Full wwPDB EM Validation Report

Aug 6, 2026 – 04:59 AM JST

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:

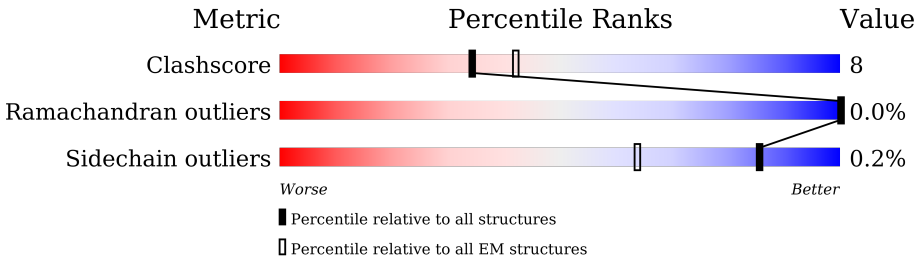
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.50

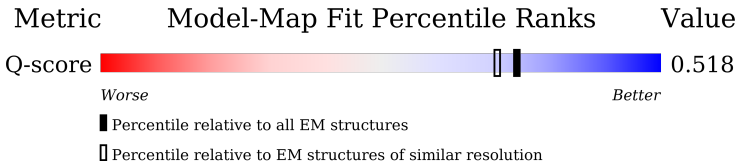
1 Overall quality at a glance

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	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
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% 19% •••
4	D	196	62% 10% • 27%

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Mol	Chain	Length	Quality of chain
5	E	97	60% 5% 35%
6	F	227	65% 7% 27%
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	65% 19% 15%
14	a	228	68% 16% 15%
15	2	246	77% 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	70% 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%

2 Entry composition (i)

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		

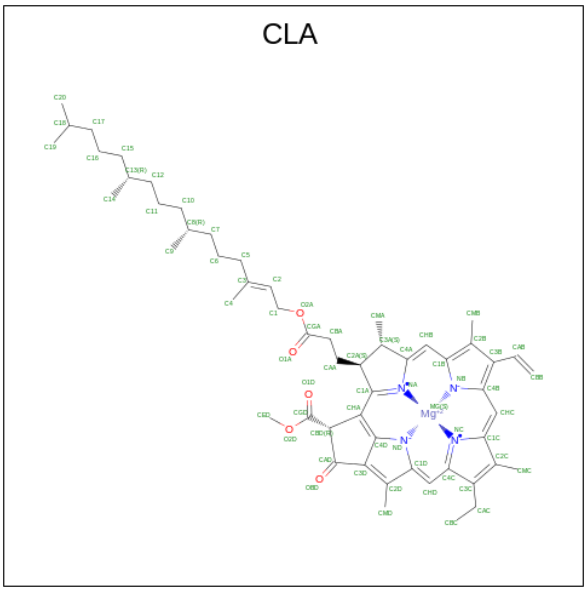
- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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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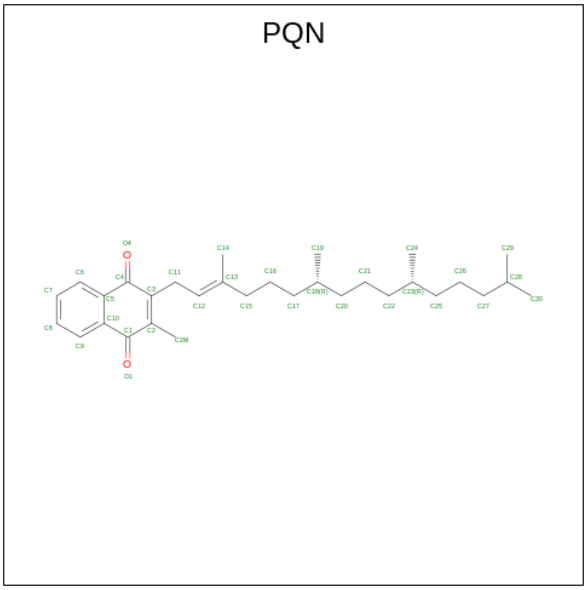
Mol	Chain	Residues	Atoms					AltConf
26	Z	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			49	40	1	4	4	
26	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			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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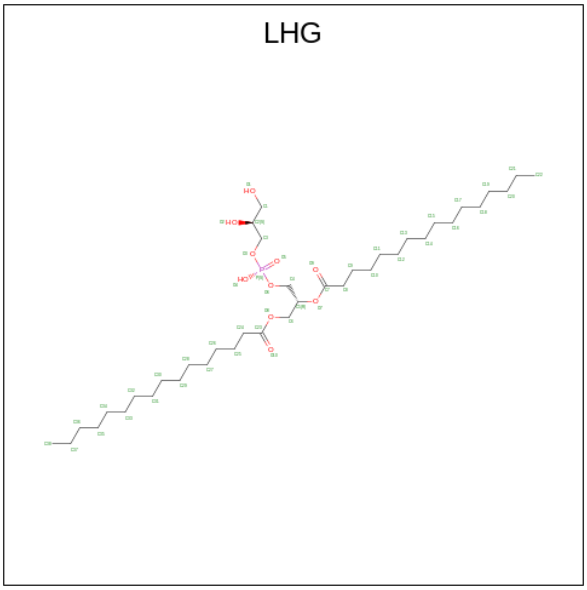
Mol	Chain	Residues	Atoms					AltConf
26	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			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: $C_{38}H_{75}O_{10}P$).



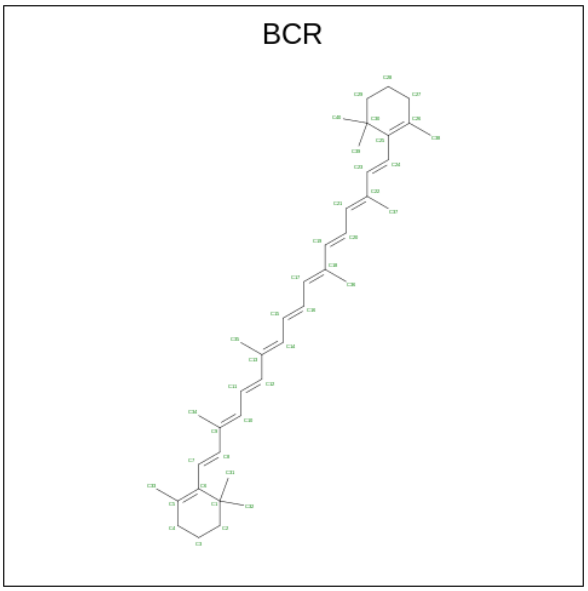
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total 49	C 38	O 10	P 1	0
28	A	1	Total 30	C 19	O 10	P 1	0
28	A	1	Total 49	C 38	O 10	P 1	0
28	B	1	Total 38	C 27	O 10	P 1	0
28	H	1	Total 49	C 38	O 10	P 1	0
28	O	1	Total 36	C 25	O 10	P 1	0
28	1	1	Total 49	C 38	O 10	P 1	0
28	a	1	Total 43	C 32	O 10	P 1	0
28	2	1	Total 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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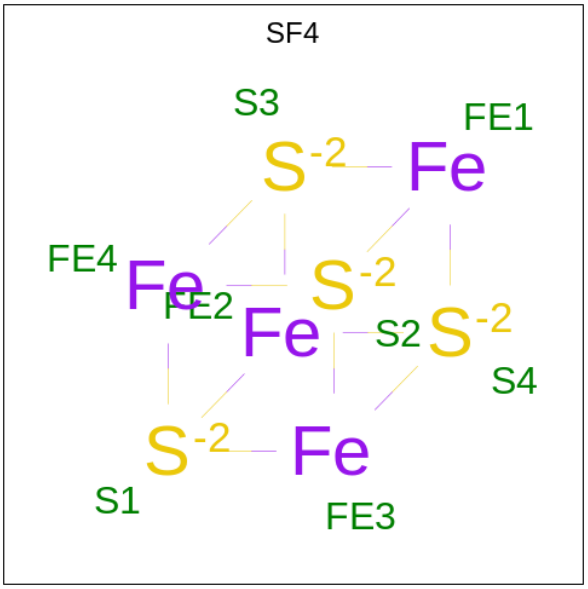
Mol	Chain	Residues	Atoms	AltConf
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	F	1	Total C 40 40	0
29	G	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	O	1	Total C 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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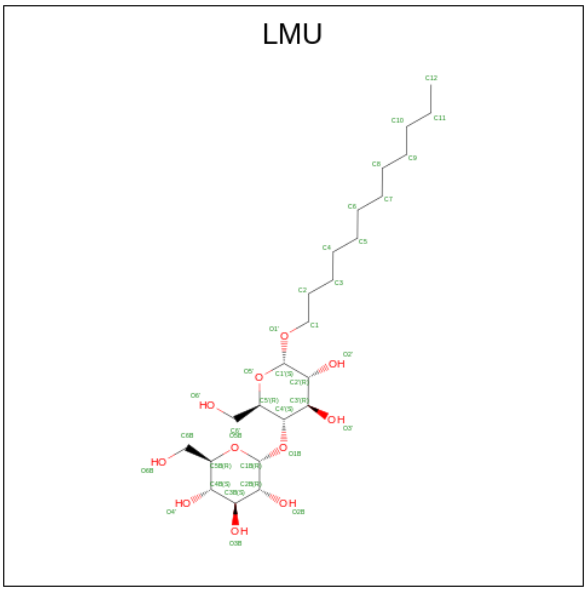
Mol	Chain	Residues	Atoms	AltConf
29	6	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	8	1	Total C 40 40	0
29	9	1	Total C 40 40	0

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



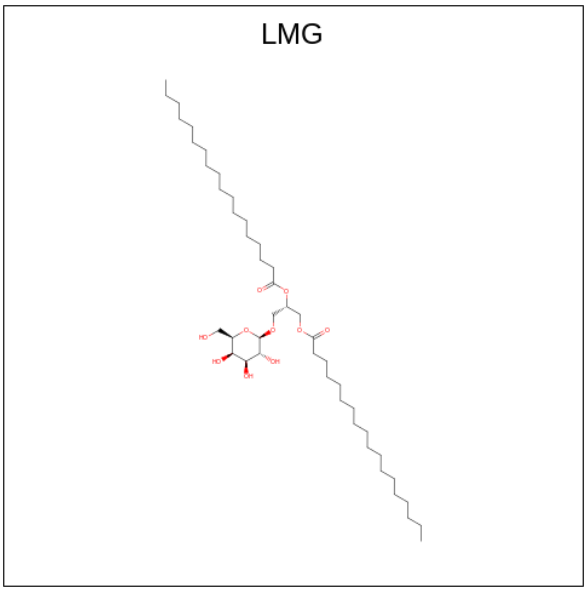
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total Fe S 8 4 4	0
30	C	1	Total Fe S 8 4 4	0
30	C	1	Total Fe S 8 4 4	0

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



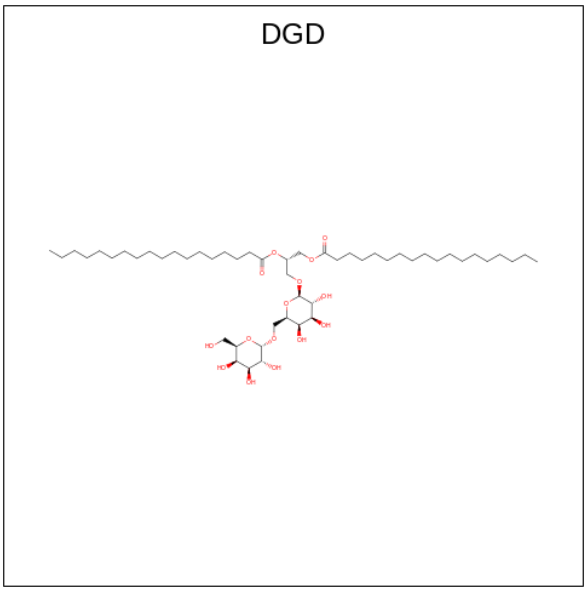
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			35	24	11	
31	A	1	Total	C	O	0
			34	24	10	
31	K	1	Total	C	O	0
			35	24	11	
31	1	1	Total	C	O	0
			35	24	11	
31	5	1	Total	C	O	0
			33	22	11	
31	5	1	Total	C	O	0
			32	21	11	
31	8	1	Total	C	O	0
			35	24	11	

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



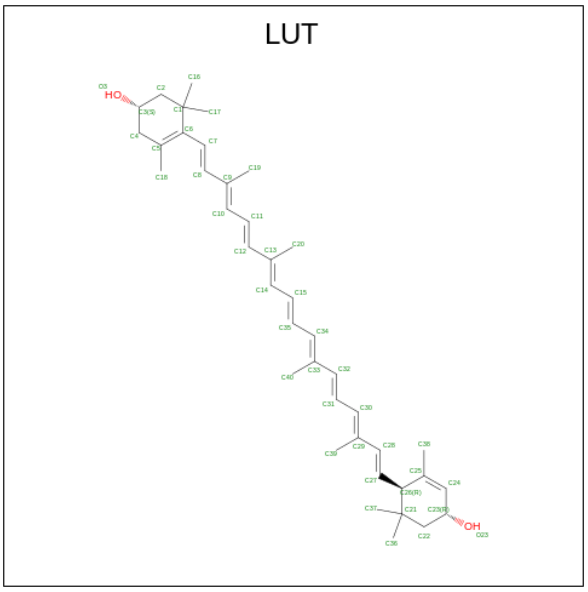
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C O 40 30 10	0
32	H	1	Total C O 55 45 10	0
32	J	1	Total C O 42 32 10	0
32	J	1	Total C O 40 30 10	0
32	L	1	Total C O 37 27 10	0
32	4	1	Total C O 40 30 10	0
32	4	1	Total C O 40 30 10	0
32	5	1	Total C O 40 30 10	0
32	8	1	Total C O 46 36 10	0
32	9	1	Total C O 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: $C_{40}H_{56}O_2$).



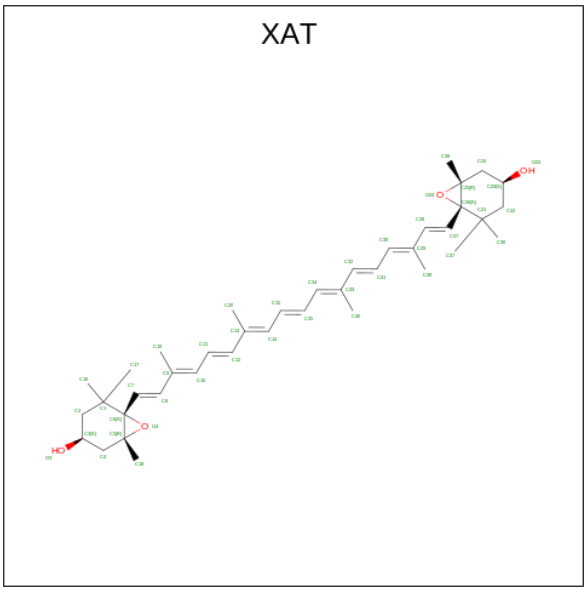
Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total	C	O	0
			42	40	2	
34	a	1	Total	C	O	0
			42	40	2	

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

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



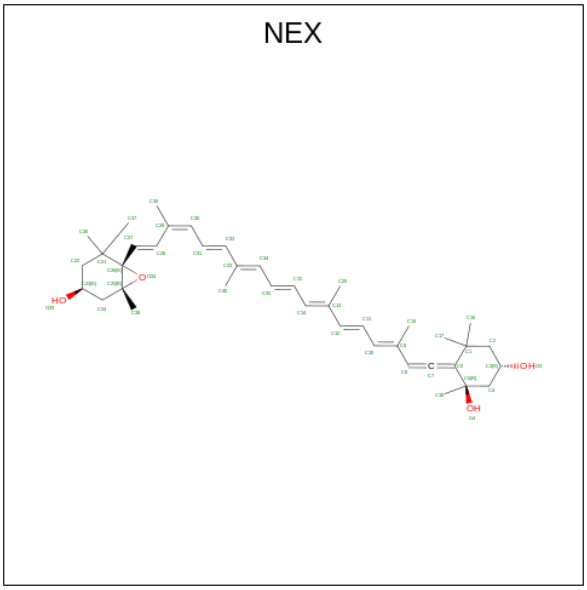
Mol	Chain	Residues	Atoms			AltConf
35	1	1	Total	C	O	0
			44	40	4	
35	a	1	Total	C	O	0
			44	40	4	
35	2	1	Total	C	O	0
			44	40	4	
35	3	1	Total	C	O	0
			44	40	4	
35	4	1	Total	C	O	0
			44	40	4	
35	5	1	Total	C	O	0
			44	40	4	
35	6	1	Total	C	O	0
			44	40	4	
35	7	1	Total	C	O	0
			44	40	4	
35	8	1	Total	C	O	0
			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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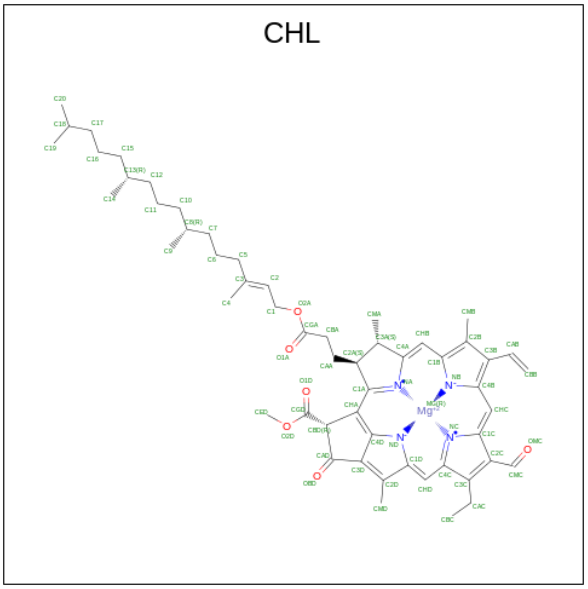
Mol	Chain	Residues	Atoms	AltConf
35	V	1	Total C O 44 40 4	0
35	W	1	Total C O 44 40 4	0

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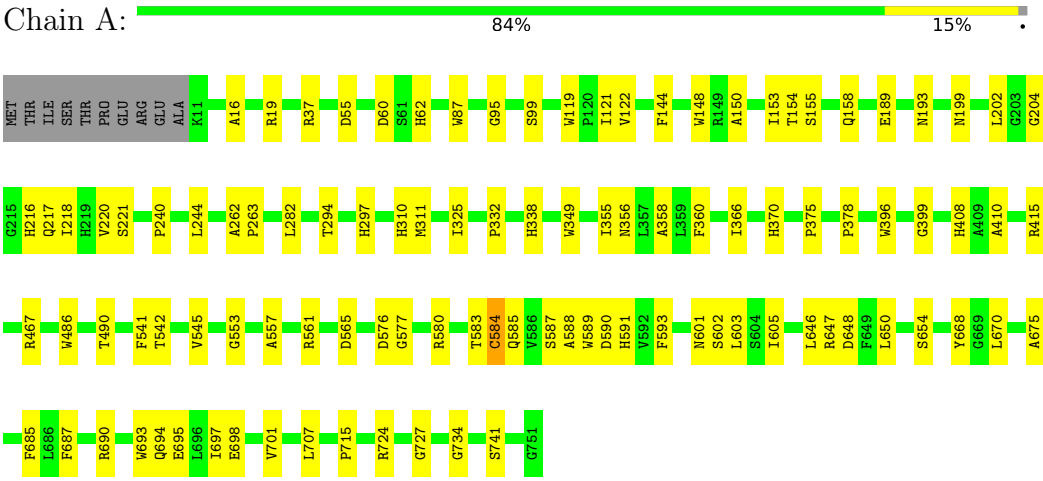
Mol	Chain	Residues	Atoms					AltConf
37	W	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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.

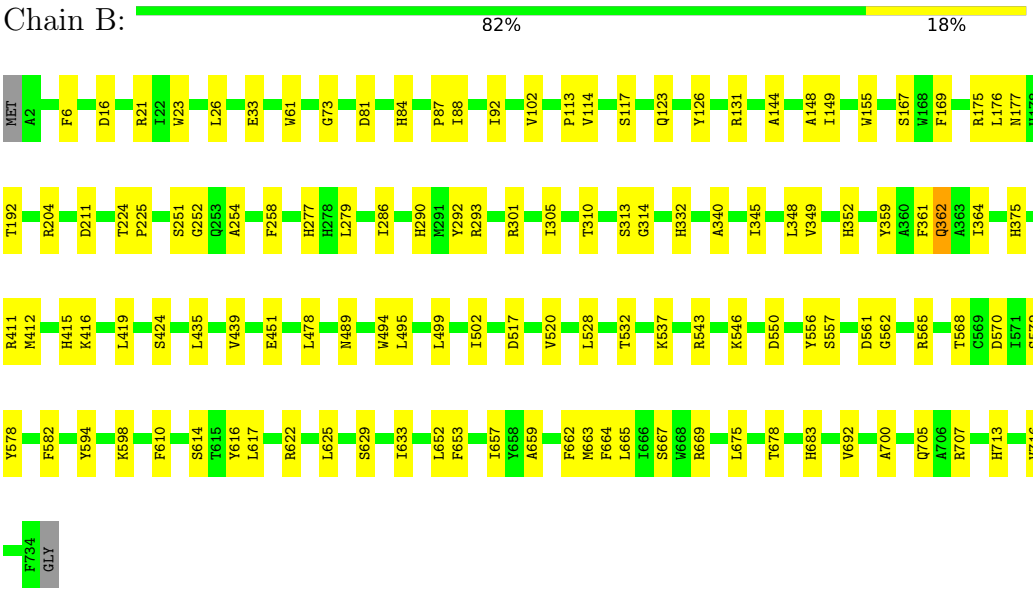
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



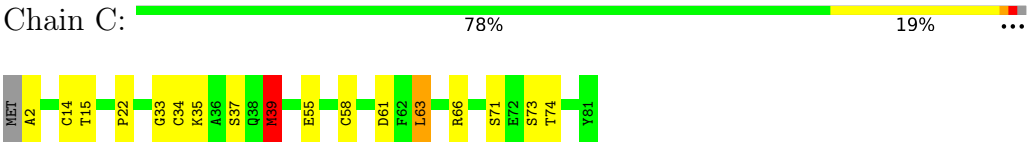
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



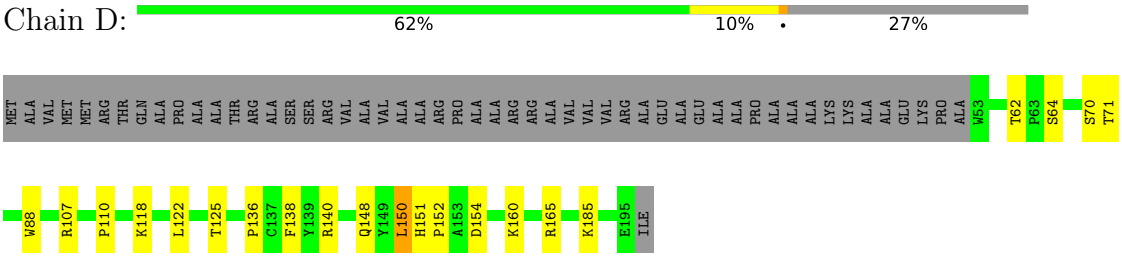
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



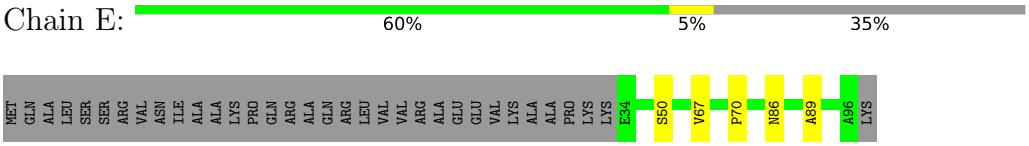
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:



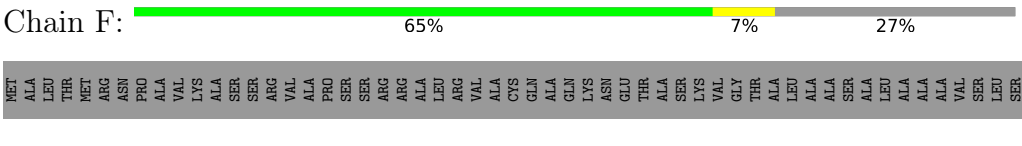
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



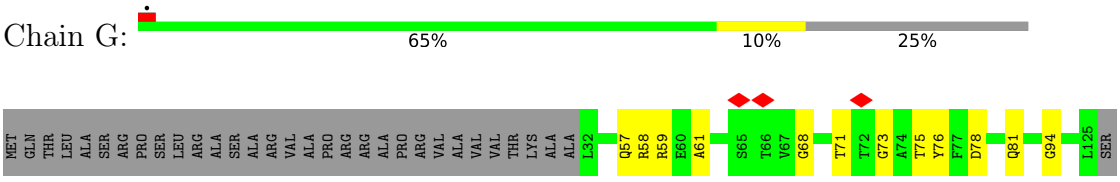
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:



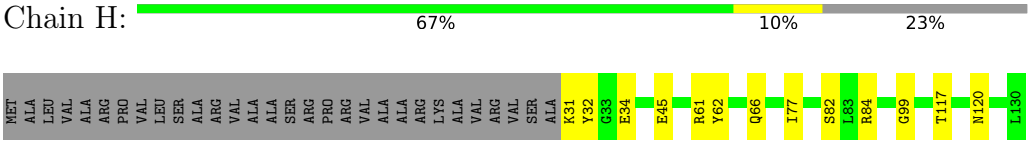
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:



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

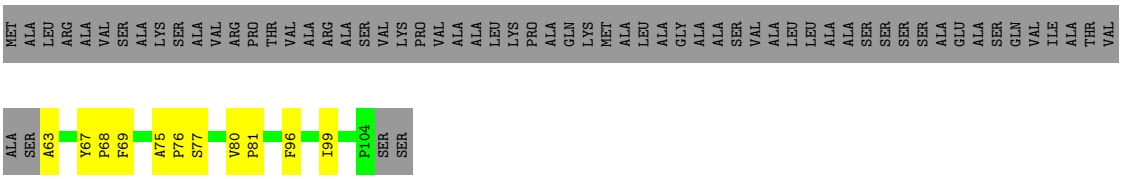
Chain H:



• Molecule 9: Photosystem I reaction center subunit VIII

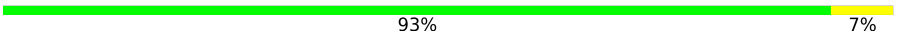
Chain I:

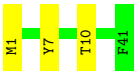




• Molecule 10: Photosystem I reaction center subunit IX

Chain J:

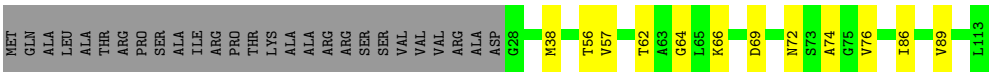




• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:

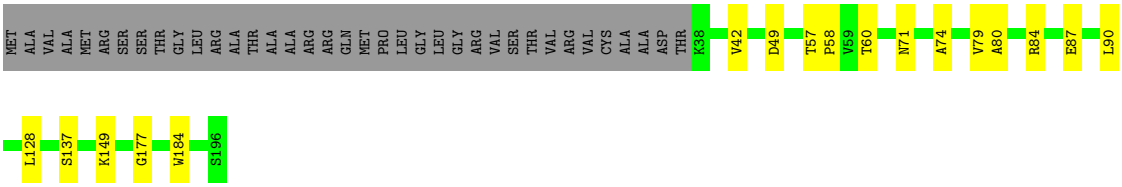




• Molecule 12: PSI subunit V

Chain L:

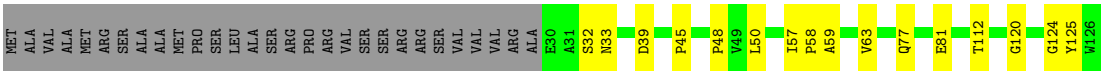




• Molecule 13: Photosystem I subunit O

Chain O:

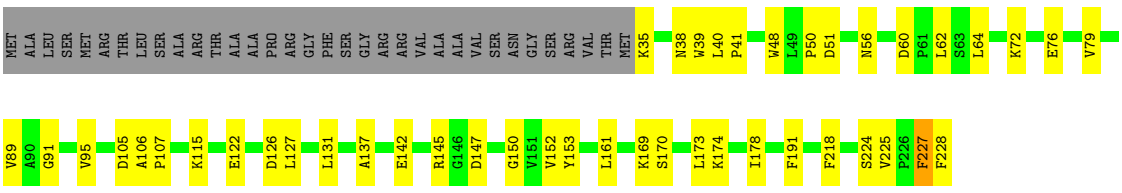




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

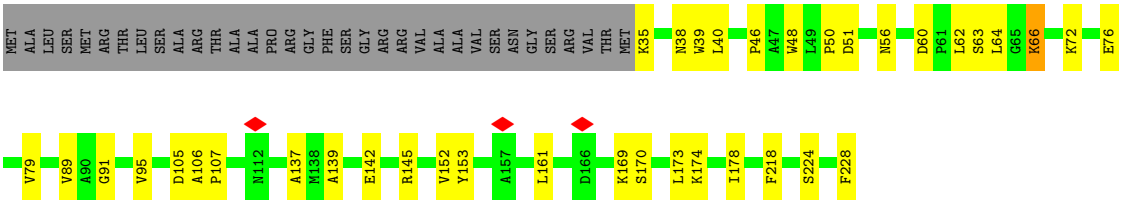




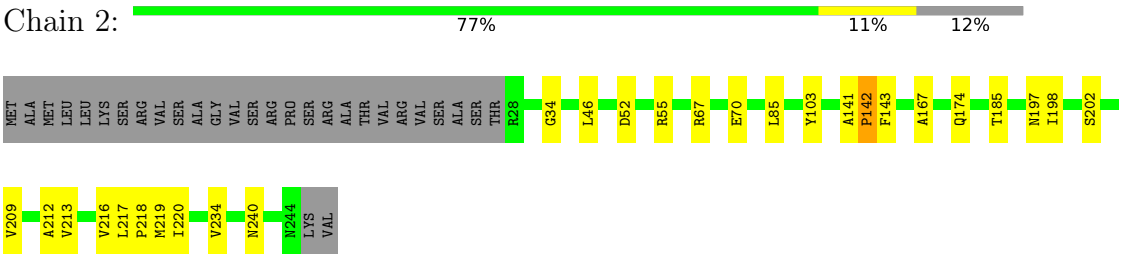
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain a:

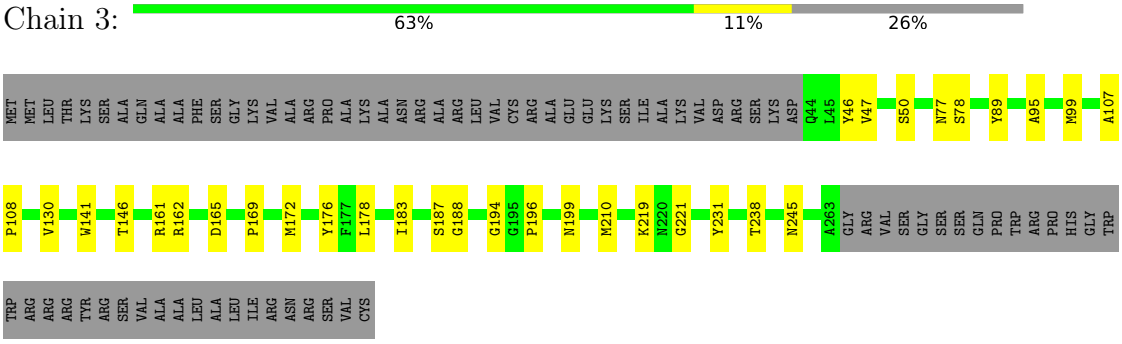




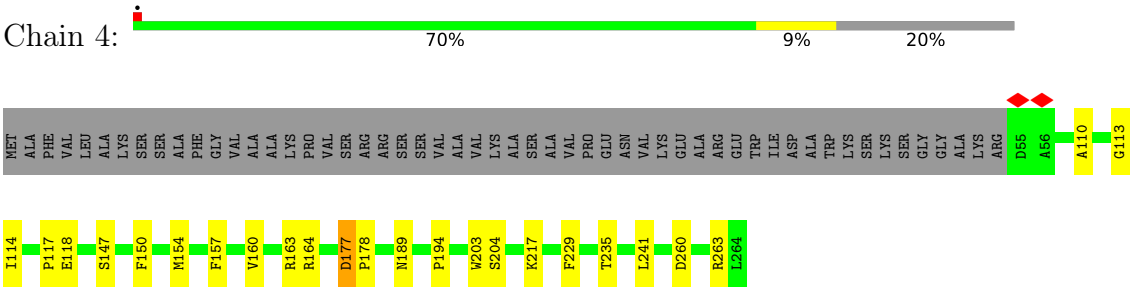
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



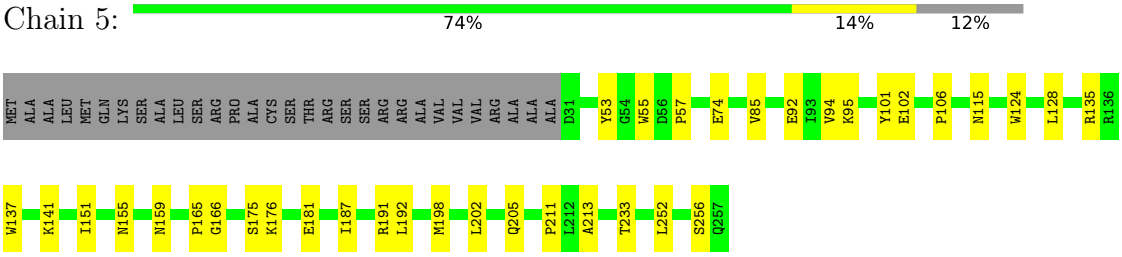
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic



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

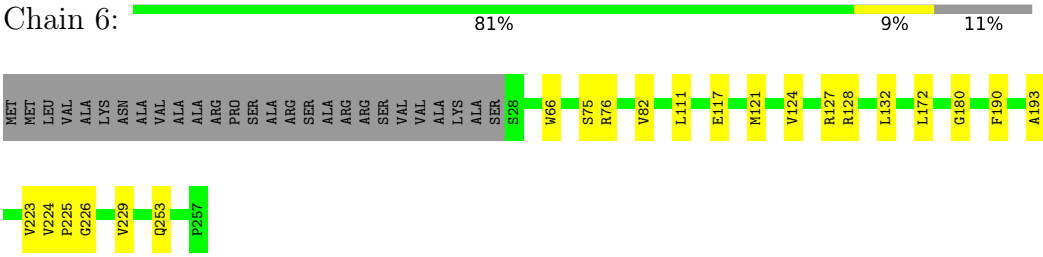


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



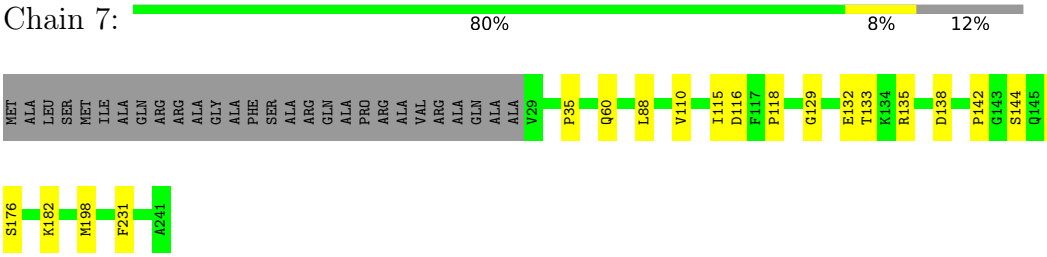
• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



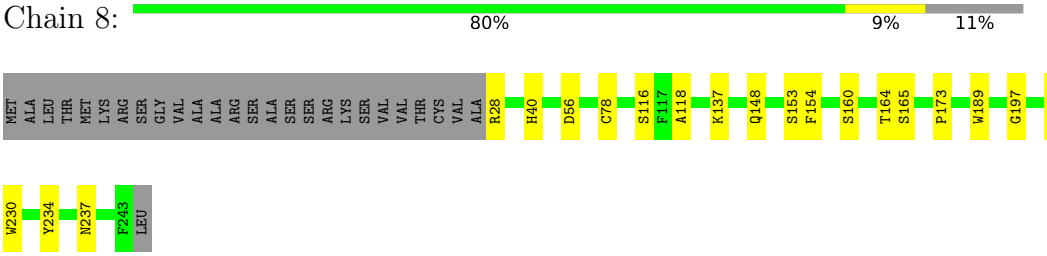
• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



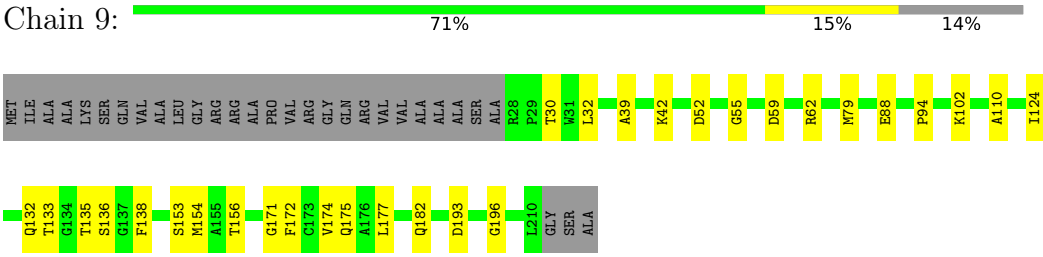
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



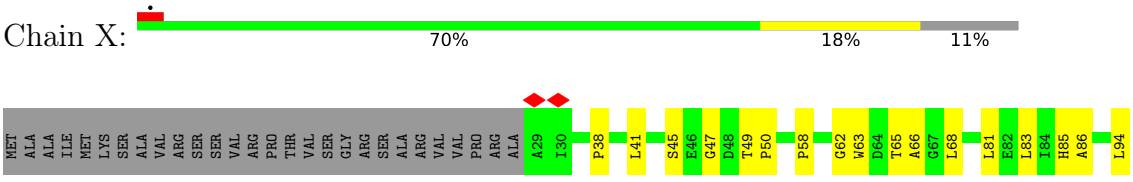
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

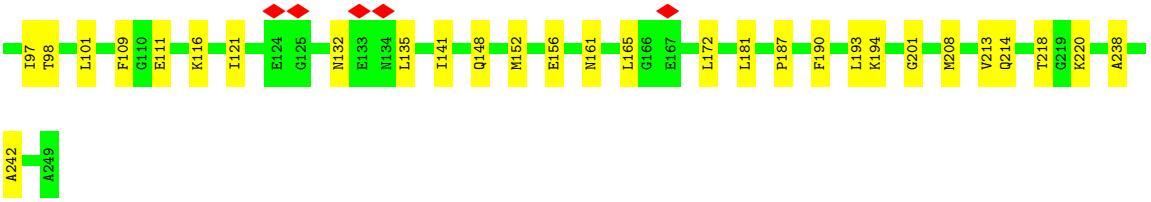
Chain 9:



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

Chain X:

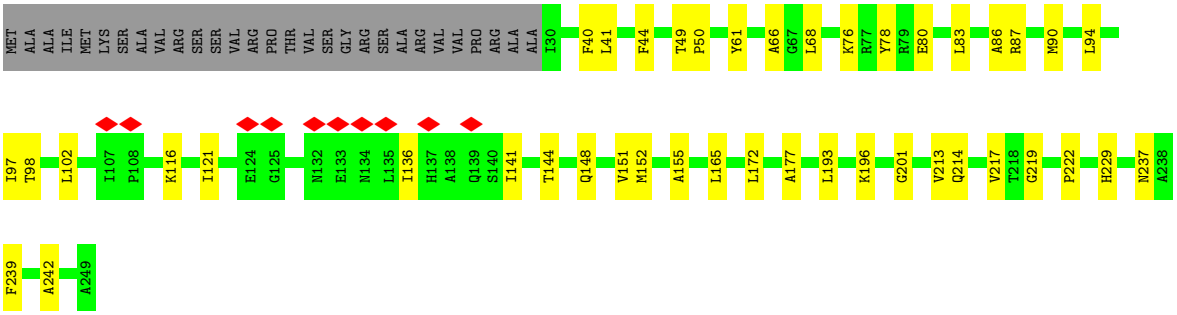




• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain W:

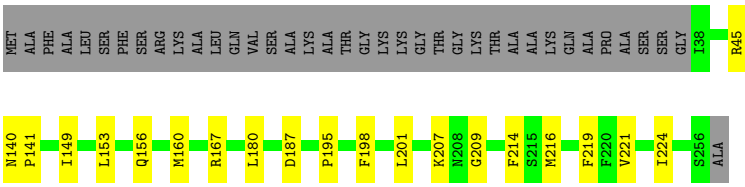




• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain Y:

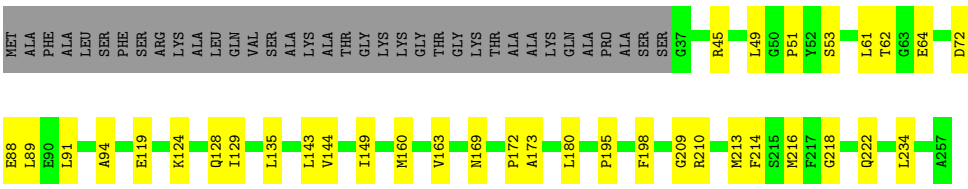




• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain Z:

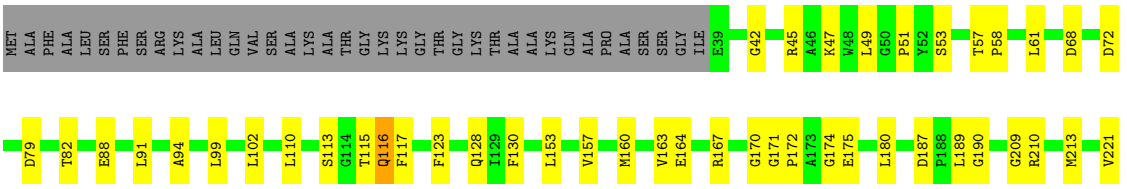


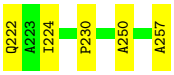


• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain U:



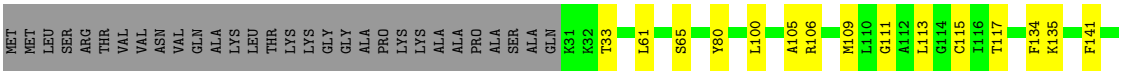


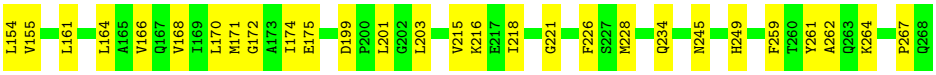


• Molecule 25: Chlorophyll a-b binding protein, chloroplastic

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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.53	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)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	713 (96%)	26 (4%)	0	100	100
2	B	731/735 (100%)	701 (96%)	30 (4%)	0	100	100
3	C	78/81 (96%)	67 (86%)	11 (14%)	0	100	100
4	D	141/196 (72%)	135 (96%)	6 (4%)	0	100	100
5	E	61/97 (63%)	57 (93%)	4 (7%)	0	100	100
6	F	163/227 (72%)	156 (96%)	7 (4%)	0	100	100
7	G	92/126 (73%)	86 (94%)	6 (6%)	0	100	100
8	H	98/130 (75%)	94 (96%)	4 (4%)	0	100	100
9	I	40/106 (38%)	35 (88%)	5 (12%)	0	100	100
10	J	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
11	K	84/113 (74%)	78 (93%)	6 (7%)	0	100	100
12	L	157/196 (80%)	146 (93%)	11 (7%)	0	100	100
13	O	95/126 (75%)	87 (92%)	8 (8%)	0	100	100
14	1	192/228 (84%)	186 (97%)	6 (3%)	0	100	100
14	a	192/228 (84%)	186 (97%)	6 (3%)	0	100	100
15	2	215/246 (87%)	203 (94%)	10 (5%)	2 (1%)	14	43
16	3	218/298 (73%)	211 (97%)	7 (3%)	0	100	100
17	4	208/264 (79%)	202 (97%)	6 (3%)	0	100	100
18	5	225/257 (88%)	211 (94%)	14 (6%)	0	100	100
19	6	228/257 (89%)	210 (92%)	18 (8%)	0	100	100
20	7	211/241 (88%)	197 (93%)	14 (7%)	0	100	100
21	8	214/243 (88%)	210 (98%)	4 (2%)	0	100	100
22	9	181/213 (85%)	165 (91%)	16 (9%)	0	100	100
23	W	218/249 (88%)	202 (93%)	16 (7%)	0	100	100
23	X	219/249 (88%)	194 (89%)	25 (11%)	0	100	100
24	U	217/257 (84%)	196 (90%)	21 (10%)	0	100	100
24	Y	217/257 (84%)	198 (91%)	19 (9%)	0	100	100
24	Z	219/257 (85%)	204 (93%)	15 (7%)	0	100	100
25	V	235/268 (88%)	222 (94%)	13 (6%)	0	100	100
All	All	5927/6937 (85%)	5590 (94%)	335 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	2	142	PRO
15	2	143	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	601/610 (98%)	600 (100%)	1 (0%)	87 87
2	B	596/597 (100%)	596 (100%)	0	100 100
3	C	69/70 (99%)	67 (97%)	2 (3%)	37 63
4	D	120/152 (79%)	120 (100%)	0	100 100
5	E	54/81 (67%)	54 (100%)	0	100 100
6	F	127/169 (75%)	127 (100%)	0	100 100
7	G	70/94 (74%)	70 (100%)	0	100 100
8	H	81/102 (79%)	81 (100%)	0	100 100
9	I	33/76 (43%)	33 (100%)	0	100 100
10	J	37/37 (100%)	37 (100%)	0	100 100
11	K	59/80 (74%)	59 (100%)	0	100 100
12	L	121/148 (82%)	121 (100%)	0	100 100
13	O	78/101 (77%)	78 (100%)	0	100 100
14	1	137/162 (85%)	135 (98%)	2 (2%)	57 72
14	a	137/162 (85%)	135 (98%)	2 (2%)	57 72
15	2	173/198 (87%)	173 (100%)	0	100 100
16	3	167/230 (73%)	167 (100%)	0	100 100
17	4	165/205 (80%)	164 (99%)	1 (1%)	78 81
18	5	184/206 (89%)	184 (100%)	0	100 100
19	6	184/203 (91%)	184 (100%)	0	100 100
20	7	164/181 (91%)	164 (100%)	0	100 100
21	8	162/183 (88%)	162 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	9	140/159 (88%)	140 (100%)	0	100 100
23	W	164/187 (88%)	164 (100%)	0	100 100
23	X	165/187 (88%)	164 (99%)	1 (1%)	78 81
24	U	168/194 (87%)	168 (100%)	0	100 100
24	Y	170/194 (88%)	170 (100%)	0	100 100
24	Z	170/194 (88%)	170 (100%)	0	100 100
25	V	178/201 (89%)	178 (100%)	0	100 100
All	All	4674/5363 (87%)	4665 (100%)	9 (0%)	85 87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	584	CYS
3	C	39	MET
3	C	63	LEU
14	1	72	LYS
14	1	227	PHE
14	a	66	LYS
14	a	72	LYS
17	4	177	ASP
23	X	165	LEU

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

Mol	Chain	Res	Type
1	A	217	GLN
1	A	268	ASN
1	A	568	ASN
1	A	609	HIS
1	A	704	HIS
2	B	99	GLN
2	B	253	GLN
2	B	445	GLN
2	B	705	GLN
3	C	16	GLN
4	D	162	ASN
5	E	87	ASN
8	H	65	ASN

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Mol	Chain	Res	Type
8	H	66	GLN
13	O	82	ASN
14	1	128	ASN
14	a	38	ASN
15	2	196	ASN
16	3	245	ASN
19	6	41	HIS
20	7	234	ASN
21	8	221	ASN
22	9	140	ASN
23	X	137	HIS
23	X	161	ASN
24	Y	140	ASN
24	U	128	GLN
24	U	147	GLN
25	V	196	GLN
23	W	161	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	1.56	1 (12%)	10,14,16	1.95	2 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	TPO	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	3.28	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	-5.21	107.48	123.21
25	V	33	TPO	CG2-CB-CA	-2.55	108.14	113.16

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	A	832	1	54,58,73	1.45	10 (18%)	65,95,113	1.46	11 (16%)
26	CLA	4	607	-	49,53,73	1.49	8 (16%)	59,89,113	1.27	6 (10%)
35	XAT	6	621	-	39,47,47	0.98	3 (7%)	54,74,74	2.42	23 (42%)
37	CHL	W	601	23	70,74,74	1.98	19 (27%)	80,114,114	2.76	24 (30%)
26	CLA	A	835	1	65,69,73	1.30	10 (15%)	78,108,113	1.28	8 (10%)
26	CLA	J	101	10	46,50,73	1.50	8 (17%)	55,85,113	1.29	6 (10%)
28	LHG	7	622	26	36,36,48	1.05	2 (5%)	39,42,54	1.02	3 (7%)
26	CLA	W	614	23	49,53,73	1.46	6 (12%)	59,89,113	1.38	3 (5%)
26	CLA	B	810	2	68,72,73	1.26	11 (16%)	81,111,113	1.38	9 (11%)
28	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	0.87	2 (3%)
28	LHG	8	622	26	48,48,48	0.91	2 (4%)	51,54,54	0.86	2 (3%)
26	CLA	F	304	6	45,49,73	1.52	8 (17%)	54,84,113	1.37	6 (11%)
32	LMG	H	205	-	55,55,55	0.86	2 (3%)	63,63,63	1.11	6 (9%)
26	CLA	8	612	21	44,49,73	1.51	8 (18%)	52,84,113	1.37	4 (7%)
26	CLA	9	611	28	46,50,73	1.50	7 (15%)	55,85,113	1.23	2 (3%)
26	CLA	B	812	2	47,51,73	1.48	8 (17%)	56,86,113	1.27	5 (8%)
26	CLA	O	2001	13	40,46,73	1.60	9 (22%)	48,80,113	1.35	5 (10%)
26	CLA	2	607	-	47,52,73	1.48	9 (19%)	56,88,113	1.38	7 (12%)
26	CLA	V	612	25	49,53,73	1.47	8 (16%)	59,89,113	1.35	5 (8%)
26	CLA	B	827	2	66,70,73	1.27	10 (15%)	79,109,113	1.34	9 (11%)
26	CLA	5	607	-	69,73,73	1.26	10 (14%)	83,113,113	1.23	8 (9%)
26	CLA	3	617	16	43,48,73	1.52	9 (20%)	51,83,113	1.40	6 (11%)
32	LMG	L	2631	-	37,37,55	1.08	2 (5%)	45,45,63	1.18	4 (8%)
26	CLA	U	613	24	63,67,73	1.33	8 (12%)	75,105,113	1.20	7 (9%)
37	CHL	Y	601	24	70,74,74	1.95	19 (27%)	80,114,114	2.86	24 (30%)
26	CLA	3	611	28	41,46,73	1.62	7 (17%)	52,81,113	1.31	4 (7%)
35	XAT	1	618	-	39,47,47	0.91	0	54,74,74	2.46	21 (38%)
26	CLA	4	608	-	69,73,73	1.25	8 (11%)	83,113,113	1.19	8 (9%)
37	CHL	X	608	-	70,73,74	1.99	16 (22%)	75,112,114	2.82	21 (28%)
28	LHG	A	847	26	29,29,48	1.16	2 (6%)	32,35,54	1.04	3 (9%)
26	CLA	Y	614	24	52,56,73	1.42	6 (11%)	62,92,113	1.29	8 (12%)
29	BCR	G	205	-	41,41,41	0.80	1 (2%)	56,56,56	1.97	15 (26%)
32	LMG	4	623	-	40,40,55	1.07	2 (5%)	48,48,63	1.15	5 (10%)
26	CLA	1	606	-	41,47,73	1.59	9 (21%)	48,80,113	1.38	6 (12%)
36	NEX	6	624	-	38,46,46	1.13	3 (7%)	50,70,70	2.40	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	Z	613	24	69,73,73	1.26	9 (13%)	83,113,113	1.22	5 (6%)
26	CLA	B	817	2	63,67,73	1.32	9 (14%)	75,105,113	1.31	6 (8%)
26	CLA	8	606	-	68,72,73	1.29	9 (13%)	82,112,113	1.13	7 (8%)
34	LUT	5	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.91	15 (29%)
26	CLA	2	604	-	46,50,73	1.50	8 (17%)	55,85,113	1.33	8 (14%)
26	CLA	A	837	1	49,53,73	1.51	11 (22%)	59,89,113	1.50	8 (13%)
32	LMG	V	2631	-	55,55,55	0.87	2 (3%)	63,63,63	1.11	5 (7%)
26	CLA	Z	604	-	54,57,73	1.50	9 (16%)	60,93,113	1.33	8 (13%)
36	NEX	5	624	-	38,46,46	1.08	1 (2%)	50,70,70	2.27	18 (36%)
26	CLA	A	829	1	69,73,73	1.27	8 (11%)	83,113,113	1.35	9 (10%)
26	CLA	6	613	-	67,72,73	1.30	9 (13%)	80,112,113	1.22	8 (10%)
29	BCR	3	622	-	41,41,41	0.89	1 (2%)	56,56,56	2.23	18 (32%)
26	CLA	G	204	7	49,53,73	1.50	9 (18%)	59,89,113	1.33	7 (11%)
26	CLA	B	828	2	69,73,73	1.28	9 (13%)	83,113,113	1.18	7 (8%)
35	XAT	4	620	-	39,47,47	0.94	2 (5%)	54,74,74	2.49	24 (44%)
26	CLA	A	838	1	54,58,73	1.42	12 (22%)	65,95,113	1.36	6 (9%)
26	CLA	7	611	28	63,67,73	1.31	9 (14%)	75,105,113	1.21	7 (9%)
37	CHL	V	608	-	52,56,74	2.17	17 (32%)	58,92,114	3.35	23 (39%)
26	CLA	4	616	17	47,51,73	1.58	9 (19%)	60,87,113	1.30	5 (8%)
26	CLA	B	839	-	69,73,73	1.28	12 (17%)	83,113,113	1.17	6 (7%)
29	BCR	4	621	-	41,41,41	0.83	1 (2%)	56,56,56	2.03	18 (32%)
37	CHL	V	609	25	65,69,74	2.00	18 (27%)	74,108,114	3.01	25 (33%)
26	CLA	8	608	-	55,59,73	1.41	10 (18%)	66,96,113	1.40	9 (13%)
28	LHG	Y	2630	26	48,48,48	0.92	2 (4%)	51,54,54	1.01	2 (3%)
28	LHG	Z	2630	26	48,48,48	0.92	2 (4%)	51,54,54	0.97	2 (3%)
26	CLA	6	611	28	46,50,73	1.49	8 (17%)	55,85,113	1.30	5 (9%)
26	CLA	K	206	11	49,53,73	1.50	8 (16%)	59,89,113	1.26	4 (6%)
26	CLA	U	612	24	46,50,73	1.50	5 (10%)	55,85,113	1.45	6 (10%)
28	LHG	2	622	26	35,35,48	1.05	2 (5%)	38,41,54	1.16	3 (7%)
26	CLA	1	601	14	57,62,73	1.36	9 (15%)	68,100,113	1.23	8 (11%)
29	BCR	6	622	-	41,41,41	0.75	0	56,56,56	2.46	25 (44%)
26	CLA	3	607	16	60,64,73	1.38	8 (13%)	75,102,113	1.23	7 (9%)
37	CHL	U	605	24	47,51,74	2.39	18 (38%)	52,86,114	3.23	21 (40%)
26	CLA	B	811	2	57,60,73	1.50	11 (19%)	68,97,113	1.35	8 (11%)
26	CLA	8	607	-	45,49,73	1.60	11 (24%)	57,84,113	1.33	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LMG	5	627	-	40,40,55	1.03	2 (5%)	48,48,63	1.02	3 (6%)
37	CHL	Z	605	24	46,50,74	2.34	18 (39%)	51,85,114	3.55	24 (47%)
29	BCR	A	848	-	41,41,41	1.01	3 (7%)	56,56,56	2.24	14 (25%)
26	CLA	A	810	1	54,58,73	1.45	8 (14%)	65,95,113	1.38	8 (12%)
26	CLA	a	614	14	58,62,73	1.37	8 (13%)	67,99,113	1.34	6 (8%)
34	LUT	a	617	-	42,43,43	0.80	1 (2%)	51,60,60	1.90	16 (31%)
26	CLA	A	825	1	69,73,73	1.27	9 (13%)	83,113,113	1.20	6 (7%)
27	PQN	A	844	-	34,34,34	3.31	9 (26%)	42,45,45	2.07	4 (9%)
26	CLA	Z	612	24	49,53,73	1.48	7 (14%)	59,89,113	1.32	7 (11%)
26	CLA	2	616	-	47,51,73	1.57	9 (19%)	60,87,113	1.33	6 (10%)
26	CLA	B	809	2	69,73,73	1.29	10 (14%)	83,113,113	1.29	8 (9%)
26	CLA	1	608	-	47,52,73	1.50	9 (19%)	56,88,113	1.30	7 (12%)
26	CLA	A	801	1	69,73,73	1.27	11 (15%)	83,113,113	1.28	7 (8%)
26	CLA	X	614	23	46,50,73	1.52	8 (17%)	55,85,113	1.30	5 (9%)
30	SF4	C	101	3	0,12,12	-	-	-		
26	CLA	Y	611	28	47,51,73	1.48	7 (14%)	56,86,113	1.27	4 (7%)
26	CLA	5	614	18	48,52,73	1.49	9 (18%)	55,87,113	1.32	5 (9%)
26	CLA	7	614	20	46,50,73	1.50	9 (19%)	55,85,113	1.31	6 (10%)
26	CLA	A	826	-	68,72,73	1.28	11 (16%)	81,111,113	1.25	7 (8%)
26	CLA	W	611	28	61,65,73	1.33	6 (9%)	73,103,113	1.15	7 (9%)
26	CLA	V	602	25	64,68,73	1.29	8 (12%)	77,107,113	1.23	8 (10%)
29	BCR	A	850	-	41,41,41	0.93	1 (2%)	56,56,56	2.02	14 (25%)
26	CLA	7	603	20	47,52,73	1.52	10 (21%)	56,88,113	1.50	7 (12%)
26	CLA	a	602	14	65,69,73	1.34	11 (16%)	78,108,113	1.24	8 (10%)
26	CLA	a	611	28	41,46,73	1.64	10 (24%)	52,81,113	1.40	10 (19%)
26	CLA	7	606	-	45,49,73	1.54	11 (24%)	54,84,113	1.28	4 (7%)
26	CLA	3	602	16	64,68,73	1.31	8 (12%)	77,107,113	1.20	8 (10%)
26	CLA	W	602	23	64,68,73	1.31	9 (14%)	77,107,113	1.17	8 (10%)
26	CLA	O	2003	-	43,48,73	1.54	9 (20%)	51,83,113	1.28	3 (5%)
31	LMU	5	628	-	34,34,36	1.19	2 (5%)	45,45,47	1.14	5 (11%)
29	BCR	a	619	-	41,41,41	0.84	0	56,56,56	2.38	22 (39%)
26	CLA	A	802	2	69,73,73	1.28	10 (14%)	83,113,113	1.39	10 (12%)
26	CLA	A	841	1	69,73,73	1.26	9 (13%)	83,113,113	1.20	6 (7%)
26	CLA	8	613	21	69,73,73	1.27	9 (13%)	83,113,113	1.16	6 (7%)
26	CLA	U	611	28	46,50,73	1.51	6 (13%)	55,85,113	1.33	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	6	609	19	49,53,73	1.50	9 (18%)	59,89,113	1.31	6 (10%)
26	CLA	U	604	-	53,56,73	1.52	10 (18%)	57,91,113	1.38	8 (14%)
26	CLA	A	818	1	64,68,73	1.30	10 (15%)	77,107,113	1.28	8 (10%)
29	BCR	L	301	-	41,41,41	0.80	0	56,56,56	2.26	24 (42%)
26	CLA	A	812	1	69,73,73	1.26	9 (13%)	83,113,113	1.19	5 (6%)
26	CLA	6	602	19	69,73,73	1.28	9 (13%)	83,113,113	1.18	8 (9%)
26	CLA	a	607	-	49,53,73	1.52	10 (20%)	59,89,113	1.21	5 (8%)
26	CLA	B	840	2	69,73,73	1.33	10 (14%)	83,113,113	1.26	5 (6%)
34	LUT	X	1621	-	42,43,43	0.81	0	51,60,60	1.74	15 (29%)
26	CLA	B	803	-	69,73,73	1.25	11 (15%)	83,113,113	1.26	6 (7%)
26	CLA	3	604	-	69,73,73	1.27	9 (13%)	83,113,113	1.19	8 (9%)
35	XAT	a	618	-	39,47,47	0.90	0	54,74,74	2.47	21 (38%)
28	LHG	9	622	26	29,29,48	1.18	2 (6%)	32,35,54	1.02	1 (3%)
26	CLA	A	843	-	68,72,73	1.29	10 (14%)	81,111,113	1.25	9 (11%)
36	NEX	V	1623	-	38,46,46	0.94	2 (5%)	50,70,70	2.30	18 (36%)
26	CLA	A	828	1	69,73,73	1.27	11 (15%)	83,113,113	1.31	10 (12%)
29	BCR	K	202	-	41,41,41	0.94	2 (4%)	56,56,56	2.28	21 (37%)
26	CLA	9	614	22	49,53,73	1.48	9 (18%)	59,89,113	1.24	7 (11%)
26	CLA	X	602	23	69,73,73	1.25	9 (13%)	83,113,113	1.20	6 (7%)
32	LMG	J	104	-	40,40,55	1.02	2 (5%)	48,48,63	1.30	6 (12%)
26	CLA	7	607	-	46,50,73	1.49	8 (17%)	55,85,113	1.20	4 (7%)
26	CLA	U	614	24	46,50,73	1.49	7 (15%)	55,85,113	1.36	5 (9%)
31	LMU	1	621	-	36,36,36	1.15	2 (5%)	47,47,47	1.00	1 (2%)
29	BCR	7	623	-	41,41,41	0.87	0	56,56,56	2.01	17 (30%)
29	BCR	3	620	-	41,41,41	0.80	0	56,56,56	2.38	23 (41%)
26	CLA	B	836	2	54,58,73	1.43	11 (20%)	65,95,113	1.46	8 (12%)
37	CHL	X	609	23	70,74,74	1.94	19 (27%)	80,114,114	2.83	25 (31%)
29	BCR	L	308	-	41,41,41	0.81	0	56,56,56	2.33	23 (41%)
29	BCR	B	844	-	41,41,41	1.08	4 (9%)	56,56,56	2.60	26 (46%)
26	CLA	Y	602	24	62,66,73	1.32	8 (12%)	74,104,113	1.23	8 (10%)
26	CLA	A	817	-	49,53,73	1.50	9 (18%)	59,89,113	1.41	6 (10%)
26	CLA	4	611	28	46,50,73	1.46	7 (15%)	55,85,113	1.35	8 (14%)
26	CLA	H	203	-	69,73,73	1.25	8 (11%)	83,113,113	1.23	5 (6%)
31	LMU	8	625	-	36,36,36	1.10	2 (5%)	47,47,47	1.24	3 (6%)
28	LHG	U	2630	26	48,48,48	0.94	2 (4%)	51,54,54	1.08	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	SF4	A	853	1,2	0,12,12	-	-	-		
26	CLA	1	611	28	61,65,73	1.33	8 (13%)	73,103,113	1.20	8 (10%)
26	CLA	6	616	19	69,73,73	1.26	10 (14%)	83,113,113	1.29	10 (12%)
26	CLA	a	613	-	58,62,73	1.40	10 (17%)	69,99,113	1.23	6 (8%)
28	LHG	3	623	-	44,44,48	0.93	2 (4%)	47,50,54	1.00	3 (6%)
31	LMU	A	857	-	36,36,36	1.09	2 (5%)	47,47,47	1.37	8 (17%)
26	CLA	B	825	-	53,57,73	1.42	8 (15%)	62,93,113	1.35	8 (12%)
26	CLA	1	610	14	42,47,73	1.56	8 (19%)	51,81,113	1.39	7 (13%)
36	NEX	Y	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.52	16 (32%)
26	CLA	V	604	-	54,58,73	1.40	8 (14%)	65,95,113	1.31	7 (10%)
26	CLA	5	619	-	47,51,73	1.60	9 (19%)	60,87,113	1.42	8 (13%)
26	CLA	F	301	-	61,65,73	1.35	9 (14%)	73,103,113	1.18	6 (8%)
26	CLA	9	610	22	61,65,73	1.36	9 (14%)	73,103,113	1.27	8 (10%)
26	CLA	9	603	22	48,52,73	1.60	13 (27%)	61,88,113	1.40	6 (9%)
28	LHG	B	851	26	37,37,48	1.04	2 (5%)	40,43,54	1.14	4 (10%)
26	CLA	B	814	2	68,72,73	1.25	9 (13%)	81,111,113	1.29	6 (7%)
26	CLA	9	607	-	49,53,73	1.45	9 (18%)	59,89,113	1.28	6 (10%)
26	CLA	1	604	-	53,57,73	1.42	8 (15%)	62,93,113	1.28	5 (8%)
28	LHG	4	622	26	48,48,48	0.91	2 (4%)	51,54,54	0.82	2 (3%)
26	CLA	V	611	28	47,51,73	1.50	7 (14%)	56,86,113	1.25	3 (5%)
37	CHL	U	608	-	48,52,74	2.21	16 (33%)	53,87,114	3.48	22 (41%)
26	CLA	Z	614	24	52,56,73	1.45	7 (13%)	62,92,113	1.28	6 (9%)
32	LMG	4	624	-	40,40,55	1.03	2 (5%)	48,48,63	1.15	5 (10%)
37	CHL	U	607	-	50,54,74	2.27	19 (38%)	56,90,114	3.35	22 (39%)
26	CLA	2	606	-	47,51,73	1.49	10 (21%)	56,86,113	1.32	5 (8%)
26	CLA	6	608	-	49,53,73	1.48	8 (16%)	59,89,113	1.35	8 (13%)
26	CLA	8	601	21	69,73,73	1.30	8 (11%)	83,113,113	1.18	6 (7%)
26	CLA	5	603	18	58,62,73	1.43	11 (18%)	73,100,113	1.35	6 (8%)
26	CLA	A	824	1	69,73,73	1.26	10 (14%)	83,113,113	1.30	6 (7%)
26	CLA	3	615	-	43,48,73	1.53	8 (18%)	51,83,113	1.31	6 (11%)
37	CHL	Z	608	-	53,57,74	2.22	19 (35%)	59,93,114	3.23	22 (37%)
37	CHL	Z	607	-	70,74,74	1.92	18 (25%)	80,114,114	2.90	21 (26%)
37	CHL	W	605	23	50,54,74	2.28	20 (40%)	56,90,114	3.38	22 (39%)
29	BCR	B	801	-	41,41,41	0.94	1 (2%)	56,56,56	2.10	18 (32%)
26	CLA	B	806	2	69,73,73	1.30	13 (18%)	83,113,113	1.38	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	B	816	2	58,62,73	1.35	9 (15%)	69,99,113	1.30	8 (11%)
26	CLA	4	606	-	43,48,73	1.55	9 (20%)	51,83,113	1.28	6 (11%)
37	CHL	V	607	-	50,54,74	2.27	19 (38%)	56,90,114	3.25	23 (41%)
37	CHL	X	606	-	48,52,74	2.28	16 (33%)	53,87,114	3.31	21 (39%)
26	CLA	U	603	24	56,60,73	1.38	7 (12%)	67,97,113	1.36	7 (10%)
26	CLA	K	201	11	49,53,73	1.46	7 (14%)	59,89,113	1.24	4 (6%)
26	CLA	Z	603	24	59,63,73	1.35	7 (11%)	71,101,113	1.41	8 (11%)
26	CLA	5	618	18	43,48,73	1.61	10 (23%)	54,83,113	1.36	7 (12%)
26	CLA	A	808	1	54,58,73	1.41	8 (14%)	65,95,113	1.35	7 (10%)
31	LMU	K	208	-	36,36,36	1.14	2 (5%)	47,47,47	1.00	3 (6%)
26	CLA	3	614	16	43,48,73	1.55	9 (20%)	51,83,113	1.36	6 (11%)
26	CLA	A	807	1	69,73,73	1.29	11 (15%)	83,113,113	1.27	6 (7%)
26	CLA	a	610	14	63,67,73	1.31	8 (12%)	76,106,113	1.15	6 (7%)
26	CLA	A	840	1	56,60,73	1.39	11 (19%)	67,97,113	1.41	9 (13%)
26	CLA	L	306	-	43,48,73	1.53	8 (18%)	51,83,113	1.35	3 (5%)
28	LHG	1	620	26	48,48,48	0.92	2 (4%)	51,54,54	0.79	2 (3%)
26	CLA	7	615	-	45,50,73	1.60	10 (22%)	56,85,113	1.33	5 (8%)
34	LUT	X	1620	-	42,43,43	0.73	0	51,60,60	1.54	9 (17%)
26	CLA	A	809	1	69,73,73	1.27	11 (15%)	83,113,113	1.31	7 (8%)
26	CLA	1	616	14	47,51,73	1.56	8 (17%)	60,87,113	1.46	9 (15%)
28	LHG	H	204	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
26	CLA	2	611	28	46,50,73	1.48	8 (17%)	55,85,113	1.35	6 (10%)
26	CLA	B	834	2	64,68,73	1.30	10 (15%)	77,107,113	1.24	7 (9%)
29	BCR	F	305	-	41,41,41	0.89	1 (2%)	56,56,56	2.34	20 (35%)
26	CLA	2	610	15	59,63,73	1.37	9 (15%)	71,101,113	1.23	7 (9%)
26	CLA	8	609	21	49,53,73	1.48	8 (16%)	59,89,113	1.33	5 (8%)
26	CLA	B	818	2	64,68,73	1.32	11 (17%)	77,107,113	1.36	8 (10%)
26	CLA	5	610	18	58,62,73	1.36	9 (15%)	69,99,113	1.22	6 (8%)
26	CLA	A	816	1	69,73,73	1.26	11 (15%)	83,113,113	1.29	7 (8%)
26	CLA	3	612	16	47,51,73	1.51	9 (19%)	56,86,113	1.24	6 (10%)
26	CLA	9	613	22	69,73,73	1.27	9 (13%)	83,113,113	1.24	6 (7%)
26	CLA	9	602	22	64,68,73	1.31	9 (14%)	77,107,113	1.27	8 (10%)
35	XAT	9	620	-	39,47,47	0.99	2 (5%)	54,74,74	2.51	19 (35%)
37	CHL	X	601	23	70,74,74	1.91	19 (27%)	80,114,114	2.85	28 (35%)
26	CLA	5	613	18	68,72,73	1.23	9 (13%)	81,111,113	1.28	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	Y	610	24	69,73,73	1.26	9 (13%)	83,113,113	1.14	7 (8%)
26	CLA	3	603	16	59,63,73	1.36	11 (18%)	71,101,113	1.39	6 (8%)
35	XAT	V	1622	-	39,47,47	0.87	0	54,74,74	2.68	20 (37%)
35	XAT	3	619	-	39,47,47	0.98	2 (5%)	54,74,74	2.60	19 (35%)
28	LHG	9	624	-	48,48,48	0.93	2 (4%)	51,54,54	0.87	2 (3%)
26	CLA	5	604	-	67,71,73	1.36	9 (13%)	84,111,113	1.20	9 (10%)
26	CLA	2	601	15	69,73,73	1.23	10 (14%)	83,113,113	1.34	8 (9%)
36	NEX	X	1623	-	38,46,46	0.90	1 (2%)	50,70,70	4.33	20 (40%)
34	LUT	V	1621	-	42,43,43	0.79	0	51,60,60	1.99	16 (31%)
35	XAT	W	1622	-	39,47,47	0.92	1 (2%)	54,74,74	4.26	25 (46%)
26	CLA	W	610	23	59,63,73	1.34	6 (10%)	71,101,113	1.26	9 (12%)
26	CLA	W	603	23	56,60,73	1.37	6 (10%)	67,97,113	1.40	8 (11%)
37	CHL	V	606	-	48,52,74	2.16	18 (37%)	53,87,114	3.32	23 (43%)
26	CLA	4	613	17	69,73,73	1.29	10 (14%)	83,113,113	1.27	9 (10%)
26	CLA	4	602	17	64,68,73	1.34	9 (14%)	77,107,113	1.22	7 (9%)
26	CLA	7	601	20	64,68,73	1.33	11 (17%)	77,107,113	1.31	9 (11%)
36	NEX	U	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.60	20 (40%)
26	CLA	6	610	19	69,73,73	1.28	8 (11%)	83,113,113	1.18	7 (8%)
26	CLA	5	617	18	54,58,73	1.41	11 (20%)	65,95,113	1.26	6 (9%)
26	CLA	B	819	-	59,63,73	1.37	8 (13%)	71,101,113	1.22	9 (12%)
26	CLA	A	831	1	69,73,73	1.29	11 (15%)	83,113,113	1.22	7 (8%)
37	CHL	W	608	-	51,55,74	2.25	18 (35%)	57,91,114	3.26	21 (36%)
26	CLA	7	612	20	48,52,73	1.50	8 (16%)	58,88,113	1.29	4 (6%)
35	XAT	X	1622	-	39,47,47	0.87	0	54,74,74	2.63	20 (37%)
26	CLA	X	610	23	69,73,73	1.26	8 (11%)	83,113,113	1.17	7 (8%)
29	BCR	1	619	-	41,41,41	0.83	0	56,56,56	2.38	22 (39%)
26	CLA	a	609	14	67,72,73	1.26	8 (11%)	80,112,113	1.19	6 (7%)
29	BCR	8	621	-	41,41,41	0.75	0	56,56,56	2.77	21 (37%)
26	CLA	1	603	14	56,61,73	1.36	8 (14%)	66,98,113	1.34	4 (6%)
26	CLA	W	612	23	49,53,73	1.48	8 (16%)	59,89,113	1.40	6 (10%)
28	LHG	5	623	26	48,48,48	0.93	2 (4%)	51,54,54	0.87	2 (3%)
35	XAT	7	620	-	39,47,47	0.99	2 (5%)	54,74,74	2.50	18 (33%)
26	CLA	A	845	28	54,58,73	1.44	10 (18%)	65,95,113	1.36	7 (10%)
35	XAT	2	620	-	39,47,47	1.05	2 (5%)	54,74,74	2.48	26 (48%)
29	BCR	5	622	-	41,41,41	0.87	2 (4%)	56,56,56	2.31	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CHL	V	601	25	70,74,74	1.95	19 (27%)	80,114,114	2.80	24 (30%)
26	CLA	X	604	-	53,57,73	1.44	6 (11%)	62,93,113	1.24	5 (8%)
37	CHL	X	605	-	50,54,74	2.42	19 (38%)	56,90,114	3.08	21 (37%)
26	CLA	5	601	18	60,64,73	1.33	7 (11%)	72,102,113	1.30	5 (6%)
26	CLA	5	612	18	44,49,73	1.52	7 (15%)	52,84,113	1.28	4 (7%)
26	CLA	9	609	22	65,69,73	1.30	9 (13%)	78,108,113	1.23	5 (6%)
26	CLA	2	609	15	49,53,73	1.52	9 (18%)	59,89,113	1.27	7 (11%)
35	XAT	8	620	-	39,47,47	1.02	2 (5%)	54,74,74	2.45	24 (44%)
26	CLA	6	617	19	49,53,73	1.46	8 (16%)	59,89,113	1.30	7 (11%)
34	LUT	U	1621	-	42,43,43	0.75	0	51,60,60	1.55	9 (17%)
26	CLA	4	610	17	65,69,73	1.27	7 (10%)	78,108,113	1.21	6 (7%)
26	CLA	8	616	21	47,51,73	1.58	7 (14%)	60,87,113	1.38	9 (15%)
26	CLA	B	807	2	56,60,73	1.44	12 (21%)	67,97,113	1.39	9 (13%)
26	CLA	L	302	12	49,53,73	1.53	8 (16%)	59,89,113	1.33	6 (10%)
32	LMG	A	860	-	40,40,55	1.00	2 (5%)	48,48,63	1.09	4 (8%)
37	CHL	U	609	24	64,68,74	2.01	17 (26%)	72,106,114	2.95	25 (34%)
29	BCR	B	847	-	41,41,41	0.92	2 (4%)	56,56,56	2.20	16 (28%)
26	CLA	3	610	16	69,73,73	1.28	8 (11%)	83,113,113	1.16	6 (7%)
34	LUT	Y	1621	-	42,43,43	0.87	1 (2%)	51,60,60	1.87	14 (27%)
26	CLA	a	608	-	47,52,73	1.50	8 (17%)	56,88,113	1.31	7 (12%)
26	CLA	9	601	22	49,53,73	1.48	8 (16%)	59,89,113	1.31	5 (8%)
26	CLA	B	808	2	69,73,73	1.27	9 (13%)	83,113,113	1.23	9 (10%)
26	CLA	V	610	25	66,70,73	1.26	7 (10%)	79,109,113	1.20	8 (10%)
26	CLA	A	834	1	69,73,73	1.30	11 (15%)	83,113,113	1.34	9 (10%)
26	CLA	3	613	16	56,61,73	1.39	9 (16%)	66,98,113	1.17	5 (7%)
26	CLA	Y	613	24	69,73,73	1.25	8 (11%)	83,113,113	1.20	6 (7%)
28	LHG	A	861	-	48,48,48	0.94	2 (4%)	51,54,54	1.00	2 (3%)
26	CLA	B	815	2	47,51,73	1.48	9 (19%)	56,86,113	1.26	4 (7%)
26	CLA	4	614	17	60,64,73	1.34	8 (13%)	72,102,113	1.25	7 (9%)
35	XAT	5	621	-	39,47,47	0.95	2 (5%)	54,74,74	2.52	18 (33%)
26	CLA	9	612	22	44,49,73	1.53	6 (13%)	52,84,113	1.21	3 (5%)
26	CLA	A	820	1	69,73,73	1.26	11 (15%)	83,113,113	1.28	9 (10%)
28	LHG	8	623	-	39,39,48	1.03	2 (5%)	42,45,54	1.07	2 (4%)
37	CHL	Y	609	24	70,74,74	1.93	20 (28%)	80,114,114	2.85	25 (31%)
26	CLA	a	606	-	47,52,73	1.52	9 (19%)	55,87,113	1.26	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	B	822	2	46,50,73	1.48	9 (19%)	55,85,113	1.29	6 (10%)
26	CLA	A	811	1	69,73,73	1.28	9 (13%)	83,113,113	1.24	5 (6%)
26	CLA	6	607	-	45,49,73	1.58	9 (20%)	57,84,113	1.35	6 (10%)
26	CLA	6	620	-	68,72,73	1.25	8 (11%)	81,111,113	1.20	5 (6%)
34	LUT	6	619	-	42,43,43	0.77	1 (2%)	51,60,60	2.07	18 (35%)
26	CLA	A	814	1	69,73,73	1.26	11 (15%)	83,113,113	1.40	10 (12%)
35	XAT	Y	1622	-	39,47,47	0.92	0	54,74,74	2.75	22 (40%)
26	CLA	1	614	14	40,45,73	1.67	9 (22%)	50,79,113	1.53	9 (18%)
26	CLA	W	604	-	51,55,73	1.47	8 (15%)	61,91,113	1.28	7 (11%)
26	CLA	K	203	-	60,64,73	1.35	10 (16%)	72,102,113	1.38	10 (13%)
31	LMU	A	858	-	34,35,36	1.26	4 (11%)	42,45,47	0.99	2 (4%)
34	LUT	Z	1621	-	42,43,43	0.79	0	51,60,60	1.41	8 (15%)
26	CLA	2	614	15	45,50,73	1.53	9 (20%)	53,85,113	1.36	8 (15%)
26	CLA	X	603	23	66,70,73	1.29	6 (9%)	79,109,113	1.29	5 (6%)
34	LUT	V	1620	-	42,43,43	0.75	0	51,60,60	1.65	10 (19%)
26	CLA	9	604	-	54,58,73	1.48	9 (16%)	68,95,113	1.30	8 (11%)
37	CHL	U	606	-	48,52,74	2.18	18 (37%)	53,87,114	3.36	21 (39%)
26	CLA	2	613	15	69,73,73	1.24	7 (10%)	83,113,113	1.12	5 (6%)
26	CLA	B	823	2	49,53,73	1.49	10 (20%)	59,89,113	1.36	7 (11%)
26	CLA	B	830	2	47,51,73	1.50	8 (17%)	56,86,113	1.37	8 (14%)
26	CLA	Z	602	24	62,66,73	1.32	8 (12%)	74,104,113	1.22	6 (8%)
26	CLA	A	804	1	69,73,73	1.25	10 (14%)	83,113,113	1.29	7 (8%)
37	CHL	W	609	23	70,74,74	1.98	18 (25%)	80,114,114	2.78	22 (27%)
26	CLA	5	609	18	69,73,73	1.29	9 (13%)	83,113,113	1.22	8 (9%)
29	BCR	A	856	-	41,41,41	0.91	2 (4%)	56,56,56	1.97	17 (30%)
34	LUT	7	619	-	42,43,43	0.91	2 (4%)	51,60,60	1.99	14 (27%)
26	CLA	6	606	-	43,48,73	1.55	8 (18%)	51,83,113	1.25	5 (9%)
26	CLA	A	833	1	49,53,73	1.49	10 (20%)	59,89,113	1.50	11 (18%)
26	CLA	G	203	7	46,50,73	1.49	8 (17%)	55,85,113	1.38	6 (10%)
37	CHL	Z	609	24	70,74,74	1.95	19 (27%)	80,114,114	2.84	25 (31%)
26	CLA	B	835	-	49,53,73	1.49	10 (20%)	59,89,113	1.33	7 (11%)
26	CLA	7	604	-	54,58,73	1.40	9 (16%)	65,95,113	1.23	6 (9%)
37	CHL	Z	606	-	50,54,74	2.29	19 (38%)	56,90,114	3.30	25 (44%)
26	CLA	7	616	20	47,51,73	1.59	10 (21%)	60,87,113	1.37	7 (11%)
26	CLA	B	804	2	45,49,73	1.48	9 (20%)	54,84,113	1.36	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	U	602	24	63,67,73	1.31	8 (12%)	75,105,113	1.20	6 (8%)
34	LUT	U	1620	-	42,43,43	0.74	0	51,60,60	1.60	10 (19%)
29	BCR	A	851	-	41,41,41	0.91	1 (2%)	56,56,56	2.29	24 (42%)
37	CHL	X	607	-	70,74,74	1.86	18 (25%)	80,114,114	2.97	24 (30%)
26	CLA	B	833	2	69,73,73	1.26	9 (13%)	83,113,113	1.15	5 (6%)
26	CLA	V	614	25	49,53,73	1.46	8 (16%)	59,89,113	1.33	6 (10%)
26	CLA	a	601	14	57,62,73	1.36	9 (15%)	68,100,113	1.24	8 (11%)
30	SF4	C	102	3	0,12,12	-	-	-		
26	CLA	2	603	15	47,52,73	1.51	9 (19%)	56,88,113	1.31	7 (12%)
31	LMU	5	629	-	33,33,36	1.21	2 (6%)	44,44,47	1.27	6 (13%)
29	BCR	B	846	-	41,41,41	0.81	1 (2%)	56,56,56	2.34	21 (37%)
26	CLA	1	602	14	65,69,73	1.33	10 (15%)	78,108,113	1.25	8 (10%)
28	LHG	V	2630	26	35,35,48	1.07	2 (5%)	38,41,54	1.08	2 (5%)
29	BCR	B	843	-	41,41,41	1.04	4 (9%)	56,56,56	1.94	18 (32%)
26	CLA	a	604	-	53,57,73	1.42	8 (15%)	62,93,113	1.27	4 (6%)
34	LUT	Z	1620	-	42,43,43	0.78	0	51,60,60	1.80	12 (23%)
26	CLA	A	854	-	69,73,73	1.30	10 (14%)	83,113,113	1.31	8 (9%)
26	CLA	a	612	14	49,53,73	1.48	9 (18%)	59,89,113	1.38	5 (8%)
36	NEX	Z	1623	-	38,46,46	1.02	1 (2%)	50,70,70	2.64	19 (38%)
26	CLA	7	610	20	69,73,73	1.29	9 (13%)	83,113,113	1.11	6 (7%)
26	CLA	A	836	1	69,73,73	1.25	10 (14%)	83,113,113	1.26	7 (8%)
26	CLA	4	609	17	61,65,73	1.33	7 (11%)	73,103,113	1.18	5 (6%)
34	LUT	2	619	-	42,43,43	0.91	2 (4%)	51,60,60	1.95	14 (27%)
26	CLA	4	603	17	48,52,73	1.56	10 (20%)	61,88,113	1.40	9 (14%)
26	CLA	6	601	19	69,73,73	1.24	8 (11%)	83,113,113	1.13	6 (7%)
28	LHG	a	620	26	42,42,48	0.98	2 (4%)	45,48,54	0.82	2 (4%)
26	CLA	K	204	11	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
34	LUT	3	618	-	42,43,43	0.83	1 (2%)	51,60,60	2.01	12 (23%)
26	CLA	B	832	2	64,68,73	1.34	9 (14%)	77,107,113	1.32	8 (10%)
26	CLA	5	616	18	45,50,73	1.60	11 (24%)	56,85,113	1.30	4 (7%)
26	CLA	A	822	-	69,73,73	1.31	9 (13%)	83,113,113	1.28	11 (13%)
29	BCR	B	845	-	41,41,41	0.93	1 (2%)	56,56,56	2.50	23 (41%)
37	CHL	V	605	25	48,52,74	2.30	18 (37%)	53,87,114	3.30	20 (37%)
26	CLA	B	824	-	69,73,73	1.27	10 (14%)	83,113,113	1.16	5 (6%)
36	NEX	W	1623	-	38,46,46	0.90	2 (5%)	50,70,70	2.54	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	L	303	12	69,73,73	1.26	9 (13%)	83,113,113	1.27	8 (9%)
28	LHG	X	2630	26	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
37	CHL	U	601	24	70,74,74	1.97	20 (28%)	80,114,114	2.75	23 (28%)
29	BCR	9	621	-	41,41,41	0.76	1 (2%)	56,56,56	2.90	18 (32%)
26	CLA	3	608	-	59,63,73	1.38	11 (18%)	71,101,113	1.18	4 (5%)
26	CLA	B	838	2	50,54,73	1.47	10 (20%)	60,90,113	1.38	7 (11%)
26	CLA	A	803	-	69,73,73	1.32	12 (17%)	83,113,113	1.21	4 (4%)
26	CLA	6	612	19	44,49,73	1.52	8 (18%)	52,84,113	1.26	5 (9%)
26	CLA	X	613	23	69,73,73	1.25	8 (11%)	83,113,113	1.14	6 (7%)
26	CLA	Y	612	24	49,53,73	1.48	7 (14%)	59,89,113	1.32	4 (6%)
29	BCR	2	623	-	41,41,41	0.86	1 (2%)	56,56,56	2.36	20 (35%)
26	CLA	1	607	-	43,48,73	1.59	10 (23%)	51,83,113	1.24	5 (9%)
34	LUT	9	619	-	42,43,43	0.87	1 (2%)	51,60,60	1.90	14 (27%)
34	LUT	W	1621	-	42,43,43	0.69	0	51,60,60	1.78	13 (25%)
26	CLA	8	610	21	64,68,73	1.28	8 (12%)	77,107,113	1.31	8 (10%)
37	CHL	W	606	-	50,54,74	2.20	19 (38%)	56,90,114	3.24	24 (42%)
26	CLA	8	603	21	48,52,73	1.58	9 (18%)	61,88,113	1.51	8 (13%)
26	CLA	A	823	1	46,50,73	1.49	9 (19%)	55,85,113	1.36	4 (7%)
26	CLA	X	612	23	47,51,73	1.49	7 (14%)	56,86,113	1.38	7 (12%)
26	CLA	W	613	23	69,73,73	1.25	8 (11%)	83,113,113	1.14	3 (3%)
29	BCR	L	309	-	41,41,41	0.78	0	56,56,56	2.40	25 (44%)
26	CLA	5	611	28	46,50,73	1.48	7 (15%)	55,85,113	1.27	7 (12%)
26	CLA	7	609	20	47,52,73	1.50	9 (19%)	55,87,113	1.24	5 (9%)
26	CLA	A	819	1	63,67,73	1.34	12 (19%)	75,105,113	1.36	7 (9%)
26	CLA	B	813	2	69,73,73	1.30	11 (15%)	83,113,113	1.21	7 (8%)
29	BCR	B	852	-	41,41,41	0.82	0	56,56,56	4.21	30 (53%)
26	CLA	6	603	19	55,59,73	1.46	10 (18%)	69,96,113	1.40	7 (10%)
26	CLA	U	610	24	60,64,73	1.32	7 (11%)	72,102,113	1.27	5 (6%)
26	CLA	Y	604	-	54,58,73	1.43	8 (14%)	65,95,113	1.23	4 (6%)
33	DGD	B	850	-	63,63,67	0.83	2 (3%)	77,77,81	1.24	7 (9%)
34	LUT	4	619	-	42,43,43	0.80	1 (2%)	51,60,60	2.02	18 (35%)
26	CLA	8	604	-	54,58,73	1.41	8 (14%)	65,95,113	1.39	9 (13%)
37	CHL	Y	605	24	46,50,74	2.47	20 (43%)	51,85,114	3.36	23 (45%)
28	LHG	3	624	26	48,48,48	0.91	2 (4%)	51,54,54	0.97	3 (5%)
26	CLA	3	609	16	64,68,73	1.33	9 (14%)	77,107,113	1.26	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	3	606	-	57,62,73	1.35	9 (15%)	68,100,113	1.36	8 (11%)
26	CLA	O	2002	-	41,46,73	1.64	9 (21%)	52,81,113	1.36	7 (13%)
26	CLA	2	612	15	48,52,73	1.49	8 (16%)	58,88,113	1.29	3 (5%)
34	LUT	1	617	-	42,43,43	0.80	1 (2%)	51,60,60	1.89	16 (31%)
28	LHG	5	625	-	48,48,48	0.91	2 (4%)	51,54,54	1.02	3 (5%)
32	LMG	J	103	-	42,42,55	0.98	2 (4%)	50,50,63	1.22	6 (12%)
26	CLA	A	821	1	57,61,73	1.37	8 (14%)	68,98,113	1.30	7 (10%)
26	CLA	A	830	1	69,73,73	1.27	10 (14%)	83,113,113	1.24	7 (8%)
26	CLA	8	611	28	46,50,73	1.50	8 (17%)	55,85,113	1.29	5 (9%)
26	CLA	Z	611	28	46,50,73	1.55	9 (19%)	58,85,113	1.38	7 (12%)
26	CLA	B	826	2	66,70,73	1.29	9 (13%)	79,109,113	1.45	6 (7%)
29	BCR	J	102	-	41,41,41	0.93	2 (4%)	56,56,56	2.40	22 (39%)
26	CLA	4	618	17	43,48,73	1.60	8 (18%)	54,83,113	1.33	5 (9%)
29	BCR	B	849	-	41,41,41	0.93	2 (4%)	56,56,56	2.53	19 (33%)
37	CHL	W	607	-	69,73,74	2.00	19 (27%)	80,113,114	2.71	24 (30%)
26	CLA	1	613	-	69,73,73	1.28	10 (14%)	83,113,113	1.15	6 (7%)
26	CLA	6	604	-	69,73,73	1.25	8 (11%)	83,113,113	1.11	7 (8%)
28	LHG	W	2630	26	33,33,48	1.13	2 (6%)	36,39,54	1.17	3 (8%)
26	CLA	8	602	21	64,68,73	1.34	9 (14%)	77,107,113	1.31	10 (12%)
26	CLA	X	611	28	49,53,73	1.48	7 (14%)	59,89,113	1.29	5 (8%)
26	CLA	F	303	-	46,50,73	1.53	10 (21%)	55,85,113	1.38	7 (12%)
26	CLA	Y	603	24	59,63,73	1.35	7 (11%)	71,101,113	1.39	7 (9%)
37	CHL	Z	601	24	70,74,74	1.91	18 (25%)	80,114,114	2.87	23 (28%)
26	CLA	4	612	17	44,49,73	1.53	7 (15%)	52,84,113	1.26	3 (5%)
28	LHG	9	623	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
26	CLA	B	805	2	69,73,73	1.27	10 (14%)	83,113,113	1.25	10 (12%)
26	CLA	V	613	25	69,73,73	1.25	8 (11%)	83,113,113	1.17	5 (6%)
26	CLA	5	606	-	43,48,73	1.55	8 (18%)	51,83,113	1.31	6 (11%)
26	CLA	B	802	2	69,73,73	1.25	10 (14%)	83,113,113	1.24	7 (8%)
26	CLA	B	841	28	69,73,73	1.25	9 (13%)	83,113,113	1.23	7 (8%)
26	CLA	1	612	14	49,53,73	1.46	9 (18%)	59,89,113	1.37	5 (8%)
26	CLA	A	827	-	62,66,73	1.34	9 (14%)	74,104,113	1.20	6 (8%)
37	CHL	Y	608	-	53,57,74	2.18	18 (33%)	59,93,114	3.31	24 (40%)
26	CLA	B	831	2	69,73,73	1.25	9 (13%)	83,113,113	1.19	6 (7%)
28	LHG	O	2631	-	35,35,48	1.07	2 (5%)	38,41,54	1.12	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CLA	6	614	19	64,68,73	1.31	8 (12%)	77,107,113	1.21	8 (10%)
37	CHL	Y	607	-	70,74,74	1.87	17 (24%)	80,114,114	2.89	23 (28%)
26	CLA	5	608	-	54,58,73	1.43	9 (16%)	65,95,113	1.22	6 (9%)
26	CLA	a	616	14	49,53,73	1.47	6 (12%)	59,89,113	1.39	8 (13%)
26	CLA	7	608	-	54,58,73	1.42	11 (20%)	65,95,113	1.34	8 (12%)
26	CLA	4	604	-	58,62,73	1.42	9 (15%)	73,100,113	1.31	8 (10%)
26	CLA	B	820	2	54,58,73	1.40	10 (18%)	65,95,113	1.37	6 (9%)
27	PQN	B	842	-	34,34,34	3.33	8 (23%)	42,45,45	2.02	7 (16%)
26	CLA	B	837	2	69,73,73	1.29	11 (15%)	83,113,113	1.32	10 (12%)
26	CLA	7	613	20	69,73,73	1.27	9 (13%)	83,113,113	1.24	6 (7%)
26	CLA	4	601	17	69,73,73	1.24	9 (13%)	83,113,113	1.23	5 (6%)
26	CLA	7	602	20	69,73,73	1.30	10 (14%)	83,113,113	1.22	7 (8%)
26	CLA	A	806	1	69,73,73	1.31	11 (15%)	83,113,113	1.40	12 (14%)
29	BCR	3	621	-	41,41,41	0.83	1 (2%)	56,56,56	1.84	15 (26%)
35	XAT	Z	1622	-	39,47,47	0.93	0	54,74,74	2.87	21 (38%)
26	CLA	Z	610	24	69,73,73	1.23	9 (13%)	83,113,113	1.19	8 (9%)
26	CLA	B	829	2	69,73,73	1.31	11 (15%)	83,113,113	1.31	10 (12%)
26	CLA	L	304	-	49,53,73	1.46	8 (16%)	59,89,113	1.30	6 (10%)
29	BCR	O	2004	-	41,41,41	0.82	0	56,56,56	1.96	14 (25%)
26	CLA	V	603	25	49,53,73	1.47	7 (14%)	59,89,113	1.46	4 (6%)
26	CLA	A	813	1	58,62,73	1.39	9 (15%)	69,99,113	1.32	8 (11%)
26	CLA	6	618	19	43,48,73	1.60	9 (20%)	54,83,113	1.43	7 (12%)
32	LMG	9	625	-	55,55,55	0.88	2 (3%)	63,63,63	1.03	6 (9%)
32	LMG	8	626	-	46,46,55	0.97	2 (4%)	54,54,63	1.10	4 (7%)
26	CLA	A	815	1	54,58,73	1.43	9 (16%)	65,95,113	1.34	5 (7%)
26	CLA	L	307	8	43,48,73	1.52	9 (20%)	51,83,113	1.42	5 (9%)
26	CLA	9	606	-	43,48,73	1.56	10 (23%)	51,83,113	1.32	4 (7%)
26	CLA	A	842	1	69,73,73	1.31	10 (14%)	83,113,113	1.35	11 (13%)
29	BCR	A	852	-	41,41,41	0.97	1 (2%)	56,56,56	2.56	26 (46%)
26	CLA	a	603	14	58,62,73	1.34	8 (13%)	69,99,113	1.33	4 (5%)
29	BCR	A	849	-	41,41,41	0.85	0	56,56,56	2.22	21 (37%)
26	CLA	1	609	14	44,48,73	1.57	9 (20%)	56,83,113	1.48	9 (16%)
35	XAT	U	1622	-	39,47,47	0.92	1 (2%)	54,74,74	4.40	22 (40%)
26	CLA	A	839	1	59,63,73	1.40	10 (16%)	71,101,113	1.34	9 (12%)
34	LUT	8	619	-	42,43,43	0.86	1 (2%)	51,60,60	1.87	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	BCR	O	2005	-	41,41,41	0.88	1 (2%)	56,56,56	3.05	23 (41%)
28	LHG	6	623	26	47,47,48	0.91	2 (4%)	50,53,54	0.96	3 (6%)
29	BCR	B	848	-	41,41,41	0.84	1 (2%)	56,56,56	2.53	14 (25%)
29	BCR	7	621	-	41,41,41	0.80	1 (2%)	56,56,56	2.28	22 (39%)
26	CLA	H	202	-	42,47,73	1.57	7 (16%)	50,82,113	1.25	3 (6%)
26	CLA	2	602	15	61,69,73	1.33	8 (13%)	70,102,113	0.96	3 (4%)
26	CLA	5	602	18	69,73,73	1.27	9 (13%)	83,113,113	1.19	7 (8%)
29	BCR	L	305	-	41,41,41	0.89	0	56,56,56	2.52	25 (44%)
26	CLA	A	805	1	56,60,73	1.41	10 (17%)	67,97,113	1.49	11 (16%)
26	CLA	B	821	2	47,51,73	1.61	9 (19%)	55,86,113	1.34	6 (10%)
34	LUT	W	1620	-	42,43,43	0.72	0	51,60,60	1.59	11 (21%)
29	BCR	K	207	-	41,41,41	0.85	1 (2%)	56,56,56	2.72	21 (37%)
34	LUT	Y	1620	-	42,43,43	0.80	0	51,60,60	3.18	18 (35%)
29	BCR	B	853	-	41,41,41	0.87	3 (7%)	56,56,56	1.81	14 (25%)
26	CLA	8	614	21	57,61,73	1.39	10 (17%)	68,98,113	1.31	7 (10%)
37	CHL	Y	606	-	50,54,74	2.24	17 (34%)	56,90,114	3.23	22 (39%)

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	A	832	1	-	11/21/97/115	-
26	CLA	4	607	-	-	5/15/91/115	-
35	XAT	6	621	-	-	0/31/93/93	0/4/4/4
37	CHL	W	601	23	-	19/41/117/117	-
26	CLA	A	835	1	-	14/35/111/115	-
26	CLA	J	101	10	-	7/12/88/115	-
28	LHG	7	622	26	-	19/41/41/53	-
26	CLA	W	614	23	-	8/15/91/115	-
26	CLA	B	810	2	-	20/37/113/115	-
28	LHG	A	846	-	-	15/53/53/53	-
28	LHG	8	622	26	-	13/53/53/53	-
26	CLA	F	304	6	-	5/10/86/115	-
32	LMG	H	205	-	-	14/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	8	612	21	-	2/10/86/115	-
26	CLA	9	611	28	-	5/12/88/115	-
26	CLA	B	812	2	-	5/13/89/115	-
26	CLA	O	2001	13	-	2/6/78/115	-
26	CLA	2	607	-	-	2/13/89/115	-
26	CLA	V	612	25	-	7/15/91/115	-
26	CLA	B	827	2	-	12/36/112/115	-
26	CLA	5	607	-	-	15/39/115/115	-
26	CLA	3	617	16	-	1/8/84/115	-
32	LMG	L	2631	-	-	4/32/52/70	0/1/1/1
26	CLA	U	613	24	-	13/32/108/115	-
37	CHL	Y	601	24	-	21/41/117/117	-
26	CLA	3	611	28	-	3/4/80/115	-
35	XAT	1	618	-	-	0/31/93/93	0/4/4/4
26	CLA	4	608	-	-	11/39/115/115	-
37	CHL	X	608	-	-	21/41/113/117	-
28	LHG	A	847	26	-	6/34/34/53	-
26	CLA	Y	614	24	-	10/19/95/115	-
29	BCR	G	205	-	-	2/29/63/63	0/2/2/2
32	LMG	4	623	-	-	6/35/55/70	0/1/1/1
26	CLA	1	606	-	-	3/7/79/115	-
36	NEX	6	624	-	-	3/27/83/83	0/3/3/3
26	CLA	Z	613	24	-	8/39/115/115	-
26	CLA	B	817	2	-	10/32/108/115	-
26	CLA	8	606	-	-	8/37/113/115	-
34	LUT	5	620	-	-	0/29/67/67	0/2/2/2
26	CLA	2	604	-	-	3/11/87/115	-
26	CLA	A	837	1	-	9/15/91/115	-
32	LMG	V	2631	-	-	12/50/70/70	0/1/1/1
26	CLA	Z	604	-	-	5/21/93/115	-
36	NEX	5	624	-	-	2/27/83/83	0/3/3/3
26	CLA	A	829	1	-	10/39/115/115	-
26	CLA	6	613	-	-	15/37/113/115	-
29	BCR	3	622	-	-	3/29/63/63	0/2/2/2
26	CLA	G	204	7	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	828	2	-	17/39/115/115	-
35	XAT	4	620	-	-	2/31/93/93	0/4/4/4
26	CLA	A	838	1	-	8/21/97/115	-
26	CLA	7	611	28	-	6/31/107/115	-
37	CHL	V	608	-	-	7/20/96/117	-
26	CLA	4	616	17	-	7/11/87/115	-
26	CLA	B	839	-	-	14/39/115/115	-
29	BCR	4	621	-	-	2/29/63/63	0/2/2/2
37	CHL	V	609	25	-	13/35/111/117	-
26	CLA	8	608	-	-	7/23/99/115	-
28	LHG	Y	2630	26	-	13/53/53/53	-
28	LHG	Z	2630	26	-	19/53/53/53	-
26	CLA	6	611	28	-	5/12/88/115	-
26	CLA	K	206	11	-	6/15/91/115	-
26	CLA	U	612	24	-	5/12/88/115	-
28	LHG	2	622	26	-	9/40/40/53	-
26	CLA	1	601	14	-	4/25/101/115	-
29	BCR	6	622	-	-	2/29/63/63	0/2/2/2
26	CLA	3	607	16	-	6/28/104/115	-
37	CHL	U	605	24	-	6/14/90/117	-
26	CLA	B	811	2	-	11/23/95/115	-
26	CLA	8	607	-	-	2/10/86/115	-
32	LMG	5	627	-	-	7/35/55/70	0/1/1/1
37	CHL	Z	605	24	-	6/12/88/117	-
29	BCR	A	848	-	-	3/29/63/63	0/2/2/2
26	CLA	A	810	1	-	7/21/97/115	-
26	CLA	a	614	14	-	9/27/99/115	-
34	LUT	a	617	-	-	4/29/67/67	0/2/2/2
26	CLA	A	825	1	-	17/39/115/115	-
27	PQN	A	844	-	-	6/23/43/43	0/2/2/2
26	CLA	Z	612	24	-	8/15/91/115	-
26	CLA	2	616	-	-	3/11/87/115	-
26	CLA	B	809	2	-	11/39/115/115	-
26	CLA	1	608	-	-	4/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	801	1	-	10/39/115/115	-
26	CLA	X	614	23	-	3/12/88/115	-
30	SF4	C	101	3	-	-	0/6/5/5
26	CLA	Y	611	28	-	9/13/89/115	-
26	CLA	5	614	18	-	9/15/87/115	-
26	CLA	7	614	20	-	3/12/88/115	-
26	CLA	A	826	-	-	8/37/113/115	-
26	CLA	W	611	28	-	9/30/106/115	-
26	CLA	V	602	25	-	8/33/109/115	-
29	BCR	A	850	-	-	2/29/63/63	0/2/2/2
26	CLA	7	603	20	-	7/13/89/115	-
26	CLA	a	602	14	-	5/35/111/115	-
26	CLA	a	611	28	-	0/4/80/115	-
26	CLA	7	606	-	-	2/10/86/115	-
26	CLA	3	602	16	-	3/33/109/115	-
26	CLA	W	602	23	-	12/33/109/115	-
26	CLA	O	2003	-	-	6/8/84/115	-
31	LMU	5	628	-	-	10/19/59/61	0/2/2/2
29	BCR	a	619	-	-	3/29/63/63	0/2/2/2
26	CLA	A	802	2	-	12/39/115/115	-
26	CLA	A	841	1	-	18/39/115/115	-
26	CLA	8	613	21	-	18/39/115/115	-
26	CLA	U	611	28	-	4/12/88/115	-
26	CLA	6	609	19	-	7/15/91/115	-
26	CLA	U	604	-	-	7/20/92/115	-
26	CLA	A	818	1	-	15/33/109/115	-
29	BCR	L	301	-	-	4/29/63/63	0/2/2/2
26	CLA	A	812	1	-	9/39/115/115	-
26	CLA	6	602	19	-	9/39/115/115	-
26	CLA	a	607	-	-	6/15/91/115	-
26	CLA	B	840	2	-	9/39/115/115	-
34	LUT	X	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	B	803	-	-	12/39/115/115	-
26	CLA	3	604	-	-	7/39/115/115	-
35	XAT	a	618	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	9	622	26	-	10/34/34/53	-
26	CLA	A	843	-	-	14/37/113/115	-
36	NEX	V	1623	-	-	7/27/83/83	0/3/3/3
26	CLA	A	828	1	-	16/39/115/115	-
29	BCR	K	202	-	-	4/29/63/63	0/2/2/2
26	CLA	9	614	22	-	5/15/91/115	-
26	CLA	X	602	23	-	13/39/115/115	-
32	LMG	J	104	-	-	12/35/55/70	0/1/1/1
26	CLA	7	607	-	-	1/12/88/115	-
26	CLA	U	614	24	-	5/12/88/115	-
31	LMU	1	621	-	-	7/21/61/61	0/2/2/2
29	BCR	7	623	-	-	3/29/63/63	0/2/2/2
29	BCR	3	620	-	-	4/29/63/63	0/2/2/2
26	CLA	B	836	2	-	5/21/97/115	-
37	CHL	X	609	23	-	26/41/117/117	-
29	BCR	L	308	-	-	6/29/63/63	0/2/2/2
29	BCR	B	844	-	-	2/29/63/63	0/2/2/2
26	CLA	Y	602	24	-	14/31/107/115	-
26	CLA	A	817	-	-	2/15/91/115	-
26	CLA	4	611	28	-	9/12/88/115	-
26	CLA	H	203	-	-	17/39/115/115	-
31	LMU	8	625	-	-	12/21/61/61	0/2/2/2
28	LHG	U	2630	26	-	21/53/53/53	-
30	SF4	A	853	1,2	-	-	0/6/5/5
26	CLA	1	611	28	-	7/30/106/115	-
26	CLA	6	616	19	-	18/39/115/115	-
26	CLA	a	613	-	-	9/26/102/115	-
28	LHG	3	623	-	-	15/49/49/53	-
31	LMU	A	857	-	-	9/21/61/61	0/2/2/2
26	CLA	B	825	-	-	4/20/96/115	-
26	CLA	1	610	14	-	2/8/80/115	-
36	NEX	Y	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	V	604	-	-	8/21/97/115	-
26	CLA	5	619	-	-	10/11/87/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	F	301	-	-	14/30/106/115	-
26	CLA	9	610	22	-	5/30/106/115	-
26	CLA	9	603	22	-	5/13/89/115	-
28	LHG	B	851	26	-	14/42/42/53	-
26	CLA	B	814	2	-	15/38/114/115	-
26	CLA	9	607	-	-	11/15/91/115	-
26	CLA	1	604	-	-	8/20/96/115	-
28	LHG	4	622	26	-	8/53/53/53	-
26	CLA	V	611	28	-	7/13/89/115	-
37	CHL	U	608	-	-	7/15/91/117	-
26	CLA	Z	614	24	-	9/19/95/115	-
32	LMG	4	624	-	-	5/35/55/70	0/1/1/1
37	CHL	U	607	-	-	11/17/93/117	-
26	CLA	2	606	-	-	3/13/89/115	-
26	CLA	6	608	-	-	8/15/91/115	-
26	CLA	8	601	21	-	16/39/115/115	-
26	CLA	5	603	18	-	5/25/101/115	-
26	CLA	A	824	1	-	11/39/115/115	-
26	CLA	3	615	-	-	3/8/84/115	-
37	CHL	Z	608	-	-	8/21/97/117	-
37	CHL	Z	607	-	-	22/41/117/117	-
37	CHL	W	605	23	-	12/17/93/117	-
29	BCR	B	801	-	-	4/29/63/63	0/2/2/2
26	CLA	B	806	2	-	19/39/115/115	-
26	CLA	B	816	2	-	10/25/101/115	-
26	CLA	4	606	-	-	4/8/84/115	-
37	CHL	V	607	-	-	12/17/93/117	-
37	CHL	X	606	-	-	6/15/91/117	-
26	CLA	U	603	24	-	10/24/100/115	-
26	CLA	K	201	11	-	7/15/91/115	-
26	CLA	Z	603	24	-	11/27/103/115	-
26	CLA	5	618	18	-	3/8/84/115	-
26	CLA	A	808	1	-	3/21/97/115	-
31	LMU	K	208	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	3	614	16	-	2/8/84/115	-
26	CLA	A	807	1	-	20/39/115/115	-
26	CLA	a	610	14	-	7/31/107/115	-
26	CLA	A	840	1	-	5/24/100/115	-
26	CLA	L	306	-	-	1/8/84/115	-
28	LHG	1	620	26	-	9/53/53/53	-
26	CLA	7	615	-	-	6/8/84/115	-
34	LUT	X	1620	-	-	4/29/67/67	0/2/2/2
26	CLA	A	809	1	-	11/39/115/115	-
26	CLA	1	616	14	-	7/11/87/115	-
28	LHG	H	204	-	-	15/53/53/53	-
26	CLA	2	611	28	-	4/12/88/115	-
26	CLA	B	834	2	-	5/33/109/115	-
29	BCR	F	305	-	-	6/29/63/63	0/2/2/2
26	CLA	2	610	15	-	5/27/103/115	-
26	CLA	8	609	21	-	2/15/91/115	-
26	CLA	B	818	2	-	11/33/109/115	-
26	CLA	5	610	18	-	6/26/102/115	-
26	CLA	A	816	1	-	15/39/115/115	-
26	CLA	3	612	16	-	5/13/89/115	-
26	CLA	9	613	22	-	14/39/115/115	-
26	CLA	9	602	22	-	7/33/109/115	-
35	XAT	9	620	-	-	0/31/93/93	0/4/4/4
37	CHL	X	601	23	-	21/41/117/117	-
26	CLA	5	613	18	-	16/37/113/115	-
26	CLA	Y	610	24	-	10/39/115/115	-
26	CLA	3	603	16	-	10/27/103/115	-
35	XAT	V	1622	-	-	2/31/93/93	0/4/4/4
35	XAT	3	619	-	-	0/31/93/93	0/4/4/4
28	LHG	9	624	-	-	17/53/53/53	-
26	CLA	5	604	-	-	12/35/111/115	-
26	CLA	2	601	15	-	8/39/115/115	-
36	NEX	X	1623	-	-	5/27/83/83	0/3/3/3
34	LUT	V	1621	-	-	3/29/67/67	0/2/2/2
35	XAT	W	1622	-	-	2/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	W	610	23	-	7/27/103/115	-
26	CLA	W	603	23	-	9/24/100/115	-
37	CHL	V	606	-	-	6/15/91/117	-
26	CLA	4	613	17	-	13/39/115/115	-
26	CLA	4	602	17	-	8/33/109/115	-
26	CLA	7	601	20	-	8/33/109/115	-
36	NEX	U	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	6	610	19	-	12/39/115/115	-
26	CLA	5	617	18	-	12/21/97/115	-
26	CLA	B	819	-	-	8/27/103/115	-
26	CLA	A	831	1	-	16/39/115/115	-
37	CHL	W	608	-	-	11/19/95/117	-
26	CLA	7	612	20	-	4/13/89/115	-
35	XAT	X	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	X	610	23	-	13/39/115/115	-
29	BCR	1	619	-	-	3/29/63/63	0/2/2/2
26	CLA	a	609	14	-	15/37/113/115	-
29	BCR	8	621	-	-	2/29/63/63	0/2/2/2
26	CLA	1	603	14	-	7/23/99/115	-
26	CLA	W	612	23	-	7/15/91/115	-
28	LHG	5	623	26	-	15/53/53/53	-
35	XAT	7	620	-	-	0/31/93/93	0/4/4/4
26	CLA	A	845	28	-	7/21/97/115	-
35	XAT	2	620	-	-	0/31/93/93	0/4/4/4
29	BCR	5	622	-	-	1/29/63/63	0/2/2/2
37	CHL	V	601	25	-	13/41/117/117	-
26	CLA	X	604	-	-	11/20/96/115	-
37	CHL	X	605	-	-	9/17/93/117	-
26	CLA	5	601	18	-	3/29/105/115	-
26	CLA	5	612	18	-	2/10/86/115	-
26	CLA	9	609	22	-	4/35/111/115	-
26	CLA	2	609	15	-	5/15/91/115	-
35	XAT	8	620	-	-	0/31/93/93	0/4/4/4
26	CLA	6	617	19	-	9/15/91/115	-
34	LUT	U	1621	-	-	5/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	4	610	17	-	8/35/111/115	-
26	CLA	8	616	21	-	5/11/87/115	-
26	CLA	B	807	2	-	4/24/100/115	-
26	CLA	L	302	12	-	8/15/91/115	-
32	LMG	A	860	-	-	9/35/55/70	0/1/1/1
37	CHL	U	609	24	-	14/34/110/117	-
29	BCR	B	847	-	-	2/29/63/63	0/2/2/2
26	CLA	3	610	16	-	14/39/115/115	-
34	LUT	Y	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	a	608	-	-	4/13/89/115	-
26	CLA	9	601	22	-	8/15/91/115	-
26	CLA	B	808	2	-	13/39/115/115	-
26	CLA	V	610	25	-	9/36/112/115	-
26	CLA	A	834	1	-	12/39/115/115	-
26	CLA	3	613	16	-	7/23/99/115	-
26	CLA	Y	613	24	-	16/39/115/115	-
28	LHG	A	861	-	-	18/53/53/53	-
26	CLA	B	815	2	-	2/13/89/115	-
26	CLA	4	614	17	-	9/29/105/115	-
35	XAT	5	621	-	-	0/31/93/93	0/4/4/4
26	CLA	9	612	22	-	2/10/86/115	-
26	CLA	A	820	1	-	8/39/115/115	-
28	LHG	8	623	-	-	12/44/44/53	-
37	CHL	Y	609	24	-	17/41/117/117	-
26	CLA	a	606	-	-	8/12/88/115	-
26	CLA	B	822	2	-	7/12/88/115	-
26	CLA	A	811	1	-	15/39/115/115	-
26	CLA	6	607	-	-	2/10/86/115	-
26	CLA	6	620	-	-	12/37/113/115	-
34	LUT	6	619	-	-	4/29/67/67	0/2/2/2
26	CLA	A	814	1	-	18/39/115/115	-
35	XAT	Y	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	1	614	14	-	0/4/76/115	-
26	CLA	W	604	-	-	6/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	K	203	-	-	10/29/105/115	-
31	LMU	A	858	-	-	10/21/57/61	0/2/2/2
34	LUT	Z	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	2	614	15	-	0/11/87/115	-
26	CLA	X	603	23	-	15/36/112/115	-
34	LUT	V	1620	-	-	4/29/67/67	0/2/2/2
26	CLA	9	604	-	-	8/20/96/115	-
37	CHL	U	606	-	-	8/15/91/117	-
26	CLA	2	613	15	-	10/39/115/115	-
26	CLA	B	823	2	-	7/15/91/115	-
26	CLA	B	830	2	-	4/13/89/115	-
26	CLA	Z	602	24	-	7/31/107/115	-
26	CLA	A	804	1	-	16/39/115/115	-
37	CHL	W	609	23	-	13/41/117/117	-
26	CLA	5	609	18	-	12/39/115/115	-
29	BCR	A	856	-	-	2/29/63/63	0/2/2/2
34	LUT	7	619	-	-	2/29/67/67	0/2/2/2
26	CLA	6	606	-	-	2/8/84/115	-
26	CLA	A	833	1	-	5/15/91/115	-
26	CLA	G	203	7	-	5/12/88/115	-
37	CHL	Z	609	24	-	18/41/117/117	-
26	CLA	B	835	-	-	2/15/91/115	-
26	CLA	7	604	-	-	8/21/97/115	-
37	CHL	Z	606	-	-	8/17/93/117	-
26	CLA	7	616	20	-	8/11/87/115	-
26	CLA	B	804	2	-	3/10/86/115	-
26	CLA	U	602	24	-	18/32/108/115	-
34	LUT	U	1620	-	-	7/29/67/67	0/2/2/2
29	BCR	A	851	-	-	2/29/63/63	0/2/2/2
37	CHL	X	607	-	-	27/41/117/117	-
26	CLA	B	833	2	-	13/39/115/115	-
26	CLA	V	614	25	-	6/15/91/115	-
26	CLA	a	601	14	-	4/25/101/115	-
30	SF4	C	102	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	2	603	15	-	7/13/89/115	-
31	LMU	5	629	-	-	11/18/58/61	0/2/2/2
29	BCR	B	846	-	-	0/29/63/63	0/2/2/2
26	CLA	1	602	14	-	5/35/111/115	-
28	LHG	V	2630	26	-	6/40/40/53	-
29	BCR	B	843	-	-	4/29/63/63	0/2/2/2
26	CLA	a	604	-	-	8/20/96/115	-
34	LUT	Z	1620	-	-	5/29/67/67	0/2/2/2
26	CLA	A	854	-	-	9/39/115/115	-
26	CLA	a	612	14	-	6/15/91/115	-
36	NEX	Z	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	7	610	20	-	7/39/115/115	-
26	CLA	A	836	1	-	9/39/115/115	-
26	CLA	4	609	17	-	5/30/106/115	-
34	LUT	2	619	-	-	2/29/67/67	0/2/2/2
26	CLA	4	603	17	-	5/13/89/115	-
26	CLA	6	601	19	-	17/39/115/115	-
28	LHG	a	620	26	-	7/47/47/53	-
26	CLA	K	204	11	-	5/15/91/115	-
34	LUT	3	618	-	-	4/29/67/67	0/2/2/2
26	CLA	B	832	2	-	12/33/109/115	-
26	CLA	5	616	18	-	4/8/84/115	-
26	CLA	A	822	-	-	6/39/115/115	-
29	BCR	B	845	-	-	9/29/63/63	0/2/2/2
37	CHL	V	605	25	-	7/15/91/117	-
26	CLA	B	824	-	-	10/39/115/115	-
36	NEX	W	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	L	303	12	-	14/39/115/115	-
28	LHG	X	2630	26	-	13/53/53/53	-
37	CHL	U	601	24	-	19/41/117/117	-
29	BCR	9	621	-	-	4/29/63/63	0/2/2/2
26	CLA	3	608	-	-	10/27/103/115	-
26	CLA	B	838	2	-	3/17/93/115	-
26	CLA	A	803	-	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	6	612	19	-	3/10/86/115	-
26	CLA	X	613	23	-	14/39/115/115	-
26	CLA	Y	612	24	-	7/15/91/115	-
29	BCR	2	623	-	-	4/29/63/63	0/2/2/2
26	CLA	1	607	-	-	2/8/84/115	-
34	LUT	9	619	-	-	4/29/67/67	0/2/2/2
34	LUT	W	1621	-	-	5/29/67/67	0/2/2/2
26	CLA	8	610	21	-	9/33/109/115	-
37	CHL	W	606	-	-	4/17/93/117	-
26	CLA	8	603	21	-	4/13/89/115	-
26	CLA	A	823	1	-	1/12/88/115	-
26	CLA	X	612	23	-	8/13/89/115	-
26	CLA	W	613	23	-	22/39/115/115	-
29	BCR	L	309	-	-	3/29/63/63	0/2/2/2
26	CLA	5	611	28	-	2/12/88/115	-
26	CLA	7	609	20	-	6/12/88/115	-
26	CLA	A	819	1	-	5/32/108/115	-
26	CLA	B	813	2	-	20/39/115/115	-
29	BCR	B	852	-	-	6/29/63/63	0/2/2/2
26	CLA	6	603	19	-	5/22/98/115	-
26	CLA	U	610	24	-	4/29/105/115	-
26	CLA	Y	604	-	-	8/21/97/115	-
33	DGD	B	850	-	-	15/51/91/95	0/2/2/2
34	LUT	4	619	-	-	4/29/67/67	0/2/2/2
26	CLA	8	604	-	-	6/21/97/115	-
37	CHL	Y	605	24	-	6/12/88/117	-
28	LHG	3	624	26	-	14/53/53/53	-
26	CLA	3	609	16	-	14/33/109/115	-
26	CLA	3	606	-	-	4/25/101/115	-
26	CLA	O	2002	-	-	0/4/80/115	-
26	CLA	2	612	15	-	7/13/89/115	-
34	LUT	1	617	-	-	4/29/67/67	0/2/2/2
28	LHG	5	625	-	-	14/53/53/53	-
32	LMG	J	103	-	-	10/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	821	1	-	14/25/101/115	-
26	CLA	A	830	1	-	13/39/115/115	-
26	CLA	8	611	28	-	6/12/88/115	-
26	CLA	Z	611	28	-	5/11/87/115	-
26	CLA	B	826	2	-	14/36/112/115	-
29	BCR	J	102	-	-	2/29/63/63	0/2/2/2
26	CLA	4	618	17	-	2/8/84/115	-
29	BCR	B	849	-	-	5/29/63/63	0/2/2/2
37	CHL	W	607	-	-	21/39/115/117	-
26	CLA	1	613	-	-	17/39/115/115	-
26	CLA	6	604	-	-	18/39/115/115	-
28	LHG	W	2630	26	-	13/38/38/53	-
26	CLA	8	602	21	-	14/33/109/115	-
26	CLA	X	611	28	-	6/15/91/115	-
26	CLA	F	303	-	-	7/12/88/115	-
26	CLA	Y	603	24	-	12/27/103/115	-
37	CHL	Z	601	24	-	16/41/117/117	-
26	CLA	4	612	17	-	4/10/86/115	-
28	LHG	9	623	-	-	20/53/53/53	-
26	CLA	B	805	2	-	11/39/115/115	-
26	CLA	V	613	25	-	20/39/115/115	-
26	CLA	5	606	-	-	3/8/84/115	-
26	CLA	B	802	2	-	18/39/115/115	-
26	CLA	B	841	28	-	15/39/115/115	-
26	CLA	1	612	14	-	6/15/91/115	-
26	CLA	A	827	-	-	7/31/107/115	-
37	CHL	Y	608	-	-	8/21/97/117	-
26	CLA	B	831	2	-	12/39/115/115	-
28	LHG	O	2631	-	-	13/40/40/53	-
26	CLA	6	614	19	-	9/33/109/115	-
37	CHL	Y	607	-	-	21/41/117/117	-
26	CLA	5	608	-	-	6/21/97/115	-
26	CLA	a	616	14	-	7/15/91/115	-
26	CLA	7	608	-	-	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	4	604	-	-	9/25/101/115	-
26	CLA	B	820	2	-	3/21/97/115	-
27	PQN	B	842	-	-	7/23/43/43	0/2/2/2
26	CLA	B	837	2	-	10/39/115/115	-
26	CLA	7	613	20	-	18/39/115/115	-
26	CLA	4	601	17	-	16/39/115/115	-
26	CLA	7	602	20	-	11/39/115/115	-
26	CLA	A	806	1	-	13/39/115/115	-
29	BCR	3	621	-	-	0/29/63/63	0/2/2/2
35	XAT	Z	1622	-	-	4/31/93/93	0/4/4/4
26	CLA	Z	610	24	-	9/39/115/115	-
26	CLA	B	829	2	-	8/39/115/115	-
26	CLA	L	304	-	-	3/15/91/115	-
29	BCR	O	2004	-	-	2/29/63/63	0/2/2/2
26	CLA	V	603	25	-	6/15/91/115	-
26	CLA	A	813	1	-	7/26/102/115	-
26	CLA	6	618	19	-	1/8/84/115	-
32	LMG	9	625	-	-	11/50/70/70	0/1/1/1
32	LMG	8	626	-	-	16/41/61/70	0/1/1/1
26	CLA	A	815	1	-	12/21/97/115	-
26	CLA	L	307	8	-	2/8/84/115	-
26	CLA	9	606	-	-	2/8/84/115	-
26	CLA	A	842	1	-	18/39/115/115	-
29	BCR	A	852	-	-	8/29/63/63	0/2/2/2
26	CLA	a	603	14	-	10/25/101/115	-
29	BCR	A	849	-	-	5/29/63/63	0/2/2/2
26	CLA	1	609	14	-	3/8/84/115	-
35	XAT	U	1622	-	-	4/31/93/93	0/4/4/4
26	CLA	A	839	1	-	10/27/103/115	-
34	LUT	8	619	-	-	4/29/67/67	0/2/2/2
29	BCR	O	2005	-	-	2/29/63/63	0/2/2/2
28	LHG	6	623	26	-	19/52/52/53	-
29	BCR	B	848	-	-	4/29/63/63	0/2/2/2
29	BCR	7	621	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	H	202	-	-	4/6/82/115	-
26	CLA	2	602	15	-	18/49/99/115	-
26	CLA	5	602	18	-	10/39/115/115	-
29	BCR	L	305	-	-	2/29/63/63	0/2/2/2
26	CLA	A	805	1	-	7/24/100/115	-
26	CLA	B	821	2	-	5/13/89/115	-
34	LUT	W	1620	-	-	6/29/67/67	0/2/2/2
29	BCR	K	207	-	-	2/29/63/63	0/2/2/2
34	LUT	Y	1620	-	-	5/29/67/67	0/2/2/2
29	BCR	B	853	-	-	4/29/63/63	0/2/2/2
26	CLA	8	614	21	-	8/25/101/115	-
37	CHL	Y	606	-	-	8/17/93/117	-

All (3510) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	842	PQN	C12-C13	9.58	1.56	1.33
27	A	844	PQN	C12-C13	9.30	1.55	1.33
27	B	842	PQN	O4-C4	7.74	1.39	1.23
27	A	844	PQN	O4-C4	7.72	1.39	1.23
27	A	844	PQN	O1-C1	7.56	1.39	1.23
27	B	842	PQN	O1-C1	7.44	1.39	1.23
27	B	842	PQN	C10-C5	-6.91	1.29	1.40
27	A	844	PQN	C10-C5	-6.61	1.29	1.40
27	A	844	PQN	C9-C10	6.61	1.50	1.39
27	A	844	PQN	C6-C5	6.52	1.50	1.39
27	B	842	PQN	C9-C10	6.51	1.50	1.39
27	B	842	PQN	C6-C5	6.46	1.50	1.39
37	X	608	CHL	C4D-C3D	-5.80	1.33	1.45
37	Y	608	CHL	O2D-CGD	5.20	1.45	1.33
37	W	605	CHL	O2D-CGD	5.18	1.45	1.33
37	W	606	CHL	O2D-CGD	5.17	1.45	1.33
37	X	605	CHL	O2D-CGD	5.17	1.45	1.33
37	Z	606	CHL	O2D-CGD	5.17	1.45	1.33
37	Y	606	CHL	O2D-CGD	5.17	1.45	1.33
37	Y	607	CHL	O2D-CGD	5.16	1.45	1.33
37	W	601	CHL	O2D-CGD	5.15	1.45	1.33
37	Z	605	CHL	O2D-CGD	5.15	1.45	1.33
37	X	601	CHL	O2D-CGD	5.15	1.45	1.33
37	U	601	CHL	O2D-CGD	5.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	U	605	CHL	O2D-CGD	5.14	1.45	1.33
37	Y	609	CHL	O2D-CGD	5.13	1.45	1.33
26	2	602	CLA	C1B-C2B	5.13	1.49	1.34
37	W	607	CHL	O2D-CGD	5.13	1.45	1.33
37	X	609	CHL	O2D-CGD	5.13	1.45	1.33
37	U	609	CHL	O2D-CGD	5.13	1.45	1.33
37	V	601	CHL	O2D-CGD	5.12	1.45	1.33
37	X	608	CHL	O2D-CGD	5.12	1.45	1.33
37	Y	605	CHL	O2D-CGD	5.11	1.45	1.33
37	V	605	CHL	O2D-CGD	5.11	1.45	1.33
37	U	606	CHL	O2D-CGD	5.11	1.45	1.33
37	X	606	CHL	O2D-CGD	5.10	1.45	1.33
37	Y	601	CHL	O2D-CGD	5.10	1.45	1.33
37	Z	601	CHL	O2D-CGD	5.09	1.45	1.33
37	Z	609	CHL	O2D-CGD	5.09	1.45	1.33
37	V	607	CHL	O2D-CGD	5.09	1.45	1.33
37	Z	608	CHL	O2D-CGD	5.09	1.45	1.33
37	V	609	CHL	O2D-CGD	5.07	1.45	1.33
37	Z	607	CHL	O2D-CGD	5.07	1.45	1.33
37	W	608	CHL	O2D-CGD	5.07	1.45	1.33
37	X	607	CHL	O2D-CGD	5.06	1.45	1.33
37	V	606	CHL	O2D-CGD	5.05	1.45	1.33
37	U	607	CHL	O2D-CGD	5.05	1.45	1.33
37	Z	606	CHL	C3D-C4D	-5.04	1.32	1.44
37	V	608	CHL	O2D-CGD	5.02	1.45	1.33
37	W	609	CHL	O2D-CGD	5.02	1.45	1.33
37	U	608	CHL	C3D-C4D	-5.02	1.32	1.44
37	X	605	CHL	CHC-C1C	5.01	1.48	1.38
37	U	609	CHL	C3D-C4D	-5.00	1.32	1.44
37	U	608	CHL	O2D-CGD	5.00	1.45	1.33
37	U	605	CHL	CHC-C1C	4.97	1.48	1.38
37	V	608	CHL	C3D-C4D	-4.97	1.33	1.44
37	Y	605	CHL	CHC-C1C	4.96	1.48	1.38
37	W	609	CHL	C3D-C4D	-4.95	1.33	1.44
37	W	607	CHL	CHC-C1C	4.94	1.48	1.38
37	V	609	CHL	C3D-C4D	-4.93	1.33	1.44
37	Y	606	CHL	C3D-C4D	-4.92	1.33	1.44
37	W	601	CHL	C3D-C4D	-4.91	1.33	1.44
37	X	606	CHL	C3D-C4D	-4.90	1.33	1.44
37	U	606	CHL	C3D-C4D	-4.90	1.33	1.44
37	X	605	CHL	C2C-C3C	4.90	1.47	1.36
37	X	609	CHL	C3D-C4D	-4.90	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	U	605	CHL	C3D-C4D	-4.89	1.33	1.44
37	Y	605	CHL	C2C-C3C	4.87	1.47	1.36
37	V	605	CHL	C3D-C4D	-4.87	1.33	1.44
37	Z	607	CHL	C3D-C4D	-4.87	1.33	1.44
37	Z	608	CHL	C3D-C4D	-4.87	1.33	1.44
37	V	606	CHL	C3D-C4D	-4.85	1.33	1.44
37	V	601	CHL	C3D-C4D	-4.85	1.33	1.44
37	U	607	CHL	CHC-C1C	4.84	1.48	1.38
37	X	605	CHL	C3D-C4D	-4.81	1.33	1.44
37	Y	605	CHL	C3D-C4D	-4.81	1.33	1.44
37	Y	609	CHL	C3D-C4D	-4.81	1.33	1.44
37	Y	601	CHL	CHC-C1C	4.81	1.48	1.38
37	Z	605	CHL	C3D-C4D	-4.80	1.33	1.44
37	Z	609	CHL	C3D-C4D	-4.79	1.33	1.44
37	Y	601	CHL	C3D-C4D	-4.78	1.33	1.44
37	X	609	CHL	C2C-C3C	4.78	1.47	1.36
37	U	605	CHL	C2C-C3C	4.77	1.47	1.36
37	Y	609	CHL	C2C-C3C	4.77	1.47	1.36
37	W	609	CHL	C2C-C3C	4.76	1.46	1.36
37	Z	606	CHL	CHC-C1C	4.76	1.48	1.38
37	U	609	CHL	C2C-C3C	4.75	1.46	1.36
37	W	601	CHL	C2C-C3C	4.75	1.46	1.36
37	X	606	CHL	CHC-C1C	4.75	1.48	1.38
37	X	605	CHL	CHD-C1D	4.74	1.47	1.38
37	U	601	CHL	C2C-C3C	4.74	1.46	1.36
37	V	607	CHL	C3D-C4D	-4.73	1.33	1.44
37	V	605	CHL	CHC-C1C	4.73	1.48	1.38
37	Z	601	CHL	C3D-C4D	-4.73	1.33	1.44
37	W	601	CHL	CHC-C1C	4.73	1.48	1.38
37	V	607	CHL	CHC-C1C	4.72	1.48	1.38
37	Y	608	CHL	C3D-C4D	-4.72	1.33	1.44
37	W	607	CHL	C3D-C4D	-4.71	1.33	1.44
37	X	608	CHL	CHC-C1C	4.71	1.48	1.38
37	U	607	CHL	C3D-C4D	-4.70	1.33	1.44
37	W	608	CHL	C3D-C4D	-4.70	1.33	1.44
37	U	605	CHL	CHD-C1D	4.70	1.47	1.38
37	V	601	CHL	CHC-C1C	4.70	1.48	1.38
37	Z	609	CHL	C2C-C3C	4.70	1.46	1.36
37	W	605	CHL	C2C-C3C	4.69	1.46	1.36
37	W	609	CHL	CHD-C1D	4.69	1.47	1.38
37	U	608	CHL	CHC-C1C	4.69	1.48	1.38
37	Z	608	CHL	C2C-C3C	4.69	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	W	608	CHL	C2C-C3C	4.68	1.46	1.36
37	V	601	CHL	C2C-C3C	4.68	1.46	1.36
37	W	607	CHL	C2C-C3C	4.68	1.46	1.37
37	Y	605	CHL	CHD-C1D	4.67	1.47	1.38
37	Y	606	CHL	CHC-C1C	4.67	1.48	1.38
37	Y	601	CHL	C2C-C3C	4.67	1.46	1.36
37	Z	608	CHL	CHC-C1C	4.67	1.48	1.38
37	U	601	CHL	CHD-C1D	4.66	1.47	1.38
37	V	609	CHL	C2C-C3C	4.66	1.46	1.36
37	U	608	CHL	C2C-C3C	4.65	1.46	1.36
37	W	605	CHL	C3D-C4D	-4.65	1.33	1.44
37	Z	609	CHL	CHD-C1D	4.64	1.47	1.38
37	X	601	CHL	C3D-C4D	-4.64	1.33	1.44
37	Y	607	CHL	C3D-C4D	-4.63	1.33	1.44
37	U	601	CHL	C3D-C4D	-4.63	1.33	1.44
37	V	605	CHL	C2C-C3C	4.61	1.46	1.36
37	W	609	CHL	CHC-C1C	4.60	1.47	1.38
37	W	606	CHL	C3D-C4D	-4.60	1.33	1.44
37	X	609	CHL	CHD-C1D	4.60	1.47	1.38
37	Y	608	CHL	CHC-C1C	4.58	1.47	1.38
37	X	608	CHL	C3D-C2D	4.57	1.46	1.36
37	W	607	CHL	CHD-C1D	4.57	1.47	1.38
37	X	607	CHL	C3D-C4D	-4.56	1.33	1.44
37	V	608	CHL	CHC-C1C	4.55	1.47	1.38
37	Z	606	CHL	C2C-C3C	4.55	1.46	1.36
37	Z	601	CHL	C2C-C3C	4.55	1.46	1.36
37	X	601	CHL	C2C-C3C	4.54	1.46	1.36
37	Z	607	CHL	CHC-C1C	4.53	1.47	1.38
37	U	607	CHL	C2C-C3C	4.53	1.46	1.36
37	X	608	CHL	C2C-C3C	4.53	1.46	1.36
37	Z	601	CHL	CHC-C1C	4.52	1.47	1.38
37	U	606	CHL	CHC-C1C	4.51	1.47	1.38
37	Z	605	CHL	C2C-C3C	4.51	1.46	1.36
37	Y	608	CHL	C2C-C3C	4.50	1.46	1.36
37	Y	609	CHL	CHD-C1D	4.50	1.47	1.38
37	W	605	CHL	O2A-CGA	4.48	1.45	1.30
37	V	607	CHL	C2C-C3C	4.48	1.46	1.36
37	V	607	CHL	O2A-CGA	4.48	1.45	1.30
37	Y	606	CHL	O2A-CGA	4.48	1.45	1.30
37	X	605	CHL	O2A-CGA	4.47	1.45	1.30
37	Z	605	CHL	CHC-C1C	4.47	1.47	1.38
37	W	608	CHL	CHC-C1C	4.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	U	609	CHL	CHD-C1D	4.44	1.47	1.38
37	V	606	CHL	CHC-C1C	4.44	1.47	1.38
37	W	608	CHL	CHD-C1D	4.44	1.47	1.38
37	W	606	CHL	O2A-CGA	4.44	1.45	1.30
37	U	601	CHL	CHC-C1C	4.43	1.47	1.38
37	V	609	CHL	CHD-C1D	4.43	1.47	1.38
37	V	608	CHL	C2C-C3C	4.42	1.46	1.36
37	V	605	CHL	CHD-C1D	4.42	1.47	1.38
37	X	606	CHL	C2C-C3C	4.42	1.46	1.36
37	W	601	CHL	CHD-C1D	4.42	1.47	1.38
28	A	861	LHG	O8-C23	4.41	1.46	1.33
37	U	607	CHL	O2A-CGA	4.41	1.45	1.30
37	X	607	CHL	CHC-C1C	4.40	1.47	1.38
37	Z	609	CHL	CHC-C1C	4.40	1.47	1.38
37	W	605	CHL	CHC-C1C	4.40	1.47	1.38
37	Z	606	CHL	O2A-CGA	4.39	1.45	1.30
37	Z	605	CHL	C3A-C2A	-4.39	1.50	1.54
37	Z	607	CHL	C2C-C3C	4.37	1.46	1.36
37	X	608	CHL	CHD-C1D	4.37	1.46	1.38
37	U	606	CHL	C2C-C3C	4.37	1.46	1.36
37	W	601	CHL	O2A-CGA	4.37	1.46	1.33
37	V	609	CHL	O2A-CGA	4.35	1.46	1.33
37	V	601	CHL	CHD-C1D	4.35	1.46	1.38
28	8	623	LHG	O8-C23	4.34	1.46	1.33
37	W	606	CHL	C2C-C3C	4.33	1.46	1.36
37	Y	607	CHL	CHC-C1C	4.32	1.47	1.38
37	Y	607	CHL	C2C-C3C	4.32	1.46	1.36
37	Y	601	CHL	CHD-C1D	4.32	1.46	1.38
37	W	609	CHL	O2A-CGA	4.31	1.45	1.33
28	W	2630	LHG	O8-C23	4.30	1.45	1.33
37	Y	601	CHL	O2A-CGA	4.29	1.45	1.33
32	L	2631	LMG	O8-C28	4.29	1.45	1.33
37	X	609	CHL	CHC-C1C	4.28	1.47	1.38
37	W	605	CHL	CHD-C1D	4.28	1.46	1.38
37	V	609	CHL	CHC-C1C	4.28	1.47	1.38
28	U	2630	LHG	O8-C23	4.28	1.45	1.33
37	Z	601	CHL	O2A-CGA	4.28	1.45	1.33
37	X	601	CHL	CHC-C1C	4.27	1.47	1.38
37	V	606	CHL	C2C-C3C	4.27	1.45	1.36
37	V	601	CHL	O2A-CGA	4.27	1.45	1.33
28	5	623	LHG	O7-C7	4.26	1.46	1.34
37	X	606	CHL	CHD-C1D	4.26	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Z	608	CHL	O2A-CGA	4.26	1.45	1.33
37	Z	608	CHL	CHD-C1D	4.26	1.46	1.38
37	X	608	CHL	O2A-CGA	4.25	1.45	1.33
28	9	622	LHG	O7-C7	4.25	1.46	1.34
37	Z	605	CHL	CHD-C1D	4.25	1.46	1.38
37	X	609	CHL	O2A-CGA	4.24	1.45	1.33
37	Z	606	CHL	CHD-C1D	4.24	1.46	1.38
37	Y	608	CHL	O2A-CGA	4.24	1.45	1.33
32	4	623	LMG	O8-C28	4.24	1.45	1.33
37	X	607	CHL	C2C-C3C	4.24	1.45	1.36
37	U	609	CHL	O2A-CGA	4.24	1.45	1.33
37	V	608	CHL	O2A-CGA	4.24	1.45	1.33
37	X	605	CHL	CHD-C4C	4.24	1.48	1.39
37	X	601	CHL	CHD-C1D	4.24	1.46	1.38
28	9	624	LHG	O8-C23	4.23	1.45	1.33
37	V	607	CHL	CHD-C1D	4.23	1.46	1.38
32	4	624	LMG	O8-C28	4.23	1.45	1.33
37	Y	609	CHL	O2A-CGA	4.22	1.45	1.33
32	4	623	LMG	O7-C10	4.21	1.46	1.34
28	V	2630	LHG	O8-C23	4.21	1.45	1.33
37	Z	607	CHL	O2A-CGA	4.19	1.45	1.33
37	X	607	CHL	O2A-CGA	4.19	1.45	1.33
28	W	2630	LHG	O7-C7	4.19	1.46	1.34
32	5	627	LMG	O8-C28	4.19	1.45	1.33
37	U	601	CHL	O2A-CGA	4.19	1.45	1.33
37	W	606	CHL	CHD-C1D	4.19	1.46	1.38
32	9	625	LMG	O8-C28	4.19	1.45	1.33
37	Y	609	CHL	CHC-C1C	4.18	1.47	1.38
37	X	601	CHL	O2A-CGA	4.17	1.45	1.33
37	U	608	CHL	CHD-C1D	4.17	1.46	1.38
28	O	2631	LHG	O8-C23	4.16	1.45	1.33
28	H	204	LHG	O8-C23	4.16	1.45	1.33
28	Z	2630	LHG	O8-C23	4.16	1.45	1.33
28	A	847	LHG	O8-C23	4.16	1.45	1.33
28	X	2630	LHG	O8-C23	4.16	1.45	1.33
36	5	624	NEX	C7-C8	-4.16	1.25	1.32
37	Z	601	CHL	CHD-C1D	4.15	1.46	1.38
37	Z	609	CHL	O2A-CGA	4.15	1.45	1.33
37	W	607	CHL	O2A-CGA	4.15	1.45	1.33
32	8	626	LMG	O8-C28	4.15	1.45	1.33
28	9	623	LHG	O8-C23	4.14	1.45	1.33
28	2	622	LHG	O7-C7	4.14	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	606	CHL	C2C-C3C	4.14	1.45	1.36
28	9	624	LHG	O7-C7	4.13	1.46	1.34
28	B	851	LHG	O8-C23	4.12	1.45	1.33
37	Y	607	CHL	O2A-CGA	4.12	1.45	1.33
28	3	624	LHG	O8-C23	4.11	1.45	1.33
37	Z	607	CHL	CHD-C1D	4.11	1.46	1.38
28	U	2630	LHG	O7-C7	4.10	1.45	1.34
32	J	103	LMG	O8-C28	4.10	1.45	1.33
37	U	606	CHL	CHD-C1D	4.10	1.46	1.38
37	U	607	CHL	CHD-C1D	4.10	1.46	1.38
37	X	605	CHL	CHC-C4B	4.08	1.48	1.39
37	U	605	CHL	CHD-C4C	4.07	1.48	1.39
37	Y	606	CHL	CHD-C1D	4.06	1.46	1.38
28	Y	2630	LHG	O8-C23	4.06	1.45	1.33
26	X	604	CLA	C1D-ND	4.06	1.42	1.37
32	V	2631	LMG	O8-C28	4.06	1.45	1.33
28	B	851	LHG	O7-C7	4.05	1.45	1.34
37	W	609	CHL	CHD-C4C	4.05	1.48	1.39
32	J	104	LMG	O8-C28	4.05	1.45	1.33
37	V	606	CHL	CHD-C1D	4.05	1.46	1.38
37	Y	608	CHL	CHD-C1D	4.05	1.46	1.38
28	5	625	LHG	O8-C23	4.04	1.45	1.33
28	Y	2630	LHG	O7-C7	4.04	1.45	1.34
33	B	850	DGD	O1G-C1A	4.04	1.45	1.33
28	X	2630	LHG	O7-C7	4.03	1.45	1.34
32	4	624	LMG	O7-C10	4.03	1.45	1.34
28	6	623	LHG	O8-C23	4.02	1.45	1.33
37	X	607	CHL	CHD-C1D	4.01	1.46	1.38
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	5	623	LHG	O8-C23	4.01	1.45	1.33
28	8	622	LHG	O7-C7	4.01	1.45	1.34
28	4	622	LHG	O8-C23	4.01	1.45	1.33
37	U	601	CHL	CHD-C4C	4.00	1.48	1.39
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
28	A	861	LHG	O7-C7	4.00	1.45	1.34
37	X	606	CHL	CHC-C4B	4.00	1.48	1.39
37	X	609	CHL	CHD-C4C	3.99	1.48	1.39
37	W	608	CHL	O2A-CGA	3.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	860	LMG	O8-C28	3.99	1.45	1.33
26	Z	614	CLA	C1D-ND	3.98	1.42	1.37
32	V	2631	LMG	O7-C10	3.98	1.45	1.34
37	W	606	CHL	CHC-C1C	3.98	1.46	1.38
37	W	607	CHL	CHD-C4C	3.98	1.48	1.39
28	Z	2630	LHG	O7-C7	3.98	1.45	1.34
37	Y	605	CHL	CHD-C4C	3.98	1.48	1.39
28	9	622	LHG	O8-C23	3.97	1.45	1.33
28	a	620	LHG	O8-C23	3.97	1.44	1.33
28	V	2630	LHG	O7-C7	3.97	1.45	1.34
28	1	620	LHG	O8-C23	3.97	1.44	1.33
28	O	2631	LHG	O7-C7	3.97	1.45	1.34
28	A	846	LHG	O8-C23	3.96	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
26	V	611	CLA	C1D-ND	3.95	1.42	1.37
37	W	608	CHL	CHD-C4C	3.95	1.48	1.39
32	A	860	LMG	O7-C10	3.95	1.45	1.34
28	3	624	LHG	O7-C7	3.95	1.45	1.34
37	Z	609	CHL	CHD-C4C	3.95	1.48	1.39
32	H	205	LMG	O8-C28	3.94	1.44	1.33
26	X	603	CLA	C1D-ND	3.94	1.42	1.37
28	7	622	LHG	O8-C23	3.94	1.44	1.33
28	3	623	LHG	O8-C23	3.93	1.44	1.33
32	J	103	LMG	O7-C10	3.93	1.45	1.34
26	B	839	CLA	C4D-ND	-3.93	1.32	1.37
37	V	608	CHL	CHD-C1D	3.93	1.46	1.38
37	U	609	CHL	CHC-C1C	3.93	1.46	1.38
32	5	627	LMG	O7-C10	3.93	1.45	1.34
26	U	610	CLA	C1D-ND	3.93	1.42	1.37
26	X	610	CLA	C1D-ND	3.92	1.42	1.37
28	6	623	LHG	O7-C7	3.92	1.45	1.34
32	J	104	LMG	O7-C10	3.91	1.45	1.34
26	U	612	CLA	C1D-ND	3.91	1.42	1.37
26	Y	611	CLA	C1D-ND	3.91	1.42	1.37
26	Y	614	CLA	C1D-ND	3.91	1.42	1.37
37	Y	607	CHL	CHD-C1D	3.91	1.46	1.38
26	X	612	CLA	C1D-ND	3.91	1.42	1.37
37	Y	609	CHL	CHD-C4C	3.91	1.48	1.39
37	Y	605	CHL	CHB-C1B	3.90	1.48	1.39
26	X	614	CLA	C1D-ND	3.90	1.42	1.37
26	8	616	CLA	C1D-ND	3.89	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	611	CLA	C1D-ND	3.89	1.42	1.37
26	W	604	CLA	C1D-ND	3.89	1.42	1.37
28	A	846	LHG	O7-C7	3.89	1.45	1.34
28	9	623	LHG	O7-C7	3.89	1.45	1.34
32	8	626	LMG	O7-C10	3.88	1.45	1.34
37	X	605	CHL	CHB-C1B	3.87	1.48	1.39
37	W	607	CHL	CHC-C4B	3.87	1.48	1.39
26	U	614	CLA	C1D-ND	3.87	1.42	1.37
37	W	601	CHL	CHD-C4C	3.87	1.48	1.39
37	U	609	CHL	CHD-C4C	3.87	1.48	1.39
28	2	622	LHG	O8-C23	3.87	1.44	1.33
37	U	605	CHL	CHB-C1B	3.86	1.48	1.39
26	A	839	CLA	C4D-ND	-3.86	1.32	1.37
28	8	622	LHG	O8-C23	3.86	1.44	1.33
26	Y	603	CLA	C1D-ND	3.85	1.42	1.37
28	7	622	LHG	O7-C7	3.85	1.45	1.34
26	W	612	CLA	C1D-ND	3.84	1.42	1.37
37	Y	605	CHL	CHC-C4B	3.84	1.48	1.39
37	U	605	CHL	CHC-C4B	3.83	1.48	1.39
26	V	610	CLA	C1D-ND	3.83	1.42	1.37
37	V	601	CHL	CHD-C4C	3.83	1.48	1.39
26	Y	612	CLA	C1D-ND	3.82	1.42	1.37
37	V	609	CHL	CHD-C4C	3.82	1.48	1.39
28	3	623	LHG	O7-C7	3.82	1.45	1.34
37	Y	606	CHL	CHC-C4B	3.82	1.48	1.39
26	A	827	CLA	C4D-ND	-3.81	1.32	1.37
37	Z	608	CHL	CHD-C4C	3.81	1.47	1.39
37	X	606	CHL	CHD-C4C	3.80	1.47	1.39
37	Y	605	CHL	OBD-CAD	3.80	1.29	1.22
26	A	854	CLA	C4D-ND	-3.80	1.32	1.37
26	Y	604	CLA	C1D-ND	3.80	1.42	1.37
37	Y	601	CHL	CHD-C4C	3.79	1.47	1.39
37	X	601	CHL	OBD-CAD	3.79	1.29	1.22
37	X	608	CHL	CHC-C4B	3.79	1.47	1.39
37	X	608	CHL	CHD-C4C	3.79	1.47	1.39
37	X	605	CHL	OBD-CAD	3.79	1.29	1.22
32	L	2631	LMG	O7-C10	3.79	1.45	1.34
26	7	601	CLA	C4D-ND	-3.78	1.32	1.37
37	Z	606	CHL	CHD-C4C	3.78	1.47	1.39
26	W	611	CLA	C1D-ND	3.78	1.42	1.37
37	W	605	CHL	OBD-CAD	3.78	1.29	1.22
26	Z	612	CLA	C1D-ND	3.78	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	822	CLA	C4D-ND	-3.78	1.32	1.37
26	U	603	CLA	C1D-ND	3.78	1.42	1.37
26	B	840	CLA	C4D-ND	-3.77	1.32	1.37
37	U	607	CHL	CHC-C4B	3.77	1.47	1.39
26	A	836	CLA	C4D-ND	-3.77	1.32	1.37
37	V	605	CHL	CHD-C4C	3.77	1.47	1.39
37	W	605	CHL	CHD-C4C	3.77	1.47	1.39
26	J	101	CLA	C1D-ND	3.77	1.42	1.37
26	Y	602	CLA	C1D-ND	3.76	1.42	1.37
26	B	821	CLA	C3C-C4C	3.75	1.46	1.40
37	W	607	CHL	OBD-CAD	3.75	1.28	1.22
26	Z	604	CLA	C1D-ND	3.75	1.42	1.37
26	X	604	CLA	C4B-NB	3.74	1.42	1.37
37	Z	606	CHL	CHC-C4B	3.74	1.47	1.39
37	U	608	CHL	CHD-C4C	3.74	1.47	1.39
37	W	601	CHL	CHC-C4B	3.73	1.47	1.39
26	3	612	CLA	C4B-NB	3.73	1.42	1.37
37	V	601	CHL	CHC-C4B	3.73	1.47	1.39
37	Z	601	CHL	CHD-C4C	3.73	1.47	1.39
26	5	611	CLA	C1D-ND	3.72	1.42	1.37
26	B	806	CLA	C4D-ND	-3.72	1.32	1.37
26	9	612	CLA	C1D-ND	3.72	1.42	1.37
26	V	602	CLA	C1D-ND	3.72	1.42	1.37
26	W	610	CLA	C1D-ND	3.72	1.42	1.37
26	B	829	CLA	C4D-ND	-3.71	1.32	1.37
26	Y	604	CLA	C4B-NB	3.71	1.42	1.37
26	Y	610	CLA	C4B-NB	3.71	1.42	1.37
26	V	603	CLA	C1D-ND	3.71	1.42	1.37
26	V	614	CLA	C1D-ND	3.71	1.42	1.37
37	Z	609	CHL	OBD-CAD	3.71	1.28	1.22
37	V	605	CHL	CHB-C1B	3.71	1.47	1.39
37	Z	601	CHL	OBD-CAD	3.71	1.28	1.22
26	L	303	CLA	C4D-ND	-3.71	1.32	1.37
33	B	850	DGD	O2G-C1B	3.70	1.44	1.34
37	Y	608	CHL	CHD-C4C	3.70	1.47	1.39
26	A	845	CLA	C4D-ND	-3.70	1.32	1.37
26	W	602	CLA	C1D-ND	3.70	1.42	1.37
37	U	601	CHL	OBD-CAD	3.70	1.28	1.22
37	V	605	CHL	OBD-CAD	3.70	1.28	1.22
26	X	611	CLA	C1D-ND	3.70	1.42	1.37
26	9	611	CLA	C1D-ND	3.69	1.42	1.37
37	W	606	CHL	OBD-CAD	3.69	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	803	CLA	C4D-ND	-3.69	1.32	1.37
37	X	609	CHL	OBD-CAD	3.69	1.28	1.22
37	U	607	CHL	CHD-C4C	3.69	1.47	1.39
26	A	841	CLA	C4D-ND	-3.69	1.32	1.37
26	X	610	CLA	C4B-NB	3.68	1.42	1.37
26	Z	603	CLA	C1D-ND	3.68	1.42	1.37
26	U	602	CLA	C1D-ND	3.68	1.42	1.37
37	U	607	CHL	OBD-CAD	3.68	1.28	1.22
37	V	607	CHL	CHC-C4B	3.67	1.47	1.39
37	V	608	CHL	CHD-C4C	3.67	1.47	1.39
26	V	612	CLA	C1D-ND	3.67	1.42	1.37
26	A	830	CLA	C4D-ND	-3.67	1.32	1.37
37	X	607	CHL	OBD-CAD	3.67	1.28	1.22
26	A	819	CLA	C4D-ND	-3.67	1.32	1.37
37	X	601	CHL	CHD-C4C	3.67	1.47	1.39
37	Y	601	CHL	CHC-C4B	3.66	1.47	1.39
37	Y	607	CHL	OBD-CAD	3.66	1.28	1.22
37	U	605	CHL	OBD-CAD	3.66	1.28	1.22
37	V	605	CHL	CHC-C4B	3.66	1.47	1.39
28	A	847	LHG	O7-C7	3.66	1.44	1.34
26	B	834	CLA	C4D-ND	-3.66	1.32	1.37
26	B	838	CLA	C4D-ND	-3.66	1.32	1.37
26	1	614	CLA	C1D-ND	3.66	1.42	1.37
37	Z	605	CHL	CHD-C4C	3.65	1.47	1.39
26	A	831	CLA	C4D-ND	-3.65	1.32	1.37
37	Z	608	CHL	CHC-C4B	3.65	1.47	1.39
26	U	613	CLA	C4B-NB	3.65	1.42	1.37
37	Z	605	CHL	OBD-CAD	3.65	1.28	1.22
26	A	820	CLA	C4D-ND	-3.65	1.32	1.37
26	B	833	CLA	C4D-ND	-3.65	1.32	1.37
37	U	609	CHL	OBD-CAD	3.65	1.28	1.22
26	6	608	CLA	C1D-ND	3.65	1.42	1.37
26	9	610	CLA	C4B-NB	3.65	1.42	1.37
37	U	606	CHL	CHD-C4C	3.65	1.47	1.39
26	U	613	CLA	C1D-ND	3.64	1.42	1.37
26	V	604	CLA	C1D-ND	3.64	1.42	1.37
26	A	825	CLA	C4D-ND	-3.64	1.32	1.37
26	W	604	CLA	C4B-NB	3.64	1.42	1.37
26	A	810	CLA	C4D-ND	-3.64	1.32	1.37
26	9	614	CLA	C4B-NB	3.64	1.42	1.37
26	U	604	CLA	C1D-ND	3.64	1.42	1.37
26	5	604	CLA	C1D-ND	3.63	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	601	CHL	OBD-CAD	3.63	1.28	1.22
26	Y	612	CLA	C4B-NB	3.63	1.42	1.37
26	W	614	CLA	C1D-ND	3.63	1.42	1.37
26	4	609	CLA	C1D-ND	3.63	1.42	1.37
26	6	602	CLA	C4D-ND	-3.63	1.32	1.37
37	W	601	CHL	OBD-CAD	3.62	1.28	1.22
26	4	611	CLA	C1D-ND	3.62	1.42	1.37
37	Y	606	CHL	CHD-C4C	3.62	1.47	1.39
26	5	601	CLA	C1D-ND	3.62	1.42	1.37
26	4	602	CLA	C4B-NB	3.62	1.42	1.37
37	Y	608	CHL	OBD-CAD	3.62	1.28	1.22
26	B	805	CLA	C4D-ND	-3.62	1.32	1.37
37	Z	607	CHL	OBD-CAD	3.62	1.28	1.22
26	1	607	CLA	C4B-NB	3.61	1.42	1.37
26	X	602	CLA	C1D-ND	3.61	1.42	1.37
26	4	612	CLA	C1D-ND	3.61	1.42	1.37
31	5	629	LMU	O5B-C1B	3.61	1.51	1.41
37	W	607	CHL	CHB-C1B	3.61	1.47	1.39
37	W	605	CHL	CHC-C4B	3.61	1.47	1.39
26	A	828	CLA	C4D-ND	-3.61	1.32	1.37
26	6	618	CLA	C1D-ND	3.61	1.42	1.37
26	7	614	CLA	C4D-ND	-3.61	1.32	1.37
37	Z	607	CHL	CHC-C4B	3.61	1.47	1.39
37	V	607	CHL	OBD-CAD	3.60	1.28	1.22
26	B	832	CLA	C4D-ND	-3.60	1.32	1.37
26	1	616	CLA	C1D-ND	3.60	1.42	1.37
26	B	815	CLA	C4D-ND	-3.60	1.32	1.37
26	A	843	CLA	C4D-ND	-3.60	1.32	1.37
26	4	604	CLA	C1D-ND	3.60	1.42	1.37
37	V	608	CHL	CHC-C4B	3.59	1.47	1.39
26	W	603	CLA	C1D-ND	3.59	1.42	1.37
26	1	602	CLA	C4D-ND	-3.59	1.32	1.37
26	a	614	CLA	C1D-ND	3.59	1.42	1.37
37	W	606	CHL	CHD-C4C	3.58	1.47	1.39
26	A	815	CLA	C4D-ND	-3.58	1.32	1.37
37	W	609	CHL	OBD-CAD	3.58	1.28	1.22
26	A	842	CLA	C4D-ND	-3.58	1.32	1.37
26	W	613	CLA	C4B-NB	3.58	1.42	1.37
26	6	601	CLA	C4D-ND	-3.58	1.32	1.37
37	V	609	CHL	OBD-CAD	3.58	1.28	1.22
37	V	607	CHL	CHD-C4C	3.58	1.47	1.39
26	5	609	CLA	C4D-ND	-3.58	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	613	CLA	C1D-ND	3.57	1.42	1.37
26	X	603	CLA	C4B-NB	3.57	1.42	1.37
26	B	837	CLA	C4D-ND	-3.57	1.32	1.37
26	3	609	CLA	C1D-ND	3.57	1.42	1.37
26	Z	610	CLA	C4B-NB	3.57	1.42	1.37
26	6	612	CLA	C1D-ND	3.57	1.42	1.37
26	9	601	CLA	C1D-ND	3.57	1.42	1.37
26	U	604	CLA	C4B-NB	3.57	1.42	1.37
26	3	602	CLA	C4D-ND	-3.57	1.32	1.37
26	Z	613	CLA	C1D-ND	3.57	1.42	1.37
26	A	834	CLA	C4D-ND	-3.57	1.32	1.37
26	8	606	CLA	C4D-ND	-3.57	1.32	1.37
26	V	611	CLA	C4B-NB	3.57	1.42	1.37
37	W	608	CHL	OBD-CAD	3.56	1.28	1.22
26	8	613	CLA	C4D-ND	-3.56	1.32	1.37
26	1	604	CLA	C1D-ND	3.56	1.42	1.37
26	2	612	CLA	C1D-ND	3.56	1.42	1.37
26	B	823	CLA	C4D-ND	-3.56	1.32	1.37
26	a	602	CLA	C4D-ND	-3.56	1.32	1.37
26	a	604	CLA	C1D-ND	3.55	1.42	1.37
26	A	824	CLA	C4D-ND	-3.55	1.32	1.37
37	X	606	CHL	CHB-C1B	3.55	1.47	1.39
36	6	624	NEX	C7-C8	-3.55	1.26	1.32
26	a	613	CLA	C4D-ND	-3.55	1.32	1.37
26	5	614	CLA	C1D-ND	3.55	1.42	1.37
26	A	806	CLA	C4D-ND	-3.55	1.32	1.37
26	Y	610	CLA	C1D-ND	3.54	1.42	1.37
26	4	613	CLA	C4B-NB	3.54	1.42	1.37
37	Y	608	CHL	CHC-C4B	3.54	1.47	1.39
26	1	608	CLA	C1D-ND	3.54	1.42	1.37
26	9	614	CLA	C1D-ND	3.54	1.42	1.37
37	V	601	CHL	OBD-CAD	3.54	1.28	1.22
37	X	606	CHL	OBD-CAD	3.54	1.28	1.22
26	B	821	CLA	C4D-ND	-3.54	1.32	1.37
26	6	604	CLA	C1D-ND	3.54	1.42	1.37
26	A	813	CLA	C4D-ND	-3.53	1.32	1.37
26	a	608	CLA	C1D-ND	3.53	1.42	1.37
26	Z	604	CLA	C4B-NB	3.53	1.42	1.37
26	A	808	CLA	C4D-ND	-3.53	1.32	1.37
26	A	812	CLA	C4D-ND	-3.53	1.32	1.37
37	X	609	CHL	CHB-C1B	3.53	1.47	1.39
26	1	606	CLA	C1D-ND	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	611	CLA	C4B-NB	3.53	1.42	1.37
26	A	832	CLA	C4D-ND	-3.53	1.32	1.37
26	B	816	CLA	C4D-ND	-3.53	1.32	1.37
26	7	611	CLA	C4D-ND	-3.53	1.32	1.37
26	B	813	CLA	C4D-ND	-3.53	1.32	1.37
26	B	809	CLA	C4D-ND	-3.53	1.32	1.37
26	F	304	CLA	C1D-ND	3.53	1.42	1.37
26	3	608	CLA	C4D-ND	-3.53	1.32	1.37
26	a	607	CLA	C4B-NB	3.53	1.42	1.37
26	A	816	CLA	C4D-ND	-3.53	1.32	1.37
26	3	612	CLA	C1D-ND	3.52	1.42	1.37
26	B	828	CLA	C4D-ND	-3.52	1.32	1.37
26	X	613	CLA	C1D-ND	3.52	1.42	1.37
26	V	613	CLA	C1D-ND	3.52	1.42	1.37
26	1	613	CLA	C4D-ND	-3.52	1.32	1.37
26	5	610	CLA	C4B-NB	3.52	1.42	1.37
26	W	602	CLA	C4B-NB	3.52	1.42	1.37
26	9	611	CLA	C4B-NB	3.52	1.42	1.37
37	Z	601	CHL	CHC-C4B	3.52	1.47	1.39
26	A	805	CLA	C4D-ND	-3.51	1.32	1.37
37	Z	607	CHL	CHD-C4C	3.51	1.47	1.39
26	3	604	CLA	C4D-ND	-3.51	1.32	1.37
26	6	604	CLA	C4D-ND	-3.51	1.32	1.37
26	7	613	CLA	C4D-ND	-3.51	1.32	1.37
26	8	601	CLA	C4D-ND	-3.51	1.32	1.37
26	W	614	CLA	C4B-NB	3.51	1.42	1.37
37	U	601	CHL	CHC-C4B	3.51	1.47	1.39
26	7	608	CLA	C4D-ND	-3.51	1.32	1.37
36	Y	1623	NEX	C7-C8	-3.51	1.26	1.32
26	2	609	CLA	C4D-ND	-3.51	1.32	1.37
26	4	608	CLA	C1D-ND	3.51	1.42	1.37
26	4	610	CLA	C1D-ND	3.51	1.42	1.37
26	6	610	CLA	C4B-NB	3.51	1.42	1.37
26	2	602	CLA	C4D-ND	-3.51	1.32	1.37
37	U	601	CHL	CHB-C1B	3.50	1.47	1.39
26	K	206	CLA	C1D-ND	3.50	1.42	1.37
26	9	612	CLA	C4B-NB	3.50	1.42	1.37
26	5	619	CLA	C1D-ND	3.50	1.42	1.37
26	a	616	CLA	C1D-ND	3.50	1.42	1.37
26	6	611	CLA	C1D-ND	3.50	1.42	1.37
37	X	607	CHL	CHD-C4C	3.49	1.47	1.39
37	Z	605	CHL	CHC-C4B	3.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L	302	CLA	C4D-ND	-3.49	1.32	1.37
26	B	804	CLA	C4D-ND	-3.49	1.32	1.37
26	7	607	CLA	C4D-ND	-3.49	1.32	1.37
26	8	604	CLA	C4D-ND	-3.49	1.32	1.37
26	3	611	CLA	C1D-ND	3.49	1.42	1.37
26	4	602	CLA	C4D-ND	-3.48	1.32	1.37
37	W	608	CHL	CHC-C4B	3.48	1.47	1.39
26	4	614	CLA	C1D-ND	3.48	1.42	1.37
37	V	606	CHL	CHC-C4B	3.48	1.47	1.39
26	Y	611	CLA	C4B-NB	3.48	1.42	1.37
37	Z	608	CHL	CHB-C1B	3.48	1.47	1.39
26	B	825	CLA	C4D-ND	-3.48	1.32	1.37
37	Z	608	CHL	OBD-CAD	3.48	1.28	1.22
26	A	829	CLA	C4D-ND	-3.47	1.32	1.37
26	5	616	CLA	C4D-ND	-3.47	1.32	1.37
26	A	823	CLA	C4D-ND	-3.47	1.32	1.37
26	1	610	CLA	C1D-ND	3.47	1.42	1.37
26	A	833	CLA	C4D-ND	-3.47	1.32	1.37
26	B	817	CLA	C4D-ND	-3.47	1.32	1.37
26	9	613	CLA	C1D-ND	3.47	1.42	1.37
37	U	608	CHL	CHC-C4B	3.47	1.47	1.39
26	A	809	CLA	C4D-ND	-3.47	1.32	1.37
37	V	606	CHL	CHD-C4C	3.47	1.47	1.39
26	B	830	CLA	C4B-NB	3.47	1.42	1.37
37	Y	607	CHL	CHD-C4C	3.46	1.47	1.39
37	W	601	CHL	CHB-C1B	3.46	1.47	1.39
26	Z	612	CLA	C4B-NB	3.46	1.42	1.37
26	6	614	CLA	C4D-ND	-3.46	1.32	1.37
26	8	608	CLA	C4D-ND	-3.46	1.32	1.37
26	5	607	CLA	C4D-ND	-3.46	1.32	1.37
26	H	202	CLA	C1D-ND	3.46	1.42	1.37
26	B	818	CLA	C4D-ND	-3.46	1.32	1.37
26	a	601	CLA	C1D-ND	3.46	1.42	1.37
26	4	618	CLA	C4B-NB	3.46	1.42	1.37
26	5	608	CLA	C4D-ND	-3.46	1.32	1.37
26	7	609	CLA	C4D-ND	-3.46	1.32	1.37
26	K	206	CLA	C4B-NB	3.45	1.42	1.37
26	9	602	CLA	C4D-ND	-3.45	1.32	1.37
26	5	618	CLA	C1D-ND	3.45	1.42	1.37
26	X	613	CLA	C4B-NB	3.45	1.42	1.37
26	Y	613	CLA	C4B-NB	3.45	1.42	1.37
26	5	612	CLA	C1D-ND	3.45	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	W	609	CHL	CHB-C1B	3.45	1.47	1.39
26	B	807	CLA	C4D-ND	-3.45	1.33	1.37
26	9	603	CLA	C4D-ND	-3.45	1.33	1.37
26	5	602	CLA	C4D-ND	-3.44	1.33	1.37
37	U	606	CHL	OBD-CAD	3.44	1.28	1.22
26	8	602	CLA	C4D-ND	-3.44	1.33	1.37
26	B	808	CLA	C4D-ND	-3.44	1.33	1.37
26	W	611	CLA	C4B-NB	3.44	1.42	1.37
37	X	607	CHL	CHC-C4B	3.44	1.47	1.39
26	X	614	CLA	C4B-NB	3.44	1.42	1.37
26	V	612	CLA	C4B-NB	3.44	1.42	1.37
26	9	603	CLA	CAB-C3B	-3.44	1.43	1.50
27	B	842	PQN	C11-C12	3.43	1.55	1.50
26	6	613	CLA	C4B-NB	3.43	1.42	1.37
26	Z	614	CLA	C4B-NB	3.43	1.42	1.37
26	1	613	CLA	C1D-ND	3.43	1.42	1.37
26	7	615	CLA	C1D-ND	3.43	1.42	1.37
37	W	609	CHL	CHC-C4B	3.43	1.47	1.39
37	Z	605	CHL	CHB-C1B	3.43	1.47	1.39
37	U	606	CHL	CHC-C4B	3.43	1.47	1.39
26	F	304	CLA	C4B-NB	3.43	1.42	1.37
26	6	614	CLA	C1D-ND	3.43	1.42	1.37
26	Z	613	CLA	C4B-NB	3.43	1.42	1.37
26	A	826	CLA	C4D-ND	-3.42	1.33	1.37
26	Z	604	CLA	CAD-C3D	-3.42	1.44	1.50
26	7	606	CLA	C4D-ND	-3.42	1.33	1.37
26	K	201	CLA	C1D-ND	3.42	1.42	1.37
26	6	616	CLA	C4D-ND	-3.42	1.33	1.37
31	K	208	LMU	O5B-C1B	3.42	1.50	1.41
26	A	821	CLA	C4D-ND	-3.42	1.33	1.37
26	6	606	CLA	C1D-ND	3.42	1.42	1.37
26	4	607	CLA	C1D-ND	3.42	1.42	1.37
26	W	610	CLA	C4B-NB	3.42	1.42	1.37
26	7	603	CLA	C1D-ND	3.42	1.42	1.37
31	5	628	LMU	O5B-C1B	3.41	1.50	1.41
26	3	610	CLA	C4B-NB	3.41	1.42	1.37
26	2	616	CLA	C1D-ND	3.41	1.42	1.37
26	X	602	CLA	C4B-NB	3.41	1.42	1.37
26	2	604	CLA	C4D-ND	-3.41	1.33	1.37
26	a	606	CLA	C4B-NB	3.41	1.42	1.37
26	4	618	CLA	C1D-ND	3.41	1.42	1.37
26	A	804	CLA	C4D-ND	-3.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	607	CLA	C4B-NB	3.41	1.42	1.37
26	a	606	CLA	C1D-ND	3.41	1.42	1.37
26	1	611	CLA	C1D-ND	3.40	1.42	1.37
26	A	802	CLA	C4D-ND	-3.40	1.33	1.37
26	5	613	CLA	C4D-ND	-3.40	1.33	1.37
26	4	616	CLA	C4B-NB	3.40	1.42	1.37
26	U	614	CLA	C4B-NB	3.40	1.42	1.37
26	a	613	CLA	C1D-ND	3.40	1.42	1.37
37	Z	607	CHL	CHB-C1B	3.40	1.47	1.39
26	2	604	CLA	C1D-ND	3.40	1.42	1.37
26	Z	602	CLA	C1D-ND	3.40	1.42	1.37
26	5	609	CLA	C1D-ND	3.40	1.42	1.37
26	a	604	CLA	C4D-ND	-3.40	1.33	1.37
26	7	602	CLA	C4D-ND	-3.40	1.33	1.37
26	a	614	CLA	C4D-ND	-3.40	1.33	1.37
26	G	204	CLA	C1D-ND	3.40	1.42	1.37
26	B	830	CLA	C1D-ND	3.39	1.42	1.37
26	2	610	CLA	C4D-ND	-3.39	1.33	1.37
37	U	609	CHL	CHB-C1B	3.39	1.47	1.39
26	a	611	CLA	C1D-ND	3.39	1.42	1.37
37	Y	606	CHL	CHB-C1B	3.39	1.47	1.39
26	V	614	CLA	C4B-NB	3.39	1.42	1.37
37	X	601	CHL	CHB-C1B	3.39	1.47	1.39
26	B	812	CLA	C4D-ND	-3.39	1.33	1.37
26	7	610	CLA	C4B-NB	3.39	1.42	1.37
26	5	608	CLA	C1D-ND	3.39	1.41	1.37
37	X	608	CHL	CHB-C1B	3.39	1.47	1.39
26	B	819	CLA	C4D-ND	-3.39	1.33	1.37
26	6	607	CLA	C4B-NB	3.39	1.41	1.37
26	4	614	CLA	C4D-ND	-3.39	1.33	1.37
26	9	607	CLA	C4D-ND	-3.38	1.33	1.37
26	2	611	CLA	C1D-ND	3.38	1.41	1.37
26	3	614	CLA	C1D-ND	3.38	1.41	1.37
26	5	617	CLA	C4D-ND	-3.38	1.33	1.37
26	Z	610	CLA	C1D-ND	3.38	1.41	1.37
26	1	606	CLA	C4B-NB	3.38	1.41	1.37
26	G	203	CLA	C1D-ND	3.38	1.41	1.37
26	X	611	CLA	C4B-NB	3.38	1.41	1.37
26	B	831	CLA	C4D-ND	-3.38	1.33	1.37
26	B	836	CLA	C4D-ND	-3.38	1.33	1.37
26	W	613	CLA	C1D-ND	3.38	1.41	1.37
26	A	835	CLA	C4D-ND	-3.38	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	606	CLA	C1D-ND	3.38	1.41	1.37
26	A	814	CLA	C4D-ND	-3.38	1.33	1.37
26	1	607	CLA	C4D-ND	-3.38	1.33	1.37
26	9	609	CLA	C1D-ND	3.38	1.41	1.37
26	V	603	CLA	C4B-NB	3.38	1.41	1.37
37	V	608	CHL	CHB-C1B	3.38	1.47	1.39
26	B	824	CLA	C4D-ND	-3.38	1.33	1.37
26	3	615	CLA	C4D-ND	-3.38	1.33	1.37
26	4	606	CLA	C4D-ND	-3.38	1.33	1.37
26	G	204	CLA	C4B-NB	3.37	1.41	1.37
26	A	822	CLA	C1D-ND	3.37	1.41	1.37
26	1	601	CLA	C1D-ND	3.37	1.41	1.37
26	6	603	CLA	C1D-ND	3.37	1.41	1.37
26	U	612	CLA	C4B-NB	3.37	1.41	1.37
26	O	2003	CLA	C1D-ND	3.37	1.41	1.37
26	Y	614	CLA	C4B-NB	3.37	1.41	1.37
37	V	607	CHL	CHB-C1B	3.37	1.47	1.39
26	8	601	CLA	C1D-ND	3.37	1.41	1.37
26	X	612	CLA	C4B-NB	3.37	1.41	1.37
26	K	203	CLA	C1D-ND	3.37	1.41	1.37
26	a	610	CLA	C1D-ND	3.36	1.41	1.37
37	Y	609	CHL	OBD-CAD	3.36	1.28	1.22
37	W	608	CHL	CHB-C1B	3.36	1.47	1.39
26	6	620	CLA	C4D-ND	-3.36	1.33	1.37
26	6	610	CLA	C1D-ND	3.36	1.41	1.37
26	8	604	CLA	C1D-ND	3.36	1.41	1.37
26	8	607	CLA	C4B-NB	3.36	1.41	1.37
37	U	608	CHL	OBD-CAD	3.36	1.28	1.22
26	B	802	CLA	C4D-ND	-3.36	1.33	1.37
37	Z	606	CHL	CHB-C1B	3.36	1.46	1.39
37	V	609	CHL	CHB-C1B	3.36	1.46	1.39
26	U	602	CLA	C4B-NB	3.36	1.41	1.37
26	2	614	CLA	C1D-ND	3.36	1.41	1.37
26	L	304	CLA	C4D-ND	-3.36	1.33	1.37
26	a	607	CLA	C1D-ND	3.36	1.41	1.37
26	V	604	CLA	C4B-NB	3.35	1.41	1.37
26	1	610	CLA	C4D-ND	-3.35	1.33	1.37
26	2	601	CLA	C4D-ND	-3.35	1.33	1.37
37	W	605	CHL	CHB-C1B	3.35	1.46	1.39
26	H	203	CLA	C1D-ND	3.35	1.41	1.37
26	1	607	CLA	C1D-ND	3.35	1.41	1.37
26	2	613	CLA	C4D-ND	-3.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	609	CLA	C4D-ND	-3.35	1.33	1.37
26	5	619	CLA	C4B-NB	3.34	1.41	1.37
26	2	609	CLA	C4B-NB	3.34	1.41	1.37
26	8	614	CLA	C4D-ND	-3.34	1.33	1.37
26	6	617	CLA	C1D-ND	3.34	1.41	1.37
37	X	609	CHL	CHC-C4B	3.34	1.46	1.39
37	Z	601	CHL	CHB-C1B	3.34	1.46	1.39
26	7	610	CLA	C4D-ND	-3.34	1.33	1.37
26	O	2002	CLA	C1D-ND	3.33	1.41	1.37
26	A	838	CLA	C4D-ND	-3.33	1.33	1.37
37	U	606	CHL	CHB-C1B	3.33	1.46	1.39
26	7	615	CLA	C4D-ND	-3.33	1.33	1.37
26	6	613	CLA	C1D-ND	3.33	1.41	1.37
26	A	817	CLA	C1D-ND	3.33	1.41	1.37
26	F	301	CLA	C4D-ND	-3.33	1.33	1.37
26	B	840	CLA	C1D-ND	3.33	1.41	1.37
26	3	614	CLA	C4B-NB	3.33	1.41	1.37
37	X	601	CHL	CHC-C4B	3.33	1.46	1.39
26	8	609	CLA	C4D-ND	-3.33	1.33	1.37
26	Z	611	CLA	C4B-NB	3.33	1.41	1.37
26	5	603	CLA	C4B-NB	3.33	1.41	1.37
26	A	837	CLA	C4D-ND	-3.33	1.33	1.37
26	B	811	CLA	C4D-ND	-3.33	1.33	1.37
26	3	607	CLA	C4D-ND	-3.33	1.33	1.37
26	2	603	CLA	C4B-NB	3.33	1.41	1.37
26	8	603	CLA	C1D-ND	3.33	1.41	1.37
26	7	612	CLA	C1D-ND	3.33	1.41	1.37
37	V	606	CHL	OBD-CAD	3.33	1.28	1.22
37	V	608	CHL	OBD-CAD	3.32	1.28	1.22
26	L	306	CLA	C4D-ND	-3.32	1.33	1.37
26	9	604	CLA	C4D-ND	-3.32	1.33	1.37
26	7	616	CLA	C1D-ND	3.32	1.41	1.37
26	B	826	CLA	C4D-ND	-3.32	1.33	1.37
26	5	604	CLA	C4B-NB	3.32	1.41	1.37
37	V	609	CHL	CHC-C4B	3.32	1.46	1.39
26	4	613	CLA	C1D-ND	3.32	1.41	1.37
37	V	601	CHL	CHB-C1B	3.31	1.46	1.39
37	W	606	CHL	CHB-C1B	3.31	1.46	1.39
26	Y	603	CLA	C4B-NB	3.31	1.41	1.37
26	V	604	CLA	C4D-ND	-3.31	1.33	1.37
26	B	822	CLA	C1D-ND	3.31	1.41	1.37
26	U	603	CLA	C4B-NB	3.31	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	611	CLA	C4D-ND	-3.31	1.33	1.37
26	A	811	CLA	C4D-ND	-3.31	1.33	1.37
26	a	609	CLA	C1D-ND	3.31	1.41	1.37
26	L	304	CLA	C1D-ND	3.31	1.41	1.37
26	9	609	CLA	C4D-ND	-3.31	1.33	1.37
26	O	2001	CLA	C4B-NB	3.31	1.41	1.37
26	L	307	CLA	C4D-ND	-3.31	1.33	1.37
26	1	604	CLA	C4D-ND	-3.31	1.33	1.37
26	4	613	CLA	C4D-ND	-3.31	1.33	1.37
31	A	858	LMU	O5B-C1B	3.31	1.50	1.41
26	F	303	CLA	C4B-NB	3.31	1.41	1.37
26	8	611	CLA	C1D-ND	3.31	1.41	1.37
26	6	611	CLA	C4D-ND	-3.30	1.33	1.37
26	a	612	CLA	C4B-NB	3.30	1.41	1.37
37	Y	607	CHL	CHB-C1B	3.30	1.46	1.39
26	3	613	CLA	C4D-ND	-3.30	1.33	1.37
26	6	607	CLA	C4D-ND	-3.30	1.33	1.37
26	2	609	CLA	C1D-ND	3.30	1.41	1.37
37	U	608	CHL	CHB-C1B	3.30	1.46	1.39
26	a	607	CLA	C4D-ND	-3.30	1.33	1.37
26	a	616	CLA	C4B-NB	3.30	1.41	1.37
26	9	604	CLA	C1D-ND	3.30	1.41	1.37
26	W	603	CLA	C4B-NB	3.30	1.41	1.37
26	A	801	CLA	C1D-ND	3.30	1.41	1.37
26	5	618	CLA	C4B-NB	3.30	1.41	1.37
31	A	858	LMU	O5'-C1'	3.30	1.50	1.41
26	7	604	CLA	C4D-ND	-3.30	1.33	1.37
26	4	601	CLA	C4D-ND	-3.30	1.33	1.37
26	4	608	CLA	C4D-ND	-3.30	1.33	1.37
26	A	840	CLA	C4D-ND	-3.29	1.33	1.37
26	B	841	CLA	C4D-ND	-3.29	1.33	1.37
26	1	603	CLA	C1D-ND	3.29	1.41	1.37
26	9	604	CLA	C4B-NB	3.29	1.41	1.37
26	4	616	CLA	C1D-ND	3.29	1.41	1.37
26	5	603	CLA	C4D-ND	-3.29	1.33	1.37
26	B	835	CLA	C4D-ND	-3.29	1.33	1.37
26	6	612	CLA	C4D-ND	-3.29	1.33	1.37
26	O	2003	CLA	C4D-ND	-3.29	1.33	1.37
26	3	606	CLA	C4D-ND	-3.29	1.33	1.37
26	6	620	CLA	C1D-ND	3.28	1.41	1.37
26	X	610	CLA	C3B-C4B	3.28	1.50	1.42
26	4	612	CLA	C4B-NB	3.28	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	601	CLA	C4B-NB	3.28	1.41	1.37
26	1	614	CLA	C4D-ND	-3.28	1.33	1.37
36	Z	1623	NEX	C7-C8	-3.28	1.26	1.32
26	3	611	CLA	C4B-NB	3.28	1.41	1.37
26	5	606	CLA	C4B-NB	3.28	1.41	1.37
26	5	612	CLA	C4B-NB	3.28	1.41	1.37
31	1	621	LMU	O5'-C1'	3.28	1.50	1.41
26	6	613	CLA	C4D-ND	-3.28	1.33	1.37
26	U	613	CLA	C4D-ND	-3.28	1.33	1.37
26	3	607	CLA	C1D-ND	3.28	1.41	1.37
26	B	822	CLA	C4D-ND	-3.28	1.33	1.37
26	4	610	CLA	C4B-NB	3.28	1.41	1.37
26	4	616	CLA	C4D-ND	-3.28	1.33	1.37
26	Y	602	CLA	C4D-ND	-3.28	1.33	1.37
26	U	604	CLA	CAD-C3D	-3.28	1.45	1.50
26	7	602	CLA	C4B-NB	3.27	1.41	1.37
26	Z	602	CLA	C4B-NB	3.27	1.41	1.37
31	8	625	LMU	O5B-C1B	3.27	1.50	1.41
26	O	2002	CLA	C4B-NB	3.27	1.41	1.37
26	1	609	CLA	C1D-ND	3.27	1.41	1.37
26	2	606	CLA	C1D-ND	3.27	1.41	1.37
26	4	604	CLA	C4D-ND	-3.27	1.33	1.37
26	8	609	CLA	C1D-ND	3.27	1.41	1.37
26	A	817	CLA	C4D-ND	-3.27	1.33	1.37
26	K	204	CLA	C4D-ND	-3.27	1.33	1.37
26	B	808	CLA	C4B-NB	3.27	1.41	1.37
26	2	616	CLA	C4B-NB	3.27	1.41	1.37
26	3	603	CLA	C4D-ND	-3.27	1.33	1.37
26	3	610	CLA	C3B-C4B	3.26	1.50	1.42
26	2	614	CLA	C4B-NB	3.26	1.41	1.37
26	L	302	CLA	CMB-C2B	-3.26	1.43	1.50
26	3	612	CLA	C3B-C4B	3.26	1.50	1.42
26	A	807	CLA	C4D-ND	-3.26	1.33	1.37
26	A	818	CLA	C4D-ND	-3.26	1.33	1.37
26	1	608	CLA	C4B-NB	3.26	1.41	1.37
26	B	810	CLA	C4D-ND	-3.26	1.33	1.37
26	3	610	CLA	C4D-ND	-3.26	1.33	1.37
26	3	614	CLA	C4D-ND	-3.26	1.33	1.37
26	9	613	CLA	C4D-ND	-3.26	1.33	1.37
26	Z	604	CLA	C4D-ND	-3.26	1.33	1.37
26	K	206	CLA	C4D-ND	-3.26	1.33	1.37
26	8	616	CLA	CAB-C3B	-3.26	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	803	CLA	C4D-ND	-3.26	1.33	1.37
26	1	604	CLA	C4B-NB	3.26	1.41	1.37
26	4	618	CLA	C4D-ND	-3.26	1.33	1.37
26	L	307	CLA	C1D-ND	3.25	1.41	1.37
26	a	610	CLA	C4D-ND	-3.25	1.33	1.37
26	a	611	CLA	C4B-NB	3.25	1.41	1.37
26	Y	602	CLA	C4B-NB	3.25	1.41	1.37
26	2	610	CLA	C4B-NB	3.25	1.41	1.37
26	4	606	CLA	C1D-ND	3.25	1.41	1.37
26	5	610	CLA	C1D-ND	3.25	1.41	1.37
31	8	625	LMU	O5'-C1'	3.25	1.50	1.41
26	Z	611	CLA	C1D-ND	3.25	1.41	1.37
26	B	820	CLA	C4D-ND	-3.25	1.33	1.37
26	6	608	CLA	C4B-NB	3.25	1.41	1.37
26	F	303	CLA	C1D-ND	3.25	1.41	1.37
26	B	827	CLA	C4D-ND	-3.25	1.33	1.37
26	B	831	CLA	C1D-ND	3.25	1.41	1.37
26	V	602	CLA	C4D-ND	-3.25	1.33	1.37
26	4	614	CLA	C4B-NB	3.25	1.41	1.37
26	O	2001	CLA	C4D-ND	-3.25	1.33	1.37
26	8	607	CLA	C1D-ND	3.25	1.41	1.37
26	a	603	CLA	C1D-ND	3.24	1.41	1.37
26	5	604	CLA	C4D-ND	-3.24	1.33	1.37
26	7	615	CLA	C4B-NB	3.24	1.41	1.37
26	6	616	CLA	C1D-ND	3.24	1.41	1.37
26	V	613	CLA	C4B-NB	3.24	1.41	1.37
37	W	609	CHL	C1D-C2D	3.24	1.51	1.45
26	3	613	CLA	C4B-NB	3.24	1.41	1.37
26	H	202	CLA	C4D-ND	-3.24	1.33	1.37
37	Z	606	CHL	OBD-CAD	3.24	1.28	1.22
26	4	603	CLA	C4D-ND	-3.24	1.33	1.37
26	1	611	CLA	C4B-NB	3.24	1.41	1.37
26	a	609	CLA	C4D-ND	-3.23	1.33	1.37
26	U	604	CLA	C4D-ND	-3.23	1.33	1.37
26	B	821	CLA	C1D-ND	3.23	1.41	1.37
26	5	610	CLA	C4D-ND	-3.23	1.33	1.37
26	1	612	CLA	C4B-NB	3.23	1.41	1.37
26	1	616	CLA	C4B-NB	3.23	1.41	1.37
26	6	609	CLA	C1D-ND	3.23	1.41	1.37
26	Z	602	CLA	C4D-ND	-3.23	1.33	1.37
26	a	602	CLA	C1D-ND	3.23	1.41	1.37
26	8	601	CLA	C4B-NB	3.23	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	857	LMU	O5B-C1B	3.23	1.50	1.41
26	8	610	CLA	C1D-ND	3.23	1.41	1.37
37	X	609	CHL	C1D-C2D	3.23	1.51	1.45
26	V	602	CLA	C4B-NB	3.23	1.41	1.37
26	6	608	CLA	C4D-ND	-3.23	1.33	1.37
26	X	602	CLA	C4D-ND	-3.23	1.33	1.37
26	7	612	CLA	C4D-ND	-3.23	1.33	1.37
26	3	604	CLA	C1D-ND	3.22	1.41	1.37
26	B	814	CLA	C4D-ND	-3.22	1.33	1.37
26	9	610	CLA	C4D-ND	-3.22	1.33	1.37
26	A	811	CLA	C1D-ND	3.22	1.41	1.37
26	a	608	CLA	C4B-NB	3.22	1.41	1.37
26	Z	603	CLA	C4B-NB	3.22	1.41	1.37
26	5	618	CLA	C4D-ND	-3.22	1.33	1.37
27	A	844	PQN	C11-C12	3.22	1.55	1.50
26	O	2002	CLA	CAB-C3B	-3.22	1.44	1.50
26	B	809	CLA	C1D-ND	3.22	1.41	1.37
26	A	801	CLA	C4D-ND	-3.22	1.33	1.37
26	6	610	CLA	C4D-ND	-3.22	1.33	1.37
26	J	101	CLA	C4B-NB	3.22	1.41	1.37
26	2	603	CLA	C4D-ND	-3.22	1.33	1.37
26	V	610	CLA	C4B-NB	3.21	1.41	1.37
26	8	607	CLA	CAB-C3B	-3.21	1.44	1.50
26	3	615	CLA	C1D-ND	3.21	1.41	1.37
26	a	604	CLA	C4B-NB	3.21	1.41	1.37
37	Y	601	CHL	CHB-C1B	3.21	1.46	1.39
26	F	303	CLA	C4D-ND	-3.21	1.33	1.37
31	1	621	LMU	O5B-C1B	3.21	1.50	1.41
26	A	812	CLA	C1D-ND	3.21	1.41	1.37
26	3	617	CLA	C1D-ND	3.21	1.41	1.37
26	2	607	CLA	C4D-ND	-3.21	1.33	1.37
26	a	608	CLA	C4D-ND	-3.21	1.33	1.37
26	7	615	CLA	CAB-C3B	-3.21	1.44	1.50
37	Z	609	CHL	CHC-C4B	3.21	1.46	1.39
26	4	607	CLA	C4D-ND	-3.21	1.33	1.37
26	G	203	CLA	C4D-ND	-3.21	1.33	1.37
26	5	616	CLA	CAB-C3B	-3.21	1.44	1.50
26	2	611	CLA	C4B-NB	3.21	1.41	1.37
26	6	602	CLA	C4B-NB	3.21	1.41	1.37
37	Y	608	CHL	CHB-C1B	3.21	1.46	1.39
31	K	208	LMU	O5'-C1'	3.21	1.50	1.41
26	A	837	CLA	C1D-ND	3.20	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	841	CLA	C1D-ND	3.20	1.41	1.37
26	6	607	CLA	C1D-ND	3.20	1.41	1.37
26	6	607	CLA	CAB-C3B	-3.20	1.44	1.50
26	5	614	CLA	C4D-ND	-3.20	1.33	1.37
26	3	602	CLA	C1D-ND	3.20	1.41	1.37
26	7	616	CLA	C4D-ND	-3.20	1.33	1.37
26	B	823	CLA	C1D-ND	3.20	1.41	1.37
26	L	306	CLA	C1D-ND	3.20	1.41	1.37
26	2	603	CLA	C1D-ND	3.20	1.41	1.37
26	7	613	CLA	C1D-ND	3.20	1.41	1.37
26	B	830	CLA	C4D-ND	-3.20	1.33	1.37
26	1	603	CLA	C4B-NB	3.20	1.41	1.37
26	5	603	CLA	CAB-C3B	-3.19	1.44	1.50
26	6	609	CLA	C4B-NB	3.19	1.41	1.37
26	L	302	CLA	C4B-NB	3.19	1.41	1.37
26	8	603	CLA	C4B-NB	3.19	1.41	1.37
26	4	603	CLA	CAB-C3B	-3.19	1.44	1.50
26	7	609	CLA	C4B-NB	3.19	1.41	1.37
37	Y	607	CHL	CHC-C4B	3.19	1.46	1.39
26	8	603	CLA	C4D-ND	-3.19	1.33	1.37
26	Z	611	CLA	C4D-ND	-3.19	1.33	1.37
26	a	603	CLA	C4B-NB	3.19	1.41	1.37
26	H	203	CLA	C4D-ND	-3.19	1.33	1.37
31	5	628	LMU	O5'-C1'	3.19	1.50	1.41
26	G	204	CLA	C4D-ND	-3.19	1.33	1.37
26	4	603	CLA	C1D-ND	3.19	1.41	1.37
26	9	606	CLA	C4B-NB	3.19	1.41	1.37
26	2	604	CLA	C4B-NB	3.18	1.41	1.37
26	U	602	CLA	C4D-ND	-3.18	1.33	1.37
26	B	821	CLA	C4B-NB	3.18	1.41	1.37
26	5	602	CLA	C4B-NB	3.18	1.41	1.37
26	1	608	CLA	C4D-ND	-3.18	1.33	1.37
26	4	609	CLA	C4B-NB	3.18	1.41	1.37
26	5	606	CLA	C1D-ND	3.18	1.41	1.37
26	W	612	CLA	C4B-NB	3.18	1.41	1.37
26	2	614	CLA	C4D-ND	-3.18	1.33	1.37
31	5	629	LMU	O5'-C1'	3.18	1.49	1.41
26	3	607	CLA	CAB-C3B	-3.18	1.44	1.50
26	K	203	CLA	C4D-ND	-3.18	1.33	1.37
37	X	607	CHL	CHB-C1B	3.18	1.46	1.39
26	O	2002	CLA	C4D-ND	-3.18	1.33	1.37
26	B	808	CLA	C1D-ND	3.18	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	819	CLA	C4B-NB	3.18	1.41	1.37
26	8	603	CLA	CAB-C3B	-3.18	1.44	1.50
26	6	601	CLA	C1D-ND	3.17	1.41	1.37
26	X	604	CLA	C4D-ND	-3.17	1.33	1.37
26	2	616	CLA	CAB-C3B	-3.17	1.44	1.50
26	7	616	CLA	CAB-C3B	-3.17	1.44	1.50
37	Y	605	CHL	C1D-C2D	3.17	1.51	1.45
26	4	618	CLA	CAB-C3B	-3.17	1.44	1.50
26	B	820	CLA	C4B-NB	3.17	1.41	1.37
26	6	611	CLA	C4B-NB	3.17	1.41	1.37
26	X	613	CLA	C4D-ND	-3.17	1.33	1.37
26	W	613	CLA	C4D-ND	-3.17	1.33	1.37
26	A	824	CLA	C1D-ND	3.17	1.41	1.37
26	8	613	CLA	C4B-NB	3.17	1.41	1.37
26	6	618	CLA	C4B-NB	3.17	1.41	1.37
26	2	612	CLA	C4D-ND	-3.17	1.33	1.37
26	9	614	CLA	C4D-ND	-3.17	1.33	1.37
26	5	619	CLA	CAB-C3B	-3.17	1.44	1.50
26	5	611	CLA	C4B-NB	3.17	1.41	1.37
26	4	604	CLA	CAB-C3B	-3.16	1.44	1.50
26	4	609	CLA	C4D-ND	-3.16	1.33	1.37
26	9	606	CLA	C1D-ND	3.16	1.41	1.37
29	B	844	BCR	C17-C18	-3.16	1.31	1.35
26	A	823	CLA	C1D-ND	3.16	1.41	1.37
26	Y	604	CLA	C4D-ND	-3.16	1.33	1.37
37	Y	609	CHL	CHC-C4B	3.16	1.46	1.39
26	7	603	CLA	C4D-ND	-3.16	1.33	1.37
26	O	2001	CLA	C1D-ND	3.16	1.41	1.37
26	H	202	CLA	C4B-NB	3.16	1.41	1.37
26	2	616	CLA	C4D-ND	-3.15	1.33	1.37
26	B	818	CLA	C1D-ND	3.15	1.41	1.37
26	8	612	CLA	C1D-ND	3.15	1.41	1.37
26	6	606	CLA	C4D-ND	-3.15	1.33	1.37
26	6	603	CLA	CAB-C3B	-3.15	1.44	1.50
26	a	609	CLA	C4B-NB	3.15	1.41	1.37
37	X	606	CHL	C3B-C4B	3.15	1.50	1.42
31	A	857	LMU	O5'-C1'	3.15	1.49	1.41
26	3	609	CLA	C4D-ND	-3.15	1.33	1.37
26	K	204	CLA	C1D-ND	3.15	1.41	1.37
26	a	612	CLA	C1D-ND	3.15	1.41	1.37
26	2	611	CLA	C4D-ND	-3.15	1.33	1.37
26	B	829	CLA	C4B-NB	3.15	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	603	CLA	C4B-NB	3.15	1.41	1.37
26	8	607	CLA	C4D-ND	-3.15	1.33	1.37
26	B	819	CLA	C1D-ND	3.15	1.41	1.37
26	4	603	CLA	C4B-NB	3.15	1.41	1.37
26	7	601	CLA	C1D-ND	3.15	1.41	1.37
26	9	603	CLA	C4B-NB	3.15	1.41	1.37
26	8	616	CLA	C4D-ND	-3.15	1.33	1.37
26	4	602	CLA	C1D-ND	3.15	1.41	1.37
26	8	616	CLA	C4B-NB	3.14	1.41	1.37
26	a	606	CLA	C4D-ND	-3.14	1.33	1.37
26	4	601	CLA	C1D-ND	3.14	1.41	1.37
26	1	609	CLA	C4D-ND	-3.14	1.33	1.37
26	5	617	CLA	C1D-ND	3.14	1.41	1.37
26	5	612	CLA	C4D-ND	-3.14	1.33	1.37
26	9	601	CLA	C4D-ND	-3.14	1.33	1.37
37	Z	609	CHL	CHB-C1B	3.14	1.46	1.39
37	U	607	CHL	CHB-C1B	3.14	1.46	1.39
26	B	835	CLA	C1D-ND	3.13	1.41	1.37
26	1	602	CLA	C1D-ND	3.13	1.41	1.37
26	4	602	CLA	C3B-C4B	3.13	1.50	1.42
37	X	608	CHL	C3B-C4B	3.13	1.50	1.42
26	B	841	CLA	C4B-NB	3.13	1.41	1.37
26	B	811	CLA	CAB-C3B	-3.13	1.44	1.50
26	4	611	CLA	C4D-ND	-3.13	1.33	1.37
26	B	811	CLA	C4B-NB	3.13	1.41	1.37
37	Y	605	CHL	MG-NA	-3.13	1.98	2.06
26	5	619	CLA	C4D-ND	-3.13	1.33	1.37
26	A	821	CLA	C1D-ND	3.13	1.41	1.37
26	7	606	CLA	C1D-ND	3.13	1.41	1.37
26	6	618	CLA	C4D-ND	-3.12	1.33	1.37
26	5	604	CLA	CAB-C3B	-3.12	1.44	1.50
26	A	838	CLA	C1D-ND	3.12	1.41	1.37
26	Y	610	CLA	C3B-C4B	3.12	1.50	1.42
26	1	612	CLA	C1D-ND	3.12	1.41	1.37
26	6	602	CLA	C1D-ND	3.12	1.41	1.37
26	a	611	CLA	C4D-ND	-3.12	1.33	1.37
26	9	606	CLA	C4D-ND	-3.12	1.33	1.37
26	3	608	CLA	C4B-NB	3.12	1.41	1.37
26	B	815	CLA	C1D-ND	3.12	1.41	1.37
26	a	601	CLA	C4D-ND	-3.12	1.33	1.37
26	3	607	CLA	C4B-NB	3.12	1.41	1.37
26	1	601	CLA	C4D-ND	-3.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	203	CLA	C4B-NB	3.11	1.41	1.37
26	5	606	CLA	C4D-ND	-3.11	1.33	1.37
26	B	840	CLA	C4B-NB	3.11	1.41	1.37
26	a	616	CLA	C4D-ND	-3.11	1.33	1.37
26	4	608	CLA	C4B-NB	3.11	1.41	1.37
26	B	829	CLA	CMB-C2B	-3.11	1.44	1.50
26	9	604	CLA	CAB-C3B	-3.11	1.44	1.50
26	B	838	CLA	C1D-ND	3.11	1.41	1.37
26	6	603	CLA	C4D-ND	-3.11	1.33	1.37
26	2	612	CLA	C4B-NB	3.11	1.41	1.37
26	7	607	CLA	C4B-NB	3.11	1.41	1.37
26	1	616	CLA	CAB-C3B	-3.11	1.44	1.50
26	1	602	CLA	C4B-NB	3.11	1.41	1.37
26	F	304	CLA	C4D-ND	-3.11	1.33	1.37
26	B	828	CLA	C1D-ND	3.11	1.41	1.37
26	F	301	CLA	C4B-NB	3.11	1.41	1.37
26	8	612	CLA	C4D-ND	-3.11	1.33	1.37
26	L	302	CLA	C1D-ND	3.11	1.41	1.37
26	5	614	CLA	C4B-NB	3.11	1.41	1.37
26	9	607	CLA	C1D-ND	3.10	1.41	1.37
26	8	610	CLA	C4D-ND	-3.10	1.33	1.37
26	6	614	CLA	C4B-NB	3.10	1.41	1.37
26	1	606	CLA	C4D-ND	-3.10	1.33	1.37
26	A	810	CLA	C1D-ND	3.10	1.41	1.37
26	3	612	CLA	C4D-ND	-3.10	1.33	1.37
26	V	613	CLA	C4D-ND	-3.10	1.33	1.37
37	V	606	CHL	CHB-C1B	3.10	1.46	1.39
26	1	612	CLA	C4D-ND	-3.10	1.33	1.37
26	A	804	CLA	C1D-ND	3.10	1.41	1.37
26	a	612	CLA	C4D-ND	-3.10	1.33	1.37
26	a	611	CLA	CAB-C3B	-3.09	1.44	1.50
26	4	612	CLA	C4D-ND	-3.09	1.33	1.37
26	7	609	CLA	C1D-ND	3.09	1.41	1.37
26	8	604	CLA	C4B-NB	3.09	1.41	1.37
26	A	837	CLA	CMB-C2B	-3.09	1.44	1.50
26	4	606	CLA	C4B-NB	3.09	1.41	1.37
26	8	602	CLA	C4B-NB	3.09	1.41	1.37
26	5	618	CLA	CAB-C3B	-3.09	1.44	1.50
26	B	812	CLA	C4B-NB	3.09	1.41	1.37
26	5	601	CLA	C4D-ND	-3.09	1.33	1.37
26	4	616	CLA	CAB-C3B	-3.09	1.44	1.50
37	X	605	CHL	C1D-C2D	3.09	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	602	CLA	C1D-ND	3.08	1.41	1.37
26	1	616	CLA	C4D-ND	-3.08	1.33	1.37
26	8	612	CLA	C4B-NB	3.08	1.41	1.37
26	Z	611	CLA	CAB-C3B	-3.08	1.44	1.50
26	A	833	CLA	C1D-ND	3.08	1.41	1.37
26	8	610	CLA	C4B-NB	3.08	1.41	1.37
26	1	609	CLA	CAB-C3B	-3.08	1.44	1.50
26	6	617	CLA	C4D-ND	-3.08	1.33	1.37
26	W	602	CLA	C4D-ND	-3.08	1.33	1.37
26	J	101	CLA	C4D-ND	-3.07	1.33	1.37
26	9	610	CLA	C3B-C4B	3.07	1.50	1.42
26	A	805	CLA	C1D-ND	3.07	1.41	1.37
26	1	611	CLA	C4D-ND	-3.07	1.33	1.37
26	2	613	CLA	C1D-ND	3.07	1.41	1.37
26	a	616	CLA	C3B-C4B	3.07	1.49	1.42
26	8	613	CLA	C1D-ND	3.07	1.41	1.37
26	6	618	CLA	CAB-C3B	-3.07	1.44	1.50
26	B	837	CLA	C4B-NB	3.07	1.41	1.37
26	5	616	CLA	C4B-NB	3.07	1.41	1.37
26	5	611	CLA	C4D-ND	-3.07	1.33	1.37
26	5	610	CLA	C3B-C4B	3.07	1.49	1.42
37	Y	606	CHL	OBD-CAD	3.07	1.27	1.22
26	a	610	CLA	C4B-NB	3.07	1.41	1.37
26	3	611	CLA	CAB-C3B	-3.07	1.44	1.50
26	9	602	CLA	C4B-NB	3.06	1.41	1.37
26	2	610	CLA	C1D-ND	3.06	1.41	1.37
26	6	606	CLA	C4B-NB	3.06	1.41	1.37
26	8	606	CLA	C4B-NB	3.06	1.41	1.37
26	2	606	CLA	C4D-ND	-3.06	1.33	1.37
26	6	612	CLA	C4B-NB	3.06	1.41	1.37
26	4	604	CLA	C4B-NB	3.06	1.41	1.37
26	B	811	CLA	CAD-C3D	-3.06	1.45	1.50
26	K	201	CLA	C4D-ND	-3.06	1.33	1.37
26	A	845	CLA	C4B-NB	3.06	1.41	1.37
26	5	603	CLA	C1D-ND	3.06	1.41	1.37
26	7	616	CLA	C4B-NB	3.06	1.41	1.37
26	H	203	CLA	C4B-NB	3.05	1.41	1.37
37	Y	609	CHL	CHB-C1B	3.05	1.46	1.39
26	a	602	CLA	C4B-NB	3.05	1.41	1.37
26	6	617	CLA	C4B-NB	3.05	1.41	1.37
26	9	612	CLA	C3B-C4B	3.05	1.49	1.42
26	9	602	CLA	C1D-ND	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	611	CLA	C4D-ND	-3.05	1.33	1.37
37	Z	606	CHL	C3B-C4B	3.05	1.49	1.42
26	A	816	CLA	C1D-ND	3.05	1.41	1.37
26	B	806	CLA	C1D-ND	3.05	1.41	1.37
26	3	617	CLA	C4D-ND	-3.05	1.33	1.37
26	2	601	CLA	C1D-ND	3.05	1.41	1.37
26	8	611	CLA	C4B-NB	3.05	1.41	1.37
26	8	614	CLA	C1D-ND	3.05	1.41	1.37
26	A	809	CLA	C1D-ND	3.04	1.41	1.37
26	A	827	CLA	C1D-ND	3.04	1.41	1.37
26	U	610	CLA	C4B-NB	3.04	1.41	1.37
26	B	832	CLA	C1D-ND	3.04	1.41	1.37
26	2	606	CLA	C4B-NB	3.04	1.41	1.37
26	7	608	CLA	C4B-NB	3.04	1.41	1.37
37	W	606	CHL	CHC-C4B	3.04	1.46	1.39
26	5	613	CLA	C4B-NB	3.04	1.41	1.37
26	5	601	CLA	C4B-NB	3.04	1.41	1.37
26	V	610	CLA	C4D-ND	-3.04	1.33	1.37
26	1	609	CLA	C4B-NB	3.04	1.41	1.37
26	W	611	CLA	C4D-ND	-3.03	1.33	1.37
26	2	604	CLA	C3B-C4B	3.03	1.49	1.42
26	9	613	CLA	C4B-NB	3.03	1.41	1.37
37	Z	609	CHL	C1D-C2D	3.03	1.51	1.45
26	2	610	CLA	C3B-C4B	3.03	1.49	1.42
26	a	603	CLA	C4D-ND	-3.03	1.33	1.37
26	4	610	CLA	C4D-ND	-3.03	1.33	1.37
26	V	611	CLA	C4D-ND	-3.03	1.33	1.37
26	9	610	CLA	C1D-ND	3.03	1.41	1.37
26	W	610	CLA	C3B-C4B	3.02	1.49	1.42
26	A	808	CLA	C1D-ND	3.02	1.41	1.37
26	A	834	CLA	C1D-ND	3.02	1.41	1.37
26	2	607	CLA	C1D-ND	3.02	1.41	1.37
26	8	608	CLA	C1D-ND	3.02	1.41	1.37
26	A	828	CLA	C1D-ND	3.02	1.41	1.37
26	1	610	CLA	C4B-NB	3.02	1.41	1.37
26	7	602	CLA	C3B-C4B	3.02	1.49	1.42
26	B	822	CLA	C4B-NB	3.02	1.41	1.37
26	8	609	CLA	C4B-NB	3.02	1.41	1.37
37	V	609	CHL	C1D-C2D	3.02	1.51	1.45
26	3	617	CLA	C4B-NB	3.02	1.41	1.37
26	K	201	CLA	C4B-NB	3.02	1.41	1.37
26	W	610	CLA	C4D-ND	-3.02	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F	301	CLA	C1D-ND	3.02	1.41	1.37
26	Z	610	CLA	C4D-ND	-3.02	1.33	1.37
26	7	604	CLA	C4B-NB	3.01	1.41	1.37
26	Y	610	CLA	C4D-ND	-3.01	1.33	1.37
26	A	807	CLA	C1D-ND	3.01	1.41	1.37
37	Y	606	CHL	C3B-C4B	3.01	1.49	1.42
26	4	601	CLA	C4B-NB	3.01	1.41	1.37
26	U	610	CLA	C4D-ND	-3.01	1.33	1.37
26	Y	613	CLA	C4D-ND	-3.00	1.33	1.37
26	5	616	CLA	C1D-ND	3.00	1.41	1.37
26	B	831	CLA	C4B-NB	3.00	1.41	1.37
26	A	811	CLA	C4B-NB	3.00	1.41	1.37
26	U	613	CLA	C3B-C4B	3.00	1.49	1.42
37	V	605	CHL	C1D-C2D	3.00	1.51	1.45
26	B	820	CLA	C1D-ND	3.00	1.41	1.37
26	3	613	CLA	C1D-ND	3.00	1.41	1.37
26	6	620	CLA	C4B-NB	3.00	1.41	1.37
26	A	825	CLA	C1D-ND	3.00	1.41	1.37
26	2	613	CLA	C4B-NB	3.00	1.41	1.37
26	B	827	CLA	C1D-ND	2.99	1.41	1.37
26	B	837	CLA	C1D-ND	2.99	1.41	1.37
26	A	842	CLA	C4B-NB	2.99	1.41	1.37
26	3	606	CLA	C1D-ND	2.99	1.41	1.37
26	A	812	CLA	C4B-NB	2.99	1.41	1.37
26	1	614	CLA	CAB-C3B	-2.99	1.44	1.50
26	A	832	CLA	C4B-NB	2.99	1.41	1.37
37	U	605	CHL	MG-NA	-2.99	1.99	2.06
26	9	612	CLA	C4D-ND	-2.99	1.33	1.37
26	A	831	CLA	C1D-ND	2.99	1.41	1.37
26	a	601	CLA	C4B-NB	2.99	1.41	1.37
26	5	607	CLA	C4B-NB	2.99	1.41	1.37
26	6	602	CLA	C3B-C4B	2.99	1.49	1.42
26	A	806	CLA	C1D-ND	2.98	1.41	1.37
26	A	843	CLA	C4B-NB	2.98	1.41	1.37
26	8	610	CLA	C3B-C4B	2.98	1.49	1.42
26	B	812	CLA	C1D-ND	2.98	1.41	1.37
26	2	607	CLA	C4B-NB	2.98	1.41	1.37
26	K	203	CLA	C4B-NB	2.98	1.41	1.37
26	A	821	CLA	C4B-NB	2.98	1.41	1.37
37	U	601	CHL	C1D-C2D	2.98	1.51	1.45
26	B	825	CLA	C1D-ND	2.98	1.41	1.37
26	3	603	CLA	C1D-ND	2.98	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	X	611	CLA	C4D-ND	-2.98	1.33	1.37
26	V	614	CLA	C4D-ND	-2.98	1.33	1.37
37	W	608	CHL	C1D-C2D	2.98	1.51	1.45
26	A	839	CLA	C1D-ND	2.98	1.41	1.37
26	B	825	CLA	C4B-NB	2.98	1.41	1.37
37	U	609	CHL	CHC-C4B	2.98	1.46	1.39
26	3	609	CLA	C4B-NB	2.98	1.41	1.37
26	7	610	CLA	C3B-C4B	2.97	1.49	1.42
26	5	609	CLA	C4B-NB	2.97	1.41	1.37
26	7	611	CLA	C1D-ND	2.97	1.41	1.37
26	A	829	CLA	C3B-C4B	2.97	1.49	1.42
26	W	604	CLA	C4D-ND	-2.97	1.33	1.37
26	B	834	CLA	C1D-ND	2.97	1.41	1.37
26	7	614	CLA	C1D-ND	2.97	1.41	1.37
26	B	816	CLA	C1D-ND	2.97	1.41	1.37
26	5	602	CLA	C1D-ND	2.97	1.41	1.37
26	5	613	CLA	C1D-ND	2.97	1.41	1.37
26	2	602	CLA	C4B-C3B	2.97	1.48	1.38
26	Z	614	CLA	C4D-ND	-2.97	1.33	1.37
26	U	604	CLA	C3B-C4B	2.97	1.49	1.42
26	A	817	CLA	C4B-NB	2.96	1.41	1.37
26	4	610	CLA	C3B-C4B	2.96	1.49	1.42
26	B	838	CLA	C4B-NB	2.96	1.41	1.37
26	1	601	CLA	C4B-NB	2.96	1.41	1.37
26	8	602	CLA	C3B-C4B	2.95	1.49	1.42
26	3	608	CLA	C1D-ND	2.95	1.41	1.37
26	6	610	CLA	C3B-C4B	2.95	1.49	1.42
26	Z	614	CLA	C3B-C4B	2.95	1.49	1.42
37	V	606	CHL	C1B-NB	-2.95	1.34	1.37
26	1	603	CLA	C4D-ND	-2.95	1.33	1.37
26	Z	602	CLA	C3B-C4B	2.95	1.49	1.42
26	A	814	CLA	C4B-NB	2.95	1.41	1.37
26	7	602	CLA	C1D-ND	2.95	1.41	1.37
26	9	603	CLA	C1D-ND	2.95	1.41	1.37
26	Z	612	CLA	C4D-ND	-2.95	1.33	1.37
26	9	607	CLA	C4B-NB	2.95	1.41	1.37
26	8	614	CLA	C4B-NB	2.95	1.41	1.37
37	Y	609	CHL	C1D-C2D	2.95	1.51	1.45
26	Y	602	CLA	C3B-C4B	2.94	1.49	1.42
37	Y	601	CHL	C1D-C2D	2.94	1.51	1.45
37	X	605	CHL	MG-NA	-2.94	1.99	2.06
26	3	610	CLA	C1D-ND	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	607	CLA	C1D-ND	2.94	1.41	1.37
26	A	829	CLA	C1D-ND	2.94	1.41	1.37
26	B	833	CLA	C1D-ND	2.94	1.41	1.37
26	7	606	CLA	C4B-NB	2.94	1.41	1.37
26	7	608	CLA	C1D-ND	2.94	1.41	1.37
26	B	829	CLA	C1D-ND	2.94	1.41	1.37
26	Y	614	CLA	C4D-ND	-2.94	1.33	1.37
26	B	805	CLA	C1D-ND	2.93	1.41	1.37
26	7	607	CLA	C1D-ND	2.93	1.41	1.37
26	a	614	CLA	C4B-NB	2.93	1.41	1.37
26	B	814	CLA	C4B-NB	2.93	1.41	1.37
26	B	816	CLA	C4B-NB	2.93	1.41	1.37
26	3	611	CLA	C4D-ND	-2.93	1.33	1.37
26	A	845	CLA	C1D-ND	2.93	1.41	1.37
26	X	614	CLA	C3B-C4B	2.93	1.49	1.42
26	A	815	CLA	C1D-ND	2.92	1.41	1.37
26	B	807	CLA	C1D-ND	2.92	1.41	1.37
37	U	605	CHL	C1D-C2D	2.92	1.51	1.45
26	A	807	CLA	C4B-NB	2.92	1.41	1.37
26	4	611	CLA	C4B-NB	2.92	1.41	1.37
26	6	601	CLA	C4B-NB	2.92	1.41	1.37
26	B	833	CLA	C4B-NB	2.92	1.41	1.37
26	7	604	CLA	C1D-ND	2.92	1.41	1.37
26	L	306	CLA	C4B-NB	2.92	1.41	1.37
26	6	616	CLA	C4B-NB	2.92	1.41	1.37
26	8	614	CLA	CMD-C2D	-2.92	1.44	1.50
26	7	612	CLA	C4B-NB	2.92	1.41	1.37
26	B	832	CLA	C4B-NB	2.92	1.41	1.37
26	A	831	CLA	C4B-NB	2.91	1.41	1.37
26	Z	610	CLA	C3B-C4B	2.91	1.49	1.42
26	A	814	CLA	C1D-ND	2.91	1.41	1.37
37	W	605	CHL	C1D-C2D	2.91	1.51	1.45
26	A	813	CLA	C1D-ND	2.91	1.41	1.37
26	W	612	CLA	C4D-ND	-2.91	1.33	1.37
26	B	813	CLA	C4B-NB	2.91	1.41	1.37
26	Z	603	CLA	C4D-ND	-2.91	1.33	1.37
26	A	818	CLA	C1D-ND	2.91	1.41	1.37
26	A	833	CLA	C4B-NB	2.91	1.41	1.37
26	A	815	CLA	C4B-NB	2.91	1.41	1.37
26	9	609	CLA	C4B-NB	2.91	1.41	1.37
26	B	807	CLA	CMD-C2D	-2.90	1.44	1.50
26	1	614	CLA	C4B-NB	2.90	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	603	CLA	C4D-ND	-2.90	1.33	1.37
26	A	823	CLA	C4B-NB	2.90	1.41	1.37
26	X	612	CLA	C4D-ND	-2.90	1.33	1.37
26	W	602	CLA	C3B-C4B	2.90	1.49	1.42
26	5	612	CLA	C3B-C4B	2.90	1.49	1.42
26	Z	613	CLA	C4D-ND	-2.89	1.33	1.37
26	3	615	CLA	C4B-NB	2.89	1.41	1.37
26	X	610	CLA	C4D-ND	-2.89	1.33	1.37
26	U	611	CLA	C4D-ND	-2.89	1.33	1.37
26	A	802	CLA	C3B-C4B	2.89	1.49	1.42
26	a	602	CLA	C3B-C4B	2.89	1.49	1.42
26	5	608	CLA	C4B-NB	2.89	1.41	1.37
26	1	607	CLA	C3B-C4B	2.89	1.49	1.42
37	Y	605	CHL	C3A-C2A	-2.89	1.51	1.54
26	A	829	CLA	C4B-NB	2.89	1.41	1.37
37	Y	605	CHL	C3D-C2D	2.89	1.47	1.39
26	A	803	CLA	CMB-C2B	-2.89	1.44	1.50
26	A	837	CLA	C4B-NB	2.89	1.41	1.37
26	B	814	CLA	C1D-ND	2.89	1.41	1.37
37	Z	605	CHL	C1D-C2D	2.89	1.51	1.45
26	1	616	CLA	C4B-C3B	2.89	1.50	1.43
26	U	611	CLA	C3B-C4B	2.88	1.49	1.42
26	4	609	CLA	C1B-C2B	2.88	1.50	1.43
26	A	845	CLA	C3B-C4B	2.88	1.49	1.42
26	3	604	CLA	C4B-NB	2.88	1.41	1.37
37	V	601	CHL	C3B-C4B	2.88	1.49	1.42
26	B	819	CLA	C3B-C4B	2.88	1.49	1.42
26	V	611	CLA	C3B-C4B	2.88	1.49	1.42
26	A	818	CLA	C4B-NB	2.88	1.41	1.37
26	A	840	CLA	C1D-ND	2.88	1.41	1.37
26	V	614	CLA	C3B-C4B	2.88	1.49	1.42
26	4	613	CLA	C3B-C4B	2.88	1.49	1.42
26	B	824	CLA	C4B-NB	2.88	1.41	1.37
26	V	602	CLA	C3B-C4B	2.88	1.49	1.42
26	a	607	CLA	C3B-C4B	2.87	1.49	1.42
29	O	2005	BCR	C30-C25	-2.87	1.49	1.53
26	L	304	CLA	C4B-NB	2.87	1.41	1.37
37	X	605	CHL	C3D-C2D	2.87	1.47	1.39
37	U	605	CHL	C3D-C2D	2.87	1.47	1.39
26	U	614	CLA	C3B-C4B	2.87	1.49	1.42
26	A	843	CLA	CMB-C2B	-2.87	1.44	1.50
26	A	813	CLA	C4B-NB	2.87	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	826	CLA	C4B-NB	2.87	1.41	1.37
37	U	609	CHL	C1D-C2D	2.86	1.51	1.45
26	A	820	CLA	C1D-ND	2.86	1.41	1.37
26	A	811	CLA	CMB-C2B	-2.86	1.44	1.50
37	Z	601	CHL	C3B-C4B	2.86	1.49	1.42
26	7	613	CLA	C4B-NB	2.86	1.41	1.37
26	5	609	CLA	CMB-C2B	-2.86	1.44	1.50
26	W	614	CLA	C4D-ND	-2.86	1.33	1.37
37	V	601	CHL	C1D-C2D	2.86	1.51	1.45
26	Y	611	CLA	C4D-ND	-2.86	1.33	1.37
26	X	614	CLA	C4D-ND	-2.85	1.33	1.37
26	B	826	CLA	C1D-ND	2.85	1.41	1.37
37	U	609	CHL	C4B-NB	-2.85	1.34	1.37
26	B	835	CLA	C4B-NB	2.85	1.41	1.37
26	O	2003	CLA	C4B-NB	2.85	1.41	1.37
26	U	610	CLA	C3B-C4B	2.85	1.49	1.42
26	1	606	CLA	C3B-C4B	2.85	1.49	1.42
26	Z	612	CLA	C3B-C4B	2.85	1.49	1.42
26	A	822	CLA	CMC-C2C	-2.85	1.44	1.50
26	1	602	CLA	C3B-C4B	2.85	1.49	1.42
26	A	834	CLA	C4B-NB	2.85	1.41	1.37
26	3	602	CLA	C4B-NB	2.85	1.41	1.37
26	X	602	CLA	C3B-C4B	2.85	1.49	1.42
26	A	835	CLA	C1D-ND	2.85	1.41	1.37
26	A	854	CLA	C4B-NB	2.85	1.41	1.37
37	W	601	CHL	C1D-C2D	2.85	1.50	1.45
26	W	604	CLA	C3B-C4B	2.85	1.49	1.42
26	A	826	CLA	CMD-C2D	-2.85	1.44	1.50
26	A	831	CLA	CMB-C2B	-2.85	1.44	1.50
26	U	603	CLA	C4D-ND	-2.85	1.33	1.37
26	A	842	CLA	CMB-C2B	-2.84	1.44	1.50
26	A	832	CLA	C1D-ND	2.84	1.41	1.37
26	B	810	CLA	C1D-ND	2.84	1.41	1.37
26	U	612	CLA	C3B-C4B	2.84	1.49	1.42
29	4	621	BCR	C30-C25	-2.84	1.49	1.53
26	7	611	CLA	C4B-NB	2.84	1.41	1.37
26	B	817	CLA	CMB-C2B	-2.84	1.44	1.50
26	U	614	CLA	C4D-ND	-2.84	1.33	1.37
26	V	603	CLA	C4D-ND	-2.84	1.33	1.37
29	K	207	BCR	C30-C25	-2.84	1.49	1.53
26	6	614	CLA	CMD-C2D	-2.84	1.44	1.50
26	A	840	CLA	C4B-NB	2.83	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	604	CLA	C4B-NB	2.83	1.41	1.37
26	A	805	CLA	C4B-NB	2.83	1.41	1.37
26	Y	611	CLA	C3B-C4B	2.83	1.49	1.42
26	A	842	CLA	CMC-C2C	-2.83	1.44	1.50
26	B	824	CLA	CMD-C2D	-2.83	1.44	1.50
26	A	810	CLA	CMD-C2D	-2.83	1.44	1.50
26	B	804	CLA	C1D-ND	2.83	1.41	1.37
26	A	807	CLA	C3B-C4B	2.83	1.49	1.42
26	8	608	CLA	C4B-NB	2.83	1.41	1.37
26	Y	612	CLA	C3B-C4B	2.83	1.49	1.42
37	Z	606	CHL	C1D-C2D	2.83	1.50	1.45
37	W	601	CHL	C3B-C4B	2.82	1.49	1.42
37	Z	608	CHL	C1D-C2D	2.82	1.50	1.45
26	A	826	CLA	C4B-NB	2.82	1.41	1.37
26	B	839	CLA	C1D-ND	2.82	1.41	1.37
34	8	619	LUT	C22-C21	-2.82	1.51	1.54
37	U	601	CHL	MG-NA	-2.82	1.99	2.06
26	9	614	CLA	C3B-C4B	2.82	1.49	1.42
26	B	807	CLA	C4B-NB	2.82	1.41	1.37
26	B	812	CLA	C3B-C4B	2.82	1.49	1.42
26	7	610	CLA	C1D-ND	2.82	1.41	1.37
26	4	612	CLA	C3B-C4B	2.82	1.49	1.42
26	B	806	CLA	CMC-C2C	-2.82	1.44	1.50
26	7	616	CLA	CMD-C2D	-2.82	1.44	1.50
26	B	803	CLA	CMD-C2D	-2.82	1.44	1.50
26	A	803	CLA	C1D-ND	2.82	1.41	1.37
26	A	832	CLA	CMB-C2B	-2.82	1.44	1.50
26	A	843	CLA	C3B-C4B	2.81	1.49	1.42
26	X	612	CLA	C3B-C4B	2.81	1.49	1.42
26	B	836	CLA	C1D-ND	2.81	1.41	1.37
26	W	611	CLA	C3B-C4B	2.81	1.49	1.42
26	V	612	CLA	C4D-ND	-2.81	1.33	1.37
26	A	839	CLA	C4B-NB	2.81	1.41	1.37
26	7	602	CLA	CMD-C2D	-2.81	1.44	1.50
26	A	808	CLA	C4B-NB	2.81	1.41	1.37
26	A	832	CLA	CMD-C2D	-2.80	1.44	1.50
37	V	605	CHL	MG-NA	-2.80	1.99	2.06
26	B	811	CLA	C1D-ND	2.80	1.41	1.37
26	A	854	CLA	CMC-C2C	-2.80	1.44	1.50
34	7	619	LUT	C22-C21	-2.80	1.51	1.54
26	L	303	CLA	C1D-ND	2.80	1.41	1.37
26	B	813	CLA	C1D-ND	2.80	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W	614	CLA	C3B-C4B	2.80	1.49	1.42
26	Z	604	CLA	C3B-C4B	2.79	1.49	1.42
26	8	604	CLA	C3B-C4B	2.79	1.49	1.42
36	6	624	NEX	C1-C6	-2.79	1.49	1.54
26	K	201	CLA	C1B-C2B	2.79	1.49	1.43
26	B	840	CLA	CMB-C2B	-2.79	1.44	1.50
26	B	809	CLA	C4B-NB	2.79	1.41	1.37
26	A	822	CLA	C3B-C4B	2.79	1.49	1.42
26	8	601	CLA	C3B-C4B	2.79	1.49	1.42
26	B	811	CLA	CMB-C2B	-2.79	1.44	1.50
26	X	611	CLA	C3B-C4B	2.79	1.49	1.42
26	A	842	CLA	C1D-ND	2.79	1.41	1.37
26	B	804	CLA	C4B-NB	2.79	1.41	1.37
26	1	610	CLA	C3B-C4B	2.79	1.49	1.42
34	9	619	LUT	C22-C21	-2.79	1.51	1.54
26	Z	603	CLA	C1B-C2B	2.79	1.49	1.43
26	2	609	CLA	C3B-C4B	2.79	1.49	1.42
37	U	608	CHL	C1D-C2D	2.79	1.50	1.45
26	9	602	CLA	C3B-C4B	2.78	1.49	1.42
26	B	836	CLA	CMD-C2D	-2.78	1.44	1.50
26	6	613	CLA	CMB-C2B	-2.78	1.44	1.50
37	Z	609	CHL	C1B-NB	-2.78	1.34	1.37
26	Z	613	CLA	C1B-C2B	2.78	1.49	1.43
26	B	839	CLA	CMB-C2B	-2.78	1.44	1.50
26	6	613	CLA	C3B-C4B	2.78	1.49	1.42
37	X	605	CHL	C3B-C4B	2.77	1.49	1.42
37	U	601	CHL	C1B-C2B	2.77	1.49	1.43
26	1	611	CLA	C3B-C4B	2.77	1.49	1.42
26	A	826	CLA	C3B-C4B	2.77	1.49	1.42
26	U	612	CLA	C4D-ND	-2.77	1.33	1.37
36	W	1623	NEX	C7-C8	-2.77	1.27	1.32
26	W	603	CLA	C4D-ND	-2.77	1.33	1.37
26	A	854	CLA	C1D-ND	2.77	1.41	1.37
26	B	802	CLA	C4B-NB	2.77	1.41	1.37
26	Y	614	CLA	C3B-C4B	2.77	1.49	1.42
26	X	604	CLA	C3B-C4B	2.77	1.49	1.42
26	7	614	CLA	C4B-NB	2.77	1.41	1.37
26	X	603	CLA	C3B-C4B	2.77	1.49	1.42
26	3	603	CLA	C4B-NB	2.77	1.41	1.37
26	U	610	CLA	C1B-C2B	2.76	1.49	1.43
26	F	304	CLA	C3B-C4B	2.76	1.49	1.42
26	V	610	CLA	C3B-C4B	2.76	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	603	CLA	CMD-C2D	-2.76	1.44	1.50
37	X	608	CHL	C1D-C2D	2.76	1.50	1.45
26	B	810	CLA	C4B-NB	2.76	1.41	1.37
26	a	606	CLA	C3B-C4B	2.76	1.49	1.42
26	L	307	CLA	C4B-NB	2.76	1.41	1.37
26	B	836	CLA	C3B-C4B	2.76	1.49	1.42
26	Y	612	CLA	C4D-ND	-2.76	1.33	1.37
37	W	606	CHL	C1B-NB	-2.76	1.34	1.37
37	Z	607	CHL	C3B-C4B	2.76	1.49	1.42
26	2	612	CLA	C3B-C4B	2.76	1.49	1.42
26	A	820	CLA	C4B-NB	2.75	1.41	1.37
26	B	803	CLA	C1D-ND	2.75	1.41	1.37
26	A	804	CLA	CMD-C2D	-2.75	1.45	1.50
26	A	842	CLA	CMD-C2D	-2.75	1.45	1.50
26	U	602	CLA	C3B-C4B	2.75	1.49	1.42
37	U	601	CHL	C3D-C2D	2.75	1.46	1.39
26	B	817	CLA	C4B-NB	2.75	1.41	1.37
26	A	828	CLA	CMD-C2D	-2.75	1.45	1.50
26	B	818	CLA	CMB-C2B	-2.75	1.45	1.50
26	A	817	CLA	CMD-C2D	-2.75	1.45	1.50
26	B	826	CLA	CMD-C2D	-2.75	1.45	1.50
37	Z	601	CHL	C1D-C2D	2.75	1.50	1.45
37	W	607	CHL	C1D-C2D	2.74	1.50	1.45
26	B	817	CLA	C1D-ND	2.74	1.41	1.37
37	W	607	CHL	MG-NA	-2.74	1.99	2.06
26	7	603	CLA	C4B-NB	2.74	1.41	1.37
26	6	608	CLA	C3B-C4B	2.74	1.49	1.42
26	a	610	CLA	C3B-C4B	2.74	1.49	1.42
26	B	815	CLA	C4B-NB	2.74	1.41	1.37
26	1	609	CLA	C1B-C2B	2.74	1.49	1.43
26	B	838	CLA	C3B-C4B	2.74	1.49	1.42
37	X	601	CHL	C1D-C2D	2.74	1.50	1.45
26	A	819	CLA	C1D-ND	2.74	1.41	1.37
26	A	827	CLA	C4B-NB	2.74	1.41	1.37
26	a	613	CLA	C4B-NB	2.74	1.41	1.37
26	V	604	CLA	C3B-C4B	2.74	1.49	1.42
26	A	825	CLA	CMB-C2B	-2.74	1.45	1.50
26	a	609	CLA	C1B-C2B	2.74	1.49	1.43
37	X	606	CHL	C3D-C2D	2.74	1.46	1.39
26	6	617	CLA	C3B-C4B	2.73	1.49	1.42
37	Y	608	CHL	C3B-C4B	2.73	1.49	1.42
37	Y	601	CHL	C3B-C4B	2.73	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	825	CLA	CMD-C2D	-2.73	1.45	1.50
26	K	204	CLA	C4B-NB	2.73	1.41	1.37
26	V	612	CLA	C3B-C4B	2.73	1.49	1.42
26	A	841	CLA	C1D-ND	2.73	1.41	1.37
36	V	1623	NEX	C7-C8	-2.73	1.27	1.32
26	A	810	CLA	C4B-NB	2.73	1.41	1.37
37	V	605	CHL	C3D-C2D	2.73	1.46	1.39
26	7	606	CLA	C3B-C4B	2.73	1.49	1.42
37	W	607	CHL	C3B-C4B	2.73	1.49	1.42
26	A	824	CLA	C4B-NB	2.73	1.41	1.37
26	3	602	CLA	C3B-C4B	2.73	1.49	1.42
29	B	849	BCR	C30-C25	-2.73	1.50	1.53
26	W	603	CLA	C1B-C2B	2.72	1.49	1.43
26	G	203	CLA	C3B-C4B	2.72	1.49	1.42
37	Y	609	CHL	C3D-C2D	2.72	1.46	1.39
26	B	818	CLA	CMD-C2D	-2.72	1.45	1.50
26	5	617	CLA	C4B-NB	2.72	1.41	1.37
26	X	613	CLA	C3B-C4B	2.72	1.49	1.42
37	X	606	CHL	MG-NA	-2.72	1.99	2.06
26	A	836	CLA	C1D-ND	2.72	1.41	1.37
26	7	612	CLA	C3B-C4B	2.72	1.49	1.42
26	B	828	CLA	C4B-NB	2.72	1.41	1.37
26	1	613	CLA	C4B-NB	2.72	1.41	1.37
26	8	606	CLA	C3B-C4B	2.71	1.49	1.42
26	A	838	CLA	CMD-C2D	-2.71	1.45	1.50
26	A	843	CLA	C1D-ND	2.71	1.41	1.37
26	A	835	CLA	C4B-NB	2.71	1.41	1.37
26	8	602	CLA	CMC-C2C	-2.71	1.45	1.50
26	B	809	CLA	CMB-C2B	-2.71	1.45	1.50
26	7	611	CLA	CMD-C2D	-2.71	1.45	1.50
26	3	614	CLA	C3B-C4B	2.71	1.49	1.42
37	Y	609	CHL	C1B-NB	-2.71	1.34	1.37
26	5	611	CLA	C3B-C4B	2.71	1.49	1.42
26	9	603	CLA	CMB-C2B	-2.70	1.45	1.50
26	Y	613	CLA	C3B-C4B	2.70	1.49	1.42
26	V	613	CLA	C3B-C4B	2.70	1.49	1.42
26	B	818	CLA	C4B-NB	2.70	1.41	1.37
26	A	819	CLA	CMD-C2D	-2.70	1.45	1.50
37	Y	605	CHL	C3B-C4B	2.70	1.49	1.42
26	X	603	CLA	C4D-ND	-2.70	1.34	1.37
26	A	816	CLA	C4B-NB	2.70	1.41	1.37
26	A	839	CLA	CMB-C2B	-2.70	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	830	CLA	CMD-C2D	-2.70	1.45	1.50
26	4	616	CLA	C1B-C2B	2.70	1.49	1.43
37	X	601	CHL	C1B-C2B	2.70	1.49	1.43
26	B	827	CLA	C4B-NB	2.69	1.41	1.37
26	A	802	CLA	C1D-ND	2.69	1.41	1.37
26	9	611	CLA	C1B-C2B	2.69	1.49	1.43
26	B	821	CLA	C3B-C4B	2.69	1.49	1.42
26	U	603	CLA	C1B-C2B	2.69	1.49	1.43
26	B	841	CLA	C3B-C4B	2.69	1.49	1.42
26	X	603	CLA	C1B-C2B	2.69	1.49	1.43
26	B	828	CLA	CMB-C2B	-2.69	1.45	1.50
29	B	848	BCR	C21-C22	-2.69	1.32	1.35
26	5	612	CLA	C1B-C2B	2.69	1.49	1.43
26	3	609	CLA	CMD-C2D	-2.69	1.45	1.50
26	X	613	CLA	C1B-C2B	2.68	1.49	1.43
26	A	803	CLA	CMD-C2D	-2.68	1.45	1.50
26	B	808	CLA	C3B-C4B	2.68	1.49	1.42
26	A	842	CLA	C3B-C4B	2.68	1.49	1.42
26	9	606	CLA	C3B-C4B	2.68	1.49	1.42
37	W	605	CHL	C3B-C4B	2.68	1.49	1.42
26	B	835	CLA	CMD-C2D	-2.68	1.45	1.50
26	B	807	CLA	CMB-C2B	-2.68	1.45	1.50
26	3	609	CLA	CMB-C2B	-2.68	1.45	1.50
29	B	849	BCR	C1-C6	-2.68	1.50	1.53
37	X	609	CHL	C3D-C2D	2.68	1.46	1.39
26	Y	613	CLA	C1B-C2B	2.67	1.49	1.43
26	2	613	CLA	C1B-C2B	2.67	1.49	1.43
26	A	806	CLA	CMD-C2D	-2.67	1.45	1.50
26	a	601	CLA	C3B-C4B	2.67	1.49	1.42
26	A	818	CLA	CMD-C2D	-2.67	1.45	1.50
26	1	602	CLA	CMD-C2D	-2.67	1.45	1.50
26	B	834	CLA	C4B-NB	2.67	1.41	1.37
36	X	1623	NEX	C7-C8	-2.67	1.27	1.32
37	X	607	CHL	C1D-C2D	2.67	1.50	1.45
26	K	206	CLA	C3B-C4B	2.67	1.49	1.42
26	L	306	CLA	C3B-C4B	2.67	1.49	1.42
29	A	850	BCR	C30-C25	-2.67	1.50	1.53
26	A	813	CLA	CMD-C2D	-2.67	1.45	1.50
26	B	839	CLA	CMD-C2D	-2.67	1.45	1.50
26	A	802	CLA	CMC-C2C	-2.67	1.45	1.50
26	W	603	CLA	C3B-C4B	2.67	1.49	1.42
26	L	304	CLA	C1B-C2B	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	813	CLA	CMB-C2B	-2.67	1.45	1.50
26	2	609	CLA	CMB-C2B	-2.67	1.45	1.50
26	5	617	CLA	CMB-C2B	-2.66	1.45	1.50
26	4	607	CLA	C3B-C4B	2.66	1.49	1.42
34	5	620	LUT	C22-C21	-2.66	1.51	1.54
26	A	826	CLA	C1D-ND	2.66	1.41	1.37
26	6	614	CLA	C3B-C4B	2.66	1.49	1.42
26	1	602	CLA	CMC-C2C	-2.66	1.45	1.50
26	A	819	CLA	CMB-C2B	-2.66	1.45	1.50
26	6	602	CLA	CMC-C2C	-2.66	1.45	1.50
26	7	601	CLA	CMD-C2D	-2.66	1.45	1.50
37	X	606	CHL	C1D-C2D	2.66	1.50	1.45
26	4	603	CLA	C1B-C2B	2.66	1.49	1.43
37	W	608	CHL	C3D-C2D	2.66	1.46	1.39
26	3	611	CLA	C1B-C2B	2.66	1.49	1.43
26	8	602	CLA	CMD-C2D	-2.66	1.45	1.50
26	9	611	CLA	C3B-C4B	2.66	1.49	1.42
26	X	611	CLA	C1B-C2B	2.66	1.49	1.43
26	B	815	CLA	CMB-C2B	-2.66	1.45	1.50
26	B	820	CLA	CMD-C2D	-2.65	1.45	1.50
26	6	611	CLA	C1B-C2B	2.65	1.49	1.43
26	9	601	CLA	C3B-C4B	2.65	1.49	1.42
26	6	609	CLA	CMB-C2B	-2.65	1.45	1.50
26	A	830	CLA	C4B-NB	2.65	1.41	1.37
26	5	606	CLA	C3B-C4B	2.65	1.49	1.42
26	a	602	CLA	CMD-C2D	-2.65	1.45	1.50
26	B	830	CLA	C3B-C4B	2.65	1.49	1.42
26	1	601	CLA	C3B-C4B	2.65	1.49	1.42
26	5	602	CLA	C3B-C4B	2.65	1.49	1.42
26	B	802	CLA	C1D-ND	2.65	1.41	1.37
26	W	613	CLA	C3B-C4B	2.65	1.49	1.42
26	6	612	CLA	C3B-C4B	2.65	1.49	1.42
26	4	606	CLA	C1B-C2B	2.65	1.49	1.43
37	Y	608	CHL	C1D-C2D	2.65	1.50	1.45
26	J	101	CLA	C3B-C4B	2.65	1.49	1.42
26	G	204	CLA	C3B-C4B	2.65	1.49	1.42
26	Y	604	CLA	C3B-C4B	2.65	1.49	1.42
26	B	836	CLA	C4B-NB	2.65	1.41	1.37
37	W	609	CHL	C3B-C4B	2.65	1.49	1.42
26	A	806	CLA	CMC-C2C	-2.64	1.45	1.50
26	a	603	CLA	C3B-C4B	2.64	1.49	1.42
34	2	619	LUT	C1-C6	-2.64	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	845	CLA	CMD-C2D	-2.64	1.45	1.50
26	A	840	CLA	CMD-C2D	-2.64	1.45	1.50
26	A	808	CLA	C3B-C4B	2.64	1.48	1.42
26	A	814	CLA	C3B-C4B	2.64	1.48	1.42
26	A	843	CLA	CMD-C2D	-2.64	1.45	1.50
26	A	815	CLA	CMC-C2C	-2.64	1.45	1.50
26	U	611	CLA	C1B-C2B	2.64	1.49	1.43
26	a	604	CLA	C3B-C4B	2.64	1.48	1.42
26	B	831	CLA	C3B-C4B	2.64	1.48	1.42
26	a	612	CLA	C3B-C4B	2.64	1.48	1.42
26	3	613	CLA	CMB-C2B	-2.64	1.45	1.50
26	3	606	CLA	C4B-NB	2.64	1.41	1.37
26	B	814	CLA	CMD-C2D	-2.64	1.45	1.50
26	B	808	CLA	CMC-C2C	-2.64	1.45	1.50
26	2	601	CLA	C4B-NB	2.63	1.41	1.37
26	B	810	CLA	C3B-C4B	2.63	1.48	1.42
26	B	808	CLA	CMB-C2B	-2.63	1.45	1.50
26	7	610	CLA	CMC-C2C	-2.63	1.45	1.50
26	2	614	CLA	C3B-C4B	2.63	1.48	1.42
37	X	607	CHL	C3B-C4B	2.63	1.48	1.42
26	O	2001	CLA	CMD-C2D	-2.63	1.45	1.50
26	B	812	CLA	CMD-C2D	-2.63	1.45	1.50
26	A	801	CLA	CMB-C2B	-2.63	1.45	1.50
37	W	605	CHL	C3D-C2D	2.63	1.46	1.39
26	7	604	CLA	C3B-C4B	2.63	1.48	1.42
26	6	606	CLA	C3B-C4B	2.63	1.48	1.42
26	A	835	CLA	CMD-C2D	-2.63	1.45	1.50
26	2	602	CLA	CMC-C2C	-2.63	1.45	1.50
26	A	809	CLA	C4B-NB	2.63	1.41	1.37
26	a	610	CLA	CMD-C2D	-2.63	1.45	1.50
26	6	616	CLA	C3B-C4B	2.63	1.48	1.42
26	B	837	CLA	CMB-C2B	-2.63	1.45	1.50
26	A	819	CLA	MG-NB	-2.63	2.00	2.05
26	B	828	CLA	CMD-C2D	-2.63	1.45	1.50
26	F	303	CLA	CMB-C2B	-2.63	1.45	1.50
26	1	604	CLA	C3B-C4B	2.63	1.48	1.42
26	8	613	CLA	CMD-C2D	-2.63	1.45	1.50
37	W	601	CHL	C1B-NB	-2.63	1.34	1.37
26	B	833	CLA	CMD-C2D	-2.63	1.45	1.50
26	V	603	CLA	C1B-C2B	2.62	1.49	1.43
37	U	607	CHL	C1D-C2D	2.62	1.50	1.45
26	2	612	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	606	CLA	C3B-C4B	2.62	1.48	1.42
26	A	824	CLA	CMB-C2B	-2.62	1.45	1.50
26	F	301	CLA	CMD-C2D	-2.62	1.45	1.50
26	3	613	CLA	C3B-C4B	2.62	1.48	1.42
26	A	805	CLA	CMD-C2D	-2.62	1.45	1.50
26	B	824	CLA	C1D-ND	2.62	1.41	1.37
26	7	609	CLA	C3B-C4B	2.62	1.48	1.42
26	A	825	CLA	C4B-NB	2.62	1.41	1.37
29	B	844	BCR	C21-C22	-2.62	1.32	1.35
26	B	832	CLA	C3B-C4B	2.62	1.48	1.42
26	B	825	CLA	C3B-C4B	2.62	1.48	1.42
26	3	604	CLA	C3B-C4B	2.62	1.48	1.42
26	A	806	CLA	CMB-C2B	-2.62	1.45	1.50
26	H	203	CLA	C3B-C4B	2.62	1.48	1.42
26	A	838	CLA	CMB-C2B	-2.62	1.45	1.50
26	K	203	CLA	CMD-C2D	-2.62	1.45	1.50
37	Y	606	CHL	C1D-C2D	2.62	1.50	1.45
26	6	606	CLA	C1B-C2B	2.62	1.49	1.43
26	O	2001	CLA	C1B-C2B	2.62	1.49	1.43
26	9	612	CLA	C1B-C2B	2.62	1.49	1.43
34	2	619	LUT	C22-C21	-2.62	1.51	1.54
26	B	813	CLA	CMD-C2D	-2.62	1.45	1.50
26	7	611	CLA	CMC-C2C	-2.62	1.45	1.50
26	5	601	CLA	C1B-C2B	2.61	1.49	1.43
26	W	612	CLA	C3B-C4B	2.61	1.48	1.42
37	W	608	CHL	C3B-C4B	2.61	1.48	1.42
26	B	809	CLA	CMC-C2C	-2.61	1.45	1.50
26	6	618	CLA	C1B-C2B	2.61	1.49	1.43
26	U	603	CLA	C3B-C4B	2.61	1.48	1.42
26	5	617	CLA	CMD-C2D	-2.61	1.45	1.50
26	A	854	CLA	C3B-C4B	2.61	1.48	1.42
26	4	610	CLA	C1B-C2B	2.61	1.49	1.43
26	9	613	CLA	C1B-C2B	2.61	1.49	1.43
26	3	613	CLA	CMD-C2D	-2.61	1.45	1.50
26	8	601	CLA	CMB-C2B	-2.61	1.45	1.50
37	W	609	CHL	C3D-C2D	2.61	1.46	1.39
26	B	832	CLA	CMB-C2B	-2.61	1.45	1.50
26	A	818	CLA	C3B-C4B	2.61	1.48	1.42
26	1	603	CLA	C3B-C4B	2.61	1.48	1.42
26	U	612	CLA	C1B-C2B	2.61	1.49	1.43
26	3	608	CLA	CMB-C2B	-2.61	1.45	1.50
26	A	822	CLA	C4B-NB	2.61	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	V	608	CHL	C1D-C2D	2.61	1.50	1.45
37	U	607	CHL	MG-NA	-2.61	2.00	2.06
37	U	607	CHL	C3B-C4B	2.61	1.48	1.42
37	Y	607	CHL	C3D-C2D	2.61	1.46	1.39
26	A	802	CLA	CMD-C2D	-2.61	1.45	1.50
26	3	606	CLA	CMB-C2B	-2.61	1.45	1.50
31	A	858	LMU	C3B-C2B	-2.61	1.48	1.52
26	A	810	CLA	C3B-C4B	2.61	1.48	1.42
26	B	840	CLA	CMD-C2D	-2.60	1.45	1.50
26	A	833	CLA	C3B-C4B	2.60	1.48	1.42
26	B	813	CLA	CMB-C2B	-2.60	1.45	1.50
26	9	603	CLA	CMD-C2D	-2.60	1.45	1.50
26	Y	603	CLA	C3B-C4B	2.60	1.48	1.42
26	8	612	CLA	C1B-C2B	2.60	1.49	1.43
37	U	608	CHL	MG-NA	-2.60	2.00	2.06
26	8	609	CLA	C3B-C4B	2.60	1.48	1.42
26	A	809	CLA	CMB-C2B	-2.60	1.45	1.50
26	U	613	CLA	C1B-C2B	2.60	1.49	1.43
26	Y	614	CLA	C1B-C2B	2.60	1.49	1.43
26	A	805	CLA	C3B-C4B	2.60	1.48	1.42
37	W	609	CHL	MG-NA	-2.60	2.00	2.06
26	a	613	CLA	CMD-C2D	-2.60	1.45	1.50
26	8	601	CLA	CMD-C2D	-2.60	1.45	1.50
37	U	606	CHL	C1D-C2D	2.60	1.50	1.45
37	Y	601	CHL	C1B-NB	-2.60	1.34	1.37
26	Z	613	CLA	CMD-C2D	-2.60	1.45	1.50
34	4	619	LUT	C22-C21	-2.60	1.51	1.54
26	7	603	CLA	CMD-C2D	-2.60	1.45	1.50
26	B	803	CLA	C4B-NB	2.60	1.41	1.37
34	3	618	LUT	C22-C21	-2.60	1.51	1.54
26	1	612	CLA	C3B-C4B	2.60	1.48	1.42
26	1	610	CLA	CMD-C2D	-2.60	1.45	1.50
26	V	612	CLA	C1B-C2B	2.60	1.49	1.43
26	2	607	CLA	C3B-C4B	2.60	1.48	1.42
26	a	602	CLA	CMC-C2C	-2.60	1.45	1.50
26	A	836	CLA	CMD-C2D	-2.60	1.45	1.50
26	V	603	CLA	C3B-C4B	2.60	1.48	1.42
26	Y	603	CLA	C1B-C2B	2.60	1.49	1.43
26	2	610	CLA	CMD-C2D	-2.60	1.45	1.50
37	U	601	CHL	C3B-C4B	2.59	1.48	1.42
37	U	605	CHL	C3B-C4B	2.59	1.48	1.42
26	L	303	CLA	C4B-NB	2.59	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	W	606	CHL	C1D-C2D	2.59	1.50	1.45
26	Z	603	CLA	C3B-C4B	2.59	1.48	1.42
37	W	609	CHL	C1B-NB	-2.59	1.34	1.37
26	9	602	CLA	CMD-C2D	-2.59	1.45	1.50
37	V	601	CHL	C3D-C2D	2.59	1.46	1.39
26	A	801	CLA	C4B-NB	2.59	1.41	1.37
26	A	835	CLA	CMB-C2B	-2.59	1.45	1.50
26	5	616	CLA	C1B-C2B	2.59	1.49	1.43
26	2	601	CLA	C3B-C4B	2.59	1.48	1.42
37	Z	609	CHL	C4B-NB	-2.59	1.34	1.37
26	a	613	CLA	CMB-C2B	-2.59	1.45	1.50
37	U	609	CHL	C3D-C2D	2.59	1.46	1.39
37	W	601	CHL	C3D-C2D	2.59	1.46	1.39
26	7	603	CLA	CMB-C2B	-2.59	1.45	1.50
26	8	616	CLA	C1B-C2B	2.59	1.49	1.43
26	8	603	CLA	CMD-C2D	-2.59	1.45	1.50
26	F	301	CLA	C3B-C4B	2.59	1.48	1.42
37	Y	605	CHL	C4B-NB	-2.59	1.34	1.37
26	B	823	CLA	C4B-NB	2.59	1.41	1.37
26	K	204	CLA	CMD-C2D	-2.59	1.45	1.50
26	9	601	CLA	C1B-C2B	2.59	1.49	1.43
29	A	852	BCR	C21-C22	-2.59	1.32	1.35
26	1	608	CLA	C3B-C4B	2.59	1.48	1.42
26	A	807	CLA	CMB-C2B	-2.58	1.45	1.50
26	5	603	CLA	CMB-C2B	-2.58	1.45	1.50
26	a	603	CLA	C1B-C2B	2.58	1.49	1.43
26	4	614	CLA	C1B-C2B	2.58	1.49	1.43
26	W	614	CLA	C1B-C2B	2.58	1.49	1.43
26	2	613	CLA	CMD-C2D	-2.58	1.45	1.50
26	A	822	CLA	CMD-C2D	-2.58	1.45	1.50
26	1	612	CLA	C1B-C2B	2.58	1.49	1.43
26	A	816	CLA	CMC-C2C	-2.58	1.45	1.50
26	B	835	CLA	CMB-C2B	-2.58	1.45	1.50
26	a	612	CLA	C1B-C2B	2.58	1.49	1.43
26	B	810	CLA	CMB-C2B	-2.58	1.45	1.50
37	W	608	CHL	C4C-C3C	2.58	1.49	1.45
26	1	603	CLA	C1B-C2B	2.58	1.49	1.43
26	a	608	CLA	C3B-C4B	2.58	1.48	1.42
26	L	303	CLA	CMB-C2B	-2.58	1.45	1.50
26	1	608	CLA	C1B-C2B	2.58	1.49	1.43
26	W	613	CLA	C1B-C2B	2.58	1.49	1.43
26	A	803	CLA	C4B-NB	2.58	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	606	CHL	C3D-C2D	2.58	1.46	1.39
37	Z	608	CHL	C3B-C4B	2.57	1.48	1.42
26	2	611	CLA	C1B-C2B	2.57	1.49	1.43
26	6	620	CLA	C3B-C4B	2.57	1.48	1.42
26	W	612	CLA	C1B-C2B	2.57	1.49	1.43
37	U	605	CHL	C1B-C2B	2.57	1.49	1.43
37	W	601	CHL	MG-NA	-2.57	2.00	2.06
26	A	820	CLA	C3B-C4B	2.57	1.48	1.42
37	Z	609	CHL	C3D-C2D	2.57	1.46	1.39
26	7	601	CLA	C4B-NB	2.57	1.40	1.37
26	2	611	CLA	C3B-C4B	2.57	1.48	1.42
26	2	614	CLA	CMD-C2D	-2.57	1.45	1.50
26	A	829	CLA	CMC-C2C	-2.57	1.45	1.50
26	B	829	CLA	C3B-C4B	2.57	1.48	1.42
37	X	608	CHL	MG-NA	-2.57	2.00	2.06
26	5	607	CLA	CMB-C2B	-2.57	1.45	1.50
26	4	612	CLA	C1B-C2B	2.57	1.49	1.43
26	L	307	CLA	C1B-C2B	2.57	1.49	1.43
26	B	813	CLA	C3B-C4B	2.57	1.48	1.42
26	A	819	CLA	CMC-C2C	-2.57	1.45	1.50
26	B	829	CLA	CMD-C2D	-2.57	1.45	1.50
26	U	614	CLA	C1B-C2B	2.57	1.49	1.43
26	B	838	CLA	CMD-C2D	-2.56	1.45	1.50
26	a	608	CLA	C1B-C2B	2.56	1.49	1.43
26	B	806	CLA	CMD-C2D	-2.56	1.45	1.50
26	B	836	CLA	C1B-NB	-2.56	1.34	1.37
37	Y	607	CHL	C1B-C2B	2.56	1.49	1.43
26	F	303	CLA	C3B-C4B	2.56	1.48	1.42
26	A	807	CLA	CMC-C2C	-2.56	1.45	1.50
26	a	614	CLA	C3B-C4B	2.56	1.48	1.42
26	6	603	CLA	CMD-C2D	-2.56	1.45	1.50
26	B	827	CLA	C3B-C4B	2.56	1.48	1.42
26	A	806	CLA	MG-NB	-2.56	2.00	2.05
26	A	834	CLA	CMD-C2D	-2.56	1.45	1.50
37	Y	607	CHL	C1B-NB	-2.56	1.34	1.37
26	6	601	CLA	C3B-C4B	2.56	1.48	1.42
26	A	854	CLA	CMB-C2B	-2.56	1.45	1.50
26	1	613	CLA	CMD-C2D	-2.56	1.45	1.50
26	A	815	CLA	C3B-C4B	2.56	1.48	1.42
37	V	607	CHL	MG-NA	-2.56	2.00	2.06
26	6	603	CLA	C1B-C2B	2.56	1.49	1.43
26	A	823	CLA	C1B-C2B	2.56	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	605	CHL	C1B-C2B	2.56	1.49	1.43
26	6	612	CLA	C1B-C2B	2.56	1.49	1.43
26	B	820	CLA	C3B-C4B	2.56	1.48	1.42
26	A	836	CLA	CMB-C2B	-2.56	1.45	1.50
26	U	602	CLA	C1B-C2B	2.55	1.49	1.43
26	8	608	CLA	CMC-C2C	-2.55	1.45	1.50
26	B	834	CLA	CMD-C2D	-2.55	1.45	1.50
26	V	613	CLA	C1B-C2B	2.55	1.49	1.43
29	B	801	BCR	C21-C22	-2.55	1.32	1.35
26	5	611	CLA	C1B-C2B	2.55	1.49	1.43
26	A	804	CLA	C1B-C2B	2.55	1.49	1.43
37	V	607	CHL	C3D-C2D	2.55	1.46	1.39
37	X	608	CHL	C1B-NB	-2.55	1.34	1.37
26	B	813	CLA	CMC-C2C	-2.55	1.45	1.50
26	Y	612	CLA	C1B-C2B	2.55	1.49	1.43
26	7	616	CLA	C1B-C2B	2.55	1.49	1.43
26	9	602	CLA	CMC-C2C	-2.55	1.45	1.50
26	7	613	CLA	C1B-C2B	2.55	1.49	1.43
26	Z	614	CLA	C1B-C2B	2.55	1.49	1.43
26	B	834	CLA	CMB-C2B	-2.55	1.45	1.50
26	B	841	CLA	CMC-C2C	-2.55	1.45	1.50
26	B	824	CLA	CMC-C2C	-2.55	1.45	1.50
26	X	614	CLA	C1B-C2B	2.55	1.49	1.43
26	A	802	CLA	C4B-NB	2.55	1.40	1.37
26	A	815	CLA	CMD-C2D	-2.55	1.45	1.50
26	8	608	CLA	CMD-C2D	-2.55	1.45	1.50
26	B	830	CLA	CMB-C2B	-2.55	1.45	1.50
26	L	306	CLA	CMC-C2C	-2.55	1.45	1.50
26	8	612	CLA	CMD-C2D	-2.55	1.45	1.50
37	Y	607	CHL	C3B-C4B	2.55	1.48	1.42
37	V	609	CHL	C3D-C2D	2.54	1.46	1.39
26	O	2002	CLA	CMD-C2D	-2.54	1.45	1.50
26	Y	611	CLA	C1B-C2B	2.54	1.49	1.43
26	5	604	CLA	C4B-C3B	2.54	1.49	1.43
37	Z	605	CHL	C1B-C2B	2.54	1.49	1.43
26	a	613	CLA	C3B-C4B	2.54	1.48	1.42
26	6	610	CLA	CMD-C2D	-2.54	1.45	1.50
26	4	608	CLA	C1B-C2B	2.54	1.49	1.43
26	O	2003	CLA	C3B-C4B	2.54	1.48	1.42
26	G	204	CLA	CMB-C2B	-2.54	1.45	1.50
37	X	605	CHL	C1B-C2B	2.54	1.49	1.43
26	A	830	CLA	C1D-ND	2.54	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	602	CLA	C1B-C2B	2.54	1.49	1.43
26	A	804	CLA	C4B-NB	2.54	1.40	1.37
26	7	610	CLA	CMB-C2B	-2.54	1.45	1.50
26	O	2002	CLA	C4B-C3B	2.54	1.49	1.43
26	5	608	CLA	C1B-C2B	2.54	1.49	1.43
26	V	611	CLA	C1B-C2B	2.54	1.49	1.43
26	B	827	CLA	CMD-C2D	-2.54	1.45	1.50
26	9	604	CLA	C4B-C3B	2.54	1.49	1.43
26	B	811	CLA	CMC-C2C	-2.54	1.45	1.50
26	B	805	CLA	CMB-C2B	-2.54	1.45	1.50
26	B	815	CLA	CMD-C2D	-2.54	1.45	1.50
26	A	820	CLA	CMD-C2D	-2.54	1.45	1.50
26	7	608	CLA	CMD-C2D	-2.54	1.45	1.50
26	A	821	CLA	C3B-C4B	2.54	1.48	1.42
29	B	843	BCR	C30-C25	-2.54	1.50	1.53
37	Z	607	CHL	C1B-C2B	2.53	1.49	1.43
26	A	813	CLA	C3B-C4B	2.53	1.48	1.42
26	A	809	CLA	CMD-C2D	-2.53	1.45	1.50
26	8	613	CLA	C3B-C4B	2.53	1.48	1.42
26	A	812	CLA	CMB-C2B	-2.53	1.45	1.50
26	B	807	CLA	CMC-C2C	-2.53	1.45	1.50
37	Y	601	CHL	C3D-C2D	2.53	1.46	1.39
26	A	836	CLA	C4B-NB	2.53	1.40	1.37
26	B	832	CLA	CMD-C2D	-2.53	1.45	1.50
26	4	613	CLA	CMB-C2B	-2.53	1.45	1.50
26	7	614	CLA	CMD-C2D	-2.53	1.45	1.50
26	B	805	CLA	C4B-NB	2.53	1.40	1.37
26	A	803	CLA	CMC-C2C	-2.53	1.45	1.50
26	7	612	CLA	CMD-C2D	-2.53	1.45	1.50
26	A	841	CLA	C4B-NB	2.53	1.40	1.37
26	A	811	CLA	CMC-C2C	-2.53	1.45	1.50
37	V	601	CHL	C1B-NB	-2.53	1.34	1.37
26	A	824	CLA	CMC-C2C	-2.53	1.45	1.50
26	A	806	CLA	C4B-NB	2.53	1.40	1.37
37	Y	606	CHL	C1B-NB	-2.53	1.34	1.37
37	Y	609	CHL	C4B-NB	-2.53	1.34	1.37
26	A	834	CLA	CMC-C2C	-2.53	1.45	1.50
26	7	604	CLA	CMD-C2D	-2.53	1.45	1.50
26	2	602	CLA	C1D-ND	2.53	1.41	1.37
26	1	613	CLA	C3B-C4B	2.53	1.48	1.42
37	W	605	CHL	C1B-C2B	2.53	1.49	1.43
26	3	608	CLA	CMD-C2D	-2.52	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	604	CLA	CMB-C2B	-2.52	1.45	1.50
26	L	302	CLA	C3B-C4B	2.52	1.48	1.42
37	X	609	CHL	C4C-C3C	2.52	1.49	1.45
26	7	609	CLA	CMD-C2D	-2.52	1.45	1.50
26	A	831	CLA	C3B-C4B	2.52	1.48	1.42
26	8	610	CLA	CMD-C2D	-2.52	1.45	1.50
26	1	613	CLA	CMB-C2B	-2.52	1.45	1.50
26	4	614	CLA	C3B-C4B	2.52	1.48	1.42
26	A	817	CLA	CMB-C2B	-2.52	1.45	1.50
37	W	607	CHL	C3D-C2D	2.52	1.46	1.39
26	A	806	CLA	C3B-C4B	2.52	1.48	1.42
26	5	613	CLA	C3B-C4B	2.52	1.48	1.42
26	J	101	CLA	C1B-C2B	2.52	1.49	1.43
26	B	822	CLA	C3B-C4B	2.52	1.48	1.42
26	5	614	CLA	C3B-C4B	2.52	1.48	1.42
26	B	829	CLA	CMC-C2C	-2.52	1.45	1.50
37	Y	609	CHL	C4C-C3C	2.52	1.49	1.45
37	V	609	CHL	MG-NA	-2.52	2.00	2.06
37	V	608	CHL	C3B-C4B	2.52	1.48	1.42
26	5	617	CLA	C1B-C2B	2.52	1.49	1.43
26	Y	602	CLA	C1B-C2B	2.52	1.49	1.43
37	W	607	CHL	C1B-C2B	2.52	1.49	1.43
26	7	601	CLA	MG-NB	-2.52	2.00	2.05
26	8	613	CLA	CMC-C2C	-2.52	1.45	1.50
26	6	607	CLA	CMC-C2C	-2.52	1.45	1.50
26	B	811	CLA	CMD-C2D	-2.51	1.45	1.50
26	8	614	CLA	C3B-C4B	2.51	1.48	1.42
26	B	833	CLA	CMC-C2C	-2.51	1.45	1.50
26	A	817	CLA	C3B-C4B	2.51	1.48	1.42
26	2	601	CLA	MG-NB	-2.51	2.00	2.05
37	V	605	CHL	C1B-C2B	2.51	1.49	1.43
26	A	841	CLA	CMC-C2C	-2.51	1.45	1.50
26	A	816	CLA	CMD-C2D	-2.51	1.45	1.50
26	A	823	CLA	C3B-C4B	2.51	1.48	1.42
26	B	837	CLA	C3B-C4B	2.51	1.48	1.42
37	V	607	CHL	C3B-C4B	2.51	1.48	1.42
26	A	825	CLA	CMD-C2D	-2.51	1.45	1.50
26	A	833	CLA	CMD-C2D	-2.51	1.45	1.50
37	V	605	CHL	C4B-NB	-2.51	1.34	1.37
26	5	601	CLA	C3B-C4B	2.51	1.48	1.42
26	B	803	CLA	CMC-C2C	-2.51	1.45	1.50
26	F	301	CLA	CMB-C2B	-2.51	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Z	607	CHL	MG-NA	-2.51	2.00	2.06
26	A	808	CLA	CMD-C2D	-2.51	1.45	1.50
37	U	605	CHL	C4B-NB	-2.51	1.34	1.37
26	4	618	CLA	C4B-C3B	2.51	1.49	1.43
26	B	816	CLA	C3B-C4B	2.51	1.48	1.42
26	2	603	CLA	C3B-C4B	2.51	1.48	1.42
26	A	836	CLA	MG-NB	-2.51	2.00	2.05
36	U	1623	NEX	C7-C8	-2.51	1.27	1.32
37	X	601	CHL	C3D-C2D	2.51	1.46	1.39
37	Z	601	CHL	C3D-C2D	2.51	1.46	1.39
26	A	821	CLA	CMD-C2D	-2.51	1.45	1.50
26	A	845	CLA	CMB-C2B	-2.51	1.45	1.50
26	3	609	CLA	CMC-C2C	-2.51	1.45	1.50
26	A	834	CLA	C3B-C4B	2.51	1.48	1.42
26	X	612	CLA	C1B-C2B	2.50	1.49	1.43
26	K	206	CLA	CMB-C2B	-2.50	1.45	1.50
37	V	605	CHL	C3B-C4B	2.50	1.48	1.42
26	9	610	CLA	CMB-C2B	-2.50	1.45	1.50
37	U	609	CHL	C4C-C3C	2.50	1.49	1.45
26	A	828	CLA	MG-NB	-2.50	2.00	2.05
37	U	609	CHL	MG-NA	-2.50	2.00	2.06
26	7	607	CLA	CMB-C2B	-2.50	1.45	1.50
37	U	601	CHL	C1B-NB	-2.50	1.34	1.37
26	7	613	CLA	CMD-C2D	-2.50	1.45	1.50
26	8	613	CLA	CMB-C2B	-2.50	1.45	1.50
26	a	612	CLA	CMD-C2D	-2.50	1.45	1.50
26	A	808	CLA	CMC-C2C	-2.50	1.45	1.50
26	7	614	CLA	C3B-C4B	2.50	1.48	1.42
26	3	604	CLA	CMB-C2B	-2.50	1.45	1.50
26	A	838	CLA	C4B-NB	2.50	1.40	1.37
26	1	601	CLA	CMD-C2D	-2.50	1.45	1.50
26	9	613	CLA	CMB-C2B	-2.50	1.45	1.50
26	B	840	CLA	CMC-C2C	-2.50	1.45	1.50
26	O	2003	CLA	C1B-C2B	2.50	1.49	1.43
26	6	609	CLA	C3B-C4B	2.49	1.48	1.42
37	Z	605	CHL	C3B-C4B	2.49	1.48	1.42
26	A	832	CLA	CMC-C2C	-2.49	1.45	1.50
26	A	839	CLA	CMC-C2C	-2.49	1.45	1.50
37	W	607	CHL	C1B-NB	-2.49	1.34	1.37
37	Z	605	CHL	C3D-C2D	2.49	1.45	1.39
26	2	609	CLA	CMC-C2C	-2.49	1.45	1.50
26	B	826	CLA	C3B-C4B	2.49	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	817	CLA	CMD-C2D	-2.49	1.45	1.50
26	X	604	CLA	C1B-C2B	2.49	1.49	1.43
26	A	805	CLA	CMC-C2C	-2.49	1.45	1.50
26	B	819	CLA	CMB-C2B	-2.49	1.45	1.50
37	U	608	CHL	C4B-NB	-2.49	1.34	1.37
26	A	801	CLA	CMD-C2D	-2.49	1.45	1.50
26	1	612	CLA	CMD-C2D	-2.49	1.45	1.50
26	X	614	CLA	CMD-C2D	-2.49	1.45	1.50
26	a	611	CLA	C4B-C3B	2.49	1.49	1.43
37	Z	607	CHL	C1D-C2D	2.49	1.50	1.45
26	B	826	CLA	CMC-C2C	-2.49	1.45	1.50
26	H	202	CLA	CMB-C2B	-2.49	1.45	1.50
26	L	307	CLA	CMC-C2C	-2.49	1.45	1.50
34	Y	1621	LUT	C1-C6	-2.49	1.50	1.53
26	W	610	CLA	C1B-C2B	2.49	1.49	1.43
37	U	605	CHL	C4C-C3C	2.49	1.49	1.45
26	B	804	CLA	C3B-C4B	2.49	1.48	1.42
26	2	616	CLA	C1B-C2B	2.49	1.49	1.43
26	7	615	CLA	C4B-C3B	2.49	1.49	1.43
26	W	611	CLA	C1B-C2B	2.49	1.49	1.43
26	9	609	CLA	C1B-C2B	2.49	1.49	1.43
26	B	828	CLA	CMC-C2C	-2.49	1.45	1.50
37	U	609	CHL	C1B-C2B	2.49	1.49	1.43
26	F	304	CLA	CMD-C2D	-2.49	1.45	1.50
26	B	803	CLA	C3B-C4B	2.49	1.48	1.42
26	G	203	CLA	C1B-C2B	2.49	1.49	1.43
26	7	608	CLA	CMB-C2B	-2.49	1.45	1.50
26	5	614	CLA	C1B-C2B	2.48	1.49	1.43
37	V	609	CHL	C1B-C2B	2.48	1.49	1.43
26	5	610	CLA	CMC-C2C	-2.48	1.45	1.50
26	5	608	CLA	CMD-C2D	-2.48	1.45	1.50
26	L	303	CLA	C3B-C4B	2.48	1.48	1.42
26	5	604	CLA	CMB-C2B	-2.48	1.45	1.50
26	7	607	CLA	C3B-C4B	2.48	1.48	1.42
26	B	814	CLA	CMC-C2C	-2.48	1.45	1.50
34	1	617	LUT	C22-C21	-2.48	1.51	1.54
26	7	602	CLA	CMC-C2C	-2.48	1.45	1.50
26	A	813	CLA	CMC-C2C	-2.48	1.45	1.50
26	4	601	CLA	CMB-C2B	-2.48	1.45	1.50
26	6	611	CLA	C3B-C4B	2.48	1.48	1.42
37	V	607	CHL	C1B-NB	-2.48	1.34	1.37
26	B	826	CLA	C1B-C2B	2.48	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z	613	CLA	C3B-C4B	2.48	1.48	1.42
26	B	824	CLA	C3B-C4B	2.47	1.48	1.42
26	O	2001	CLA	C3B-C4B	2.47	1.48	1.42
26	L	303	CLA	CMD-C2D	-2.47	1.45	1.50
26	3	610	CLA	CMC-C2C	-2.47	1.45	1.50
26	6	607	CLA	C4B-C3B	2.47	1.49	1.43
26	W	602	CLA	C1B-C2B	2.47	1.49	1.43
26	A	825	CLA	C1B-C2B	2.47	1.49	1.43
26	4	618	CLA	C1B-C2B	2.47	1.49	1.43
26	B	812	CLA	CMB-C2B	-2.47	1.45	1.50
26	K	204	CLA	CMC-C2C	-2.47	1.45	1.50
37	Y	601	CHL	MG-NA	-2.47	2.00	2.06
26	B	820	CLA	C1B-C2B	2.47	1.49	1.43
26	B	822	CLA	C1B-C2B	2.47	1.49	1.43
26	A	811	CLA	CMD-C2D	-2.47	1.45	1.50
26	A	826	CLA	CMB-C2B	-2.47	1.45	1.50
26	K	204	CLA	C3B-C4B	2.47	1.48	1.42
26	A	831	CLA	CMC-C2C	-2.47	1.45	1.50
26	A	833	CLA	CMB-C2B	-2.47	1.45	1.50
26	3	614	CLA	CMD-C2D	-2.47	1.45	1.50
26	7	609	CLA	CMB-C2B	-2.47	1.45	1.50
26	8	611	CLA	CMD-C2D	-2.47	1.45	1.50
37	X	601	CHL	C3B-C4B	2.47	1.48	1.42
34	a	617	LUT	C22-C21	-2.47	1.51	1.54
26	7	612	CLA	C1B-C2B	2.47	1.49	1.43
26	L	307	CLA	C3B-C4B	2.47	1.48	1.42
26	2	603	CLA	CMD-C2D	-2.47	1.45	1.50
26	8	611	CLA	CMB-C2B	-2.47	1.45	1.50
26	5	618	CLA	C4B-C3B	2.47	1.49	1.43
37	Z	608	CHL	C1B-C2B	2.47	1.49	1.43
37	Y	607	CHL	C4B-NB	-2.47	1.34	1.37
26	A	816	CLA	CMB-C2B	-2.47	1.45	1.50
37	W	608	CHL	C1B-C2B	2.47	1.49	1.43
26	A	818	CLA	CMB-C2B	-2.47	1.45	1.50
26	4	604	CLA	C1B-C2B	2.47	1.49	1.43
26	4	609	CLA	C3B-C4B	2.47	1.48	1.42
37	Y	609	CHL	C3B-C4B	2.46	1.48	1.42
37	U	606	CHL	C3D-C2D	2.46	1.45	1.39
26	9	610	CLA	CMD-C2D	-2.46	1.45	1.50
26	5	603	CLA	C1B-C2B	2.46	1.49	1.43
26	6	614	CLA	C1B-C2B	2.46	1.49	1.43
37	Z	607	CHL	C4B-NB	-2.46	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	601	CLA	CMD-C2D	-2.46	1.45	1.50
26	9	614	CLA	C1B-C2B	2.46	1.49	1.43
34	6	619	LUT	C22-C21	-2.46	1.51	1.54
26	3	617	CLA	C3B-C4B	2.46	1.48	1.42
26	8	608	CLA	C3B-C4B	2.46	1.48	1.42
29	7	621	BCR	C1-C6	-2.46	1.50	1.53
37	Z	609	CHL	MG-NA	-2.46	2.00	2.06
26	7	604	CLA	CMC-C2C	-2.46	1.45	1.50
26	A	834	CLA	MG-NB	-2.46	2.00	2.05
26	4	602	CLA	CMD-C2D	-2.46	1.45	1.50
26	B	816	CLA	CMB-C2B	-2.46	1.45	1.50
37	Z	606	CHL	C3D-C2D	2.46	1.45	1.39
37	U	606	CHL	C3B-C4B	2.46	1.48	1.42
26	4	613	CLA	CMD-C2D	-2.46	1.45	1.50
26	4	614	CLA	CMD-C2D	-2.46	1.45	1.50
26	B	837	CLA	CMD-C2D	-2.46	1.45	1.50
26	4	603	CLA	CMD-C2D	-2.46	1.45	1.50
26	B	821	CLA	CMB-C2B	-2.46	1.45	1.50
26	9	609	CLA	CMD-C2D	-2.46	1.45	1.50
26	K	206	CLA	C1B-C2B	2.46	1.49	1.43
37	U	607	CHL	C3D-C2D	2.46	1.45	1.39
26	B	810	CLA	CMD-C2D	-2.46	1.45	1.50
26	8	616	CLA	C4B-C3B	2.46	1.49	1.43
26	Y	604	CLA	CMB-C2B	-2.46	1.45	1.50
26	7	602	CLA	CMB-C2B	-2.46	1.45	1.50
26	8	603	CLA	CMB-C2B	-2.46	1.45	1.50
37	X	607	CHL	C3D-C2D	2.46	1.45	1.39
26	7	601	CLA	C3B-C4B	2.45	1.48	1.42
26	3	607	CLA	C1B-C2B	2.45	1.49	1.43
37	X	607	CHL	C1B-C2B	2.45	1.49	1.43
26	8	607	CLA	C4B-C3B	2.45	1.49	1.43
26	K	201	CLA	C3B-C4B	2.45	1.48	1.42
26	3	604	CLA	CMC-C2C	-2.45	1.45	1.50
26	A	801	CLA	C1B-C2B	2.45	1.49	1.43
26	7	616	CLA	C4B-C3B	2.45	1.49	1.43
26	4	611	CLA	C3B-C4B	2.45	1.48	1.42
26	A	801	CLA	CMC-C2C	-2.45	1.45	1.50
26	A	807	CLA	CMD-C2D	-2.45	1.45	1.50
26	B	814	CLA	C3B-C4B	2.45	1.48	1.42
26	A	805	CLA	CMB-C2B	-2.45	1.45	1.50
26	9	604	CLA	CMD-C2D	-2.45	1.45	1.50
26	K	203	CLA	C3B-C4B	2.45	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	604	CLA	CMD-C2D	-2.45	1.45	1.50
26	H	203	CLA	C1B-C2B	2.45	1.49	1.43
26	3	610	CLA	CMB-C2B	-2.45	1.45	1.50
26	8	607	CLA	CMD-C2D	-2.45	1.45	1.50
26	2	606	CLA	C1B-C2B	2.45	1.49	1.43
26	B	805	CLA	C3B-C4B	2.45	1.48	1.42
26	B	805	CLA	CMD-C2D	-2.45	1.45	1.50
26	Z	611	CLA	CMD-C2D	-2.45	1.45	1.50
26	H	202	CLA	C3B-C4B	2.45	1.48	1.42
26	5	607	CLA	MG-NB	-2.45	2.00	2.05
37	X	605	CHL	C4B-NB	-2.45	1.34	1.37
26	3	615	CLA	C3B-C4B	2.44	1.48	1.42
37	Y	607	CHL	MG-NA	-2.44	2.00	2.06
26	9	604	CLA	CMB-C2B	-2.44	1.45	1.50
26	7	604	CLA	CMB-C2B	-2.44	1.45	1.50
37	Z	607	CHL	C1B-NB	-2.44	1.34	1.37
26	5	603	CLA	CMD-C2D	-2.44	1.45	1.50
37	U	606	CHL	C1B-NB	-2.44	1.34	1.37
26	A	827	CLA	CMD-C2D	-2.44	1.45	1.50
26	3	602	CLA	CMC-C2C	-2.44	1.45	1.50
26	4	608	CLA	C3B-C4B	2.44	1.48	1.42
26	5	604	CLA	CMD-C2D	-2.44	1.45	1.50
26	7	601	CLA	CMB-C2B	-2.44	1.45	1.50
26	A	833	CLA	C1B-NB	-2.44	1.34	1.37
37	Y	608	CHL	C3D-C2D	2.44	1.45	1.39
26	2	603	CLA	C1B-C2B	2.44	1.49	1.43
26	Z	602	CLA	C1B-C2B	2.44	1.49	1.43
26	7	613	CLA	CMC-C2C	-2.44	1.45	1.50
26	A	816	CLA	C1B-C2B	2.44	1.49	1.43
26	4	602	CLA	CMC-C2C	-2.44	1.45	1.50
26	9	606	CLA	CMD-C2D	-2.44	1.45	1.50
26	B	835	CLA	C3B-C4B	2.44	1.48	1.42
26	Z	612	CLA	C1B-C2B	2.44	1.49	1.43
37	U	605	CHL	C1B-NB	-2.44	1.34	1.37
26	A	817	CLA	C1B-C2B	2.44	1.49	1.43
26	3	603	CLA	C1B-C2B	2.44	1.49	1.43
26	3	615	CLA	CMC-C2C	-2.44	1.45	1.50
26	B	839	CLA	CMC-C2C	-2.43	1.45	1.50
26	2	606	CLA	C3B-C4B	2.43	1.48	1.42
26	A	829	CLA	CMD-C2D	-2.43	1.45	1.50
26	A	814	CLA	CMC-C2C	-2.43	1.45	1.50
26	L	304	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	823	CLA	CMD-C2D	-2.43	1.45	1.50
26	5	602	CLA	CMC-C2C	-2.43	1.45	1.50
26	B	824	CLA	CMB-C2B	-2.43	1.45	1.50
26	B	831	CLA	C1B-C2B	2.43	1.49	1.43
26	3	610	CLA	CMD-C2D	-2.43	1.45	1.50
26	a	602	CLA	C1B-C2B	2.43	1.49	1.43
26	5	604	CLA	C1B-C2B	2.43	1.49	1.43
26	2	606	CLA	CMD-C2D	-2.43	1.45	1.50
26	6	617	CLA	CMD-C2D	-2.43	1.45	1.50
26	A	821	CLA	CMC-C2C	-2.43	1.45	1.50
26	B	827	CLA	CMB-C2B	-2.43	1.45	1.50
26	6	620	CLA	CMB-C2B	-2.43	1.45	1.50
26	8	614	CLA	C1B-C2B	2.43	1.49	1.43
26	B	804	CLA	CMD-C2D	-2.43	1.45	1.50
26	B	834	CLA	C3B-C4B	2.43	1.48	1.42
26	4	602	CLA	CMB-C2B	-2.43	1.45	1.50
26	A	840	CLA	C3B-C4B	2.43	1.48	1.42
26	B	831	CLA	CMD-C2D	-2.43	1.45	1.50
26	a	609	CLA	CMD-C2D	-2.43	1.45	1.50
37	Z	601	CHL	MG-NA	-2.43	2.00	2.06
37	U	608	CHL	C3D-C2D	2.43	1.45	1.39
37	Z	601	CHL	C1B-C2B	2.43	1.49	1.43
26	A	830	CLA	MG-NB	-2.43	2.01	2.05
26	A	811	CLA	C3B-C4B	2.43	1.48	1.42
26	3	615	CLA	C1B-C2B	2.42	1.49	1.43
26	B	813	CLA	MG-NB	-2.42	2.01	2.05
26	1	606	CLA	C1B-C2B	2.42	1.49	1.43
37	Y	606	CHL	MG-NA	-2.42	2.00	2.06
37	V	601	CHL	MG-NA	-2.42	2.00	2.06
26	a	609	CLA	C3B-C4B	2.42	1.48	1.42
37	Z	608	CHL	MG-NA	-2.42	2.00	2.06
26	H	202	CLA	C1B-C2B	2.42	1.49	1.43
26	1	610	CLA	C1B-C2B	2.42	1.49	1.43
26	A	821	CLA	C1B-C2B	2.42	1.49	1.43
26	A	834	CLA	CMB-C2B	-2.42	1.45	1.50
26	B	802	CLA	CMD-C2D	-2.42	1.45	1.50
26	5	616	CLA	CMD-C2D	-2.42	1.45	1.50
26	8	609	CLA	CMD-C2D	-2.42	1.45	1.50
26	7	602	CLA	CHC-C1C	2.42	1.43	1.38
26	7	610	CLA	CMD-C2D	-2.42	1.45	1.50
26	K	203	CLA	CMB-C2B	-2.42	1.45	1.50
26	A	839	CLA	MG-NB	-2.42	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	609	CLA	CMD-C2D	-2.42	1.45	1.50
26	5	618	CLA	C1B-C2B	2.42	1.48	1.43
26	5	602	CLA	C1B-C2B	2.42	1.48	1.43
26	A	819	CLA	MG-ND	-2.42	2.01	2.05
26	A	814	CLA	CMB-C2B	-2.42	1.45	1.50
26	B	836	CLA	CMC-C2C	-2.42	1.45	1.50
26	A	841	CLA	CMD-C2D	-2.42	1.45	1.50
26	4	611	CLA	C1B-C2B	2.41	1.48	1.43
26	B	820	CLA	CMB-C2B	-2.41	1.45	1.50
26	A	820	CLA	CMB-C2B	-2.41	1.45	1.50
26	a	612	CLA	CMB-C2B	-2.41	1.45	1.50
26	A	826	CLA	CMC-C2C	-2.41	1.45	1.50
26	1	609	CLA	CMD-C2D	-2.41	1.45	1.50
37	Y	605	CHL	C1B-NB	-2.41	1.34	1.37
37	V	609	CHL	C3B-C4B	2.41	1.48	1.42
26	B	833	CLA	C3B-C4B	2.41	1.48	1.42
26	6	604	CLA	CMB-C2B	-2.41	1.45	1.50
26	A	827	CLA	CMB-C2B	-2.41	1.45	1.50
26	5	608	CLA	C3B-C4B	2.41	1.48	1.42
26	O	2001	CLA	CMC-C2C	-2.41	1.45	1.50
26	5	618	CLA	CMD-C2D	-2.41	1.45	1.50
26	8	606	CLA	CMC-C2C	-2.41	1.45	1.50
26	5	607	CLA	C3B-C4B	2.41	1.48	1.42
26	3	609	CLA	C3B-C4B	2.41	1.48	1.42
26	4	610	CLA	CMC-C2C	-2.41	1.45	1.50
37	V	606	CHL	C3B-C4B	2.41	1.48	1.42
26	B	807	CLA	MG-NB	-2.41	2.01	2.05
26	A	831	CLA	CMD-C2D	-2.41	1.45	1.50
37	V	609	CHL	C1B-NB	-2.41	1.34	1.37
26	5	619	CLA	C1B-C2B	2.41	1.48	1.43
26	7	608	CLA	C3B-C4B	2.41	1.48	1.42
37	X	609	CHL	C3B-C4B	2.41	1.48	1.42
26	F	303	CLA	CMD-C2D	-2.41	1.45	1.50
26	1	604	CLA	CMB-C2B	-2.41	1.45	1.50
37	Z	608	CHL	C4B-NB	-2.41	1.34	1.37
26	2	610	CLA	CMC-C2C	-2.41	1.45	1.50
26	7	607	CLA	CMD-C2D	-2.41	1.45	1.50
26	4	604	CLA	C4B-C3B	2.41	1.48	1.43
26	B	817	CLA	CMC-C2C	-2.41	1.45	1.50
26	4	607	CLA	CMB-C2B	-2.41	1.45	1.50
26	8	611	CLA	C1B-C2B	2.40	1.48	1.43
37	X	601	CHL	C1B-NB	-2.40	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	V	607	CHL	C1B-C2B	2.40	1.48	1.43
26	B	836	CLA	CMB-C2B	-2.40	1.45	1.50
26	2	616	CLA	C4B-C3B	2.40	1.48	1.43
26	4	613	CLA	C1B-C2B	2.40	1.48	1.43
26	A	817	CLA	CMC-C2C	-2.40	1.45	1.50
26	L	307	CLA	CMD-C2D	-2.40	1.45	1.50
26	7	613	CLA	CMB-C2B	-2.40	1.45	1.50
26	7	607	CLA	C1B-C2B	2.40	1.48	1.43
26	9	606	CLA	C1B-C2B	2.40	1.48	1.43
26	4	609	CLA	CMD-C2D	-2.40	1.45	1.50
26	A	842	CLA	MG-NB	-2.40	2.01	2.05
37	Z	606	CHL	C1B-NB	-2.40	1.34	1.37
26	3	603	CLA	MG-NB	-2.40	2.01	2.05
26	B	818	CLA	CMC-C2C	-2.40	1.45	1.50
26	1	606	CLA	CMB-C2B	-2.40	1.45	1.50
26	3	608	CLA	C3B-C4B	2.40	1.48	1.42
26	A	812	CLA	CMD-C2D	-2.40	1.45	1.50
26	A	815	CLA	CMB-C2B	-2.40	1.45	1.50
26	5	619	CLA	CMD-C2D	-2.40	1.45	1.50
26	6	617	CLA	CMB-C2B	-2.40	1.45	1.50
37	Y	605	CHL	C4C-C3C	2.40	1.49	1.45
26	H	203	CLA	CMD-C2D	-2.40	1.45	1.50
26	4	610	CLA	CMD-C2D	-2.40	1.45	1.50
26	V	613	CLA	CMD-C2D	-2.40	1.45	1.50
37	U	609	CHL	C1B-NB	-2.40	1.34	1.37
37	W	606	CHL	C3D-C2D	2.40	1.45	1.39
26	8	603	CLA	C1B-C2B	2.39	1.48	1.43
26	a	607	CLA	CMD-C2D	-2.39	1.45	1.50
26	4	616	CLA	C4B-C3B	2.39	1.48	1.43
37	Z	606	CHL	MG-NA	-2.39	2.00	2.06
26	A	828	CLA	C3B-C4B	2.39	1.48	1.42
37	W	601	CHL	C4B-NB	-2.39	1.34	1.37
26	B	802	CLA	CMC-C2C	-2.39	1.45	1.50
26	B	837	CLA	CMC-C2C	-2.39	1.45	1.50
26	K	204	CLA	C1B-C2B	2.39	1.48	1.43
26	A	843	CLA	MG-NB	-2.39	2.01	2.05
26	A	839	CLA	CMD-C2D	-2.39	1.45	1.50
26	B	810	CLA	CMC-C2C	-2.39	1.45	1.50
26	3	611	CLA	C4B-C3B	2.39	1.48	1.43
26	3	617	CLA	CMB-C2B	-2.39	1.45	1.50
26	8	610	CLA	CMC-C2C	-2.39	1.45	1.50
26	8	612	CLA	C3B-C4B	2.39	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	603	CLA	C4B-C3B	2.39	1.48	1.43
26	6	616	CLA	CMB-C2B	-2.39	1.45	1.50
26	B	819	CLA	CMD-C2D	-2.39	1.45	1.50
26	1	607	CLA	CMD-C2D	-2.39	1.45	1.50
26	4	601	CLA	C3B-C4B	2.39	1.48	1.42
37	X	601	CHL	MG-NA	-2.39	2.00	2.06
26	A	822	CLA	CMB-C2B	-2.39	1.45	1.50
26	8	606	CLA	C1B-C2B	2.39	1.48	1.43
26	A	827	CLA	C3B-C4B	2.39	1.48	1.42
26	9	613	CLA	C3B-C4B	2.39	1.48	1.42
26	a	604	CLA	CMB-C2B	-2.39	1.45	1.50
26	6	620	CLA	CMD-C2D	-2.39	1.45	1.50
26	B	838	CLA	CMC-C2C	-2.39	1.45	1.50
26	6	620	CLA	C1B-C2B	2.39	1.48	1.43
26	7	616	CLA	CMC-C2C	-2.39	1.45	1.50
26	a	603	CLA	CMD-C2D	-2.38	1.45	1.50
26	5	616	CLA	CMB-C2B	-2.38	1.45	1.50
26	Y	604	CLA	C1B-C2B	2.38	1.48	1.43
26	B	806	CLA	CMB-C2B	-2.38	1.45	1.50
26	1	602	CLA	C1B-C2B	2.38	1.48	1.43
26	A	839	CLA	C3B-C4B	2.38	1.48	1.42
29	K	202	BCR	C17-C18	-2.38	1.32	1.35
26	A	826	CLA	MG-NB	-2.38	2.01	2.05
26	1	614	CLA	C1B-C2B	2.38	1.48	1.43
34	7	619	LUT	C1-C6	-2.38	1.50	1.53
26	a	606	CLA	C1B-C2B	2.38	1.48	1.43
26	B	809	CLA	CMD-C2D	-2.38	1.45	1.50
26	K	203	CLA	C1B-C2B	2.38	1.48	1.43
26	2	610	CLA	CMB-C2B	-2.38	1.45	1.50
26	5	613	CLA	C1B-C2B	2.38	1.48	1.43
26	A	837	CLA	CMD-C2D	-2.38	1.45	1.50
26	8	609	CLA	CMB-C2B	-2.38	1.45	1.50
37	U	608	CHL	C3B-C4B	2.38	1.48	1.42
26	B	839	CLA	MG-NB	-2.38	2.01	2.05
26	A	812	CLA	C3B-C4B	2.38	1.48	1.42
37	Z	607	CHL	C3D-C2D	2.38	1.45	1.39
37	V	609	CHL	C4B-NB	-2.38	1.34	1.37
26	B	805	CLA	CMC-C2C	-2.38	1.45	1.50
26	8	607	CLA	C1B-C2B	2.38	1.48	1.43
26	5	609	CLA	CMD-C2D	-2.38	1.45	1.50
26	5	619	CLA	CMB-C2B	-2.38	1.45	1.50
26	4	601	CLA	CMD-C2D	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	608	CLA	CMB-C2B	-2.37	1.45	1.50
26	A	835	CLA	C3B-C4B	2.37	1.48	1.42
26	1	614	CLA	C4B-C3B	2.37	1.48	1.43
26	F	304	CLA	C1B-C2B	2.37	1.48	1.43
26	F	304	CLA	CMC-C2C	-2.37	1.45	1.50
26	1	612	CLA	CMB-C2B	-2.37	1.45	1.50
26	B	805	CLA	C1B-NB	-2.37	1.34	1.37
26	6	604	CLA	C3B-C4B	2.37	1.48	1.42
26	1	608	CLA	CMD-C2D	-2.37	1.45	1.50
26	B	802	CLA	C1B-C2B	2.37	1.48	1.43
37	W	601	CHL	C1B-C2B	2.37	1.48	1.43
29	9	621	BCR	C21-C22	-2.37	1.32	1.35
26	5	619	CLA	C4B-C3B	2.37	1.48	1.43
26	A	832	CLA	C3B-C4B	2.37	1.48	1.42
26	a	606	CLA	CMB-C2B	-2.37	1.45	1.50
26	9	609	CLA	CMB-C2B	-2.37	1.45	1.50
26	a	614	CLA	C1B-C2B	2.37	1.48	1.43
26	a	601	CLA	CMC-C2C	-2.37	1.45	1.50
26	9	613	CLA	CMD-C2D	-2.37	1.45	1.50
37	V	607	CHL	C4B-NB	-2.37	1.34	1.37
26	B	819	CLA	CMC-C2C	-2.37	1.45	1.50
26	F	304	CLA	CMB-C2B	-2.37	1.45	1.50
26	K	204	CLA	CMB-C2B	-2.37	1.45	1.50
26	6	620	CLA	CMC-C2C	-2.37	1.45	1.50
26	5	606	CLA	CMB-C2B	-2.37	1.45	1.50
26	9	603	CLA	C1B-C2B	2.37	1.48	1.43
26	B	818	CLA	MG-NB	-2.37	2.01	2.05
26	A	821	CLA	CMB-C2B	-2.37	1.45	1.50
26	B	823	CLA	CMB-C2B	-2.37	1.45	1.50
26	a	608	CLA	CMD-C2D	-2.37	1.45	1.50
37	Z	609	CHL	C3B-C4B	2.37	1.48	1.42
26	1	603	CLA	CMD-C2D	-2.37	1.45	1.50
26	4	612	CLA	CMD-C2D	-2.37	1.45	1.50
26	B	825	CLA	C1B-C2B	2.36	1.48	1.43
26	A	828	CLA	CMB-C2B	-2.36	1.45	1.50
26	7	615	CLA	CMB-C2B	-2.36	1.45	1.50
37	V	605	CHL	C1B-NB	-2.36	1.34	1.37
26	4	616	CLA	CMD-C2D	-2.36	1.45	1.50
26	B	802	CLA	CMB-C2B	-2.36	1.45	1.50
37	V	606	CHL	C3D-C2D	2.36	1.45	1.39
26	Z	604	CLA	CMB-C2B	-2.36	1.45	1.50
26	B	808	CLA	CMD-C2D	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	9	607	CLA	C1B-C2B	2.36	1.48	1.43
26	a	602	CLA	CMB-C2B	-2.36	1.45	1.50
26	7	606	CLA	CMD-C2D	-2.36	1.45	1.50
26	a	610	CLA	C1B-C2B	2.36	1.48	1.43
37	Y	601	CHL	C1B-C2B	2.36	1.48	1.43
37	W	609	CHL	C4B-NB	-2.36	1.34	1.37
26	3	617	CLA	C1B-C2B	2.36	1.48	1.43
26	5	601	CLA	CMD-C2D	-2.36	1.45	1.50
26	3	606	CLA	MG-NB	-2.36	2.01	2.05
37	X	609	CHL	MG-NA	-2.36	2.00	2.06
37	Y	607	CHL	C1D-C2D	2.36	1.50	1.45
26	2	611	CLA	CMD-C2D	-2.36	1.45	1.50
26	W	604	CLA	CMB-C2B	-2.36	1.45	1.50
26	8	608	CLA	MG-NB	-2.36	2.01	2.05
26	2	603	CLA	CMB-C2B	-2.36	1.45	1.50
26	A	806	CLA	C1B-NB	-2.36	1.34	1.37
37	X	607	CHL	C1B-NB	-2.36	1.34	1.37
37	V	607	CHL	C1D-C2D	2.36	1.50	1.45
26	3	607	CLA	C4B-C3B	2.36	1.48	1.43
26	B	806	CLA	C1B-C2B	2.35	1.48	1.43
26	1	602	CLA	CMB-C2B	-2.35	1.45	1.50
26	A	828	CLA	C4B-NB	2.35	1.40	1.37
29	B	846	BCR	C30-C25	-2.35	1.50	1.53
35	8	620	XAT	C22-C21	-2.35	1.50	1.54
37	Z	608	CHL	C3D-C2D	2.35	1.45	1.39
26	H	203	CLA	CMB-C2B	-2.35	1.45	1.50
26	A	823	CLA	CMD-C2D	-2.35	1.45	1.50
37	X	605	CHL	C4C-C3C	2.35	1.49	1.45
26	1	604	CLA	CMD-C2D	-2.35	1.45	1.50
26	Z	611	CLA	CMB-C2B	-2.35	1.45	1.50
26	9	609	CLA	C3B-C4B	2.35	1.48	1.42
26	8	612	CLA	CMC-C2C	-2.35	1.45	1.50
26	K	203	CLA	MG-NB	-2.35	2.01	2.05
26	A	829	CLA	CMB-C2B	-2.35	1.45	1.50
26	B	829	CLA	C1B-NB	-2.35	1.34	1.37
37	U	608	CHL	C1B-C2B	2.35	1.48	1.43
26	A	810	CLA	CMC-C2C	-2.35	1.45	1.50
26	a	606	CLA	CMC-C2C	-2.35	1.45	1.50
26	a	616	CLA	CMD-C2D	-2.35	1.45	1.50
26	B	836	CLA	MG-NB	-2.35	2.01	2.05
26	A	825	CLA	CMC-C2C	-2.35	1.45	1.50
26	a	604	CLA	CMD-C2D	-2.35	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	608	CHL	C1B-NB	-2.35	1.34	1.37
37	W	608	CHL	C1B-NB	-2.35	1.34	1.37
26	B	812	CLA	CMC-C2C	-2.35	1.45	1.50
26	B	835	CLA	C1B-C2B	2.35	1.48	1.43
37	Z	605	CHL	MG-NA	-2.35	2.00	2.06
26	A	841	CLA	CMB-C2B	-2.35	1.45	1.50
26	8	614	CLA	CMB-C2B	-2.35	1.45	1.50
26	A	830	CLA	CMB-C2B	-2.35	1.45	1.50
26	6	607	CLA	C1B-C2B	2.35	1.48	1.43
26	5	606	CLA	C1B-C2B	2.35	1.48	1.43
37	U	607	CHL	C1B-NB	-2.35	1.34	1.37
26	B	814	CLA	CMB-C2B	-2.34	1.45	1.50
26	7	612	CLA	CMC-C2C	-2.34	1.45	1.50
26	a	609	CLA	CMB-C2B	-2.34	1.45	1.50
26	B	832	CLA	CMC-C2C	-2.34	1.45	1.50
37	X	606	CHL	C1B-C2B	2.34	1.48	1.43
37	W	606	CHL	C4C-C3C	2.34	1.49	1.45
26	B	804	CLA	CMB-C2B	-2.34	1.45	1.50
26	A	837	CLA	CMC-C2C	-2.34	1.45	1.50
26	7	608	CLA	C1B-C2B	2.34	1.48	1.43
29	B	847	BCR	C30-C25	-2.34	1.50	1.53
26	B	840	CLA	MG-NB	-2.34	2.01	2.05
37	W	605	CHL	C4C-C3C	2.34	1.49	1.45
26	X	602	CLA	C1B-C2B	2.34	1.48	1.43
26	B	822	CLA	CMD-C2D	-2.34	1.45	1.50
26	2	607	CLA	CMB-C2B	-2.34	1.45	1.50
37	U	601	CHL	C4C-C3C	2.34	1.49	1.45
37	V	601	CHL	C1B-C2B	2.34	1.48	1.43
37	W	609	CHL	C4C-C3C	2.34	1.49	1.45
26	B	812	CLA	C1B-C2B	2.34	1.48	1.43
26	B	834	CLA	C1B-C2B	2.34	1.48	1.43
26	1	601	CLA	CMC-C2C	-2.34	1.45	1.50
26	1	611	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	B	833	CLA	C1B-C2B	2.34	1.48	1.43
26	A	840	CLA	CMB-C2B	-2.33	1.45	1.50
26	3	617	CLA	CMD-C2D	-2.33	1.45	1.50
26	A	845	CLA	CMC-C2C	-2.33	1.45	1.50
26	2	614	CLA	CMB-C2B	-2.33	1.45	1.50
26	B	817	CLA	C3B-C4B	2.33	1.48	1.42
26	7	603	CLA	C3B-C4B	2.33	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	615	CLA	CMB-C2B	-2.33	1.45	1.50
26	6	604	CLA	C1B-C2B	2.33	1.48	1.43
26	A	830	CLA	C3B-C4B	2.33	1.48	1.42
26	9	609	CLA	CMC-C2C	-2.33	1.45	1.50
26	B	839	CLA	C4B-NB	2.33	1.40	1.37
37	U	607	CHL	C4B-NB	-2.33	1.34	1.37
26	A	841	CLA	C1B-C2B	2.33	1.48	1.43
26	2	604	CLA	CMC-C2C	-2.33	1.45	1.50
26	B	825	CLA	CMC-C2C	-2.33	1.45	1.50
26	1	606	CLA	CMC-C2C	-2.33	1.45	1.50
26	6	613	CLA	CMC-C2C	-2.33	1.45	1.50
26	B	811	CLA	C1B-C2B	2.33	1.48	1.43
26	B	823	CLA	C3B-C4B	2.33	1.48	1.42
37	W	608	CHL	C4B-NB	-2.33	1.34	1.37
26	6	618	CLA	C4B-C3B	2.33	1.48	1.43
26	A	826	CLA	MG-ND	-2.33	2.01	2.05
26	A	809	CLA	C1B-NB	-2.33	1.34	1.37
37	W	607	CHL	C4B-NB	-2.33	1.34	1.37
26	B	804	CLA	C1B-C2B	2.33	1.48	1.43
26	A	835	CLA	CMC-C2C	-2.33	1.45	1.50
26	9	607	CLA	C3B-C4B	2.33	1.48	1.42
26	A	840	CLA	MG-NB	-2.33	2.01	2.05
26	7	614	CLA	C1B-C2B	2.33	1.48	1.43
26	B	802	CLA	C3B-C4B	2.33	1.48	1.42
26	4	603	CLA	CMC-C2C	-2.33	1.45	1.50
26	7	611	CLA	CMB-C2B	-2.33	1.45	1.50
26	9	602	CLA	C1B-C2B	2.33	1.48	1.43
26	A	841	CLA	MG-NB	-2.33	2.01	2.05
26	1	609	CLA	CMB-C2B	-2.33	1.45	1.50
27	A	844	PQN	C10-C1	2.33	1.52	1.48
26	7	606	CLA	MG-NB	-2.32	2.01	2.05
26	K	204	CLA	MG-NB	-2.32	2.01	2.05
26	3	612	CLA	CMD-C2D	-2.32	1.45	1.50
26	B	814	CLA	C1B-C2B	2.32	1.48	1.43
26	B	810	CLA	C1B-NB	-2.32	1.34	1.37
26	a	609	CLA	CMC-C2C	-2.32	1.45	1.50
26	6	617	CLA	C1B-C2B	2.32	1.48	1.43
26	6	602	CLA	CMD-C2D	-2.32	1.45	1.50
26	G	203	CLA	CMD-C2D	-2.32	1.45	1.50
26	A	804	CLA	CMC-C2C	-2.32	1.45	1.50
37	Z	601	CHL	C1B-NB	-2.32	1.34	1.37
26	7	611	CLA	C1B-C2B	2.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	809	CLA	C3B-C4B	2.32	1.48	1.42
26	8	603	CLA	C4B-C3B	2.32	1.48	1.43
26	6	616	CLA	C1B-C2B	2.32	1.48	1.43
26	7	603	CLA	C1B-C2B	2.32	1.48	1.43
37	U	606	CHL	C1B-C2B	2.32	1.48	1.43
26	a	614	CLA	CMB-C2B	-2.32	1.45	1.50
26	B	832	CLA	C1B-C2B	2.32	1.48	1.43
26	L	304	CLA	C3B-C4B	2.32	1.48	1.42
26	V	614	CLA	C1B-C2B	2.32	1.48	1.43
37	X	606	CHL	C1B-NB	-2.32	1.34	1.37
26	B	804	CLA	CMC-C2C	-2.32	1.45	1.50
26	8	602	CLA	CMB-C2B	-2.32	1.45	1.50
26	7	606	CLA	CMB-C2B	-2.32	1.45	1.50
26	B	807	CLA	C3B-C4B	2.32	1.48	1.42
26	A	840	CLA	CMC-C2C	-2.32	1.45	1.50
26	B	840	CLA	C3B-C4B	2.31	1.48	1.42
37	V	608	CHL	C3D-C2D	2.31	1.45	1.39
26	1	616	CLA	C1B-C2B	2.31	1.48	1.43
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	V	604	CLA	C1B-C2B	2.31	1.48	1.43
26	A	813	CLA	MG-NB	-2.31	2.01	2.05
29	B	847	BCR	C1-C6	-2.31	1.50	1.53
26	A	826	CLA	C1B-NB	-2.31	1.34	1.37
37	Z	609	CHL	C4C-C3C	2.31	1.49	1.45
26	B	827	CLA	CMC-C2C	-2.31	1.45	1.50
26	1	613	CLA	CMC-C2C	-2.31	1.45	1.50
26	A	820	CLA	CMC-C2C	-2.31	1.45	1.50
26	B	815	CLA	CMC-C2C	-2.31	1.45	1.50
26	5	602	CLA	CMD-C2D	-2.31	1.45	1.50
26	2	614	CLA	C1B-C2B	2.31	1.48	1.43
26	5	602	CLA	CMB-C2B	-2.31	1.45	1.50
26	B	802	CLA	MG-NB	-2.31	2.01	2.05
26	A	809	CLA	C3B-C4B	2.31	1.48	1.42
26	G	204	CLA	CMD-C2D	-2.31	1.45	1.50
26	A	808	CLA	C1B-C2B	2.31	1.48	1.43
26	8	611	CLA	C3B-C4B	2.31	1.48	1.42
26	A	824	CLA	CMD-C2D	-2.31	1.45	1.50
26	L	302	CLA	CMC-C2C	-2.31	1.45	1.50
26	O	2003	CLA	CMD-C2D	-2.31	1.45	1.50
26	6	610	CLA	CMC-C2C	-2.31	1.45	1.50
26	B	831	CLA	CMC-C2C	-2.31	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	604	CLA	CMC-C2C	-2.31	1.45	1.50
26	6	602	CLA	C1B-C2B	2.31	1.48	1.43
26	A	833	CLA	CMC-C2C	-2.31	1.45	1.50
26	1	616	CLA	CMD-C2D	-2.30	1.45	1.50
37	V	608	CHL	C1B-C2B	2.30	1.48	1.43
26	5	606	CLA	CMC-C2C	-2.30	1.45	1.50
37	V	608	CHL	C1B-NB	-2.30	1.35	1.37
26	B	828	CLA	MG-NB	-2.30	2.01	2.05
26	A	812	CLA	CMC-C2C	-2.30	1.45	1.50
26	3	608	CLA	CMC-C2C	-2.30	1.45	1.50
26	7	611	CLA	C3B-C4B	2.30	1.48	1.42
26	B	806	CLA	C4B-NB	2.30	1.40	1.37
26	Y	610	CLA	C1B-C2B	2.30	1.48	1.43
26	B	817	CLA	MG-NB	-2.30	2.01	2.05
26	3	606	CLA	C1B-C2B	2.30	1.48	1.43
26	6	607	CLA	CMB-C2B	-2.30	1.45	1.50
26	2	613	CLA	C3B-C4B	2.30	1.48	1.42
26	8	604	CLA	C1B-C2B	2.30	1.48	1.43
26	5	614	CLA	CMD-C2D	-2.30	1.45	1.50
26	9	606	CLA	CMB-C2B	-2.30	1.45	1.50
26	Z	603	CLA	CMD-C2D	-2.30	1.45	1.50
26	9	610	CLA	CMC-C2C	-2.30	1.45	1.50
26	A	835	CLA	MG-NB	-2.30	2.01	2.05
37	U	607	CHL	C1B-C2B	2.30	1.48	1.43
26	A	841	CLA	C3B-C4B	2.30	1.48	1.42
26	7	613	CLA	C3B-C4B	2.30	1.48	1.42
26	A	807	CLA	C1B-NB	-2.30	1.35	1.37
26	5	609	CLA	CMC-C2C	-2.30	1.45	1.50
26	6	612	CLA	CMC-C2C	-2.30	1.45	1.50
26	a	604	CLA	C1B-C2B	2.30	1.48	1.43
26	a	616	CLA	C1B-C2B	2.30	1.48	1.43
26	4	607	CLA	C1B-C2B	2.30	1.48	1.43
26	A	803	CLA	C3B-C4B	2.30	1.48	1.42
26	A	825	CLA	MG-NB	-2.30	2.01	2.05
26	Z	611	CLA	C1B-C2B	2.30	1.48	1.43
26	B	838	CLA	C1B-C2B	2.29	1.48	1.43
26	3	612	CLA	C1B-C2B	2.29	1.48	1.43
26	B	826	CLA	MG-NB	-2.29	2.01	2.05
26	7	603	CLA	CMC-C2C	-2.29	1.45	1.50
26	L	306	CLA	C1B-C2B	2.29	1.48	1.43
26	B	822	CLA	CMB-C2B	-2.29	1.45	1.50
26	2	607	CLA	CMD-C2D	-2.29	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	601	CLA	CMB-C2B	-2.29	1.45	1.50
26	7	603	CLA	MG-NB	-2.29	2.01	2.05
26	3	606	CLA	CMC-C2C	-2.29	1.45	1.50
26	3	615	CLA	CMD-C2D	-2.29	1.45	1.50
26	2	601	CLA	CMD-C2D	-2.29	1.45	1.50
26	B	830	CLA	C1B-C2B	2.29	1.48	1.43
26	W	604	CLA	C1B-C2B	2.29	1.48	1.43
26	2	607	CLA	MG-NB	-2.29	2.01	2.05
26	B	828	CLA	C3B-C4B	2.29	1.48	1.42
26	A	829	CLA	MG-NB	-2.29	2.01	2.05
26	1	614	CLA	CMB-C2B	-2.29	1.45	1.50
26	3	603	CLA	CMB-C2B	-2.29	1.45	1.50
37	Y	608	CHL	C1B-C2B	2.29	1.48	1.43
26	3	607	CLA	CMD-C2D	-2.29	1.45	1.50
26	3	607	CLA	CMB-C2B	-2.29	1.45	1.50
27	A	844	PQN	C5-C4	2.29	1.52	1.48
26	L	306	CLA	CMD-C2D	-2.29	1.46	1.50
26	6	601	CLA	C1B-C2B	2.29	1.48	1.43
26	B	816	CLA	MG-NB	-2.29	2.01	2.05
26	B	833	CLA	CMB-C2B	-2.29	1.46	1.50
37	W	606	CHL	C1B-C2B	2.29	1.48	1.43
26	4	616	CLA	CMC-C2C	-2.29	1.46	1.50
37	W	605	CHL	MG-NA	-2.29	2.00	2.06
26	9	613	CLA	CMC-C2C	-2.29	1.46	1.50
26	9	606	CLA	CMC-C2C	-2.28	1.46	1.50
26	B	831	CLA	CMB-C2B	-2.28	1.46	1.50
26	9	607	CLA	CMB-C2B	-2.28	1.46	1.50
29	A	848	BCR	C30-C25	-2.28	1.50	1.53
26	A	802	CLA	CMB-C2B	-2.28	1.46	1.50
26	2	606	CLA	CMC-C2C	-2.28	1.46	1.50
26	2	613	CLA	CMB-C2B	-2.28	1.46	1.50
37	Y	608	CHL	C2C-C1C	2.28	1.49	1.44
26	7	614	CLA	MG-NB	-2.28	2.01	2.05
26	A	823	CLA	CMB-C2B	-2.28	1.46	1.50
26	X	610	CLA	CHC-C1C	2.28	1.43	1.38
26	B	841	CLA	C1B-C2B	2.28	1.48	1.43
26	F	301	CLA	CMC-C2C	-2.28	1.46	1.50
26	B	806	CLA	C3B-C4B	2.28	1.48	1.42
26	A	814	CLA	CMD-C2D	-2.28	1.46	1.50
26	B	815	CLA	C3B-C4B	2.28	1.48	1.42
26	G	204	CLA	C1B-C2B	2.28	1.48	1.43
26	8	609	CLA	C1B-C2B	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L	304	CLA	CMC-C2C	-2.28	1.46	1.50
26	5	604	CLA	CMC-C2C	-2.28	1.46	1.50
26	5	607	CLA	CMC-C2C	-2.28	1.46	1.50
26	6	604	CLA	CMD-C2D	-2.28	1.46	1.50
37	U	601	CHL	C4B-NB	-2.28	1.35	1.37
26	V	610	CLA	C1B-C2B	2.28	1.48	1.43
26	Z	602	CLA	CMC-C2C	-2.28	1.46	1.50
26	4	606	CLA	CMB-C2B	-2.28	1.46	1.50
26	9	604	CLA	CMC-C2C	-2.28	1.46	1.50
26	A	838	CLA	MG-NB	-2.28	2.01	2.05
26	A	814	CLA	C1B-NB	-2.28	1.35	1.37
26	O	2001	CLA	CMB-C2B	-2.27	1.46	1.50
26	6	609	CLA	CMD-C2D	-2.27	1.46	1.50
26	4	601	CLA	C1B-C2B	2.27	1.48	1.43
26	5	608	CLA	CMB-C2B	-2.27	1.46	1.50
26	L	302	CLA	MG-NB	-2.27	2.01	2.05
37	X	609	CHL	C1B-C2B	2.27	1.48	1.43
26	A	804	CLA	MG-NB	-2.27	2.01	2.05
26	3	606	CLA	CMD-C2D	-2.27	1.46	1.50
26	B	803	CLA	C1B-C2B	2.27	1.48	1.43
26	9	602	CLA	CMB-C2B	-2.27	1.46	1.50
26	B	816	CLA	CMD-C2D	-2.27	1.46	1.50
26	F	303	CLA	C1B-C2B	2.27	1.48	1.43
26	H	202	CLA	CMD-C2D	-2.27	1.46	1.50
26	A	854	CLA	CMD-C2D	-2.27	1.46	1.50
26	O	2002	CLA	CMC-C2C	-2.27	1.46	1.50
26	a	607	CLA	CMB-C2B	-2.27	1.46	1.50
26	A	815	CLA	MG-NB	-2.27	2.01	2.05
26	B	820	CLA	CMC-C2C	-2.27	1.46	1.50
26	6	613	CLA	CMD-C2D	-2.27	1.46	1.50
26	A	840	CLA	C1B-C2B	2.27	1.48	1.43
26	4	603	CLA	C4B-C3B	2.27	1.48	1.43
26	B	803	CLA	CMB-C2B	-2.27	1.46	1.50
26	8	606	CLA	CMB-C2B	-2.27	1.46	1.50
26	B	830	CLA	CMD-C2D	-2.26	1.46	1.50
26	K	206	CLA	CMC-C2C	-2.26	1.46	1.50
26	a	614	CLA	MG-NB	-2.26	2.01	2.05
26	a	611	CLA	C1B-C2B	2.26	1.48	1.43
26	1	602	CLA	MG-NB	-2.26	2.01	2.05
26	9	603	CLA	CMC-C2C	-2.26	1.46	1.50
26	3	602	CLA	CMD-C2D	-2.26	1.46	1.50
26	5	606	CLA	CMD-C2D	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	616	CLA	C4B-C3B	2.26	1.48	1.43
26	A	803	CLA	MG-NB	-2.26	2.01	2.05
37	Y	609	CHL	MG-NA	-2.26	2.00	2.06
26	A	808	CLA	CMB-C2B	-2.26	1.46	1.50
26	a	613	CLA	C1B-C2B	2.26	1.48	1.43
26	a	613	CLA	CMC-C2C	-2.26	1.46	1.50
26	4	606	CLA	CMD-C2D	-2.26	1.46	1.50
26	A	837	CLA	MG-NB	-2.26	2.01	2.05
26	B	824	CLA	MG-ND	-2.26	2.01	2.05
26	A	818	CLA	CMC-C2C	-2.26	1.46	1.50
26	A	824	CLA	C1B-C2B	2.26	1.48	1.43
26	A	827	CLA	C1B-C2B	2.26	1.48	1.43
26	A	838	CLA	C1B-C2B	2.26	1.48	1.43
37	V	608	CHL	MG-NA	-2.26	2.00	2.06
26	A	802	CLA	MG-ND	-2.26	2.01	2.05
26	A	837	CLA	C1B-C2B	2.26	1.48	1.43
26	K	201	CLA	CMD-C2D	-2.26	1.46	1.50
26	1	604	CLA	C1B-C2B	2.26	1.48	1.43
29	A	851	BCR	C21-C22	-2.26	1.32	1.35
37	W	606	CHL	C3B-C4B	2.26	1.48	1.42
26	A	814	CLA	C1B-C2B	2.26	1.48	1.43
26	5	608	CLA	CMC-C2C	-2.25	1.46	1.50
26	5	614	CLA	CMB-C2B	-2.25	1.46	1.50
26	B	823	CLA	MG-NB	-2.25	2.01	2.05
26	2	610	CLA	CHC-C1C	2.25	1.43	1.38
37	Z	606	CHL	C2C-C1C	2.25	1.49	1.44
26	a	602	CLA	MG-NB	-2.25	2.01	2.05
26	5	603	CLA	C4B-C3B	2.25	1.48	1.43
26	O	2003	CLA	CMB-C2B	-2.25	1.46	1.50
26	3	614	CLA	CMB-C2B	-2.25	1.46	1.50
26	B	817	CLA	MG-ND	-2.25	2.01	2.05
26	O	2002	CLA	C1B-C2B	2.25	1.48	1.43
37	X	601	CHL	C4B-NB	-2.25	1.35	1.37
26	U	613	CLA	CMC-C2C	-2.25	1.46	1.50
26	B	806	CLA	MG-NB	-2.25	2.01	2.05
26	7	614	CLA	CMC-C2C	-2.25	1.46	1.50
26	3	614	CLA	C1B-C2B	2.25	1.48	1.43
26	7	606	CLA	C1B-C2B	2.25	1.48	1.43
26	2	601	CLA	CMC-C2C	-2.25	1.46	1.50
26	B	821	CLA	C1B-C2B	2.25	1.48	1.43
26	B	838	CLA	MG-NB	-2.25	2.01	2.05
26	A	810	CLA	CMB-C2B	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	604	CLA	CMD-C2D	-2.25	1.46	1.50
26	Z	602	CLA	CHC-C1C	2.25	1.43	1.38
26	A	834	CLA	C1B-C2B	2.25	1.48	1.43
37	Z	608	CHL	C1B-NB	-2.25	1.35	1.37
26	a	601	CLA	C1B-C2B	2.25	1.48	1.43
26	1	609	CLA	CMC-C2C	-2.25	1.46	1.50
26	4	607	CLA	CMD-C2D	-2.25	1.46	1.50
37	X	608	CHL	C1B-C2B	2.25	1.48	1.43
26	A	819	CLA	C4B-NB	2.24	1.40	1.37
26	4	608	CLA	CMB-C2B	-2.24	1.46	1.50
26	5	613	CLA	CMB-C2B	-2.24	1.46	1.50
26	1	601	CLA	C1B-C2B	2.24	1.48	1.43
26	6	603	CLA	CMC-C2C	-2.24	1.46	1.50
26	8	611	CLA	CMC-C2C	-2.24	1.46	1.50
37	V	606	CHL	C2C-C1C	2.24	1.49	1.44
37	X	607	CHL	MG-NA	-2.24	2.00	2.06
26	B	808	CLA	C1B-C2B	2.24	1.48	1.43
37	W	607	CHL	C4C-C3C	2.24	1.48	1.44
26	A	832	CLA	C1B-NB	-2.24	1.35	1.37
26	7	601	CLA	CMC-C2C	-2.24	1.46	1.50
26	8	604	CLA	CMC-C2C	-2.24	1.46	1.50
26	9	604	CLA	C1B-C2B	2.24	1.48	1.43
26	6	608	CLA	C1B-C2B	2.24	1.48	1.43
26	B	838	CLA	CMB-C2B	-2.24	1.46	1.50
26	3	611	CLA	CMD-C2D	-2.24	1.46	1.50
26	A	812	CLA	C1B-C2B	2.24	1.48	1.43
26	1	614	CLA	CMD-C2D	-2.24	1.46	1.50
26	9	601	CLA	CMD-C2D	-2.24	1.46	1.50
26	A	807	CLA	MG-NB	-2.24	2.01	2.05
26	8	602	CLA	C1B-C2B	2.24	1.48	1.43
37	W	606	CHL	C4B-NB	-2.24	1.35	1.37
26	7	615	CLA	C1B-C2B	2.24	1.48	1.43
26	2	602	CLA	CMD-C2D	-2.24	1.46	1.50
26	3	610	CLA	CHC-C1C	2.24	1.43	1.38
26	8	610	CLA	C1B-C2B	2.24	1.48	1.43
37	Z	606	CHL	C4C-C3C	2.24	1.48	1.45
37	X	609	CHL	C4B-NB	-2.24	1.35	1.37
26	F	303	CLA	CMC-C2C	-2.24	1.46	1.50
26	1	613	CLA	C1B-C2B	2.24	1.48	1.43
26	7	608	CLA	MG-NB	-2.24	2.01	2.05
26	A	825	CLA	C3B-C4B	2.24	1.48	1.42
26	H	203	CLA	CMC-C2C	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	606	CLA	CMD-C2D	-2.24	1.46	1.50
37	Y	601	CHL	C2C-C1C	2.23	1.49	1.44
37	V	606	CHL	C1D-C2D	2.23	1.49	1.45
26	5	609	CLA	C3B-C4B	2.23	1.48	1.42
26	8	614	CLA	CMC-C2C	-2.23	1.46	1.50
37	W	608	CHL	MG-NA	-2.23	2.01	2.06
26	1	610	CLA	CMC-C2C	-2.23	1.46	1.50
26	Y	610	CLA	CMB-C2B	-2.23	1.46	1.50
26	A	824	CLA	C3B-C4B	2.23	1.48	1.42
26	B	810	CLA	MG-NB	-2.23	2.01	2.05
26	B	823	CLA	C1B-C2B	2.23	1.48	1.43
26	B	841	CLA	CMD-C2D	-2.23	1.46	1.50
26	a	611	CLA	CMD-C2D	-2.23	1.46	1.50
26	a	614	CLA	CMD-C2D	-2.23	1.46	1.50
26	B	809	CLA	MG-NB	-2.23	2.01	2.05
26	A	811	CLA	C1B-C2B	2.23	1.48	1.43
26	8	613	CLA	C1B-C2B	2.23	1.48	1.43
35	7	620	XAT	O24-C25	-2.23	1.43	1.46
26	Z	604	CLA	C1B-C2B	2.23	1.48	1.43
26	A	837	CLA	C3B-C4B	2.23	1.48	1.42
26	2	616	CLA	CMD-C2D	-2.23	1.46	1.50
26	9	601	CLA	CMB-C2B	-2.23	1.46	1.50
26	Y	611	CLA	CMD-C2D	-2.23	1.46	1.50
37	Z	605	CHL	C1B-NB	-2.23	1.35	1.37
37	V	608	CHL	C4B-NB	-2.23	1.35	1.37
26	3	602	CLA	C1B-C2B	2.23	1.48	1.43
26	9	611	CLA	CMD-C2D	-2.23	1.46	1.50
26	8	601	CLA	CMC-C2C	-2.23	1.46	1.50
26	A	831	CLA	C1B-NB	-2.23	1.35	1.37
26	B	841	CLA	CMB-C2B	-2.23	1.46	1.50
35	8	620	XAT	O24-C25	-2.23	1.43	1.46
26	3	613	CLA	C1B-C2B	2.22	1.48	1.43
26	1	606	CLA	CMD-C2D	-2.22	1.46	1.50
26	A	827	CLA	MG-NB	-2.22	2.01	2.05
26	a	607	CLA	C1B-C2B	2.22	1.48	1.43
26	A	814	CLA	MG-NB	-2.22	2.01	2.05
26	3	608	CLA	MG-NB	-2.22	2.01	2.05
26	6	610	CLA	CMB-C2B	-2.22	1.46	1.50
26	K	206	CLA	CMD-C2D	-2.22	1.46	1.50
37	Z	605	CHL	C4C-C3C	2.22	1.48	1.45
26	5	613	CLA	CMC-C2C	-2.22	1.46	1.50
26	A	818	CLA	C1B-C2B	2.22	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	838	CLA	C1B-NB	-2.22	1.35	1.37
26	7	601	CLA	MG-ND	-2.22	2.01	2.05
26	4	609	CLA	CMC-C2C	-2.22	1.46	1.50
26	B	836	CLA	C1B-C2B	2.22	1.48	1.43
26	Z	611	CLA	C4B-C3B	2.22	1.48	1.43
26	B	815	CLA	C1B-C2B	2.22	1.48	1.43
29	B	845	BCR	C1-C6	-2.22	1.50	1.53
37	X	607	CHL	C4B-NB	-2.22	1.35	1.37
26	W	603	CLA	CMD-C2D	-2.22	1.46	1.50
26	2	614	CLA	CMC-C2C	-2.22	1.46	1.50
26	a	610	CLA	CMC-C2C	-2.22	1.46	1.50
26	5	610	CLA	CMB-C2B	-2.22	1.46	1.50
26	6	614	CLA	CMC-C2C	-2.22	1.46	1.50
26	A	831	CLA	MG-NB	-2.22	2.01	2.05
26	5	607	CLA	CMD-C2D	-2.22	1.46	1.50
26	1	601	CLA	CMB-C2B	-2.22	1.46	1.50
26	4	603	CLA	CMB-C2B	-2.21	1.46	1.50
26	A	822	CLA	MG-NB	-2.21	2.01	2.05
26	1	611	CLA	CMD-C2D	-2.21	1.46	1.50
26	8	612	CLA	CMB-C2B	-2.21	1.46	1.50
26	A	838	CLA	CMC-C2C	-2.21	1.46	1.50
26	A	832	CLA	MG-NB	-2.21	2.01	2.05
26	6	608	CLA	CMC-C2C	-2.21	1.46	1.50
26	2	601	CLA	CMB-C2B	-2.21	1.46	1.50
37	Y	601	CHL	C4B-NB	-2.21	1.35	1.37
26	B	811	CLA	C4B-C3B	2.21	1.48	1.43
26	8	607	CLA	CMB-C2B	-2.21	1.46	1.50
26	B	807	CLA	MG-ND	-2.21	2.01	2.05
26	A	830	CLA	C1B-C2B	2.21	1.48	1.43
26	5	612	CLA	CMD-C2D	-2.21	1.46	1.50
26	9	607	CLA	CMC-C2C	-2.21	1.46	1.50
26	W	613	CLA	CMD-C2D	-2.21	1.46	1.50
26	F	301	CLA	C1B-C2B	2.21	1.48	1.43
35	U	1622	XAT	O24-C25	-2.21	1.43	1.46
26	1	614	CLA	MG-NB	-2.21	2.01	2.05
26	B	824	CLA	C1B-C2B	2.21	1.48	1.43
26	Z	610	CLA	CMC-C2C	-2.21	1.46	1.50
29	3	622	BCR	C30-C25	-2.21	1.50	1.53
26	B	823	CLA	CMC-C2C	-2.21	1.46	1.50
26	L	302	CLA	CMD-C2D	-2.20	1.46	1.50
26	1	609	CLA	C4B-C3B	2.20	1.48	1.43
26	A	837	CLA	C1B-NB	-2.20	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	604	CLA	CMC-C2C	-2.20	1.46	1.50
26	5	613	CLA	CMD-C2D	-2.20	1.46	1.50
26	A	805	CLA	MG-NB	-2.20	2.01	2.05
26	J	101	CLA	CMB-C2B	-2.20	1.46	1.50
26	4	606	CLA	CMC-C2C	-2.20	1.46	1.50
26	3	603	CLA	MG-ND	-2.20	2.01	2.05
26	B	834	CLA	MG-NB	-2.20	2.01	2.05
26	6	606	CLA	CMD-C2D	-2.20	1.46	1.50
26	6	611	CLA	CMC-C2C	-2.20	1.46	1.50
26	8	606	CLA	CMD-C2D	-2.20	1.46	1.50
26	7	604	CLA	C1B-C2B	2.20	1.48	1.43
26	B	835	CLA	MG-NB	-2.20	2.01	2.05
26	B	813	CLA	C1B-NB	-2.20	1.35	1.37
26	8	610	CLA	CMB-C2B	-2.20	1.46	1.50
26	A	823	CLA	MG-NB	-2.20	2.01	2.05
26	B	825	CLA	CMB-C2B	-2.20	1.46	1.50
37	X	607	CHL	C4C-C3C	2.20	1.48	1.45
26	7	608	CLA	CMC-C2C	-2.20	1.46	1.50
26	W	612	CLA	CMD-C2D	-2.20	1.46	1.50
26	2	606	CLA	CMB-C2B	-2.20	1.46	1.50
26	8	609	CLA	CMC-C2C	-2.20	1.46	1.50
26	a	613	CLA	MG-NB	-2.20	2.01	2.05
26	6	601	CLA	CMD-C2D	-2.20	1.46	1.50
26	6	606	CLA	CMB-C2B	-2.20	1.46	1.50
26	6	607	CLA	CMD-C2D	-2.19	1.46	1.50
26	6	618	CLA	CMD-C2D	-2.19	1.46	1.50
29	A	848	BCR	C1-C6	-2.19	1.50	1.53
26	A	809	CLA	CMC-C2C	-2.19	1.46	1.50
26	Z	613	CLA	CMB-C2B	-2.19	1.46	1.50
26	9	603	CLA	MG-NB	-2.19	2.01	2.05
26	6	608	CLA	CMD-C2D	-2.19	1.46	1.50
26	A	834	CLA	MG-ND	-2.19	2.01	2.05
26	6	612	CLA	CMB-C2B	-2.19	1.46	1.50
26	7	606	CLA	CMC-C2C	-2.19	1.46	1.50
35	6	621	XAT	O24-C25	-2.19	1.43	1.46
27	B	842	PQN	C5-C4	2.19	1.52	1.48
26	8	614	CLA	MG-NB	-2.19	2.01	2.05
37	Y	601	CHL	C4C-C3C	2.19	1.48	1.45
26	4	616	CLA	CMB-C2B	-2.19	1.46	1.50
26	B	830	CLA	CMC-C2C	-2.19	1.46	1.50
26	a	612	CLA	CMC-C2C	-2.19	1.46	1.50
26	A	824	CLA	MG-NB	-2.19	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	610	CLA	CMD-C2D	-2.19	1.46	1.50
29	B	844	BCR	C16-C15	-2.19	1.30	1.36
26	A	838	CLA	C3B-C4B	2.19	1.47	1.42
26	2	604	CLA	C1B-C2B	2.19	1.48	1.43
26	6	606	CLA	CMC-C2C	-2.19	1.46	1.50
37	X	606	CHL	C4C-C3C	2.19	1.48	1.45
26	6	614	CLA	CMB-C2B	-2.19	1.46	1.50
37	Y	609	CHL	C1B-C2B	2.19	1.48	1.43
26	B	839	CLA	CHC-C4B	-2.19	1.34	1.39
26	2	601	CLA	MG-ND	-2.19	2.01	2.05
26	3	612	CLA	CMC-C2C	-2.19	1.46	1.50
26	6	602	CLA	CMB-C2B	-2.18	1.46	1.50
29	5	622	BCR	C30-C25	-2.18	1.50	1.53
26	6	609	CLA	C1B-C2B	2.18	1.48	1.43
26	A	828	CLA	MG-ND	-2.18	2.01	2.05
26	9	601	CLA	CMC-C2C	-2.18	1.46	1.50
26	Y	613	CLA	CMD-C2D	-2.18	1.46	1.50
26	2	610	CLA	MG-NB	-2.18	2.01	2.05
26	1	607	CLA	CMB-C2B	-2.18	1.46	1.50
26	2	612	CLA	CMD-C2D	-2.18	1.46	1.50
26	8	604	CLA	CMD-C2D	-2.18	1.46	1.50
26	B	818	CLA	C3B-C4B	2.18	1.47	1.42
29	A	848	BCR	C19-C18	2.18	1.50	1.45
26	4	602	CLA	CHC-C1C	2.18	1.43	1.38
26	1	612	CLA	CMC-C2C	-2.18	1.46	1.50
26	Z	614	CLA	CMD-C2D	-2.18	1.46	1.50
26	5	618	CLA	CMB-C2B	-2.18	1.46	1.50
26	A	830	CLA	CMC-C2C	-2.18	1.46	1.50
26	A	806	CLA	MG-ND	-2.18	2.01	2.05
26	B	808	CLA	CAC-C3C	-2.18	1.45	1.51
26	B	834	CLA	CMC-C2C	-2.18	1.46	1.50
26	9	607	CLA	CMD-C2D	-2.18	1.46	1.50
26	Y	613	CLA	CMC-C2C	-2.18	1.46	1.50
26	B	826	CLA	CMB-C2B	-2.18	1.46	1.50
26	6	609	CLA	MG-NB	-2.18	2.01	2.05
26	O	2003	CLA	CMC-C2C	-2.17	1.46	1.50
26	7	607	CLA	CMC-C2C	-2.17	1.46	1.50
26	B	827	CLA	MG-NB	-2.17	2.01	2.05
26	1	607	CLA	C1B-C2B	2.17	1.48	1.43
26	1	613	CLA	MG-NB	-2.17	2.01	2.05
26	A	827	CLA	CMC-C2C	-2.17	1.46	1.50
26	a	603	CLA	CMC-C2C	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	607	CLA	CMC-C2C	-2.17	1.46	1.50
26	3	609	CLA	MG-NB	-2.17	2.01	2.05
26	9	606	CLA	MG-NB	-2.17	2.01	2.05
26	A	836	CLA	CMC-C2C	-2.17	1.46	1.50
26	A	843	CLA	CMC-C2C	-2.17	1.46	1.50
26	V	603	CLA	CMD-C2D	-2.17	1.46	1.50
26	U	604	CLA	C1B-C2B	2.17	1.48	1.43
37	X	605	CHL	C1B-NB	-2.17	1.35	1.37
26	6	603	CLA	CMB-C2B	-2.17	1.46	1.50
26	B	824	CLA	MG-NB	-2.17	2.01	2.05
29	B	853	BCR	C1-C6	-2.17	1.50	1.53
26	3	604	CLA	C1B-C2B	2.17	1.48	1.43
26	B	836	CLA	MG-ND	-2.17	2.01	2.05
26	O	2002	CLA	CMB-C2B	-2.17	1.46	1.50
29	J	102	BCR	C17-C18	-2.17	1.32	1.35
37	Z	609	CHL	CHB-C4A	-2.17	1.32	1.37
26	A	804	CLA	CMB-C2B	-2.17	1.46	1.50
26	A	810	CLA	C1B-C2B	2.17	1.48	1.43
26	B	818	CLA	MG-ND	-2.17	2.01	2.05
26	X	613	CLA	CMB-C2B	-2.17	1.46	1.50
26	3	614	CLA	CMC-C2C	-2.17	1.46	1.50
26	6	611	CLA	CMB-C2B	-2.17	1.46	1.50
26	2	612	CLA	CMB-C2B	-2.17	1.46	1.50
26	5	607	CLA	MG-ND	-2.17	2.01	2.05
26	4	604	CLA	CMB-C2B	-2.16	1.46	1.50
26	V	612	CLA	CMD-C2D	-2.16	1.46	1.50
26	2	606	CLA	MG-NB	-2.16	2.01	2.05
26	a	601	CLA	MG-NB	-2.16	2.01	2.05
26	B	821	CLA	CMD-C2D	-2.16	1.46	1.50
26	A	830	CLA	MG-ND	-2.16	2.01	2.05
26	B	839	CLA	C3B-C4B	2.16	1.47	1.42
26	A	845	CLA	C1B-C2B	2.16	1.48	1.43
26	Y	614	CLA	CMD-C2D	-2.16	1.46	1.50
26	8	608	CLA	C1B-C2B	2.16	1.48	1.43
26	5	617	CLA	CMC-C2C	-2.16	1.46	1.50
26	1	611	CLA	CMB-C2B	-2.16	1.46	1.50
37	V	606	CHL	C4B-NB	-2.16	1.35	1.37
26	A	819	CLA	C3B-C4B	2.16	1.47	1.42
26	G	203	CLA	CMB-C2B	-2.16	1.46	1.50
26	U	603	CLA	CMD-C2D	-2.16	1.46	1.50
26	A	828	CLA	CMC-C2C	-2.16	1.46	1.50
26	B	829	CLA	CAC-C3C	-2.16	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	7	614	CLA	CMB-C2B	-2.16	1.46	1.50
26	V	602	CLA	CMC-C2C	-2.16	1.46	1.50
26	A	842	CLA	C1B-NB	-2.16	1.35	1.37
26	B	828	CLA	C1B-C2B	2.15	1.48	1.43
26	8	603	CLA	CMC-C2C	-2.15	1.46	1.50
26	Z	610	CLA	CMB-C2B	-2.15	1.46	1.50
26	B	807	CLA	C1B-NB	-2.15	1.35	1.37
26	Z	610	CLA	CHC-C1C	2.15	1.42	1.38
37	V	609	CHL	C4C-C3C	2.15	1.48	1.45
26	6	616	CLA	CMD-C2D	-2.15	1.46	1.50
26	U	602	CLA	CMB-C2B	-2.15	1.46	1.50
26	6	618	CLA	CMB-C2B	-2.15	1.46	1.50
26	A	815	CLA	C1B-C2B	2.15	1.48	1.43
37	W	609	CHL	C1B-C2B	2.15	1.48	1.43
26	B	822	CLA	CMC-C2C	-2.15	1.46	1.50
26	A	820	CLA	MG-NB	-2.15	2.01	2.05
26	A	834	CLA	C1B-NB	-2.15	1.35	1.37
26	Y	602	CLA	CMC-C2C	-2.15	1.46	1.50
26	G	203	CLA	CMC-C2C	-2.15	1.46	1.50
26	2	603	CLA	CMC-C2C	-2.15	1.46	1.50
26	6	601	CLA	CMC-C2C	-2.15	1.46	1.50
26	A	801	CLA	MG-NB	-2.15	2.01	2.05
26	a	601	CLA	CMB-C2B	-2.15	1.46	1.50
29	B	843	BCR	C17-C18	-2.15	1.32	1.35
26	Y	603	CLA	CMB-C2B	-2.15	1.46	1.50
26	1	604	CLA	CMC-C2C	-2.15	1.46	1.50
26	a	611	CLA	CMB-C2B	-2.15	1.46	1.50
37	W	607	CHL	C4D-CHA	2.15	1.46	1.38
26	7	609	CLA	C1B-C2B	2.15	1.48	1.43
26	B	804	CLA	MG-NB	-2.15	2.01	2.05
37	V	601	CHL	C2C-C1C	2.15	1.49	1.44
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	V	604	CLA	CMB-C2B	-2.15	1.46	1.50
26	4	608	CLA	CMC-C2C	-2.15	1.46	1.50
26	L	306	CLA	CMB-C2B	-2.14	1.46	1.50
26	a	607	CLA	CMC-C2C	-2.14	1.46	1.50
26	3	603	CLA	CMC-C2C	-2.14	1.46	1.50
26	A	816	CLA	C3B-C4B	2.14	1.47	1.42
37	X	608	CHL	C4C-C3C	2.14	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	840	CLA	C1B-C2B	2.14	1.48	1.43
26	X	602	CLA	CMC-C2C	-2.14	1.46	1.50
26	V	613	CLA	CMC-C2C	-2.14	1.46	1.50
26	A	835	CLA	C1B-C2B	2.14	1.48	1.43
26	B	809	CLA	C1B-C2B	2.14	1.48	1.43
26	6	610	CLA	C1B-C2B	2.14	1.48	1.43
26	6	618	CLA	CMC-C2C	-2.14	1.46	1.50
26	9	614	CLA	CMB-C2B	-2.14	1.46	1.50
37	Z	601	CHL	C2C-C1C	2.14	1.49	1.44
26	1	606	CLA	MG-NB	-2.14	2.01	2.05
26	B	816	CLA	C1B-C2B	2.14	1.48	1.43
26	A	804	CLA	MG-ND	-2.14	2.01	2.05
26	A	819	CLA	CHC-C4B	-2.14	1.34	1.39
29	B	853	BCR	C30-C25	-2.14	1.50	1.53
26	Z	602	CLA	CMD-C2D	-2.14	1.46	1.50
26	5	602	CLA	MG-NB	-2.14	2.01	2.05
26	Y	610	CLA	CHC-C1C	2.14	1.42	1.38
26	B	832	CLA	MG-NB	-2.14	2.01	2.05
26	1	603	CLA	CMC-C2C	-2.14	1.46	1.50
26	V	603	CLA	CMB-C2B	-2.14	1.46	1.50
26	A	845	CLA	C1B-NB	-2.14	1.35	1.37
26	9	610	CLA	CHC-C1C	2.14	1.42	1.38
26	3	608	CLA	C1B-C2B	2.13	1.48	1.43
37	X	601	CHL	C4C-C3C	2.13	1.48	1.45
37	W	601	CHL	C2C-C1C	2.13	1.49	1.44
26	8	606	CLA	MG-NB	-2.13	2.01	2.05
26	a	610	CLA	CMB-C2B	-2.13	1.46	1.50
26	V	611	CLA	CMD-C2D	-2.13	1.46	1.50
26	4	612	CLA	CMC-C2C	-2.13	1.46	1.50
29	B	844	BCR	C1-C6	-2.13	1.50	1.53
26	B	837	CLA	CAC-C3C	-2.13	1.45	1.51
26	3	613	CLA	MG-NB	-2.13	2.01	2.05
26	2	616	CLA	CMB-C2B	-2.13	1.46	1.50
26	5	616	CLA	CMC-C2C	-2.13	1.46	1.50
26	W	602	CLA	CMC-C2C	-2.13	1.46	1.50
26	A	836	CLA	C1B-C2B	2.13	1.48	1.43
37	Z	608	CHL	C2C-C1C	2.13	1.49	1.44
26	7	611	CLA	MG-NB	-2.13	2.01	2.05
26	5	610	CLA	C1B-C2B	2.13	1.48	1.43
26	7	615	CLA	CMD-C2D	-2.13	1.46	1.50
26	3	606	CLA	C3B-C4B	2.13	1.47	1.42
26	A	803	CLA	C1B-C2B	2.13	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	614	CLA	CMD-C2D	-2.13	1.46	1.50
26	5	609	CLA	MG-NB	-2.13	2.01	2.05
26	6	613	CLA	C1B-C2B	2.13	1.48	1.43
26	A	838	CLA	CHC-C4B	-2.13	1.34	1.39
26	A	807	CLA	MG-ND	-2.13	2.01	2.05
26	F	303	CLA	CAC-C3C	-2.13	1.45	1.51
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	U	602	CLA	CMD-C2D	-2.13	1.46	1.50
26	A	819	CLA	C1B-C2B	2.13	1.48	1.43
26	4	611	CLA	CMD-C2D	-2.13	1.46	1.50
35	6	621	XAT	C22-C21	-2.12	1.51	1.54
26	8	604	CLA	CMB-C2B	-2.12	1.46	1.50
26	A	817	CLA	MG-NB	-2.12	2.01	2.05
26	A	843	CLA	C1B-NB	-2.12	1.35	1.37
26	1	610	CLA	CMB-C2B	-2.12	1.46	1.50
26	X	613	CLA	CMD-C2D	-2.12	1.46	1.50
26	V	604	CLA	CMD-C2D	-2.12	1.46	1.50
37	Z	607	CHL	C4C-C3C	2.12	1.48	1.45
37	W	605	CHL	C1B-NB	-2.12	1.35	1.37
35	2	620	XAT	O24-C25	-2.12	1.43	1.46
26	B	839	CLA	MG-ND	-2.12	2.01	2.05
26	A	804	CLA	C3B-C4B	2.12	1.47	1.42
26	6	603	CLA	MG-NB	-2.12	2.01	2.05
26	5	617	CLA	CAC-C3C	-2.12	1.45	1.51
26	L	304	CLA	CMB-C2B	-2.12	1.46	1.50
26	2	602	CLA	CMB-C2B	-2.12	1.45	1.50
26	6	616	CLA	CMC-C2C	-2.12	1.46	1.50
35	2	620	XAT	C22-C21	-2.12	1.51	1.54
26	G	204	CLA	CMC-C2C	-2.12	1.46	1.50
26	6	612	CLA	CMD-C2D	-2.12	1.46	1.50
26	Z	603	CLA	CMB-C2B	-2.12	1.46	1.50
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	3	608	CLA	C1B-NB	-2.12	1.35	1.37
37	V	605	CHL	C4C-C3C	2.12	1.48	1.45
26	B	831	CLA	MG-NB	-2.12	2.01	2.05
37	X	605	CHL	C2C-C1C	2.12	1.49	1.44
26	7	612	CLA	CMB-C2B	-2.12	1.46	1.50
26	3	604	CLA	MG-NB	-2.12	2.01	2.05
37	U	607	CHL	CHB-C4A	-2.12	1.32	1.37
35	3	619	XAT	C22-C21	-2.12	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	854	CLA	MG-ND	-2.12	2.01	2.05
26	1	602	CLA	C1B-NB	-2.11	1.35	1.37
37	X	601	CHL	C4D-CHA	2.11	1.45	1.38
26	Z	612	CLA	CMC-C2C	-2.11	1.46	1.50
26	4	601	CLA	CMC-C2C	-2.11	1.46	1.50
26	Y	610	CLA	CMC-C2C	-2.11	1.46	1.50
26	9	603	CLA	C4B-C3B	2.11	1.48	1.43
26	2	611	CLA	CMB-C2B	-2.11	1.46	1.50
26	B	841	CLA	MG-NB	-2.11	2.01	2.05
26	5	619	CLA	CMC-C2C	-2.11	1.46	1.50
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	X	604	CLA	CMB-C2B	-2.11	1.46	1.50
26	A	811	CLA	MG-NB	-2.11	2.01	2.05
26	a	607	CLA	CHC-C1C	2.11	1.42	1.38
26	9	612	CLA	CMD-C2D	-2.11	1.46	1.50
26	A	840	CLA	MG-ND	-2.11	2.01	2.05
26	5	617	CLA	MG-NB	-2.11	2.01	2.05
26	5	609	CLA	C1B-C2B	2.11	1.48	1.43
29	B	853	BCR	C21-C22	-2.11	1.33	1.35
26	B	829	CLA	MG-NB	-2.11	2.01	2.05
26	A	809	CLA	C1B-C2B	2.11	1.48	1.43
26	4	606	CLA	MG-NB	-2.11	2.01	2.05
37	Y	608	CHL	MG-NA	-2.11	2.01	2.06
26	W	602	CLA	CMD-C2D	-2.11	1.46	1.50
26	W	613	CLA	CMC-C2C	-2.11	1.46	1.50
26	V	614	CLA	CHC-C1C	2.11	1.42	1.38
26	B	818	CLA	CHC-C4B	-2.11	1.34	1.39
37	Z	609	CHL	C1B-C2B	2.11	1.48	1.43
26	6	608	CLA	CMB-C2B	-2.11	1.46	1.50
26	3	602	CLA	CMB-C2B	-2.11	1.46	1.50
26	8	601	CLA	MG-NB	-2.11	2.01	2.05
35	3	619	XAT	O4-C5	-2.11	1.43	1.46
26	4	613	CLA	MG-NB	-2.11	2.01	2.05
26	A	819	CLA	C1B-NB	-2.11	1.35	1.37
26	W	613	CLA	CMB-C2B	-2.11	1.46	1.50
26	Z	610	CLA	C1B-C2B	2.11	1.48	1.43
26	A	833	CLA	MG-NB	-2.10	2.01	2.05
26	U	602	CLA	CMC-C2C	-2.10	1.46	1.50
26	5	601	CLA	CMB-C2B	-2.10	1.46	1.50
37	U	606	CHL	C2C-C1C	2.10	1.49	1.44
26	a	604	CLA	CMC-C2C	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	806	CLA	CAC-C3C	-2.10	1.45	1.51
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	U	606	CHL	C4B-NB	-2.10	1.35	1.37
37	W	605	CHL	C4B-NB	-2.10	1.35	1.37
26	B	813	CLA	MG-ND	-2.10	2.01	2.05
37	W	606	CHL	C4D-CHA	2.10	1.45	1.38
26	X	611	CLA	CMD-C2D	-2.10	1.46	1.50
26	9	613	CLA	CHC-C4B	-2.10	1.34	1.39
26	4	613	CLA	CMC-C2C	-2.10	1.46	1.50
26	7	602	CLA	MG-NB	-2.10	2.01	2.05
37	W	601	CHL	C4C-C3C	2.10	1.48	1.45
26	X	610	CLA	C1B-C2B	2.10	1.48	1.43
26	A	836	CLA	MG-ND	-2.10	2.01	2.05
26	A	854	CLA	MG-NB	-2.10	2.01	2.05
26	6	611	CLA	CMD-C2D	-2.10	1.46	1.50
26	X	610	CLA	CMB-C2B	-2.10	1.46	1.50
37	U	601	CHL	C4D-CHA	2.10	1.45	1.38
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	1	607	CLA	CMC-C2C	-2.10	1.46	1.50
26	Y	612	CLA	CMC-C2C	-2.10	1.46	1.50
37	U	606	CHL	C4C-C3C	2.09	1.48	1.45
26	a	602	CLA	C1B-NB	-2.09	1.35	1.37
26	5	603	CLA	MG-NB	-2.09	2.01	2.05
37	U	608	CHL	C1B-NB	-2.09	1.35	1.37
26	A	842	CLA	MG-ND	-2.09	2.01	2.05
26	A	801	CLA	CHC-C4B	-2.09	1.34	1.39
26	1	603	CLA	CMB-C2B	-2.09	1.46	1.50
26	5	616	CLA	MG-NB	-2.09	2.01	2.05
26	A	823	CLA	CMC-C2C	-2.09	1.46	1.50
26	Y	602	CLA	CMD-C2D	-2.09	1.46	1.50
26	A	818	CLA	MG-NB	-2.09	2.01	2.05
26	4	608	CLA	CMD-C2D	-2.09	1.46	1.50
26	4	611	CLA	CMC-C2C	-2.09	1.46	1.50
37	V	606	CHL	C4C-C3C	2.09	1.48	1.45
26	L	307	CLA	CMB-C2B	-2.09	1.46	1.50
26	A	826	CLA	C1B-C2B	2.09	1.48	1.43
26	B	810	CLA	C1B-C2B	2.09	1.48	1.43
26	Y	602	CLA	CHC-C1C	2.09	1.42	1.38
26	K	203	CLA	MG-ND	-2.09	2.01	2.05
26	L	307	CLA	MG-NB	-2.09	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	603	CLA	CMC-C2C	-2.09	1.46	1.50
26	5	612	CLA	CMC-C2C	-2.09	1.46	1.50
26	5	611	CLA	CMB-C2B	-2.09	1.46	1.50
26	B	818	CLA	C1B-C2B	2.09	1.48	1.43
26	9	603	CLA	CHC-C4B	-2.09	1.34	1.39
26	A	831	CLA	C1B-C2B	2.09	1.48	1.43
35	6	621	XAT	O4-C5	-2.09	1.43	1.46
26	Y	613	CLA	CMB-C2B	-2.09	1.46	1.50
26	V	612	CLA	CMB-C2B	-2.09	1.46	1.50
26	B	816	CLA	CMC-C2C	-2.08	1.46	1.50
26	Z	611	CLA	CMC-C2C	-2.08	1.46	1.50
26	W	612	CLA	CMC-C2C	-2.08	1.46	1.50
37	V	601	CHL	C4B-NB	-2.08	1.35	1.37
26	B	834	CLA	MG-ND	-2.08	2.01	2.05
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	A	824	CLA	CHC-C4B	-2.08	1.34	1.39
26	W	614	CLA	CMD-C2D	-2.08	1.46	1.50
26	B	810	CLA	MG-ND	-2.08	2.01	2.05
37	U	605	CHL	C2C-C1C	2.08	1.49	1.44
26	A	843	CLA	MG-ND	-2.08	2.01	2.05
26	Z	614	CLA	CMB-C2B	-2.08	1.46	1.50
26	7	606	CLA	MG-ND	-2.08	2.01	2.05
26	B	806	CLA	CAC-C3C	-2.08	1.45	1.51
26	9	610	CLA	C1B-C2B	2.08	1.48	1.43
26	8	602	CLA	MG-NB	-2.08	2.01	2.05
35	4	620	XAT	O24-C25	-2.08	1.43	1.46
37	Y	609	CHL	CHB-C4A	-2.08	1.32	1.37
26	B	823	CLA	MG-ND	-2.08	2.01	2.05
26	B	835	CLA	CMC-C2C	-2.08	1.46	1.50
26	6	617	CLA	CMC-C2C	-2.08	1.46	1.50
26	1	613	CLA	C1B-NB	-2.08	1.35	1.37
35	5	621	XAT	O24-C25	-2.08	1.43	1.46
26	3	614	CLA	MG-NB	-2.08	2.01	2.05
26	7	616	CLA	CHC-C1C	2.08	1.42	1.38
26	U	614	CLA	CHC-C1C	2.08	1.42	1.38
37	X	609	CHL	C1B-NB	-2.08	1.35	1.37
35	9	620	XAT	O24-C25	-2.08	1.43	1.46
36	V	1623	NEX	O24-C25	-2.08	1.43	1.46
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	839	CLA	C1B-C2B	2.08	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	2	623	BCR	C30-C25	-2.08	1.50	1.53
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	X	603	CLA	CMB-C2B	-2.07	1.46	1.50
26	V	612	CLA	CMC-C2C	-2.07	1.46	1.50
26	W	604	CLA	CMD-C2D	-2.07	1.46	1.50
26	B	813	CLA	C1B-C2B	2.07	1.48	1.43
26	7	601	CLA	C1B-C2B	2.07	1.48	1.43
26	U	610	CLA	CMC-C2C	-2.07	1.46	1.50
26	U	613	CLA	CMD-C2D	-2.07	1.46	1.50
26	1	607	CLA	CHC-C1C	2.07	1.42	1.38
26	A	828	CLA	C1B-NB	-2.07	1.35	1.37
26	a	613	CLA	C1B-NB	-2.07	1.35	1.37
26	W	602	CLA	CMB-C2B	-2.07	1.46	1.50
35	5	621	XAT	O4-C5	-2.07	1.43	1.46
26	7	610	CLA	CHC-C1C	2.07	1.42	1.38
26	1	607	CLA	MG-NB	-2.07	2.01	2.05
26	U	603	CLA	CMB-C2B	-2.07	1.46	1.50
26	1	608	CLA	CMB-C2B	-2.07	1.46	1.50
26	5	610	CLA	CHC-C1C	2.07	1.42	1.38
26	X	602	CLA	CHC-C1C	2.07	1.42	1.38
26	3	612	CLA	CHC-C1C	2.07	1.42	1.38
26	V	611	CLA	CMB-C2B	-2.07	1.46	1.50
26	A	845	CLA	MG-NB	-2.07	2.01	2.05
29	G	205	BCR	C1-C6	-2.07	1.50	1.53
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	2	609	CLA	C1B-C2B	2.07	1.48	1.43
26	W	612	CLA	CMB-C2B	-2.07	1.46	1.50
26	U	604	CLA	CHC-C1C	2.07	1.42	1.38
26	5	618	CLA	CMC-C2C	-2.07	1.46	1.50
26	X	613	CLA	CMC-C2C	-2.07	1.46	1.50
26	B	827	CLA	C1B-C2B	2.07	1.48	1.43
26	B	820	CLA	MG-ND	-2.07	2.01	2.05
37	V	605	CHL	C2C-C1C	2.07	1.49	1.44
26	3	617	CLA	CMC-C2C	-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	614	CLA	MG-NB	-2.06	2.01	2.05
26	5	614	CLA	CMC-C2C	-2.06	1.46	1.50
37	Y	608	CHL	C4B-NB	-2.06	1.35	1.37
26	B	803	CLA	MG-ND	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	W	605	CHL	C2C-C1C	2.06	1.49	1.44
26	7	613	CLA	CHC-C4B	-2.06	1.34	1.39
26	U	614	CLA	CMD-C2D	-2.06	1.46	1.50
26	B	806	CLA	C1B-NB	-2.06	1.35	1.37
26	4	607	CLA	CMC-C2C	-2.06	1.46	1.50
26	4	618	CLA	CMD-C2D	-2.06	1.46	1.50
26	W	602	CLA	CHC-C1C	2.06	1.42	1.38
26	B	835	CLA	MG-ND	-2.06	2.01	2.05
26	2	606	CLA	MG-ND	-2.06	2.01	2.05
26	A	816	CLA	CAC-C3C	-2.06	1.45	1.51
26	2	612	CLA	CMC-C2C	-2.06	1.46	1.50
26	5	607	CLA	C1B-C2B	2.06	1.48	1.43
26	K	201	CLA	CMB-C2B	-2.06	1.46	1.50
26	Y	603	CLA	CMD-C2D	-2.06	1.46	1.50
26	3	609	CLA	C1B-C2B	2.06	1.48	1.43
35	4	620	XAT	C22-C21	-2.06	1.51	1.54
29	B	843	BCR	C14-C13	-2.06	1.33	1.35
37	V	607	CHL	C4D-CHA	2.06	1.45	1.38
26	A	816	CLA	CHC-C4B	-2.06	1.34	1.39
29	K	202	BCR	C30-C25	-2.06	1.50	1.53
26	B	827	CLA	CAC-C3C	-2.06	1.45	1.51
26	B	807	CLA	C1B-C2B	2.06	1.48	1.43
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	3	612	CLA	CMB-C2B	-2.06	1.46	1.50
26	a	603	CLA	CMB-C2B	-2.06	1.46	1.50
26	V	610	CLA	CMC-C2C	-2.06	1.46	1.50
26	B	809	CLA	CAC-C3C	-2.06	1.45	1.51
26	A	820	CLA	C1B-NB	-2.06	1.35	1.37
26	4	614	CLA	MG-NB	-2.06	2.01	2.05
26	a	608	CLA	CMB-C2B	-2.06	1.46	1.50
26	a	612	CLA	MG-NB	-2.06	2.01	2.05
26	B	837	CLA	C1B-C2B	2.06	1.48	1.43
26	6	602	CLA	MG-NB	-2.06	2.01	2.05
26	A	836	CLA	C3B-C4B	2.05	1.47	1.42
29	F	305	BCR	C30-C25	-2.05	1.50	1.53
26	B	839	CLA	C1B-NB	-2.05	1.35	1.37
26	X	612	CLA	CMC-C2C	-2.05	1.46	1.50
26	9	603	CLA	C3B-C2B	-2.05	1.36	1.44
26	A	832	CLA	MG-ND	-2.05	2.01	2.05
26	V	614	CLA	CMB-C2B	-2.05	1.46	1.50
26	a	611	CLA	MG-NB	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	613	CLA	CMB-C2B	-2.05	1.46	1.50
26	A	803	CLA	CAC-C3C	-2.05	1.45	1.51
26	A	837	CLA	CHC-C4B	-2.05	1.34	1.39
37	Y	605	CHL	C2C-C1C	2.05	1.49	1.44
26	8	616	CLA	CHC-C1C	2.05	1.42	1.38
26	W	604	CLA	CHC-C1C	2.05	1.42	1.38
37	Z	605	CHL	C4B-NB	-2.05	1.35	1.37
26	Y	611	CLA	CMB-C2B	-2.05	1.46	1.50
26	7	610	CLA	C1B-NB	-2.05	1.35	1.37
26	A	828	CLA	C1B-C2B	2.05	1.48	1.43
26	3	613	CLA	CMC-C2C	-2.05	1.46	1.50
37	U	607	CHL	C4D-CHA	2.05	1.45	1.38
26	B	811	CLA	MG-NB	-2.05	2.01	2.05
26	K	203	CLA	CMC-C2C	-2.05	1.46	1.50
37	Y	605	CHL	C4D-CHA	2.05	1.45	1.38
26	J	101	CLA	CMD-C2D	-2.05	1.46	1.50
26	a	608	CLA	CMC-C2C	-2.05	1.46	1.50
37	Y	606	CHL	C4C-C3C	2.05	1.48	1.45
37	Z	608	CHL	C4C-C3C	2.05	1.48	1.45
26	Y	604	CLA	CMC-C2C	-2.05	1.46	1.50
26	A	809	CLA	MG-ND	-2.05	2.01	2.05
26	A	802	CLA	CAC-C3C	-2.05	1.45	1.51
26	A	833	CLA	C1B-C2B	2.05	1.48	1.43
26	2	601	CLA	C1B-C2B	2.05	1.48	1.43
26	a	607	CLA	MG-NB	-2.04	2.01	2.05
26	B	805	CLA	MG-ND	-2.04	2.01	2.05
26	2	611	CLA	CMC-C2C	-2.04	1.46	1.50
26	B	803	CLA	C1B-NB	-2.04	1.35	1.37
35	9	620	XAT	C22-C21	-2.04	1.51	1.54
36	W	1623	NEX	O24-C25	-2.04	1.43	1.46
26	A	820	CLA	C1B-C2B	2.04	1.48	1.43
26	A	813	CLA	MG-ND	-2.04	2.01	2.05
26	Z	610	CLA	CMD-C2D	-2.04	1.46	1.50
29	J	102	BCR	C30-C25	-2.04	1.51	1.53
26	2	607	CLA	C1B-C2B	2.04	1.48	1.43
26	W	610	CLA	CHC-C1C	2.04	1.42	1.38
37	X	609	CHL	CMC-C2C	2.04	1.49	1.45
26	B	806	CLA	CHC-C4B	-2.04	1.34	1.39
26	2	602	CLA	CAC-C3C	-2.04	1.45	1.51
26	V	602	CLA	CMD-C2D	-2.04	1.46	1.50
26	B	821	CLA	CMC-C2C	-2.04	1.45	1.50
26	J	101	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	613	CLA	CHC-C1C	2.04	1.42	1.38
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
36	6	624	NEX	O24-C25	-2.04	1.43	1.46
26	7	615	CLA	CMC-C2C	-2.04	1.46	1.50
26	B	803	CLA	MG-NB	-2.04	2.01	2.05
26	W	611	CLA	CHC-C1C	2.04	1.42	1.38
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	A	802	CLA	C1B-NB	-2.04	1.35	1.37
37	W	605	CHL	C4D-CHA	2.04	1.45	1.38
26	A	814	CLA	MG-ND	-2.04	2.01	2.05
26	3	603	CLA	CHC-C4B	-2.04	1.34	1.39
29	A	856	BCR	C1-C6	-2.04	1.51	1.53
26	B	840	CLA	MG-ND	-2.04	2.01	2.05
26	7	603	CLA	MG-ND	-2.04	2.01	2.05
26	X	602	CLA	CMD-C2D	-2.04	1.46	1.50
26	6	609	CLA	CMC-C2C	-2.03	1.46	1.50
37	Z	606	CHL	C4B-NB	-2.03	1.35	1.37
26	B	839	CLA	C1B-C2B	2.03	1.48	1.43
26	B	819	CLA	MG-NB	-2.03	2.01	2.05
26	A	801	CLA	CAC-C3C	-2.03	1.45	1.51
26	6	613	CLA	MG-NB	-2.03	2.01	2.05
35	7	620	XAT	C22-C21	-2.03	1.51	1.54
29	3	621	BCR	C1-C6	-2.03	1.51	1.53
26	X	614	CLA	CMB-C2B	-2.03	1.46	1.50
26	4	614	CLA	CMC-C2C	-2.03	1.46	1.50
26	X	610	CLA	CMC-C2C	-2.03	1.46	1.50
26	U	610	CLA	CMD-C2D	-2.03	1.46	1.50
26	L	303	CLA	C1B-C2B	2.03	1.48	1.43
26	5	617	CLA	CHC-C4B	-2.03	1.34	1.39
26	a	611	CLA	CMC-C2C	-2.03	1.46	1.50
26	9	611	CLA	CMB-C2B	-2.03	1.46	1.50
37	V	607	CHL	C4C-C3C	2.03	1.48	1.45
26	4	603	CLA	MG-NB	-2.03	2.01	2.05
26	Y	610	CLA	CMD-C2D	-2.03	1.46	1.50
26	Z	613	CLA	MG-NB	-2.03	2.01	2.05
26	Z	613	CLA	CMC-C2C	-2.03	1.46	1.50
26	B	807	CLA	CHC-C4B	-2.03	1.34	1.39
26	9	614	CLA	CMD-C2D	-2.03	1.46	1.50
26	U	604	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	606	CLA	C1B-NB	-2.03	1.35	1.37
26	U	611	CLA	CMB-C2B	-2.03	1.46	1.50
29	B	843	BCR	C1-C6	-2.03	1.51	1.53
26	A	801	CLA	C3B-C4B	2.03	1.47	1.42
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	4	604	CLA	CMD-C2D	-2.02	1.46	1.50
26	5	611	CLA	CMD-C2D	-2.02	1.46	1.50
26	O	2001	CLA	MG-NB	-2.02	2.01	2.05
26	1	611	CLA	MG-NB	-2.02	2.01	2.05
29	A	856	BCR	C21-C22	-2.02	1.33	1.35
26	5	617	CLA	C3B-C4B	2.02	1.47	1.42
37	V	601	CHL	C4C-C3C	2.02	1.48	1.45
26	9	607	CLA	MG-NB	-2.02	2.01	2.05
26	A	820	CLA	CAC-C3C	-2.02	1.45	1.51
37	U	606	CHL	MG-NA	-2.02	2.01	2.06
26	Y	612	CLA	CMD-C2D	-2.02	1.46	1.50
26	V	613	CLA	CMB-C2B	-2.02	1.46	1.50
26	a	602	CLA	MG-ND	-2.02	2.01	2.05
26	X	602	CLA	CMB-C2B	-2.02	1.46	1.50
26	V	610	CLA	CMD-C2D	-2.02	1.46	1.50
26	7	608	CLA	CAC-C3C	-2.02	1.45	1.51
37	Y	609	CHL	CMC-C2C	2.02	1.49	1.45
26	2	603	CLA	CHC-C4B	-2.02	1.34	1.39
26	7	601	CLA	C1B-NB	-2.02	1.35	1.37
26	5	614	CLA	MG-NB	-2.02	2.01	2.05
26	A	818	CLA	CHC-C4B	-2.02	1.34	1.39
26	B	829	CLA	CHC-C4B	-2.02	1.34	1.39
26	2	604	CLA	CMB-C2B	-2.02	1.46	1.50
26	A	831	CLA	CHC-C4B	-2.02	1.34	1.39
26	B	837	CLA	C1B-NB	-2.02	1.35	1.37
26	7	608	CLA	MG-ND	-2.02	2.01	2.05
26	3	603	CLA	C3B-C4B	2.02	1.47	1.42
37	V	606	CHL	CHB-C4A	-2.02	1.32	1.37
26	Z	604	CLA	CMD-C2D	-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	A	840	CLA	CHC-C4B	-2.02	1.34	1.39
26	2	616	CLA	CMC-C2C	-2.02	1.46	1.50
37	V	606	CHL	C4D-CHA	2.01	1.45	1.38
26	A	812	CLA	CHC-C4B	-2.01	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	616	CLA	O2A-CGA	2.01	1.37	1.30
26	9	614	CLA	CMC-C2C	-2.01	1.46	1.50
31	A	858	LMU	C3B-C4B	-2.01	1.49	1.52
26	A	854	CLA	C1B-C2B	2.01	1.48	1.43
37	Z	601	CHL	CMC-C2C	2.01	1.49	1.45
26	V	602	CLA	CHC-C1C	2.01	1.42	1.38
26	B	838	CLA	C1B-NB	-2.01	1.35	1.37
26	8	614	CLA	MG-ND	-2.01	2.01	2.05
26	4	618	CLA	CMB-C2B	-2.01	1.46	1.50
26	2	607	CLA	CMC-C2C	-2.01	1.46	1.50
26	8	607	CLA	CHC-C1C	2.01	1.42	1.38
26	8	607	CLA	MG-NB	-2.01	2.01	2.05
26	7	609	CLA	CMC-C2C	-2.01	1.46	1.50
26	A	805	CLA	MG-ND	-2.01	2.01	2.05
26	9	603	CLA	C1B-NB	-2.01	1.35	1.37
26	7	609	CLA	MG-NB	-2.01	2.01	2.05
26	5	603	CLA	CAC-C3C	-2.01	1.46	1.51
26	Y	604	CLA	CMD-C2D	-2.01	1.46	1.50
26	A	803	CLA	C1B-NB	-2.01	1.35	1.37
37	Y	606	CHL	CHB-C4A	-2.01	1.32	1.37
26	A	805	CLA	CAC-C3C	-2.01	1.46	1.51
26	1	608	CLA	CMC-C2C	-2.01	1.46	1.50
26	8	608	CLA	MG-ND	-2.01	2.01	2.05
37	W	606	CHL	CMC-C2C	2.01	1.49	1.45
26	A	807	CLA	CAC-C3C	-2.01	1.46	1.51
37	Z	606	CHL	CHB-C4A	-2.00	1.32	1.37
26	7	602	CLA	MG-ND	-2.00	2.01	2.05
29	5	622	BCR	C23-C22	2.00	1.50	1.45
26	V	604	CLA	CMC-C2C	-2.00	1.46	1.50
26	1	616	CLA	CHC-C1C	2.00	1.42	1.38
26	6	616	CLA	MG-ND	-2.00	2.01	2.05
35	W	1622	XAT	O24-C25	-2.00	1.43	1.46
26	Z	604	CLA	CMC-C2C	-2.00	1.46	1.50
26	1	608	CLA	MG-NB	-2.00	2.01	2.05
26	X	612	CLA	CMB-C2B	-2.00	1.46	1.50
37	U	601	CHL	CMC-C2C	2.00	1.49	1.45
26	Z	612	CLA	CMB-C2B	-2.00	1.46	1.50
26	9	614	CLA	CHC-C1C	2.00	1.42	1.38
26	L	303	CLA	CMC-C2C	-2.00	1.46	1.50
26	X	611	CLA	CMB-C2B	-2.00	1.46	1.50
26	7	615	CLA	MG-NB	-2.00	2.01	2.05
26	X	614	CLA	CHC-C1C	2.00	1.42	1.38

All (4551) 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	-17.41	81.69	107.37
35	W	1622	XAT	C37-C21-C36	-17.39	81.72	107.37
29	B	852	BCR	C32-C1-C6	-16.31	83.85	110.30
35	U	1622	XAT	C37-C21-C22	-15.46	82.13	108.98
35	W	1622	XAT	C37-C21-C22	-14.80	83.27	108.98
29	O	2005	BCR	C40-C30-C25	-11.15	92.21	110.30
29	B	848	BCR	C24-C23-C22	-10.84	109.86	126.23
36	X	1623	NEX	C16-C1-C6	10.55	119.91	110.47
29	B	852	BCR	C8-C9-C10	10.45	134.98	118.94
36	W	1623	NEX	O24-C25-C24	10.41	121.20	113.38
29	K	207	BCR	C40-C30-C25	-10.05	93.99	110.30
37	U	607	CHL	C2B-C1B-NB	9.97	116.92	110.23
29	9	621	BCR	C24-C23-C22	-9.94	111.22	126.23
37	X	607	CHL	C2B-C1B-NB	9.85	116.83	110.23
37	Y	601	CHL	C2B-C1B-NB	9.68	116.72	110.23
29	B	852	BCR	C34-C9-C10	-9.63	109.43	122.92
37	Y	608	CHL	C2B-C1B-NB	9.57	116.65	110.23
29	8	621	BCR	C33-C5-C6	9.56	135.26	124.53
37	Z	609	CHL	C2B-C1B-NB	9.52	116.61	110.23
37	W	605	CHL	C2B-C1B-NB	9.43	116.55	110.23
37	Y	607	CHL	C2B-C1B-NB	9.41	116.54	110.23
37	V	606	CHL	C2B-C1B-NB	9.32	116.48	110.23
37	V	607	CHL	C2B-C1B-NB	9.31	116.47	110.23
37	Z	607	CHL	C2B-C1B-NB	9.31	116.47	110.23
37	V	601	CHL	C2B-C1B-NB	9.26	116.44	110.23
37	Y	609	CHL	C2B-C1B-NB	9.26	116.44	110.23
37	V	609	CHL	C2B-C1B-NB	9.24	116.42	110.23
34	Y	1620	LUT	C15-C35-C34	-9.23	104.57	123.47
37	U	608	CHL	C2B-C1B-NB	9.21	116.41	110.23
37	W	609	CHL	CMD-C2D-C1D	9.17	140.88	124.71
37	W	608	CHL	C2B-C1B-NB	9.15	116.37	110.23
37	Z	608	CHL	CMD-C2D-C1D	9.08	140.71	124.71
37	V	608	CHL	C2B-C1B-NB	9.05	116.30	110.23
37	Z	606	CHL	C2B-C1B-NB	9.04	116.29	110.23
37	Z	601	CHL	C2B-C1B-NB	9.02	116.28	110.23
37	V	609	CHL	CMD-C2D-C1D	9.01	140.59	124.71
37	X	608	CHL	C2B-C1B-NB	8.99	116.26	110.23
36	Z	1623	NEX	O24-C25-C24	8.98	120.13	113.38
37	U	606	CHL	C2B-C1B-NB	8.97	116.25	110.23
37	Z	605	CHL	C2B-C1B-NB	8.96	116.24	110.23
36	Y	1623	NEX	O24-C25-C24	8.96	120.11	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	X	609	CHL	CMD-C2D-C1D	8.95	140.49	124.71
37	Z	609	CHL	CMD-C2D-C1D	8.86	140.32	124.71
37	V	608	CHL	CMD-C2D-C1D	8.79	140.20	124.71
37	U	608	CHL	CMD-C2D-C1D	8.79	140.20	124.71
34	Y	1620	LUT	C20-C13-C14	-8.72	110.70	122.92
36	U	1623	NEX	O24-C25-C24	8.70	119.92	113.38
37	Z	605	CHL	CMD-C2D-C1D	8.70	140.04	124.71
37	X	601	CHL	CMD-C2D-C1D	8.68	140.02	124.71
37	X	601	CHL	C2B-C1B-NB	8.68	116.05	110.23
37	Z	606	CHL	CMD-C2D-C1D	8.66	139.98	124.71
37	Y	601	CHL	CMD-C2D-C1D	8.66	139.97	124.71
37	Z	608	CHL	C2B-C1B-NB	8.65	116.03	110.23
35	5	621	XAT	O24-C25-C24	8.64	119.87	113.38
29	B	852	BCR	C32-C1-C31	-8.63	82.04	108.53
37	Z	607	CHL	C2C-C3C-C4C	-8.63	100.34	106.49
37	Y	608	CHL	C1D-ND-C4D	-8.62	100.21	106.33
37	V	608	CHL	C1D-ND-C4D	-8.62	100.21	106.33
37	W	609	CHL	C2B-C1B-NB	8.61	116.01	110.23
37	Z	607	CHL	CMD-C2D-C1D	8.59	139.86	124.71
27	A	844	PQN	C11-C12-C13	-8.57	112.52	126.79
37	W	601	CHL	C2B-C1B-NB	8.57	115.98	110.23
37	X	607	CHL	CMD-C2D-C1D	8.55	139.79	124.71
36	X	1623	NEX	C17-C1-C16	-8.54	82.31	108.53
37	U	609	CHL	CMD-C2D-C1D	8.51	139.72	124.71
37	Z	601	CHL	CMD-C2D-C1D	8.51	139.71	124.71
37	Y	607	CHL	C2C-C3C-C4C	-8.49	100.44	106.49
37	V	601	CHL	CMD-C2D-C1D	8.47	139.64	124.71
37	Y	608	CHL	CMD-C2D-C1D	8.46	139.62	124.71
37	W	607	CHL	CMD-C2D-C1D	8.46	139.62	124.71
37	X	607	CHL	C2C-C3C-C4C	-8.45	100.47	106.49
37	W	601	CHL	CMD-C2D-C1D	8.43	139.57	124.71
37	W	605	CHL	CMD-C2D-C1D	8.42	139.56	124.71
37	W	606	CHL	CMD-C2D-C1D	8.42	139.56	124.71
37	X	608	CHL	C1D-ND-C4D	-8.42	100.35	106.33
37	Y	606	CHL	C2B-C1B-NB	8.42	115.88	110.23
37	Z	605	CHL	C1D-ND-C4D	-8.40	100.37	106.33
37	Y	609	CHL	CMD-C2D-C1D	8.38	139.49	124.71
37	W	605	CHL	C1D-ND-C4D	-8.38	100.38	106.33
37	Y	605	CHL	CMD-C2D-C1D	8.38	139.48	124.71
37	W	608	CHL	CMD-C2D-C1D	8.37	139.46	124.71
37	X	607	CHL	C1D-ND-C4D	-8.36	100.39	106.33
37	X	609	CHL	C2B-C1B-NB	8.34	115.82	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	U	608	CHL	C1D-ND-C4D	-8.33	100.42	106.33
37	U	601	CHL	CMD-C2D-C1D	8.32	139.37	124.71
37	U	609	CHL	C2B-C1B-NB	8.32	115.81	110.23
37	V	605	CHL	CMD-C2D-C1D	8.31	139.37	124.71
37	X	606	CHL	C2B-C1B-NB	8.31	115.81	110.23
37	V	609	CHL	C1D-ND-C4D	-8.30	100.44	106.33
37	W	606	CHL	C2B-C1B-NB	8.28	115.78	110.23
37	U	601	CHL	C2B-C1B-NB	8.28	115.78	110.23
37	Z	606	CHL	C1D-ND-C4D	-8.25	100.47	106.33
37	U	606	CHL	C1D-ND-C4D	-8.25	100.48	106.33
37	U	607	CHL	CMD-C2D-C1D	8.24	139.24	124.71
37	Z	601	CHL	C1D-ND-C4D	-8.24	100.48	106.33
37	Y	607	CHL	C1D-ND-C4D	-8.22	100.49	106.33
35	U	1622	XAT	C36-C21-C22	8.20	123.24	108.98
37	Y	605	CHL	CHD-C1D-ND	-8.19	116.93	124.45
37	X	605	CHL	CMD-C2D-C1D	8.17	139.12	124.71
35	U	1622	XAT	O24-C25-C24	8.17	119.52	113.38
37	W	608	CHL	C1D-ND-C4D	-8.16	100.53	106.33
37	V	601	CHL	C1D-ND-C4D	-8.16	100.54	106.33
37	X	608	CHL	CMD-C2D-C1D	8.15	139.08	124.71
37	U	606	CHL	CMD-C2D-C1D	8.14	139.06	124.71
37	U	605	CHL	CMD-C2D-C1D	8.11	139.01	124.71
35	4	620	XAT	O4-C5-C4	8.11	119.47	113.38
37	Y	606	CHL	C1D-ND-C4D	-8.11	100.58	106.33
37	V	607	CHL	C2C-C3C-C4C	-8.09	100.72	106.49
36	X	1623	NEX	O24-C25-C24	8.08	119.45	113.38
35	Z	1622	XAT	O24-C25-C24	8.07	119.45	113.38
37	V	605	CHL	C2B-C1B-NB	8.05	115.63	110.23
37	W	607	CHL	C2B-C1B-NB	7.99	115.59	110.23
37	Y	606	CHL	CMD-C2D-C1D	7.98	138.78	124.71
29	J	102	BCR	C28-C27-C26	-7.94	99.91	114.08
35	W	1622	XAT	C36-C21-C22	7.90	122.71	108.98
37	Y	601	CHL	C1D-ND-C4D	-7.89	100.73	106.33
37	X	608	CHL	C2C-C3C-C4C	-7.89	100.86	106.49
37	Z	608	CHL	C1D-ND-C4D	-7.88	100.74	106.33
37	V	606	CHL	CMD-C2D-C1D	7.88	138.59	124.71
37	X	606	CHL	CMD-C2D-C1D	7.76	138.39	124.71
37	U	607	CHL	C1D-ND-C4D	-7.75	100.83	106.33
36	V	1623	NEX	O24-C25-C24	7.75	119.21	113.38
37	W	606	CHL	C1D-ND-C4D	-7.73	100.84	106.33
37	X	606	CHL	C2C-C3C-C4C	-7.72	100.98	106.49
37	U	608	CHL	C2C-C3C-C4C	-7.72	100.99	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	X	609	CHL	C1D-ND-C4D	-7.71	100.86	106.33
34	9	619	LUT	C8-C7-C6	-7.70	105.58	127.20
35	7	620	XAT	O4-C5-C4	7.70	119.17	113.38
37	W	609	CHL	CHD-C1D-ND	-7.67	117.40	124.45
37	X	606	CHL	C1D-ND-C4D	-7.66	100.89	106.33
37	Y	607	CHL	CMD-C2D-C1D	7.65	138.19	124.71
37	Z	607	CHL	C1D-ND-C4D	-7.63	100.91	106.33
37	V	607	CHL	CMD-C2D-C1D	7.63	138.16	124.71
34	4	619	LUT	C8-C7-C6	-7.62	105.81	127.20
37	U	609	CHL	C1D-ND-C4D	-7.61	100.93	106.33
37	X	605	CHL	C2B-C1B-NB	7.59	115.32	110.23
37	Y	606	CHL	C2C-C3C-C4C	-7.58	101.08	106.49
37	V	608	CHL	C2C-C3C-C4C	-7.56	101.10	106.49
37	Y	609	CHL	C1D-ND-C4D	-7.55	100.97	106.33
37	X	601	CHL	C1D-ND-C4D	-7.55	100.97	106.33
37	U	607	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
34	Y	1620	LUT	C11-C10-C9	-7.54	116.55	127.31
37	Z	605	CHL	C2C-C3C-C4C	-7.54	101.12	106.49
37	U	609	CHL	C2C-C3C-C4C	-7.53	101.12	106.49
37	V	606	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
37	V	605	CHL	CHD-C1D-ND	-7.51	117.56	124.45
37	U	605	CHL	C2B-C1B-NB	7.49	115.25	110.23
37	W	608	CHL	C2C-C3C-C4C	-7.49	101.15	106.49
37	Y	605	CHL	C2B-C1B-NB	7.45	115.23	110.23
35	X	1622	XAT	O24-C25-C24	7.45	118.98	113.38
37	U	606	CHL	C2C-C3C-C4C	-7.44	101.19	106.49
35	Z	1622	XAT	C15-C14-C13	-7.40	116.74	127.31
37	Z	608	CHL	C2C-C3C-C4C	-7.39	101.22	106.49
27	B	842	PQN	C11-C12-C13	-7.39	114.50	126.79
37	V	607	CHL	C1D-ND-C4D	-7.38	101.09	106.33
35	3	619	XAT	O24-C25-C24	7.36	118.91	113.38
37	W	601	CHL	C1D-ND-C4D	-7.34	101.12	106.33
35	a	618	XAT	O4-C5-C4	7.33	118.89	113.38
37	Y	607	CHL	C2D-C1D-ND	7.32	115.50	110.10
37	V	606	CHL	C1D-ND-C4D	-7.30	101.15	106.33
37	Y	608	CHL	C2D-C1D-ND	7.30	115.48	110.10
37	W	605	CHL	C2C-C3C-C4C	-7.29	101.29	106.49
37	X	609	CHL	CHD-C1D-ND	-7.29	117.75	124.45
37	Z	609	CHL	C1D-ND-C4D	-7.29	101.16	106.33
37	V	605	CHL	C1D-ND-C4D	-7.27	101.17	106.33
37	Z	606	CHL	C2C-C3C-C4C	-7.25	101.32	106.49
37	W	609	CHL	C2C-C3C-C4C	-7.25	101.32	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Y	605	CHL	C2C-C3C-C4C	-7.25	101.32	106.49
37	U	605	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
37	W	609	CHL	C1D-ND-C4D	-7.21	101.21	106.33
37	X	605	CHL	CHD-C1D-ND	-7.21	117.83	124.45
37	X	607	CHL	C2D-C1D-ND	7.20	115.41	110.10
37	V	605	CHL	C2C-C3C-C4C	-7.20	101.36	106.49
35	X	1622	XAT	O4-C5-C4	7.19	118.78	113.38
35	1	618	XAT	O4-C5-C4	7.19	118.78	113.38
27	A	844	PQN	C14-C13-C15	-7.17	103.22	115.27
26	B	826	CLA	C4A-NA-C1A	7.15	109.92	106.71
35	W	1622	XAT	O24-C25-C24	7.15	118.75	113.38
37	Y	609	CHL	C2C-C3C-C4C	-7.15	101.39	106.49
37	W	607	CHL	C2C-C3C-C4C	-7.14	101.19	106.49
37	V	608	CHL	C2D-C1D-ND	7.13	115.36	110.10
29	B	849	BCR	C39-C30-C25	-7.10	98.79	110.30
29	O	2005	BCR	C24-C23-C22	-7.10	115.51	126.23
35	9	620	XAT	O24-C25-C24	7.09	118.71	113.38
37	Y	601	CHL	C2C-C3C-C4C	-7.09	101.44	106.49
29	A	852	BCR	C24-C23-C22	-7.07	115.55	126.23
35	7	620	XAT	O24-C25-C24	7.07	118.69	113.38
37	W	601	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
37	Z	609	CHL	CHD-C1D-ND	-7.03	118.00	124.45
35	Y	1622	XAT	O4-C5-C4	7.00	118.64	113.38
36	X	1623	NEX	C2-C1-C6	6.99	116.01	109.21
35	Y	1622	XAT	O24-C25-C24	6.98	118.63	113.38
35	Y	1622	XAT	C15-C14-C13	-6.95	117.39	127.31
37	U	601	CHL	C1D-ND-C4D	-6.94	101.41	106.33
37	U	605	CHL	CHD-C1D-ND	-6.92	118.09	124.45
37	X	609	CHL	C2C-C3C-C4C	-6.92	101.55	106.49
37	W	605	CHL	C2D-C1D-ND	6.91	115.20	110.10
37	Y	608	CHL	C2C-C3C-C4C	-6.90	101.57	106.49
37	V	609	CHL	CHD-C1D-ND	-6.90	118.11	124.45
37	X	605	CHL	C1D-ND-C4D	-6.90	101.44	106.33
37	Z	601	CHL	C2D-C1D-ND	6.87	115.17	110.10
37	X	601	CHL	C2C-C3C-C4C	-6.87	101.59	106.49
35	V	1622	XAT	O4-C5-C4	6.86	118.53	113.38
37	Z	609	CHL	C2C-C3C-C4C	-6.84	101.61	106.49
26	A	837	CLA	C4A-NA-C1A	6.84	109.78	106.71
37	Y	609	CHL	CHD-C1D-ND	-6.83	118.18	124.45
37	V	609	CHL	C2C-C3C-C4C	-6.82	101.63	106.49
26	B	810	CLA	C4A-NA-C1A	6.82	109.77	106.71
29	B	852	BCR	C7-C8-C9	-6.81	115.94	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Y	1620	LUT	C12-C13-C14	6.80	129.38	118.94
29	B	852	BCR	C31-C1-C6	6.80	121.33	110.30
37	U	601	CHL	CHD-C1D-ND	-6.79	118.21	124.45
37	W	606	CHL	C2C-C3C-C4C	-6.78	101.66	106.49
36	6	624	NEX	O24-C25-C24	6.76	118.46	113.38
37	Z	601	CHL	C2C-C3C-C4C	-6.75	101.68	106.49
29	A	850	BCR	C8-C7-C6	-6.75	108.26	127.20
37	W	607	CHL	C1D-ND-C4D	-6.75	101.54	106.33
34	Y	1620	LUT	C15-C14-C13	6.74	136.94	127.31
37	V	601	CHL	C2C-C3C-C4C	-6.74	101.68	106.49
29	F	305	BCR	C36-C18-C17	-6.74	113.48	122.92
37	Z	605	CHL	C2D-C1D-ND	6.74	115.07	110.10
37	U	605	CHL	C1D-ND-C4D	-6.73	101.55	106.33
29	5	622	BCR	C23-C24-C25	-6.73	108.31	127.20
35	9	620	XAT	O4-C5-C4	6.72	118.43	113.38
34	7	619	LUT	C8-C7-C6	-6.71	108.36	127.20
37	Y	601	CHL	CHD-C1D-ND	-6.71	118.29	124.45
29	B	848	BCR	C23-C22-C21	-6.71	108.65	118.94
37	U	608	CHL	C2D-C1D-ND	6.70	115.04	110.10
29	B	845	BCR	C37-C22-C21	-6.68	113.57	122.92
37	Z	601	CHL	CHD-C1D-ND	-6.67	118.33	124.45
35	W	1622	XAT	O4-C5-C4	6.66	118.39	113.38
37	U	606	CHL	C2D-C1D-ND	6.65	115.01	110.10
37	W	606	CHL	C2D-C1D-ND	6.65	115.01	110.10
37	U	607	CHL	C2D-C1D-ND	6.65	115.00	110.10
26	7	613	CLA	C4A-NA-C1A	6.65	109.69	106.71
37	X	605	CHL	C2C-C3C-C4C	-6.65	101.75	106.49
37	X	606	CHL	CHD-C1D-ND	-6.64	118.35	124.45
26	8	603	CLA	C4A-NA-C1A	6.64	109.69	106.71
37	Y	606	CHL	C2D-C1D-ND	6.63	114.99	110.10
37	V	601	CHL	CHD-C1D-ND	-6.62	118.37	124.45
29	A	848	BCR	C38-C26-C25	-6.61	117.11	124.53
26	Z	603	CLA	C4A-NA-C1A	6.60	109.67	106.71
37	X	601	CHL	C2D-C1D-ND	6.60	114.97	110.10
26	3	603	CLA	C4A-NA-C1A	6.60	109.67	106.71
37	U	601	CHL	C2C-C3C-C4C	-6.59	101.79	106.49
29	2	623	BCR	C28-C27-C26	-6.59	102.31	114.08
35	Z	1622	XAT	O4-C5-C4	6.59	118.33	113.38
26	K	204	CLA	C4A-NA-C1A	6.58	109.66	106.71
29	3	622	BCR	C38-C26-C25	-6.56	117.16	124.53
35	8	620	XAT	O4-C5-C4	6.55	118.30	113.38
26	1	603	CLA	C4A-NA-C1A	6.53	109.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	601	CHL	CHD-C1D-ND	-6.52	118.46	124.45
37	W	608	CHL	C2D-C1D-ND	6.52	114.91	110.10
37	Z	605	CHL	CHD-C1D-ND	-6.49	118.49	124.45
26	a	603	CLA	C4A-NA-C1A	6.47	109.61	106.71
37	Y	601	CHL	C2D-C1D-ND	6.45	114.86	110.10
37	Z	607	CHL	C2D-C1D-ND	6.45	114.86	110.10
37	Z	608	CHL	C2D-C1D-ND	6.44	114.85	110.10
37	Y	605	CHL	C1D-ND-C4D	-6.44	101.76	106.33
26	B	809	CLA	C4A-NA-C1A	6.44	109.60	106.71
26	V	603	CLA	C4A-NA-C1A	6.44	109.60	106.71
37	V	601	CHL	C2D-C1D-ND	6.44	114.85	110.10
26	5	603	CLA	C4A-NA-C1A	6.43	109.59	106.71
37	V	607	CHL	C2D-C1D-ND	6.43	114.84	110.10
36	5	624	NEX	C38-C25-C26	-6.42	111.49	122.26
29	3	620	BCR	C3-C4-C5	-6.42	102.61	114.08
37	V	609	CHL	C2D-C1D-ND	6.41	114.83	110.10
37	U	608	CHL	CHD-C1D-ND	-6.41	118.57	124.45
35	6	621	XAT	O4-C5-C4	6.40	118.19	113.38
29	7	623	BCR	C8-C7-C6	-6.39	109.27	127.20
35	6	621	XAT	O24-C25-C24	6.37	118.17	113.38
29	B	844	BCR	C27-C26-C25	-6.37	113.48	122.73
37	X	606	CHL	C2D-C1D-ND	6.37	114.80	110.10
26	A	819	CLA	C4A-NA-C1A	6.36	109.57	106.71
26	B	806	CLA	C4A-NA-C1A	6.35	109.56	106.71
29	L	301	BCR	C8-C7-C6	-6.35	109.36	127.20
37	U	609	CHL	CHD-C1D-ND	-6.35	118.62	124.45
26	7	603	CLA	C4A-NA-C1A	6.33	109.55	106.71
26	A	814	CLA	C4A-NA-C1A	6.33	109.55	106.71
34	8	619	LUT	C8-C7-C6	-6.33	109.44	127.20
34	Y	1620	LUT	C35-C15-C14	6.32	136.42	123.47
37	W	607	CHL	CHD-C1D-ND	-6.31	118.65	124.45
29	A	848	BCR	C8-C7-C6	-6.29	109.54	127.20
26	W	603	CLA	C4A-NA-C1A	6.29	109.53	106.71
37	X	608	CHL	C2D-C1D-ND	6.28	114.73	110.10
26	A	815	CLA	C4A-NA-C1A	6.27	109.53	106.71
29	8	621	BCR	C40-C30-C25	6.27	120.47	110.30
29	9	621	BCR	C28-C27-C26	-6.25	102.91	114.08
37	W	605	CHL	CHD-C1D-ND	-6.25	118.71	124.45
26	A	823	CLA	C4A-NA-C1A	6.25	109.52	106.71
29	O	2005	BCR	C39-C30-C25	6.24	120.43	110.30
29	L	305	BCR	C34-C9-C8	-6.24	108.24	118.08
37	Z	608	CHL	CHD-C1D-ND	-6.24	118.72	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Z	606	CHL	CHD-C1D-ND	-6.24	118.72	124.45
37	W	608	CHL	CHD-C1D-ND	-6.23	118.73	124.45
37	X	601	CHL	CHD-C1D-ND	-6.22	118.74	124.45
29	A	851	BCR	C40-C30-C25	6.22	120.38	110.30
29	A	852	BCR	C28-C27-C26	-6.22	102.98	114.08
26	A	828	CLA	C4A-NA-C1A	6.21	109.50	106.71
26	A	816	CLA	C4A-NA-C1A	6.21	109.50	106.71
29	B	846	BCR	C23-C24-C25	-6.20	109.79	127.20
37	V	608	CHL	CHD-C1D-ND	-6.19	118.76	124.45
37	Y	608	CHL	CHD-C1D-ND	-6.19	118.77	124.45
29	K	202	BCR	C28-C27-C26	-6.18	103.03	114.08
29	B	846	BCR	C38-C26-C25	-6.18	117.59	124.53
26	B	837	CLA	C4A-NA-C1A	6.17	109.48	106.71
35	U	1622	XAT	O4-C5-C4	6.17	118.01	113.38
35	V	1622	XAT	O24-C25-C24	6.16	118.01	113.38
35	5	621	XAT	O4-C5-C4	6.16	118.01	113.38
37	V	606	CHL	C2D-C1D-ND	6.16	114.64	110.10
37	Z	607	CHL	CHD-C1D-ND	-6.16	118.80	124.45
29	8	621	BCR	C38-C26-C25	-6.15	117.62	124.53
26	X	603	CLA	C4A-NA-C1A	6.13	109.46	106.71
37	X	608	CHL	CHD-C1D-ND	-6.13	118.82	124.45
37	Y	606	CHL	CHD-C1D-ND	-6.13	118.82	124.45
26	A	809	CLA	C4A-NA-C1A	6.12	109.46	106.71
37	Y	609	CHL	C2D-C1D-ND	6.11	114.61	110.10
26	A	802	CLA	C4A-NA-C1A	6.11	109.45	106.71
35	3	619	XAT	O4-C5-C4	6.10	117.96	113.38
26	A	834	CLA	C4A-NA-C1A	6.09	109.44	106.71
37	X	609	CHL	O2D-CGD-CBD	6.09	122.09	111.27
26	6	603	CLA	C4A-NA-C1A	6.08	109.44	106.71
26	2	601	CLA	C4A-NA-C1A	6.08	109.44	106.71
37	Z	606	CHL	C2D-C1D-ND	6.07	114.58	110.10
26	A	821	CLA	C4A-NA-C1A	6.07	109.44	106.71
29	F	305	BCR	C28-C27-C26	-6.06	103.25	114.08
29	B	845	BCR	C33-C5-C6	-6.06	117.72	124.53
26	3	606	CLA	C4A-NA-C1A	6.04	109.42	106.71
37	U	601	CHL	CHB-C1B-NB	-6.03	117.87	124.26
26	W	614	CLA	C4A-NA-C1A	6.01	109.41	106.71
34	3	618	LUT	C8-C7-C6	-6.00	110.34	127.20
26	B	820	CLA	C4A-NA-C1A	6.00	109.41	106.71
37	U	607	CHL	CHD-C1D-ND	-6.00	118.94	124.45
36	W	1623	NEX	C11-C10-C9	-5.99	118.76	127.31
37	V	605	CHL	C2D-C1D-ND	5.99	114.52	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	U	607	CHL	C3B-C2B-C1B	-5.98	99.94	107.16
37	U	609	CHL	C2D-C1D-ND	5.97	114.51	110.10
35	3	619	XAT	C18-C5-C6	-5.96	112.27	122.26
35	3	619	XAT	C38-C25-C26	-5.96	112.27	122.26
29	A	848	BCR	C23-C24-C25	-5.95	110.49	127.20
26	Z	613	CLA	C4A-NA-C1A	5.94	109.38	106.71
29	A	856	BCR	C8-C7-C6	-5.94	110.52	127.20
26	B	824	CLA	C4A-NA-C1A	5.92	109.37	106.71
29	B	849	BCR	C20-C21-C22	-5.91	118.87	127.31
26	Y	603	CLA	C4A-NA-C1A	5.91	109.36	106.71
26	B	811	CLA	C4A-NA-C1A	5.90	109.36	106.71
37	Y	605	CHL	CHB-C1B-NB	-5.90	118.01	124.26
36	6	624	NEX	C38-C25-C26	-5.90	112.37	122.26
29	4	621	BCR	C23-C24-C25	-5.89	110.67	127.20
29	O	2004	BCR	C8-C7-C6	-5.89	110.67	127.20
26	L	303	CLA	C4A-NA-C1A	5.88	109.35	106.71
26	6	618	CLA	C4A-NA-C1A	5.87	109.35	106.71
37	V	606	CHL	C3C-C4C-NC	5.86	117.14	110.57
29	9	621	BCR	C23-C22-C21	-5.86	109.96	118.94
26	U	612	CLA	C4A-NA-C1A	5.84	109.33	106.71
26	1	612	CLA	C4A-NA-C1A	5.83	109.33	106.71
35	7	620	XAT	C18-C5-C6	-5.83	112.49	122.26
37	Y	609	CHL	O2D-CGD-CBD	5.82	121.61	111.27
26	U	603	CLA	C4A-NA-C1A	5.80	109.31	106.71
36	W	1623	NEX	C15-C14-C13	-5.80	119.03	127.31
26	B	836	CLA	C4A-NA-C1A	5.79	109.31	106.71
26	a	612	CLA	C4A-NA-C1A	5.79	109.31	106.71
29	6	622	BCR	C40-C30-C25	5.79	119.69	110.30
26	5	601	CLA	C4A-NA-C1A	5.78	109.30	106.71
35	2	620	XAT	O24-C25-C24	5.76	117.71	113.38
26	B	841	CLA	C4A-NA-C1A	5.76	109.30	106.71
37	X	607	CHL	CHD-C1D-ND	-5.76	119.16	124.45
37	W	607	CHL	C2D-C1D-ND	5.76	114.35	110.10
37	U	606	CHL	CHD-C1D-ND	-5.75	119.17	124.45
37	W	601	CHL	C2D-C1D-ND	5.75	114.34	110.10
29	8	621	BCR	C4-C5-C6	-5.75	114.39	122.73
26	a	609	CLA	C4A-NA-C1A	5.75	109.29	106.71
26	B	838	CLA	C4A-NA-C1A	5.74	109.29	106.71
37	X	609	CHL	C2D-C1D-ND	5.74	114.33	110.10
26	L	307	CLA	C4A-NA-C1A	5.73	109.28	106.71
26	B	813	CLA	C4A-NA-C1A	5.73	109.28	106.71
26	4	603	CLA	C4A-NA-C1A	5.73	109.28	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	613	CLA	C4A-NA-C1A	5.72	109.28	106.71
35	1	618	XAT	O24-C25-C24	5.72	117.68	113.38
36	U	1623	NEX	C20-C13-C12	5.72	127.09	118.08
26	A	839	CLA	C4A-NA-C1A	5.72	109.28	106.71
26	B	840	CLA	C4A-NA-C1A	5.72	109.28	106.71
37	Z	609	CHL	C2D-C1D-ND	5.71	114.31	110.10
29	K	207	BCR	C40-C30-C39	-5.71	90.99	108.53
35	U	1622	XAT	C15-C14-C13	-5.71	119.17	127.31
26	B	827	CLA	C4A-NA-C1A	5.70	109.27	106.71
29	1	619	BCR	C33-C5-C6	-5.70	118.13	124.53
29	L	305	BCR	C33-C5-C6	-5.70	118.13	124.53
37	Y	607	CHL	C3C-C4C-NC	5.69	116.95	110.57
29	6	622	BCR	C33-C5-C6	-5.69	118.14	124.53
37	U	609	CHL	O2D-CGD-CBD	5.68	121.37	111.27
26	A	806	CLA	C4A-NA-C1A	5.68	109.26	106.71
26	A	824	CLA	C4A-NA-C1A	5.67	109.26	106.71
29	a	619	BCR	C33-C5-C6	-5.67	118.16	124.53
35	a	618	XAT	O24-C25-C24	5.67	117.64	113.38
37	U	601	CHL	C2D-C1D-ND	5.67	114.28	110.10
29	B	846	BCR	C28-C27-C26	-5.67	103.96	114.08
26	B	831	CLA	C4A-NA-C1A	5.67	109.25	106.71
26	6	620	CLA	C4A-NA-C1A	5.67	109.25	106.71
35	6	621	XAT	C38-C25-C26	-5.66	112.77	122.26
29	3	620	BCR	C40-C30-C25	5.66	119.48	110.30
26	B	803	CLA	C4A-NA-C1A	5.66	109.25	106.71
29	L	309	BCR	C39-C30-C25	5.65	119.47	110.30
26	B	814	CLA	C4A-NA-C1A	5.64	109.24	106.71
26	B	807	CLA	C4A-NA-C1A	5.64	109.24	106.71
37	W	607	CHL	CHB-C1B-NB	-5.64	118.29	124.26
37	V	607	CHL	C3B-C2B-C1B	-5.63	100.36	107.16
29	B	801	BCR	C16-C17-C18	-5.63	119.28	127.31
26	1	609	CLA	C4A-NA-C1A	5.62	109.23	106.71
26	V	613	CLA	C4A-NA-C1A	5.60	109.22	106.71
26	A	805	CLA	C4A-NA-C1A	5.59	109.22	106.71
37	Y	607	CHL	CHD-C1D-ND	-5.57	119.34	124.45
29	7	621	BCR	C23-C24-C25	-5.57	111.57	127.20
26	1	602	CLA	C4A-NA-C1A	5.56	109.20	106.71
37	Y	601	CHL	C3B-C2B-C1B	-5.55	100.46	107.16
26	A	835	CLA	C4A-NA-C1A	5.55	109.20	106.71
29	K	207	BCR	C39-C30-C25	5.55	119.30	110.30
29	B	847	BCR	C38-C26-C25	-5.54	118.30	124.53
35	W	1622	XAT	C38-C25-C26	-5.54	112.98	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	X	607	CHL	C3C-C4C-NC	5.54	116.78	110.57
29	9	621	BCR	C33-C5-C6	-5.54	118.31	124.53
29	J	102	BCR	C20-C21-C22	-5.53	119.42	127.31
29	5	622	BCR	C8-C7-C6	-5.53	111.68	127.20
26	4	609	CLA	C4A-NA-C1A	5.53	109.19	106.71
36	5	624	NEX	O24-C25-C24	5.52	117.53	113.38
26	8	608	CLA	C4A-NA-C1A	5.52	109.19	106.71
37	U	605	CHL	C2D-C1D-ND	5.52	114.17	110.10
29	B	852	BCR	C32-C1-C2	-5.51	86.85	108.91
26	A	829	CLA	C4A-NA-C1A	5.51	109.18	106.71
34	a	617	LUT	C8-C7-C6	-5.51	111.74	127.20
26	A	811	CLA	C4A-NA-C1A	5.51	109.18	106.71
26	F	303	CLA	C4A-NA-C1A	5.50	109.18	106.71
37	U	608	CHL	C3B-C2B-C1B	-5.50	100.53	107.16
35	8	620	XAT	C18-C5-C6	-5.50	113.05	122.26
26	2	611	CLA	C4A-NA-C1A	5.49	109.18	106.71
37	X	605	CHL	C2D-C1D-ND	5.48	114.14	110.10
26	A	804	CLA	C4A-NA-C1A	5.48	109.17	106.71
29	B	852	BCR	C20-C21-C22	-5.48	119.50	127.31
36	U	1623	NEX	C35-C34-C33	-5.47	119.50	127.31
37	V	608	CHL	C3C-C4C-NC	5.47	116.70	110.57
35	9	620	XAT	C18-C5-C6	-5.47	113.09	122.26
29	8	621	BCR	C23-C24-C25	-5.47	111.84	127.20
37	Z	607	CHL	C3B-C2B-C1B	-5.46	100.57	107.16
35	4	620	XAT	O24-C25-C38	5.46	121.60	115.06
37	Z	609	CHL	O2D-CGD-CBD	5.46	120.97	111.27
26	9	609	CLA	C4A-NA-C1A	5.46	109.16	106.71
29	9	621	BCR	C7-C8-C9	5.46	134.48	126.23
26	G	203	CLA	C4A-NA-C1A	5.46	109.16	106.71
29	L	305	BCR	C11-C10-C9	-5.45	119.53	127.31
26	8	612	CLA	C4A-NA-C1A	5.45	109.16	106.71
34	1	617	LUT	C8-C7-C6	-5.44	111.91	127.20
27	B	842	PQN	C15-C13-C12	-5.44	110.11	121.12
29	6	622	BCR	C38-C26-C25	-5.44	118.42	124.53
37	U	606	CHL	C3C-C4C-NC	5.44	116.67	110.57
26	A	817	CLA	C4A-NA-C1A	5.43	109.15	106.71
26	B	804	CLA	C4A-NA-C1A	5.43	109.15	106.71
26	5	602	CLA	C4A-NA-C1A	5.43	109.15	106.71
29	L	308	BCR	C7-C8-C9	-5.43	118.03	126.23
26	A	854	CLA	C4A-NA-C1A	5.43	109.15	106.71
37	W	606	CHL	C3C-C4C-NC	5.43	116.66	110.57
37	X	607	CHL	C3B-C2B-C1B	-5.43	100.61	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	849	BCR	C28-C27-C26	-5.43	104.39	114.08
35	V	1622	XAT	C18-C5-C6	-5.42	113.17	122.26
29	O	2005	BCR	C40-C30-C39	-5.42	91.89	108.53
29	a	619	BCR	C8-C7-C6	-5.42	111.98	127.20
26	7	608	CLA	C4A-NA-C1A	5.42	109.14	106.71
29	1	619	BCR	C8-C7-C6	-5.42	111.99	127.20
26	Y	613	CLA	C4A-NA-C1A	5.42	109.14	106.71
29	a	619	BCR	C40-C30-C25	5.41	119.07	110.30
37	Z	607	CHL	C3C-C4C-NC	5.41	116.64	110.57
26	K	201	CLA	C4A-NA-C1A	5.40	109.13	106.71
37	V	607	CHL	CHD-C1D-ND	-5.40	119.49	124.45
29	1	619	BCR	C40-C30-C25	5.40	119.06	110.30
26	U	611	CLA	C4A-NA-C1A	5.40	109.13	106.71
26	a	602	CLA	C4A-NA-C1A	5.39	109.13	106.71
37	Y	607	CHL	C3B-C2B-C1B	-5.39	100.65	107.16
37	W	605	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
26	6	611	CLA	C4A-NA-C1A	5.39	109.13	106.71
29	3	620	BCR	C38-C26-C25	-5.38	118.48	124.53
37	W	609	CHL	C2D-C1D-ND	5.38	114.07	110.10
36	X	1623	NEX	C17-C1-C2	-5.38	84.90	109.05
26	B	833	CLA	C4A-NA-C1A	5.37	109.12	106.71
29	9	621	BCR	C27-C26-C25	-5.37	114.93	122.73
26	L	304	CLA	C4A-NA-C1A	5.37	109.12	106.71
37	V	606	CHL	O2D-CGD-CBD	5.36	120.80	111.27
35	V	1622	XAT	C38-C25-C26	-5.36	113.28	122.26
26	A	801	CLA	C4A-NA-C1A	5.36	109.12	106.71
26	B	805	CLA	C4A-NA-C1A	5.36	109.11	106.71
35	5	621	XAT	C18-C5-C6	-5.36	113.28	122.26
37	Y	605	CHL	C2D-C1D-ND	5.35	114.05	110.10
26	a	601	CLA	C4A-NA-C1A	5.35	109.11	106.71
26	a	616	CLA	C4A-NA-C1A	5.35	109.11	106.71
26	A	807	CLA	C4A-NA-C1A	5.34	109.11	106.71
37	Z	605	CHL	C3C-C4C-NC	5.34	116.56	110.57
37	Y	608	CHL	C3C-C4C-NC	5.33	116.55	110.57
34	W	1621	LUT	C15-C14-C13	-5.33	119.70	127.31
37	Z	608	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
29	O	2004	BCR	C3-C4-C5	-5.33	104.57	114.08
35	X	1622	XAT	C38-C25-C26	-5.32	113.34	122.26
36	X	1623	NEX	C15-C14-C13	-5.32	119.71	127.31
37	Y	605	CHL	O2D-CGD-CBD	5.32	120.72	111.27
37	V	609	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
26	A	813	CLA	C4A-NA-C1A	5.32	109.10	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	606	CLA	C4A-NA-C1A	5.32	109.10	106.71
26	A	838	CLA	C4A-NA-C1A	5.31	109.09	106.71
37	V	609	CHL	O2D-CGD-CBD	5.30	120.69	111.27
37	V	608	CHL	C3D-C2D-C1D	-5.30	98.60	105.83
26	9	613	CLA	C4A-NA-C1A	5.29	109.08	106.71
29	B	848	BCR	C8-C7-C6	-5.29	112.34	127.20
26	A	842	CLA	C4A-NA-C1A	5.29	109.08	106.71
26	K	203	CLA	C4A-NA-C1A	5.28	109.08	106.71
29	A	852	BCR	C3-C4-C5	-5.28	104.66	114.08
26	9	601	CLA	C4A-NA-C1A	5.28	109.08	106.71
35	U	1622	XAT	C38-C25-C26	-5.27	113.43	122.26
29	A	852	BCR	C37-C22-C23	5.26	126.37	118.08
26	V	612	CLA	C4A-NA-C1A	5.26	109.07	106.71
34	6	619	LUT	C8-C7-C6	-5.26	112.43	127.20
37	X	606	CHL	O2D-CGD-CBD	5.26	120.61	111.27
35	a	618	XAT	C38-C25-C26	-5.26	113.45	122.26
37	U	605	CHL	O2D-CGD-CBD	5.25	120.59	111.27
35	Z	1622	XAT	C6-C7-C8	-5.25	114.90	125.99
37	Y	608	CHL	C3D-C2D-C1D	-5.25	98.67	105.83
29	G	205	BCR	C8-C7-C6	-5.24	112.49	127.20
36	Z	1623	NEX	C15-C14-C13	-5.24	119.83	127.31
29	L	308	BCR	C28-C27-C26	-5.24	104.73	114.08
37	U	608	CHL	C3D-C2D-C1D	-5.23	98.69	105.83
37	Z	609	CHL	C3B-C2B-C1B	-5.23	100.84	107.16
35	1	618	XAT	C38-C25-C26	-5.23	113.49	122.26
37	U	605	CHL	CHB-C1B-NB	-5.23	118.72	124.26
37	X	607	CHL	C3D-C2D-C1D	-5.23	98.69	105.83
26	U	610	CLA	C4A-NA-C1A	5.23	109.06	106.71
26	A	830	CLA	C4A-NA-C1A	5.22	109.05	106.71
26	A	836	CLA	C4A-NA-C1A	5.22	109.05	106.71
34	2	619	LUT	C21-C26-C27	-5.22	106.10	112.70
37	W	605	CHL	C3C-C4C-NC	5.22	116.42	110.57
29	7	621	BCR	C8-C7-C6	-5.22	112.55	127.20
37	V	607	CHL	C3C-C4C-NC	5.22	116.42	110.57
26	2	613	CLA	C4A-NA-C1A	5.22	109.05	106.71
37	V	608	CHL	C3B-C2B-C1B	-5.21	100.87	107.16
37	V	605	CHL	C3B-C2B-C1B	-5.21	100.87	107.16
37	W	608	CHL	C3B-C2B-C1B	-5.21	100.87	107.16
26	A	803	CLA	C4A-NA-C1A	5.20	109.04	106.71
26	B	832	CLA	C4A-NA-C1A	5.20	109.04	106.71
37	U	609	CHL	C3B-C2B-C1B	-5.20	100.89	107.16
26	9	611	CLA	C4A-NA-C1A	5.19	109.04	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	F	305	BCR	C38-C26-C25	-5.19	118.70	124.53
26	B	816	CLA	C4A-NA-C1A	5.19	109.04	106.71
37	Z	605	CHL	C3B-C2B-C1B	-5.18	100.91	107.16
37	X	605	CHL	C3B-C2B-C1B	-5.18	100.91	107.16
37	W	606	CHL	CHD-C1D-ND	-5.17	119.70	124.45
37	V	605	CHL	O2D-CGD-CBD	5.17	120.46	111.27
37	Y	605	CHL	C3B-C2B-C1B	-5.17	100.92	107.16
26	5	619	CLA	C4A-NA-C1A	5.17	109.03	106.71
37	U	606	CHL	C3B-C2B-C1B	-5.17	100.93	107.16
35	2	620	XAT	O4-C5-C4	5.16	117.26	113.38
29	B	852	BCR	C15-C16-C17	-5.16	112.91	123.47
26	9	606	CLA	C4A-NA-C1A	5.16	109.02	106.71
37	Y	607	CHL	C3D-C2D-C1D	-5.16	98.80	105.83
26	1	601	CLA	C4A-NA-C1A	5.15	109.02	106.71
37	Y	608	CHL	C3B-C2B-C1B	-5.15	100.95	107.16
37	X	608	CHL	C3C-C4C-NC	5.15	116.34	110.57
29	A	849	BCR	C20-C21-C22	-5.14	119.97	127.31
37	Z	606	CHL	C3D-C4D-ND	5.14	118.56	110.24
26	1	616	CLA	C4A-NA-C1A	5.14	109.02	106.71
37	X	601	CHL	C3C-C4C-NC	5.14	116.33	110.57
35	U	1622	XAT	C18-C5-C6	-5.14	113.65	122.26
29	L	309	BCR	C38-C26-C25	-5.14	118.76	124.53
37	Z	601	CHL	C3C-C4C-NC	5.14	116.33	110.57
29	B	844	BCR	C16-C17-C18	-5.13	119.98	127.31
37	Z	608	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
37	V	601	CHL	C3B-C2B-C1B	-5.13	100.97	107.16
26	4	608	CLA	C4A-NA-C1A	5.13	109.01	106.71
37	X	605	CHL	CHB-C1B-NB	-5.12	118.84	124.26
27	B	842	PQN	C14-C13-C15	-5.12	106.66	115.27
37	W	605	CHL	O2D-CGD-CBD	5.12	120.36	111.27
37	X	601	CHL	C3D-C2D-C1D	-5.12	98.85	105.83
37	U	605	CHL	C3B-C2B-C1B	-5.11	100.99	107.16
26	5	616	CLA	C4A-NA-C1A	5.11	109.00	106.71
37	W	601	CHL	O2D-CGD-CBD	5.11	120.35	111.27
37	Z	606	CHL	C3C-C4C-NC	5.11	116.30	110.57
37	U	601	CHL	C3B-C2B-C1B	-5.11	100.99	107.16
37	U	607	CHL	C3C-C4C-NC	5.11	116.30	110.57
26	6	602	CLA	C4A-NA-C1A	5.11	109.00	106.71
26	W	613	CLA	C4A-NA-C1A	5.11	109.00	106.71
37	X	601	CHL	C3B-C2B-C1B	-5.11	101.00	107.16
34	3	618	LUT	C18-C5-C6	-5.10	118.80	124.53
37	Y	606	CHL	C3C-C4C-NC	5.10	116.29	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	K	207	BCR	C30-C25-C26	-5.10	115.43	122.61
26	9	602	CLA	C4A-NA-C1A	5.10	109.00	106.71
37	X	601	CHL	CHB-C1B-NB	-5.09	118.86	124.26
29	4	621	BCR	C33-C5-C6	-5.09	118.81	124.53
37	Z	608	CHL	C3C-C4C-NC	5.09	116.28	110.57
29	2	623	BCR	C33-C5-C6	-5.09	118.82	124.53
37	W	607	CHL	C3B-C2B-C1B	-5.09	101.02	107.16
37	V	609	CHL	C3D-C4D-ND	5.09	118.47	110.24
37	W	608	CHL	C3C-C4C-NC	5.08	116.27	110.57
26	4	614	CLA	C4A-NA-C1A	5.08	108.99	106.71
37	W	605	CHL	C3D-C2D-C1D	-5.08	98.90	105.83
26	4	604	CLA	C4A-NA-C1A	5.08	108.99	106.71
36	Z	1623	NEX	C2-C1-C6	5.07	114.14	109.21
37	V	606	CHL	C3B-C2B-C1B	-5.07	101.04	107.16
37	Z	605	CHL	C3D-C2D-C1D	-5.07	98.91	105.83
37	W	601	CHL	C3B-C2B-C1B	-5.07	101.04	107.16
26	A	841	CLA	C4A-NA-C1A	5.07	108.98	106.71
35	U	1622	XAT	C31-C30-C29	-5.06	120.08	127.31
26	3	617	CLA	C4A-NA-C1A	5.06	108.98	106.71
29	L	301	BCR	C34-C9-C10	-5.06	115.84	122.92
29	6	622	BCR	C23-C24-C25	-5.05	113.01	127.20
37	U	608	CHL	C3C-C4C-NC	5.05	116.24	110.57
26	W	612	CLA	C4A-NA-C1A	5.05	108.98	106.71
37	X	609	CHL	C3D-C4D-ND	5.05	118.40	110.24
26	a	608	CLA	C4A-NA-C1A	5.05	108.97	106.71
37	U	609	CHL	C3C-C4C-NC	5.05	116.23	110.57
35	V	1622	XAT	O4-C5-C18	5.05	121.10	115.06
37	Y	601	CHL	C3C-C4C-NC	5.04	116.23	110.57
29	K	207	BCR	C40-C30-C29	-5.04	88.75	108.91
37	Z	601	CHL	C3D-C2D-C1D	-5.04	98.95	105.83
29	B	849	BCR	C33-C5-C6	-5.03	118.88	124.53
37	U	607	CHL	C3D-C2D-C1D	-5.03	98.96	105.83
26	A	810	CLA	C4A-NA-C1A	5.03	108.97	106.71
37	V	609	CHL	C3D-C2D-C1D	-5.03	98.97	105.83
35	2	620	XAT	C18-C5-C6	-5.03	113.83	122.26
26	1	608	CLA	C4A-NA-C1A	5.02	108.97	106.71
26	V	604	CLA	C4A-NA-C1A	5.02	108.97	106.71
26	2	614	CLA	C4A-NA-C1A	5.02	108.96	106.71
26	A	833	CLA	C4A-NA-C1A	5.02	108.96	106.71
26	A	825	CLA	C4A-NA-C1A	5.01	108.96	106.71
37	W	606	CHL	C3D-C2D-C1D	-5.01	99.00	105.83
35	Z	1622	XAT	C38-C25-C26	-5.01	113.87	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	O	2005	BCR	C20-C21-C22	-5.00	120.17	127.31
26	8	602	CLA	C4A-NA-C1A	5.00	108.95	106.71
37	Z	607	CHL	C3D-C2D-C1D	-5.00	99.01	105.83
29	O	2005	BCR	C8-C7-C6	-5.00	113.17	127.20
37	Z	607	CHL	CHB-C1B-NB	-5.00	118.97	124.26
34	Y	1621	LUT	C7-C8-C9	-5.00	118.69	126.23
36	Z	1623	NEX	C17-C1-C6	-5.00	106.00	110.47
37	Y	601	CHL	C3D-C2D-C1D	-5.00	99.01	105.83
29	5	622	BCR	C3-C4-C5	-4.99	105.16	114.08
26	6	609	CLA	C4A-NA-C1A	4.99	108.95	106.71
37	V	601	CHL	C3D-C4D-ND	4.99	118.31	110.24
37	Y	609	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
35	3	619	XAT	O4-C5-C18	4.98	121.03	115.06
26	A	826	CLA	C4A-NA-C1A	4.98	108.95	106.71
37	Y	606	CHL	C3D-C2D-C1D	-4.98	99.04	105.83
26	U	614	CLA	C4A-NA-C1A	4.98	108.94	106.71
35	Y	1622	XAT	C38-C25-C26	-4.98	113.92	122.26
37	Z	605	CHL	C3D-C4D-ND	4.97	118.28	110.24
37	V	606	CHL	CHD-C1D-ND	-4.97	119.89	124.45
37	W	608	CHL	C3D-C4D-ND	4.97	118.27	110.24
26	3	611	CLA	C4A-NA-C1A	4.96	108.94	106.71
26	8	606	CLA	C4A-NA-C1A	4.96	108.94	106.71
26	6	616	CLA	C4A-NA-C1A	4.95	108.93	106.71
26	7	611	CLA	C4A-NA-C1A	4.94	108.93	106.71
37	V	607	CHL	CHB-C1B-NB	-4.94	119.02	124.26
37	U	606	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
26	F	304	CLA	C4A-NA-C1A	4.94	108.92	106.71
26	6	606	CLA	C4A-NA-C1A	4.94	108.92	106.71
26	9	603	CLA	C4A-NA-C1A	4.94	108.92	106.71
34	V	1621	LUT	C11-C10-C9	-4.94	120.27	127.31
37	Y	606	CHL	C3D-C4D-ND	4.93	118.21	110.24
26	A	840	CLA	C4A-NA-C1A	4.93	108.92	106.71
26	8	611	CLA	C4A-NA-C1A	4.92	108.92	106.71
35	2	620	XAT	C38-C25-C26	-4.92	114.01	122.26
29	2	623	BCR	C7-C8-C9	-4.92	118.80	126.23
37	W	609	CHL	C3D-C4D-ND	4.92	118.20	110.24
37	U	609	CHL	C3D-C2D-C1D	-4.92	99.12	105.83
35	5	621	XAT	O4-C5-C18	4.92	120.95	115.06
29	B	852	BCR	C15-C14-C13	-4.92	120.29	127.31
26	4	613	CLA	C4A-NA-C1A	4.92	108.92	106.71
37	U	609	CHL	C3D-C4D-ND	4.92	118.19	110.24
37	W	608	CHL	C3D-C2D-C1D	-4.91	99.12	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	W	1622	XAT	C18-C5-C6	-4.91	114.03	122.26
29	K	202	BCR	C30-C25-C26	-4.91	115.69	122.61
29	K	202	BCR	C20-C21-C22	-4.91	120.30	127.31
37	Y	609	CHL	C3C-C4C-NC	4.91	116.08	110.57
37	V	605	CHL	C3D-C2D-C1D	-4.91	99.13	105.83
29	9	621	BCR	C34-C9-C8	4.91	125.81	118.08
37	X	606	CHL	C3D-C2D-C1D	-4.91	99.13	105.83
37	Z	601	CHL	C3B-C2B-C1B	-4.91	101.24	107.16
35	9	620	XAT	C38-C25-C26	-4.91	114.04	122.26
29	B	847	BCR	C23-C24-C25	-4.91	113.42	127.20
26	A	818	CLA	C4A-NA-C1A	4.90	108.91	106.71
34	W	1621	LUT	C11-C10-C9	-4.90	120.31	127.31
26	O	2003	CLA	C4A-NA-C1A	4.90	108.91	106.71
29	A	850	BCR	C23-C24-C25	-4.90	113.45	127.20
26	B	817	CLA	C4A-NA-C1A	4.89	108.91	106.71
37	U	608	CHL	C3D-C4D-ND	4.89	118.15	110.24
29	B	845	BCR	C34-C9-C10	-4.89	116.07	122.92
26	A	820	CLA	C4A-NA-C1A	4.89	108.90	106.71
26	A	808	CLA	C4A-NA-C1A	4.89	108.90	106.71
37	V	605	CHL	C3C-C4C-NC	4.89	116.05	110.57
34	7	619	LUT	C18-C5-C6	4.89	130.01	124.53
35	V	1622	XAT	C31-C30-C29	-4.89	120.34	127.31
35	W	1622	XAT	C37-C21-C26	-4.88	96.86	110.05
36	V	1623	NEX	C15-C14-C13	-4.88	120.34	127.31
37	V	601	CHL	C3D-C2D-C1D	-4.88	99.18	105.83
37	Y	609	CHL	C3B-C2B-C1B	-4.87	101.28	107.16
26	7	615	CLA	C4A-NA-C1A	4.87	108.90	106.71
37	Z	605	CHL	O2D-CGD-CBD	4.87	119.92	111.27
29	B	847	BCR	C24-C23-C22	-4.87	118.88	126.23
37	X	608	CHL	C1D-C2D-C3D	-4.87	99.83	106.94
29	B	844	BCR	C20-C21-C22	-4.87	120.36	127.31
29	7	621	BCR	C40-C30-C25	4.86	118.19	110.30
29	O	2005	BCR	C40-C30-C29	-4.86	89.45	108.91
37	X	606	CHL	C3C-C4C-NC	4.86	116.02	110.57
26	B	839	CLA	C4A-NA-C1A	4.85	108.89	106.71
37	X	606	CHL	C3D-C4D-ND	4.85	118.08	110.24
26	1	606	CLA	C4A-NA-C1A	4.85	108.89	106.71
37	W	605	CHL	C3D-C4D-ND	4.84	118.07	110.24
34	Y	1620	LUT	C11-C12-C13	-4.84	112.81	126.42
26	A	827	CLA	C4A-NA-C1A	4.84	108.88	106.71
26	B	835	CLA	C4A-NA-C1A	4.84	108.88	106.71
35	4	620	XAT	C18-C5-C6	-4.84	114.15	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	U	606	CHL	C3D-C4D-ND	4.84	118.06	110.24
36	U	1623	NEX	C38-C25-C26	-4.83	114.16	122.26
35	U	1622	XAT	O4-C5-C18	4.83	120.84	115.06
36	6	624	NEX	C5-C6-C1	4.83	124.49	119.70
36	6	624	NEX	C2-C1-C6	4.83	113.91	109.21
26	B	812	CLA	C4A-NA-C1A	4.83	108.88	106.71
37	X	609	CHL	C3D-C2D-C1D	-4.83	99.24	105.83
37	W	607	CHL	C3D-C2D-C1D	-4.83	99.24	105.83
37	V	601	CHL	C3C-C4C-NC	4.82	115.98	110.57
35	U	1622	XAT	C27-C28-C29	-4.82	118.05	125.53
26	3	613	CLA	C4A-NA-C1A	4.82	108.87	106.71
37	W	609	CHL	C3B-C2B-C1B	-4.82	101.35	107.16
26	8	607	CLA	C4A-NA-C1A	4.82	108.87	106.71
37	V	607	CHL	C3D-C2D-C1D	-4.81	99.26	105.83
29	L	308	BCR	C3-C4-C5	-4.81	105.48	114.08
35	V	1622	XAT	C15-C14-C13	-4.81	120.44	127.31
29	B	848	BCR	C28-C27-C26	-4.81	105.48	114.08
34	Y	1620	LUT	C7-C8-C9	-4.81	118.96	126.23
37	Y	609	CHL	C3D-C4D-ND	4.81	118.02	110.24
37	V	605	CHL	C3D-C4D-ND	4.81	118.02	110.24
36	Z	1623	NEX	C27-C28-C29	-4.81	118.07	125.53
26	H	203	CLA	C4A-NA-C1A	4.81	108.87	106.71
26	7	601	CLA	C4A-NA-C1A	4.81	108.87	106.71
36	Y	1623	NEX	C38-C25-C26	-4.80	114.21	122.26
26	2	616	CLA	C4A-NA-C1A	4.80	108.87	106.71
29	2	623	BCR	C8-C7-C6	-4.80	113.71	127.20
37	X	605	CHL	C3D-C4D-ND	4.80	118.01	110.24
29	G	205	BCR	C20-C21-C22	-4.80	120.46	127.31
26	3	609	CLA	C4A-NA-C1A	4.80	108.86	106.71
37	W	601	CHL	C3C-C4C-NC	4.80	115.95	110.57
37	V	608	CHL	C3D-C4D-ND	4.80	118.00	110.24
26	A	831	CLA	C4A-NA-C1A	4.80	108.86	106.71
26	2	607	CLA	C4A-NA-C1A	4.80	108.86	106.71
37	V	609	CHL	C3C-C4C-NC	4.79	115.94	110.57
26	4	606	CLA	C4A-NA-C1A	4.79	108.86	106.71
37	Z	609	CHL	C3D-C2D-C1D	-4.79	99.29	105.83
37	Z	606	CHL	C3B-C2B-C1B	-4.78	101.39	107.16
37	W	601	CHL	C3D-C4D-ND	4.78	117.97	110.24
36	Y	1623	NEX	C27-C28-C29	-4.78	118.11	125.53
37	W	609	CHL	C3D-C2D-C1D	-4.78	99.31	105.83
26	3	608	CLA	C4A-NA-C1A	4.78	108.85	106.71
29	F	305	BCR	C20-C21-C22	-4.78	120.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	614	CLA	C4A-NA-C1A	4.77	108.85	106.71
26	5	606	CLA	C4A-NA-C1A	4.77	108.85	106.71
34	U	1620	LUT	C15-C14-C13	-4.77	120.50	127.31
37	Y	608	CHL	C3D-C4D-ND	4.77	117.95	110.24
26	Z	611	CLA	C4A-NA-C1A	4.76	108.85	106.71
37	W	601	CHL	C3D-C2D-C1D	-4.76	99.33	105.83
37	W	607	CHL	C3C-C4C-NC	4.76	115.77	110.57
26	9	610	CLA	C4A-NA-C1A	4.76	108.85	106.71
34	X	1621	LUT	C35-C34-C33	-4.76	120.52	127.31
37	Z	606	CHL	O2D-CGD-CBD	4.76	119.72	111.27
37	X	606	CHL	C3B-C2B-C1B	-4.75	101.43	107.16
26	V	611	CLA	C4A-NA-C1A	4.75	108.84	106.71
36	V	1623	NEX	C38-C25-C26	-4.75	114.31	122.26
29	2	623	BCR	C20-C21-C22	-4.74	120.54	127.31
34	2	619	LUT	C1-C6-C5	-4.74	115.93	122.61
29	B	849	BCR	C27-C26-C25	-4.74	115.84	122.73
27	B	842	PQN	C14-C13-C12	-4.74	111.52	123.68
26	A	812	CLA	C4A-NA-C1A	4.73	108.83	106.71
34	9	619	LUT	C21-C26-C27	-4.73	106.72	112.70
37	Z	601	CHL	C3D-C4D-ND	4.73	117.89	110.24
26	B	808	CLA	C4A-NA-C1A	4.73	108.83	106.71
37	X	608	CHL	C3B-C2B-C1B	-4.72	101.46	107.16
37	U	605	CHL	C3D-C2D-C1D	-4.72	99.38	105.83
26	8	616	CLA	C4A-NA-C1A	4.72	108.83	106.71
36	X	1623	NEX	C38-C25-C26	-4.72	114.36	122.26
37	Y	605	CHL	C3D-C2D-C1D	-4.71	99.40	105.83
37	X	605	CHL	C3D-C2D-C1D	-4.71	99.40	105.83
37	X	605	CHL	O2D-CGD-CBD	4.71	119.64	111.27
26	G	204	CLA	C4A-NA-C1A	4.71	108.82	106.71
36	6	624	NEX	O24-C25-C38	4.71	120.70	115.06
37	U	605	CHL	C3D-C4D-ND	4.71	117.85	110.24
29	A	849	BCR	C24-C23-C22	-4.71	119.12	126.23
37	W	609	CHL	C3C-C4C-NC	4.71	115.85	110.57
36	X	1623	NEX	C27-C28-C29	-4.70	118.23	125.53
37	V	608	CHL	O2D-CGD-CBD	4.70	119.63	111.27
37	Z	606	CHL	C3D-C2D-C1D	-4.70	99.42	105.83
26	5	609	CLA	C4A-NA-C1A	4.70	108.82	106.71
37	Y	601	CHL	C3D-C4D-ND	4.70	117.84	110.24
34	2	619	LUT	C8-C7-C6	-4.70	114.01	127.20
29	5	622	BCR	C38-C26-C25	-4.70	119.25	124.53
34	V	1621	LUT	C15-C14-C13	-4.70	120.61	127.31
37	X	609	CHL	C3B-C2B-C1B	-4.69	101.50	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	X	609	CHL	C3C-C4C-NC	4.69	115.83	110.57
37	V	606	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
37	Z	601	CHL	O2D-CGD-CBD	4.69	119.59	111.27
26	B	802	CLA	C4A-NA-C1A	4.68	108.81	106.71
26	8	601	CLA	C4A-NA-C1A	4.68	108.81	106.71
36	5	624	NEX	C26-C27-C28	-4.68	116.10	125.99
37	Z	609	CHL	C3D-C4D-ND	4.68	117.81	110.24
26	2	612	CLA	C4A-NA-C1A	4.68	108.81	106.71
26	4	602	CLA	C4A-NA-C1A	4.68	108.81	106.71
35	X	1622	XAT	C18-C5-C6	-4.67	114.43	122.26
27	A	844	PQN	C15-C13-C12	-4.67	111.66	121.12
26	7	612	CLA	C4A-NA-C1A	4.67	108.81	106.71
26	3	607	CLA	C4A-NA-C1A	4.67	108.80	106.71
26	Z	602	CLA	C4A-NA-C1A	4.67	108.80	106.71
37	U	601	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
35	7	620	XAT	C38-C25-C26	-4.66	114.44	122.26
29	K	202	BCR	C36-C18-C19	4.66	125.43	118.08
26	5	607	CLA	C4A-NA-C1A	4.66	108.80	106.71
26	X	613	CLA	C4A-NA-C1A	4.66	108.80	106.71
35	U	1622	XAT	C37-C21-C26	-4.66	97.47	110.05
26	a	614	CLA	C4A-NA-C1A	4.66	108.80	106.71
26	8	609	CLA	C4A-NA-C1A	4.66	108.80	106.71
29	G	205	BCR	C16-C17-C18	-4.66	120.67	127.31
29	B	849	BCR	C23-C24-C25	-4.65	114.13	127.20
35	Y	1622	XAT	C6-C7-C8	-4.65	116.15	125.99
26	6	617	CLA	C4A-NA-C1A	4.65	108.80	106.71
37	U	606	CHL	O2D-CGD-CBD	4.65	119.53	111.27
37	Y	607	CHL	C3D-C4D-ND	4.65	117.75	110.24
36	Y	1623	NEX	C35-C34-C33	-4.64	120.68	127.31
26	3	604	CLA	C4A-NA-C1A	4.64	108.79	106.71
26	8	614	CLA	C4A-NA-C1A	4.64	108.79	106.71
29	B	801	BCR	C20-C21-C22	-4.64	120.68	127.31
29	B	853	BCR	C24-C23-C22	-4.64	119.22	126.23
26	5	617	CLA	C4A-NA-C1A	4.64	108.79	106.71
26	7	616	CLA	C4A-NA-C1A	4.64	108.79	106.71
29	B	849	BCR	C7-C8-C9	-4.64	119.23	126.23
26	5	604	CLA	C4A-NA-C1A	4.64	108.79	106.71
26	6	607	CLA	C4A-NA-C1A	4.64	108.79	106.71
35	a	618	XAT	O24-C25-C38	4.64	120.61	115.06
29	J	102	BCR	C36-C18-C19	4.63	125.38	118.08
26	X	602	CLA	C4A-NA-C1A	4.63	108.79	106.71
29	B	846	BCR	C3-C4-C5	-4.63	105.81	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	606	CLA	C4A-NA-C1A	4.63	108.79	106.71
36	Z	1623	NEX	C38-C25-C26	-4.63	114.50	122.26
29	1	619	BCR	C23-C24-C25	-4.63	114.21	127.20
34	5	620	LUT	C21-C26-C27	-4.63	106.85	112.70
29	B	849	BCR	C38-C26-C25	4.62	129.72	124.53
37	V	601	CHL	O2D-CGD-CBD	4.62	119.48	111.27
29	L	305	BCR	C33-C5-C4	4.62	122.49	113.62
35	Y	1622	XAT	C18-C5-C6	-4.62	114.52	122.26
26	O	2001	CLA	C4A-NA-C1A	4.62	108.78	106.71
29	7	623	BCR	C38-C26-C25	-4.61	119.35	124.53
26	1	614	CLA	C4A-NA-C1A	4.61	108.78	106.71
26	5	612	CLA	C4A-NA-C1A	4.61	108.78	106.71
29	a	619	BCR	C23-C24-C25	-4.61	114.25	127.20
35	1	618	XAT	O24-C25-C38	4.61	120.58	115.06
35	a	618	XAT	C18-C5-C6	-4.61	114.54	122.26
26	L	306	CLA	C4A-NA-C1A	4.61	108.78	106.71
26	3	615	CLA	C4A-NA-C1A	4.61	108.78	106.71
26	B	822	CLA	C4A-NA-C1A	4.60	108.78	106.71
26	9	607	CLA	C4A-NA-C1A	4.60	108.78	106.71
37	X	607	CHL	C3D-C4D-ND	4.60	117.69	110.24
35	V	1622	XAT	O24-C25-C38	4.60	120.57	115.06
35	X	1622	XAT	C15-C14-C13	-4.60	120.74	127.31
37	Y	601	CHL	CHB-C1B-NB	-4.60	119.39	124.26
37	W	609	CHL	O2D-CGD-CBD	4.60	119.44	111.27
26	8	604	CLA	C4A-NA-C1A	4.60	108.77	106.71
35	1	618	XAT	C18-C5-C6	-4.60	114.56	122.26
29	7	623	BCR	C20-C21-C22	-4.59	120.75	127.31
37	Y	605	CHL	C3D-C4D-ND	4.58	117.65	110.24
35	8	620	XAT	O24-C25-C38	4.58	120.55	115.06
26	B	828	CLA	C4A-NA-C1A	4.58	108.77	106.71
26	8	613	CLA	C4A-NA-C1A	4.58	108.77	106.71
26	A	832	CLA	C4A-NA-C1A	4.58	108.76	106.71
37	U	601	CHL	C3D-C4D-ND	4.57	117.64	110.24
37	Y	601	CHL	O2D-CGD-CBD	4.57	119.39	111.27
26	4	616	CLA	C4A-NA-C1A	4.57	108.76	106.71
37	U	608	CHL	O2D-CGD-CBD	4.57	119.39	111.27
29	L	309	BCR	C7-C8-C9	-4.56	119.34	126.23
26	X	612	CLA	C4A-NA-C1A	4.56	108.76	106.71
29	2	623	BCR	C38-C26-C25	-4.56	119.40	124.53
37	Z	609	CHL	C3C-C4C-NC	4.56	115.69	110.57
36	W	1623	NEX	C38-C25-C26	-4.56	114.61	122.26
29	L	309	BCR	C23-C24-C25	-4.56	114.39	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	843	CLA	C4A-NA-C1A	4.56	108.75	106.71
29	B	801	BCR	C28-C27-C26	-4.55	105.95	114.08
26	B	834	CLA	C4A-NA-C1A	4.55	108.75	106.71
26	X	611	CLA	C4A-NA-C1A	4.55	108.75	106.71
34	U	1621	LUT	C15-C14-C13	-4.55	120.81	127.31
37	Z	608	CHL	C3D-C4D-ND	4.55	117.60	110.24
26	4	618	CLA	C4A-NA-C1A	4.55	108.75	106.71
26	6	613	CLA	C4A-NA-C1A	4.54	108.75	106.71
26	9	604	CLA	C4A-NA-C1A	4.54	108.75	106.71
26	K	206	CLA	C4A-NA-C1A	4.54	108.75	106.71
26	7	606	CLA	C4A-NA-C1A	4.54	108.75	106.71
29	7	621	BCR	C28-C27-C26	-4.54	105.98	114.08
35	W	1622	XAT	C11-C10-C9	-4.54	120.84	127.31
26	B	823	CLA	C4A-NA-C1A	4.53	108.74	106.71
37	U	601	CHL	O2D-CGD-CBD	4.53	119.32	111.27
29	B	844	BCR	C15-C16-C17	-4.53	114.19	123.47
26	B	821	CLA	C4A-NA-C1A	4.53	108.74	106.71
29	A	851	BCR	C37-C22-C23	4.53	125.21	118.08
35	U	1622	XAT	C6-C7-C8	-4.53	116.42	125.99
29	J	102	BCR	C15-C16-C17	-4.52	114.21	123.47
37	Y	606	CHL	O2D-CGD-CBD	4.52	119.31	111.27
35	3	619	XAT	C6-C7-C8	-4.52	116.43	125.99
26	F	301	CLA	C4A-NA-C1A	4.52	108.74	106.71
26	4	610	CLA	C4A-NA-C1A	4.52	108.74	106.71
29	3	621	BCR	C8-C7-C6	-4.52	114.52	127.20
36	Y	1623	NEX	C15-C14-C13	-4.51	120.87	127.31
34	Z	1620	LUT	C11-C10-C9	-4.51	120.87	127.31
26	4	601	CLA	C4A-NA-C1A	4.51	108.73	106.71
26	X	614	CLA	C4A-NA-C1A	4.51	108.73	106.71
35	9	620	XAT	C26-C27-C28	-4.51	116.46	125.99
34	V	1621	LUT	C7-C8-C9	-4.51	119.43	126.23
37	V	605	CHL	CHB-C1B-NB	-4.50	119.49	124.26
37	U	607	CHL	C3D-C4D-ND	4.50	117.52	110.24
26	Y	604	CLA	C4A-NA-C1A	4.50	108.73	106.71
35	Z	1622	XAT	C26-C27-C28	-4.50	116.48	125.99
34	V	1620	LUT	C11-C10-C9	-4.50	120.89	127.31
26	J	101	CLA	C4A-NA-C1A	4.50	108.73	106.71
29	a	619	BCR	C20-C21-C22	-4.49	120.90	127.31
35	Z	1622	XAT	C18-C5-C6	-4.49	114.73	122.26
35	6	621	XAT	C18-C5-C6	-4.49	114.74	122.26
29	6	622	BCR	C8-C7-C6	-4.48	114.61	127.20
26	Z	614	CLA	C4A-NA-C1A	4.48	108.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Z	607	CHL	C3D-C4D-ND	4.48	117.48	110.24
26	6	608	CLA	C4A-NA-C1A	4.48	108.72	106.71
29	B	843	BCR	C16-C17-C18	-4.47	120.93	127.31
26	B	818	CLA	C4A-NA-C1A	4.47	108.72	106.71
26	5	610	CLA	C4A-NA-C1A	4.47	108.72	106.71
26	5	611	CLA	C4A-NA-C1A	4.47	108.72	106.71
34	6	619	LUT	C18-C5-C6	-4.47	119.51	124.53
29	A	848	BCR	C36-C18-C17	-4.47	116.66	122.92
29	K	207	BCR	C29-C30-C25	4.47	117.36	110.48
35	5	621	XAT	C38-C25-C26	-4.47	114.78	122.26
29	K	207	BCR	C20-C21-C22	-4.46	120.95	127.31
36	5	624	NEX	O24-C25-C38	4.46	120.40	115.06
34	Z	1620	LUT	C7-C8-C9	-4.46	119.50	126.23
29	B	847	BCR	C33-C5-C6	-4.46	119.52	124.53
26	6	610	CLA	C4A-NA-C1A	4.45	108.71	106.71
35	5	621	XAT	C6-C7-C8	-4.44	116.60	125.99
26	4	611	CLA	C4A-NA-C1A	4.44	108.70	106.71
29	A	850	BCR	C20-C21-C22	-4.44	120.98	127.31
37	Y	608	CHL	O2D-CGD-CBD	4.44	119.15	111.27
26	A	845	CLA	CMB-C2B-C1B	-4.44	118.61	125.37
34	W	1620	LUT	C11-C10-C9	-4.43	120.98	127.31
37	Y	606	CHL	CAC-C3C-C4C	4.43	130.56	124.81
37	V	608	CHL	CHD-C4C-C3C	-4.43	118.33	124.84
26	7	610	CLA	C4A-NA-C1A	4.43	108.70	106.71
29	1	619	BCR	C20-C21-C22	-4.43	120.99	127.31
35	W	1622	XAT	O4-C5-C18	4.42	120.36	115.06
26	5	608	CLA	C4A-NA-C1A	4.42	108.69	106.71
29	5	622	BCR	C33-C5-C6	-4.41	119.57	124.53
26	V	614	CLA	C4A-NA-C1A	4.41	108.69	106.71
29	6	622	BCR	C28-C27-C26	-4.41	106.20	114.08
29	O	2004	BCR	C20-C21-C22	-4.41	121.01	127.31
29	B	852	BCR	C19-C18-C17	-4.41	112.17	118.94
37	Z	608	CHL	CHB-C1B-NB	-4.41	119.59	124.26
29	B	847	BCR	C3-C4-C5	-4.40	106.21	114.08
26	2	609	CLA	C4A-NA-C1A	4.39	108.68	106.71
37	Y	607	CHL	CHB-C1B-NB	-4.39	119.61	124.26
26	B	836	CLA	CMB-C2B-C1B	-4.39	118.68	125.37
37	V	607	CHL	C3D-C4D-ND	4.39	117.34	110.24
29	B	843	BCR	C20-C21-C22	-4.39	121.05	127.31
37	Y	606	CHL	C3B-C2B-C1B	-4.38	101.87	107.16
37	W	606	CHL	C3B-C2B-C1B	-4.38	101.87	107.16
37	Y	605	CHL	C3C-C4C-NC	4.38	115.49	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	X	1620	LUT	C7-C8-C9	-4.38	119.61	126.23
35	8	620	XAT	O24-C25-C24	4.38	116.67	113.38
29	B	801	BCR	C37-C22-C23	4.37	124.97	118.08
26	L	302	CLA	C4A-NA-C1A	4.37	108.67	106.71
26	H	202	CLA	C4A-NA-C1A	4.36	108.67	106.71
26	7	602	CLA	C4A-NA-C1A	4.36	108.67	106.71
37	W	606	CHL	C3D-C4D-ND	4.36	117.29	110.24
26	B	830	CLA	C4A-NA-C1A	4.36	108.67	106.71
35	4	620	XAT	C6-C7-C8	-4.36	116.78	125.99
26	U	604	CLA	C4A-NA-C1A	4.35	108.66	106.71
34	6	619	LUT	C16-C1-C6	4.35	117.36	110.30
37	U	601	CHL	C3C-C4C-NC	4.35	115.45	110.57
26	7	604	CLA	C4A-NA-C1A	4.35	108.66	106.71
29	B	845	BCR	C24-C23-C22	-4.34	119.68	126.23
32	H	205	LMG	O7-C10-C11	4.34	120.85	111.50
37	X	601	CHL	C3D-C4D-ND	4.34	117.25	110.24
29	K	207	BCR	C7-C8-C9	-4.34	119.68	126.23
36	U	1623	NEX	C27-C28-C29	-4.33	118.81	125.53
29	L	309	BCR	C16-C17-C18	-4.33	121.14	127.31
35	2	620	XAT	O4-C5-C18	4.33	120.24	115.06
32	J	103	LMG	O7-C10-C11	4.33	120.83	111.50
36	Z	1623	NEX	C31-C30-C29	-4.33	121.14	127.31
29	O	2005	BCR	C30-C25-C26	-4.32	116.53	122.61
29	B	843	BCR	C7-C8-C9	-4.32	119.71	126.23
29	B	844	BCR	C19-C18-C17	-4.32	112.31	118.94
37	U	605	CHL	C3C-C4C-NC	4.31	115.41	110.57
37	U	606	CHL	CHD-C4C-C3C	-4.31	118.50	124.84
37	V	606	CHL	C3D-C4D-ND	4.31	117.22	110.24
29	3	621	BCR	C33-C5-C6	-4.31	119.69	124.53
29	L	301	BCR	C28-C27-C26	-4.31	106.38	114.08
29	O	2005	BCR	C29-C30-C25	4.31	117.12	110.48
35	W	1622	XAT	C15-C14-C13	-4.31	121.16	127.31
29	B	843	BCR	C37-C22-C23	4.31	124.87	118.08
37	Y	608	CHL	CHD-C4C-C3C	-4.31	118.51	124.84
26	Y	614	CLA	C4A-NA-C1A	4.31	108.64	106.71
35	8	620	XAT	C38-C25-C26	-4.31	115.04	122.26
26	5	618	CLA	C4A-NA-C1A	4.30	108.64	106.71
26	7	607	CLA	C4A-NA-C1A	4.30	108.64	106.71
26	5	614	CLA	C4A-NA-C1A	4.30	108.64	106.71
29	B	844	BCR	C38-C26-C25	4.30	129.35	124.53
34	3	618	LUT	C19-C9-C8	-4.30	111.31	118.08
37	W	601	CHL	CHB-C1B-NB	-4.30	119.71	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	V	606	CHL	CHD-C4C-C3C	-4.29	118.53	124.84
28	2	622	LHG	O7-C7-C8	4.29	120.75	111.50
35	Y	1622	XAT	O24-C25-C38	4.28	120.19	115.06
34	5	620	LUT	C35-C15-C14	-4.28	114.70	123.47
29	5	622	BCR	C37-C22-C21	-4.28	116.92	122.92
26	3	602	CLA	C4A-NA-C1A	4.28	108.63	106.71
29	3	622	BCR	C16-C17-C18	-4.28	121.20	127.31
29	7	621	BCR	C20-C21-C22	-4.28	121.20	127.31
26	A	829	CLA	CMB-C2B-C1B	-4.27	118.86	125.37
36	Y	1623	NEX	C16-C1-C6	-4.27	106.65	110.47
29	B	847	BCR	C8-C7-C6	-4.27	115.20	127.20
35	2	620	XAT	O24-C25-C38	4.27	120.17	115.06
37	U	607	CHL	O2D-CGD-CBD	4.27	118.86	111.27
26	V	602	CLA	C4A-NA-C1A	4.27	108.62	106.71
37	Z	601	CHL	CHB-C1B-NB	-4.26	119.74	124.26
37	U	607	CHL	CHB-C1B-NB	-4.26	119.74	124.26
36	V	1623	NEX	C27-C28-C29	-4.26	118.92	125.53
29	A	851	BCR	C3-C4-C5	-4.26	106.47	114.08
29	B	844	BCR	C7-C8-C9	-4.26	119.79	126.23
34	V	1621	LUT	C31-C30-C29	-4.26	121.24	127.31
29	B	852	BCR	C23-C24-C25	-4.25	115.26	127.20
37	Z	608	CHL	O2D-CGD-CBD	4.25	118.83	111.27
37	Y	607	CHL	CHD-C4C-C3C	-4.25	118.59	124.84
29	B	846	BCR	C20-C21-C22	-4.25	121.25	127.31
37	X	607	CHL	CAC-C3C-C4C	4.24	130.32	124.81
29	8	621	BCR	C20-C21-C22	-4.24	121.26	127.31
35	9	620	XAT	C6-C7-C8	-4.24	117.03	125.99
29	L	301	BCR	C20-C21-C22	-4.24	121.27	127.31
27	A	844	PQN	C14-C13-C12	-4.23	112.82	123.68
35	X	1622	XAT	O24-C25-C38	4.23	120.13	115.06
35	V	1622	XAT	C35-C34-C33	-4.23	121.27	127.31
26	4	607	CLA	C4A-NA-C1A	4.23	108.61	106.71
37	W	606	CHL	C3B-C4B-NB	4.23	114.44	110.52
37	W	607	CHL	C3D-C4D-ND	4.22	117.07	110.24
34	V	1620	LUT	C35-C34-C33	-4.22	121.29	127.31
35	V	1622	XAT	C11-C10-C9	-4.22	121.29	127.31
37	U	607	CHL	CHD-C4C-C3C	-4.22	118.64	124.84
29	A	852	BCR	C36-C18-C17	-4.21	117.03	122.92
26	A	826	CLA	CMB-C2B-C1B	-4.21	118.96	125.37
29	L	305	BCR	C3-C4-C5	-4.21	106.56	114.08
35	Z	1622	XAT	C35-C34-C33	-4.21	121.31	127.31
29	3	622	BCR	C3-C4-C5	-4.19	106.59	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	848	BCR	C37-C22-C23	4.19	124.68	118.08
26	W	610	CLA	C4A-NA-C1A	4.19	108.59	106.71
37	X	607	CHL	CHD-C4C-C3C	-4.19	118.69	124.84
32	8	626	LMG	O7-C10-C11	4.19	120.52	111.50
29	B	852	BCR	C35-C13-C12	-4.19	111.48	118.08
34	a	617	LUT	C18-C5-C6	-4.18	119.83	124.53
29	B	845	BCR	C29-C30-C25	4.18	116.91	110.48
29	9	621	BCR	C38-C26-C25	4.17	129.21	124.53
26	1	604	CLA	C4A-NA-C1A	4.17	108.58	106.71
37	Z	607	CHL	CAC-C3C-C4C	4.16	130.21	124.81
29	9	621	BCR	C8-C9-C10	-4.16	112.56	118.94
37	X	608	CHL	O2D-CGD-CBD	4.16	118.43	111.49
29	B	847	BCR	C15-C16-C17	-4.16	114.96	123.47
35	Z	1622	XAT	C35-C15-C14	-4.15	114.97	123.47
37	U	601	CHL	CMB-C2B-C1B	4.15	131.69	125.37
26	2	610	CLA	C4A-NA-C1A	4.15	108.57	106.71
34	1	617	LUT	C18-C5-C6	-4.15	119.87	124.53
29	B	853	BCR	C37-C22-C23	4.14	124.61	118.08
29	L	308	BCR	C30-C25-C24	4.14	127.50	115.78
33	B	850	DGD	O2G-C1B-C2B	4.14	120.43	111.50
26	6	604	CLA	C4A-NA-C1A	4.14	108.57	106.71
37	W	608	CHL	O2D-CGD-CBD	4.14	118.63	111.27
29	9	621	BCR	C16-C17-C18	-4.14	121.40	127.31
35	Z	1622	XAT	O24-C25-C38	4.14	120.01	115.06
35	2	620	XAT	C35-C15-C14	-4.14	115.00	123.47
29	A	852	BCR	C34-C9-C10	-4.14	117.13	122.92
35	X	1622	XAT	O4-C5-C18	4.13	120.01	115.06
26	2	603	CLA	C4A-NA-C1A	4.13	108.56	106.71
26	a	613	CLA	C4A-NA-C1A	4.13	108.56	106.71
29	B	845	BCR	C3-C4-C5	-4.13	106.71	114.08
34	5	620	LUT	C3-C4-C5	-4.13	103.63	111.85
36	5	624	NEX	C5-C6-C1	4.13	123.79	119.70
29	9	621	BCR	C20-C21-C22	-4.12	121.43	127.31
36	W	1623	NEX	C27-C28-C29	-4.12	119.14	125.53
37	X	601	CHL	CMB-C2B-C1B	4.12	131.64	125.37
29	A	848	BCR	C20-C21-C22	-4.12	121.43	127.31
26	a	604	CLA	C4A-NA-C1A	4.11	108.56	106.71
37	W	606	CHL	CAC-C3C-C4C	4.11	130.15	124.81
37	Z	601	CHL	CHD-C4C-C3C	-4.11	118.80	124.84
26	Z	604	CLA	C4A-NA-C1A	4.11	108.55	106.71
29	3	620	BCR	C28-C27-C26	-4.11	106.74	114.08
34	8	619	LUT	C18-C5-C6	-4.11	119.91	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	849	BCR	C1-C6-C5	-4.10	116.83	122.61
29	O	2005	BCR	C16-C17-C18	-4.10	121.45	127.31
37	Y	609	CHL	C3B-C4B-NB	4.10	114.32	110.52
29	A	851	BCR	C16-C17-C18	-4.09	121.47	127.31
35	Z	1622	XAT	O4-C5-C18	4.09	119.96	115.06
36	U	1623	NEX	O24-C25-C38	4.09	119.96	115.06
36	Z	1623	NEX	C5-C6-C1	4.09	123.75	119.70
35	U	1622	XAT	C35-C34-C33	-4.08	121.48	127.31
26	6	612	CLA	C4A-NA-C1A	4.08	108.54	106.71
37	W	606	CHL	O2D-CGD-CBD	4.08	118.52	111.27
34	Y	1620	LUT	C35-C34-C33	4.08	133.13	127.31
28	O	2631	LHG	O7-C7-C8	4.08	120.29	111.50
26	B	815	CLA	C4A-NA-C1A	4.07	108.54	106.71
26	W	604	CLA	C4A-NA-C1A	4.07	108.54	106.71
37	Z	607	CHL	O2D-CGD-CBD	4.07	118.51	111.27
35	Y	1622	XAT	C31-C30-C29	-4.07	121.50	127.31
36	X	1623	NEX	O24-C25-C38	4.07	119.93	115.06
29	3	622	BCR	C20-C21-C22	-4.06	121.52	127.31
26	1	613	CLA	C4A-NA-C1A	4.05	108.53	106.71
29	A	851	BCR	C20-C21-C22	-4.05	121.53	127.31
36	X	1623	NEX	C35-C34-C33	-4.05	121.53	127.31
29	3	620	BCR	C23-C24-C25	-4.05	115.83	127.20
37	X	607	CHL	O2D-CGD-CBD	4.05	118.46	111.27
37	U	608	CHL	CHD-C4C-C3C	-4.05	118.89	124.84
35	4	620	XAT	C38-C25-C26	-4.05	115.48	122.26
29	L	309	BCR	C20-C21-C22	-4.04	121.54	127.31
29	O	2005	BCR	C36-C18-C17	-4.04	117.26	122.92
26	B	829	CLA	C4A-NA-C1A	4.04	108.52	106.71
26	Y	602	CLA	C4A-NA-C1A	4.04	108.52	106.71
37	W	607	CHL	O2D-CGD-CBD	4.04	118.44	111.27
26	B	818	CLA	C4-C3-C5	4.03	122.06	115.27
26	a	611	CLA	C4A-NA-C1A	4.03	108.52	106.71
32	V	2631	LMG	O7-C10-C11	4.03	120.19	111.50
35	4	620	XAT	O24-C25-C24	4.03	116.41	113.38
28	U	2630	LHG	O7-C7-C8	4.03	120.19	111.50
37	X	605	CHL	C3C-C4C-NC	4.02	115.08	110.57
37	X	601	CHL	O2D-CGD-CBD	4.02	118.42	111.27
26	B	829	CLA	CMB-C2B-C1B	-4.02	119.25	125.37
26	9	614	CLA	C4A-NA-C1A	4.01	108.51	106.71
28	W	2630	LHG	O7-C7-C8	4.00	120.12	111.50
29	L	305	BCR	C37-C22-C21	-4.00	117.33	122.92
35	X	1622	XAT	C6-C7-C8	-3.99	117.55	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	611	CLA	C4A-NA-C1A	3.99	108.50	106.71
37	W	606	CHL	CHD-C4C-C3C	-3.99	118.98	124.84
29	K	207	BCR	C24-C23-C22	-3.99	120.21	126.23
34	U	1621	LUT	C11-C10-C9	-3.98	121.62	127.31
29	O	2004	BCR	C24-C23-C22	-3.98	120.22	126.23
29	1	619	BCR	C36-C18-C17	-3.98	117.35	122.92
26	3	612	CLA	C4A-NA-C1A	3.98	108.50	106.71
26	A	836	CLA	C4-C3-C5	3.98	121.96	115.27
36	U	1623	NEX	C20-C13-C14	-3.98	117.35	122.92
37	Z	608	CHL	CHD-C4C-C3C	-3.97	119.00	124.84
35	3	619	XAT	C26-C27-C28	-3.97	117.59	125.99
26	B	825	CLA	C4A-NA-C1A	3.97	108.49	106.71
37	U	609	CHL	C3B-C4B-NB	3.97	114.20	110.52
34	7	619	LUT	C21-C26-C27	-3.97	107.69	112.70
29	B	852	BCR	C10-C11-C12	-3.96	110.85	123.22
29	B	848	BCR	C16-C17-C18	-3.96	121.65	127.31
34	W	1621	LUT	C35-C34-C33	-3.96	121.66	127.31
26	6	601	CLA	C4A-NA-C1A	3.96	108.49	106.71
35	Y	1622	XAT	O4-C5-C18	3.96	119.80	115.06
37	V	606	CHL	CAC-C3C-C4C	3.96	129.94	124.81
36	V	1623	NEX	C17-C1-C6	-3.96	106.93	110.47
29	L	301	BCR	C15-C16-C17	-3.95	115.38	123.47
34	2	619	LUT	C11-C10-C9	-3.95	121.67	127.31
29	L	308	BCR	C23-C22-C21	-3.95	112.88	118.94
35	W	1622	XAT	C6-C7-C8	-3.95	117.64	125.99
29	5	622	BCR	C36-C18-C17	-3.94	117.41	122.92
26	7	614	CLA	C4A-NA-C1A	3.93	108.47	106.71
29	J	102	BCR	C39-C30-C25	-3.93	103.93	110.30
37	Z	606	CHL	CHD-C4C-C3C	-3.93	119.07	124.84
29	a	619	BCR	C36-C18-C17	-3.92	117.42	122.92
29	B	844	BCR	C30-C25-C26	-3.92	117.09	122.61
26	U	602	CLA	C4A-NA-C1A	3.92	108.47	106.71
35	W	1622	XAT	O24-C25-C38	3.92	119.75	115.06
29	B	844	BCR	C37-C22-C23	3.92	124.26	118.08
29	B	848	BCR	C38-C26-C25	3.92	128.93	124.53
26	3	610	CLA	C4A-NA-C1A	3.92	108.47	106.71
26	Y	612	CLA	C4A-NA-C1A	3.92	108.47	106.71
29	L	305	BCR	C20-C21-C22	-3.92	121.72	127.31
37	X	606	CHL	CAC-C3C-C4C	3.92	129.89	124.81
31	A	857	LMU	C1'-C2'-C3'	3.92	118.15	110.00
35	9	620	XAT	O4-C5-C18	3.92	119.75	115.06
29	B	852	BCR	C37-C22-C21	-3.91	117.44	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	851	BCR	C30-C25-C24	3.91	126.85	115.78
29	L	308	BCR	C37-C22-C23	3.91	124.24	118.08
26	8	610	CLA	C4A-NA-C1A	3.91	108.46	106.71
29	3	622	BCR	C23-C24-C25	-3.91	116.22	127.20
33	B	850	DGD	O6D-C5D-C6D	3.91	114.56	106.67
29	3	620	BCR	C20-C21-C22	-3.91	121.73	127.31
26	O	2002	CLA	C4A-NA-C1A	3.91	108.46	106.71
29	B	844	BCR	C15-C14-C13	-3.91	121.73	127.31
29	A	849	BCR	C38-C26-C27	3.90	121.12	113.62
37	Y	606	CHL	CHD-C4C-C3C	-3.90	119.11	124.84
29	G	205	BCR	C38-C26-C25	-3.90	120.15	124.53
29	3	622	BCR	C7-C8-C9	-3.90	120.35	126.23
32	H	205	LMG	C8-O7-C10	-3.89	108.21	117.79
32	J	104	LMG	O7-C10-C11	3.89	119.88	111.50
29	L	309	BCR	C36-C18-C17	-3.89	117.48	122.92
34	3	618	LUT	C11-C10-C9	-3.88	121.78	127.31
37	X	608	CHL	CHD-C4C-C3C	-3.88	119.14	124.84
31	5	629	LMU	O5B-C1B-C2B	3.87	118.55	110.35
29	B	845	BCR	C36-C18-C19	3.87	124.18	118.08
37	X	608	CHL	CHB-C1B-NB	-3.87	120.16	124.26
29	1	619	BCR	C38-C26-C25	-3.86	120.19	124.53
29	B	849	BCR	C37-C22-C23	-3.86	111.99	118.08
29	4	621	BCR	C3-C4-C5	-3.86	107.18	114.08
29	L	309	BCR	C4-C5-C6	-3.86	117.12	122.73
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
29	B	844	BCR	C36-C18-C19	3.86	124.16	118.08
35	8	620	XAT	C26-C27-C28	-3.86	117.84	125.99
37	U	605	CHL	CAC-C3C-C4C	3.85	129.81	124.81
37	X	607	CHL	CHB-C1B-NB	-3.85	120.18	124.26
34	X	1620	LUT	C11-C10-C9	-3.85	121.82	127.31
29	a	619	BCR	C38-C26-C25	-3.85	120.21	124.53
37	Z	609	CHL	CHB-C1B-NB	-3.85	120.19	124.26
26	W	602	CLA	C4A-NA-C1A	3.85	108.44	106.71
29	B	852	BCR	C35-C13-C14	3.84	128.31	122.92
37	V	607	CHL	CHD-C4C-C3C	-3.84	119.19	124.84
29	B	847	BCR	C20-C21-C22	-3.84	121.83	127.31
29	F	305	BCR	C30-C25-C26	-3.84	117.20	122.61
35	7	620	XAT	C6-C7-C8	-3.84	117.88	125.99
35	Z	1622	XAT	C31-C30-C29	-3.83	121.84	127.31
37	Z	601	CHL	CMB-C2B-C1B	3.83	131.20	125.37
29	5	622	BCR	C20-C21-C22	-3.83	121.85	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	856	BCR	C20-C21-C22	-3.83	121.85	127.31
29	L	308	BCR	C20-C19-C18	-3.82	115.67	126.42
28	X	2630	LHG	O7-C7-C8	3.82	119.74	111.50
29	3	621	BCR	C20-C21-C22	-3.82	121.85	127.31
34	5	620	LUT	C8-C7-C6	-3.82	116.48	127.20
29	9	621	BCR	C37-C22-C23	3.82	124.09	118.08
34	3	618	LUT	C18-C5-C4	3.82	121.42	114.36
29	3	622	BCR	C16-C15-C14	-3.81	115.67	123.47
26	6	614	CLA	C4A-NA-C1A	3.81	108.42	106.71
37	Z	605	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
37	Y	607	CHL	CAC-C3C-C4C	3.81	129.75	124.81
29	J	102	BCR	C23-C24-C25	-3.80	116.53	127.20
29	K	202	BCR	C27-C26-C25	-3.80	117.21	122.73
37	Y	601	CHL	CHD-C4C-C3C	-3.80	119.26	124.84
29	O	2004	BCR	C36-C18-C17	-3.80	117.60	122.92
31	8	625	LMU	C1'-C2'-C3'	3.79	117.89	110.00
35	X	1622	XAT	C11-C10-C9	-3.79	121.91	127.31
35	8	620	XAT	O4-C5-C18	3.78	119.59	115.06
26	Z	612	CLA	C4A-NA-C1A	3.78	108.41	106.71
37	X	601	CHL	CHD-C4C-C3C	-3.78	119.28	124.84
29	A	849	BCR	C36-C18-C19	3.78	124.03	118.08
29	4	621	BCR	C38-C26-C25	-3.78	120.28	124.53
29	9	621	BCR	C3-C4-C5	-3.78	107.33	114.08
29	7	621	BCR	C38-C26-C25	-3.78	120.29	124.53
29	B	852	BCR	C11-C10-C9	3.78	132.70	127.31
26	4	612	CLA	C4A-NA-C1A	3.77	108.40	106.71
29	B	846	BCR	C37-C22-C23	3.77	124.02	118.08
37	W	605	CHL	CHD-C4C-C3C	-3.77	119.29	124.84
29	B	853	BCR	C7-C8-C9	-3.77	120.54	126.23
29	A	849	BCR	C27-C26-C25	-3.76	117.27	122.73
34	Y	1621	LUT	C15-C14-C13	-3.76	121.94	127.31
26	4	613	CLA	C1-O2A-CGA	3.76	126.31	116.44
26	1	610	CLA	C4A-NA-C1A	3.76	108.39	106.71
37	X	609	CHL	C3B-C4B-NB	3.76	114.00	110.52
37	V	609	CHL	C3B-C4B-NB	3.75	114.00	110.52
37	Y	607	CHL	C3B-C4B-NB	3.75	113.99	110.52
37	W	609	CHL	CHB-C1B-NB	-3.75	120.29	124.26
29	4	621	BCR	C20-C21-C22	-3.74	121.97	127.31
29	F	305	BCR	C38-C26-C27	3.74	120.81	113.62
32	5	627	LMG	O7-C10-C11	3.74	119.57	111.50
34	Y	1621	LUT	C35-C34-C33	-3.74	121.97	127.31
36	5	624	NEX	C39-C29-C30	-3.74	117.68	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	851	LHG	O7-C7-C8	3.74	119.56	111.50
35	Y	1622	XAT	C26-C27-C28	-3.74	118.08	125.99
26	7	602	CLA	C3B-C4B-NB	-3.74	107.05	110.52
29	O	2005	BCR	C38-C26-C25	-3.74	120.33	124.53
29	A	850	BCR	C16-C17-C18	-3.74	121.98	127.31
29	2	623	BCR	C16-C17-C18	-3.73	121.98	127.31
29	B	801	BCR	C16-C15-C14	-3.73	115.83	123.47
29	1	619	BCR	C28-C27-C26	-3.73	107.42	114.08
36	W	1623	NEX	C35-C34-C33	-3.72	122.00	127.31
29	B	847	BCR	C36-C18-C19	3.72	123.94	118.08
34	Y	1621	LUT	C1-C6-C5	-3.72	117.37	122.61
29	a	619	BCR	C28-C27-C26	-3.72	107.44	114.08
35	Z	1622	XAT	C11-C10-C9	-3.72	122.01	127.31
29	A	849	BCR	C3-C4-C5	-3.72	107.44	114.08
36	6	624	NEX	C26-C27-C28	-3.71	118.14	125.99
37	W	607	CHL	CHC-C4B-NB	-3.71	120.33	124.26
37	Z	607	CHL	CHD-C4C-C3C	-3.71	119.39	124.84
26	B	826	CLA	O2D-CGD-O1D	-3.71	116.59	123.84
29	L	305	BCR	C32-C1-C6	-3.70	104.29	110.30
36	Y	1623	NEX	C11-C10-C9	-3.70	122.03	127.31
29	B	849	BCR	C16-C17-C18	-3.69	122.04	127.31
29	B	853	BCR	C33-C5-C6	-3.69	120.38	124.53
37	X	608	CHL	CHC-C4B-NB	-3.69	120.35	124.26
37	Z	609	CHL	C3B-C4B-NB	3.69	113.94	110.52
35	2	620	XAT	C6-C7-C8	-3.69	118.20	125.99
37	X	608	CHL	CAC-C3C-C4C	3.69	129.59	124.81
34	X	1620	LUT	C15-C14-C13	-3.69	122.05	127.31
37	Y	607	CHL	O2D-CGD-CBD	3.69	117.82	111.27
37	X	601	CHL	C3B-C4B-NB	3.69	113.93	110.52
37	W	605	CHL	CHB-C1B-NB	-3.68	120.36	124.26
35	2	620	XAT	C27-C28-C29	-3.68	119.82	125.53
34	7	619	LUT	C19-C9-C8	-3.68	112.28	118.08
37	W	608	CHL	CAC-C3C-C4C	3.68	129.59	124.81
37	V	601	CHL	CHB-C1B-NB	-3.68	120.36	124.26
37	V	601	CHL	CHD-C4C-C3C	-3.68	119.44	124.84
37	X	607	CHL	C3B-C4B-NB	3.68	113.92	110.52
29	B	852	BCR	C36-C18-C19	3.67	123.87	118.08
29	L	308	BCR	C16-C17-C18	-3.67	122.07	127.31
34	W	1620	LUT	C35-C34-C33	-3.67	122.07	127.31
28	A	861	LHG	O7-C7-C8	3.67	119.42	111.50
26	B	830	CLA	CHD-C1D-ND	-3.67	121.08	124.45
26	a	610	CLA	C4A-NA-C1A	3.67	108.36	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Z	1620	LUT	C15-C14-C13	-3.66	122.09	127.31
28	9	622	LHG	O7-C7-C8	3.66	119.39	111.50
29	3	620	BCR	C11-C10-C9	-3.66	122.09	127.31
26	B	825	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
26	1	607	CLA	C4A-NA-C1A	3.66	108.35	106.71
29	B	852	BCR	C37-C22-C23	3.66	123.84	118.08
26	8	610	CLA	CMB-C2B-C1B	-3.66	119.80	125.37
29	B	845	BCR	C7-C8-C9	-3.66	120.71	126.23
26	A	822	CLA	C4A-NA-C1A	3.65	108.35	106.71
26	2	604	CLA	C4A-NA-C1A	3.65	108.35	106.71
29	2	623	BCR	C11-C10-C9	-3.65	122.10	127.31
35	U	1622	XAT	C15-C35-C34	-3.65	116.00	123.47
28	Z	2630	LHG	O7-C7-C8	3.65	119.37	111.50
37	W	601	CHL	CHC-C4B-NB	-3.65	120.40	124.26
29	A	848	BCR	C37-C22-C21	-3.64	117.82	122.92
29	F	305	BCR	C16-C15-C14	-3.64	116.01	123.47
29	K	202	BCR	C37-C22-C23	3.64	123.81	118.08
26	Y	611	CLA	C4A-NA-C1A	3.64	108.34	106.71
37	U	605	CHL	CHC-C4B-NB	-3.63	120.41	124.26
28	9	623	LHG	O7-C7-C8	3.63	119.33	111.50
29	B	801	BCR	C33-C5-C6	-3.63	120.45	124.53
35	8	620	XAT	C6-C7-C8	-3.63	118.31	125.99
29	A	852	BCR	C38-C26-C25	-3.63	120.45	124.53
36	V	1623	NEX	C15-C35-C34	-3.63	116.04	123.47
35	V	1622	XAT	C27-C28-C29	-3.63	119.90	125.53
36	U	1623	NEX	C31-C30-C29	-3.63	122.13	127.31
37	V	607	CHL	O2D-CGD-CBD	3.63	117.71	111.27
29	B	845	BCR	C37-C22-C23	3.63	123.79	118.08
26	Y	610	CLA	C4A-NA-C1A	3.62	108.33	106.71
36	U	1623	NEX	C15-C14-C13	-3.62	122.14	127.31
29	7	621	BCR	C33-C5-C6	-3.62	120.46	124.53
28	H	204	LHG	O7-C7-C8	3.62	119.30	111.50
26	3	610	CLA	C3B-C4B-NB	-3.62	107.16	110.52
29	7	623	BCR	C28-C27-C26	-3.62	107.62	114.08
26	A	854	CLA	CMB-C2B-C1B	-3.62	119.86	125.37
36	Y	1623	NEX	O24-C25-C38	3.62	119.39	115.06
28	V	2630	LHG	O7-C7-C8	3.62	119.29	111.50
28	3	624	LHG	O7-C7-C8	3.61	119.29	111.50
34	Y	1621	LUT	C11-C10-C9	-3.61	122.15	127.31
37	W	606	CHL	C1C-C2C-C3C	-3.61	104.25	107.11
34	8	619	LUT	C19-C9-C8	-3.60	112.40	118.08
37	U	606	CHL	CAC-C3C-C4C	3.60	129.48	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	6	621	XAT	C6-C7-C8	-3.60	118.39	125.99
29	3	620	BCR	C16-C17-C18	-3.59	122.18	127.31
29	B	801	BCR	C24-C23-C22	-3.59	120.80	126.23
37	X	606	CHL	CHC-C4B-NB	-3.59	120.45	124.26
37	V	609	CHL	CHB-C1B-NB	-3.59	120.45	124.26
34	V	1620	LUT	C15-C14-C13	-3.59	122.18	127.31
29	L	308	BCR	C30-C25-C26	-3.59	117.56	122.61
29	K	207	BCR	C11-C10-C9	-3.59	122.19	127.31
29	B	846	BCR	C8-C7-C6	-3.59	117.12	127.20
35	U	1622	XAT	O24-C25-C38	3.59	119.35	115.06
29	A	856	BCR	C33-C5-C6	-3.59	120.50	124.53
29	8	621	BCR	C8-C7-C6	-3.58	117.13	127.20
31	1	621	LMU	C1B-O1B-C4'	-3.58	109.10	117.96
29	3	621	BCR	C23-C24-C25	-3.58	117.14	127.20
28	5	625	LHG	O7-C7-C8	3.58	119.21	111.50
29	K	207	BCR	C39-C30-C29	3.58	123.21	108.91
29	3	620	BCR	C24-C23-C22	-3.57	120.84	126.23
28	9	624	LHG	O7-C7-C8	3.57	119.19	111.50
35	6	621	XAT	O4-C5-C18	3.56	119.33	115.06
34	U	1621	LUT	C35-C34-C33	-3.56	122.23	127.31
37	Z	605	CHL	C3B-C4B-NB	3.56	113.82	110.52
35	W	1622	XAT	C35-C34-C33	-3.56	122.23	127.31
37	W	608	CHL	CHD-C4C-C3C	-3.56	119.61	124.84
37	Y	606	CHL	CHC-C4B-NB	-3.56	120.49	124.26
34	5	620	LUT	C7-C8-C9	-3.55	120.86	126.23
37	Y	609	CHL	CHB-C1B-NB	-3.55	120.50	124.26
29	A	851	BCR	C23-C22-C21	-3.55	113.50	118.94
29	6	622	BCR	C20-C21-C22	-3.55	122.25	127.31
36	6	624	NEX	C39-C29-C30	-3.55	117.95	122.92
35	1	618	XAT	O4-C5-C18	3.55	119.30	115.06
37	V	609	CHL	CHD-C4C-C3C	-3.54	119.63	124.84
36	Y	1623	NEX	C5-C6-C1	3.54	123.21	119.70
29	B	845	BCR	C33-C5-C4	3.54	120.42	113.62
29	B	853	BCR	C20-C21-C22	-3.54	122.26	127.31
37	X	609	CHL	CAC-C3C-C4C	3.54	129.40	124.81
29	B	849	BCR	C3-C4-C5	-3.54	107.76	114.08
34	8	619	LUT	C16-C1-C6	3.54	116.04	110.30
29	7	623	BCR	C16-C17-C18	-3.54	122.26	127.31
35	X	1622	XAT	C35-C34-C33	-3.53	122.27	127.31
29	L	301	BCR	C36-C18-C19	3.53	123.64	118.08
29	8	621	BCR	C36-C18-C19	3.53	123.64	118.08
35	X	1622	XAT	C26-C27-C28	-3.53	118.53	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	608	CHL	C3B-C4B-NB	3.53	113.79	110.52
29	L	309	BCR	C8-C9-C10	-3.53	113.53	118.94
29	G	205	BCR	C16-C15-C14	-3.52	116.25	123.47
29	3	622	BCR	C11-C10-C9	-3.52	122.28	127.31
26	5	613	CLA	C4-C3-C5	3.52	121.20	115.27
37	V	607	CHL	CAC-C3C-C4C	3.52	129.38	124.81
32	4	624	LMG	O7-C10-C11	3.52	119.09	111.50
29	K	202	BCR	C16-C17-C18	-3.52	122.29	127.31
31	8	625	LMU	C2'-C3'-C4'	3.52	117.71	109.68
26	A	845	CLA	C4A-NA-C1A	3.52	108.29	106.71
26	X	604	CLA	C4A-NA-C1A	3.52	108.29	106.71
29	A	852	BCR	C7-C8-C9	-3.51	120.92	126.23
37	Z	605	CHL	CHB-C1B-NB	-3.51	120.54	124.26
29	O	2005	BCR	C3-C4-C5	-3.51	107.81	114.08
28	6	623	LHG	O7-C7-C8	3.51	119.07	111.50
37	W	601	CHL	CHD-C4C-C3C	-3.51	119.68	124.84
29	F	305	BCR	C36-C18-C19	3.51	123.61	118.08
29	7	623	BCR	C36-C18-C19	3.51	123.61	118.08
29	B	846	BCR	C30-C25-C24	3.51	125.70	115.78
35	1	618	XAT	C6-C7-C8	-3.50	118.59	125.99
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
37	Z	606	CHL	CAC-C3C-C4C	3.50	129.35	124.81
26	a	607	CLA	C4A-NA-C1A	3.49	108.28	106.71
26	8	604	CLA	C1-C2-C3	-3.49	121.10	126.75
26	8	610	CLA	C4-C3-C5	3.49	121.15	115.27
29	G	205	BCR	C36-C18-C17	-3.49	118.03	122.92
35	6	621	XAT	O24-C25-C38	3.49	119.24	115.06
29	A	856	BCR	C36-C18-C19	3.49	123.58	118.08
35	Z	1622	XAT	C4-C3-C2	-3.49	104.03	110.77
29	1	619	BCR	C37-C22-C23	3.49	123.57	118.08
29	B	845	BCR	C8-C9-C10	3.49	124.29	118.94
37	X	606	CHL	CHB-C1B-NB	-3.49	120.57	124.26
29	4	621	BCR	C16-C17-C18	-3.48	122.34	127.31
29	8	621	BCR	C37-C22-C21	-3.48	118.05	122.92
29	3	620	BCR	C7-C8-C9	-3.48	120.98	126.23
26	7	609	CLA	C4A-NA-C1A	3.47	108.27	106.71
28	Y	2630	LHG	O7-C7-C8	3.47	118.99	111.50
35	a	618	XAT	O4-C5-C18	3.47	119.22	115.06
37	Z	609	CHL	CAC-C3C-C4C	3.47	129.31	124.81
29	3	621	BCR	C37-C22-C23	3.47	123.54	118.08
35	9	620	XAT	C35-C15-C14	-3.47	116.37	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	849	BCR	C16-C17-C18	-3.47	122.36	127.31
26	A	814	CLA	C4-C3-C5	3.47	121.10	115.27
35	X	1622	XAT	C4-C3-C2	-3.46	104.09	110.77
29	B	844	BCR	C28-C27-C26	-3.45	107.91	114.08
31	A	858	LMU	C6B-C5B-C4B	-3.45	108.72	113.54
37	X	605	CHL	CHC-C4B-NB	-3.45	120.60	124.26
29	B	844	BCR	C24-C23-C22	-3.45	121.02	126.23
29	B	844	BCR	C21-C20-C19	-3.45	112.45	123.22
37	Y	605	CHL	CAC-C3C-C4C	3.45	129.29	124.81
29	A	851	BCR	C28-C27-C26	-3.45	107.92	114.08
29	6	622	BCR	C16-C17-C18	-3.44	122.39	127.31
29	9	621	BCR	C1-C6-C5	-3.44	117.76	122.61
26	2	610	CLA	C3B-C4B-NB	-3.44	107.32	110.52
26	4	613	CLA	O2A-CGA-O1A	-3.44	114.91	123.59
26	V	610	CLA	C4A-NA-C1A	3.44	108.25	106.71
35	6	621	XAT	C38-C25-C24	3.44	118.15	114.28
26	W	610	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
29	A	856	BCR	C16-C17-C18	-3.44	122.40	127.31
37	W	609	CHL	CAC-C3C-C4C	3.44	129.27	124.81
37	U	608	CHL	CHB-C1B-NB	-3.44	120.62	124.26
29	A	852	BCR	C31-C1-C6	-3.44	104.73	110.30
36	Z	1623	NEX	O24-C25-C38	3.43	119.17	115.06
29	J	102	BCR	C24-C23-C22	-3.43	121.05	126.23
35	2	620	XAT	C12-C13-C14	-3.43	113.68	118.94
35	Y	1622	XAT	C27-C28-C29	-3.43	120.21	125.53
26	Z	610	CLA	C4A-NA-C1A	3.42	108.25	106.71
35	4	620	XAT	C35-C15-C14	-3.42	116.46	123.47
29	a	619	BCR	C37-C22-C23	3.42	123.47	118.08
37	W	608	CHL	CHB-C1B-NB	-3.42	120.64	124.26
37	Y	609	CHL	CAC-C3C-C4C	3.42	129.25	124.81
29	L	305	BCR	C34-C9-C10	3.42	127.71	122.92
34	W	1620	LUT	C7-C8-C9	-3.42	121.07	126.23
36	V	1623	NEX	O24-C25-C38	3.42	119.15	115.06
29	J	102	BCR	C7-C8-C9	-3.42	121.07	126.23
29	L	301	BCR	C40-C30-C25	-3.41	104.76	110.30
29	A	849	BCR	C11-C10-C9	-3.41	122.44	127.31
26	Z	604	CLA	CMB-C2B-C1B	-3.41	120.17	125.37
37	Z	601	CHL	C1-C2-C3	-3.41	120.14	126.04
35	5	621	XAT	C8-C9-C10	-3.41	113.71	118.94
35	1	618	XAT	C26-C27-C28	-3.41	118.79	125.99
26	A	840	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
26	A	804	CLA	O2D-CGD-O1D	-3.40	117.19	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	K	202	BCR	C15-C16-C17	-3.40	116.50	123.47
34	6	619	LUT	C18-C5-C4	3.40	120.65	114.36
29	2	623	BCR	C39-C30-C25	-3.40	104.78	110.30
28	8	623	LHG	O7-C7-C8	3.40	118.82	111.50
37	W	609	CHL	CMD-C2D-C3D	-3.40	119.80	127.61
32	L	2631	LMG	C8-O7-C10	-3.39	109.44	117.79
34	Z	1620	LUT	C35-C34-C33	-3.39	122.47	127.31
29	A	850	BCR	C38-C26-C25	-3.39	120.72	124.53
34	5	620	LUT	C17-C1-C6	-3.39	104.80	110.30
34	5	620	LUT	C28-C29-C30	-3.39	113.74	118.94
29	F	305	BCR	C24-C23-C22	-3.39	121.12	126.23
37	U	609	CHL	CHB-C1B-NB	-3.39	120.67	124.26
26	Y	602	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
35	W	1622	XAT	C26-C27-C28	-3.38	118.84	125.99
26	A	802	CLA	CMB-C2B-C1B	-3.38	120.22	125.37
26	U	613	CLA	C4A-NA-C1A	3.38	108.23	106.71
29	L	308	BCR	C38-C26-C25	-3.38	120.73	124.53
37	W	605	CHL	C3B-C4B-NB	3.38	113.65	110.52
26	W	611	CLA	C4A-NA-C1A	3.38	108.22	106.71
29	A	856	BCR	C37-C22-C23	3.38	123.40	118.08
29	A	848	BCR	C16-C17-C18	-3.38	122.49	127.31
26	U	604	CLA	CMB-C2B-C1B	-3.38	120.22	125.37
29	G	205	BCR	C11-C10-C9	-3.37	122.50	127.31
37	Y	608	CHL	C3B-C4B-NB	3.37	113.64	110.52
37	U	609	CHL	CMB-C2B-C1B	3.37	130.50	125.37
36	Z	1623	NEX	C15-C35-C34	-3.37	116.57	123.47
29	8	621	BCR	C15-C16-C17	-3.37	116.58	123.47
26	9	612	CLA	C4A-NA-C1A	3.37	108.22	106.71
28	7	622	LHG	O7-C7-C8	3.36	118.75	111.50
26	1	602	CLA	CMB-C2B-C1B	-3.36	120.25	125.37
29	B	846	BCR	C11-C10-C9	-3.36	122.51	127.31
26	B	819	CLA	C4A-NA-C1A	3.36	108.22	106.71
34	U	1620	LUT	C7-C8-C9	-3.36	121.16	126.23
35	a	618	XAT	C26-C27-C28	-3.36	118.89	125.99
34	X	1621	LUT	C35-C15-C14	-3.36	116.59	123.47
26	A	854	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
29	O	2005	BCR	C39-C30-C29	3.36	122.33	108.91
29	3	621	BCR	C11-C10-C9	-3.35	122.52	127.31
35	U	1622	XAT	C11-C10-C9	-3.35	122.52	127.31
31	5	629	LMU	C1B-C2B-C3B	3.35	116.98	110.00
29	7	621	BCR	C37-C22-C23	3.35	123.36	118.08
35	3	619	XAT	C38-C25-C24	3.35	118.05	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	8	621	BCR	C37-C22-C23	3.35	123.36	118.08
29	B	852	BCR	C8-C7-C6	-3.35	117.80	127.20
29	K	202	BCR	C7-C8-C9	-3.35	121.17	126.23
34	1	617	LUT	C21-C26-C27	-3.35	108.47	112.70
34	a	617	LUT	C21-C26-C27	-3.34	108.47	112.70
37	V	605	CHL	CAC-C3C-C4C	3.34	129.15	124.81
37	Z	605	CHL	CAC-C3C-C4C	3.34	129.15	124.81
29	A	851	BCR	C7-C8-C9	-3.34	121.19	126.23
29	O	2005	BCR	C31-C1-C6	-3.34	104.88	110.30
26	1	604	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
34	V	1620	LUT	C7-C8-C9	-3.34	121.19	126.23
29	B	845	BCR	C16-C17-C18	-3.33	122.55	127.31
26	a	604	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
29	B	849	BCR	C33-C5-C4	3.33	120.02	113.62
29	B	844	BCR	C11-C10-C9	-3.33	122.55	127.31
26	A	829	CLA	CMB-C2B-C3B	3.33	134.66	126.59
29	5	622	BCR	C37-C22-C23	3.33	123.33	118.08
37	X	601	CHL	CAC-C3C-C4C	3.33	129.13	124.81
35	Y	1622	XAT	C35-C15-C14	-3.33	116.65	123.47
26	A	805	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
36	X	1623	NEX	C39-C29-C30	-3.33	118.26	122.92
29	3	622	BCR	C28-C27-C26	-3.33	108.14	114.08
26	a	602	CLA	CMB-C2B-C1B	-3.33	120.30	125.37
26	B	810	CLA	CAA-C2A-C3A	-3.32	103.68	112.78
35	3	619	XAT	O24-C25-C38	3.32	119.03	115.06
29	A	850	BCR	C33-C5-C6	-3.32	120.80	124.53
35	X	1622	XAT	C31-C30-C29	-3.31	122.58	127.31
35	W	1622	XAT	C31-C30-C29	-3.31	122.58	127.31
26	X	610	CLA	C4A-NA-C1A	3.31	108.20	106.71
29	G	205	BCR	C7-C8-C9	-3.31	121.23	126.23
29	4	621	BCR	C11-C10-C9	-3.31	122.59	127.31
35	Y	1622	XAT	C4-C3-C2	-3.31	104.38	110.77
35	7	620	XAT	C27-C28-C29	-3.31	120.40	125.53
26	8	602	CLA	CMB-C2B-C1B	-3.31	120.33	125.37
28	5	623	LHG	O7-C7-C8	3.30	118.62	111.50
29	G	205	BCR	C36-C18-C19	3.30	123.28	118.08
37	Z	606	CHL	CHC-C4B-NB	-3.30	120.76	124.26
26	A	820	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
29	L	305	BCR	C15-C14-C13	-3.30	122.61	127.31
29	L	305	BCR	C8-C9-C10	3.30	124.00	118.94
35	4	620	XAT	C27-C28-C29	-3.29	120.42	125.53
29	O	2004	BCR	C16-C17-C18	-3.29	122.61	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	822	CLA	CMB-C2B-C1B	-3.29	120.36	125.37
35	W	1622	XAT	C27-C28-C29	-3.29	120.42	125.53
36	Z	1623	NEX	C11-C10-C9	-3.29	122.62	127.31
37	V	605	CHL	CHD-C4C-C3C	-3.29	120.01	124.84
32	4	623	LMG	O7-C10-C11	3.28	118.58	111.50
34	Y	1620	LUT	C32-C33-C34	-3.28	113.91	118.94
29	K	202	BCR	C37-C22-C21	-3.28	118.33	122.92
37	W	606	CHL	CHB-C1B-NB	-3.28	120.79	124.26
29	A	850	BCR	C11-C10-C9	-3.28	122.63	127.31
26	9	613	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
26	1	614	CLA	C2A-C3A-C4A	-3.28	102.65	106.26
29	B	801	BCR	C29-C30-C25	3.27	115.52	110.48
29	L	309	BCR	C2-C1-C6	3.27	115.52	110.48
29	L	301	BCR	C4-C5-C6	-3.27	117.98	122.73
37	X	606	CHL	CHD-C4C-C3C	-3.27	120.03	124.84
37	U	609	CHL	CHD-C4C-C3C	-3.27	120.03	124.84
29	7	623	BCR	C36-C18-C17	-3.27	118.34	122.92
26	B	827	CLA	CHB-C4A-NA	3.27	129.03	124.51
34	V	1621	LUT	C35-C34-C33	-3.26	122.65	127.31
37	X	601	CHL	C1C-C2C-C3C	-3.26	104.52	107.11
29	B	849	BCR	C30-C25-C26	-3.26	118.02	122.61
29	B	852	BCR	C2-C1-C6	3.26	115.50	110.48
37	V	601	CHL	CHC-C4B-NB	-3.26	120.81	124.26
37	X	609	CHL	C1C-C2C-C3C	-3.26	104.53	107.11
29	5	622	BCR	C36-C18-C19	3.26	123.21	118.08
26	B	810	CLA	CHB-C4A-NA	3.26	129.02	124.51
35	Y	1622	XAT	C35-C34-C33	-3.26	122.66	127.31
35	6	621	XAT	C27-C28-C29	-3.26	120.48	125.53
35	6	621	XAT	C26-C27-C28	-3.25	119.12	125.99
29	B	801	BCR	C21-C20-C19	-3.25	113.08	123.22
37	U	609	CHL	C1C-C2C-C3C	-3.25	104.54	107.11
26	A	826	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
29	O	2005	BCR	C23-C24-C25	-3.25	118.09	127.20
34	Y	1621	LUT	C2-C3-C4	3.24	114.75	110.30
29	B	846	BCR	C24-C25-C26	-3.24	113.60	121.46
36	V	1623	NEX	C39-C29-C30	-3.24	118.38	122.92
37	Z	606	CHL	C4A-NA-C1A	-3.24	105.25	106.71
37	U	601	CHL	C3B-C4B-NB	3.24	113.52	110.52
37	V	608	CHL	CAC-C3C-C4C	3.24	129.01	124.81
37	Z	601	CHL	C4-C3-C5	3.23	120.70	115.27
26	U	610	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
36	U	1623	NEX	C16-C1-C6	3.23	113.36	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Z	601	CHL	C3B-C4B-NB	3.23	113.51	110.52
26	1	616	CLA	CMB-C2B-C3B	3.23	131.95	123.59
37	Y	605	CHL	CHC-C4B-NB	-3.23	120.84	124.26
35	U	1622	XAT	C31-C32-C33	-3.23	117.35	126.42
26	2	607	CLA	C3B-C4B-NB	-3.22	107.53	110.52
37	Z	607	CHL	CMB-C2B-C1B	3.22	130.28	125.37
34	W	1621	LUT	C31-C30-C29	-3.22	122.72	127.31
29	L	305	BCR	C16-C17-C18	-3.22	122.72	127.31
37	U	608	CHL	C3B-C4B-NB	3.21	113.50	110.52
26	A	832	CLA	CAA-C2A-C1A	-3.21	101.44	111.97
26	A	817	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
37	Y	609	CHL	C1C-C2C-C3C	-3.21	104.57	107.11
26	9	610	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
29	L	308	BCR	C21-C20-C19	-3.21	113.21	123.22
36	5	624	NEX	C38-C25-C24	3.21	117.89	114.28
36	Y	1623	NEX	C39-C29-C30	-3.20	118.44	122.92
26	2	604	CLA	CMB-C2B-C1B	-3.20	120.49	125.37
29	6	622	BCR	C36-C18-C19	3.20	123.12	118.08
35	1	618	XAT	C35-C15-C14	-3.20	116.92	123.47
35	7	620	XAT	C26-C27-C28	-3.20	119.23	125.99
37	W	607	CHL	CMB-C2B-C1B	3.20	130.24	125.37
29	B	846	BCR	C38-C26-C27	3.20	119.76	113.62
37	X	609	CHL	CMD-C2D-C3D	-3.20	120.26	127.61
26	B	838	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
34	Z	1620	LUT	C30-C31-C32	-3.19	113.25	123.22
26	Y	611	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
37	V	609	CHL	C1C-C2C-C3C	-3.19	104.58	107.11
29	2	623	BCR	C36-C18-C17	-3.19	118.45	122.92
29	3	620	BCR	C39-C30-C25	-3.19	105.12	110.30
34	X	1621	LUT	C30-C31-C32	-3.18	113.28	123.22
35	a	618	XAT	C35-C15-C14	-3.18	116.95	123.47
37	X	605	CHL	CAC-C3C-C4C	3.18	128.94	124.81
29	3	622	BCR	C37-C22-C23	3.18	123.09	118.08
29	A	851	BCR	C24-C25-C26	-3.18	113.75	121.46
29	B	849	BCR	C36-C18-C19	3.18	123.09	118.08
29	J	102	BCR	C38-C26-C25	-3.18	120.95	124.53
26	B	807	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
35	W	1622	XAT	C36-C21-C26	3.18	118.63	110.05
37	U	609	CHL	CAC-C3C-C4C	3.18	128.93	124.81
34	a	617	LUT	C16-C1-C6	3.18	115.45	110.30
26	A	809	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
32	A	860	LMG	O1-C1-C2	3.17	113.26	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1	617	LUT	C16-C1-C6	3.17	115.45	110.30
29	B	846	BCR	C7-C8-C9	-3.17	121.44	126.23
34	3	618	LUT	C16-C1-C6	3.17	115.44	110.30
37	W	606	CHL	CMB-C2B-C1B	3.17	130.20	125.37
32	L	2631	LMG	O7-C10-C11	3.17	118.33	111.50
34	6	619	LUT	C19-C9-C8	-3.17	113.08	118.08
37	V	608	CHL	C3B-C4B-NB	3.17	113.45	110.52
37	W	606	CHL	CHB-C4A-NA	3.16	128.88	124.51
26	8	602	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
37	U	601	CHL	CAC-C3C-C4C	3.16	128.91	124.81
37	W	605	CHL	CAC-C3C-C4C	3.15	128.90	124.81
32	J	104	LMG	C6-C5-C4	-3.15	105.62	113.00
34	4	619	LUT	C21-C26-C27	-3.15	108.72	112.70
37	U	601	CHL	C1C-C2C-C3C	-3.15	104.61	107.11
29	L	309	BCR	C15-C14-C13	-3.15	122.81	127.31
29	K	207	BCR	C36-C18-C19	3.15	123.04	118.08
29	B	852	BCR	C33-C5-C6	-3.15	120.99	124.53
26	A	832	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
26	B	837	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
29	K	202	BCR	C15-C14-C13	-3.15	122.82	127.31
37	Z	609	CHL	CMD-C2D-C3D	-3.15	120.37	127.61
35	V	1622	XAT	C6-C7-C8	-3.15	119.34	125.99
26	A	813	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
26	1	610	CLA	CBD-CHA-C1A	3.15	132.21	128.50
29	3	620	BCR	C36-C18-C17	-3.15	118.52	122.92
37	W	609	CHL	C3B-C4B-NB	3.15	113.43	110.52
26	U	614	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
37	Z	607	CHL	CHC-C4B-NB	-3.14	120.93	124.26
29	B	846	BCR	C36-C18-C19	3.14	123.03	118.08
29	A	856	BCR	C11-C10-C9	-3.14	122.82	127.31
37	U	607	CHL	CAC-C3C-C4C	3.14	128.89	124.81
27	B	842	PQN	C11-C3-C4	-3.14	115.14	118.50
26	V	602	CLA	CMB-C2B-C1B	-3.14	120.59	125.37
32	A	860	LMG	O7-C10-C11	3.13	118.25	111.50
35	4	620	XAT	C8-C9-C10	-3.13	114.13	118.94
35	7	620	XAT	O24-C25-C38	3.13	118.81	115.06
26	Y	614	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
26	A	843	CLA	CHB-C1B-NB	3.13	127.57	124.26
37	U	608	CHL	CMB-C2B-C1B	3.13	130.13	125.37
28	8	622	LHG	O7-C7-C8	3.13	118.24	111.50
26	1	609	CLA	CAB-C3B-C2B	3.13	131.70	123.59
29	L	308	BCR	C33-C5-C4	3.13	119.62	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	3	620	BCR	C37-C22-C23	3.13	123.00	118.08
29	7	621	BCR	C36-C18-C19	3.13	123.00	118.08
26	B	827	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
26	A	833	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
35	7	620	XAT	O4-C5-C18	3.12	118.80	115.06
37	Y	608	CHL	CHB-C1B-NB	-3.12	120.95	124.26
36	W	1623	NEX	C31-C30-C29	-3.12	122.86	127.31
34	Y	1620	LUT	C30-C31-C32	-3.12	113.48	123.22
35	V	1622	XAT	C26-C27-C28	-3.12	119.40	125.99
37	V	609	CHL	CMD-C2D-C3D	-3.12	120.44	127.61
28	A	847	LHG	O7-C7-C8	3.12	118.22	111.50
37	X	607	CHL	CHB-C4A-NA	3.12	128.82	124.51
29	L	309	BCR	C3-C4-C5	-3.12	108.51	114.08
26	U	604	CLA	CHB-C1B-NB	3.11	127.55	124.26
37	X	607	CHL	CMB-C2B-C1B	3.11	130.11	125.37
34	W	1620	LUT	C15-C14-C13	-3.11	122.87	127.31
37	Y	601	CHL	CAC-C3C-C4C	3.11	128.85	124.81
37	Z	608	CHL	CMD-C2D-C3D	-3.11	120.46	127.61
35	X	1622	XAT	C10-C11-C12	-3.11	113.52	123.22
26	A	840	CLA	O2D-CGD-CBD	3.11	116.79	111.27
37	Z	607	CHL	C3B-C4B-NB	3.11	113.40	110.52
26	9	602	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
26	V	612	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
29	J	102	BCR	C19-C18-C17	-3.10	114.19	118.94
26	5	619	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
26	B	820	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
29	B	843	BCR	C11-C10-C9	-3.10	122.89	127.31
29	A	850	BCR	C36-C18-C19	3.10	122.95	118.08
29	6	622	BCR	C11-C10-C9	-3.09	122.89	127.31
29	K	207	BCR	C23-C24-C25	-3.09	118.52	127.20
26	B	810	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
35	7	620	XAT	C35-C15-C14	-3.09	117.14	123.47
26	B	826	CLA	C1-C2-C3	-3.09	120.69	126.04
37	Y	608	CHL	C1C-C2C-C3C	-3.09	104.66	107.11
26	Z	614	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
34	6	619	LUT	C22-C23-C24	3.09	115.25	111.74
37	W	609	CHL	CHD-C4C-C3C	-3.09	120.30	124.84
26	B	836	CLA	CMB-C2B-C3B	3.09	134.06	126.59
36	X	1623	NEX	C16-C1-C2	3.09	122.91	109.05
26	7	601	CLA	CMB-C2B-C1B	-3.08	120.67	125.37
26	L	302	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
37	V	609	CHL	CAC-C3C-C4C	3.08	128.81	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	849	BCR	C7-C8-C9	-3.08	121.58	126.23
26	X	610	CLA	CHB-C1B-NB	3.08	127.52	124.26
37	U	608	CHL	C4A-NA-C1A	-3.08	105.32	106.71
29	6	622	BCR	C7-C8-C9	-3.08	121.58	126.23
26	5	607	CLA	C3B-C4B-NB	-3.08	107.66	110.52
34	8	619	LUT	C18-C5-C4	3.08	120.06	114.36
34	Z	1621	LUT	C35-C34-C33	-3.08	122.91	127.31
35	V	1622	XAT	C31-C32-C33	-3.08	117.76	126.42
37	U	601	CHL	CHC-C4B-NB	-3.08	121.00	124.26
37	Y	609	CHL	CHD-C4C-C3C	-3.08	120.32	124.84
35	2	620	XAT	C10-C11-C12	-3.08	113.62	123.22
29	2	623	BCR	C23-C24-C25	-3.07	118.57	127.20
37	Z	601	CHL	C1C-C2C-C3C	-3.07	104.67	107.11
26	A	845	CLA	CMB-C2B-C3B	3.07	134.03	126.59
26	2	610	CLA	CHB-C1B-NB	3.07	127.51	124.26
36	U	1623	NEX	C11-C12-C13	3.07	135.05	126.42
29	1	619	BCR	C30-C25-C24	3.07	124.47	115.78
26	2	601	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
26	O	2002	CLA	CMB-C2B-C3B	3.07	131.54	123.59
26	B	840	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
29	8	621	BCR	C1-C6-C5	-3.07	118.29	122.61
29	a	619	BCR	C30-C25-C24	3.07	124.46	115.78
26	Y	603	CLA	CHB-C4A-NA	3.07	128.75	124.51
28	5	625	LHG	C5-O7-C7	-3.07	110.24	117.79
34	X	1621	LUT	C10-C11-C12	-3.06	113.67	123.22
26	B	815	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
35	X	1622	XAT	C27-C28-C29	-3.06	120.78	125.53
29	6	622	BCR	C38-C26-C27	3.06	119.49	113.62
26	X	612	CLA	CAA-C2A-C3A	-3.06	104.41	112.78
36	Y	1623	NEX	C24-C23-C22	-3.06	104.87	110.77
37	W	601	CHL	C4-C3-C5	3.05	120.41	115.27
37	U	608	CHL	CAC-C3C-C4C	3.05	128.77	124.81
37	V	601	CHL	CAC-C3C-C4C	3.05	128.77	124.81
37	U	606	CHL	C3B-C4B-NB	3.05	113.35	110.52
34	U	1620	LUT	C18-C5-C6	-3.05	121.10	124.53
26	B	812	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
26	X	603	CLA	CHB-C4A-NA	3.05	128.73	124.51
29	A	851	BCR	C36-C18-C19	3.05	122.88	118.08
26	A	814	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
28	3	623	LHG	O7-C7-C8	3.05	118.07	111.50
26	Z	603	CLA	CHB-C4A-NA	3.05	128.73	124.51
26	a	614	CLA	O2D-CGD-O1D	-3.05	117.88	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	6	619	LUT	C35-C15-C14	-3.05	117.23	123.47
37	Z	606	CHL	CMD-C2D-C3D	-3.05	120.61	127.61
34	Y	1620	LUT	C18-C5-C6	-3.05	121.11	124.53
29	K	202	BCR	C11-C10-C9	-3.05	122.96	127.31
26	4	614	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
29	L	301	BCR	C23-C24-C25	-3.04	118.65	127.20
26	W	612	CLA	CHB-C4A-NA	3.04	128.72	124.51
35	2	620	XAT	C28-C29-C30	-3.04	114.27	118.94
26	B	803	CLA	CHB-C4A-NA	3.04	128.72	124.51
29	B	852	BCR	C40-C30-C25	-3.04	105.36	110.30
29	6	622	BCR	C39-C30-C25	-3.04	105.36	110.30
26	A	838	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
29	A	848	BCR	C24-C23-C22	-3.04	121.64	126.23
35	2	620	XAT	C32-C33-C34	-3.04	114.28	118.94
29	A	852	BCR	C15-C16-C17	-3.04	117.25	123.47
29	B	848	BCR	C20-C21-C22	-3.04	122.98	127.31
29	L	301	BCR	C7-C8-C9	-3.03	121.65	126.23
26	7	616	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
26	6	620	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
36	W	1623	NEX	C11-C12-C13	-3.03	117.90	126.42
28	9	623	LHG	C5-O7-C7	-3.03	110.33	117.79
29	L	305	BCR	C37-C22-C23	3.03	122.85	118.08
26	A	824	CLA	C4-C3-C5	3.03	120.36	115.27
26	8	616	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
34	9	619	LUT	C8-C9-C10	3.02	123.58	118.94
37	Z	605	CHL	CAA-C2A-C3A	-3.02	109.04	116.10
26	B	818	CLA	CHC-C4B-NB	3.02	127.46	124.26
26	5	610	CLA	C3B-C4B-NB	-3.02	107.71	110.52
29	a	619	BCR	C16-C17-C18	-3.02	123.00	127.31
26	A	808	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
26	V	614	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
29	A	849	BCR	C30-C25-C26	-3.02	118.36	122.61
29	a	619	BCR	C24-C25-C26	-3.02	114.16	121.46
28	4	622	LHG	O7-C7-C8	3.01	117.99	111.50
29	L	308	BCR	C2-C1-C6	3.01	115.12	110.48
35	Y	1622	XAT	C24-C23-C22	-3.01	104.96	110.77
26	U	602	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
29	1	619	BCR	C24-C25-C26	-3.01	114.17	121.46
26	Y	603	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
37	Y	608	CHL	CHB-C4A-NA	3.01	128.68	124.51
29	6	622	BCR	C37-C22-C23	3.01	122.82	118.08
36	Y	1623	NEX	C2-C1-C6	3.01	112.14	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	852	BCR	C2-C1-C6	3.01	115.11	110.48
29	O	2004	BCR	C31-C1-C6	-3.01	105.42	110.30
26	A	830	CLA	C3B-C4B-NB	-3.01	107.72	110.52
26	K	203	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
26	1	616	CLA	C3B-C4B-NB	-3.01	108.22	110.23
34	Z	1621	LUT	C10-C11-C12	-3.01	113.84	123.22
26	A	810	CLA	CHB-C4A-NA	3.00	128.67	124.51
37	V	607	CHL	CMB-C2B-C1B	3.00	129.94	125.37
26	B	808	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
26	A	812	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
26	A	837	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
26	5	602	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
29	2	623	BCR	C32-C1-C6	-3.00	105.44	110.30
26	W	602	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
37	Z	609	CHL	CHD-C4C-C3C	-2.99	120.44	124.84
35	8	620	XAT	C18-C5-C4	2.99	117.65	114.28
34	X	1621	LUT	C16-C1-C6	-2.99	105.44	110.30
29	a	619	BCR	C7-C8-C9	-2.99	121.71	126.23
26	A	839	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
29	O	2005	BCR	C7-C8-C9	-2.99	121.71	126.23
34	V	1621	LUT	C7-C6-C5	2.99	128.71	121.46
29	B	853	BCR	C16-C17-C18	-2.99	123.04	127.31
36	U	1623	NEX	C39-C29-C30	-2.99	118.73	122.92
26	X	604	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
26	A	810	CLA	CHD-C1D-ND	-2.99	121.71	124.45
26	a	610	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
34	V	1621	LUT	C22-C23-C24	-2.99	108.34	111.74
26	B	818	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
29	B	843	BCR	C16-C15-C14	-2.99	117.36	123.47
29	A	850	BCR	C36-C18-C17	-2.99	118.74	122.92
29	A	856	BCR	C36-C18-C17	-2.99	118.74	122.92
26	W	612	CLA	CAA-C2A-C3A	-2.98	104.60	112.78
31	A	857	LMU	C2'-C3'-C4'	2.98	116.50	109.68
29	7	621	BCR	C38-C26-C27	2.98	119.35	113.62
26	2	613	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
29	B	843	BCR	C15-C14-C13	-2.98	123.05	127.31
37	Y	605	CHL	C4A-NA-C1A	2.98	108.05	106.71
26	9	614	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
26	B	821	CLA	C4C-C3C-C2C	-2.98	105.59	108.89
29	B	848	BCR	C27-C26-C25	-2.98	118.41	122.73
37	U	607	CHL	CMB-C2B-C1B	2.98	129.91	125.37
29	A	852	BCR	C38-C26-C27	2.98	119.33	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	X	610	CLA	C3B-C4B-NB	-2.98	107.75	110.52
29	1	619	BCR	C16-C17-C18	-2.98	123.06	127.31
37	W	607	CHL	CHD-C4C-C3C	-2.97	120.33	124.98
26	X	610	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
35	5	621	XAT	C10-C11-C12	-2.97	113.94	123.22
29	2	623	BCR	C38-C26-C27	2.97	119.33	113.62
34	6	619	LUT	C3-C4-C5	-2.97	105.94	111.85
26	B	805	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
29	K	202	BCR	C33-C5-C4	-2.97	107.91	113.62
26	7	615	CLA	CMB-C2B-C3B	2.97	131.29	123.59
29	A	852	BCR	C23-C22-C21	-2.97	114.38	118.94
29	A	849	BCR	C33-C5-C6	-2.97	121.19	124.53
26	Z	603	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	8	603	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
36	6	624	NEX	C19-C9-C10	2.97	127.08	122.92
26	B	841	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
26	6	602	CLA	C3B-C4B-NB	-2.97	107.76	110.52
26	Y	603	CLA	CAA-C2A-C3A	-2.97	104.66	112.78
26	A	812	CLA	CHD-C1D-ND	-2.97	121.73	124.45
29	3	622	BCR	C24-C23-C22	-2.97	121.75	126.23
26	A	825	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
26	2	611	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
26	B	814	CLA	CHB-C4A-NA	2.96	128.61	124.51
26	W	603	CLA	CHB-C4A-NA	2.96	128.61	124.51
34	6	619	LUT	C11-C10-C9	-2.96	123.08	127.31
29	1	619	BCR	C7-C8-C9	-2.96	121.76	126.23
29	4	621	BCR	C7-C8-C9	-2.96	121.76	126.23
26	7	610	CLA	C3B-C4B-NB	-2.96	107.77	110.52
26	1	616	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
37	V	606	CHL	CHB-C4A-NA	2.96	128.60	124.51
26	6	603	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
29	B	801	BCR	C40-C30-C25	2.96	115.10	110.30
26	8	604	CLA	CMB-C2B-C1B	-2.96	120.86	125.37
26	2	616	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
35	8	620	XAT	C10-C11-C12	-2.96	113.99	123.22
36	6	624	NEX	C15-C35-C34	-2.95	117.42	123.47
26	H	203	CLA	CHB-C4A-NA	2.95	128.60	124.51
35	1	618	XAT	C27-C28-C29	-2.95	120.95	125.53
37	Y	601	CHL	CMB-C2B-C1B	2.95	129.87	125.37
29	8	621	BCR	C38-C26-C27	2.95	119.29	113.62
26	9	601	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
29	8	621	BCR	C8-C9-C10	-2.95	114.42	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	309	BCR	C36-C18-C19	2.95	122.72	118.08
29	a	619	BCR	C38-C26-C27	2.95	119.28	113.62
28	3	623	LHG	C5-O7-C7	-2.95	110.54	117.79
37	W	605	CHL	C1C-C2C-C3C	-2.95	104.78	107.11
26	8	614	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
37	X	609	CHL	O2D-CGD-O1D	-2.95	118.08	123.84
37	V	601	CHL	C3B-C4B-NB	2.94	113.25	110.52
26	Y	612	CLA	CHB-C4A-NA	2.94	128.58	124.51
34	4	619	LUT	C8-C9-C10	2.94	123.46	118.94
26	Z	613	CLA	CHC-C4B-NB	2.94	127.37	124.26
29	7	621	BCR	C36-C18-C17	-2.94	118.80	122.92
29	G	205	BCR	C24-C23-C22	-2.94	121.79	126.23
37	U	606	CHL	CMB-C2B-C1B	2.94	129.85	125.37
29	1	619	BCR	C38-C26-C27	2.94	119.27	113.62
26	4	601	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
26	A	802	CLA	CHB-C4A-NA	2.94	128.58	124.51
34	5	620	LUT	C35-C34-C33	-2.94	123.11	127.31
26	Z	611	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
26	8	613	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
34	W	1620	LUT	C21-C26-C27	-2.94	108.99	112.70
26	6	613	CLA	CHD-C1D-ND	-2.93	121.76	124.45
26	A	826	CLA	CMB-C2B-C3B	2.93	133.70	126.59
37	X	606	CHL	OMC-CMC-C2C	-2.93	119.05	125.69
34	7	619	LUT	C8-C9-C10	2.93	123.44	118.94
26	6	602	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
35	3	619	XAT	C8-C9-C10	-2.93	114.44	118.94
34	6	619	LUT	C21-C26-C27	-2.93	109.00	112.70
26	8	606	CLA	C3B-C4B-NB	-2.93	107.80	110.52
29	5	622	BCR	C24-C25-C26	-2.92	114.38	121.46
26	3	609	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
37	V	608	CHL	CHB-C1B-NB	-2.92	121.16	124.26
29	J	102	BCR	C10-C11-C12	-2.92	114.10	123.22
26	6	607	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
26	6	608	CLA	CHD-C1D-ND	-2.92	121.77	124.45
26	B	834	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
26	U	603	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
35	4	620	XAT	C18-C5-C4	2.92	117.56	114.28
37	U	601	CHL	C1-C2-C3	-2.92	120.99	126.04
26	B	806	CLA	CHB-C4A-NA	2.92	128.55	124.51
37	V	606	CHL	C3B-C4B-NB	2.92	113.22	110.52
26	a	616	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
29	B	843	BCR	C15-C16-C17	-2.92	117.50	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	610	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
26	G	203	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
29	F	305	BCR	C12-C13-C14	-2.91	114.47	118.94
37	Z	608	CHL	CMB-C2B-C1B	2.91	129.81	125.37
37	X	607	CHL	CAA-C2A-C3A	-2.91	104.80	112.78
35	W	1622	XAT	C4-C3-C2	-2.91	105.15	110.77
29	3	622	BCR	C36-C18-C17	-2.91	118.84	122.92
26	2	601	CLA	CMB-C2B-C1B	-2.91	120.94	125.37
29	A	852	BCR	C20-C21-C22	-2.91	123.16	127.31
26	B	817	CLA	CHB-C4A-NA	2.91	128.53	124.51
37	Y	608	CHL	CAC-C3C-C4C	2.91	128.58	124.81
37	Z	609	CHL	C1C-C2C-C3C	-2.91	104.81	107.11
26	Z	610	CLA	CHB-C1B-NB	2.91	127.33	124.26
34	5	620	LUT	C11-C10-C9	-2.91	123.16	127.31
35	V	1622	XAT	C24-C23-C22	-2.91	105.16	110.77
37	Y	607	CHL	CMB-C2B-C1B	2.90	129.79	125.37
26	W	604	CLA	CMB-C2B-C1B	-2.90	120.95	125.37
26	6	620	CLA	CHB-C4A-NA	2.90	128.52	124.51
35	9	620	XAT	O24-C25-C38	2.90	118.53	115.06
37	W	608	CHL	CMB-C2B-C1B	2.90	129.79	125.37
35	a	618	XAT	C27-C28-C29	-2.90	121.03	125.53
29	L	305	BCR	C36-C18-C19	2.90	122.64	118.08
26	8	604	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
26	W	614	CLA	CHB-C4A-NA	2.90	128.52	124.51
26	7	616	CLA	C3B-C4B-NB	-2.90	108.29	110.23
29	O	2005	BCR	C2-C1-C6	2.90	114.94	110.48
29	3	622	BCR	C8-C7-C6	-2.90	119.06	127.20
26	B	822	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
37	Y	609	CHL	CHB-C4A-NA	2.90	128.52	124.51
26	B	816	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
37	U	606	CHL	CHB-C1B-NB	-2.90	121.19	124.26
36	X	1623	NEX	C28-C29-C30	2.89	123.38	118.94
26	V	603	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
26	7	607	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
26	a	611	CLA	C3B-C4B-NB	-2.89	108.29	110.23
29	K	202	BCR	C38-C26-C27	2.89	119.17	113.62
26	B	823	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
29	B	845	BCR	C15-C16-C17	-2.89	117.56	123.47
29	O	2005	BCR	C33-C5-C6	-2.89	121.28	124.53
35	Y	1622	XAT	C11-C10-C9	-2.89	123.19	127.31
26	A	854	CLA	CMB-C2B-C3B	2.89	133.58	126.59
26	8	608	CLA	O2D-CGD-O1D	-2.89	118.19	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	623	BCR	C11-C10-C9	-2.89	123.19	127.31
26	5	604	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
26	8	611	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
26	V	604	CLA	CMB-C2B-C1B	-2.88	120.98	125.37
34	2	619	LUT	C7-C8-C9	-2.88	121.88	126.23
26	A	835	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
35	U	1622	XAT	C36-C21-C26	2.88	117.83	110.05
26	5	609	CLA	CHD-C1D-ND	-2.88	121.81	124.45
37	Z	601	CHL	CHC-C4B-NB	-2.88	121.21	124.26
37	Z	601	CHL	CAC-C3C-C4C	2.88	128.55	124.81
35	3	619	XAT	C10-C11-C12	-2.88	114.23	123.22
29	5	622	BCR	C16-C17-C18	-2.88	123.20	127.31
35	4	620	XAT	C12-C13-C14	-2.88	114.52	118.94
29	B	844	BCR	C33-C5-C6	-2.88	121.30	124.53
34	W	1620	LUT	C35-C15-C14	-2.88	117.58	123.47
26	L	303	CLA	CHD-C1D-ND	-2.88	121.81	124.45
34	4	619	LUT	C16-C1-C6	2.88	114.97	110.30
29	B	847	BCR	C11-C10-C9	-2.88	123.21	127.31
26	A	841	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
26	A	818	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
29	6	622	BCR	C37-C22-C21	-2.87	118.90	122.92
26	6	601	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
29	K	207	BCR	C16-C17-C18	-2.87	123.21	127.31
29	B	844	BCR	C37-C22-C21	-2.87	118.90	122.92
37	Y	601	CHL	CMD-C2D-C3D	-2.87	121.01	127.61
26	Z	612	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
37	V	609	CHL	CHB-C4A-NA	2.87	128.47	124.51
26	8	610	CLA	CMB-C2B-C3B	2.87	133.53	126.59
37	U	601	CHL	C4-C3-C5	2.87	120.09	115.27
26	A	842	CLA	CHB-C1B-NB	2.86	127.29	124.26
26	B	803	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
29	L	309	BCR	C16-C15-C14	-2.86	117.61	123.47
29	3	620	BCR	C30-C25-C24	2.86	123.87	115.78
26	5	613	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
37	Z	608	CHL	C3B-C4B-NB	2.86	113.17	110.52
32	J	104	LMG	O8-C28-C29	2.86	120.89	111.91
35	6	621	XAT	C10-C11-C12	-2.86	114.29	123.22
26	A	808	CLA	C1-C2-C3	-2.86	122.12	126.75
37	V	601	CHL	C1C-C2C-C3C	-2.86	104.84	107.11
29	O	2004	BCR	C7-C8-C9	-2.86	121.92	126.23
29	F	305	BCR	C16-C17-C18	-2.86	123.23	127.31
29	K	207	BCR	C8-C7-C6	-2.86	119.18	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Z	605	CHL	CMD-C2D-C3D	-2.86	121.05	127.61
26	4	602	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
26	O	2001	CLA	CBD-CHA-C1A	2.86	131.87	128.50
37	V	605	CHL	CMB-C2B-C1B	2.85	129.72	125.37
29	3	621	BCR	C7-C8-C9	-2.85	121.92	126.23
26	A	842	CLA	CMB-C2B-C1B	-2.85	121.03	125.37
26	1	606	CLA	CBD-CHA-C1A	2.85	131.07	128.06
29	A	848	BCR	C24-C25-C26	-2.85	114.56	121.46
34	2	619	LUT	C28-C29-C30	-2.85	114.57	118.94
26	A	833	CLA	CHD-C1D-ND	-2.85	121.84	124.45
26	6	610	CLA	C3B-C4B-NB	-2.85	107.87	110.52
34	8	619	LUT	C8-C9-C10	2.85	123.31	118.94
26	X	602	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	O	2004	BCR	C36-C18-C19	2.85	122.56	118.08
34	U	1620	LUT	C21-C26-C27	-2.84	109.11	112.70
35	9	620	XAT	C10-C11-C12	-2.84	114.34	123.22
26	6	616	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
26	B	841	CLA	C3B-C4B-NB	-2.84	107.88	110.52
28	U	2630	LHG	O8-C23-C24	2.84	120.83	111.91
26	H	203	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
29	a	619	BCR	C11-C10-C9	-2.84	123.26	127.31
37	X	609	CHL	CHD-C4C-C3C	-2.84	120.67	124.84
29	A	848	BCR	C30-C25-C24	2.84	123.81	115.78
37	W	607	CHL	CAC-C3C-C4C	2.84	129.36	125.04
37	U	601	CHL	CHD-C4C-C3C	-2.84	120.67	124.84
29	L	308	BCR	C38-C26-C27	2.84	119.07	113.62
26	Y	613	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
36	5	624	NEX	C17-C1-C6	-2.84	107.93	110.47
29	B	845	BCR	C20-C21-C22	-2.84	123.26	127.31
35	9	620	XAT	C38-C25-C24	2.84	117.47	114.28
26	U	603	CLA	CHB-C4A-NA	2.83	128.43	124.51
37	W	601	CHL	CMD-C2D-C3D	-2.83	121.09	127.61
26	Y	610	CLA	C3B-C4B-NB	-2.83	107.89	110.52
29	B	843	BCR	C36-C18-C19	2.83	122.54	118.08
26	7	611	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
37	W	605	CHL	CMB-C2B-C1B	2.83	129.68	125.37
26	6	611	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
34	W	1621	LUT	C15-C35-C34	-2.83	117.68	123.47
37	U	608	CHL	C2A-C3A-C4A	-2.83	97.30	101.87
29	A	849	BCR	C37-C22-C21	-2.83	118.96	122.92
29	1	619	BCR	C11-C10-C9	-2.83	123.28	127.31
28	A	861	LHG	O8-C23-C24	2.83	120.78	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	853	BCR	C15-C16-C17	-2.83	117.68	123.47
37	U	608	CHL	CMD-C2D-C3D	-2.83	121.11	127.61
26	9	610	CLA	O2D-CGD-CBD	2.83	116.29	111.27
26	U	610	CLA	CHB-C4A-NA	2.83	128.42	124.51
26	A	803	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	B	832	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
37	Y	605	CHL	CMD-C2D-C3D	-2.82	121.12	127.61
26	A	831	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	9	610	CLA	C3B-C4B-NB	-2.82	107.90	110.52
37	Y	601	CHL	C3B-C4B-NB	2.82	113.13	110.52
26	A	807	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	V	613	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	8	623	LHG	O8-C23-C24	2.82	120.77	111.91
37	U	605	CHL	CMB-C2B-C1B	2.82	129.67	125.37
29	B	847	BCR	C36-C18-C17	-2.82	118.97	122.92
29	B	853	BCR	C36-C18-C19	2.82	122.52	118.08
29	9	621	BCR	C36-C18-C17	-2.82	118.97	122.92
29	F	305	BCR	C7-C8-C9	-2.82	121.97	126.23
26	4	602	CLA	CHB-C1B-NB	2.82	127.24	124.26
33	B	850	DGD	O1G-C1A-C2A	2.82	120.76	111.91
26	B	819	CLA	C3B-C4B-NB	-2.82	107.90	110.52
26	B	826	CLA	CHB-C4A-NA	2.82	128.41	124.51
29	L	309	BCR	C37-C22-C21	-2.82	118.97	122.92
26	U	612	CLA	CHB-C4A-NA	2.82	128.41	124.51
26	3	604	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
31	A	857	LMU	C1B-O1B-C4'	-2.82	110.99	117.96
26	A	805	CLA	CHB-C4A-NA	2.82	128.41	124.51
37	X	601	CHL	CMD-C2D-C3D	-2.82	121.13	127.61
26	a	608	CLA	O2D-CGD-O1D	-2.82	117.69	124.09
34	8	619	LUT	C38-C25-C24	-2.82	117.53	123.56
37	Z	607	CHL	CMD-C2D-C3D	-2.82	121.13	127.61
37	W	607	CHL	CMD-C2D-C3D	-2.82	121.14	127.61
26	4	610	CLA	CHB-C4A-NA	2.82	128.41	124.51
26	H	203	CLA	CAA-C2A-C3A	-2.81	105.07	112.78
26	5	610	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
32	4	623	LMG	O8-C28-C29	2.81	120.73	111.91
26	9	607	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
29	B	847	BCR	C37-C22-C21	-2.81	118.99	122.92
29	A	851	BCR	C2-C1-C6	2.81	114.81	110.48
35	4	620	XAT	C26-C27-C28	-2.81	120.05	125.99
35	1	618	XAT	C10-C11-C12	-2.81	114.45	123.22
29	B	852	BCR	C31-C1-C2	2.81	120.14	108.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	609	CHL	O2A-CGA-CBA	2.81	120.72	111.91
26	A	813	CLA	C3B-C4B-NB	-2.81	107.91	110.52
26	4	602	CLA	C3B-C4B-NB	-2.81	107.91	110.52
26	A	819	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	L	303	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	B	829	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	8	607	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
29	B	845	BCR	C1-C6-C5	-2.81	118.66	122.61
26	7	602	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
37	V	607	CHL	C3B-C4B-NB	2.81	113.12	110.52
29	B	853	BCR	C37-C22-C21	-2.81	118.99	122.92
26	3	612	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
37	U	601	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
26	4	603	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
35	a	618	XAT	C10-C11-C12	-2.80	114.46	123.22
26	A	833	CLA	CMB-C2B-C1B	-2.80	121.10	125.37
37	U	609	CHL	CMD-C2D-C3D	-2.80	121.16	127.61
29	B	846	BCR	C15-C16-C17	-2.80	117.73	123.47
34	8	619	LUT	C11-C10-C9	-2.80	123.31	127.31
29	7	623	BCR	C23-C24-C25	-2.80	119.33	127.20
29	3	620	BCR	C8-C7-C6	-2.80	119.33	127.20
35	8	620	XAT	C35-C34-C33	-2.80	123.31	127.31
37	Z	608	CHL	CAC-C3C-C4C	2.80	128.44	124.81
26	4	604	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	B	806	CLA	C5-C3-C2	2.80	126.78	121.12
26	K	206	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	1	608	CLA	O2D-CGD-O1D	-2.80	117.73	124.09
29	8	621	BCR	C15-C14-C13	-2.80	123.32	127.31
26	A	816	CLA	C1-C2-C3	-2.80	121.20	126.04
29	A	849	BCR	C38-C26-C25	-2.80	121.39	124.53
26	A	840	CLA	CAA-CBA-CGA	-2.80	105.08	113.25
35	8	620	XAT	C27-C28-C29	-2.80	121.19	125.53
26	9	611	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
37	V	601	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
37	V	608	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
26	6	614	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
26	A	834	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	B	832	CLA	C5-C3-C2	2.79	126.77	121.12
35	8	620	XAT	C35-C15-C14	-2.79	117.75	123.47
26	V	604	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
32	J	103	LMG	O8-C28-C29	2.79	120.67	111.91
26	6	604	CLA	O2D-CGD-O1D	-2.79	118.38	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	W	1623	NEX	C39-C29-C30	-2.79	119.01	122.92
26	A	845	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	1	614	CLA	CAB-C3B-C2B	2.79	130.82	123.59
26	V	612	CLA	CHB-C4A-NA	2.79	128.37	124.51
26	W	613	CLA	CHB-C4A-NA	2.79	128.37	124.51
29	4	621	BCR	C36-C18-C17	-2.79	119.02	122.92
26	4	608	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	B	827	CLA	CMA-C3A-C4A	-2.79	104.28	111.77
29	3	622	BCR	C37-C22-C21	-2.79	119.02	122.92
29	L	308	BCR	C4-C5-C6	-2.79	118.68	122.73
29	A	849	BCR	C15-C14-C13	-2.79	123.33	127.31
26	B	802	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
26	B	833	CLA	CHD-C1D-ND	-2.79	121.89	124.45
37	X	601	CHL	O2A-CGA-CBA	2.79	120.65	111.91
26	8	609	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
26	A	802	CLA	CAA-C2A-C1A	-2.79	102.85	111.97
26	9	604	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
34	4	619	LUT	C12-C13-C14	-2.78	114.67	118.94
29	A	851	BCR	C24-C23-C22	-2.78	122.03	126.23
29	3	620	BCR	C15-C14-C13	-2.78	123.34	127.31
26	V	603	CLA	CHB-C4A-NA	2.78	128.36	124.51
26	7	606	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	L	304	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	6	608	CLA	CHB-C4A-NA	2.78	128.36	124.51
37	V	608	CHL	CHB-C4A-NA	2.78	128.36	124.51
26	B	833	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	Z	610	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	3	609	CLA	CHB-C4A-NA	2.78	128.36	124.51
26	A	818	CLA	CMB-C2B-C1B	-2.78	121.14	125.37
29	3	621	BCR	C32-C1-C6	-2.78	105.79	110.30
28	a	620	LHG	O8-C23-C24	2.78	120.63	111.91
29	5	622	BCR	C30-C25-C24	2.78	123.64	115.78
34	X	1621	LUT	C15-C14-C13	-2.78	123.34	127.31
26	9	609	CLA	CHD-C1D-ND	-2.78	121.90	124.45
34	4	619	LUT	C18-C5-C6	-2.78	121.41	124.53
26	Z	602	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
26	J	101	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
34	4	619	LUT	C35-C15-C14	-2.78	117.79	123.47
26	7	608	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
26	B	837	CLA	CHD-C1D-ND	-2.77	121.90	124.45
26	V	602	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
26	Y	612	CLA	O2D-CGD-O1D	-2.77	118.42	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	613	CLA	CMB-C2B-C1B	-2.77	121.15	125.37
37	Z	605	CHL	CMB-C2B-C1B	2.77	129.59	125.37
29	B	843	BCR	C24-C23-C22	-2.77	122.05	126.23
37	Y	605	CHL	CMB-C2B-C1B	2.77	129.59	125.37
26	a	603	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
29	A	856	BCR	C38-C26-C25	-2.77	121.42	124.53
29	7	621	BCR	C15-C16-C17	-2.77	117.80	123.47
26	A	806	CLA	CAA-C2A-C1A	-2.77	102.90	111.97
26	4	616	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
26	W	604	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
34	4	619	LUT	C19-C9-C8	-2.77	113.72	118.08
26	1	611	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
36	Z	1623	NEX	C26-C27-C28	-2.77	120.14	125.99
26	7	603	CLA	O2D-CGD-O1D	-2.77	117.81	124.09
26	A	836	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
28	V	2630	LHG	O8-C23-C24	2.77	120.59	111.91
34	Y	1620	LUT	C40-C33-C32	2.77	122.44	118.08
26	Z	611	CLA	CAB-C3B-C2B	2.77	130.76	123.59
26	F	304	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
29	A	851	BCR	C40-C30-C29	-2.76	97.86	108.91
26	A	843	CLA	C3B-C4B-NB	-2.76	107.95	110.52
37	V	608	CHL	O2A-CGA-CBA	2.76	120.57	111.91
29	B	847	BCR	C7-C8-C9	-2.76	122.06	126.23
35	5	621	XAT	C15-C35-C34	-2.76	117.82	123.47
26	B	804	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	2	604	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
34	3	618	LUT	C38-C25-C24	-2.76	117.66	123.56
32	J	103	LMG	C8-O7-C10	-2.76	111.00	117.79
26	A	807	CLA	C3B-C4B-NB	-2.76	107.96	110.52
28	B	851	LHG	O8-C23-C24	2.76	120.56	111.91
26	9	613	CLA	C1-C2-C3	-2.76	121.28	126.04
35	9	620	XAT	C8-C9-C10	-2.76	114.71	118.94
26	B	805	CLA	CMB-C2B-C1B	-2.76	121.17	125.37
28	1	620	LHG	O8-C23-C24	2.75	120.55	111.91
35	W	1622	XAT	C7-C8-C9	-2.75	121.26	125.53
37	W	601	CHL	CAC-C3C-C4C	2.75	128.38	124.81
37	W	608	CHL	CHB-C4A-NA	2.75	128.32	124.51
26	A	814	CLA	CMB-C2B-C1B	-2.75	121.18	125.37
35	W	1622	XAT	C10-C11-C12	-2.75	114.63	123.22
26	8	612	CLA	CHB-C4A-NA	2.75	128.32	124.51
37	Y	605	CHL	O2D-CGD-O1D	-2.75	118.46	123.84
26	F	304	CLA	CHD-C1D-ND	-2.75	121.92	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	J	102	BCR	C29-C30-C25	2.75	114.72	110.48
35	5	621	XAT	O24-C25-C38	2.75	118.35	115.06
34	4	619	LUT	C2-C3-C4	2.75	114.07	110.30
26	X	602	CLA	CHB-C4A-NA	2.75	128.32	124.51
29	O	2004	BCR	C2-C1-C6	2.75	114.71	110.48
26	V	610	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
32	9	625	LMG	O8-C28-C29	2.75	120.54	111.91
28	W	2630	LHG	O8-C23-C24	2.75	120.53	111.91
26	3	610	CLA	CHB-C1B-NB	2.75	127.17	124.26
26	B	824	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
33	B	850	DGD	C2G-O2G-C1B	-2.75	111.02	117.79
29	L	309	BCR	C37-C22-C23	2.75	122.41	118.08
29	6	622	BCR	C36-C18-C17	-2.75	119.08	122.92
26	4	613	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
35	3	619	XAT	C27-C28-C29	-2.75	121.27	125.53
37	V	605	CHL	C3B-C4B-NB	2.75	113.06	110.52
26	U	614	CLA	CHB-C4A-NA	2.75	128.31	124.51
29	B	852	BCR	C24-C23-C22	-2.74	122.09	126.23
29	K	202	BCR	C33-C5-C6	2.74	127.61	124.53
26	8	606	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
26	U	612	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
31	A	857	LMU	O5B-C5B-C4B	2.74	114.67	109.69
26	L	304	CLA	CHB-C4A-NA	2.74	128.30	124.51
34	W	1621	LUT	C36-C21-C26	2.74	113.70	109.55
26	Y	604	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	3	621	BCR	C40-C30-C25	-2.74	105.85	110.30
26	X	603	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
26	5	603	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
26	A	822	CLA	CMB-C2B-C3B	2.74	133.22	126.59
29	L	301	BCR	C3-C4-C5	-2.74	109.19	114.08
37	X	605	CHL	CMB-C2B-C1B	2.74	129.54	125.37
26	8	601	CLA	C3B-C4B-NB	-2.74	107.97	110.52
26	V	611	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
26	A	824	CLA	CHD-C1D-ND	-2.74	121.94	124.45
29	2	623	BCR	C3-C4-C5	-2.74	109.19	114.08
26	4	613	CLA	C3B-C4B-NB	-2.74	107.98	110.52
26	3	606	CLA	CHC-C4B-NB	2.74	127.15	124.26
34	U	1620	LUT	C11-C10-C9	-2.73	123.41	127.31
35	U	1622	XAT	C4-C3-C2	-2.73	105.50	110.77
26	A	820	CLA	O2D-CGD-CBD	2.73	116.12	111.27
26	X	611	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
26	3	607	CLA	CHD-C1D-ND	-2.73	121.94	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	613	CLA	CHD-C1D-ND	-2.73	121.94	124.45
32	8	626	LMG	O8-C28-C29	2.73	120.48	111.91
37	Y	601	CHL	CHC-C4B-NB	-2.73	121.37	124.26
36	5	624	NEX	C31-C30-C29	-2.73	123.41	127.31
26	A	828	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
37	V	601	CHL	CMB-C2B-C1B	2.73	129.53	125.37
29	G	205	BCR	C37-C22-C23	2.73	122.38	118.08
26	W	604	CLA	CHB-C1B-NB	2.73	127.14	124.26
29	B	845	BCR	C11-C10-C9	-2.73	123.42	127.31
37	Z	601	CHL	CMD-C2D-C3D	-2.73	121.34	127.61
36	X	1623	NEX	C11-C10-C9	-2.73	123.42	127.31
34	V	1620	LUT	C30-C31-C32	-2.73	114.71	123.22
26	O	2001	CLA	O2D-CGD-O1D	-2.73	117.90	124.09
26	1	613	CLA	CMB-C2B-C1B	-2.73	121.22	125.37
29	8	621	BCR	C28-C27-C26	-2.73	109.21	114.08
36	W	1623	NEX	O24-C25-C38	2.72	118.32	115.06
26	3	607	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
29	A	850	BCR	C24-C23-C22	-2.72	122.12	126.23
34	Y	1621	LUT	C16-C1-C6	-2.72	105.88	110.30
36	5	624	NEX	C15-C35-C34	-2.72	117.90	123.47
37	X	606	CHL	O2D-CGD-O1D	-2.72	118.52	123.84
26	B	819	CLA	CHB-C1B-NB	2.72	127.14	124.26
26	W	603	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
26	X	612	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	5	608	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
26	1	614	CLA	CHC-C4B-NB	2.72	127.14	124.26
26	A	807	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	U	611	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	V	614	CLA	CHB-C4A-NA	2.72	128.27	124.51
34	V	1621	LUT	C15-C35-C34	-2.72	117.91	123.47
26	A	827	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
28	H	204	LHG	O8-C23-C24	2.71	120.43	111.91
26	1	614	CLA	O2D-CGD-O1D	-2.71	117.93	124.09
26	A	802	CLA	CMB-C2B-C3B	2.71	133.16	126.59
35	2	620	XAT	C30-C31-C32	-2.71	114.75	123.22
26	A	801	CLA	CHC-C4B-NB	2.71	127.13	124.26
29	4	621	BCR	C40-C30-C25	-2.71	105.90	110.30
29	7	621	BCR	C37-C22-C21	-2.71	119.12	122.92
26	6	613	CLA	CHB-C1B-NB	2.71	127.13	124.26
29	G	205	BCR	C28-C27-C26	-2.71	109.24	114.08
26	A	839	CLA	CHB-C1B-NB	2.71	127.13	124.26
29	2	623	BCR	C30-C25-C26	-2.71	118.80	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	X	614	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
26	8	607	CLA	CMB-C2B-C3B	2.71	130.61	123.59
26	L	307	CLA	O2D-CGD-O1D	-2.71	117.94	124.09
35	7	620	XAT	C28-C29-C30	-2.71	114.79	118.94
26	8	604	CLA	CHD-C1D-ND	-2.71	121.97	124.45
29	6	622	BCR	C30-C25-C24	2.71	123.44	115.78
29	L	308	BCR	C33-C5-C6	-2.71	121.49	124.53
37	U	609	CHL	CHB-C4A-NA	2.71	128.25	124.51
26	5	618	CLA	CMB-C2B-C3B	2.71	130.60	123.59
29	6	622	BCR	C3-C4-C5	-2.70	109.25	114.08
26	4	611	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
26	3	617	CLA	O2D-CGD-O1D	-2.70	117.95	124.09
26	B	823	CLA	C3B-C4B-NB	-2.70	108.01	110.52
37	W	601	CHL	C3B-C4B-NB	2.70	113.02	110.52
26	5	619	CLA	CHB-C4A-NA	2.70	128.25	124.51
29	B	845	BCR	C8-C7-C6	-2.70	119.61	127.20
34	1	617	LUT	C11-C10-C9	-2.70	123.45	127.31
31	5	628	LMU	C1'-C2'-C3'	2.70	115.62	110.00
29	8	621	BCR	C3-C4-C5	-2.70	109.25	114.08
29	L	308	BCR	C24-C25-C26	-2.70	114.92	121.46
26	L	303	CLA	CHB-C4A-NA	2.70	128.25	124.51
37	V	609	CHL	CMB-C2B-C1B	2.70	129.48	125.37
36	W	1623	NEX	C15-C35-C34	-2.70	117.94	123.47
26	B	817	CLA	C4-C3-C5	2.70	119.81	115.27
37	X	601	CHL	CHB-C4A-NA	2.70	128.24	124.51
26	V	604	CLA	CHB-C4A-NA	2.70	128.24	124.51
37	Y	607	CHL	CHB-C4A-NA	2.70	128.24	124.51
36	6	624	NEX	C28-C29-C30	2.70	123.08	118.94
29	L	305	BCR	C30-C25-C26	-2.70	118.81	122.61
26	1	601	CLA	O2D-CGD-O1D	-2.70	117.97	124.09
37	X	608	CHL	C3B-C4B-NB	2.70	113.02	110.52
26	A	806	CLA	CMB-C2B-C1B	-2.70	121.26	125.37
26	5	610	CLA	CHB-C4A-NA	2.70	128.24	124.51
37	W	608	CHL	CMD-C2D-C3D	-2.70	121.41	127.61
29	B	801	BCR	C39-C30-C25	-2.69	105.93	110.30
37	V	609	CHL	O2D-CGD-O1D	-2.69	118.57	123.84
34	Y	1620	LUT	C10-C11-C12	2.69	131.62	123.22
37	V	609	CHL	C1-O2A-CGA	2.69	123.51	116.44
36	Y	1623	NEX	C4-C3-C2	-2.69	105.57	110.77
26	5	611	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
34	9	619	LUT	C19-C9-C8	-2.69	113.83	118.08
29	B	849	BCR	C23-C22-C21	2.69	123.07	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	609	CHL	CHC-C4B-NB	-2.69	121.41	124.26
35	X	1622	XAT	C24-C23-C22	-2.69	105.58	110.77
26	W	613	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
35	4	620	XAT	C10-C11-C12	-2.69	114.82	123.22
26	F	301	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
26	F	303	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
26	3	611	CLA	O2D-CGD-O1D	-2.69	117.98	124.09
37	W	601	CHL	O2A-CGA-CBA	2.69	120.34	111.91
29	1	619	BCR	C36-C18-C19	2.69	122.31	118.08
26	1	609	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
37	Y	609	CHL	O2A-CGA-CBA	2.69	120.34	111.91
26	W	614	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
35	4	620	XAT	C35-C34-C33	-2.69	123.47	127.31
26	X	612	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
26	U	604	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
36	X	1623	NEX	C11-C12-C13	-2.69	118.87	126.42
34	1	617	LUT	C35-C15-C14	-2.68	117.97	123.47
26	5	617	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
26	A	819	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	2	609	CLA	C3B-C4B-NB	-2.68	108.03	110.52
26	B	810	CLA	C1-C2-C3	-2.68	121.40	126.04
26	Y	610	CLA	CHB-C4A-NA	2.68	128.22	124.51
37	Y	608	CHL	CMB-C2B-C1B	2.68	129.46	125.37
26	J	101	CLA	CHD-C1D-ND	-2.68	121.99	124.45
26	A	843	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
29	3	621	BCR	C37-C22-C21	-2.68	119.17	122.92
37	W	601	CHL	C1C-C2C-C3C	-2.68	104.98	107.11
35	9	620	XAT	C12-C13-C14	-2.68	114.83	118.94
37	W	606	CHL	CMD-C2D-C3D	-2.68	121.44	127.61
34	3	618	LUT	C8-C9-C10	2.68	123.06	118.94
26	2	604	CLA	CMB-C2B-C3B	2.68	133.08	126.59
29	L	301	BCR	C29-C30-C25	2.68	114.61	110.48
35	Z	1622	XAT	C11-C12-C13	-2.68	118.89	126.42
29	7	621	BCR	C16-C17-C18	-2.68	123.48	127.31
26	3	617	CLA	CHB-C4A-NA	2.68	128.22	124.51
37	X	609	CHL	CHB-C1B-NB	-2.68	121.42	124.26
26	a	612	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
26	A	806	CLA	CHB-C4A-NA	2.68	128.22	124.51
34	Y	1620	LUT	C38-C25-C24	-2.68	117.83	123.56
29	A	849	BCR	C36-C18-C17	-2.68	119.17	122.92
29	B	848	BCR	C16-C15-C14	-2.68	117.99	123.47
26	7	611	CLA	CHC-C4B-NB	2.68	127.09	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	807	CLA	CHB-C1B-NB	2.68	127.09	124.26
26	A	832	CLA	CHB-C4A-NA	2.67	128.21	124.51
29	J	102	BCR	C37-C22-C21	-2.67	119.18	122.92
26	6	608	CLA	C3B-C4B-NB	-2.67	108.03	110.52
34	a	617	LUT	C35-C15-C14	-2.67	118.00	123.47
26	7	615	CLA	CAB-C3B-C2B	2.67	130.52	123.59
26	9	609	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
26	9	607	CLA	CHD-C1D-ND	-2.67	122.00	124.45
26	6	613	CLA	O2D-CGD-O1D	-2.67	118.02	124.09
26	A	809	CLA	CHB-C4A-NA	2.67	128.21	124.51
26	A	833	CLA	CHB-C4A-NA	2.67	128.21	124.51
26	6	617	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
37	X	609	CHL	CHB-C4A-NA	2.67	128.20	124.51
26	5	614	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
37	V	605	CHL	CHC-C4B-NB	-2.67	121.43	124.26
26	B	836	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
34	5	620	LUT	C30-C31-C32	-2.67	114.89	123.22
26	B	809	CLA	CHD-C1D-ND	-2.67	122.00	124.45
35	6	621	XAT	C28-C29-C30	-2.67	114.85	118.94
26	A	805	CLA	CMB-C2B-C1B	-2.67	121.31	125.37
37	X	608	CHL	CMB-C2B-C1B	2.67	129.43	125.37
26	7	614	CLA	CHC-C4B-NB	2.67	127.08	124.26
26	6	610	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
29	A	852	BCR	C8-C9-C10	2.67	123.03	118.94
29	A	849	BCR	C15-C16-C17	-2.67	118.01	123.47
37	W	606	CHL	CAA-C2A-C1A	2.67	120.71	111.97
37	Y	609	CHL	CMD-C2D-C3D	-2.67	121.48	127.61
26	4	616	CLA	CAB-C3B-C2B	2.67	130.50	123.59
37	X	605	CHL	CMD-C2D-C3D	-2.67	121.48	127.61
32	9	625	LMG	O7-C10-C11	2.66	117.24	111.50
26	2	602	CLA	O2D-CGD-O1D	-2.66	118.04	124.09
32	V	2631	LMG	O1-C1-C2	2.66	112.46	108.30
36	V	1623	NEX	C24-C23-C22	-2.66	105.63	110.77
26	A	842	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
37	U	609	CHL	O2D-CGD-O1D	-2.66	118.63	123.84
34	V	1620	LUT	C35-C15-C14	-2.66	118.02	123.47
26	A	806	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	a	607	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	4	607	CLA	CHD-C1D-ND	-2.66	122.01	124.45
26	3	603	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	3	613	CLA	O2D-CGD-O1D	-2.66	118.05	124.09
37	Z	609	CHL	O2A-CGA-CBA	2.66	120.25	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	621	BCR	C32-C1-C6	-2.66	105.99	110.30
26	4	618	CLA	O2D-CGD-O1D	-2.66	118.06	124.09
37	V	605	CHL	CMD-C2D-C3D	-2.66	121.50	127.61
34	7	619	LUT	C16-C1-C6	-2.66	105.99	110.30
26	1	603	CLA	CHB-C4A-NA	2.66	128.18	124.51
26	B	804	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	a	601	CLA	O2D-CGD-O1D	-2.65	118.06	124.09
26	O	2002	CLA	CAB-C3B-C2B	2.65	130.47	123.59
26	A	806	CLA	CHD-C1D-ND	-2.65	122.02	124.45
34	5	620	LUT	C18-C5-C6	-2.65	121.55	124.53
26	1	607	CLA	C3B-C4B-NB	-2.65	108.05	110.52
26	6	608	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
26	V	602	CLA	CMB-C2B-C3B	2.65	133.01	126.59
37	X	607	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
26	A	831	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
37	X	605	CHL	CHD-C4C-C3C	-2.65	120.94	124.84
26	1	612	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
26	L	302	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
26	B	829	CLA	CHD-C1D-ND	-2.65	122.02	124.45
29	6	622	BCR	C33-C5-C4	2.65	118.70	113.62
29	a	619	BCR	C36-C18-C19	2.65	122.25	118.08
29	3	622	BCR	C38-C26-C27	2.65	118.70	113.62
28	A	846	LHG	O7-C7-C8	2.65	117.21	111.50
35	7	620	XAT	C10-C11-C12	-2.65	114.96	123.22
34	8	619	LUT	C35-C15-C14	-2.65	118.05	123.47
26	5	609	CLA	C1-C2-C3	-2.65	121.47	126.04
26	L	306	CLA	O2D-CGD-O1D	-2.65	118.08	124.09
29	A	852	BCR	C10-C11-C12	-2.64	114.96	123.22
35	4	620	XAT	C32-C33-C34	-2.64	114.88	118.94
26	7	614	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
26	2	612	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
26	K	204	CLA	CHB-C4A-NA	2.64	128.17	124.51
26	A	829	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
37	Y	607	CHL	CHC-C4B-NB	-2.64	121.46	124.26
37	W	605	CHL	CMD-C2D-C3D	-2.64	121.54	127.61
26	9	604	CLA	CMB-C2B-C3B	2.64	130.43	123.59
26	7	613	CLA	CHB-C4A-NA	2.64	128.16	124.51
29	B	848	BCR	C32-C1-C6	-2.64	106.02	110.30
37	U	605	CHL	O2D-CGD-O1D	-2.64	118.68	123.84
29	7	621	BCR	C11-C10-C9	-2.64	123.55	127.31
29	L	309	BCR	C10-C11-C12	-2.64	114.99	123.22
32	4	624	LMG	O8-C28-C29	2.64	120.18	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	B	850	DGD	C1D-O6D-C5D	-2.64	108.52	113.69
26	A	809	CLA	C1-C2-C3	-2.64	121.48	126.04
29	J	102	BCR	C8-C9-C10	-2.64	114.90	118.94
26	Z	612	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	U	613	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
37	X	608	CHL	O2A-CGA-CBA	2.63	120.18	111.91
26	B	809	CLA	CHB-C4A-NA	2.63	128.16	124.51
26	B	816	CLA	C3B-C4B-NB	-2.63	108.07	110.52
35	7	620	XAT	C18-C5-C4	2.63	117.24	114.28
29	F	305	BCR	C11-C10-C9	-2.63	123.55	127.31
26	a	603	CLA	CHB-C4A-NA	2.63	128.15	124.51
34	2	619	LUT	C15-C35-C34	-2.63	118.08	123.47
37	X	601	CHL	C1-C2-C3	-2.63	121.49	126.04
26	a	614	CLA	CHC-C4B-NB	2.63	127.04	124.26
29	8	621	BCR	C11-C10-C9	-2.63	123.56	127.31
26	a	613	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
34	4	619	LUT	C10-C11-C12	-2.63	115.01	123.22
26	B	806	CLA	C1-C2-C3	-2.63	121.50	126.04
26	1	611	CLA	C5-C3-C2	2.63	126.44	121.12
34	Y	1621	LUT	C38-C25-C24	-2.63	117.93	123.56
29	7	621	BCR	C30-C25-C24	2.63	123.21	115.78
29	A	852	BCR	C37-C22-C21	-2.62	119.25	122.92
34	Z	1620	LUT	C15-C35-C34	-2.62	118.10	123.47
26	A	811	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
26	B	837	CLA	C3B-C4B-NB	-2.62	108.08	110.52
35	1	618	XAT	C12-C13-C14	-2.62	114.92	118.94
29	L	309	BCR	C11-C10-C9	-2.62	123.57	127.31
26	8	612	CLA	O2D-CGD-O1D	-2.62	118.13	124.09
34	1	617	LUT	C28-C29-C30	-2.62	114.92	118.94
37	Z	605	CHL	C1C-C2C-C3C	-2.62	105.03	107.11
26	B	817	CLA	C3B-C4B-NB	-2.62	108.08	110.52
29	L	301	BCR	C36-C18-C17	-2.62	119.25	122.92
26	A	823	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
35	3	619	XAT	C4-C3-C2	-2.62	105.71	110.77
26	9	610	CLA	CHD-C1D-ND	-2.62	122.05	124.45
26	A	824	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
28	A	847	LHG	C5-O7-C7	-2.62	111.34	117.79
26	B	831	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
34	a	617	LUT	C28-C29-C30	-2.62	114.92	118.94
26	7	602	CLA	CHB-C1B-NB	2.62	127.03	124.26
29	B	853	BCR	C11-C10-C9	-2.62	123.57	127.31
26	8	616	CLA	C3B-C4B-NB	-2.62	108.48	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	O	2004	BCR	C33-C5-C6	-2.62	121.59	124.53
35	a	618	XAT	C12-C13-C14	-2.62	114.93	118.94
35	9	620	XAT	C28-C29-C30	-2.62	114.93	118.94
26	B	829	CLA	CMB-C2B-C3B	2.62	132.92	126.59
26	7	606	CLA	C3B-C4B-NB	-2.61	108.09	110.52
26	B	819	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
26	B	828	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
26	X	602	CLA	CMB-C2B-C1B	-2.61	121.39	125.37
26	2	603	CLA	CHC-C4B-NB	2.61	127.02	124.26
34	a	617	LUT	C11-C10-C9	-2.61	123.58	127.31
29	4	621	BCR	C8-C7-C6	-2.61	119.87	127.20
37	U	605	CHL	CMD-C2D-C3D	-2.61	121.61	127.61
36	6	624	NEX	C24-C23-C22	-2.61	105.73	110.77
26	5	606	CLA	C3B-C4B-NB	-2.61	108.09	110.52
37	Z	606	CHL	C2A-C1A-CHA	-2.61	119.30	123.86
26	8	603	CLA	C3B-C4B-NB	-2.61	108.48	110.23
31	5	628	LMU	C1B-O1B-C4'	-2.61	111.51	117.96
26	B	838	CLA	CMB-C2B-C1B	-2.61	121.40	125.37
37	Y	607	CHL	O2A-CGA-CBA	2.61	120.09	111.91
37	Y	601	CHL	C1-C2-C3	-2.61	121.53	126.04
37	U	606	CHL	CHB-C4A-NA	2.61	128.12	124.51
32	A	860	LMG	C7-O1-C1	-2.61	108.64	113.74
37	Z	608	CHL	CHC-C4B-NB	-2.61	121.50	124.26
37	Y	608	CHL	O2A-CGA-CBA	2.61	120.09	111.91
34	9	619	LUT	C35-C15-C14	-2.61	118.14	123.47
35	Z	1622	XAT	C18-C5-C4	2.61	117.21	114.28
29	L	301	BCR	C37-C22-C23	2.61	122.18	118.08
34	Z	1620	LUT	C38-C25-C24	-2.61	117.98	123.56
26	1	613	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
34	X	1620	LUT	C18-C5-C6	-2.60	121.60	124.53
26	7	601	CLA	CMB-C2B-C3B	2.60	132.90	126.59
26	5	614	CLA	CHC-C4B-NB	2.60	127.01	124.26
29	7	623	BCR	C37-C22-C21	-2.60	119.28	122.92
26	3	610	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
26	8	616	CLA	CHB-C4A-NA	2.60	128.11	124.51
37	Y	601	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
26	2	610	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
28	O	2631	LHG	C5-O7-C7	-2.60	111.39	117.79
37	X	607	CHL	O2A-CGA-CBA	2.60	120.07	111.91
35	6	621	XAT	C4-C3-C2	-2.60	105.75	110.77
26	4	604	CLA	CMB-C2B-C3B	2.60	130.33	123.59
26	5	619	CLA	C2A-C1A-CHA	2.60	128.40	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	V	2631	LMG	O8-C28-C29	2.60	120.06	111.91
26	8	610	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	A	842	CLA	C4-C3-C5	2.60	119.64	115.27
26	5	617	CLA	C1-C2-C3	-2.60	122.55	126.75
31	5	629	LMU	C1'-O5'-C5'	-2.60	108.59	113.69
34	V	1620	LUT	C18-C5-C6	-2.60	121.61	124.53
26	2	616	CLA	CAB-C3B-C2B	2.60	130.32	123.59
26	A	835	CLA	CHB-C4A-NA	2.60	128.10	124.51
36	6	624	NEX	C27-C28-C29	-2.60	121.50	125.53
26	5	607	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
29	3	620	BCR	C38-C26-C27	2.60	118.61	113.62
26	5	601	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
26	A	828	CLA	C3B-C4B-NB	-2.60	108.11	110.52
37	V	606	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
26	5	618	CLA	CAB-C3B-C2B	2.59	130.31	123.59
29	B	852	BCR	C29-C30-C25	2.59	114.47	110.48
26	3	606	CLA	CHB-C4A-NA	2.59	128.10	124.51
26	8	601	CLA	CHB-C1B-NB	2.59	127.00	124.26
29	B	844	BCR	C16-C15-C14	-2.59	118.17	123.47
29	O	2004	BCR	C11-C10-C9	-2.59	123.61	127.31
26	A	833	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
34	V	1620	LUT	C38-C25-C24	-2.59	118.02	123.56
26	B	823	CLA	CHC-C4B-NB	2.59	127.00	124.26
29	F	305	BCR	C19-C18-C17	2.59	122.91	118.94
26	B	813	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
29	O	2005	BCR	C16-C15-C14	-2.59	118.17	123.47
29	7	623	BCR	C38-C26-C27	2.59	118.59	113.62
26	2	609	CLA	CHB-C1B-NB	2.59	127.00	124.26
26	A	805	CLA	O2D-CGD-CBD	2.59	115.87	111.27
37	Z	608	CHL	O2A-CGA-CBA	2.59	120.03	111.91
26	8	616	CLA	O1D-CGD-CBD	2.59	129.78	124.48
37	W	608	CHL	C1C-C2C-C3C	-2.59	105.06	107.11
26	O	2003	CLA	O2D-CGD-O1D	-2.59	118.22	124.09
29	L	301	BCR	C33-C5-C4	2.59	118.58	113.62
26	5	602	CLA	C3B-C4B-NB	-2.59	108.12	110.52
29	B	843	BCR	C30-C25-C26	-2.59	118.97	122.61
26	Z	602	CLA	CHB-C4A-NA	2.59	128.09	124.51
26	7	601	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
26	Z	614	CLA	CHB-C4A-NA	2.58	128.09	124.51
34	X	1621	LUT	C7-C8-C9	-2.58	122.33	126.23
28	B	851	LHG	C5-O7-C7	-2.58	111.43	117.79
26	1	616	CLA	CMB-C2B-C1B	-2.58	121.43	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	9	602	CLA	CMB-C2B-C1B	-2.58	121.43	125.37
34	3	618	LUT	C21-C26-C27	-2.58	109.44	112.70
35	8	620	XAT	C12-C13-C14	-2.58	114.98	118.94
26	A	823	CLA	CHD-C1D-ND	-2.58	122.08	124.45
26	6	613	CLA	C1-C2-C3	-2.58	121.58	126.04
26	W	610	CLA	CHB-C4A-NA	2.58	128.08	124.51
26	4	607	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
37	V	607	CHL	CHC-C4B-NB	-2.58	121.53	124.26
26	B	820	CLA	CHB-C4A-NA	2.58	128.08	124.51
31	A	857	LMU	C4B-C3B-C2B	2.58	115.33	110.82
36	X	1623	NEX	C26-C27-C28	-2.58	120.54	125.99
34	Z	1620	LUT	C35-C15-C14	-2.58	118.19	123.47
26	8	601	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
37	X	609	CHL	O2A-CGA-CBA	2.58	120.00	111.91
35	3	619	XAT	C28-C29-C30	-2.58	114.99	118.94
29	L	305	BCR	C15-C16-C17	-2.58	118.19	123.47
26	4	603	CLA	CAB-C3B-C2B	2.58	130.27	123.59
34	4	619	LUT	C18-C5-C4	2.58	119.13	114.36
29	A	849	BCR	C1-C6-C5	-2.58	118.98	122.61
26	A	805	CLA	CHD-C1D-ND	-2.58	122.09	124.45
26	A	830	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
26	A	832	CLA	C3B-C4B-NB	-2.58	108.13	110.52
34	U	1620	LUT	C15-C35-C34	-2.58	118.20	123.47
26	B	809	CLA	O2D-CGD-O1D	-2.57	118.80	123.84
36	Z	1623	NEX	C24-C23-C22	-2.57	105.80	110.77
26	A	810	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
26	A	801	CLA	CBA-CAA-C2A	-2.57	106.27	113.86
26	a	616	CLA	CMB-C2B-C1B	-2.57	121.45	125.37
29	7	621	BCR	C7-C8-C9	-2.57	122.35	126.23
26	A	837	CLA	CHB-C4A-NA	2.57	128.07	124.51
34	V	1621	LUT	C11-C12-C13	-2.57	119.19	126.42
29	A	848	BCR	C19-C18-C17	2.57	122.89	118.94
26	a	601	CLA	CHB-C1B-NB	2.57	126.98	124.26
26	3	612	CLA	C3B-C4B-NB	-2.57	108.13	110.52
35	9	620	XAT	C35-C34-C33	-2.57	123.64	127.31
31	K	208	LMU	C3B-C4B-C5B	2.57	114.83	110.24
37	V	608	CHL	CMB-C2B-C1B	2.57	129.28	125.37
26	3	602	CLA	CHB-C4A-NA	2.57	128.07	124.51
34	Z	1621	LUT	C15-C14-C13	-2.57	123.64	127.31
37	Y	601	CHL	O2A-CGA-CBA	2.57	119.97	111.91
29	3	622	BCR	C33-C5-C6	-2.57	121.64	124.53
37	Y	601	CHL	C4-C3-C5	2.57	119.59	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	601	CHL	CMB-C2B-C1B	2.57	129.28	125.37
29	4	621	BCR	C37-C22-C23	2.57	122.12	118.08
37	Y	608	CHL	CMD-C2D-C3D	-2.57	121.71	127.61
26	6	617	CLA	CHD-C1D-ND	-2.57	122.09	124.45
29	L	305	BCR	C30-C25-C24	2.57	123.04	115.78
37	X	608	CHL	C4-C3-C5	2.57	119.59	115.27
26	4	618	CLA	CMB-C2B-C3B	2.57	130.24	123.59
29	L	301	BCR	C10-C11-C12	-2.57	115.21	123.22
29	L	309	BCR	C34-C9-C8	2.57	122.12	118.08
35	5	621	XAT	C12-C13-C14	-2.56	115.00	118.94
26	G	204	CLA	CHB-C1B-NB	2.56	126.97	124.26
29	B	847	BCR	C15-C14-C13	-2.56	123.65	127.31
26	7	612	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
29	7	623	BCR	C24-C23-C22	-2.56	122.36	126.23
32	L	2631	LMG	O8-C28-C29	2.56	119.95	111.91
26	A	810	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
37	V	609	CHL	C2A-C1A-CHA	-2.56	119.38	123.86
26	a	606	CLA	C3B-C4B-NB	-2.56	108.14	110.52
26	7	610	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	8	608	CLA	CHB-C4A-NA	2.56	128.05	124.51
29	L	308	BCR	C1-C6-C5	-2.56	119.01	122.61
29	G	205	BCR	C32-C1-C6	-2.56	106.15	110.30
26	V	610	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	A	838	CLA	CHB-C4A-NA	2.56	128.05	124.51
31	A	857	LMU	C3B-C4B-C5B	2.56	114.80	110.24
26	5	608	CLA	CHC-C4B-NB	2.56	126.96	124.26
26	2	616	CLA	CHB-C4A-NA	2.56	128.05	124.51
29	B	853	BCR	C15-C14-C13	-2.56	123.66	127.31
26	2	614	CLA	O2D-CGD-O1D	-2.56	118.28	124.09
26	7	616	CLA	CMB-C2B-C3B	2.56	130.21	123.59
26	1	601	CLA	C3B-C4B-NB	-2.56	108.14	110.52
37	W	609	CHL	C4-C3-C5	2.56	119.57	115.27
26	4	603	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	B	826	CLA	O2D-CGD-CBD	2.55	115.81	111.27
29	B	846	BCR	C37-C22-C21	-2.55	119.34	122.92
26	4	611	CLA	CHD-C1D-ND	-2.55	122.11	124.45
29	J	102	BCR	C38-C26-C27	2.55	118.52	113.62
26	8	604	CLA	CMB-C2B-C3B	2.55	132.77	126.59
26	a	611	CLA	CAB-C3B-C2B	2.55	130.21	123.59
26	a	601	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	7	602	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	Z	611	CLA	CMB-C2B-C3B	2.55	130.20	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	607	CLA	C3B-C4B-NB	-2.55	108.15	110.52
26	a	602	CLA	CMB-C2B-C3B	2.55	132.76	126.59
37	W	607	CHL	O2A-CGA-CBA	2.55	119.91	111.91
29	B	844	BCR	C3-C4-C5	-2.55	109.53	114.08
26	2	613	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	3	610	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	3	608	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
26	6	601	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	6	611	CLA	CHB-C4A-NA	2.55	128.04	124.51
29	5	622	BCR	C32-C1-C6	-2.55	106.17	110.30
26	5	616	CLA	CAB-C3B-C2B	2.55	130.19	123.59
29	K	202	BCR	C24-C23-C22	-2.55	122.39	126.23
26	1	612	CLA	CHB-C4A-NA	2.55	128.03	124.51
26	8	610	CLA	C4-C3-C2	-2.55	117.14	123.68
26	6	616	CLA	C3B-C4B-NB	-2.55	108.15	110.52
26	W	612	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
34	V	1621	LUT	C1-C6-C5	-2.55	119.03	122.61
26	1	602	CLA	CMB-C2B-C3B	2.55	132.76	126.59
26	U	613	CLA	CAC-C3C-C4C	2.55	128.11	124.81
26	A	821	CLA	CHB-C4A-NA	2.55	128.03	124.51
26	8	602	CLA	CMB-C2B-C3B	2.55	132.75	126.59
35	V	1622	XAT	C38-C25-C24	2.55	117.14	114.28
26	8	612	CLA	CHC-C4B-NB	2.55	126.95	124.26
37	U	609	CHL	C4-C3-C5	2.54	119.55	115.27
26	W	611	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	a	610	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
37	Y	609	CHL	CMB-C2B-C1B	2.54	129.24	125.37
34	a	617	LUT	C35-C34-C33	-2.54	123.68	127.31
37	V	606	CHL	CHB-C1B-NB	-2.54	121.56	124.26
26	B	802	CLA	CHC-C4B-NB	2.54	126.95	124.26
37	U	605	CHL	CHD-C4C-C3C	-2.54	121.10	124.84
26	7	604	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	7	616	CLA	CAB-C3B-C2B	2.54	130.18	123.59
26	1	606	CLA	C3B-C4B-NB	-2.54	108.16	110.52
29	A	852	BCR	C21-C20-C19	-2.54	115.28	123.22
34	X	1621	LUT	C22-C23-C24	-2.54	108.85	111.74
26	A	822	CLA	C7-C6-C5	-2.54	106.46	113.36
32	V	2631	LMG	C7-O1-C1	-2.54	108.78	113.74
26	6	618	CLA	CHB-C4A-NA	2.54	128.02	124.51
26	X	610	CLA	CHB-C4A-NA	2.54	128.02	124.51
29	B	849	BCR	C16-C15-C14	-2.54	118.27	123.47
26	B	822	CLA	CHC-C4B-NB	2.54	126.94	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	814	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
26	B	818	CLA	CHB-C4A-NA	2.54	128.02	124.51
26	1	609	CLA	CHC-C4B-NB	2.54	126.94	124.26
29	A	852	BCR	C1-C6-C5	-2.54	119.04	122.61
29	B	852	BCR	C1-C6-C5	-2.54	119.04	122.61
26	a	614	CLA	CHD-C1D-ND	-2.54	122.12	124.45
26	7	610	CLA	CHB-C1B-NB	2.54	126.94	124.26
29	A	856	BCR	C7-C8-C9	-2.54	122.40	126.23
29	B	844	BCR	C40-C30-C25	-2.54	106.19	110.30
26	7	613	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
26	A	829	CLA	CHD-C1D-ND	-2.53	122.12	124.45
37	X	609	CHL	C4-C3-C5	2.53	119.53	115.27
29	B	843	BCR	C11-C12-C13	-2.53	119.30	126.42
37	U	601	CHL	O2A-CGA-CBA	2.53	119.86	111.91
26	9	603	CLA	CHC-C4B-NB	2.53	126.94	124.26
26	8	603	CLA	CAB-C3B-C2B	2.53	130.15	123.59
32	4	623	LMG	O1-C1-C2	2.53	112.26	108.30
35	4	620	XAT	C24-C23-C22	-2.53	105.88	110.77
26	4	606	CLA	O2D-CGD-O1D	-2.53	118.34	124.09
26	Y	610	CLA	CHB-C1B-NB	2.53	126.94	124.26
26	7	603	CLA	CHB-C4A-NA	2.53	128.01	124.51
29	A	851	BCR	C31-C1-C6	-2.53	106.19	110.30
26	5	611	CLA	CHD-C1D-ND	-2.53	122.13	124.45
26	H	203	CLA	CHD-C1D-ND	-2.53	122.13	124.45
26	6	614	CLA	CHD-C1D-ND	-2.53	122.13	124.45
26	Y	614	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	G	203	CLA	CHB-C4A-NA	2.53	128.01	124.51
37	V	601	CHL	O2A-CGA-CBA	2.53	119.84	111.91
29	O	2005	BCR	C36-C18-C19	2.53	122.06	118.08
26	A	832	CLA	C1-C2-C3	-2.53	122.66	126.75
34	9	619	LUT	C16-C1-C6	2.53	114.40	110.30
37	U	607	CHL	CMD-C2D-C3D	-2.53	121.80	127.61
26	1	604	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	Z	603	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
26	A	801	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
26	Z	610	CLA	CHB-C4A-NA	2.53	128.00	124.51
26	G	204	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
26	B	811	CLA	CHB-C4A-NA	2.53	128.00	124.51
29	8	621	BCR	C39-C30-C25	-2.52	106.20	110.30
26	1	601	CLA	CHB-C1B-NB	2.52	126.93	124.26
26	6	603	CLA	CAB-C3B-C2B	2.52	130.13	123.59
26	U	613	CLA	CHB-C4A-NA	2.52	128.00	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	606	CLA	O2D-CGD-O1D	-2.52	118.36	124.09
26	A	816	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
26	A	818	CLA	CHD-C1D-ND	-2.52	122.14	124.45
26	2	601	CLA	C3B-C4B-NB	-2.52	108.17	110.52
26	A	837	CLA	CHC-C4B-NB	2.52	126.93	124.26
26	9	602	CLA	C1-C2-C3	-2.52	121.68	126.04
26	2	614	CLA	CHD-C1D-ND	-2.52	122.14	124.45
26	Z	613	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
26	a	612	CLA	CHB-C4A-NA	2.52	128.00	124.51
26	1	614	CLA	CHD-C1D-ND	-2.52	122.14	124.45
29	3	620	BCR	C36-C18-C19	2.52	122.05	118.08
34	Z	1620	LUT	C39-C29-C28	2.52	122.05	118.08
26	7	608	CLA	C3B-C4B-NB	-2.52	108.18	110.52
26	3	607	CLA	CAB-C3B-C2B	2.52	130.12	123.59
34	1	617	LUT	C35-C34-C33	-2.52	123.72	127.31
29	A	852	BCR	C12-C13-C14	-2.52	115.08	118.94
26	1	611	CLA	C3B-C4B-NB	-2.52	108.18	110.52
29	4	621	BCR	C33-C5-C4	2.52	118.45	113.62
26	5	619	CLA	CAB-C3B-C2B	2.52	130.11	123.59
26	4	606	CLA	CHC-C4B-NB	2.52	126.92	124.26
26	B	816	CLA	C1-C2-C3	-2.52	121.69	126.04
36	X	1623	NEX	C24-C23-C22	-2.52	105.92	110.77
26	5	612	CLA	O2D-CGD-O1D	-2.51	118.38	124.09
37	V	606	CHL	CAA-C2A-C1A	2.51	120.21	111.97
29	4	621	BCR	C11-C12-C13	-2.51	119.35	126.42
36	6	624	NEX	C10-C11-C12	-2.51	115.37	123.22
37	Z	609	CHL	O2D-CGD-O1D	-2.51	118.92	123.84
26	B	811	CLA	O2D-CGD-O1D	-2.51	118.38	124.09
34	8	619	LUT	C21-C26-C27	-2.51	109.52	112.70
26	A	804	CLA	C1-C2-C3	-2.51	121.70	126.04
26	1	601	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	1	607	CLA	CHD-C1D-ND	-2.51	122.15	124.45
26	1	602	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
36	5	624	NEX	C24-C23-C22	-2.51	105.92	110.77
26	X	613	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
26	W	611	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
26	4	609	CLA	CHD-C1D-ND	-2.51	122.15	124.45
35	2	620	XAT	C26-C27-C28	-2.51	120.69	125.99
26	2	611	CLA	CHB-C4A-NA	2.51	127.98	124.51
29	B	801	BCR	C23-C22-C21	-2.51	115.09	118.94
35	a	618	XAT	C8-C9-C10	-2.51	115.09	118.94
34	V	1621	LUT	C38-C25-C24	-2.51	118.19	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Y	609	CHL	O2D-CGD-O1D	-2.51	118.93	123.84
26	5	619	CLA	CMB-C2B-C3B	2.51	130.09	123.59
26	7	604	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
26	6	616	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	5	612	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	8	607	CLA	CAB-C3B-C2B	2.51	130.09	123.59
26	9	609	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	A	832	CLA	CHB-C1B-NB	2.51	126.91	124.26
26	B	831	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	a	602	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
37	U	606	CHL	CMD-C2D-C3D	-2.51	121.85	127.61
26	K	203	CLA	CAA-CBA-CGA	-2.51	105.93	113.25
26	a	604	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	a	609	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	2	601	CLA	CMB-C2B-C3B	2.50	132.65	126.59
37	X	606	CHL	CMB-C2B-C1B	2.50	129.18	125.37
26	1	603	CLA	O2D-CGD-O1D	-2.50	118.40	124.09
26	2	607	CLA	O2D-CGD-O1D	-2.50	118.40	124.09
26	a	611	CLA	CMB-C2B-C3B	2.50	130.08	123.59
26	K	201	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
37	X	605	CHL	C1C-C2C-C3C	-2.50	105.13	107.11
26	6	606	CLA	O2D-CGD-O1D	-2.50	118.41	124.09
26	6	606	CLA	CHB-C4A-NA	2.50	127.97	124.51
34	6	619	LUT	C12-C13-C14	-2.50	115.10	118.94
26	9	603	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
34	X	1620	LUT	C31-C30-C29	-2.50	123.74	127.31
26	A	835	CLA	C3B-C4B-NB	-2.50	108.20	110.52
26	7	608	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	A	845	CLA	CHB-C1B-NB	2.50	126.90	124.26
37	Y	609	CHL	C4-C3-C5	2.50	119.47	115.27
36	Z	1623	NEX	C5-C4-C3	2.50	114.70	111.75
28	A	847	LHG	O8-C23-C24	2.50	119.75	111.91
26	1	609	CLA	CAB-C3B-C4B	-2.50	121.56	125.37
32	8	626	LMG	C8-O7-C10	-2.50	111.64	117.79
26	4	613	CLA	O2A-CGA-CBA	2.50	119.74	111.91
26	Y	611	CLA	CHB-C4A-NA	2.50	127.97	124.51
29	L	309	BCR	C40-C30-C25	-2.50	106.25	110.30
29	B	843	BCR	C23-C22-C21	-2.50	115.11	118.94
26	4	608	CLA	CHD-C1D-ND	-2.50	122.16	124.45
26	B	809	CLA	C3B-C4B-NB	-2.49	108.20	110.52
26	B	821	CLA	CHD-C1D-ND	-2.49	122.16	124.45
26	5	604	CLA	CMB-C2B-C3B	2.49	130.05	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	840	CLA	CMB-C2B-C1B	-2.49	121.57	125.37
26	4	612	CLA	O2D-CGD-O1D	-2.49	118.43	124.09
37	Y	609	CHL	CHC-C4B-NB	-2.49	121.62	124.26
37	Z	607	CHL	CED-O2D-CGD	2.49	121.57	115.94
35	2	620	XAT	C20-C13-C12	2.49	122.00	118.08
26	A	802	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
26	4	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
29	B	848	BCR	C29-C30-C25	2.49	114.31	110.48
26	A	815	CLA	CHB-C4A-NA	2.49	127.95	124.51
36	U	1623	NEX	C11-C10-C9	-2.49	123.76	127.31
36	5	624	NEX	C28-C29-C30	2.49	122.76	118.94
26	3	607	CLA	CHB-C4A-NA	2.49	127.95	124.51
26	5	617	CLA	CHB-C4A-NA	2.49	127.95	124.51
26	3	614	CLA	C3B-C4B-NB	-2.49	108.21	110.52
26	6	618	CLA	CAB-C3B-C2B	2.49	130.04	123.59
26	4	604	CLA	CHB-C4A-NA	2.49	127.95	124.51
26	B	817	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
26	B	835	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
26	B	832	CLA	CHB-C4A-NA	2.49	127.95	124.51
26	3	603	CLA	CHB-C4A-NA	2.49	127.95	124.51
37	Z	609	CHL	C1-C2-C3	-2.49	121.74	126.04
26	A	830	CLA	CHC-C4B-NB	2.49	126.89	124.26
29	K	202	BCR	C36-C18-C17	-2.49	119.44	122.92
29	K	202	BCR	C19-C18-C17	-2.49	115.13	118.94
35	7	620	XAT	C38-C25-C24	2.49	117.08	114.28
26	3	606	CLA	O2D-CGD-O1D	-2.49	118.45	124.09
29	B	849	BCR	C36-C18-C17	-2.48	119.44	122.92
26	5	606	CLA	CHB-C4A-NA	2.48	127.95	124.51
26	K	204	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
34	W	1621	LUT	C38-C25-C24	-2.48	118.25	123.56
26	Z	604	CLA	CHB-C1B-NB	2.48	126.89	124.26
26	A	843	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
26	9	603	CLA	CAB-C3B-C2B	2.48	130.02	123.59
29	3	621	BCR	C15-C16-C17	-2.48	118.39	123.47
26	A	837	CLA	CHD-C1D-ND	-2.48	122.17	124.45
26	B	808	CLA	C1D-ND-C4D	-2.48	104.57	106.33
29	L	301	BCR	C29-C28-C27	-2.48	105.83	111.38
26	L	302	CLA	CHD-C1D-ND	-2.48	122.17	124.45
26	9	606	CLA	CHB-C4A-NA	2.48	127.94	124.51
26	a	611	CLA	O2D-CGD-O1D	-2.48	118.46	124.09
26	B	825	CLA	CMB-C2B-C1B	-2.48	121.59	125.37
26	A	840	CLA	CHB-C1B-NB	2.48	126.88	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	608	CLA	CHB-C4A-NA	2.48	127.94	124.51
29	B	801	BCR	C24-C25-C26	2.48	127.47	121.46
26	U	603	CLA	C2A-C1A-CHA	2.48	128.19	123.86
26	B	825	CLA	CHD-C1D-ND	-2.48	122.18	124.45
26	A	842	CLA	C1-C2-C3	-2.48	121.76	126.04
37	X	609	CHL	C2A-C1A-CHA	-2.48	119.53	123.86
26	a	601	CLA	C3B-C4B-NB	-2.48	108.22	110.52
35	a	618	XAT	C28-C29-C30	-2.48	115.14	118.94
26	6	612	CLA	O2D-CGD-O1D	-2.48	118.47	124.09
26	6	601	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
26	Z	610	CLA	C3B-C4B-NB	-2.47	108.22	110.52
35	1	618	XAT	C28-C29-C30	-2.47	115.14	118.94
37	X	607	CHL	CHC-C4B-NB	-2.47	121.64	124.26
26	9	603	CLA	CHB-C1B-NB	2.47	126.88	124.26
26	A	839	CLA	C3B-C4B-NB	-2.47	108.22	110.52
26	9	607	CLA	C3B-C4B-NB	-2.47	108.22	110.52
26	A	824	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	L	307	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	X	611	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	4	618	CLA	CAB-C3B-C2B	2.47	130.00	123.59
26	A	822	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
26	1	609	CLA	CHB-C4A-NA	2.47	127.93	124.51
29	A	850	BCR	C16-C15-C14	-2.47	118.41	123.47
26	2	606	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	3	615	CLA	O2D-CGD-O1D	-2.47	118.48	124.09
34	Z	1621	LUT	C38-C25-C24	-2.47	118.28	123.56
32	J	104	LMG	O1-C1-C2	2.47	112.16	108.30
26	9	614	CLA	C3B-C4B-NB	-2.47	108.22	110.52
26	O	2002	CLA	O2D-CGD-O1D	-2.47	118.48	124.09
26	6	618	CLA	O2D-CGD-O1D	-2.47	118.49	124.09
37	Z	606	CHL	C3B-C4B-NB	2.47	112.80	110.52
37	Z	608	CHL	C1C-C2C-C3C	-2.47	105.16	107.11
26	B	810	CLA	C11-C10-C8	-2.47	107.94	115.92
37	Y	609	CHL	O1D-CGD-CBD	-2.47	119.44	124.48
29	L	305	BCR	C38-C26-C25	-2.47	121.76	124.53
29	F	305	BCR	C8-C9-C10	-2.47	115.16	118.94
26	A	804	CLA	CHB-C4A-NA	2.47	127.92	124.51
26	9	607	CLA	CHB-C4A-NA	2.47	127.92	124.51
29	3	620	BCR	C15-C16-C17	-2.46	118.43	123.47
26	a	607	CLA	CHD-C1D-ND	-2.46	122.19	124.45
28	O	2631	LHG	O8-C23-C24	2.46	119.64	111.91
34	a	617	LUT	C1-C6-C5	-2.46	119.14	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	623	BCR	C32-C1-C6	2.46	114.29	110.30
26	a	609	CLA	CHC-C4B-NB	2.46	126.86	124.26
28	3	623	LHG	O8-C23-C24	2.46	119.64	111.91
26	A	817	CLA	CHB-C4A-NA	2.46	127.92	124.51
26	4	604	CLA	CAB-C3B-C2B	2.46	129.97	123.59
26	Z	604	CLA	CMB-C2B-C3B	2.46	132.55	126.59
26	3	603	CLA	C2D-C1D-ND	-2.46	108.29	110.10
34	X	1621	LUT	C18-C5-C6	-2.46	121.76	124.53
29	2	623	BCR	C37-C22-C23	2.46	121.95	118.08
26	8	608	CLA	C3B-C4B-NB	-2.46	108.23	110.52
26	6	609	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
29	A	849	BCR	C11-C12-C13	-2.46	119.50	126.42
35	1	618	XAT	C8-C9-C10	-2.46	115.17	118.94
35	X	1622	XAT	C15-C35-C34	-2.46	118.44	123.47
37	W	605	CHL	C4D-CHA-C1A	-2.46	118.26	121.25
26	A	827	CLA	CHD-C1D-ND	-2.46	122.19	124.45
26	L	303	CLA	C4-C3-C5	2.46	119.41	115.27
26	X	603	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
26	A	812	CLA	CHB-C4A-NA	2.46	127.91	124.51
28	6	623	LHG	C5-O7-C7	-2.46	111.74	117.79
34	X	1620	LUT	C15-C35-C34	-2.46	118.44	123.47
35	5	621	XAT	C30-C31-C32	-2.46	115.55	123.22
35	2	620	XAT	C35-C34-C33	-2.46	123.80	127.31
37	V	601	CHL	CHB-C4A-NA	2.46	127.91	124.51
29	L	305	BCR	C7-C6-C5	-2.46	115.51	121.46
29	6	622	BCR	C32-C1-C6	-2.46	106.31	110.30
26	A	822	CLA	CHB-C1B-NB	2.46	126.86	124.26
26	5	617	CLA	CHC-C4B-NB	2.46	126.86	124.26
35	8	620	XAT	C4-C3-C2	-2.45	106.03	110.77
26	Y	610	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
26	B	821	CLA	CHC-C1C-C2C	-2.45	123.93	129.77
26	B	813	CLA	C3B-C4B-NB	-2.45	108.24	110.52
26	7	616	CLA	CHB-C4A-NA	2.45	127.91	124.51
26	X	614	CLA	CHB-C4A-NA	2.45	127.91	124.51
34	U	1621	LUT	C38-C25-C24	-2.45	118.31	123.56
26	2	607	CLA	CHB-C1B-NB	2.45	126.86	124.26
37	V	605	CHL	O2D-CGD-O1D	-2.45	119.04	123.84
37	W	601	CHL	C1-C2-C3	-2.45	121.80	126.04
26	B	819	CLA	CMB-C2B-C1B	-2.45	121.63	125.37
37	V	606	CHL	CMD-C2D-C3D	-2.45	121.97	127.61
37	Z	609	CHL	CHB-C4A-NA	2.45	127.90	124.51
35	a	618	XAT	C35-C34-C33	-2.45	123.81	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	301	BCR	C37-C22-C21	-2.45	119.49	122.92
26	A	845	CLA	C1-C2-C3	-2.45	122.78	126.75
34	4	619	LUT	C28-C29-C30	-2.45	115.18	118.94
27	B	842	PQN	C26-C25-C23	-2.45	108.00	115.92
26	A	817	CLA	CHD-C1D-ND	-2.45	122.20	124.45
26	Y	613	CLA	CHB-C4A-NA	2.45	127.90	124.51
26	a	616	CLA	C3B-C4B-NB	-2.45	108.24	110.52
37	Z	606	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
37	V	605	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
26	K	203	CLA	C3B-C4B-NB	-2.45	108.24	110.52
26	A	819	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
26	5	604	CLA	CAB-C3B-C2B	2.45	129.93	123.59
26	9	614	CLA	CHD-C1D-ND	-2.45	122.20	124.45
35	8	620	XAT	C24-C23-C22	-2.45	106.05	110.77
34	7	619	LUT	C15-C35-C34	-2.45	118.46	123.47
29	B	801	BCR	C36-C18-C19	2.45	121.93	118.08
26	A	834	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
26	1	602	CLA	CHB-C4A-NA	2.45	127.89	124.51
26	5	604	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
36	6	624	NEX	C31-C30-C29	-2.44	123.82	127.31
37	Z	601	CHL	O2A-CGA-CBA	2.44	119.58	111.91
26	A	808	CLA	CHD-C1D-ND	-2.44	122.21	124.45
26	B	805	CLA	CHD-C1D-ND	-2.44	122.21	124.45
26	5	607	CLA	CHC-C4B-NB	2.44	126.84	124.26
29	L	305	BCR	C36-C18-C17	-2.44	119.50	122.92
26	1	614	CLA	CMB-C2B-C3B	2.44	129.92	123.59
35	2	620	XAT	C37-C21-C36	-2.44	103.77	107.37
26	F	304	CLA	CHB-C4A-NA	2.44	127.89	124.51
26	8	602	CLA	CHB-C4A-NA	2.44	127.89	124.51
37	W	607	CHL	C4-C3-C5	2.44	119.38	115.27
34	7	619	LUT	C38-C25-C24	-2.44	118.33	123.56
37	W	609	CHL	C1C-C2C-C3C	-2.44	105.18	107.11
26	1	608	CLA	CHB-C4A-NA	2.44	127.89	124.51
35	6	621	XAT	C8-C9-C10	-2.44	115.19	118.94
26	6	607	CLA	CMB-C2B-C3B	2.44	129.92	123.59
26	A	803	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
35	1	618	XAT	C35-C34-C33	-2.44	123.83	127.31
26	2	603	CLA	O2D-CGD-O1D	-2.44	118.55	124.09
26	V	613	CLA	CHB-C4A-NA	2.44	127.89	124.51
35	V	1622	XAT	C7-C8-C9	-2.44	121.74	125.53
37	W	605	CHL	O2D-CGD-O1D	-2.44	119.07	123.84
26	5	607	CLA	CHB-C4A-NA	2.44	127.88	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	607	CHL	C3B-C4B-NB	2.44	112.78	110.52
29	G	205	BCR	C23-C24-C25	-2.44	120.36	127.20
26	9	612	CLA	O2D-CGD-O1D	-2.44	118.56	124.09
26	2	614	CLA	CHB-C1B-NB	2.44	126.84	124.26
26	A	817	CLA	O2D-CGD-CBD	2.44	115.60	111.27
26	F	303	CLA	CHD-C1D-ND	-2.44	122.22	124.45
26	2	611	CLA	CHC-C4B-NB	2.44	126.84	124.26
34	a	617	LUT	C18-C5-C4	2.44	118.87	114.36
26	A	842	CLA	C3B-C4B-NB	-2.44	108.26	110.52
26	3	611	CLA	CAB-C3B-C2B	2.43	129.90	123.59
36	6	624	NEX	C15-C14-C13	-2.43	123.84	127.31
26	5	607	CLA	CHB-C1B-NB	2.43	126.83	124.26
26	8	611	CLA	CHC-C4B-NB	2.43	126.83	124.26
26	1	607	CLA	O2D-CGD-O1D	-2.43	118.57	124.09
26	B	807	CLA	C1-C2-C3	-2.43	121.84	126.04
26	4	601	CLA	CHB-C4A-NA	2.43	127.87	124.51
26	4	602	CLA	CHD-C1D-ND	-2.43	122.22	124.45
26	A	814	CLA	CHB-C4A-NA	2.43	127.87	124.51
26	1	601	CLA	CHC-C4B-NB	2.43	126.83	124.26
34	1	617	LUT	C10-C11-C12	-2.43	115.64	123.22
26	3	603	CLA	CHC-C4B-NB	2.43	126.83	124.26
26	B	830	CLA	CHB-C4A-NA	2.43	127.87	124.51
34	X	1620	LUT	C38-C25-C24	-2.43	118.36	123.56
26	W	610	CLA	C1-C2-C3	-2.43	121.84	126.04
31	K	208	LMU	C1'-C2'-C3'	2.43	115.05	110.00
34	Z	1621	LUT	C30-C31-C32	-2.43	115.64	123.22
26	A	819	CLA	CHC-C4B-NB	2.43	126.83	124.26
26	4	614	CLA	CHC-C4B-NB	2.43	126.83	124.26
26	9	613	CLA	CHD-C1D-ND	-2.43	122.22	124.45
26	B	822	CLA	CHB-C4A-NA	2.43	127.87	124.51
26	1	610	CLA	CHB-C4A-NA	2.43	127.87	124.51
34	7	619	LUT	C35-C15-C14	-2.43	118.50	123.47
26	5	618	CLA	O2D-CGD-O1D	-2.43	118.58	124.09
26	W	610	CLA	CHD-C1D-ND	-2.43	122.22	124.45
26	Z	604	CLA	O2D-CGD-O1D	-2.43	119.10	123.84
29	O	2005	BCR	C28-C29-C30	-2.42	105.93	114.60
26	3	604	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
26	4	612	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	Y	602	CLA	CHB-C4A-NA	2.42	127.86	124.51
32	9	625	LMG	O1-C1-C2	2.42	112.09	108.30
26	8	603	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	9	606	CLA	O2D-CGD-O1D	-2.42	118.58	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	806	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
26	A	841	CLA	CHC-C4B-NB	2.42	126.82	124.26
26	6	604	CLA	CHD-C1D-ND	-2.42	122.23	124.45
26	L	303	CLA	C3B-C4B-NB	-2.42	108.27	110.52
26	6	603	CLA	C3B-C4B-NB	-2.42	108.61	110.23
26	L	302	CLA	CHB-C1B-NB	2.42	126.82	124.26
26	2	616	CLA	CMB-C2B-C3B	2.42	129.87	123.59
26	3	607	CLA	CMB-C2B-C3B	2.42	129.86	123.59
26	B	834	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	a	608	CLA	CHB-C4A-NA	2.42	127.86	124.51
34	a	617	LUT	C8-C9-C10	2.42	122.65	118.94
26	B	839	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
26	Y	614	CLA	CHD-C1D-ND	-2.42	122.23	124.45
26	B	812	CLA	C3B-C4B-NB	-2.42	108.27	110.52
29	9	621	BCR	C33-C5-C4	2.42	118.26	113.62
34	4	619	LUT	C38-C25-C24	-2.42	118.39	123.56
26	B	832	CLA	CHD-C1D-ND	-2.42	122.23	124.45
26	V	614	CLA	CHD-C1D-ND	-2.42	122.23	124.45
26	B	817	CLA	CHB-C1B-NB	2.42	126.81	124.26
26	B	827	CLA	CHD-C1D-ND	-2.41	122.23	124.45
26	2	612	CLA	CHB-C4A-NA	2.41	127.85	124.51
26	5	613	CLA	CHC-C4B-NB	2.41	126.81	124.26
26	B	807	CLA	CHD-C1D-ND	-2.41	122.24	124.45
26	5	606	CLA	CHB-C1B-NB	2.41	126.81	124.26
26	A	815	CLA	C1-C2-C3	-2.41	122.85	126.75
26	K	201	CLA	CHB-C4A-NA	2.41	127.85	124.51
34	7	619	LUT	C12-C13-C14	-2.41	115.24	118.94
26	V	602	CLA	CHB-C4A-NA	2.41	127.85	124.51
34	W	1620	LUT	C18-C5-C6	-2.41	121.82	124.53
34	6	619	LUT	C35-C34-C33	-2.41	123.87	127.31
26	B	836	CLA	CHB-C4A-NA	2.41	127.85	124.51
26	1	613	CLA	CHB-C1B-NB	2.41	126.81	124.26
26	B	832	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
26	7	609	CLA	CHD-C1D-ND	-2.41	122.24	124.45
26	A	829	CLA	CHB-C1B-NB	2.41	126.81	124.26
29	5	622	BCR	C11-C10-C9	-2.41	123.87	127.31
34	Y	1620	LUT	C8-C9-C10	2.41	122.64	118.94
26	7	612	CLA	CHB-C4A-NA	2.41	127.84	124.51
26	8	611	CLA	CHB-C4A-NA	2.41	127.84	124.51
32	V	2631	LMG	C8-O7-C10	-2.41	111.86	117.79
26	8	608	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
26	1	614	CLA	CHB-C1B-NB	2.41	126.81	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	X	1622	XAT	C7-C8-C9	-2.41	121.79	125.53
26	a	602	CLA	CHB-C4A-NA	2.41	127.84	124.51
34	6	619	LUT	C10-C11-C12	-2.41	115.71	123.22
26	6	610	CLA	CHB-C4A-NA	2.41	127.84	124.51
26	A	840	CLA	CHC-C4B-NB	2.40	126.80	124.26
26	a	613	CLA	CHB-C1B-NB	2.40	126.80	124.26
29	3	622	BCR	C33-C5-C4	2.40	118.24	113.62
35	8	620	XAT	C7-C8-C9	-2.40	121.80	125.53
26	A	835	CLA	CHC-C4B-NB	2.40	126.80	124.26
26	3	612	CLA	CHB-C1B-NB	2.40	126.80	124.26
37	Y	607	CHL	CED-O2D-CGD	2.40	121.37	115.94
29	L	308	BCR	C15-C14-C13	-2.40	123.88	127.31
26	a	612	CLA	CHC-C4B-NB	2.40	126.80	124.26
26	U	611	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
26	1	612	CLA	CHC-C4B-NB	2.40	126.80	124.26
34	X	1621	LUT	C38-C25-C24	-2.40	118.42	123.56
26	6	609	CLA	CHD-C1D-ND	-2.40	122.25	124.45
26	F	303	CLA	CHC-C4B-NB	2.40	126.80	124.26
26	5	613	CLA	CHB-C4A-NA	2.40	127.83	124.51
37	Y	606	CHL	C3B-C4B-NB	2.40	112.74	110.52
26	A	820	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	B	823	CLA	CHB-C4A-NA	2.40	127.83	124.51
34	1	617	LUT	C1-C6-C5	-2.40	119.23	122.61
37	U	606	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
26	K	203	CLA	CAA-C2A-C1A	2.40	119.84	111.97
34	V	1621	LUT	C1-C2-C3	2.40	119.06	113.64
26	B	841	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	H	202	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	8	614	CLA	CHC-C4B-NB	2.40	126.79	124.26
26	V	611	CLA	CHB-C4A-NA	2.40	127.83	124.51
34	1	617	LUT	C18-C5-C4	2.40	118.79	114.36
26	B	840	CLA	CHD-C1D-ND	-2.40	122.25	124.45
26	a	609	CLA	O2D-CGD-O1D	-2.39	118.65	124.09
29	B	843	BCR	C36-C18-C17	-2.39	119.57	122.92
35	7	620	XAT	C8-C9-C10	-2.39	115.27	118.94
37	U	607	CHL	C3B-C4B-NB	2.39	112.74	110.52
29	4	621	BCR	C15-C14-C13	-2.39	123.89	127.31
26	L	306	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	4	609	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	4	614	CLA	CHD-C1D-ND	-2.39	122.25	124.45
26	A	836	CLA	CHC-C4B-NB	2.39	126.79	124.26
26	a	614	CLA	CHB-C1B-NB	2.39	126.79	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	Y	1623	NEX	C28-C29-C30	2.39	122.61	118.94
34	a	617	LUT	C10-C11-C12	-2.39	115.75	123.22
29	J	102	BCR	C3-C4-C5	-2.39	109.81	114.08
26	2	606	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
26	B	837	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
26	Y	604	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	a	610	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	2	603	CLA	CHB-C4A-NA	2.39	127.82	124.51
37	U	605	CHL	C4D-CHA-C1A	-2.39	118.34	121.25
26	6	614	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
26	A	822	CLA	CHB-C4A-NA	2.39	127.81	124.51
26	B	808	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
26	5	603	CLA	CAB-C3B-C2B	2.39	129.78	123.59
35	1	618	XAT	C4-C3-C2	-2.39	106.16	110.77
34	W	1621	LUT	C11-C12-C13	-2.39	119.71	126.42
26	X	612	CLA	CHC-C4B-NB	2.39	126.78	124.26
26	9	613	CLA	CHB-C4A-NA	2.38	127.81	124.51
29	B	846	BCR	C2-C1-C6	2.38	114.15	110.48
29	L	305	BCR	C11-C12-C13	-2.38	119.72	126.42
26	3	614	CLA	O2D-CGD-O1D	-2.38	118.68	124.09
26	6	607	CLA	CAB-C3B-C2B	2.38	129.77	123.59
26	A	804	CLA	CHC-C4B-NB	2.38	126.78	124.26
36	Z	1623	NEX	C39-C29-C30	-2.38	119.58	122.92
37	Y	605	CHL	CHD-C4C-C3C	-2.38	121.34	124.84
26	3	614	CLA	CHB-C1B-NB	2.38	126.78	124.26
26	2	604	CLA	C3B-C4B-NB	-2.38	108.31	110.52
35	Z	1622	XAT	C19-C9-C8	2.38	121.83	118.08
26	8	609	CLA	CHB-C4A-NA	2.38	127.80	124.51
34	U	1620	LUT	C20-C13-C14	-2.38	119.59	122.92
26	5	602	CLA	CHB-C4A-NA	2.38	127.80	124.51
34	6	619	LUT	C38-C25-C24	-2.38	118.47	123.56
26	B	827	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
26	A	813	CLA	CHB-C1B-NB	2.38	126.78	124.26
26	2	604	CLA	CHB-C1B-NB	2.38	126.78	124.26
26	6	617	CLA	CHB-C4A-NA	2.38	127.80	124.51
34	Y	1621	LUT	C7-C6-C5	2.38	127.22	121.46
26	B	830	CLA	CAC-C3C-C4C	2.38	127.89	124.81
26	A	828	CLA	CHB-C1B-NB	2.38	126.77	124.26
26	A	820	CLA	CHD-C1D-ND	-2.38	122.27	124.45
35	7	620	XAT	C30-C31-C32	-2.38	115.80	123.22
26	A	843	CLA	CAA-CBA-CGA	-2.38	106.31	113.25
26	V	614	CLA	C3B-C4B-NB	-2.38	108.31	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	816	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	X	613	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	A	828	CLA	CMB-C2B-C1B	-2.38	121.75	125.37
26	U	612	CLA	CAA-C2A-C3A	-2.38	108.32	114.26
26	3	606	CLA	C1-C2-C3	-2.38	121.94	126.04
26	6	611	CLA	CHC-C4B-NB	2.37	126.77	124.26
26	B	826	CLA	C3B-C4B-NB	-2.37	108.31	110.52
29	K	202	BCR	C11-C12-C13	-2.37	119.75	126.42
29	3	620	BCR	C23-C22-C21	-2.37	115.30	118.94
26	V	610	CLA	CHB-C1B-NB	2.37	126.77	124.26
35	V	1622	XAT	C15-C35-C34	-2.37	118.61	123.47
35	2	620	XAT	C18-C5-C4	2.37	116.95	114.28
26	B	819	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
29	B	845	BCR	C23-C22-C21	2.37	122.58	118.94
29	L	301	BCR	C8-C9-C10	2.37	122.58	118.94
37	W	606	CHL	CED-O2D-CGD	2.37	121.30	115.94
26	A	818	CLA	CHB-C1B-NB	2.37	126.77	124.26
26	B	835	CLA	CHB-C1B-NB	2.37	126.77	124.26
26	V	604	CLA	CHB-C1B-NB	2.37	126.77	124.26
26	B	811	CLA	CAB-C3B-C2B	2.37	129.74	123.59
32	9	625	LMG	C8-O7-C10	-2.37	111.95	117.79
26	9	604	CLA	CAB-C3B-C2B	2.37	129.74	123.59
37	X	607	CHL	C4-C3-C5	2.37	119.26	115.27
26	8	607	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	6	610	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
37	Z	609	CHL	C4-C3-C5	2.37	119.26	115.27
26	U	614	CLA	CHD-C1D-ND	-2.37	122.28	124.45
29	L	305	BCR	C1-C6-C7	2.37	122.48	115.78
26	6	610	CLA	CHD-C1D-ND	-2.37	122.28	124.45
29	4	621	BCR	C37-C22-C21	-2.37	119.61	122.92
26	K	206	CLA	CHD-C1D-ND	-2.37	122.28	124.45
26	A	834	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	4	610	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
29	L	305	BCR	C24-C23-C22	-2.37	122.66	126.23
26	B	835	CLA	CMB-C2B-C1B	-2.37	121.76	125.37
26	A	825	CLA	CHB-C4A-NA	2.37	127.78	124.51
26	3	612	CLA	CHB-C4A-NA	2.37	127.78	124.51
26	U	602	CLA	CHD-C1D-ND	-2.37	122.28	124.45
26	5	609	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
36	U	1623	NEX	C31-C32-C33	-2.37	119.77	126.42
26	L	307	CLA	CMB-C2B-C1B	-2.37	121.77	125.37
29	A	852	BCR	C4-C5-C6	-2.37	119.30	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K	203	CLA	CHB-C4A-NA	2.37	127.78	124.51
26	2	601	CLA	CHB-C1B-NB	2.37	126.76	124.26
26	5	606	CLA	CHC-C4B-NB	2.37	126.76	124.26
29	B	843	BCR	C24-C25-C26	2.37	127.19	121.46
26	B	835	CLA	CHC-C4B-NB	2.36	126.76	124.26
26	Z	611	CLA	O2D-CGD-CBD	2.36	115.47	111.27
32	J	103	LMG	O6-C5-C6	2.36	112.31	106.44
26	2	607	CLA	CHB-C4A-NA	2.36	127.78	124.51
26	5	609	CLA	CHB-C1B-NB	2.36	126.76	124.26
29	B	801	BCR	C8-C7-C6	-2.36	120.57	127.20
26	8	611	CLA	CHD-C1D-ND	-2.36	122.28	124.45
26	5	603	CLA	CHB-C4A-NA	2.36	127.78	124.51
37	Z	607	CHL	CAA-C2A-C3A	-2.36	106.31	112.78
37	Y	606	CHL	CMD-C2D-C3D	-2.36	122.18	127.61
37	W	601	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
26	V	602	CLA	C1-C2-C3	-2.36	121.96	126.04
26	7	604	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
28	3	624	LHG	C5-O7-C7	-2.36	111.98	117.79
37	Z	607	CHL	O2A-CGA-CBA	2.36	119.31	111.91
26	A	815	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
36	6	624	NEX	C5-C4-C3	2.36	114.54	111.75
26	A	807	CLA	CHD-C1D-ND	-2.36	122.29	124.45
36	5	624	NEX	C27-C28-C29	-2.36	121.87	125.53
26	3	602	CLA	CHD-C1D-ND	-2.36	122.29	124.45
26	A	808	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	B	824	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	4	606	CLA	C3B-C4B-NB	-2.36	108.33	110.52
37	Y	605	CHL	C4D-CHA-C1A	-2.36	118.38	121.25
29	3	620	BCR	C11-C12-C13	-2.36	119.80	126.42
26	7	604	CLA	C3B-C4B-NB	-2.36	108.33	110.52
35	a	618	XAT	C4-C3-C2	-2.35	106.23	110.77
26	A	822	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
29	A	856	BCR	C37-C22-C21	-2.35	119.62	122.92
26	7	603	CLA	CHC-C4B-NB	2.35	126.75	124.26
37	Y	606	CHL	CMB-C2B-C1B	2.35	128.95	125.37
26	W	604	CLA	CHB-C4A-NA	2.35	127.77	124.51
26	7	614	CLA	CHD-C1D-ND	-2.35	122.29	124.45
26	8	614	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
29	B	846	BCR	C16-C17-C18	-2.35	123.95	127.31
37	V	609	CHL	C4-C3-C5	2.35	119.23	115.27
35	Z	1622	XAT	C40-C33-C32	2.35	121.78	118.08
26	7	609	CLA	CHB-C1B-NB	2.35	126.75	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	822	CLA	C3B-C4B-NB	-2.35	108.33	110.52
26	A	802	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
34	1	617	LUT	C8-C9-C10	2.35	122.55	118.94
36	V	1623	NEX	C28-C29-C30	2.35	122.55	118.94
26	4	604	CLA	CHD-C1D-ND	-2.35	122.29	124.45
26	8	601	CLA	CHD-C1D-ND	-2.35	122.29	124.45
26	4	613	CLA	CHB-C4A-NA	2.35	127.76	124.51
26	1	606	CLA	CHB-C1B-NB	2.35	126.75	124.26
37	W	608	CHL	CHC-C4B-NB	-2.35	121.77	124.26
35	a	618	XAT	C30-C31-C32	-2.35	115.88	123.22
26	A	832	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
26	3	617	CLA	CHD-C1D-ND	-2.35	122.30	124.45
26	6	614	CLA	C2D-C1D-ND	-2.35	108.37	110.10
26	A	806	CLA	O1D-CGD-CBD	2.35	129.29	124.48
29	A	856	BCR	C15-C14-C13	-2.35	123.96	127.31
26	6	603	CLA	CMB-C2B-C3B	2.35	129.67	123.59
26	7	614	CLA	C3B-C4B-NB	-2.35	108.34	110.52
26	F	301	CLA	CHB-C4A-NA	2.35	127.76	124.51
36	V	1623	NEX	C26-C27-C28	-2.35	121.03	125.99
26	W	603	CLA	CMB-C2B-C1B	-2.35	121.80	125.37
29	B	852	BCR	C3-C4-C5	-2.35	109.89	114.08
26	3	615	CLA	CHC-C4B-NB	2.35	126.74	124.26
26	5	609	CLA	CHB-C4A-NA	2.35	127.75	124.51
26	A	823	CLA	CHB-C4A-NA	2.34	127.75	124.51
35	1	618	XAT	C30-C31-C32	-2.34	115.90	123.22
35	9	620	XAT	C18-C5-C4	2.34	116.92	114.28
26	6	607	CLA	CHB-C4A-NA	2.34	127.75	124.51
37	X	601	CHL	C4-C3-C5	2.34	119.21	115.27
37	V	606	CHL	O2D-CGD-O1D	-2.34	119.26	123.84
26	1	603	CLA	CHD-C1D-ND	-2.34	122.30	124.45
34	2	619	LUT	C35-C15-C14	-2.34	118.68	123.47
29	A	851	BCR	C8-C7-C6	-2.34	120.62	127.20
34	6	619	LUT	C31-C30-C29	-2.34	123.97	127.31
37	Y	608	CHL	CHC-C4B-NB	-2.34	121.78	124.26
26	B	815	CLA	CHB-C4A-NA	2.34	127.75	124.51
26	9	601	CLA	CHB-C4A-NA	2.34	127.75	124.51
26	J	101	CLA	C3B-C4B-NB	-2.34	108.34	110.52
26	X	612	CLA	CHB-C1B-NB	2.34	126.73	124.26
37	U	609	CHL	O2A-CGA-CBA	2.34	119.25	111.91
26	4	613	CLA	CHD-C1D-ND	-2.34	122.30	124.45
28	A	846	LHG	O8-C23-C24	2.34	119.25	111.91
26	A	820	CLA	CMB-C2B-C1B	-2.34	121.81	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Y	605	CHL	CAA-C2A-C3A	-2.34	110.64	116.10
26	A	834	CLA	C3B-C4B-NB	-2.34	108.34	110.52
29	6	622	BCR	C30-C25-C26	-2.34	119.32	122.61
26	A	842	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
37	W	607	CHL	OMC-CMC-C2C	-2.34	120.40	125.69
29	7	621	BCR	C24-C25-C26	-2.34	115.80	121.46
29	3	621	BCR	C36-C18-C19	2.34	121.76	118.08
35	3	619	XAT	C15-C35-C34	-2.34	118.69	123.47
26	A	854	CLA	C2B-C1B-NB	2.34	111.80	110.23
28	5	623	LHG	O8-C23-C24	2.34	119.24	111.91
26	5	613	CLA	C3B-C4B-NB	-2.33	108.35	110.52
34	7	619	LUT	C1-C6-C5	-2.33	119.33	122.61
34	Z	1620	LUT	C16-C1-C6	-2.33	106.51	110.30
26	7	613	CLA	CHC-C4B-NB	2.33	126.73	124.26
29	G	205	BCR	C37-C22-C21	-2.33	119.65	122.92
26	B	821	CLA	O2D-CGD-O1D	-2.33	118.79	124.09
26	A	836	CLA	CHB-C4A-NA	2.33	127.74	124.51
26	K	206	CLA	CHB-C4A-NA	2.33	127.74	124.51
37	Z	605	CHL	O2D-CGD-O1D	-2.33	119.28	123.84
26	7	608	CLA	CHC-C4B-NB	2.33	126.73	124.26
26	B	834	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
26	F	301	CLA	CHD-C1D-ND	-2.33	122.31	124.45
31	5	628	LMU	C2'-C3'-C4'	2.33	115.01	109.68
26	Z	602	CLA	C3B-C4B-NB	-2.33	108.35	110.52
26	9	604	CLA	C3B-C4B-NB	-2.33	108.67	110.23
37	V	606	CHL	CAA-C2A-C3A	-2.33	106.39	112.78
37	Y	606	CHL	OMC-CMC-C2C	-2.33	120.42	125.69
37	U	607	CHL	OMC-CMC-C2C	-2.33	120.42	125.69
26	3	604	CLA	CHB-C4A-NA	2.33	127.73	124.51
26	B	814	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
34	9	619	LUT	C38-C25-C24	-2.33	118.58	123.56
26	a	608	CLA	CHD-C1D-ND	-2.33	122.31	124.45
26	8	613	CLA	C3B-C4B-NB	-2.33	108.36	110.52
29	A	851	BCR	C15-C16-C17	-2.33	118.71	123.47
34	W	1621	LUT	C36-C21-C22	-2.33	105.03	109.44
26	U	612	CLA	CHB-C1B-NB	2.33	126.72	124.26
26	3	609	CLA	CBA-CAA-C2A	2.33	120.73	113.86
28	5	625	LHG	O8-C23-C24	2.33	119.20	111.91
29	6	622	BCR	C15-C14-C13	-2.32	123.99	127.31
26	U	610	CLA	C1-C2-C3	-2.32	122.02	126.04
26	K	203	CLA	CHC-C4B-NB	2.32	126.72	124.26
26	2	614	CLA	CMB-C2B-C1B	-2.32	121.83	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	601	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
37	X	606	CHL	C3B-C4B-NB	2.32	112.67	110.52
26	Z	602	CLA	CHB-C1B-NB	2.32	126.72	124.26
28	6	623	LHG	O8-C23-C24	2.32	119.20	111.91
26	B	829	CLA	CHB-C1B-NB	2.32	126.72	124.26
26	2	609	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
26	B	802	CLA	CBA-CAA-C2A	-2.32	107.01	113.86
26	1	616	CLA	CHD-C1D-ND	-2.32	122.32	124.45
26	a	601	CLA	CHD-C1D-ND	-2.32	122.32	124.45
26	a	601	CLA	CHC-C4B-NB	2.32	126.71	124.26
26	A	815	CLA	C3B-C4B-NB	-2.32	108.36	110.52
26	A	821	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
37	Z	606	CHL	CMB-C2B-C1B	2.32	128.90	125.37
26	a	606	CLA	CHB-C1B-NB	2.32	126.71	124.26
26	8	603	CLA	CMB-C2B-C3B	2.32	129.60	123.59
34	X	1621	LUT	C20-C13-C12	2.32	121.73	118.08
26	8	613	CLA	CHB-C4A-NA	2.32	127.72	124.51
37	U	607	CHL	CHB-C4A-NA	2.32	127.72	124.51
26	A	834	CLA	C4-C3-C2	-2.32	117.73	123.68
34	V	1621	LUT	C16-C1-C6	-2.32	106.54	110.30
26	8	608	CLA	CHC-C4B-NB	2.32	126.71	124.26
26	9	614	CLA	CHB-C1B-NB	2.32	126.71	124.26
26	U	613	CLA	CHB-C1B-NB	2.32	126.71	124.26
26	9	604	CLA	CHB-C4A-NA	2.32	127.72	124.51
26	1	604	CLA	CHD-C1D-ND	-2.32	122.33	124.45
26	B	815	CLA	CHC-C4B-NB	2.32	126.71	124.26
26	B	833	CLA	CHB-C4A-NA	2.31	127.71	124.51
35	2	620	XAT	C38-C25-C24	2.31	116.88	114.28
34	V	1621	LUT	C18-C5-C6	2.31	127.13	124.53
26	A	805	CLA	C3B-C4B-NB	-2.31	108.37	110.52
29	4	621	BCR	C36-C18-C19	2.31	121.72	118.08
34	X	1621	LUT	C19-C9-C8	2.31	121.72	118.08
35	1	618	XAT	C37-C21-C22	2.31	113.00	108.98
26	a	609	CLA	CHD-C1D-ND	-2.31	122.33	124.45
26	5	601	CLA	CHB-C4A-NA	2.31	127.71	124.51
32	J	104	LMG	C8-O7-C10	-2.31	112.10	117.79
26	B	836	CLA	CHB-C1B-NB	2.31	126.70	124.26
26	4	603	CLA	CHC-C4B-NB	2.31	126.70	124.26
26	5	611	CLA	CHC-C4B-NB	2.31	126.70	124.26
37	Z	605	CHL	CHB-C4A-NA	2.31	127.71	124.51
26	X	603	CLA	C2A-C1A-CHA	2.31	127.90	123.86
32	9	625	LMG	C1-O6-C5	-2.31	109.15	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	5	620	LUT	C39-C29-C28	2.31	121.72	118.08
26	A	808	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
26	W	602	CLA	CHB-C1B-NB	2.31	126.70	124.26
26	B	802	CLA	CHB-C4A-NA	2.31	127.71	124.51
26	7	607	CLA	CHB-C4A-NA	2.31	127.71	124.51
37	X	608	CHL	C1-C2-C3	-2.31	122.05	126.04
26	8	616	CLA	CMB-C2B-C3B	2.31	129.58	123.59
26	A	811	CLA	CHB-C4A-NA	2.31	127.71	124.51
26	A	824	CLA	CHC-C4B-NB	2.31	126.70	124.26
29	L	305	BCR	C4-C5-C6	-2.31	119.38	122.73
26	W	603	CLA	C2A-C1A-CHA	2.31	127.90	123.86
26	1	601	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
26	A	822	CLA	O2A-C1-C2	-2.31	102.57	108.64
26	8	613	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
26	7	603	CLA	CHD-C1D-ND	-2.31	122.33	124.45
26	F	301	CLA	C3B-C4B-NB	-2.31	108.37	110.52
37	U	605	CHL	C3B-C4B-NB	2.31	112.66	110.52
29	B	853	BCR	C32-C1-C6	-2.31	106.56	110.30
26	7	606	CLA	CHB-C4A-NA	2.31	127.70	124.51
26	1	601	CLA	CHD-C1D-ND	-2.31	122.33	124.45
26	W	611	CLA	CHB-C1B-NB	2.31	126.70	124.26
26	4	610	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
29	9	621	BCR	C29-C28-C27	-2.31	106.22	111.38
26	B	837	CLA	CHB-C1B-NB	2.30	126.70	124.26
26	9	609	CLA	CHC-C4B-NB	2.30	126.70	124.26
26	B	825	CLA	CHB-C4A-NA	2.30	127.70	124.51
26	L	303	CLA	O2D-CGD-CBD	2.30	115.36	111.27
26	A	820	CLA	C7-C6-C5	-2.30	107.10	113.36
26	B	802	CLA	C3B-C4B-NB	-2.30	108.38	110.52
31	5	629	LMU	C6'-C5'-C4'	-2.30	106.62	113.33
26	J	101	CLA	CHB-C4A-NA	2.30	127.70	124.51
35	8	620	XAT	C8-C9-C10	-2.30	115.41	118.94
26	B	807	CLA	CHC-C4B-NB	2.30	126.69	124.26
26	1	608	CLA	CHD-C1D-ND	-2.30	122.34	124.45
26	a	616	CLA	CHB-C4A-NA	2.30	127.70	124.51
26	Z	613	CLA	CHB-C4A-NA	2.30	127.70	124.51
26	A	841	CLA	C3B-C4B-NB	-2.30	108.38	110.52
26	A	843	CLA	C1-C2-C3	-2.30	122.06	126.04
34	9	619	LUT	C18-C5-C6	-2.30	121.94	124.53
26	6	616	CLA	CHD-C1D-ND	-2.30	122.34	124.45
29	B	845	BCR	C28-C27-C26	-2.30	109.97	114.08
34	Z	1620	LUT	C18-C5-C6	-2.30	121.94	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	4	619	LUT	C1-C6-C5	-2.30	119.37	122.61
26	A	814	CLA	CHD-C1D-ND	-2.30	122.34	124.45
26	5	618	CLA	C3B-C4B-NB	-2.30	108.69	110.23
26	A	813	CLA	CHD-C1D-ND	-2.30	122.34	124.45
26	1	611	CLA	CHB-C1B-NB	2.30	126.69	124.26
29	A	851	BCR	C11-C10-C9	-2.30	124.03	127.31
29	6	622	BCR	C15-C16-C17	-2.30	118.77	123.47
26	7	608	CLA	CAA-CBA-CGA	-2.30	106.54	113.25
26	K	203	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
29	A	852	BCR	C19-C18-C17	2.30	122.47	118.94
26	Y	612	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
36	Z	1623	NEX	C30-C31-C32	-2.30	116.05	123.22
26	L	304	CLA	CHD-C1D-ND	-2.30	122.34	124.45
26	2	609	CLA	CHB-C4A-NA	2.30	127.69	124.51
29	B	845	BCR	C15-C14-C13	-2.30	124.03	127.31
36	5	624	NEX	C2-C1-C6	2.30	111.44	109.21
35	7	620	XAT	C32-C33-C34	-2.30	115.42	118.94
26	A	818	CLA	CHB-C4A-NA	2.30	127.69	124.51
26	6	616	CLA	C4-C3-C5	2.30	119.13	115.27
35	8	620	XAT	C38-C25-C24	2.30	116.86	114.28
34	X	1620	LUT	C35-C34-C33	-2.29	124.03	127.31
26	7	611	CLA	CHB-C4A-NA	2.29	127.69	124.51
37	U	607	CHL	CMA-C3A-C4A	-2.29	105.61	111.77
32	A	860	LMG	O8-C28-C29	2.29	119.11	111.91
29	A	851	BCR	C30-C25-C26	-2.29	119.39	122.61
37	V	601	CHL	C1-C2-C3	-2.29	122.08	126.04
29	B	852	BCR	C1-C6-C7	2.29	122.26	115.78
26	B	830	CLA	CHD-C1D-C2D	2.29	130.29	125.48
35	4	620	XAT	C4-C3-C2	-2.29	106.35	110.77
29	K	207	BCR	C32-C1-C6	-2.29	106.58	110.30
29	A	856	BCR	C40-C30-C25	2.29	114.02	110.30
29	4	621	BCR	C15-C16-C17	-2.29	118.78	123.47
26	8	614	CLA	CHB-C4A-NA	2.29	127.68	124.51
37	V	608	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
35	U	1622	XAT	C10-C11-C12	-2.29	116.07	123.22
26	8	602	CLA	CHD-C1D-ND	-2.29	122.35	124.45
36	Y	1623	NEX	C26-C27-C28	-2.29	121.15	125.99
26	X	611	CLA	CHC-C4B-NB	2.29	126.68	124.26
26	A	806	CLA	C3B-C4B-NB	-2.29	108.39	110.52
26	a	611	CLA	CAA-C2A-C3A	-2.29	110.76	116.10
29	A	856	BCR	C30-C25-C24	2.29	122.25	115.78
26	6	616	CLA	CBC-CAC-C3C	2.29	118.74	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	X	2630	LHG	O8-C23-C24	2.29	119.09	111.91
26	3	614	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	L	308	BCR	C31-C1-C6	-2.29	106.59	110.30
26	6	613	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
26	8	608	CLA	CHB-C1B-NB	2.29	126.68	124.26
34	9	619	LUT	C10-C11-C12	-2.29	116.08	123.22
26	W	610	CLA	CHB-C1B-NB	2.29	126.68	124.26
37	X	605	CHL	O2D-CGD-O1D	-2.29	119.37	123.84
31	8	625	LMU	O5'-C1'-C2'	2.29	115.19	110.35
26	A	825	CLA	CHC-C4B-NB	2.29	126.68	124.26
26	A	826	CLA	CHB-C1B-NB	2.29	126.68	124.26
26	4	609	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
26	3	602	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
26	a	604	CLA	CHD-C1D-ND	-2.29	122.35	124.45
26	9	610	CLA	CHB-C1B-NB	2.28	126.68	124.26
29	A	850	BCR	C31-C1-C6	-2.28	106.59	110.30
35	Z	1622	XAT	C24-C23-C22	-2.28	106.36	110.77
36	U	1623	NEX	C24-C23-C22	-2.28	106.36	110.77
26	8	604	CLA	CHB-C4A-NA	2.28	127.67	124.51
26	9	602	CLA	O2D-CGD-CBD	2.28	115.33	111.27
34	Y	1621	LUT	C30-C31-C32	-2.28	116.09	123.22
26	F	304	CLA	CHC-C4B-NB	2.28	126.67	124.26
35	a	618	XAT	C37-C21-C22	2.28	112.95	108.98
26	1	609	CLA	CHD-C1D-ND	-2.28	122.36	124.45
29	L	309	BCR	C33-C5-C6	2.28	127.09	124.53
26	B	816	CLA	CHC-C4B-NB	2.28	126.67	124.26
37	Z	601	CHL	O2D-CGD-O1D	-2.28	119.38	123.84
26	9	606	CLA	C3B-C4B-NB	-2.28	108.40	110.52
29	7	621	BCR	C15-C14-C13	-2.28	124.06	127.31
26	A	810	CLA	C3B-C4B-NB	-2.28	108.40	110.52
26	6	606	CLA	C3B-C4B-NB	-2.28	108.40	110.52
29	a	619	BCR	C11-C12-C13	-2.28	120.02	126.42
29	a	619	BCR	C32-C1-C6	-2.28	106.60	110.30
26	2	610	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
26	B	805	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
26	X	602	CLA	CHB-C1B-NB	2.28	126.67	124.26
35	7	620	XAT	C7-C8-C9	-2.28	122.00	125.53
37	Y	601	CHL	O2D-CGD-O1D	-2.28	119.39	123.84
26	6	613	CLA	CHB-C4A-NA	2.28	127.66	124.51
34	7	619	LUT	C3-C4-C5	2.28	116.39	111.85
29	3	621	BCR	C16-C17-C18	-2.28	124.06	127.31
35	V	1622	XAT	C4-C3-C2	-2.27	106.38	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	617	CLA	CHC-C4B-NB	2.27	126.67	124.26
29	A	851	BCR	C15-C14-C13	-2.27	124.06	127.31
35	8	620	XAT	C31-C30-C29	-2.27	124.06	127.31
26	9	610	CLA	CHB-C4A-NA	2.27	127.66	124.51
26	4	618	CLA	CHD-C1D-ND	-2.27	122.36	124.45
34	X	1621	LUT	C11-C10-C9	-2.27	124.06	127.31
37	X	609	CHL	O1D-CGD-CBD	-2.27	119.83	124.48
34	Z	1621	LUT	C19-C9-C8	2.27	121.66	118.08
26	8	607	CLA	C3B-C4B-NB	-2.27	108.71	110.23
26	8	616	CLA	CAB-C3B-C2B	2.27	129.48	123.59
29	6	622	BCR	C1-C6-C7	2.27	122.21	115.78
26	U	604	CLA	CMB-C2B-C3B	2.27	132.09	126.59
26	U	604	CLA	CHB-C4A-NA	2.27	127.65	124.51
26	6	604	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
36	X	1623	NEX	C20-C13-C14	-2.27	119.74	122.92
26	A	830	CLA	CHB-C4A-NA	2.27	127.65	124.51
26	6	609	CLA	CHB-C4A-NA	2.27	127.65	124.51
26	6	614	CLA	CHC-C4B-NB	2.27	126.66	124.26
34	5	620	LUT	C11-C12-C13	-2.27	120.04	126.42
37	Z	606	CHL	CHB-C4A-NA	2.27	127.65	124.51
37	Y	606	CHL	C2A-C1A-CHA	-2.27	119.89	123.86
26	5	604	CLA	C3B-C4B-NB	-2.27	108.71	110.23
31	K	208	LMU	O5'-C1'-C2'	2.27	115.15	110.35
26	a	601	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
26	a	611	CLA	CMA-C3A-C2A	-2.27	110.80	116.10
26	5	603	CLA	C4-C3-C5	2.27	119.09	115.27
37	V	608	CHL	C1C-C2C-C3C	-2.27	105.31	107.11
26	A	843	CLA	CHD-C1D-ND	-2.27	122.37	124.45
26	A	838	CLA	C2D-C1D-ND	-2.27	108.43	110.10
34	2	619	LUT	C15-C14-C13	-2.27	124.07	127.31
36	5	624	NEX	C15-C14-C13	-2.27	124.07	127.31
26	4	614	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
26	B	837	CLA	CHB-C4A-NA	2.27	127.65	124.51
26	4	613	CLA	CHB-C1B-NB	2.27	126.66	124.26
29	1	619	BCR	C32-C1-C6	-2.27	106.62	110.30
37	X	601	CHL	C4A-NA-C1A	2.27	107.72	106.71
37	X	609	CHL	CMB-C2B-C1B	2.27	128.82	125.37
26	A	805	CLA	CMB-C2B-C3B	2.27	132.08	126.59
29	A	849	BCR	C37-C22-C23	2.27	121.65	118.08
32	9	625	LMG	C12-C11-C10	-2.27	105.38	113.62
26	B	807	CLA	O2D-CGD-CBD	2.27	115.29	111.27
26	5	610	CLA	O2A-CGA-O1A	-2.26	117.88	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	5	620	LUT	C18-C5-C4	2.26	118.55	114.36
26	L	304	CLA	CHC-C4B-NB	2.26	126.65	124.26
26	5	609	CLA	CHC-C4B-NB	2.26	126.65	124.26
35	W	1622	XAT	C35-C15-C14	-2.26	118.84	123.47
26	B	838	CLA	C3B-C4B-NB	-2.26	108.42	110.52
26	5	618	CLA	CHB-C4A-NA	2.26	127.64	124.51
26	Y	614	CLA	CHC-C4B-NB	2.26	126.65	124.26
26	B	810	CLA	C3B-C4B-NB	-2.26	108.42	110.52
26	1	616	CLA	CHB-C4A-NA	2.26	127.64	124.51
26	2	604	CLA	CHB-C4A-NA	2.26	127.64	124.51
29	J	102	BCR	C30-C25-C26	-2.26	119.43	122.61
32	5	627	LMG	O8-C28-C29	2.26	119.00	111.91
32	4	623	LMG	C6-C5-C4	-2.26	107.71	113.00
37	V	607	CHL	C4D-CHA-C1A	-2.26	118.50	121.25
29	B	848	BCR	C37-C22-C21	2.26	126.09	122.92
26	4	610	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
26	B	807	CLA	CHB-C1B-NB	2.26	126.65	124.26
32	4	623	LMG	O6-C5-C6	2.26	112.05	106.44
26	7	615	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
26	1	616	CLA	CAB-C3B-C2B	2.26	129.44	123.59
26	5	618	CLA	CHD-C1D-ND	-2.26	122.38	124.45
29	B	849	BCR	C11-C12-C13	-2.26	120.07	126.42
29	A	850	BCR	C37-C22-C21	-2.26	119.76	122.92
26	8	614	CLA	C1-C2-C3	-2.26	122.14	126.04
26	U	604	CLA	CHD-C1D-ND	-2.26	122.38	124.45
26	4	608	CLA	CHC-C4B-NB	2.26	126.65	124.26
26	7	603	CLA	C2D-C1D-ND	-2.26	108.44	110.10
29	L	301	BCR	C15-C14-C13	-2.26	124.09	127.31
29	F	305	BCR	C8-C7-C6	-2.26	120.87	127.20
26	6	618	CLA	C3B-C4B-NB	-2.25	108.72	110.23
26	B	807	CLA	CHB-C4A-NA	2.25	127.63	124.51
26	B	806	CLA	C9-C8-C10	-2.25	103.13	111.29
29	A	852	BCR	C8-C7-C6	-2.25	120.87	127.20
26	B	808	CLA	CHB-C4A-NA	2.25	127.63	124.51
34	X	1621	LUT	C39-C29-C28	2.25	121.63	118.08
26	B	825	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
34	Y	1621	LUT	C31-C30-C29	-2.25	124.10	127.31
29	B	844	BCR	C11-C12-C13	-2.25	120.09	126.42
37	U	601	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
26	B	833	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
26	A	837	CLA	O2D-CGD-CBD	2.25	115.27	111.27
29	B	853	BCR	C1-C6-C5	-2.25	119.44	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	837	CLA	O2D-CGD-CBD	2.25	115.27	111.27
28	U	2630	LHG	C5-O7-C7	-2.25	112.25	117.79
37	V	601	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
26	6	618	CLA	CMB-C2B-C3B	2.25	129.42	123.59
26	8	610	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
35	a	618	XAT	C32-C33-C34	-2.25	115.49	118.94
26	A	842	CLA	CHD-C1D-ND	-2.25	122.39	124.45
26	3	606	CLA	CHD-C1D-ND	-2.25	122.39	124.45
26	3	610	CLA	CHD-C1D-ND	-2.25	122.39	124.45
26	6	603	CLA	CHB-C4A-NA	2.25	127.62	124.51
26	a	611	CLA	CHB-C1B-NB	2.25	126.64	124.26
35	8	620	XAT	C28-C29-C30	-2.25	115.49	118.94
26	A	816	CLA	CHB-C4A-NA	2.25	127.62	124.51
26	6	613	CLA	C3B-C4B-NB	-2.25	108.43	110.52
26	V	603	CLA	CAA-C2A-C3A	-2.25	106.63	112.78
29	A	851	BCR	C33-C5-C6	-2.25	122.01	124.53
29	3	620	BCR	C24-C25-C26	-2.25	116.02	121.46
29	1	619	BCR	C11-C12-C13	-2.25	120.11	126.42
26	7	613	CLA	CHD-C1D-ND	-2.24	122.39	124.45
26	A	804	CLA	O2D-CGD-CBD	2.24	115.26	111.27
29	F	305	BCR	C10-C11-C12	-2.24	116.21	123.22
26	B	823	CLA	CHD-C1D-ND	-2.24	122.39	124.45
26	W	602	CLA	CMB-C2B-C1B	-2.24	121.95	125.37
26	6	610	CLA	CHB-C1B-NB	2.24	126.63	124.26
26	9	607	CLA	CHC-C4B-NB	2.24	126.63	124.26
37	U	606	CHL	O2D-CGD-O1D	-2.24	119.45	123.84
26	W	603	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
36	V	1623	NEX	C20-C13-C14	-2.24	119.78	122.92
26	G	203	CLA	CAA-C2A-C3A	-2.24	108.66	114.26
26	V	604	CLA	CMB-C2B-C3B	2.24	132.02	126.59
26	V	614	CLA	CHB-C1B-NB	2.24	126.63	124.26
26	A	841	CLA	CHB-C4A-NA	2.24	127.61	124.51
26	B	831	CLA	C3B-C4B-NB	-2.24	108.44	110.52
37	Y	605	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
26	B	828	CLA	CHC-C4B-NB	2.24	126.63	124.26
26	B	819	CLA	CHD-C1D-ND	-2.24	122.39	124.45
32	H	205	LMG	O8-C28-C29	2.24	118.94	111.91
26	7	610	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
26	3	604	CLA	CHB-C1B-NB	2.24	126.63	124.26
26	O	2002	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
26	4	604	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
29	L	301	BCR	C31-C1-C6	2.24	113.93	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	617	LUT	C19-C9-C8	-2.24	114.55	118.08
26	A	822	CLA	CHD-C1D-ND	-2.24	122.40	124.45
36	Z	1623	NEX	C35-C34-C33	-2.24	124.12	127.31
34	U	1621	LUT	C18-C5-C6	-2.24	122.02	124.53
37	X	601	CHL	CHC-C4B-NB	-2.24	121.89	124.26
34	Y	1621	LUT	C1-C2-C3	2.24	118.70	113.64
26	9	610	CLA	C4-C3-C5	2.24	119.03	115.27
26	A	842	CLA	CHB-C4A-NA	2.24	127.61	124.51
26	B	834	CLA	CHD-C1D-ND	-2.24	122.40	124.45
34	6	619	LUT	C17-C1-C6	-2.24	106.67	110.30
37	V	608	CHL	C2A-C1A-CHA	-2.24	119.95	123.86
36	5	624	NEX	C35-C34-C33	-2.24	124.12	127.31
36	U	1623	NEX	C2-C1-C6	-2.24	107.04	109.21
26	2	606	CLA	CAC-C3C-C4C	2.24	127.71	124.81
35	Y	1622	XAT	C40-C33-C32	2.24	121.60	118.08
35	3	619	XAT	C24-C23-C22	-2.23	106.46	110.77
37	X	606	CHL	CMD-C2D-C3D	-2.23	122.47	127.61
26	U	602	CLA	C1-C2-C3	-2.23	122.18	126.04
26	B	838	CLA	CHD-C1D-ND	-2.23	122.40	124.45
26	B	805	CLA	CHB-C4A-NA	2.23	127.60	124.51
26	B	839	CLA	CAC-C3C-C4C	2.23	127.71	124.81
35	2	620	XAT	C8-C9-C10	-2.23	115.51	118.94
26	2	604	CLA	CHD-C1D-ND	-2.23	122.40	124.45
26	A	806	CLA	C5-C3-C2	2.23	125.64	121.12
37	W	606	CHL	C4D-C3D-CAD	2.23	110.73	108.10
35	6	621	XAT	C12-C13-C14	-2.23	115.52	118.94
37	Y	601	CHL	C4D-CHA-C1A	-2.23	118.53	121.25
35	4	620	XAT	C28-C29-C30	-2.23	115.52	118.94
28	Z	2630	LHG	O8-C23-C24	2.23	118.91	111.91
26	A	802	CLA	C3A-C2A-C1A	2.23	104.68	101.34
34	U	1621	LUT	C30-C31-C32	-2.23	116.26	123.22
26	B	813	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
26	3	608	CLA	CHD-C1D-ND	-2.23	122.41	124.45
37	V	606	CHL	C4D-CHA-C1A	-2.23	118.54	121.25
26	3	614	CLA	CHC-C4B-NB	2.23	126.62	124.26
29	8	621	BCR	C11-C12-C13	-2.23	120.16	126.42
26	B	828	CLA	CHD-C1D-ND	-2.23	122.41	124.45
37	W	605	CHL	CHC-C4B-NB	-2.23	121.90	124.26
29	A	851	BCR	C16-C15-C14	-2.23	118.91	123.47
29	2	623	BCR	C33-C5-C4	2.23	117.89	113.62
26	G	203	CLA	C3B-C4B-NB	-2.23	108.45	110.52
26	A	811	CLA	O1D-CGD-CBD	2.23	129.04	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Z	604	CLA	C1-C2-C3	-2.23	123.15	126.75
26	U	603	CLA	CHC-C4B-NB	2.23	126.61	124.26
28	9	624	LHG	O8-C23-C24	2.23	118.89	111.91
37	Y	609	CHL	C1-C2-C3	-2.22	122.19	126.04
26	X	614	CLA	C3B-C4B-NB	-2.22	108.45	110.52
26	W	611	CLA	C3B-C4B-NB	-2.22	108.45	110.52
26	A	839	CLA	C5-C3-C2	2.22	125.62	121.12
34	4	619	LUT	C30-C31-C32	-2.22	116.28	123.22
35	8	620	XAT	C32-C33-C34	-2.22	115.53	118.94
34	V	1620	LUT	C39-C29-C28	2.22	121.58	118.08
26	5	608	CLA	CHD-C1D-ND	-2.22	122.41	124.45
26	6	602	CLA	CHB-C4A-NA	2.22	127.59	124.51
26	X	604	CLA	CHB-C4A-NA	2.22	127.59	124.51
26	A	845	CLA	O1D-CGD-CBD	2.22	129.03	124.48
26	8	613	CLA	CHB-C1B-NB	2.22	126.61	124.26
35	2	620	XAT	C40-C33-C34	2.22	126.03	122.92
26	A	829	CLA	CHB-C4A-NA	2.22	127.58	124.51
34	W	1620	LUT	C38-C25-C24	-2.22	118.81	123.56
26	Z	612	CLA	CHC-C4B-NB	2.22	126.61	124.26
26	a	608	CLA	C3B-C4B-NB	-2.22	108.46	110.52
37	Z	608	CHL	C4D-CHA-C1A	-2.22	118.55	121.25
26	7	609	CLA	CHB-C4A-NA	2.22	127.58	124.51
28	Y	2630	LHG	C26-C25-C24	-2.22	105.21	113.19
34	Z	1620	LUT	C28-C29-C30	-2.22	115.54	118.94
26	B	822	CLA	CHD-C1D-ND	-2.22	122.42	124.45
26	a	611	CLA	CHB-C4A-NA	2.22	127.58	124.51
37	Y	607	CHL	CAA-C2A-C3A	-2.22	106.70	112.78
26	Y	602	CLA	CHD-C1D-ND	-2.22	122.42	124.45
26	3	608	CLA	C3B-C4B-NB	-2.22	108.46	110.52
37	V	609	CHL	C4D-CHA-C1A	-2.22	118.55	121.25
37	V	606	CHL	O1D-CGD-CBD	-2.22	119.95	124.48
32	J	103	LMG	C7-O1-C1	-2.22	109.41	113.74
26	A	835	CLA	O2D-CGD-CBD	2.22	115.21	111.27
26	6	606	CLA	CHC-C4B-NB	2.22	126.60	124.26
26	B	830	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
29	3	621	BCR	C15-C14-C13	-2.22	124.15	127.31
26	B	829	CLA	CHC-C1C-NC	2.22	127.56	124.20
29	J	102	BCR	C30-C25-C24	2.22	122.05	115.78
29	8	621	BCR	C32-C1-C6	-2.22	106.71	110.30
29	7	623	BCR	C37-C22-C23	2.22	121.57	118.08
37	V	607	CHL	CMA-C3A-C4A	-2.21	105.82	111.77
31	A	857	LMU	O5'-C1'-C2'	2.21	115.04	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5	622	BCR	C33-C5-C4	2.21	117.87	113.62
26	7	608	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	5	604	CLA	CHB-C4A-NA	2.21	127.57	124.51
29	1	619	BCR	C15-C14-C13	-2.21	124.15	127.31
26	Z	612	CLA	CHB-C1B-NB	2.21	126.60	124.26
26	W	611	CLA	CHC-C4B-NB	2.21	126.60	124.26
29	J	102	BCR	C32-C1-C6	-2.21	106.71	110.30
26	O	2002	CLA	CAA-C2A-C3A	-2.21	110.93	116.10
26	B	812	CLA	CHB-C4A-NA	2.21	127.57	124.51
26	A	816	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	G	204	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	B	816	CLA	CHB-C1B-NB	2.21	126.60	124.26
29	B	846	BCR	C19-C18-C17	-2.21	115.55	118.94
36	U	1623	NEX	C12-C13-C14	-2.21	115.55	118.94
35	Y	1622	XAT	C30-C31-C32	-2.21	116.31	123.22
29	B	843	BCR	C32-C1-C6	-2.21	106.71	110.30
26	9	603	CLA	CMB-C2B-C3B	2.21	129.32	123.59
26	5	614	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	B	819	CLA	CHB-C4A-NA	2.21	127.57	124.51
28	3	624	LHG	O8-C23-C24	2.21	118.84	111.91
26	1	606	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	A	829	CLA	C4-C3-C5	2.21	118.99	115.27
26	A	812	CLA	O1D-CGD-CBD	2.21	129.00	124.48
26	B	807	CLA	C3B-C4B-NB	-2.21	108.47	110.52
26	B	829	CLA	C3C-C4C-NC	-2.21	108.09	110.57
26	a	616	CLA	CMB-C2B-C3B	2.21	131.94	126.59
26	2	613	CLA	CHC-C4B-NB	2.21	126.59	124.26
26	L	303	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
26	a	613	CLA	CMB-C2B-C3B	2.21	131.94	126.59
26	6	601	CLA	O2D-CGD-CBD	2.21	115.19	111.27
35	4	620	XAT	O4-C5-C18	2.21	117.70	115.06
26	X	610	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
26	A	831	CLA	CHD-C1D-ND	-2.21	122.43	124.45
26	A	835	CLA	CHD-C1D-ND	-2.21	122.43	124.45
26	A	820	CLA	CHB-C1B-NB	2.21	126.59	124.26
26	9	613	CLA	CHC-C4B-NB	2.21	126.59	124.26
26	6	604	CLA	CHB-C4A-NA	2.21	127.56	124.51
26	8	601	CLA	CHB-C4A-NA	2.21	127.56	124.51
26	6	614	CLA	C3B-C4B-NB	-2.21	108.47	110.52
29	7	621	BCR	C39-C30-C25	-2.21	106.72	110.30
35	6	621	XAT	C35-C34-C33	-2.21	124.16	127.31
26	U	612	CLA	CHC-C4B-NB	2.20	126.59	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	1	618	XAT	C32-C33-C34	-2.20	115.56	118.94
29	B	845	BCR	C16-C15-C14	-2.20	118.96	123.47
26	6	602	CLA	CHD-C1D-ND	-2.20	122.43	124.45
26	X	614	CLA	CHD-C1D-ND	-2.20	122.43	124.45
36	U	1623	NEX	O4-C5-C18	-2.20	105.47	109.39
31	5	629	LMU	C1B-O1B-C4'	-2.20	112.51	117.96
26	6	609	CLA	CHB-C1B-NB	2.20	126.59	124.26
34	V	1621	LUT	C3-C4-C5	-2.20	107.47	111.85
26	5	611	CLA	CHB-C4A-NA	2.20	127.56	124.51
26	W	602	CLA	CHB-C4A-NA	2.20	127.56	124.51
26	9	614	CLA	CHC-C4B-NB	2.20	126.59	124.26
29	L	301	BCR	C34-C9-C8	2.20	121.55	118.08
26	A	810	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
26	U	613	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
26	A	840	CLA	CHB-C4A-NA	2.20	127.56	124.51
34	U	1620	LUT	C38-C25-C24	-2.20	118.85	123.56
26	8	614	CLA	C3B-C4B-NB	-2.20	108.47	110.52
34	Y	1620	LUT	C16-C1-C6	-2.20	106.73	110.30
28	8	622	LHG	O8-C23-C24	2.20	118.81	111.91
26	A	831	CLA	CAA-CBA-CGA	-2.20	106.82	113.25
34	1	617	LUT	C19-C9-C8	-2.20	114.61	118.08
29	3	622	BCR	C30-C25-C26	-2.20	119.52	122.61
26	6	608	CLA	CHB-C1B-NB	2.20	126.58	124.26
26	B	827	CLA	C3B-C4B-NB	-2.20	108.47	110.52
37	Z	606	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
31	5	628	LMU	O5'-C1'-C2'	2.20	115.00	110.35
26	A	805	CLA	CHB-C1B-NB	2.20	126.58	124.26
26	7	614	CLA	CHB-C1B-NB	2.20	126.58	124.26
29	a	619	BCR	C15-C14-C13	-2.20	124.17	127.31
29	B	845	BCR	C36-C18-C17	-2.20	119.84	122.92
34	Y	1621	LUT	C17-C1-C6	-2.20	106.73	110.30
35	6	621	XAT	C18-C5-C4	2.20	116.75	114.28
37	Z	609	CHL	CHC-C4B-NB	-2.20	121.93	124.26
26	2	613	CLA	CHD-C1D-ND	-2.20	122.44	124.45
26	3	617	CLA	C3B-C4B-NB	-2.20	108.48	110.52
35	2	620	XAT	C7-C8-C9	-2.20	122.12	125.53
26	5	608	CLA	CHB-C4A-NA	2.20	127.55	124.51
26	2	609	CLA	CHD-C1D-ND	-2.20	122.44	124.45
28	a	620	LHG	O7-C7-C8	2.20	116.23	111.50
26	4	614	CLA	C3B-C4B-NB	-2.20	108.48	110.52
37	Z	606	CHL	C4D-CHA-C1A	-2.20	118.58	121.25
32	4	624	LMG	O8-C28-O10	-2.20	118.05	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	842	PQN	C24-C23-C22	-2.19	103.34	111.29
26	3	604	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
37	X	601	CHL	CED-O2D-CGD	2.19	120.90	115.94
26	B	813	CLA	CHB-C1B-NB	2.19	126.58	124.26
34	W	1620	LUT	C39-C29-C28	2.19	121.53	118.08
29	B	844	BCR	C8-C7-C6	-2.19	121.04	127.20
29	L	305	BCR	C39-C30-C25	2.19	113.86	110.30
26	3	615	CLA	CHB-C1B-NB	2.19	126.58	124.26
37	U	609	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
26	B	816	CLA	CHD-C1D-ND	-2.19	122.44	124.45
29	L	309	BCR	C11-C12-C13	-2.19	120.26	126.42
26	A	819	CLA	CMB-C2B-C3B	2.19	131.90	126.59
26	a	616	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	5	602	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	V	602	CLA	CHD-C1D-ND	-2.19	122.44	124.45
37	V	607	CHL	CMD-C2D-C3D	-2.19	122.57	127.61
26	W	603	CLA	CHC-C4B-NB	2.19	126.58	124.26
29	B	844	BCR	C29-C30-C25	2.19	113.85	110.48
26	1	609	CLA	CMA-C3A-C2A	-2.19	110.99	116.10
37	V	607	CHL	CED-O2D-CGD	2.19	120.89	115.94
26	4	616	CLA	CMB-C2B-C3B	2.19	129.26	123.59
29	B	853	BCR	C33-C5-C4	2.19	117.82	113.62
29	A	848	BCR	C23-C22-C21	2.19	122.30	118.94
26	5	607	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	Y	603	CLA	C2A-C1A-CHA	2.19	127.69	123.86
26	A	841	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
34	W	1620	LUT	C30-C31-C32	-2.19	116.39	123.22
26	A	813	CLA	CHC-C4B-NB	2.19	126.57	124.26
26	4	611	CLA	CHC-C4B-NB	2.19	126.57	124.26
34	a	617	LUT	C15-C35-C34	-2.19	119.00	123.47
26	a	603	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	B	832	CLA	C3B-C4B-NB	-2.19	108.49	110.52
29	2	623	BCR	C11-C12-C13	-2.19	120.28	126.42
26	5	601	CLA	CHD-C1D-ND	-2.19	122.45	124.45
26	B	811	CLA	O1D-CGD-CBD	2.18	127.48	120.14
26	B	840	CLA	C2D-C1D-ND	-2.18	108.49	110.10
26	B	838	CLA	CHB-C4A-NA	2.18	127.53	124.51
26	A	821	CLA	O1D-CGD-CBD	2.18	128.95	124.48
26	7	615	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	2	611	CLA	C3B-C4B-NB	-2.18	108.49	110.52
26	O	2003	CLA	CHB-C4A-NA	2.18	127.53	124.51
28	1	620	LHG	O7-C7-C8	2.18	116.20	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	W	1621	LUT	C21-C26-C25	2.18	115.33	111.42
26	7	601	CLA	CHB-C1B-NB	2.18	126.57	124.26
37	U	608	CHL	O2D-CGD-O1D	-2.18	119.57	123.84
34	8	619	LUT	C36-C21-C26	2.18	112.85	109.55
26	A	821	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	7	602	CLA	CHD-C1D-ND	-2.18	122.45	124.45
29	3	620	BCR	C30-C25-C26	-2.18	119.54	122.61
26	6	620	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	Y	602	CLA	O2D-CGD-CBD	2.18	115.14	111.27
26	7	608	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
26	L	302	CLA	CHB-C4A-NA	2.18	127.53	124.51
26	B	820	CLA	CHC-C4B-NB	2.18	126.56	124.26
29	K	207	BCR	C15-C16-C17	-2.18	119.01	123.47
26	B	831	CLA	CHD-C1D-ND	-2.18	122.45	124.45
37	Z	605	CHL	C4D-CHA-C1A	-2.18	118.60	121.25
26	8	616	CLA	O2A-CGA-O1A	-2.18	117.87	123.30
26	A	828	CLA	CHB-C4A-NA	2.18	127.52	124.51
26	3	607	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
26	8	609	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	X	611	CLA	CHB-C1B-NB	2.18	126.56	124.26
26	A	813	CLA	CHB-C4A-NA	2.18	127.52	124.51
26	3	615	CLA	CHB-C4A-NA	2.18	127.52	124.51
26	6	604	CLA	CHC-C4B-NB	2.18	126.56	124.26
26	4	604	CLA	C3B-C4B-NB	-2.18	108.77	110.23
26	Z	604	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	1	611	CLA	CHB-C4A-NA	2.18	127.52	124.51
26	2	603	CLA	CHB-C1B-NB	2.18	126.56	124.26
34	3	618	LUT	C15-C35-C34	-2.17	119.02	123.47
26	X	602	CLA	CMB-C2B-C3B	2.17	131.85	126.59
26	A	813	CLA	C1-C2-C3	-2.17	122.28	126.04
29	J	102	BCR	C34-C9-C8	2.17	121.50	118.08
29	B	846	BCR	C15-C14-C13	-2.17	124.21	127.31
26	Z	603	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
26	3	602	CLA	C3B-C4B-NB	-2.17	108.50	110.52
34	7	619	LUT	C18-C5-C4	-2.17	110.33	114.36
26	A	816	CLA	CHC-C4B-NB	2.17	126.56	124.26
26	1	612	CLA	CHB-C1B-NB	2.17	126.56	124.26
35	8	620	XAT	C15-C35-C34	-2.17	119.02	123.47
26	B	839	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	B	805	CLA	C3B-C4B-NB	-2.17	108.50	110.52
26	A	838	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
34	1	617	LUT	C15-C35-C34	-2.17	119.02	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	617	LUT	C38-C25-C24	-2.17	118.91	123.56
26	K	203	CLA	CHB-C1B-NB	2.17	126.56	124.26
26	3	613	CLA	CHB-C4A-NA	2.17	127.52	124.51
34	2	619	LUT	C19-C9-C8	-2.17	114.66	118.08
37	Y	606	CHL	CHB-C1B-NB	-2.17	121.96	124.26
26	8	603	CLA	CHC-C4B-NB	2.17	126.56	124.26
26	U	602	CLA	CHB-C4A-NA	2.17	127.52	124.51
26	1	613	CLA	CMB-C2B-C3B	2.17	131.85	126.59
26	V	610	CLA	C3B-C4B-NB	-2.17	108.50	110.52
26	A	837	CLA	CHB-C1B-NB	2.17	126.56	124.26
37	U	609	CHL	C2A-C1A-CHA	-2.17	120.06	123.86
37	X	609	CHL	C4D-CHA-C1A	-2.17	118.61	121.25
34	U	1620	LUT	C39-C29-C28	2.17	121.50	118.08
26	W	602	CLA	CHD-C1D-ND	-2.17	122.46	124.45
28	B	851	LHG	O8-C23-O10	-2.17	118.12	123.59
26	Y	613	CLA	CAC-C3C-C4C	2.17	127.62	124.81
26	A	833	CLA	CMB-C2B-C3B	2.17	131.84	126.59
26	3	613	CLA	C3B-C4B-NB	-2.17	108.50	110.52
26	2	606	CLA	O1D-CGD-CBD	2.17	128.92	124.48
35	6	621	XAT	C35-C15-C14	-2.17	119.03	123.47
26	8	606	CLA	CHB-C4A-NA	2.17	127.51	124.51
26	O	2001	CLA	C3B-C4B-NB	-2.17	108.50	110.52
26	7	601	CLA	O1D-CGD-CBD	2.17	128.92	124.48
26	8	602	CLA	C3B-C4B-NB	-2.17	108.51	110.52
29	B	847	BCR	C33-C5-C4	2.17	117.78	113.62
37	X	606	CHL	C4D-CHA-C1A	-2.17	118.61	121.25
29	2	623	BCR	C16-C15-C14	-2.17	119.04	123.47
26	8	606	CLA	CHB-C1B-NB	2.17	126.55	124.26
26	8	606	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
26	H	202	CLA	O2D-CGD-O1D	-2.16	119.17	124.09
36	Z	1623	NEX	C40-C33-C32	2.16	121.49	118.08
28	2	622	LHG	O8-C23-C24	2.16	118.70	111.91
26	5	610	CLA	CHB-C1B-NB	2.16	126.55	124.26
26	4	607	CLA	C3B-C4B-NB	-2.16	108.51	110.52
26	Y	613	CLA	CHC-C4B-NB	2.16	126.55	124.26
26	F	303	CLA	CHB-C4A-NA	2.16	127.50	124.51
35	3	619	XAT	C12-C13-C14	-2.16	115.62	118.94
34	Z	1621	LUT	C18-C5-C6	-2.16	122.10	124.53
26	4	611	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
33	B	850	DGD	O2G-C1B-O1B	-2.16	118.48	123.70
34	1	617	LUT	C38-C25-C24	-2.16	118.93	123.56
26	B	831	CLA	O2A-CGA-O1A	-2.16	118.14	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	602	CLA	CHB-C1B-NB	2.16	126.55	124.26
37	W	609	CHL	C1-C2-C3	-2.16	122.31	126.04
29	A	848	BCR	C28-C27-C26	-2.16	110.22	114.08
37	U	606	CHL	C2A-C1A-CHA	-2.16	120.08	123.86
34	2	619	LUT	C22-C23-C24	2.16	114.20	111.74
26	3	611	CLA	CMB-C2B-C3B	2.16	129.19	123.59
26	B	839	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
37	Y	606	CHL	O2D-CGD-O1D	-2.16	119.62	123.84
26	1	607	CLA	CHB-C4A-NA	2.16	127.50	124.51
26	2	610	CLA	CHB-C4A-NA	2.16	127.50	124.51
26	a	614	CLA	O2D-CGD-CBD	2.16	115.11	111.27
26	6	620	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
36	U	1623	NEX	O24-C25-C26	-2.16	57.17	58.96
26	B	805	CLA	CHB-C1B-NB	2.16	126.54	124.26
29	3	621	BCR	C36-C18-C17	-2.16	119.90	122.92
26	Z	603	CLA	C2A-C1A-CHA	2.16	127.63	123.86
29	1	619	BCR	C37-C22-C21	-2.16	119.90	122.92
34	V	1621	LUT	C30-C31-C32	-2.16	116.49	123.22
26	Z	604	CLA	CHB-C4A-NA	2.16	127.49	124.51
26	Y	602	CLA	CMB-C2B-C1B	-2.16	122.09	125.37
26	B	805	CLA	CMB-C2B-C3B	2.16	131.81	126.59
26	B	806	CLA	CMC-C2C-C1C	-2.16	121.76	125.04
26	4	603	CLA	CMB-C2B-C3B	2.16	129.17	123.59
29	K	207	BCR	C28-C29-C30	-2.15	106.90	114.60
26	6	607	CLA	C3B-C4B-NB	-2.15	108.79	110.23
26	Y	614	CLA	CHB-C1B-NB	2.15	126.54	124.26
26	F	303	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
26	1	608	CLA	C3B-C4B-NB	-2.15	108.52	110.52
26	9	604	CLA	CHB-C1B-NB	2.15	126.53	124.26
26	Z	611	CLA	CHB-C1B-NB	2.15	126.53	124.26
26	B	840	CLA	CHB-C4A-NA	2.15	127.49	124.51
32	4	624	LMG	O1-C1-C2	2.15	111.66	108.30
35	5	621	XAT	C24-C23-C22	-2.15	106.62	110.77
26	F	301	CLA	CHB-C1B-NB	2.15	126.53	124.26
29	7	623	BCR	C15-C14-C13	-2.15	124.24	127.31
26	Z	614	CLA	C3B-C4B-NB	-2.15	108.52	110.52
26	A	834	CLA	CAA-CBA-CGA	-2.15	106.97	113.25
35	Y	1622	XAT	C18-C5-C4	2.15	116.70	114.28
26	A	801	CLA	CHB-C4A-NA	2.15	127.48	124.51
29	B	801	BCR	C37-C22-C21	-2.15	119.91	122.92
26	A	814	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
26	5	617	CLA	O2A-CGA-O1A	-2.15	118.17	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	854	CLA	C11-C10-C8	-2.15	108.98	115.92
26	9	612	CLA	CHB-C4A-NA	2.15	127.48	124.51
26	a	612	CLA	CHB-C1B-NB	2.15	126.53	124.26
26	K	204	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	2	614	CLA	CHB-C4A-NA	2.14	127.48	124.51
26	B	828	CLA	CHB-C4A-NA	2.14	127.48	124.51
36	V	1623	NEX	C19-C9-C8	2.14	123.89	118.93
26	1	602	CLA	O1D-CGD-CBD	2.14	128.87	124.48
26	B	820	CLA	C3B-C4B-NB	-2.14	108.53	110.52
26	8	609	CLA	CMB-C2B-C1B	-2.14	122.10	125.37
26	W	604	CLA	CMB-C2B-C3B	2.14	131.78	126.59
26	8	602	CLA	CHB-C1B-NB	2.14	126.53	124.26
26	8	603	CLA	CHB-C1B-NB	2.14	126.53	124.26
26	B	838	CLA	CMB-C2B-C3B	2.14	131.78	126.59
26	Y	610	CLA	CHD-C1D-ND	-2.14	122.48	124.45
26	9	602	CLA	CMB-C2B-C3B	2.14	131.78	126.59
26	B	841	CLA	CHB-C1B-NB	2.14	126.52	124.26
37	Z	609	CHL	O1D-CGD-CBD	-2.14	120.10	124.48
26	4	611	CLA	C3B-C4B-NB	-2.14	108.53	110.52
26	3	602	CLA	C1-C2-C3	-2.14	122.34	126.04
26	Z	614	CLA	CHB-C1B-NB	2.14	126.52	124.26
36	Z	1623	NEX	C11-C12-C13	-2.14	120.40	126.42
26	X	613	CLA	CAC-C3C-C4C	2.14	127.59	124.81
26	1	611	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
32	L	2631	LMG	O1-C1-C2	2.14	111.64	108.30
37	W	601	CHL	CHB-C4A-NA	2.14	127.47	124.51
34	W	1621	LUT	C37-C21-C26	-2.14	106.31	109.55
37	U	607	CHL	CHC-C4B-NB	-2.14	121.99	124.26
26	A	833	CLA	O2D-CGD-CBD	2.14	115.07	111.27
26	4	603	CLA	O2A-CGA-O1A	-2.14	117.97	123.30
26	a	606	CLA	CHD-C1D-ND	-2.14	122.49	124.45
26	5	619	CLA	O2D-CGD-CBD	2.14	115.06	111.27
26	A	819	CLA	C3B-C4B-NB	-2.14	108.53	110.52
26	7	609	CLA	C3B-C4B-NB	-2.14	108.53	110.52
26	Z	612	CLA	C3B-C4B-NB	-2.14	108.53	110.52
26	A	806	CLA	C3C-C4C-NC	-2.14	108.17	110.57
34	3	618	LUT	C15-C14-C13	-2.14	124.26	127.31
35	4	620	XAT	C37-C21-C36	-2.14	104.22	107.37
26	B	812	CLA	CHB-C1B-NB	2.14	126.52	124.26
35	4	620	XAT	C19-C9-C8	2.14	121.44	118.08
37	W	605	CHL	CHB-C4A-NA	2.14	127.47	124.51
26	Z	611	CLA	CHB-C4A-NA	2.13	127.46	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	Y	1622	XAT	C7-C8-C9	-2.13	122.22	125.53
26	V	613	CLA	C3B-C4B-NB	-2.13	108.53	110.52
26	6	616	CLA	CHC-C4B-NB	2.13	126.52	124.26
26	6	617	CLA	CHB-C1B-NB	2.13	126.52	124.26
26	4	611	CLA	CMB-C2B-C3B	2.13	131.76	126.59
35	3	619	XAT	C35-C15-C14	-2.13	119.10	123.47
26	1	614	CLA	C3B-C4B-NB	-2.13	108.80	110.23
26	B	809	CLA	CHC-C4B-NB	2.13	126.52	124.26
26	3	606	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
26	4	608	CLA	C3B-C4B-NB	-2.13	108.54	110.52
29	a	619	BCR	C1-C6-C7	2.13	121.81	115.78
26	2	601	CLA	CHB-C4A-NA	2.13	127.46	124.51
34	9	619	LUT	C17-C1-C6	-2.13	106.84	110.30
26	5	616	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
26	A	832	CLA	O2D-CGD-CBD	2.13	115.06	111.27
26	A	833	CLA	CBA-CAA-C2A	2.13	120.15	113.86
29	A	856	BCR	C16-C15-C14	-2.13	119.11	123.47
29	9	621	BCR	C15-C14-C13	-2.13	124.27	127.31
29	1	619	BCR	C1-C6-C7	2.13	121.81	115.78
26	A	817	CLA	CAC-C3C-C4C	2.13	127.57	124.81
36	5	624	NEX	C35-C15-C14	-2.13	119.11	123.47
26	7	603	CLA	CHB-C1B-NB	2.13	126.51	124.26
26	A	843	CLA	C11-C12-C13	-2.13	109.04	115.92
34	9	619	LUT	C28-C29-C30	-2.13	115.67	118.94
37	U	605	CHL	C1C-C2C-C3C	-2.13	105.42	107.11
26	A	842	CLA	CMB-C2B-C3B	2.13	131.74	126.59
26	G	204	CLA	CHC-C4B-NB	2.13	126.51	124.26
37	W	608	CHL	O2D-CGD-O1D	-2.13	119.68	123.84
26	B	821	CLA	CHB-C4A-NA	2.13	127.45	124.51
29	B	843	BCR	C37-C22-C21	-2.13	119.94	122.92
26	A	825	CLA	CHD-C1D-ND	-2.13	122.50	124.45
26	3	604	CLA	CHD-C1D-ND	-2.13	122.50	124.45
26	3	615	CLA	C3B-C4B-NB	-2.13	108.54	110.52
37	Z	609	CHL	CMB-C2B-C1B	2.13	128.61	125.37
35	4	620	XAT	C40-C33-C34	2.13	125.90	122.92
26	W	610	CLA	CMB-C2B-C1B	-2.12	122.13	125.37
34	W	1620	LUT	C11-C12-C13	-2.12	120.45	126.42
26	B	814	CLA	C1-C2-C3	-2.12	122.37	126.04
26	6	603	CLA	CHD-C1D-ND	-2.12	122.50	124.45
29	A	852	BCR	C16-C17-C18	-2.12	124.28	127.31
26	6	616	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
26	A	828	CLA	CMB-C2B-C3B	2.12	131.72	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	608	CLA	CHC-C4B-NB	2.12	126.50	124.26
31	A	858	LMU	O5B-C1B-C2B	2.12	115.10	111.31
29	K	207	BCR	C11-C12-C13	-2.12	120.46	126.42
26	3	609	CLA	C3B-C4B-NB	-2.12	108.55	110.52
26	1	609	CLA	CMB-C2B-C3B	2.12	129.08	123.59
31	5	628	LMU	O5B-C5B-C4B	2.12	113.54	109.69
37	X	607	CHL	C4D-C3D-CAD	2.12	110.59	108.10
29	5	622	BCR	C15-C14-C13	-2.12	124.29	127.31
37	X	601	CHL	C4D-C3D-CAD	2.12	110.59	108.10
29	B	843	BCR	C20-C19-C18	-2.12	120.47	126.42
26	7	611	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
26	a	602	CLA	CHB-C1B-NB	2.12	126.50	124.26
26	A	854	CLA	O1D-CGD-CBD	2.12	128.82	124.48
26	B	809	CLA	O1D-CGD-CBD	2.12	128.82	124.48
35	Y	1622	XAT	C10-C11-C12	-2.12	116.61	123.22
26	A	814	CLA	CMB-C2B-C3B	2.12	131.71	126.59
26	U	602	CLA	CMB-C2B-C1B	-2.12	122.15	125.37
28	U	2630	LHG	C6-C5-C4	-2.12	106.78	111.79
26	4	607	CLA	CHB-C4A-NA	2.12	127.44	124.51
26	Z	603	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
26	6	604	CLA	CHB-C1B-NB	2.11	126.50	124.26
29	L	309	BCR	C35-C13-C14	2.11	125.89	122.92
35	6	621	XAT	C15-C35-C34	-2.11	119.14	123.47
26	A	854	CLA	CMD-C2D-C3D	2.11	132.48	127.61
26	9	602	CLA	CHB-C4A-NA	2.11	127.44	124.51
26	5	619	CLA	C3B-C4B-NB	-2.11	108.81	110.23
29	F	305	BCR	C23-C24-C25	-2.11	121.27	127.20
26	A	805	CLA	C4-C3-C2	-2.11	118.26	123.68
26	B	830	CLA	C2D-C1D-ND	-2.11	108.55	110.10
34	6	619	LUT	C15-C35-C34	-2.11	119.15	123.47
26	X	604	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
26	8	602	CLA	C1-C2-C3	-2.11	122.39	126.04
26	W	612	CLA	CHC-C4B-NB	2.11	126.49	124.26
26	A	828	CLA	CAA-CBA-CGA	-2.11	107.08	113.25
29	F	305	BCR	C37-C22-C21	-2.11	119.97	122.92
26	B	814	CLA	CHD-C1D-ND	-2.11	122.51	124.45
26	B	818	CLA	CHD-C1D-ND	-2.11	122.51	124.45
26	A	831	CLA	CHB-C4A-NA	2.11	127.43	124.51
26	B	835	CLA	CHB-C4A-NA	2.11	127.43	124.51
26	1	613	CLA	CHB-C4A-NA	2.11	127.43	124.51
29	A	852	BCR	C16-C15-C14	-2.11	119.15	123.47
26	3	602	CLA	O2A-CGA-O1A	-2.11	118.27	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	621	BCR	C24-C23-C22	-2.11	123.05	126.23
26	U	614	CLA	CHB-C1B-NB	2.11	126.49	124.26
36	X	1623	NEX	O24-C25-C26	-2.11	57.21	58.96
26	B	808	CLA	C11-C10-C8	-2.11	109.10	115.92
35	W	1622	XAT	O4-C5-C6	-2.11	57.21	58.96
29	F	305	BCR	C35-C13-C12	2.11	121.40	118.08
26	Y	604	CLA	CHB-C1B-NB	2.11	126.49	124.26
26	O	2002	CLA	CMA-C3A-C2A	-2.11	111.18	116.10
35	3	619	XAT	C18-C5-C4	2.11	116.65	114.28
37	X	607	CHL	C6-C5-C3	-2.11	107.93	113.45
26	5	603	CLA	CHD-C1D-ND	-2.11	122.52	124.45
26	Z	602	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
35	6	621	XAT	C37-C21-C26	-2.11	104.36	110.05
37	X	601	CHL	CAA-C2A-C1A	2.11	118.88	111.97
26	A	814	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
34	U	1620	LUT	C31-C30-C29	-2.11	124.30	127.31
29	K	202	BCR	C16-C15-C14	-2.11	119.16	123.47
26	Z	610	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
29	A	850	BCR	C7-C8-C9	-2.11	123.05	126.23
26	4	607	CLA	CHB-C1B-NB	2.10	126.48	124.26
26	B	811	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
26	2	609	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
26	A	839	CLA	CHD-C1D-ND	-2.10	122.52	124.45
26	a	607	CLA	CHB-C4A-NA	2.10	127.42	124.51
26	A	825	CLA	O1D-CGD-CBD	2.10	128.78	124.48
29	B	849	BCR	C15-C14-C13	-2.10	124.31	127.31
34	W	1621	LUT	C31-C32-C33	-2.10	120.51	126.42
26	A	821	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
35	2	620	XAT	C4-C3-C2	-2.10	106.72	110.77
26	O	2001	CLA	CHB-C4A-NA	2.10	127.42	124.51
26	4	606	CLA	CHB-C4A-NA	2.10	127.42	124.51
26	B	803	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
26	Z	612	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
26	B	811	CLA	C4-C3-C2	-2.10	118.29	123.68
26	5	608	CLA	C3B-C4B-NB	-2.10	108.57	110.52
29	B	801	BCR	C30-C25-C26	-2.10	119.66	122.61
26	5	601	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
26	A	818	CLA	CMB-C2B-C3B	2.10	131.67	126.59
34	Z	1621	LUT	C35-C15-C14	-2.10	119.17	123.47
26	B	823	CLA	O2A-CGA-O1A	-2.10	118.07	123.30
26	Y	602	CLA	CHB-C1B-NB	2.10	126.48	124.26
26	6	609	CLA	C3B-C4B-NB	-2.10	108.57	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Y	608	CHL	O2D-CGD-O1D	-2.10	119.74	123.84
26	9	601	CLA	CHD-C1D-ND	-2.10	122.53	124.45
26	A	805	CLA	CHC-C4B-NB	2.10	126.48	124.26
26	B	828	CLA	CHB-C1B-NB	2.10	126.48	124.26
26	B	808	CLA	C3B-C4B-NB	-2.10	108.57	110.52
34	4	619	LUT	C36-C21-C26	2.10	112.72	109.55
26	X	612	CLA	C2A-C1A-CHA	2.10	127.53	123.86
26	B	820	CLA	C1-C2-C3	-2.10	123.36	126.75
26	6	612	CLA	CHD-C1D-ND	-2.10	122.53	124.45
26	a	602	CLA	O1D-CGD-CBD	2.10	128.77	124.48
26	6	611	CLA	C3B-C4B-NB	-2.10	108.57	110.52
26	F	303	CLA	CHB-C1B-NB	2.10	126.48	124.26
35	V	1622	XAT	C11-C12-C13	-2.10	120.53	126.42
29	A	851	BCR	C36-C18-C17	-2.10	119.99	122.92
26	B	819	CLA	CMB-C2B-C3B	2.10	131.66	126.59
26	B	805	CLA	O1D-CGD-CBD	2.10	128.77	124.48
26	W	610	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
26	L	304	CLA	O2A-CGA-O1A	-2.09	118.08	123.30
36	V	1623	NEX	O24-C25-C26	-2.09	57.23	58.96
26	A	834	CLA	CHB-C1B-NB	2.09	126.47	124.26
26	1	602	CLA	CHB-C1B-NB	2.09	126.47	124.26
26	3	602	CLA	O1D-CGD-CBD	2.09	128.77	124.48
26	W	612	CLA	C2A-C1A-CHA	2.09	127.52	123.86
26	A	802	CLA	CHD-C1D-ND	-2.09	122.53	124.45
35	4	620	XAT	C30-C31-C32	-2.09	116.68	123.22
26	5	614	CLA	C3B-C4B-NB	-2.09	108.57	110.52
26	1	611	CLA	CHD-C1D-ND	-2.09	122.53	124.45
34	1	617	LUT	C12-C13-C14	-2.09	115.73	118.94
26	3	613	CLA	CHB-C1B-NB	2.09	126.47	124.26
26	A	827	CLA	C3B-C4B-NB	-2.09	108.57	110.52
26	7	612	CLA	C3B-C4B-NB	-2.09	108.57	110.52
26	8	604	CLA	C3B-C4B-NB	-2.09	108.57	110.52
26	A	818	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
29	1	619	BCR	C24-C23-C22	-2.09	123.08	126.23
26	A	826	CLA	CHB-C4A-NA	2.09	127.40	124.51
26	1	608	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
26	B	825	CLA	CMB-C2B-C3B	2.09	131.65	126.59
26	7	602	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
26	2	611	CLA	CHD-C1D-ND	-2.09	122.53	124.45
26	9	602	CLA	C3B-C4B-NB	-2.09	108.58	110.52
31	A	857	LMU	C1B-C2B-C3B	2.09	114.34	110.00
28	7	622	LHG	P-O6-C4	-2.09	109.44	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	2	623	BCR	C36-C18-C19	2.09	121.37	118.08
26	V	610	CLA	C1-C2-C3	-2.09	122.43	126.04
26	V	610	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
34	9	619	LUT	C2-C3-C4	2.09	113.16	110.30
26	W	602	CLA	C1-C2-C3	-2.09	122.44	126.04
26	A	809	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
26	8	608	CLA	CHD-C1D-ND	-2.09	122.54	124.45
35	W	1622	XAT	C15-C35-C34	-2.09	119.20	123.47
26	K	204	CLA	C3B-C4B-NB	-2.09	108.58	110.52
26	6	618	CLA	CHC-C4B-NB	2.09	126.47	124.26
26	a	613	CLA	CHB-C4A-NA	2.09	127.40	124.51
34	U	1621	LUT	C21-C26-C27	-2.09	110.06	112.70
26	a	608	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
37	V	607	CHL	CHB-C4A-NA	2.08	127.39	124.51
37	V	601	CHL	C4-C3-C5	2.08	118.78	115.27
26	B	804	CLA	C3B-C4B-NB	-2.08	108.58	110.52
35	6	621	XAT	C15-C14-C13	-2.08	124.33	127.31
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	3	604	CLA	CAA-CBA-CGA	-2.08	107.16	113.25
29	L	301	BCR	C1-C6-C5	-2.08	119.68	122.61
34	5	620	LUT	C38-C25-C24	-2.08	119.10	123.56
26	8	604	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
34	2	619	LUT	C38-C25-C24	-2.08	119.10	123.56
26	A	836	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
37	U	607	CHL	CBB-CAB-C3B	-2.08	117.26	127.62
37	Z	605	CHL	C2A-C1A-CHA	-2.08	120.22	123.85
26	A	828	CLA	CAA-C2A-C1A	-2.08	105.16	111.97
26	3	612	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
26	B	818	CLA	C6-C5-C3	2.08	118.91	113.45
29	A	849	BCR	C29-C30-C25	2.08	113.68	110.48
26	2	607	CLA	CHD-C1D-ND	-2.08	122.54	124.45
26	8	606	CLA	CHD-C1D-ND	-2.08	122.54	124.45
29	K	202	BCR	C23-C24-C25	-2.08	121.36	127.20
26	B	829	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
37	X	608	CHL	OMC-CMC-C2C	-2.08	120.98	125.69
35	5	621	XAT	C19-C9-C8	2.08	121.35	118.08
34	X	1621	LUT	C28-C29-C30	-2.08	115.75	118.94
36	6	624	NEX	C17-C1-C6	-2.08	108.61	110.47
35	Z	1622	XAT	C30-C31-C32	-2.08	116.73	123.22
26	A	801	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
29	B	844	BCR	C39-C30-C25	2.08	113.67	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	813	CLA	CHB-C4A-NA	2.08	127.39	124.51
29	L	308	BCR	C20-C21-C22	2.08	130.28	127.31
34	a	617	LUT	C12-C13-C14	-2.08	115.75	118.94
26	A	806	CLA	CMB-C2B-C3B	2.08	131.62	126.59
29	L	308	BCR	C29-C30-C25	2.08	113.68	110.48
26	A	836	CLA	O1D-CGD-CBD	2.08	128.74	124.48
26	B	824	CLA	O1D-CGD-CBD	2.08	128.74	124.48
26	A	829	CLA	C3B-C4B-NB	-2.08	108.59	110.52
26	6	602	CLA	O2D-CGD-CBD	2.08	114.96	111.27
26	9	604	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
26	K	201	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
26	B	818	CLA	CHB-C1B-NB	2.08	126.45	124.26
26	6	601	CLA	C3B-C4B-NB	-2.08	108.59	110.52
26	B	811	CLA	C3B-C4B-NB	-2.07	108.84	110.23
26	4	616	CLA	C3B-C4B-NB	-2.07	108.84	110.23
29	B	848	BCR	C21-C20-C19	-2.07	116.74	123.22
37	Y	607	CHL	C1-C2-C3	-2.07	122.46	126.04
26	a	616	CLA	CHB-C1B-NB	2.07	126.45	124.26
26	4	608	CLA	CAC-C3C-C4C	2.07	127.50	124.81
37	Y	606	CHL	CED-O2D-CGD	2.07	120.63	115.94
26	3	609	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
26	8	608	CLA	CMB-C2B-C1B	-2.07	122.21	125.37
26	B	803	CLA	CMB-C2B-C3B	2.07	131.60	126.59
29	7	623	BCR	C11-C12-C13	-2.07	120.60	126.42
26	5	616	CLA	CHB-C4A-NA	2.07	127.37	124.51
29	B	846	BCR	C32-C1-C6	-2.07	106.94	110.30
26	B	834	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
26	U	603	CLA	CHA-C1A-NA	-2.07	121.66	126.40
26	V	604	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
34	4	619	LUT	C22-C23-C24	2.07	114.10	111.74
26	U	603	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	A	856	BCR	C15-C16-C17	-2.07	119.24	123.47
26	2	607	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
29	a	619	BCR	C37-C22-C21	-2.07	120.03	122.92
37	V	607	CHL	OMC-CMC-C2C	-2.07	121.01	125.69
35	4	620	XAT	C36-C21-C26	2.07	115.63	110.05
34	Y	1621	LUT	C18-C5-C4	2.07	118.19	114.36
26	9	614	CLA	CHB-C4A-NA	2.07	127.37	124.51
29	B	847	BCR	C40-C30-C25	-2.07	106.95	110.30
26	B	827	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
37	U	608	CHL	CHC-C4B-NB	-2.07	122.07	124.26
29	B	844	BCR	C2-C1-C6	-2.07	107.30	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	602	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
26	6	608	CLA	O2A-CGA-O1A	-2.07	118.15	123.30
26	2	603	CLA	O2A-CGA-O1A	-2.07	118.15	123.30
26	5	611	CLA	CHB-C1B-NB	2.06	126.44	124.26
26	4	609	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
26	V	612	CLA	O2A-CGA-O1A	-2.06	118.15	123.30
26	6	614	CLA	CHB-C4A-NA	2.06	127.37	124.51
26	2	610	CLA	C4-C3-C5	2.06	118.74	115.27
35	1	618	XAT	O24-C25-C26	-2.06	57.25	58.96
35	9	620	XAT	C4-C3-C2	-2.06	106.79	110.77
29	L	301	BCR	C27-C26-C25	-2.06	119.74	122.73
26	Y	603	CLA	CHC-C4B-NB	2.06	126.44	124.26
37	U	609	CHL	C1-C2-C3	-2.06	122.48	126.04
26	A	834	CLA	CMB-C2B-C3B	2.06	131.58	126.59
29	J	102	BCR	C27-C26-C25	-2.06	119.74	122.73
26	A	839	CLA	CHC-C4B-NB	2.06	126.44	124.26
26	B	839	CLA	CHB-C4A-NA	2.06	127.36	124.51
26	4	610	CLA	CHD-C1D-ND	-2.06	122.56	124.45
37	W	607	CHL	C4D-CHA-C1A	-2.06	118.74	121.25
26	1	608	CLA	CHC-C4B-NB	2.06	126.44	124.26
34	2	619	LUT	C8-C9-C10	2.06	122.10	118.94
26	G	204	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
29	5	622	BCR	C15-C16-C17	-2.06	119.25	123.47
34	Y	1620	LUT	C39-C29-C28	2.06	121.32	118.08
33	B	850	DGD	C1D-C2D-C3D	2.06	114.28	110.00
36	U	1623	NEX	C10-C11-C12	2.06	129.64	123.22
35	6	621	XAT	C24-C23-C22	-2.06	106.80	110.77
26	A	827	CLA	CHB-C4A-NA	2.06	127.36	124.51
26	B	813	CLA	O1D-CGD-CBD	2.06	128.69	124.48
26	A	810	CLA	CHA-C1A-NA	-2.06	121.69	126.40
26	L	307	CLA	CMB-C2B-C3B	2.06	131.57	126.59
37	Y	605	CHL	C3B-C4B-NB	2.06	112.42	110.52
34	7	619	LUT	C11-C10-C9	-2.06	124.38	127.31
26	B	835	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
26	A	820	CLA	C3B-C4B-NB	-2.06	108.61	110.52
26	3	606	CLA	C3B-C4B-NB	-2.06	108.61	110.52
35	U	1622	XAT	O4-C5-C6	-2.06	57.26	58.96
26	B	808	CLA	C16-C15-C13	-2.06	109.28	115.92
26	X	610	CLA	CHB-C1B-C2B	-2.06	121.43	127.24
35	Y	1622	XAT	O4-C5-C6	-2.06	57.26	58.96
32	5	627	LMG	C8-O7-C10	-2.05	112.73	117.79
31	5	629	LMU	O5'-C5'-C6'	2.05	111.54	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	802	CLA	CHB-C1B-NB	2.05	126.43	124.26
26	B	822	CLA	CHB-C1B-NB	2.05	126.43	124.26
26	Z	613	CLA	CHB-C1B-NB	2.05	126.43	124.26
26	7	601	CLA	CHB-C4A-NA	2.05	127.35	124.51
37	W	606	CHL	CBC-CAC-C3C	-2.05	106.77	112.43
26	A	809	CLA	CHC-C4B-NB	2.05	126.43	124.26
26	A	827	CLA	CHC-C4B-NB	2.05	126.43	124.26
36	Y	1623	NEX	O24-C25-C26	-2.05	57.26	58.96
29	7	623	BCR	C30-C25-C26	-2.05	119.72	122.61
26	A	801	CLA	C2A-C1A-CHA	2.05	127.45	123.86
28	4	622	LHG	O8-C23-C24	2.05	118.35	111.91
26	6	608	CLA	CHC-C4B-NB	2.05	126.43	124.26
26	Z	610	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
26	B	824	CLA	C3B-C4B-NB	-2.05	108.61	110.52
26	1	610	CLA	C3B-C4B-NB	-2.05	108.61	110.52
26	2	601	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	W	604	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	F	304	CLA	CMA-C3A-C2A	-2.05	111.31	116.10
26	A	809	CLA	O2D-CGD-CBD	2.05	114.91	111.27
26	a	611	CLA	CHD-C1D-ND	-2.05	122.57	124.45
34	4	619	LUT	C17-C1-C6	-2.05	106.97	110.30
26	5	613	CLA	C4-C3-C2	-2.05	118.42	123.68
26	Y	610	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
32	H	205	LMG	O5-C6-C5	-2.05	104.26	111.29
37	W	606	CHL	CAA-C2A-C3A	-2.05	107.16	112.78
37	Z	608	CHL	C4D-C3D-CAD	2.05	110.51	108.10
26	A	833	CLA	CHB-C1B-NB	2.05	126.43	124.26
37	Y	608	CHL	C4D-CHA-C1A	-2.05	118.75	121.25
35	a	618	XAT	O24-C25-C26	-2.05	57.26	58.96
37	Y	608	CHL	CED-O2D-CGD	2.05	120.57	115.94
29	A	856	BCR	C30-C25-C26	-2.05	119.73	122.61
36	V	1623	NEX	C31-C30-C29	-2.05	124.39	127.31
26	2	602	CLA	CHD-C1D-ND	-2.05	122.57	124.45
26	4	603	CLA	CHD-C1D-ND	-2.05	122.57	124.45
26	5	604	CLA	CHB-C1B-NB	2.05	126.42	124.26
26	Y	603	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	A	803	CLA	CMB-C2B-C3B	2.05	131.55	126.59
26	Y	614	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
37	X	605	CHL	C3B-C4B-NB	2.05	112.41	110.52
32	4	624	LMG	C7-O1-C1	-2.05	109.74	113.74
26	9	601	CLA	O2A-CGA-O1A	-2.05	118.20	123.30
32	H	205	LMG	C9-C8-C7	-2.05	106.95	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	841	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
35	2	620	XAT	O4-C5-C6	-2.05	57.26	58.96
29	a	619	BCR	C24-C23-C22	-2.05	123.14	126.23
26	A	830	CLA	C7-C6-C5	-2.05	107.80	113.36
37	Z	605	CHL	CHC-C4B-NB	-2.05	122.09	124.26
26	7	613	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
36	W	1623	NEX	C2-C1-C6	2.04	111.20	109.21
26	U	610	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
26	Y	613	CLA	CHB-C1B-NB	2.04	126.42	124.26
26	7	601	CLA	C3B-C4B-NB	-2.04	108.62	110.52
29	O	2005	BCR	C38-C26-C27	2.04	117.54	113.62
26	G	203	CLA	CHD-C1D-ND	-2.04	122.58	124.45
29	K	207	BCR	C36-C18-C17	-2.04	120.06	122.92
26	Y	611	CLA	CHB-C1B-NB	2.04	126.42	124.26
26	A	804	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
34	2	619	LUT	C11-C12-C13	-2.04	120.68	126.42
26	B	836	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
29	B	801	BCR	C7-C8-C9	-2.04	123.15	126.23
26	A	828	CLA	CHC-C4B-NB	2.04	126.42	124.26
26	7	616	CLA	CHC-C4B-NB	2.04	126.42	124.26
29	6	622	BCR	C24-C25-C26	-2.04	116.52	121.46
26	A	835	CLA	C7-C6-C5	-2.04	107.82	113.36
26	2	614	CLA	CHC-C4B-NB	2.04	126.42	124.26
26	A	839	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	G	204	CLA	C3B-C4B-NB	-2.04	108.62	110.52
26	6	612	CLA	CHB-C4A-NA	2.04	127.33	124.51
37	W	607	CHL	C1-C2-C3	-2.04	122.52	126.04
26	X	613	CLA	CHD-C1D-ND	-2.04	122.58	124.45
26	7	610	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
28	X	2630	LHG	C5-O7-C7	-2.04	112.77	117.79
29	L	309	BCR	C15-C16-C17	-2.04	119.30	123.47
35	X	1622	XAT	C18-C5-C4	2.04	116.57	114.28
26	A	811	CLA	C1-C2-C3	-2.04	122.52	126.04
26	A	832	CLA	CHC-C4B-NB	2.04	126.41	124.26
26	B	832	CLA	C4-C3-C5	-2.04	111.84	115.27
34	V	1620	LUT	C11-C12-C13	-2.04	120.69	126.42
26	X	604	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
29	L	309	BCR	C12-C13-C14	-2.04	115.82	118.94
34	X	1620	LUT	C39-C29-C28	2.04	121.28	118.08
26	1	610	CLA	C2A-C1A-CHA	2.04	125.87	122.71
26	U	604	CLA	C3B-C4B-NB	-2.04	108.63	110.52
26	V	613	CLA	CHC-C4B-NB	2.03	126.41	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	W	603	CLA	CMB-C2B-C3B	2.03	131.51	126.59
26	B	806	CLA	CHC-C1C-NC	2.03	127.29	124.20
26	5	607	CLA	O2D-CGD-CBD	2.03	114.88	111.27
26	4	606	CLA	CHB-C1B-NB	2.03	126.41	124.26
26	5	602	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
26	7	601	CLA	C4-C3-C2	-2.03	118.46	123.68
26	5	609	CLA	C3B-C4B-NB	-2.03	108.63	110.52
26	6	612	CLA	CHC-C4B-NB	2.03	126.41	124.26
37	Z	606	CHL	CHB-C1B-C2B	-2.03	121.50	127.24
26	J	101	CLA	CHC-C4B-NB	2.03	126.41	124.26
29	5	622	BCR	C7-C8-C9	-2.03	123.17	126.23
26	7	611	CLA	O1D-CGD-CBD	2.03	128.64	124.48
36	V	1623	NEX	C40-C33-C32	2.03	121.28	118.08
26	4	614	CLA	CHB-C4A-NA	2.03	127.32	124.51
26	8	610	CLA	C6-C5-C3	2.03	118.78	113.45
35	6	621	XAT	C7-C8-C9	-2.03	122.38	125.53
34	9	619	LUT	C12-C13-C14	-2.03	115.83	118.94
26	W	611	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	6	616	CLA	CHB-C1B-NB	2.03	126.41	124.26
26	B	836	CLA	O1D-CGD-CBD	2.03	128.64	124.48
26	1	606	CLA	CHB-C4A-NA	2.03	127.32	124.51
26	3	609	CLA	CHB-C1B-NB	2.03	126.41	124.26
26	B	810	CLA	O2D-CGD-CBD	2.03	114.87	111.27
26	2	614	CLA	C3B-C4B-NB	-2.03	108.63	110.52
35	5	621	XAT	C4-C3-C2	-2.03	106.86	110.77
35	2	620	XAT	C11-C10-C9	-2.03	124.42	127.31
29	B	844	BCR	C33-C5-C4	2.03	117.51	113.62
26	7	607	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	U	613	CLA	CHD-C1D-ND	-2.03	122.59	124.45
32	J	103	LMG	O8-C28-O10	-2.03	118.48	123.59
26	a	610	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
37	X	608	CHL	O2D-CGD-O1D	-2.03	119.88	123.84
37	W	609	CHL	O2D-CGD-O1D	-2.03	119.88	123.84
26	1	616	CLA	CHB-C1B-NB	2.03	126.40	124.26
26	Z	603	CLA	CHC-C4B-NB	2.03	126.40	124.26
26	B	827	CLA	CMB-C2B-C3B	2.03	131.49	126.59
29	A	851	BCR	C39-C30-C25	-2.03	107.01	110.30
26	B	810	CLA	C2A-C1A-CHA	2.03	127.40	123.86
26	K	203	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	5	612	CLA	CMB-C2B-C1B	-2.02	122.28	125.37
26	a	610	CLA	C3B-C4B-NB	-2.02	108.64	110.52
26	B	834	CLA	O2D-CGD-CBD	2.02	114.86	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	J	102	BCR	C7-C6-C5	2.02	126.36	121.46
26	A	831	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
29	B	852	BCR	C27-C26-C25	-2.02	119.79	122.73
26	X	613	CLA	CHC-C4B-NB	2.02	126.40	124.26
26	A	837	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
34	W	1621	LUT	C7-C8-C9	-2.02	123.18	126.23
26	B	830	CLA	C3C-C4C-NC	-2.02	108.30	110.57
26	4	601	CLA	C1-C2-C3	-2.02	122.55	126.04
26	5	611	CLA	C3B-C4B-NB	-2.02	108.64	110.52
26	B	802	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
35	9	620	XAT	C24-C23-C22	-2.02	106.87	110.77
26	A	814	CLA	CHB-C1B-NB	2.02	126.40	124.26
35	X	1622	XAT	C31-C32-C33	-2.02	120.74	126.42
26	A	839	CLA	O2D-CGD-CBD	2.02	114.86	111.27
35	8	620	XAT	C30-C31-C32	-2.02	116.91	123.22
26	a	602	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
34	U	1621	LUT	C11-C12-C13	-2.02	120.74	126.42
35	5	621	XAT	C38-C25-C24	2.02	116.55	114.28
26	A	806	CLA	CHB-C1B-NB	2.02	126.39	124.26
26	5	604	CLA	CHD-C1D-ND	-2.02	122.60	124.45
26	8	602	CLA	O2D-CGD-CBD	2.02	114.85	111.27
32	H	205	LMG	O7-C10-O9	-2.02	118.83	123.70
26	4	602	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
26	B	808	CLA	C1-C2-C3	-2.02	122.55	126.04
26	Y	602	CLA	C1-C2-C3	-2.02	122.55	126.04
34	U	1621	LUT	C15-C35-C34	-2.02	119.34	123.47
29	B	845	BCR	C30-C25-C26	-2.02	119.77	122.61
29	O	2004	BCR	C37-C22-C21	-2.02	120.10	122.92
35	W	1622	XAT	C30-C31-C32	-2.02	116.92	123.22
26	2	603	CLA	CAC-C3C-C4C	2.02	127.43	124.81
26	B	809	CLA	CHB-C1B-NB	2.02	126.39	124.26
26	B	837	CLA	CHC-C4B-NB	2.02	126.39	124.26
26	5	602	CLA	CHB-C1B-NB	2.02	126.39	124.26
37	U	608	CHL	C4D-CHA-C1A	-2.02	118.80	121.25
26	4	608	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
34	9	619	LUT	C30-C31-C32	-2.02	116.93	123.22
26	B	803	CLA	C3B-C4B-NB	-2.02	108.64	110.52
35	5	621	XAT	C35-C15-C14	-2.02	119.34	123.47
26	2	616	CLA	C3B-C4B-NB	-2.02	108.88	110.23
26	A	808	CLA	CHB-C1B-NB	2.01	126.39	124.26
29	A	852	BCR	C27-C26-C25	-2.01	119.81	122.73
26	B	829	CLA	O1D-CGD-CBD	2.01	128.60	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	607	CHL	C1C-C2C-C3C	-2.01	105.52	107.11
26	B	828	CLA	C3B-C4B-NB	-2.01	108.65	110.52
36	5	624	NEX	C16-C1-C6	-2.01	108.67	110.47
37	Z	606	CHL	CED-O2D-CGD	2.01	120.49	115.94
26	A	840	CLA	CMB-C2B-C3B	2.01	131.46	126.59
26	V	612	CLA	O2D-CGD-CBD	2.01	114.84	111.27
26	V	610	CLA	CAA-CBA-CGA	-2.01	107.37	113.25
26	A	833	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
26	a	609	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
37	V	609	CHL	CHC-C4B-NB	-2.01	122.13	124.26
29	L	308	BCR	C15-C16-C17	-2.01	119.35	123.47
37	X	601	CHL	CAA-C2A-C3A	-2.01	107.27	112.78
26	3	603	CLA	CAC-C3C-C4C	2.01	127.42	124.81
35	a	618	XAT	C38-C25-C24	2.01	116.54	114.28
26	W	602	CLA	O2D-CGD-CBD	2.01	114.84	111.27
37	X	605	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
26	8	616	CLA	CHD-C1D-ND	-2.01	122.61	124.45
26	A	838	CLA	O1D-CGD-CBD	2.01	128.60	124.48
32	J	104	LMG	C7-O1-C1	-2.01	109.81	113.74
28	7	622	LHG	O8-C23-C24	2.01	118.21	111.91
34	3	618	LUT	C3-C4-C5	-2.01	107.85	111.85
26	Y	614	CLA	C3B-C4B-NB	-2.01	108.65	110.52
26	V	602	CLA	CHB-C1B-NB	2.01	126.38	124.26
26	1	604	CLA	O1D-CGD-CBD	2.01	128.59	124.48
26	A	830	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
26	U	611	CLA	CHD-C1D-ND	-2.01	122.61	124.45
26	A	832	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
29	A	848	BCR	C11-C12-C13	-2.01	120.78	126.42
26	A	826	CLA	O1D-CGD-CBD	2.01	128.59	124.48
26	B	841	CLA	CHD-C1D-ND	-2.01	122.61	124.45
26	B	837	CLA	C4-C3-C5	2.01	118.65	115.27
26	4	602	CLA	CHB-C4A-NA	2.01	127.29	124.51
26	7	611	CLA	CHB-C1B-NB	2.01	126.38	124.26
26	B	825	CLA	O1D-CGD-CBD	2.01	128.59	124.48
35	1	618	XAT	C38-C25-C24	2.01	116.54	114.28
26	1	602	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
26	4	603	CLA	C3B-C4B-NB	-2.01	108.89	110.23
26	6	617	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
28	2	622	LHG	C6-C5-C4	-2.01	107.04	111.79
26	6	617	CLA	O1D-CGD-CBD	2.00	128.59	124.48
26	A	816	CLA	O1D-CGD-CBD	2.00	128.59	124.48
29	O	2004	BCR	C38-C26-C25	-2.00	122.28	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	7	604	CLA	CHB-C1B-NB	2.00	126.38	124.26
29	K	207	BCR	C16-C15-C14	-2.00	119.37	123.47
36	V	1623	NEX	C30-C31-C32	-2.00	116.97	123.22
37	V	608	CHL	C4D-CHA-C1A	-2.00	118.81	121.25
26	Z	614	CLA	CHD-C1D-ND	-2.00	122.61	124.45
28	W	2630	LHG	C5-O7-C7	-2.00	112.86	117.79
26	A	821	CLA	C3B-C4B-NB	-2.00	108.66	110.52
37	Y	607	CHL	CMD-C2D-C3D	-2.00	123.01	127.61
35	Z	1622	XAT	C39-C29-C28	2.00	121.23	118.08
32	8	626	LMG	O7-C10-O9	-2.00	118.86	123.70
26	6	602	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
26	W	610	CLA	O2D-CGD-CBD	2.00	114.83	111.27
26	1	610	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
29	B	846	BCR	C21-C20-C19	-2.00	116.97	123.22
26	Z	610	CLA	O2D-CGD-CBD	2.00	114.82	111.27

There are no chirality outliers.

All (3788) 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	C2A-CAA-CBA-CGA
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	814	CLA	CHA-CBD-CGD-O1D
26	A	814	CLA	CHA-CBD-CGD-O2D
26	A	815	CLA	CBD-CGD-O2D-CED
26	A	816	CLA	C1A-C2A-CAA-CBA
26	A	816	CLA	C3A-C2A-CAA-CBA
26	A	816	CLA	CHA-CBD-CGD-O1D
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

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Mol	Chain	Res	Type	Atoms
26	A	821	CLA	C3A-C2A-CAA-CBA
26	A	821	CLA	CHA-CBD-CGD-O1D
26	A	821	CLA	CHA-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	CHA-CBD-CGD-O1D
26	A	828	CLA	CHA-CBD-CGD-O2D
26	A	828	CLA	CAD-CBD-CGD-O1D
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	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	841	CLA	CHA-CBD-CGD-O1D
26	A	841	CLA	CHA-CBD-CGD-O2D
26	A	845	CLA	C1A-C2A-CAA-CBA
26	A	854	CLA	CHA-CBD-CGD-O1D
26	A	854	CLA	CHA-CBD-CGD-O2D
26	B	802	CLA	CHA-CBD-CGD-O1D
26	B	802	CLA	CHA-CBD-CGD-O2D
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	CHA-CBD-CGD-O1D
26	B	813	CLA	CHA-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	818	CLA	C4-C3-C5-C6
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	823	CLA	CHA-CBD-CGD-O1D
26	B	823	CLA	CHA-CBD-CGD-O2D
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	C2B-C3B-CAB-CBB
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-O2D
26	B	835	CLA	CBD-CGD-O2D-CED
26	B	839	CLA	C2A-CAA-CBA-CGA
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	J	101	CLA	CHA-CBD-CGD-O1D
26	J	101	CLA	CHA-CBD-CGD-O2D
26	K	201	CLA	C2B-C3B-CAB-CBB
26	K	201	CLA	C4B-C3B-CAB-CBB
26	K	203	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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	302	CLA	CHA-CBD-CGD-O1D
26	L	302	CLA	CHA-CBD-CGD-O2D
26	L	303	CLA	C2-C3-C5-C6
26	L	303	CLA	C4-C3-C5-C6
26	O	2003	CLA	C2B-C3B-CAB-CBB
26	O	2003	CLA	C4B-C3B-CAB-CBB
26	1	601	CLA	C4B-C3B-CAB-CBB
26	1	603	CLA	C2B-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	1	611	CLA	CHA-CBD-CGD-O1D
26	1	611	CLA	CHA-CBD-CGD-O2D
26	1	613	CLA	CHA-CBD-CGD-O1D
26	1	613	CLA	CHA-CBD-CGD-O2D
26	1	616	CLA	CHA-CBD-CGD-O1D
26	1	616	CLA	CHA-CBD-CGD-O2D
26	a	601	CLA	C4B-C3B-CAB-CBB
26	a	603	CLA	C2B-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	a	613	CLA	CHA-CBD-CGD-O1D
26	a	613	CLA	CHA-CBD-CGD-O2D
26	a	616	CLA	CHA-CBD-CGD-O1D
26	a	616	CLA	CHA-CBD-CGD-O2D
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	602	CLA	C4B-C3B-CAB-CBB
26	2	604	CLA	CBD-CGD-O2D-CED
26	2	610	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
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	611	CLA	CHA-CBD-CGD-O1D
26	2	611	CLA	CHA-CBD-CGD-O2D
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	C2B-C3B-CAB-CBB
26	3	608	CLA	C4B-C3B-CAB-CBB
26	3	609	CLA	C3A-C2A-CAA-CBA
26	3	609	CLA	C2A-CAA-CBA-CGA
26	3	609	CLA	C2B-C3B-CAB-CBB
26	3	609	CLA	C4B-C3B-CAB-CBB
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	614	CLA	C2B-C3B-CAB-CBB
26	3	614	CLA	C4B-C3B-CAB-CBB
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	604	CLA	CHA-CBD-CGD-O1D
26	4	604	CLA	CHA-CBD-CGD-O2D
26	4	604	CLA	C11-C10-C8-C7
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	CBD-CGD-O2D-CED
26	4	618	CLA	C1A-C2A-CAA-CBA
26	5	601	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	5	601	CLA	C4B-C3B-CAB-CBB
26	5	602	CLA	CHA-CBD-CGD-O1D
26	5	602	CLA	CHA-CBD-CGD-O2D
26	5	604	CLA	CHA-CBD-CGD-O1D
26	5	604	CLA	CHA-CBD-CGD-O2D
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	C2B-C3B-CAB-CBB
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	CHA-CBD-CGD-O1D
26	5	617	CLA	CHA-CBD-CGD-O2D
26	5	617	CLA	CAD-CBD-CGD-O1D
26	5	617	CLA	CBD-CGD-O2D-CED
26	5	618	CLA	C1A-C2A-CAA-CBA
26	5	618	CLA	C3A-C2A-CAA-CBA
26	5	619	CLA	CHA-CBD-CGD-O2D
26	6	601	CLA	CHA-CBD-CGD-O1D
26	6	607	CLA	CHA-CBD-CGD-O1D
26	6	607	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	611	CLA	CHA-CBD-CGD-O1D
26	6	611	CLA	CHA-CBD-CGD-O2D
26	6	612	CLA	C1A-C2A-CAA-CBA
26	6	612	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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	CHA-CBD-CGD-O1D
26	7	601	CLA	CHA-CBD-CGD-O2D
26	7	601	CLA	CAD-CBD-CGD-O1D
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	613	CLA	CHA-CBD-CGD-O1D
26	7	613	CLA	CHA-CBD-CGD-O2D
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	CHA-CBD-CGD-O1D
26	8	606	CLA	CHA-CBD-CGD-O2D
26	8	606	CLA	CBD-CGD-O2D-CED
26	8	607	CLA	CBD-CGD-O2D-CED
26	8	608	CLA	C2B-C3B-CAB-CBB
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	8	614	CLA	CHA-CBD-CGD-O1D
26	8	614	CLA	CHA-CBD-CGD-O2D
26	9	601	CLA	CHA-CBD-CGD-O1D
26	9	601	CLA	CHA-CBD-CGD-O2D
26	9	604	CLA	O1A-CGA-O2A-C1
26	9	606	CLA	C1A-C2A-CAA-CBA
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	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	9	610	CLA	C4B-C3B-CAB-CBB
26	9	611	CLA	C4B-C3B-CAB-CBB
26	9	611	CLA	CHA-CBD-CGD-O1D
26	9	611	CLA	CHA-CBD-CGD-O2D
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	9	613	CLA	CHA-CBD-CGD-O1D
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	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	CHA-CBD-CGD-O1D
26	X	611	CLA	CHA-CBD-CGD-O2D
26	X	611	CLA	CAD-CBD-CGD-O1D
26	X	612	CLA	C2B-C3B-CAB-CBB
26	X	612	CLA	C4B-C3B-CAB-CBB
26	X	613	CLA	CHA-CBD-CGD-O1D
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	602	CLA	CHA-CBD-CGD-O1D
26	Y	602	CLA	CHA-CBD-CGD-O2D
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	611	CLA	CHA-CBD-CGD-O1D
26	Y	611	CLA	CHA-CBD-CGD-O2D
26	Y	613	CLA	CHA-CBD-CGD-O1D
26	Y	613	CLA	CHA-CBD-CGD-O2D
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

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Mol	Chain	Res	Type	Atoms
26	Z	610	CLA	C2-C3-C5-C6
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	603	CLA	CHA-CBD-CGD-O1D
26	U	603	CLA	CHA-CBD-CGD-O2D
26	U	611	CLA	C4B-C3B-CAB-CBB
26	U	612	CLA	C2B-C3B-CAB-CBB
26	U	612	CLA	C4B-C3B-CAB-CBB
26	U	613	CLA	CHA-CBD-CGD-O1D
26	U	613	CLA	CHA-CBD-CGD-O2D
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	613	CLA	CHA-CBD-CGD-O1D
26	V	613	CLA	CHA-CBD-CGD-O2D
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	611	CLA	C1A-C2A-CAA-CBA
26	W	612	CLA	C2B-C3B-CAB-CBB
26	W	612	CLA	C4B-C3B-CAB-CBB
26	W	613	CLA	C2B-C3B-CAB-CBB
26	W	613	CLA	C4B-C3B-CAB-CBB
26	W	613	CLA	CHA-CBD-CGD-O1D
26	W	613	CLA	CHA-CBD-CGD-O2D
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	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	C4-O6-P-O3
28	B	851	LHG	C3-O3-P-O4
28	B	851	LHG	C3-O3-P-O5
28	B	851	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
28	H	204	LHG	C4-O6-P-O4
28	H	204	LHG	O7-C5-C6-O8
28	1	620	LHG	O1-C1-C2-C3
28	1	620	LHG	C3-O3-P-O4
28	a	620	LHG	O1-C1-C2-C3
28	a	620	LHG	C3-O3-P-O4
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-O6
28	3	623	LHG	C4-O6-P-O5
28	3	624	LHG	C3-O3-P-O5
28	5	623	LHG	C3-O3-P-O4
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	C4-O6-P-O5
28	7	622	LHG	C3-O3-P-O6
28	8	622	LHG	C4-O6-P-O4
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	O7-C5-C6-O8
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
28	Z	2630	LHG	O1-C1-C2-C3
28	U	2630	LHG	C3-O3-P-O6
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

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Mol	Chain	Res	Type	Atoms
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	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	847	BCR	C37-C22-C23-C24
29	B	848	BCR	C21-C22-C23-C24
29	B	848	BCR	C37-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	852	BCR	C7-C8-C9-C34
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	305	BCR	C7-C8-C9-C10
29	L	305	BCR	C7-C8-C9-C34
29	L	308	BCR	C5-C6-C7-C8
29	L	308	BCR	C7-C8-C9-C10
29	L	308	BCR	C7-C8-C9-C34
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
29	a	619	BCR	C23-C24-C25-C30
29	2	623	BCR	C7-C8-C9-C10
29	3	620	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
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	C37-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	K	208	LMU	C2-C1-O1'-C1'
31	5	628	LMU	C2'-C1'-O1'-C1
31	5	628	LMU	O5'-C1'-O1'-C1
31	5	628	LMU	C2-C1-O1'-C1'
31	8	625	LMU	C2'-C1'-O1'-C1
31	8	625	LMU	O5'-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	4	619	LUT	C7-C8-C9-C10
34	4	619	LUT	C7-C8-C9-C19
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	9	619	LUT	C7-C8-C9-C10
34	9	619	LUT	C7-C8-C9-C19
34	Y	1620	LUT	C13-C14-C15-C35
34	Y	1621	LUT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	Y	1621	LUT	C7-C8-C9-C19
34	U	1620	LUT	C31-C32-C33-C40
34	V	1620	LUT	C7-C8-C9-C10
34	V	1620	LUT	C7-C8-C9-C19
34	V	1621	LUT	C7-C8-C9-C10
34	V	1621	LUT	C7-C8-C9-C19
34	W	1620	LUT	C7-C8-C9-C10
34	W	1620	LUT	C7-C8-C9-C19
34	W	1621	LUT	C7-C8-C9-C10
35	4	620	XAT	C21-C26-C27-C28
35	4	620	XAT	C25-C26-C27-C28
35	X	1622	XAT	C11-C12-C13-C14
35	X	1622	XAT	C11-C12-C13-C20
35	Z	1622	XAT	C11-C12-C13-C20
35	U	1622	XAT	C11-C12-C13-C14
35	U	1622	XAT	C11-C12-C13-C20
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	601	CHL	C2A-CAA-CBA-CGA
37	X	606	CHL	C1A-C2A-CAA-CBA
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	CHA-CBD-CGD-O1D
37	X	609	CHL	CHA-CBD-CGD-O2D
37	Y	605	CHL	C3C-C2C-CMC-OMC
37	Y	606	CHL	C3C-C2C-CMC-OMC
37	Z	601	CHL	C2-C3-C5-C6
37	Z	601	CHL	C4-C3-C5-C6
37	Z	605	CHL	C1C-C2C-CMC-OMC
37	Z	605	CHL	C3C-C2C-CMC-OMC
37	Z	606	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	Z	606	CHL	C3A-C2A-CAA-CBA
37	Z	607	CHL	C1A-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	C3C-C2C-CMC-OMC
37	U	606	CHL	C3C-C2C-CMC-OMC
37	U	607	CHL	C1A-C2A-CAA-CBA
37	U	607	CHL	C3A-C2A-CAA-CBA
37	U	607	CHL	C2B-C3B-CAB-CBB
37	U	607	CHL	C4B-C3B-CAB-CBB
37	U	607	CHL	C1C-C2C-CMC-OMC
37	U	607	CHL	C3C-C2C-CMC-OMC
37	U	608	CHL	C1A-C2A-CAA-CBA
37	U	608	CHL	C3A-C2A-CAA-CBA
37	U	609	CHL	C1C-C2C-CMC-OMC
37	U	609	CHL	C3C-C2C-CMC-OMC
37	V	605	CHL	C3C-C2C-CMC-OMC
37	V	606	CHL	C2B-C3B-CAB-CBB
37	V	606	CHL	C4B-C3B-CAB-CBB
37	V	607	CHL	C1A-C2A-CAA-CBA
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	C3C-C2C-CMC-OMC
37	V	609	CHL	C1C-C2C-CMC-OMC
37	V	609	CHL	C3C-C2C-CMC-OMC
37	W	605	CHL	C3C-C2C-CMC-OMC
37	W	605	CHL	CHA-CBD-CGD-O1D
37	W	605	CHL	CHA-CBD-CGD-O2D
37	W	607	CHL	C3C-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

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Mol	Chain	Res	Type	Atoms
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
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	829	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

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Mol	Chain	Res	Type	Atoms
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	613	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
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	811	CLA	O1D-CGD-O2D-CED
26	A	815	CLA	O1D-CGD-O2D-CED
26	2	606	CLA	O1D-CGD-O2D-CED
26	3	604	CLA	O1D-CGD-O2D-CED
26	6	617	CLA	O1D-CGD-O2D-CED
26	Z	612	CLA	O1D-CGD-O2D-CED
26	V	614	CLA	O1D-CGD-O2D-CED
37	U	607	CHL	O1D-CGD-O2D-CED
26	B	806	CLA	O1D-CGD-O2D-CED
26	B	814	CLA	O1D-CGD-O2D-CED
26	B	822	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

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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	X	602	CLA	O1D-CGD-O2D-CED
26	Y	604	CLA	O1D-CGD-O2D-CED
26	V	613	CLA	O1D-CGD-O2D-CED
26	W	614	CLA	O1D-CGD-O2D-CED
37	Z	608	CHL	O1D-CGD-O2D-CED
26	A	839	CLA	CBA-CGA-O2A-C1
26	8	604	CLA	CBA-CGA-O2A-C1
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
26	A	835	CLA	C4C-C3C-CAC-CBC
26	A	818	CLA	O1A-CGA-O2A-C1
26	A	821	CLA	O1A-CGA-O2A-C1
26	B	831	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
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	6	614	CLA	O1D-CGD-O2D-CED
26	7	608	CLA	O1D-CGD-O2D-CED
26	7	612	CLA	O1D-CGD-O2D-CED
26	A	810	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
37	Z	607	CHL	O1D-CGD-O2D-CED
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
26	B	809	CLA	O1D-CGD-O2D-CED
26	2	612	CLA	O1D-CGD-O2D-CED
26	6	608	CLA	O1D-CGD-O2D-CED
26	X	612	CLA	O1D-CGD-O2D-CED
37	V	608	CHL	O1D-CGD-O2D-CED
28	9	623	LHG	O9-C7-O7-C5
32	H	205	LMG	O9-C10-O7-C8
26	A	822	CLA	O1A-CGA-O2A-C1
26	4	609	CLA	O1A-CGA-O2A-C1
26	B	813	CLA	C4C-C3C-CAC-CBC
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

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Mol	Chain	Res	Type	Atoms
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
37	W	601	CHL	C3-C5-C6-C7
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
27	A	844	PQN	C15-C16-C17-C18
32	8	626	LMG	C11-C10-O7-C8
33	B	850	DGD	C2B-C1B-O2G-C2G
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	837	CLA	CBD-CGD-O2D-CED
26	5	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	7	613	CLA	CBD-CGD-O2D-CED
26	Y	614	CLA	O1A-CGA-O2A-C1
26	B	821	CLA	CBA-CGA-O2A-C1
26	A	805	CLA	C3-C5-C6-C7
31	K	208	LMU	O5'-C5'-C6'-O6'
26	A	818	CLA	C4-C3-C5-C6
26	A	842	CLA	C4-C3-C5-C6
26	B	817	CLA	C4-C3-C5-C6
26	A	842	CLA	C2-C3-C5-C6
26	B	818	CLA	C2-C3-C5-C6
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	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	B	824	CLA	C2A-CAA-CBA-CGA
26	B	831	CLA	C2A-CAA-CBA-CGA
26	4	601	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	606	CHL	C2A-CAA-CBA-CGA
37	Z	607	CHL	C2A-CAA-CBA-CGA
37	W	605	CHL	C2A-CAA-CBA-CGA
37	W	607	CHL	C2A-CAA-CBA-CGA
26	Y	603	CLA	O1A-CGA-O2A-C1
28	3	624	LHG	O10-C23-O8-C6
26	V	603	CLA	O1D-CGD-O2D-CED
37	U	606	CHL	O1D-CGD-O2D-CED
37	U	608	CHL	O1D-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
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
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
31	8	625	LMU	O5'-C5'-C6'-O6'
26	A	835	CLA	C2C-C3C-CAC-CBC
26	A	845	CLA	O1D-CGD-O2D-CED
26	B	840	CLA	O1D-CGD-O2D-CED
27	A	844	PQN	C11-C12-C13-C14
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	A	831	CLA	O1D-CGD-O2D-CED
26	B	810	CLA	O1D-CGD-O2D-CED
26	B	816	CLA	O1D-CGD-O2D-CED
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
37	V	607	CHL	O1D-CGD-O2D-CED
32	L	2631	LMG	O9-C10-O7-C8
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

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Mol	Chain	Res	Type	Atoms
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	B	813	CLA	C2C-C3C-CAC-CBC
26	A	802	CLA	O1D-CGD-O2D-CED
26	4	608	CLA	O1D-CGD-O2D-CED
35	Z	1622	XAT	C13-C14-C15-C35
36	X	1623	NEX	C9-C10-C11-C12
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
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
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	B	813	CLA	C3-C5-C6-C7
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	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	U	603	CLA	O1D-CGD-O2D-CED
28	3	623	LHG	C8-C7-O7-C5
31	5	629	LMU	O5B-C1B-O1B-C4'
26	A	821	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	7	604	CLA	O1A-CGA-O2A-C1
37	Y	601	CHL	O1A-CGA-O2A-C1
28	1	620	LHG	C14-C15-C16-C17
32	H	205	LMG	C4-C5-C6-O5
26	A	835	CLA	O1D-CGD-O2D-CED
26	A	841	CLA	CBD-CGD-O2D-CED
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	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	839	CLA	O1D-CGD-O2D-CED
26	Y	614	CLA	O1D-CGD-O2D-CED
31	A	857	LMU	O5B-C5B-C6B-O6B
26	5	613	CLA	C4-C3-C5-C6
26	8	610	CLA	C4-C3-C5-C6
26	5	613	CLA	C2-C3-C5-C6
26	8	610	CLA	C2-C3-C5-C6
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
31	5	629	LMU	O5B-C5B-C6B-O6B
26	A	805	CLA	O1A-CGA-O2A-C1
26	A	816	CLA	O1A-CGA-O2A-C1
26	B	802	CLA	O1A-CGA-O2A-C1
26	Y	613	CLA	O1D-CGD-O2D-CED
26	6	616	CLA	C2C-C3C-CAC-CBC
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	830	CLA	CBD-CGD-O2D-CED
26	1	609	CLA	CBD-CGD-O2D-CED
26	W	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	K	208	LMU	C4'-C5'-C6'-O6'
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
26	6	616	CLA	O1D-CGD-O2D-CED
26	U	602	CLA	O1D-CGD-O2D-CED
26	B	813	CLA	O1D-CGD-O2D-CED
26	H	203	CLA	O1D-CGD-O2D-CED
26	8	616	CLA	O1D-CGD-O2D-CED
37	X	605	CHL	O1D-CGD-O2D-CED
28	X	2630	LHG	C1-C2-C3-O3
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
26	B	814	CLA	C3-C5-C6-C7
26	6	613	CLA	C3-C5-C6-C7
26	U	610	CLA	O1D-CGD-O2D-CED
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	2	613	CLA	C15-C16-C17-C18
26	B	804	CLA	CBD-CGD-O2D-CED
26	L	304	CLA	CBD-CGD-O2D-CED
26	W	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	A	844	PQN	C23-C25-C26-C27
37	X	601	CHL	C5-C6-C7-C8
37	X	607	CHL	C13-C15-C16-C17
32	V	2631	LMG	O6-C5-C6-O5
37	X	601	CHL	O1A-CGA-O2A-C1
31	A	857	LMU	C4B-C5B-C6B-O6B
31	5	629	LMU	C4B-C5B-C6B-O6B
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
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	Y	614	CLA	O2A-C1-C2-C3
31	K	208	LMU	C2'-C1'-O1'-C1
28	7	622	LHG	O7-C5-C6-O8
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
37	U	601	CHL	C4-C3-C5-C6
26	B	817	CLA	C2-C3-C5-C6
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
26	F	304	CLA	O1D-CGD-O2D-CED
26	3	608	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	3	609	CLA	CBD-CGD-O2D-CED
28	Y	2630	LHG	C24-C25-C26-C27
31	A	858	LMU	C5'-C4'-O1B-C1B
26	5	602	CLA	C8-C10-C11-C12
26	B	811	CLA	C2A-CAA-CBA-CGA
26	9	613	CLA	C2A-CAA-CBA-CGA
37	V	607	CHL	C2A-CAA-CBA-CGA
29	B	849	BCR	C37-C22-C23-C24
29	B	852	BCR	C11-C12-C13-C35
29	L	308	BCR	C36-C18-C19-C20
29	2	623	BCR	C7-C8-C9-C34
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	6	619	LUT	C7-C8-C9-C19
34	7	619	LUT	C7-C8-C9-C19
34	8	619	LUT	C7-C8-C9-C19
34	X	1620	LUT	C7-C8-C9-C19
34	Z	1620	LUT	C7-C8-C9-C19
34	W	1620	LUT	C27-C28-C29-C39
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	3	618	LUT	C7-C8-C9-C10
34	6	619	LUT	C7-C8-C9-C10
34	7	619	LUT	C7-C8-C9-C10
34	8	619	LUT	C7-C8-C9-C10
34	X	1620	LUT	C7-C8-C9-C10
34	Z	1620	LUT	C11-C12-C13-C14
26	A	814	CLA	O1A-CGA-O2A-C1
37	Z	601	CHL	O1A-CGA-O2A-C1
26	A	824	CLA	C10-C11-C12-C13
26	A	828	CLA	C13-C15-C16-C17
26	B	828	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	6	601	CLA	C13-C15-C16-C17
26	V	602	CLA	C10-C11-C12-C13
26	W	602	CLA	C10-C11-C12-C13
37	X	607	CHL	C8-C10-C11-C12
26	A	827	CLA	O1D-CGD-O2D-CED
26	A	814	CLA	CBD-CGD-O2D-CED
26	Y	602	CLA	CBD-CGD-O2D-CED
26	A	816	CLA	O1D-CGD-O2D-CED
26	3	609	CLA	C3-C5-C6-C7
26	9	610	CLA	C8-C10-C11-C12
26	A	810	CLA	CBA-CGA-O2A-C1
26	A	832	CLA	CBA-CGA-O2A-C1
26	B	828	CLA	CBA-CGA-O2A-C1
26	5	602	CLA	CBA-CGA-O2A-C1
26	8	601	CLA	CBA-CGA-O2A-C1
26	A	814	CLA	C8-C10-C11-C12
26	B	833	CLA	C8-C10-C11-C12
26	B	839	CLA	C13-C15-C16-C17
26	B	839	CLA	C15-C16-C17-C18
26	a	609	CLA	C5-C6-C7-C8
26	3	603	CLA	C5-C6-C7-C8
26	3	604	CLA	C15-C16-C17-C18
26	4	601	CLA	C5-C6-C7-C8
26	6	613	CLA	C5-C6-C7-C8
37	Z	601	CHL	C5-C6-C7-C8
37	V	601	CHL	C13-C15-C16-C17
37	W	609	CHL	C15-C16-C17-C18
28	7	622	LHG	C23-C24-C25-C26
26	6	602	CLA	O1D-CGD-O2D-CED
28	Y	2630	LHG	O10-C23-O8-C6
26	Y	612	CLA	O1D-CGD-O2D-CED
26	A	829	CLA	C5-C6-C7-C8
26	A	829	CLA	C10-C11-C12-C13
26	A	831	CLA	C10-C11-C12-C13
26	A	834	CLA	C10-C11-C12-C13
26	A	836	CLA	C5-C6-C7-C8
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	813	CLA	C5-C6-C7-C8
26	B	816	CLA	C5-C6-C7-C8
26	B	824	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	B	834	CLA	C8-C10-C11-C12
26	1	613	CLA	C8-C10-C11-C12
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	6	616	CLA	C13-C15-C16-C17
26	7	613	CLA	C15-C16-C17-C18
26	8	610	CLA	C10-C11-C12-C13
26	9	602	CLA	C5-C6-C7-C8
26	Y	603	CLA	C5-C6-C7-C8
26	V	613	CLA	C13-C15-C16-C17
27	B	842	PQN	C15-C16-C17-C18
27	B	842	PQN	C25-C26-C27-C28
37	X	608	CHL	C13-C15-C16-C17
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	U	601	CHL	C13-C15-C16-C17
37	W	601	CHL	C13-C15-C16-C17
37	W	601	CHL	C15-C16-C17-C18
26	V	611	CLA	O1D-CGD-O2D-CED
28	5	623	LHG	C7-C8-C9-C10
28	5	625	LHG	C7-C8-C9-C10
28	6	623	LHG	C23-C24-C25-C26
28	X	2630	LHG	C7-C8-C9-C10
28	V	2630	LHG	C23-C24-C25-C26
32	4	624	LMG	C28-C29-C30-C31
31	5	629	LMU	O5'-C5'-C6'-O6'
26	B	832	CLA	CBD-CGD-O2D-CED
26	4	604	CLA	O1D-CGD-O2D-CED
26	4	607	CLA	O1D-CGD-O2D-CED
26	7	602	CLA	O1D-CGD-O2D-CED
26	A	802	CLA	C15-C16-C17-C18
26	A	825	CLA	C10-C11-C12-C13
26	3	607	CLA	C5-C6-C7-C8
37	Z	601	CHL	C13-C15-C16-C17
37	V	601	CHL	C15-C16-C17-C18
37	W	609	CHL	C13-C15-C16-C17
26	Y	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	5	610	CLA	O1D-CGD-O2D-CED
26	6	620	CLA	O1D-CGD-O2D-CED
28	3	623	LHG	O9-C7-O7-C5
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	W	604	CLA	O1D-CGD-O2D-CED
28	a	620	LHG	C23-C24-C25-C26
28	3	623	LHG	C7-C8-C9-C10
26	a	603	CLA	CBD-CGD-O2D-CED
26	B	826	CLA	C13-C15-C16-C17
37	U	606	CHL	C2A-CAA-CBA-CGA
37	V	605	CHL	C2A-CAA-CBA-CGA
37	V	606	CHL	C2A-CAA-CBA-CGA
26	Z	614	CLA	O2A-C1-C2-C3
26	A	843	CLA	C10-C11-C12-C13
26	B	809	CLA	C13-C15-C16-C17
26	A	843	CLA	C12-C13-C15-C16
26	B	802	CLA	C11-C10-C8-C7
26	B	831	CLA	C12-C13-C15-C16
26	B	839	CLA	C11-C10-C8-C7
26	B	841	CLA	C11-C10-C8-C7
26	H	203	CLA	C12-C13-C15-C16
26	5	607	CLA	C6-C7-C8-C10
26	5	613	CLA	C6-C7-C8-C10
26	9	613	CLA	C11-C12-C13-C15
26	X	603	CLA	C6-C7-C8-C10
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
28	1	620	LHG	C23-C24-C25-C26
26	A	818	CLA	C2A-CAA-CBA-CGA
26	A	821	CLA	C2A-CAA-CBA-CGA
26	A	822	CLA	C2A-CAA-CBA-CGA
26	6	617	CLA	C2A-CAA-CBA-CGA
37	X	605	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
37	U	607	CHL	C2A-CAA-CBA-CGA
37	W	606	CHL	C2A-CAA-CBA-CGA
26	A	837	CLA	O1D-CGD-O2D-CED
26	A	838	CLA	O1D-CGD-O2D-CED
26	1	610	CLA	O1D-CGD-O2D-CED
26	a	610	CLA	O1D-CGD-O2D-CED
26	4	602	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	824	CLA	C13-C15-C16-C17
26	A	831	CLA	C5-C6-C7-C8
26	A	854	CLA	C5-C6-C7-C8
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	4	608	CLA	C5-C6-C7-C8
26	A	801	CLA	O1A-CGA-O2A-C1
26	U	602	CLA	O1A-CGA-O2A-C1
26	B	823	CLA	CBD-CGD-O2D-CED
26	A	816	CLA	C8-C10-C11-C12
26	A	825	CLA	C13-C15-C16-C17
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	B	824	CLA	O1D-CGD-O2D-CED
26	A	829	CLA	C15-C16-C17-C18
26	1	601	CLA	C5-C6-C7-C8
26	a	601	CLA	C5-C6-C7-C8
26	3	609	CLA	C8-C10-C11-C12
26	7	601	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	W	609	CHL	C10-C11-C12-C13
26	A	825	CLA	O1D-CGD-O2D-CED
26	8	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	5	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	8	601	CLA	O1A-CGA-O2A-C1
26	9	613	CLA	O1A-CGA-O2A-C1
37	X	608	CHL	O1A-CGA-O2A-C1
26	3	613	CLA	CAA-CBA-CGA-O2A
28	Y	2630	LHG	C11-C10-C9-C8
26	A	806	CLA	C5-C6-C7-C8
26	A	829	CLA	C13-C15-C16-C17
26	B	818	CLA	C8-C10-C11-C12
26	V	613	CLA	C8-C10-C11-C12
37	U	609	CHL	C8-C10-C11-C12
37	V	601	CHL	C5-C6-C7-C8
26	Y	611	CLA	O1D-CGD-O2D-CED
26	A	810	CLA	O1A-CGA-O2A-C1
28	A	861	LHG	C8-C7-O7-C5
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	8	602	CLA	C10-C11-C12-C13
37	Y	607	CHL	C13-C15-C16-C17
37	U	601	CHL	C5-C6-C7-C8
28	A	847	LHG	C3-O3-P-O6
28	A	861	LHG	C3-O3-P-O6
28	H	204	LHG	C4-O6-P-O3
28	O	2631	LHG	C3-O3-P-O6
28	1	620	LHG	C3-O3-P-O6
28	a	620	LHG	C3-O3-P-O6
28	2	622	LHG	C3-O3-P-O6
28	3	624	LHG	C3-O3-P-O6
28	5	623	LHG	C3-O3-P-O6
28	6	623	LHG	C3-O3-P-O6
28	6	623	LHG	C4-O6-P-O3
28	8	623	LHG	C4-O6-P-O3
28	9	622	LHG	C4-O6-P-O3
28	9	623	LHG	C3-O3-P-O6
28	9	623	LHG	C4-O6-P-O3
28	Z	2630	LHG	C4-O6-P-O3
28	W	2630	LHG	C3-O3-P-O6
28	W	2630	LHG	C4-O6-P-O3
28	3	623	LHG	C23-C24-C25-C26
26	A	834	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
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	4	611	CLA	O1D-CGD-O2D-CED
26	7	613	CLA	O1D-CGD-O2D-CED
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	Y	608	CHL	O2A-C1-C2-C3
37	Z	608	CHL	O2A-C1-C2-C3
28	6	623	LHG	C7-C8-C9-C10
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	7	622	LHG	C1-C2-C3-O3
28	A	861	LHG	O9-C7-O7-C5
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	A	818	CLA	C2-C3-C5-C6
26	B	809	CLA	C15-C16-C17-C18
26	B	833	CLA	C13-C15-C16-C17
26	5	613	CLA	C10-C11-C12-C13
26	6	610	CLA	C8-C10-C11-C12
37	X	609	CHL	C5-C6-C7-C8
26	A	814	CLA	C2A-CAA-CBA-CGA
26	A	841	CLA	C2A-CAA-CBA-CGA
26	B	828	CLA	C2A-CAA-CBA-CGA
26	2	602	CLA	C2A-CAA-CBA-CGA
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
26	Y	610	CLA	C2A-CAA-CBA-CGA
37	Z	608	CHL	C2A-CAA-CBA-CGA
31	K	208	LMU	O5B-C5B-C6B-O6B
26	L	303	CLA	C3-C5-C6-C7
26	J	101	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

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Mol	Chain	Res	Type	Atoms
28	9	624	LHG	C24-C23-O8-C6
37	Z	609	CHL	CBA-CGA-O2A-C1
26	B	816	CLA	CAA-CBA-CGA-O2A
26	B	827	CLA	C10-C11-C12-C13
32	9	625	LMG	C19-C20-C21-C22
37	Z	605	CHL	CBD-CGD-O2D-CED
28	O	2631	LHG	C8-C7-O7-C5
28	5	625	LHG	C8-C7-O7-C5
26	B	837	CLA	C13-C15-C16-C17
26	B	810	CLA	C2A-CAA-CBA-CGA
26	5	613	CLA	C2A-CAA-CBA-CGA
28	5	623	LHG	C11-C12-C13-C14
28	8	622	LHG	C15-C16-C17-C18
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	842	CLA	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	602	CLA	CBA-CGA-O2A-C1
28	7	622	LHG	C11-C12-C13-C14
28	9	624	LHG	C30-C31-C32-C33
28	O	2631	LHG	O9-C7-O7-C5
28	5	625	LHG	O9-C7-O7-C5
28	6	623	LHG	C27-C28-C29-C30
26	U	604	CLA	O1D-CGD-O2D-CED
26	B	828	CLA	O1A-CGA-O2A-C1
28	3	624	LHG	O6-C4-C5-O7
28	6	623	LHG	C28-C29-C30-C31
32	8	626	LMG	C17-C18-C19-C20
26	A	812	CLA	O1D-CGD-O2D-CED
26	A	829	CLA	C8-C10-C11-C12
37	W	608	CHL	CBA-CGA-O2A-C1
28	7	622	LHG	C10-C11-C12-C13
28	8	622	LHG	C29-C30-C31-C32
26	X	613	CLA	C3-C5-C6-C7
32	V	2631	LMG	C10-C11-C12-C13
26	5	604	CLA	O1D-CGD-O2D-CED
32	J	104	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
26	A	841	CLA	CBA-CGA-O2A-C1
28	7	622	LHG	C24-C23-O8-C6
28	9	624	LHG	C28-C29-C30-C31
28	Z	2630	LHG	C10-C11-C12-C13
28	U	2630	LHG	C27-C28-C29-C30
32	9	625	LMG	C12-C13-C14-C15
26	3	610	CLA	C8-C10-C11-C12
37	X	609	CHL	C15-C16-C17-C18
26	B	808	CLA	C16-C17-C18-C20
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	608	CHL	C16-C17-C18-C20
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	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	822	CLA	C4-C3-C5-C6
32	H	205	LMG	C31-C32-C33-C34
26	1	613	CLA	C2-C3-C5-C6
26	a	613	CLA	C2-C3-C5-C6
26	3	604	CLA	C2-C3-C5-C6
26	6	613	CLA	C2-C3-C5-C6
26	X	613	CLA	C2-C3-C5-C6
26	A	836	CLA	C11-C10-C8-C9
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	1	613	CLA	C11-C12-C13-C14
26	a	609	CLA	C11-C12-C13-C14
26	5	607	CLA	C6-C7-C8-C9
26	6	610	CLA	C11-C12-C13-C14
26	7	610	CLA	C14-C13-C15-C16
26	9	613	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
26	7	606	CLA	O1D-CGD-O2D-CED
26	A	832	CLA	C2A-CAA-CBA-CGA
26	6	616	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	Y	614	CLA	C2A-CAA-CBA-CGA
26	W	613	CLA	C2A-CAA-CBA-CGA
37	W	608	CHL	C2A-CAA-CBA-CGA
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
34	2	619	LUT	C7-C8-C9-C19
34	Z	1620	LUT	C11-C12-C13-C20
34	U	1620	LUT	C7-C8-C9-C19
34	W	1621	LUT	C7-C8-C9-C19
28	5	625	LHG	C27-C28-C29-C30
28	W	2630	LHG	O1-C1-C2-C3
34	2	619	LUT	C7-C8-C9-C10
34	Z	1620	LUT	C7-C8-C9-C10
34	U	1620	LUT	C7-C8-C9-C10
26	A	802	CLA	C3-C5-C6-C7
32	4	624	LMG	O6-C5-C6-O5
37	Z	601	CHL	C15-C16-C17-C18
31	8	625	LMU	C4-C5-C6-C7
32	H	205	LMG	C33-C34-C35-C36
28	H	204	LHG	C10-C11-C12-C13
28	5	623	LHG	C28-C29-C30-C31
28	Y	2630	LHG	C18-C19-C20-C21
31	5	628	LMU	C6-C7-C8-C9
32	L	2631	LMG	C12-C13-C14-C15
32	4	623	LMG	C31-C32-C33-C34
32	9	625	LMG	C35-C36-C37-C38
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

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Mol	Chain	Res	Type	Atoms
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
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
37	U	606	CHL	C4B-C3B-CAB-CBB
37	U	608	CHL	C4B-C3B-CAB-CBB
37	U	609	CHL	C4B-C3B-CAB-CBB
26	A	831	CLA	C16-C17-C18-C20
26	B	808	CLA	C16-C17-C18-C19
26	3	603	CLA	C6-C7-C8-C9
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	609	CHL	C16-C17-C18-C19
37	X	609	CHL	C16-C17-C18-C20
37	Y	601	CHL	C16-C17-C18-C19
37	Y	609	CHL	C16-C17-C18-C19
32	J	104	LMG	O6-C1-O1-C7
26	B	802	CLA	C5-C6-C7-C8
26	B	831	CLA	C13-C15-C16-C17
37	X	607	CHL	C10-C11-C12-C13
28	A	861	LHG	C17-C18-C19-C20
28	5	623	LHG	C16-C17-C18-C19
28	8	622	LHG	C9-C10-C11-C12
31	A	857	LMU	C6-C7-C8-C9
26	1	613	CLA	CBD-CGD-O2D-CED
26	a	613	CLA	CBD-CGD-O2D-CED
26	2	613	CLA	CBD-CGD-O2D-CED
37	V	606	CHL	O1D-CGD-O2D-CED
28	9	623	LHG	C34-C35-C36-C37
32	8	626	LMG	C18-C19-C20-C21
31	A	858	LMU	C4'-C5'-C6'-O6'
28	4	622	LHG	C10-C11-C12-C13
26	4	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
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
28	1	620	LHG	C28-C29-C30-C31
28	a	620	LHG	C28-C29-C30-C31
28	5	623	LHG	C11-C10-C9-C8
31	8	625	LMU	C3'-C4'-O1B-C1B
37	X	609	CHL	O1D-CGD-O2D-CED
37	Z	606	CHL	O1D-CGD-O2D-CED
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	1	606	CLA	CBD-CGD-O2D-CED
26	a	606	CLA	C3A-C2A-CAA-CBA
26	a	606	CLA	CBD-CGD-O2D-CED
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
26	A	842	CLA	C15-C16-C17-C18
36	V	1623	NEX	C9-C10-C11-C12
31	8	625	LMU	C2-C1-O1'-C1'
31	A	857	LMU	C11-C10-C9-C8
31	K	208	LMU	C4-C5-C6-C7
26	B	836	CLA	O1D-CGD-O2D-CED
26	A	831	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	3	603	CLA	C6-C7-C8-C10
26	W	602	CLA	C11-C12-C13-C15
37	X	607	CHL	C16-C17-C18-C19
37	X	608	CHL	C16-C17-C18-C19
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	V	601	CHL	C16-C17-C18-C20
37	V	609	CHL	C11-C12-C13-C15
37	W	609	CHL	C16-C17-C18-C20
31	8	625	LMU	C11-C10-C9-C8
26	A	839	CLA	O1D-CGD-O2D-CED
37	Z	609	CHL	O1D-CGD-O2D-CED
32	J	103	LMG	C7-C8-C9-O8
26	A	836	CLA	CBD-CGD-O2D-CED
31	1	621	LMU	C4'-C5'-C6'-O6'
31	K	208	LMU	C3-C4-C5-C6
32	A	860	LMG	C16-C17-C18-C19
26	B	803	CLA	O2A-C1-C2-C3
26	8	614	CLA	O1D-CGD-O2D-CED
26	A	804	CLA	C3-C5-C6-C7
28	B	851	LHG	C23-C24-C25-C26
28	A	861	LHG	C33-C34-C35-C36
28	3	624	LHG	C32-C33-C34-C35
28	5	625	LHG	C16-C17-C18-C19
26	2	610	CLA	C5-C6-C7-C8
26	A	826	CLA	C4-C3-C5-C6
26	K	203	CLA	C4-C3-C5-C6
26	9	609	CLA	C4-C3-C5-C6
37	Y	607	CHL	C4-C3-C5-C6
37	Z	607	CHL	C4-C3-C5-C6
26	B	841	CLA	CBA-CGA-O2A-C1
28	H	204	LHG	C24-C23-O8-C6
26	A	807	CLA	C2-C3-C5-C6
26	B	816	CLA	C2-C3-C5-C6
26	K	203	CLA	C2-C3-C5-C6
37	Y	607	CHL	C2-C3-C5-C6
28	3	624	LHG	C8-C7-O7-C5
28	1	620	LHG	O1-C1-C2-O2
28	a	620	LHG	O1-C1-C2-O2
28	Z	2630	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
28	A	846	LHG	C13-C14-C15-C16
28	9	623	LHG	C16-C17-C18-C19
28	9	623	LHG	C25-C26-C27-C28
26	X	612	CLA	C2A-CAA-CBA-CGA
26	1	602	CLA	O1A-CGA-O2A-C1
26	a	602	CLA	O1A-CGA-O2A-C1
26	4	601	CLA	C16-C17-C18-C20
26	5	613	CLA	C16-C17-C18-C19
37	Y	609	CHL	C16-C17-C18-C20
37	U	601	CHL	C16-C17-C18-C20
26	A	812	CLA	C2B-C3B-CAB-CBB
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	A	841	CLA	C2B-C3B-CAB-CBB
26	B	802	CLA	C2B-C3B-CAB-CBB
26	B	837	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	1	601	CLA	C2B-C3B-CAB-CBB
26	1	607	CLA	C2B-C3B-CAB-CBB
26	a	601	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	4	602	CLA	C2B-C3B-CAB-CBB
26	5	611	CLA	C2B-C3B-CAB-CBB
26	5	617	CLA	C2B-C3B-CAB-CBB
26	6	604	CLA	C2B-C3B-CAB-CBB
26	6	611	CLA	C2B-C3B-CAB-CBB
26	6	614	CLA	C2B-C3B-CAB-CBB
26	6	620	CLA	C2B-C3B-CAB-CBB
26	7	610	CLA	C2B-C3B-CAB-CBB
26	8	601	CLA	C2B-C3B-CAB-CBB
26	8	613	CLA	C2B-C3B-CAB-CBB
26	9	607	CLA	C2B-C3B-CAB-CBB
26	9	611	CLA	C2B-C3B-CAB-CBB
26	9	614	CLA	C2B-C3B-CAB-CBB
26	X	603	CLA	C2B-C3B-CAB-CBB
26	Y	603	CLA	C2B-C3B-CAB-CBB
26	Y	612	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	Z	610	CLA	C2B-C3B-CAB-CBB
26	Z	613	CLA	C2B-C3B-CAB-CBB
26	U	611	CLA	C2B-C3B-CAB-CBB
26	V	603	CLA	C2B-C3B-CAB-CBB
26	V	611	CLA	C2B-C3B-CAB-CBB
26	V	613	CLA	C2B-C3B-CAB-CBB
26	W	611	CLA	C2B-C3B-CAB-CBB
37	U	606	CHL	C2B-C3B-CAB-CBB
37	U	608	CHL	C2B-C3B-CAB-CBB
37	U	609	CHL	C2B-C3B-CAB-CBB
26	A	830	CLA	C13-C15-C16-C17
26	7	602	CLA	C13-C15-C16-C17
37	Y	601	CHL	C8-C10-C11-C12
28	A	846	LHG	C29-C30-C31-C32
31	8	625	LMU	C5'-C4'-O1B-C1B
26	A	807	CLA	O1A-CGA-O2A-C1
28	5	625	LHG	C1-C2-C3-O3
31	5	628	LMU	C5-C6-C7-C8
28	3	624	LHG	O9-C7-O7-C5
28	H	204	LHG	C32-C33-C34-C35
26	A	834	CLA	C5-C6-C7-C8
26	B	805	CLA	C10-C11-C12-C13
26	B	841	CLA	C13-C15-C16-C17
26	A	841	CLA	O1A-CGA-O2A-C1
37	Z	609	CHL	O1A-CGA-O2A-C1
31	A	858	LMU	C1-C2-C3-C4
32	8	626	LMG	C14-C15-C16-C17
26	3	602	CLA	C11-C12-C13-C14
29	A	848	BCR	C1-C6-C7-C8
29	A	848	BCR	C5-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

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Mol	Chain	Res	Type	Atoms
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	K	202	BCR	C5-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
29	5	622	BCR	C23-C24-C25-C30
29	7	623	BCR	C5-C6-C7-C8
29	7	623	BCR	C23-C24-C25-C26
34	4	619	LUT	C5-C6-C7-C8
34	6	619	LUT	C1-C6-C7-C8
34	9	619	LUT	C1-C6-C7-C8
34	9	619	LUT	C5-C6-C7-C8
34	X	1620	LUT	C1-C6-C7-C8
34	X	1620	LUT	C5-C6-C7-C8
34	Y	1620	LUT	C1-C6-C7-C8
34	Y	1620	LUT	C5-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
34	W	1621	LUT	C5-C6-C7-C8
31	A	858	LMU	C6-C7-C8-C9
26	B	818	CLA	C5-C6-C7-C8
26	a	609	CLA	C13-C15-C16-C17
27	B	842	PQN	C20-C21-C22-C23
28	B	851	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
28	6	623	LHG	C8-C7-O7-C5
32	A	860	LMG	C11-C10-O7-C8
26	Z	603	CLA	O1D-CGD-O2D-CED
26	2	601	CLA	C15-C16-C17-C18
26	8	613	CLA	C5-C6-C7-C8
26	8	613	CLA	C10-C11-C12-C13
26	B	816	CLA	C2-C1-O2A-CGA
26	A	814	CLA	C4-C3-C5-C6
26	B	808	CLA	C4-C3-C5-C6
26	B	814	CLA	C4-C3-C5-C6
26	B	816	CLA	C4-C3-C5-C6
26	F	301	CLA	C4-C3-C5-C6
26	X	613	CLA	C4-C3-C5-C6
26	V	613	CLA	C4-C3-C5-C6
26	A	807	CLA	C11-C10-C8-C7
26	A	814	CLA	C11-C10-C8-C7
26	A	822	CLA	C2-C3-C5-C6
26	A	824	CLA	C11-C10-C8-C7
26	A	826	CLA	C2-C3-C5-C6
26	B	802	CLA	C6-C7-C8-C10
26	B	808	CLA	C2-C3-C5-C6
26	B	810	CLA	C2-C3-C5-C6
26	B	814	CLA	C2-C3-C5-C6
26	B	827	CLA	C12-C13-C15-C16
26	B	833	CLA	C6-C7-C8-C10
26	H	203	CLA	C11-C10-C8-C7
26	1	613	CLA	C11-C12-C13-C15
26	a	609	CLA	C11-C12-C13-C15
26	a	609	CLA	C12-C13-C15-C16
26	5	609	CLA	C11-C10-C8-C7
26	6	601	CLA	C11-C10-C8-C7
26	7	610	CLA	C12-C13-C15-C16
26	8	601	CLA	C11-C12-C13-C15
26	8	613	CLA	C11-C10-C8-C7
26	9	609	CLA	C2-C3-C5-C6
26	9	613	CLA	C11-C10-C8-C7
26	Y	613	CLA	C12-C13-C15-C16
26	V	613	CLA	C2-C3-C5-C6
26	V	613	CLA	C6-C7-C8-C10
26	W	613	CLA	C11-C12-C13-C15
37	X	608	CHL	C6-C7-C8-C10
37	X	609	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
37	Z	607	CHL	C2-C3-C5-C6
37	U	601	CHL	C6-C7-C8-C10
37	V	601	CHL	C11-C12-C13-C15
37	W	601	CHL	C6-C7-C8-C10
37	W	601	CHL	C11-C10-C8-C7
26	A	806	CLA	C3-C5-C6-C7
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
28	5	623	LHG	C12-C13-C14-C15
26	A	807	CLA	C15-C16-C17-C18
26	a	609	CLA	C10-C11-C12-C13
37	X	601	CHL	C15-C16-C17-C18
26	B	819	CLA	CBD-CGD-O2D-CED
26	7	616	CLA	CBD-CGD-O2D-CED
26	1	613	CLA	C16-C17-C18-C19
26	6	604	CLA	C16-C17-C18-C20
37	W	607	CHL	C16-C17-C18-C19
26	A	821	CLA	O1D-CGD-O2D-CED
32	5	627	LMG	C28-C29-C30-C31
26	A	813	CLA	CBA-CGA-O2A-C1
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
32	J	103	LMG	C29-C28-O8-C9
26	A	803	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	A	824	CLA	C8-C10-C11-C12
26	A	825	CLA	C15-C16-C17-C18
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	W	601	CHL	C8-C10-C11-C12
26	3	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	B	817	CLA	C10-C11-C12-C13
28	O	2631	LHG	C7-C8-C9-C10
26	B	804	CLA	O1D-CGD-O2D-CED
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	A	801	CLA	C3-C5-C6-C7
26	L	304	CLA	O1D-CGD-O2D-CED
28	9	623	LHG	C17-C18-C19-C20
28	U	2630	LHG	C9-C10-C11-C12
26	B	841	CLA	O1A-CGA-O2A-C1
26	B	837	CLA	CBD-CGD-O2D-CED
26	3	612	CLA	CBD-CGD-O2D-CED
26	B	833	CLA	CBA-CGA-O2A-C1
37	U	609	CHL	CBA-CGA-O2A-C1
26	B	831	CLA	C16-C17-C18-C20
26	B	832	CLA	C11-C12-C13-C15
26	A	806	CLA	C10-C11-C12-C13
26	B	810	CLA	C5-C6-C7-C8
26	5	609	CLA	C13-C15-C16-C17
28	X	2630	LHG	C28-C29-C30-C31
28	A	846	LHG	C7-C8-C9-C10
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	A	846	LHG	C31-C32-C33-C34
37	U	601	CHL	C10-C11-C12-C13
26	L	302	CLA	CBD-CGD-O2D-CED
26	B	838	CLA	CBA-CGA-O2A-C1
28	H	204	LHG	O10-C23-O8-C6
28	B	851	LHG	O9-C7-O7-C5
28	6	623	LHG	O9-C7-O7-C5
32	A	860	LMG	O9-C10-O7-C8
32	J	104	LMG	O9-C10-O7-C8
32	4	624	LMG	O9-C10-O7-C8
28	2	622	LHG	C23-C24-C25-C26
28	A	846	LHG	C25-C26-C27-C28
33	B	850	DGD	O6E-C5E-C6E-O5E
28	Z	2630	LHG	C11-C12-C13-C14
26	A	842	CLA	C16-C17-C18-C19
37	X	601	CHL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
28	B	851	LHG	C27-C28-C29-C30
26	B	806	CLA	C8-C10-C11-C12
37	Z	609	CHL	C13-C15-C16-C17
26	A	807	CLA	C4-C3-C5-C6
26	B	810	CLA	C4-C3-C5-C6
26	A	814	CLA	C2-C3-C5-C6
26	F	301	CLA	C2-C3-C5-C6
26	W	613	CLA	C2-C3-C5-C6
37	U	601	CHL	C2-C3-C5-C6
31	A	858	LMU	C3'-C4'-O1B-C1B
26	A	809	CLA	C14-C13-C15-C16
26	A	814	CLA	C11-C10-C8-C9
26	A	816	CLA	C11-C10-C8-C9
26	A	824	CLA	C11-C10-C8-C9
26	B	802	CLA	C6-C7-C8-C9
26	B	810	CLA	C11-C10-C8-C9
26	B	831	CLA	C14-C13-C15-C16
26	H	203	CLA	C11-C10-C8-C9
26	H	203	CLA	C14-C13-C15-C16
26	a	609	CLA	C14-C13-C15-C16
26	4	602	CLA	C6-C7-C8-C9
26	4	610	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	8	606	CLA	C11-C12-C13-C14
26	9	613	CLA	C11-C12-C13-C14
26	X	603	CLA	C6-C7-C8-C9
26	X	603	CLA	C14-C13-C15-C16
26	Y	613	CLA	C14-C13-C15-C16
26	W	613	CLA	C14-C13-C15-C16
37	X	601	CHL	C11-C10-C8-C9
37	Z	601	CHL	C11-C10-C8-C9
37	Z	607	CHL	C6-C7-C8-C9
37	W	601	CHL	C11-C10-C8-C9
28	3	623	LHG	C28-C29-C30-C31
26	U	613	CLA	C3-C5-C6-C7
37	V	601	CHL	C3-C5-C6-C7
26	A	825	CLA	C2A-CAA-CBA-CGA
26	A	842	CLA	C2A-CAA-CBA-CGA
26	B	807	CLA	C2A-CAA-CBA-CGA
26	4	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
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
31	5	628	LMU	C3'-C4'-O1B-C1B
32	9	625	LMG	C22-C23-C24-C25
26	3	607	CLA	CBA-CGA-O2A-C1
29	3	620	BCR	C37-C22-C23-C24
34	U	1621	LUT	C7-C8-C9-C19
26	1	609	CLA	O1D-CGD-O2D-CED
28	Z	2630	LHG	C25-C26-C27-C28
34	U	1620	LUT	C31-C32-C33-C34
35	U	1622	XAT	C31-C32-C33-C34
31	8	625	LMU	C1-C2-C3-C4
26	A	813	CLA	O1A-CGA-O2A-C1
26	A	815	CLA	O1A-CGA-O2A-C1
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
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

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Mol	Chain	Res	Type	Atoms
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
37	X	607	CHL	C1A-C2A-CAA-CBA
37	Y	609	CHL	C1A-C2A-CAA-CBA
37	U	609	CHL	C1A-C2A-CAA-CBA
37	V	605	CHL	C1A-C2A-CAA-CBA
37	V	606	CHL	C1A-C2A-CAA-CBA
37	V	609	CHL	C1A-C2A-CAA-CBA
37	W	605	CHL	C1A-C2A-CAA-CBA
37	W	608	CHL	C1A-C2A-CAA-CBA
26	B	832	CLA	C11-C12-C13-C14
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
28	8	623	LHG	O9-C7-O7-C5
32	9	625	LMG	O9-C10-O7-C8
26	A	843	CLA	C11-C10-C8-C7
26	A	830	CLA	O1D-CGD-O2D-CED
26	A	854	CLA	C10-C11-C12-C13
26	B	806	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	3	609	CLA	C5-C6-C7-C8
26	V	602	CLA	C8-C10-C11-C12
26	U	604	CLA	CAD-CBD-CGD-O2D
28	3	623	LHG	C4-O6-P-O3
26	A	804	CLA	C2C-C3C-CAC-CBC
32	V	2631	LMG	C32-C33-C34-C35
33	B	850	DGD	C1B-C2B-C3B-C4B
26	5	613	CLA	C3-C5-C6-C7
26	A	841	CLA	O1D-CGD-O2D-CED
32	V	2631	LMG	C4-C5-C6-O5
26	B	802	CLA	C10-C11-C12-C13
26	L	303	CLA	C10-C11-C12-C13
26	1	613	CLA	C10-C11-C12-C13
26	X	610	CLA	C5-C6-C7-C8
26	Y	610	CLA	C5-C6-C7-C8
37	X	609	CHL	C8-C10-C11-C12
26	6	603	CLA	CBA-CGA-O2A-C1
37	X	609	CHL	CBA-CGA-O2A-C1
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	U	2630	LHG	C17-C18-C19-C20
31	5	629	LMU	C2-C3-C4-C5
26	B	831	CLA	C16-C17-C18-C19
37	X	607	CHL	C16-C17-C18-C20
28	9	623	LHG	C26-C27-C28-C29
26	9	610	CLA	C3-C5-C6-C7
26	B	803	CLA	C10-C11-C12-C13
37	X	606	CHL	C2A-CAA-CBA-CGA
28	A	861	LHG	C7-C8-C9-C10
26	A	840	CLA	C2C-C3C-CAC-CBC
28	B	851	LHG	C29-C30-C31-C32
31	5	629	LMU	C3-C4-C5-C6
28	W	2630	LHG	C1-C2-C3-O3
26	W	613	CLA	C4-C3-C5-C6
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

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Mol	Chain	Res	Type	Atoms
26	9	611	CLA	C3A-C2A-CAA-CBA
26	9	612	CLA	C3A-C2A-CAA-CBA
31	5	628	LMU	C5'-C4'-O1B-C1B
31	5	629	LMU	C4-C5-C6-C7
26	A	816	CLA	C10-C11-C12-C13
37	W	607	CHL	C15-C16-C17-C18
31	A	857	LMU	C3'-C4'-O1B-C1B
26	8	602	CLA	O1A-CGA-O2A-C1
28	5	625	LHG	C24-C25-C26-C27
26	A	837	CLA	C2A-CAA-CBA-CGA
26	A	807	CLA	C16-C17-C18-C19
26	B	811	CLA	C6-C7-C8-C10
26	8	602	CLA	C11-C12-C13-C15
26	W	613	CLA	O1D-CGD-O2D-CED
26	U	602	CLA	C11-C12-C13-C14
28	H	204	LHG	C4-C5-C6-O8
28	4	622	LHG	C14-C15-C16-C17
32	5	627	LMG	C7-C8-C9-O8
32	8	626	LMG	O1-C7-C8-C9
32	8	626	LMG	C7-C8-C9-O8
26	B	839	CLA	C10-C11-C12-C13
32	J	103	LMG	O10-C28-O8-C9
26	3	609	CLA	O1D-CGD-O2D-CED
26	B	812	CLA	C2A-CAA-CBA-CGA
26	B	805	CLA	C13-C15-C16-C17
26	8	613	CLA	C15-C16-C17-C18
26	U	610	CLA	C5-C6-C7-C8
26	4	604	CLA	C11-C10-C8-C9
26	4	610	CLA	C14-C13-C15-C16
37	X	601	CHL	CAA-CBA-CGA-O2A
26	3	607	CLA	O1A-CGA-O2A-C1
26	W	603	CLA	O1A-CGA-O2A-C1
28	3	624	LHG	C9-C10-C11-C12
37	U	609	CHL	C2C-C3C-CAC-CBC
26	A	834	CLA	C8-C10-C11-C12
26	V	610	CLA	C8-C10-C11-C12
31	5	629	LMU	C6-C7-C8-C9
31	A	857	LMU	C5'-C4'-O1B-C1B
32	H	205	LMG	C16-C17-C18-C19
26	A	819	CLA	C11-C12-C13-C14
26	B	814	CLA	C16-C17-C18-C19
26	6	616	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	B	816	CLA	C2A-CAA-CBA-CGA
32	J	104	LMG	O6-C5-C6-O5
26	W	611	CLA	C4-C3-C5-C6
28	A	861	LHG	C35-C36-C37-C38
28	9	622	LHG	O10-C23-O8-C6
26	A	825	CLA	CBA-CGA-O2A-C1
26	B	839	CLA	CBA-CGA-O2A-C1
26	7	610	CLA	CBA-CGA-O2A-C1
31	5	628	LMU	O5'-C5'-C6'-O6'
28	6	623	LHG	C34-C35-C36-C37
32	V	2631	LMG	C22-C23-C24-C25
26	A	816	CLA	C15-C16-C17-C18
26	3	602	CLA	C10-C11-C12-C13
26	L	302	CLA	C2A-CAA-CBA-CGA
26	U	613	CLA	C2A-CAA-CBA-CGA
37	U	601	CHL	C15-C16-C17-C18
26	B	811	CLA	C2-C1-O2A-CGA
32	9	625	LMG	C24-C25-C26-C27
31	A	858	LMU	C2-C3-C4-C5
31	1	621	LMU	C4-C5-C6-C7
26	A	814	CLA	O1D-CGD-O2D-CED
26	a	603	CLA	O1D-CGD-O2D-CED
26	A	812	CLA	C15-C16-C17-C18
26	A	830	CLA	C8-C10-C11-C12
32	8	626	LMG	C22-C23-C24-C25
26	8	614	CLA	CBA-CGA-O2A-C1
28	2	622	LHG	C24-C23-O8-C6
26	A	801	CLA	C16-C17-C18-C19
26	B	811	CLA	C6-C7-C8-C9
28	9	623	LHG	C7-C8-C9-C10
26	2	616	CLA	CBD-CGD-O2D-CED
31	1	621	LMU	C3-C4-C5-C6
31	1	621	LMU	C6-C7-C8-C9
26	A	827	CLA	C10-C11-C12-C13
37	Z	605	CHL	O1D-CGD-O2D-CED
26	B	833	CLA	O1A-CGA-O2A-C1
26	6	603	CLA	O1A-CGA-O2A-C1
37	U	609	CHL	O1A-CGA-O2A-C1
28	A	861	LHG	C15-C16-C17-C18
32	J	104	LMG	C17-C18-C19-C20
28	H	204	LHG	C7-C8-C9-C10
26	A	801	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	Y	609	CHL	C15-C16-C17-C18
37	Z	607	CHL	C10-C11-C12-C13
37	W	607	CHL	C8-C10-C11-C12
32	V	2631	LMG	C15-C16-C17-C18
27	B	842	PQN	C23-C25-C26-C27
26	A	825	CLA	O1A-CGA-O2A-C1
37	X	609	CHL	O1A-CGA-O2A-C1
37	W	601	CHL	C4-C3-C5-C6
26	6	616	CLA	C15-C16-C17-C18
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	A	831	CLA	C12-C13-C15-C16
26	B	802	CLA	C11-C12-C13-C15
26	B	806	CLA	C11-C12-C13-C15
26	B	806	CLA	C12-C13-C15-C16
26	B	810	CLA	C11-C10-C8-C7
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	X	610	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	Z	601	CHL	C11-C10-C8-C7
37	V	601	CHL	C6-C7-C8-C10
37	W	607	CHL	C11-C12-C13-C15
31	A	858	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
26	A	802	CLA	C14-C13-C15-C16
26	A	804	CLA	C11-C12-C13-C14
26	A	804	CLA	C14-C13-C15-C16
26	A	820	CLA	C11-C10-C8-C9
26	A	826	CLA	C11-C10-C8-C9
26	A	842	CLA	C11-C10-C8-C9
26	A	842	CLA	C11-C12-C13-C14
26	B	806	CLA	C11-C12-C13-C14
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	610	CLA	C11-C10-C8-C9
26	2	602	CLA	C11-C10-C8-C9
26	2	602	CLA	C14-C13-C15-C16
26	4	610	CLA	C6-C7-C8-C9
26	5	607	CLA	C14-C13-C15-C16
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	8	601	CLA	C11-C12-C13-C14
26	8	602	CLA	C11-C10-C8-C9
26	X	602	CLA	C6-C7-C8-C9
26	X	613	CLA	C11-C10-C8-C9
26	U	613	CLA	C11-C10-C8-C9
26	V	602	CLA	C6-C7-C8-C9
26	V	613	CLA	C14-C13-C15-C16
37	X	607	CHL	C14-C13-C15-C16
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
26	X	603	CLA	CBD-CGD-O2D-CED
32	A	860	LMG	C15-C16-C17-C18
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	Z	612	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	W	614	CLA	C2A-CAA-CBA-CGA
32	8	626	LMG	C21-C22-C23-C24
26	Z	610	CLA	CBD-CGD-O2D-CED
35	W	1622	XAT	C11-C12-C13-C20
26	A	807	CLA	C16-C17-C18-C20
26	B	832	CLA	O1D-CGD-O2D-CED
34	U	1621	LUT	C7-C8-C9-C10
34	W	1620	LUT	C27-C28-C29-C30
35	Z	1622	XAT	C11-C12-C13-C14
32	J	104	LMG	C18-C19-C20-C21
26	6	616	CLA	C3-C5-C6-C7
37	Y	609	CHL	C10-C11-C12-C13
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	A	816	CLA	C13-C15-C16-C17
26	7	613	CLA	C10-C11-C12-C13
26	8	613	CLA	C8-C10-C11-C12
26	B	841	CLA	CBD-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
37	Z	609	CHL	C4B-C3B-CAB-CBB
26	8	602	CLA	C11-C12-C13-C14
26	W	613	CLA	C8-C10-C11-C12
28	5	623	LHG	O6-C4-C5-C6
26	7	611	CLA	CBA-CGA-O2A-C1
37	W	601	CHL	CBA-CGA-O2A-C1
37	W	605	CHL	CBD-CGD-O2D-CED
37	Z	607	CHL	C15-C16-C17-C18
37	W	601	CHL	C5-C6-C7-C8
26	W	603	CLA	CAA-CBA-CGA-O2A
26	B	823	CLA	O1D-CGD-O2D-CED
26	U	602	CLA	C4-C3-C5-C6
37	Y	601	CHL	C13-C15-C16-C17
26	7	610	CLA	O1A-CGA-O2A-C1
33	B	850	DGD	C9B-CAB-CBB-CCB
37	W	608	CHL	O1A-CGA-O2A-C1
26	A	843	CLA	C8-C10-C11-C12
37	Y	607	CHL	C10-C11-C12-C13
37	Y	606	CHL	C2A-CAA-CBA-CGA
26	2	601	CLA	CBA-CGA-O2A-C1
37	W	607	CHL	CAA-CBA-CGA-O2A
26	H	203	CLA	C3A-C2A-CAA-CBA
26	6	609	CLA	C3A-C2A-CAA-CBA
26	7	615	CLA	CBD-CGD-O2D-CED
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
26	L	302	CLA	O1D-CGD-O2D-CED
34	Z	1621	LUT	C29-C30-C31-C32
36	Z	1623	NEX	C9-C10-C11-C12
26	1	603	CLA	CBA-CGA-O2A-C1
26	a	603	CLA	CBA-CGA-O2A-C1
31	A	857	LMU	C2-C1-O1'-C1'
31	1	621	LMU	C2-C1-O1'-C1'
26	A	804	CLA	C10-C11-C12-C13
28	9	624	LHG	C17-C18-C19-C20
26	B	803	CLA	CBA-CGA-O2A-C1
37	Y	608	CHL	CBA-CGA-O2A-C1
28	7	622	LHG	C9-C10-C11-C12
32	5	627	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
37	U	609	CHL	C11-C12-C13-C14
26	A	806	CLA	C13-C15-C16-C17
26	6	610	CLA	C15-C16-C17-C18
37	X	607	CHL	C15-C16-C17-C18
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
28	7	622	LHG	C26-C27-C28-C29
26	A	843	CLA	O2A-C1-C2-C3
26	7	602	CLA	C3-C5-C6-C7
26	U	602	CLA	C3-C5-C6-C7
28	8	623	LHG	C32-C33-C34-C35
33	B	850	DGD	C7B-C8B-C9B-CAB
26	A	824	CLA	C4-C3-C5-C6
26	9	602	CLA	C4-C3-C5-C6
37	Y	601	CHL	C4-C3-C5-C6
26	W	611	CLA	C2-C3-C5-C6
26	A	836	CLA	O1D-CGD-O2D-CED
37	X	605	CHL	C3C-C2C-CMC-OMC
37	Y	607	CHL	C3C-C2C-CMC-OMC
37	Z	608	CHL	C3C-C2C-CMC-OMC
26	B	839	CLA	O1A-CGA-O2A-C1
26	a	614	CLA	O1A-CGA-O2A-C1
26	8	614	CLA	O1A-CGA-O2A-C1
26	2	613	CLA	O1D-CGD-O2D-CED
26	A	829	CLA	C2A-CAA-CBA-CGA
28	8	623	LHG	O1-C1-C2-O2
28	5	623	LHG	O6-C4-C5-O7
26	A	803	CLA	CBD-CGD-O2D-CED
26	6	604	CLA	CBA-CGA-O2A-C1
26	7	616	CLA	O1D-CGD-O2D-CED
26	9	602	CLA	C11-C12-C13-C15
26	A	843	CLA	C13-C15-C16-C17
31	A	857	LMU	C7-C8-C9-C10
26	A	835	CLA	C2B-C3B-CAB-CBB
26	B	821	CLA	C2B-C3B-CAB-CBB
26	F	304	CLA	C2B-C3B-CAB-CBB
26	4	606	CLA	C2B-C3B-CAB-CBB
26	6	608	CLA	C2B-C3B-CAB-CBB
26	7	608	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	9	601	CLA	C2B-C3B-CAB-CBB
26	X	610	CLA	C2B-C3B-CAB-CBB
26	X	613	CLA	C2B-C3B-CAB-CBB
37	X	609	CHL	C2B-C3B-CAB-CBB
37	Z	609	CHL	C2B-C3B-CAB-CBB
26	3	612	CLA	O1D-CGD-O2D-CED
26	6	604	CLA	C15-C16-C17-C18
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
28	O	2631	LHG	O7-C5-C6-O8
32	5	627	LMG	O7-C8-C9-O8
26	B	837	CLA	C10-C11-C12-C13
26	B	819	CLA	O1D-CGD-O2D-CED
28	Z	2630	LHG	C14-C15-C16-C17
31	A	858	LMU	C5-C6-C7-C8
32	9	625	LMG	O6-C1-O1-C7
28	6	623	LHG	C14-C15-C16-C17
26	Y	602	CLA	C3-C5-C6-C7
26	A	843	CLA	C4-C3-C5-C6
26	A	805	CLA	C2-C1-O2A-CGA
26	A	814	CLA	C2-C1-O2A-CGA
26	B	806	CLA	C2-C1-O2A-CGA
26	9	602	CLA	C2-C3-C5-C6
26	A	806	CLA	C6-C7-C8-C9
26	A	811	CLA	C6-C7-C8-C9
26	A	811	CLA	C11-C10-C8-C9
26	A	814	CLA	C14-C13-C15-C16
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	3	610	CLA	C11-C10-C8-C9
26	5	604	CLA	C11-C12-C13-C14
26	6	620	CLA	C11-C12-C13-C14
26	8	610	CLA	C6-C7-C8-C9
26	Y	610	CLA	C11-C12-C13-C14
26	Z	613	CLA	C11-C10-C8-C9
26	U	613	CLA	C6-C7-C8-C9
26	V	610	CLA	C11-C10-C8-C9
26	W	613	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
37	Y	609	CHL	C14-C13-C15-C16
37	W	607	CHL	C11-C12-C13-C14
26	H	203	CLA	CBA-CGA-O2A-C1
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	836	CLA	O1A-CGA-O2A-C1
28	3	624	LHG	C11-C10-C9-C8
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	Y	602	CLA	O1D-CGD-O2D-CED
26	5	609	CLA	C16-C17-C18-C20
29	A	850	BCR	C5-C6-C7-C8
29	A	852	BCR	C1-C6-C7-C8
29	A	852	BCR	C23-C24-C25-C30
29	B	845	BCR	C23-C24-C25-C30
29	F	305	BCR	C1-C6-C7-C8
29	O	2004	BCR	C23-C24-C25-C30
29	4	621	BCR	C1-C6-C7-C8
34	X	1621	LUT	C1-C6-C7-C8
34	X	1621	LUT	C5-C6-C7-C8
34	Z	1621	LUT	C1-C6-C7-C8
34	Z	1621	LUT	C5-C6-C7-C8
34	W	1620	LUT	C5-C6-C7-C8
37	X	608	CHL	C10-C11-C12-C13
26	1	613	CLA	O1D-CGD-O2D-CED
28	O	2631	LHG	C26-C27-C28-C29
26	a	613	CLA	O1D-CGD-O2D-CED
26	J	101	CLA	C1A-C2A-CAA-CBA
26	L	306	CLA	C1A-C2A-CAA-CBA
26	4	611	CLA	C1A-C2A-CAA-CBA
36	Z	1623	NEX	C31-C32-C33-C34
37	X	608	CHL	C5-C6-C7-C8
32	J	103	LMG	C17-C18-C19-C20
32	J	103	LMG	C21-C22-C23-C24
26	A	801	CLA	C16-C17-C18-C20
26	3	608	CLA	C3-C5-C6-C7
28	9	624	LHG	C34-C35-C36-C37
28	A	847	LHG	O6-C4-C5-C6
28	6	623	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
28	9	623	LHG	O6-C4-C5-C6
32	V	2631	LMG	C33-C34-C35-C36
26	A	802	CLA	C12-C13-C15-C16
26	A	806	CLA	C6-C7-C8-C10
26	A	809	CLA	C11-C12-C13-C15
26	A	820	CLA	C11-C10-C8-C7
26	A	828	CLA	C11-C10-C8-C7
26	A	830	CLA	C6-C7-C8-C10
26	A	842	CLA	C11-C10-C8-C7
26	A	842	CLA	C11-C12-C13-C15
26	A	843	CLA	C2-C3-C5-C6
26	B	805	CLA	C11-C12-C13-C15
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	608	CLA	C11-C10-C8-C7
26	4	610	CLA	C6-C7-C8-C10
26	5	604	CLA	C11-C10-C8-C7
26	5	607	CLA	C12-C13-C15-C16
26	5	609	CLA	C11-C12-C13-C15
26	6	601	CLA	C6-C7-C8-C10
26	6	616	CLA	C11-C12-C13-C15
26	6	620	CLA	C11-C12-C13-C15
26	8	613	CLA	C11-C12-C13-C15
26	X	602	CLA	C6-C7-C8-C10
26	X	610	CLA	C11-C12-C13-C15
26	X	613	CLA	C6-C7-C8-C10
26	X	613	CLA	C11-C10-C8-C7
26	Y	613	CLA	C11-C10-C8-C7
26	Z	602	CLA	C11-C10-C8-C7
26	Z	613	CLA	C11-C10-C8-C7
26	U	602	CLA	C6-C7-C8-C10
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	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
37	X	607	CHL	C12-C13-C15-C16
37	X	608	CHL	C12-C13-C15-C16
37	X	609	CHL	C11-C12-C13-C15
37	Y	601	CHL	C11-C10-C8-C7
37	Y	601	CHL	C11-C12-C13-C15
37	Y	607	CHL	C11-C10-C8-C7
37	Z	607	CHL	C12-C13-C15-C16
37	U	601	CHL	C12-C13-C15-C16
37	W	601	CHL	C11-C12-C13-C15
26	Z	604	CLA	O1A-CGA-O2A-C1
26	A	811	CLA	C13-C15-C16-C17
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
28	4	622	LHG	C30-C31-C32-C33
26	6	613	CLA	CBA-CGA-O2A-C1
26	4	604	CLA	C2A-CAA-CBA-CGA
26	B	810	CLA	C15-C16-C17-C18
26	B	827	CLA	C8-C10-C11-C12
26	1	603	CLA	C2A-CAA-CBA-CGA
26	a	603	CLA	C2A-CAA-CBA-CGA
26	A	854	CLA	C15-C16-C17-C18
26	2	601	CLA	C8-C10-C11-C12
26	A	831	CLA	CBA-CGA-O2A-C1
26	B	826	CLA	CBA-CGA-O2A-C1
32	A	860	LMG	C29-C28-O8-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	CAD-CBD-CGD-O2D
26	A	818	CLA	CAD-CBD-CGD-O2D
26	A	826	CLA	CAD-CBD-CGD-O2D
26	A	827	CLA	CAD-CBD-CGD-O2D
26	A	837	CLA	CAD-CBD-CGD-O2D
26	B	804	CLA	CAD-CBD-CGD-O2D
26	B	809	CLA	CAD-CBD-CGD-O2D
26	B	812	CLA	CAD-CBD-CGD-O2D
26	B	816	CLA	CAD-CBD-CGD-O2D
26	B	834	CLA	CAD-CBD-CGD-O2D
26	F	301	CLA	CAD-CBD-CGD-O2D
26	F	303	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	F	304	CLA	CAD-CBD-CGD-O2D
26	G	203	CLA	CAD-CBD-CGD-O2D
26	1	612	CLA	CAD-CBD-CGD-O2D
26	a	602	CLA	CAD-CBD-CGD-O2D
26	a	603	CLA	CAD-CBD-CGD-O2D
26	a	612	CLA	CAD-CBD-CGD-O2D
26	2	606	CLA	CAD-CBD-CGD-O2D
26	3	604	CLA	CAD-CBD-CGD-O2D
26	4	607	CLA	CAD-CBD-CGD-O2D
26	4	609	CLA	CAD-CBD-CGD-O2D
26	4	610	CLA	CAD-CBD-CGD-O2D
26	5	614	CLA	CAD-CBD-CGD-O2D
26	5	617	CLA	CAD-CBD-CGD-O2D
26	6	609	CLA	CAD-CBD-CGD-O2D
26	6	620	CLA	CAD-CBD-CGD-O2D
26	7	601	CLA	CAD-CBD-CGD-O2D
26	7	616	CLA	CAD-CBD-CGD-O2D
26	X	604	CLA	CAD-CBD-CGD-O2D
26	X	611	CLA	CAD-CBD-CGD-O2D
26	X	612	CLA	CAD-CBD-CGD-O2D
26	Y	603	CLA	CAD-CBD-CGD-O2D
26	Z	614	CLA	CAD-CBD-CGD-O2D
26	U	612	CLA	CAD-CBD-CGD-O2D
26	V	602	CLA	CAD-CBD-CGD-O2D
26	V	604	CLA	CAD-CBD-CGD-O2D
26	V	611	CLA	CAD-CBD-CGD-O2D
26	W	603	CLA	CAD-CBD-CGD-O2D
26	W	604	CLA	CAD-CBD-CGD-O2D
36	V	1623	NEX	C7-C8-C9-C19
37	Y	606	CHL	CAD-CBD-CGD-O2D
37	U	606	CHL	CAD-CBD-CGD-O2D
31	1	621	LMU	O5'-C5'-C6'-O6'
32	8	626	LMG	C20-C21-C22-C23
26	A	803	CLA	C13-C15-C16-C17
26	2	613	CLA	C13-C15-C16-C17
32	4	623	LMG	C10-C11-C12-C13
28	H	204	LHG	C15-C16-C17-C18
28	8	623	LHG	C24-C23-O8-C6
28	9	623	LHG	C35-C36-C37-C38
31	A	858	LMU	O5'-C1'-O1'-C1
26	A	842	CLA	C8-C10-C11-C12
26	5	604	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	8	625	LMU	C6-C7-C8-C9
32	9	625	LMG	C7-C8-C9-O8
26	8	608	CLA	CBD-CGD-O2D-CED
26	K	203	CLA	O1A-CGA-O2A-C1
26	6	613	CLA	O1A-CGA-O2A-C1
37	Y	608	CHL	O1A-CGA-O2A-C1
37	Y	609	CHL	O1A-CGA-O2A-C1
28	9	623	LHG	C12-C13-C14-C15
28	A	846	LHG	O6-C4-C5-O7
28	6	623	LHG	O6-C4-C5-O7
26	B	803	CLA	C5-C6-C7-C8
26	B	810	CLA	C3-C5-C6-C7
37	Y	607	CHL	C3-C5-C6-C7
26	B	832	CLA	CAA-CBA-CGA-O2A
26	2	602	CLA	NC-C1C-CHC-C4B
26	B	826	CLA	O1A-CGA-O2A-C1
26	A	806	CLA	CHA-CBD-CGD-O1D
26	A	809	CLA	CHA-CBD-CGD-O1D
26	A	809	CLA	CHA-CBD-CGD-O2D
26	A	815	CLA	CHA-CBD-CGD-O1D
26	A	816	CLA	CHA-CBD-CGD-O2D
26	A	825	CLA	CHA-CBD-CGD-O1D
26	A	832	CLA	CHA-CBD-CGD-O1D
26	A	845	CLA	CHA-CBD-CGD-O1D
26	A	845	CLA	CHA-CBD-CGD-O2D
26	B	826	CLA	CHA-CBD-CGD-O1D
26	B	833	CLA	CHA-CBD-CGD-O1D
26	B	841	CLA	CHA-CBD-CGD-O1D
26	1	604	CLA	CHA-CBD-CGD-O1D
26	a	604	CLA	CHA-CBD-CGD-O1D
26	a	614	CLA	CHA-CBD-CGD-O1D
26	a	614	CLA	CHA-CBD-CGD-O2D
26	3	609	CLA	CHA-CBD-CGD-O1D
26	4	616	CLA	CHA-CBD-CGD-O1D
26	5	619	CLA	CHA-CBD-CGD-O1D
26	6	601	CLA	CHA-CBD-CGD-O2D
26	7	611	CLA	CHA-CBD-CGD-O1D
26	9	613	CLA	CHA-CBD-CGD-O2D
26	X	613	CLA	CHA-CBD-CGD-O2D
26	Z	611	CLA	CHA-CBD-CGD-O1D
26	Z	611	CLA	CHA-CBD-CGD-O2D
26	Z	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	Z	612	CLA	CHA-CBD-CGD-O2D
26	U	602	CLA	CHA-CBD-CGD-O1D
26	U	602	CLA	CHA-CBD-CGD-O2D
37	Y	605	CHL	CHA-CBD-CGD-O1D
37	Y	605	CHL	CHA-CBD-CGD-O2D
37	U	605	CHL	CHA-CBD-CGD-O1D
37	U	605	CHL	CHA-CBD-CGD-O2D
37	Y	606	CHL	CBD-CGD-O2D-CED
26	B	803	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
31	8	625	LMU	C2-C3-C4-C5
32	A	860	LMG	O1-C7-C8-O7
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	831	CLA	O1A-CGA-O2A-C1
26	4	613	CLA	C16-C17-C18-C20
26	5	609	CLA	C16-C17-C18-C19
26	X	603	CLA	O1D-CGD-O2D-CED
37	Y	606	CHL	O1D-CGD-O2D-CED
28	9	623	LHG	C30-C31-C32-C33
26	B	832	CLA	C3-C5-C6-C7
26	B	828	CLA	C4-C3-C5-C6
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	Z	610	CLA	O1D-CGD-O2D-CED
28	7	622	LHG	O9-C7-O7-C5
26	A	826	CLA	C8-C10-C11-C12
26	A	841	CLA	C11-C12-C13-C14
26	5	604	CLA	C6-C7-C8-C9
26	8	613	CLA	C11-C12-C13-C14
26	X	602	CLA	C14-C13-C15-C16
26	W	613	CLA	C6-C7-C8-C9
28	Z	2630	LHG	C15-C16-C17-C18
33	B	850	DGD	CAB-CBB-CCB-CDB
37	W	605	CHL	O1D-CGD-O2D-CED
28	U	2630	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
26	2	602	CLA	C13-C15-C16-C17
28	A	846	LHG	C30-C31-C32-C33
28	O	2631	LHG	C10-C11-C12-C13
31	5	628	LMU	C7-C8-C9-C10
26	6	610	CLA	C2A-CAA-CBA-CGA
26	V	604	CLA	C2A-CAA-CBA-CGA
29	B	849	BCR	C7-C8-C9-C10
26	A	838	CLA	C1A-C2A-CAA-CBA
26	B	821	CLA	CHA-CBD-CGD-O2D
26	H	202	CLA	CHA-CBD-CGD-O2D
26	L	302	CLA	C1A-C2A-CAA-CBA
26	L	307	CLA	CHA-CBD-CGD-O2D
26	2	603	CLA	CHA-CBD-CGD-O2D
26	4	610	CLA	C1A-C2A-CAA-CBA
26	6	610	CLA	C1A-C2A-CAA-CBA
26	6	613	CLA	CHA-CBD-CGD-O2D
26	X	602	CLA	C1A-C2A-CAA-CBA
26	Z	604	CLA	C1A-C2A-CAA-CBA
26	Z	610	CLA	C1A-C2A-CAA-CBA
37	W	601	CHL	C1A-C2A-CAA-CBA
37	W	607	CHL	C1A-C2A-CAA-CBA
26	4	613	CLA	C16-C17-C18-C19
26	A	830	CLA	C5-C6-C7-C8
26	B	819	CLA	CBA-CGA-O2A-C1
26	B	829	CLA	CBA-CGA-O2A-C1
28	O	2631	LHG	C27-C28-C29-C30
28	X	2630	LHG	C27-C28-C29-C30
34	X	1621	LUT	C29-C30-C31-C32
35	Y	1622	XAT	C13-C14-C15-C35
28	5	625	LHG	C3-O3-P-O6
28	7	622	LHG	C4-O6-P-O3
28	Y	2630	LHG	C4-O6-P-O3
28	V	2630	LHG	C4-O6-P-O3
37	X	608	CHL	CAD-CBD-CGD-O2D
32	L	2631	LMG	C13-C14-C15-C16
26	A	828	CLA	C4-C3-C5-C6
26	B	827	CLA	C4-C3-C5-C6
32	9	625	LMG	O7-C10-C11-C12
28	Y	2630	LHG	C2-C3-O3-P
26	B	828	CLA	C2-C3-C5-C6
37	W	601	CHL	C2-C3-C5-C6
26	A	813	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	A	839	CLA	C4B-C3B-CAB-CBB
26	A	842	CLA	C4B-C3B-CAB-CBB
26	B	811	CLA	CAD-CBD-CGD-O1D
26	B	811	CLA	CAD-CBD-CGD-O2D
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	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	613	CLA	C4B-C3B-CAB-CBB
26	6	613	CLA	C4B-C3B-CAB-CBB
26	Y	610	CLA	C4B-C3B-CAB-CBB
28	A	847	LHG	C3-O3-P-O5
28	A	861	LHG	C4-O6-P-O4
28	O	2631	LHG	C3-O3-P-O5
28	2	622	LHG	C3-O3-P-O5
28	3	623	LHG	C3-O3-P-O4
28	3	623	LHG	C4-O6-P-O4
28	3	624	LHG	C3-O3-P-O4
28	6	623	LHG	C4-O6-P-O4
28	7	622	LHG	C3-O3-P-O4
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	C4-O6-P-O4
28	V	2630	LHG	C4-O6-P-O4
28	W	2630	LHG	C4-O6-P-O4
37	X	601	CHL	C4B-C3B-CAB-CBB
37	X	607	CHL	C4B-C3B-CAB-CBB
37	X	609	CHL	C4B-C3B-CAB-CBB
37	Y	601	CHL	C4B-C3B-CAB-CBB
37	Y	607	CHL	C4B-C3B-CAB-CBB
37	Y	609	CHL	C4B-C3B-CAB-CBB
37	Z	605	CHL	C4B-C3B-CAB-CBB
37	Z	608	CHL	C4B-C3B-CAB-CBB
37	U	605	CHL	C4B-C3B-CAB-CBB
37	V	605	CHL	C4B-C3B-CAB-CBB
37	V	607	CHL	C4B-C3B-CAB-CBB
37	V	608	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
37	V	609	CHL	C4B-C3B-CAB-CBB
37	W	605	CHL	C4B-C3B-CAB-CBB
37	W	606	CHL	C4B-C3B-CAB-CBB
37	W	608	CHL	C4B-C3B-CAB-CBB
37	W	609	CHL	C4B-C3B-CAB-CBB
26	V	613	CLA	C16-C17-C18-C19
28	Z	2630	LHG	C32-C33-C34-C35
26	6	620	CLA	O2A-C1-C2-C3
26	X	604	CLA	O2A-C1-C2-C3
26	a	610	CLA	C5-C6-C7-C8
37	W	607	CHL	C5-C6-C7-C8
28	7	622	LHG	O6-C4-C5-C6
26	A	811	CLA	C8-C10-C11-C12
26	7	613	CLA	C13-C15-C16-C17
26	8	601	CLA	C13-C15-C16-C17
37	W	609	CHL	C5-C6-C7-C8
37	V	609	CHL	C3-C5-C6-C7
28	6	623	LHG	C12-C13-C14-C15
26	U	602	CLA	C10-C11-C12-C13
26	A	806	CLA	CAD-CBD-CGD-O1D
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	825	CLA	CAD-CBD-CGD-O1D
26	A	831	CLA	CAD-CBD-CGD-O1D
26	A	845	CLA	CAD-CBD-CGD-O1D
26	B	813	CLA	CAD-CBD-CGD-O1D
26	B	841	CLA	CAD-CBD-CGD-O1D
26	6	601	CLA	CAD-CBD-CGD-O1D
26	Y	602	CLA	CAD-CBD-CGD-O1D
26	Y	611	CLA	CAD-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	7	601	CLA	CBA-CGA-O2A-C1
28	U	2630	LHG	C1-C2-C3-O3
26	A	802	CLA	C11-C10-C8-C7
26	A	807	CLA	C6-C7-C8-C10
26	A	818	CLA	C11-C10-C8-C7
26	A	828	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
26	A	841	CLA	C11-C10-C8-C7
26	A	842	CLA	C12-C13-C15-C16
26	B	808	CLA	C11-C10-C8-C7
26	B	808	CLA	C12-C13-C15-C16
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	O	2001	CLA	CAD-CBD-CGD-O2D
26	1	613	CLA	C11-C10-C8-C7
26	3	613	CLA	CAD-CBD-CGD-O2D
26	5	613	CLA	C11-C10-C8-C7
26	5	619	CLA	C3A-C2A-CAA-CBA
26	6	610	CLA	C6-C7-C8-C10
26	6	610	CLA	C11-C12-C13-C15
26	6	611	CLA	C3A-C2A-CAA-CBA
26	7	603	CLA	CHA-CBD-CGD-O1D
26	7	609	CLA	CHA-CBD-CGD-O2D
26	7	615	CLA	CHA-CBD-CGD-O2D
26	X	610	CLA	C11-C10-C8-C7
26	Y	602	CLA	C6-C7-C8-C10
26	V	610	CLA	C11-C12-C13-C15
26	W	613	CLA	C6-C7-C8-C10
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
37	Y	607	CHL	C12-C13-C15-C16
37	Z	601	CHL	C6-C7-C8-C10
37	Z	601	CHL	C11-C12-C13-C15
37	W	601	CHL	C12-C13-C15-C16
37	W	607	CHL	C12-C13-C15-C16
28	A	861	LHG	C28-C29-C30-C31
36	W	1623	NEX	C13-C14-C15-C35
26	A	819	CLA	CAA-CBA-CGA-O2A
26	B	827	CLA	CAA-CBA-CGA-O2A
28	U	2630	LHG	C7-C8-C9-C10
28	7	622	LHG	C8-C7-O7-C5
31	K	208	LMU	C6-C7-C8-C9
32	A	860	LMG	O10-C28-O8-C9
26	7	615	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	8	603	CLA	C2A-CAA-CBA-CGA
26	O	2003	CLA	CAD-CBD-CGD-O1D
26	a	614	CLA	C1A-C2A-CAA-CBA
26	3	615	CLA	CAD-CBD-CGD-O1D
26	4	612	CLA	CAD-CBD-CGD-O1D
28	4	622	LHG	C25-C26-C27-C28
28	Z	2630	LHG	C4-C5-C6-O8
32	A	860	LMG	O1-C7-C8-C9
32	J	103	LMG	O1-C7-C8-C9
37	X	601	CHL	C1C-C2C-CMC-OMC
37	X	605	CHL	C1C-C2C-CMC-OMC
37	Y	605	CHL	C1C-C2C-CMC-OMC
37	Y	606	CHL	C1C-C2C-CMC-OMC
37	Y	607	CHL	C1C-C2C-CMC-OMC
37	Z	608	CHL	C1C-C2C-CMC-OMC
37	U	605	CHL	C1C-C2C-CMC-OMC
37	U	606	CHL	C1C-C2C-CMC-OMC
37	V	605	CHL	C1C-C2C-CMC-OMC
37	V	608	CHL	C1C-C2C-CMC-OMC
37	W	605	CHL	C1C-C2C-CMC-OMC
37	W	607	CHL	C1C-C2C-CMC-OMC
37	W	608	CHL	C1C-C2C-CMC-OMC
26	B	829	CLA	O1A-CGA-O2A-C1
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
26	V	613	CLA	C16-C17-C18-C20
26	B	832	CLA	C5-C6-C7-C8
27	A	844	PQN	C18-C20-C21-C22
26	A	803	CLA	O1D-CGD-O2D-CED
26	2	616	CLA	O1D-CGD-O2D-CED
26	7	601	CLA	O1A-CGA-O2A-C1
28	8	623	LHG	O10-C23-O8-C6
26	5	613	CLA	C15-C16-C17-C18
26	V	613	CLA	CBA-CGA-O2A-C1
28	Z	2630	LHG	C18-C19-C20-C21
26	B	828	CLA	C8-C10-C11-C12
26	7	610	CLA	C15-C16-C17-C18
26	A	809	CLA	C11-C12-C13-C14
26	A	828	CLA	C11-C10-C8-C9
26	A	831	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	B	805	CLA	C11-C12-C13-C14
26	B	806	CLA	C14-C13-C15-C16
26	B	808	CLA	C14-C13-C15-C16
26	B	810	CLA	C6-C7-C8-C9
26	B	839	CLA	C11-C10-C8-C9
26	6	601	CLA	C6-C7-C8-C9
26	6	613	CLA	C11-C10-C8-C9
26	X	613	CLA	C6-C7-C8-C9
26	Y	613	CLA	C11-C10-C8-C9
26	Z	602	CLA	C11-C10-C8-C9
26	U	602	CLA	C6-C7-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	Z	607	CHL	C14-C13-C15-C16
37	U	601	CHL	C14-C13-C15-C16
26	A	831	CLA	C3-C5-C6-C7
26	W	602	CLA	C3-C5-C6-C7
26	B	819	CLA	O1A-CGA-O2A-C1
33	B	850	DGD	C2A-C3A-C4A-C5A
26	B	838	CLA	O1A-CGA-O2A-C1
36	U	1623	NEX	C10-C11-C12-C13
26	V	613	CLA	O1A-CGA-O2A-C1
29	A	849	BCR	C21-C22-C23-C24
26	A	815	CLA	C2B-C3B-CAB-CBB
26	A	832	CLA	C2B-C3B-CAB-CBB
26	A	839	CLA	C2B-C3B-CAB-CBB
26	A	842	CLA	C2B-C3B-CAB-CBB
26	G	204	CLA	C2B-C3B-CAB-CBB
26	K	204	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	3	606	CLA	C2B-C3B-CAB-CBB
26	4	609	CLA	C2B-C3B-CAB-CBB
26	4	613	CLA	C2B-C3B-CAB-CBB
26	5	607	CLA	C2B-C3B-CAB-CBB
26	5	608	CLA	C2B-C3B-CAB-CBB
26	6	606	CLA	C2B-C3B-CAB-CBB
26	6	610	CLA	C2B-C3B-CAB-CBB
26	6	617	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	7	603	CLA	C2B-C3B-CAB-CBB
26	8	611	CLA	C2B-C3B-CAB-CBB
26	Y	604	CLA	C2B-C3B-CAB-CBB
26	Y	610	CLA	C2B-C3B-CAB-CBB
26	Y	613	CLA	C2B-C3B-CAB-CBB
26	Z	602	CLA	C2B-C3B-CAB-CBB
26	Z	614	CLA	C2B-C3B-CAB-CBB
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	602	CLA	C2B-C3B-CAB-CBB
26	W	614	CLA	C2B-C3B-CAB-CBB
37	Z	608	CHL	C2B-C3B-CAB-CBB
37	V	607	CHL	C2B-C3B-CAB-CBB
37	V	608	CHL	C2B-C3B-CAB-CBB
37	W	606	CHL	C2B-C3B-CAB-CBB
26	A	804	CLA	C4C-C3C-CAC-CBC
26	H	203	CLA	C15-C16-C17-C18
32	V	2631	LMG	C16-C17-C18-C19
26	A	824	CLA	C2-C3-C5-C6
26	B	827	CLA	C2-C3-C5-C6
32	H	205	LMG	C30-C31-C32-C33
26	B	825	CLA	C1-C2-C3-C4
26	1	604	CLA	C1-C2-C3-C4
26	a	604	CLA	C1-C2-C3-C4
26	X	604	CLA	C1-C2-C3-C4
26	U	604	CLA	C1-C2-C3-C4
28	A	861	LHG	C6-C5-O7-C7
28	8	623	LHG	C6-C5-O7-C7
32	8	626	LMG	C9-C8-O7-C10
26	B	841	CLA	O1D-CGD-O2D-CED
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
37	U	609	CHL	C4C-C3C-CAC-CBC
26	A	838	CLA	CBA-CGA-O2A-C1
26	A	835	CLA	C2-C1-O2A-CGA
26	B	805	CLA	C2-C1-O2A-CGA
26	B	826	CLA	C2-C1-O2A-CGA
26	B	828	CLA	C2-C1-O2A-CGA
26	9	604	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
26	9	610	CLA	C2-C1-O2A-CGA
37	W	609	CHL	C2-C1-O2A-CGA
26	B	837	CLA	O1D-CGD-O2D-CED
26	8	611	CLA	O1D-CGD-O2D-CED
31	5	629	LMU	C1-C2-C3-C4
26	Z	604	CLA	CHA-CBD-CGD-O1D
26	Z	604	CLA	CHA-CBD-CGD-O2D
26	8	610	CLA	CBA-CGA-O2A-C1
26	8	610	CLA	O1A-CGA-O2A-C1
26	5	607	CLA	C13-C15-C16-C17
37	Z	609	CHL	C4-C3-C5-C6
29	A	851	BCR	C1-C6-C7-C8
29	L	309	BCR	C5-C6-C7-C8
29	2	623	BCR	C23-C24-C25-C30
34	W	1620	LUT	C1-C6-C7-C8
26	A	828	CLA	C2-C3-C5-C6
32	V	2631	LMG	O9-C10-O7-C8
28	9	624	LHG	C15-C16-C17-C18
26	1	603	CLA	C6-C7-C8-C10
26	a	603	CLA	C6-C7-C8-C10
32	V	2631	LMG	C11-C10-O7-C8
32	H	205	LMG	O6-C1-O1-C7
28	Z	2630	LHG	O7-C5-C6-O8
28	A	846	LHG	C4-O6-P-O3
28	B	851	LHG	C4-O6-P-O3
28	H	204	LHG	C3-O3-P-O6
28	O	2631	LHG	C4-O6-P-O3
28	3	624	LHG	C4-O6-P-O3
28	4	622	LHG	C3-O3-P-O6
28	5	625	LHG	C4-O6-P-O3
28	8	622	LHG	C3-O3-P-O6
28	8	623	LHG	C3-O3-P-O6
28	9	624	LHG	C3-O3-P-O6
28	X	2630	LHG	C3-O3-P-O6
28	Z	2630	LHG	C3-O3-P-O6
28	V	2630	LHG	C3-O3-P-O6
28	H	204	LHG	C26-C27-C28-C29
31	1	621	LMU	O1'-C1-C2-C3
26	B	837	CLA	C5-C6-C7-C8
33	B	850	DGD	C1G-C2G-C3G-O3G
26	A	803	CLA	C4-C3-C5-C6
32	4	623	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
26	B	839	CLA	C12-C13-C15-C16
26	6	613	CLA	C6-C7-C8-C10
26	7	613	CLA	C11-C10-C8-C7
37	Z	609	CHL	C6-C7-C8-C10
28	4	622	LHG	C29-C30-C31-C32
26	B	813	CLA	C11-C10-C8-C9
26	B	813	CLA	C11-C12-C13-C14
26	B	833	CLA	C6-C7-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	X	610	CLA	C14-C13-C15-C16
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	X	609	CHL	C11-C12-C13-C14
37	Y	607	CHL	C14-C13-C15-C16
37	W	607	CHL	C14-C13-C15-C16
36	U	1623	NEX	C33-C34-C35-C15
26	A	819	CLA	C10-C11-C12-C13
28	U	2630	LHG	C11-C10-C9-C8
26	A	818	CLA	C8-C10-C11-C12
26	B	832	CLA	C10-C11-C12-C13
26	9	604	CLA	C3-C5-C6-C7
28	5	625	LHG	C15-C16-C17-C18
36	Y	1623	NEX	C31-C32-C33-C40
37	X	601	CHL	CAA-CBA-CGA-O1A
26	7	602	CLA	C16-C17-C18-C20
28	8	622	LHG	C12-C13-C14-C15
26	A	838	CLA	O1A-CGA-O2A-C1
37	X	609	CHL	C10-C11-C12-C13
35	V	1622	XAT	C31-C32-C33-C34
36	6	624	NEX	C11-C12-C13-C14
26	A	841	CLA	C3-C5-C6-C7
26	4	610	CLA	C12-C13-C15-C16
28	8	622	LHG	C1-C2-C3-O3
26	B	806	CLA	C2-C3-C5-C6
26	U	602	CLA	C2-C3-C5-C6
37	Y	601	CHL	C2-C3-C5-C6
26	X	604	CLA	CBA-CGA-O2A-C1
26	5	619	CLA	O1D-CGD-O2D-CED
26	B	833	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	6	601	CLA	C5-C6-C7-C8
26	X	604	CLA	O1A-CGA-O2A-C1
26	8	611	CLA	CBD-CGD-O2D-CED
26	A	817	CLA	C4B-C3B-CAB-CBB
26	A	827	CLA	C4B-C3B-CAB-CBB
26	A	832	CLA	C4B-C3B-CAB-CBB
26	H	203	CLA	C4B-C3B-CAB-CBB
26	K	204	CLA	C4B-C3B-CAB-CBB
26	L	303	CLA	C4B-C3B-CAB-CBB
26	4	601	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	X	604	CLA	C4B-C3B-CAB-CBB
26	Y	602	CLA	C4B-C3B-CAB-CBB
26	Y	613	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	Y	605	CHL	C4B-C3B-CAB-CBB
26	A	813	CLA	C2A-CAA-CBA-CGA
26	A	837	CLA	CAA-CBA-CGA-O1A
35	X	1622	XAT	C9-C10-C11-C12
26	B	802	CLA	C13-C15-C16-C17
26	7	615	CLA	CAA-CBA-CGA-O2A
28	9	623	LHG	C31-C32-C33-C34
28	4	622	LHG	C13-C14-C15-C16
28	H	204	LHG	C23-C24-C25-C26
26	A	814	CLA	C16-C17-C18-C19
37	U	601	CHL	C3-C5-C6-C7
26	B	811	CLA	C4-C3-C5-C6
26	A	811	CLA	C2-C3-C5-C6
28	B	851	LHG	C11-C10-C9-C8
26	A	836	CLA	C10-C11-C12-C13
28	A	861	LHG	O2-C2-C3-O3
28	5	625	LHG	C17-C18-C19-C20
26	B	814	CLA	C2-C1-O2A-CGA
26	F	301	CLA	C2-C1-O2A-CGA
26	H	203	CLA	C2-C1-O2A-CGA
26	8	601	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
37	X	608	CHL	C2-C1-O2A-CGA
31	5	629	LMU	C4'-C5'-C6'-O6'
33	B	850	DGD	C4B-C5B-C6B-C7B
26	A	838	CLA	C2A-CAA-CBA-CGA
26	1	602	CLA	C2A-CAA-CBA-CGA
26	a	602	CLA	C2A-CAA-CBA-CGA
26	a	606	CLA	C2A-CAA-CBA-CGA
26	2	612	CLA	C2A-CAA-CBA-CGA
26	3	607	CLA	C2A-CAA-CBA-CGA
26	9	602	CLA	C2A-CAA-CBA-CGA
26	Z	602	CLA	C2A-CAA-CBA-CGA
28	9	624	LHG	O7-C5-C6-O8
37	Y	601	CHL	C2A-CAA-CBA-CGA
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
26	5	614	CLA	CAA-CBA-CGA-O2A
26	3	609	CLA	C4C-C3C-CAC-CBC
26	A	828	CLA	O1A-CGA-O2A-C1
28	8	623	LHG	C30-C31-C32-C33
28	U	2630	LHG	C30-C31-C32-C33
26	a	607	CLA	CAA-CBA-CGA-O2A
26	7	611	CLA	C3-C5-C6-C7
26	A	811	CLA	C4-C3-C5-C6
26	B	806	CLA	C4-C3-C5-C6
37	V	609	CHL	C4-C3-C5-C6
26	A	826	CLA	C14-C13-C15-C16
26	A	834	CLA	C11-C12-C13-C14
26	L	303	CLA	C14-C13-C15-C16
26	6	604	CLA	C11-C10-C8-C9
26	X	602	CLA	C11-C12-C13-C14
37	X	601	CHL	C6-C7-C8-C9
37	Y	607	CHL	C6-C7-C8-C9
26	1	603	CLA	C6-C7-C8-C9
26	a	603	CLA	C6-C7-C8-C9
26	7	602	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	1	612	CLA	CAA-CBA-CGA-O1A
26	a	607	CLA	CAA-CBA-CGA-O1A
28	U	2630	LHG	C23-C24-C25-C26
26	A	828	CLA	CBA-CGA-O2A-C1
26	Y	604	CLA	CBA-CGA-O2A-C1
28	W	2630	LHG	C26-C27-C28-C29
28	3	623	LHG	C4-C5-C6-O8
28	9	624	LHG	C4-C5-C6-O8
28	U	2630	LHG	C4-C5-C6-O8
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	Y	2630	LHG	C12-C13-C14-C15
26	2	603	CLA	CAA-CBA-CGA-O1A
37	U	608	CHL	C2A-CAA-CBA-CGA
26	G	204	CLA	C2A-CAA-CBA-CGA
28	Z	2630	LHG	C12-C13-C14-C15
32	H	205	LMG	C13-C14-C15-C16
26	a	612	CLA	CAA-CBA-CGA-O1A
26	4	603	CLA	CAA-CBA-CGA-O2A
26	V	612	CLA	CAA-CBA-CGA-O1A
35	V	1622	XAT	C31-C32-C33-C40
26	L	302	CLA	CAA-CBA-CGA-O2A
26	6	617	CLA	CAA-CBA-CGA-O1A
32	8	626	LMG	C7-C8-O7-C10
26	8	602	CLA	C4-C3-C5-C6
26	8	608	CLA	O1D-CGD-O2D-CED
26	B	814	CLA	C1A-C2A-CAA-CBA
26	B	827	CLA	C1A-C2A-CAA-CBA
26	B	832	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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
37	Y	601	CHL	C1A-C2A-CAA-CBA
37	Z	609	CHL	C1A-C2A-CAA-CBA
37	X	607	CHL	CBA-CGA-O2A-C1
26	A	811	CLA	C6-C7-C8-C10
26	A	841	CLA	C12-C13-C15-C16
26	B	802	CLA	C12-C13-C15-C16
26	6	604	CLA	C11-C10-C8-C7
26	7	613	CLA	C11-C12-C13-C15
26	A	802	CLA	C5-C6-C7-C8
26	4	607	CLA	CAA-CBA-CGA-O1A
26	5	614	CLA	CAA-CBA-CGA-O1A
26	7	609	CLA	CAA-CBA-CGA-O1A
28	B	851	LHG	C24-C25-C26-C27
28	9	624	LHG	C16-C17-C18-C19
37	Z	607	CHL	C8-C10-C11-C12
37	X	601	CHL	C3C-C2C-CMC-OMC
26	A	801	CLA	CAA-CBA-CGA-O2A
26	B	817	CLA	CBA-CGA-O2A-C1
26	7	609	CLA	CAA-CBA-CGA-O2A
26	7	612	CLA	CAA-CBA-CGA-O1A
28	8	622	LHG	C18-C19-C20-C21
26	A	807	CLA	C2A-CAA-CBA-CGA
37	V	609	CHL	C10-C11-C12-C13
32	H	205	LMG	C28-C29-C30-C31
26	Y	612	CLA	CAA-CBA-CGA-O1A
26	2	603	CLA	C2C-C3C-CAC-CBC
28	9	624	LHG	C31-C32-C33-C34
26	5	619	CLA	CBD-CGD-O2D-CED
26	4	601	CLA	C4-C3-C5-C6
26	A	809	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	A	813	CLA	C2B-C3B-CAB-CBB
26	A	817	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	H	203	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	613	CLA	C2B-C3B-CAB-CBB
26	4	601	CLA	C2B-C3B-CAB-CBB
26	4	608	CLA	C2B-C3B-CAB-CBB
26	6	609	CLA	C2B-C3B-CAB-CBB
26	6	613	CLA	C2B-C3B-CAB-CBB
26	X	604	CLA	C2B-C3B-CAB-CBB
26	Y	602	CLA	C2B-C3B-CAB-CBB
26	U	602	CLA	C2B-C3B-CAB-CBB
37	X	601	CHL	C2B-C3B-CAB-CBB
37	X	607	CHL	C2B-C3B-CAB-CBB
37	Y	601	CHL	C2B-C3B-CAB-CBB
37	Y	605	CHL	C2B-C3B-CAB-CBB
37	Y	607	CHL	C2B-C3B-CAB-CBB
37	Y	608	CHL	C2B-C3B-CAB-CBB
37	Y	609	CHL	C2B-C3B-CAB-CBB
37	Z	605	CHL	C2B-C3B-CAB-CBB
37	U	605	CHL	C2B-C3B-CAB-CBB
37	V	605	CHL	C2B-C3B-CAB-CBB
37	V	609	CHL	C2B-C3B-CAB-CBB
37	W	605	CHL	C2B-C3B-CAB-CBB
37	W	608	CHL	C2B-C3B-CAB-CBB
37	W	609	CHL	C2B-C3B-CAB-CBB
26	L	302	CLA	CAA-CBA-CGA-O1A
26	7	603	CLA	CAA-CBA-CGA-O2A
26	V	612	CLA	CAA-CBA-CGA-O2A
26	4	601	CLA	C13-C15-C16-C17
26	Y	604	CLA	O1A-CGA-O2A-C1
32	5	627	LMG	C12-C13-C14-C15
26	6	601	CLA	C16-C17-C18-C20
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

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Mol	Chain	Res	Type	Atoms
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	A	837	CLA	CAA-CBA-CGA-O2A
26	2	603	CLA	CAA-CBA-CGA-O2A
26	W	612	CLA	CAA-CBA-CGA-O2A
28	W	2630	LHG	O7-C5-C6-O8
37	W	607	CHL	C10-C11-C12-C13
26	A	840	CLA	C4C-C3C-CAC-CBC
37	X	609	CHL	C2C-C3C-CAC-CBC
34	U	1621	LUT	C29-C30-C31-C32
36	Y	1623	NEX	C33-C34-C35-C15
26	5	616	CLA	CAA-CBA-CGA-O2A
26	7	612	CLA	CAA-CBA-CGA-O2A
37	Y	606	CHL	CAA-CBA-CGA-O1A
26	V	610	CLA	C13-C15-C16-C17
26	A	839	CLA	C6-C7-C8-C10
26	B	810	CLA	C16-C17-C18-C19
26	B	819	CLA	C6-C7-C8-C10
28	6	623	LHG	C17-C18-C19-C20
32	A	860	LMG	C11-C12-C13-C14
26	3	608	CLA	C5-C6-C7-C8
26	4	603	CLA	CAA-CBA-CGA-O1A
26	7	615	CLA	CAA-CBA-CGA-O1A
37	Y	606	CHL	CAA-CBA-CGA-O2A
28	A	861	LHG	C14-C15-C16-C17
32	J	103	LMG	C22-C23-C24-C25
26	A	815	CLA	C2-C1-O2A-CGA
26	A	828	CLA	C2-C1-O2A-CGA
26	B	840	CLA	C2-C1-O2A-CGA
26	8	610	CLA	C2-C1-O2A-CGA
26	8	613	CLA	C2-C1-O2A-CGA
26	9	609	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
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	9	623	LHG	C11-C12-C13-C14
26	A	833	CLA	CAA-CBA-CGA-O2A
26	1	612	CLA	CAA-CBA-CGA-O2A
26	a	612	CLA	CAA-CBA-CGA-O2A
26	6	617	CLA	CAA-CBA-CGA-O2A
26	9	601	CLA	CAA-CBA-CGA-O2A
37	Z	606	CHL	CAA-CBA-CGA-O2A
26	5	610	CLA	C5-C6-C7-C8
26	F	301	CLA	C6-C7-C8-C9
37	V	601	CHL	C11-C10-C8-C9
37	W	607	CHL	C11-C10-C8-C9
26	4	607	CLA	CAA-CBA-CGA-O2A
26	W	612	CLA	CAA-CBA-CGA-O1A
26	8	601	CLA	C10-C11-C12-C13
26	A	824	CLA	C2A-CAA-CBA-CGA
26	A	830	CLA	C2A-CAA-CBA-CGA
26	7	602	CLA	C2A-CAA-CBA-CGA
26	2	602	CLA	C16-C17-C18-C19
26	B	817	CLA	O1A-CGA-O2A-C1
26	a	610	CLA	O1A-CGA-O2A-C1
37	X	607	CHL	O1A-CGA-O2A-C1
29	B	801	BCR	C5-C6-C7-C8
29	G	205	BCR	C23-C24-C25-C30
29	K	202	BCR	C1-C6-C7-C8
29	3	622	BCR	C1-C6-C7-C8
37	Y	609	CHL	C2C-C3C-CAC-CBC
32	5	627	LMG	O1-C7-C8-C9
26	7	603	CLA	CAA-CBA-CGA-O1A
28	a	620	LHG	C27-C28-C29-C30
28	3	623	LHG	C24-C25-C26-C27
33	B	850	DGD	C4A-C5A-C6A-C7A
26	A	825	CLA	C4-C3-C5-C6
26	A	827	CLA	C4-C3-C5-C6
26	a	602	CLA	C10-C11-C12-C13
27	A	844	PQN	C12-C13-C15-C16
26	B	818	CLA	C3-C5-C6-C7
26	G	204	CLA	CAA-CBA-CGA-O2A
26	Y	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
37	Z	606	CHL	CAA-CBA-CGA-O1A
28	1	620	LHG	C27-C28-C29-C30
31	5	628	LMU	O5B-C1B-O1B-C4'
26	1	602	CLA	C10-C11-C12-C13
26	V	603	CLA	CAA-CBA-CGA-O2A
26	B	809	CLA	O1A-CGA-O2A-C1
26	A	818	CLA	C11-C12-C13-C15
26	Y	613	CLA	C16-C17-C18-C20
28	9	623	LHG	O6-C4-C5-O7
28	X	2630	LHG	O6-C4-C5-O7
37	W	607	CHL	CAA-CBA-CGA-O1A
26	1	616	CLA	CAA-CBA-CGA-O2A
26	a	616	CLA	CAA-CBA-CGA-O2A
26	U	604	CLA	CAD-CBD-CGD-O1D
37	X	608	CHL	CAD-CBD-CGD-O1D
28	O	2631	LHG	C11-C12-C13-C14
26	6	601	CLA	CBA-CGA-O2A-C1
26	1	608	CLA	CAA-CBA-CGA-O2A
26	a	608	CLA	CAA-CBA-CGA-O2A
26	5	616	CLA	CAA-CBA-CGA-O1A
26	W	614	CLA	CAA-CBA-CGA-O2A
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	1	604	CLA	C4B-C3B-CAB-CBB
26	1	606	CLA	C4B-C3B-CAB-CBB
26	a	604	CLA	C4B-C3B-CAB-CBB
26	a	606	CLA	C4B-C3B-CAB-CBB
26	4	608	CLA	C4B-C3B-CAB-CBB
26	5	609	CLA	C4B-C3B-CAB-CBB
26	6	602	CLA	C4B-C3B-CAB-CBB
26	7	604	CLA	C4B-C3B-CAB-CBB
26	8	606	CLA	C4B-C3B-CAB-CBB
26	U	602	CLA	C4B-C3B-CAB-CBB
26	W	610	CLA	C4B-C3B-CAB-CBB
26	8	613	CLA	C16-C17-C18-C20
28	A	861	LHG	O6-C4-C5-C6
28	X	2630	LHG	O6-C4-C5-C6
26	W	603	CLA	C4-C3-C5-C6
37	X	607	CHL	C4-C3-C5-C6
37	Y	609	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	W	603	CLA	CAA-CBA-CGA-O1A
26	A	831	CLA	C11-C12-C13-C15
26	B	810	CLA	C6-C7-C8-C10
26	6	602	CLA	C11-C12-C13-C15
26	4	608	CLA	C4C-C3C-CAC-CBC
34	Y	1621	LUT	C29-C30-C31-C32
35	Z	1622	XAT	C33-C34-C35-C15
32	8	626	LMG	C2-C1-O1-C7
32	8	626	LMG	O7-C8-C9-O8
26	a	610	CLA	CBA-CGA-O2A-C1
26	5	607	CLA	C3-C5-C6-C7
26	9	603	CLA	CAA-CBA-CGA-O2A
26	7	611	CLA	O2A-C1-C2-C3
26	U	604	CLA	O2A-C1-C2-C3
26	A	807	CLA	CAA-CBA-CGA-O2A
26	B	806	CLA	CAA-CBA-CGA-O2A
26	3	608	CLA	C2A-CAA-CBA-CGA
37	V	609	CHL	O1D-CGD-O2D-CED
26	B	833	CLA	C10-C11-C12-C13
26	V	603	CLA	CAA-CBA-CGA-O1A
29	B	852	BCR	C11-C10-C9-C34
28	U	2630	LHG	O7-C7-C8-C9
28	9	623	LHG	C14-C15-C16-C17
26	Y	610	CLA	C4-C3-C5-C6
37	U	609	CHL	C4-C3-C5-C6
37	W	609	CHL	C4-C3-C5-C6
26	A	826	CLA	C15-C16-C17-C18
26	Y	602	CLA	C5-C6-C7-C8
28	9	624	LHG	O9-C7-O7-C5
26	A	833	CLA	CAA-CBA-CGA-O1A
26	9	601	CLA	CAA-CBA-CGA-O1A
26	4	601	CLA	C2-C3-C5-C6
28	8	622	LHG	O8-C23-C24-C25
26	A	835	CLA	C12-C13-C15-C16
26	A	802	CLA	C11-C10-C8-C9
26	A	818	CLA	C11-C10-C8-C9
26	B	814	CLA	C11-C12-C13-C14
26	1	613	CLA	C11-C10-C8-C9
26	6	610	CLA	C6-C7-C8-C9
26	7	601	CLA	C6-C7-C8-C9
26	8	613	CLA	C11-C10-C8-C9
26	X	610	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
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
37	W	601	CHL	C14-C13-C15-C16
28	Y	2630	LHG	C16-C17-C18-C19
26	6	608	CLA	CAA-CBA-CGA-O1A
26	A	803	CLA	C3A-C2A-CAA-CBA
26	X	612	CLA	C3A-C2A-CAA-CBA
26	U	603	CLA	C3A-C2A-CAA-CBA
26	V	604	CLA	C3A-C2A-CAA-CBA
26	A	830	CLA	CAA-CBA-CGA-O2A
26	4	613	CLA	CAA-CBA-CGA-O2A
26	U	603	CLA	CAA-CBA-CGA-O2A
26	1	608	CLA	CAA-CBA-CGA-O1A
26	a	608	CLA	CAA-CBA-CGA-O1A
26	8	603	CLA	CAA-CBA-CGA-O2A
26	W	614	CLA	CAA-CBA-CGA-O1A
37	W	605	CHL	CAA-CBA-CGA-O2A
26	A	808	CLA	CAD-CBD-CGD-O2D
26	A	820	CLA	CAD-CBD-CGD-O2D
26	A	824	CLA	CAD-CBD-CGD-O2D
26	A	835	CLA	CAD-CBD-CGD-O2D
26	A	838	CLA	CAD-CBD-CGD-O2D
26	B	805	CLA	CAD-CBD-CGD-O2D
26	B	817	CLA	CAD-CBD-CGD-O2D
26	B	827	CLA	CAD-CBD-CGD-O2D
26	B	838	CLA	CAD-CBD-CGD-O2D
26	B	839	CLA	CAD-CBD-CGD-O2D
26	L	303	CLA	CAD-CBD-CGD-O2D
26	L	304	CLA	CAD-CBD-CGD-O2D
26	1	602	CLA	CAD-CBD-CGD-O2D
26	2	609	CLA	CAD-CBD-CGD-O2D
26	2	610	CLA	CAD-CBD-CGD-O2D
26	2	613	CLA	CAD-CBD-CGD-O2D
26	2	616	CLA	CAD-CBD-CGD-O2D
26	3	608	CLA	CAD-CBD-CGD-O2D
26	3	610	CLA	CAD-CBD-CGD-O2D
26	3	612	CLA	CAD-CBD-CGD-O2D
26	4	601	CLA	CAD-CBD-CGD-O2D
26	4	603	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	5	610	CLA	CAD-CBD-CGD-O2D
26	6	614	CLA	CAD-CBD-CGD-O2D
26	7	602	CLA	CAD-CBD-CGD-O2D
26	8	601	CLA	CAD-CBD-CGD-O2D
26	X	610	CLA	CAD-CBD-CGD-O2D
26	Y	612	CLA	CAD-CBD-CGD-O2D
26	Y	614	CLA	CAD-CBD-CGD-O2D
26	Z	603	CLA	CAD-CBD-CGD-O2D
26	V	612	CLA	CAD-CBD-CGD-O2D
26	V	614	CLA	CAD-CBD-CGD-O2D
26	W	614	CLA	CAD-CBD-CGD-O2D
36	X	1623	NEX	C7-C8-C9-C19
37	X	606	CHL	CAD-CBD-CGD-O2D
37	X	607	CHL	CAD-CBD-CGD-O2D
37	Z	606	CHL	CAD-CBD-CGD-O2D
37	V	605	CHL	CAD-CBD-CGD-O2D
37	V	607	CHL	CAD-CBD-CGD-O2D
37	W	606	CHL	CAD-CBD-CGD-O2D
26	2	602	CLA	C16-C17-C18-C20
26	6	601	CLA	C16-C17-C18-C19
28	B	851	LHG	C11-C12-C13-C14
26	5	619	CLA	C2A-CAA-CBA-CGA
26	5	601	CLA	C3-C5-C6-C7
26	A	806	CLA	CAA-CBA-CGA-O2A
26	B	829	CLA	C4-C3-C5-C6
26	3	608	CLA	C4-C3-C5-C6
26	7	602	CLA	C4-C3-C5-C6
26	B	841	CLA	C3-C5-C6-C7
27	B	842	PQN	C12-C13-C15-C16
37	U	609	CHL	C2-C3-C5-C6
26	A	835	CLA	CAA-CBA-CGA-O2A
28	Y	2630	LHG	C14-C15-C16-C17
29	A	848	BCR	C21-C22-C23-C24
29	B	845	BCR	C21-C22-C23-C24
26	6	620	CLA	C3-C5-C6-C7
32	H	205	LMG	C7-C8-C9-O8
32	J	104	LMG	C7-C8-C9-O8
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	G	204	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	1	616	CLA	CAA-CBA-CGA-O1A
26	a	616	CLA	CAA-CBA-CGA-O1A
26	5	619	CLA	CAA-CBA-CGA-O2A
26	9	607	CLA	CAA-CBA-CGA-O1A
26	9	607	CLA	CAA-CBA-CGA-O2A
28	9	624	LHG	C14-C15-C16-C17
32	H	205	LMG	C14-C15-C16-C17
26	A	821	CLA	CAA-CBA-CGA-O2A
26	A	840	CLA	CAA-CBA-CGA-O2A
26	H	203	CLA	CAA-CBA-CGA-O2A
26	Z	613	CLA	CAA-CBA-CGA-O2A
26	8	603	CLA	CAA-CBA-CGA-O1A
26	A	804	CLA	O2A-C1-C2-C3
26	B	806	CLA	O2A-C1-C2-C3
26	B	810	CLA	O2A-C1-C2-C3
26	B	817	CLA	O2A-C1-C2-C3
37	Z	607	CHL	O2A-C1-C2-C3
37	V	601	CHL	O2A-C1-C2-C3
32	J	104	LMG	C31-C32-C33-C34
37	X	609	CHL	C4C-C3C-CAC-CBC
28	B	851	LHG	C24-C23-O8-C6
26	9	603	CLA	C2A-CAA-CBA-CGA
26	9	607	CLA	C2A-CAA-CBA-CGA
26	9	603	CLA	CAA-CBA-CGA-O1A
37	W	605	CHL	CAA-CBA-CGA-O1A
26	a	612	CLA	O1D-CGD-O2D-CED
28	Z	2630	LHG	C11-C10-C9-C8
26	1	612	CLA	O1D-CGD-O2D-CED
26	A	806	CLA	CHA-CBD-CGD-O2D
26	A	807	CLA	CHA-CBD-CGD-O1D
26	A	811	CLA	CHA-CBD-CGD-O1D
26	A	815	CLA	CHA-CBD-CGD-O2D
26	A	825	CLA	CHA-CBD-CGD-O2D
26	A	832	CLA	CHA-CBD-CGD-O2D
26	A	835	CLA	CHA-CBD-CGD-O2D
26	B	814	CLA	CHA-CBD-CGD-O1D
26	B	822	CLA	CHA-CBD-CGD-O1D
26	B	822	CLA	CHA-CBD-CGD-O2D
26	B	826	CLA	CHA-CBD-CGD-O2D
26	B	828	CLA	CHA-CBD-CGD-O1D
26	B	828	CLA	CHA-CBD-CGD-O2D
26	B	841	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	1	604	CLA	CHA-CBD-CGD-O2D
26	1	609	CLA	CHA-CBD-CGD-O2D
26	1	612	CLA	CHA-CBD-CGD-O2D
26	a	604	CLA	CHA-CBD-CGD-O2D
26	a	612	CLA	CHA-CBD-CGD-O2D
26	4	611	CLA	CHA-CBD-CGD-O1D
26	4	611	CLA	CHA-CBD-CGD-O2D
26	5	607	CLA	CHA-CBD-CGD-O1D
26	5	607	CLA	CHA-CBD-CGD-O2D
26	7	604	CLA	CHA-CBD-CGD-O1D
26	7	604	CLA	CHA-CBD-CGD-O2D
26	7	611	CLA	CHA-CBD-CGD-O2D
26	7	616	CLA	CHA-CBD-CGD-O2D
26	8	602	CLA	CHA-CBD-CGD-O1D
26	8	602	CLA	CHA-CBD-CGD-O2D
26	8	603	CLA	CHA-CBD-CGD-O2D
26	9	603	CLA	CHA-CBD-CGD-O1D
26	9	603	CLA	CHA-CBD-CGD-O2D
26	9	604	CLA	CHA-CBD-CGD-O1D
26	9	604	CLA	CHA-CBD-CGD-O2D
26	9	607	CLA	CHA-CBD-CGD-O1D
26	9	607	CLA	CHA-CBD-CGD-O2D
26	X	602	CLA	CHA-CBD-CGD-O1D
26	X	603	CLA	CHA-CBD-CGD-O1D
26	X	603	CLA	CHA-CBD-CGD-O2D
26	U	611	CLA	CHA-CBD-CGD-O1D
26	U	611	CLA	CHA-CBD-CGD-O2D
26	W	602	CLA	CHA-CBD-CGD-O1D
26	W	602	CLA	CHA-CBD-CGD-O2D
26	W	612	CLA	CHA-CBD-CGD-O1D
26	W	612	CLA	CHA-CBD-CGD-O2D
37	X	601	CHL	CHA-CBD-CGD-O1D
37	X	601	CHL	CHA-CBD-CGD-O2D
37	Y	601	CHL	CHA-CBD-CGD-O2D
37	V	601	CHL	CHA-CBD-CGD-O1D
37	V	601	CHL	CHA-CBD-CGD-O2D
26	3	608	CLA	C2-C3-C5-C6
28	H	204	LHG	C11-C12-C13-C14
26	6	608	CLA	CAA-CBA-CGA-O2A
26	A	818	CLA	CAA-CBA-CGA-O2A
26	B	813	CLA	CAA-CBA-CGA-O2A
26	9	613	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	X	2630	LHG	O7-C5-C6-O8
28	7	622	LHG	C29-C30-C31-C32
32	V	2631	LMG	C39-C40-C41-C42
26	6	602	CLA	C2A-CAA-CBA-CGA
26	W	612	CLA	C2A-CAA-CBA-CGA
26	B	819	CLA	C6-C7-C8-C9
26	B	823	CLA	CAA-CBA-CGA-O2A
37	Z	609	CHL	C10-C11-C12-C13
26	Z	602	CLA	C3-C5-C6-C7
26	A	813	CLA	CAA-CBA-CGA-O2A
26	B	841	CLA	CAA-CBA-CGA-O2A
26	W	602	CLA	CAA-CBA-CGA-O2A
28	9	622	LHG	O8-C23-C24-C25
26	a	606	CLA	CAA-CBA-CGA-O2A
26	4	602	CLA	C4-C3-C5-C6
37	W	607	CHL	C4-C3-C5-C6
26	W	613	CLA	C10-C11-C12-C13
26	A	829	CLA	C12-C13-C15-C16
26	B	840	CLA	C11-C10-C8-C7
26	6	604	CLA	C6-C7-C8-C10
26	W	603	CLA	C2-C3-C5-C6
26	A	839	CLA	C6-C7-C8-C9
26	B	810	CLA	C16-C17-C18-C20
26	4	614	CLA	C5-C6-C7-C8
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	6	604	CLA	C11-C12-C13-C14
26	7	613	CLA	C11-C10-C8-C9
26	X	610	CLA	C6-C7-C8-C9
37	X	607	CHL	C11-C10-C8-C9
26	A	814	CLA	C13-C15-C16-C17
26	A	824	CLA	C2B-C3B-CAB-CBB
26	A	827	CLA	C2B-C3B-CAB-CBB
26	B	836	CLA	C2B-C3B-CAB-CBB
26	3	617	CLA	C2B-C3B-CAB-CBB
26	W	610	CLA	C2B-C3B-CAB-CBB
37	X	605	CHL	C2B-C3B-CAB-CBB
26	6	609	CLA	CAA-CBA-CGA-O2A
37	Y	609	CHL	C4C-C3C-CAC-CBC
26	A	807	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	A	835	CLA	CAA-CBA-CGA-O1A
26	5	619	CLA	CAA-CBA-CGA-O1A
26	B	806	CLA	C2A-CAA-CBA-CGA
26	B	809	CLA	CBA-CGA-O2A-C1
28	3	624	LHG	C23-C24-C25-C26
28	U	2630	LHG	O9-C7-C8-C9
26	A	830	CLA	C10-C11-C12-C13
26	A	802	CLA	C4-C3-C5-C6
26	7	613	CLA	C4-C3-C5-C6
26	6	616	CLA	C4C-C3C-CAC-CBC
28	8	623	LHG	O1-C1-C2-C3
26	B	811	CLA	C2-C3-C5-C6
28	3	623	LHG	C11-C10-C9-C8
26	A	840	CLA	CAA-CBA-CGA-O1A
31	5	629	LMU	C2B-C1B-O1B-C4'
29	K	207	BCR	C7-C8-C9-C10
32	4	624	LMG	C29-C30-C31-C32
26	Z	614	CLA	CBA-CGA-O2A-C1
26	6	601	CLA	O1A-CGA-O2A-C1
26	A	803	CLA	C1A-C2A-CAA-CBA
26	A	806	CLA	C1A-C2A-CAA-CBA
26	A	807	CLA	C1A-C2A-CAA-CBA
26	F	301	CLA	C1A-C2A-CAA-CBA
26	K	204	CLA	C1A-C2A-CAA-CBA
26	O	2001	CLA	CHA-CBD-CGD-O2D
26	O	2003	CLA	CHA-CBD-CGD-O2D
26	1	606	CLA	CAD-CBD-CGD-O2D
26	a	606	CLA	CAD-CBD-CGD-O2D
26	2	602	CLA	CHA-CBD-CGD-O2D
26	2	604	CLA	C1A-C2A-CAA-CBA
26	2	609	CLA	C1A-C2A-CAA-CBA
26	3	606	CLA	CHA-CBD-CGD-O2D
26	3	611	CLA	CHA-CBD-CGD-O2D
26	3	613	CLA	CHA-CBD-CGD-O2D
26	6	608	CLA	C1A-C2A-CAA-CBA
26	7	603	CLA	CHA-CBD-CGD-O2D
26	X	612	CLA	C1A-C2A-CAA-CBA
26	U	603	CLA	C1A-C2A-CAA-CBA
37	Y	607	CHL	C1A-C2A-CAA-CBA
37	U	601	CHL	C1A-C2A-CAA-CBA
28	X	2630	LHG	C19-C20-C21-C22
26	A	830	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	B	803	CLA	C15-C16-C17-C18
26	U	613	CLA	O1D-CGD-O2D-CED
26	A	808	CLA	C2-C1-O2A-CGA
26	A	839	CLA	C2-C1-O2A-CGA
26	4	608	CLA	C13-C15-C16-C17
26	B	832	CLA	CBA-CGA-O2A-C1
26	H	203	CLA	CAA-CBA-CGA-O1A
26	Z	613	CLA	CAA-CBA-CGA-O1A
37	V	607	CHL	CAA-CBA-CGA-O2A
33	B	850	DGD	C2B-C3B-C4B-C5B
26	B	837	CLA	C2A-CAA-CBA-CGA
26	W	610	CLA	C2A-CAA-CBA-CGA
28	H	204	LHG	C17-C18-C19-C20
26	8	613	CLA	C16-C17-C18-C19
26	B	806	CLA	CAA-CBA-CGA-O1A
26	4	613	CLA	CAA-CBA-CGA-O1A
28	A	861	LHG	C10-C11-C12-C13
26	7	616	CLA	CAA-CBA-CGA-O2A
37	Z	607	CHL	CAA-CBA-CGA-O2A
28	Y	2630	LHG	C5-C4-O6-P
26	A	806	CLA	CAA-CBA-CGA-O1A
26	1	612	CLA	CBD-CGD-O2D-CED
26	2	609	CLA	CAA-CBA-CGA-O2A
37	X	605	CHL	CAA-CBA-CGA-O2A
37	U	607	CHL	CAA-CBA-CGA-O2A
26	L	303	CLA	C13-C15-C16-C17
26	7	602	CLA	C4B-C3B-CAB-CBB
28	A	846	LHG	C4-O6-P-O5
28	B	851	LHG	C4-O6-P-O5
28	O	2631	LHG	C4-O6-P-O5
28	5	625	LHG	C4-O6-P-O5
28	8	622	LHG	C3-O3-P-O5
28	8	622	LHG	C4-O6-P-O5
28	Z	2630	LHG	C3-O3-P-O5
28	U	2630	LHG	C3-O3-P-O4
37	X	605	CHL	C4B-C3B-CAB-CBB
37	Y	608	CHL	C4B-C3B-CAB-CBB
37	Z	607	CHL	C4B-C3B-CAB-CBB
26	9	613	CLA	CAA-CBA-CGA-O1A
28	8	622	LHG	O10-C23-C24-C25
26	X	602	CLA	CAA-CBA-CGA-O2A
26	W	611	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	A	846	LHG	O6-C4-C5-C6
28	A	846	LHG	C11-C12-C13-C14
26	4	616	CLA	CAA-CBA-CGA-O2A
29	B	801	BCR	C1-C6-C7-C8
26	6	604	CLA	C13-C15-C16-C17
26	A	821	CLA	CAA-CBA-CGA-O1A
26	a	606	CLA	CAA-CBA-CGA-O1A
26	A	804	CLA	C2A-CAA-CBA-CGA
26	B	813	CLA	C2A-CAA-CBA-CGA
26	A	843	CLA	C6-C7-C8-C10
28	1	620	LHG	C17-C18-C19-C20
26	B	823	CLA	CAA-CBA-CGA-O1A
26	8	608	CLA	CAA-CBA-CGA-O2A
37	Y	607	CHL	CAA-CBA-CGA-O2A
32	4	623	LMG	C28-C29-C30-C31
37	X	609	CHL	C4-C3-C5-C6
37	Y	609	CHL	C2-C3-C5-C6
26	6	609	CLA	CAA-CBA-CGA-O1A
26	A	811	CLA	CAD-CBD-CGD-O1D
26	A	837	CLA	CAD-CBD-CGD-O1D
26	A	843	CLA	CAD-CBD-CGD-O1D
26	B	805	CLA	CAD-CBD-CGD-O1D
26	B	814	CLA	CAD-CBD-CGD-O1D
26	B	822	CLA	CAD-CBD-CGD-O1D
26	B	825	CLA	CAD-CBD-CGD-O1D
26	B	826	CLA	CAD-CBD-CGD-O1D
26	K	201	CLA	CAD-CBD-CGD-O1D
26	4	611	CLA	CAD-CBD-CGD-O1D
26	4	616	CLA	CAD-CBD-CGD-O1D
26	5	619	CLA	CAD-CBD-CGD-O1D
26	6	604	CLA	CAD-CBD-CGD-O1D
26	8	616	CLA	CAD-CBD-CGD-O1D
26	X	602	CLA	CAD-CBD-CGD-O1D
36	V	1623	NEX	C7-C8-C9-C10
37	X	601	CHL	CAD-CBD-CGD-O1D
37	X	605	CHL	CAD-CBD-CGD-O1D
26	A	840	CLA	CBD-CGD-O2D-CED
26	a	612	CLA	CBD-CGD-O2D-CED
26	A	813	CLA	CAA-CBA-CGA-O1A
26	W	602	CLA	CAA-CBA-CGA-O1A
26	A	822	CLA	CAA-CBA-CGA-O2A
26	A	802	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	A	807	CLA	C6-C7-C8-C9
26	A	841	CLA	C14-C13-C15-C16
26	B	803	CLA	C14-C13-C15-C16
26	B	828	CLA	C11-C10-C8-C9
26	B	840	CLA	C11-C10-C8-C9
26	7	602	CLA	C6-C7-C8-C9
26	7	613	CLA	C11-C12-C13-C14
26	8	613	CLA	C14-C13-C15-C16
37	U	607	CHL	CAA-CBA-CGA-O1A
26	B	827	CLA	O1A-CGA-O2A-C1
26	B	832	CLA	O1A-CGA-O2A-C1
26	W	604	CLA	O1A-CGA-O2A-C1
26	B	841	CLA	CAA-CBA-CGA-O1A
28	9	622	LHG	O10-C23-C24-C25
26	A	805	CLA	CAA-CBA-CGA-O2A
32	J	103	LMG	O7-C10-C11-C12
37	V	608	CHL	CAA-CBA-CGA-O2A
26	W	611	CLA	C5-C6-C7-C8
26	B	807	CLA	O1A-CGA-O2A-C1
26	a	613	CLA	O1A-CGA-O2A-C1
26	A	818	CLA	CAA-CBA-CGA-O1A
26	L	303	CLA	C2A-CAA-CBA-CGA
26	6	603	CLA	CAA-CBA-CGA-O2A
26	6	616	CLA	CAA-CBA-CGA-O2A
26	A	809	CLA	C8-C10-C11-C12
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	5	613	CLA	C2-C1-O2A-CGA
26	B	831	CLA	C4-C3-C5-C6
26	6	614	CLA	C4-C3-C5-C6
26	B	824	CLA	C5-C6-C7-C8
26	6	613	CLA	C10-C11-C12-C13
26	A	801	CLA	C12-C13-C15-C16
26	A	810	CLA	C3A-C2A-CAA-CBA
26	A	812	CLA	C11-C12-C13-C15
26	A	816	CLA	C6-C7-C8-C10
26	A	825	CLA	C2-C3-C5-C6
26	B	803	CLA	C6-C7-C8-C10
26	F	301	CLA	C3A-C2A-CAA-CBA
26	H	202	CLA	CHA-CBD-CGD-O1D
26	L	307	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	O	2003	CLA	CHA-CBD-CGD-O1D
26	O	2003	CLA	CAD-CBD-CGD-O2D
26	a	609	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	609	CLA	C6-C7-C8-C10
26	3	610	CLA	C6-C7-C8-C10
26	3	611	CLA	CHA-CBD-CGD-O1D
26	3	611	CLA	CAD-CBD-CGD-O2D
26	3	613	CLA	CHA-CBD-CGD-O1D
26	4	612	CLA	CAD-CBD-CGD-O2D
26	4	614	CLA	C6-C7-C8-C10
26	5	606	CLA	CAD-CBD-CGD-O2D
26	5	616	CLA	CBD-CGD-O2D-CED
26	5	618	CLA	CHA-CBD-CGD-O1D
26	6	612	CLA	CHA-CBD-CGD-O1D
26	6	613	CLA	CAD-CBD-CGD-O2D
26	6	618	CLA	CAD-CBD-CGD-O2D
26	7	607	CLA	C3A-C2A-CAA-CBA
26	8	613	CLA	C12-C13-C15-C16
26	X	602	CLA	C12-C13-C15-C16
26	X	610	CLA	C6-C7-C8-C10
26	Y	610	CLA	C12-C13-C15-C16
26	Z	611	CLA	C3A-C2A-CAA-CBA
37	X	609	CHL	C3A-C2A-CAA-CBA
37	Y	609	CHL	C11-C12-C13-C15
26	7	616	CLA	CAA-CBA-CGA-O1A
26	a	609	CLA	CAA-CBA-CGA-O2A
26	a	614	CLA	CAA-CBA-CGA-O2A
26	6	601	CLA	CAA-CBA-CGA-O2A
26	8	604	CLA	CAA-CBA-CGA-O2A
28	2	622	LHG	O8-C23-C24-C25
28	4	622	LHG	O8-C23-C24-C25
26	Z	614	CLA	O1A-CGA-O2A-C1
29	K	207	BCR	C21-C22-C23-C24
29	1	619	BCR	C11-C12-C13-C14
29	a	619	BCR	C11-C12-C13-C14
29	3	622	BCR	C17-C18-C19-C20
35	Y	1622	XAT	C11-C12-C13-C14
35	W	1622	XAT	C11-C12-C13-C14
36	Y	1623	NEX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	a	609	CLA	CAA-CBA-CGA-O1A
26	W	611	CLA	CAA-CBA-CGA-O1A
34	U	1620	LUT	C33-C34-C35-C15
26	Y	602	CLA	CAA-CBA-CGA-O2A
28	W	2630	LHG	O7-C7-C8-C9
32	V	2631	LMG	O6-C1-O1-C7
26	6	601	CLA	C8-C10-C11-C12
26	1	613	CLA	O1A-CGA-O2A-C1
26	B	832	CLA	CAA-CBA-CGA-O1A
26	a	614	CLA	CAA-CBA-CGA-O1A
26	6	603	CLA	CAA-CBA-CGA-O1A
26	6	616	CLA	CAA-CBA-CGA-O1A
26	W	604	CLA	CBA-CGA-O2A-C1
37	V	607	CHL	CAA-CBA-CGA-O1A
37	X	607	CHL	CAA-CBA-CGA-O2A
26	B	806	CLA	C10-C11-C12-C13
26	3	610	CLA	C13-C15-C16-C17
26	B	813	CLA	CAA-CBA-CGA-O1A
26	4	616	CLA	C2A-CAA-CBA-CGA
26	6	603	CLA	C2A-CAA-CBA-CGA
26	A	809	CLA	C13-C15-C16-C17
26	4	608	CLA	C8-C10-C11-C12
26	9	613	CLA	C15-C16-C17-C18
26	Y	610	CLA	O1D-CGD-O2D-CED
26	9	602	CLA	CAA-CBA-CGA-O2A
26	V	602	CLA	CAA-CBA-CGA-O2A
28	W	2630	LHG	O8-C23-C24-C25
26	4	616	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

290 monomers are involved in 664 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	4	607	CLA	1	0
35	6	621	XAT	1	0
37	W	601	CHL	3	0
26	A	835	CLA	2	0
26	W	614	CLA	4	0
26	F	304	CLA	1	0
26	8	612	CLA	2	0
26	V	612	CLA	2	0
26	B	827	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	5	607	CLA	2	0
26	U	613	CLA	3	0
37	Y	601	CHL	6	0
35	1	618	XAT	3	0
37	X	608	CHL	3	0
29	G	205	BCR	4	0
26	1	606	CLA	1	0
36	6	624	NEX	6	0
26	Z	613	CLA	4	0
26	B	817	CLA	1	0
26	8	606	CLA	1	0
34	5	620	LUT	4	0
26	A	837	CLA	1	0
32	V	2631	LMG	2	0
36	5	624	NEX	1	0
26	A	829	CLA	5	0
29	3	622	BCR	7	0
26	B	828	CLA	2	0
35	4	620	XAT	3	0
26	7	611	CLA	4	0
37	V	608	CHL	2	0
26	4	616	CLA	1	0
26	B	839	CLA	1	0
29	4	621	BCR	5	0
37	V	609	CHL	3	0
28	Y	2630	LHG	6	0
28	Z	2630	LHG	9	0
26	1	601	CLA	2	0
29	6	622	BCR	1	0
37	U	605	CHL	1	0
32	5	627	LMG	1	0
29	A	848	BCR	3	0
34	a	617	LUT	5	0
26	A	825	CLA	3	0
27	A	844	PQN	2	0
26	Z	612	CLA	1	0
26	X	614	CLA	1	0
26	7	614	CLA	2	0
26	V	602	CLA	3	0
29	A	850	BCR	8	0
26	a	611	CLA	1	0
26	W	602	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	619	BCR	3	0
26	A	802	CLA	3	0
26	A	841	CLA	4	0
26	8	613	CLA	2	0
26	6	609	CLA	1	0
26	U	604	CLA	3	0
26	A	818	CLA	1	0
29	L	301	BCR	10	0
26	A	812	CLA	1	0
26	6	602	CLA	1	0
26	a	607	CLA	1	0
26	B	840	CLA	1	0
34	X	1621	LUT	6	0
26	B	803	CLA	2	0
35	a	618	XAT	3	0
28	9	622	LHG	1	0
26	A	843	CLA	2	0
36	V	1623	NEX	11	0
29	K	202	BCR	5	0
26	X	602	CLA	4	0
29	7	623	BCR	5	0
29	3	620	BCR	8	0
37	X	609	CHL	4	0
29	L	308	BCR	7	0
29	B	844	BCR	6	0
26	Y	602	CLA	2	0
26	4	611	CLA	1	0
28	U	2630	LHG	1	0
26	1	611	CLA	1	0
26	6	616	CLA	1	0
26	a	613	CLA	1	0
28	3	623	LHG	1	0
31	A	857	LMU	1	0
26	B	825	CLA	2	0
36	Y	1623	NEX	2	0
26	5	619	CLA	3	0
26	F	301	CLA	1	0
26	9	610	CLA	1	0
26	1	604	CLA	1	0
37	U	608	CHL	3	0
26	Z	614	CLA	1	0
37	U	607	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	2	606	CLA	1	0
26	6	608	CLA	1	0
26	5	603	CLA	1	0
26	A	824	CLA	2	0
37	Z	608	CHL	2	0
37	Z	607	CHL	3	0
37	W	605	CHL	2	0
29	B	801	BCR	7	0
26	B	816	CLA	1	0
26	4	606	CLA	1	0
37	V	607	CHL	4	0
26	Z	603	CLA	1	0
26	A	808	CLA	2	0
26	A	807	CLA	3	0
26	A	840	CLA	1	0
26	7	615	CLA	1	0
34	X	1620	LUT	6	0
26	A	809	CLA	1	0
26	B	834	CLA	3	0
29	F	305	BCR	7	0
26	B	818	CLA	1	0
26	5	610	CLA	1	0
26	A	816	CLA	1	0
26	3	612	CLA	1	0
26	9	613	CLA	2	0
37	X	601	CHL	7	0
26	5	613	CLA	1	0
26	Y	610	CLA	2	0
35	V	1622	XAT	6	0
35	3	619	XAT	2	0
36	X	1623	NEX	2	0
34	V	1621	LUT	5	0
35	W	1622	XAT	3	0
26	W	610	CLA	1	0
26	W	603	CLA	2	0
37	V	606	CHL	2	0
26	7	601	CLA	1	0
26	6	610	CLA	3	0
26	B	819	CLA	1	0
26	A	831	CLA	1	0
35	X	1622	XAT	3	0
26	X	610	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	1	619	BCR	2	0
29	8	621	BCR	3	0
26	W	612	CLA	1	0
28	5	623	LHG	6	0
35	7	620	XAT	1	0
35	2	620	XAT	1	0
29	5	622	BCR	2	0
37	V	601	CHL	4	0
26	X	604	CLA	1	0
26	9	609	CLA	1	0
35	8	620	XAT	1	0
34	U	1621	LUT	2	0
26	L	302	CLA	3	0
32	A	860	LMG	1	0
37	U	609	CHL	3	0
29	B	847	BCR	4	0
26	3	610	CLA	1	0
34	Y	1621	LUT	4	0
26	B	808	CLA	3	0
26	V	610	CLA	3	0
26	A	834	CLA	2	0
26	3	613	CLA	1	0
26	Y	613	CLA	4	0
35	5	621	XAT	2	0
26	A	820	CLA	2	0
37	Y	609	CHL	3	0
26	a	606	CLA	1	0
26	B	822	CLA	1	0
26	6	607	CLA	1	0
34	6	619	LUT	5	0
35	Y	1622	XAT	3	0
26	K	203	CLA	1	0
34	Z	1621	LUT	4	0
26	X	603	CLA	1	0
34	V	1620	LUT	5	0
37	U	606	CHL	2	0
26	2	613	CLA	3	0
26	B	830	CLA	1	0
26	Z	602	CLA	4	0
37	W	609	CHL	1	0
29	A	856	BCR	10	0
34	7	619	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	6	606	CLA	1	0
37	Z	609	CHL	3	0
26	B	835	CLA	1	0
26	7	604	CLA	1	0
37	Z	606	CHL	3	0
26	7	616	CLA	1	0
26	U	602	CLA	1	0
34	U	1620	LUT	6	0
29	A	851	BCR	6	0
37	X	607	CHL	2	0
26	B	833	CLA	2	0
26	V	614	CLA	1	0
26	a	601	CLA	3	0
30	C	102	SF4	1	0
29	B	846	BCR	3	0
28	V	2630	LHG	3	0
29	B	843	BCR	9	0
26	a	604	CLA	1	0
34	Z	1620	LUT	6	0
26	A	854	CLA	5	0
36	Z	1623	NEX	3	0
26	4	609	CLA	1	0
34	2	619	LUT	7	0
26	6	601	CLA	1	0
28	a	620	LHG	1	0
26	K	204	CLA	2	0
34	3	618	LUT	7	0
26	A	822	CLA	4	0
29	B	845	BCR	3	0
37	V	605	CHL	1	0
26	B	824	CLA	1	0
36	W	1623	NEX	2	0
26	L	303	CLA	2	0
28	X	2630	LHG	6	0
37	U	601	CHL	4	0
29	9	621	BCR	7	0
26	3	608	CLA	1	0
26	A	803	CLA	3	0
26	X	613	CLA	4	0
29	2	623	BCR	5	0
26	1	607	CLA	1	0
34	9	619	LUT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	W	1621	LUT	4	0
26	8	610	CLA	1	0
37	W	606	CHL	1	0
26	X	612	CLA	1	0
26	W	613	CLA	4	0
29	L	309	BCR	4	0
26	5	611	CLA	7	0
26	7	609	CLA	1	0
26	A	819	CLA	2	0
26	B	813	CLA	2	0
29	B	852	BCR	6	0
26	U	610	CLA	4	0
33	B	850	DGD	1	0
34	4	619	LUT	3	0
26	8	604	CLA	1	0
37	Y	605	CHL	1	0
28	3	624	LHG	2	0
26	3	606	CLA	1	0
34	1	617	LUT	6	0
26	A	821	CLA	1	0
26	A	830	CLA	1	0
26	8	611	CLA	2	0
26	Z	611	CLA	3	0
29	J	102	BCR	8	0
26	4	618	CLA	1	0
29	B	849	BCR	2	0
37	W	607	CHL	3	0
26	1	613	CLA	1	0
28	W	2630	LHG	1	0
26	X	611	CLA	2	0
26	F	303	CLA	4	0
26	Y	603	CLA	3	0
37	Z	601	CHL	4	0
26	V	613	CLA	4	0
26	B	802	CLA	1	0
26	A	827	CLA	1	0
37	Y	608	CHL	2	0
28	O	2631	LHG	1	0
26	6	614	CLA	2	0
37	Y	607	CHL	3	0
27	B	842	PQN	3	0
26	B	837	CLA	2	0

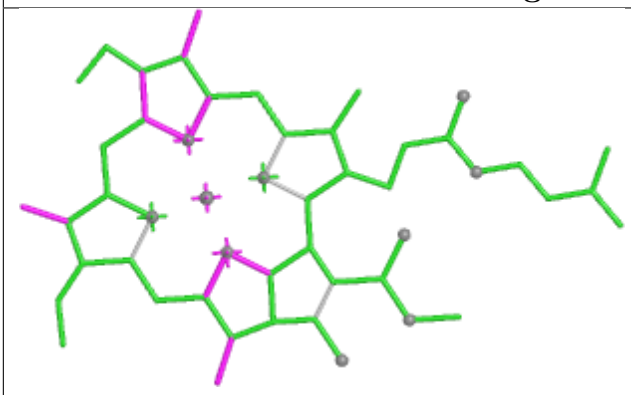
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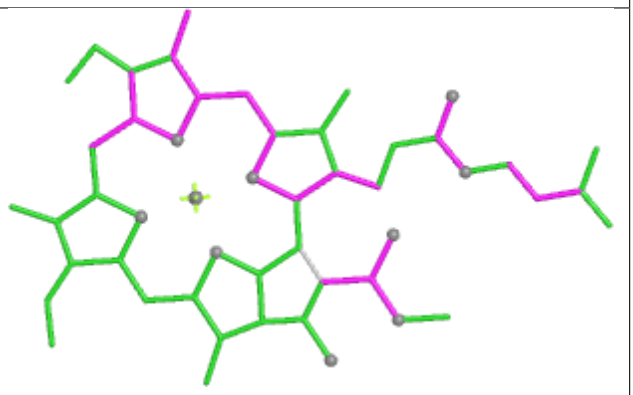
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	7	613	CLA	2	0
26	4	601	CLA	1	0
26	7	602	CLA	1	0
26	A	806	CLA	2	0
29	3	621	BCR	4	0
35	Z	1622	XAT	5	0
26	Z	610	CLA	5	0
29	O	2004	BCR	3	0
32	9	625	LMG	2	0
32	8	626	LMG	3	0
26	A	815	CLA	2	0
26	L	307	CLA	2	0
29	A	852	BCR	10	0
26	a	603	CLA	1	0
29	A	849	BCR	5	0
35	U	1622	XAT	5	0
34	8	619	LUT	6	0
29	O	2005	BCR	6	0
29	B	848	BCR	2	0
29	7	621	BCR	3	0
26	5	602	CLA	2	0
29	L	305	BCR	8	0
26	A	805	CLA	1	0
26	B	821	CLA	3	0
34	W	1620	LUT	4	0
29	K	207	BCR	3	0
34	Y	1620	LUT	5	0
29	B	853	BCR	3	0
37	Y	606	CHL	2	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.

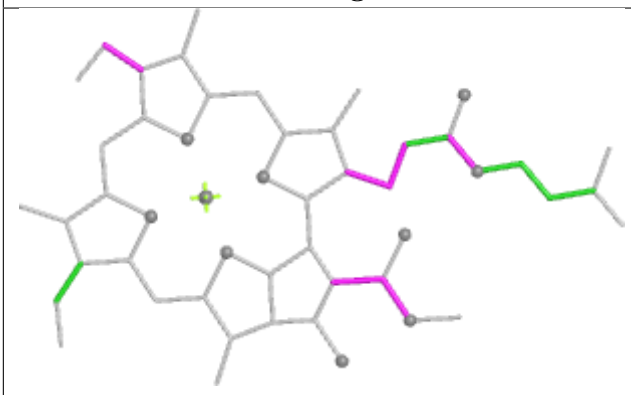
Ligand CLA A 832



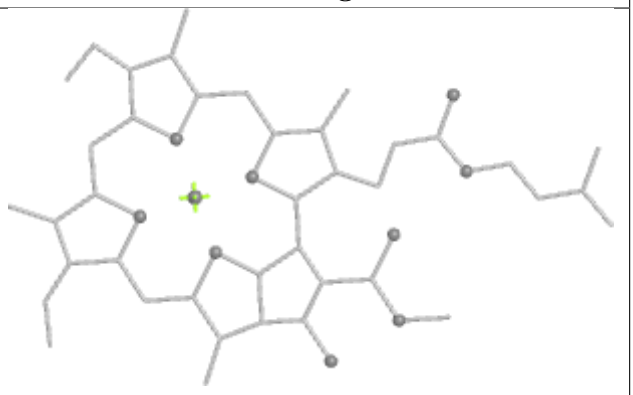
Bond lengths



Bond angles

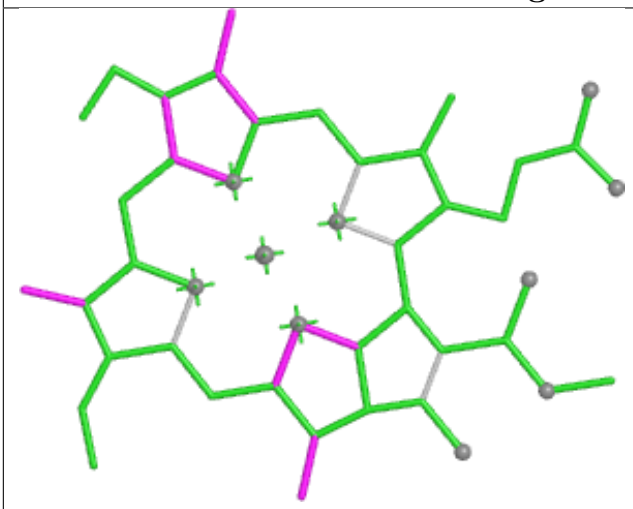


Torsions

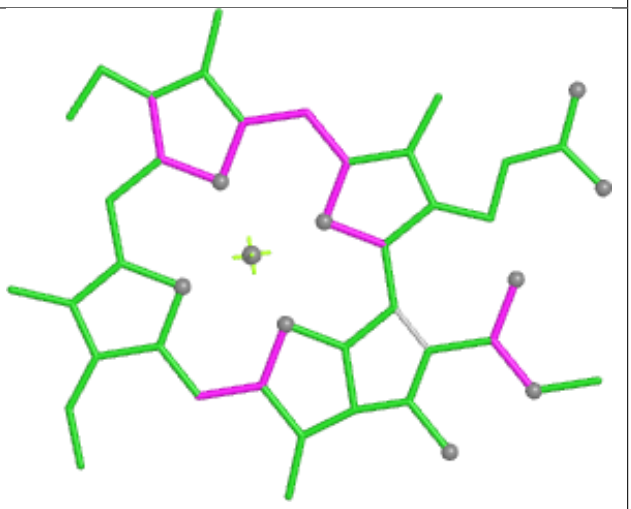


Rings

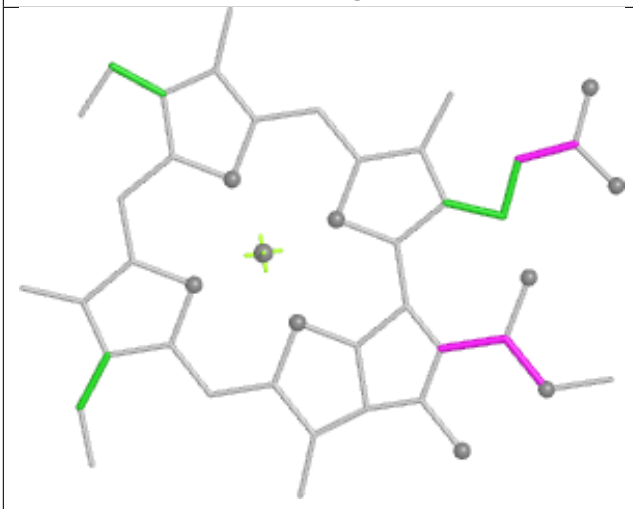
Ligand CLA 4 607



Bond lengths



Bond angles

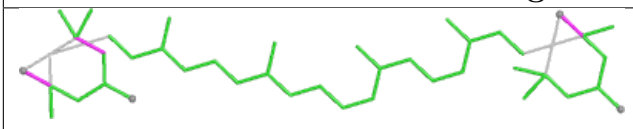


Torsions

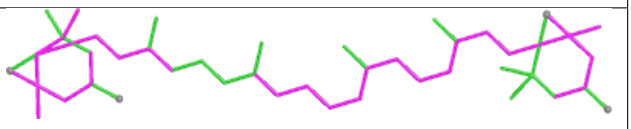


Rings

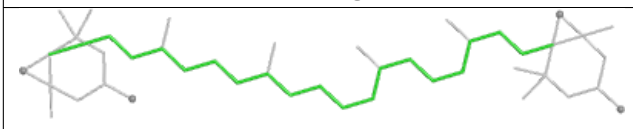
Ligand XAT 6 621



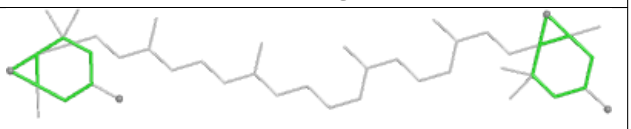
Bond lengths



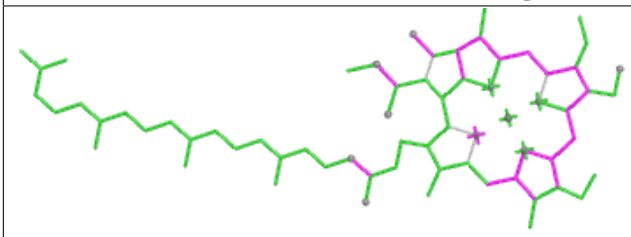
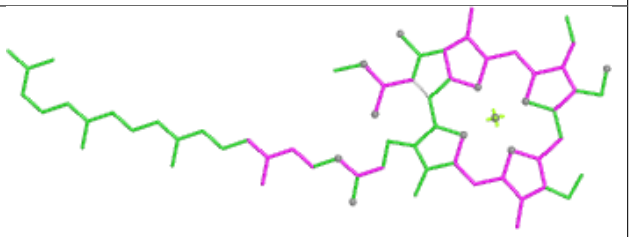
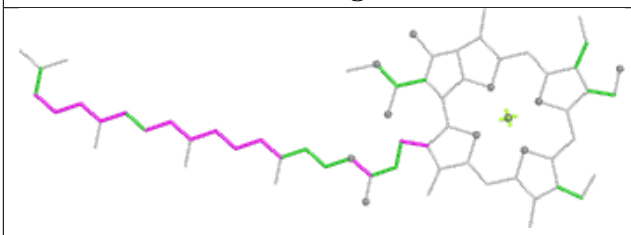
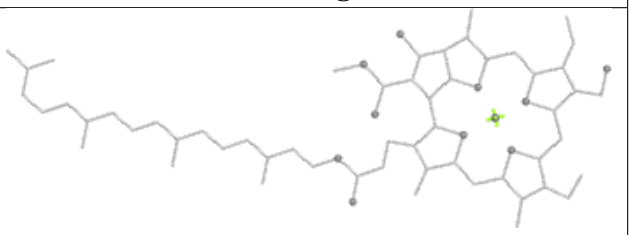
Bond angles

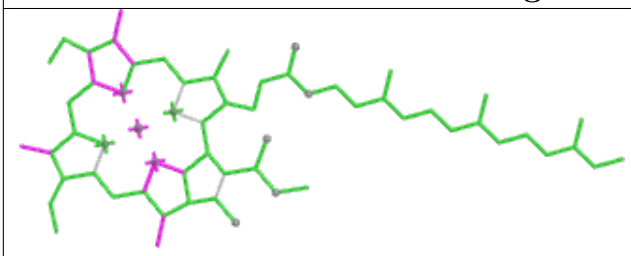
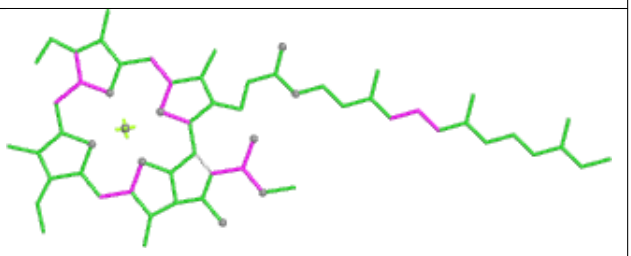
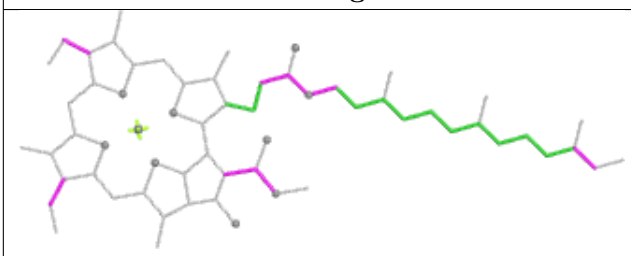
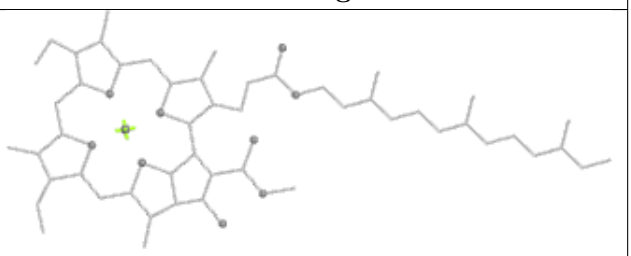


Torsions

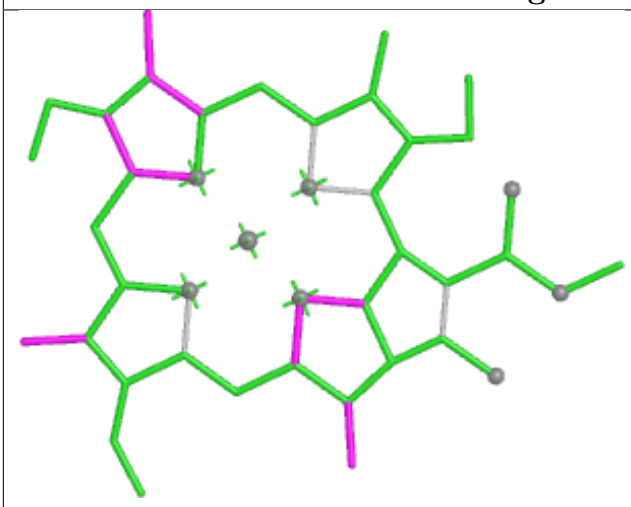


Rings

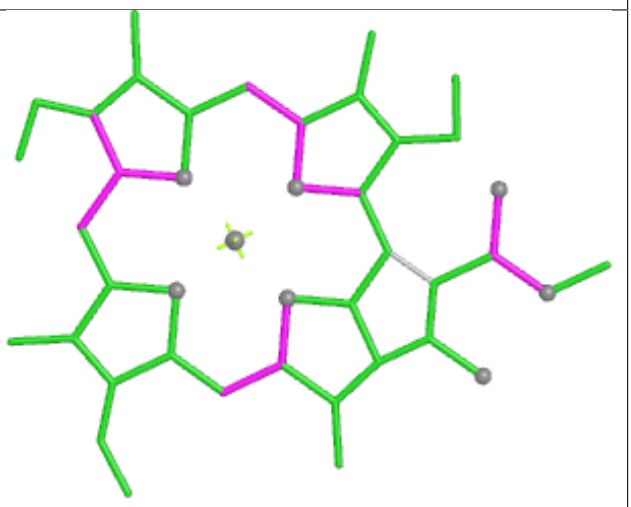
Ligand CHL W 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

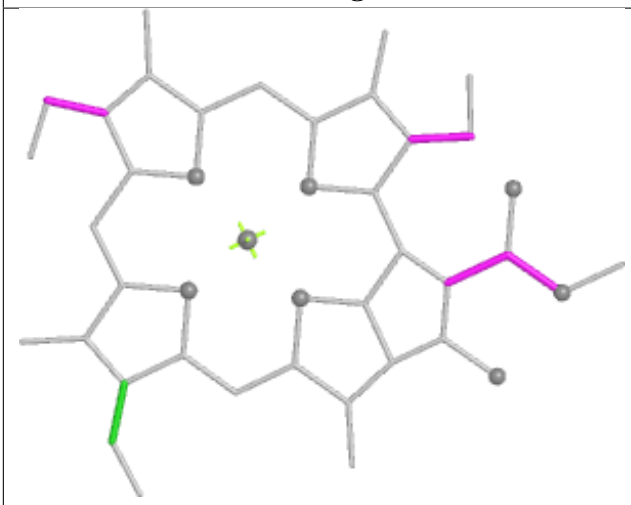
Ligand CLA J 101



Bond lengths



Bond angles

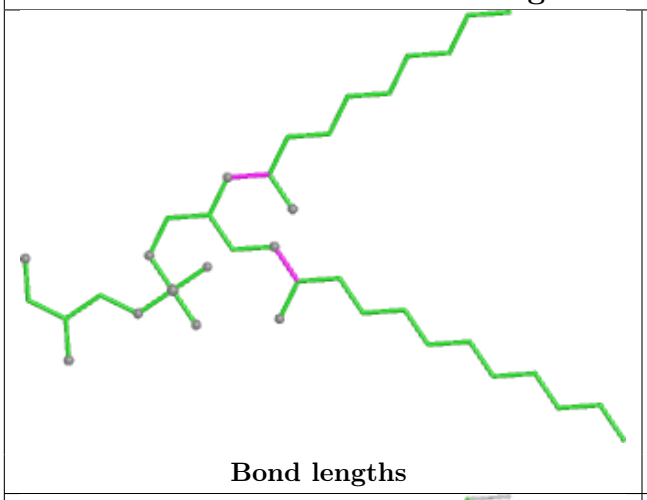


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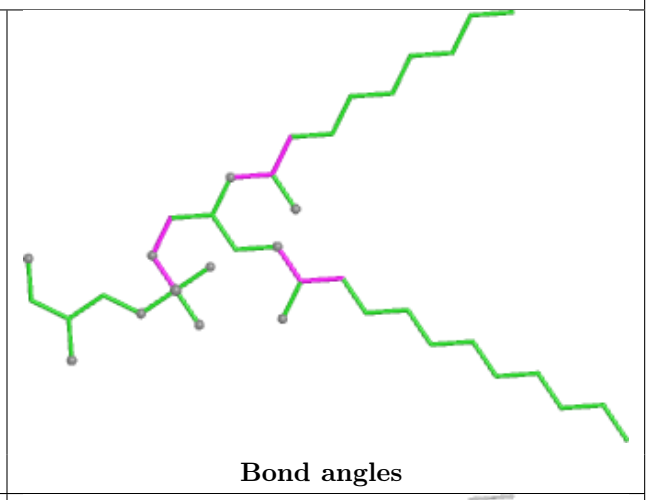


Rings

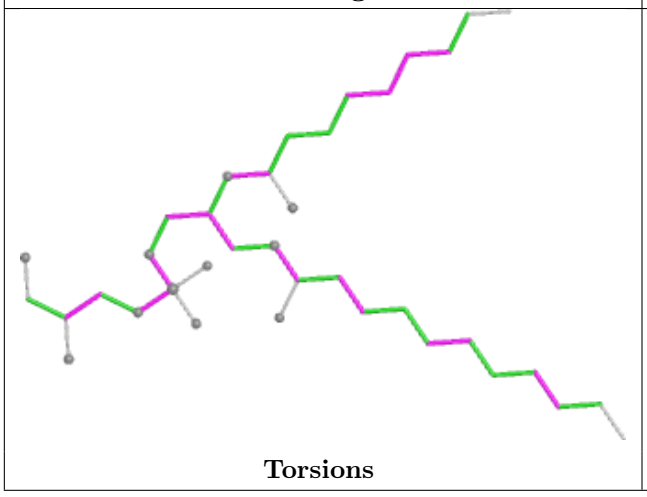
Ligand LHG 7 622



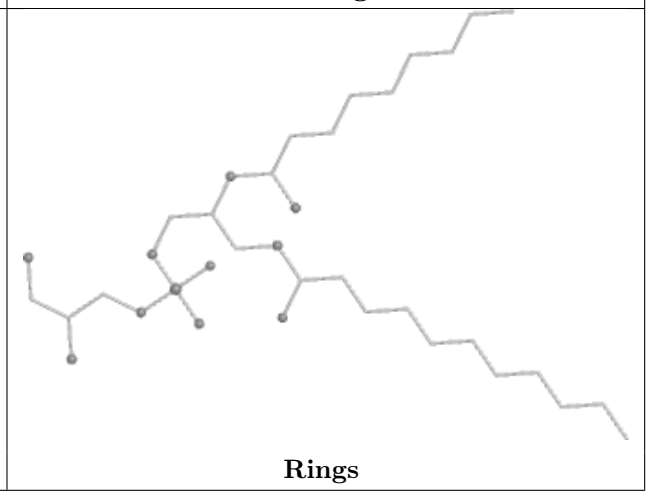
Bond lengths



Bond angles

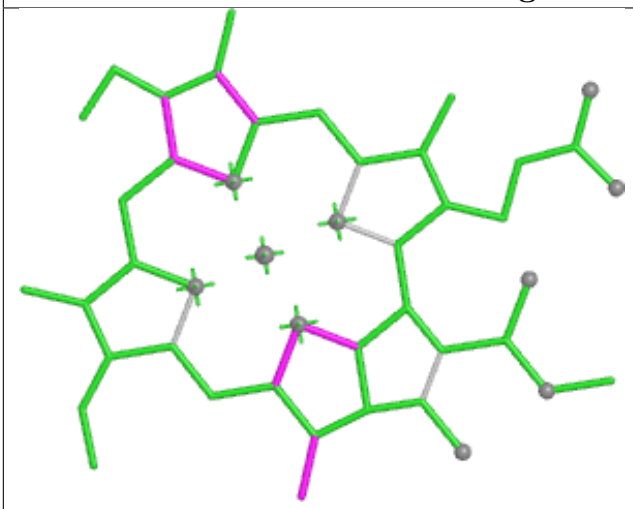


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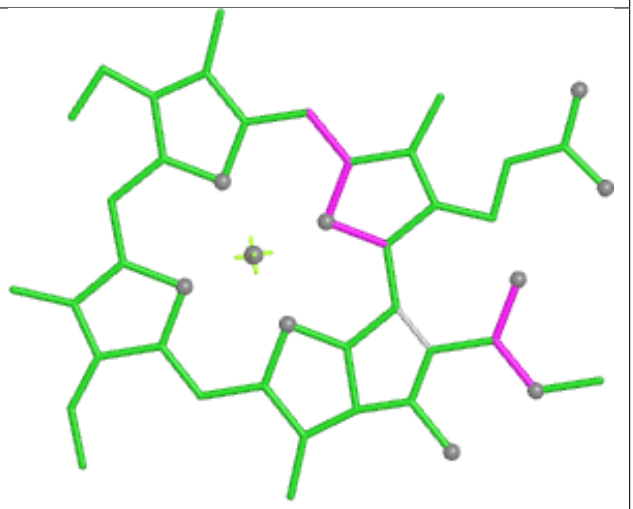


Rings

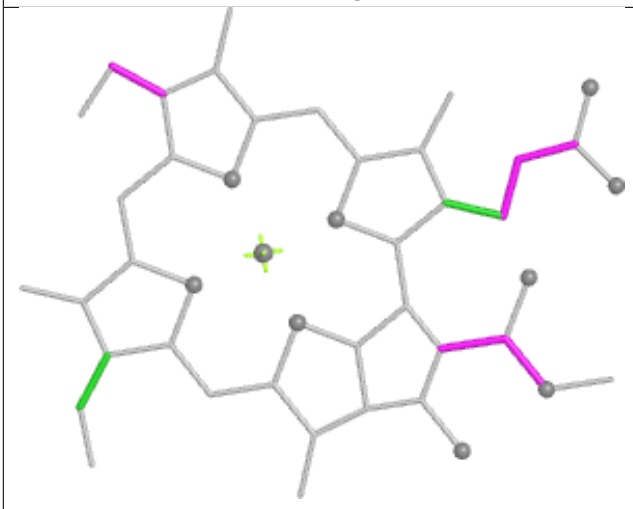
Ligand CLA W 614



Bond lengths



Bond angles

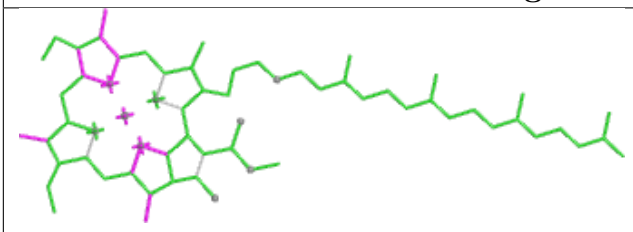


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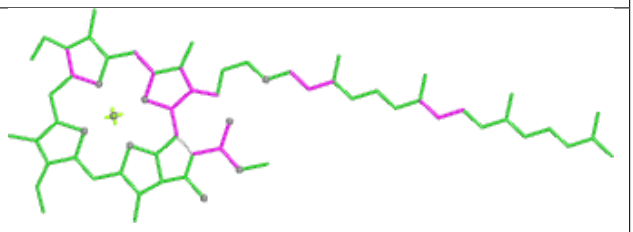


Rings

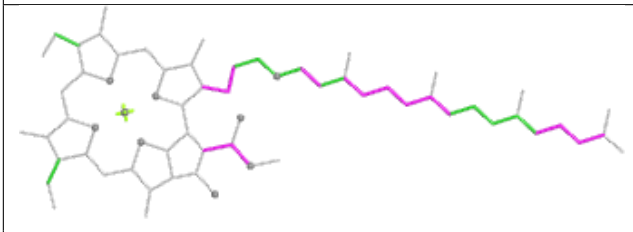
Ligand CLA B 810



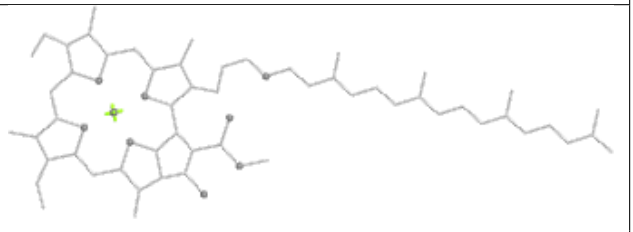
Bond lengths



Bond angles

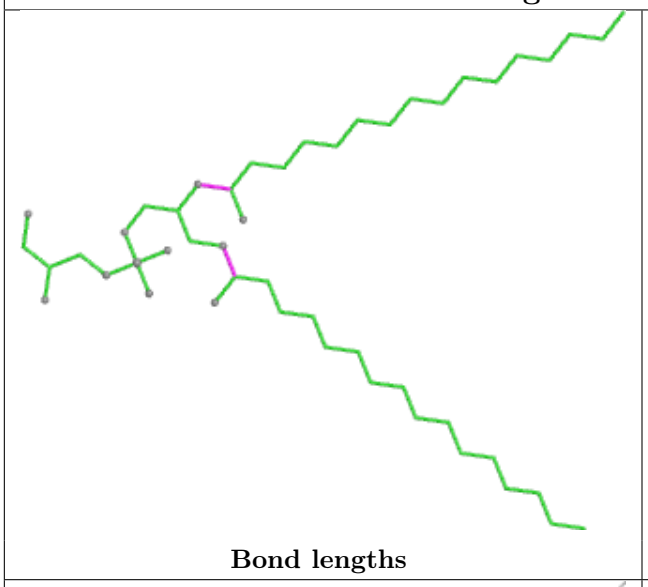


Torsions

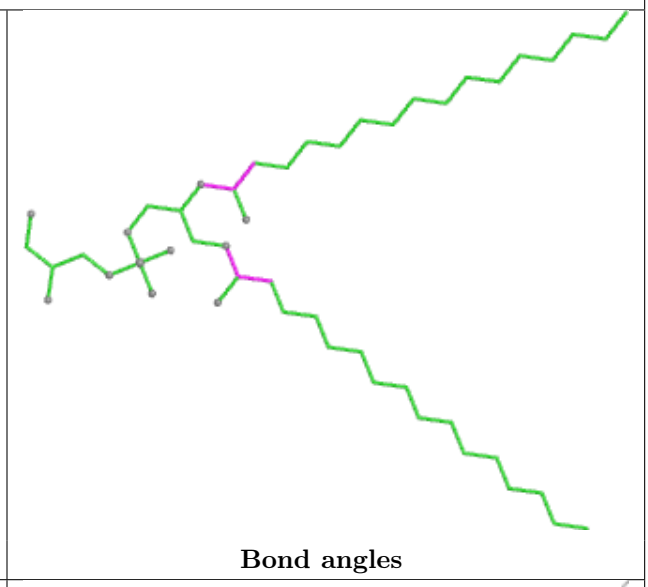


Rings

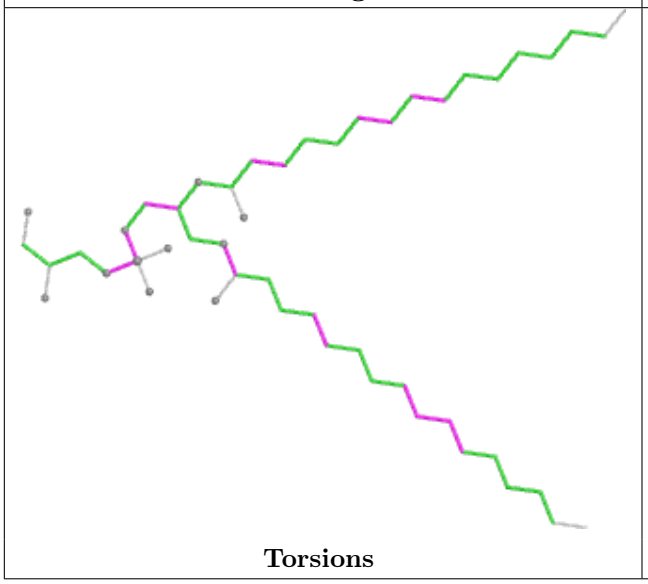
Ligand LHG A 846



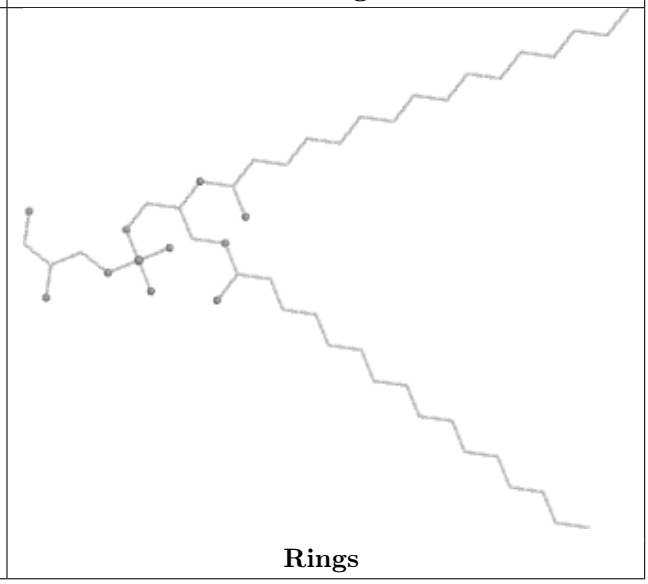
Bond lengths



Bond angles

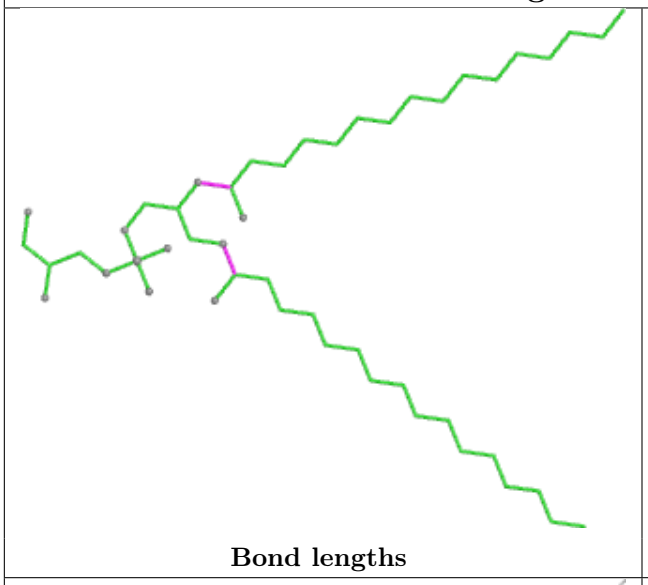


Torsions

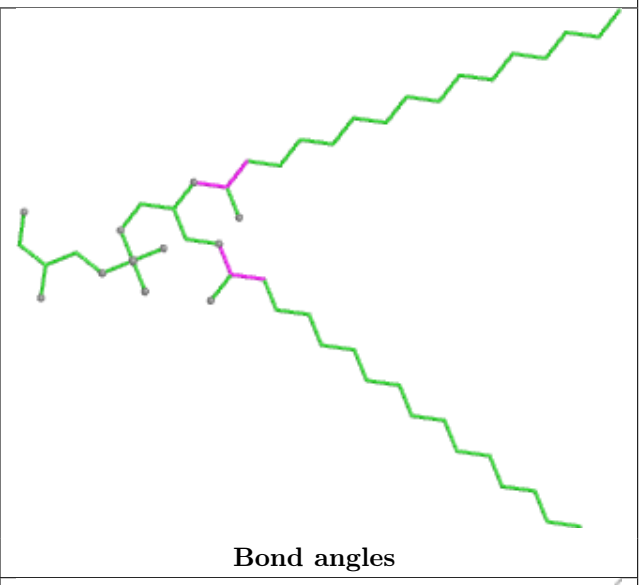


Rings

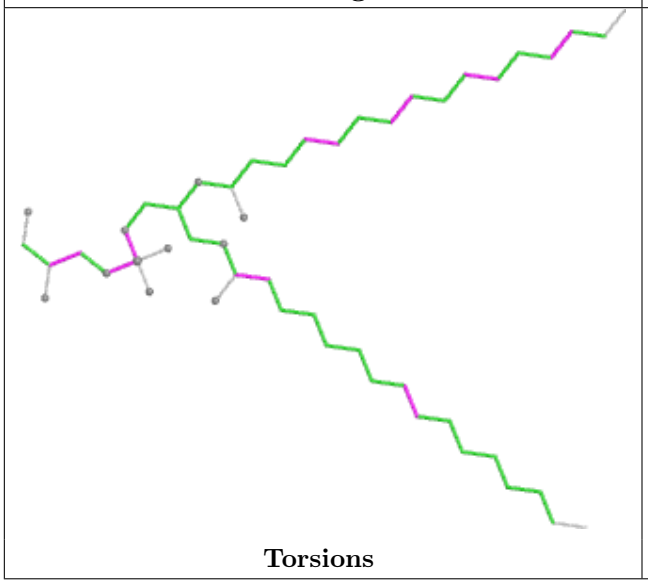
Ligand LHG 8 622



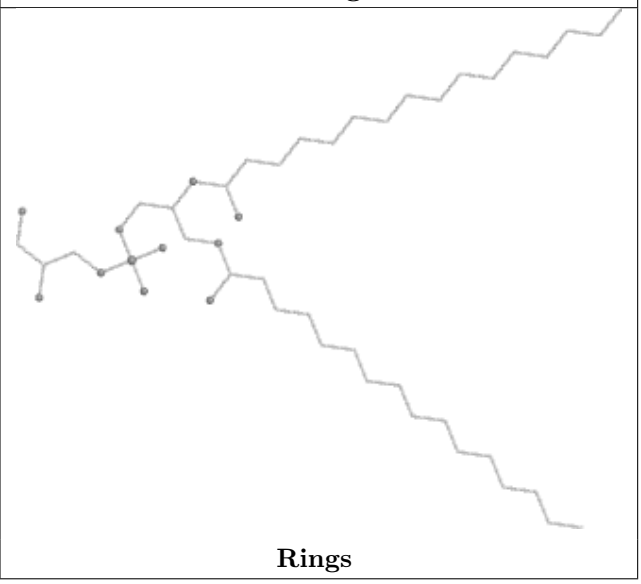
Bond lengths



Bond angles

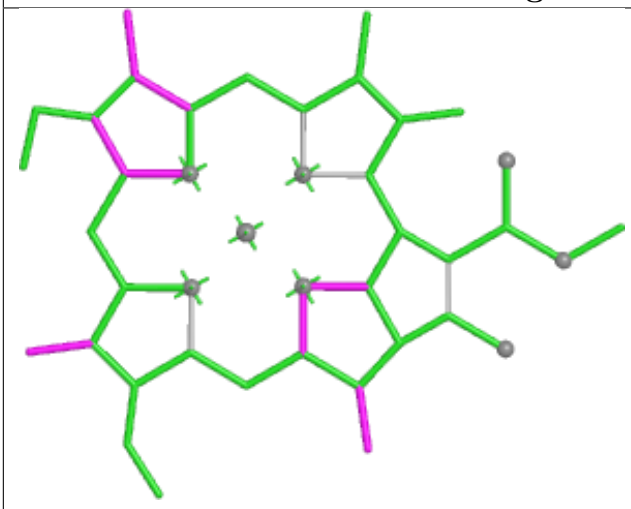


Torsions

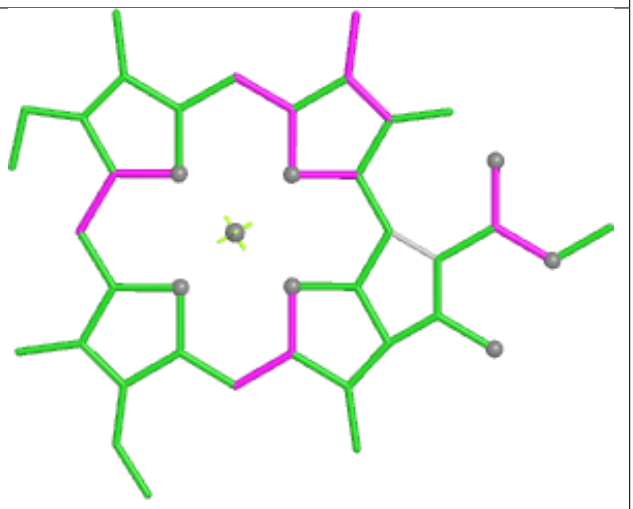


Rings

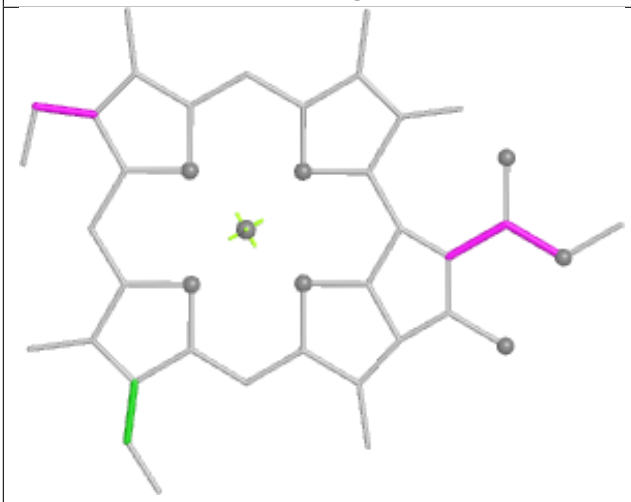
Ligand CLA F 304



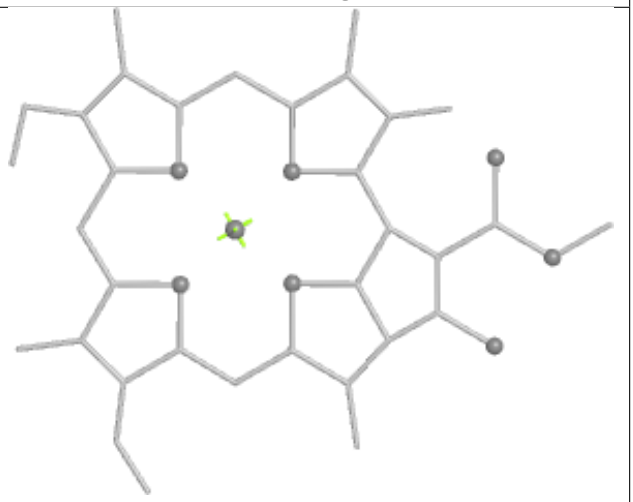
Bond lengths



Bond angles

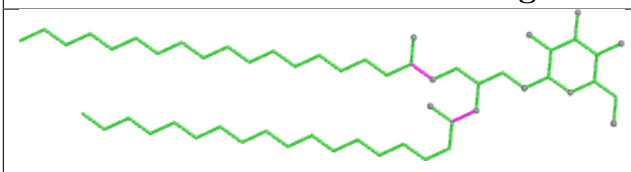


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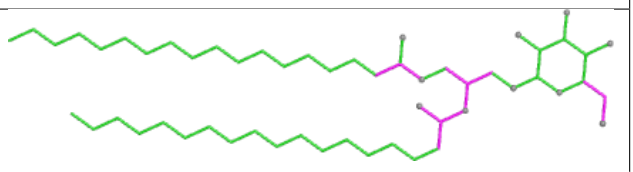


Rings

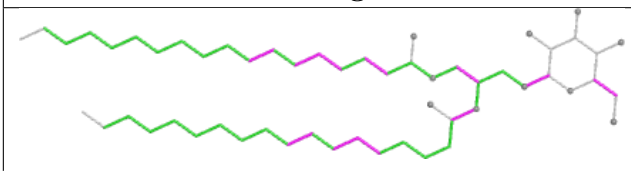
Ligand LMG H 205



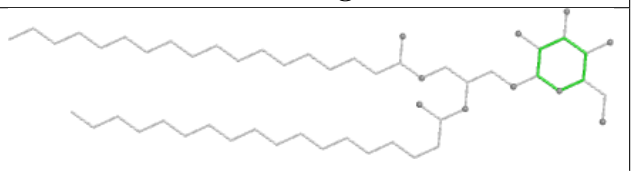
Bond lengths



Bond angles

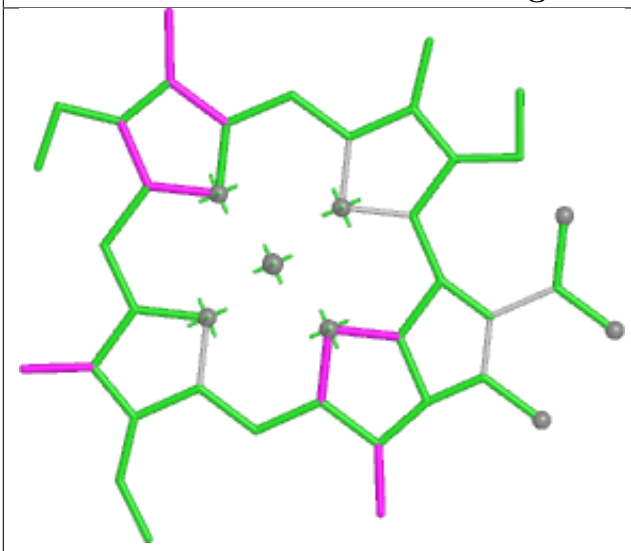


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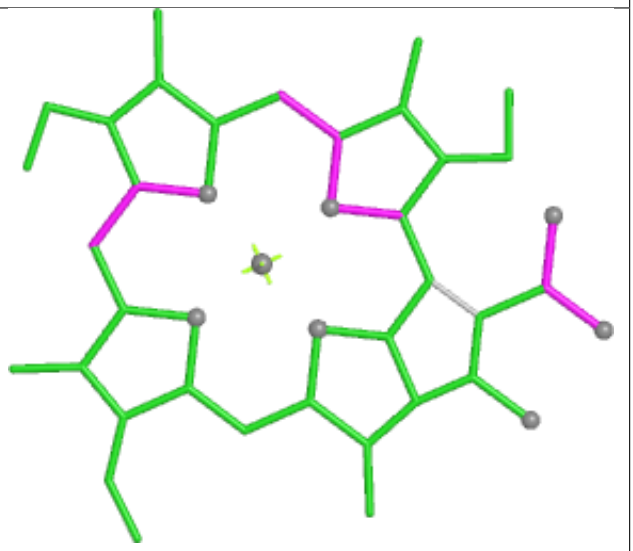


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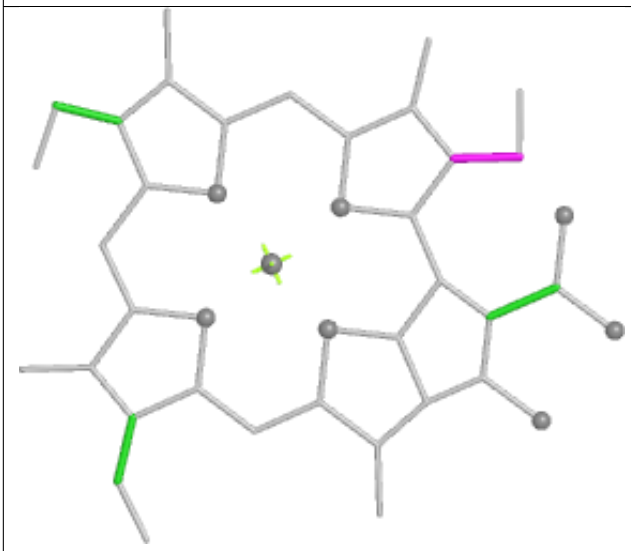
Ligand CLA 8 612



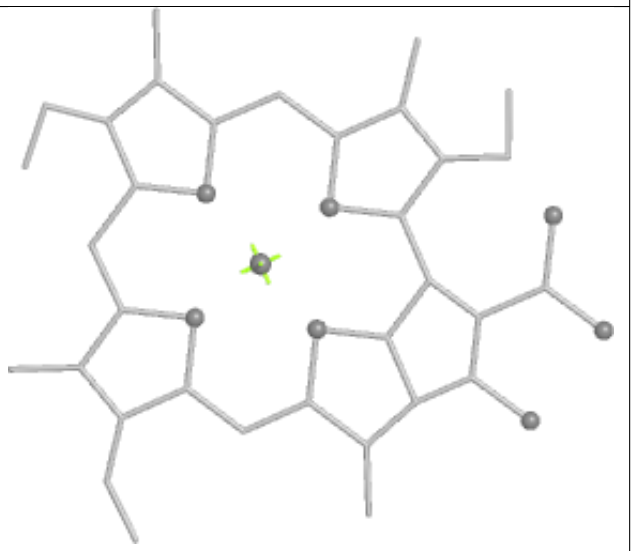
Bond lengths



Bond angles

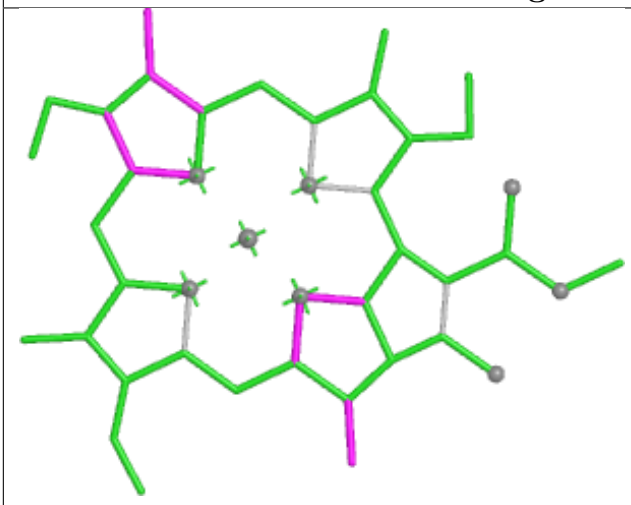


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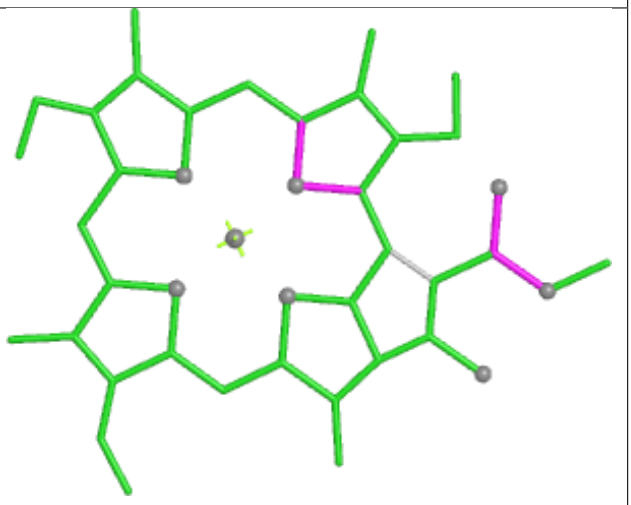


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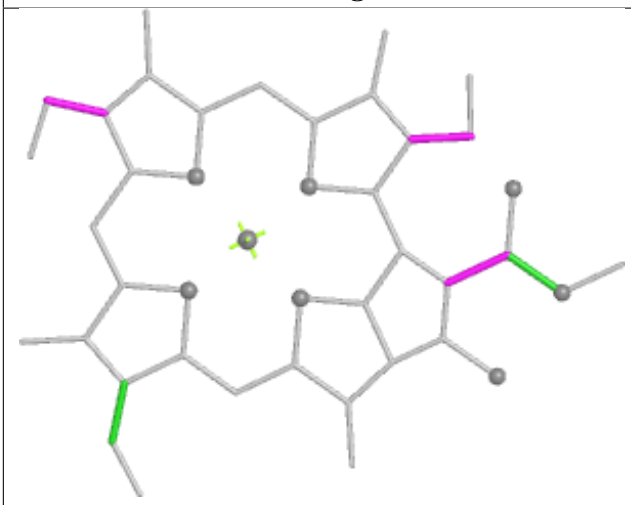
Ligand CLA 9 611



Bond lengths



Bond angles

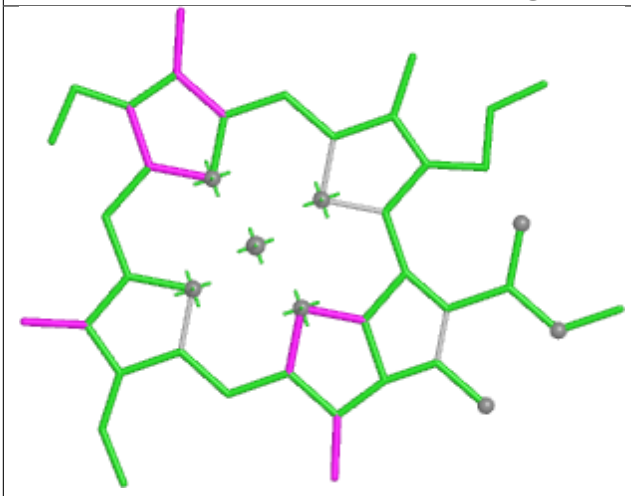


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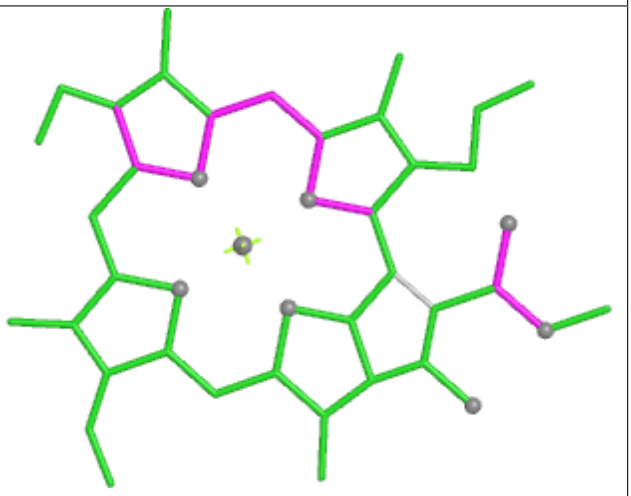


Rings

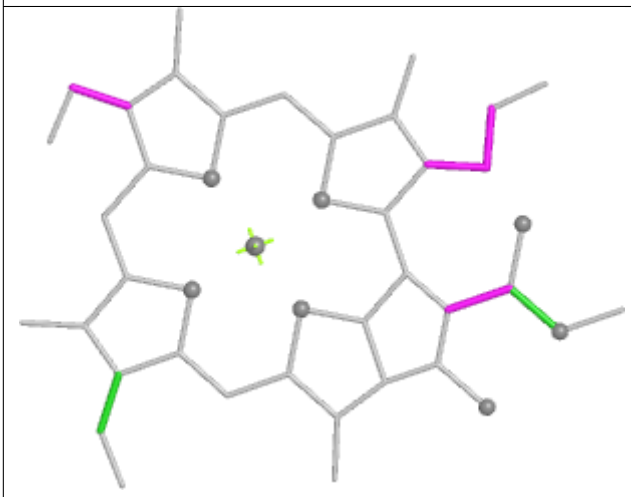
Ligand CLA B 812



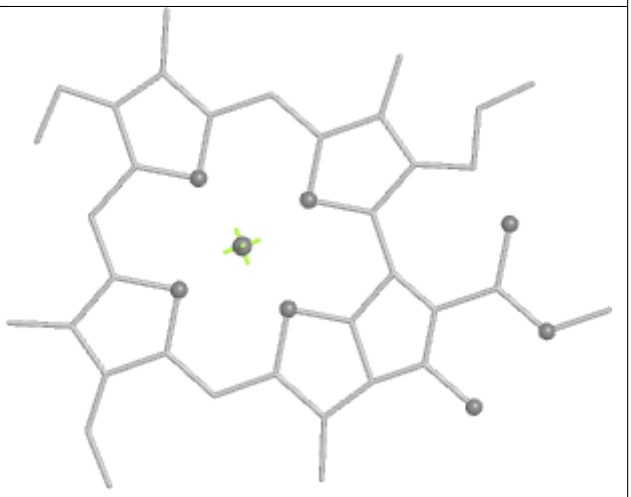
Bond lengths



Bond angles

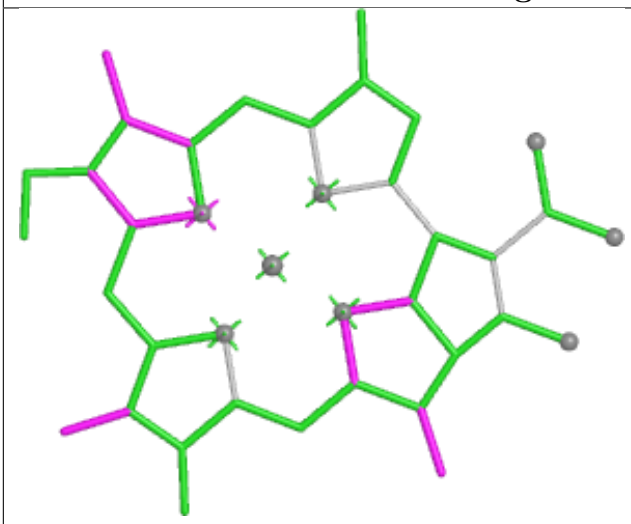


Torsions



Rings

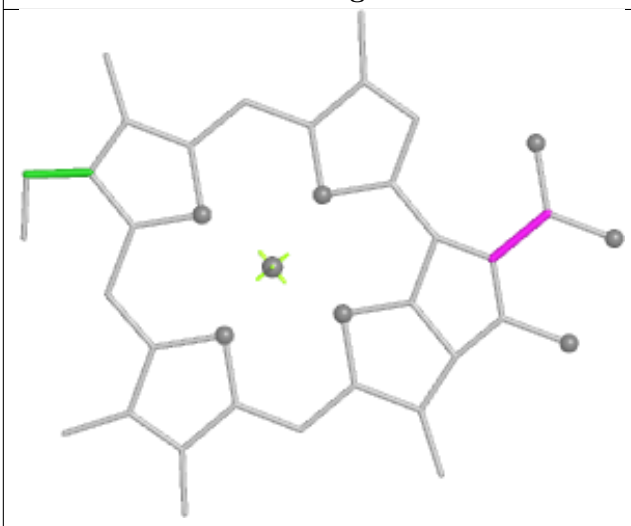
Ligand CLA O 2001



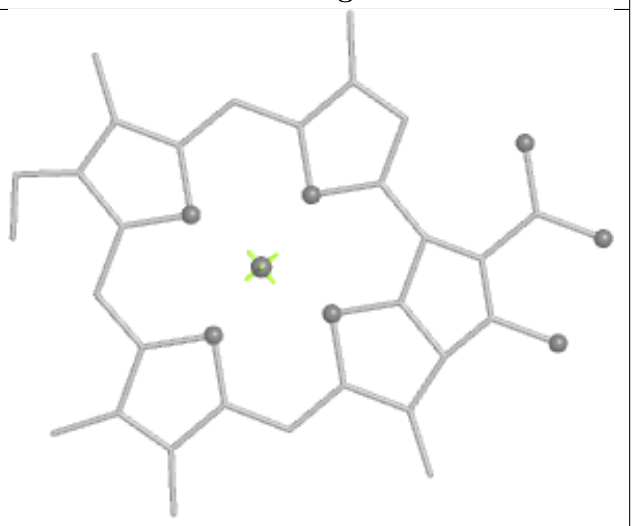
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Bond angles

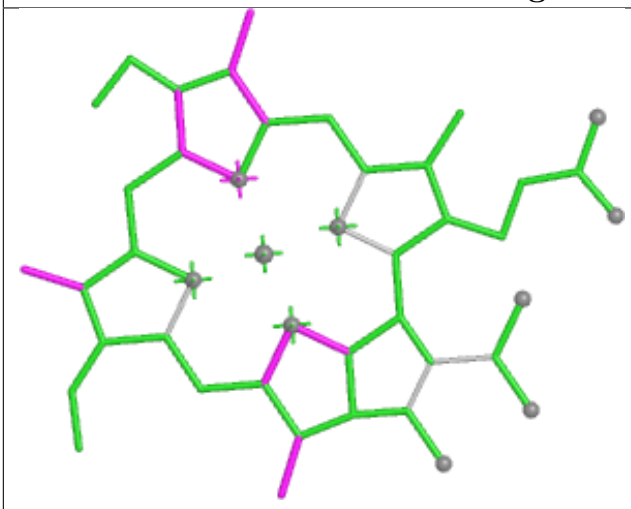


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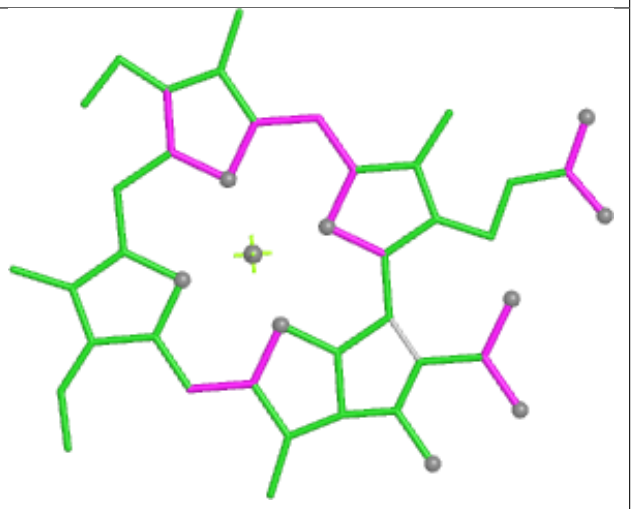


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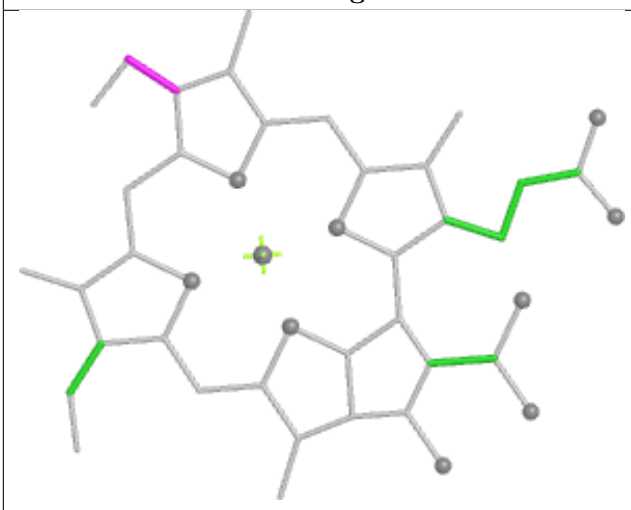
Ligand CLA 2 607



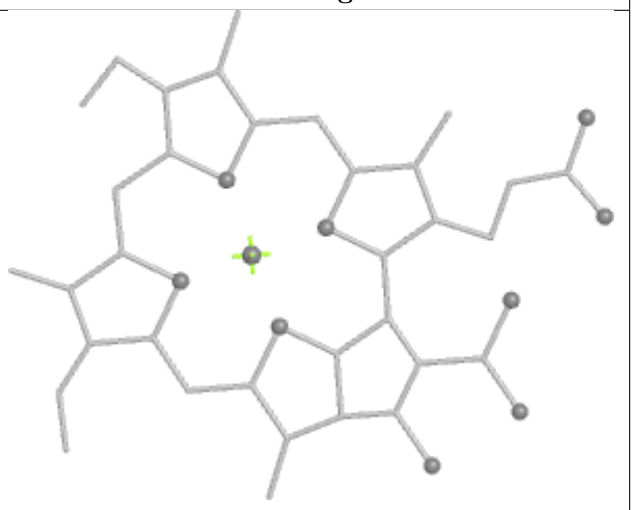
Bond lengths



Bond angles

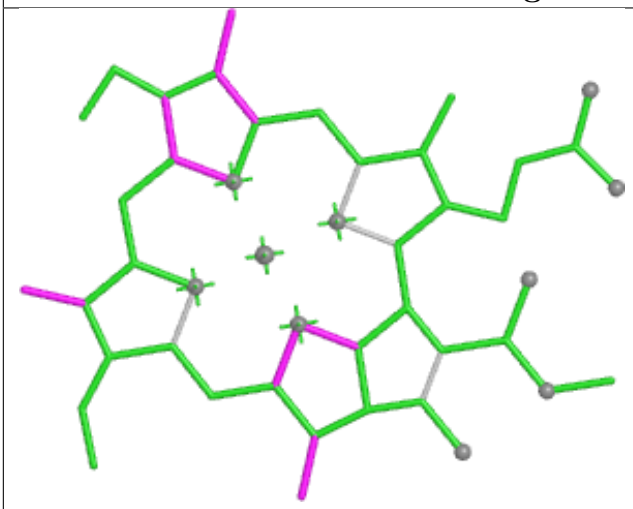


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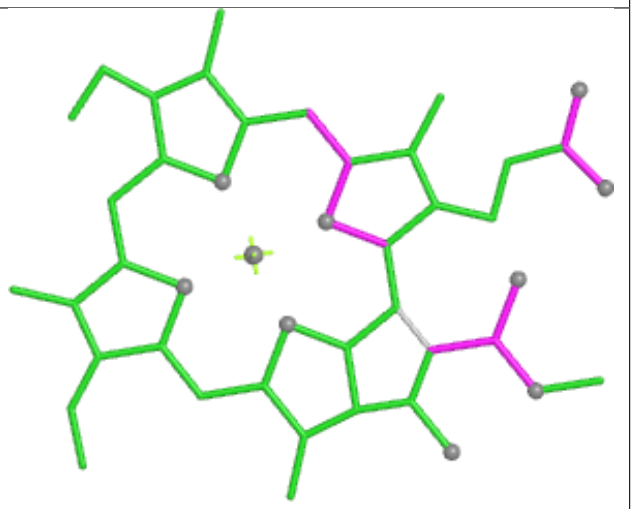


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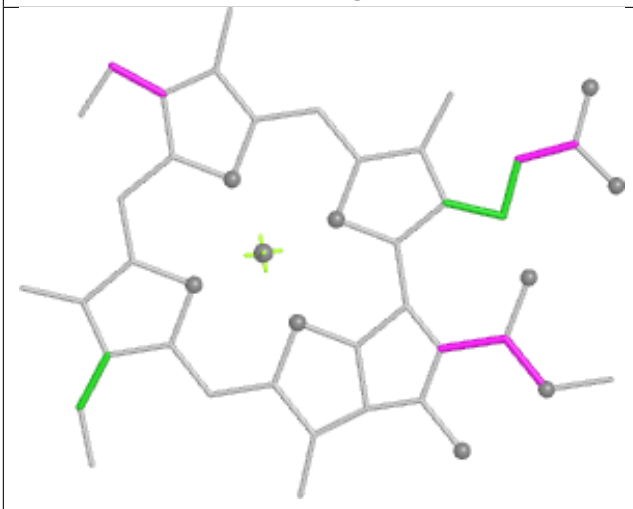
Ligand CLA V 612



Bond lengths



Bond angles

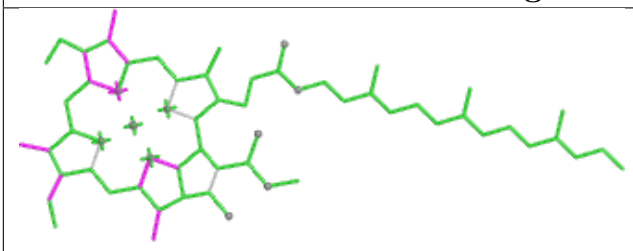


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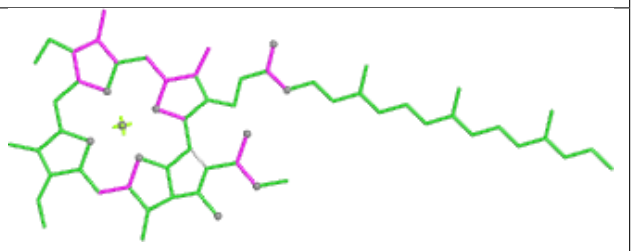


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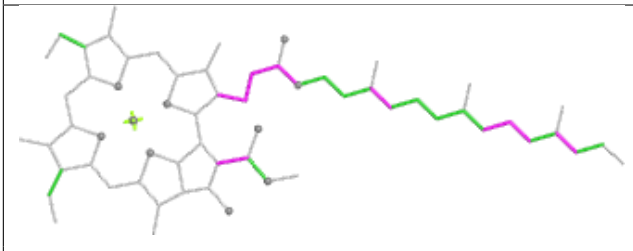
Ligand CLA B 827



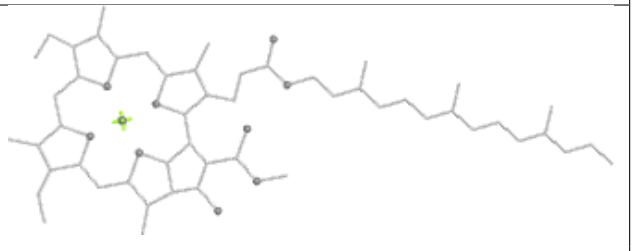
Bond lengths



Bond angles

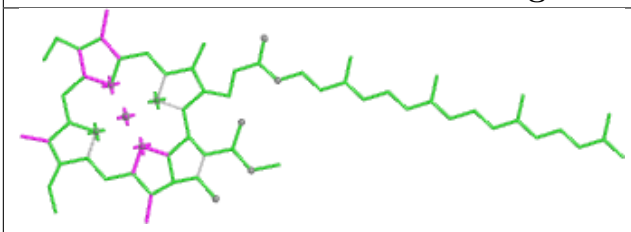


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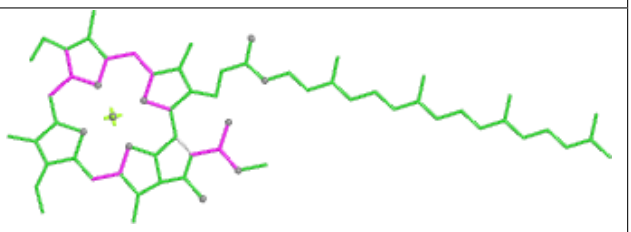


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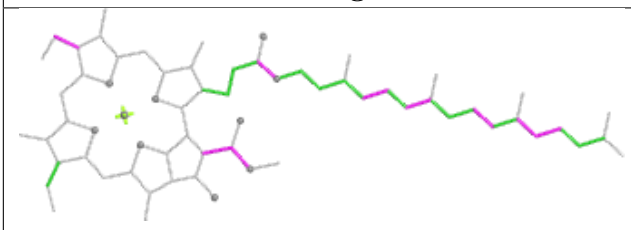
Ligand CLA 5 607



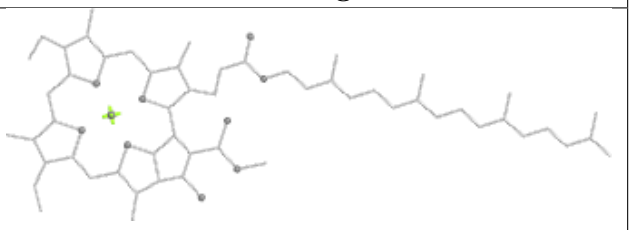
Bond lengths



Bond angles

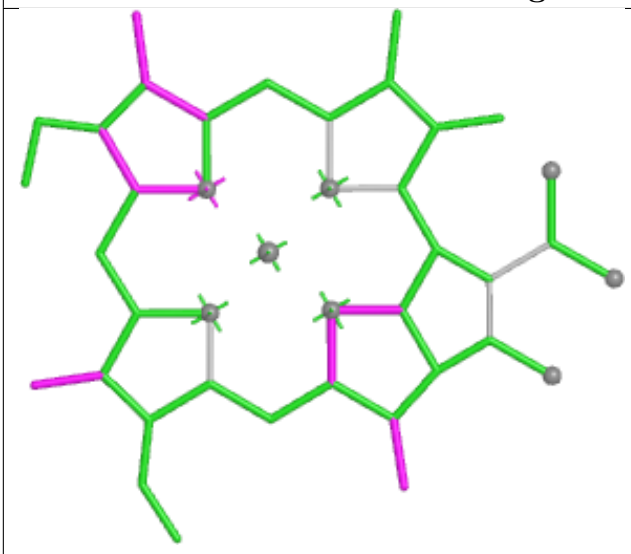


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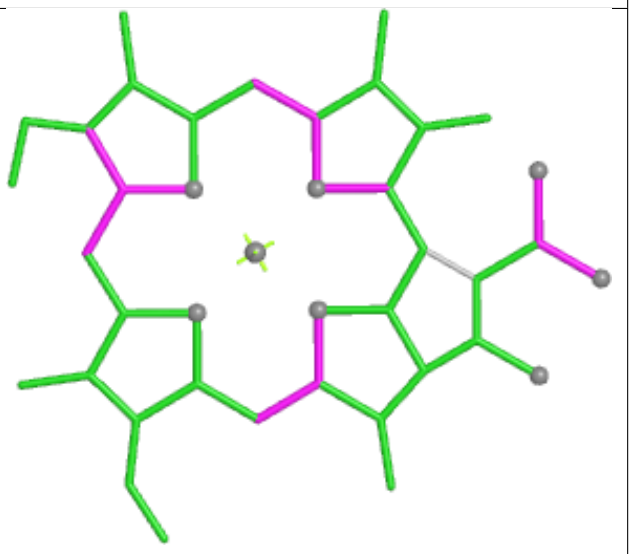


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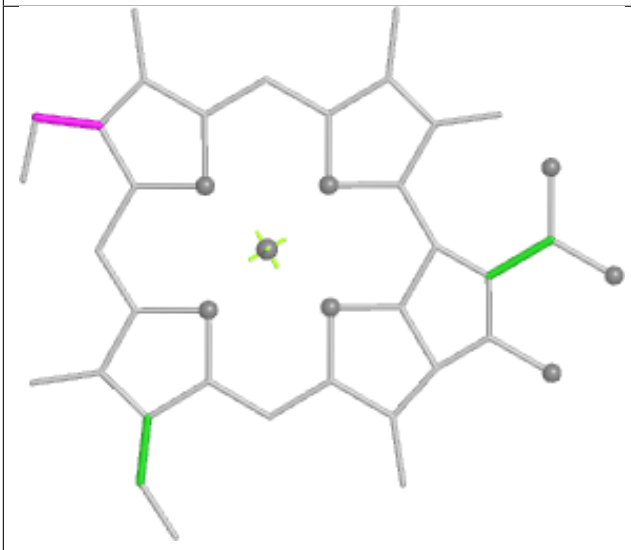
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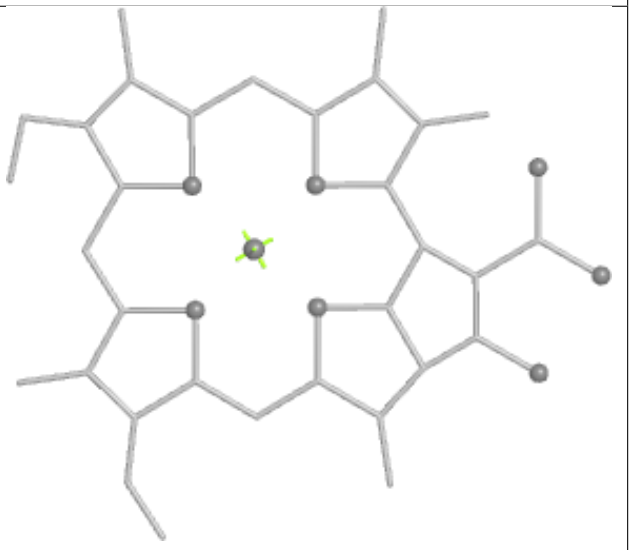
Bond lengths



Bond angles

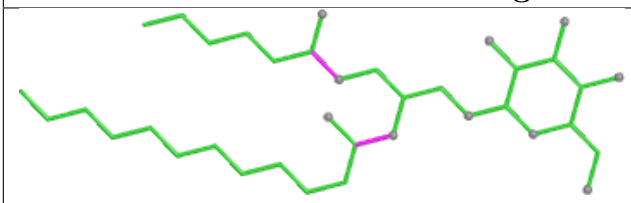


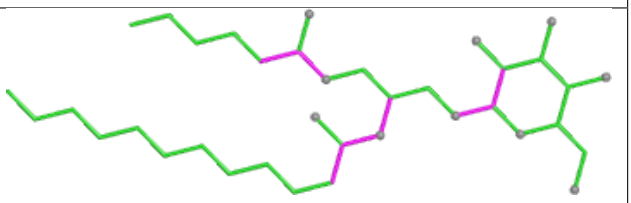
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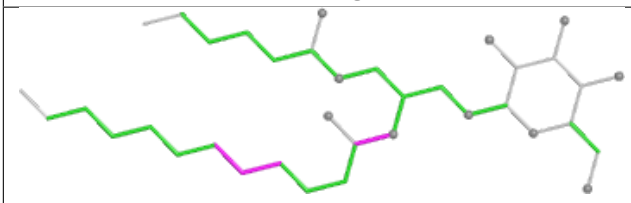


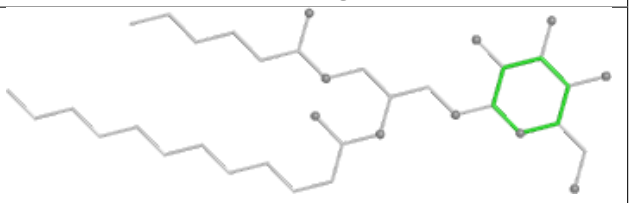
Rings

Ligand LMG L 2631

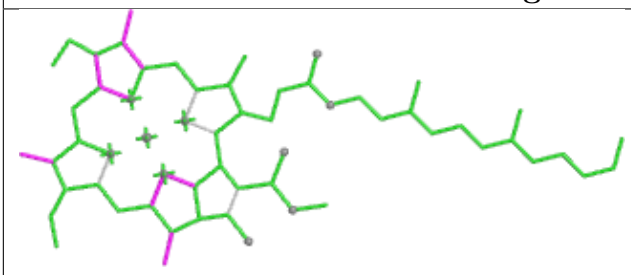

Bond lengths

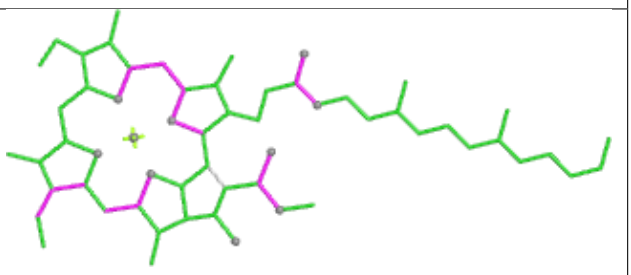

Bond angles

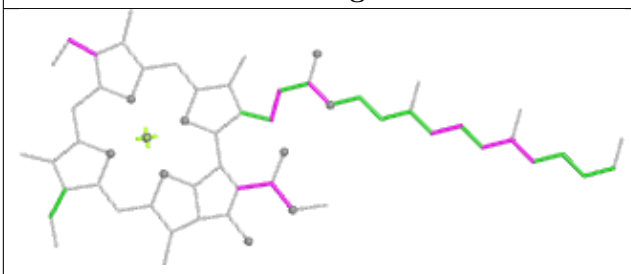

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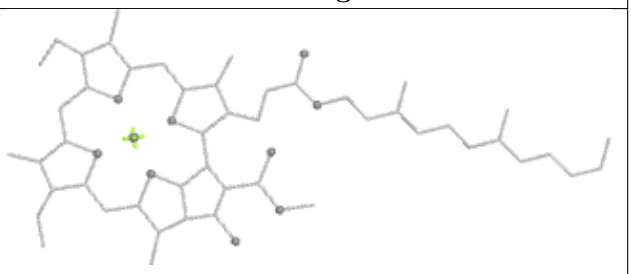

Rings

Ligand CLA U 613

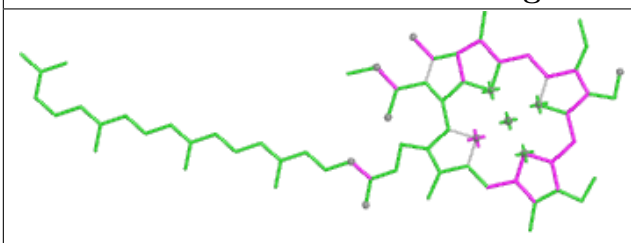

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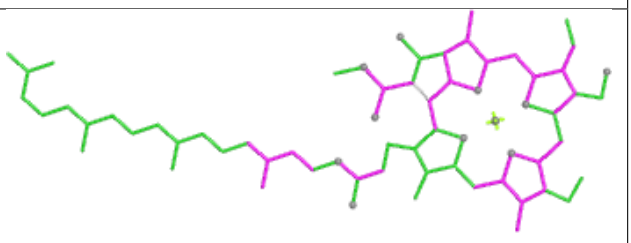

Bond angles

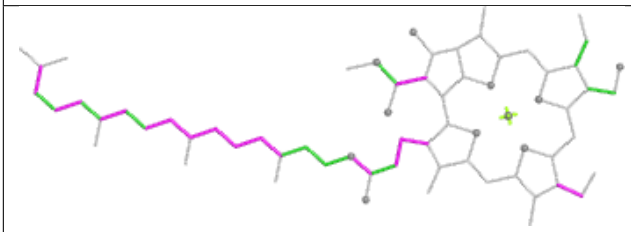

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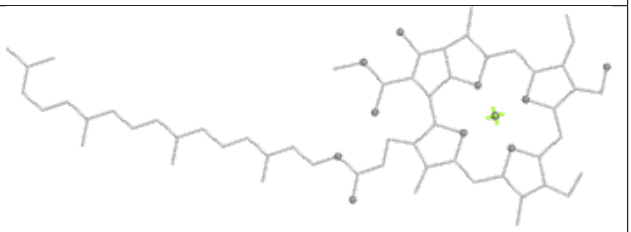

Rings

Ligand CHL Y 601

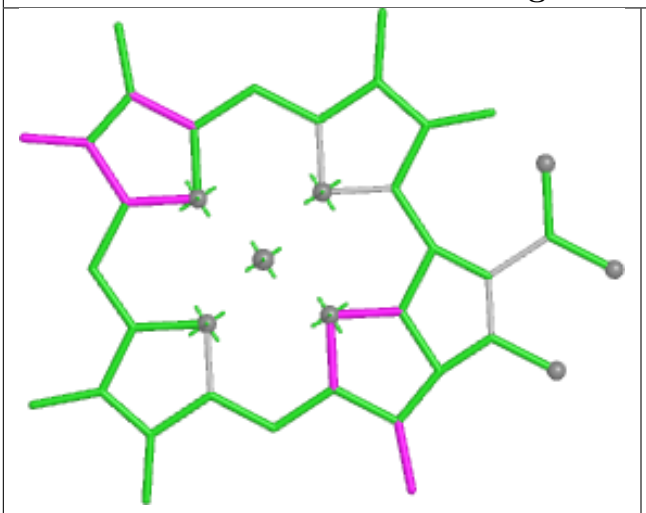

Bond lengths


Bond angles

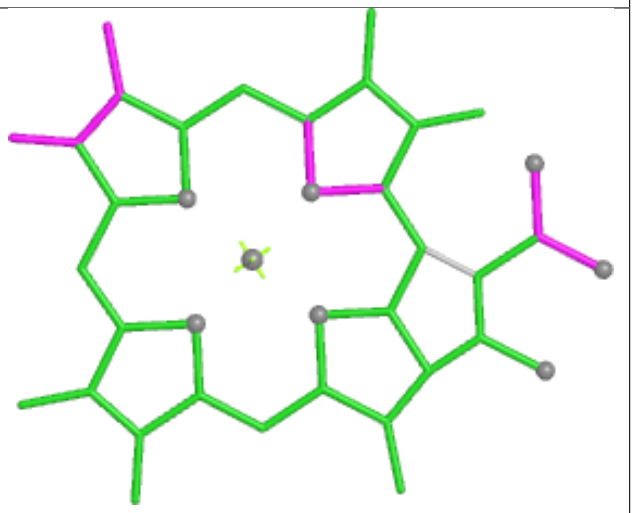

Torsions


Rings

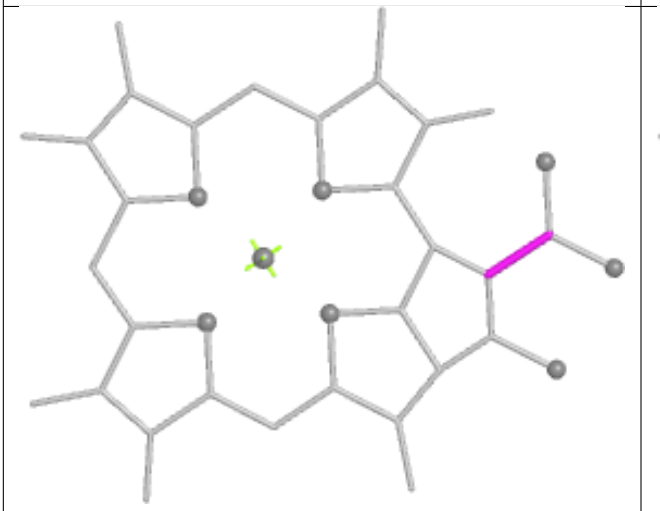
Ligand CLA 3 611



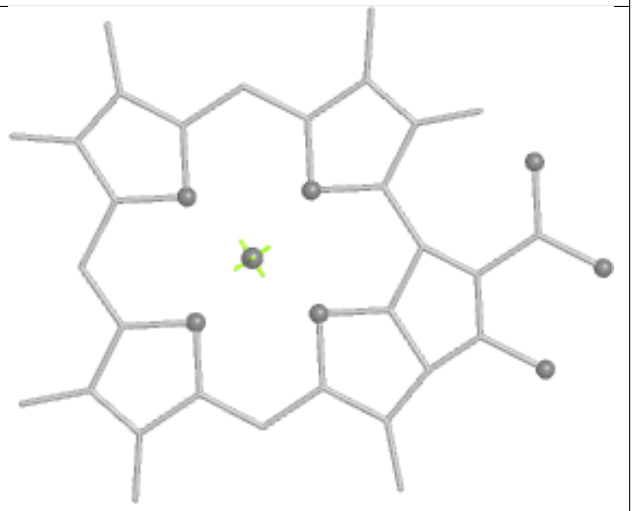
Bond lengths



Bond angles

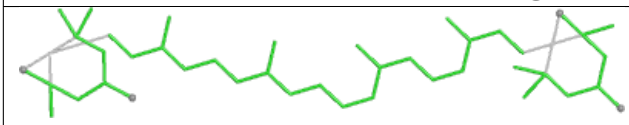


Torsions

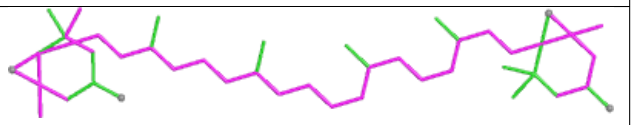


Rings

Ligand XAT 1 618



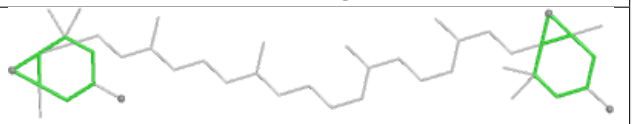
Bond lengths



Bond angles

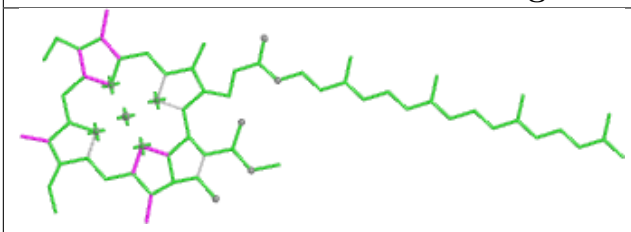


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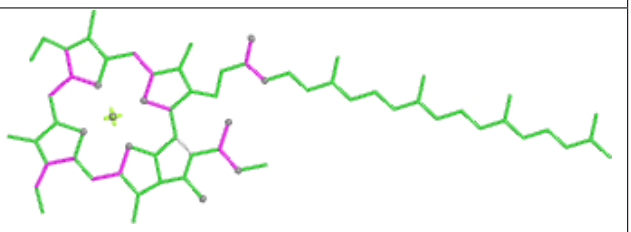


Rings

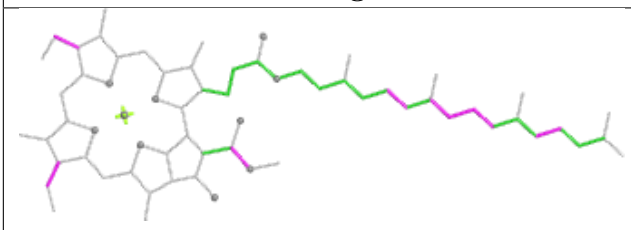
Ligand CLA 4 608



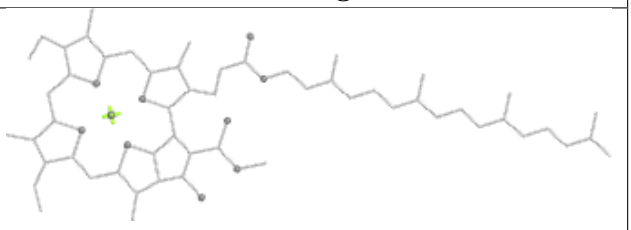
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Bond angles

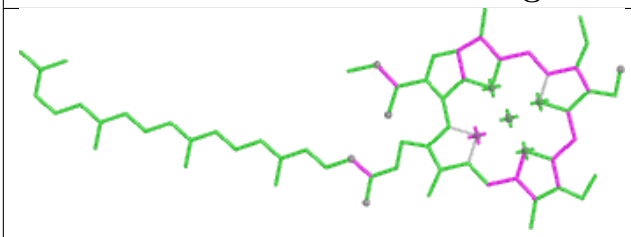


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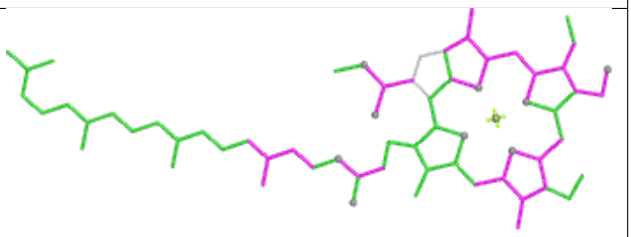


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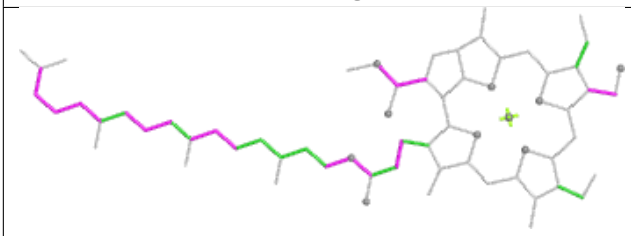
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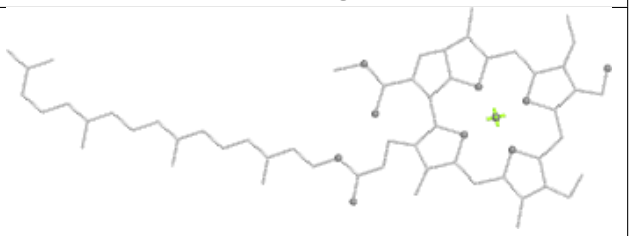
Bond lengths



Bond angles

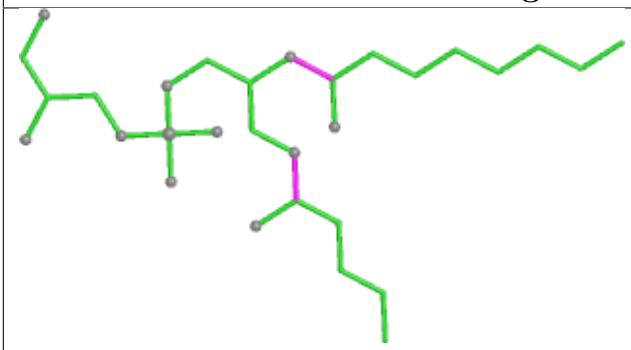


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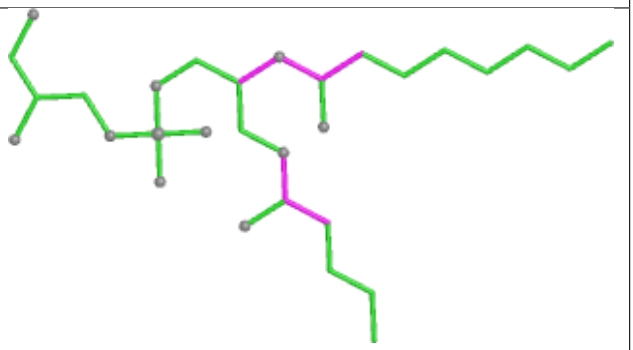


Rings

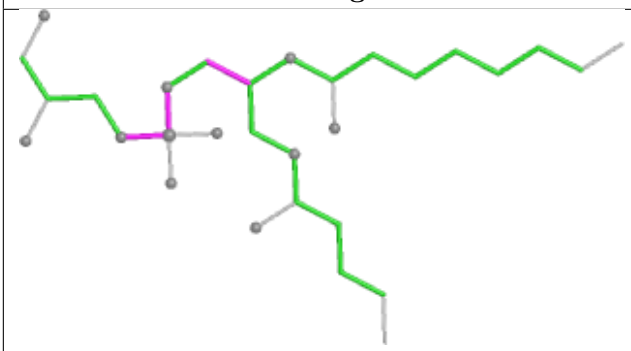
Ligand LHG A 847



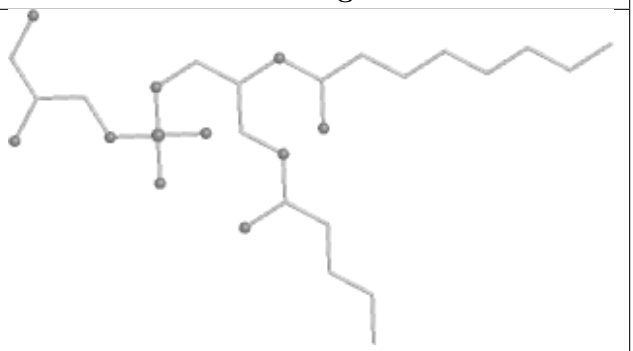
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Bond angles

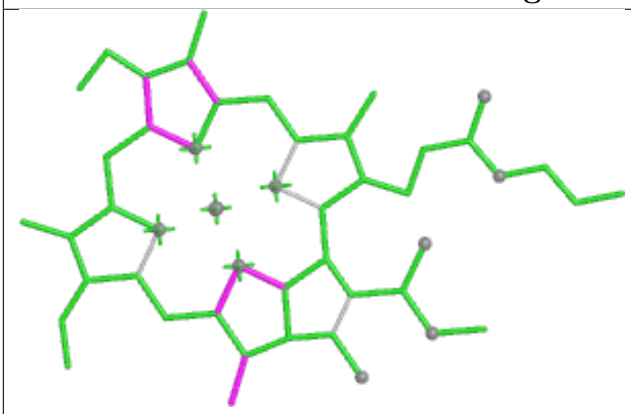


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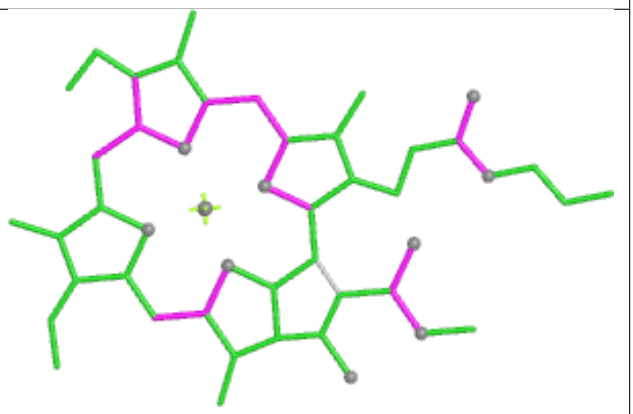


Rings

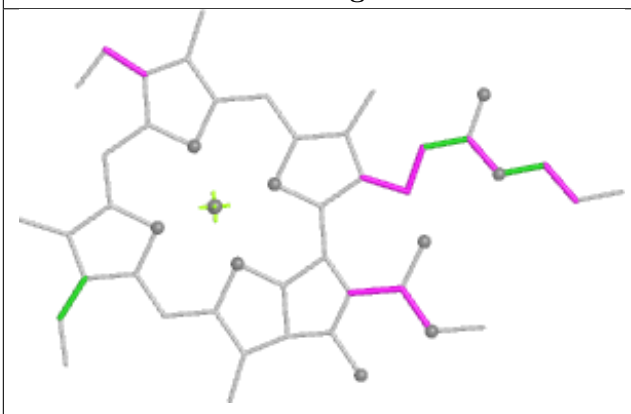
Ligand CLA Y 614



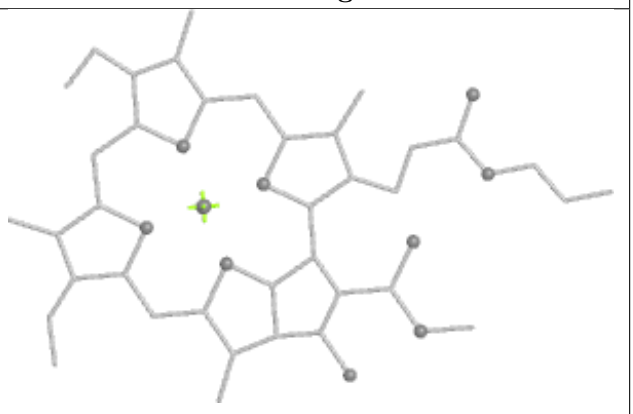
Bond lengths



Bond angles

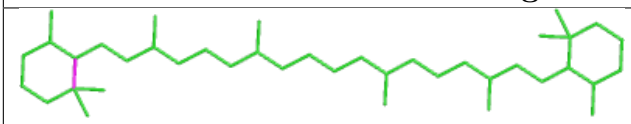


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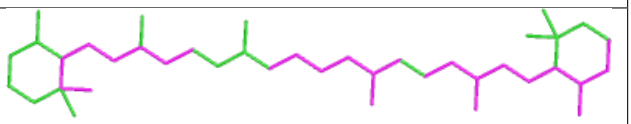


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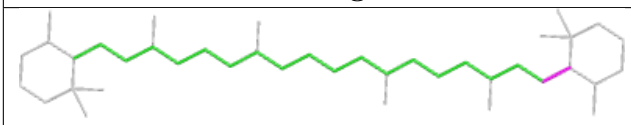
Ligand BCR G 205



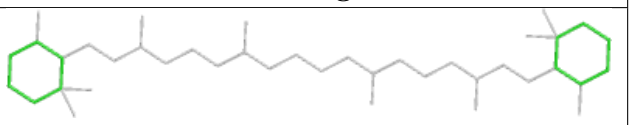
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Bond angles

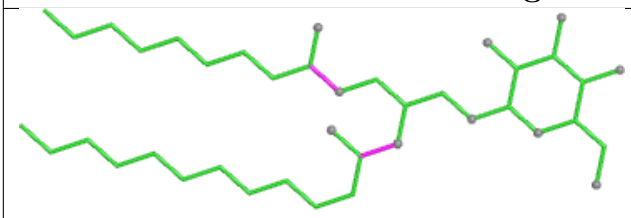


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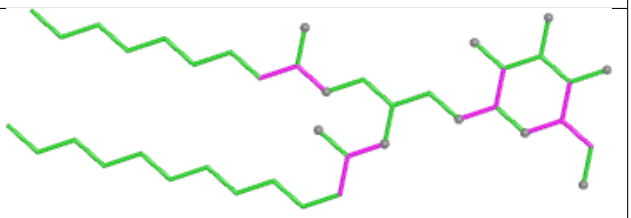


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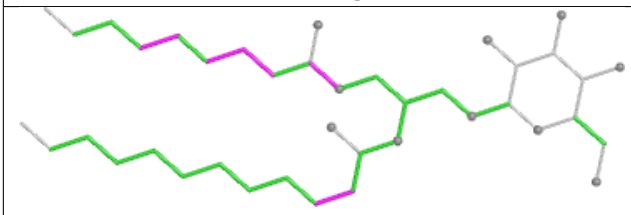
Ligand LMG 4 623



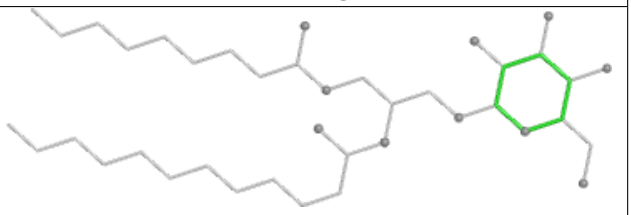
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Bond angles

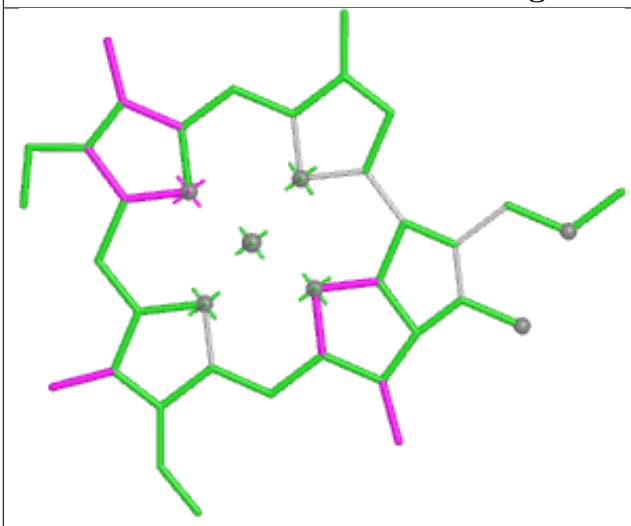


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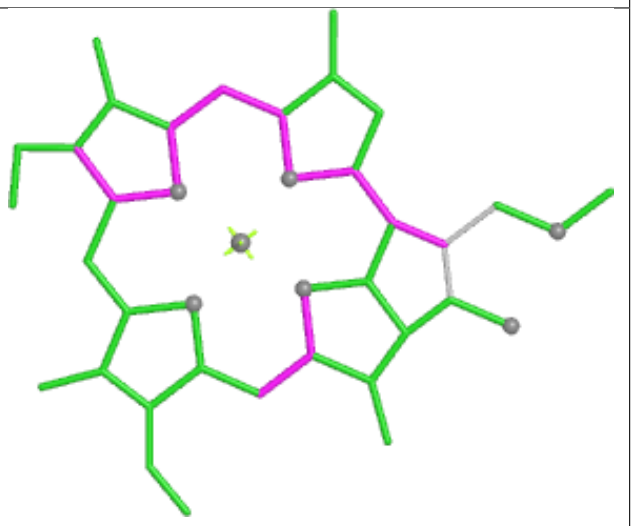


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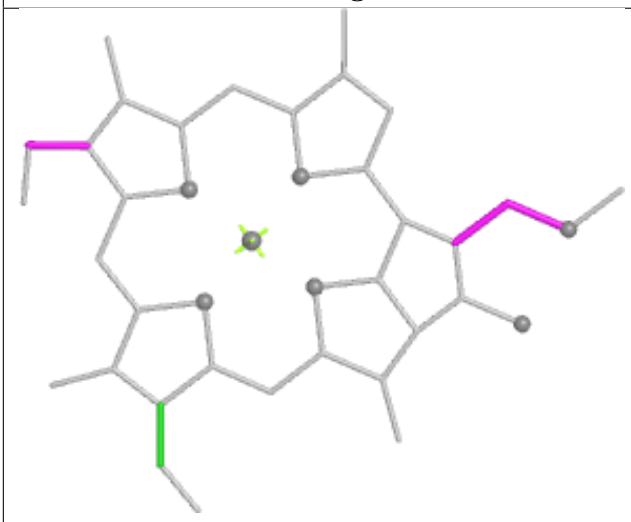
Ligand CLA 1 606



Bond lengths



Bond angles

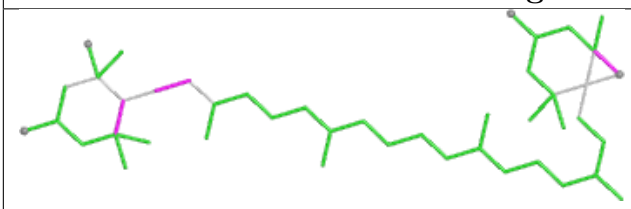


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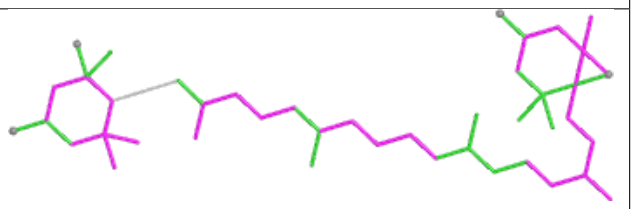


Rings

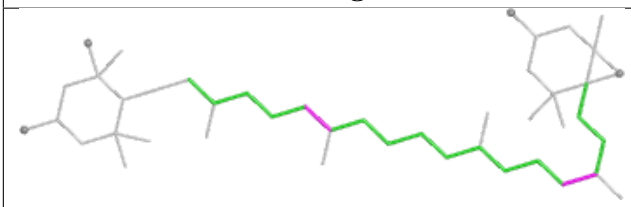
Ligand NEX 6 624



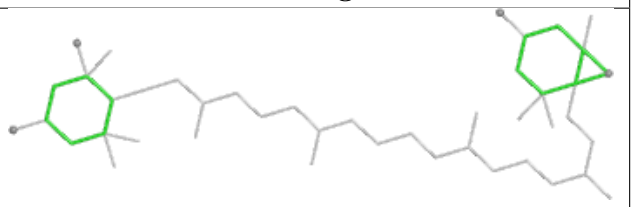
Bond lengths



Bond angles

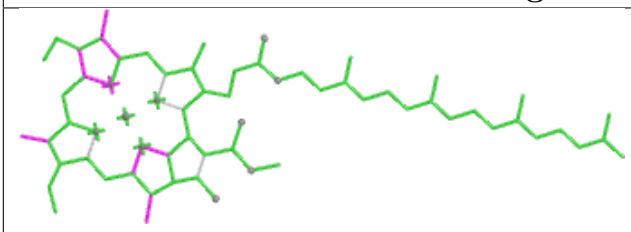


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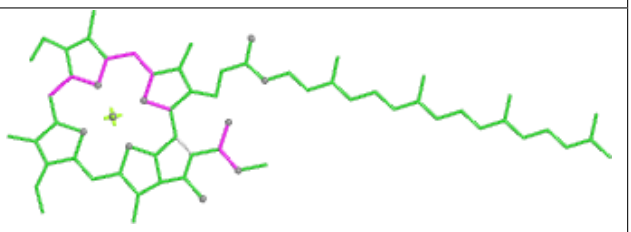


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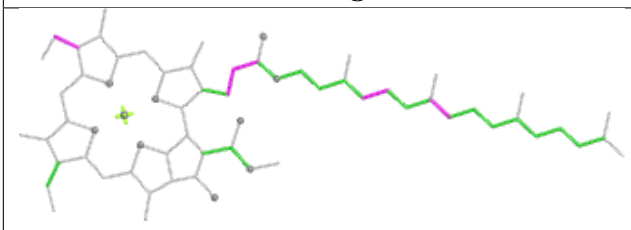
Ligand CLA Z 613



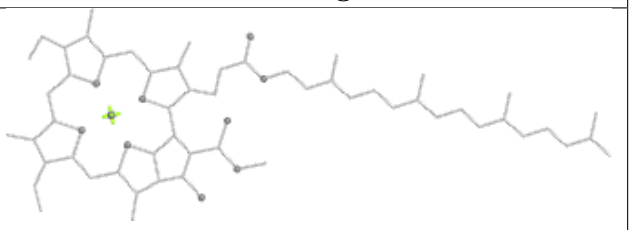
Bond lengths



Bond angles

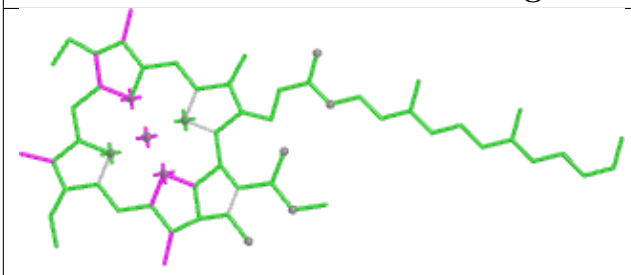


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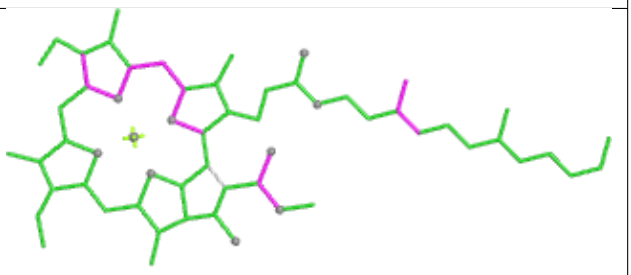


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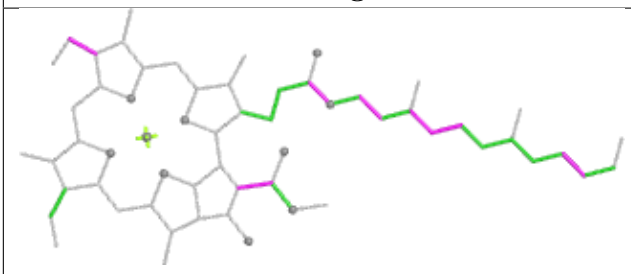
Ligand CLA B 817



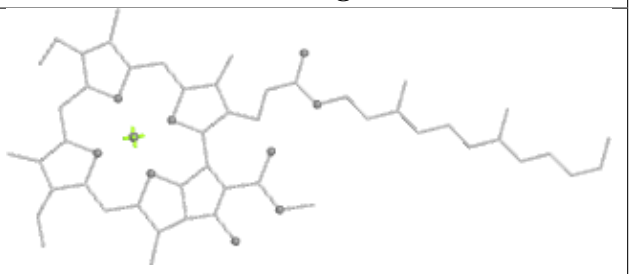
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Bond angles

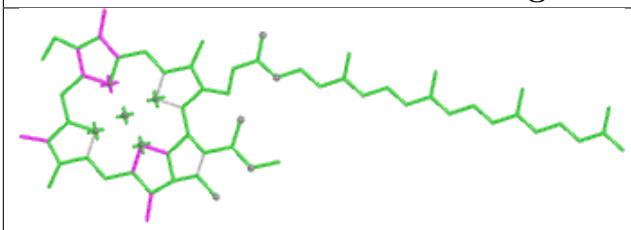


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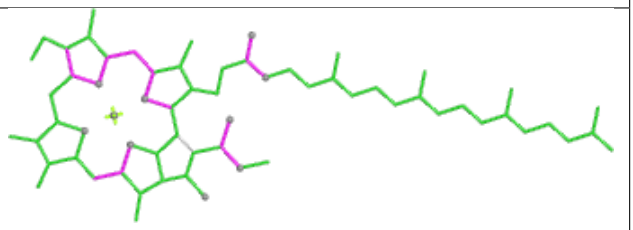


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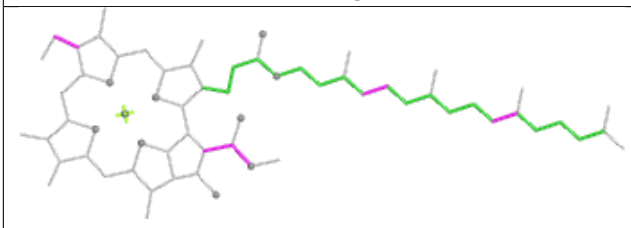
Ligand CLA 8 606



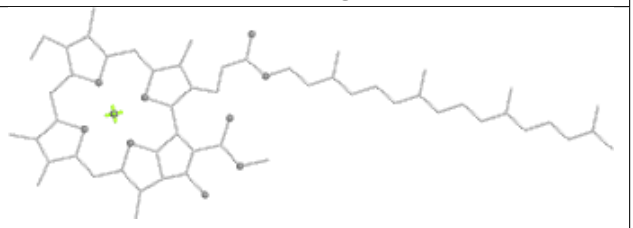
Bond lengths



Bond angles



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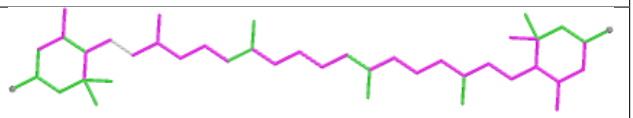


Rings

Ligand LUT 5 620



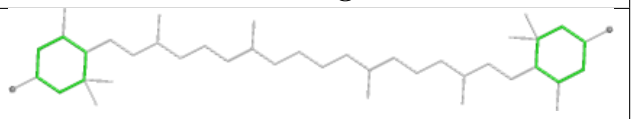
Bond lengths



Bond angles

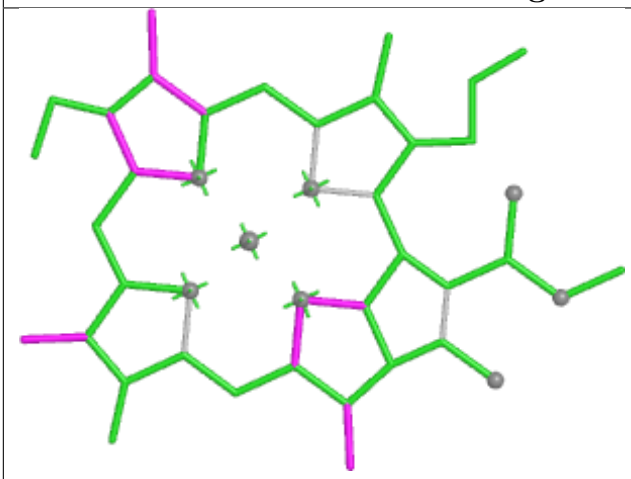


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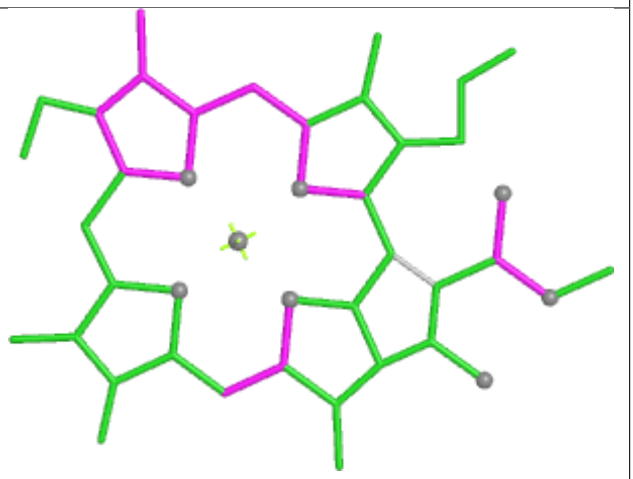


Rings

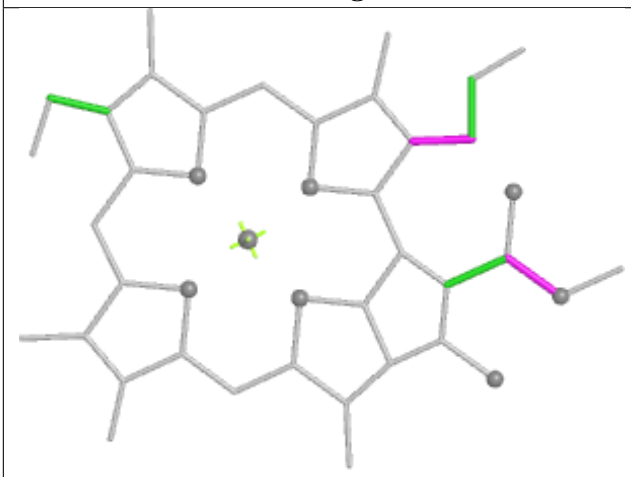
Ligand CLA 2 604



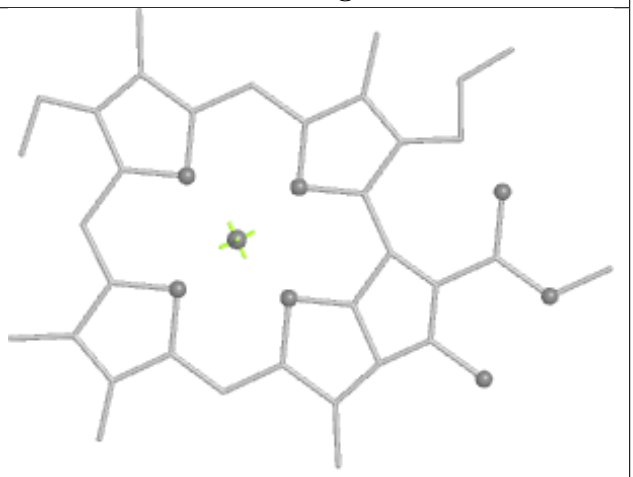
Bond lengths



Bond angles

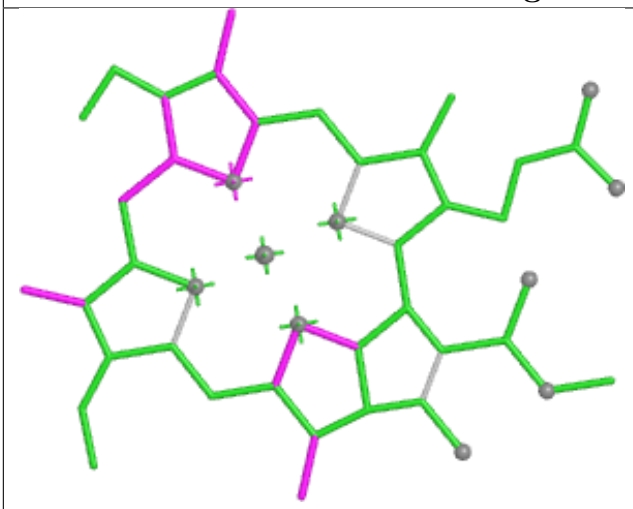


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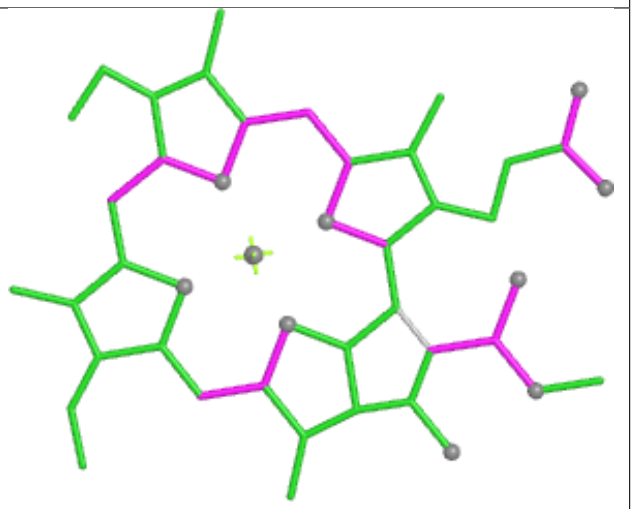


Rings

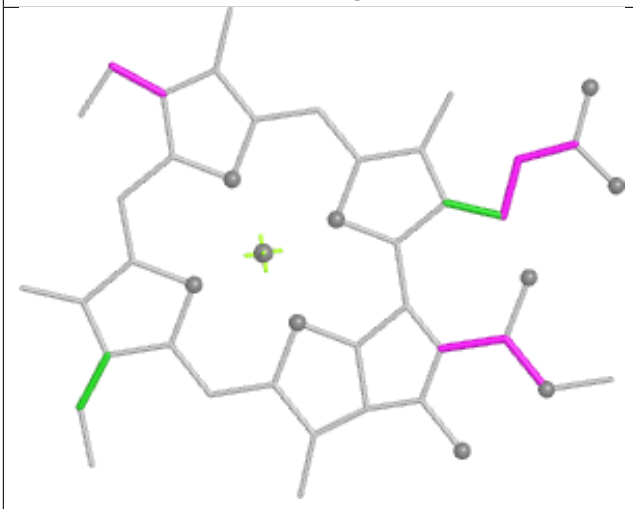
Ligand CLA A 837



Bond lengths



Bond angles

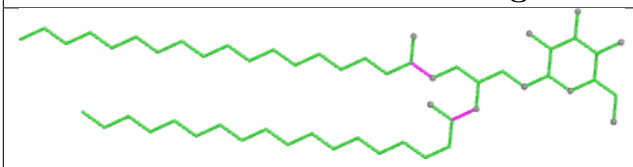


Torsions

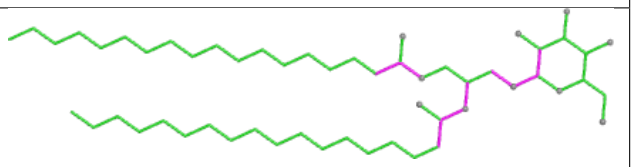


Rings

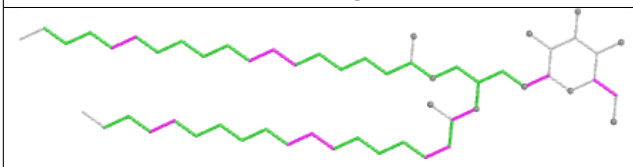
Ligand LMG V 2631



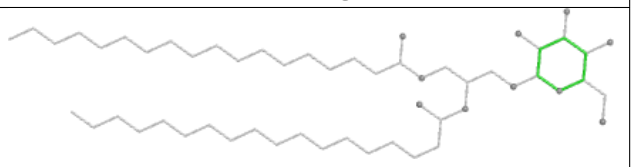
Bond lengths



Bond angles

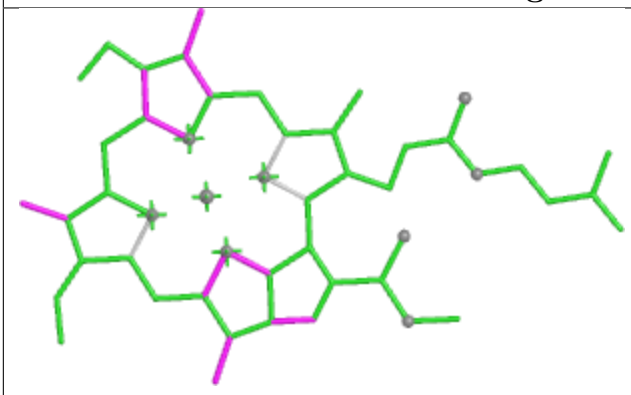


Torsions

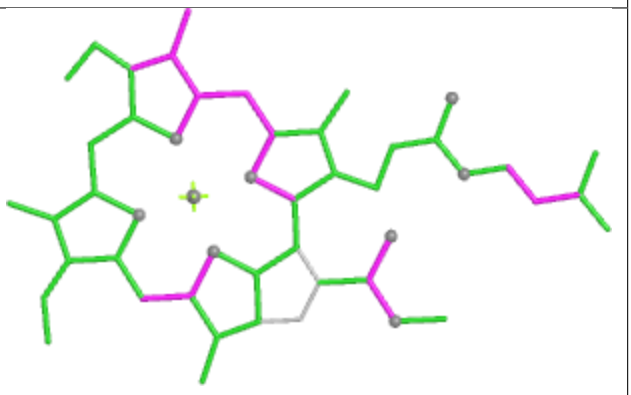


Rings

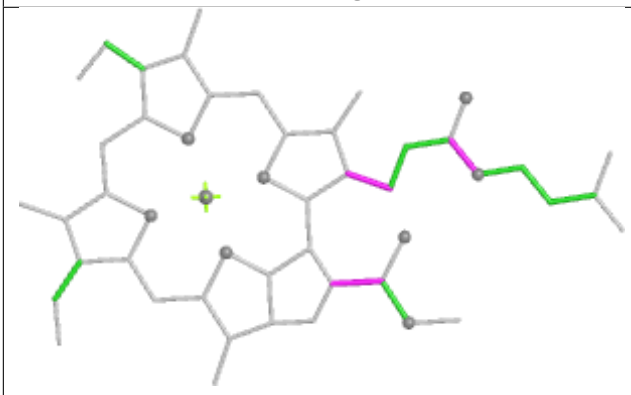
Ligand CLA Z 604



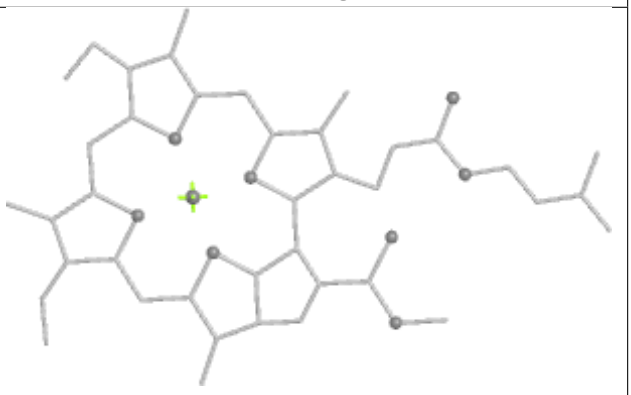
Bond lengths



Bond angles

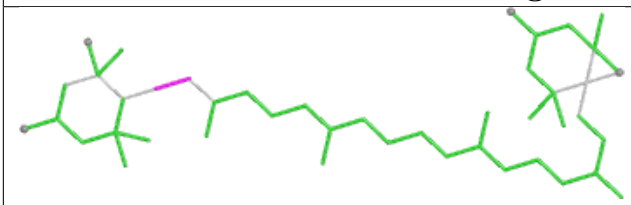


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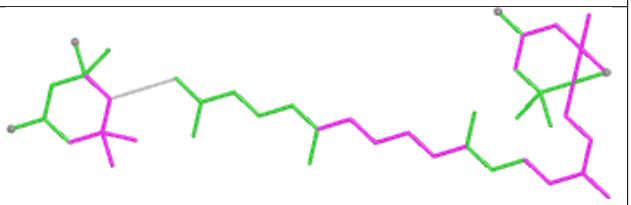


Rings

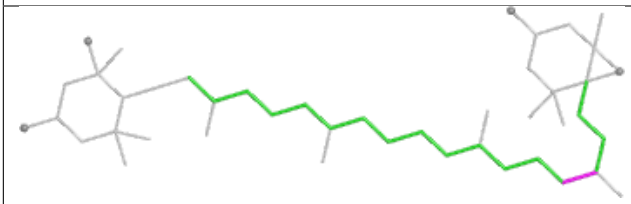
Ligand NEX 5 624



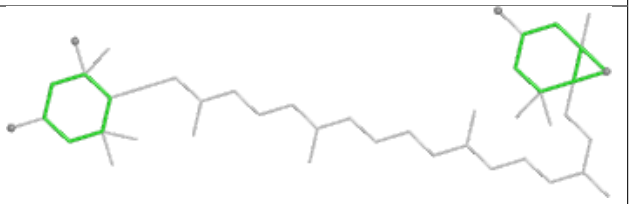
Bond lengths



Bond angles

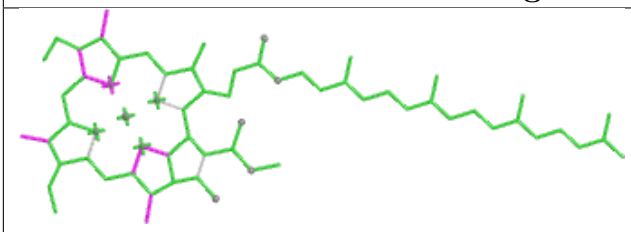


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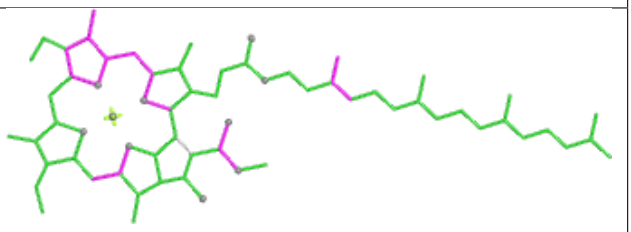


Rings

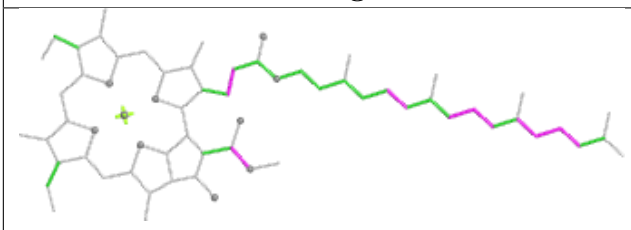
Ligand CLA A 829



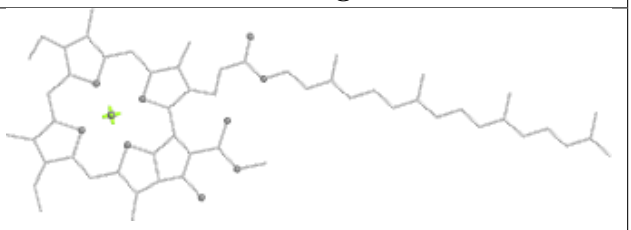
Bond lengths



Bond angles

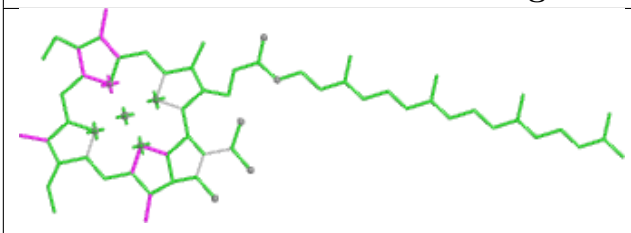


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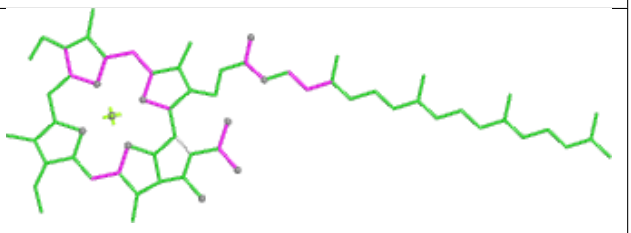


Rings

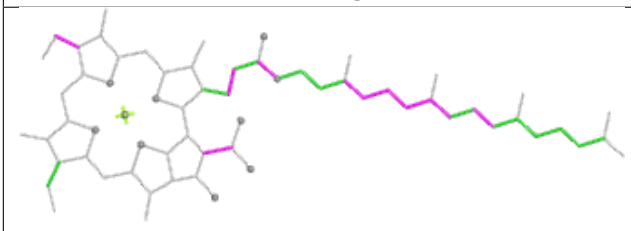
Ligand CLA 6 613



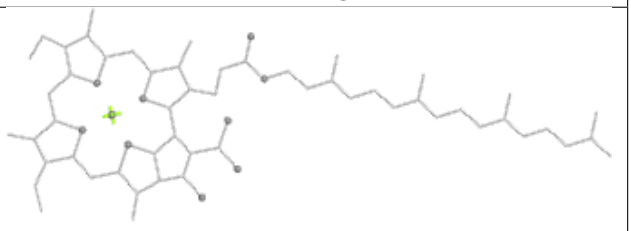
Bond lengths



Bond angles

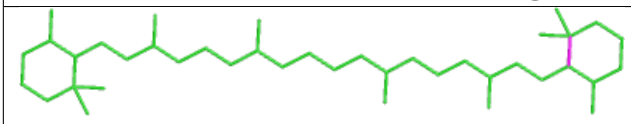


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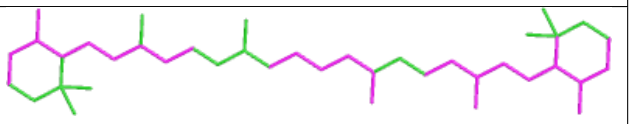


Rings

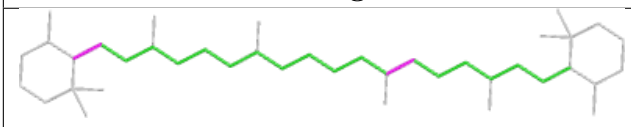
Ligand BCR 3 622



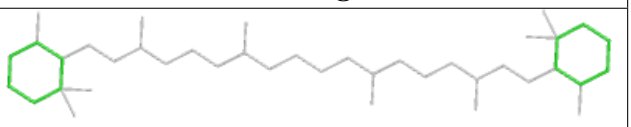
Bond lengths



Bond angles

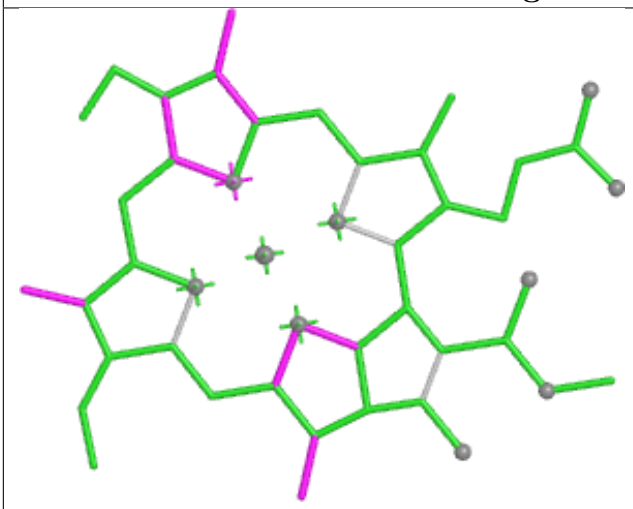


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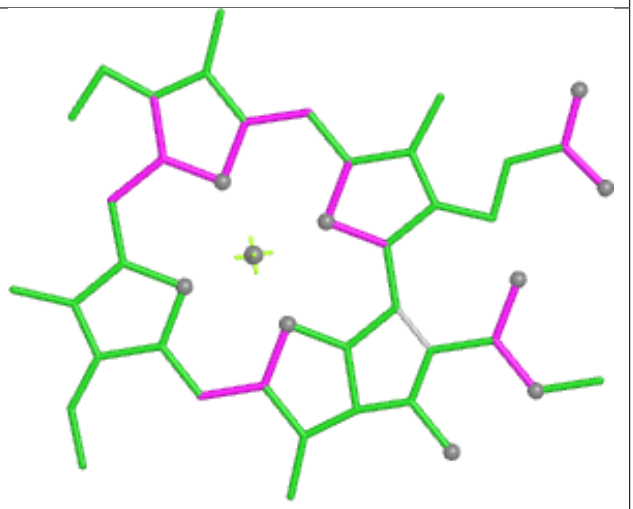


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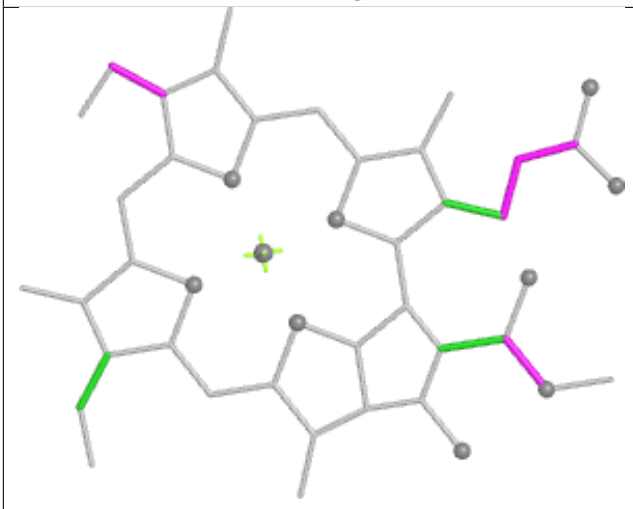
Ligand CLA G 204



Bond lengths



Bond angles

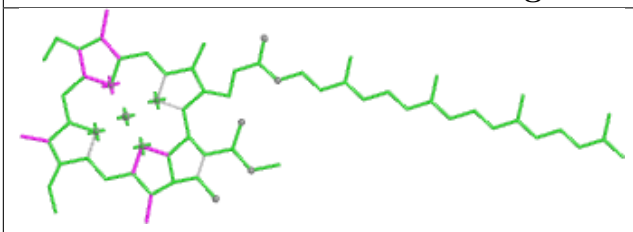


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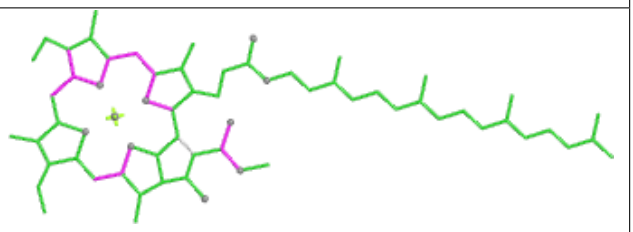


Rings

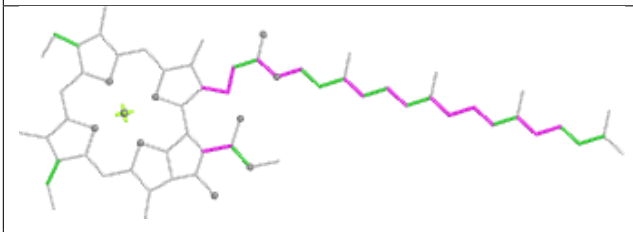
Ligand CLA B 828



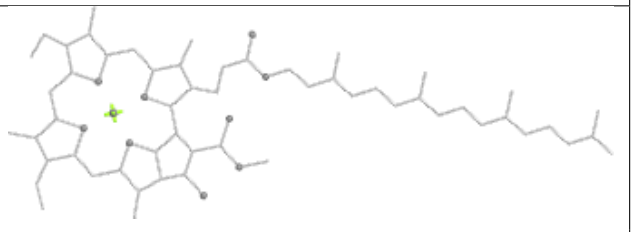
Bond lengths



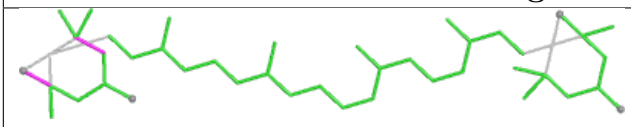
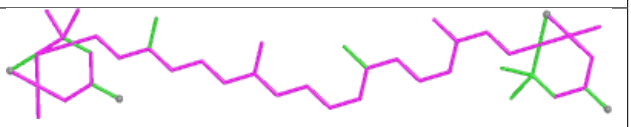
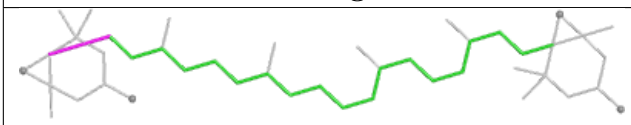
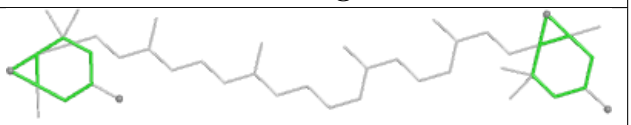
Bond angles

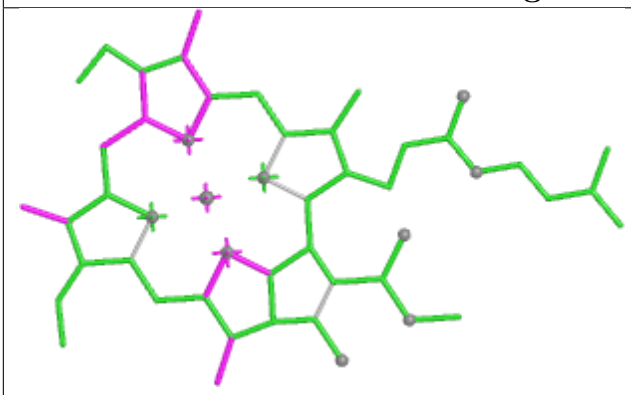
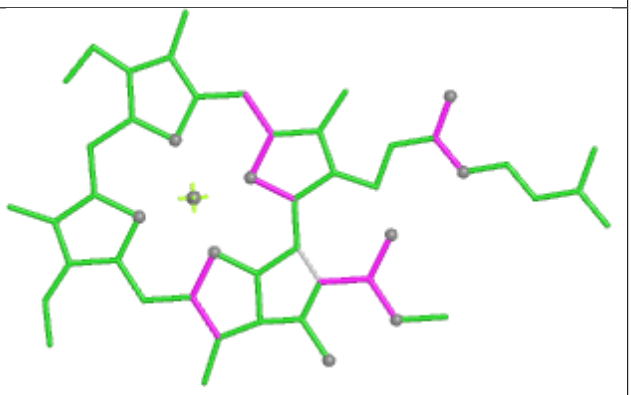
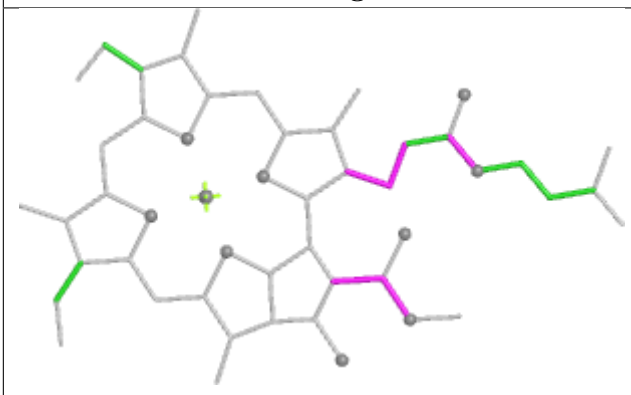
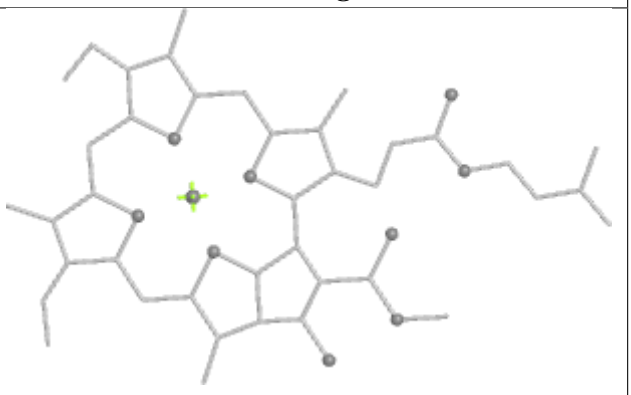


Torsions

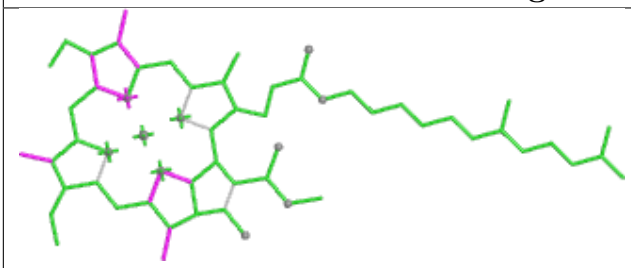


Rings

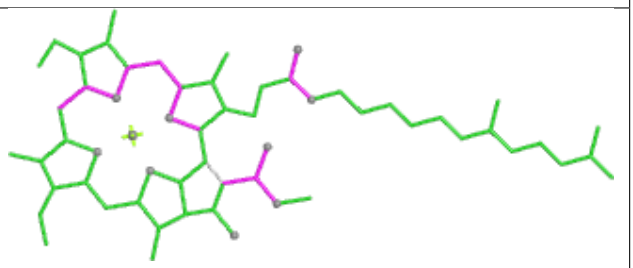
Ligand XAT 4 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

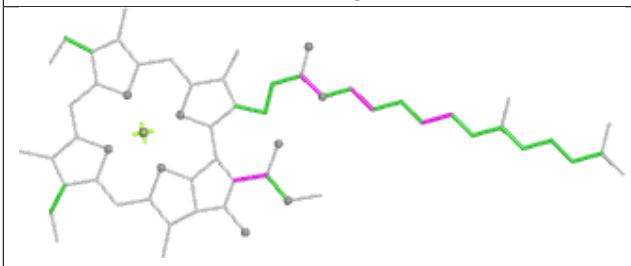
Ligand CLA 7 611



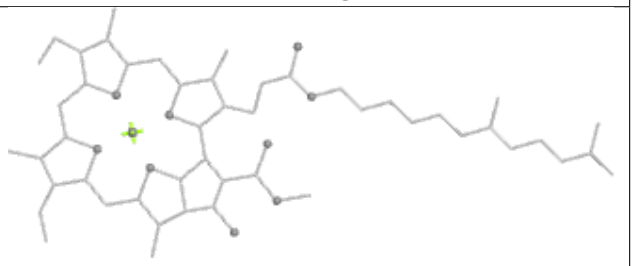
Bond lengths



Bond angles

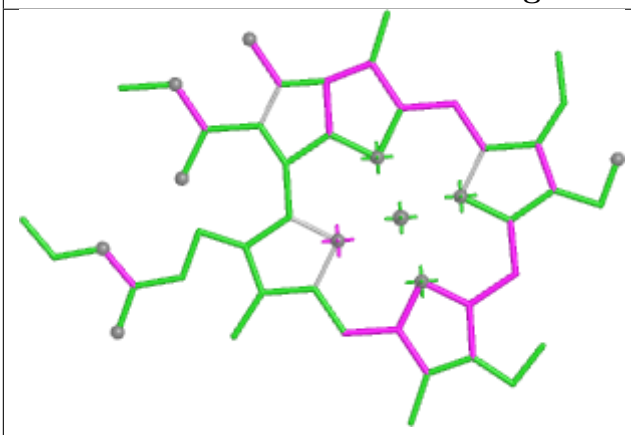


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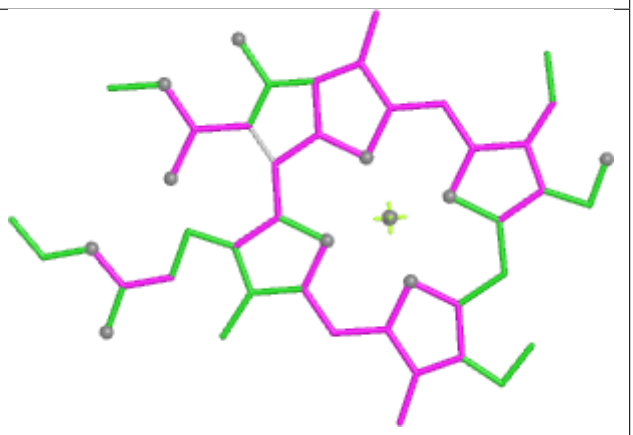


Rings

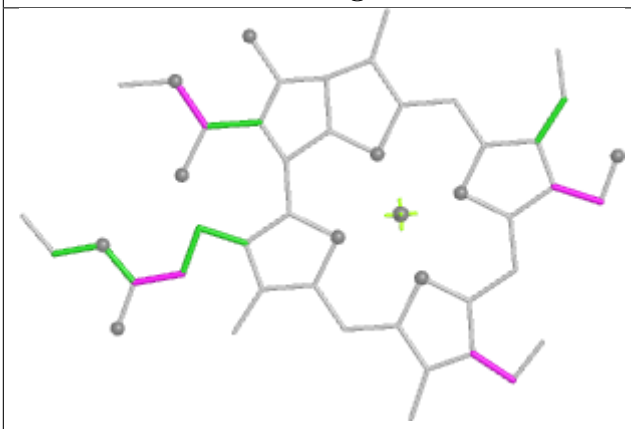
Ligand CHL V 608



Bond lengths



Bond angles

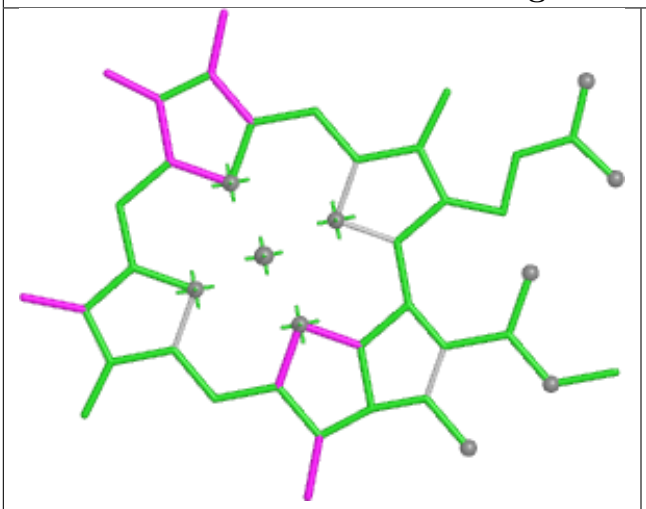


Torsions

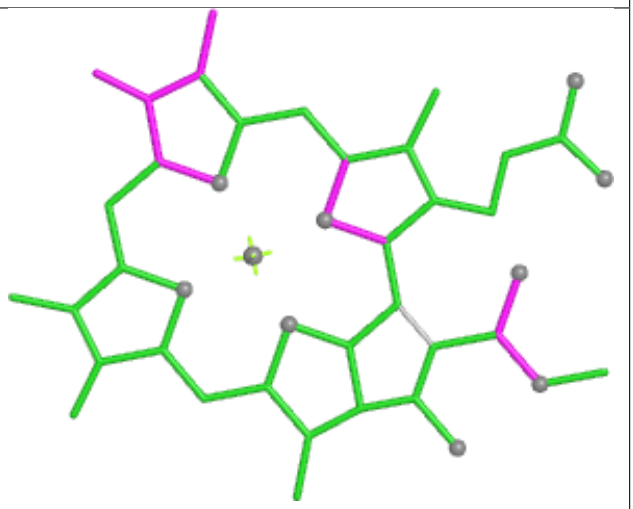


Rings

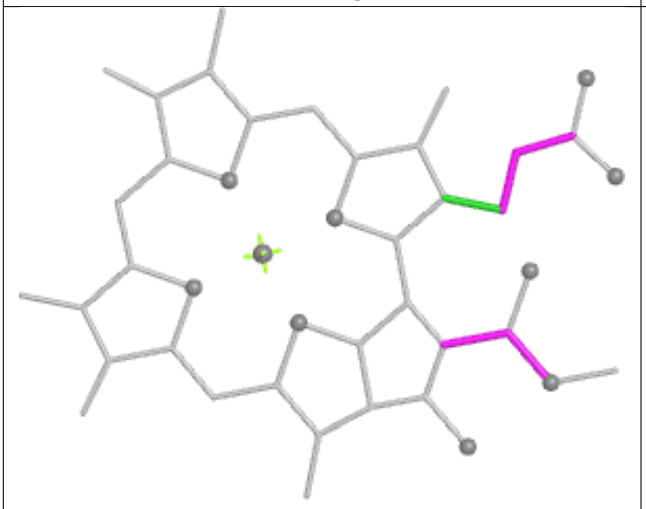
Ligand CLA 4 616



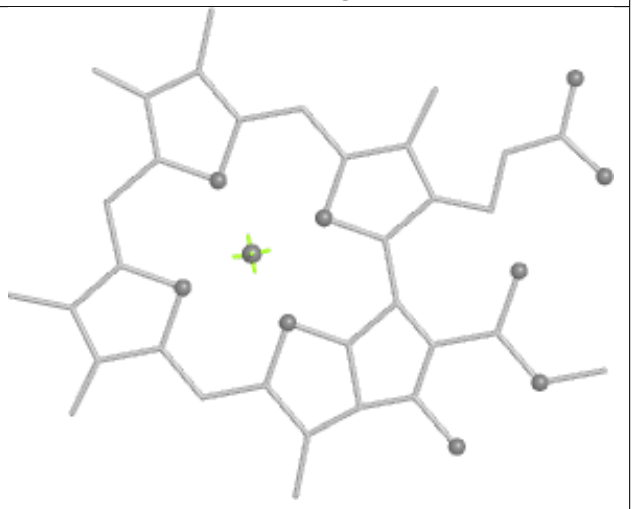
Bond lengths



Bond angles

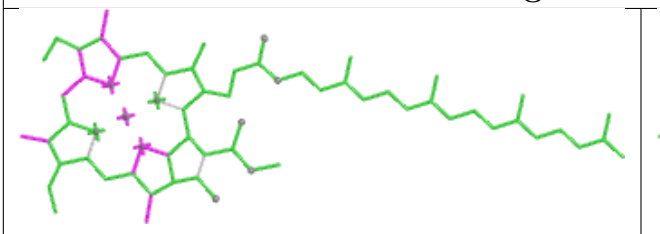


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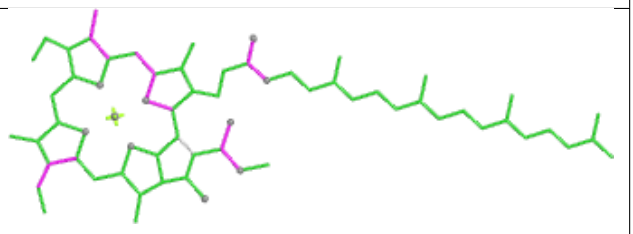


Rings

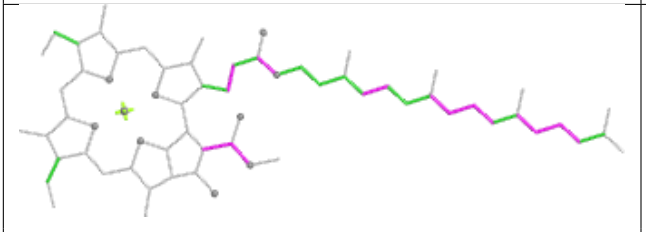
Ligand CLA B 839



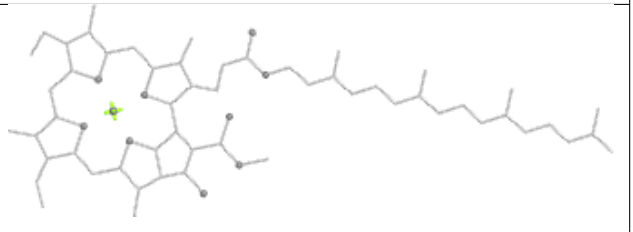
Bond lengths



Bond angles

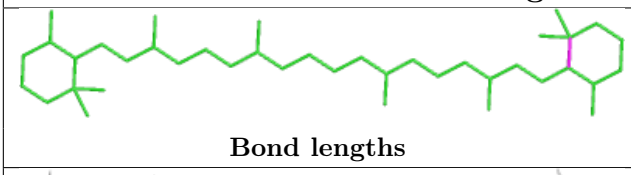


Torsions

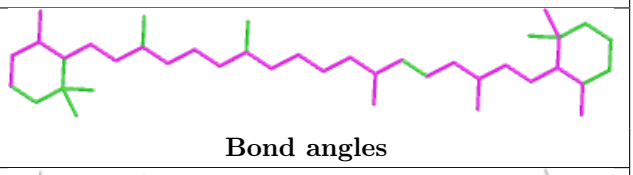


Rings

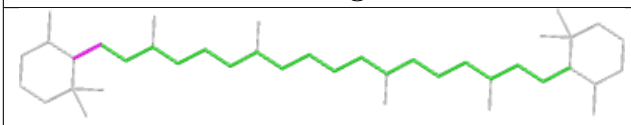
Ligand BCR 4 621



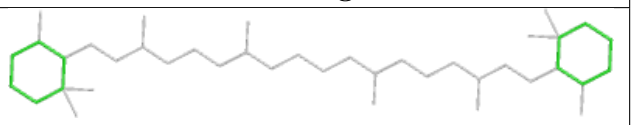
Bond lengths



Bond angles

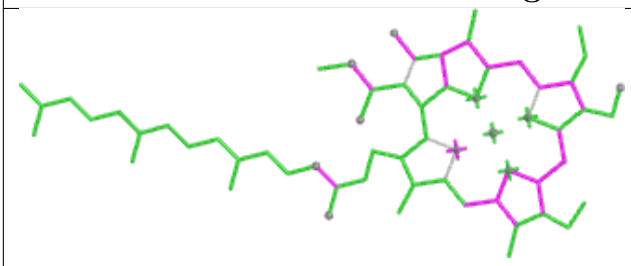


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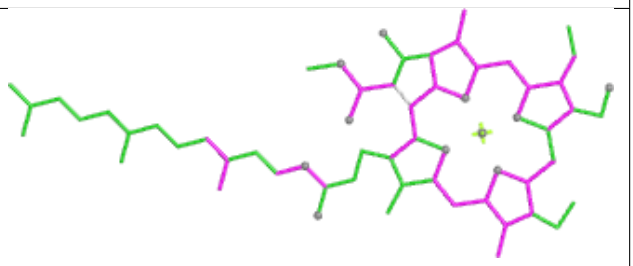


Rings

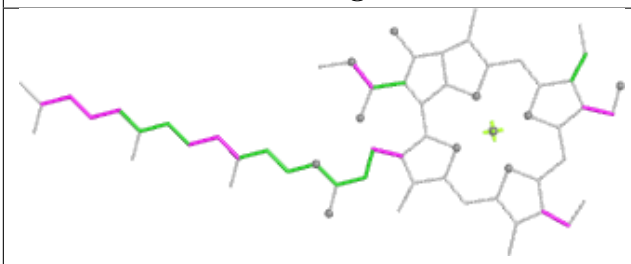
Ligand CHL V 609



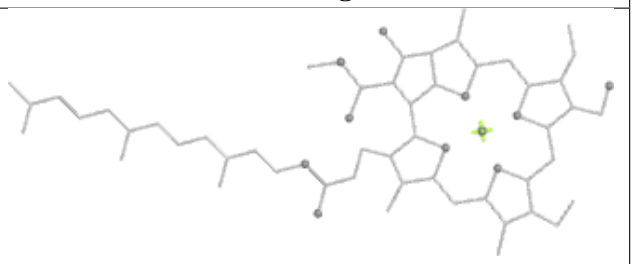
Bond lengths



Bond angles

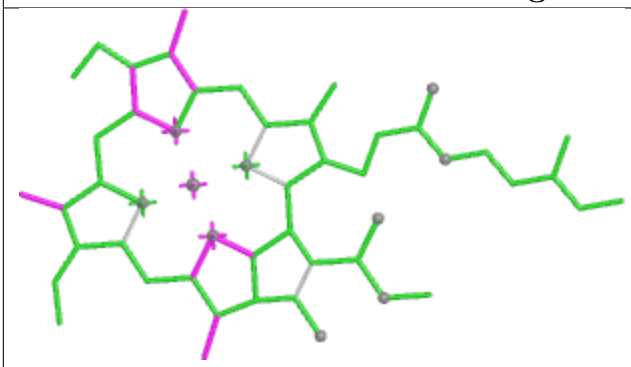


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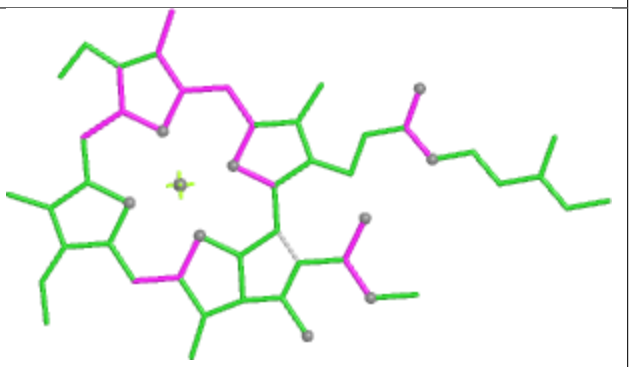


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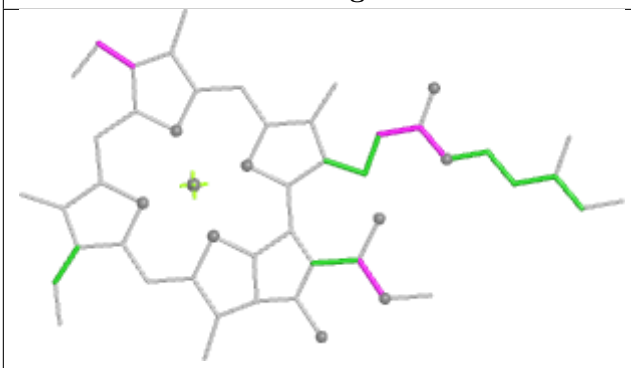
Ligand CLA 8 608



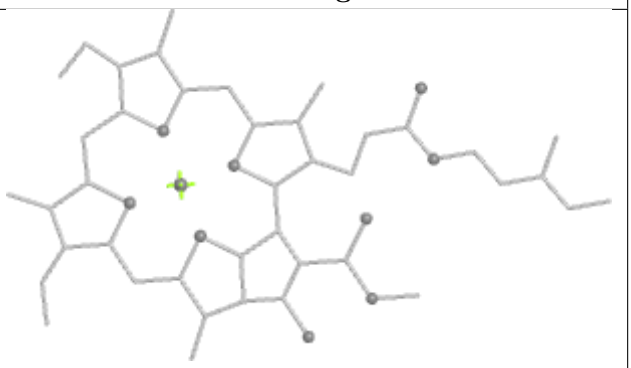
Bond lengths



Bond angles

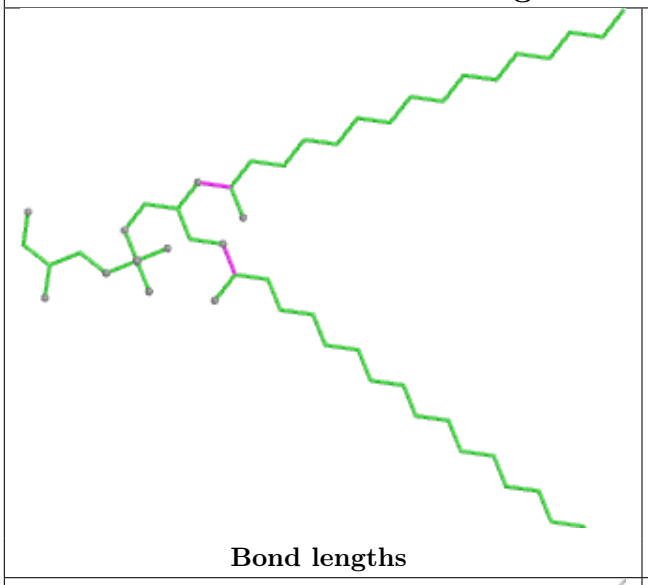


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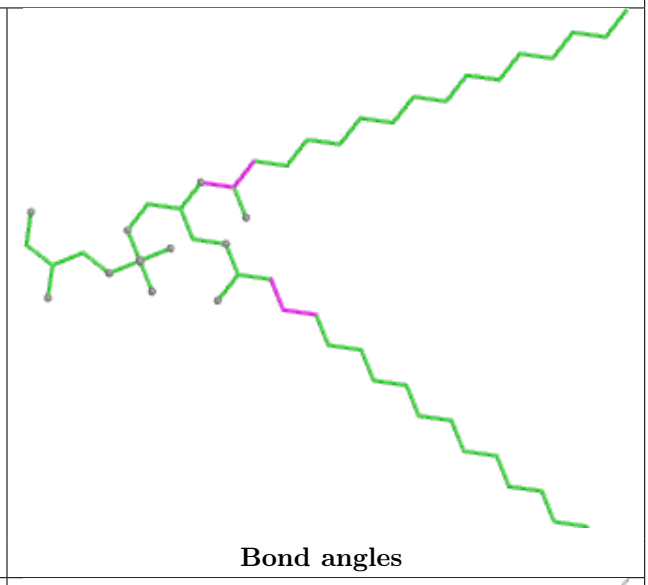


Rings

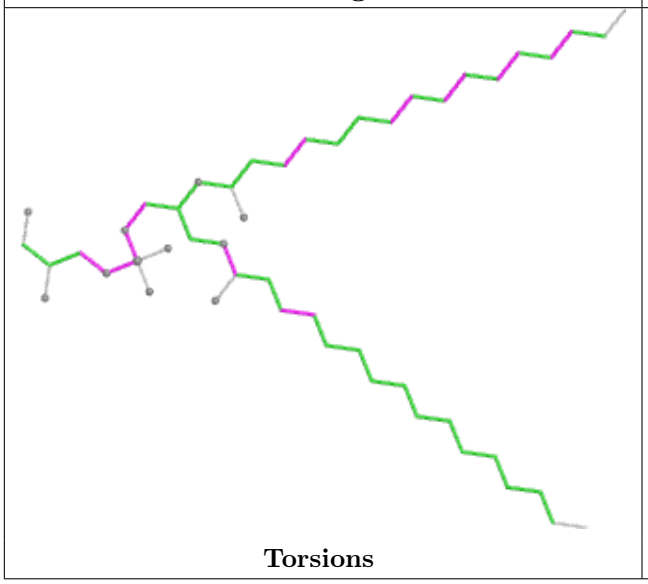
Ligand LHG Y 2630



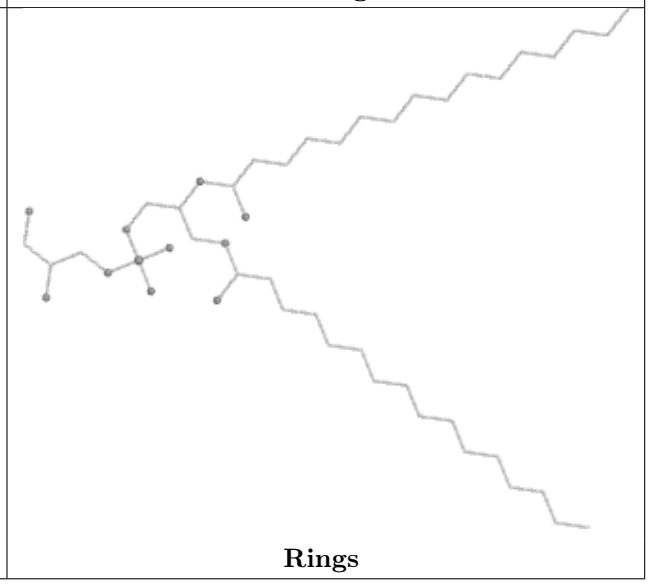
Bond lengths



Bond angles

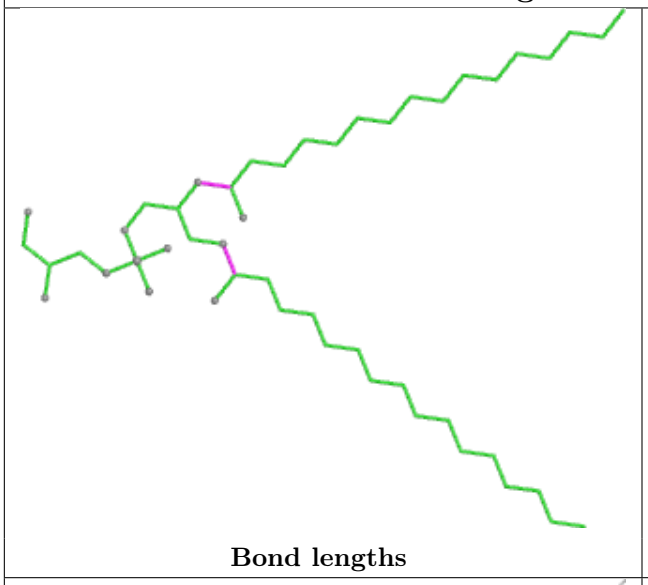


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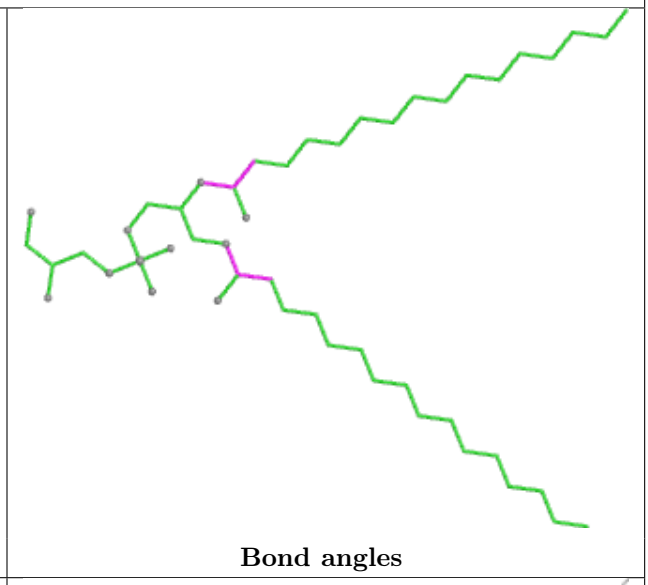


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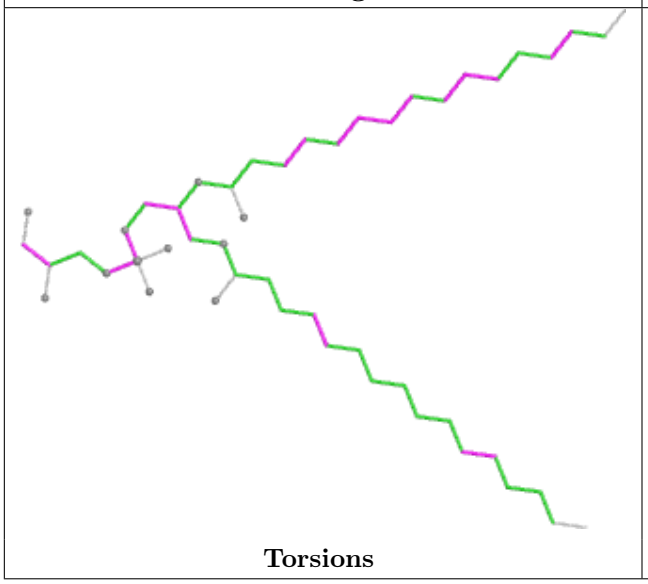
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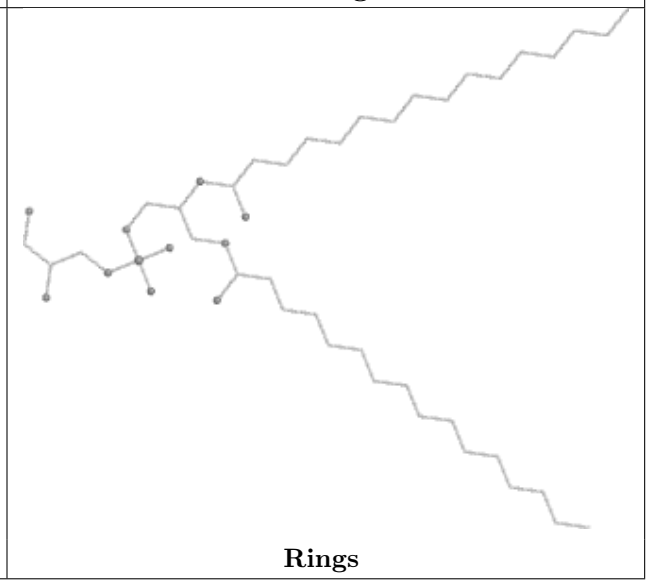
Bond lengths



Bond angles

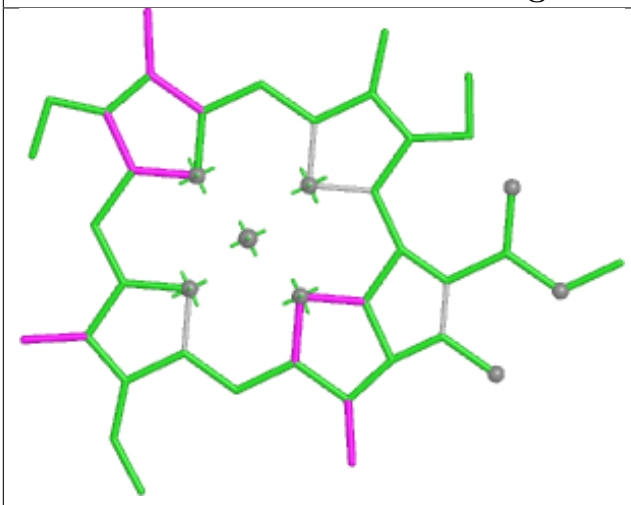


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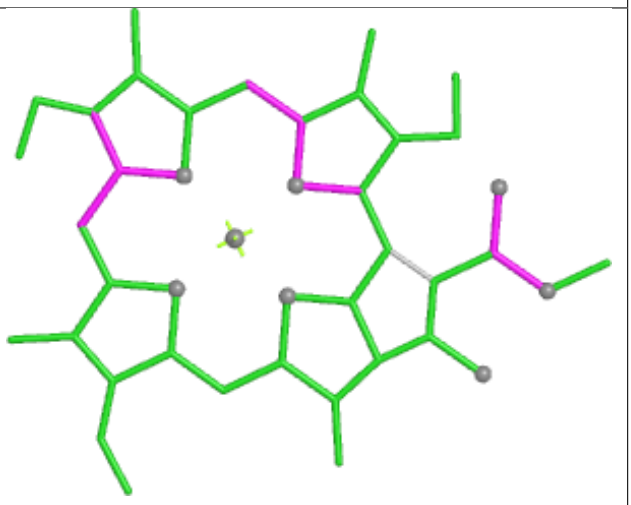


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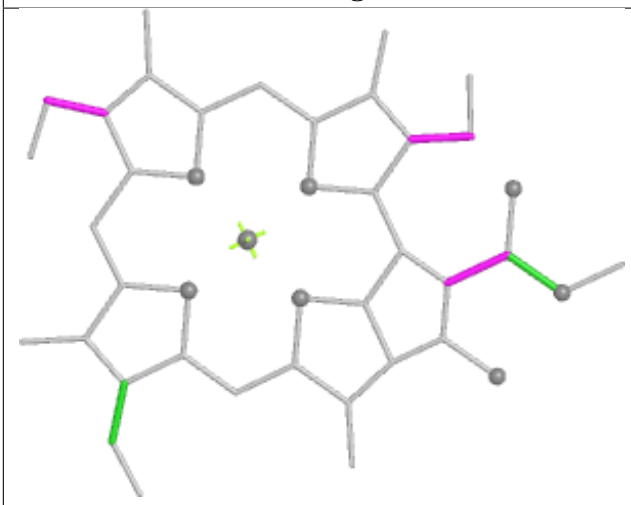
Ligand CLA 6 611



Bond lengths



Bond angles

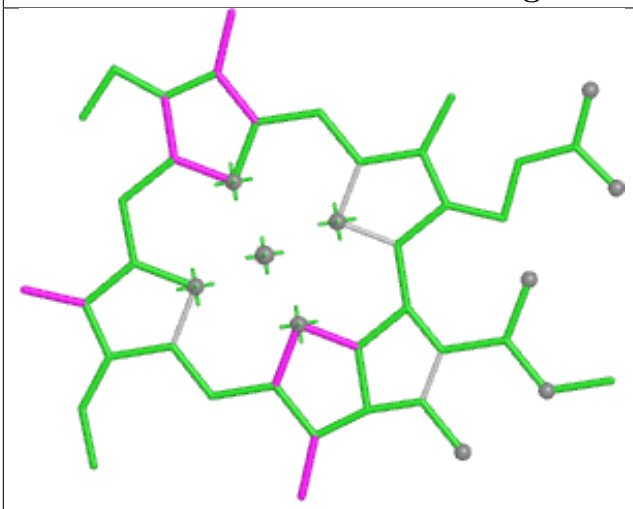


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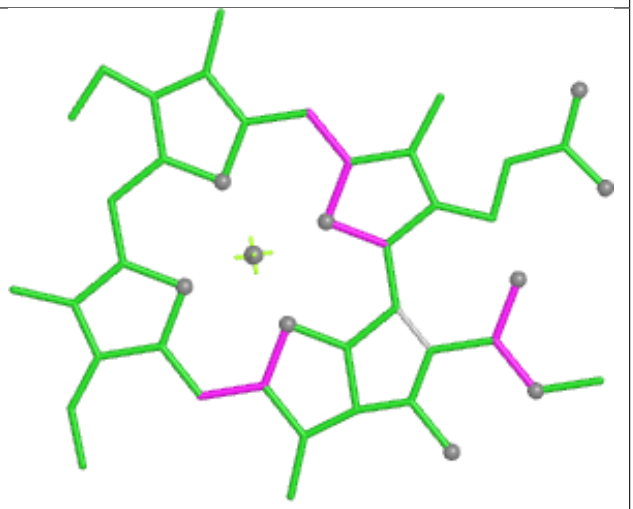


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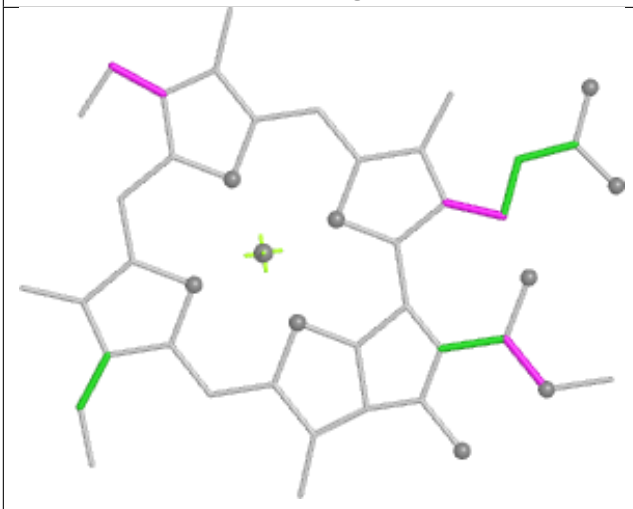
Ligand CLA K 206



Bond lengths



Bond angles

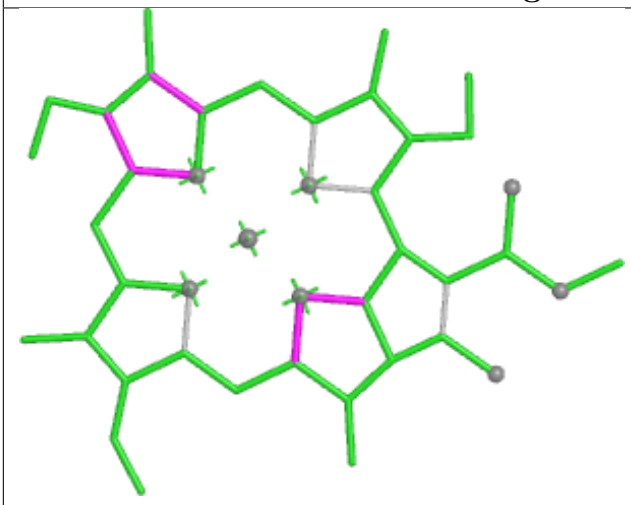


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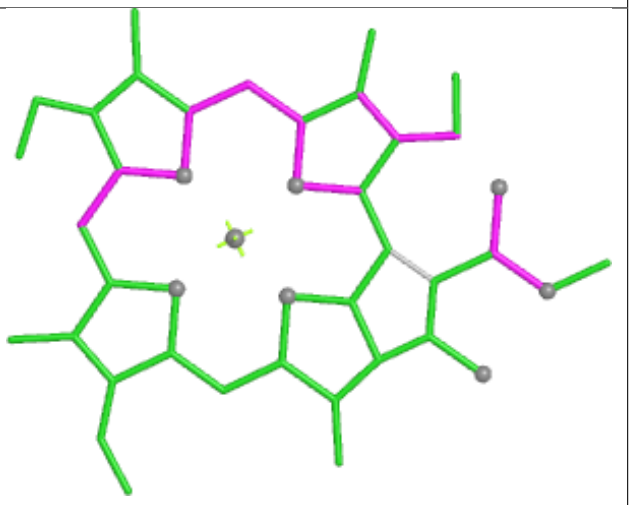


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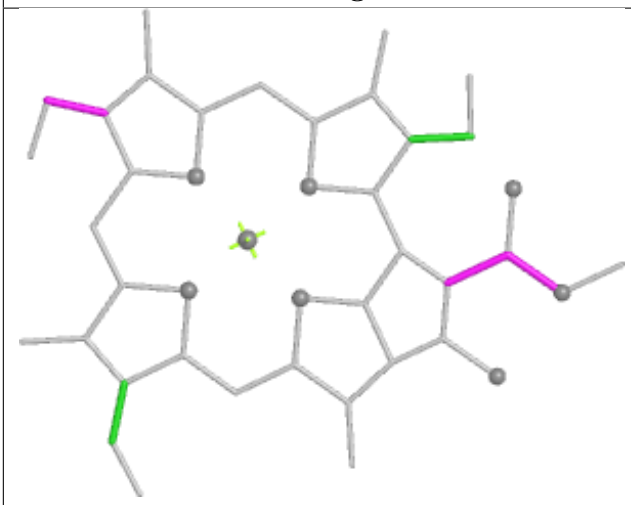
Ligand CLA U 612



Bond lengths



Bond angles

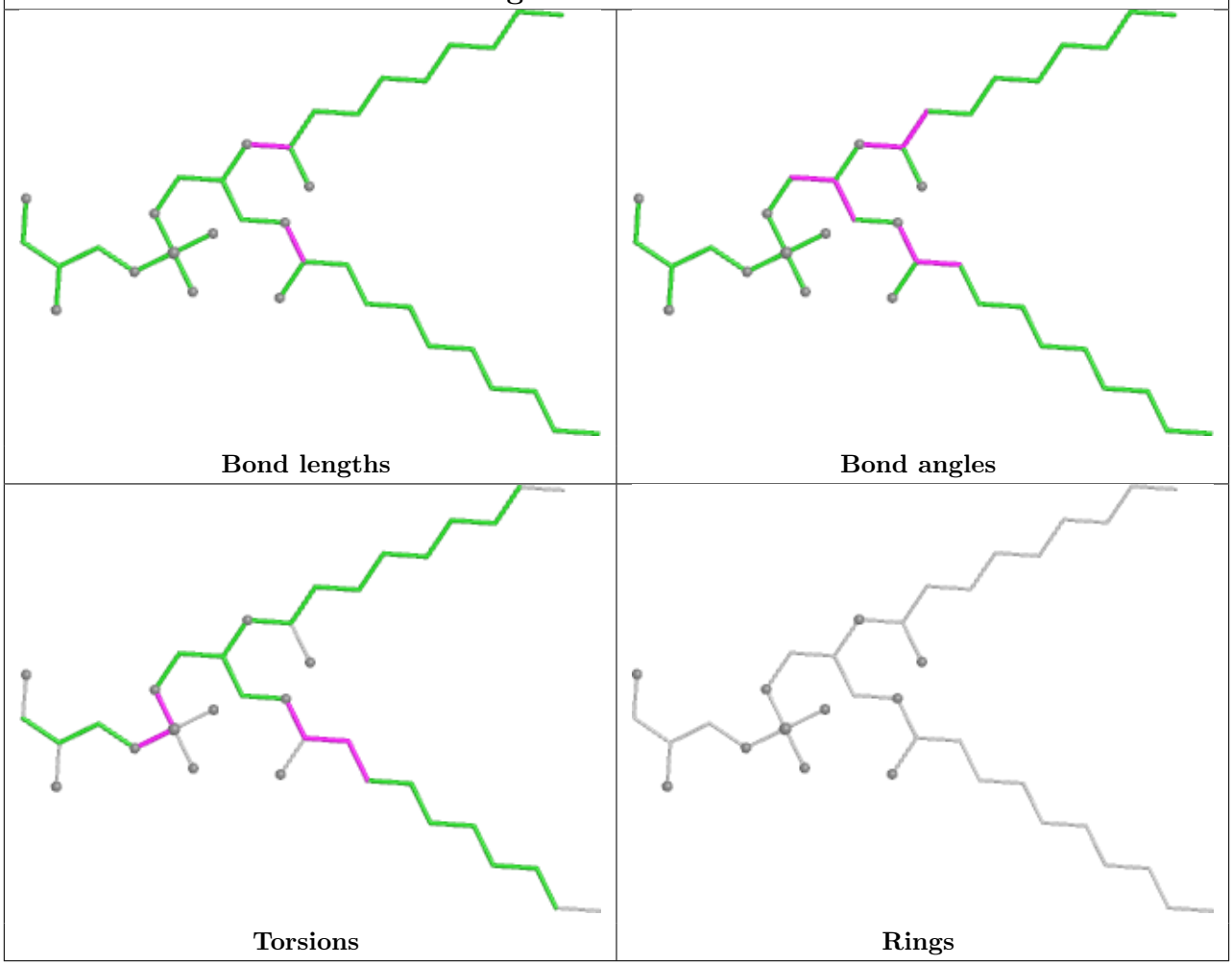


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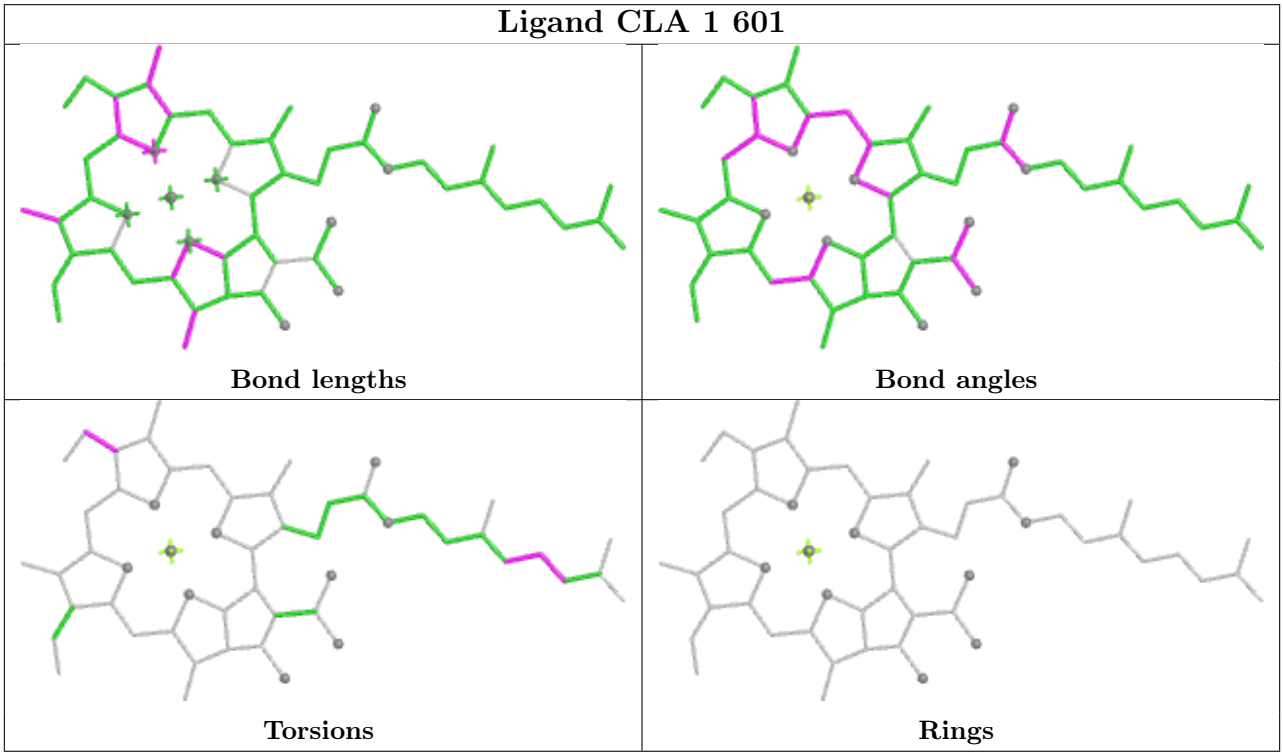


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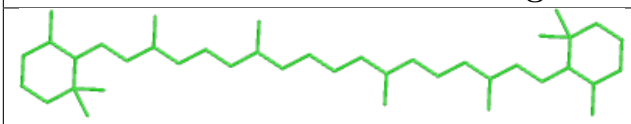
Ligand LHG 2 622



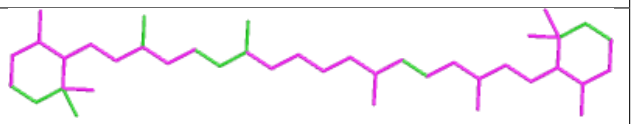
Ligand CLA 1 601



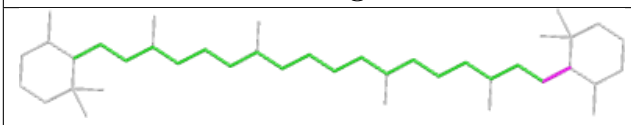
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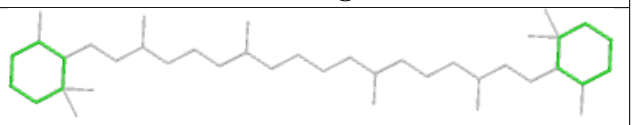
Bond lengths



Bond angles

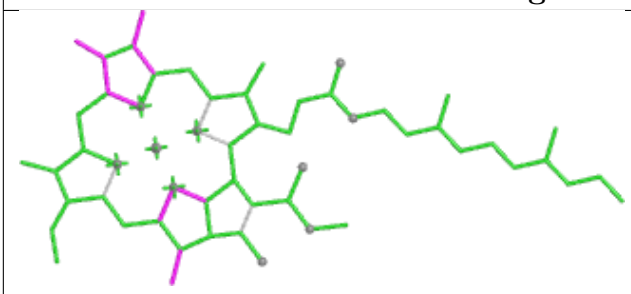


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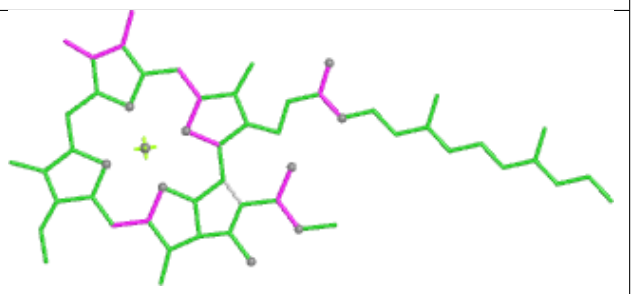


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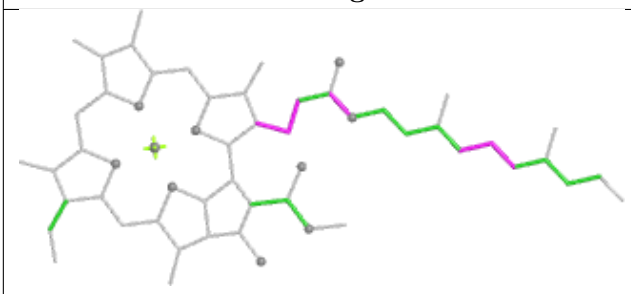
Ligand CLA 3 607



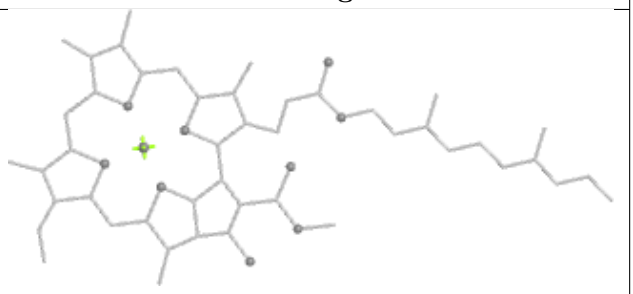
Bond lengths



Bond angles

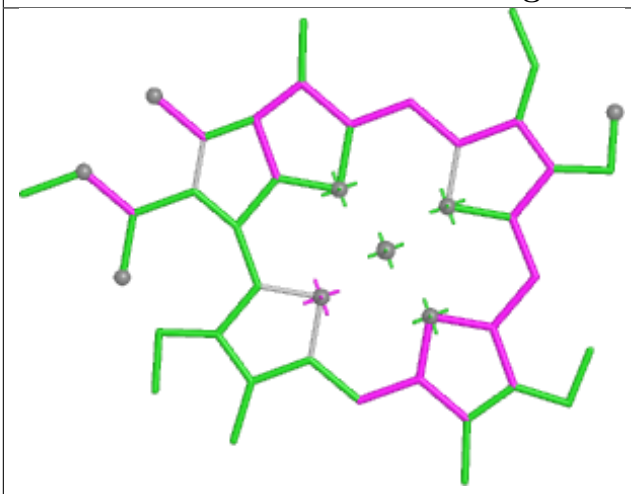


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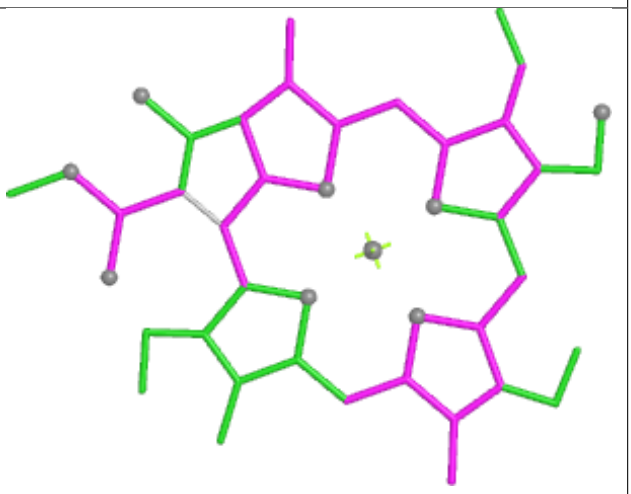


Rings

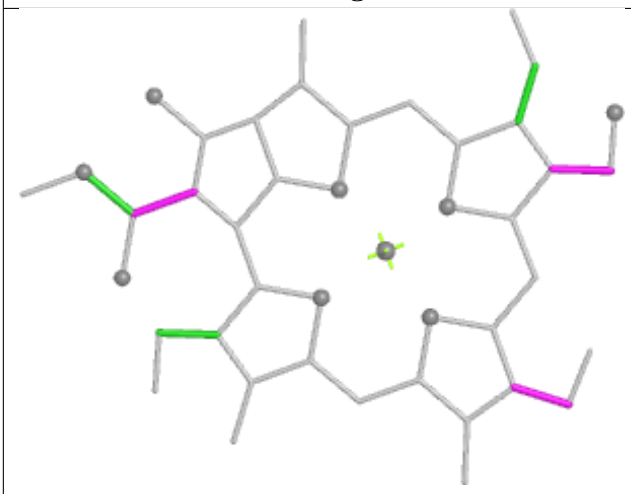
Ligand CHL U 605



Bond lengths



Bond angles

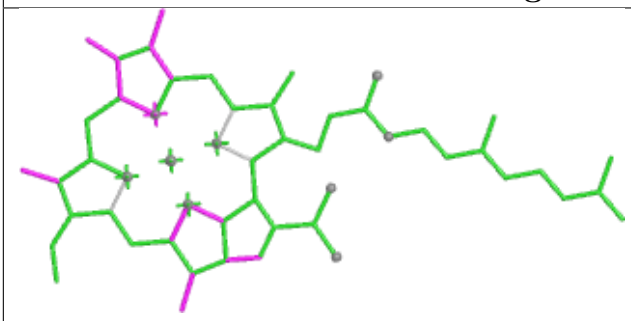


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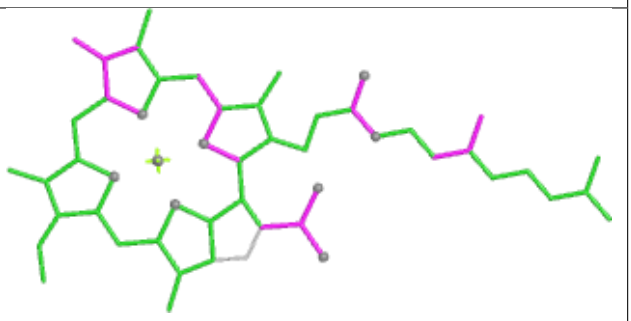


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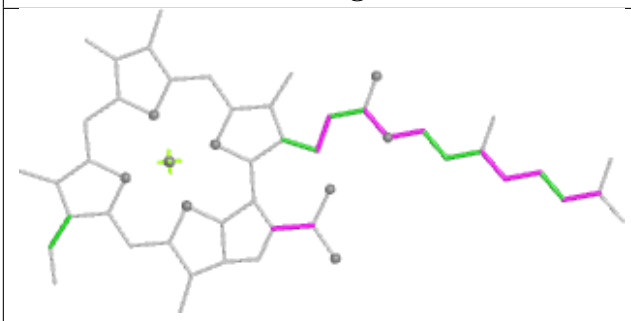
Ligand CLA B 811



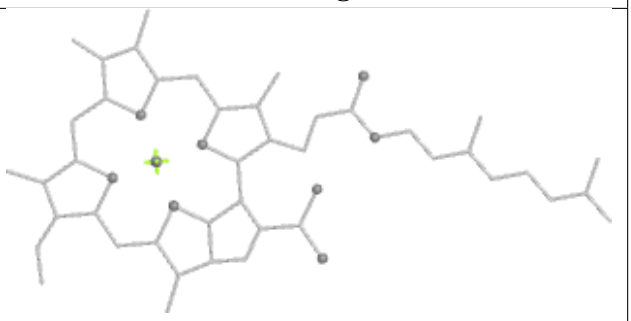
Bond lengths



Bond angles

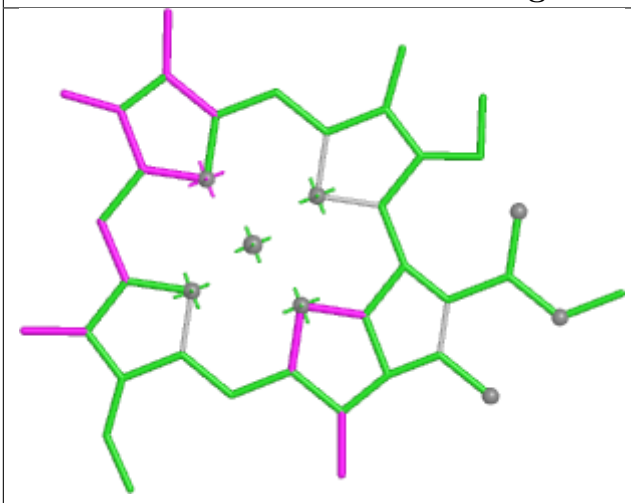


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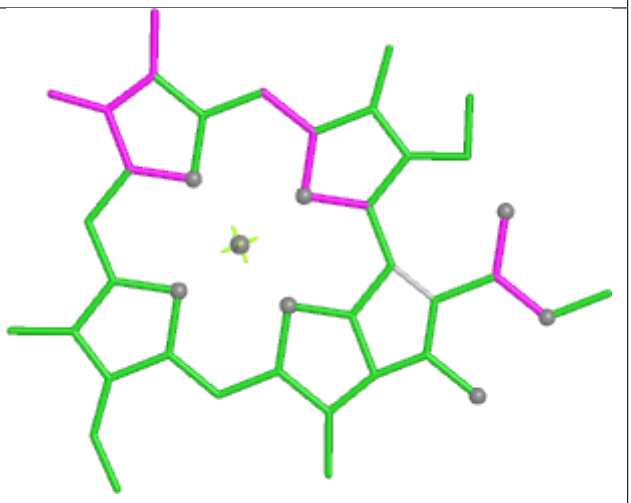


Rings

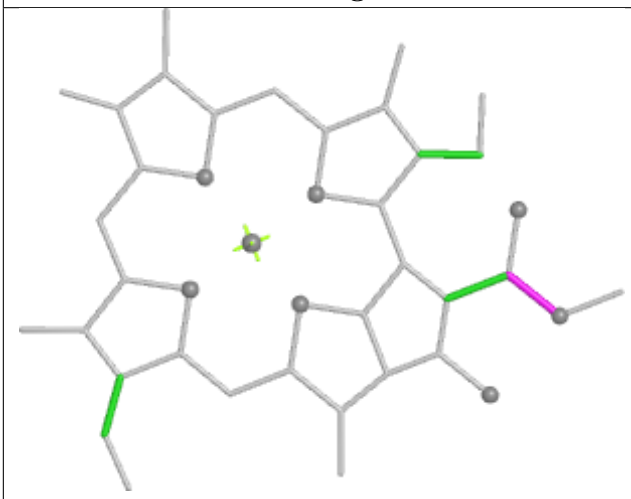
Ligand CLA 8 607



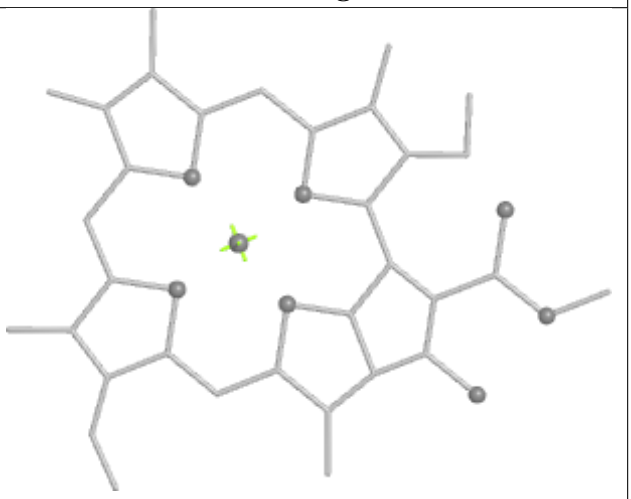
Bond lengths



Bond angles

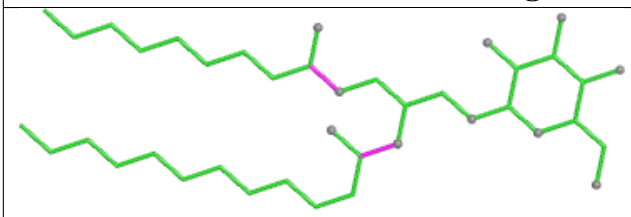


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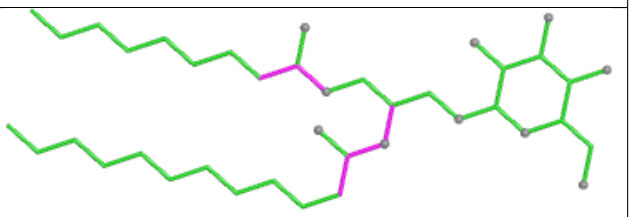


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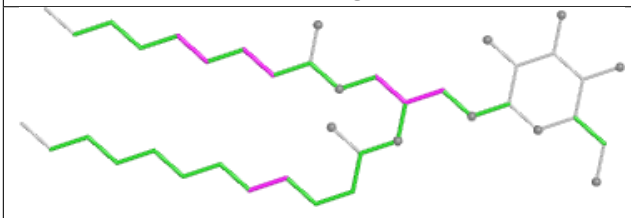
Ligand LMG 5 627



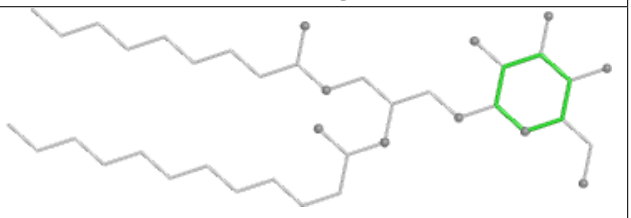
Bond lengths



Bond angles

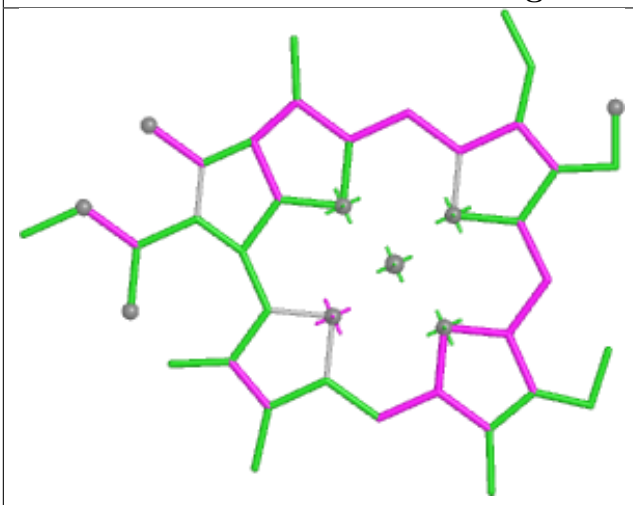


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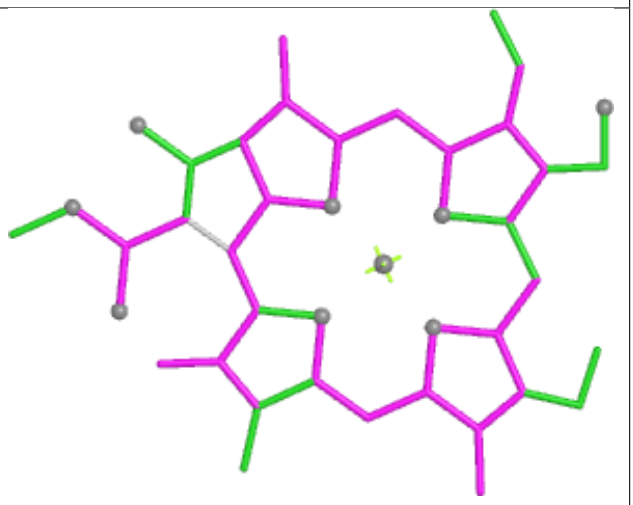


Rings

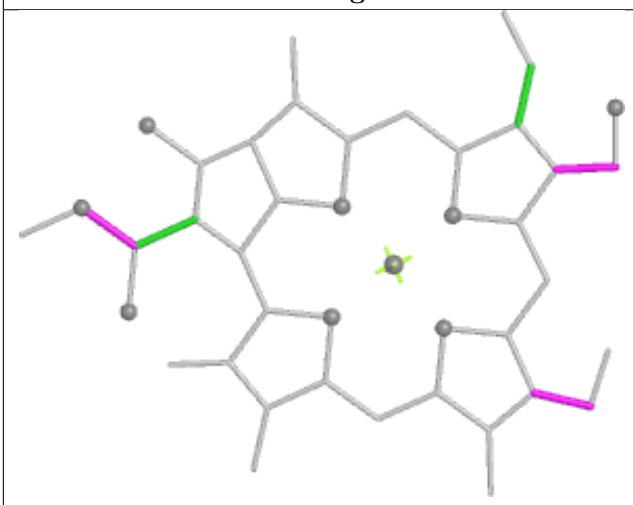
Ligand CHL Z 605



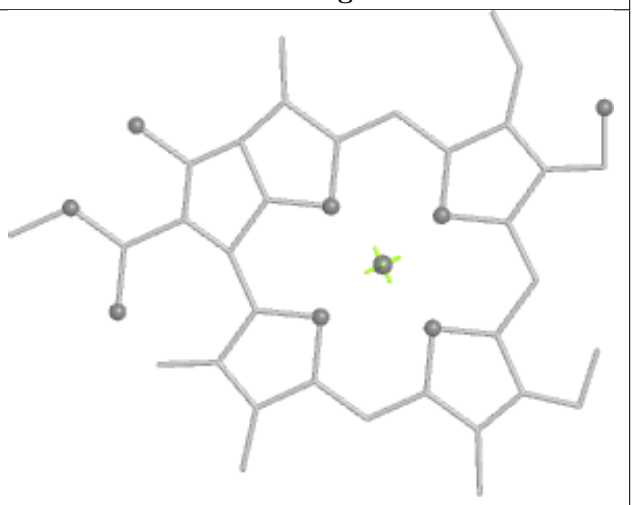
Bond lengths



Bond angles

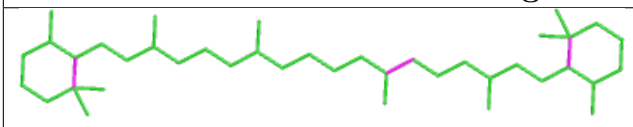


Torsions

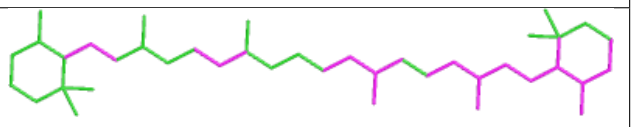


Rings

Ligand BCR A 848



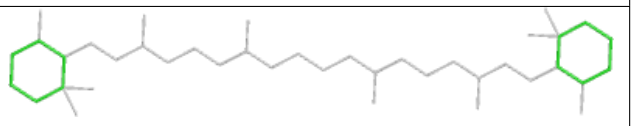
Bond lengths



Bond angles

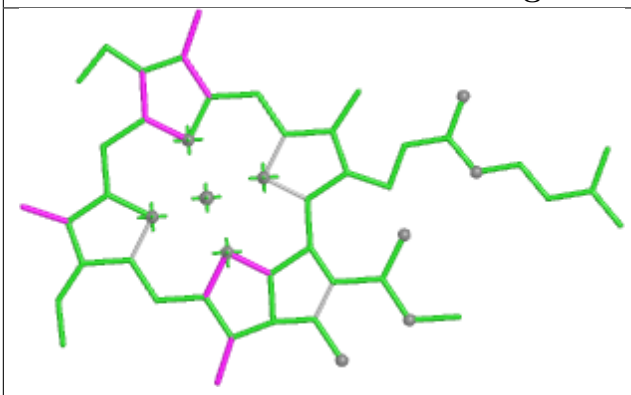


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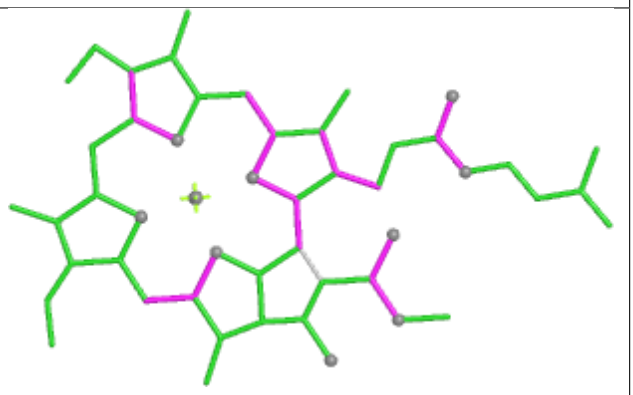


Rings

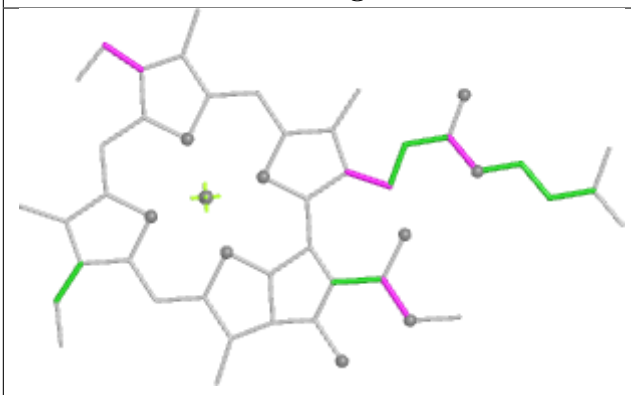
Ligand CLA A 810



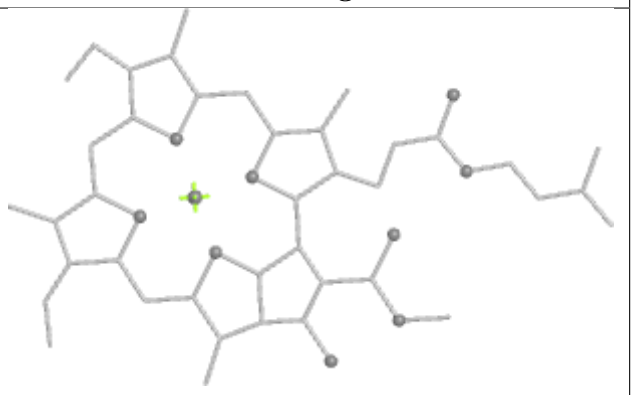
Bond lengths



Bond angles

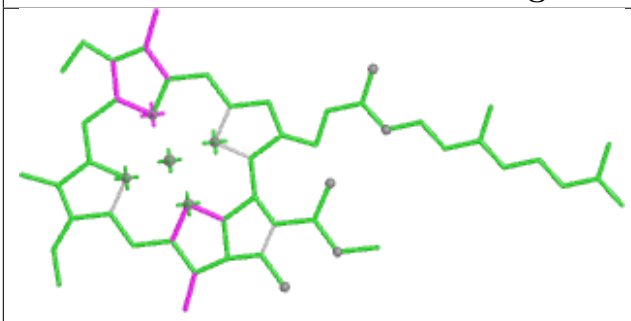


Torsions

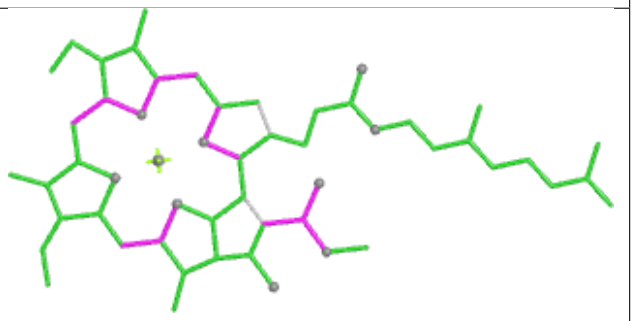


Rings

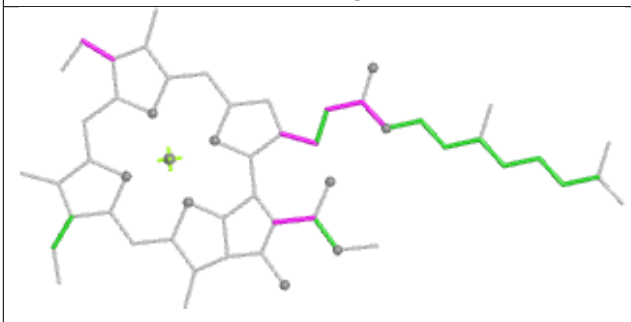
Ligand CLA a 614



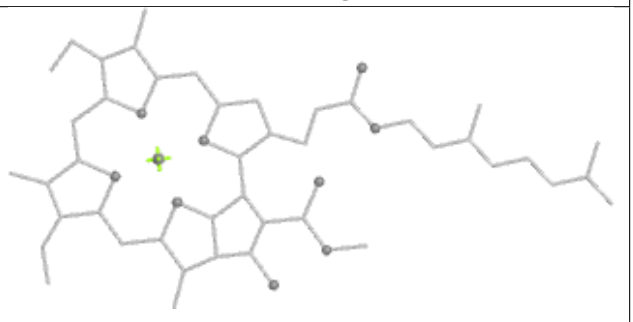
Bond lengths



Bond angles

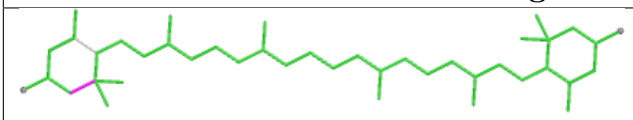


Torsions

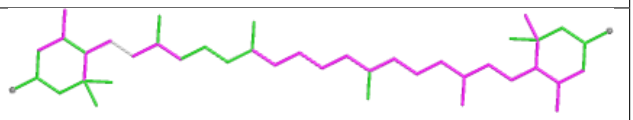


Rings

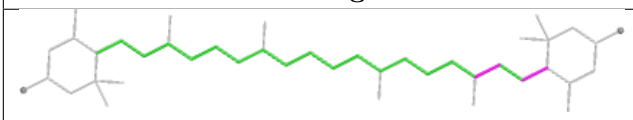
Ligand LUT a 617



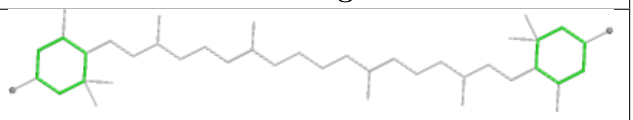
Bond lengths



Bond angles

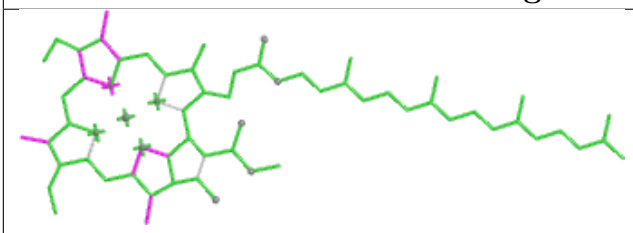


Torsions

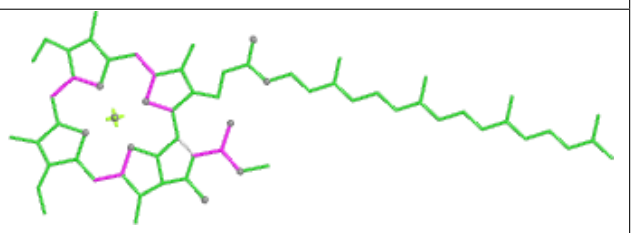


Rings

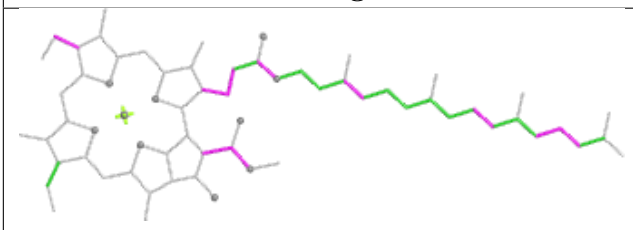
Ligand CLA A 825



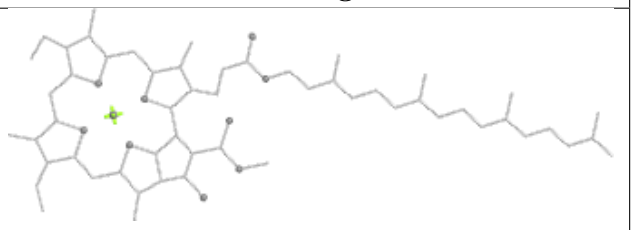
Bond lengths



Bond angles

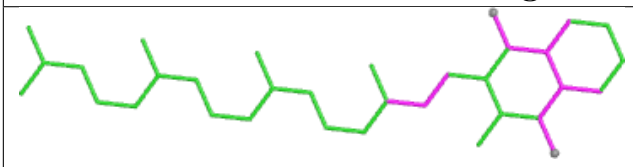


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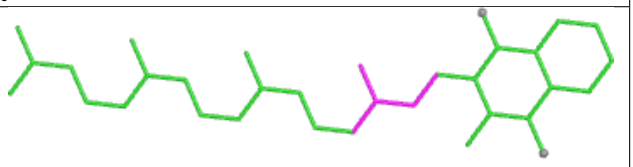


Rings

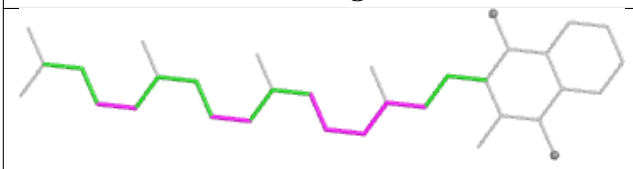
Ligand PQN A 844



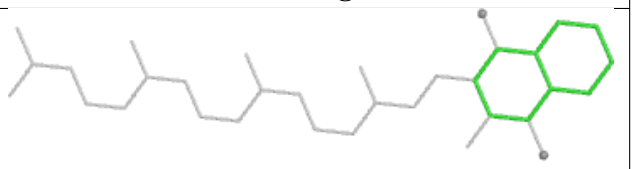
Bond lengths



Bond angles

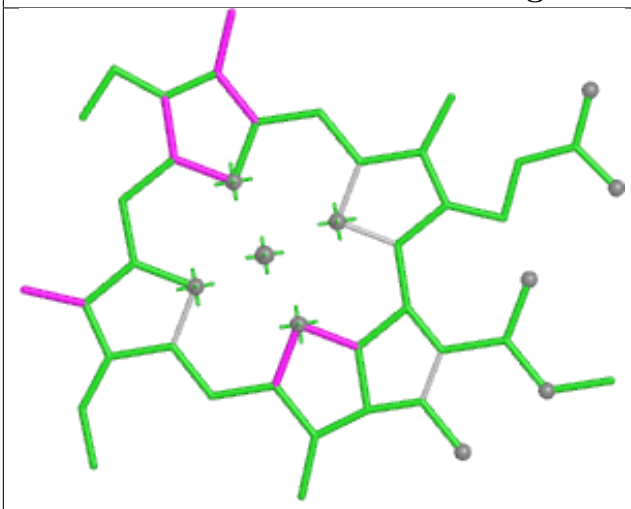


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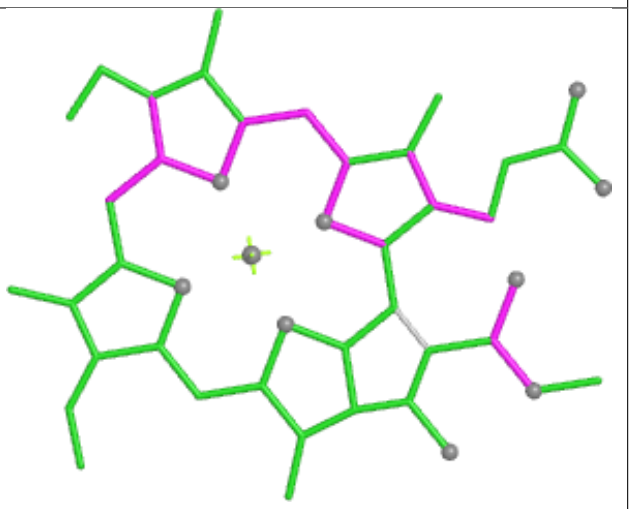


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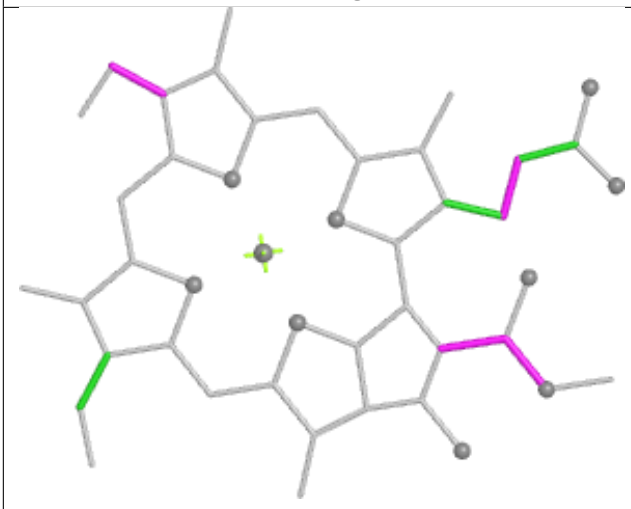
Ligand CLA Z 612



Bond lengths



Bond angles

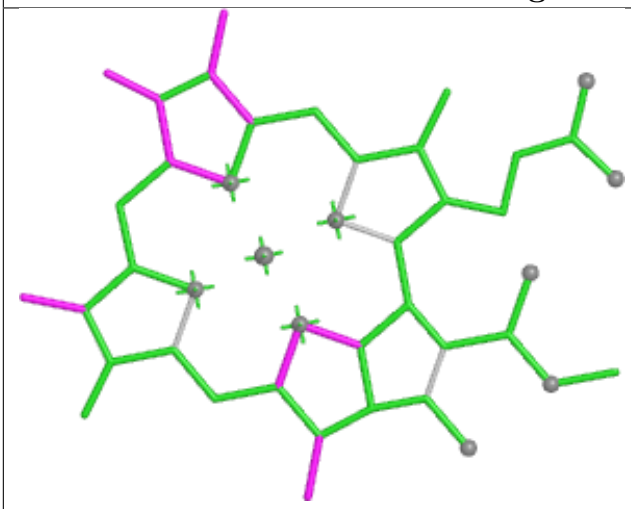


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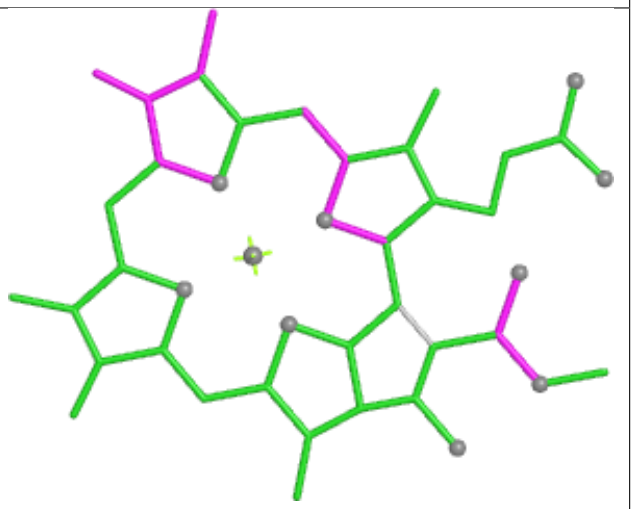


Rings

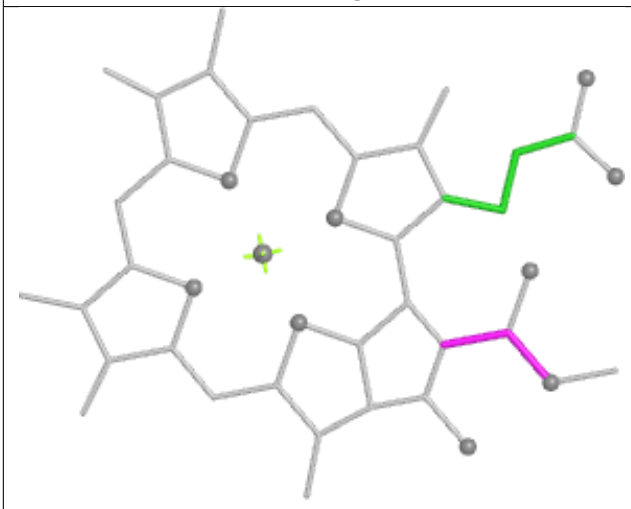
Ligand CLA 2 616



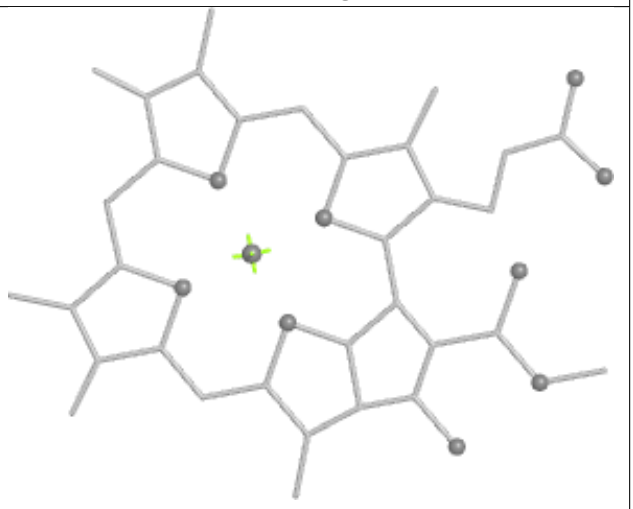
Bond lengths



Bond angles

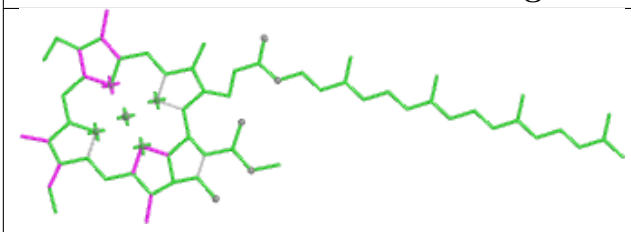


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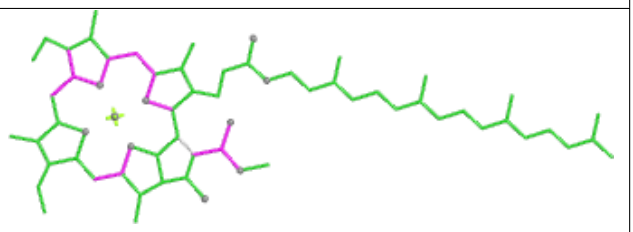


Rings

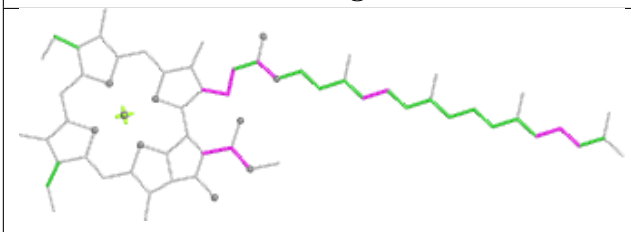
Ligand CLA B 809



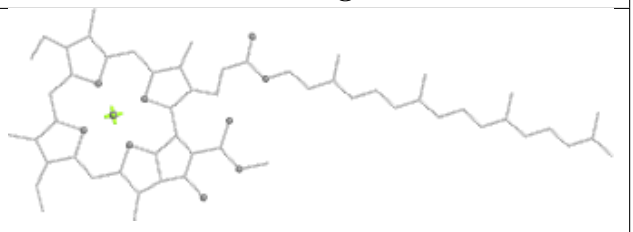
Bond lengths



Bond angles

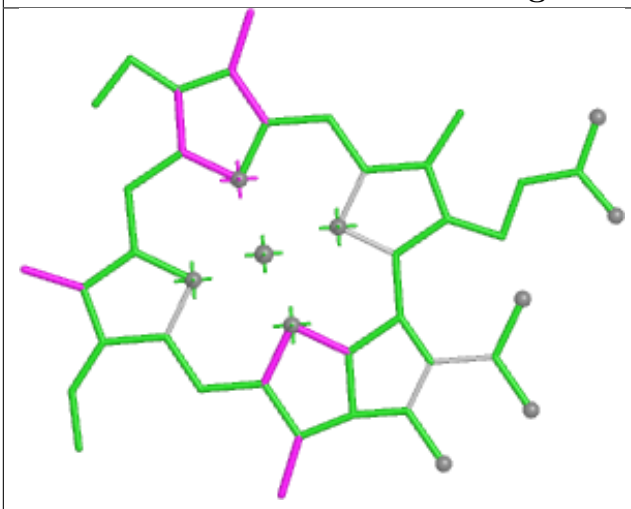


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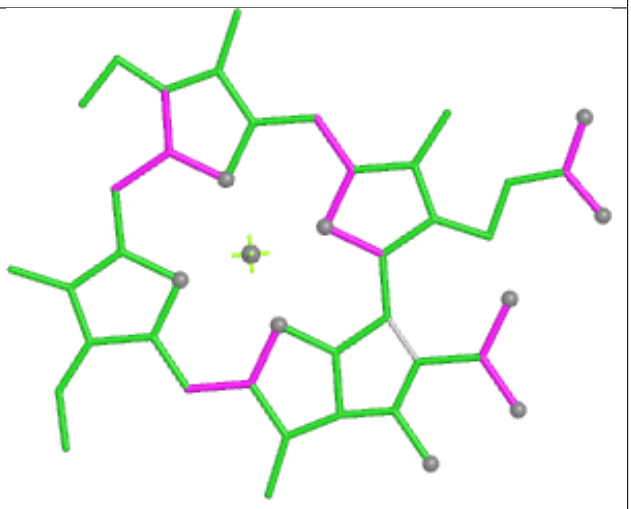


Rings

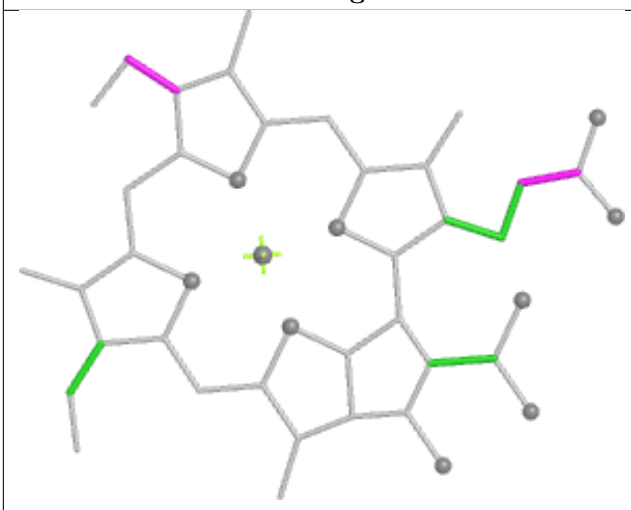
Ligand CLA 1 608



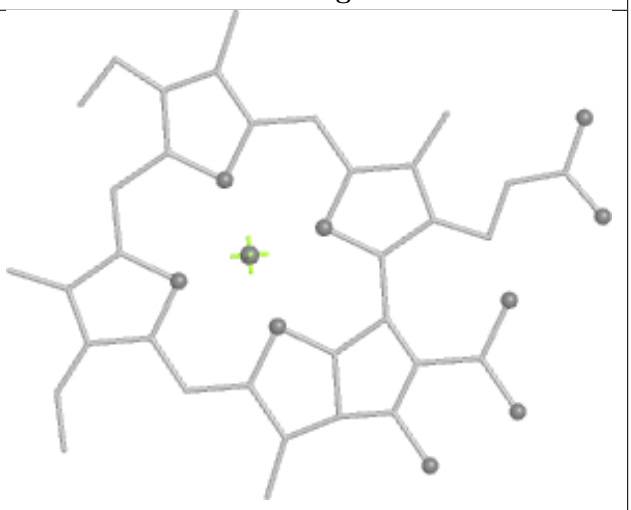
Bond lengths



Bond angles

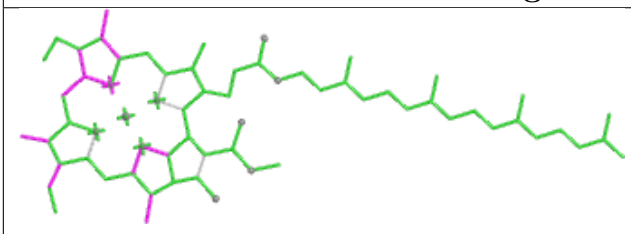


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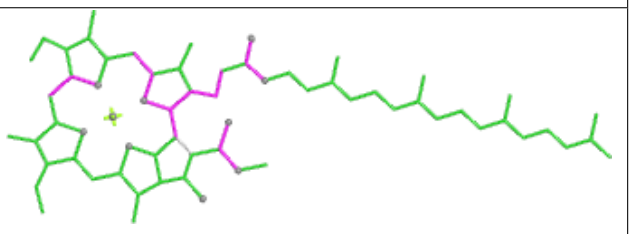


Rings

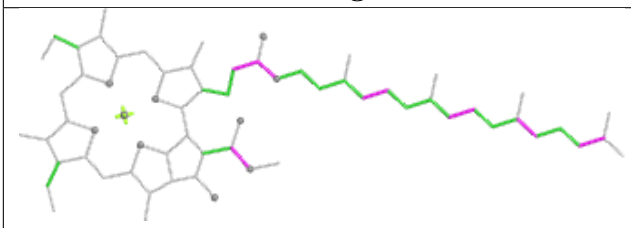
Ligand CLA A 801



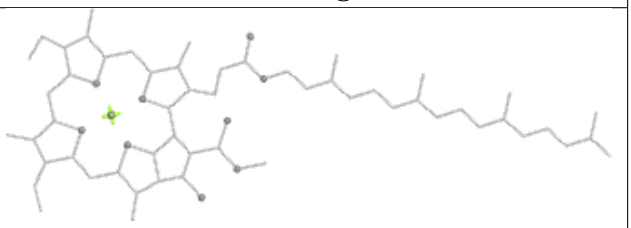
Bond lengths



Bond angles

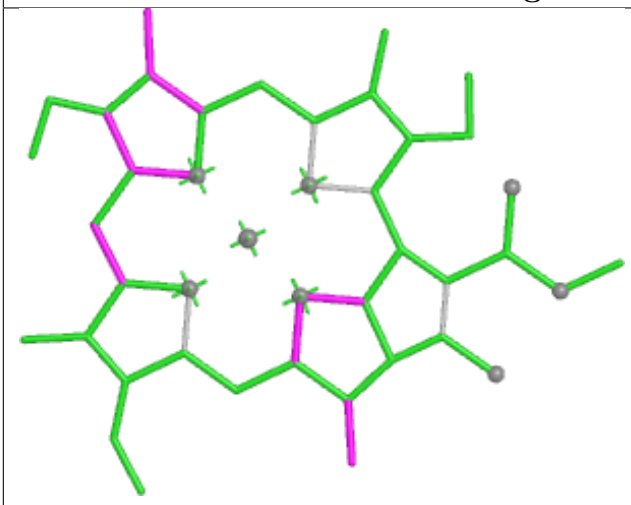


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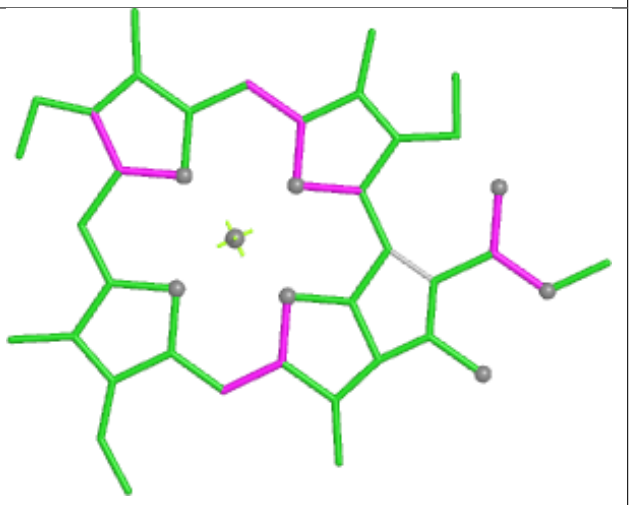


Rings

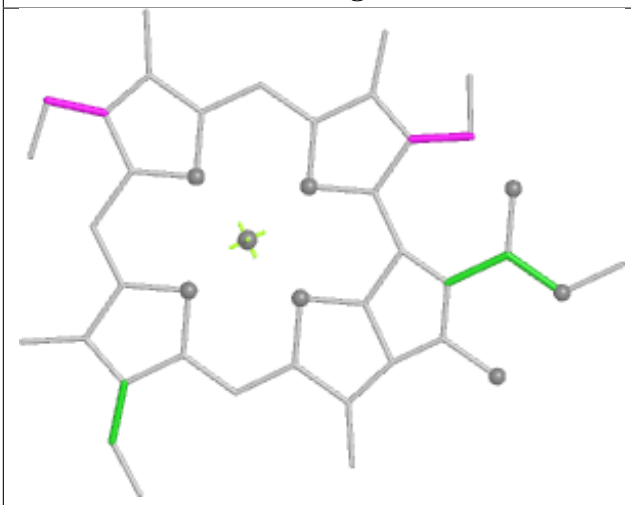
Ligand CLA X 614



Bond lengths



Bond angles

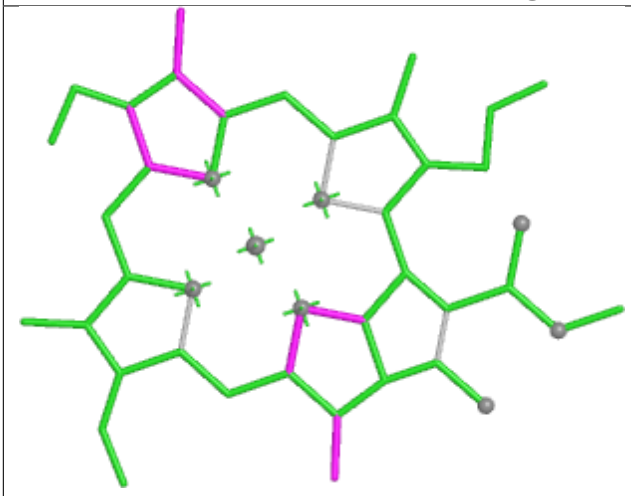


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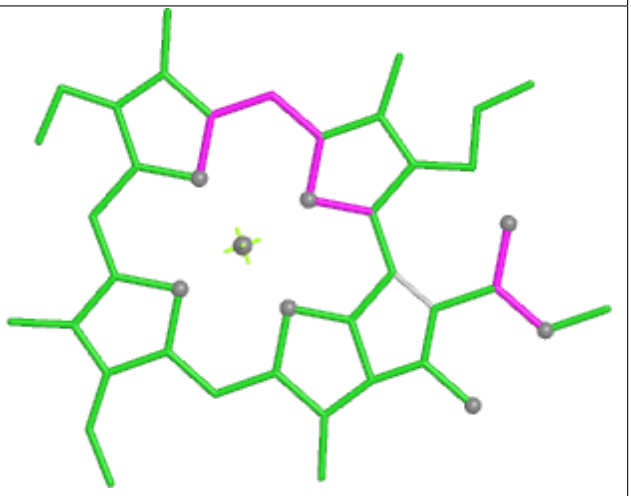


Rings

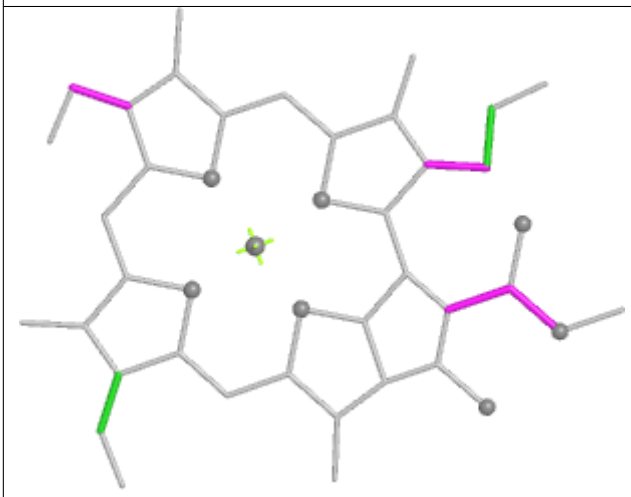
Ligand CLA Y 611



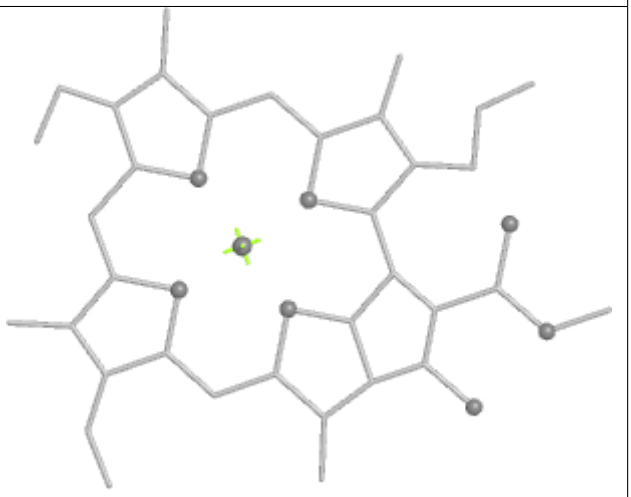
Bond lengths



Bond angles

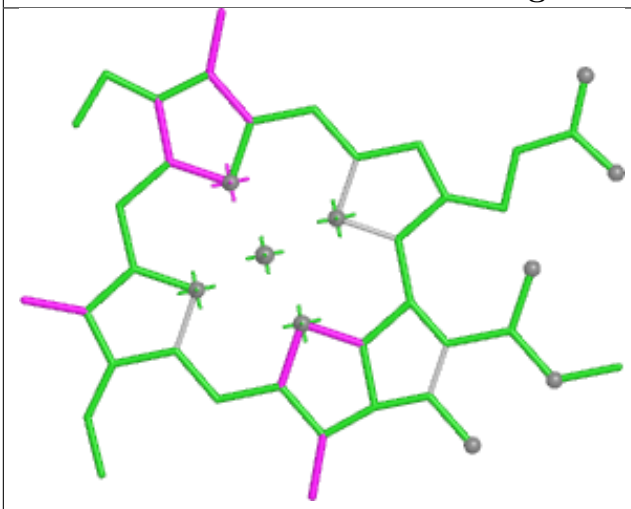


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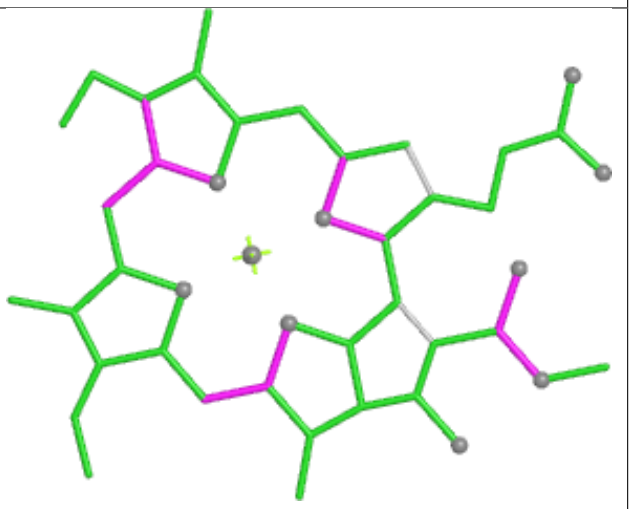


Rings

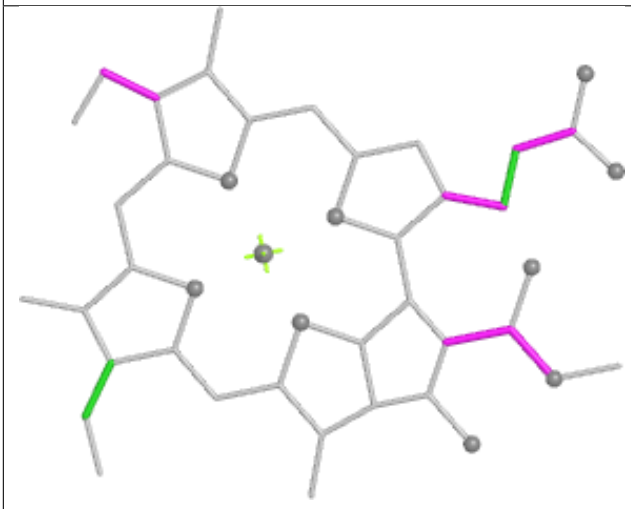
Ligand CLA 5 614



Bond lengths



Bond angles

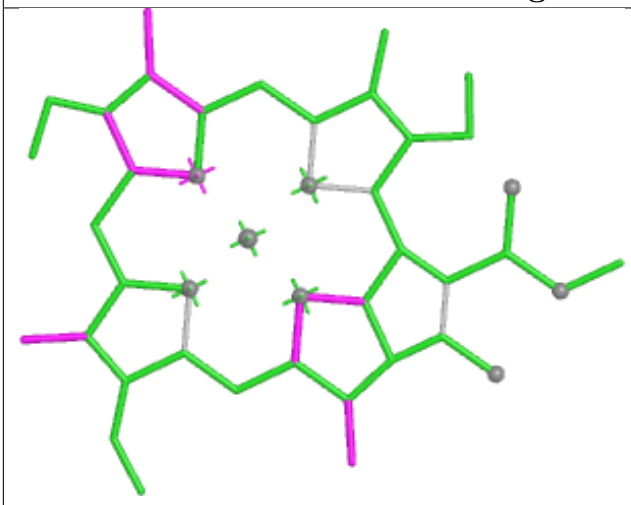


Torsions

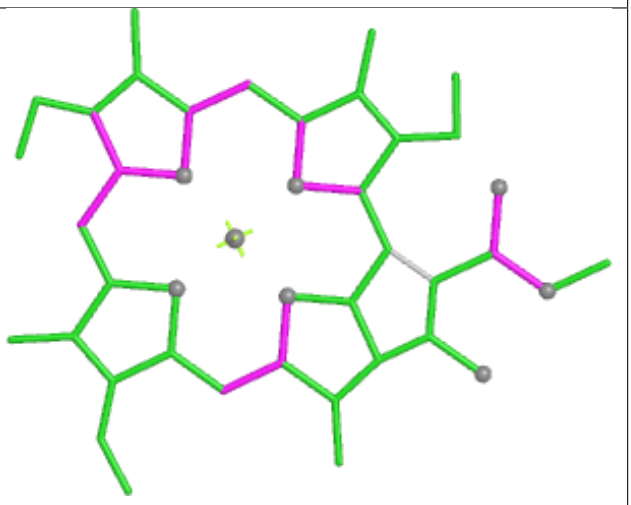


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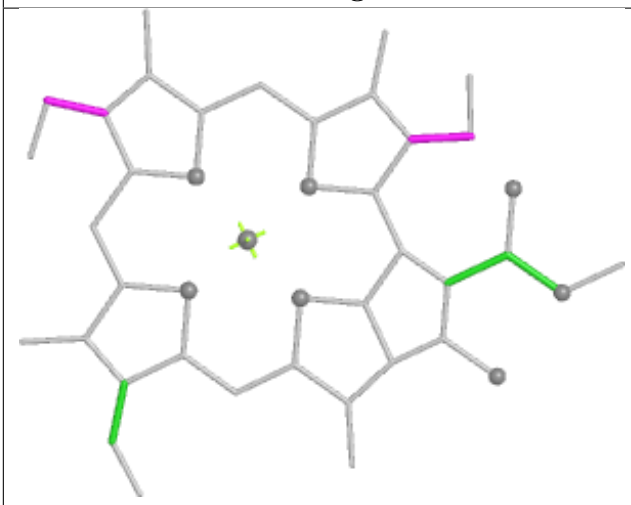
Ligand CLA 7 614



Bond lengths



Bond angles

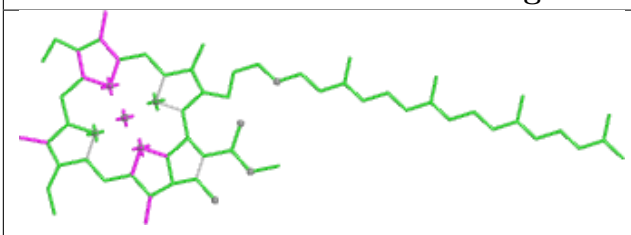


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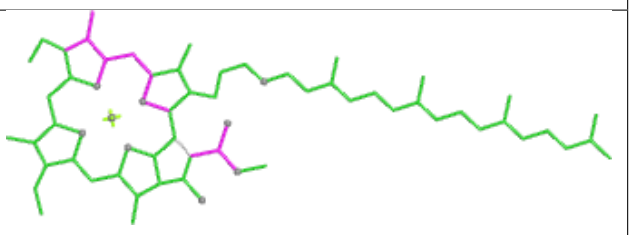


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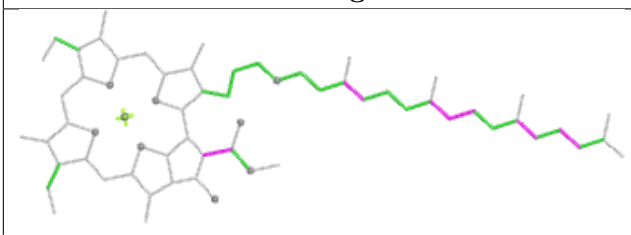
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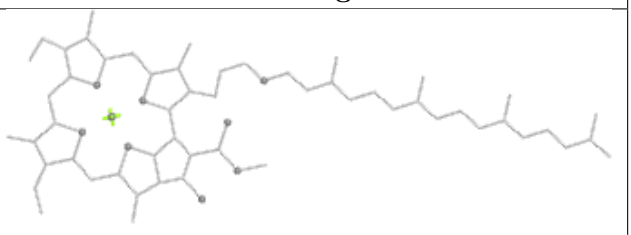
Bond lengths



Bond angles

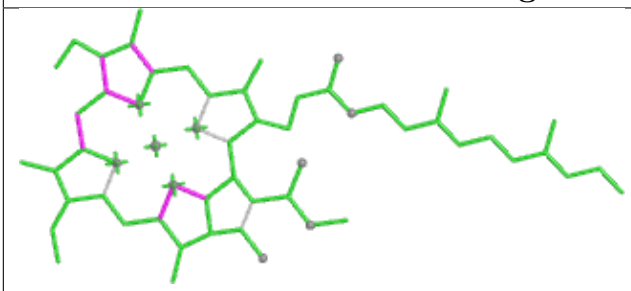


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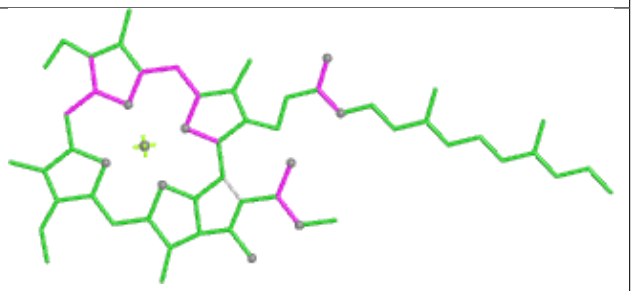


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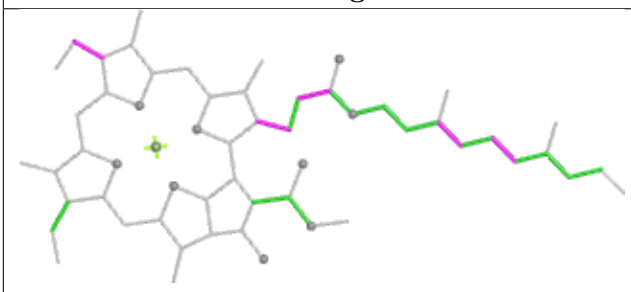
Ligand CLA W 611



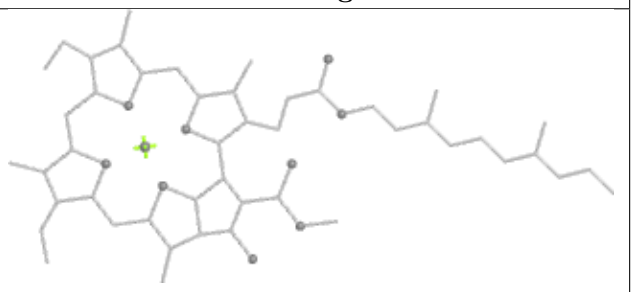
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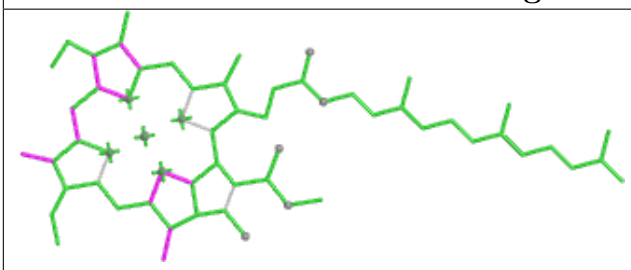


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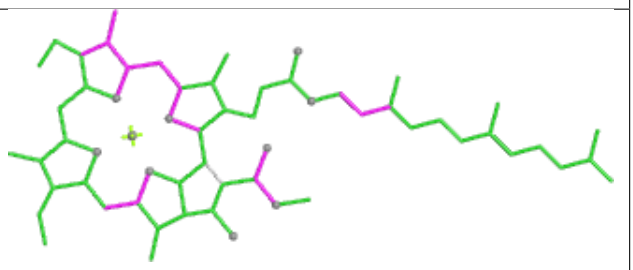


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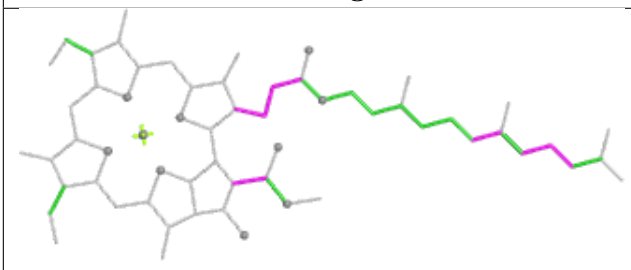
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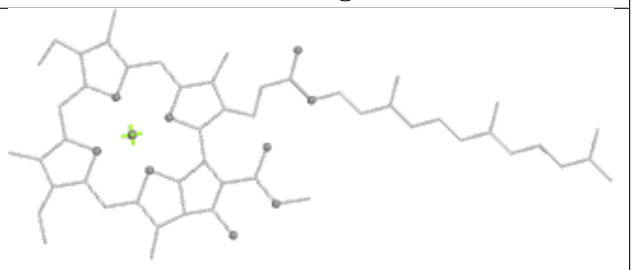
Bond lengths



Bond angles

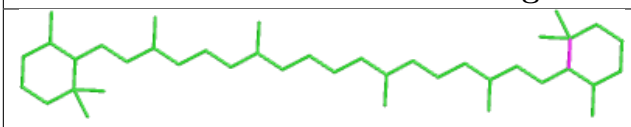


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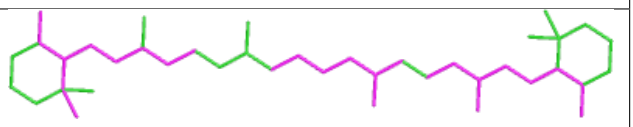


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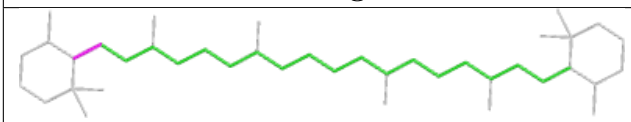
Ligand BCR A 850



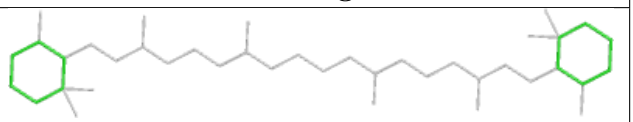
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Bond angles

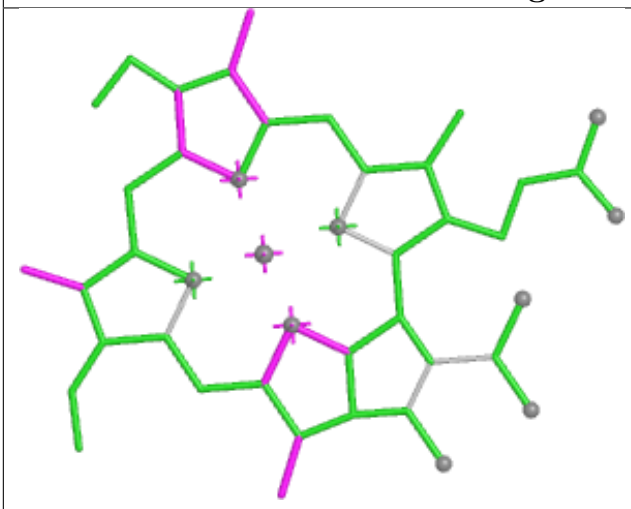


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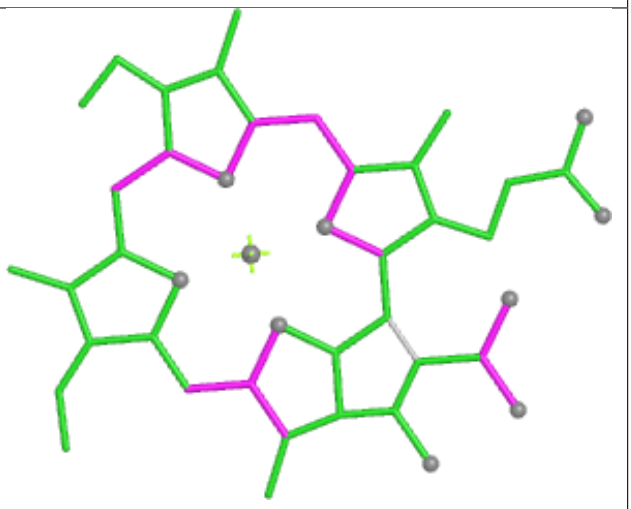


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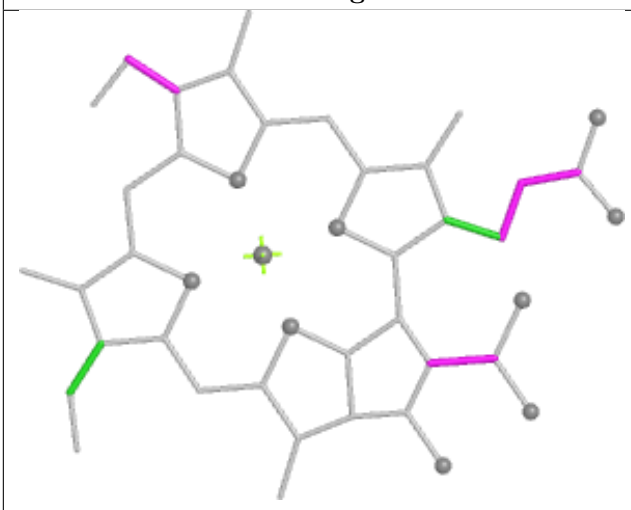
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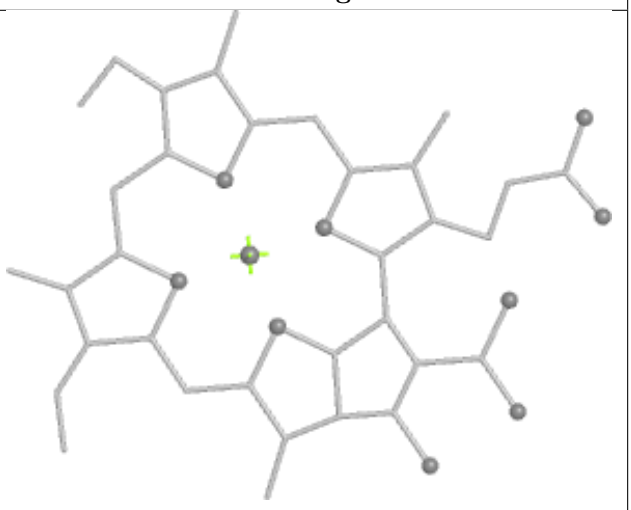
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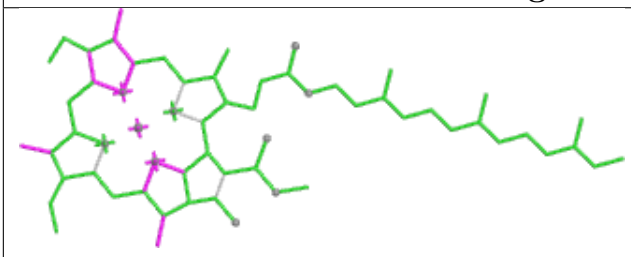


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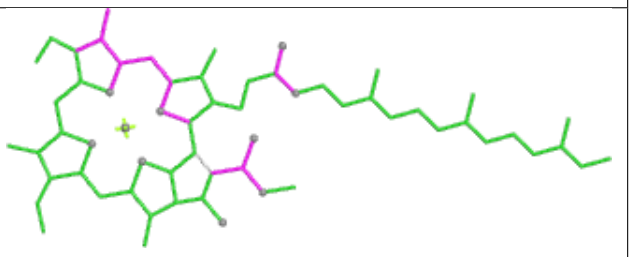


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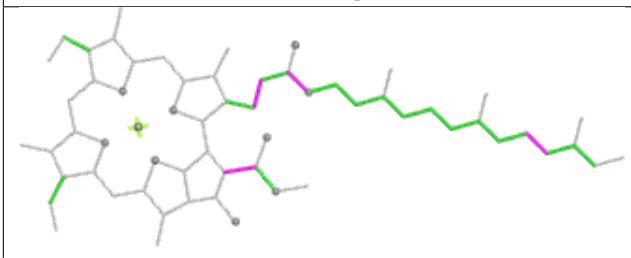
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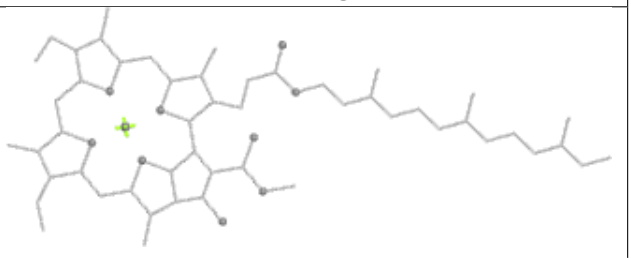
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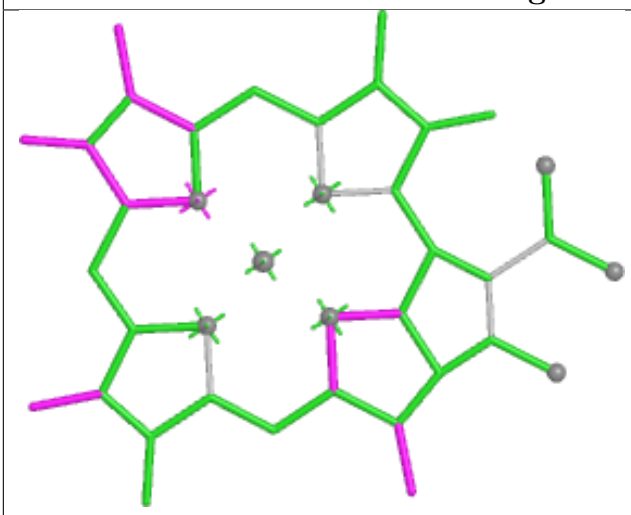


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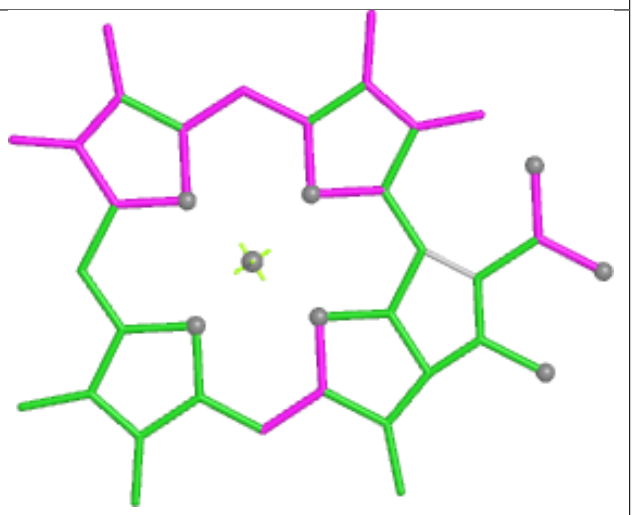


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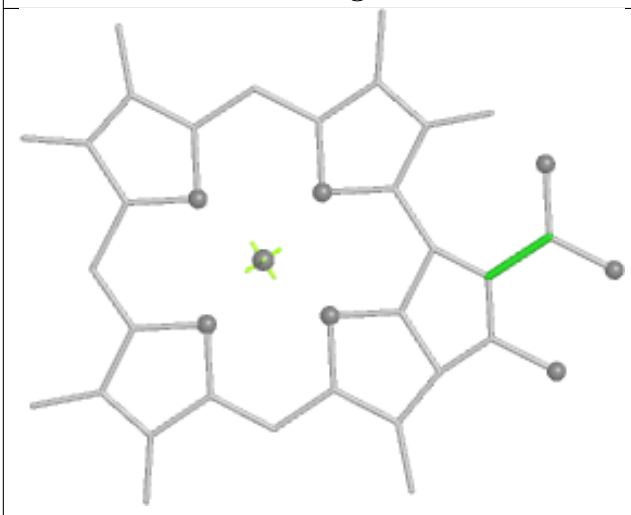
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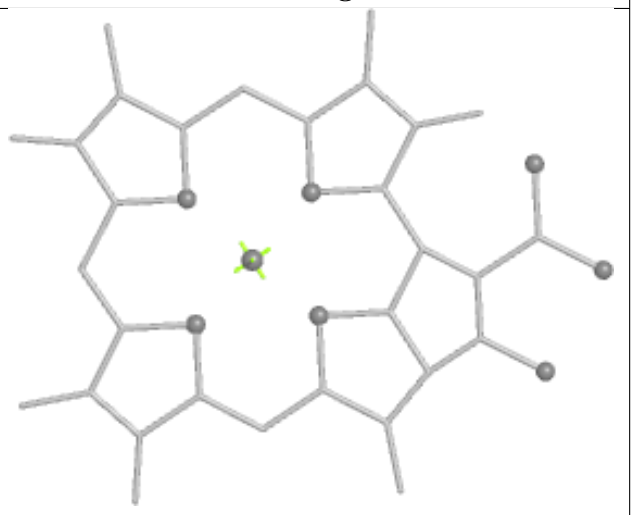
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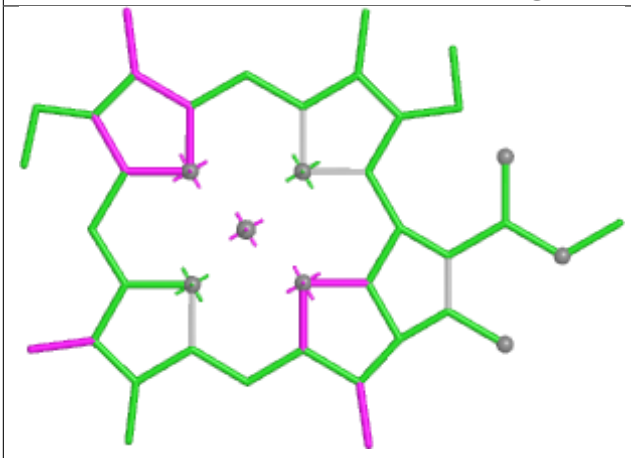


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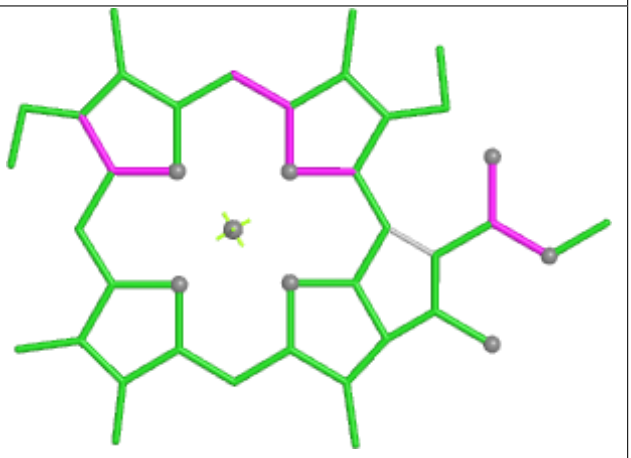


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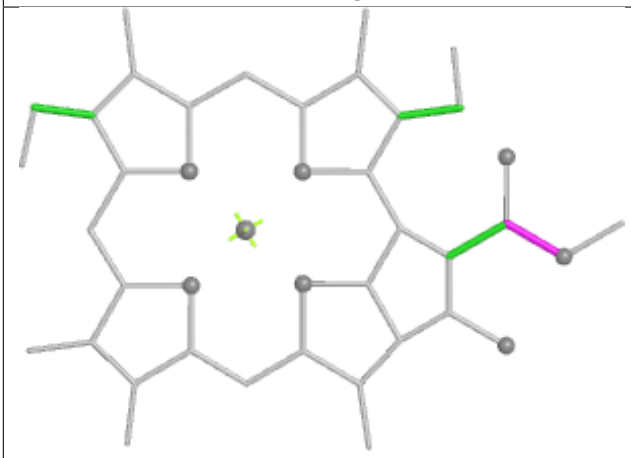
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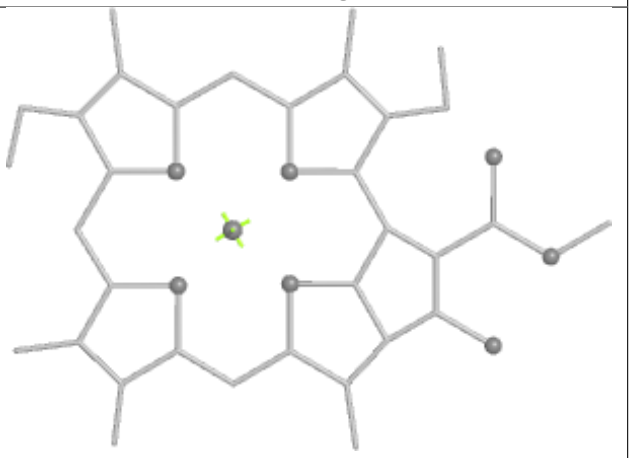
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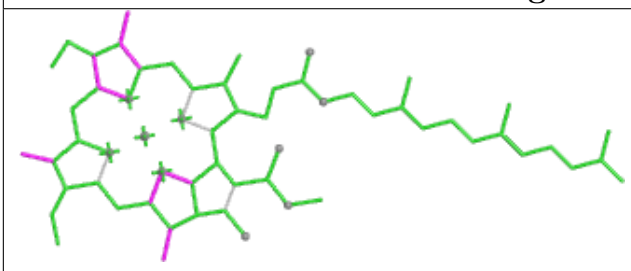


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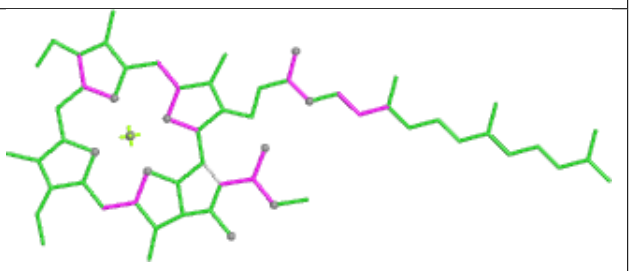


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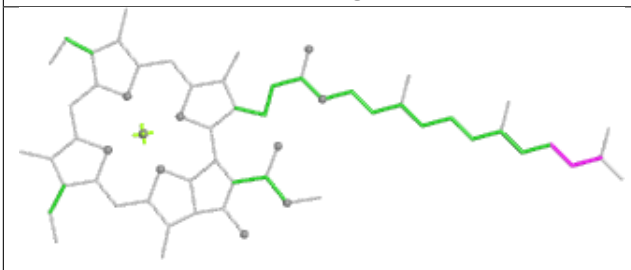
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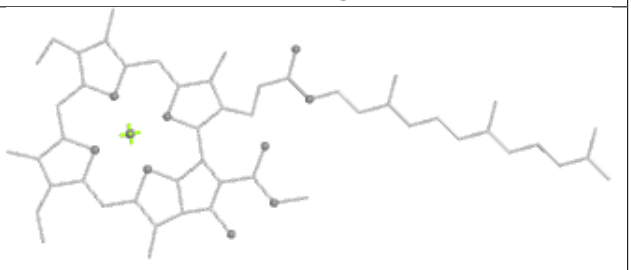
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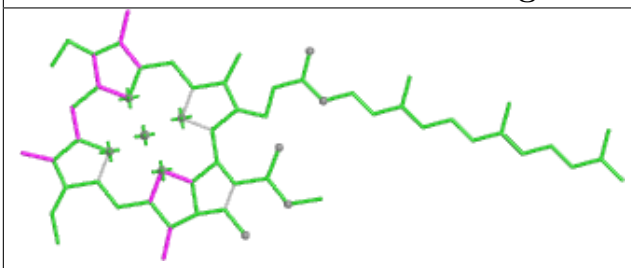


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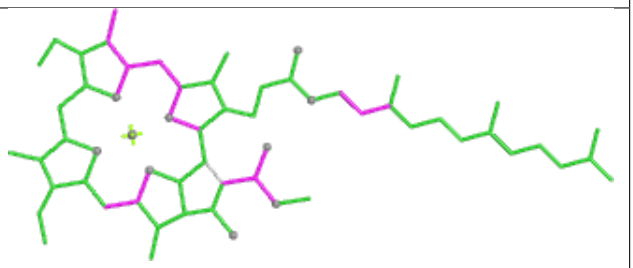


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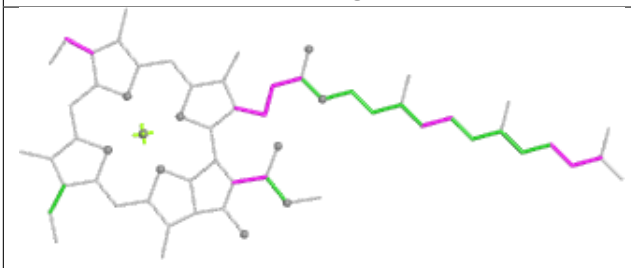
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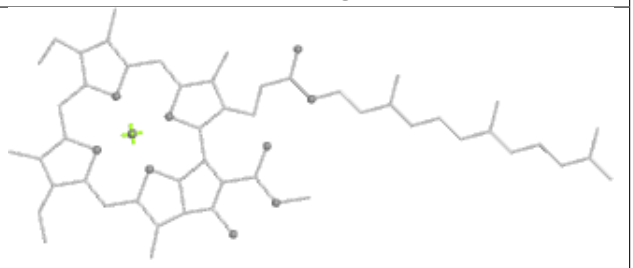
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Bond angles

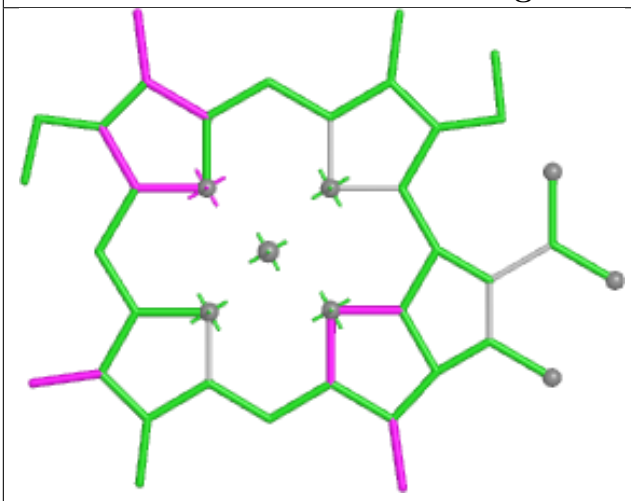


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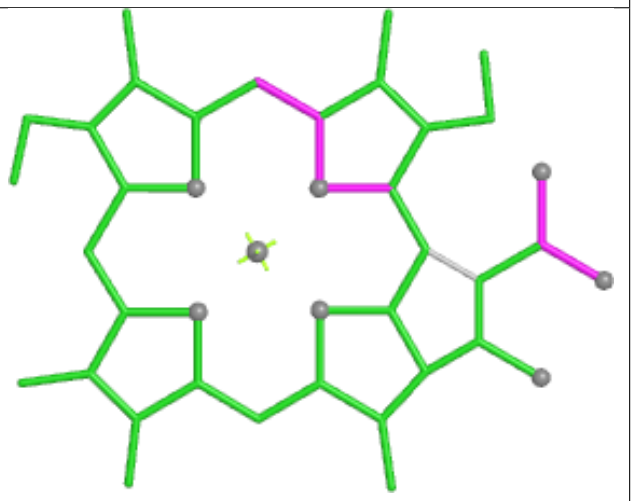


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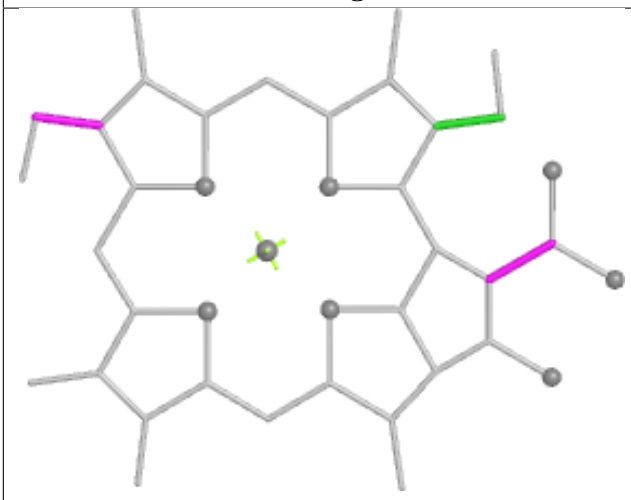
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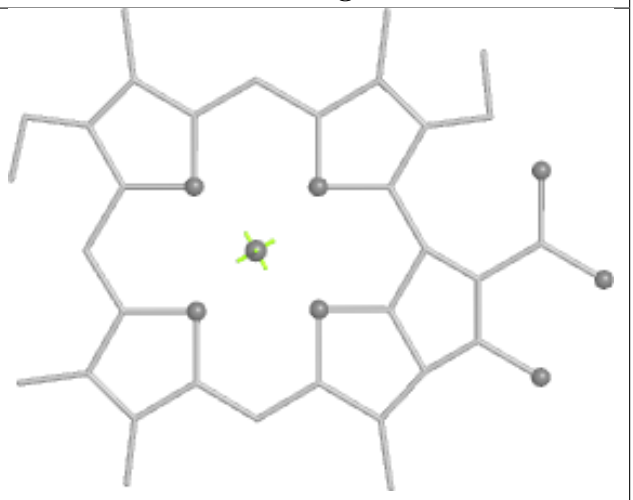
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Bond angles

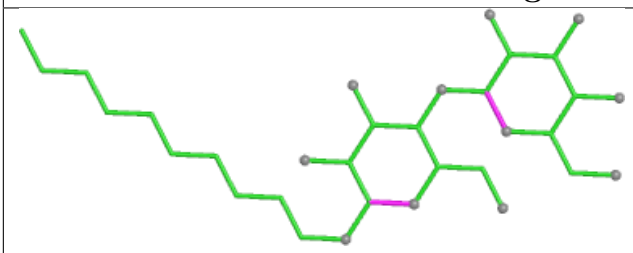


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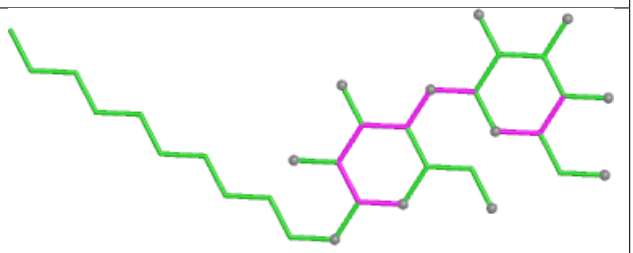


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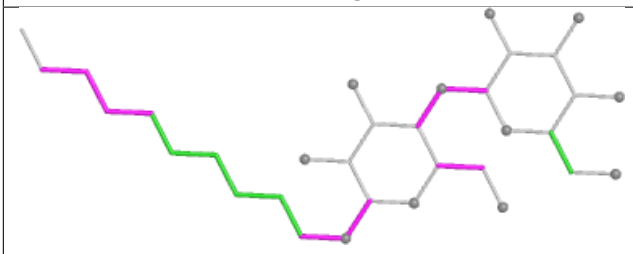
Ligand LMU 5 628



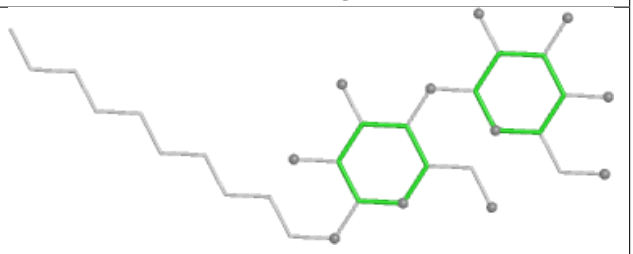
Bond lengths



Bond angles

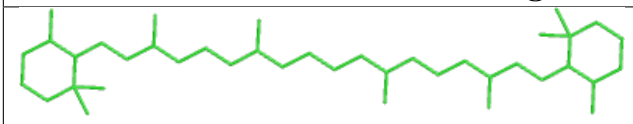


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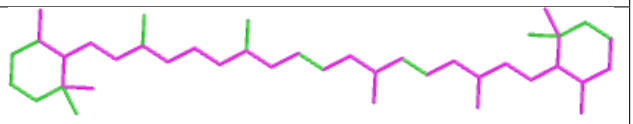


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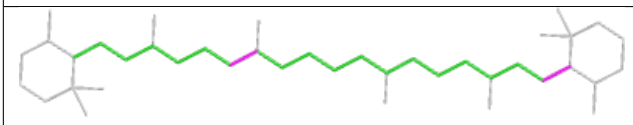
Ligand BCR a 619



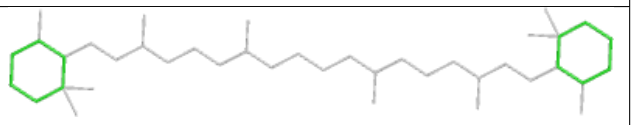
Bond lengths



Bond angles

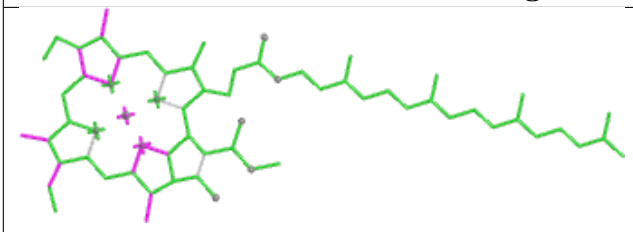


Torsions

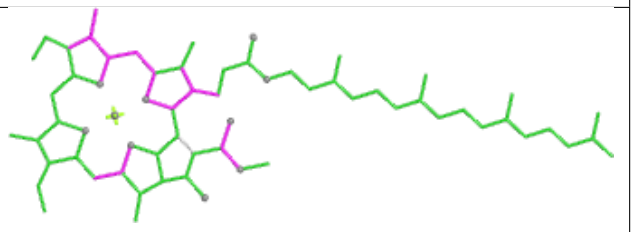


Rings

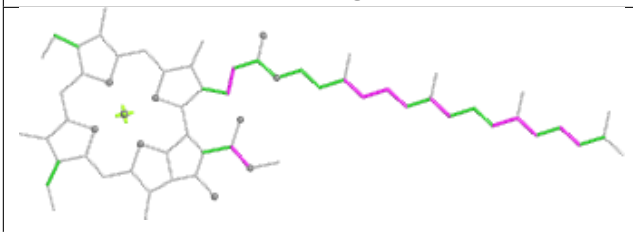
Ligand CLA A 802



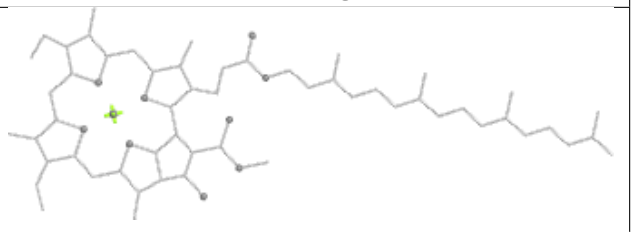
Bond lengths



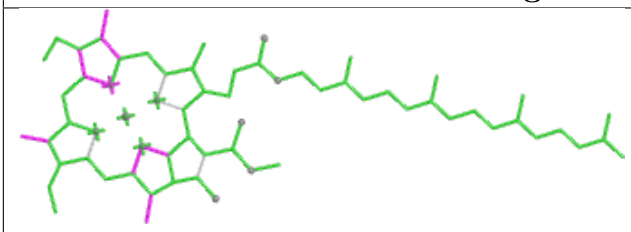
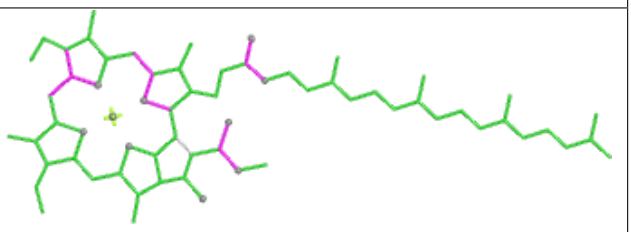
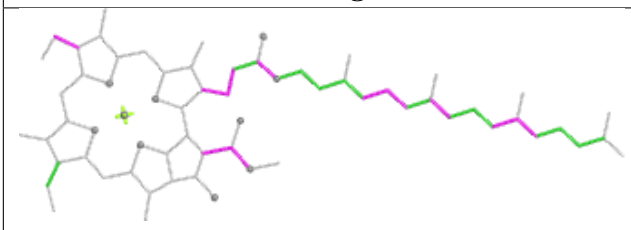
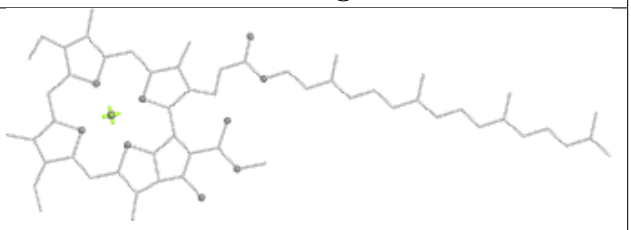
Bond angles

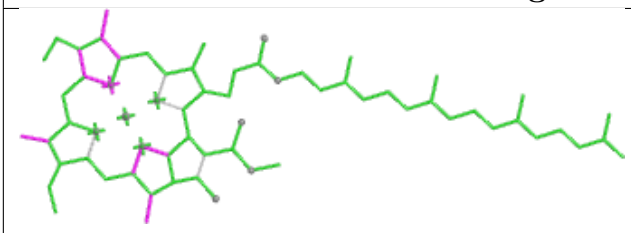
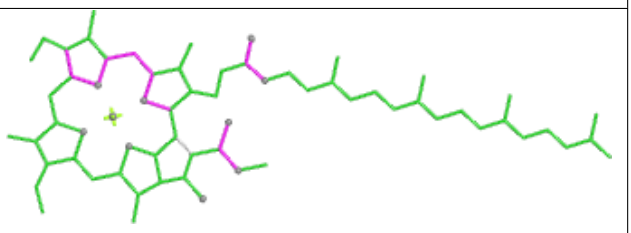
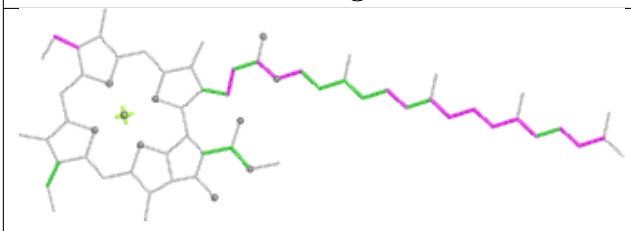
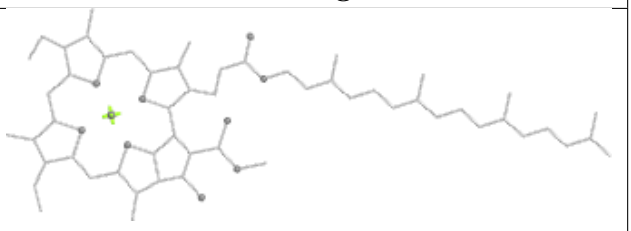


Torsions

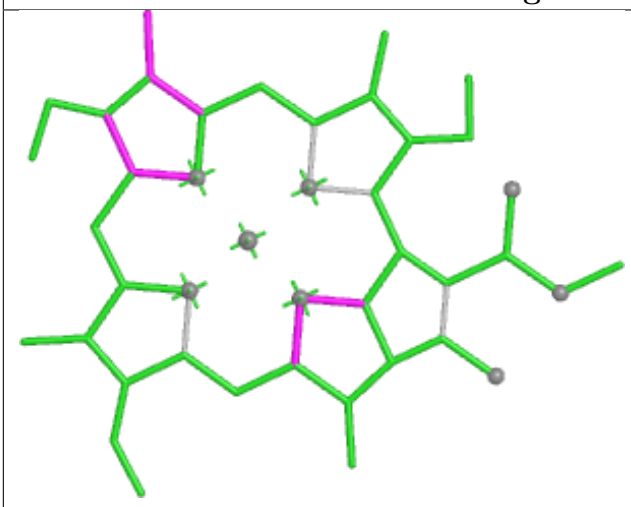


Rings

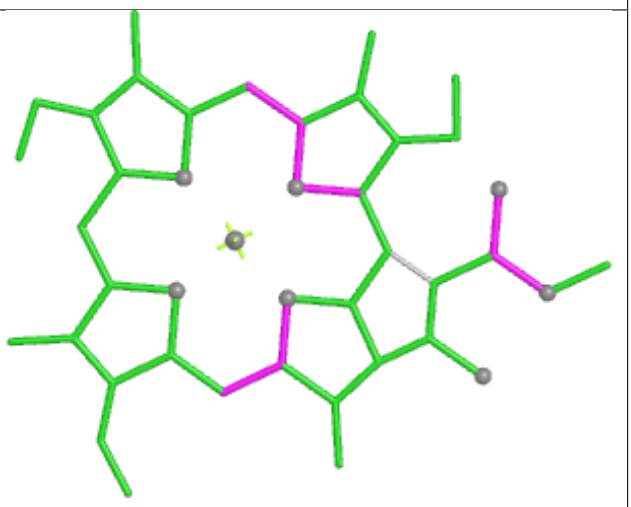
Ligand CLA A 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 8 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

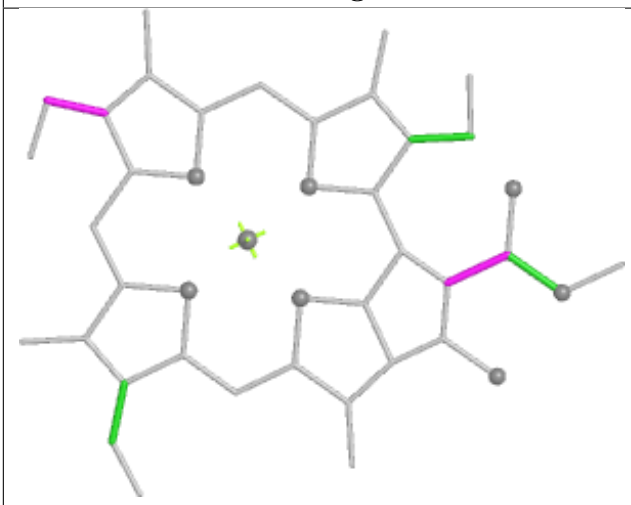
Ligand CLA U 611



Bond lengths



Bond angles

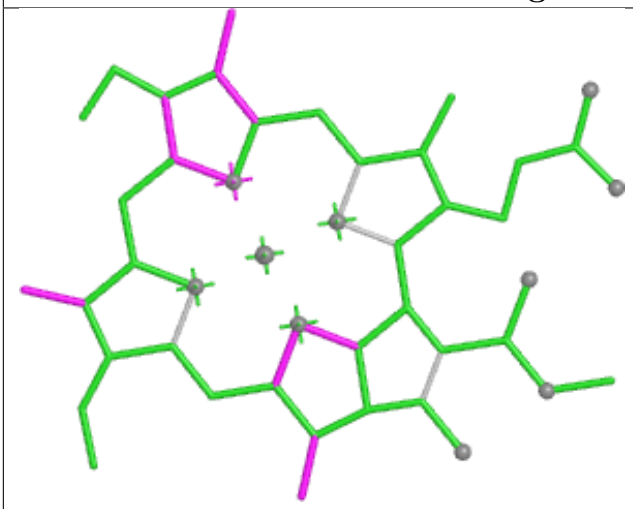


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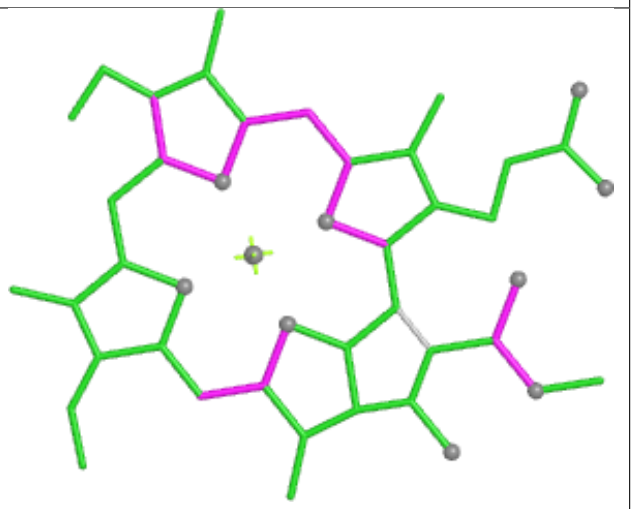


Rings

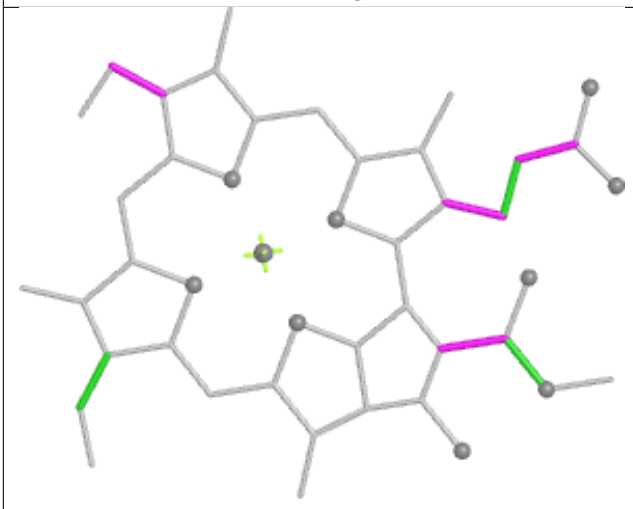
Ligand CLA 6 609



Bond lengths



Bond angles

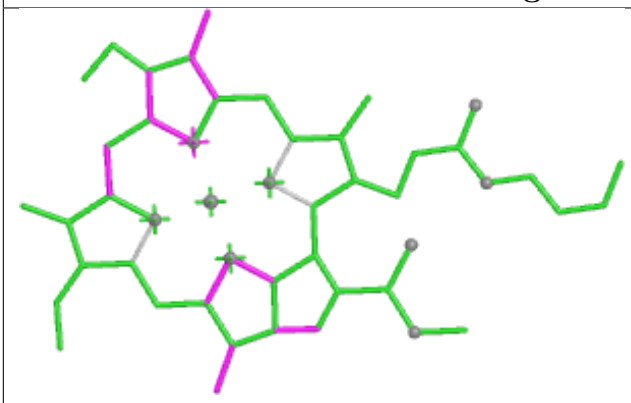


Torsions

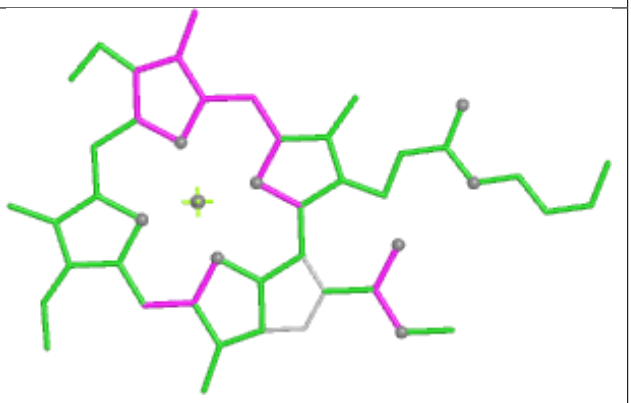


Rings

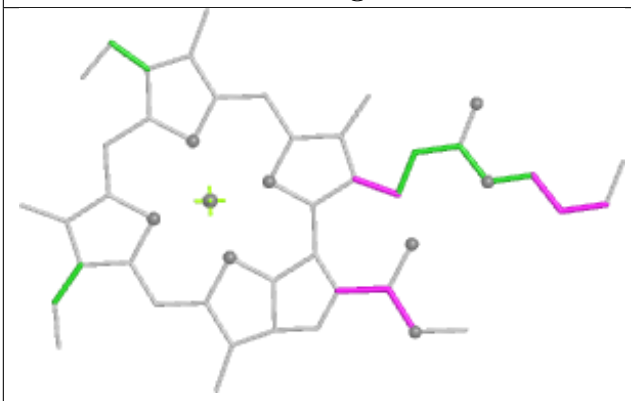
Ligand CLA U 604



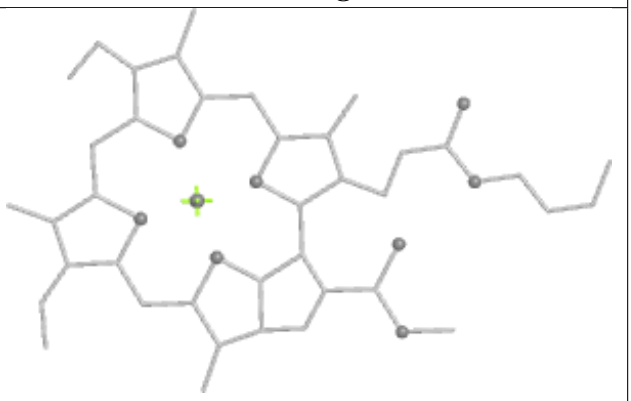
Bond lengths



Bond angles

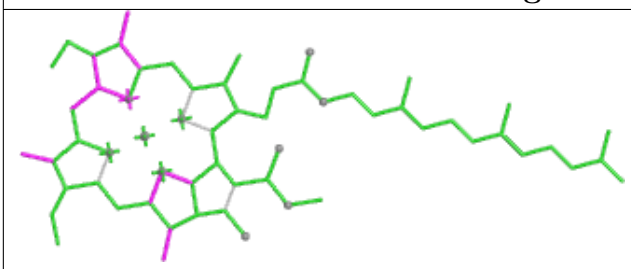


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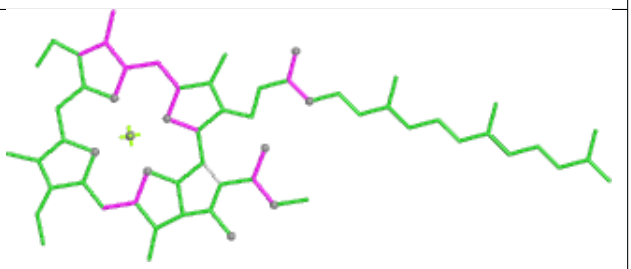


Rings

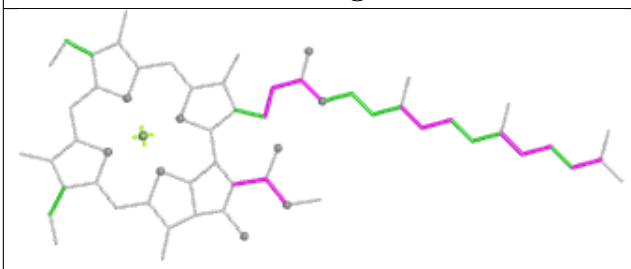
Ligand CLA A 818



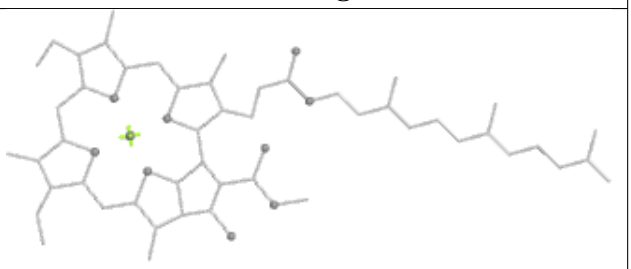
Bond lengths



Bond angles

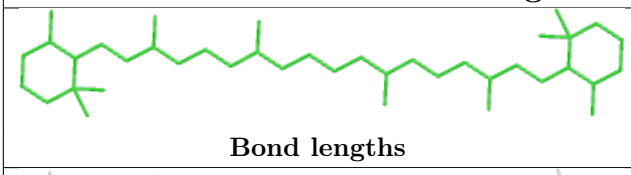


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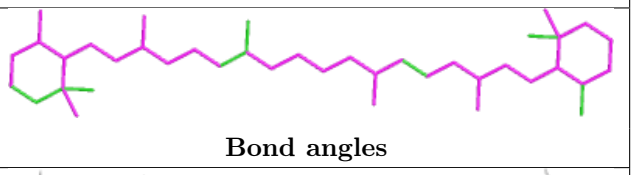


Rings

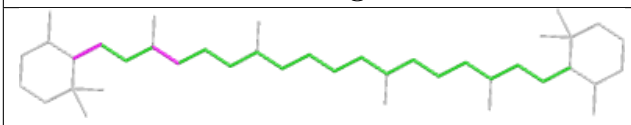
Ligand BCR L 301



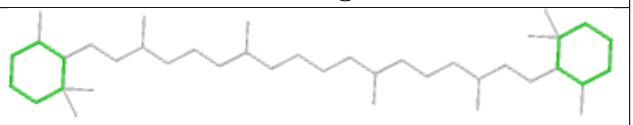
Bond lengths



Bond angles

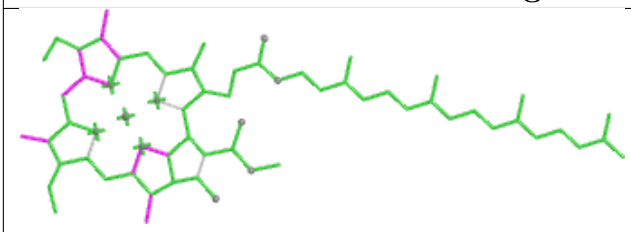


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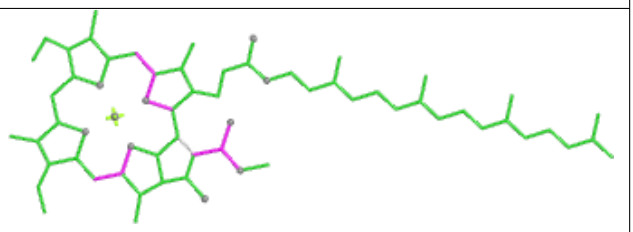


Rings

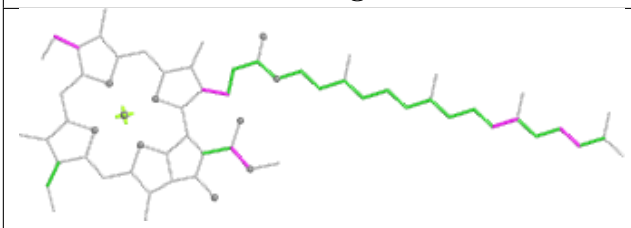
Ligand CLA A 812



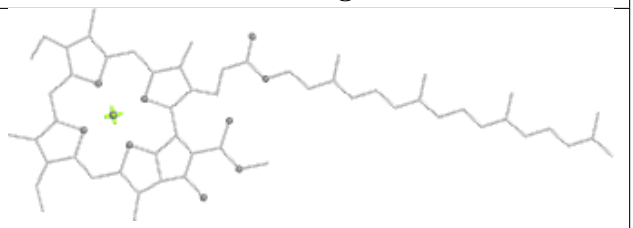
Bond lengths



Bond angles

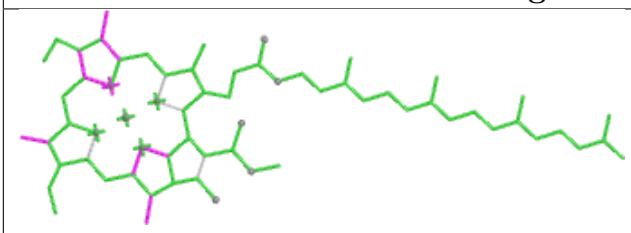


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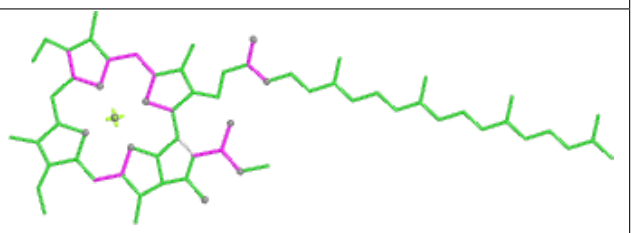


Rings

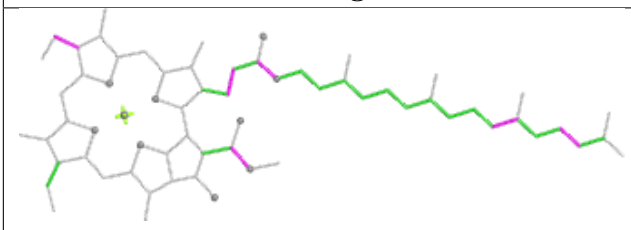
Ligand CLA 6 602



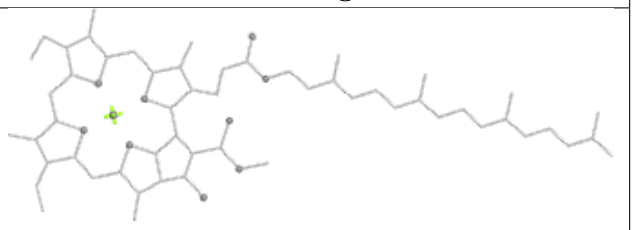
Bond lengths



Bond angles

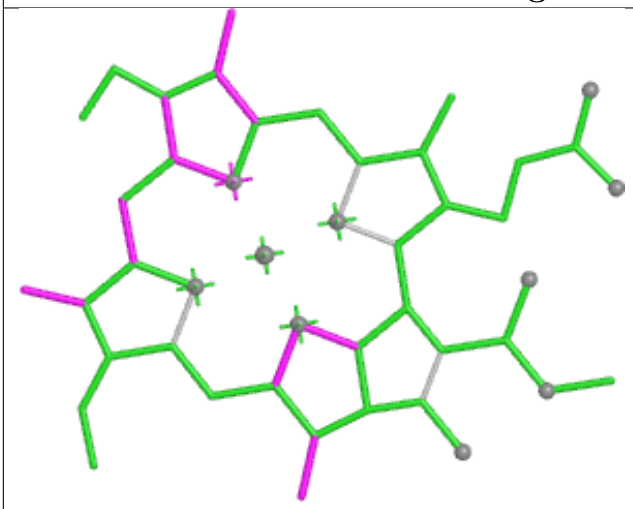


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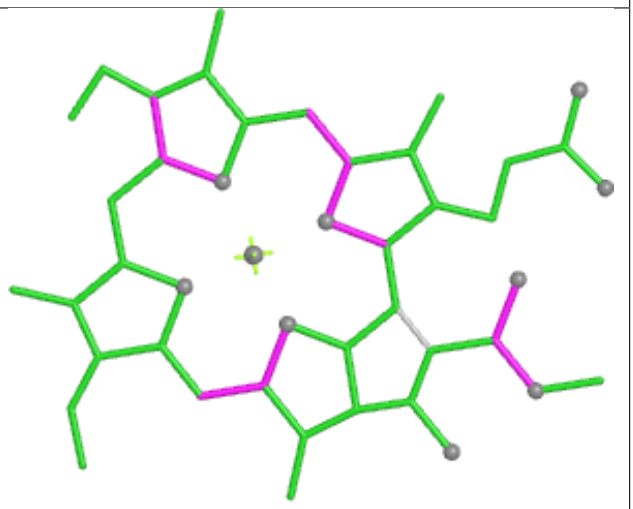


Rings

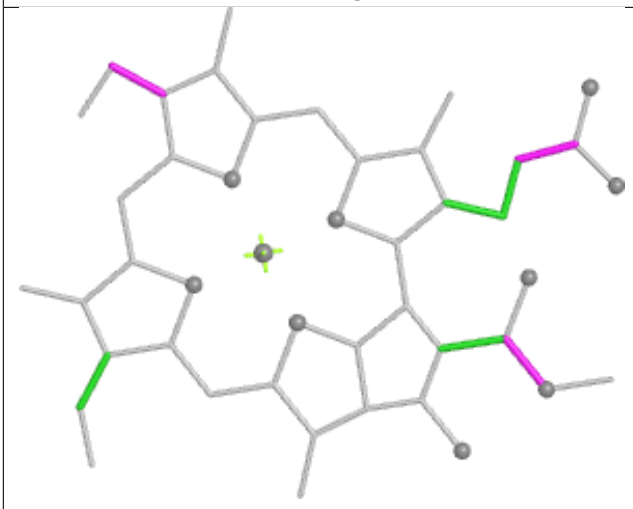
Ligand CLA a 607



Bond lengths



Bond angles

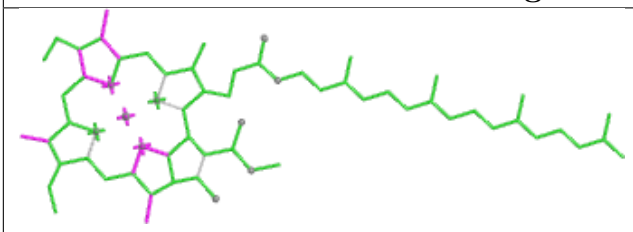


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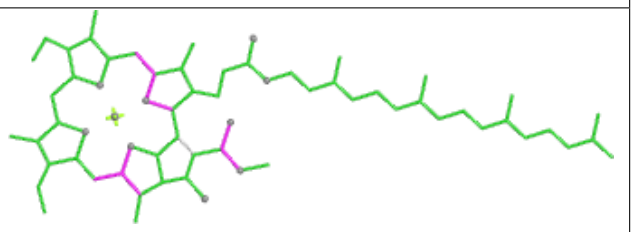


Rings

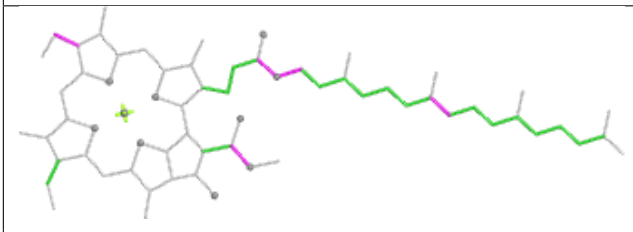
Ligand CLA B 840



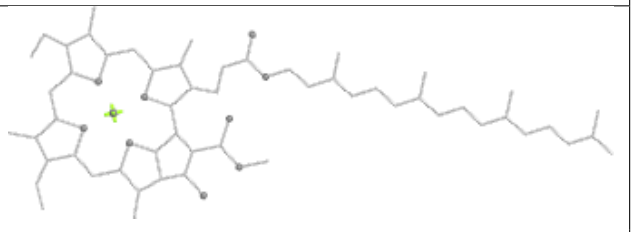
Bond lengths



Bond angles

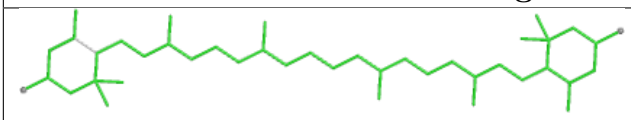


Torsions

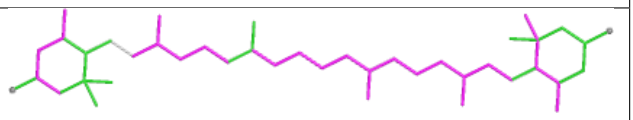


Rings

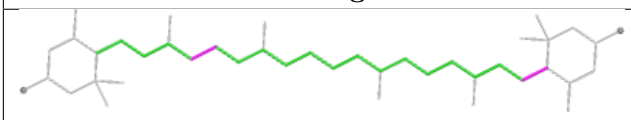
Ligand LUT X 1621



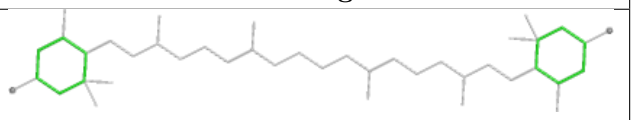
Bond lengths



Bond angles

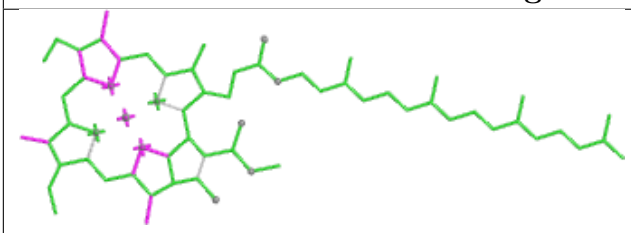


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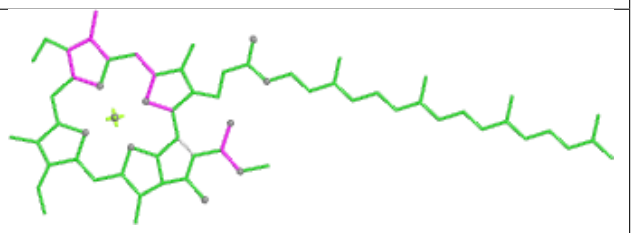


Rings

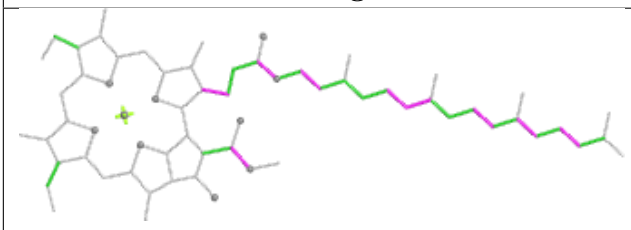
Ligand CLA B 803



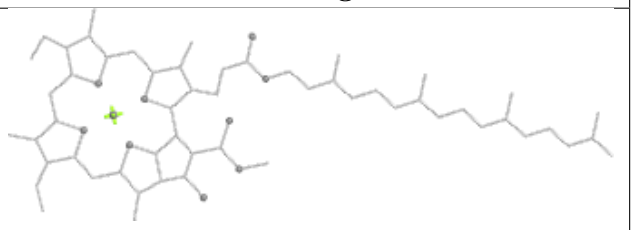
Bond lengths



Bond angles

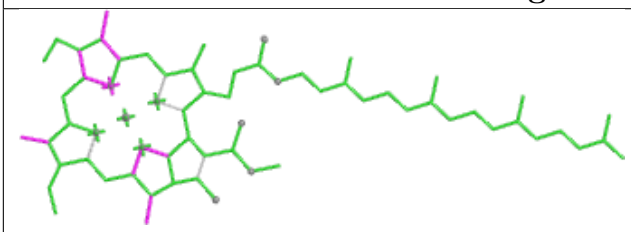


Torsions

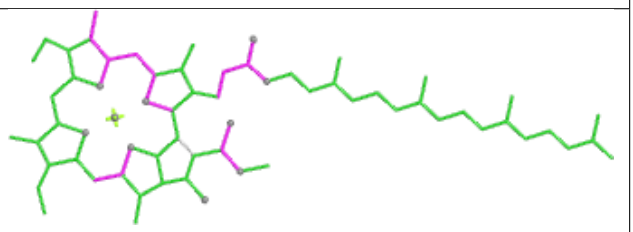


Rings

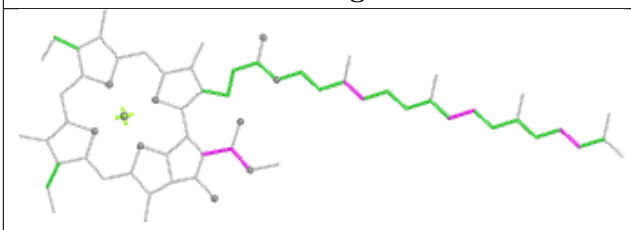
Ligand CLA 3 604



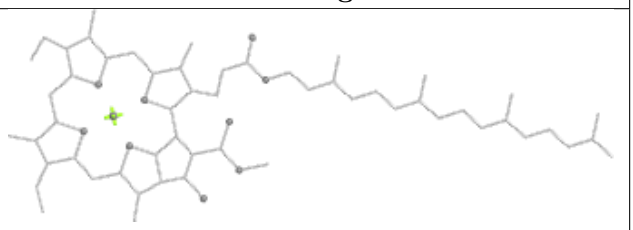
Bond lengths



Bond angles

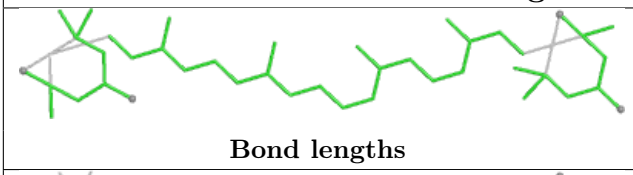


Torsions

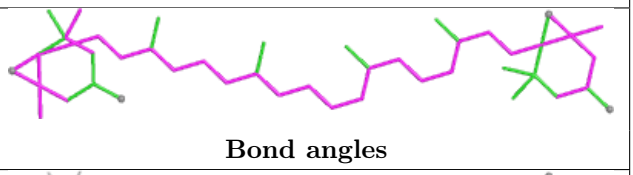


Rings

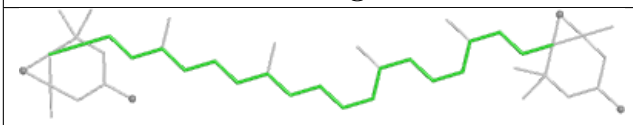
Ligand XAT a 618



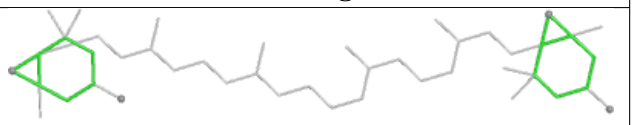
Bond lengths



Bond angles

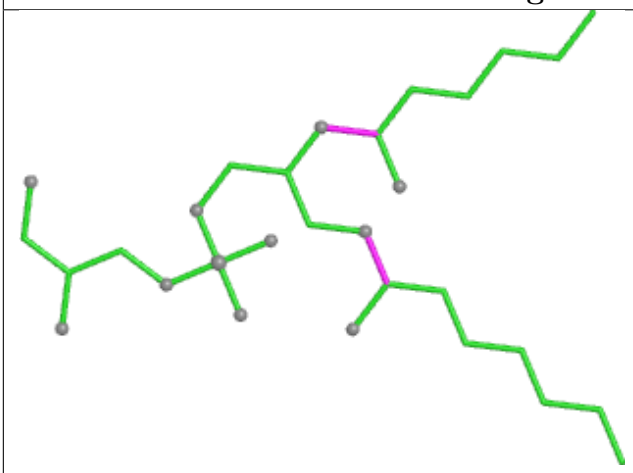


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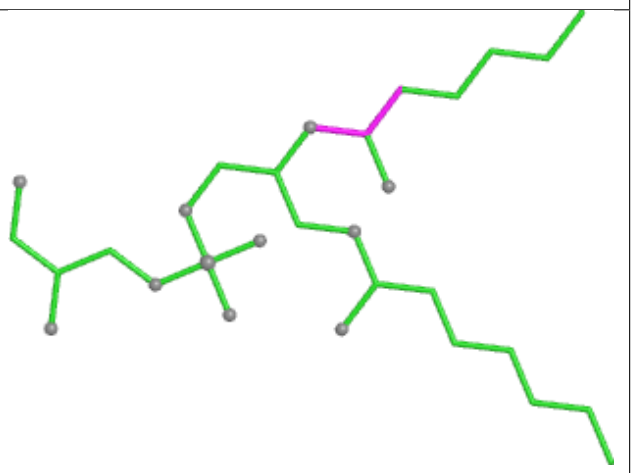


Rings

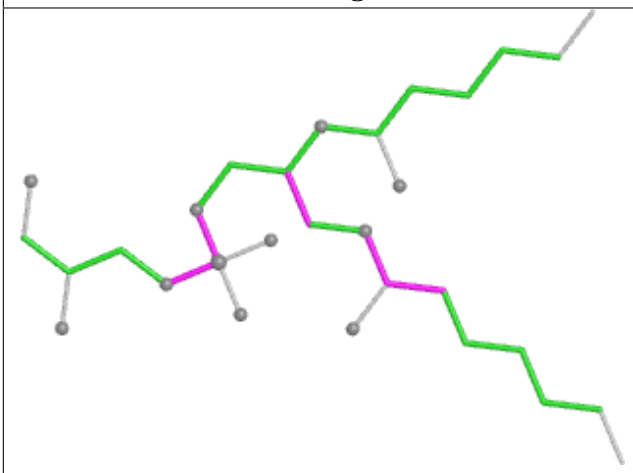
Ligand LHG 9 622



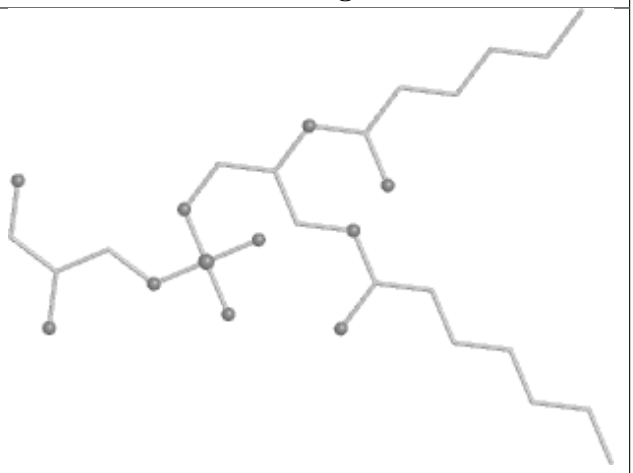
Bond lengths



Bond angles

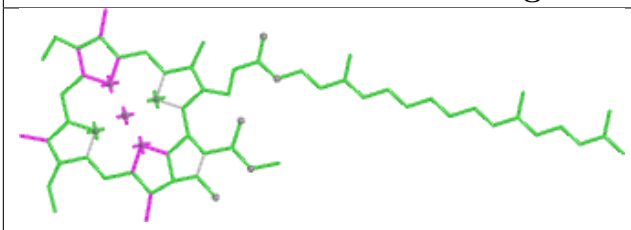


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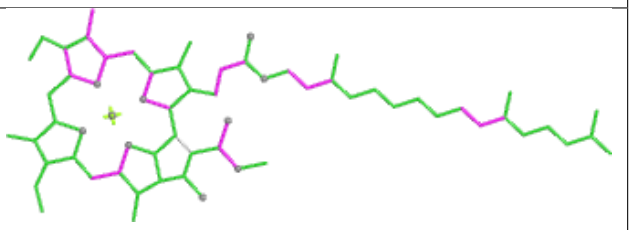


Rings

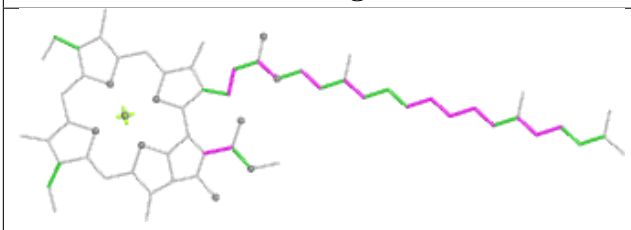
Ligand CLA A 843



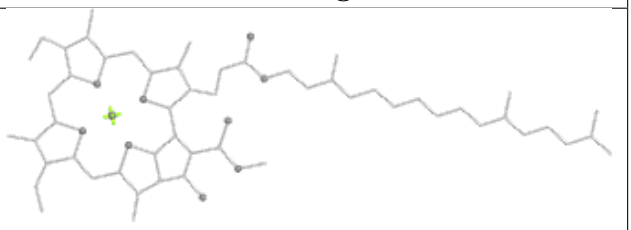
Bond lengths



Bond angles

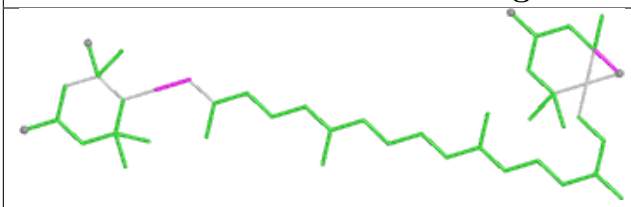


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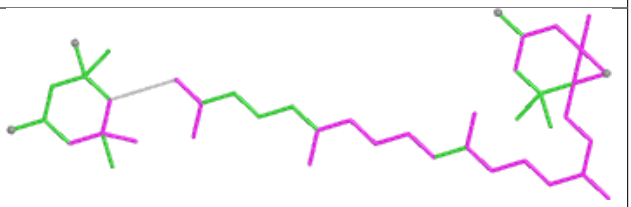


Rings

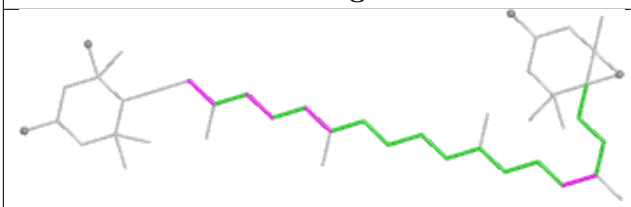
Ligand NEX V 1623



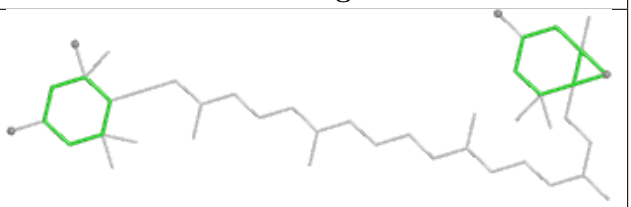
Bond lengths



Bond angles

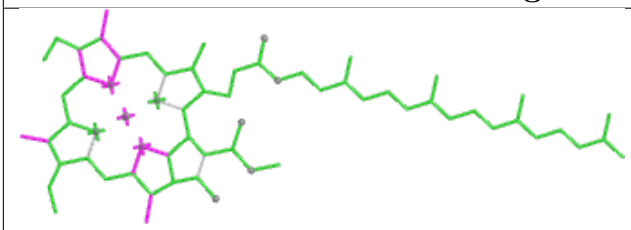


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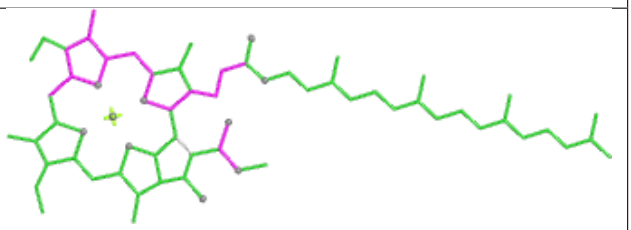


Rings

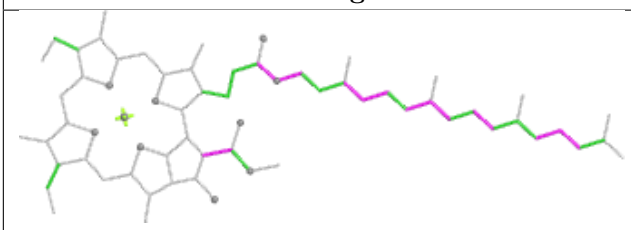
Ligand CLA A 828



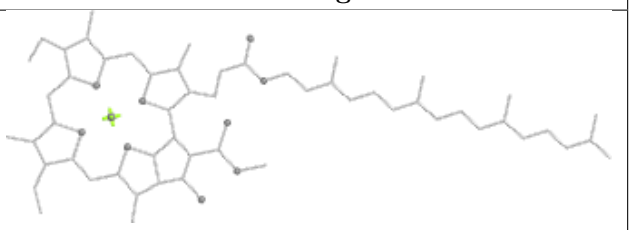
Bond lengths



Bond angles

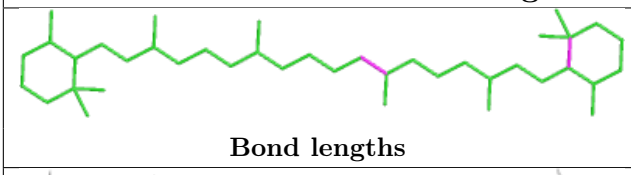


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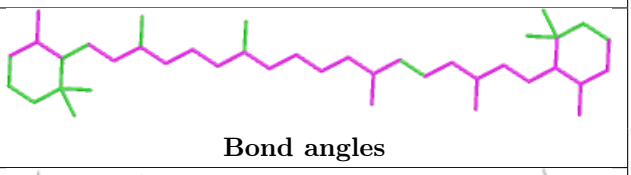


Rings

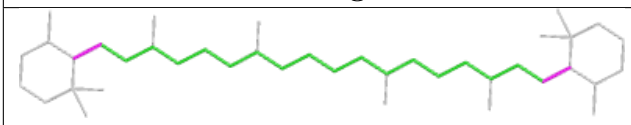
Ligand BCR K 202



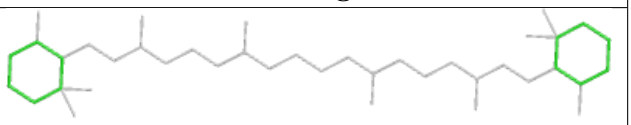
Bond lengths



Bond angles

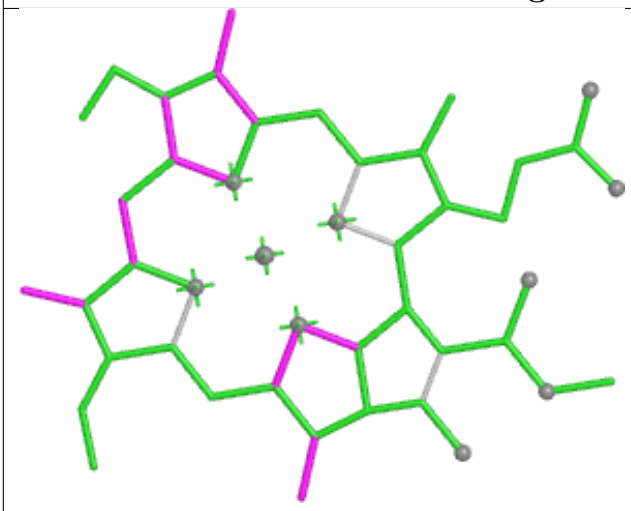


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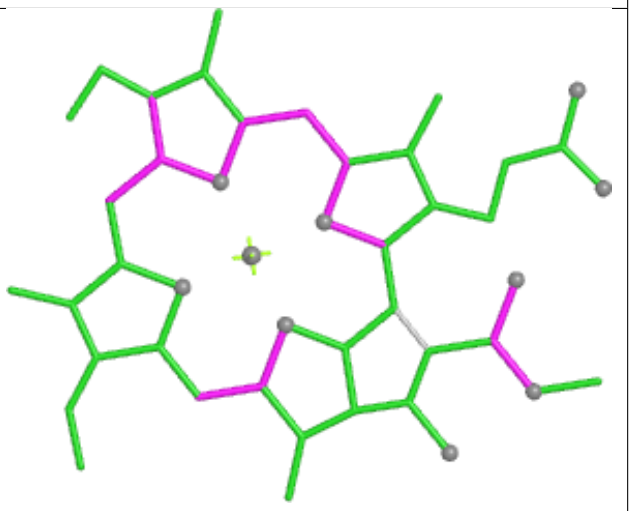


Rings

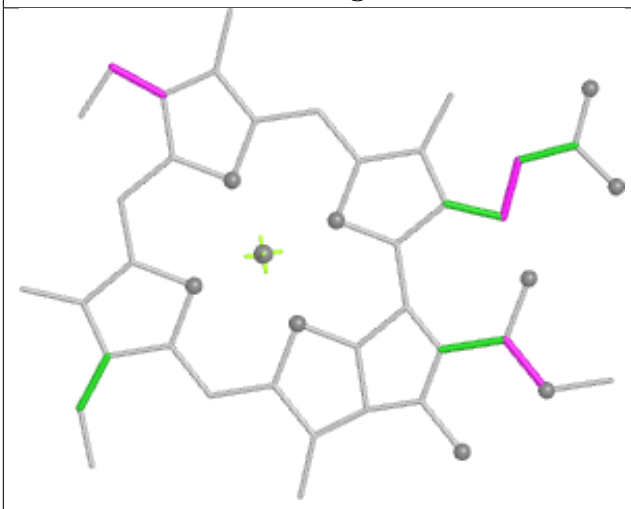
Ligand CLA 9 614



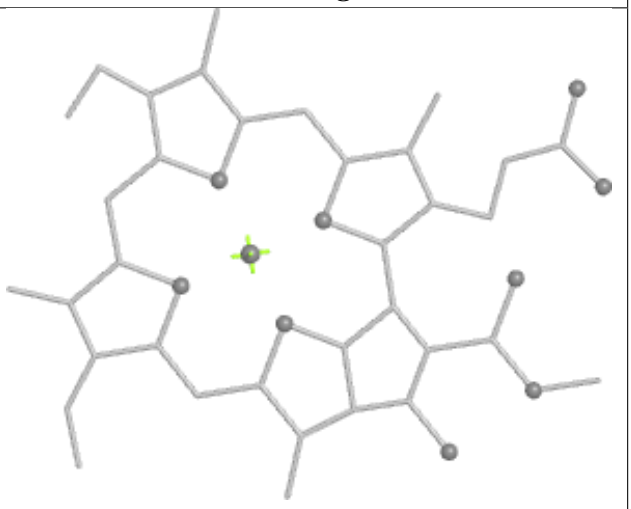
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Bond angles

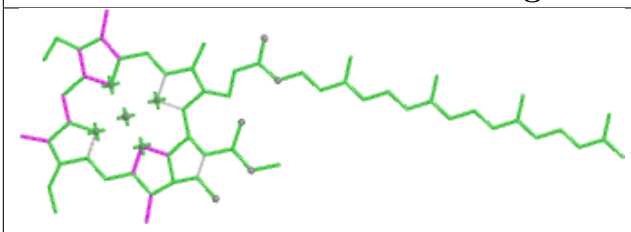


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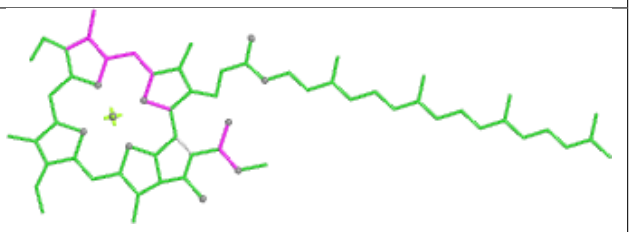


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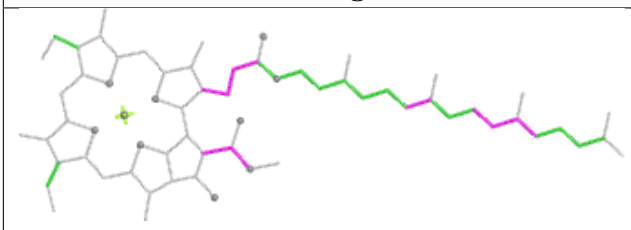
Ligand CLA X 602



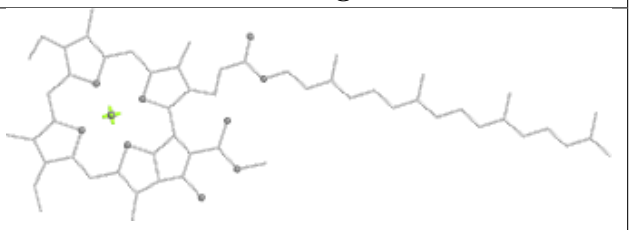
Bond lengths



Bond angles

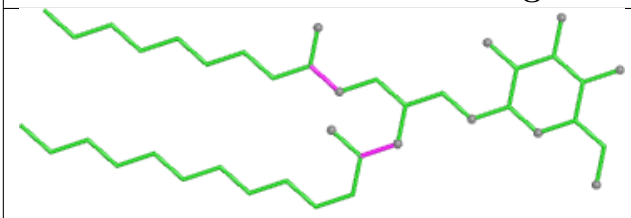


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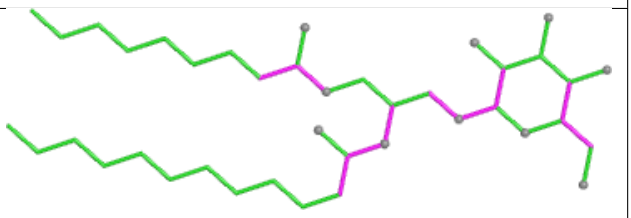


Rings

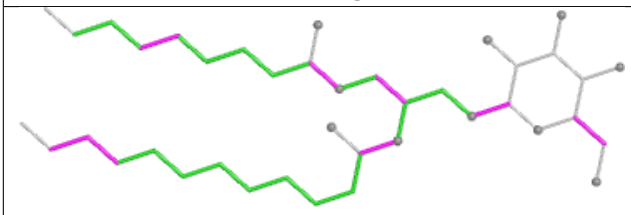
Ligand LMG J 104



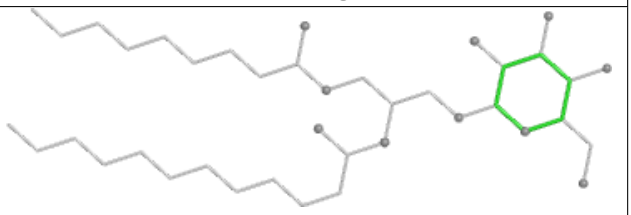
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Bond angles

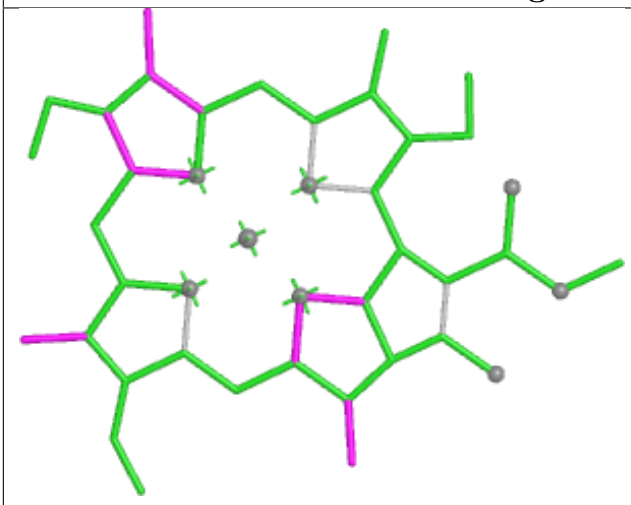


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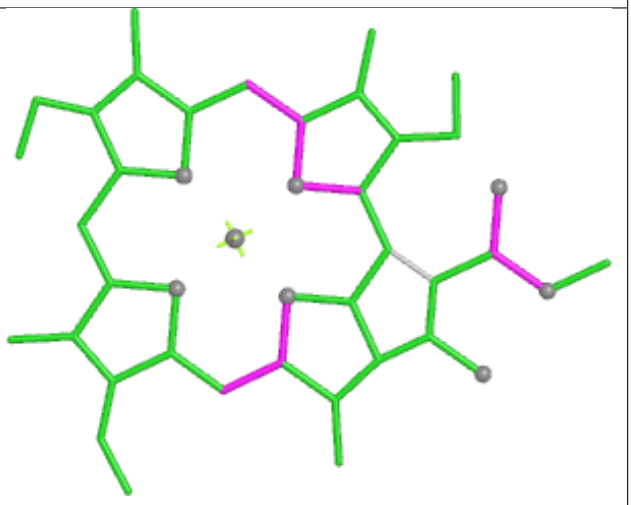


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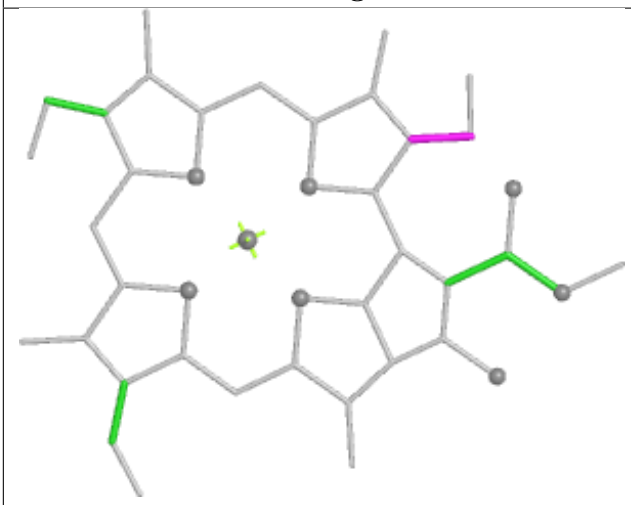
Ligand CLA 7 607



Bond lengths



Bond angles

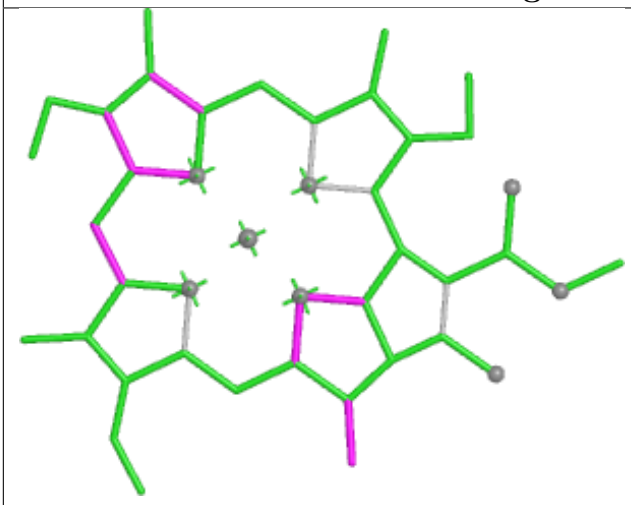


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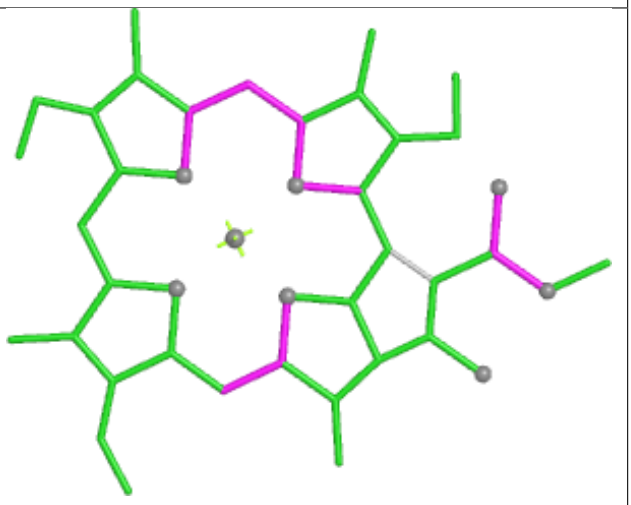


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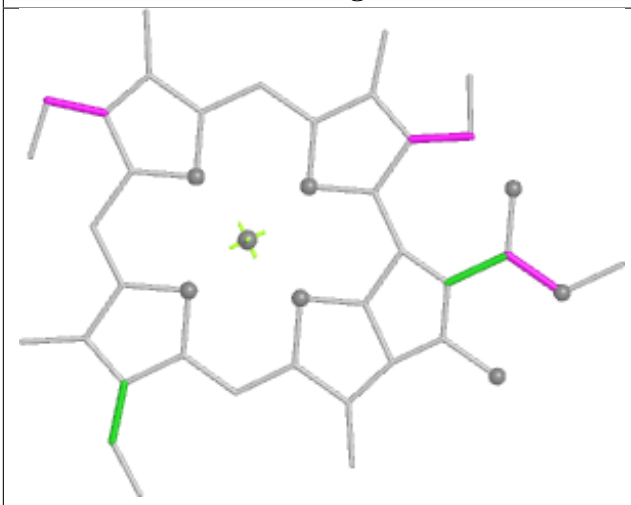
Ligand CLA U 614



Bond lengths



Bond angles

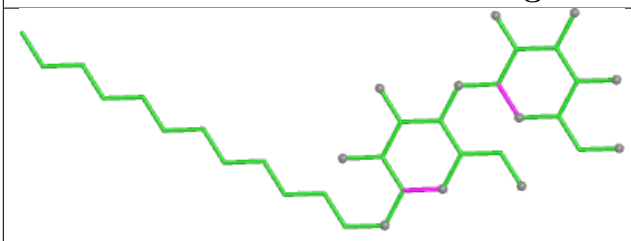


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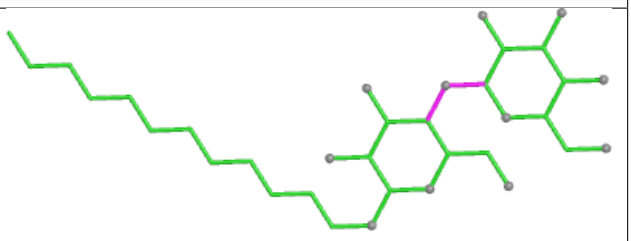


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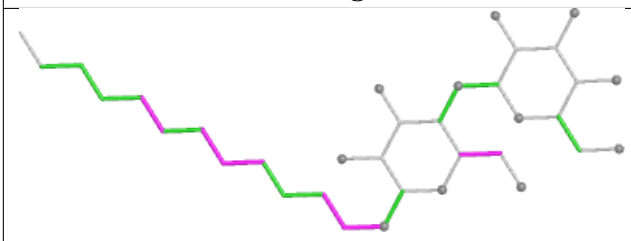
Ligand LMU 1 621



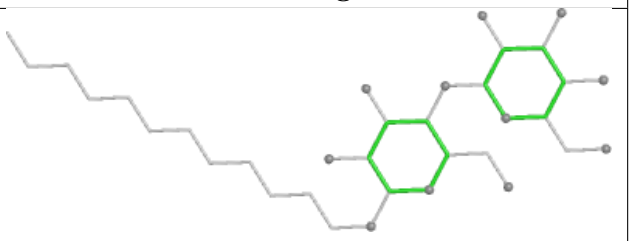
Bond lengths



Bond angles

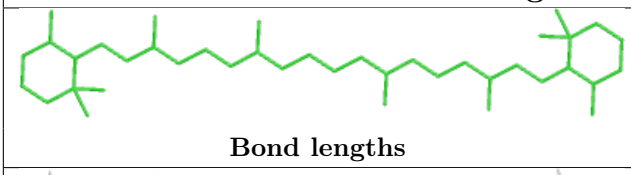


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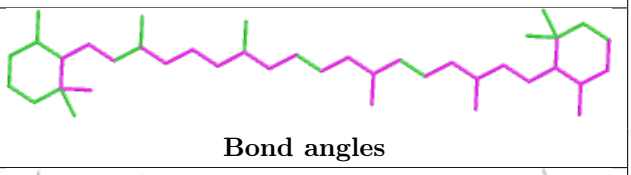


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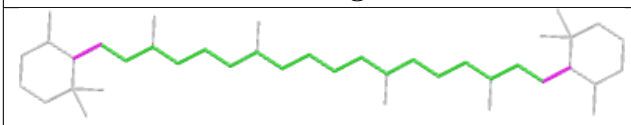
Ligand BCR 7 623



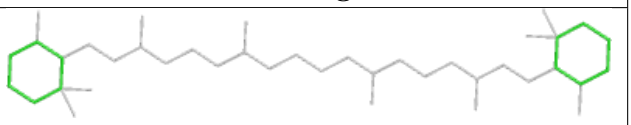
Bond lengths



Bond angles



Torsions



Rings

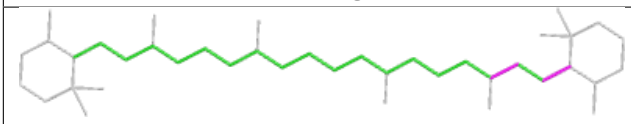
Ligand BCR 3 620



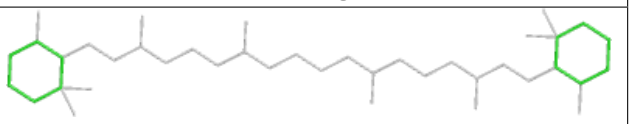
Bond lengths



Bond angles

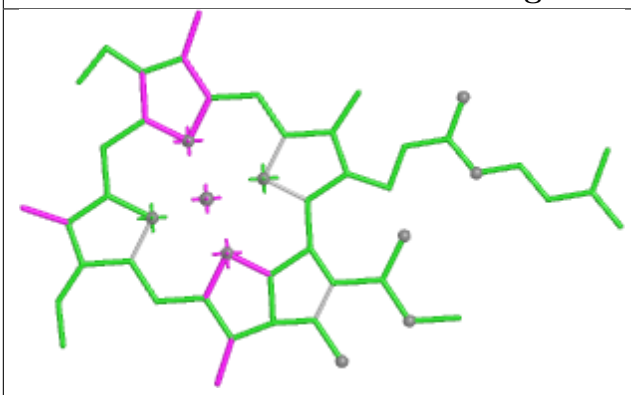


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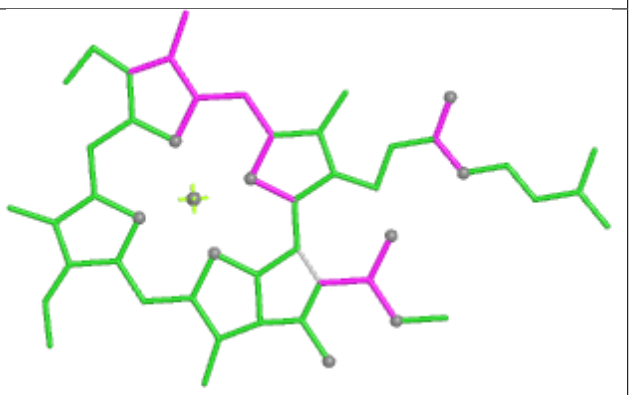


Rings

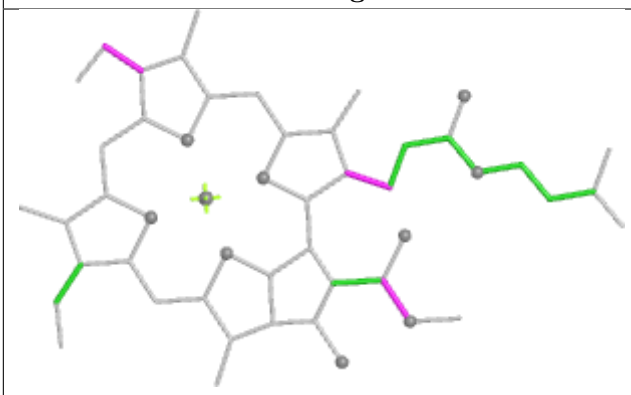
Ligand CLA B 836



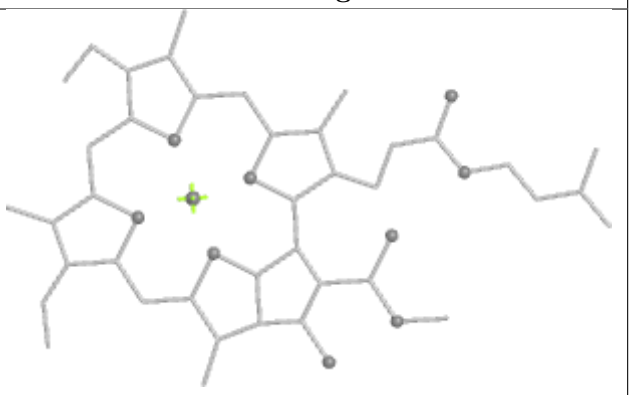
Bond lengths



Bond angles

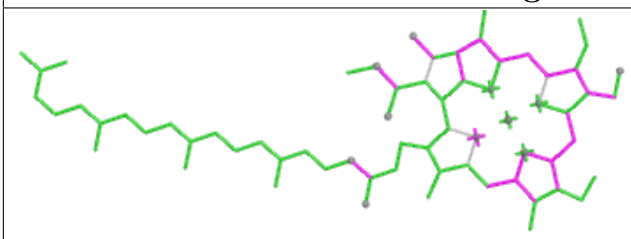


Torsions

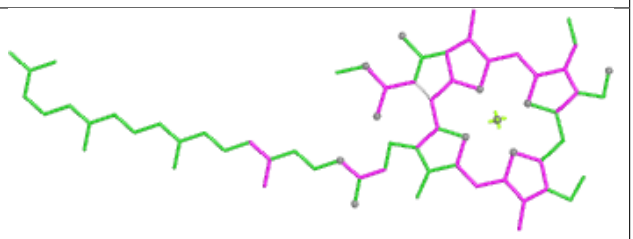


Rings

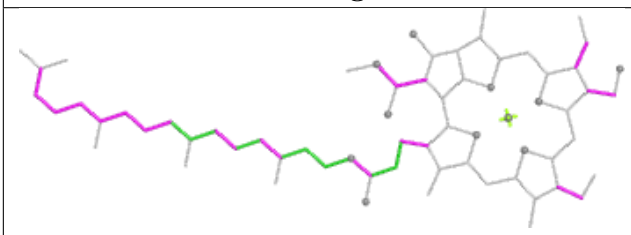
Ligand CHL X 609



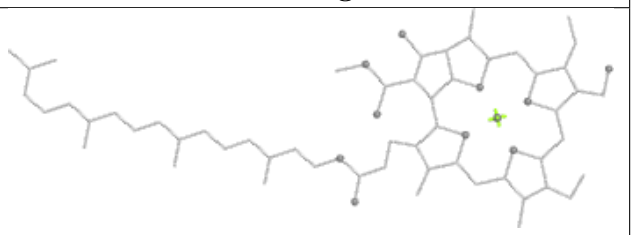
Bond lengths



Bond angles

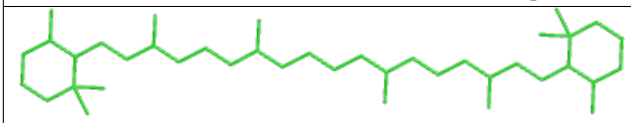


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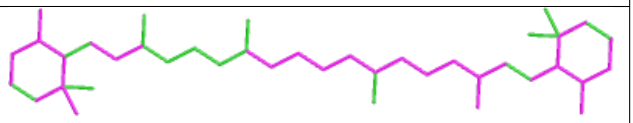


Rings

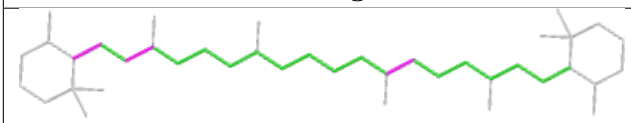
Ligand BCR L 308



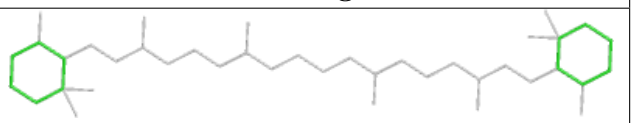
Bond lengths



Bond angles

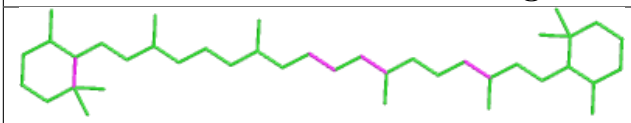


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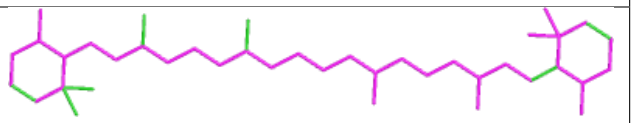


Rings

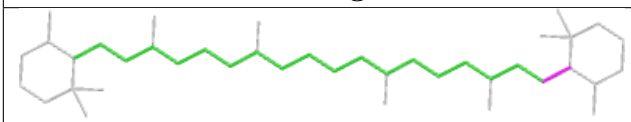
Ligand BCR B 844



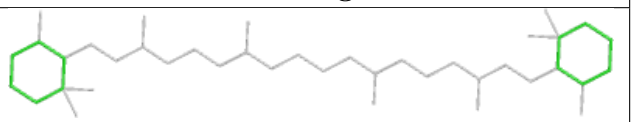
Bond lengths



Bond angles

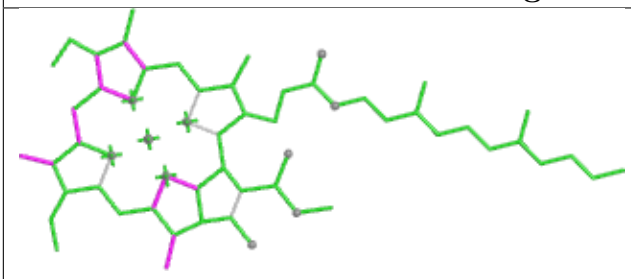


Torsions

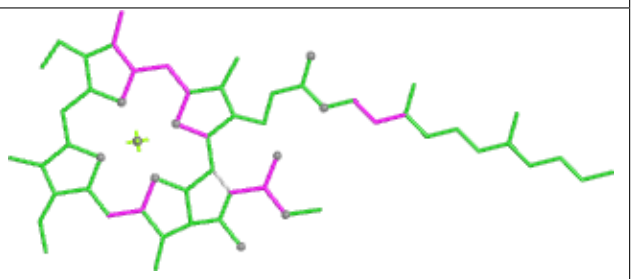


Rings

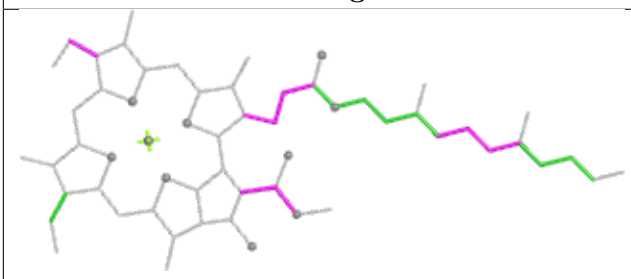
Ligand CLA Y 602



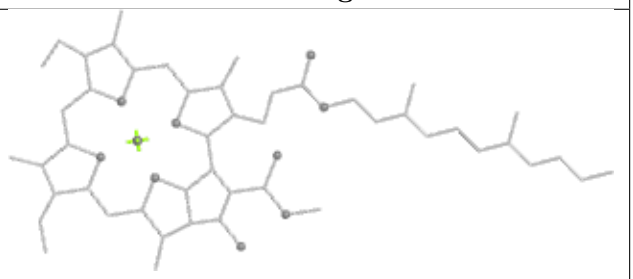
Bond lengths



Bond angles

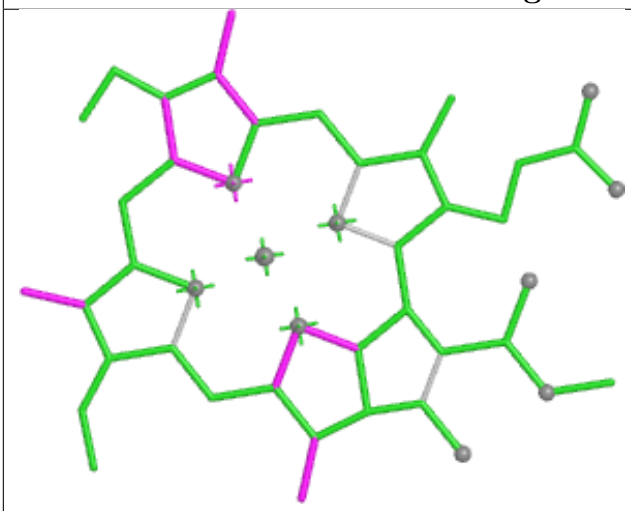


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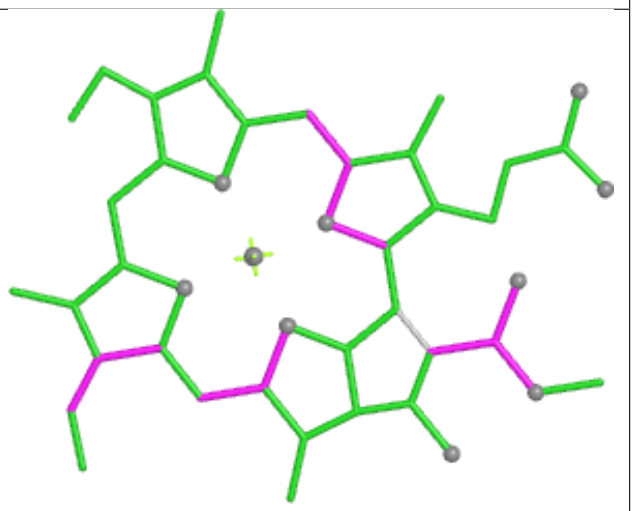


Rings

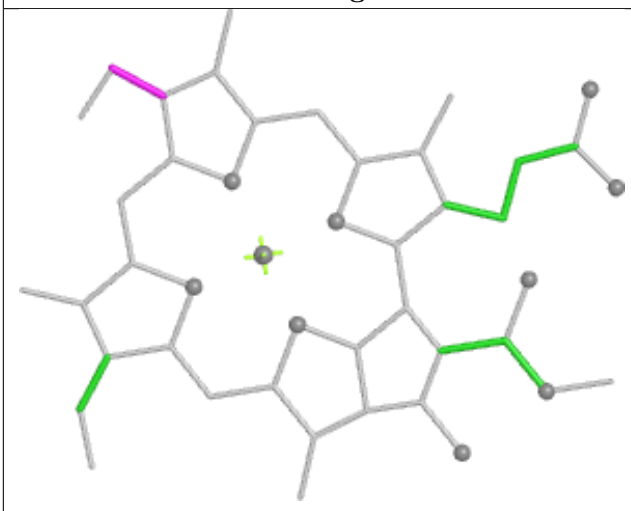
Ligand CLA A 817



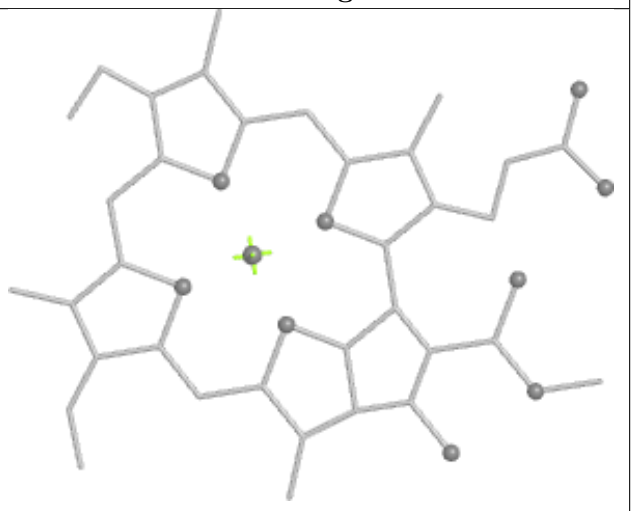
Bond lengths



Bond angles

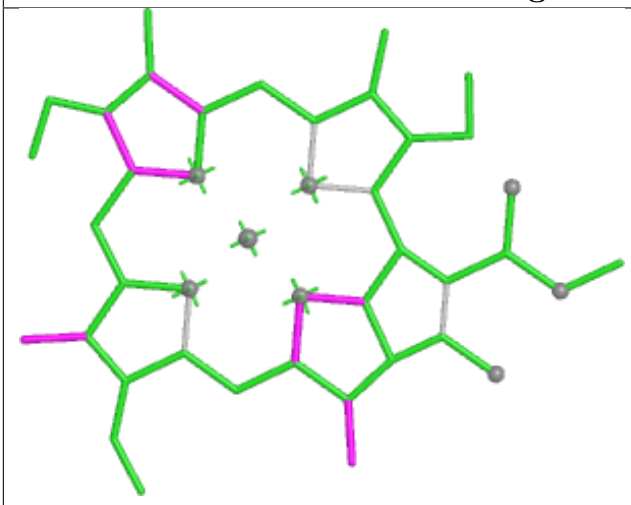


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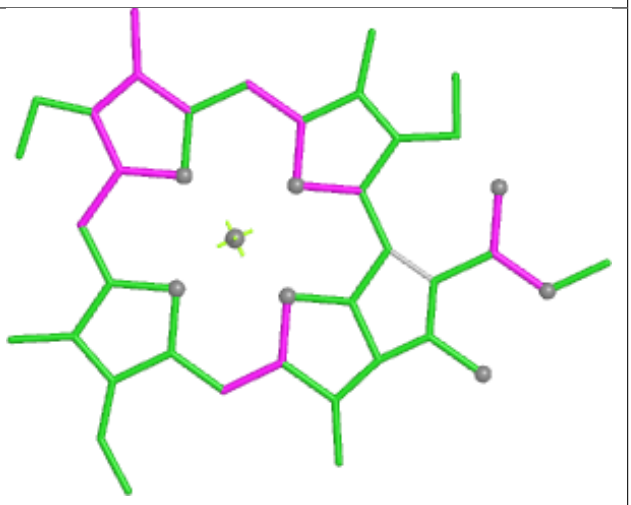


Rings

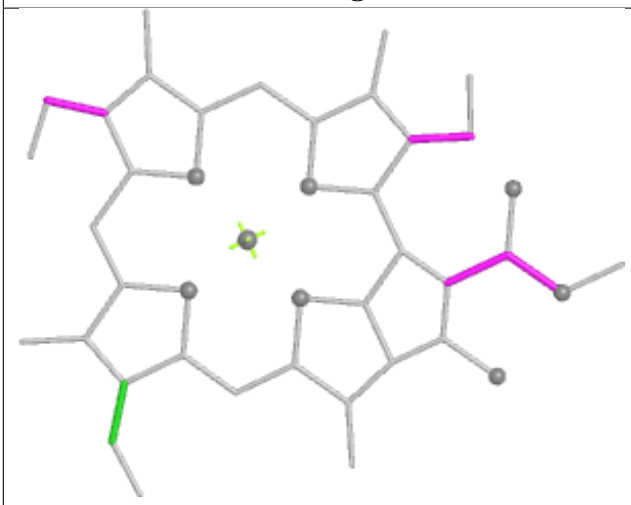
Ligand CLA 4 611



Bond lengths



Bond angles

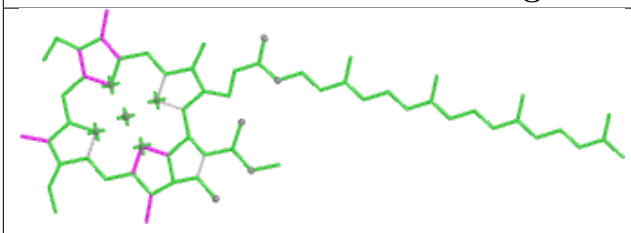


Torsions

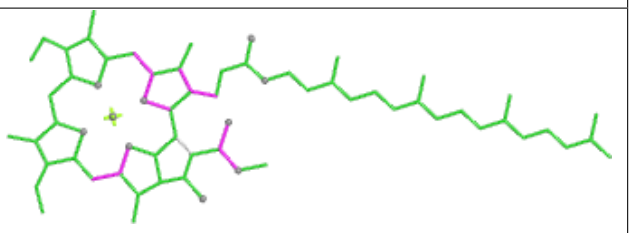


Rings

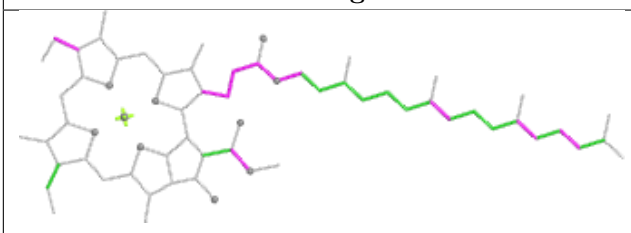
Ligand CLA H 203



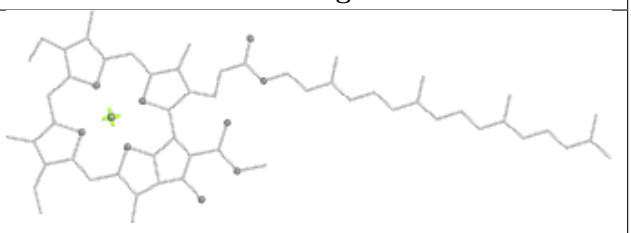
Bond lengths



Bond angles

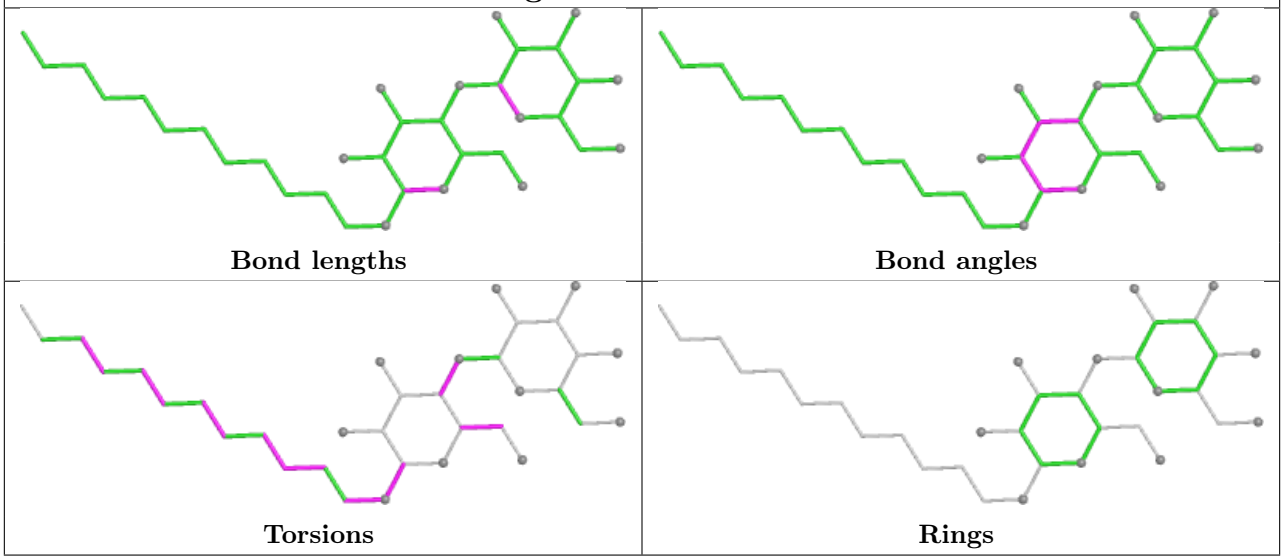


Torsions

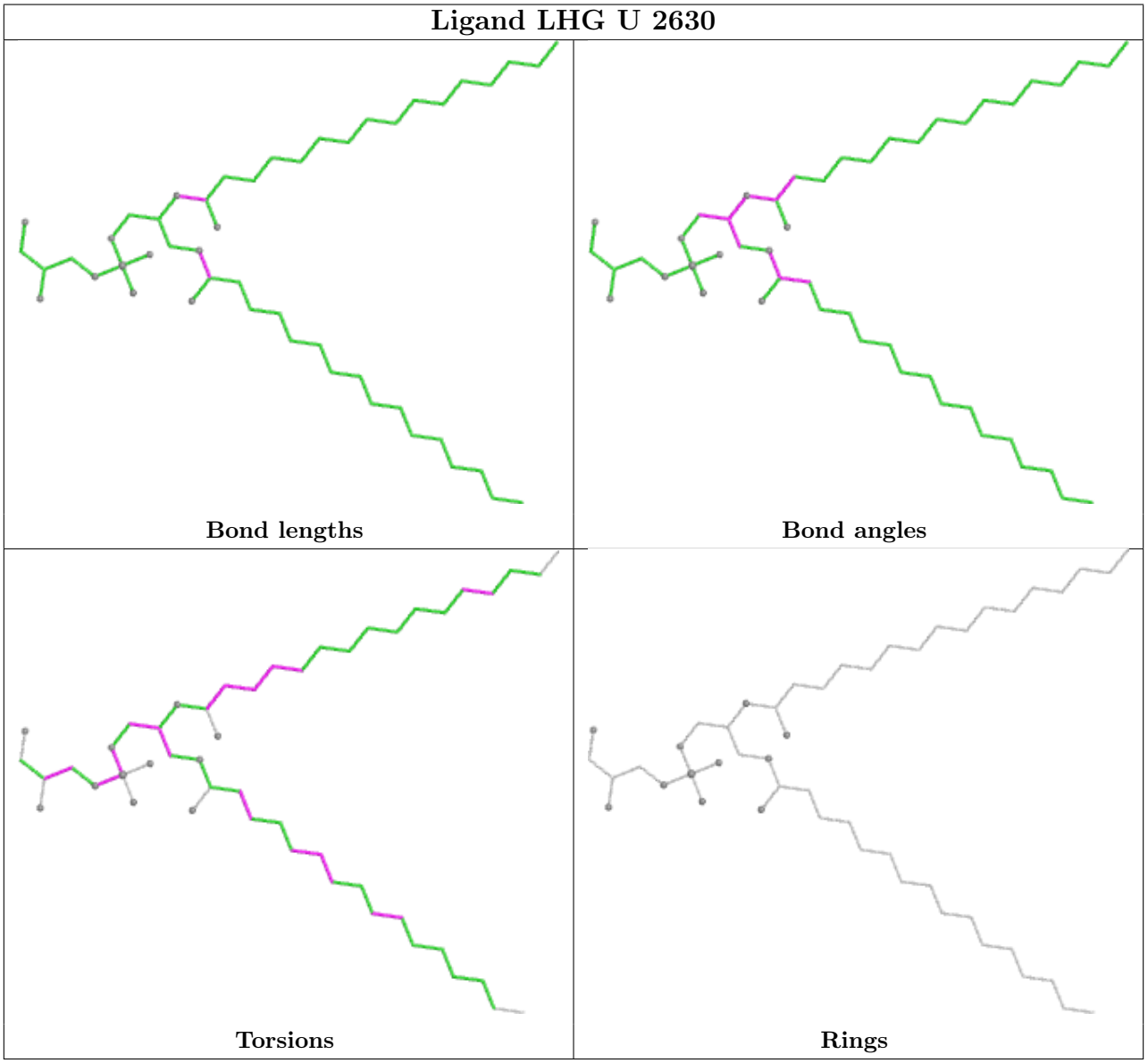


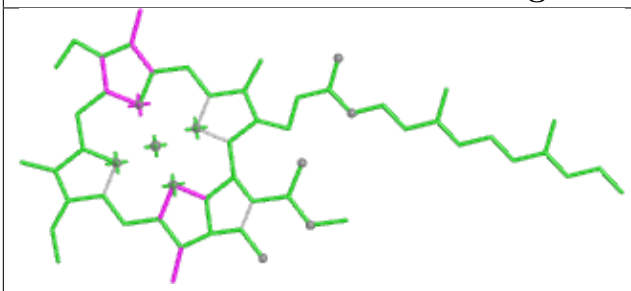
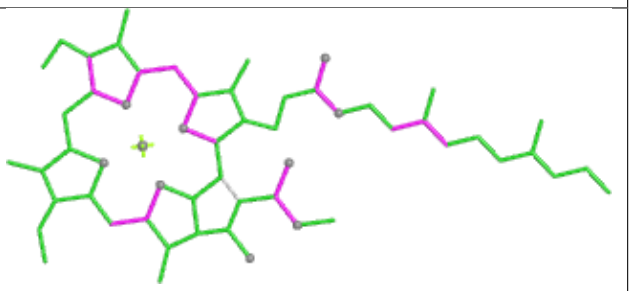
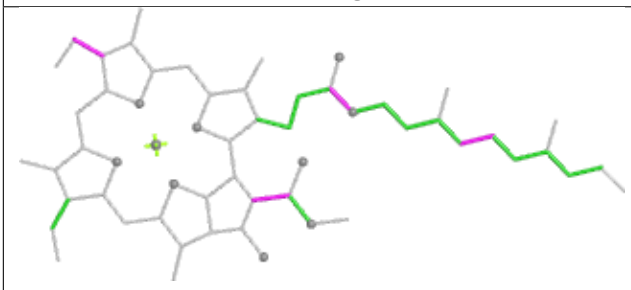
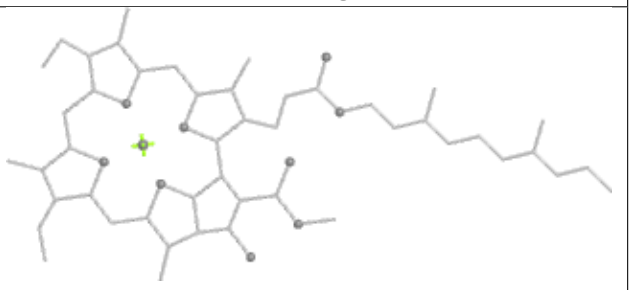
Rings

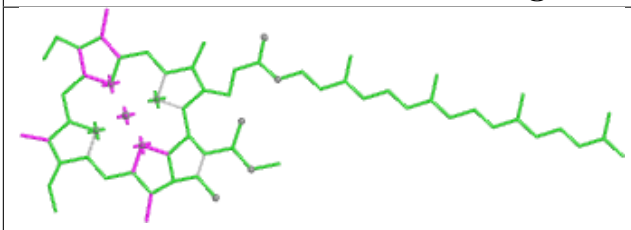
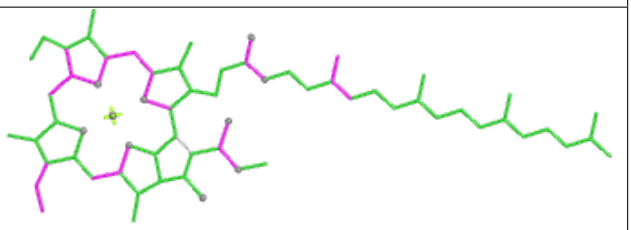
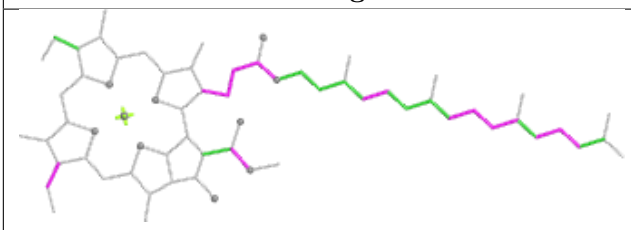
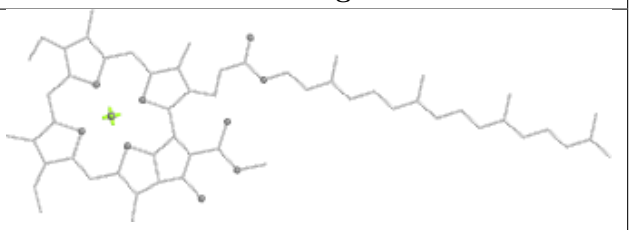
Ligand LMU 8 625



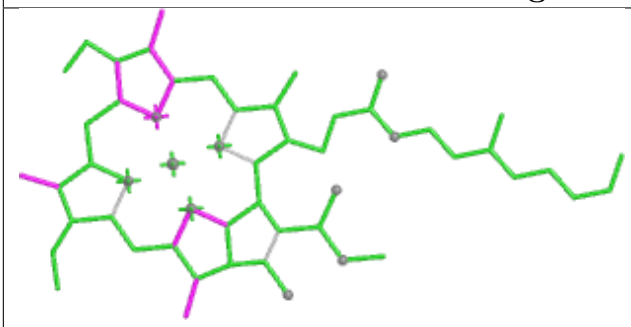
Ligand LHG U 2630



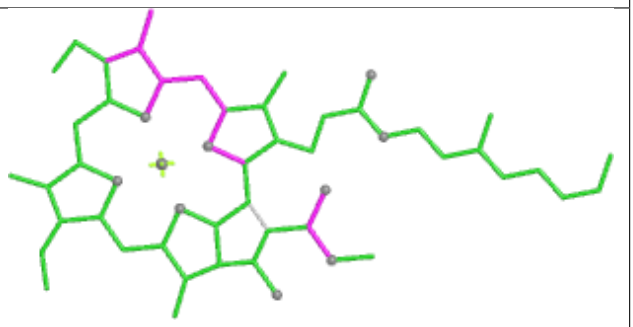
Ligand CLA 1 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

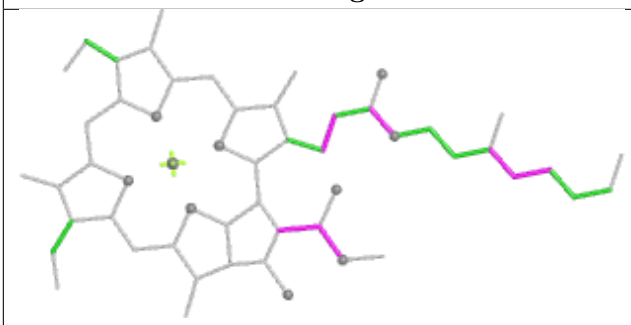
Ligand CLA a 613



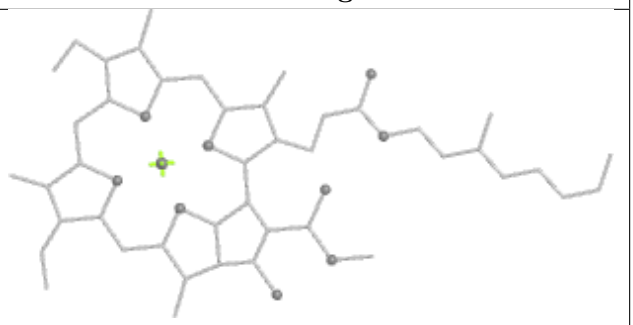
Bond lengths



Bond angles

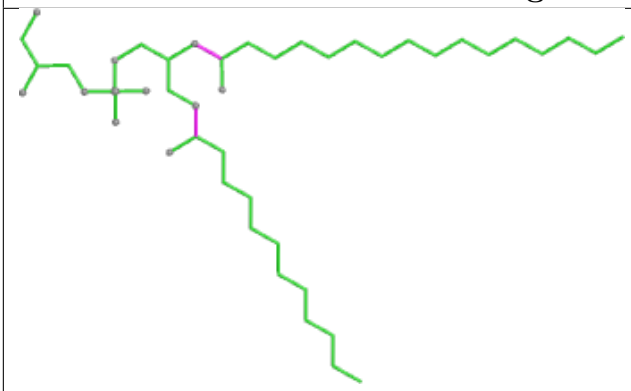


Torsions

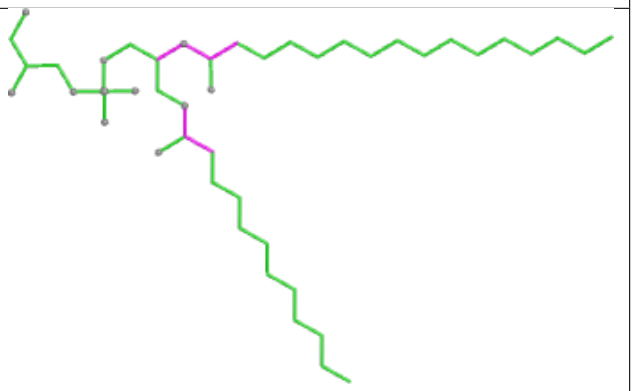


Rings

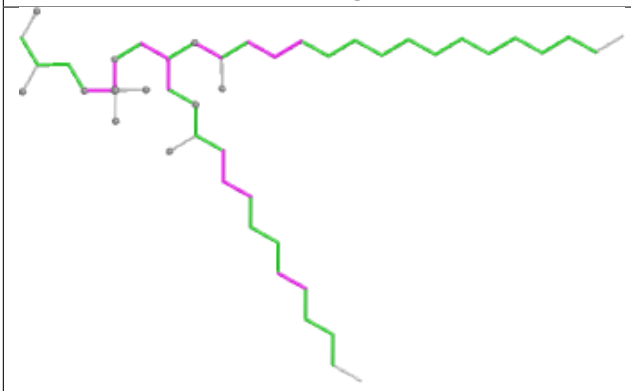
Ligand LHG 3 623



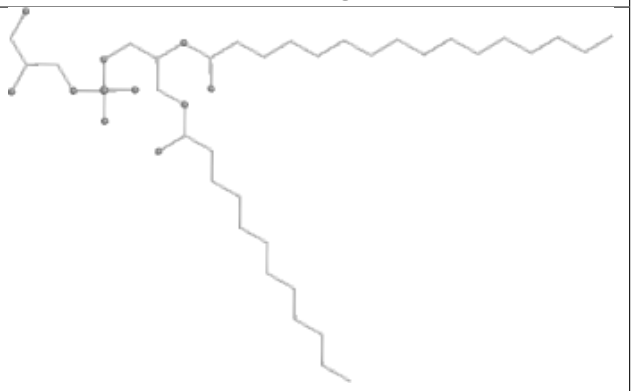
Bond lengths



Bond angles

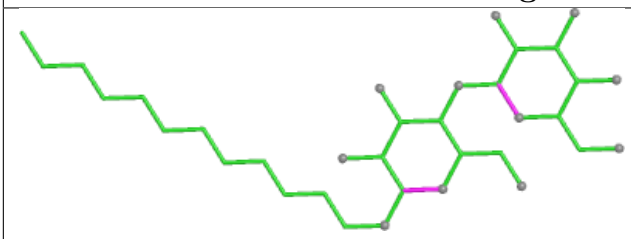


Torsions

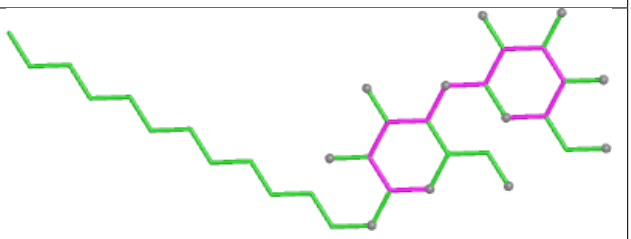


Rings

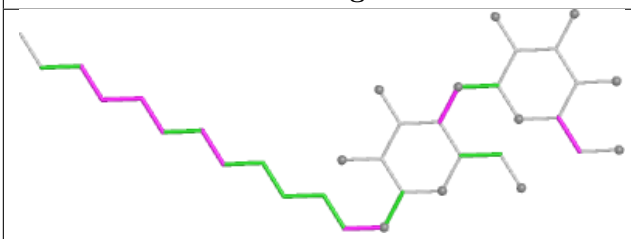
Ligand LMU A 857



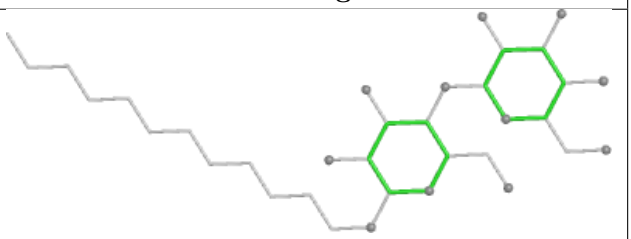
Bond lengths



Bond angles

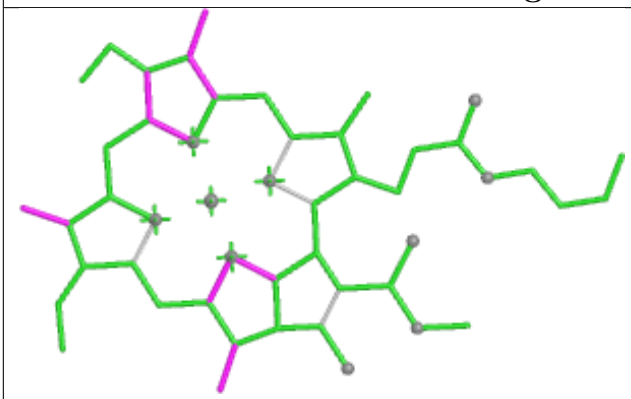


Torsions

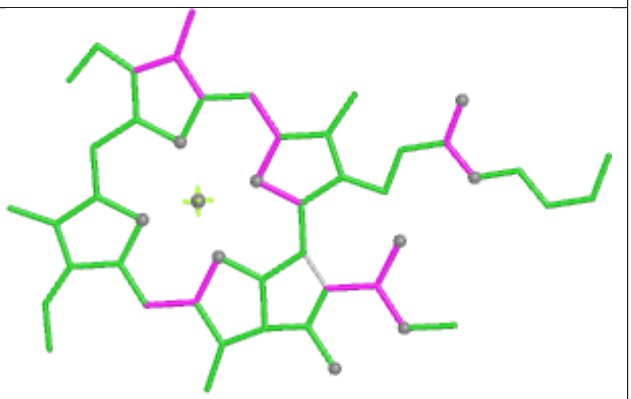


Rings

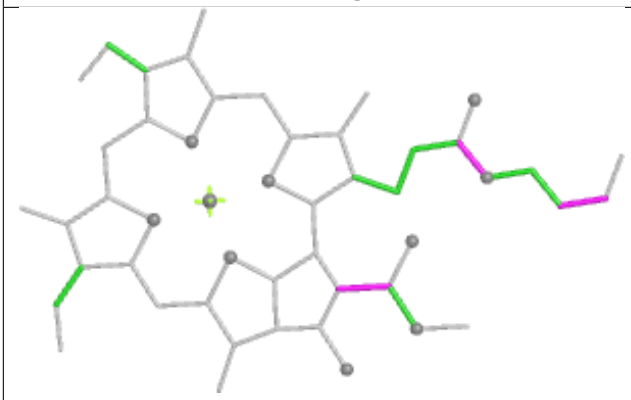
Ligand CLA B 825



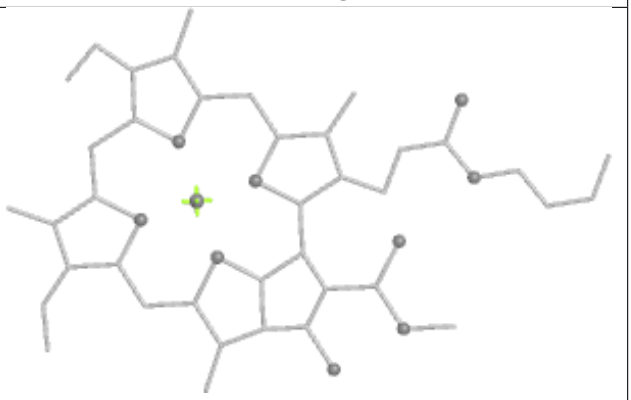
Bond lengths



Bond angles

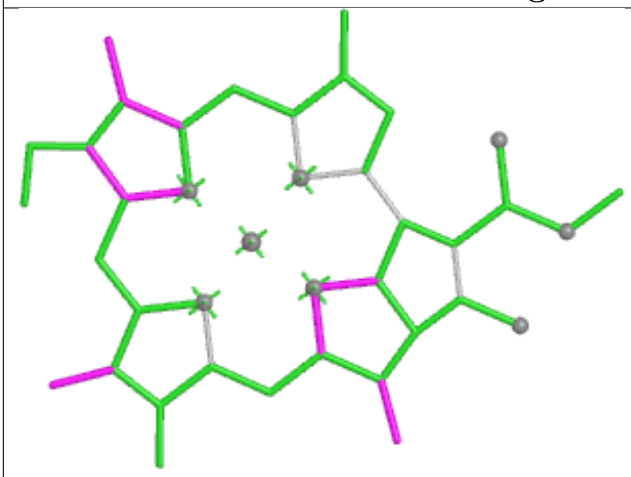


Torsions

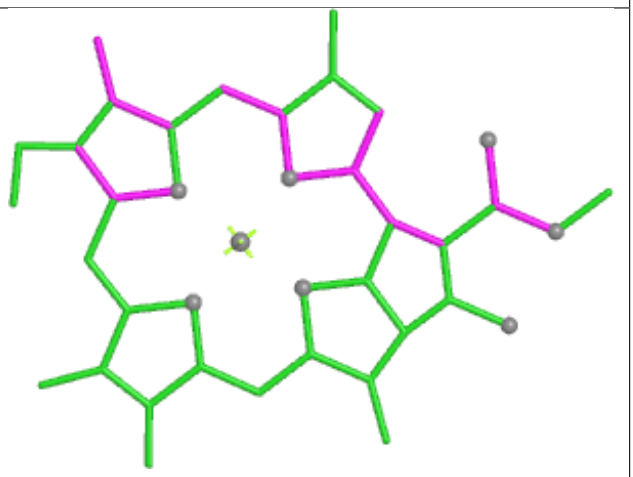


Rings

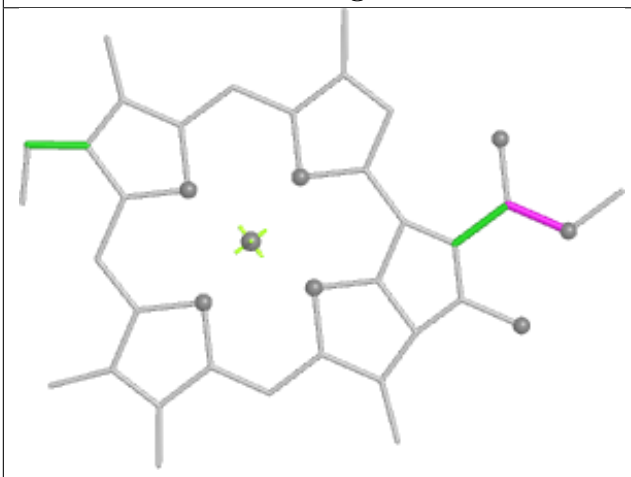
Ligand CLA 1 610



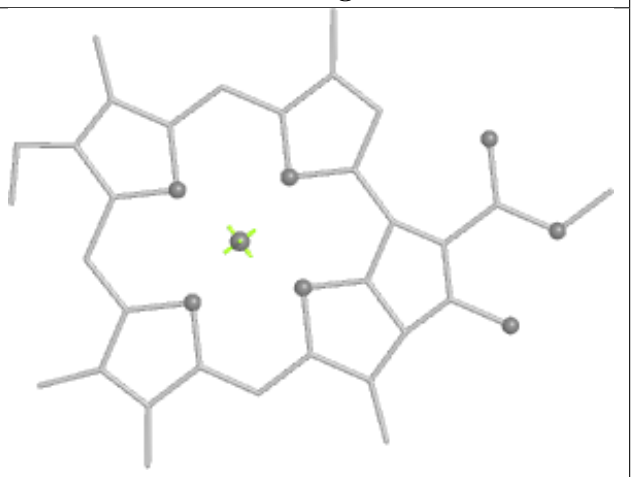
Bond lengths



Bond angles

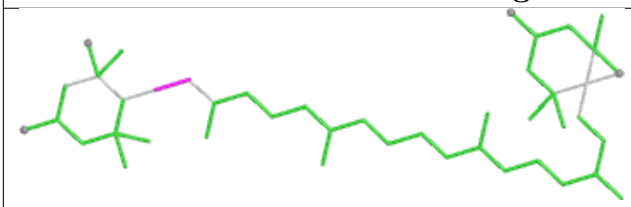


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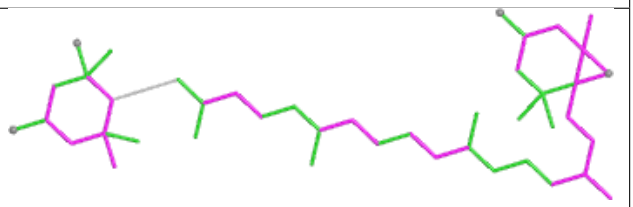


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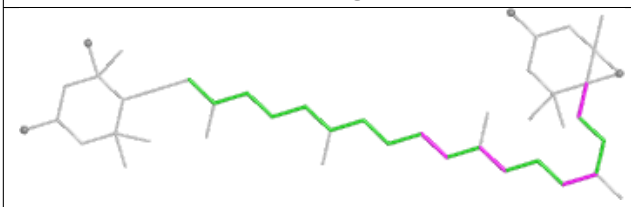
Ligand NEX Y 1623



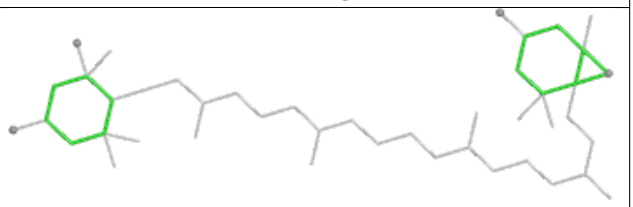
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Bond angles

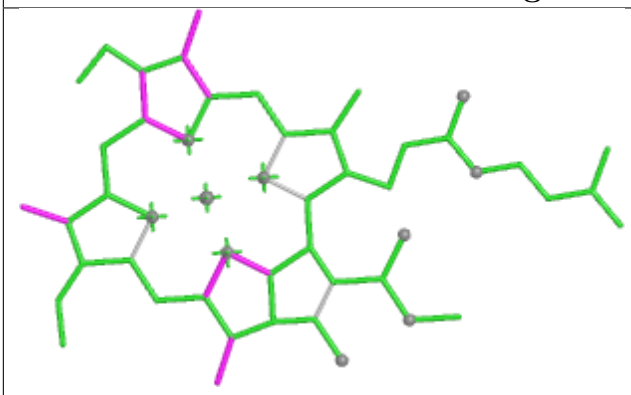


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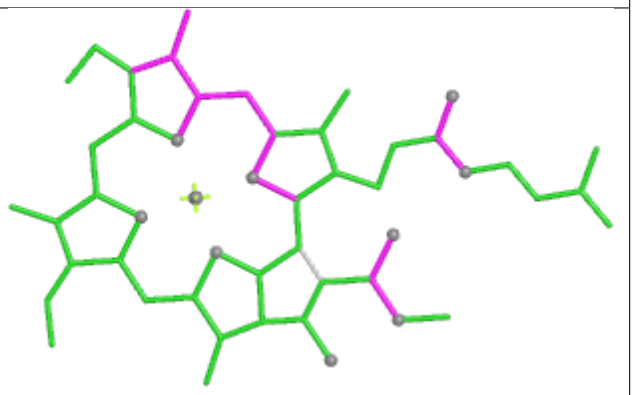


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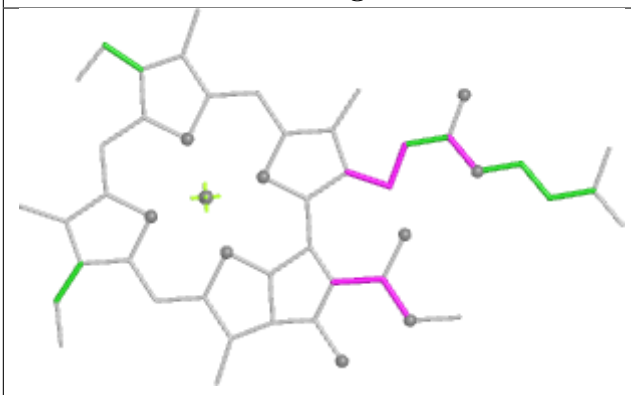
Ligand CLA V 604



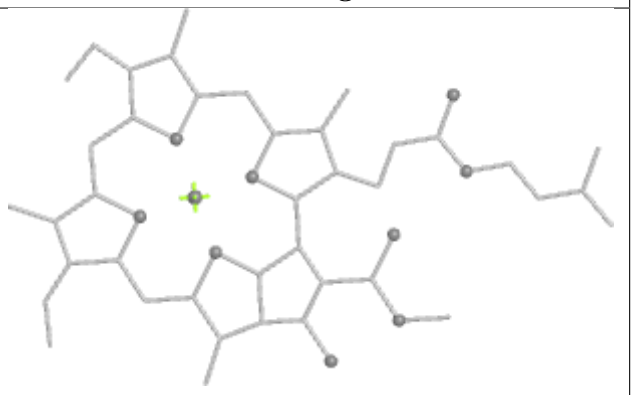
Bond lengths



Bond angles

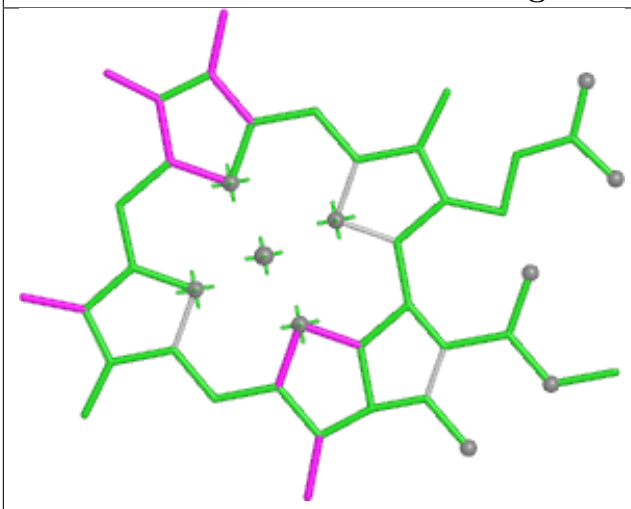


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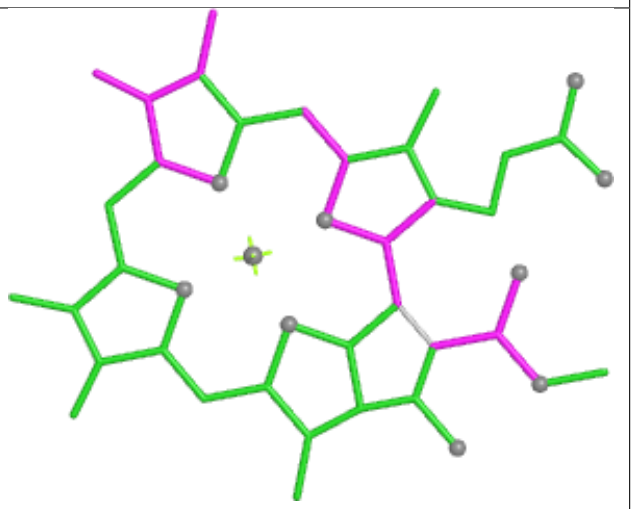


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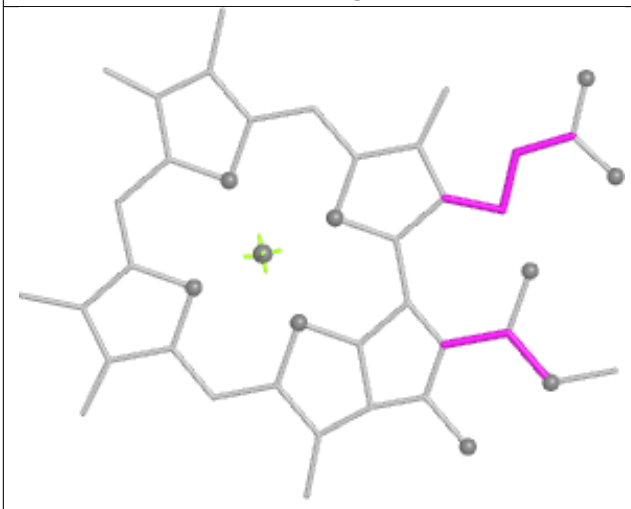
Ligand CLA 5 619



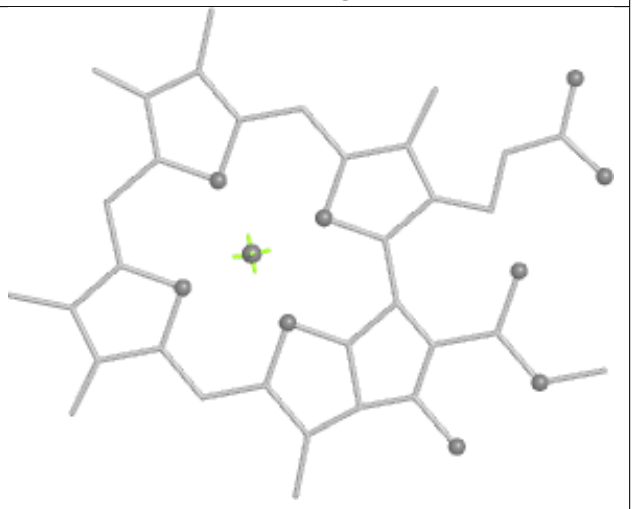
Bond lengths



Bond angles

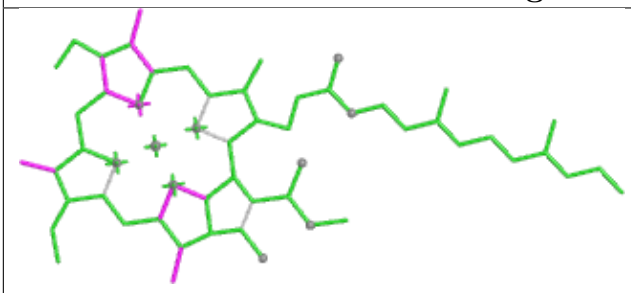


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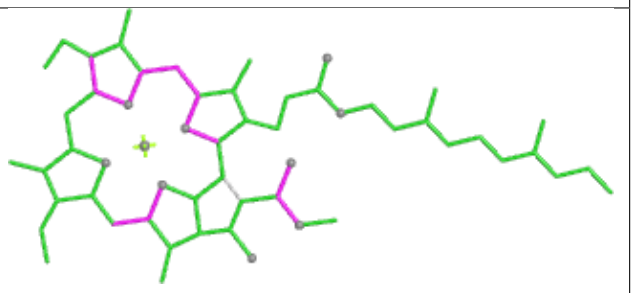


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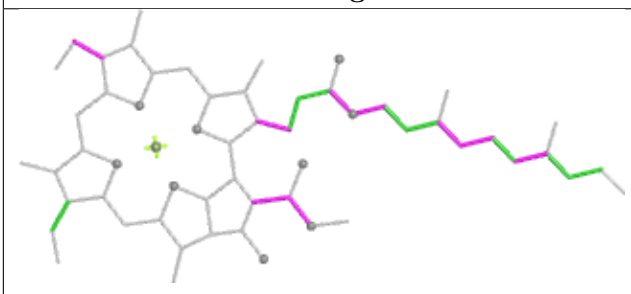
Ligand CLA F 301



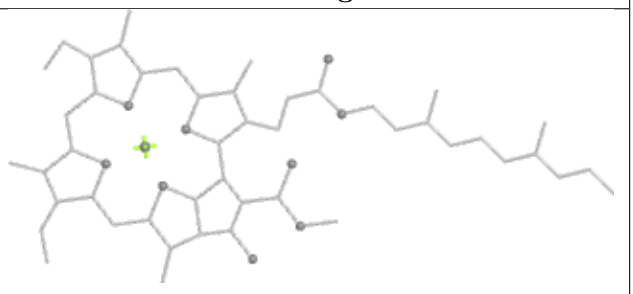
Bond lengths



Bond angles

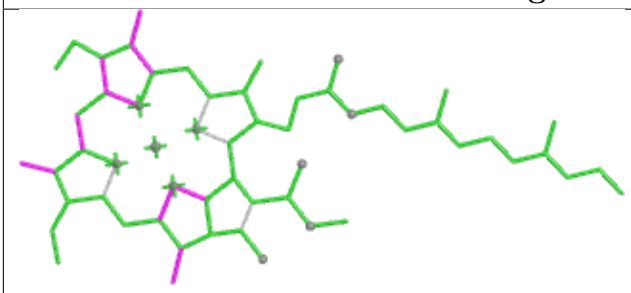


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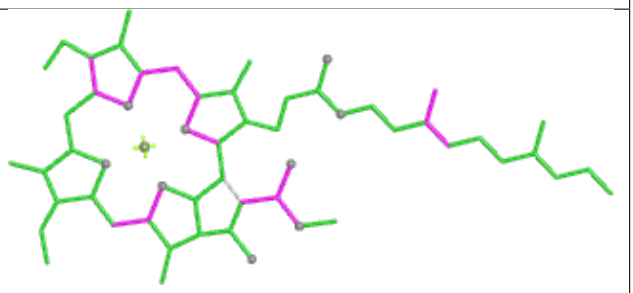


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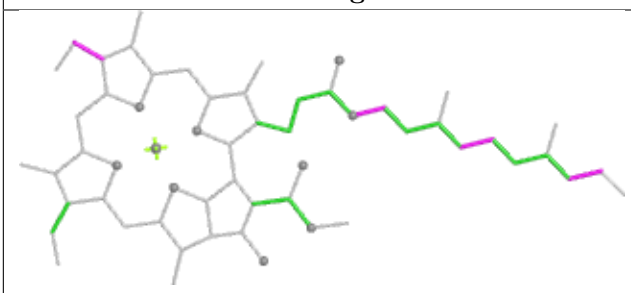
Ligand CLA 9 610



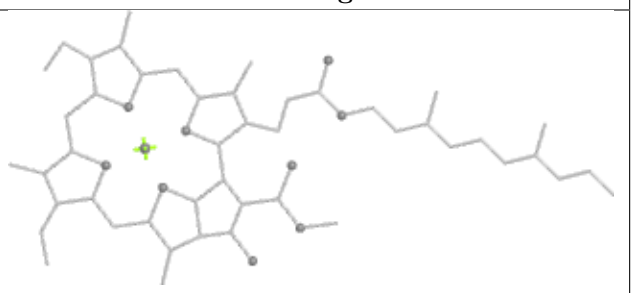
Bond lengths



Bond angles

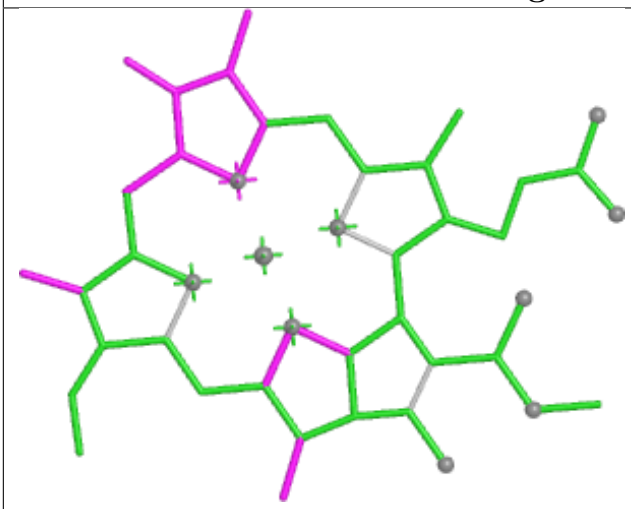


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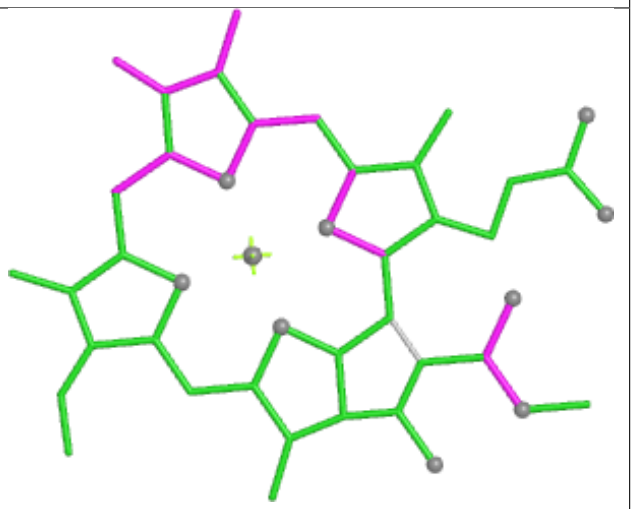


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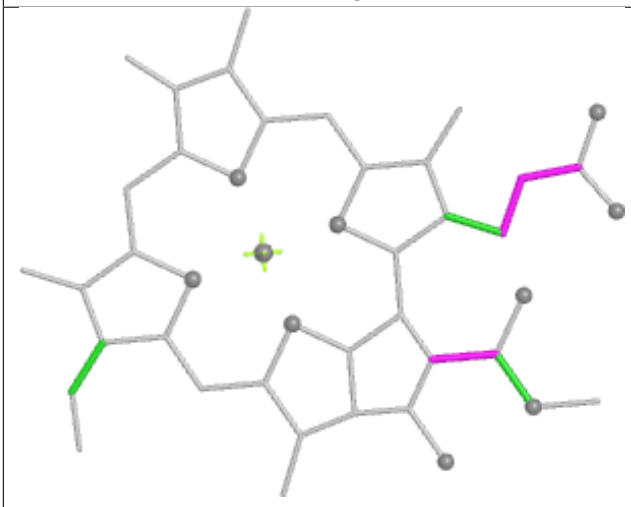
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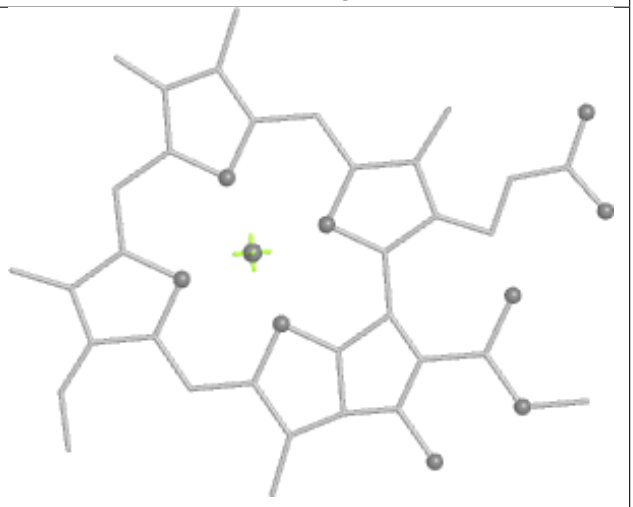
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Bond angles

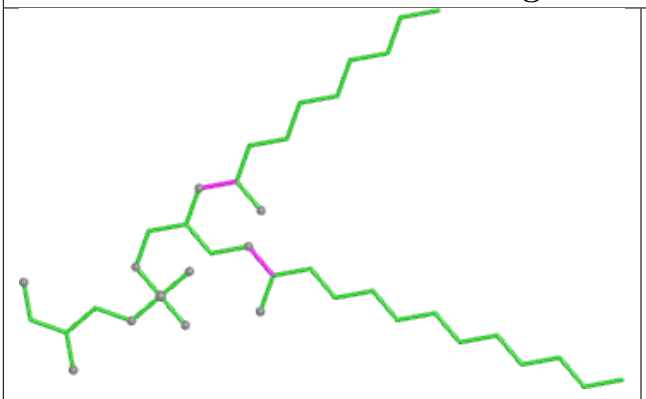


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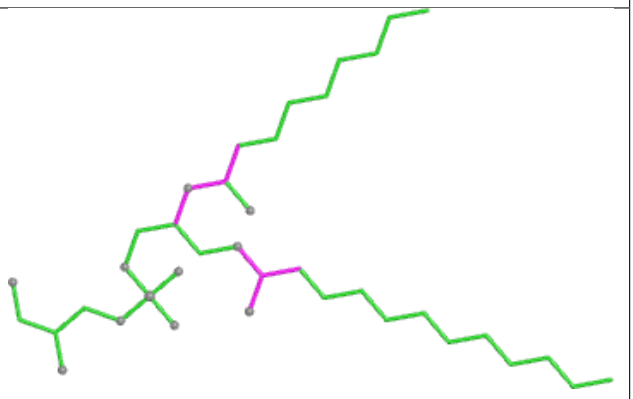


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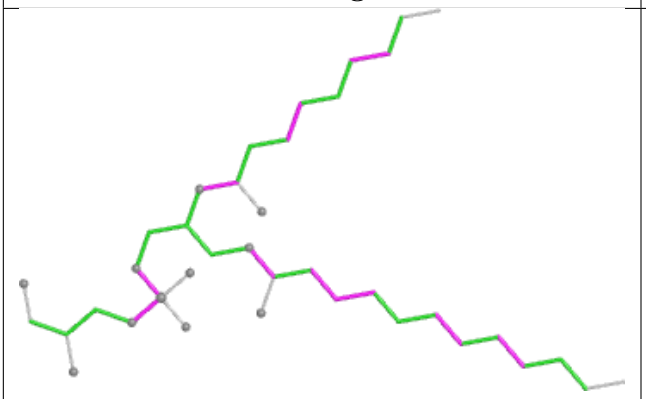
Ligand LHG B 851



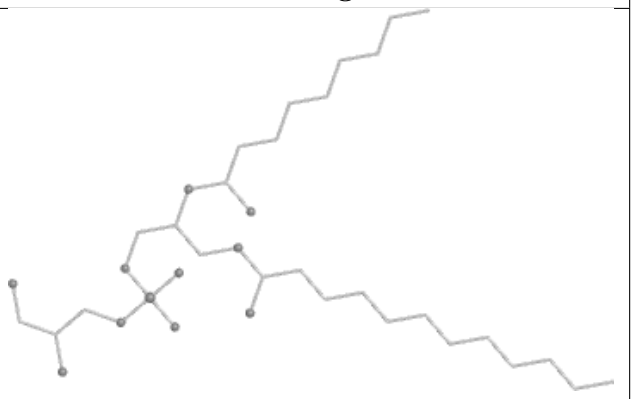
Bond lengths



Bond angles

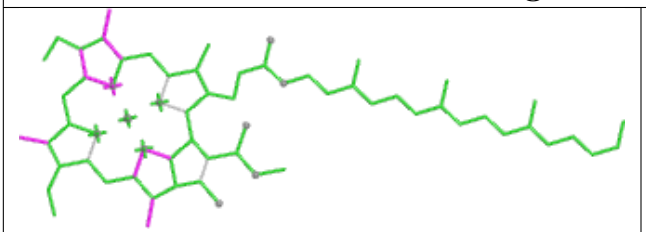


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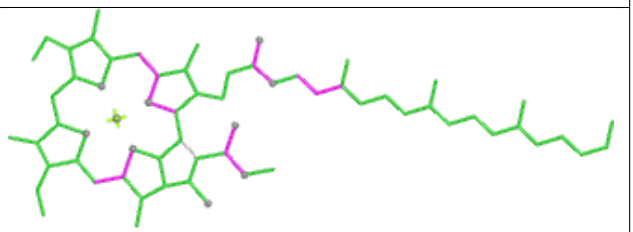


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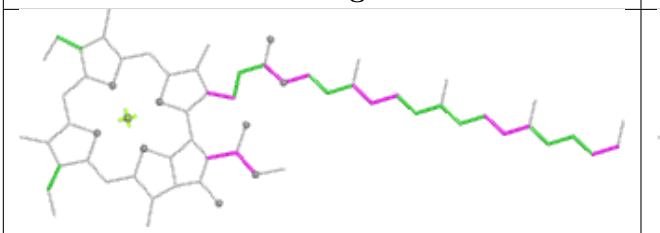
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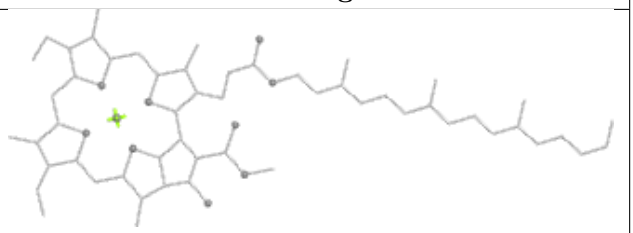
Bond lengths



Bond angles

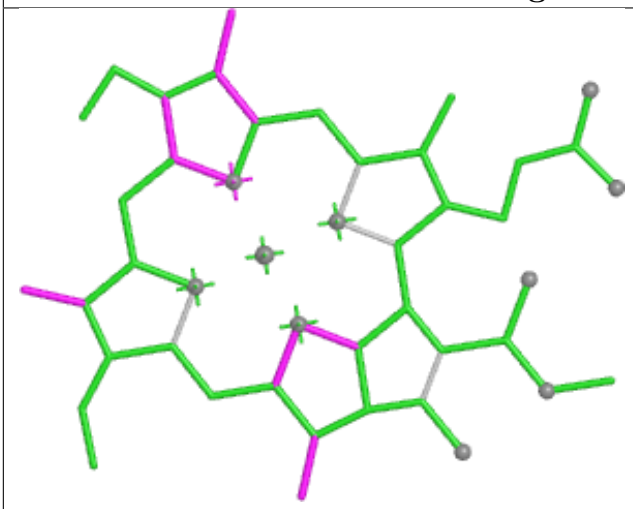


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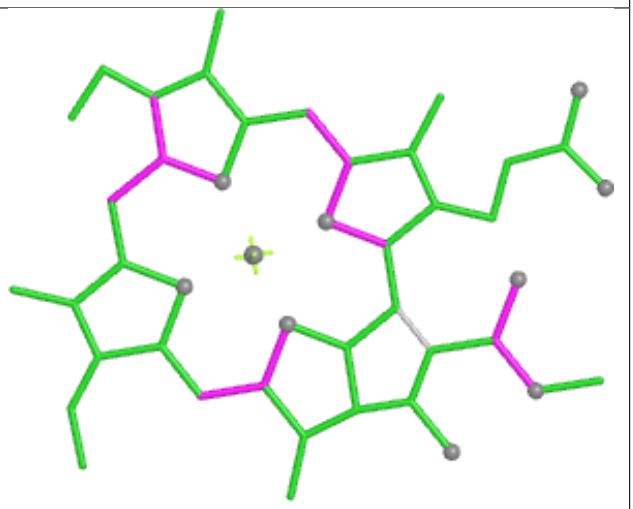


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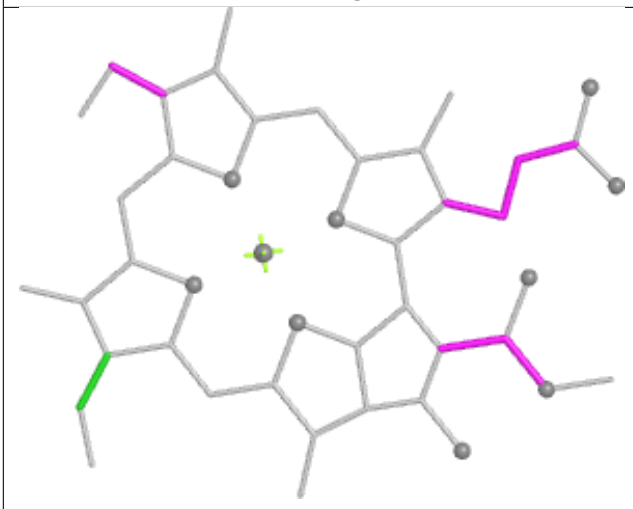
Ligand CLA 9 607



Bond lengths



Bond angles

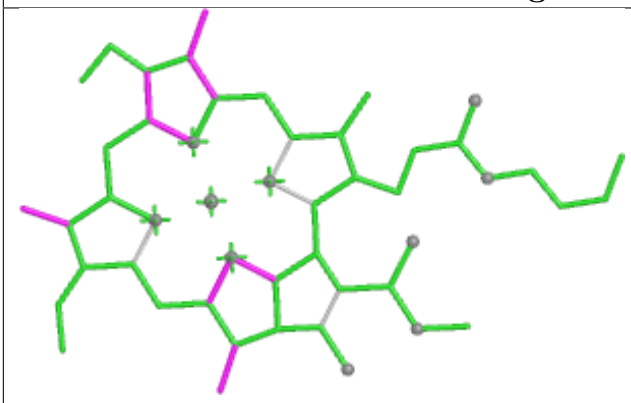


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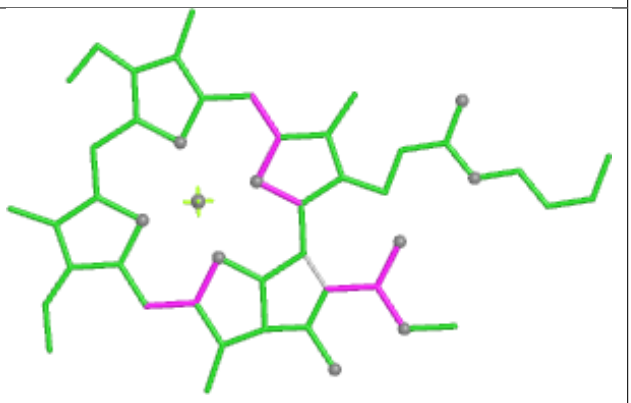


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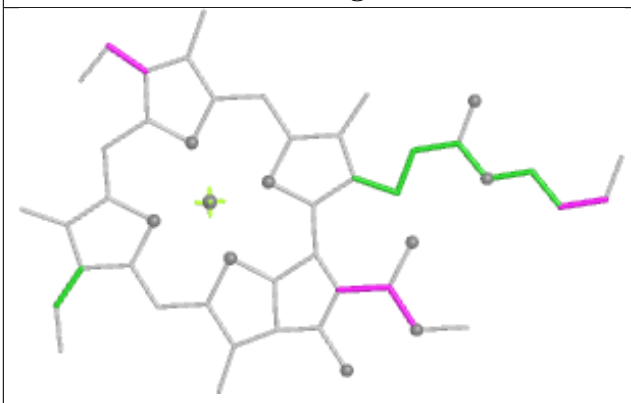
Ligand CLA 1 604



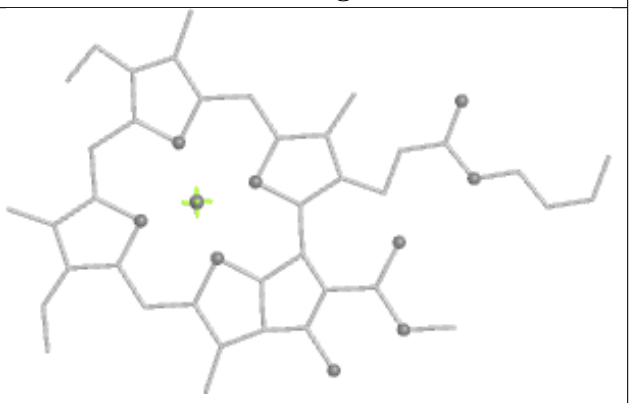
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Bond angles

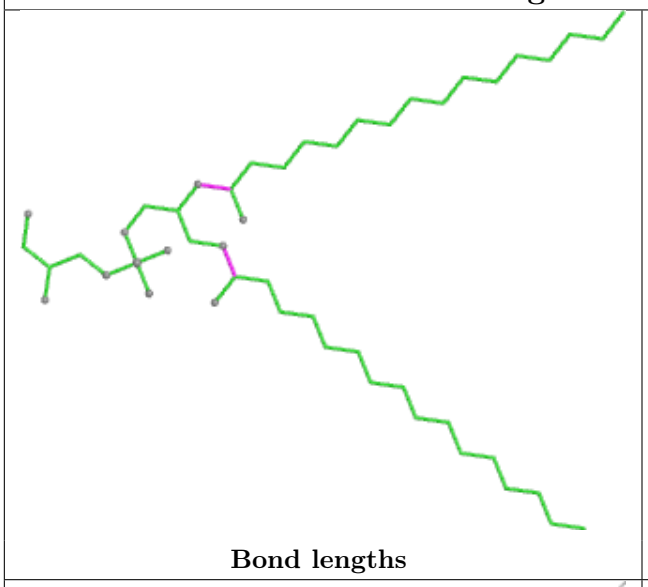


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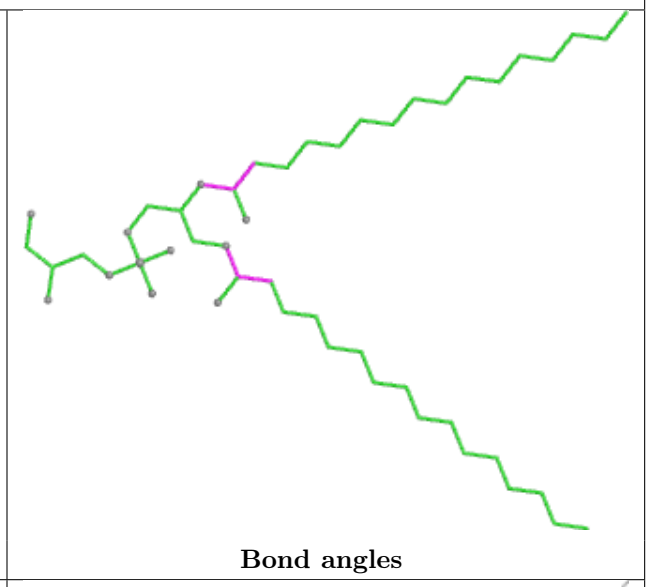


Rings

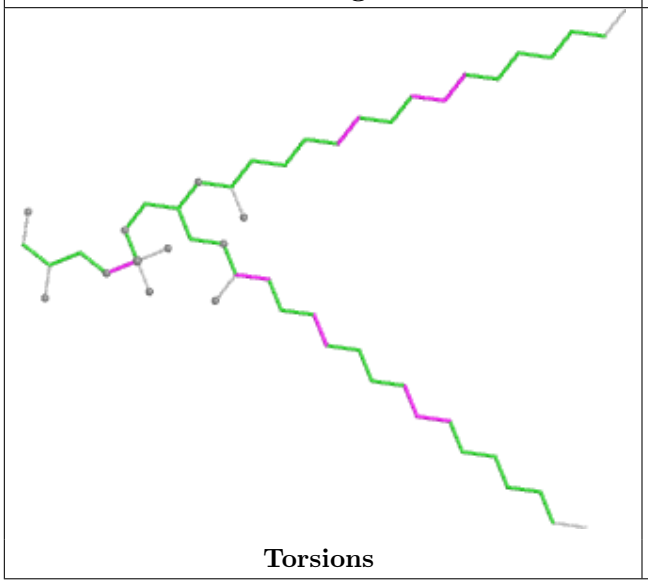
Ligand LHG 4 622



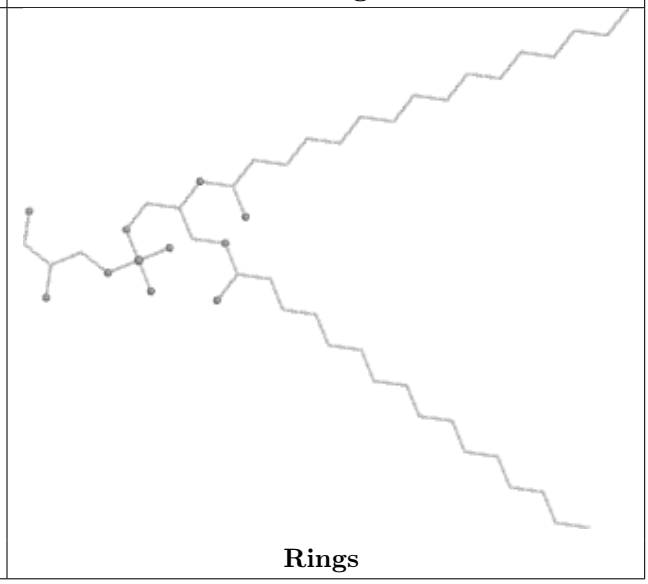
Bond lengths



Bond angles

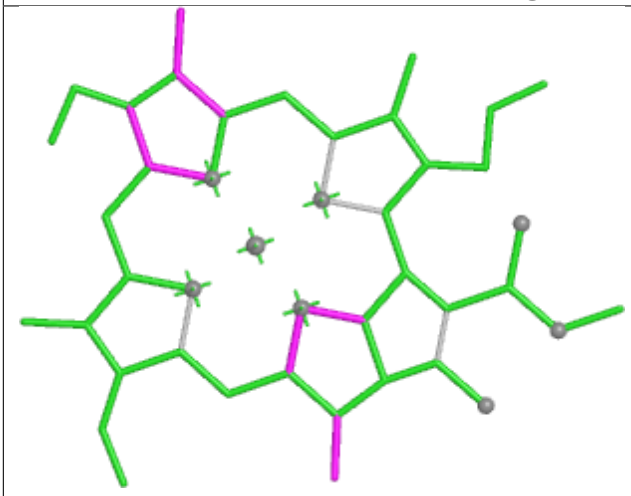


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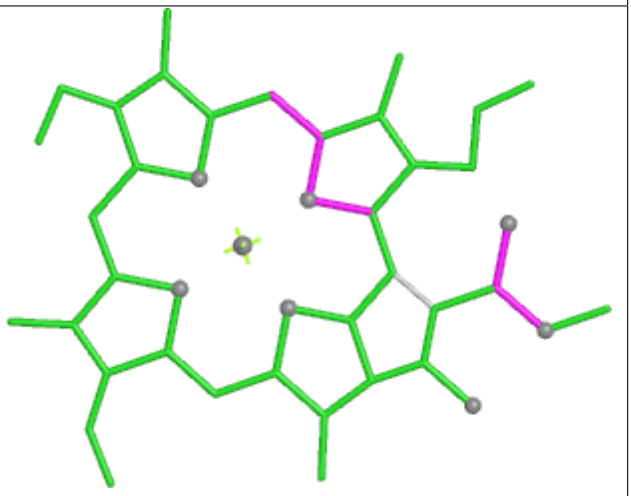


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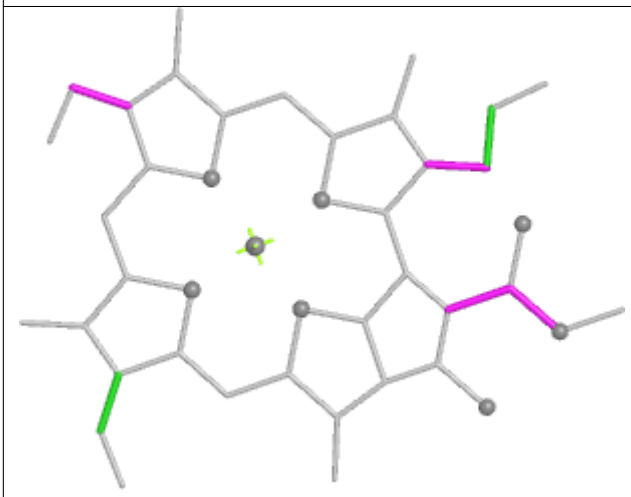
Ligand CLA V 611



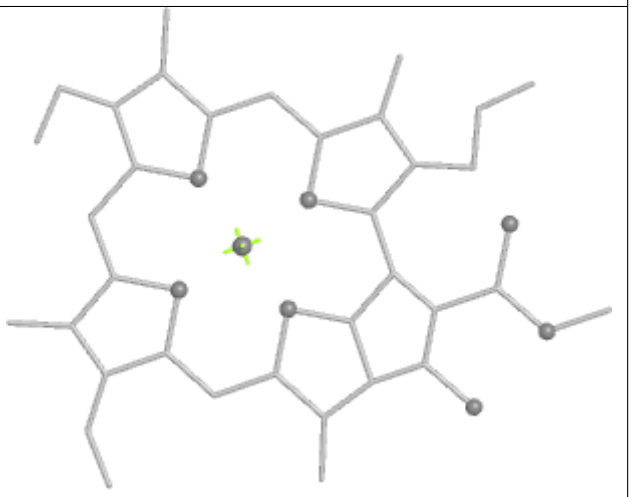
Bond lengths



Bond angles

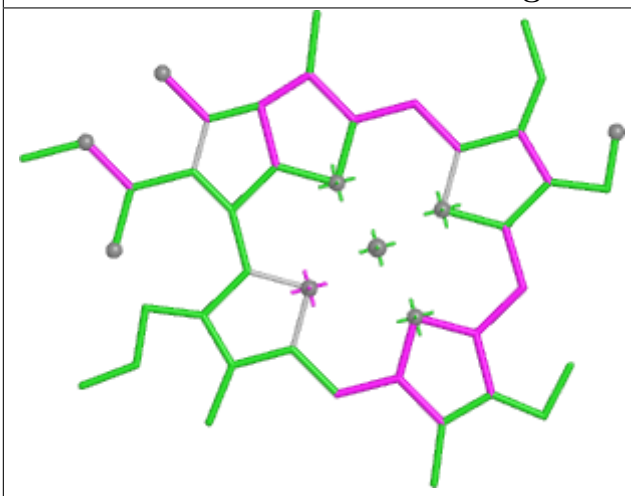


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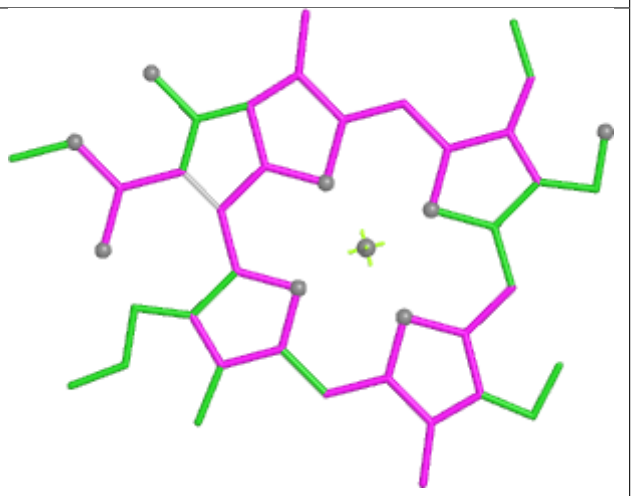


Rings

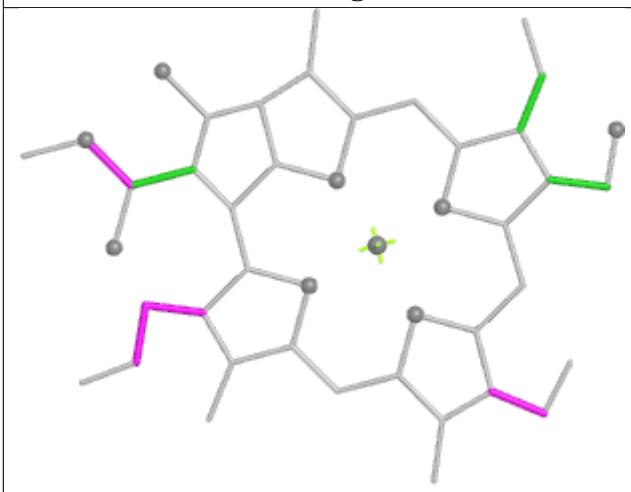
Ligand CHL U 608



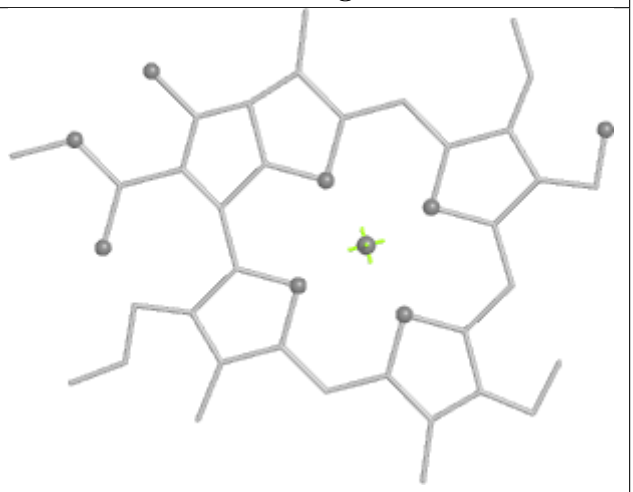
Bond lengths



Bond angles

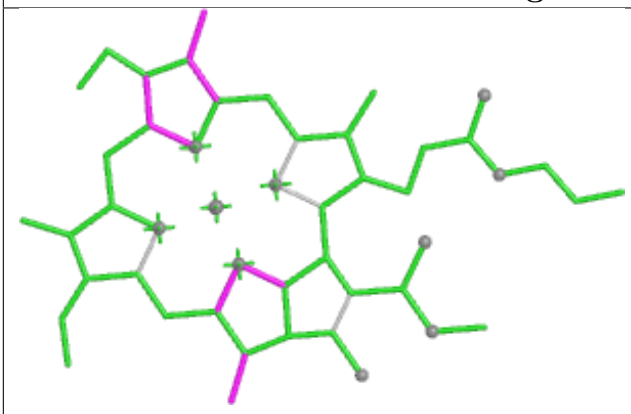


Torsions

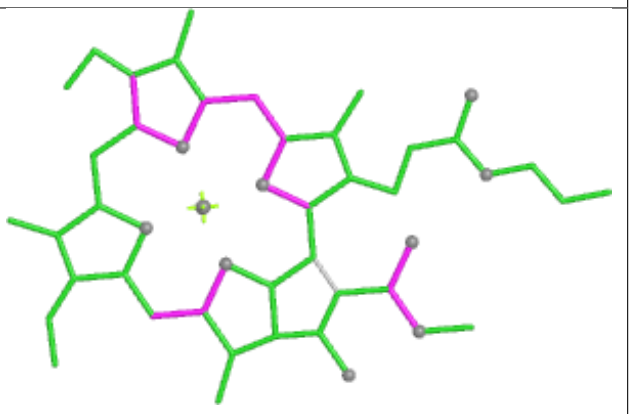


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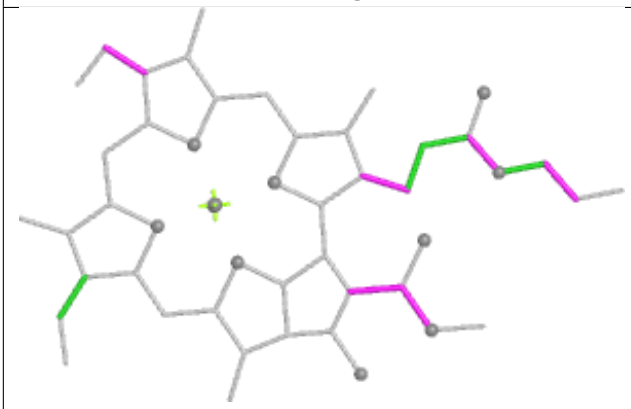
Ligand CLA Z 614



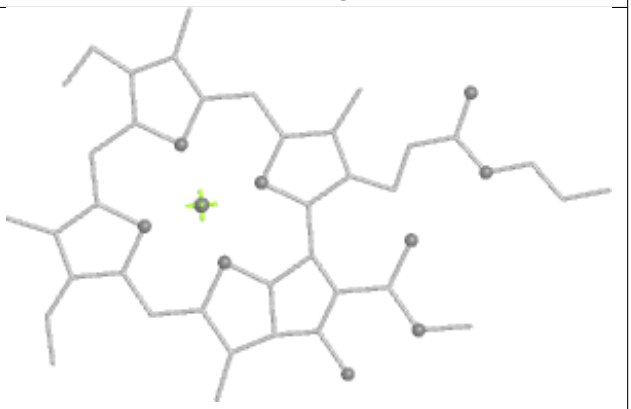
Bond lengths



Bond angles

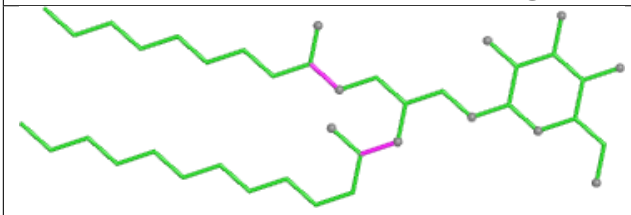


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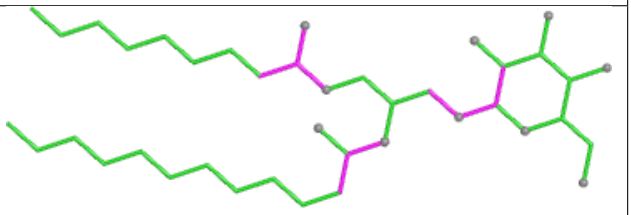


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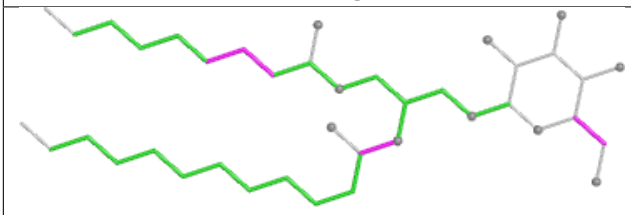
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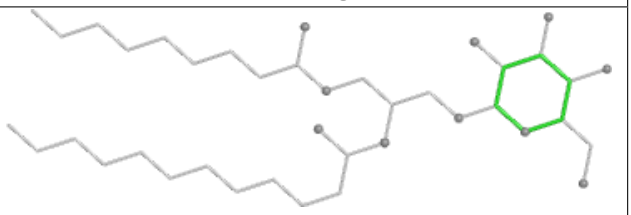
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Bond angles

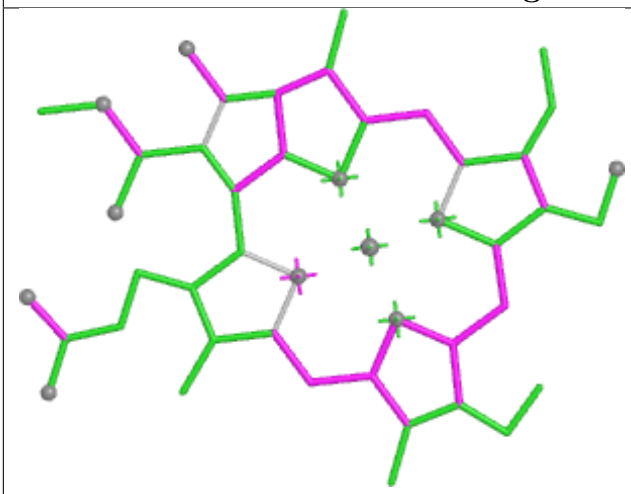


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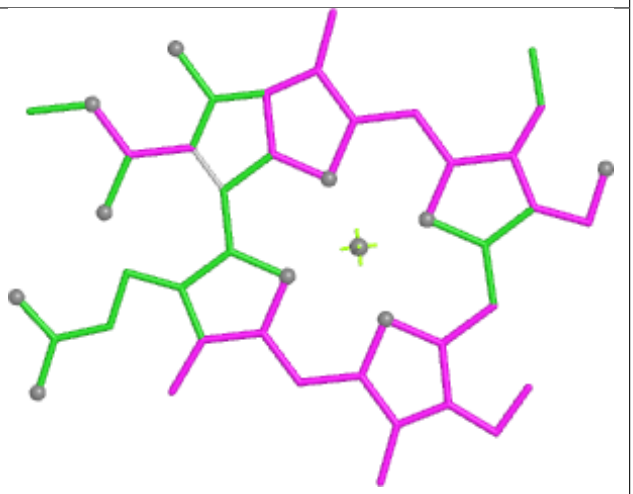


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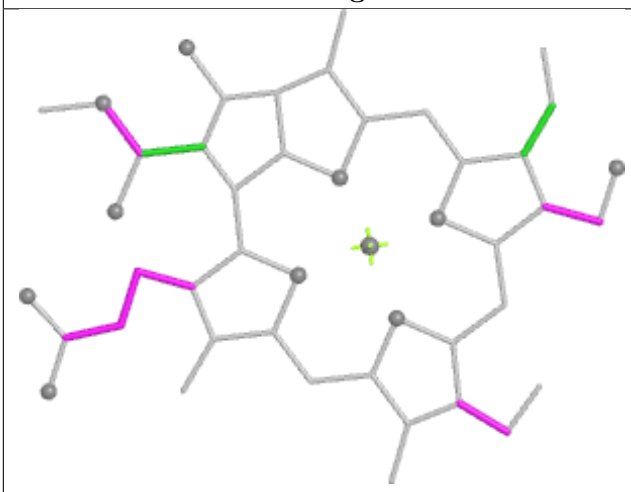
Ligand CHL U 607



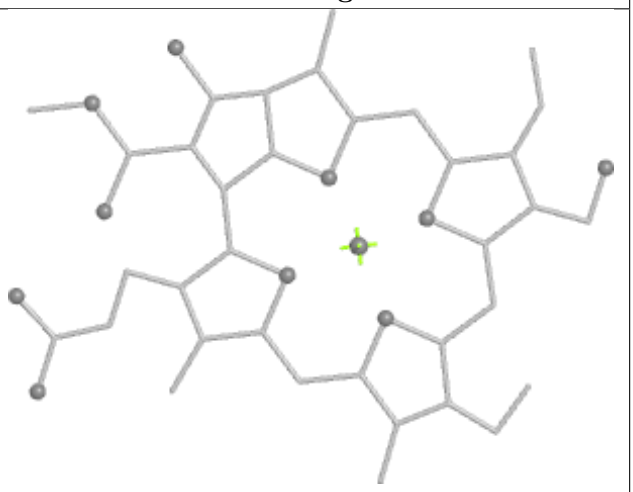
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Bond angles

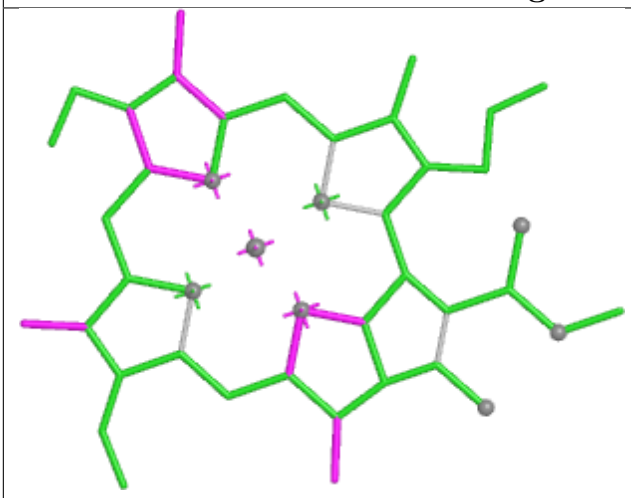


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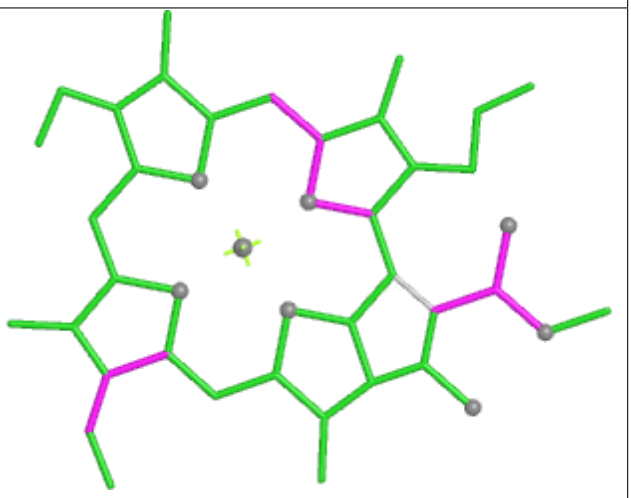


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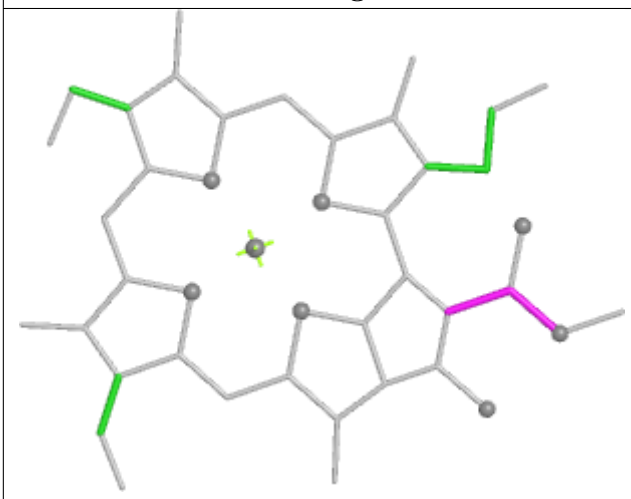
Ligand CLA 2 606



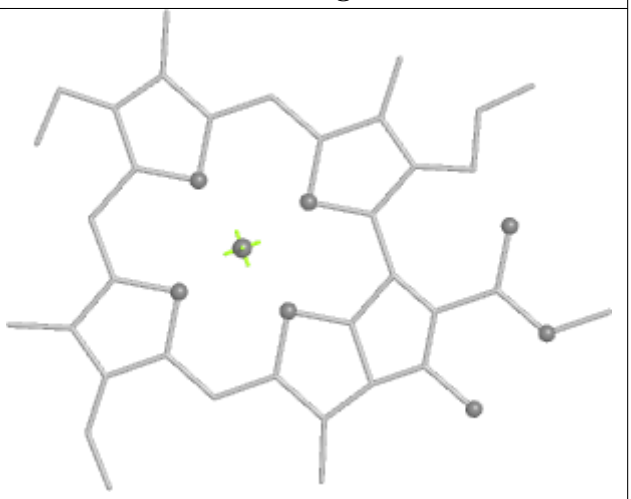
Bond lengths



Bond angles

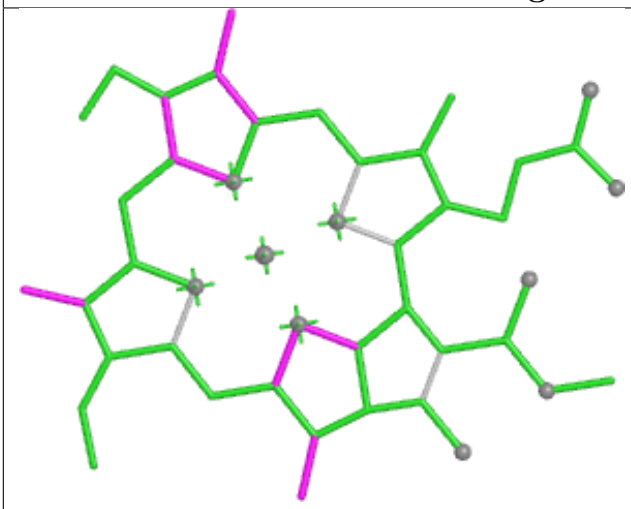


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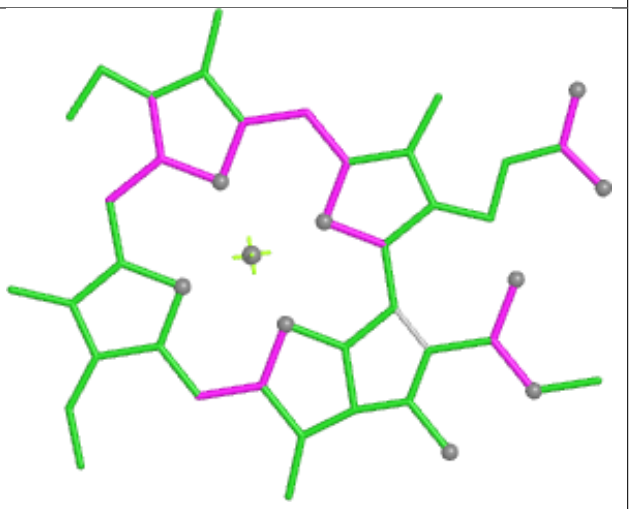


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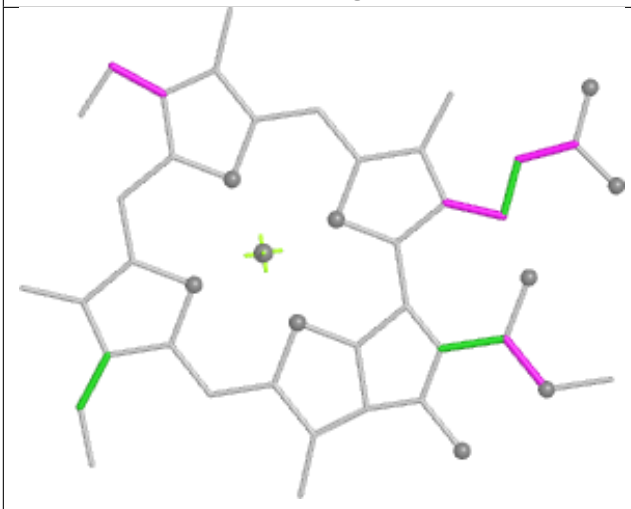
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Bond lengths



Bond angles

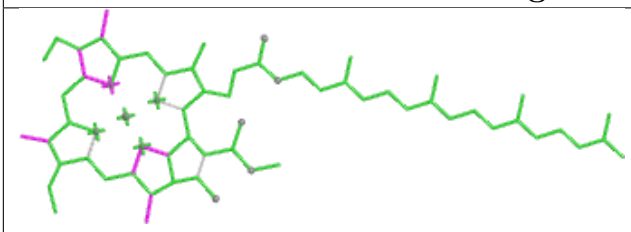


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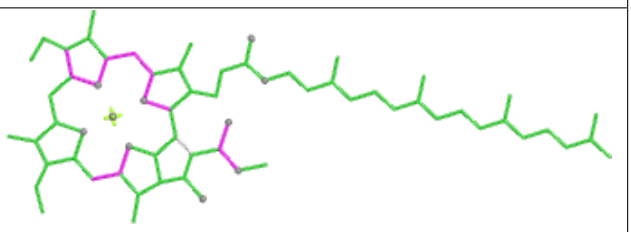


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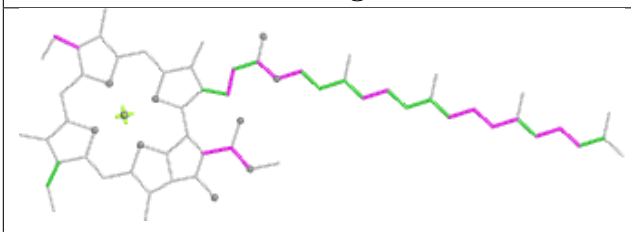
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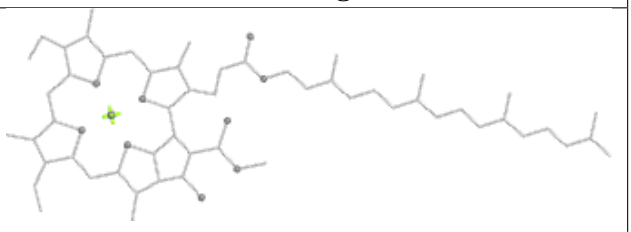
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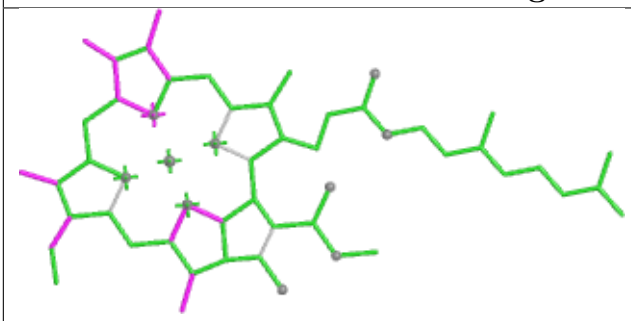


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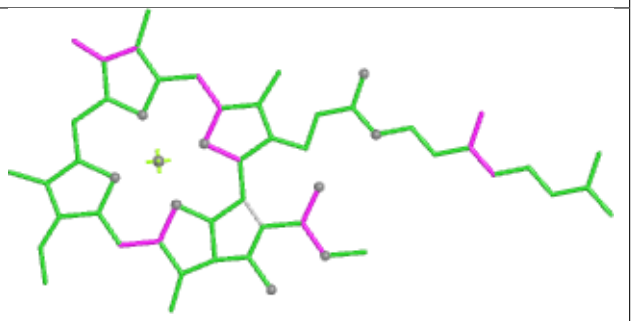


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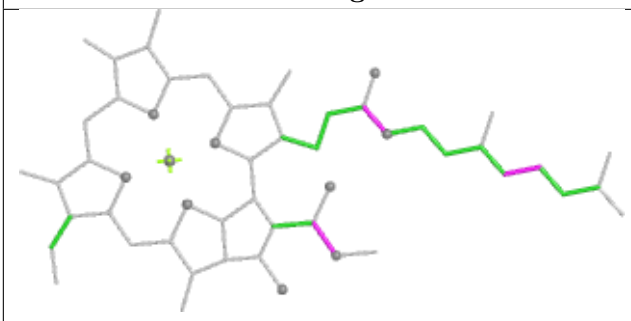
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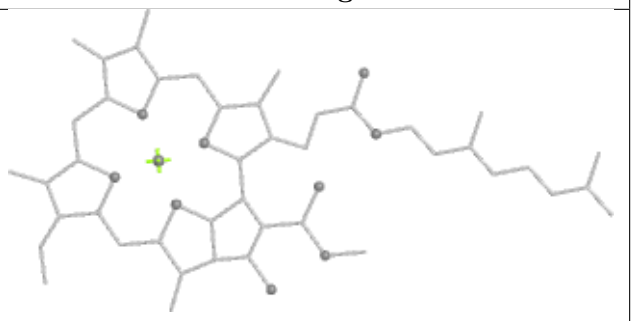
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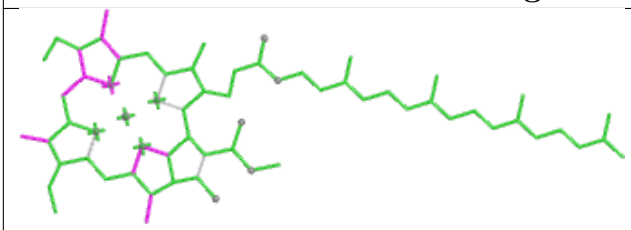


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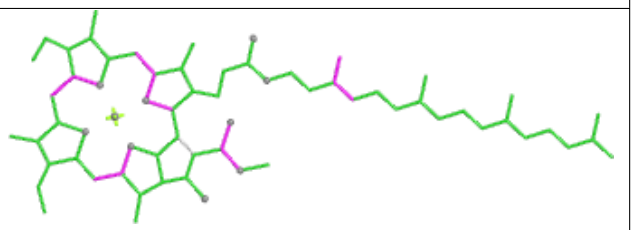


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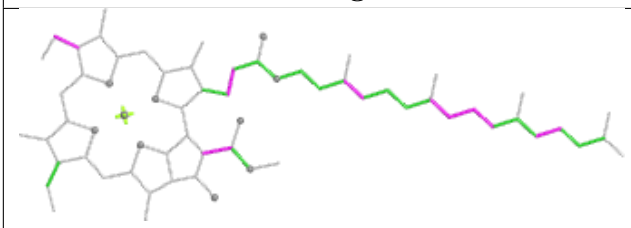
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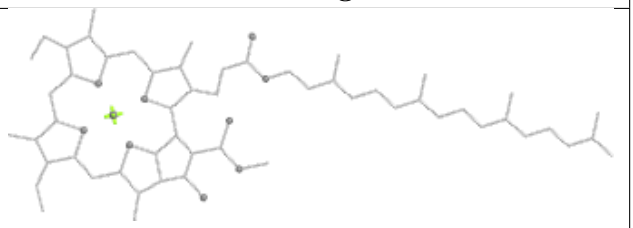
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Bond angles

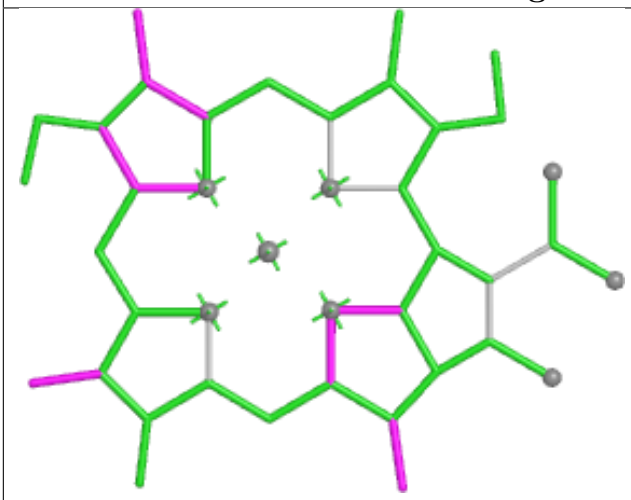


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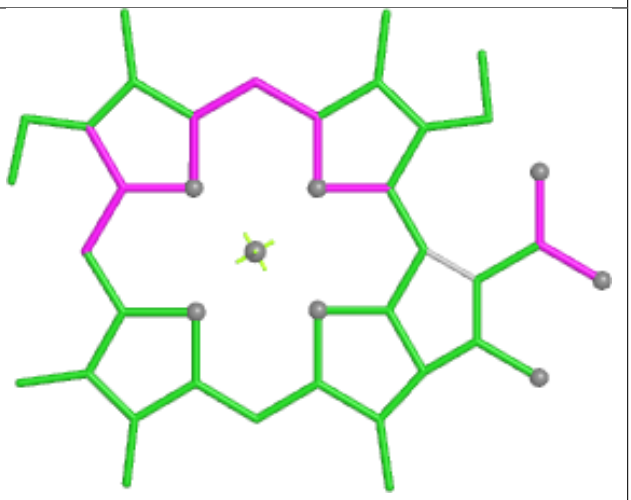


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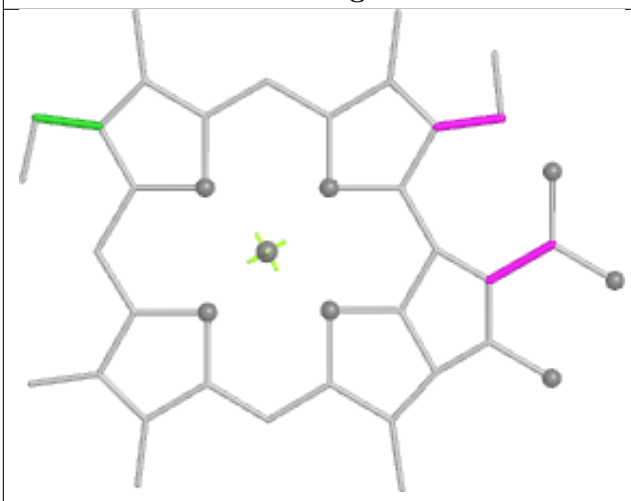
Ligand CLA 3 615



Bond lengths



Bond angles

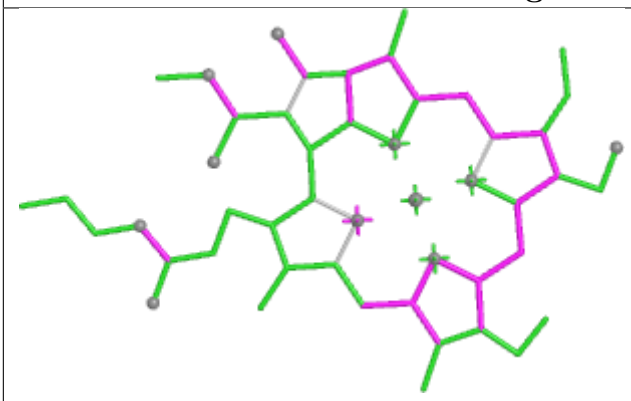


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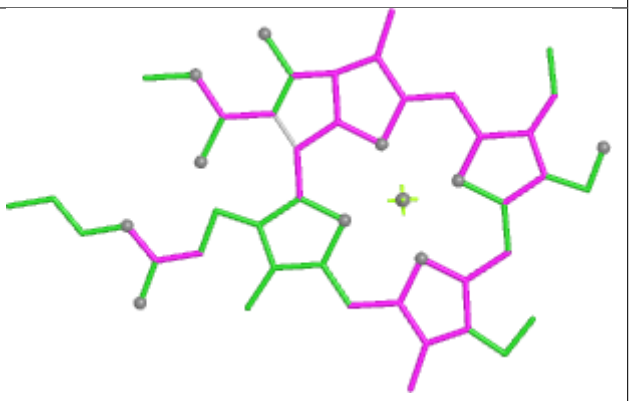


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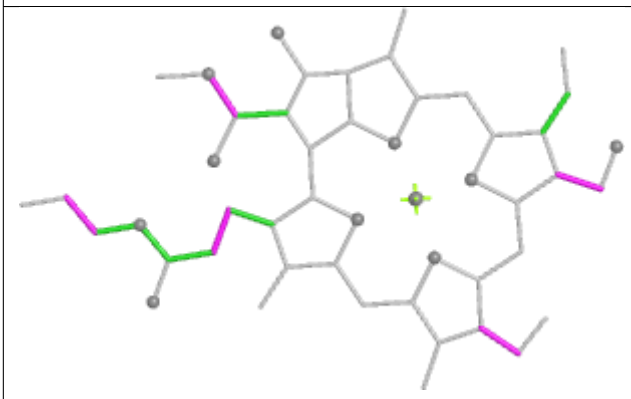
Ligand CHL Z 608



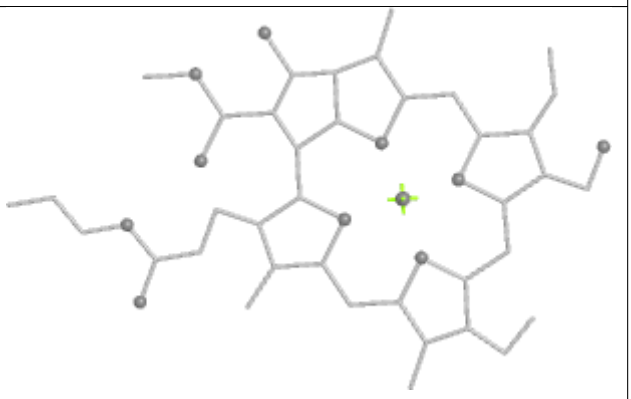
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Bond angles

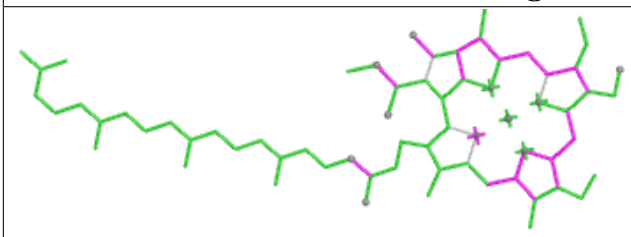


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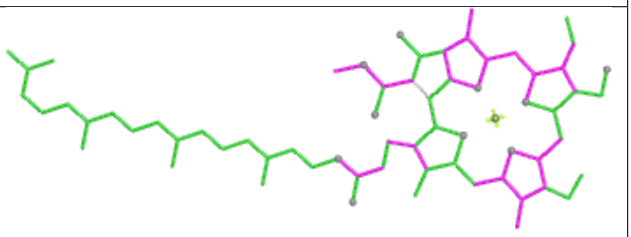


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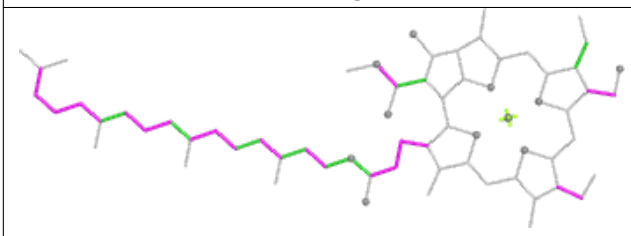
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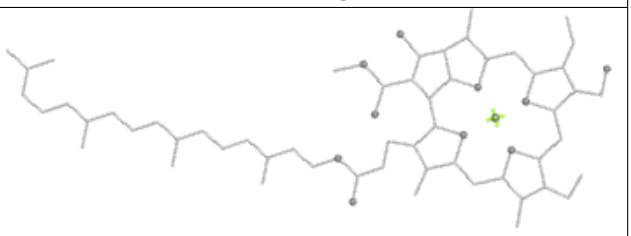
Bond lengths



Bond angles

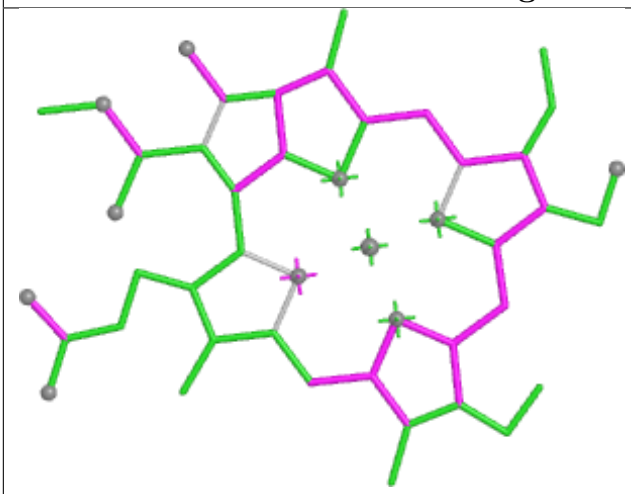


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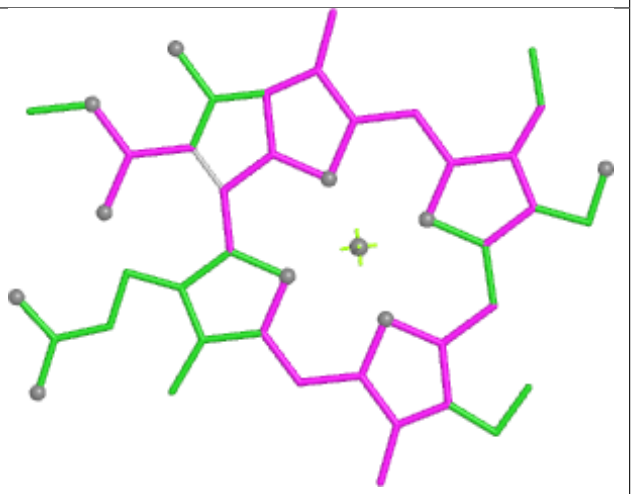


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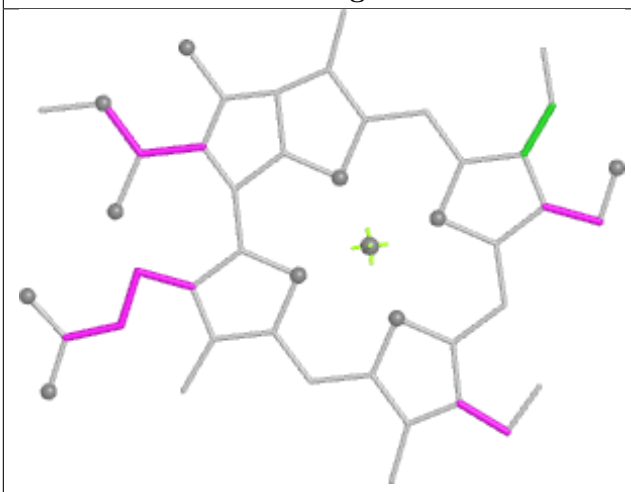
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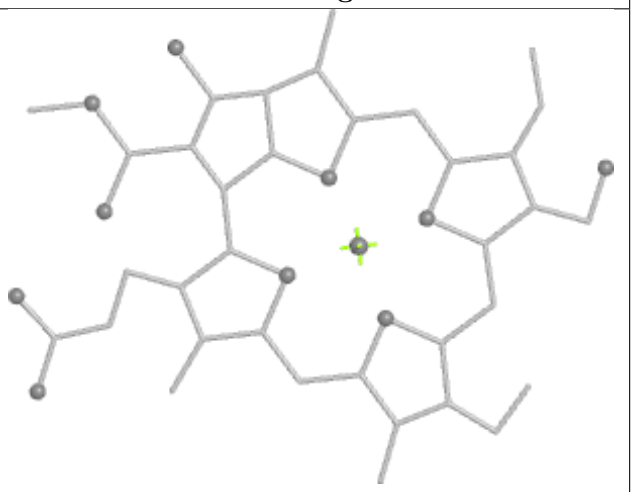
Bond lengths



Bond angles



Torsions

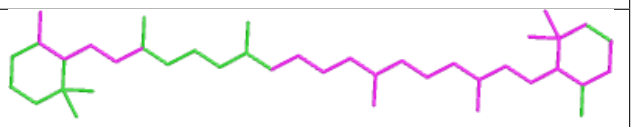


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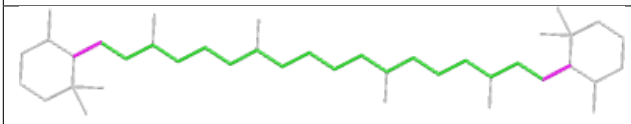
Ligand BCR B 801



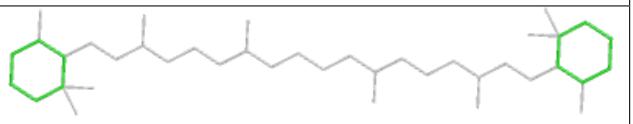
Bond lengths



Bond angles

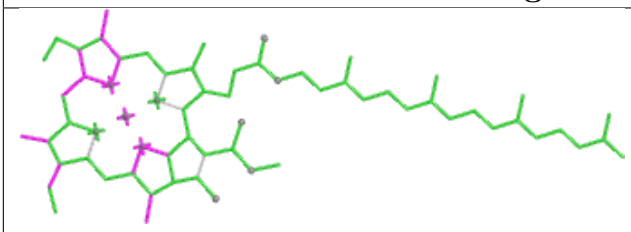


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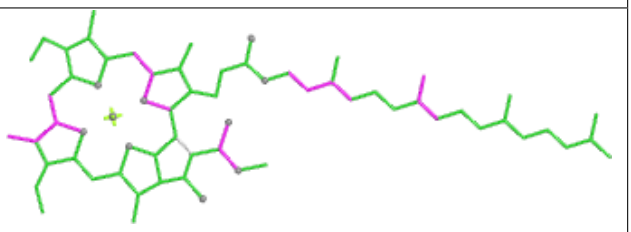


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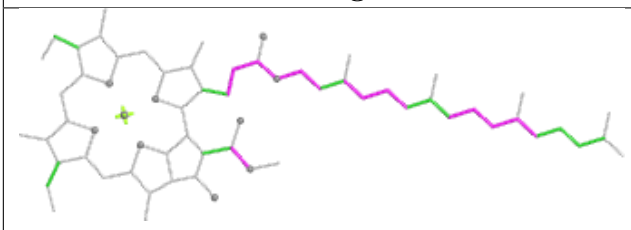
Ligand CLA B 806



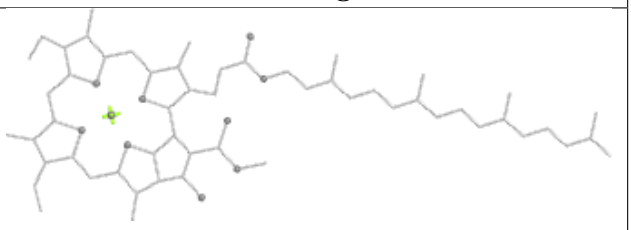
Bond lengths



Bond angles

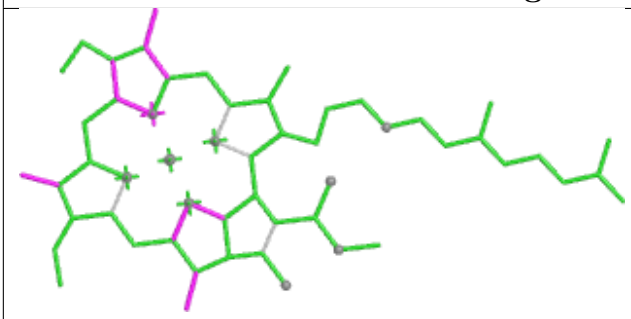


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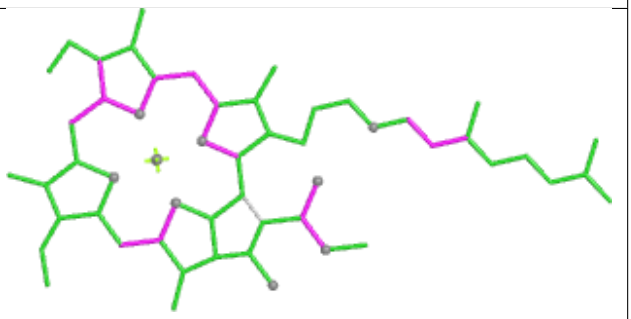


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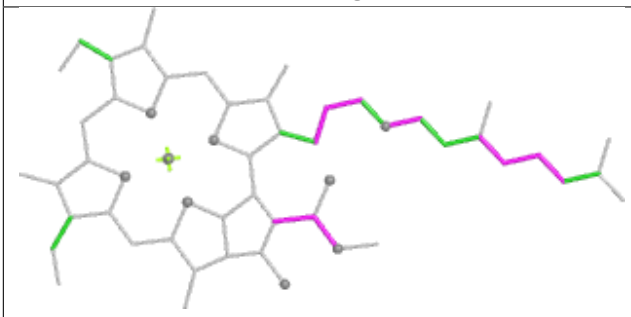
Ligand CLA B 816



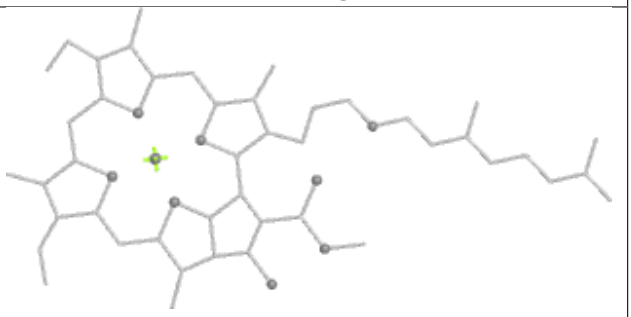
Bond lengths



Bond angles

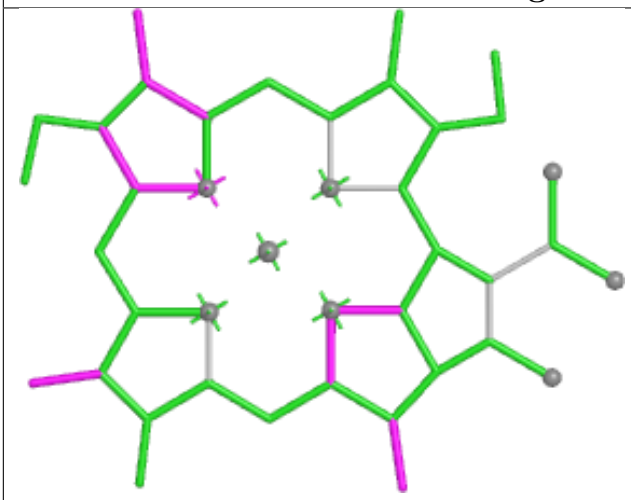


Torsions

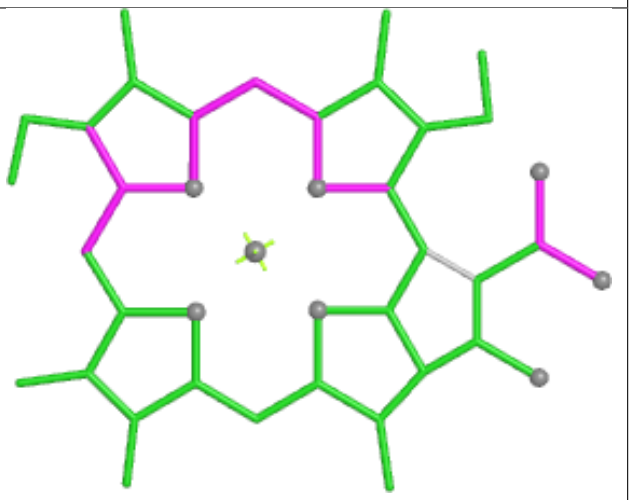


Rings

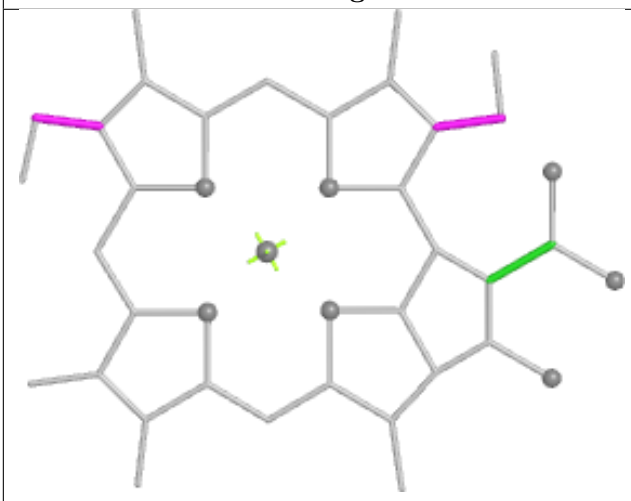
Ligand CLA 4 606



Bond lengths



Bond angles

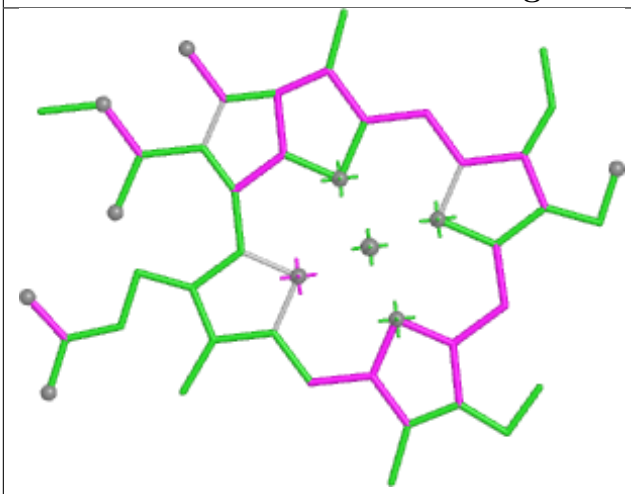


Torsions

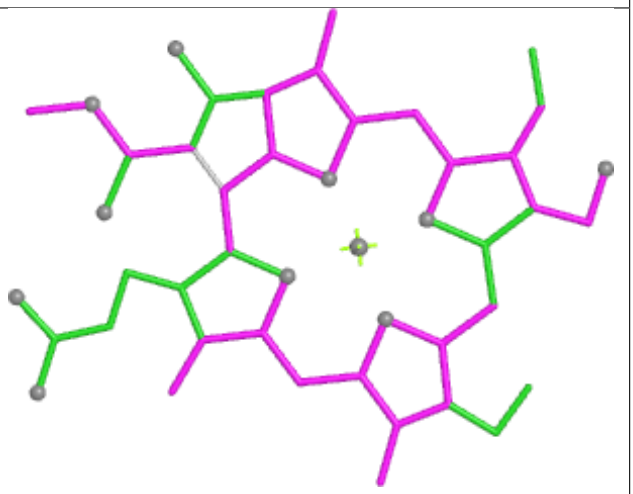


Rings

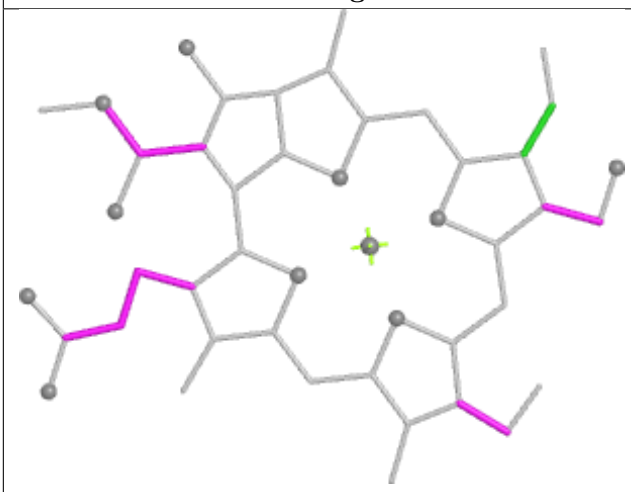
Ligand CHL V 607



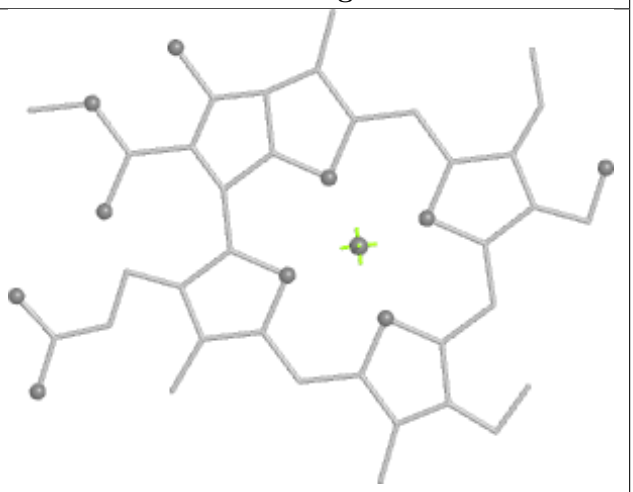
Bond lengths



Bond angles

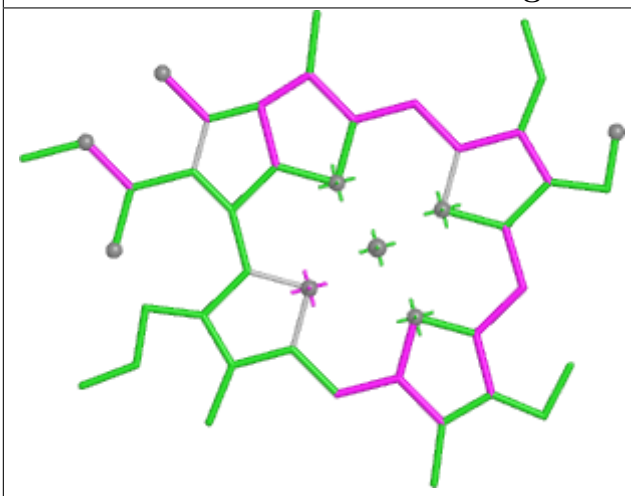


Torsions

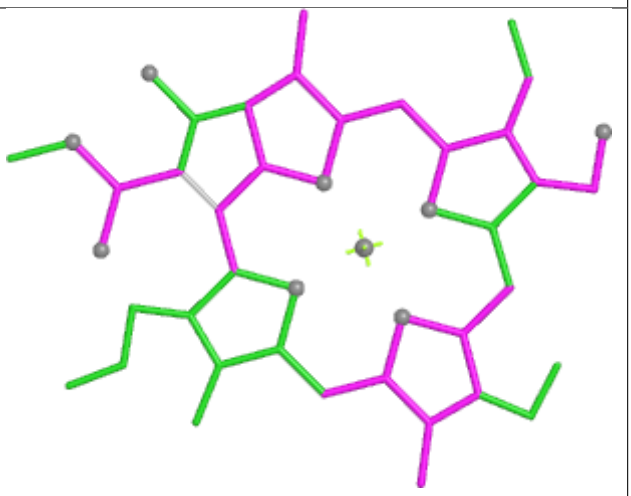


Rings

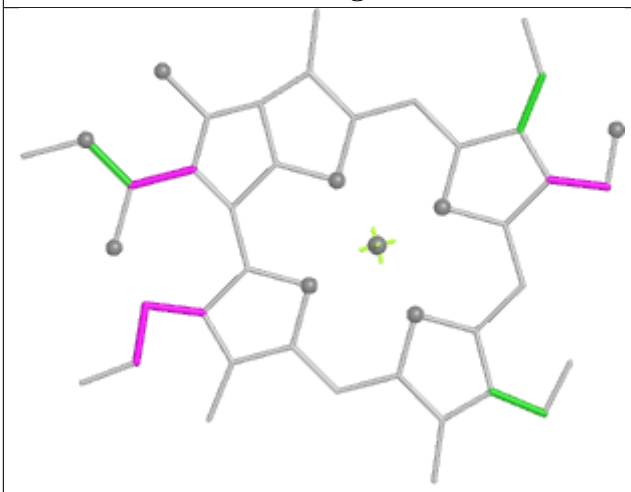
Ligand CHL X 606



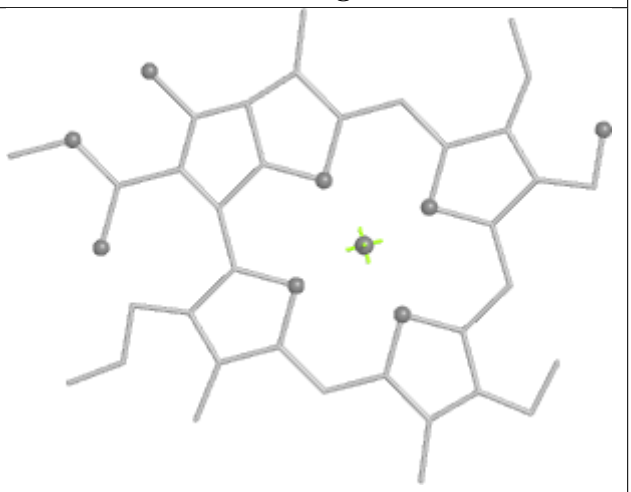
Bond lengths



Bond angles

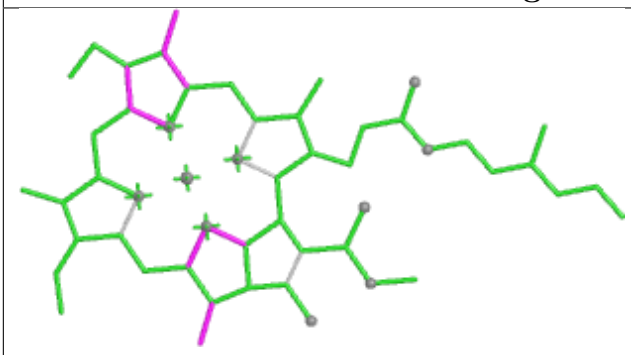


Torsions

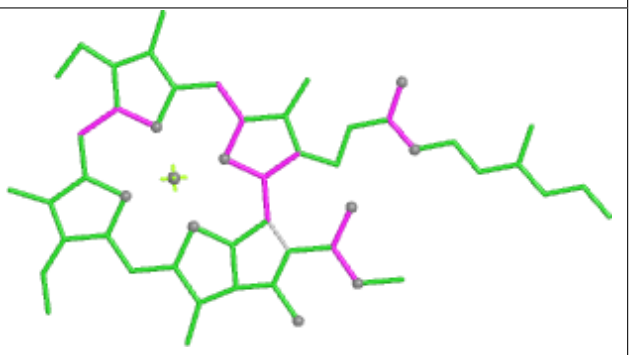


Rings

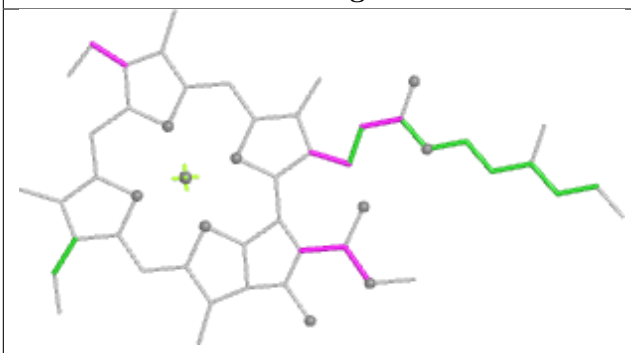
Ligand CLA U 603



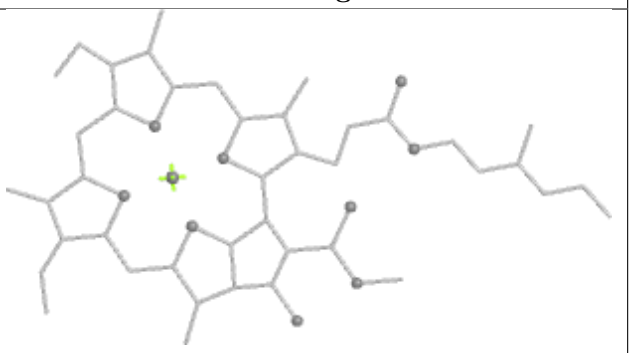
Bond lengths



Bond angles

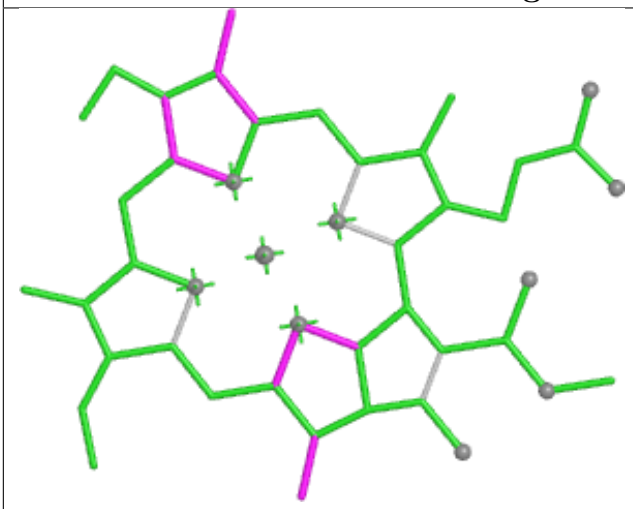


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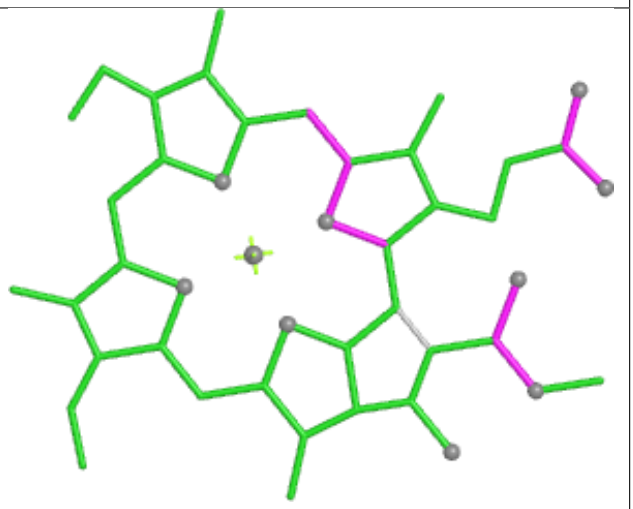


Rings

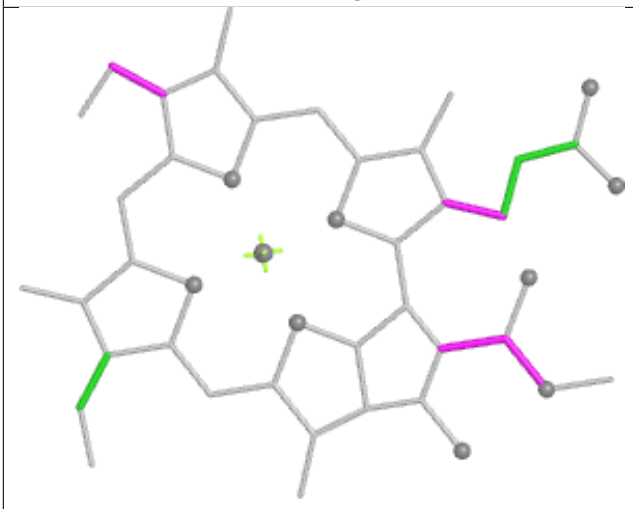
Ligand CLA K 201



Bond lengths



Bond angles

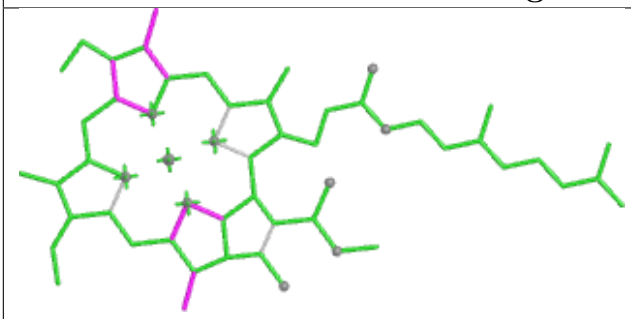


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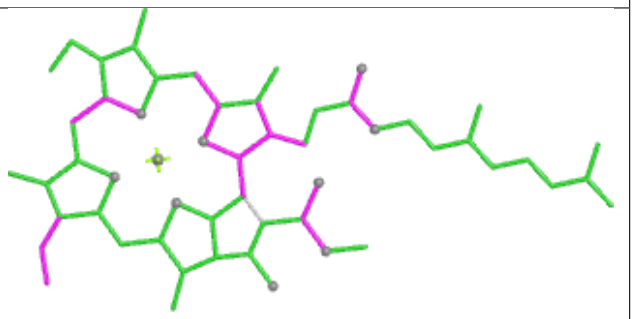


Rings

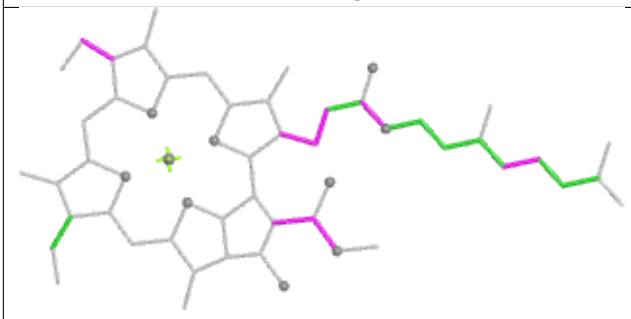
Ligand CLA Z 603



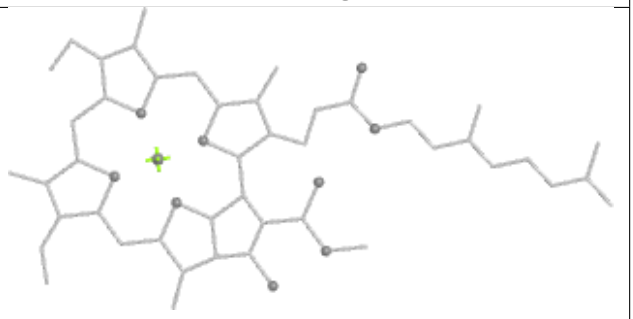
Bond lengths



Bond angles

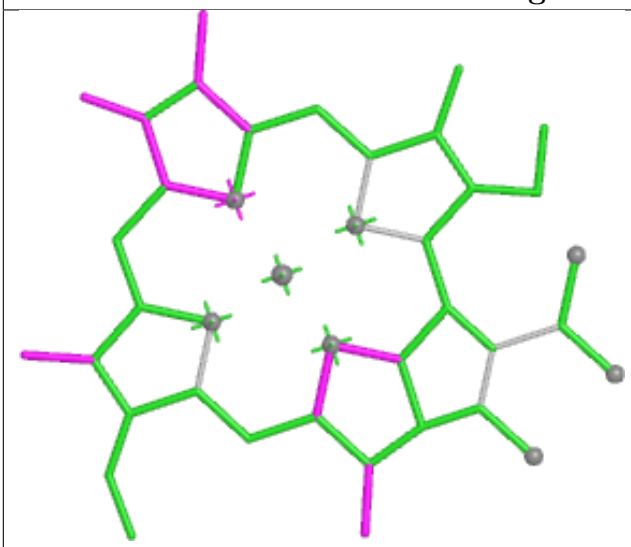


Torsions

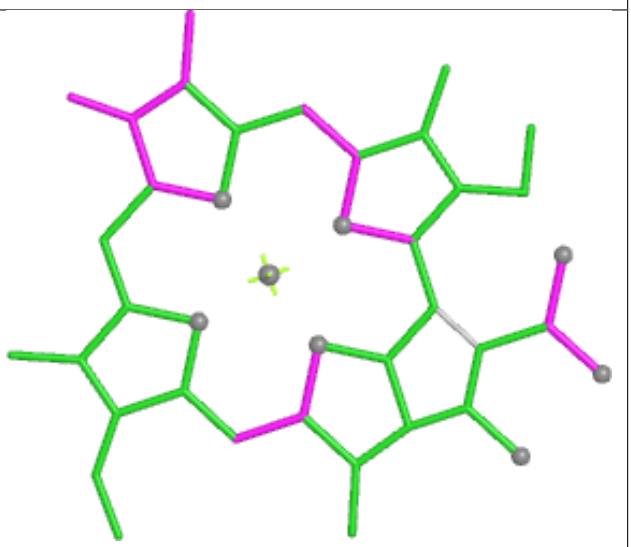


Rings

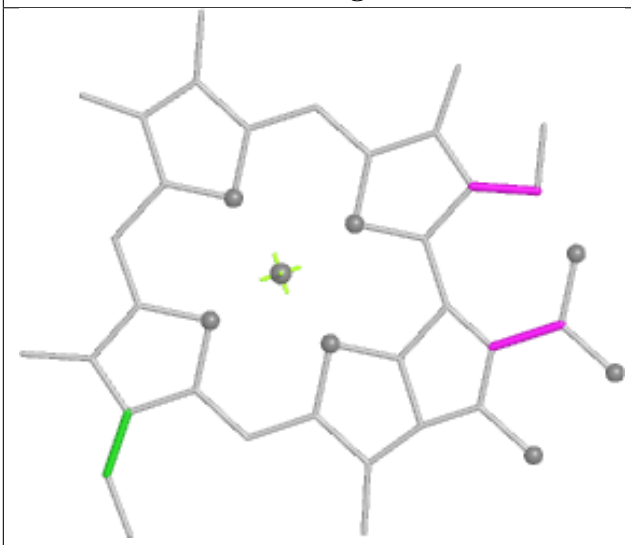
Ligand CLA 5 618



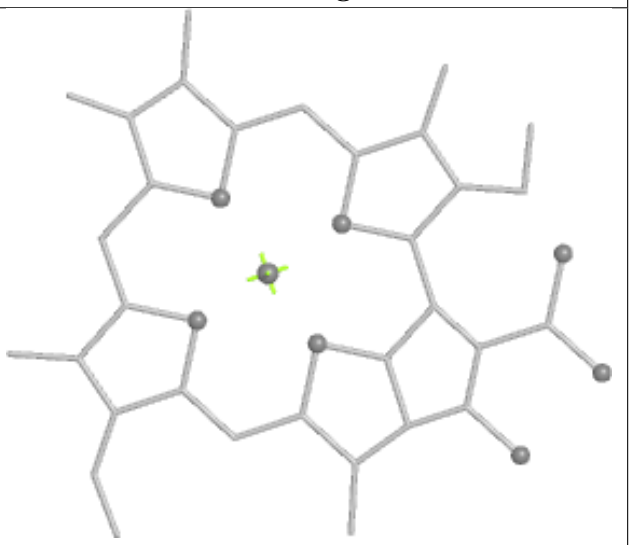
Bond lengths



Bond angles

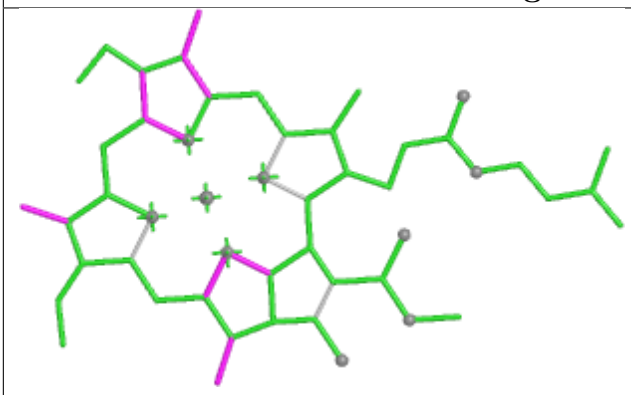


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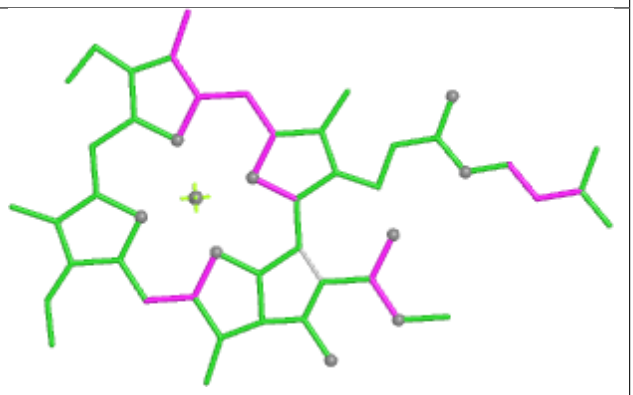


Rings

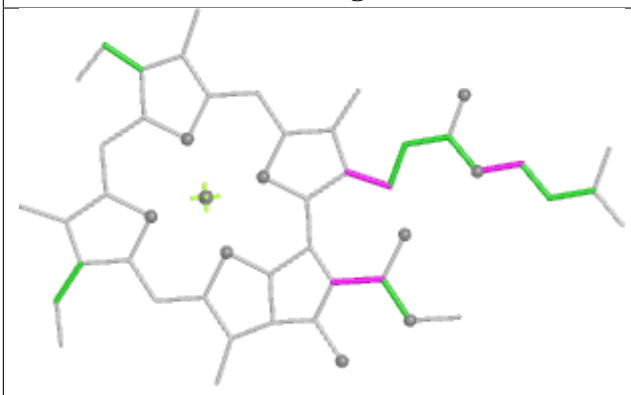
Ligand CLA A 808



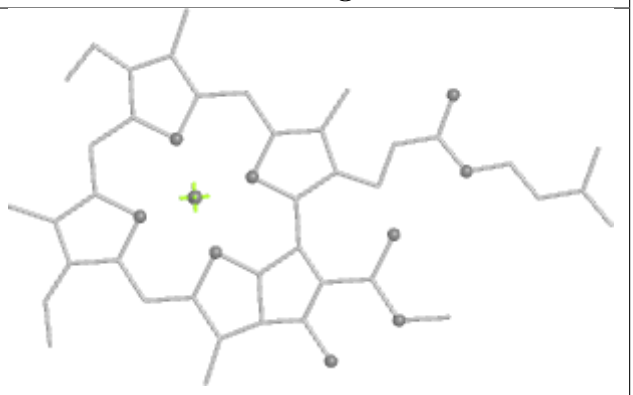
Bond lengths



Bond angles

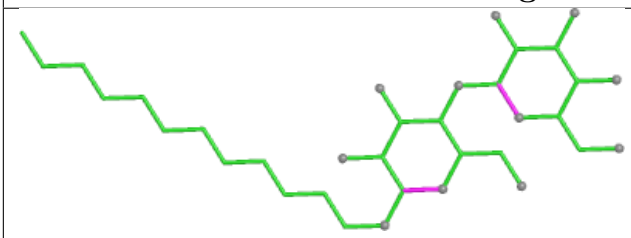


Torsions

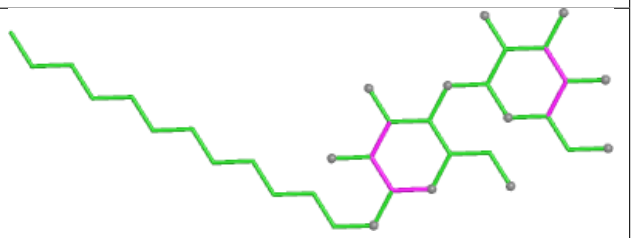


Rings

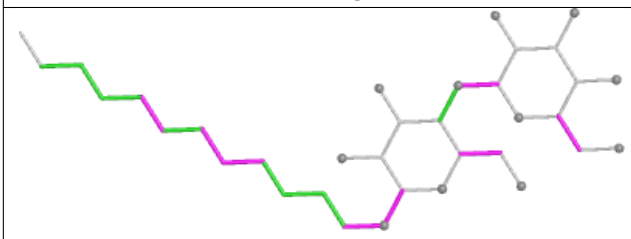
Ligand LMU K 208



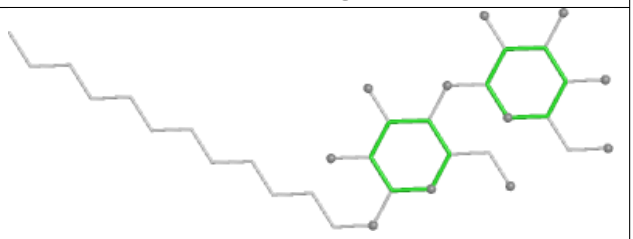
Bond lengths



Bond angles

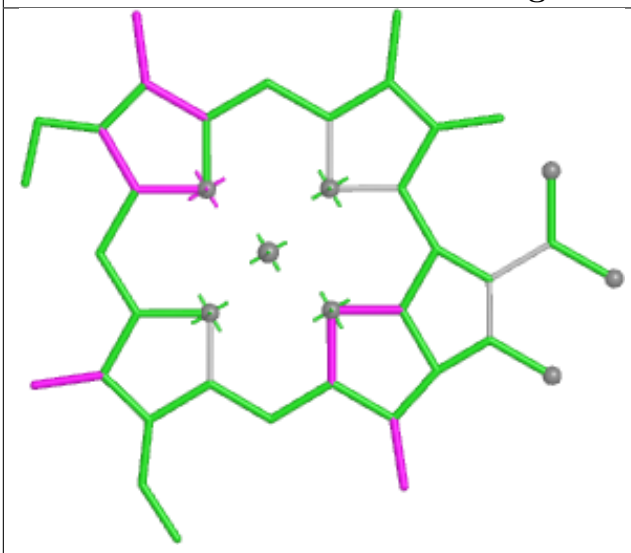


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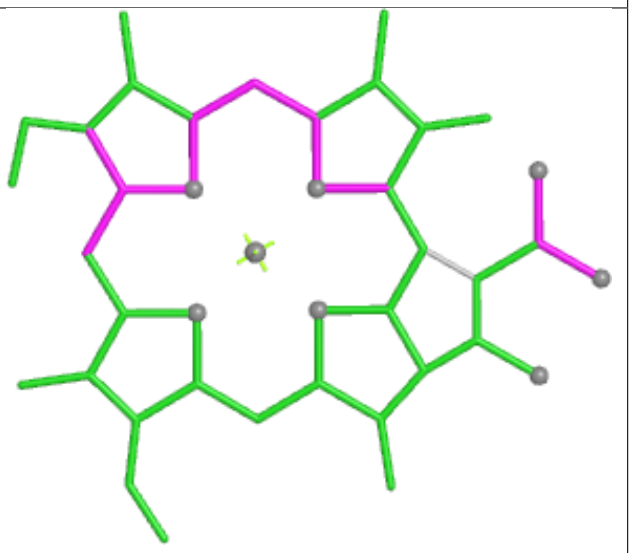


Rings

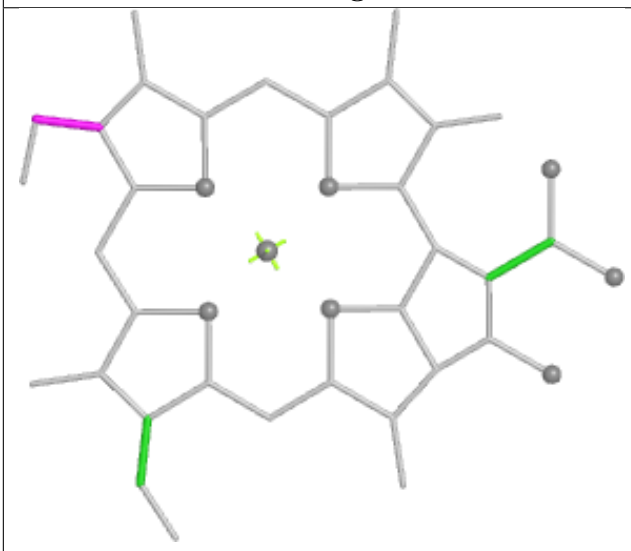
Ligand CLA 3 614



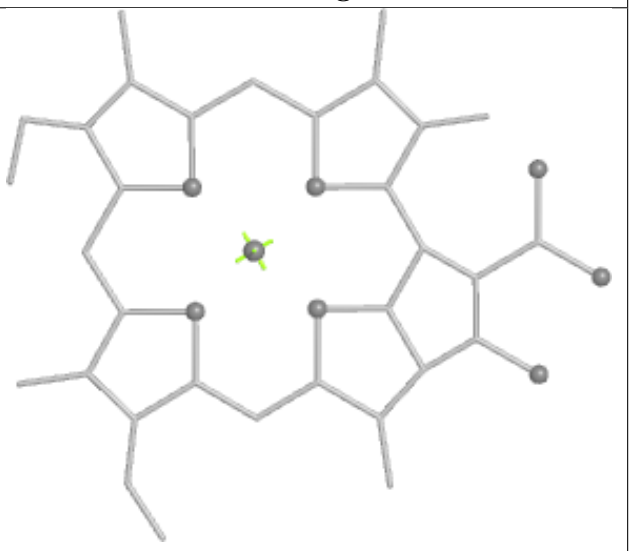
Bond lengths



Bond angles

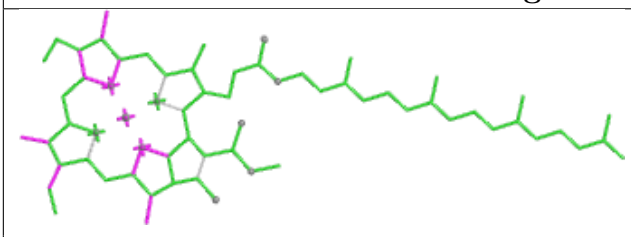


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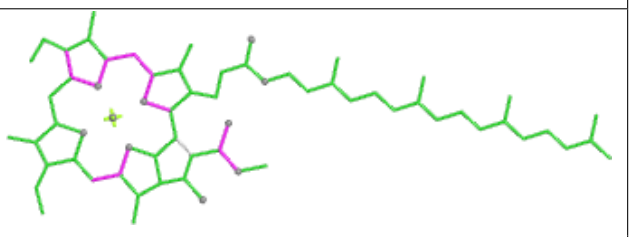


Rings

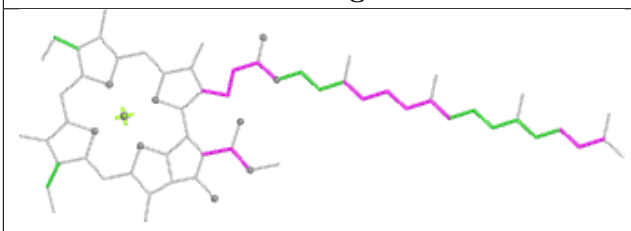
Ligand CLA A 807



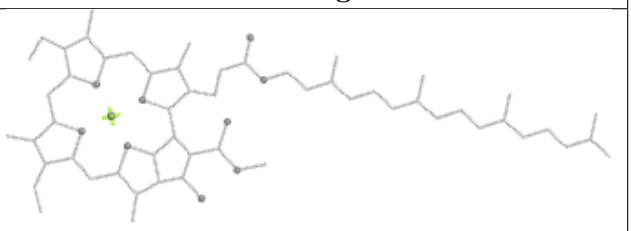
Bond lengths



Bond angles

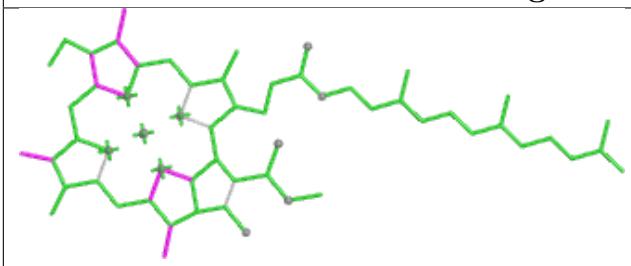


Torsions

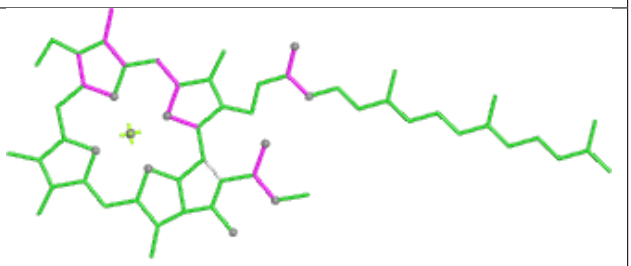


Rings

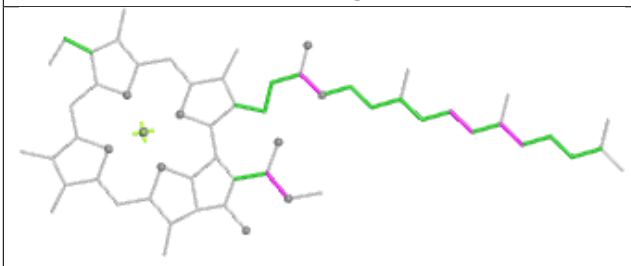
Ligand CLA a 610



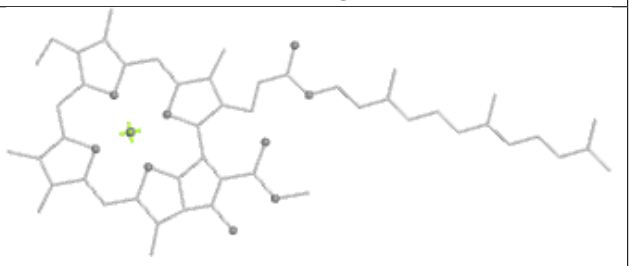
Bond lengths



Bond angles

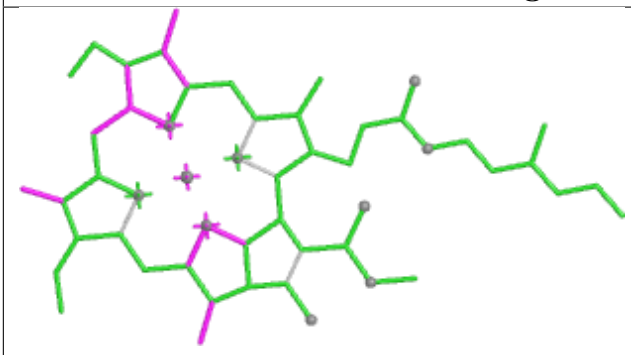


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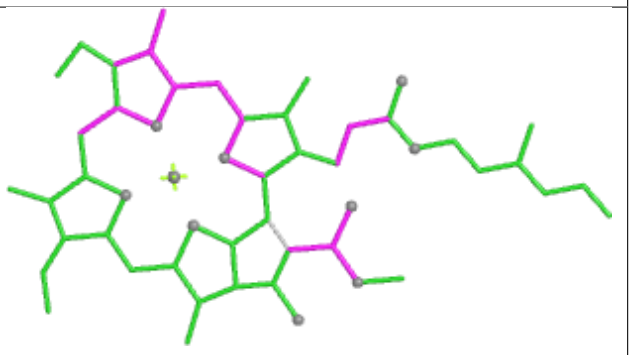


Rings

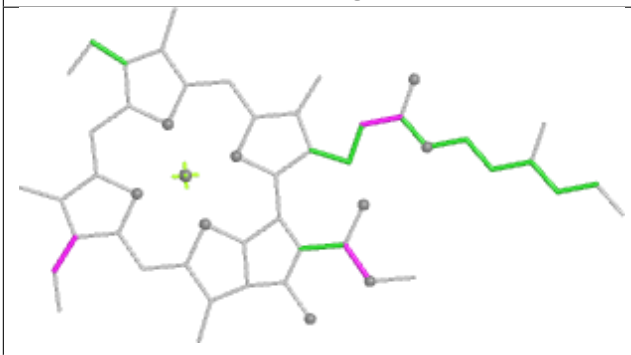
Ligand CLA A 840



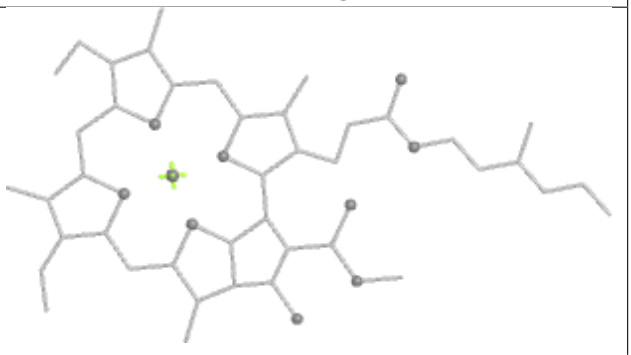
Bond lengths



Bond angles

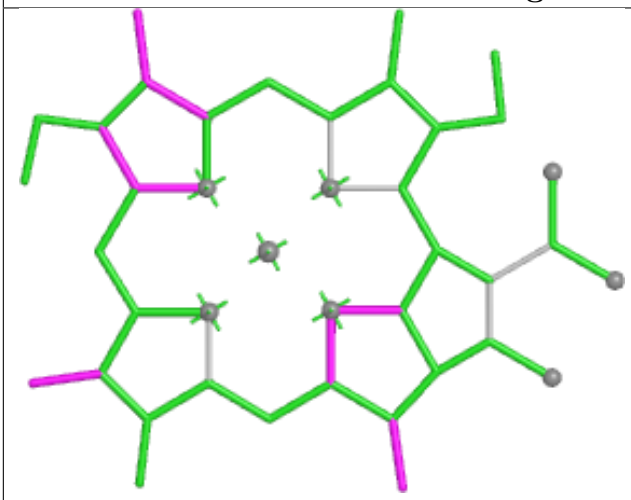


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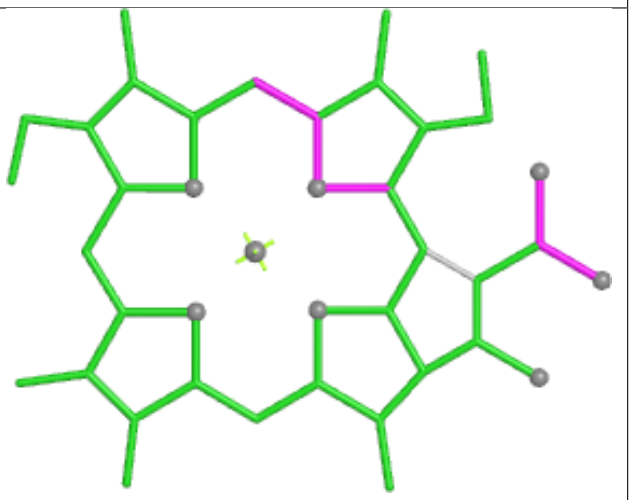


Rings

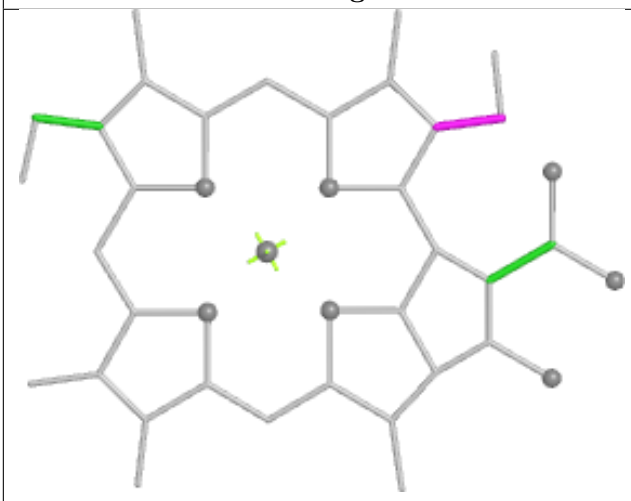
Ligand CLA L 306



Bond lengths



Bond angles

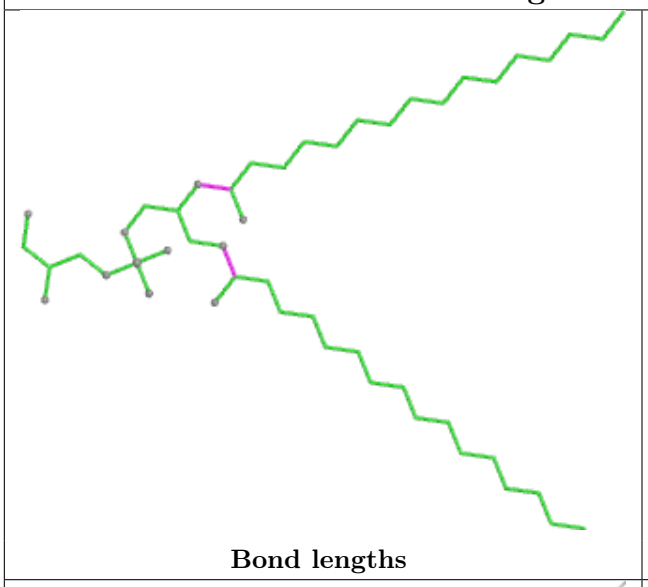


Torsions

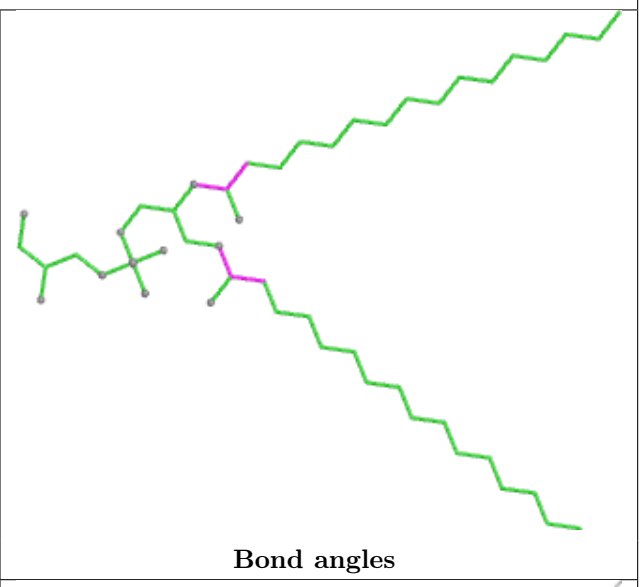


Rings

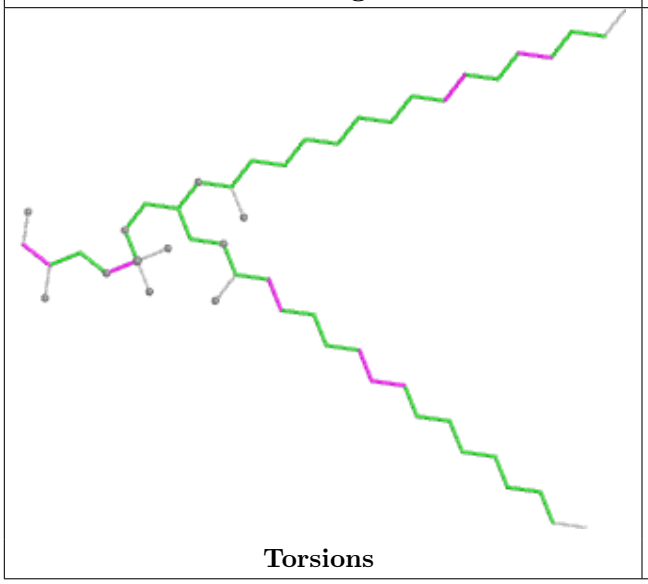
Ligand LHG 1 620



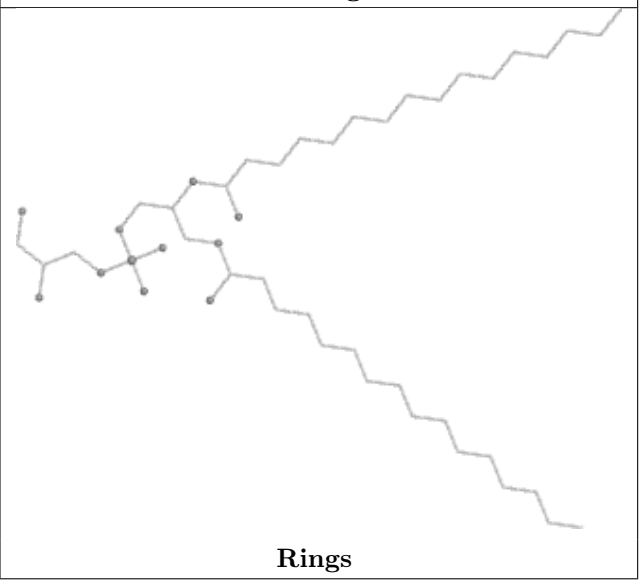
Bond lengths



Bond angles

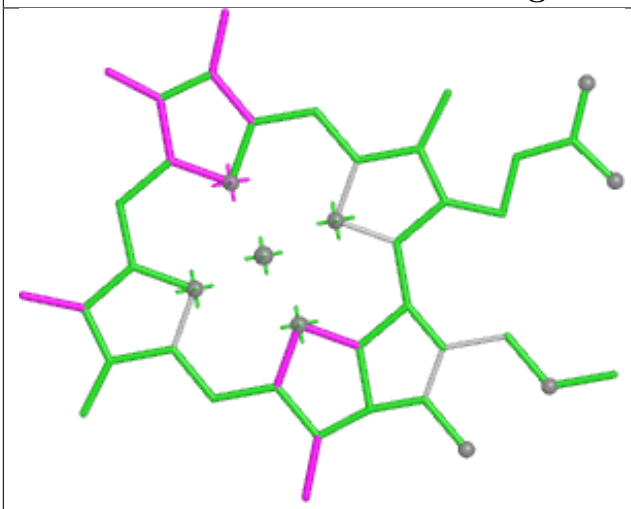


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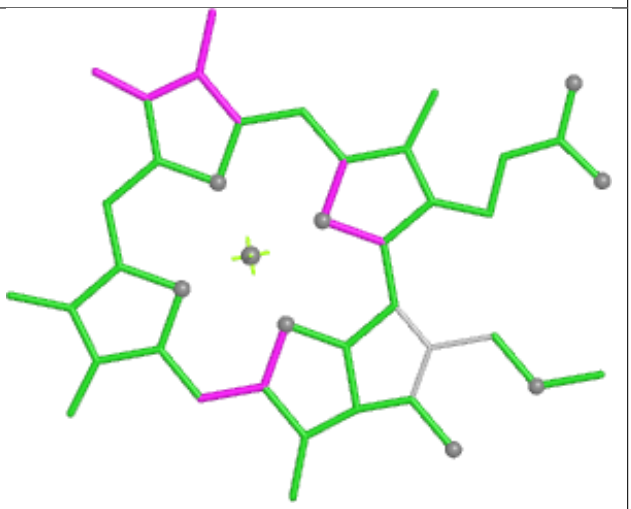


Rings

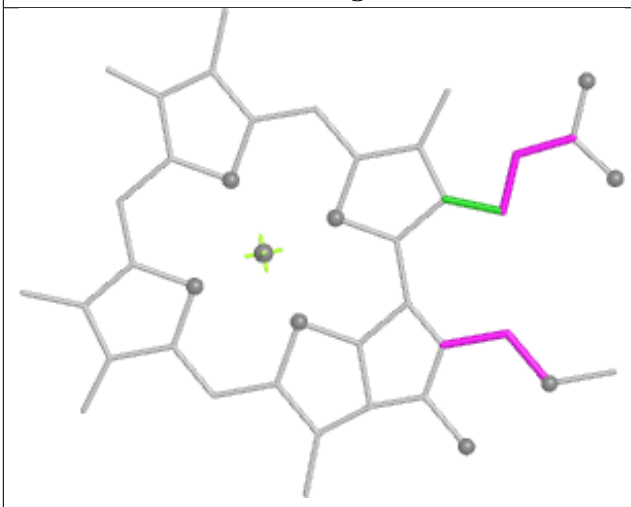
Ligand CLA 7 615



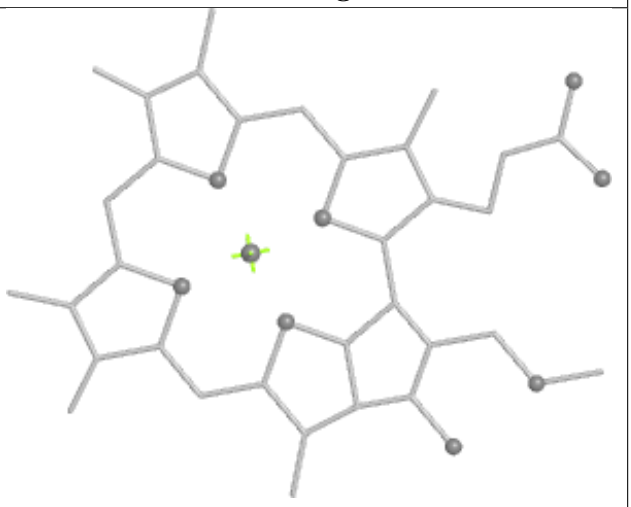
Bond lengths



Bond angles

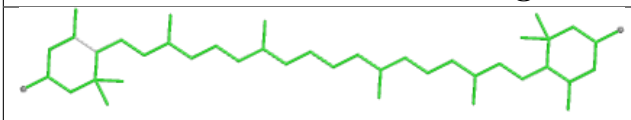


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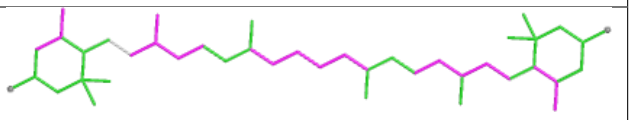


Rings

Ligand LUT X 1620



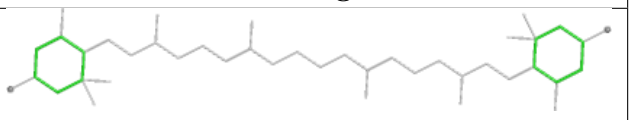
Bond lengths



Bond angles

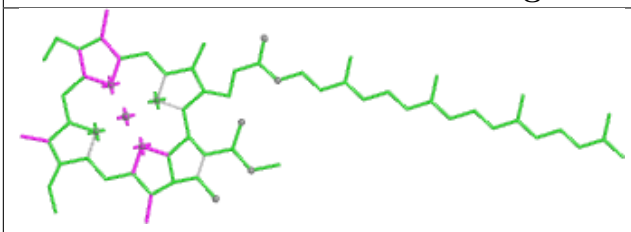


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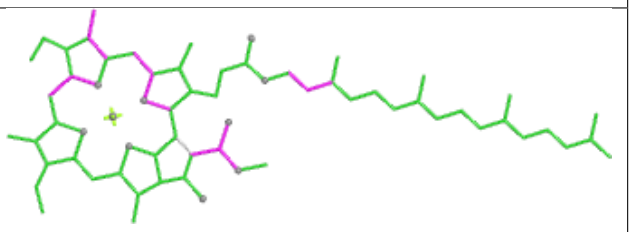


Rings

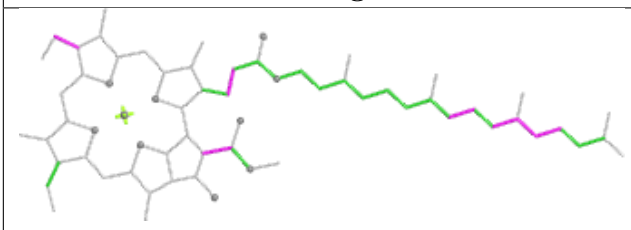
Ligand CLA A 809



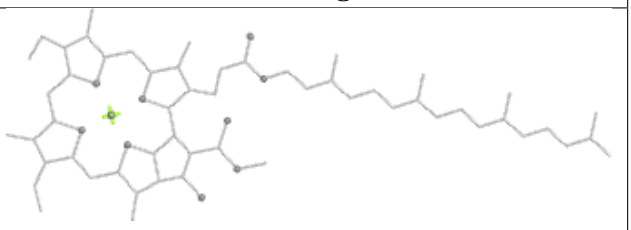
Bond lengths



Bond angles

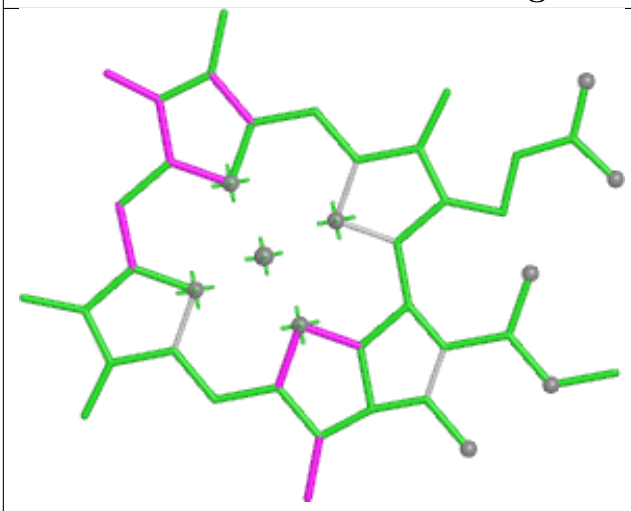


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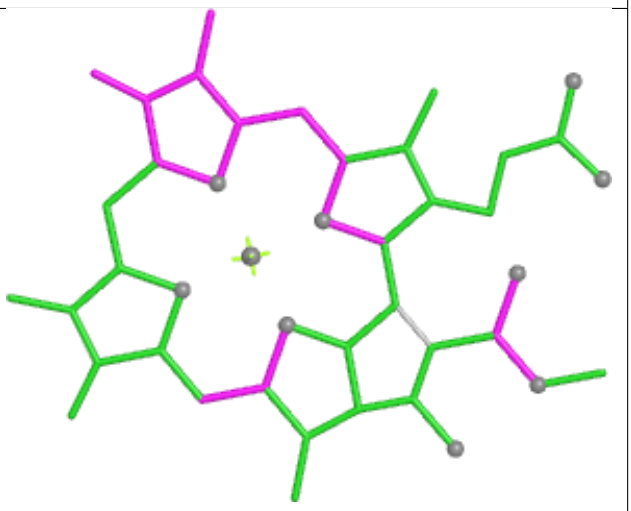


Rings

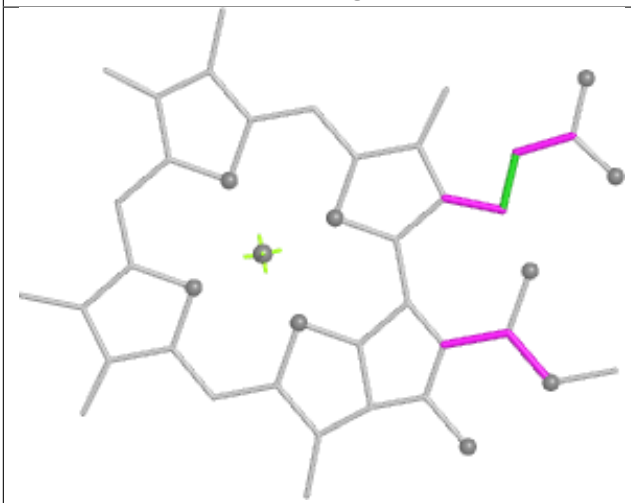
Ligand CLA 1 616



Bond lengths



Bond angles

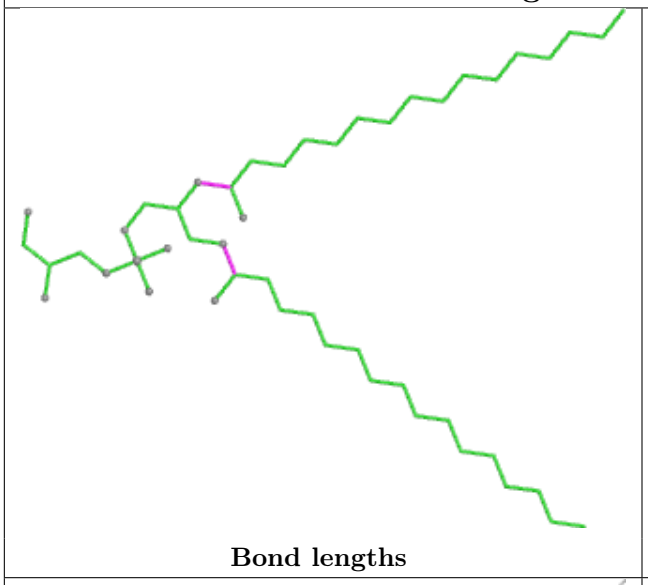


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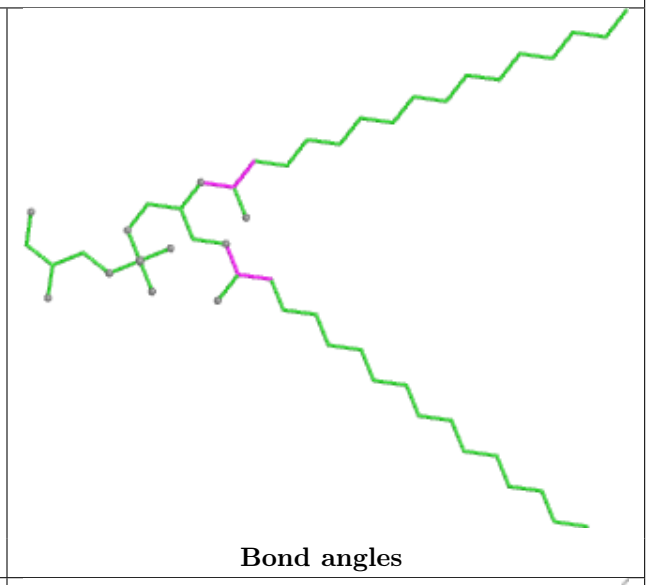


Rings

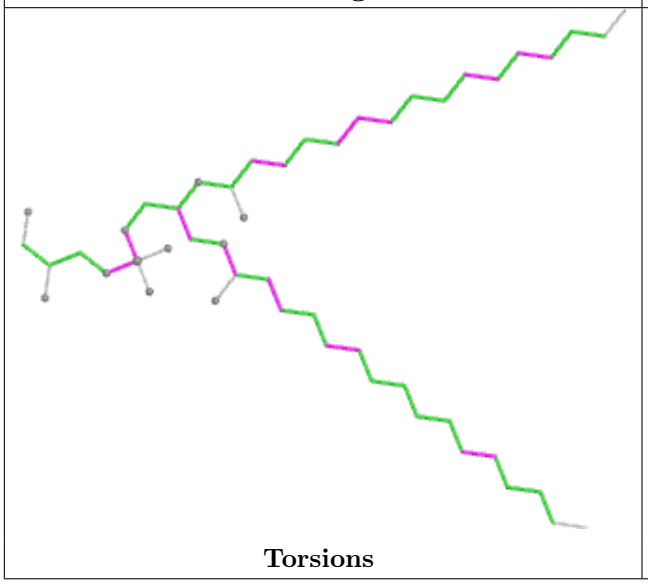
Ligand LHG H 204



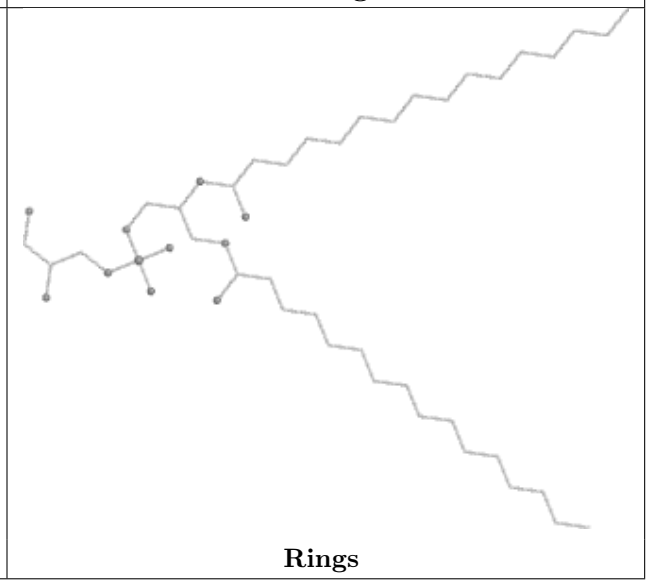
Bond lengths



Bond angles

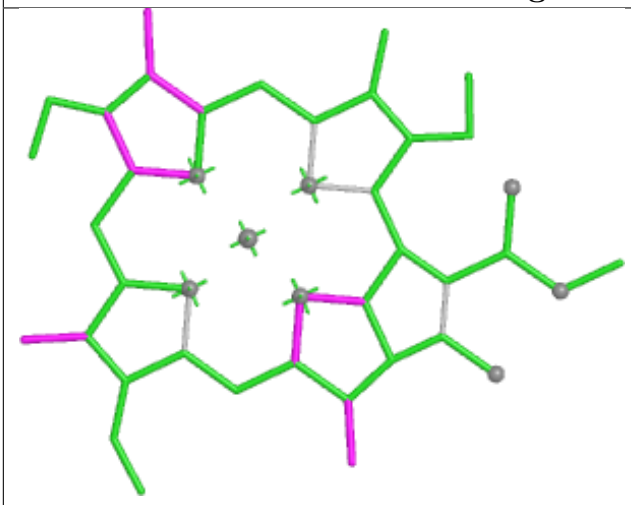


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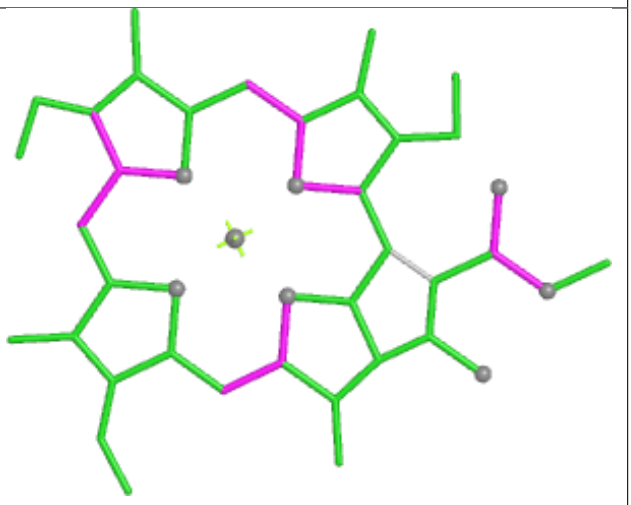


Rings

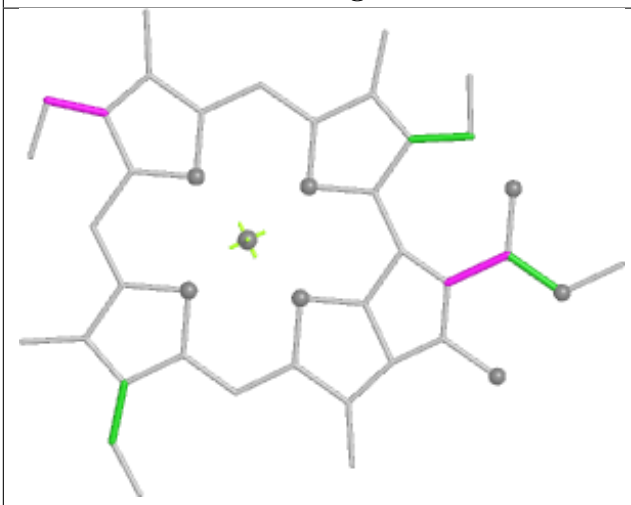
Ligand CLA 2 611



Bond lengths



Bond angles

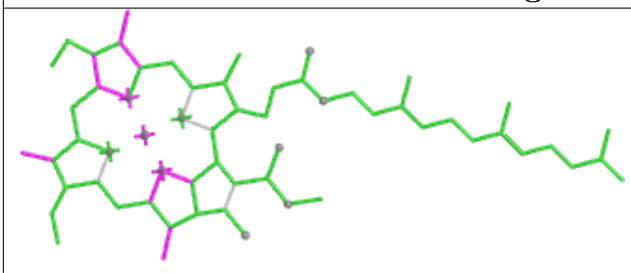


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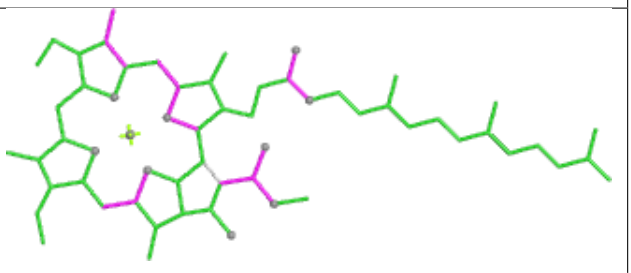


Rings

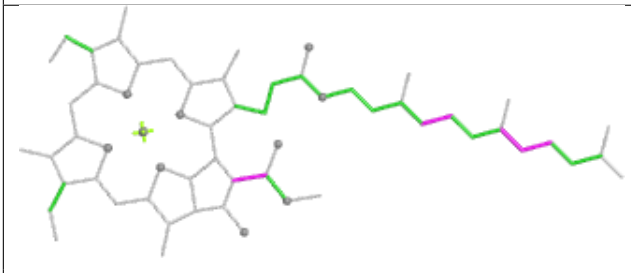
Ligand CLA B 834



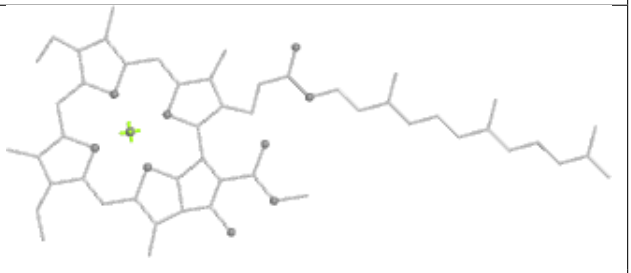
Bond lengths



Bond angles

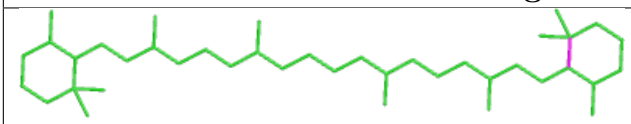


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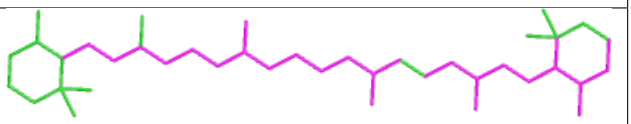


Rings

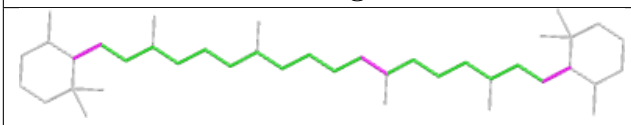
Ligand BCR F 305



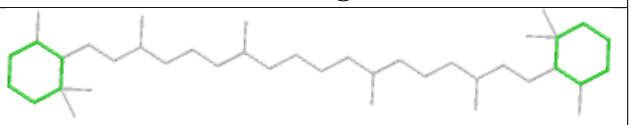
Bond lengths



Bond angles

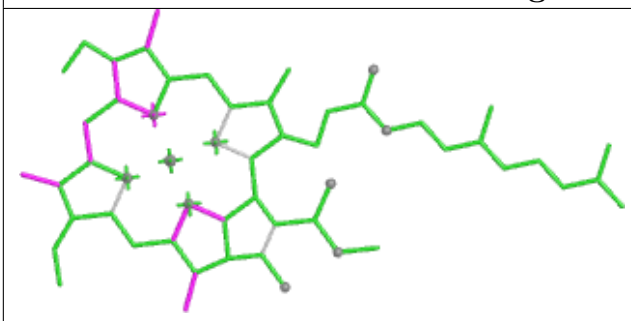


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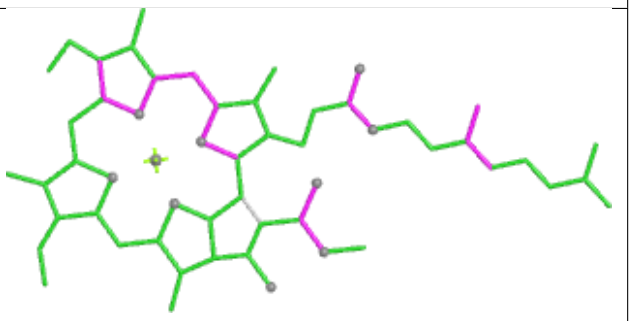


Rings

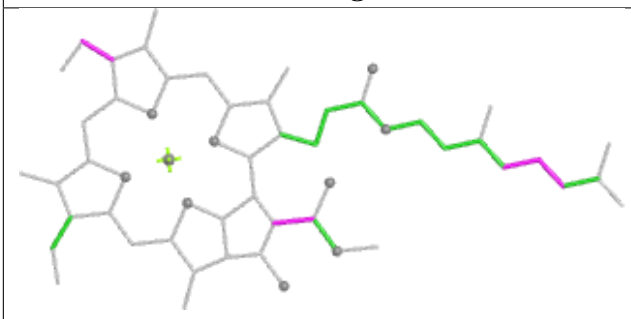
Ligand CLA 2 610



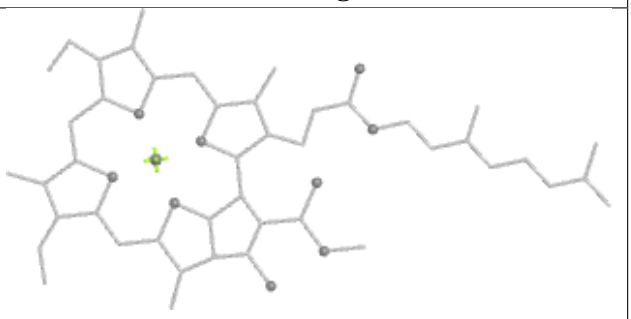
Bond lengths



Bond angles

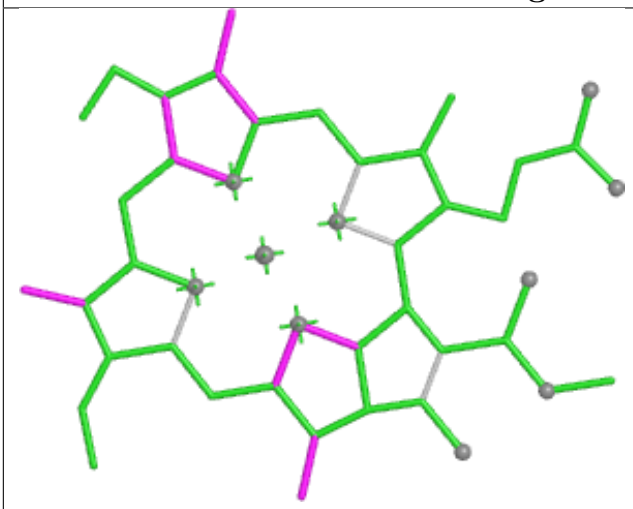


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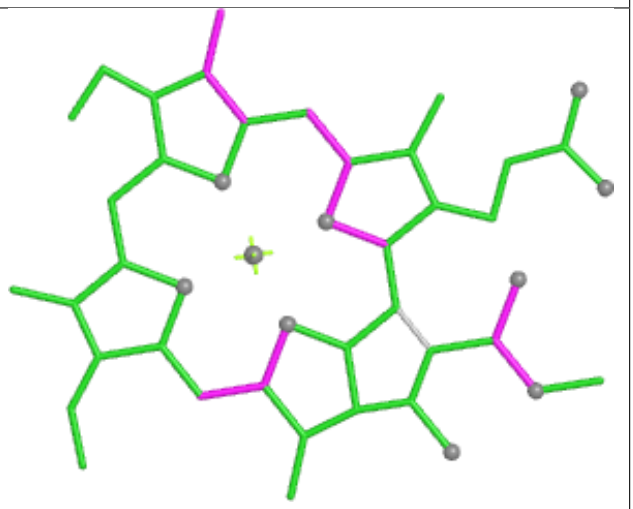


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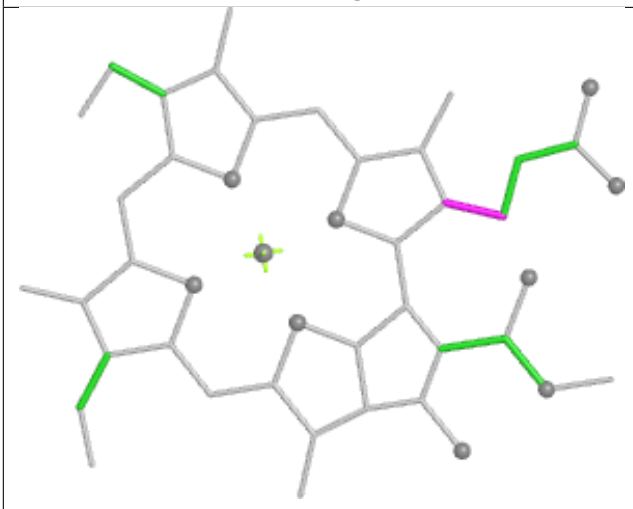
Ligand CLA 8 609



Bond lengths



Bond angles

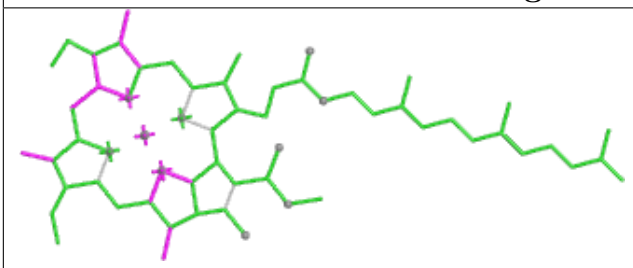


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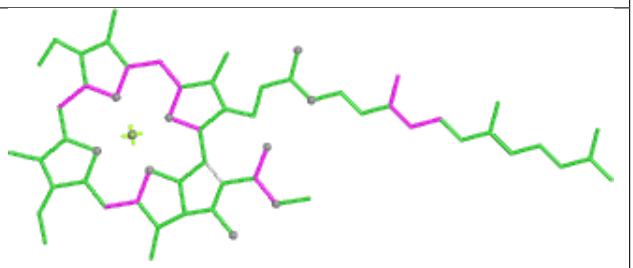


Rings

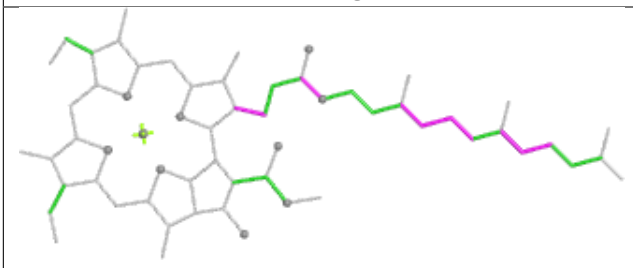
Ligand CLA B 818



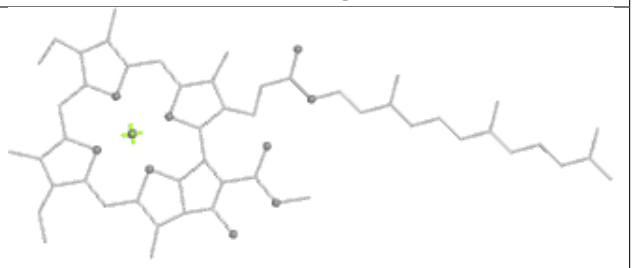
Bond lengths



Bond angles

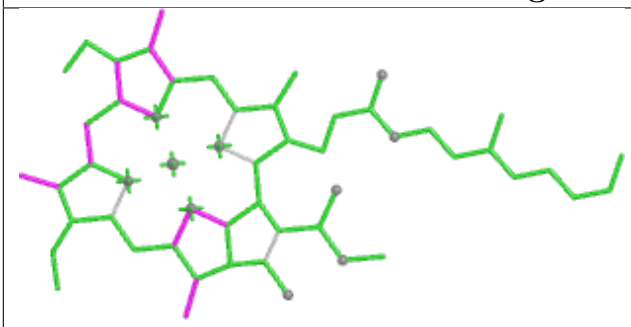


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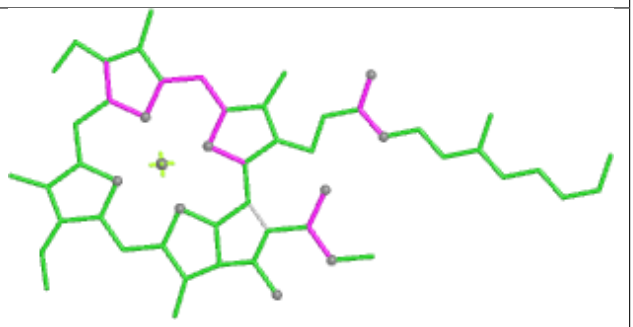


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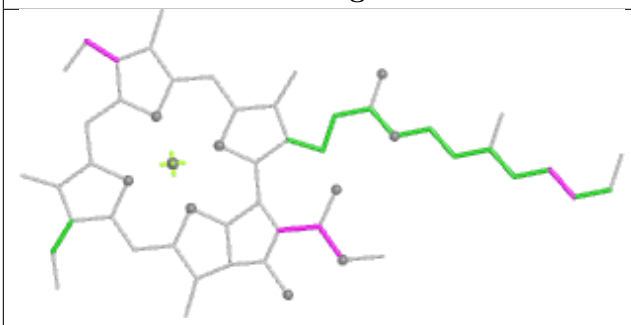
Ligand CLA 5 610



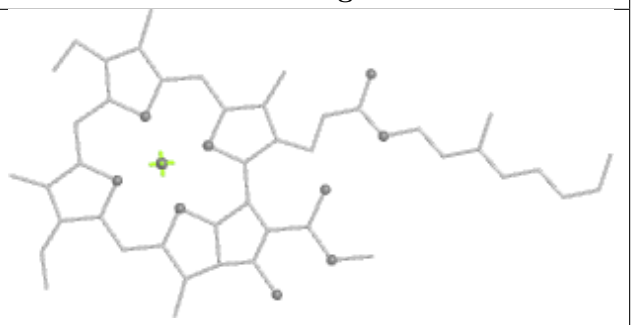
Bond lengths



Bond angles

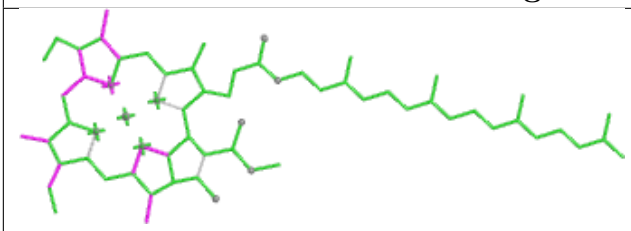


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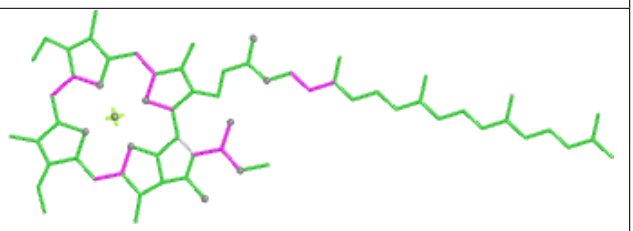


Rings

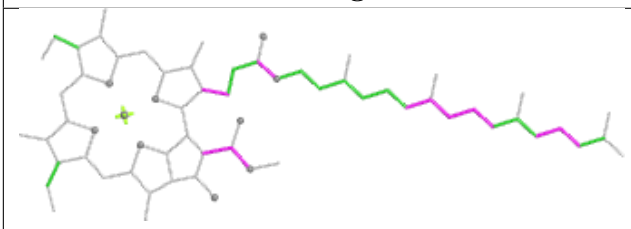
Ligand CLA A 816



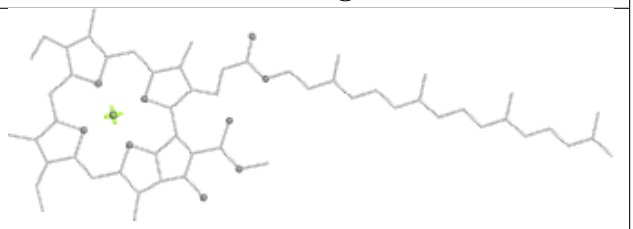
Bond lengths



Bond angles

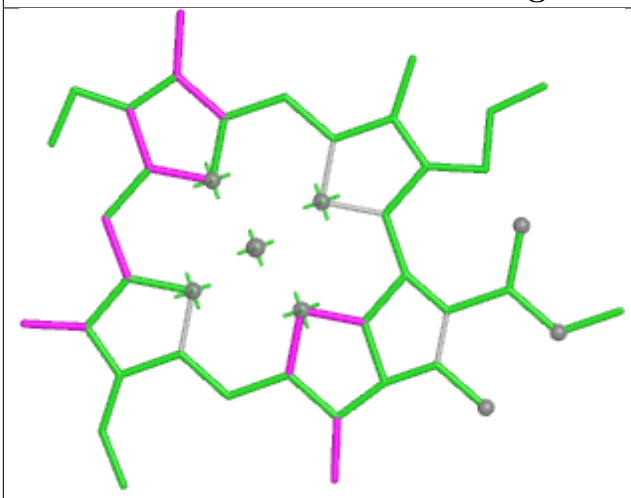


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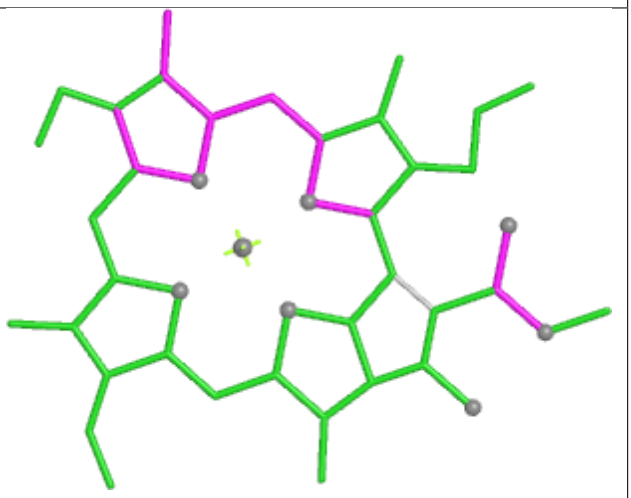


Rings

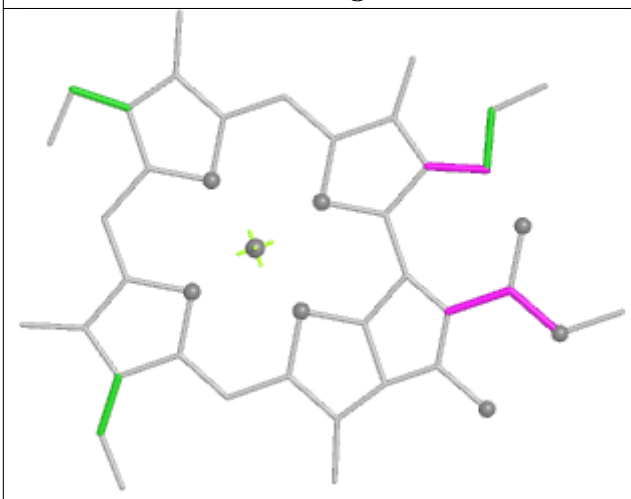
Ligand CLA 3 612



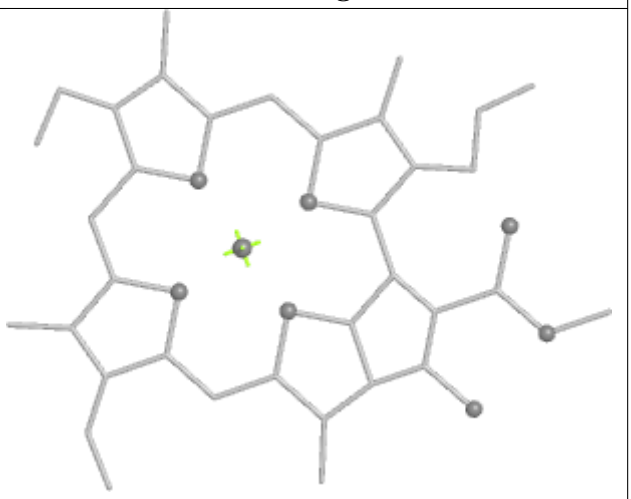
Bond lengths



Bond angles

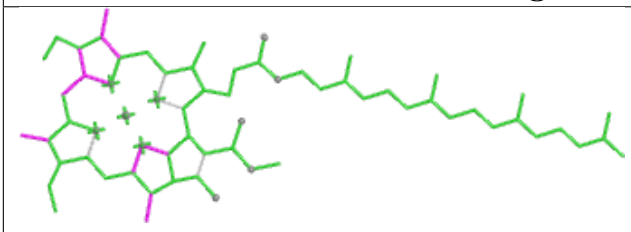


Torsions

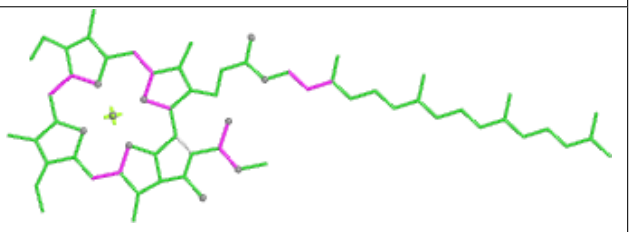


Rings

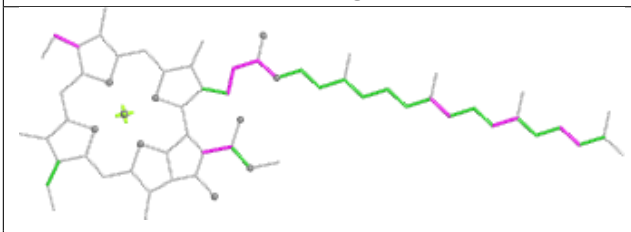
Ligand CLA 9 613



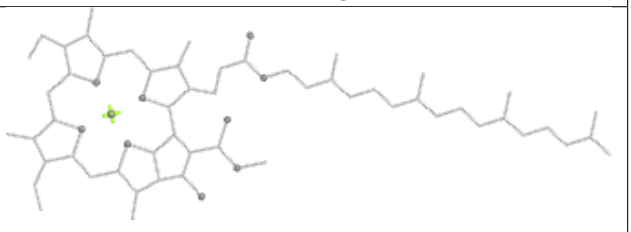
Bond lengths



Bond angles

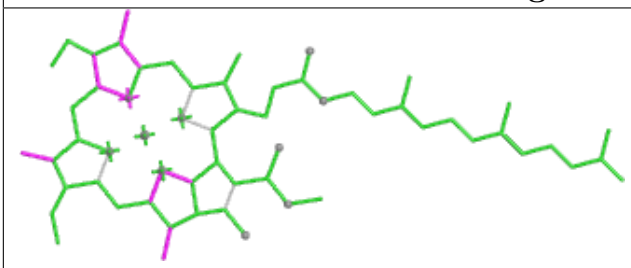


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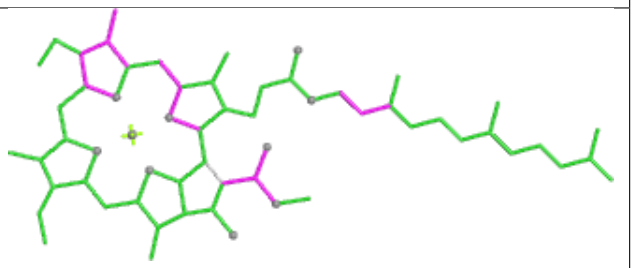


Rings

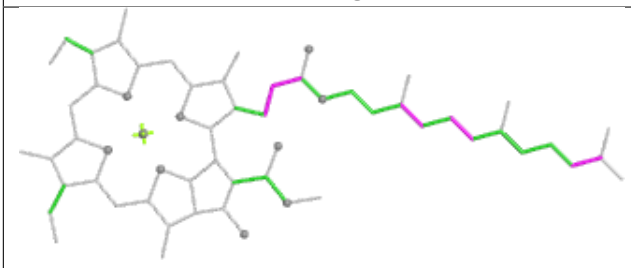
Ligand CLA 9 602



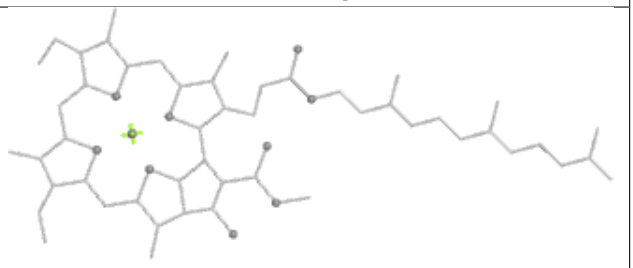
Bond lengths



Bond angles

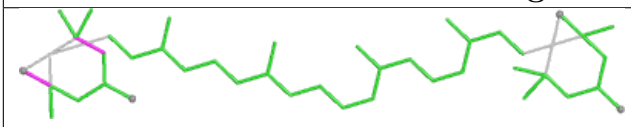


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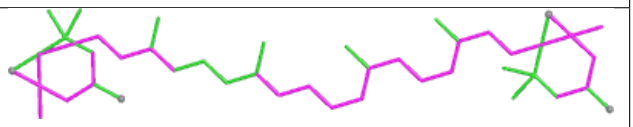


Rings

Ligand XAT 9 620



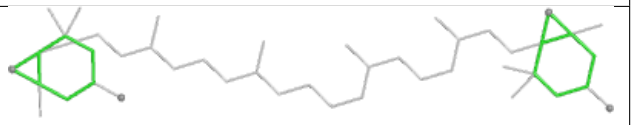
Bond lengths



Bond angles

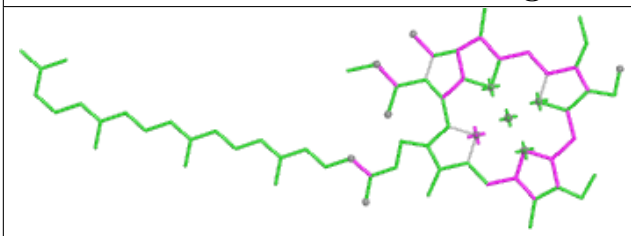


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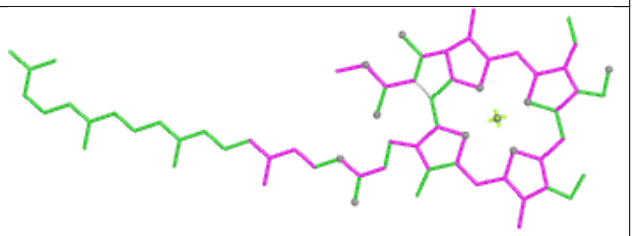


Rings

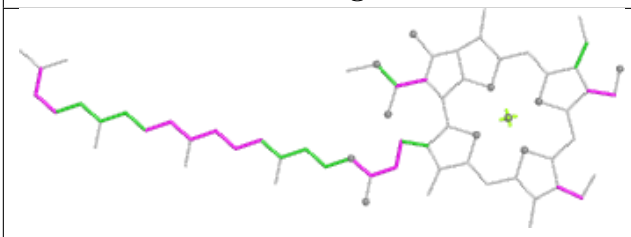
Ligand CHL X 601



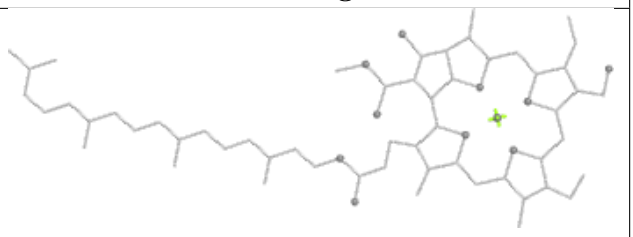
Bond lengths



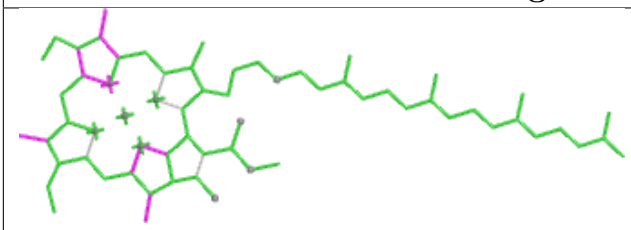
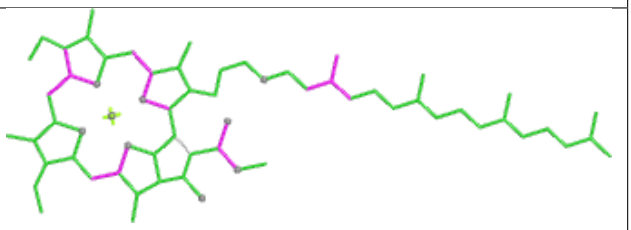
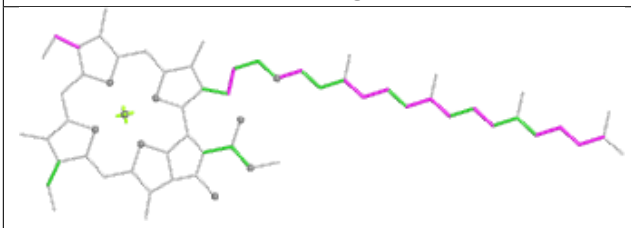
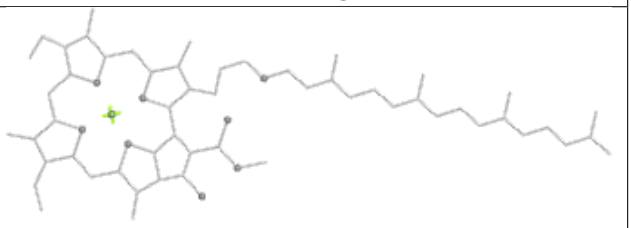
Bond angles

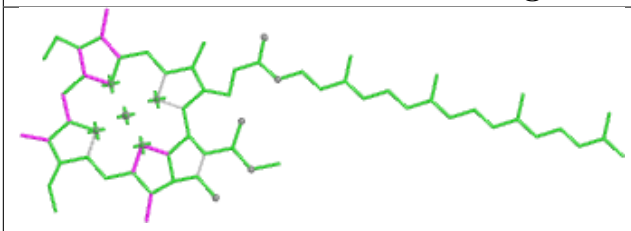
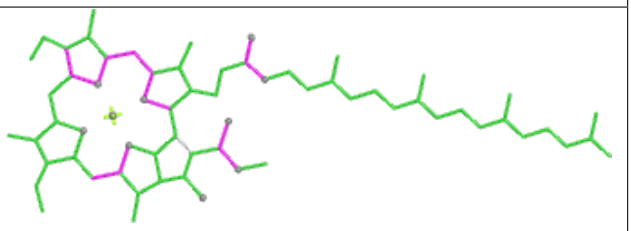
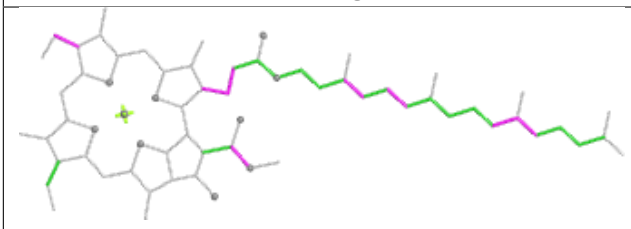
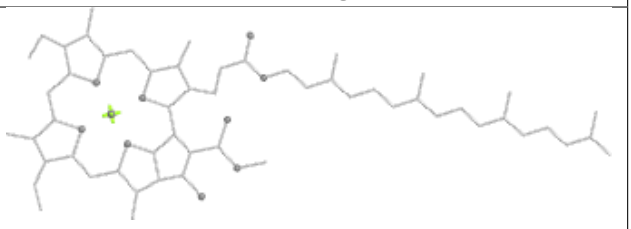


Torsions

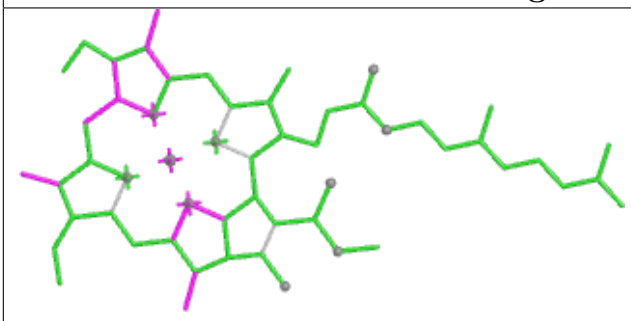


Rings

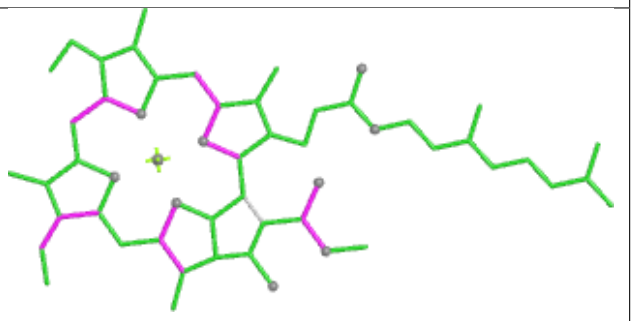
Ligand CLA 5 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

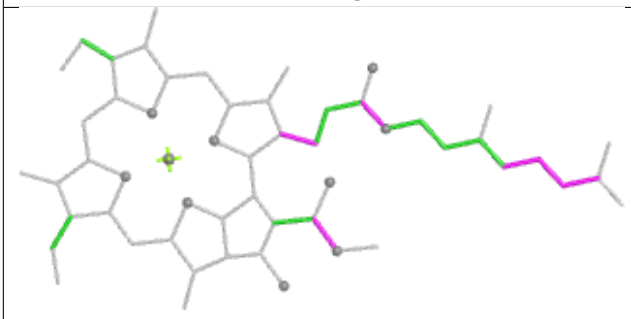
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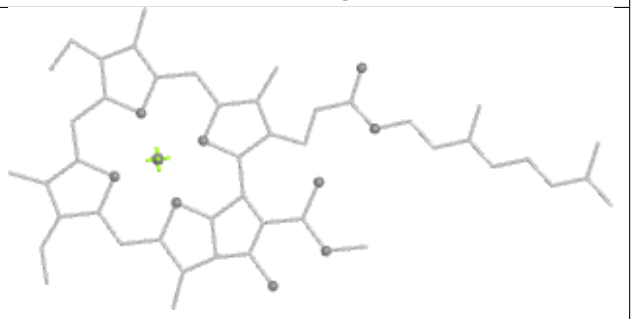
Bond lengths



Bond angles

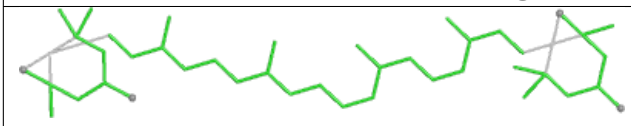


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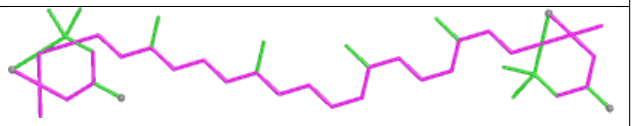


Rings

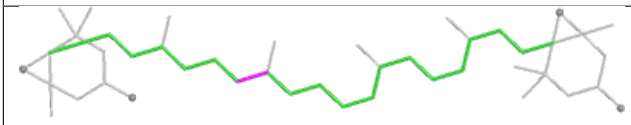
Ligand XAT V 1622



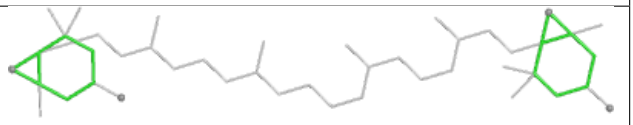
Bond lengths



Bond angles

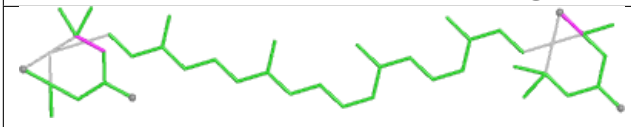


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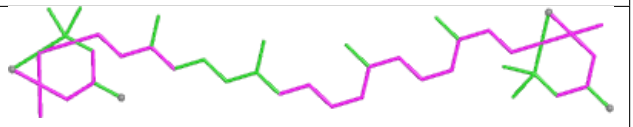


Rings

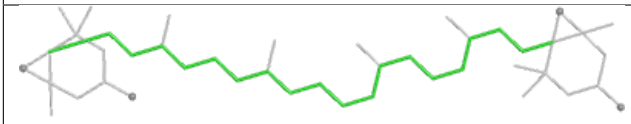
Ligand XAT 3 619



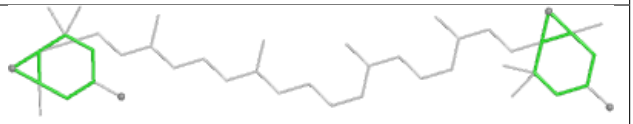
Bond lengths



Bond angles

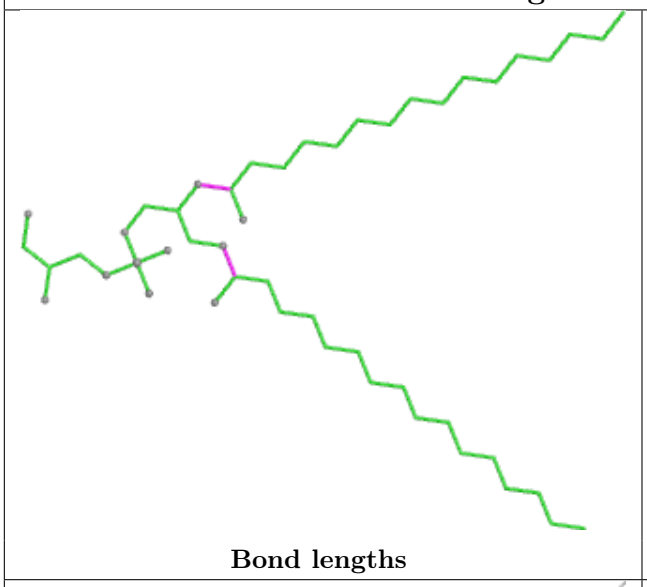


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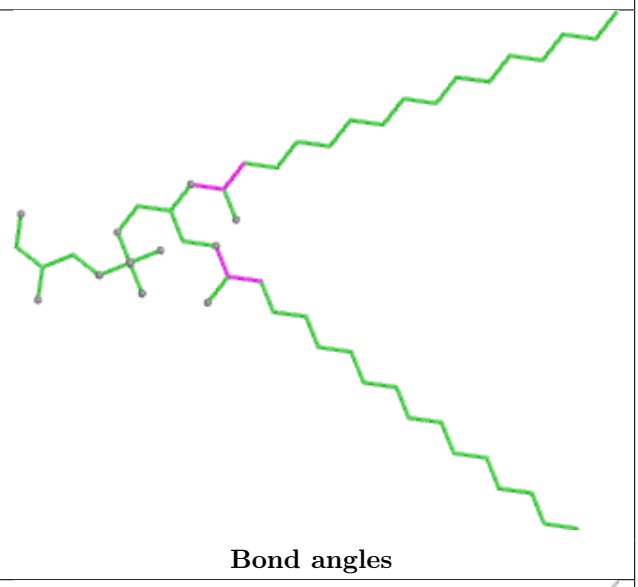


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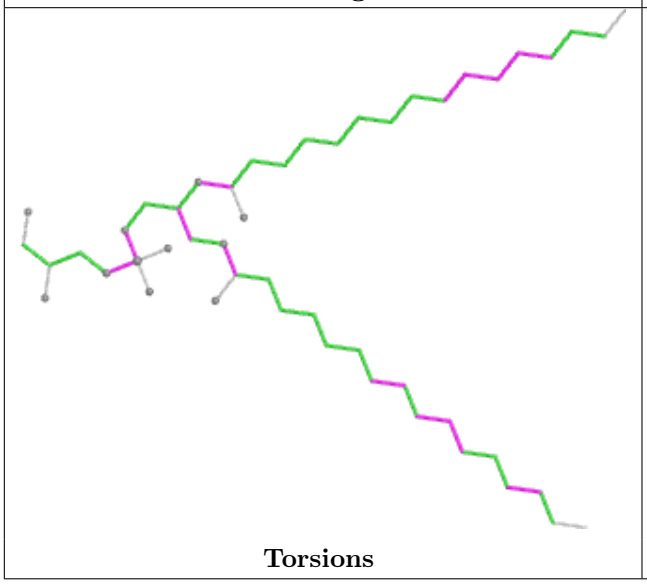
Ligand LHG 9 624



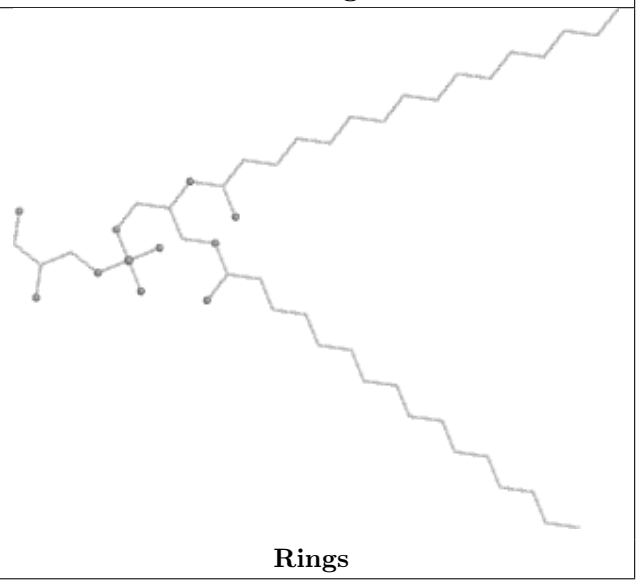
Bond lengths



Bond angles

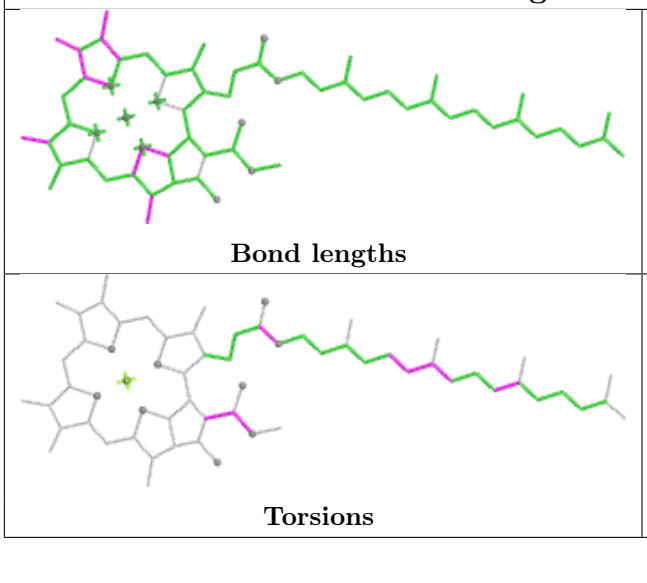


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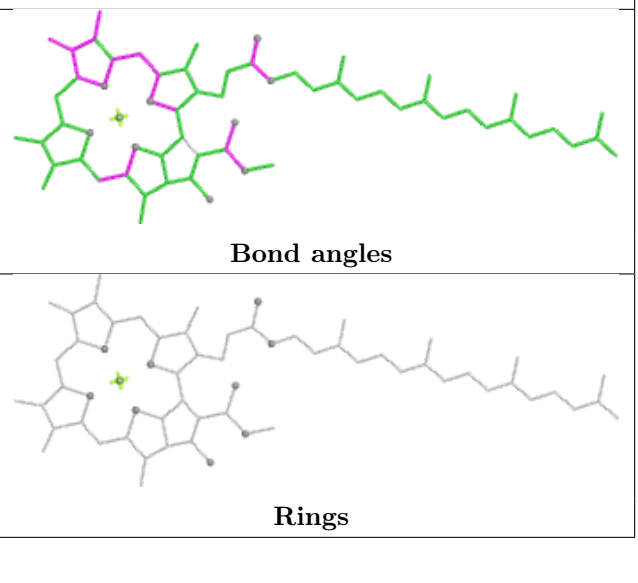


Rings

Ligand CLA 5 604



Bond lengths

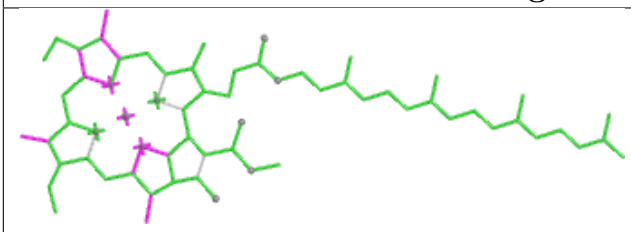


Bond angles

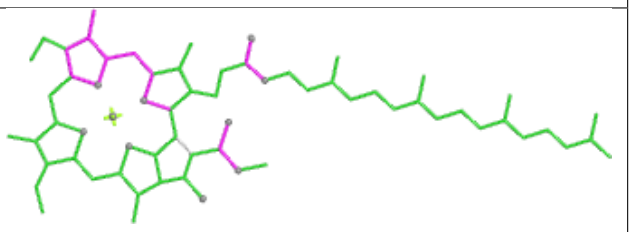
Torsions

Rings

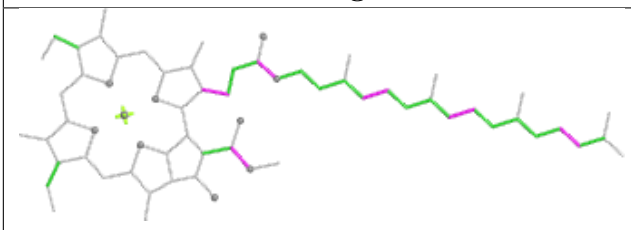
Ligand CLA 2 601



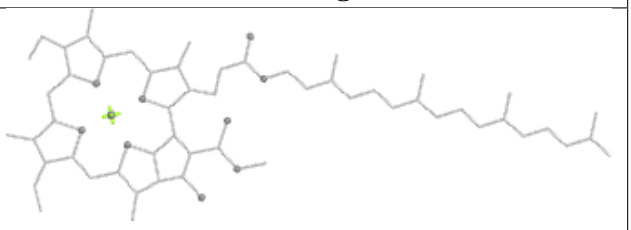
Bond lengths



Bond angles



Torsions



Rings

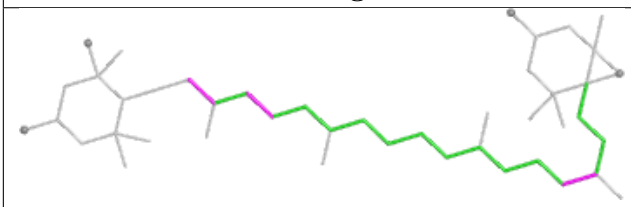
Ligand NEX X 1623



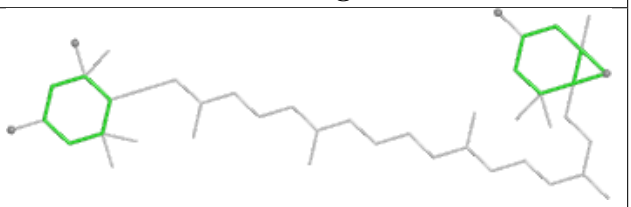
Bond lengths



Bond angles

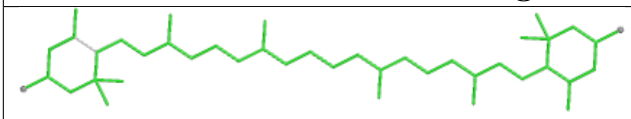


Torsions

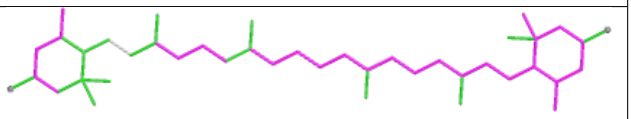


Rings

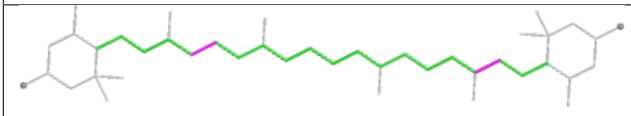
Ligand LUT V 1621



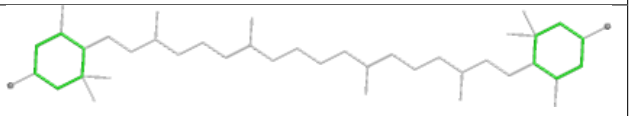
Bond lengths



Bond angles

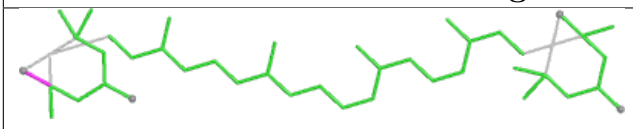


Torsions

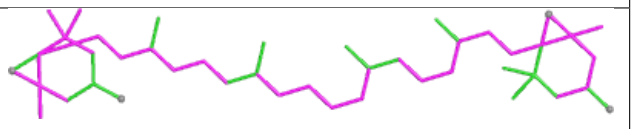


Rings

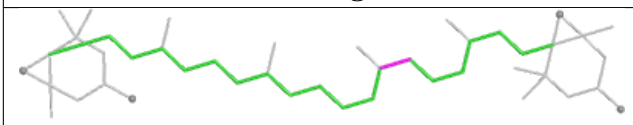
Ligand XAT W 1622



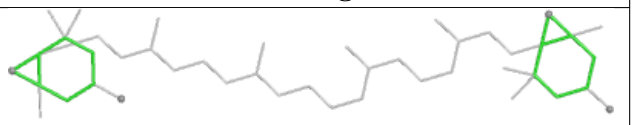
Bond lengths



Bond angles

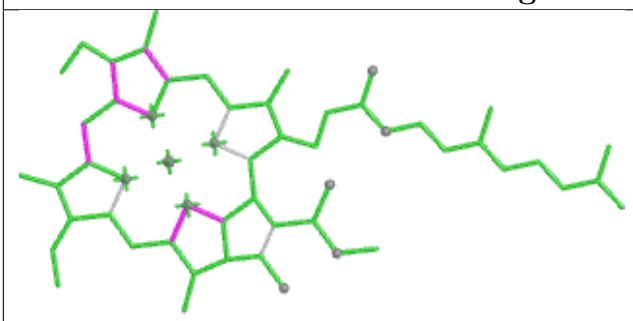


Torsions

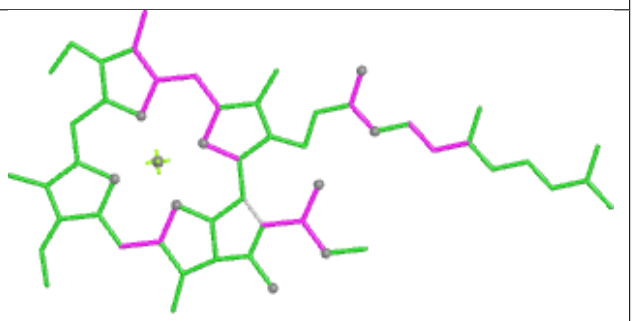


Rings

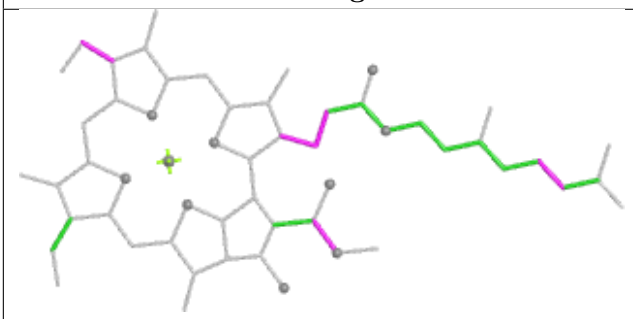
Ligand CLA W 610



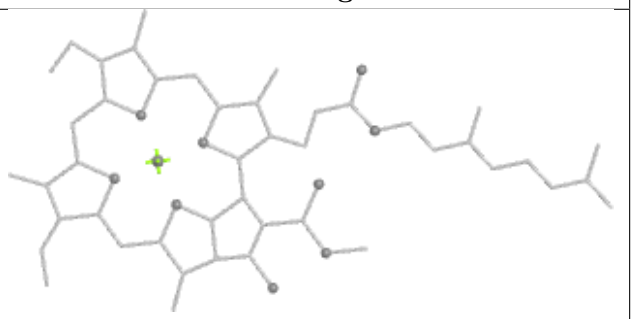
Bond lengths



Bond angles

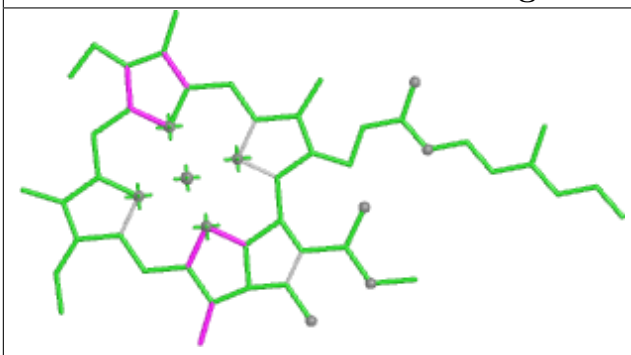


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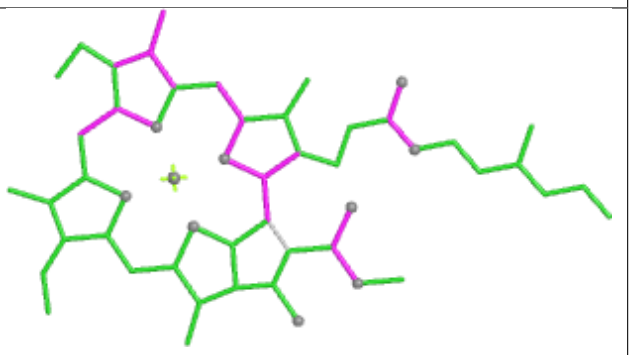


Rings

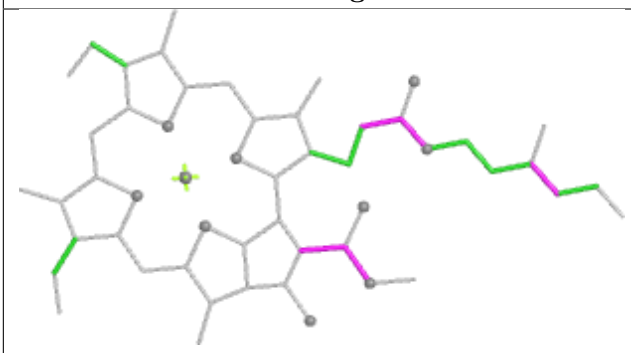
Ligand CLA W 603



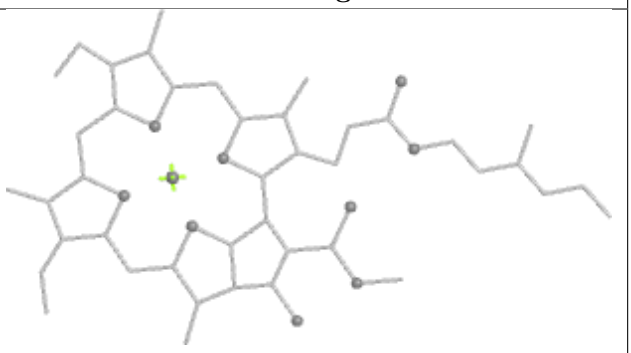
Bond lengths



Bond angles

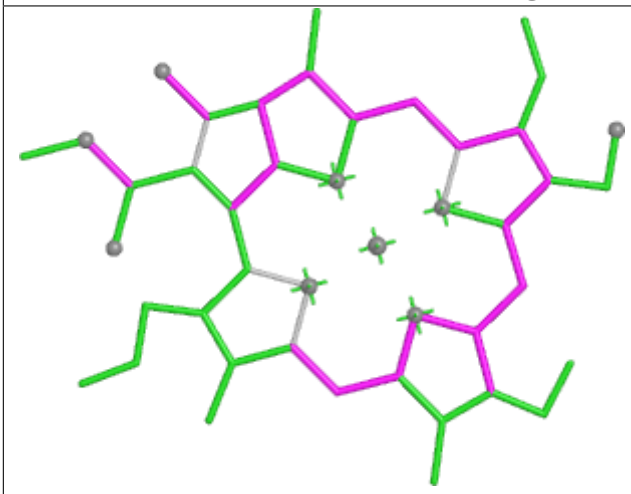


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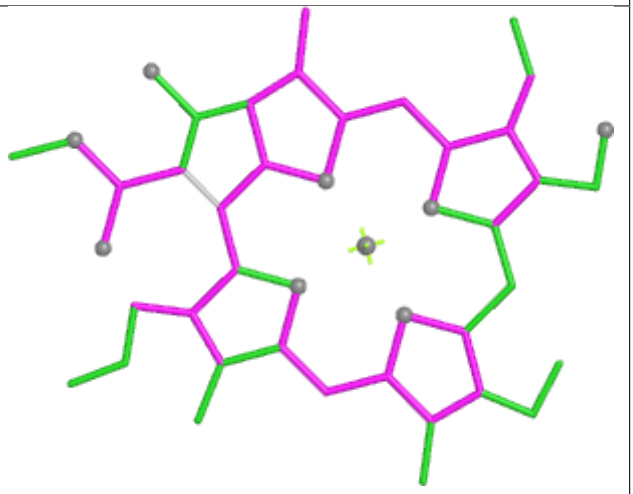


Rings

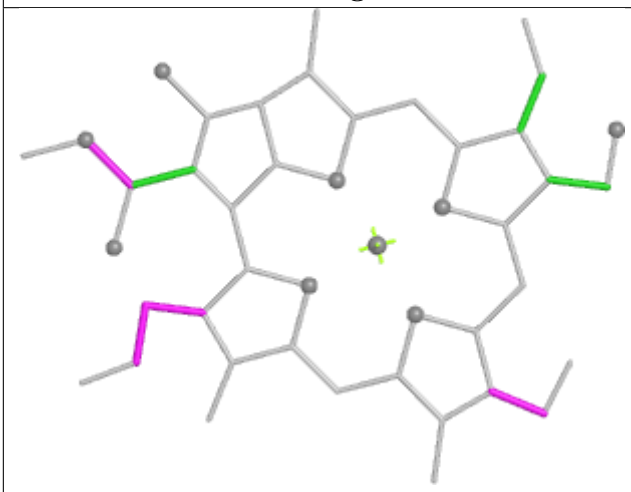
Ligand CHL V 606



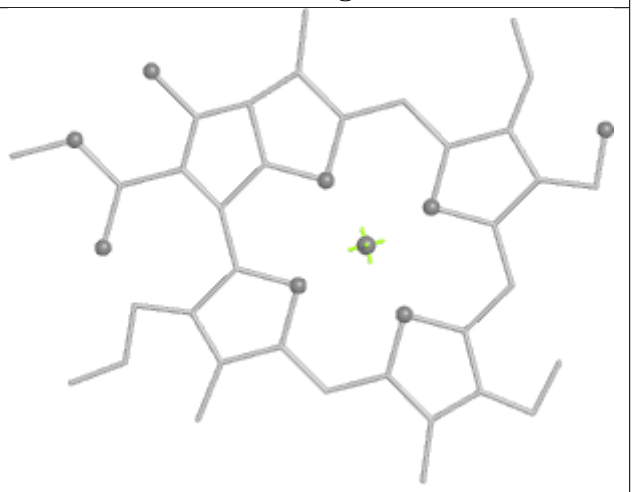
Bond lengths



Bond angles

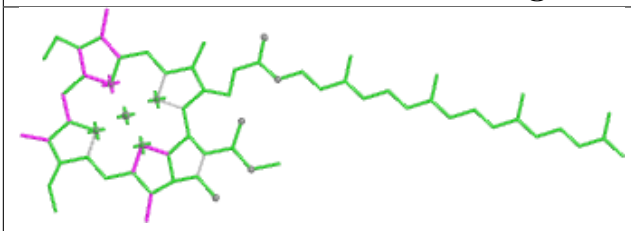


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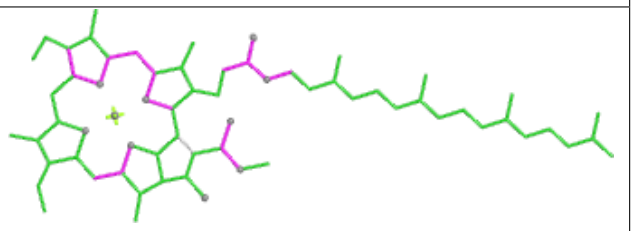


Rings

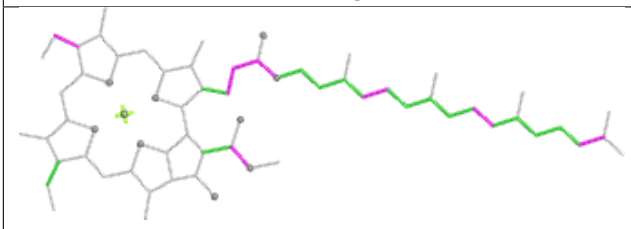
Ligand CLA 4 613



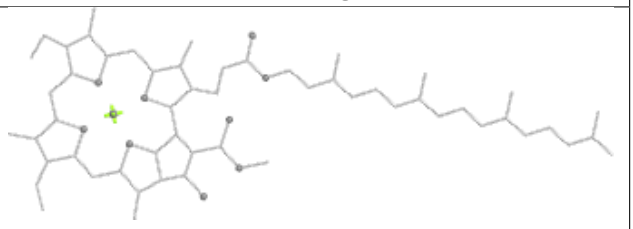
Bond lengths



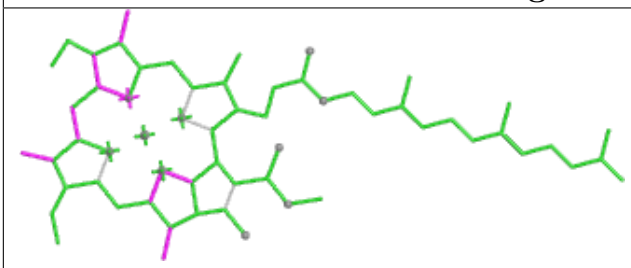
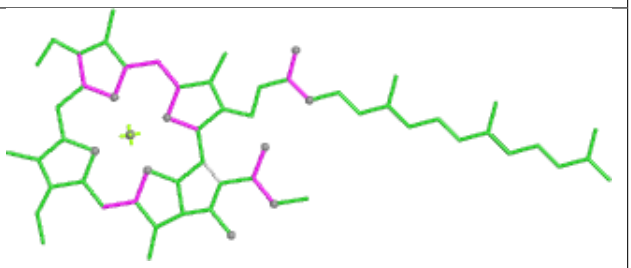
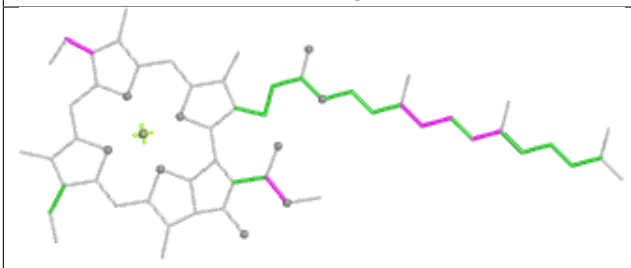
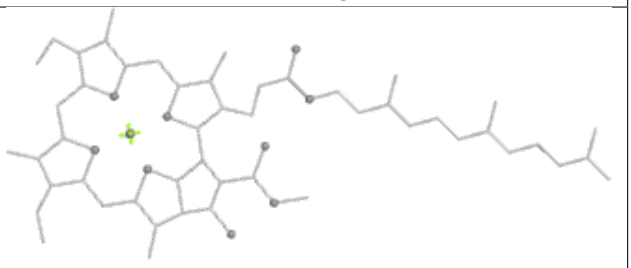
Bond angles

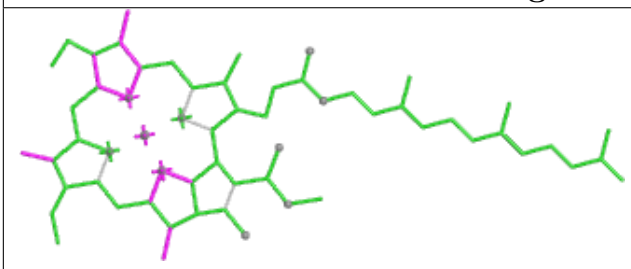
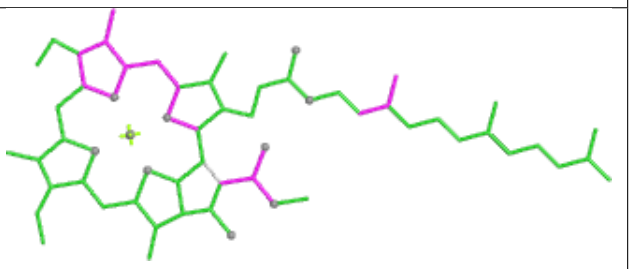
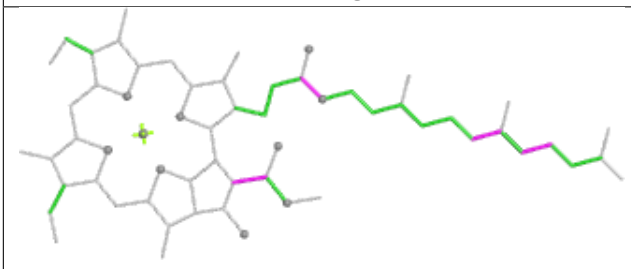
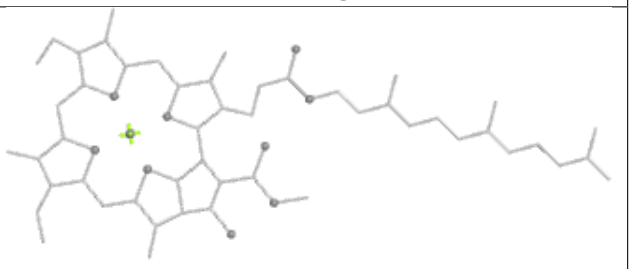


Torsions

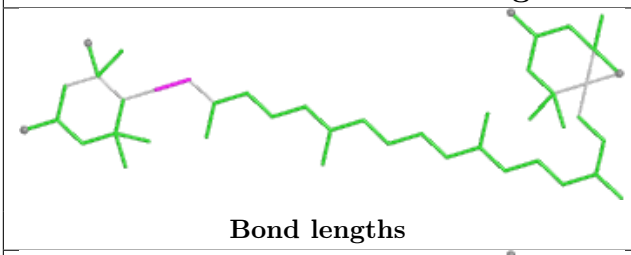


Rings

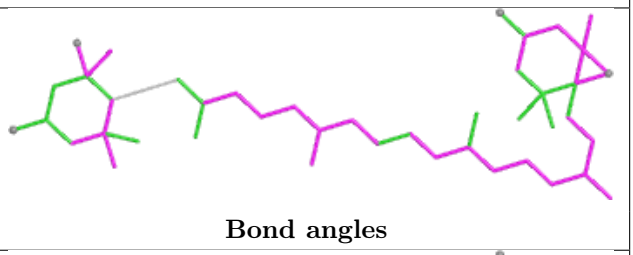
Ligand CLA 4 602	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 7 601	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

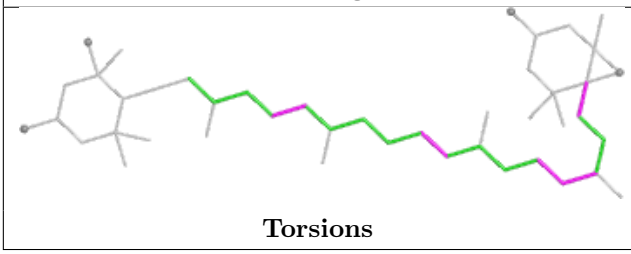
Ligand NEX U 1623



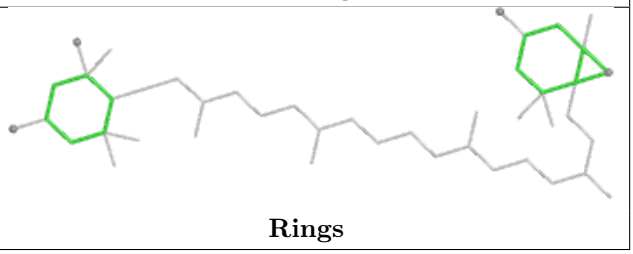
Bond lengths



Bond angles

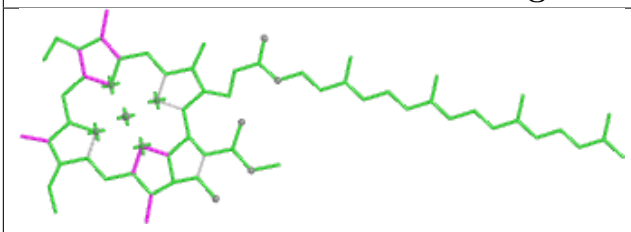


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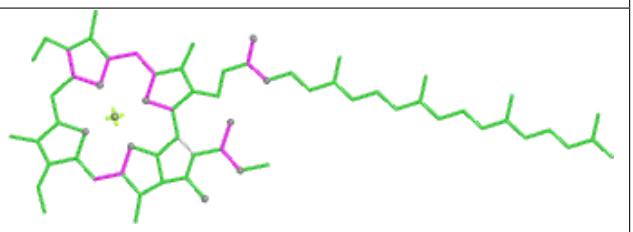


Rings

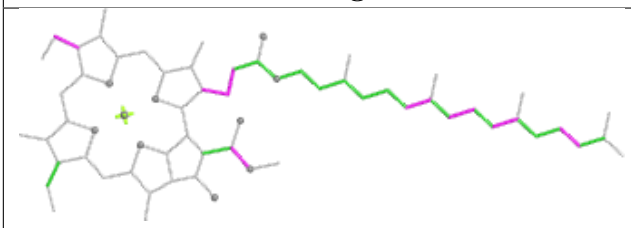
Ligand CLA 6 610



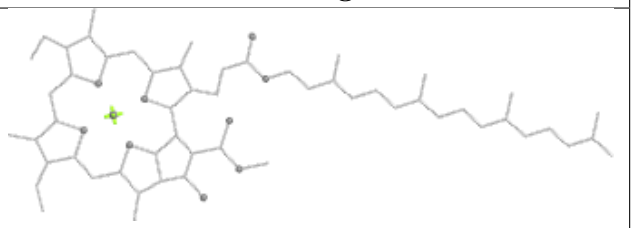
Bond lengths



Bond angles

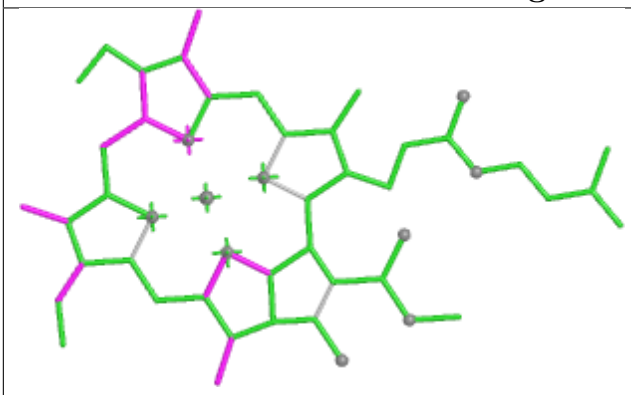


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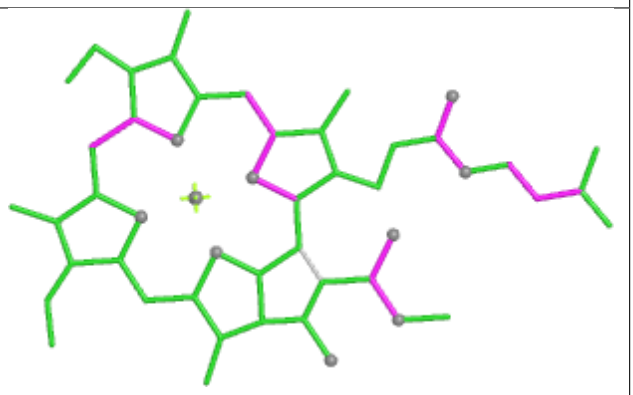


Rings

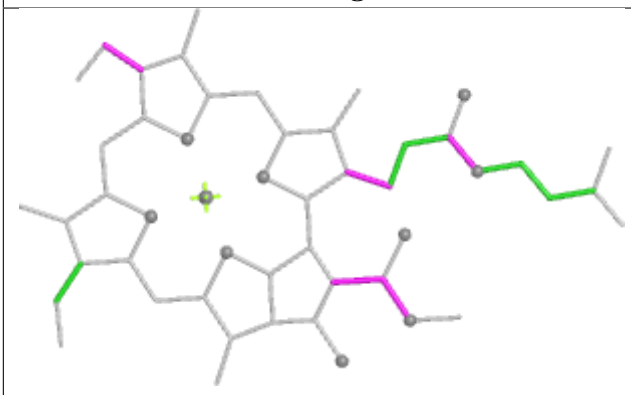
Ligand CLA 5 617



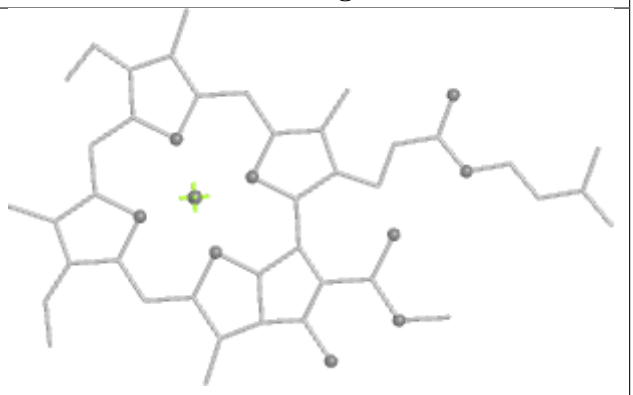
Bond lengths



Bond angles

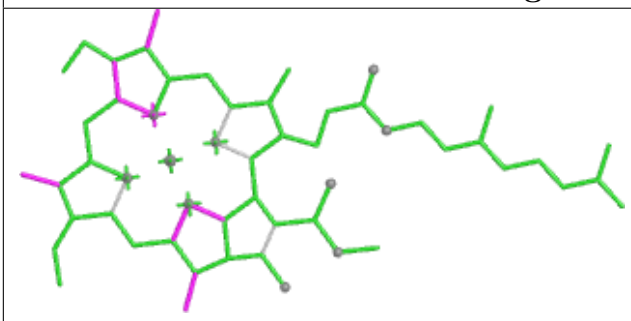


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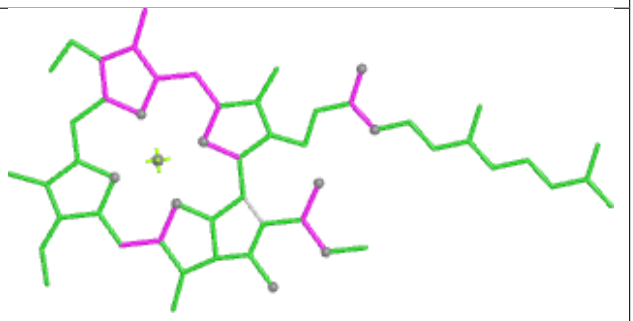


Rings

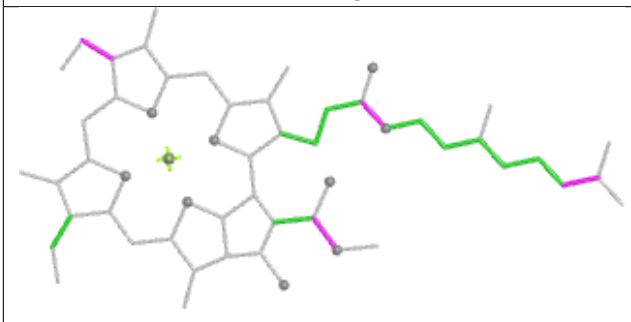
Ligand CLA B 819



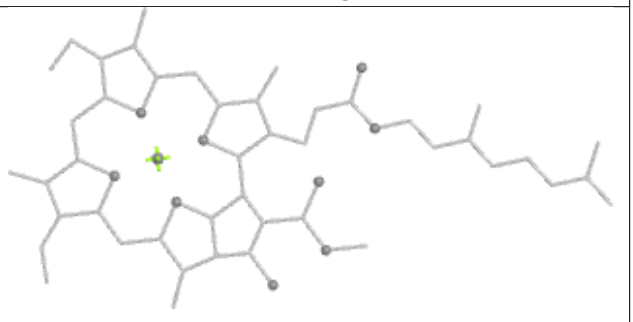
Bond lengths



Bond angles

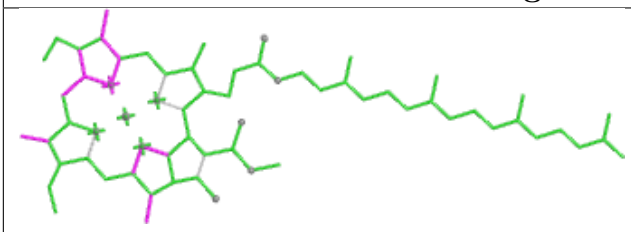


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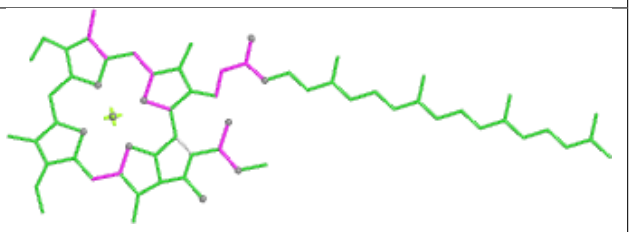


Rings

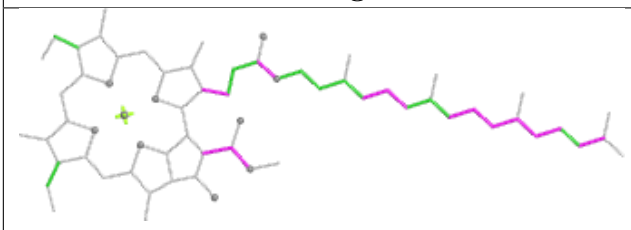
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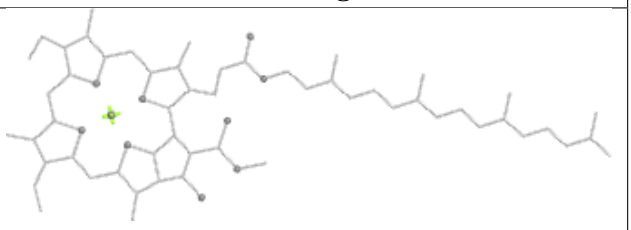
Bond lengths



Bond angles

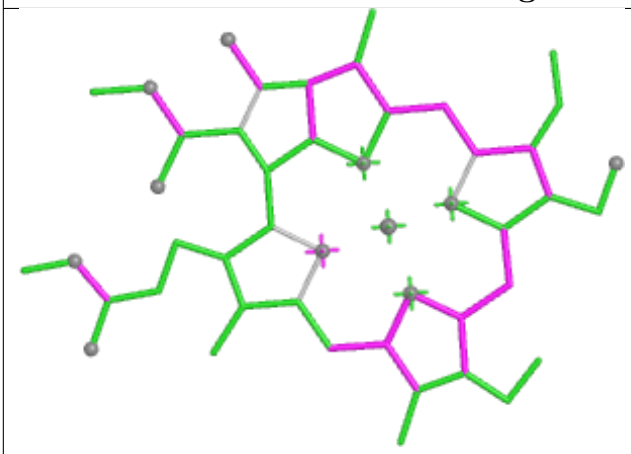


Torsions

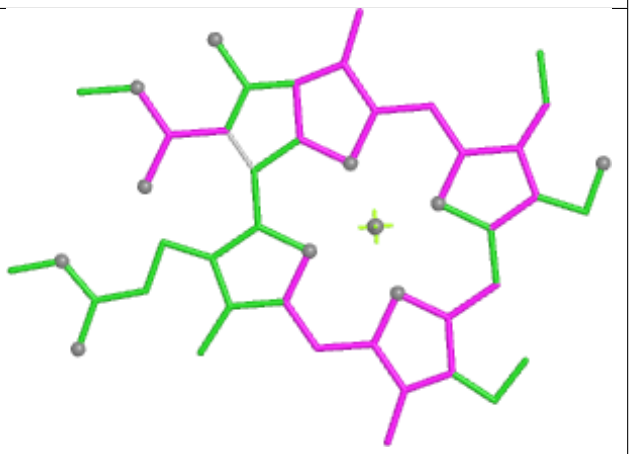


Rings

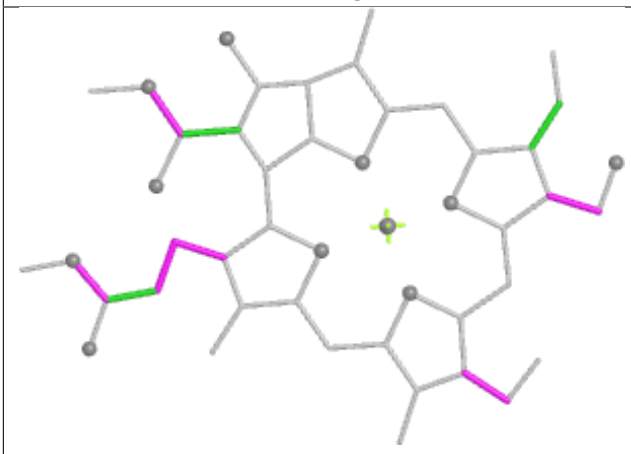
Ligand CHL W 608



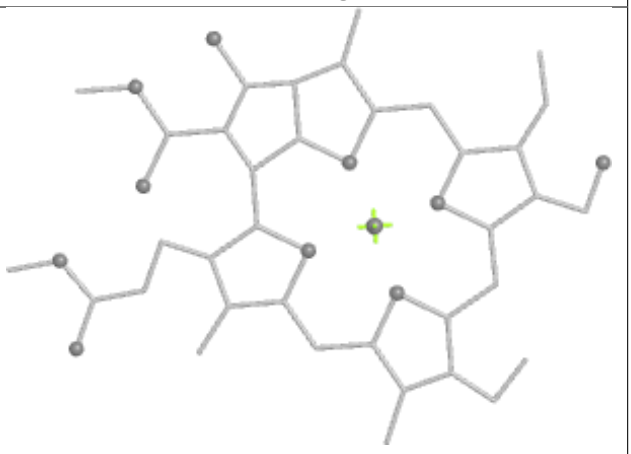
Bond lengths



Bond angles

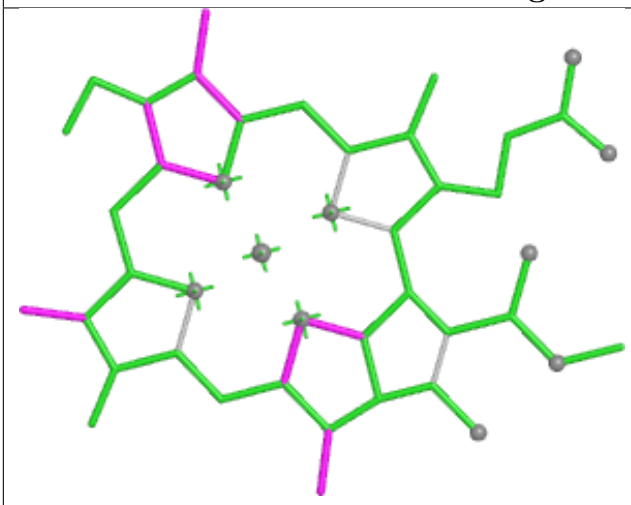


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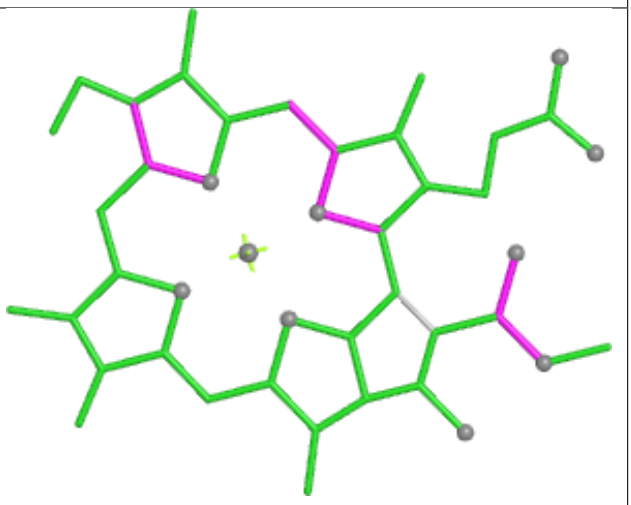


Rings

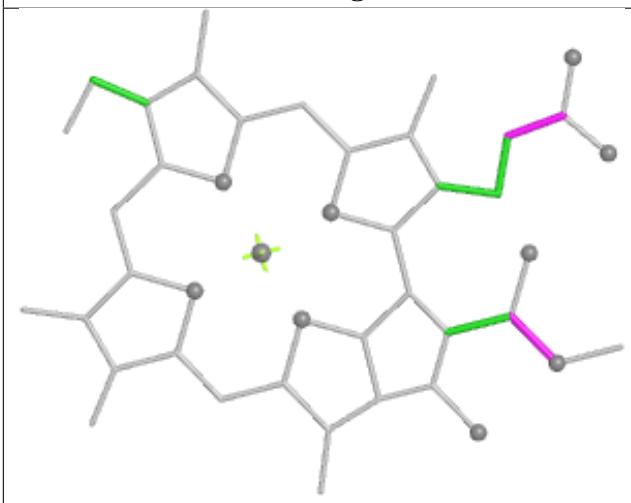
Ligand CLA 7 612



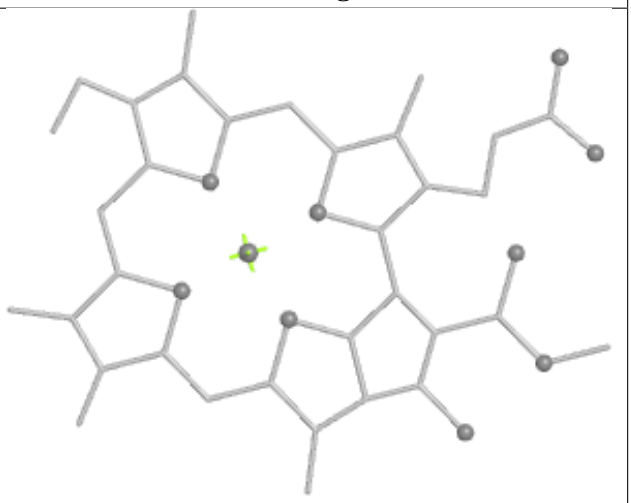
Bond lengths



Bond angles

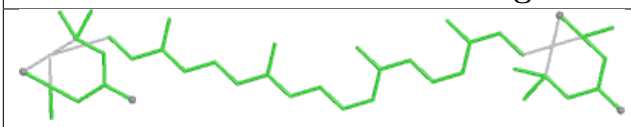


Torsions

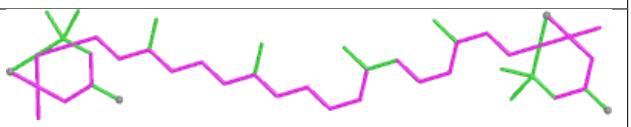


Rings

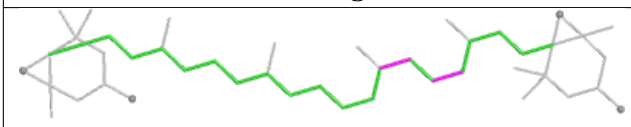
Ligand XAT X 1622



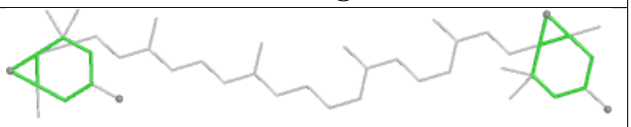
Bond lengths



Bond angles

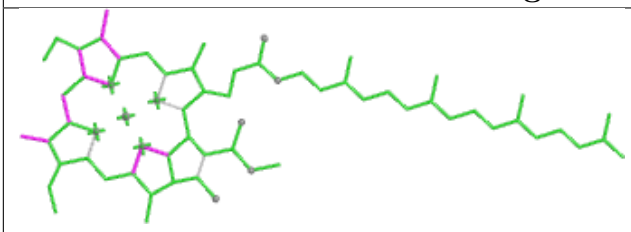


Torsions

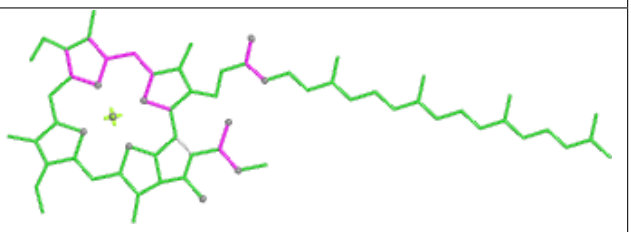


Rings

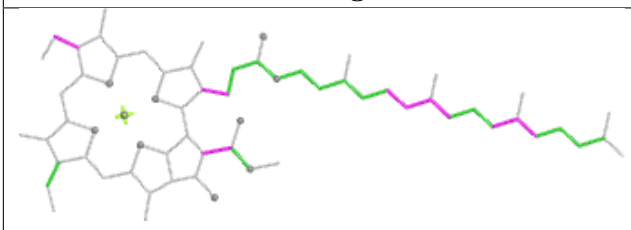
Ligand CLA X 610



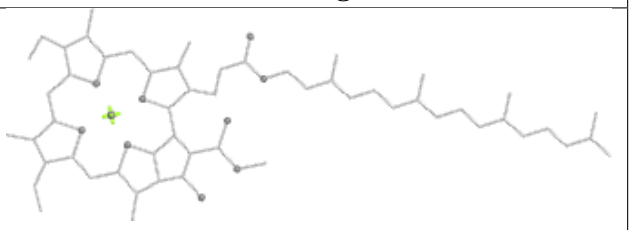
Bond lengths



Bond angles



Torsions

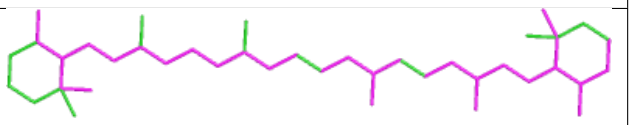


Rings

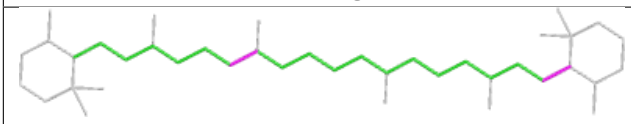
Ligand BCR 1 619



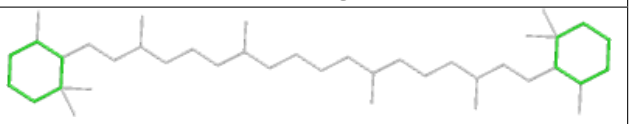
Bond lengths



Bond angles

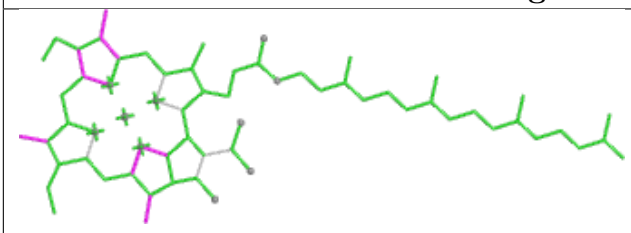


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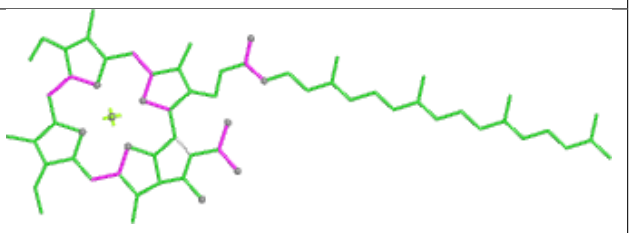


Rings

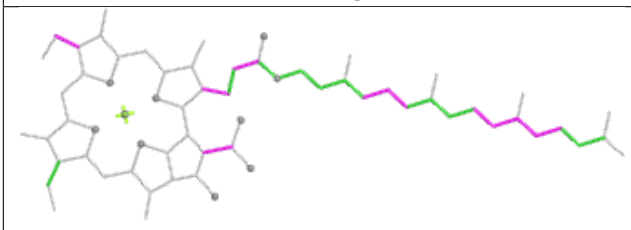
Ligand CLA a 609



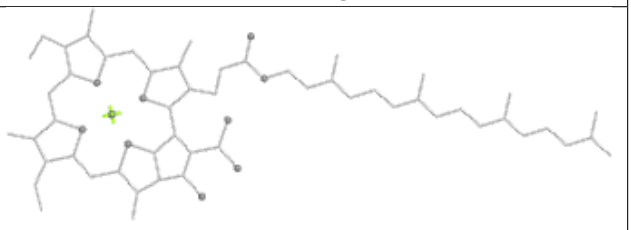
Bond lengths



Bond angles

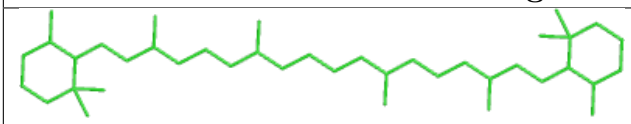


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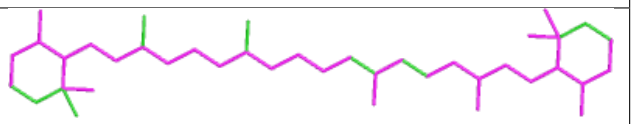


Rings

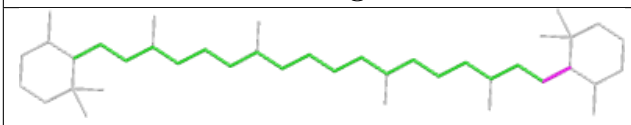
Ligand BCR 8 621



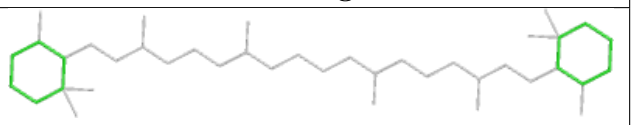
Bond lengths



Bond angles

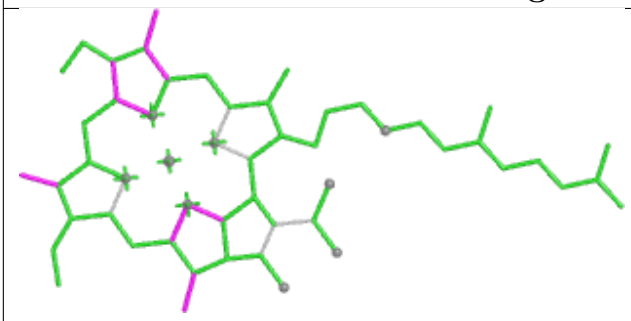


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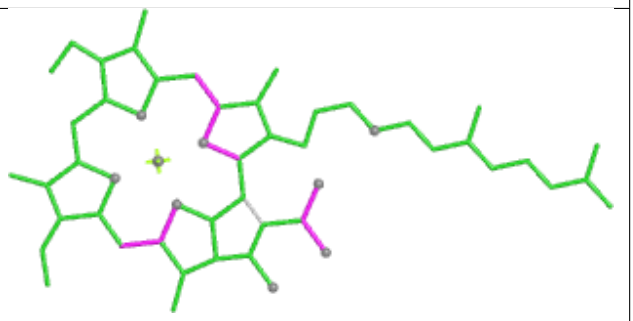


Rings

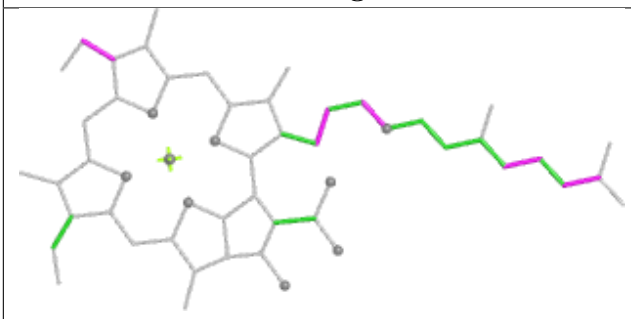
Ligand CLA 1 603



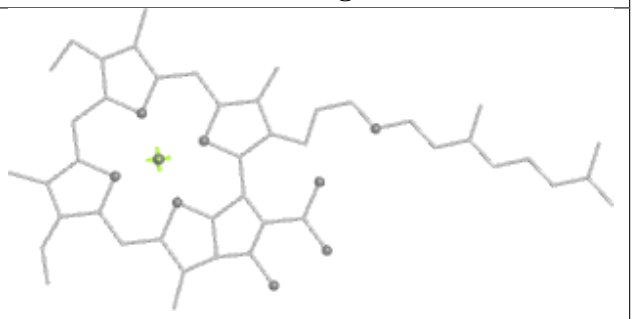
Bond lengths



Bond angles

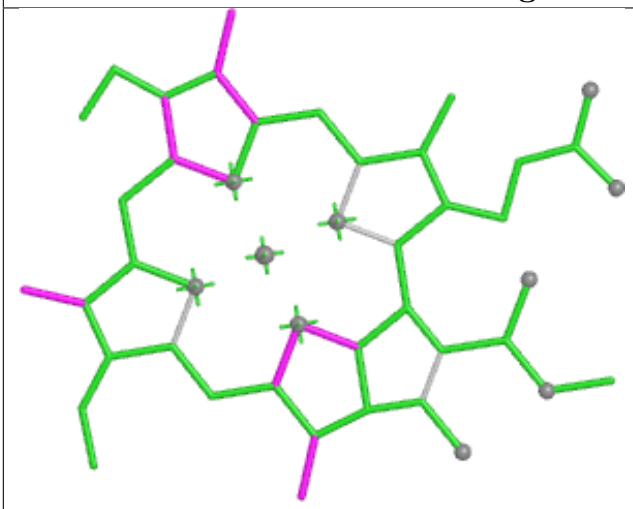


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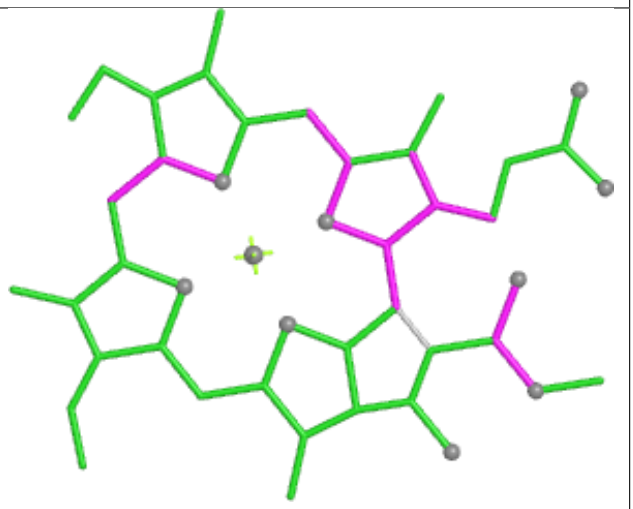


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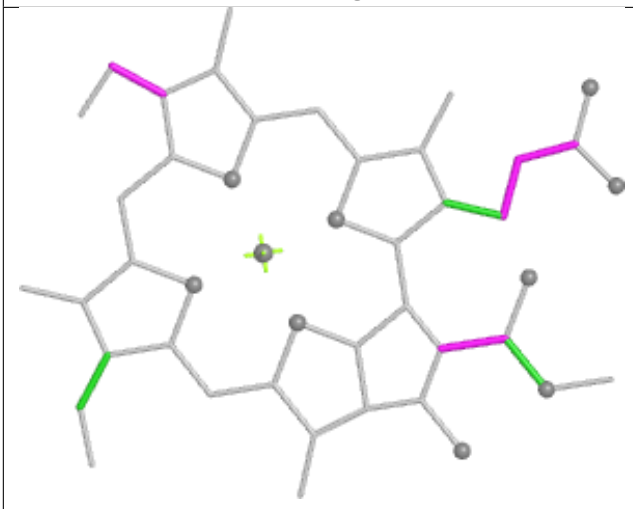
Ligand CLA W 612



Bond lengths



Bond angles

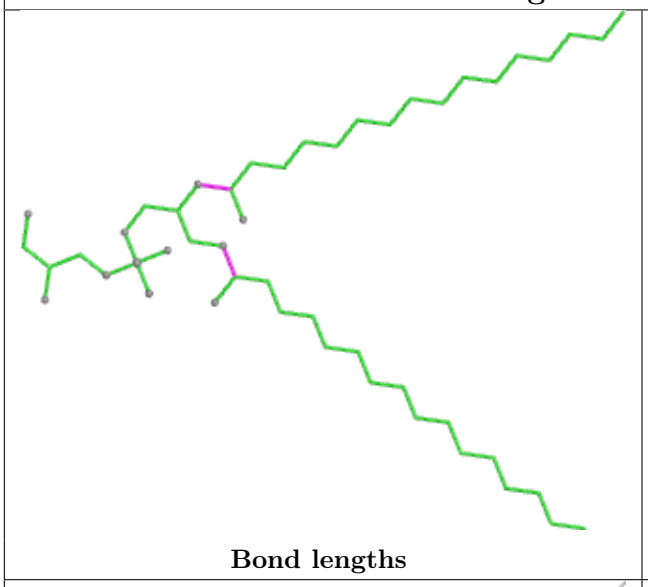


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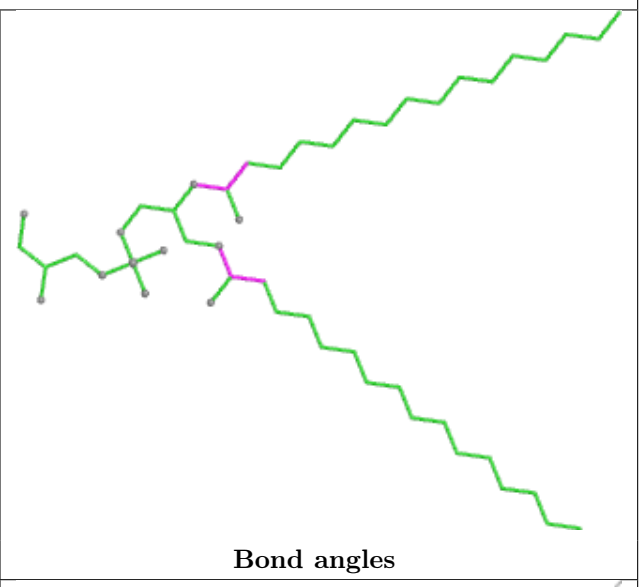


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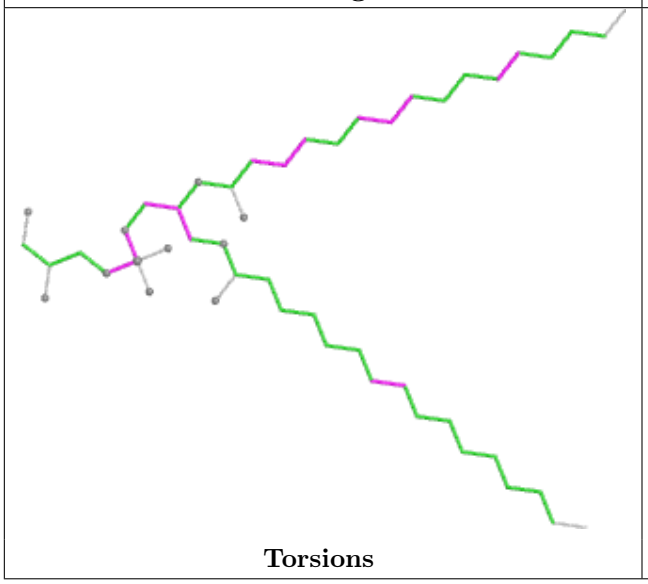
Ligand LHG 5 623



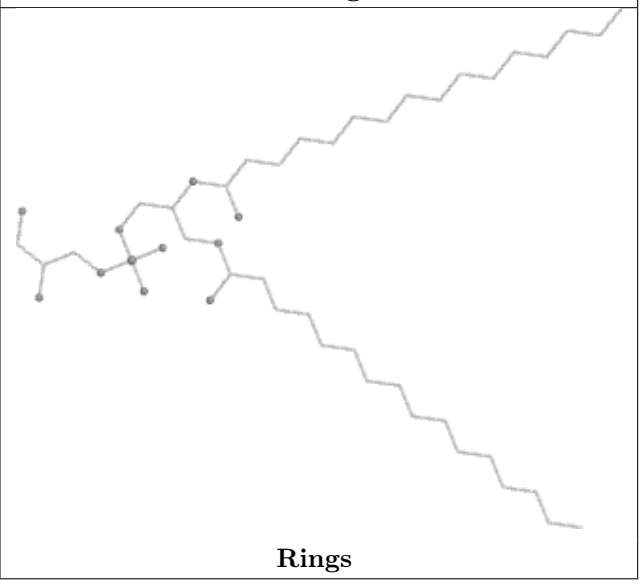
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Bond angles

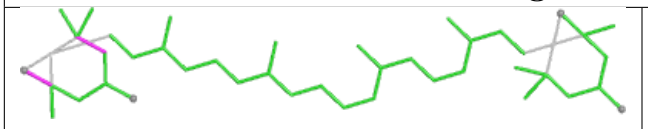


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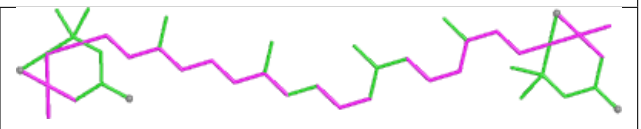


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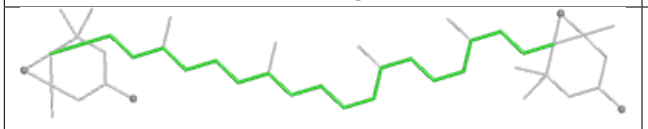
Ligand XAT 7 620



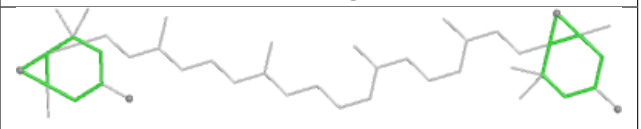
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Bond angles

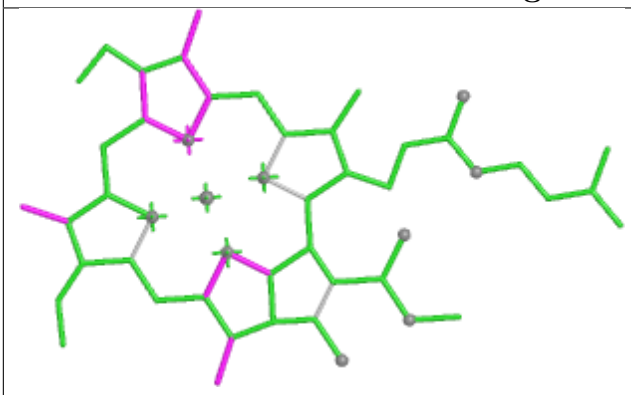


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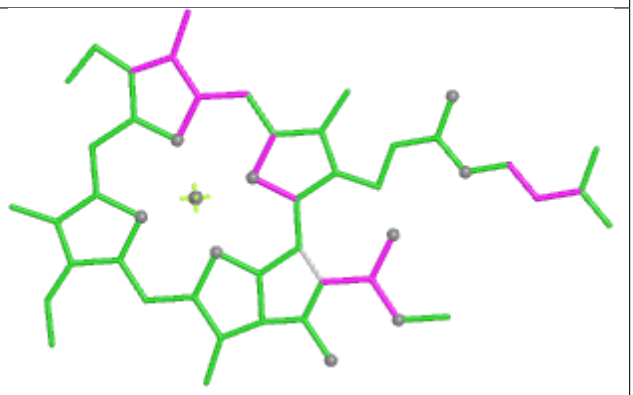


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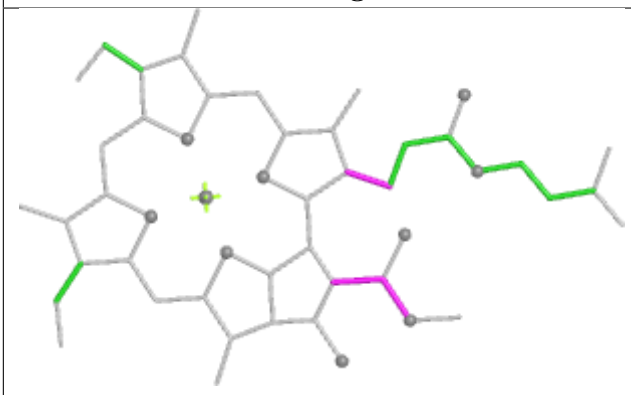
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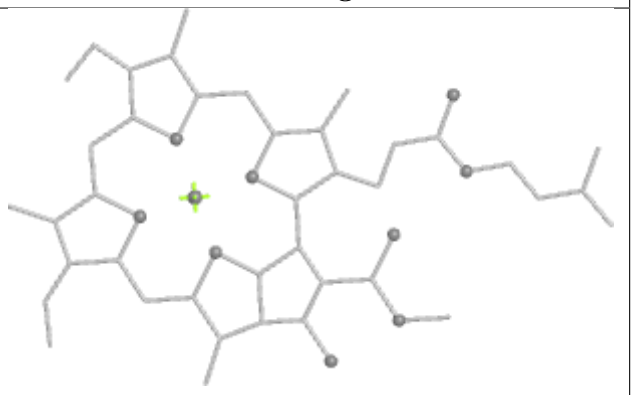
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Bond angles

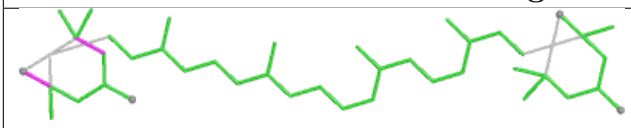


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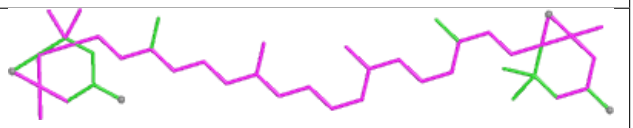


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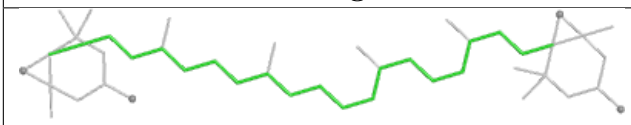
Ligand XAT 2 620



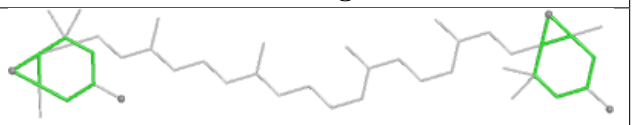
Bond lengths



Bond angles

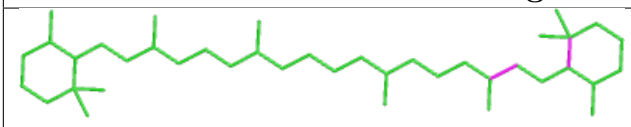


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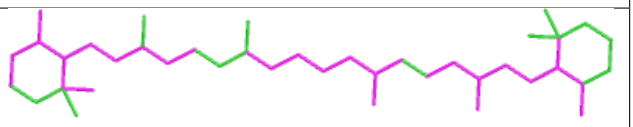


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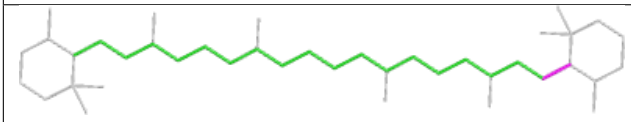
Ligand BCR 5 622



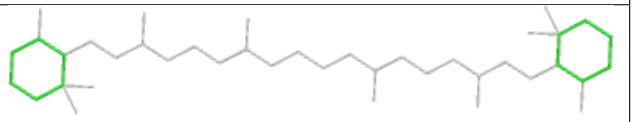
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Bond angles

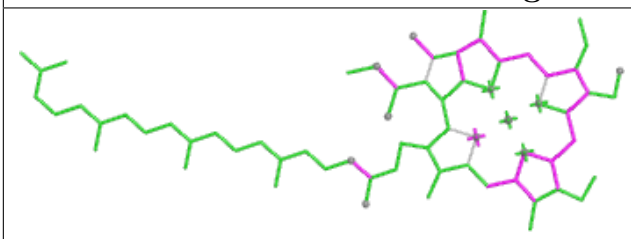


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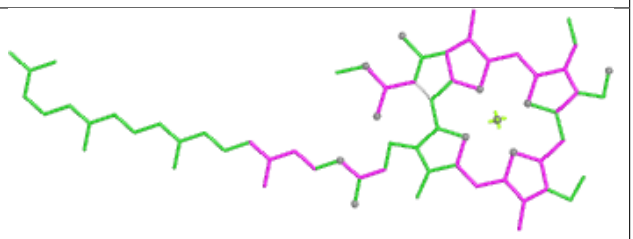


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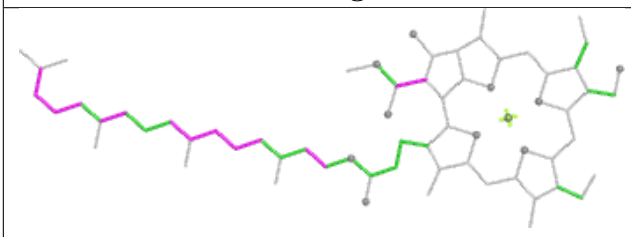
Ligand CHL V 601



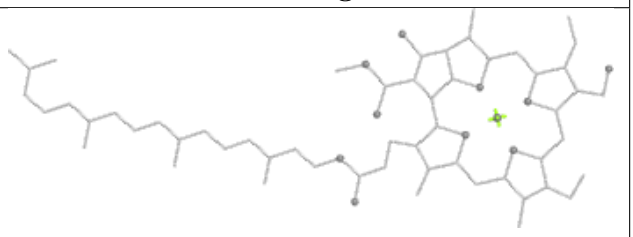
Bond lengths



Bond angles

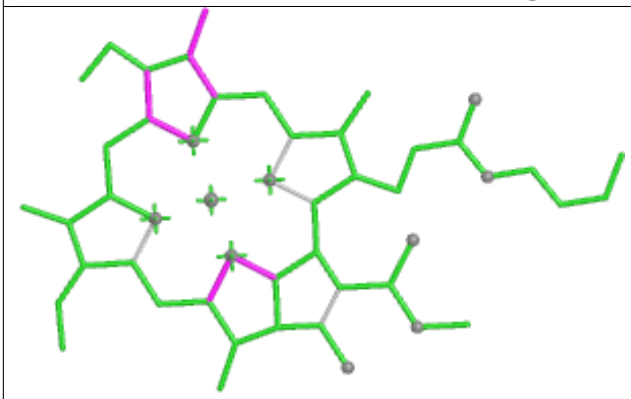


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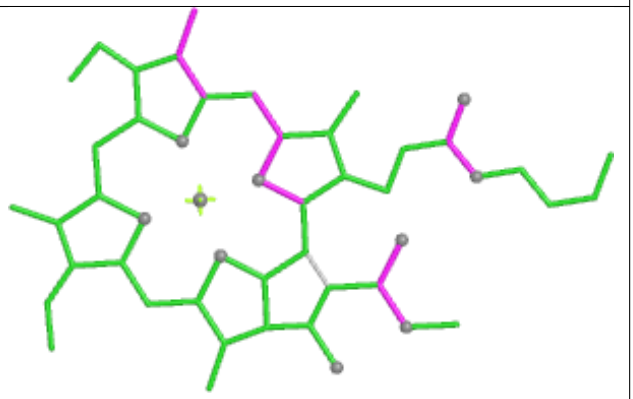


Rings

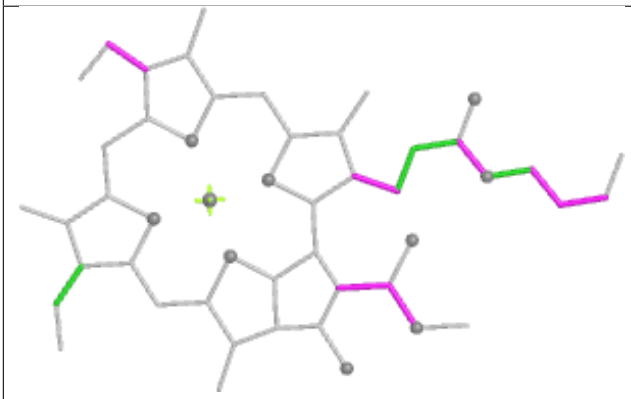
Ligand CLA X 604



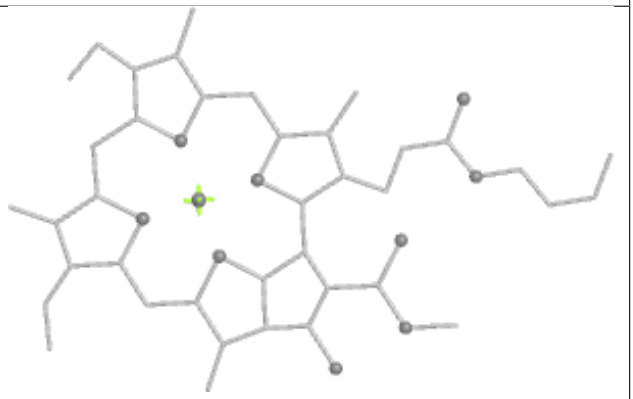
Bond lengths



Bond angles

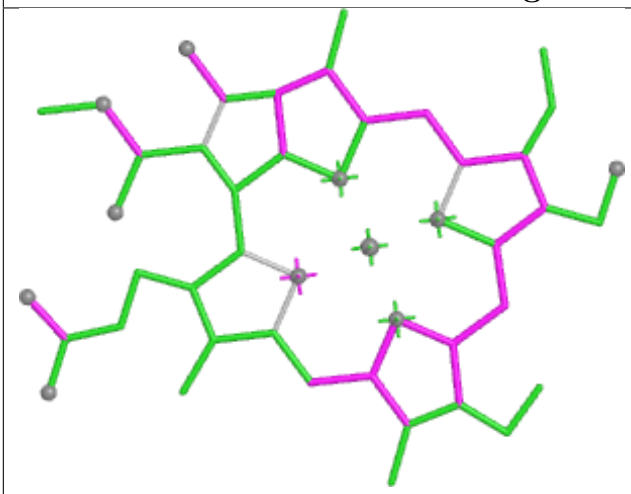


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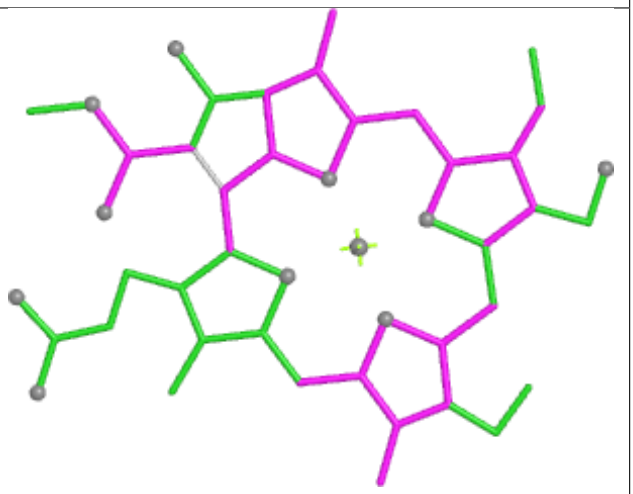


Rings

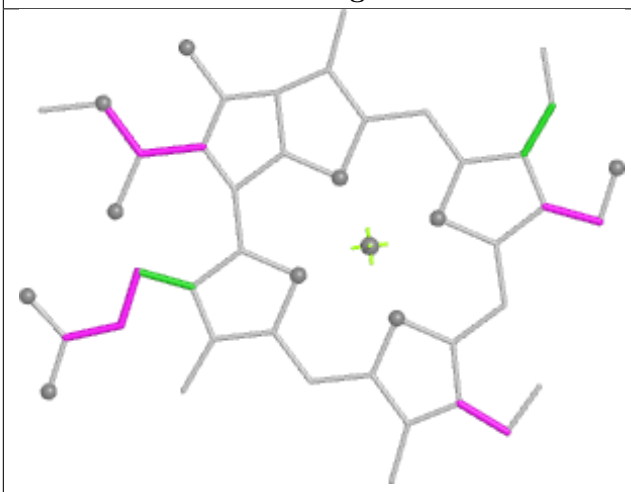
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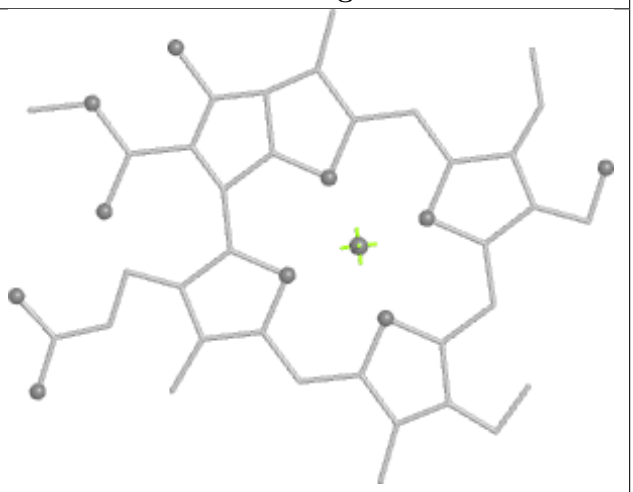
Bond lengths



Bond angles

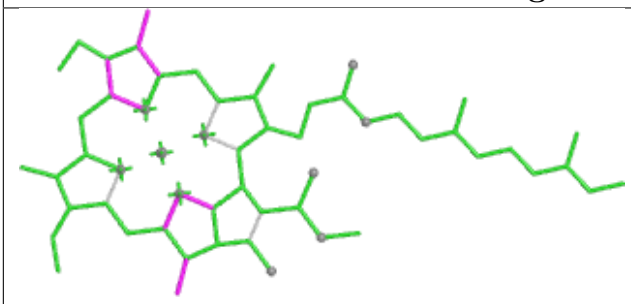


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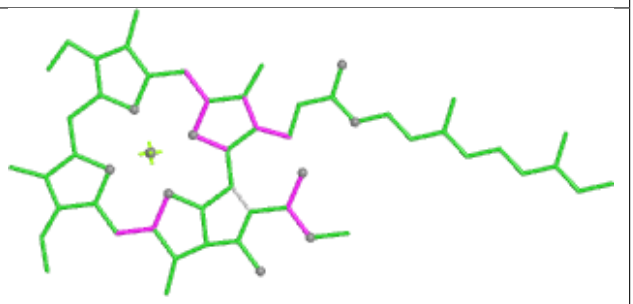


Rings

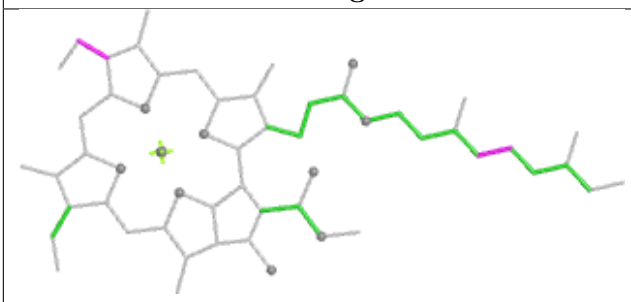
Ligand CLA 5 601



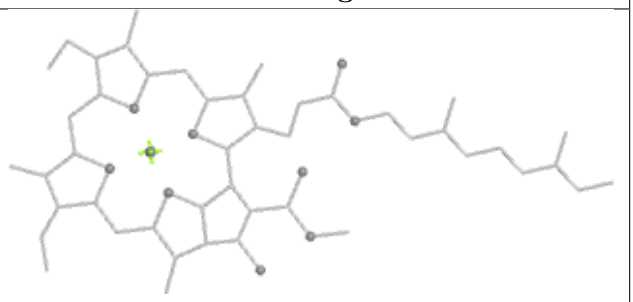
Bond lengths



Bond angles

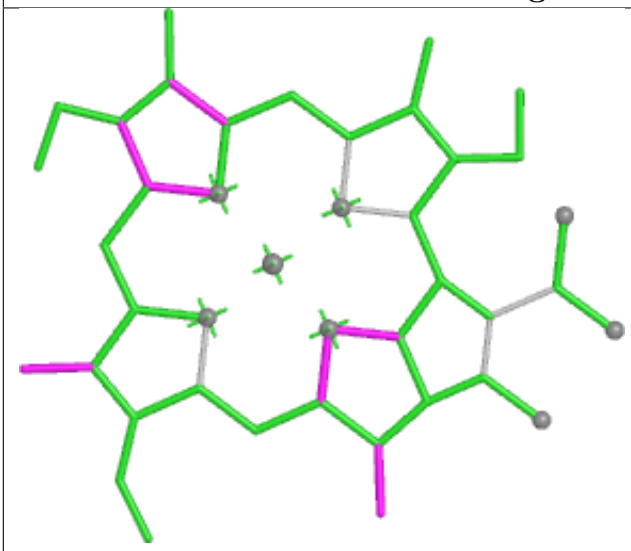


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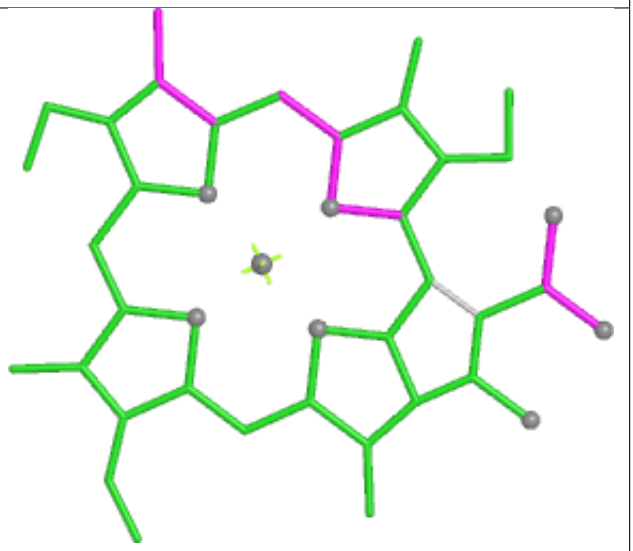


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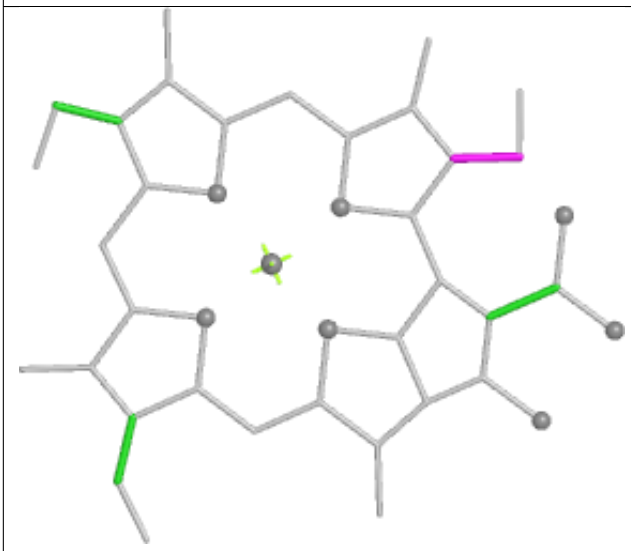
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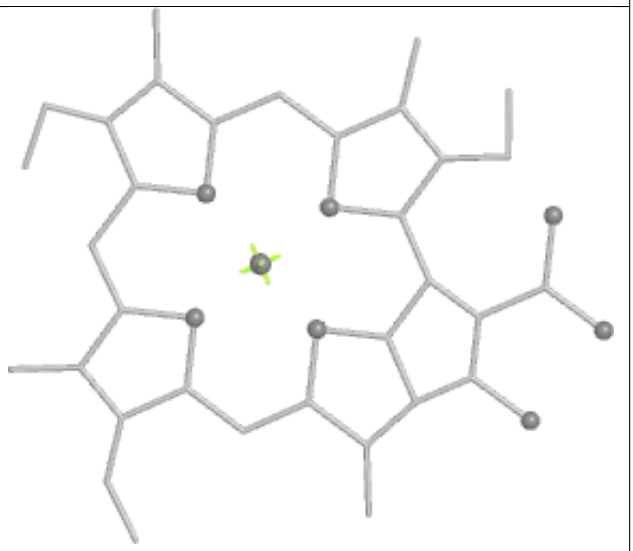
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Bond angles

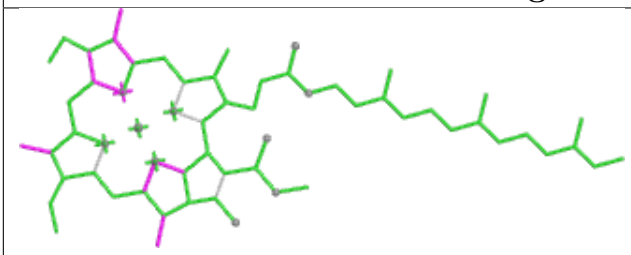


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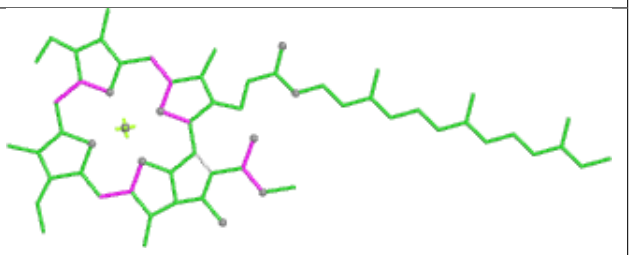


Rings

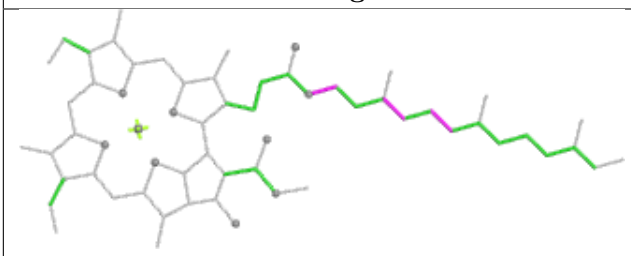
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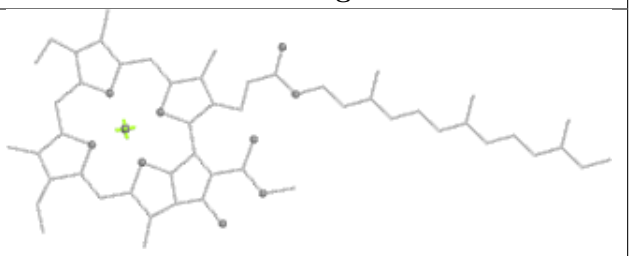
Bond lengths



Bond angles

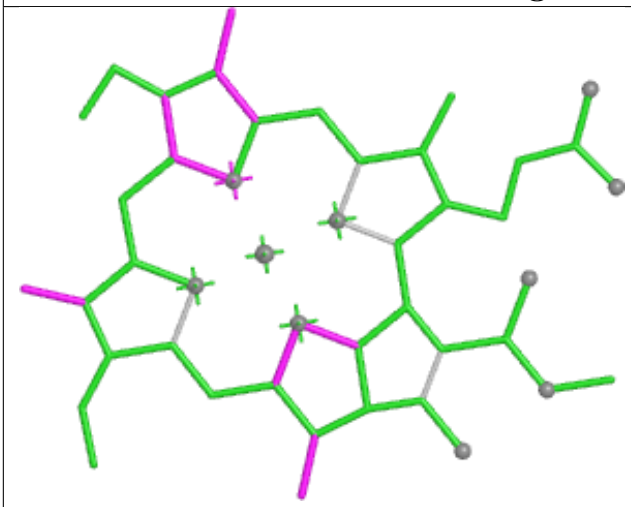


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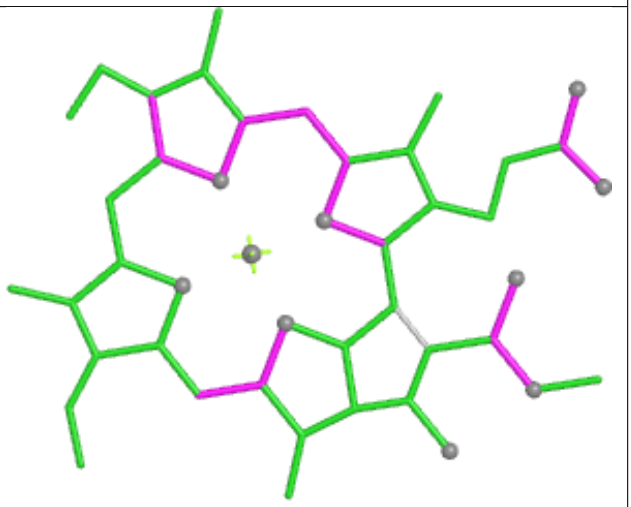


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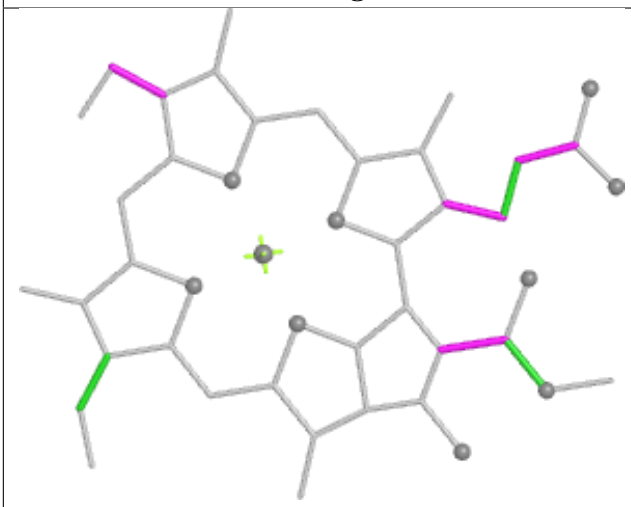
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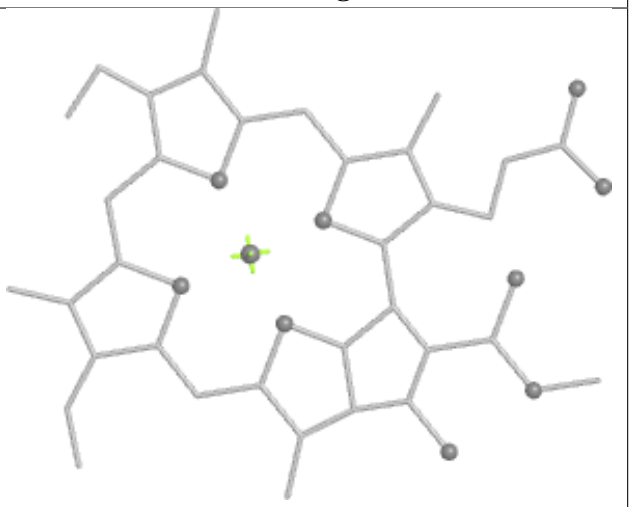
Bond lengths



Bond angles

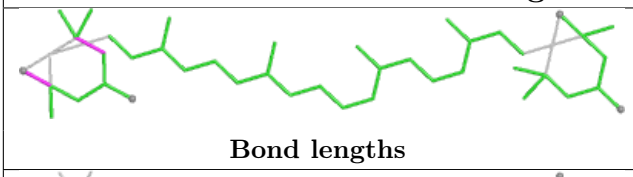


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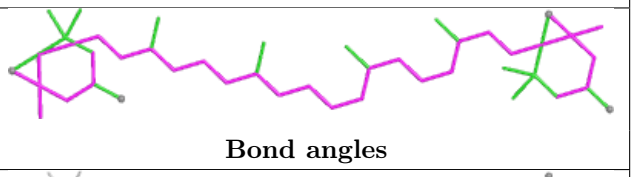


Rings

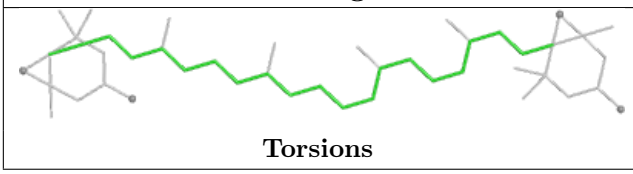
Ligand XAT 8 620



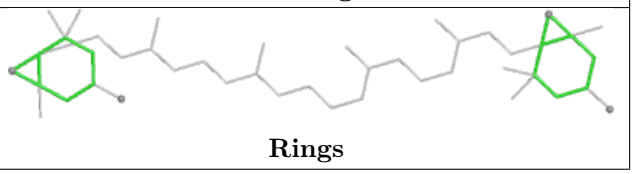
Bond lengths



Bond angles

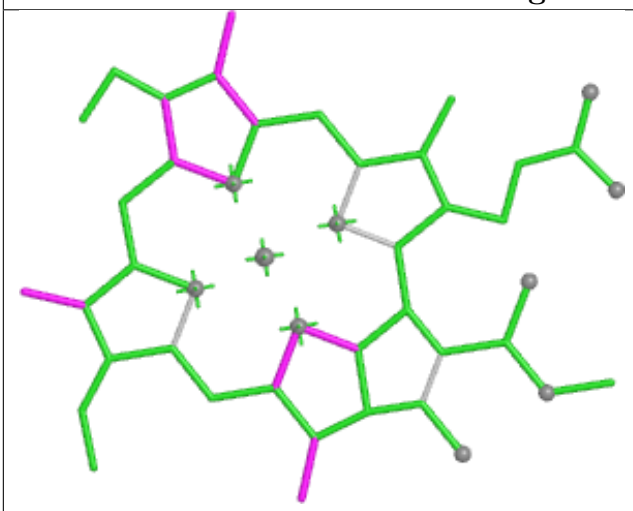


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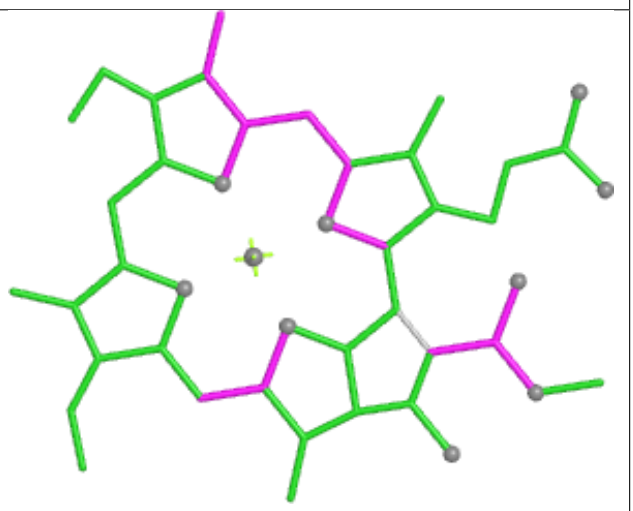


Rings

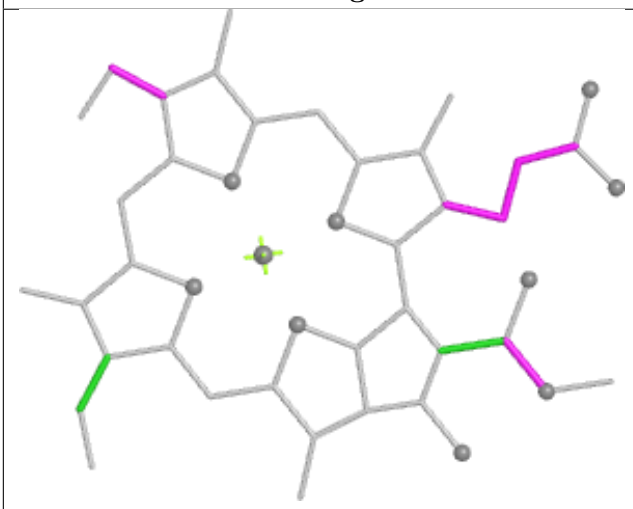
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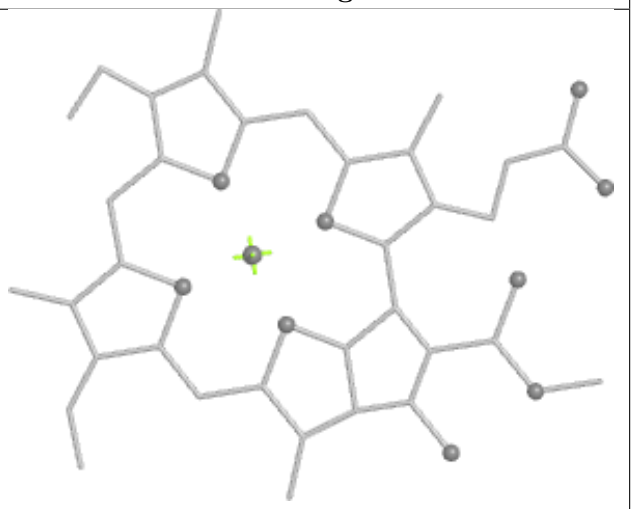
Bond lengths



Bond angles

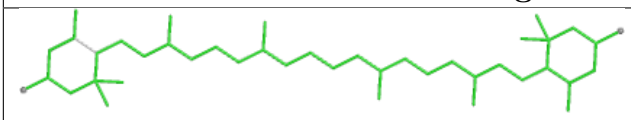


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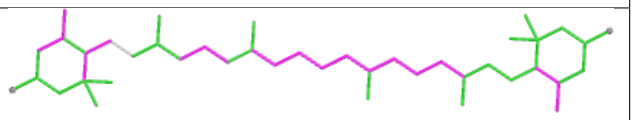


Rings

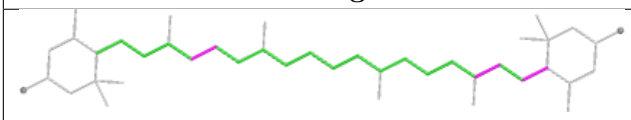
Ligand LUT U 1621



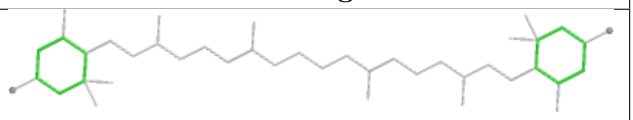
Bond lengths



Bond angles

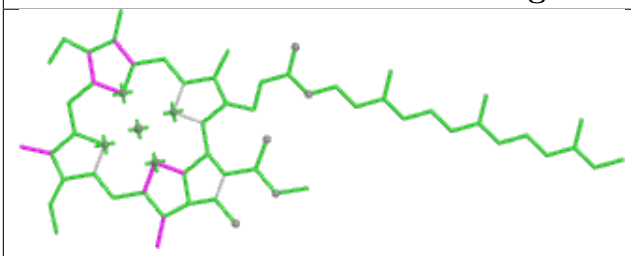


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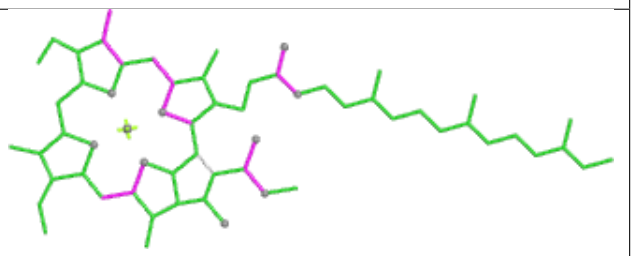


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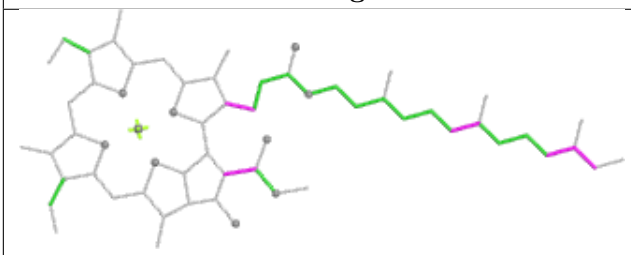
Ligand CLA 4 610



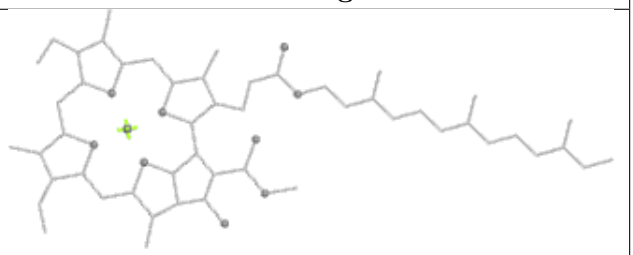
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Bond angles

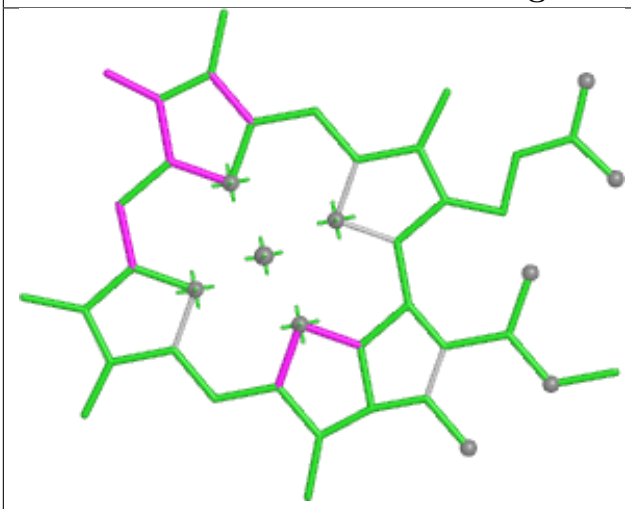


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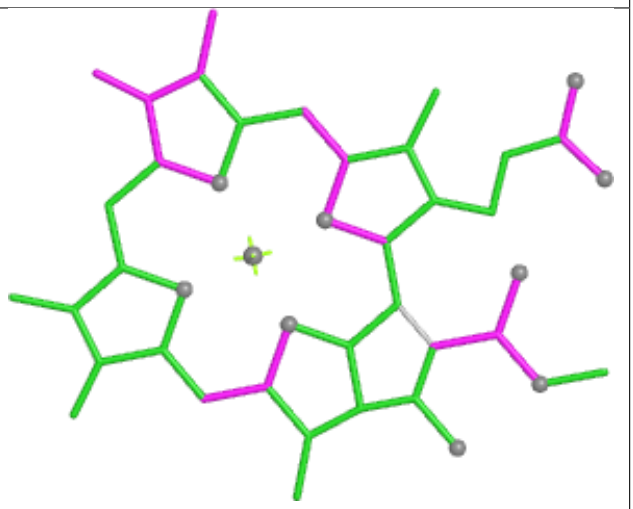


Rings

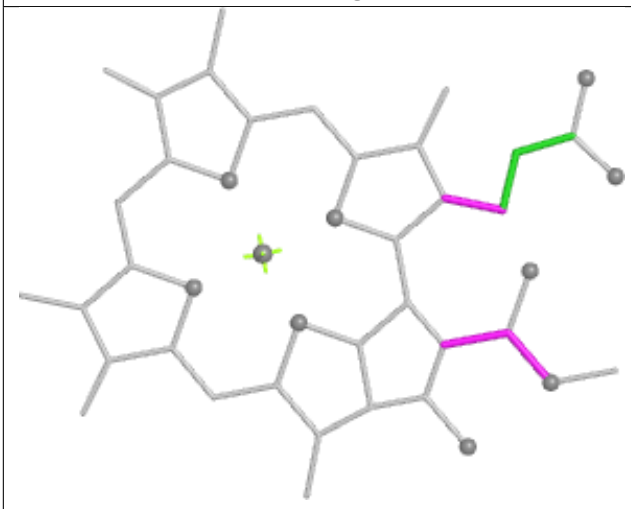
Ligand CLA 8 616



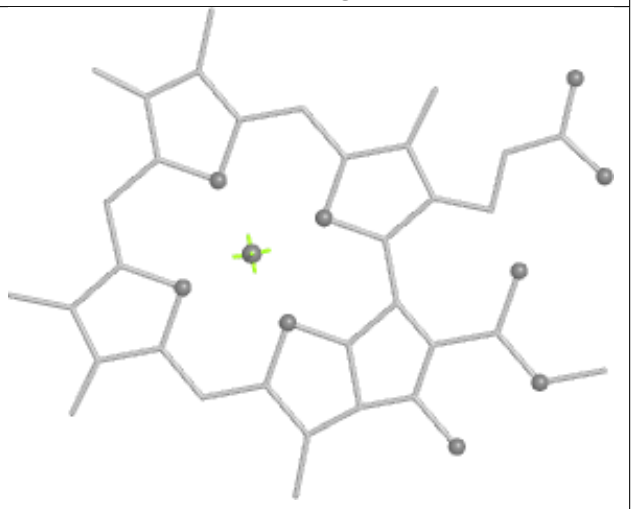
Bond lengths



Bond angles

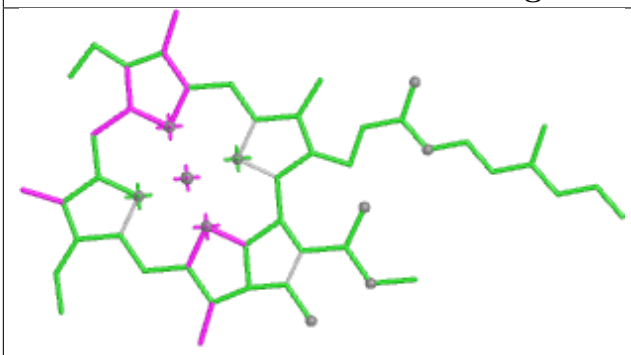


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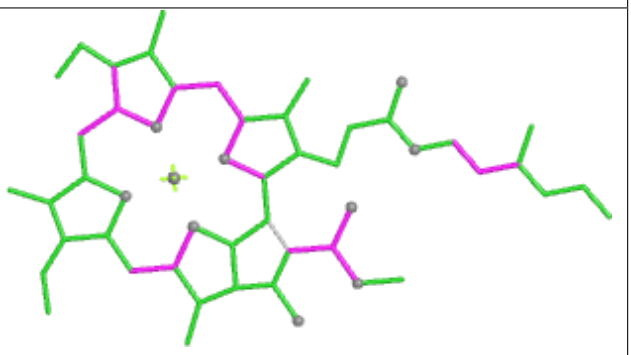


Rings

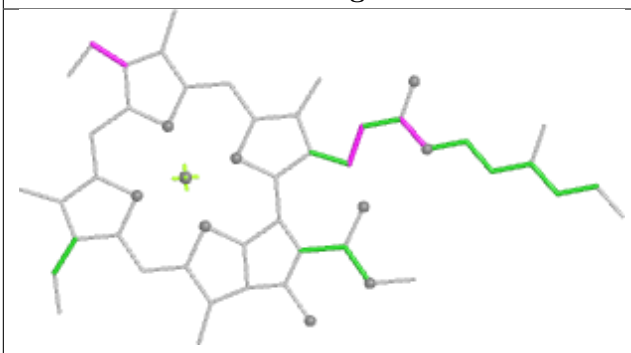
Ligand CLA B 807



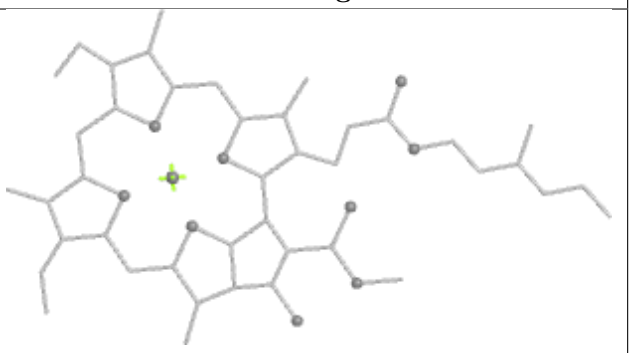
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Bond angles

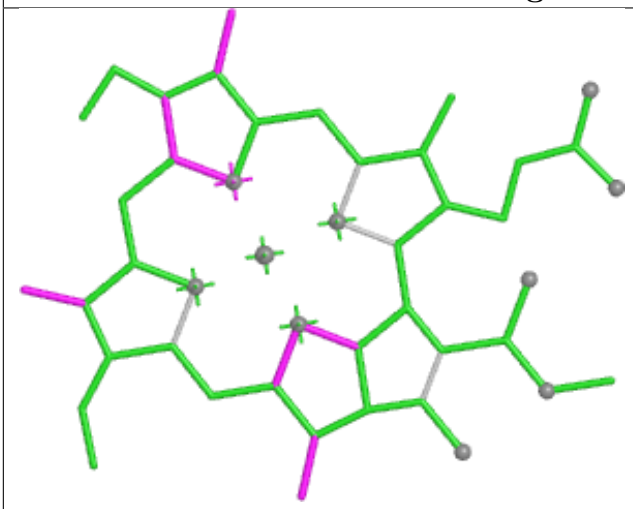


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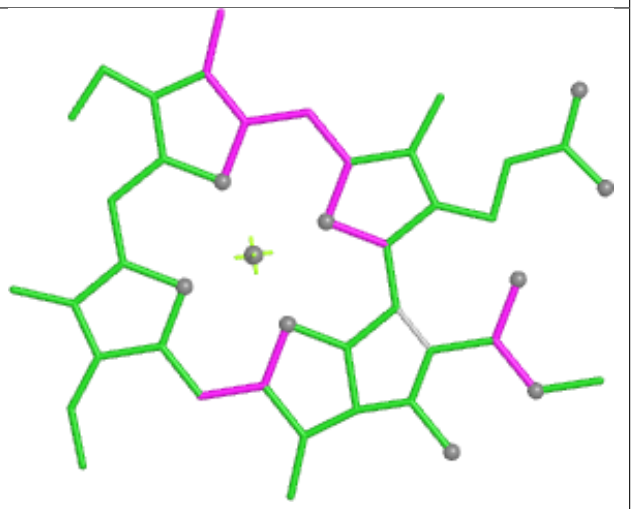


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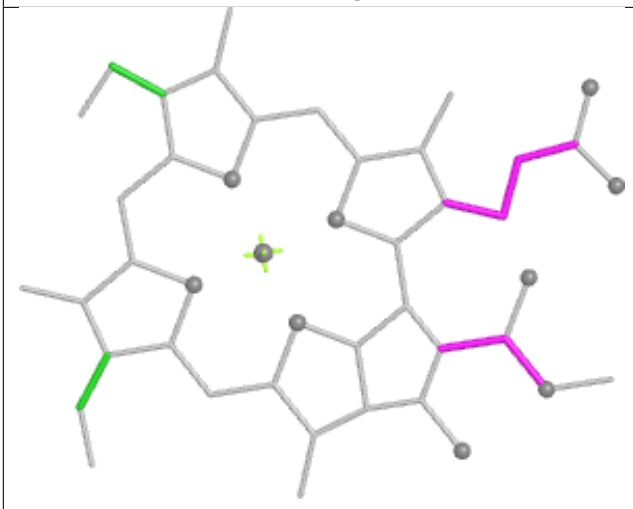
Ligand CLA L 302



Bond lengths



Bond angles

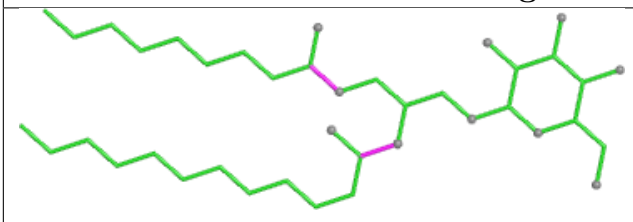


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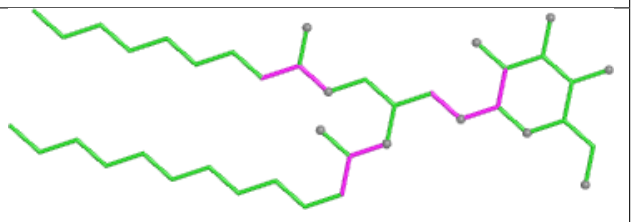


Rings

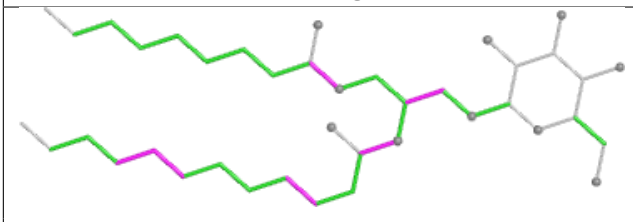
Ligand LMG A 860



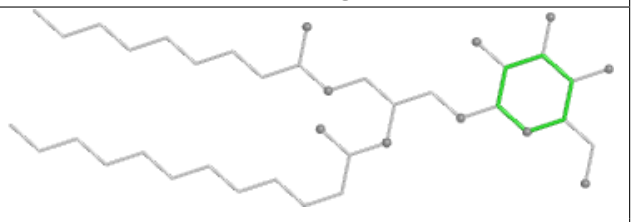
Bond lengths



Bond angles

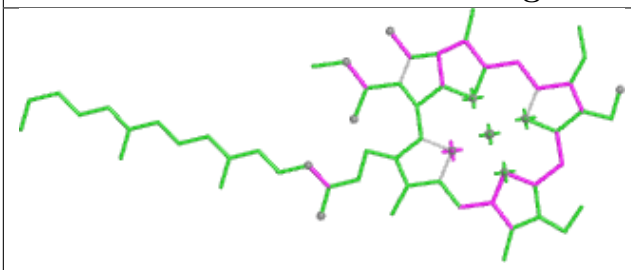


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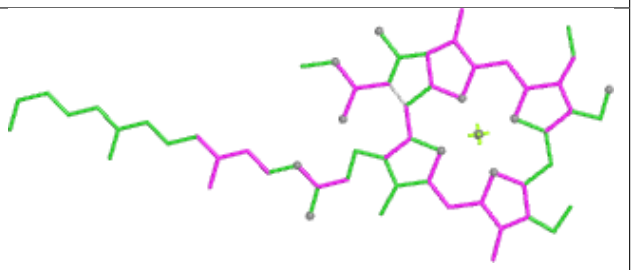


Rings

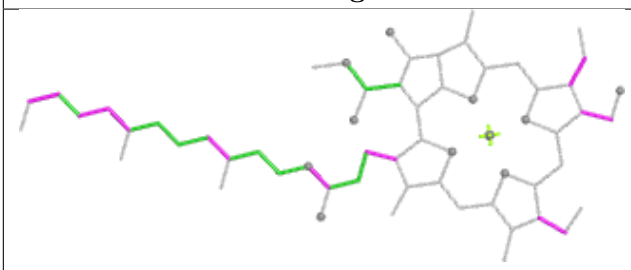
Ligand CHL U 609



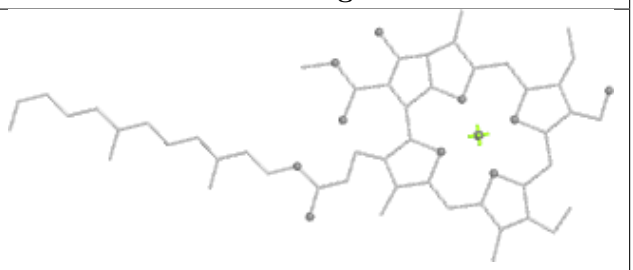
Bond lengths



Bond angles

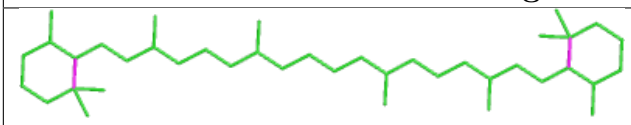


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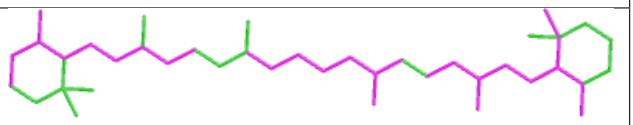


Rings

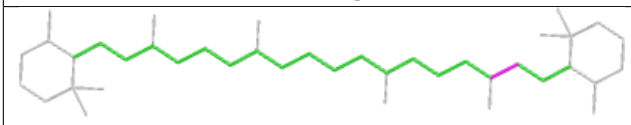
Ligand BCR B 847



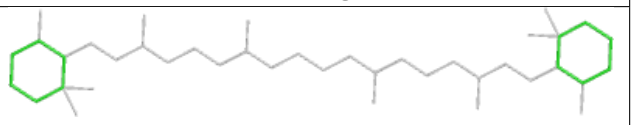
Bond lengths



Bond angles

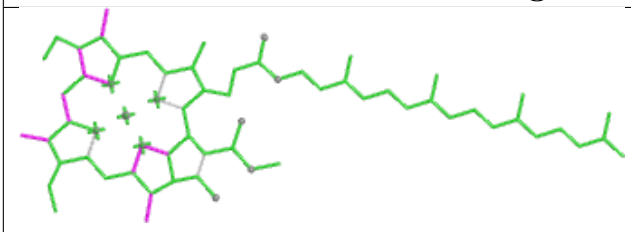


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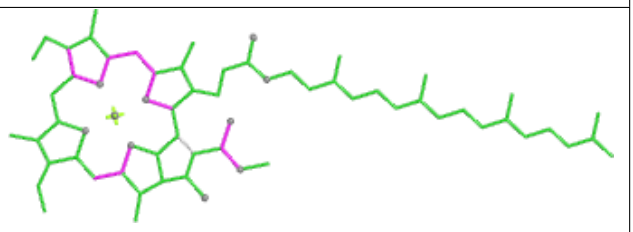


Rings

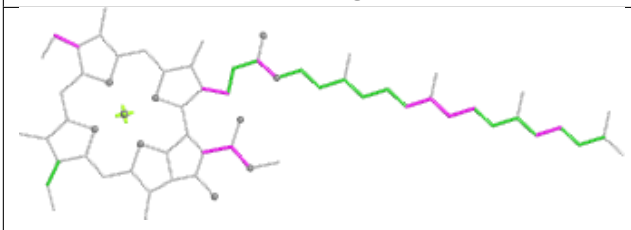
Ligand CLA 3 610



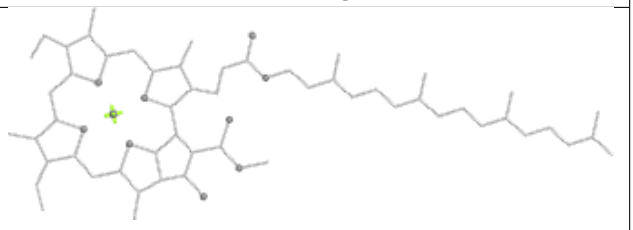
Bond lengths



Bond angles

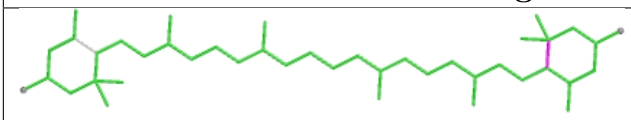


Torsions

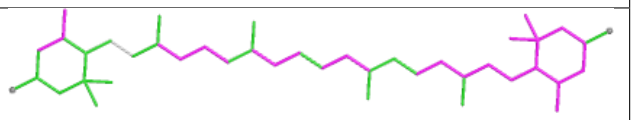


Rings

Ligand LUT Y 1621



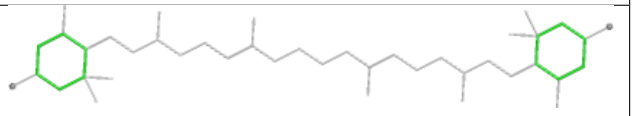
Bond lengths



Bond angles

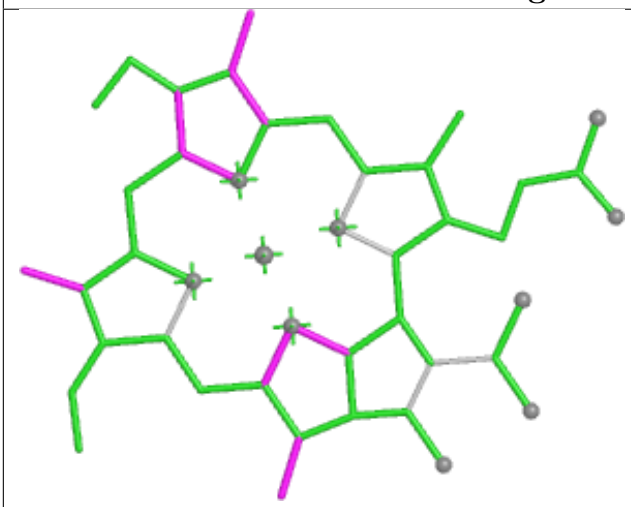


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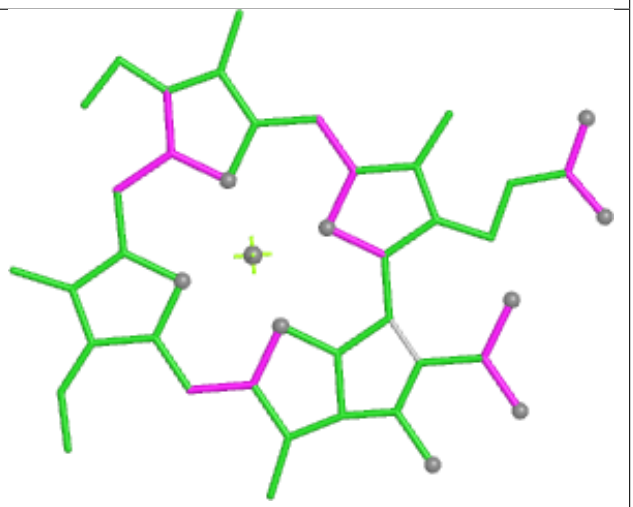


Rings

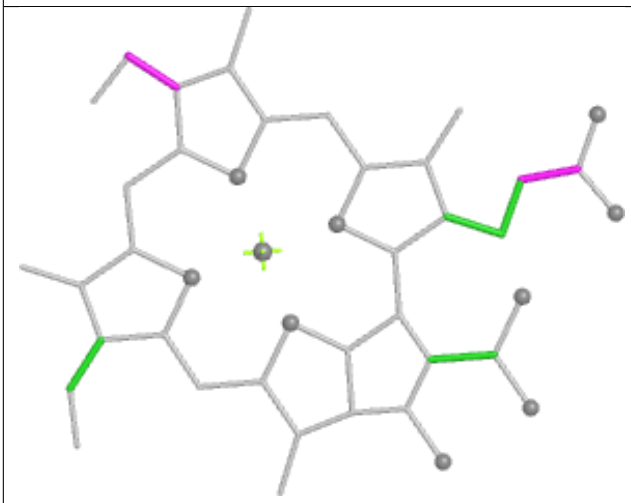
Ligand CLA a 608



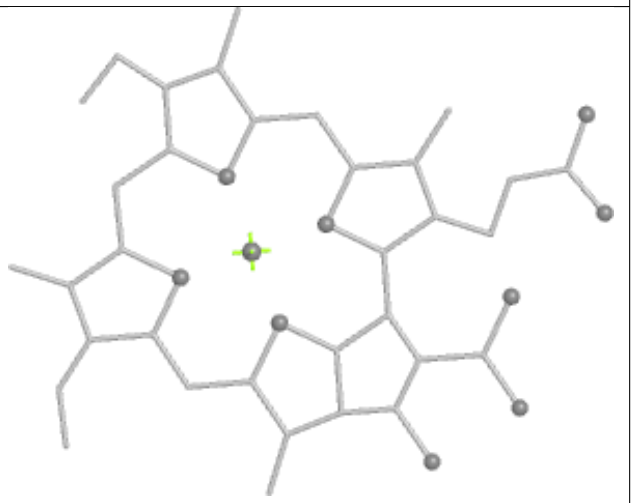
Bond lengths



Bond angles

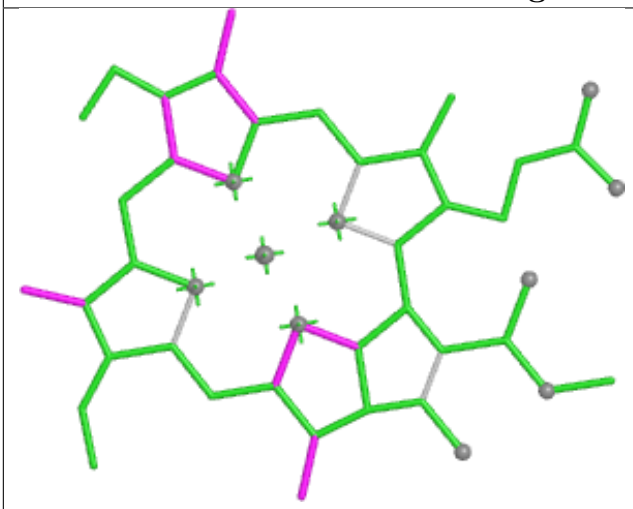


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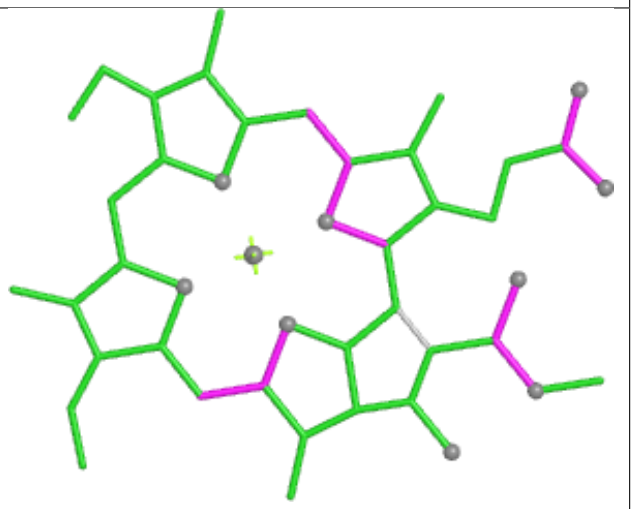


Rings

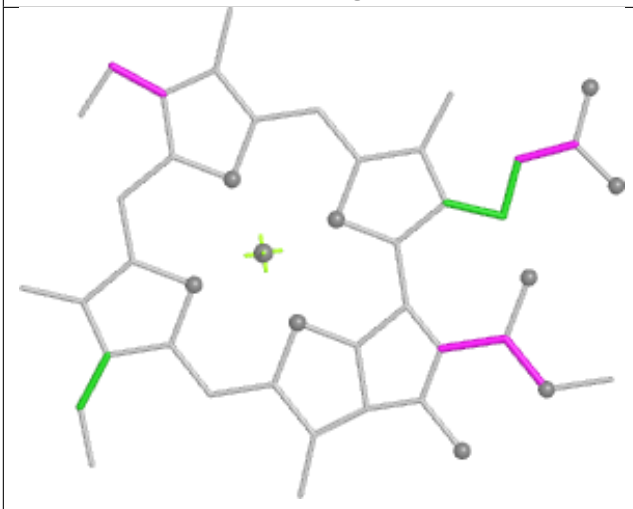
Ligand CLA 9 601



Bond lengths



Bond angles

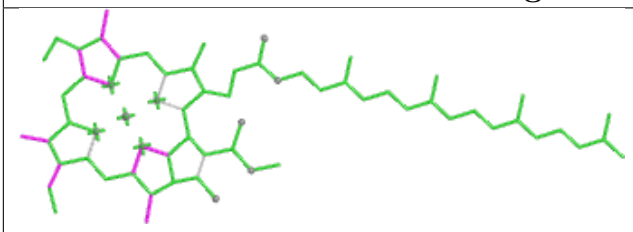


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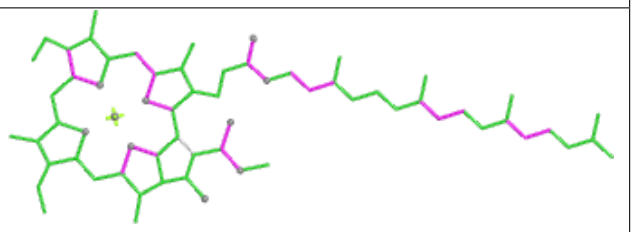


Rings

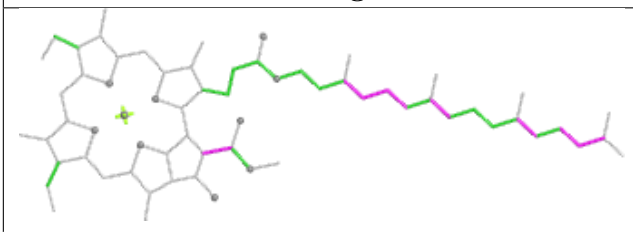
Ligand CLA B 808



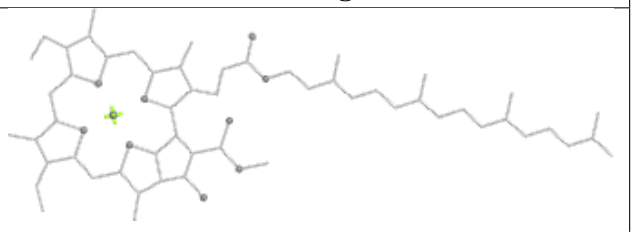
Bond lengths



Bond angles

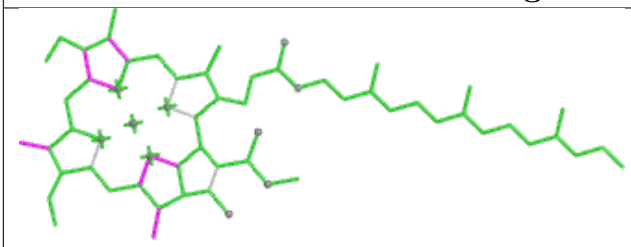


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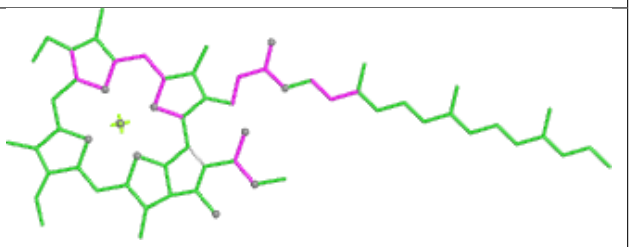


Rings

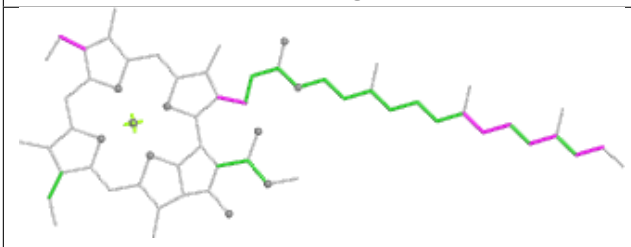
Ligand CLA V 610



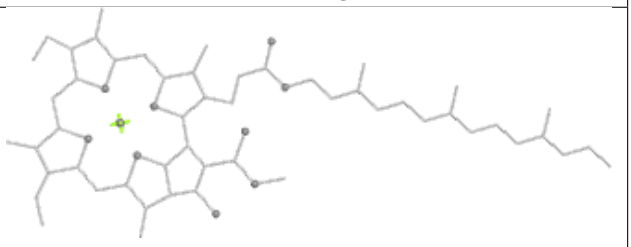
Bond lengths



Bond angles

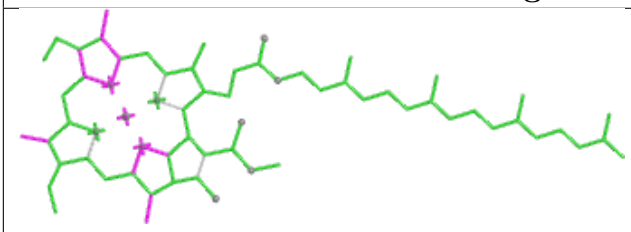


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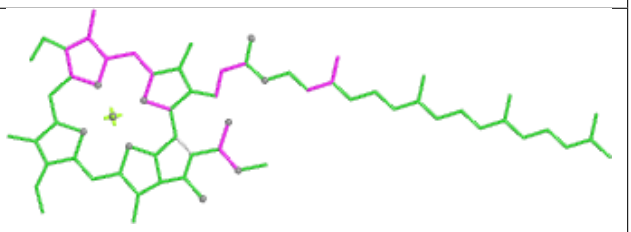


Rings

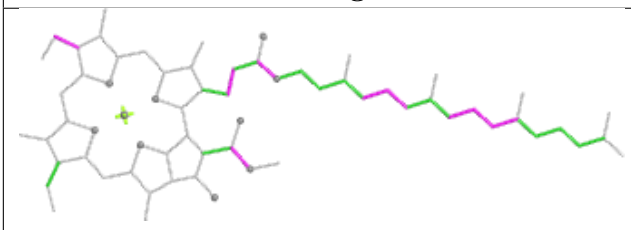
Ligand CLA A 834



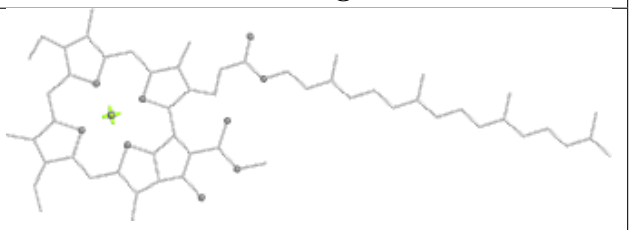
Bond lengths



Bond angles

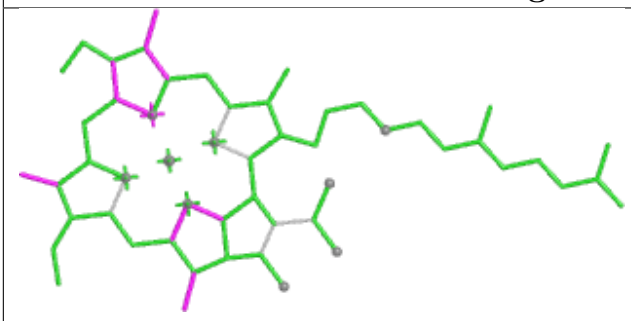


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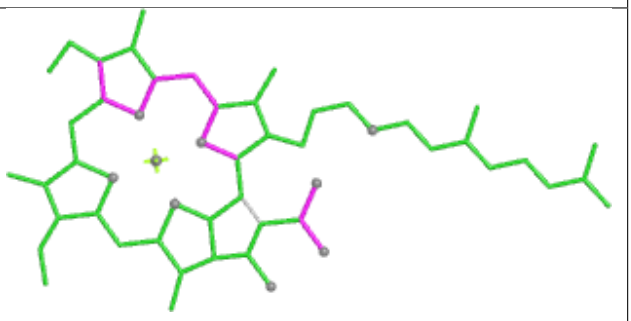


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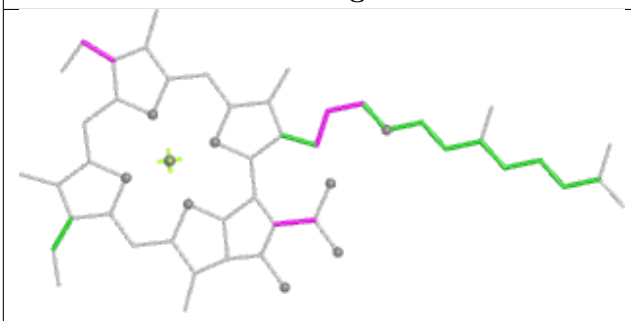
Ligand CLA 3 613



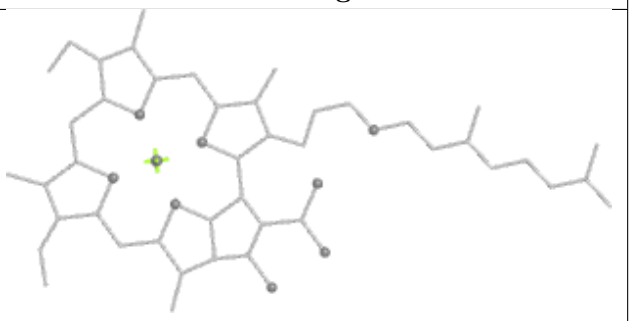
Bond lengths



Bond angles

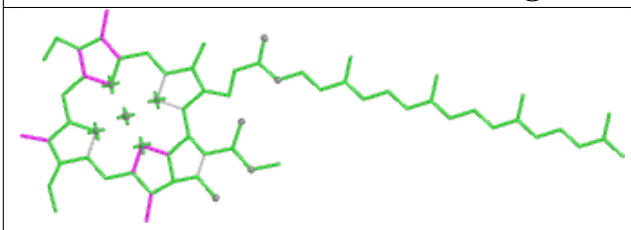


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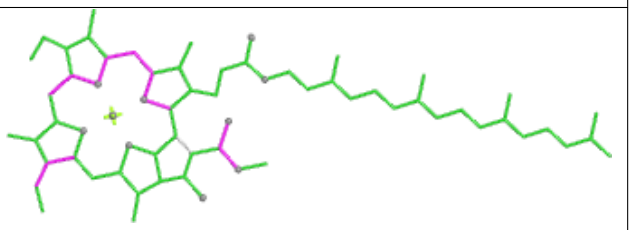


Rings

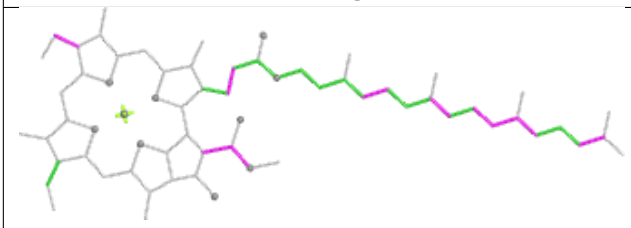
Ligand CLA Y 613



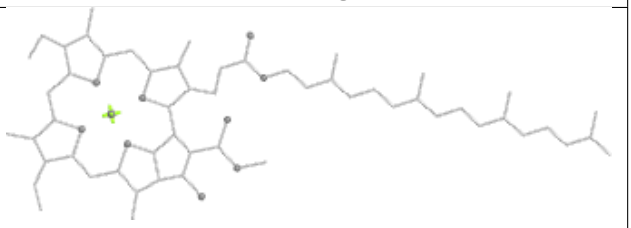
Bond lengths



Bond angles

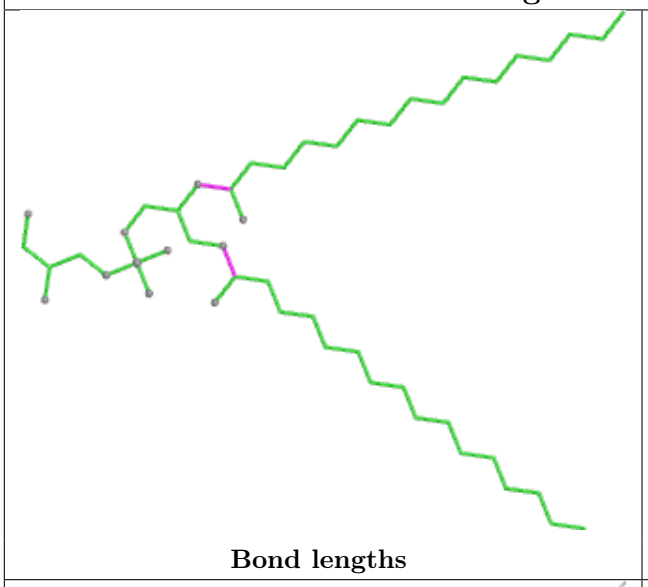


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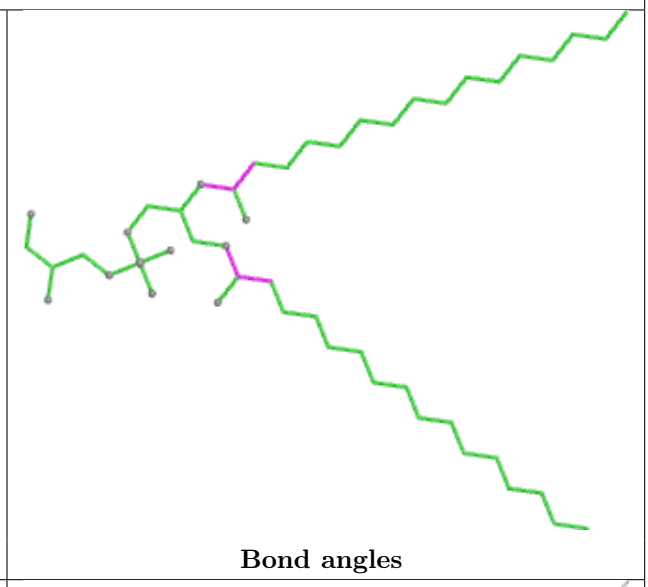


Rings

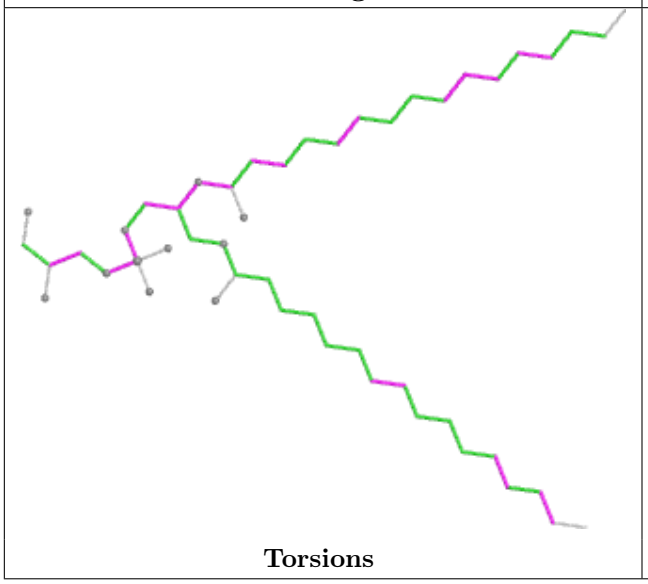
Ligand LHG A 861



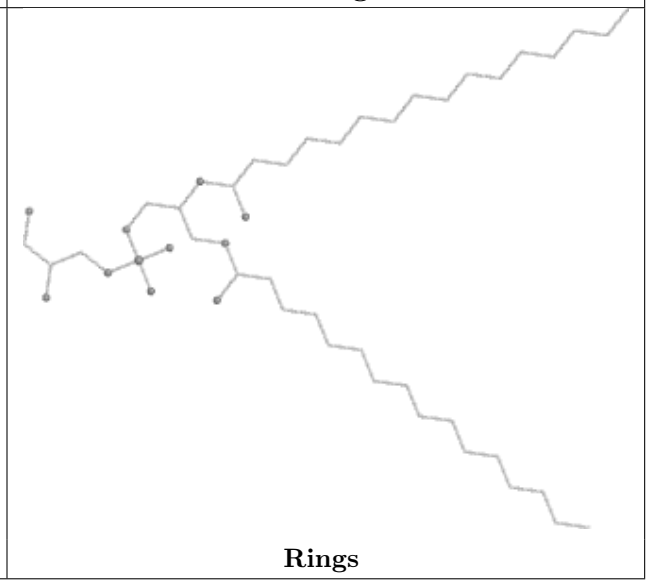
Bond lengths



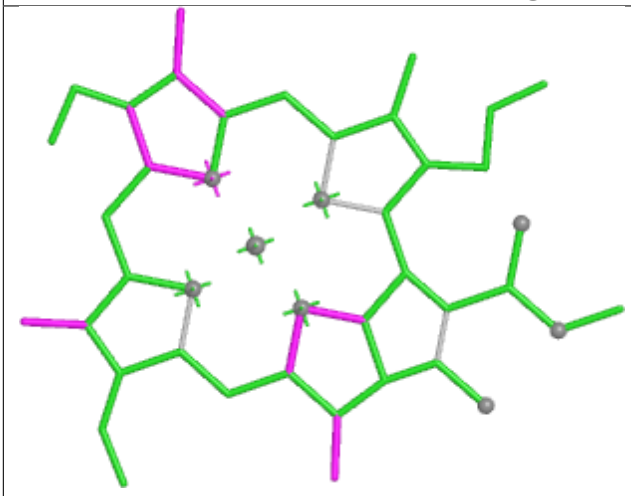
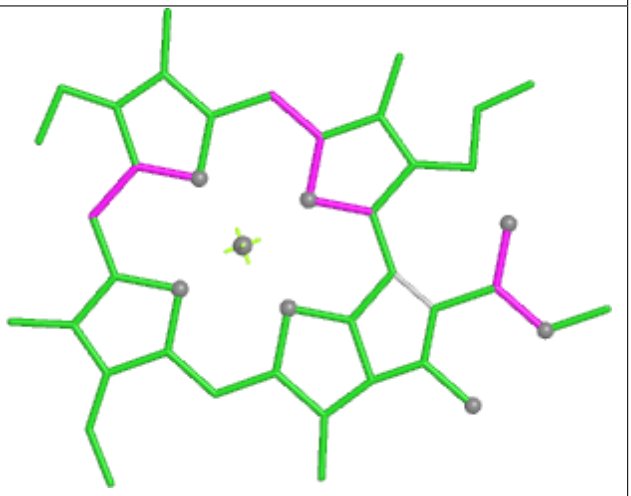
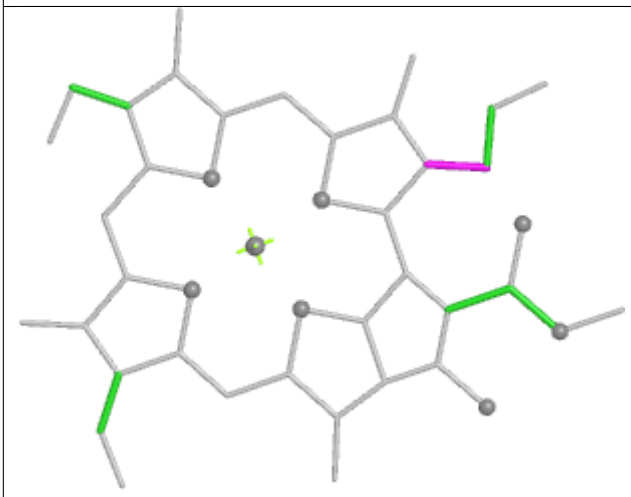
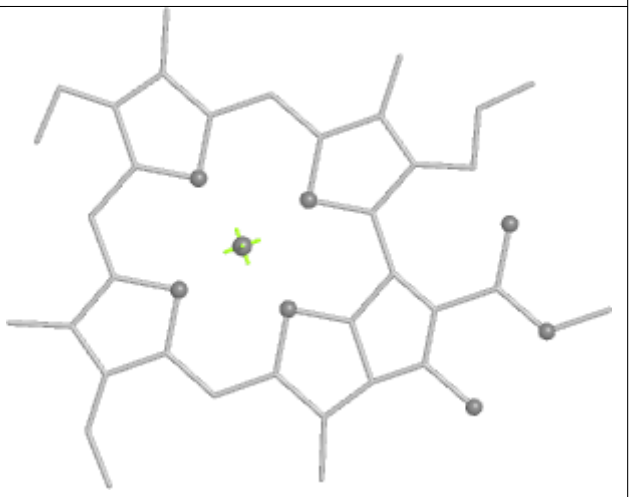
Bond angles



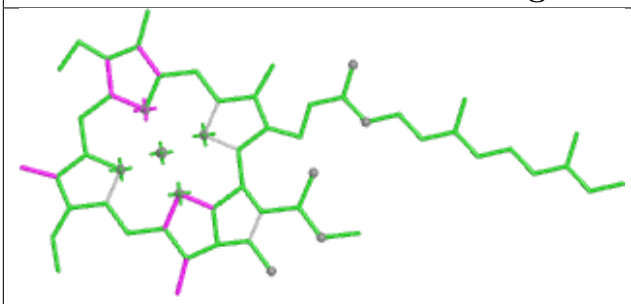
Torsions



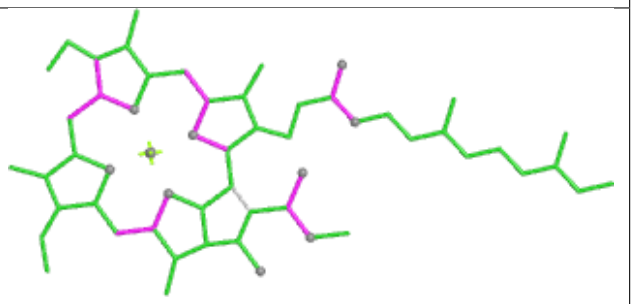
Rings

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

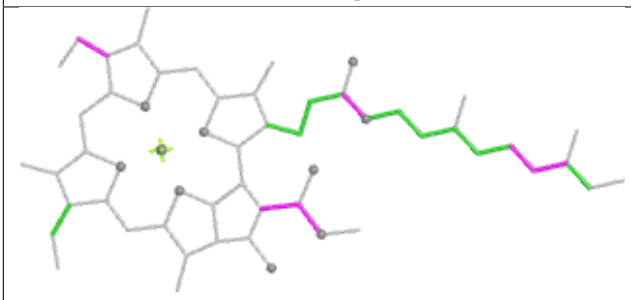
Ligand CLA 4 614



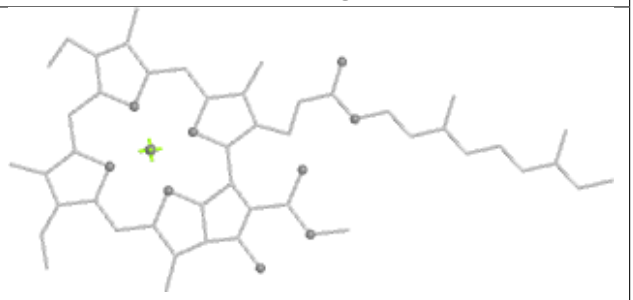
Bond lengths



Bond angles

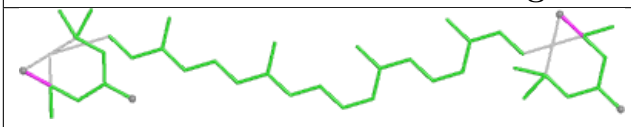


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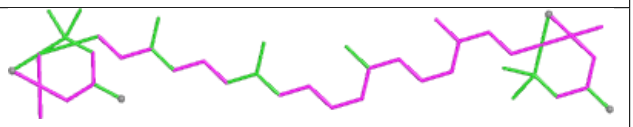


Rings

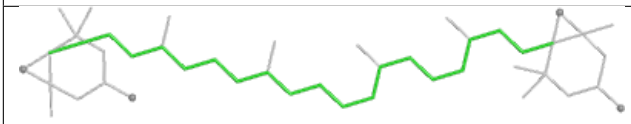
Ligand XAT 5 621



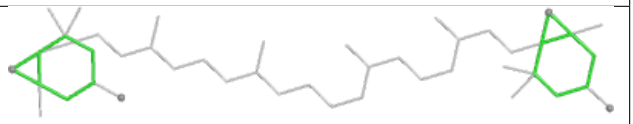
Bond lengths



Bond angles

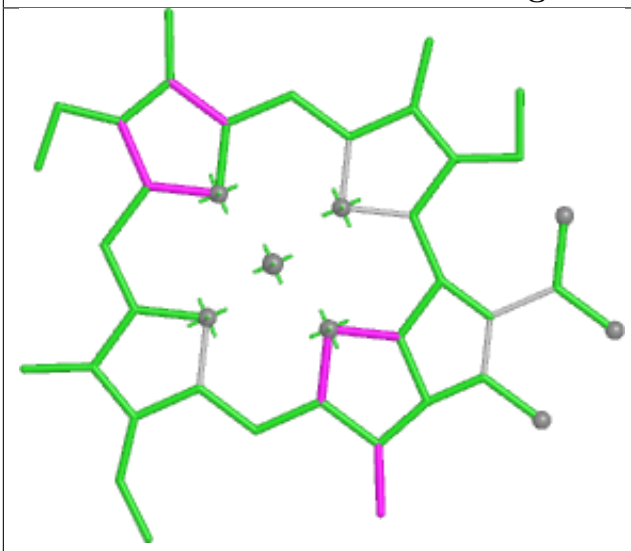


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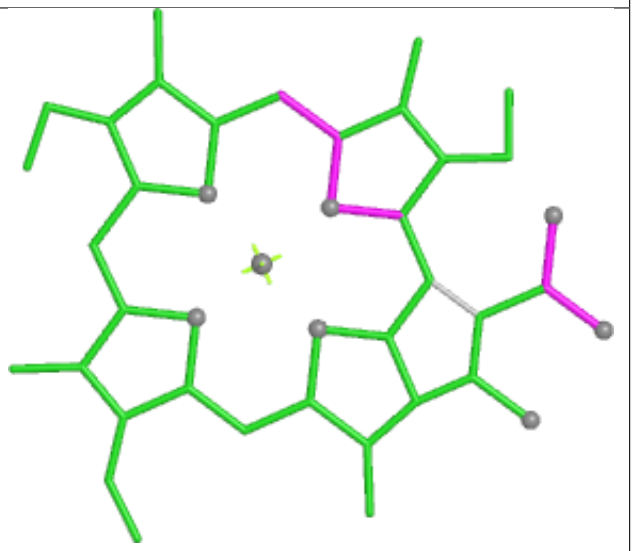


Rings

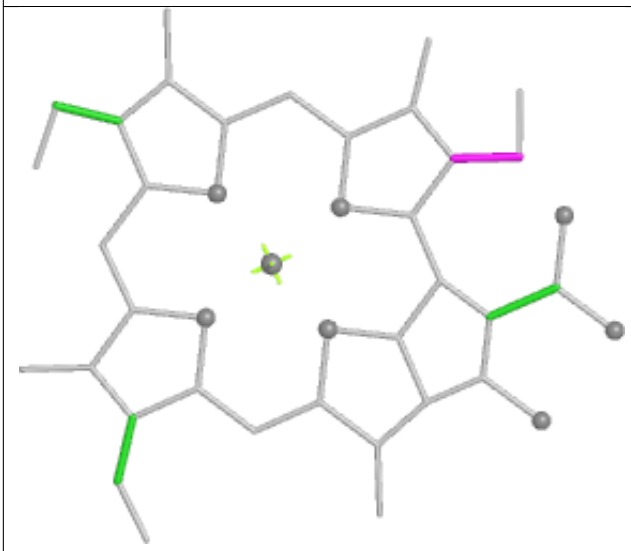
Ligand CLA 9 612



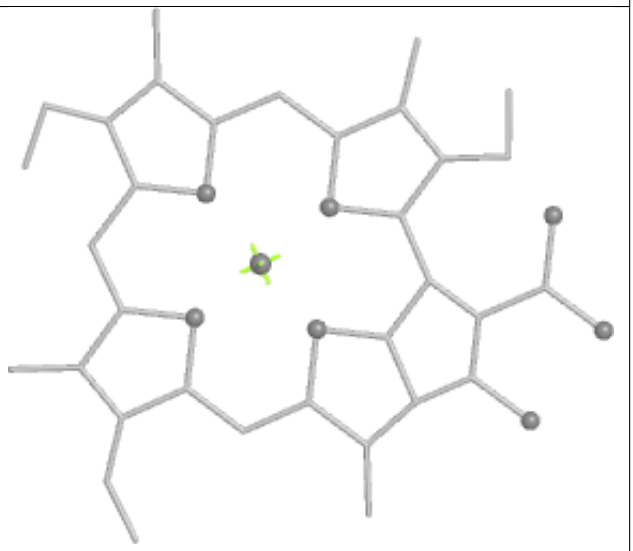
Bond lengths



Bond angles

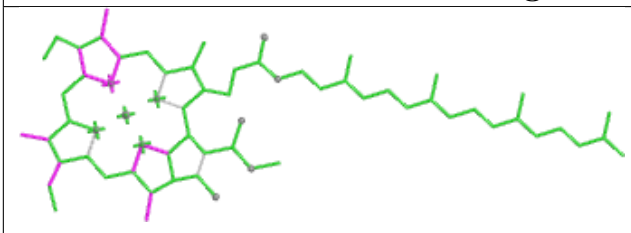


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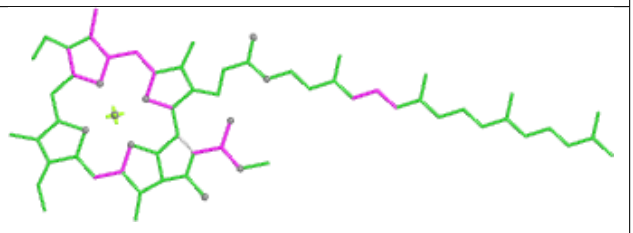


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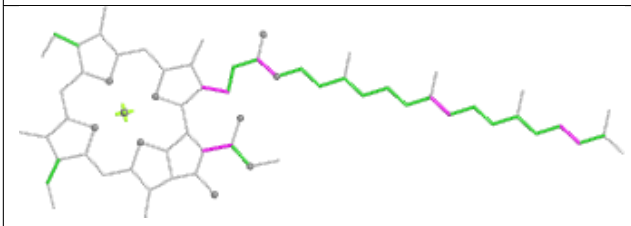
Ligand CLA A 820



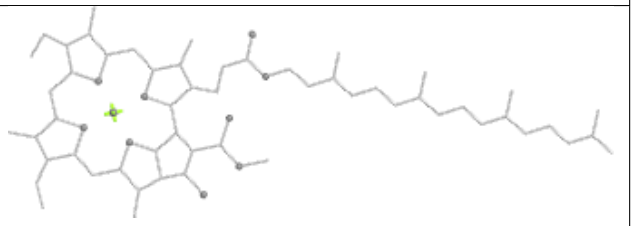
Bond lengths



Bond angles

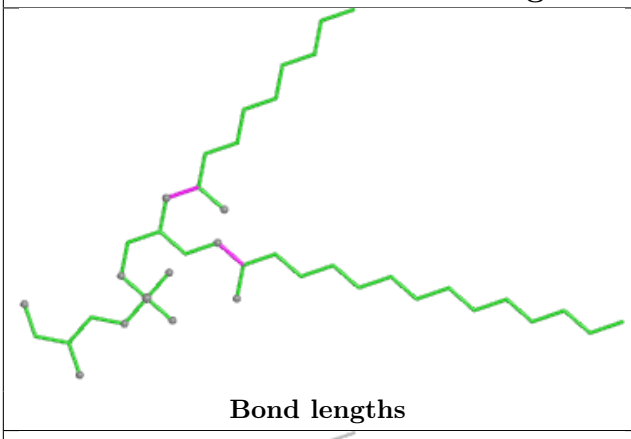


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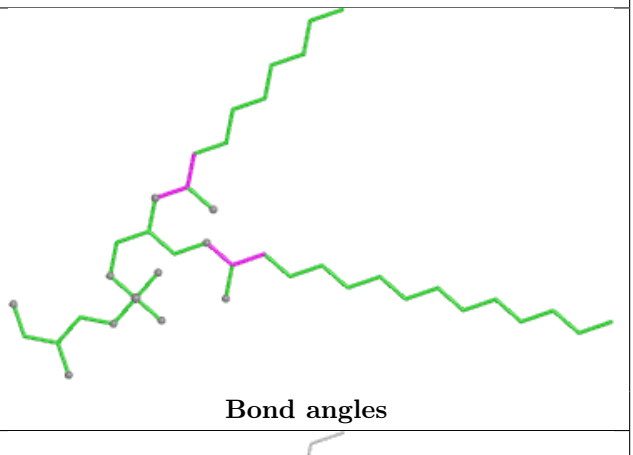


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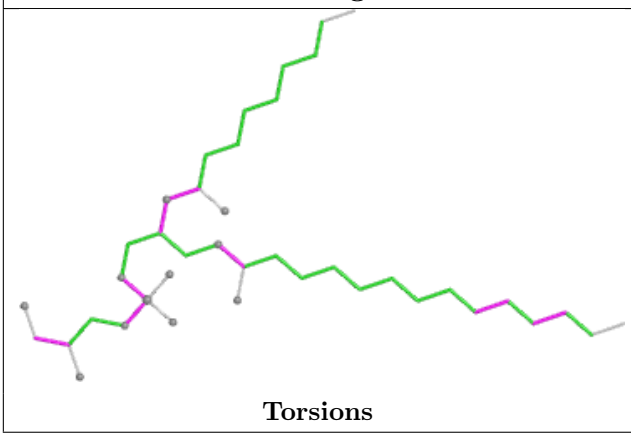
Ligand LHG 8 623



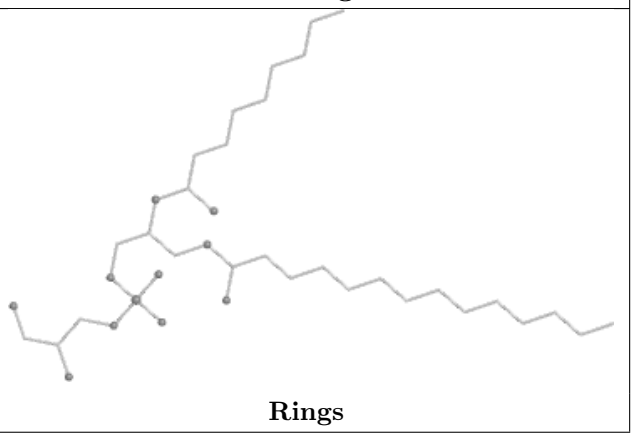
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Bond angles

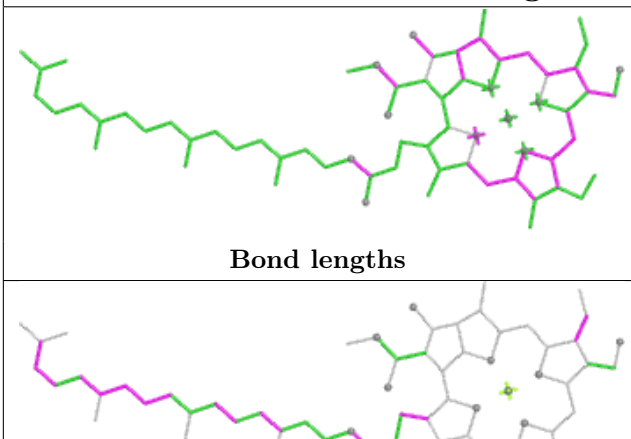


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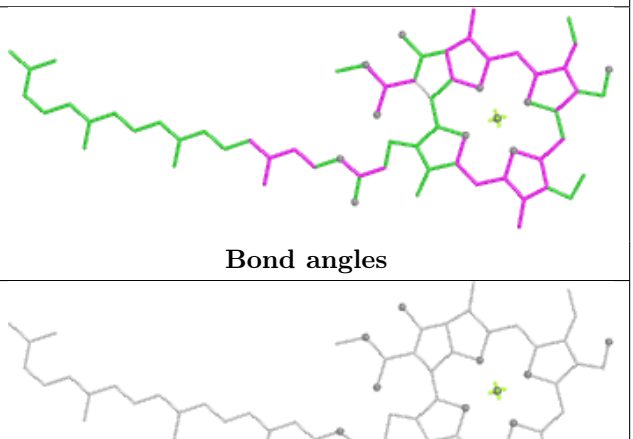


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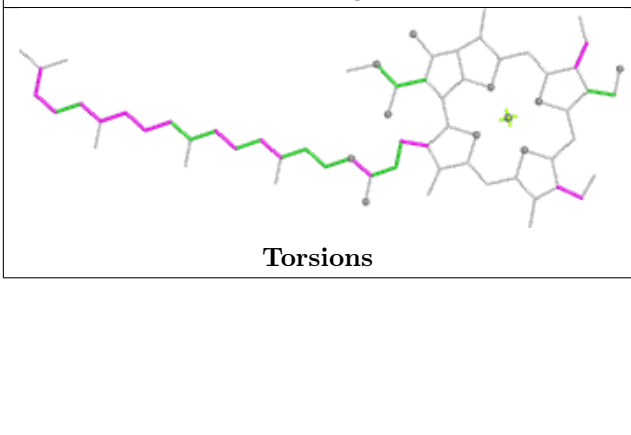
Ligand CHL Y 609



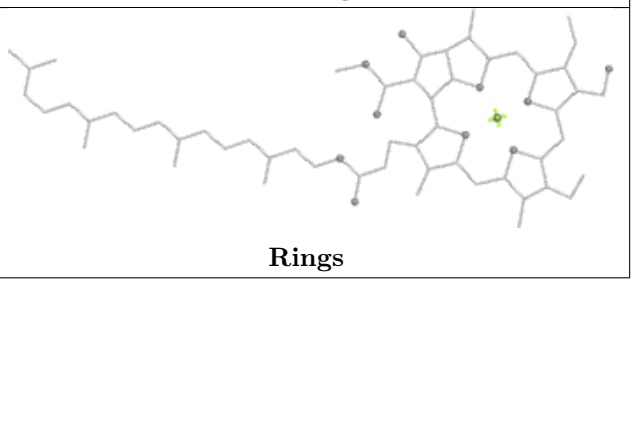
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Bond angles

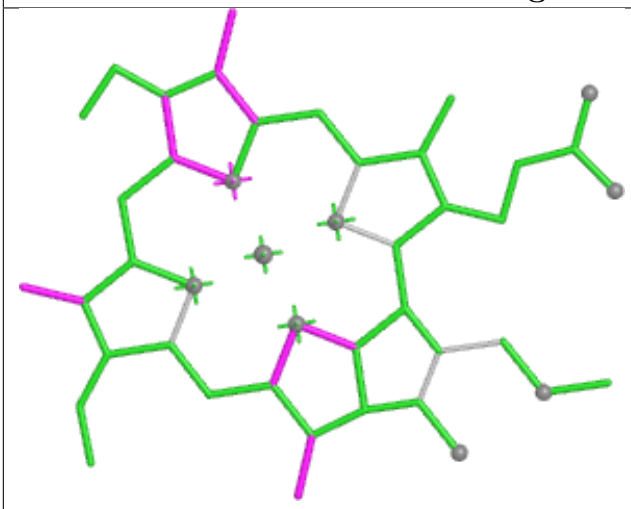


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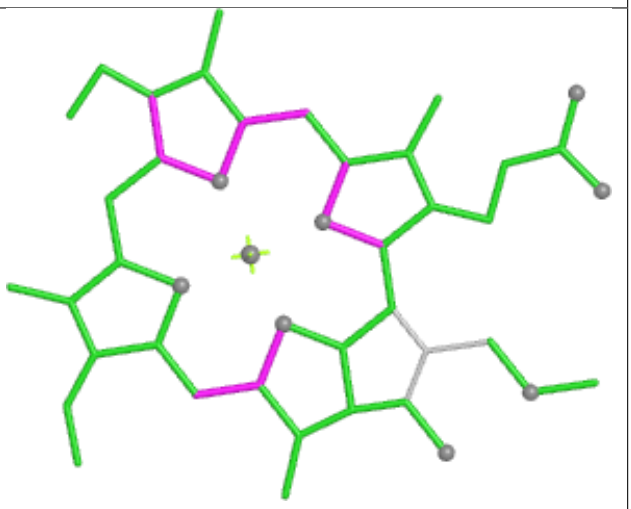


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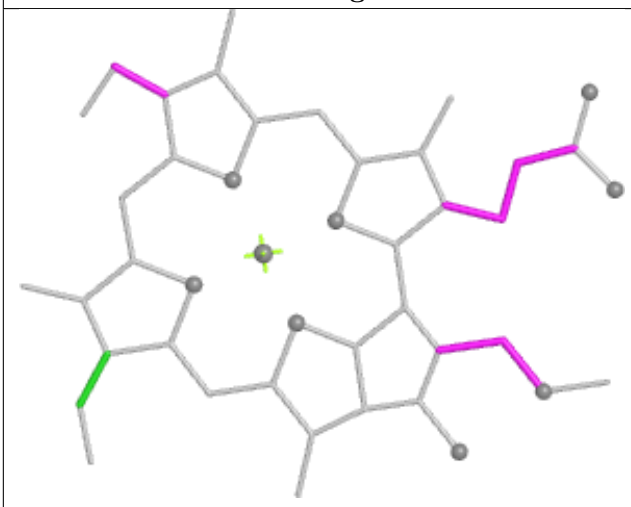
Ligand CLA a 606



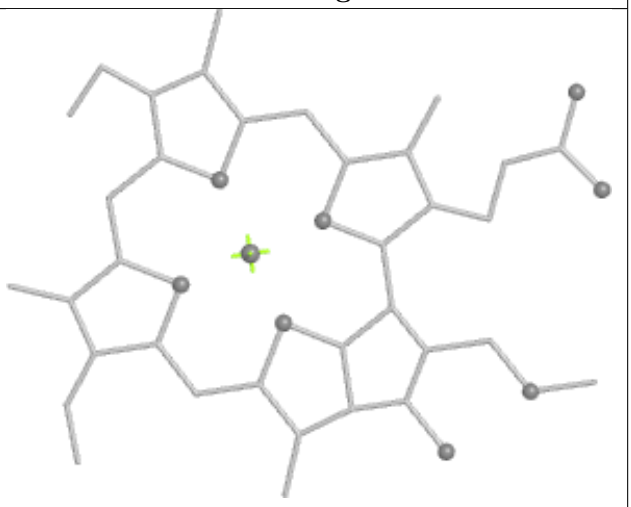
Bond lengths



Bond angles

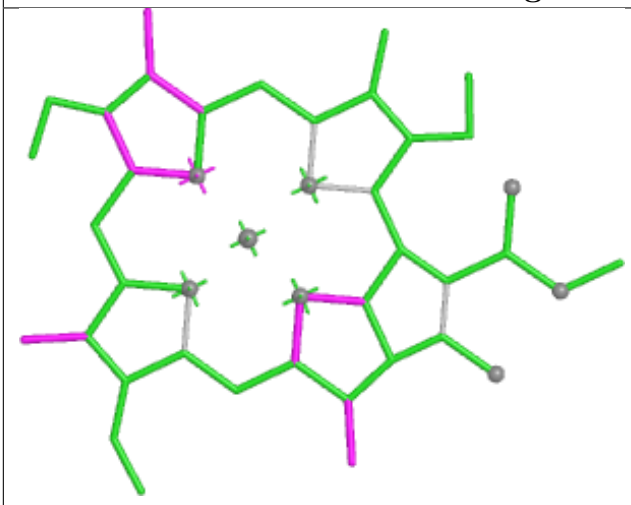


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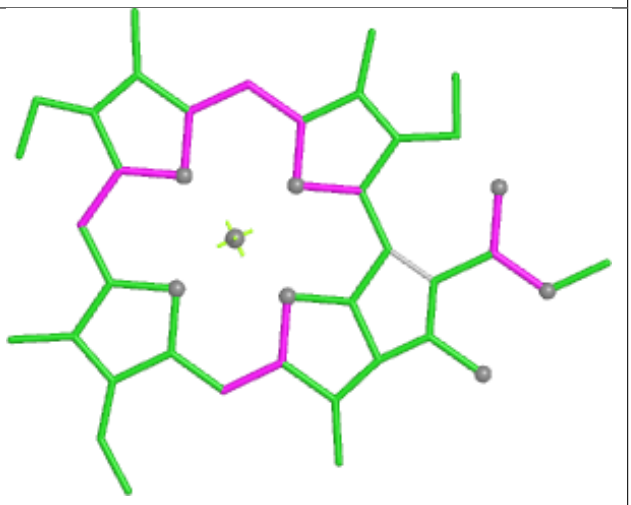


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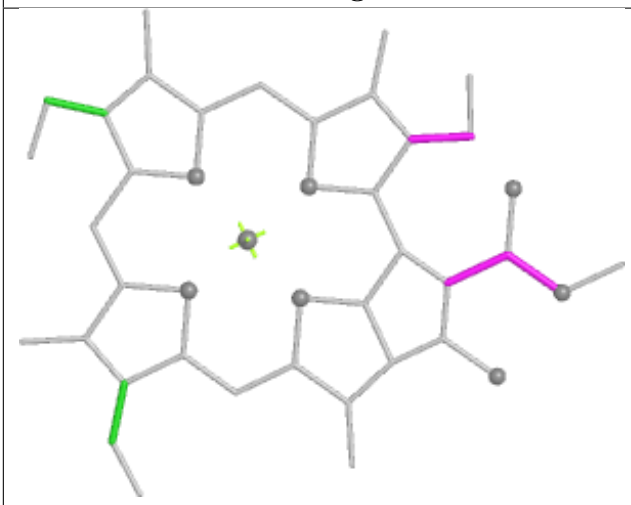
Ligand CLA B 822



Bond lengths



Bond angles

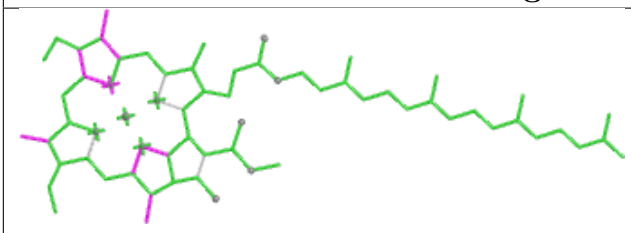


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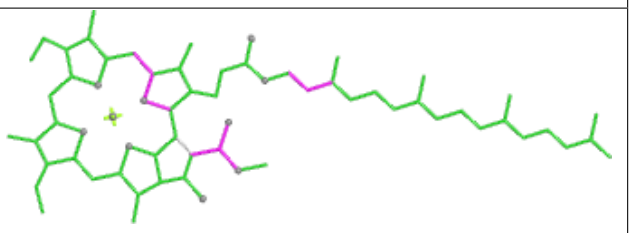


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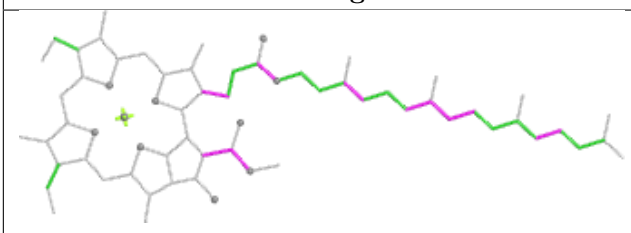
Ligand CLA A 811



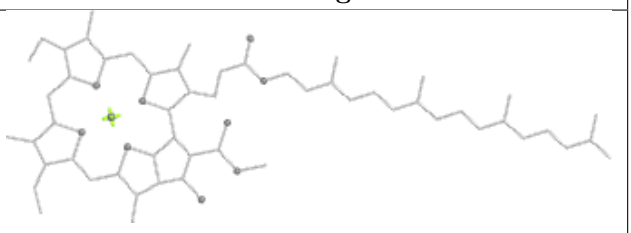
Bond lengths



Bond angles

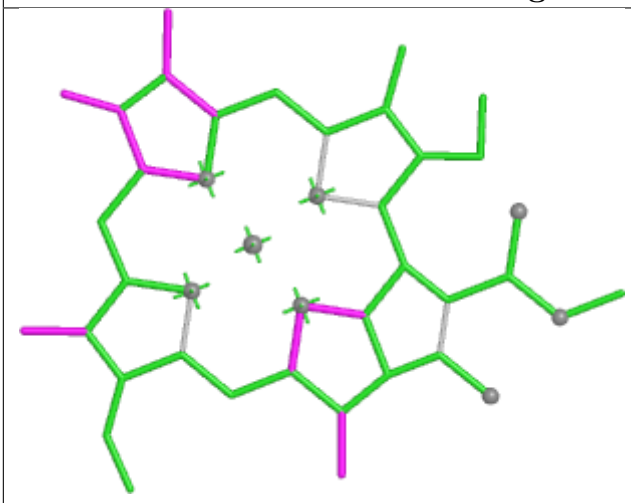


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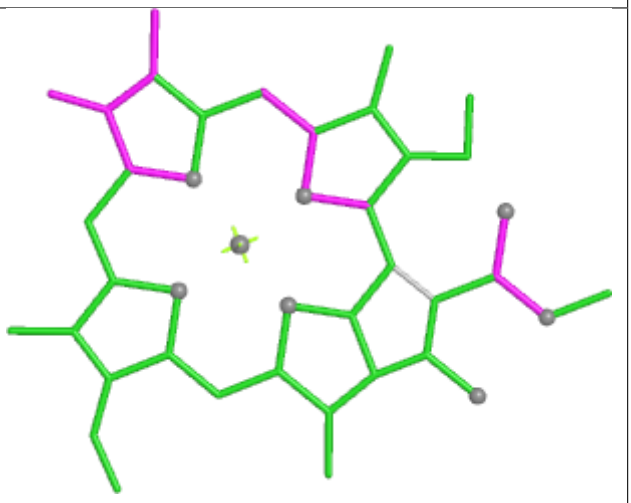


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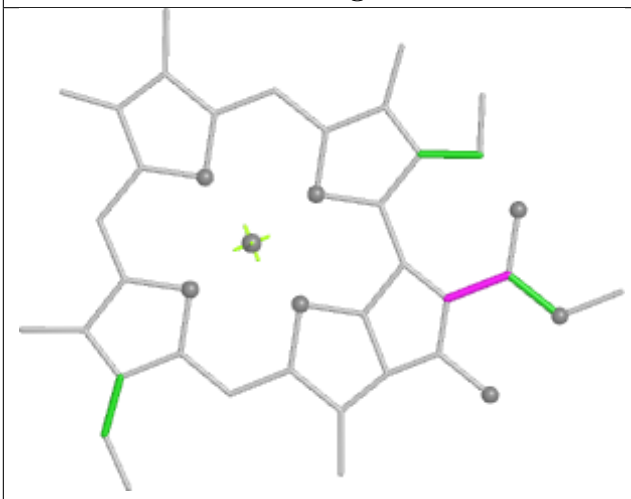
Ligand CLA 6 607



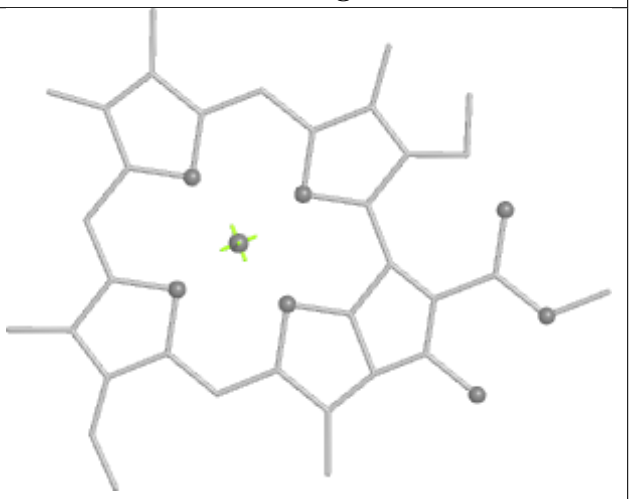
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Bond angles

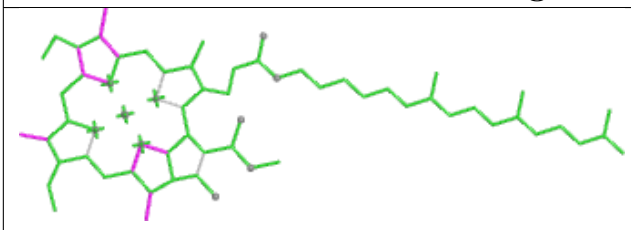


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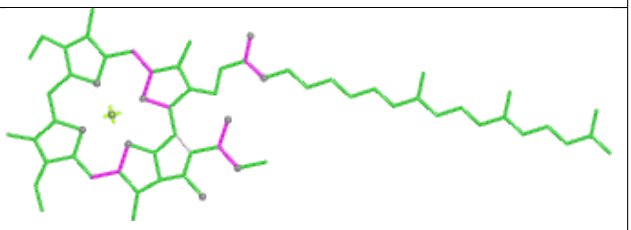


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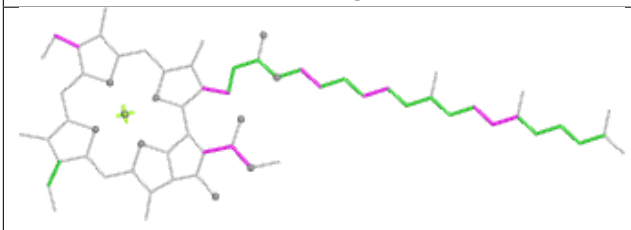
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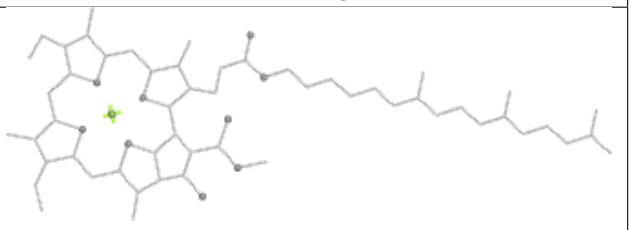
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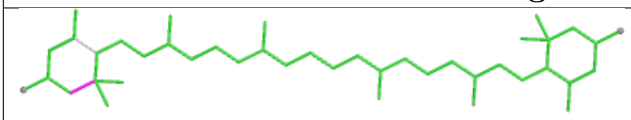


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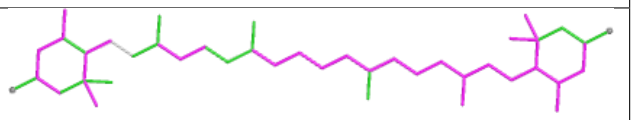


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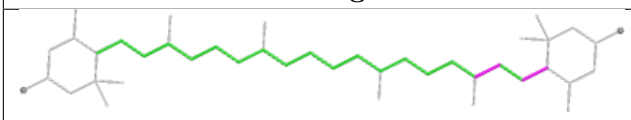
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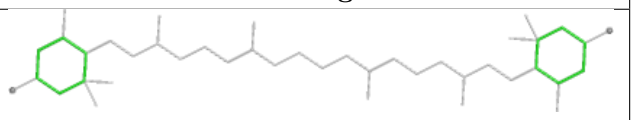
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Bond angles

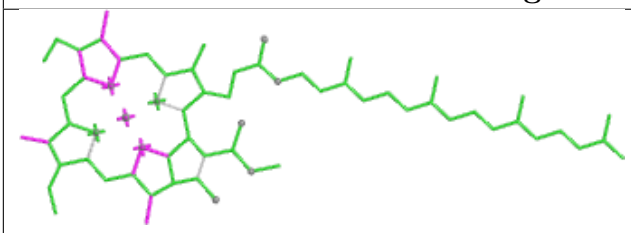


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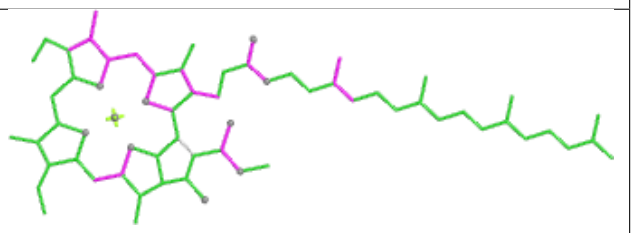


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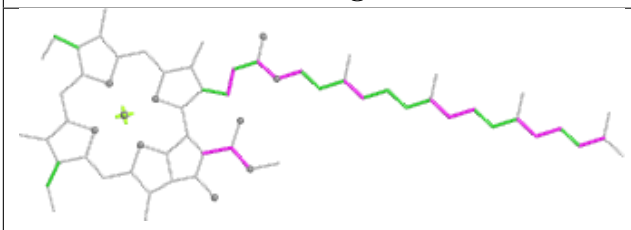
Ligand CLA A 814



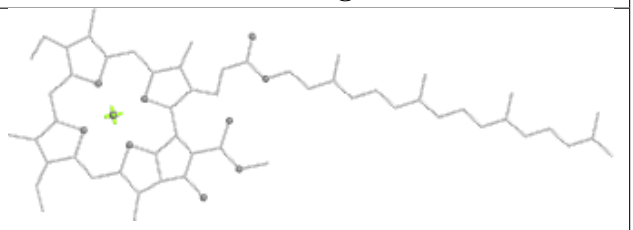
Bond lengths



Bond angles

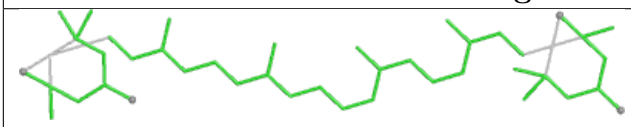


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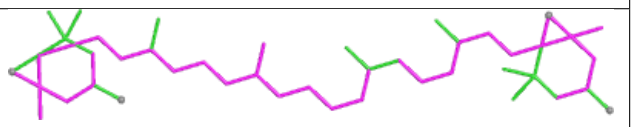


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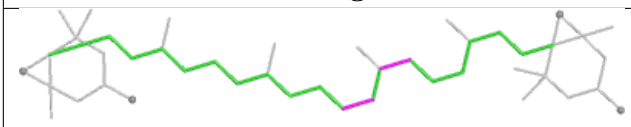
Ligand XAT Y 1622



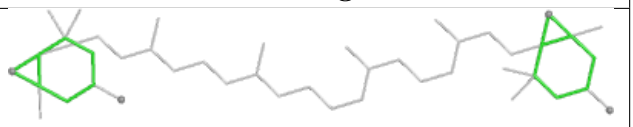
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Bond angles

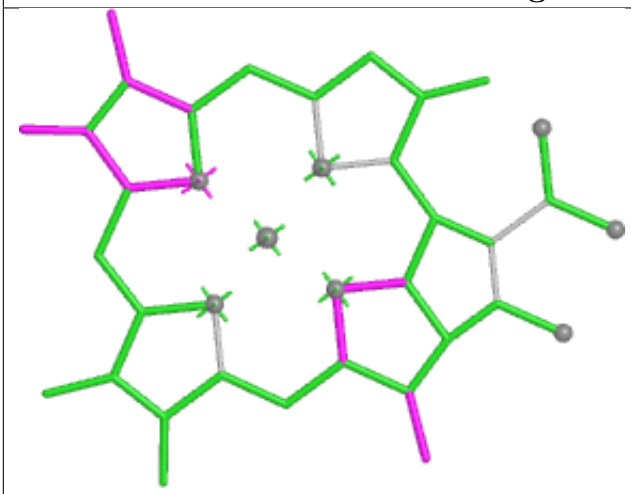


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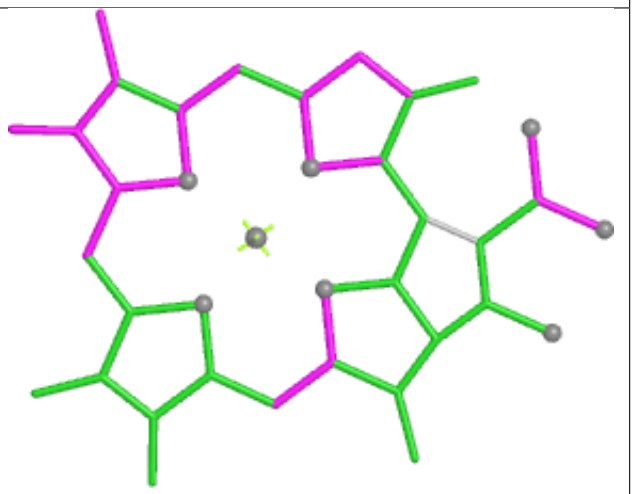


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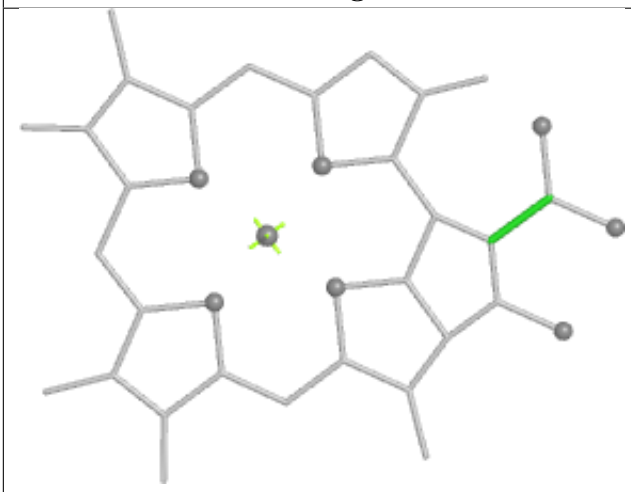
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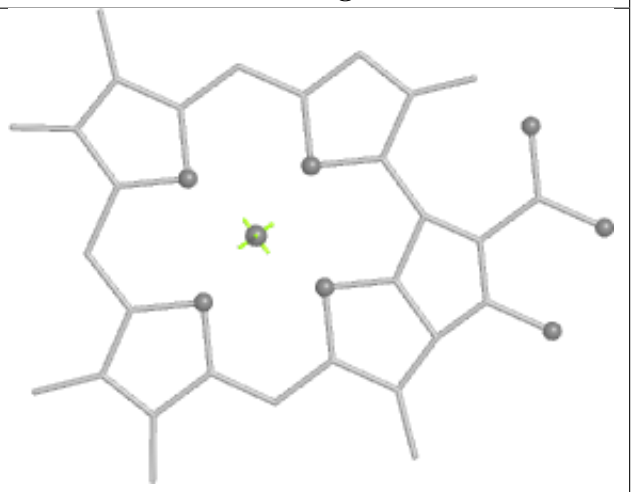
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Bond angles

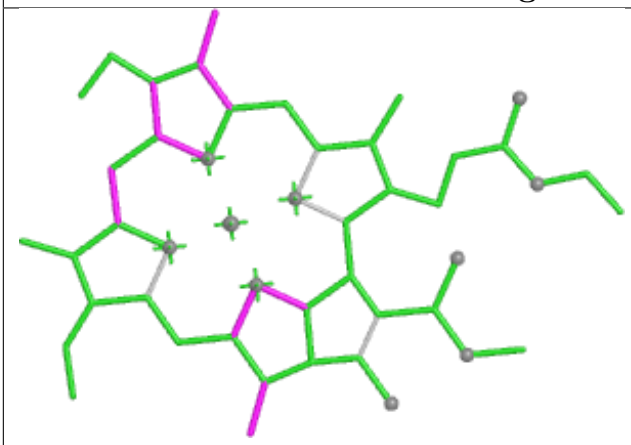


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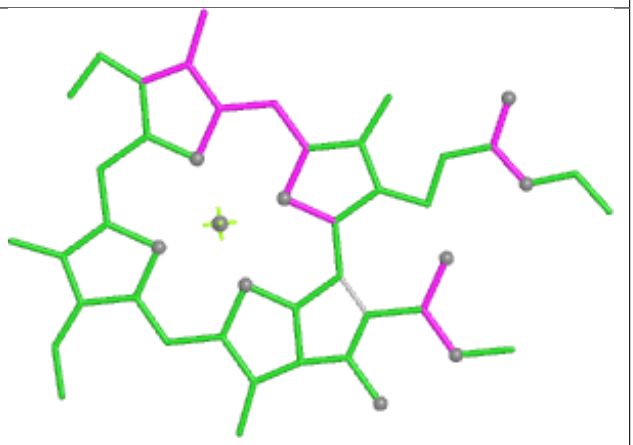


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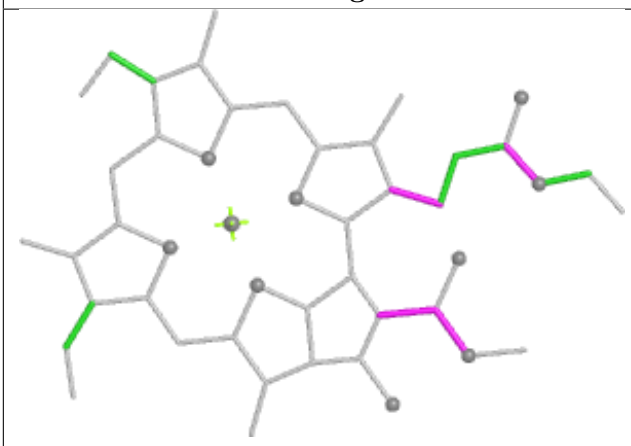
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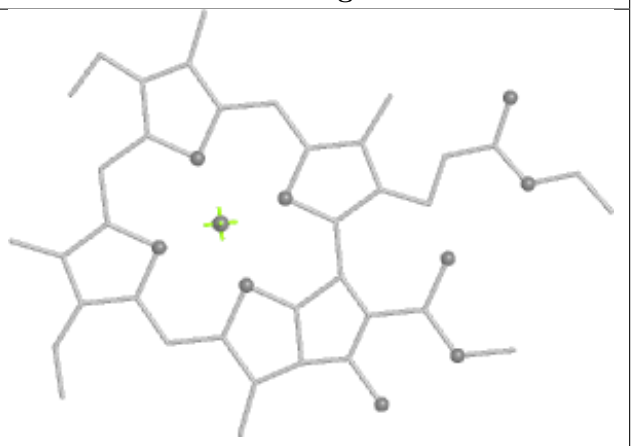
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Bond angles

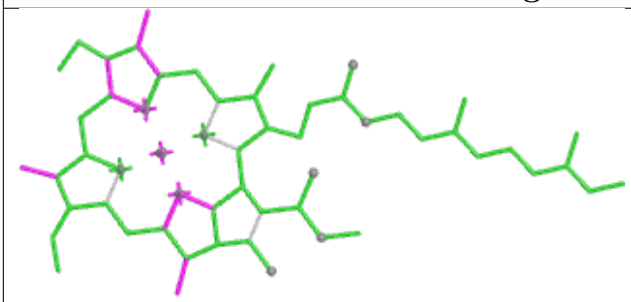


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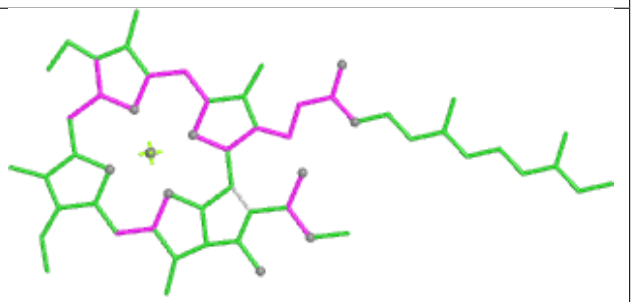


Rings

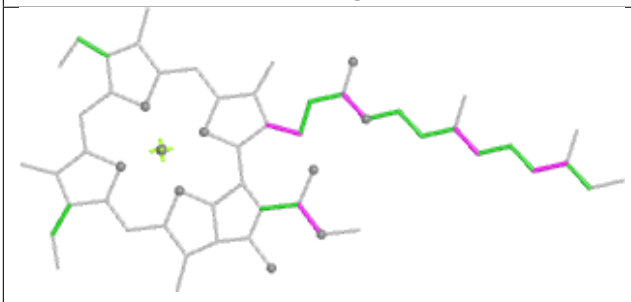
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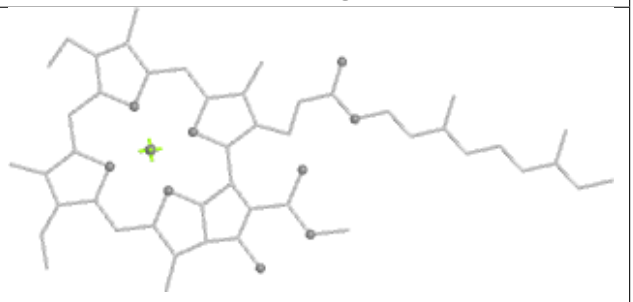
Bond lengths



Bond angles

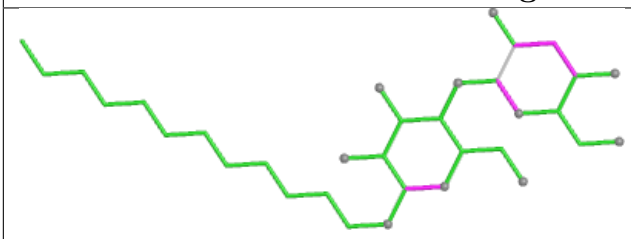


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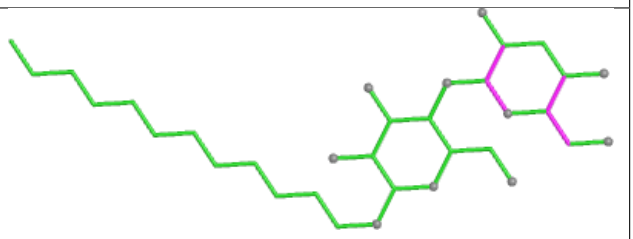


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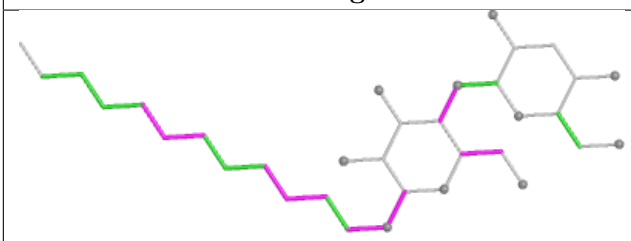
Ligand LMU A 858



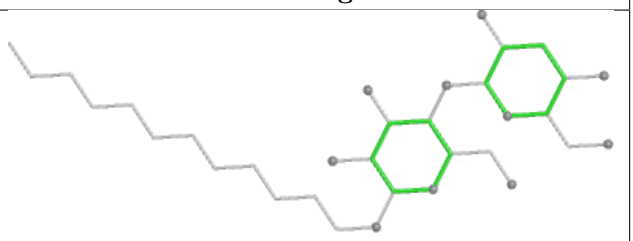
Bond lengths



Bond angles



Torsions

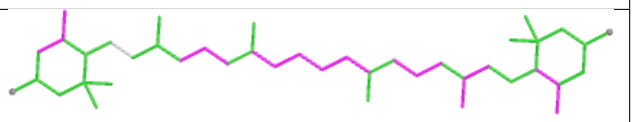


Rings

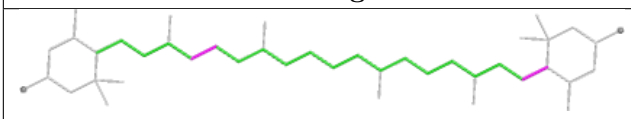
Ligand LUT Z 1621



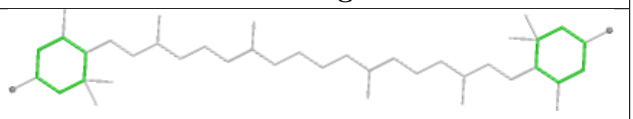
Bond lengths



Bond angles

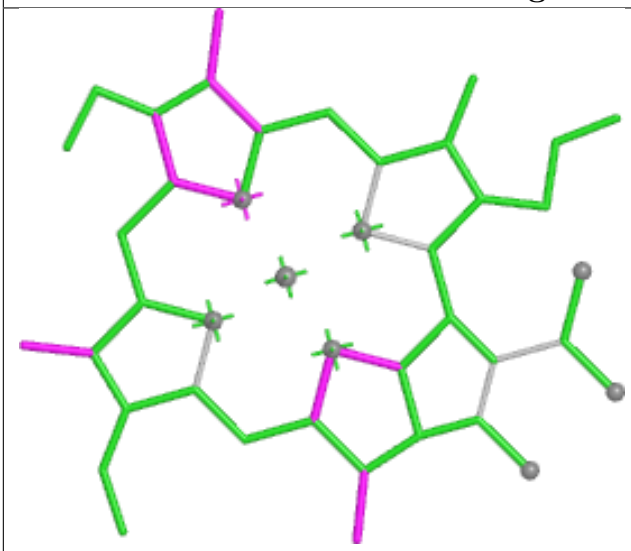


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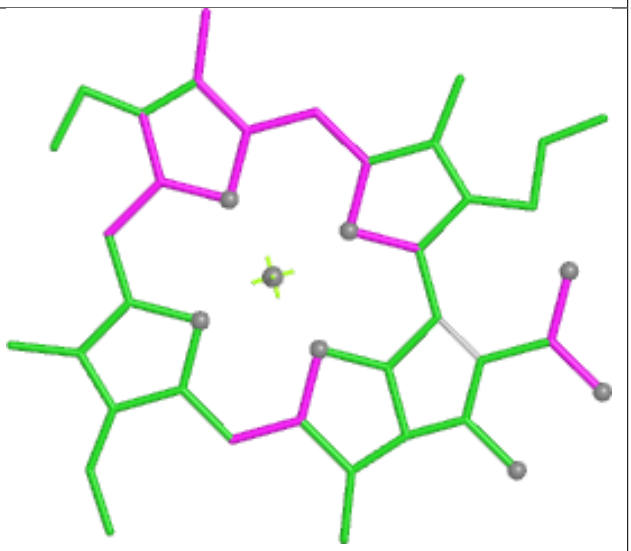


Rings

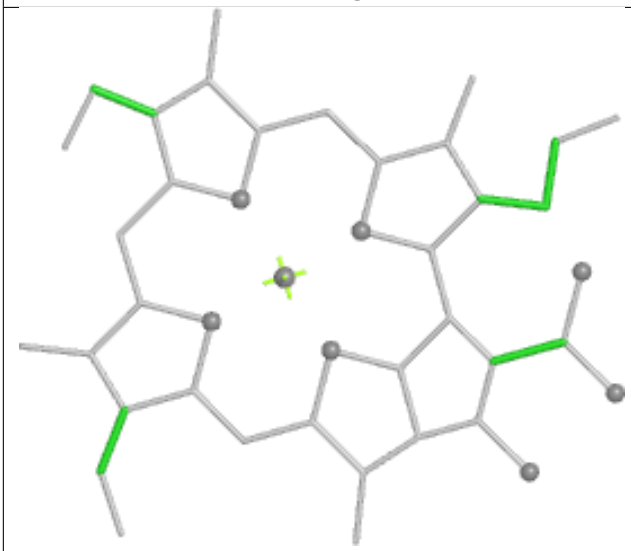
Ligand CLA 2 614



Bond lengths



Bond angles

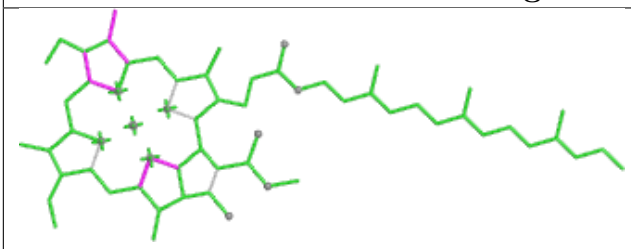


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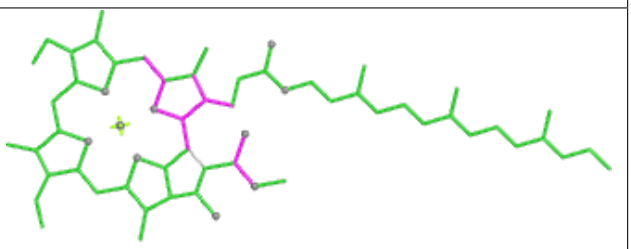


Rings

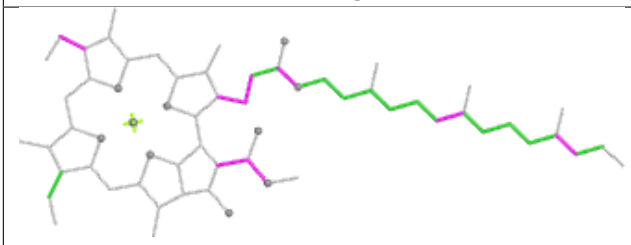
Ligand CLA X 603



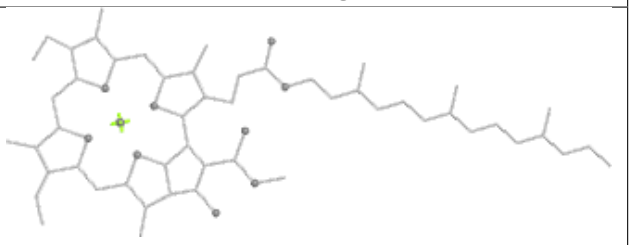
Bond lengths



Bond angles



Torsions

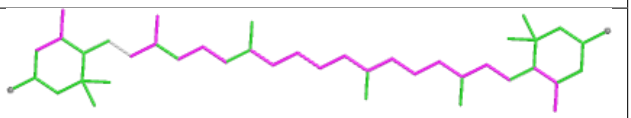


Rings

Ligand LUT V 1620



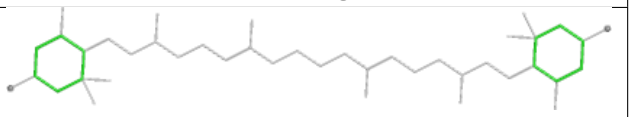
Bond lengths



Bond angles

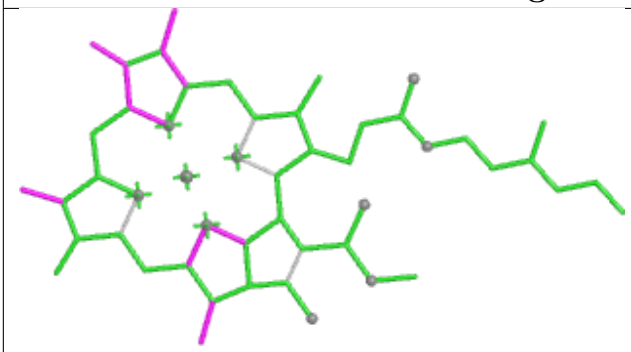


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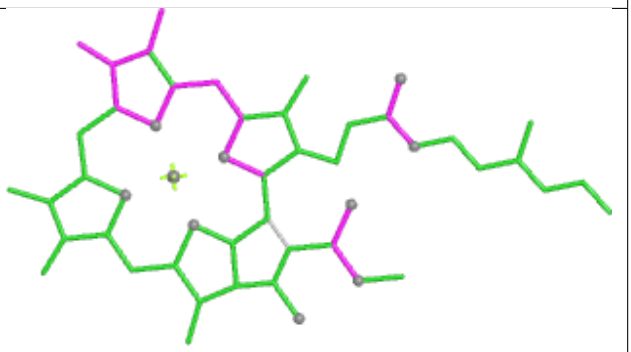


Rings

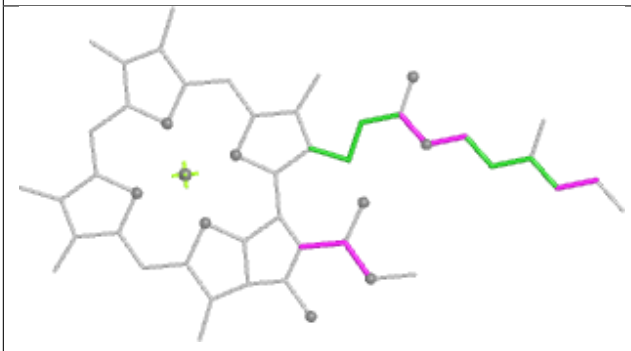
Ligand CLA 9 604



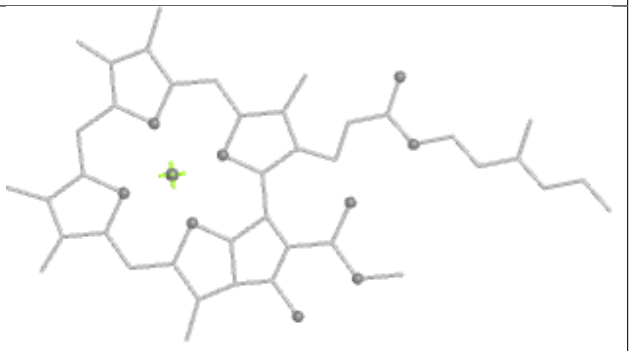
Bond lengths



Bond angles

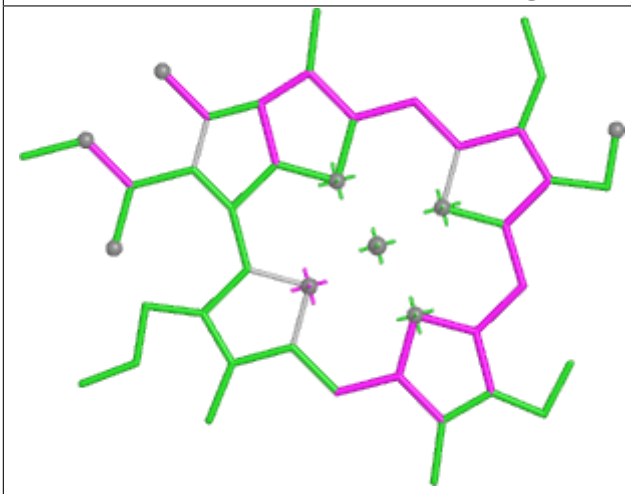


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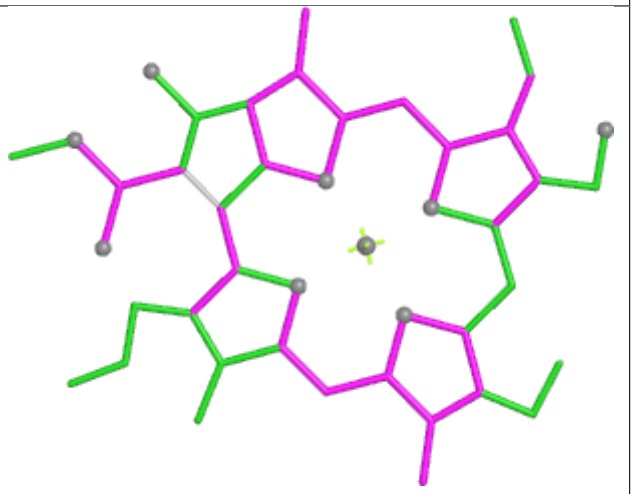


Rings

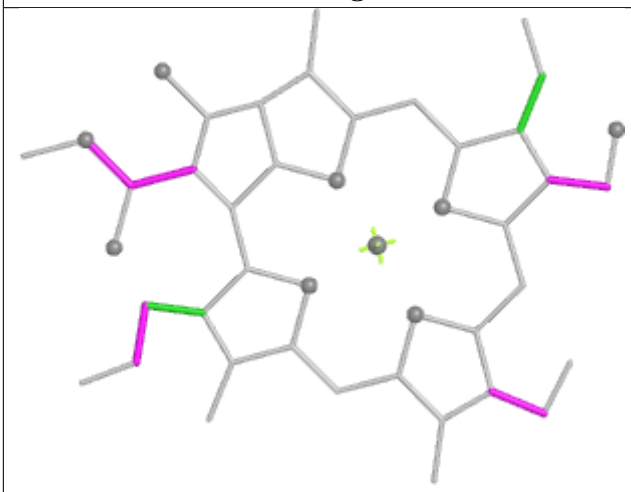
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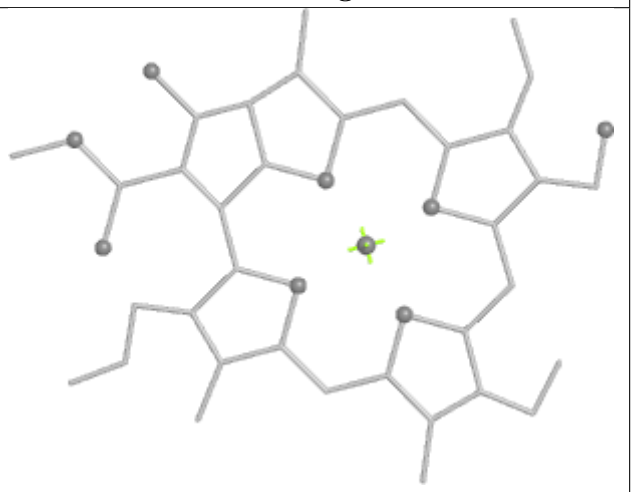
Bond lengths



Bond angles

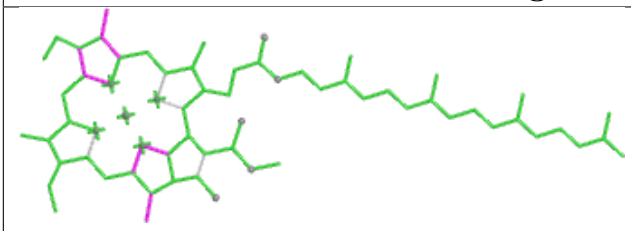


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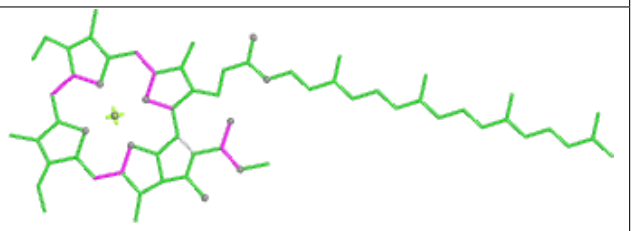


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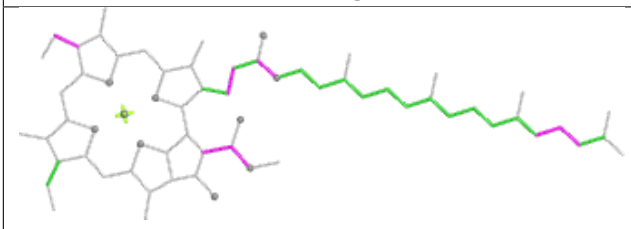
Ligand CLA 2 613



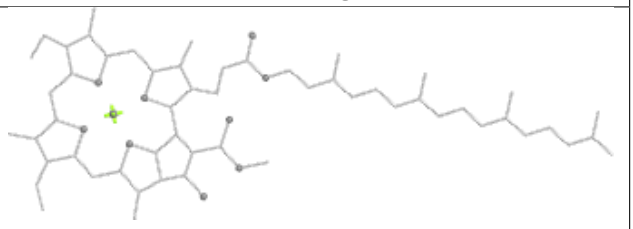
Bond lengths



Bond angles

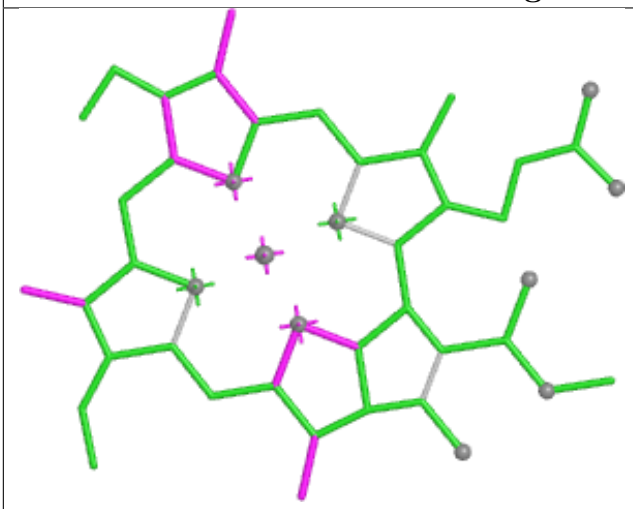


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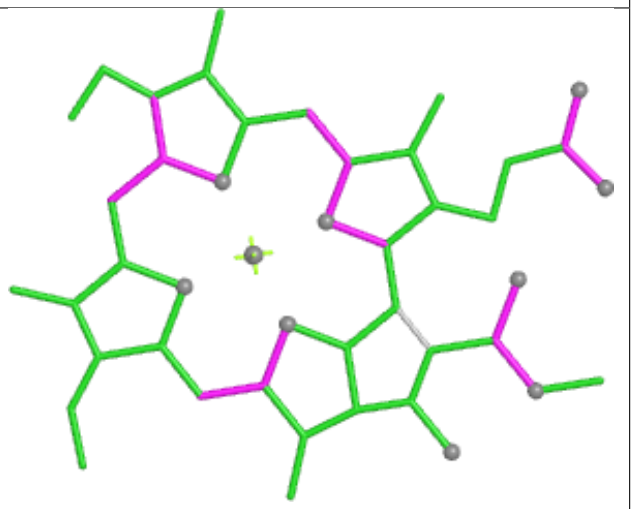


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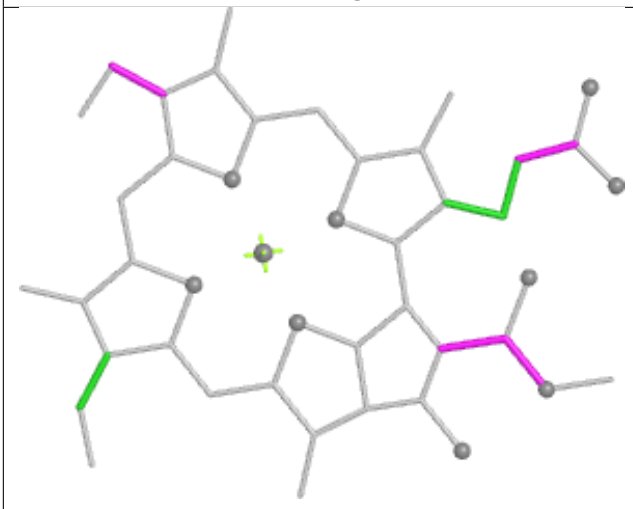
Ligand CLA B 823



Bond lengths



Bond angles

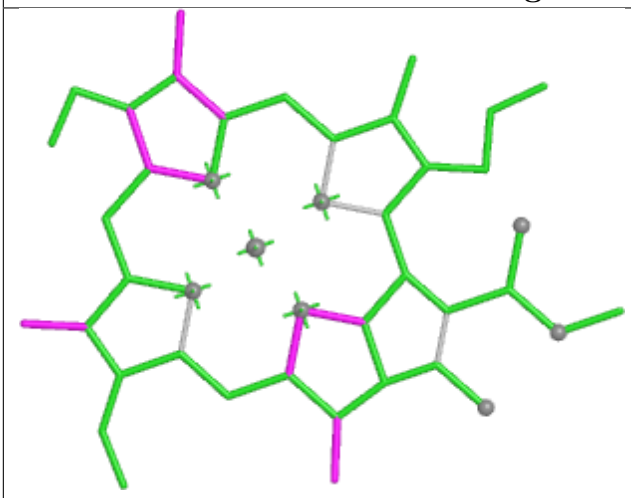


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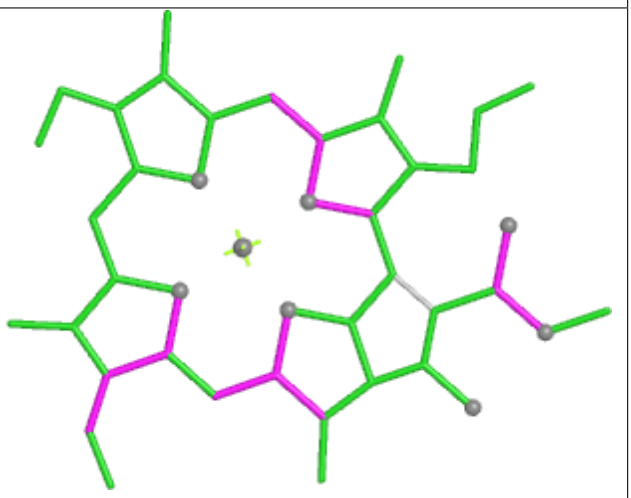


Rings

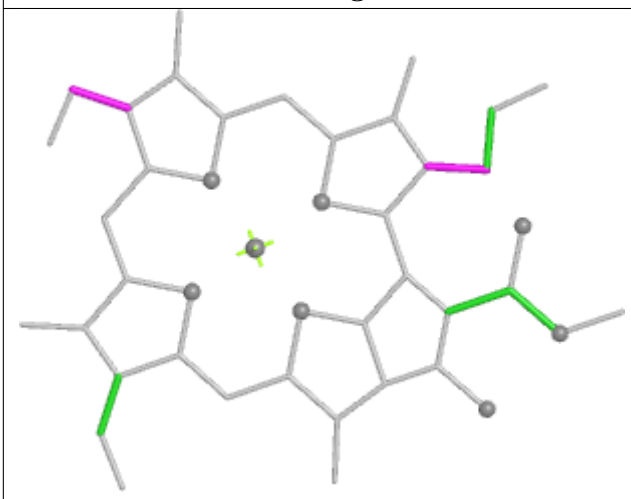
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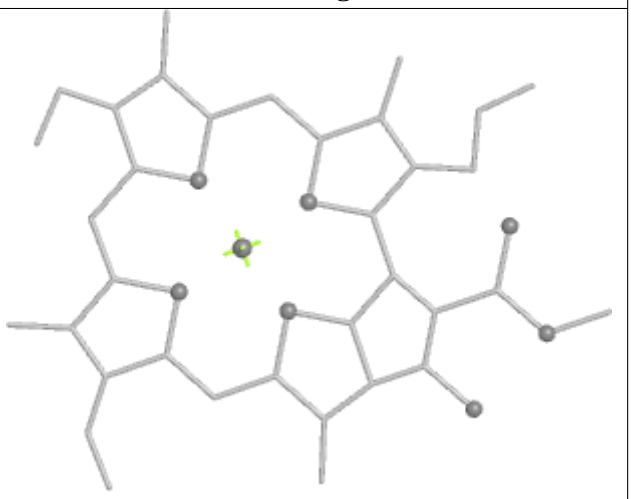
Bond lengths



Bond angles

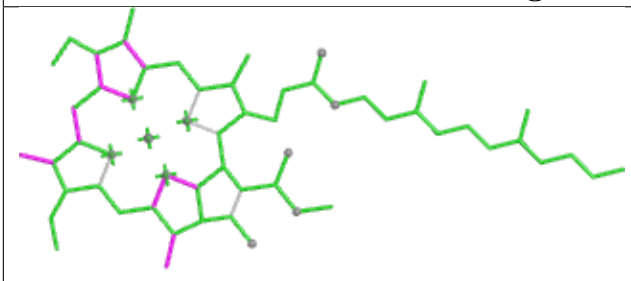


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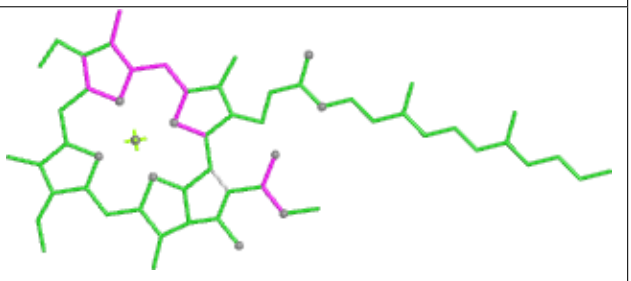


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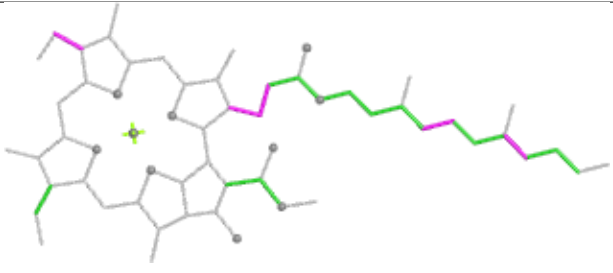
Ligand CLA Z 602



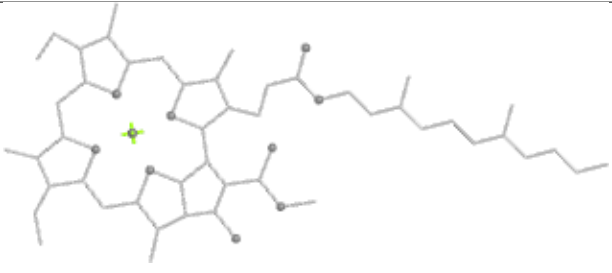
Bond lengths



Bond angles

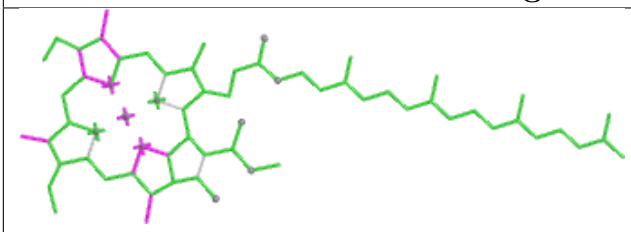


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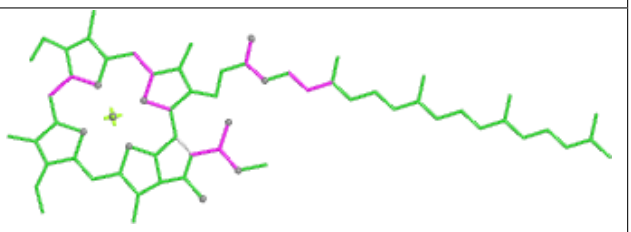


Rings

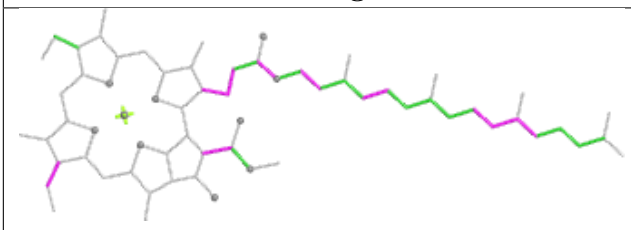
Ligand CLA A 804



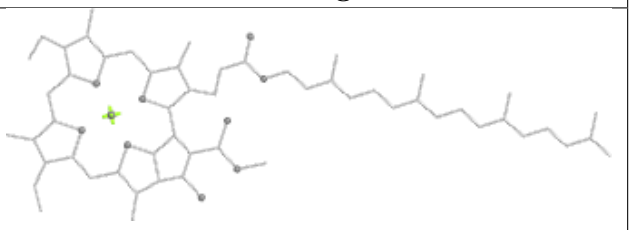
Bond lengths



Bond angles

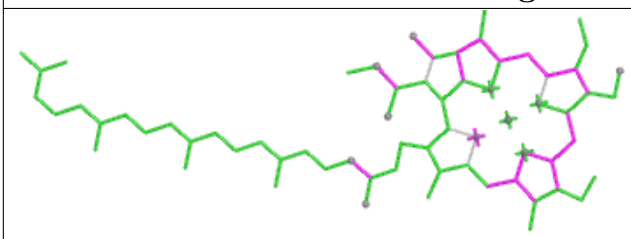


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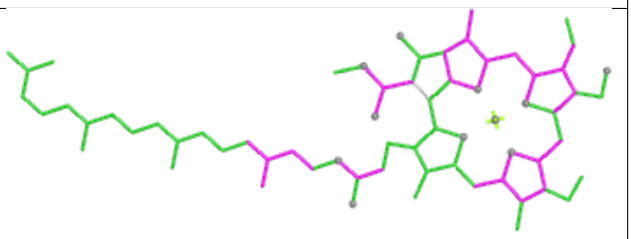


Rings

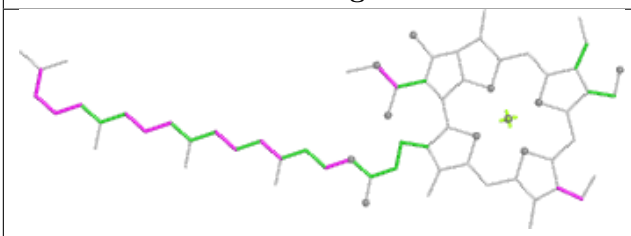
Ligand CHL W 609



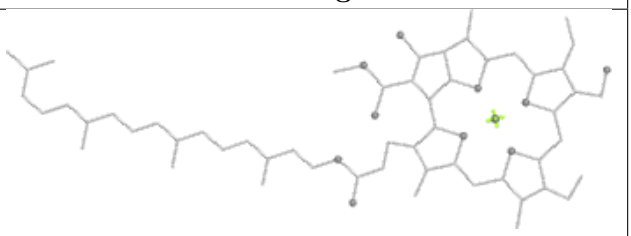
Bond lengths



Bond angles

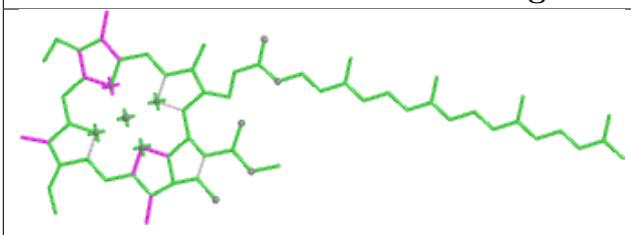


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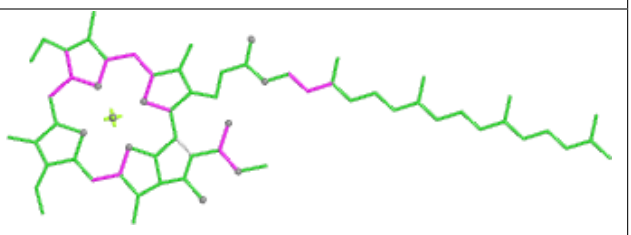


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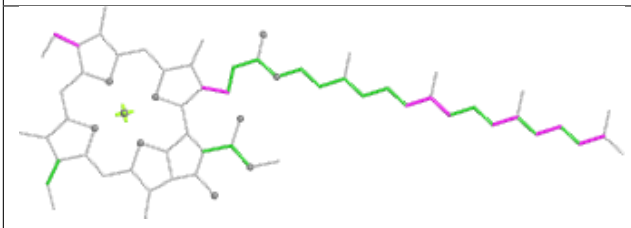
Ligand CLA 5 609



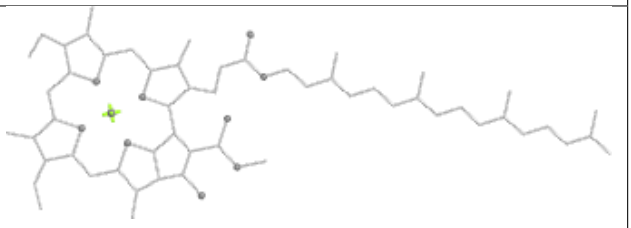
Bond lengths



Bond angles

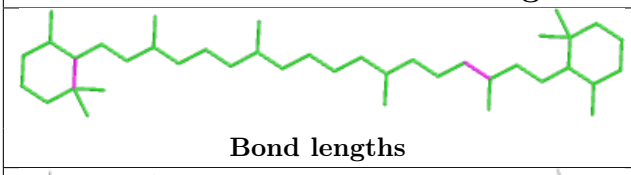


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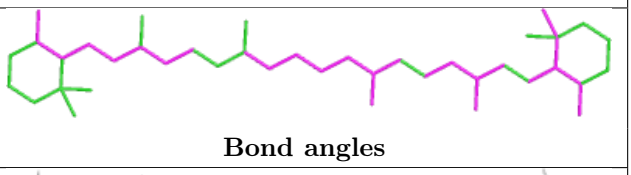


Rings

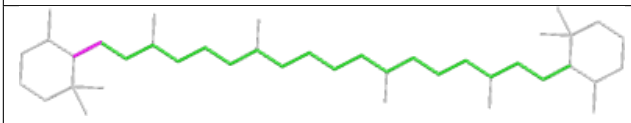
Ligand BCR A 856



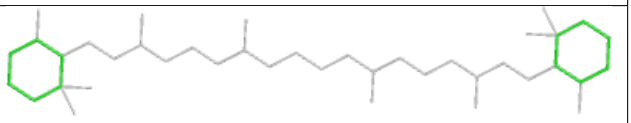
Bond lengths



Bond angles



Torsions



Rings

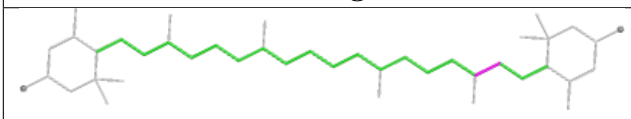
Ligand LUT 7 619



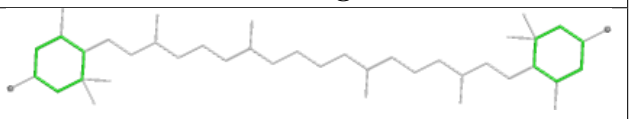
Bond lengths



Bond angles

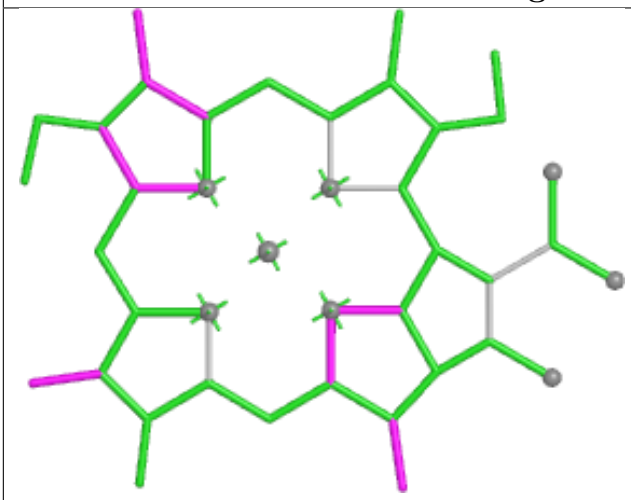


Torsions

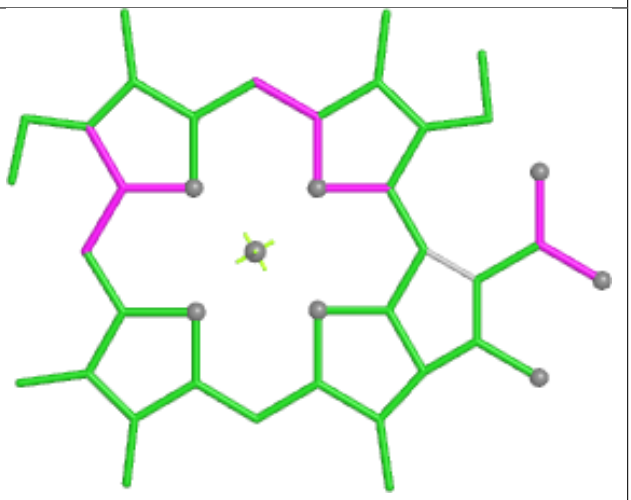


Rings

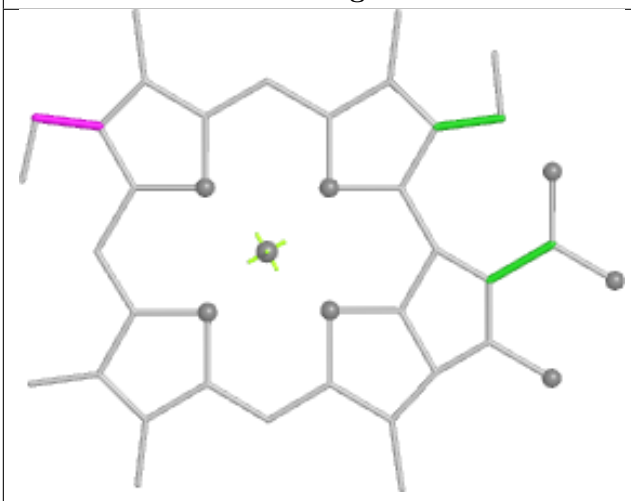
Ligand CLA 6 606



Bond lengths



Bond angles

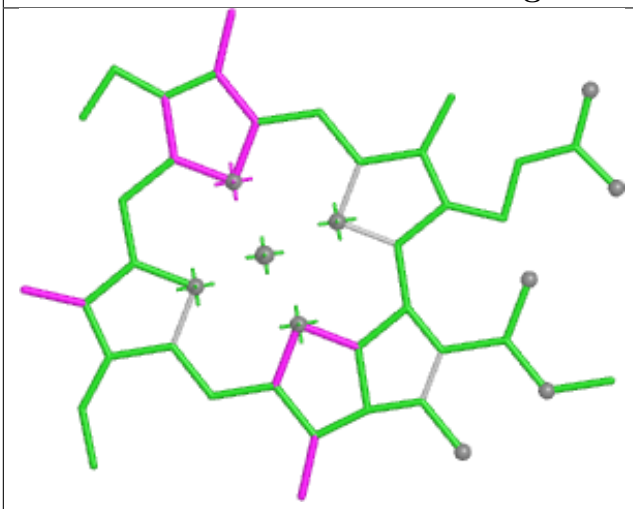


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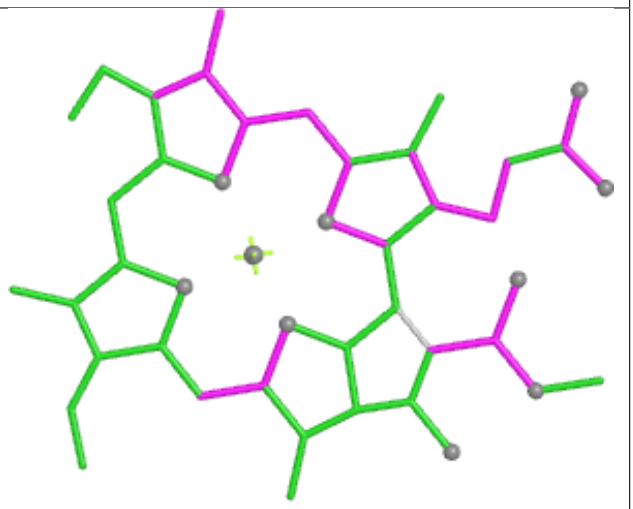


Rings

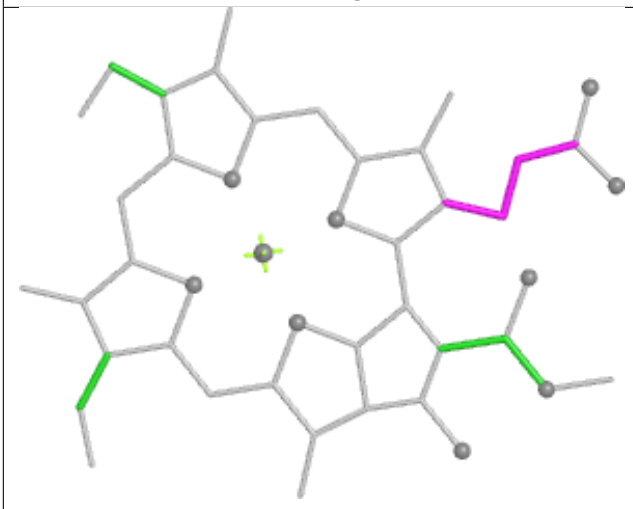
Ligand CLA A 833



Bond lengths



Bond angles

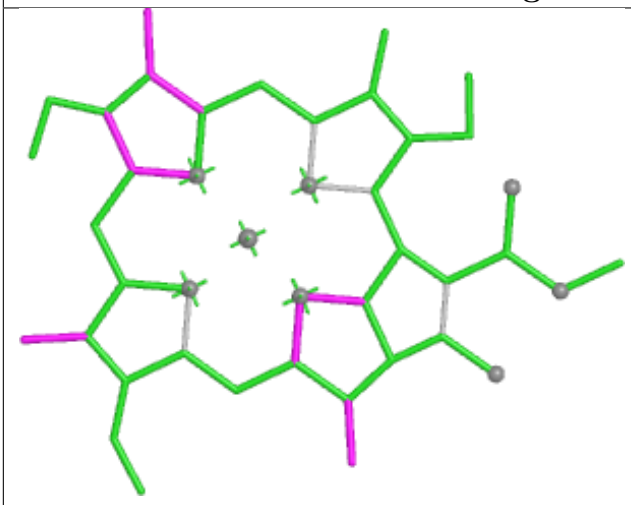


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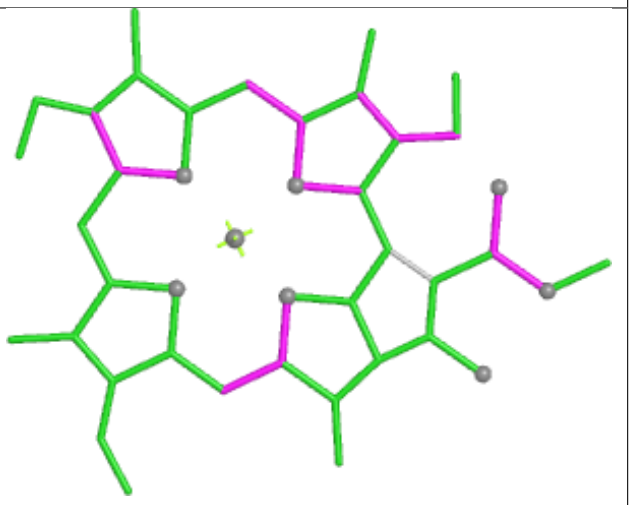


Rings

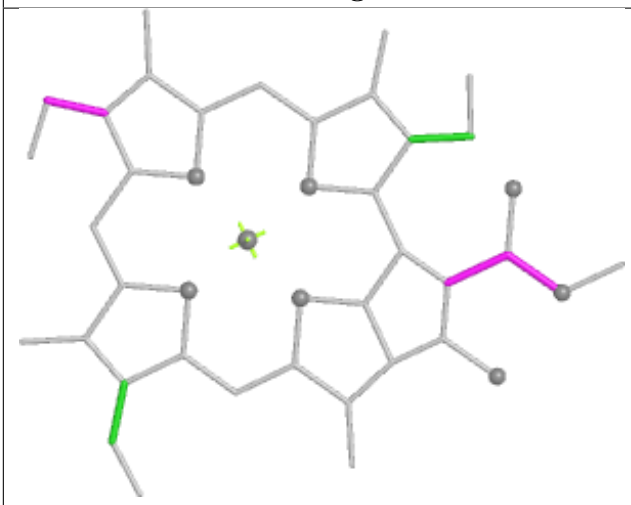
Ligand CLA G 203



Bond lengths



Bond angles

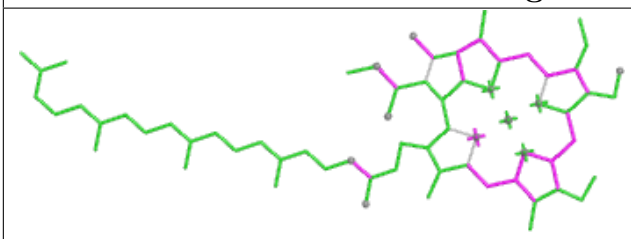


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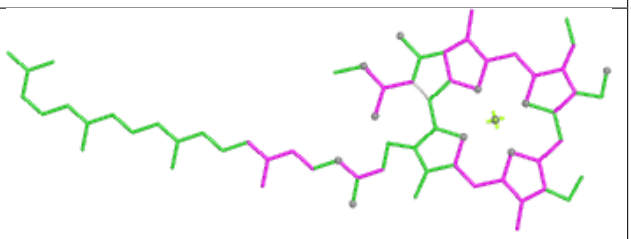


Rings

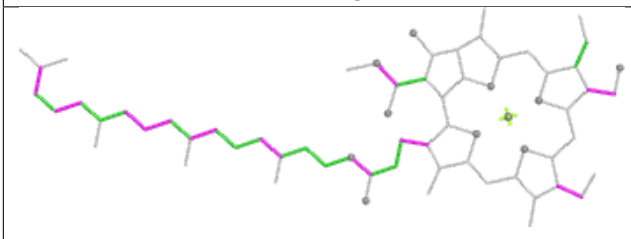
Ligand CHL Z 609



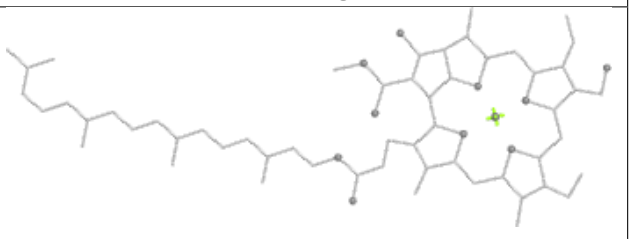
Bond lengths



Bond angles

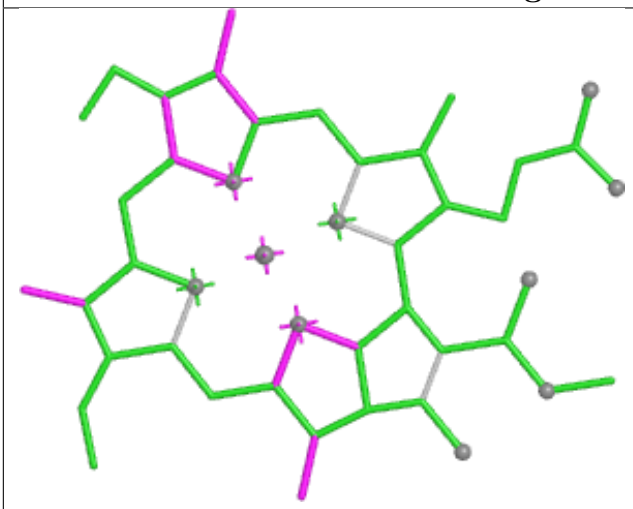


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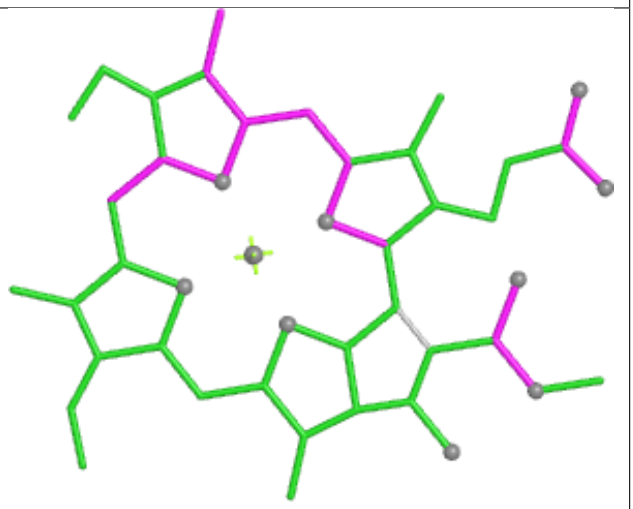


Rings

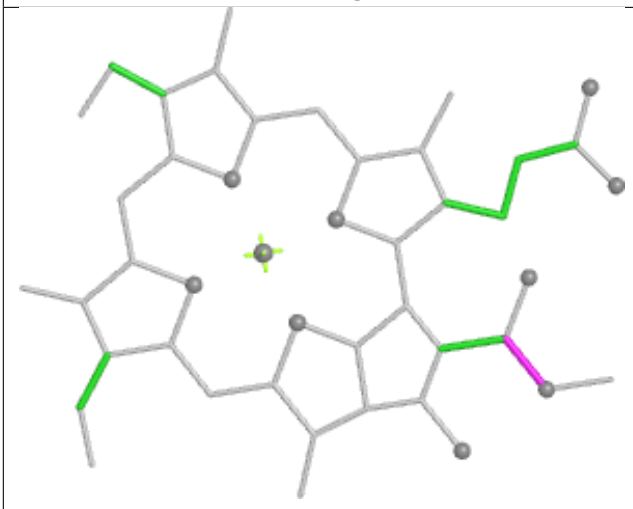
Ligand CLA B 835



Bond lengths



Bond angles

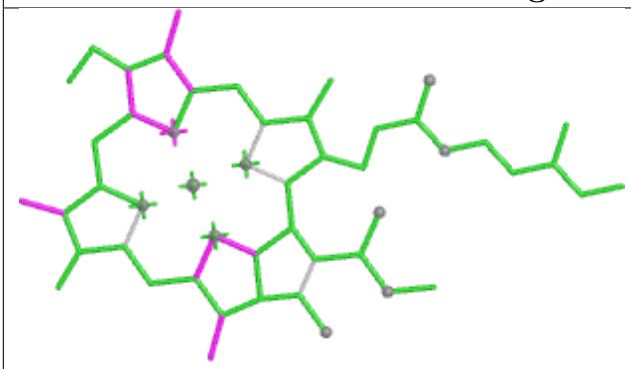


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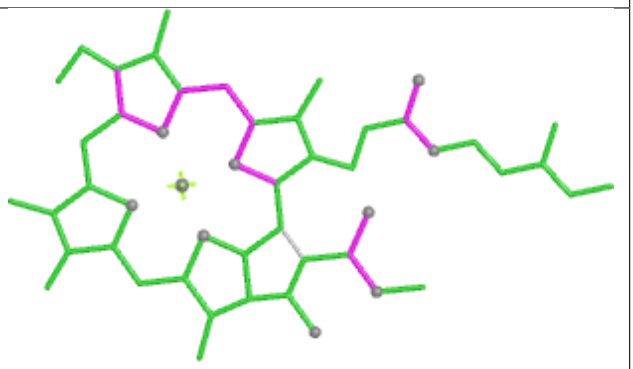


Rings

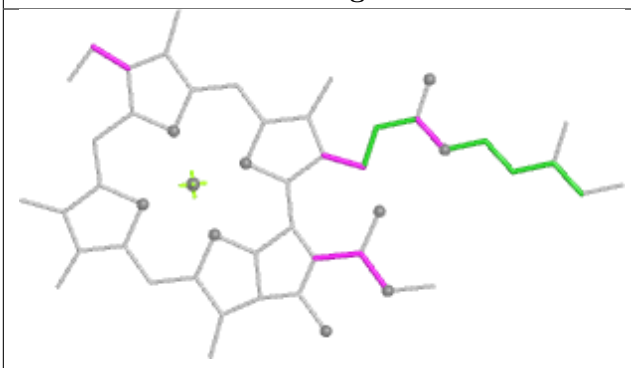
Ligand CLA 7 604



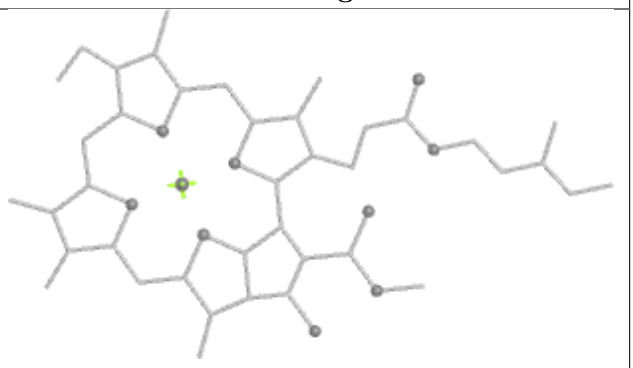
Bond lengths



Bond angles

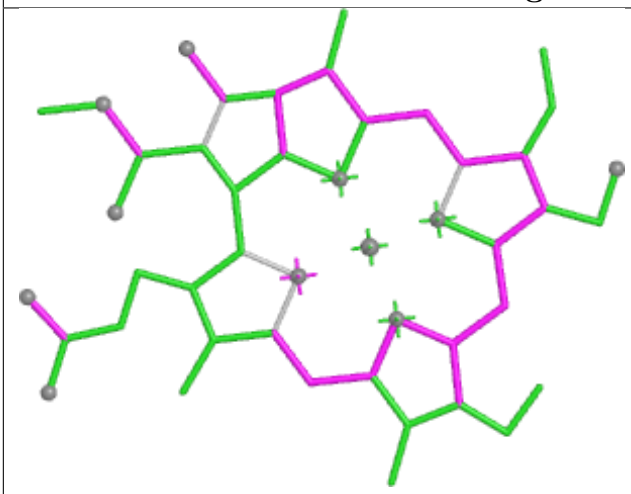


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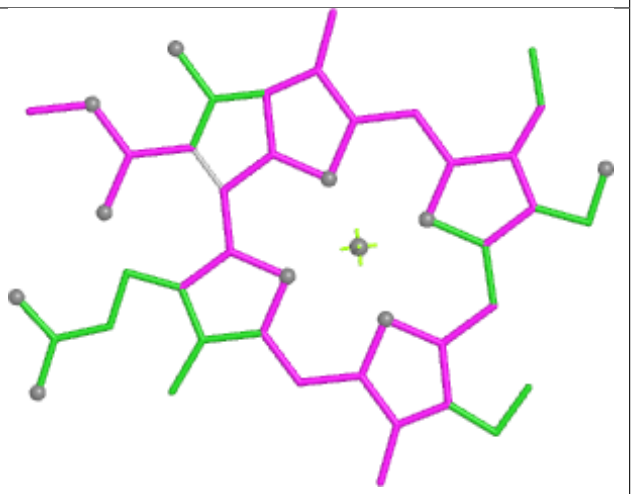


Rings

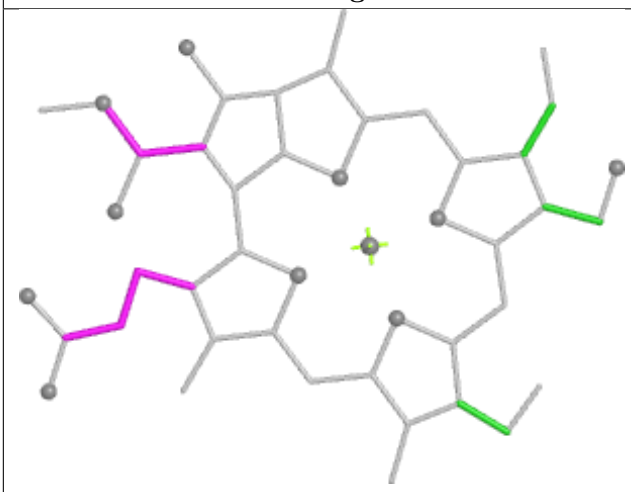
Ligand CHL Z 606



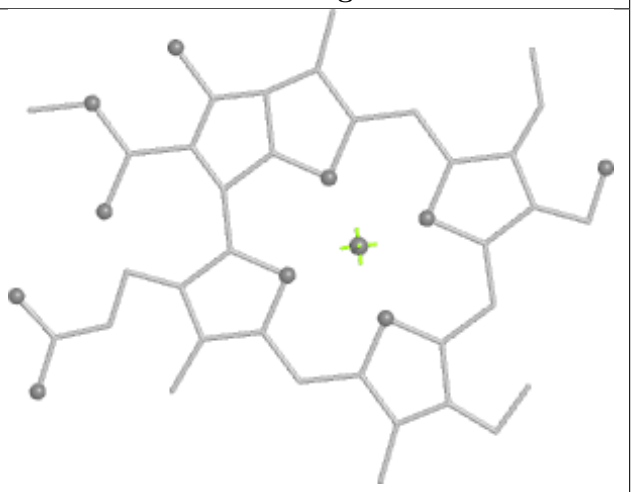
Bond lengths



Bond angles

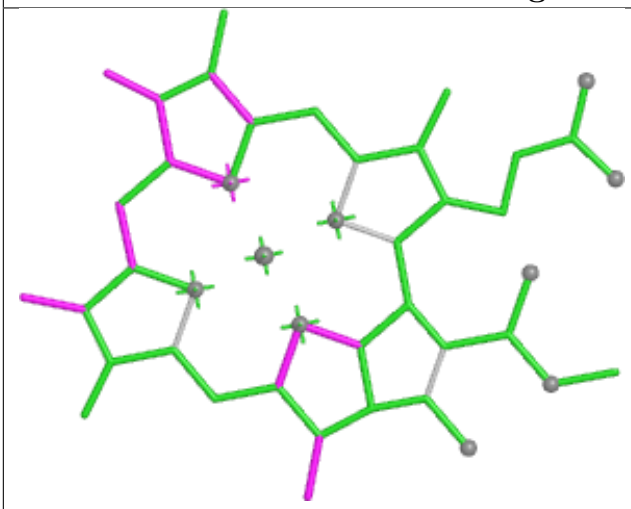


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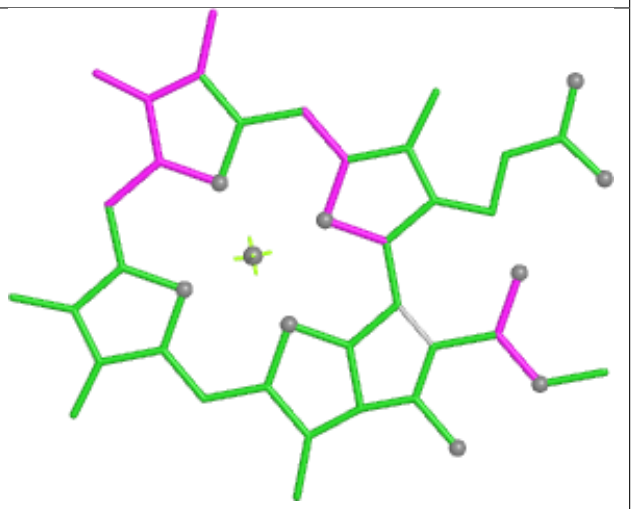


Rings

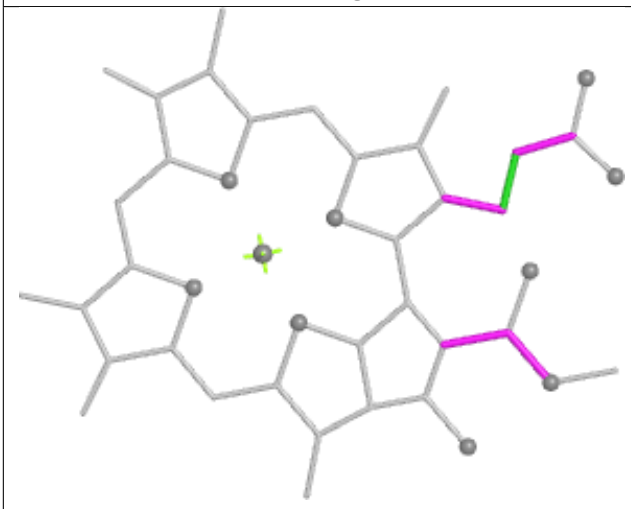
Ligand CLA 7 616



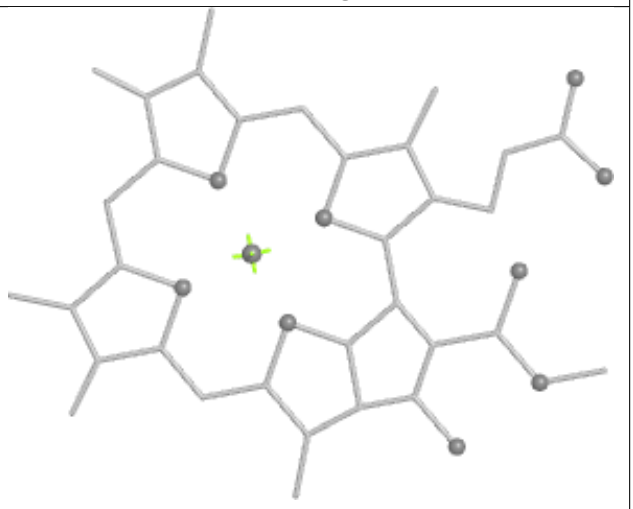
Bond lengths



Bond angles

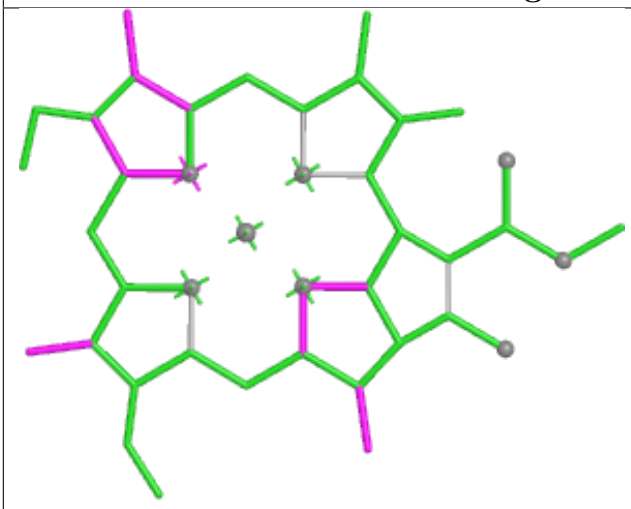


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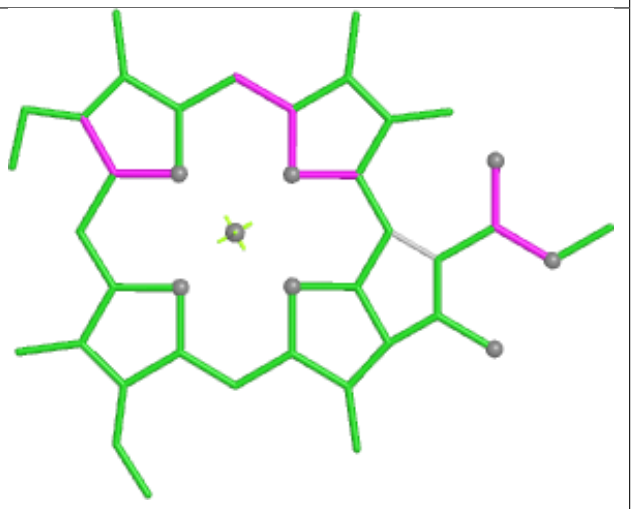


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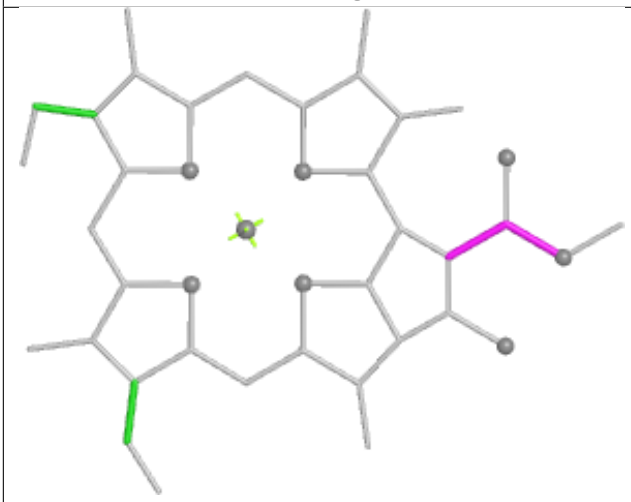
Ligand CLA B 804



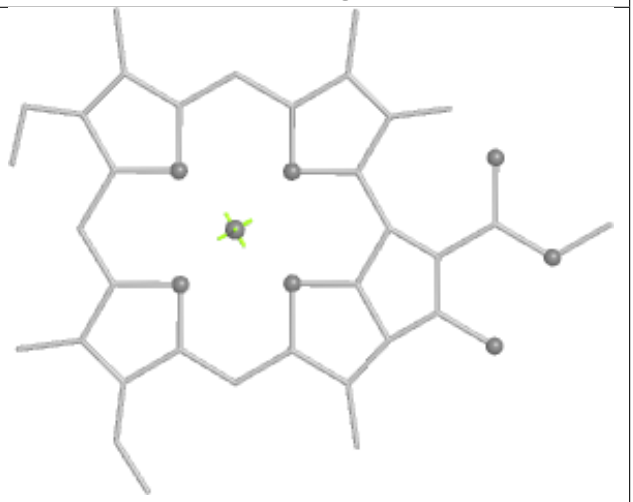
Bond lengths



Bond angles

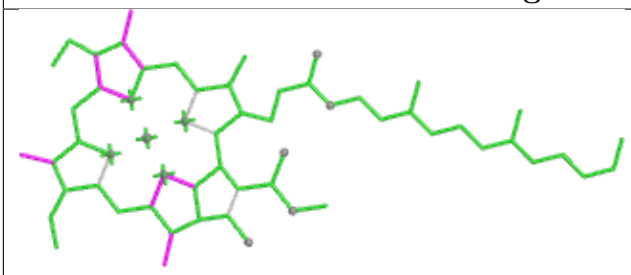


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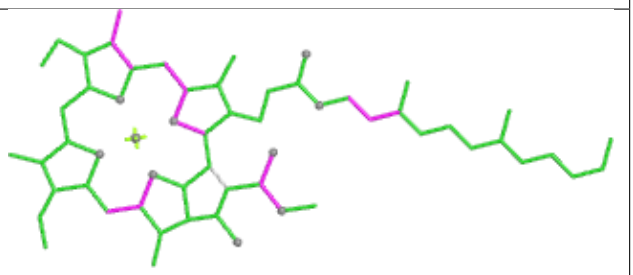


Rings

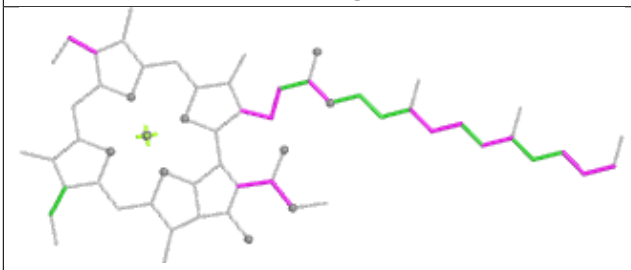
Ligand CLA U 602



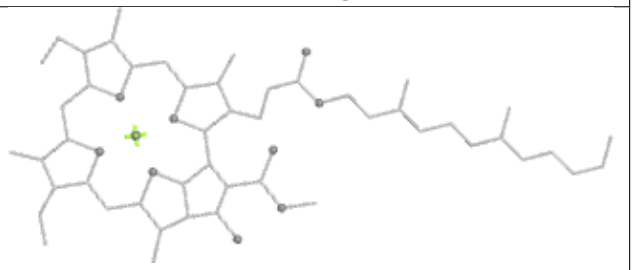
Bond lengths



Bond angles

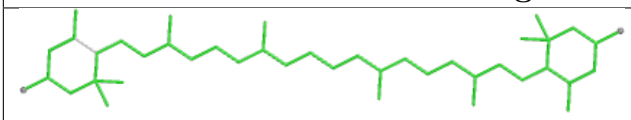


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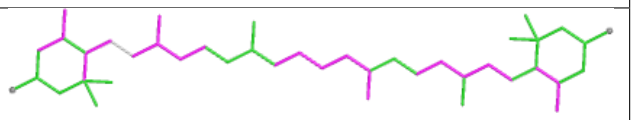


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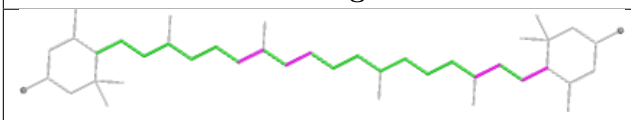
Ligand LUT U 1620



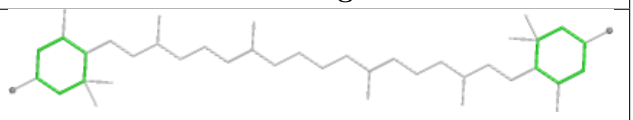
Bond lengths



Bond angles



Torsions

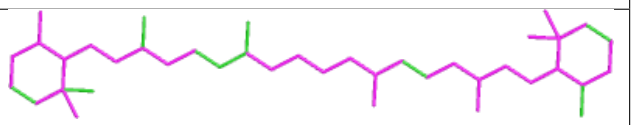


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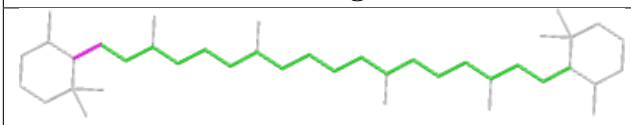
Ligand BCR A 851



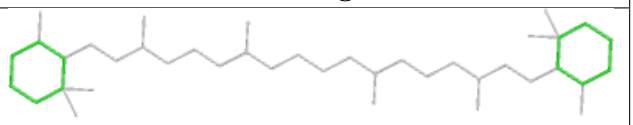
Bond lengths



Bond angles

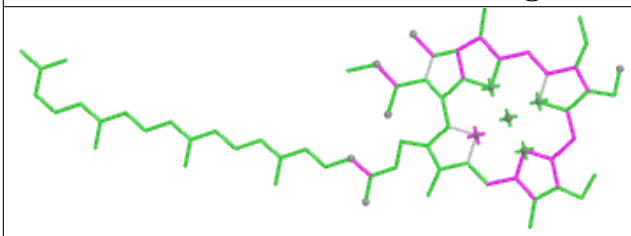


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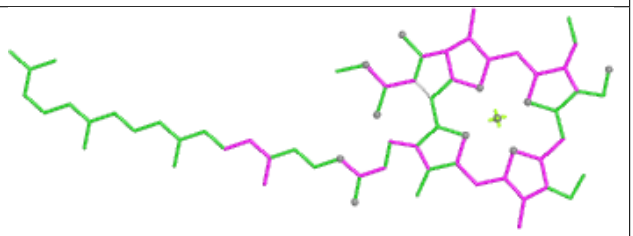


Rings

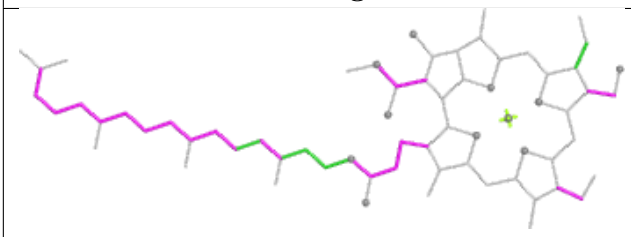
Ligand CHL X 607



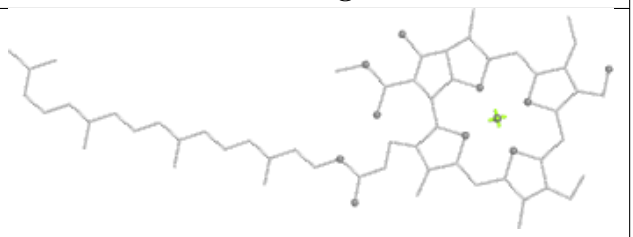
Bond lengths



Bond angles

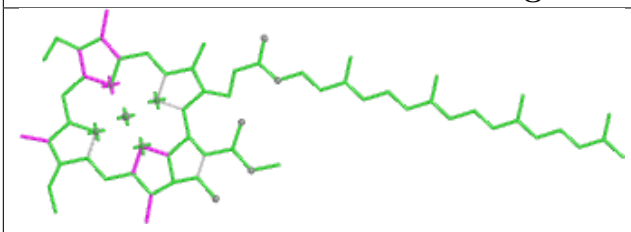


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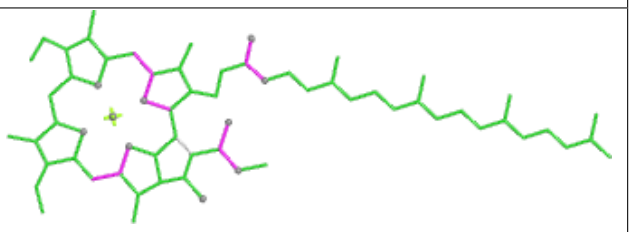


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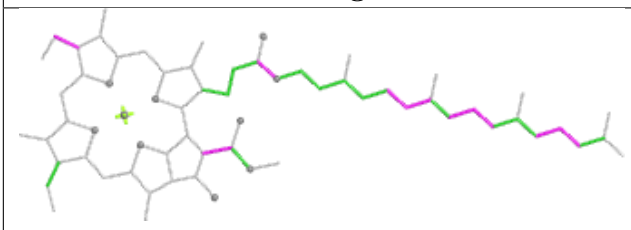
Ligand CLA B 833



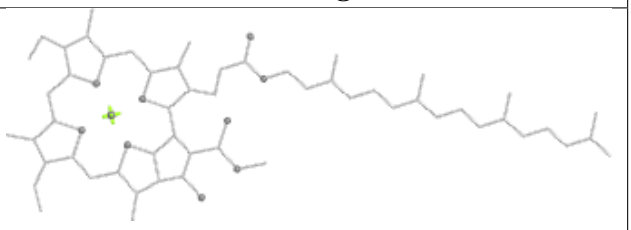
Bond lengths



Bond angles

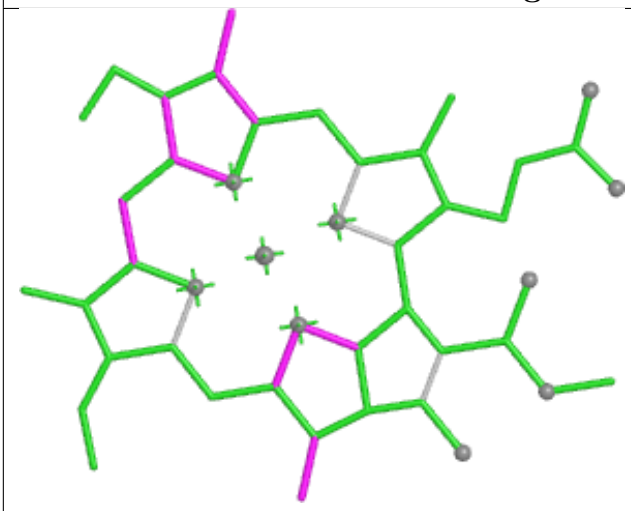


Torsions

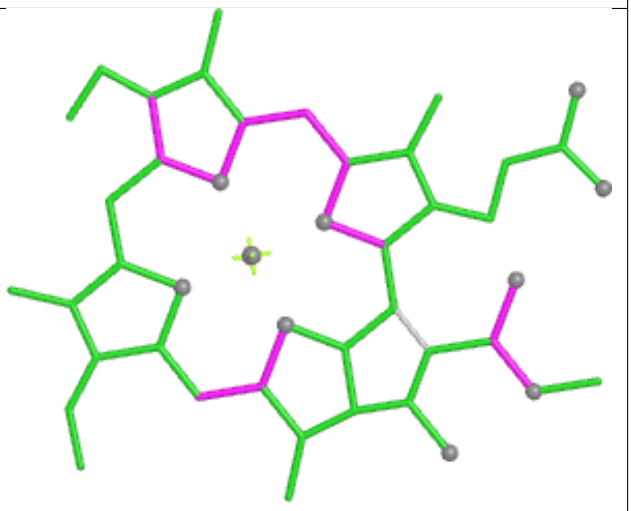


Rings

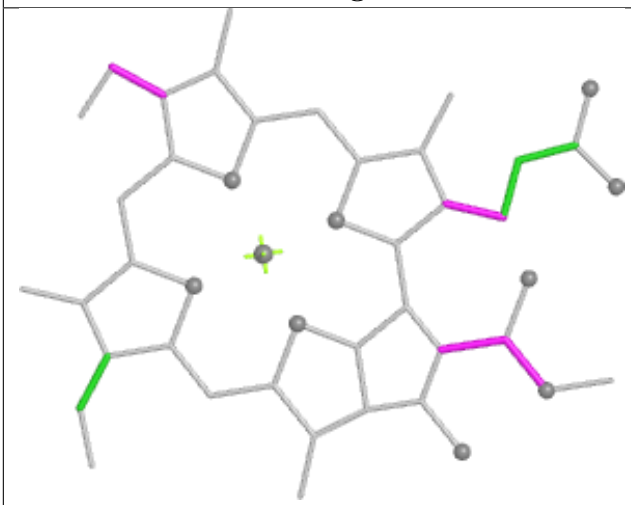
Ligand CLA V 614



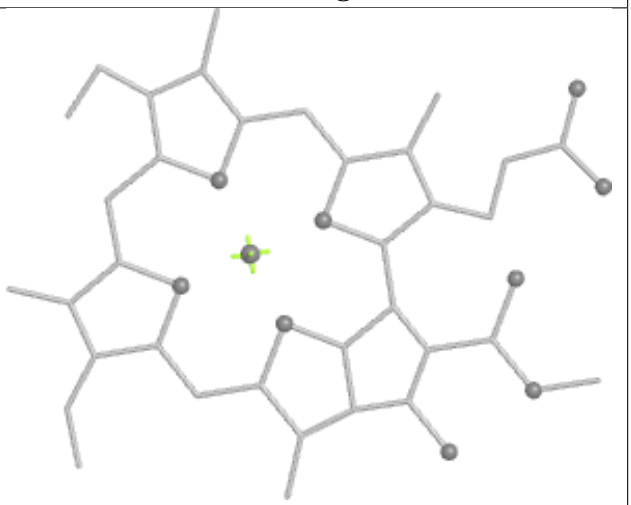
Bond lengths



Bond angles

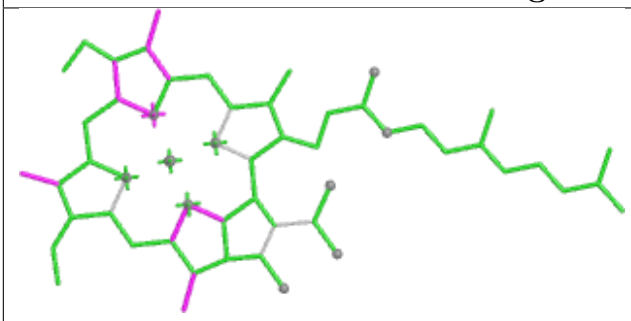


Torsions

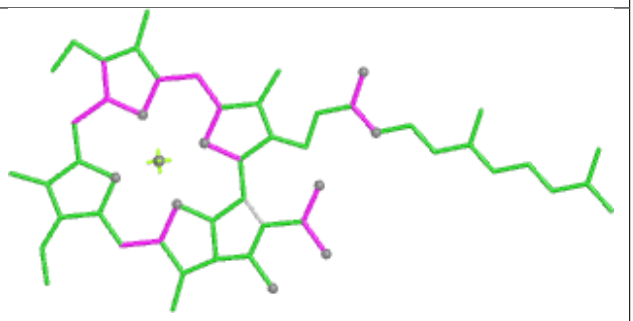


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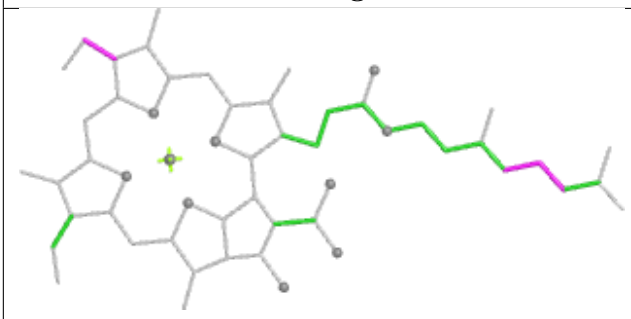
Ligand CLA a 601



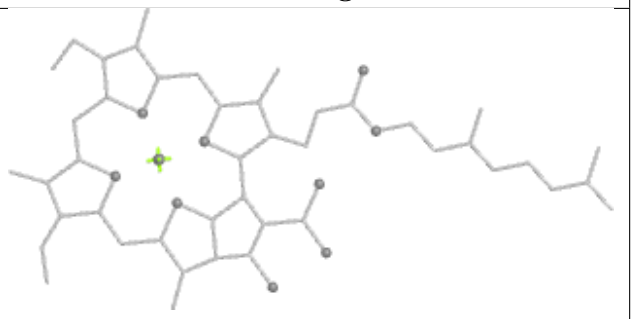
Bond lengths



Bond angles

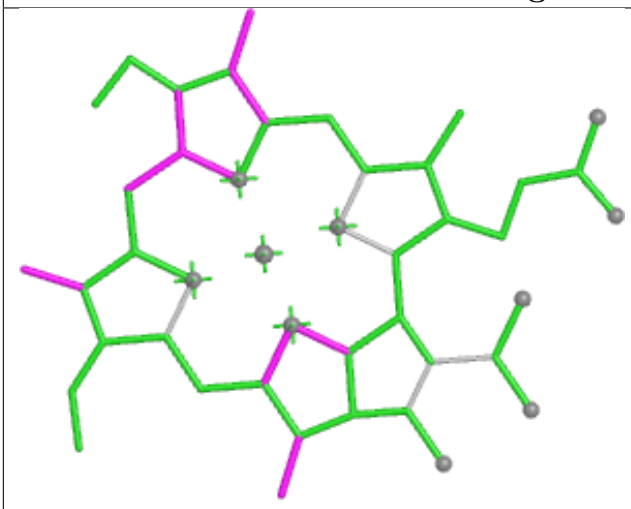


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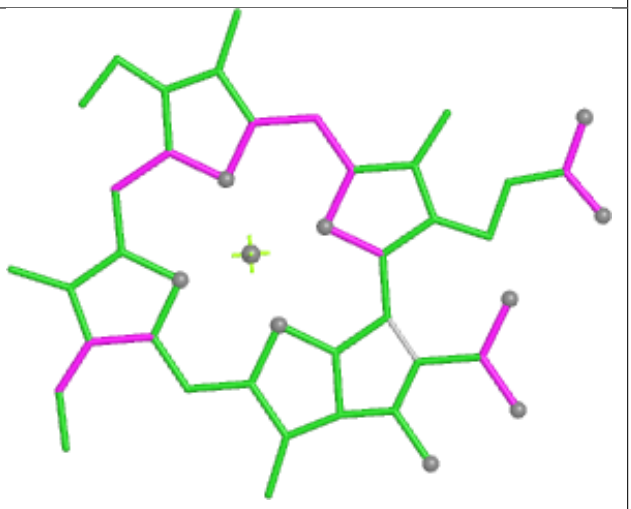


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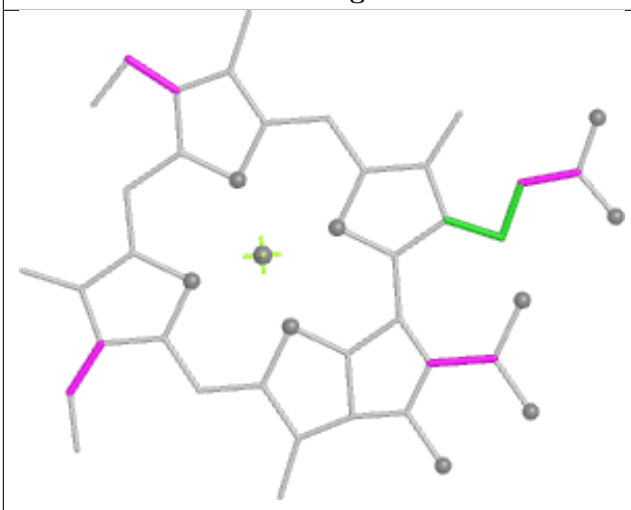
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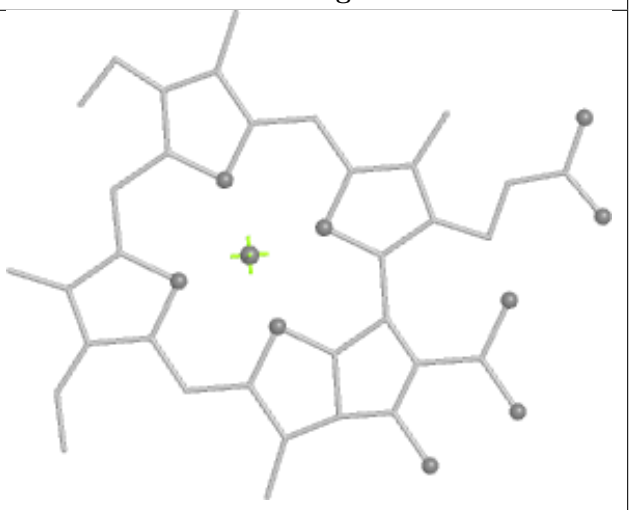
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Bond angles

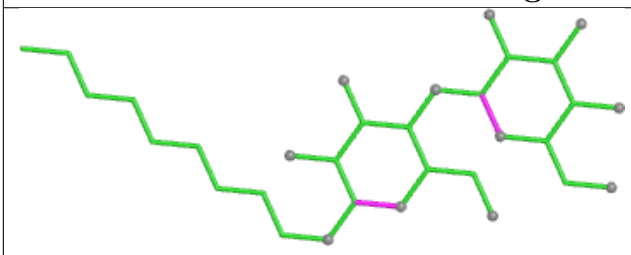


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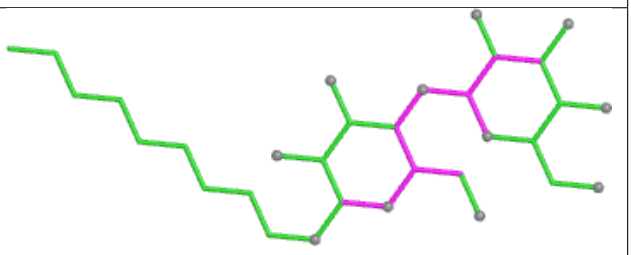


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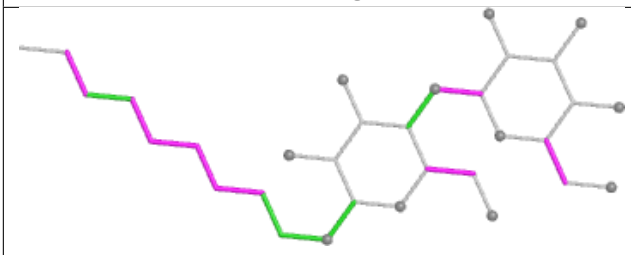
Ligand LMU 5 629



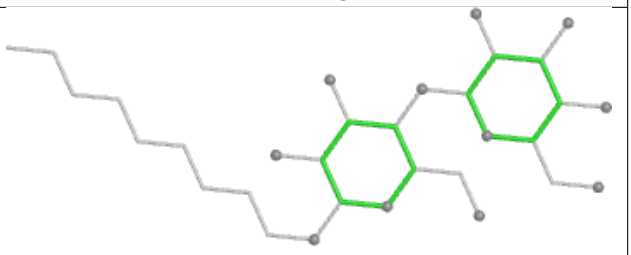
Bond lengths



Bond angles

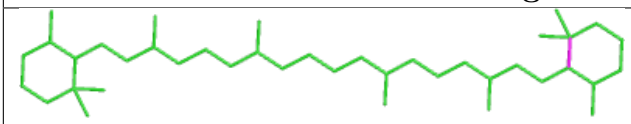


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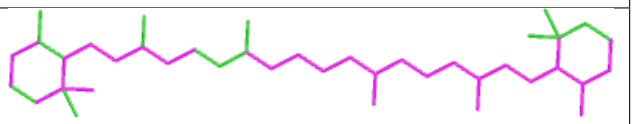


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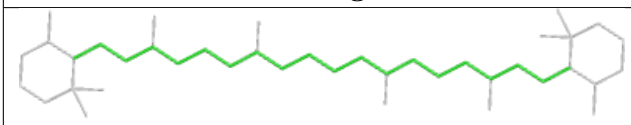
Ligand BCR B 846



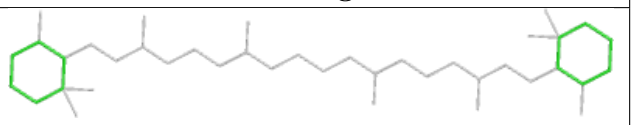
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Bond angles

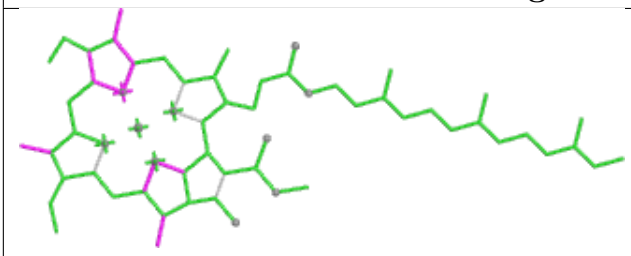


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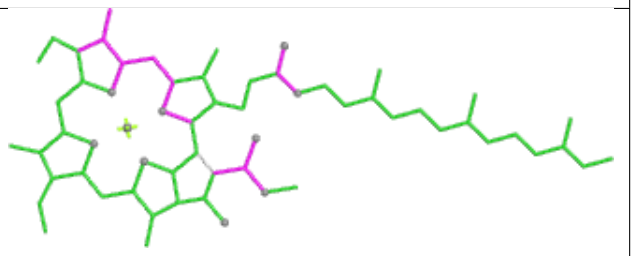


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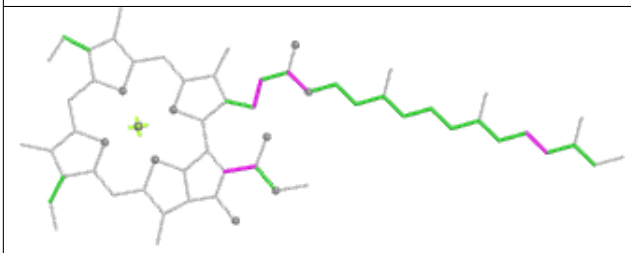
Ligand CLA 1 602



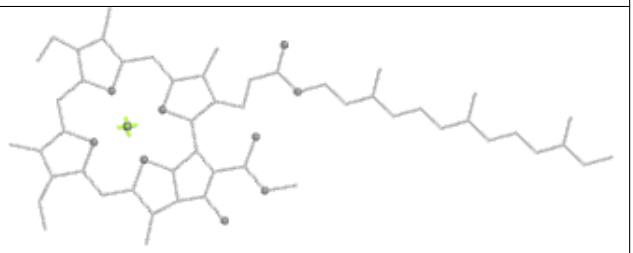
Bond lengths



Bond angles

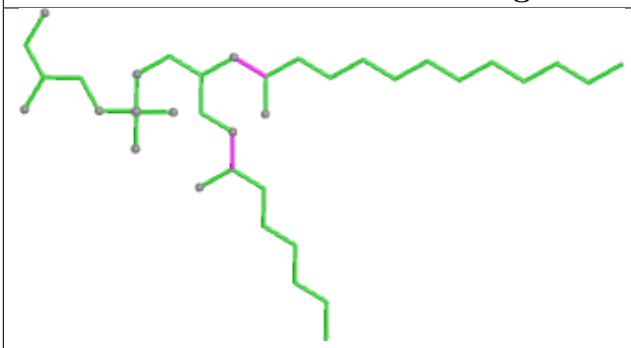


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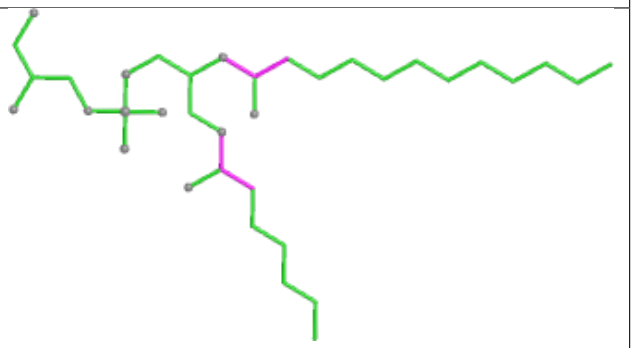


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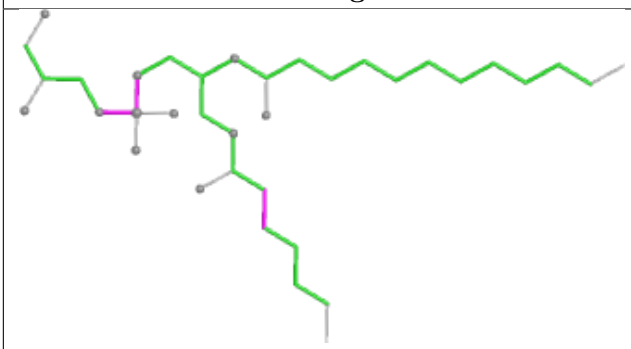
Ligand LHG V 2630



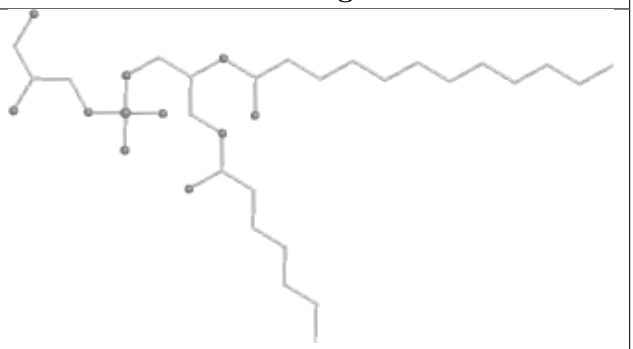
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Bond angles

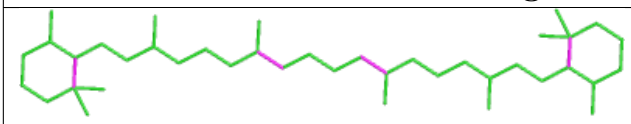


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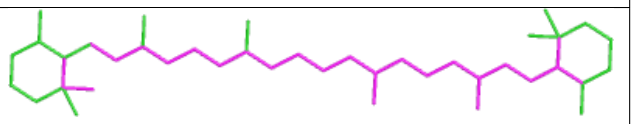


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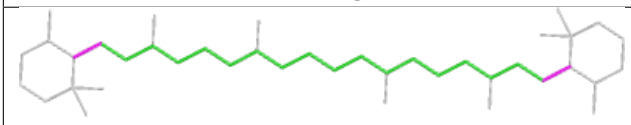
Ligand BCR B 843



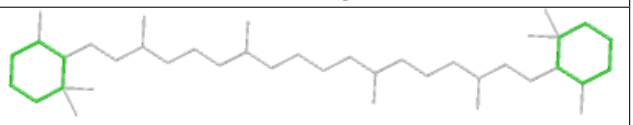
Bond lengths



Bond angles

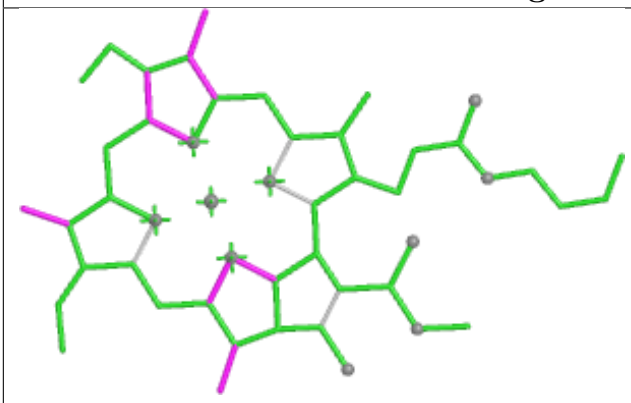


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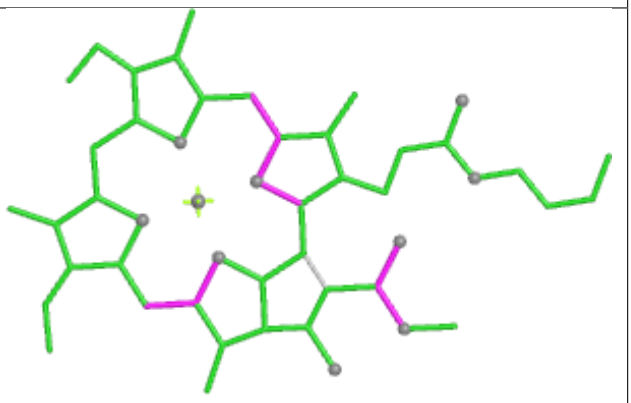


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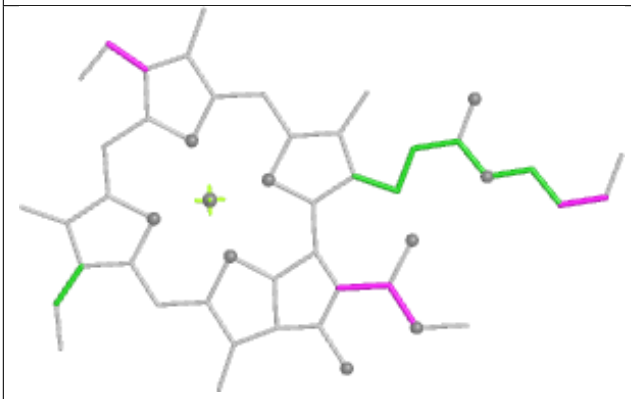
Ligand CLA a 604



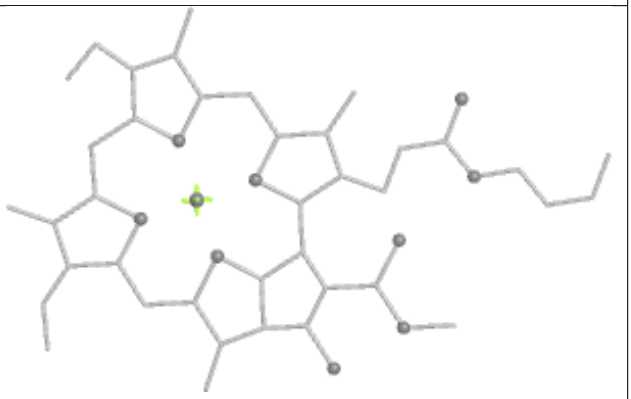
Bond lengths



Bond angles



Torsions

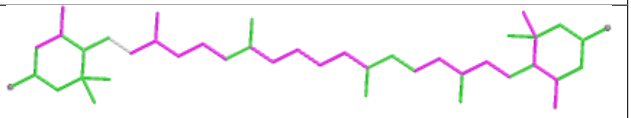


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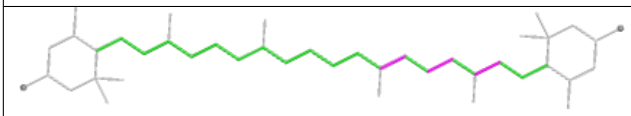
Ligand LUT Z 1620



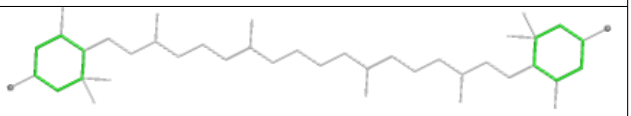
Bond lengths



Bond angles

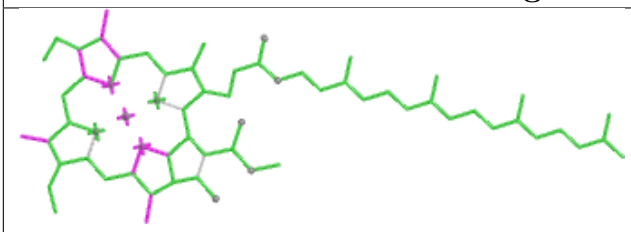


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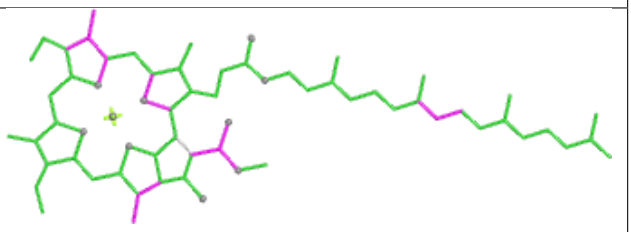


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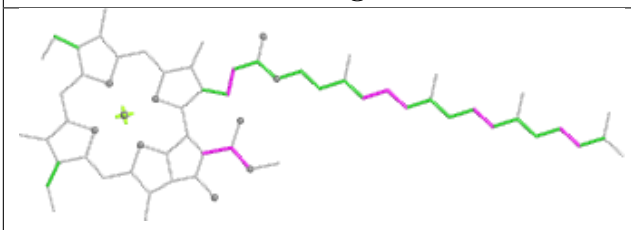
Ligand CLA A 854



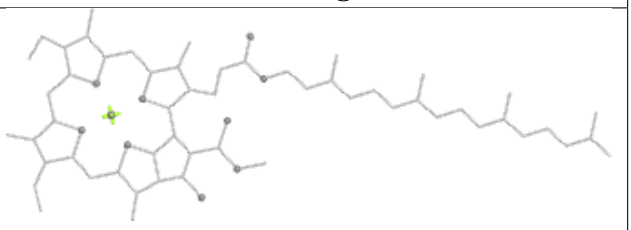
Bond lengths



Bond angles

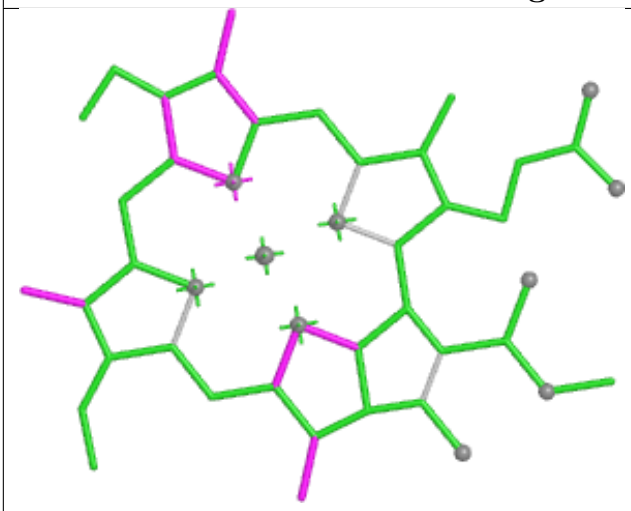


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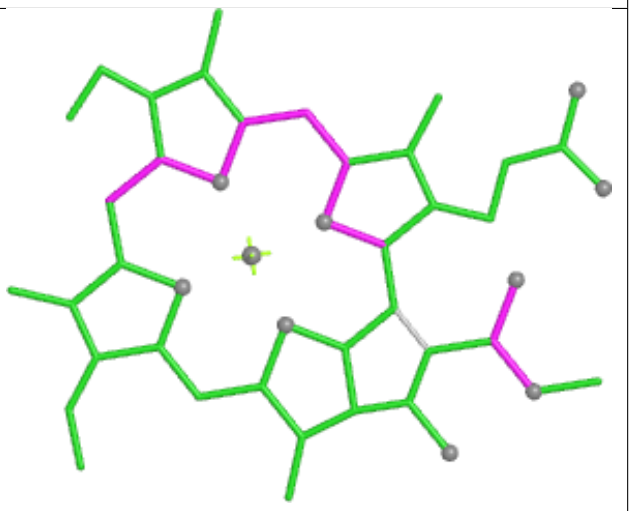


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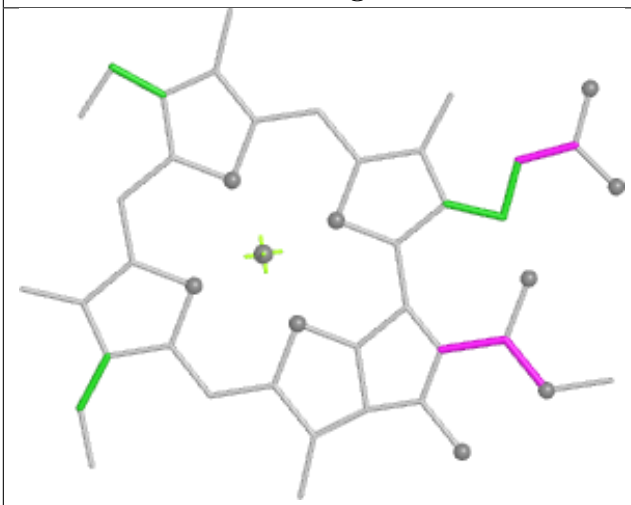
Ligand CLA a 612



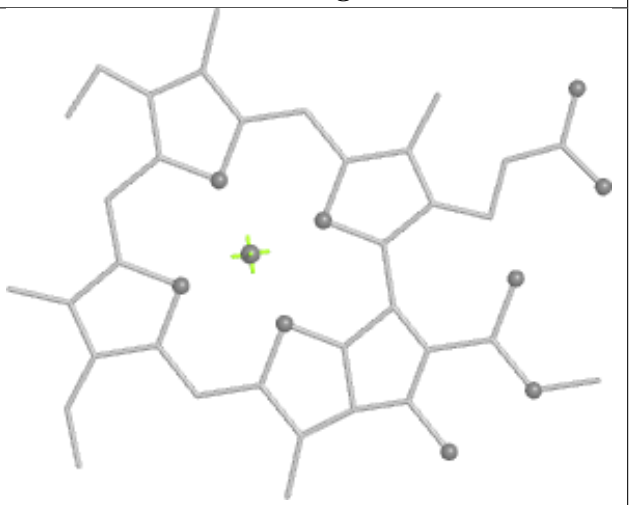
Bond lengths



Bond angles

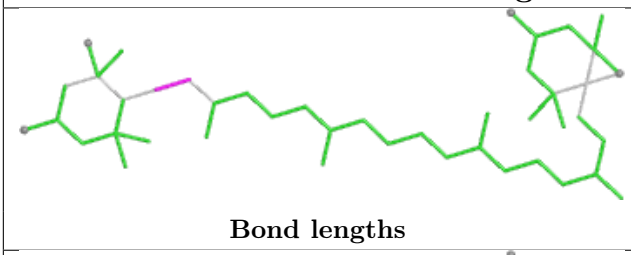


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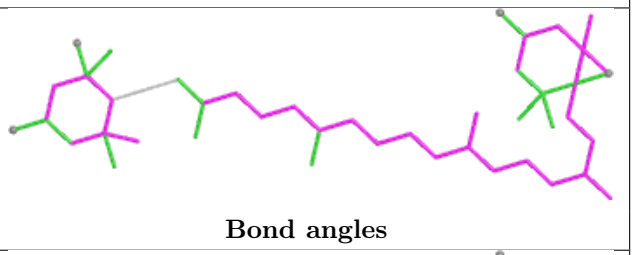


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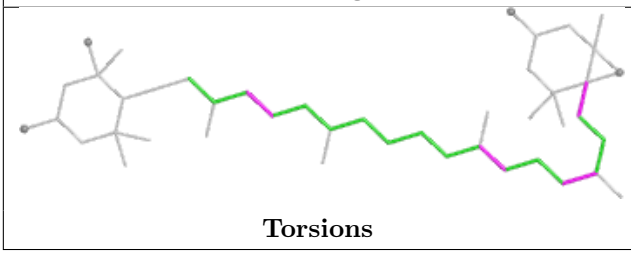
Ligand NEX Z 1623



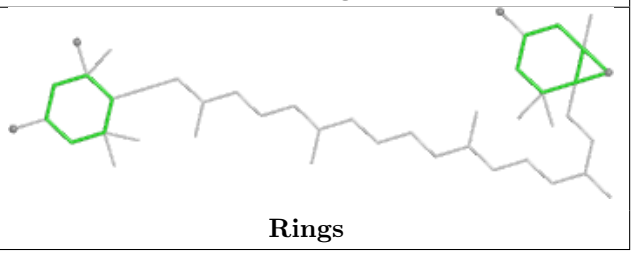
Bond lengths



Bond angles

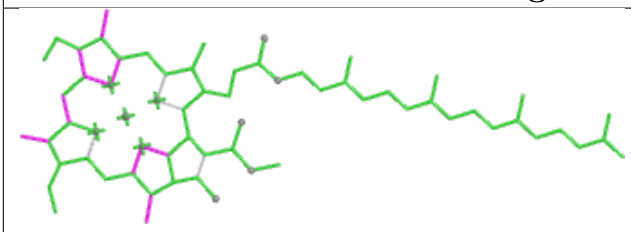


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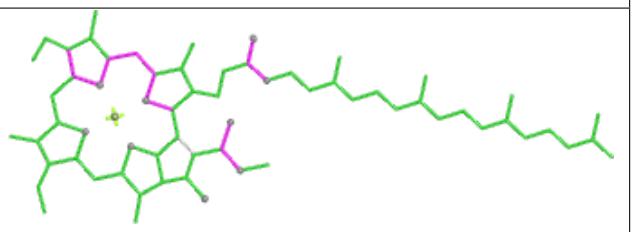


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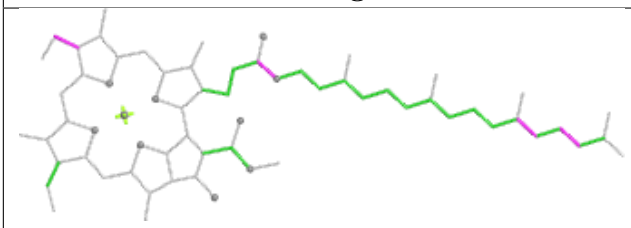
Ligand CLA 7 610



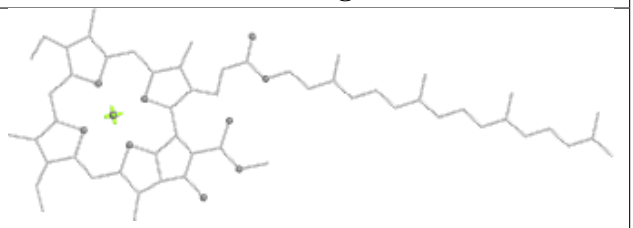
Bond lengths



Bond angles

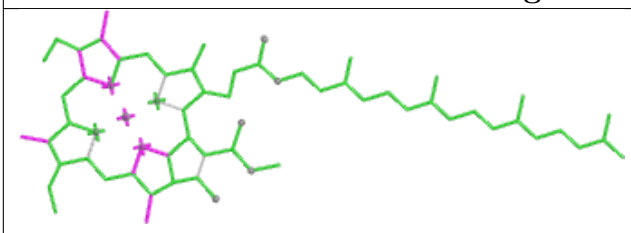


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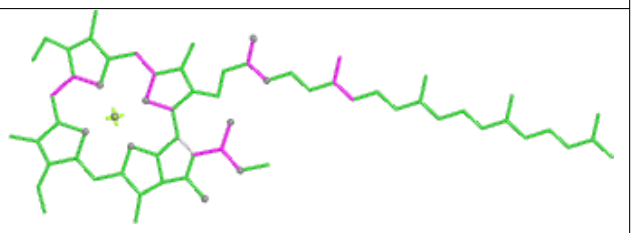


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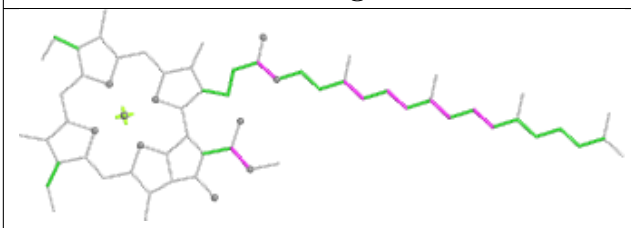
Ligand CLA A 836



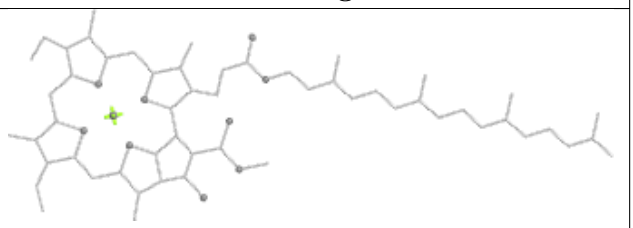
Bond lengths



Bond angles

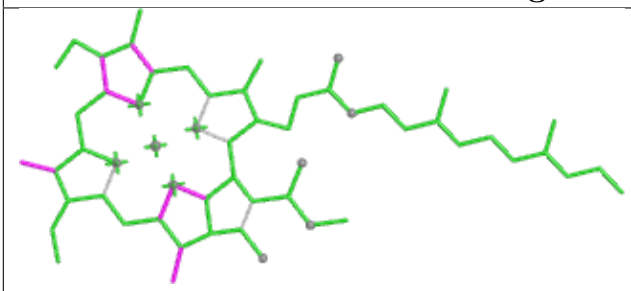


Torsions

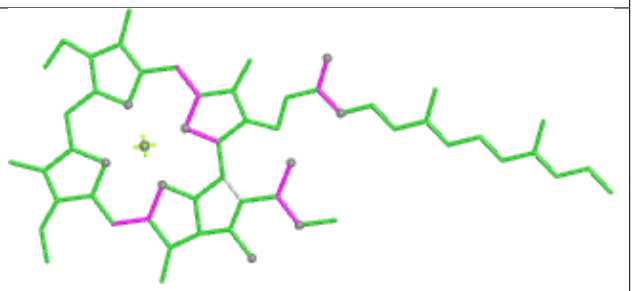


Rings

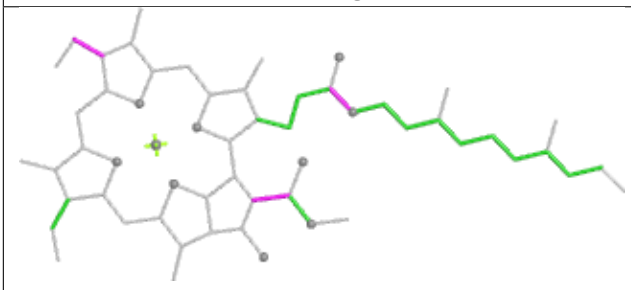
Ligand CLA 4 609



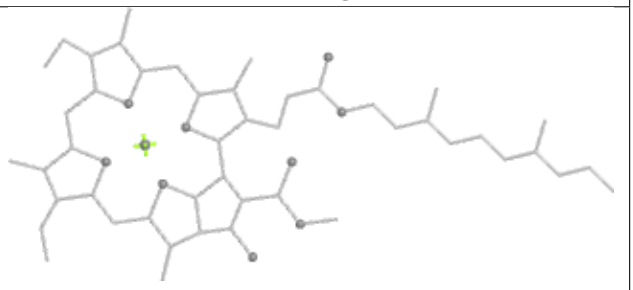
Bond lengths



Bond angles



Torsions

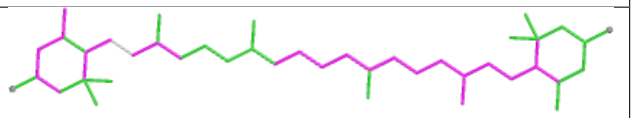


Rings

Ligand LUT 2 619



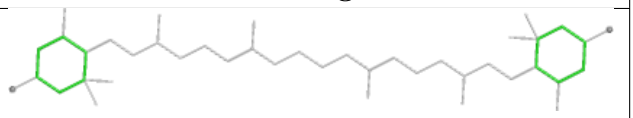
Bond lengths



Bond angles

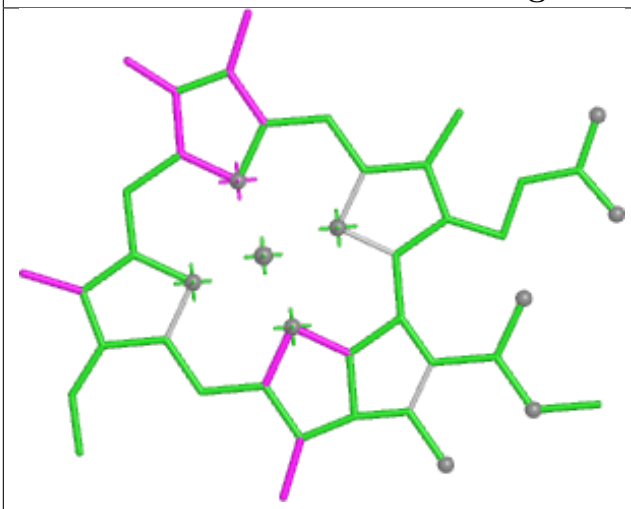


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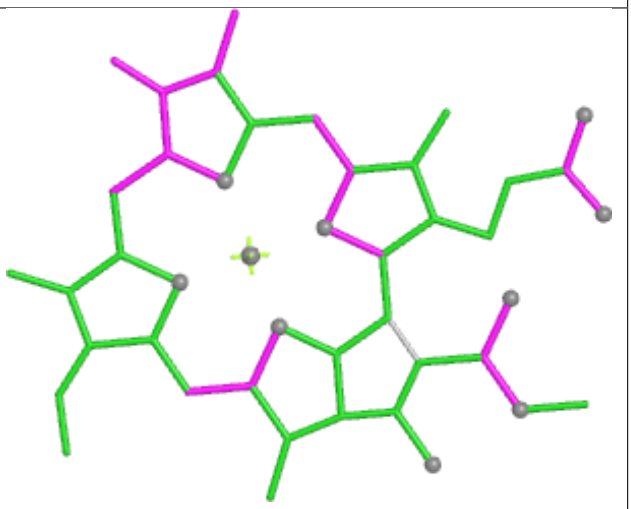


Rings

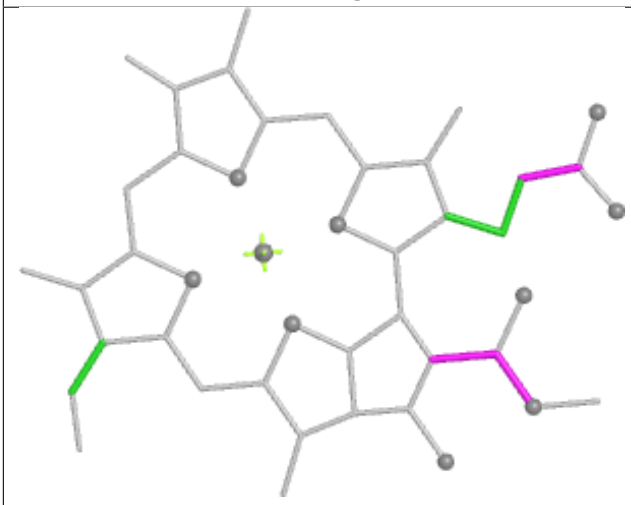
Ligand CLA 4 603



Bond lengths



Bond angles

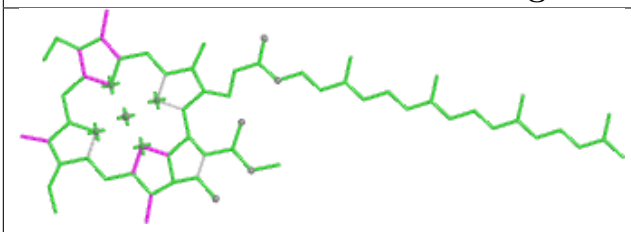


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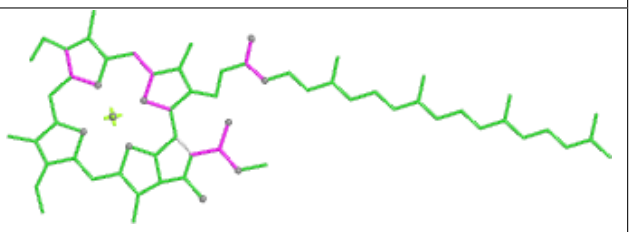


Rings

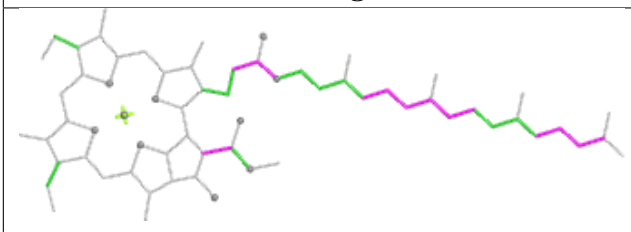
Ligand CLA 6 601



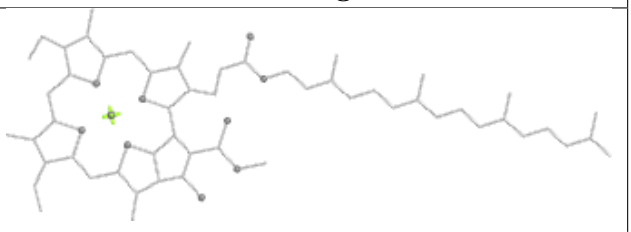
Bond lengths



Bond angles

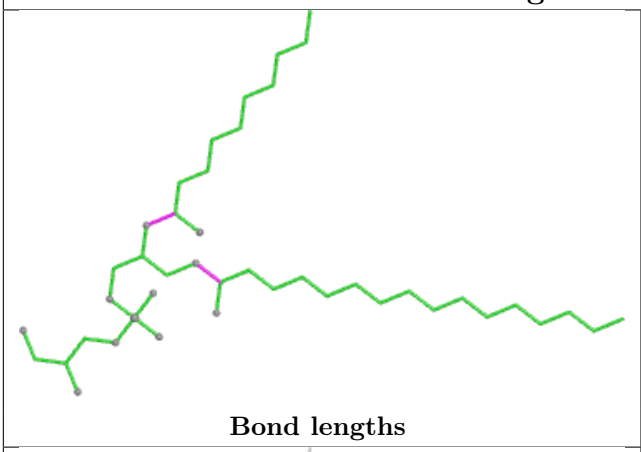


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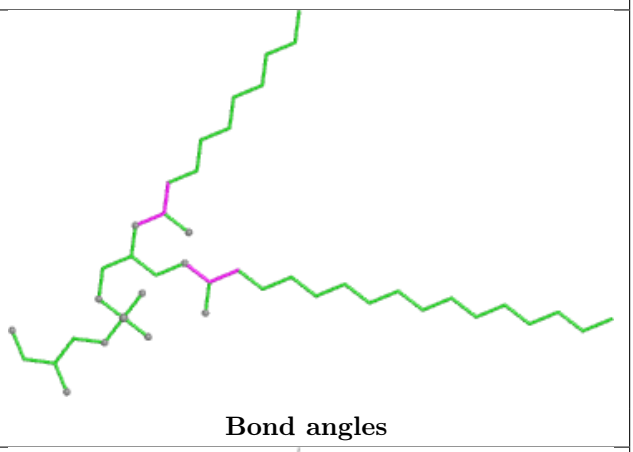


Rings

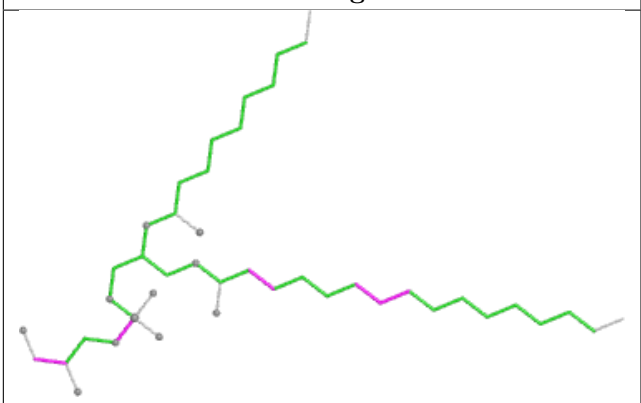
Ligand LHG a 620



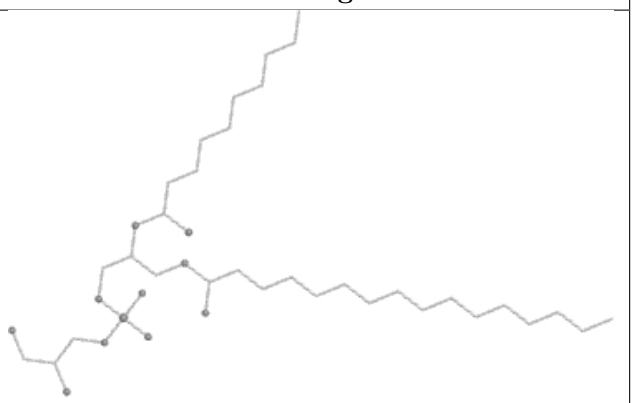
Bond lengths



Bond angles

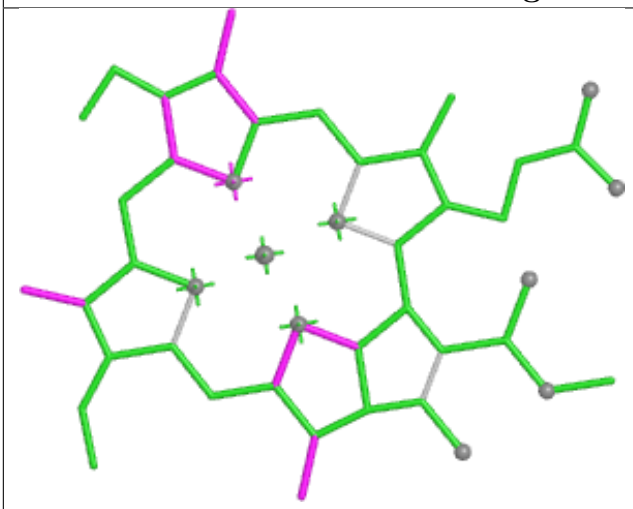


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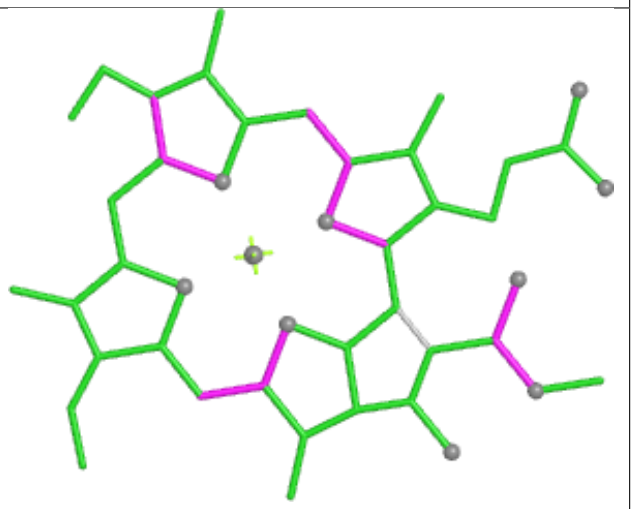


Rings

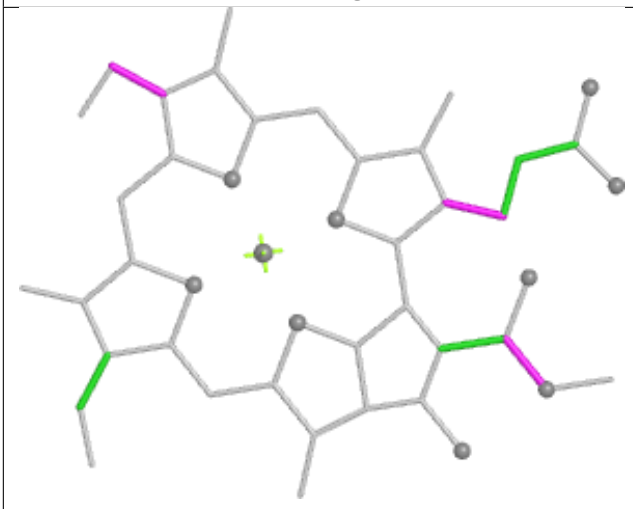
Ligand CLA K 204



Bond lengths



Bond angles

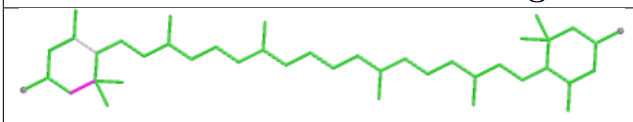


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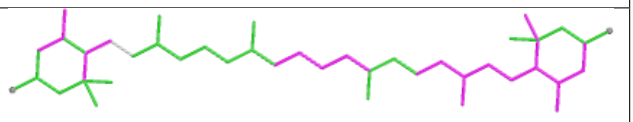


Rings

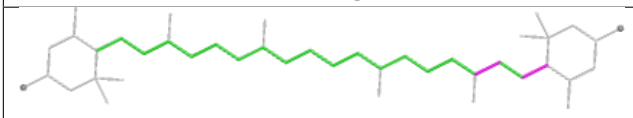
Ligand LUT 3 618



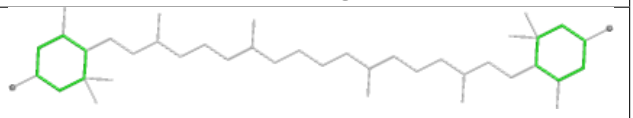
Bond lengths



Bond angles

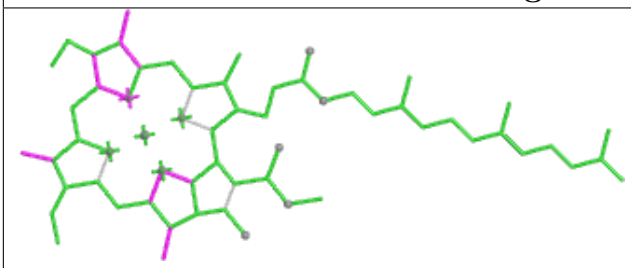


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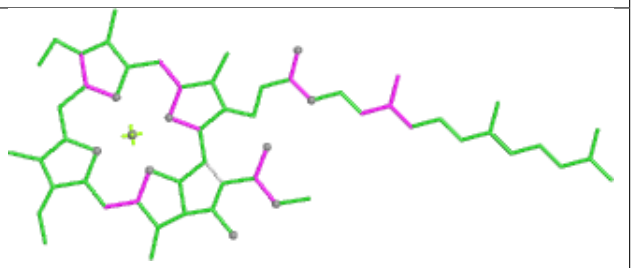


Rings

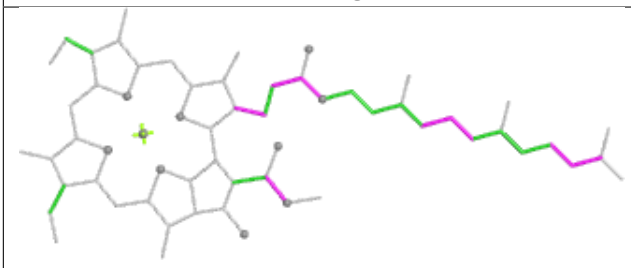
Ligand CLA B 832



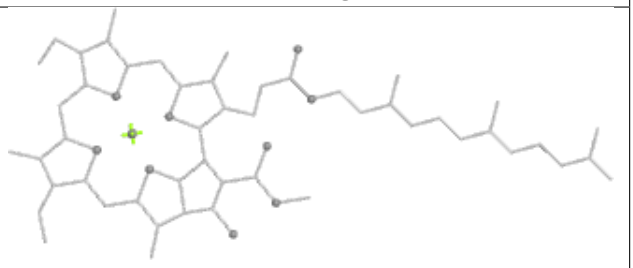
Bond lengths



Bond angles

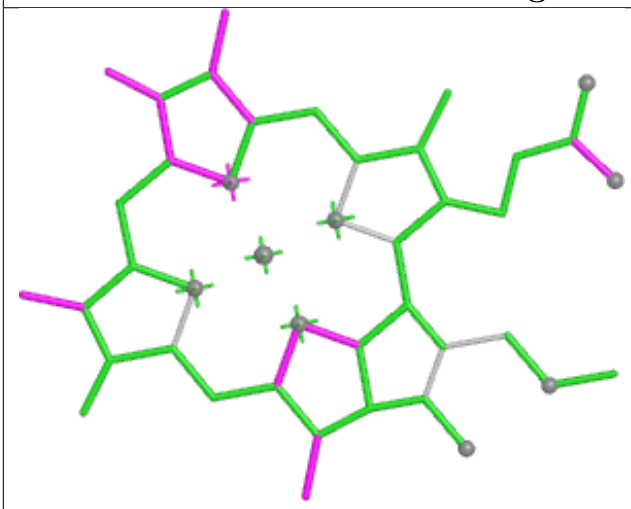


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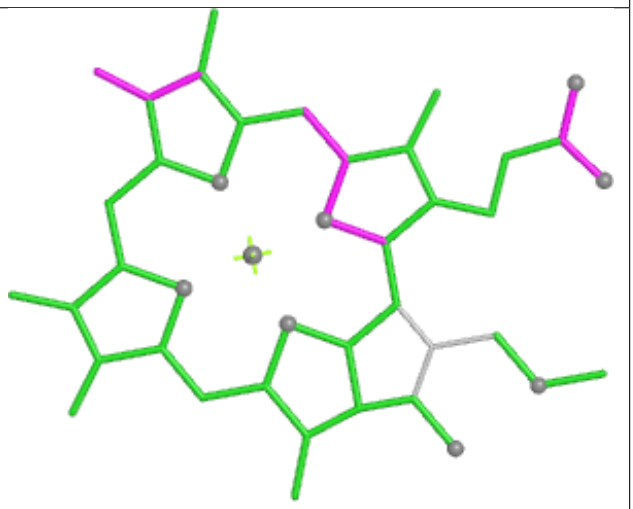


Rings

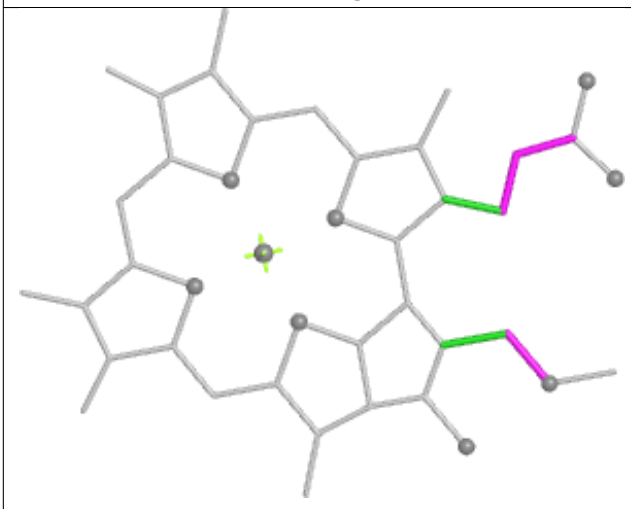
Ligand CLA 5 616



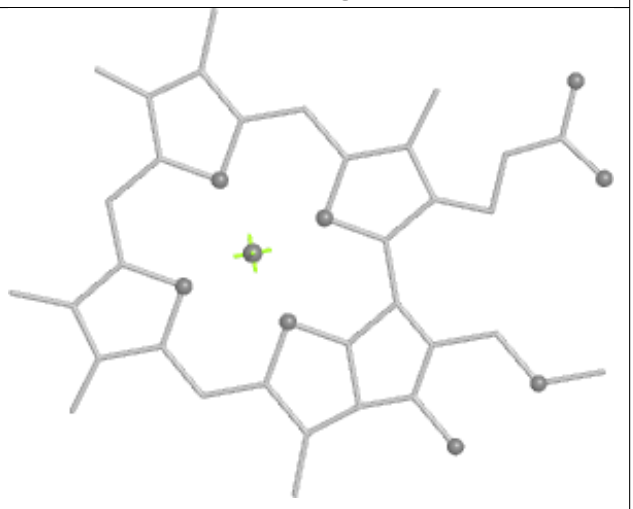
Bond lengths



Bond angles

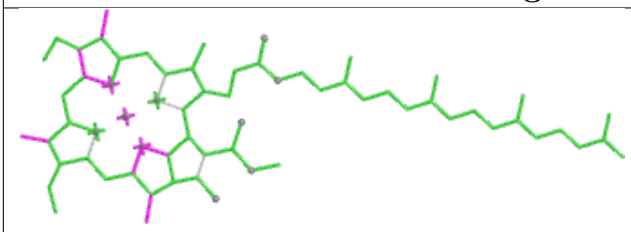


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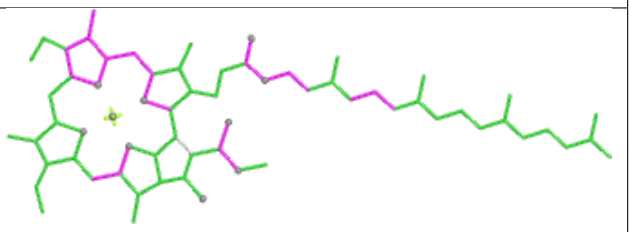


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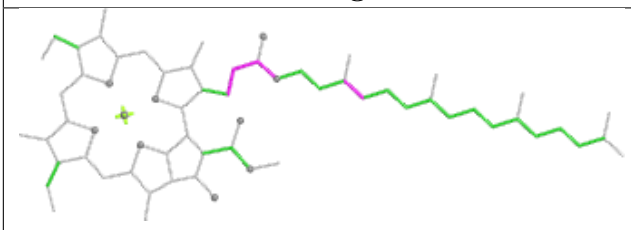
Ligand CLA A 822



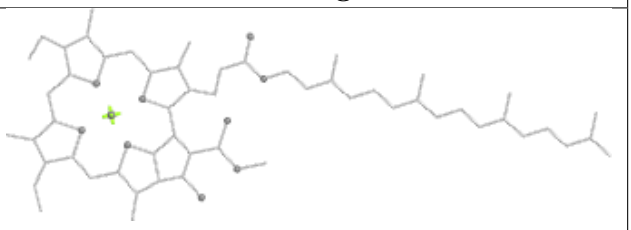
Bond lengths



Bond angles



Torsions



Rings

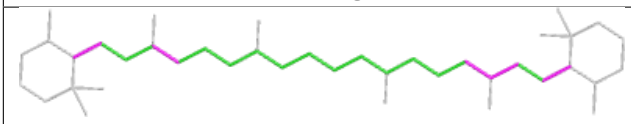
Ligand BCR B 845



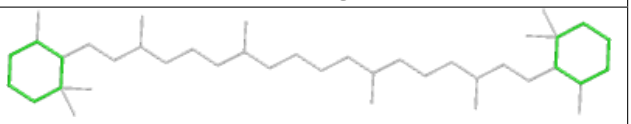
Bond lengths



Bond angles

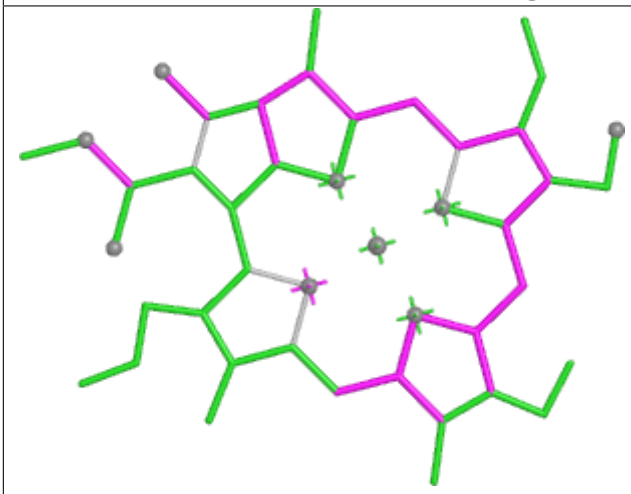


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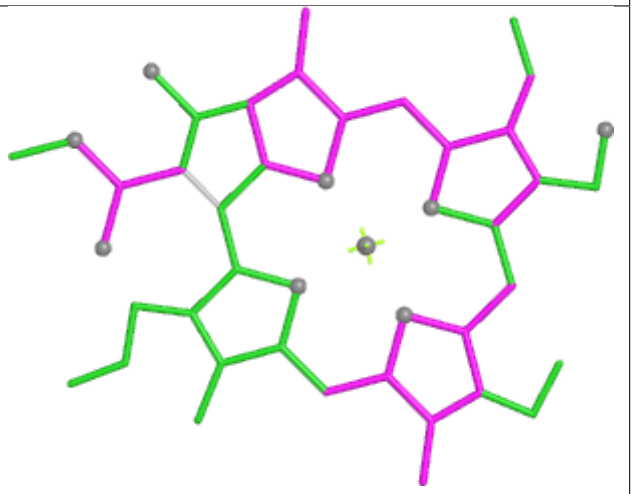


Rings

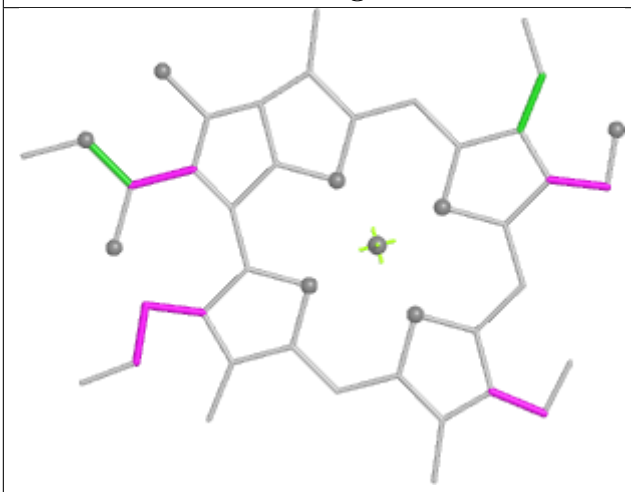
Ligand CHL V 605



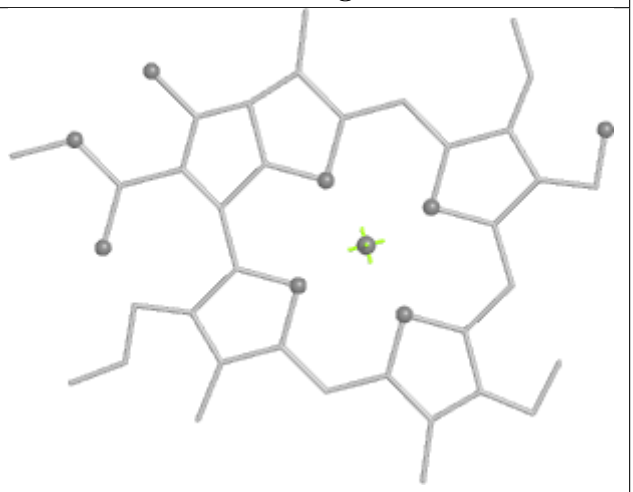
Bond lengths



Bond angles

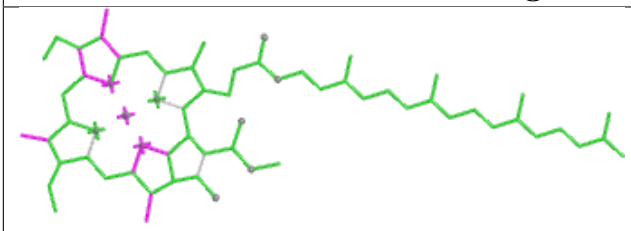


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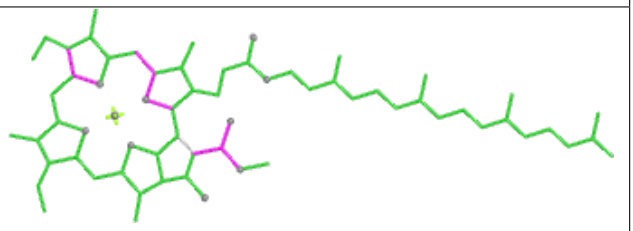


Rings

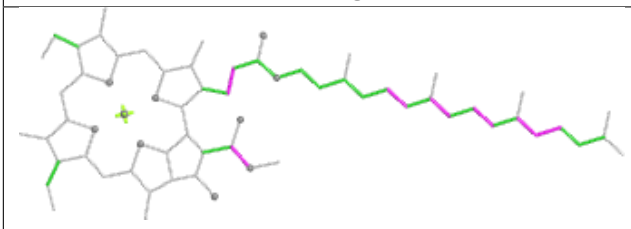
Ligand CLA B 824



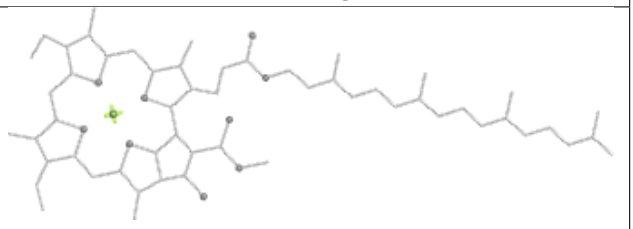
Bond lengths



Bond angles

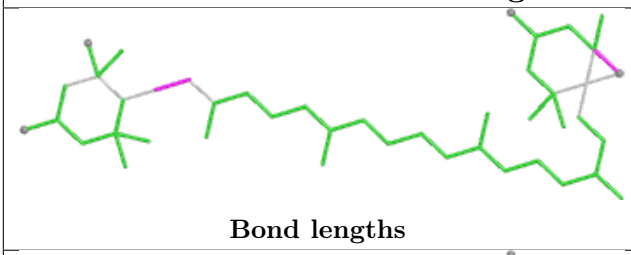


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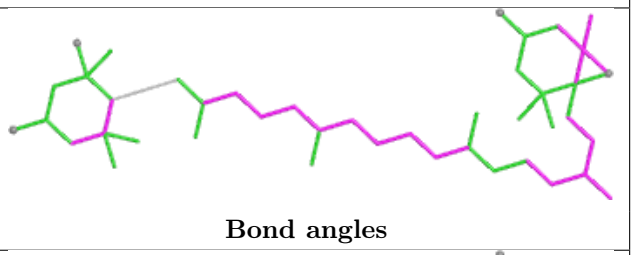


Rings

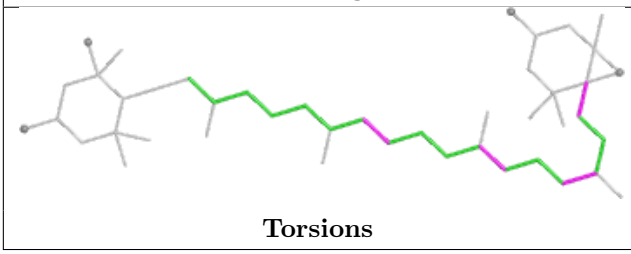
Ligand NEX W 1623



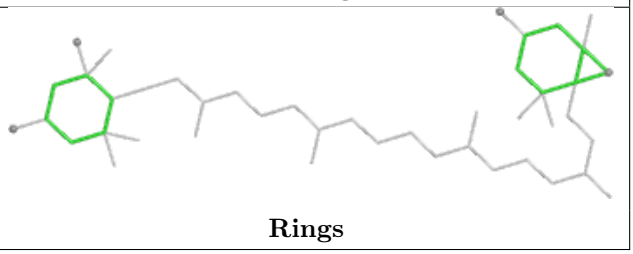
Bond lengths



Bond angles

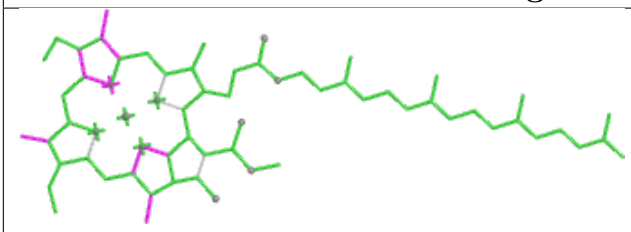


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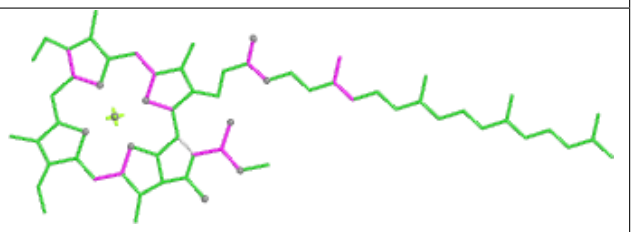


Rings

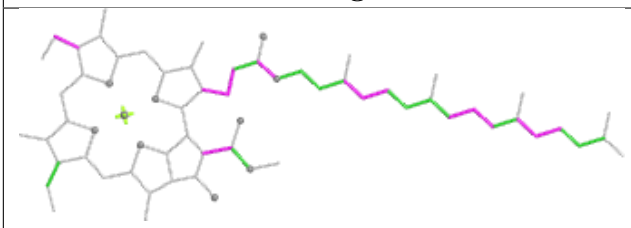
Ligand CLA L 303



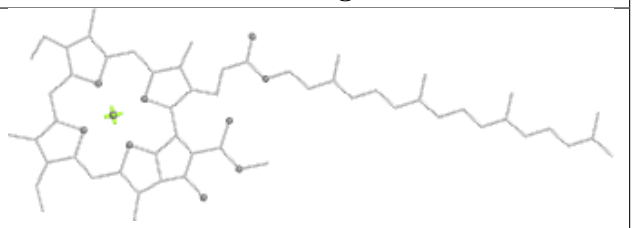
Bond lengths



Bond angles

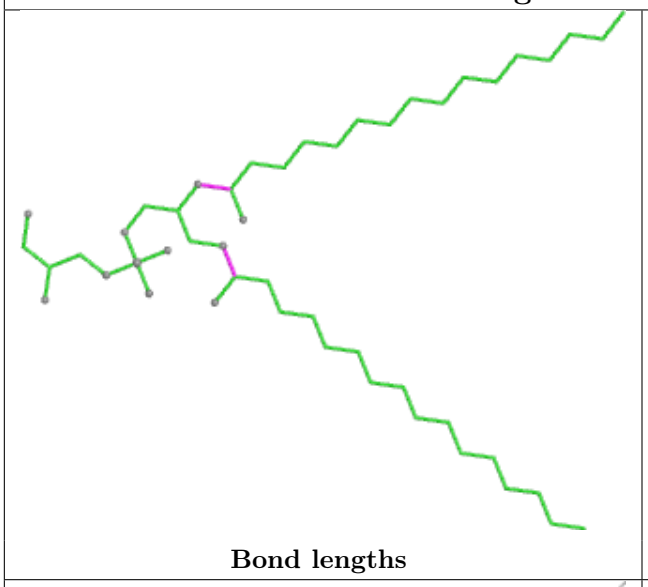


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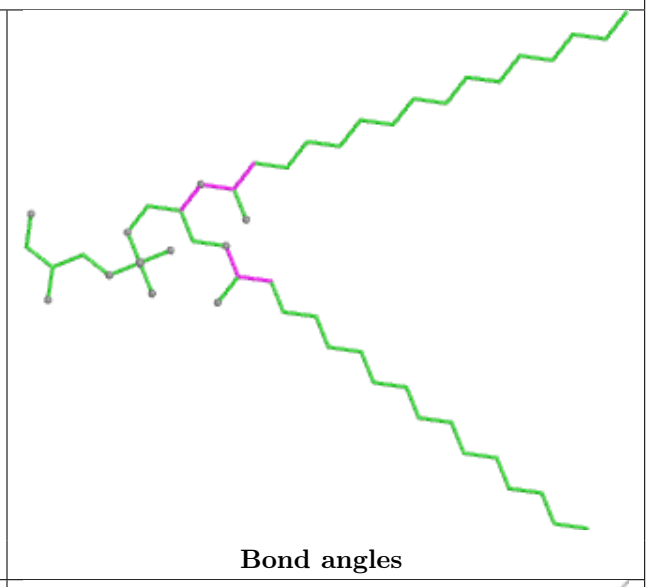


Rings

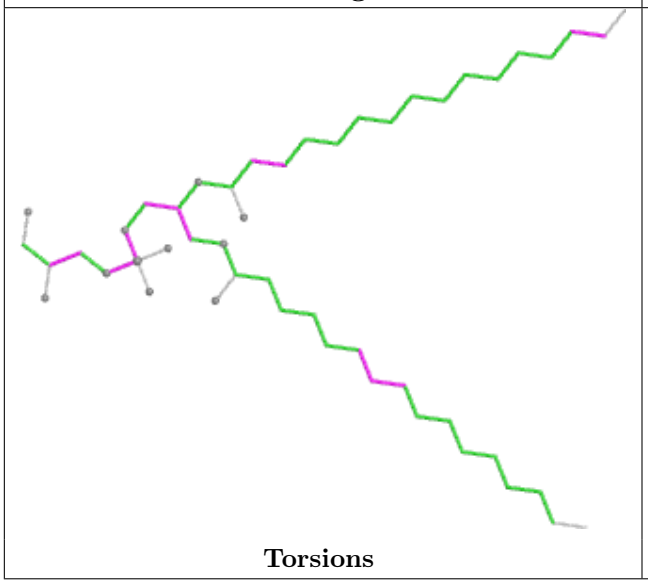
Ligand LHG X 2630



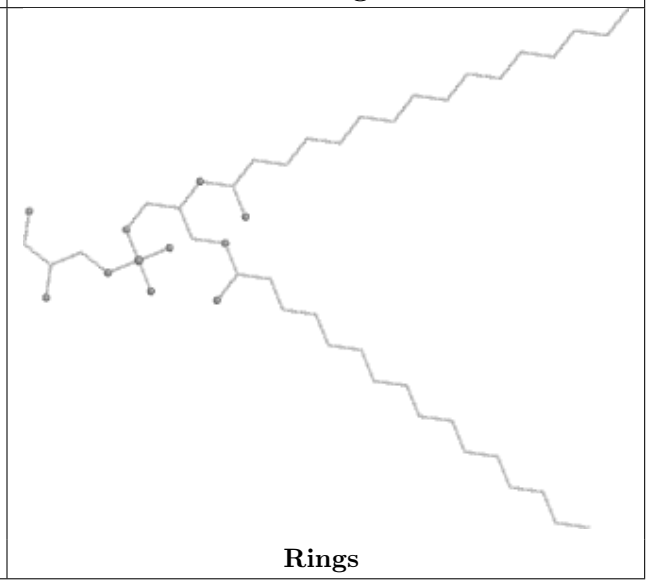
Bond lengths



Bond angles

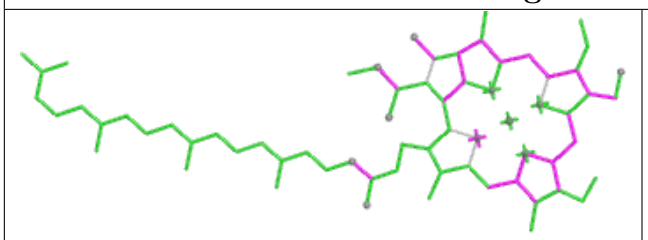


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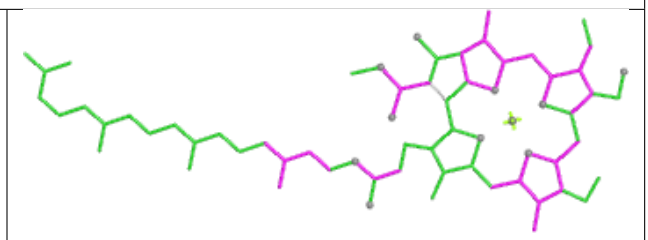


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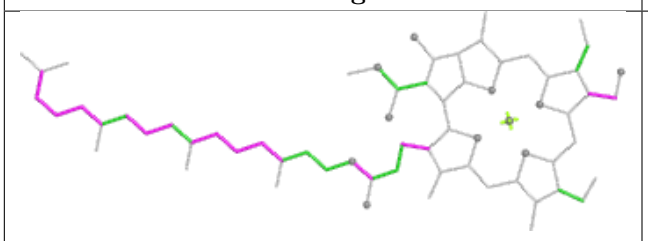
Ligand CHL U 601



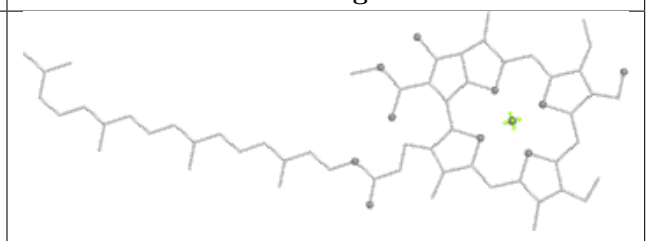
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Bond angles

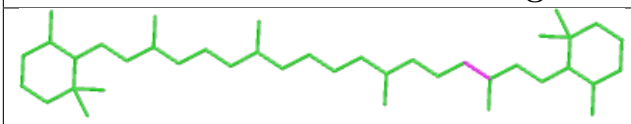


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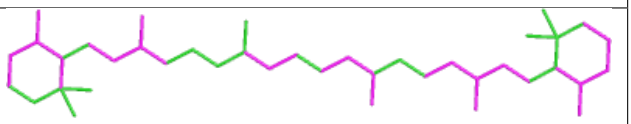


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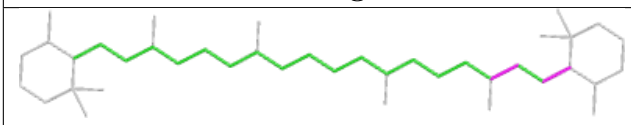
Ligand BCR 9 621



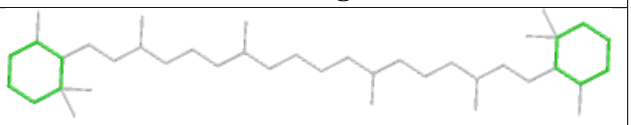
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Bond angles

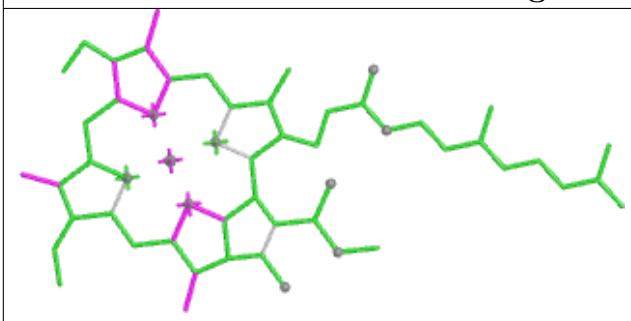


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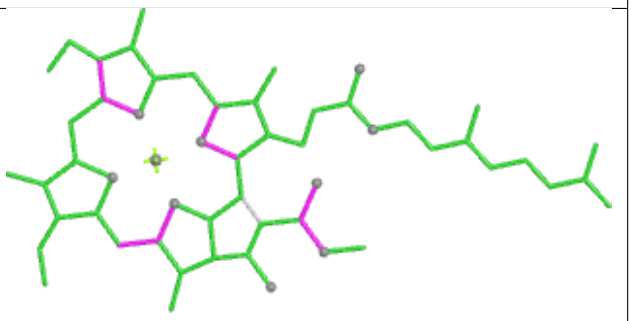


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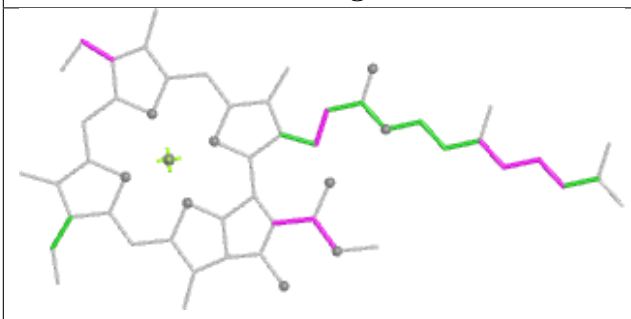
Ligand CLA 3 608



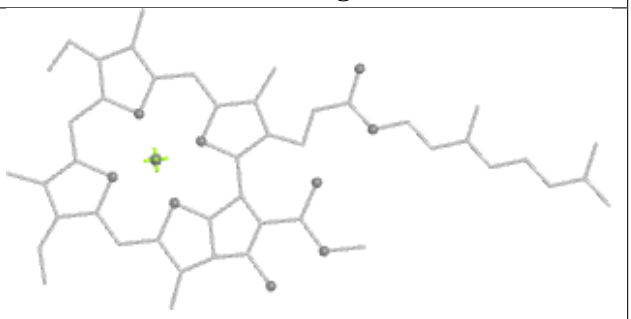
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Bond angles

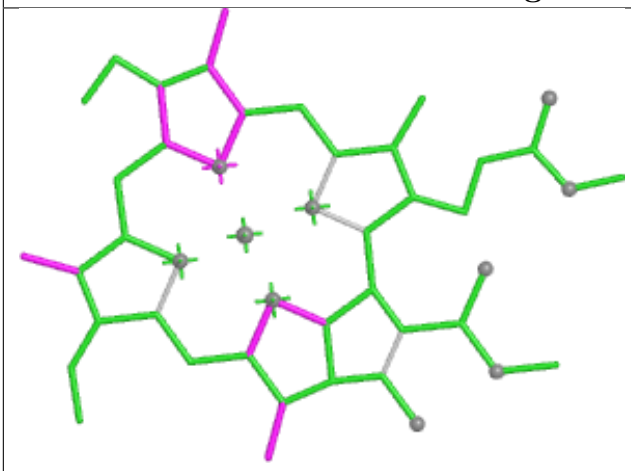


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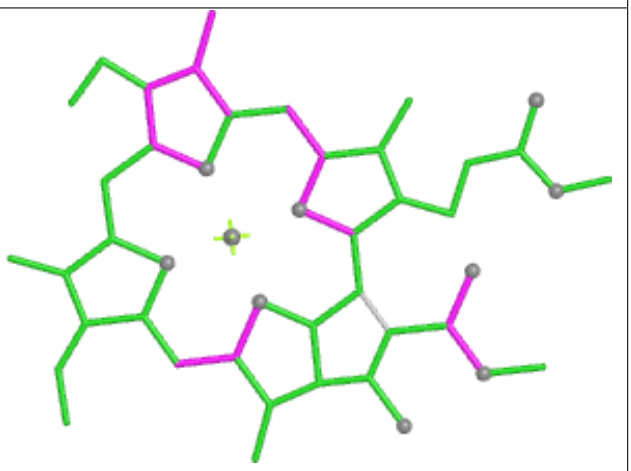


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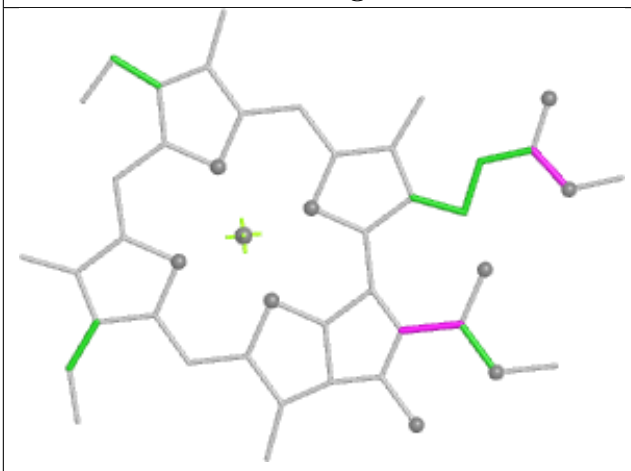
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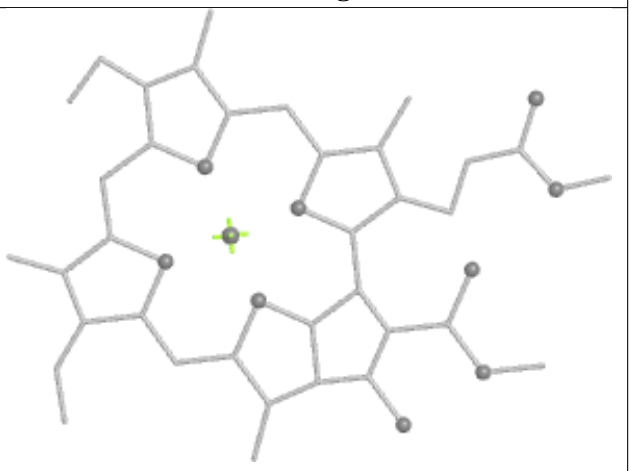
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Bond angles

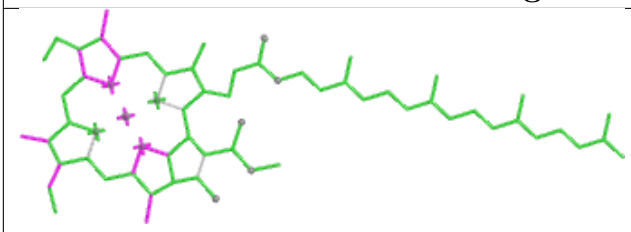


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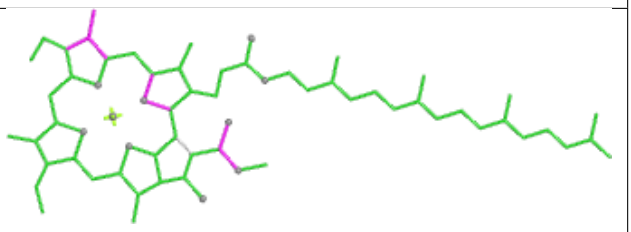


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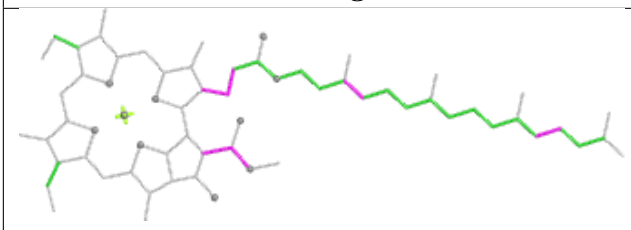
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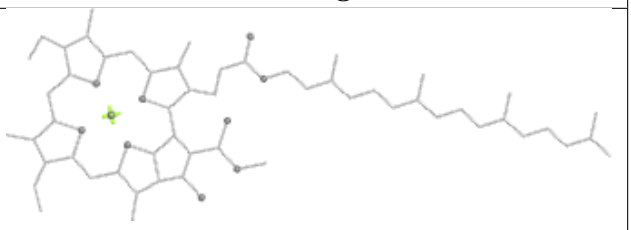
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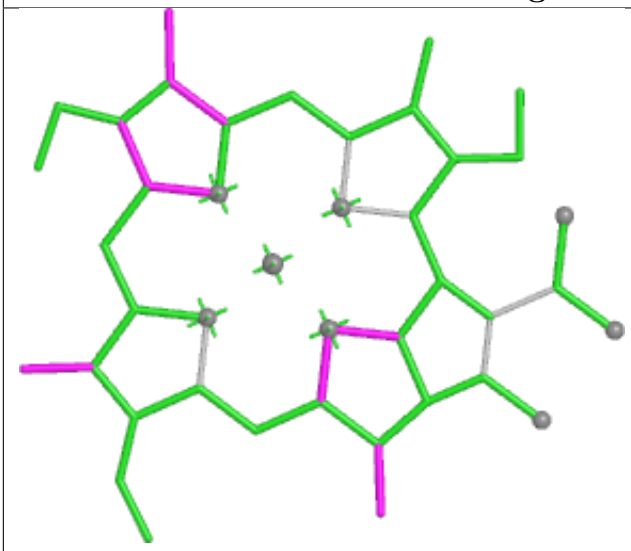


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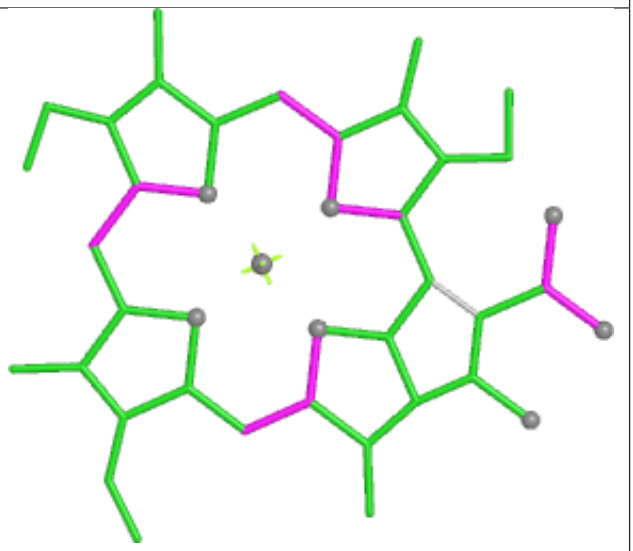


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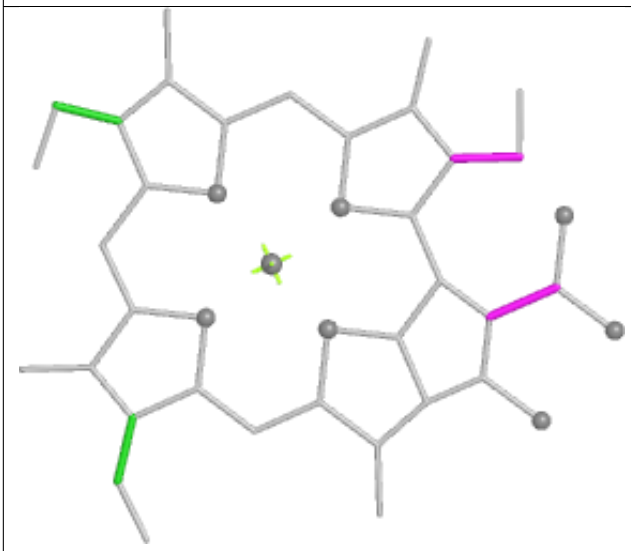
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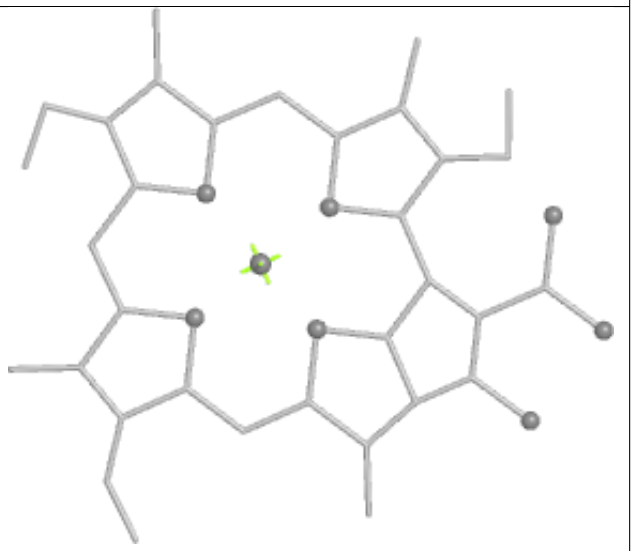
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Bond angles

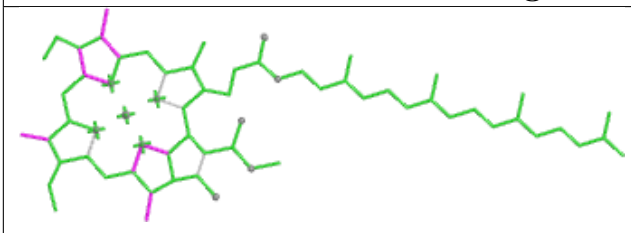


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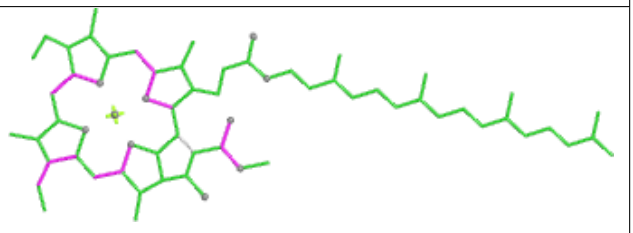


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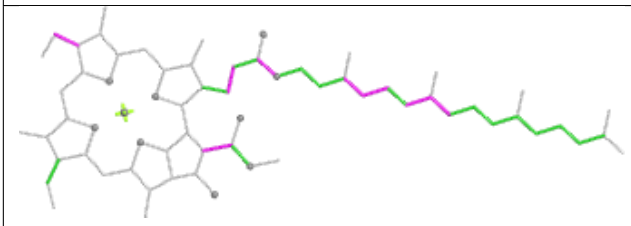
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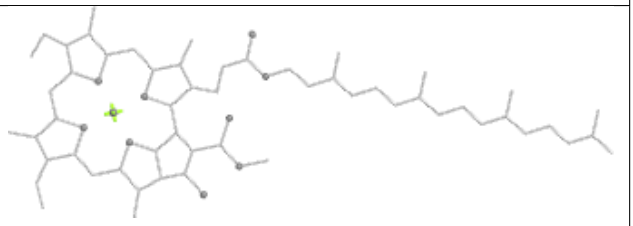
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Bond angles

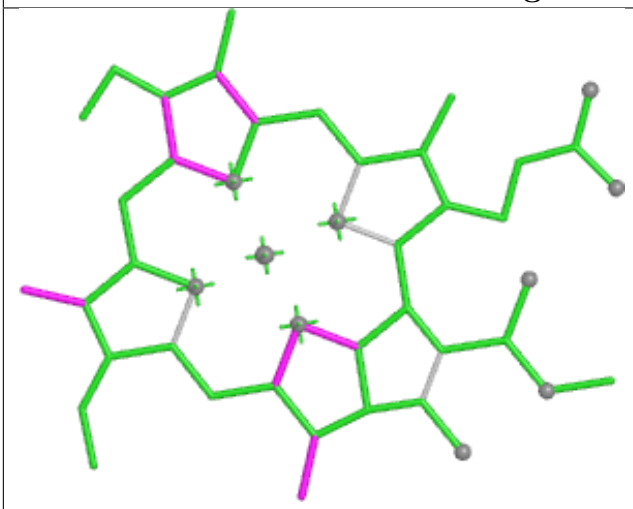


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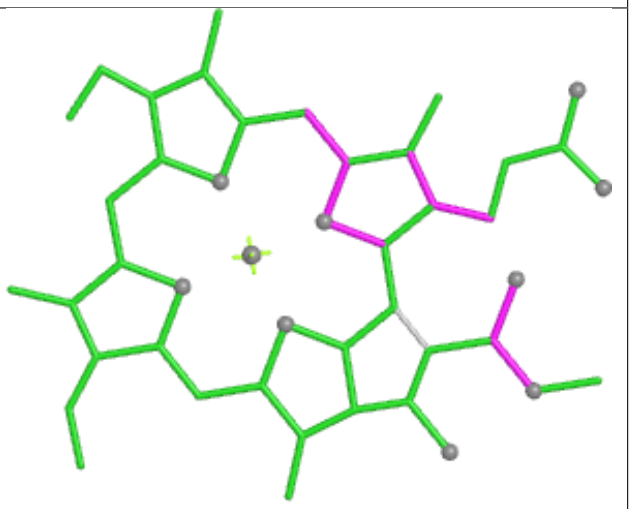


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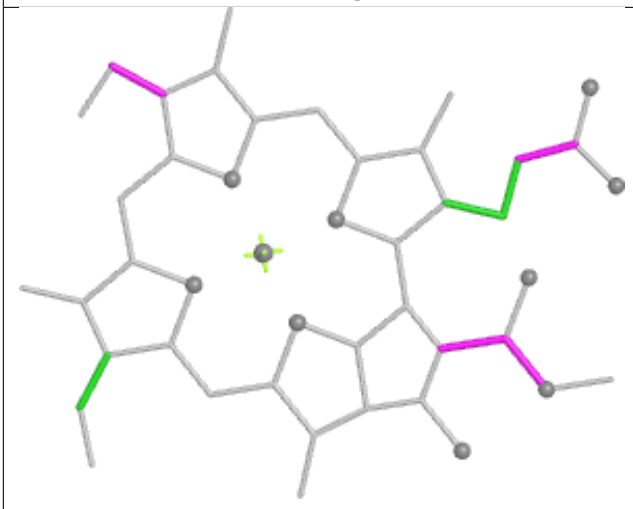
Ligand CLA Y 612



Bond lengths



Bond angles

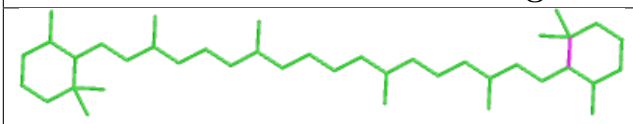


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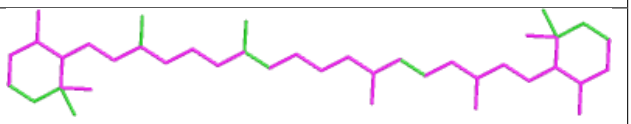


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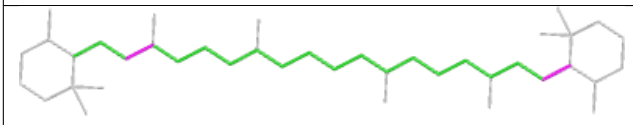
Ligand BCR 2 623



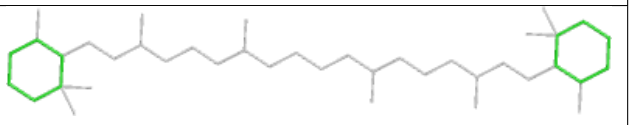
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Bond angles

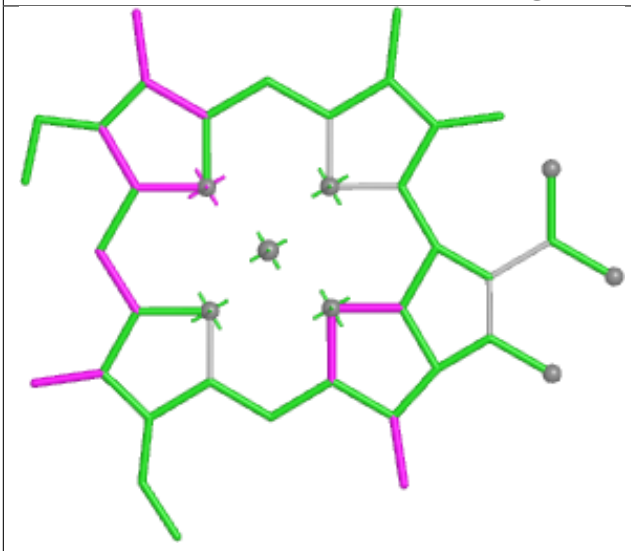


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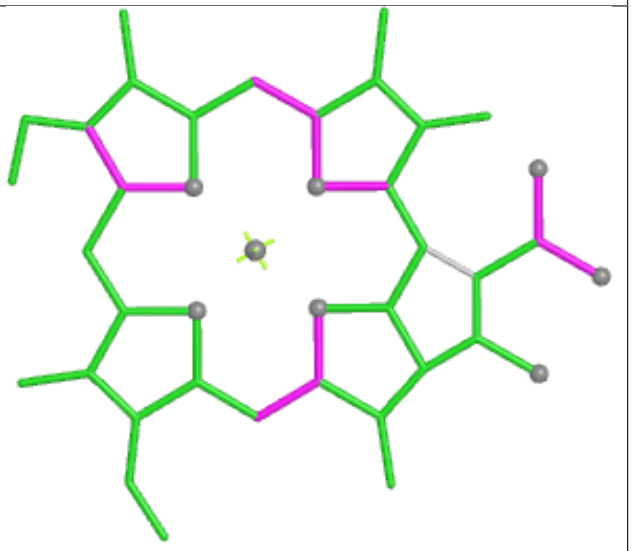


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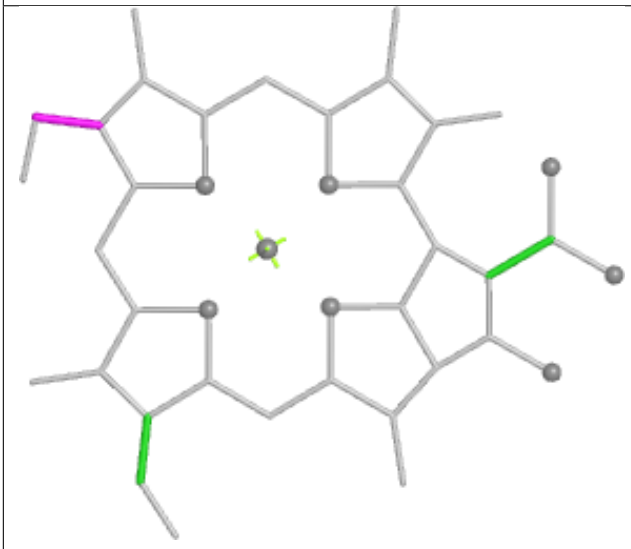
Ligand CLA 1 607



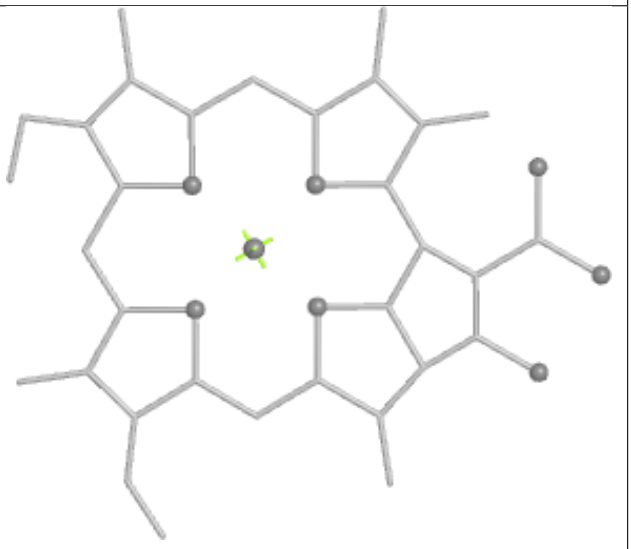
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Bond angles

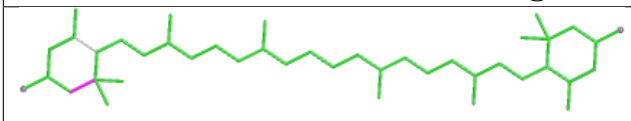


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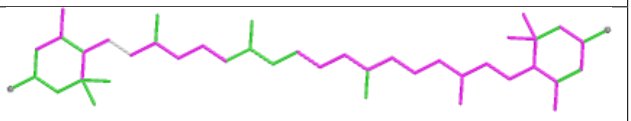


Rings

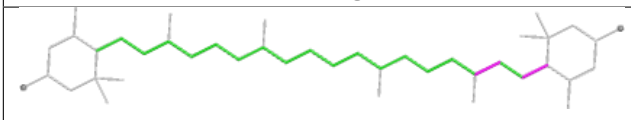
Ligand LUT 9 619



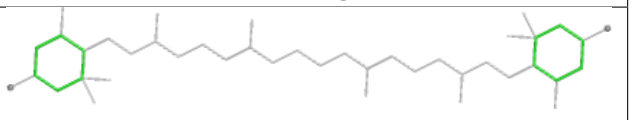
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Bond angles

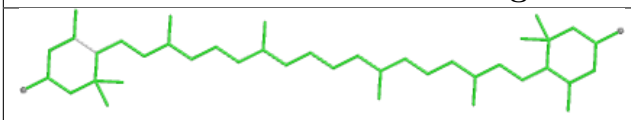


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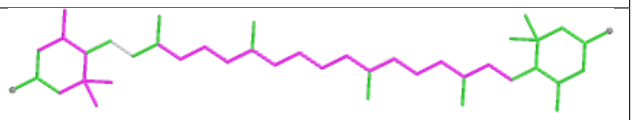


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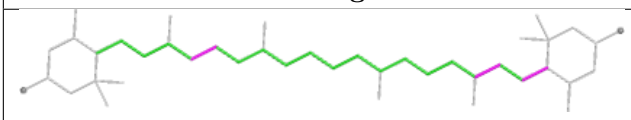
Ligand LUT W 1621



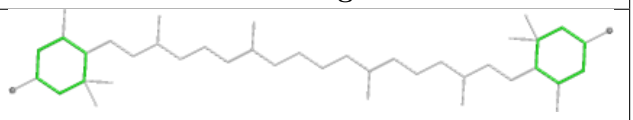
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Bond angles

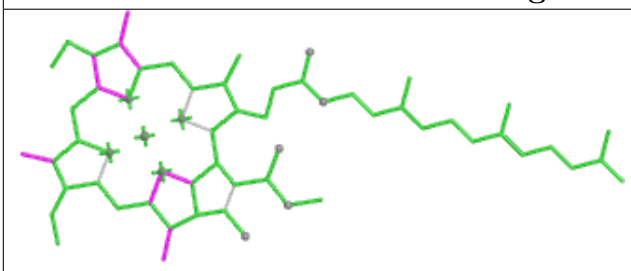


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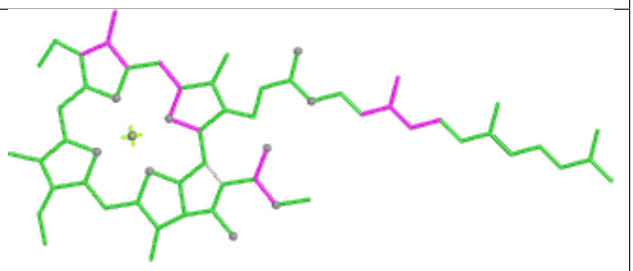


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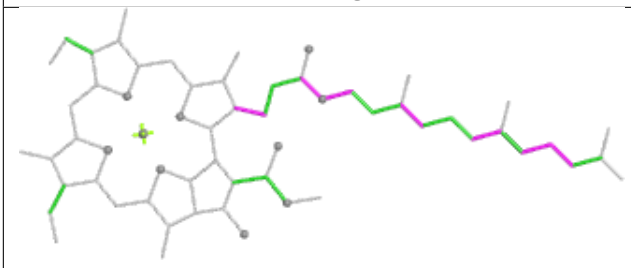
Ligand CLA 8 610



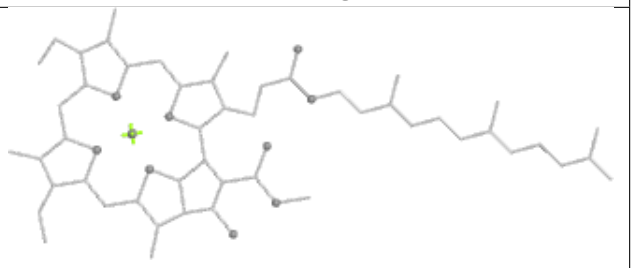
Bond lengths



Bond angles

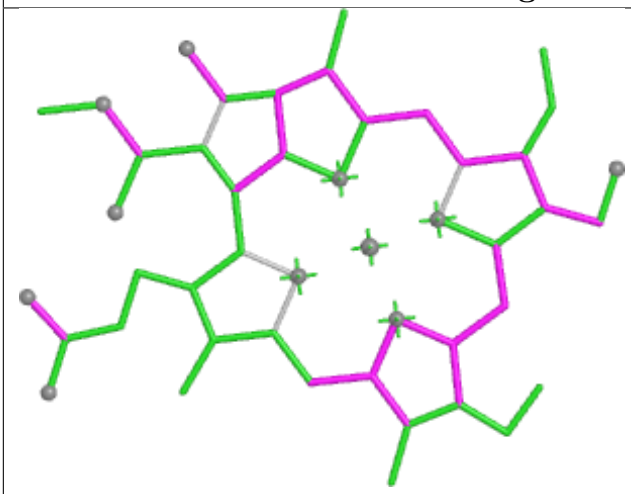


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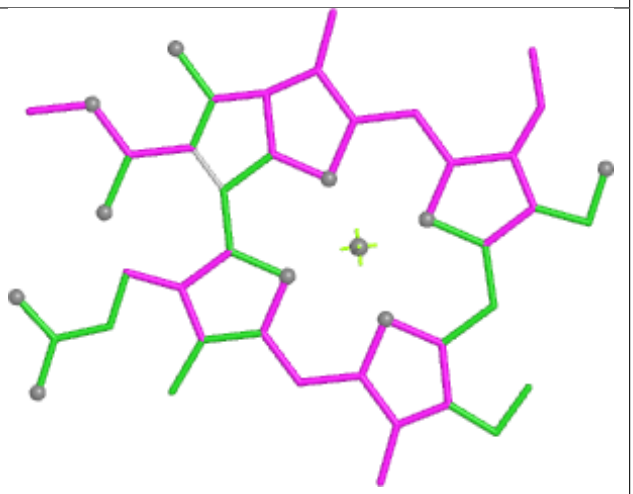


Rings

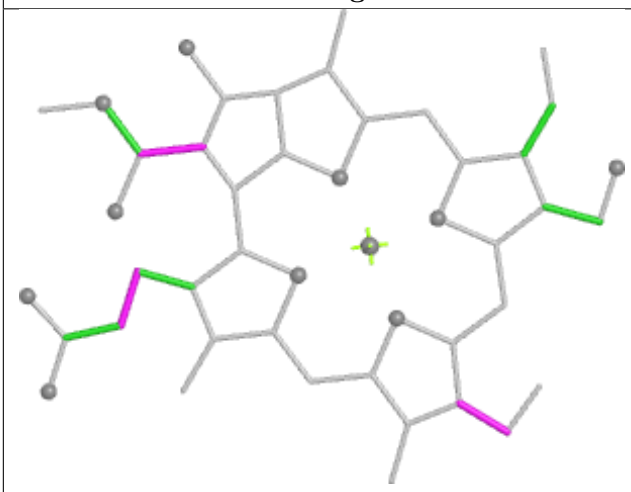
Ligand CHL W 606



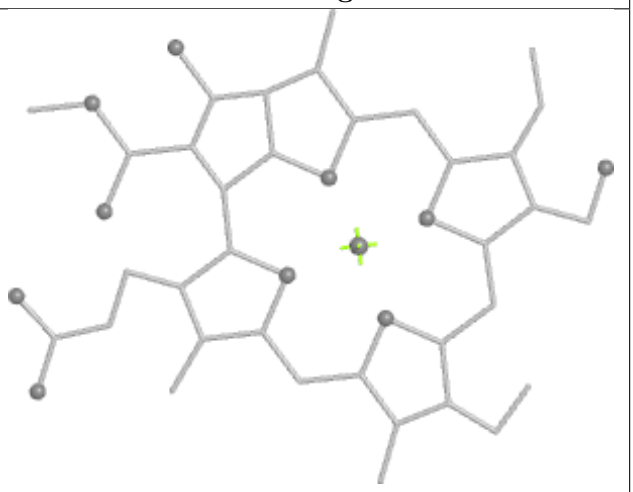
Bond lengths



Bond angles

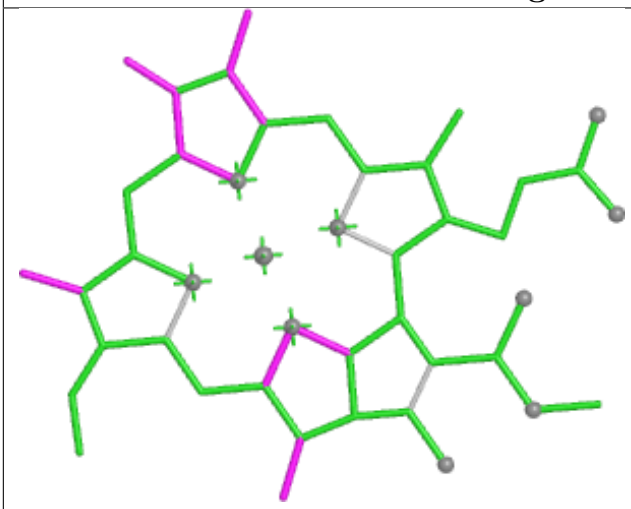


Torsions

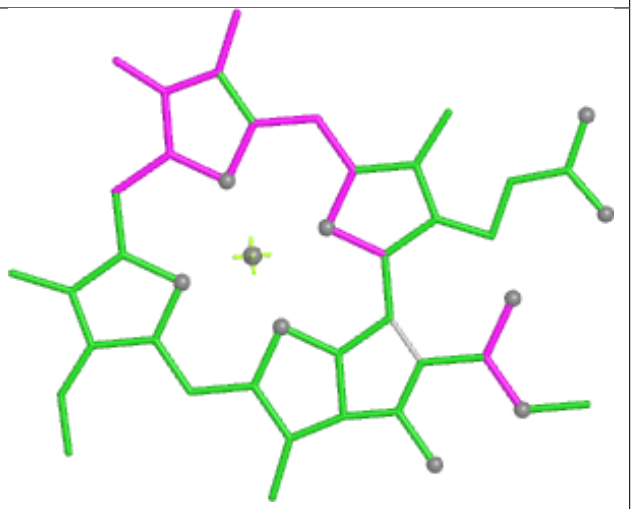


Rings

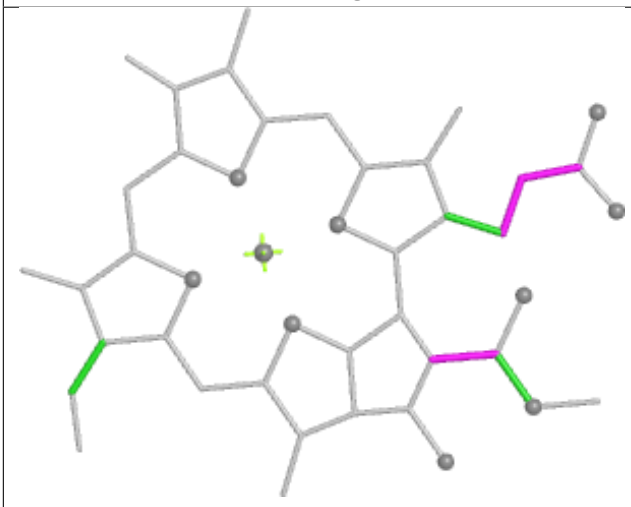
Ligand CLA 8 603



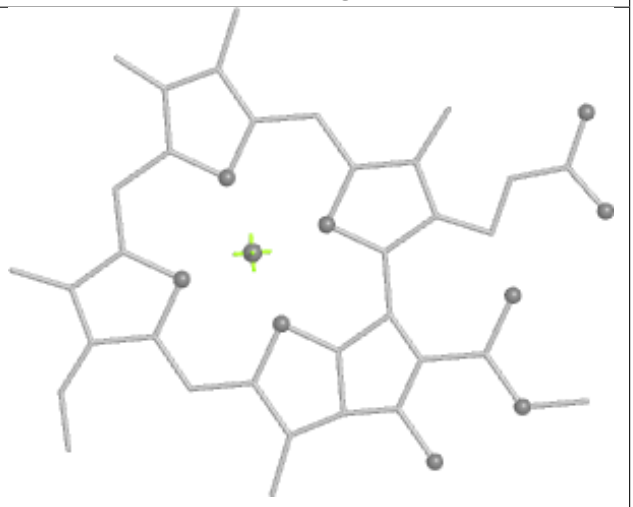
Bond lengths



Bond angles

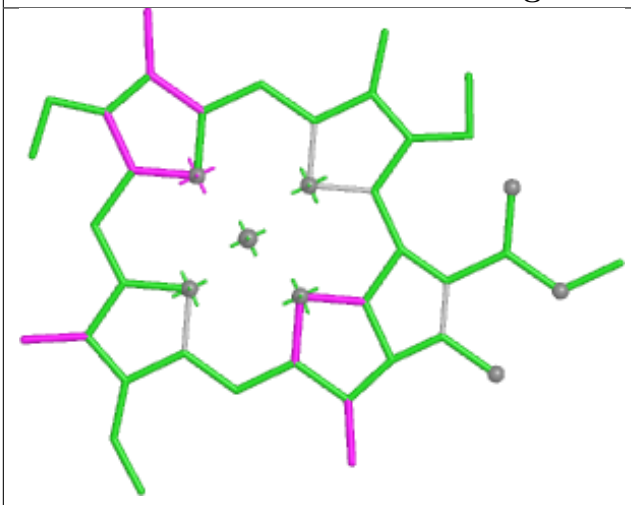


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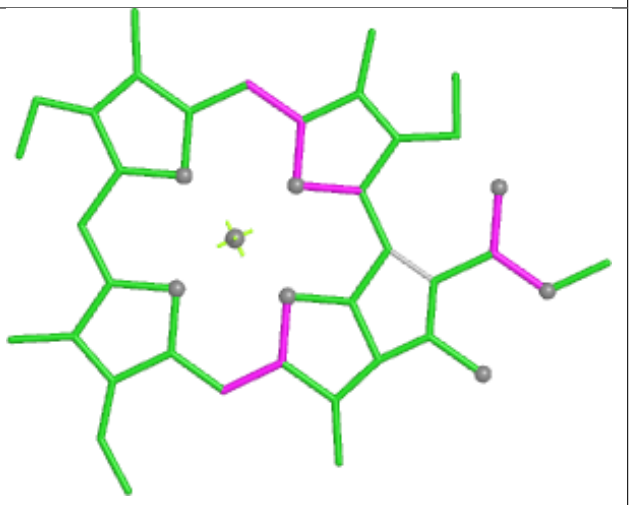


Rings

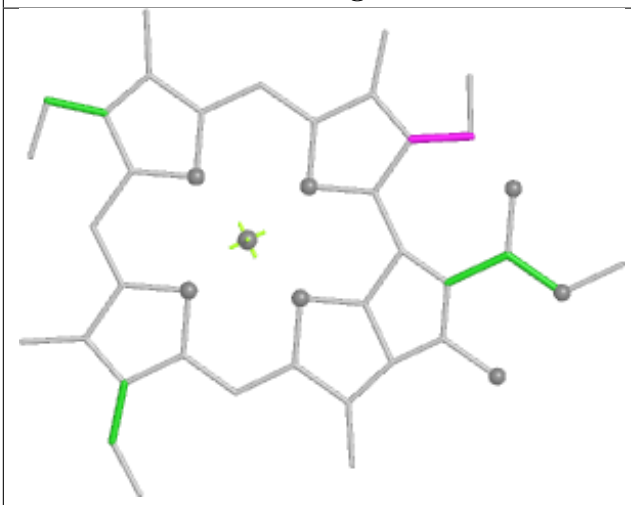
Ligand CLA A 823



Bond lengths



Bond angles

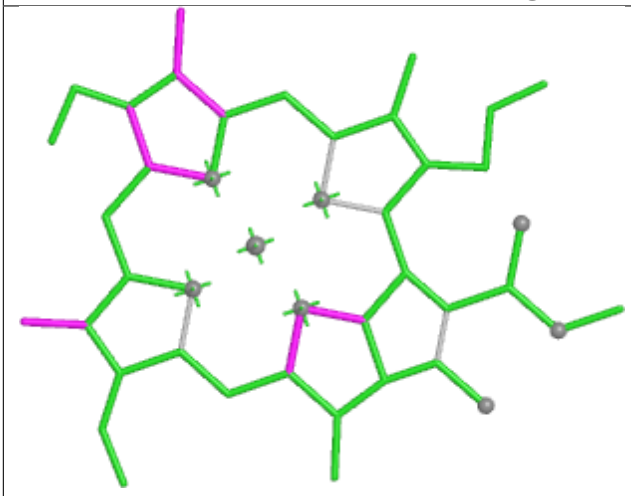


Torsions

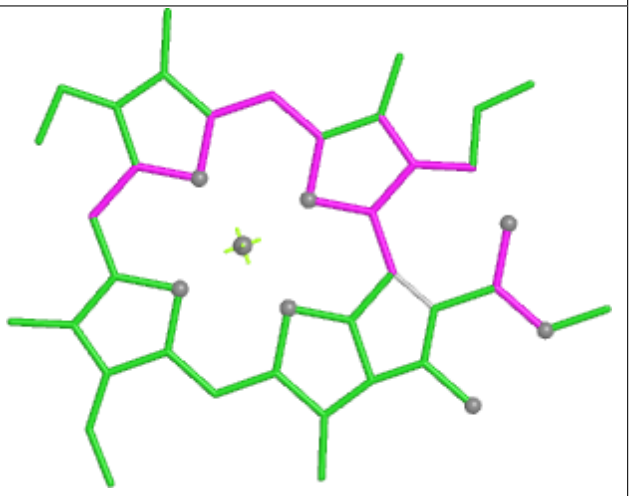


Rings

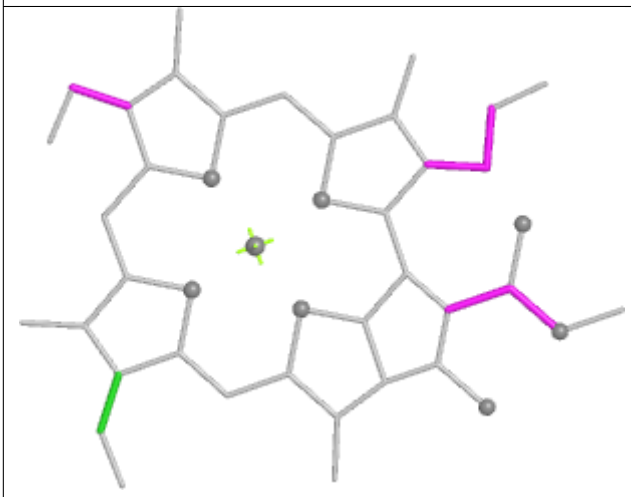
Ligand CLA X 612



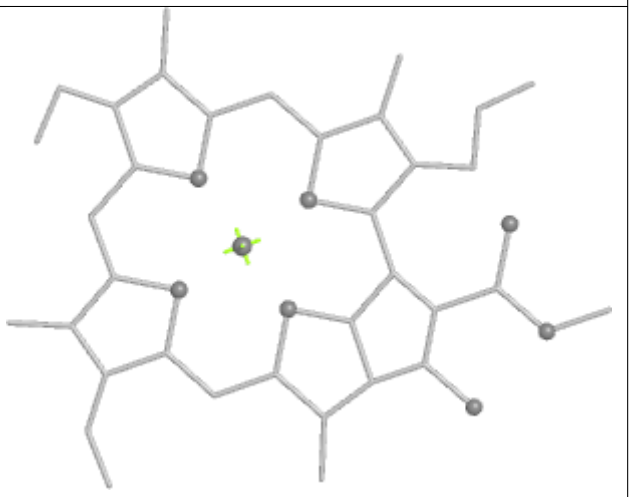
Bond lengths



Bond angles

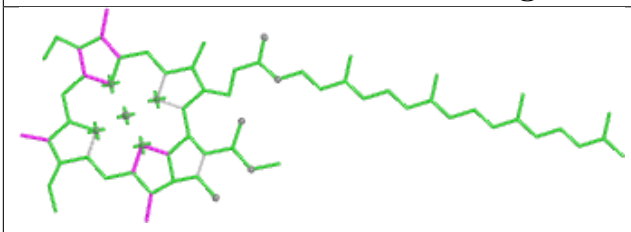


Torsions

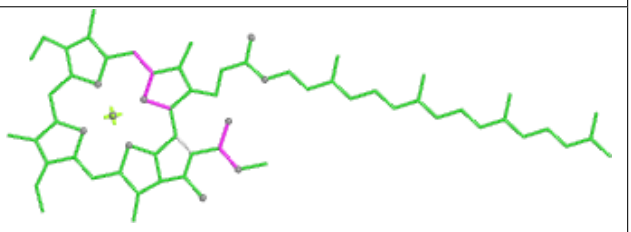


Rings

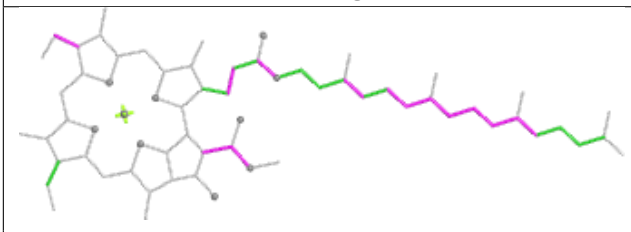
Ligand CLA W 613



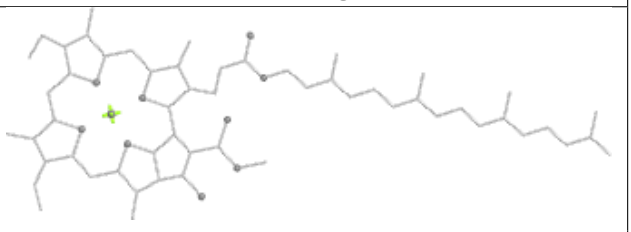
Bond lengths



Bond angles

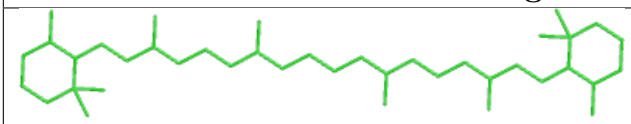


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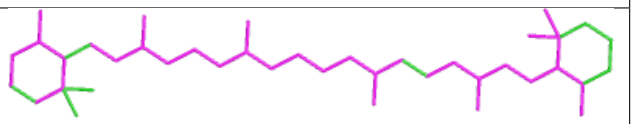


Rings

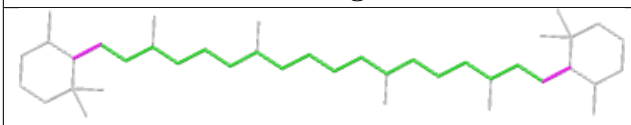
Ligand BCR L 309



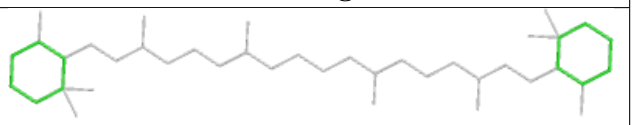
Bond lengths



Bond angles

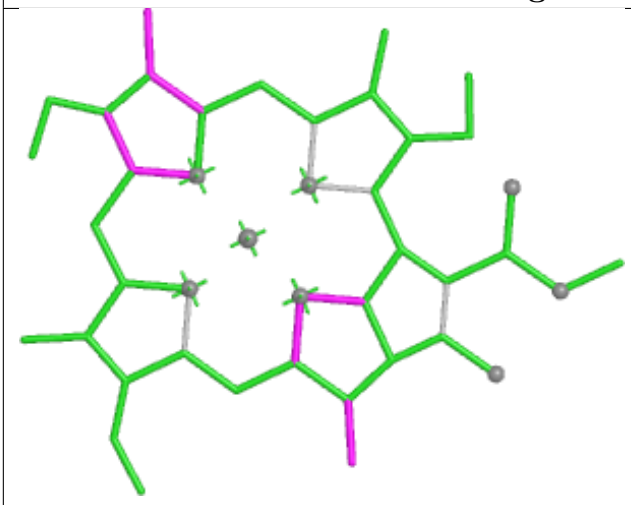


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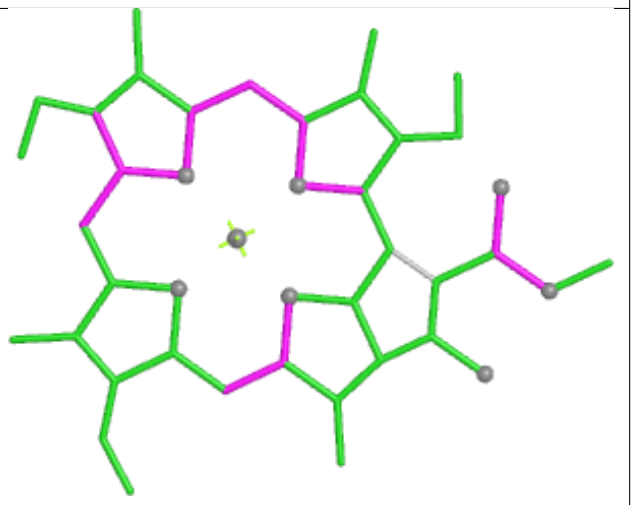


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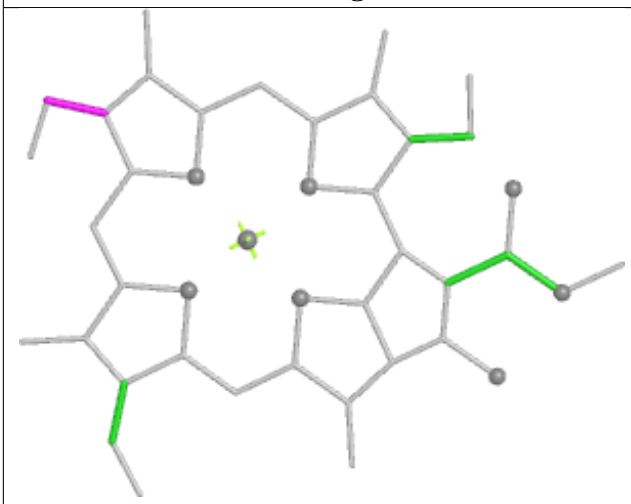
Ligand CLA 5 611



Bond lengths



Bond angles

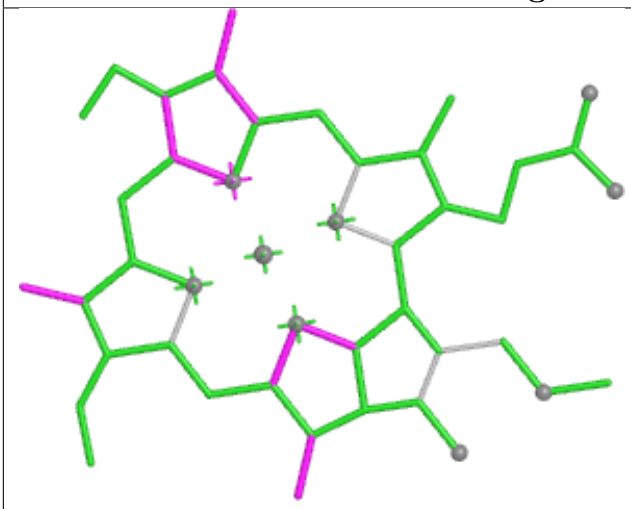


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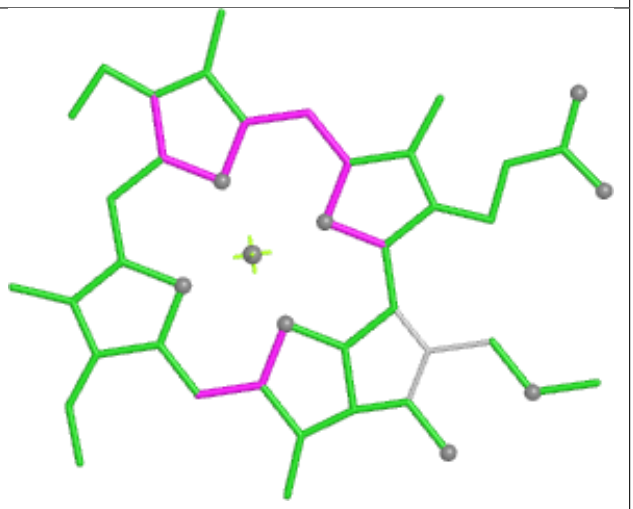


Rings

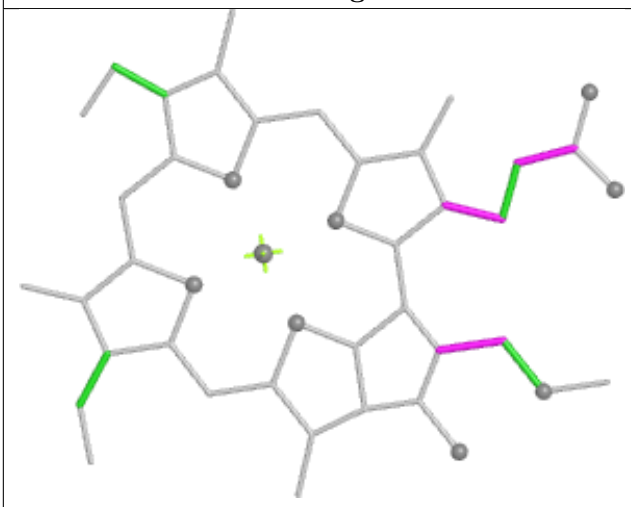
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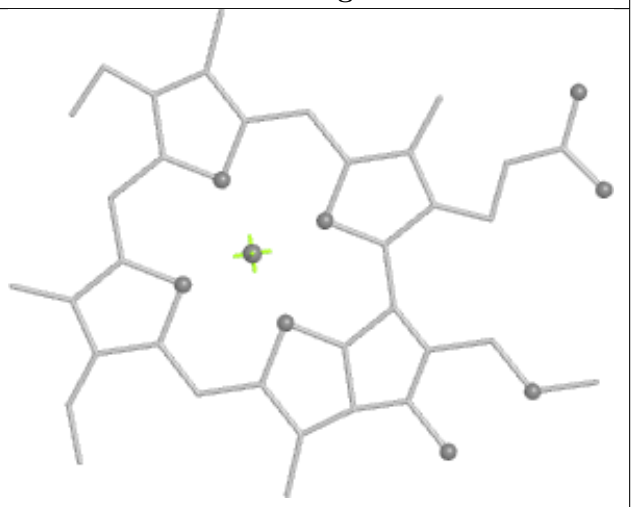
Bond lengths



Bond angles

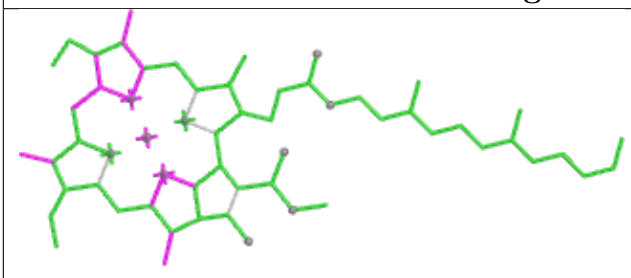


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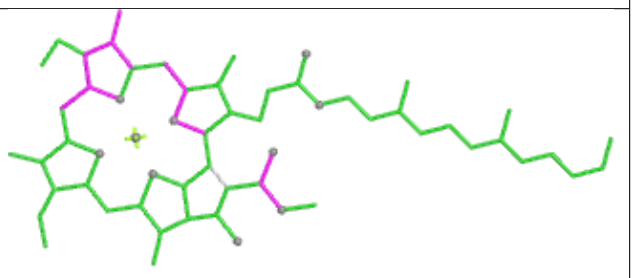


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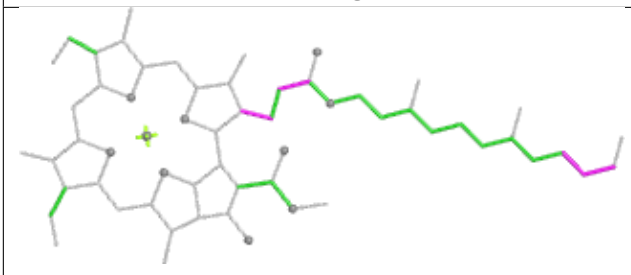
Ligand CLA A 819



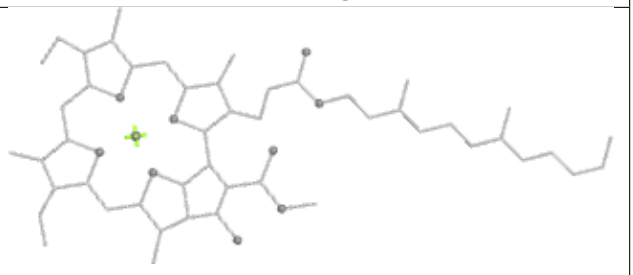
Bond lengths



Bond angles

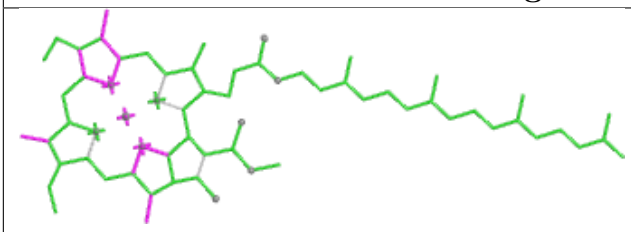


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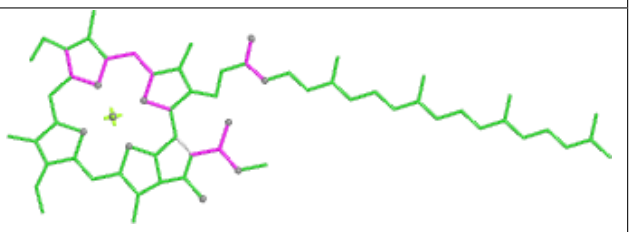


Rings

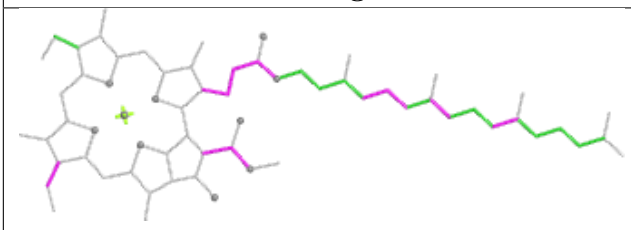
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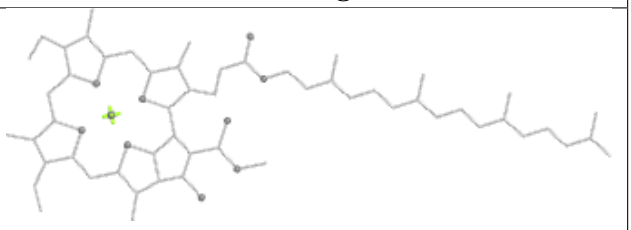
Bond lengths



Bond angles



Torsions



Rings

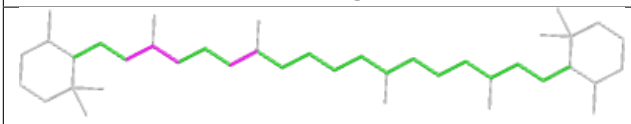
Ligand BCR B 852



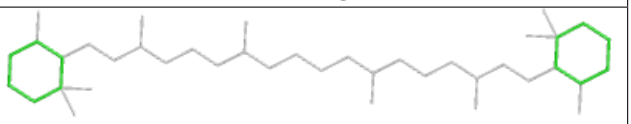
Bond lengths



Bond angles

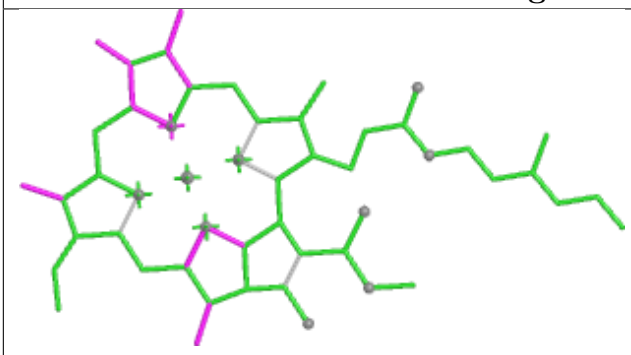


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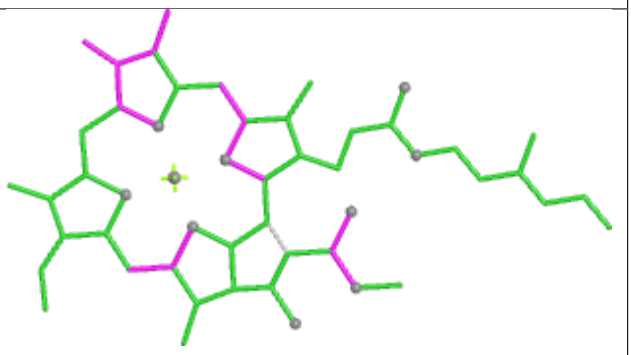


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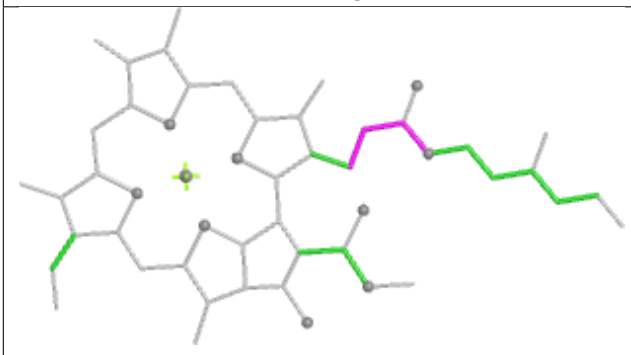
Ligand CLA 6 603



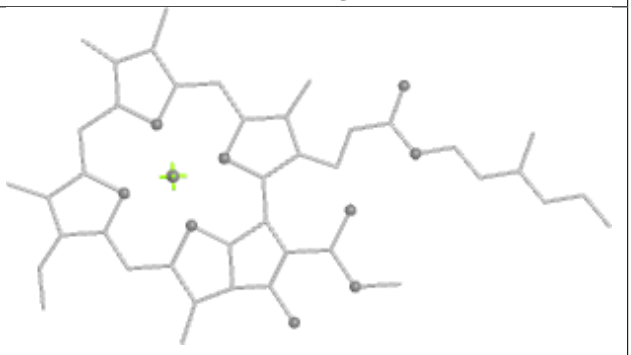
Bond lengths



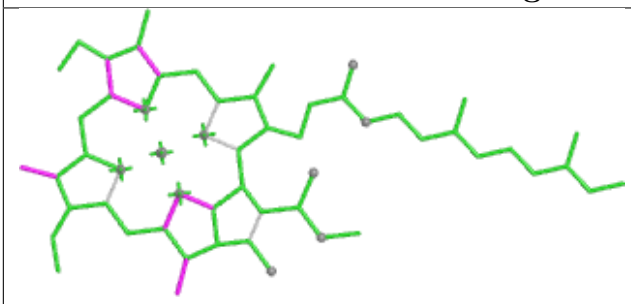
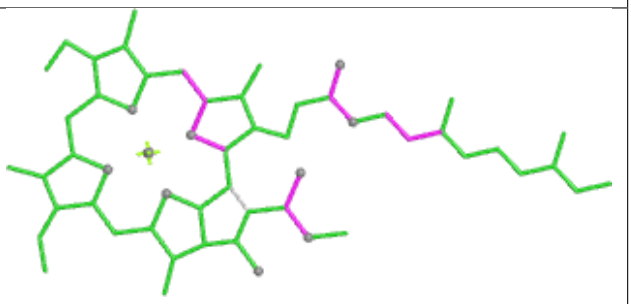
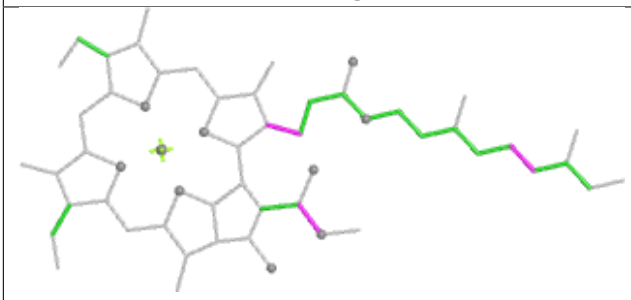
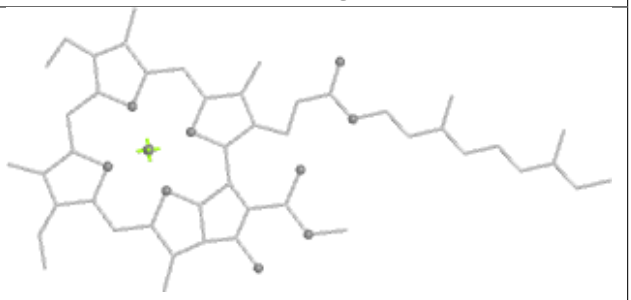
Bond angles

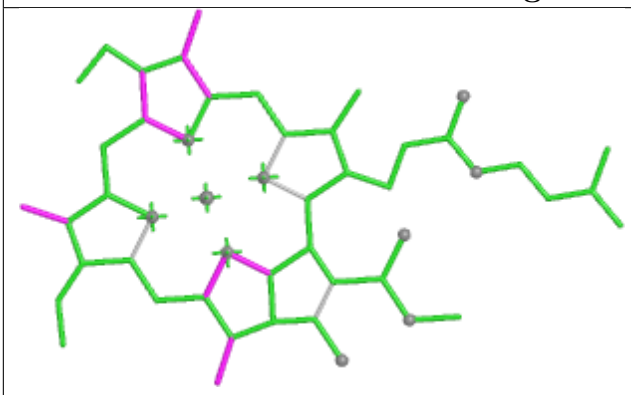
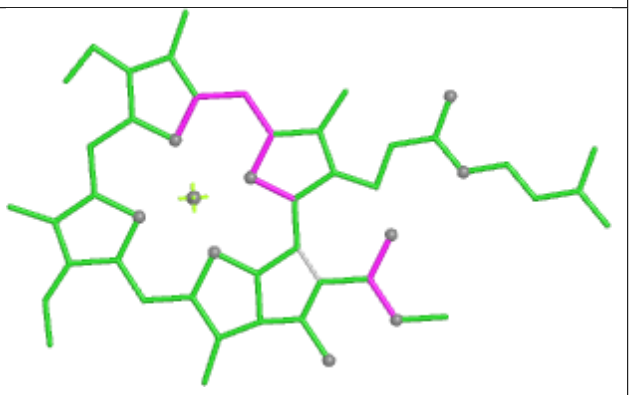
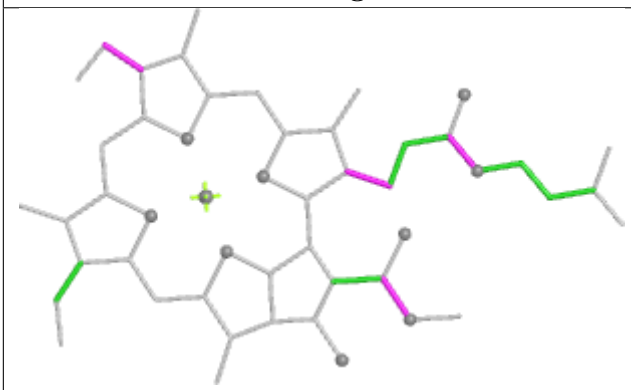
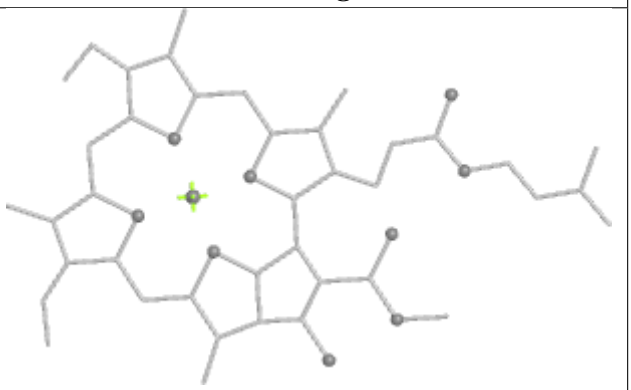


Torsions

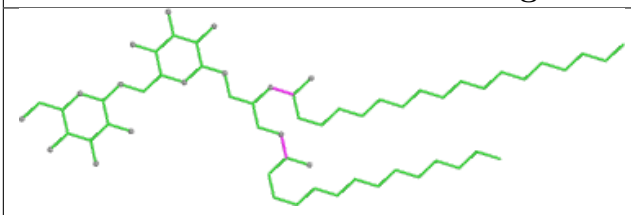


Rings

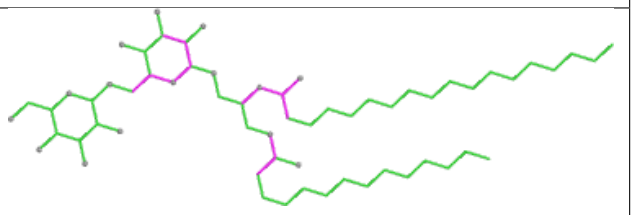
Ligand CLA U 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

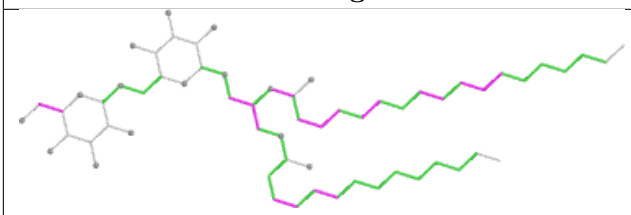
Ligand DGD B 850



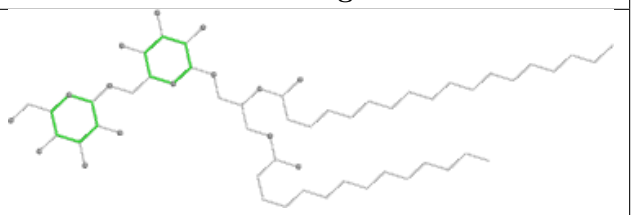
Bond lengths



Bond angles



Torsions

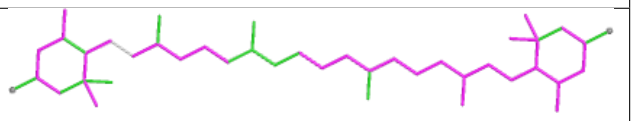


Rings

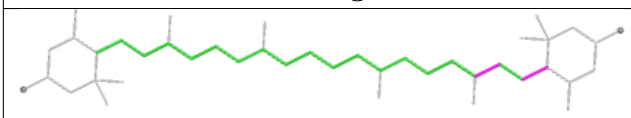
Ligand LUT 4 619



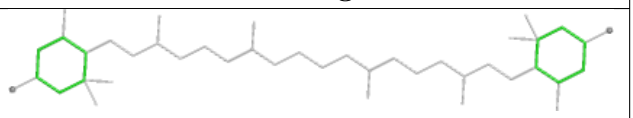
Bond lengths



Bond angles

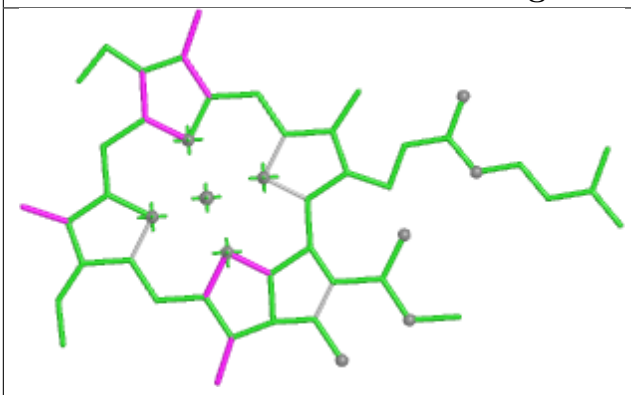


Torsions

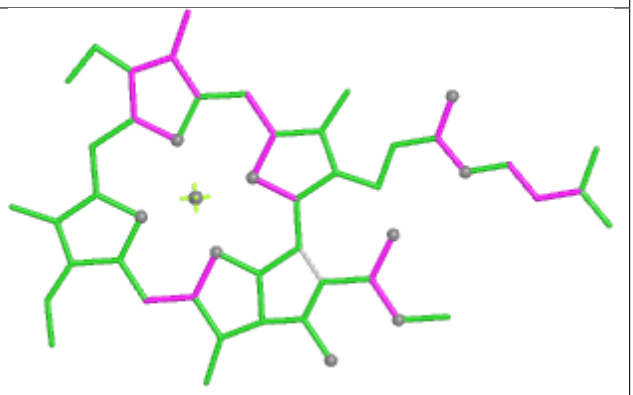


Rings

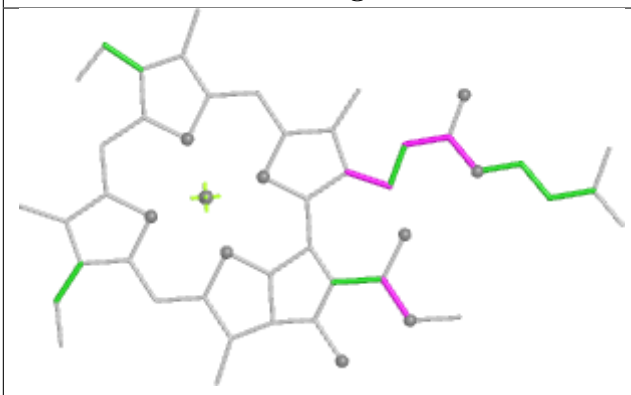
Ligand CLA 8 604



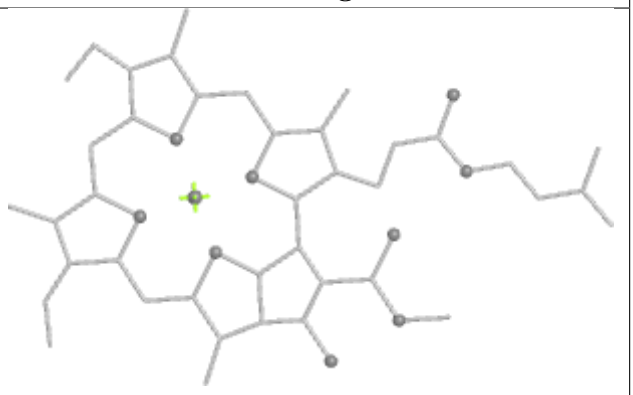
Bond lengths



Bond angles

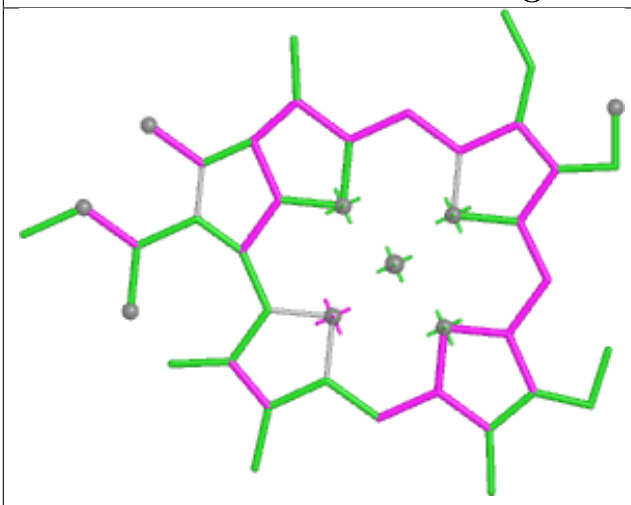


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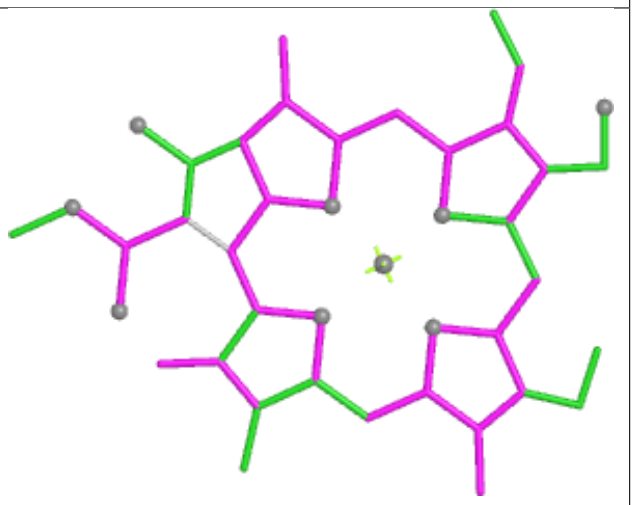


Rings

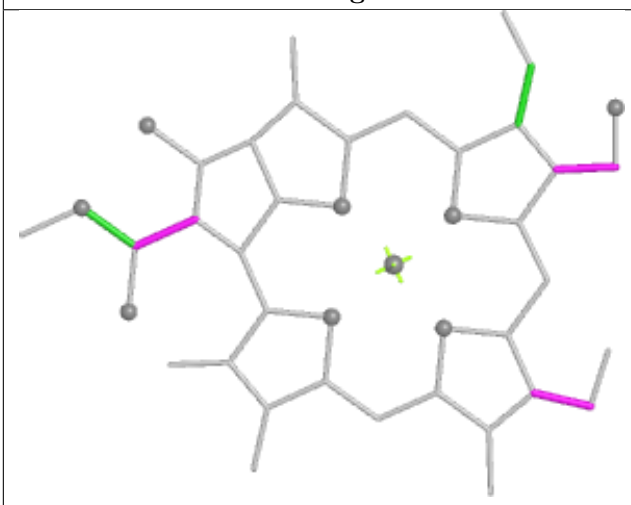
Ligand CHL Y 605



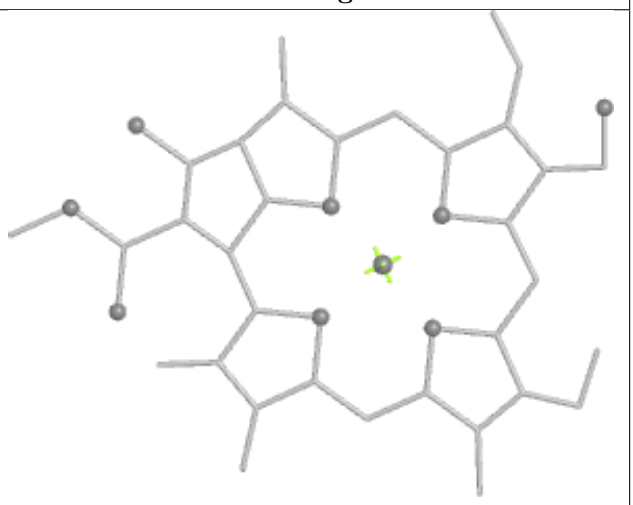
Bond lengths



Bond angles

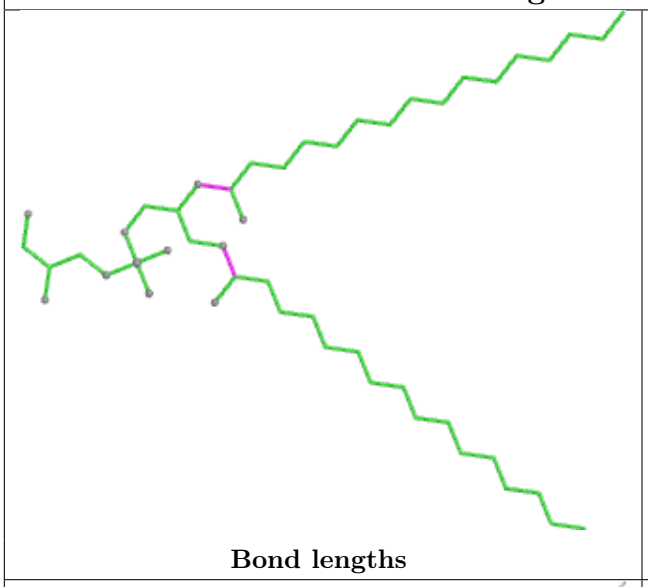


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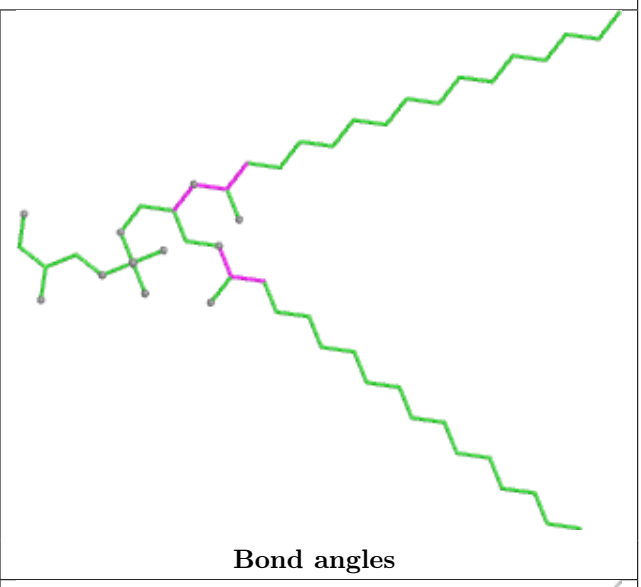


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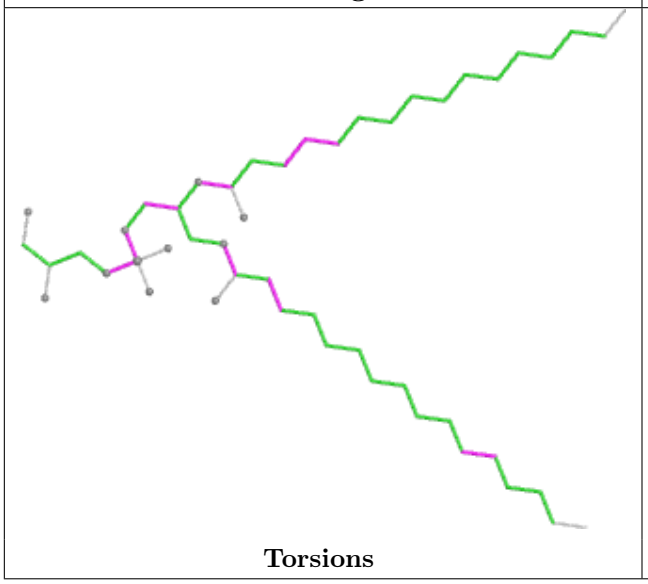
Ligand LHG 3 624



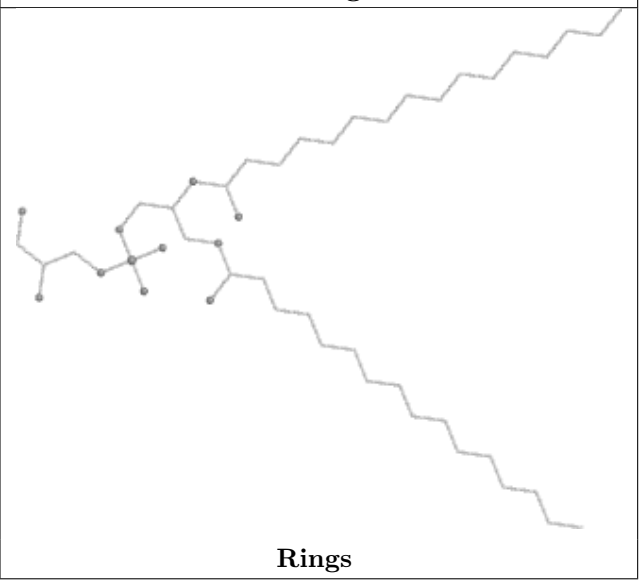
Bond lengths



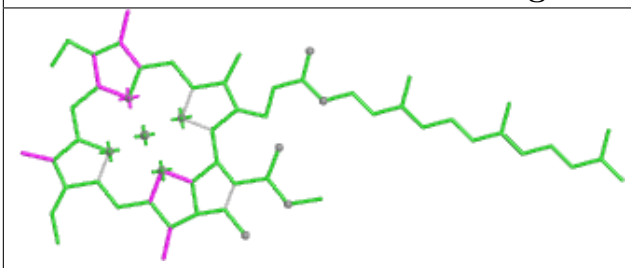
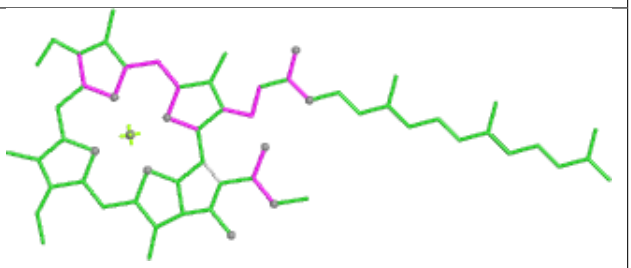
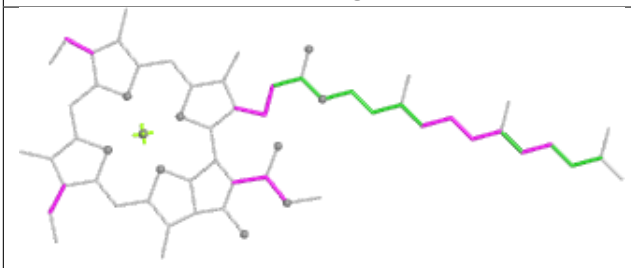
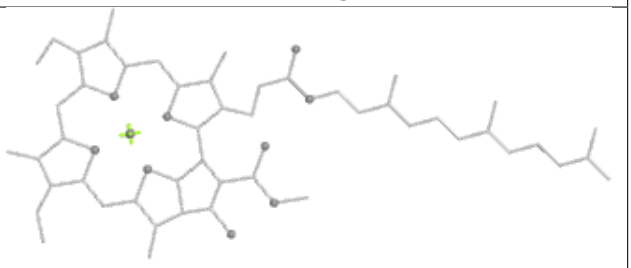
Bond angles

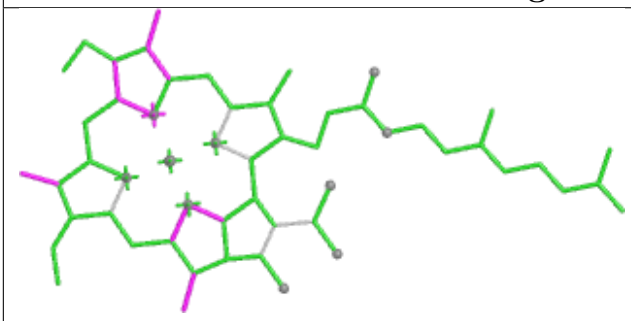
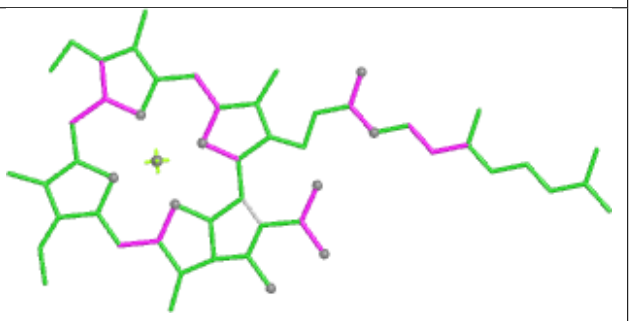
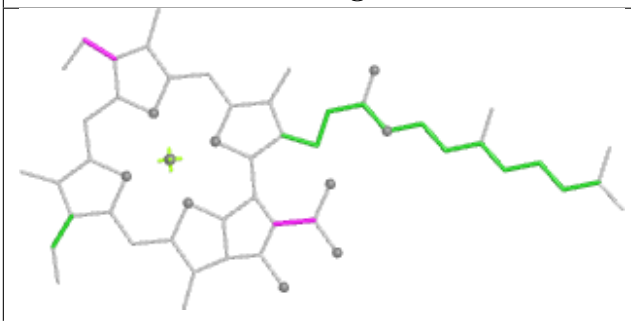
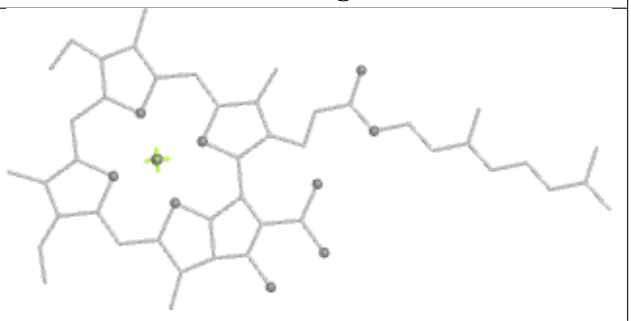


Torsions

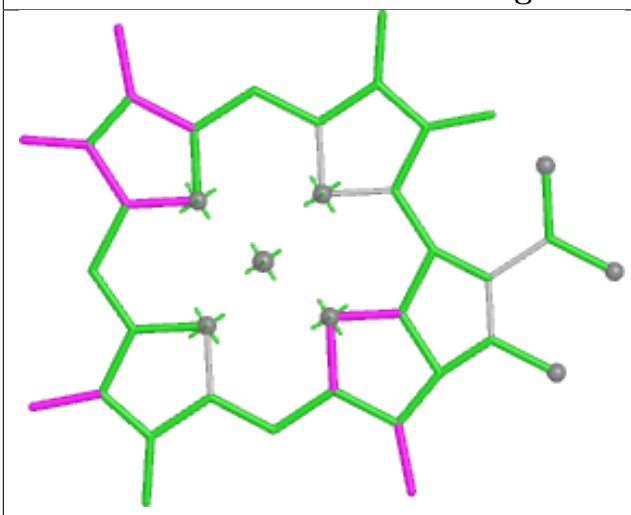


Rings

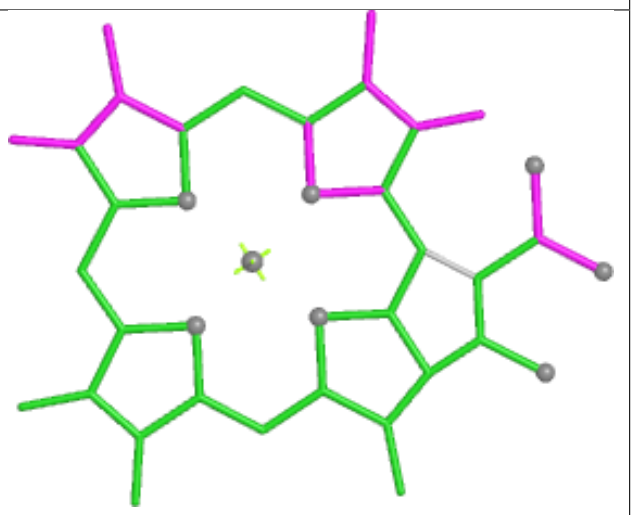
Ligand CLA 3 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

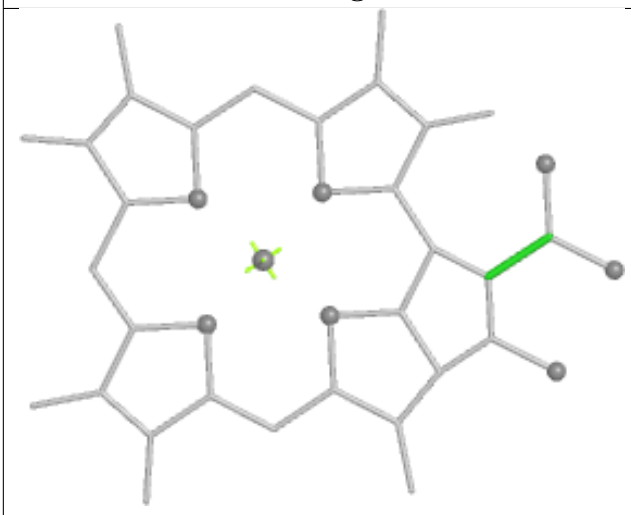
Ligand CLA O 2002



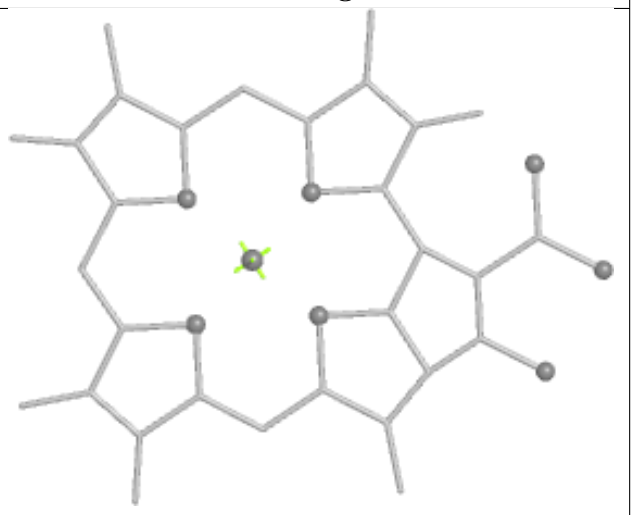
Bond lengths



Bond angles

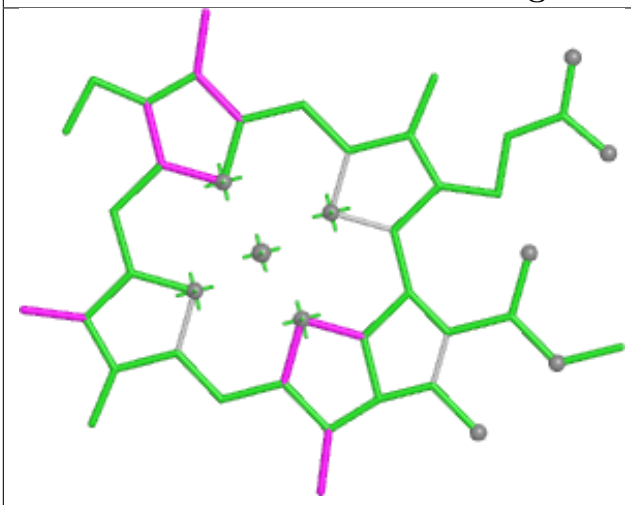


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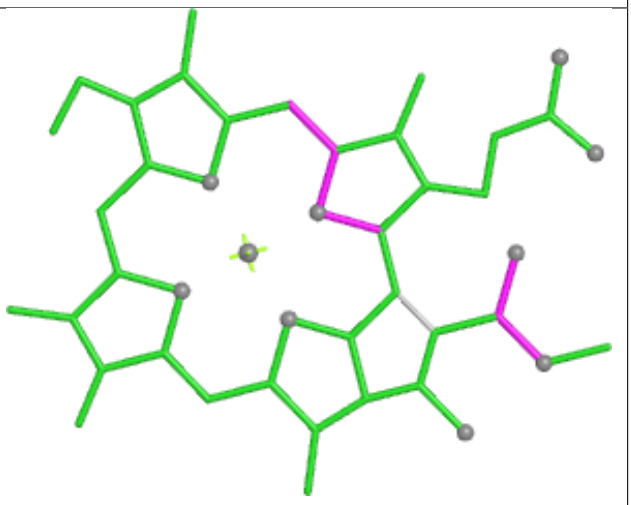


Rings

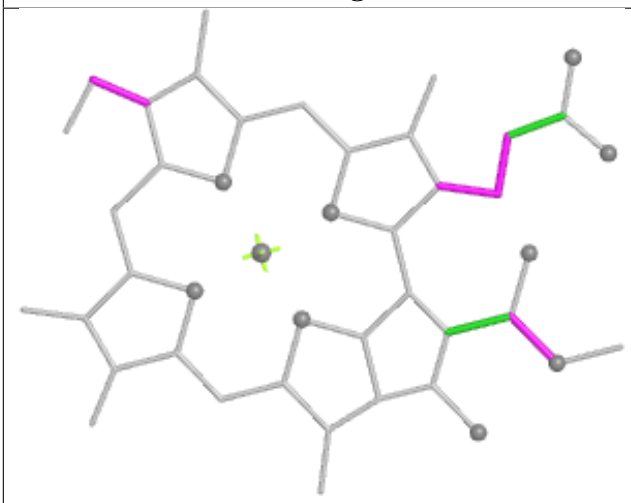
Ligand CLA 2 612



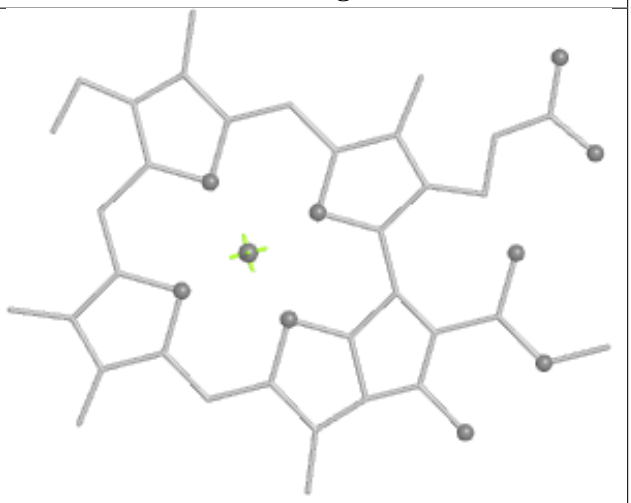
Bond lengths



Bond angles

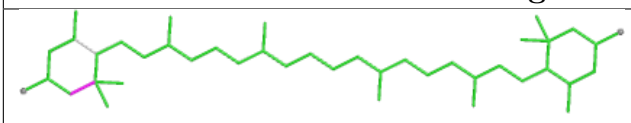


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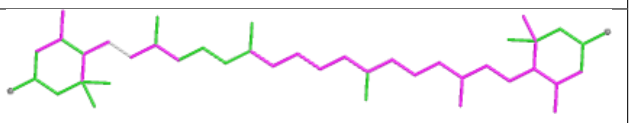


Rings

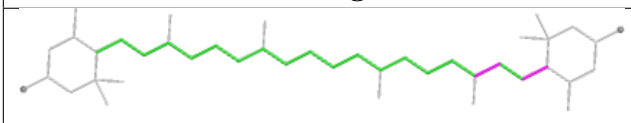
Ligand LUT 1 617



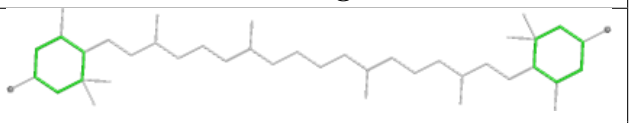
Bond lengths



Bond angles

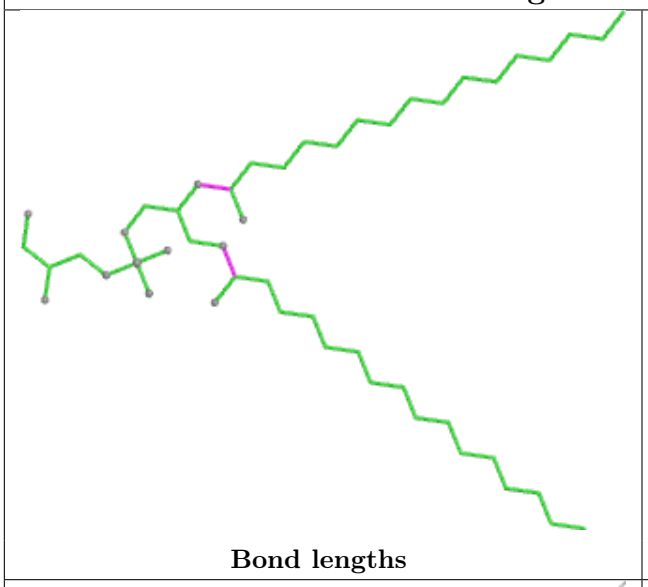


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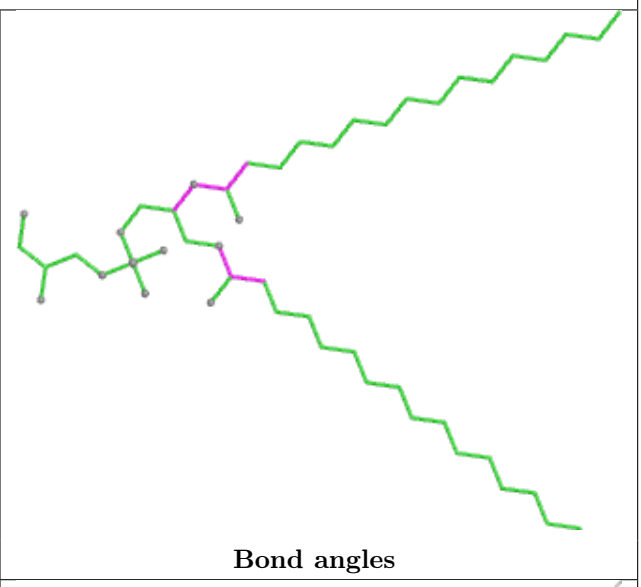


Rings

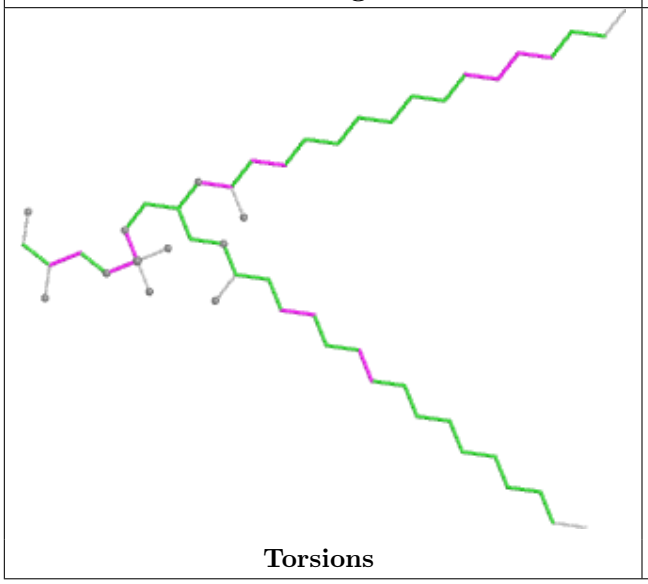
Ligand LHG 5 625



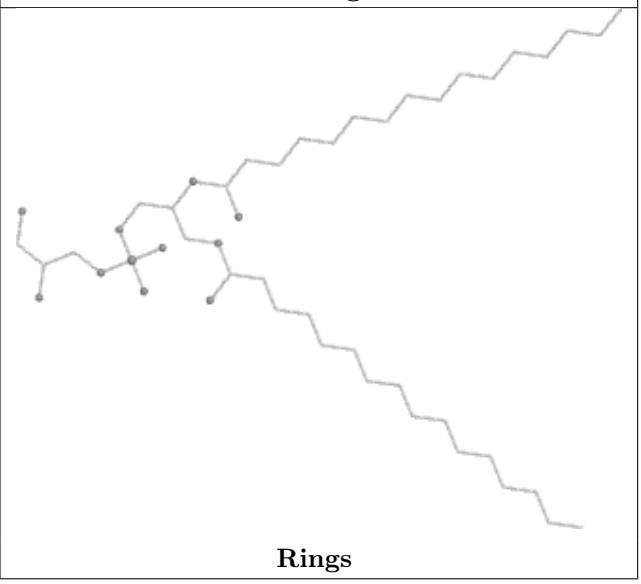
Bond lengths



Bond angles

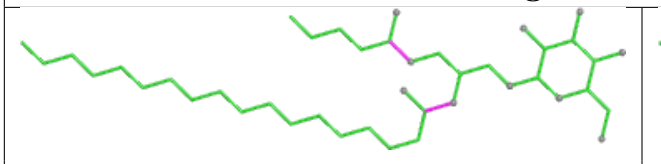


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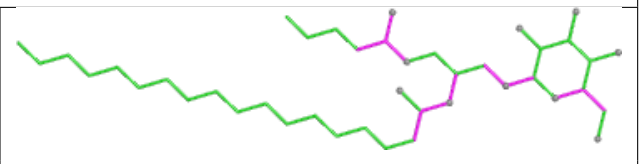


Rings

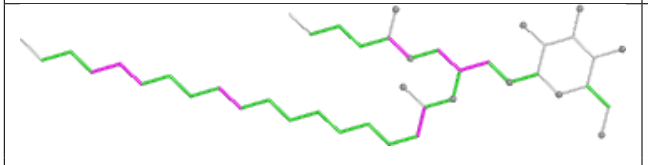
Ligand LMG J 103



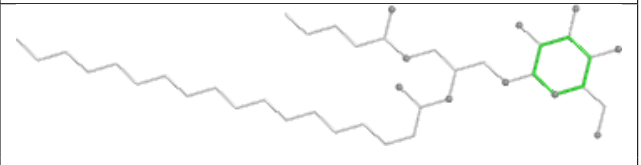
Bond lengths



Bond angles

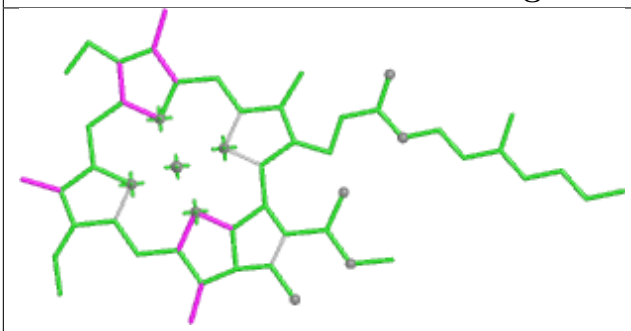


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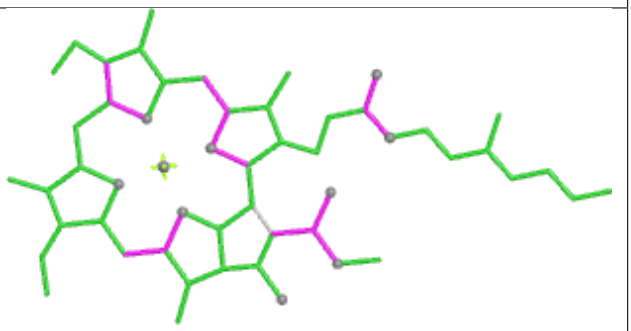


Rings

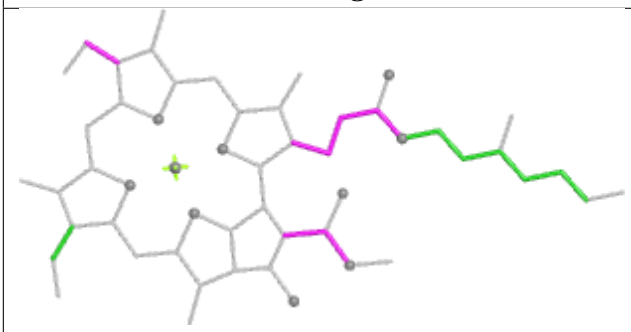
Ligand CLA A 821



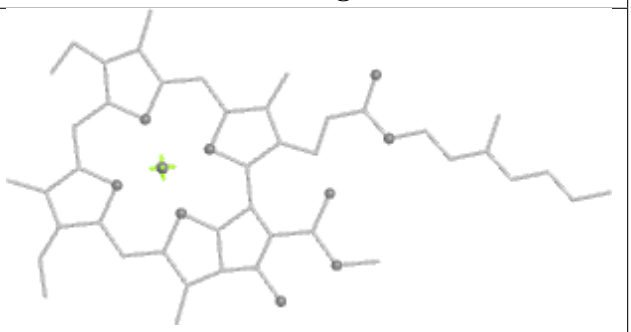
Bond lengths



Bond angles

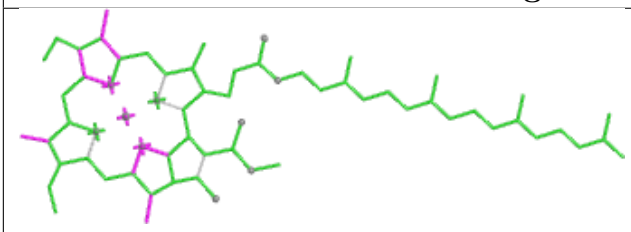


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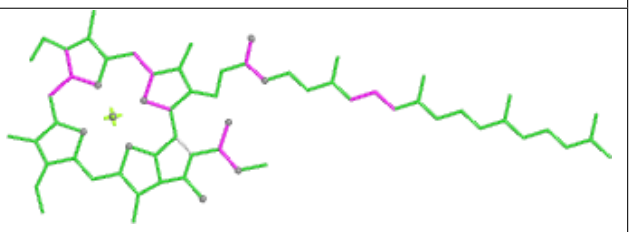


Rings

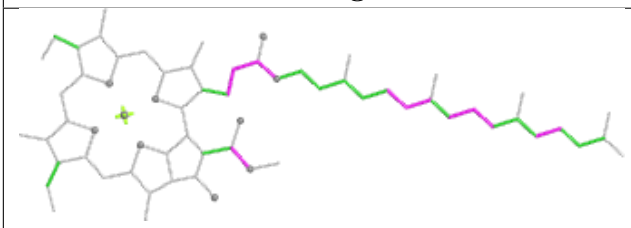
Ligand CLA A 830



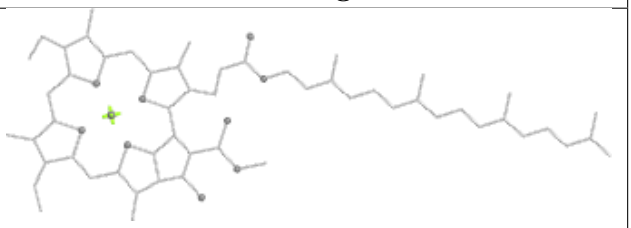
Bond lengths



Bond angles

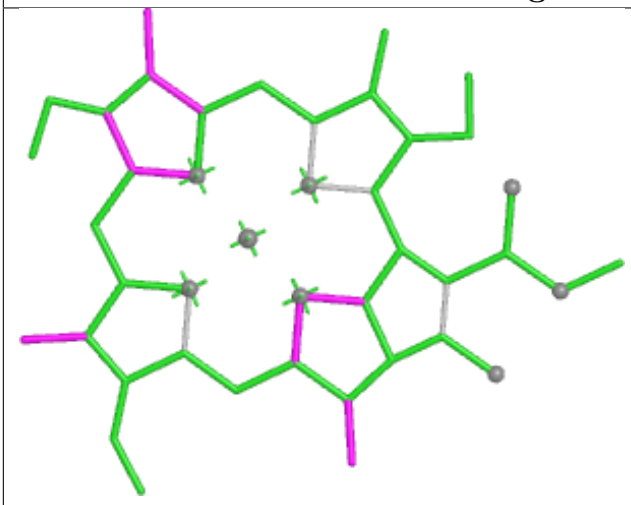


Torsions

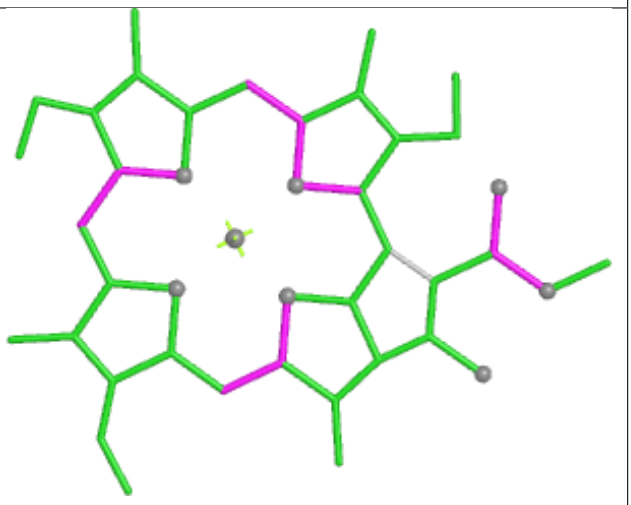


Rings

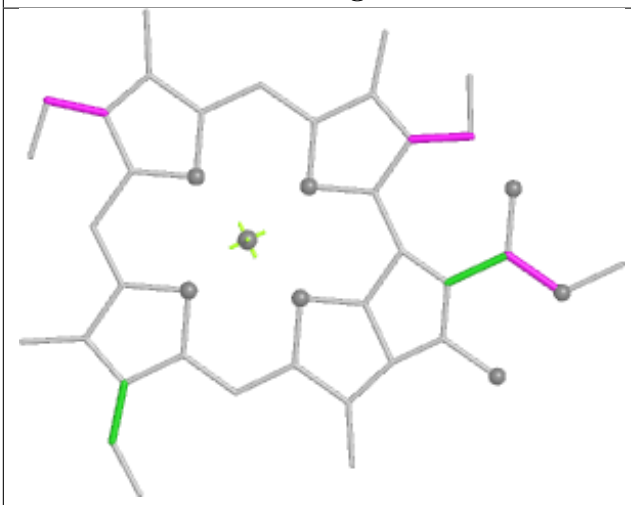
Ligand CLA 8 611



Bond lengths



Bond angles

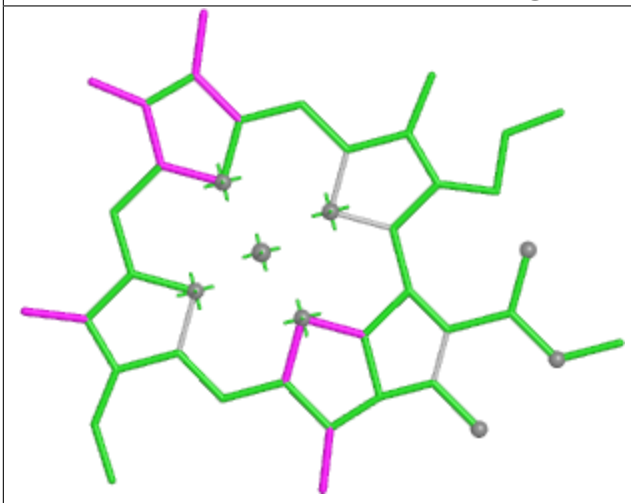


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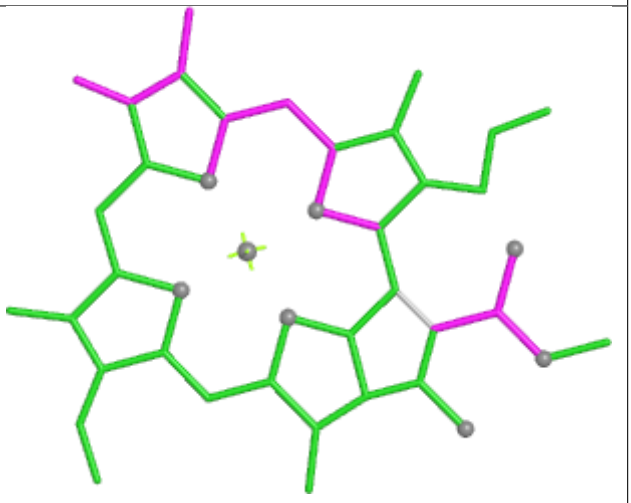


Rings

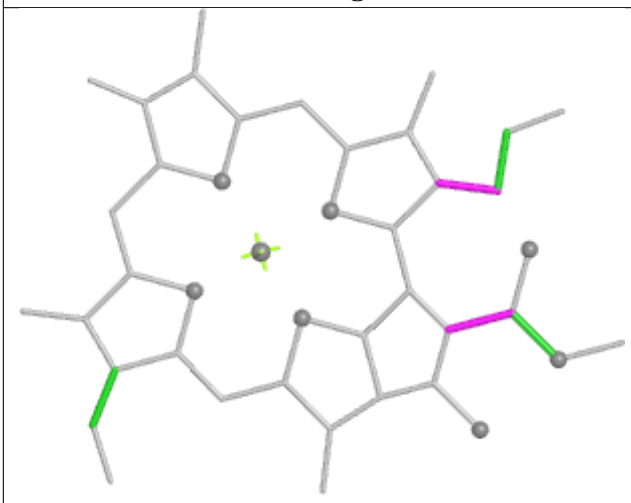
Ligand CLA Z 611



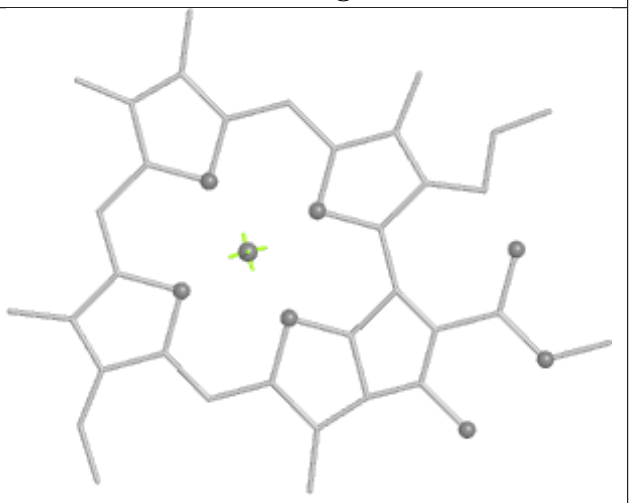
Bond lengths



Bond angles

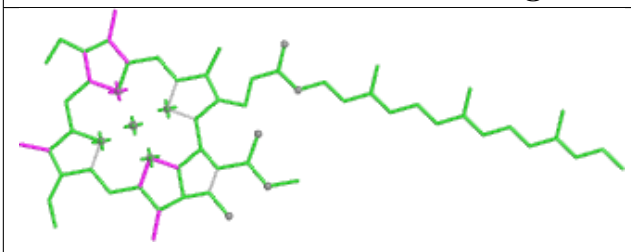


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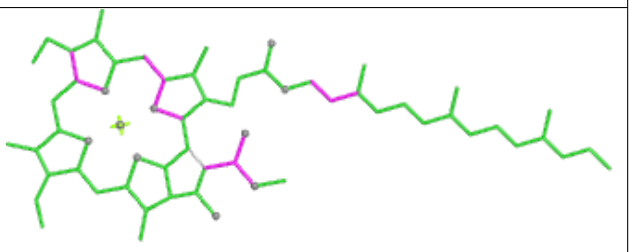


Rings

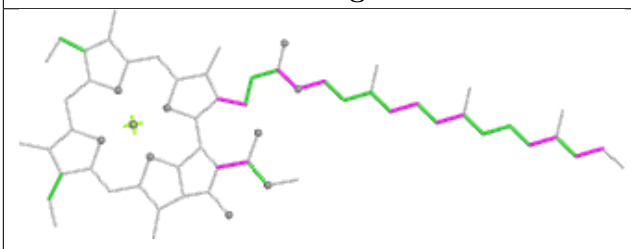
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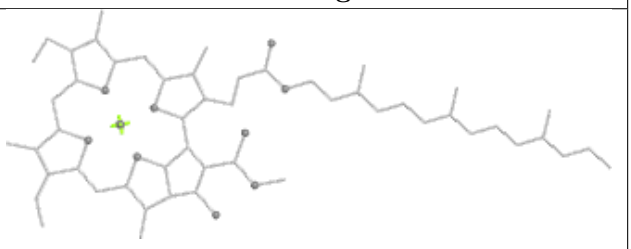
Bond lengths



Bond angles

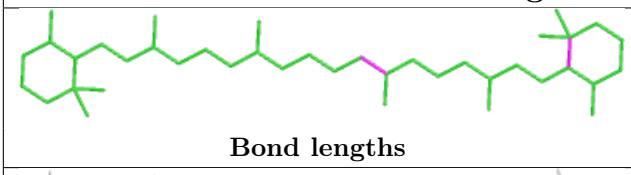


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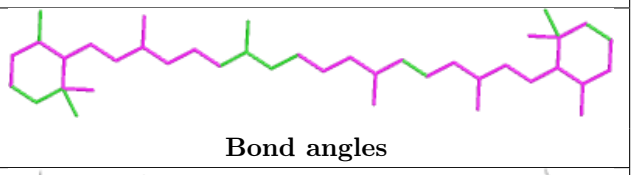


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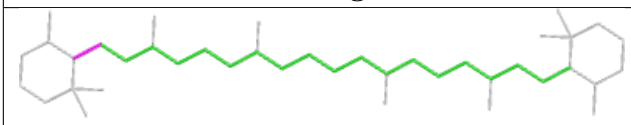
Ligand BCR J 102



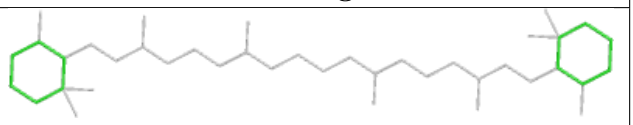
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Bond angles

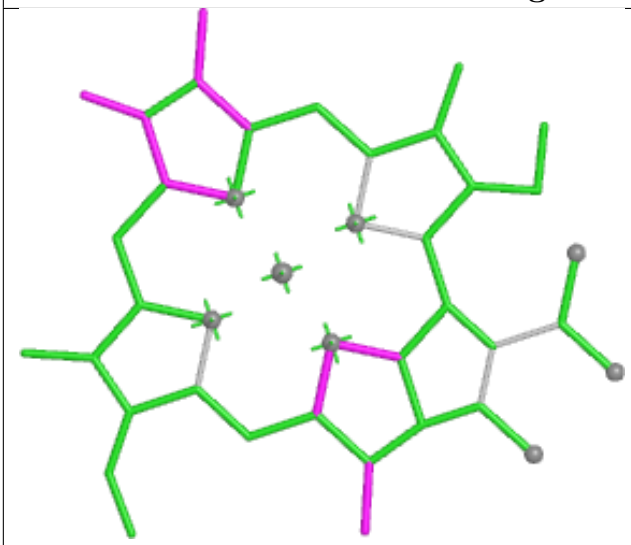


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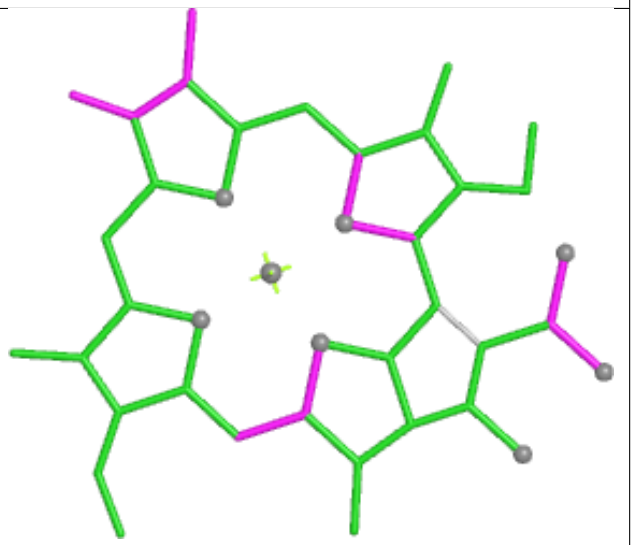


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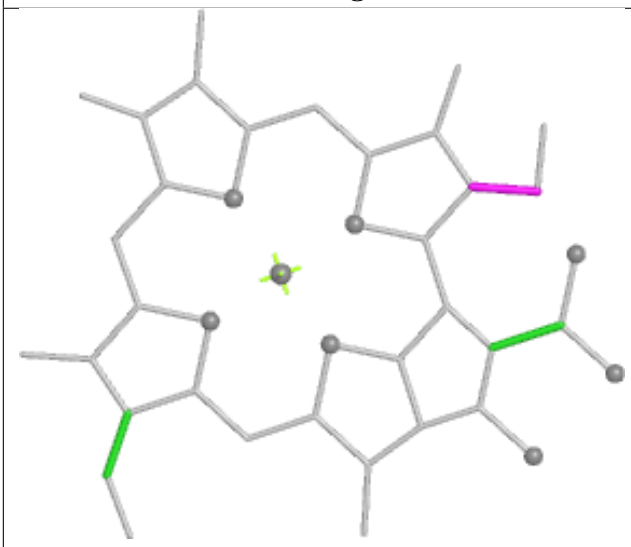
Ligand CLA 4 618



Bond lengths



Bond angles

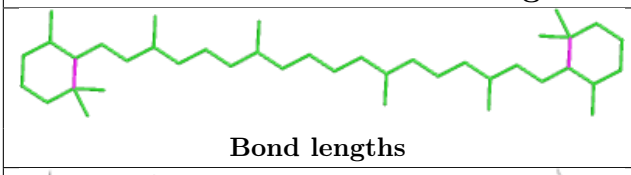


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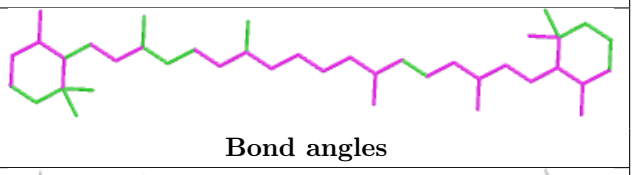


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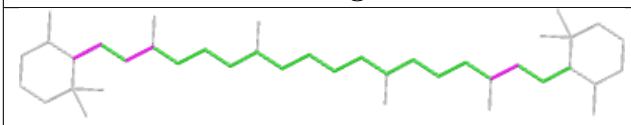
Ligand BCR B 849



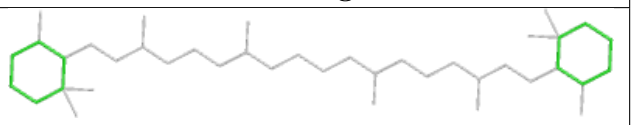
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Bond angles

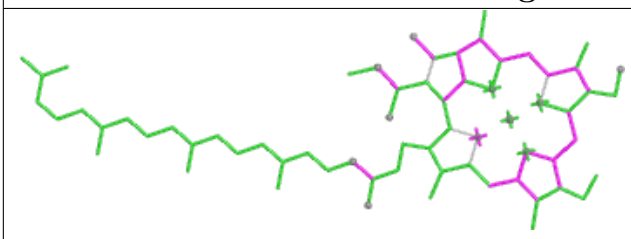


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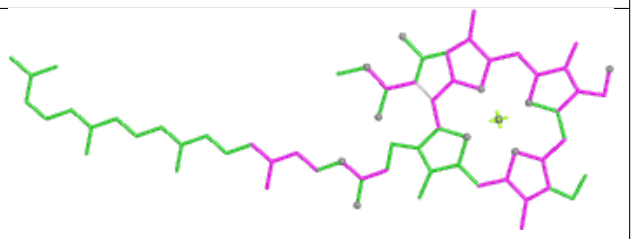


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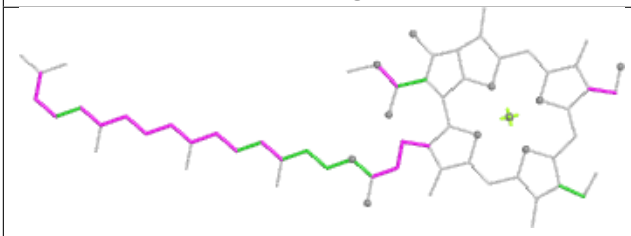
Ligand CHL W 607



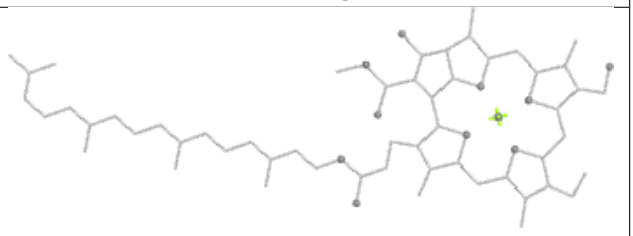
Bond lengths



Bond angles

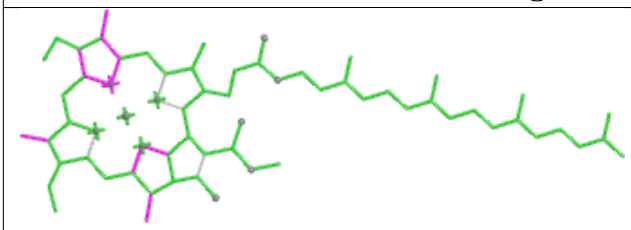


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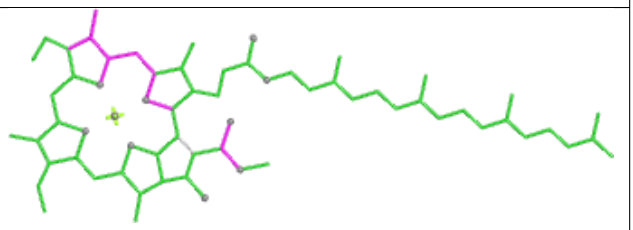


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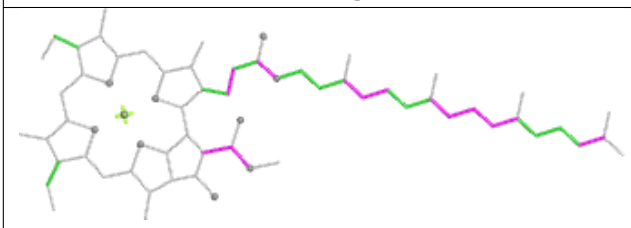
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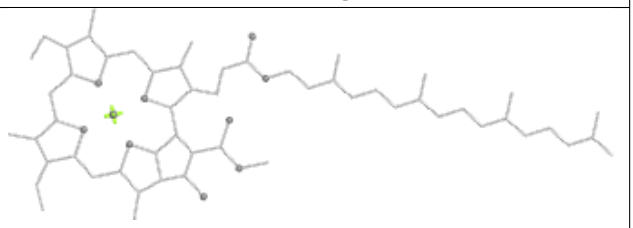
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Bond angles

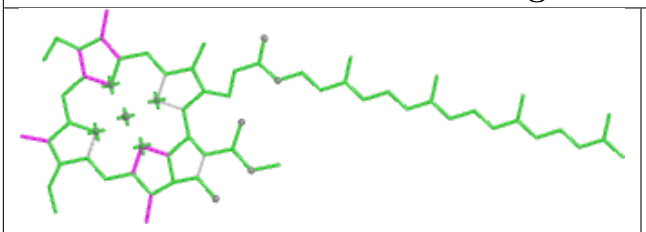


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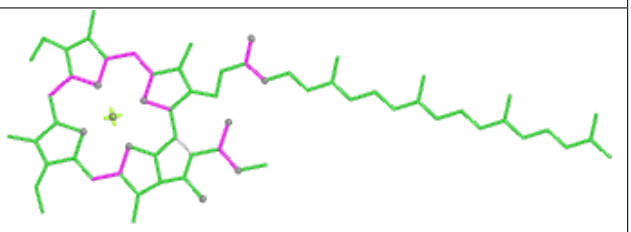


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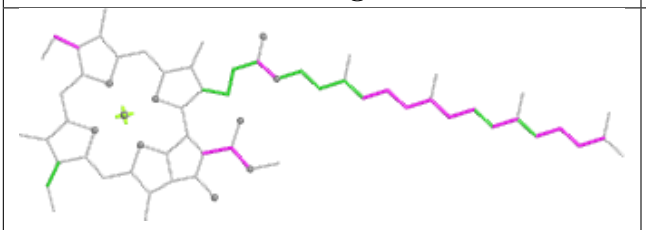
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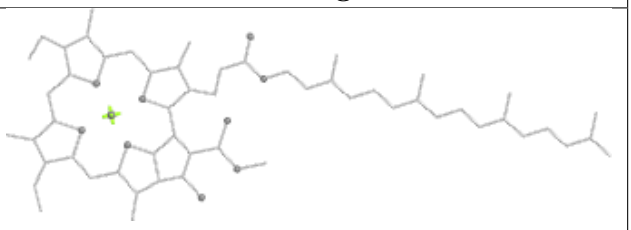
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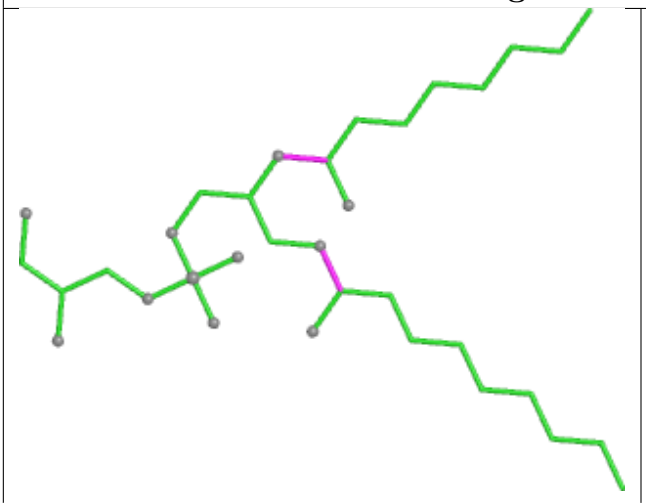


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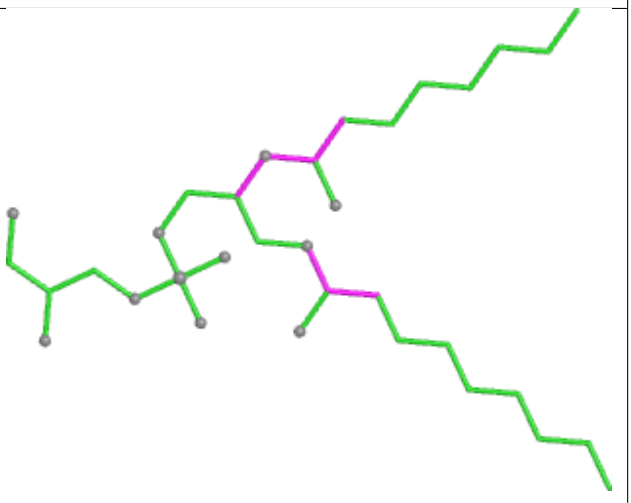


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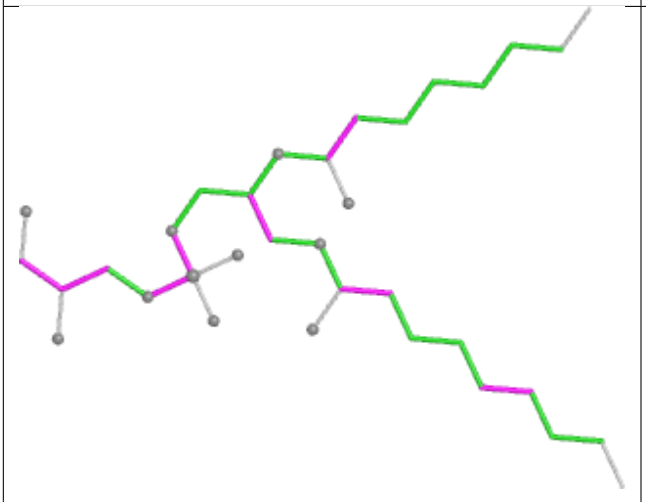
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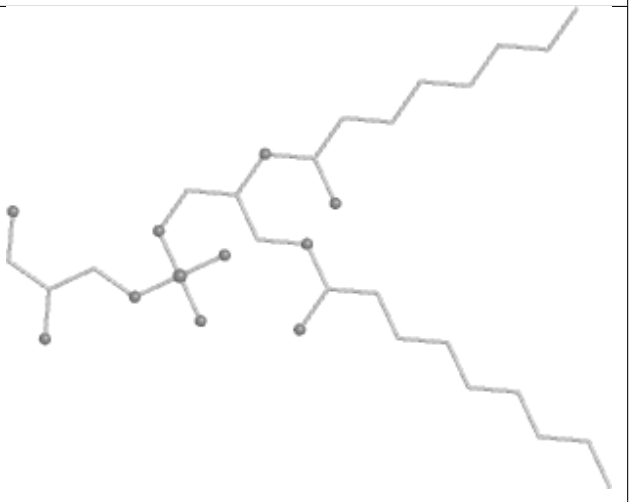
Bond lengths



Bond angles

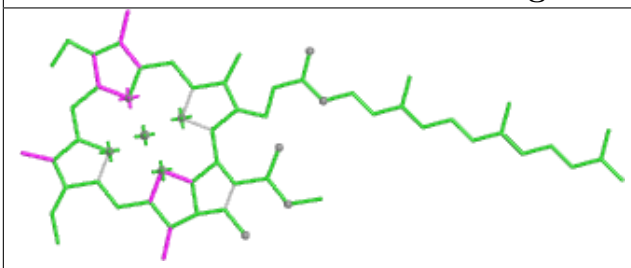


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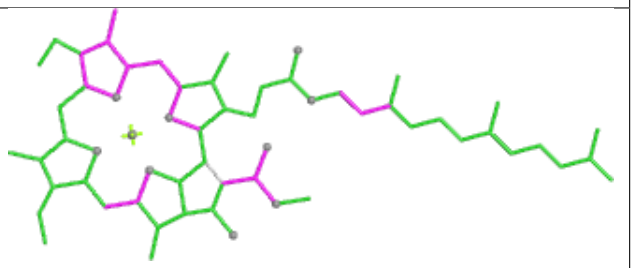


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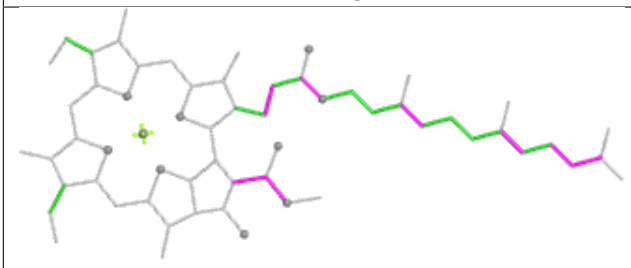
Ligand CLA 8 602



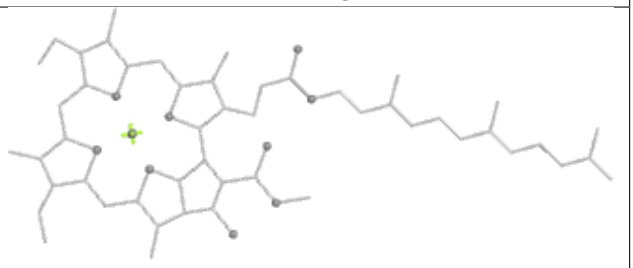
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Bond angles

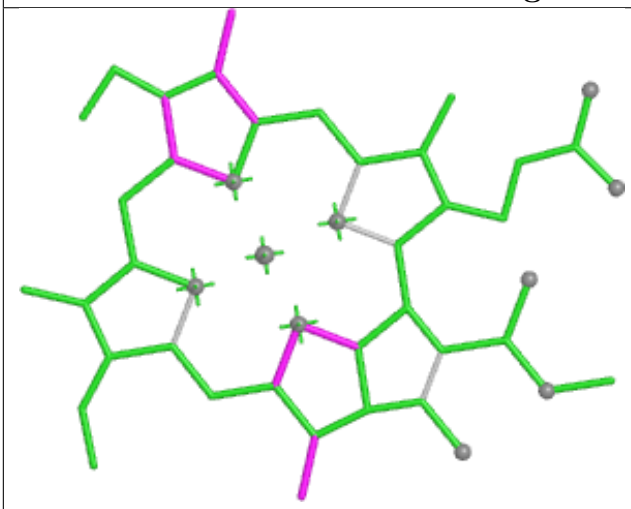


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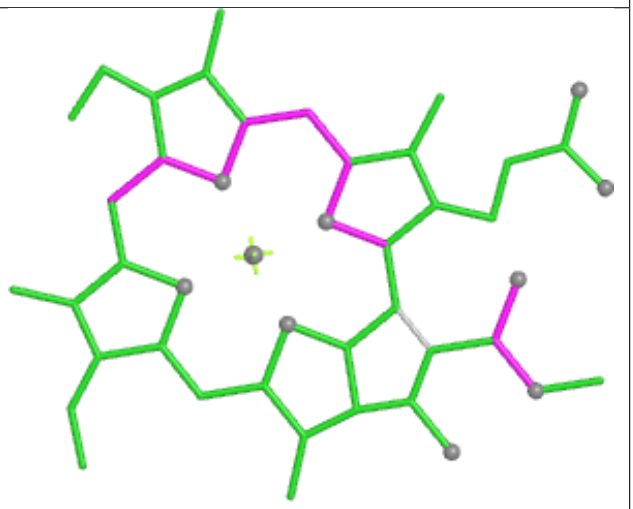


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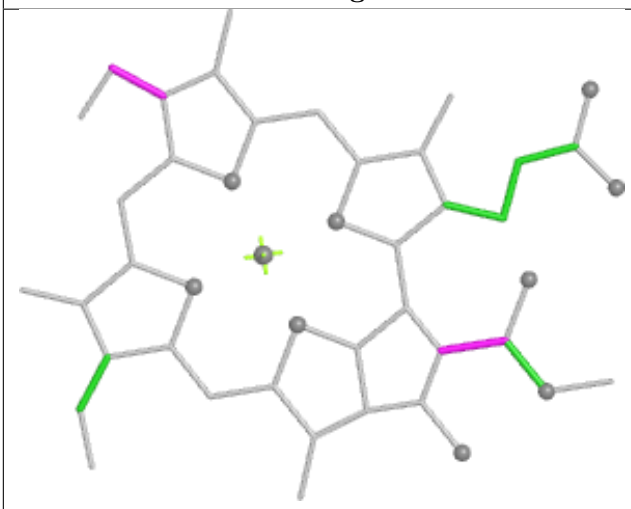
Ligand CLA X 611



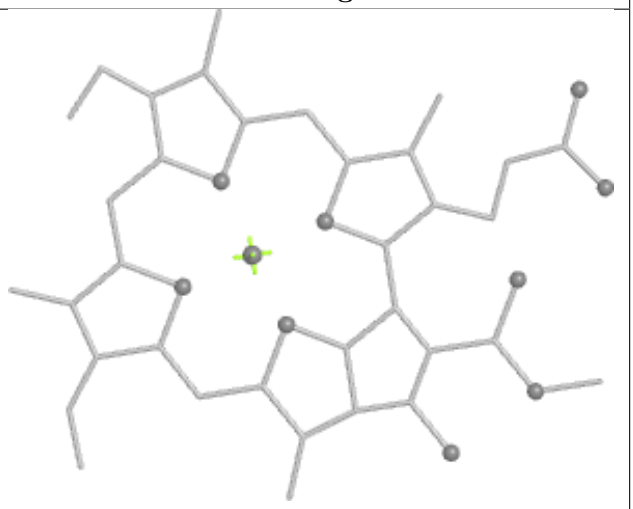
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Bond angles

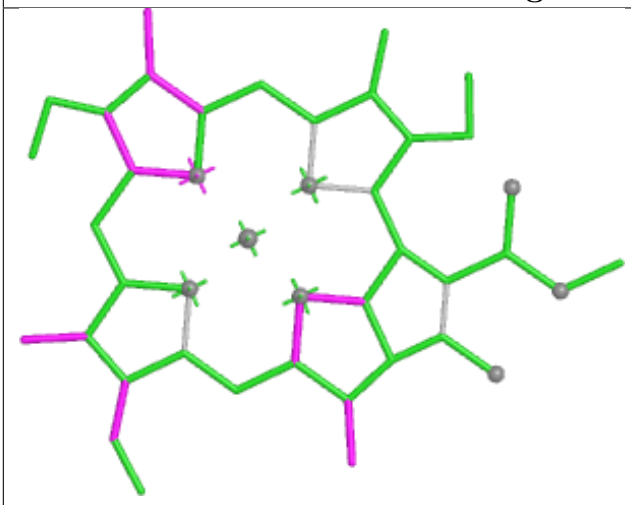


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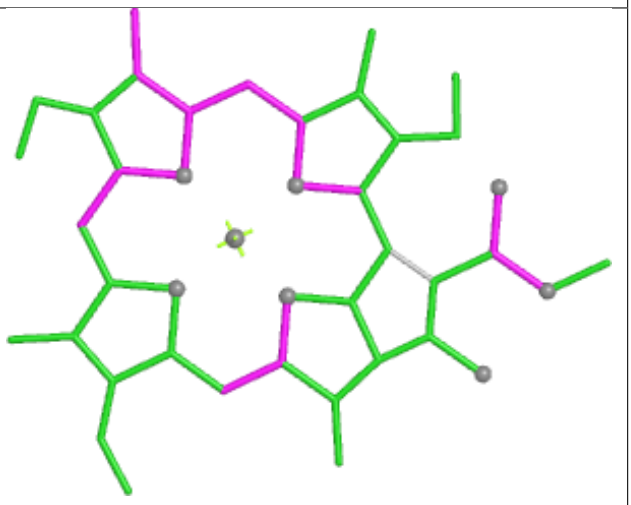


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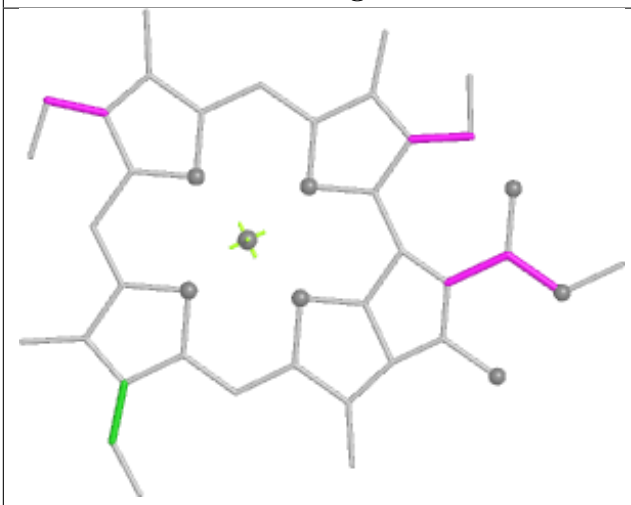
Ligand CLA F 303



Bond lengths



Bond angles

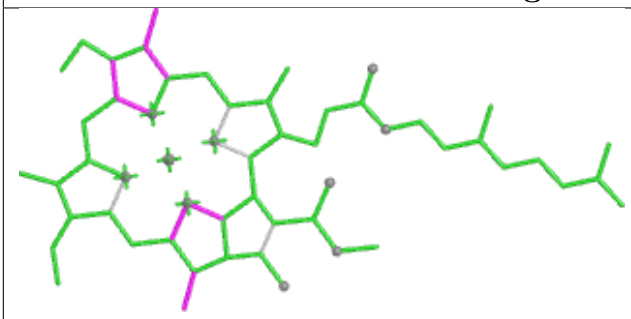


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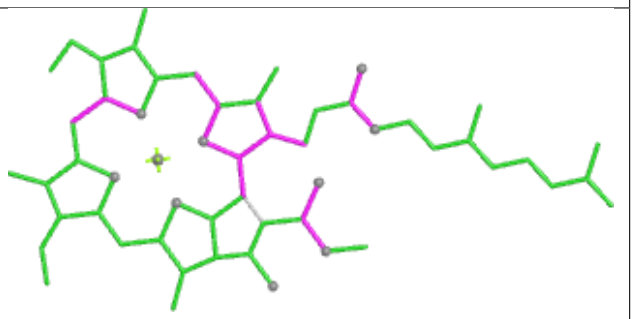


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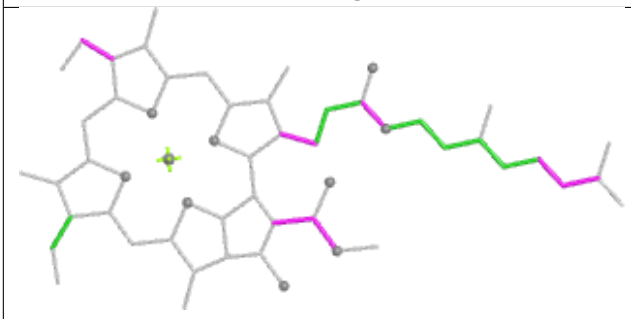
Ligand CLA Y 603



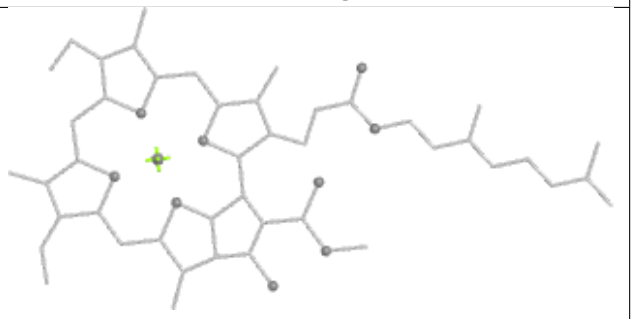
Bond lengths



Bond angles

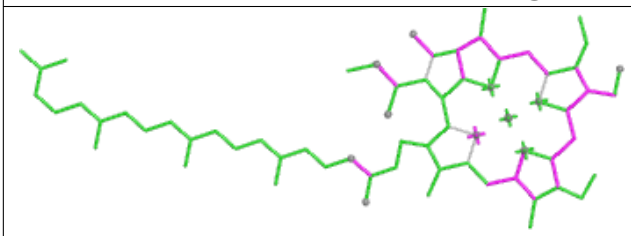


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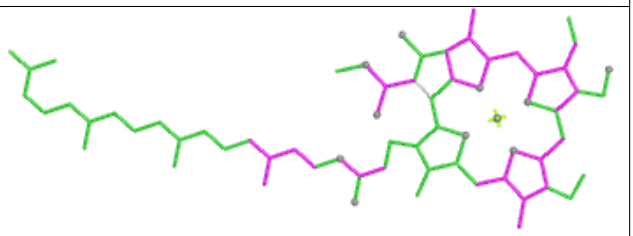


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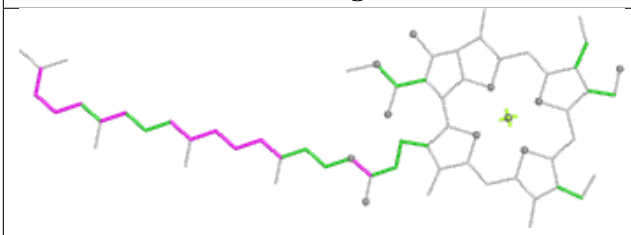
Ligand CHL Z 601



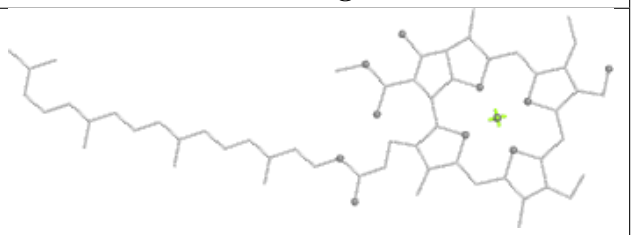
Bond lengths



Bond angles

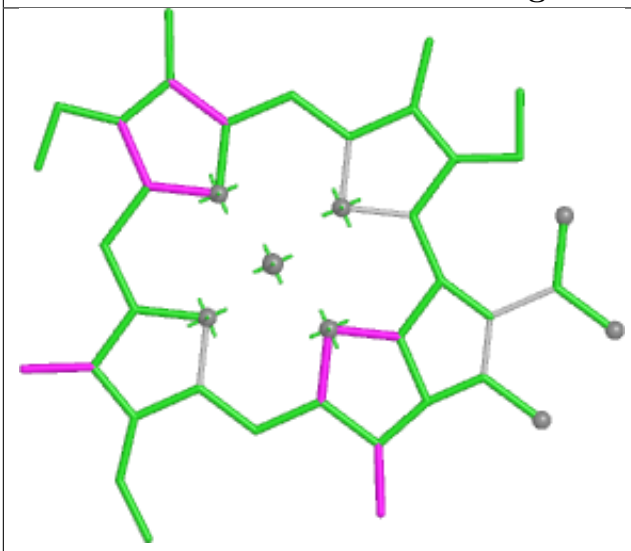


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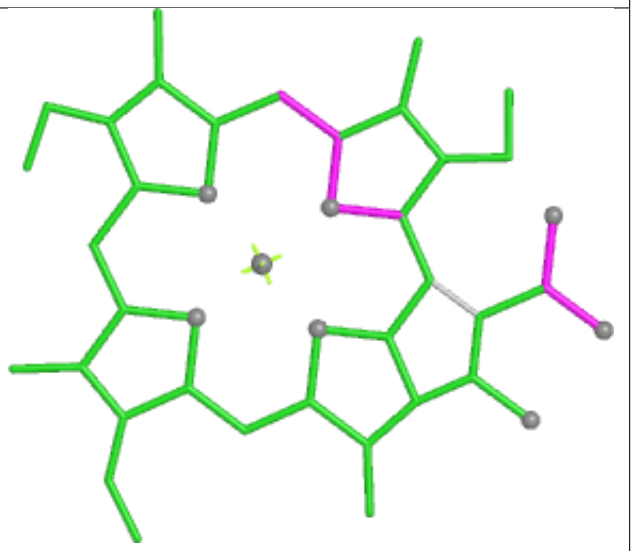


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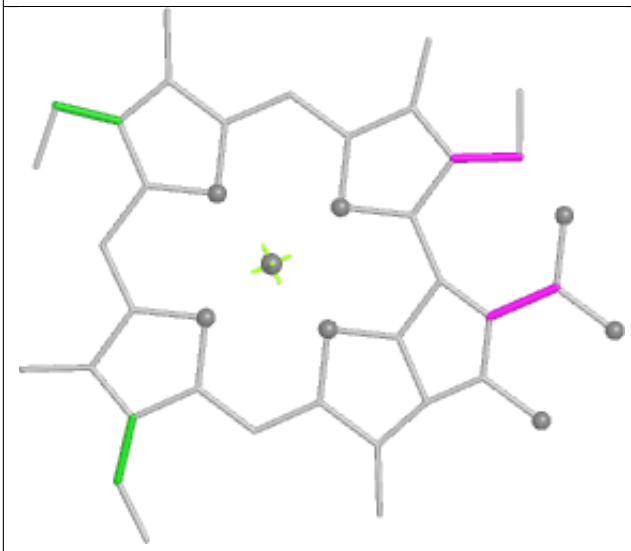
Ligand CLA 4 612



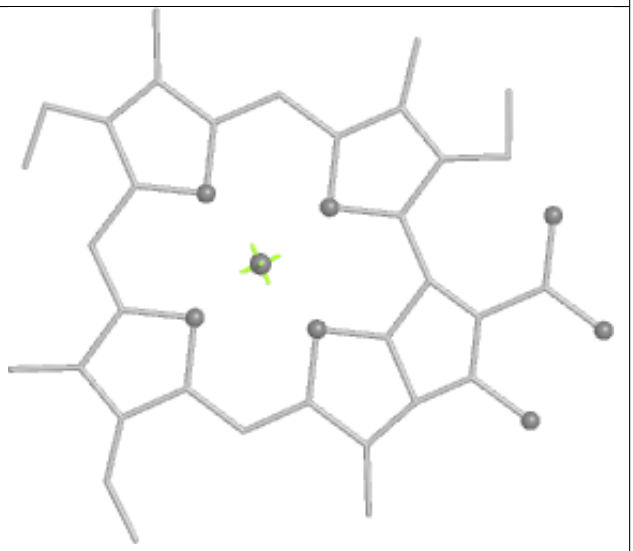
Bond lengths



Bond angles

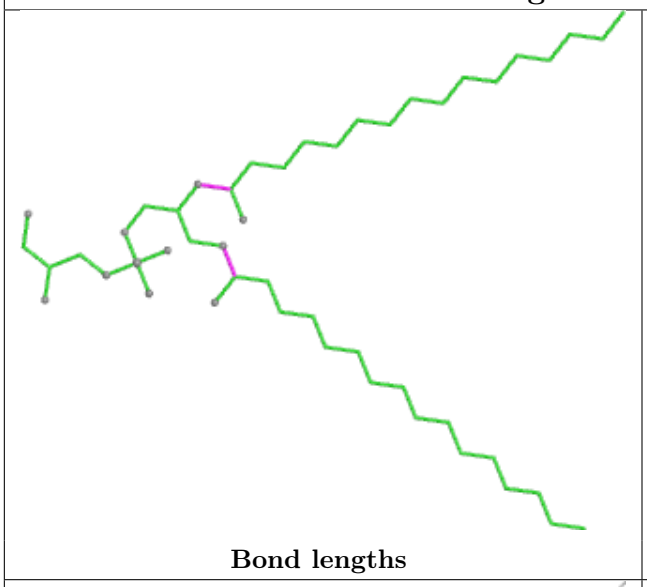


Torsions

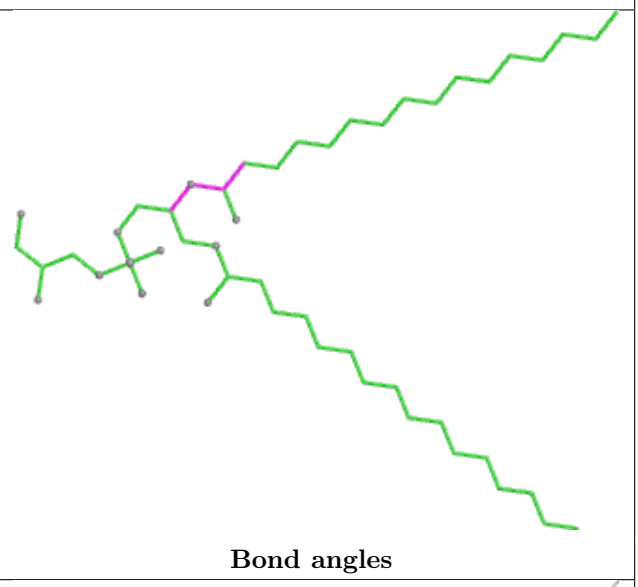


Rings

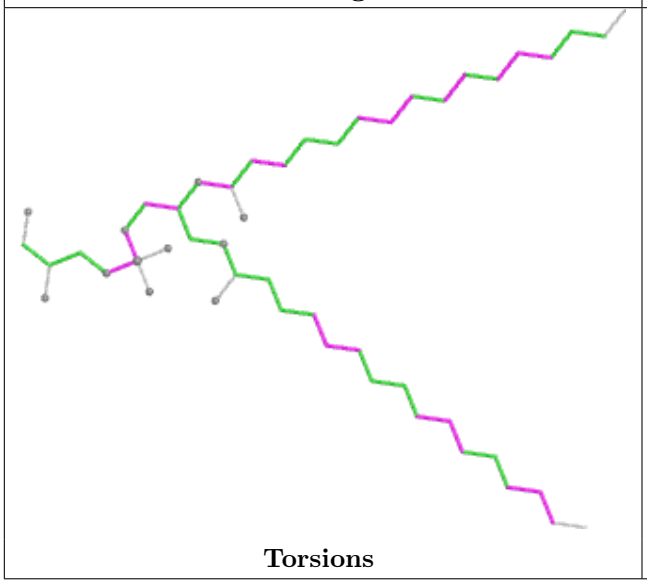
Ligand LHG 9 623



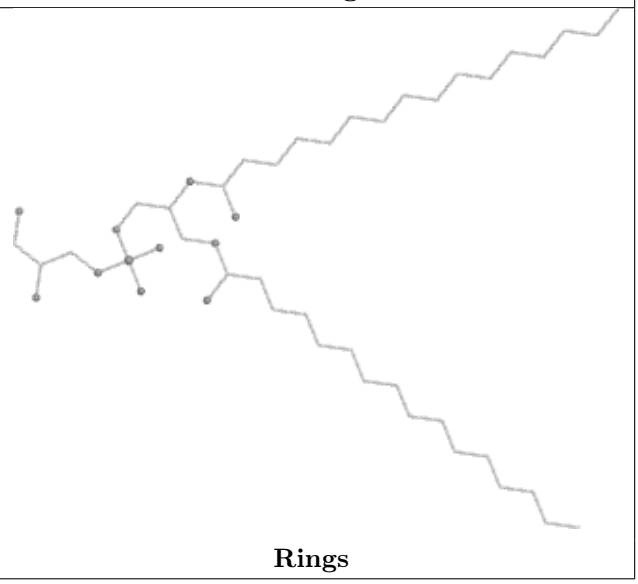
Bond lengths



Bond angles

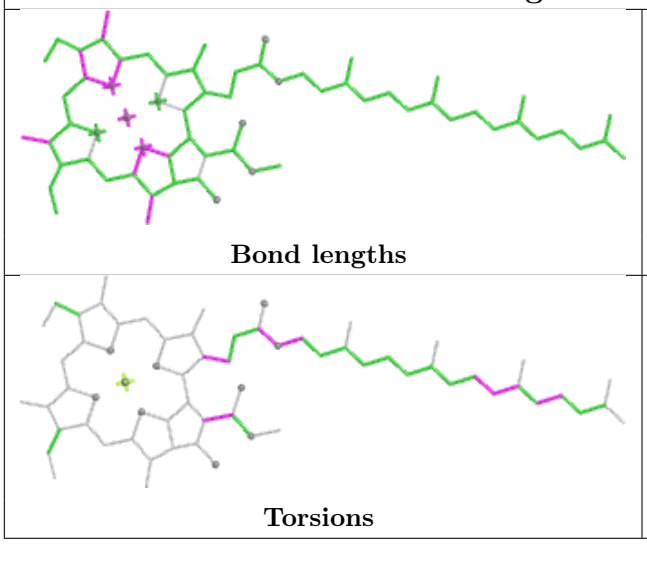


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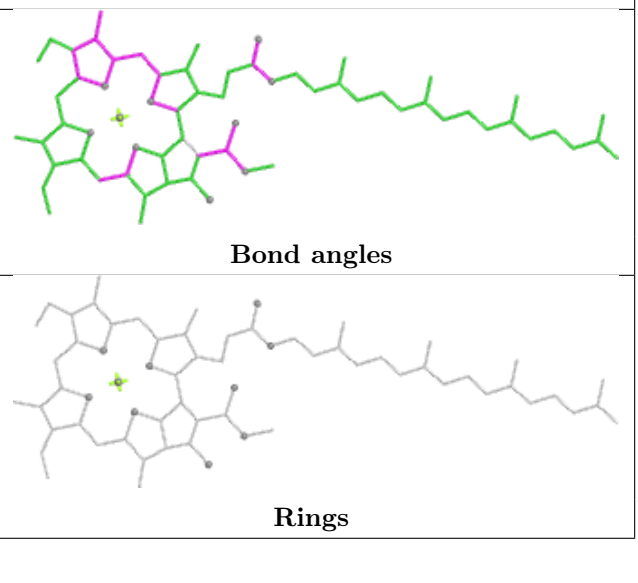


Rings

Ligand CLA B 805



Bond lengths

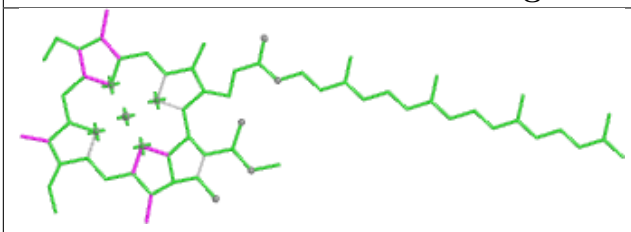


Bond angles

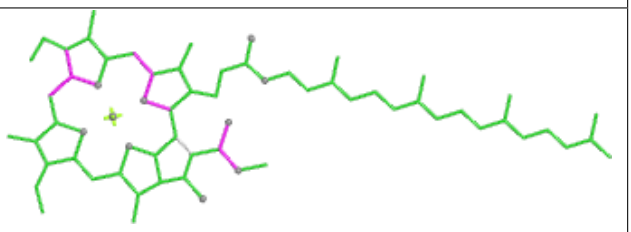
Torsions

Rings

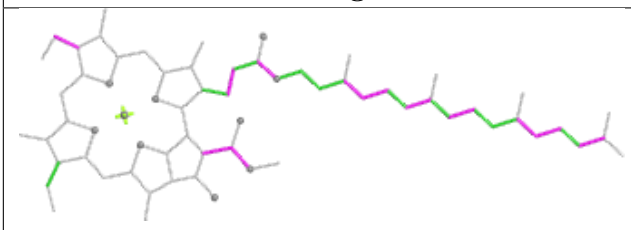
Ligand CLA V 613



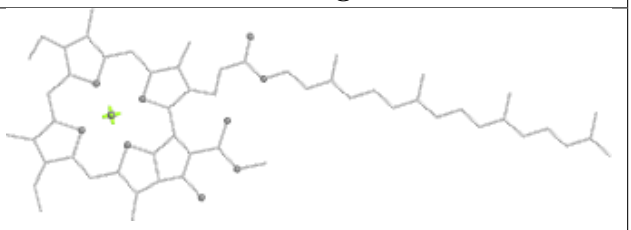
Bond lengths



Bond angles

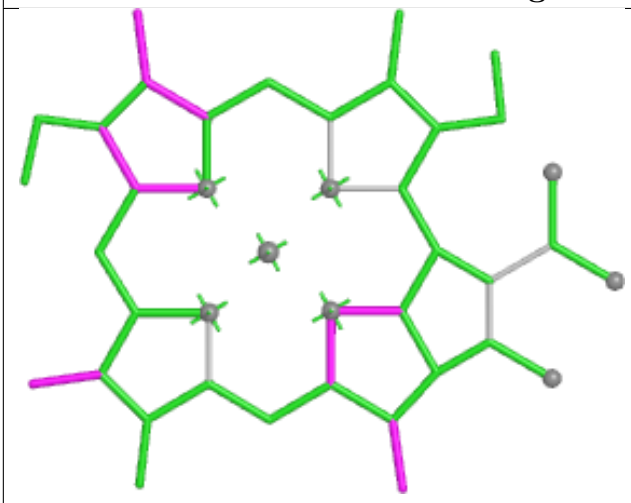


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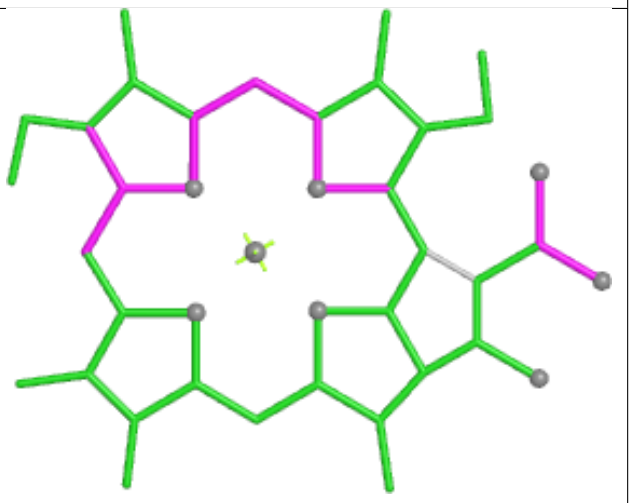


Rings

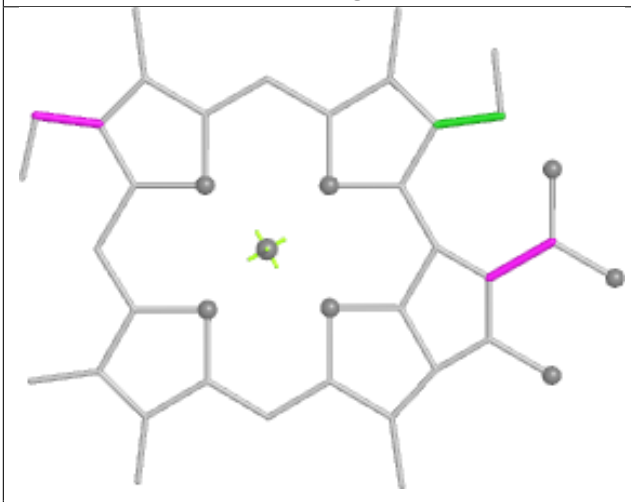
Ligand CLA 5 606



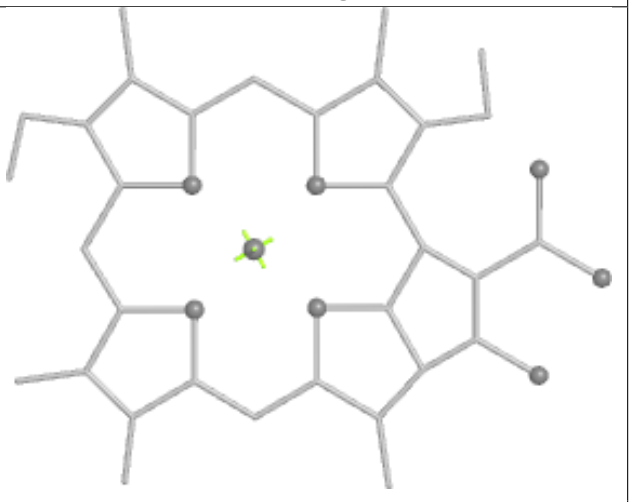
Bond lengths



Bond angles

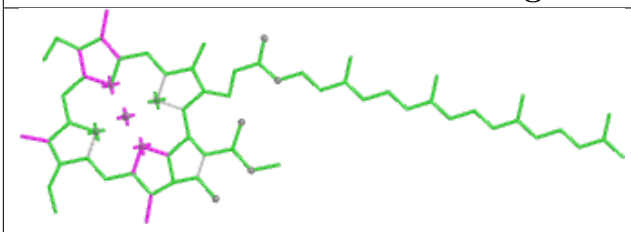


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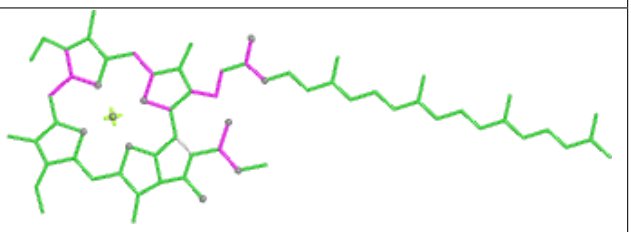


Rings

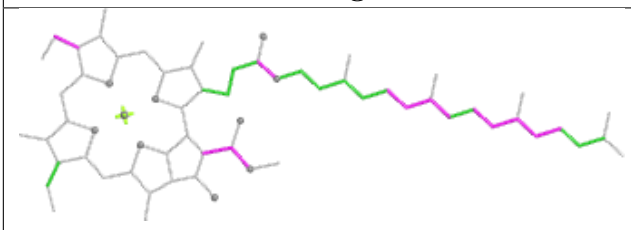
Ligand CLA B 802



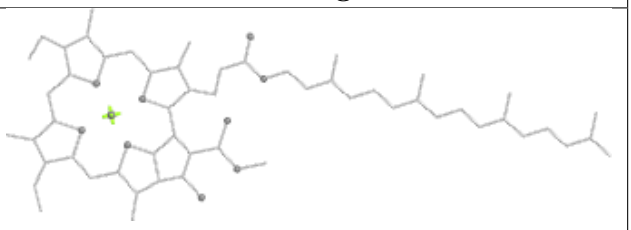
Bond lengths



Bond angles

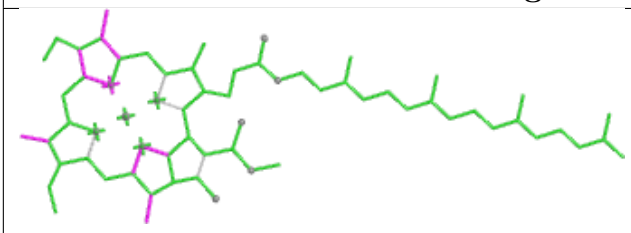


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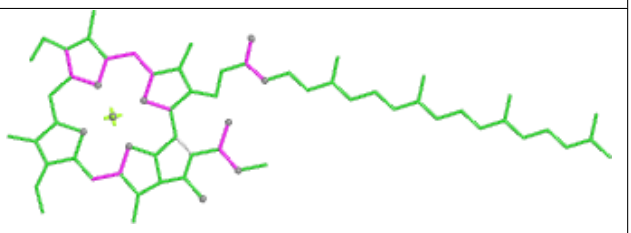


Rings

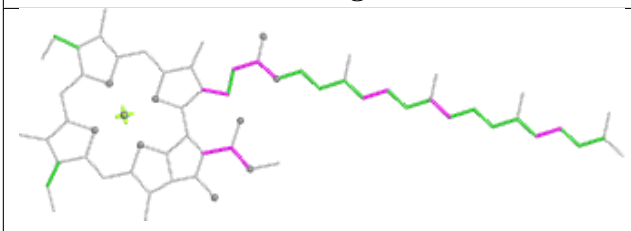
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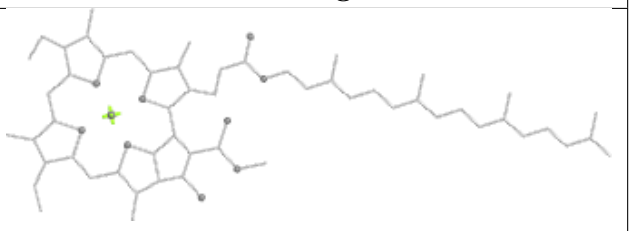
Bond lengths



Bond angles

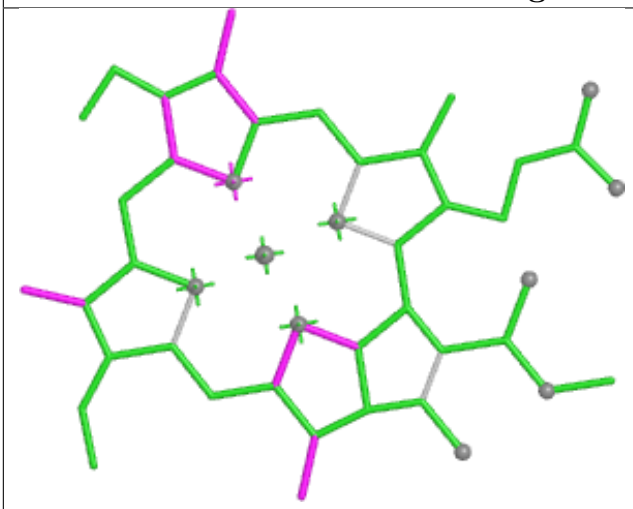


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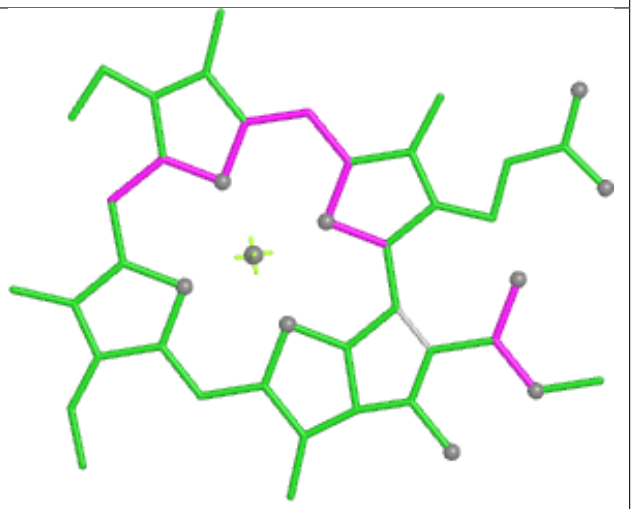


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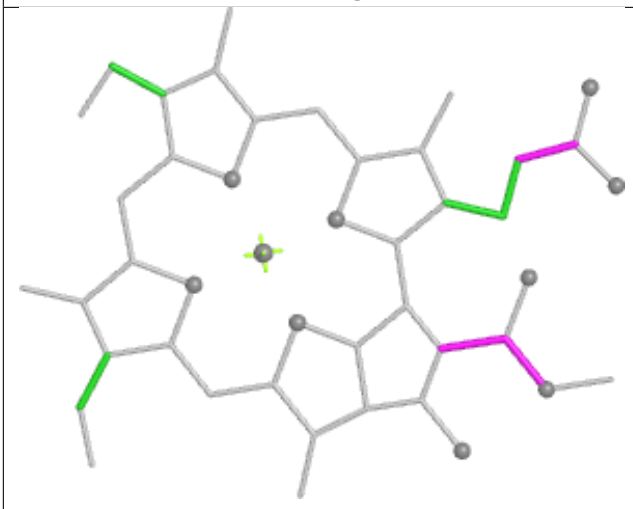
Ligand CLA 1 612



Bond lengths



Bond angles

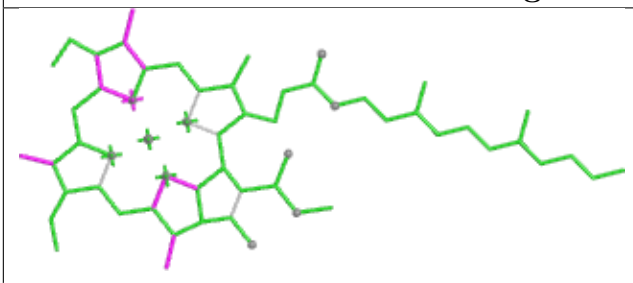


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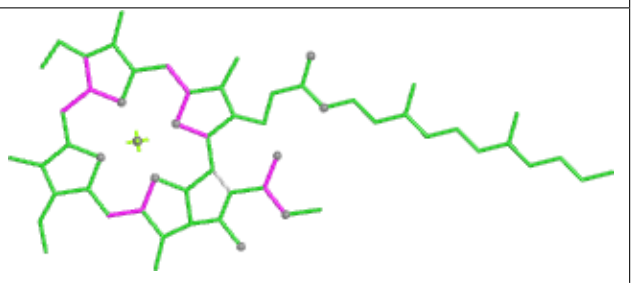


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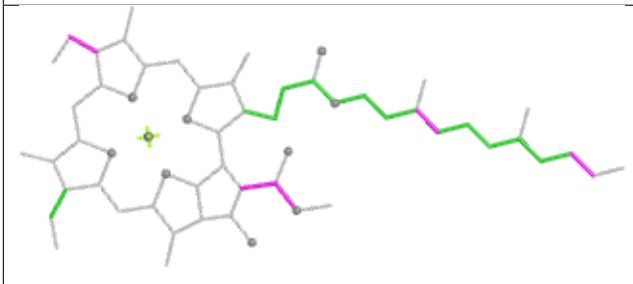
Ligand CLA A 827



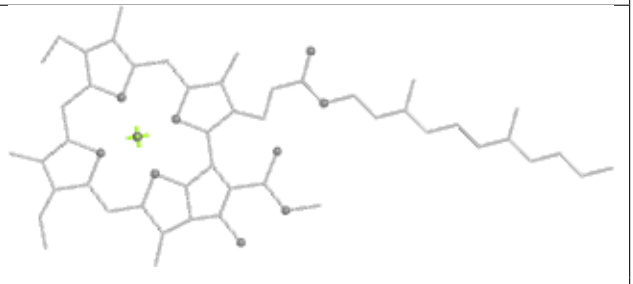
Bond lengths



Bond angles

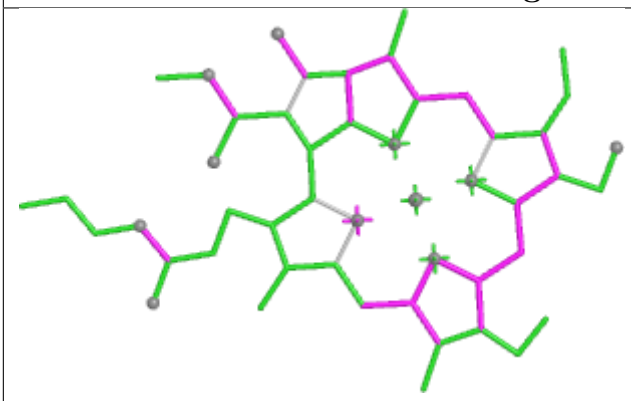


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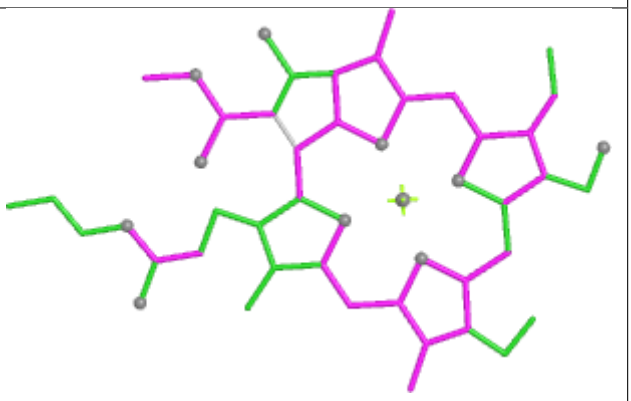


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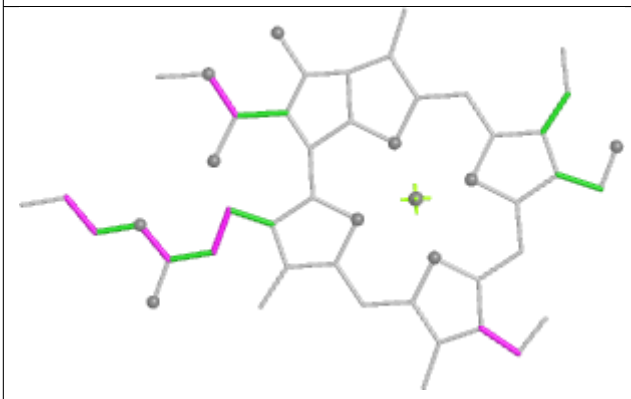
Ligand CHL Y 608



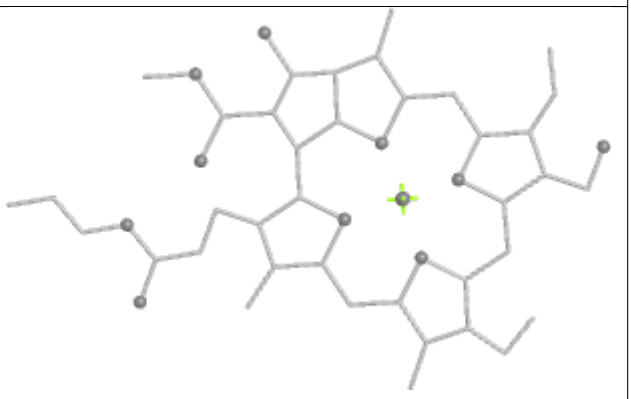
Bond lengths



Bond angles

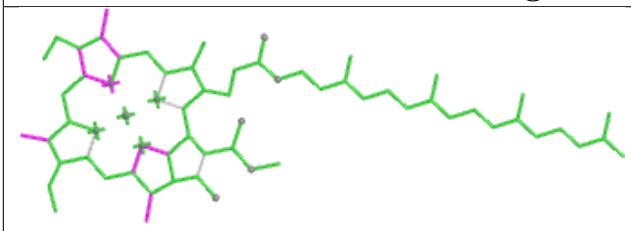


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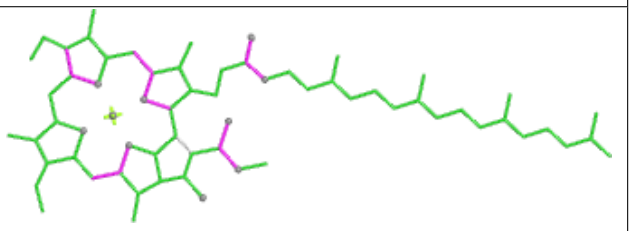


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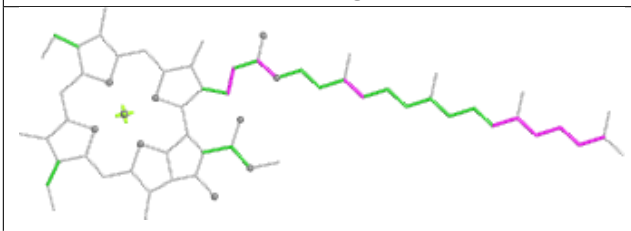
Ligand CLA B 831



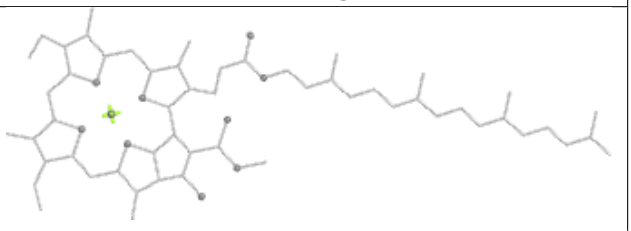
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Bond angles

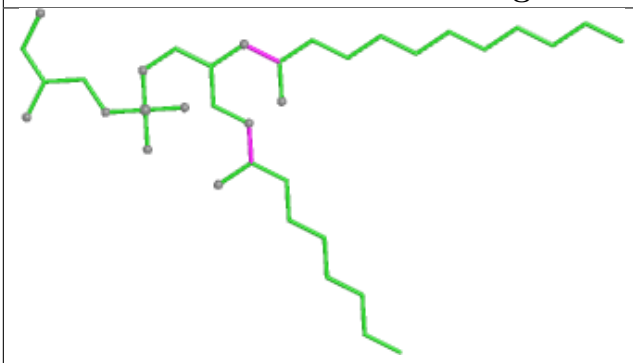


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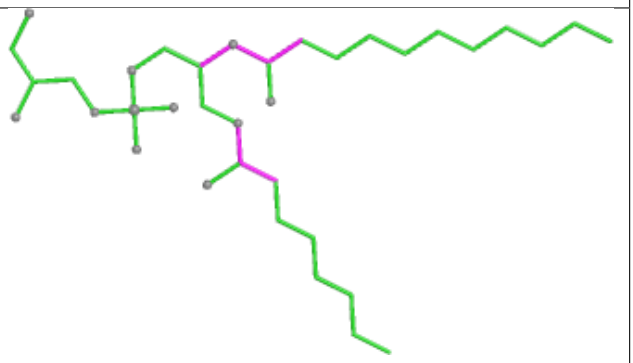


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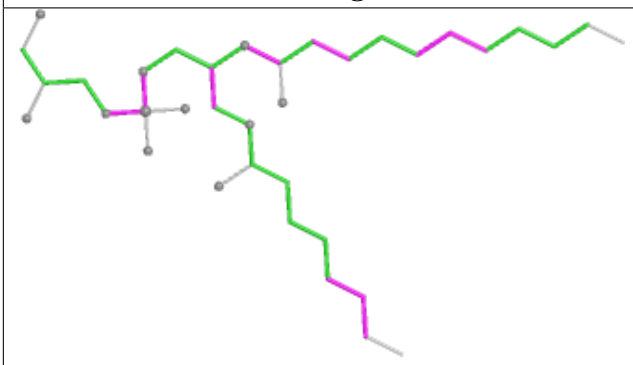
Ligand LHG O 2631



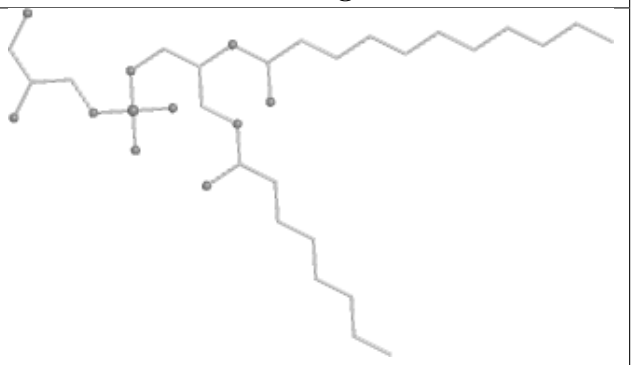
Bond lengths



Bond angles

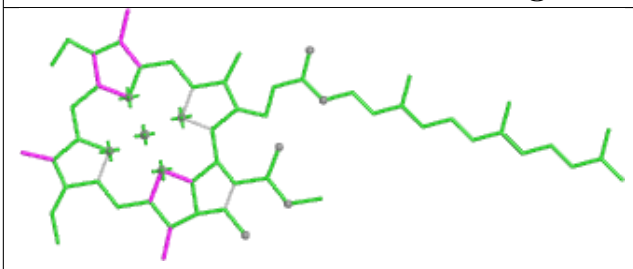


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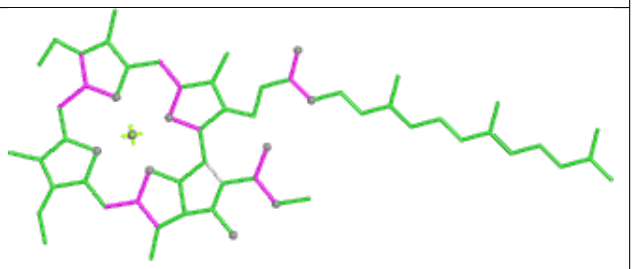


Rings

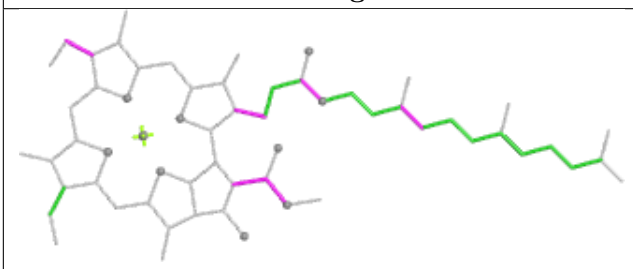
Ligand CLA 6 614



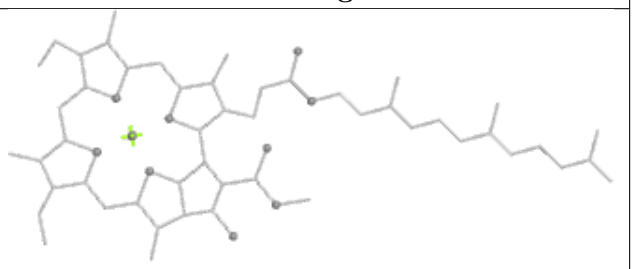
Bond lengths



Bond angles

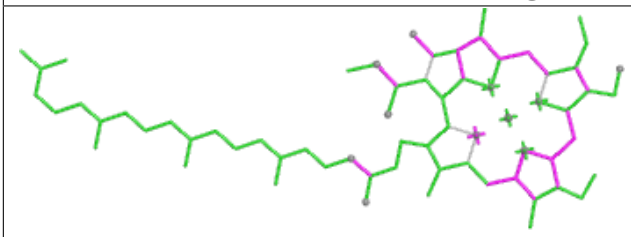


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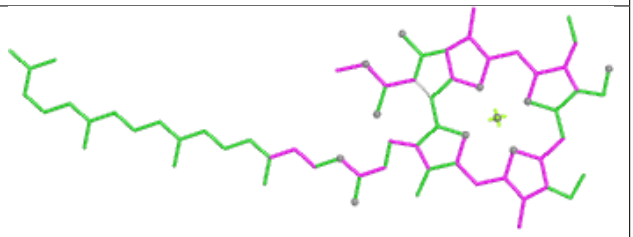


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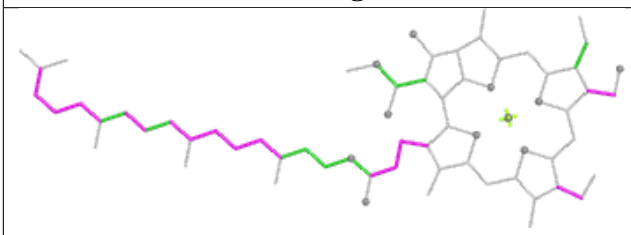
Ligand CHL Y 607



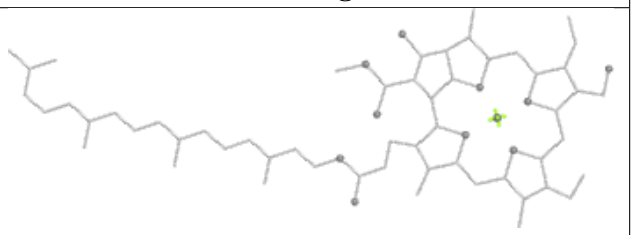
Bond lengths



Bond angles

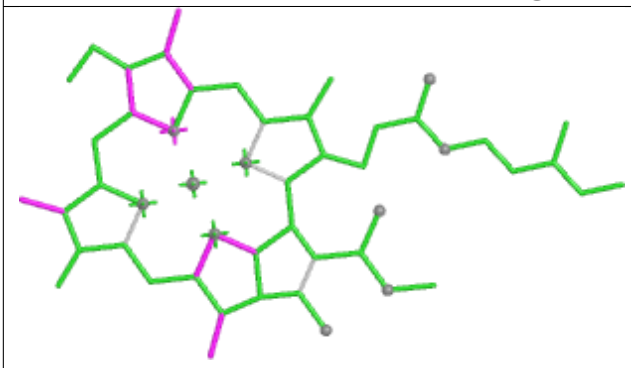


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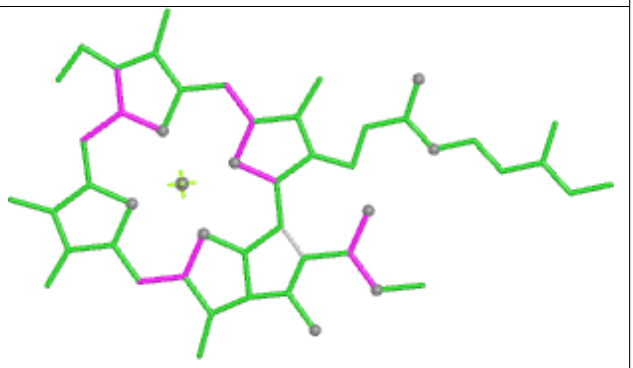


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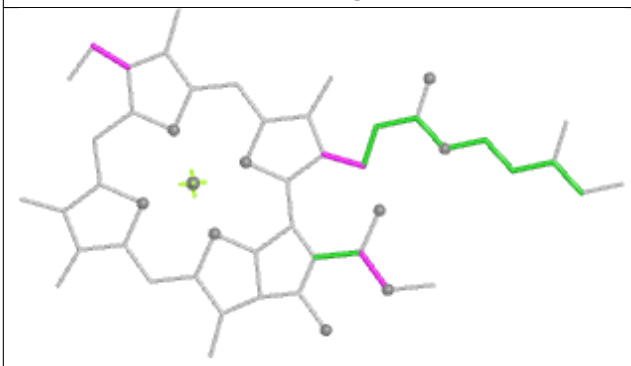
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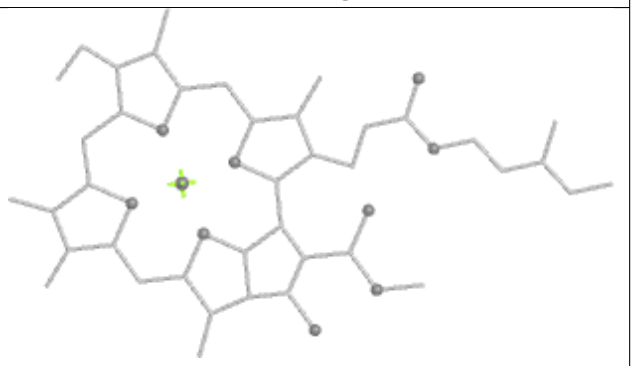
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Bond angles

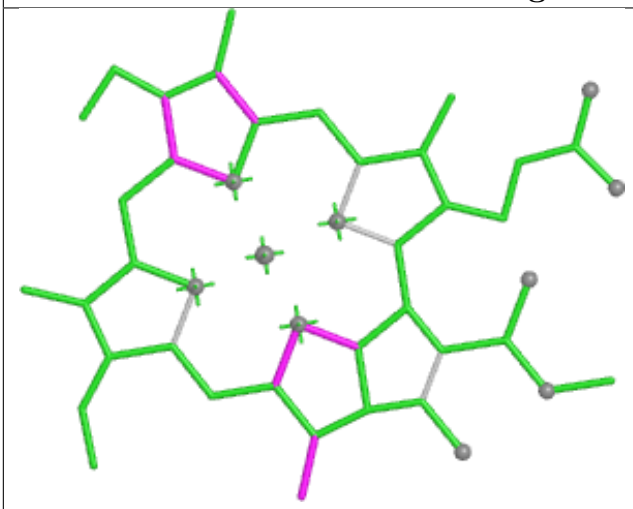


Torsions

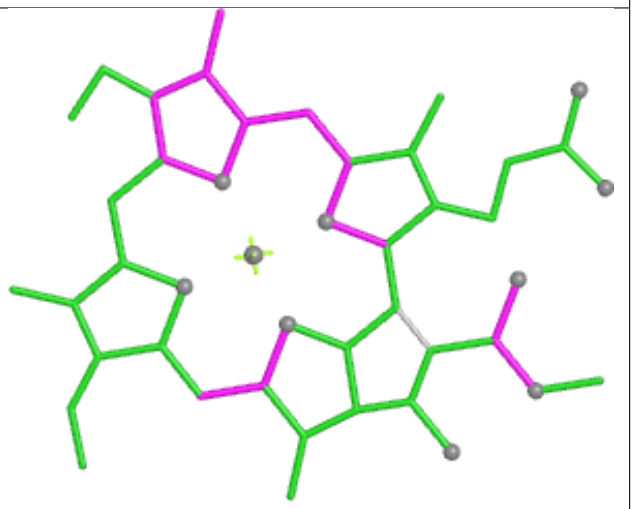


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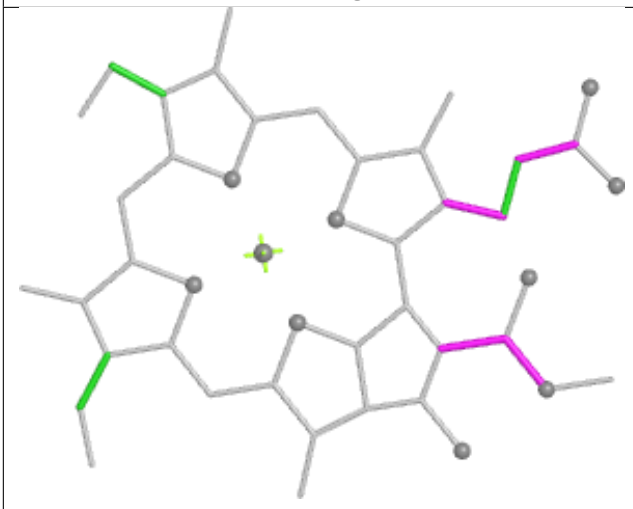
Ligand CLA a 616



Bond lengths



Bond angles

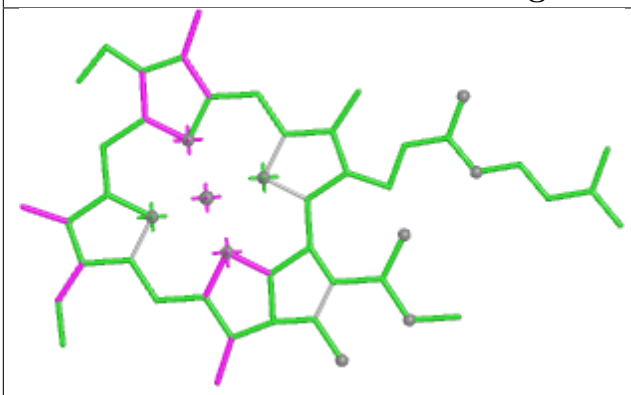


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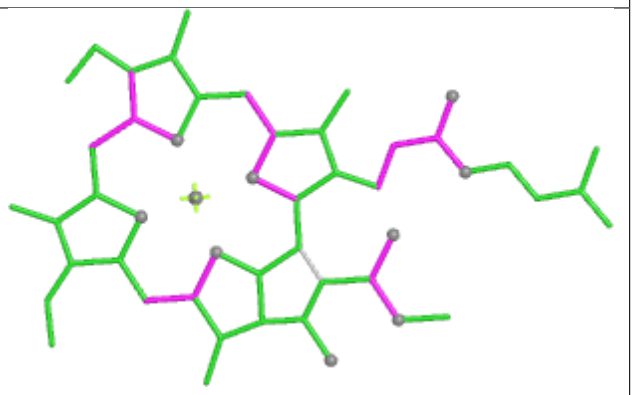


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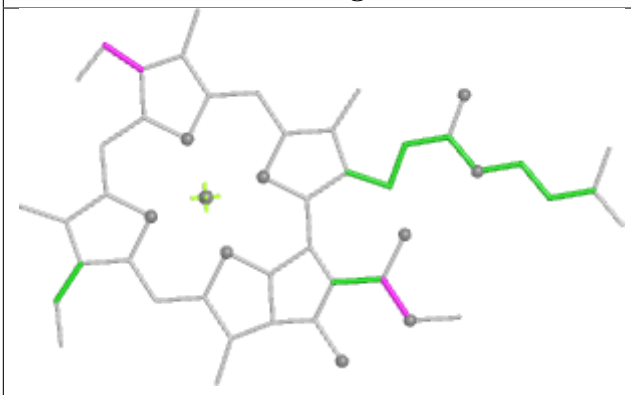
Ligand CLA 7 608



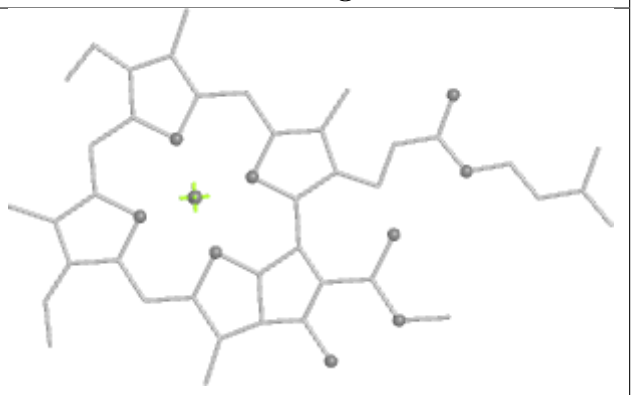
Bond lengths



Bond angles

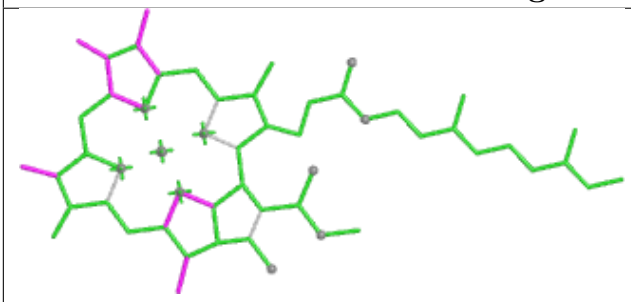


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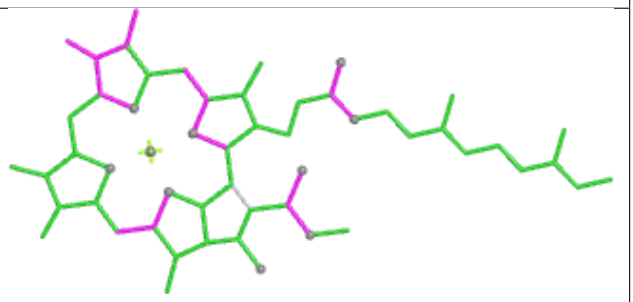


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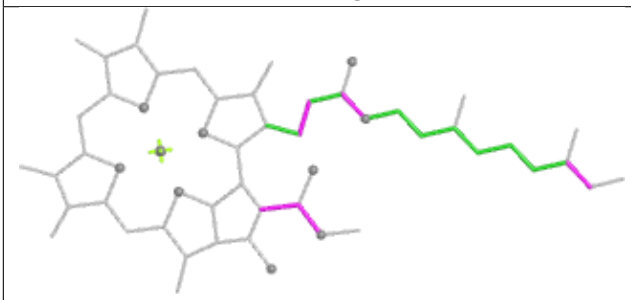
Ligand CLA 4 604



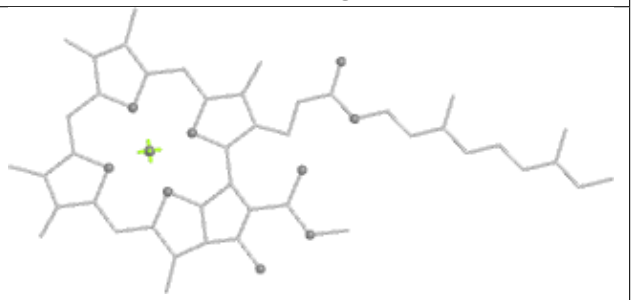
Bond lengths



Bond angles

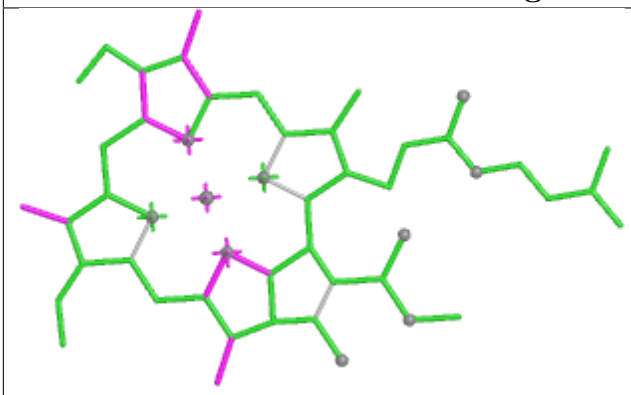


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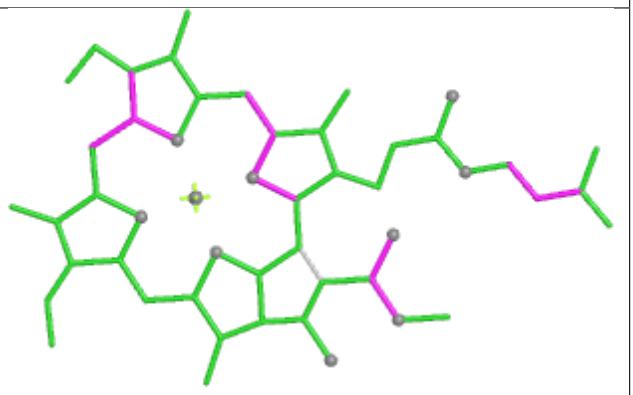


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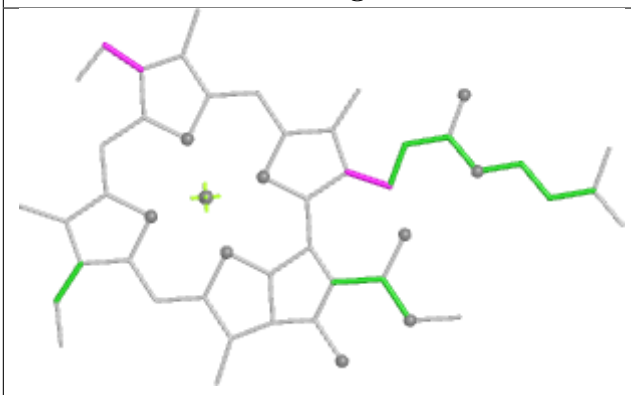
Ligand CLA B 820



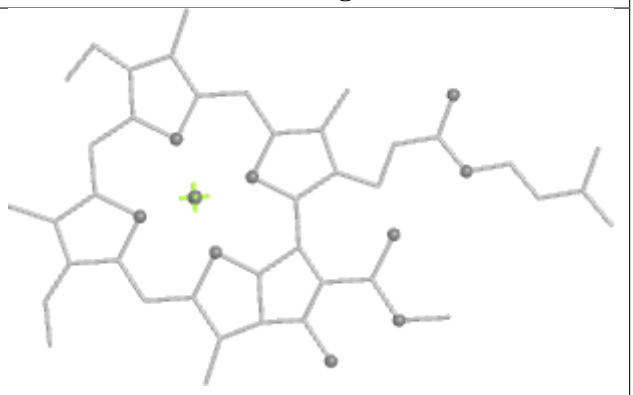
Bond lengths



Bond angles

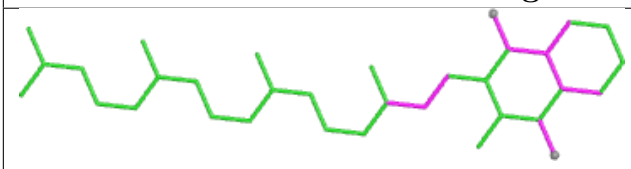


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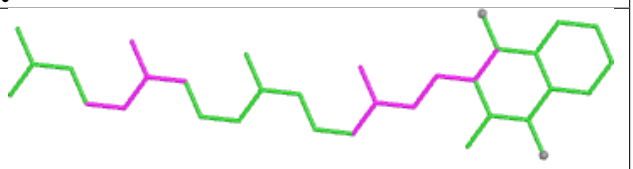


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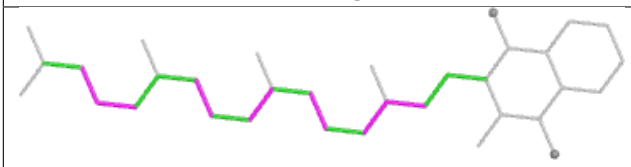
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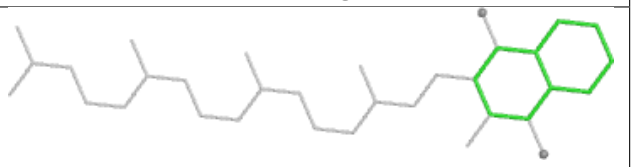
Bond lengths



Bond angles

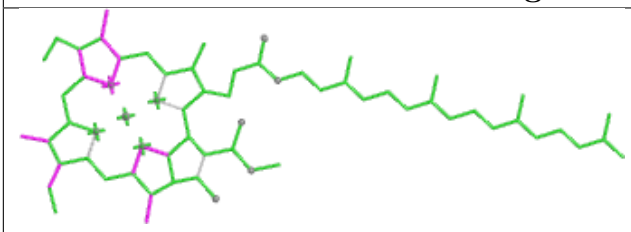


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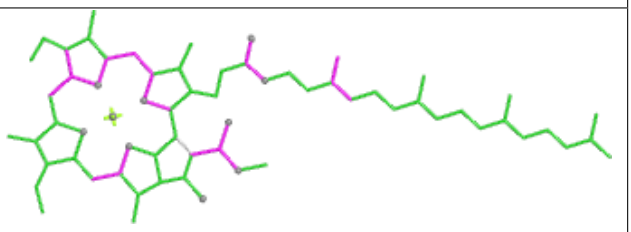


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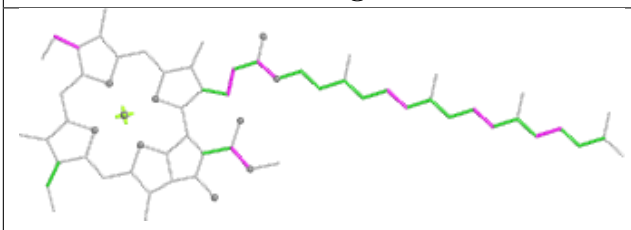
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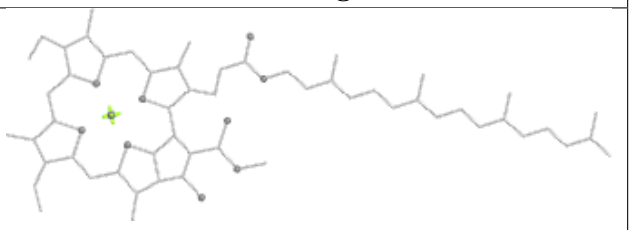
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Bond angles

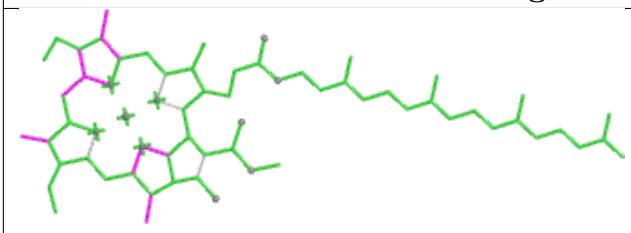


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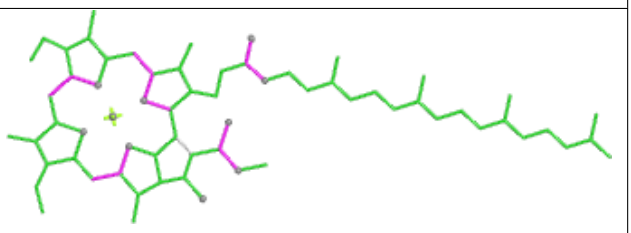


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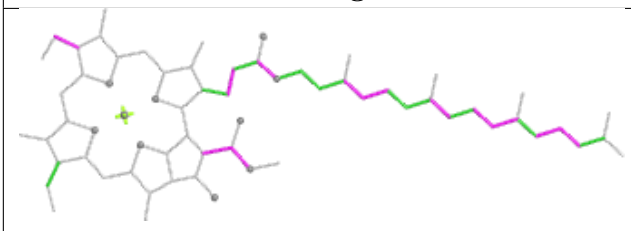
Ligand CLA 7 613



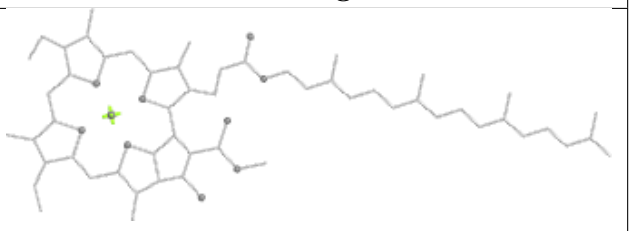
Bond lengths



Bond angles

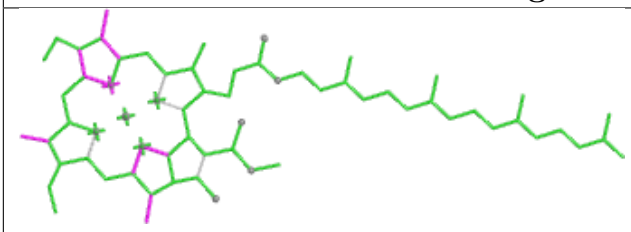


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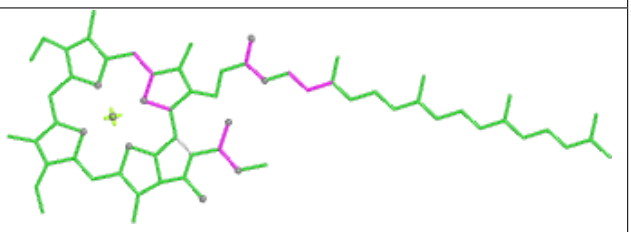


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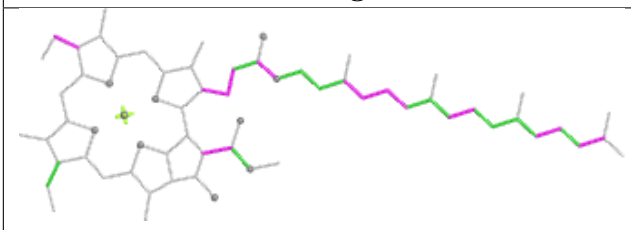
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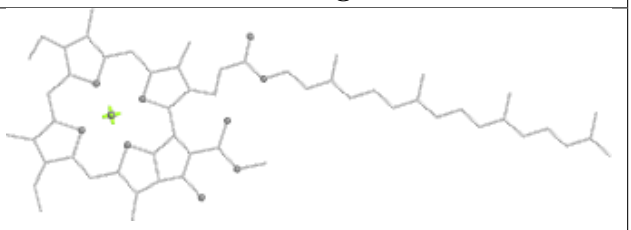
Bond lengths



Bond angles

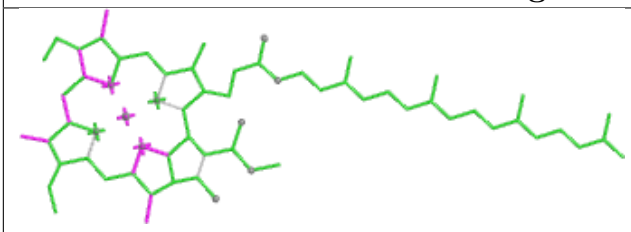


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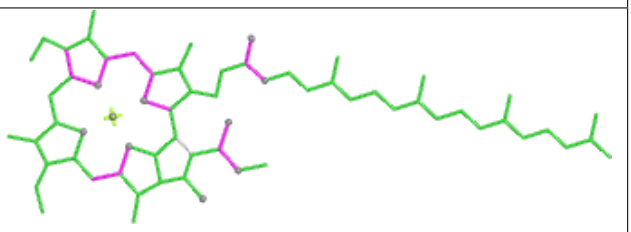


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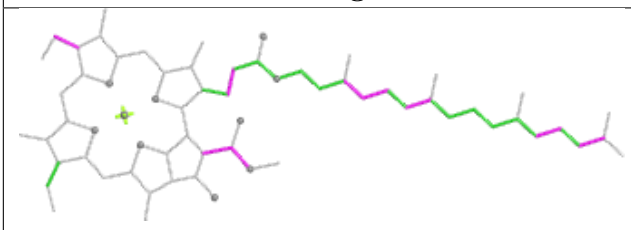
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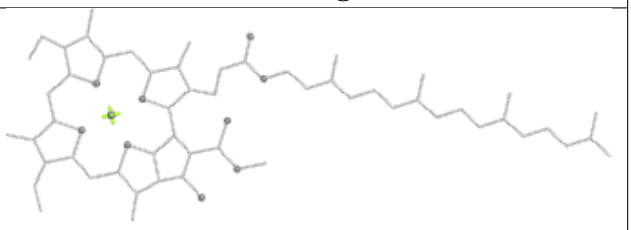
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Bond angles

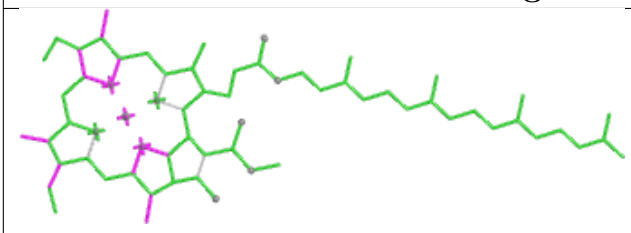


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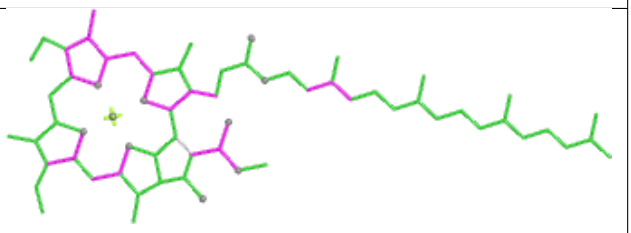


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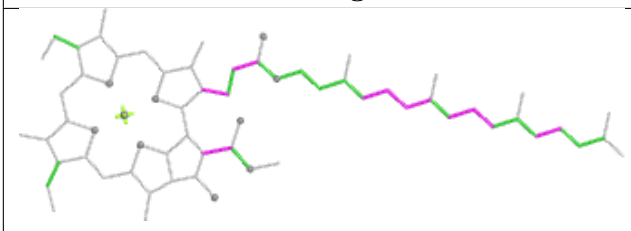
Ligand CLA A 806



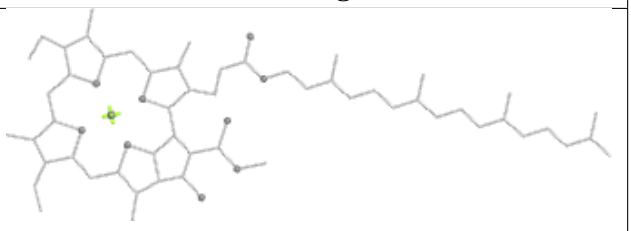
Bond lengths



Bond angles

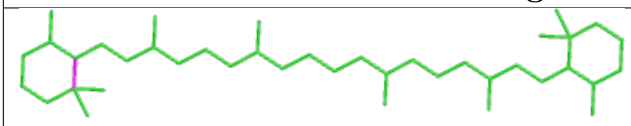


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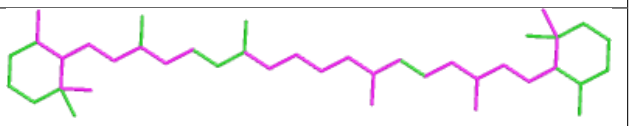


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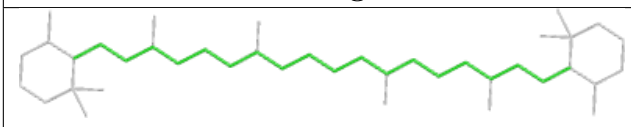
Ligand BCR 3 621



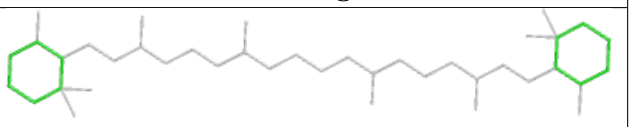
Bond lengths



Bond angles

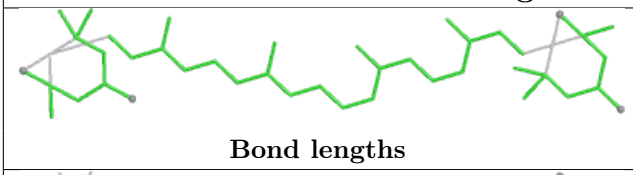


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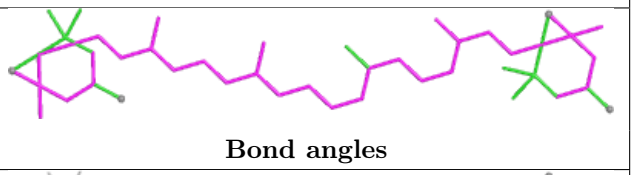


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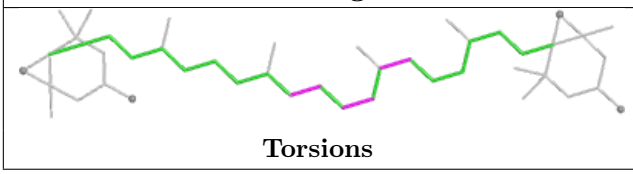
Ligand XAT Z 1622



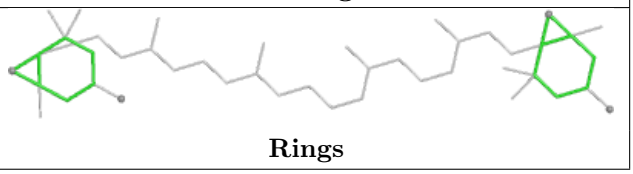
Bond lengths



Bond angles

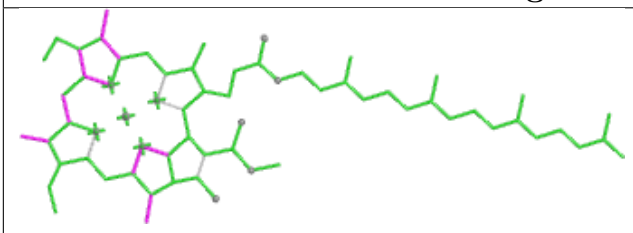


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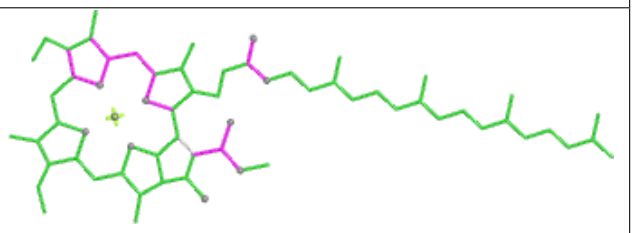


Rings

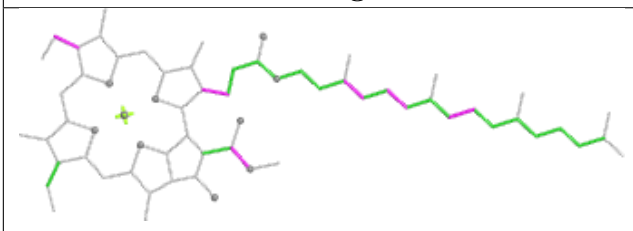
Ligand CLA Z 610



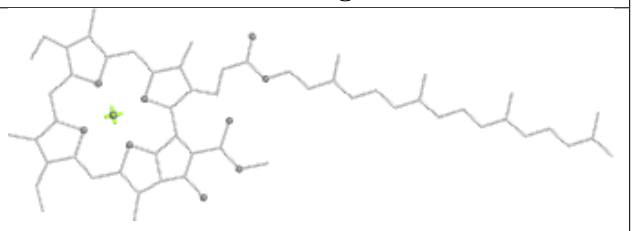
Bond lengths



Bond angles

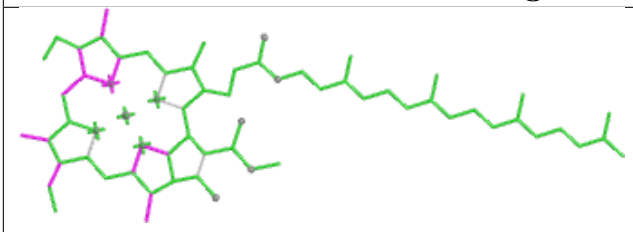


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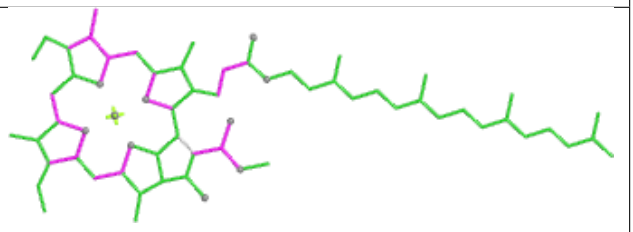


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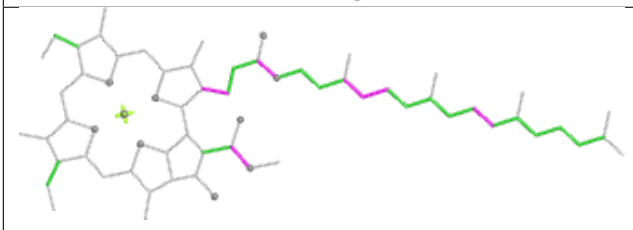
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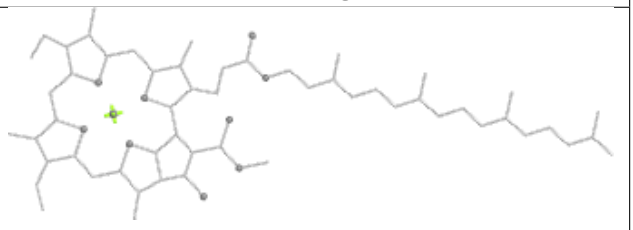
Bond lengths



Bond angles

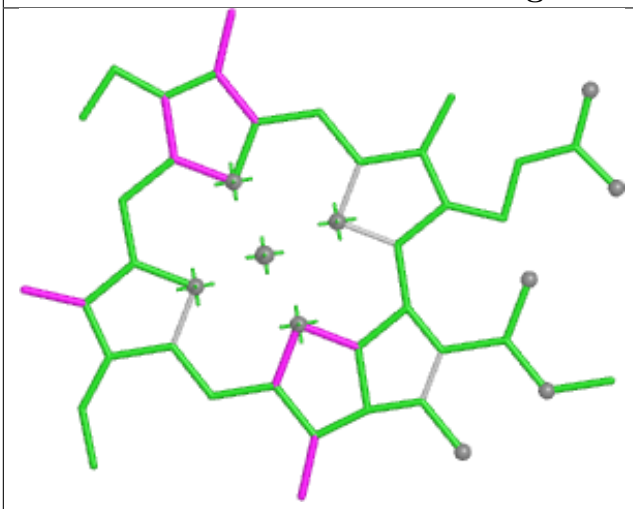


Torsions

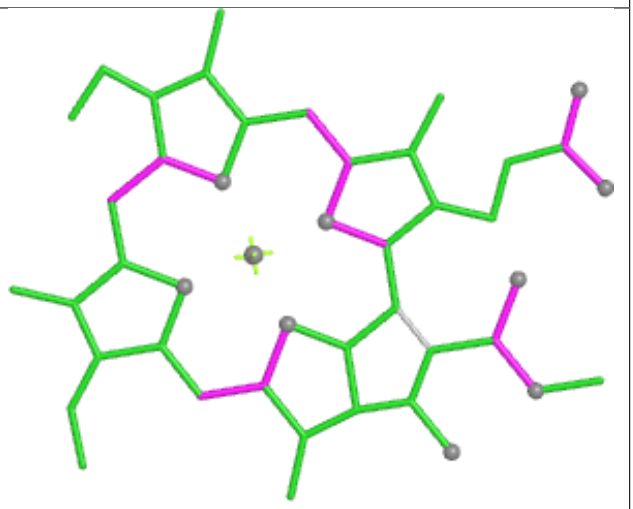


Rings

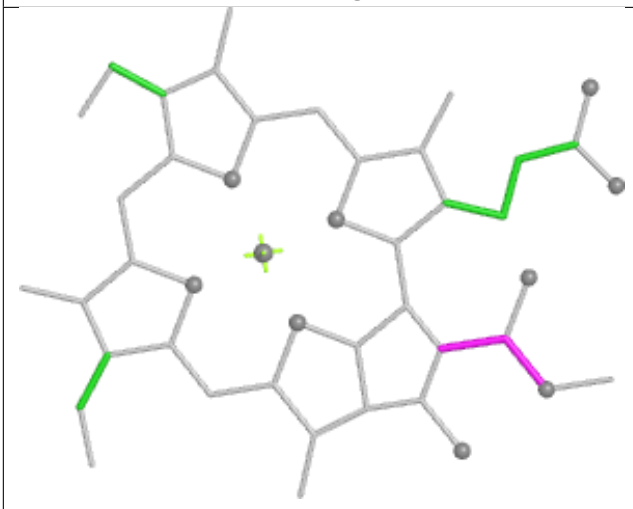
Ligand CLA L 304



Bond lengths



Bond angles

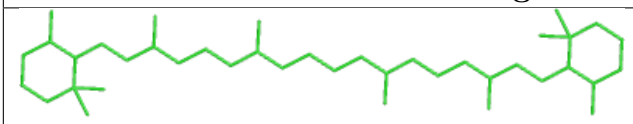


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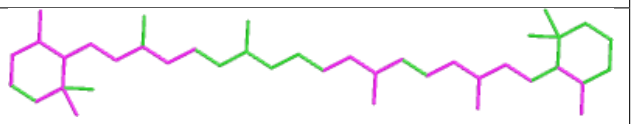


Rings

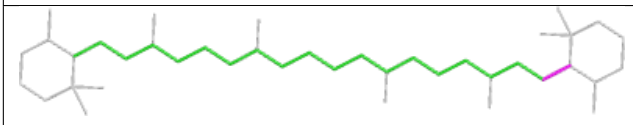
Ligand BCR O 2004



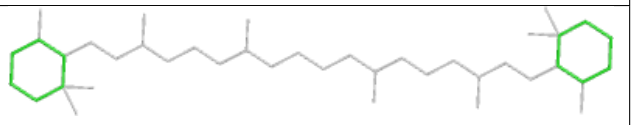
Bond lengths



Bond angles

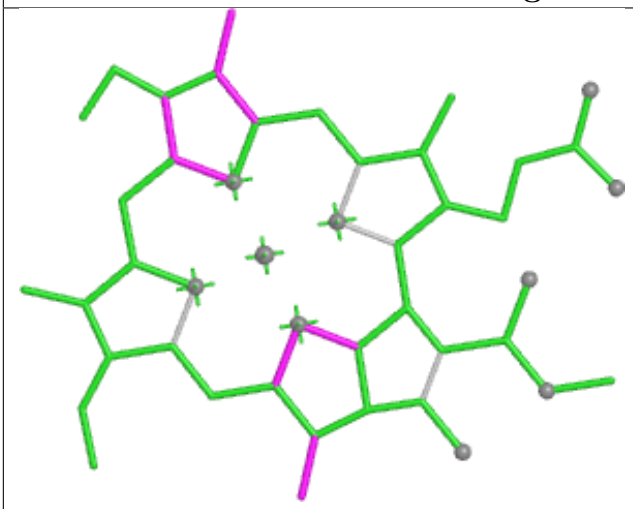


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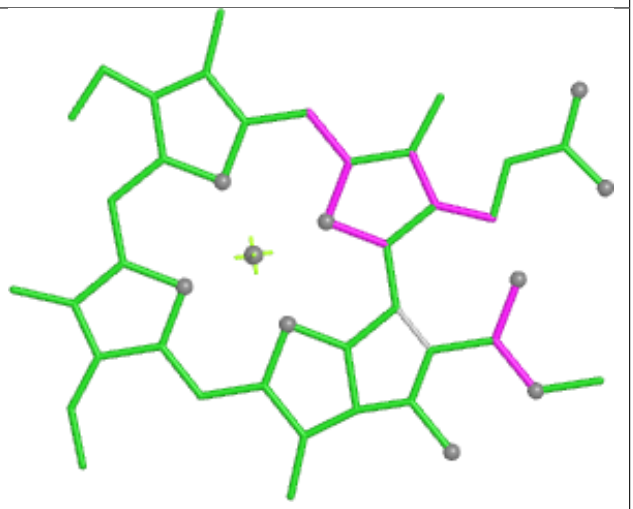


Rings

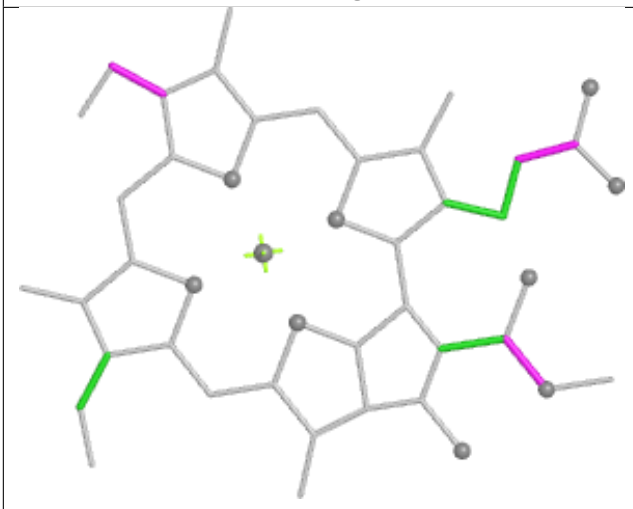
Ligand CLA V 603



Bond lengths



Bond angles

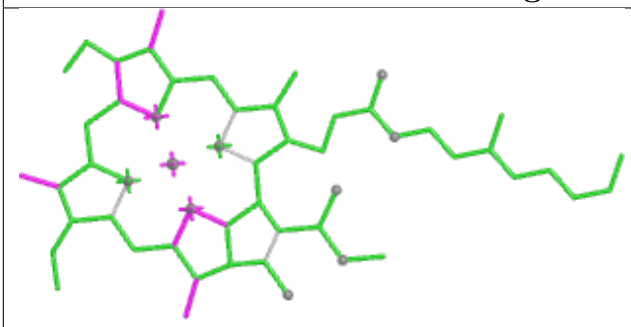


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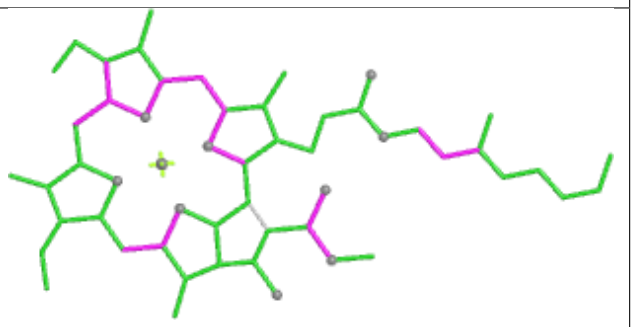


Rings

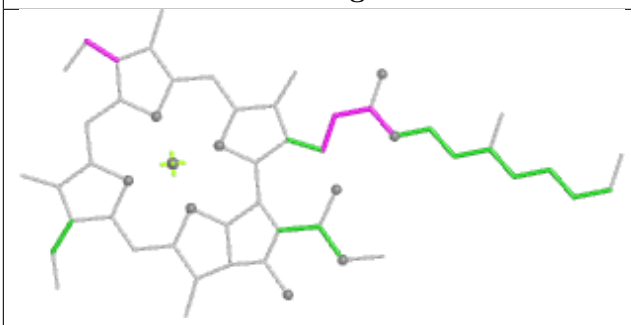
Ligand CLA A 813



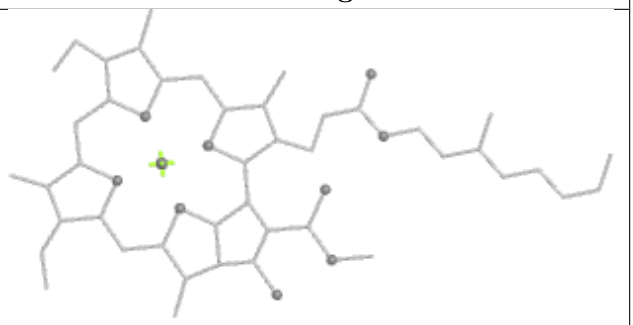
Bond lengths



Bond angles

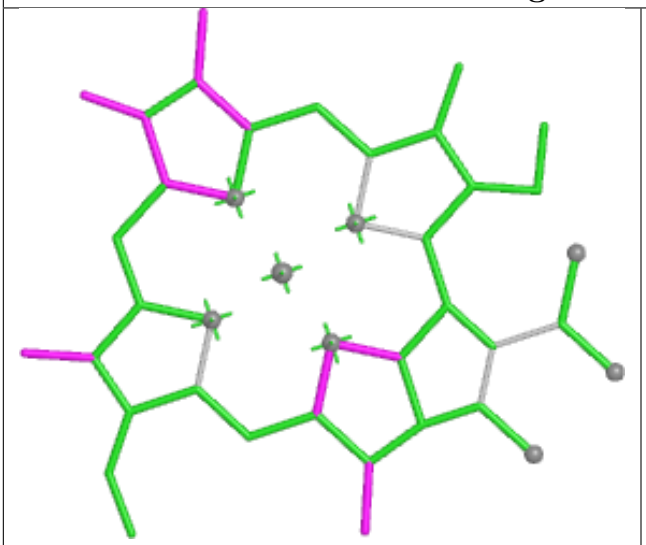


Torsions



Rings

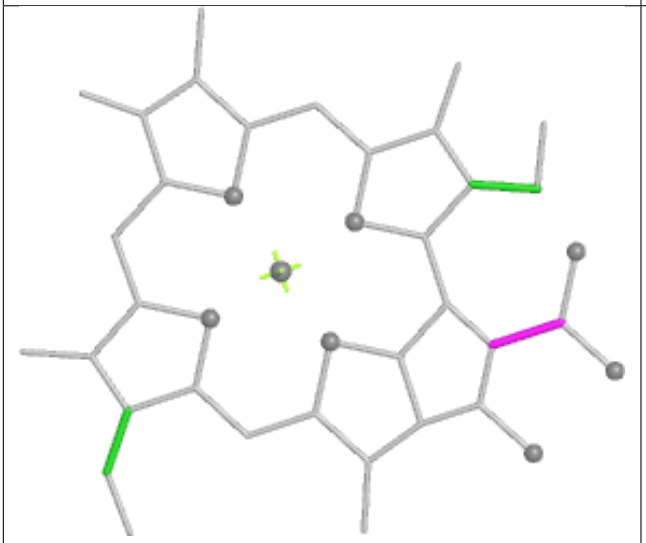
Ligand CLA 6 618



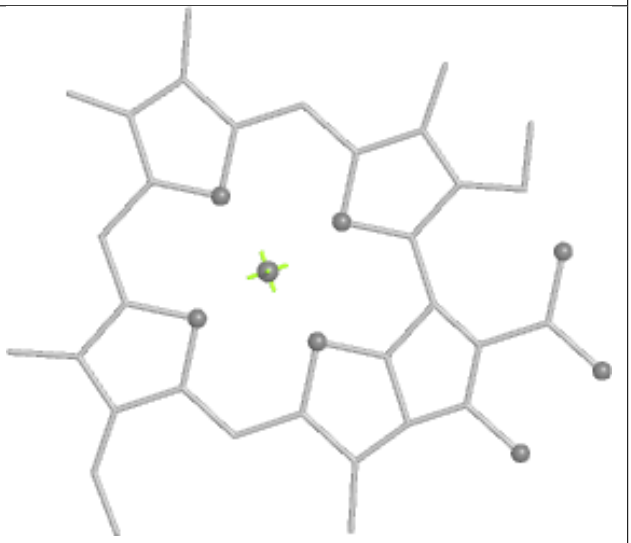
Bond lengths



Bond angles

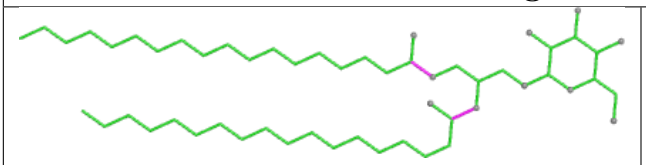


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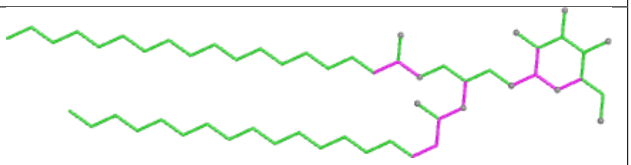


Rings

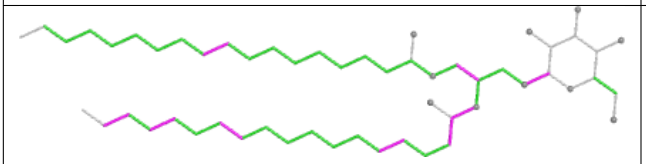
Ligand LMG 9 625



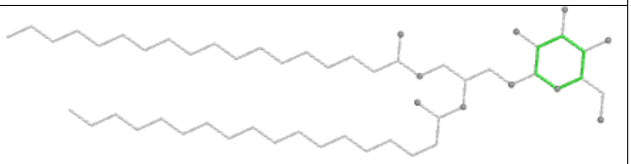
Bond lengths



Bond angles

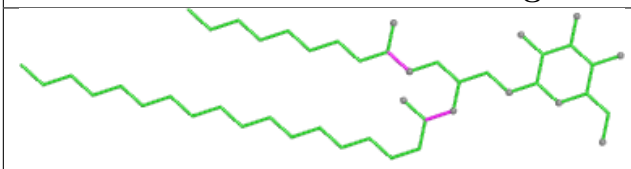


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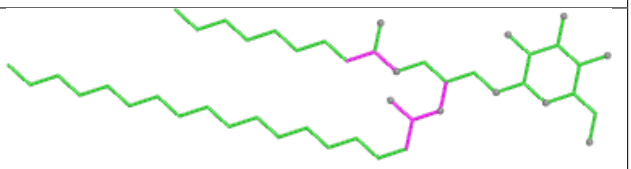


Rings

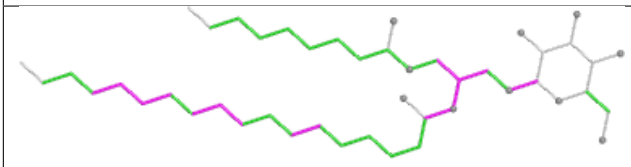
Ligand LMG 8 626



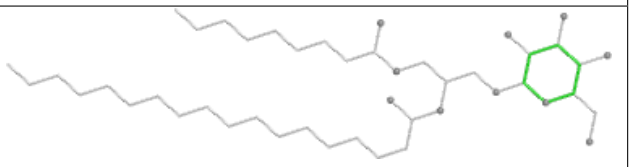
Bond lengths



Bond angles

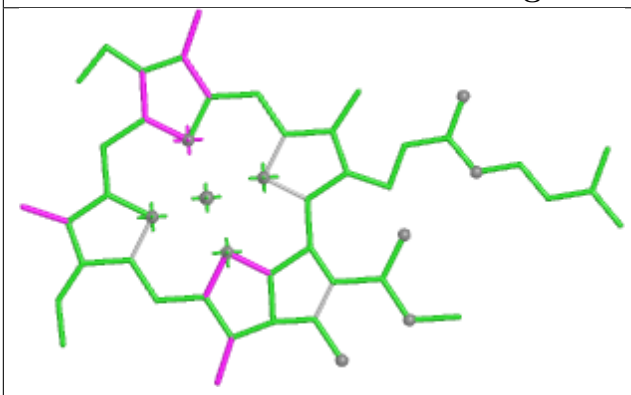


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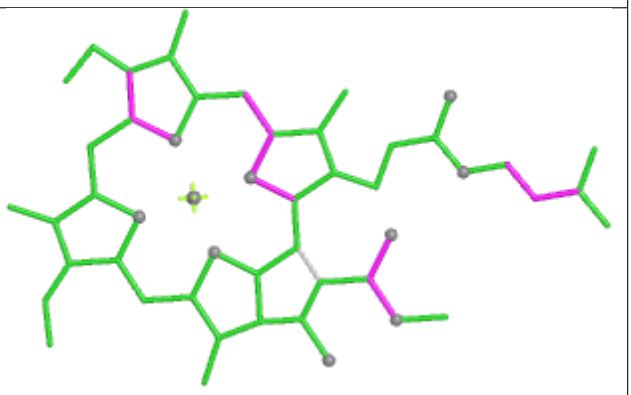


Rings

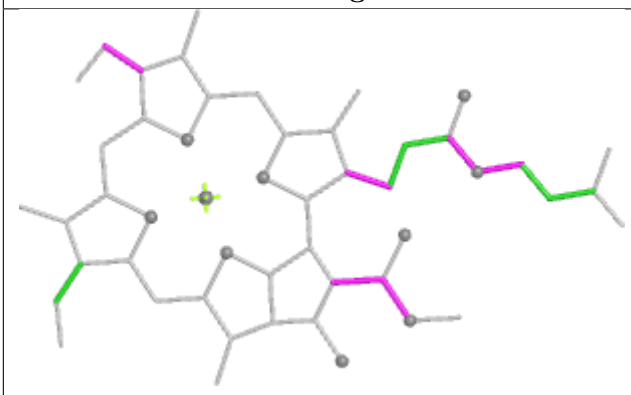
Ligand CLA A 815



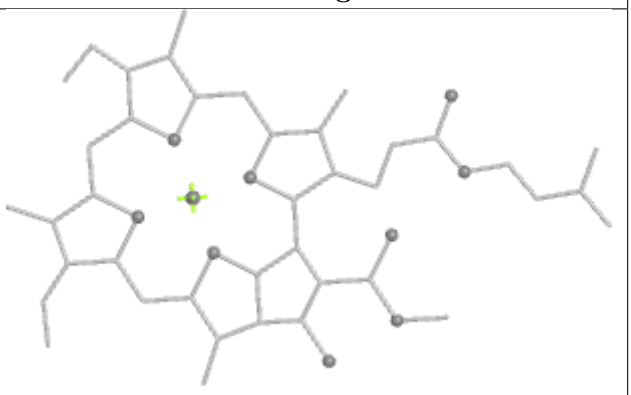
Bond lengths



Bond angles

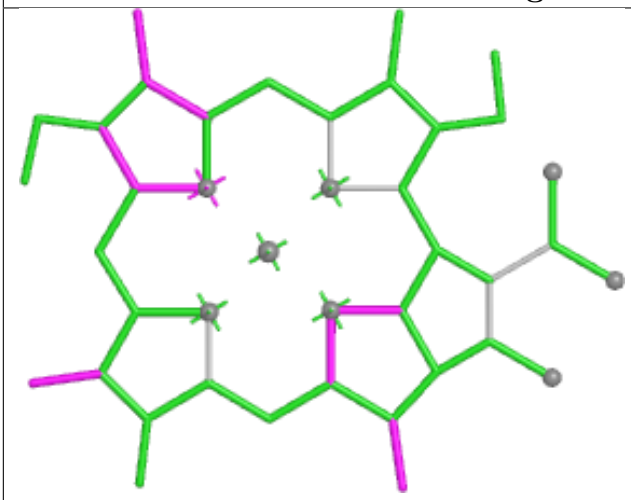


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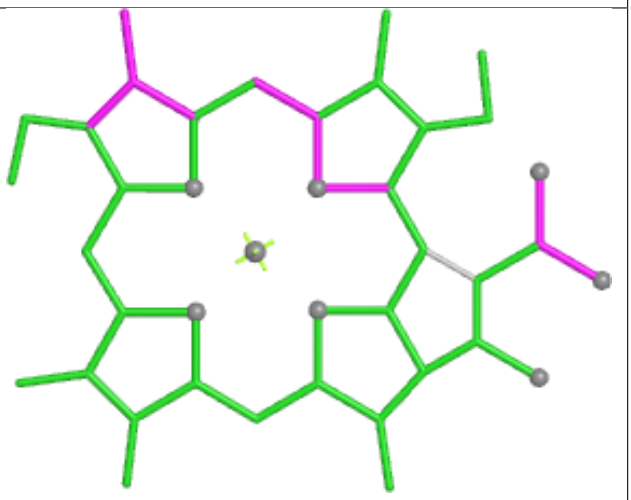


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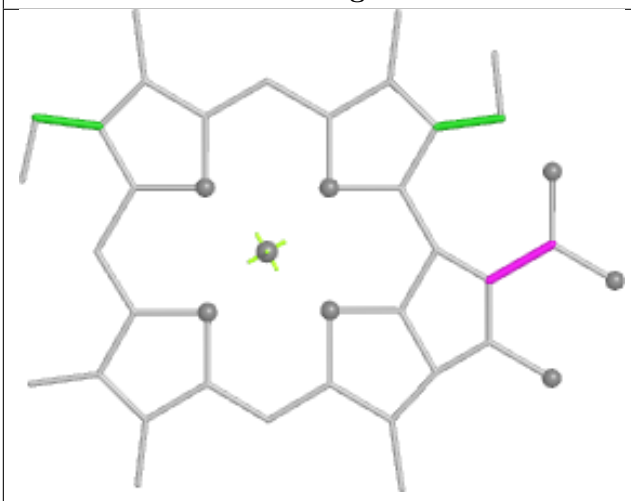
Ligand CLA L 307



Bond lengths



Bond angles

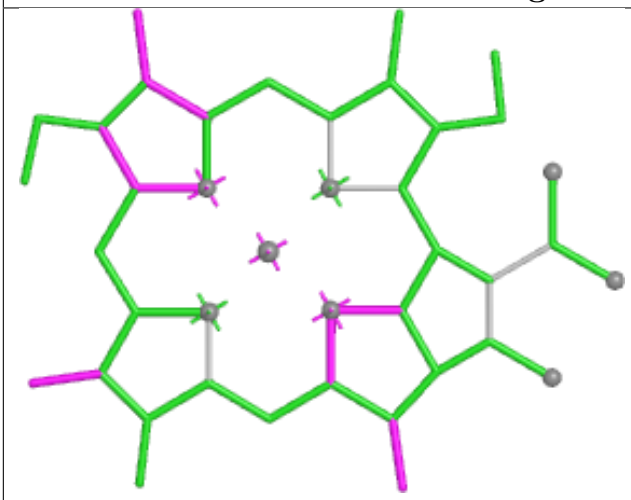


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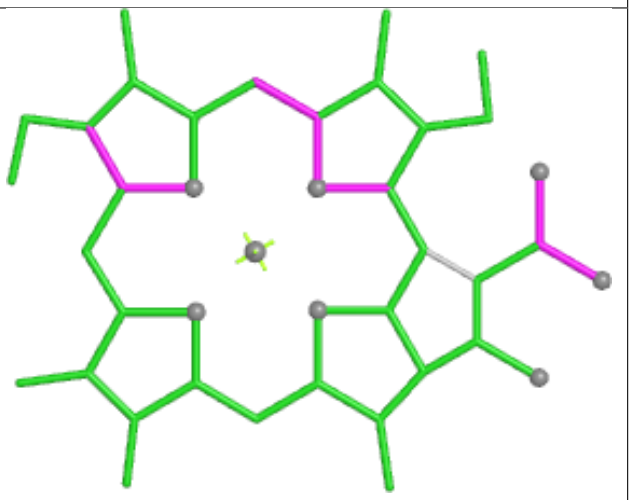


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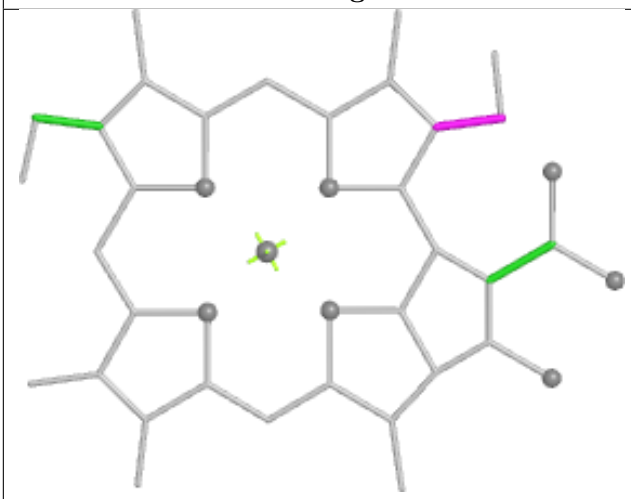
Ligand CLA 9 606



Bond lengths



Bond angles

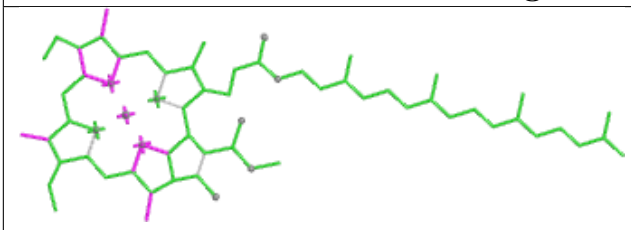


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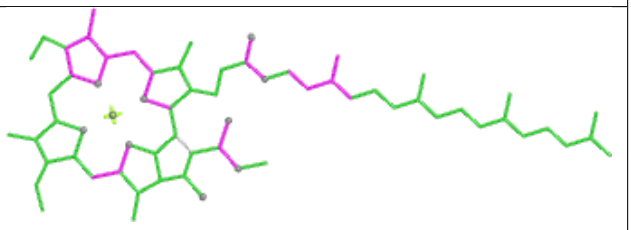


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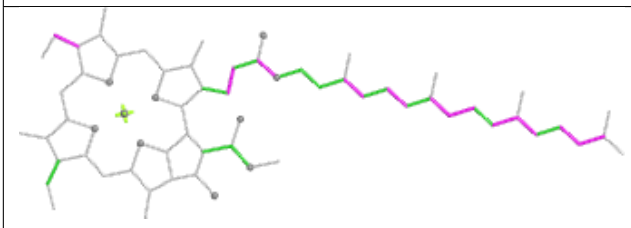
Ligand CLA A 842



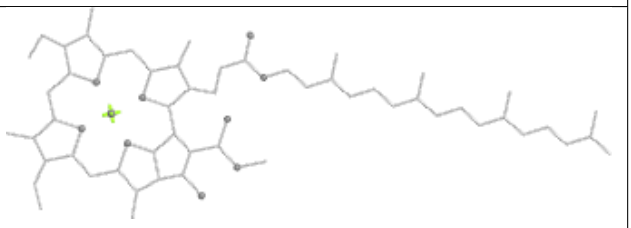
Bond lengths



Bond angles

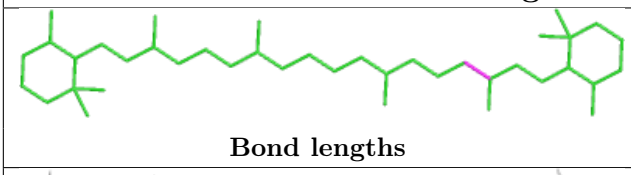


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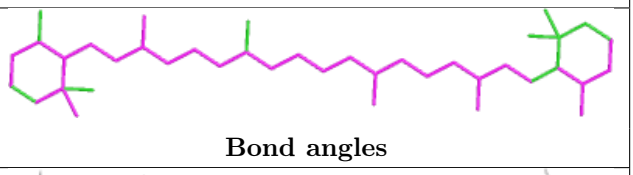


Rings

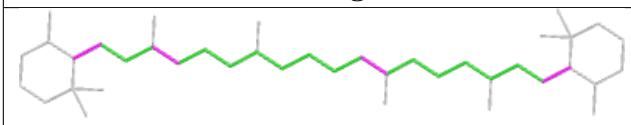
Ligand BCR A 852



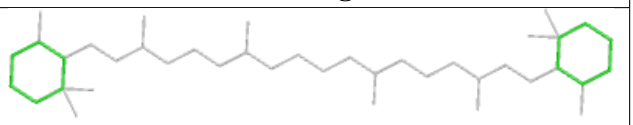
Bond lengths



Bond angles

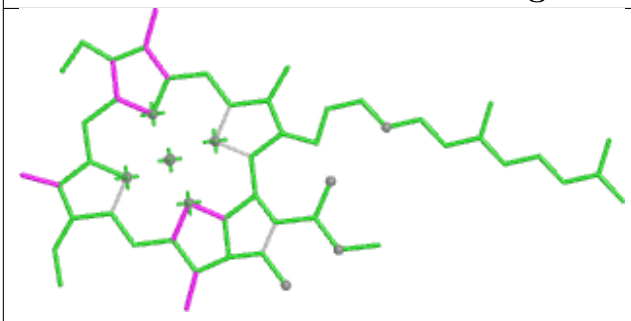


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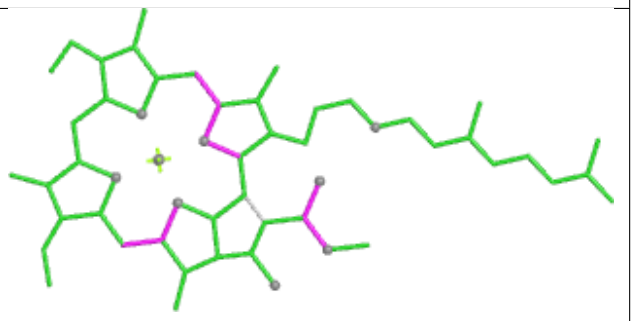


Rings

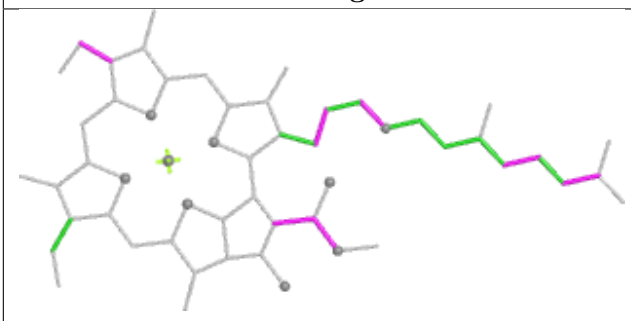
Ligand CLA a 603



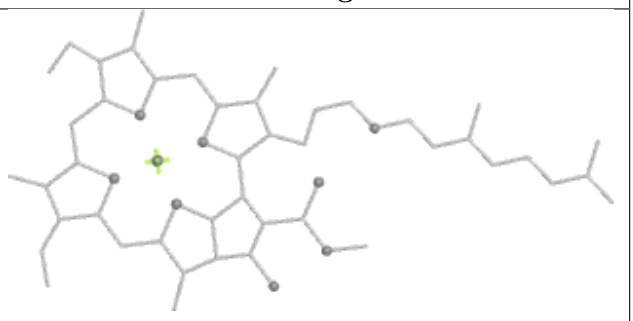
Bond lengths



Bond angles

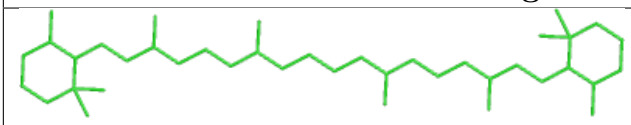


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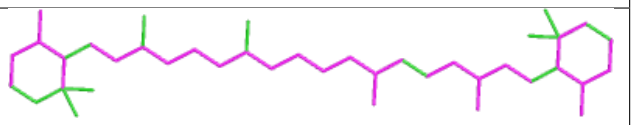


Rings

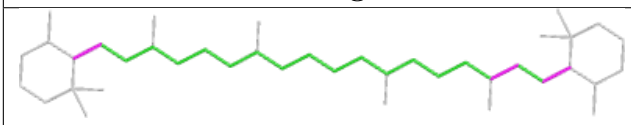
Ligand BCR A 849



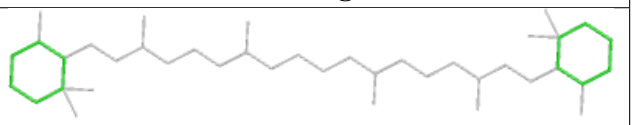
Bond lengths



Bond angles

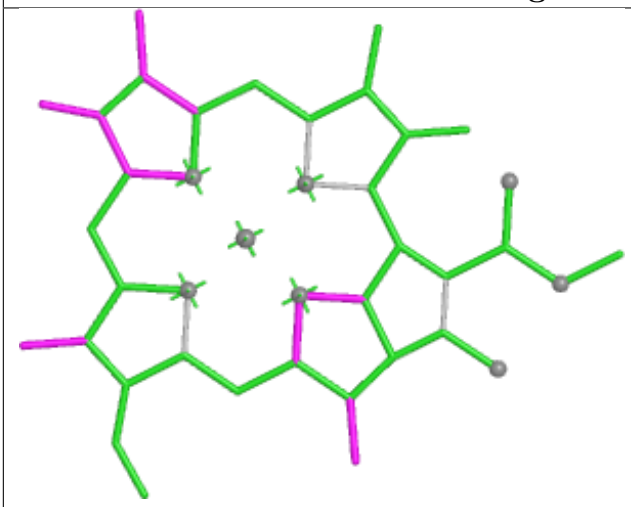


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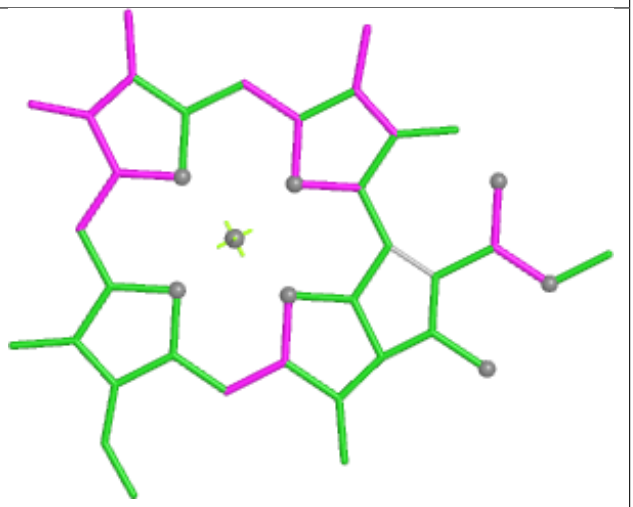


Rings

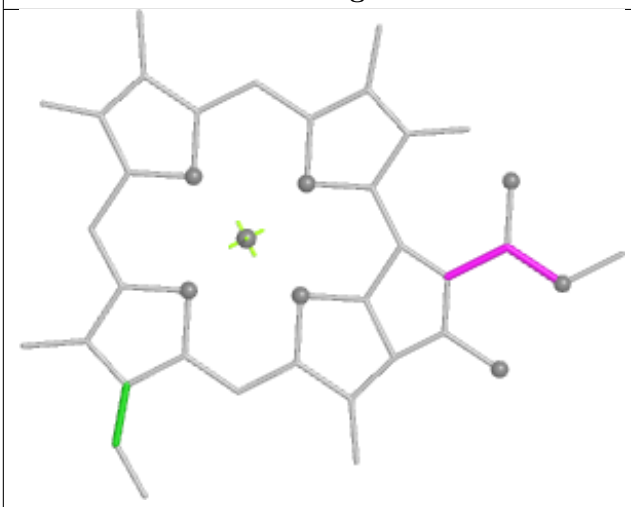
Ligand CLA 1 609



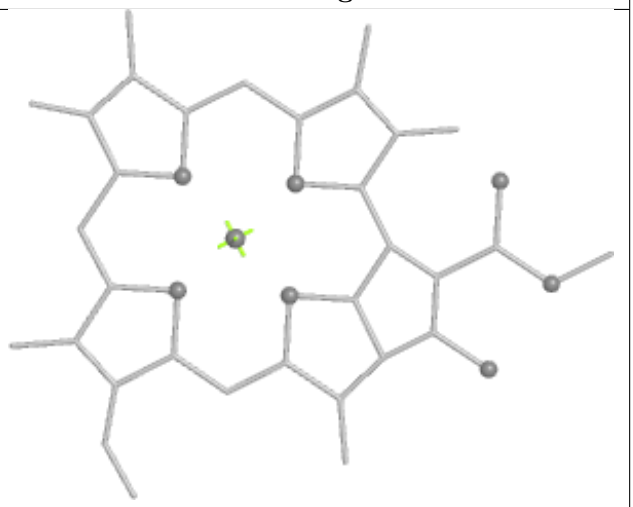
Bond lengths



Bond angles

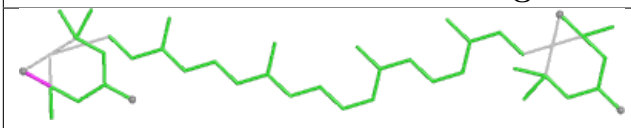


Torsions

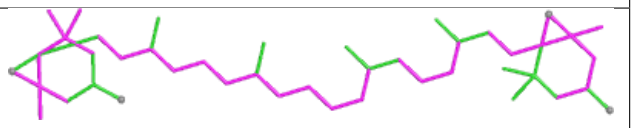


Rings

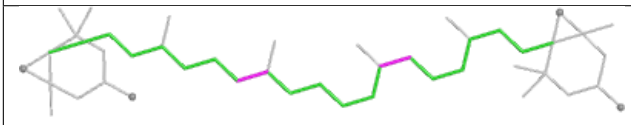
Ligand XAT U 1622



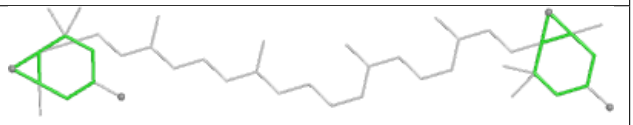
Bond lengths



Bond angles

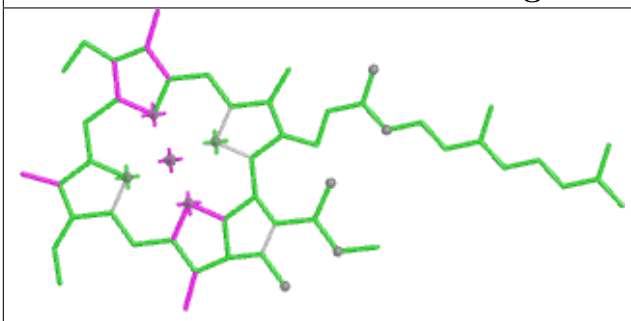


Torsions

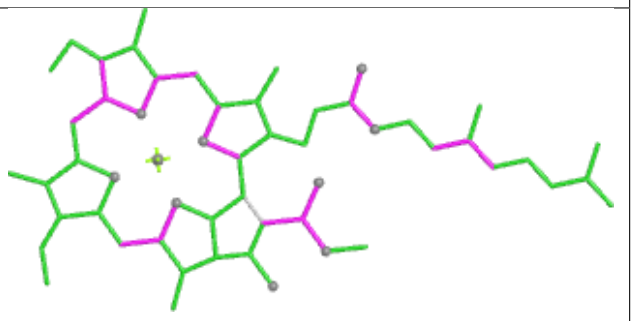


Rings

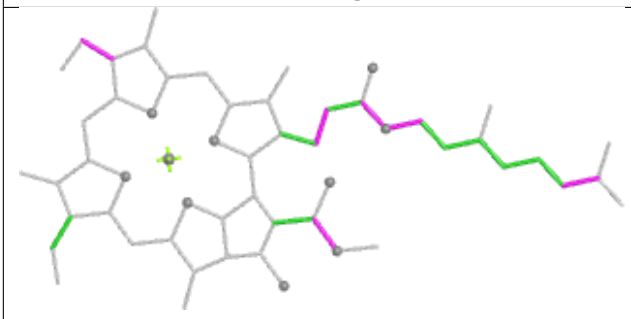
Ligand CLA A 839



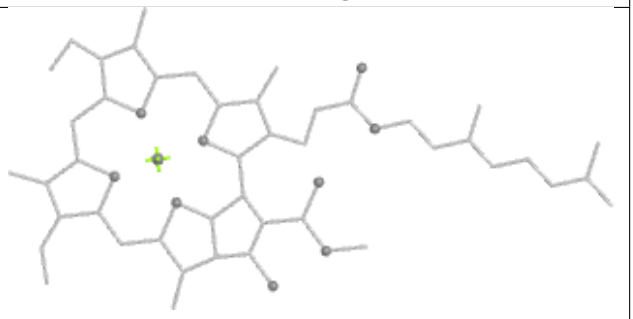
Bond lengths



Bond angles

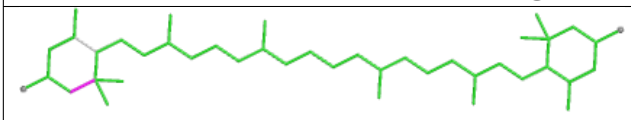


Torsions

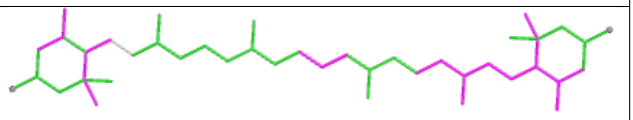


Rings

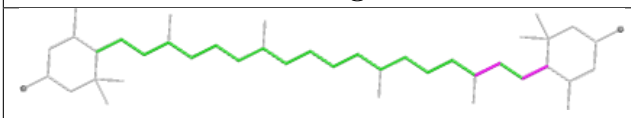
Ligand LUT 8 619



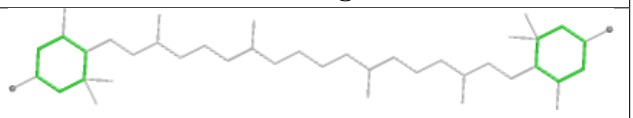
Bond lengths



Bond angles

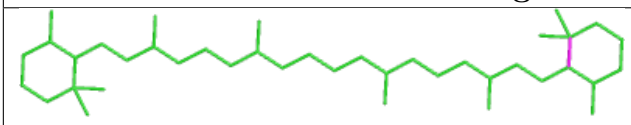


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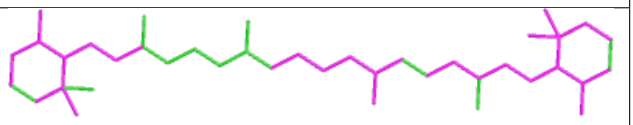


Rings

Ligand BCR O 2005



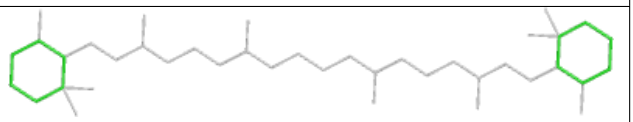
Bond lengths



Bond angles

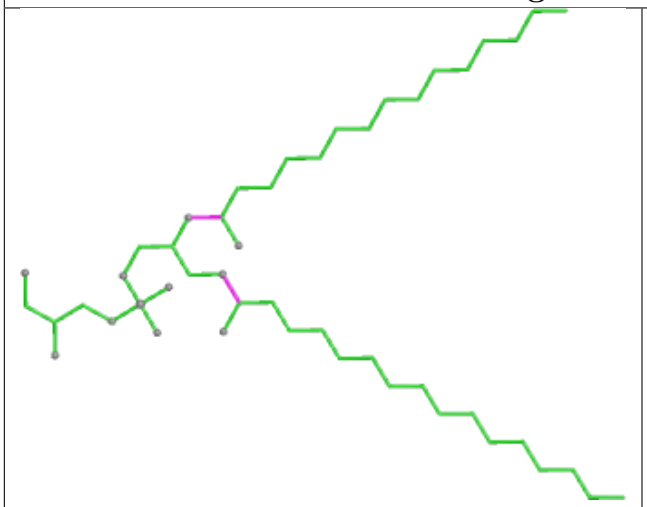


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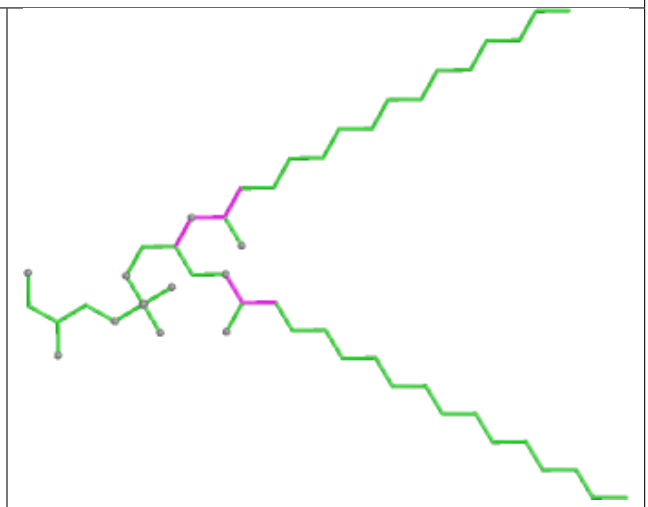


Rings

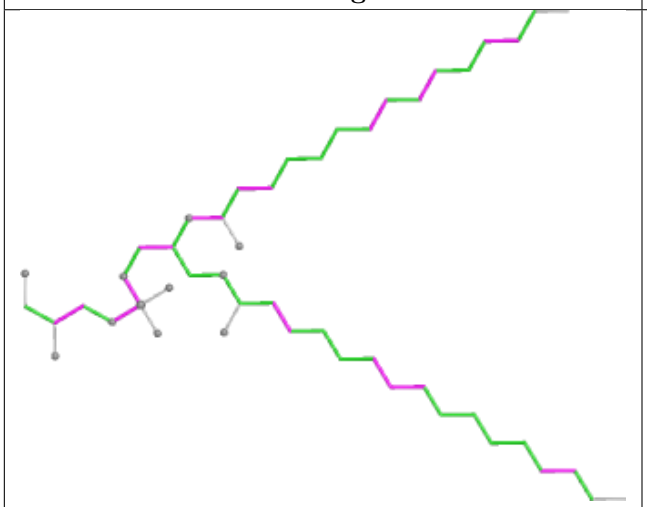
Ligand LHG 6 623



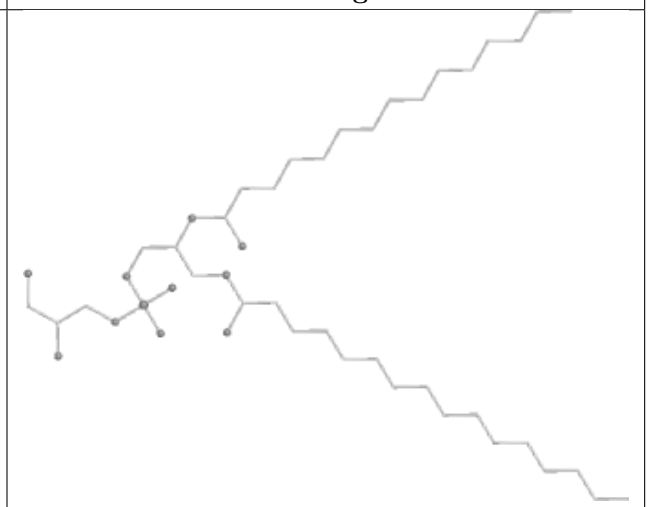
Bond lengths



Bond angles

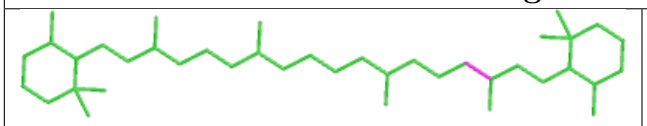


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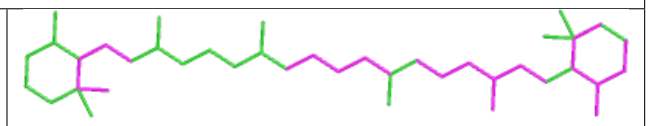


Rings

Ligand BCR B 848



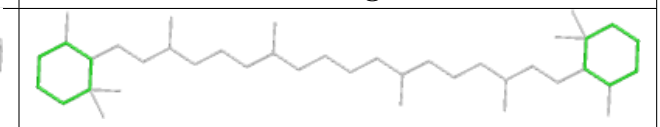
Bond lengths



Bond angles

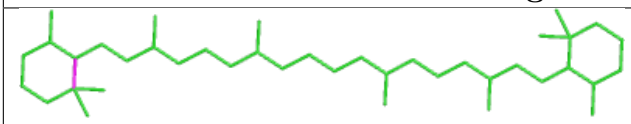


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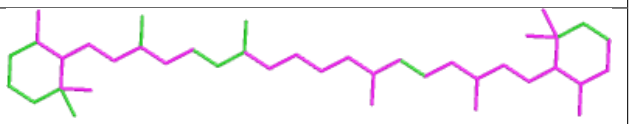


Rings

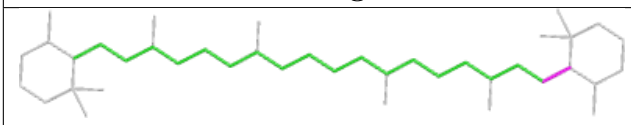
Ligand BCR 7 621



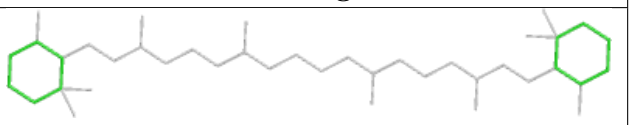
Bond lengths



Bond angles

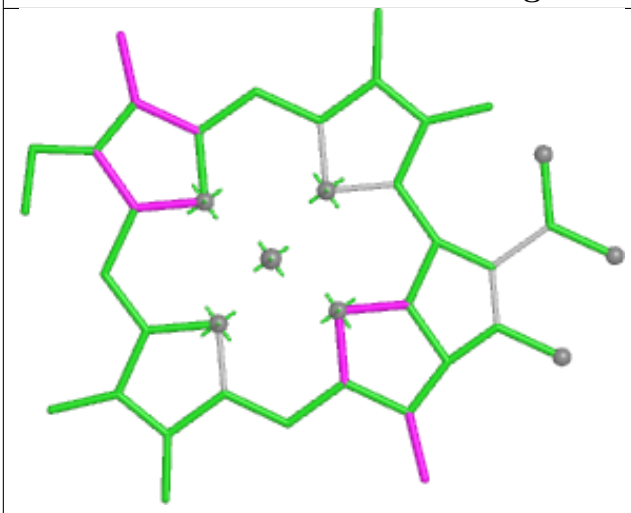


Torsions



Rings

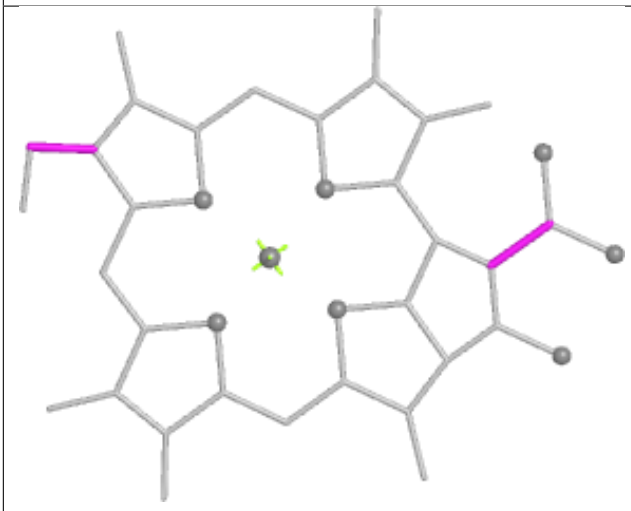
Ligand CLA H 202



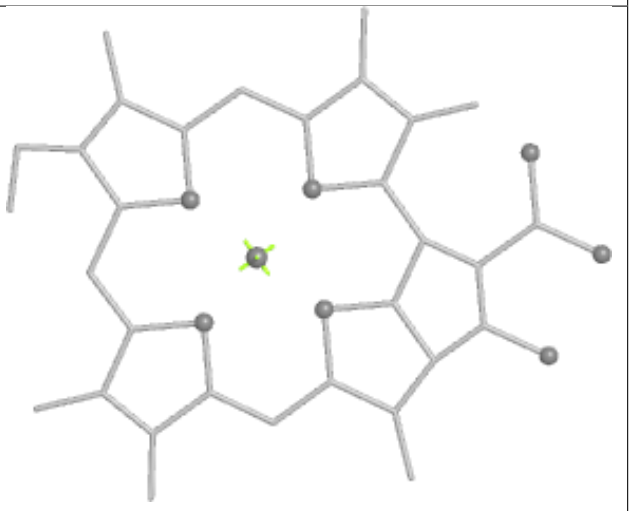
Bond lengths



Bond angles

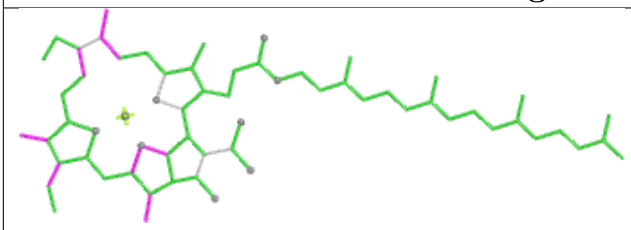


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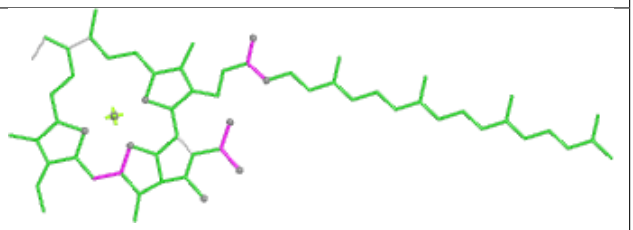


Rings

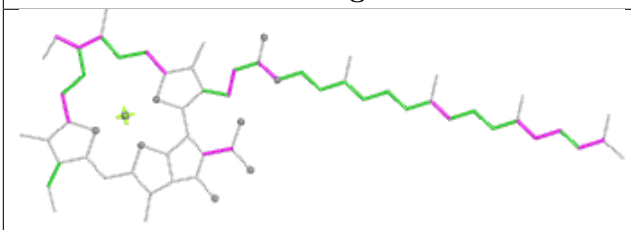
Ligand CLA 2 602



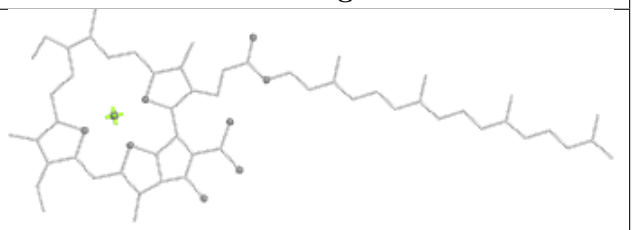
Bond lengths



Bond angles

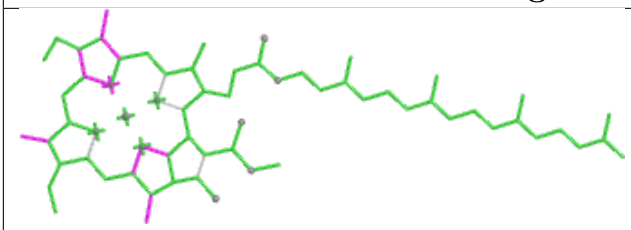


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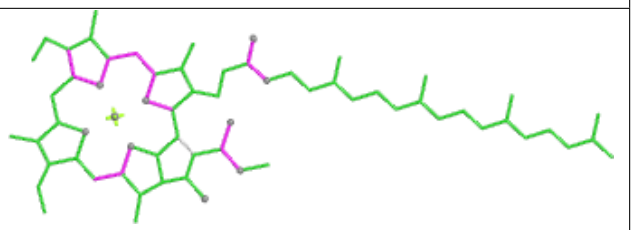


Rings

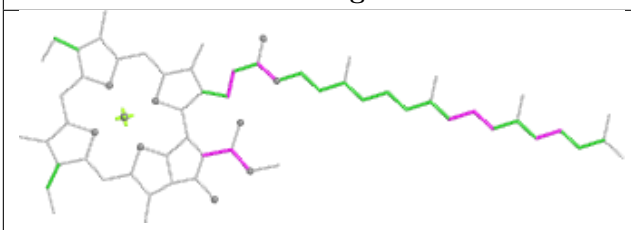
Ligand CLA 5 602



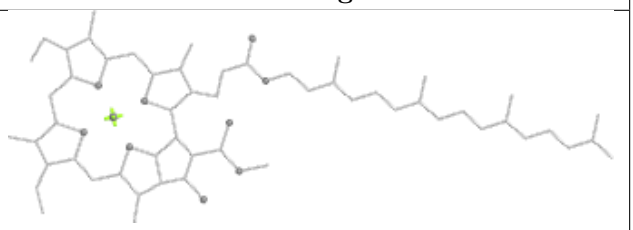
Bond lengths



Bond angles

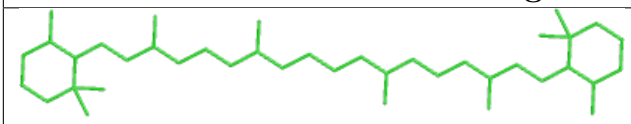


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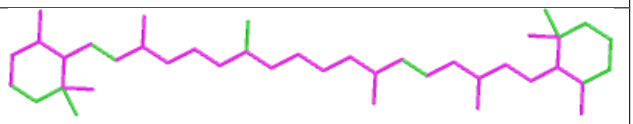


Rings

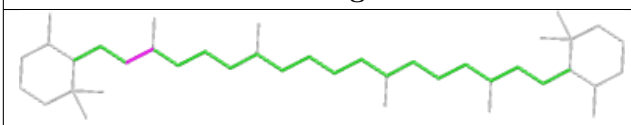
Ligand BCR L 305



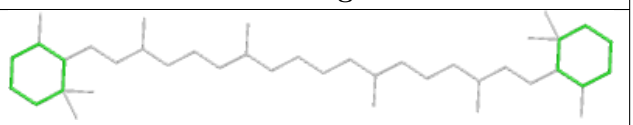
Bond lengths



Bond angles

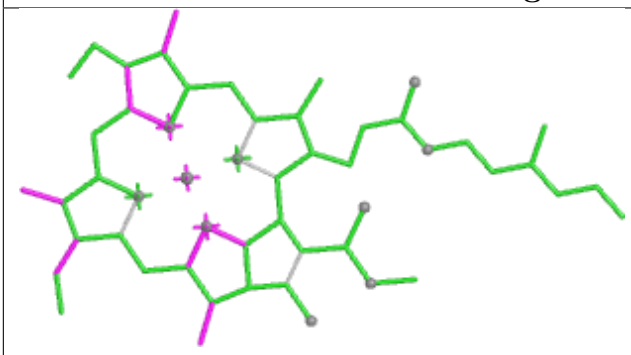


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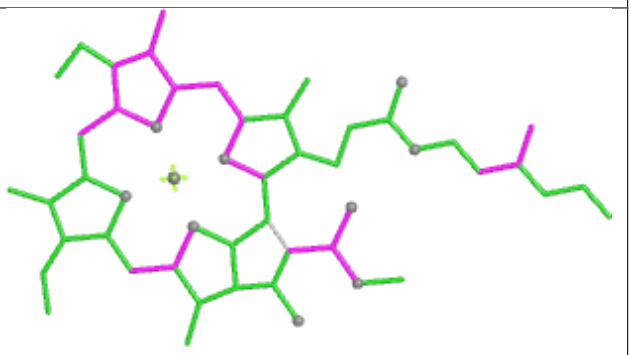


Rings

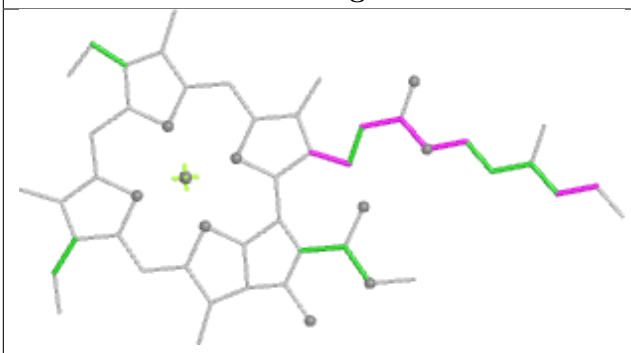
Ligand CLA A 805



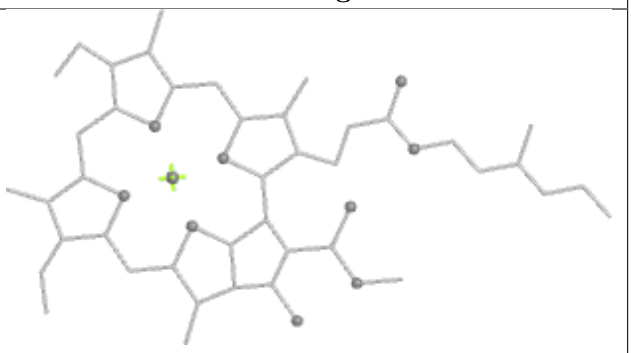
Bond lengths



Bond angles

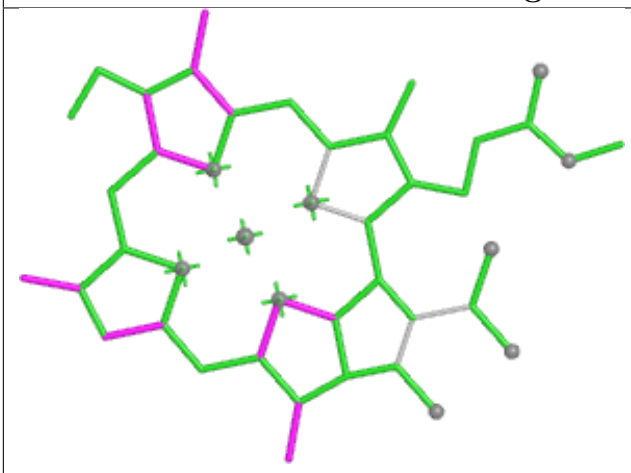


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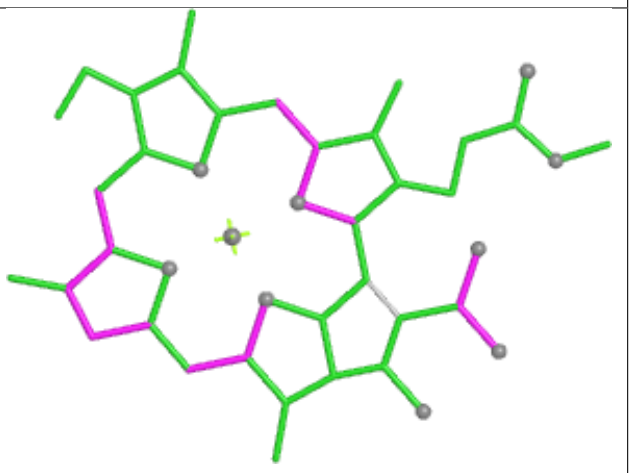


Rings

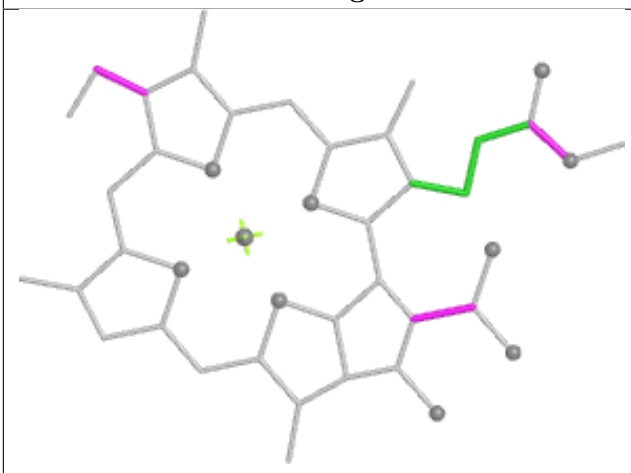
Ligand CLA B 821



Bond lengths



Bond angles

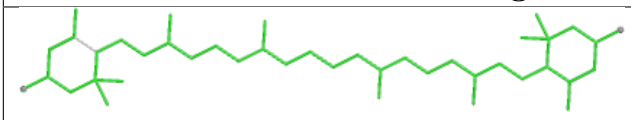


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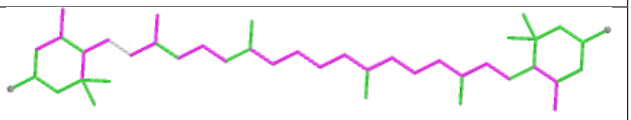


Rings

Ligand LUT W 1620



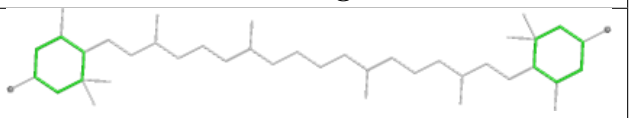
Bond lengths



Bond angles



Torsions

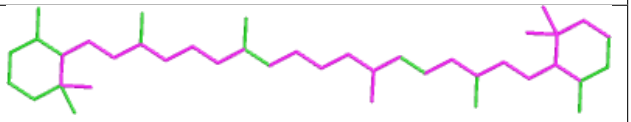


Rings

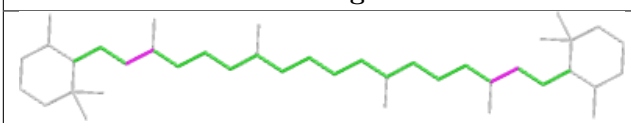
Ligand BCR K 207



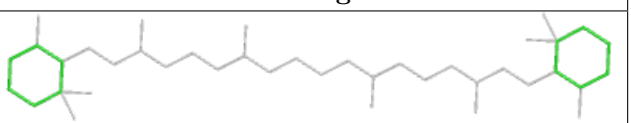
Bond lengths



Bond angles

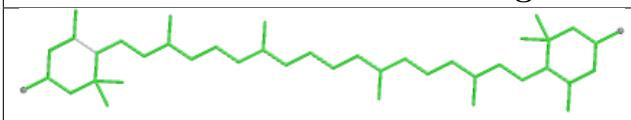


Torsions

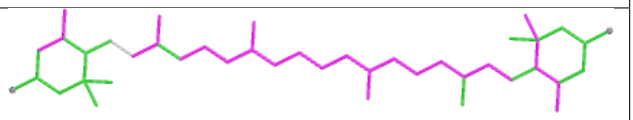


Rings

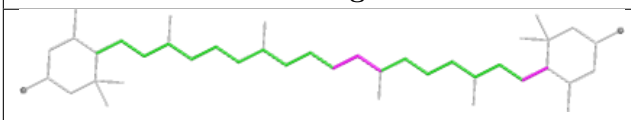
Ligand LUT Y 1620



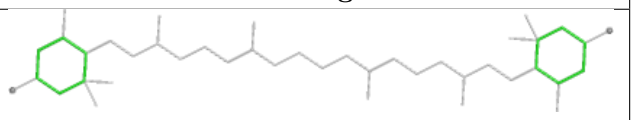
Bond lengths



Bond angles



Torsions

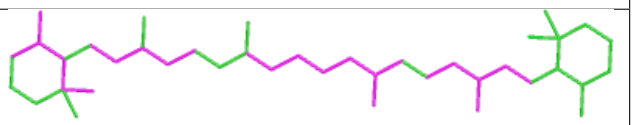


Rings

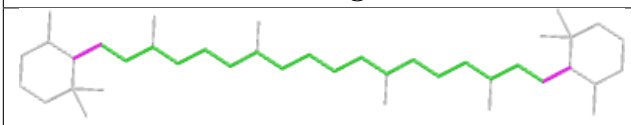
Ligand BCR B 853



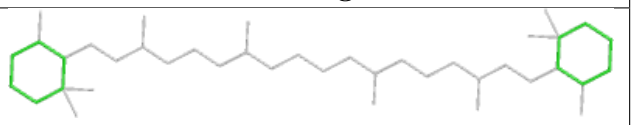
Bond lengths



Bond angles

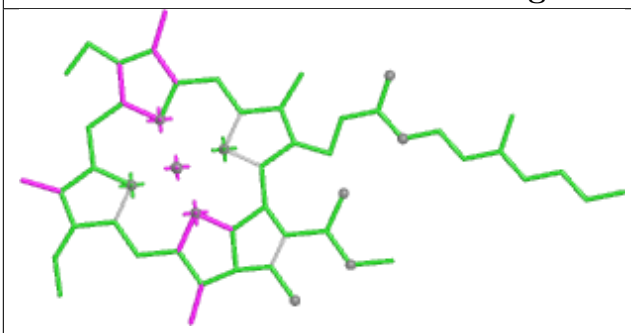


Torsions

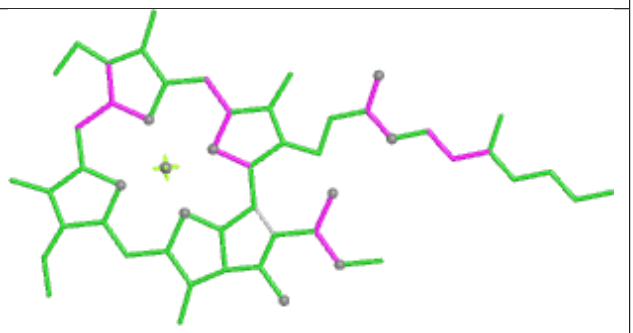


Rings

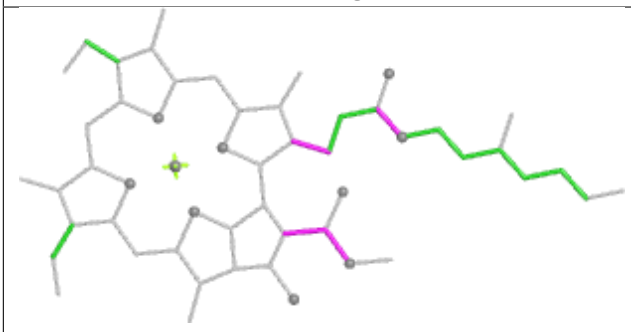
Ligand CLA 8 614



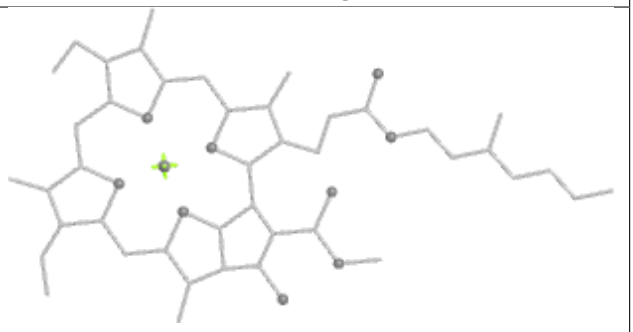
Bond lengths



Bond angles

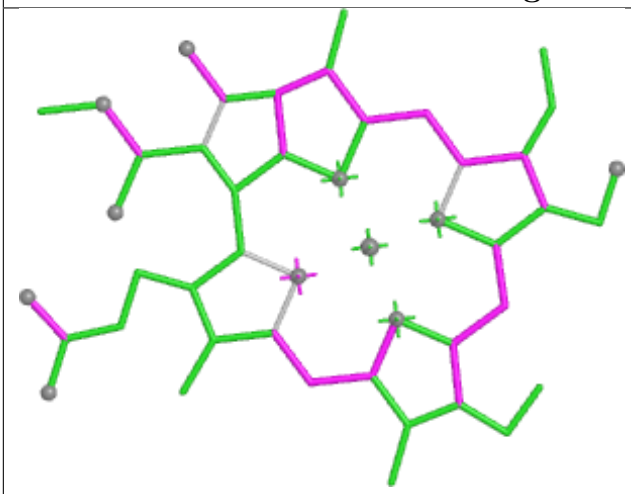


Torsions

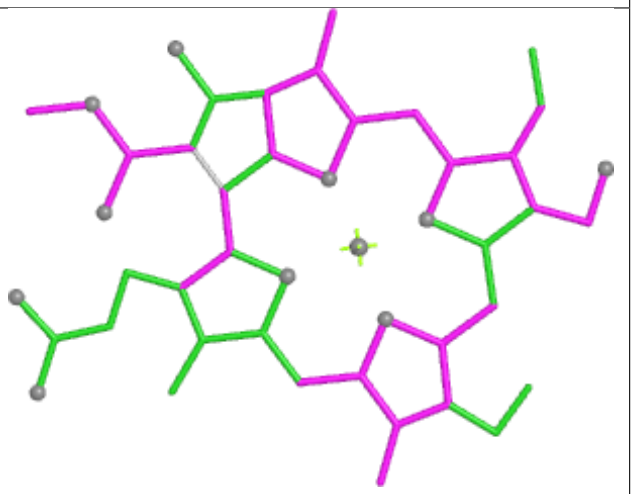


Rings

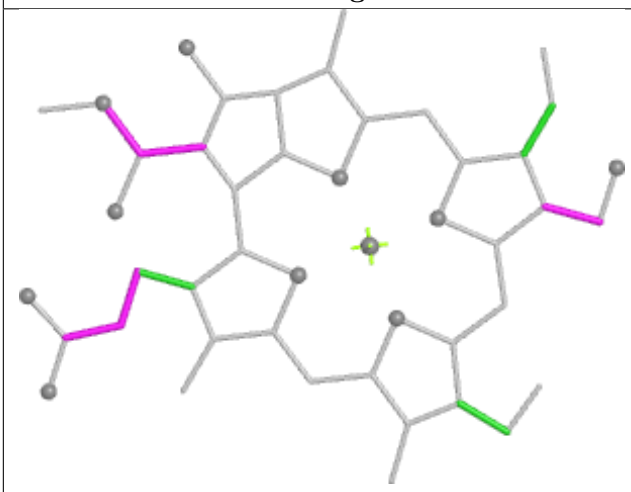
Ligand CHL Y 606



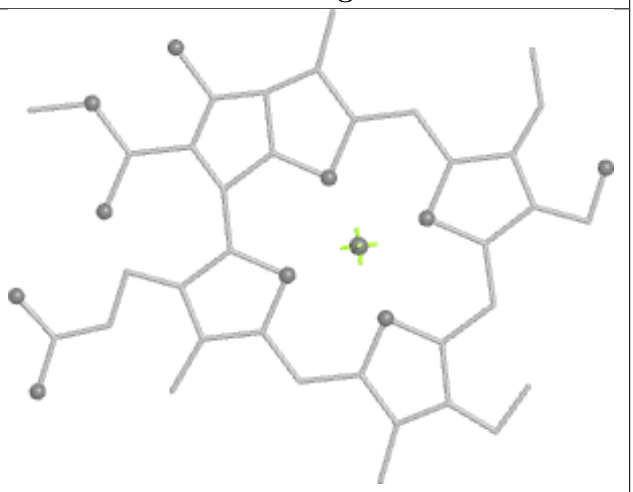
Bond lengths



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.

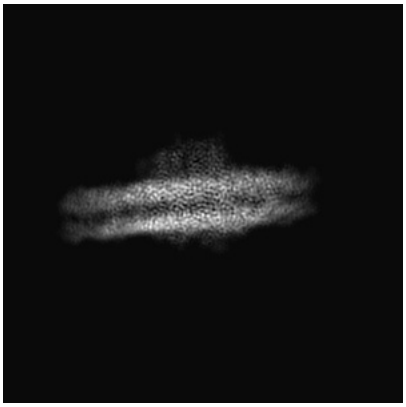
6 Map visualisation

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

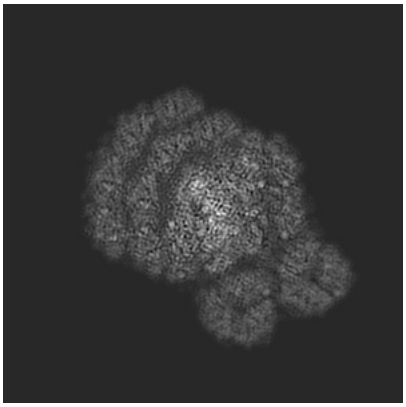
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

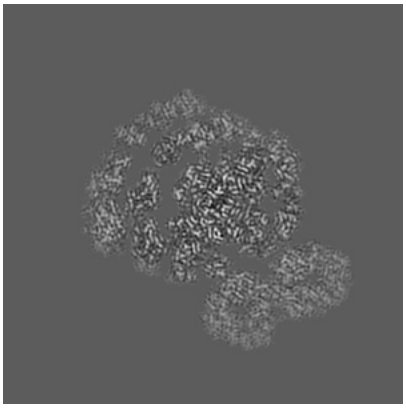
6.2.1 Primary map



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)

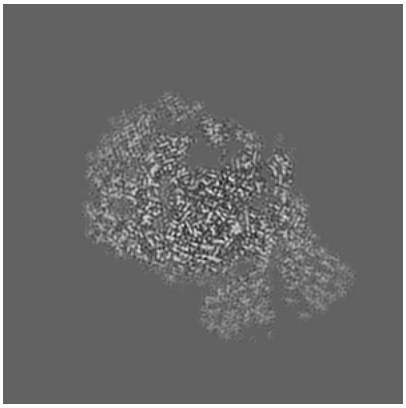
6.3.1 Primary map



X Index: 194



Y Index: 153

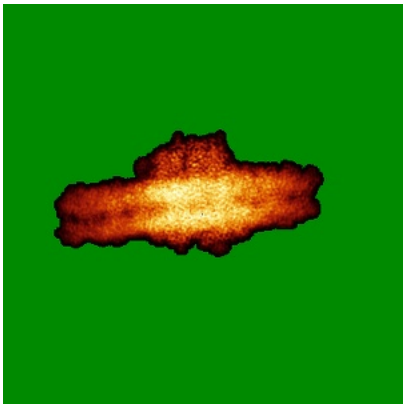


Z Index: 190

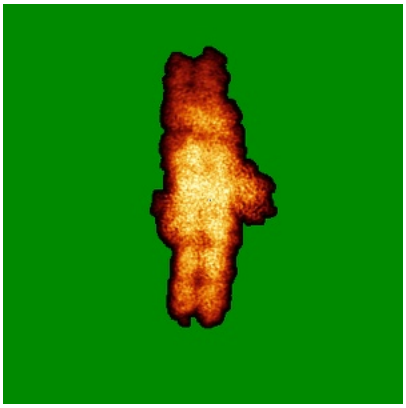
The images above show the largest variance slices of the map in three orthogonal directions.

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

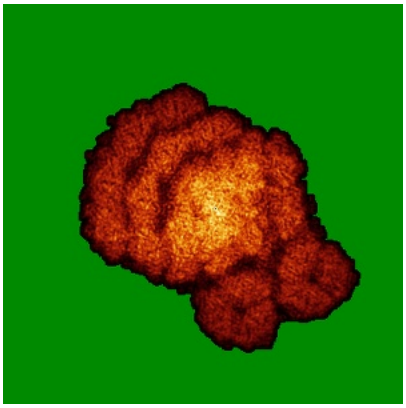
6.4.1 Primary map



X



Y

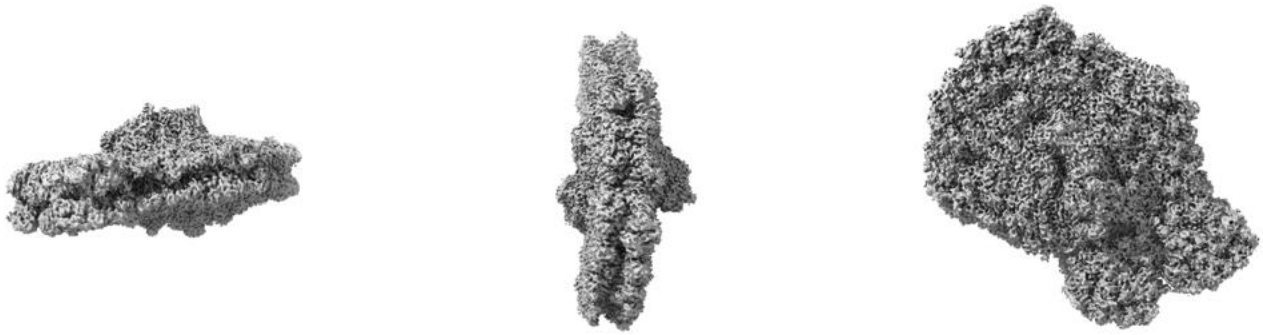


Z

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.

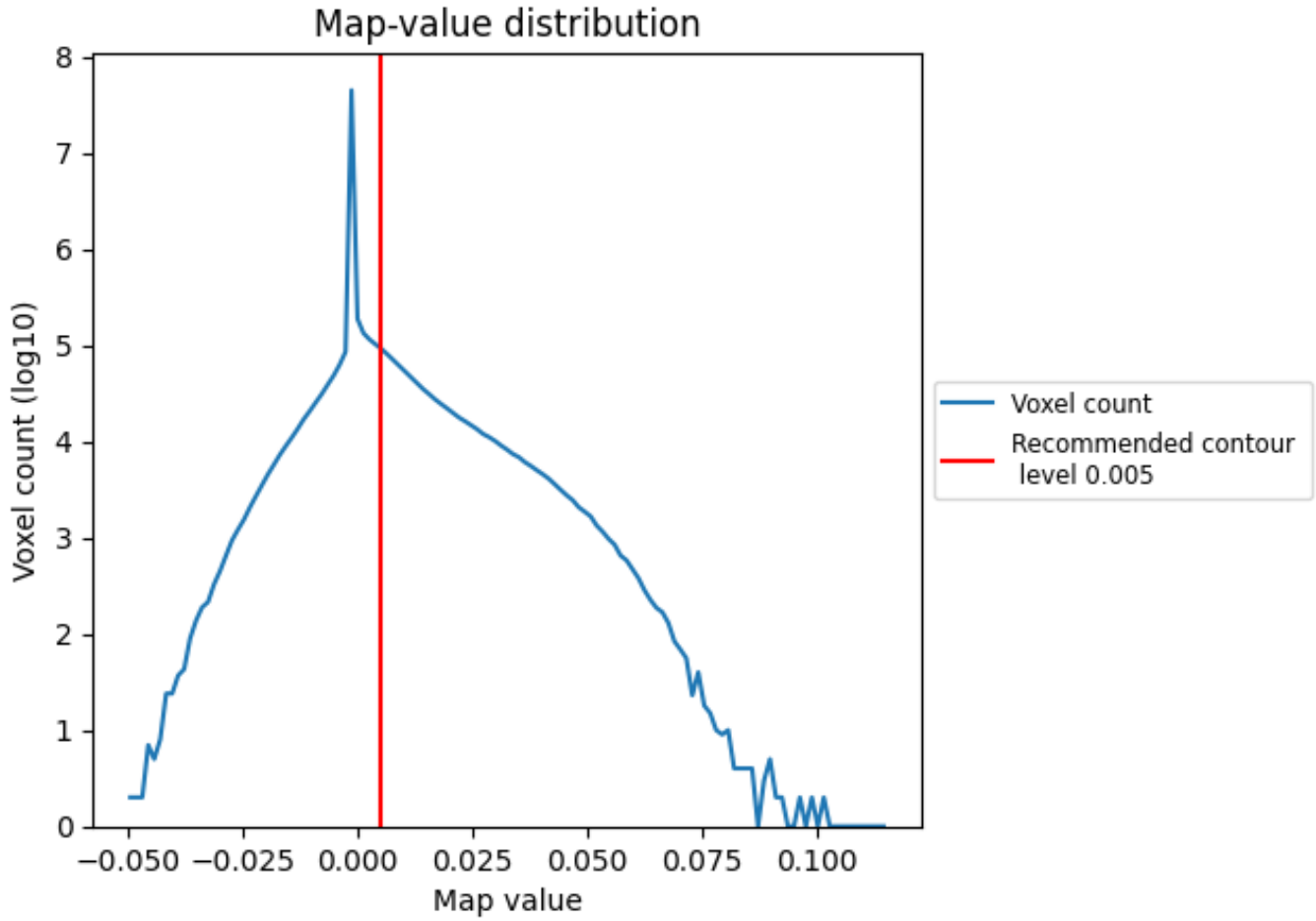
6.6 Mask visualisation (i)

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

7 Map analysis

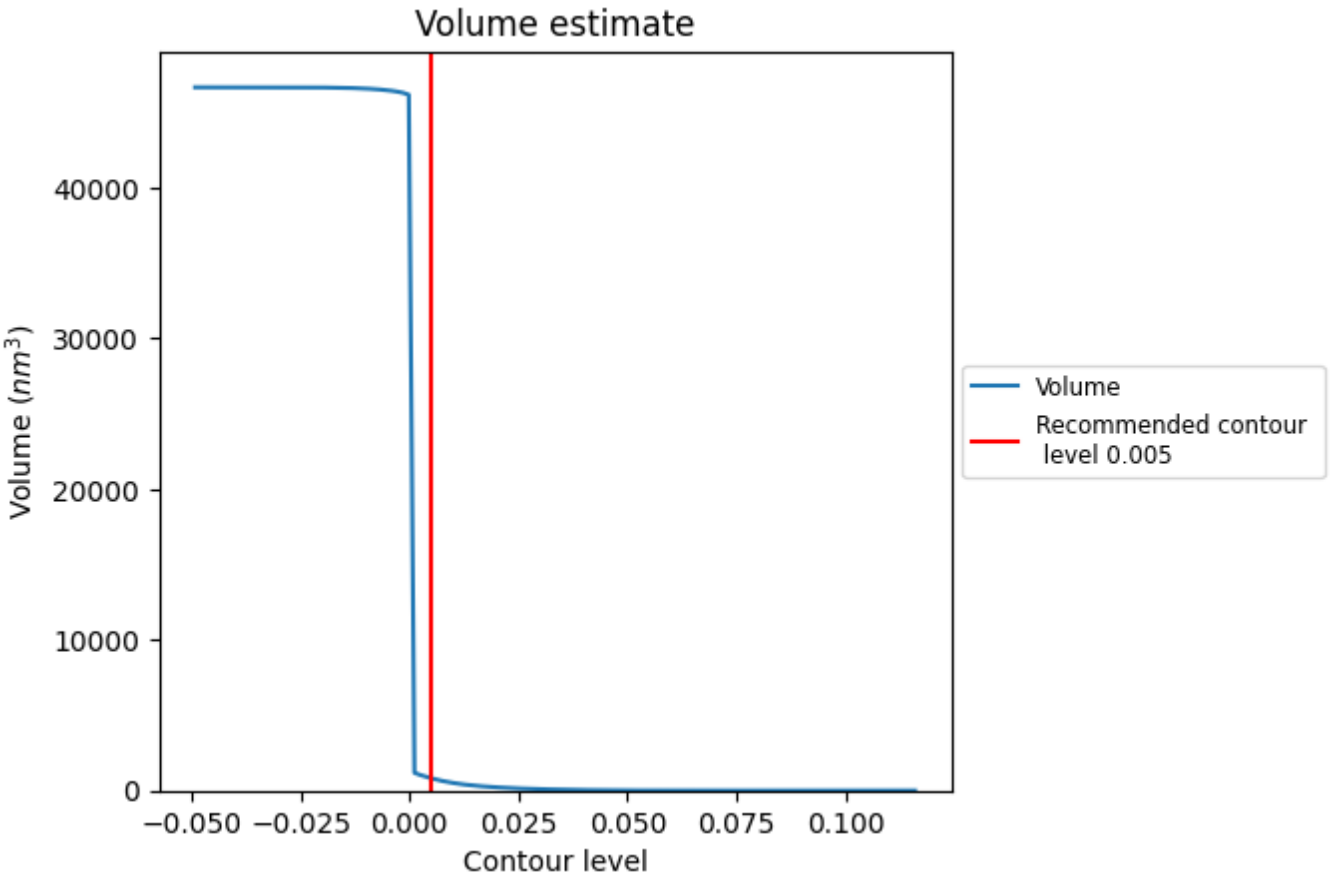
This section contains the results of statistical analysis of the map.

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.

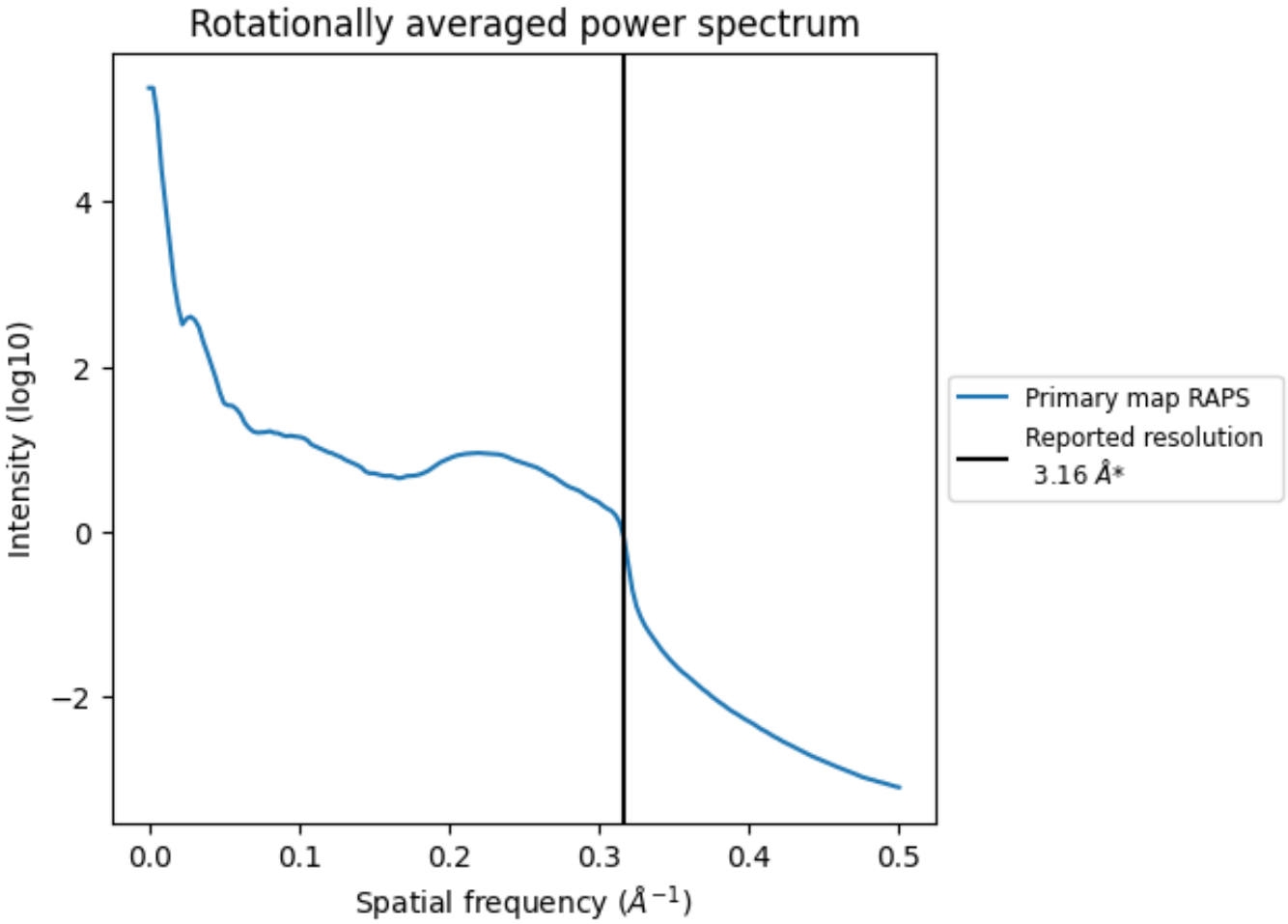
7.2 Volume estimate



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 $Å^{-1}$

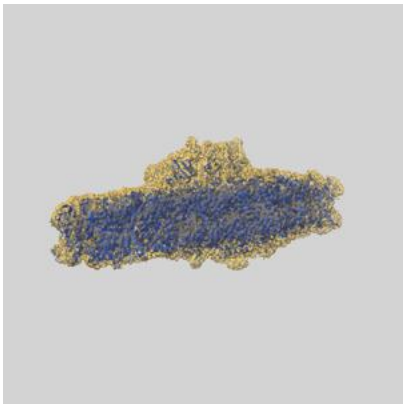
8 Fourier-Shell correlation

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

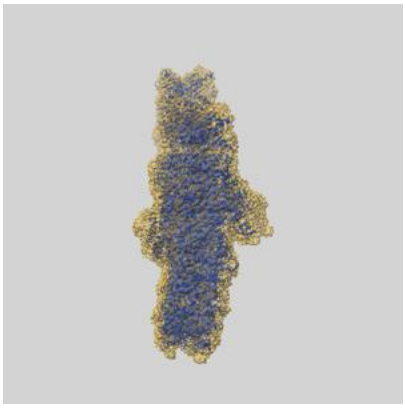
9 Map-model fit

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 37.

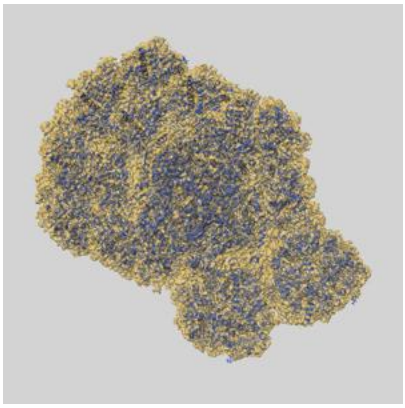
9.1 Map-model overlay



X



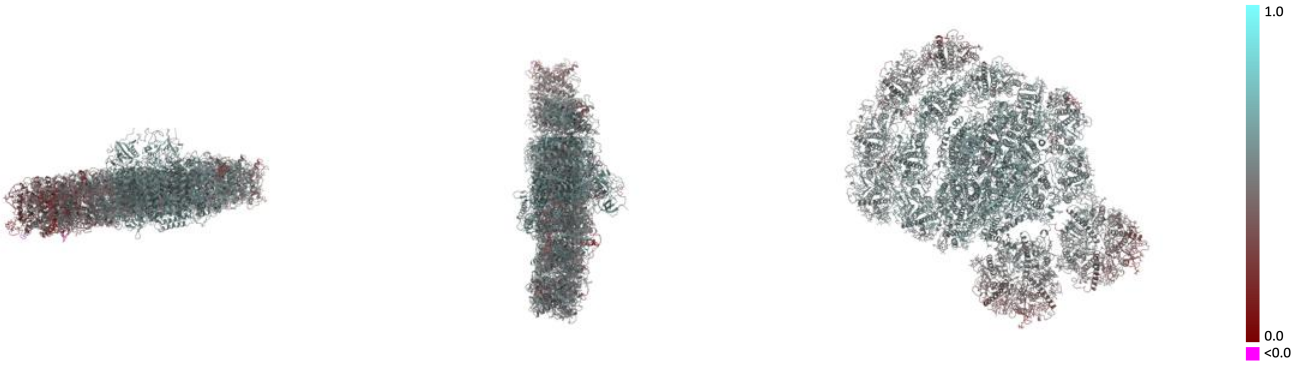
Y



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.

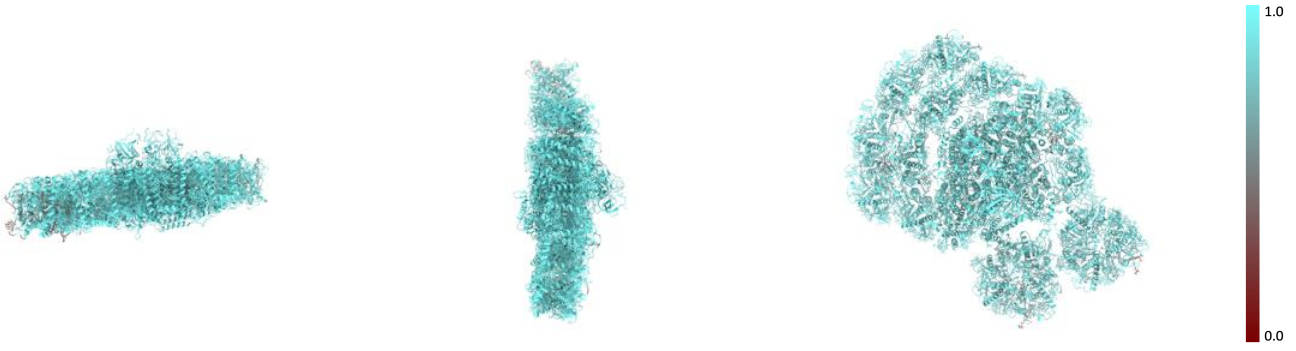
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

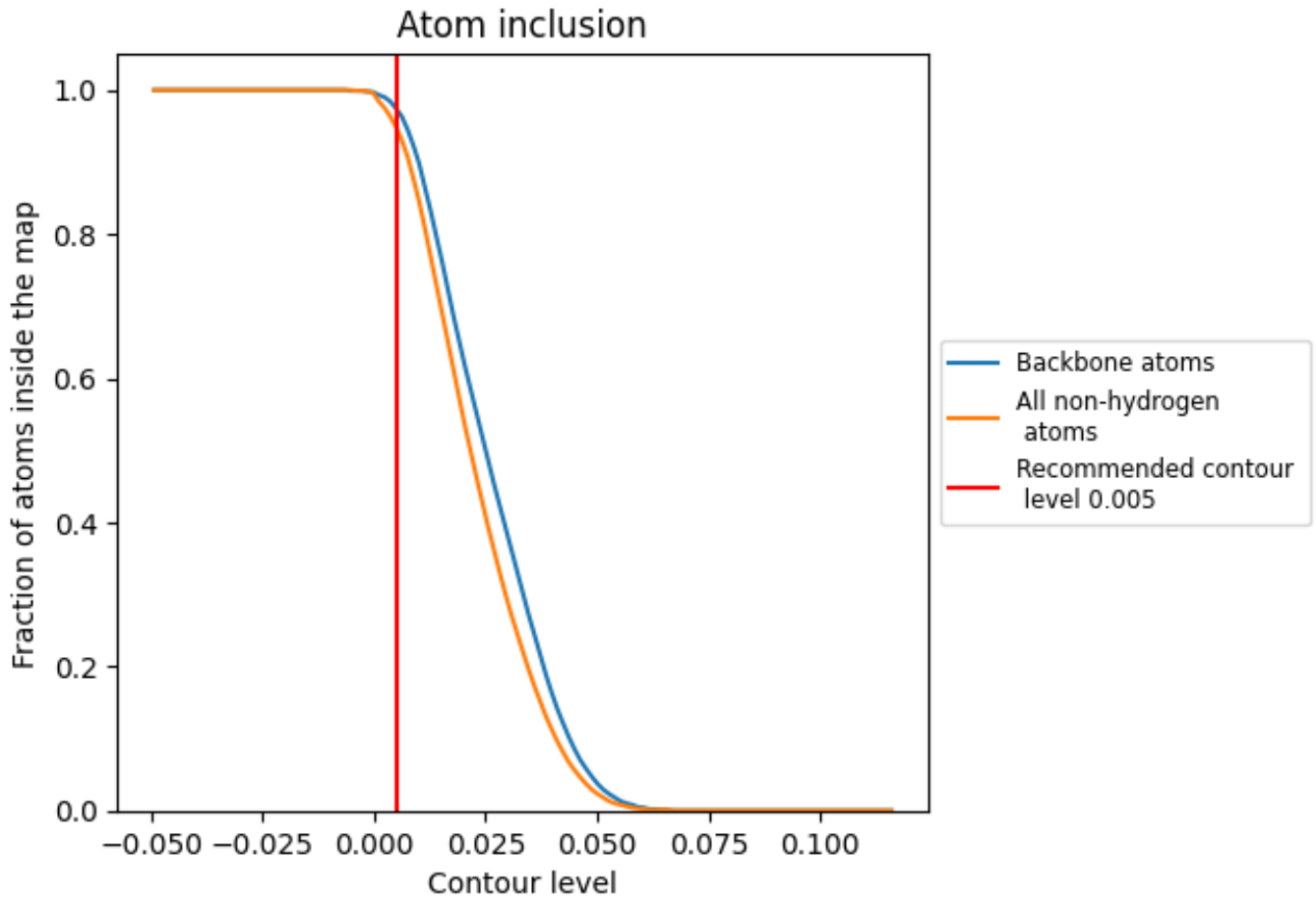
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

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

