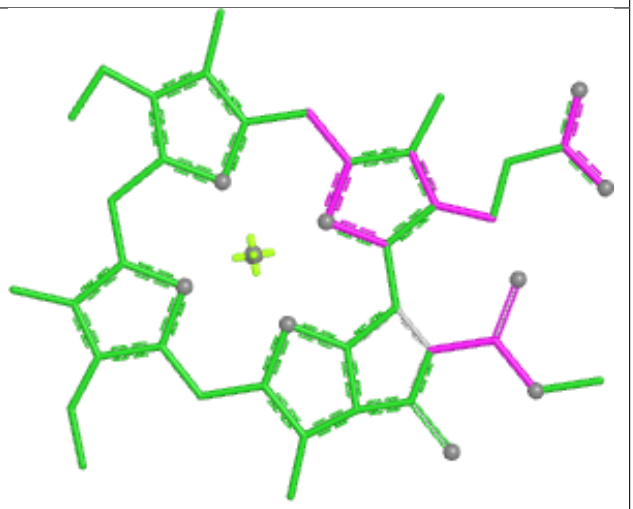


Rings

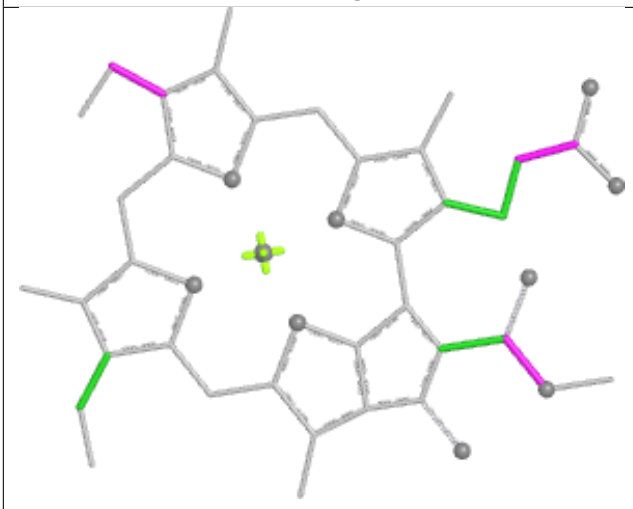
Ligand CLA V 612



Bond lengths



Bond angles

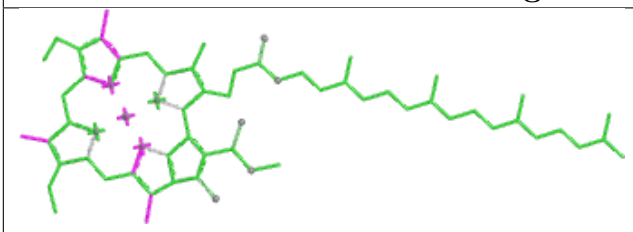


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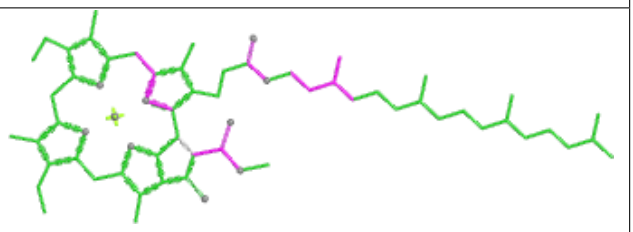


Rings

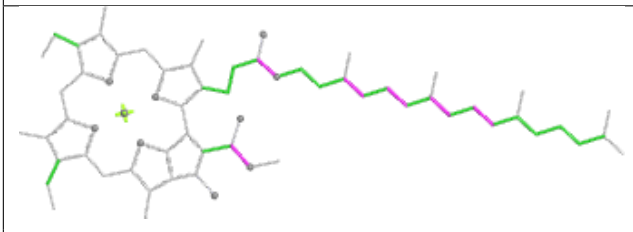
Ligand CLA A 836



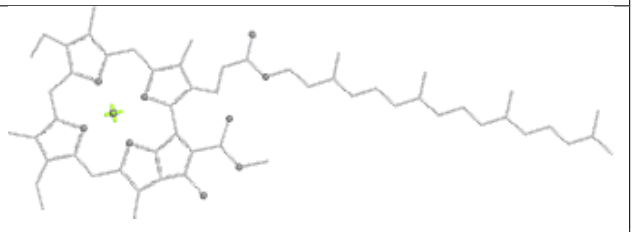
Bond lengths



Bond angles

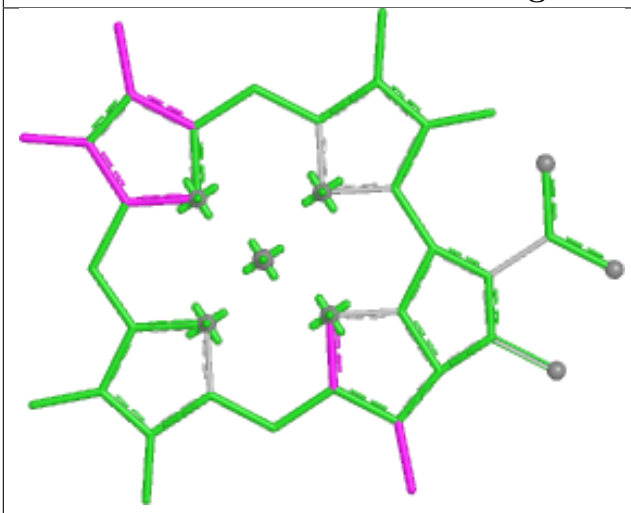


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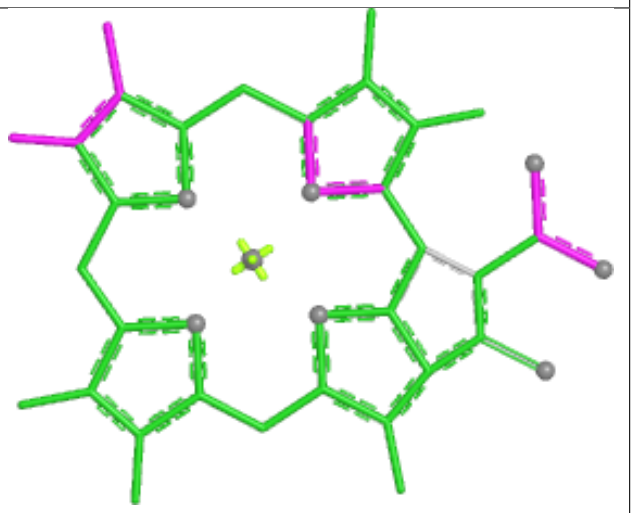


Rings

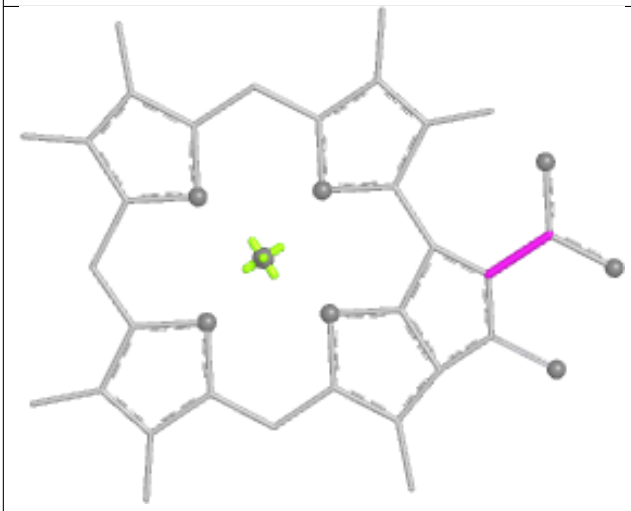
Ligand CLA 3 611



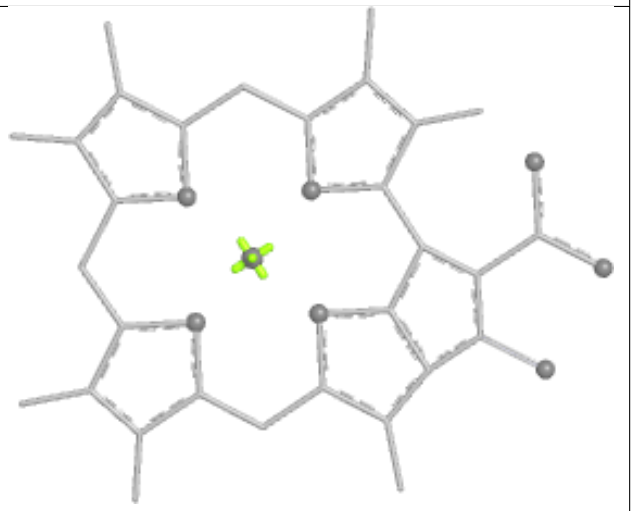
Bond lengths



Bond angles

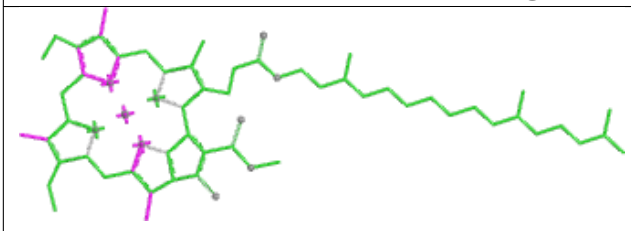


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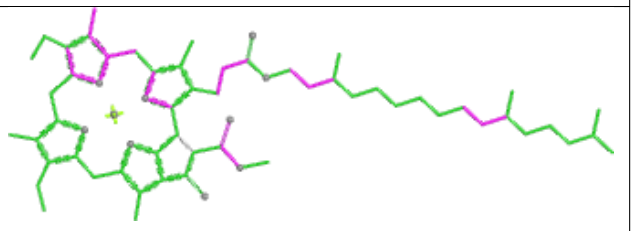


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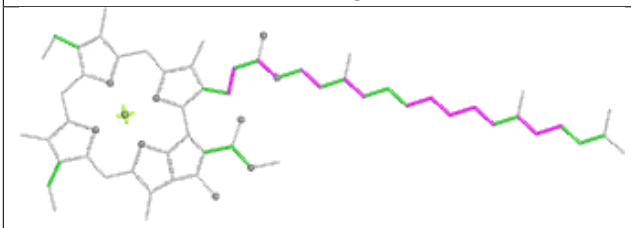
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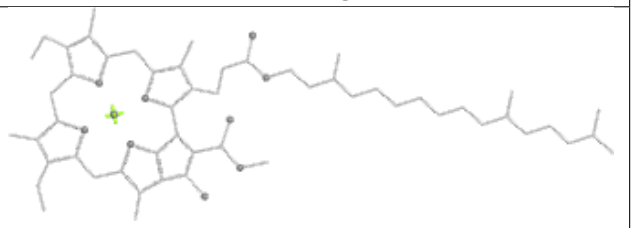
Bond lengths



Bond angles

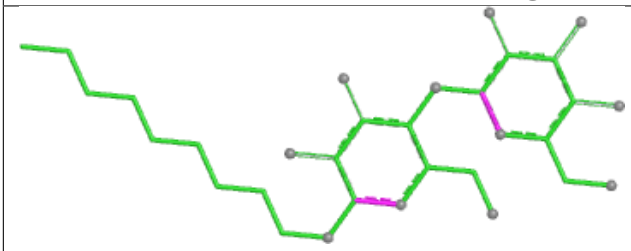


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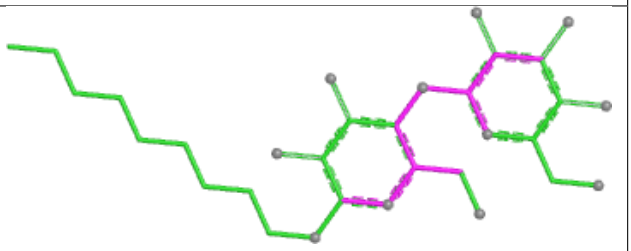


Rings

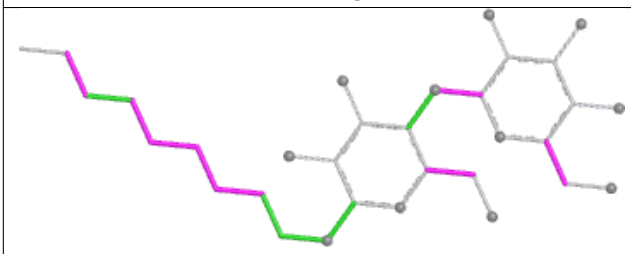
Ligand LMU 5 629



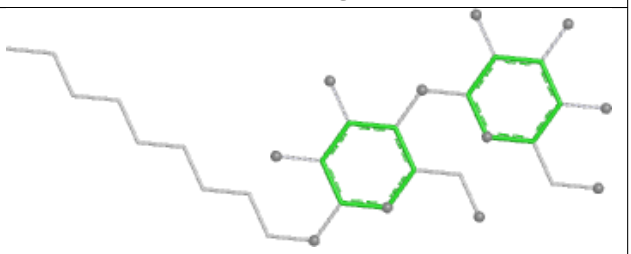
Bond lengths



Bond angles

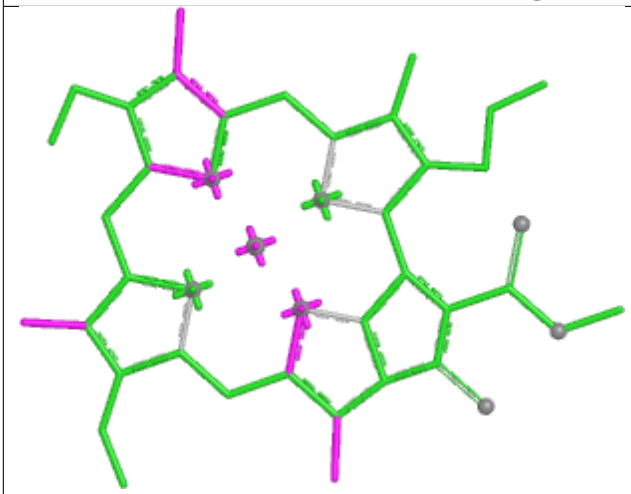


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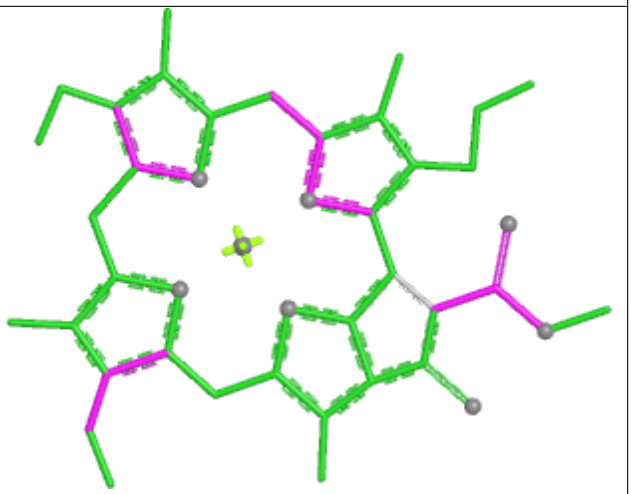


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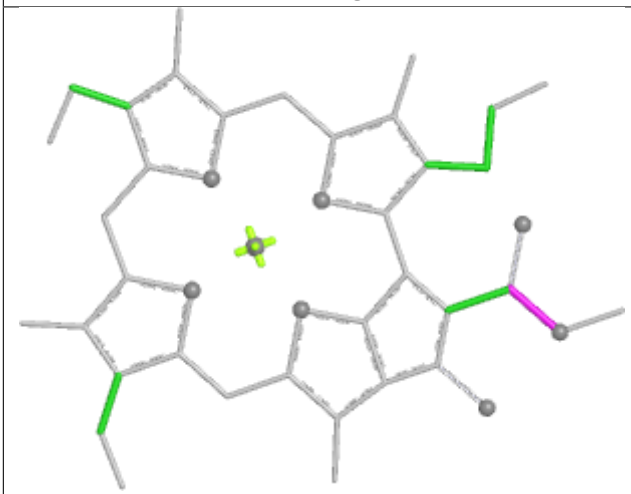
Ligand CLA 2 606



Bond lengths



Bond angles

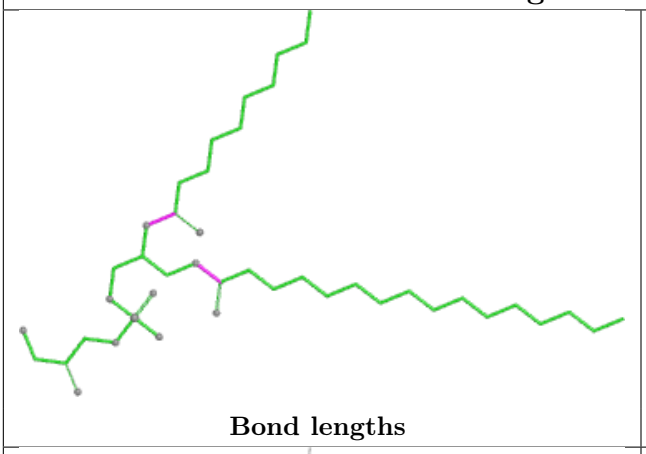


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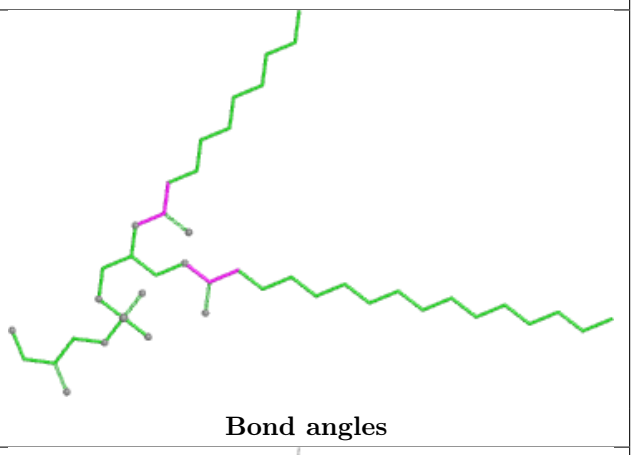


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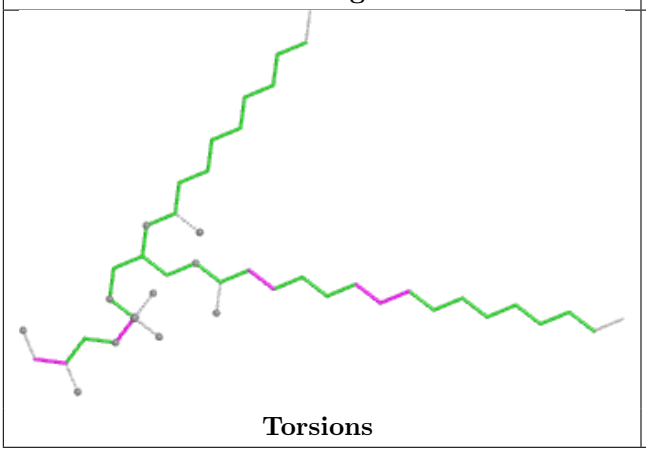
Ligand LHG a 620



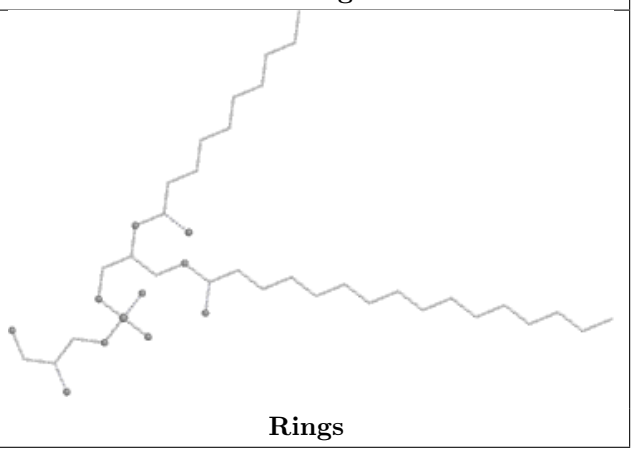
Bond lengths



Bond angles

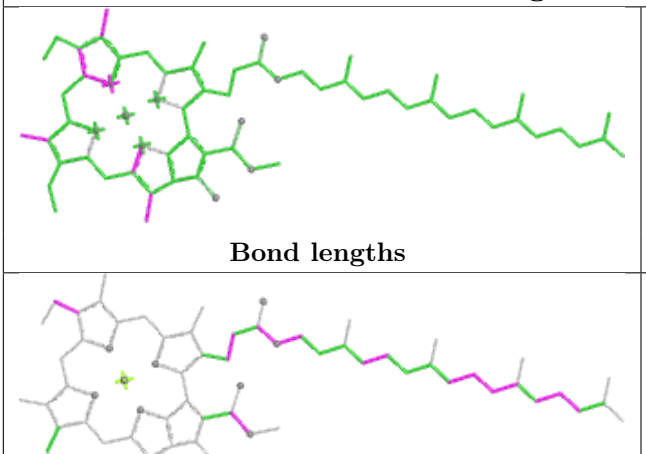


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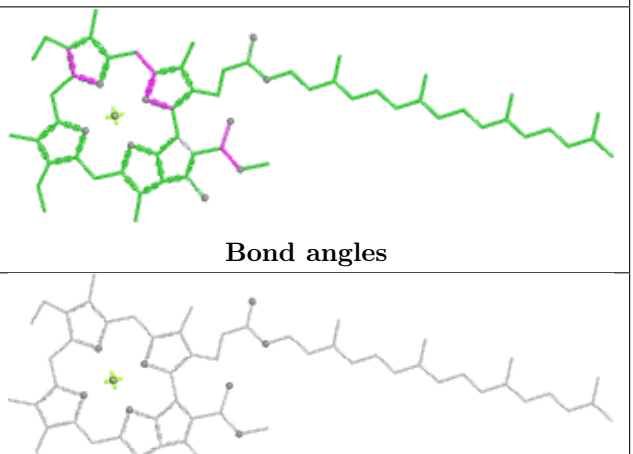


Rings

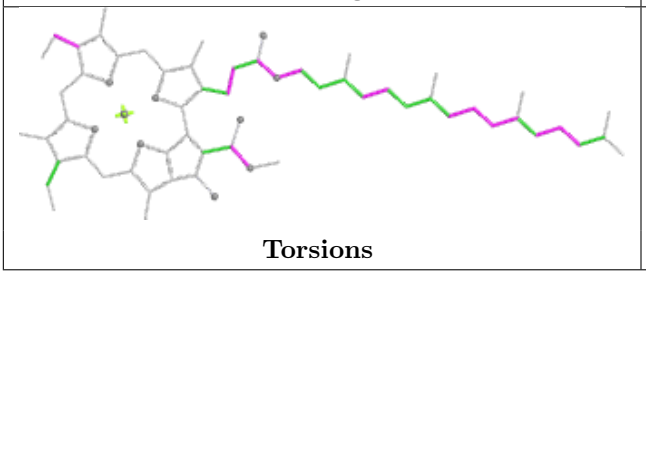
Ligand CLA 8 601



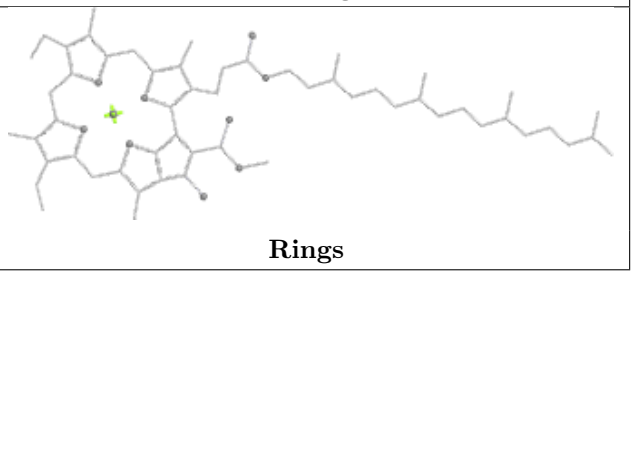
Bond lengths



Bond angles

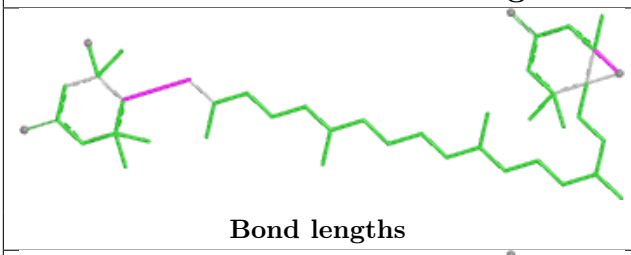


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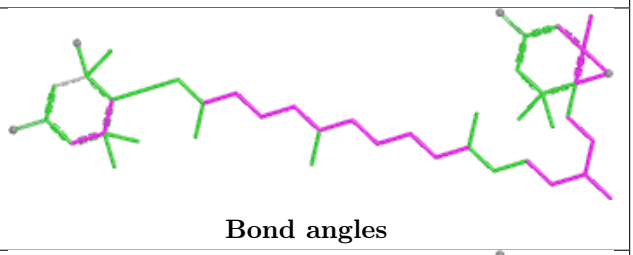


Rings

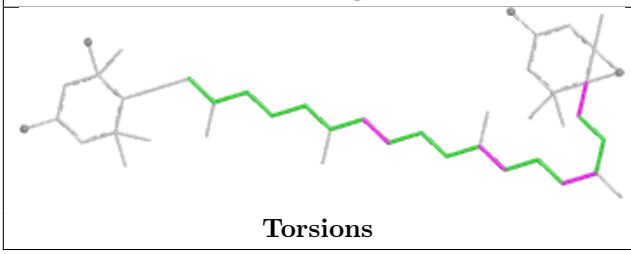
Ligand NEX W 1623



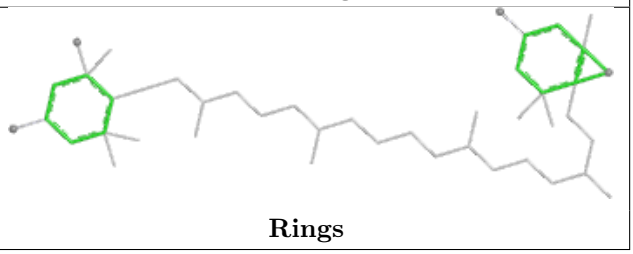
Bond lengths



Bond angles

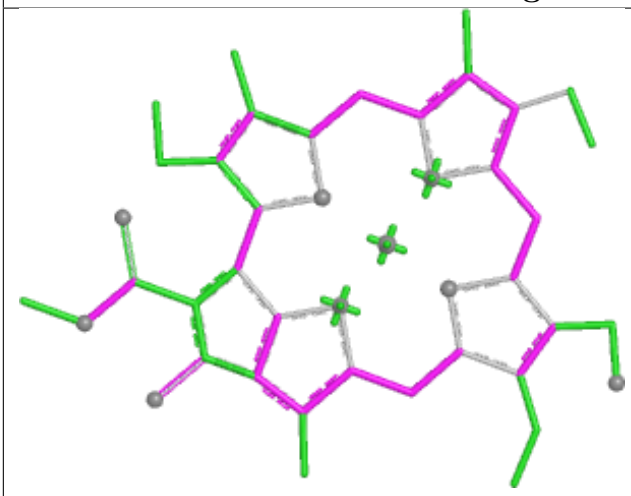


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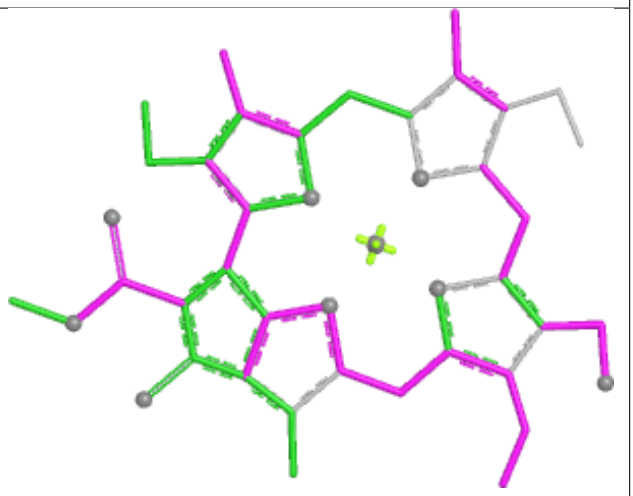


Rings

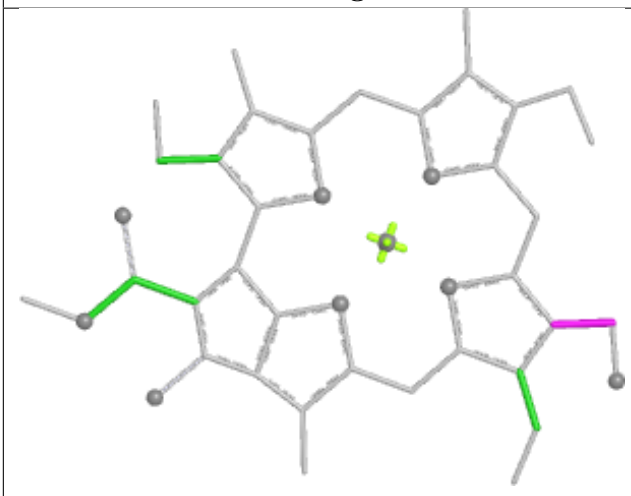
Ligand CHL U 605



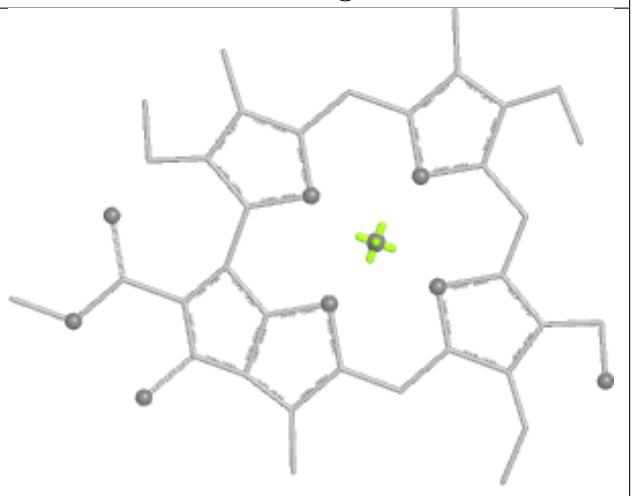
Bond lengths



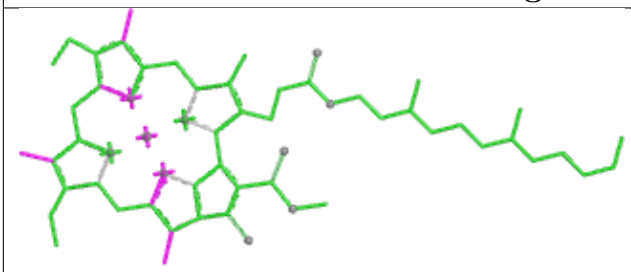
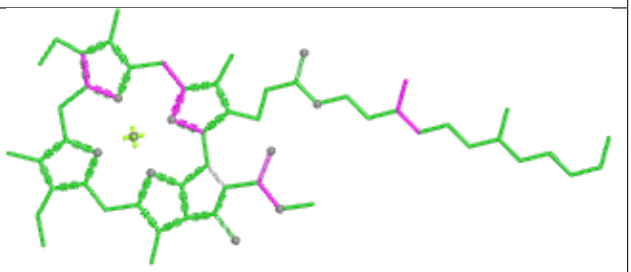
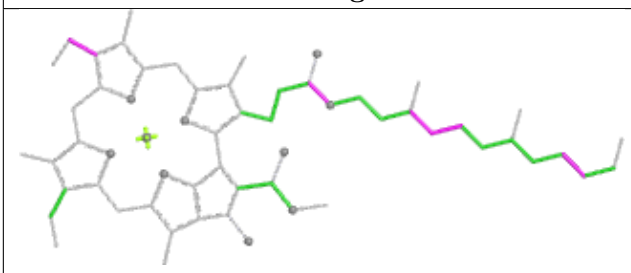
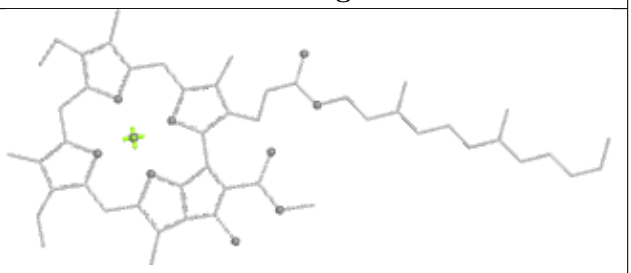
Bond angles



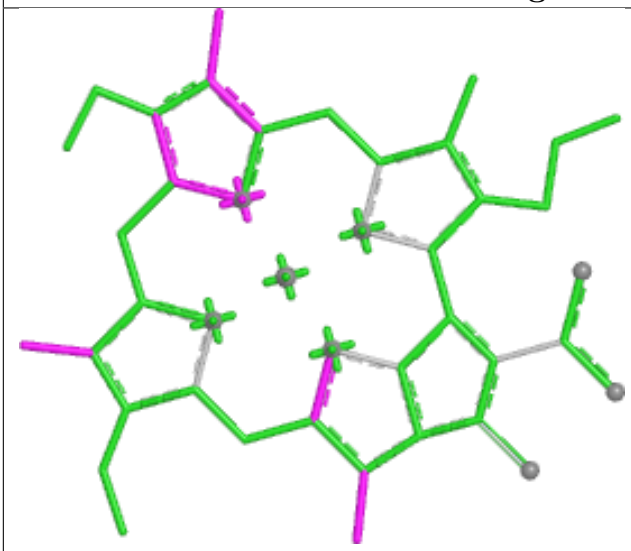
Torsions



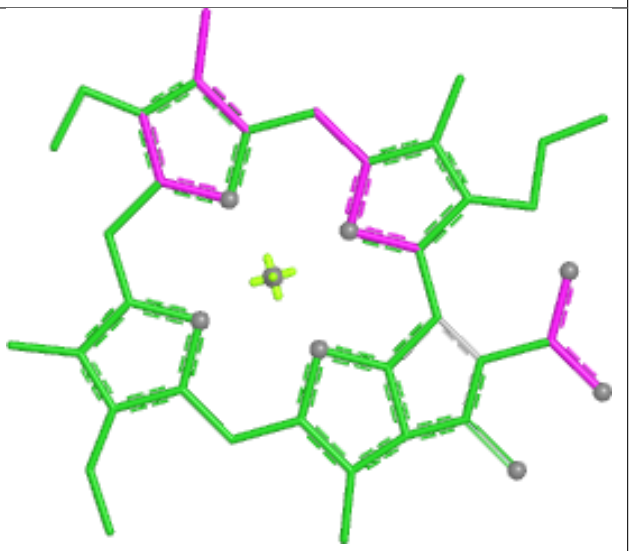
Rings

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

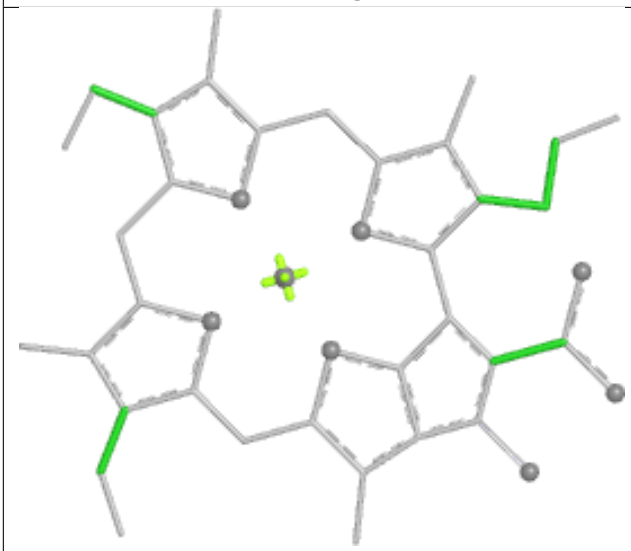
Ligand CLA 2 614



Bond lengths



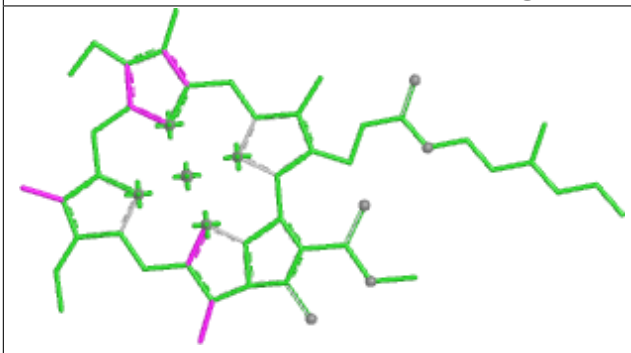
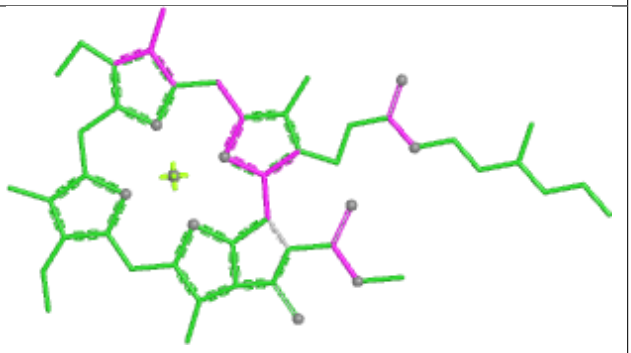
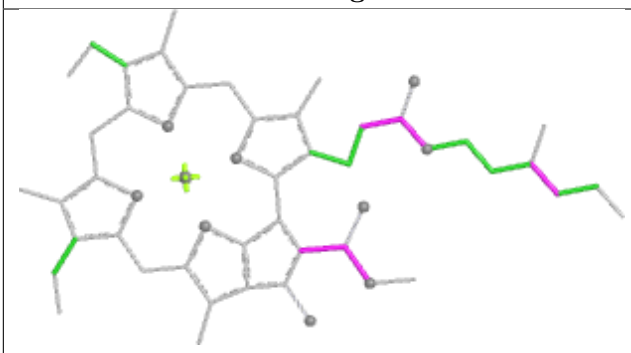
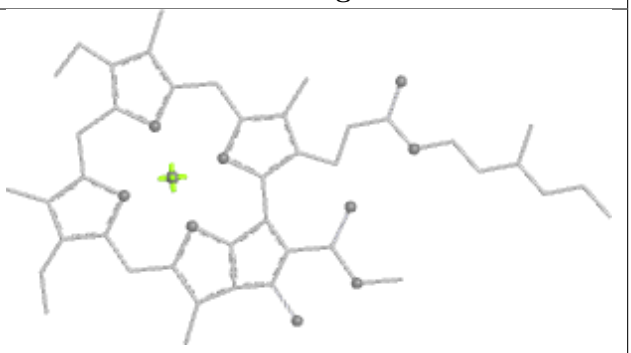
Bond angles

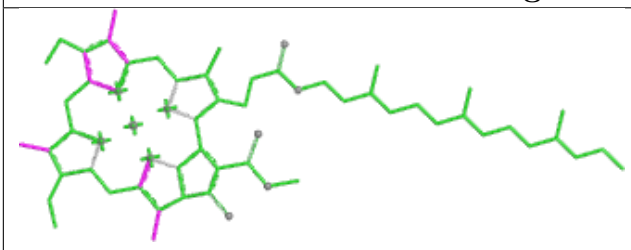
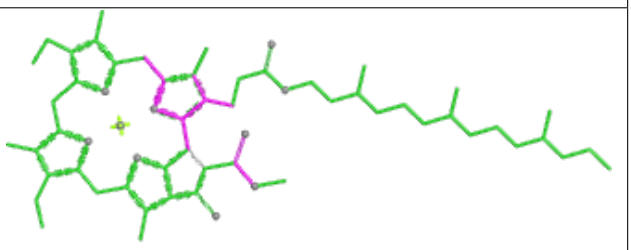
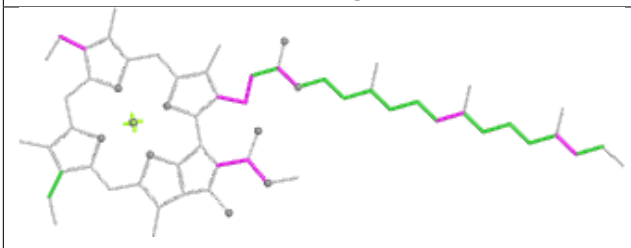
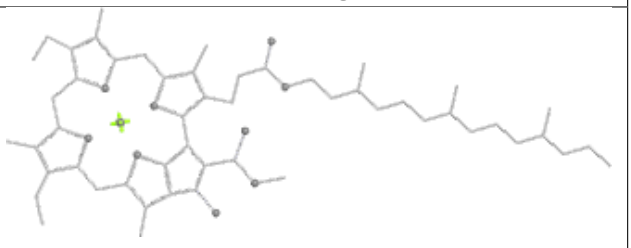


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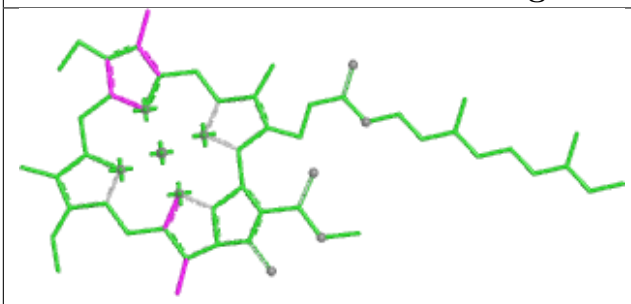


Rings

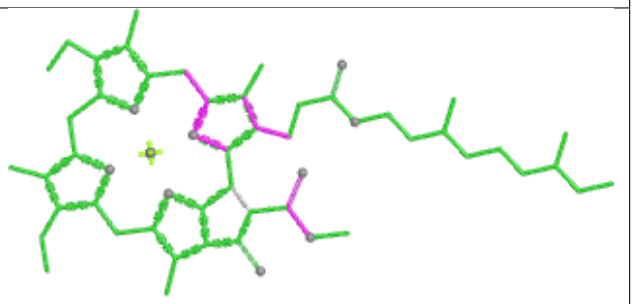
Ligand CLA W 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA X 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

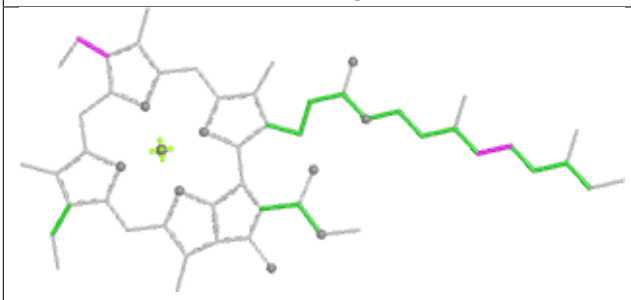
Ligand CLA 5 601



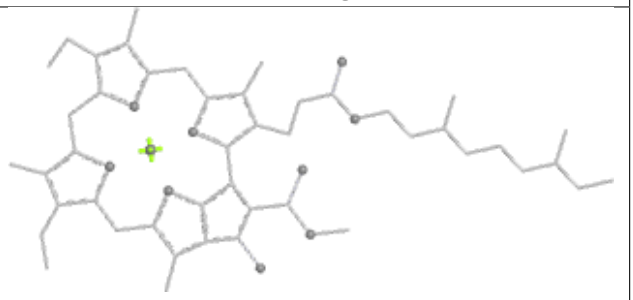
Bond lengths



Bond angles

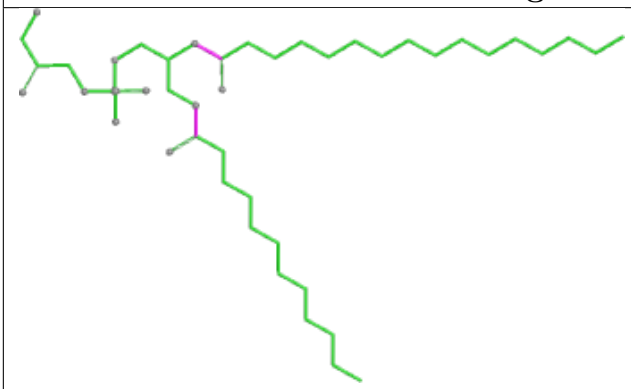


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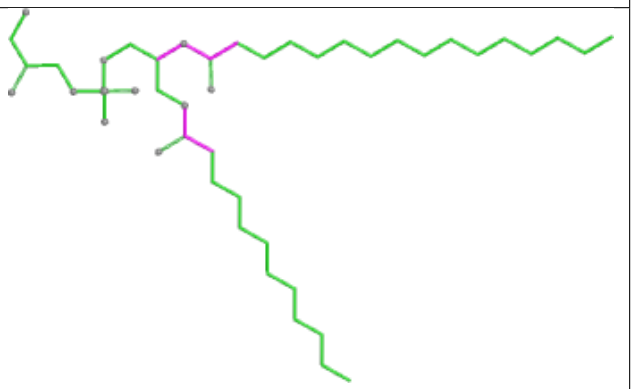


Rings

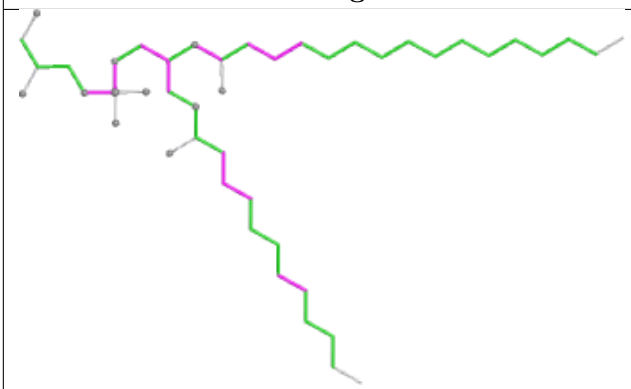
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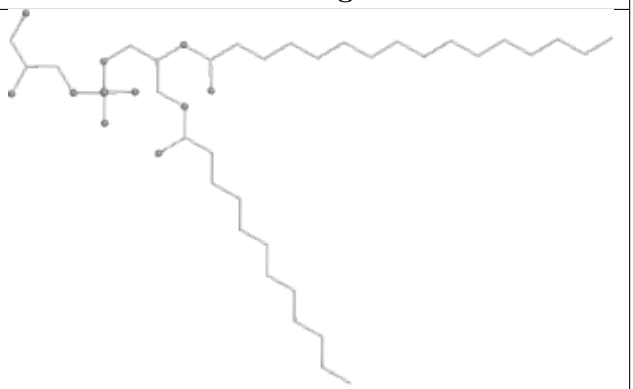
Bond lengths



Bond angles

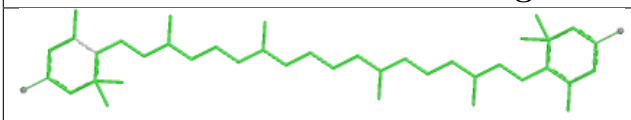


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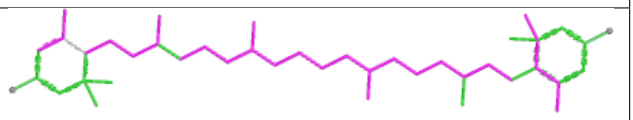


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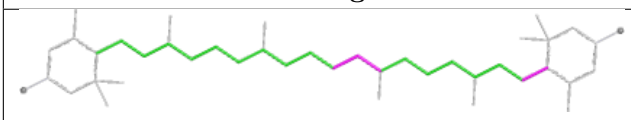
Ligand LUT Y 1620



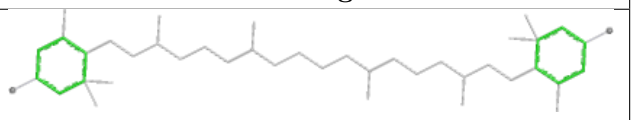
Bond lengths



Bond angles

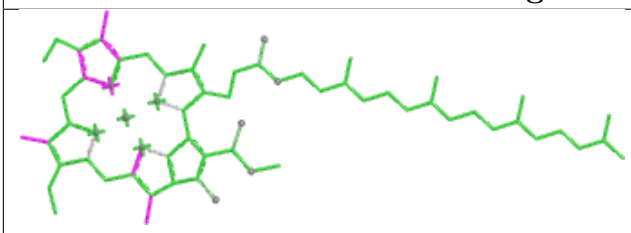


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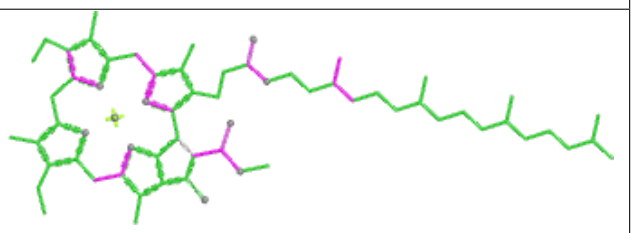


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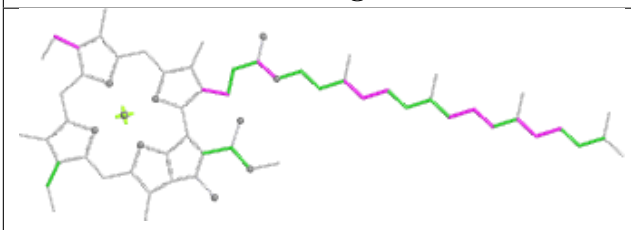
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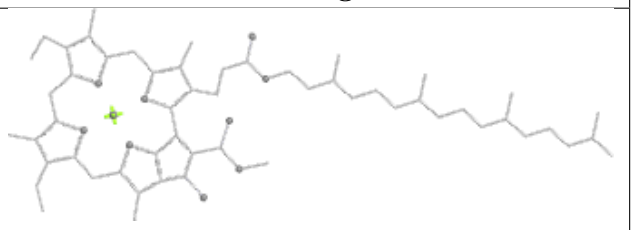
Bond lengths



Bond angles

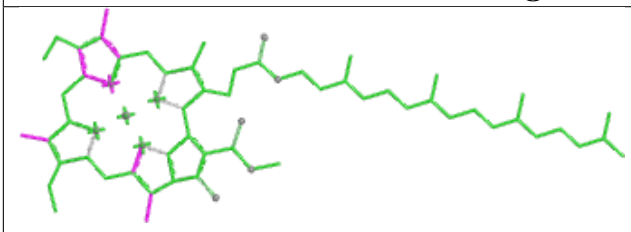


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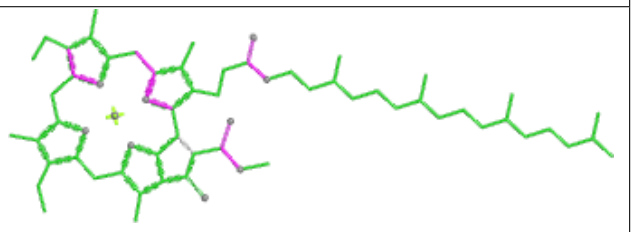


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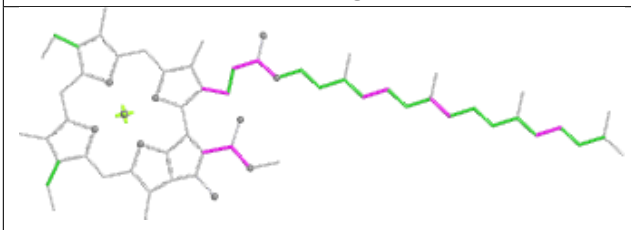
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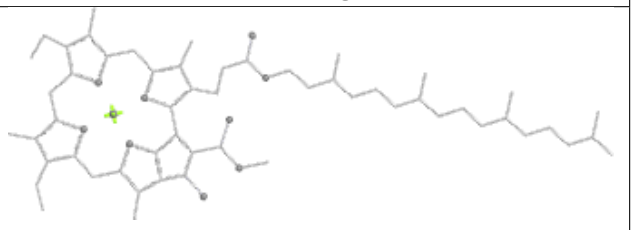
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Bond angles

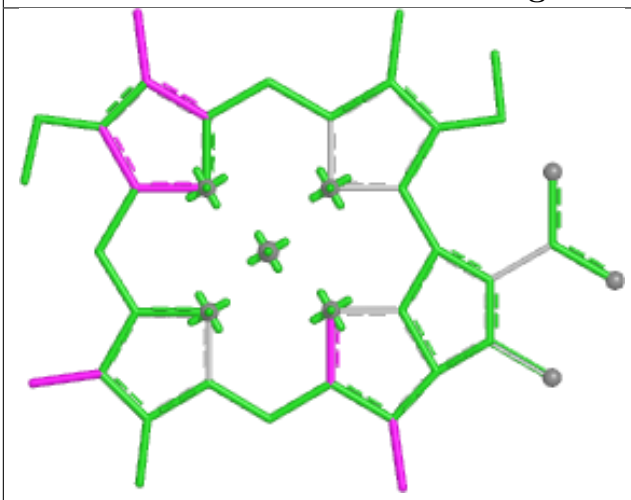


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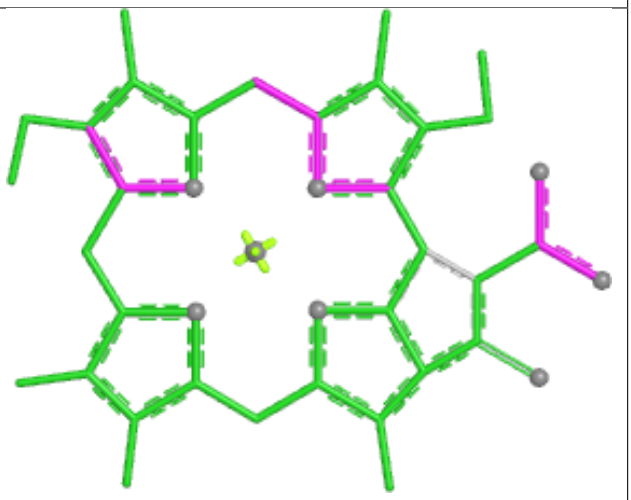


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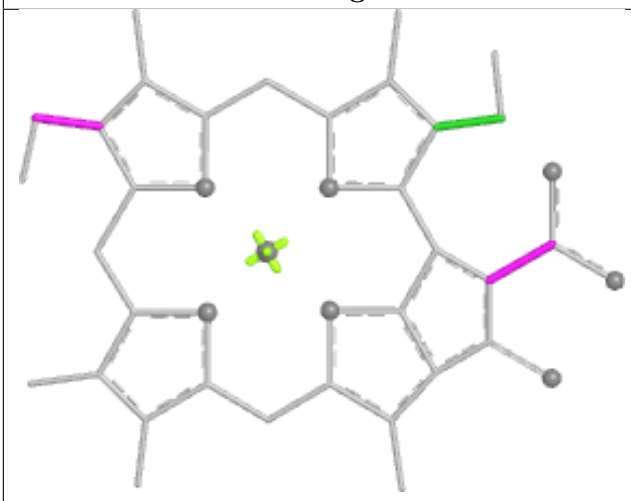
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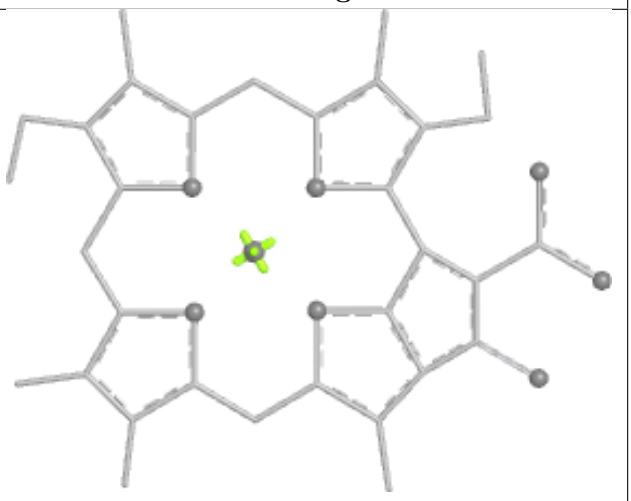
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Bond angles

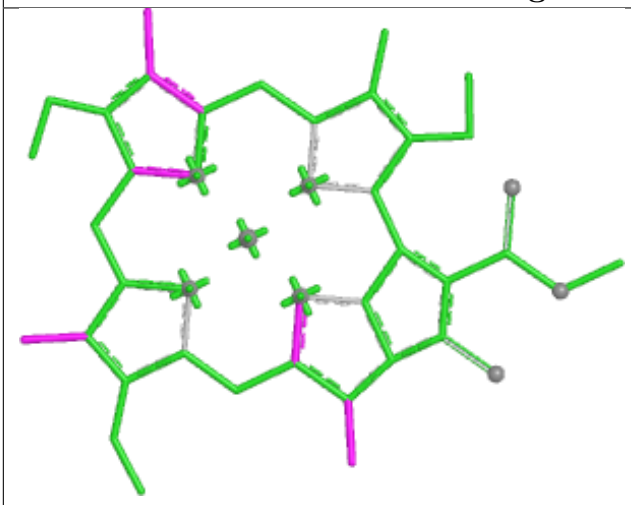


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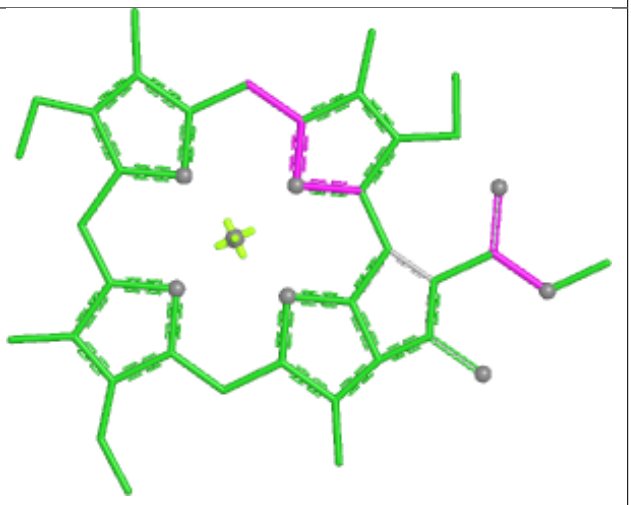


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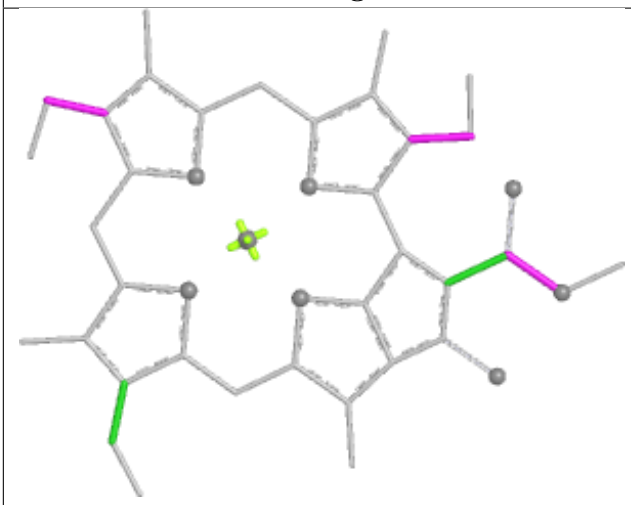
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Bond lengths



Bond angles

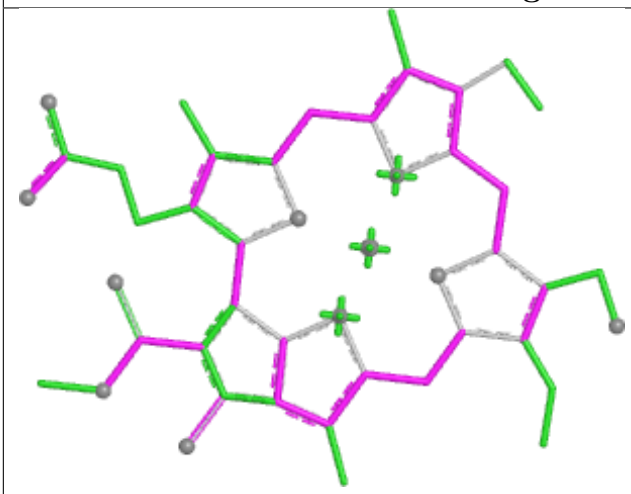


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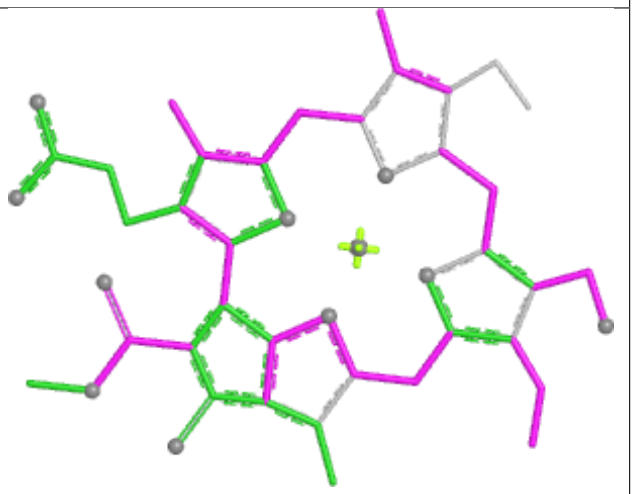


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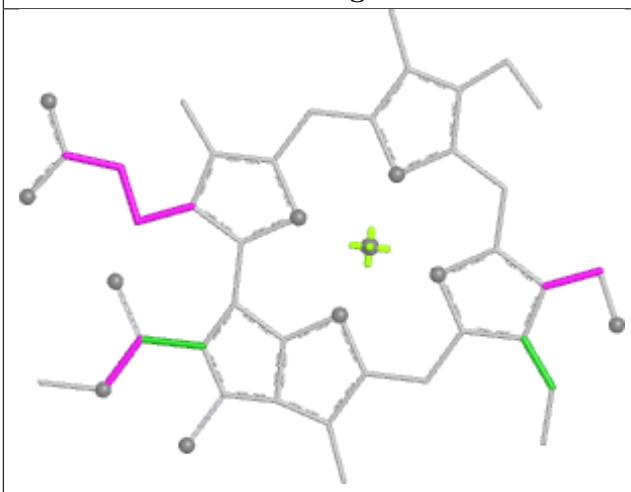
Ligand CHL U 607



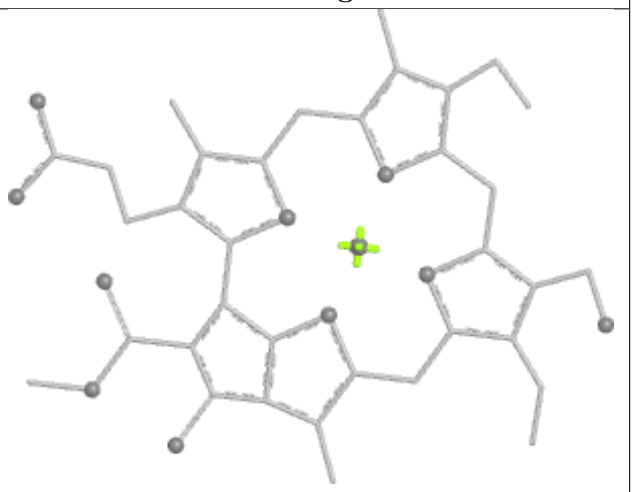
Bond lengths



Bond angles

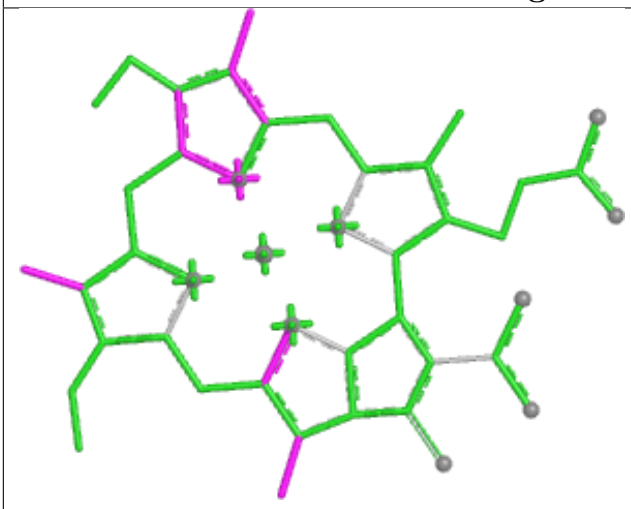


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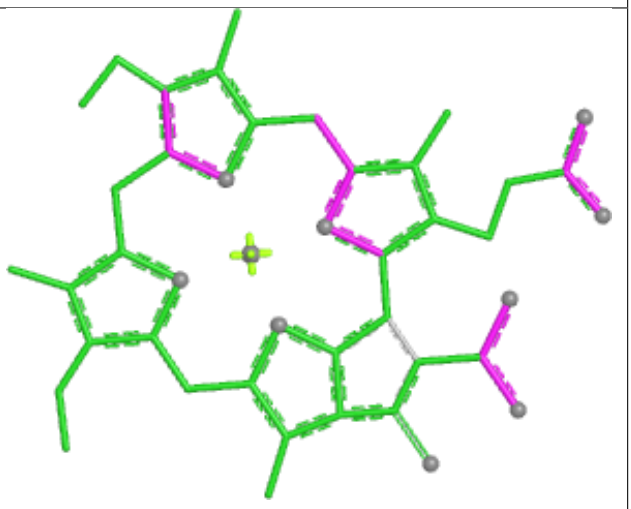


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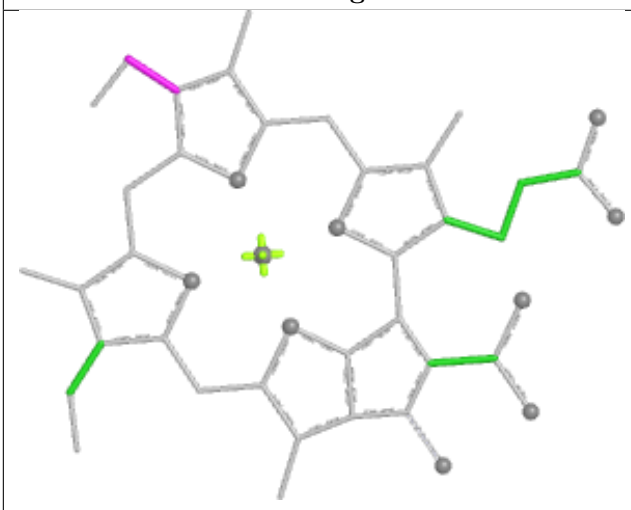
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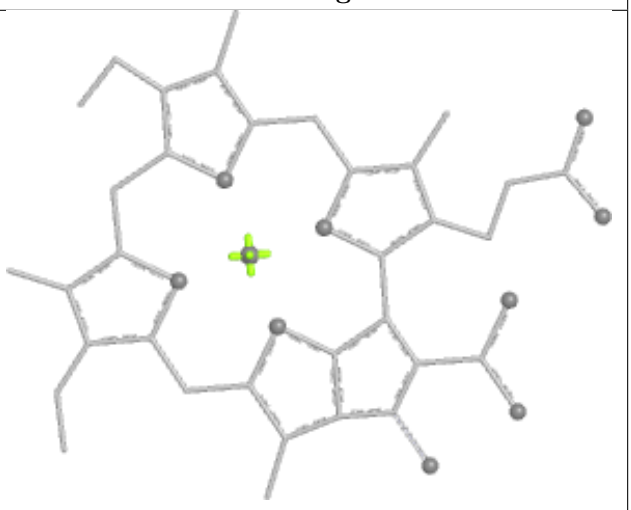
Bond lengths



Bond angles

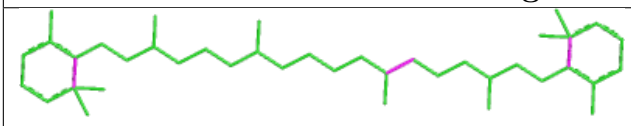


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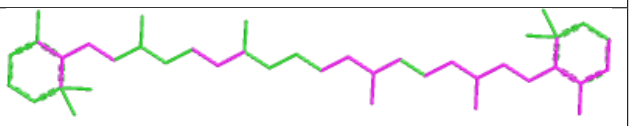


Rings

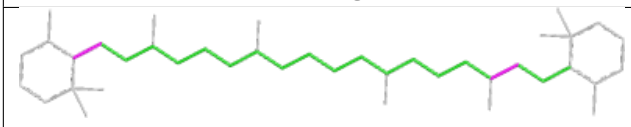
Ligand BCR A 848



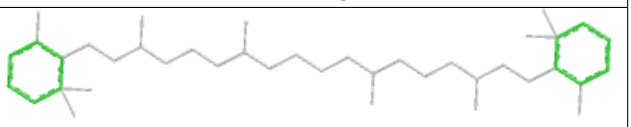
Bond lengths



Bond angles

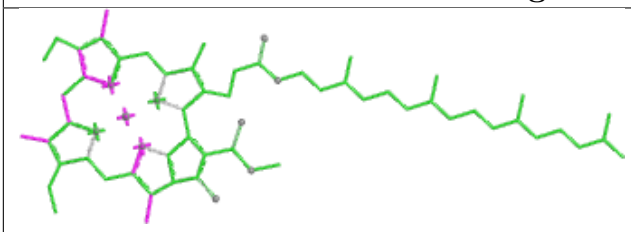


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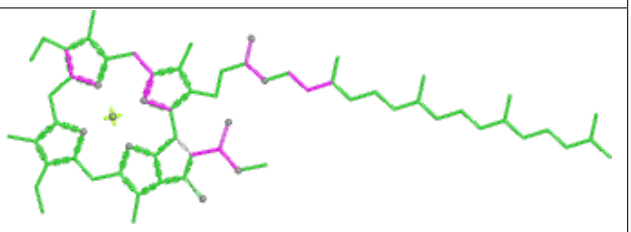


Rings

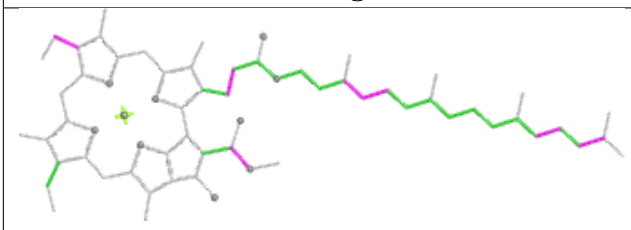
Ligand CLA 7 602



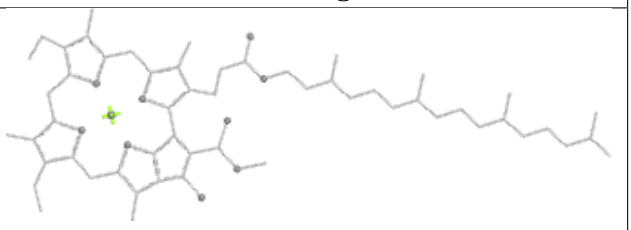
Bond lengths



Bond angles

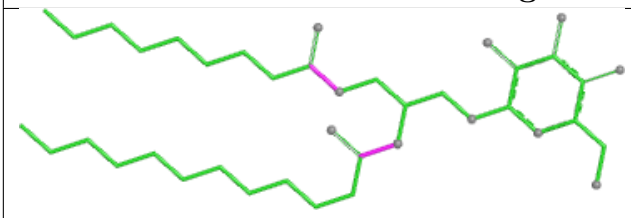


Torsions

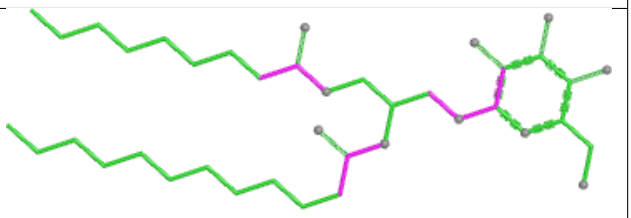


Rings

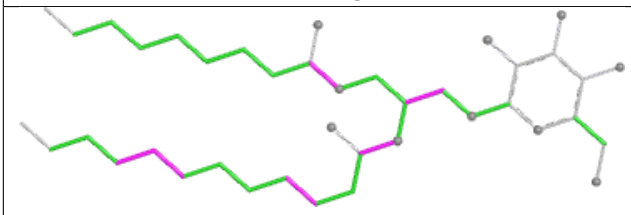
Ligand LMG A 860



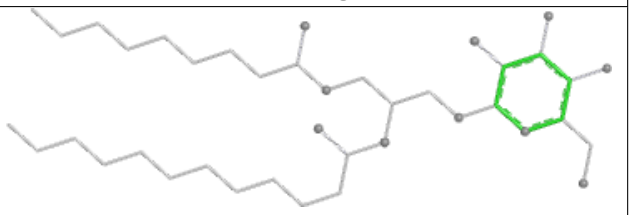
Bond lengths



Bond angles

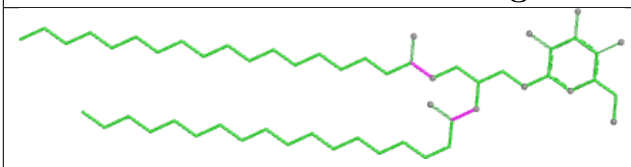


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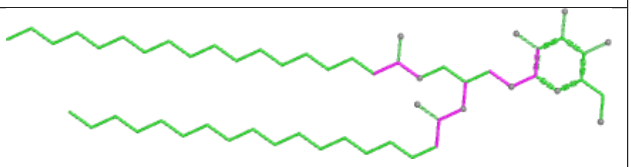


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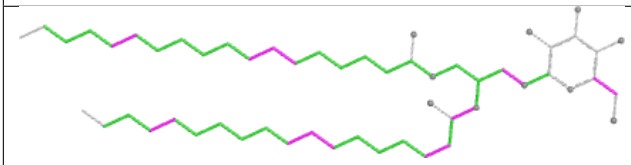
Ligand LMG V 2631



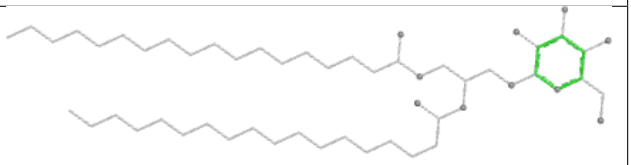
Bond lengths



Bond angles

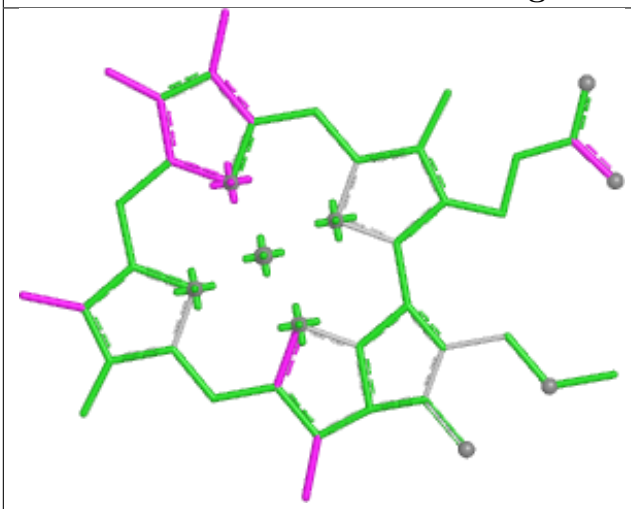


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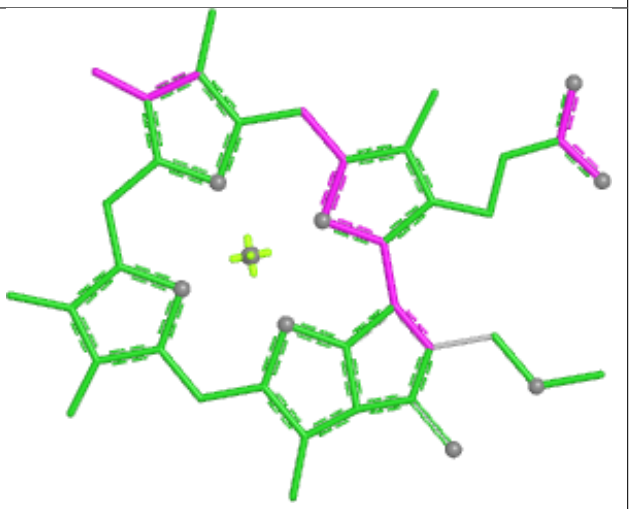


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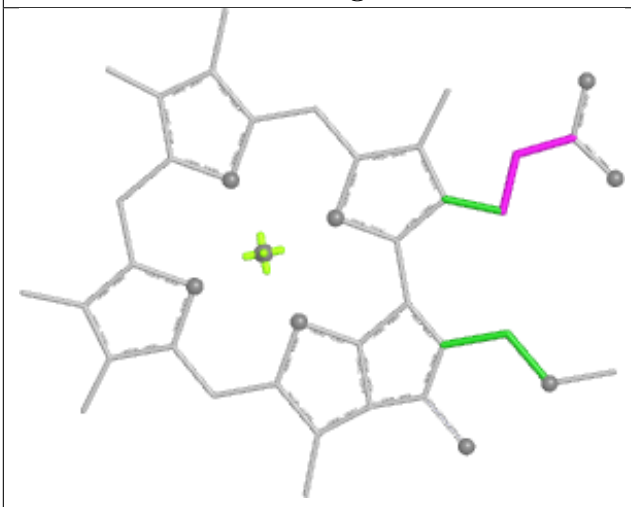
Ligand CLA 5 616



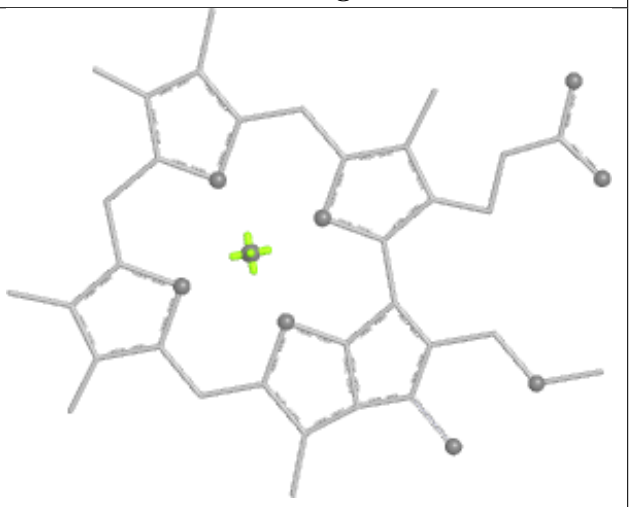
Bond lengths



Bond angles

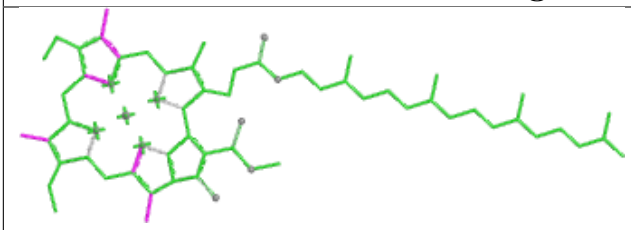


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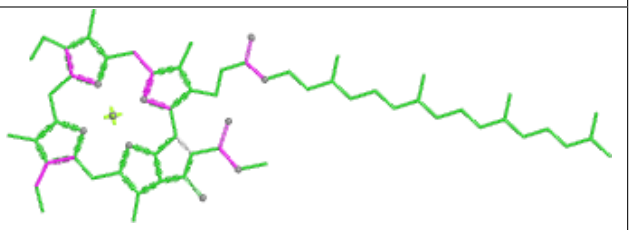


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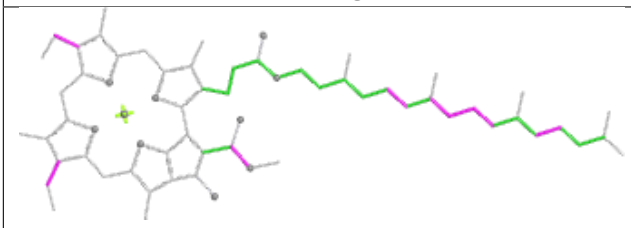
Ligand CLA 4 608



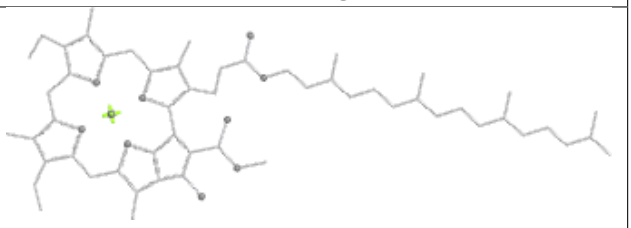
Bond lengths



Bond angles

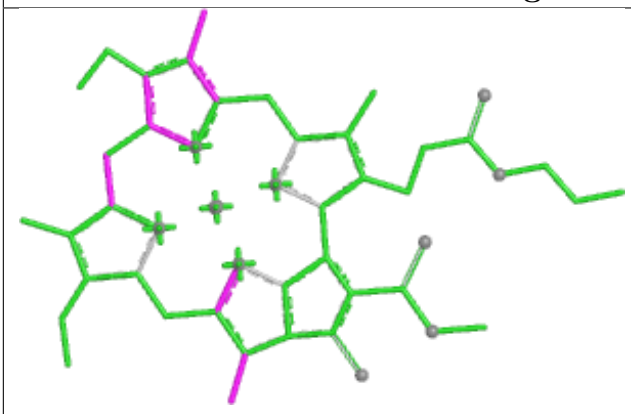


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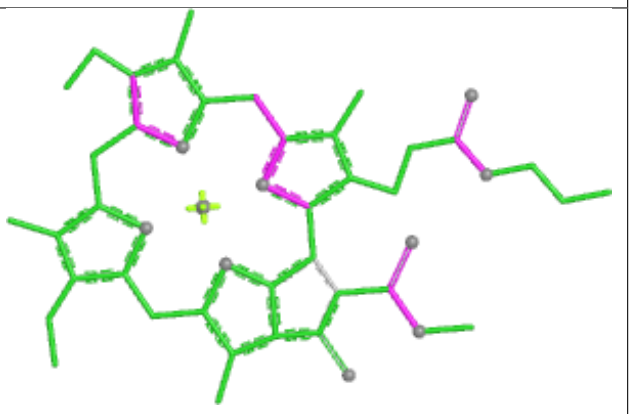


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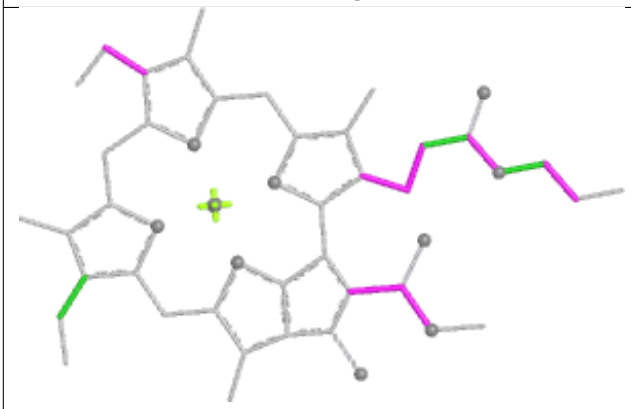
Ligand CLA Y 614



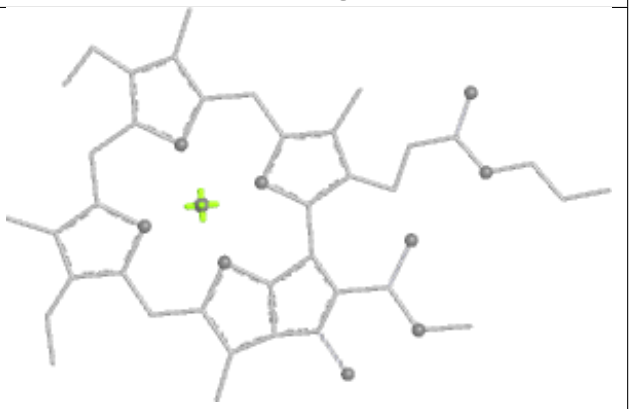
Bond lengths



Bond angles

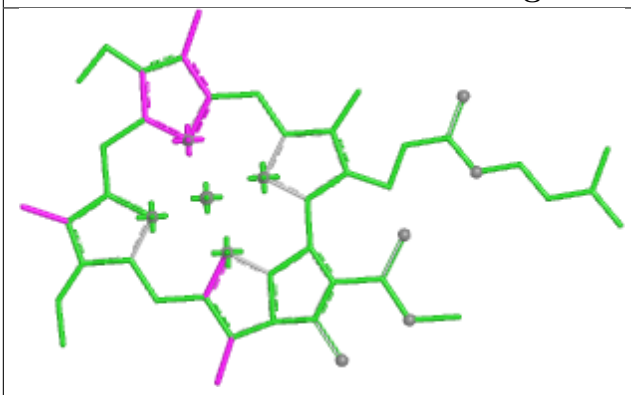


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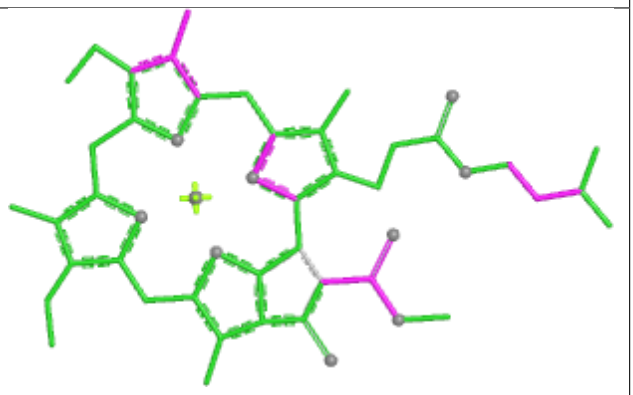


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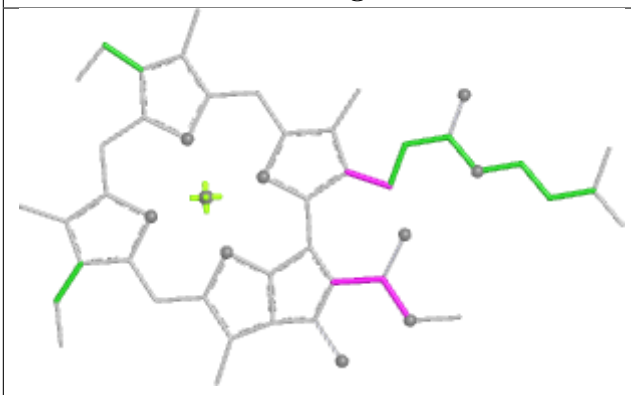
Ligand CLA A 845



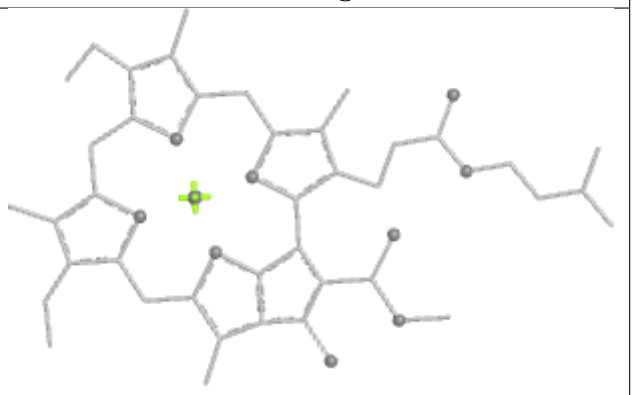
Bond lengths



Bond angles

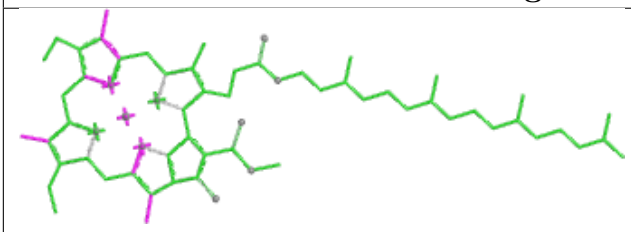


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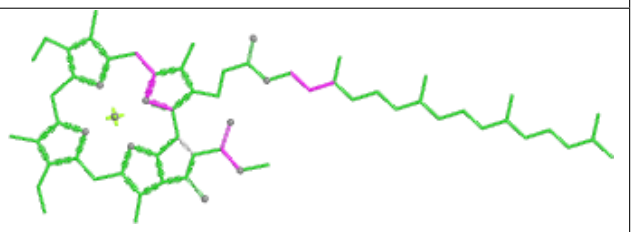


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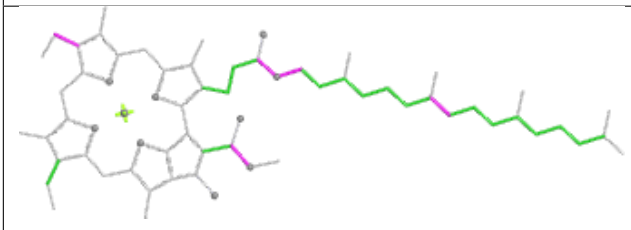
Ligand CLA B 840



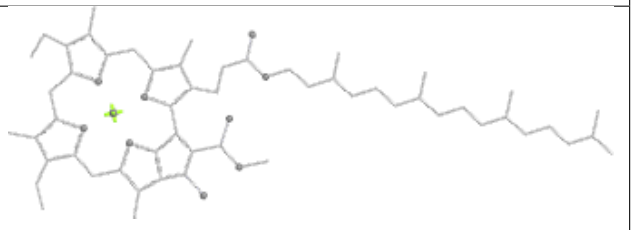
Bond lengths



Bond angles

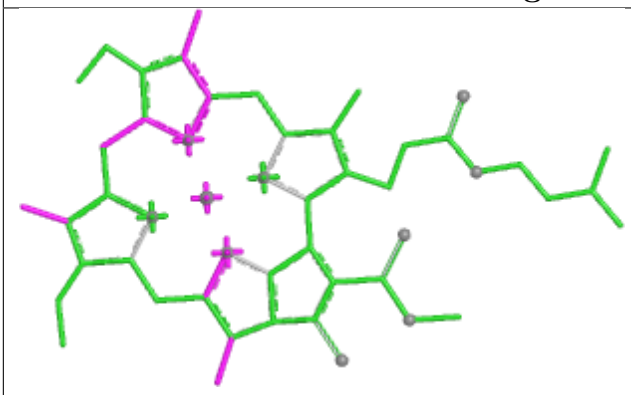


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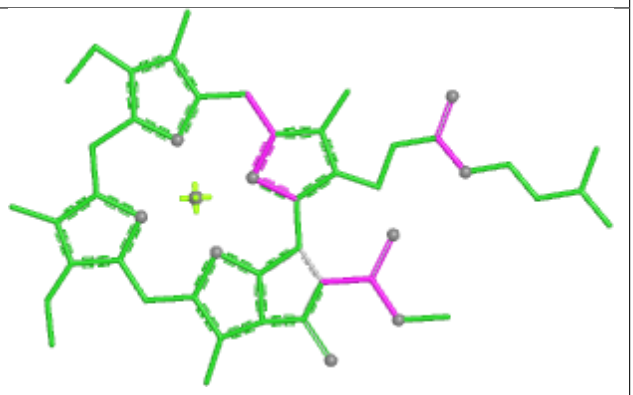


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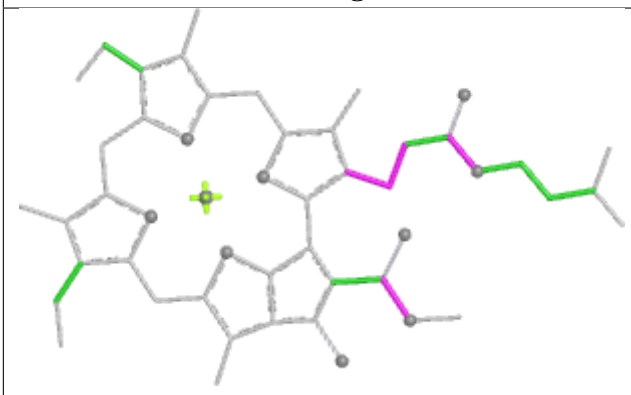
Ligand CLA A 838



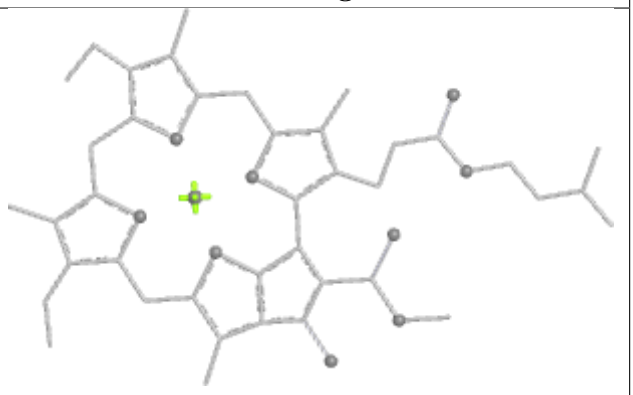
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Bond angles

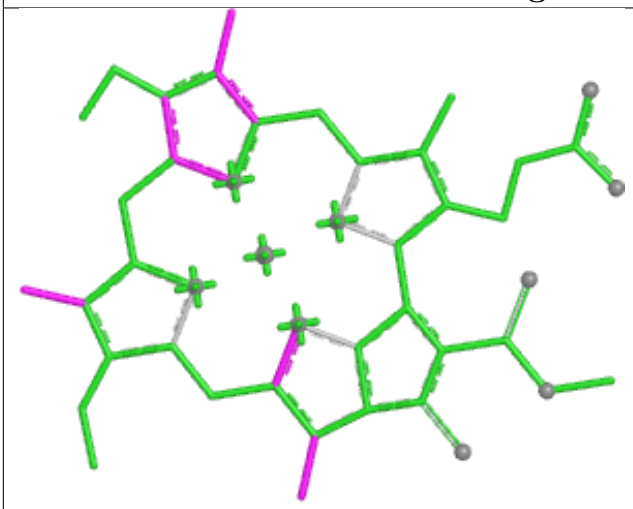


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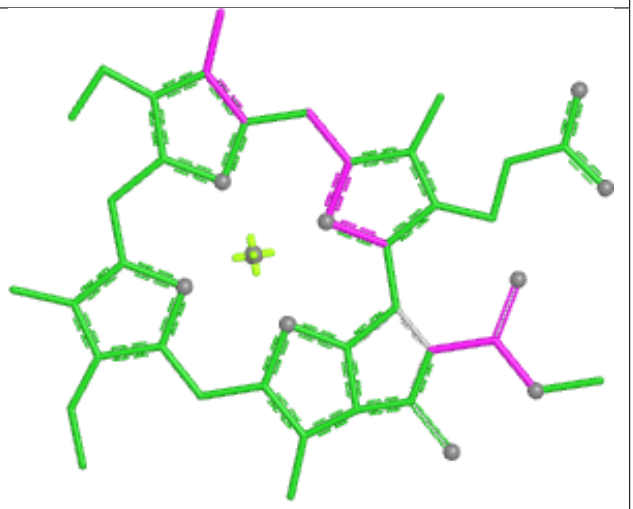


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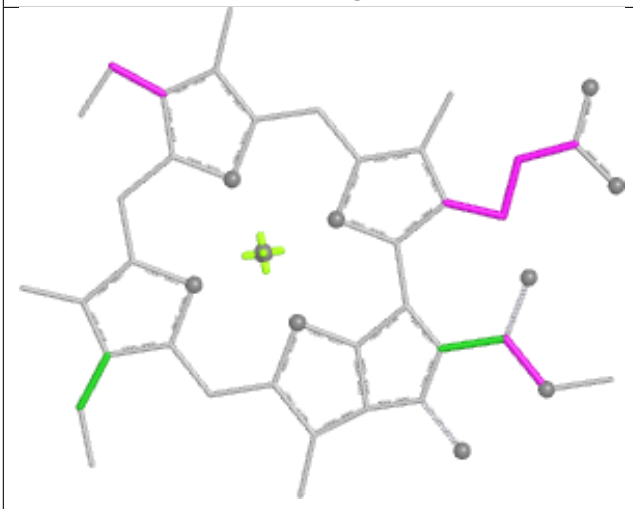
Ligand CLA 6 617



Bond lengths



Bond angles

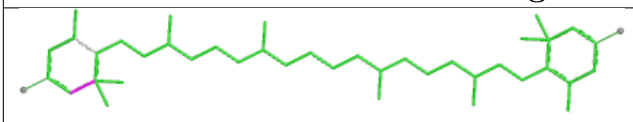


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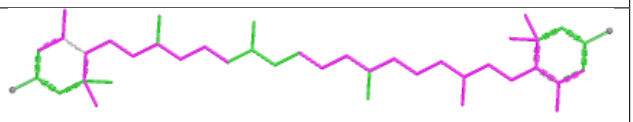


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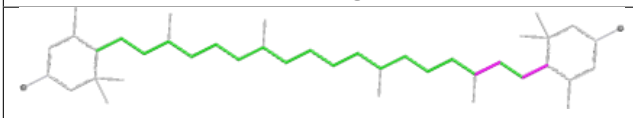
Ligand LUT 4 619



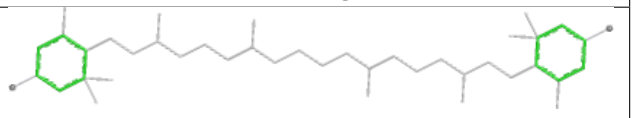
Bond lengths



Bond angles

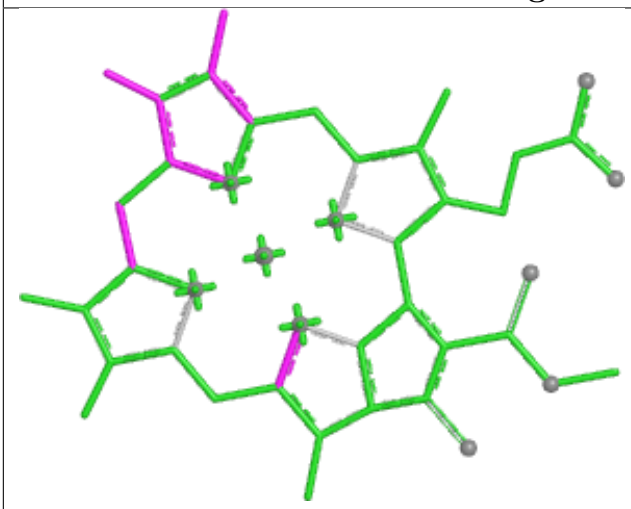


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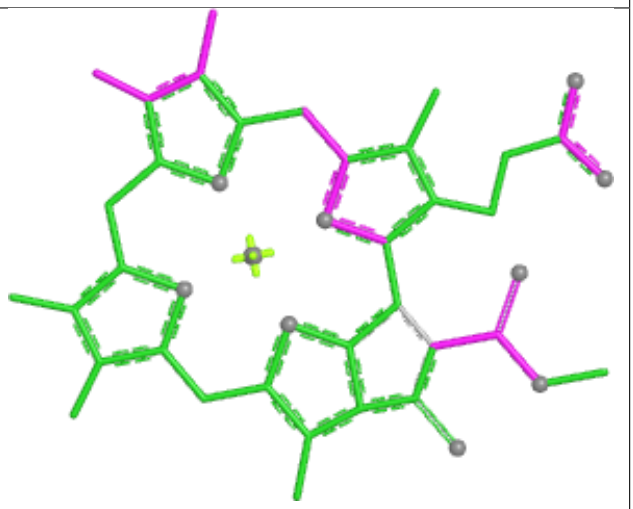


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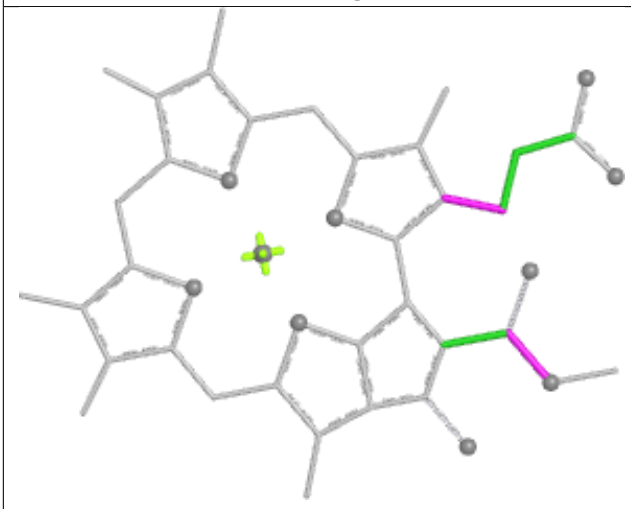
Ligand CLA 8 616



Bond lengths



Bond angles

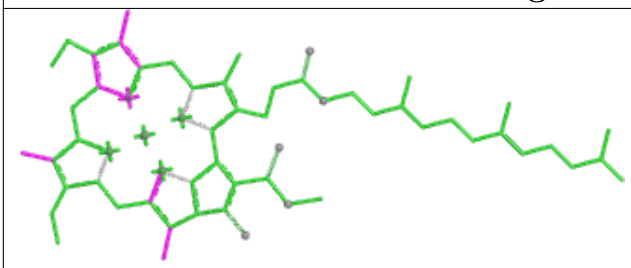


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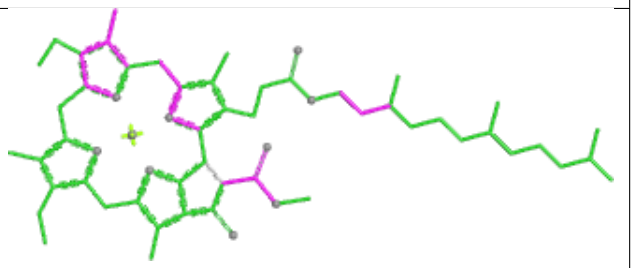


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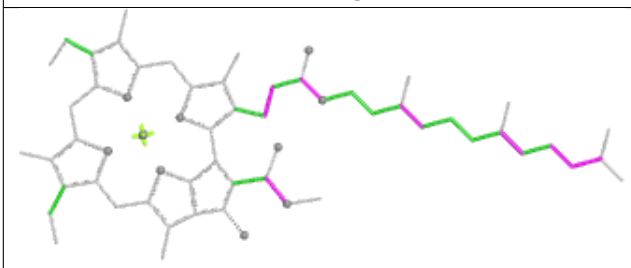
Ligand CLA 8 602



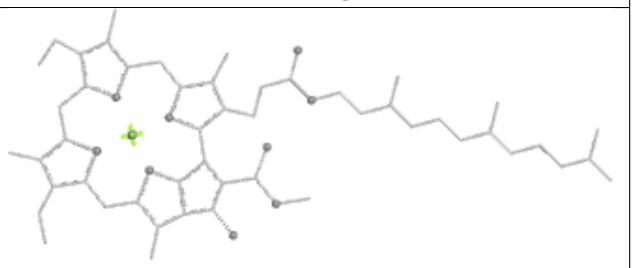
Bond lengths



Bond angles

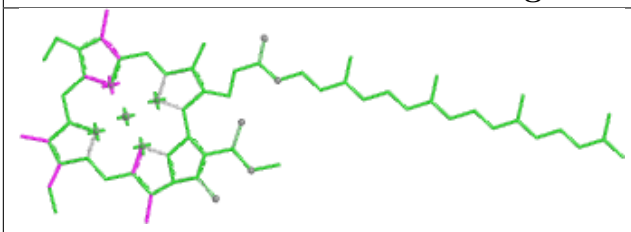


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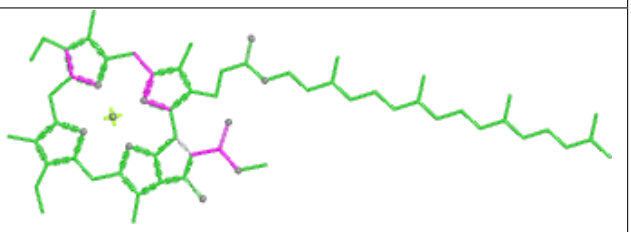


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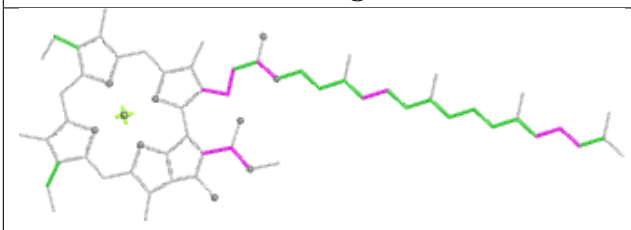
Ligand CLA B 809



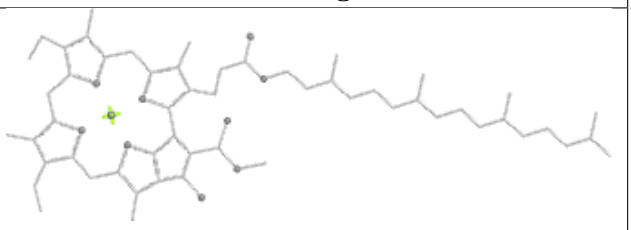
Bond lengths



Bond angles

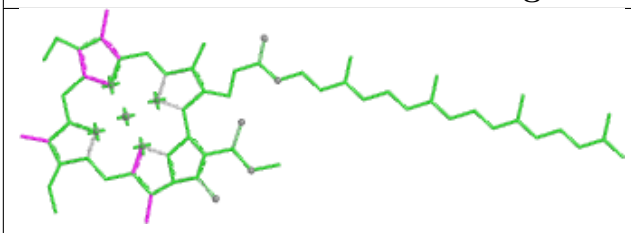


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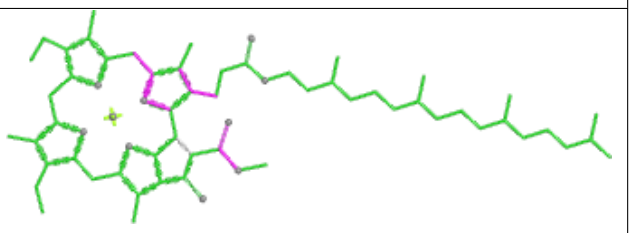


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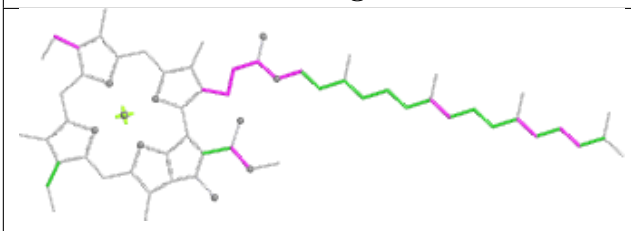
Ligand CLA H 203



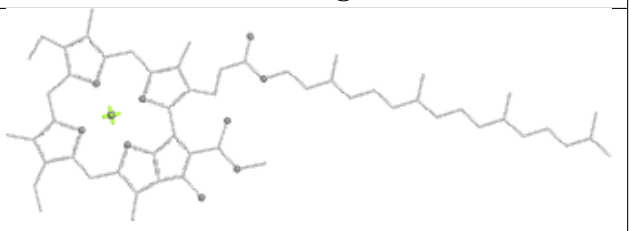
Bond lengths



Bond angles

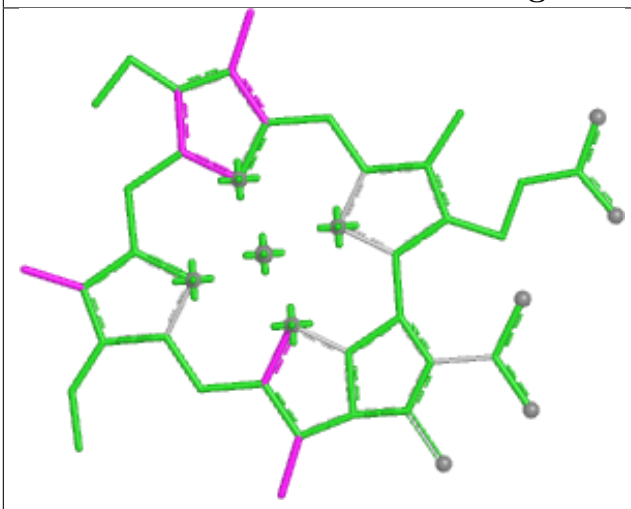


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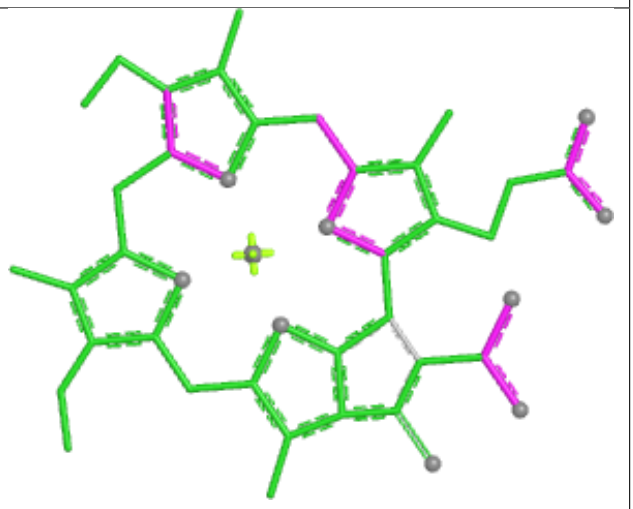


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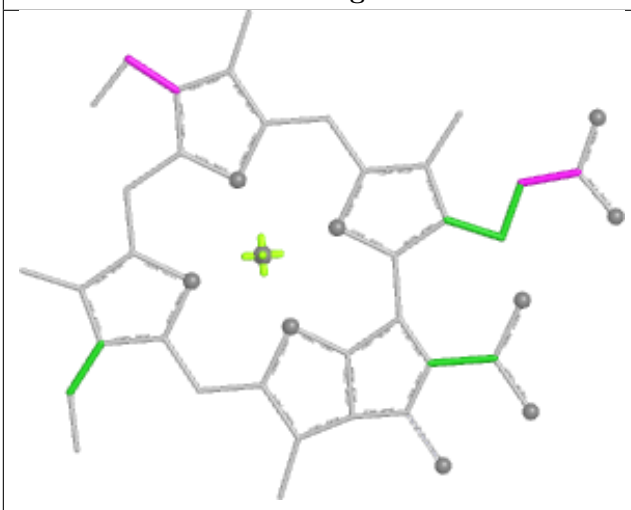
Ligand CLA a 608



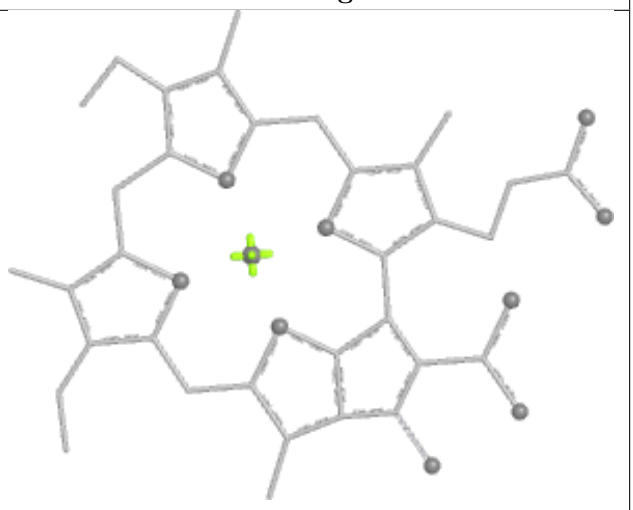
Bond lengths



Bond angles

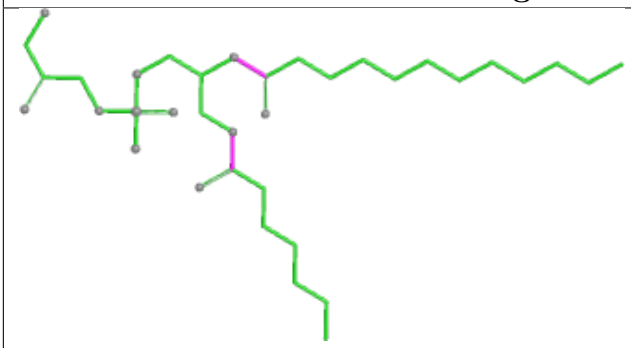


Torsions

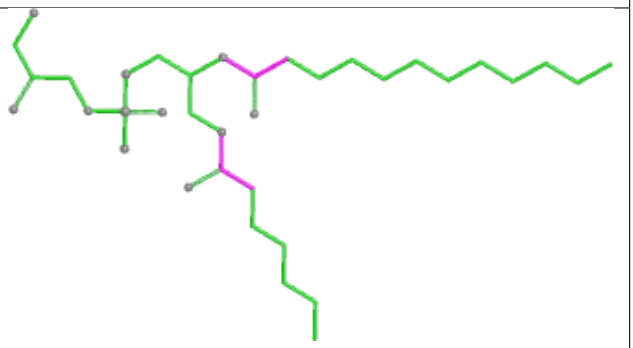


Rings

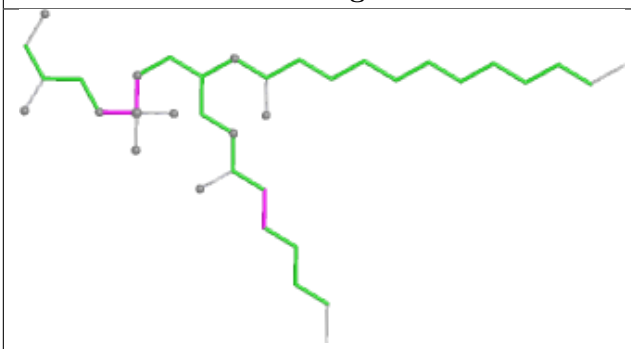
Ligand LHG V 2630



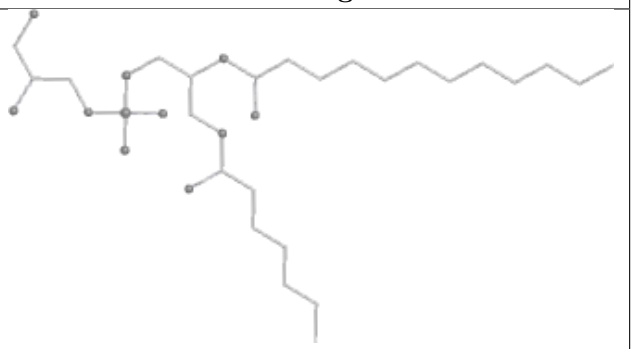
Bond lengths



Bond angles

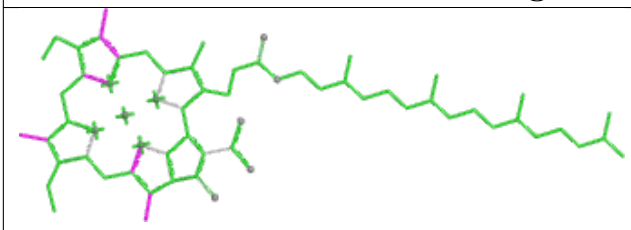


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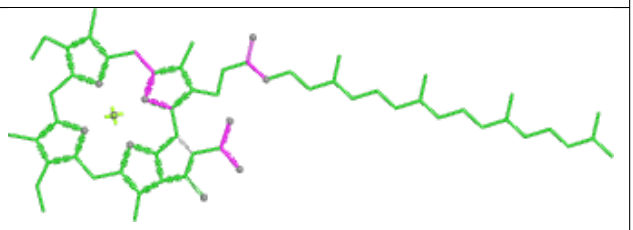


Rings

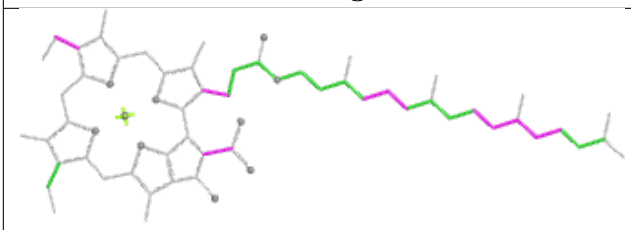
Ligand CLA a 609



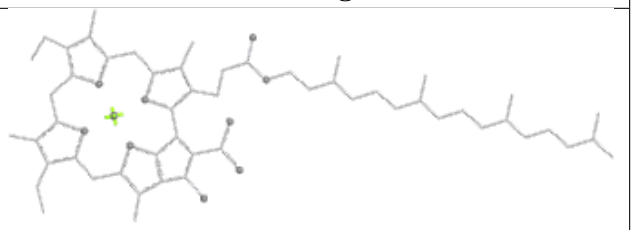
Bond lengths



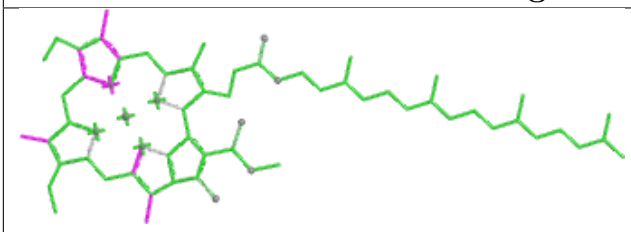
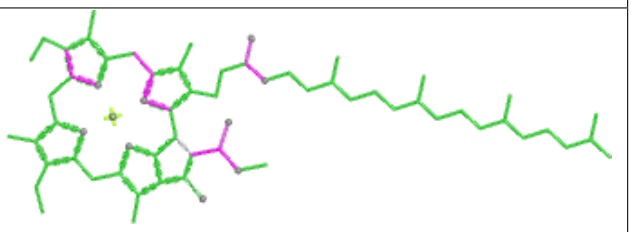
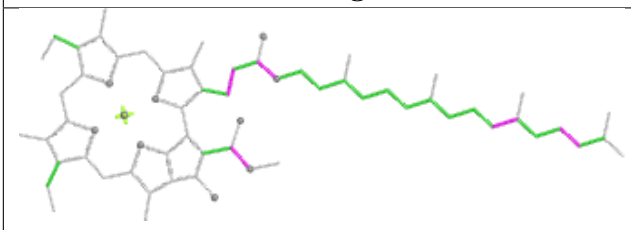
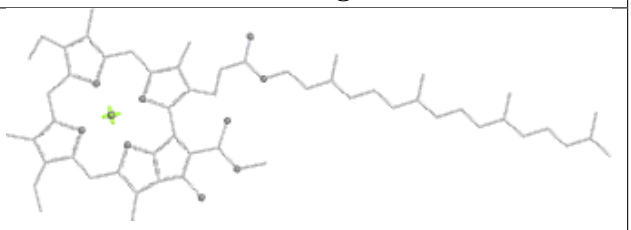
Bond angles

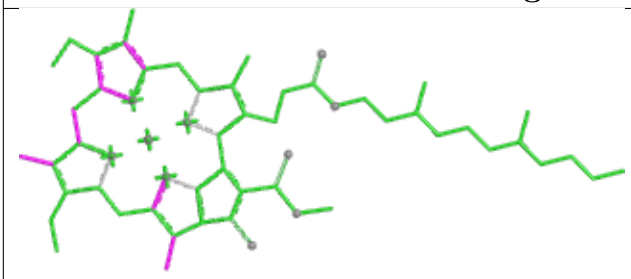
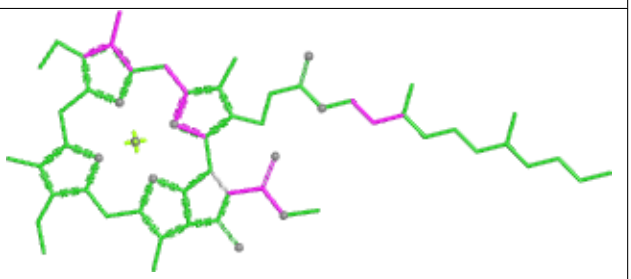
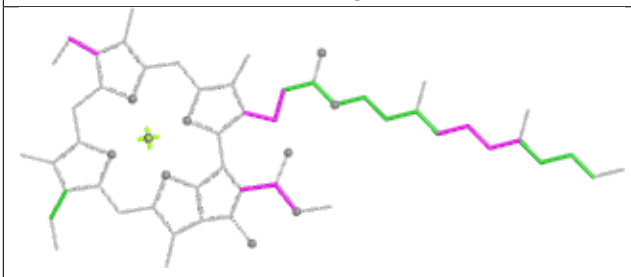
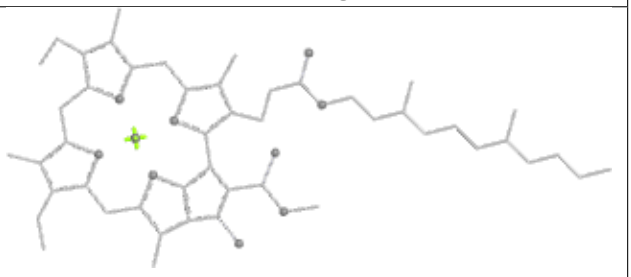


Torsions

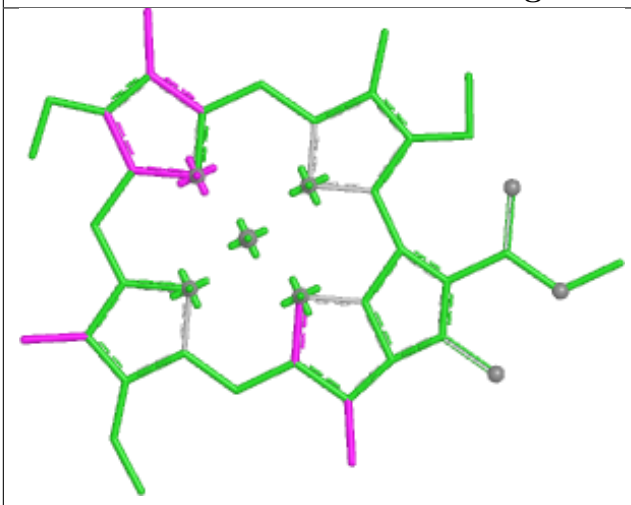


Rings

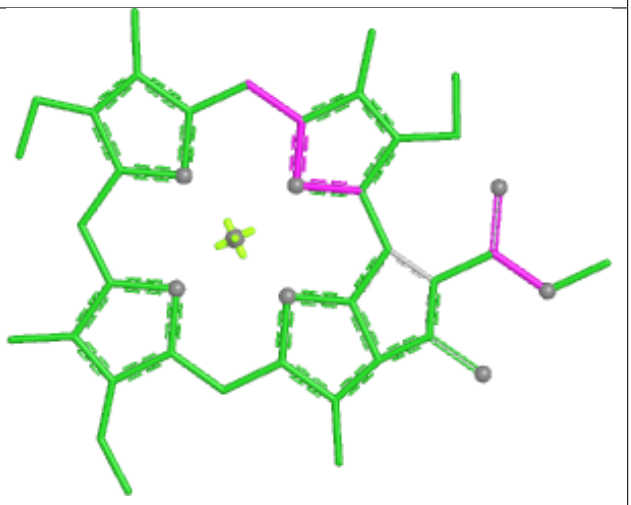
Ligand CLA 6 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Y 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

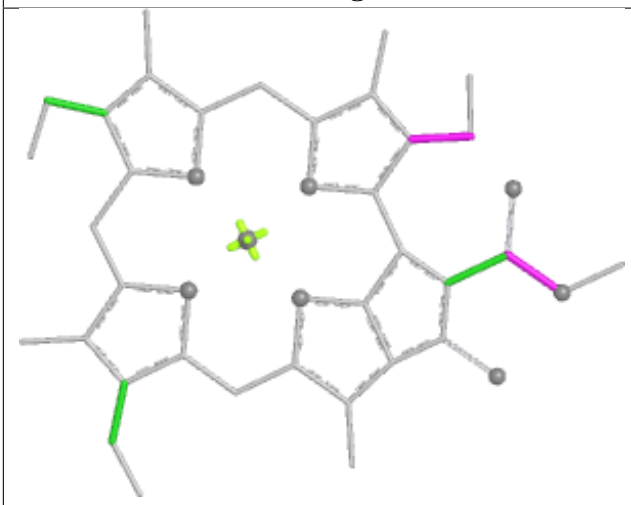
Ligand CLA B 822



Bond lengths



Bond angles

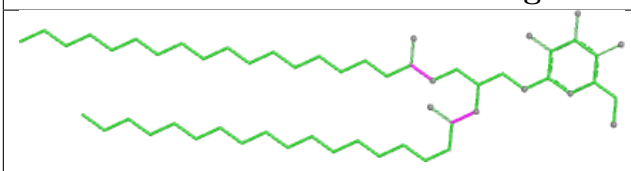


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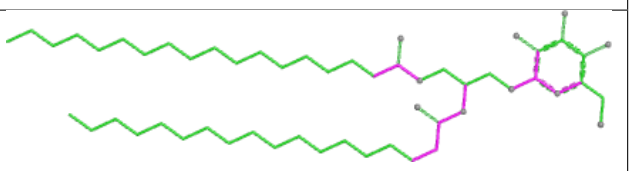


Rings

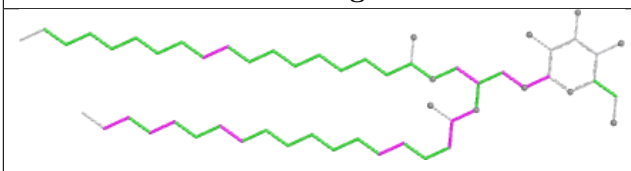
Ligand LMG 9 625



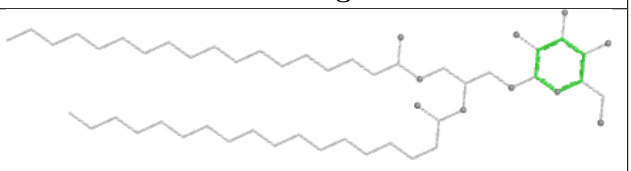
Bond lengths



Bond angles

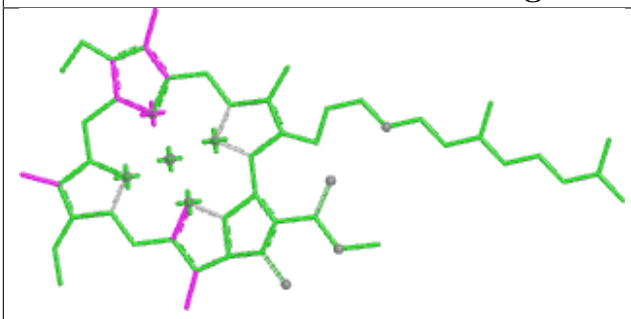


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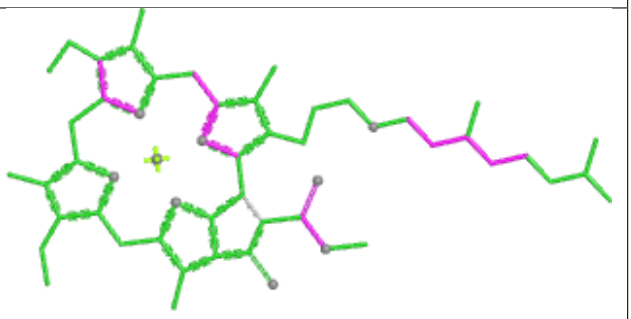


Rings

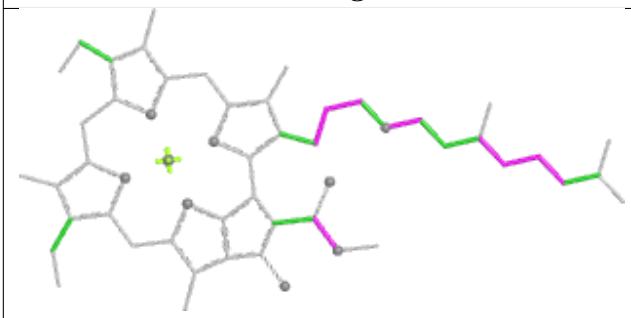
Ligand CLA B 816



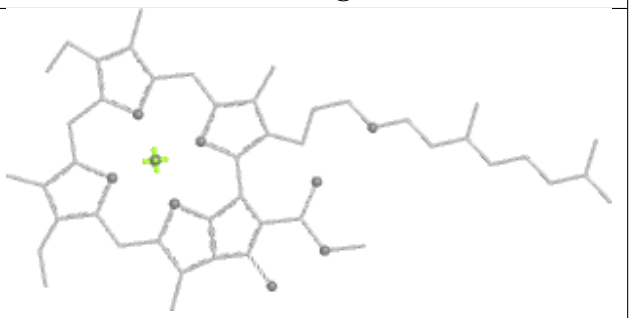
Bond lengths



Bond angles

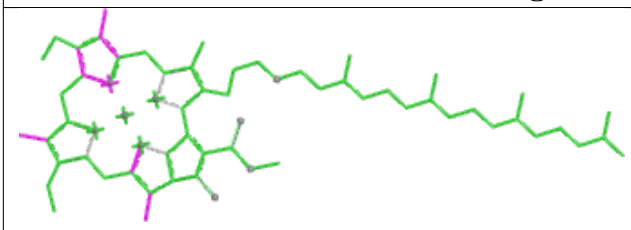


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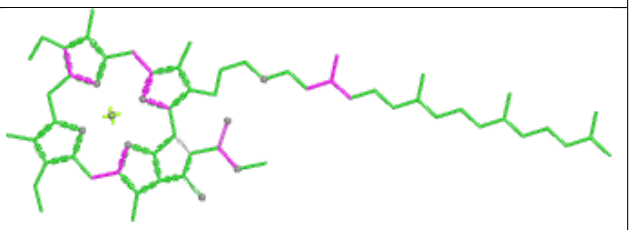


Rings

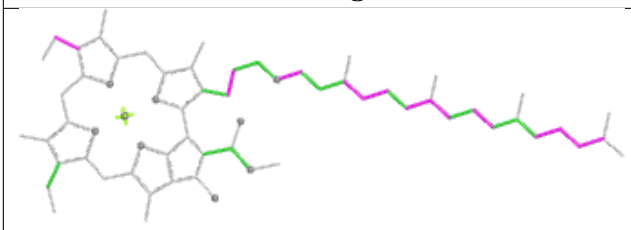
Ligand CLA 5 613



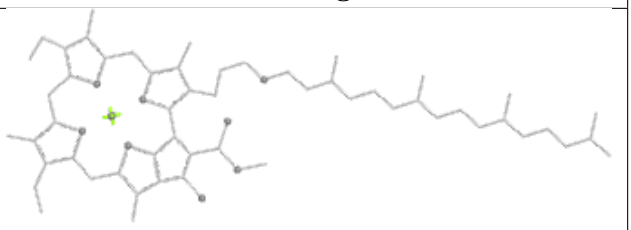
Bond lengths



Bond angles

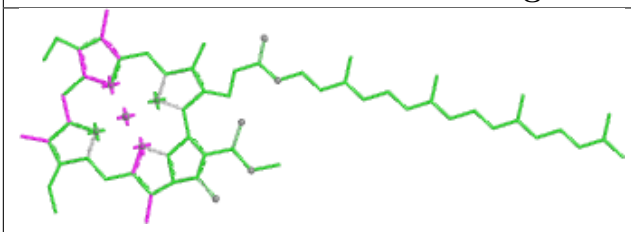


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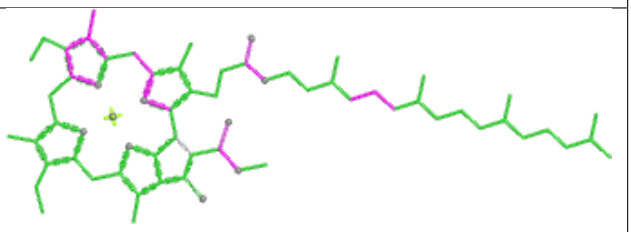


Rings

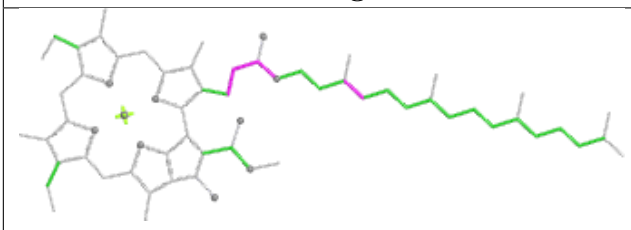
Ligand CLA A 822



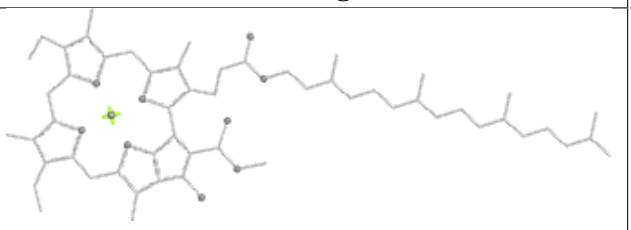
Bond lengths



Bond angles

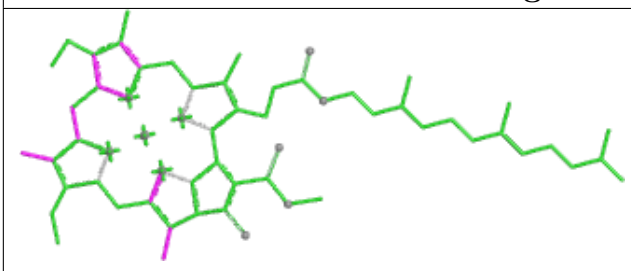


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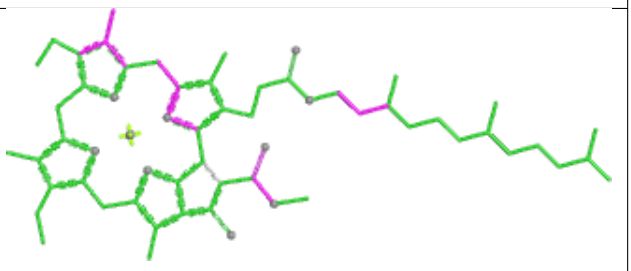


Rings

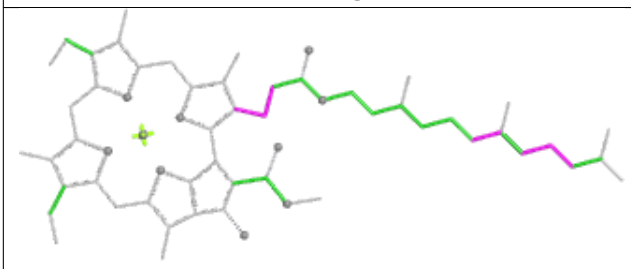
Ligand CLA V 602



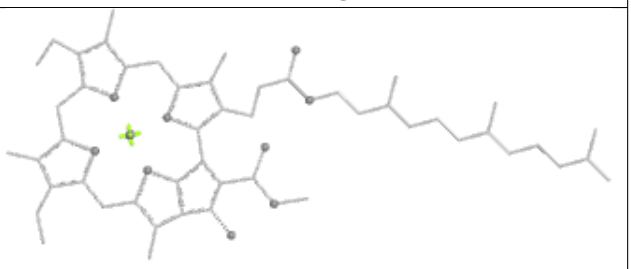
Bond lengths



Bond angles

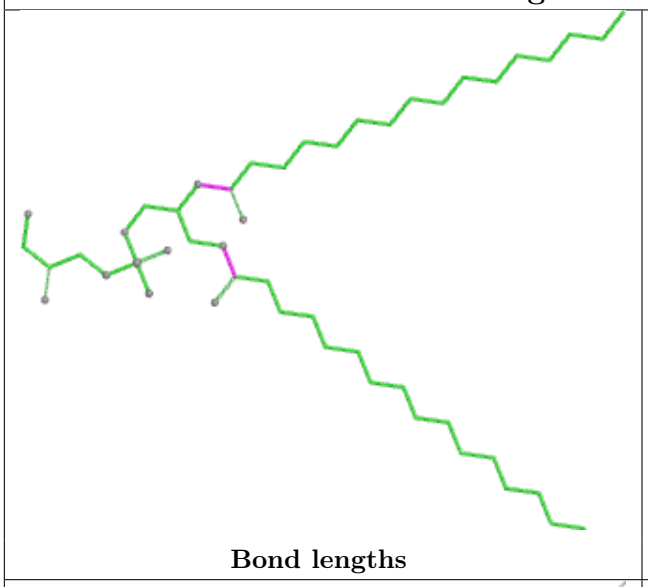


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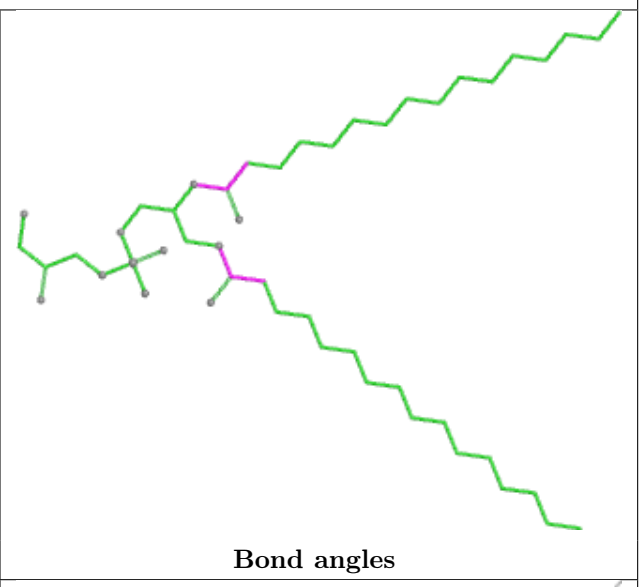


Rings

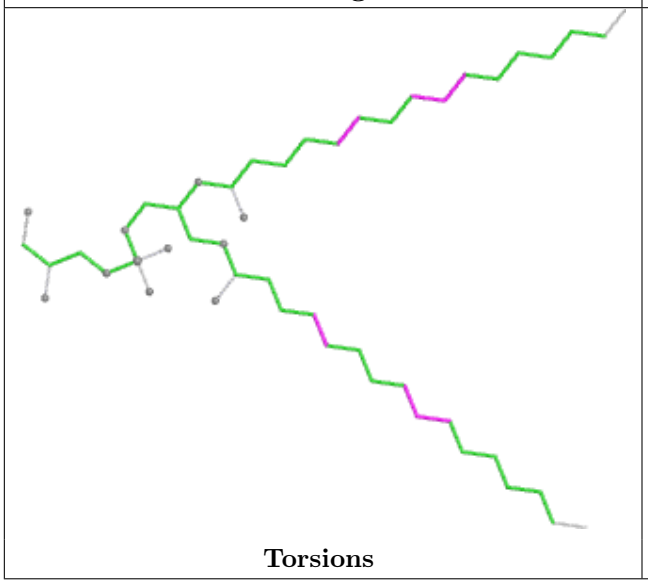
Ligand LHG 4 622



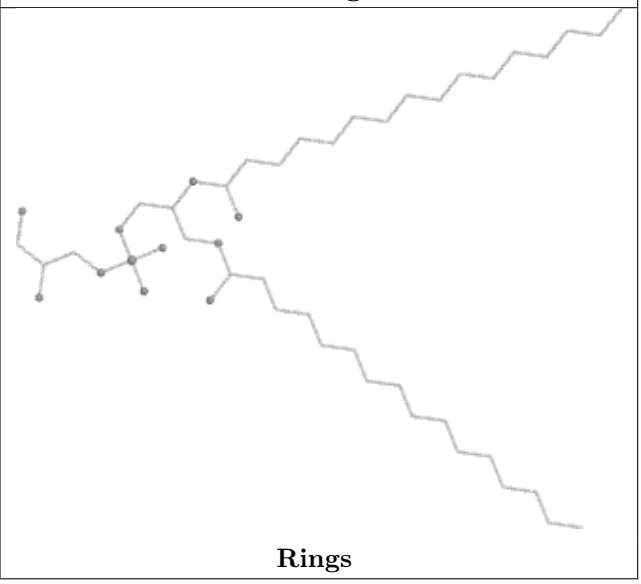
Bond lengths



Bond angles

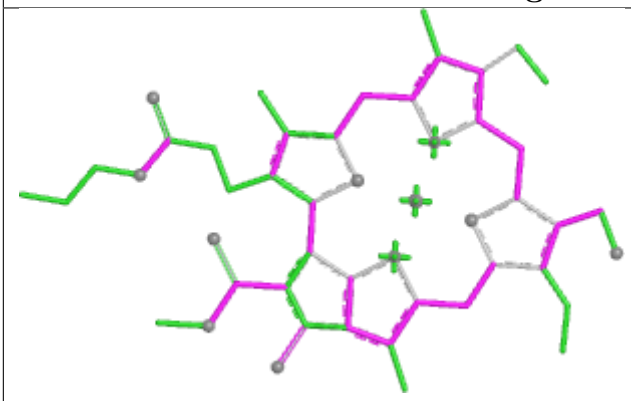


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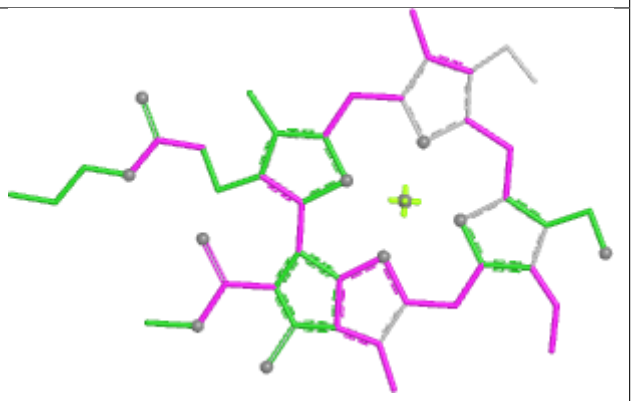


Rings

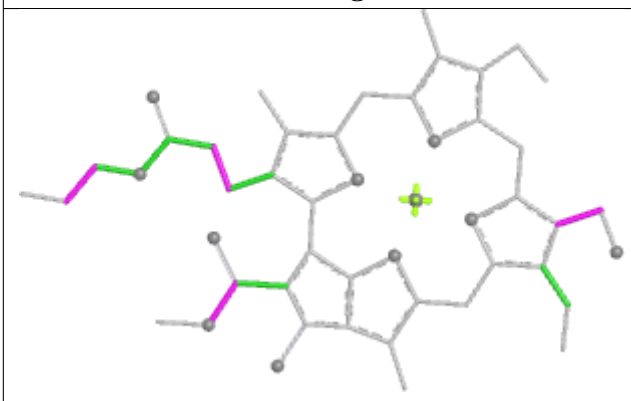
Ligand CHL Z 608



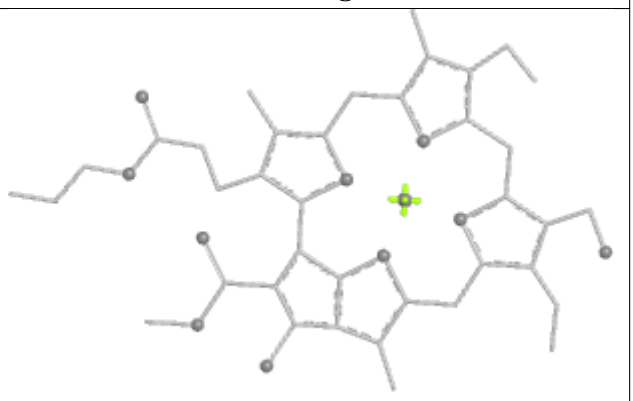
Bond lengths



Bond angles

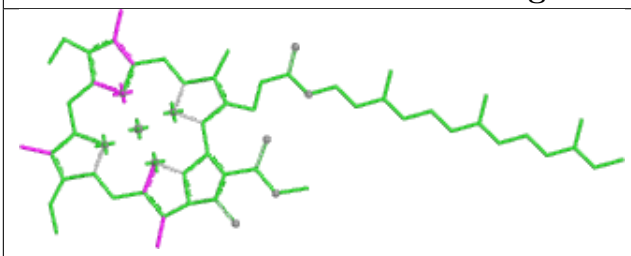


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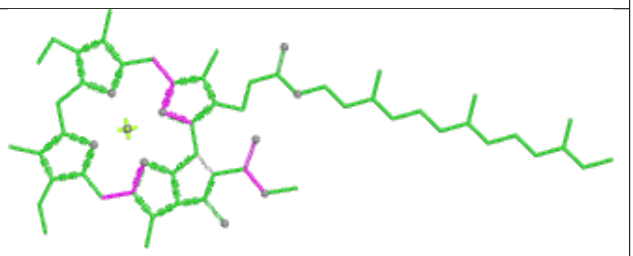


Rings

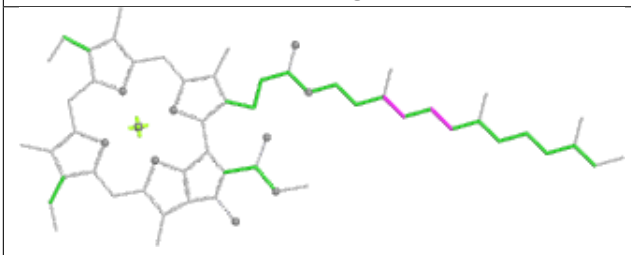
Ligand CLA 9 609



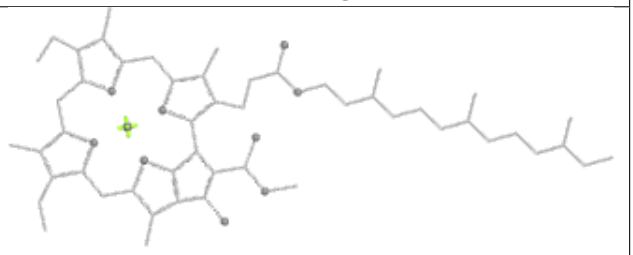
Bond lengths



Bond angles

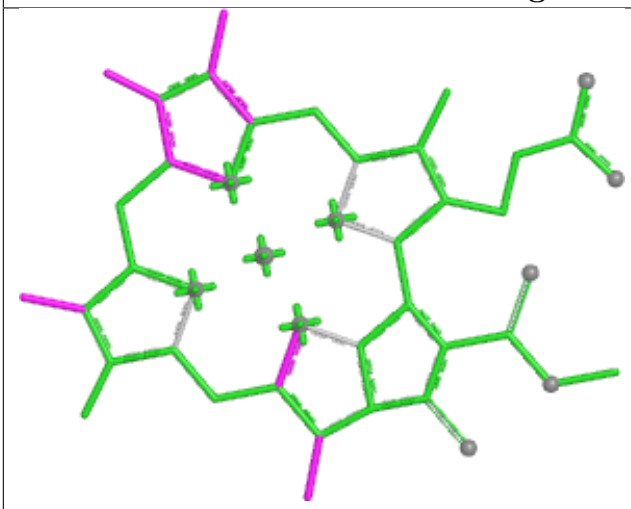


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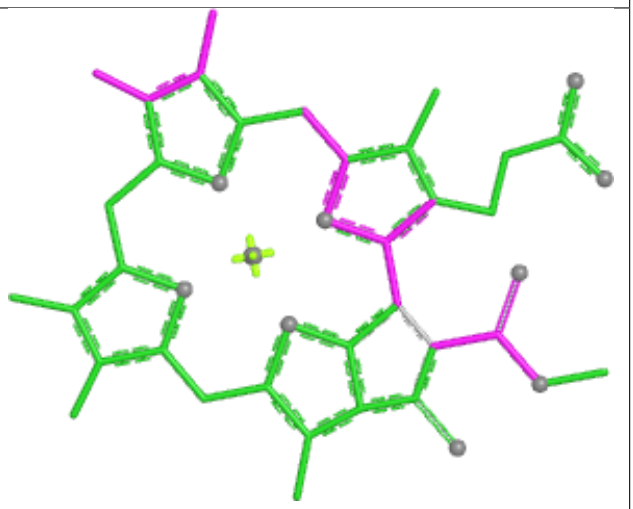


Rings

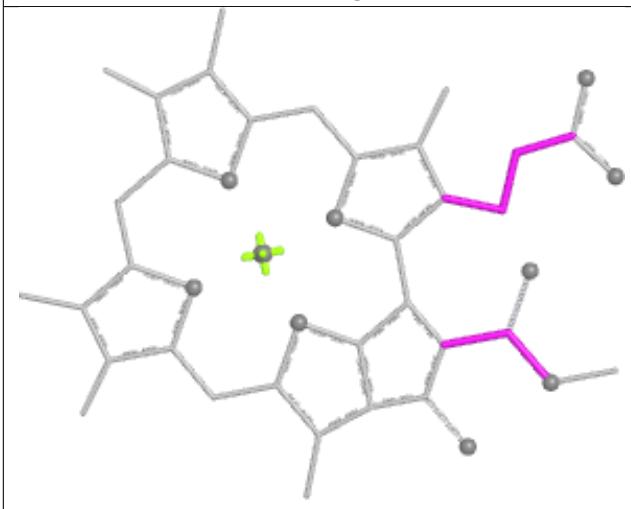
Ligand CLA 5 619



Bond lengths



Bond angles

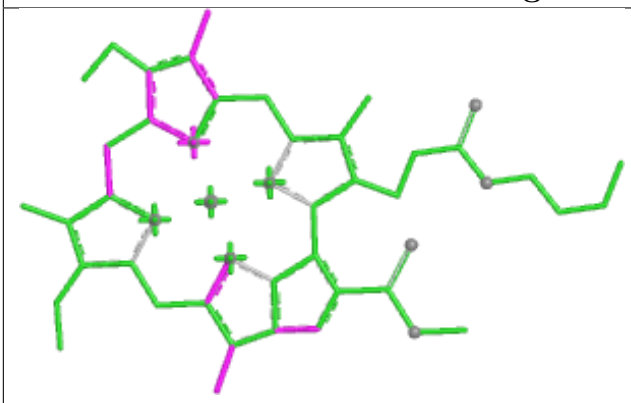


Torsions

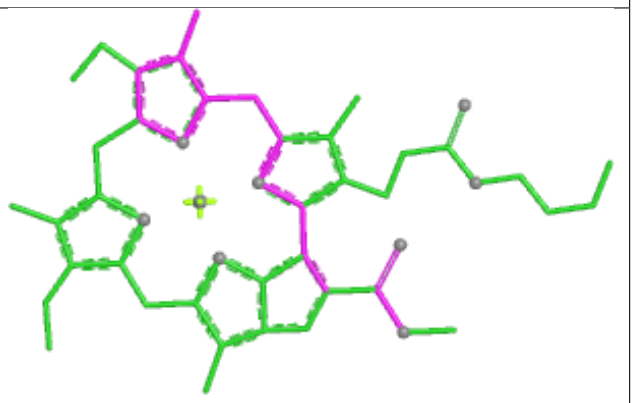


Rings

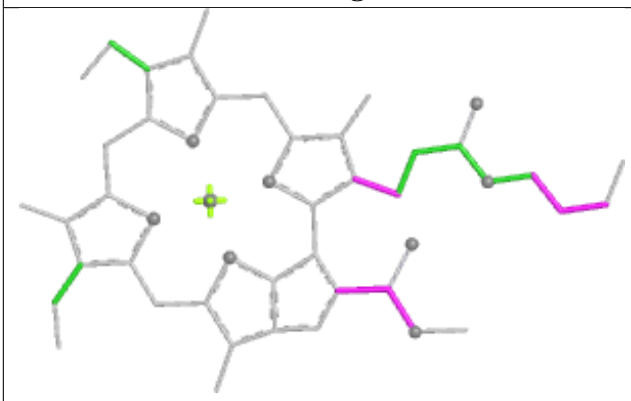
Ligand CLA U 604



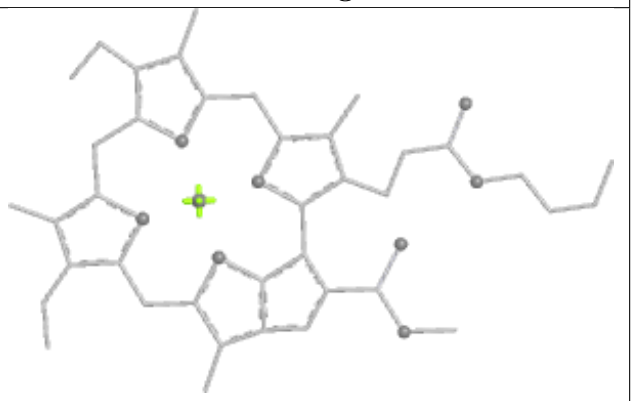
Bond lengths



Bond angles

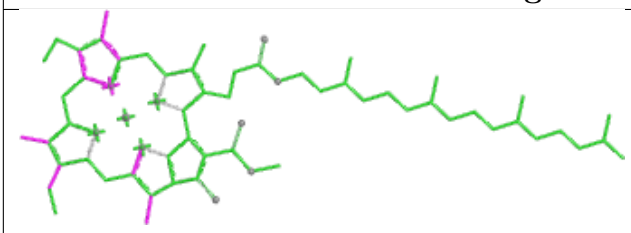


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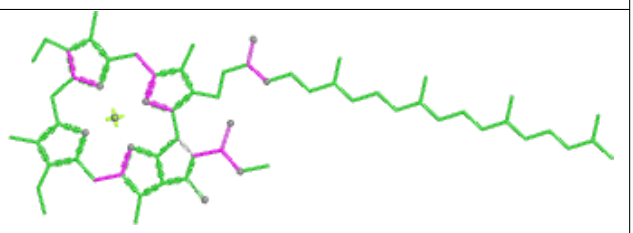


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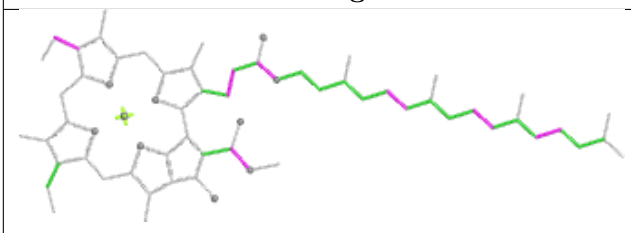
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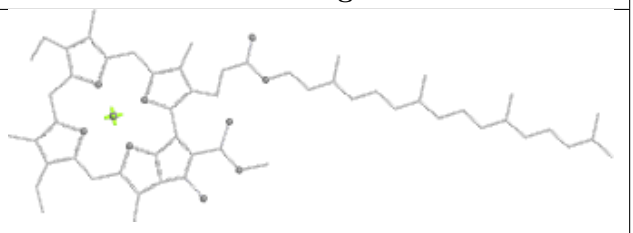
Bond lengths



Bond angles

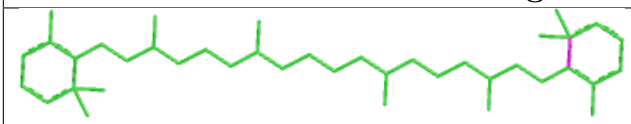


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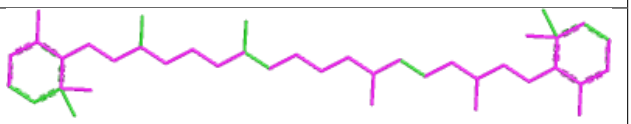


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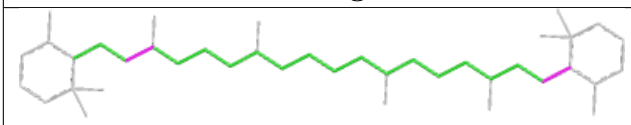
Ligand BCR 2 623



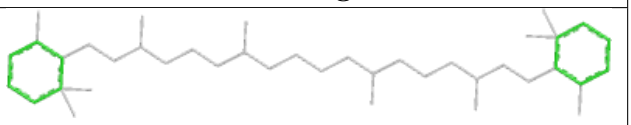
Bond lengths



Bond angles

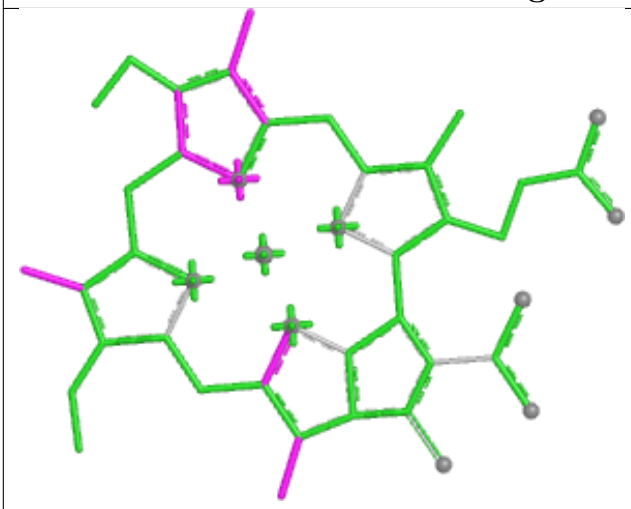


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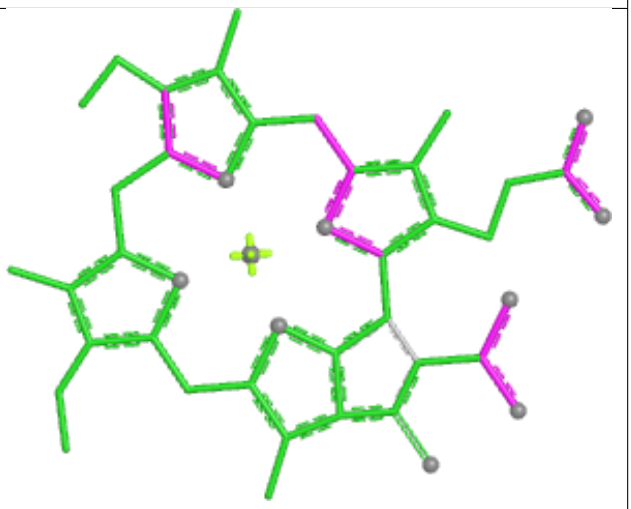


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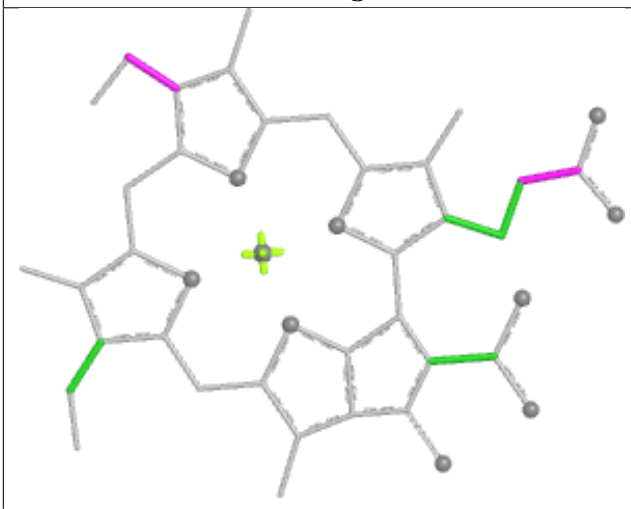
Ligand CLA 1 608



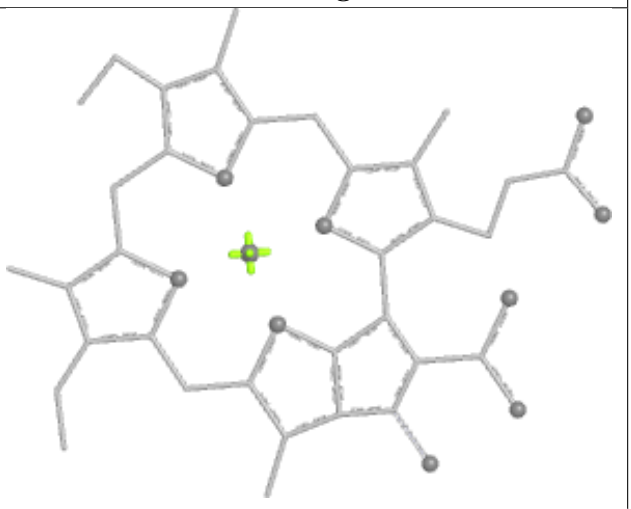
Bond lengths



Bond angles

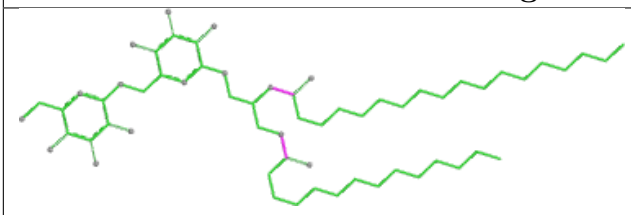


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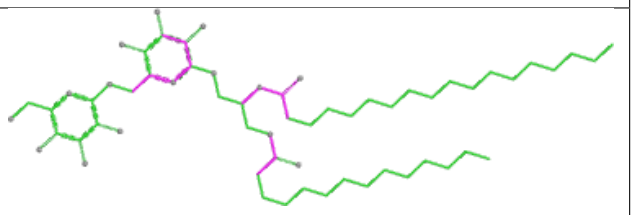


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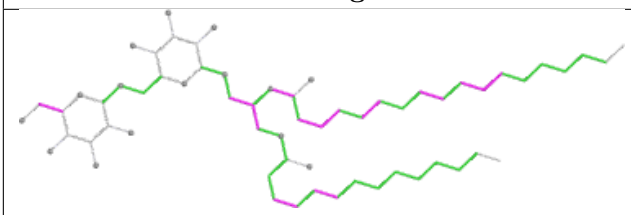
Ligand DGD B 850



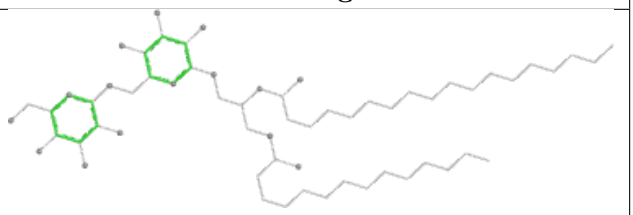
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Bond angles

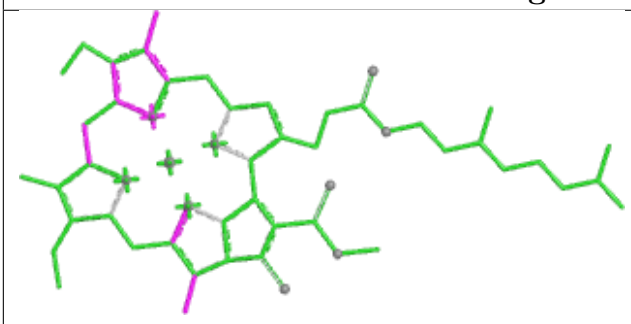


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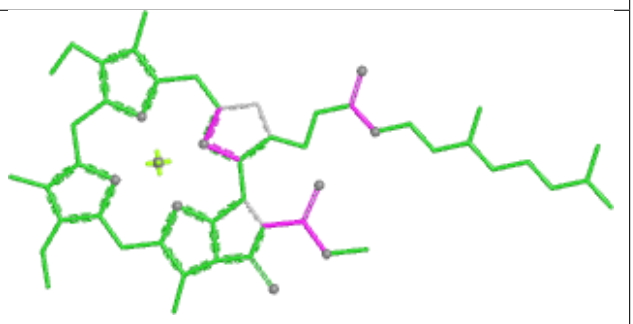


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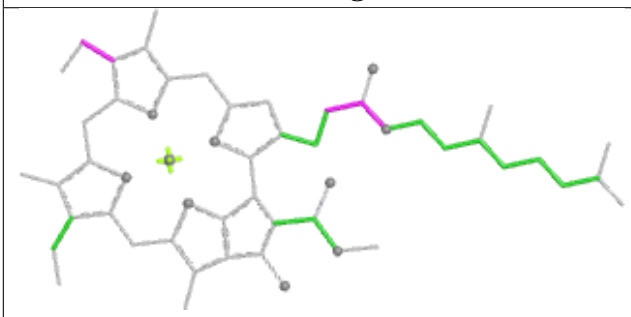
Ligand CLA a 614



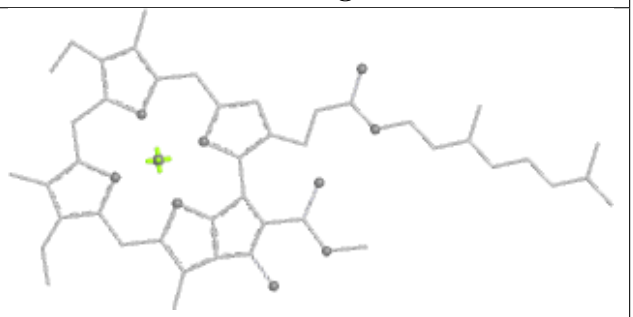
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Bond angles

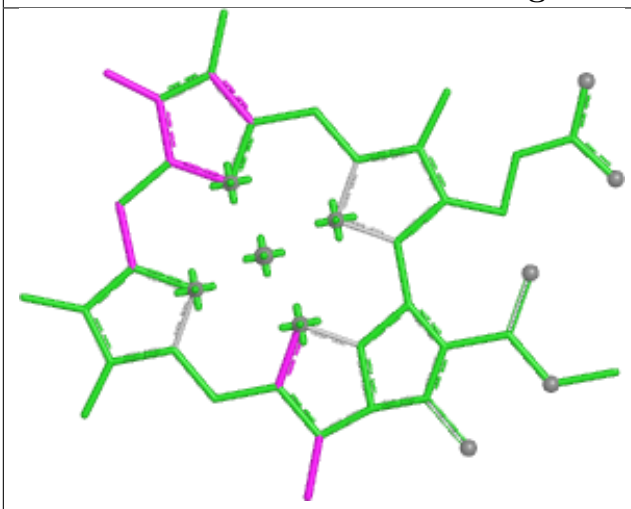


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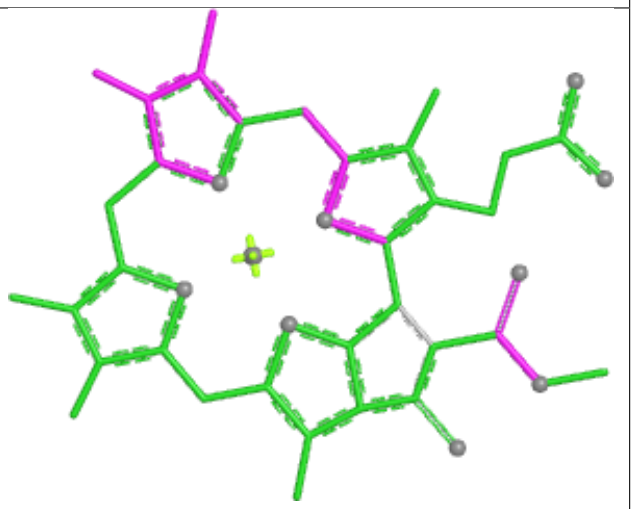


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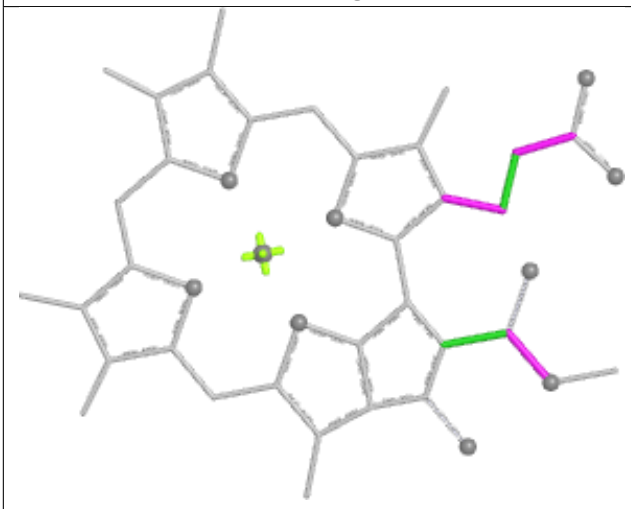
Ligand CLA 1 616



Bond lengths



Bond angles

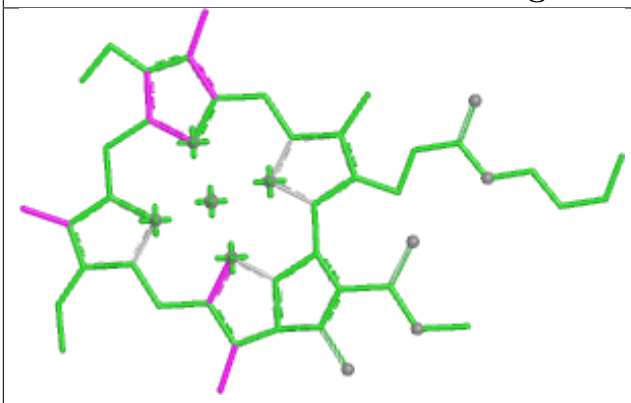


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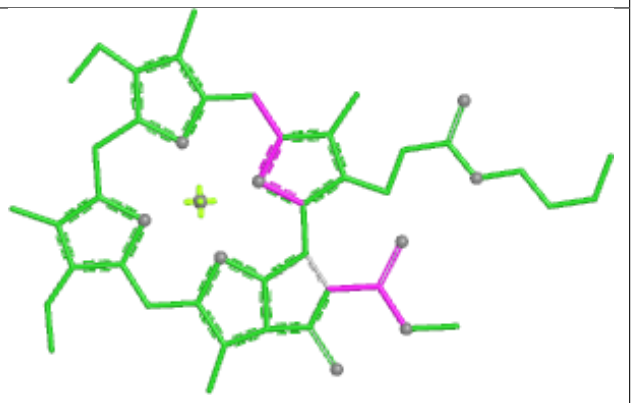


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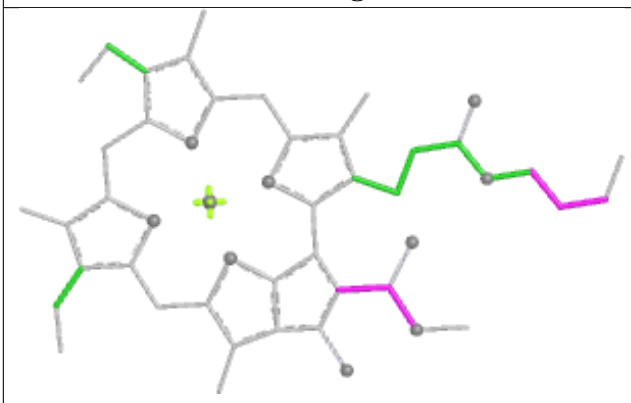
Ligand CLA a 604



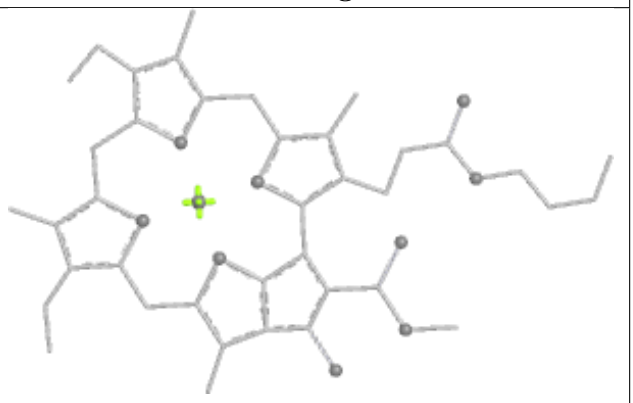
Bond lengths



Bond angles

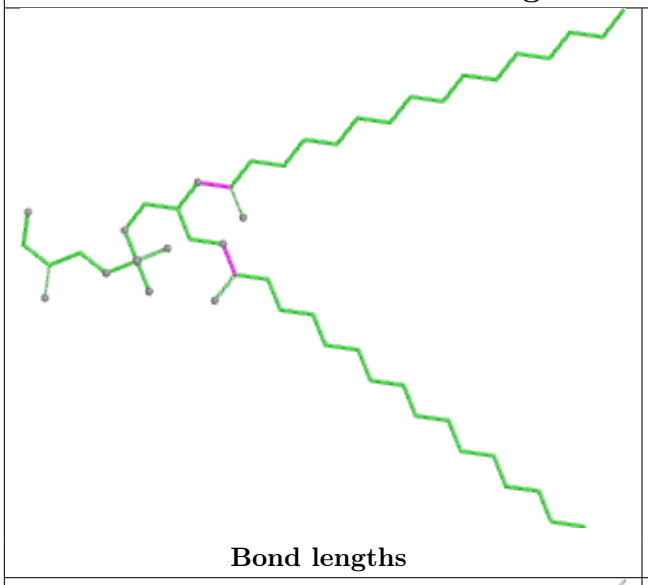


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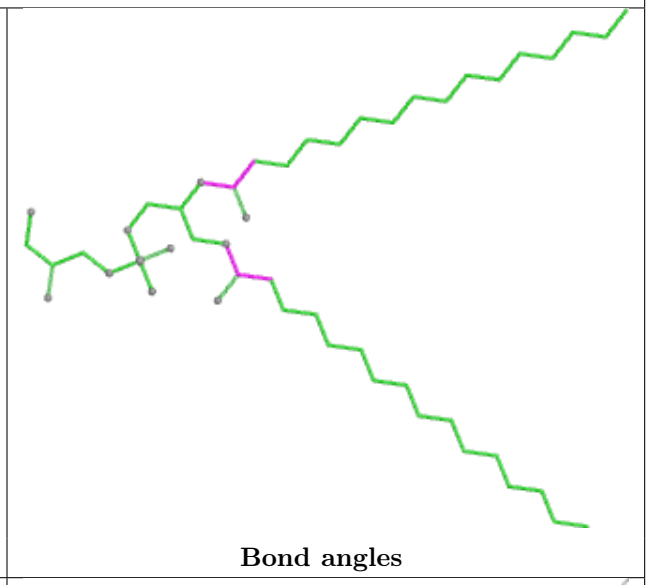


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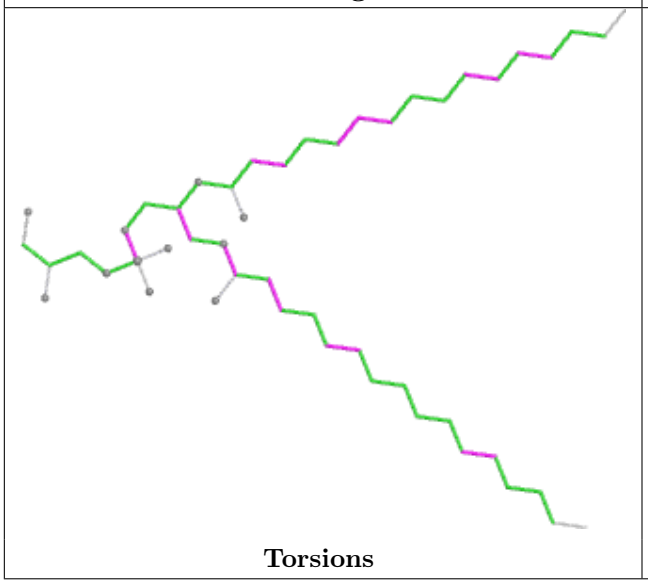
Ligand LHG H 204



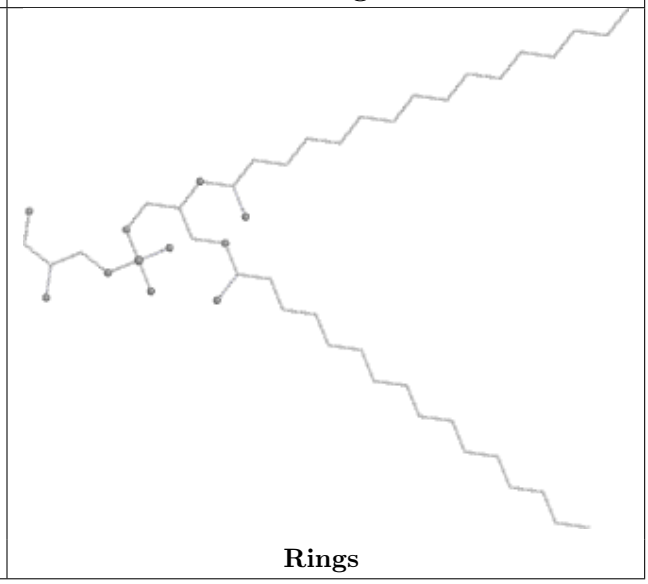
Bond lengths



Bond angles

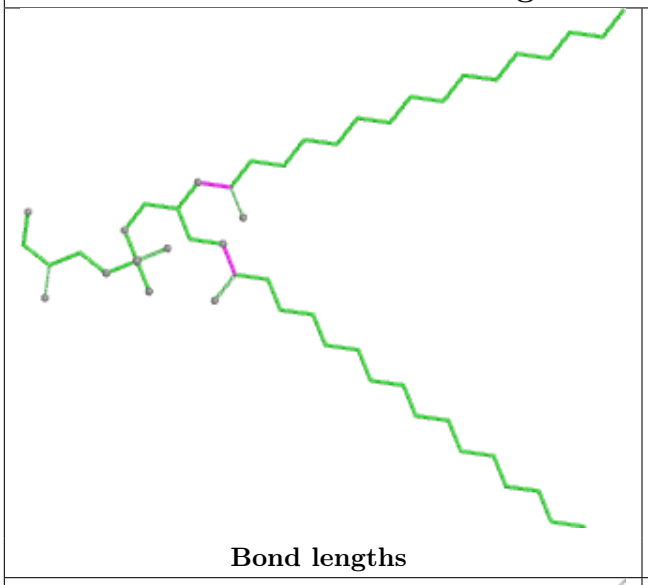


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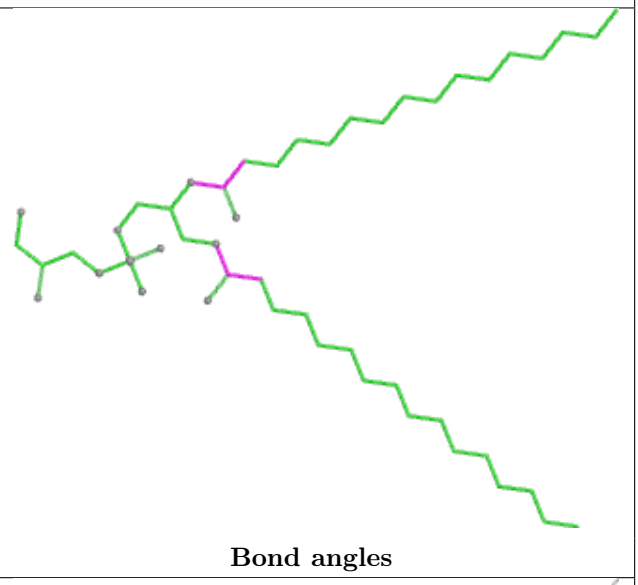


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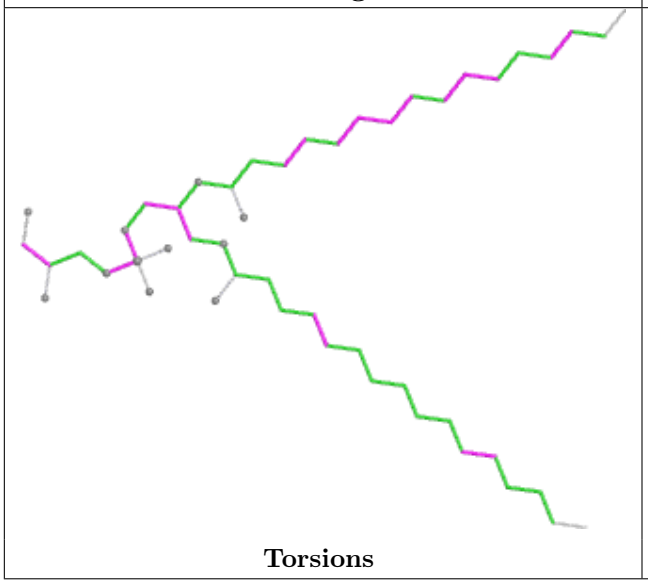
Ligand LHG Z 2630



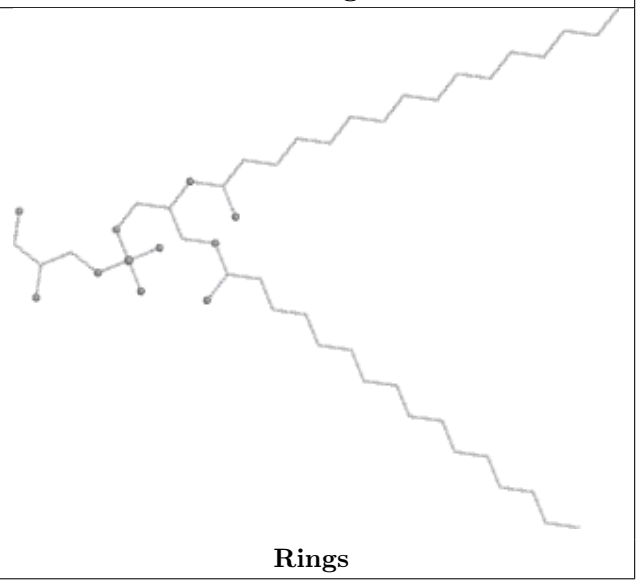
Bond lengths



Bond angles

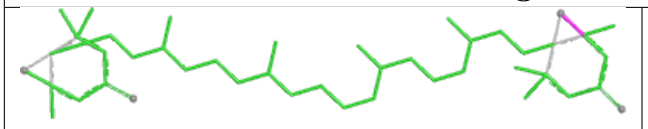


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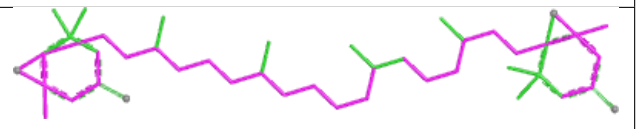


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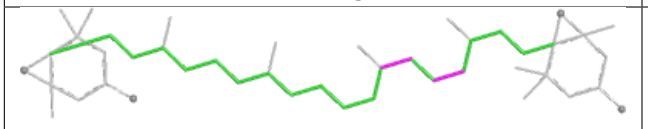
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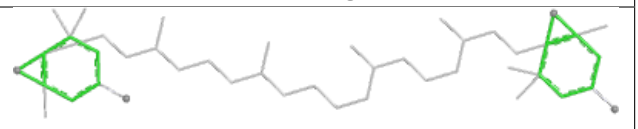
Bond lengths



Bond angles

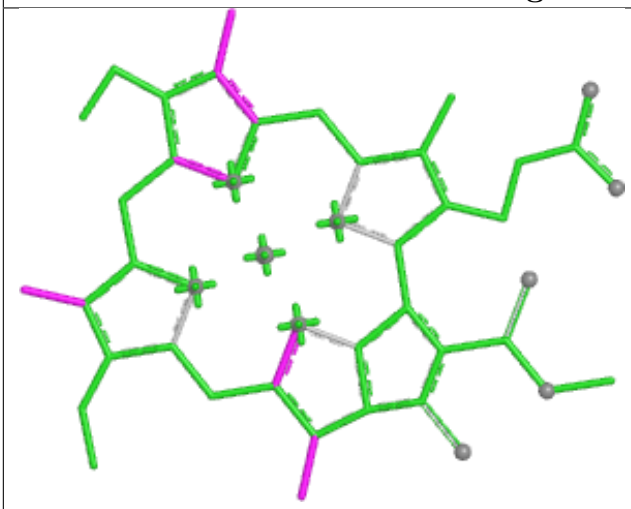


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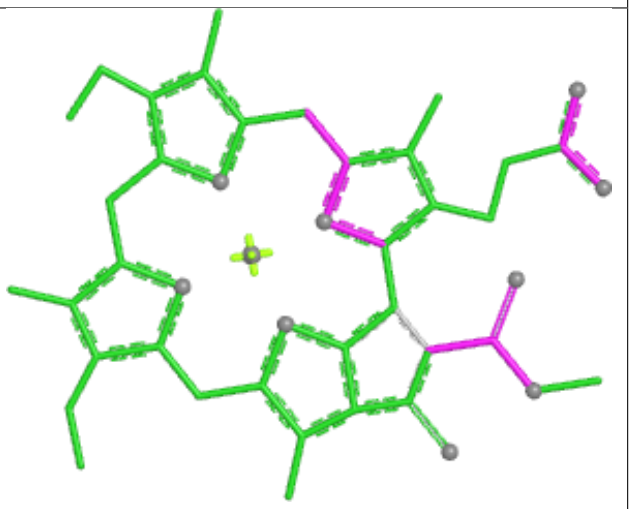


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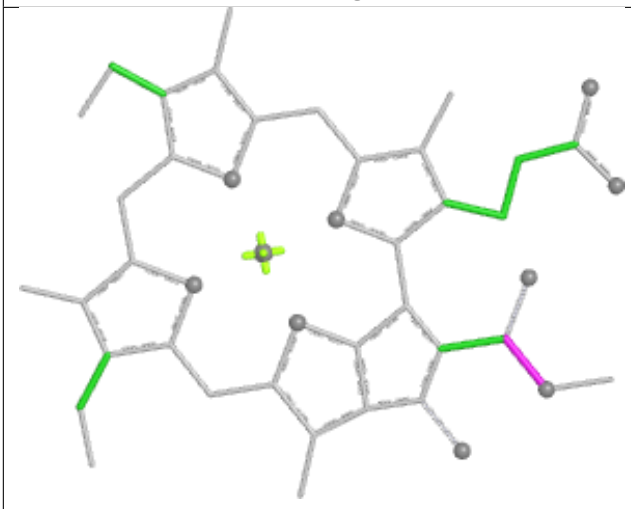
Ligand CLA L 304



Bond lengths



Bond angles

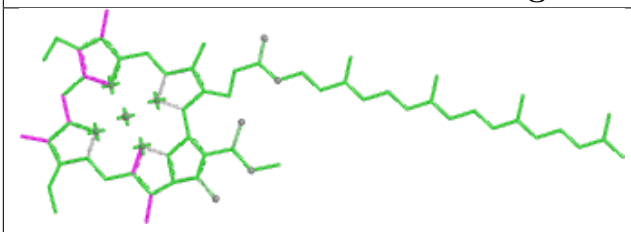


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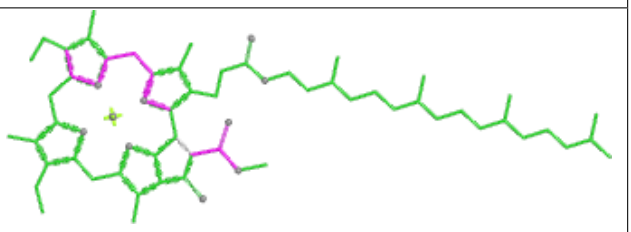


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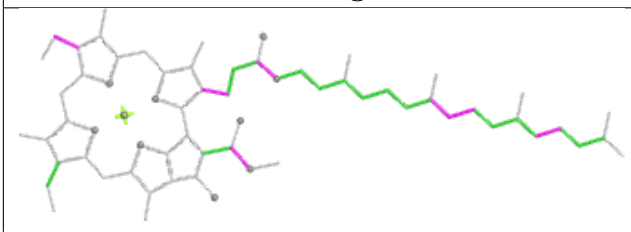
Ligand CLA 3 610



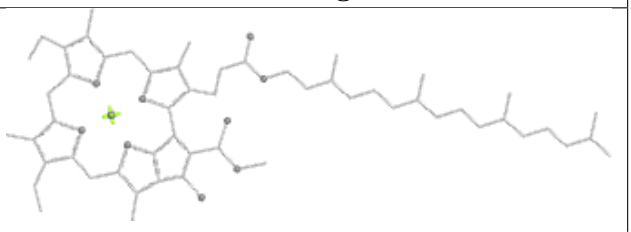
Bond lengths



Bond angles

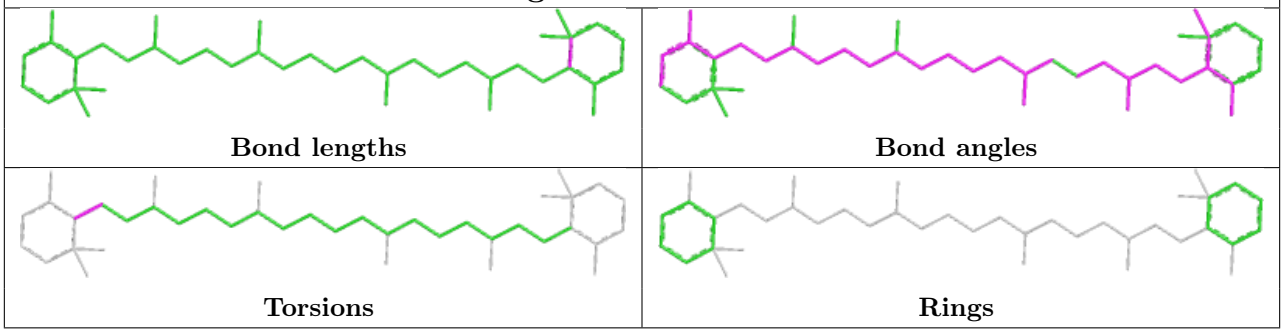


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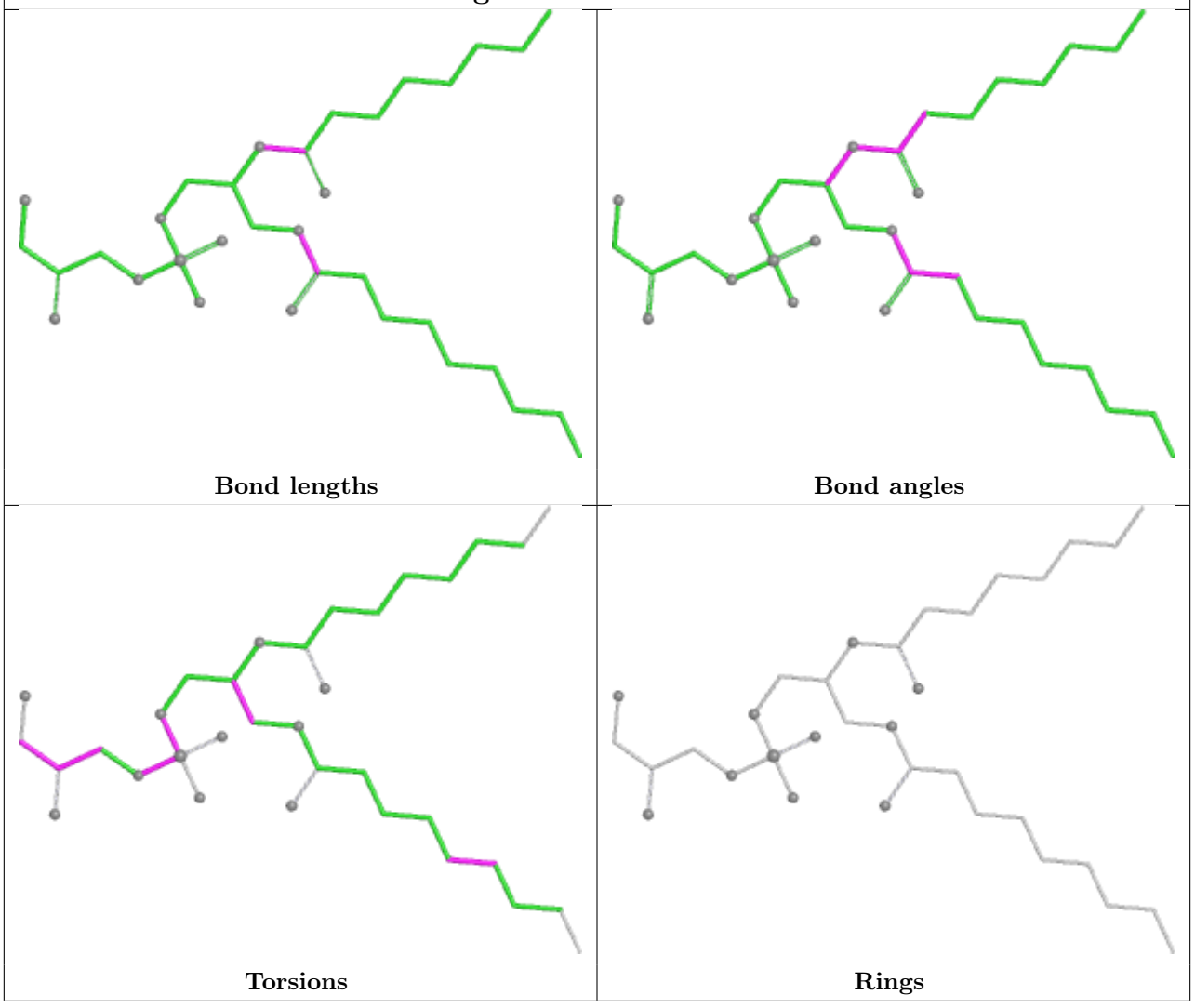


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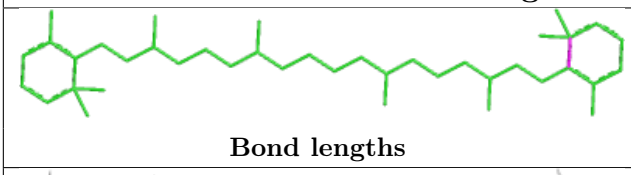
Ligand BCR 4 621

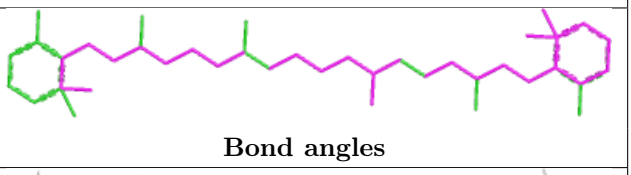


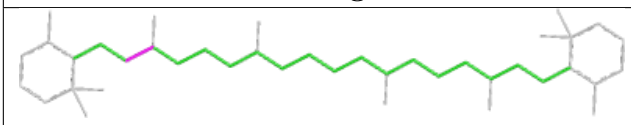
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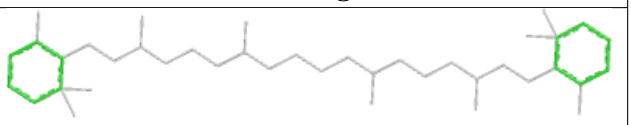


Ligand BCR K 207

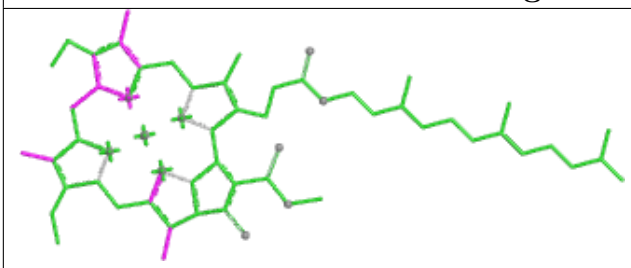

Bond lengths

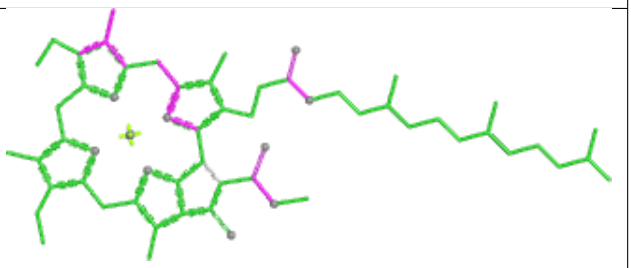

Bond angles

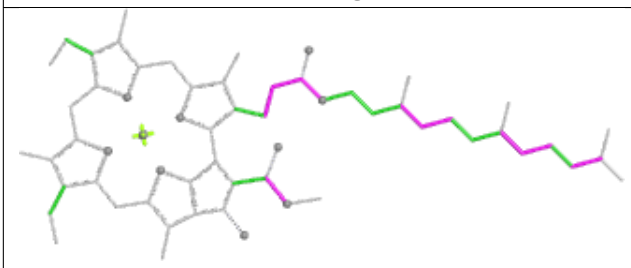

Torsions

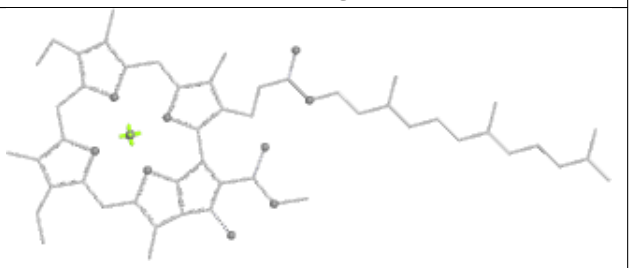

Rings

Ligand CLA A 818

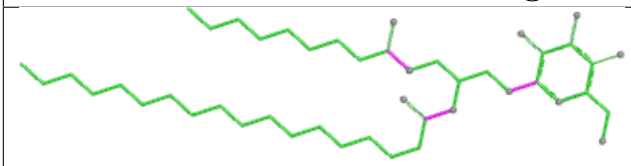

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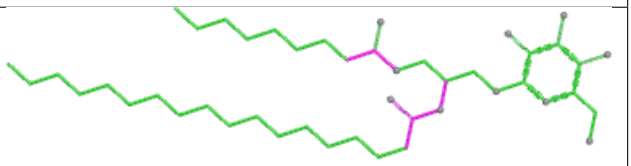

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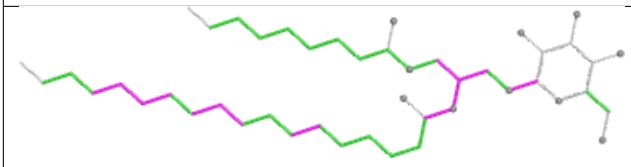

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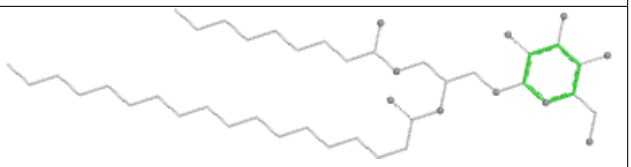

Rings

Ligand LMG 8 626

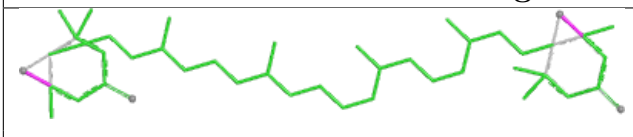

Bond lengths


Bond angles

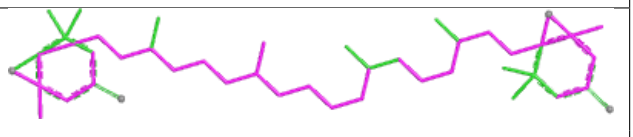

Torsions


Rings

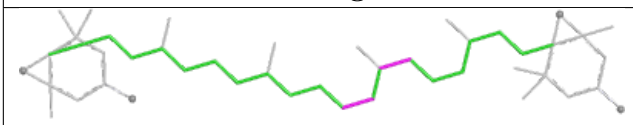
Ligand XAT Y 1622



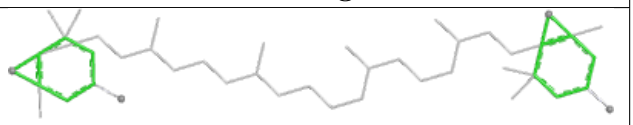
Bond lengths



Bond angles

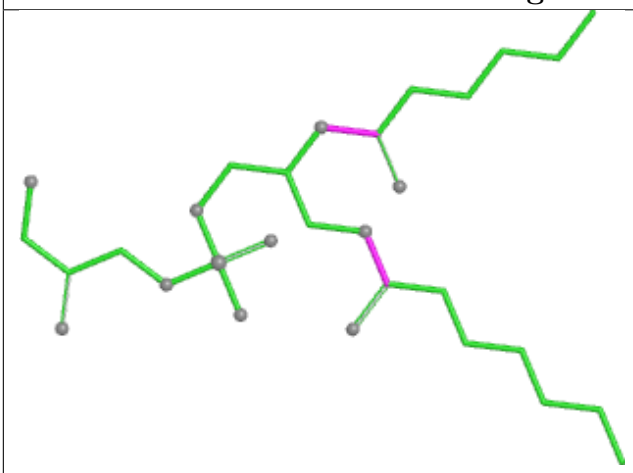


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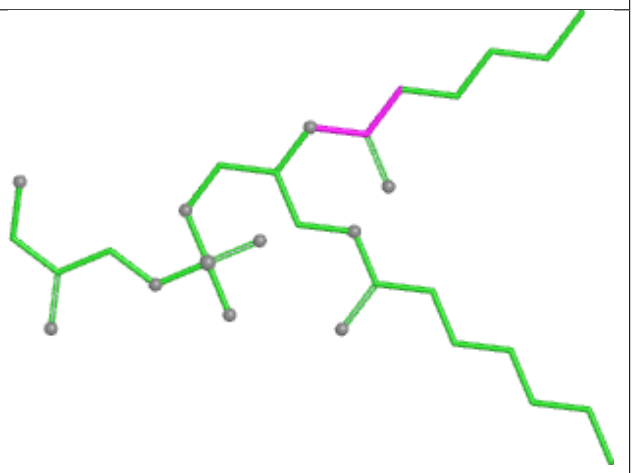


Rings

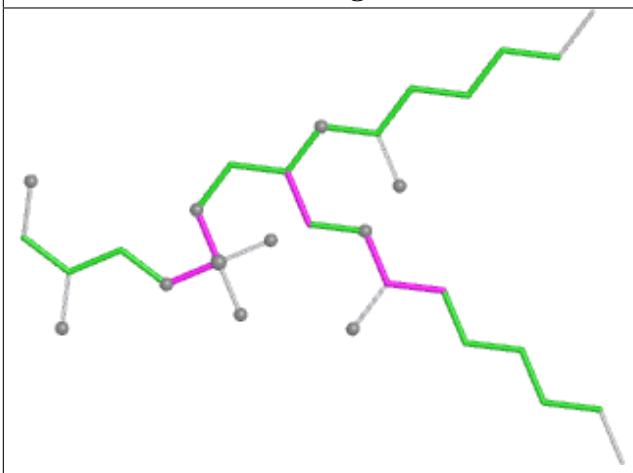
Ligand LHG 9 622



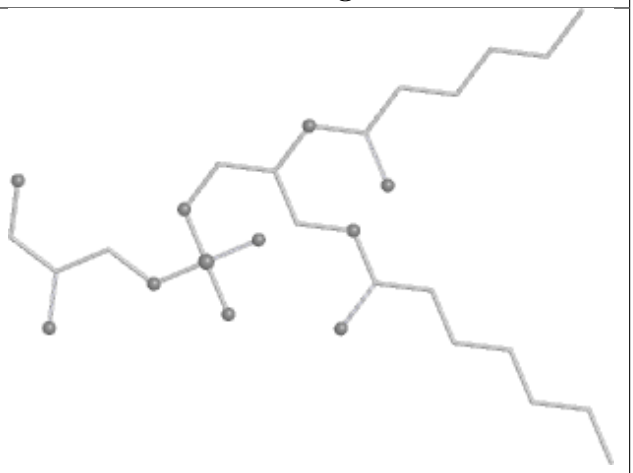
Bond lengths



Bond angles

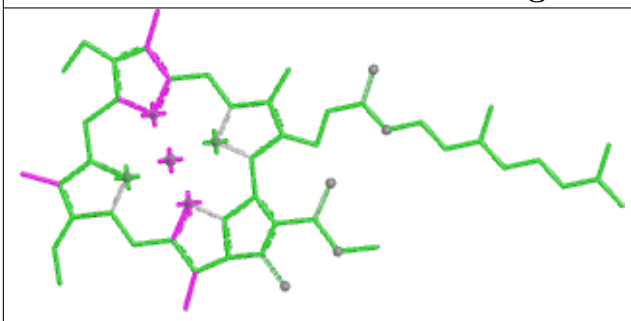


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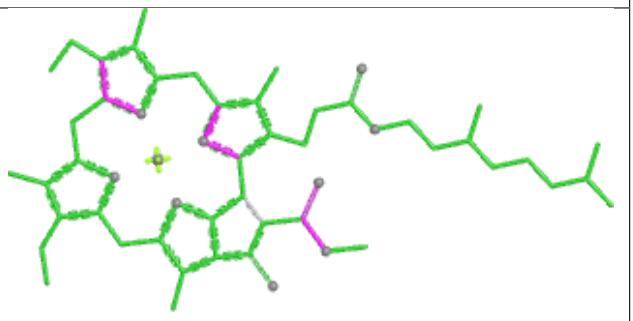


Rings

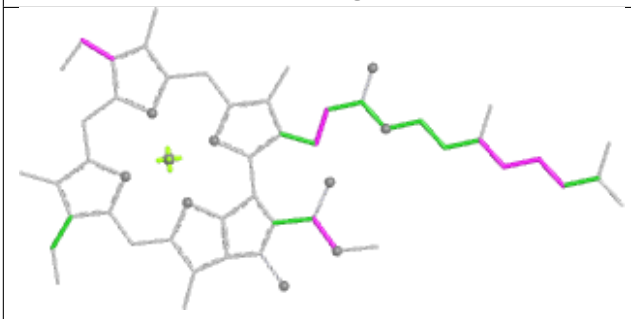
Ligand CLA 3 608



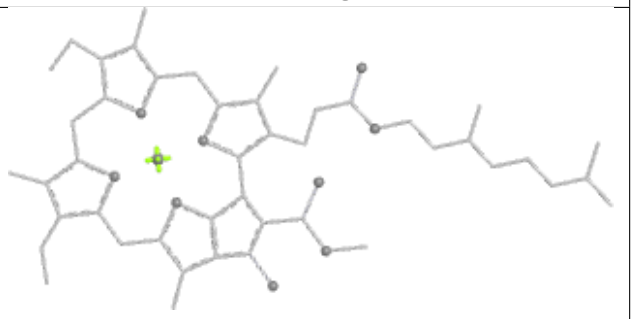
Bond lengths



Bond angles

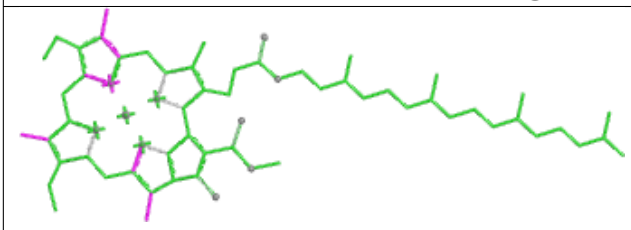


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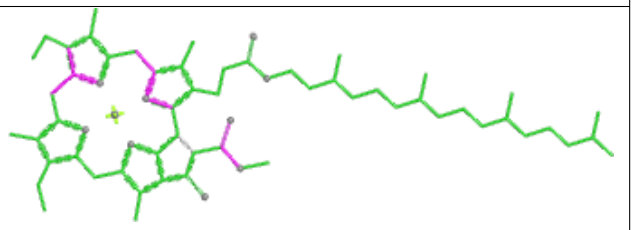


Rings

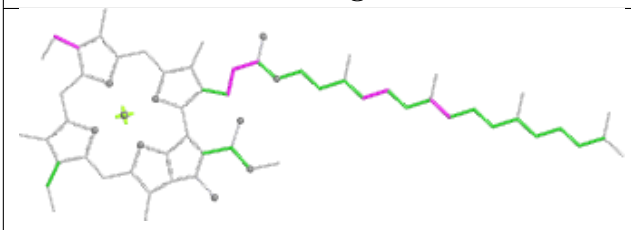
Ligand CLA Z 613



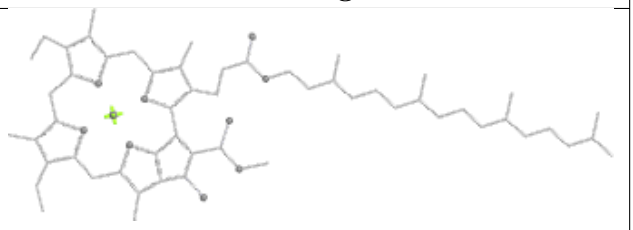
Bond lengths



Bond angles

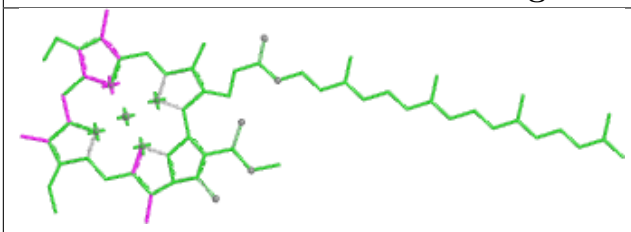


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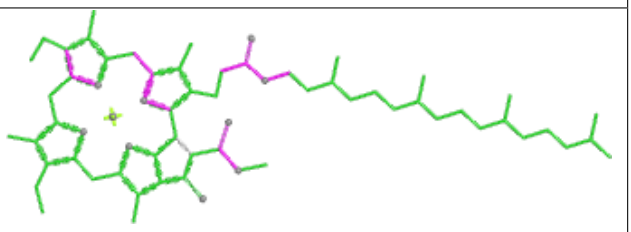


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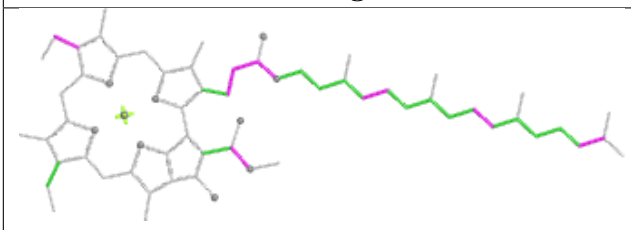
Ligand CLA 4 613



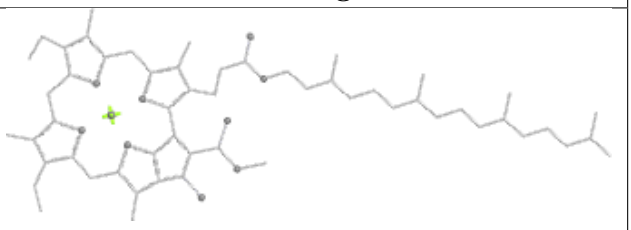
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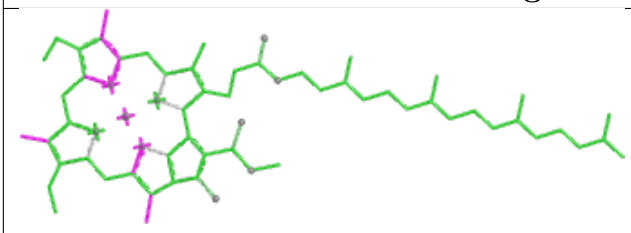


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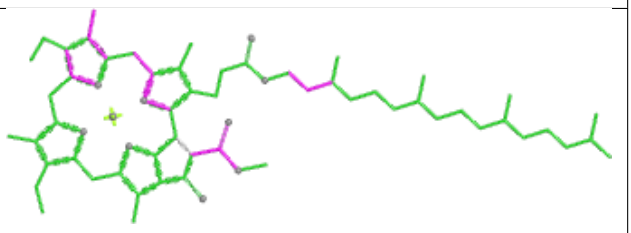


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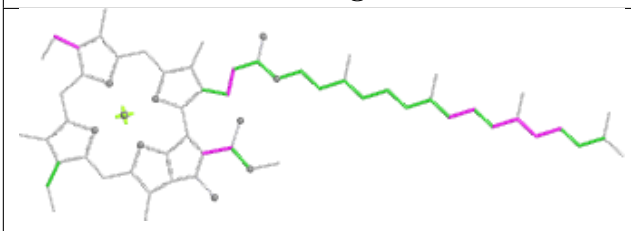
Ligand CLA A 809



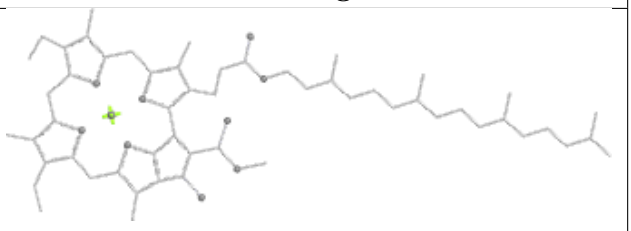
Bond lengths



Bond angles

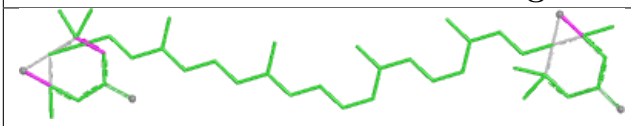


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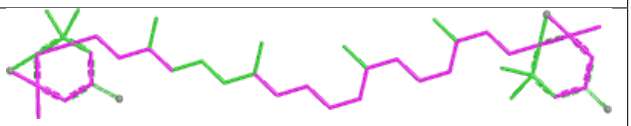


Rings

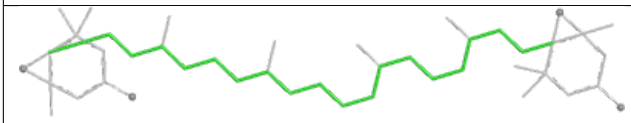
Ligand XAT 9 620



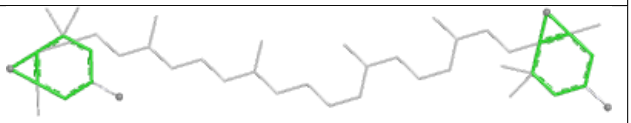
Bond lengths



Bond angles

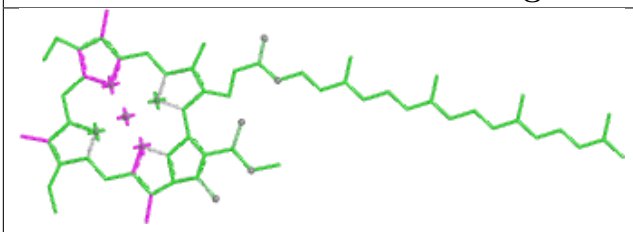


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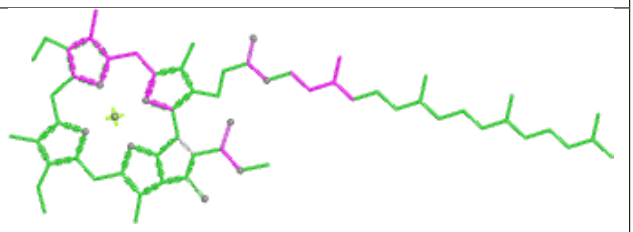


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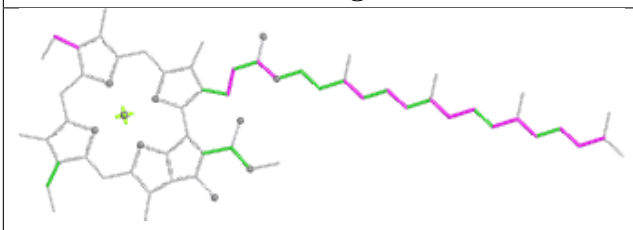
Ligand CLA A 842



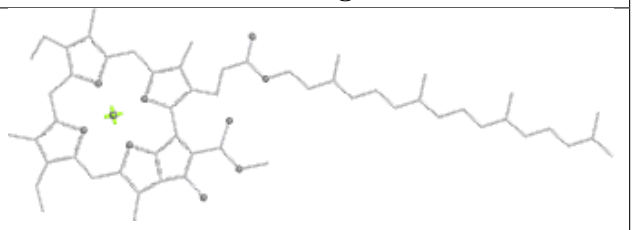
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Bond angles

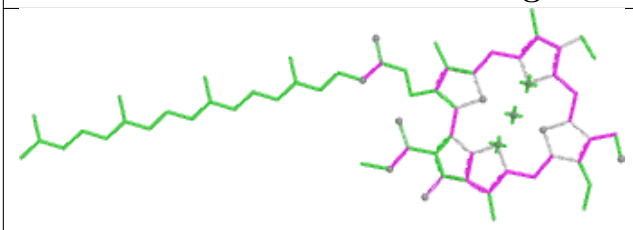


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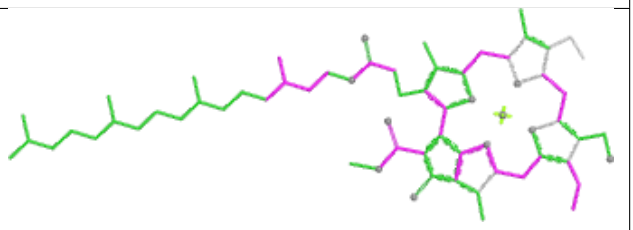


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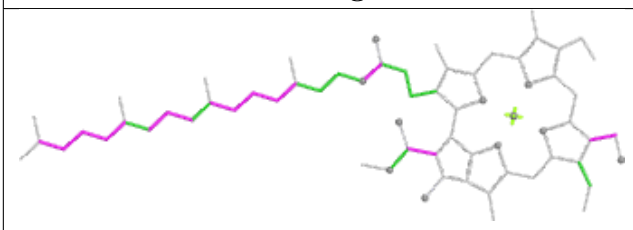
Ligand CHL U 601



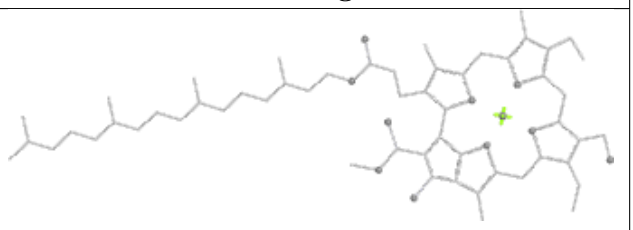
Bond lengths



Bond angles

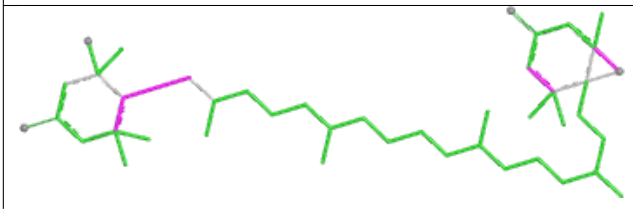


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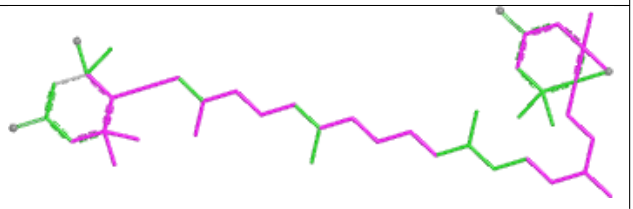


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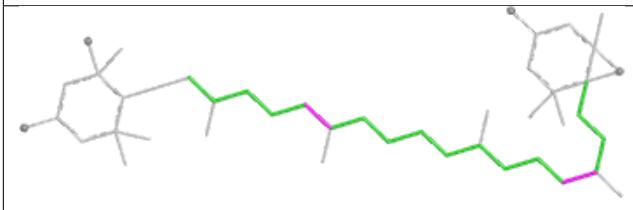
Ligand NEX 6 624



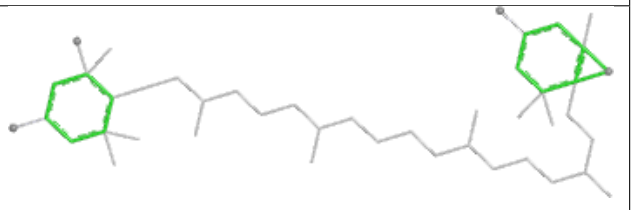
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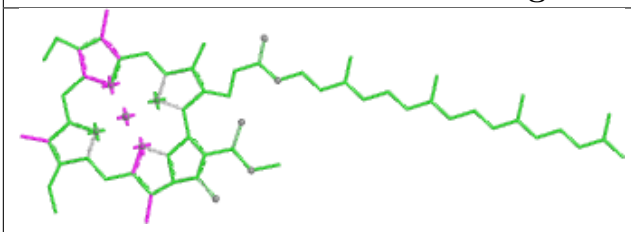


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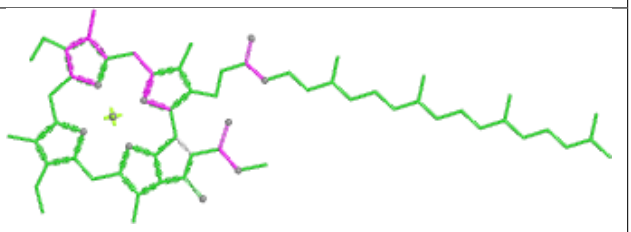


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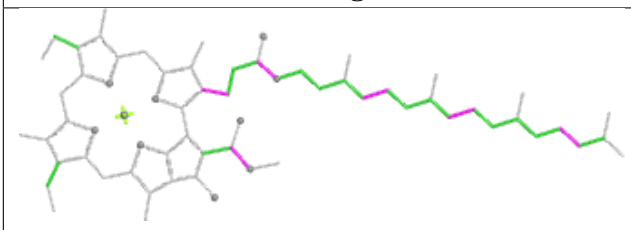
Ligand CLA 2 601



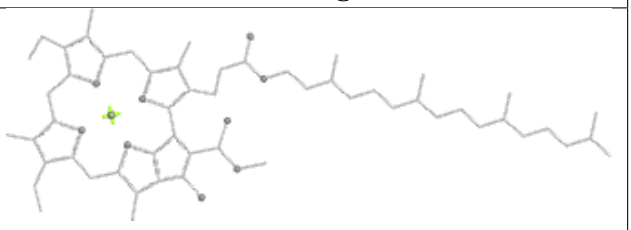
Bond lengths



Bond angles

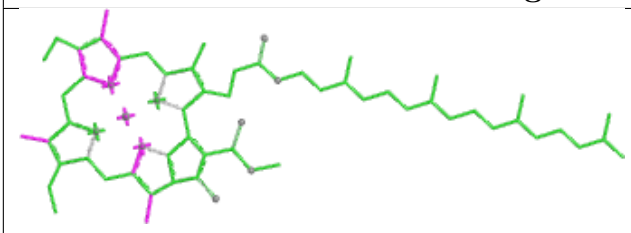


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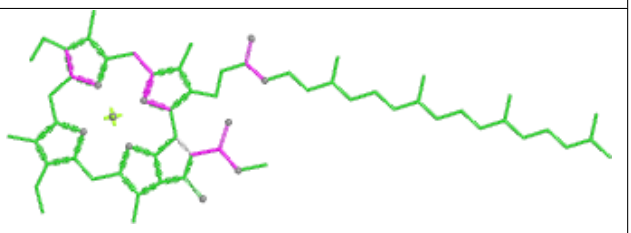


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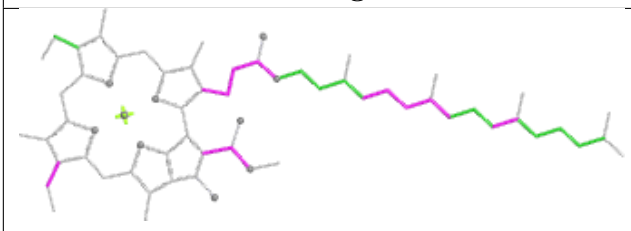
Ligand CLA B 813



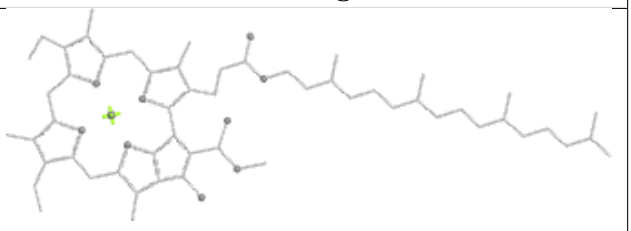
Bond lengths



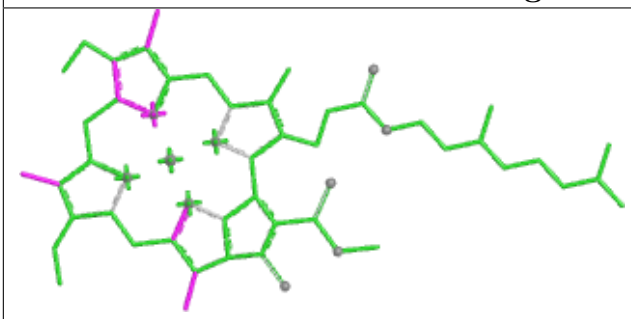
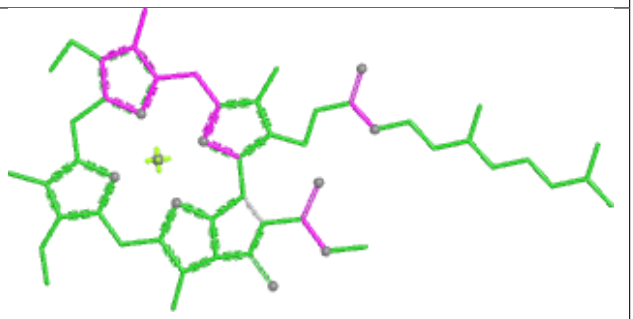
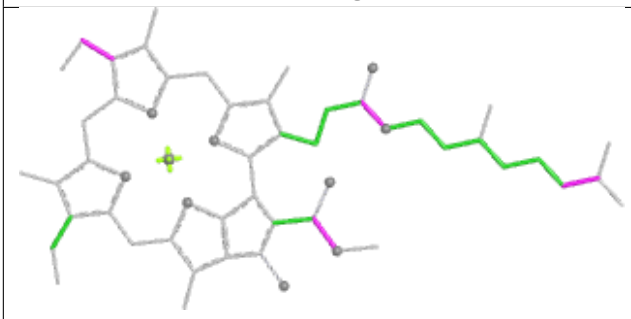
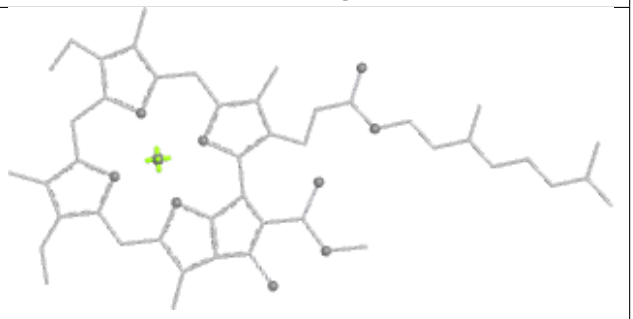
Bond angles



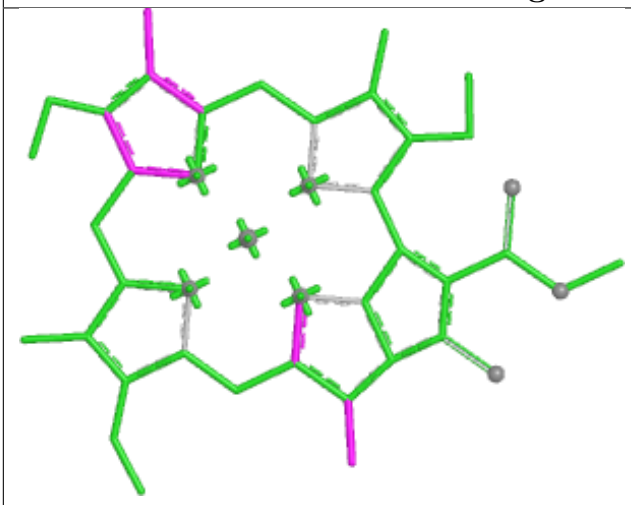
Torsions



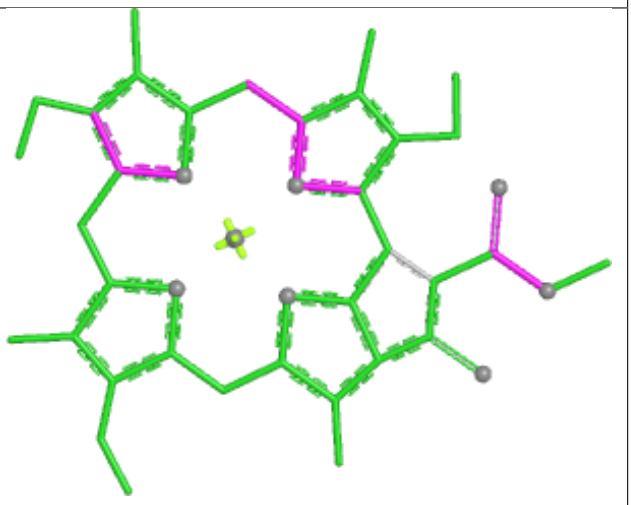
Rings

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

Ligand CLA 5 611



Bond lengths



Bond angles

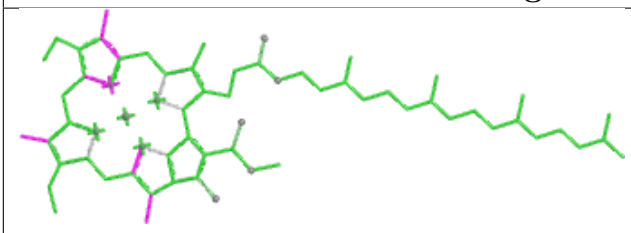


Torsions

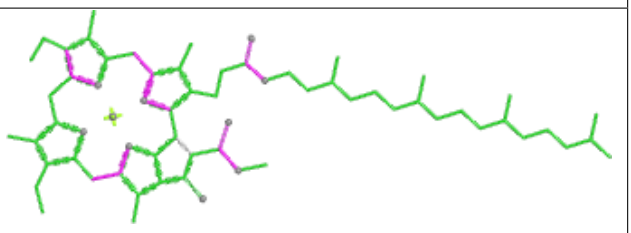


Rings

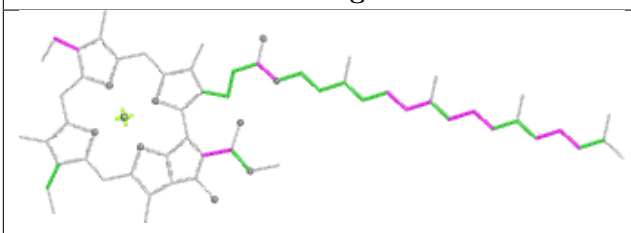
Ligand CLA B 833



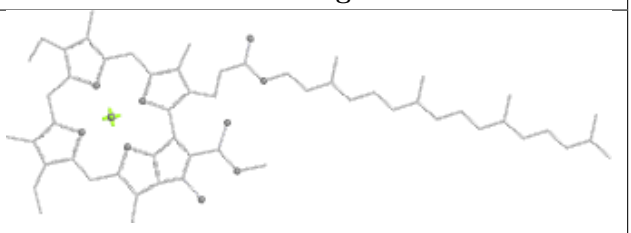
Bond lengths



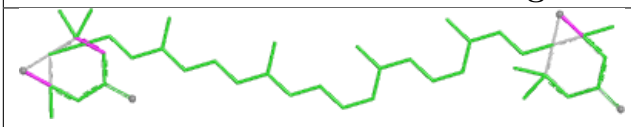
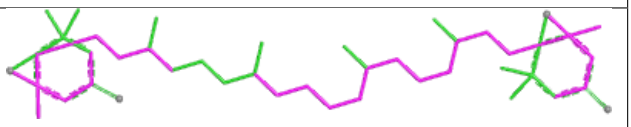
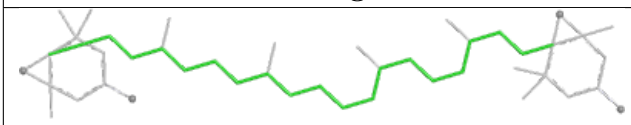
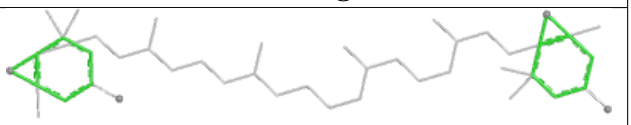
Bond angles

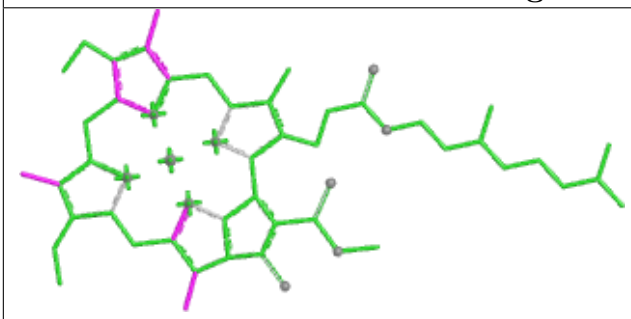
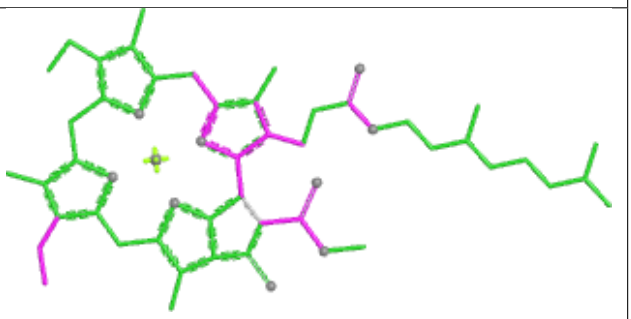
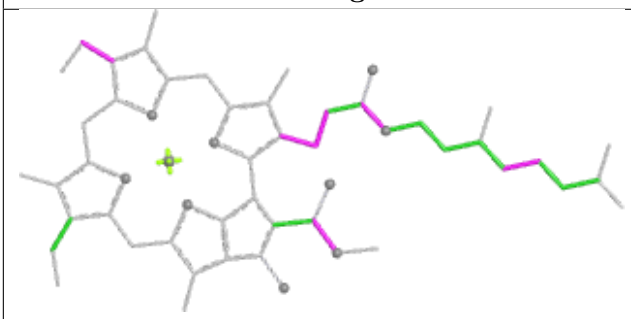
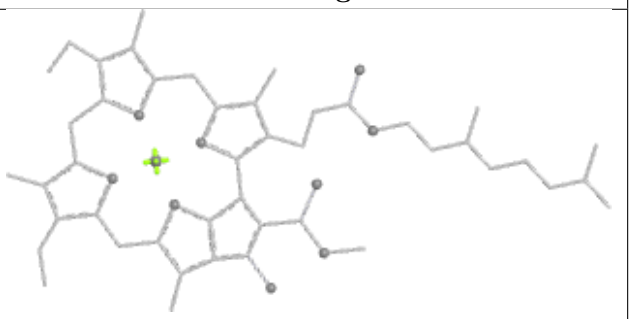


Torsions

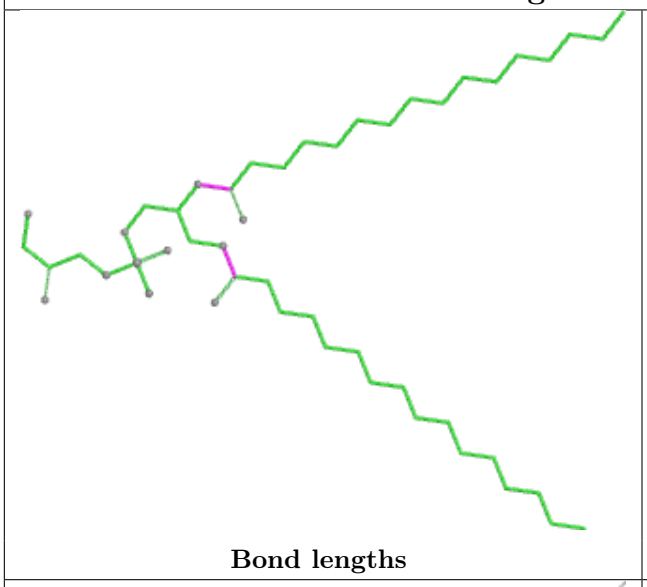


Rings

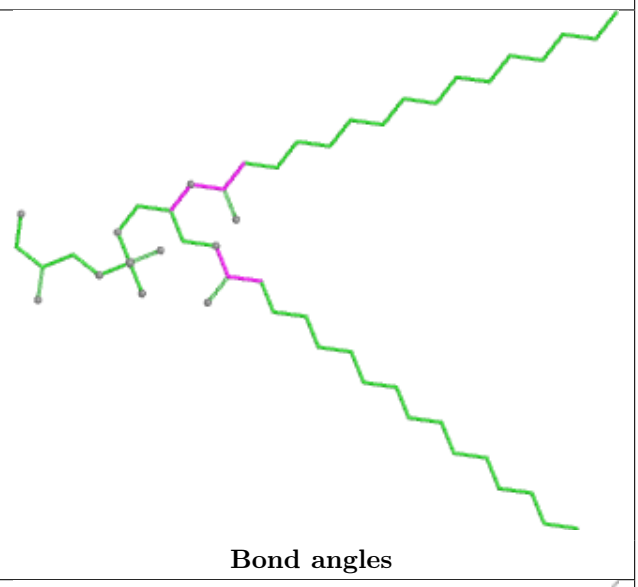
Ligand XAT 3 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

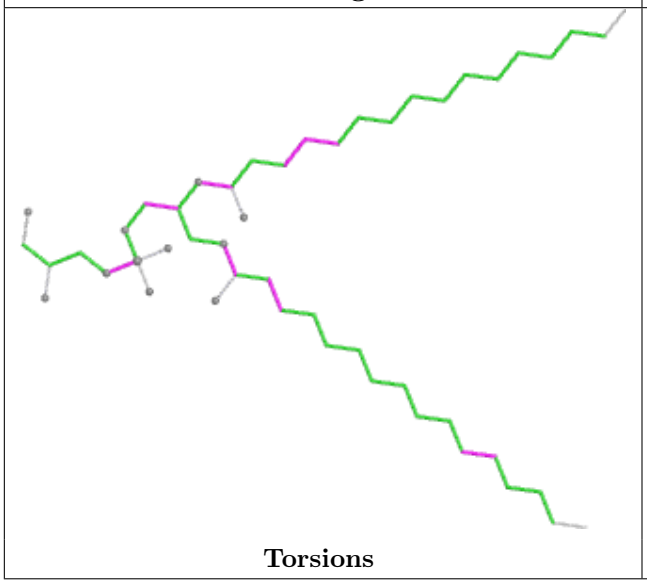
Ligand LHG 3 624



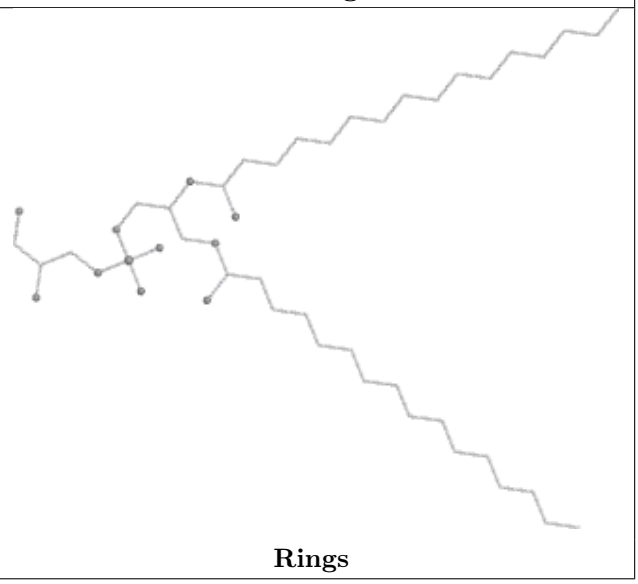
Bond lengths



Bond angles

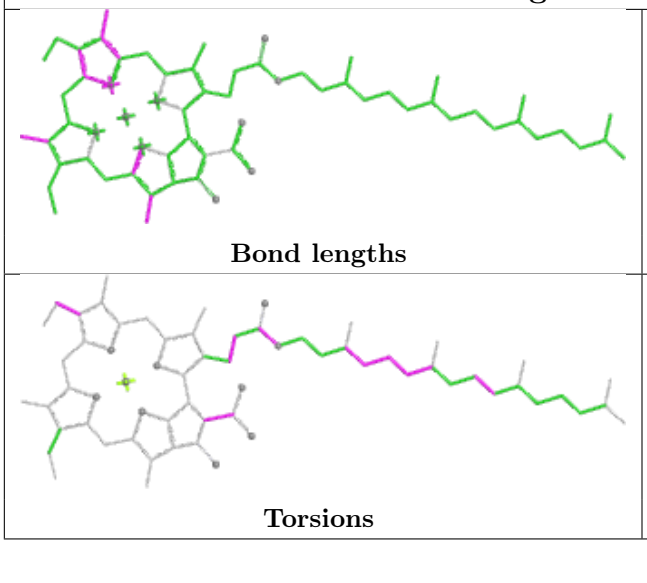


Torsions

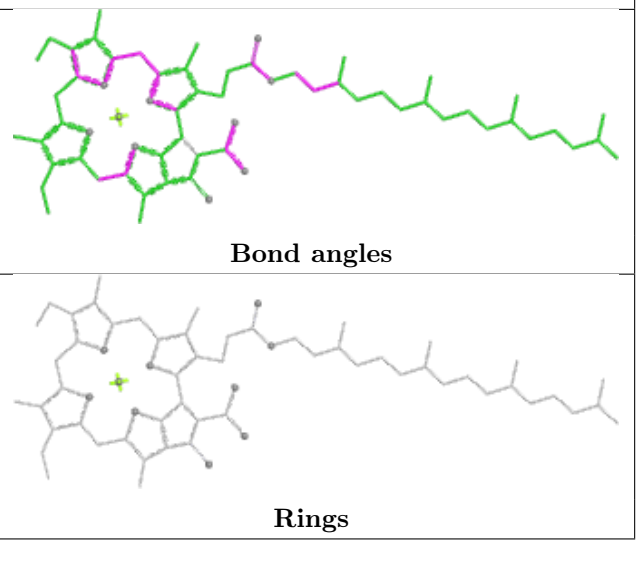


Rings

Ligand CLA 6 613



Bond lengths

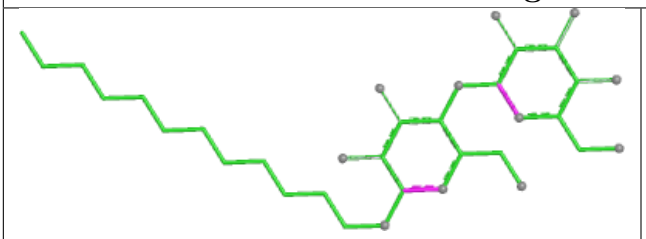


Bond angles

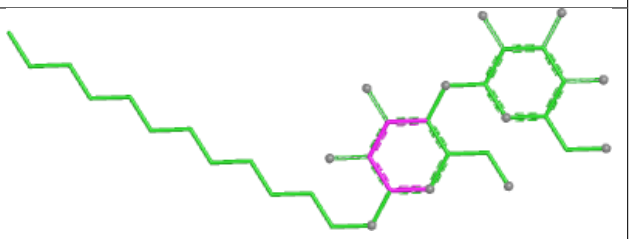
Torsions

Rings

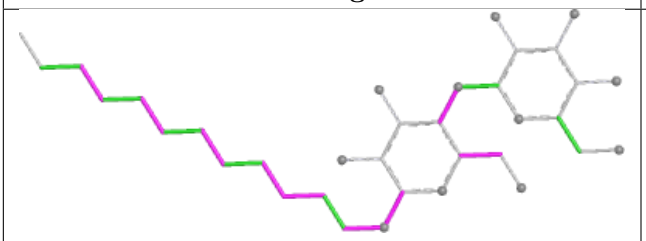
Ligand LMU 8 625



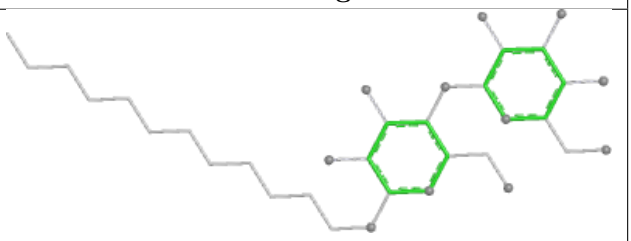
Bond lengths



Bond angles

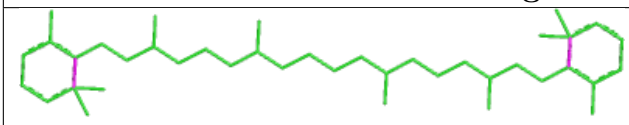


Torsions

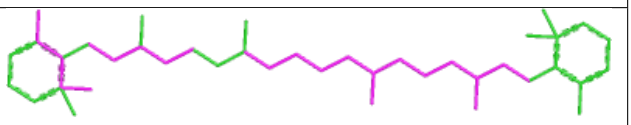


Rings

Ligand BCR B 853



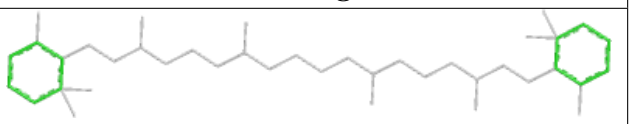
Bond lengths



Bond angles

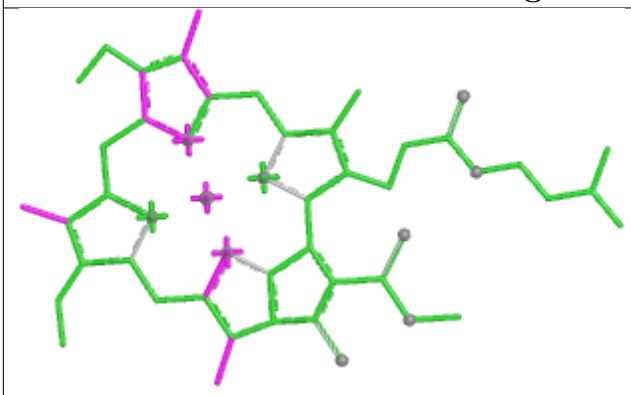


Torsions

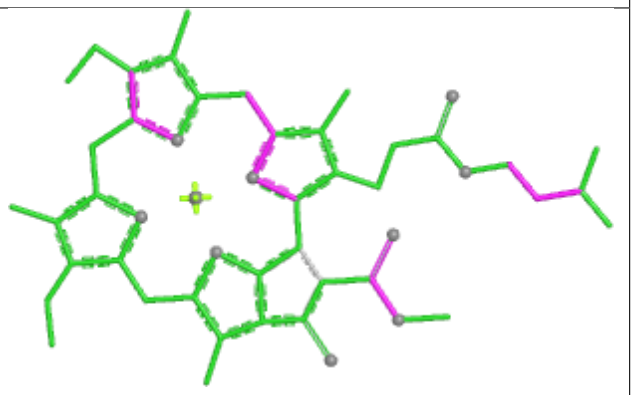


Rings

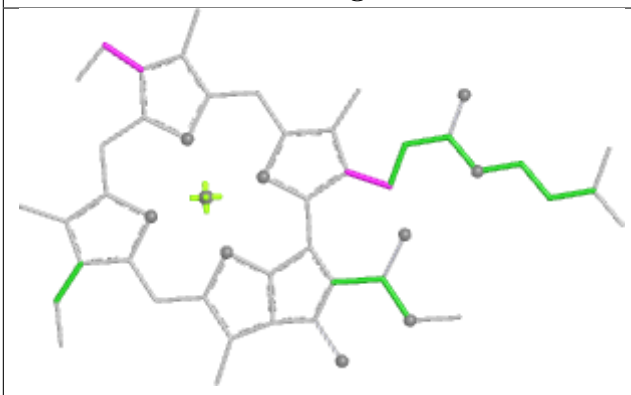
Ligand CLA B 820



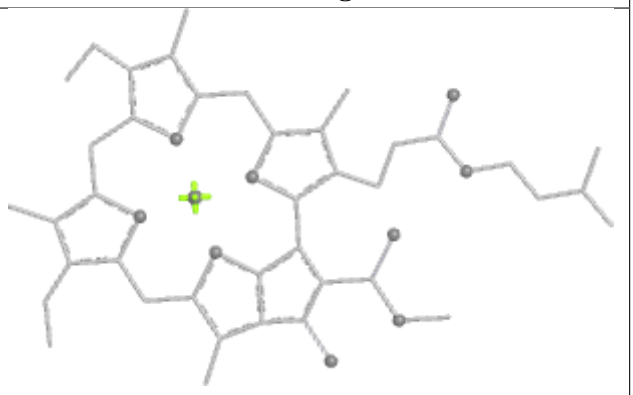
Bond lengths



Bond angles

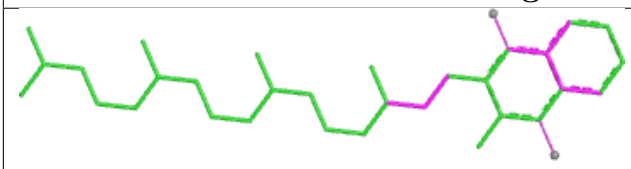


Torsions

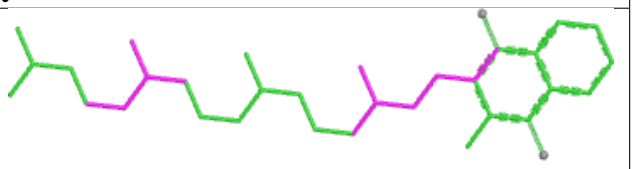


Rings

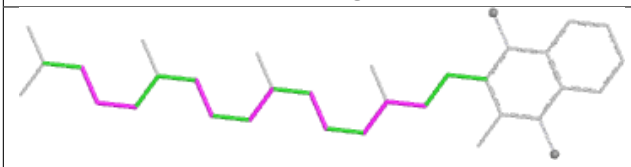
Ligand PQN B 842



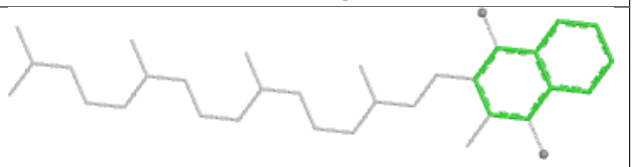
Bond lengths



Bond angles

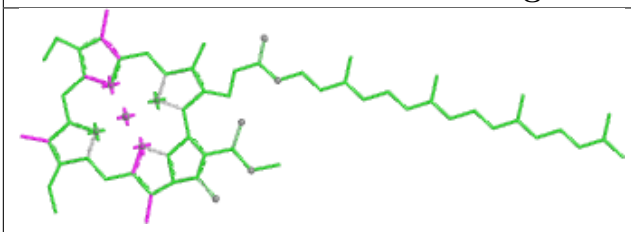


Torsions

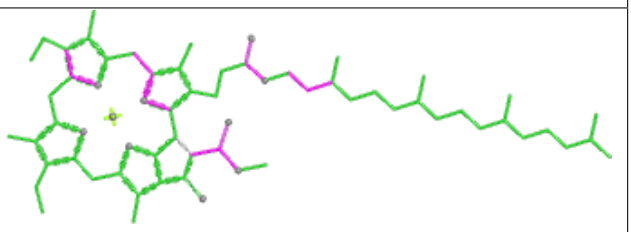


Rings

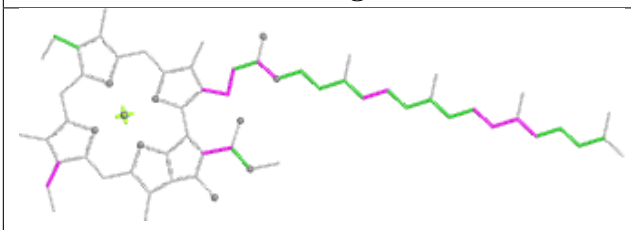
Ligand CLA A 804



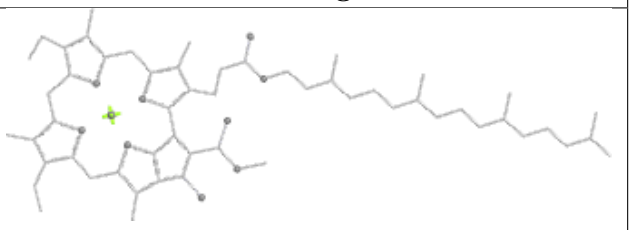
Bond lengths



Bond angles

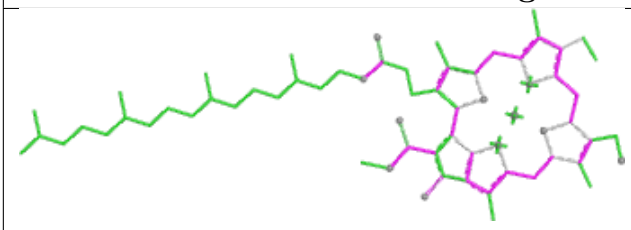


Torsions

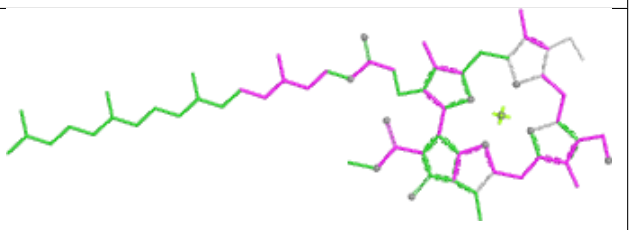


Rings

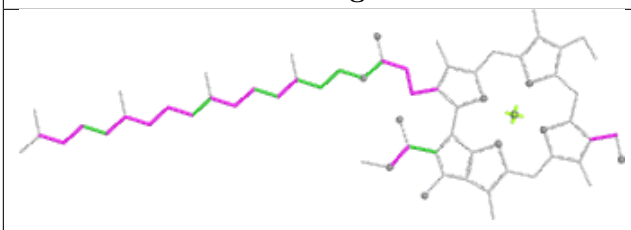
Ligand CHL W 607



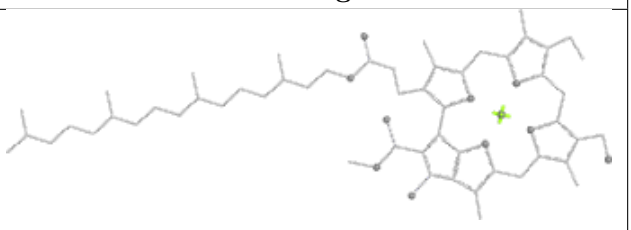
Bond lengths



Bond angles

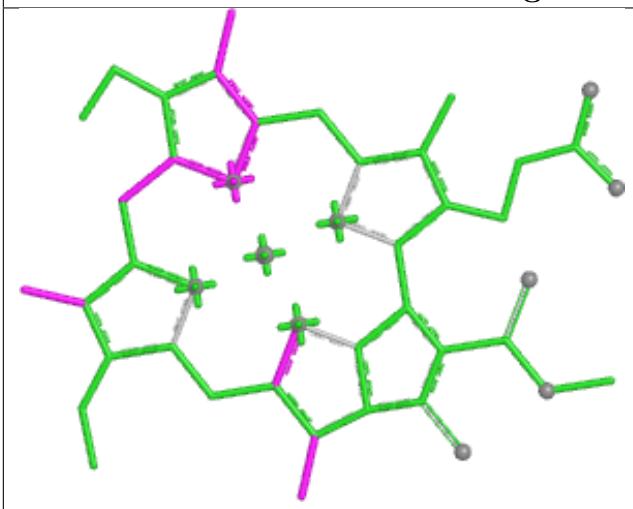


Torsions

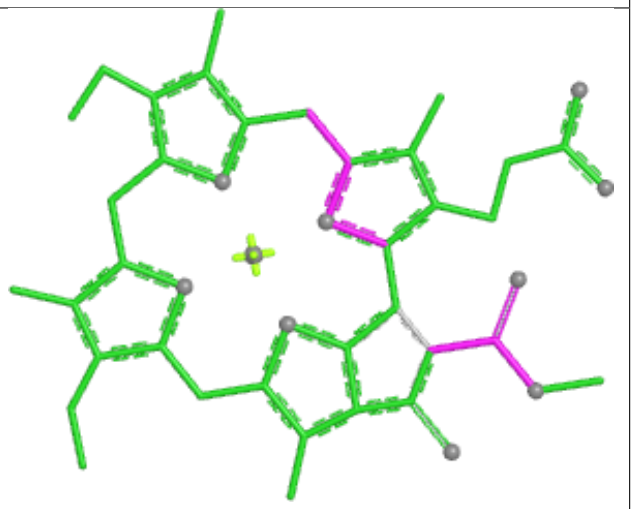


Rings

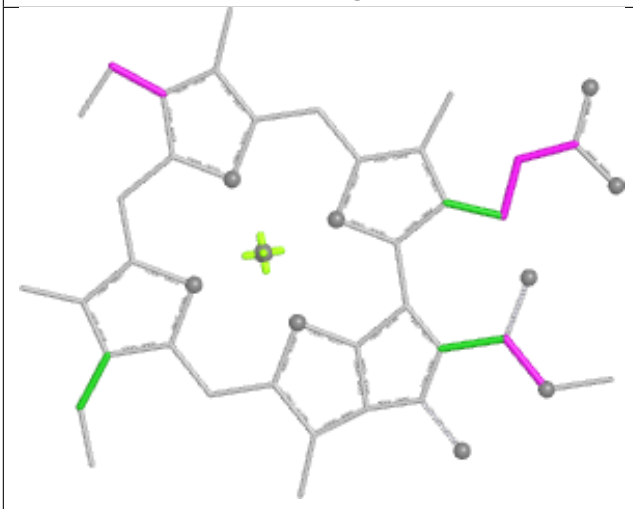
Ligand CLA A 837



Bond lengths



Bond angles

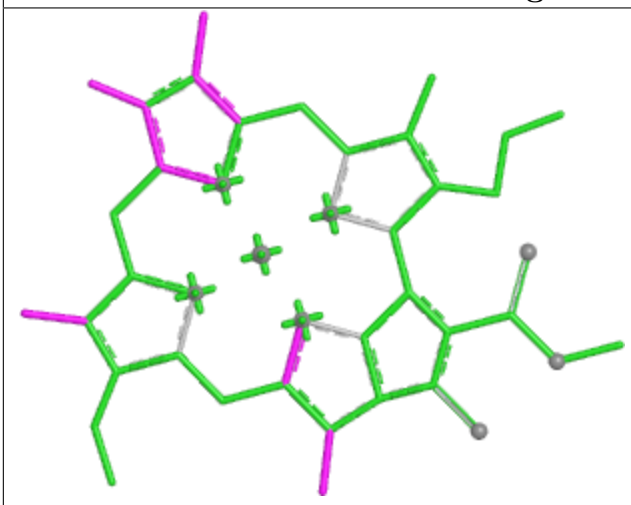


Torsions

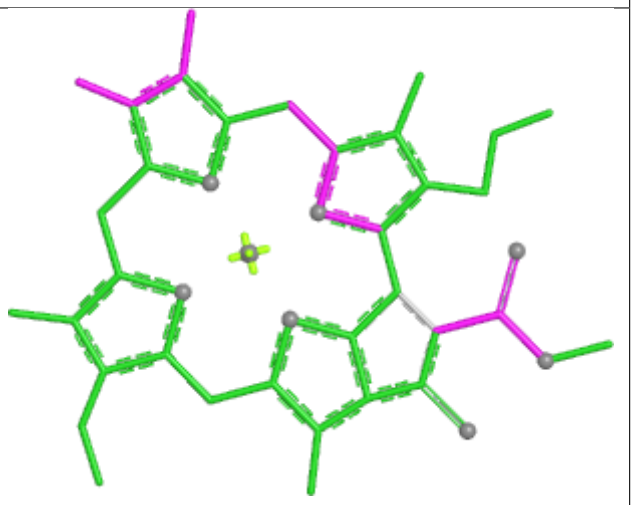


Rings

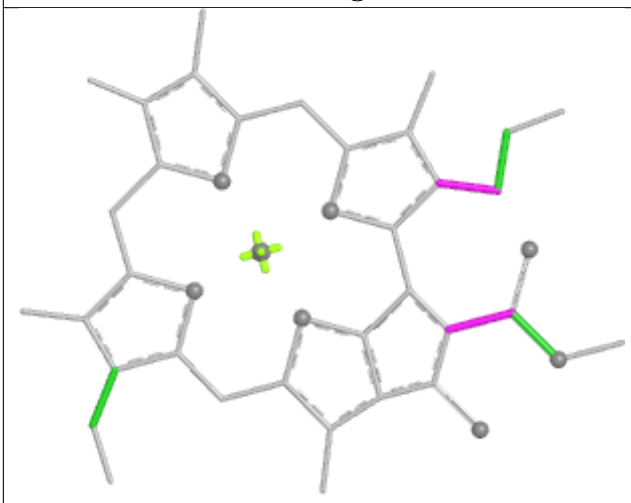
Ligand CLA Z 611



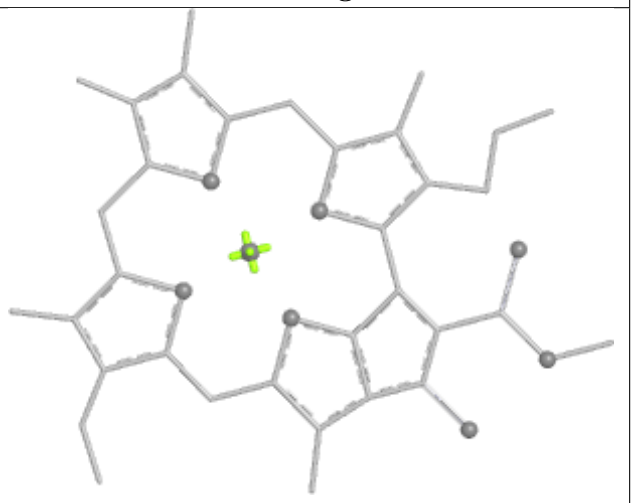
Bond lengths



Bond angles

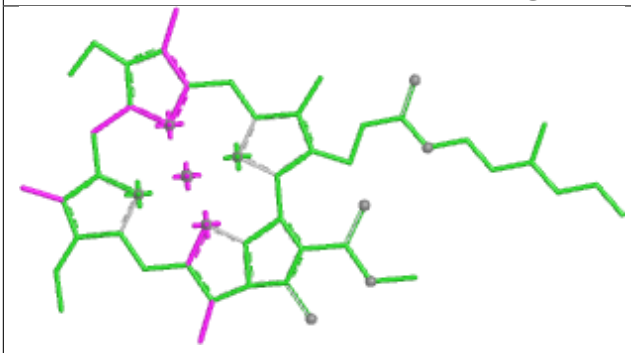


Torsions

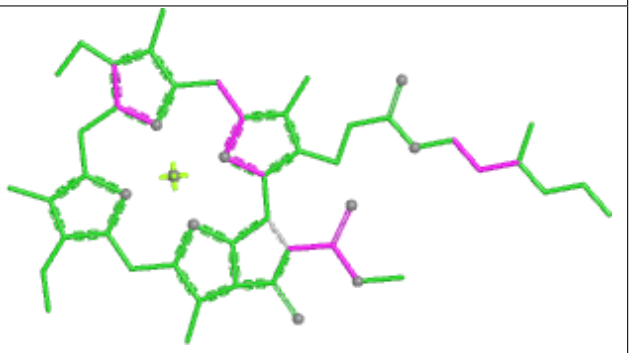


Rings

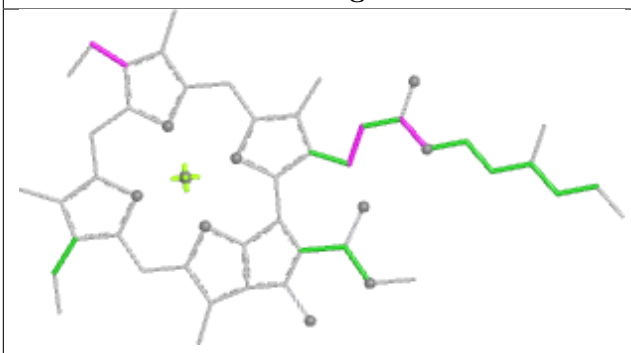
Ligand CLA B 807



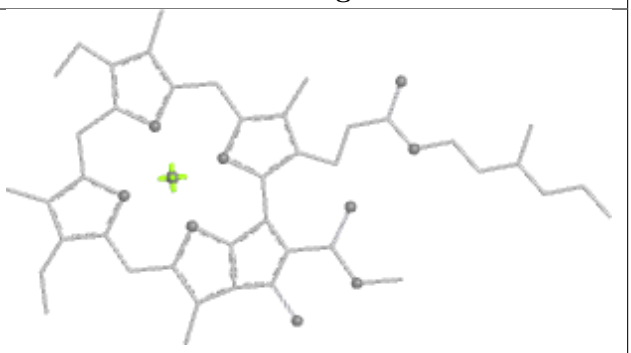
Bond lengths



Bond angles

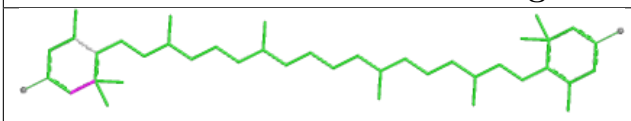


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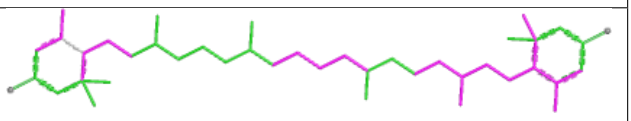


Rings

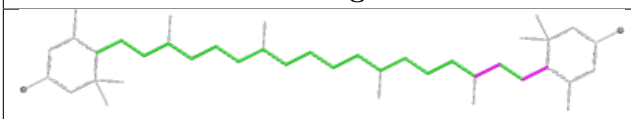
Ligand LUT 3 618



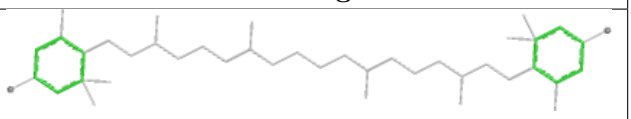
Bond lengths



Bond angles

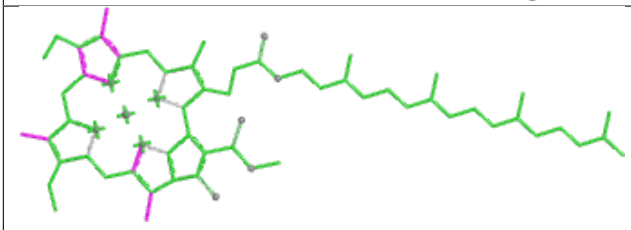


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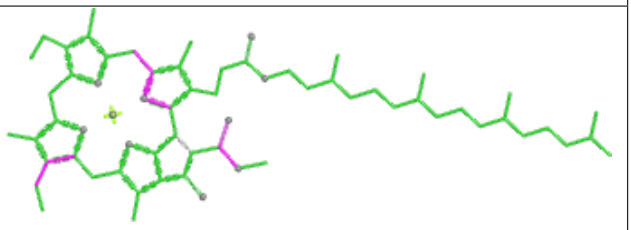


Rings

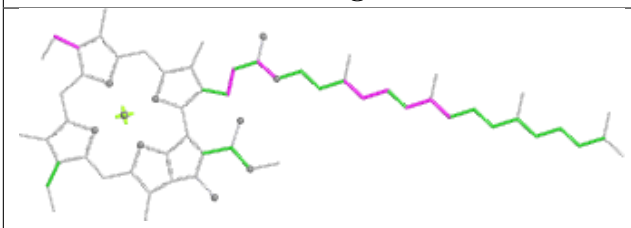
Ligand CLA X 613



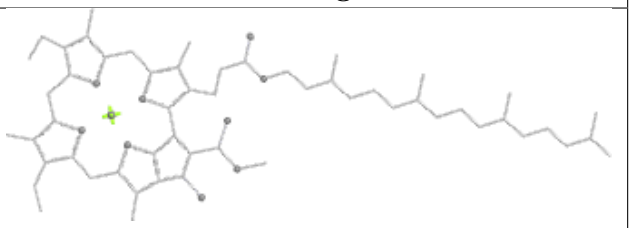
Bond lengths



Bond angles

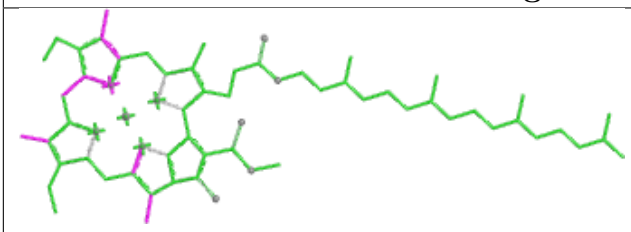


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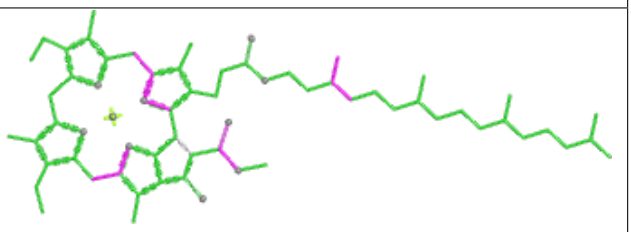


Rings

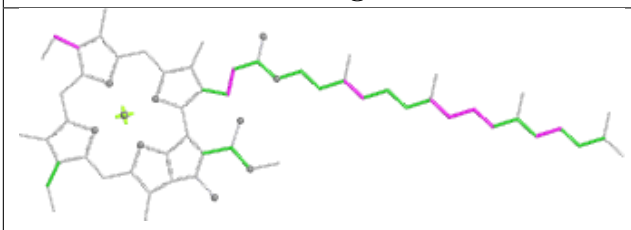
Ligand CLA A 824



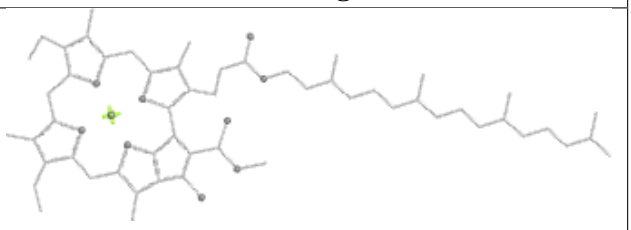
Bond lengths



Bond angles

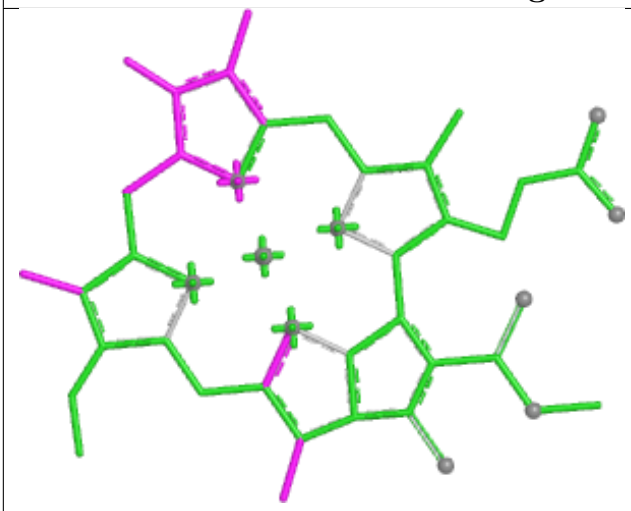


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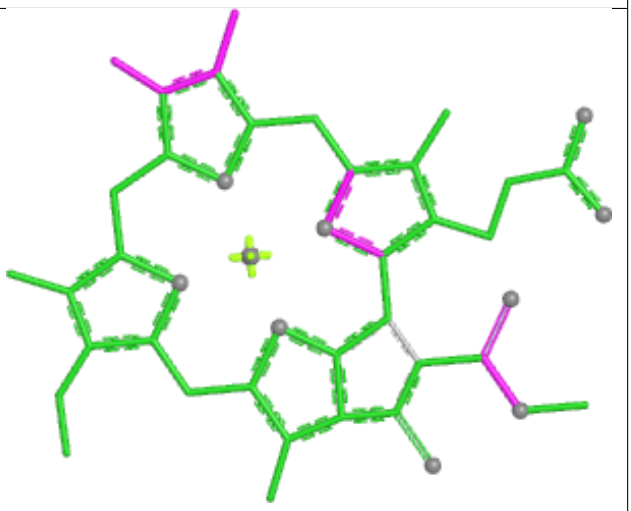


Rings

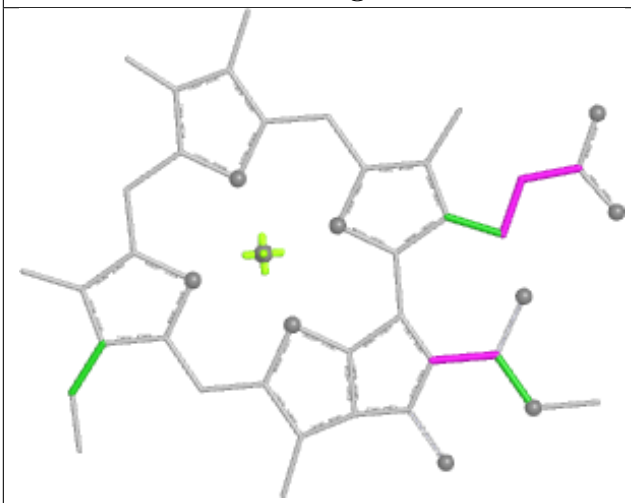
Ligand CLA 9 603



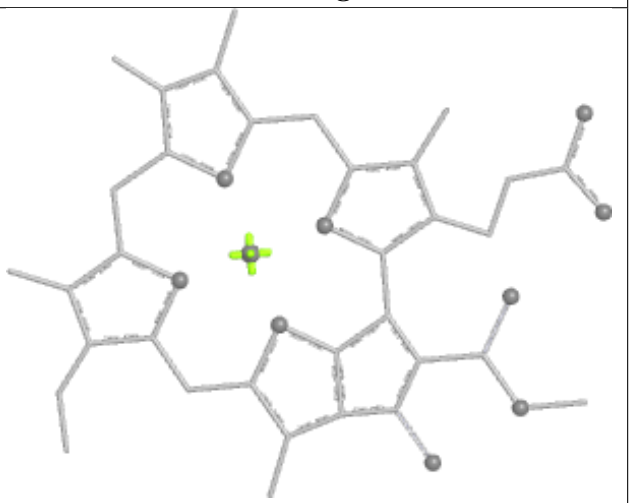
Bond lengths



Bond angles

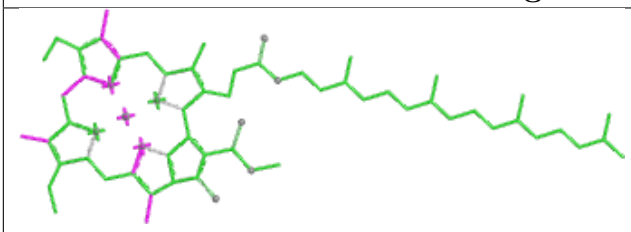


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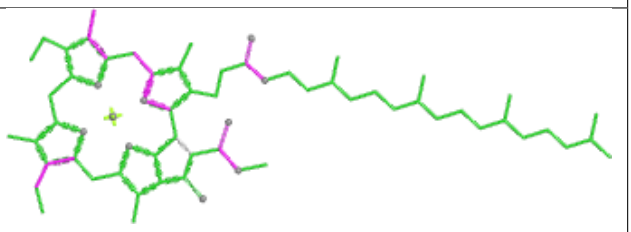


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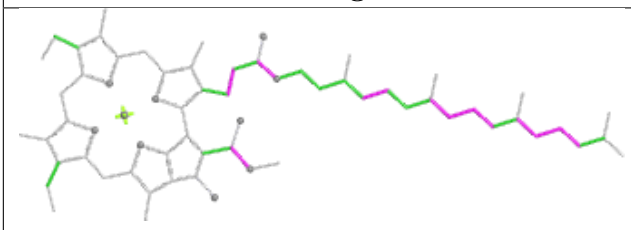
Ligand CLA B 839



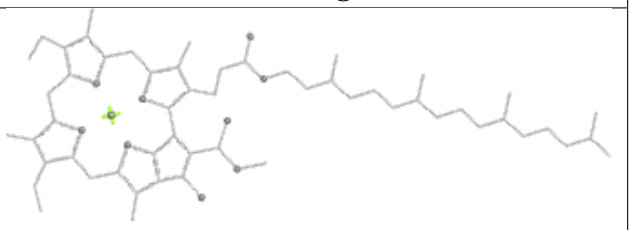
Bond lengths



Bond angles

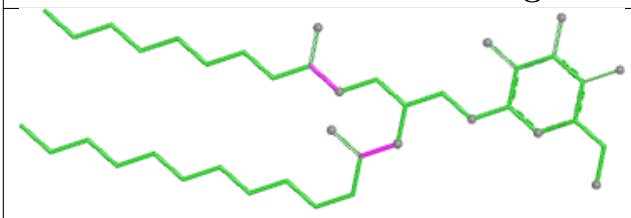


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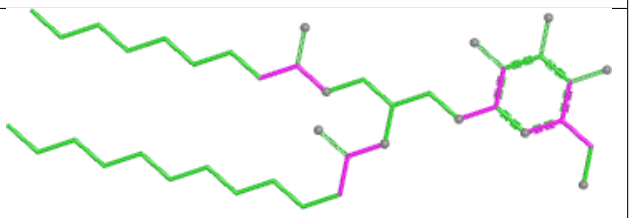


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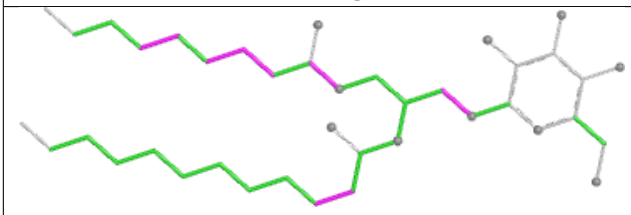
Ligand LMG 4 623



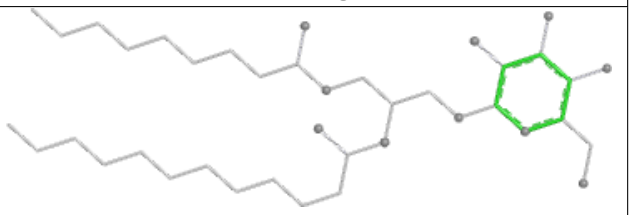
Bond lengths



Bond angles

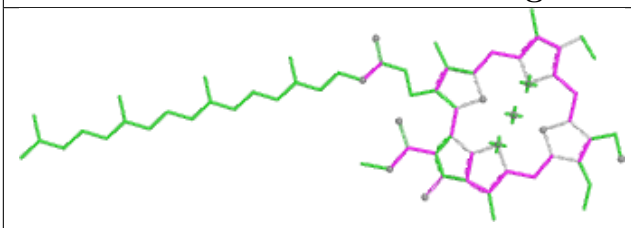


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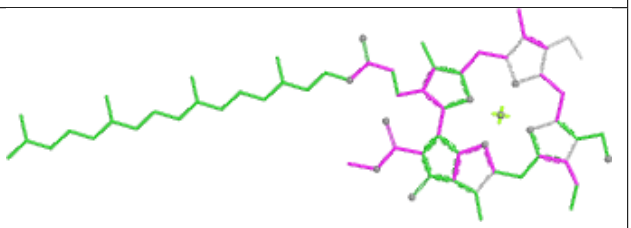


Rings

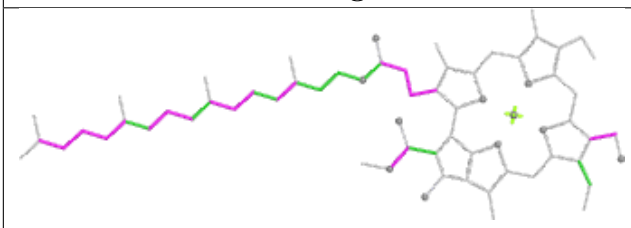
Ligand CHL Z 607



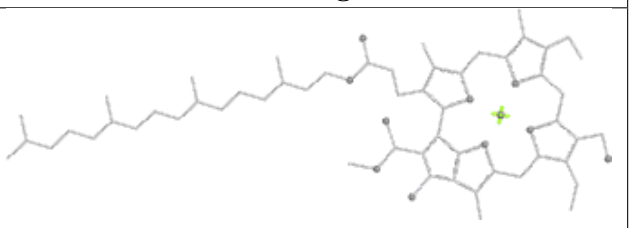
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Bond angles

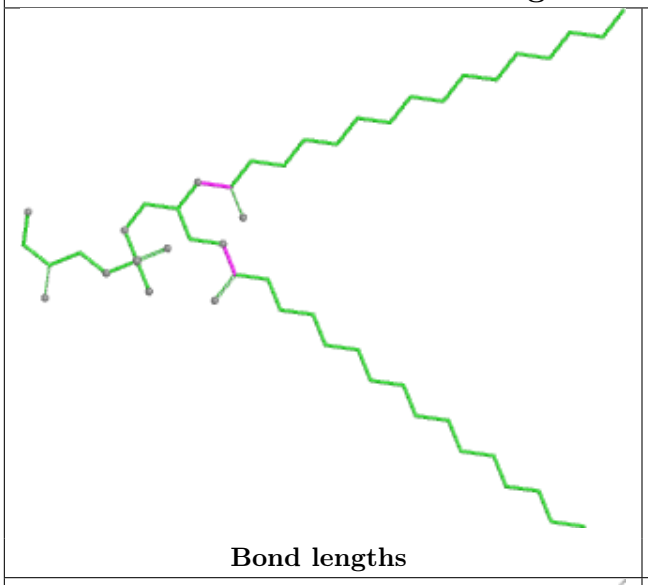


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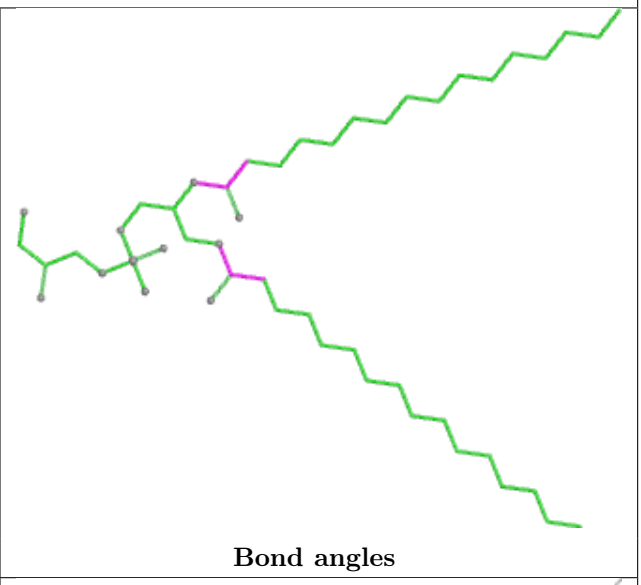


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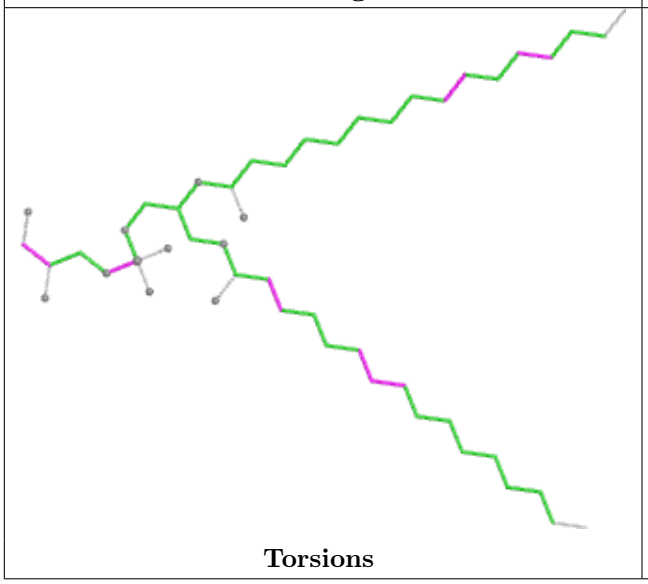
Ligand LHG 1 620



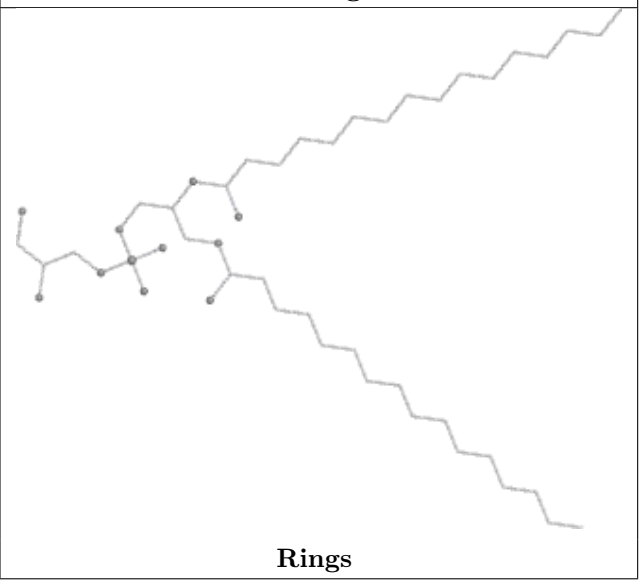
Bond lengths



Bond angles



Torsions

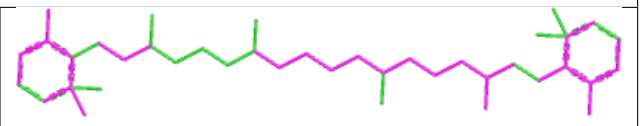


Rings

Ligand BCR L 308



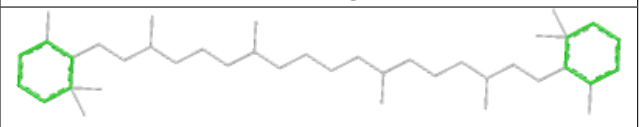
Bond lengths



Bond angles

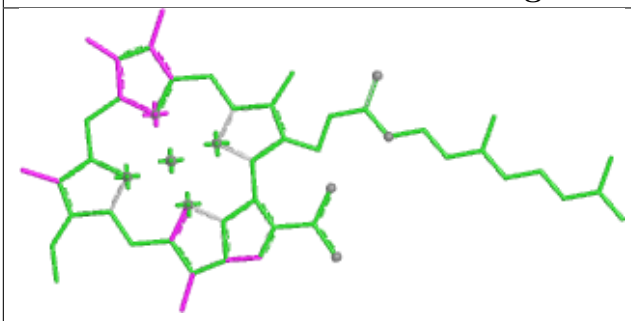


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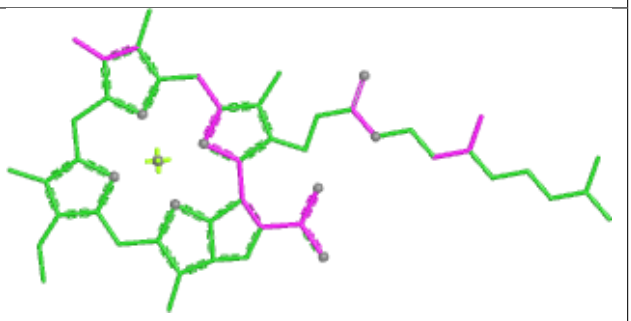


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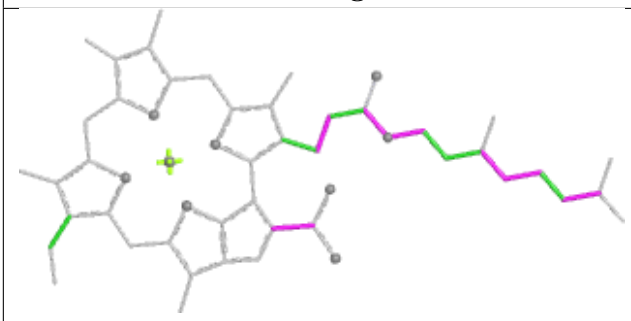
Ligand CLA B 811



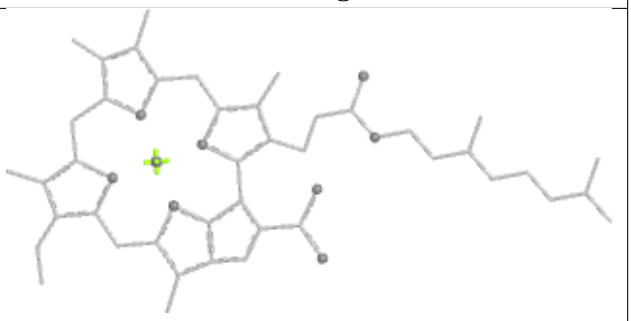
Bond lengths



Bond angles

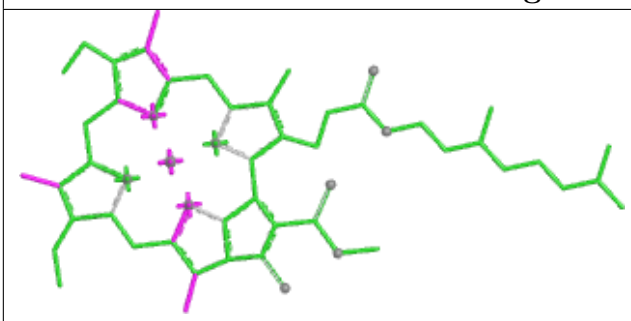


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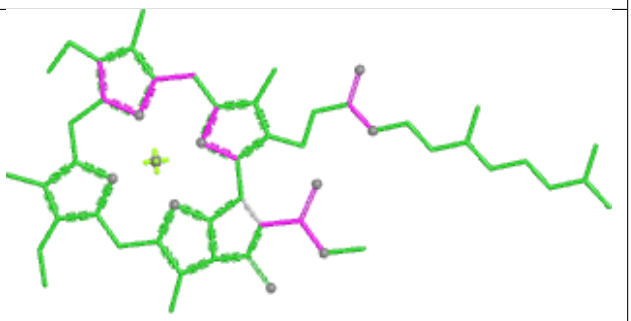


Rings

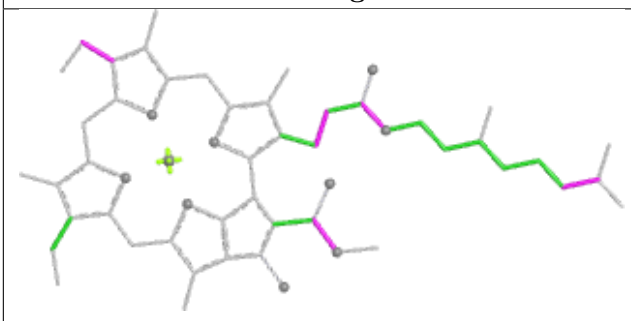
Ligand CLA A 839



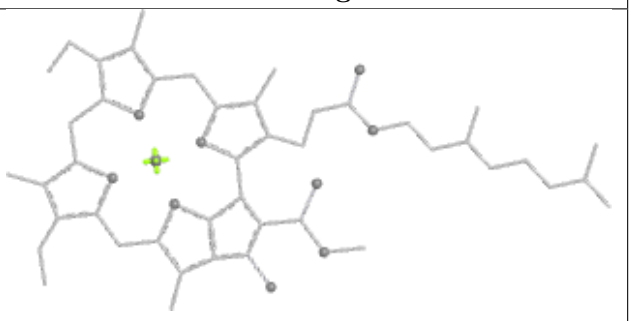
Bond lengths



Bond angles

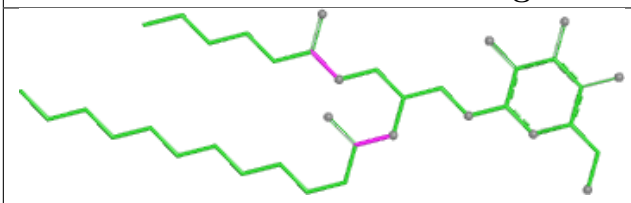


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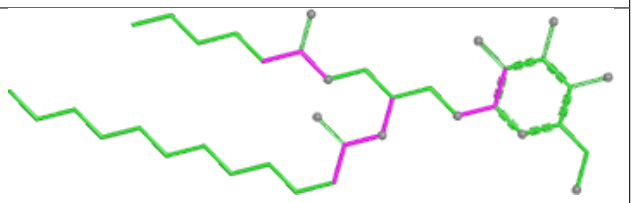


Rings

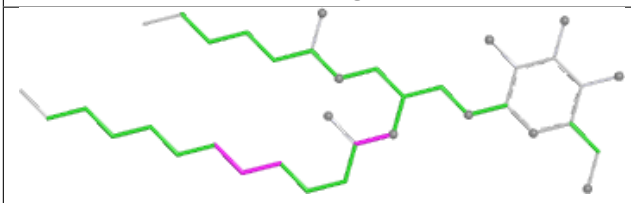
Ligand LMG L 2631



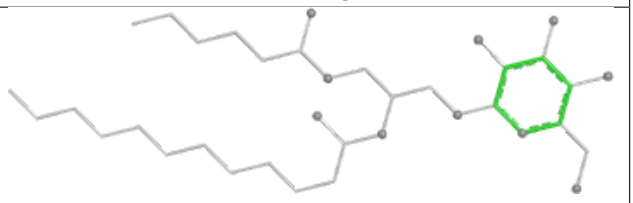
Bond lengths



Bond angles

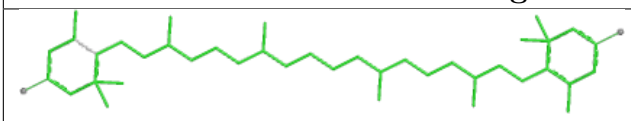


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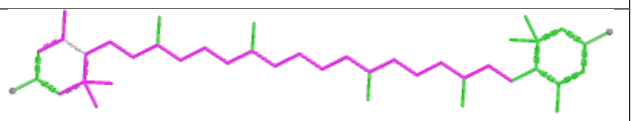


Rings

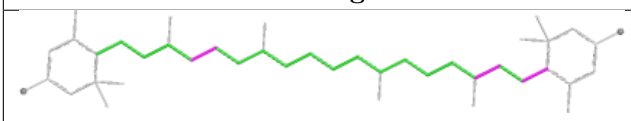
Ligand LUT W 1621



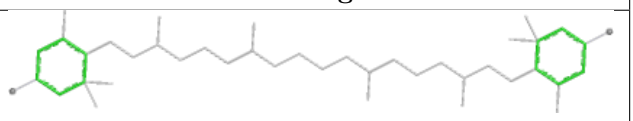
Bond lengths



Bond angles

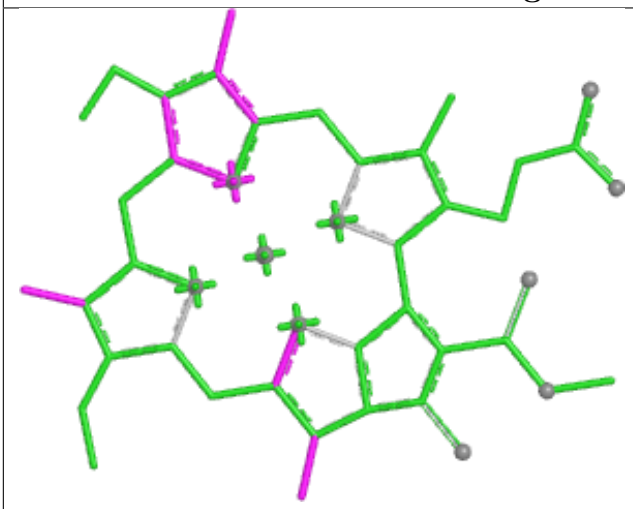


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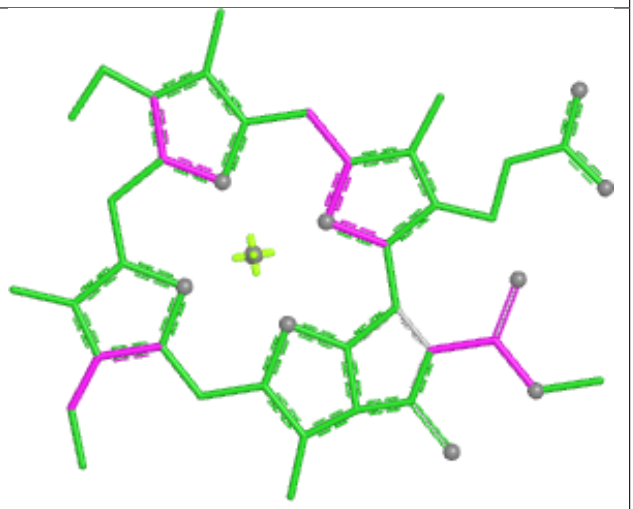


Rings

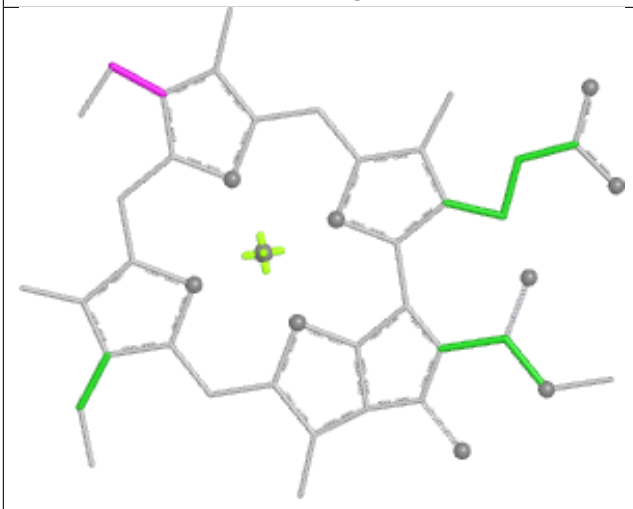
Ligand CLA A 817



Bond lengths



Bond angles

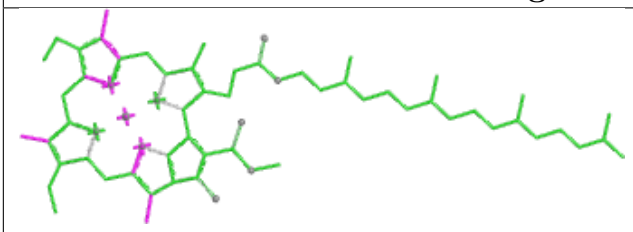


Torsions

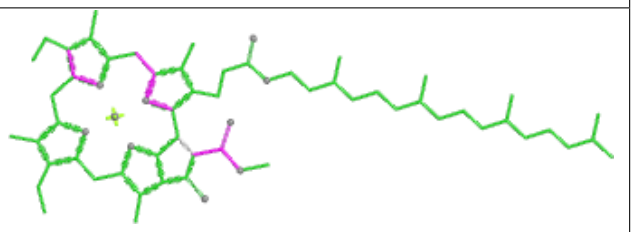


Rings

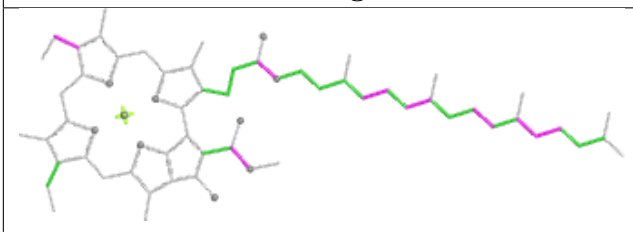
Ligand CLA 5 607



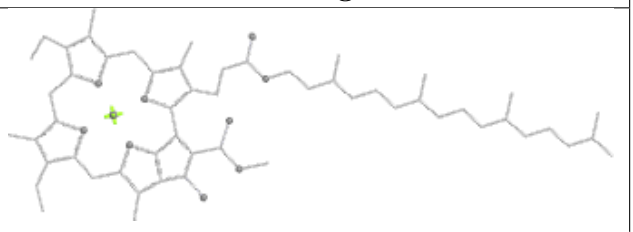
Bond lengths



Bond angles

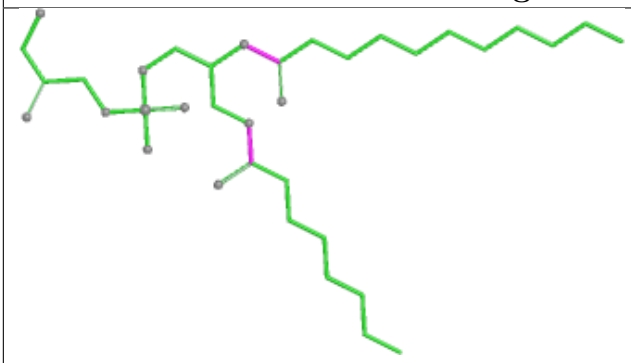


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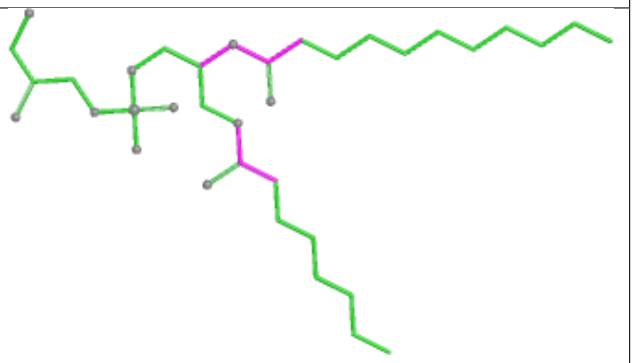


Rings

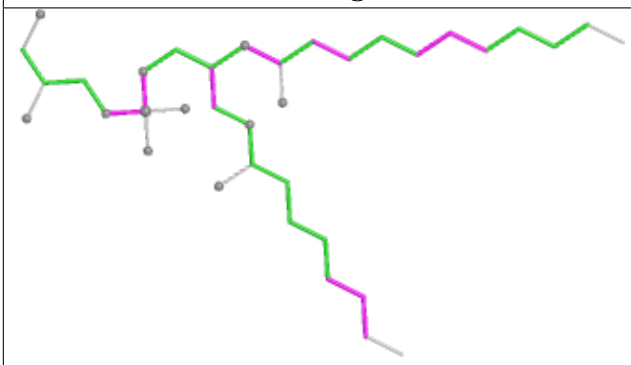
Ligand LHG O 2631



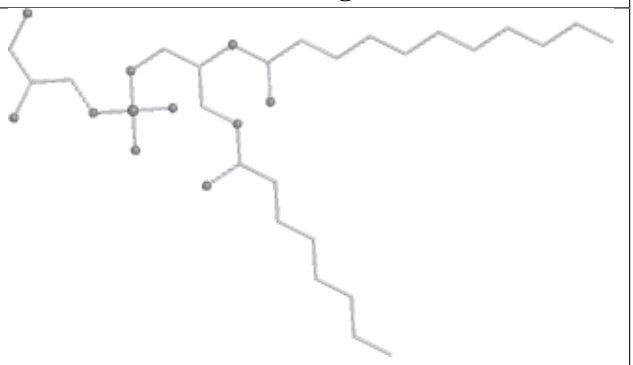
Bond lengths



Bond angles

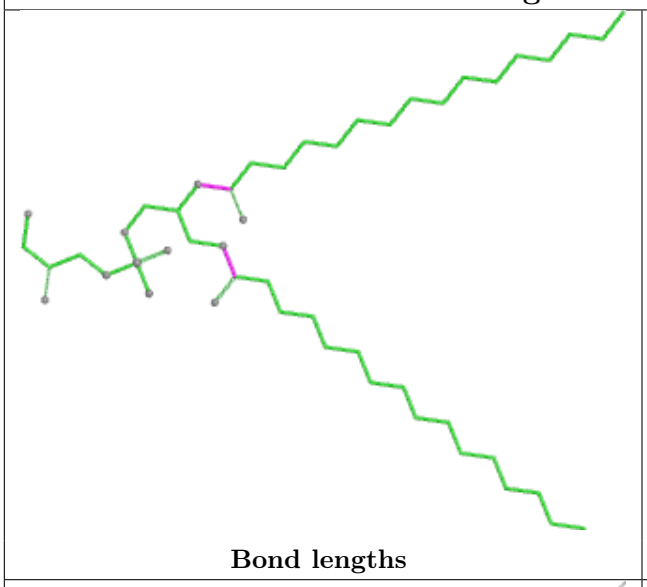


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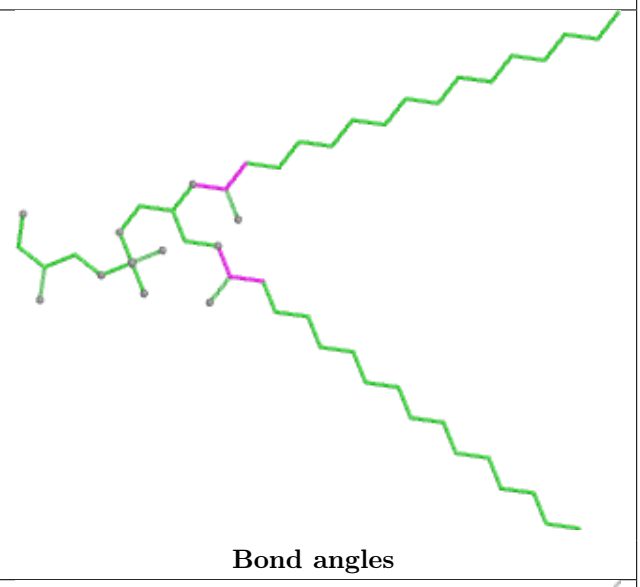


Rings

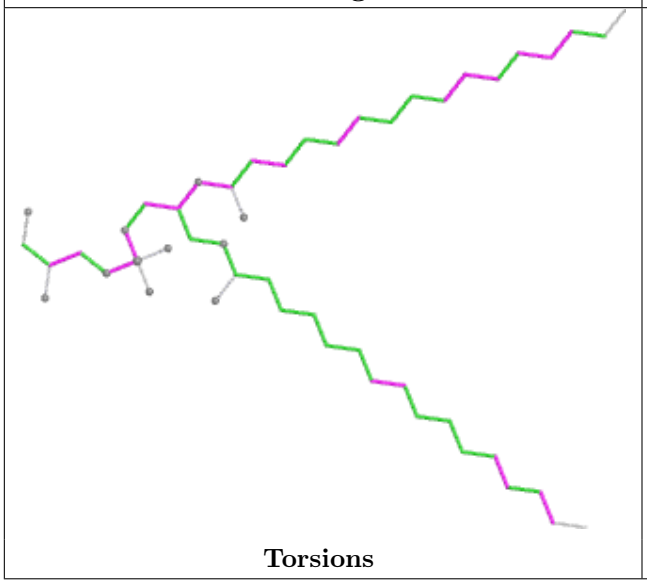
Ligand LHG A 861



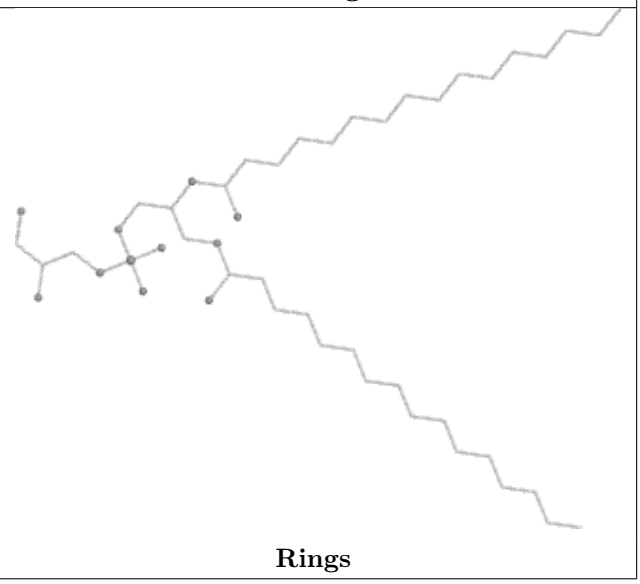
Bond lengths



Bond angles



Torsions

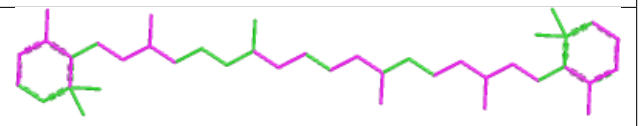


Rings

Ligand BCR 9 621



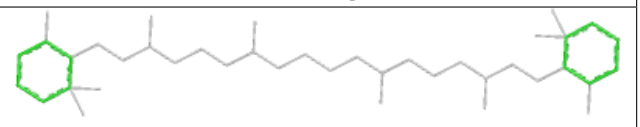
Bond lengths



Bond angles

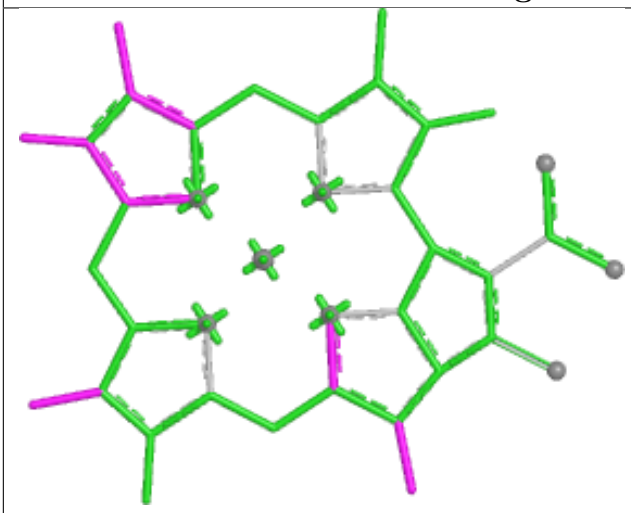


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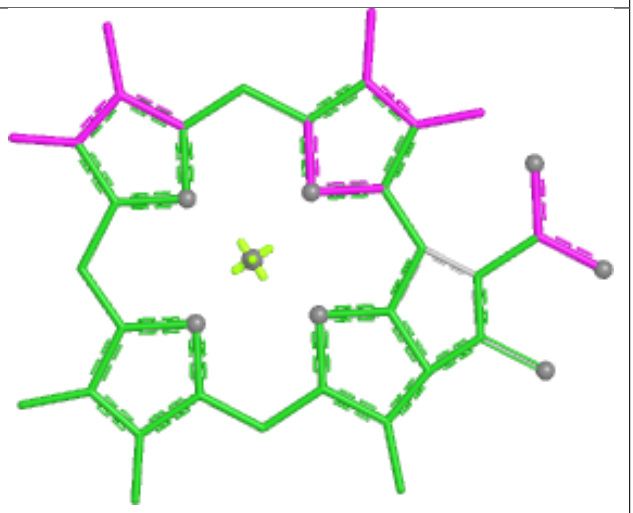


Rings

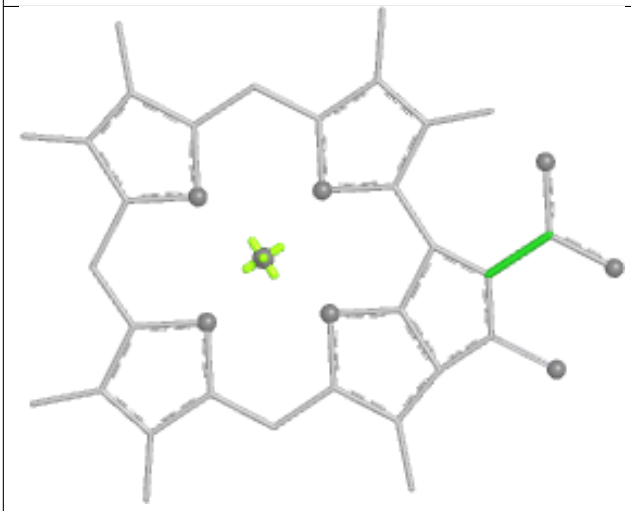
Ligand CLA O 2002



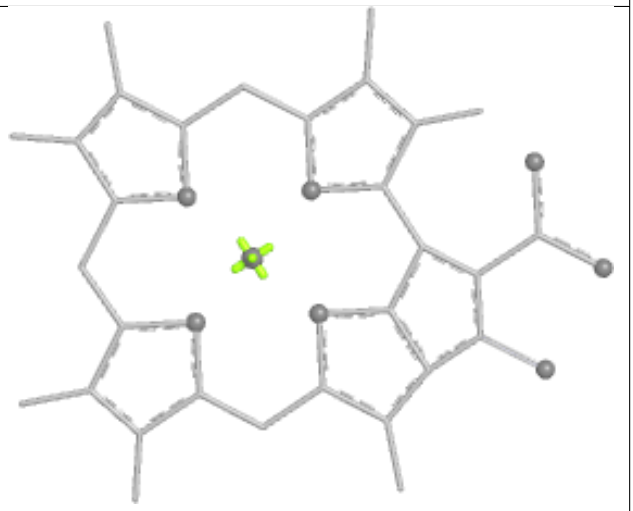
Bond lengths



Bond angles

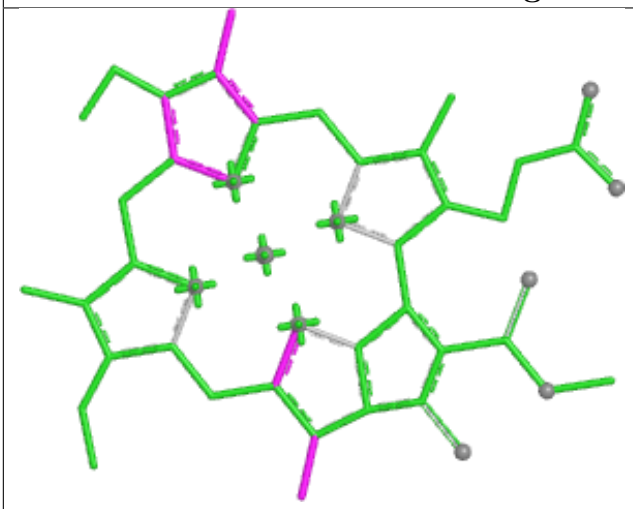


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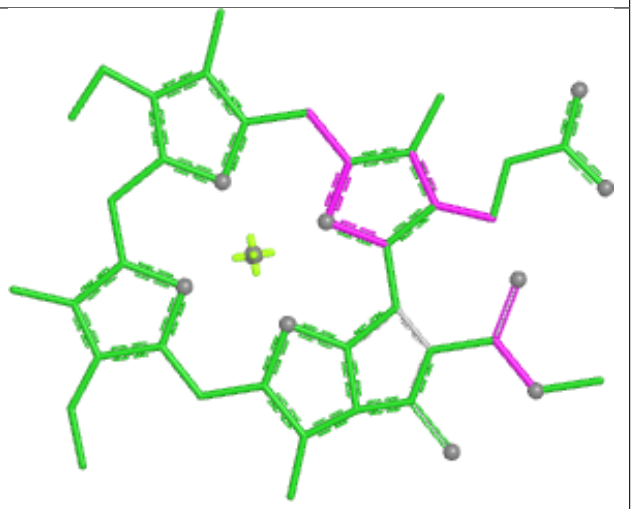


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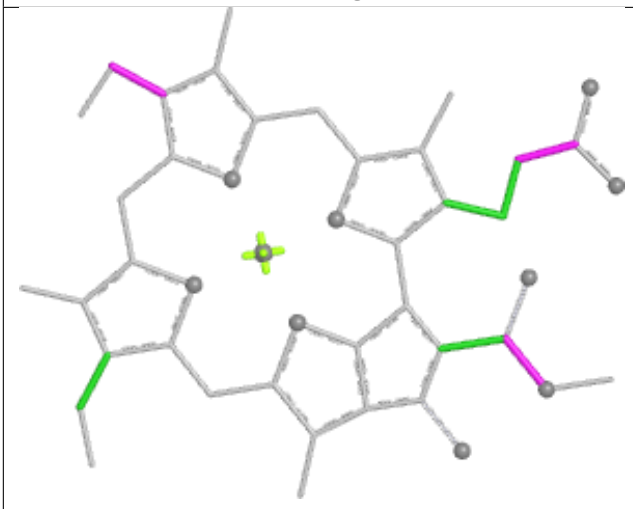
Ligand CLA V 603



Bond lengths



Bond angles

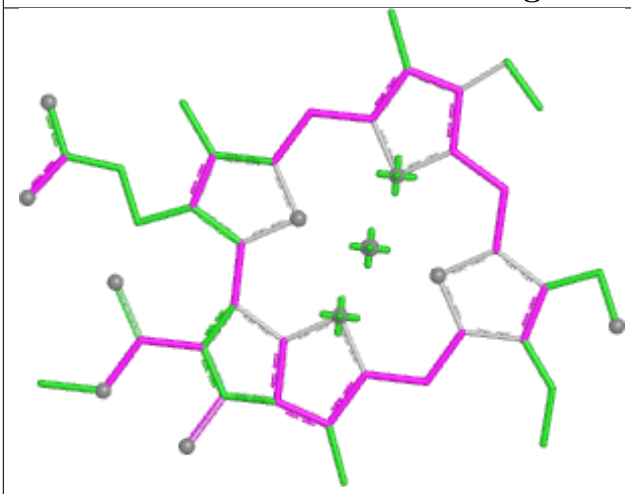


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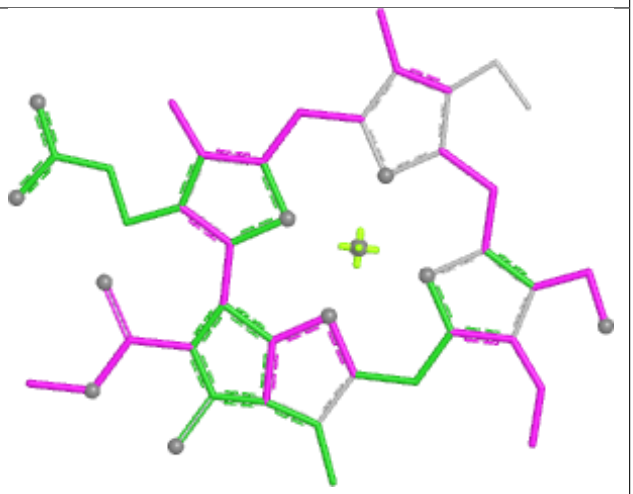


Rings

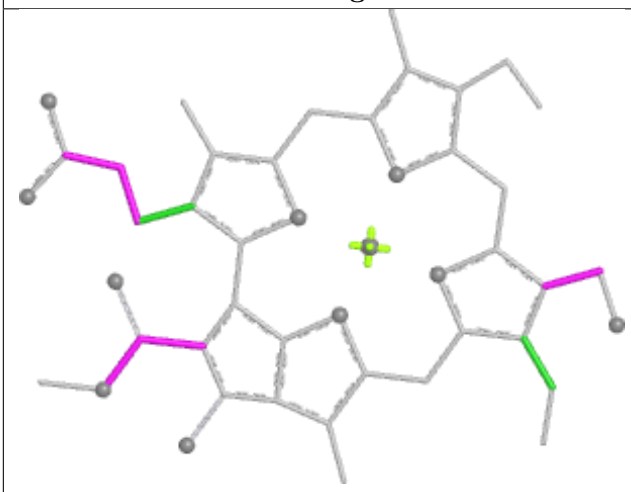
Ligand CHL Y 606



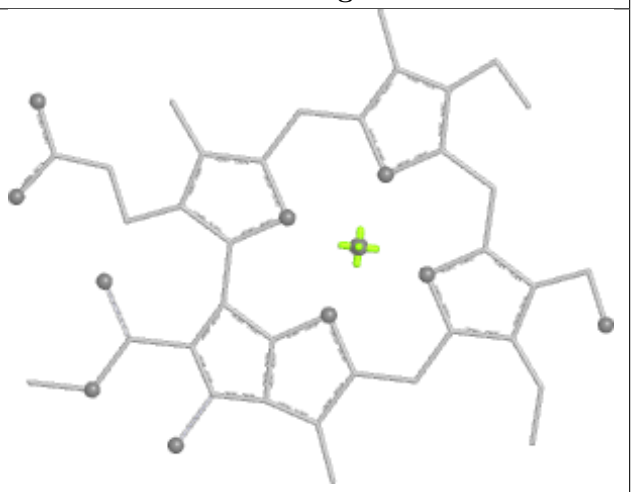
Bond lengths



Bond angles

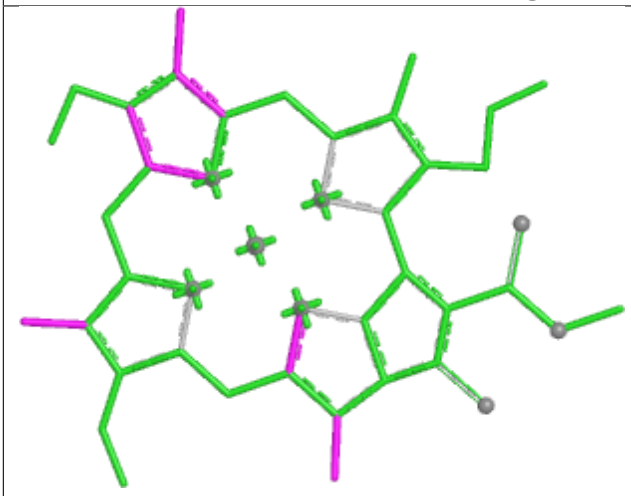


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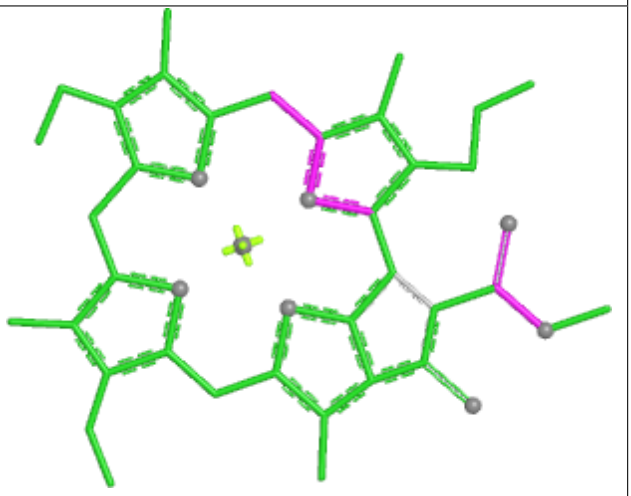


Rings

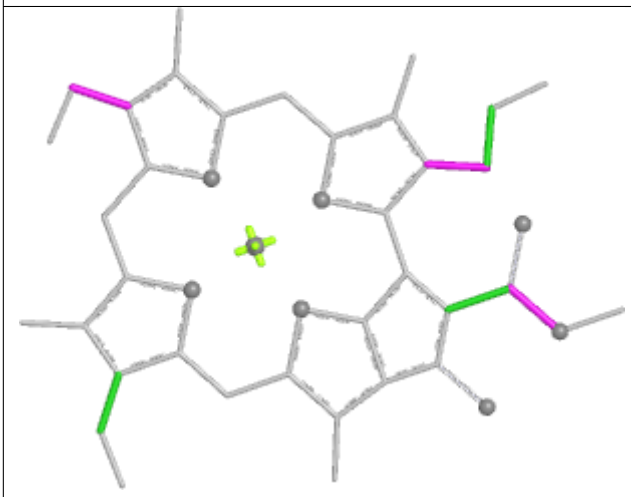
Ligand CLA V 611



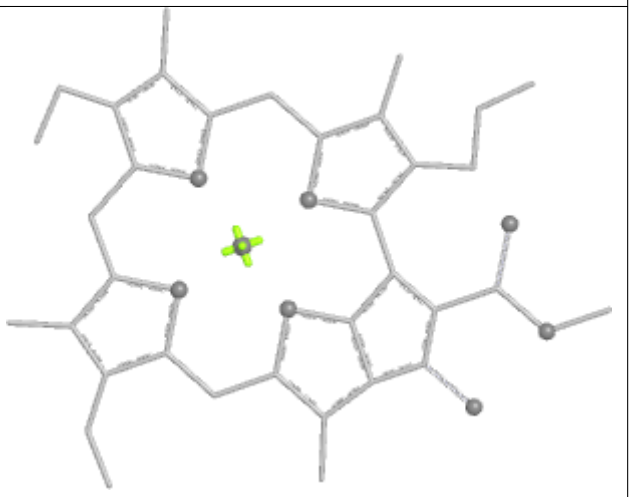
Bond lengths



Bond angles

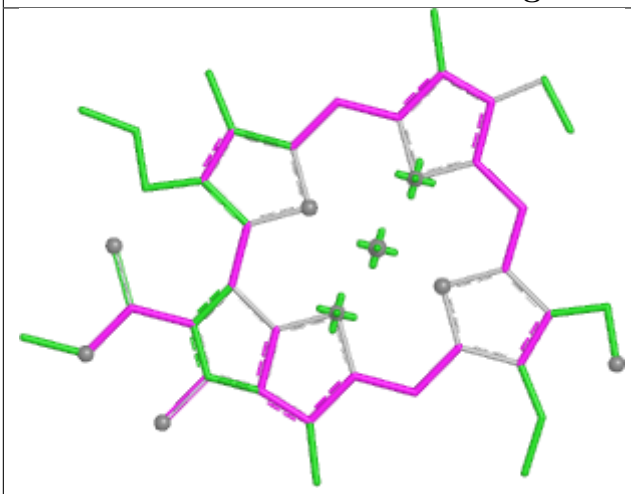


Torsions

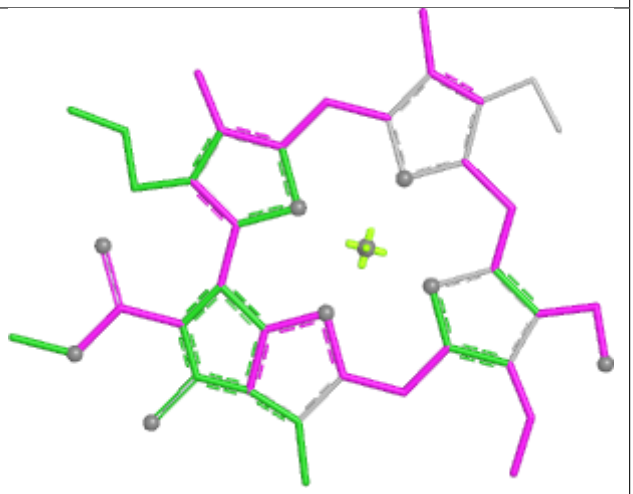


Rings

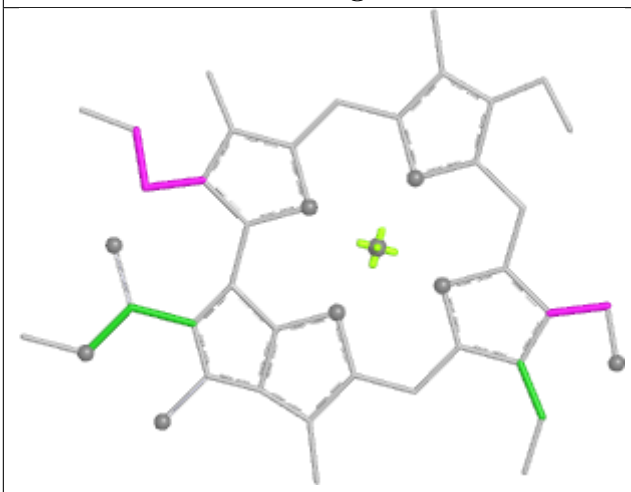
Ligand CHL V 605



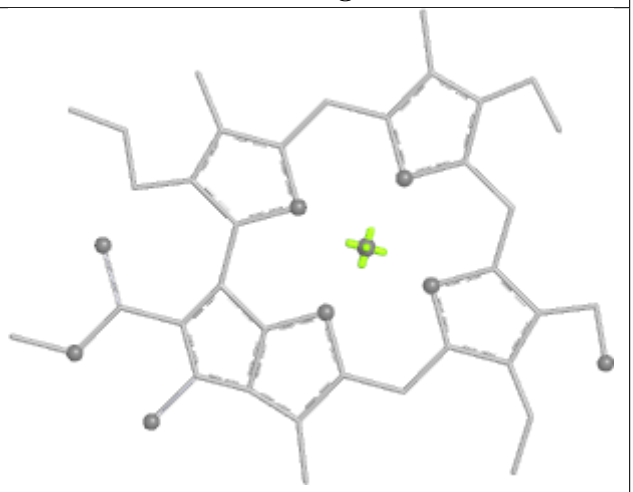
Bond lengths



Bond angles

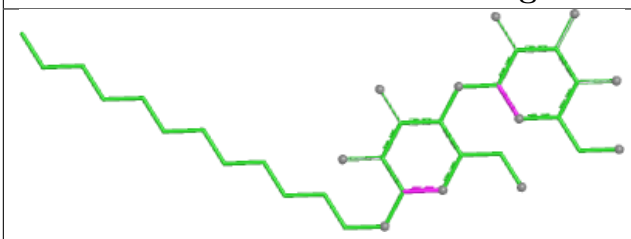


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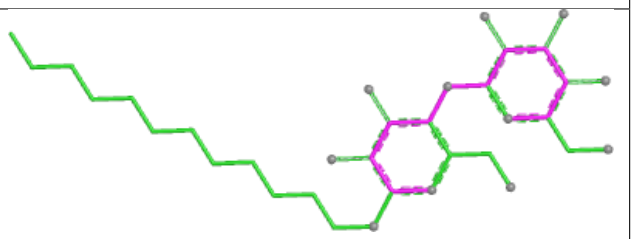


Rings

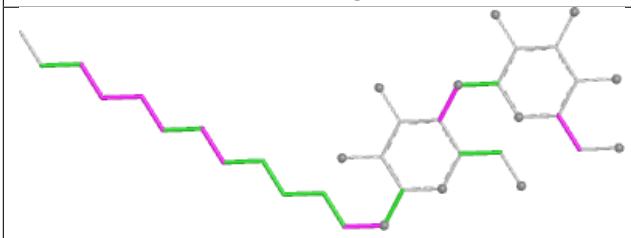
Ligand LMU A 857



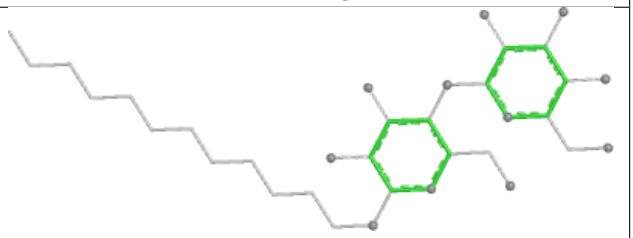
Bond lengths



Bond angles

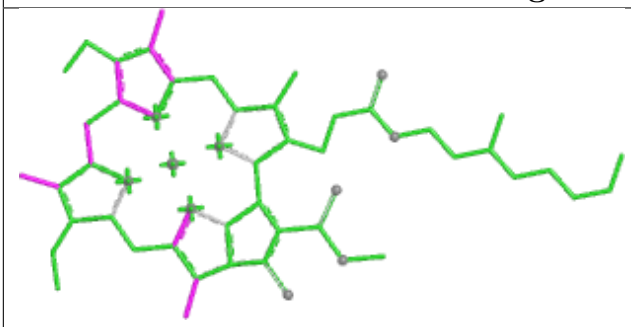


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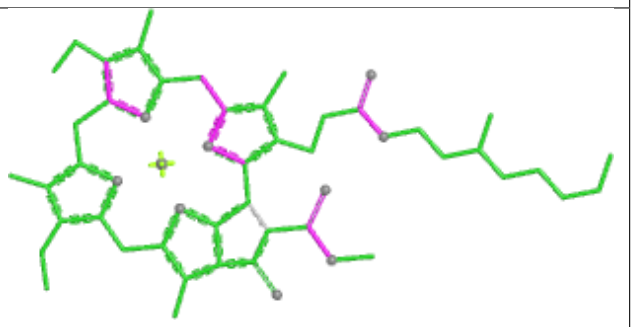


Rings

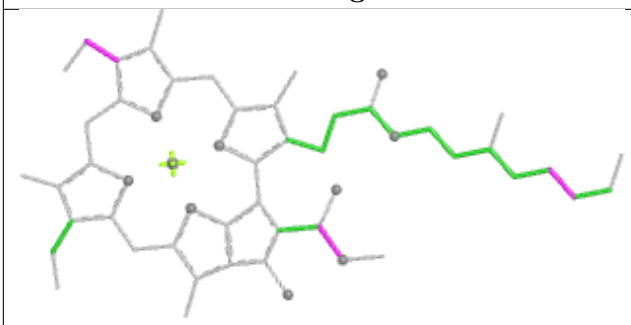
Ligand CLA 5 610



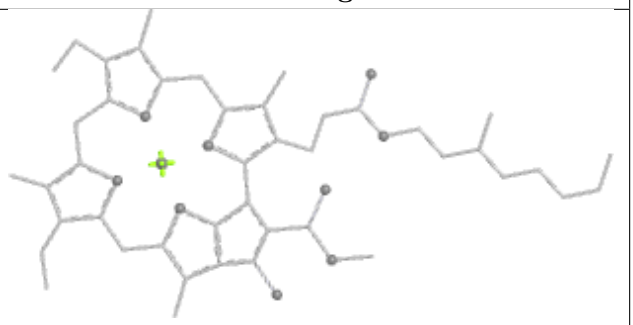
Bond lengths



Bond angles

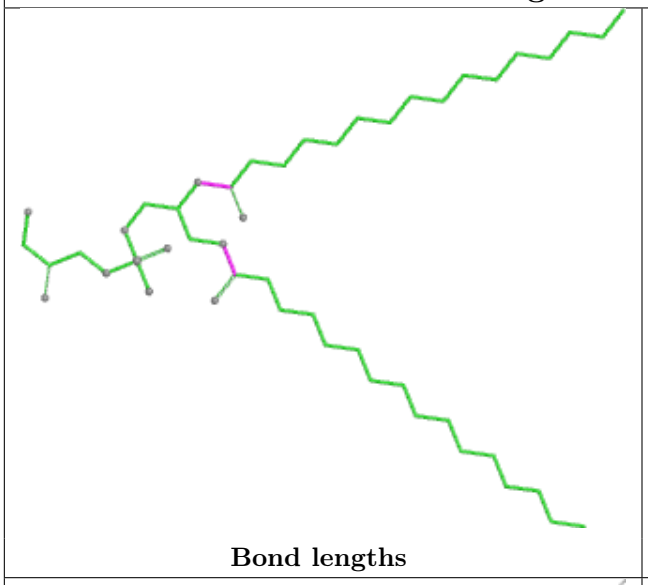


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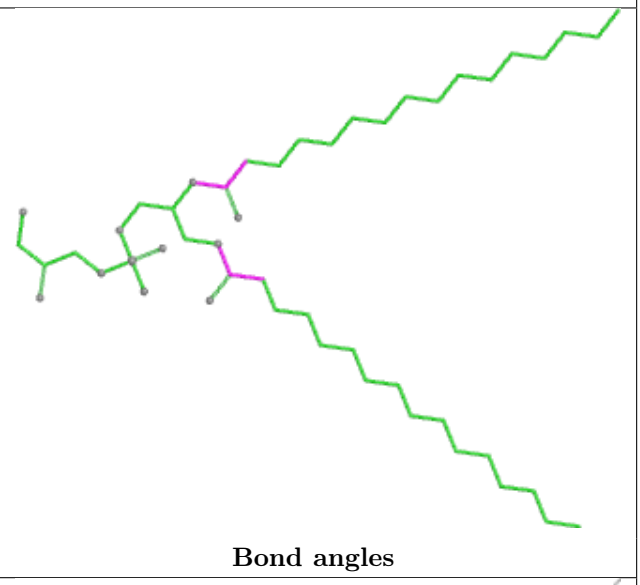


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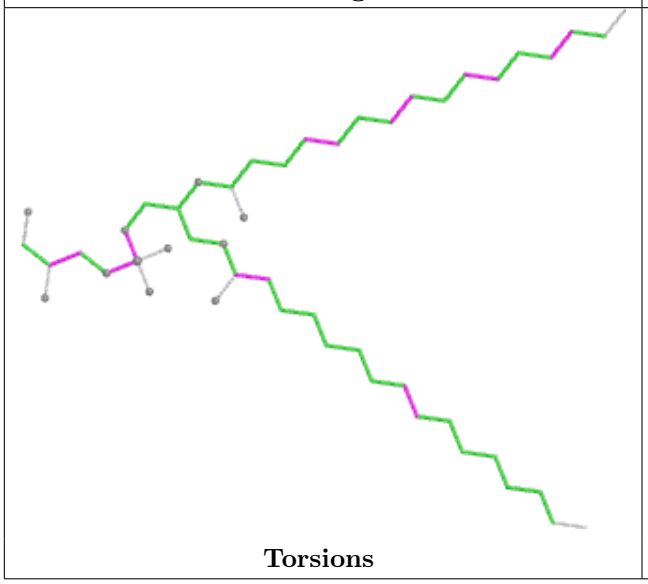
Ligand LHG 8 622



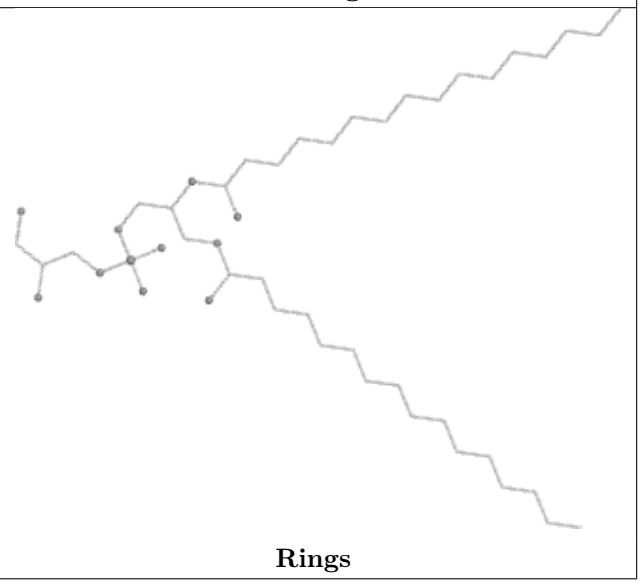
Bond lengths



Bond angles

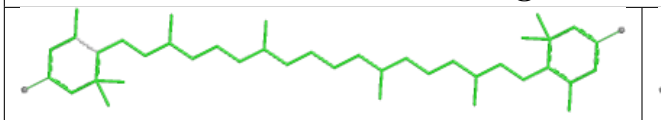


Torsions



Rings

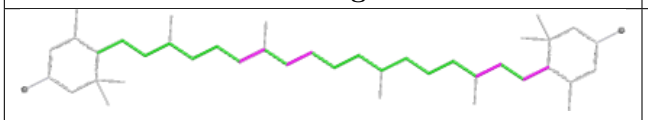
Ligand LUT U 1620



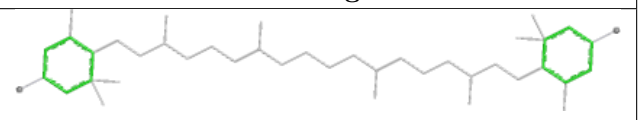
Bond lengths



Bond angles

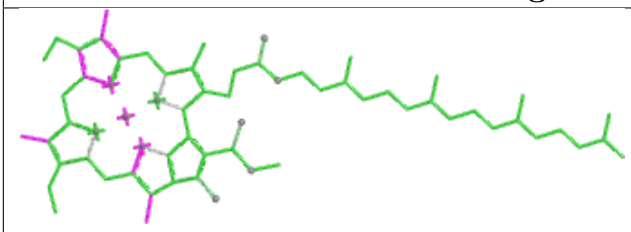


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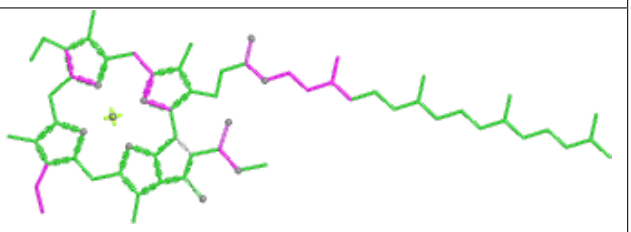


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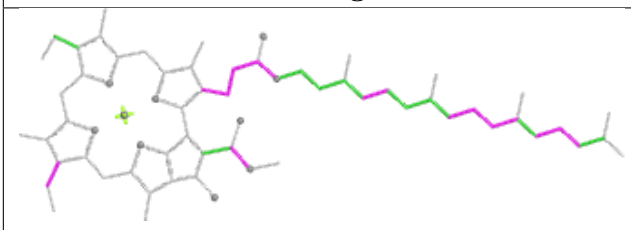
Ligand CLA 6 616



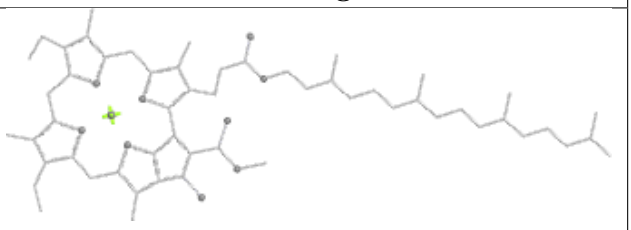
Bond lengths



Bond angles

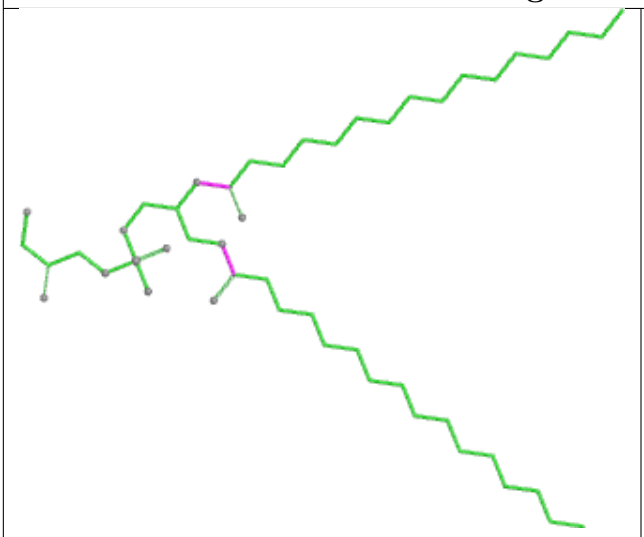


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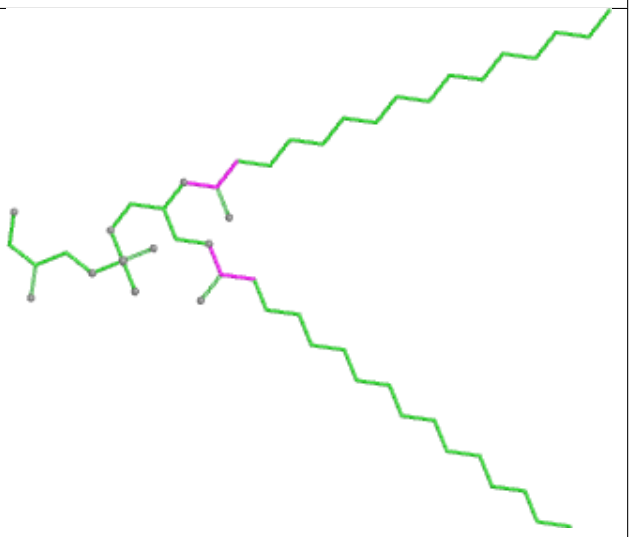


Rings

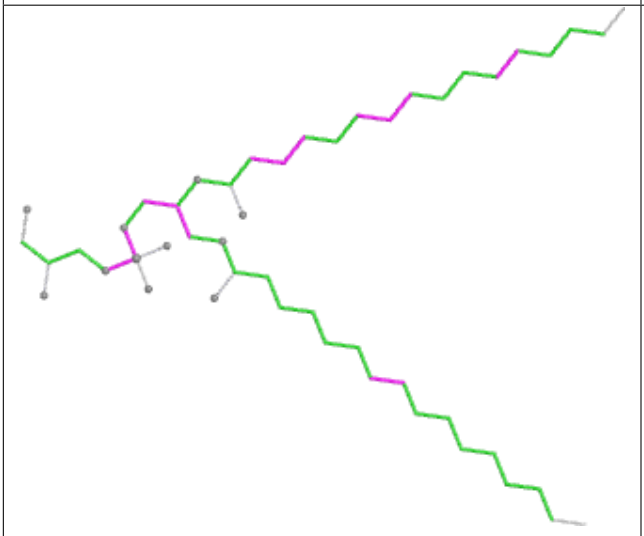
Ligand LHG 5 623



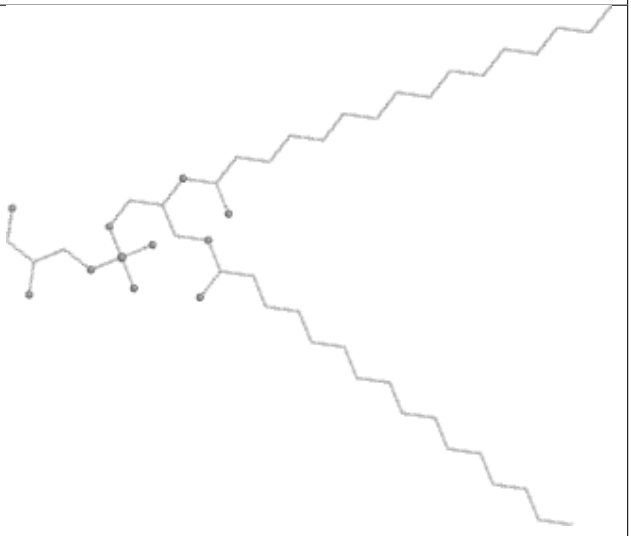
Bond lengths



Bond angles

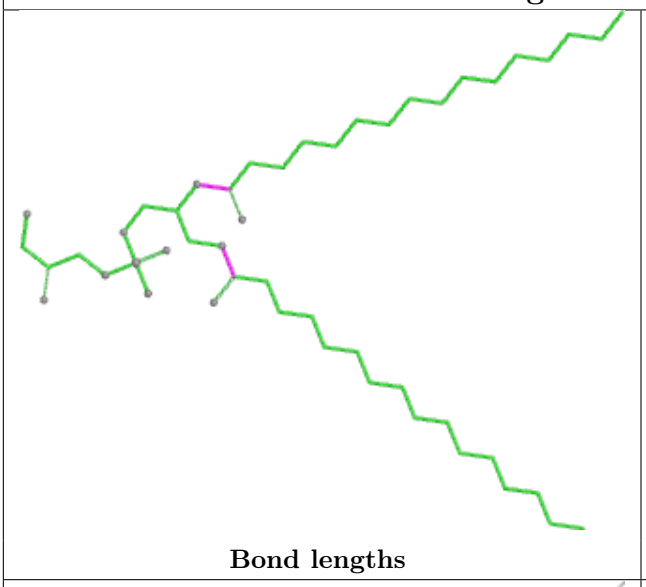


Torsions

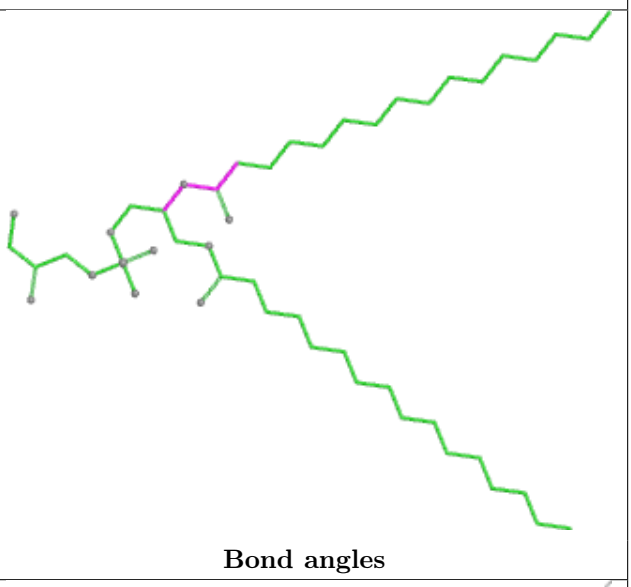


Rings

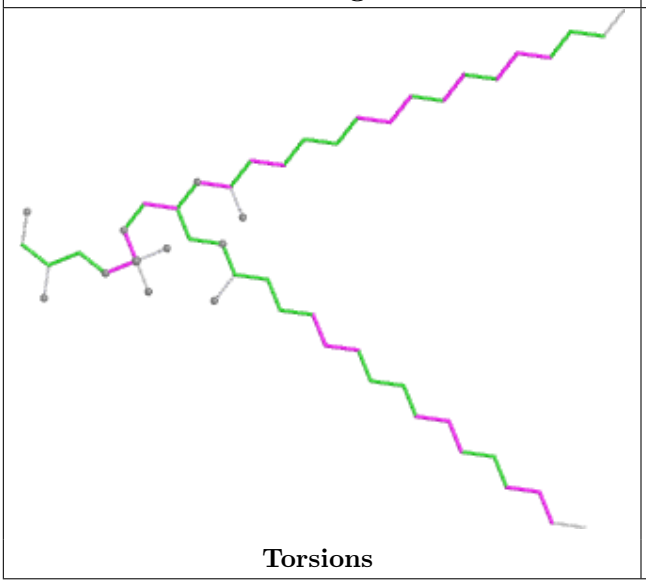
Ligand LHG 9 623



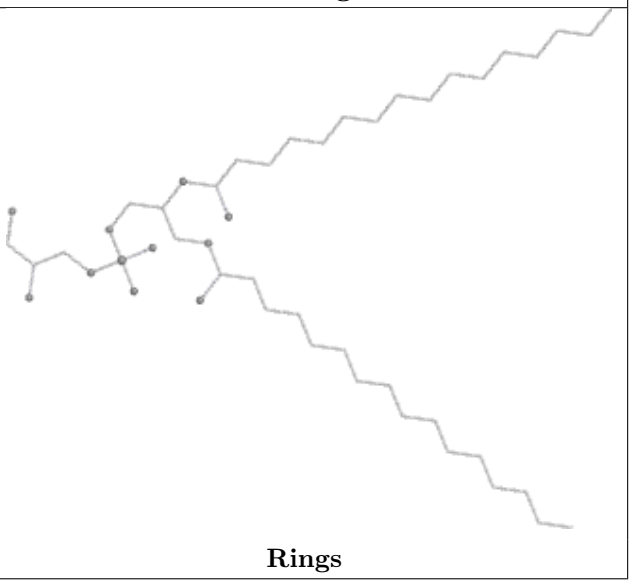
Bond lengths



Bond angles



Torsions

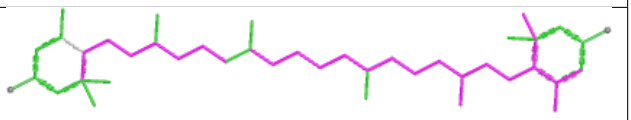


Rings

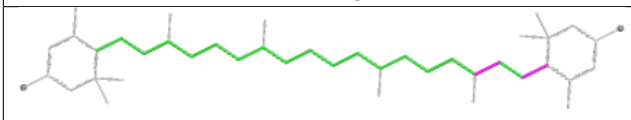
Ligand LUT 1 617



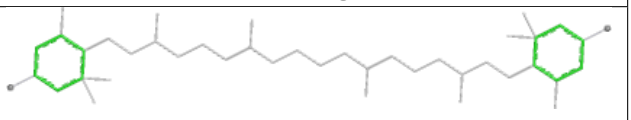
Bond lengths



Bond angles

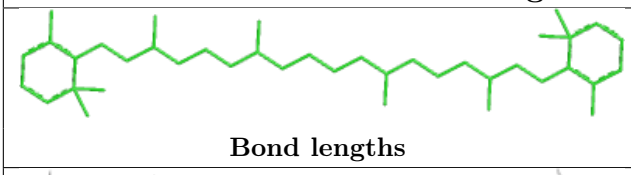


Torsions

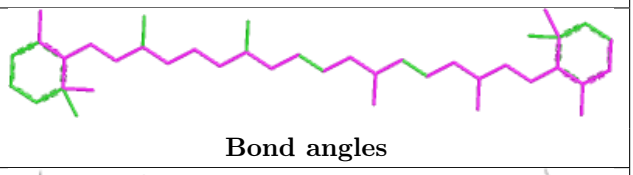


Rings

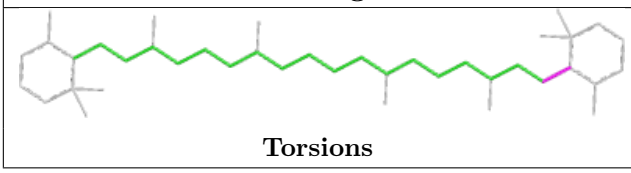
Ligand BCR 1 619



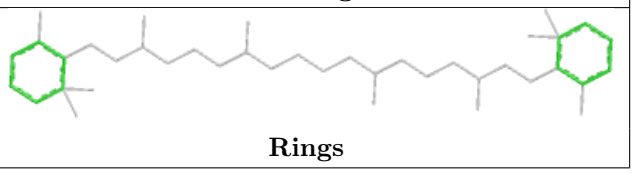
Bond lengths



Bond angles

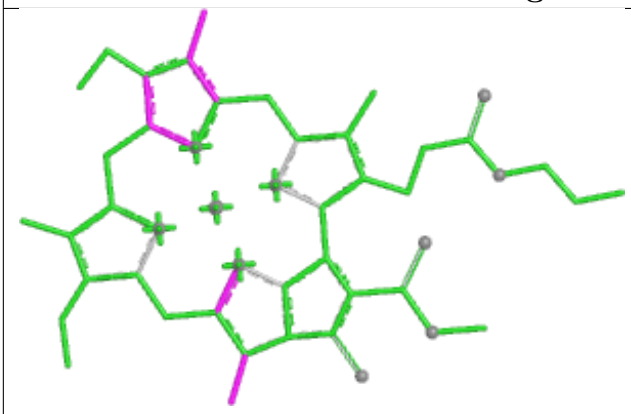


Torsions

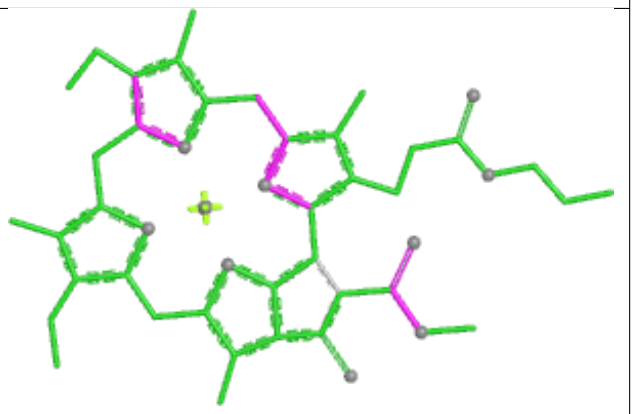


Rings

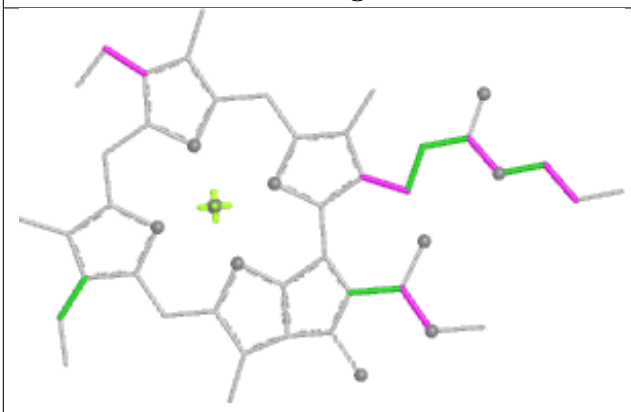
Ligand CLA Z 614



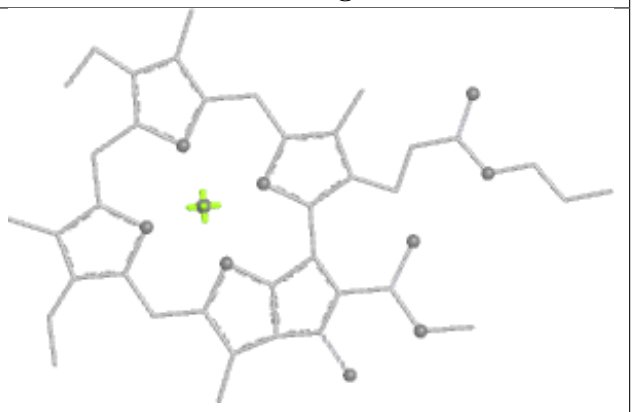
Bond lengths



Bond angles

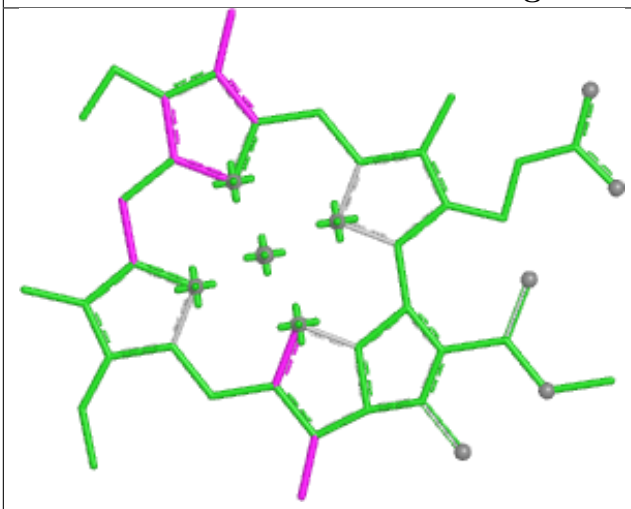


Torsions

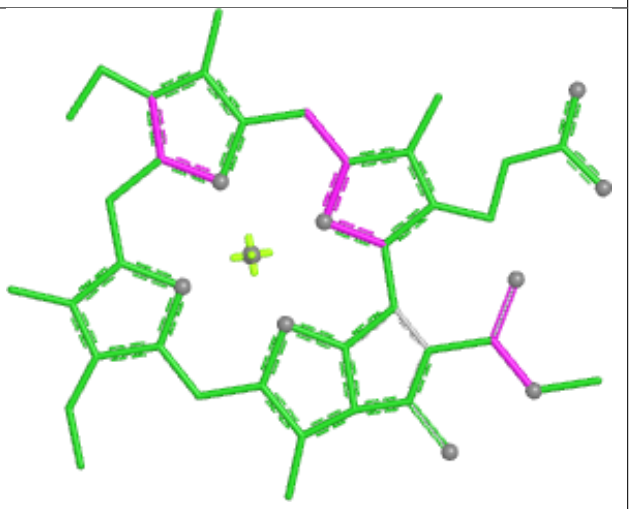


Rings

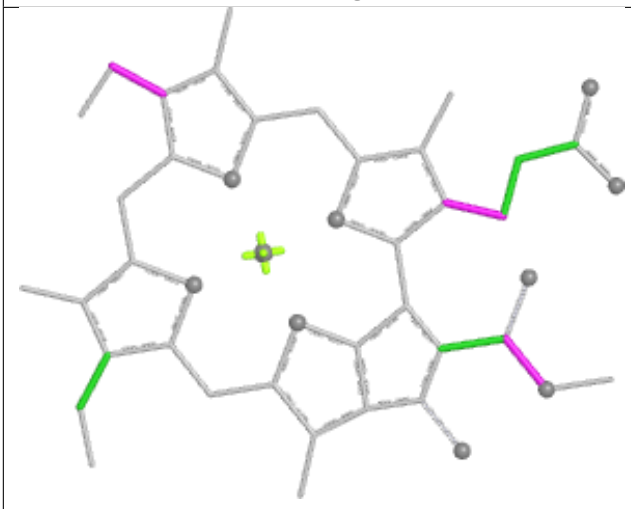
Ligand CLA V 614



Bond lengths



Bond angles

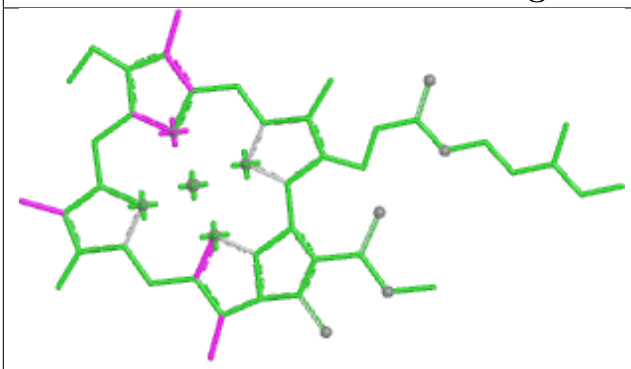


Torsions

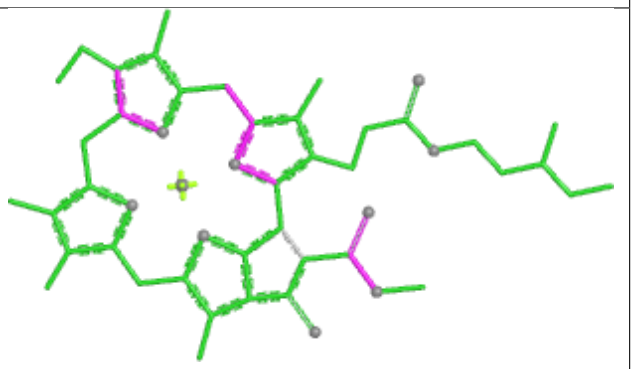


Rings

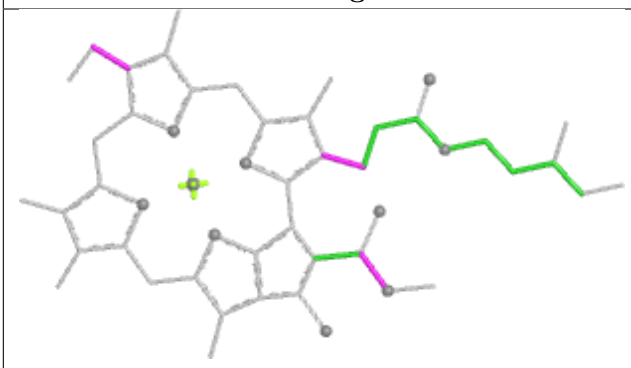
Ligand CLA 5 608



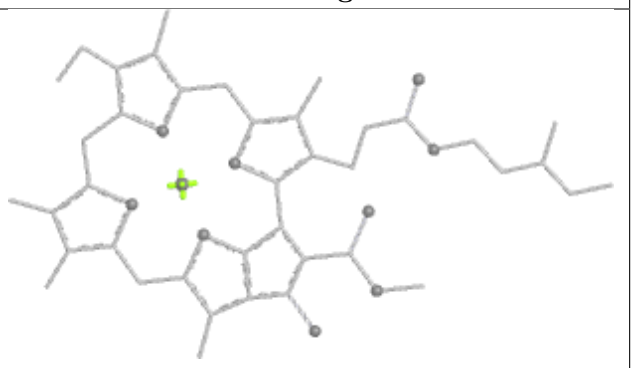
Bond lengths



Bond angles

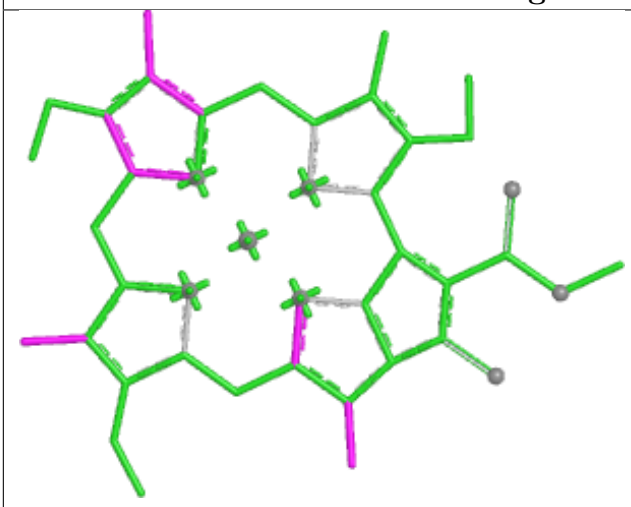


Torsions

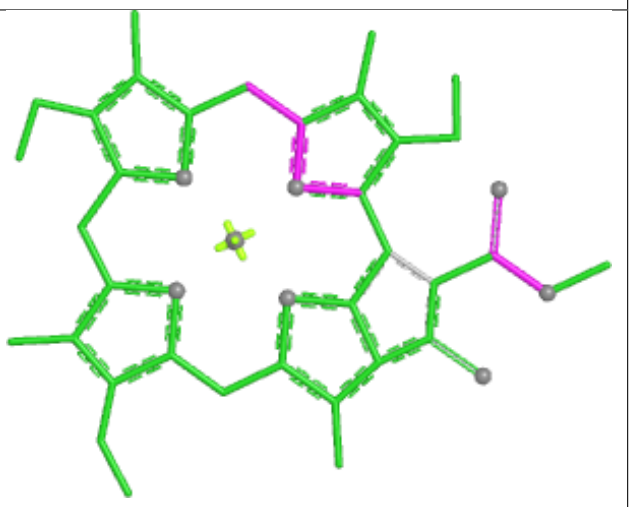


Rings

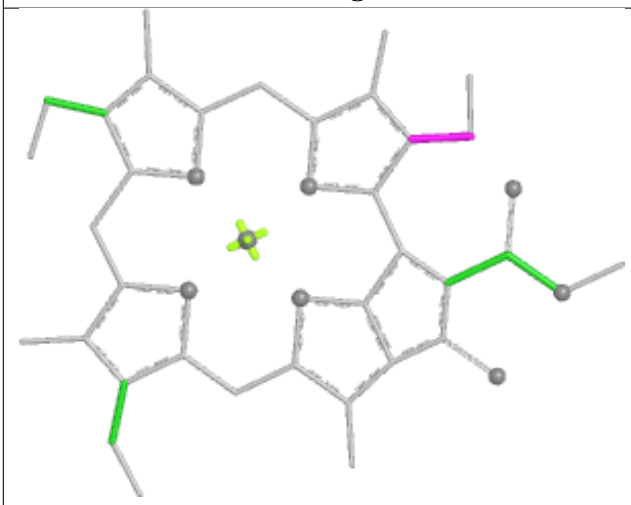
Ligand CLA 7 607



Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

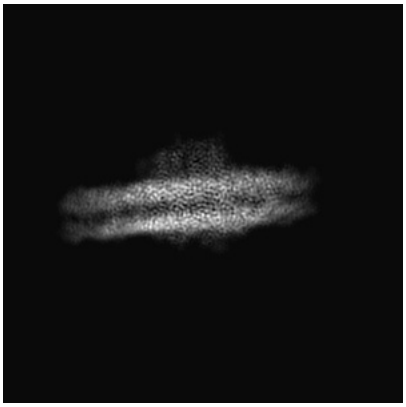
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30926. 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

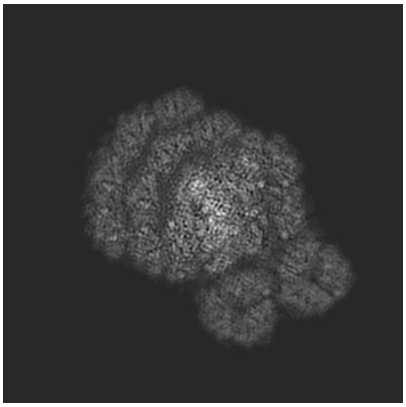
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

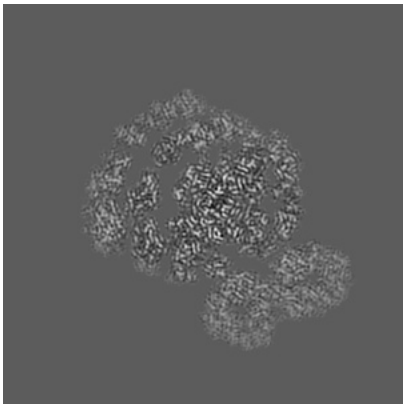
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

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

6.3 Largest variance slices (i)

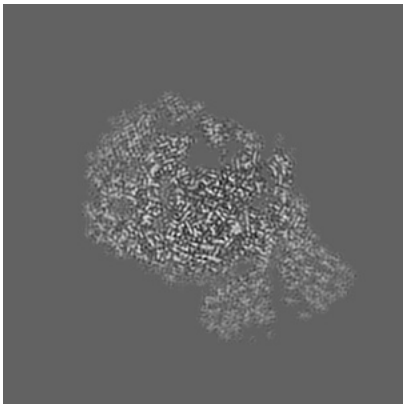
6.3.1 Primary map



X Index: 194



Y Index: 153

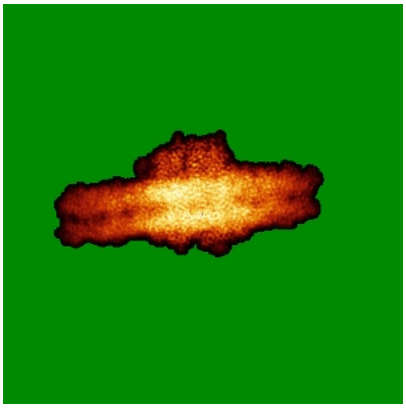


Z Index: 190

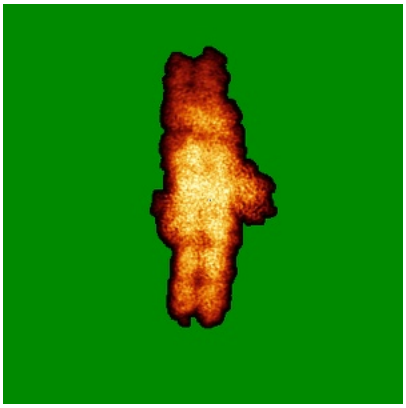
The images above show the largest variance slices of the map in three orthogonal directions.

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

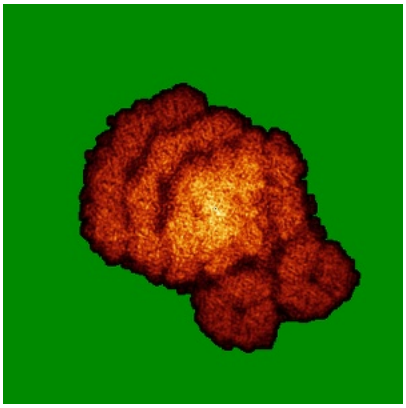
6.4.1 Primary map



X



Y

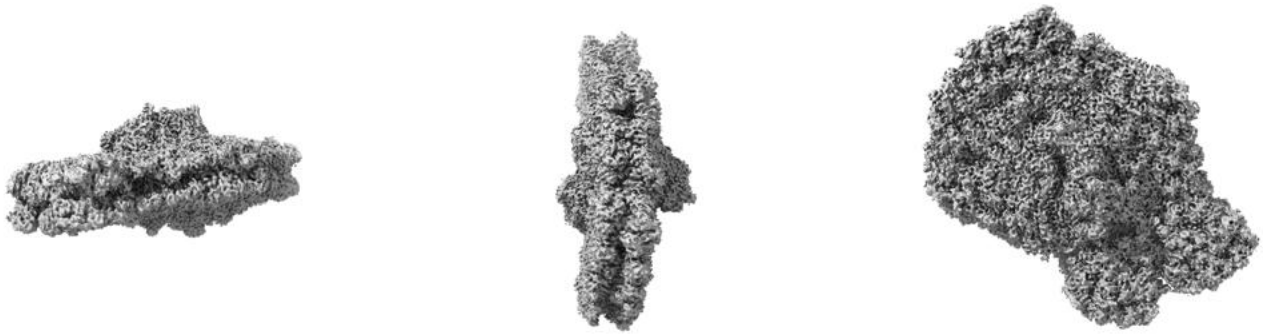


Z

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

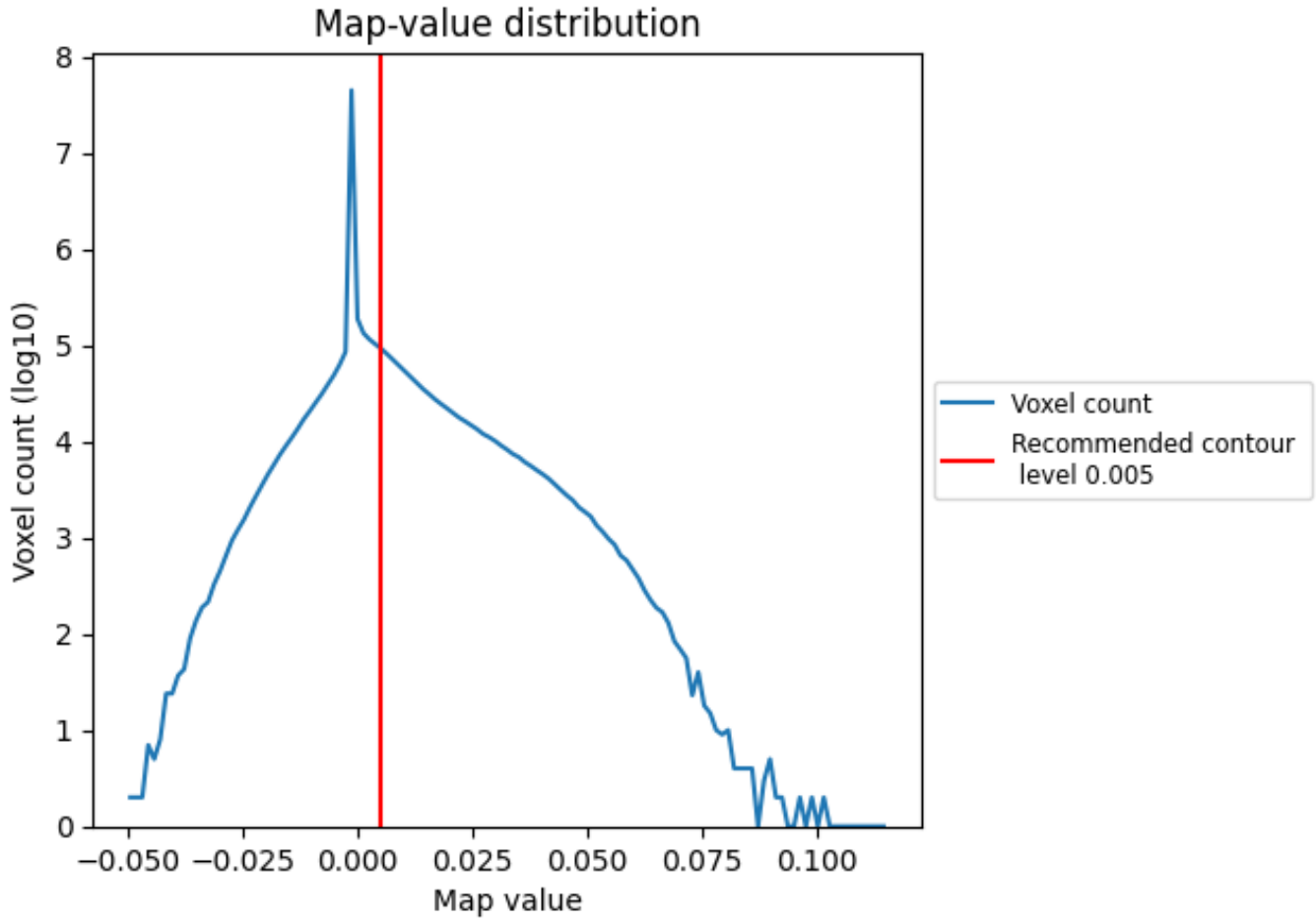
6.6 Mask visualisation (i)

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

7 Map analysis

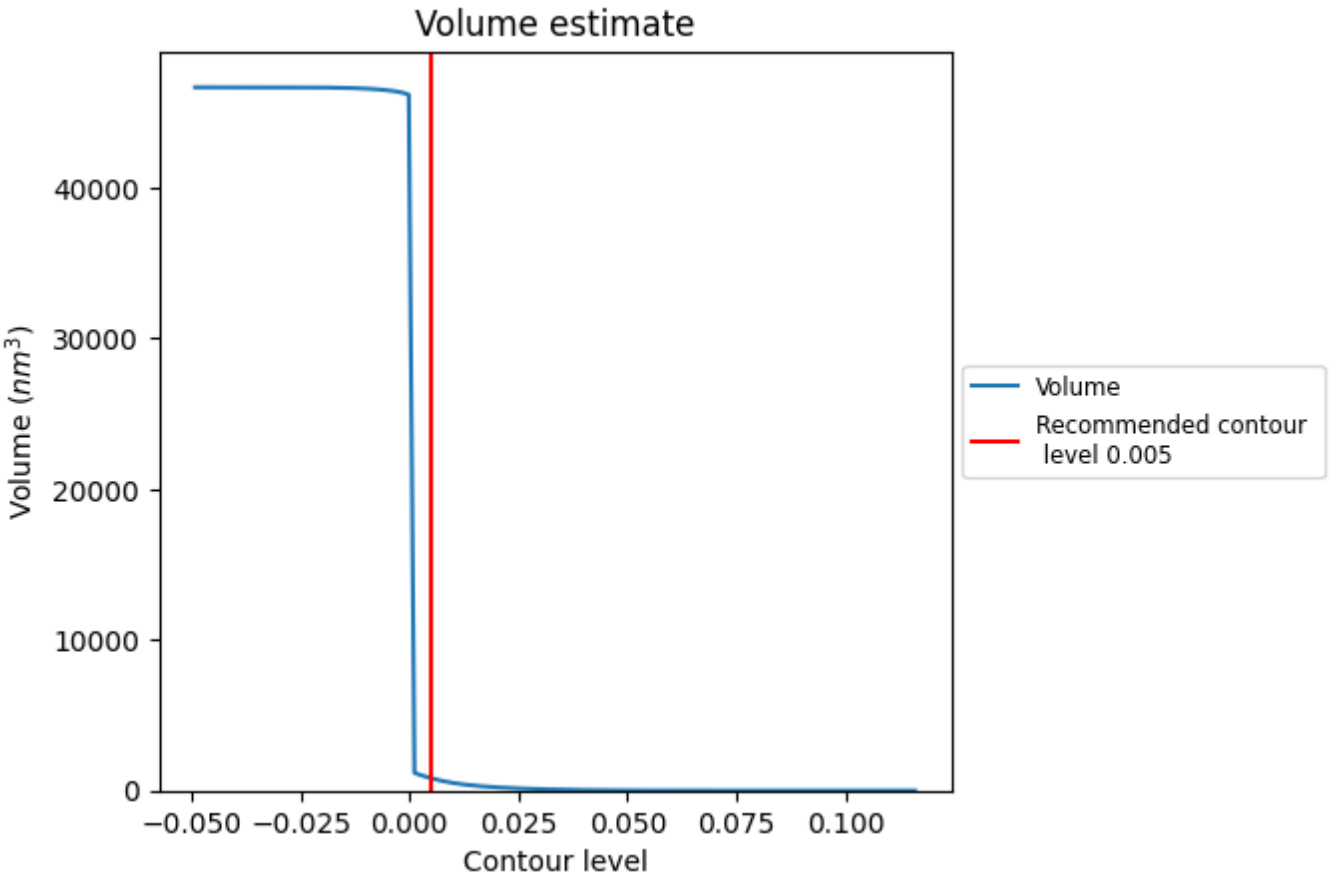
This section contains the results of statistical analysis of the map.

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.

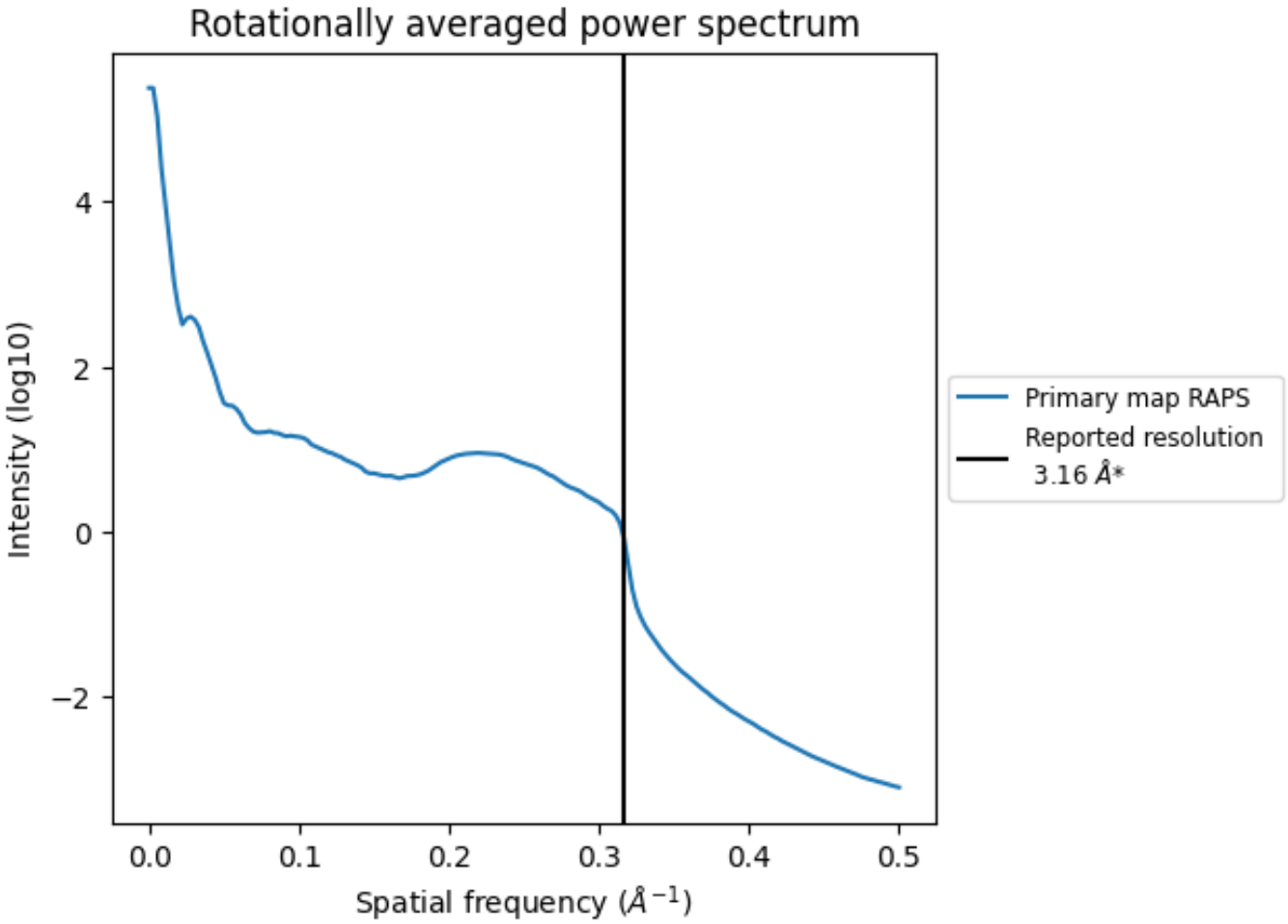
7.2 Volume estimate



The volume at the recommended contour level is 811 nm^3; this corresponds to an approximate mass of 733 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 0.316 $Å^{-1}$

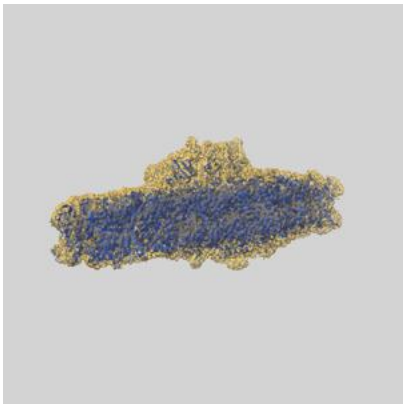
8 Fourier-Shell correlation

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

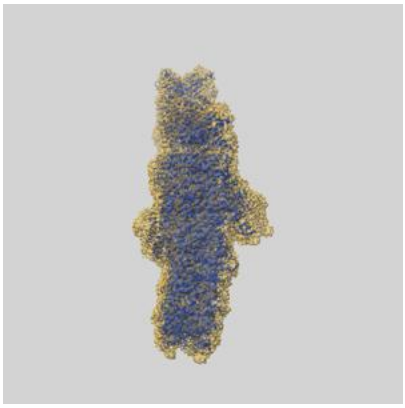
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30926 and PDB model 7DZ8. Per-residue inclusion information can be found in section 3 on page 45.

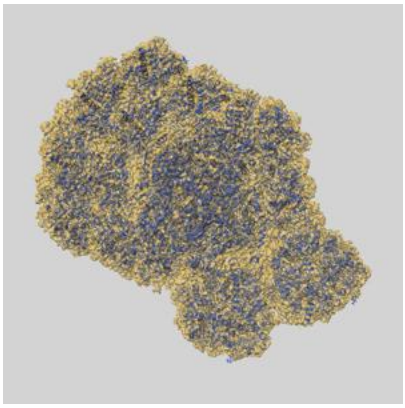
9.1 Map-model overlay



X



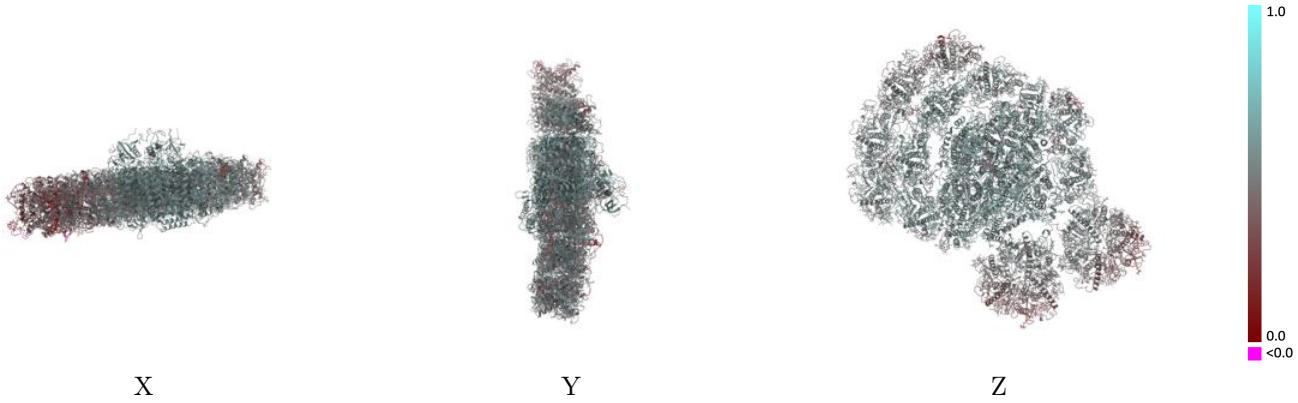
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

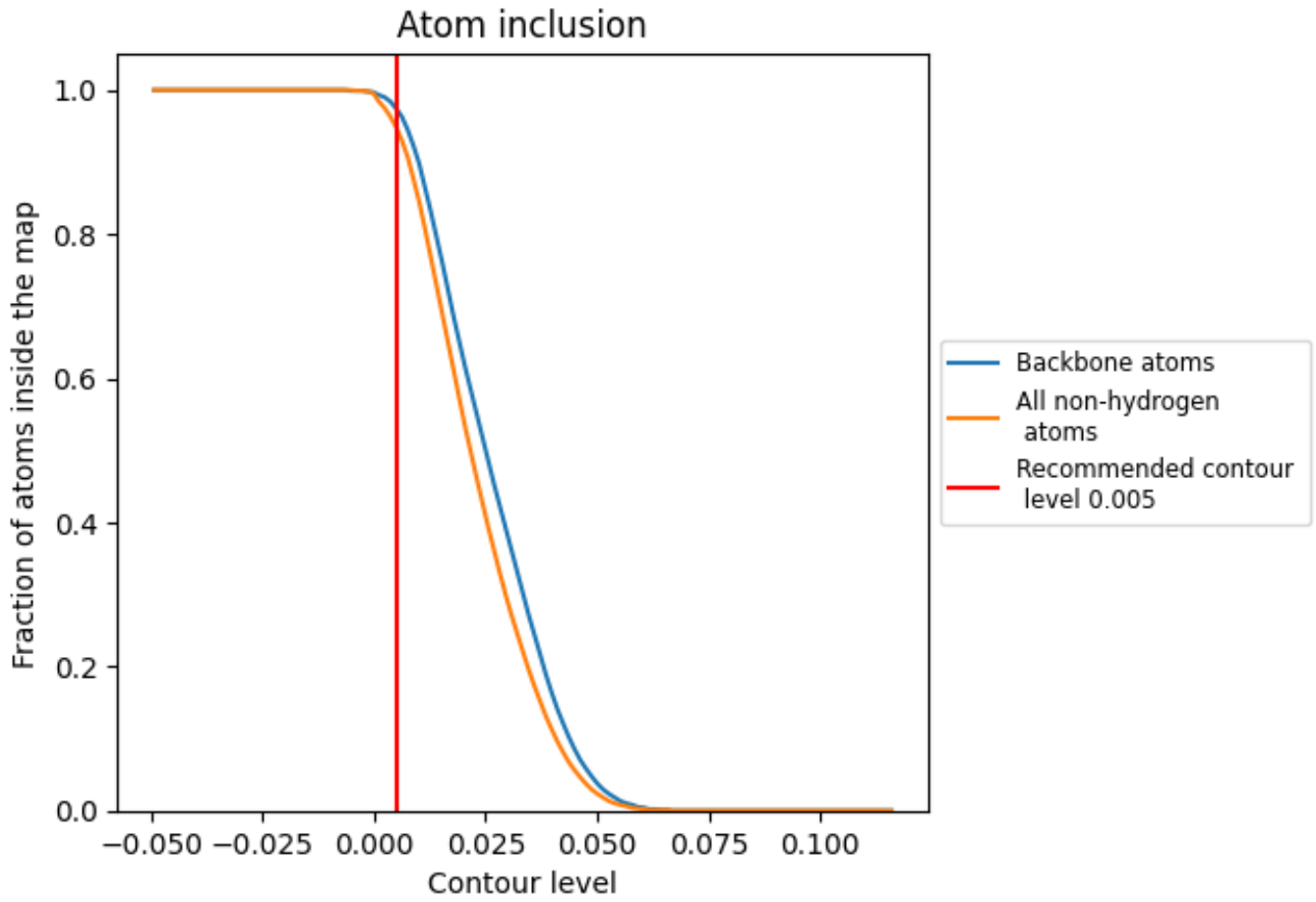


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9480	0.5180
1	0.9450	0.5180
2	0.9720	0.5370
3	0.9620	0.5530
4	0.9300	0.4740
5	0.9380	0.5160
6	0.9480	0.5130
7	0.9750	0.5640
8	0.9680	0.5530
9	0.9410	0.5060
A	0.9810	0.5850
B	0.9750	0.5810
C	0.9700	0.5390
D	0.9900	0.5690
E	0.9900	0.5660
F	0.9890	0.5650
G	0.9410	0.5040
H	0.9700	0.5480
I	0.9430	0.5380
J	0.9610	0.5550
K	0.9690	0.5310
L	0.9740	0.5570
O	0.9750	0.5400
U	0.9200	0.4270
V	0.9480	0.4950
W	0.8530	0.3620
X	0.8550	0.3700
Y	0.8830	0.4070
Z	0.9350	0.4990
a	0.8970	0.4270

