Full wwPDB EM Validation Report ⓘ

Aug 7, 2026 – 04:15 AM JST

PDB ID	:	8Z11 / pdb_00008z11
EMDB ID	:	EMD-39717
Title	:	Cryo-EM structure of haptophyte photosystem I
Authors	:	He, F.Y.; Zhao, L.S.; Li, K.; Zhang, Y.Z.; Liu, L.N.
Deposited on	:	2024-04-10
Resolution	:	2.74 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:

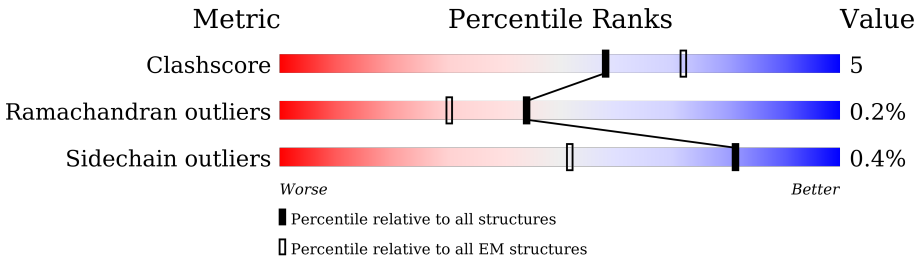
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

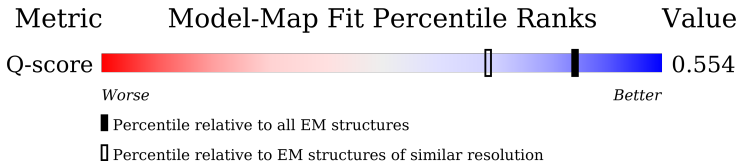
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.74 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.





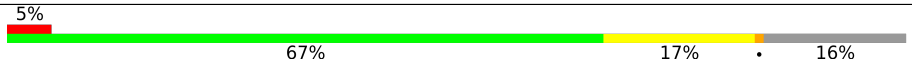
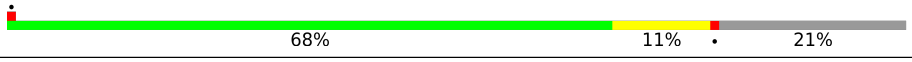
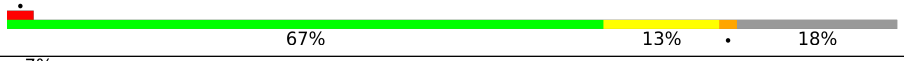
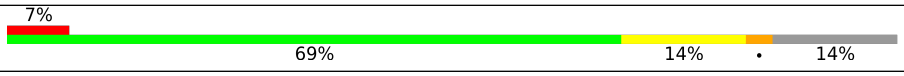
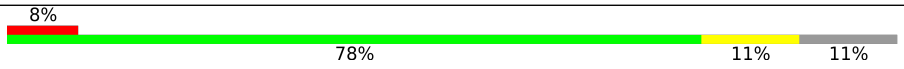
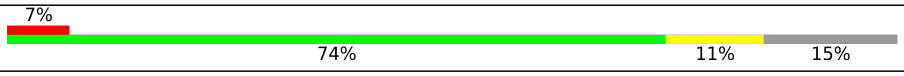
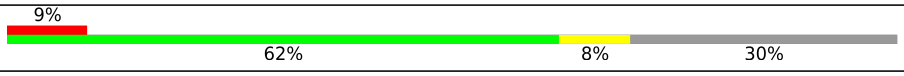
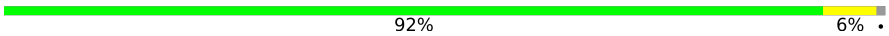
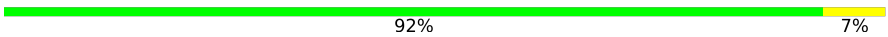
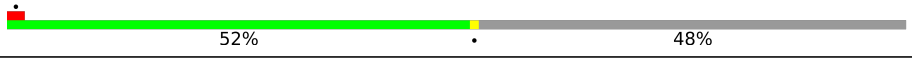
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10492 (2.24 - 3.24)

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	209	78% 7% • 14%
2	B	209	56% 16% • 24%
3	C	205	16% 76% 11% 14%
4	D	245	62% 10% • 27%

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Mol	Chain	Length	Quality of chain
5	E	206	
6	F	240	
7	G	198	
8	H	198	
9	I	194	
10	J	200	
11	K	202	
12	L	229	
13	M	217	
13	P	217	
13	W	217	
14	N	224	
15	O	206	
15	R	206	
15	T	206	
16	Q	187	
17	S	235	
18	U	203	
19	V	122	
20	a	752	
21	b	734	
22	c	81	
23	d	142	
24	e	124	
25	f	184	

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Mol	Chain	Length	Quality of chain
26	i	36	6% 89% 8%
27	j	40	82% 18%
28	k	92	72% 24%
29	l	145	94% 5%
30	m	30	93% 7%
31	r	133	62% 6% 32%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	DD6	J	317	X	-	-	-
34	DD6	K	315	X	-	-	-
34	DD6	O	313	X	-	-	-
34	DD6	S	321	X	-	-	-
37	A86	O	312	X	-	-	-

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 73546 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 iFCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	180	Total	C	N	O	S	0	0
			1403	910	230	254	9		

- Molecule 2 is a protein called iFCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	158	Total	C	N	O	S	0	0
			1194	770	197	219	8		

- Molecule 3 is a protein called iFCPI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	177	Total	C	N	O	S	0	0
			1346	872	223	244	7		

- Molecule 4 is a protein called iFCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	178	Total	C	N	O	S	1	0
			1392	910	220	254	8		

- Molecule 5 is a protein called iFCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	176	Total	C	N	O	S	0	0
			1316	854	212	240	10		

- Molecule 6 is a protein called iFCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	210	Total	C	N	O	S	0	0
			1573	1006	266	290	11		

- Molecule 7 is a protein called iFCPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	167	Total	C	N	O	S	0	0
			1235	794	204	227	10		

- Molecule 8 is a protein called iFCPI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	167	Total	C	N	O	S	0	0
			1266	808	212	233	13		

- Molecule 9 is a protein called iFCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	154	Total	C	N	O	S	0	0
			1190	770	198	213	9		

- Molecule 10 is a protein called iFCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	171	Total	C	N	O	S	0	0
			1253	803	212	227	11		

- Molecule 11 is a protein called iFCPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	166	Total	C	N	O	S	0	0
			1280	837	217	219	7		

- Molecule 12 is a protein called iFCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	198	Total	C	N	O	S	0	0
			1479	960	246	266	7		

- Molecule 13 is a protein called iFCPI-15/14/16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	193	Total	C	N	O	S	0	0
			1465	949	247	263	6		
13	P	193	Total	C	N	O	S	0	0
			1465	949	247	263	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	193	Total	C	N	O	S	0	0
			1465	949	247	263	6		

- Molecule 14 is a protein called iFCPI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	194	Total	C	N	O	S	0	0
			1451	941	247	255	8		

- Molecule 15 is a protein called iFCPI-20/19/21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	175	Total	C	N	O	S	0	0
			1299	842	215	237	5		
15	R	175	Total	C	N	O	S	0	0
			1299	842	215	237	5		
15	T	175	Total	C	N	O	S	0	0
			1299	842	215	237	5		

- Molecule 16 is a protein called iFCPI-18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	157	Total	C	N	O	S	0	0
			1210	775	205	221	9		

- Molecule 17 is a protein called iFCPI-22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	205	Total	C	N	O	S	0	0
			1597	1046	264	279	8		

- Molecule 18 is a protein called iFCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	142	Total	C	N	O	S	0	0
			1084	698	180	199	7		

- Molecule 19 is a protein called L-iFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	47	Total	C	N	O	S	0	0
			357	229	60	66	2		

- Molecule 20 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	741	Total	C	N	O	S	0	0
			5826	3810	991	995	30		

- Molecule 21 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	732	Total	C	N	O	S	0	0
			5818	3832	981	984	21		

- Molecule 22 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	80	Total	C	N	O	S	0	0
			596	364	105	116	11		

- Molecule 23 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	137	Total	C	N	O	S	0	0
			1080	698	181	198	3		

- Molecule 24 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	65	Total	C	N	O	S	0	0
			504	320	87	94	3		

- Molecule 25 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	161	Total	C	N	O	S	0	0
			1243	804	211	224	4		

- Molecule 26 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	i	33	Total	C	N	O	S	0	0
			258	179	34	44	1		

- Molecule 27 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	j	40	Total	C	N	O	S	0	0
			316	210	47	57	2		

- Molecule 28 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	k	70	Total	C	N	O	S	0	0
			503	327	80	90	6		

- Molecule 29 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	l	143	Total	C	N	O	S	0	0
			1081	710	173	196	2		

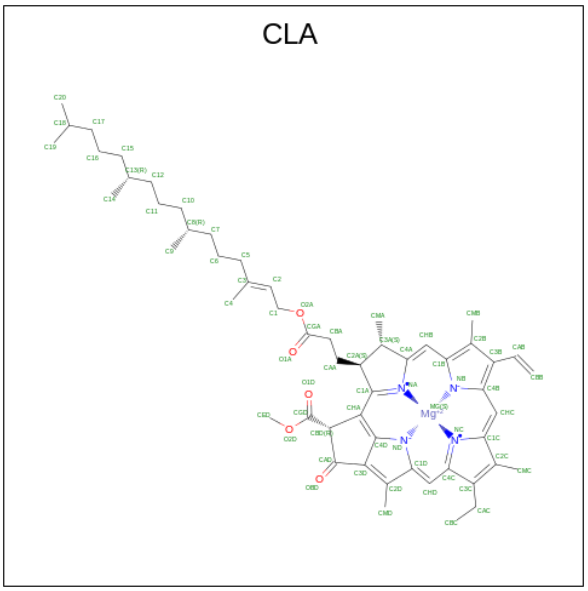
- Molecule 30 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	m	30	Total	C	N	O	S	0	0
			219	145	35	37	2		

- Molecule 31 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	r	91	Total	C	N	O	S	0	0
			682	441	111	129	1		

- Molecule 32 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
32	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
32	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
32	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	B	1	Total 40	C 32	Mg 1	N 4	O 3	0
32	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	B	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	C	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
32	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	C	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
32	D	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	D	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
32	F	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
32	G	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
32	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
32	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	H	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	H	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
32	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	I	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
32	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	J	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	J	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
32	J	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	J	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	J	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
32	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
32	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	L	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
32	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
32	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
32	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	M	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	M	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
32	M	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
32	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	M	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
32	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	M	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	O	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
32	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	P	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
32	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	Q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	Q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	Q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	Q	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	Q	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
32	Q	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
32	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
32	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	R	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	S	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	S	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
32	S	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
32	S	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
32	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	T	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	U	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
32	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	V	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
32	V	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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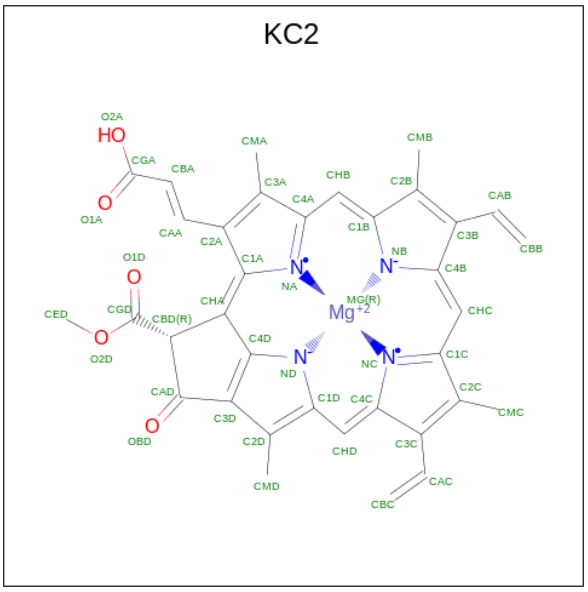
Mol	Chain	Residues	Atoms					AltConf
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
32	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	f	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
32	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 33 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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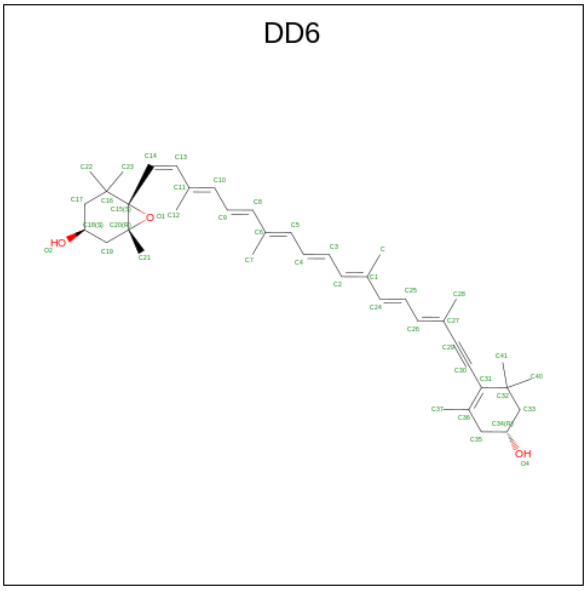
Mol	Chain	Residues	Atoms					AltConf
33	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 34 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			43	40	3	
34	A	1	Total	C	O	0
			43	40	3	
34	A	1	Total	C	O	0
			43	40	3	
34	A	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			43	40	3	
34	C	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	F	1	Total	C	O	0
			43	40	3	
34	F	1	Total	C	O	0
			43	40	3	
34	F	1	Total	C	O	0
			43	40	3	
34	G	1	Total	C	O	0
			43	40	3	
34	H	1	Total	C	O	0
			43	40	3	
34	H	1	Total	C	O	0
			43	40	3	
34	H	1	Total	C	O	0
			43	40	3	
34	I	1	Total	C	O	0
			43	40	3	
34	I	1	Total	C	O	0
			43	40	3	
34	I	1	Total	C	O	0
			43	40	3	

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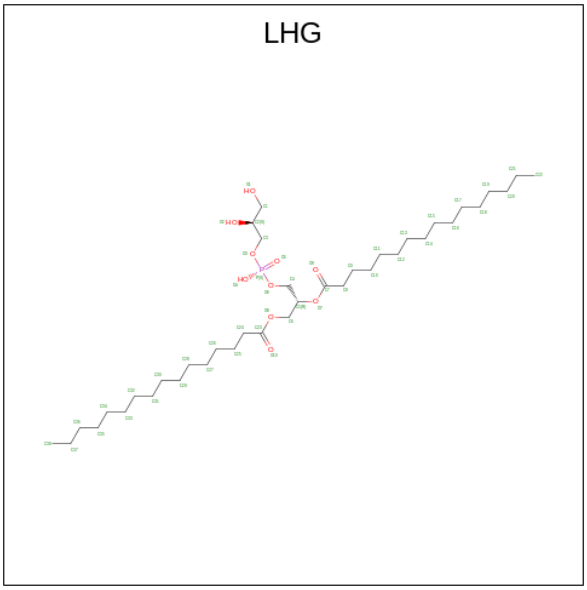
Mol	Chain	Residues	Atoms			AltConf
34	I	1	Total	C	O	0
			43	40	3	
34	J	1	Total	C	O	0
			43	40	3	
34	J	1	Total	C	O	0
			43	40	3	
34	J	1	Total	C	O	0
			43	40	3	
34	J	1	Total	C	O	0
			43	40	3	
34	K	1	Total	C	O	0
			43	40	3	
34	K	1	Total	C	O	0
			43	40	3	
34	L	1	Total	C	O	0
			43	40	3	
34	M	1	Total	C	O	0
			43	40	3	
34	N	1	Total	C	O	0
			43	40	3	
34	N	1	Total	C	O	0
			43	40	3	
34	N	1	Total	C	O	0
			43	40	3	
34	O	1	Total	C	O	0
			43	40	3	
34	P	1	Total	C	O	0
			43	40	3	
34	Q	1	Total	C	O	0
			43	40	3	
34	Q	1	Total	C	O	0
			43	40	3	
34	Q	1	Total	C	O	0
			43	40	3	
34	Q	1	Total	C	O	0
			43	40	3	
34	R	1	Total	C	O	0
			43	40	3	
34	S	1	Total	C	O	0
			43	40	3	
34	T	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms	AltConf
34	U	1	Total C O 43 40 3	0
34	V	1	Total C O 43 40 3	0
34	W	1	Total C O 43 40 3	0
34	j	1	Total C O 43 40 3	0
34	k	1	Total C O 43 40 3	0

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



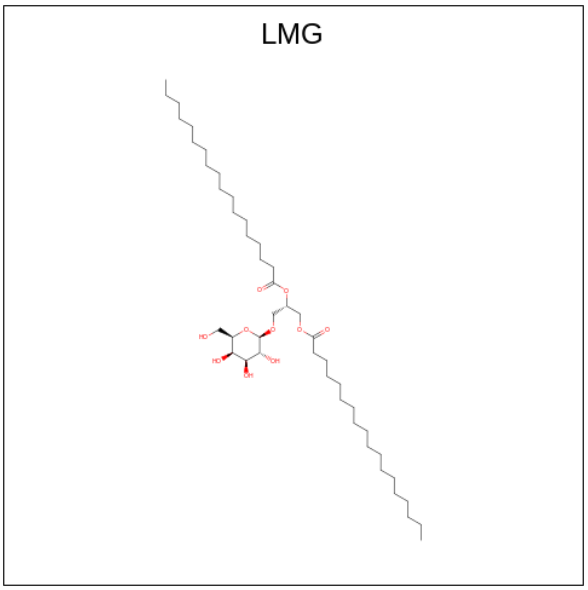
Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total C O P 40 29 10 1	0
35	B	1	Total C O P 31 20 10 1	0
35	D	1	Total C O P 48 37 10 1	0
35	E	1	Total C O P 46 35 10 1	0
35	E	1	Total C O P 46 35 10 1	0
35	F	1	Total C O P 41 30 10 1	0

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Mol	Chain	Residues	Atoms				AltConf
35	F	1	Total	C	O	P	0
			40	29	10	1	
35	I	1	Total	C	O	P	0
			46	35	10	1	
35	I	1	Total	C	O	P	0
			37	26	10	1	
35	M	1	Total	C	O	P	0
			46	35	10	1	
35	P	1	Total	C	O	P	0
			46	35	10	1	
35	W	1	Total	C	O	P	0
			46	35	10	1	
35	a	1	Total	C	O	P	0
			48	37	10	1	
35	a	1	Total	C	O	P	0
			30	19	10	1	
35	a	1	Total	C	O	P	0
			38	27	10	1	
35	f	1	Total	C	O	P	0
			47	36	10	1	

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



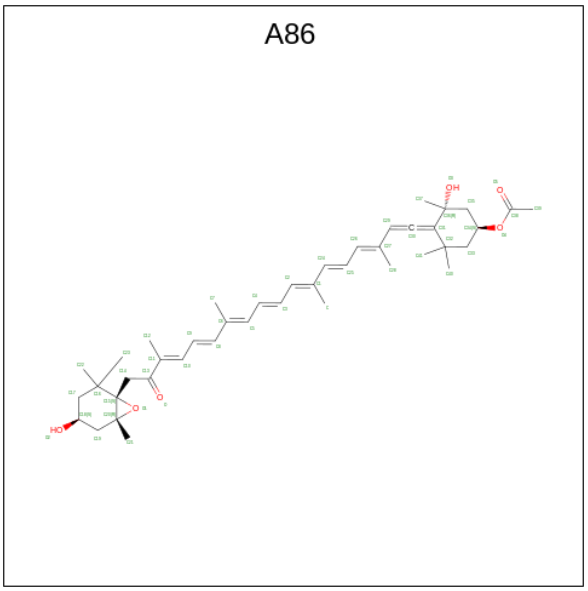
Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			36	26	10	

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Mol	Chain	Residues	Atoms	AltConf
36	A	1	Total C O 40 30 10	0
36	D	1	Total C O 30 20 10	0
36	D	1	Total C O 36 26 10	0
36	D	1	Total C O 40 30 10	0
36	D	1	Total C O 35 25 10	0
36	E	1	Total C O 40 30 10	0
36	E	1	Total C O 31 21 10	0
36	E	1	Total C O 40 30 10	0
36	F	1	Total C O 40 30 10	0
36	F	1	Total C O 33 23 10	0
36	L	1	Total C O 37 27 10	0
36	M	1	Total C O 40 30 10	0
36	N	1	Total C O 40 30 10	0
36	P	1	Total C O 45 35 10	0
36	S	1	Total C O 33 23 10	0
36	T	1	Total C O 37 27 10	0
36	W	1	Total C O 39 29 10	0
36	j	1	Total C O 38 28 10	0
36	l	1	Total C O 49 39 10	0

- Molecule 37 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
37	C	1	Total C O 48 42 6	0
37	C	1	Total C O 48 42 6	0
37	D	1	Total C O 48 42 6	0
37	D	1	Total C O 48 42 6	0
37	F	1	Total C O 48 42 6	0
37	F	1	Total C O 48 42 6	0
37	F	1	Total C O 48 42 6	0
37	G	1	Total C O 48 42 6	0
37	G	1	Total C O 48 42 6	0
37	H	1	Total C O 48 42 6	0
37	J	1	Total C O 48 42 6	0
37	K	1	Total C O 48 42 6	0
37	K	1	Total C O 48 42 6	0
37	K	1	Total C O 48 42 6	0

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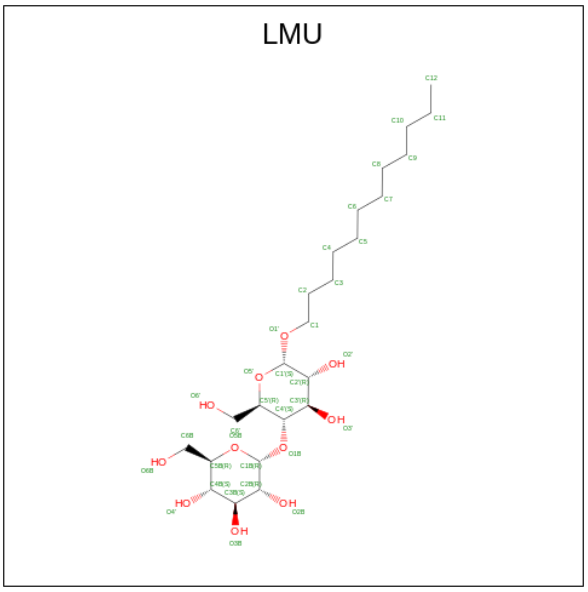
Mol	Chain	Residues	Atoms			AltConf
37	L	1	Total	C	O	0
			48	42	6	
37	L	1	Total	C	O	0
			48	42	6	
37	L	1	Total	C	O	0
			48	42	6	
37	L	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	N	1	Total	C	O	0
			48	42	6	
37	N	1	Total	C	O	0
			48	42	6	
37	N	1	Total	C	O	0
			48	42	6	
37	N	1	Total	C	O	0
			48	42	6	
37	O	1	Total	C	O	0
			48	42	6	
37	O	1	Total	C	O	0
			48	42	6	
37	P	1	Total	C	O	0
			48	42	6	
37	P	1	Total	C	O	0
			48	42	6	
37	P	1	Total	C	O	0
			48	42	6	
37	P	1	Total	C	O	0
			48	42	6	
37	Q	1	Total	C	O	0
			48	42	6	

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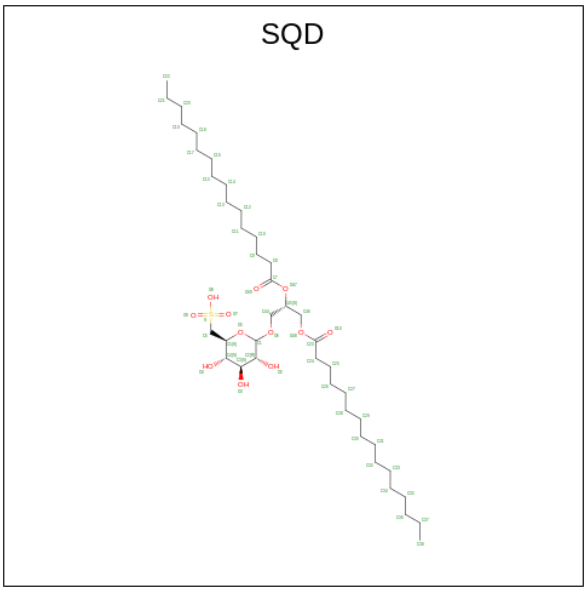
Mol	Chain	Residues	Atoms	AltConf
37	Q	1	Total C O 48 42 6	0
37	R	1	Total C O 48 42 6	0
37	R	1	Total C O 48 42 6	0
37	S	1	Total C O 48 42 6	0
37	S	1	Total C O 48 42 6	0
37	S	1	Total C O 48 42 6	0
37	S	1	Total C O 48 42 6	0
37	S	1	Total C O 48 42 6	0
37	S	1	Total C O 48 42 6	0
37	S	1	Total C O 48 42 6	0
37	T	1	Total C O 48 42 6	0
37	T	1	Total C O 48 42 6	0
37	T	1	Total C O 48 42 6	0
37	U	1	Total C O 48 42 6	0
37	W	1	Total C O 48 42 6	0
37	W	1	Total C O 48 42 6	0
37	W	1	Total C O 48 42 6	0
37	W	1	Total C O 48 42 6	0
37	r	1	Total C O 48 42 6	0

- Molecule 38 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



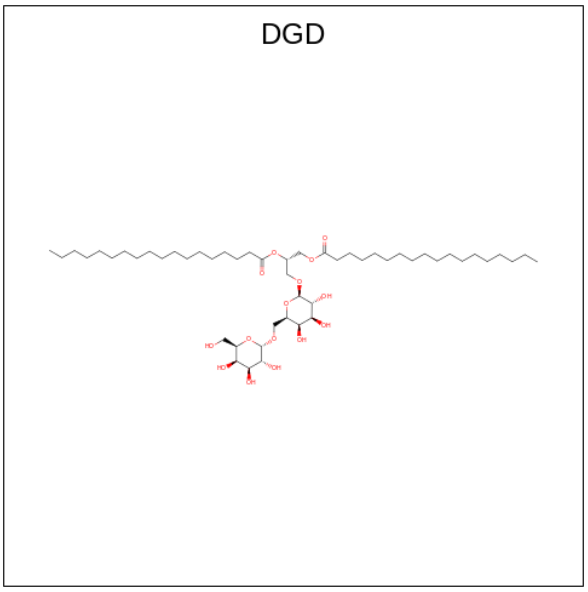
Mol	Chain	Residues	Atoms			AltConf
38	D	1	Total	C	O	0
			35	24	11	
38	I	1	Total	C	O	0
			35	24	11	
38	J	1	Total	C	O	0
			35	24	11	
38	V	1	Total	C	O	0
			34	23	11	
38	j	1	Total	C	O	0
			34	23	11	

- Molecule 39 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
39	H	1	Total	C	O	S	0
			43	30	12	1	
39	k	1	Total	C	O	S	0
			36	23	12	1	

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



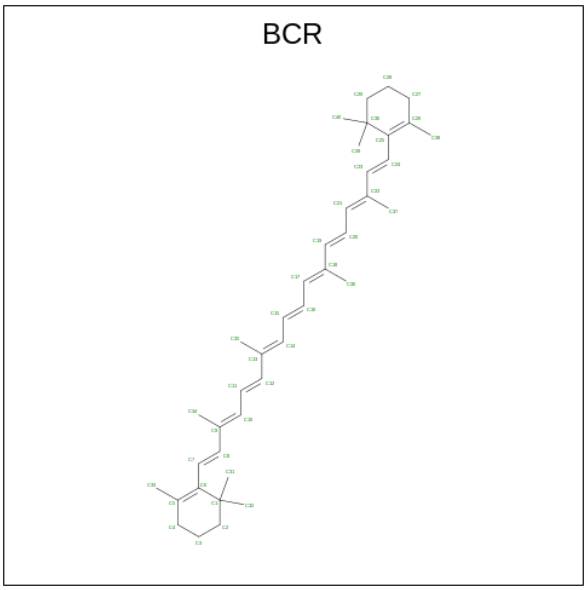
Mol	Chain	Residues	Atoms			AltConf
40	Q	1	Total	C	O	0
			56	41	15	

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Mol	Chain	Residues	Atoms	AltConf
40	b	1	Total C O 56 41 15	0

- Molecule 41 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



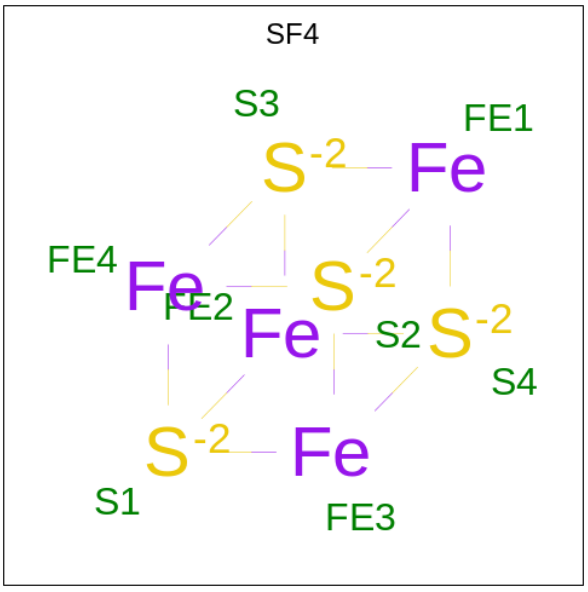
Mol	Chain	Residues	Atoms	AltConf
41	U	1	Total C 40 40	0
41	a	1	Total C 40 40	0
41	a	1	Total C 40 40	0
41	a	1	Total C 40 40	0
41	a	1	Total C 40 40	0
41	a	1	Total C 40 40	0
41	b	1	Total C 40 40	0
41	b	1	Total C 40 40	0
41	b	1	Total C 40 40	0
41	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
41	b	1	Total C 40 40	0
41	f	1	Total C 40 40	0
41	i	1	Total C 40 40	0
41	j	1	Total C 40 40	0
41	k	1	Total C 40 40	0
41	l	1	Total C 40 40	0
41	l	1	Total C 40 40	0
41	m	1	Total C 40 40	0
41	r	1	Total C 40 40	0
41	r	1	Total C 40 40	0

- Molecule 42 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



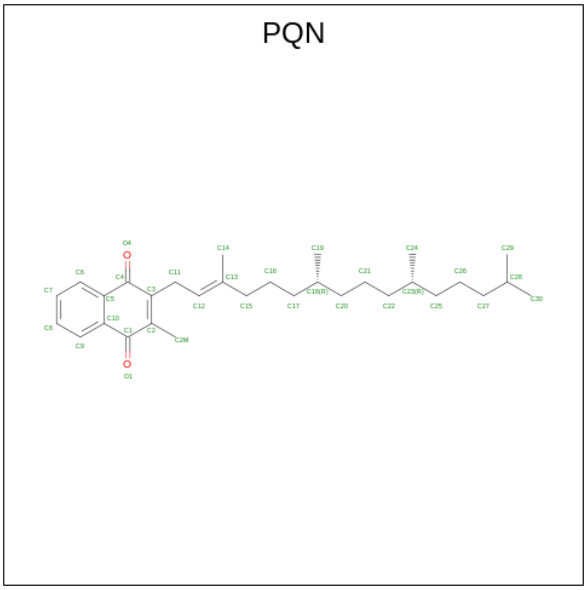
Mol	Chain	Residues	Atoms	AltConf
42	a	1	Total Fe S 8 4 4	0

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Mol	Chain	Residues	Atoms	AltConf
42	c	1	Total Fe S 8 4 4	0
42	c	1	Total Fe S 8 4 4	0

- Molecule 43 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



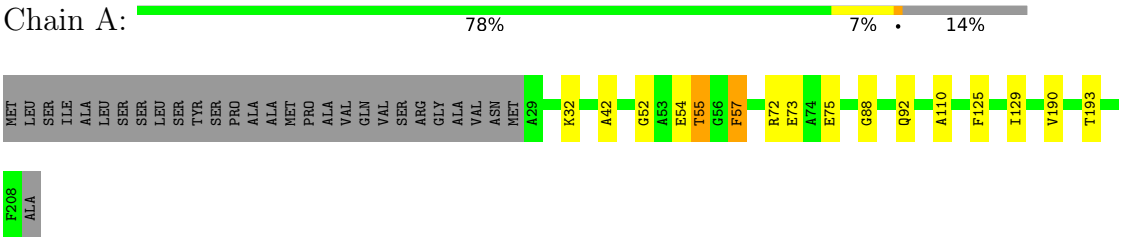
Mol	Chain	Residues	Atoms	AltConf
43	a	1	Total C O 33 31 2	0
43	b	1	Total C O 33 31 2	0

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.

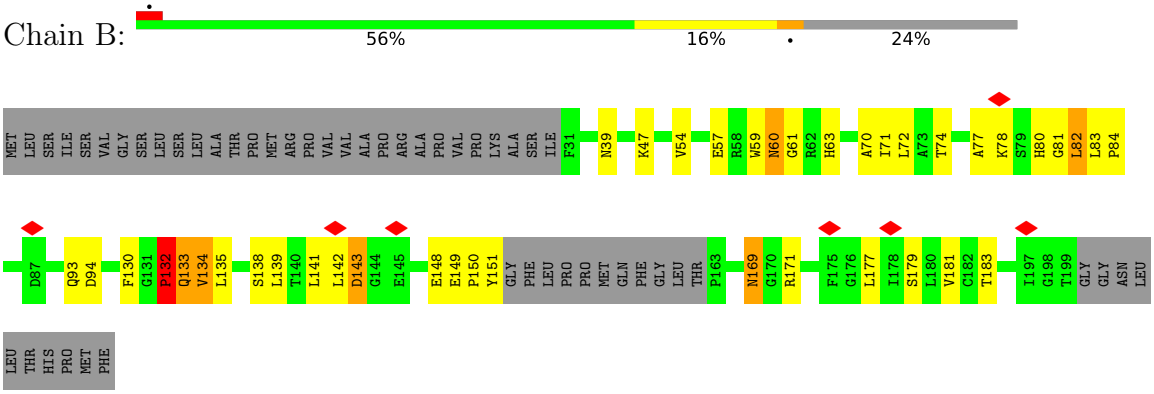
• Molecule 1: iFCPI-7

Chain A:



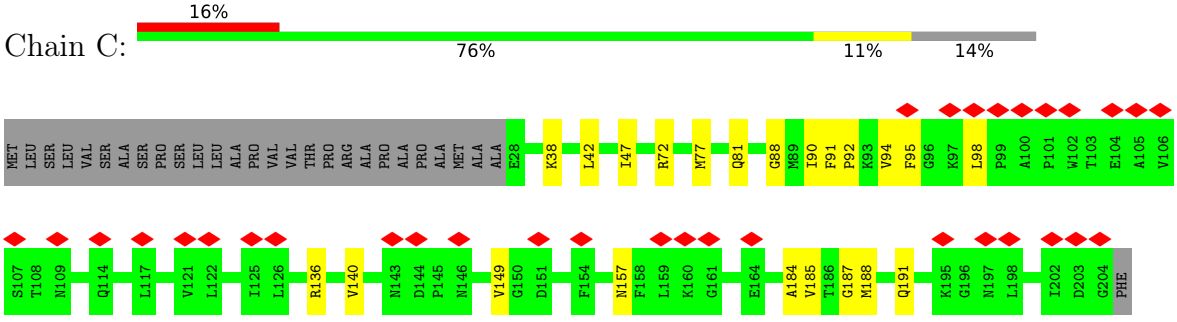
• Molecule 2: iFCPI-1

Chain B:



• Molecule 3: iFCPI-11

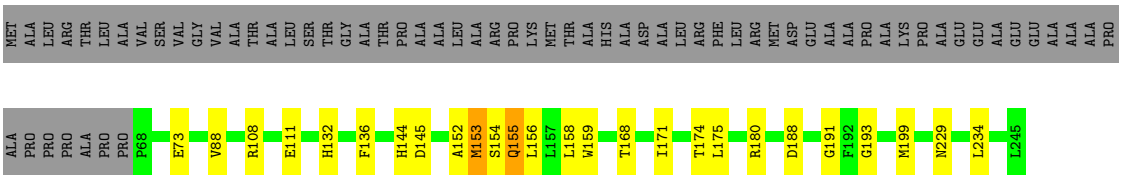
Chain C:



• Molecule 4: iFCPI-6

Chain D:

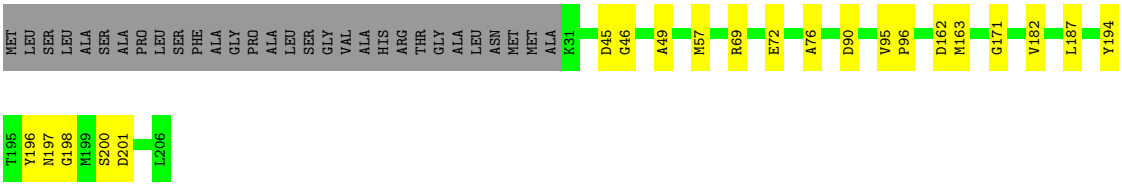




• Molecule 5: iFCPI-5

Chain E:

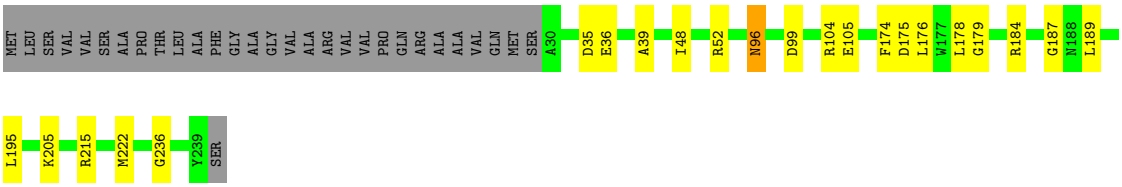




• Molecule 6: iFCPI-8

Chain F:

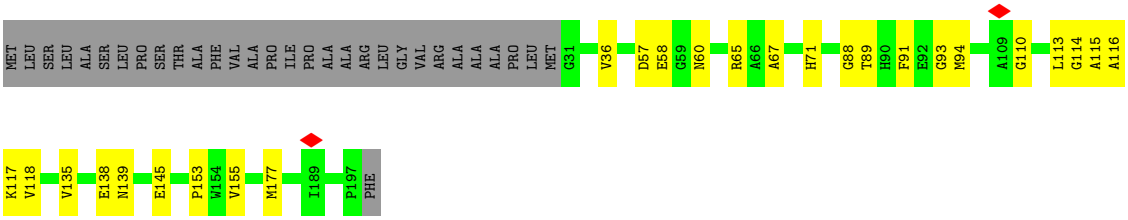




• Molecule 7: iFCPI-13

Chain G:

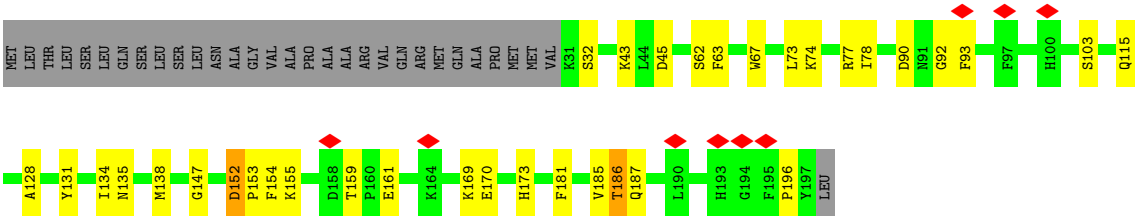




• Molecule 8: iFCPI-10

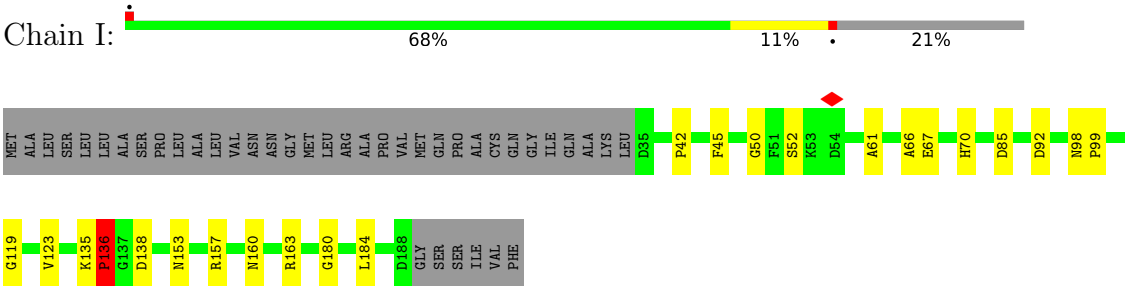
Chain H:





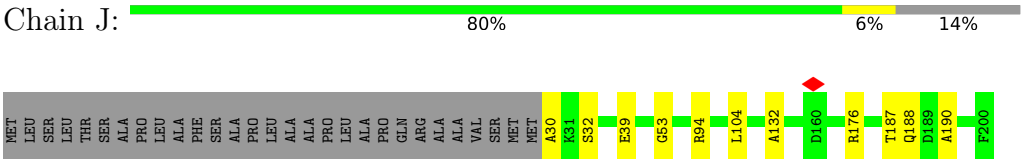
• Molecule 9: iFCPI-3

Chain I:



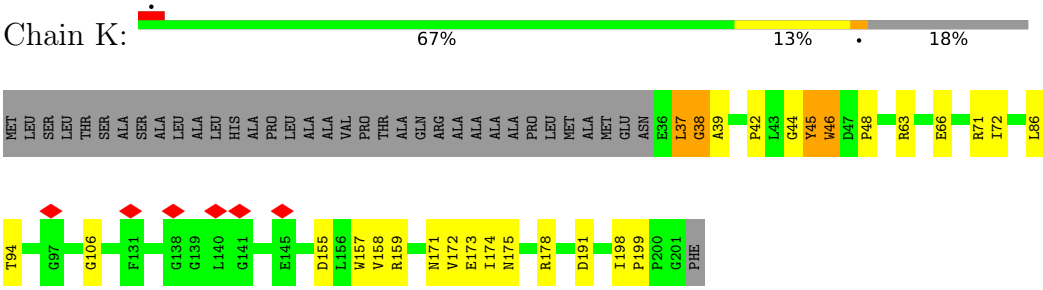
• Molecule 10: iFCPI-9

Chain J:



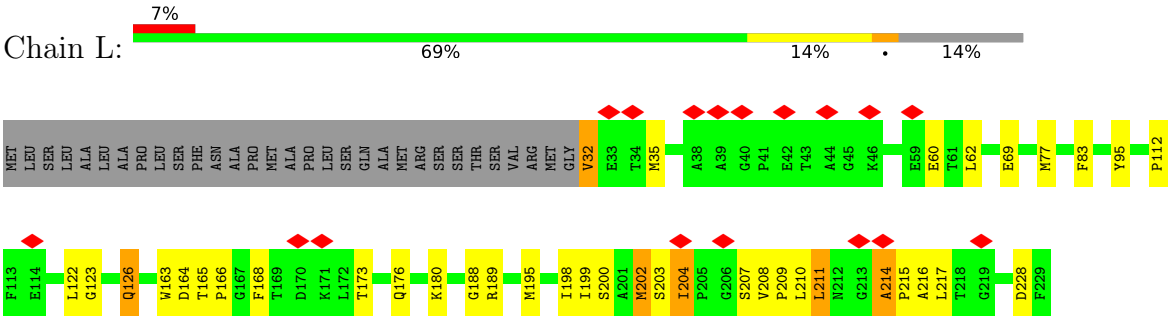
• Molecule 11: iFCPI-4

Chain K:



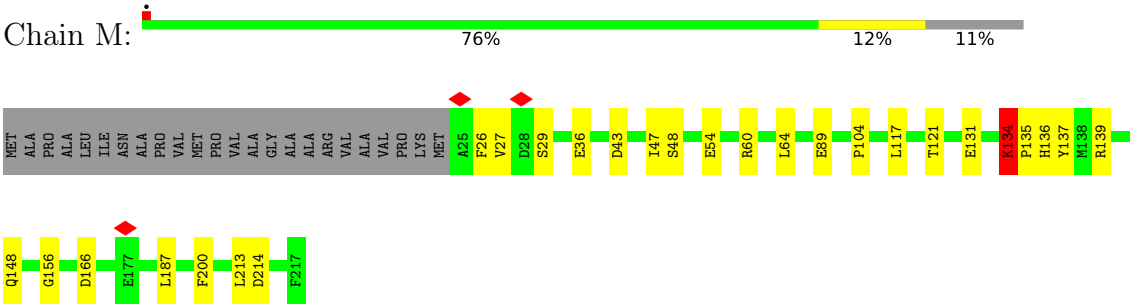
• Molecule 12: iFCPI-12

Chain L:



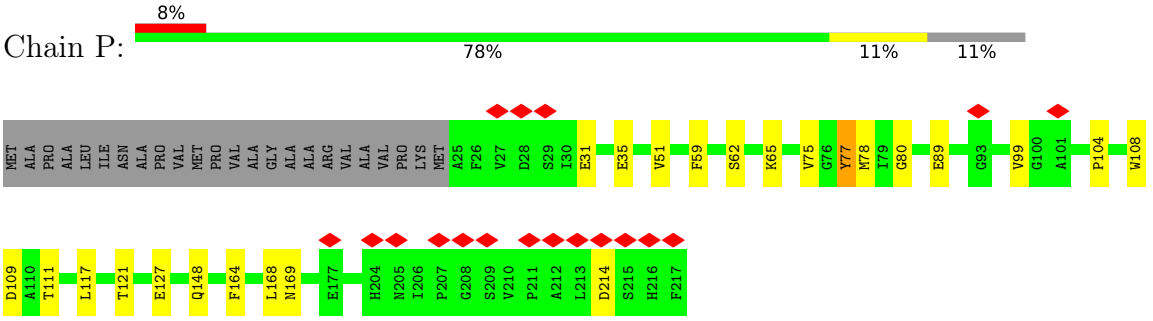
• Molecule 13: iFCPI-15/14/16

Chain M:



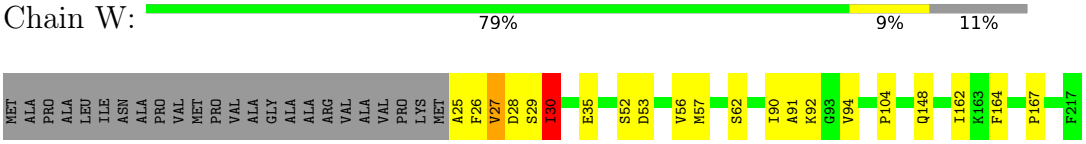
• Molecule 13: iFCPI-15/14/16

Chain P:



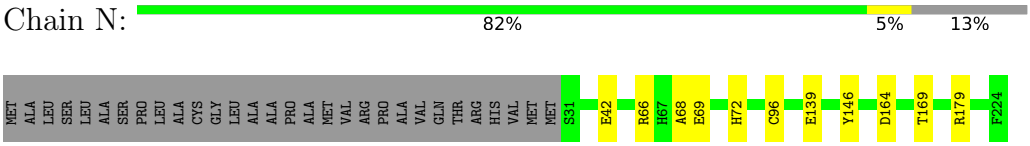
• Molecule 13: iFCPI-15/14/16

Chain W:



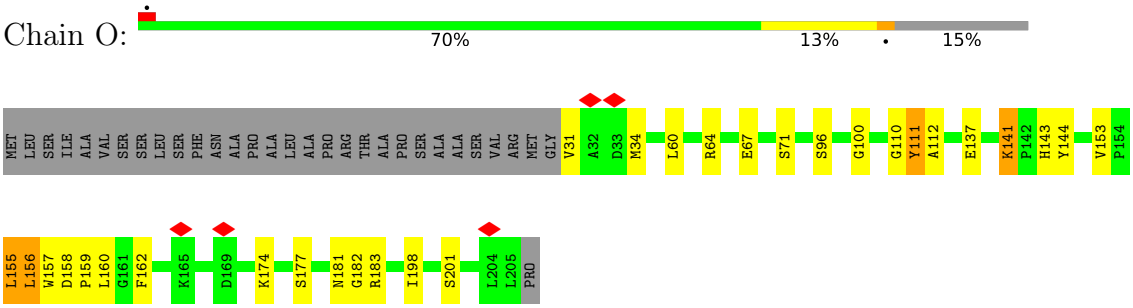
• Molecule 14: iFCPI-17

Chain N:



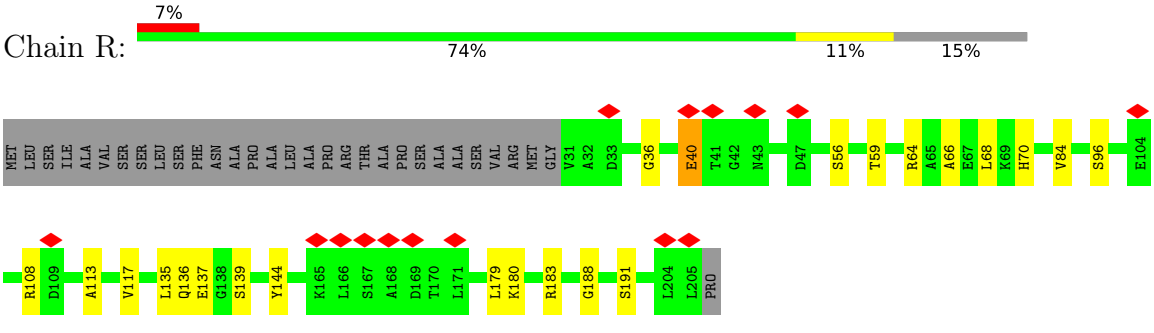
• Molecule 15: iFCPI-20/19/21

Chain O:



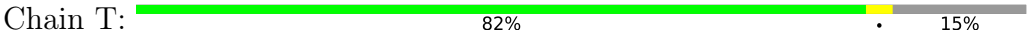
• Molecule 15: iFCPI-20/19/21

Chain R:



• Molecule 15: iFCPI-20/19/21

Chain T:

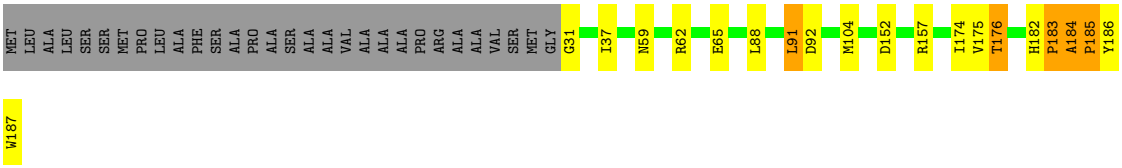




• Molecule 16: iFCPI-18

Chain Q:

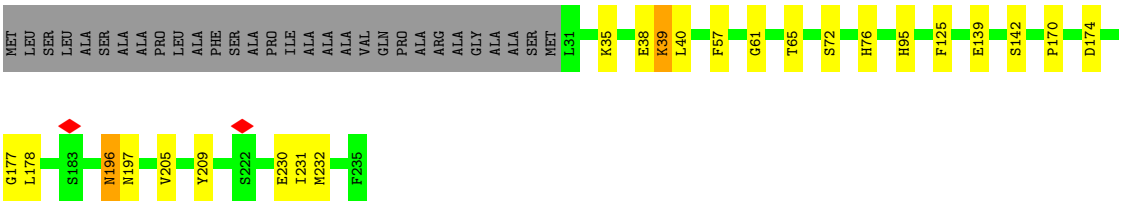




• Molecule 17: iFCPI-22

Chain S:

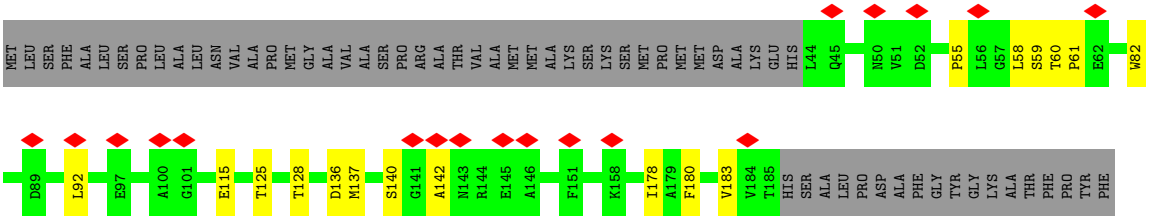




• Molecule 18: iFCPI-2

Chain U:

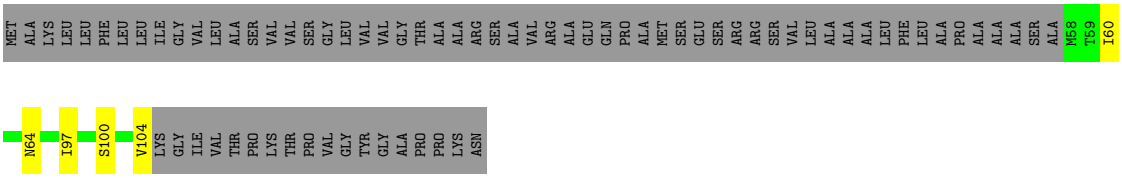




• Molecule 19: L-iFP

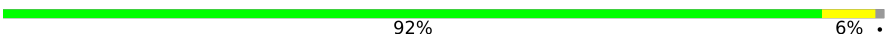
Chain V:

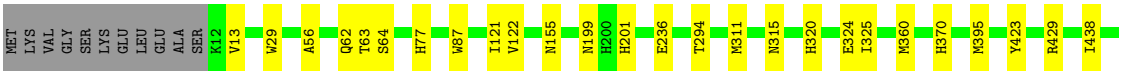


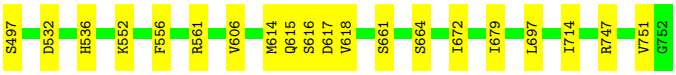


• Molecule 20: Photosystem I P700 chlorophyll a apoprotein A1

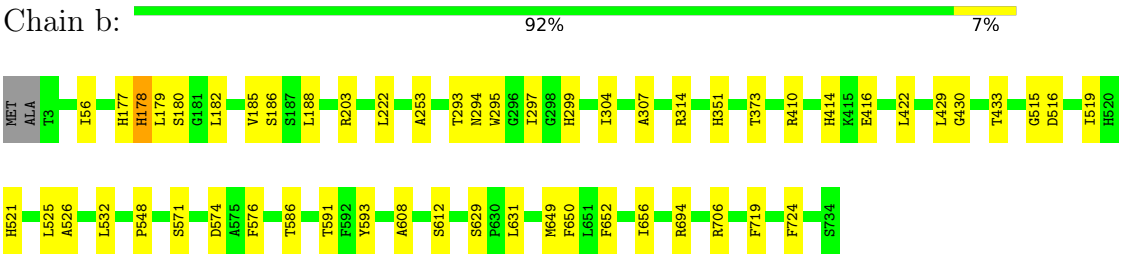
Chain a:



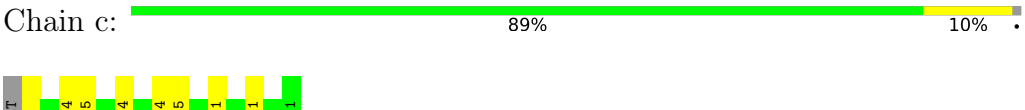




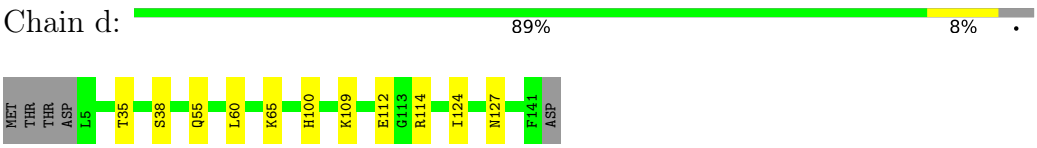
• Molecule 21: Photosystem I P700 chlorophyll a apoprotein A2



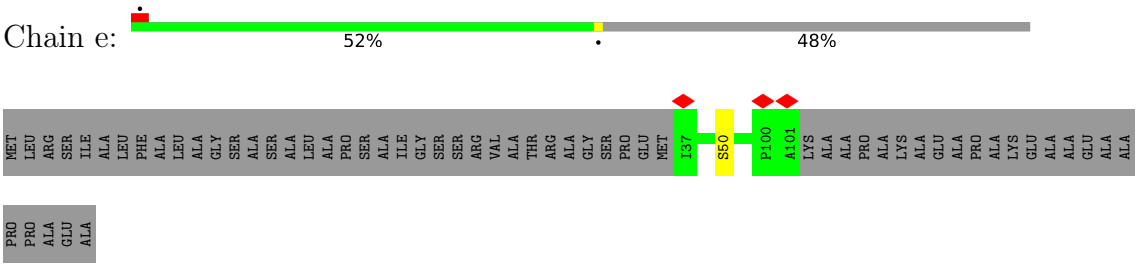
• Molecule 22: Photosystem I iron-sulfur center



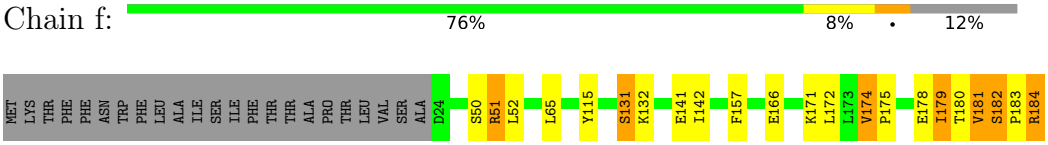
• Molecule 23: Photosystem I reaction center subunit II



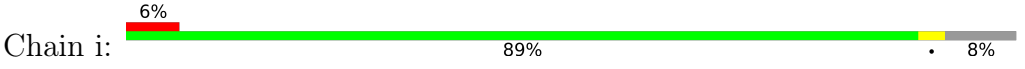
• Molecule 24: PsaE

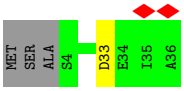


• Molecule 25: Photosystem I reaction center subunit III



• Molecule 26: Photosystem I reaction center subunit VIII

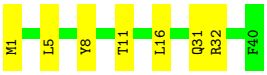




• Molecule 27: Photosystem I reaction center subunit IX

Chain j:





• Molecule 28: PsaK

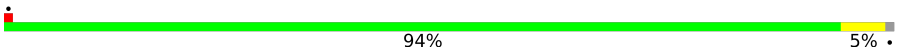
Chain k:

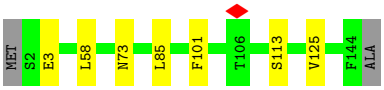




• Molecule 29: Photosystem I reaction center subunit XI

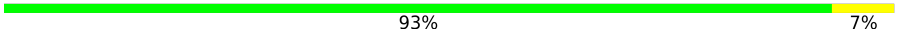
Chain l:





• Molecule 30: Photosystem I reaction center subunit XII

Chain m:

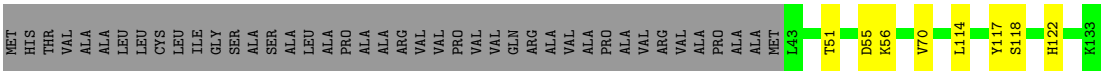




• Molecule 31: PsaR

Chain r:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	148236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.577	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.065	Depositor
Map value standard deviation	0.129	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DD6, SF4, CLA, LMG, DGD, SQD, LMU, PQN, BCR, KC2, A86, LHG

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	0.71	8/1443 (0.6%)	0.60	2/1956 (0.1%)
2	B	0.60	2/1224 (0.2%)	0.75	4/1661 (0.2%)
3	C	0.43	0/1377	0.50	0/1864
4	D	0.59	2/1432 (0.1%)	0.53	3/1939 (0.2%)
5	E	0.60	2/1350 (0.1%)	0.56	3/1839 (0.2%)
6	F	0.46	0/1616	0.50	2/2193 (0.1%)
7	G	0.42	0/1265	0.59	4/1722 (0.2%)
8	H	0.47	1/1297 (0.1%)	0.59	2/1751 (0.1%)
9	I	0.54	1/1219 (0.1%)	0.47	0/1646
10	J	0.34	0/1282	0.46	0/1729
11	K	0.60	4/1321 (0.3%)	0.57	2/1792 (0.1%)
12	L	0.58	0/1519	0.66	2/2057 (0.1%)
13	M	0.37	0/1505	0.51	1/2041 (0.0%)
13	P	0.49	1/1505 (0.1%)	0.52	1/2041 (0.0%)
13	W	0.51	1/1505 (0.1%)	0.56	1/2041 (0.0%)
14	N	0.21	0/1491	0.45	0/2023
15	O	0.51	3/1333 (0.2%)	0.60	3/1815 (0.2%)
15	R	0.28	0/1333	0.46	0/1815
15	T	0.23	0/1333	0.43	0/1815
16	Q	0.53	4/1244 (0.3%)	0.61	8/1690 (0.5%)
17	S	0.60	6/1650 (0.4%)	0.53	1/2234 (0.0%)
18	U	0.33	0/1107	0.53	1/1494 (0.1%)
19	V	0.26	0/369	0.49	0/503
20	a	0.37	6/6019 (0.1%)	0.38	2/8193 (0.0%)
21	b	0.48	11/6029 (0.2%)	0.42	3/8226 (0.0%)
22	c	0.43	0/606	0.41	0/822
23	d	0.36	0/1105	0.46	0/1492
24	e	0.25	0/515	0.44	0/699
25	f	0.89	7/1273 (0.5%)	0.66	4/1723 (0.2%)
26	i	0.20	0/265	0.38	0/363
27	j	0.19	0/323	0.34	0/439
28	k	0.22	0/512	0.46	0/693

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	l	0.19	0/1109	0.36	0/1510
30	m	0.19	0/220	0.33	0/298
31	r	0.18	0/700	0.37	0/957
All	All	0.47	59/49396 (0.1%)	0.50	49/67076 (0.1%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	177	HIS	C-O	-8.09	1.14	1.24
21	b	180	SER	CA-C	-7.74	1.42	1.52
20	a	423	TYR	CA-C	-7.54	1.43	1.52
5	E	162	ASP	CA-C	-7.53	1.42	1.52
8	H	32	SER	CA-C	-7.52	1.43	1.52
16	Q	176	THR	CA-C	-7.36	1.42	1.52
25	f	181	VAL	N-CA	-7.05	1.38	1.46
17	S	196	ASN	N-CA	-6.81	1.37	1.46
1	A	57	PHE	C-O	-6.78	1.16	1.24
4	D	155	GLN	CA-C	-6.78	1.43	1.52
1	A	73	GLU	CA-C	-6.62	1.43	1.52
1	A	57	PHE	N-CA	-6.52	1.38	1.46
9	I	138	ASP	CA-C	-6.51	1.45	1.53
21	b	179	LEU	CA-C	-6.42	1.44	1.52
17	S	196	ASN	CA-CB	-6.39	1.42	1.53
15	O	112	ALA	CA-C	-6.20	1.45	1.52
20	a	616	SER	CA-C	-6.19	1.44	1.52
1	A	73	GLU	N-CA	-6.18	1.37	1.46
11	K	45	TYR	CA-C	-6.17	1.45	1.52
21	b	177	HIS	CA-C	-6.10	1.45	1.52
21	b	179	LEU	C-O	-6.08	1.16	1.24
17	S	38	GLU	CA-C	-6.06	1.44	1.52
25	f	131	SER	CA-C	-6.04	1.44	1.52
1	A	57	PHE	CA-C	-6.03	1.45	1.52
21	b	297	ILE	C-O	-5.98	1.17	1.24
2	B	39	ASN	CA-C	-5.97	1.45	1.52
20	a	615	GLN	C-O	-5.81	1.16	1.24
21	b	178	HIS	C-O	-5.79	1.15	1.24
11	K	37	LEU	CA-C	-5.79	1.45	1.52
17	S	196	ASN	C-N	-5.74	1.26	1.33
20	a	618	VAL	C-O	-5.68	1.17	1.24
21	b	295	TRP	CA-C	-5.65	1.45	1.53
16	Q	176	THR	CA-CB	-5.64	1.43	1.53
25	f	141	GLU	CA-C	-5.60	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	77	TYR	CA-C	-5.54	1.47	1.52
15	O	111	TYR	CA-C	-5.54	1.44	1.52
16	Q	91	LEU	CA-C	-5.54	1.46	1.52
11	K	38	GLY	CA-C	-5.52	1.44	1.51
4	D	152	ALA	CA-C	-5.40	1.44	1.52
5	E	163	MET	N-CA	-5.40	1.39	1.46
21	b	180	SER	C-O	-5.39	1.17	1.24
17	S	196	ASN	CA-C	-5.30	1.45	1.52
1	A	57	PHE	CA-CB	-5.29	1.45	1.53
20	a	615	GLN	CA-C	-5.29	1.45	1.52
21	b	180	SER	N-CA	-5.23	1.39	1.46
25	f	174	VAL	CA-C	-5.23	1.47	1.52
17	S	39	LYS	CA-C	-5.20	1.45	1.52
20	a	616	SER	N-CA	-5.17	1.39	1.46
13	W	27	VAL	CA-C	-5.13	1.45	1.52
1	A	55	THR	C-O	-5.11	1.18	1.24
16	Q	176	THR	C-O	-5.10	1.17	1.24
25	f	172	LEU	CA-C	-5.08	1.46	1.52
11	K	46	TRP	CA-C	-5.07	1.47	1.53
25	f	178	GLU	CA-C	-5.07	1.46	1.53
25	f	178	GLU	N-CA	-5.04	1.41	1.46
2	B	132	PRO	CA-C	-5.03	1.45	1.52
21	b	297	ILE	N-CA	-5.02	1.40	1.46
1	A	73	GLU	C-O	-5.00	1.17	1.24
15	O	141	LYS	CA-CB	-5.00	1.47	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	77	TYR	N-CA-C	-9.22	100.67	112.93
4	D	153	MET	N-CA-C	-8.49	103.36	114.31
2	B	133	GLN	N-CA-C	-8.40	99.00	110.68
7	G	93	GLY	N-CA-C	8.26	122.44	110.80
13	M	134	LYS	N-CA-C	8.21	123.64	112.55
5	E	163	MET	N-CA-C	-8.03	103.62	113.50
15	O	155	LEU	N-CA-C	-7.47	101.22	110.41
21	b	576	PHE	N-CA-C	-7.17	101.99	111.24
25	f	181	VAL	N-CA-C	-7.12	98.25	108.42
12	L	211	LEU	N-CA-C	-6.94	101.98	111.56
6	F	96	ASN	N-CA-C	-6.83	103.29	111.69
1	A	73	GLU	N-CA-C	-6.75	104.85	113.23
21	b	295	TRP	N-CA-C	-6.72	98.38	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	f	132	LYS	N-CA-C	-6.72	104.72	113.12
2	B	60	ASN	N-CA-C	-6.68	103.69	110.97
17	S	39	LYS	N-CA-C	-6.61	105.37	113.50
16	Q	88	LEU	O-C-N	6.58	127.46	121.80
5	E	162	ASP	N-CA-C	-6.38	105.65	113.50
4	D	156	LEU	N-CA-C	-6.32	105.70	113.41
12	L	202	MET	N-CA-C	-6.14	103.91	111.40
11	K	45	TYR	N-CA-C	-6.12	101.36	110.23
7	G	118	VAL	CA-C-N	-6.03	113.76	119.85
7	G	118	VAL	C-N-CA	-6.03	113.76	119.85
1	A	52	GLY	N-CA-C	-5.88	106.84	115.72
25	f	51	ARG	N-CA-C	-5.87	105.22	112.38
2	B	47	LYS	N-CA-C	5.86	118.44	111.71
18	U	59	SER	N-CA-C	5.75	118.04	109.59
16	Q	92	ASP	N-CA-C	-5.70	106.46	113.41
6	F	175	ASP	O-C-N	-5.68	115.67	122.15
13	W	30	ILE	CB-CA-C	5.63	120.53	111.29
20	a	614	MET	O-C-N	-5.49	115.52	122.27
8	H	152	ASP	CA-C-N	-5.48	113.54	119.24
8	H	152	ASP	C-N-CA	-5.48	113.54	119.24
16	Q	185	PRO	N-CA-C	-5.47	106.72	113.84
16	Q	184	ALA	CA-C-N	-5.44	114.01	119.56
16	Q	184	ALA	C-N-CA	-5.44	114.01	119.56
2	B	82	LEU	N-CA-C	-5.43	104.90	112.45
7	G	116	ALA	N-CA-C	-5.39	105.80	112.38
21	b	177	HIS	N-CA-C	5.24	117.07	111.36
15	O	141	LYS	CA-C-N	-5.24	113.30	119.84
15	O	141	LYS	C-N-CA	-5.24	113.30	119.84
4	D	155	GLN	N-CA-C	-5.18	106.96	113.28
16	Q	184	ALA	N-CA-C	5.12	120.44	113.16
16	Q	91	LEU	N-CA-C	-5.12	101.36	109.59
11	K	42	PRO	N-CA-C	-5.09	106.19	113.47
20	a	617	ASP	N-CA-C	5.09	121.19	114.12
16	Q	175	VAL	O-C-N	-5.05	116.62	121.83
5	E	182	VAL	O-C-N	-5.03	116.67	121.90
25	f	179	ILE	N-CA-C	-5.00	101.01	108.46

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	1403	0	1381	14	0
2	B	1194	0	1157	35	0
3	C	1346	0	1366	16	0
4	D	1392	0	1340	20	0
5	E	1316	0	1319	11	0
6	F	1573	0	1548	22	0
7	G	1235	0	1231	24	0
8	H	1266	0	1241	27	0
9	I	1190	0	1194	14	0
10	J	1253	0	1243	8	0
11	K	1280	0	1275	29	0
12	L	1479	0	1476	51	0
13	M	1465	0	1469	18	0
13	P	1465	0	1469	20	0
13	W	1465	0	1469	24	0
14	N	1451	0	1475	8	0
15	O	1299	0	1315	23	0
15	R	1299	0	1315	16	0
15	T	1299	0	1315	5	0
16	Q	1210	0	1167	16	0
17	S	1597	0	1552	22	0
18	U	1084	0	1081	14	0
19	V	357	0	352	5	0
20	a	5826	0	5714	35	0
21	b	5818	0	5647	41	0
22	c	596	0	578	9	0
23	d	1080	0	1095	7	0
24	e	504	0	493	1	0
25	f	1243	0	1252	22	0
26	i	258	0	268	1	0
27	j	316	0	328	5	0
28	k	503	0	523	3	0
29	l	1081	0	1091	6	0
30	m	219	0	243	1	0
31	r	682	0	665	7	0
32	A	583	0	573	7	0
32	B	321	0	242	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	C	402	0	351	3	0
32	D	679	0	640	6	0
32	E	644	0	573	0	0
32	F	527	0	456	4	0
32	G	350	0	291	0	0
32	H	418	0	321	5	0
32	I	506	0	480	3	0
32	J	500	0	410	4	0
32	K	301	0	259	4	0
32	L	422	0	333	10	0
32	M	381	0	343	5	0
32	N	316	0	274	6	0
32	O	367	0	326	4	0
32	P	357	0	307	3	0
32	Q	481	0	423	1	0
32	R	336	0	269	1	0
32	S	446	0	366	1	0
32	T	360	0	305	2	0
32	U	265	0	193	3	0
32	V	163	0	143	0	0
32	W	410	0	403	14	0
32	a	2658	0	2697	23	0
32	b	2403	0	2432	17	0
32	f	152	0	127	0	0
32	j	45	0	33	1	0
32	k	165	0	147	7	0
32	l	175	0	177	0	0
32	r	105	0	92	0	0
33	A	45	0	0	2	0
33	C	45	0	0	0	0
33	E	45	0	0	0	0
33	F	90	0	0	2	0
33	G	90	0	0	1	0
33	H	45	0	0	0	0
33	I	90	0	0	4	0
33	J	90	0	0	0	0
33	K	180	0	0	3	0
33	L	225	0	0	0	0
33	M	270	0	0	1	0
33	N	315	0	0	2	0
33	O	135	0	0	1	0
33	P	225	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Q	90	0	0	0	0
33	R	180	0	0	1	0
33	S	180	0	0	5	0
33	T	135	0	0	0	0
33	U	45	0	0	0	0
33	W	270	0	0	1	0
34	A	172	0	0	2	0
34	B	43	0	0	0	0
34	C	43	0	0	0	0
34	D	215	0	0	2	0
34	E	172	0	0	0	0
34	F	129	0	0	0	0
34	G	43	0	0	0	0
34	H	129	0	0	0	0
34	I	172	0	0	2	0
34	J	172	0	0	1	0
34	K	86	0	0	0	0
34	L	43	0	0	1	0
34	M	43	0	0	3	0
34	N	129	0	0	0	0
34	O	43	0	0	0	0
34	P	43	0	0	0	0
34	Q	172	0	0	0	0
34	R	43	0	0	0	0
34	S	43	0	0	2	0
34	T	43	0	0	0	0
34	U	43	0	0	1	0
34	V	43	0	0	0	0
34	W	43	0	0	1	0
34	j	43	0	0	0	0
34	k	43	0	0	1	0
35	A	40	0	50	0	0
35	B	31	0	32	2	0
35	D	48	0	69	0	0
35	E	92	0	130	0	0
35	F	81	0	102	2	0
35	I	83	0	109	0	0
35	M	46	0	65	0	0
35	P	46	0	65	1	0
35	W	46	0	65	0	0
35	a	116	0	145	7	0
35	f	47	0	67	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	A	76	0	92	1	0
36	D	141	0	162	1	0
36	E	111	0	132	0	0
36	F	73	0	86	18	0
36	L	37	0	44	0	0
36	M	40	0	48	9	0
36	N	40	0	49	5	0
36	P	45	0	59	7	0
36	S	33	0	34	8	0
36	T	37	0	44	2	0
36	W	39	0	46	11	0
36	j	38	0	46	1	0
36	l	49	0	69	5	0
37	C	96	0	0	0	0
37	D	96	0	0	1	0
37	F	144	0	0	2	0
37	G	96	0	0	0	0
37	H	48	0	0	1	0
37	J	48	0	0	0	0
37	K	144	0	0	0	0
37	L	192	0	0	4	0
37	M	288	0	0	6	0
37	N	192	0	0	0	0
37	O	96	0	0	0	0
37	P	192	0	0	1	0
37	Q	96	0	0	2	0
37	R	96	0	0	2	0
37	S	336	0	0	2	0
37	T	144	0	0	1	0
37	U	48	0	0	0	0
37	W	192	0	0	2	0
37	r	48	0	0	0	0
38	D	35	0	46	2	0
38	I	35	0	46	3	0
38	J	35	0	46	3	0
38	V	34	0	41	3	0
38	j	34	0	41	0	0
39	H	43	0	50	16	0
39	k	36	0	36	6	0
40	Q	56	0	70	3	0
40	b	56	0	70	0	0
41	U	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	a	200	0	280	2	0
41	b	200	0	280	6	0
41	f	40	0	56	0	0
41	i	40	0	56	0	0
41	j	40	0	56	0	0
41	k	40	0	56	1	0
41	l	80	0	112	1	0
41	m	40	0	56	0	0
41	r	80	0	112	0	0
42	a	8	0	0	0	0
42	c	16	0	0	1	0
43	a	33	0	46	0	0
43	b	33	0	46	0	0
All	All	73546	0	65101	651	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (651) 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)
20:a:497:SER:OG	35:a:851:LHG:C4	1.80	1.27
20:a:497:SER:OG	35:a:851:LHG:HC41	1.10	1.25
33:I:309:KC2:O1A	36:l:201:LMG:O3	1.52	1.20
34:A:313:DD6:C28	36:N:301:LMG:H322	1.77	1.14
37:S:315:A86:C39	36:S:322:LMG:H291	1.79	1.11
17:S:174:ASP:OD1	17:S:177:GLY:N	1.87	1.07
32:N:312:CLA:CAA	36:W:320:LMG:H152	1.86	1.05
22:c:2:SER:N	22:c:71:SER:HG	1.58	1.00
33:S:312:KC2:O2A	36:S:322:LMG:O1	1.62	0.98
1:A:57:PHE:HE1	32:A:301:CLA:HBC3	1.30	0.95
17:S:174:ASP:CG	17:S:177:GLY:HA2	1.92	0.95
32:k:203:CLA:HBB2	39:k:206:SQD:H251	1.48	0.93
13:W:91:ALA:HB3	13:W:94:VAL:HG12	1.50	0.93
17:S:174:ASP:OD1	17:S:177:GLY:CA	2.18	0.92
33:A:310:KC2:O2A	36:N:301:LMG:O4	1.59	0.92
6:F:48:ILE:CD1	36:F:320:LMG:O4	2.18	0.91
33:F:310:KC2:CMA	36:F:319:LMG:H112	2.00	0.91
32:k:203:CLA:CAB	39:k:206:SQD:H462	2.00	0.90
32:M:311:CLA:CBA	36:P:318:LMG:H151	2.02	0.90
36:F:320:LMG:H291	32:b:826:CLA:H12	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:N:312:CLA:CAA	36:W:320:LMG:C15	2.48	0.90
32:M:311:CLA:CGA	36:P:318:LMG:H151	2.03	0.89
12:L:83:PHE:CE2	12:L:198:ILE:HD13	2.09	0.88
36:M:320:LMG:C16	32:W:312:CLA:HBA2	2.04	0.87
33:I:309:KC2:O1A	36:l:201:LMG:C3	2.08	0.87
7:G:88:GLY:C	11:K:89:PRO:HG3	2.00	0.86
34:A:313:DD6:C28	36:N:301:LMG:C32	2.54	0.85
36:M:320:LMG:H161	32:W:312:CLA:CGA	2.07	0.85
35:F:318:LHG:O1	36:F:320:LMG:HC61	1.77	0.84
7:G:89:THR:N	11:K:89:PRO:HG3	1.91	0.84
36:M:320:LMG:H162	32:W:312:CLA:HBA2	1.57	0.84
15:O:153:VAL:HG11	15:O:156:LEU:HD12	1.58	0.84
13:W:92:LYS:HB2	36:W:320:LMG:HC2	1.59	0.83
11:K:106:GLY:HA3	11:K:191:ASP:OD2	1.79	0.82
20:a:497:SER:HG	35:a:851:LHG:C4	1.91	0.82
32:k:203:CLA:HAB	39:k:206:SQD:H462	1.62	0.82
10:J:30:ALA:O	10:J:39:GLU:OE2	1.97	0.81
12:L:83:PHE:CZ	12:L:198:ILE:HD13	2.15	0.81
36:M:320:LMG:H161	32:W:312:CLA:CBA	2.11	0.80
17:S:174:ASP:OD2	17:S:177:GLY:HA2	1.81	0.79
22:c:2:SER:N	22:c:71:SER:OG	2.15	0.79
1:A:54:GLU:O	1:A:55:THR:C	2.25	0.78
4:D:88:VAL:O	4:D:108:ARG:NH2	2.17	0.78
5:E:197:ASN:HB2	5:E:201:ASP:OD1	1.84	0.77
13:W:91:ALA:HB3	13:W:94:VAL:CG1	2.15	0.77
20:a:497:SER:CB	35:a:851:LHG:HC41	2.16	0.75
25:f:174:VAL:CG1	25:f:179:ILE:HD11	2.17	0.75
13:W:62:SER:OG	32:W:309:CLA:OBD	2.05	0.75
37:D:322:A86:O3	32:M:309:CLA:O1D	2.04	0.74
12:L:217:LEU:HD11	32:L:311:CLA:HMD3	1.70	0.74
18:U:137:MET:HA	18:U:142:ALA:HB3	1.68	0.74
37:M:315:A86:C28	36:M:320:LMG:H342	2.18	0.72
33:G:309:KC2:CMA	28:k:111:ILE:HG21	2.19	0.72
5:E:69:ARG:NH1	5:E:72:GLU:OE2	2.21	0.72
36:F:320:LMG:H121	35:F:321:LHG:H271	1.71	0.72
12:L:210:LEU:HD23	37:L:315:A86:C38	2.19	0.72
32:a:836:CLA:O2A	34:k:205:DD6:O2	2.06	0.72
6:F:39:ALA:HB2	36:F:320:LMG:HC4	1.71	0.72
13:P:169:ASN:O	15:R:56:SER:OG	2.08	0.71
4:D:108:ARG:NH1	4:D:111:GLU:OE2	2.23	0.71
12:L:122:LEU:O	12:L:126:GLN:HG2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:GLN:OE1	2:B:93:GLN:N	2.24	0.71
12:L:83:PHE:CE2	12:L:198:ILE:CD1	2.73	0.71
36:F:319:LMG:H301	32:J:312:CLA:C6	2.20	0.71
11:K:38:GLY:HA2	11:K:174:ILE:HD11	1.72	0.70
13:M:214:ASP:OD2	37:M:318:A86:O2	2.09	0.70
15:T:64:ARG:NH1	15:T:67:GLU:OE1	2.24	0.70
22:c:61:ASP:OD2	24:e:50:SER:OG	2.04	0.70
11:K:175:ASN:ND2	32:K:301:CLA:O1D	2.24	0.70
1:A:57:PHE:CE1	32:A:301:CLA:HBC3	2.22	0.70
25:f:115:TYR:OH	25:f:157:PHE:O	2.09	0.69
37:S:315:A86:C39	36:S:322:LMG:C29	2.67	0.69
13:W:162:ILE:O	37:W:302:A86:O2	2.11	0.69
33:P:312:KC2:O1A	36:P:318:LMG:O3	1.98	0.69
11:K:71:ARG:NH1	11:K:173:GLU:OE2	2.26	0.69
13:P:168:LEU:O	15:R:59:THR:OG1	2.11	0.69
3:C:94:VAL:HG12	3:C:95:PHE:CD1	2.28	0.68
36:F:319:LMG:H301	32:J:312:CLA:H62	1.75	0.68
14:N:66:ARG:NH1	14:N:69:GLU:OE1	2.26	0.68
13:M:43:ASP:OD1	34:M:316:DD6:O4	2.12	0.68
1:A:57:PHE:HE1	32:A:301:CLA:CBC	2.04	0.68
8:H:77:ARG:NH2	8:H:147:GLY:O	2.26	0.68
10:J:32:SER:OG	10:J:53:GLY:O	2.12	0.68
25:f:181:VAL:CG1	25:f:184:ARG:NH2	2.57	0.68
12:L:228:ASP:OD1	12:L:228:ASP:O	2.13	0.67
22:c:24:ASP:OD2	23:d:100:HIS:ND1	2.27	0.67
2:B:70:ALA:O	2:B:74:THR:HG23	1.95	0.67
15:O:198:ILE:O	15:O:201:SER:OG	2.12	0.66
12:L:32:VAL:HG13	12:L:62:LEU:HD11	1.78	0.66
14:N:179:ARG:NH1	33:N:303:KC2:O1A	2.28	0.66
4:D:144:HIS:CD2	4:D:153:MET:HE2	2.30	0.66
11:K:38:GLY:HA2	11:K:174:ILE:CD1	2.25	0.66
9:I:153:ASN:OD1	9:I:157:ARG:NH1	2.28	0.66
12:L:60:GLU:OE2	12:L:60:GLU:N	2.27	0.66
20:a:395:MET:HE2	20:a:606:VAL:HG11	1.77	0.66
21:b:410:ARG:NE	32:b:826:CLA:OBD	2.29	0.66
8:H:135:ASN:HA	39:H:315:SQD:H81	1.78	0.66
32:b:827:CLA:O1A	27:j:31:GLN:NE2	2.28	0.65
21:b:548:PRO:HB3	25:f:183:PRO:CG	2.26	0.65
3:C:38:LYS:NZ	3:C:42:LEU:O	2.29	0.65
14:N:96:CYS:SG	33:N:314:KC2:OBD	2.55	0.65
16:Q:37:ILE:O	16:Q:62:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:W:92:LYS:CB	36:W:320:LMG:O4	2.44	0.65
21:b:608:ALA:O	21:b:612:SER:OG	2.14	0.65
12:L:202:MET:HE1	12:L:217:LEU:HA	1.79	0.65
6:F:236:GLY:O	37:F:312:A86:O2	2.15	0.65
15:T:35:GLU:O	15:T:64:ARG:NH2	2.29	0.65
11:K:94:THR:OG1	33:K:309:KC2:O1A	2.10	0.65
12:L:95:TYR:O	37:L:316:A86:O3	2.14	0.65
33:A:310:KC2:C2A	36:N:301:LMG:H302	2.26	0.65
5:E:57:MET:HB2	28:k:85:ILE:HD13	1.80	0.64
12:L:209:PRO:O	12:L:210:LEU:HB3	1.96	0.64
33:M:313:KC2:CMA	36:M:320:LMG:H111	2.27	0.64
21:b:516:ASP:OD2	21:b:593:TYR:OH	2.13	0.64
5:E:76:ALA:HB1	5:E:171:GLY:HA3	1.78	0.64
1:A:88:GLY:O	1:A:92:GLN:HG3	1.98	0.64
5:E:49:ALA:O	5:E:69:ARG:NH2	2.31	0.64
13:M:89:GLU:OE2	13:M:89:GLU:N	2.30	0.64
32:M:311:CLA:HBA1	36:P:318:LMG:H151	1.80	0.64
17:S:174:ASP:OD1	17:S:177:GLY:HA2	1.88	0.64
8:H:115:GLN:O	8:H:115:GLN:NE2	2.30	0.63
13:M:36:GLU:HG3	37:M:317:A86:C18	2.28	0.63
32:N:312:CLA:CAA	36:W:320:LMG:H151	2.27	0.63
33:S:312:KC2:O2A	36:S:322:LMG:HC91	1.99	0.63
13:W:92:LYS:HB3	36:W:320:LMG:O4	1.99	0.63
4:D:153:MET:HE3	32:D:315:CLA:CHD	2.28	0.63
4:D:229:ASN:ND2	4:D:234:LEU:O	2.31	0.63
15:O:174:LYS:NZ	33:O:302:KC2:O1A	2.32	0.63
16:Q:31:GLY:N	16:Q:59:ASN:OD1	2.32	0.62
14:N:139:GLU:OE2	14:N:146:TYR:OH	2.12	0.62
33:S:312:KC2:O2A	36:S:322:LMG:C9	2.48	0.62
6:F:48:ILE:HD13	36:F:320:LMG:O4	2.00	0.62
25:f:181:VAL:CG1	25:f:184:ARG:CZ	2.78	0.62
36:M:320:LMG:C16	32:W:312:CLA:CBA	2.70	0.62
2:B:77:ALA:HB1	2:B:82:LEU:HB2	1.82	0.61
21:b:571:SER:OG	21:b:574:ASP:OD2	2.16	0.61
7:G:145:GLU:OE1	7:G:145:GLU:N	2.33	0.61
9:I:66:ALA:O	9:I:70:HIS:ND1	2.32	0.61
36:F:319:LMG:H352	32:J:312:CLA:H112	1.82	0.61
12:L:173:THR:OG1	12:L:176:GLN:OE1	2.13	0.61
17:S:174:ASP:CG	17:S:177:GLY:CA	2.67	0.61
36:T:301:LMG:O5	36:T:301:LMG:O4	2.11	0.61
23:d:124:ILE:O	23:d:127:ASN:ND2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:M:320:LMG:H161	32:W:312:CLA:O2A	1.99	0.61
32:k:203:CLA:CBB	39:k:206:SQD:H251	2.27	0.61
8:H:63:PHE:CZ	39:H:315:SQD:H262	2.36	0.61
27:j:32:ARG:NH2	32:j:101:CLA:O1D	2.34	0.61
4:D:175:LEU:O	38:D:324:LMU:H6'2	2.01	0.61
20:a:294:THR:HG23	32:a:814:CLA:HMA3	1.82	0.60
13:M:60:ARG:NH2	32:M:310:CLA:O1D	2.34	0.60
8:H:93:PHE:O	32:H:309:CLA:HMD2	2.00	0.60
6:F:174:PHE:HE1	36:F:320:LMG:O9	1.84	0.60
2:B:142:LEU:O	2:B:143:ASP:C	2.43	0.60
18:U:58:LEU:HD13	32:U:305:CLA:O1A	2.02	0.60
21:b:307:ALA:HB3	32:b:833:CLA:CED	2.32	0.60
7:G:57:ASP:OD1	7:G:58:GLU:N	2.34	0.60
6:F:104:ARG:NH2	32:F:307:CLA:O1D	2.35	0.59
12:L:112:PRO:O	34:L:319:DD6:O2	2.18	0.59
11:K:106:GLY:CA	11:K:191:ASP:OD2	2.49	0.59
2:B:83:LEU:O	2:B:84:PRO:C	2.45	0.59
13:M:104:PRO:O	34:M:316:DD6:O2	2.19	0.59
37:W:316:A86:C35	36:W:320:LMG:H291	2.31	0.59
3:C:94:VAL:HG12	3:C:95:PHE:N	2.17	0.59
22:c:14:CYS:O	22:c:15:THR:HG22	2.01	0.59
7:G:139:ASN:OD1	38:I:315:LMU:C6'	2.51	0.59
36:S:322:LMG:HC1	36:S:322:LMG:H112	1.84	0.59
32:W:310:CLA:C6	32:W:310:CLA:HED3	2.32	0.59
11:K:63:ARG:NH1	11:K:66:GLU:OE1	2.35	0.59
15:R:135:LEU:O	15:R:139:SER:OG	2.13	0.59
2:B:179:SER:O	2:B:183:THR:HG23	2.03	0.58
33:I:309:KC2:CGA	36:l:201:LMG:O3	2.46	0.58
11:K:38:GLY:CA	11:K:174:ILE:HD11	2.34	0.58
8:H:134:ILE:HG22	39:H:315:SQD:H101	1.85	0.58
8:H:159:THR:OG1	8:H:161:GLU:OE2	2.15	0.58
12:L:123:GLY:HA2	12:L:126:GLN:HG3	1.85	0.58
17:S:178:LEU:O	17:S:178:LEU:HD12	2.04	0.58
6:F:99:ASP:OD2	6:F:179:GLY:HA2	2.03	0.58
12:L:165:THR:N	12:L:166:PRO:CD	2.67	0.58
15:R:136:GLN:NE2	37:R:313:A86:O2	2.37	0.58
7:G:153:PRO:HB2	11:K:158:VAL:HG13	1.86	0.58
15:O:67:GLU:OE2	15:O:183:ARG:NH1	2.37	0.58
15:O:159:PRO:HG2	32:O:304:CLA:C1D	2.34	0.58
4:D:145:ASP:OD1	34:D:318:DD6:O2	2.22	0.58
32:H:306:CLA:HED1	39:H:315:SQD:H282	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:196:ASN:N	17:S:196:ASN:HD22	2.02	0.57
22:c:14:CYS:N	42:c:101:SF4:S2	2.70	0.57
21:b:548:PRO:HB3	25:f:183:PRO:HG3	1.85	0.57
15:O:155:LEU:O	15:O:156:LEU:HB2	2.03	0.57
13:W:104:PRO:O	34:W:317:DD6:O4	2.22	0.57
21:b:548:PRO:HB3	25:f:183:PRO:HG2	1.87	0.56
1:A:54:GLU:HG2	1:A:55:THR:N	2.20	0.56
20:a:121:ILE:HG13	20:a:122:VAL:HG13	1.87	0.56
21:b:430:GLY:HA2	21:b:525:LEU:HD22	1.87	0.56
4:D:132:HIS:ND1	4:D:136:PHE:O	2.38	0.56
23:d:109:LYS:O	23:d:114:ARG:NH1	2.39	0.56
15:O:96:SER:O	15:O:100:GLY:N	2.39	0.56
7:G:138:GLU:OE2	9:I:42:PRO:HA	2.05	0.56
11:K:37:LEU:HD22	11:K:171:ASN:OD1	2.05	0.56
11:K:93:SER:OG	33:K:309:KC2:O2A	2.19	0.56
16:Q:184:ALA:O	16:Q:186:TYR:CE2	2.59	0.56
18:U:82:TRP:HZ3	18:U:183:VAL:HG11	1.70	0.56
3:C:136:ARG:O	3:C:140:VAL:HG23	2.06	0.56
4:D:155:GLN:O	4:D:159:TRP:HD1	1.88	0.56
9:I:119:GLY:O	9:I:123:VAL:HG13	2.05	0.56
15:R:36:GLY:O	15:R:183:ARG:NH2	2.39	0.56
16:Q:91:LEU:HD21	16:Q:104:MET:SD	2.46	0.56
16:Q:174:ILE:HD11	16:Q:186:TYR:CE2	2.41	0.56
13:W:148:GLN:O	13:W:164:PHE:N	2.37	0.56
10:J:187:THR:O	10:J:188:GLN:C	2.47	0.55
32:W:310:CLA:HED3	32:W:310:CLA:H61	1.86	0.55
21:b:410:ARG:O	21:b:414:HIS:ND1	2.39	0.55
23:d:38:SER:OG	23:d:55:GLN:O	2.24	0.55
32:Q:303:CLA:HMB3	32:Q:303:CLA:HBB1	1.88	0.55
29:l:58:LEU:HD22	29:l:85:LEU:HD23	1.88	0.55
12:L:217:LEU:CD1	32:L:311:CLA:HMD3	2.36	0.55
15:R:66:ALA:O	15:R:70:HIS:ND1	2.37	0.55
2:B:80:HIS:O	2:B:81:GLY:C	2.47	0.55
13:P:77:TYR:CZ	13:P:104:PRO:HB2	2.41	0.55
18:U:125:THR:O	18:U:128:THR:OG1	2.23	0.55
15:O:160:LEU:HG	32:O:304:CLA:HMD2	1.89	0.55
20:a:63:THR:OG1	20:a:64:SER:N	2.41	0.54
13:M:26:PHE:O	13:M:29:SER:OG	2.24	0.54
20:a:497:SER:OG	35:a:851:LHG:C5	2.53	0.54
11:K:72:ILE:HD12	32:K:304:CLA:HMD2	1.87	0.54
2:B:60:ASN:O	2:B:61:GLY:C	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:W:314:KC2:O1A	36:W:320:LMG:O3	2.10	0.54
23:d:112:GLU:N	23:d:112:GLU:OE2	2.41	0.54
2:B:133:GLN:O	2:B:134:VAL:C	2.46	0.54
8:H:74:LYS:NZ	32:H:305:CLA:O1D	2.37	0.54
21:b:293:THR:OG1	32:b:817:CLA:OBD	2.24	0.54
6:F:39:ALA:HB2	36:F:320:LMG:C4	2.38	0.54
25:f:182:SER:CB	25:f:183:PRO:CD	2.86	0.54
13:P:75:VAL:HG23	13:P:78:MET:HE2	1.90	0.53
15:R:137:GLU:OE2	15:R:144:TYR:OH	2.18	0.53
12:L:32:VAL:HG12	32:L:309:CLA:HED3	1.91	0.53
12:L:202:MET:HE1	12:L:217:LEU:CA	2.38	0.53
25:f:181:VAL:HG11	25:f:184:ARG:NH2	2.23	0.53
7:G:115:ALA:C	7:G:117:LYS:N	2.65	0.53
12:L:214:ALA:N	12:L:215:PRO:CD	2.71	0.53
2:B:138:SER:OG	2:B:139:LEU:N	2.41	0.53
3:C:187:GLY:O	3:C:188:MET:C	2.51	0.53
16:Q:91:LEU:HD21	16:Q:104:MET:HE1	1.89	0.53
32:a:832:CLA:H143	35:a:851:LHG:C18	2.38	0.53
21:b:422:LEU:HD13	21:b:532:LEU:HA	1.91	0.53
35:P:317:LHG:O2	35:P:317:LHG:O9	2.26	0.53
6:F:48:ILE:HD11	36:F:320:LMG:O4	2.04	0.53
20:a:201:HIS:ND1	32:a:822:CLA:OBD	2.40	0.53
19:V:104:VAL:CG1	38:V:205:LMU:H6D	2.38	0.53
7:G:91:PHE:CE1	11:K:86:LEU:HD12	2.44	0.53
21:b:526:ALA:HB1	21:b:586:THR:HB	1.91	0.53
7:G:153:PRO:HB2	11:K:158:VAL:CG1	2.39	0.52
15:T:109:ASP:OD1	15:T:112:ALA:HB3	2.09	0.52
25:f:181:VAL:HG12	25:f:184:ARG:CZ	2.38	0.52
11:K:39:ALA:HB2	32:K:306:CLA:CED	2.40	0.52
15:O:71:SER:HB3	15:O:182:GLY:HA3	1.92	0.52
12:L:32:VAL:HG13	12:L:62:LEU:HD21	1.91	0.52
12:L:200:SER:O	12:L:204:ILE:N	2.43	0.52
13:P:62:SER:OG	32:P:307:CLA:OBD	2.24	0.52
17:S:205:VAL:CG1	17:S:209:TYR:CZ	2.92	0.52
20:a:679:ILE:HD11	32:a:833:CLA:HAB	1.92	0.52
9:I:67:GLU:OE1	9:I:163:ARG:NH1	2.42	0.52
21:b:222:LEU:HD11	32:b:814:CLA:O1A	2.10	0.52
5:E:90:ASP:OD2	5:E:194:TYR:OH	2.19	0.52
7:G:139:ASN:OD1	38:I:315:LMU:H6D	2.10	0.52
12:L:166:PRO:HG2	12:L:168:PHE:CE2	2.45	0.52
10:J:94:ARG:NH2	10:J:104:LEU:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:198:ILE:HG22	12:L:198:ILE:O	2.10	0.51
33:P:312:KC2:C1C	36:P:318:LMG:H392	2.40	0.51
11:K:38:GLY:CA	11:K:174:ILE:CD1	2.87	0.51
12:L:77:MET:HE3	12:L:188:GLY:CA	2.41	0.51
33:S:312:KC2:O2A	36:S:322:LMG:C8	2.58	0.51
18:U:178:ILE:HD11	32:U:305:CLA:HMC3	1.93	0.51
13:W:25:ALA:O	13:W:26:PHE:C	2.49	0.51
21:b:182:LEU:O	21:b:186:SER:OG	2.19	0.51
2:B:77:ALA:O	2:B:82:LEU:N	2.36	0.51
6:F:48:ILE:HD13	36:F:320:LMG:HO4	1.75	0.51
11:K:172:VAL:HG23	32:K:301:CLA:OBD	2.11	0.51
17:S:61:GLY:O	17:S:65:THR:HG23	2.11	0.51
6:F:52:ARG:NH1	6:F:178:LEU:O	2.44	0.51
12:L:77:MET:HE3	12:L:188:GLY:N	2.26	0.51
15:T:177:SER:OG	32:T:302:CLA:O2D	2.28	0.51
21:b:293:THR:O	21:b:294:ASN:HB2	2.11	0.51
31:r:55:ASP:OD1	31:r:56:LYS:N	2.44	0.51
2:B:132:PRO:HD2	29:l:125:VAL:HG21	1.93	0.51
39:H:315:SQD:H4	39:H:315:SQD:O7	2.10	0.51
12:L:123:GLY:HA2	12:L:126:GLN:CG	2.41	0.51
13:M:134:LYS:O	13:M:135:PRO:C	2.51	0.51
13:M:156:GLY:O	37:M:301:A86:O2	2.29	0.51
25:f:166:GLU:HG2	25:f:171:LYS:HB2	1.92	0.51
8:H:62:SER:HB3	31:r:70:VAL:HG22	1.93	0.51
9:I:85:ASP:OD2	9:I:184:LEU:N	2.41	0.51
16:Q:184:ALA:O	16:Q:186:TYR:CD2	2.62	0.51
17:S:230:GLU:O	17:S:232:MET:N	2.43	0.51
18:U:115:GLU:OE1	18:U:115:GLU:N	2.42	0.51
25:f:180:THR:C	25:f:181:VAL:HG23	2.34	0.51
3:C:88:GLY:O	3:C:92:PRO:CD	2.59	0.51
6:F:105:GLU:OE1	6:F:187:GLY:N	2.42	0.51
32:b:833:CLA:H42	32:b:834:CLA:O1A	2.12	0.50
8:H:181:PHE:O	8:H:185:VAL:HG12	2.10	0.50
12:L:210:LEU:O	12:L:210:LEU:HG	2.11	0.50
33:S:312:KC2:O2A	36:S:322:LMG:C7	2.57	0.50
21:b:429:LEU:O	21:b:433:THR:OG1	2.23	0.50
13:W:90:ILE:CG2	13:W:94:VAL:HG13	2.42	0.50
20:a:532:ASP:O	20:a:536:HIS:ND1	2.42	0.50
2:B:54:VAL:HG21	2:B:150:PRO:HA	1.91	0.50
12:L:204:ILE:HD13	32:L:310:CLA:HMD1	1.93	0.50
13:P:77:TYR:O	13:P:80:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:ALA:HA	2:B:82:LEU:HD12	1.93	0.50
3:C:47:ILE:O	3:C:72:ARG:NH2	2.45	0.50
17:S:57:PHE:H	17:S:65:THR:HG21	1.76	0.50
36:W:320:LMG:O10	36:W:320:LMG:H121	2.12	0.50
12:L:200:SER:O	12:L:203:SER:N	2.45	0.50
36:M:320:LMG:H301	32:W:312:CLA:O1A	2.11	0.50
15:O:157:TRP:O	15:O:158:ASP:C	2.52	0.50
2:B:80:HIS:ND1	2:B:82:LEU:HD21	2.27	0.50
13:P:65:LYS:NZ	13:P:127:GLU:OE1	2.37	0.50
37:M:317:A86:C24	36:P:318:LMG:H171	2.41	0.50
32:a:828:CLA:H72	32:a:828:CLA:H41	1.93	0.50
13:M:27:VAL:HG11	13:M:48:SER:HB2	1.94	0.49
15:O:137:GLU:OE2	15:O:144:TYR:OH	2.21	0.49
16:Q:91:LEU:HD21	16:Q:104:MET:CE	2.42	0.49
32:a:828:CLA:H41	32:a:828:CLA:C7	2.41	0.49
21:b:631:LEU:HD21	21:b:650:PHE:CD1	2.47	0.49
20:a:77:HIS:ND1	32:a:821:CLA:OBD	2.42	0.49
2:B:169:ASN:N	2:B:169:ASN:HD22	2.11	0.49
7:G:113:LEU:O	7:G:114:GLY:C	2.54	0.49
9:I:50:GLY:O	9:I:52:SER:N	2.45	0.49
13:P:31:GLU:OE2	13:P:31:GLU:N	2.40	0.49
20:a:438:ILE:HG13	20:a:556:PHE:HE2	1.76	0.49
14:N:164:ASP:OD2	14:N:169:THR:HG22	2.12	0.49
12:L:195:MET:O	12:L:199:ILE:HG13	2.13	0.49
13:M:54:GLU:OE1	13:M:139:ARG:NH1	2.45	0.49
18:U:137:MET:HA	18:U:142:ALA:CB	2.41	0.49
4:D:73:GLU:O	32:D:304:CLA:HMA3	2.13	0.49
30:m:5:GLY:O	30:m:9:VAL:HG13	2.13	0.49
4:D:168:THR:HA	4:D:171:ILE:HG22	1.95	0.49
12:L:198:ILE:O	12:L:198:ILE:CG2	2.61	0.49
12:L:209:PRO:HG2	32:L:310:CLA:HHB	1.95	0.49
7:G:67:ALA:O	7:G:71:HIS:ND1	2.43	0.49
3:C:184:ALA:O	3:C:185:VAL:C	2.52	0.48
4:D:144:HIS:CD2	4:D:153:MET:CE	2.96	0.48
20:a:29:TRP:CZ3	32:a:810:CLA:H43	2.48	0.48
20:a:697:LEU:HD21	32:a:802:CLA:CED	2.43	0.48
12:L:198:ILE:O	12:L:202:MET:HG2	2.13	0.48
13:W:25:ALA:O	13:W:56:VAL:CG1	2.60	0.48
32:k:201:CLA:HMC3	41:k:204:BCR:H383	1.94	0.48
14:N:66:ARG:NH2	32:N:311:CLA:O1D	2.44	0.48
15:O:157:TRP:HA	15:O:157:TRP:CE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:661:SER:O	20:a:664:SER:OG	2.32	0.48
1:A:72:ARG:NH2	1:A:75:GLU:OE1	2.44	0.48
7:G:139:ASN:OD1	38:I:315:LMU:H6E	2.13	0.48
1:A:110:ALA:HB1	32:A:309:CLA:CED	2.43	0.48
2:B:60:ASN:O	2:B:63:HIS:N	2.46	0.48
2:B:130:PHE:CZ	35:B:308:LHG:H242	2.48	0.48
7:G:135:VAL:HG22	32:I:301:CLA:HBB1	1.96	0.48
8:H:152:ASP:O	8:H:153:PRO:C	2.53	0.48
12:L:217:LEU:HD11	32:L:311:CLA:CMD	2.42	0.48
13:P:109:ASP:OD1	13:P:109:ASP:N	2.43	0.48
20:a:370:HIS:ND1	32:a:828:CLA:OBD	2.43	0.48
13:M:131:GLU:OE2	13:M:137:TYR:OH	2.21	0.48
15:O:155:LEU:O	15:O:156:LEU:CB	2.61	0.48
13:W:53:ASP:OD1	13:W:53:ASP:O	2.32	0.48
2:B:132:PRO:HB2	2:B:134:VAL:HG23	1.95	0.48
36:F:320:LMG:HC5	21:b:314:ARG:CZ	2.44	0.48
8:H:154:PHE:O	8:H:155:LYS:C	2.57	0.48
12:L:209:PRO:O	12:L:210:LEU:CB	2.62	0.48
13:M:47:ILE:HD12	34:M:316:DD6:O4	2.13	0.48
19:V:104:VAL:CG1	38:V:205:LMU:C6'	2.91	0.48
4:D:153:MET:HE3	32:D:315:CLA:C4C	2.44	0.47
9:I:92:ASP:OD2	34:I:311:DD6:O2	2.32	0.47
12:L:69:GLU:OE2	12:L:189:ARG:NE	2.44	0.47
12:L:209:PRO:HD2	32:L:310:CLA:C1B	2.45	0.47
8:H:78:ILE:HD12	32:H:305:CLA:HMD2	1.96	0.47
8:H:135:ASN:HA	39:H:315:SQD:C8	2.44	0.47
13:W:35:GLU:OE1	13:W:35:GLU:N	2.46	0.47
9:I:61:ALA:HB1	9:I:136:PRO:HG3	1.94	0.47
19:V:104:VAL:HG12	38:V:205:LMU:H6D	1.96	0.47
1:A:72:ARG:HG3	1:A:72:ARG:O	2.15	0.47
39:H:315:SQD:H191	41:b:845:BCR:H24C	1.96	0.47
9:I:135:LYS:O	9:I:136:PRO:C	2.57	0.47
3:C:90:ILE:HG23	3:C:188:MET:HE1	1.97	0.47
4:D:191:GLY:O	13:W:52:SER:OG	2.27	0.47
7:G:117:LYS:O	7:G:117:LYS:HG3	2.15	0.47
8:H:73:LEU:HD22	8:H:170:GLU:OE2	2.15	0.47
39:H:315:SQD:O49	39:H:315:SQD:C46	2.60	0.47
13:P:117:LEU:O	13:P:121:THR:OG1	2.27	0.47
17:S:205:VAL:HG12	17:S:209:TYR:CE2	2.50	0.47
18:U:55:PRO:O	34:U:309:DD6:O4	2.33	0.47
20:a:552:LYS:HG3	20:a:556:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:714:ILE:CD1	25:f:142:ILE:HG23	2.45	0.47
20:a:714:ILE:HD11	25:f:142:ILE:HG23	1.97	0.47
21:b:188:LEU:HD21	41:b:845:BCR:H331	1.97	0.47
13:P:89:GLU:OE1	13:P:89:GLU:N	2.48	0.47
36:T:301:LMG:HO4	36:T:301:LMG:HO5	1.62	0.47
21:b:574:ASP:OD1	21:b:706:ARG:NH1	2.47	0.47
21:b:694:ARG:NH2	26:i:33:ASP:OD2	2.48	0.47
8:H:77:ARG:NH1	8:H:170:GLU:OE2	2.48	0.47
33:I:309:KC2:CMB	36:l:201:LMG:H331	2.45	0.47
16:Q:62:ARG:NH2	16:Q:65:GLU:OE1	2.48	0.47
6:F:96:ASN:HA	36:F:320:LMG:HC71	1.97	0.46
19:V:97:ILE:O	19:V:100:SER:OG	2.30	0.46
2:B:141:LEU:HD11	2:B:148:GLU:HG3	1.96	0.46
13:P:108:TRP:O	13:P:111:THR:OG1	2.33	0.46
16:Q:184:ALA:HB1	37:Q:316:A86:C17	2.45	0.46
36:l:201:LMG:H312	36:l:201:LMG:H161	1.97	0.46
38:D:324:LMU:H6D	36:D:325:LMG:HC72	1.97	0.46
10:J:30:ALA:O	10:J:39:GLU:CD	2.58	0.46
13:P:75:VAL:O	13:P:75:VAL:HG22	2.15	0.46
16:Q:184:ALA:CB	37:Q:316:A86:C17	2.94	0.46
2:B:77:ALA:HA	2:B:82:LEU:HG	1.98	0.46
15:O:31:VAL:HA	15:O:34:MET:HG2	1.98	0.46
20:a:155:ASN:C	20:a:155:ASN:OD1	2.56	0.46
20:a:311:MET:HE1	32:a:820:CLA:C3D	2.45	0.46
32:a:838:CLA:H72	32:a:838:CLA:H41	1.96	0.46
6:F:195:LEU:HD11	38:J:318:LMU:C1	2.45	0.46
7:G:36:VAL:O	7:G:65:ARG:NH2	2.49	0.46
7:G:60:ASN:ND2	9:I:45:PHE:O	2.38	0.46
12:L:180:LYS:NZ	37:L:315:A86:O2	2.48	0.46
15:O:34:MET:O	15:O:64:ARG:NH1	2.47	0.46
13:P:99:VAL:HG23	32:P:311:CLA:CED	2.46	0.46
18:U:60:THR:O	18:U:61:PRO:C	2.59	0.46
25:f:174:VAL:HG11	25:f:179:ILE:HG12	1.97	0.46
8:H:67:TRP:HH2	39:H:315:SQD:H151	1.80	0.46
15:R:188:GLY:HA3	37:R:312:A86:C29	2.46	0.46
21:b:178:HIS:HE1	32:b:816:CLA:NC	2.13	0.46
12:L:202:MET:CE	12:L:217:LEU:HB3	2.46	0.46
12:L:210:LEU:HD23	37:L:315:A86:C39	2.46	0.46
17:S:205:VAL:HG12	17:S:209:TYR:CZ	2.51	0.46
32:W:310:CLA:O1A	32:W:311:CLA:H41	2.16	0.46
21:b:652:PHE:CE2	21:b:656:ILE:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:174:VAL:HG22	25:f:175:PRO:HD2	1.98	0.46
39:H:315:SQD:H192	41:b:845:BCR:H372	1.97	0.45
18:U:128:THR:CG2	41:U:310:BCR:H342	2.45	0.45
11:K:37:LEU:O	11:K:63:ARG:NH2	2.49	0.45
2:B:78:LYS:HA	2:B:83:LEU:CD2	2.46	0.45
12:L:77:MET:HE3	12:L:188:GLY:HA2	1.98	0.45
12:L:209:PRO:HG2	32:L:310:CLA:CHB	2.46	0.45
15:R:96:SER:OG	33:R:311:KC2:O1A	2.27	0.45
6:F:205:LYS:NZ	33:F:302:KC2:O1A	2.45	0.45
5:E:187:LEU:CD2	5:E:196:TYR:OH	2.64	0.45
6:F:195:LEU:HD11	38:J:318:LMU:H12	1.97	0.45
32:N:312:CLA:HBD	36:W:320:LMG:H152	1.99	0.45
6:F:222:MET:HA	6:F:222:MET:HE2	1.99	0.45
8:H:67:TRP:CH2	39:H:315:SQD:H151	2.52	0.45
13:M:117:LEU:O	13:M:121:THR:OG1	2.27	0.45
21:b:351:HIS:ND1	32:b:828:CLA:OBD	2.43	0.45
5:E:95:VAL:HG22	5:E:96:PRO:HD2	1.99	0.45
11:K:171:ASN:O	11:K:175:ASN:ND2	2.50	0.45
12:L:163:TRP:O	12:L:164:ASP:C	2.57	0.45
36:N:301:LMG:HC72	36:N:301:LMG:HC2	1.70	0.45
13:P:214:ASP:OD2	37:P:316:A86:O2	2.35	0.45
16:Q:152:ASP:OD2	16:Q:157:ARG:NH1	2.50	0.45
20:a:360:MET:HE3	32:a:823:CLA:HBC3	1.99	0.45
32:A:303:CLA:H42	32:A:303:CLA:HMA2	1.99	0.45
6:F:176:LEU:HD11	6:F:184:ARG:CG	2.47	0.45
8:H:131:TYR:CE1	39:H:315:SQD:H141	2.51	0.45
12:L:209:PRO:HG3	32:L:310:CLA:HMA1	1.99	0.45
15:O:141:LYS:O	15:O:143:HIS:N	2.50	0.45
17:S:170:PRO:HD2	34:S:321:DD6:C22	2.47	0.45
3:C:88:GLY:O	3:C:92:PRO:HD3	2.17	0.45
39:H:315:SQD:H142	39:H:315:SQD:H112	1.32	0.45
8:H:138:MET:HG3	39:H:315:SQD:H82	1.99	0.44
15:R:188:GLY:O	15:R:191:SER:OG	2.23	0.44
20:a:320:HIS:HB3	20:a:325:ILE:HD11	1.99	0.44
2:B:94:ASP:O	29:l:73:ASN:ND2	2.50	0.44
12:L:200:SER:C	12:L:202:MET:N	2.71	0.44
12:L:214:ALA:C	12:L:216:ALA:N	2.73	0.44
13:W:29:SER:O	13:W:30:ILE:C	2.61	0.44
2:B:132:PRO:C	2:B:134:VAL:N	2.74	0.44
7:G:110:GLY:O	7:G:114:GLY:N	2.46	0.44
12:L:35:MET:HE3	12:L:62:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:77:TYR:O	13:P:78:MET:C	2.57	0.44
32:a:834:CLA:H41	32:a:834:CLA:H61	1.78	0.44
21:b:373:THR:HG23	21:b:591:THR:HG21	1.98	0.44
4:D:174:THR:OG1	4:D:180:ARG:O	2.23	0.44
9:I:99:PRO:O	34:I:312:DD6:O4	2.36	0.44
40:Q:318:DGD:CHB	32:S:305:CLA:HBC1	2.47	0.44
32:a:803:CLA:HED2	27:j:16:LEU:HD22	2.00	0.44
21:b:307:ALA:HB2	31:r:51:THR:OG1	2.16	0.44
11:K:155:ASP:OD1	11:K:155:ASP:N	2.51	0.44
15:R:64:ARG:NH2	32:R:308:CLA:O1D	2.50	0.44
13:W:167:PRO:HG3	32:W:306:CLA:C2D	2.48	0.44
32:W:310:CLA:HED3	32:W:310:CLA:H62	1.97	0.44
1:A:110:ALA:HB1	32:A:309:CLA:HED3	2.00	0.44
6:F:189:LEU:HD11	37:F:313:A86:O2	2.18	0.44
17:S:40:LEU:HG	17:S:196:ASN:HD21	1.82	0.44
32:a:832:CLA:C14	35:a:851:LHG:C18	2.95	0.44
8:H:196:PRO:O	37:H:314:A86:O2	2.35	0.44
13:P:51:VAL:HG21	13:P:59:PHE:CE2	2.53	0.44
17:S:196:ASN:O	17:S:197:ASN:C	2.60	0.44
21:b:307:ALA:HB2	31:r:51:THR:CB	2.48	0.44
8:H:186:THR:O	8:H:187:GLN:C	2.60	0.44
12:L:204:ILE:HG23	12:L:207:SER:HB2	1.99	0.44
14:N:42:GLU:N	14:N:42:GLU:OE1	2.51	0.44
20:a:236:GLU:OE1	20:a:236:GLU:N	2.50	0.44
21:b:299:HIS:HB3	21:b:304:ILE:HD11	1.99	0.44
21:b:631:LEU:HD22	21:b:724:PHE:HA	2.00	0.44
11:K:46:TRP:C	11:K:48:PRO:HD3	2.42	0.43
13:M:60:ARG:NH1	13:M:187:LEU:HD11	2.33	0.43
14:N:68:ALA:O	14:N:72:HIS:ND1	2.51	0.43
9:I:98:ASN:ND2	9:I:180:GLY:O	2.50	0.43
15:T:62:TRP:NE1	32:T:307:CLA:O1A	2.49	0.43
36:A:317:LMG:HC91	36:A:318:LMG:H142	2.00	0.43
13:W:28:ASP:O	13:W:29:SER:C	2.60	0.43
20:a:56:ALA:O	20:a:62:GLN:NE2	2.48	0.43
21:b:203:ARG:NH2	21:b:253:ALA:O	2.47	0.43
4:D:193:GLY:O	4:D:199:MET:HE2	2.17	0.43
25:f:174:VAL:HG13	25:f:179:ILE:HD11	1.99	0.43
27:j:1:MET:CB	27:j:5:LEU:HD23	2.49	0.43
2:B:177:LEU:O	2:B:181:VAL:HG23	2.18	0.43
5:E:198:GLY:C	5:E:200:SER:N	2.74	0.43
25:f:174:VAL:HG12	25:f:179:ILE:HD11	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:180:THR:C	25:f:181:VAL:CG2	2.91	0.43
2:B:132:PRO:C	2:B:134:VAL:H	2.27	0.43
6:F:189:LEU:HD12	32:F:304:CLA:HMD2	2.01	0.43
8:H:169:LYS:O	8:H:173:HIS:ND1	2.51	0.43
15:R:84:VAL:O	15:R:108:ARG:NH2	2.52	0.43
32:b:811:CLA:HBC1	32:b:830:CLA:H93	2.00	0.43
4:D:188:ASP:OD1	34:D:316:DD6:O2	2.36	0.43
13:M:148:GLN:NE2	13:M:166:ASP:OD1	2.49	0.43
15:R:40:GLU:HB2	15:R:180:LYS:NZ	2.34	0.43
20:a:429:ARG:NH1	29:l:3:GLU:OE1	2.52	0.43
21:b:307:ALA:HB3	32:b:833:CLA:HED3	2.01	0.43
11:K:38:GLY:HA2	11:K:178:ARG:HH22	1.83	0.43
13:P:75:VAL:HG13	32:P:311:CLA:HMC1	2.00	0.43
2:B:130:PHE:CZ	35:B:308:LHG:C24	3.01	0.43
6:F:35:ASP:OD1	6:F:36:GLU:N	2.52	0.43
10:J:176:ARG:NH1	34:J:317:DD6:O4	2.52	0.43
16:Q:182:HIS:O	16:Q:183:PRO:O	2.37	0.43
34:S:321:DD6:C22	34:S:321:DD6:C19	2.94	0.43
13:W:26:PHE:CD2	13:W:28:ASP:HB2	2.54	0.43
1:A:72:ARG:NH2	32:A:307:CLA:O1D	2.45	0.43
20:a:87:TRP:NE1	32:a:824:CLA:OBD	2.49	0.43
22:c:14:CYS:O	22:c:15:THR:CG2	2.66	0.43
2:B:71:ILE:HD12	2:B:72:LEU:N	2.34	0.42
13:W:25:ALA:HA	13:W:57:MET:HG2	2.01	0.42
15:O:141:LYS:HD3	15:O:141:LYS:HA	1.87	0.42
16:Q:185:PRO:O	16:Q:186:TYR:HB2	2.19	0.42
15:R:40:GLU:HB2	15:R:180:LYS:HZ1	1.85	0.42
32:a:823:CLA:H12	41:a:843:BCR:H371	2.01	0.42
3:C:191:GLN:OE1	32:C:308:CLA:NA	2.52	0.42
13:M:60:ARG:HD3	13:M:64:LEU:HD23	2.00	0.42
23:d:35:THR:HG22	23:d:60:LEU:HD13	1.99	0.42
41:l:206:BCR:C8	41:l:206:BCR:H331	2.48	0.42
1:A:190:VAL:O	1:A:193:THR:OG1	2.33	0.42
2:B:77:ALA:HA	2:B:82:LEU:CD1	2.49	0.42
3:C:77:MET:HG3	32:C:305:CLA:HMD2	2.02	0.42
4:D:73:GLU:OE2	4:D:73:GLU:N	2.47	0.42
4:D:168:THR:HB	32:D:308:CLA:HMA1	2.01	0.42
6:F:215:ARG:HB3	32:F:307:CLA:HBC2	2.02	0.42
7:G:117:LYS:O	7:G:117:LYS:CG	2.66	0.42
37:T:313:A86:O	37:T:313:A86:C21	2.67	0.42
20:a:324:GLU:OE1	20:a:324:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:51:ARG:HD3	25:f:65:LEU:HD21	2.01	0.42
18:U:82:TRP:CZ3	18:U:183:VAL:HG11	2.52	0.42
37:M:317:A86:C24	36:P:318:LMG:C17	2.97	0.42
13:W:92:LYS:HB2	36:W:320:LMG:O4	2.19	0.42
21:b:649:MET:HE1	32:b:822:CLA:H42	2.02	0.42
25:f:50:SER:C	25:f:52:LEU:N	2.77	0.42
27:j:8:TYR:O	27:j:11:THR:HG22	2.20	0.42
3:C:81:GLN:OE1	32:C:305:CLA:HBC3	2.20	0.42
40:Q:318:DGD:HE61	17:S:125:PHE:CZ	2.55	0.42
2:B:54:VAL:HG11	2:B:151:TYR:CD1	2.54	0.42
3:C:91:PHE:O	3:C:92:PRO:C	2.63	0.42
7:G:71:HIS:HB3	7:G:177:MET:HE2	2.02	0.42
8:H:43:LYS:C	8:H:45:ASP:OD1	2.63	0.42
39:H:315:SQD:H441	39:H:315:SQD:O2	2.20	0.42
10:J:187:THR:O	10:J:190:ALA:N	2.53	0.42
21:b:293:THR:OG1	21:b:293:THR:O	2.38	0.42
2:B:59:TRP:O	2:B:60:ASN:C	2.60	0.42
2:B:77:ALA:HA	2:B:82:LEU:CG	2.49	0.42
7:G:155:VAL:O	11:K:157:TRP:O	2.38	0.42
17:S:35:LYS:O	17:S:39:LYS:HG2	2.19	0.42
18:U:180:PHE:HA	18:U:183:VAL:HG22	2.01	0.42
21:b:185:VAL:HG11	41:b:841:BCR:H341	2.01	0.42
21:b:515:GLY:O	21:b:519:ILE:HG22	2.19	0.42
8:H:128:ALA:HB1	32:b:817:CLA:C5	2.50	0.42
32:I:303:CLA:H62	32:I:303:CLA:H41	1.92	0.42
12:L:35:MET:HB2	32:L:309:CLA:CED	2.49	0.42
16:Q:187:TRP:CD1	40:Q:318:DGD:HG11	2.55	0.42
13:W:91:ALA:CB	13:W:94:VAL:CG1	2.93	0.42
20:a:747:ARG:O	20:a:751:VAL:HG22	2.20	0.42
32:a:805:CLA:H193	41:a:846:BCR:H21C	2.01	0.42
32:D:314:CLA:H41	32:D:314:CLA:H62	1.73	0.41
8:H:90:ASP:OD1	8:H:103:SER:OG	2.24	0.41
28:k:63:MET:CE	28:k:65:ILE:HD11	2.50	0.41
7:G:94:MET:O	7:G:94:MET:HG2	2.20	0.41
39:H:315:SQD:O4	39:H:315:SQD:H1	2.20	0.41
15:O:34:MET:HG3	15:O:60:LEU:HD13	2.02	0.41
13:P:35:GLU:OE1	13:P:35:GLU:N	2.49	0.41
13:P:148:GLN:O	13:P:164:PHE:N	2.48	0.41
18:U:136:ASP:O	18:U:140:SER:HB2	2.20	0.41
20:a:13:VAL:N	20:a:315:ASN:OD1	2.51	0.41
32:k:203:CLA:HBB2	39:k:206:SQD:C25	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:ASP:OD1	5:E:46:GLY:N	2.54	0.41
15:O:159:PRO:HG2	32:O:304:CLA:C2D	2.50	0.41
32:b:833:CLA:H41	31:r:117:TYR:CE1	2.56	0.41
29:l:101:PHE:O	29:l:113:SER:OG	2.37	0.41
3:C:72:ARG:HG3	3:C:149:VAL:HG11	2.01	0.41
9:I:160:ASN:ND2	32:I:301:CLA:O1D	2.47	0.41
15:O:158:ASP:CG	15:O:162:PHE:H	2.27	0.41
19:V:60:ILE:N	19:V:64:ASN:OD1	2.53	0.41
2:B:132:PRO:HD2	29:l:125:VAL:CG2	2.51	0.41
5:E:187:LEU:HD22	5:E:196:TYR:OH	2.20	0.41
15:R:113:ALA:O	15:R:117:VAL:HG23	2.20	0.41
17:S:72:SER:OG	17:S:76:HIS:CE1	2.73	0.41
31:r:114:LEU:O	31:r:118:SER:N	2.47	0.41
1:A:125:PHE:CZ	1:A:129:ILE:HD11	2.55	0.41
32:D:307:CLA:C9	32:W:310:CLA:H41	2.51	0.41
11:K:38:GLY:N	11:K:174:ILE:HD11	2.36	0.41
11:K:198:ILE:HD12	11:K:199:PRO:HD2	2.03	0.41
13:W:92:LYS:CD	13:W:92:LYS:C	2.93	0.41
22:c:54:CYS:SG	22:c:55:GLU:N	2.93	0.41
22:c:14:CYS:C	22:c:15:THR:HG22	2.46	0.41
12:L:208:VAL:HB	12:L:211:LEU:HB3	2.03	0.41
32:b:835:CLA:H41	32:b:835:CLA:H62	1.77	0.41
32:F:304:CLA:C9	38:J:318:LMU:H92	2.50	0.41
8:H:152:ASP:OD1	8:H:152:ASP:N	2.54	0.41
32:H:301:CLA:HMC1	10:J:132:ALA:HB2	2.03	0.41
11:K:159:ARG:NE	33:K:303:KC2:O2A	2.54	0.41
13:M:200:PHE:HA	13:M:213:LEU:HD21	2.03	0.41
17:S:57:PHE:N	17:S:65:THR:HG21	2.36	0.41
17:S:139:GLU:O	17:S:142:SER:OG	2.34	0.41
20:a:199:ASN:HB3	32:a:817:CLA:HMD2	2.01	0.41
20:a:561:ARG:O	23:d:65:LYS:NZ	2.52	0.41
20:a:672:ILE:HD11	32:a:807:CLA:HMC2	2.01	0.41
32:a:852:CLA:H152	41:b:843:BCR:H362	2.03	0.41
32:k:203:CLA:C3B	39:k:206:SQD:H442	2.51	0.41
21:b:56:ILE:HD12	32:b:807:CLA:CBB	2.50	0.41
21:b:649:MET:HE2	21:b:719:PHE:CD2	2.55	0.41
36:j:104:LMG:HC1	36:j:104:LMG:HC92	2.03	0.41
4:D:171:ILE:HA	4:D:174:THR:HG22	2.02	0.40
36:F:319:LMG:H352	32:J:312:CLA:C11	2.48	0.40
18:U:92:LEU:O	32:U:306:CLA:HMD1	2.21	0.40
2:B:148:GLU:O	2:B:149:GLU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:ASN:OD1	3:C:157:ASN:N	2.52	0.40
21:b:416:GLU:OE2	25:f:181:VAL:HG13	2.21	0.40
2:B:57:GLU:OE2	2:B:171:ARG:NH1	2.55	0.40
36:F:320:LMG:HC91	36:F:320:LMG:C11	2.52	0.40
7:G:114:GLY:O	7:G:117:LYS:N	2.54	0.40
32:N:310:CLA:H61	32:N:310:CLA:H41	1.94	0.40
15:O:156:LEU:HD22	32:O:304:CLA:C2B	2.52	0.40
15:R:68:LEU:HD21	15:R:179:LEU:HD21	2.03	0.40
15:O:110:GLY:O	15:O:111:TYR:C	2.62	0.40
15:O:177:SER:O	15:O:181:ASN:ND2	2.52	0.40
13:W:90:ILE:HG22	13:W:94:VAL:HG13	2.03	0.40
21:b:521:HIS:CD2	35:f:205:LHG:H383	2.57	0.40
1:A:32:LYS:O	1:A:42:ALA:N	2.54	0.40
16:Q:176:THR:O	16:Q:176:THR:HG22	2.21	0.40
21:b:307:ALA:HB2	31:r:51:THR:HB	2.04	0.40
32:b:831:CLA:HBB1	41:b:843:BCR:H363	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	178/209 (85%)	175 (98%)	3 (2%)	0	100 100
2	B	154/209 (74%)	144 (94%)	8 (5%)	2 (1%)	9 16
3	C	175/205 (85%)	168 (96%)	6 (3%)	1 (1%)	21 36
4	D	177/245 (72%)	173 (98%)	4 (2%)	0	100 100
5	E	174/206 (84%)	161 (92%)	13 (8%)	0	100 100
6	F	208/240 (87%)	200 (96%)	8 (4%)	0	100 100
7	G	165/198 (83%)	158 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	165/198 (83%)	158 (96%)	6 (4%)	1 (1%)	21	36
9	I	152/194 (78%)	146 (96%)	5 (3%)	1 (1%)	18	32
10	J	169/200 (84%)	166 (98%)	3 (2%)	0	100	100
11	K	164/202 (81%)	157 (96%)	6 (4%)	1 (1%)	21	36
12	L	196/229 (86%)	190 (97%)	5 (3%)	1 (0%)	24	40
13	M	191/217 (88%)	183 (96%)	7 (4%)	1 (0%)	24	40
13	P	191/217 (88%)	183 (96%)	8 (4%)	0	100	100
13	W	191/217 (88%)	181 (95%)	9 (5%)	1 (0%)	24	40
14	N	192/224 (86%)	184 (96%)	8 (4%)	0	100	100
15	O	173/206 (84%)	160 (92%)	12 (7%)	1 (1%)	21	36
15	R	173/206 (84%)	167 (96%)	6 (4%)	0	100	100
15	T	173/206 (84%)	162 (94%)	11 (6%)	0	100	100
16	Q	155/187 (83%)	152 (98%)	2 (1%)	1 (1%)	21	36
17	S	203/235 (86%)	192 (95%)	10 (5%)	1 (0%)	24	40
18	U	140/203 (69%)	133 (95%)	7 (5%)	0	100	100
19	V	45/122 (37%)	43 (96%)	2 (4%)	0	100	100
20	a	739/752 (98%)	711 (96%)	28 (4%)	0	100	100
21	b	730/734 (100%)	708 (97%)	22 (3%)	0	100	100
22	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
23	d	135/142 (95%)	129 (96%)	6 (4%)	0	100	100
24	e	63/124 (51%)	57 (90%)	6 (10%)	0	100	100
25	f	159/184 (86%)	154 (97%)	5 (3%)	0	100	100
26	i	31/36 (86%)	31 (100%)	0	0	100	100
27	j	38/40 (95%)	38 (100%)	0	0	100	100
28	k	68/92 (74%)	68 (100%)	0	0	100	100
29	l	141/145 (97%)	137 (97%)	4 (3%)	0	100	100
30	m	28/30 (93%)	28 (100%)	0	0	100	100
31	r	89/133 (67%)	89 (100%)	0	0	100	100
All	All	6203/7268 (85%)	5960 (96%)	231 (4%)	12 (0%)	44	62

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	GLY
9	I	136	PRO
11	K	44	GLY
13	M	136	HIS
15	O	156	LEU
16	Q	183	PRO
2	B	143	ASP
3	C	98	LEU
13	W	30	ILE
12	L	214	ALA
17	S	231	ILE
2	B	134	VAL

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	148/170 (87%)	148 (100%)	0	100 100
2	B	117/159 (74%)	114 (97%)	3 (3%)	40 62
3	C	143/164 (87%)	143 (100%)	0	100 100
4	D	143/186 (77%)	141 (99%)	2 (1%)	59 74
5	E	137/157 (87%)	137 (100%)	0	100 100
6	F	161/183 (88%)	161 (100%)	0	100 100
7	G	126/148 (85%)	126 (100%)	0	100 100
8	H	133/158 (84%)	132 (99%)	1 (1%)	73 83
9	I	125/156 (80%)	124 (99%)	1 (1%)	73 83
10	J	122/143 (85%)	122 (100%)	0	100 100
11	K	129/153 (84%)	128 (99%)	1 (1%)	73 83
12	L	151/176 (86%)	148 (98%)	3 (2%)	48 67
13	M	148/164 (90%)	147 (99%)	1 (1%)	76 85
13	P	148/164 (90%)	148 (100%)	0	100 100
13	W	148/164 (90%)	147 (99%)	1 (1%)	76 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	N	150/172 (87%)	150 (100%)	0	100 100
15	O	133/156 (85%)	133 (100%)	0	100 100
15	R	133/156 (85%)	132 (99%)	1 (1%)	73 83
15	T	133/156 (85%)	133 (100%)	0	100 100
16	Q	124/142 (87%)	124 (100%)	0	100 100
17	S	160/177 (90%)	159 (99%)	1 (1%)	78 87
18	U	110/156 (70%)	110 (100%)	0	100 100
19	V	41/94 (44%)	41 (100%)	0	100 100
20	a	607/616 (98%)	607 (100%)	0	100 100
21	b	590/591 (100%)	589 (100%)	1 (0%)	87 94
22	c	68/69 (99%)	68 (100%)	0	100 100
23	d	116/121 (96%)	116 (100%)	0	100 100
24	e	53/88 (60%)	53 (100%)	0	100 100
25	f	127/147 (86%)	124 (98%)	3 (2%)	43 63
26	i	30/32 (94%)	30 (100%)	0	100 100
27	j	36/36 (100%)	36 (100%)	0	100 100
28	k	53/70 (76%)	53 (100%)	0	100 100
29	l	117/118 (99%)	117 (100%)	0	100 100
30	m	22/22 (100%)	22 (100%)	0	100 100
31	r	71/99 (72%)	70 (99%)	1 (1%)	59 74
All	All	4953/5663 (88%)	4933 (100%)	20 (0%)	81 90

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	132	PRO
2	B	135	LEU
2	B	169	ASN
4	D	154	SER
4	D	158	LEU
8	H	186	THR
9	I	136	PRO
11	K	45	TYR
12	L	32	VAL
12	L	126	GLN

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Mol	Chain	Res	Type
12	L	204	ILE
13	M	134	LYS
15	R	40	GLU
17	S	95	HIS
13	W	27	VAL
21	b	629	SER
25	f	131	SER
25	f	182	SER
25	f	184	ARG
31	r	122	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	60	ASN
2	B	133	GLN
2	B	169	ASN
3	C	166	GLN
4	D	144	HIS
6	F	124	GLN
6	F	129	HIS
8	H	187	GLN
13	M	169	ASN
13	M	189	ASN
14	N	187	ASN
13	P	169	ASN
16	Q	51	ASN
16	Q	182	HIS
17	S	90	GLN
17	S	163	ASN
17	S	196	ASN
18	U	133	GLN
13	W	118	GLN
13	W	205	ASN
20	a	31	GLN
20	a	106	GLN
20	a	124	GLN
20	a	182	HIS
20	a	193	ASN
21	b	53	HIS
21	b	178	HIS
21	b	275	HIS

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Mol	Chain	Res	Type
22	c	38	GLN
25	f	140	ASN
28	k	76	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

517 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	$\#\|Z\| > 2$
32	CLA	H	308	8	45,49,73	2.32	10 (22%)	54,84,113	1.87	9 (16%)
32	CLA	P	311	-	64,68,73	1.80	9 (14%)	77,107,113	1.44	10 (12%)
37	A86	G	311	-	44,50,50	0.56	1 (2%)	51,76,76	0.88	2 (3%)
37	A86	P	313	-	44,50,50	0.57	1 (2%)	51,76,76	1.28	2 (3%)
32	CLA	Q	310	-	50,54,73	2.10	9 (18%)	60,90,113	1.67	9 (15%)
37	A86	W	318	-	44,50,50	0.36	0	51,76,76	1.34	4 (7%)
39	SQD	H	315	-	42,43,54	1.32	4 (9%)	51,54,65	1.39	6 (11%)
32	CLA	Q	309	-	49,53,73	2.06	9 (18%)	59,89,113	1.63	5 (8%)
32	CLA	b	820	-	68,72,73	1.78	9 (13%)	81,111,113	1.46	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	A86	T	313	-	44,50,50	0.78	1 (2%)	51,76,76	1.05	2 (3%)
36	LMG	P	318	-	45,45,55	0.97	2 (4%)	53,53,63	1.15	4 (7%)
37	A86	P	316	-	44,50,50	0.44	0	51,76,76	1.61	5 (9%)
33	KC2	O	302	-	49,53,53	1.89	4 (8%)	62,89,89	1.34	9 (14%)
32	CLA	L	314	-	49,53,73	2.12	9 (18%)	59,89,113	1.61	7 (11%)
41	BCR	a	843	-	41,41,41	0.16	0	56,56,56	0.41	0
32	CLA	A	304	-	69,73,73	1.74	9 (13%)	83,113,113	1.41	9 (10%)
33	KC2	W	314	13,36	49,53,53	1.90	4 (8%)	62,89,89	1.34	8 (12%)
32	CLA	C	309	-	47,51,73	2.16	9 (19%)	56,86,113	1.63	7 (12%)
34	DD6	H	313	-	39,45,45	0.21	0	52,67,67	0.92	4 (7%)
32	CLA	S	304	-	46,50,73	2.14	9 (19%)	55,85,113	1.62	7 (12%)
34	DD6	I	312	-	39,45,45	0.20	0	52,67,67	0.68	1 (1%)
36	LMG	D	302	-	30,30,55	1.17	3 (10%)	38,38,63	1.40	5 (13%)
34	DD6	E	319	-	39,45,45	0.18	0	52,67,67	0.80	3 (5%)
34	DD6	J	314	-	39,45,45	0.25	0	52,67,67	0.65	1 (1%)
32	CLA	P	305	13	64,68,73	1.81	9 (14%)	77,107,113	1.44	7 (9%)
32	CLA	M	306	13	66,70,73	1.81	9 (13%)	79,109,113	1.45	7 (8%)
32	CLA	R	308	15	64,68,73	1.80	9 (14%)	77,107,113	1.49	9 (11%)
33	KC2	S	302	17	49,53,53	1.90	4 (8%)	62,89,89	1.34	8 (12%)
32	CLA	J	301	10	49,53,73	2.09	9 (18%)	59,89,113	1.57	7 (11%)
37	A86	Q	311	-	44,50,50	0.44	0	51,76,76	0.89	2 (3%)
33	KC2	E	313	-	49,53,53	1.88	4 (8%)	62,89,89	1.34	8 (12%)
34	DD6	Q	312	-	39,45,45	0.18	0	52,67,67	0.77	1 (1%)
42	SF4	c	101	22	0,12,12	-	-	-		
32	CLA	b	805	-	69,73,73	1.69	9 (13%)	83,113,113	1.32	8 (9%)
32	CLA	M	312	-	64,68,73	1.82	9 (14%)	77,107,113	1.46	7 (9%)
32	CLA	N	309	14	54,58,73	2.04	9 (16%)	65,95,113	1.69	9 (13%)
32	CLA	k	203	-	59,63,73	1.88	9 (15%)	71,101,113	1.55	10 (14%)
37	A86	Q	316	-	44,50,50	0.57	1 (2%)	51,76,76	0.45	0
33	KC2	R	303	-	49,53,53	1.91	4 (8%)	62,89,89	1.35	8 (12%)
32	CLA	b	813	-	49,53,73	2.07	9 (18%)	59,89,113	1.61	7 (11%)
32	CLA	W	306	-	59,63,73	1.90	9 (15%)	71,101,113	1.52	7 (9%)
34	DD6	H	311	-	39,45,45	0.23	0	52,67,67	1.03	4 (7%)
34	DD6	C	310	-	39,45,45	0.19	0	52,67,67	0.81	2 (3%)
33	KC2	L	313	-	49,53,53	1.88	4 (8%)	62,89,89	1.36	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DD6	O	313	-	39,45,45	0.18	0	52,67,67	1.22	4 (7%)
34	DD6	V	202	-	39,45,45	0.19	0	52,67,67	0.96	3 (5%)
32	CLA	J	307	10	59,63,73	1.93	10 (16%)	71,101,113	1.69	9 (12%)
32	CLA	b	808	21	69,73,73	1.72	9 (13%)	83,113,113	1.34	7 (8%)
32	CLA	F	309	-	59,63,73	1.88	9 (15%)	71,101,113	1.47	6 (8%)
32	CLA	H	307	-	64,68,73	1.85	9 (14%)	77,107,113	1.49	8 (10%)
32	CLA	E	314	-	54,58,73	2.01	9 (16%)	65,95,113	1.59	8 (12%)
32	CLA	r	202	-	49,53,73	2.09	9 (18%)	59,89,113	1.63	6 (10%)
35	LHG	I	318	32	36,36,48	1.05	2 (5%)	39,42,54	1.29	4 (10%)
32	CLA	L	307	-	61,65,73	1.87	9 (14%)	73,103,113	1.50	8 (10%)
33	KC2	M	307	-	49,53,53	1.91	4 (8%)	62,89,89	1.31	8 (12%)
33	KC2	K	309	11	49,53,53	1.89	4 (8%)	62,89,89	1.36	10 (16%)
32	CLA	D	311	4	69,73,73	1.74	9 (13%)	83,113,113	1.38	8 (9%)
32	CLA	B	309	-	59,63,73	1.88	9 (15%)	71,101,113	1.41	6 (8%)
33	KC2	P	301	-	49,53,53	1.89	4 (8%)	62,89,89	1.33	9 (14%)
32	CLA	a	810	-	66,70,73	1.76	9 (13%)	79,109,113	1.43	8 (10%)
43	PQN	b	847	-	34,34,34	0.42	0	42,45,45	0.67	1 (2%)
41	BCR	k	204	-	41,41,41	0.14	0	56,56,56	0.38	0
36	LMG	l	201	33	49,49,55	0.89	2 (4%)	57,57,63	1.48	12 (21%)
32	CLA	G	306	7	60,64,73	1.91	9 (15%)	72,102,113	1.64	10 (13%)
32	CLA	b	835	-	64,68,73	1.79	9 (14%)	77,107,113	1.50	9 (11%)
32	CLA	D	309	4	49,53,73	2.10	9 (18%)	59,89,113	1.65	7 (11%)
32	CLA	H	309	-	49,53,73	2.16	9 (18%)	59,89,113	1.66	8 (13%)
37	A86	D	322	-	44,50,50	0.47	1 (2%)	51,76,76	0.92	2 (3%)
32	CLA	a	836	20	59,63,73	1.90	9 (15%)	71,101,113	1.47	7 (9%)
32	CLA	E	312	-	64,68,73	1.82	9 (14%)	77,107,113	1.43	7 (9%)
32	CLA	U	305	18	49,53,73	2.15	9 (18%)	59,89,113	1.76	10 (16%)
34	DD6	E	317	-	39,45,45	0.20	0	52,67,67	0.94	3 (5%)
32	CLA	L	309	-	49,53,73	2.13	9 (18%)	59,89,113	1.65	7 (11%)
36	LMG	W	320	33,37	39,39,55	1.05	2 (5%)	47,47,63	1.13	3 (6%)
32	CLA	U	302	18	49,53,73	2.12	9 (18%)	59,89,113	1.63	9 (15%)
32	CLA	C	305	-	64,68,73	1.92	9 (14%)	77,107,113	1.57	9 (11%)
33	KC2	W	305	13	49,53,53	1.85	4 (8%)	62,89,89	1.36	7 (11%)
32	CLA	a	833	-	69,73,73	1.72	9 (13%)	83,113,113	1.40	7 (8%)
32	CLA	R	309	15	45,49,73	2.29	10 (22%)	54,84,113	1.83	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	R	307	15	49,53,73	2.08	9 (18%)	59,89,113	1.63	7 (11%)
34	DD6	G	312	-	39,45,45	0.24	0	52,67,67	0.86	4 (7%)
41	BCR	l	205	-	41,41,41	0.11	0	56,56,56	0.33	0
33	KC2	I	309	9,36	49,53,53	1.87	4 (8%)	62,89,89	1.37	8 (12%)
32	CLA	F	311	-	49,53,73	2.10	9 (18%)	59,89,113	1.69	7 (11%)
34	DD6	D	317	-	39,45,45	0.17	0	52,67,67	1.01	3 (5%)
35	LHG	F	321	-	39,39,48	0.69	2 (5%)	42,45,54	1.16	2 (4%)
34	DD6	M	316	-	39,45,45	0.18	0	52,67,67	0.79	1 (1%)
34	DD6	R	314	-	39,45,45	0.18	0	52,67,67	0.83	1 (1%)
35	LHG	a	851	-	37,37,48	1.01	2 (5%)	40,43,54	1.27	5 (12%)
32	CLA	M	305	-	54,58,73	1.96	9 (16%)	65,95,113	1.54	11 (16%)
32	CLA	Q	305	16	55,59,73	1.94	9 (16%)	66,96,113	1.54	6 (9%)
33	KC2	T	311	15	49,53,53	1.88	4 (8%)	62,89,89	1.38	10 (16%)
32	CLA	Q	303	16	64,68,73	1.88	10 (15%)	77,107,113	1.65	9 (11%)
34	DD6	I	313	-	39,45,45	0.19	0	52,67,67	0.79	2 (3%)
32	CLA	a	815	20	54,58,73	1.93	9 (16%)	65,95,113	1.53	7 (10%)
32	CLA	T	310	-	59,63,73	1.91	9 (15%)	71,101,113	1.56	8 (11%)
32	CLA	b	837	21	69,73,73	1.77	9 (13%)	83,113,113	1.52	7 (8%)
32	CLA	J	312	-	62,66,73	1.88	9 (14%)	74,104,113	1.45	8 (10%)
32	CLA	K	301	-	49,53,73	2.11	9 (18%)	59,89,113	1.62	7 (11%)
36	LMG	A	318	-	40,40,55	0.95	2 (5%)	48,48,63	1.28	6 (12%)
32	CLA	H	306	8	54,58,73	2.01	9 (16%)	65,95,113	1.57	6 (9%)
33	KC2	N	302	14	49,53,53	1.89	4 (8%)	62,89,89	1.33	8 (12%)
37	A86	W	316	36	44,50,50	0.62	1 (2%)	51,76,76	0.69	1 (1%)
32	CLA	L	311	-	43,48,73	2.30	9 (20%)	52,82,113	1.97	10 (19%)
32	CLA	a	841	20	69,73,73	1.72	9 (13%)	83,113,113	1.38	7 (8%)
32	CLA	S	309	-	64,68,73	1.79	9 (14%)	77,107,113	1.47	9 (11%)
35	LHG	E	321	-	45,45,48	0.92	2 (4%)	48,51,54	1.15	3 (6%)
34	DD6	Q	314	-	39,45,45	0.17	0	52,67,67	0.67	2 (3%)
32	CLA	a	832	-	64,68,73	1.80	9 (14%)	77,107,113	1.48	5 (6%)
32	CLA	S	311	-	54,58,73	2.02	9 (16%)	65,95,113	1.65	8 (12%)
32	CLA	T	308	15	64,68,73	1.84	9 (14%)	77,107,113	1.57	14 (18%)
34	DD6	K	315	-	39,45,45	0.18	0	52,67,67	1.18	3 (5%)
35	LHG	F	318	-	40,40,48	0.71	1 (2%)	43,46,54	1.11	2 (4%)
33	KC2	A	310	1	49,53,53	1.90	4 (8%)	62,89,89	1.34	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	LMG	D	321	-	40,40,55	0.82	0	48,48,63	1.29	6 (12%)
33	KC2	J	310	10	49,53,53	1.90	4 (8%)	62,89,89	1.33	8 (12%)
34	DD6	H	312	-	39,45,45	0.20	0	52,67,67	0.90	3 (5%)
32	CLA	Q	301	33	64,68,73	1.86	9 (14%)	77,107,113	1.48	7 (9%)
32	CLA	b	818	-	69,73,73	1.77	9 (13%)	83,113,113	1.42	8 (9%)
32	CLA	l	203	35	69,73,73	1.79	9 (13%)	83,113,113	1.32	7 (8%)
32	CLA	O	305	15	69,73,73	1.70	9 (13%)	83,113,113	1.40	8 (9%)
35	LHG	a	850	32	29,29,48	0.84	0	32,35,54	1.23	3 (9%)
32	CLA	M	308	13	61,65,73	1.89	9 (14%)	73,103,113	1.55	11 (15%)
32	CLA	I	305	9	60,64,73	1.91	9 (15%)	72,102,113	1.58	8 (11%)
32	CLA	R	304	-	49,53,73	2.10	9 (18%)	59,89,113	1.66	8 (13%)
32	CLA	B	301	-	43,48,73	2.25	9 (20%)	52,82,113	1.86	9 (17%)
32	CLA	G	301	-	49,53,73	2.15	9 (18%)	59,89,113	1.64	7 (11%)
32	CLA	a	817	20	65,69,73	1.78	9 (13%)	78,108,113	1.44	8 (10%)
32	CLA	b	828	21	65,69,73	1.82	9 (13%)	78,108,113	1.50	8 (10%)
35	LHG	D	320	-	47,47,48	0.64	0	50,53,54	1.17	3 (6%)
32	CLA	B	303	-	49,53,73	2.10	9 (18%)	59,89,113	1.57	5 (8%)
37	A86	K	312	-	44,50,50	0.50	1 (2%)	51,76,76	0.74	1 (1%)
41	BCR	a	844	-	41,41,41	0.16	0	56,56,56	0.40	0
32	CLA	H	310	-	50,54,73	2.12	9 (18%)	60,90,113	1.59	7 (11%)
34	DD6	N	321	-	39,45,45	0.16	0	52,67,67	0.89	1 (1%)
33	KC2	L	302	12	49,53,53	1.91	4 (8%)	62,89,89	1.33	9 (14%)
32	CLA	a	820	-	69,73,73	1.75	9 (13%)	83,113,113	1.48	9 (10%)
37	A86	M	315	-	44,50,50	0.36	0	51,76,76	1.19	3 (5%)
32	CLA	D	306	4	64,68,73	1.78	9 (14%)	77,107,113	1.48	10 (12%)
33	KC2	R	311	15	49,53,53	1.88	4 (8%)	62,89,89	1.33	9 (14%)
32	CLA	b	821	21	59,63,73	1.87	9 (15%)	71,101,113	1.55	7 (9%)
32	CLA	K	304	11	49,53,73	2.11	9 (18%)	59,89,113	1.67	7 (11%)
37	A86	N	315	-	44,50,50	0.54	1 (2%)	51,76,76	0.79	1 (1%)
32	CLA	a	852	-	69,73,73	1.75	9 (13%)	83,113,113	1.31	9 (10%)
32	CLA	R	310	-	59,63,73	1.89	9 (15%)	71,101,113	1.48	6 (8%)
33	KC2	T	304	15	49,53,53	1.87	4 (8%)	62,89,89	1.35	8 (12%)
37	A86	M	314	-	44,50,50	0.60	1 (2%)	51,76,76	0.82	2 (3%)
32	CLA	a	822	-	66,70,73	1.76	9 (13%)	79,109,113	1.43	10 (12%)
37	A86	N	317	-	44,50,50	0.61	1 (2%)	51,76,76	0.84	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DD6	P	315	-	39,45,45	0.25	0	52,67,67	0.89	4 (7%)
32	CLA	I	303	9	59,63,73	1.93	9 (15%)	71,101,113	1.64	9 (12%)
37	A86	R	313	-	44,50,50	0.56	1 (2%)	51,76,76	1.01	2 (3%)
32	CLA	l	202	-	49,53,73	2.07	9 (18%)	59,89,113	1.65	7 (11%)
32	CLA	F	322	-	64,68,73	1.86	9 (14%)	77,107,113	1.52	9 (11%)
32	CLA	b	806	-	69,73,73	1.77	9 (13%)	83,113,113	1.40	7 (8%)
37	A86	N	316	-	44,50,50	0.56	1 (2%)	51,76,76	1.37	3 (5%)
32	CLA	H	301	8	49,53,73	2.15	9 (18%)	59,89,113	1.75	9 (15%)
35	LHG	E	301	-	45,45,48	0.65	1 (2%)	48,51,54	1.10	2 (4%)
32	CLA	a	823	-	69,73,73	1.73	9 (13%)	83,113,113	1.41	8 (9%)
34	DD6	Q	313	-	39,45,45	0.21	0	52,67,67	0.64	1 (1%)
37	A86	r	204	-	44,50,50	0.44	1 (2%)	51,76,76	1.00	2 (3%)
35	LHG	a	849	-	47,47,48	0.63	1 (2%)	50,53,54	1.16	3 (6%)
36	LMG	L	320	-	37,37,55	0.82	1 (2%)	45,45,63	1.24	5 (11%)
32	CLA	f	201	-	64,68,73	1.79	9 (14%)	77,107,113	1.36	7 (9%)
38	LMU	D	324	-	36,36,36	0.38	0	47,47,47	0.85	0
32	CLA	U	307	-	49,53,73	2.15	9 (18%)	59,89,113	1.70	8 (13%)
32	CLA	W	313	-	64,68,73	1.86	9 (14%)	77,107,113	1.51	8 (10%)
34	DD6	E	318	-	39,45,45	0.17	0	52,67,67	0.73	3 (5%)
36	LMG	S	322	33	33,33,55	1.10	2 (6%)	41,41,63	1.27	3 (7%)
35	LHG	B	308	-	30,30,48	1.11	2 (6%)	33,36,54	1.20	4 (12%)
32	CLA	R	301	-	49,53,73	2.15	9 (18%)	59,89,113	1.74	8 (13%)
33	KC2	N	307	14	49,53,53	1.89	4 (8%)	62,89,89	1.34	7 (11%)
32	CLA	J	308	-	49,53,73	2.15	9 (18%)	59,89,113	1.73	8 (13%)
37	A86	H	314	-	44,50,50	0.38	0	51,76,76	1.15	3 (5%)
33	KC2	K	303	11	49,53,53	1.90	4 (8%)	62,89,89	1.34	9 (14%)
32	CLA	U	306	-	49,53,73	2.13	9 (18%)	59,89,113	1.63	7 (11%)
36	LMG	A	317	-	36,36,55	1.07	2 (5%)	44,44,63	1.32	4 (9%)
32	CLA	l	204	29	69,73,73	1.79	9 (13%)	83,113,113	1.48	11 (13%)
32	CLA	b	832	-	69,73,73	1.77	9 (13%)	83,113,113	1.43	6 (7%)
33	KC2	R	302	15	49,53,53	1.91	4 (8%)	62,89,89	1.37	9 (14%)
32	CLA	E	308	5	69,73,73	1.73	9 (13%)	83,113,113	1.35	7 (8%)
33	KC2	M	313	13,36	49,53,53	1.88	4 (8%)	62,89,89	1.34	9 (14%)
37	A86	S	314	-	44,50,50	0.30	0	51,76,76	1.65	6 (11%)
32	CLA	Q	308	-	49,53,73	2.12	9 (18%)	59,89,113	1.65	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	b	810	21	64,68,73	1.77	9 (14%)	77,107,113	1.34	6 (7%)
32	CLA	a	812	20	59,63,73	1.88	9 (15%)	71,101,113	1.67	10 (14%)
32	CLA	b	802	-	69,73,73	1.70	9 (13%)	83,113,113	1.47	8 (9%)
32	CLA	K	308	11	69,73,73	1.78	9 (13%)	83,113,113	1.41	7 (8%)
32	CLA	a	819	20	69,73,73	1.72	9 (13%)	83,113,113	1.37	7 (8%)
32	CLA	C	306	3	69,73,73	1.81	9 (13%)	83,113,113	1.48	8 (9%)
37	A86	L	316	-	44,50,50	0.44	1 (2%)	51,76,76	1.50	2 (3%)
32	CLA	A	302	35	64,68,73	1.81	9 (14%)	77,107,113	1.37	5 (6%)
35	LHG	M	319	-	45,45,48	0.64	0	48,51,54	1.18	4 (8%)
34	DD6	A	315	-	39,45,45	0.19	0	52,67,67	0.90	3 (5%)
32	CLA	K	307	11	45,49,73	2.26	10 (22%)	54,84,113	1.67	9 (16%)
32	CLA	a	814	20	69,73,73	1.70	9 (13%)	83,113,113	1.53	11 (13%)
32	CLA	D	315	-	49,53,73	2.05	9 (18%)	59,89,113	1.70	7 (11%)
32	CLA	G	308	-	58,62,73	1.94	9 (15%)	69,99,113	1.53	7 (10%)
34	DD6	J	315	-	39,45,45	0.18	0	52,67,67	0.88	2 (3%)
35	LHG	A	316	-	39,39,48	0.70	1 (2%)	42,45,54	1.16	2 (4%)
33	KC2	C	303	-	49,53,53	1.91	4 (8%)	62,89,89	1.32	7 (11%)
35	LHG	W	319	32	45,45,48	0.72	1 (2%)	48,51,54	1.16	4 (8%)
32	CLA	P	308	13	49,53,73	2.08	9 (18%)	59,89,113	1.58	7 (11%)
32	CLA	W	312	13	64,68,73	1.82	9 (14%)	77,107,113	1.42	7 (9%)
32	CLA	O	308	-	49,53,73	2.13	9 (18%)	59,89,113	1.68	8 (13%)
33	KC2	N	303	14	49,53,53	1.88	4 (8%)	62,89,89	1.38	9 (14%)
32	CLA	I	308	-	59,63,73	1.93	9 (15%)	71,101,113	1.58	7 (9%)
33	KC2	N	304	14	49,53,53	1.84	4 (8%)	62,89,89	1.37	9 (14%)
32	CLA	A	305	1	65,69,73	1.82	9 (13%)	78,108,113	1.46	7 (8%)
32	CLA	F	306	6	59,63,73	1.91	9 (15%)	71,101,113	1.50	8 (11%)
32	CLA	a	838	-	69,73,73	1.72	9 (13%)	83,113,113	1.46	9 (10%)
32	CLA	b	817	21	59,63,73	1.87	9 (15%)	71,101,113	1.50	7 (9%)
37	A86	O	312	-	44,50,50	0.47	1 (2%)	51,76,76	0.92	3 (5%)
32	CLA	B	306	-	49,53,73	2.11	9 (18%)	59,89,113	1.65	7 (11%)
32	CLA	b	804	21	69,73,73	1.75	9 (13%)	83,113,113	1.50	10 (12%)
33	KC2	P	306	-	49,53,53	1.90	4 (8%)	62,89,89	1.31	8 (12%)
37	A86	J	313	-	44,50,50	0.47	1 (2%)	51,76,76	1.82	5 (9%)
32	CLA	D	312	4	59,63,73	1.92	9 (15%)	71,101,113	1.52	9 (12%)
32	CLA	a	840	-	69,73,73	1.74	9 (13%)	83,113,113	1.44	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	b	814	-	49,53,73	2.05	9 (18%)	59,89,113	1.60	7 (11%)
32	CLA	E	306	5	64,68,73	1.86	9 (14%)	77,107,113	1.47	7 (9%)
32	CLA	T	305	-	49,53,73	2.14	9 (18%)	59,89,113	1.68	9 (15%)
41	BCR	f	202	-	41,41,41	0.11	0	56,56,56	0.38	0
32	CLA	C	302	-	45,49,73	2.27	10 (22%)	54,84,113	1.79	7 (12%)
32	CLA	k	202	-	59,63,73	1.90	9 (15%)	71,101,113	1.46	5 (7%)
36	LMG	M	320	33	40,40,55	1.08	2 (5%)	48,48,63	1.09	3 (6%)
33	KC2	H	303	-	49,53,53	1.91	4 (8%)	62,89,89	1.33	7 (11%)
32	CLA	I	317	35	69,73,73	1.73	9 (13%)	83,113,113	1.40	6 (7%)
32	CLA	K	310	-	49,53,73	2.14	9 (18%)	59,89,113	1.73	8 (13%)
32	CLA	G	307	-	43,48,73	2.26	9 (20%)	52,82,113	1.93	9 (17%)
42	SF4	c	102	-	0,12,12	-	-	-		
36	LMG	E	302	-	40,40,55	1.11	4 (10%)	48,48,63	1.55	8 (16%)
32	CLA	N	311	14	64,68,73	1.80	9 (14%)	77,107,113	1.40	8 (10%)
33	KC2	L	303	-	49,53,53	1.87	4 (8%)	62,89,89	1.36	9 (14%)
32	CLA	I	306	9	69,73,73	1.75	9 (13%)	83,113,113	1.43	6 (7%)
32	CLA	D	314	4	56,60,73	1.84	9 (16%)	67,97,113	1.51	10 (14%)
32	CLA	a	825	20	69,73,73	1.71	9 (13%)	83,113,113	1.30	7 (8%)
37	A86	M	317	-	44,50,50	0.73	1 (2%)	51,76,76	0.55	1 (1%)
32	CLA	C	304	3	47,51,73	2.21	9 (19%)	56,86,113	1.85	10 (17%)
33	KC2	S	303	17	49,53,53	1.86	4 (8%)	62,89,89	1.36	9 (14%)
41	BCR	a	845	-	41,41,41	0.15	0	56,56,56	0.37	0
43	PQN	a	848	-	34,34,34	0.39	0	42,45,45	0.99	1 (2%)
32	CLA	D	305	-	62,66,73	1.84	9 (14%)	74,104,113	1.49	7 (9%)
32	CLA	A	308	-	59,63,73	1.87	9 (15%)	71,101,113	1.45	6 (8%)
32	CLA	W	310	13	64,68,73	1.81	9 (14%)	77,107,113	1.43	8 (10%)
32	CLA	f	203	25	49,53,73	2.08	9 (18%)	59,89,113	1.64	5 (8%)
37	A86	U	308	-	44,50,50	0.65	1 (2%)	51,76,76	1.16	3 (5%)
32	CLA	E	315	-	50,54,73	2.07	9 (18%)	60,90,113	1.62	8 (13%)
37	A86	P	319	-	44,50,50	0.49	1 (2%)	51,76,76	0.80	2 (3%)
32	CLA	I	307	-	49,53,73	2.10	9 (18%)	59,89,113	1.71	8 (13%)
32	CLA	V	201	-	62,66,73	1.86	9 (14%)	74,104,113	1.45	7 (9%)
41	BCR	b	844	-	41,41,41	0.14	0	56,56,56	0.49	0
33	KC2	P	312	13	49,53,53	1.90	4 (8%)	62,89,89	1.35	9 (14%)
32	CLA	P	309	-	65,69,73	1.81	10 (15%)	78,108,113	1.44	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	b	836	-	69,73,73	1.74	9 (13%)	83,113,113	1.45	7 (8%)
37	A86	K	311	-	44,50,50	0.60	1 (2%)	51,76,76	0.83	2 (3%)
41	BCR	r	203	-	41,41,41	0.14	0	56,56,56	0.42	0
42	SF4	a	847	-	0,12,12	-	-	-		
32	CLA	Q	307	16	66,70,73	1.78	9 (13%)	79,109,113	1.39	7 (8%)
34	DD6	I	310	-	39,45,45	0.15	0	52,67,67	0.88	3 (5%)
34	DD6	S	321	-	39,45,45	0.46	0	52,67,67	1.56	5 (9%)
32	CLA	T	309	-	49,53,73	2.12	9 (18%)	59,89,113	1.63	7 (11%)
32	CLA	F	304	-	59,63,73	1.91	9 (15%)	71,101,113	1.55	9 (12%)
32	CLA	b	833	-	66,70,73	1.78	9 (13%)	79,109,113	1.51	7 (8%)
32	CLA	a	809	-	64,68,73	1.80	9 (14%)	77,107,113	1.49	7 (9%)
32	CLA	U	301	18	43,48,73	2.25	9 (20%)	52,82,113	1.81	9 (17%)
32	CLA	r	201	-	64,68,73	1.89	9 (14%)	77,107,113	1.54	9 (11%)
37	A86	D	323	-	44,50,50	0.38	0	51,76,76	0.90	3 (5%)
32	CLA	a	828	-	62,66,73	1.81	9 (14%)	74,104,113	1.53	9 (12%)
32	CLA	a	802	-	67,71,73	1.75	9 (13%)	80,110,113	1.47	11 (13%)
34	DD6	D	316	-	39,45,45	0.20	0	52,67,67	0.93	3 (5%)
37	A86	O	311	-	44,50,50	0.33	0	51,76,76	0.96	2 (3%)
32	CLA	F	301	-	43,48,73	2.25	9 (20%)	52,82,113	1.86	9 (17%)
33	KC2	K	302	11	49,53,53	1.87	4 (8%)	62,89,89	1.36	7 (11%)
35	LHG	P	317	-	45,45,48	0.63	0	48,51,54	1.16	4 (8%)
32	CLA	U	303	18	49,53,73	2.10	9 (18%)	59,89,113	1.73	9 (15%)
32	CLA	G	304	-	59,63,73	1.89	9 (15%)	71,101,113	1.49	8 (11%)
37	A86	S	318	-	44,50,50	0.45	1 (2%)	51,76,76	0.92	3 (5%)
37	A86	W	315	-	44,50,50	0.57	1 (2%)	51,76,76	1.11	2 (3%)
33	KC2	Q	317	32	49,53,53	1.85	4 (8%)	62,89,89	1.42	8 (12%)
41	BCR	b	841	-	41,41,41	0.13	0	56,56,56	0.41	0
32	CLA	O	307	15	64,68,73	1.83	9 (14%)	77,107,113	1.47	8 (10%)
32	CLA	b	812	21	69,73,73	1.72	9 (13%)	83,113,113	1.40	7 (8%)
34	DD6	N	319	-	39,45,45	0.16	0	52,67,67	0.98	3 (5%)
32	CLA	D	313	-	62,66,73	1.84	9 (14%)	74,104,113	1.47	7 (9%)
38	LMU	J	318	-	36,36,36	0.69	0	47,47,47	1.01	1 (2%)
36	LMG	D	303	-	36,36,55	1.03	2 (5%)	44,44,63	1.48	7 (15%)
41	BCR	i	101	-	41,41,41	0.20	0	56,56,56	0.53	0
37	A86	C	311	-	44,50,50	0.67	1 (2%)	51,76,76	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	A	307	1	64,68,73	1.84	9 (14%)	77,107,113	1.49	8 (10%)
34	DD6	J	316	-	39,45,45	0.19	0	52,67,67	0.73	3 (5%)
36	LMG	j	104	-	38,38,55	1.09	3 (7%)	46,46,63	1.48	6 (13%)
36	LMG	T	301	-	37,37,55	0.93	1 (2%)	45,45,63	1.27	6 (13%)
41	BCR	a	854	-	41,41,41	0.17	0	56,56,56	0.44	0
32	CLA	a	818	20	64,68,73	1.83	9 (14%)	77,107,113	1.66	11 (14%)
32	CLA	L	312	-	64,68,73	1.81	9 (14%)	77,107,113	1.40	7 (9%)
33	KC2	L	305	12	49,53,53	1.89	4 (8%)	62,89,89	1.37	8 (12%)
32	CLA	a	803	20	67,71,73	1.75	9 (13%)	80,110,113	1.48	8 (10%)
33	KC2	W	304	13	49,53,53	1.87	4 (8%)	62,89,89	1.35	9 (14%)
36	LMG	N	301	-	40,40,55	1.07	2 (5%)	48,48,63	1.16	4 (8%)
32	CLA	H	305	8	49,53,73	2.09	9 (18%)	59,89,113	1.75	8 (13%)
34	DD6	A	314	-	39,45,45	0.19	0	52,67,67	0.70	1 (1%)
32	CLA	a	830	20	69,73,73	1.78	9 (13%)	83,113,113	1.43	9 (10%)
32	CLA	Q	306	16	66,70,73	1.80	9 (13%)	79,109,113	1.49	9 (11%)
32	CLA	I	301	-	69,73,73	1.74	9 (13%)	83,113,113	1.38	5 (6%)
37	A86	P	314	-	44,50,50	0.43	1 (2%)	51,76,76	1.19	3 (5%)
32	CLA	f	204	-	51,55,73	2.06	9 (17%)	61,91,113	1.60	8 (13%)
34	DD6	A	313	-	39,45,45	0.15	0	52,67,67	0.80	2 (3%)
32	CLA	E	305	5	59,63,73	1.89	9 (15%)	71,101,113	1.48	7 (9%)
33	KC2	M	321	15	49,53,53	1.87	4 (8%)	62,89,89	1.39	7 (11%)
37	A86	M	318	-	44,50,50	0.42	1 (2%)	51,76,76	0.85	4 (7%)
33	KC2	G	309	7	49,53,53	1.88	4 (8%)	62,89,89	1.39	8 (12%)
33	KC2	L	306	12	49,53,53	1.89	4 (8%)	62,89,89	1.35	9 (14%)
41	BCR	j	102	-	41,41,41	0.16	0	56,56,56	0.48	0
32	CLA	b	838	-	69,73,73	1.82	9 (13%)	83,113,113	1.52	8 (9%)
37	A86	S	320	-	44,50,50	0.47	1 (2%)	51,76,76	0.58	0
32	CLA	M	309	13	49,53,73	2.06	9 (18%)	59,89,113	1.63	6 (10%)
32	CLA	H	304	-	49,53,73	2.15	9 (18%)	59,89,113	1.80	9 (15%)
32	CLA	b	819	-	69,73,73	1.71	9 (13%)	83,113,113	1.32	8 (9%)
34	DD6	T	314	-	39,45,45	0.19	0	52,67,67	0.85	3 (5%)
32	CLA	a	835	20	69,73,73	1.72	9 (13%)	83,113,113	1.37	6 (7%)
36	LMG	D	325	-	35,35,55	1.06	2 (5%)	43,43,63	1.48	7 (16%)
41	BCR	b	842	-	41,41,41	0.23	0	56,56,56	0.57	1 (1%)
32	CLA	a	831	20	64,68,73	1.82	9 (14%)	77,107,113	1.45	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	KC2	M	304	13	49,53,53	1.91	4 (8%)	62,89,89	1.33	6 (9%)
32	CLA	j	101	27	49,53,73	2.09	9 (18%)	59,89,113	1.59	6 (10%)
33	KC2	U	304	18	49,53,53	1.87	4 (8%)	62,89,89	1.36	7 (11%)
33	KC2	F	302	6	49,53,53	1.90	4 (8%)	62,89,89	1.35	9 (14%)
32	CLA	b	816	-	66,70,73	1.77	9 (13%)	79,109,113	1.37	7 (8%)
32	CLA	V	203	19	59,63,73	1.88	9 (15%)	71,101,113	1.47	6 (8%)
32	CLA	C	307	3	64,68,73	1.83	9 (14%)	77,107,113	1.54	10 (12%)
40	DGD	b	846	-	57,57,67	0.88	2 (3%)	71,71,81	1.31	6 (8%)
32	CLA	A	309	1	69,73,73	1.74	9 (13%)	83,113,113	1.39	7 (8%)
32	CLA	A	306	1	69,73,73	1.74	9 (13%)	83,113,113	1.34	6 (7%)
32	CLA	E	303	5	49,53,73	2.05	9 (18%)	59,89,113	1.61	6 (10%)
32	CLA	J	306	10	59,63,73	1.85	9 (15%)	71,101,113	1.53	8 (11%)
37	A86	F	317	-	44,50,50	0.52	1 (2%)	51,76,76	0.63	2 (3%)
33	KC2	G	302	-	49,53,53	1.88	4 (8%)	62,89,89	1.33	7 (11%)
32	CLA	D	308	4	59,63,73	1.92	9 (15%)	71,101,113	1.59	8 (11%)
33	KC2	Q	302	-	49,53,53	1.87	4 (8%)	62,89,89	1.32	8 (12%)
32	CLA	F	308	6	50,54,73	2.12	9 (18%)	60,90,113	1.61	7 (11%)
34	DD6	B	307	-	39,45,45	0.19	0	52,67,67	0.78	3 (5%)
32	CLA	W	307	13	49,53,73	2.10	9 (18%)	59,89,113	1.61	7 (11%)
33	KC2	F	310	6,36	49,53,53	1.86	4 (8%)	62,89,89	1.35	9 (14%)
34	DD6	F	316	-	39,45,45	0.21	0	52,67,67	1.38	3 (5%)
32	CLA	F	307	6	64,68,73	1.81	9 (14%)	77,107,113	1.45	8 (10%)
32	CLA	G	303	7	59,63,73	1.89	9 (15%)	71,101,113	1.63	11 (15%)
37	A86	L	318	-	44,50,50	0.67	1 (2%)	51,76,76	1.09	2 (3%)
32	CLA	Q	304	-	54,58,73	1.97	9 (16%)	65,95,113	1.59	9 (13%)
32	CLA	N	313	-	64,68,73	1.83	9 (14%)	77,107,113	1.48	8 (10%)
32	CLA	T	306	15	64,68,73	1.80	9 (14%)	77,107,113	1.37	6 (7%)
37	A86	L	317	-	44,50,50	0.51	1 (2%)	51,76,76	1.20	3 (5%)
34	DD6	D	318	-	39,45,45	0.19	0	52,67,67	0.61	0
32	CLA	a	806	-	64,68,73	1.80	9 (14%)	77,107,113	1.43	8 (10%)
32	CLA	b	803	21	69,73,73	1.71	9 (13%)	83,113,113	1.33	6 (7%)
32	CLA	W	309	13	69,73,73	1.74	9 (13%)	83,113,113	1.38	7 (8%)
32	CLA	J	302	-	49,53,73	2.09	9 (18%)	59,89,113	1.63	7 (11%)
32	CLA	b	827	21	54,58,73	1.99	9 (16%)	65,95,113	1.53	7 (10%)
37	A86	R	312	-	44,50,50	0.56	1 (2%)	51,76,76	0.77	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	b	815	21	69,73,73	1.69	9 (13%)	83,113,113	1.41	8 (9%)
39	SQD	k	206	-	35,36,54	1.46	5 (14%)	44,47,65	1.49	7 (15%)
37	A86	S	316	-	44,50,50	0.62	1 (2%)	51,76,76	1.21	3 (5%)
33	KC2	N	308	14	49,53,53	1.87	4 (8%)	62,89,89	1.33	8 (12%)
32	CLA	E	307	5	59,63,73	1.85	9 (15%)	71,101,113	1.48	6 (8%)
34	DD6	L	319	-	39,45,45	0.20	0	52,67,67	1.23	3 (5%)
32	CLA	L	308	12	49,53,73	2.10	9 (18%)	59,89,113	1.63	7 (11%)
32	CLA	b	824	21	62,66,73	1.82	9 (14%)	74,104,113	1.43	6 (8%)
33	KC2	W	308	-	49,53,53	1.85	4 (8%)	62,89,89	1.36	9 (14%)
32	CLA	D	307	4	65,69,73	1.81	9 (13%)	78,108,113	1.57	10 (12%)
32	CLA	O	304	-	49,53,73	2.14	9 (18%)	59,89,113	1.74	9 (15%)
32	CLA	b	811	21	54,58,73	1.95	9 (16%)	65,95,113	1.58	8 (12%)
34	DD6	F	314	-	39,45,45	0.23	0	52,67,67	0.86	3 (5%)
33	KC2	R	305	15	49,53,53	1.90	4 (8%)	62,89,89	1.36	6 (9%)
32	CLA	a	834	20	69,73,73	1.73	9 (13%)	83,113,113	1.37	6 (7%)
32	CLA	b	831	-	64,68,73	1.77	9 (14%)	77,107,113	1.37	7 (9%)
41	BCR	b	845	-	41,41,41	0.16	0	56,56,56	0.29	0
32	CLA	a	807	-	69,73,73	1.78	9 (13%)	83,113,113	1.50	9 (10%)
33	KC2	P	302	13	49,53,53	1.91	4 (8%)	62,89,89	1.37	9 (14%)
32	CLA	a	808	20	54,58,73	2.01	9 (16%)	65,95,113	1.59	8 (12%)
32	CLA	P	310	-	45,49,73	2.29	10 (22%)	54,84,113	1.80	7 (12%)
32	CLA	W	311	13	69,73,73	1.73	9 (13%)	83,113,113	1.35	7 (8%)
34	DD6	I	311	-	39,45,45	0.17	0	52,67,67	0.70	1 (1%)
37	A86	G	310	-	44,50,50	0.38	0	51,76,76	1.25	2 (3%)
32	CLA	A	301	1	49,53,73	2.05	9 (18%)	59,89,113	1.59	8 (13%)
32	CLA	a	853	-	69,73,73	1.73	9 (13%)	83,113,113	1.43	10 (12%)
32	CLA	V	204	-	54,58,73	1.98	9 (16%)	65,95,113	1.54	6 (9%)
33	KC2	O	303	15	49,53,53	1.86	4 (8%)	62,89,89	1.31	8 (12%)
41	BCR	b	843	-	41,41,41	0.12	0	56,56,56	0.55	0
32	CLA	E	309	5	62,66,73	1.81	9 (14%)	74,104,113	1.51	8 (10%)
32	CLA	A	303	1	66,70,73	1.77	9 (13%)	79,109,113	1.43	7 (8%)
34	DD6	E	316	-	39,45,45	0.19	0	52,67,67	0.95	3 (5%)
32	CLA	b	826	-	53,57,73	2.05	9 (16%)	62,93,113	1.68	9 (14%)
37	A86	M	322	-	44,50,50	0.43	1 (2%)	51,76,76	0.65	1 (1%)
32	CLA	a	837	20	59,63,73	1.93	9 (15%)	71,101,113	1.59	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	DGD	Q	318	-	57,57,67	0.92	2 (3%)	71,71,81	1.15	6 (8%)
32	CLA	P	304	-	49,53,73	2.13	9 (18%)	59,89,113	1.68	10 (16%)
32	CLA	a	813	20	49,53,73	2.13	9 (18%)	59,89,113	1.76	8 (13%)
34	DD6	Q	315	-	39,45,45	0.18	0	52,67,67	0.74	2 (3%)
32	CLA	a	839	20	59,63,73	1.88	9 (15%)	71,101,113	1.55	8 (11%)
32	CLA	b	822	21	69,73,73	1.69	9 (13%)	83,113,113	1.41	9 (10%)
32	CLA	M	311	13	49,53,73	2.13	9 (18%)	59,89,113	1.74	8 (13%)
32	CLA	S	305	17	67,71,73	1.78	9 (13%)	80,110,113	1.38	6 (7%)
32	CLA	T	302	15	49,53,73	2.15	9 (18%)	59,89,113	1.66	8 (13%)
35	LHG	I	314	-	45,45,48	0.64	0	48,51,54	1.18	2 (4%)
37	A86	S	319	-	44,50,50	0.37	0	51,76,76	0.94	2 (3%)
32	CLA	b	825	21	64,68,73	1.78	10 (15%)	77,107,113	1.44	6 (7%)
34	DD6	N	318	-	39,45,45	0.18	0	52,67,67	0.88	2 (3%)
37	A86	S	315	-	44,50,50	0.55	1 (2%)	51,76,76	1.37	3 (5%)
33	KC2	S	312	17,36	49,53,53	1.74	4 (8%)	62,89,89	1.34	7 (11%)
32	CLA	b	830	21	65,69,73	1.82	9 (13%)	78,108,113	1.64	11 (14%)
37	A86	N	320	-	44,50,50	0.62	1 (2%)	51,76,76	0.55	1 (1%)
37	A86	W	302	-	44,50,50	0.45	1 (2%)	51,76,76	0.68	1 (1%)
33	KC2	P	303	13	49,53,53	1.90	4 (8%)	62,89,89	1.31	6 (9%)
35	LHG	f	205	-	46,46,48	0.59	0	49,52,54	1.10	2 (4%)
32	CLA	R	306	15	49,53,73	2.09	9 (18%)	59,89,113	1.70	7 (11%)
32	CLA	O	309	-	66,70,73	1.79	9 (13%)	79,109,113	1.45	8 (10%)
32	CLA	b	823	-	69,73,73	1.71	9 (13%)	83,113,113	1.40	8 (9%)
34	DD6	F	315	-	39,45,45	0.19	0	52,67,67	1.01	3 (5%)
32	CLA	E	311	5	49,53,73	2.11	9 (18%)	59,89,113	1.71	8 (13%)
32	CLA	C	301	3	49,53,73	2.10	9 (18%)	59,89,113	1.59	8 (13%)
32	CLA	N	312	-	45,49,73	2.23	10 (22%)	54,84,113	1.69	7 (12%)
32	CLA	S	313	17	49,53,73	2.11	9 (18%)	59,89,113	1.67	7 (11%)
34	DD6	j	103	-	39,45,45	0.18	0	52,67,67	0.83	1 (1%)
33	KC2	T	303	-	49,53,53	1.90	4 (8%)	62,89,89	1.35	9 (14%)
32	CLA	D	304	4	64,68,73	1.83	9 (14%)	77,107,113	1.45	7 (9%)
36	LMG	F	319	33	40,40,55	1.01	2 (5%)	48,48,63	1.08	2 (4%)
34	DD6	D	301	-	39,45,45	0.20	0	52,67,67	0.78	2 (3%)
32	CLA	D	310	4	69,73,73	1.76	9 (13%)	83,113,113	1.52	11 (13%)
32	CLA	O	306	15	49,53,73	2.09	9 (18%)	59,89,113	1.63	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	CLA	b	834	21	64,68,73	1.82	9 (14%)	77,107,113	1.47	7 (9%)
32	CLA	B	304	-	50,54,73	2.15	9 (18%)	60,90,113	1.71	9 (15%)
32	CLA	N	310	14	59,63,73	1.92	9 (15%)	71,101,113	1.59	6 (8%)
32	CLA	N	305	-	54,58,73	2.03	9 (16%)	65,95,113	1.62	8 (12%)
32	CLA	I	302	9	59,63,73	1.87	9 (15%)	71,101,113	1.50	8 (11%)
32	CLA	B	302	2	49,53,73	2.04	9 (18%)	59,89,113	1.61	8 (13%)
32	CLA	M	310	13	66,70,73	1.74	9 (13%)	79,109,113	1.38	6 (7%)
32	CLA	E	304	-	64,68,73	1.87	9 (14%)	77,107,113	1.51	7 (9%)
32	CLA	J	304	10	59,63,73	1.94	10 (16%)	71,101,113	1.63	11 (15%)
32	CLA	I	304	9	49,53,73	2.10	9 (18%)	59,89,113	1.66	8 (13%)
36	LMG	F	320	-	33,33,55	1.11	3 (9%)	41,41,63	1.27	4 (9%)
32	CLA	L	304	-	49,53,73	2.05	9 (18%)	59,89,113	1.60	9 (15%)
33	KC2	O	310	15	49,53,53	1.88	4 (8%)	62,89,89	1.34	9 (14%)
38	LMU	I	315	-	36,36,36	0.35	0	47,47,47	1.18	5 (10%)
38	LMU	V	205	-	35,35,36	0.48	0	46,46,47	1.16	3 (6%)
37	A86	F	313	-	44,50,50	0.44	1 (2%)	51,76,76	0.93	3 (5%)
32	CLA	J	305	10	56,60,73	1.96	9 (16%)	67,97,113	1.51	8 (11%)
34	DD6	K	313	-	39,45,45	0.19	0	52,67,67	0.64	2 (3%)
32	CLA	a	805	20	69,73,73	1.82	12 (17%)	83,113,113	1.53	11 (13%)
37	A86	K	314	-	44,50,50	0.58	1 (2%)	51,76,76	1.15	4 (7%)
32	CLA	G	305	7	49,53,73	2.05	9 (18%)	59,89,113	1.57	8 (13%)
32	CLA	B	305	-	49,53,73	2.16	9 (18%)	59,89,113	1.75	8 (13%)
32	CLA	S	308	17	48,52,73	2.18	10 (20%)	58,87,113	1.96	10 (17%)
37	A86	M	301	-	44,50,50	0.47	1 (2%)	51,76,76	0.64	2 (3%)
32	CLA	E	310	5	49,53,73	2.07	9 (18%)	59,89,113	1.57	6 (10%)
41	BCR	l	206	-	41,41,41	0.23	0	56,56,56	0.92	3 (5%)
32	CLA	C	308	3	49,53,73	2.12	9 (18%)	59,89,113	1.78	11 (18%)
33	KC2	K	305	11	49,53,53	1.87	4 (8%)	62,89,89	1.38	7 (11%)
37	A86	T	315	-	44,50,50	0.54	1 (2%)	51,76,76	0.52	1 (1%)
32	CLA	a	821	20	59,63,73	1.88	9 (15%)	71,101,113	1.47	6 (8%)
33	KC2	J	303	10	49,53,53	1.87	4 (8%)	62,89,89	1.34	7 (11%)
32	CLA	a	804	20	62,66,73	1.82	9 (14%)	74,104,113	1.49	8 (10%)
32	CLA	b	809	21	49,53,73	2.07	9 (18%)	59,89,113	1.61	6 (10%)
34	DD6	J	317	-	39,45,45	0.18	0	52,67,67	0.97	3 (5%)
33	KC2	I	316	12	49,53,53	1.88	4 (8%)	62,89,89	1.34	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DD6	A	312	-	39,45,45	0.21	0	52,67,67	0.94	4 (7%)
32	CLA	L	310	-	43,48,73	2.26	9 (20%)	52,82,113	1.94	8 (15%)
33	KC2	N	314	14	49,53,53	1.90	4 (8%)	62,89,89	1.34	8 (12%)
32	CLA	H	302	-	45,49,73	2.33	10 (22%)	54,84,113	1.85	8 (14%)
32	CLA	b	807	21	64,68,73	1.87	9 (14%)	77,107,113	1.60	8 (10%)
37	A86	C	312	-	44,50,50	0.41	1 (2%)	51,76,76	1.25	2 (3%)
33	KC2	N	306	14	49,53,53	1.86	4 (8%)	62,89,89	1.34	9 (14%)
33	KC2	S	306	17	49,53,53	1.86	4 (8%)	62,89,89	1.32	8 (12%)
32	CLA	O	301	15	49,53,73	2.16	9 (18%)	59,89,113	1.69	8 (13%)
33	KC2	M	303	13	49,53,53	1.89	4 (8%)	62,89,89	1.29	5 (8%)
36	LMG	E	322	-	40,40,55	1.08	2 (5%)	48,48,63	1.34	3 (6%)
32	CLA	a	801	-	69,73,73	1.69	9 (13%)	83,113,113	1.38	10 (12%)
32	CLA	S	310	17	49,53,73	2.08	9 (18%)	59,89,113	1.63	7 (11%)
37	A86	L	315	-	44,50,50	0.51	1 (2%)	51,76,76	1.03	3 (5%)
32	CLA	P	307	13	49,53,73	2.10	9 (18%)	59,89,113	1.67	7 (11%)
41	BCR	U	310	-	41,41,41	0.15	0	56,56,56	0.39	0
32	CLA	a	842	-	59,63,73	1.89	9 (15%)	71,101,113	1.46	6 (8%)
32	CLA	k	201	28	59,63,73	1.88	9 (15%)	71,101,113	1.49	7 (9%)
32	CLA	a	816	20	49,53,73	2.06	9 (18%)	59,89,113	1.64	6 (10%)
34	DD6	D	319	-	39,45,45	0.18	0	52,67,67	0.87	3 (5%)
32	CLA	A	311	-	49,53,73	2.09	9 (18%)	59,89,113	1.69	6 (10%)
32	CLA	F	303	6	66,70,73	1.78	9 (13%)	79,109,113	1.39	8 (10%)
32	CLA	J	311	-	49,53,73	2.08	9 (18%)	59,89,113	1.72	7 (11%)
32	CLA	L	301	-	49,53,73	2.12	9 (18%)	59,89,113	1.63	7 (11%)
32	CLA	b	801	-	64,68,73	1.83	9 (14%)	77,107,113	1.57	8 (10%)
37	A86	F	312	-	44,50,50	0.57	1 (2%)	51,76,76	1.34	3 (5%)
34	DD6	W	317	-	39,45,45	0.20	0	52,67,67	0.67	2 (3%)
32	CLA	J	309	-	49,53,73	2.08	9 (18%)	59,89,113	1.62	7 (11%)
32	CLA	b	839	21	69,73,73	1.72	9 (13%)	83,113,113	1.32	6 (7%)
41	BCR	a	846	-	41,41,41	0.15	0	56,56,56	0.38	0
32	CLA	T	307	15	54,58,73	2.00	9 (16%)	65,95,113	1.55	7 (10%)
32	CLA	S	307	-	56,60,73	1.98	9 (16%)	67,97,113	1.86	12 (17%)
32	CLA	S	301	-	49,53,73	2.16	9 (18%)	59,89,113	1.77	9 (15%)
37	A86	T	312	-	44,50,50	0.81	1 (2%)	51,76,76	1.12	3 (5%)
32	CLA	a	827	-	69,73,73	1.73	9 (13%)	83,113,113	1.45	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DD6	U	309	-	39,45,45	0.19	0	52,67,67	0.97	4 (7%)
38	LMU	j	105	-	35,35,36	0.27	0	46,46,47	1.09	3 (6%)
32	CLA	a	826	20	69,73,73	1.71	9 (13%)	83,113,113	1.34	6 (7%)
41	BCR	m	101	-	41,41,41	0.14	0	56,56,56	0.43	0
32	CLA	b	840	-	65,69,73	1.79	9 (13%)	78,108,113	1.37	6 (7%)
32	CLA	K	306	-	64,68,73	1.80	9 (14%)	77,107,113	1.54	11 (14%)
33	KC2	W	301	15	49,53,53	1.87	4 (8%)	62,89,89	1.36	9 (14%)
34	DD6	k	205	-	39,45,45	0.18	0	52,67,67	0.84	4 (7%)
33	KC2	M	302	13	49,53,53	1.87	4 (8%)	62,89,89	1.33	8 (12%)
32	CLA	a	811	20	59,63,73	1.90	9 (15%)	71,101,113	1.52	8 (11%)
32	CLA	b	829	21	59,63,73	1.89	9 (15%)	71,101,113	1.53	7 (9%)
32	CLA	a	824	-	65,69,73	1.76	9 (13%)	78,108,113	1.44	7 (8%)
37	A86	S	317	-	44,50,50	0.49	1 (2%)	51,76,76	1.42	2 (3%)
41	BCR	r	205	-	41,41,41	0.16	0	56,56,56	0.36	0
32	CLA	F	305	-	53,57,73	2.04	9 (16%)	64,94,113	1.69	8 (12%)
32	CLA	a	829	-	64,68,73	1.85	9 (14%)	77,107,113	1.48	7 (9%)
36	LMG	E	320	-	31,31,55	1.12	2 (6%)	39,39,63	1.54	7 (17%)
33	KC2	W	303	13	49,53,53	1.87	4 (8%)	62,89,89	1.34	9 (14%)

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
32	CLA	H	308	8	-	3/10/86/115	-
32	CLA	P	311	-	-	13/33/109/115	-
37	A86	G	311	-	-	4/34/90/90	1/3/3/3
37	A86	P	313	-	-	7/34/90/90	1/3/3/3
32	CLA	Q	310	-	-	4/17/93/115	-
37	A86	W	318	-	-	6/34/90/90	0/3/3/3
39	SQD	H	315	-	-	23/38/58/69	0/1/1/1
32	CLA	Q	309	-	-	3/15/91/115	-
32	CLA	b	820	-	-	7/38/114/115	-
37	A86	T	313	-	-	9/34/90/90	0/3/3/3
36	LMG	P	318	-	-	20/40/60/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	P	316	-	-	7/34/90/90	0/3/3/3
33	KC2	O	302	-	-	8/15/71/71	-
32	CLA	L	314	-	-	7/15/91/115	-
41	BCR	a	843	-	-	4/29/63/63	0/2/2/2
32	CLA	A	304	-	-	10/39/115/115	-
33	KC2	W	314	13,36	-	7/15/71/71	-
32	CLA	C	309	-	-	3/13/89/115	-
34	DD6	H	313	-	-	2/26/80/80	0/3/3/3
32	CLA	S	304	-	-	2/12/88/115	-
34	DD6	I	312	-	-	0/26/80/80	0/3/3/3
36	LMG	D	302	-	-	9/25/45/70	0/1/1/1
34	DD6	E	319	-	-	0/26/80/80	0/3/3/3
34	DD6	J	314	-	-	2/26/80/80	0/3/3/3
32	CLA	P	305	13	-	12/33/109/115	-
32	CLA	M	306	13	-	3/36/112/115	-
32	CLA	R	308	15	-	3/33/109/115	-
33	KC2	S	302	17	-	4/15/71/71	-
32	CLA	J	301	10	-	3/15/91/115	-
37	A86	Q	311	-	-	8/34/90/90	0/3/3/3
33	KC2	E	313	-	-	8/15/71/71	-
34	DD6	Q	312	-	-	1/26/80/80	0/3/3/3
42	SF4	c	101	22	-	-	0/6/5/5
32	CLA	b	805	-	-	6/39/115/115	-
32	CLA	M	312	-	-	10/33/109/115	-
32	CLA	N	309	14	-	4/21/97/115	-
32	CLA	k	203	-	-	9/27/103/115	-
37	A86	Q	316	-	-	6/34/90/90	0/3/3/3
33	KC2	R	303	-	-	5/15/71/71	-
32	CLA	b	813	-	-	4/15/91/115	-
32	CLA	W	306	-	-	6/27/103/115	-
34	DD6	H	311	-	-	0/26/80/80	0/3/3/3
34	DD6	C	310	-	-	0/26/80/80	0/3/3/3
33	KC2	L	313	-	-	8/15/71/71	-
34	DD6	O	313	-	1/1/12/24	0/26/80/80	0/3/3/3
34	DD6	V	202	-	-	4/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	J	307	10	-	6/27/103/115	-
32	CLA	b	808	21	-	9/39/115/115	-
32	CLA	F	309	-	-	5/27/103/115	-
32	CLA	H	307	-	-	12/33/109/115	-
32	CLA	E	314	-	-	2/21/97/115	-
32	CLA	r	202	-	-	1/15/91/115	-
35	LHG	I	318	32	-	16/41/41/53	-
32	CLA	L	307	-	-	2/30/106/115	-
33	KC2	M	307	-	-	3/15/71/71	-
33	KC2	K	309	11	-	8/15/71/71	-
32	CLA	D	311	4	-	6/39/115/115	-
32	CLA	B	309	-	-	5/27/103/115	-
33	KC2	P	301	-	-	9/15/71/71	-
32	CLA	a	810	-	-	14/36/112/115	-
43	PQN	b	847	-	-	1/23/43/43	0/2/2/2
41	BCR	k	204	-	-	4/29/63/63	0/2/2/2
36	LMG	l	201	33	-	23/44/64/70	0/1/1/1
32	CLA	G	306	7	-	11/29/105/115	-
32	CLA	b	835	-	-	7/33/109/115	-
32	CLA	D	309	4	-	2/15/91/115	-
32	CLA	H	309	-	-	7/15/91/115	-
37	A86	D	322	-	-	4/34/90/90	0/3/3/3
32	CLA	a	836	20	-	9/27/103/115	-
32	CLA	E	312	-	-	8/33/109/115	-
32	CLA	U	305	18	-	7/15/91/115	-
34	DD6	E	317	-	-	0/26/80/80	0/3/3/3
32	CLA	L	309	-	-	5/15/91/115	-
36	LMG	W	320	33,37	-	13/34/54/70	0/1/1/1
32	CLA	U	302	18	-	4/15/91/115	-
32	CLA	C	305	-	-	8/33/109/115	-
33	KC2	W	305	13	-	4/15/71/71	-
32	CLA	a	833	-	-	4/39/115/115	-
32	CLA	R	309	15	-	3/10/86/115	-
32	CLA	R	307	15	-	2/15/91/115	-
34	DD6	G	312	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	BCR	l	205	-	-	4/29/63/63	0/2/2/2
33	KC2	I	309	9,36	-	8/15/71/71	-
32	CLA	F	311	-	-	0/15/91/115	-
34	DD6	D	317	-	-	0/26/80/80	0/3/3/3
35	LHG	F	321	-	-	16/44/44/53	-
34	DD6	M	316	-	-	1/26/80/80	0/3/3/3
34	DD6	R	314	-	-	0/26/80/80	0/3/3/3
35	LHG	a	851	-	-	8/42/42/53	-
32	CLA	M	305	-	-	3/21/97/115	-
32	CLA	Q	305	16	-	5/23/99/115	-
33	KC2	T	311	15	-	5/15/71/71	-
32	CLA	Q	303	16	-	6/33/109/115	-
34	DD6	I	313	-	-	0/26/80/80	0/3/3/3
32	CLA	a	815	20	-	1/21/97/115	-
32	CLA	T	310	-	-	4/27/103/115	-
32	CLA	b	837	21	-	13/39/115/115	-
32	CLA	J	312	-	-	12/31/107/115	-
32	CLA	K	301	-	-	4/15/91/115	-
36	LMG	A	318	-	-	9/35/55/70	0/1/1/1
32	CLA	H	306	8	-	3/21/97/115	-
33	KC2	N	302	14	-	5/15/71/71	-
37	A86	W	316	36	-	5/34/90/90	0/3/3/3
32	CLA	L	311	-	-	2/10/82/115	-
32	CLA	a	841	20	-	11/39/115/115	-
32	CLA	S	309	-	-	15/33/109/115	-
35	LHG	E	321	-	-	18/50/50/53	-
34	DD6	Q	314	-	-	1/26/80/80	0/3/3/3
32	CLA	a	832	-	-	5/33/109/115	-
34	DD6	K	315	-	1/1/12/24	1/26/80/80	0/3/3/3
32	CLA	S	311	-	-	5/21/97/115	-
32	CLA	T	308	15	-	7/33/109/115	-
35	LHG	F	318	-	-	15/45/45/53	-
33	KC2	A	310	1	-	5/15/71/71	-
36	LMG	D	321	-	-	16/35/55/70	0/1/1/1
33	KC2	J	310	10	-	8/15/71/71	-
34	DD6	H	312	-	-	2/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	Q	301	33	-	6/33/109/115	-
32	CLA	b	818	-	-	9/39/115/115	-
32	CLA	l	203	35	-	16/39/115/115	-
32	CLA	O	305	15	-	8/39/115/115	-
35	LHG	a	850	32	-	13/34/34/53	-
32	CLA	M	308	13	-	9/30/106/115	-
32	CLA	I	305	9	-	6/29/105/115	-
32	CLA	R	304	-	-	5/15/91/115	-
32	CLA	B	301	-	-	3/10/82/115	-
32	CLA	G	301	-	-	6/15/91/115	-
32	CLA	a	817	20	-	9/35/111/115	-
32	CLA	b	828	21	-	7/35/111/115	-
35	LHG	D	320	-	-	23/52/52/53	-
32	CLA	B	303	-	-	3/15/91/115	-
37	A86	K	312	-	-	7/34/90/90	0/3/3/3
41	BCR	a	844	-	-	2/29/63/63	0/2/2/2
32	CLA	H	310	-	-	3/17/93/115	-
34	DD6	N	321	-	-	2/26/80/80	0/3/3/3
33	KC2	L	302	12	-	4/15/71/71	-
32	CLA	a	820	-	-	10/39/115/115	-
37	A86	M	315	-	-	4/34/90/90	0/3/3/3
32	CLA	D	306	4	-	9/33/109/115	-
33	KC2	R	311	15	-	4/15/71/71	-
32	CLA	b	821	21	-	3/27/103/115	-
32	CLA	K	304	11	-	5/15/91/115	-
37	A86	N	315	-	-	2/34/90/90	0/3/3/3
32	CLA	a	852	-	-	11/39/115/115	-
32	CLA	R	310	-	-	6/27/103/115	-
33	KC2	T	304	15	-	3/15/71/71	-
37	A86	M	314	-	-	4/34/90/90	1/3/3/3
32	CLA	a	822	-	-	10/36/112/115	-
37	A86	N	317	-	-	8/34/90/90	0/3/3/3
34	DD6	P	315	-	-	0/26/80/80	0/3/3/3
32	CLA	I	303	9	-	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	R	313	-	-	4/34/90/90	0/3/3/3
32	CLA	l	202	-	-	5/15/91/115	-
32	CLA	F	322	-	-	10/33/109/115	-
32	CLA	b	806	-	-	10/39/115/115	-
37	A86	N	316	-	-	14/34/90/90	0/3/3/3
32	CLA	H	301	8	-	8/15/91/115	-
35	LHG	E	301	-	-	18/50/50/53	-
32	CLA	a	823	-	-	5/39/115/115	-
34	DD6	Q	313	-	-	0/26/80/80	0/3/3/3
37	A86	r	204	-	-	8/34/90/90	0/3/3/3
35	LHG	a	849	-	-	22/52/52/53	-
36	LMG	L	320	-	-	13/32/52/70	0/1/1/1
32	CLA	f	201	-	-	4/33/109/115	-
38	LMU	D	324	-	-	11/21/61/61	0/2/2/2
32	CLA	U	307	-	-	5/15/91/115	-
32	CLA	W	313	-	-	5/33/109/115	-
34	DD6	E	318	-	-	1/26/80/80	0/3/3/3
36	LMG	S	322	33	-	13/28/48/70	0/1/1/1
35	LHG	B	308	-	-	18/35/35/53	-
32	CLA	R	301	-	-	4/15/91/115	-
33	KC2	N	307	14	-	4/15/71/71	-
32	CLA	J	308	-	-	6/15/91/115	-
37	A86	H	314	-	-	5/34/90/90	0/3/3/3
33	KC2	K	303	11	-	8/15/71/71	-
32	CLA	U	306	-	-	8/15/91/115	-
36	LMG	A	317	-	-	15/31/51/70	0/1/1/1
32	CLA	l	204	29	-	15/39/115/115	-
32	CLA	b	832	-	-	9/39/115/115	-
33	KC2	R	302	15	-	5/15/71/71	-
32	CLA	E	308	5	-	11/39/115/115	-
33	KC2	M	313	13,36	-	7/15/71/71	-
37	A86	S	314	-	-	6/34/90/90	0/3/3/3
32	CLA	Q	308	-	-	5/15/91/115	-
32	CLA	b	810	21	-	5/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	a	812	20	-	7/27/103/115	-
32	CLA	b	802	-	-	3/39/115/115	-
32	CLA	K	308	11	-	12/39/115/115	-
32	CLA	a	819	20	-	14/39/115/115	-
32	CLA	C	306	3	-	14/39/115/115	-
37	A86	L	316	-	-	8/34/90/90	0/3/3/3
32	CLA	A	302	35	-	4/33/109/115	-
35	LHG	M	319	-	-	18/50/50/53	-
34	DD6	A	315	-	-	3/26/80/80	0/3/3/3
32	CLA	K	307	11	-	4/10/86/115	-
32	CLA	a	814	20	-	10/39/115/115	-
32	CLA	D	315	-	-	4/15/91/115	-
32	CLA	G	308	-	-	6/26/102/115	-
34	DD6	J	315	-	-	1/26/80/80	0/3/3/3
35	LHG	A	316	-	-	21/44/44/53	-
33	KC2	C	303	-	-	9/15/71/71	-
35	LHG	W	319	32	-	18/50/50/53	-
32	CLA	P	308	13	-	2/15/91/115	-
32	CLA	W	312	13	-	12/33/109/115	-
32	CLA	O	308	-	-	6/15/91/115	-
33	KC2	N	303	14	-	7/15/71/71	-
32	CLA	I	308	-	-	8/27/103/115	-
33	KC2	N	304	14	-	8/15/71/71	-
32	CLA	A	305	1	-	6/35/111/115	-
32	CLA	F	306	6	-	5/27/103/115	-
32	CLA	a	838	-	-	5/39/115/115	-
32	CLA	b	817	21	-	11/27/103/115	-
37	A86	O	312	-	1/1/14/25	4/34/90/90	0/3/3/3
32	CLA	B	306	-	-	4/15/91/115	-
32	CLA	b	804	21	-	19/39/115/115	-
33	KC2	P	306	-	-	5/15/71/71	-
37	A86	J	313	-	-	8/34/90/90	0/3/3/3
32	CLA	D	312	4	-	6/27/103/115	-
32	CLA	a	840	-	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	b	814	-	-	6/15/91/115	-
32	CLA	E	306	5	-	7/33/109/115	-
32	CLA	T	305	-	-	12/15/91/115	-
41	BCR	f	202	-	-	2/29/63/63	0/2/2/2
32	CLA	C	302	-	-	0/10/86/115	-
32	CLA	k	202	-	-	10/27/103/115	-
36	LMG	M	320	33	-	9/35/55/70	0/1/1/1
33	KC2	H	303	-	-	8/15/71/71	-
32	CLA	I	317	35	-	3/39/115/115	-
32	CLA	K	310	-	-	6/15/91/115	-
32	CLA	G	307	-	-	2/10/82/115	-
42	SF4	c	102	-	-	-	0/6/5/5
36	LMG	E	302	-	-	19/35/55/70	0/1/1/1
32	CLA	N	311	14	-	7/33/109/115	-
33	KC2	L	303	-	-	4/15/71/71	-
32	CLA	I	306	9	-	7/39/115/115	-
32	CLA	D	314	4	-	7/24/100/115	-
32	CLA	a	825	20	-	2/39/115/115	-
37	A86	M	317	-	-	7/34/90/90	1/3/3/3
32	CLA	C	304	3	-	4/13/89/115	-
33	KC2	S	303	17	-	6/15/71/71	-
41	BCR	a	845	-	-	4/29/63/63	0/2/2/2
43	PQN	a	848	-	-	8/23/43/43	0/2/2/2
32	CLA	D	305	-	-	9/31/107/115	-
32	CLA	A	308	-	-	3/27/103/115	-
32	CLA	W	310	13	-	12/33/109/115	-
32	CLA	f	203	25	-	2/15/91/115	-
37	A86	U	308	-	-	2/34/90/90	1/3/3/3
32	CLA	E	315	-	-	5/17/93/115	-
37	A86	P	319	-	-	4/34/90/90	0/3/3/3
32	CLA	I	307	-	-	6/15/91/115	-
32	CLA	V	201	-	-	6/31/107/115	-
41	BCR	b	844	-	-	4/29/63/63	0/2/2/2
33	KC2	P	312	13	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	P	309	-	-	7/35/111/115	-
32	CLA	b	836	-	-	9/39/115/115	-
37	A86	K	311	-	-	8/34/90/90	0/3/3/3
41	BCR	r	203	-	-	5/29/63/63	0/2/2/2
42	SF4	a	847	-	-	-	0/6/5/5
32	CLA	Q	307	16	-	8/36/112/115	-
34	DD6	I	310	-	-	1/26/80/80	0/3/3/3
34	DD6	S	321	-	1/1/12/24	5/26/80/80	0/3/3/3
32	CLA	T	309	-	-	4/15/91/115	-
32	CLA	F	304	-	-	3/27/103/115	-
32	CLA	b	833	-	-	10/36/112/115	-
32	CLA	a	809	-	-	8/33/109/115	-
32	CLA	U	301	18	-	3/10/82/115	-
32	CLA	r	201	-	-	8/33/109/115	-
37	A86	D	323	-	-	10/34/90/90	0/3/3/3
32	CLA	a	828	-	-	7/31/107/115	-
32	CLA	a	802	-	-	10/37/113/115	-
34	DD6	D	316	-	-	1/26/80/80	0/3/3/3
37	A86	O	311	-	-	4/34/90/90	0/3/3/3
32	CLA	F	301	-	-	2/10/82/115	-
33	KC2	K	302	11	-	6/15/71/71	-
35	LHG	P	317	-	-	20/50/50/53	-
32	CLA	U	303	18	-	3/15/91/115	-
32	CLA	G	304	-	-	4/27/103/115	-
37	A86	S	318	-	-	4/34/90/90	0/3/3/3
37	A86	W	315	-	-	7/34/90/90	0/3/3/3
33	KC2	Q	317	32	-	8/15/71/71	-
41	BCR	b	841	-	-	0/29/63/63	0/2/2/2
32	CLA	O	307	15	-	7/33/109/115	-
32	CLA	b	812	21	-	11/39/115/115	-
34	DD6	N	319	-	-	1/26/80/80	0/3/3/3
32	CLA	D	313	-	-	11/31/107/115	-
38	LMU	J	318	-	-	4/21/61/61	0/2/2/2
36	LMG	D	303	-	-	16/31/51/70	0/1/1/1
41	BCR	i	101	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	C	311	-	-	8/34/90/90	0/3/3/3
32	CLA	A	307	1	-	5/33/109/115	-
34	DD6	J	316	-	-	0/26/80/80	0/3/3/3
36	LMG	j	104	-	-	21/33/53/70	0/1/1/1
36	LMG	T	301	-	-	14/32/52/70	0/1/1/1
41	BCR	a	854	-	-	5/29/63/63	0/2/2/2
32	CLA	a	818	20	-	10/33/109/115	-
32	CLA	L	312	-	-	8/33/109/115	-
33	KC2	L	305	12	-	11/15/71/71	-
32	CLA	a	803	20	-	8/37/113/115	-
33	KC2	W	304	13	-	5/15/71/71	-
36	LMG	N	301	-	-	19/35/55/70	0/1/1/1
32	CLA	H	305	8	-	5/15/91/115	-
34	DD6	A	314	-	-	1/26/80/80	0/3/3/3
32	CLA	a	830	20	-	11/39/115/115	-
32	CLA	Q	306	16	-	14/36/112/115	-
32	CLA	I	301	-	-	12/39/115/115	-
37	A86	P	314	-	-	4/34/90/90	0/3/3/3
32	CLA	f	204	-	-	1/18/94/115	-
34	DD6	A	313	-	-	3/26/80/80	0/3/3/3
32	CLA	E	305	5	-	1/27/103/115	-
33	KC2	M	321	15	-	5/15/71/71	-
37	A86	M	318	-	-	4/34/90/90	0/3/3/3
33	KC2	G	309	7	-	9/15/71/71	-
33	KC2	L	306	12	-	6/15/71/71	-
41	BCR	j	102	-	-	5/29/63/63	0/2/2/2
32	CLA	b	838	-	-	10/39/115/115	-
37	A86	S	320	-	-	6/34/90/90	0/3/3/3
32	CLA	M	309	13	-	7/15/91/115	-
32	CLA	H	304	-	-	7/15/91/115	-
32	CLA	b	819	-	-	4/39/115/115	-
34	DD6	T	314	-	-	1/26/80/80	0/3/3/3
32	CLA	a	835	20	-	11/39/115/115	-
36	LMG	D	325	-	-	9/30/50/70	0/1/1/1
41	BCR	b	842	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	a	831	20	-	4/33/109/115	-
33	KC2	M	304	13	-	6/15/71/71	-
32	CLA	j	101	27	-	4/15/91/115	-
33	KC2	U	304	18	-	6/15/71/71	-
33	KC2	F	302	6	-	8/15/71/71	-
32	CLA	b	816	-	-	8/36/112/115	-
32	CLA	V	203	19	-	4/27/103/115	-
32	CLA	C	307	3	-	9/33/109/115	-
40	DGD	b	846	-	-	21/45/85/95	0/2/2/2
32	CLA	A	309	1	-	12/39/115/115	-
32	CLA	A	306	1	-	9/39/115/115	-
32	CLA	E	303	5	-	4/15/91/115	-
32	CLA	J	306	10	-	7/27/103/115	-
37	A86	F	317	-	-	7/34/90/90	0/3/3/3
33	KC2	G	302	-	-	9/15/71/71	-
32	CLA	D	308	4	-	4/27/103/115	-
33	KC2	Q	302	-	-	7/15/71/71	-
32	CLA	F	308	6	-	3/17/93/115	-
34	DD6	B	307	-	-	2/26/80/80	0/3/3/3
32	CLA	W	307	13	-	7/15/91/115	-
33	KC2	F	310	6,36	-	8/15/71/71	-
34	DD6	F	316	-	-	3/26/80/80	0/3/3/3
32	CLA	F	307	6	-	5/33/109/115	-
32	CLA	G	303	7	-	10/27/103/115	-
37	A86	L	318	-	-	4/34/90/90	0/3/3/3
32	CLA	Q	304	-	-	3/21/97/115	-
32	CLA	N	313	-	-	9/33/109/115	-
32	CLA	T	306	15	-	5/33/109/115	-
37	A86	L	317	-	-	10/34/90/90	0/3/3/3
34	DD6	D	318	-	-	2/26/80/80	0/3/3/3
32	CLA	a	806	-	-	7/33/109/115	-
32	CLA	b	803	21	-	9/39/115/115	-
32	CLA	W	309	13	-	6/39/115/115	-
32	CLA	J	302	-	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	b	827	21	-	4/21/97/115	-
37	A86	R	312	-	-	3/34/90/90	0/3/3/3
32	CLA	b	815	21	-	7/39/115/115	-
39	SQD	k	206	-	-	13/31/51/69	0/1/1/1
37	A86	S	316	-	-	2/34/90/90	0/3/3/3
33	KC2	N	308	14	-	5/15/71/71	-
32	CLA	E	307	5	-	8/27/103/115	-
34	DD6	L	319	-	-	2/26/80/80	0/3/3/3
32	CLA	L	308	12	-	4/15/91/115	-
32	CLA	b	824	21	-	8/31/107/115	-
33	KC2	W	308	-	-	6/15/71/71	-
32	CLA	D	307	4	-	6/35/111/115	-
32	CLA	O	304	-	-	2/15/91/115	-
32	CLA	b	811	21	-	6/21/97/115	-
34	DD6	F	314	-	-	1/26/80/80	0/3/3/3
33	KC2	R	305	15	-	5/15/71/71	-
32	CLA	a	834	20	-	7/39/115/115	-
32	CLA	b	831	-	-	14/33/109/115	-
41	BCR	b	845	-	-	2/29/63/63	0/2/2/2
32	CLA	a	807	-	-	9/39/115/115	-
33	KC2	P	302	13	-	9/15/71/71	-
32	CLA	a	808	20	-	3/21/97/115	-
32	CLA	P	310	-	-	3/10/86/115	-
32	CLA	W	311	13	-	13/39/115/115	-
34	DD6	I	311	-	-	1/26/80/80	0/3/3/3
37	A86	G	310	-	-	10/34/90/90	0/3/3/3
32	CLA	A	301	1	-	5/15/91/115	-
32	CLA	a	853	-	-	10/39/115/115	-
32	CLA	V	204	-	-	3/21/97/115	-
33	KC2	O	303	15	-	6/15/71/71	-
41	BCR	b	843	-	-	2/29/63/63	0/2/2/2
32	CLA	E	309	5	-	10/31/107/115	-
32	CLA	A	303	1	-	11/36/112/115	-
34	DD6	E	316	-	-	0/26/80/80	0/3/3/3
32	CLA	b	826	-	-	4/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	M	322	-	-	4/34/90/90	0/3/3/3
32	CLA	a	837	20	-	7/27/103/115	-
40	DGD	Q	318	-	-	27/45/85/95	0/2/2/2
32	CLA	P	304	-	-	6/15/91/115	-
32	CLA	a	813	20	-	6/15/91/115	-
34	DD6	Q	315	-	-	1/26/80/80	0/3/3/3
32	CLA	a	839	20	-	7/27/103/115	-
32	CLA	b	822	21	-	7/39/115/115	-
32	CLA	M	311	13	-	7/15/91/115	-
32	CLA	S	305	17	-	6/37/113/115	-
32	CLA	T	302	15	-	6/15/91/115	-
35	LHG	I	314	-	-	22/50/50/53	-
37	A86	S	319	-	-	7/34/90/90	0/3/3/3
32	CLA	b	825	21	-	8/33/109/115	-
34	DD6	N	318	-	-	2/26/80/80	0/3/3/3
37	A86	S	315	-	-	3/34/90/90	1/3/3/3
33	KC2	S	312	17,36	-	4/15/71/71	-
32	CLA	b	830	21	-	7/35/111/115	-
37	A86	N	320	-	-	0/34/90/90	0/3/3/3
37	A86	W	302	-	-	1/34/90/90	0/3/3/3
33	KC2	P	303	13	-	3/15/71/71	-
35	LHG	f	205	-	-	26/51/51/53	-
32	CLA	R	306	15	-	4/15/91/115	-
32	CLA	O	309	-	-	7/36/112/115	-
32	CLA	b	823	-	-	10/39/115/115	-
34	DD6	F	315	-	-	3/26/80/80	0/3/3/3
32	CLA	E	311	5	-	3/15/91/115	-
32	CLA	C	301	3	-	3/15/91/115	-
32	CLA	N	312	-	-	6/10/86/115	-
32	CLA	S	313	17	-	6/15/91/115	-
34	DD6	j	103	-	-	1/26/80/80	0/3/3/3
33	KC2	T	303	-	-	8/15/71/71	-
32	CLA	D	304	4	-	10/33/109/115	-
36	LMG	F	319	33	-	16/35/55/70	0/1/1/1
34	DD6	D	301	-	-	2/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	D	310	4	-	6/39/115/115	-
32	CLA	O	306	15	-	5/15/91/115	-
32	CLA	b	834	21	-	3/33/109/115	-
32	CLA	B	304	-	-	7/17/93/115	-
32	CLA	N	310	14	-	7/27/103/115	-
32	CLA	N	305	-	-	6/21/97/115	-
32	CLA	I	302	9	-	8/27/103/115	-
32	CLA	B	302	2	-	6/15/91/115	-
32	CLA	M	310	13	-	4/36/112/115	-
32	CLA	E	304	-	-	4/33/109/115	-
32	CLA	J	304	10	-	5/27/103/115	-
32	CLA	I	304	9	-	5/15/91/115	-
36	LMG	F	320	-	-	7/28/48/70	0/1/1/1
32	CLA	L	304	-	-	2/15/91/115	-
33	KC2	O	310	15	-	6/15/71/71	-
38	LMU	I	315	-	-	6/21/61/61	0/2/2/2
38	LMU	V	205	-	-	6/20/60/61	0/2/2/2
37	A86	F	313	-	-	5/34/90/90	0/3/3/3
32	CLA	J	305	10	-	3/24/100/115	-
34	DD6	K	313	-	-	0/26/80/80	0/3/3/3
32	CLA	a	805	20	-	15/39/115/115	-
37	A86	K	314	-	-	4/34/90/90	0/3/3/3
32	CLA	G	305	7	-	5/15/91/115	-
32	CLA	B	305	-	-	5/15/91/115	-
32	CLA	S	308	17	-	4/15/91/115	-
37	A86	M	301	-	-	6/34/90/90	0/3/3/3
32	CLA	E	310	5	-	7/15/91/115	-
41	BCR	l	206	-	-	5/29/63/63	0/2/2/2
32	CLA	C	308	3	-	4/15/91/115	-
33	KC2	K	305	11	-	4/15/71/71	-
37	A86	T	315	-	-	4/34/90/90	0/3/3/3
32	CLA	a	821	20	-	7/27/103/115	-
33	KC2	J	303	10	-	8/15/71/71	-
32	CLA	a	804	20	-	4/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	b	809	21	-	5/15/91/115	-
34	DD6	J	317	-	1/1/12/24	0/26/80/80	0/3/3/3
33	KC2	I	316	12	-	8/15/71/71	-
34	DD6	A	312	-	-	0/26/80/80	0/3/3/3
32	CLA	L	310	-	-	4/10/82/115	-
33	KC2	N	314	14	-	6/15/71/71	-
32	CLA	H	302	-	-	5/10/86/115	-
32	CLA	b	807	21	-	10/33/109/115	-
37	A86	C	312	-	-	6/34/90/90	0/3/3/3
33	KC2	N	306	14	-	4/15/71/71	-
33	KC2	S	306	17	-	6/15/71/71	-
32	CLA	O	301	15	-	5/15/91/115	-
33	KC2	M	303	13	-	2/15/71/71	-
36	LMG	E	322	-	-	12/35/55/70	0/1/1/1
32	CLA	a	801	-	-	5/39/115/115	-
32	CLA	S	310	17	-	9/15/91/115	-
37	A86	L	315	-	-	4/34/90/90	0/3/3/3
32	CLA	P	307	13	-	0/15/91/115	-
41	BCR	U	310	-	-	4/29/63/63	0/2/2/2
32	CLA	a	842	-	-	8/27/103/115	-
32	CLA	k	201	28	-	9/27/103/115	-
32	CLA	a	816	20	-	7/15/91/115	-
34	DD6	D	319	-	-	2/26/80/80	0/3/3/3
32	CLA	A	311	-	-	7/15/91/115	-
32	CLA	F	303	6	-	10/36/112/115	-
32	CLA	J	311	-	-	2/15/91/115	-
32	CLA	L	301	-	-	7/15/91/115	-
32	CLA	b	801	-	-	6/33/109/115	-
37	A86	F	312	-	-	2/34/90/90	0/3/3/3
34	DD6	W	317	-	-	1/26/80/80	0/3/3/3
32	CLA	J	309	-	-	2/15/91/115	-
32	CLA	b	839	21	-	12/39/115/115	-
41	BCR	a	846	-	-	2/29/63/63	0/2/2/2
32	CLA	T	307	15	-	4/21/97/115	-
32	CLA	S	307	-	-	2/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	S	301	-	-	3/15/91/115	-
37	A86	T	312	-	-	4/34/90/90	0/3/3/3
32	CLA	a	827	-	-	11/39/115/115	-
34	DD6	U	309	-	-	0/26/80/80	0/3/3/3
38	LMU	j	105	-	-	12/20/60/61	0/2/2/2
32	CLA	a	826	20	-	16/39/115/115	-
41	BCR	m	101	-	-	1/29/63/63	0/2/2/2
32	CLA	b	840	-	-	9/35/111/115	-
32	CLA	K	306	-	-	10/33/109/115	-
33	KC2	W	301	15	-	5/15/71/71	-
34	DD6	k	205	-	-	1/26/80/80	0/3/3/3
33	KC2	M	302	13	-	6/15/71/71	-
32	CLA	a	811	20	-	5/27/103/115	-
32	CLA	b	829	21	-	8/27/103/115	-
32	CLA	a	824	-	-	7/35/111/115	-
37	A86	S	317	-	-	6/34/90/90	0/3/3/3
41	BCR	r	205	-	-	2/29/63/63	0/2/2/2
32	CLA	F	305	-	-	1/19/95/115	-
32	CLA	a	829	-	-	7/33/109/115	-
36	LMG	E	320	-	-	13/26/46/70	0/1/1/1
33	KC2	W	303	13	-	6/15/71/71	-

All (2897) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	S	312	KC2	MG-ND	-10.20	1.85	2.05
33	K	303	KC2	MG-ND	-10.20	1.85	2.05
33	N	308	KC2	MG-ND	-10.20	1.85	2.05
33	W	305	KC2	MG-ND	-10.13	1.85	2.05
33	P	303	KC2	MG-ND	-10.08	1.85	2.05
33	T	304	KC2	MG-ND	-10.03	1.85	2.05
33	N	303	KC2	MG-ND	-10.00	1.86	2.05
33	K	302	KC2	MG-ND	-9.99	1.86	2.05
33	P	306	KC2	MG-ND	-9.98	1.86	2.05
33	F	302	KC2	MG-ND	-9.98	1.86	2.05
33	M	304	KC2	MG-ND	-9.98	1.86	2.05
33	W	303	KC2	MG-ND	-9.97	1.86	2.05
33	O	310	KC2	MG-ND	-9.97	1.86	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	302	KC2	MG-ND	-9.96	1.86	2.05
33	L	313	KC2	MG-ND	-9.96	1.86	2.05
33	O	303	KC2	MG-ND	-9.95	1.86	2.05
33	R	302	KC2	MG-ND	-9.93	1.86	2.05
33	W	314	KC2	MG-ND	-9.93	1.86	2.05
33	K	305	KC2	MG-ND	-9.93	1.86	2.05
33	T	303	KC2	MG-ND	-9.93	1.86	2.05
33	P	312	KC2	MG-ND	-9.93	1.86	2.05
33	E	313	KC2	MG-ND	-9.92	1.86	2.05
33	W	304	KC2	MG-ND	-9.92	1.86	2.05
33	M	313	KC2	MG-ND	-9.91	1.86	2.05
33	S	303	KC2	MG-ND	-9.89	1.86	2.05
33	Q	317	KC2	MG-ND	-9.89	1.86	2.05
33	L	303	KC2	MG-ND	-9.89	1.86	2.05
33	I	309	KC2	MG-ND	-9.87	1.86	2.05
33	P	302	KC2	MG-ND	-9.86	1.86	2.05
33	O	302	KC2	MG-ND	-9.86	1.86	2.05
33	M	321	KC2	MG-ND	-9.86	1.86	2.05
33	L	302	KC2	MG-ND	-9.86	1.86	2.05
33	R	303	KC2	MG-ND	-9.84	1.86	2.05
33	W	308	KC2	MG-ND	-9.83	1.86	2.05
33	A	310	KC2	MG-ND	-9.83	1.86	2.05
33	L	305	KC2	MG-ND	-9.83	1.86	2.05
33	N	314	KC2	MG-ND	-9.82	1.86	2.05
33	W	301	KC2	MG-ND	-9.82	1.86	2.05
33	N	307	KC2	MG-ND	-9.82	1.86	2.05
33	L	306	KC2	MG-ND	-9.81	1.86	2.05
33	T	311	KC2	MG-ND	-9.81	1.86	2.05
33	Q	302	KC2	MG-ND	-9.80	1.86	2.05
33	M	303	KC2	MG-ND	-9.80	1.86	2.05
33	G	302	KC2	MG-ND	-9.79	1.86	2.05
33	N	306	KC2	MG-ND	-9.79	1.86	2.05
33	S	306	KC2	MG-ND	-9.79	1.86	2.05
33	N	304	KC2	MG-ND	-9.79	1.86	2.05
33	U	304	KC2	MG-ND	-9.78	1.86	2.05
33	R	305	KC2	MG-ND	-9.77	1.86	2.05
33	H	303	KC2	MG-ND	-9.76	1.86	2.05
33	S	302	KC2	MG-ND	-9.75	1.86	2.05
33	M	307	KC2	MG-ND	-9.74	1.86	2.05
33	G	309	KC2	MG-ND	-9.74	1.86	2.05
33	R	311	KC2	MG-ND	-9.73	1.86	2.05
33	P	301	KC2	MG-ND	-9.72	1.86	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	I	316	KC2	MG-ND	-9.71	1.86	2.05
33	M	302	KC2	MG-ND	-9.71	1.86	2.05
33	C	303	KC2	MG-ND	-9.70	1.86	2.05
33	J	303	KC2	MG-ND	-9.68	1.86	2.05
33	K	309	KC2	MG-ND	-9.67	1.86	2.05
33	J	310	KC2	MG-ND	-9.65	1.86	2.05
33	F	310	KC2	MG-ND	-9.64	1.86	2.05
32	S	304	CLA	C1D-ND	7.45	1.46	1.37
32	l	203	CLA	C1D-ND	7.44	1.46	1.37
32	K	307	CLA	C1D-ND	7.43	1.46	1.37
32	H	310	CLA	C1D-ND	7.41	1.46	1.37
32	P	310	CLA	C1D-ND	7.41	1.46	1.37
32	C	309	CLA	C1D-ND	7.38	1.46	1.37
32	F	311	CLA	C1D-ND	7.38	1.46	1.37
32	G	305	CLA	C1D-ND	7.33	1.46	1.37
32	G	301	CLA	C1D-ND	7.33	1.46	1.37
32	a	811	CLA	C1D-ND	7.32	1.46	1.37
32	F	308	CLA	C1D-ND	7.32	1.46	1.37
32	F	301	CLA	C1D-ND	7.32	1.46	1.37
32	C	306	CLA	C1D-ND	7.30	1.46	1.37
32	a	842	CLA	C1D-ND	7.30	1.46	1.37
32	T	309	CLA	C1D-ND	7.29	1.46	1.37
32	a	822	CLA	C1D-ND	7.29	1.46	1.37
32	L	301	CLA	C1D-ND	7.29	1.46	1.37
32	T	302	CLA	C1D-ND	7.28	1.46	1.37
32	B	309	CLA	C1D-ND	7.27	1.46	1.37
32	W	307	CLA	C1D-ND	7.27	1.46	1.37
32	b	819	CLA	C1D-ND	7.27	1.46	1.37
32	k	202	CLA	C1D-ND	7.26	1.46	1.37
32	r	201	CLA	C1D-ND	7.25	1.46	1.37
32	C	301	CLA	C1D-ND	7.25	1.46	1.37
32	U	301	CLA	C1D-ND	7.25	1.46	1.37
32	L	312	CLA	C1D-ND	7.24	1.46	1.37
32	H	306	CLA	C1D-ND	7.23	1.46	1.37
32	F	303	CLA	C1D-ND	7.23	1.46	1.37
32	J	302	CLA	C1D-ND	7.22	1.46	1.37
32	H	302	CLA	C1D-ND	7.22	1.46	1.37
32	J	305	CLA	C1D-ND	7.22	1.46	1.37
32	b	817	CLA	C1D-ND	7.21	1.46	1.37
32	E	305	CLA	C1D-ND	7.21	1.46	1.37
32	L	310	CLA	C1D-ND	7.21	1.46	1.37
32	E	303	CLA	C1D-ND	7.20	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	811	CLA	C1D-ND	7.19	1.46	1.37
32	J	301	CLA	C1D-ND	7.18	1.46	1.37
32	j	101	CLA	C1D-ND	7.18	1.46	1.37
32	M	309	CLA	C1D-ND	7.17	1.46	1.37
32	L	308	CLA	C1D-ND	7.16	1.46	1.37
32	N	311	CLA	C1D-ND	7.16	1.46	1.37
32	f	204	CLA	C1D-ND	7.16	1.46	1.37
32	E	314	CLA	C1D-ND	7.16	1.46	1.37
32	E	310	CLA	C1D-ND	7.15	1.46	1.37
32	K	308	CLA	C1D-ND	7.15	1.46	1.37
32	S	305	CLA	C1D-ND	7.15	1.46	1.37
32	U	302	CLA	C1D-ND	7.15	1.46	1.37
32	G	308	CLA	C1D-ND	7.15	1.46	1.37
32	P	308	CLA	C1D-ND	7.15	1.46	1.37
32	b	801	CLA	C1D-ND	7.15	1.46	1.37
32	K	301	CLA	C1D-ND	7.14	1.46	1.37
32	B	301	CLA	C1D-ND	7.14	1.46	1.37
32	M	306	CLA	C1D-ND	7.14	1.46	1.37
32	P	309	CLA	C1D-ND	7.14	1.46	1.37
32	M	312	CLA	C1D-ND	7.13	1.46	1.37
32	O	308	CLA	C1D-ND	7.13	1.46	1.37
32	D	312	CLA	C1D-ND	7.12	1.46	1.37
32	K	304	CLA	C1D-ND	7.12	1.46	1.37
32	L	304	CLA	C1D-ND	7.11	1.46	1.37
32	D	304	CLA	C1D-ND	7.11	1.46	1.37
32	a	817	CLA	C1D-ND	7.11	1.46	1.37
32	C	304	CLA	C1D-ND	7.11	1.46	1.37
32	R	301	CLA	C1D-ND	7.11	1.46	1.37
32	H	308	CLA	C1D-ND	7.11	1.46	1.37
32	b	816	CLA	C1D-ND	7.10	1.46	1.37
32	I	302	CLA	C1D-ND	7.10	1.46	1.37
32	A	306	CLA	C1D-ND	7.10	1.46	1.37
32	R	309	CLA	C1D-ND	7.10	1.46	1.37
32	b	806	CLA	C1D-ND	7.10	1.46	1.37
32	W	312	CLA	C1D-ND	7.09	1.46	1.37
32	b	829	CLA	C1D-ND	7.09	1.46	1.37
32	J	312	CLA	C1D-ND	7.09	1.46	1.37
32	E	315	CLA	C1D-ND	7.08	1.46	1.37
32	L	314	CLA	C1D-ND	7.08	1.46	1.37
32	B	303	CLA	C1D-ND	7.08	1.46	1.37
32	E	311	CLA	C1D-ND	7.08	1.46	1.37
32	L	309	CLA	C1D-ND	7.08	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	L	311	CLA	C1D-ND	7.08	1.46	1.37
32	C	302	CLA	C1D-ND	7.07	1.46	1.37
32	A	302	CLA	C1D-ND	7.07	1.46	1.37
32	C	307	CLA	C1D-ND	7.06	1.46	1.37
32	Q	308	CLA	C1D-ND	7.06	1.46	1.37
32	R	310	CLA	C1D-ND	7.06	1.46	1.37
32	P	305	CLA	C1D-ND	7.05	1.46	1.37
32	O	301	CLA	C1D-ND	7.05	1.46	1.37
32	N	312	CLA	C1D-ND	7.05	1.46	1.37
32	E	308	CLA	C1D-ND	7.05	1.46	1.37
32	T	307	CLA	C1D-ND	7.04	1.46	1.37
32	a	804	CLA	C1D-ND	7.04	1.46	1.37
32	f	203	CLA	C1D-ND	7.04	1.46	1.37
32	U	307	CLA	C1D-ND	7.04	1.46	1.37
32	N	313	CLA	C1D-ND	7.04	1.46	1.37
32	R	308	CLA	C1D-ND	7.04	1.46	1.37
32	Q	310	CLA	C1D-ND	7.03	1.46	1.37
32	Q	307	CLA	C1D-ND	7.03	1.46	1.37
32	T	305	CLA	C1D-ND	7.03	1.46	1.37
32	G	307	CLA	C1D-ND	7.03	1.46	1.37
32	S	311	CLA	C1D-ND	7.02	1.46	1.37
32	a	808	CLA	C1D-ND	7.02	1.46	1.37
32	S	301	CLA	C1D-ND	7.02	1.46	1.37
32	F	322	CLA	C1D-ND	7.00	1.46	1.37
32	M	305	CLA	C1D-ND	7.00	1.46	1.37
32	P	307	CLA	C1D-ND	6.99	1.46	1.37
32	M	310	CLA	C1D-ND	6.99	1.46	1.37
32	B	305	CLA	C1D-ND	6.98	1.46	1.37
32	H	305	CLA	C1D-ND	6.98	1.46	1.37
32	b	821	CLA	C1D-ND	6.98	1.46	1.37
32	T	308	CLA	C1D-ND	6.98	1.46	1.37
32	F	307	CLA	C1D-ND	6.98	1.46	1.37
32	O	307	CLA	C1D-ND	6.97	1.46	1.37
32	H	307	CLA	C1D-ND	6.97	1.46	1.37
32	H	309	CLA	C1D-ND	6.97	1.46	1.37
32	W	311	CLA	C1D-ND	6.97	1.46	1.37
32	R	304	CLA	C1D-ND	6.97	1.46	1.37
32	P	311	CLA	C1D-ND	6.97	1.46	1.37
32	D	309	CLA	C1D-ND	6.97	1.46	1.37
32	S	310	CLA	C1D-ND	6.96	1.46	1.37
32	B	306	CLA	C1D-ND	6.96	1.46	1.37
32	a	815	CLA	C1D-ND	6.96	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	O	304	CLA	C1D-ND	6.96	1.46	1.37
32	A	301	CLA	C1D-ND	6.95	1.46	1.37
32	b	839	CLA	C1D-ND	6.95	1.46	1.37
32	S	308	CLA	C1D-ND	6.95	1.46	1.37
32	R	307	CLA	C1D-ND	6.94	1.46	1.37
32	W	310	CLA	C1D-ND	6.94	1.46	1.37
32	a	803	CLA	C1D-ND	6.94	1.46	1.37
32	b	827	CLA	C1D-ND	6.94	1.46	1.37
32	b	835	CLA	C1D-ND	6.94	1.46	1.37
32	I	305	CLA	C1D-ND	6.94	1.46	1.37
32	V	204	CLA	C1D-ND	6.93	1.46	1.37
32	a	853	CLA	C1D-ND	6.93	1.46	1.37
32	J	311	CLA	C1D-ND	6.92	1.46	1.37
32	I	307	CLA	C1D-ND	6.92	1.46	1.37
32	a	831	CLA	C1D-ND	6.92	1.46	1.37
32	C	308	CLA	C1D-ND	6.92	1.46	1.37
32	J	308	CLA	C1D-ND	6.92	1.46	1.37
32	b	818	CLA	C1D-ND	6.91	1.46	1.37
32	D	311	CLA	C1D-ND	6.91	1.46	1.37
32	F	305	CLA	C1D-ND	6.91	1.46	1.37
32	K	310	CLA	C1D-ND	6.91	1.46	1.37
32	O	309	CLA	C1D-ND	6.91	1.46	1.37
32	a	825	CLA	C1D-ND	6.91	1.46	1.37
32	I	306	CLA	C1D-ND	6.91	1.46	1.37
32	T	310	CLA	C1D-ND	6.91	1.46	1.37
32	W	313	CLA	C1D-ND	6.90	1.46	1.37
32	k	201	CLA	C1D-ND	6.90	1.46	1.37
32	S	313	CLA	C1D-ND	6.90	1.46	1.37
32	D	305	CLA	C1D-ND	6.90	1.46	1.37
32	a	839	CLA	C1D-ND	6.90	1.46	1.37
32	b	808	CLA	C1D-ND	6.90	1.46	1.37
32	a	813	CLA	C1D-ND	6.90	1.46	1.37
32	S	309	CLA	C1D-ND	6.90	1.46	1.37
32	Q	309	CLA	C1D-ND	6.90	1.46	1.37
32	a	818	CLA	C1D-ND	6.89	1.46	1.37
32	Q	301	CLA	C1D-ND	6.89	1.46	1.37
32	a	809	CLA	C1D-ND	6.89	1.46	1.37
32	l	202	CLA	C1D-ND	6.89	1.46	1.37
32	D	306	CLA	C1D-ND	6.89	1.46	1.37
32	H	301	CLA	C1D-ND	6.88	1.46	1.37
32	a	816	CLA	C1D-ND	6.88	1.46	1.37
32	D	310	CLA	C1D-ND	6.88	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	827	CLA	C1D-ND	6.88	1.46	1.37
32	J	307	CLA	C1D-ND	6.87	1.46	1.37
32	a	829	CLA	C1D-ND	6.87	1.46	1.37
32	r	202	CLA	C1D-ND	6.87	1.46	1.37
32	U	305	CLA	C1D-ND	6.87	1.46	1.37
32	G	304	CLA	C1D-ND	6.86	1.46	1.37
32	K	306	CLA	C1D-ND	6.86	1.46	1.37
32	V	201	CLA	C1D-ND	6.86	1.46	1.37
32	V	203	CLA	C1D-ND	6.86	1.46	1.37
32	a	826	CLA	C1D-ND	6.86	1.46	1.37
32	b	834	CLA	C1D-ND	6.85	1.46	1.37
32	A	309	CLA	C1D-ND	6.85	1.46	1.37
32	I	304	CLA	C1D-ND	6.85	1.46	1.37
32	J	304	CLA	C1D-ND	6.85	1.46	1.37
32	A	307	CLA	C1D-ND	6.84	1.46	1.37
32	A	308	CLA	C1D-ND	6.84	1.46	1.37
32	M	311	CLA	C1D-ND	6.84	1.46	1.37
32	D	313	CLA	C1D-ND	6.84	1.46	1.37
32	b	840	CLA	C1D-ND	6.84	1.46	1.37
32	a	837	CLA	C1D-ND	6.84	1.46	1.37
32	O	306	CLA	C1D-ND	6.83	1.46	1.37
32	F	306	CLA	C1D-ND	6.83	1.46	1.37
32	N	305	CLA	C1D-ND	6.83	1.46	1.37
32	a	806	CLA	C1D-ND	6.83	1.46	1.37
32	U	306	CLA	C1D-ND	6.83	1.46	1.37
32	G	303	CLA	C1D-ND	6.83	1.46	1.37
32	Q	305	CLA	C1D-ND	6.83	1.46	1.37
32	b	809	CLA	C1D-ND	6.83	1.46	1.37
32	D	315	CLA	C1D-ND	6.83	1.46	1.37
32	E	304	CLA	C1D-ND	6.83	1.46	1.37
32	M	308	CLA	C1D-ND	6.82	1.46	1.37
32	a	821	CLA	C1D-ND	6.82	1.46	1.37
32	F	309	CLA	C1D-ND	6.81	1.46	1.37
32	b	826	CLA	C1D-ND	6.81	1.46	1.37
32	T	306	CLA	C1D-ND	6.81	1.46	1.37
32	E	312	CLA	C1D-ND	6.81	1.46	1.37
32	J	309	CLA	C1D-ND	6.81	1.46	1.37
32	J	306	CLA	C1D-ND	6.80	1.46	1.37
32	b	814	CLA	C1D-ND	6.79	1.46	1.37
32	A	303	CLA	C1D-ND	6.79	1.46	1.37
32	A	305	CLA	C1D-ND	6.79	1.46	1.37
32	b	838	CLA	C1D-ND	6.78	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	834	CLA	C1D-ND	6.78	1.46	1.37
32	C	305	CLA	C1D-ND	6.78	1.46	1.37
32	Q	304	CLA	C1D-ND	6.78	1.46	1.37
32	a	805	CLA	MG-ND	-6.78	1.92	2.05
32	I	317	CLA	C1D-ND	6.77	1.46	1.37
32	a	833	CLA	C1D-ND	6.77	1.46	1.37
32	a	830	CLA	C1D-ND	6.77	1.46	1.37
32	a	841	CLA	C1D-ND	6.77	1.46	1.37
32	Q	306	CLA	C1D-ND	6.77	1.46	1.37
32	I	301	CLA	C1D-ND	6.77	1.46	1.37
32	b	820	CLA	C1D-ND	6.75	1.46	1.37
32	I	308	CLA	C1D-ND	6.75	1.46	1.37
32	b	837	CLA	C1D-ND	6.75	1.46	1.37
32	a	835	CLA	C1D-ND	6.75	1.46	1.37
32	a	836	CLA	C1D-ND	6.75	1.46	1.37
32	a	840	CLA	C1D-ND	6.74	1.46	1.37
32	b	812	CLA	C1D-ND	6.74	1.46	1.37
32	P	304	CLA	C1D-ND	6.74	1.46	1.37
32	A	311	CLA	C1D-ND	6.73	1.46	1.37
32	N	310	CLA	C1D-ND	6.73	1.46	1.37
32	b	813	CLA	C1D-ND	6.73	1.46	1.37
32	b	807	CLA	C1D-ND	6.72	1.46	1.37
32	A	304	CLA	C1D-ND	6.72	1.46	1.37
32	a	828	CLA	C1D-ND	6.72	1.46	1.37
32	W	306	CLA	C1D-ND	6.72	1.46	1.37
32	B	304	CLA	C1D-ND	6.71	1.46	1.37
32	R	306	CLA	C1D-ND	6.71	1.46	1.37
32	G	306	CLA	C1D-ND	6.71	1.46	1.37
32	D	308	CLA	C1D-ND	6.69	1.46	1.37
32	Q	303	CLA	C1D-ND	6.68	1.46	1.37
32	b	828	CLA	C1D-ND	6.68	1.46	1.37
32	b	824	CLA	C1D-ND	6.68	1.46	1.37
32	F	304	CLA	C1D-ND	6.67	1.46	1.37
32	a	820	CLA	C1D-ND	6.65	1.46	1.37
32	H	304	CLA	C1D-ND	6.65	1.46	1.37
32	f	201	CLA	C1D-ND	6.64	1.46	1.37
32	b	831	CLA	C1D-ND	6.64	1.45	1.37
32	I	303	CLA	C1D-ND	6.64	1.45	1.37
32	E	309	CLA	C1D-ND	6.63	1.45	1.37
32	E	307	CLA	C1D-ND	6.62	1.45	1.37
32	a	807	CLA	C1D-ND	6.62	1.45	1.37
32	O	305	CLA	C1D-ND	6.60	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	819	CLA	C1D-ND	6.60	1.45	1.37
32	U	303	CLA	C1D-ND	6.59	1.45	1.37
32	W	309	CLA	C1D-ND	6.56	1.45	1.37
32	L	307	CLA	C1D-ND	6.56	1.45	1.37
32	a	810	CLA	C1D-ND	6.55	1.45	1.37
33	R	305	KC2	C4B-NB	6.54	1.45	1.37
32	a	805	CLA	MG-NB	-6.54	1.92	2.05
32	a	824	CLA	C1D-ND	6.54	1.45	1.37
32	B	302	CLA	C1D-ND	6.53	1.45	1.37
32	a	814	CLA	C1D-ND	6.53	1.45	1.37
32	b	803	CLA	C1D-ND	6.52	1.45	1.37
32	l	204	CLA	C1D-ND	6.51	1.45	1.37
32	b	810	CLA	C1D-ND	6.50	1.45	1.37
32	b	822	CLA	C1D-ND	6.50	1.45	1.37
32	a	801	CLA	MG-ND	-6.49	1.92	2.05
32	E	306	CLA	C1D-ND	6.49	1.45	1.37
32	b	830	CLA	C1D-ND	6.48	1.45	1.37
32	D	307	CLA	C1D-ND	6.45	1.45	1.37
32	b	802	CLA	MG-ND	-6.45	1.93	2.05
32	b	804	CLA	C1D-ND	6.43	1.45	1.37
32	J	312	CLA	MG-NB	-6.42	1.93	2.05
32	b	832	CLA	C1D-ND	6.41	1.45	1.37
32	N	309	CLA	C1D-ND	6.41	1.45	1.37
32	D	314	CLA	MG-ND	-6.40	1.93	2.05
32	b	825	CLA	C1D-ND	6.39	1.45	1.37
32	a	852	CLA	C1D-ND	6.39	1.45	1.37
32	b	833	CLA	C1D-ND	6.36	1.45	1.37
32	b	805	CLA	MG-ND	-6.34	1.93	2.05
32	b	836	CLA	C1D-ND	6.32	1.45	1.37
32	C	308	CLA	MG-NB	-6.31	1.93	2.05
32	k	203	CLA	C1D-ND	6.29	1.45	1.37
32	a	823	CLA	C1D-ND	6.29	1.45	1.37
32	S	307	CLA	C1D-ND	6.29	1.45	1.37
33	C	303	KC2	C4B-NB	6.28	1.45	1.37
33	J	310	KC2	C4B-NB	6.28	1.45	1.37
33	S	302	KC2	C4B-NB	6.27	1.45	1.37
32	b	815	CLA	C1D-ND	6.25	1.45	1.37
32	a	838	CLA	C1D-ND	6.24	1.45	1.37
33	M	303	KC2	C4B-NB	6.23	1.45	1.37
33	L	305	KC2	C4B-NB	6.19	1.45	1.37
32	b	823	CLA	C1D-ND	6.17	1.45	1.37
33	M	321	KC2	C4B-NB	6.16	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	832	CLA	C1D-ND	6.16	1.45	1.37
33	H	303	KC2	C4B-NB	6.15	1.45	1.37
33	N	307	KC2	C4B-NB	6.14	1.45	1.37
33	A	310	KC2	C4B-NB	6.14	1.45	1.37
33	I	316	KC2	C4B-NB	6.13	1.45	1.37
33	F	302	KC2	C4B-NB	6.13	1.45	1.37
33	G	309	KC2	C4B-NB	6.12	1.45	1.37
32	N	309	CLA	MG-ND	-6.12	1.93	2.05
32	b	836	CLA	MG-ND	-6.11	1.93	2.05
32	a	812	CLA	MG-NB	-6.08	1.93	2.05
33	K	309	KC2	C4B-NB	6.06	1.45	1.37
33	J	303	KC2	C4B-NB	6.05	1.45	1.37
33	P	301	KC2	C4B-NB	6.05	1.45	1.37
32	a	823	CLA	MG-ND	-6.05	1.93	2.05
33	E	313	KC2	C4B-NB	6.05	1.45	1.37
32	F	322	CLA	MG-ND	-6.04	1.93	2.05
33	K	305	KC2	C4B-NB	6.04	1.45	1.37
32	L	307	CLA	MG-ND	-6.04	1.93	2.05
33	P	302	KC2	C4B-NB	6.03	1.45	1.37
33	P	312	KC2	C4B-NB	6.02	1.45	1.37
32	a	838	CLA	MG-ND	-6.01	1.93	2.05
33	R	311	KC2	C4B-NB	5.99	1.45	1.37
32	a	830	CLA	MG-ND	-5.99	1.93	2.05
33	Q	302	KC2	C4B-NB	5.99	1.45	1.37
33	G	302	KC2	C4B-NB	5.98	1.45	1.37
32	a	852	CLA	MG-ND	-5.97	1.93	2.05
33	M	307	KC2	C4B-NB	5.97	1.45	1.37
33	N	314	KC2	C4B-NB	5.97	1.45	1.37
33	R	302	KC2	C4B-NB	5.96	1.45	1.37
32	l	204	CLA	MG-NA	-5.96	1.92	2.06
33	W	314	KC2	C4B-NB	5.96	1.45	1.37
33	T	311	KC2	C4B-NB	5.95	1.45	1.37
33	R	303	KC2	C4B-NB	5.95	1.45	1.37
32	T	305	CLA	MG-ND	-5.95	1.94	2.05
33	O	302	KC2	C4B-NB	5.94	1.45	1.37
32	H	304	CLA	C1B-NB	5.94	1.45	1.37
33	P	306	KC2	C4B-NB	5.93	1.45	1.37
32	a	802	CLA	C1D-ND	5.93	1.45	1.37
32	a	802	CLA	MG-ND	-5.93	1.94	2.05
32	a	818	CLA	MG-ND	-5.93	1.94	2.05
33	L	313	KC2	C4B-NB	5.93	1.45	1.37
33	L	302	KC2	C4B-NB	5.92	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	F	310	KC2	C4B-NB	5.92	1.45	1.37
32	C	306	CLA	MG-NB	-5.92	1.94	2.05
32	P	310	CLA	C1B-NB	5.92	1.45	1.37
33	W	301	KC2	C4B-NB	5.91	1.45	1.37
33	L	306	KC2	C4B-NB	5.90	1.45	1.37
32	b	802	CLA	C1D-ND	5.90	1.45	1.37
32	b	810	CLA	MG-ND	-5.90	1.94	2.05
32	E	306	CLA	MG-NB	-5.90	1.94	2.05
32	H	302	CLA	MG-NB	-5.90	1.94	2.05
32	I	304	CLA	MG-ND	-5.89	1.94	2.05
33	M	302	KC2	C4B-NB	5.89	1.45	1.37
32	b	832	CLA	MG-NB	-5.89	1.94	2.05
32	b	838	CLA	MG-ND	-5.88	1.94	2.05
32	b	832	CLA	MG-ND	-5.87	1.94	2.05
32	R	301	CLA	C1B-NB	5.87	1.45	1.37
33	O	310	KC2	C4B-NB	5.87	1.45	1.37
32	G	307	CLA	C1B-NB	5.86	1.45	1.37
32	B	304	CLA	C1B-NB	5.86	1.45	1.37
32	R	309	CLA	C1B-NB	5.86	1.45	1.37
33	S	306	KC2	C4B-NB	5.86	1.45	1.37
32	C	302	CLA	C1B-NB	5.85	1.45	1.37
32	b	802	CLA	MG-NB	-5.85	1.94	2.05
32	a	812	CLA	MG-ND	-5.85	1.94	2.05
32	b	825	CLA	MG-ND	-5.85	1.94	2.05
32	W	310	CLA	MG-NB	-5.84	1.94	2.05
32	C	305	CLA	MG-NB	-5.84	1.94	2.05
32	C	306	CLA	MG-ND	-5.84	1.94	2.05
32	C	305	CLA	C1B-NB	5.83	1.45	1.37
33	U	304	KC2	C4B-NB	5.83	1.45	1.37
32	H	301	CLA	MG-ND	-5.83	1.94	2.05
32	J	309	CLA	MG-ND	-5.83	1.94	2.05
32	U	303	CLA	MG-ND	-5.83	1.94	2.05
32	U	301	CLA	C1B-NB	5.83	1.44	1.37
32	H	304	CLA	MG-ND	-5.82	1.94	2.05
32	N	305	CLA	MG-ND	-5.82	1.94	2.05
32	b	815	CLA	MG-ND	-5.81	1.94	2.05
33	M	313	KC2	C4B-NB	5.81	1.44	1.37
32	O	308	CLA	C1B-NB	5.81	1.44	1.37
32	M	308	CLA	MG-ND	-5.81	1.94	2.05
32	b	807	CLA	MG-NA	-5.81	1.92	2.06
32	J	305	CLA	MG-ND	-5.80	1.94	2.05
32	O	306	CLA	MG-ND	-5.80	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	805	CLA	C1D-ND	5.80	1.44	1.37
32	r	201	CLA	C1B-NB	5.80	1.44	1.37
32	B	304	CLA	MG-NA	-5.80	1.92	2.06
32	C	305	CLA	MG-ND	-5.80	1.94	2.05
32	C	304	CLA	C1B-NB	5.79	1.44	1.37
32	H	308	CLA	C1B-NB	5.79	1.44	1.37
33	T	303	KC2	C4B-NB	5.79	1.44	1.37
32	N	310	CLA	MG-NB	-5.78	1.94	2.05
32	S	307	CLA	MG-NA	-5.78	1.92	2.06
32	L	310	CLA	C1B-NB	5.78	1.44	1.37
32	J	307	CLA	C1B-NB	5.77	1.44	1.37
32	L	311	CLA	C1B-NB	5.77	1.44	1.37
32	B	305	CLA	C1B-NB	5.77	1.44	1.37
32	H	302	CLA	C1B-NB	5.77	1.44	1.37
32	C	305	CLA	MG-NA	-5.77	1.92	2.06
32	U	307	CLA	C1B-NB	5.77	1.44	1.37
32	H	308	CLA	MG-NB	-5.77	1.94	2.05
32	a	801	CLA	MG-NB	-5.76	1.94	2.05
32	B	301	CLA	C1B-NB	5.76	1.44	1.37
32	C	304	CLA	MG-NB	-5.76	1.94	2.05
32	l	204	CLA	MG-ND	-5.76	1.94	2.05
33	I	309	KC2	C4B-NB	5.76	1.44	1.37
32	S	307	CLA	MG-ND	-5.76	1.94	2.05
33	K	303	KC2	C4B-NB	5.76	1.44	1.37
32	O	306	CLA	MG-NB	-5.76	1.94	2.05
32	H	301	CLA	MG-NB	-5.76	1.94	2.05
33	N	306	KC2	C4B-NB	5.76	1.44	1.37
32	L	311	CLA	MG-ND	-5.75	1.94	2.05
33	Q	317	KC2	C4B-NB	5.75	1.44	1.37
32	Q	308	CLA	MG-NB	-5.75	1.94	2.05
32	B	302	CLA	MG-ND	-5.74	1.94	2.05
32	O	301	CLA	MG-NB	-5.74	1.94	2.05
32	b	840	CLA	MG-ND	-5.74	1.94	2.05
32	J	308	CLA	MG-NB	-5.74	1.94	2.05
32	K	310	CLA	C1B-NB	5.74	1.44	1.37
32	F	305	CLA	MG-ND	-5.74	1.94	2.05
32	b	816	CLA	MG-ND	-5.73	1.94	2.05
32	b	826	CLA	C1B-NB	5.73	1.44	1.37
32	H	305	CLA	MG-ND	-5.73	1.94	2.05
32	l	204	CLA	MG-NB	-5.73	1.94	2.05
33	W	308	KC2	C4B-NB	5.73	1.44	1.37
32	b	826	CLA	MG-ND	-5.73	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	S	308	CLA	MG-ND	-5.73	1.94	2.05
32	b	838	CLA	MG-NB	-5.73	1.94	2.05
32	F	322	CLA	MG-NB	-5.72	1.94	2.05
32	N	310	CLA	MG-ND	-5.72	1.94	2.05
32	f	203	CLA	C1B-NB	5.72	1.44	1.37
32	b	809	CLA	MG-ND	-5.72	1.94	2.05
32	a	807	CLA	MG-NA	-5.72	1.92	2.06
32	H	304	CLA	MG-NB	-5.72	1.94	2.05
32	T	309	CLA	C1B-NB	5.71	1.44	1.37
32	O	301	CLA	C1B-NB	5.71	1.44	1.37
32	S	310	CLA	C1B-NB	5.71	1.44	1.37
32	F	304	CLA	MG-NB	-5.71	1.94	2.05
32	b	801	CLA	C1B-NB	5.71	1.44	1.37
32	b	813	CLA	MG-ND	-5.71	1.94	2.05
33	N	302	KC2	C4B-NB	5.71	1.44	1.37
32	a	821	CLA	MG-ND	-5.71	1.94	2.05
32	r	201	CLA	MG-ND	-5.71	1.94	2.05
32	f	204	CLA	MG-ND	-5.70	1.94	2.05
32	W	313	CLA	MG-NB	-5.70	1.94	2.05
32	a	822	CLA	MG-ND	-5.70	1.94	2.05
32	b	838	CLA	C1B-NB	5.70	1.44	1.37
32	W	309	CLA	MG-ND	-5.70	1.94	2.05
32	P	304	CLA	MG-ND	-5.70	1.94	2.05
32	K	310	CLA	MG-ND	-5.70	1.94	2.05
32	L	309	CLA	MG-ND	-5.70	1.94	2.05
32	M	311	CLA	MG-ND	-5.70	1.94	2.05
32	T	302	CLA	C1B-NB	5.69	1.44	1.37
32	G	308	CLA	C1B-NB	5.69	1.44	1.37
32	S	301	CLA	C1B-NB	5.69	1.44	1.37
32	U	305	CLA	C1B-NB	5.69	1.44	1.37
32	L	309	CLA	MG-NB	-5.69	1.94	2.05
32	a	807	CLA	MG-ND	-5.69	1.94	2.05
33	W	303	KC2	C4B-NB	5.68	1.44	1.37
32	E	314	CLA	C1B-NB	5.68	1.44	1.37
32	F	308	CLA	C1B-NB	5.68	1.44	1.37
32	U	306	CLA	MG-ND	-5.68	1.94	2.05
32	A	306	CLA	MG-NB	-5.68	1.94	2.05
32	a	832	CLA	MG-ND	-5.68	1.94	2.05
32	S	311	CLA	MG-NA	-5.68	1.92	2.06
32	E	311	CLA	C1B-NB	5.68	1.44	1.37
32	H	310	CLA	C1B-NB	5.68	1.44	1.37
32	G	301	CLA	MG-NB	-5.68	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	I	303	CLA	MG-NB	-5.68	1.94	2.05
32	a	820	CLA	MG-ND	-5.67	1.94	2.05
32	H	308	CLA	MG-ND	-5.67	1.94	2.05
32	D	312	CLA	MG-ND	-5.67	1.94	2.05
32	T	308	CLA	MG-NB	-5.67	1.94	2.05
32	b	808	CLA	MG-ND	-5.67	1.94	2.05
32	N	309	CLA	MG-NB	-5.67	1.94	2.05
32	S	313	CLA	C1B-NB	5.66	1.44	1.37
32	K	304	CLA	C1B-NB	5.66	1.44	1.37
32	a	812	CLA	C1D-ND	5.66	1.44	1.37
32	D	308	CLA	MG-ND	-5.66	1.94	2.05
32	a	819	CLA	MG-ND	-5.66	1.94	2.05
32	B	306	CLA	MG-ND	-5.66	1.94	2.05
32	Q	303	CLA	C1B-NB	5.66	1.44	1.37
32	b	806	CLA	C1B-NB	5.66	1.44	1.37
32	b	803	CLA	MG-ND	-5.66	1.94	2.05
32	K	308	CLA	C1B-NB	5.66	1.44	1.37
33	S	303	KC2	C4B-NB	5.66	1.44	1.37
32	M	305	CLA	MG-ND	-5.66	1.94	2.05
32	a	829	CLA	MG-NB	-5.66	1.94	2.05
32	l	203	CLA	MG-ND	-5.65	1.94	2.05
32	F	301	CLA	C1B-NB	5.65	1.44	1.37
32	b	826	CLA	MG-NB	-5.65	1.94	2.05
32	U	305	CLA	MG-ND	-5.65	1.94	2.05
32	W	313	CLA	MG-ND	-5.65	1.94	2.05
32	L	314	CLA	C1B-NB	5.65	1.44	1.37
32	O	304	CLA	C1B-NB	5.65	1.44	1.37
32	P	307	CLA	C1B-NB	5.65	1.44	1.37
32	r	201	CLA	MG-NB	-5.65	1.94	2.05
32	A	304	CLA	MG-ND	-5.65	1.94	2.05
32	b	831	CLA	MG-ND	-5.65	1.94	2.05
32	E	308	CLA	MG-NB	-5.65	1.94	2.05
32	a	808	CLA	MG-NB	-5.65	1.94	2.05
32	E	307	CLA	MG-ND	-5.65	1.94	2.05
32	a	818	CLA	MG-NB	-5.65	1.94	2.05
32	b	836	CLA	MG-NB	-5.65	1.94	2.05
32	H	309	CLA	C1B-NB	5.64	1.44	1.37
32	I	308	CLA	MG-NB	-5.64	1.94	2.05
32	E	309	CLA	MG-ND	-5.64	1.94	2.05
32	j	101	CLA	C1B-NB	5.64	1.44	1.37
32	b	830	CLA	MG-ND	-5.64	1.94	2.05
32	C	307	CLA	MG-ND	-5.64	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	306	CLA	MG-ND	-5.64	1.94	2.05
32	r	202	CLA	MG-ND	-5.64	1.94	2.05
32	a	842	CLA	C1B-NB	5.64	1.44	1.37
32	b	819	CLA	MG-ND	-5.64	1.94	2.05
32	U	305	CLA	MG-NB	-5.63	1.94	2.05
32	E	308	CLA	MG-ND	-5.63	1.94	2.05
32	J	304	CLA	MG-ND	-5.63	1.94	2.05
32	a	828	CLA	MG-ND	-5.63	1.94	2.05
32	a	839	CLA	MG-ND	-5.63	1.94	2.05
32	U	305	CLA	MG-NA	-5.63	1.92	2.06
32	B	304	CLA	MG-ND	-5.63	1.94	2.05
33	K	302	KC2	C4B-NB	5.63	1.44	1.37
32	b	805	CLA	MG-NB	-5.63	1.94	2.05
32	E	304	CLA	C1B-NB	5.63	1.44	1.37
32	A	303	CLA	MG-ND	-5.63	1.94	2.05
32	b	828	CLA	MG-ND	-5.62	1.94	2.05
32	Q	303	CLA	MG-NA	-5.62	1.92	2.06
32	a	841	CLA	MG-ND	-5.62	1.94	2.05
32	H	308	CLA	MG-NA	-5.62	1.92	2.06
32	H	301	CLA	MG-NA	-5.62	1.92	2.06
32	A	311	CLA	MG-ND	-5.62	1.94	2.05
32	a	824	CLA	MG-ND	-5.62	1.94	2.05
32	O	304	CLA	MG-ND	-5.62	1.94	2.05
32	b	820	CLA	MG-ND	-5.62	1.94	2.05
32	S	301	CLA	MG-NB	-5.62	1.94	2.05
32	N	309	CLA	MG-NA	-5.62	1.92	2.06
32	I	303	CLA	MG-ND	-5.61	1.94	2.05
32	U	307	CLA	MG-ND	-5.61	1.94	2.05
32	Q	301	CLA	C1B-NB	5.61	1.44	1.37
32	D	308	CLA	C1B-NB	5.61	1.44	1.37
32	B	303	CLA	MG-ND	-5.61	1.94	2.05
32	M	312	CLA	C1B-NB	5.61	1.44	1.37
32	T	307	CLA	MG-NB	-5.61	1.94	2.05
32	b	812	CLA	MG-ND	-5.61	1.94	2.05
32	a	830	CLA	C1B-NB	5.61	1.44	1.37
32	L	301	CLA	C1B-NB	5.61	1.44	1.37
32	O	305	CLA	MG-ND	-5.60	1.94	2.05
32	Q	308	CLA	MG-ND	-5.60	1.94	2.05
32	a	815	CLA	MG-ND	-5.60	1.94	2.05
32	a	813	CLA	C1B-NB	5.60	1.44	1.37
32	C	308	CLA	MG-NA	-5.60	1.93	2.06
32	a	830	CLA	MG-NB	-5.60	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	827	CLA	MG-ND	-5.60	1.94	2.05
32	b	830	CLA	MG-NA	-5.60	1.93	2.06
32	H	301	CLA	C1B-NB	5.60	1.44	1.37
32	b	807	CLA	MG-NB	-5.60	1.94	2.05
32	L	311	CLA	MG-NB	-5.60	1.94	2.05
32	Q	303	CLA	MG-ND	-5.60	1.94	2.05
32	M	308	CLA	MG-NB	-5.59	1.94	2.05
32	a	834	CLA	MG-ND	-5.59	1.94	2.05
32	J	302	CLA	C1B-NB	5.59	1.44	1.37
32	a	807	CLA	MG-NB	-5.59	1.94	2.05
32	f	201	CLA	MG-ND	-5.59	1.94	2.05
32	F	306	CLA	MG-ND	-5.59	1.94	2.05
32	G	306	CLA	MG-NB	-5.59	1.94	2.05
32	a	837	CLA	MG-ND	-5.59	1.94	2.05
32	H	309	CLA	MG-NA	-5.59	1.93	2.06
32	U	306	CLA	MG-NB	-5.59	1.94	2.05
32	Q	310	CLA	MG-NB	-5.59	1.94	2.05
32	b	821	CLA	MG-ND	-5.59	1.94	2.05
32	I	308	CLA	MG-NA	-5.59	1.93	2.06
32	S	301	CLA	MG-NA	-5.59	1.93	2.06
32	B	303	CLA	C1B-NB	5.59	1.44	1.37
32	I	307	CLA	C1B-NB	5.58	1.44	1.37
32	J	305	CLA	C1B-NB	5.58	1.44	1.37
32	Q	301	CLA	MG-NB	-5.58	1.94	2.05
32	C	304	CLA	MG-NA	-5.58	1.93	2.06
32	O	307	CLA	MG-NB	-5.58	1.94	2.05
32	I	303	CLA	MG-NA	-5.58	1.93	2.06
32	P	304	CLA	MG-NA	-5.58	1.93	2.06
32	J	308	CLA	C1B-NB	5.58	1.44	1.37
32	U	301	CLA	MG-NB	-5.58	1.94	2.05
32	S	311	CLA	MG-NB	-5.58	1.94	2.05
32	a	811	CLA	MG-ND	-5.58	1.94	2.05
32	H	309	CLA	MG-NB	-5.58	1.94	2.05
32	I	305	CLA	MG-ND	-5.58	1.94	2.05
32	T	308	CLA	MG-ND	-5.58	1.94	2.05
32	a	833	CLA	MG-ND	-5.58	1.94	2.05
33	W	304	KC2	C4B-NB	5.57	1.44	1.37
32	N	305	CLA	MG-NB	-5.57	1.94	2.05
32	a	836	CLA	MG-ND	-5.57	1.94	2.05
32	a	813	CLA	MG-ND	-5.57	1.94	2.05
32	D	309	CLA	MG-NB	-5.57	1.94	2.05
32	J	308	CLA	MG-ND	-5.57	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	821	CLA	MG-NB	-5.57	1.94	2.05
32	Q	301	CLA	MG-ND	-5.57	1.94	2.05
32	M	311	CLA	C1B-NB	5.57	1.44	1.37
32	Q	306	CLA	MG-ND	-5.57	1.94	2.05
32	b	826	CLA	MG-NA	-5.57	1.93	2.06
32	I	306	CLA	C1B-NB	5.57	1.44	1.37
32	W	313	CLA	MG-NA	-5.57	1.93	2.06
32	Q	309	CLA	MG-ND	-5.57	1.94	2.05
32	F	305	CLA	C1B-NB	5.57	1.44	1.37
32	a	814	CLA	MG-ND	-5.56	1.94	2.05
32	E	304	CLA	MG-ND	-5.56	1.94	2.05
32	A	301	CLA	MG-ND	-5.56	1.94	2.05
32	W	307	CLA	MG-ND	-5.56	1.94	2.05
32	O	307	CLA	MG-ND	-5.56	1.94	2.05
32	Q	304	CLA	MG-ND	-5.56	1.94	2.05
32	a	803	CLA	C1B-NB	5.56	1.44	1.37
32	A	307	CLA	MG-NB	-5.56	1.94	2.05
32	S	307	CLA	MG-NB	-5.56	1.94	2.05
32	a	826	CLA	MG-ND	-5.56	1.94	2.05
32	P	308	CLA	MG-ND	-5.55	1.94	2.05
32	R	304	CLA	C1B-NB	5.55	1.44	1.37
32	O	309	CLA	C1B-NB	5.55	1.44	1.37
32	T	310	CLA	MG-ND	-5.55	1.94	2.05
32	a	829	CLA	C1B-NB	5.55	1.44	1.37
32	N	305	CLA	MG-NA	-5.55	1.93	2.06
32	b	838	CLA	MG-NA	-5.55	1.93	2.06
32	U	307	CLA	MG-NB	-5.55	1.94	2.05
32	D	312	CLA	C1B-NB	5.55	1.44	1.37
32	b	814	CLA	MG-ND	-5.55	1.94	2.05
32	W	307	CLA	C1B-NB	5.55	1.44	1.37
32	a	806	CLA	MG-ND	-5.55	1.94	2.05
32	F	304	CLA	MG-ND	-5.55	1.94	2.05
32	P	309	CLA	MG-ND	-5.55	1.94	2.05
32	a	831	CLA	MG-ND	-5.55	1.94	2.05
32	O	301	CLA	MG-ND	-5.54	1.94	2.05
32	W	306	CLA	MG-ND	-5.54	1.94	2.05
32	a	837	CLA	MG-NA	-5.54	1.93	2.06
32	Q	310	CLA	C1B-NB	5.54	1.44	1.37
32	S	305	CLA	C1B-NB	5.54	1.44	1.37
32	b	811	CLA	MG-ND	-5.54	1.94	2.05
32	a	813	CLA	MG-NA	-5.54	1.93	2.06
32	C	309	CLA	C1B-NB	5.54	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	k	203	CLA	MG-NB	-5.54	1.94	2.05
32	N	311	CLA	MG-ND	-5.54	1.94	2.05
32	L	304	CLA	MG-ND	-5.54	1.94	2.05
32	N	313	CLA	C1B-NB	5.54	1.44	1.37
32	r	202	CLA	C1B-NB	5.54	1.44	1.37
32	R	306	CLA	MG-ND	-5.53	1.94	2.05
32	T	306	CLA	MG-ND	-5.53	1.94	2.05
32	G	304	CLA	MG-ND	-5.53	1.94	2.05
32	P	307	CLA	MG-ND	-5.53	1.94	2.05
32	D	304	CLA	C1B-NB	5.53	1.44	1.37
32	a	810	CLA	MG-ND	-5.53	1.94	2.05
32	C	304	CLA	MG-ND	-5.53	1.94	2.05
32	M	311	CLA	MG-NB	-5.53	1.94	2.05
32	S	301	CLA	MG-ND	-5.53	1.94	2.05
32	E	303	CLA	C1B-NB	5.53	1.44	1.37
32	G	305	CLA	MG-ND	-5.53	1.94	2.05
32	K	301	CLA	MG-ND	-5.53	1.94	2.05
32	G	301	CLA	C1B-NB	5.53	1.44	1.37
32	B	305	CLA	MG-ND	-5.53	1.94	2.05
32	R	309	CLA	MG-ND	-5.53	1.94	2.05
32	N	312	CLA	C1B-NB	5.52	1.44	1.37
32	a	836	CLA	MG-NB	-5.52	1.94	2.05
33	M	304	KC2	C4B-NB	5.52	1.44	1.37
32	B	305	CLA	MG-NA	-5.52	1.93	2.06
32	f	204	CLA	C1B-NB	5.52	1.44	1.37
32	U	303	CLA	MG-NA	-5.52	1.93	2.06
32	T	302	CLA	MG-NB	-5.52	1.94	2.05
32	L	311	CLA	MG-NA	-5.52	1.93	2.06
32	W	311	CLA	MG-ND	-5.52	1.94	2.05
32	C	301	CLA	MG-ND	-5.52	1.94	2.05
32	C	302	CLA	MG-ND	-5.52	1.94	2.05
32	T	305	CLA	MG-NA	-5.52	1.93	2.06
32	b	828	CLA	C1B-NB	5.52	1.44	1.37
32	R	301	CLA	MG-NB	-5.52	1.94	2.05
32	A	307	CLA	MG-ND	-5.52	1.94	2.05
32	Q	310	CLA	MG-ND	-5.52	1.94	2.05
32	S	309	CLA	MG-ND	-5.52	1.94	2.05
32	A	305	CLA	C1B-NB	5.52	1.44	1.37
32	J	304	CLA	MG-NA	-5.52	1.93	2.06
32	k	202	CLA	C1B-NB	5.52	1.44	1.37
32	F	308	CLA	MG-NB	-5.52	1.94	2.05
32	J	307	CLA	MG-NA	-5.52	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	P	305	CLA	C1B-NB	5.52	1.44	1.37
32	S	305	CLA	MG-ND	-5.52	1.94	2.05
32	J	304	CLA	MG-NB	-5.51	1.94	2.05
32	K	304	CLA	MG-ND	-5.51	1.94	2.05
32	V	203	CLA	MG-ND	-5.51	1.94	2.05
32	a	840	CLA	MG-ND	-5.51	1.94	2.05
32	b	827	CLA	MG-ND	-5.51	1.94	2.05
32	D	313	CLA	C1B-NB	5.51	1.44	1.37
32	I	305	CLA	MG-NB	-5.51	1.94	2.05
32	C	301	CLA	C1B-NB	5.51	1.44	1.37
32	N	313	CLA	MG-ND	-5.51	1.94	2.05
32	E	305	CLA	MG-ND	-5.51	1.94	2.05
32	I	301	CLA	C1B-NB	5.51	1.44	1.37
32	H	304	CLA	MG-NA	-5.51	1.93	2.06
32	H	306	CLA	MG-NB	-5.51	1.94	2.05
32	a	818	CLA	C1B-NB	5.51	1.44	1.37
32	L	310	CLA	MG-NA	-5.51	1.93	2.06
32	L	312	CLA	C1B-NB	5.51	1.44	1.37
32	E	311	CLA	MG-ND	-5.51	1.94	2.05
32	E	309	CLA	MG-NB	-5.51	1.94	2.05
32	D	305	CLA	C1B-NB	5.51	1.44	1.37
32	I	302	CLA	C1B-NB	5.51	1.44	1.37
32	A	305	CLA	MG-ND	-5.51	1.94	2.05
32	b	837	CLA	MG-NB	-5.51	1.94	2.05
32	L	314	CLA	MG-ND	-5.50	1.94	2.05
32	a	820	CLA	MG-NB	-5.50	1.94	2.05
32	K	308	CLA	MG-ND	-5.50	1.94	2.05
32	R	304	CLA	MG-ND	-5.50	1.94	2.05
32	a	835	CLA	MG-ND	-5.50	1.94	2.05
32	Q	305	CLA	MG-NB	-5.50	1.94	2.05
32	Q	306	CLA	MG-NB	-5.50	1.94	2.05
32	b	816	CLA	MG-NB	-5.50	1.94	2.05
32	b	822	CLA	MG-ND	-5.50	1.94	2.05
32	R	306	CLA	C1B-NB	5.50	1.44	1.37
32	b	807	CLA	C1B-NB	5.50	1.44	1.37
32	E	306	CLA	MG-ND	-5.50	1.94	2.05
32	P	304	CLA	C1B-NB	5.50	1.44	1.37
33	N	303	KC2	C4B-NB	5.50	1.44	1.37
32	b	833	CLA	C1B-NB	5.50	1.44	1.37
32	U	303	CLA	MG-NB	-5.50	1.94	2.05
32	J	301	CLA	C1B-NB	5.50	1.44	1.37
32	R	310	CLA	C1B-NB	5.50	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	804	CLA	MG-ND	-5.50	1.94	2.05
32	L	308	CLA	C1B-NB	5.50	1.44	1.37
32	b	807	CLA	MG-ND	-5.50	1.94	2.05
32	J	301	CLA	MG-ND	-5.50	1.94	2.05
32	F	311	CLA	C1B-NB	5.50	1.44	1.37
32	H	306	CLA	C1B-NB	5.50	1.44	1.37
32	E	306	CLA	MG-NA	-5.50	1.93	2.06
32	K	301	CLA	C1B-NB	5.49	1.44	1.37
32	l	203	CLA	MG-NB	-5.49	1.94	2.05
32	a	832	CLA	MG-NB	-5.49	1.94	2.05
32	F	309	CLA	MG-NB	-5.49	1.94	2.05
32	R	307	CLA	MG-NB	-5.49	1.94	2.05
32	A	309	CLA	C1B-NB	5.49	1.44	1.37
32	K	307	CLA	MG-ND	-5.49	1.94	2.05
32	E	303	CLA	MG-ND	-5.49	1.94	2.05
32	J	311	CLA	MG-ND	-5.49	1.94	2.05
32	l	202	CLA	MG-ND	-5.49	1.94	2.05
32	V	201	CLA	C1B-NB	5.49	1.44	1.37
32	F	303	CLA	MG-ND	-5.49	1.94	2.05
32	k	201	CLA	MG-ND	-5.49	1.94	2.05
32	Q	309	CLA	C1B-NB	5.49	1.44	1.37
32	a	853	CLA	MG-ND	-5.49	1.94	2.05
32	H	302	CLA	MG-NA	-5.49	1.93	2.06
32	E	315	CLA	MG-ND	-5.48	1.94	2.05
32	a	837	CLA	C1B-NB	5.48	1.44	1.37
33	O	303	KC2	C4B-NB	5.48	1.44	1.37
32	b	809	CLA	MG-NB	-5.48	1.94	2.05
32	H	307	CLA	C1B-NB	5.48	1.44	1.37
32	U	302	CLA	MG-NB	-5.48	1.94	2.05
32	Q	303	CLA	MG-NB	-5.48	1.94	2.05
32	R	301	CLA	MG-ND	-5.48	1.94	2.05
32	F	303	CLA	C1B-NB	5.48	1.44	1.37
32	a	808	CLA	MG-ND	-5.47	1.94	2.05
32	G	306	CLA	MG-NA	-5.47	1.93	2.06
32	N	309	CLA	C1B-NB	5.47	1.44	1.37
32	E	305	CLA	C1B-NB	5.47	1.44	1.37
32	M	306	CLA	C1B-NB	5.47	1.44	1.37
33	N	304	KC2	C4B-NB	5.47	1.44	1.37
32	J	308	CLA	MG-NA	-5.47	1.93	2.06
32	W	312	CLA	MG-ND	-5.47	1.94	2.05
32	J	304	CLA	C1B-NB	5.47	1.44	1.37
32	S	304	CLA	C1B-NB	5.47	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	T	308	CLA	C1B-NB	5.47	1.44	1.37
32	U	306	CLA	C1B-NB	5.47	1.44	1.37
32	T	306	CLA	C1B-NB	5.47	1.44	1.37
32	O	304	CLA	MG-NB	-5.47	1.94	2.05
32	R	309	CLA	MG-NA	-5.47	1.93	2.06
32	I	317	CLA	MG-ND	-5.47	1.94	2.05
32	B	301	CLA	MG-ND	-5.47	1.94	2.05
32	P	308	CLA	C1B-NB	5.47	1.44	1.37
32	E	304	CLA	MG-NB	-5.47	1.94	2.05
32	O	301	CLA	MG-NA	-5.47	1.93	2.06
32	K	301	CLA	MG-NB	-5.47	1.94	2.05
32	W	312	CLA	C1B-NB	5.47	1.44	1.37
32	a	837	CLA	MG-NB	-5.46	1.95	2.05
32	Q	304	CLA	C1B-NB	5.46	1.44	1.37
32	F	306	CLA	MG-NB	-5.46	1.95	2.05
32	A	311	CLA	MG-NB	-5.46	1.95	2.05
32	D	309	CLA	MG-ND	-5.46	1.95	2.05
32	b	804	CLA	MG-NB	-5.46	1.95	2.05
32	b	823	CLA	MG-NA	-5.46	1.93	2.06
32	b	828	CLA	MG-NB	-5.46	1.95	2.05
32	E	315	CLA	C1B-NB	5.46	1.44	1.37
32	H	309	CLA	MG-ND	-5.46	1.95	2.05
32	a	829	CLA	MG-ND	-5.46	1.95	2.05
32	P	311	CLA	MG-ND	-5.46	1.95	2.05
32	S	304	CLA	MG-ND	-5.46	1.95	2.05
32	O	309	CLA	MG-ND	-5.46	1.95	2.05
32	U	302	CLA	MG-ND	-5.46	1.95	2.05
32	U	307	CLA	MG-NA	-5.46	1.93	2.06
32	H	310	CLA	MG-ND	-5.46	1.95	2.05
32	K	306	CLA	MG-ND	-5.46	1.95	2.05
32	C	302	CLA	MG-NB	-5.46	1.95	2.05
32	L	301	CLA	MG-NB	-5.46	1.95	2.05
32	V	201	CLA	MG-ND	-5.46	1.95	2.05
32	a	823	CLA	MG-NB	-5.46	1.95	2.05
32	k	201	CLA	C1B-NB	5.45	1.44	1.37
32	b	837	CLA	MG-ND	-5.45	1.95	2.05
32	R	308	CLA	MG-ND	-5.45	1.95	2.05
32	D	310	CLA	MG-NB	-5.45	1.95	2.05
32	b	818	CLA	MG-NB	-5.45	1.95	2.05
32	I	317	CLA	C1B-NB	5.45	1.44	1.37
32	a	832	CLA	MG-NA	-5.45	1.93	2.06
32	a	831	CLA	C1B-NB	5.45	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	307	CLA	C1B-NB	5.45	1.44	1.37
32	M	308	CLA	C1B-NB	5.45	1.44	1.37
32	U	302	CLA	C1B-NB	5.45	1.44	1.37
32	L	310	CLA	MG-ND	-5.45	1.95	2.05
32	A	308	CLA	MG-ND	-5.45	1.95	2.05
32	a	804	CLA	MG-ND	-5.45	1.95	2.05
32	G	306	CLA	MG-ND	-5.45	1.95	2.05
32	B	304	CLA	MG-NB	-5.44	1.95	2.05
32	D	304	CLA	MG-ND	-5.44	1.95	2.05
32	T	302	CLA	MG-ND	-5.44	1.95	2.05
32	b	827	CLA	MG-NB	-5.44	1.95	2.05
32	b	824	CLA	MG-NB	-5.44	1.95	2.05
32	V	204	CLA	C1B-NB	5.44	1.44	1.37
32	a	811	CLA	C1B-NB	5.44	1.44	1.37
32	b	837	CLA	MG-NA	-5.44	1.93	2.06
32	U	306	CLA	MG-NA	-5.44	1.93	2.06
32	I	305	CLA	MG-NA	-5.44	1.93	2.06
32	a	802	CLA	MG-NA	-5.43	1.93	2.06
32	U	303	CLA	C1B-NB	5.43	1.44	1.37
32	P	304	CLA	MG-NB	-5.43	1.95	2.05
32	b	818	CLA	MG-ND	-5.43	1.95	2.05
32	D	311	CLA	MG-ND	-5.43	1.95	2.05
32	j	101	CLA	MG-ND	-5.43	1.95	2.05
32	B	309	CLA	C1B-NB	5.43	1.44	1.37
32	H	307	CLA	MG-ND	-5.43	1.95	2.05
32	b	817	CLA	MG-ND	-5.43	1.95	2.05
32	S	307	CLA	C1B-NB	5.43	1.44	1.37
32	R	310	CLA	MG-ND	-5.43	1.95	2.05
32	A	302	CLA	MG-ND	-5.43	1.95	2.05
32	B	306	CLA	C1B-NB	5.43	1.44	1.37
32	B	309	CLA	MG-ND	-5.43	1.95	2.05
32	E	315	CLA	MG-NB	-5.43	1.95	2.05
32	k	203	CLA	C1B-NB	5.43	1.44	1.37
32	G	303	CLA	C1B-NB	5.42	1.44	1.37
32	b	828	CLA	MG-NA	-5.42	1.93	2.06
32	H	302	CLA	MG-ND	-5.42	1.95	2.05
32	T	310	CLA	C1B-NB	5.42	1.44	1.37
32	H	305	CLA	MG-NB	-5.42	1.95	2.05
32	H	310	CLA	MG-NB	-5.42	1.95	2.05
32	a	812	CLA	MG-NA	-5.42	1.93	2.06
32	J	306	CLA	MG-ND	-5.42	1.95	2.05
32	T	310	CLA	MG-NB	-5.42	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	315	CLA	C1B-NB	5.42	1.44	1.37
32	F	311	CLA	MG-ND	-5.42	1.95	2.05
32	P	305	CLA	MG-ND	-5.42	1.95	2.05
32	k	202	CLA	MG-ND	-5.42	1.95	2.05
32	a	817	CLA	C1B-NB	5.42	1.44	1.37
32	a	825	CLA	MG-ND	-5.42	1.95	2.05
32	H	307	CLA	MG-NB	-5.42	1.95	2.05
32	D	307	CLA	MG-NB	-5.42	1.95	2.05
32	M	306	CLA	MG-ND	-5.42	1.95	2.05
32	W	306	CLA	MG-NA	-5.42	1.93	2.06
32	a	821	CLA	C1B-NB	5.42	1.44	1.37
32	E	304	CLA	MG-NA	-5.42	1.93	2.06
32	b	839	CLA	MG-ND	-5.41	1.95	2.05
32	a	816	CLA	MG-ND	-5.41	1.95	2.05
32	L	307	CLA	MG-NB	-5.41	1.95	2.05
32	V	204	CLA	MG-ND	-5.41	1.95	2.05
32	W	310	CLA	MG-ND	-5.41	1.95	2.05
32	a	816	CLA	C1B-NB	5.41	1.44	1.37
32	I	307	CLA	MG-ND	-5.41	1.95	2.05
32	b	818	CLA	C1B-NB	5.41	1.44	1.37
32	A	309	CLA	MG-ND	-5.41	1.95	2.05
32	G	307	CLA	MG-NA	-5.41	1.93	2.06
32	I	308	CLA	C1B-NB	5.41	1.44	1.37
32	C	307	CLA	MG-NB	-5.41	1.95	2.05
32	T	309	CLA	MG-ND	-5.41	1.95	2.05
32	D	315	CLA	MG-ND	-5.41	1.95	2.05
32	A	303	CLA	C1B-NB	5.41	1.44	1.37
32	P	310	CLA	MG-ND	-5.41	1.95	2.05
32	a	813	CLA	MG-NB	-5.41	1.95	2.05
32	a	852	CLA	MG-NB	-5.40	1.95	2.05
32	E	312	CLA	C1B-NB	5.40	1.44	1.37
32	B	301	CLA	MG-NB	-5.40	1.95	2.05
32	G	303	CLA	MG-ND	-5.40	1.95	2.05
32	b	830	CLA	MG-NB	-5.40	1.95	2.05
32	l	203	CLA	C1B-NB	5.40	1.44	1.37
32	A	304	CLA	C1B-NB	5.40	1.44	1.37
32	I	306	CLA	MG-ND	-5.40	1.95	2.05
32	K	307	CLA	MG-NB	-5.40	1.95	2.05
32	L	301	CLA	MG-ND	-5.40	1.95	2.05
32	I	301	CLA	MG-ND	-5.39	1.95	2.05
32	L	308	CLA	MG-NB	-5.39	1.95	2.05
32	a	840	CLA	MG-NB	-5.39	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	309	CLA	MG-ND	-5.39	1.95	2.05
32	b	818	CLA	MG-NA	-5.39	1.93	2.06
32	a	822	CLA	MG-NB	-5.39	1.95	2.05
32	I	302	CLA	MG-ND	-5.39	1.95	2.05
32	E	312	CLA	MG-ND	-5.39	1.95	2.05
32	b	821	CLA	C1B-NB	5.39	1.44	1.37
32	K	308	CLA	MG-NB	-5.39	1.95	2.05
32	a	809	CLA	C1B-NB	5.39	1.44	1.37
32	D	307	CLA	MG-NA	-5.39	1.93	2.06
32	K	307	CLA	C1B-NB	5.39	1.44	1.37
32	R	308	CLA	C1B-NB	5.39	1.44	1.37
32	J	302	CLA	MG-ND	-5.39	1.95	2.05
32	G	307	CLA	MG-ND	-5.39	1.95	2.05
32	I	308	CLA	MG-ND	-5.39	1.95	2.05
32	K	310	CLA	MG-NB	-5.39	1.95	2.05
32	b	837	CLA	C1B-NB	5.39	1.44	1.37
32	L	309	CLA	C1B-NB	5.38	1.44	1.37
32	O	304	CLA	MG-NA	-5.38	1.93	2.06
32	k	203	CLA	MG-ND	-5.38	1.95	2.05
32	a	834	CLA	C1B-NB	5.38	1.44	1.37
32	S	310	CLA	MG-ND	-5.38	1.95	2.05
32	F	306	CLA	C1B-NB	5.38	1.44	1.37
32	I	305	CLA	C1B-NB	5.38	1.44	1.37
32	J	311	CLA	C1B-NB	5.38	1.44	1.37
32	b	824	CLA	MG-ND	-5.38	1.95	2.05
32	N	312	CLA	MG-ND	-5.38	1.95	2.05
32	b	834	CLA	C1B-NB	5.38	1.44	1.37
32	F	305	CLA	MG-NA	-5.38	1.93	2.06
32	O	308	CLA	MG-ND	-5.38	1.95	2.05
32	R	301	CLA	MG-NA	-5.38	1.93	2.06
32	M	312	CLA	MG-ND	-5.38	1.95	2.05
32	b	840	CLA	C1B-NB	5.38	1.44	1.37
32	b	820	CLA	MG-NA	-5.38	1.93	2.06
32	E	310	CLA	MG-ND	-5.38	1.95	2.05
32	G	304	CLA	C1B-NB	5.38	1.44	1.37
32	N	311	CLA	C1B-NB	5.38	1.44	1.37
32	W	309	CLA	MG-NB	-5.38	1.95	2.05
32	a	836	CLA	C1B-NB	5.37	1.44	1.37
32	D	312	CLA	MG-NB	-5.37	1.95	2.05
32	J	301	CLA	MG-NB	-5.37	1.95	2.05
32	b	833	CLA	MG-ND	-5.37	1.95	2.05
32	Q	307	CLA	MG-ND	-5.37	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	305	CLA	MG-ND	-5.37	1.95	2.05
32	D	308	CLA	MG-NB	-5.37	1.95	2.05
32	K	306	CLA	MG-NB	-5.37	1.95	2.05
32	D	307	CLA	MG-ND	-5.37	1.95	2.05
32	V	203	CLA	MG-NB	-5.37	1.95	2.05
32	K	310	CLA	MG-NA	-5.37	1.93	2.06
32	b	809	CLA	C1B-NB	5.37	1.44	1.37
32	C	308	CLA	MG-ND	-5.37	1.95	2.05
32	Q	308	CLA	C1B-NB	5.37	1.44	1.37
32	F	309	CLA	MG-ND	-5.36	1.95	2.05
32	I	304	CLA	C1B-NB	5.36	1.44	1.37
33	T	304	KC2	C4B-NB	5.36	1.44	1.37
32	W	306	CLA	MG-NB	-5.36	1.95	2.05
32	b	835	CLA	MG-ND	-5.36	1.95	2.05
32	A	305	CLA	MG-NB	-5.36	1.95	2.05
32	E	310	CLA	C1B-NB	5.36	1.44	1.37
32	M	310	CLA	MG-ND	-5.36	1.95	2.05
32	a	810	CLA	MG-NB	-5.36	1.95	2.05
32	D	310	CLA	MG-ND	-5.36	1.95	2.05
32	F	307	CLA	MG-ND	-5.36	1.95	2.05
32	S	309	CLA	MG-NB	-5.36	1.95	2.05
32	S	313	CLA	MG-ND	-5.36	1.95	2.05
32	a	838	CLA	MG-NB	-5.36	1.95	2.05
32	k	203	CLA	MG-NA	-5.36	1.93	2.06
32	M	309	CLA	MG-NB	-5.36	1.95	2.05
32	D	310	CLA	MG-NA	-5.36	1.93	2.06
32	F	304	CLA	MG-NA	-5.36	1.93	2.06
32	R	306	CLA	MG-NA	-5.36	1.93	2.06
32	N	305	CLA	C1B-NB	5.36	1.44	1.37
32	Q	305	CLA	MG-ND	-5.36	1.95	2.05
32	W	313	CLA	C1B-NB	5.35	1.44	1.37
32	F	301	CLA	MG-NB	-5.35	1.95	2.05
32	W	311	CLA	MG-NB	-5.35	1.95	2.05
32	A	304	CLA	MG-NB	-5.35	1.95	2.05
32	D	309	CLA	C1B-NB	5.35	1.44	1.37
32	a	808	CLA	C1B-NB	5.35	1.44	1.37
32	b	830	CLA	C1B-NB	5.35	1.44	1.37
32	Q	309	CLA	MG-NB	-5.35	1.95	2.05
32	H	306	CLA	MG-ND	-5.35	1.95	2.05
32	b	817	CLA	C1B-NB	5.35	1.44	1.37
32	G	307	CLA	MG-NB	-5.35	1.95	2.05
32	a	828	CLA	C1B-NB	5.35	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	823	CLA	MG-ND	-5.35	1.95	2.05
32	a	825	CLA	MG-NB	-5.34	1.95	2.05
32	b	810	CLA	MG-NB	-5.34	1.95	2.05
32	b	816	CLA	C1B-NB	5.34	1.44	1.37
32	U	301	CLA	MG-ND	-5.34	1.95	2.05
32	H	305	CLA	MG-NA	-5.34	1.93	2.06
32	R	309	CLA	MG-NB	-5.34	1.95	2.05
32	S	311	CLA	MG-ND	-5.34	1.95	2.05
32	M	311	CLA	MG-NA	-5.34	1.93	2.06
32	R	307	CLA	MG-ND	-5.34	1.95	2.05
32	O	308	CLA	MG-NA	-5.34	1.93	2.06
32	B	302	CLA	MG-NB	-5.34	1.95	2.05
32	a	842	CLA	MG-ND	-5.34	1.95	2.05
32	B	305	CLA	MG-NB	-5.34	1.95	2.05
32	T	307	CLA	MG-ND	-5.33	1.95	2.05
32	P	311	CLA	C1B-NB	5.33	1.44	1.37
32	b	804	CLA	C1B-NB	5.33	1.44	1.37
32	S	308	CLA	MG-NB	-5.33	1.95	2.05
32	M	305	CLA	C1B-NB	5.33	1.44	1.37
32	b	820	CLA	C1B-NB	5.33	1.44	1.37
32	I	303	CLA	C1B-NB	5.33	1.44	1.37
32	b	804	CLA	MG-NA	-5.33	1.93	2.06
32	C	302	CLA	MG-NA	-5.33	1.93	2.06
32	b	815	CLA	MG-NB	-5.32	1.95	2.05
32	I	307	CLA	MG-NB	-5.32	1.95	2.05
32	J	309	CLA	MG-NB	-5.32	1.95	2.05
32	A	308	CLA	C1B-NB	5.32	1.44	1.37
32	L	308	CLA	MG-ND	-5.32	1.95	2.05
32	a	809	CLA	MG-ND	-5.32	1.95	2.05
32	O	308	CLA	MG-NB	-5.32	1.95	2.05
32	P	309	CLA	C1B-NB	5.32	1.44	1.37
32	W	309	CLA	C1B-NB	5.32	1.44	1.37
32	D	304	CLA	MG-NB	-5.32	1.95	2.05
33	L	303	KC2	C4B-NB	5.31	1.44	1.37
32	J	312	CLA	MG-NA	-5.31	1.93	2.06
32	G	301	CLA	MG-ND	-5.31	1.95	2.05
32	b	820	CLA	MG-NB	-5.31	1.95	2.05
32	a	852	CLA	MG-NA	-5.31	1.93	2.06
32	F	305	CLA	MG-NB	-5.31	1.95	2.05
32	b	819	CLA	MG-NB	-5.31	1.95	2.05
32	Q	307	CLA	C1B-NB	5.31	1.44	1.37
32	a	808	CLA	MG-NA	-5.31	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	309	CLA	MG-NB	-5.31	1.95	2.05
32	A	302	CLA	C1B-NB	5.31	1.44	1.37
32	b	803	CLA	MG-NB	-5.31	1.95	2.05
32	b	801	CLA	MG-ND	-5.31	1.95	2.05
32	F	307	CLA	C1B-NB	5.31	1.44	1.37
32	a	804	CLA	C1B-NB	5.31	1.44	1.37
32	b	834	CLA	MG-NB	-5.31	1.95	2.05
32	B	303	CLA	MG-NB	-5.31	1.95	2.05
32	Q	307	CLA	MG-NB	-5.31	1.95	2.05
32	T	305	CLA	MG-NB	-5.31	1.95	2.05
32	A	311	CLA	MG-NA	-5.31	1.93	2.06
32	C	301	CLA	MG-NB	-5.31	1.95	2.05
32	S	305	CLA	MG-NB	-5.31	1.95	2.05
32	E	311	CLA	MG-NB	-5.30	1.95	2.05
32	a	829	CLA	MG-NA	-5.30	1.93	2.06
32	O	307	CLA	C1B-NB	5.30	1.44	1.37
32	G	301	CLA	MG-NA	-5.30	1.93	2.06
32	W	306	CLA	C1B-NB	5.30	1.44	1.37
32	V	201	CLA	MG-NB	-5.30	1.95	2.05
32	S	311	CLA	C1B-NB	5.30	1.44	1.37
32	Q	310	CLA	MG-NA	-5.30	1.93	2.06
32	R	307	CLA	C1B-NB	5.30	1.44	1.37
32	f	203	CLA	MG-ND	-5.30	1.95	2.05
32	G	308	CLA	MG-NB	-5.30	1.95	2.05
32	a	826	CLA	C1B-NB	5.30	1.44	1.37
32	A	311	CLA	C1B-NB	5.29	1.44	1.37
32	D	307	CLA	C1B-NB	5.29	1.44	1.37
32	B	306	CLA	MG-NB	-5.29	1.95	2.05
32	F	301	CLA	MG-ND	-5.29	1.95	2.05
32	J	312	CLA	MG-ND	-5.29	1.95	2.05
32	I	304	CLA	MG-NB	-5.29	1.95	2.05
32	F	308	CLA	MG-NA	-5.29	1.93	2.06
32	E	307	CLA	C1B-NB	5.29	1.44	1.37
32	G	303	CLA	MG-NA	-5.29	1.93	2.06
32	A	307	CLA	MG-NA	-5.29	1.93	2.06
32	F	322	CLA	C1B-NB	5.29	1.44	1.37
32	P	310	CLA	MG-NB	-5.29	1.95	2.05
32	S	309	CLA	C1B-NB	5.29	1.44	1.37
32	P	309	CLA	MG-NB	-5.29	1.95	2.05
32	U	302	CLA	MG-NA	-5.29	1.93	2.06
32	L	314	CLA	MG-NB	-5.29	1.95	2.05
32	T	305	CLA	C1B-NB	5.29	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	839	CLA	C1B-NB	5.29	1.44	1.37
32	M	306	CLA	MG-NB	-5.29	1.95	2.05
32	L	312	CLA	MG-ND	-5.28	1.95	2.05
32	G	308	CLA	MG-ND	-5.28	1.95	2.05
33	N	308	KC2	C4B-NB	5.28	1.44	1.37
32	G	305	CLA	MG-NB	-5.28	1.95	2.05
32	D	311	CLA	C1B-NB	5.28	1.44	1.37
32	L	304	CLA	C1B-NB	5.28	1.44	1.37
32	J	311	CLA	MG-NB	-5.28	1.95	2.05
32	P	310	CLA	MG-NA	-5.28	1.93	2.06
32	C	307	CLA	C1B-NB	5.28	1.44	1.37
32	B	306	CLA	MG-NA	-5.28	1.93	2.06
32	b	806	CLA	MG-NB	-5.28	1.95	2.05
32	f	201	CLA	C1B-NB	5.28	1.44	1.37
32	G	303	CLA	MG-NB	-5.28	1.95	2.05
32	a	806	CLA	C1B-NB	5.28	1.44	1.37
32	a	802	CLA	MG-NB	-5.28	1.95	2.05
32	a	801	CLA	C1D-ND	5.27	1.44	1.37
32	b	829	CLA	MG-NB	-5.27	1.95	2.05
32	M	310	CLA	C1B-NB	5.27	1.44	1.37
32	A	302	CLA	MG-NB	-5.27	1.95	2.05
32	K	304	CLA	MG-NA	-5.27	1.93	2.06
32	a	833	CLA	C1B-NB	5.27	1.44	1.37
32	F	308	CLA	MG-ND	-5.27	1.95	2.05
32	b	829	CLA	MG-ND	-5.27	1.95	2.05
32	f	204	CLA	MG-NB	-5.27	1.95	2.05
32	b	813	CLA	C1B-NB	5.27	1.44	1.37
32	V	203	CLA	C1B-NB	5.27	1.44	1.37
32	M	309	CLA	MG-ND	-5.27	1.95	2.05
32	a	852	CLA	C1B-NB	5.27	1.44	1.37
32	r	202	CLA	MG-NB	-5.26	1.95	2.05
32	D	311	CLA	MG-NB	-5.26	1.95	2.05
32	A	301	CLA	MG-NB	-5.26	1.95	2.05
32	C	309	CLA	MG-NB	-5.26	1.95	2.05
32	S	308	CLA	MG-NA	-5.26	1.93	2.06
32	b	831	CLA	C1B-NB	5.26	1.44	1.37
32	J	311	CLA	MG-NA	-5.25	1.93	2.06
32	a	803	CLA	MG-ND	-5.25	1.95	2.05
32	b	823	CLA	MG-NB	-5.25	1.95	2.05
32	b	833	CLA	MG-NB	-5.25	1.95	2.05
32	b	827	CLA	MG-NA	-5.25	1.93	2.06
32	a	827	CLA	MG-NB	-5.25	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	L	310	CLA	MG-NB	-5.25	1.95	2.05
33	P	303	KC2	C4B-NB	5.25	1.44	1.37
32	I	301	CLA	MG-NB	-5.25	1.95	2.05
32	b	813	CLA	MG-NB	-5.25	1.95	2.05
32	N	311	CLA	MG-NB	-5.24	1.95	2.05
32	b	801	CLA	MG-NA	-5.24	1.93	2.06
32	F	301	CLA	MG-NA	-5.24	1.93	2.06
32	I	307	CLA	MG-NA	-5.24	1.93	2.06
32	N	312	CLA	MG-NB	-5.24	1.95	2.05
32	W	307	CLA	MG-NB	-5.24	1.95	2.05
32	a	835	CLA	C1B-NB	5.24	1.44	1.37
32	b	824	CLA	C1B-NB	5.24	1.44	1.37
32	a	831	CLA	MG-NB	-5.24	1.95	2.05
32	T	309	CLA	MG-NB	-5.23	1.95	2.05
32	a	840	CLA	MG-NA	-5.23	1.93	2.06
32	a	806	CLA	MG-NB	-5.23	1.95	2.05
32	A	305	CLA	MG-NA	-5.23	1.93	2.06
32	b	833	CLA	MG-NA	-5.23	1.93	2.06
32	E	310	CLA	MG-NB	-5.23	1.95	2.05
32	a	806	CLA	MG-NA	-5.23	1.93	2.06
32	S	313	CLA	MG-NA	-5.22	1.93	2.06
32	P	311	CLA	MG-NB	-5.22	1.95	2.05
32	a	839	CLA	MG-NB	-5.22	1.95	2.05
33	W	305	KC2	C4B-NB	5.22	1.44	1.37
32	E	308	CLA	C1B-NB	5.22	1.44	1.37
32	J	309	CLA	C1B-NB	5.22	1.44	1.37
32	b	834	CLA	MG-ND	-5.22	1.95	2.05
32	D	306	CLA	MG-ND	-5.22	1.95	2.05
32	M	308	CLA	MG-NA	-5.22	1.93	2.06
32	b	827	CLA	C1B-NB	5.22	1.44	1.37
32	S	308	CLA	C1B-NB	5.22	1.44	1.37
32	L	314	CLA	MG-NA	-5.22	1.93	2.06
32	J	302	CLA	MG-NB	-5.22	1.95	2.05
32	B	301	CLA	MG-NA	-5.22	1.93	2.06
32	a	824	CLA	C1B-NB	5.22	1.44	1.37
32	A	308	CLA	MG-NB	-5.22	1.95	2.05
32	b	808	CLA	MG-NB	-5.22	1.95	2.05
32	V	204	CLA	MG-NA	-5.21	1.93	2.06
32	b	840	CLA	MG-NB	-5.21	1.95	2.05
32	b	814	CLA	MG-NB	-5.21	1.95	2.05
32	D	308	CLA	MG-NA	-5.21	1.93	2.06
32	D	305	CLA	MG-NB	-5.21	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	V	204	CLA	MG-NB	-5.21	1.95	2.05
32	D	314	CLA	MG-NB	-5.21	1.95	2.05
32	I	317	CLA	MG-NB	-5.21	1.95	2.05
32	Q	305	CLA	C1B-NB	5.21	1.44	1.37
32	b	814	CLA	C1B-NB	5.21	1.44	1.37
32	F	307	CLA	MG-NB	-5.21	1.95	2.05
32	k	202	CLA	MG-NB	-5.21	1.95	2.05
32	Q	306	CLA	C1B-NB	5.21	1.44	1.37
32	a	820	CLA	C1B-NB	5.21	1.44	1.37
32	R	304	CLA	MG-NB	-5.21	1.95	2.05
32	r	201	CLA	MG-NA	-5.21	1.93	2.06
32	M	309	CLA	C1B-NB	5.20	1.44	1.37
32	b	834	CLA	MG-NA	-5.20	1.93	2.06
32	I	306	CLA	MG-NB	-5.20	1.95	2.05
32	E	306	CLA	C1B-NB	5.20	1.44	1.37
32	S	310	CLA	MG-NB	-5.20	1.95	2.05
32	T	307	CLA	MG-NA	-5.20	1.93	2.06
32	W	312	CLA	MG-NB	-5.20	1.95	2.05
32	R	308	CLA	MG-NB	-5.20	1.95	2.05
32	b	832	CLA	MG-NA	-5.20	1.93	2.06
32	S	313	CLA	MG-NB	-5.20	1.95	2.05
32	D	310	CLA	C1B-NB	5.20	1.44	1.37
32	B	302	CLA	MG-NA	-5.20	1.93	2.06
32	a	840	CLA	C1B-NB	5.20	1.44	1.37
32	O	307	CLA	MG-NA	-5.19	1.93	2.06
32	L	307	CLA	C1B-NB	5.19	1.44	1.37
32	a	835	CLA	MG-NB	-5.19	1.95	2.05
32	D	313	CLA	MG-NA	-5.19	1.93	2.06
32	F	309	CLA	MG-NA	-5.19	1.93	2.06
32	b	821	CLA	MG-NB	-5.19	1.95	2.05
32	K	306	CLA	MG-NA	-5.19	1.94	2.06
32	N	310	CLA	C1B-NB	5.19	1.44	1.37
32	J	307	CLA	MG-NB	-5.19	1.95	2.05
32	A	301	CLA	C1B-NB	5.18	1.44	1.37
32	a	815	CLA	C1B-NB	5.18	1.44	1.37
32	f	201	CLA	MG-NB	-5.18	1.95	2.05
32	T	307	CLA	C1B-NB	5.18	1.44	1.37
32	J	306	CLA	MG-NA	-5.18	1.94	2.06
32	b	832	CLA	C1B-NB	5.18	1.44	1.37
32	E	314	CLA	MG-ND	-5.18	1.95	2.05
32	b	829	CLA	MG-NA	-5.18	1.94	2.06
32	b	825	CLA	MG-NB	-5.18	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	l	202	CLA	MG-NB	-5.18	1.95	2.05
32	Q	301	CLA	MG-NA	-5.17	1.94	2.06
32	R	306	CLA	MG-NB	-5.17	1.95	2.05
32	b	812	CLA	MG-NB	-5.17	1.95	2.05
32	F	306	CLA	MG-NA	-5.17	1.94	2.06
32	E	312	CLA	MG-NB	-5.17	1.95	2.05
32	a	853	CLA	MG-NB	-5.17	1.95	2.05
32	A	303	CLA	MG-NB	-5.17	1.95	2.05
32	R	310	CLA	MG-NB	-5.17	1.95	2.05
32	V	201	CLA	MG-NA	-5.16	1.94	2.06
32	l	202	CLA	C1B-NB	5.16	1.44	1.37
32	K	304	CLA	MG-NB	-5.16	1.95	2.05
32	a	828	CLA	MG-NB	-5.16	1.95	2.05
32	b	831	CLA	MG-NB	-5.16	1.95	2.05
32	D	313	CLA	MG-ND	-5.16	1.95	2.05
32	E	311	CLA	MG-NA	-5.16	1.94	2.06
32	b	811	CLA	C1B-NB	5.16	1.44	1.37
32	D	315	CLA	MG-NA	-5.16	1.94	2.06
32	a	853	CLA	C1B-NB	5.16	1.44	1.37
32	a	819	CLA	MG-NB	-5.15	1.95	2.05
32	W	309	CLA	MG-NA	-5.15	1.94	2.06
32	D	313	CLA	MG-NB	-5.15	1.95	2.05
32	E	314	CLA	MG-NB	-5.15	1.95	2.05
32	R	304	CLA	MG-NA	-5.15	1.94	2.06
32	T	306	CLA	MG-NB	-5.15	1.95	2.05
32	E	314	CLA	MG-NA	-5.15	1.94	2.06
32	b	835	CLA	MG-NA	-5.15	1.94	2.06
32	E	312	CLA	MG-NA	-5.15	1.94	2.06
32	a	817	CLA	MG-ND	-5.15	1.95	2.05
32	b	829	CLA	C1B-NB	5.15	1.44	1.37
32	a	814	CLA	MG-NB	-5.14	1.95	2.05
32	Q	304	CLA	MG-NA	-5.14	1.94	2.06
32	C	306	CLA	C1B-NB	5.14	1.44	1.37
32	D	306	CLA	C1B-NB	5.14	1.44	1.37
32	N	313	CLA	MG-NB	-5.14	1.95	2.05
32	Q	308	CLA	MG-NA	-5.14	1.94	2.06
32	T	302	CLA	MG-NA	-5.14	1.94	2.06
32	F	311	CLA	MG-NB	-5.13	1.95	2.05
32	P	307	CLA	MG-NB	-5.13	1.95	2.05
32	a	811	CLA	MG-NB	-5.13	1.95	2.05
32	D	314	CLA	MG-NA	-5.13	1.94	2.06
32	b	806	CLA	MG-ND	-5.13	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	306	CLA	MG-NA	-5.13	1.94	2.06
32	b	836	CLA	MG-NA	-5.12	1.94	2.06
32	D	304	CLA	MG-NA	-5.12	1.94	2.06
32	a	832	CLA	C1B-NB	5.12	1.44	1.37
32	T	309	CLA	MG-NA	-5.12	1.94	2.06
32	O	305	CLA	C1B-NB	5.12	1.44	1.37
32	T	308	CLA	MG-NA	-5.12	1.94	2.06
32	M	312	CLA	MG-NB	-5.12	1.95	2.05
32	D	309	CLA	MG-NA	-5.12	1.94	2.06
32	L	307	CLA	MG-NA	-5.12	1.94	2.06
32	F	322	CLA	MG-NA	-5.11	1.94	2.06
32	J	306	CLA	C1B-NB	5.11	1.44	1.37
32	a	826	CLA	MG-NB	-5.11	1.95	2.05
32	T	310	CLA	MG-NA	-5.11	1.94	2.06
32	J	306	CLA	MG-NB	-5.11	1.95	2.05
32	a	802	CLA	C1B-NB	5.11	1.44	1.37
32	J	307	CLA	MG-ND	-5.11	1.95	2.05
32	I	304	CLA	MG-NA	-5.11	1.94	2.06
32	a	810	CLA	C1B-NB	5.11	1.44	1.37
32	F	309	CLA	C1B-NB	5.10	1.44	1.37
32	H	307	CLA	MG-NA	-5.10	1.94	2.06
32	b	823	CLA	C1B-NB	5.10	1.44	1.37
32	P	305	CLA	MG-NB	-5.10	1.95	2.05
32	a	839	CLA	C1B-NB	5.10	1.44	1.37
32	a	807	CLA	C1B-NB	5.10	1.44	1.37
32	M	310	CLA	MG-NB	-5.09	1.95	2.05
32	a	831	CLA	MG-NA	-5.09	1.94	2.06
32	a	820	CLA	MG-NA	-5.09	1.94	2.06
32	a	816	CLA	MG-NB	-5.09	1.95	2.05
32	a	838	CLA	C1B-NB	5.09	1.44	1.37
32	l	204	CLA	C1B-NB	5.09	1.44	1.37
32	A	306	CLA	C1B-NB	5.09	1.44	1.37
32	F	303	CLA	MG-NB	-5.09	1.95	2.05
32	b	801	CLA	MG-NB	-5.08	1.95	2.05
32	j	101	CLA	MG-NB	-5.08	1.95	2.05
32	O	306	CLA	C1B-NB	5.08	1.44	1.37
32	W	310	CLA	MG-NA	-5.08	1.94	2.06
32	L	308	CLA	MG-NA	-5.07	1.94	2.06
32	P	307	CLA	MG-NA	-5.07	1.94	2.06
32	a	830	CLA	MG-NA	-5.07	1.94	2.06
32	G	305	CLA	C1B-NB	5.07	1.44	1.37
32	b	812	CLA	C1B-NB	5.07	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	H	310	CLA	MG-NA	-5.06	1.94	2.06
32	b	822	CLA	MG-NA	-5.06	1.94	2.06
32	D	315	CLA	MG-NB	-5.05	1.95	2.05
32	a	815	CLA	MG-NB	-5.05	1.95	2.05
32	L	301	CLA	MG-NA	-5.05	1.94	2.06
32	a	827	CLA	C1B-NB	5.05	1.44	1.37
32	k	201	CLA	MG-NB	-5.05	1.95	2.05
32	a	834	CLA	MG-NB	-5.05	1.95	2.05
32	Q	305	CLA	MG-NA	-5.05	1.94	2.06
32	O	305	CLA	MG-NB	-5.05	1.95	2.05
32	b	822	CLA	MG-NB	-5.04	1.95	2.05
32	b	806	CLA	MG-NA	-5.04	1.94	2.06
32	E	307	CLA	MG-NB	-5.04	1.95	2.05
32	G	304	CLA	MG-NA	-5.04	1.94	2.06
32	P	308	CLA	MG-NB	-5.04	1.95	2.05
32	a	833	CLA	MG-NB	-5.04	1.95	2.05
32	G	304	CLA	MG-NB	-5.04	1.95	2.05
32	G	308	CLA	MG-NA	-5.04	1.94	2.06
32	R	310	CLA	MG-NA	-5.04	1.94	2.06
32	E	315	CLA	MG-NA	-5.04	1.94	2.06
32	P	311	CLA	MG-NA	-5.04	1.94	2.06
32	a	809	CLA	MG-NA	-5.04	1.94	2.06
32	a	804	CLA	MG-NB	-5.04	1.95	2.05
32	L	309	CLA	MG-NA	-5.03	1.94	2.06
32	B	303	CLA	MG-NA	-5.03	1.94	2.06
32	a	816	CLA	MG-NA	-5.03	1.94	2.06
32	B	309	CLA	MG-NB	-5.03	1.95	2.05
32	a	819	CLA	MG-NA	-5.03	1.94	2.06
32	b	817	CLA	MG-NB	-5.03	1.95	2.05
32	f	203	CLA	MG-NB	-5.03	1.95	2.05
32	b	822	CLA	C1B-NB	5.03	1.44	1.37
32	Q	304	CLA	MG-NB	-5.02	1.95	2.05
32	M	309	CLA	MG-NA	-5.02	1.94	2.06
32	F	304	CLA	C1B-NB	5.02	1.44	1.37
32	J	305	CLA	MG-NB	-5.02	1.95	2.05
32	a	819	CLA	C1B-NB	5.02	1.44	1.37
32	W	310	CLA	C1B-NB	5.02	1.44	1.37
32	O	309	CLA	MG-NB	-5.02	1.95	2.05
32	a	853	CLA	MG-NA	-5.02	1.94	2.06
32	a	827	CLA	MG-NA	-5.02	1.94	2.06
32	b	825	CLA	C1B-NB	5.01	1.43	1.37
32	b	824	CLA	MG-NA	-5.01	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	E	305	CLA	MG-NB	-5.01	1.95	2.05
32	D	311	CLA	MG-NA	-5.01	1.94	2.06
32	a	823	CLA	C1B-NB	5.01	1.43	1.37
32	P	305	CLA	MG-NA	-5.01	1.94	2.06
32	A	301	CLA	MG-NA	-5.01	1.94	2.06
32	l	202	CLA	MG-NA	-5.00	1.94	2.06
32	a	810	CLA	MG-NA	-5.00	1.94	2.06
32	K	308	CLA	MG-NA	-5.00	1.94	2.06
32	H	306	CLA	MG-NA	-5.00	1.94	2.06
32	E	303	CLA	MG-NB	-5.00	1.95	2.05
32	M	305	CLA	MG-NB	-4.99	1.95	2.05
32	K	306	CLA	C1B-NB	4.99	1.43	1.37
32	b	835	CLA	C1B-NB	4.99	1.43	1.37
32	a	841	CLA	C1B-NB	4.99	1.43	1.37
32	D	305	CLA	MG-NA	-4.99	1.94	2.06
32	E	309	CLA	MG-NA	-4.98	1.94	2.06
32	F	307	CLA	MG-NA	-4.98	1.94	2.06
32	a	841	CLA	MG-NB	-4.98	1.95	2.05
32	a	814	CLA	C1B-NB	4.98	1.43	1.37
32	a	818	CLA	MG-NA	-4.98	1.94	2.06
32	N	313	CLA	MG-NA	-4.98	1.94	2.06
32	a	805	CLA	MG-NA	-4.98	1.94	2.06
32	G	306	CLA	C1B-NB	4.98	1.43	1.37
32	a	836	CLA	MG-NA	-4.97	1.94	2.06
32	O	309	CLA	MG-NA	-4.97	1.94	2.06
32	H	305	CLA	C1B-NB	4.97	1.43	1.37
32	K	301	CLA	MG-NA	-4.96	1.94	2.06
32	S	310	CLA	MG-NA	-4.96	1.94	2.06
32	f	201	CLA	MG-NA	-4.96	1.94	2.06
32	S	304	CLA	MG-NB	-4.96	1.96	2.05
32	a	842	CLA	MG-NB	-4.96	1.96	2.05
32	N	310	CLA	MG-NA	-4.96	1.94	2.06
32	b	815	CLA	MG-NA	-4.96	1.94	2.06
32	R	307	CLA	MG-NA	-4.96	1.94	2.06
32	Q	306	CLA	MG-NA	-4.95	1.94	2.06
32	L	304	CLA	MG-NB	-4.95	1.96	2.05
32	b	811	CLA	MG-NB	-4.95	1.96	2.05
32	W	311	CLA	C1B-NB	4.95	1.43	1.37
32	N	312	CLA	MG-NA	-4.95	1.94	2.06
32	b	825	CLA	MG-NA	-4.95	1.94	2.06
32	J	301	CLA	MG-NA	-4.95	1.94	2.06
32	L	312	CLA	MG-NB	-4.94	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	T	306	CLA	MG-NA	-4.94	1.94	2.06
32	E	309	CLA	C1B-NB	4.94	1.43	1.37
32	a	801	CLA	C1B-NB	4.94	1.43	1.37
32	C	301	CLA	MG-NA	-4.93	1.94	2.06
32	I	301	CLA	MG-NA	-4.93	1.94	2.06
32	A	304	CLA	MG-NA	-4.93	1.94	2.06
32	a	824	CLA	MG-NA	-4.93	1.94	2.06
32	a	835	CLA	MG-NA	-4.93	1.94	2.06
32	J	302	CLA	MG-NA	-4.92	1.94	2.06
32	b	839	CLA	MG-NB	-4.92	1.96	2.05
32	b	819	CLA	C1B-NB	4.92	1.43	1.37
32	a	839	CLA	MG-NA	-4.91	1.94	2.06
32	a	803	CLA	MG-NB	-4.91	1.96	2.05
32	C	309	CLA	MG-NA	-4.91	1.94	2.06
32	a	809	CLA	MG-NB	-4.91	1.96	2.05
32	a	804	CLA	MG-NA	-4.91	1.94	2.06
32	k	201	CLA	MG-NA	-4.91	1.94	2.06
32	a	803	CLA	MG-NA	-4.91	1.94	2.06
32	M	312	CLA	MG-NA	-4.91	1.94	2.06
32	a	825	CLA	MG-NA	-4.91	1.94	2.06
32	I	306	CLA	MG-NA	-4.90	1.94	2.06
32	J	312	CLA	C1B-NB	4.90	1.43	1.37
32	b	810	CLA	C1B-NB	4.90	1.43	1.37
32	b	814	CLA	MG-NA	-4.90	1.94	2.06
32	O	305	CLA	MG-NA	-4.90	1.94	2.06
32	a	823	CLA	MG-NA	-4.90	1.94	2.06
32	B	302	CLA	C1B-NB	4.89	1.43	1.37
32	b	808	CLA	C1B-NB	4.89	1.43	1.37
32	D	306	CLA	MG-NB	-4.89	1.96	2.05
32	A	308	CLA	MG-NA	-4.89	1.94	2.06
32	C	307	CLA	MG-NA	-4.88	1.94	2.06
32	F	311	CLA	MG-NA	-4.88	1.94	2.06
32	b	836	CLA	C1B-NB	4.88	1.43	1.37
32	r	202	CLA	MG-NA	-4.88	1.94	2.06
32	W	312	CLA	MG-NA	-4.88	1.94	2.06
32	a	833	CLA	MG-NA	-4.88	1.94	2.06
32	b	835	CLA	MG-NB	-4.88	1.96	2.05
32	b	812	CLA	MG-NA	-4.88	1.94	2.06
32	E	307	CLA	MG-NA	-4.87	1.94	2.06
32	b	831	CLA	MG-NA	-4.87	1.94	2.06
32	b	809	CLA	MG-NA	-4.87	1.94	2.06
32	C	306	CLA	MG-NA	-4.86	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	T	312	A86	C32-C31	-4.86	1.46	1.54
32	I	317	CLA	MG-NA	-4.86	1.94	2.06
32	U	301	CLA	MG-NA	-4.86	1.94	2.06
32	Q	309	CLA	MG-NA	-4.86	1.94	2.06
32	a	825	CLA	C1B-NB	4.86	1.43	1.37
32	b	815	CLA	C1B-NB	4.86	1.43	1.37
32	V	203	CLA	MG-NA	-4.85	1.94	2.06
32	D	306	CLA	MG-NA	-4.85	1.94	2.06
32	a	841	CLA	MG-NA	-4.84	1.94	2.06
32	b	821	CLA	MG-NA	-4.84	1.94	2.06
32	D	312	CLA	MG-NA	-4.84	1.94	2.06
32	b	802	CLA	MG-NA	-4.84	1.94	2.06
32	I	302	CLA	MG-NB	-4.84	1.96	2.05
32	j	101	CLA	MG-NA	-4.84	1.94	2.06
32	A	309	CLA	MG-NA	-4.84	1.94	2.06
32	O	306	CLA	MG-NA	-4.84	1.94	2.06
32	b	803	CLA	MG-NA	-4.83	1.94	2.06
32	a	834	CLA	MG-NA	-4.83	1.94	2.06
32	b	813	CLA	MG-NA	-4.83	1.94	2.06
32	b	803	CLA	C1B-NB	4.83	1.43	1.37
32	b	805	CLA	MG-NA	-4.82	1.94	2.06
32	b	840	CLA	MG-NA	-4.82	1.94	2.06
32	J	305	CLA	MG-NA	-4.81	1.94	2.06
32	W	311	CLA	MG-NA	-4.81	1.94	2.06
32	b	839	CLA	MG-NA	-4.81	1.94	2.06
32	a	838	CLA	MG-NA	-4.81	1.94	2.06
32	A	302	CLA	MG-NA	-4.80	1.94	2.06
32	M	305	CLA	MG-NA	-4.80	1.94	2.06
32	L	312	CLA	MG-NA	-4.80	1.94	2.06
32	a	824	CLA	MG-NB	-4.80	1.96	2.05
32	I	302	CLA	MG-NA	-4.80	1.94	2.06
32	a	828	CLA	MG-NA	-4.79	1.94	2.06
32	f	203	CLA	MG-NA	-4.79	1.94	2.06
32	J	309	CLA	MG-NA	-4.79	1.94	2.06
32	f	204	CLA	MG-NA	-4.78	1.94	2.06
32	a	814	CLA	MG-NA	-4.78	1.94	2.06
32	S	309	CLA	MG-NA	-4.78	1.94	2.06
32	P	309	CLA	MG-NA	-4.77	1.94	2.06
32	E	310	CLA	MG-NA	-4.77	1.94	2.06
32	a	817	CLA	MG-NA	-4.76	1.95	2.06
32	W	307	CLA	MG-NA	-4.75	1.95	2.06
32	a	801	CLA	MG-NA	-4.75	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	808	CLA	MG-NA	-4.75	1.95	2.06
32	L	304	CLA	MG-NA	-4.75	1.95	2.06
32	a	826	CLA	MG-NA	-4.75	1.95	2.06
32	k	202	CLA	MG-NA	-4.74	1.95	2.06
32	P	308	CLA	MG-NA	-4.73	1.95	2.06
32	Q	307	CLA	MG-NA	-4.73	1.95	2.06
32	A	303	CLA	MG-NA	-4.73	1.95	2.06
32	b	805	CLA	C1B-NB	4.72	1.43	1.37
32	l	203	CLA	MG-NA	-4.71	1.95	2.06
32	A	306	CLA	MG-NA	-4.70	1.95	2.06
32	a	821	CLA	MG-NA	-4.70	1.95	2.06
32	D	314	CLA	C1D-ND	4.70	1.43	1.37
32	b	817	CLA	MG-NA	-4.69	1.95	2.06
32	b	810	CLA	MG-NA	-4.67	1.95	2.06
32	a	815	CLA	MG-NA	-4.67	1.95	2.06
32	b	811	CLA	MG-NA	-4.66	1.95	2.06
32	R	308	CLA	MG-NA	-4.66	1.95	2.06
32	N	311	CLA	MG-NA	-4.66	1.95	2.06
32	a	811	CLA	MG-NA	-4.64	1.95	2.06
32	E	303	CLA	MG-NA	-4.63	1.95	2.06
39	k	206	SQD	O8-S	4.61	1.63	1.47
32	a	817	CLA	MG-NB	-4.61	1.96	2.05
32	b	802	CLA	C1B-NB	4.59	1.43	1.37
32	a	822	CLA	C1B-NB	4.58	1.43	1.37
32	S	305	CLA	MG-NA	-4.58	1.95	2.06
33	M	307	KC2	C1B-NB	4.57	1.43	1.37
32	B	309	CLA	MG-NA	-4.56	1.95	2.06
32	K	307	CLA	MG-NA	-4.55	1.95	2.06
39	H	315	SQD	O8-S	4.55	1.63	1.47
32	E	305	CLA	MG-NA	-4.54	1.95	2.06
32	E	308	CLA	MG-NA	-4.53	1.95	2.06
32	M	310	CLA	MG-NA	-4.53	1.95	2.06
32	a	842	CLA	MG-NA	-4.51	1.95	2.06
33	P	303	KC2	C4C-NC	4.51	1.44	1.37
36	E	322	LMG	O8-C28	4.50	1.46	1.33
37	T	313	A86	C32-C31	-4.49	1.47	1.54
39	H	315	SQD	O48-C23	4.49	1.46	1.33
32	b	816	CLA	MG-NA	-4.45	1.95	2.06
32	F	303	CLA	MG-NA	-4.45	1.95	2.06
36	E	322	LMG	O7-C10	4.44	1.46	1.34
32	C	308	CLA	C1B-NB	4.44	1.43	1.37
36	A	317	LMG	O7-C10	4.41	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	M	320	LMG	O8-C28	4.36	1.46	1.33
40	b	846	DGD	O2G-C1B	4.36	1.46	1.34
32	S	304	CLA	C4B-NB	4.35	1.43	1.37
37	M	317	A86	C32-C31	-4.35	1.47	1.54
32	G	305	CLA	MG-NA	-4.32	1.96	2.06
33	M	304	KC2	C4C-NC	4.32	1.44	1.37
33	L	302	KC2	C1B-NB	4.31	1.43	1.37
32	S	313	CLA	C4B-NB	4.28	1.43	1.37
39	k	206	SQD	O48-C23	4.27	1.45	1.33
33	M	304	KC2	C1B-NB	4.26	1.43	1.37
33	R	303	KC2	C1B-NB	4.25	1.43	1.37
32	b	819	CLA	MG-NA	-4.25	1.96	2.06
32	a	842	CLA	C4B-NB	4.24	1.43	1.37
36	W	320	LMG	O8-C28	4.24	1.45	1.33
32	K	307	CLA	C3A-C2A	-4.24	1.50	1.54
32	a	817	CLA	C4B-NB	4.24	1.43	1.37
32	a	822	CLA	MG-NA	-4.23	1.96	2.06
36	N	301	LMG	O7-C10	4.23	1.46	1.34
33	P	302	KC2	C1B-NB	4.22	1.43	1.37
33	J	310	KC2	C1B-NB	4.21	1.43	1.37
32	S	304	CLA	MG-NA	-4.21	1.96	2.06
36	P	318	LMG	O8-C28	4.21	1.45	1.33
35	I	318	LHG	O7-C7	4.20	1.46	1.34
36	N	301	LMG	O8-C28	4.20	1.45	1.33
33	N	303	KC2	C1B-NB	4.20	1.42	1.37
33	M	313	KC2	C1B-NB	4.20	1.42	1.37
33	H	303	KC2	C1B-NB	4.19	1.42	1.37
36	M	320	LMG	O7-C10	4.18	1.46	1.34
32	L	314	CLA	C4B-NB	4.18	1.42	1.37
33	T	303	KC2	C1B-NB	4.18	1.42	1.37
36	F	319	LMG	O7-C10	4.17	1.46	1.34
33	P	303	KC2	C1B-NB	4.17	1.42	1.37
32	P	310	CLA	C4B-NB	4.17	1.42	1.37
39	k	206	SQD	O47-C7	4.16	1.46	1.34
33	N	314	KC2	C1B-NB	4.16	1.42	1.37
33	P	312	KC2	C1B-NB	4.16	1.42	1.37
33	S	312	KC2	C4B-NB	4.16	1.42	1.37
32	T	302	CLA	C4B-NB	4.15	1.42	1.37
32	B	305	CLA	C4B-NB	4.14	1.42	1.37
33	W	304	KC2	C1B-NB	4.14	1.42	1.37
33	C	303	KC2	C1B-NB	4.14	1.42	1.37
33	P	301	KC2	C1B-NB	4.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	L	306	KC2	C1B-NB	4.13	1.42	1.37
32	f	203	CLA	C4B-NB	4.13	1.42	1.37
33	N	314	KC2	C4C-NC	4.12	1.44	1.37
33	R	303	KC2	C4C-NC	4.11	1.44	1.37
32	C	309	CLA	C4B-NB	4.11	1.42	1.37
32	F	308	CLA	C4B-NB	4.11	1.42	1.37
33	L	303	KC2	C4C-NC	4.11	1.43	1.37
32	J	309	CLA	C4B-NB	4.10	1.42	1.37
33	L	303	KC2	C1B-NB	4.10	1.42	1.37
33	A	310	KC2	C1B-NB	4.10	1.42	1.37
33	I	316	KC2	C1B-NB	4.10	1.42	1.37
33	O	303	KC2	C1B-NB	4.10	1.42	1.37
32	a	824	CLA	C4B-NB	4.09	1.42	1.37
32	G	307	CLA	C4B-NB	4.09	1.42	1.37
32	a	812	CLA	MG-NC	-4.09	1.96	2.06
32	L	311	CLA	C4B-NB	4.09	1.42	1.37
33	N	302	KC2	C1B-NB	4.09	1.42	1.37
32	H	309	CLA	C4B-NB	4.09	1.42	1.37
36	E	320	LMG	O8-C28	4.08	1.45	1.33
35	a	851	LHG	O8-C23	4.07	1.45	1.33
32	T	309	CLA	C4B-NB	4.07	1.42	1.37
32	B	304	CLA	C4B-NB	4.07	1.42	1.37
33	R	302	KC2	C1B-NB	4.07	1.42	1.37
36	j	104	LMG	O8-C28	4.07	1.45	1.33
32	H	310	CLA	C4B-NB	4.07	1.42	1.37
32	O	308	CLA	C4B-NB	4.06	1.42	1.37
32	C	302	CLA	C4B-NB	4.06	1.42	1.37
32	E	314	CLA	C4B-NB	4.06	1.42	1.37
40	Q	318	DGD	O2G-C1B	4.06	1.45	1.34
32	G	308	CLA	C4B-NB	4.06	1.42	1.37
36	D	303	LMG	O8-C28	4.05	1.45	1.33
32	B	309	CLA	C4B-NB	4.05	1.42	1.37
32	F	301	CLA	C4B-NB	4.05	1.42	1.37
32	H	307	CLA	C4B-NB	4.04	1.42	1.37
32	U	301	CLA	C4B-NB	4.04	1.42	1.37
33	H	303	KC2	C4C-NC	4.04	1.43	1.37
33	K	309	KC2	C1B-NB	4.04	1.42	1.37
33	N	302	KC2	C4C-NC	4.04	1.43	1.37
36	P	318	LMG	O7-C10	4.04	1.45	1.34
36	S	322	LMG	O8-C28	4.04	1.45	1.33
32	B	301	CLA	C4B-NB	4.04	1.42	1.37
32	S	305	CLA	C4B-NB	4.03	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	833	CLA	C4B-NB	4.03	1.42	1.37
32	T	305	CLA	C4B-NB	4.03	1.42	1.37
32	F	311	CLA	C4B-NB	4.02	1.42	1.37
32	J	305	CLA	C4B-NB	4.02	1.42	1.37
33	O	302	KC2	C1B-NB	4.02	1.42	1.37
32	H	302	CLA	C4B-NB	4.02	1.42	1.37
32	r	202	CLA	C4B-NB	4.02	1.42	1.37
36	l	201	LMG	O7-C10	4.02	1.45	1.34
36	D	302	LMG	O8-C28	4.02	1.45	1.33
37	C	311	A86	C32-C31	-4.02	1.47	1.54
37	L	318	A86	C32-C31	-4.02	1.47	1.54
32	D	312	CLA	C4B-NB	4.02	1.42	1.37
33	C	303	KC2	C4C-NC	4.02	1.43	1.37
33	K	309	KC2	C4C-NC	4.02	1.43	1.37
32	L	312	CLA	C4B-NB	4.02	1.42	1.37
32	L	301	CLA	C4B-NB	4.01	1.42	1.37
33	G	302	KC2	C1B-NB	4.01	1.42	1.37
33	S	302	KC2	C1B-NB	4.01	1.42	1.37
32	O	309	CLA	C4B-NB	4.01	1.42	1.37
32	O	304	CLA	C4B-NB	4.01	1.42	1.37
33	W	314	KC2	C1B-NB	4.01	1.42	1.37
32	K	307	CLA	C4B-NB	4.00	1.42	1.37
33	T	304	KC2	C1B-NB	4.00	1.42	1.37
33	R	302	KC2	C4C-NC	4.00	1.43	1.37
33	N	307	KC2	C1B-NB	4.00	1.42	1.37
32	a	809	CLA	C4B-NB	4.00	1.42	1.37
32	C	301	CLA	C4B-NB	3.99	1.42	1.37
32	G	301	CLA	C4B-NB	3.99	1.42	1.37
32	C	308	CLA	MG-NC	-3.99	1.96	2.06
32	J	302	CLA	C4B-NB	3.99	1.42	1.37
33	M	302	KC2	C4C-NC	3.99	1.43	1.37
40	Q	318	DGD	O1G-C1A	3.99	1.45	1.33
32	M	312	CLA	C4B-NB	3.99	1.42	1.37
33	R	311	KC2	C1B-NB	3.99	1.42	1.37
32	R	301	CLA	C4B-NB	3.98	1.42	1.37
33	T	311	KC2	C1B-NB	3.98	1.42	1.37
32	R	309	CLA	C4B-NB	3.98	1.42	1.37
32	L	310	CLA	C4B-NB	3.98	1.42	1.37
32	S	310	CLA	C4B-NB	3.97	1.42	1.37
32	b	811	CLA	C4B-NB	3.97	1.42	1.37
32	Q	303	CLA	C4B-NB	3.97	1.42	1.37
32	b	813	CLA	C4B-NB	3.97	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	E	312	CLA	C4B-NB	3.97	1.42	1.37
36	W	320	LMG	O7-C10	3.96	1.45	1.34
32	a	811	CLA	C4B-NB	3.96	1.42	1.37
33	K	303	KC2	C1B-NB	3.96	1.42	1.37
33	S	302	KC2	C4C-NC	3.95	1.43	1.37
32	B	303	CLA	C4B-NB	3.95	1.42	1.37
32	I	308	CLA	C4B-NB	3.95	1.42	1.37
32	S	308	CLA	C4B-NB	3.95	1.42	1.37
32	f	204	CLA	C4B-NB	3.95	1.42	1.37
32	V	203	CLA	C4B-NB	3.94	1.42	1.37
32	D	306	CLA	C4B-NB	3.94	1.42	1.37
32	C	305	CLA	C4B-NB	3.94	1.42	1.37
33	F	310	KC2	C1B-NB	3.94	1.42	1.37
32	k	202	CLA	C4B-NB	3.94	1.42	1.37
32	R	304	CLA	C4B-NB	3.94	1.42	1.37
33	M	302	KC2	C1B-NB	3.94	1.42	1.37
33	P	302	KC2	C4C-NC	3.94	1.43	1.37
32	l	202	CLA	C4B-NB	3.94	1.42	1.37
32	M	305	CLA	C4B-NB	3.94	1.42	1.37
32	D	311	CLA	C4B-NB	3.93	1.42	1.37
32	E	307	CLA	C4B-NB	3.93	1.42	1.37
35	E	321	LHG	O8-C23	3.93	1.44	1.33
32	a	803	CLA	C4B-NB	3.93	1.42	1.37
33	Q	302	KC2	C1B-NB	3.93	1.42	1.37
32	I	307	CLA	C4B-NB	3.93	1.42	1.37
32	P	307	CLA	C4B-NB	3.93	1.42	1.37
32	U	302	CLA	C4B-NB	3.93	1.42	1.37
32	b	806	CLA	C4B-NB	3.93	1.42	1.37
32	E	305	CLA	C4B-NB	3.93	1.42	1.37
37	N	320	A86	C32-C31	-3.92	1.48	1.54
32	N	313	CLA	C4B-NB	3.92	1.42	1.37
32	D	308	CLA	C4B-NB	3.92	1.42	1.37
32	a	836	CLA	C4B-NB	3.92	1.42	1.37
33	M	303	KC2	C1B-NB	3.92	1.42	1.37
32	a	805	CLA	C1D-ND	3.92	1.42	1.37
32	P	308	CLA	C4B-NB	3.92	1.42	1.37
33	N	306	KC2	C1B-NB	3.92	1.42	1.37
32	H	304	CLA	C4B-NB	3.92	1.42	1.37
32	P	305	CLA	C4B-NB	3.92	1.42	1.37
32	V	201	CLA	C4B-NB	3.91	1.42	1.37
32	a	805	CLA	MG-NC	-3.91	1.97	2.06
32	B	306	CLA	C4B-NB	3.91	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	H	315	SQD	O47-C7	3.91	1.45	1.34
32	b	839	CLA	C4B-NB	3.91	1.42	1.37
32	W	307	CLA	C4B-NB	3.91	1.42	1.37
33	R	311	KC2	C4C-NC	3.91	1.43	1.37
32	j	101	CLA	C4B-NB	3.90	1.42	1.37
32	G	304	CLA	C4B-NB	3.90	1.42	1.37
32	N	309	CLA	MG-NC	-3.90	1.97	2.06
33	L	306	KC2	C4C-NC	3.90	1.43	1.37
32	I	317	CLA	C4B-NB	3.90	1.42	1.37
32	B	304	CLA	MG-NC	-3.90	1.97	2.06
32	U	306	CLA	C4B-NB	3.90	1.42	1.37
32	K	301	CLA	C4B-NB	3.90	1.42	1.37
32	K	308	CLA	C4B-NB	3.89	1.42	1.37
33	O	310	KC2	C1B-NB	3.89	1.42	1.37
32	K	310	CLA	C4B-NB	3.89	1.42	1.37
36	j	104	LMG	O7-C10	3.89	1.45	1.34
32	b	834	CLA	C4B-NB	3.89	1.42	1.37
32	Q	306	CLA	C4B-NB	3.89	1.42	1.37
32	T	310	CLA	C4B-NB	3.89	1.42	1.37
33	W	314	KC2	C4C-NC	3.89	1.43	1.37
33	P	301	KC2	C4C-NC	3.89	1.43	1.37
32	E	310	CLA	C4B-NB	3.88	1.42	1.37
32	M	306	CLA	C4B-NB	3.88	1.42	1.37
32	Q	307	CLA	C4B-NB	3.88	1.42	1.37
32	U	305	CLA	C4B-NB	3.88	1.42	1.37
32	S	307	CLA	MG-NC	-3.88	1.97	2.06
33	J	303	KC2	C4C-NC	3.88	1.43	1.37
33	G	309	KC2	C1B-NB	3.88	1.42	1.37
32	b	820	CLA	C4B-NB	3.88	1.42	1.37
33	N	308	KC2	C1B-NB	3.88	1.42	1.37
32	Q	310	CLA	C4B-NB	3.88	1.42	1.37
32	N	312	CLA	C4B-NB	3.88	1.42	1.37
32	a	822	CLA	C4B-NB	3.88	1.42	1.37
32	E	304	CLA	C4B-NB	3.87	1.42	1.37
32	I	304	CLA	C4B-NB	3.87	1.42	1.37
33	I	309	KC2	C1B-NB	3.87	1.42	1.37
32	C	307	CLA	C4B-NB	3.87	1.42	1.37
32	S	301	CLA	C4B-NB	3.87	1.42	1.37
33	U	304	KC2	C1B-NB	3.87	1.42	1.37
33	W	303	KC2	C1B-NB	3.87	1.42	1.37
33	L	302	KC2	C4C-NC	3.87	1.43	1.37
32	H	306	CLA	C4B-NB	3.87	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	201	CLA	C4B-NB	3.87	1.42	1.37
32	E	306	CLA	MG-NC	-3.87	1.97	2.06
32	I	301	CLA	C4B-NB	3.86	1.42	1.37
32	a	827	CLA	C4B-NB	3.86	1.42	1.37
32	A	305	CLA	C4B-NB	3.86	1.42	1.37
32	E	303	CLA	C4B-NB	3.86	1.42	1.37
36	D	303	LMG	O7-C10	3.86	1.45	1.34
32	U	307	CLA	C4B-NB	3.86	1.42	1.37
32	a	814	CLA	C4B-NB	3.86	1.42	1.37
35	E	321	LHG	O7-C7	3.86	1.45	1.34
32	O	301	CLA	C4B-NB	3.86	1.42	1.37
32	r	201	CLA	C4B-NB	3.86	1.42	1.37
33	J	310	KC2	C4C-NC	3.86	1.43	1.37
32	k	201	CLA	C4B-NB	3.86	1.42	1.37
36	S	322	LMG	O7-C10	3.86	1.45	1.34
32	I	306	CLA	C4B-NB	3.86	1.42	1.37
33	G	302	KC2	C4C-NC	3.85	1.43	1.37
35	B	308	LHG	O8-C23	3.85	1.44	1.33
33	T	304	KC2	C4C-NC	3.85	1.43	1.37
32	a	839	CLA	C4B-NB	3.85	1.42	1.37
32	V	204	CLA	C4B-NB	3.85	1.42	1.37
32	b	829	CLA	C4B-NB	3.85	1.42	1.37
32	l	204	CLA	MG-NC	-3.85	1.97	2.06
32	H	308	CLA	C4B-NB	3.85	1.42	1.37
33	W	303	KC2	C4C-NC	3.84	1.43	1.37
32	R	310	CLA	C4B-NB	3.84	1.42	1.37
33	K	302	KC2	C4C-NC	3.84	1.43	1.37
32	D	305	CLA	C4B-NB	3.84	1.42	1.37
32	E	311	CLA	C4B-NB	3.84	1.42	1.37
32	N	312	CLA	C3A-C2A	-3.84	1.50	1.54
32	F	305	CLA	C4B-NB	3.84	1.42	1.37
33	P	306	KC2	C4C-NC	3.84	1.43	1.37
32	a	804	CLA	C4B-NB	3.84	1.42	1.37
32	G	306	CLA	MG-NC	-3.84	1.97	2.06
37	S	316	A86	C32-C31	-3.84	1.48	1.54
32	b	801	CLA	C4B-NB	3.84	1.42	1.37
33	L	305	KC2	C1B-NB	3.84	1.42	1.37
37	U	308	A86	C32-C31	-3.83	1.48	1.54
36	D	325	LMG	O8-C28	3.83	1.44	1.33
33	O	302	KC2	C4C-NC	3.83	1.43	1.37
32	l	203	CLA	C4B-NB	3.83	1.42	1.37
32	L	304	CLA	C4B-NB	3.83	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	320	LMG	O8-C28	3.83	1.44	1.33
33	M	307	KC2	C4C-NC	3.83	1.43	1.37
32	J	301	CLA	C4B-NB	3.83	1.42	1.37
33	L	313	KC2	C1B-NB	3.83	1.42	1.37
32	G	305	CLA	C4B-NB	3.83	1.42	1.37
33	P	312	KC2	C4C-NC	3.83	1.43	1.37
32	F	307	CLA	C4B-NB	3.82	1.42	1.37
35	I	318	LHG	O8-C23	3.82	1.44	1.33
36	A	317	LMG	O8-C28	3.82	1.44	1.33
32	a	813	CLA	C4B-NB	3.82	1.42	1.37
32	a	837	CLA	C4B-NB	3.82	1.42	1.37
33	F	302	KC2	C1B-NB	3.82	1.42	1.37
33	N	307	KC2	C4C-NC	3.82	1.43	1.37
32	M	308	CLA	C4B-NB	3.81	1.42	1.37
33	U	304	KC2	C4C-NC	3.81	1.43	1.37
32	P	304	CLA	C4B-NB	3.81	1.42	1.37
32	D	315	CLA	C4B-NB	3.81	1.42	1.37
32	S	311	CLA	MG-NC	-3.81	1.97	2.06
33	E	313	KC2	C4C-NC	3.81	1.43	1.37
32	b	835	CLA	C4B-NB	3.81	1.42	1.37
33	I	309	KC2	C4C-NC	3.81	1.43	1.37
33	A	310	KC2	C4C-NC	3.80	1.43	1.37
32	a	834	CLA	C4B-NB	3.80	1.42	1.37
33	N	304	KC2	C4C-NC	3.80	1.43	1.37
33	N	306	KC2	C4C-NC	3.80	1.43	1.37
32	b	814	CLA	C4B-NB	3.80	1.42	1.37
32	a	816	CLA	C4B-NB	3.80	1.42	1.37
32	M	311	CLA	C4B-NB	3.79	1.42	1.37
33	T	303	KC2	C4C-NC	3.79	1.43	1.37
32	b	821	CLA	C4B-NB	3.79	1.42	1.37
32	H	309	CLA	MG-NC	-3.79	1.97	2.06
32	b	817	CLA	C4B-NB	3.78	1.42	1.37
33	K	305	KC2	C4C-NC	3.78	1.43	1.37
32	K	304	CLA	C4B-NB	3.78	1.42	1.37
33	P	306	KC2	C1B-NB	3.78	1.42	1.37
36	F	319	LMG	O8-C28	3.78	1.44	1.33
32	P	311	CLA	C4B-NB	3.78	1.42	1.37
32	C	305	CLA	MG-NC	-3.78	1.97	2.06
32	b	840	CLA	C4B-NB	3.78	1.42	1.37
32	R	308	CLA	C4B-NB	3.78	1.42	1.37
32	Q	301	CLA	C4B-NB	3.78	1.42	1.37
32	W	312	CLA	C4B-NB	3.78	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	313	CLA	C4B-NB	3.78	1.42	1.37
33	G	309	KC2	C4C-NC	3.77	1.43	1.37
33	W	301	KC2	C1B-NB	3.77	1.42	1.37
35	B	308	LHG	O7-C7	3.77	1.44	1.34
32	A	309	CLA	C4B-NB	3.77	1.42	1.37
32	R	307	CLA	C4B-NB	3.77	1.42	1.37
32	L	309	CLA	C4B-NB	3.77	1.42	1.37
32	F	303	CLA	C4B-NB	3.76	1.42	1.37
32	a	833	CLA	C4B-NB	3.76	1.42	1.37
36	D	302	LMG	O7-C10	3.76	1.44	1.34
32	R	306	CLA	C4B-NB	3.76	1.42	1.37
33	N	304	KC2	C1B-NB	3.76	1.42	1.37
32	C	306	CLA	C4B-NB	3.76	1.42	1.37
37	W	316	A86	C32-C31	-3.76	1.48	1.54
32	T	306	CLA	C4B-NB	3.76	1.42	1.37
33	T	311	KC2	C4C-NC	3.76	1.43	1.37
32	b	824	CLA	C4B-NB	3.76	1.42	1.37
33	J	303	KC2	C1B-NB	3.76	1.42	1.37
33	F	302	KC2	C4C-NC	3.75	1.43	1.37
32	a	852	CLA	MG-NC	-3.75	1.97	2.06
33	F	310	KC2	C4C-NC	3.75	1.43	1.37
33	N	303	KC2	C4C-NC	3.75	1.43	1.37
33	O	310	KC2	C4C-NC	3.75	1.43	1.37
32	S	308	CLA	MG-NC	-3.75	1.97	2.06
32	F	304	CLA	MG-NC	-3.75	1.97	2.06
35	a	851	LHG	O7-C7	3.75	1.44	1.34
33	K	302	KC2	C1B-NB	3.75	1.42	1.37
33	W	304	KC2	C4C-NC	3.74	1.43	1.37
32	A	308	CLA	C4B-NB	3.74	1.42	1.37
32	a	808	CLA	C4B-NB	3.74	1.42	1.37
32	H	301	CLA	C4B-NB	3.74	1.42	1.37
33	S	306	KC2	C1B-NB	3.74	1.42	1.37
32	I	303	CLA	MG-NC	-3.74	1.97	2.06
32	H	302	CLA	MG-NC	-3.74	1.97	2.06
32	P	309	CLA	C4B-NB	3.74	1.42	1.37
32	a	829	CLA	C4B-NB	3.73	1.42	1.37
36	D	325	LMG	O7-C10	3.73	1.44	1.34
33	S	303	KC2	C1B-NB	3.73	1.42	1.37
32	E	315	CLA	C4B-NB	3.73	1.42	1.37
32	G	306	CLA	C4B-NB	3.73	1.42	1.37
32	N	311	CLA	C4B-NB	3.73	1.42	1.37
32	a	802	CLA	MG-NC	-3.73	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Q	304	CLA	C4B-NB	3.73	1.42	1.37
32	a	805	CLA	C3D-C4D	-3.73	1.35	1.44
33	M	313	KC2	C4C-NC	3.72	1.43	1.37
32	Q	308	CLA	C4B-NB	3.72	1.42	1.37
32	D	314	CLA	MG-NC	-3.72	1.97	2.06
33	W	301	KC2	C4C-NC	3.72	1.43	1.37
36	E	302	LMG	C4-C5	3.72	1.60	1.53
33	L	313	KC2	C4C-NC	3.72	1.43	1.37
32	a	831	CLA	C4B-NB	3.72	1.42	1.37
32	a	815	CLA	C4B-NB	3.72	1.42	1.37
32	a	823	CLA	C4B-NB	3.72	1.42	1.37
32	B	302	CLA	C4B-NB	3.71	1.42	1.37
32	N	305	CLA	C4B-NB	3.71	1.42	1.37
32	a	853	CLA	C4B-NB	3.71	1.42	1.37
32	T	308	CLA	C4B-NB	3.71	1.42	1.37
32	C	304	CLA	MG-NC	-3.71	1.97	2.06
32	b	808	CLA	C4B-NB	3.71	1.42	1.37
32	A	302	CLA	C4B-NB	3.70	1.42	1.37
33	W	308	KC2	C4C-NC	3.70	1.43	1.37
36	l	201	LMG	O8-C28	3.70	1.44	1.33
32	Q	303	CLA	MG-NC	-3.70	1.97	2.06
32	L	308	CLA	C4B-NB	3.70	1.42	1.37
32	a	819	CLA	C4B-NB	3.70	1.42	1.37
32	b	830	CLA	C4B-NB	3.70	1.42	1.37
32	J	311	CLA	C4B-NB	3.70	1.42	1.37
32	W	309	CLA	C4B-NB	3.70	1.42	1.37
32	P	304	CLA	MG-NC	-3.70	1.97	2.06
32	H	305	CLA	C4B-NB	3.70	1.42	1.37
32	b	812	CLA	C4B-NB	3.69	1.42	1.37
32	b	819	CLA	C4B-NB	3.69	1.42	1.37
32	b	807	CLA	MG-NC	-3.69	1.97	2.06
32	T	305	CLA	MG-NC	-3.69	1.97	2.06
33	M	303	KC2	C4C-NC	3.68	1.43	1.37
32	b	803	CLA	C4B-NB	3.68	1.42	1.37
32	b	818	CLA	C4B-NB	3.68	1.42	1.37
32	b	827	CLA	C4B-NB	3.68	1.42	1.37
32	F	322	CLA	C4B-NB	3.67	1.42	1.37
32	W	306	CLA	C4B-NB	3.67	1.42	1.37
32	A	311	CLA	C4B-NB	3.67	1.42	1.37
33	E	313	KC2	C1B-NB	3.67	1.42	1.37
32	a	807	CLA	MG-NC	-3.67	1.97	2.06
32	L	307	CLA	C4B-NB	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Q	302	KC2	C4C-NC	3.67	1.43	1.37
32	a	820	CLA	C4B-NB	3.67	1.42	1.37
32	B	305	CLA	MG-NC	-3.67	1.97	2.06
33	S	303	KC2	C4C-NC	3.66	1.43	1.37
32	a	841	CLA	C4B-NB	3.66	1.42	1.37
33	S	306	KC2	C4C-NC	3.66	1.43	1.37
32	F	306	CLA	C4B-NB	3.66	1.42	1.37
32	b	838	CLA	MG-NC	-3.66	1.97	2.06
33	I	316	KC2	C4C-NC	3.66	1.43	1.37
33	O	303	KC2	C4C-NC	3.66	1.43	1.37
32	M	310	CLA	C4B-NB	3.66	1.42	1.37
32	W	313	CLA	C4B-NB	3.65	1.42	1.37
32	D	304	CLA	C4B-NB	3.65	1.42	1.37
32	T	307	CLA	C4B-NB	3.65	1.42	1.37
32	L	311	CLA	MG-NC	-3.65	1.97	2.06
37	M	314	A86	C32-C31	-3.65	1.48	1.54
32	S	307	CLA	C4B-NB	3.64	1.42	1.37
32	A	303	CLA	C4B-NB	3.64	1.42	1.37
32	a	825	CLA	C4B-NB	3.64	1.42	1.37
32	a	838	CLA	C4B-NB	3.64	1.42	1.37
32	J	307	CLA	C4B-NB	3.64	1.42	1.37
32	J	308	CLA	C4B-NB	3.64	1.42	1.37
33	W	305	KC2	C4C-NC	3.64	1.43	1.37
37	N	317	A86	C32-C31	-3.64	1.48	1.54
32	A	301	CLA	C4B-NB	3.63	1.42	1.37
32	D	307	CLA	MG-NC	-3.63	1.97	2.06
32	O	306	CLA	C4B-NB	3.63	1.42	1.37
33	L	305	KC2	C4C-NC	3.63	1.43	1.37
32	N	305	CLA	MG-NC	-3.62	1.97	2.06
32	D	310	CLA	MG-NC	-3.62	1.97	2.06
32	k	203	CLA	C4B-NB	3.62	1.42	1.37
33	R	305	KC2	C1B-NB	3.62	1.42	1.37
32	H	308	CLA	MG-NC	-3.62	1.97	2.06
36	E	320	LMG	O7-C10	3.62	1.44	1.34
32	a	810	CLA	C4B-NB	3.61	1.42	1.37
32	E	304	CLA	MG-NC	-3.61	1.97	2.06
32	E	306	CLA	C4B-NB	3.61	1.42	1.37
37	Q	316	A86	C32-C31	-3.61	1.48	1.54
37	K	311	A86	C32-C31	-3.61	1.48	1.54
33	W	308	KC2	C1B-NB	3.61	1.42	1.37
32	I	305	CLA	C4B-NB	3.60	1.42	1.37
32	F	305	CLA	MG-NC	-3.60	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	J	308	CLA	MG-NC	-3.60	1.97	2.06
32	S	301	CLA	MG-NC	-3.60	1.97	2.06
32	I	305	CLA	MG-NC	-3.59	1.97	2.06
32	F	309	CLA	C4B-NB	3.59	1.42	1.37
32	M	309	CLA	C4B-NB	3.59	1.42	1.37
32	D	309	CLA	C4B-NB	3.59	1.42	1.37
32	a	813	CLA	MG-NC	-3.59	1.97	2.06
32	U	306	CLA	MG-NC	-3.59	1.97	2.06
32	a	807	CLA	C4B-NB	3.59	1.42	1.37
32	a	826	CLA	C4B-NB	3.59	1.42	1.37
32	a	837	CLA	MG-NC	-3.58	1.97	2.06
32	N	310	CLA	C4B-NB	3.58	1.42	1.37
33	R	305	KC2	C4C-NC	3.58	1.43	1.37
32	H	301	CLA	MG-NC	-3.58	1.97	2.06
32	O	301	CLA	MG-NC	-3.58	1.97	2.06
32	Q	309	CLA	C4B-NB	3.58	1.42	1.37
32	b	806	CLA	MG-NC	-3.58	1.97	2.06
36	F	320	LMG	O7-C10	3.58	1.44	1.34
32	W	313	CLA	MG-NC	-3.58	1.97	2.06
32	F	309	CLA	MG-NC	-3.57	1.97	2.06
32	D	307	CLA	C4B-NB	3.57	1.42	1.37
32	N	309	CLA	C4B-NB	3.57	1.42	1.37
32	b	823	CLA	C4B-NB	3.57	1.42	1.37
32	H	305	CLA	MG-NC	-3.57	1.97	2.06
32	R	307	CLA	MG-NC	-3.57	1.97	2.06
32	b	834	CLA	MG-NC	-3.56	1.97	2.06
32	I	303	CLA	C4B-NB	3.56	1.42	1.37
32	b	831	CLA	C4B-NB	3.56	1.42	1.37
32	a	801	CLA	MG-NC	-3.56	1.97	2.06
32	R	306	CLA	MG-NC	-3.56	1.97	2.06
32	C	304	CLA	C4B-NB	3.56	1.42	1.37
32	b	807	CLA	C4B-NB	3.56	1.42	1.37
32	U	303	CLA	C4B-NB	3.56	1.42	1.37
32	U	307	CLA	MG-NC	-3.55	1.97	2.06
32	K	304	CLA	MG-NC	-3.55	1.97	2.06
32	a	802	CLA	C4B-NB	3.55	1.42	1.37
32	G	301	CLA	MG-NC	-3.55	1.97	2.06
32	b	816	CLA	C4B-NB	3.55	1.42	1.37
32	b	826	CLA	MG-NC	-3.55	1.97	2.06
32	b	837	CLA	C4B-NB	3.55	1.42	1.37
32	G	303	CLA	C4B-NB	3.55	1.42	1.37
32	J	307	CLA	MG-NC	-3.55	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	307	CLA	C4B-NB	3.54	1.42	1.37
33	K	303	KC2	C4C-NC	3.54	1.43	1.37
32	b	830	CLA	MG-NC	-3.54	1.97	2.06
32	b	810	CLA	C4B-NB	3.54	1.42	1.37
33	N	308	KC2	C4C-NC	3.54	1.43	1.37
32	b	837	CLA	MG-NC	-3.54	1.97	2.06
32	Q	310	CLA	MG-NC	-3.53	1.97	2.06
32	C	306	CLA	MG-NC	-3.53	1.97	2.06
32	a	808	CLA	MG-NC	-3.53	1.97	2.06
32	k	203	CLA	MG-NC	-3.53	1.97	2.06
32	S	309	CLA	C4B-NB	3.53	1.42	1.37
32	B	306	CLA	MG-NC	-3.53	1.97	2.06
32	M	311	CLA	MG-NC	-3.53	1.97	2.06
32	I	302	CLA	C4B-NB	3.53	1.42	1.37
32	D	310	CLA	C4B-NB	3.52	1.42	1.37
32	a	821	CLA	C4B-NB	3.52	1.42	1.37
32	b	832	CLA	C4B-NB	3.52	1.42	1.37
33	M	321	KC2	C4C-NC	3.52	1.43	1.37
32	W	311	CLA	C4B-NB	3.52	1.42	1.37
32	U	305	CLA	MG-NC	-3.52	1.97	2.06
32	O	304	CLA	MG-NC	-3.51	1.97	2.06
32	J	304	CLA	MG-NC	-3.51	1.97	2.06
32	F	304	CLA	C4B-NB	3.51	1.42	1.37
33	Q	317	KC2	C4C-NC	3.51	1.43	1.37
32	R	309	CLA	MG-NC	-3.51	1.97	2.06
32	D	313	CLA	MG-NC	-3.51	1.97	2.06
32	R	309	CLA	C3A-C2A	-3.50	1.51	1.54
32	L	310	CLA	MG-NC	-3.50	1.97	2.06
32	b	836	CLA	C4B-NB	3.50	1.42	1.37
32	F	308	CLA	MG-NC	-3.50	1.98	2.06
32	b	818	CLA	MG-NC	-3.50	1.98	2.06
32	b	809	CLA	C4B-NB	3.50	1.42	1.37
32	E	308	CLA	C4B-NB	3.50	1.42	1.37
37	G	311	A86	C32-C31	-3.50	1.48	1.54
32	W	310	CLA	MG-NC	-3.49	1.98	2.06
32	K	310	CLA	MG-NC	-3.49	1.98	2.06
32	A	304	CLA	C4B-NB	3.49	1.42	1.37
32	K	306	CLA	C4B-NB	3.49	1.42	1.37
33	M	321	KC2	C1B-NB	3.49	1.42	1.37
32	J	312	CLA	C4B-NB	3.49	1.42	1.37
32	G	307	CLA	MG-NC	-3.49	1.98	2.06
32	S	311	CLA	C4B-NB	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	822	CLA	C4B-NB	3.49	1.42	1.37
32	Q	305	CLA	C4B-NB	3.49	1.42	1.37
32	I	308	CLA	MG-NC	-3.48	1.98	2.06
32	b	833	CLA	MG-NC	-3.48	1.98	2.06
32	N	310	CLA	MG-NC	-3.48	1.98	2.06
32	b	815	CLA	C4B-NB	3.48	1.42	1.37
32	T	302	CLA	MG-NC	-3.48	1.98	2.06
32	E	314	CLA	MG-NC	-3.48	1.98	2.06
32	L	307	CLA	MG-NC	-3.47	1.98	2.06
32	T	307	CLA	MG-NC	-3.47	1.98	2.06
32	Q	308	CLA	MG-NC	-3.47	1.98	2.06
32	U	303	CLA	MG-NC	-3.47	1.98	2.06
32	a	835	CLA	C4B-NB	3.47	1.42	1.37
32	J	312	CLA	MG-NC	-3.47	1.98	2.06
37	K	314	A86	C32-C31	-3.46	1.48	1.54
32	b	820	CLA	MG-NC	-3.46	1.98	2.06
32	a	806	CLA	C4B-NB	3.46	1.42	1.37
32	G	303	CLA	MG-NC	-3.46	1.98	2.06
32	b	823	CLA	MG-NC	-3.46	1.98	2.06
32	D	306	CLA	MG-NC	-3.46	1.98	2.06
32	F	301	CLA	MG-NC	-3.45	1.98	2.06
32	a	829	CLA	MG-NC	-3.45	1.98	2.06
32	b	828	CLA	MG-NC	-3.45	1.98	2.06
32	J	306	CLA	MG-NC	-3.45	1.98	2.06
32	F	306	CLA	MG-NC	-3.45	1.98	2.06
32	W	306	CLA	MG-NC	-3.45	1.98	2.06
32	U	302	CLA	MG-NC	-3.44	1.98	2.06
32	b	826	CLA	C4B-NB	3.44	1.42	1.37
32	a	840	CLA	MG-NC	-3.44	1.98	2.06
32	H	304	CLA	MG-NC	-3.43	1.98	2.06
32	K	306	CLA	MG-NC	-3.43	1.98	2.06
32	a	830	CLA	C4B-NB	3.42	1.42	1.37
32	I	307	CLA	MG-NC	-3.42	1.98	2.06
32	R	301	CLA	MG-NC	-3.42	1.98	2.06
32	b	825	CLA	C4B-NB	3.42	1.42	1.37
37	W	315	A86	C32-C31	-3.42	1.48	1.54
32	O	308	CLA	MG-NC	-3.42	1.98	2.06
32	P	310	CLA	MG-NC	-3.42	1.98	2.06
32	A	306	CLA	C4B-NB	3.42	1.42	1.37
32	a	840	CLA	C4B-NB	3.42	1.42	1.37
32	a	832	CLA	MG-NC	-3.42	1.98	2.06
32	b	827	CLA	MG-NC	-3.41	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	828	CLA	C4B-NB	3.41	1.42	1.37
40	b	846	DGD	O1G-C1A	3.41	1.43	1.33
32	r	201	CLA	MG-NC	-3.40	1.98	2.06
32	W	309	CLA	MG-NC	-3.40	1.98	2.06
32	A	307	CLA	MG-NC	-3.40	1.98	2.06
32	D	309	CLA	MG-NC	-3.40	1.98	2.06
32	I	304	CLA	MG-NC	-3.40	1.98	2.06
32	b	804	CLA	C4B-NB	3.40	1.42	1.37
32	D	308	CLA	MG-NC	-3.39	1.98	2.06
33	K	305	KC2	C1B-NB	3.39	1.42	1.37
32	E	311	CLA	MG-NC	-3.39	1.98	2.06
32	S	313	CLA	MG-NC	-3.39	1.98	2.06
32	b	805	CLA	C4B-NB	3.39	1.42	1.37
32	O	306	CLA	MG-NC	-3.39	1.98	2.06
32	b	804	CLA	MG-NC	-3.39	1.98	2.06
32	b	801	CLA	MG-NC	-3.39	1.98	2.06
32	L	308	CLA	MG-NC	-3.38	1.98	2.06
37	T	315	A86	C32-C31	-3.38	1.48	1.54
32	M	306	CLA	MG-NC	-3.38	1.98	2.06
32	A	311	CLA	MG-NC	-3.38	1.98	2.06
32	H	307	CLA	MG-NC	-3.37	1.98	2.06
32	a	818	CLA	C4B-NB	3.37	1.41	1.37
32	R	304	CLA	MG-NC	-3.37	1.98	2.06
32	D	304	CLA	MG-NC	-3.37	1.98	2.06
32	l	204	CLA	C4B-NB	3.37	1.41	1.37
32	O	305	CLA	C4B-NB	3.37	1.41	1.37
33	Q	317	KC2	C1B-NB	3.37	1.41	1.37
37	R	313	A86	C32-C31	-3.37	1.48	1.54
32	A	305	CLA	MG-NC	-3.36	1.98	2.06
32	B	301	CLA	MG-NC	-3.36	1.98	2.06
32	a	801	CLA	C4B-NB	3.36	1.41	1.37
32	H	308	CLA	C3A-C2A	-3.36	1.51	1.54
32	H	306	CLA	MG-NC	-3.36	1.98	2.06
32	C	302	CLA	MG-NC	-3.36	1.98	2.06
32	b	832	CLA	MG-NC	-3.35	1.98	2.06
32	V	201	CLA	MG-NC	-3.35	1.98	2.06
32	J	304	CLA	C4B-NB	3.35	1.41	1.37
32	M	309	CLA	MG-NC	-3.35	1.98	2.06
32	G	308	CLA	MG-NC	-3.35	1.98	2.06
32	M	308	CLA	MG-NC	-3.35	1.98	2.06
32	b	829	CLA	MG-NC	-3.35	1.98	2.06
33	W	305	KC2	C1B-NB	3.35	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	L	314	CLA	MG-NC	-3.35	1.98	2.06
32	C	309	CLA	MG-NC	-3.34	1.98	2.06
32	E	315	CLA	MG-NC	-3.34	1.98	2.06
37	S	315	A86	C32-C31	-3.34	1.49	1.54
32	P	307	CLA	MG-NC	-3.34	1.98	2.06
32	a	853	CLA	MG-NC	-3.34	1.98	2.06
32	a	832	CLA	C4B-NB	3.34	1.41	1.37
32	a	819	CLA	MG-NC	-3.34	1.98	2.06
37	P	313	A86	C32-C31	-3.33	1.49	1.54
32	G	304	CLA	MG-NC	-3.33	1.98	2.06
32	P	311	CLA	MG-NC	-3.33	1.98	2.06
32	a	820	CLA	MG-NC	-3.33	1.98	2.06
32	Q	305	CLA	MG-NC	-3.32	1.98	2.06
32	H	302	CLA	C3A-C2A	-3.32	1.51	1.54
32	J	309	CLA	MG-NC	-3.32	1.98	2.06
32	J	311	CLA	MG-NC	-3.32	1.98	2.06
32	V	204	CLA	MG-NC	-3.32	1.98	2.06
32	b	838	CLA	C4B-NB	3.32	1.41	1.37
32	O	305	CLA	MG-NC	-3.31	1.98	2.06
32	Q	301	CLA	MG-NC	-3.31	1.98	2.06
32	H	310	CLA	MG-NC	-3.31	1.98	2.06
32	T	310	CLA	MG-NC	-3.30	1.98	2.06
32	K	308	CLA	MG-NC	-3.30	1.98	2.06
32	C	307	CLA	MG-NC	-3.30	1.98	2.06
32	D	314	CLA	C1B-NB	3.30	1.41	1.37
32	a	806	CLA	MG-NC	-3.30	1.98	2.06
32	L	309	CLA	MG-NC	-3.30	1.98	2.06
32	Q	306	CLA	MG-NC	-3.29	1.98	2.06
32	E	309	CLA	C4B-NB	3.29	1.41	1.37
32	a	836	CLA	MG-NC	-3.29	1.98	2.06
32	K	301	CLA	MG-NC	-3.29	1.98	2.06
32	O	307	CLA	MG-NC	-3.29	1.98	2.06
32	D	311	CLA	MG-NC	-3.29	1.98	2.06
32	E	309	CLA	MG-NC	-3.29	1.98	2.06
32	a	809	CLA	MG-NC	-3.29	1.98	2.06
32	U	301	CLA	MG-NC	-3.29	1.98	2.06
32	F	322	CLA	MG-NC	-3.28	1.98	2.06
32	l	202	CLA	MG-NC	-3.28	1.98	2.06
32	Q	304	CLA	MG-NC	-3.28	1.98	2.06
32	I	302	CLA	MG-NC	-3.28	1.98	2.06
32	a	852	CLA	C4B-NB	3.28	1.41	1.37
32	k	201	CLA	MG-NC	-3.28	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	T	309	CLA	MG-NC	-3.27	1.98	2.06
32	A	306	CLA	MG-NC	-3.27	1.98	2.06
32	O	307	CLA	C4B-NB	3.27	1.41	1.37
32	a	814	CLA	MG-NC	-3.27	1.98	2.06
32	a	825	CLA	MG-NC	-3.26	1.98	2.06
32	R	310	CLA	MG-NC	-3.26	1.98	2.06
37	F	312	A86	C32-C31	-3.26	1.49	1.54
32	L	301	CLA	MG-NC	-3.25	1.98	2.06
32	b	815	CLA	MG-NC	-3.25	1.98	2.06
32	b	813	CLA	MG-NC	-3.25	1.98	2.06
32	b	835	CLA	MG-NC	-3.25	1.98	2.06
32	a	827	CLA	MG-NC	-3.25	1.98	2.06
32	F	311	CLA	MG-NC	-3.25	1.98	2.06
32	A	301	CLA	MG-NC	-3.24	1.98	2.06
32	b	836	CLA	MG-NC	-3.24	1.98	2.06
32	B	303	CLA	MG-NC	-3.24	1.98	2.06
32	b	802	CLA	MG-NC	-3.23	1.98	2.06
32	a	831	CLA	MG-NC	-3.23	1.98	2.06
37	N	316	A86	C32-C31	-3.23	1.49	1.54
32	r	202	CLA	MG-NC	-3.23	1.98	2.06
32	E	308	CLA	MG-NC	-3.22	1.98	2.06
32	O	309	CLA	MG-NC	-3.22	1.98	2.06
32	T	308	CLA	MG-NC	-3.22	1.98	2.06
32	D	315	CLA	MG-NC	-3.21	1.98	2.06
32	C	302	CLA	C3A-C2A	-3.21	1.51	1.54
37	R	312	A86	C32-C31	-3.21	1.49	1.54
32	E	312	CLA	MG-NC	-3.21	1.98	2.06
32	N	313	CLA	MG-NC	-3.21	1.98	2.06
32	D	312	CLA	MG-NC	-3.21	1.98	2.06
32	b	824	CLA	MG-NC	-3.20	1.98	2.06
32	P	305	CLA	MG-NC	-3.20	1.98	2.06
32	a	803	CLA	MG-NC	-3.20	1.98	2.06
32	J	306	CLA	C4B-NB	3.20	1.41	1.37
32	J	301	CLA	MG-NC	-3.20	1.98	2.06
32	a	839	CLA	MG-NC	-3.19	1.98	2.06
32	A	302	CLA	MG-NC	-3.19	1.98	2.06
32	a	833	CLA	MG-NC	-3.19	1.98	2.06
32	I	306	CLA	MG-NC	-3.19	1.98	2.06
32	b	828	CLA	C4B-NB	3.19	1.41	1.37
32	N	312	CLA	MG-NC	-3.19	1.98	2.06
32	f	201	CLA	MG-NC	-3.19	1.98	2.06
32	a	816	CLA	MG-NC	-3.19	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	I	301	CLA	MG-NC	-3.18	1.98	2.06
32	J	302	CLA	MG-NC	-3.18	1.98	2.06
32	F	307	CLA	MG-NC	-3.18	1.98	2.06
32	W	312	CLA	MG-NC	-3.18	1.98	2.06
32	T	306	CLA	MG-NC	-3.18	1.98	2.06
32	D	305	CLA	MG-NC	-3.18	1.98	2.06
32	A	309	CLA	MG-NC	-3.17	1.98	2.06
32	M	305	CLA	MG-NC	-3.17	1.98	2.06
32	a	812	CLA	C3A-C2A	-3.17	1.45	1.54
32	b	825	CLA	MG-NC	-3.17	1.98	2.06
32	S	310	CLA	MG-NC	-3.17	1.98	2.06
32	a	817	CLA	MG-NC	-3.17	1.98	2.06
32	f	204	CLA	MG-NC	-3.17	1.98	2.06
32	W	310	CLA	C4B-NB	3.17	1.41	1.37
32	Q	307	CLA	MG-NC	-3.17	1.98	2.06
32	a	834	CLA	MG-NC	-3.17	1.98	2.06
32	C	301	CLA	MG-NC	-3.17	1.98	2.06
32	M	312	CLA	MG-NC	-3.17	1.98	2.06
32	P	310	CLA	C3A-C2A	-3.16	1.51	1.54
32	V	203	CLA	MG-NC	-3.16	1.98	2.06
32	J	305	CLA	MG-NC	-3.16	1.98	2.06
32	C	308	CLA	C4B-NB	3.16	1.41	1.37
32	b	822	CLA	MG-NC	-3.15	1.98	2.06
32	A	308	CLA	MG-NC	-3.15	1.98	2.06
32	a	812	CLA	C3D-C4D	-3.14	1.37	1.44
32	b	809	CLA	MG-NC	-3.14	1.98	2.06
32	b	805	CLA	MG-NC	-3.14	1.98	2.06
32	E	310	CLA	MG-NC	-3.14	1.98	2.06
32	S	309	CLA	MG-NC	-3.14	1.98	2.06
32	b	808	CLA	MG-NC	-3.14	1.98	2.06
32	b	814	CLA	MG-NC	-3.14	1.98	2.06
32	l	203	CLA	MG-NC	-3.14	1.98	2.06
32	W	307	CLA	MG-NC	-3.13	1.98	2.06
32	a	830	CLA	MG-NC	-3.13	1.98	2.06
32	L	304	CLA	MG-NC	-3.13	1.98	2.06
32	f	203	CLA	MG-NC	-3.13	1.98	2.06
32	a	810	CLA	MG-NC	-3.12	1.98	2.06
32	a	828	CLA	MG-NC	-3.12	1.98	2.06
32	j	101	CLA	MG-NC	-3.12	1.98	2.06
32	P	308	CLA	MG-NC	-3.12	1.98	2.06
32	k	202	CLA	MG-NC	-3.11	1.98	2.06
32	b	839	CLA	MG-NC	-3.11	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	F	317	A86	C32-C31	-3.11	1.49	1.54
32	a	818	CLA	MG-NC	-3.11	1.98	2.06
32	E	307	CLA	MG-NC	-3.11	1.98	2.06
32	b	812	CLA	MG-NC	-3.10	1.98	2.06
32	L	312	CLA	MG-NC	-3.10	1.98	2.06
32	b	821	CLA	MG-NC	-3.10	1.98	2.06
32	S	305	CLA	MG-NC	-3.09	1.98	2.06
32	a	804	CLA	MG-NC	-3.09	1.98	2.06
32	A	304	CLA	MG-NC	-3.09	1.98	2.06
32	a	824	CLA	MG-NC	-3.08	1.98	2.06
32	a	841	CLA	MG-NC	-3.08	1.98	2.06
32	B	302	CLA	MG-NC	-3.08	1.99	2.06
32	N	311	CLA	MG-NC	-3.08	1.99	2.06
32	a	805	CLA	C1D-C2D	-3.07	1.39	1.45
32	I	317	CLA	MG-NC	-3.07	1.99	2.06
32	b	803	CLA	MG-NC	-3.07	1.99	2.06
32	b	817	CLA	MG-NC	-3.07	1.99	2.06
32	F	303	CLA	MG-NC	-3.06	1.99	2.06
32	S	308	CLA	C2C-C1C	3.06	1.45	1.40
32	a	822	CLA	MG-NC	-3.06	1.99	2.06
32	a	835	CLA	MG-NC	-3.05	1.99	2.06
32	b	840	CLA	MG-NC	-3.04	1.99	2.06
32	P	309	CLA	MG-NC	-3.04	1.99	2.06
32	B	309	CLA	MG-NC	-3.03	1.99	2.06
32	A	303	CLA	MG-NC	-3.03	1.99	2.06
32	Q	309	CLA	MG-NC	-3.02	1.99	2.06
32	a	823	CLA	MG-NC	-3.02	1.99	2.06
32	E	305	CLA	MG-NC	-3.02	1.99	2.06
37	N	315	A86	C32-C31	-3.01	1.49	1.54
32	W	311	CLA	MG-NC	-3.01	1.99	2.06
32	a	826	CLA	MG-NC	-3.00	1.99	2.06
32	b	810	CLA	MG-NC	-3.00	1.99	2.06
32	K	307	CLA	MG-NC	-2.99	1.99	2.06
32	a	811	CLA	MG-NC	-2.99	1.99	2.06
37	L	315	A86	C32-C31	-2.98	1.49	1.54
32	a	838	CLA	MG-NC	-2.98	1.99	2.06
32	a	842	CLA	MG-NC	-2.98	1.99	2.06
32	a	815	CLA	MG-NC	-2.97	1.99	2.06
32	b	811	CLA	MG-NC	-2.97	1.99	2.06
37	L	317	A86	C32-C31	-2.96	1.49	1.54
32	G	305	CLA	MG-NC	-2.96	1.99	2.06
36	E	302	LMG	O1-C1	2.96	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	314	CLA	C3D-C4D	-2.95	1.37	1.44
32	R	308	CLA	MG-NC	-2.94	1.99	2.06
32	a	821	CLA	MG-NC	-2.93	1.99	2.06
32	b	831	CLA	MG-NC	-2.92	1.99	2.06
32	E	303	CLA	MG-NC	-2.90	1.99	2.06
37	P	319	A86	C32-C31	-2.89	1.49	1.54
32	b	819	CLA	MG-NC	-2.88	1.99	2.06
32	M	310	CLA	MG-NC	-2.88	1.99	2.06
32	S	304	CLA	MG-NC	-2.86	1.99	2.06
37	M	301	A86	C32-C31	-2.84	1.49	1.54
37	S	317	A86	C32-C31	-2.82	1.49	1.54
39	H	315	SQD	C6-S	-2.80	1.67	1.77
37	K	312	A86	C32-C31	-2.75	1.49	1.54
32	a	812	CLA	C1D-C2D	-2.72	1.40	1.45
32	a	805	CLA	C1B-NB	2.72	1.41	1.37
37	W	302	A86	C32-C31	-2.71	1.50	1.54
37	D	322	A86	C32-C31	-2.71	1.50	1.54
36	A	318	LMG	C4-C5	2.69	1.58	1.53
39	k	206	SQD	C6-S	-2.69	1.67	1.77
32	D	314	CLA	C1D-C2D	-2.67	1.40	1.45
37	S	320	A86	C32-C31	-2.63	1.50	1.54
32	b	816	CLA	MG-NC	-2.60	2.00	2.06
37	F	313	A86	C32-C31	-2.59	1.50	1.54
37	L	316	A86	C32-C31	-2.58	1.50	1.54
32	b	802	CLA	C4B-NB	2.55	1.40	1.37
32	N	310	CLA	C3D-C4D	-2.52	1.38	1.44
35	W	319	LHG	O7-C5	-2.52	1.40	1.46
32	b	802	CLA	C3D-C4D	-2.51	1.38	1.44
37	M	318	A86	C32-C31	-2.49	1.50	1.54
32	a	805	CLA	C1C-NC	-2.47	1.34	1.37
32	a	823	CLA	C1D-C2D	-2.46	1.40	1.45
32	a	822	CLA	C1D-C2D	-2.44	1.40	1.45
33	S	312	KC2	C4C-NC	2.44	1.41	1.37
32	C	306	CLA	C3D-C4D	-2.44	1.38	1.44
37	S	318	A86	C32-C31	-2.44	1.50	1.54
37	M	322	A86	C32-C31	-2.42	1.50	1.54
32	C	308	CLA	C3D-C4D	-2.42	1.38	1.44
32	a	805	CLA	C3A-C2A	-2.41	1.47	1.54
32	f	201	CLA	C1D-C2D	-2.41	1.40	1.45
32	b	819	CLA	C1D-C2D	-2.40	1.40	1.45
32	a	832	CLA	C1D-C2D	-2.40	1.40	1.45
32	a	830	CLA	C1D-C2D	-2.40	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	802	CLA	C1D-C2D	-2.38	1.40	1.45
32	f	204	CLA	C3D-C4D	-2.38	1.38	1.44
32	b	836	CLA	C1D-C2D	-2.38	1.40	1.45
32	b	832	CLA	C1D-C2D	-2.38	1.40	1.45
37	P	314	A86	C32-C31	-2.37	1.50	1.54
32	a	836	CLA	C1D-C2D	-2.36	1.40	1.45
32	a	838	CLA	C3D-C4D	-2.35	1.38	1.44
32	b	833	CLA	C1D-C2D	-2.35	1.40	1.45
32	A	302	CLA	C1D-C2D	-2.35	1.40	1.45
32	b	805	CLA	C1D-C2D	-2.35	1.40	1.45
32	b	832	CLA	C3D-C4D	-2.35	1.38	1.44
32	b	823	CLA	C1D-C2D	-2.35	1.40	1.45
32	b	815	CLA	C3D-C4D	-2.35	1.38	1.44
32	a	852	CLA	C1D-C2D	-2.35	1.40	1.45
36	L	320	LMG	O7-C8	-2.35	1.40	1.46
32	a	825	CLA	C1D-C2D	-2.35	1.40	1.45
32	b	831	CLA	C1D-C2D	-2.34	1.40	1.45
32	a	820	CLA	C3D-C4D	-2.34	1.38	1.44
32	K	307	CLA	C1D-C2D	-2.34	1.40	1.45
32	A	303	CLA	C3D-C4D	-2.34	1.38	1.44
32	b	816	CLA	C1D-C2D	-2.34	1.40	1.45
32	a	821	CLA	C3D-C4D	-2.34	1.38	1.44
32	Q	303	CLA	C1D-C2D	-2.34	1.40	1.45
32	a	821	CLA	C1D-C2D	-2.33	1.40	1.45
32	b	836	CLA	C3D-C4D	-2.33	1.38	1.44
32	Q	306	CLA	C3D-C4D	-2.33	1.38	1.44
32	b	824	CLA	C1D-C2D	-2.33	1.40	1.45
32	b	828	CLA	C3D-C4D	-2.33	1.38	1.44
32	G	305	CLA	C1D-C2D	-2.33	1.40	1.45
32	N	311	CLA	C1D-C2D	-2.33	1.40	1.45
32	S	305	CLA	C1D-C2D	-2.33	1.40	1.45
32	a	833	CLA	C3D-C4D	-2.33	1.38	1.44
32	b	809	CLA	C1D-C2D	-2.33	1.40	1.45
32	T	307	CLA	C1D-C2D	-2.33	1.40	1.45
32	S	304	CLA	C1D-C2D	-2.32	1.40	1.45
32	D	306	CLA	C1D-C2D	-2.32	1.40	1.45
32	a	823	CLA	C3D-C4D	-2.32	1.38	1.44
32	W	311	CLA	C1D-C2D	-2.32	1.40	1.45
32	b	810	CLA	C1D-C2D	-2.32	1.40	1.45
32	O	306	CLA	C3D-C4D	-2.32	1.38	1.44
32	A	304	CLA	C1D-C2D	-2.32	1.40	1.45
32	a	832	CLA	C3D-C4D	-2.32	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	306	CLA	C1D-C2D	-2.31	1.40	1.45
32	A	303	CLA	C1D-C2D	-2.31	1.40	1.45
32	b	808	CLA	C1D-C2D	-2.31	1.40	1.45
32	b	815	CLA	C1D-C2D	-2.31	1.40	1.45
32	Q	301	CLA	C1D-C2D	-2.31	1.40	1.45
32	b	820	CLA	C1D-C2D	-2.31	1.40	1.45
32	S	311	CLA	C3D-C4D	-2.31	1.39	1.44
32	S	309	CLA	C1D-C2D	-2.31	1.40	1.45
32	T	310	CLA	C3D-C4D	-2.31	1.39	1.44
32	a	819	CLA	C1D-C2D	-2.31	1.40	1.45
32	T	307	CLA	C3D-C4D	-2.31	1.39	1.44
32	b	817	CLA	C1D-C2D	-2.31	1.40	1.45
32	b	803	CLA	C3D-C4D	-2.31	1.39	1.44
32	b	803	CLA	C1D-C2D	-2.30	1.40	1.45
32	J	307	CLA	C3D-C4D	-2.30	1.39	1.44
32	b	811	CLA	C1D-C2D	-2.30	1.40	1.45
32	l	203	CLA	C1D-C2D	-2.30	1.40	1.45
32	F	303	CLA	C1D-C2D	-2.30	1.40	1.45
32	b	822	CLA	C1D-C2D	-2.30	1.40	1.45
32	W	313	CLA	C1D-C2D	-2.30	1.40	1.45
32	W	310	CLA	C3D-C4D	-2.30	1.39	1.44
32	E	306	CLA	C3D-C4D	-2.30	1.39	1.44
32	a	807	CLA	C3D-C4D	-2.30	1.39	1.44
32	a	810	CLA	C3D-C4D	-2.30	1.39	1.44
32	W	312	CLA	C1D-C2D	-2.30	1.40	1.45
32	D	310	CLA	C1D-C2D	-2.29	1.40	1.45
32	A	308	CLA	C1D-C2D	-2.29	1.40	1.45
32	a	828	CLA	C1D-C2D	-2.29	1.40	1.45
32	F	306	CLA	C3D-C4D	-2.29	1.39	1.44
32	E	309	CLA	C1D-C2D	-2.29	1.40	1.45
32	b	825	CLA	C1D-C2D	-2.29	1.40	1.45
32	J	309	CLA	C3D-C4D	-2.29	1.39	1.44
32	O	306	CLA	C1D-C2D	-2.29	1.40	1.45
32	b	839	CLA	C1D-C2D	-2.29	1.40	1.45
32	J	304	CLA	C3D-C4D	-2.29	1.39	1.44
32	b	812	CLA	C3D-C4D	-2.29	1.39	1.44
32	D	309	CLA	C3D-C4D	-2.29	1.39	1.44
32	U	306	CLA	C1D-C2D	-2.29	1.40	1.45
32	a	801	CLA	C1D-C2D	-2.29	1.40	1.45
32	I	305	CLA	C3D-C4D	-2.29	1.39	1.44
32	F	307	CLA	C1D-C2D	-2.29	1.40	1.45
32	J	305	CLA	C1D-C2D	-2.29	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	r	202	CLA	C1D-C2D	-2.29	1.40	1.45
32	a	842	CLA	C1D-C2D	-2.29	1.40	1.45
32	K	301	CLA	C3D-C4D	-2.29	1.39	1.44
32	L	307	CLA	C1D-C2D	-2.29	1.40	1.45
32	a	827	CLA	C1D-C2D	-2.29	1.40	1.45
32	b	811	CLA	C3D-C4D	-2.28	1.39	1.44
32	a	834	CLA	C1D-C2D	-2.28	1.40	1.45
32	b	830	CLA	C3D-C4D	-2.28	1.39	1.44
32	b	813	CLA	C3D-C4D	-2.28	1.39	1.44
32	H	307	CLA	C1D-C2D	-2.28	1.40	1.45
32	a	841	CLA	C1D-C2D	-2.28	1.40	1.45
32	F	309	CLA	C3D-C4D	-2.28	1.39	1.44
32	I	308	CLA	C3D-C4D	-2.28	1.39	1.44
32	W	309	CLA	C1D-C2D	-2.28	1.40	1.45
32	E	305	CLA	C1D-C2D	-2.28	1.40	1.45
32	V	203	CLA	C1D-C2D	-2.28	1.40	1.45
32	b	809	CLA	C3D-C4D	-2.27	1.39	1.44
32	A	306	CLA	C1D-C2D	-2.27	1.40	1.45
32	k	203	CLA	C1D-C2D	-2.27	1.40	1.45
32	J	309	CLA	C1D-C2D	-2.27	1.40	1.45
32	G	306	CLA	C3D-C4D	-2.27	1.39	1.44
32	b	825	CLA	C3D-C4D	-2.27	1.39	1.44
32	W	309	CLA	C3D-C4D	-2.27	1.39	1.44
32	a	831	CLA	C3D-C4D	-2.27	1.39	1.44
32	b	830	CLA	C1D-C2D	-2.27	1.40	1.45
32	a	816	CLA	C3D-C4D	-2.27	1.39	1.44
32	a	829	CLA	C1D-C2D	-2.27	1.40	1.45
32	a	812	CLA	C3B-C2B	-2.27	1.33	1.41
32	l	204	CLA	C3D-C4D	-2.27	1.39	1.44
32	J	312	CLA	C3D-C4D	-2.27	1.39	1.44
32	W	310	CLA	C1D-C2D	-2.27	1.40	1.45
32	b	818	CLA	C3D-C4D	-2.27	1.39	1.44
32	a	814	CLA	C3D-C4D	-2.27	1.39	1.44
32	I	302	CLA	C1D-C2D	-2.27	1.40	1.45
32	T	306	CLA	C1D-C2D	-2.27	1.40	1.45
32	I	306	CLA	C1D-C2D	-2.27	1.40	1.45
32	J	302	CLA	C1D-C2D	-2.27	1.40	1.45
32	a	833	CLA	C1D-C2D	-2.27	1.40	1.45
32	D	308	CLA	C1D-C2D	-2.27	1.40	1.45
32	R	306	CLA	C3D-C4D	-2.27	1.39	1.44
32	B	302	CLA	C1D-C2D	-2.27	1.40	1.45
32	a	803	CLA	C1D-C2D	-2.27	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	811	CLA	C1D-C2D	-2.27	1.40	1.45
32	b	840	CLA	C1D-C2D	-2.27	1.40	1.45
37	r	204	A86	C32-C31	-2.27	1.50	1.54
32	b	833	CLA	C3D-C4D	-2.27	1.39	1.44
32	a	824	CLA	C1D-C2D	-2.27	1.40	1.45
32	E	307	CLA	C3D-C4D	-2.27	1.39	1.44
32	Q	305	CLA	C3D-C4D	-2.27	1.39	1.44
32	S	307	CLA	C3D-C4D	-2.27	1.39	1.44
32	C	308	CLA	C1D-C2D	-2.27	1.40	1.45
32	D	309	CLA	C1D-C2D	-2.27	1.40	1.45
32	E	312	CLA	C1D-C2D	-2.27	1.40	1.45
32	A	307	CLA	C3D-C4D	-2.27	1.39	1.44
32	P	308	CLA	C1D-C2D	-2.26	1.40	1.45
32	a	835	CLA	C1D-C2D	-2.26	1.40	1.45
32	a	826	CLA	C3D-C4D	-2.26	1.39	1.44
32	I	317	CLA	C1D-C2D	-2.26	1.40	1.45
32	O	305	CLA	C1D-C2D	-2.26	1.40	1.45
32	B	306	CLA	C1D-C2D	-2.26	1.40	1.45
32	N	310	CLA	C1D-C2D	-2.26	1.40	1.45
32	l	202	CLA	C1D-C2D	-2.26	1.40	1.45
32	b	812	CLA	C1D-C2D	-2.26	1.40	1.45
32	Q	306	CLA	C1D-C2D	-2.26	1.40	1.45
32	A	309	CLA	C3D-C4D	-2.26	1.39	1.44
32	l	203	CLA	C3D-C4D	-2.26	1.39	1.44
32	A	309	CLA	C1D-C2D	-2.26	1.40	1.45
32	I	301	CLA	C1D-C2D	-2.26	1.40	1.45
32	a	831	CLA	C1D-C2D	-2.26	1.40	1.45
32	L	307	CLA	C3D-C4D	-2.26	1.39	1.44
32	b	804	CLA	C3D-C4D	-2.26	1.39	1.44
32	a	824	CLA	C3D-C4D	-2.26	1.39	1.44
32	a	835	CLA	C3D-C4D	-2.26	1.39	1.44
32	B	309	CLA	C1D-C2D	-2.26	1.40	1.45
32	Q	308	CLA	C1D-C2D	-2.26	1.40	1.45
32	I	303	CLA	C3D-C4D	-2.26	1.39	1.44
32	A	301	CLA	C1D-C2D	-2.26	1.40	1.45
32	B	303	CLA	C1D-C2D	-2.26	1.40	1.45
32	K	306	CLA	C1D-C2D	-2.26	1.40	1.45
32	G	303	CLA	C3D-C4D	-2.26	1.39	1.44
32	b	823	CLA	C3D-C4D	-2.26	1.39	1.44
32	E	308	CLA	C1D-C2D	-2.26	1.40	1.45
32	b	826	CLA	C3D-C4D	-2.26	1.39	1.44
32	N	305	CLA	C1D-C2D	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	853	CLA	C3D-C4D	-2.25	1.39	1.44
32	C	307	CLA	C1D-C2D	-2.25	1.40	1.45
32	L	309	CLA	C1D-C2D	-2.25	1.40	1.45
32	D	313	CLA	C3D-C4D	-2.25	1.39	1.44
32	a	809	CLA	C3D-C4D	-2.25	1.39	1.44
32	b	834	CLA	C3D-C4D	-2.25	1.39	1.44
32	M	312	CLA	C1D-C2D	-2.25	1.40	1.45
32	a	826	CLA	C1D-C2D	-2.25	1.40	1.45
32	E	315	CLA	C1D-C2D	-2.25	1.40	1.45
32	Q	307	CLA	C1D-C2D	-2.25	1.40	1.45
32	k	202	CLA	C1D-C2D	-2.25	1.40	1.45
32	A	311	CLA	C3D-C4D	-2.25	1.39	1.44
32	E	310	CLA	C1D-C2D	-2.25	1.40	1.45
32	a	818	CLA	C1D-C2D	-2.25	1.40	1.45
32	I	302	CLA	C3D-C4D	-2.25	1.39	1.44
32	a	807	CLA	C1D-C2D	-2.25	1.40	1.45
32	N	313	CLA	C1D-C2D	-2.25	1.40	1.45
32	a	817	CLA	C1D-C2D	-2.25	1.40	1.45
32	A	304	CLA	C3D-C4D	-2.25	1.39	1.44
32	A	311	CLA	C1D-C2D	-2.25	1.40	1.45
32	V	204	CLA	C1D-C2D	-2.25	1.40	1.45
32	D	307	CLA	C3D-C4D	-2.25	1.39	1.44
32	a	830	CLA	C3D-C4D	-2.25	1.39	1.44
32	k	203	CLA	C3D-C4D	-2.25	1.39	1.44
32	W	306	CLA	C1D-C2D	-2.25	1.40	1.45
32	I	306	CLA	C3D-C4D	-2.25	1.39	1.44
32	b	824	CLA	C3D-C4D	-2.25	1.39	1.44
32	J	311	CLA	C1D-C2D	-2.25	1.40	1.45
32	f	204	CLA	C1D-C2D	-2.25	1.40	1.45
32	T	305	CLA	C3D-C4D	-2.25	1.39	1.44
32	a	839	CLA	C3D-C4D	-2.25	1.39	1.44
32	I	317	CLA	C3D-C4D	-2.25	1.39	1.44
32	b	838	CLA	C3D-C4D	-2.25	1.39	1.44
32	A	307	CLA	C1D-C2D	-2.25	1.40	1.45
32	J	312	CLA	C1D-C2D	-2.25	1.40	1.45
32	E	309	CLA	C3D-C4D	-2.25	1.39	1.44
32	a	841	CLA	C3D-C4D	-2.25	1.39	1.44
32	k	201	CLA	C1D-C2D	-2.24	1.40	1.45
32	J	306	CLA	C3D-C4D	-2.24	1.39	1.44
32	T	308	CLA	C1D-C2D	-2.24	1.40	1.45
32	l	204	CLA	C1D-C2D	-2.24	1.40	1.45
32	b	806	CLA	C1D-C2D	-2.24	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	829	CLA	C1D-C2D	-2.24	1.40	1.45
32	O	305	CLA	C3D-C4D	-2.24	1.39	1.44
32	F	309	CLA	C1D-C2D	-2.24	1.40	1.45
32	D	308	CLA	C3D-C4D	-2.24	1.39	1.44
32	H	305	CLA	C3D-C4D	-2.24	1.39	1.44
32	I	301	CLA	C3D-C4D	-2.24	1.39	1.44
32	b	807	CLA	C3D-C4D	-2.24	1.39	1.44
32	P	304	CLA	C1D-C2D	-2.24	1.40	1.45
32	a	819	CLA	C3D-C4D	-2.24	1.39	1.44
32	C	301	CLA	C1D-C2D	-2.24	1.40	1.45
32	a	806	CLA	C1D-C2D	-2.24	1.40	1.45
32	K	306	CLA	C3D-C4D	-2.24	1.39	1.44
32	W	307	CLA	C1D-C2D	-2.24	1.40	1.45
32	a	804	CLA	C1D-C2D	-2.24	1.40	1.45
32	a	840	CLA	C3D-C4D	-2.24	1.39	1.44
32	G	304	CLA	C3D-C4D	-2.24	1.39	1.44
32	M	310	CLA	C3D-C4D	-2.24	1.39	1.44
32	D	313	CLA	C1D-C2D	-2.24	1.40	1.45
32	I	304	CLA	C1D-C2D	-2.24	1.40	1.45
32	a	838	CLA	C1D-C2D	-2.24	1.40	1.45
32	a	853	CLA	C1D-C2D	-2.24	1.40	1.45
32	E	306	CLA	C1D-C2D	-2.24	1.40	1.45
32	R	306	CLA	C1D-C2D	-2.24	1.40	1.45
32	E	312	CLA	C3D-C4D	-2.24	1.39	1.44
32	K	301	CLA	C1D-C2D	-2.23	1.40	1.45
32	J	306	CLA	C1D-C2D	-2.23	1.40	1.45
32	a	820	CLA	C1D-C2D	-2.23	1.40	1.45
32	r	201	CLA	C3D-C4D	-2.23	1.39	1.44
32	S	308	CLA	C1D-C2D	-2.23	1.40	1.45
32	b	837	CLA	C3D-C4D	-2.23	1.39	1.44
32	a	808	CLA	C1D-C2D	-2.23	1.40	1.45
32	D	310	CLA	C3D-C4D	-2.23	1.39	1.44
32	Q	305	CLA	C1D-C2D	-2.23	1.40	1.45
32	L	301	CLA	C1D-C2D	-2.23	1.40	1.45
32	A	308	CLA	C3D-C4D	-2.23	1.39	1.44
32	Q	309	CLA	C1D-C2D	-2.23	1.40	1.45
32	T	302	CLA	C1D-C2D	-2.23	1.40	1.45
32	F	306	CLA	C1D-C2D	-2.23	1.40	1.45
32	L	308	CLA	C1D-C2D	-2.23	1.40	1.45
32	b	822	CLA	C3D-C4D	-2.23	1.39	1.44
32	C	305	CLA	C1D-C2D	-2.23	1.40	1.45
32	E	303	CLA	C1D-C2D	-2.23	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	F	322	CLA	C1D-C2D	-2.23	1.40	1.45
32	P	309	CLA	C1D-C2D	-2.23	1.40	1.45
32	S	313	CLA	C1D-C2D	-2.23	1.40	1.45
32	D	305	CLA	C1D-C2D	-2.23	1.40	1.45
32	b	810	CLA	C3D-C4D	-2.23	1.39	1.44
32	L	311	CLA	C3D-C4D	-2.23	1.39	1.44
32	W	313	CLA	C3D-C4D	-2.23	1.39	1.44
32	a	822	CLA	C3D-C4D	-2.23	1.39	1.44
32	b	840	CLA	C3D-C4D	-2.23	1.39	1.44
32	a	827	CLA	C3D-C4D	-2.23	1.39	1.44
32	E	304	CLA	C1D-C2D	-2.23	1.40	1.45
32	F	304	CLA	C3D-C4D	-2.23	1.39	1.44
32	V	201	CLA	C3D-C4D	-2.23	1.39	1.44
32	F	304	CLA	C1D-C2D	-2.22	1.40	1.45
32	E	304	CLA	C3D-C4D	-2.22	1.39	1.44
32	M	310	CLA	C1D-C2D	-2.22	1.40	1.45
32	a	815	CLA	C1D-C2D	-2.22	1.40	1.45
32	J	304	CLA	C1C-C2C	2.22	1.48	1.44
32	b	826	CLA	C1D-C2D	-2.22	1.40	1.45
32	a	813	CLA	C3D-C4D	-2.22	1.39	1.44
32	H	304	CLA	C3D-C4D	-2.22	1.39	1.44
32	T	306	CLA	C3D-C4D	-2.22	1.39	1.44
32	T	308	CLA	C3D-C4D	-2.22	1.39	1.44
32	H	304	CLA	C1D-C2D	-2.22	1.40	1.45
32	Q	303	CLA	C3D-C4D	-2.22	1.39	1.44
32	O	309	CLA	C1D-C2D	-2.22	1.40	1.45
32	J	304	CLA	C1D-C2D	-2.22	1.40	1.45
32	a	839	CLA	C1D-C2D	-2.22	1.40	1.45
32	a	811	CLA	C3D-C4D	-2.22	1.39	1.44
32	b	808	CLA	C3D-C4D	-2.22	1.39	1.44
32	E	315	CLA	C3D-C4D	-2.22	1.39	1.44
32	Q	308	CLA	C3D-C4D	-2.22	1.39	1.44
32	b	820	CLA	C3D-C4D	-2.22	1.39	1.44
32	N	309	CLA	C1D-C2D	-2.22	1.40	1.45
32	K	304	CLA	C3D-C4D	-2.22	1.39	1.44
32	N	313	CLA	C3D-C4D	-2.22	1.39	1.44
32	Q	309	CLA	C3D-C4D	-2.22	1.39	1.44
32	b	813	CLA	C1D-C2D	-2.22	1.40	1.45
32	b	839	CLA	C3D-C4D	-2.22	1.39	1.44
32	H	309	CLA	C1D-C2D	-2.22	1.40	1.45
32	N	309	CLA	C3D-C4D	-2.22	1.39	1.44
32	a	837	CLA	C1D-C2D	-2.22	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	H	310	CLA	C1D-C2D	-2.22	1.41	1.45
32	a	840	CLA	C1D-C2D	-2.22	1.41	1.45
32	A	305	CLA	C3D-C4D	-2.22	1.39	1.44
32	O	304	CLA	C1D-C2D	-2.21	1.41	1.45
32	A	302	CLA	C3D-C4D	-2.21	1.39	1.44
32	M	308	CLA	C3D-C4D	-2.21	1.39	1.44
32	k	201	CLA	C3D-C4D	-2.21	1.39	1.44
32	G	304	CLA	C1D-C2D	-2.21	1.41	1.45
32	a	818	CLA	C3D-C4D	-2.21	1.39	1.44
32	D	307	CLA	C1D-C2D	-2.21	1.41	1.45
32	F	307	CLA	C3D-C4D	-2.21	1.39	1.44
32	b	816	CLA	C3D-C4D	-2.21	1.39	1.44
35	E	301	LHG	P-O6	2.21	1.68	1.59
32	b	828	CLA	C1D-C2D	-2.21	1.41	1.45
32	H	306	CLA	C1D-C2D	-2.21	1.41	1.45
32	I	303	CLA	C1D-C2D	-2.21	1.41	1.45
32	D	305	CLA	C3D-C4D	-2.21	1.39	1.44
32	M	306	CLA	C1D-C2D	-2.21	1.41	1.45
32	Q	310	CLA	C3D-C4D	-2.21	1.39	1.44
32	a	806	CLA	C3D-C4D	-2.21	1.39	1.44
32	S	305	CLA	C3D-C4D	-2.21	1.39	1.44
32	N	312	CLA	C1D-C2D	-2.21	1.41	1.45
32	J	308	CLA	C3D-C4D	-2.21	1.39	1.44
32	C	306	CLA	C1D-C2D	-2.21	1.41	1.45
32	C	309	CLA	C1D-C2D	-2.21	1.41	1.45
32	b	838	CLA	C1D-C2D	-2.21	1.41	1.45
32	j	101	CLA	C1D-C2D	-2.21	1.41	1.45
32	b	829	CLA	C3D-C4D	-2.21	1.39	1.44
32	F	305	CLA	C1D-C2D	-2.20	1.41	1.45
32	b	834	CLA	C1D-C2D	-2.20	1.41	1.45
32	b	814	CLA	C1D-C2D	-2.20	1.41	1.45
32	r	201	CLA	C1D-C2D	-2.20	1.41	1.45
32	G	305	CLA	C3D-C4D	-2.20	1.39	1.44
32	S	313	CLA	C3D-C4D	-2.20	1.39	1.44
32	P	309	CLA	C3D-C4D	-2.20	1.39	1.44
32	b	837	CLA	C1D-C2D	-2.20	1.41	1.45
32	f	203	CLA	C1D-C2D	-2.20	1.41	1.45
32	E	308	CLA	C3D-C4D	-2.20	1.39	1.44
32	R	307	CLA	C3D-C4D	-2.20	1.39	1.44
32	a	837	CLA	C3D-C4D	-2.20	1.39	1.44
32	E	307	CLA	C1D-C2D	-2.20	1.41	1.45
32	I	308	CLA	C1D-C2D	-2.20	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	306	CLA	C3D-C4D	-2.20	1.39	1.44
32	K	308	CLA	C1D-C2D	-2.20	1.41	1.45
32	S	301	CLA	C1D-C2D	-2.20	1.41	1.45
32	J	311	CLA	C3D-C4D	-2.20	1.39	1.44
32	D	306	CLA	C3D-C4D	-2.20	1.39	1.44
32	r	202	CLA	C3D-C4D	-2.20	1.39	1.44
32	J	308	CLA	C1D-C2D	-2.20	1.41	1.45
32	E	305	CLA	C3D-C4D	-2.20	1.39	1.44
32	b	831	CLA	C3D-C4D	-2.20	1.39	1.44
32	L	314	CLA	C1D-C2D	-2.20	1.41	1.45
32	a	815	CLA	C3D-C4D	-2.20	1.39	1.44
32	V	204	CLA	C3D-C4D	-2.20	1.39	1.44
32	b	817	CLA	C3D-C4D	-2.20	1.39	1.44
32	M	309	CLA	C3D-C4D	-2.20	1.39	1.44
32	D	311	CLA	C1D-C2D	-2.20	1.41	1.45
32	N	305	CLA	C3D-C4D	-2.20	1.39	1.44
32	O	307	CLA	C1D-C2D	-2.20	1.41	1.45
32	S	309	CLA	C3D-C4D	-2.20	1.39	1.44
32	Q	304	CLA	C1D-C2D	-2.20	1.41	1.45
32	Q	304	CLA	C3D-C4D	-2.20	1.39	1.44
32	k	202	CLA	C3D-C4D	-2.20	1.39	1.44
32	a	828	CLA	C3D-C4D	-2.19	1.39	1.44
32	M	311	CLA	C1D-C2D	-2.19	1.41	1.45
32	a	813	CLA	C1D-C2D	-2.19	1.41	1.45
37	C	312	A86	C32-C31	-2.19	1.50	1.54
32	Q	301	CLA	C3D-C4D	-2.19	1.39	1.44
32	W	312	CLA	C3D-C4D	-2.19	1.39	1.44
32	J	301	CLA	C1D-C2D	-2.19	1.41	1.45
32	P	311	CLA	C3D-C4D	-2.19	1.39	1.44
32	C	307	CLA	C3D-C4D	-2.19	1.39	1.44
32	D	315	CLA	C3D-C4D	-2.19	1.39	1.44
32	F	311	CLA	C3D-C4D	-2.19	1.39	1.44
32	M	306	CLA	C3D-C4D	-2.19	1.39	1.44
32	N	311	CLA	C3D-C4D	-2.19	1.39	1.44
32	K	310	CLA	C3D-C4D	-2.19	1.39	1.44
32	O	304	CLA	C3D-C4D	-2.19	1.39	1.44
32	O	307	CLA	C3D-C4D	-2.19	1.39	1.44
32	b	827	CLA	C1D-C2D	-2.19	1.41	1.45
32	A	306	CLA	C3D-C4D	-2.19	1.39	1.44
32	D	304	CLA	C1D-C2D	-2.19	1.41	1.45
32	D	312	CLA	C1D-C2D	-2.19	1.41	1.45
32	W	311	CLA	C3D-C4D	-2.19	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	303	CLA	C1D-C2D	-2.19	1.41	1.45
32	H	301	CLA	C1D-C2D	-2.19	1.41	1.45
32	P	304	CLA	C3D-C4D	-2.19	1.39	1.44
32	P	307	CLA	C1D-C2D	-2.19	1.41	1.45
32	P	311	CLA	C1D-C2D	-2.19	1.41	1.45
32	b	806	CLA	C3D-C4D	-2.19	1.39	1.44
32	R	308	CLA	C1D-C2D	-2.19	1.41	1.45
32	O	301	CLA	C1D-C2D	-2.19	1.41	1.45
32	E	314	CLA	C3D-C4D	-2.19	1.39	1.44
32	R	304	CLA	C1D-C2D	-2.19	1.41	1.45
32	b	818	CLA	C1D-C2D	-2.19	1.41	1.45
32	a	836	CLA	C3D-C4D	-2.19	1.39	1.44
32	b	821	CLA	C1D-C2D	-2.19	1.41	1.45
36	T	301	LMG	C7-C8	2.18	1.57	1.50
32	I	307	CLA	C1D-C2D	-2.18	1.41	1.45
32	M	308	CLA	C1D-C2D	-2.18	1.41	1.45
32	J	302	CLA	C3D-C4D	-2.18	1.39	1.44
32	S	308	CLA	C3D-C4D	-2.18	1.39	1.44
32	N	312	CLA	C3D-C4D	-2.18	1.39	1.44
32	B	304	CLA	C1D-C2D	-2.18	1.41	1.45
32	V	201	CLA	C1D-C2D	-2.18	1.41	1.45
32	H	306	CLA	C3D-C4D	-2.18	1.39	1.44
32	L	308	CLA	C3D-C4D	-2.18	1.39	1.44
32	V	203	CLA	C3D-C4D	-2.18	1.39	1.44
32	K	310	CLA	C1D-C2D	-2.18	1.41	1.45
32	M	305	CLA	C1D-C2D	-2.18	1.41	1.45
32	R	307	CLA	C1D-C2D	-2.18	1.41	1.45
32	U	305	CLA	C3D-C4D	-2.18	1.39	1.44
32	b	814	CLA	C3D-C4D	-2.18	1.39	1.44
32	H	307	CLA	C3D-C4D	-2.18	1.39	1.44
32	E	310	CLA	C3D-C4D	-2.18	1.39	1.44
32	U	302	CLA	C1D-C2D	-2.18	1.41	1.45
32	A	301	CLA	C3D-C4D	-2.18	1.39	1.44
37	J	313	A86	C32-C31	-2.18	1.50	1.54
32	a	808	CLA	C3D-C4D	-2.18	1.39	1.44
32	E	314	CLA	C1D-C2D	-2.18	1.41	1.45
32	I	304	CLA	C3D-C4D	-2.18	1.39	1.44
32	a	834	CLA	C3D-C4D	-2.18	1.39	1.44
32	a	852	CLA	C3D-C4D	-2.18	1.39	1.44
32	A	305	CLA	C1D-C2D	-2.18	1.41	1.45
32	b	804	CLA	C1D-C2D	-2.18	1.41	1.45
32	K	308	CLA	C3D-C4D	-2.18	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	F	303	CLA	C3D-C4D	-2.18	1.39	1.44
32	P	307	CLA	C3D-C4D	-2.18	1.39	1.44
32	J	305	CLA	C3D-C4D	-2.18	1.39	1.44
32	S	307	CLA	C1D-C2D	-2.18	1.41	1.45
32	U	303	CLA	C3D-C4D	-2.18	1.39	1.44
32	B	306	CLA	C3D-C4D	-2.18	1.39	1.44
32	D	304	CLA	C3D-C4D	-2.18	1.39	1.44
32	R	308	CLA	C3D-C4D	-2.18	1.39	1.44
32	b	835	CLA	C3D-C4D	-2.18	1.39	1.44
32	L	312	CLA	C1D-C2D	-2.17	1.41	1.45
39	k	206	SQD	O6-C1	2.17	1.43	1.40
32	b	835	CLA	C1D-C2D	-2.17	1.41	1.45
32	a	829	CLA	C3D-C4D	-2.17	1.39	1.44
32	D	312	CLA	C3D-C4D	-2.17	1.39	1.44
32	Q	310	CLA	C1D-C2D	-2.17	1.41	1.45
32	F	305	CLA	C3D-C4D	-2.17	1.39	1.44
32	a	803	CLA	C3D-C4D	-2.17	1.39	1.44
32	a	810	CLA	C1D-C2D	-2.17	1.41	1.45
32	a	804	CLA	C3D-C4D	-2.17	1.39	1.44
32	a	816	CLA	C1D-C2D	-2.17	1.41	1.45
32	f	201	CLA	C3D-C4D	-2.17	1.39	1.44
33	S	312	KC2	C1B-NB	2.17	1.40	1.37
32	G	301	CLA	C3D-C4D	-2.17	1.39	1.44
32	P	305	CLA	C3D-C4D	-2.17	1.39	1.44
32	I	307	CLA	C3D-C4D	-2.17	1.39	1.44
32	F	308	CLA	C1D-C2D	-2.17	1.41	1.45
32	I	305	CLA	C1D-C2D	-2.17	1.41	1.45
32	U	307	CLA	C3D-C4D	-2.17	1.39	1.44
32	R	304	CLA	C3D-C4D	-2.17	1.39	1.44
32	T	309	CLA	C1D-C2D	-2.17	1.41	1.45
32	T	310	CLA	C1D-C2D	-2.17	1.41	1.45
32	L	312	CLA	C3D-C4D	-2.16	1.39	1.44
32	B	305	CLA	C1D-C2D	-2.16	1.41	1.45
32	R	310	CLA	C3D-C4D	-2.16	1.39	1.44
32	b	821	CLA	C3D-C4D	-2.16	1.39	1.44
32	G	308	CLA	C1D-C2D	-2.16	1.41	1.45
32	L	304	CLA	C1D-C2D	-2.16	1.41	1.45
32	L	314	CLA	C3D-C4D	-2.16	1.39	1.44
32	M	309	CLA	C1D-C2D	-2.16	1.41	1.45
32	a	825	CLA	C3D-C4D	-2.16	1.39	1.44
32	O	301	CLA	C3D-C4D	-2.16	1.39	1.44
32	F	322	CLA	C3D-C4D	-2.16	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	308	CLA	C3D-C4D	-2.16	1.39	1.44
32	C	305	CLA	C3D-C4D	-2.16	1.39	1.44
32	U	307	CLA	C1D-C2D	-2.16	1.41	1.45
32	a	817	CLA	C3D-C4D	-2.16	1.39	1.44
32	S	310	CLA	C1D-C2D	-2.16	1.41	1.45
32	a	814	CLA	C1D-C2D	-2.16	1.41	1.45
32	C	301	CLA	C3D-C4D	-2.16	1.39	1.44
32	E	311	CLA	C3D-C4D	-2.16	1.39	1.44
32	H	301	CLA	C3D-C4D	-2.16	1.39	1.44
32	U	301	CLA	C1D-C2D	-2.16	1.41	1.45
32	B	305	CLA	C3D-C4D	-2.16	1.39	1.44
32	L	310	CLA	C3D-C4D	-2.16	1.39	1.44
32	G	301	CLA	C1D-C2D	-2.16	1.41	1.45
32	a	809	CLA	C1D-C2D	-2.16	1.41	1.45
32	S	310	CLA	C3D-C4D	-2.15	1.39	1.44
32	B	303	CLA	C3D-C4D	-2.15	1.39	1.44
32	a	805	CLA	CHD-C4C	-2.15	1.34	1.39
32	O	309	CLA	C3D-C4D	-2.15	1.39	1.44
32	C	304	CLA	C1D-C2D	-2.15	1.41	1.45
32	b	807	CLA	C1D-C2D	-2.15	1.41	1.45
32	G	307	CLA	C3D-C4D	-2.15	1.39	1.44
32	b	827	CLA	C3D-C4D	-2.15	1.39	1.44
32	R	309	CLA	C1D-C2D	-2.15	1.41	1.45
32	U	303	CLA	C1D-C2D	-2.15	1.41	1.45
32	C	304	CLA	C3D-C4D	-2.15	1.39	1.44
32	Q	307	CLA	C3D-C4D	-2.15	1.39	1.44
32	b	819	CLA	C3D-C4D	-2.15	1.39	1.44
32	D	311	CLA	C3D-C4D	-2.15	1.39	1.44
32	E	303	CLA	C3D-C4D	-2.15	1.39	1.44
32	l	202	CLA	C3D-C4D	-2.15	1.39	1.44
32	S	301	CLA	C3D-C4D	-2.15	1.39	1.44
32	L	304	CLA	C3D-C4D	-2.14	1.39	1.44
32	E	311	CLA	C1D-C2D	-2.14	1.41	1.45
32	F	311	CLA	C1D-C2D	-2.14	1.41	1.45
32	L	309	CLA	C3D-C4D	-2.14	1.39	1.44
32	C	302	CLA	C1D-C2D	-2.14	1.41	1.45
32	M	311	CLA	C3D-C4D	-2.14	1.39	1.44
32	H	309	CLA	C3D-C4D	-2.14	1.39	1.44
32	M	312	CLA	C3D-C4D	-2.14	1.39	1.44
32	O	308	CLA	C1D-C2D	-2.14	1.41	1.45
32	C	302	CLA	C3D-C4D	-2.14	1.39	1.44
32	j	101	CLA	C3D-C4D	-2.14	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	O	312	A86	C32-C31	-2.14	1.51	1.54
32	B	302	CLA	C3D-C4D	-2.14	1.39	1.44
32	R	301	CLA	C3D-C4D	-2.14	1.39	1.44
32	H	308	CLA	C1D-C2D	-2.14	1.41	1.45
32	R	301	CLA	C1D-C2D	-2.13	1.41	1.45
32	T	305	CLA	C1D-C2D	-2.13	1.41	1.45
32	P	305	CLA	C1D-C2D	-2.13	1.41	1.45
32	U	305	CLA	C1D-C2D	-2.13	1.41	1.45
32	W	307	CLA	C3D-C4D	-2.13	1.39	1.44
32	T	302	CLA	C3D-C4D	-2.13	1.39	1.44
32	a	842	CLA	C3D-C4D	-2.13	1.39	1.44
32	R	310	CLA	C1D-C2D	-2.13	1.41	1.45
32	D	315	CLA	C1D-C2D	-2.13	1.41	1.45
32	H	308	CLA	C3D-C4D	-2.13	1.39	1.44
32	U	306	CLA	C3D-C4D	-2.13	1.39	1.44
32	b	801	CLA	C3D-C4D	-2.13	1.39	1.44
32	B	301	CLA	C1D-C2D	-2.12	1.41	1.45
32	P	308	CLA	C3D-C4D	-2.12	1.39	1.44
36	E	302	LMG	C4-C3	2.12	1.57	1.52
32	M	305	CLA	C3D-C4D	-2.12	1.39	1.44
32	f	203	CLA	C3D-C4D	-2.12	1.39	1.44
32	F	301	CLA	C3D-C4D	-2.12	1.39	1.44
32	S	311	CLA	C1D-C2D	-2.12	1.41	1.45
32	b	802	CLA	C1D-C2D	-2.12	1.41	1.45
32	b	805	CLA	C3D-C4D	-2.12	1.39	1.44
32	K	304	CLA	C1D-C2D	-2.11	1.41	1.45
32	D	314	CLA	C3A-C2A	-2.11	1.48	1.54
32	R	309	CLA	C3D-C4D	-2.11	1.39	1.44
32	O	308	CLA	C3D-C4D	-2.11	1.39	1.44
32	H	302	CLA	C1D-C2D	-2.11	1.41	1.45
36	F	320	LMG	O7-C8	-2.11	1.41	1.46
32	U	301	CLA	C3D-C4D	-2.10	1.39	1.44
32	P	310	CLA	C3D-C4D	-2.10	1.39	1.44
32	F	308	CLA	C3D-C4D	-2.10	1.39	1.44
32	B	301	CLA	C3D-C4D	-2.10	1.39	1.44
32	F	301	CLA	C1D-C2D	-2.10	1.41	1.45
32	G	307	CLA	C1D-C2D	-2.10	1.41	1.45
32	T	309	CLA	C3D-C4D	-2.09	1.39	1.44
32	L	311	CLA	C1D-C2D	-2.09	1.41	1.45
32	H	302	CLA	C3D-C4D	-2.09	1.39	1.44
32	P	310	CLA	C1D-C2D	-2.09	1.41	1.45
32	a	802	CLA	C3D-C4D	-2.09	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	J	307	CLA	C1D-C2D	-2.09	1.41	1.45
32	L	301	CLA	C3D-C4D	-2.09	1.39	1.44
32	C	309	CLA	C3D-C4D	-2.08	1.39	1.44
36	j	104	LMG	O1-C1	2.08	1.43	1.40
32	B	309	CLA	C3D-C4D	-2.08	1.39	1.44
32	J	301	CLA	C3D-C4D	-2.08	1.39	1.44
32	b	825	CLA	C3A-C2A	-2.08	1.48	1.54
32	J	307	CLA	C1C-C2C	2.08	1.48	1.44
32	K	307	CLA	C3D-C4D	-2.08	1.39	1.44
32	b	801	CLA	C1D-C2D	-2.07	1.41	1.45
32	U	302	CLA	C3D-C4D	-2.07	1.39	1.44
32	L	310	CLA	C1D-C2D	-2.07	1.41	1.45
32	H	310	CLA	C3D-C4D	-2.06	1.39	1.44
32	B	304	CLA	C3D-C4D	-2.06	1.39	1.44
36	E	302	LMG	C7-C8	2.06	1.57	1.50
35	F	318	LHG	P-O6	2.05	1.67	1.59
36	A	318	LMG	O1-C1	2.05	1.43	1.40
35	A	316	LHG	P-O6	2.04	1.67	1.59
32	a	805	CLA	C1C-C2C	-2.04	1.40	1.44
32	Q	303	CLA	C1C-C2C	2.04	1.48	1.44
32	S	304	CLA	C3D-C4D	-2.04	1.39	1.44
35	F	321	LHG	P-O6	2.03	1.67	1.59
32	H	305	CLA	C1D-C2D	-2.03	1.41	1.45
35	a	849	LHG	O7-C5	-2.03	1.41	1.46
36	D	302	LMG	O7-C8	-2.03	1.41	1.46
32	a	801	CLA	C3D-C4D	-2.03	1.39	1.44
35	F	321	LHG	O7-C5	-2.03	1.41	1.46
32	P	309	CLA	C1C-C2C	2.02	1.48	1.44

All (3137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	S	307	CLA	C4A-NA-C1A	-8.62	102.83	106.71
37	S	317	A86	O1-C20-C19	8.49	119.76	113.38
32	a	818	CLA	C4A-NA-C1A	-8.34	102.95	106.71
34	S	321	DD6	O1-C20-C19	-8.32	107.14	113.38
32	S	308	CLA	C1C-NC-C4C	-8.20	103.02	106.71
37	J	313	A86	O1-C20-C19	8.15	119.50	113.38
37	L	316	A86	O1-C20-C19	8.11	119.47	113.38
32	b	837	CLA	C4A-NA-C1A	-7.90	103.15	106.71
32	b	838	CLA	C4A-NA-C1A	-7.83	103.18	106.71
37	N	316	A86	O1-C20-C19	-7.82	107.51	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	807	CLA	C4A-NA-C1A	-7.77	103.22	106.71
32	Q	303	CLA	C4A-NA-C1A	-7.60	103.29	106.71
32	M	311	CLA	C4A-NA-C1A	-7.54	103.32	106.71
32	H	304	CLA	C4A-NA-C1A	-7.52	103.32	106.71
37	P	316	A86	C33-C32-C31	7.51	116.51	109.21
32	I	303	CLA	C4A-NA-C1A	-7.51	103.33	106.71
32	S	301	CLA	C4A-NA-C1A	-7.46	103.35	106.71
32	R	301	CLA	C4A-NA-C1A	-7.44	103.36	106.71
32	L	311	CLA	C4A-NA-C1A	-7.43	103.37	106.71
32	b	830	CLA	C4A-NA-C1A	-7.43	103.37	106.71
32	J	304	CLA	C4A-NA-C1A	-7.32	103.41	106.71
32	H	308	CLA	C4A-NA-C1A	-7.32	103.42	106.71
32	G	307	CLA	C4A-NA-C1A	-7.30	103.42	106.71
32	U	303	CLA	C4A-NA-C1A	-7.28	103.43	106.71
32	C	305	CLA	C4A-NA-C1A	-7.26	103.44	106.71
32	a	813	CLA	C4A-NA-C1A	-7.26	103.44	106.71
32	H	301	CLA	C4A-NA-C1A	-7.23	103.45	106.71
32	b	801	CLA	C4A-NA-C1A	-7.23	103.46	106.71
32	D	308	CLA	C4A-NA-C1A	-7.20	103.47	106.71
32	E	304	CLA	C4A-NA-C1A	-7.19	103.47	106.71
32	K	310	CLA	C4A-NA-C1A	-7.18	103.48	106.71
32	b	836	CLA	C4A-NA-C1A	-7.18	103.48	106.71
32	U	305	CLA	C4A-NA-C1A	-7.17	103.48	106.71
37	S	315	A86	O1-C20-C19	7.16	118.76	113.38
32	a	837	CLA	C4A-NA-C1A	-7.13	103.50	106.71
32	R	309	CLA	C4A-NA-C1A	-7.13	103.50	106.71
32	H	302	CLA	C4A-NA-C1A	-7.12	103.50	106.71
32	J	307	CLA	C4A-NA-C1A	-7.11	103.51	106.71
32	E	311	CLA	C4A-NA-C1A	-7.10	103.52	106.71
32	C	302	CLA	C4A-NA-C1A	-7.06	103.53	106.71
32	O	304	CLA	C4A-NA-C1A	-7.03	103.54	106.71
32	F	322	CLA	C4A-NA-C1A	-7.03	103.55	106.71
37	G	310	A86	O1-C20-C19	7.03	118.66	113.38
37	P	313	A86	O1-C20-C19	-7.02	108.11	113.38
32	L	310	CLA	C4A-NA-C1A	-6.99	103.56	106.71
32	b	828	CLA	C4A-NA-C1A	-6.98	103.57	106.71
32	J	308	CLA	C4A-NA-C1A	-6.96	103.58	106.71
32	A	311	CLA	C4A-NA-C1A	-6.95	103.58	106.71
32	b	802	CLA	C4A-NA-C1A	-6.94	103.58	106.71
32	a	814	CLA	C4A-NA-C1A	-6.94	103.59	106.71
32	N	309	CLA	C4A-NA-C1A	-6.92	103.59	106.71
32	b	804	CLA	C4A-NA-C1A	-6.92	103.59	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	C	304	CLA	C4A-NA-C1A	-6.91	103.60	106.71
32	J	311	CLA	C4A-NA-C1A	-6.91	103.60	106.71
32	I	305	CLA	C4A-NA-C1A	-6.87	103.62	106.71
32	D	307	CLA	C4A-NA-C1A	-6.86	103.62	106.71
32	U	307	CLA	C4A-NA-C1A	-6.84	103.63	106.71
32	a	805	CLA	C4A-NA-C1A	-6.84	103.63	106.71
32	I	307	CLA	C4A-NA-C1A	-6.83	103.63	106.71
32	a	820	CLA	C4A-NA-C1A	-6.83	103.63	106.71
37	F	312	A86	O1-C20-C19	6.83	118.51	113.38
32	C	308	CLA	C1D-ND-C4D	-6.82	101.49	106.33
32	P	310	CLA	C4A-NA-C1A	-6.81	103.64	106.71
32	a	838	CLA	C4A-NA-C1A	-6.80	103.65	106.71
32	B	305	CLA	C4A-NA-C1A	-6.80	103.65	106.71
32	W	313	CLA	C4A-NA-C1A	-6.80	103.65	106.71
32	a	807	CLA	C4A-NA-C1A	-6.78	103.66	106.71
32	a	827	CLA	C4A-NA-C1A	-6.77	103.66	106.71
32	l	204	CLA	C4A-NA-C1A	-6.76	103.67	106.71
32	a	839	CLA	C4A-NA-C1A	-6.72	103.68	106.71
32	F	305	CLA	C4A-NA-C1A	-6.72	103.69	106.71
32	b	832	CLA	C4A-NA-C1A	-6.72	103.69	106.71
32	B	301	CLA	C4A-NA-C1A	-6.71	103.69	106.71
32	a	832	CLA	C4A-NA-C1A	-6.70	103.69	106.71
32	E	309	CLA	C4A-NA-C1A	-6.68	103.70	106.71
32	a	830	CLA	C4A-NA-C1A	-6.65	103.72	106.71
32	D	315	CLA	C4A-NA-C1A	-6.64	103.72	106.71
32	Q	301	CLA	C4A-NA-C1A	-6.64	103.72	106.71
32	H	305	CLA	C4A-NA-C1A	-6.64	103.72	106.71
32	N	310	CLA	C4A-NA-C1A	-6.64	103.72	106.71
32	I	317	CLA	C4A-NA-C1A	-6.62	103.73	106.71
32	b	826	CLA	C4A-NA-C1A	-6.61	103.73	106.71
32	C	307	CLA	C4A-NA-C1A	-6.59	103.74	106.71
34	L	319	DD6	O1-C20-C19	-6.58	108.44	113.38
32	I	308	CLA	C4A-NA-C1A	-6.58	103.75	106.71
32	A	307	CLA	C4A-NA-C1A	-6.56	103.76	106.71
32	b	820	CLA	C4A-NA-C1A	-6.56	103.76	106.71
32	r	201	CLA	C4A-NA-C1A	-6.55	103.76	106.71
32	C	306	CLA	C4A-NA-C1A	-6.52	103.78	106.71
32	l	202	CLA	C4A-NA-C1A	-6.50	103.78	106.71
32	N	305	CLA	C4A-NA-C1A	-6.49	103.79	106.71
32	k	203	CLA	C4A-NA-C1A	-6.47	103.80	106.71
32	L	307	CLA	C4A-NA-C1A	-6.46	103.80	106.71
32	B	304	CLA	C4A-NA-C1A	-6.45	103.80	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	C	306	CLA	C1D-ND-C4D	-6.42	101.78	106.33
32	a	829	CLA	C4A-NA-C1A	-6.41	103.82	106.71
32	S	313	CLA	C4A-NA-C1A	-6.41	103.83	106.71
32	F	301	CLA	C4A-NA-C1A	-6.41	103.83	106.71
32	T	310	CLA	C4A-NA-C1A	-6.38	103.84	106.71
32	P	307	CLA	C4A-NA-C1A	-6.38	103.84	106.71
32	b	833	CLA	C1D-ND-C4D	-6.37	101.81	106.33
32	R	304	CLA	C4A-NA-C1A	-6.36	103.85	106.71
32	a	812	CLA	C4A-NA-C1A	-6.35	103.85	106.71
32	J	307	CLA	C1D-ND-C4D	-6.35	101.82	106.33
32	D	310	CLA	C4A-NA-C1A	-6.29	103.88	106.71
32	N	310	CLA	C1D-ND-C4D	-6.29	101.87	106.33
32	M	306	CLA	C1D-ND-C4D	-6.29	101.87	106.33
32	G	308	CLA	C1D-ND-C4D	-6.28	101.87	106.33
32	H	306	CLA	C1D-ND-C4D	-6.28	101.87	106.33
32	R	306	CLA	C4A-NA-C1A	-6.28	103.88	106.71
32	b	834	CLA	C1D-ND-C4D	-6.27	101.88	106.33
32	G	306	CLA	C4A-NA-C1A	-6.27	103.89	106.71
32	T	310	CLA	C1D-ND-C4D	-6.26	101.89	106.33
37	C	312	A86	O1-C20-C19	6.26	118.08	113.38
32	J	312	CLA	C1D-ND-C4D	-6.26	101.89	106.33
32	C	308	CLA	C4A-NA-C1A	-6.25	103.89	106.71
37	U	308	A86	O1-C20-C19	-6.25	108.69	113.38
32	O	301	CLA	C4A-NA-C1A	-6.25	103.90	106.71
32	O	309	CLA	C4A-NA-C1A	-6.25	103.90	106.71
32	a	804	CLA	C4A-NA-C1A	-6.25	103.90	106.71
32	b	818	CLA	C4A-NA-C1A	-6.24	103.90	106.71
32	G	303	CLA	C1D-ND-C4D	-6.24	101.90	106.33
32	I	304	CLA	C4A-NA-C1A	-6.24	103.90	106.71
32	b	835	CLA	C4A-NA-C1A	-6.24	103.90	106.71
32	F	311	CLA	C1D-ND-C4D	-6.23	101.91	106.33
32	G	301	CLA	C1D-ND-C4D	-6.23	101.91	106.33
32	G	303	CLA	C4A-NA-C1A	-6.23	103.90	106.71
32	O	308	CLA	C4A-NA-C1A	-6.23	103.90	106.71
32	D	309	CLA	C4A-NA-C1A	-6.23	103.91	106.71
32	Q	306	CLA	C4A-NA-C1A	-6.23	103.91	106.71
32	W	306	CLA	C4A-NA-C1A	-6.23	103.91	106.71
32	T	302	CLA	C1D-ND-C4D	-6.23	101.91	106.33
32	F	311	CLA	C4A-NA-C1A	-6.23	103.91	106.71
37	S	314	A86	C33-C32-C31	6.22	115.26	109.21
32	G	306	CLA	C1D-ND-C4D	-6.22	101.91	106.33
32	S	311	CLA	C4A-NA-C1A	-6.22	103.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	I	302	CLA	C1D-ND-C4D	-6.22	101.92	106.33
32	L	309	CLA	C4A-NA-C1A	-6.21	103.91	106.71
32	a	821	CLA	C4A-NA-C1A	-6.21	103.91	106.71
32	P	305	CLA	C1D-ND-C4D	-6.21	101.92	106.33
32	D	312	CLA	C4A-NA-C1A	-6.21	103.91	106.71
32	U	306	CLA	C4A-NA-C1A	-6.21	103.92	106.71
32	E	315	CLA	C1D-ND-C4D	-6.21	101.92	106.33
32	H	307	CLA	C1D-ND-C4D	-6.20	101.93	106.33
32	E	314	CLA	C1D-ND-C4D	-6.20	101.93	106.33
32	R	308	CLA	C4A-NA-C1A	-6.20	103.92	106.71
32	A	304	CLA	C1D-ND-C4D	-6.20	101.93	106.33
32	D	304	CLA	C1D-ND-C4D	-6.20	101.93	106.33
32	A	305	CLA	C4A-NA-C1A	-6.19	103.92	106.71
32	T	307	CLA	C1D-ND-C4D	-6.19	101.94	106.33
32	S	311	CLA	C1D-ND-C4D	-6.19	101.94	106.33
32	a	809	CLA	C1D-ND-C4D	-6.18	101.94	106.33
32	P	309	CLA	C4A-NA-C1A	-6.18	103.93	106.71
32	a	803	CLA	C4A-NA-C1A	-6.18	103.93	106.71
32	J	306	CLA	C1D-ND-C4D	-6.17	101.95	106.33
32	N	313	CLA	C4A-NA-C1A	-6.17	103.93	106.71
32	a	833	CLA	C4A-NA-C1A	-6.17	103.93	106.71
32	U	301	CLA	C1D-ND-C4D	-6.17	101.95	106.33
32	H	302	CLA	C1D-ND-C4D	-6.17	101.95	106.33
32	A	305	CLA	C1D-ND-C4D	-6.17	101.95	106.33
32	I	308	CLA	C1D-ND-C4D	-6.17	101.95	106.33
32	A	303	CLA	C1D-ND-C4D	-6.16	101.96	106.33
32	N	313	CLA	C1D-ND-C4D	-6.16	101.96	106.33
32	F	303	CLA	C1D-ND-C4D	-6.16	101.96	106.33
37	T	313	A86	O1-C20-C19	-6.16	108.76	113.38
32	b	829	CLA	C1D-ND-C4D	-6.16	101.96	106.33
32	F	301	CLA	C1D-ND-C4D	-6.15	101.96	106.33
32	D	313	CLA	C1D-ND-C4D	-6.15	101.97	106.33
32	f	204	CLA	C1D-ND-C4D	-6.15	101.97	106.33
32	S	305	CLA	C1D-ND-C4D	-6.15	101.97	106.33
32	W	310	CLA	C1D-ND-C4D	-6.15	101.97	106.33
32	a	831	CLA	C4A-NA-C1A	-6.15	103.94	106.71
32	Q	310	CLA	C1D-ND-C4D	-6.14	101.97	106.33
32	a	828	CLA	C4A-NA-C1A	-6.14	103.94	106.71
32	b	821	CLA	C4A-NA-C1A	-6.14	103.94	106.71
32	I	306	CLA	C1D-ND-C4D	-6.14	101.97	106.33
37	M	315	A86	O1-C20-C19	-6.14	108.77	113.38
32	L	312	CLA	C1D-ND-C4D	-6.13	101.98	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	R	308	CLA	C1D-ND-C4D	-6.13	101.98	106.33
32	a	808	CLA	C1D-ND-C4D	-6.13	101.98	106.33
32	Q	308	CLA	C1D-ND-C4D	-6.13	101.98	106.33
32	C	304	CLA	C1D-ND-C4D	-6.13	101.98	106.33
32	H	310	CLA	C1D-ND-C4D	-6.12	101.98	106.33
32	K	308	CLA	C1D-ND-C4D	-6.12	101.98	106.33
32	Q	308	CLA	C4A-NA-C1A	-6.12	103.95	106.71
32	T	309	CLA	C4A-NA-C1A	-6.12	103.95	106.71
32	F	308	CLA	C1D-ND-C4D	-6.12	101.99	106.33
32	a	823	CLA	C4A-NA-C1A	-6.12	103.95	106.71
32	E	306	CLA	C1D-ND-C4D	-6.12	101.99	106.33
32	a	836	CLA	C4A-NA-C1A	-6.12	103.96	106.71
32	f	203	CLA	C4A-NA-C1A	-6.12	103.96	106.71
32	T	308	CLA	C4A-NA-C1A	-6.11	103.96	106.71
32	E	310	CLA	C1D-ND-C4D	-6.11	101.99	106.33
32	A	309	CLA	C1D-ND-C4D	-6.11	101.99	106.33
32	b	818	CLA	C1D-ND-C4D	-6.11	101.99	106.33
32	b	824	CLA	C1D-ND-C4D	-6.11	101.99	106.33
32	F	309	CLA	C1D-ND-C4D	-6.11	102.00	106.33
32	a	840	CLA	C1D-ND-C4D	-6.11	102.00	106.33
32	K	308	CLA	C4A-NA-C1A	-6.11	103.96	106.71
32	F	307	CLA	C1D-ND-C4D	-6.10	102.00	106.33
32	K	304	CLA	C4A-NA-C1A	-6.10	103.96	106.71
32	a	840	CLA	C4A-NA-C1A	-6.10	103.96	106.71
32	R	307	CLA	C1D-ND-C4D	-6.10	102.00	106.33
32	Q	305	CLA	C1D-ND-C4D	-6.10	102.00	106.33
37	S	316	A86	O1-C20-C19	-6.09	108.81	113.38
32	E	303	CLA	C1D-ND-C4D	-6.09	102.01	106.33
34	F	316	DD6	C14-C13-C11	6.09	134.98	125.53
32	P	309	CLA	C1D-ND-C4D	-6.09	102.01	106.33
32	P	310	CLA	C1D-ND-C4D	-6.09	102.01	106.33
32	D	310	CLA	C1D-ND-C4D	-6.09	102.01	106.33
32	b	826	CLA	C1D-ND-C4D	-6.09	102.01	106.33
32	b	809	CLA	C4A-NA-C1A	-6.08	103.97	106.71
32	D	307	CLA	C1D-ND-C4D	-6.08	102.01	106.33
32	a	820	CLA	C1D-ND-C4D	-6.08	102.01	106.33
32	A	307	CLA	C1D-ND-C4D	-6.08	102.02	106.33
32	E	305	CLA	C1D-ND-C4D	-6.08	102.02	106.33
32	b	806	CLA	C1D-ND-C4D	-6.08	102.02	106.33
32	a	811	CLA	C4A-NA-C1A	-6.08	103.97	106.71
32	I	305	CLA	C1D-ND-C4D	-6.07	102.02	106.33
32	a	809	CLA	C4A-NA-C1A	-6.07	103.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	O	308	CLA	C1D-ND-C4D	-6.07	102.02	106.33
32	B	305	CLA	C1D-ND-C4D	-6.07	102.03	106.33
32	J	302	CLA	C1D-ND-C4D	-6.07	102.03	106.33
32	M	310	CLA	C1D-ND-C4D	-6.07	102.03	106.33
32	J	306	CLA	C4A-NA-C1A	-6.07	103.98	106.71
32	E	311	CLA	C1D-ND-C4D	-6.06	102.03	106.33
32	D	305	CLA	C1D-ND-C4D	-6.06	102.03	106.33
32	D	311	CLA	C1D-ND-C4D	-6.06	102.03	106.33
32	L	310	CLA	C1D-ND-C4D	-6.06	102.03	106.33
32	f	203	CLA	C1D-ND-C4D	-6.06	102.03	106.33
32	k	201	CLA	C1D-ND-C4D	-6.06	102.03	106.33
32	D	309	CLA	C1D-ND-C4D	-6.05	102.03	106.33
32	P	307	CLA	C1D-ND-C4D	-6.05	102.03	106.33
32	a	811	CLA	C1D-ND-C4D	-6.05	102.03	106.33
32	b	817	CLA	C1D-ND-C4D	-6.05	102.03	106.33
32	U	301	CLA	C4A-NA-C1A	-6.05	103.98	106.71
32	Q	306	CLA	C1D-ND-C4D	-6.05	102.04	106.33
32	S	310	CLA	C1D-ND-C4D	-6.05	102.04	106.33
32	K	306	CLA	C1D-ND-C4D	-6.05	102.04	106.33
32	a	803	CLA	C1D-ND-C4D	-6.05	102.04	106.33
32	Q	304	CLA	C4A-NA-C1A	-6.05	103.99	106.71
32	B	301	CLA	C1D-ND-C4D	-6.05	102.04	106.33
32	C	301	CLA	C1D-ND-C4D	-6.04	102.04	106.33
32	R	306	CLA	C1D-ND-C4D	-6.04	102.04	106.33
37	P	314	A86	O1-C20-C19	6.04	117.92	113.38
32	S	310	CLA	C4A-NA-C1A	-6.04	103.99	106.71
32	a	817	CLA	C1D-ND-C4D	-6.04	102.04	106.33
32	a	831	CLA	C1D-ND-C4D	-6.04	102.04	106.33
32	M	309	CLA	C1D-ND-C4D	-6.04	102.05	106.33
32	V	204	CLA	C1D-ND-C4D	-6.04	102.05	106.33
32	a	813	CLA	C1D-ND-C4D	-6.04	102.05	106.33
32	Q	309	CLA	C4A-NA-C1A	-6.04	103.99	106.71
32	M	312	CLA	C1D-ND-C4D	-6.04	102.05	106.33
32	r	201	CLA	C1D-ND-C4D	-6.04	102.05	106.33
32	V	201	CLA	C1D-ND-C4D	-6.03	102.05	106.33
32	a	853	CLA	C1D-ND-C4D	-6.03	102.05	106.33
32	C	309	CLA	C1D-ND-C4D	-6.03	102.05	106.33
32	k	202	CLA	C1D-ND-C4D	-6.03	102.05	106.33
32	E	312	CLA	C4A-NA-C1A	-6.03	104.00	106.71
32	G	307	CLA	C1D-ND-C4D	-6.03	102.05	106.33
32	L	301	CLA	C1D-ND-C4D	-6.03	102.05	106.33
32	U	307	CLA	C1D-ND-C4D	-6.03	102.05	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	T	308	CLA	C1D-ND-C4D	-6.02	102.06	106.33
32	W	307	CLA	C1D-ND-C4D	-6.02	102.06	106.33
32	R	310	CLA	C1D-ND-C4D	-6.02	102.06	106.33
32	b	801	CLA	C1D-ND-C4D	-6.02	102.06	106.33
32	A	308	CLA	C1D-ND-C4D	-6.02	102.06	106.33
32	F	304	CLA	C1D-ND-C4D	-6.01	102.06	106.33
32	R	301	CLA	C1D-ND-C4D	-6.01	102.06	106.33
32	O	309	CLA	C1D-ND-C4D	-6.01	102.06	106.33
32	H	306	CLA	C4A-NA-C1A	-6.01	104.00	106.71
32	K	301	CLA	C4A-NA-C1A	-6.01	104.00	106.71
32	D	306	CLA	C1D-ND-C4D	-6.01	102.07	106.33
32	K	301	CLA	C1D-ND-C4D	-6.01	102.07	106.33
32	J	302	CLA	C4A-NA-C1A	-6.01	104.00	106.71
32	b	834	CLA	C4A-NA-C1A	-6.01	104.00	106.71
32	Q	309	CLA	C1D-ND-C4D	-6.01	102.07	106.33
32	P	304	CLA	C4A-NA-C1A	-6.01	104.01	106.71
32	O	301	CLA	C1D-ND-C4D	-6.00	102.07	106.33
32	T	302	CLA	C4A-NA-C1A	-6.00	104.01	106.71
32	r	202	CLA	C4A-NA-C1A	-6.00	104.01	106.71
32	L	308	CLA	C1D-ND-C4D	-6.00	102.07	106.33
32	Q	307	CLA	C1D-ND-C4D	-6.00	102.07	106.33
32	b	803	CLA	C4A-NA-C1A	-6.00	104.01	106.71
32	L	311	CLA	C1D-ND-C4D	-6.00	102.08	106.33
32	E	308	CLA	C1D-ND-C4D	-5.99	102.08	106.33
32	I	301	CLA	C1D-ND-C4D	-5.99	102.08	106.33
32	J	308	CLA	C1D-ND-C4D	-5.99	102.08	106.33
32	S	313	CLA	C1D-ND-C4D	-5.99	102.08	106.33
32	a	814	CLA	C1D-ND-C4D	-5.99	102.08	106.33
32	I	303	CLA	C1D-ND-C4D	-5.99	102.08	106.33
32	C	307	CLA	C1D-ND-C4D	-5.99	102.08	106.33
32	J	309	CLA	C1D-ND-C4D	-5.99	102.08	106.33
32	a	842	CLA	C1D-ND-C4D	-5.99	102.08	106.33
32	r	202	CLA	C1D-ND-C4D	-5.98	102.08	106.33
32	S	301	CLA	C1D-ND-C4D	-5.98	102.09	106.33
32	O	307	CLA	C4A-NA-C1A	-5.98	104.02	106.71
32	a	836	CLA	C1D-ND-C4D	-5.98	102.09	106.33
32	A	303	CLA	C4A-NA-C1A	-5.97	104.02	106.71
32	N	312	CLA	C1D-ND-C4D	-5.97	102.09	106.33
32	K	304	CLA	C1D-ND-C4D	-5.97	102.09	106.33
32	A	302	CLA	C1D-ND-C4D	-5.97	102.09	106.33
32	N	311	CLA	C1D-ND-C4D	-5.97	102.09	106.33
32	H	305	CLA	C1D-ND-C4D	-5.97	102.09	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	309	CLA	C4A-NA-C1A	-5.97	104.02	106.71
32	F	306	CLA	C1D-ND-C4D	-5.97	102.10	106.33
32	b	837	CLA	C1D-ND-C4D	-5.97	102.10	106.33
32	J	311	CLA	C1D-ND-C4D	-5.96	102.10	106.33
32	P	311	CLA	C1D-ND-C4D	-5.96	102.10	106.33
32	H	309	CLA	C1D-ND-C4D	-5.96	102.10	106.33
32	Q	301	CLA	C1D-ND-C4D	-5.96	102.10	106.33
32	G	304	CLA	C1D-ND-C4D	-5.96	102.10	106.33
32	O	307	CLA	C1D-ND-C4D	-5.95	102.11	106.33
32	E	312	CLA	C1D-ND-C4D	-5.95	102.11	106.33
32	l	203	CLA	C1D-ND-C4D	-5.95	102.11	106.33
32	a	819	CLA	C4A-NA-C1A	-5.95	104.03	106.71
32	Q	303	CLA	C1D-ND-C4D	-5.95	102.11	106.33
32	b	827	CLA	C1D-ND-C4D	-5.95	102.11	106.33
32	H	304	CLA	C1D-ND-C4D	-5.95	102.11	106.33
32	a	822	CLA	C1D-ND-C4D	-5.95	102.11	106.33
32	b	833	CLA	C4A-NA-C1A	-5.95	104.03	106.71
32	U	302	CLA	C1D-ND-C4D	-5.94	102.11	106.33
32	D	305	CLA	C4A-NA-C1A	-5.94	104.03	106.71
32	R	304	CLA	C1D-ND-C4D	-5.94	102.11	106.33
32	M	308	CLA	C1D-ND-C4D	-5.94	102.11	106.33
32	A	306	CLA	C1D-ND-C4D	-5.94	102.12	106.33
32	I	307	CLA	C1D-ND-C4D	-5.94	102.12	106.33
32	a	833	CLA	C1D-ND-C4D	-5.94	102.12	106.33
34	O	313	DD6	O1-C20-C19	-5.94	108.92	113.38
32	b	839	CLA	C1D-ND-C4D	-5.94	102.12	106.33
32	a	839	CLA	C1D-ND-C4D	-5.93	102.12	106.33
32	b	816	CLA	C1D-ND-C4D	-5.93	102.12	106.33
32	C	302	CLA	C1D-ND-C4D	-5.93	102.12	106.33
32	a	807	CLA	C1D-ND-C4D	-5.93	102.12	106.33
32	b	832	CLA	C1D-ND-C4D	-5.93	102.12	106.33
32	W	312	CLA	C1D-ND-C4D	-5.93	102.12	106.33
32	a	816	CLA	C1D-ND-C4D	-5.92	102.13	106.33
32	b	811	CLA	C1D-ND-C4D	-5.92	102.13	106.33
32	H	309	CLA	C4A-NA-C1A	-5.92	104.04	106.71
32	D	312	CLA	C1D-ND-C4D	-5.92	102.13	106.33
32	O	306	CLA	C1D-ND-C4D	-5.92	102.13	106.33
32	F	305	CLA	C1D-ND-C4D	-5.92	102.13	106.33
32	b	821	CLA	C1D-ND-C4D	-5.92	102.13	106.33
32	T	309	CLA	C1D-ND-C4D	-5.92	102.13	106.33
32	j	101	CLA	C1D-ND-C4D	-5.92	102.13	106.33
32	a	806	CLA	C1D-ND-C4D	-5.92	102.13	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	835	CLA	C1D-ND-C4D	-5.92	102.13	106.33
32	b	809	CLA	C1D-ND-C4D	-5.92	102.13	106.33
37	K	314	A86	O1-C20-C19	5.91	117.82	113.38
32	b	815	CLA	C1D-ND-C4D	-5.91	102.14	106.33
32	E	304	CLA	C1D-ND-C4D	-5.90	102.14	106.33
32	b	825	CLA	C4A-NA-C1A	-5.90	104.05	106.71
36	E	322	LMG	O7-C10-C11	5.90	124.22	111.50
32	C	305	CLA	C1D-ND-C4D	-5.90	102.14	106.33
32	b	828	CLA	C1D-ND-C4D	-5.90	102.15	106.33
32	a	815	CLA	C1D-ND-C4D	-5.89	102.15	106.33
32	M	308	CLA	C4A-NA-C1A	-5.89	104.06	106.71
40	b	846	DGD	O2G-C1B-C2B	5.89	124.20	111.50
32	V	203	CLA	C4A-NA-C1A	-5.89	104.06	106.71
32	R	309	CLA	C1D-ND-C4D	-5.89	102.15	106.33
32	f	204	CLA	C4A-NA-C1A	-5.89	104.06	106.71
32	B	306	CLA	C1D-ND-C4D	-5.89	102.15	106.33
32	O	305	CLA	C1D-ND-C4D	-5.89	102.15	106.33
32	S	309	CLA	C1D-ND-C4D	-5.89	102.15	106.33
32	I	306	CLA	C4A-NA-C1A	-5.89	104.06	106.71
32	a	837	CLA	C1D-ND-C4D	-5.89	102.15	106.33
32	H	308	CLA	C1D-ND-C4D	-5.88	102.16	106.33
32	K	310	CLA	C1D-ND-C4D	-5.88	102.16	106.33
32	V	203	CLA	C1D-ND-C4D	-5.88	102.16	106.33
32	k	201	CLA	C4A-NA-C1A	-5.88	104.06	106.71
32	D	308	CLA	C1D-ND-C4D	-5.88	102.16	106.33
32	D	315	CLA	C1D-ND-C4D	-5.88	102.16	106.33
32	E	305	CLA	C4A-NA-C1A	-5.87	104.06	106.71
32	L	304	CLA	C1D-ND-C4D	-5.87	102.16	106.33
32	Q	310	CLA	C4A-NA-C1A	-5.87	104.07	106.71
32	W	312	CLA	C4A-NA-C1A	-5.87	104.07	106.71
32	O	304	CLA	C1D-ND-C4D	-5.87	102.17	106.33
32	b	819	CLA	C1D-ND-C4D	-5.87	102.17	106.33
32	G	308	CLA	C4A-NA-C1A	-5.87	104.07	106.71
32	W	309	CLA	C4A-NA-C1A	-5.87	104.07	106.71
32	b	812	CLA	C1D-ND-C4D	-5.87	102.17	106.33
37	L	318	A86	O1-C20-C19	5.87	117.79	113.38
32	D	306	CLA	C4A-NA-C1A	-5.86	104.07	106.71
32	J	304	CLA	C1D-ND-C4D	-5.86	102.17	106.33
32	I	317	CLA	C1D-ND-C4D	-5.86	102.17	106.33
32	A	311	CLA	C1D-ND-C4D	-5.85	102.18	106.33
32	a	826	CLA	C1D-ND-C4D	-5.85	102.18	106.33
32	L	309	CLA	C1D-ND-C4D	-5.85	102.18	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	J	301	CLA	C1D-ND-C4D	-5.84	102.19	106.33
32	b	813	CLA	C4A-NA-C1A	-5.84	104.08	106.71
32	b	807	CLA	C1D-ND-C4D	-5.84	102.19	106.33
32	E	309	CLA	C1D-ND-C4D	-5.83	102.19	106.33
32	a	804	CLA	C1D-ND-C4D	-5.83	102.19	106.33
32	b	813	CLA	C1D-ND-C4D	-5.83	102.19	106.33
32	a	832	CLA	C1D-ND-C4D	-5.83	102.19	106.33
32	W	313	CLA	C1D-ND-C4D	-5.83	102.19	106.33
32	a	810	CLA	C1D-ND-C4D	-5.83	102.19	106.33
32	l	202	CLA	C1D-ND-C4D	-5.83	102.19	106.33
32	H	307	CLA	C4A-NA-C1A	-5.83	104.09	106.71
32	a	825	CLA	C1D-ND-C4D	-5.82	102.20	106.33
32	b	840	CLA	C1D-ND-C4D	-5.82	102.20	106.33
32	R	310	CLA	C4A-NA-C1A	-5.81	104.09	106.71
32	E	307	CLA	C1D-ND-C4D	-5.81	102.20	106.33
32	a	821	CLA	C1D-ND-C4D	-5.81	102.20	106.33
32	P	308	CLA	C1D-ND-C4D	-5.81	102.21	106.33
32	T	306	CLA	C1D-ND-C4D	-5.81	102.21	106.33
32	a	819	CLA	C1D-ND-C4D	-5.81	102.21	106.33
32	T	305	CLA	C4A-NA-C1A	-5.81	104.09	106.71
32	L	301	CLA	C4A-NA-C1A	-5.81	104.10	106.71
32	a	808	CLA	C4A-NA-C1A	-5.80	104.10	106.71
32	A	301	CLA	C1D-ND-C4D	-5.80	102.22	106.33
32	b	820	CLA	C1D-ND-C4D	-5.79	102.22	106.33
32	b	814	CLA	C1D-ND-C4D	-5.79	102.22	106.33
32	b	835	CLA	C1D-ND-C4D	-5.79	102.22	106.33
32	J	305	CLA	C1D-ND-C4D	-5.79	102.22	106.33
32	S	304	CLA	C1D-ND-C4D	-5.78	102.23	106.33
36	E	302	LMG	C7-O1-C1	5.78	125.04	113.74
32	a	816	CLA	C4A-NA-C1A	-5.78	104.11	106.71
32	b	804	CLA	C1D-ND-C4D	-5.78	102.23	106.33
32	B	303	CLA	C1D-ND-C4D	-5.77	102.24	106.33
32	b	822	CLA	C1D-ND-C4D	-5.77	102.24	106.33
32	J	309	CLA	C4A-NA-C1A	-5.77	104.11	106.71
32	b	812	CLA	C4A-NA-C1A	-5.77	104.11	106.71
32	a	812	CLA	C1D-ND-C4D	-5.77	102.24	106.33
32	K	307	CLA	C1D-ND-C4D	-5.77	102.24	106.33
32	L	314	CLA	C1D-ND-C4D	-5.76	102.24	106.33
32	a	829	CLA	C1D-ND-C4D	-5.76	102.24	106.33
32	W	309	CLA	C1D-ND-C4D	-5.76	102.24	106.33
32	b	802	CLA	C1D-ND-C4D	-5.75	102.25	106.33
32	b	831	CLA	C1D-ND-C4D	-5.75	102.25	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	311	CLA	C1D-ND-C4D	-5.75	102.25	106.33
32	Q	304	CLA	C1D-ND-C4D	-5.75	102.25	106.33
32	P	305	CLA	C4A-NA-C1A	-5.75	104.12	106.71
32	S	307	CLA	C1D-ND-C4D	-5.75	102.25	106.33
32	b	838	CLA	C1D-ND-C4D	-5.75	102.25	106.33
32	H	301	CLA	C1D-ND-C4D	-5.75	102.25	106.33
32	b	825	CLA	C1D-ND-C4D	-5.75	102.25	106.33
32	U	305	CLA	C1D-ND-C4D	-5.74	102.25	106.33
32	M	305	CLA	C1D-ND-C4D	-5.74	102.26	106.33
32	G	305	CLA	C1D-ND-C4D	-5.74	102.26	106.33
32	b	823	CLA	C1D-ND-C4D	-5.74	102.26	106.33
32	a	824	CLA	C4A-NA-C1A	-5.73	104.13	106.71
32	B	306	CLA	C4A-NA-C1A	-5.73	104.13	106.71
32	S	308	CLA	C4A-NA-C1A	-5.73	104.13	106.71
32	F	307	CLA	C4A-NA-C1A	-5.72	104.14	106.71
32	I	302	CLA	C4A-NA-C1A	-5.71	104.14	106.71
32	a	802	CLA	C4A-NA-C1A	-5.71	104.14	106.71
32	a	827	CLA	C1D-ND-C4D	-5.71	102.28	106.33
32	L	314	CLA	C4A-NA-C1A	-5.71	104.14	106.71
32	a	834	CLA	C1D-ND-C4D	-5.71	102.28	106.33
32	E	315	CLA	C4A-NA-C1A	-5.70	104.14	106.71
32	W	311	CLA	C1D-ND-C4D	-5.70	102.29	106.33
32	B	309	CLA	C1D-ND-C4D	-5.69	102.29	106.33
32	b	836	CLA	C1D-ND-C4D	-5.69	102.29	106.33
32	b	829	CLA	C4A-NA-C1A	-5.69	104.15	106.71
32	W	306	CLA	C1D-ND-C4D	-5.69	102.29	106.33
32	a	823	CLA	C1D-ND-C4D	-5.69	102.29	106.33
32	a	838	CLA	C1D-ND-C4D	-5.68	102.30	106.33
32	a	818	CLA	C1D-ND-C4D	-5.68	102.30	106.33
32	M	312	CLA	C4A-NA-C1A	-5.68	104.15	106.71
32	W	307	CLA	C4A-NA-C1A	-5.68	104.15	106.71
32	a	828	CLA	C1D-ND-C4D	-5.68	102.30	106.33
32	F	306	CLA	C4A-NA-C1A	-5.67	104.16	106.71
32	a	841	CLA	C1D-ND-C4D	-5.65	102.32	106.33
32	b	803	CLA	C1D-ND-C4D	-5.65	102.32	106.33
32	P	304	CLA	C1D-ND-C4D	-5.65	102.32	106.33
37	J	313	A86	C34-O4-C38	5.65	128.42	117.90
32	L	308	CLA	C4A-NA-C1A	-5.64	104.17	106.71
32	I	304	CLA	C1D-ND-C4D	-5.63	102.33	106.33
32	M	306	CLA	C4A-NA-C1A	-5.63	104.17	106.71
32	l	204	CLA	C1D-ND-C4D	-5.63	102.34	106.33
32	F	309	CLA	C4A-NA-C1A	-5.63	104.18	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	U	306	CLA	C1D-ND-C4D	-5.63	102.34	106.33
32	b	808	CLA	C1D-ND-C4D	-5.63	102.34	106.33
32	P	311	CLA	C4A-NA-C1A	-5.62	104.18	106.71
32	Q	305	CLA	C4A-NA-C1A	-5.62	104.18	106.71
32	b	830	CLA	C1D-ND-C4D	-5.61	102.35	106.33
32	a	835	CLA	C4A-NA-C1A	-5.61	104.19	106.71
32	A	304	CLA	C4A-NA-C1A	-5.60	104.19	106.71
32	F	322	CLA	C1D-ND-C4D	-5.60	102.36	106.33
32	I	301	CLA	C4A-NA-C1A	-5.59	104.19	106.71
32	j	101	CLA	C4A-NA-C1A	-5.59	104.19	106.71
32	a	830	CLA	C1D-ND-C4D	-5.59	102.36	106.33
32	k	203	CLA	C1D-ND-C4D	-5.59	102.37	106.33
32	E	308	CLA	C4A-NA-C1A	-5.59	104.19	106.71
32	E	303	CLA	C4A-NA-C1A	-5.58	104.20	106.71
32	a	824	CLA	C1D-ND-C4D	-5.58	102.37	106.33
32	T	305	CLA	C1D-ND-C4D	-5.58	102.37	106.33
32	S	308	CLA	C1D-ND-C4D	-5.57	102.38	106.33
32	b	814	CLA	C4A-NA-C1A	-5.57	104.20	106.71
32	b	815	CLA	C4A-NA-C1A	-5.57	104.20	106.71
32	U	302	CLA	C4A-NA-C1A	-5.56	104.21	106.71
32	a	834	CLA	C4A-NA-C1A	-5.55	104.21	106.71
32	b	810	CLA	C1D-ND-C4D	-5.55	102.39	106.33
37	P	316	A86	C34-O4-C38	5.54	128.23	117.90
32	V	201	CLA	C4A-NA-C1A	-5.54	104.21	106.71
32	G	301	CLA	C4A-NA-C1A	-5.54	104.22	106.71
32	b	808	CLA	C4A-NA-C1A	-5.54	104.22	106.71
32	N	312	CLA	C4A-NA-C1A	-5.54	104.22	106.71
32	a	801	CLA	CHD-C1D-ND	-5.53	119.37	124.45
32	b	822	CLA	C4A-NA-C1A	-5.53	104.22	106.71
32	B	302	CLA	C4A-NA-C1A	-5.53	104.22	106.71
34	J	317	DD6	O1-C20-C19	-5.52	109.23	113.38
32	B	304	CLA	C1D-ND-C4D	-5.52	102.41	106.33
32	a	806	CLA	C4A-NA-C1A	-5.52	104.22	106.71
32	a	853	CLA	C4A-NA-C1A	-5.52	104.23	106.71
32	V	204	CLA	C4A-NA-C1A	-5.51	104.23	106.71
32	b	823	CLA	C4A-NA-C1A	-5.50	104.23	106.71
32	O	305	CLA	C4A-NA-C1A	-5.50	104.23	106.71
32	N	309	CLA	C1D-ND-C4D	-5.49	102.44	106.33
32	R	307	CLA	C4A-NA-C1A	-5.49	104.24	106.71
32	H	305	CLA	CHD-C1D-ND	-5.48	119.42	124.45
33	N	308	KC2	C4D-C3D-CAD	5.48	111.11	107.42
32	E	306	CLA	C4A-NA-C1A	-5.48	104.24	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	311	CLA	C4A-NA-C1A	-5.47	104.25	106.71
32	E	307	CLA	C4A-NA-C1A	-5.47	104.25	106.71
32	U	303	CLA	C1D-ND-C4D	-5.46	102.45	106.33
32	N	305	CLA	C1D-ND-C4D	-5.46	102.45	106.33
32	a	817	CLA	C4A-NA-C1A	-5.46	104.25	106.71
32	D	313	CLA	C4A-NA-C1A	-5.45	104.25	106.71
37	S	314	A86	C34-O4-C38	5.45	128.06	117.90
32	M	309	CLA	C4A-NA-C1A	-5.45	104.25	106.71
32	L	304	CLA	C4A-NA-C1A	-5.45	104.26	106.71
32	f	201	CLA	C1D-ND-C4D	-5.44	102.47	106.33
34	K	315	DD6	O1-C20-C19	-5.44	109.30	113.38
32	G	306	CLA	CHD-C1D-ND	-5.43	119.46	124.45
32	F	308	CLA	C4A-NA-C1A	-5.43	104.27	106.71
32	O	306	CLA	C4A-NA-C1A	-5.42	104.27	106.71
32	b	806	CLA	C4A-NA-C1A	-5.42	104.27	106.71
32	P	308	CLA	C4A-NA-C1A	-5.41	104.27	106.71
33	L	313	KC2	C4D-C3D-CAD	5.41	111.07	107.42
32	D	304	CLA	C4A-NA-C1A	-5.39	104.28	106.71
32	b	827	CLA	C4A-NA-C1A	-5.39	104.28	106.71
32	a	841	CLA	C4A-NA-C1A	-5.39	104.28	106.71
37	L	315	A86	C33-C32-C31	5.38	114.44	109.21
32	k	202	CLA	C4A-NA-C1A	-5.38	104.29	106.71
32	D	311	CLA	C4A-NA-C1A	-5.37	104.29	106.71
32	b	801	CLA	CHD-C1D-ND	-5.37	119.52	124.45
32	W	310	CLA	C4A-NA-C1A	-5.37	104.29	106.71
32	S	305	CLA	C4A-NA-C1A	-5.35	104.30	106.71
37	C	312	A86	C21-C20-C19	-5.34	108.28	114.28
32	L	312	CLA	C4A-NA-C1A	-5.33	104.31	106.71
32	A	308	CLA	C4A-NA-C1A	-5.32	104.31	106.71
32	a	842	CLA	C4A-NA-C1A	-5.32	104.31	106.71
32	L	307	CLA	C1D-ND-C4D	-5.30	102.57	106.33
32	a	815	CLA	C4A-NA-C1A	-5.30	104.32	106.71
32	E	314	CLA	C4A-NA-C1A	-5.30	104.32	106.71
32	A	306	CLA	C4A-NA-C1A	-5.29	104.33	106.71
32	T	307	CLA	C4A-NA-C1A	-5.29	104.33	106.71
32	J	307	CLA	CHD-C1D-ND	-5.29	119.59	124.45
32	l	203	CLA	C4A-NA-C1A	-5.29	104.33	106.71
32	G	304	CLA	C4A-NA-C1A	-5.28	104.33	106.71
32	a	812	CLA	CHD-C1D-ND	-5.28	119.60	124.45
32	A	301	CLA	C4A-NA-C1A	-5.28	104.33	106.71
32	M	310	CLA	C4A-NA-C1A	-5.28	104.33	106.71
37	W	315	A86	O1-C20-C19	-5.27	109.42	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	N	319	DD6	C14-C13-C11	5.26	133.70	125.53
32	N	311	CLA	C4A-NA-C1A	-5.26	104.34	106.71
32	S	309	CLA	C4A-NA-C1A	-5.25	104.34	106.71
32	b	840	CLA	C4A-NA-C1A	-5.25	104.34	106.71
32	B	302	CLA	C1D-ND-C4D	-5.25	102.61	106.33
32	H	310	CLA	C4A-NA-C1A	-5.25	104.35	106.71
32	J	305	CLA	C4A-NA-C1A	-5.25	104.35	106.71
37	W	318	A86	C36-C31-C32	5.24	124.90	119.70
32	C	309	CLA	C4A-NA-C1A	-5.23	104.35	106.71
32	F	303	CLA	C4A-NA-C1A	-5.22	104.36	106.71
37	T	312	A86	O1-C20-C19	5.22	117.30	113.38
32	a	852	CLA	C1D-ND-C4D	-5.22	102.63	106.33
32	b	817	CLA	C4A-NA-C1A	-5.22	104.36	106.71
37	J	313	A86	C21-C20-C19	-5.21	108.42	114.28
32	K	306	CLA	CHD-C1D-ND	-5.21	119.67	124.45
32	b	816	CLA	C4A-NA-C1A	-5.20	104.37	106.71
33	L	306	KC2	C4D-C3D-CAD	5.19	110.92	107.42
32	a	810	CLA	CHD-C1D-ND	-5.19	119.69	124.45
32	Q	307	CLA	C4A-NA-C1A	-5.18	104.38	106.71
37	H	314	A86	O1-C20-C19	5.18	117.27	113.38
37	S	315	A86	C21-C20-C19	-5.18	108.45	114.28
32	F	304	CLA	C4A-NA-C1A	-5.16	104.38	106.71
32	B	303	CLA	C4A-NA-C1A	-5.16	104.39	106.71
32	T	305	CLA	CHD-C1D-ND	-5.16	119.71	124.45
37	W	318	A86	C33-C32-C31	5.15	114.22	109.21
32	b	807	CLA	CHD-C1D-ND	-5.15	119.72	124.45
35	I	318	LHG	O7-C7-C8	5.15	122.59	111.50
32	b	802	CLA	CHD-C1D-ND	-5.15	119.72	124.45
32	F	304	CLA	CHD-C1D-ND	-5.14	119.73	124.45
32	a	805	CLA	C1D-ND-C4D	-5.13	102.69	106.33
32	E	306	CLA	CHD-C1D-ND	-5.13	119.74	124.45
32	L	311	CLA	CHD-C1D-ND	-5.12	119.75	124.45
32	S	311	CLA	CHD-C1D-ND	-5.12	119.75	124.45
37	G	311	A86	O1-C20-C19	5.12	117.22	113.38
37	S	319	A86	O1-C20-C19	5.12	117.22	113.38
32	N	309	CLA	CHD-C1D-ND	-5.11	119.75	124.45
32	a	826	CLA	C4A-NA-C1A	-5.11	104.41	106.71
32	T	306	CLA	C4A-NA-C1A	-5.10	104.42	106.71
39	H	315	SQD	O47-C7-C8	5.09	122.48	111.50
32	C	301	CLA	C4A-NA-C1A	-5.09	104.42	106.71
32	a	810	CLA	C4A-NA-C1A	-5.08	104.42	106.71
32	l	204	CLA	CHD-C1D-ND	-5.08	119.79	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	805	CLA	C4A-NA-C1A	-5.07	104.43	106.71
33	N	302	KC2	C4D-C3D-CAD	5.07	110.84	107.42
32	S	304	CLA	C4A-NA-C1A	-5.07	104.43	106.71
32	E	310	CLA	C4A-NA-C1A	-5.06	104.43	106.71
33	R	305	KC2	C4D-C3D-CAD	5.06	110.83	107.42
32	K	306	CLA	C4A-NA-C1A	-5.06	104.43	106.71
32	M	305	CLA	C4A-NA-C1A	-5.04	104.44	106.71
34	F	316	DD6	O1-C20-C19	-5.04	109.60	113.38
32	a	816	CLA	CHD-C1D-ND	-5.04	119.82	124.45
33	N	307	KC2	C4D-C3D-CAD	5.03	110.81	107.42
32	b	811	CLA	C4A-NA-C1A	-5.03	104.44	106.71
33	Q	317	KC2	C4D-C3D-CAD	5.03	110.81	107.42
33	W	301	KC2	C4D-C3D-CAD	5.03	110.81	107.42
32	D	307	CLA	CHD-C1D-ND	-5.03	119.84	124.45
37	L	317	A86	O1-C20-C19	5.02	117.16	113.38
32	C	305	CLA	CHD-C1D-ND	-5.02	119.84	124.45
32	D	314	CLA	CHD-C1D-ND	-5.02	119.84	124.45
33	T	311	KC2	C4D-C3D-CAD	5.02	110.80	107.42
32	L	310	CLA	CHD-C1D-ND	-5.02	119.84	124.45
33	W	314	KC2	C4D-C3D-CAD	5.01	110.80	107.42
32	H	302	CLA	CHD-C1D-ND	-5.00	119.86	124.45
37	O	311	A86	O1-C20-C19	5.00	117.14	113.38
36	D	325	LMG	O7-C10-C11	5.00	122.28	111.50
32	D	314	CLA	C1D-ND-C4D	-5.00	102.78	106.33
43	a	848	PQN	C11-C3-C4	-5.00	113.15	118.50
33	G	309	KC2	C4D-C3D-CAD	5.00	110.79	107.42
32	B	304	CLA	CHD-C1D-ND	-4.99	119.87	124.45
32	F	311	CLA	CHD-C1D-ND	-4.97	119.89	124.45
33	M	304	KC2	C4D-C3D-CAD	4.96	110.76	107.42
33	M	321	KC2	C4D-C3D-CAD	4.96	110.76	107.42
32	I	306	CLA	CHD-C1D-ND	-4.96	119.90	124.45
33	P	312	KC2	C4D-C3D-CAD	4.96	110.76	107.42
32	B	305	CLA	CHD-C1D-ND	-4.95	119.90	124.45
32	K	307	CLA	C4A-NA-C1A	-4.95	104.48	106.71
33	O	310	KC2	C4D-C3D-CAD	4.95	110.76	107.42
32	a	802	CLA	CHD-C1D-ND	-4.95	119.91	124.45
32	a	822	CLA	C4A-NA-C1A	-4.95	104.48	106.71
32	P	310	CLA	CHD-C1D-ND	-4.94	119.92	124.45
32	S	307	CLA	CHD-C1D-ND	-4.94	119.92	124.45
32	C	308	CLA	CHD-C1D-ND	-4.93	119.92	124.45
33	P	301	KC2	C4D-C3D-CAD	4.93	110.75	107.42
33	K	309	KC2	C4D-C3D-CAD	4.93	110.74	107.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	R	311	KC2	C4D-C3D-CAD	4.91	110.73	107.42
32	K	304	CLA	CHD-C1D-ND	-4.91	119.94	124.45
36	E	320	LMG	O7-C10-C11	4.91	122.08	111.50
34	D	317	DD6	C14-C13-C11	4.91	133.15	125.53
32	b	839	CLA	C4A-NA-C1A	-4.91	104.50	106.71
32	D	310	CLA	CHD-C1D-ND	-4.91	119.94	124.45
33	G	302	KC2	C4D-C3D-CAD	4.91	110.73	107.42
33	I	316	KC2	C4D-C3D-CAD	4.91	110.73	107.42
32	a	852	CLA	CHD-C1D-ND	-4.90	119.95	124.45
33	F	310	KC2	C4D-C3D-CAD	4.90	110.72	107.42
33	K	305	KC2	C4D-C3D-CAD	4.89	110.72	107.42
32	N	310	CLA	CHD-C1D-ND	-4.89	119.96	124.45
32	a	837	CLA	CHD-C1D-ND	-4.89	119.96	124.45
33	R	303	KC2	C4D-C3D-CAD	4.89	110.72	107.42
33	S	303	KC2	C4D-C3D-CAD	4.88	110.71	107.42
32	b	837	CLA	CHD-C1D-ND	-4.88	119.97	124.45
37	r	204	A86	O1-C20-C19	-4.88	109.72	113.38
32	I	304	CLA	CHD-C1D-ND	-4.88	119.97	124.45
32	D	313	CLA	CHD-C1D-ND	-4.87	119.97	124.45
32	b	824	CLA	C4A-NA-C1A	-4.87	104.52	106.71
32	J	301	CLA	C4A-NA-C1A	-4.87	104.52	106.71
33	N	314	KC2	C4D-C3D-CAD	4.87	110.70	107.42
37	H	314	A86	C21-C20-C19	-4.87	108.81	114.28
32	C	304	CLA	CHD-C1D-ND	-4.86	119.98	124.45
32	b	810	CLA	C4A-NA-C1A	-4.86	104.52	106.71
32	R	309	CLA	CHD-C1D-ND	-4.86	119.99	124.45
32	B	309	CLA	C4A-NA-C1A	-4.86	104.52	106.71
32	E	314	CLA	CHD-C1D-ND	-4.86	119.99	124.45
37	L	316	A86	C33-C32-C31	4.86	113.93	109.21
32	W	310	CLA	CHD-C1D-ND	-4.85	119.99	124.45
32	A	302	CLA	C4A-NA-C1A	-4.85	104.52	106.71
33	W	308	KC2	C4D-C3D-CAD	4.85	110.69	107.42
32	G	303	CLA	CHD-C1D-ND	-4.85	120.00	124.45
32	a	809	CLA	CHD-C1D-ND	-4.85	120.00	124.45
32	F	305	CLA	CHD-C1D-ND	-4.84	120.00	124.45
33	F	302	KC2	C4D-C3D-CAD	4.84	110.69	107.42
32	a	802	CLA	C1D-ND-C4D	-4.84	102.89	106.33
33	L	305	KC2	C4D-C3D-CAD	4.84	110.68	107.42
32	S	308	CLA	CHD-C1D-ND	-4.84	120.01	124.45
32	O	307	CLA	CHD-C1D-ND	-4.83	120.01	124.45
32	J	304	CLA	CHD-C1D-ND	-4.83	120.01	124.45
33	J	310	KC2	C4D-C3D-CAD	4.83	110.68	107.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	F	308	CLA	CHD-C1D-ND	-4.83	120.02	124.45
32	G	301	CLA	CHD-C1D-ND	-4.83	120.02	124.45
33	P	303	KC2	C4D-C3D-CAD	4.83	110.68	107.42
32	T	310	CLA	CHD-C1D-ND	-4.83	120.02	124.45
33	A	310	KC2	C4D-C3D-CAD	4.83	110.67	107.42
32	b	826	CLA	CHD-C1D-ND	-4.83	120.02	124.45
32	O	308	CLA	CHD-C1D-ND	-4.82	120.02	124.45
32	Q	310	CLA	CHD-C1D-ND	-4.82	120.02	124.45
32	A	305	CLA	CHD-C1D-ND	-4.82	120.02	124.45
33	E	313	KC2	C4D-C3D-CAD	4.82	110.67	107.42
33	K	303	KC2	C4D-C3D-CAD	4.82	110.67	107.42
32	G	305	CLA	C4A-NA-C1A	-4.82	104.54	106.71
32	b	804	CLA	CHD-C1D-ND	-4.82	120.03	124.45
33	N	303	KC2	C4D-C3D-CAD	4.81	110.67	107.42
33	I	309	KC2	C4D-C3D-CAD	4.81	110.67	107.42
32	M	309	CLA	CHD-C1D-ND	-4.81	120.03	124.45
32	T	302	CLA	CHD-C1D-ND	-4.81	120.03	124.45
33	P	302	KC2	C4D-C3D-CAD	4.81	110.66	107.42
33	W	303	KC2	C4D-C3D-CAD	4.81	110.66	107.42
32	b	806	CLA	CHD-C1D-ND	-4.81	120.04	124.45
32	a	840	CLA	CHD-C1D-ND	-4.80	120.04	124.45
32	F	301	CLA	CHD-C1D-ND	-4.80	120.04	124.45
32	S	301	CLA	CHD-C1D-ND	-4.80	120.04	124.45
32	b	835	CLA	CHD-C1D-ND	-4.80	120.04	124.45
32	R	306	CLA	CHD-C1D-ND	-4.80	120.05	124.45
36	A	317	LMG	O7-C10-C11	4.80	121.84	111.50
32	D	306	CLA	CHD-C1D-ND	-4.80	120.05	124.45
32	L	312	CLA	CHD-C1D-ND	-4.80	120.05	124.45
32	a	808	CLA	CHD-C1D-ND	-4.80	120.05	124.45
32	b	833	CLA	CHD-C1D-ND	-4.80	120.05	124.45
32	b	834	CLA	CHD-C1D-ND	-4.80	120.05	124.45
32	a	839	CLA	CHD-C1D-ND	-4.79	120.05	124.45
37	S	314	A86	O4-C34-C33	4.79	119.53	107.59
32	a	820	CLA	CHD-C1D-ND	-4.79	120.05	124.45
32	b	818	CLA	CHD-C1D-ND	-4.79	120.05	124.45
32	N	305	CLA	CHD-C1D-ND	-4.79	120.05	124.45
32	J	306	CLA	CHD-C1D-ND	-4.78	120.06	124.45
32	C	306	CLA	CHD-C1D-ND	-4.78	120.06	124.45
32	O	301	CLA	CHD-C1D-ND	-4.78	120.06	124.45
32	b	838	CLA	CHD-C1D-ND	-4.78	120.06	124.45
32	G	307	CLA	CHD-C1D-ND	-4.77	120.07	124.45
32	b	827	CLA	CHD-C1D-ND	-4.77	120.07	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	K	310	CLA	CHD-C1D-ND	-4.77	120.07	124.45
32	a	807	CLA	CHD-C1D-ND	-4.77	120.07	124.45
32	J	308	CLA	CHD-C1D-ND	-4.76	120.08	124.45
32	I	305	CLA	CHD-C1D-ND	-4.76	120.08	124.45
33	M	302	KC2	C4D-C3D-CAD	4.76	110.63	107.42
32	P	304	CLA	CHD-C1D-ND	-4.76	120.08	124.45
32	G	308	CLA	CHD-C1D-ND	-4.75	120.08	124.45
32	a	814	CLA	CHD-C1D-ND	-4.75	120.09	124.45
33	M	313	KC2	C4D-C3D-CAD	4.75	110.62	107.42
32	I	307	CLA	CHD-C1D-ND	-4.75	120.09	124.45
32	L	308	CLA	CHD-C1D-ND	-4.75	120.09	124.45
32	a	805	CLA	CHD-C1D-ND	-4.75	120.09	124.45
32	A	311	CLA	CHD-C1D-ND	-4.75	120.09	124.45
33	H	303	KC2	C4D-C3D-CAD	4.75	110.62	107.42
32	R	307	CLA	CHD-C1D-ND	-4.75	120.09	124.45
32	I	303	CLA	CHD-C1D-ND	-4.74	120.09	124.45
32	M	308	CLA	CHD-C1D-ND	-4.74	120.10	124.45
32	O	306	CLA	CHD-C1D-ND	-4.74	120.10	124.45
32	f	201	CLA	C4A-NA-C1A	-4.74	104.58	106.71
32	C	307	CLA	CHD-C1D-ND	-4.73	120.10	124.45
32	a	813	CLA	CHD-C1D-ND	-4.73	120.10	124.45
32	B	302	CLA	CHD-C1D-ND	-4.73	120.11	124.45
32	b	822	CLA	CHD-C1D-ND	-4.73	120.11	124.45
32	k	203	CLA	CHD-C1D-ND	-4.73	120.11	124.45
32	J	312	CLA	CHD-C1D-ND	-4.73	120.11	124.45
32	Q	304	CLA	CHD-C1D-ND	-4.73	120.11	124.45
32	U	303	CLA	CHD-C1D-ND	-4.73	120.11	124.45
32	U	307	CLA	CHD-C1D-ND	-4.72	120.11	124.45
33	N	306	KC2	C4D-C3D-CAD	4.72	110.61	107.42
32	D	311	CLA	CHD-C1D-ND	-4.72	120.12	124.45
32	W	306	CLA	CHD-C1D-ND	-4.72	120.12	124.45
33	W	304	KC2	C4D-C3D-CAD	4.72	110.60	107.42
32	S	310	CLA	CHD-C1D-ND	-4.72	120.12	124.45
32	H	301	CLA	CHD-C1D-ND	-4.72	120.12	124.45
32	Q	305	CLA	CHD-C1D-ND	-4.72	120.12	124.45
32	L	304	CLA	CHD-C1D-ND	-4.72	120.12	124.45
32	M	306	CLA	CHD-C1D-ND	-4.72	120.12	124.45
32	J	311	CLA	CHD-C1D-ND	-4.71	120.12	124.45
33	S	306	KC2	C4D-C3D-CAD	4.71	110.60	107.42
32	D	315	CLA	CHD-C1D-ND	-4.71	120.13	124.45
32	L	309	CLA	CHD-C1D-ND	-4.71	120.13	124.45
32	P	307	CLA	CHD-C1D-ND	-4.70	120.13	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Q	307	CLA	CHD-C1D-ND	-4.70	120.14	124.45
32	W	309	CLA	CHD-C1D-ND	-4.70	120.14	124.45
32	b	820	CLA	CHD-C1D-ND	-4.70	120.14	124.45
32	F	306	CLA	CHD-C1D-ND	-4.69	120.14	124.45
32	S	313	CLA	CHD-C1D-ND	-4.69	120.14	124.45
32	G	304	CLA	CHD-C1D-ND	-4.69	120.14	124.45
32	A	307	CLA	CHD-C1D-ND	-4.69	120.14	124.45
32	E	307	CLA	CHD-C1D-ND	-4.69	120.14	124.45
32	D	308	CLA	CHD-C1D-ND	-4.69	120.15	124.45
33	T	303	KC2	C4D-C3D-CAD	4.69	110.58	107.42
32	R	301	CLA	CHD-C1D-ND	-4.69	120.15	124.45
32	U	302	CLA	CHD-C1D-ND	-4.69	120.15	124.45
33	O	302	KC2	C4D-C3D-CAD	4.69	110.58	107.42
32	D	309	CLA	CHD-C1D-ND	-4.68	120.15	124.45
32	J	301	CLA	CHD-C1D-ND	-4.68	120.15	124.45
32	R	310	CLA	CHD-C1D-ND	-4.68	120.15	124.45
32	a	806	CLA	CHD-C1D-ND	-4.68	120.15	124.45
33	O	303	KC2	C4D-C3D-CAD	4.68	110.58	107.42
32	E	308	CLA	CHD-C1D-ND	-4.68	120.15	124.45
32	I	317	CLA	CHD-C1D-ND	-4.68	120.15	124.45
32	a	817	CLA	CHD-C1D-ND	-4.68	120.15	124.45
32	E	304	CLA	CHD-C1D-ND	-4.68	120.16	124.45
32	Q	301	CLA	CHD-C1D-ND	-4.68	120.16	124.45
32	M	311	CLA	CHD-C1D-ND	-4.68	120.16	124.45
32	O	305	CLA	CHD-C1D-ND	-4.68	120.16	124.45
32	b	828	CLA	CHD-C1D-ND	-4.68	120.16	124.45
32	a	818	CLA	CHD-C1D-ND	-4.67	120.16	124.45
32	U	301	CLA	CHD-C1D-ND	-4.67	120.16	124.45
33	C	303	KC2	C4D-C3D-CAD	4.67	110.57	107.42
33	L	303	KC2	C4D-C3D-CAD	4.67	110.57	107.42
32	N	313	CLA	CHD-C1D-ND	-4.67	120.17	124.45
32	b	814	CLA	CHD-C1D-ND	-4.67	120.17	124.45
33	S	302	KC2	C4D-C3D-CAD	4.66	110.56	107.42
32	P	311	CLA	CHD-C1D-ND	-4.66	120.17	124.45
32	l	202	CLA	CHD-C1D-ND	-4.66	120.17	124.45
32	C	309	CLA	CHD-C1D-ND	-4.66	120.17	124.45
33	K	302	KC2	C4D-C3D-CAD	4.66	110.56	107.42
32	B	306	CLA	CHD-C1D-ND	-4.66	120.17	124.45
32	H	309	CLA	CHD-C1D-ND	-4.66	120.18	124.45
32	P	305	CLA	CHD-C1D-ND	-4.66	120.18	124.45
33	U	304	KC2	C4D-C3D-CAD	4.65	110.56	107.42
32	A	306	CLA	CHD-C1D-ND	-4.65	120.18	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Q	306	CLA	CHD-C1D-ND	-4.65	120.18	124.45
32	a	829	CLA	CHD-C1D-ND	-4.65	120.18	124.45
33	T	304	KC2	C4D-C3D-CAD	4.65	110.56	107.42
33	M	303	KC2	C4D-C3D-CAD	4.65	110.55	107.42
32	L	307	CLA	CHD-C1D-ND	-4.65	120.18	124.45
32	E	315	CLA	CHD-C1D-ND	-4.65	120.18	124.45
32	H	310	CLA	CHD-C1D-ND	-4.64	120.19	124.45
32	F	307	CLA	CHD-C1D-ND	-4.64	120.19	124.45
32	H	307	CLA	CHD-C1D-ND	-4.64	120.19	124.45
32	M	305	CLA	CHD-C1D-ND	-4.64	120.19	124.45
32	a	825	CLA	C4A-NA-C1A	-4.64	104.62	106.71
32	D	304	CLA	CHD-C1D-ND	-4.64	120.19	124.45
32	D	305	CLA	CHD-C1D-ND	-4.64	120.19	124.45
32	R	308	CLA	CHD-C1D-ND	-4.64	120.19	124.45
32	a	838	CLA	CHD-C1D-ND	-4.64	120.19	124.45
32	B	301	CLA	CHD-C1D-ND	-4.64	120.19	124.45
32	P	309	CLA	CHD-C1D-ND	-4.63	120.19	124.45
32	V	201	CLA	CHD-C1D-ND	-4.63	120.20	124.45
32	b	805	CLA	CHD-C1D-ND	-4.63	120.20	124.45
32	E	309	CLA	CHD-C1D-ND	-4.63	120.20	124.45
33	M	307	KC2	C4D-C3D-CAD	4.63	110.54	107.42
37	R	313	A86	O1-C20-C19	4.62	116.86	113.38
32	b	812	CLA	CHD-C1D-ND	-4.62	120.21	124.45
32	b	813	CLA	CHD-C1D-ND	-4.62	120.21	124.45
32	T	308	CLA	CHD-C1D-ND	-4.62	120.21	124.45
32	J	312	CLA	C4A-NA-C1A	-4.62	104.63	106.71
32	K	308	CLA	CHD-C1D-ND	-4.62	120.21	124.45
33	N	304	KC2	C4D-C3D-CAD	4.62	110.53	107.42
37	L	317	A86	C21-C20-C19	-4.62	109.09	114.28
37	R	313	A86	C21-C20-C19	-4.62	109.09	114.28
32	Q	308	CLA	CHD-C1D-ND	-4.61	120.21	124.45
32	U	305	CLA	CHD-C1D-ND	-4.61	120.21	124.45
32	O	309	CLA	CHD-C1D-ND	-4.61	120.22	124.45
32	b	830	CLA	CHD-C1D-ND	-4.61	120.22	124.45
32	b	805	CLA	C1D-ND-C4D	-4.61	103.06	106.33
32	K	301	CLA	CHD-C1D-ND	-4.61	120.22	124.45
32	b	831	CLA	C4A-NA-C1A	-4.61	104.64	106.71
37	T	312	A86	C21-C20-C19	-4.60	109.10	114.28
32	N	312	CLA	CHD-C1D-ND	-4.60	120.22	124.45
32	a	803	CLA	CHD-C1D-ND	-4.60	120.22	124.45
32	J	302	CLA	CHD-C1D-ND	-4.60	120.22	124.45
32	f	204	CLA	CHD-C1D-ND	-4.60	120.22	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	k	201	CLA	CHD-C1D-ND	-4.60	120.22	124.45
33	P	306	KC2	C4D-C3D-CAD	4.60	110.52	107.42
32	H	304	CLA	CHD-C1D-ND	-4.60	120.23	124.45
32	b	809	CLA	CHD-C1D-ND	-4.60	120.23	124.45
32	W	313	CLA	CHD-C1D-ND	-4.60	120.23	124.45
32	F	322	CLA	CHD-C1D-ND	-4.60	120.23	124.45
32	L	301	CLA	CHD-C1D-ND	-4.60	120.23	124.45
32	b	829	CLA	CHD-C1D-ND	-4.59	120.23	124.45
32	a	804	CLA	CHD-C1D-ND	-4.59	120.23	124.45
32	H	306	CLA	CHD-C1D-ND	-4.59	120.23	124.45
32	a	833	CLA	CHD-C1D-ND	-4.59	120.23	124.45
32	M	312	CLA	CHD-C1D-ND	-4.59	120.23	124.45
33	R	302	KC2	C4D-C3D-CAD	4.59	110.52	107.42
32	D	312	CLA	CHD-C1D-ND	-4.59	120.24	124.45
32	M	310	CLA	CHD-C1D-ND	-4.59	120.24	124.45
32	b	821	CLA	CHD-C1D-ND	-4.59	120.24	124.45
32	B	303	CLA	CHD-C1D-ND	-4.59	120.24	124.45
32	j	101	CLA	CHD-C1D-ND	-4.59	120.24	124.45
32	V	204	CLA	CHD-C1D-ND	-4.59	120.24	124.45
32	a	834	CLA	CHD-C1D-ND	-4.59	120.24	124.45
32	H	308	CLA	CHD-C1D-ND	-4.58	120.24	124.45
32	W	307	CLA	CHD-C1D-ND	-4.58	120.24	124.45
32	b	817	CLA	CHD-C1D-ND	-4.58	120.24	124.45
32	R	304	CLA	CHD-C1D-ND	-4.58	120.24	124.45
32	E	312	CLA	CHD-C1D-ND	-4.58	120.24	124.45
32	T	309	CLA	CHD-C1D-ND	-4.58	120.24	124.45
32	E	311	CLA	CHD-C1D-ND	-4.58	120.25	124.45
32	a	831	CLA	CHD-C1D-ND	-4.58	120.25	124.45
32	a	853	CLA	CHD-C1D-ND	-4.58	120.25	124.45
32	E	310	CLA	CHD-C1D-ND	-4.57	120.25	124.45
32	T	307	CLA	CHD-C1D-ND	-4.57	120.25	124.45
32	J	305	CLA	CHD-C1D-ND	-4.57	120.25	124.45
32	C	302	CLA	CHD-C1D-ND	-4.57	120.25	124.45
32	O	304	CLA	CHD-C1D-ND	-4.57	120.26	124.45
32	F	309	CLA	CHD-C1D-ND	-4.57	120.26	124.45
32	T	306	CLA	CHD-C1D-ND	-4.56	120.26	124.45
32	r	202	CLA	CHD-C1D-ND	-4.56	120.26	124.45
41	l	206	BCR	C7-C8-C9	4.56	133.13	126.23
32	I	302	CLA	CHD-C1D-ND	-4.56	120.26	124.45
32	I	308	CLA	CHD-C1D-ND	-4.56	120.26	124.45
32	I	301	CLA	CHD-C1D-ND	-4.56	120.27	124.45
32	W	312	CLA	CHD-C1D-ND	-4.56	120.27	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	311	CLA	CHD-C1D-ND	-4.56	120.27	124.45
33	J	303	KC2	C4D-C3D-CAD	4.55	110.49	107.42
32	a	852	CLA	C4A-NA-C1A	-4.55	104.66	106.71
32	b	836	CLA	CHD-C1D-ND	-4.55	120.27	124.45
32	f	203	CLA	CHD-C1D-ND	-4.55	120.27	124.45
32	a	801	CLA	C4A-NA-C1A	-4.55	104.66	106.71
32	a	827	CLA	CHD-C1D-ND	-4.55	120.27	124.45
32	b	815	CLA	CHD-C1D-ND	-4.55	120.28	124.45
34	N	321	DD6	C14-C13-C11	4.55	132.59	125.53
32	L	314	CLA	CHD-C1D-ND	-4.55	120.28	124.45
32	r	201	CLA	CHD-C1D-ND	-4.55	120.28	124.45
32	b	819	CLA	C4A-NA-C1A	-4.54	104.66	106.71
34	j	103	DD6	C14-C13-C11	4.54	132.57	125.53
32	b	825	CLA	CHD-C1D-ND	-4.54	120.29	124.45
32	a	815	CLA	CHD-C1D-ND	-4.53	120.29	124.45
32	A	302	CLA	CHD-C1D-ND	-4.53	120.29	124.45
32	A	309	CLA	CHD-C1D-ND	-4.53	120.29	124.45
32	a	842	CLA	CHD-C1D-ND	-4.52	120.30	124.45
32	a	824	CLA	CHD-C1D-ND	-4.52	120.30	124.45
32	k	202	CLA	CHD-C1D-ND	-4.52	120.30	124.45
32	Q	303	CLA	CHD-C1D-ND	-4.52	120.30	124.45
32	b	803	CLA	CHD-C1D-ND	-4.52	120.30	124.45
33	Q	302	KC2	C4D-C3D-CAD	4.51	110.46	107.42
32	a	835	CLA	CHD-C1D-ND	-4.51	120.31	124.45
32	S	309	CLA	CHD-C1D-ND	-4.51	120.31	124.45
32	Q	309	CLA	CHD-C1D-ND	-4.51	120.31	124.45
32	E	303	CLA	CHD-C1D-ND	-4.50	120.31	124.45
32	a	823	CLA	CHD-C1D-ND	-4.50	120.32	124.45
32	b	839	CLA	CHD-C1D-ND	-4.50	120.32	124.45
36	D	303	LMG	O7-C10-C11	4.49	121.18	111.50
32	a	811	CLA	CHD-C1D-ND	-4.49	120.33	124.45
32	b	832	CLA	CHD-C1D-ND	-4.48	120.34	124.45
32	l	203	CLA	CHD-C1D-ND	-4.48	120.34	124.45
32	N	311	CLA	CHD-C1D-ND	-4.48	120.34	124.45
32	b	811	CLA	CHD-C1D-ND	-4.48	120.34	124.45
32	a	828	CLA	CHD-C1D-ND	-4.47	120.34	124.45
32	K	307	CLA	CHD-C1D-ND	-4.46	120.35	124.45
32	U	306	CLA	CHD-C1D-ND	-4.46	120.35	124.45
34	F	315	DD6	C14-C13-C11	4.46	132.45	125.53
32	b	824	CLA	CHD-C1D-ND	-4.46	120.36	124.45
37	S	314	A86	C36-C31-C32	4.46	124.12	119.70
32	A	308	CLA	CHD-C1D-ND	-4.45	120.36	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	826	CLA	CHD-C1D-ND	-4.45	120.36	124.45
32	a	825	CLA	CHD-C1D-ND	-4.45	120.36	124.45
32	b	840	CLA	CHD-C1D-ND	-4.45	120.37	124.45
32	J	309	CLA	CHD-C1D-ND	-4.44	120.37	124.45
32	V	203	CLA	CHD-C1D-ND	-4.44	120.37	124.45
32	A	304	CLA	CHD-C1D-ND	-4.44	120.38	124.45
32	S	304	CLA	CHD-C1D-ND	-4.42	120.39	124.45
32	a	819	CLA	CHD-C1D-ND	-4.42	120.39	124.45
32	A	301	CLA	CHD-C1D-ND	-4.42	120.39	124.45
37	J	313	A86	O4-C34-C35	4.41	118.58	107.59
32	B	309	CLA	CHD-C1D-ND	-4.41	120.40	124.45
33	L	302	KC2	C4D-C3D-CAD	4.40	110.39	107.42
32	F	303	CLA	CHD-C1D-ND	-4.40	120.41	124.45
32	E	305	CLA	CHD-C1D-ND	-4.39	120.42	124.45
32	a	832	CLA	CHD-C1D-ND	-4.39	120.42	124.45
32	P	308	CLA	CHD-C1D-ND	-4.39	120.42	124.45
33	W	305	KC2	C4D-C3D-CAD	4.38	110.38	107.42
32	f	201	CLA	CHD-C1D-ND	-4.37	120.43	124.45
32	b	810	CLA	CHD-C1D-ND	-4.37	120.44	124.45
33	S	312	KC2	C1D-ND-C4D	4.37	109.44	106.33
32	S	305	CLA	CHD-C1D-ND	-4.36	120.44	124.45
32	b	808	CLA	CHD-C1D-ND	-4.36	120.44	124.45
36	N	301	LMG	O7-C10-C11	4.36	120.90	111.50
32	a	821	CLA	CHD-C1D-ND	-4.35	120.46	124.45
32	a	841	CLA	CHD-C1D-ND	-4.34	120.47	124.45
32	C	301	CLA	CHD-C1D-ND	-4.34	120.47	124.45
33	W	305	KC2	C1D-ND-C4D	4.33	109.41	106.33
32	A	303	CLA	CHD-C1D-ND	-4.32	120.48	124.45
34	V	202	DD6	C14-C13-C11	4.32	132.23	125.53
36	M	320	LMG	O7-C10-C11	4.32	120.81	111.50
32	D	314	CLA	C4A-NA-C1A	-4.31	104.77	106.71
32	a	838	CLA	CHB-C1B-NB	-4.31	119.70	124.26
32	a	822	CLA	CHD-C1D-ND	-4.30	120.50	124.45
32	b	823	CLA	CHD-C1D-ND	-4.30	120.50	124.45
32	a	830	CLA	CHD-C1D-ND	-4.27	120.53	124.45
32	a	801	CLA	CHB-C1B-NB	-4.27	119.73	124.26
39	k	206	SQD	O47-C7-C8	4.27	120.70	111.50
32	b	805	CLA	CHB-C1B-NB	-4.26	119.74	124.26
32	a	836	CLA	CHD-C1D-ND	-4.25	120.55	124.45
36	j	104	LMG	O1-C1-C2	4.25	114.93	108.30
32	G	305	CLA	CHD-C1D-ND	-4.24	120.56	124.45
32	b	831	CLA	CHB-C1B-NB	-4.24	119.77	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	B	302	CLA	CHB-C1B-NB	-4.23	119.78	124.26
35	a	851	LHG	O7-C7-C8	4.21	120.58	111.50
32	b	816	CLA	CHD-C1D-ND	-4.21	120.59	124.45
35	I	314	LHG	O4-P-O5	4.21	133.03	112.24
36	F	319	LMG	O7-C10-C11	4.21	120.56	111.50
37	F	312	A86	C33-C32-C31	4.20	113.30	109.21
35	f	205	LHG	O4-P-O5	4.20	133.01	112.24
35	a	849	LHG	O4-P-O5	4.20	132.98	112.24
32	b	831	CLA	CHD-C1D-ND	-4.18	120.61	124.45
35	A	316	LHG	O4-P-O5	4.18	132.91	112.24
32	b	820	CLA	CHB-C1B-NB	-4.18	119.83	124.26
32	a	801	CLA	C1D-ND-C4D	-4.17	103.37	106.33
36	P	318	LMG	O7-C10-C11	4.17	120.49	111.50
35	E	301	LHG	O4-P-O5	4.17	132.84	112.24
35	M	319	LHG	O4-P-O5	4.16	132.80	112.24
35	a	850	LHG	O4-P-O5	4.15	132.77	112.24
35	F	321	LHG	O4-P-O5	4.15	132.77	112.24
36	l	201	LMG	O7-C10-C11	4.15	120.44	111.50
35	D	320	LHG	O4-P-O5	4.14	132.72	112.24
32	b	819	CLA	CHD-C1D-ND	-4.14	120.65	124.45
37	M	314	A86	C21-C20-C19	-4.13	109.63	114.28
35	E	321	LHG	O7-C7-C8	4.12	120.39	111.50
35	B	308	LHG	O7-C7-C8	4.11	120.37	111.50
32	b	830	CLA	O2A-C1-C2	4.11	119.43	108.64
35	F	318	LHG	O4-P-O5	4.10	132.53	112.24
37	C	311	A86	C21-C20-C19	-4.10	109.66	114.28
36	j	104	LMG	O7-C10-C11	4.09	120.31	111.50
35	W	319	LHG	O4-P-O5	4.09	132.45	112.24
32	T	305	CLA	CHB-C1B-NB	-4.08	119.94	124.26
40	Q	318	DGD	O2G-C1B-C2B	4.07	120.28	111.50
32	P	304	CLA	CHB-C1B-NB	-4.07	119.95	124.26
34	J	315	DD6	O1-C20-C19	-4.06	110.33	113.38
34	Q	315	DD6	C14-C13-C11	4.06	131.82	125.53
33	K	302	KC2	C1D-ND-C4D	4.05	109.21	106.33
32	a	812	CLA	CHB-C1B-NB	-4.05	119.97	124.26
37	F	313	A86	O1-C20-C19	-4.04	110.35	113.38
32	b	835	CLA	CHB-C1B-NB	-4.04	119.98	124.26
35	P	317	LHG	O4-P-O5	4.03	132.16	112.24
34	U	309	DD6	C14-C13-C11	4.03	131.78	125.53
34	K	315	DD6	C14-C13-C11	4.03	131.78	125.53
32	b	812	CLA	CHB-C1B-NB	-4.02	120.00	124.26
32	a	822	CLA	CHB-C1B-NB	-4.02	120.00	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	S	322	LMG	O7-C10-C11	4.00	120.13	111.50
36	F	320	LMG	O7-C10-C11	4.00	120.13	111.50
32	D	314	CLA	CHB-C1B-NB	-4.00	120.02	124.26
33	M	321	KC2	C1D-ND-C4D	3.99	109.17	106.33
32	a	828	CLA	CHB-C1B-NB	-3.99	120.04	124.26
32	L	310	CLA	CHB-C1B-NB	-3.98	120.04	124.26
34	A	313	DD6	C14-C13-C11	3.98	131.71	125.53
37	P	316	A86	O4-C34-C35	3.98	117.50	107.59
37	P	319	A86	O1-C20-C19	3.97	116.37	113.38
36	W	320	LMG	O7-C10-C11	3.97	120.05	111.50
33	R	302	KC2	C1D-ND-C4D	3.97	109.15	106.33
32	J	312	CLA	CHB-C1B-NB	-3.96	120.07	124.26
33	K	305	KC2	C1D-ND-C4D	3.93	109.13	106.33
37	R	312	A86	C33-C32-C31	3.93	113.03	109.21
33	N	303	KC2	C1D-ND-C4D	3.91	109.12	106.33
32	Q	303	CLA	CHB-C1B-NB	-3.91	120.12	124.26
32	a	802	CLA	CHB-C1B-NB	-3.91	120.12	124.26
32	a	803	CLA	CHB-C1B-NB	-3.90	120.13	124.26
33	F	302	KC2	C1D-ND-C4D	3.90	109.11	106.33
32	a	824	CLA	CHB-C1B-NB	-3.90	120.13	124.26
36	D	302	LMG	O7-C10-C11	3.90	119.90	111.50
33	P	302	KC2	C1D-ND-C4D	3.89	109.10	106.33
32	b	822	CLA	CHB-C1B-NB	-3.88	120.15	124.26
34	E	317	DD6	O1-C20-C19	-3.88	110.47	113.38
34	H	312	DD6	C14-C13-C11	3.88	131.55	125.53
37	D	322	A86	O1-C20-C19	3.88	116.30	113.38
32	b	829	CLA	CHB-C1B-NB	-3.88	120.15	124.26
37	W	318	A86	C21-C20-C19	-3.88	109.92	114.28
33	M	303	KC2	CHD-C1D-ND	-3.87	120.16	124.26
32	b	801	CLA	CHB-C1B-NB	-3.87	120.16	124.26
33	U	304	KC2	C1D-ND-C4D	3.86	109.08	106.33
32	M	305	CLA	CHB-C1B-NB	-3.86	120.17	124.26
32	a	823	CLA	CHB-C1B-NB	-3.86	120.17	124.26
32	a	818	CLA	C1-C2-C3	-3.85	119.38	126.04
33	E	313	KC2	C1D-ND-C4D	3.85	109.07	106.33
32	b	834	CLA	CHB-C1B-NB	-3.84	120.19	124.26
32	b	811	CLA	CHB-C1B-NB	-3.84	120.19	124.26
32	M	308	CLA	CHB-C1B-NB	-3.84	120.20	124.26
33	N	304	KC2	CHD-C1D-ND	-3.84	120.20	124.26
33	G	309	KC2	C1D-ND-C4D	3.83	109.05	106.33
33	S	303	KC2	CHD-C1D-ND	-3.82	120.21	124.26
32	Q	304	CLA	CHB-C1B-NB	-3.82	120.22	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	H	303	KC2	CHD-C1D-ND	-3.81	120.22	124.26
34	T	314	DD6	O1-C20-C19	-3.81	110.52	113.38
32	M	306	CLA	CHB-C1B-NB	-3.80	120.23	124.26
33	M	313	KC2	C1D-ND-C4D	3.80	109.04	106.33
32	A	301	CLA	CHB-C1B-NB	-3.80	120.23	124.26
32	D	315	CLA	CHB-C1B-NB	-3.79	120.24	124.26
33	T	303	KC2	C1D-ND-C4D	3.79	109.03	106.33
32	J	311	CLA	CHB-C1B-NB	-3.79	120.25	124.26
33	L	305	KC2	C1D-ND-C4D	3.79	109.03	106.33
32	C	301	CLA	CHB-C1B-NB	-3.78	120.25	124.26
32	b	802	CLA	CHB-C1B-NB	-3.78	120.26	124.26
33	U	304	KC2	CHD-C1D-ND	-3.78	120.26	124.26
34	A	315	DD6	O1-C20-C19	-3.78	110.55	113.38
32	a	816	CLA	CHB-C1B-NB	-3.78	120.26	124.26
33	W	304	KC2	C1D-ND-C4D	3.77	109.02	106.33
33	W	303	KC2	C1D-ND-C4D	3.77	109.01	106.33
32	R	309	CLA	CHB-C1B-NB	-3.77	120.27	124.26
33	I	309	KC2	C1D-ND-C4D	3.76	109.01	106.33
34	H	311	DD6	C32-C31-C36	-3.76	117.32	122.63
32	H	305	CLA	CHB-C1B-NB	-3.76	120.27	124.26
32	K	306	CLA	CHB-C1B-NB	-3.76	120.28	124.26
33	O	302	KC2	C1D-ND-C4D	3.76	109.00	106.33
33	L	303	KC2	C1D-ND-C4D	3.76	109.00	106.33
32	a	852	CLA	CHB-C1B-NB	-3.76	120.28	124.26
34	I	310	DD6	C14-C13-C11	3.75	131.36	125.53
33	P	306	KC2	C1D-ND-C4D	3.75	109.00	106.33
33	P	303	KC2	C1D-ND-C4D	3.75	109.00	106.33
32	b	840	CLA	CHB-C1B-NB	-3.75	120.29	124.26
32	b	825	CLA	CHB-C1B-NB	-3.75	120.29	124.26
32	S	308	CLA	CHB-C1B-NB	-3.75	120.29	124.26
32	W	306	CLA	CHB-C1B-NB	-3.75	120.29	124.26
32	P	311	CLA	CHB-C1B-NB	-3.75	120.29	124.26
33	M	302	KC2	C1D-ND-C4D	3.74	109.00	106.33
33	L	302	KC2	CHD-C1D-ND	-3.74	120.29	124.26
33	N	306	KC2	C1D-ND-C4D	3.74	108.99	106.33
33	M	307	KC2	CHD-C1D-ND	-3.73	120.31	124.26
33	O	303	KC2	CHD-C1D-ND	-3.73	120.31	124.26
32	N	305	CLA	CHB-C1B-NB	-3.73	120.31	124.26
32	a	830	CLA	CHB-C1B-NB	-3.73	120.31	124.26
37	N	317	A86	C34-O4-C38	3.72	124.84	117.90
33	A	310	KC2	C1D-ND-C4D	3.72	108.98	106.33
32	D	306	CLA	CHB-C1B-NB	-3.72	120.32	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	P	312	KC2	C1D-ND-C4D	3.72	108.98	106.33
33	K	303	KC2	CHD-C1D-ND	-3.72	120.32	124.26
32	B	303	CLA	CHB-C1B-NB	-3.72	120.32	124.26
32	D	304	CLA	CHB-C1B-NB	-3.72	120.32	124.26
32	E	314	CLA	CHB-C1B-NB	-3.72	120.32	124.26
33	L	303	KC2	CHD-C1D-ND	-3.72	120.32	124.26
32	a	808	CLA	CHB-C1B-NB	-3.72	120.32	124.26
32	a	832	CLA	CHB-C1B-NB	-3.72	120.32	124.26
32	b	826	CLA	CHB-C1B-NB	-3.71	120.33	124.26
33	S	306	KC2	CHD-C1D-ND	-3.71	120.33	124.26
37	S	316	A86	C34-O4-C38	3.71	124.81	117.90
33	O	310	KC2	CHD-C1D-ND	-3.71	120.33	124.26
32	P	308	CLA	CHB-C1B-NB	-3.71	120.33	124.26
33	N	314	KC2	C1D-ND-C4D	3.71	108.97	106.33
33	R	303	KC2	C1D-ND-C4D	3.70	108.97	106.33
32	E	307	CLA	CHB-C1B-NB	-3.70	120.34	124.26
32	b	830	CLA	CHB-C1B-NB	-3.70	120.34	124.26
32	G	304	CLA	CHB-C1B-NB	-3.70	120.34	124.26
32	R	306	CLA	CHB-C1B-NB	-3.70	120.34	124.26
33	W	305	KC2	CHD-C1D-ND	-3.70	120.34	124.26
33	W	308	KC2	C1D-ND-C4D	3.70	108.96	106.33
32	b	823	CLA	CHB-C1B-NB	-3.69	120.35	124.26
33	C	303	KC2	CHD-C1D-ND	-3.69	120.35	124.26
33	R	311	KC2	CHD-C1D-ND	-3.69	120.35	124.26
32	b	824	CLA	CHB-C1B-NB	-3.69	120.35	124.26
34	D	316	DD6	C14-C13-C11	3.69	131.26	125.53
32	K	310	CLA	CHB-C1B-NB	-3.69	120.35	124.26
33	J	310	KC2	CHD-C1D-ND	-3.69	120.35	124.26
33	L	302	KC2	C1D-ND-C4D	3.69	108.96	106.33
32	a	829	CLA	CHB-C1B-NB	-3.69	120.35	124.26
32	P	305	CLA	CHB-C1B-NB	-3.69	120.35	124.26
32	J	301	CLA	CHB-C1B-NB	-3.68	120.36	124.26
33	I	309	KC2	CHD-C1D-ND	-3.68	120.36	124.26
32	a	806	CLA	CHB-C1B-NB	-3.68	120.36	124.26
33	W	301	KC2	CHD-C1D-ND	-3.68	120.36	124.26
32	I	303	CLA	CHB-C1B-NB	-3.68	120.36	124.26
32	b	827	CLA	CHB-C1B-NB	-3.68	120.36	124.26
33	Q	302	KC2	CHD-C1D-ND	-3.68	120.36	124.26
33	T	304	KC2	CHD-C1D-ND	-3.68	120.36	124.26
33	I	316	KC2	CHD-C1D-ND	-3.67	120.37	124.26
32	a	811	CLA	CHB-C1B-NB	-3.67	120.37	124.26
32	a	813	CLA	CHB-C1B-NB	-3.67	120.37	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	S	313	CLA	CHB-C1B-NB	-3.67	120.37	124.26
32	I	317	CLA	CHB-C1B-NB	-3.67	120.38	124.26
33	N	307	KC2	C1D-ND-C4D	3.66	108.94	106.33
33	S	302	KC2	C1D-ND-C4D	3.66	108.94	106.33
33	K	302	KC2	CHD-C1D-ND	-3.66	120.38	124.26
32	L	314	CLA	CHB-C1B-NB	-3.66	120.38	124.26
32	J	305	CLA	CHB-C1B-NB	-3.66	120.38	124.26
32	a	826	CLA	CHB-C1B-NB	-3.66	120.38	124.26
32	b	814	CLA	CHB-C1B-NB	-3.66	120.38	124.26
33	G	302	KC2	C1D-ND-C4D	3.66	108.94	106.33
32	b	810	CLA	CHB-C1B-NB	-3.66	120.39	124.26
33	W	314	KC2	C1D-ND-C4D	3.66	108.93	106.33
33	C	303	KC2	C1D-ND-C4D	3.65	108.93	106.33
33	Q	302	KC2	C1D-ND-C4D	3.65	108.93	106.33
32	b	808	CLA	CHB-C1B-NB	-3.65	120.39	124.26
32	F	301	CLA	CHB-C1B-NB	-3.65	120.39	124.26
32	I	304	CLA	CHB-C1B-NB	-3.65	120.39	124.26
32	L	311	CLA	CBD-CHA-C1A	3.65	132.80	128.50
32	U	307	CLA	CHB-C1B-NB	-3.65	120.39	124.26
32	G	301	CLA	CHB-C1B-NB	-3.65	120.39	124.26
33	W	304	KC2	CHD-C1D-ND	-3.65	120.39	124.26
32	B	305	CLA	CHB-C1B-NB	-3.65	120.39	124.26
32	F	306	CLA	CHB-C1B-NB	-3.65	120.39	124.26
33	J	303	KC2	CHD-C1D-ND	-3.65	120.39	124.26
32	H	310	CLA	CHB-C1B-NB	-3.65	120.39	124.26
32	b	833	CLA	CHB-C1B-NB	-3.65	120.39	124.26
33	T	311	KC2	C1D-ND-C4D	3.65	108.93	106.33
32	F	308	CLA	CHB-C1B-NB	-3.65	120.40	124.26
32	I	305	CLA	CHB-C1B-NB	-3.65	120.40	124.26
34	D	319	DD6	C14-C13-C11	3.65	131.19	125.53
33	P	301	KC2	CHD-C1D-ND	-3.65	120.40	124.26
32	S	309	CLA	CHB-C1B-NB	-3.65	120.40	124.26
32	V	204	CLA	CHB-C1B-NB	-3.65	120.40	124.26
33	F	310	KC2	CHD-C1D-ND	-3.65	120.40	124.26
33	N	314	KC2	CHD-C1D-ND	-3.65	120.40	124.26
37	D	322	A86	C34-O4-C38	3.64	124.69	117.90
37	K	311	A86	C34-O4-C38	3.64	124.68	117.90
37	O	312	A86	C34-O4-C38	3.64	124.68	117.90
33	A	310	KC2	CHD-C1D-ND	-3.64	120.40	124.26
33	S	302	KC2	CHD-C1D-ND	-3.64	120.40	124.26
32	D	313	CLA	CHB-C1B-NB	-3.64	120.41	124.26
32	H	301	CLA	CHB-C1B-NB	-3.64	120.41	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	S	318	A86	C34-O4-C38	3.64	124.67	117.90
33	J	303	KC2	C1D-ND-C4D	3.64	108.92	106.33
33	R	305	KC2	C1D-ND-C4D	3.64	108.92	106.33
32	R	307	CLA	CHB-C1B-NB	-3.64	120.41	124.26
33	K	309	KC2	CHD-C1D-ND	-3.64	120.41	124.26
33	Q	317	KC2	C1D-ND-C4D	3.63	108.92	106.33
33	P	312	KC2	CHD-C1D-ND	-3.63	120.41	124.26
32	W	309	CLA	CHB-C1B-NB	-3.63	120.41	124.26
32	a	810	CLA	CHB-C1B-NB	-3.63	120.41	124.26
32	a	835	CLA	CHB-C1B-NB	-3.63	120.41	124.26
33	O	303	KC2	C1D-ND-C4D	3.63	108.91	106.33
33	R	311	KC2	C1D-ND-C4D	3.63	108.91	106.33
37	W	315	A86	C34-O4-C38	3.63	124.66	117.90
32	b	839	CLA	CHB-C1B-NB	-3.63	120.42	124.26
32	R	304	CLA	CHB-C1B-NB	-3.63	120.42	124.26
33	P	301	KC2	C1D-ND-C4D	3.63	108.91	106.33
32	U	305	CLA	CHB-C1B-NB	-3.63	120.42	124.26
34	O	313	DD6	C14-C13-C11	3.62	131.15	125.53
32	a	807	CLA	CHB-C1B-NB	-3.62	120.42	124.26
32	f	201	CLA	CHB-C1B-NB	-3.62	120.42	124.26
33	M	304	KC2	C1D-ND-C4D	3.62	108.91	106.33
32	K	304	CLA	CHB-C1B-NB	-3.62	120.42	124.26
32	a	853	CLA	CHB-C1B-NB	-3.62	120.42	124.26
32	a	805	CLA	CAA-C2A-C1A	-3.62	100.11	111.97
32	H	308	CLA	CHB-C1B-NB	-3.62	120.42	124.26
32	a	831	CLA	CHB-C1B-NB	-3.62	120.43	124.26
37	N	315	A86	C34-O4-C38	3.62	124.63	117.90
33	R	303	KC2	CHD-C1D-ND	-3.61	120.43	124.26
32	B	306	CLA	CHB-C1B-NB	-3.61	120.43	124.26
32	F	304	CLA	CHB-C1B-NB	-3.61	120.43	124.26
32	V	203	CLA	CHB-C1B-NB	-3.61	120.43	124.26
33	N	304	KC2	C1D-ND-C4D	3.61	108.90	106.33
32	a	825	CLA	CHB-C1B-NB	-3.61	120.43	124.26
33	N	303	KC2	CHD-C1D-ND	-3.61	120.44	124.26
33	W	314	KC2	CHD-C1D-ND	-3.61	120.44	124.26
32	O	306	CLA	CHB-C1B-NB	-3.61	120.44	124.26
32	U	302	CLA	CHB-C1B-NB	-3.61	120.44	124.26
33	H	303	KC2	C1D-ND-C4D	3.61	108.90	106.33
33	W	301	KC2	C1D-ND-C4D	3.60	108.89	106.33
32	L	301	CLA	CHB-C1B-NB	-3.60	120.44	124.26
33	W	303	KC2	CHD-C1D-ND	-3.60	120.45	124.26
33	T	311	KC2	CHD-C1D-ND	-3.60	120.45	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	M	313	KC2	CHD-C1D-ND	-3.60	120.45	124.26
37	U	308	A86	C34-O4-C38	3.60	124.60	117.90
32	b	817	CLA	CHB-C1B-NB	-3.59	120.45	124.26
37	P	314	A86	C34-O4-C38	3.59	124.59	117.90
32	Q	309	CLA	CHB-C1B-NB	-3.59	120.45	124.26
32	a	839	CLA	CHB-C1B-NB	-3.59	120.45	124.26
33	L	306	KC2	C1D-ND-C4D	3.59	108.89	106.33
32	C	309	CLA	CHB-C1B-NB	-3.59	120.46	124.26
33	G	309	KC2	CHD-C1D-ND	-3.59	120.46	124.26
33	P	302	KC2	CHD-C1D-ND	-3.59	120.46	124.26
32	N	311	CLA	CHB-C1B-NB	-3.59	120.46	124.26
33	O	302	KC2	CHD-C1D-ND	-3.59	120.46	124.26
32	B	304	CLA	CHB-C1B-NB	-3.58	120.46	124.26
33	G	302	KC2	CHD-C1D-ND	-3.58	120.46	124.26
32	E	311	CLA	CHB-C1B-NB	-3.58	120.47	124.26
32	a	819	CLA	CHB-C1B-NB	-3.58	120.47	124.26
32	a	834	CLA	CHB-C1B-NB	-3.58	120.47	124.26
32	N	313	CLA	CHB-C1B-NB	-3.58	120.47	124.26
32	C	306	CLA	CHB-C1B-NB	-3.58	120.47	124.26
32	J	308	CLA	CHB-C1B-NB	-3.58	120.47	124.26
32	G	307	CLA	CBD-CHA-C1A	3.58	132.72	128.50
32	F	311	CLA	CHB-C1B-NB	-3.58	120.47	124.26
32	F	305	CLA	CHB-C1B-NB	-3.58	120.47	124.26
32	a	817	CLA	CHB-C1B-NB	-3.58	120.47	124.26
34	D	316	DD6	O1-C20-C19	-3.58	110.70	113.38
32	O	304	CLA	CHB-C1B-NB	-3.57	120.47	124.26
33	R	305	KC2	CHD-C1D-ND	-3.57	120.47	124.26
32	L	311	CLA	CHB-C1B-NB	-3.57	120.47	124.26
32	A	302	CLA	CHB-C1B-NB	-3.57	120.47	124.26
32	T	309	CLA	CHB-C1B-NB	-3.57	120.47	124.26
33	L	305	KC2	CHD-C1D-ND	-3.57	120.47	124.26
37	M	315	A86	C34-O4-C38	3.57	124.55	117.90
32	E	305	CLA	CHB-C1B-NB	-3.57	120.48	124.26
33	N	302	KC2	CHD-C1D-ND	-3.57	120.48	124.26
32	G	306	CLA	CHB-C1B-NB	-3.57	120.48	124.26
32	I	308	CLA	CHB-C1B-NB	-3.57	120.48	124.26
32	N	309	CLA	CHC-C4B-NB	-3.57	120.48	124.26
32	a	815	CLA	CHB-C1B-NB	-3.57	120.48	124.26
34	I	311	DD6	C14-C13-C11	3.57	131.07	125.53
32	Q	310	CLA	CHB-C1B-NB	-3.57	120.48	124.26
33	M	302	KC2	CHD-C1D-ND	-3.57	120.48	124.26
33	N	307	KC2	CHD-C1D-ND	-3.57	120.48	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	F	302	KC2	CHD-C1D-ND	-3.56	120.48	124.26
33	T	303	KC2	CHD-C1D-ND	-3.56	120.48	124.26
32	T	306	CLA	CHB-C1B-NB	-3.56	120.48	124.26
33	L	306	KC2	CHD-C1D-ND	-3.56	120.48	124.26
36	j	104	LMG	O8-C28-C29	3.56	123.09	111.91
32	D	310	CLA	CHB-C1B-NB	-3.56	120.49	124.26
32	L	308	CLA	CHB-C1B-NB	-3.56	120.49	124.26
32	L	310	CLA	CBD-CHA-C1A	3.56	132.70	128.50
32	T	307	CLA	CHB-C1B-NB	-3.56	120.49	124.26
32	J	307	CLA	CAA-C2A-C1A	-3.56	100.31	111.97
32	G	308	CLA	CHB-C1B-NB	-3.56	120.49	124.26
32	a	841	CLA	CHB-C1B-NB	-3.56	120.49	124.26
32	L	312	CLA	CHB-C1B-NB	-3.56	120.49	124.26
32	P	310	CLA	CHB-C1B-NB	-3.55	120.50	124.26
32	a	827	CLA	CHB-C1B-NB	-3.55	120.50	124.26
33	K	305	KC2	CHD-C1D-ND	-3.55	120.50	124.26
33	T	304	KC2	C1D-ND-C4D	3.55	108.86	106.33
32	C	302	CLA	CHB-C1B-NB	-3.55	120.50	124.26
32	R	310	CLA	CHB-C1B-NB	-3.55	120.50	124.26
32	Q	305	CLA	CHB-C1B-NB	-3.55	120.50	124.26
37	N	316	A86	C34-O4-C38	3.55	124.50	117.90
37	W	318	A86	C34-O4-C38	3.54	124.50	117.90
32	W	313	CLA	CHB-C1B-NB	-3.54	120.51	124.26
33	L	313	KC2	CHD-C1D-ND	-3.54	120.51	124.26
33	N	308	KC2	C1D-ND-C4D	3.54	108.85	106.33
37	Q	311	A86	C34-O4-C38	3.54	124.50	117.90
32	A	307	CLA	CHB-C1B-NB	-3.54	120.51	124.26
32	D	312	CLA	CHB-C1B-NB	-3.53	120.52	124.26
32	S	307	CLA	CHC-C4B-NB	-3.53	120.52	124.26
32	D	311	CLA	CHB-C1B-NB	-3.53	120.52	124.26
32	J	306	CLA	CHB-C1B-NB	-3.53	120.52	124.26
32	O	301	CLA	CHB-C1B-NB	-3.53	120.52	124.26
32	l	202	CLA	CHB-C1B-NB	-3.53	120.52	124.26
32	G	303	CLA	CHB-C1B-NB	-3.53	120.52	124.26
32	D	308	CLA	CHB-C1B-NB	-3.53	120.52	124.26
33	K	303	KC2	C1D-ND-C4D	3.53	108.84	106.33
32	N	312	CLA	CHB-C1B-NB	-3.53	120.52	124.26
32	S	301	CLA	CHB-C1B-NB	-3.53	120.52	124.26
32	U	303	CLA	CHB-C1B-NB	-3.53	120.52	124.26
33	W	308	KC2	CHD-C1D-ND	-3.53	120.52	124.26
33	N	306	KC2	CHD-C1D-ND	-3.53	120.52	124.26
34	E	316	DD6	C14-C13-C11	3.53	131.00	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	G	307	CLA	CHB-C1B-NB	-3.53	120.52	124.26
37	S	317	A86	C34-O4-C38	3.53	124.47	117.90
32	j	101	CLA	CHB-C1B-NB	-3.53	120.52	124.26
32	L	304	CLA	CHB-C1B-NB	-3.52	120.53	124.26
32	b	816	CLA	CHB-C1B-NB	-3.52	120.53	124.26
32	Q	301	CLA	CHB-C1B-NB	-3.52	120.53	124.26
32	Q	307	CLA	CHB-C1B-NB	-3.52	120.53	124.26
32	V	201	CLA	CHB-C1B-NB	-3.52	120.53	124.26
32	J	302	CLA	CHB-C1B-NB	-3.52	120.53	124.26
33	J	310	KC2	C1D-ND-C4D	3.52	108.83	106.33
33	L	313	KC2	C1D-ND-C4D	3.52	108.83	106.33
32	f	203	CLA	CHB-C1B-NB	-3.52	120.53	124.26
32	L	309	CLA	CHB-C1B-NB	-3.52	120.53	124.26
34	E	316	DD6	O1-C20-C19	-3.52	110.74	113.38
33	O	310	KC2	C1D-ND-C4D	3.51	108.83	106.33
32	O	308	CLA	CHB-C1B-NB	-3.51	120.54	124.26
32	H	302	CLA	CHB-C1B-NB	-3.51	120.54	124.26
32	S	307	CLA	C3A-C2A-C1A	-3.51	96.08	101.34
33	M	303	KC2	C1D-ND-C4D	3.51	108.83	106.33
37	C	311	A86	C34-O4-C38	3.51	124.44	117.90
32	H	307	CLA	CHB-C1B-NB	-3.51	120.54	124.26
32	W	312	CLA	CHB-C1B-NB	-3.51	120.54	124.26
32	I	301	CLA	CHB-C1B-NB	-3.51	120.55	124.26
33	S	303	KC2	C1D-ND-C4D	3.51	108.83	106.33
32	A	308	CLA	CHB-C1B-NB	-3.50	120.55	124.26
33	E	313	KC2	CHD-C1D-ND	-3.50	120.55	124.26
32	F	307	CLA	CHB-C1B-NB	-3.50	120.55	124.26
32	C	305	CLA	CHB-C1B-NB	-3.50	120.55	124.26
32	E	309	CLA	CHB-C1B-NB	-3.50	120.55	124.26
38	V	205	LMU	C1B-O1B-C4'	-3.50	109.31	117.96
32	Q	306	CLA	CHB-C1B-NB	-3.50	120.56	124.26
32	a	836	CLA	CHB-C1B-NB	-3.50	120.56	124.26
32	a	837	CLA	CHB-C1B-NB	-3.50	120.56	124.26
32	H	304	CLA	CHB-C1B-NB	-3.49	120.56	124.26
32	H	309	CLA	CHB-C1B-NB	-3.49	120.56	124.26
34	M	316	DD6	C14-C13-C11	3.49	130.95	125.53
33	I	316	KC2	C1D-ND-C4D	3.49	108.81	106.33
32	b	813	CLA	CHB-C1B-NB	-3.49	120.56	124.26
37	r	204	A86	C34-O4-C38	3.49	124.40	117.90
32	A	311	CLA	CHB-C1B-NB	-3.49	120.56	124.26
32	J	307	CLA	CHB-C1B-NB	-3.49	120.56	124.26
32	J	304	CLA	CHB-C1B-NB	-3.49	120.56	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	W	316	A86	C34-O4-C38	3.49	124.39	117.90
36	S	322	LMG	O8-C28-C29	3.49	120.52	111.38
32	E	303	CLA	CHB-C1B-NB	-3.49	120.57	124.26
32	T	302	CLA	CHB-C1B-NB	-3.49	120.57	124.26
33	K	309	KC2	C1D-ND-C4D	3.49	108.81	106.33
32	B	309	CLA	CHB-C1B-NB	-3.48	120.57	124.26
32	D	305	CLA	CHB-C1B-NB	-3.48	120.57	124.26
33	M	304	KC2	CHD-C1D-ND	-3.48	120.57	124.26
33	F	310	KC2	C1D-ND-C4D	3.48	108.81	106.33
33	M	321	KC2	CHD-C1D-ND	-3.48	120.57	124.26
32	C	308	CLA	CHB-C1B-NB	-3.48	120.57	124.26
32	b	821	CLA	CHB-C1B-NB	-3.48	120.57	124.26
33	R	302	KC2	CHD-C1D-ND	-3.48	120.57	124.26
32	O	307	CLA	CHB-C1B-NB	-3.48	120.57	124.26
33	Q	317	KC2	CHD-C1D-ND	-3.48	120.57	124.26
38	j	105	LMU	C1B-O1B-C4'	-3.48	109.35	117.96
32	k	201	CLA	CHB-C1B-NB	-3.48	120.58	124.26
33	M	307	KC2	C1D-ND-C4D	3.48	108.80	106.33
32	b	806	CLA	CHC-C4B-NB	-3.47	120.58	124.26
32	I	307	CLA	CHB-C1B-NB	-3.47	120.58	124.26
32	T	310	CLA	CHB-C1B-NB	-3.47	120.58	124.26
32	E	315	CLA	CHB-C1B-NB	-3.47	120.58	124.26
32	M	312	CLA	CHB-C1B-NB	-3.47	120.58	124.26
32	R	301	CLA	CHB-C1B-NB	-3.47	120.58	124.26
37	D	323	A86	C34-O4-C38	3.47	124.36	117.90
32	M	310	CLA	CHB-C1B-NB	-3.47	120.58	124.26
32	T	308	CLA	CHB-C1B-NB	-3.47	120.58	124.26
32	K	308	CLA	CHB-C1B-NB	-3.47	120.58	124.26
32	C	308	CLA	C3D-C4D-ND	3.47	115.85	110.24
37	K	314	A86	C34-O4-C38	3.47	124.36	117.90
32	L	307	CLA	CHB-C1B-NB	-3.47	120.59	124.26
37	Q	311	A86	C36-C31-C32	-3.47	116.26	119.70
32	M	309	CLA	CHB-C1B-NB	-3.46	120.59	124.26
32	K	301	CLA	CHB-C1B-NB	-3.46	120.59	124.26
32	a	840	CLA	CHB-C1B-NB	-3.46	120.59	124.26
32	B	301	CLA	CHB-C1B-NB	-3.46	120.59	124.26
37	L	318	A86	C34-O4-C38	3.46	124.35	117.90
32	A	305	CLA	CHB-C1B-NB	-3.46	120.59	124.26
32	a	804	CLA	CHB-C1B-NB	-3.46	120.60	124.26
32	b	836	CLA	CHB-C1B-NB	-3.46	120.60	124.26
37	P	313	A86	C34-O4-C38	3.46	124.33	117.90
32	W	307	CLA	CHB-C1B-NB	-3.45	120.60	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	828	CLA	CHB-C1B-NB	-3.45	120.60	124.26
32	E	310	CLA	CHB-C1B-NB	-3.45	120.60	124.26
32	K	307	CLA	CHB-C1B-NB	-3.45	120.60	124.26
32	D	309	CLA	CHB-C1B-NB	-3.45	120.61	124.26
34	J	315	DD6	C14-C13-C11	3.45	130.88	125.53
32	A	303	CLA	CHB-C1B-NB	-3.45	120.61	124.26
32	R	308	CLA	CHB-C1B-NB	-3.45	120.61	124.26
32	I	306	CLA	CHB-C1B-NB	-3.44	120.61	124.26
34	R	314	DD6	C14-C13-C11	3.44	130.87	125.53
33	S	312	KC2	CHD-C1D-ND	-3.44	120.61	124.26
32	O	305	CLA	CHB-C1B-NB	-3.44	120.61	124.26
32	U	301	CLA	CBD-CHA-C1A	3.44	132.56	128.50
32	I	302	CLA	CHB-C1B-NB	-3.44	120.61	124.26
32	f	204	CLA	CHB-C1B-NB	-3.44	120.61	124.26
37	M	318	A86	O1-C20-C19	3.44	115.97	113.38
32	F	309	CLA	CHB-C1B-NB	-3.44	120.62	124.26
32	a	805	CLA	CHB-C1B-NB	-3.44	120.62	124.26
32	r	201	CLA	CHB-C1B-NB	-3.44	120.62	124.26
32	l	204	CLA	CHB-C1B-NB	-3.43	120.62	124.26
32	k	202	CLA	CHB-C1B-NB	-3.43	120.62	124.26
32	H	306	CLA	CHB-C1B-NB	-3.43	120.63	124.26
32	S	310	CLA	CHB-C1B-NB	-3.43	120.63	124.26
32	b	809	CLA	CHB-C1B-NB	-3.43	120.63	124.26
32	E	312	CLA	CHB-C1B-NB	-3.43	120.63	124.26
32	a	809	CLA	CHB-C1B-NB	-3.43	120.63	124.26
32	b	818	CLA	CHB-C1B-NB	-3.43	120.63	124.26
33	S	306	KC2	C1D-ND-C4D	3.42	108.77	106.33
32	M	311	CLA	CHB-C1B-NB	-3.42	120.64	124.26
32	P	309	CLA	CHB-C1B-NB	-3.42	120.64	124.26
32	a	821	CLA	CHB-C1B-NB	-3.42	120.64	124.26
33	P	306	KC2	CHD-C1D-ND	-3.42	120.64	124.26
32	b	815	CLA	CHB-C1B-NB	-3.42	120.64	124.26
32	E	304	CLA	CHB-C1B-NB	-3.41	120.64	124.26
32	Q	308	CLA	CHB-C1B-NB	-3.41	120.64	124.26
32	S	304	CLA	CHB-C1B-NB	-3.41	120.65	124.26
32	a	842	CLA	CHB-C1B-NB	-3.41	120.65	124.26
36	D	325	LMG	O8-C28-C29	3.41	122.61	111.91
33	N	302	KC2	C1D-ND-C4D	3.41	108.75	106.33
32	a	833	CLA	CHB-C1B-NB	-3.40	120.66	124.26
37	F	312	A86	C34-O4-C38	3.40	124.23	117.90
32	k	203	CLA	CHB-C1B-NB	-3.40	120.66	124.26
32	A	304	CLA	CHB-C1B-NB	-3.39	120.67	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	K	312	A86	C34-O4-C38	3.39	124.21	117.90
32	U	301	CLA	CHB-C1B-NB	-3.38	120.67	124.26
32	l	203	CLA	CHB-C1B-NB	-3.38	120.67	124.26
36	D	325	LMG	C1-O6-C5	-3.38	107.06	113.69
32	E	306	CLA	CHB-C1B-NB	-3.38	120.68	124.26
32	M	312	CLA	C1-C2-C3	-3.37	120.21	126.04
32	A	306	CLA	CHB-C1B-NB	-3.37	120.69	124.26
32	D	307	CLA	CHB-C1B-NB	-3.36	120.70	124.26
32	W	311	CLA	CHB-C1B-NB	-3.36	120.70	124.26
32	U	306	CLA	CHB-C1B-NB	-3.36	120.70	124.26
32	S	305	CLA	CHB-C1B-NB	-3.36	120.70	124.26
34	P	315	DD6	O1-C20-C19	-3.35	110.86	113.38
32	b	819	CLA	CHB-C1B-NB	-3.35	120.71	124.26
32	a	818	CLA	CHB-C1B-NB	-3.35	120.71	124.26
32	N	310	CLA	CHB-C1B-NB	-3.35	120.71	124.26
32	G	305	CLA	CHB-C1B-NB	-3.34	120.72	124.26
36	E	302	LMG	O1-C7-C8	-3.34	102.83	110.90
32	F	322	CLA	CHB-C1B-NB	-3.33	120.73	124.26
33	P	303	KC2	CHD-C1D-ND	-3.33	120.73	124.26
32	N	309	CLA	CHB-C1B-NB	-3.33	120.73	124.26
32	b	837	CLA	CHB-C1B-NB	-3.33	120.73	124.26
32	E	308	CLA	CHB-C1B-NB	-3.33	120.73	124.26
32	b	804	CLA	CHB-C1B-NB	-3.32	120.74	124.26
32	P	307	CLA	CHB-C1B-NB	-3.32	120.75	124.26
34	H	311	DD6	C14-C13-C11	3.31	130.67	125.53
39	k	206	SQD	O48-C23-C24	3.31	122.29	111.91
32	S	311	CLA	CHC-C4B-NB	-3.31	120.76	124.26
40	Q	318	DGD	O1G-C1A-C2A	3.30	122.26	111.91
33	S	312	KC2	C4D-C3D-CAD	3.30	109.64	107.42
34	S	321	DD6	C23-C16-C15	3.29	118.94	110.05
34	H	313	DD6	O1-C20-C19	-3.29	110.91	113.38
32	F	303	CLA	CHB-C1B-NB	-3.29	120.78	124.26
34	E	319	DD6	O1-C20-C19	-3.28	110.92	113.38
32	O	309	CLA	CHB-C1B-NB	-3.28	120.79	124.26
32	r	202	CLA	CHB-C1B-NB	-3.27	120.79	124.26
36	E	320	LMG	O1-C1-C2	3.27	113.40	108.30
32	J	309	CLA	CHB-C1B-NB	-3.26	120.80	124.26
38	I	315	LMU	C3'-C4'-C5'	-3.26	103.45	110.93
34	V	202	DD6	O1-C20-C19	-3.25	110.94	113.38
32	S	311	CLA	CHB-C1B-NB	-3.25	120.82	124.26
32	S	307	CLA	CHB-C1B-NB	-3.25	120.82	124.26
32	W	310	CLA	CHB-C1B-NB	-3.25	120.82	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	K	311	A86	O1-C20-C19	3.24	115.81	113.38
32	b	838	CLA	CHB-C1B-NB	-3.24	120.83	124.26
40	b	846	DGD	O1G-C1A-C2A	3.24	122.06	111.91
37	W	302	A86	O1-C20-C19	3.23	115.81	113.38
32	A	309	CLA	CHB-C1B-NB	-3.23	120.84	124.26
32	C	307	CLA	CHB-C1B-NB	-3.23	120.84	124.26
32	F	301	CLA	CBD-CHA-C1A	3.23	132.31	128.50
37	P	316	A86	O1-C20-C19	-3.23	110.96	113.38
36	A	318	LMG	C7-O1-C1	3.23	120.04	113.74
32	b	807	CLA	CHB-C1B-NB	-3.22	120.84	124.26
32	a	824	CLA	CHC-C4B-NB	-3.22	120.84	124.26
32	a	820	CLA	C1-C2-C3	-3.22	120.47	126.04
32	b	821	CLA	C1-C2-C3	-3.22	120.47	126.04
36	S	322	LMG	C8-O7-C10	-3.22	109.87	117.79
32	b	802	CLA	C3D-C4D-ND	3.22	115.44	110.24
32	b	803	CLA	CHB-C1B-NB	-3.22	120.85	124.26
32	C	304	CLA	CHB-C1B-NB	-3.21	120.86	124.26
36	D	303	LMG	C7-O1-C1	-3.21	107.47	113.74
33	N	308	KC2	CHD-C1D-ND	-3.20	120.87	124.26
32	B	301	CLA	CBD-CHA-C1A	3.19	132.26	128.50
36	M	320	LMG	O8-C28-C29	3.19	121.92	111.91
37	S	319	A86	C33-C32-C31	3.18	112.31	109.21
32	b	811	CLA	C1-C2-C3	-3.18	121.61	126.75
32	b	833	CLA	C3D-C4D-ND	3.16	115.35	110.24
34	L	319	DD6	C21-C20-C19	3.16	117.83	114.28
37	N	317	A86	O1-C20-C19	3.15	115.75	113.38
32	D	314	CLA	C2C-C1C-NC	3.15	112.92	109.97
34	N	318	DD6	C32-C31-C36	-3.15	118.19	122.63
32	N	310	CLA	C3D-C4D-ND	3.15	115.33	110.24
32	F	304	CLA	C1-C2-C3	-3.15	120.60	126.04
37	F	313	A86	C33-C32-C31	3.14	112.27	109.21
32	b	804	CLA	C1-C2-C3	3.14	131.48	126.04
32	b	806	CLA	CHB-C1B-NB	-3.14	120.94	124.26
34	A	312	DD6	O1-C20-C19	-3.13	111.03	113.38
32	T	310	CLA	C3D-C4D-ND	3.13	115.31	110.24
32	Q	303	CLA	CHC-C4B-NB	-3.13	120.94	124.26
32	I	308	CLA	C3D-C4D-ND	3.12	115.29	110.24
39	H	315	SQD	O48-C23-C24	3.12	121.70	111.91
34	D	317	DD6	C33-C34-C35	-3.12	106.03	110.30
35	a	851	LHG	O8-C23-C24	3.12	121.70	111.91
32	E	306	CLA	C3D-C4D-ND	3.12	115.28	110.24
32	J	307	CLA	C3D-C4D-ND	3.12	115.28	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	D	301	DD6	C14-C13-C11	3.12	130.36	125.53
36	l	201	LMG	C3-C4-C5	3.11	115.79	110.24
34	H	313	DD6	C14-C13-C11	3.11	130.36	125.53
38	J	318	LMU	C1'-O5'-C5'	3.11	119.80	113.69
36	D	325	LMG	C8-O7-C10	-3.11	110.13	117.79
34	S	321	DD6	O1-C20-C15	-3.11	56.38	58.96
34	Q	313	DD6	C14-C13-C11	3.09	130.33	125.53
36	E	322	LMG	O7-C10-O9	-3.08	116.25	123.70
37	P	319	A86	C21-C20-C19	-3.08	110.82	114.28
32	a	820	CLA	C3D-C4D-ND	3.08	115.22	110.24
32	G	308	CLA	C3D-C4D-ND	3.07	115.20	110.24
36	D	302	LMG	C7-O1-C1	-3.07	107.74	113.74
37	O	312	A86	O3-C36-C37	3.05	114.83	109.39
36	l	201	LMG	C6-C5-C4	-3.05	105.86	113.00
32	M	306	CLA	C3D-C4D-ND	3.04	115.16	110.24
32	b	834	CLA	C3D-C4D-ND	3.04	115.16	110.24
35	E	321	LHG	O8-C23-C24	3.04	121.46	111.91
32	G	303	CLA	C3D-C4D-ND	3.04	115.16	110.24
34	H	312	DD6	C32-C31-C36	-3.04	118.34	122.63
32	H	307	CLA	C3D-C4D-ND	3.04	115.15	110.24
32	a	833	CLA	CHC-C4B-NB	-3.03	121.05	124.26
34	C	310	DD6	C32-C31-C36	-3.03	118.35	122.63
32	U	301	CLA	C3D-C4D-ND	3.03	115.14	110.24
32	S	309	CLA	O2A-C1-C2	-3.03	100.67	108.64
32	F	304	CLA	C3D-C4D-ND	3.03	115.14	110.24
32	J	312	CLA	C3D-C4D-ND	3.03	115.14	110.24
32	C	306	CLA	C3D-C4D-ND	3.03	115.13	110.24
32	G	306	CLA	CAA-C2A-C1A	-3.03	102.06	111.97
32	J	309	CLA	CHC-C4B-NB	-3.03	121.05	124.26
32	L	307	CLA	CHC-C4B-NB	-3.03	121.05	124.26
32	S	311	CLA	C3D-C4D-ND	3.02	115.13	110.24
32	a	840	CLA	C3D-C4D-ND	3.02	115.12	110.24
32	C	304	CLA	C3D-C4D-ND	3.02	115.12	110.24
32	O	309	CLA	CHC-C4B-NB	-3.02	121.06	124.26
32	D	307	CLA	C3D-C4D-ND	3.02	115.12	110.24
32	b	818	CLA	C3D-C4D-ND	3.02	115.12	110.24
34	O	313	DD6	C32-C31-C36	-3.01	118.38	122.63
32	a	814	CLA	C3D-C4D-ND	3.01	115.11	110.24
34	H	311	DD6	O1-C20-C19	-3.01	111.12	113.38
32	b	815	CLA	C3D-C4D-ND	3.01	115.10	110.24
38	I	315	LMU	O1B-C4'-C3'	3.01	115.28	107.28
32	R	308	CLA	CMC-C2C-C1C	3.01	129.62	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	P	305	CLA	C3D-C4D-ND	3.00	115.10	110.24
32	A	305	CLA	C3D-C4D-ND	3.00	115.10	110.24
32	A	304	CLA	C3D-C4D-ND	3.00	115.09	110.24
32	G	301	CLA	C3D-C4D-ND	3.00	115.09	110.24
32	E	314	CLA	C3D-C4D-ND	3.00	115.09	110.24
32	F	301	CLA	C3D-C4D-ND	3.00	115.08	110.24
32	D	304	CLA	C3D-C4D-ND	2.99	115.08	110.24
39	H	315	SQD	O7-S-C6	2.99	110.49	106.94
32	F	309	CLA	C3D-C4D-ND	2.99	115.08	110.24
34	L	319	DD6	C14-C13-C11	2.99	130.17	125.53
32	M	308	CLA	C3D-C4D-ND	2.99	115.07	110.24
32	Q	310	CLA	C3D-C4D-ND	2.99	115.07	110.24
40	Q	318	DGD	C1D-O6D-C5D	2.98	119.54	113.69
32	R	306	CLA	C3D-C4D-ND	2.98	115.06	110.24
32	B	305	CLA	C3D-C4D-ND	2.98	115.05	110.24
32	B	301	CLA	C3D-C4D-ND	2.98	115.05	110.24
34	J	314	DD6	C14-C13-C11	2.97	130.15	125.53
32	H	302	CLA	C3D-C4D-ND	2.97	115.05	110.24
32	H	309	CLA	C3D-C4D-ND	2.97	115.05	110.24
32	H	306	CLA	C3D-C4D-ND	2.97	115.04	110.24
32	K	306	CLA	CAA-C2A-C1A	-2.97	102.25	111.97
32	a	801	CLA	CHA-C1A-NA	-2.97	119.61	126.40
32	a	814	CLA	CHB-C1B-NB	-2.96	121.12	124.26
32	b	832	CLA	CHB-C1B-NB	-2.96	121.12	124.26
32	b	826	CLA	C3D-C4D-ND	2.96	115.02	110.24
32	a	809	CLA	C3D-C4D-ND	2.96	115.02	110.24
32	G	307	CLA	C3D-C4D-ND	2.96	115.02	110.24
32	a	807	CLA	C3D-C4D-ND	2.96	115.02	110.24
33	Q	317	KC2	C2A-C3A-C4A	2.96	108.68	106.49
32	F	307	CLA	C3D-C4D-ND	2.96	115.02	110.24
32	a	832	CLA	C3D-C4D-ND	2.96	115.02	110.24
34	E	316	DD6	C21-C20-C19	2.96	117.61	114.28
32	D	313	CLA	C3D-C4D-ND	2.96	115.02	110.24
37	S	318	A86	C36-C31-C32	-2.96	116.76	119.70
32	G	306	CLA	C3D-C4D-ND	2.96	115.02	110.24
34	I	312	DD6	C14-C13-C11	2.95	130.12	125.53
32	b	837	CLA	C3D-C4D-ND	2.95	115.02	110.24
32	D	305	CLA	C3D-C4D-ND	2.95	115.02	110.24
34	A	314	DD6	C14-C13-C11	2.95	130.11	125.53
32	D	310	CLA	C3D-C4D-ND	2.95	115.01	110.24
34	J	317	DD6	C14-C13-C11	2.95	130.11	125.53
32	S	307	CLA	C2A-C3A-C4A	-2.95	97.11	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	I	303	CLA	C3D-C4D-ND	2.95	115.01	110.24
32	J	308	CLA	C3D-C4D-ND	2.95	115.01	110.24
32	b	832	CLA	C3D-C4D-ND	2.95	115.01	110.24
32	N	313	CLA	C3D-C4D-ND	2.94	115.00	110.24
34	F	316	DD6	C21-C20-C19	2.94	117.59	114.28
32	a	812	CLA	C1-C2-C3	-2.94	120.95	126.04
32	a	805	CLA	C2C-C1C-NC	2.94	112.73	109.97
36	l	201	LMG	O8-C28-C29	2.94	121.14	111.91
32	I	305	CLA	C3D-C4D-ND	2.94	115.00	110.24
32	K	308	CLA	C3D-C4D-ND	2.94	114.99	110.24
32	T	308	CLA	C3D-C4D-ND	2.94	114.99	110.24
36	F	320	LMG	O8-C28-C29	2.94	121.13	111.91
32	D	315	CLA	C3D-C4D-ND	2.94	114.99	110.24
32	T	302	CLA	C3D-C4D-ND	2.94	114.99	110.24
34	H	313	DD6	C32-C31-C36	-2.94	118.49	122.63
32	F	311	CLA	C3D-C4D-ND	2.94	114.99	110.24
32	E	311	CLA	C3D-C4D-ND	2.94	114.99	110.24
32	O	308	CLA	C3D-C4D-ND	2.94	114.99	110.24
32	J	306	CLA	C3D-C4D-ND	2.93	114.98	110.24
32	S	307	CLA	C3D-C4D-ND	2.93	114.98	110.24
36	D	321	LMG	O1-C7-C8	-2.93	103.83	110.90
32	Q	308	CLA	C3D-C4D-ND	2.93	114.98	110.24
34	A	315	DD6	C14-C13-C11	2.93	130.08	125.53
32	A	307	CLA	C3D-C4D-ND	2.93	114.97	110.24
32	O	301	CLA	C3D-C4D-ND	2.92	114.97	110.24
32	F	308	CLA	C3D-C4D-ND	2.92	114.97	110.24
34	G	312	DD6	O1-C20-C19	-2.92	111.19	113.38
32	P	307	CLA	C3D-C4D-ND	2.92	114.97	110.24
32	Q	305	CLA	C3D-C4D-ND	2.92	114.97	110.24
32	V	201	CLA	C3D-C4D-ND	2.92	114.97	110.24
32	b	801	CLA	C3D-C4D-ND	2.92	114.96	110.24
32	H	305	CLA	C3D-C4D-ND	2.92	114.96	110.24
32	O	307	CLA	C3D-C4D-ND	2.92	114.96	110.24
32	Q	309	CLA	C3D-C4D-ND	2.92	114.96	110.24
32	a	814	CLA	CHC-C4B-NB	-2.92	121.17	124.26
37	L	317	A86	C33-C32-C31	2.91	112.04	109.21
32	K	307	CLA	CAA-C2A-C3A	-2.91	109.30	116.10
32	a	813	CLA	C3D-C4D-ND	2.91	114.95	110.24
32	a	853	CLA	C3D-C4D-ND	2.91	114.95	110.24
32	G	303	CLA	CAA-C2A-C1A	-2.91	102.44	111.97
32	C	307	CLA	C3D-C4D-ND	2.91	114.95	110.24
34	E	317	DD6	C14-C13-C11	2.91	130.04	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	309	CLA	C3D-C4D-ND	2.91	114.94	110.24
32	O	305	CLA	C3D-C4D-ND	2.91	114.94	110.24
32	K	306	CLA	C3D-C4D-ND	2.91	114.94	110.24
32	b	822	CLA	CAA-C2A-C1A	-2.90	102.46	111.97
32	R	301	CLA	C3D-C4D-ND	2.90	114.94	110.24
32	E	315	CLA	C3D-C4D-ND	2.90	114.93	110.24
32	a	809	CLA	CHC-C4B-NB	-2.90	121.18	124.26
32	I	301	CLA	C3D-C4D-ND	2.90	114.93	110.24
32	a	808	CLA	C3D-C4D-ND	2.90	114.93	110.24
32	J	311	CLA	C3D-C4D-ND	2.90	114.93	110.24
34	B	307	DD6	C14-C13-C11	2.90	130.03	125.53
32	I	306	CLA	C3D-C4D-ND	2.90	114.93	110.24
37	D	323	A86	O1-C20-C19	2.90	115.56	113.38
32	L	312	CLA	C3D-C4D-ND	2.90	114.93	110.24
32	S	310	CLA	C3D-C4D-ND	2.90	114.92	110.24
32	D	311	CLA	C3D-C4D-ND	2.90	114.92	110.24
36	E	302	LMG	O1-C1-C2	2.90	112.82	108.30
32	I	302	CLA	C3D-C4D-ND	2.89	114.92	110.24
32	R	308	CLA	C3D-C4D-ND	2.89	114.92	110.24
32	b	806	CLA	C3D-C4D-ND	2.89	114.92	110.24
32	R	310	CLA	C3D-C4D-ND	2.89	114.92	110.24
32	S	301	CLA	C3D-C4D-ND	2.89	114.92	110.24
32	E	312	CLA	C3D-C4D-ND	2.89	114.91	110.24
32	f	203	CLA	C3D-C4D-ND	2.89	114.91	110.24
32	E	303	CLA	C3D-C4D-ND	2.89	114.91	110.24
36	j	104	LMG	C7-O1-C1	2.89	119.39	113.74
32	b	824	CLA	C3D-C4D-ND	2.89	114.91	110.24
32	b	828	CLA	C3D-C4D-ND	2.89	114.91	110.24
32	b	829	CLA	C3D-C4D-ND	2.89	114.91	110.24
35	B	308	LHG	O8-C23-C24	2.89	120.97	111.91
32	a	836	CLA	C3D-C4D-ND	2.89	114.91	110.24
34	F	315	DD6	O1-C20-C19	2.89	115.55	113.38
32	E	309	CLA	C3D-C4D-ND	2.89	114.91	110.24
32	b	809	CLA	C3D-C4D-ND	2.88	114.90	110.24
32	a	833	CLA	C3D-C4D-ND	2.88	114.90	110.24
32	O	309	CLA	C3D-C4D-ND	2.88	114.90	110.24
32	K	310	CLA	C3D-C4D-ND	2.88	114.90	110.24
32	b	807	CLA	C3D-C4D-ND	2.88	114.90	110.24
32	D	309	CLA	C3D-C4D-ND	2.88	114.90	110.24
32	f	204	CLA	C3D-C4D-ND	2.88	114.90	110.24
32	G	304	CLA	C3D-C4D-ND	2.88	114.89	110.24
32	J	304	CLA	C3D-C4D-ND	2.88	114.89	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	k	201	CLA	C3D-C4D-ND	2.88	114.89	110.24
32	C	305	CLA	C3D-C4D-ND	2.87	114.89	110.24
32	a	831	CLA	C3D-C4D-ND	2.87	114.89	110.24
32	E	310	CLA	C3D-C4D-ND	2.87	114.89	110.24
32	Q	303	CLA	C3D-C4D-ND	2.87	114.89	110.24
32	W	310	CLA	C3D-C4D-ND	2.87	114.89	110.24
32	b	813	CLA	C3D-C4D-ND	2.87	114.89	110.24
32	P	310	CLA	C3D-C4D-ND	2.87	114.88	110.24
32	F	306	CLA	C3D-C4D-ND	2.87	114.88	110.24
32	J	309	CLA	C3D-C4D-ND	2.87	114.88	110.24
32	L	310	CLA	C3D-C4D-ND	2.87	114.88	110.24
32	R	306	CLA	CHC-C4B-NB	-2.87	121.22	124.26
37	M	318	A86	C33-C32-C31	2.87	112.00	109.21
32	E	304	CLA	C3D-C4D-ND	2.87	114.88	110.24
32	V	204	CLA	C3D-C4D-ND	2.87	114.88	110.24
32	a	814	CLA	C1-C2-C3	-2.87	121.08	126.04
32	C	302	CLA	C3D-C4D-ND	2.87	114.87	110.24
32	J	302	CLA	C3D-C4D-ND	2.86	114.87	110.24
32	M	309	CLA	C3D-C4D-ND	2.86	114.87	110.24
32	U	307	CLA	C3D-C4D-ND	2.86	114.87	110.24
35	D	320	LHG	O8-C23-C24	2.86	120.89	111.91
32	K	304	CLA	C3D-C4D-ND	2.86	114.87	110.24
32	D	308	CLA	C3D-C4D-ND	2.86	114.87	110.24
32	a	837	CLA	C3D-C4D-ND	2.86	114.86	110.24
34	J	316	DD6	C14-C13-C11	2.86	129.97	125.53
36	D	303	LMG	O7-C8-C9	2.86	118.75	108.40
32	L	311	CLA	C3D-C4D-ND	2.86	114.86	110.24
32	a	820	CLA	CHB-C1B-NB	-2.86	121.23	124.26
32	I	307	CLA	C3D-C4D-ND	2.86	114.86	110.24
32	T	307	CLA	C3D-C4D-ND	2.85	114.86	110.24
32	a	838	CLA	C3D-C4D-ND	2.85	114.85	110.24
32	b	827	CLA	C3D-C4D-ND	2.85	114.85	110.24
32	H	310	CLA	C3D-C4D-ND	2.85	114.85	110.24
32	M	312	CLA	C3D-C4D-ND	2.85	114.85	110.24
32	R	307	CLA	C3D-C4D-ND	2.85	114.85	110.24
32	r	202	CLA	C3D-C4D-ND	2.85	114.85	110.24
32	H	304	CLA	C3D-C4D-ND	2.85	114.85	110.24
32	b	823	CLA	C3D-C4D-ND	2.85	114.85	110.24
32	a	817	CLA	C3D-C4D-ND	2.85	114.85	110.24
36	l	201	LMG	C1-C2-C3	-2.85	104.06	110.00
32	C	301	CLA	C3D-C4D-ND	2.85	114.84	110.24
32	P	309	CLA	C3D-C4D-ND	2.85	114.84	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	835	CLA	C3D-C4D-ND	2.85	114.84	110.24
32	b	821	CLA	C3D-C4D-ND	2.85	114.84	110.24
37	G	310	A86	C36-C31-C32	-2.85	116.87	119.70
34	A	312	DD6	C14-C13-C11	2.85	129.95	125.53
32	R	309	CLA	C3D-C4D-ND	2.84	114.84	110.24
32	a	838	CLA	C1-C2-C3	2.84	130.96	126.04
32	A	303	CLA	C3D-C4D-ND	2.84	114.84	110.24
32	Q	306	CLA	C3D-C4D-ND	2.84	114.84	110.24
32	R	304	CLA	C3D-C4D-ND	2.84	114.84	110.24
32	r	201	CLA	C3D-C4D-ND	2.84	114.84	110.24
32	W	307	CLA	C3D-C4D-ND	2.84	114.83	110.24
32	L	301	CLA	C3D-C4D-ND	2.84	114.83	110.24
32	Q	301	CLA	C3D-C4D-ND	2.84	114.83	110.24
32	A	311	CLA	C3D-C4D-ND	2.84	114.83	110.24
36	T	301	LMG	O6-C1-O1	-2.84	103.26	109.97
32	H	309	CLA	CHC-C4B-NB	-2.83	121.26	124.26
32	I	317	CLA	C3D-C4D-ND	2.83	114.82	110.24
32	T	308	CLA	C1-C2-C3	-2.83	121.14	126.04
32	Q	303	CLA	C3A-C2A-C1A	-2.83	97.10	101.34
32	F	303	CLA	C3D-C4D-ND	2.83	114.82	110.24
32	S	313	CLA	C3D-C4D-ND	2.83	114.82	110.24
32	C	309	CLA	C3D-C4D-ND	2.83	114.81	110.24
32	H	308	CLA	C3D-C4D-ND	2.83	114.81	110.24
32	D	307	CLA	C11-C10-C8	2.83	125.06	115.92
32	S	305	CLA	C3D-C4D-ND	2.83	114.81	110.24
32	P	311	CLA	C3D-C4D-ND	2.82	114.81	110.24
32	a	803	CLA	C3D-C4D-ND	2.82	114.81	110.24
32	F	305	CLA	C1-C2-C3	-2.82	122.18	126.75
32	a	806	CLA	C3D-C4D-ND	2.82	114.80	110.24
32	C	305	CLA	C3A-C2A-C1A	-2.82	97.11	101.34
32	L	308	CLA	C3D-C4D-ND	2.82	114.80	110.24
32	Q	304	CLA	C3D-C4D-ND	2.82	114.80	110.24
32	T	309	CLA	C3D-C4D-ND	2.82	114.80	110.24
32	a	815	CLA	C3D-C4D-ND	2.82	114.80	110.24
32	O	304	CLA	C3D-C4D-ND	2.82	114.80	110.24
32	b	817	CLA	C3D-C4D-ND	2.82	114.80	110.24
32	b	825	CLA	C3D-C4D-ND	2.82	114.79	110.24
32	F	305	CLA	C3D-C4D-ND	2.81	114.79	110.24
32	b	804	CLA	C3D-C4D-ND	2.81	114.79	110.24
32	W	312	CLA	C3D-C4D-ND	2.81	114.79	110.24
32	a	816	CLA	C3D-C4D-ND	2.81	114.79	110.24
32	a	826	CLA	C3D-C4D-ND	2.81	114.79	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	839	CLA	C3D-C4D-ND	2.81	114.79	110.24
35	a	851	LHG	C5-O7-C7	-2.81	110.87	117.79
34	k	205	DD6	C14-C13-C11	2.81	129.89	125.53
32	A	308	CLA	C3D-C4D-ND	2.81	114.78	110.24
32	U	302	CLA	C3D-C4D-ND	2.81	114.78	110.24
32	Q	307	CLA	C3D-C4D-ND	2.81	114.78	110.24
32	W	309	CLA	C3D-C4D-ND	2.81	114.78	110.24
32	K	301	CLA	C3D-C4D-ND	2.80	114.77	110.24
32	C	304	CLA	CHC-C4B-NB	-2.80	121.29	124.26
34	I	313	DD6	O1-C20-C19	2.80	115.49	113.38
32	A	302	CLA	C3D-C4D-ND	2.80	114.77	110.24
32	k	203	CLA	C3D-C4D-ND	2.80	114.77	110.24
32	H	301	CLA	C3D-C4D-ND	2.80	114.77	110.24
32	D	312	CLA	C3D-C4D-ND	2.80	114.76	110.24
32	b	812	CLA	C3D-C4D-ND	2.80	114.76	110.24
32	D	306	CLA	C3D-C4D-ND	2.80	114.76	110.24
39	k	206	SQD	O8-S-C6	2.79	110.19	105.74
32	M	311	CLA	C3D-C4D-ND	2.79	114.75	110.24
36	F	319	LMG	O8-C28-C29	2.79	120.67	111.91
32	T	306	CLA	C3D-C4D-ND	2.79	114.75	110.24
32	a	819	CLA	C3D-C4D-ND	2.79	114.75	110.24
32	k	202	CLA	C3D-C4D-ND	2.79	114.75	110.24
34	E	317	DD6	C21-C20-C19	2.79	117.42	114.28
35	a	849	LHG	O8-C23-C24	2.79	120.65	111.91
32	N	312	CLA	C3D-C4D-ND	2.78	114.74	110.24
32	E	307	CLA	C3D-C4D-ND	2.78	114.74	110.24
32	M	310	CLA	C3D-C4D-ND	2.78	114.74	110.24
32	b	838	CLA	C3D-C4D-ND	2.78	114.74	110.24
32	b	836	CLA	C3D-C4D-ND	2.78	114.73	110.24
32	L	304	CLA	C3D-C4D-ND	2.78	114.73	110.24
32	a	842	CLA	C3D-C4D-ND	2.78	114.73	110.24
33	W	308	KC2	CHB-C1B-NB	2.77	127.00	124.45
32	V	203	CLA	C3D-C4D-ND	2.77	114.72	110.24
32	b	822	CLA	C3D-C4D-ND	2.77	114.72	110.24
32	a	829	CLA	C3D-C4D-ND	2.77	114.72	110.24
32	E	305	CLA	C3D-C4D-ND	2.77	114.72	110.24
32	S	309	CLA	C3D-C4D-ND	2.77	114.71	110.24
32	U	305	CLA	C3D-C4D-ND	2.77	114.71	110.24
32	b	820	CLA	C3D-C4D-ND	2.77	114.71	110.24
32	j	101	CLA	C3D-C4D-ND	2.77	114.71	110.24
32	C	306	CLA	CHC-C4B-NB	-2.76	121.33	124.26
36	W	320	LMG	O8-C28-C29	2.76	120.58	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	839	CLA	C3D-C4D-ND	2.76	114.71	110.24
32	l	202	CLA	C3D-C4D-ND	2.76	114.71	110.24
36	E	320	LMG	O6-C1-C2	-2.76	104.50	110.35
37	F	313	A86	C36-C31-C32	-2.76	116.95	119.70
32	F	307	CLA	CMC-C2C-C1C	2.76	129.25	125.04
32	N	309	CLA	C3D-C4D-ND	2.76	114.70	110.24
34	A	312	DD6	C21-C20-C19	2.76	117.38	114.28
32	a	818	CLA	C3D-C4D-ND	2.75	114.69	110.24
32	b	814	CLA	C3D-C4D-ND	2.75	114.69	110.24
36	N	301	LMG	O8-C28-C29	2.75	120.55	111.91
32	J	305	CLA	C3D-C4D-ND	2.75	114.69	110.24
36	E	320	LMG	C1-O6-C5	-2.75	108.29	113.69
32	O	306	CLA	C3D-C4D-ND	2.75	114.68	110.24
32	F	305	CLA	CHC-C4B-NB	-2.75	121.35	124.26
35	A	316	LHG	O8-C23-C24	2.75	120.53	111.91
36	L	320	LMG	O6-C1-O1	-2.75	103.47	109.97
32	b	823	CLA	C1-C2-C3	-2.75	121.29	126.04
32	b	840	CLA	C3D-C4D-ND	2.75	114.68	110.24
32	a	817	CLA	CHC-C4B-NB	-2.75	121.35	124.26
32	N	311	CLA	C3D-C4D-ND	2.75	114.68	110.24
32	a	811	CLA	C3D-C4D-ND	2.75	114.68	110.24
32	b	835	CLA	C3D-C4D-ND	2.75	114.68	110.24
36	l	201	LMG	O6-C1-C2	-2.75	104.54	110.35
39	k	206	SQD	O7-S-C6	2.74	110.20	106.94
32	A	301	CLA	C3D-C4D-ND	2.74	114.67	110.24
32	B	306	CLA	C3D-C4D-ND	2.74	114.67	110.24
32	A	306	CLA	C3D-C4D-ND	2.74	114.67	110.24
32	U	303	CLA	C3D-C4D-ND	2.74	114.66	110.24
36	P	318	LMG	O8-C28-C29	2.74	120.49	111.91
32	W	313	CLA	C3D-C4D-ND	2.74	114.66	110.24
32	L	309	CLA	C3D-C4D-ND	2.73	114.65	110.24
32	L	314	CLA	C3D-C4D-ND	2.73	114.65	110.24
32	J	301	CLA	C3D-C4D-ND	2.73	114.65	110.24
32	P	307	CLA	CHC-C4B-NB	-2.73	121.37	124.26
32	P	304	CLA	C3D-C4D-ND	2.73	114.65	110.24
32	b	803	CLA	C3D-C4D-ND	2.73	114.65	110.24
34	V	202	DD6	C21-C20-C19	2.72	117.34	114.28
39	H	315	SQD	O8-S-C6	2.72	110.08	105.74
32	B	304	CLA	C3D-C4D-ND	2.72	114.64	110.24
32	W	306	CLA	C3D-C4D-ND	2.72	114.64	110.24
32	I	304	CLA	C3D-C4D-ND	2.72	114.63	110.24
32	a	827	CLA	C3D-C4D-ND	2.72	114.63	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	810	CLA	C3D-C4D-ND	2.72	114.63	110.24
32	b	811	CLA	C3D-C4D-ND	2.72	114.63	110.24
32	a	834	CLA	C3D-C4D-ND	2.72	114.63	110.24
32	a	804	CLA	C3D-C4D-ND	2.71	114.63	110.24
32	U	306	CLA	C3D-C4D-ND	2.71	114.63	110.24
37	O	311	A86	C33-C32-C31	2.71	111.85	109.21
32	T	308	CLA	CMC-C2C-C1C	2.71	129.17	125.04
37	S	314	A86	O1-C20-C19	2.71	115.42	113.38
32	O	305	CLA	CHC-C4B-NB	-2.71	121.39	124.26
32	l	204	CLA	C3D-C4D-ND	2.71	114.63	110.24
34	F	314	DD6	C33-C34-C35	2.71	114.02	110.30
36	N	301	LMG	C8-O7-C10	-2.71	111.11	117.79
32	C	304	CLA	CBA-CAA-C2A	2.71	119.74	114.02
32	E	308	CLA	C3D-C4D-ND	2.71	114.62	110.24
37	M	322	A86	C36-C31-C32	-2.71	117.01	119.70
36	D	321	LMG	O6-C1-O1	-2.71	103.56	109.97
41	l	206	BCR	C8-C9-C10	2.71	123.09	118.94
36	E	320	LMG	O8-C28-C29	2.71	120.40	111.91
32	B	303	CLA	C3D-C4D-ND	2.70	114.61	110.24
35	I	318	LHG	O8-C23-C24	2.70	120.39	111.91
32	r	202	CLA	CHC-C4B-NB	-2.70	121.40	124.26
33	T	304	KC2	C4B-C3B-C2B	2.70	108.97	106.75
34	F	314	DD6	C32-C31-C36	-2.70	118.82	122.63
38	V	205	LMU	C1B-C2B-C3B	2.70	115.62	110.00
35	W	319	LHG	O8-C23-C24	2.70	120.37	111.91
32	a	812	CLA	C3D-C4D-ND	2.70	114.60	110.24
32	a	824	CLA	C3D-C4D-ND	2.70	114.60	110.24
32	b	830	CLA	C3D-C4D-ND	2.70	114.60	110.24
34	U	309	DD6	C32-C31-C36	-2.69	118.83	122.63
32	M	305	CLA	C3D-C4D-ND	2.69	114.59	110.24
32	a	821	CLA	C3D-C4D-ND	2.69	114.59	110.24
32	H	304	CLA	C3A-C2A-C1A	-2.69	97.31	101.34
32	K	306	CLA	CAA-C2A-C3A	2.69	120.14	112.78
32	B	304	CLA	CHC-C4B-NB	-2.69	121.41	124.26
32	O	307	CLA	CMC-C2C-C1C	2.69	129.13	125.04
32	a	825	CLA	C3D-C4D-ND	2.69	114.59	110.24
32	b	810	CLA	C3D-C4D-ND	2.69	114.58	110.24
36	D	303	LMG	O8-C28-C29	2.69	120.34	111.91
32	b	816	CLA	C3D-C4D-ND	2.68	114.58	110.24
32	a	823	CLA	C3D-C4D-ND	2.68	114.58	110.24
34	N	318	DD6	O1-C20-C19	-2.68	111.37	113.38
32	b	831	CLA	C3D-C4D-ND	2.68	114.57	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	W	320	LMG	C8-O7-C10	-2.68	111.20	117.79
33	H	303	KC2	CHB-C1B-NB	2.68	126.91	124.45
32	W	311	CLA	C3D-C4D-ND	2.67	114.56	110.24
32	a	828	CLA	C3D-C4D-ND	2.67	114.56	110.24
33	K	309	KC2	CHB-C1B-NB	2.66	126.90	124.45
36	P	318	LMG	C8-O7-C10	-2.66	111.25	117.79
32	P	308	CLA	C3D-C4D-ND	2.66	114.53	110.24
35	M	319	LHG	O8-C23-C24	2.65	120.23	111.91
32	a	830	CLA	C3D-C4D-ND	2.64	114.51	110.24
32	a	818	CLA	CHA-C1A-NA	-2.64	120.35	126.40
32	J	312	CLA	CHC-C4B-NB	-2.64	121.47	124.26
32	F	322	CLA	CHA-C1A-NA	-2.64	120.36	126.40
36	D	321	LMG	O1-C1-C2	-2.64	104.19	108.30
36	D	302	LMG	O8-C28-C29	2.63	120.17	111.91
32	M	305	CLA	C1-C2-C3	-2.63	122.50	126.75
32	a	812	CLA	CHC-C4B-NB	-2.63	121.47	124.26
32	S	308	CLA	C3D-C4D-ND	2.63	114.48	110.24
36	E	302	LMG	O6-C5-C4	2.62	114.46	109.69
32	a	841	CLA	C3D-C4D-ND	2.62	114.48	110.24
37	N	316	A86	C33-C32-C31	2.62	111.76	109.21
32	D	314	CLA	C3D-C4D-ND	2.62	114.48	110.24
32	F	322	CLA	C3D-C4D-ND	2.62	114.48	110.24
34	k	205	DD6	O1-C20-C15	-2.62	56.79	58.96
38	j	105	LMU	O5B-C1B-C2B	-2.62	104.81	110.35
34	Q	312	DD6	O1-C20-C19	-2.62	111.42	113.38
37	S	314	A86	O4-C34-C35	2.62	114.11	107.59
36	A	318	LMG	O1-C1-C2	-2.61	104.22	108.30
32	I	303	CLA	CHC-C4B-NB	-2.61	121.49	124.26
33	K	303	KC2	CHB-C1B-NB	2.61	126.86	124.45
32	a	805	CLA	C3D-C4D-ND	2.61	114.46	110.24
34	E	319	DD6	C14-C13-C11	2.61	129.58	125.53
32	N	313	CLA	C1-C2-C3	-2.61	121.53	126.04
33	S	306	KC2	CHD-C4C-NC	2.61	128.16	124.20
34	T	314	DD6	C21-C20-C19	2.60	117.20	114.28
32	C	307	CLA	CAA-C2A-C3A	2.59	119.88	112.78
36	A	317	LMG	C9-C8-C7	-2.59	105.65	111.79
35	I	314	LHG	O8-C23-C24	2.59	120.04	111.91
33	C	303	KC2	CHB-C1B-NB	2.59	126.83	124.45
32	f	204	CLA	CHC-C4B-NB	-2.59	121.52	124.26
32	l	203	CLA	C3D-C4D-ND	2.59	114.42	110.24
33	I	316	KC2	CHD-C4C-NC	2.59	128.12	124.20
34	S	321	DD6	C22-C16-C15	-2.58	103.07	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	M	317	A86	C21-C20-C19	-2.58	111.37	114.28
36	E	320	LMG	C8-O7-C10	-2.58	111.43	117.79
32	B	309	CLA	C3D-C4D-ND	2.58	114.41	110.24
32	b	819	CLA	C3D-C4D-ND	2.58	114.41	110.24
32	l	204	CLA	C3A-C2A-C1A	-2.58	97.47	101.34
35	F	321	LHG	O8-C23-C24	2.58	120.00	111.91
34	D	319	DD6	C33-C34-C35	2.57	113.83	110.30
33	L	305	KC2	C4C-C3C-C2C	2.57	109.16	107.11
32	b	808	CLA	C3D-C4D-ND	2.57	114.39	110.24
32	a	802	CLA	CHC-C4B-NB	-2.57	121.54	124.26
32	S	309	CLA	C1-C2-C3	2.56	130.47	126.04
32	N	305	CLA	C3D-C4D-ND	2.56	114.38	110.24
34	K	313	DD6	C14-C13-C11	2.56	129.50	125.53
32	a	801	CLA	C4D-CHA-C1A	-2.56	118.14	121.25
32	T	305	CLA	C3D-C4D-ND	2.56	114.37	110.24
32	Q	303	CLA	CBA-CAA-C2A	2.56	121.41	113.86
32	L	307	CLA	C3D-C4D-ND	2.55	114.36	110.24
32	a	822	CLA	C3D-C4D-ND	2.55	114.36	110.24
32	a	852	CLA	C3D-C4D-ND	2.55	114.36	110.24
33	F	310	KC2	CHB-C1B-NB	2.55	126.80	124.45
36	l	201	LMG	C1-O6-C5	-2.55	108.69	113.69
33	P	312	KC2	CHB-C1B-NB	2.55	126.79	124.45
33	N	303	KC2	C4B-C3B-C2B	2.55	108.84	106.75
32	E	314	CLA	CHC-C4B-NB	-2.55	121.56	124.26
32	S	308	CLA	CHC-C4B-NB	-2.54	121.56	124.26
36	A	318	LMG	O6-C5-C4	2.54	114.31	109.69
32	a	830	CLA	C11-C12-C13	2.54	124.13	115.92
33	Q	317	KC2	C3A-C4A-NA	-2.54	107.80	110.57
34	A	315	DD6	C21-C20-C19	2.54	117.14	114.28
32	f	201	CLA	C3D-C4D-ND	2.54	114.35	110.24
33	O	303	KC2	CHB-C1B-NB	2.54	126.78	124.45
32	T	308	CLA	CAA-C2A-C3A	2.54	119.72	112.78
37	P	314	A86	C36-C31-C32	-2.53	117.18	119.70
32	K	307	CLA	C3D-C4D-ND	2.53	114.34	110.24
32	S	304	CLA	C3D-C4D-ND	2.53	114.34	110.24
33	W	301	KC2	CHD-C4C-NC	2.53	128.04	124.20
32	b	834	CLA	CHC-C4B-NB	-2.53	121.58	124.26
32	b	819	CLA	CMA-C3A-C4A	2.53	118.57	111.77
36	E	302	LMG	O6-C1-O1	-2.53	103.98	109.97
33	G	309	KC2	C4C-C3C-C2C	2.53	109.12	107.11
38	I	315	LMU	C1-O1'-C1'	-2.53	109.65	113.84
35	P	317	LHG	O8-C23-C24	2.52	119.82	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	b	842	BCR	C7-C8-C9	2.52	130.04	126.23
37	M	315	A86	C33-C32-C31	2.52	111.66	109.21
36	E	320	LMG	O7-C10-O9	-2.52	117.61	123.70
33	P	306	KC2	CHB-C1B-NB	2.52	126.77	124.45
34	C	310	DD6	C14-C13-C11	2.52	129.44	125.53
32	E	304	CLA	CHC-C4B-NB	-2.52	121.59	124.26
32	b	828	CLA	CAA-C2A-C1A	-2.51	103.73	111.97
33	M	307	KC2	CHD-C4C-NC	2.51	128.01	124.20
32	H	307	CLA	CBA-CAA-C2A	2.51	121.28	113.86
32	G	305	CLA	C3D-C4D-ND	2.51	114.30	110.24
33	T	304	KC2	CHB-C1B-NB	2.51	126.76	124.45
32	D	308	CLA	CHC-C4B-NB	-2.51	121.60	124.26
43	b	847	PQN	C11-C3-C4	-2.51	115.82	118.50
34	W	317	DD6	C14-C13-C11	2.51	129.42	125.53
33	I	316	KC2	CHB-C1B-NB	2.51	126.76	124.45
33	J	303	KC2	CHB-C1B-NB	2.50	126.76	124.45
33	W	301	KC2	CHB-C1B-NB	2.50	126.75	124.45
33	N	304	KC2	CHD-C4C-NC	2.50	128.00	124.20
37	K	314	A86	C21-C20-C19	-2.50	111.47	114.28
37	C	311	A86	O1-C20-C19	2.50	115.26	113.38
32	A	309	CLA	C1-C2-C3	-2.50	121.72	126.04
36	D	302	LMG	C8-O7-C10	-2.50	111.64	117.79
33	K	303	KC2	CHD-C4C-NC	2.50	127.99	124.20
33	N	307	KC2	CHB-C1B-NB	2.50	126.75	124.45
33	J	310	KC2	CHB-C1B-NB	2.50	126.75	124.45
33	I	309	KC2	CHB-C1B-NB	2.49	126.75	124.45
33	W	303	KC2	CHB-C1B-NB	2.49	126.75	124.45
33	W	305	KC2	CHB-C1B-NB	2.49	126.75	124.45
33	M	313	KC2	CHB-C1B-NB	2.49	126.74	124.45
32	O	305	CLA	CBA-CAA-C2A	2.49	121.22	113.86
33	N	306	KC2	C4B-C3B-C2B	2.49	108.80	106.75
32	B	302	CLA	C3D-C4D-ND	2.49	114.27	110.24
32	H	301	CLA	C3A-C2A-C1A	-2.49	97.61	101.34
35	a	850	LHG	O8-C23-C24	2.49	119.72	111.91
33	N	302	KC2	CHB-C1B-NB	2.49	126.74	124.45
33	N	314	KC2	CHB-C1B-NB	2.49	126.74	124.45
32	T	308	CLA	CAA-C2A-C1A	-2.48	103.83	111.97
33	P	303	KC2	C4B-C3B-C2B	2.48	108.79	106.75
40	Q	318	DGD	O4D-C4D-C3D	-2.48	104.61	110.35
33	M	321	KC2	CHB-C4A-NA	2.48	128.11	124.20
35	W	319	LHG	C11-C10-C9	-2.48	101.85	114.42
32	E	306	CLA	CHC-C4B-NB	-2.48	121.64	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	H	301	CLA	CHC-C4B-NB	-2.48	121.64	124.26
33	Q	302	KC2	CHB-C1B-NB	2.48	126.73	124.45
35	a	849	LHG	C11-C10-C9	-2.47	101.86	114.42
34	S	321	DD6	C21-C20-C19	2.47	117.06	114.28
32	D	311	CLA	C1-C2-C3	-2.47	121.77	126.04
33	S	306	KC2	CHB-C1B-NB	2.47	126.73	124.45
32	b	802	CLA	CHC-C4B-NB	-2.47	121.64	124.26
34	F	315	DD6	C32-C31-C36	-2.47	119.15	122.63
37	M	314	A86	C36-C31-C32	-2.47	117.25	119.70
32	D	307	CLA	CMC-C2C-C1C	2.47	128.80	125.04
32	G	306	CLA	CMC-C2C-C1C	2.47	128.80	125.04
33	P	301	KC2	CHB-C1B-NB	2.47	126.72	124.45
34	E	318	DD6	C14-C13-C11	2.46	129.35	125.53
32	b	830	CLA	CHC-C4B-NB	-2.46	121.65	124.26
36	l	201	LMG	O1-C1-C2	2.46	112.15	108.30
32	H	305	CLA	CHC-C4B-NB	-2.46	121.65	124.26
32	I	304	CLA	CHC-C4B-NB	-2.46	121.65	124.26
33	L	302	KC2	C4B-C3B-C2B	2.46	108.77	106.75
32	a	822	CLA	CHA-C1A-NA	-2.46	120.77	126.40
32	T	305	CLA	CHC-C4B-NB	-2.46	121.66	124.26
33	Q	302	KC2	CHD-C4C-NC	2.46	127.93	124.20
32	B	306	CLA	CHC-C4B-NB	-2.45	121.66	124.26
33	W	305	KC2	CHD-C4C-NC	2.45	127.92	124.20
33	N	308	KC2	CHB-C1B-NB	2.45	126.70	124.45
32	E	308	CLA	CHA-C1A-NA	-2.45	120.79	126.40
32	D	306	CLA	CHC-C4B-NB	-2.45	121.67	124.26
32	S	307	CLA	C2A-C1A-CHA	2.44	128.13	123.86
33	O	302	KC2	CHB-C1B-NB	2.44	126.70	124.45
33	J	310	KC2	CHD-C4C-NC	2.44	127.91	124.20
32	b	811	CLA	CHC-C4B-NB	-2.44	121.67	124.26
37	T	315	A86	O1-C20-C19	-2.44	111.55	113.38
32	F	322	CLA	O2A-C1-C2	2.44	115.05	108.64
32	a	810	CLA	CMC-C2C-C1C	2.44	128.76	125.04
32	S	304	CLA	C2C-C1C-NC	2.44	112.26	109.97
33	N	306	KC2	CHB-C1B-NB	2.44	126.70	124.45
33	L	305	KC2	CHB-C4A-NA	2.44	128.05	124.20
33	N	314	KC2	C4C-C3C-C2C	2.44	109.05	107.11
33	A	310	KC2	CHB-C1B-NB	2.44	126.69	124.45
32	f	201	CLA	C1-C2-C3	-2.43	121.83	126.04
36	E	302	LMG	O7-C10-O9	-2.43	117.82	123.70
32	A	304	CLA	CMC-C2C-C1C	2.43	128.74	125.04
33	S	312	KC2	CHB-C1B-NB	2.43	126.69	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	H	305	CLA	CHD-C1D-C2D	2.43	130.58	125.48
32	D	310	CLA	CAA-C2A-C3A	2.43	119.43	112.78
32	a	802	CLA	C3D-C4D-ND	2.43	114.17	110.24
33	M	302	KC2	CHB-C1B-NB	2.43	126.69	124.45
33	R	305	KC2	CHD-C4C-NC	2.43	127.89	124.20
32	a	840	CLA	C1-C2-C3	-2.43	121.85	126.04
33	R	311	KC2	CHB-C1B-NB	2.42	126.68	124.45
33	K	305	KC2	CHB-C4A-NA	2.42	128.02	124.20
34	G	312	DD6	C32-C31-C36	-2.42	119.21	122.63
32	b	807	CLA	CHC-C4B-NB	-2.42	121.69	124.26
32	a	822	CLA	CMA-C3A-C4A	2.42	118.28	111.77
32	H	302	CLA	CHA-C1A-NA	-2.42	120.86	126.40
32	C	305	CLA	CHC-C4B-NB	-2.42	121.70	124.26
34	G	312	DD6	C14-C13-C11	2.42	129.28	125.53
33	K	302	KC2	CHB-C1B-NB	2.42	126.68	124.45
33	Q	317	KC2	CHB-C1B-NB	2.42	126.67	124.45
33	S	302	KC2	CHB-C1B-NB	2.41	126.67	124.45
33	O	310	KC2	CHB-C1B-NB	2.41	126.67	124.45
33	N	307	KC2	CHD-C4C-NC	2.41	127.86	124.20
33	S	303	KC2	CHD-C4C-NC	2.41	127.86	124.20
33	F	302	KC2	CHB-C1B-NB	2.41	126.67	124.45
32	b	805	CLA	CHA-C1A-NA	-2.41	120.88	126.40
33	P	302	KC2	C4B-C3B-C2B	2.41	108.73	106.75
33	J	303	KC2	CHD-C4C-NC	2.41	127.86	124.20
33	U	304	KC2	C4C-C3C-C2C	2.41	109.03	107.11
32	D	305	CLA	C1-C2-C3	-2.41	121.88	126.04
33	M	321	KC2	CHD-C4C-NC	2.41	127.85	124.20
33	T	311	KC2	CHB-C1B-NB	2.40	126.66	124.45
32	W	313	CLA	CHC-C4B-NB	-2.40	121.72	124.26
36	A	318	LMG	O1-C7-C8	-2.40	105.11	110.90
33	M	304	KC2	C4B-C3B-C2B	2.40	108.72	106.75
33	G	302	KC2	CHB-C1B-NB	2.40	126.66	124.45
32	a	801	CLA	CHD-C1D-C2D	2.40	130.51	125.48
37	S	318	A86	O1-C20-C19	2.40	115.18	113.38
33	J	310	KC2	C4C-C3C-C2C	2.40	109.02	107.11
32	a	811	CLA	C2C-C1C-NC	2.40	112.22	109.97
37	H	314	A86	C36-C31-C32	-2.40	117.32	119.70
35	E	301	LHG	O8-C23-C24	2.40	119.43	111.91
32	J	304	CLA	CBA-CAA-C2A	2.39	120.93	113.86
33	R	302	KC2	CHB-C4A-NA	2.39	127.98	124.20
32	a	828	CLA	CBA-CAA-C2A	2.39	120.93	113.86
36	E	322	LMG	O8-C28-C29	2.39	119.42	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	H	308	CLA	CHC-C4B-NB	-2.39	121.72	124.26
33	K	305	KC2	CHB-C1B-NB	2.39	126.65	124.45
32	P	309	CLA	CMC-C2C-C1C	2.39	128.68	125.04
39	k	206	SQD	O6-C1-C2	2.39	112.03	108.30
33	L	306	KC2	CHB-C1B-NB	2.39	126.65	124.45
34	E	319	DD6	C21-C20-C19	2.39	116.97	114.28
34	Q	314	DD6	C14-C13-C11	2.39	129.23	125.53
32	a	852	CLA	CHC-C4B-NB	-2.39	121.73	124.26
32	G	303	CLA	CAA-C2A-C3A	2.38	119.31	112.78
33	K	302	KC2	CHD-C4C-NC	2.38	127.82	124.20
32	a	802	CLA	CAA-C2A-C1A	-2.38	104.17	111.97
37	G	311	A86	C21-C20-C19	-2.38	111.60	114.28
33	M	307	KC2	CHB-C1B-NB	2.38	126.64	124.45
32	a	804	CLA	CHC-C4B-NB	-2.38	121.73	124.26
33	W	314	KC2	CHB-C1B-NB	2.38	126.64	124.45
33	M	303	KC2	CHB-C1B-NB	2.38	126.64	124.45
33	R	305	KC2	CHB-C1B-NB	2.38	126.64	124.45
32	C	308	CLA	CHC-C4B-NB	-2.38	121.74	124.26
39	k	206	SQD	O5-C1-C2	-2.38	105.31	110.35
32	a	807	CLA	CHC-C4B-NB	-2.37	121.74	124.26
32	a	838	CLA	CHA-C1A-NA	-2.37	120.96	126.40
33	A	310	KC2	CHD-C4C-NC	2.37	127.80	124.20
32	b	804	CLA	CHC-C4B-NB	-2.37	121.75	124.26
32	a	827	CLA	C1-C2-C3	-2.37	121.94	126.04
33	R	303	KC2	CHB-C1B-NB	2.37	126.63	124.45
36	F	320	LMG	C8-O7-C10	-2.37	111.96	117.79
33	H	303	KC2	CHD-C4C-NC	2.37	127.80	124.20
33	L	305	KC2	CHD-C4C-NC	2.37	127.79	124.20
33	P	302	KC2	CHD-C4C-NC	2.37	127.79	124.20
33	S	312	KC2	C4C-C3C-C2C	2.36	108.99	107.11
33	S	302	KC2	CHD-C4C-NC	2.36	127.79	124.20
36	T	301	LMG	O1-C7-C8	-2.36	105.20	110.90
33	G	309	KC2	CHB-C1B-NB	2.36	126.62	124.45
34	T	314	DD6	C14-C13-C11	2.36	129.19	125.53
33	W	308	KC2	CHD-C4C-NC	2.36	127.78	124.20
32	Q	306	CLA	O2A-C1-C2	-2.36	102.44	108.64
32	S	309	CLA	CBA-CAA-C2A	2.36	120.82	113.86
37	F	317	A86	O1-C20-C19	-2.36	111.61	113.38
32	K	306	CLA	C1-C2-C3	-2.36	121.97	126.04
33	O	302	KC2	CHD-C4C-NC	2.36	127.78	124.20
32	a	820	CLA	O2A-C1-C2	2.35	114.82	108.64
36	T	301	LMG	O1-C1-C2	-2.35	104.63	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	303	KC2	CHD-C4C-NC	2.35	127.78	124.20
32	H	304	CLA	CHC-C4B-NB	-2.35	121.77	124.26
32	b	837	CLA	CHC-C4B-NB	-2.35	121.77	124.26
34	D	319	DD6	C32-C31-C36	-2.35	119.31	122.63
32	U	305	CLA	CHC-C4B-NB	-2.35	121.77	124.26
32	a	807	CLA	C1-C2-C3	-2.35	121.98	126.04
33	E	313	KC2	CHB-C1B-NB	2.35	126.61	124.45
40	b	846	DGD	O1G-C1G-C2G	2.35	115.27	108.43
33	P	301	KC2	CHD-C4C-NC	2.35	127.77	124.20
35	f	205	LHG	O8-C23-C24	2.35	119.28	111.91
33	K	305	KC2	CHD-C4C-NC	2.35	127.76	124.20
33	M	313	KC2	CHD-C4C-NC	2.35	127.76	124.20
37	L	315	A86	C21-C20-C19	-2.34	111.64	114.28
33	W	301	KC2	C4C-C3C-C2C	2.34	108.97	107.11
33	W	304	KC2	C4B-C3B-C2B	2.34	108.67	106.75
33	L	302	KC2	C4C-C3C-C2C	2.34	108.97	107.11
33	L	303	KC2	C4C-C3C-C2C	2.34	108.97	107.11
35	I	318	LHG	O7-C7-O9	-2.34	118.05	123.70
37	T	313	A86	C21-C20-C19	-2.34	111.65	114.28
33	P	306	KC2	CHD-C4C-NC	2.34	127.75	124.20
36	D	325	LMG	C7-O1-C1	-2.34	109.17	113.74
32	l	204	CLA	CHC-C4B-NB	-2.34	121.78	124.26
32	F	304	CLA	CMC-C2C-C1C	2.33	128.59	125.04
32	D	314	CLA	CHC-C1C-C2C	-2.33	120.25	126.73
33	M	303	KC2	CHD-C4C-NC	2.33	127.74	124.20
34	P	315	DD6	C32-C31-C36	-2.33	119.34	122.63
33	W	305	KC2	C4C-C3C-C2C	2.33	108.97	107.11
32	J	305	CLA	CHC-C4B-NB	-2.33	121.79	124.26
32	T	308	CLA	O2A-C1-C2	2.33	114.76	108.64
33	L	303	KC2	CHB-C1B-NB	2.33	126.59	124.45
33	W	304	KC2	CHD-C4C-NC	2.33	127.74	124.20
33	G	309	KC2	CHD-C4C-NC	2.33	127.73	124.20
39	H	315	SQD	O9-S-C6	2.33	109.70	106.94
34	H	311	DD6	C21-C20-C19	2.33	116.90	114.28
36	T	301	LMG	O2-C2-C1	-2.33	104.39	110.05
33	S	306	KC2	C4C-C3C-C2C	2.33	108.96	107.11
35	D	320	LHG	C11-C10-C9	-2.33	102.62	114.42
32	b	801	CLA	CHD-C1D-C2D	2.33	130.36	125.48
33	L	306	KC2	C4B-C3B-C2B	2.33	108.66	106.75
33	L	305	KC2	CHB-C1B-NB	2.33	126.59	124.45
32	a	812	CLA	CHD-C1D-C2D	2.33	130.36	125.48
32	J	306	CLA	CHC-C4B-NB	-2.32	121.80	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	k	203	CLA	CBA-CAA-C2A	2.32	120.72	113.86
32	C	302	CLA	CHC-C4B-NB	-2.32	121.80	124.26
32	G	305	CLA	C2C-C1C-NC	2.32	112.15	109.97
33	E	313	KC2	CHD-C4C-NC	2.32	127.72	124.20
33	P	312	KC2	CHD-C4C-NC	2.32	127.72	124.20
32	J	304	CLA	CMC-C2C-C1C	2.32	128.57	125.04
34	k	205	DD6	C32-C31-C36	2.32	125.91	122.63
32	a	805	CLA	CHC-C1C-C2C	-2.32	120.29	126.73
32	a	830	CLA	CHA-C1A-NA	-2.32	121.09	126.40
32	b	835	CLA	CHC-C4B-NB	-2.32	121.80	124.26
32	S	307	CLA	CHA-C1A-NA	-2.32	121.09	126.40
33	T	304	KC2	C4C-C3C-C2C	2.32	108.95	107.11
32	Q	303	CLA	CHA-C1A-NA	-2.32	121.09	126.40
32	a	837	CLA	CHC-C4B-NB	-2.32	121.81	124.26
32	J	307	CLA	CHD-C1D-C2D	2.31	130.33	125.48
36	E	302	LMG	O3-C3-C2	-2.31	105.00	110.35
33	M	302	KC2	CHD-C4C-NC	2.31	127.71	124.20
33	P	303	KC2	CHB-C1B-NB	2.31	126.58	124.45
32	b	815	CLA	CAA-C2A-C3A	2.31	119.11	112.78
37	K	314	A86	C36-C31-C32	-2.31	117.40	119.70
32	G	306	CLA	CHC-C4B-NB	-2.31	121.81	124.26
33	S	312	KC2	CHD-C4C-NC	2.31	127.71	124.20
33	F	310	KC2	CHD-C4C-NC	2.31	127.71	124.20
33	L	306	KC2	CHD-C4C-NC	2.31	127.71	124.20
32	a	829	CLA	CHA-C1A-NA	-2.31	121.11	126.40
33	L	313	KC2	CHB-C1B-NB	2.31	126.58	124.45
32	U	303	CLA	CHC-C4B-NB	-2.31	121.81	124.26
32	b	838	CLA	CHC-C4B-NB	-2.31	121.81	124.26
33	U	304	KC2	CHB-C4A-NA	2.31	127.84	124.20
33	L	303	KC2	C4B-C3B-C2B	2.31	108.65	106.75
36	l	201	LMG	O6-C5-C6	2.31	112.17	106.44
36	D	325	LMG	O7-C10-O9	-2.31	118.13	123.70
32	C	307	CLA	CHC-C4B-NB	-2.31	121.81	124.26
33	T	303	KC2	C4B-C3B-C2B	2.31	108.65	106.75
32	U	305	CLA	C3A-C2A-C1A	-2.31	97.89	101.34
32	b	815	CLA	CHC-C4B-NB	-2.31	121.82	124.26
32	J	307	CLA	CMC-C2C-C1C	2.30	128.55	125.04
33	T	303	KC2	CHD-C4C-NC	2.30	127.70	124.20
36	D	303	LMG	C8-O7-C10	2.30	123.46	117.79
32	b	802	CLA	CHA-C1A-NA	-2.30	121.12	126.40
32	U	306	CLA	CHC-C4B-NB	-2.30	121.82	124.26
32	D	310	CLA	CBA-CAA-C2A	2.30	120.66	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	304	CLA	C1-C2-C3	-2.30	122.06	126.04
36	F	320	LMG	C7-O1-C1	-2.30	109.24	113.74
33	J	303	KC2	CHB-C4A-NA	2.30	127.83	124.20
32	W	313	CLA	CHA-C1A-NA	-2.30	121.13	126.40
37	N	320	A86	C33-C32-C31	2.30	111.45	109.21
33	U	304	KC2	CHB-C1B-NB	2.30	126.57	124.45
32	T	305	CLA	CHD-C1D-C2D	2.30	130.30	125.48
33	I	309	KC2	CHD-C4C-NC	2.30	127.69	124.20
33	U	304	KC2	CHD-C4C-NC	2.30	127.69	124.20
33	L	302	KC2	CHD-C4C-NC	2.30	127.69	124.20
33	N	304	KC2	C4C-C3C-C2C	2.29	108.94	107.11
32	F	309	CLA	CHC-C4B-NB	-2.29	121.83	124.26
32	B	302	CLA	CHA-C1A-NA	-2.29	121.14	126.40
32	b	805	CLA	C4D-CHA-C1A	-2.29	118.46	121.25
32	a	802	CLA	C4D-CHA-C1A	-2.29	118.46	121.25
32	b	805	CLA	C3D-C4D-ND	2.29	113.95	110.24
32	a	806	CLA	C2C-C1C-NC	2.29	112.12	109.97
34	P	315	DD6	C33-C34-C35	2.29	113.44	110.30
32	H	302	CLA	CHC-C4B-NB	-2.29	121.83	124.26
33	W	314	KC2	C4C-C3C-C2C	2.29	108.93	107.11
32	M	308	CLA	CAA-C2A-C1A	-2.29	104.48	111.97
32	M	308	CLA	CAA-C2A-C3A	2.29	119.04	112.78
32	b	823	CLA	CBA-CAA-C2A	2.29	120.61	113.86
32	k	203	CLA	O2A-C1-C2	2.29	114.64	108.64
32	b	819	CLA	CHA-C1A-NA	-2.29	121.16	126.40
33	M	321	KC2	CHB-C1B-NB	2.29	126.55	124.45
34	U	309	DD6	C33-C34-C35	2.29	113.43	110.30
33	F	310	KC2	C4C-C3C-C2C	2.28	108.93	107.11
32	I	303	CLA	CHA-C1A-NA	-2.28	121.17	126.40
32	H	308	CLA	CHA-C1A-NA	-2.28	121.17	126.40
32	L	311	CLA	CHC-C4B-NB	-2.28	121.84	124.26
32	Q	310	CLA	CHC-C4B-NB	-2.28	121.84	124.26
33	W	304	KC2	CHB-C1B-NB	2.28	126.55	124.45
33	S	303	KC2	C4C-C3C-C2C	2.28	108.93	107.11
32	b	830	CLA	C1-O2A-CGA	2.28	122.43	116.44
32	D	307	CLA	CHC-C4B-NB	-2.28	121.84	124.26
32	G	308	CLA	CHC-C4B-NB	-2.28	121.84	124.26
32	I	307	CLA	CHC-C4B-NB	-2.28	121.84	124.26
32	b	802	CLA	CHD-C1D-C2D	2.28	130.26	125.48
32	a	852	CLA	CHB-C4A-NA	2.28	127.66	124.51
33	I	309	KC2	CHB-C4A-NA	2.28	127.80	124.20
33	K	305	KC2	C4C-C3C-C2C	2.28	108.92	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	A	318	LMG	O2-C2-C1	-2.28	104.51	110.05
33	M	307	KC2	C4B-C3B-C2B	2.28	108.62	106.75
32	b	829	CLA	CHC-C4B-NB	-2.28	121.85	124.26
32	B	301	CLA	CHC-C4B-NB	-2.28	121.85	124.26
32	D	315	CLA	CHC-C4B-NB	-2.27	121.85	124.26
32	a	853	CLA	C1-C2-C3	-2.27	122.11	126.04
32	S	311	CLA	CHD-C1D-C2D	2.27	130.25	125.48
32	S	301	CLA	CHC-C4B-NB	-2.27	121.85	124.26
33	K	303	KC2	C4B-C3B-C2B	2.27	108.62	106.75
32	W	307	CLA	C2C-C1C-NC	2.27	112.10	109.97
33	K	309	KC2	CHD-C4C-NC	2.27	127.64	124.20
33	M	307	KC2	CHC-C4B-NB	2.27	126.54	124.45
33	S	312	KC2	CHB-C4A-NA	2.27	127.78	124.20
32	b	807	CLA	CHD-C1D-C2D	2.27	130.24	125.48
41	l	206	BCR	C11-C10-C9	2.27	130.55	127.31
32	N	305	CLA	CHC-C4B-NB	-2.27	121.86	124.26
36	D	321	LMG	O3-C3-C2	-2.27	105.11	110.35
32	b	827	CLA	CHC-C4B-NB	-2.27	121.86	124.26
32	C	304	CLA	CHA-C1A-NA	-2.26	121.21	126.40
34	J	316	DD6	O1-C20-C19	-2.26	111.68	113.38
32	H	304	CLA	CHA-C1A-NA	-2.26	121.21	126.40
40	b	846	DGD	O1G-C1A-O1A	-2.26	117.88	123.59
33	I	309	KC2	C4C-C3C-C2C	2.26	108.91	107.11
32	U	302	CLA	CHC-C4B-NB	-2.26	121.86	124.26
37	F	317	A86	C21-C20-C19	-2.26	111.73	114.28
33	R	311	KC2	CHD-C4C-NC	2.26	127.64	124.20
34	I	313	DD6	C14-C13-C11	2.26	129.04	125.53
32	N	309	CLA	CHD-C1D-C2D	2.26	130.22	125.48
32	I	308	CLA	C3A-C2A-C1A	-2.26	97.95	101.34
33	N	304	KC2	CHB-C1B-NB	2.26	126.53	124.45
32	a	820	CLA	CHC-C4B-NB	-2.26	121.86	124.26
32	a	802	CLA	CHA-C1A-NA	-2.26	121.22	126.40
33	G	302	KC2	CHD-C4C-NC	2.26	127.63	124.20
32	D	310	CLA	CAA-C2A-C1A	-2.26	104.57	111.97
35	M	319	LHG	C11-C10-C9	-2.26	102.96	114.42
36	D	302	LMG	C1-O6-C5	-2.26	109.26	113.69
33	T	311	KC2	CHD-C4C-NC	2.26	127.63	124.20
32	L	311	CLA	CHD-C1D-C2D	2.26	130.21	125.48
32	B	305	CLA	CHC-C4B-NB	-2.26	121.87	124.26
32	H	301	CLA	CHA-C1A-NA	-2.26	121.23	126.40
33	N	303	KC2	CHB-C4A-NA	2.26	127.76	124.20
32	l	202	CLA	CHC-C4B-NB	-2.25	121.87	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	R	305	KC2	C4C-C3C-C2C	2.25	108.91	107.11
32	L	307	CLA	CHA-C1A-NA	-2.25	121.23	126.40
32	a	841	CLA	C1-C2-C3	-2.25	122.14	126.04
32	a	808	CLA	CHC-C4B-NB	-2.25	121.87	124.26
32	f	201	CLA	CHC-C4B-NB	-2.25	121.87	124.26
34	W	317	DD6	O1-C20-C15	-2.25	57.09	58.96
36	D	321	LMG	O7-C10-O9	-2.25	118.26	123.70
32	J	304	CLA	CHC-C4B-NB	-2.25	121.87	124.26
32	C	304	CLA	C3A-C2A-C1A	-2.25	97.97	101.34
36	D	325	LMG	O8-C28-O10	-2.25	117.92	123.59
32	b	832	CLA	O2A-C1-C2	2.25	114.54	108.64
32	a	838	CLA	CHC-C4B-NB	-2.25	121.88	124.26
35	M	319	LHG	C20-C19-C18	-2.25	103.01	114.42
32	b	817	CLA	CBA-CAA-C2A	2.25	120.50	113.86
32	a	818	CLA	C3A-C2A-C1A	-2.25	97.97	101.34
34	D	316	DD6	C21-C20-C19	2.25	116.81	114.28
37	P	316	A86	O4-C34-C33	2.24	113.18	107.59
35	a	850	LHG	O8-C23-O10	-2.24	117.93	123.59
33	L	313	KC2	CHB-C4A-NA	2.24	127.74	124.20
32	G	303	CLA	CHC-C4B-NB	-2.24	121.88	124.26
33	P	306	KC2	CHC-C4B-NB	2.24	126.52	124.45
33	T	303	KC2	CHB-C1B-NB	2.24	126.52	124.45
32	C	301	CLA	C2C-C1C-NC	2.24	112.07	109.97
32	J	307	CLA	CHC-C4B-NB	-2.24	121.88	124.26
33	A	310	KC2	C4C-C3C-C2C	2.24	108.89	107.11
32	a	827	CLA	CHA-C1A-NA	-2.24	121.27	126.40
32	O	306	CLA	CHA-C1A-NA	-2.24	121.27	126.40
32	a	813	CLA	CHC-C4B-NB	-2.24	121.89	124.26
33	M	304	KC2	CHB-C1B-NB	2.24	126.51	124.45
33	K	302	KC2	C4C-C3C-C2C	2.24	108.89	107.11
33	N	303	KC2	CHB-C1B-NB	2.24	126.51	124.45
32	J	312	CLA	CHA-C1A-NA	-2.24	121.28	126.40
32	S	304	CLA	CHA-C1A-NA	-2.24	121.28	126.40
33	R	311	KC2	CHC-C4B-NB	2.23	126.51	124.45
32	a	814	CLA	CHA-C1A-NA	-2.23	121.28	126.40
32	a	811	CLA	CHA-C1A-NA	-2.23	121.28	126.40
32	C	305	CLA	CHA-C1A-NA	-2.23	121.28	126.40
32	A	304	CLA	CBA-CAA-C2A	2.23	120.45	113.86
32	a	830	CLA	C2C-C1C-NC	2.23	112.06	109.97
32	A	304	CLA	CAA-C2A-C3A	2.23	118.89	112.78
33	N	304	KC2	CHC-C4B-NB	2.23	126.50	124.45
32	K	304	CLA	CHC-C4B-NB	-2.23	121.90	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	Q	317	KC2	CHD-C4C-NC	2.23	127.59	124.20
33	N	306	KC2	CHB-C4A-NA	2.23	127.72	124.20
32	b	824	CLA	CHC-C4B-NB	-2.23	121.90	124.26
32	U	307	CLA	CHC-C4B-NB	-2.23	121.90	124.26
32	S	301	CLA	CHA-C1A-NA	-2.23	121.30	126.40
32	b	803	CLA	CHC-C4B-NB	-2.23	121.90	124.26
32	b	804	CLA	CAA-C2A-C1A	-2.23	104.68	111.97
33	R	303	KC2	C4C-C3C-C2C	2.23	108.88	107.11
32	O	304	CLA	CAA-C2A-C1A	-2.23	104.68	111.97
33	G	309	KC2	CHB-C4A-NA	2.23	127.71	124.20
33	N	306	KC2	CHD-C4C-NC	2.22	127.58	124.20
32	M	311	CLA	CHA-C1A-NA	-2.22	121.30	126.40
32	C	301	CLA	CHC-C4B-NB	-2.22	121.90	124.26
33	O	310	KC2	CHB-C4A-NA	2.22	127.71	124.20
33	Q	302	KC2	C4C-C3C-C2C	2.22	108.88	107.11
32	D	310	CLA	CHC-C4B-NB	-2.22	121.91	124.26
32	L	312	CLA	CHC-C4B-NB	-2.22	121.91	124.26
35	P	317	LHG	C20-C19-C18	-2.22	103.15	114.42
33	G	302	KC2	CHB-C4A-NA	2.22	127.70	124.20
33	P	306	KC2	C4C-C3C-C2C	2.22	108.88	107.11
33	L	302	KC2	CHC-C4B-NB	2.22	126.49	124.45
32	J	308	CLA	CHA-C1A-NA	-2.22	121.32	126.40
33	O	302	KC2	C4C-C3C-C2C	2.22	108.88	107.11
33	T	311	KC2	C4C-C3C-C2C	2.22	108.88	107.11
32	b	833	CLA	CHC-C4B-NB	-2.22	121.91	124.26
33	M	313	KC2	C4B-C3B-C2B	2.22	108.57	106.75
33	T	304	KC2	CHC-C4B-NB	2.22	126.49	124.45
32	H	304	CLA	CBA-CAA-C2A	2.22	120.41	113.86
32	a	810	CLA	CHD-C1D-C2D	2.22	130.13	125.48
33	W	305	KC2	CHC-C4B-NB	2.22	126.49	124.45
32	I	308	CLA	CHC-C4B-NB	-2.22	121.91	124.26
32	a	828	CLA	CHA-C1A-NA	-2.21	121.33	126.40
32	L	310	CLA	CHD-C1D-C2D	2.21	130.12	125.48
33	F	302	KC2	CHB-C4A-NA	2.21	127.69	124.20
32	l	204	CLA	CHD-C1D-C2D	2.21	130.12	125.48
33	M	313	KC2	CHC-C4B-NB	2.21	126.49	124.45
33	N	308	KC2	CHD-C4C-NC	2.21	127.56	124.20
33	N	308	KC2	CHC-C4B-NB	2.21	126.49	124.45
33	H	303	KC2	C4C-C3C-C2C	2.21	108.87	107.11
32	O	301	CLA	CHC-C4B-NB	-2.21	121.92	124.26
32	C	308	CLA	CHC-C1C-C2C	-2.21	120.59	126.73
33	K	309	KC2	C3A-C4A-NA	-2.21	108.16	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	314	CLA	CGD-CBD-CAD	-2.21	103.58	110.73
34	A	313	DD6	O1-C20-C15	-2.21	57.13	58.96
32	W	309	CLA	C2C-C1C-NC	2.21	112.04	109.97
32	D	313	CLA	CHC-C4B-NB	-2.21	121.92	124.26
32	S	311	CLA	CBA-CAA-C2A	2.21	120.38	113.86
36	j	104	LMG	C1-O6-C5	2.21	118.02	113.69
32	F	311	CLA	CHD-C1D-C2D	2.21	130.11	125.48
33	O	303	KC2	CHD-C4C-NC	2.21	127.55	124.20
32	U	303	CLA	CHA-C1A-NA	-2.21	121.35	126.40
36	l	201	LMG	C8-O7-C10	-2.21	112.36	117.79
32	b	838	CLA	CHA-C1A-NA	-2.21	121.35	126.40
32	K	308	CLA	CHC-C4B-NB	-2.20	121.92	124.26
37	M	318	A86	C36-C31-C32	2.20	121.88	119.70
33	N	304	KC2	C4B-C3B-C2B	2.20	108.56	106.75
32	D	308	CLA	CHA-C1A-NA	-2.20	121.35	126.40
33	M	302	KC2	CHB-C4A-NA	2.20	127.68	124.20
33	F	302	KC2	CHD-C4C-NC	2.20	127.55	124.20
36	D	321	LMG	O2-C2-C1	-2.20	104.69	110.05
32	G	304	CLA	C1-C2-C3	-2.20	122.23	126.04
32	a	822	CLA	O2A-C1-C2	-2.20	102.85	108.64
32	U	303	CLA	C3A-C2A-C1A	-2.20	98.04	101.34
34	K	315	DD6	O1-C20-C15	-2.20	57.14	58.96
33	W	308	KC2	C3A-C4A-NA	-2.20	108.17	110.57
32	C	307	CLA	CHA-C1A-NA	-2.20	121.36	126.40
32	M	308	CLA	CBA-CAA-C2A	2.20	120.35	113.86
32	Q	310	CLA	CBA-CAA-C2A	2.20	120.35	113.86
32	a	816	CLA	CHD-C1D-C2D	2.20	130.09	125.48
32	D	314	CLA	CHA-C1A-NA	-2.20	121.36	126.40
36	A	318	LMG	O3-C3-C2	-2.20	105.27	110.35
32	W	312	CLA	C1-C2-C3	-2.20	122.24	126.04
32	C	305	CLA	CHD-C1D-C2D	2.20	130.09	125.48
32	H	305	CLA	CHA-C1A-NA	-2.20	121.37	126.40
33	W	308	KC2	C2A-C3A-C4A	2.20	108.11	106.49
32	b	808	CLA	C2C-C1C-NC	2.20	112.03	109.97
32	D	314	CLA	CHD-C1D-C2D	2.20	130.08	125.48
35	P	317	LHG	C11-C10-C9	-2.19	103.28	114.42
33	K	309	KC2	C2A-C3A-C4A	2.19	108.11	106.49
32	r	201	CLA	CHC-C4B-NB	-2.19	121.93	124.26
32	b	816	CLA	CHA-C1A-NA	-2.19	121.37	126.40
33	T	303	KC2	CHC-C4B-NB	2.19	126.47	124.45
32	A	301	CLA	C2C-C1C-NC	2.19	112.03	109.97
32	a	814	CLA	CBA-CAA-C2A	2.19	120.33	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	L	311	CLA	CHA-C1A-NA	-2.19	121.48	126.41
33	K	303	KC2	CHB-C4A-NA	2.19	127.66	124.20
32	V	201	CLA	CHC-C4B-NB	-2.19	121.94	124.26
33	S	302	KC2	C4B-C3B-C2B	2.19	108.55	106.75
32	K	304	CLA	CHD-C1D-C2D	2.19	130.07	125.48
33	N	303	KC2	CHC-C4B-NB	2.19	126.47	124.45
33	S	303	KC2	CHB-C1B-NB	2.19	126.47	124.45
32	N	309	CLA	CHA-C1A-NA	-2.19	121.39	126.40
32	E	312	CLA	CHC-C4B-NB	-2.19	121.94	124.26
36	L	320	LMG	O7-C10-O9	-2.19	118.42	123.70
36	D	303	LMG	O1-C1-C2	2.19	111.72	108.30
36	L	320	LMG	O1-C1-C2	-2.19	104.89	108.30
32	F	304	CLA	CHC-C4B-NB	-2.19	121.94	124.26
32	L	310	CLA	CHC-C4B-NB	-2.19	121.94	124.26
33	W	303	KC2	CHD-C4C-NC	2.19	127.52	124.20
33	I	316	KC2	C4C-C3C-C2C	2.19	108.85	107.11
33	L	306	KC2	CHC-C4B-NB	2.19	126.46	124.45
33	P	312	KC2	CHC-C4B-NB	2.19	126.46	124.45
32	G	307	CLA	CHC-C4B-NB	-2.18	121.94	124.26
32	P	304	CLA	CHC-C4B-NB	-2.18	121.94	124.26
33	Q	302	KC2	CHB-C4A-NA	2.18	127.65	124.20
33	L	305	KC2	CHC-C4B-NB	2.18	126.46	124.45
32	J	304	CLA	CHA-C1A-NA	-2.18	121.40	126.40
37	M	301	A86	C33-C32-C31	2.18	111.33	109.21
32	a	842	CLA	CHC-C4B-NB	-2.18	121.95	124.26
32	a	815	CLA	C1-C2-C3	-2.18	123.22	126.75
32	G	301	CLA	CHC-C4B-NB	-2.18	121.95	124.26
32	A	306	CLA	CHA-C1A-NA	-2.18	121.40	126.40
32	a	819	CLA	CHC-C4B-NB	-2.18	121.95	124.26
33	E	313	KC2	CHC-C4B-NB	2.18	126.46	124.45
32	E	306	CLA	CHD-C1D-C2D	2.18	130.05	125.48
33	P	302	KC2	CHB-C1B-NB	2.18	126.46	124.45
33	W	304	KC2	CHC-C4B-NB	2.18	126.46	124.45
32	a	821	CLA	CHA-C1A-NA	-2.18	121.41	126.40
33	A	310	KC2	CHB-C4A-NA	2.18	127.64	124.20
33	F	310	KC2	C3A-C4A-NA	-2.18	108.19	110.57
32	b	830	CLA	CHA-C1A-NA	-2.18	121.41	126.40
33	T	303	KC2	CHB-C4A-NA	2.18	127.64	124.20
33	W	301	KC2	CHC-C4B-NB	2.18	126.45	124.45
32	I	304	CLA	CHD-C1D-C2D	2.18	130.05	125.48
32	C	306	CLA	CHA-C1A-NA	-2.18	121.41	126.40
33	J	303	KC2	C4C-C3C-C2C	2.18	108.84	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	S	308	CLA	CHA-C1A-NA	-2.18	121.41	126.40
32	r	201	CLA	CHA-C1A-NA	-2.18	121.41	126.40
32	a	827	CLA	CHC-C4B-NB	-2.18	121.95	124.26
33	W	303	KC2	C4B-C3B-C2B	2.17	108.54	106.75
33	L	313	KC2	CHC-C4B-NB	2.17	126.45	124.45
32	a	814	CLA	CAA-C2A-C3A	2.17	118.73	112.78
32	H	307	CLA	CHC-C4B-NB	-2.17	121.96	124.26
33	Q	317	KC2	CHC-C4B-NB	2.17	126.45	124.45
32	K	310	CLA	CHC-C4B-NB	-2.17	121.96	124.26
33	P	302	KC2	CHB-C4A-NA	2.17	127.63	124.20
32	B	304	CLA	CAA-C2A-C1A	-2.17	104.86	111.97
33	F	302	KC2	C4C-C3C-C2C	2.17	108.84	107.11
32	I	305	CLA	CHC-C4B-NB	-2.17	121.96	124.26
32	a	802	CLA	CHB-C4A-NA	2.17	127.51	124.51
32	L	309	CLA	CHA-C1A-NA	-2.17	121.43	126.40
32	D	306	CLA	C2C-C1C-NC	2.17	112.00	109.97
32	b	812	CLA	C2C-C1C-NC	2.17	112.00	109.97
32	W	311	CLA	CBA-CAA-C2A	2.17	120.27	113.86
32	H	302	CLA	CHD-C1D-C2D	2.17	130.03	125.48
33	R	302	KC2	C4B-C3B-C2B	2.17	108.53	106.75
36	L	320	LMG	O3-C3-C2	-2.17	105.33	110.35
33	C	303	KC2	C4C-C3C-C2C	2.17	108.84	107.11
33	S	302	KC2	C4C-C3C-C2C	2.17	108.84	107.11
32	a	830	CLA	CHB-C4A-NA	2.17	127.51	124.51
32	b	835	CLA	CHB-C4A-NA	2.17	127.51	124.51
32	a	837	CLA	C3A-C2A-C1A	-2.17	98.09	101.34
33	K	309	KC2	C4C-C3C-C2C	2.17	108.83	107.11
33	R	311	KC2	C4C-C3C-C2C	2.17	108.83	107.11
32	F	304	CLA	CHD-C1D-C2D	2.17	130.02	125.48
33	K	303	KC2	C4C-C3C-C2C	2.17	108.83	107.11
32	S	307	CLA	CHD-C1D-C2D	2.17	130.02	125.48
38	j	105	LMU	C1-O1'-C1'	-2.16	110.25	113.84
32	a	825	CLA	C2C-C1C-NC	2.16	112.00	109.97
40	b	846	DGD	O3G-C3G-C2G	2.16	116.12	110.90
33	K	303	KC2	CHC-C4B-NB	2.16	126.44	124.45
32	O	304	CLA	CHC-C4B-NB	-2.16	121.97	124.26
32	M	305	CLA	CHA-C1A-NA	-2.16	121.44	126.40
33	P	301	KC2	C4C-C3C-C2C	2.16	108.83	107.11
32	D	312	CLA	CHA-C1A-NA	-2.16	121.44	126.40
33	L	303	KC2	CHB-C4A-NA	2.16	127.61	124.20
32	T	305	CLA	C4D-CHA-C1A	-2.16	118.62	121.25
32	S	308	CLA	C2C-C1C-CHC	-2.16	120.44	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	k	206	SQD	O48-C23-O10	-2.16	118.13	123.59
34	E	318	DD6	C21-C20-C19	2.16	116.71	114.28
32	b	831	CLA	C2C-C1C-NC	2.16	112.00	109.97
33	P	312	KC2	C4C-C3C-C2C	2.16	108.83	107.11
32	T	307	CLA	C1-C2-C3	-2.16	123.25	126.75
33	M	307	KC2	CHB-C4A-NA	2.16	127.61	124.20
32	a	825	CLA	CHC-C4B-NB	-2.16	121.97	124.26
32	a	805	CLA	CHD-C1D-C2D	2.16	130.01	125.48
33	O	302	KC2	CHB-C4A-NA	2.16	127.61	124.20
33	W	304	KC2	CHB-C4A-NA	2.16	127.61	124.20
33	W	314	KC2	CHB-C4A-NA	2.16	127.61	124.20
32	J	306	CLA	CHB-C4A-NA	2.16	127.50	124.51
32	J	308	CLA	CHC-C4B-NB	-2.16	121.97	124.26
33	L	303	KC2	CHC-C4B-NB	2.16	126.44	124.45
32	P	310	CLA	CHC-C4B-NB	-2.16	121.97	124.26
32	b	826	CLA	CHC-C4B-NB	-2.16	121.97	124.26
32	D	310	CLA	CHA-C1A-NA	-2.16	121.45	126.40
32	U	305	CLA	CHA-C1A-NA	-2.16	121.45	126.40
32	k	203	CLA	CHC-C4B-NB	-2.16	121.97	124.26
32	N	305	CLA	CHA-C1A-NA	-2.16	121.46	126.40
32	S	313	CLA	CHC-C4B-NB	-2.16	121.97	124.26
32	b	823	CLA	CHC-C4B-NB	-2.16	121.97	124.26
32	B	305	CLA	CHD-C1D-C2D	2.16	130.00	125.48
32	a	852	CLA	CHA-C1A-NA	-2.16	121.46	126.40
33	O	310	KC2	CHC-C4B-NB	2.16	126.44	124.45
32	L	314	CLA	CHC-C4B-NB	-2.16	121.97	124.26
32	P	310	CLA	CHD-C1D-C2D	2.16	130.00	125.48
33	M	313	KC2	C4C-C3C-C2C	2.15	108.83	107.11
35	I	318	LHG	O8-C23-O10	-2.15	118.15	123.59
32	O	301	CLA	CHA-C1A-NA	-2.15	121.46	126.40
32	J	311	CLA	CHC-C4B-NB	-2.15	121.98	124.26
32	K	308	CLA	CHA-C1A-NA	-2.15	121.47	126.40
32	J	304	CLA	C3A-C2A-C1A	-2.15	98.11	101.34
32	O	308	CLA	CHC-C4B-NB	-2.15	121.98	124.26
33	O	303	KC2	CHC-C4B-NB	2.15	126.43	124.45
32	F	305	CLA	CHD-C1D-C2D	2.15	129.99	125.48
33	S	302	KC2	CHB-C4A-NA	2.15	127.59	124.20
34	N	319	DD6	O1-C20-C19	-2.15	111.77	113.38
32	P	311	CLA	CHA-C1A-NA	-2.15	121.47	126.40
32	M	305	CLA	C2C-C1C-NC	2.15	111.99	109.97
32	a	822	CLA	CHC-C4B-NB	-2.15	121.98	124.26
37	J	313	A86	C33-C32-C31	2.15	111.30	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	S	307	CLA	CAA-C2A-C1A	-2.15	104.93	111.97
37	M	318	A86	C21-C20-C19	-2.15	111.86	114.28
32	H	310	CLA	CHC-C4B-NB	-2.15	121.98	124.26
32	W	310	CLA	CGD-CBD-CAD	-2.15	103.77	110.73
35	F	318	LHG	O8-C23-C24	2.15	118.65	111.91
32	b	811	CLA	C2C-C1C-NC	2.15	111.98	109.97
33	O	310	KC2	CHD-C4C-NC	2.15	127.46	124.20
32	a	804	CLA	CBA-CAA-C2A	2.15	120.20	113.86
32	a	822	CLA	C2C-C1C-NC	2.15	111.98	109.97
32	C	308	CLA	CHD-C1D-C2D	2.15	129.98	125.48
33	N	314	KC2	CHC-C4B-NB	2.14	126.42	124.45
33	W	303	KC2	CHB-C4A-NA	2.14	127.58	124.20
32	b	819	CLA	C2C-C1C-NC	2.14	111.98	109.97
32	T	302	CLA	CHC-C4B-NB	-2.14	121.99	124.26
32	b	818	CLA	CHC-C4B-NB	-2.14	121.99	124.26
32	l	203	CLA	CHA-C1A-NA	-2.14	121.49	126.40
32	B	304	CLA	CHD-C1D-C2D	2.14	129.97	125.48
32	I	304	CLA	CHA-C1A-NA	-2.14	121.49	126.40
32	L	304	CLA	CHC-C4B-NB	-2.14	121.99	124.26
33	O	303	KC2	CHB-C4A-NA	2.14	127.58	124.20
32	b	835	CLA	CHD-C1D-C2D	2.14	129.97	125.48
33	E	313	KC2	CHB-C4A-NA	2.14	127.58	124.20
33	W	301	KC2	CHB-C4A-NA	2.14	127.58	124.20
33	S	303	KC2	C4B-C3B-C2B	2.14	108.51	106.75
33	S	303	KC2	CHC-C4B-NB	2.14	126.42	124.45
32	a	839	CLA	CHA-C1A-NA	-2.14	121.50	126.40
32	a	837	CLA	CHD-C1D-C2D	2.14	129.97	125.48
33	S	303	KC2	CHB-C4A-NA	2.14	127.58	124.20
32	a	801	CLA	C2A-C1A-CHA	2.14	127.60	123.86
33	T	311	KC2	C4B-C3B-C2B	2.14	108.51	106.75
32	N	311	CLA	CHC-C4B-NB	-2.14	121.99	124.26
33	I	316	KC2	CHC-C4B-NB	2.14	126.42	124.45
32	b	820	CLA	C2C-C1C-NC	2.14	111.97	109.97
32	T	308	CLA	CHA-C1A-NA	-2.14	121.50	126.40
33	N	303	KC2	CHD-C4C-NC	2.14	127.44	124.20
32	K	306	CLA	CHC-C4B-NB	-2.14	122.00	124.26
33	L	306	KC2	CHB-C4A-NA	2.14	127.57	124.20
36	T	301	LMG	O7-C10-O9	-2.14	118.54	123.70
33	T	311	KC2	CHC-C4B-NB	2.13	126.42	124.45
33	W	314	KC2	CHD-C4C-NC	2.13	127.44	124.20
32	P	304	CLA	CHB-C4A-NA	2.13	127.46	124.51
32	a	807	CLA	C3A-C2A-C1A	-2.13	98.14	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	J	304	CLA	CHD-C1D-C2D	2.13	129.96	125.48
32	a	801	CLA	C3D-C4D-ND	2.13	113.69	110.24
33	F	310	KC2	CHC-C4B-NB	2.13	126.42	124.45
32	F	307	CLA	CHC-C4B-NB	-2.13	122.00	124.26
33	F	310	KC2	C2A-C3A-C4A	2.13	108.07	106.49
32	S	308	CLA	CHD-C1D-C2D	2.13	129.96	125.48
32	b	837	CLA	CHD-C1D-C2D	2.13	129.96	125.48
32	M	312	CLA	CHC-C4B-NB	-2.13	122.00	124.26
32	R	309	CLA	CHC-C4B-NB	-2.13	122.00	124.26
33	E	313	KC2	C4C-C3C-C2C	2.13	108.81	107.11
32	U	302	CLA	CMC-C2C-C1C	2.13	128.29	125.04
32	E	311	CLA	CHC-C4B-NB	-2.13	122.00	124.26
33	J	310	KC2	CHB-C4A-NA	2.13	127.56	124.20
32	r	201	CLA	CAA-C2A-C3A	2.13	118.61	112.78
32	R	309	CLA	CHD-C1D-C2D	2.13	129.95	125.48
33	A	310	KC2	CHC-C4B-NB	2.13	126.41	124.45
33	G	309	KC2	CHC-C4B-NB	2.13	126.41	124.45
32	T	310	CLA	CHD-C1D-C2D	2.13	129.95	125.48
32	R	301	CLA	CHC-C4B-NB	-2.13	122.00	124.26
32	R	307	CLA	CHC-C4B-NB	-2.13	122.00	124.26
32	Q	306	CLA	C1-C2-C3	2.13	129.72	126.04
32	P	311	CLA	CHC-C4B-NB	-2.13	122.00	124.26
32	S	310	CLA	CHC-C4B-NB	-2.13	122.00	124.26
32	C	304	CLA	CHD-C1D-C2D	2.13	129.94	125.48
38	I	315	LMU	O5'-C1'-C2'	2.13	114.85	110.35
32	G	306	CLA	CHD-C1D-C2D	2.13	129.94	125.48
32	C	309	CLA	CHC-C4B-NB	-2.13	122.01	124.26
32	F	308	CLA	CHC-C4B-NB	-2.13	122.01	124.26
34	D	317	DD6	O1-C20-C15	-2.13	57.20	58.96
32	a	840	CLA	CHC-C4B-NB	-2.12	122.01	124.26
33	N	302	KC2	CHB-C4A-NA	2.12	127.55	124.20
32	a	809	CLA	CHD-C1D-C2D	2.12	129.93	125.48
32	a	820	CLA	CHD-C1D-C2D	2.12	129.93	125.48
38	V	205	LMU	O5'-C5'-C6'	2.12	111.71	106.44
32	O	306	CLA	CHC-C4B-NB	-2.12	122.01	124.26
33	T	303	KC2	C4C-C3C-C2C	2.12	108.80	107.11
32	a	812	CLA	CGD-CBD-CAD	-2.12	103.86	110.73
32	F	301	CLA	CHD-C1D-C2D	2.12	129.93	125.48
32	a	818	CLA	CHC-C4B-NB	-2.12	122.01	124.26
32	Q	308	CLA	CHA-C1A-NA	-2.12	121.55	126.40
32	U	306	CLA	CHA-C1A-NA	-2.12	121.55	126.40
33	T	304	KC2	CHD-C4C-NC	2.12	127.42	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	307	CLA	CHD-C1D-C2D	2.12	129.92	125.48
32	O	308	CLA	CHD-C1D-C2D	2.12	129.92	125.48
32	G	305	CLA	CHA-C1A-NA	-2.12	121.55	126.40
32	A	307	CLA	CHA-C1A-NA	-2.12	121.55	126.40
32	M	308	CLA	CHD-C1D-C2D	2.12	129.92	125.48
32	b	839	CLA	CHC-C4B-NB	-2.12	122.02	124.26
32	D	310	CLA	CHD-C1D-C2D	2.12	129.92	125.48
33	O	303	KC2	C4B-C3B-C2B	2.12	108.49	106.75
32	E	309	CLA	CHA-C1A-NA	-2.12	121.55	126.40
32	M	305	CLA	CHB-C4A-NA	2.12	127.44	124.51
32	a	841	CLA	CHB-C4A-NA	2.11	127.44	124.51
33	L	303	KC2	CHD-C4C-NC	2.11	127.41	124.20
32	F	308	CLA	CHD-C1D-C2D	2.11	129.91	125.48
33	N	302	KC2	C4B-C3B-C2B	2.11	108.49	106.75
32	a	839	CLA	CHD-C1D-C2D	2.11	129.91	125.48
33	O	310	KC2	C4C-C3C-C2C	2.11	108.79	107.11
32	Q	304	CLA	CHC-C4B-NB	-2.11	122.02	124.26
34	F	314	DD6	C14-C13-C11	2.11	128.81	125.53
32	M	308	CLA	C2C-C1C-NC	2.11	111.95	109.97
32	C	307	CLA	CBA-CAA-C2A	2.11	120.10	113.86
33	W	308	KC2	CHC-C4B-NB	2.11	126.39	124.45
32	N	305	CLA	CHD-C1D-C2D	2.11	129.91	125.48
32	N	310	CLA	CHD-C1D-C2D	2.11	129.91	125.48
33	P	301	KC2	CHB-C4A-NA	2.11	127.53	124.20
32	A	303	CLA	C2C-C1C-NC	2.11	111.95	109.97
32	E	311	CLA	CHA-C1A-NA	-2.11	121.56	126.40
32	a	823	CLA	CHA-C1A-NA	-2.11	121.56	126.40
32	a	828	CLA	CAA-C2A-C3A	2.11	118.56	112.78
36	D	303	LMG	C12-C11-C10	-2.11	105.95	113.62
32	F	301	CLA	CHC-C4B-NB	-2.11	122.02	124.26
32	F	306	CLA	CHC-C4B-NB	-2.11	122.02	124.26
32	Q	308	CLA	CHC-C4B-NB	-2.11	122.02	124.26
32	l	204	CLA	CHA-C1A-NA	-2.11	121.57	126.40
33	H	303	KC2	C4B-C3B-C2B	2.11	108.48	106.75
32	Q	310	CLA	CHD-C1D-C2D	2.11	129.90	125.48
32	F	311	CLA	CHC-C4B-NB	-2.11	122.03	124.26
32	G	301	CLA	CHD-C1D-C2D	2.11	129.90	125.48
32	b	838	CLA	CHD-C1D-C2D	2.11	129.90	125.48
32	k	203	CLA	CHA-C1A-NA	-2.11	121.57	126.40
32	D	313	CLA	CHD-C1D-C2D	2.11	129.90	125.48
33	K	309	KC2	CHC-C4B-NB	2.11	126.39	124.45
33	W	314	KC2	CHC-C4B-NB	2.11	126.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	305	CLA	CHC-C4B-NB	-2.11	122.03	124.26
32	K	310	CLA	CHD-C1D-C2D	2.11	129.90	125.48
32	P	304	CLA	CHD-C1D-C2D	2.11	129.90	125.48
33	N	304	KC2	CHB-C4A-NA	2.11	127.52	124.20
33	N	306	KC2	CHC-C4B-NB	2.11	126.39	124.45
34	G	312	DD6	C21-C20-C19	2.10	116.65	114.28
37	M	301	A86	O1-C20-C19	2.10	114.96	113.38
32	L	301	CLA	CHC-C4B-NB	-2.10	122.03	124.26
32	b	818	CLA	CHD-C1D-C2D	2.10	129.89	125.48
32	J	312	CLA	CBA-CAA-C2A	2.10	120.08	113.86
32	K	307	CLA	CHA-C1A-NA	-2.10	121.58	126.40
32	b	809	CLA	CHA-C1A-NA	-2.10	121.58	126.40
33	R	302	KC2	CHD-C4C-NC	2.10	127.39	124.20
32	b	810	CLA	CHA-C1A-NA	-2.10	121.58	126.40
32	T	305	CLA	CHA-C1A-NA	-2.10	121.58	126.40
32	I	306	CLA	CHD-C1D-C2D	2.10	129.89	125.48
32	I	302	CLA	CHC-C4B-NB	-2.10	122.03	124.26
32	F	303	CLA	CHA-C1A-NA	-2.10	121.58	126.40
37	L	315	A86	O4-C34-C33	2.10	112.83	107.59
34	Q	314	DD6	O1-C20-C19	-2.10	111.80	113.38
33	P	301	KC2	CHC-C4B-NB	2.10	126.39	124.45
33	P	302	KC2	C4C-C3C-C2C	2.10	108.78	107.11
32	K	301	CLA	CHC-C4B-NB	-2.10	122.03	124.26
33	P	306	KC2	CHB-C4A-NA	2.10	127.51	124.20
32	D	315	CLA	CHD-C1D-C2D	2.10	129.88	125.48
32	S	301	CLA	CHD-C1D-C2D	2.10	129.88	125.48
32	a	802	CLA	CHD-C1D-C2D	2.10	129.88	125.48
32	a	852	CLA	CHD-C1D-C2D	2.10	129.88	125.48
32	b	827	CLA	CHD-C1D-C2D	2.10	129.88	125.48
32	H	306	CLA	CHC-C4B-NB	-2.10	122.03	124.26
32	a	829	CLA	CHC-C4B-NB	-2.10	122.03	124.26
32	a	818	CLA	O2A-C1-C2	2.10	114.15	108.64
33	M	321	KC2	C4C-C3C-C2C	2.10	108.78	107.11
32	R	301	CLA	CHA-C1A-NA	-2.10	121.59	126.40
32	W	310	CLA	CHC-C4B-NB	-2.10	122.04	124.26
33	R	303	KC2	C4B-C3B-C2B	2.10	108.47	106.75
32	O	307	CLA	CHD-C1D-C2D	2.10	129.88	125.48
32	a	839	CLA	C1-C2-C3	-2.10	122.42	126.04
32	a	840	CLA	CHD-C1D-C2D	2.10	129.88	125.48
32	a	807	CLA	CHD-C1D-C2D	2.10	129.88	125.48
32	a	805	CLA	CBA-CAA-C2A	2.10	120.05	113.86
32	F	303	CLA	C2C-C1C-NC	2.10	111.94	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Q	304	CLA	CHD-C1D-C2D	2.10	129.88	125.48
32	a	828	CLA	C1-C2-C3	2.10	129.67	126.04
32	A	311	CLA	CHD-C1D-C2D	2.10	129.88	125.48
32	J	301	CLA	CHC-C4B-NB	-2.10	122.04	124.26
32	E	314	CLA	CHD-C1D-C2D	2.09	129.87	125.48
32	M	309	CLA	CHD-C1D-C2D	2.09	129.87	125.48
32	I	302	CLA	C2C-C1C-NC	2.09	111.93	109.97
32	T	310	CLA	CHC-C4B-NB	-2.09	122.04	124.26
32	D	306	CLA	CHD-C1D-C2D	2.09	129.87	125.48
32	a	823	CLA	C2C-C1C-NC	2.09	111.93	109.97
32	T	302	CLA	CHD-C1D-C2D	2.09	129.87	125.48
32	R	304	CLA	CHB-C4A-NA	2.09	127.41	124.51
33	N	302	KC2	CHC-C4B-NB	2.09	126.38	124.45
37	T	312	A86	C36-C31-C32	-2.09	117.62	119.70
32	a	836	CLA	CHA-C1A-NA	-2.09	121.61	126.40
32	H	308	CLA	C2A-C1A-CHA	2.09	127.50	123.85
32	b	826	CLA	CHD-C1D-C2D	2.09	129.87	125.48
33	R	302	KC2	CHB-C1B-NB	2.09	126.38	124.45
33	W	308	KC2	C4C-C3C-C2C	2.09	108.78	107.11
32	l	204	CLA	CHB-C4A-NA	2.09	127.40	124.51
32	T	306	CLA	CHC-C4B-NB	-2.09	122.04	124.26
33	O	302	KC2	CHC-C4B-NB	2.09	126.38	124.45
32	U	307	CLA	CHA-C1A-NA	-2.09	121.61	126.40
32	Q	304	CLA	CBA-CAA-C2A	2.09	120.03	113.86
32	Q	306	CLA	CBA-CAA-C2A	2.09	120.03	113.86
32	k	203	CLA	CHD-C1D-C2D	2.09	129.86	125.48
32	b	836	CLA	CHA-C1A-NA	-2.09	121.61	126.40
32	a	805	CLA	C1D-CHD-C4C	-2.09	121.55	126.06
32	E	305	CLA	C2C-C1C-NC	2.09	111.93	109.97
32	a	803	CLA	C2C-C1C-NC	2.09	111.93	109.97
32	R	306	CLA	CHD-C1D-C2D	2.09	129.86	125.48
32	a	812	CLA	CHA-C1A-NA	-2.09	121.62	126.40
32	A	309	CLA	CHC-C4B-NB	-2.09	122.05	124.26
35	E	321	LHG	O8-C23-O10	-2.09	118.32	123.59
32	H	307	CLA	O2A-C1-C2	2.09	114.12	108.64
32	b	822	CLA	CHD-C1D-C2D	2.09	129.86	125.48
36	M	320	LMG	O7-C10-O9	-2.09	118.66	123.70
32	M	305	CLA	CHC-C1C-C2C	-2.09	120.93	126.73
32	G	307	CLA	CHD-C1D-C2D	2.09	129.86	125.48
32	C	306	CLA	CHD-C1D-C2D	2.09	129.85	125.48
32	C	307	CLA	CHD-C1D-C2D	2.09	129.85	125.48
32	J	308	CLA	CHD-C1D-C2D	2.09	129.85	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	I	305	CLA	CHD-C1D-C2D	2.08	129.85	125.48
33	I	309	KC2	CHC-C4B-NB	2.08	126.37	124.45
33	R	311	KC2	CHB-C4A-NA	2.08	127.49	124.20
32	b	818	CLA	CHA-C1A-NA	-2.08	121.62	126.40
32	L	304	CLA	CHD-C1D-C2D	2.08	129.85	125.48
32	a	814	CLA	CHD-C1D-C2D	2.08	129.85	125.48
32	b	813	CLA	CHC-C4B-NB	-2.08	122.05	124.26
32	O	301	CLA	CHD-C1D-C2D	2.08	129.85	125.48
32	a	818	CLA	CHD-C1D-C2D	2.08	129.85	125.48
37	D	323	A86	C36-C31-C32	-2.08	117.63	119.70
33	K	302	KC2	CHB-C4A-NA	2.08	127.48	124.20
32	A	308	CLA	C2C-C1C-NC	2.08	111.92	109.97
34	k	205	DD6	C23-C16-C15	2.08	115.66	110.05
33	W	304	KC2	C4C-C3C-C2C	2.08	108.77	107.11
32	b	808	CLA	CHA-C1A-NA	-2.08	121.63	126.40
34	B	307	DD6	C32-C31-C36	2.08	125.57	122.63
34	Q	315	DD6	O1-C20-C15	-2.08	57.24	58.96
35	W	319	LHG	C27-C26-C25	-2.08	103.86	114.42
32	M	311	CLA	CHC-C4B-NB	-2.08	122.06	124.26
32	W	311	CLA	CHC-C4B-NB	-2.08	122.06	124.26
33	J	310	KC2	C4B-C3B-C2B	2.08	108.46	106.75
32	b	830	CLA	C3A-C2A-C1A	-2.08	98.22	101.34
36	T	301	LMG	C7-O1-C1	2.08	117.80	113.74
32	C	308	CLA	CHA-C1A-NA	-2.08	121.64	126.40
32	B	302	CLA	CHB-C4A-NA	2.08	127.39	124.51
32	D	306	CLA	CHC-C1C-C2C	-2.08	120.96	126.73
40	Q	318	DGD	C3E-C4E-C5E	2.08	113.94	110.24
32	R	310	CLA	CHD-C1D-C2D	2.08	129.84	125.48
32	U	303	CLA	CHD-C1D-C2D	2.08	129.84	125.48
32	b	825	CLA	CHC-C4B-NB	-2.08	122.06	124.26
32	b	828	CLA	CHC-C4B-NB	-2.08	122.06	124.26
32	G	307	CLA	CHA-C1A-NA	-2.08	121.74	126.41
32	b	816	CLA	CAC-C3C-C4C	2.08	127.50	124.81
32	b	804	CLA	CHD-C1D-C2D	2.08	129.83	125.48
34	B	307	DD6	O1-C20-C15	-2.08	57.24	58.96
32	D	306	CLA	CHB-C4A-NA	2.08	127.38	124.51
32	F	322	CLA	CHC-C4B-NB	-2.08	122.06	124.26
33	R	302	KC2	CHC-C4B-NB	2.08	126.36	124.45
32	N	311	CLA	CBA-CAA-C2A	2.07	119.99	113.86
32	B	306	CLA	CHA-C1A-NA	-2.07	121.65	126.40
32	b	806	CLA	CHD-C1D-C2D	2.07	129.83	125.48
33	O	302	KC2	C4B-C3B-C2B	2.07	108.46	106.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	F	306	CLA	CHB-C4A-NA	2.07	127.38	124.51
32	a	835	CLA	CHB-C4A-NA	2.07	127.38	124.51
32	J	305	CLA	CHA-C1A-NA	-2.07	121.65	126.40
32	W	306	CLA	CHD-C1D-C2D	2.07	129.83	125.48
33	N	306	KC2	C4C-C3C-C2C	2.07	108.76	107.11
32	E	315	CLA	CHC-C4B-NB	-2.07	122.06	124.26
32	a	837	CLA	CHA-C1A-NA	-2.07	121.65	126.40
32	P	311	CLA	O2A-C1-C2	-2.07	103.19	108.64
32	b	829	CLA	CHA-C1A-NA	-2.07	121.65	126.40
34	N	319	DD6	O1-C20-C15	-2.07	57.24	58.96
32	A	304	CLA	CHC-C4B-NB	-2.07	122.06	124.26
33	N	308	KC2	C4B-C3B-C2B	2.07	108.45	106.75
32	E	307	CLA	CHD-C1D-C2D	2.07	129.83	125.48
32	J	301	CLA	CHD-C1D-C2D	2.07	129.83	125.48
33	T	311	KC2	CHB-C4A-NA	2.07	127.47	124.20
37	S	316	A86	O4-C34-C33	-2.07	102.44	107.59
32	L	312	CLA	CHD-C1D-C2D	2.07	129.82	125.48
32	a	808	CLA	CHD-C1D-C2D	2.07	129.82	125.48
33	P	303	KC2	CHB-C4A-NA	2.07	127.47	124.20
32	K	306	CLA	CHD-C1D-C2D	2.07	129.82	125.48
32	W	309	CLA	CHD-C1D-C2D	2.07	129.82	125.48
32	B	302	CLA	CHD-C1D-C2D	2.07	129.82	125.48
33	P	301	KC2	C4B-C3B-C2B	2.07	108.45	106.75
32	b	822	CLA	CHC-C4B-NB	-2.07	122.07	124.26
33	W	303	KC2	CHC-C4B-NB	2.07	126.36	124.45
32	b	805	CLA	CHD-C1D-C2D	2.07	129.82	125.48
33	L	306	KC2	C4C-C3C-C2C	2.07	108.76	107.11
33	N	307	KC2	C4C-C3C-C2C	2.07	108.76	107.11
32	B	309	CLA	CHA-C1A-NA	-2.07	121.66	126.40
32	b	826	CLA	CHA-C1A-NA	-2.07	121.66	126.40
33	N	307	KC2	CHB-C4A-NA	2.07	127.46	124.20
32	A	303	CLA	CHB-C4A-NA	2.07	127.37	124.51
32	L	307	CLA	CHD-C1D-C2D	2.07	129.82	125.48
32	M	311	CLA	CHD-C1D-C2D	2.07	129.81	125.48
32	D	311	CLA	CHC-C4B-NB	-2.07	122.07	124.26
32	H	301	CLA	CHD-C1D-C2D	2.07	129.81	125.48
35	B	308	LHG	O8-C23-O10	-2.07	118.38	123.59
33	R	303	KC2	CHB-C4A-NA	2.07	127.46	124.20
32	b	834	CLA	CHD-C1D-C2D	2.07	129.81	125.48
34	U	309	DD6	O1-C20-C15	-2.07	57.25	58.96
32	N	312	CLA	CAA-C2A-C1A	-2.07	106.71	111.81
32	A	305	CLA	CHD-C1D-C2D	2.06	129.81	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	I	310	DD6	O1-C20-C15	-2.06	57.25	58.96
36	j	104	LMG	O8-C28-O10	-2.06	118.38	123.59
32	b	804	CLA	CHA-C1A-NA	-2.06	121.67	126.40
32	I	307	CLA	CHD-C1D-C2D	2.06	129.81	125.48
32	Q	304	CLA	CHB-C4A-NA	2.06	127.36	124.51
32	b	817	CLA	C2C-C1C-NC	2.06	111.90	109.97
32	G	304	CLA	CHC-C4B-NB	-2.06	122.07	124.26
32	I	317	CLA	CHD-C1D-C2D	2.06	129.81	125.48
37	O	312	A86	C33-C32-C31	2.06	111.22	109.21
33	P	312	KC2	CHB-C4A-NA	2.06	127.45	124.20
36	A	317	LMG	O7-C8-C7	2.06	115.86	108.40
32	S	310	CLA	CHD-C1D-C2D	2.06	129.80	125.48
32	N	309	CLA	C1-C2-C3	-2.06	123.42	126.75
33	R	303	KC2	CHC-C4B-NB	2.06	126.35	124.45
32	R	301	CLA	CHD-C1D-C2D	2.06	129.80	125.48
33	W	303	KC2	C4C-C3C-C2C	2.06	108.75	107.11
32	a	817	CLA	C2C-C1C-NC	2.06	111.90	109.97
32	a	853	CLA	CHB-C4A-NA	2.06	127.36	124.51
32	G	303	CLA	CHD-C1D-C2D	2.06	129.80	125.48
32	a	806	CLA	CHD-C1D-C2D	2.06	129.80	125.48
32	C	302	CLA	CHA-C1A-NA	-2.06	121.68	126.40
32	k	201	CLA	CHC-C4B-NB	-2.06	122.08	124.26
32	O	305	CLA	CHD-C1D-C2D	2.06	129.80	125.48
32	b	828	CLA	CHD-C1D-C2D	2.06	129.80	125.48
34	O	313	DD6	C33-C34-C35	2.06	113.12	110.30
32	L	304	CLA	CHB-C4A-NA	2.06	127.36	124.51
32	N	313	CLA	CHC-C4B-NB	-2.06	122.08	124.26
32	a	813	CLA	CHA-C1A-NA	-2.06	121.69	126.40
33	T	311	KC2	C2A-C3A-C4A	2.06	108.01	106.49
33	M	313	KC2	CHB-C4A-NA	2.06	127.44	124.20
34	E	318	DD6	O1-C20-C19	-2.06	111.84	113.38
32	G	304	CLA	CHD-C1D-C2D	2.06	129.79	125.48
32	R	307	CLA	CHD-C1D-C2D	2.06	129.79	125.48
32	L	308	CLA	CHD-C1D-C2D	2.06	129.79	125.48
36	N	301	LMG	O7-C10-O9	-2.06	118.73	123.70
32	F	306	CLA	CHD-C1D-C2D	2.05	129.79	125.48
32	R	304	CLA	CHC-C4B-NB	-2.05	122.08	124.26
32	U	302	CLA	CHD-C1D-C2D	2.05	129.79	125.48
32	b	826	CLA	CHB-C4A-NA	2.05	127.35	124.51
32	a	806	CLA	CAA-C2A-C1A	-2.05	105.25	111.97
34	D	301	DD6	C32-C31-C36	2.05	125.53	122.63
32	D	309	CLA	CHC-C4B-NB	-2.05	122.08	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	J	309	CLA	CHA-C1A-NA	-2.05	121.69	126.40
32	b	820	CLA	CHD-C1D-C2D	2.05	129.79	125.48
33	K	309	KC2	C4B-C3B-C2B	2.05	108.44	106.75
32	P	308	CLA	CHA-C1A-NA	-2.05	121.70	126.40
32	a	803	CLA	CHC-C4B-NB	-2.05	122.08	124.26
32	Q	305	CLA	CHD-C1D-C2D	2.05	129.78	125.48
32	K	306	CLA	CBA-CAA-C2A	2.05	119.92	113.86
35	a	851	LHG	O7-C7-O9	-2.05	118.74	123.70
33	L	302	KC2	CHB-C4A-NA	2.05	127.44	124.20
32	B	305	CLA	CHA-C1A-NA	-2.05	121.70	126.40
32	G	308	CLA	CHD-C1D-C2D	2.05	129.78	125.48
32	J	311	CLA	CHD-C1D-C2D	2.05	129.78	125.48
32	W	310	CLA	CHD-C1D-C2D	2.05	129.78	125.48
36	l	201	LMG	O8-C28-O10	-2.05	118.42	123.59
32	V	204	CLA	CHC-C4B-NB	-2.05	122.09	124.26
32	B	301	CLA	CHD-C1D-C2D	2.05	129.78	125.48
32	P	307	CLA	CHD-C1D-C2D	2.05	129.78	125.48
32	W	306	CLA	CHC-C4B-NB	-2.05	122.09	124.26
32	H	309	CLA	CHD-C1D-C2D	2.05	129.78	125.48
33	N	308	KC2	CHB-C4A-NA	2.05	127.43	124.20
32	C	301	CLA	CHC-C1C-C2C	-2.05	121.04	126.73
32	M	306	CLA	CHD-C1D-C2D	2.05	129.78	125.48
32	r	201	CLA	CAA-C2A-C1A	-2.05	105.26	111.97
32	a	813	CLA	CHD-C1D-C2D	2.05	129.78	125.48
32	E	308	CLA	C2C-C1C-NC	2.05	111.89	109.97
32	b	833	CLA	CHD-C1D-C2D	2.05	129.77	125.48
39	H	315	SQD	O47-C7-O49	-2.05	118.76	123.70
32	b	835	CLA	CHA-C1A-NA	-2.05	121.71	126.40
34	P	315	DD6	O1-C20-C15	-2.05	57.27	58.96
32	A	307	CLA	CHD-C1D-C2D	2.05	129.77	125.48
32	D	308	CLA	CHD-C1D-C2D	2.05	129.77	125.48
36	L	320	LMG	O2-C2-C1	-2.05	105.08	110.05
32	U	307	CLA	CHD-C1D-C2D	2.04	129.77	125.48
33	C	303	KC2	CHB-C4A-NA	2.04	127.43	124.20
34	H	313	DD6	C21-C20-C19	2.04	116.58	114.28
32	O	306	CLA	CHD-C1D-C2D	2.04	129.77	125.48
32	L	311	CLA	C2A-C1A-CHA	2.04	125.88	122.71
32	a	810	CLA	CBA-CAA-C2A	2.04	119.90	113.86
37	U	308	A86	C36-C31-C32	-2.04	117.67	119.70
33	M	304	KC2	CHB-C4A-NA	2.04	127.42	124.20
32	l	203	CLA	C2C-C1C-NC	2.04	111.89	109.97
32	U	301	CLA	CHD-C1D-C2D	2.04	129.76	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	J	317	DD6	O1-C20-C15	-2.04	57.27	58.96
32	a	811	CLA	CHC-C1C-C2C	-2.04	121.06	126.73
32	b	813	CLA	CHD-C1D-C2D	2.04	129.76	125.48
33	W	301	KC2	C4B-C3B-C2B	2.04	108.43	106.75
32	T	308	CLA	CBA-CAA-C2A	2.04	119.89	113.86
32	O	304	CLA	CHA-C1A-NA	-2.04	121.72	126.40
33	S	306	KC2	CHC-C4B-NB	2.04	126.33	124.45
32	a	853	CLA	CHA-C1A-NA	-2.04	121.72	126.40
32	O	307	CLA	CAA-C2A-C1A	-2.04	105.29	111.97
32	D	309	CLA	CHD-C1D-C2D	2.04	129.76	125.48
32	M	306	CLA	C2C-C1C-NC	2.04	111.88	109.97
32	I	307	CLA	CHA-C1A-NA	-2.04	121.72	126.40
32	B	301	CLA	CHA-C1A-NA	-2.04	121.82	126.41
33	M	302	KC2	C4B-C3B-C2B	2.04	108.43	106.75
32	T	302	CLA	CHA-C1A-NA	-2.04	121.72	126.40
32	E	304	CLA	CHD-C1D-C2D	2.04	129.76	125.48
32	N	313	CLA	CHD-C1D-C2D	2.04	129.76	125.48
33	N	302	KC2	C4C-C3C-C2C	2.04	108.73	107.11
32	V	201	CLA	CHD-C1D-C2D	2.04	129.76	125.48
40	b	846	DGD	O1B-C1B-C2B	-2.04	115.78	123.73
33	L	302	KC2	CHB-C1B-NB	2.04	126.33	124.45
33	R	302	KC2	C4C-C3C-C2C	2.04	108.73	107.11
32	l	204	CLA	C4D-CHA-C1A	-2.04	118.77	121.25
32	E	309	CLA	CHC-C4B-NB	-2.04	122.10	124.26
33	S	306	KC2	C4B-C3B-C2B	2.04	108.42	106.75
32	a	801	CLA	CHC-C4B-NB	-2.04	122.10	124.26
32	V	203	CLA	CHA-C1A-NA	-2.04	121.73	126.40
32	A	301	CLA	CHB-C4A-NA	2.04	127.33	124.51
32	T	309	CLA	CHD-C1D-C2D	2.04	129.75	125.48
34	H	312	DD6	O1-C20-C15	-2.04	57.27	58.96
32	a	853	CLA	CHC-C4B-NB	-2.04	122.10	124.26
32	K	307	CLA	C2C-C1C-NC	2.04	111.88	109.97
40	Q	318	DGD	O2G-C1B-O1B	-2.04	118.78	123.70
32	b	830	CLA	CHD-C1D-C2D	2.03	129.75	125.48
32	D	307	CLA	CHA-C1A-NA	-2.03	121.74	126.40
32	b	822	CLA	CAA-C2A-C3A	2.03	118.35	112.78
32	M	308	CLA	CHC-C1C-C2C	-2.03	121.08	126.73
32	C	308	CLA	C2C-C1C-NC	2.03	111.88	109.97
33	N	314	KC2	CHD-C4C-NC	2.03	127.29	124.20
33	P	312	KC2	C4B-C3B-C2B	2.03	108.42	106.75
32	I	303	CLA	C3A-C2A-C1A	-2.03	98.29	101.34
32	b	807	CLA	C2A-C3A-C4A	-2.03	98.59	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	L	309	CLA	CHD-C1D-C2D	2.03	129.74	125.48
32	T	308	CLA	CHC-C4B-NB	-2.03	122.11	124.26
32	F	322	CLA	CHD-C1D-C2D	2.03	129.74	125.48
33	N	314	KC2	CHB-C4A-NA	2.03	127.41	124.20
32	P	311	CLA	CHD-C1D-C2D	2.03	129.74	125.48
32	J	302	CLA	CHC-C4B-NB	-2.03	122.11	124.26
32	T	307	CLA	CHC-C4B-NB	-2.03	122.11	124.26
32	b	801	CLA	CHA-C1A-NA	-2.03	121.75	126.40
32	U	302	CLA	CHA-C1A-NA	-2.03	121.75	126.40
32	S	313	CLA	CHD-C1D-C2D	2.03	129.74	125.48
34	K	313	DD6	C32-C31-C36	2.03	125.50	122.63
33	F	302	KC2	C4B-C3B-C2B	2.03	108.42	106.75
36	A	317	LMG	C1-O6-C5	-2.03	109.70	113.69
32	U	305	CLA	CHD-C1D-C2D	2.03	129.74	125.48
32	M	305	CLA	CHD-C1D-C2D	2.03	129.74	125.48
32	a	817	CLA	CHD-C1D-C2D	2.03	129.74	125.48
32	T	310	CLA	C1-C2-C3	-2.03	122.53	126.04
32	b	814	CLA	CHA-C1A-NA	-2.03	121.75	126.40
32	T	309	CLA	CHC-C4B-NB	-2.03	122.11	124.26
32	C	309	CLA	CHD-C1D-C2D	2.03	129.74	125.48
32	E	305	CLA	CHA-C1A-NA	-2.03	121.75	126.40
36	P	318	LMG	O7-C10-O9	-2.03	118.80	123.70
32	D	311	CLA	CHD-C1D-C2D	2.03	129.73	125.48
32	E	312	CLA	CHD-C1D-C2D	2.03	129.73	125.48
32	b	836	CLA	CHD-C1D-C2D	2.03	129.73	125.48
33	I	316	KC2	C4B-C3B-C2B	2.03	108.42	106.75
33	R	311	KC2	C4B-C3B-C2B	2.03	108.42	106.75
32	b	814	CLA	CHD-C1D-C2D	2.03	129.73	125.48
32	a	836	CLA	CHC-C4B-NB	-2.03	122.11	124.26
32	P	308	CLA	C2C-C1C-NC	2.03	111.87	109.97
32	H	309	CLA	CHA-C1A-NA	-2.03	121.76	126.40
32	J	305	CLA	CHD-C1D-C2D	2.03	129.73	125.48
32	P	309	CLA	CHA-C1A-NA	-2.03	121.76	126.40
32	a	808	CLA	C2C-C1C-NC	2.03	111.87	109.97
32	Q	308	CLA	CHD-C1D-C2D	2.03	129.73	125.48
32	D	312	CLA	O2A-C1-C2	2.03	113.96	108.64
32	f	204	CLA	CHA-C1A-NA	-2.03	121.76	126.40
34	I	310	DD6	C32-C31-C36	-2.03	119.77	122.63
32	T	308	CLA	CHD-C1D-C2D	2.03	129.73	125.48
32	f	204	CLA	CHD-C1D-C2D	2.03	129.73	125.48
32	Q	306	CLA	CHA-C1A-NA	-2.03	121.76	126.40
32	j	101	CLA	CHD-C1D-C2D	2.02	129.73	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	304	CLA	CHD-C1D-C2D	2.02	129.73	125.48
32	D	312	CLA	CHD-C1D-C2D	2.02	129.72	125.48
32	a	838	CLA	CHD-C1D-C2D	2.02	129.72	125.48
32	G	306	CLA	C4D-CHA-C1A	-2.02	118.79	121.25
33	O	310	KC2	C4B-C3B-C2B	2.02	108.41	106.75
32	R	308	CLA	CHD-C1D-C2D	2.02	129.72	125.48
32	F	303	CLA	CHC-C4B-NB	-2.02	122.11	124.26
33	I	316	KC2	CHB-C4A-NA	2.02	127.39	124.20
32	E	303	CLA	C2C-C1C-NC	2.02	111.87	109.97
35	B	308	LHG	O7-C7-O9	-2.02	118.81	123.70
32	M	310	CLA	CBA-CAA-C2A	2.02	119.83	113.86
32	L	304	CLA	CHA-C1A-NA	-2.02	121.77	126.40
34	A	312	DD6	C33-C34-C35	2.02	113.07	110.30
32	E	315	CLA	CHD-C1D-C2D	2.02	129.72	125.48
32	b	812	CLA	CHD-C1D-C2D	2.02	129.72	125.48
32	G	305	CLA	CHC-C1C-C2C	-2.02	121.11	126.73
33	F	302	KC2	CHC-C4B-NB	2.02	126.31	124.45
33	P	302	KC2	CHC-C4B-NB	2.02	126.31	124.45
32	I	303	CLA	CHD-C1D-C2D	2.02	129.72	125.48
32	P	305	CLA	CHD-C1D-C2D	2.02	129.72	125.48
32	W	307	CLA	CHD-C1D-C2D	2.02	129.72	125.48
32	a	823	CLA	CHD-C1D-C2D	2.02	129.72	125.48
33	G	302	KC2	C4C-C3C-C2C	2.02	108.72	107.11
38	I	315	LMU	C2'-C3'-C4'	-2.02	105.07	109.68
32	O	309	CLA	C11-C10-C8	2.02	122.45	115.92
32	U	301	CLA	C2C-C1C-NC	2.02	111.86	109.97
32	H	308	CLA	CHD-C1D-C2D	2.02	129.72	125.48
32	L	314	CLA	CHD-C1D-C2D	2.02	129.72	125.48
32	J	302	CLA	C2C-C1C-NC	2.02	111.86	109.97
32	Q	310	CLA	CHA-C1A-NA	-2.02	121.77	126.40
32	U	301	CLA	CHA-C1A-NA	-2.02	121.87	126.41
33	N	303	KC2	C4C-C3C-C2C	2.02	108.72	107.11
32	L	308	CLA	CHC-C4B-NB	-2.02	122.12	124.26
32	E	311	CLA	CHD-C1D-C2D	2.02	129.71	125.48
36	E	302	LMG	O2-C2-C1	-2.02	105.14	110.05
32	A	307	CLA	CHC-C4B-NB	-2.02	122.12	124.26
32	C	308	CLA	CHC-C1C-NC	2.02	127.26	124.20
32	P	304	CLA	CHA-C1A-NA	-2.02	121.78	126.40
33	M	302	KC2	C4C-C3C-C2C	2.02	108.72	107.11
32	F	307	CLA	CHD-C1D-C2D	2.02	129.71	125.48
32	P	311	CLA	CHB-C4A-NA	2.02	127.30	124.51
32	a	804	CLA	CHD-C1D-C2D	2.02	129.71	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	Q	301	CLA	CHD-C1D-C2D	2.01	129.71	125.48
32	Q	301	CLA	CHC-C4B-NB	-2.01	122.12	124.26
32	Q	307	CLA	CHC-C4B-NB	-2.01	122.12	124.26
32	b	840	CLA	CHA-C1A-NA	-2.01	121.78	126.40
32	P	305	CLA	C2C-C1C-NC	2.01	111.86	109.97
32	b	821	CLA	CHD-C1D-C2D	2.01	129.70	125.48
32	R	308	CLA	CHA-C1A-NA	-2.01	121.79	126.40
32	E	314	CLA	C1-C2-C3	-2.01	123.49	126.75
34	J	316	DD6	C32-C31-C36	-2.01	119.79	122.63
32	a	819	CLA	C2C-C1C-NC	2.01	111.86	109.97
32	D	305	CLA	CHD-C1D-C2D	2.01	129.70	125.48
32	a	853	CLA	CHD-C1D-C2D	2.01	129.70	125.48
32	J	306	CLA	CHD-C1D-C2D	2.01	129.70	125.48
37	S	315	A86	C36-C31-C32	-2.01	117.70	119.70
32	A	301	CLA	CHC-C1C-C2C	-2.01	121.14	126.73
32	I	302	CLA	CHB-C4A-NA	2.01	127.29	124.51
36	l	201	LMG	O7-C10-O9	-2.01	118.84	123.70
32	E	310	CLA	CHD-C1D-C2D	2.01	129.70	125.48
32	a	815	CLA	CHD-C1D-C2D	2.01	129.70	125.48
32	N	311	CLA	CHA-C1A-NA	-2.01	121.79	126.40
32	K	307	CLA	CMA-C3A-C4A	2.01	117.18	111.77
32	K	310	CLA	CHA-C1A-NA	-2.01	121.80	126.40
32	R	304	CLA	CHD-C1D-C2D	2.01	129.69	125.48
32	a	824	CLA	CHD-C1D-C2D	2.01	129.69	125.48
32	k	201	CLA	CHD-C1D-C2D	2.01	129.69	125.48
32	S	301	CLA	C3A-C2A-C1A	-2.01	98.33	101.34
32	O	304	CLA	CHD-C1D-C2D	2.01	129.69	125.48
32	a	833	CLA	CHD-C1D-C2D	2.01	129.69	125.48
32	U	305	CLA	C4D-CHA-C1A	-2.01	118.80	121.25
32	G	303	CLA	CHB-C4A-NA	2.01	127.29	124.51
32	E	309	CLA	CHD-C1D-C2D	2.01	129.69	125.48
32	D	312	CLA	CHC-C4B-NB	-2.01	122.13	124.26
32	a	803	CLA	CHB-C4A-NA	2.01	127.29	124.51
32	W	313	CLA	CHD-C1D-C2D	2.01	129.69	125.48
32	a	827	CLA	CHD-C1D-C2D	2.01	129.69	125.48
32	a	831	CLA	CHB-C4A-NA	2.01	127.29	124.51
32	L	301	CLA	CAA-C2A-C1A	-2.01	105.40	111.97
32	I	305	CLA	CHB-C4A-NA	2.01	127.29	124.51
35	a	851	LHG	C26-C25-C24	-2.01	105.98	113.19
32	b	815	CLA	CHD-C1D-C2D	2.01	129.69	125.48
32	R	308	CLA	CBA-CAA-C2A	2.01	119.78	113.86
32	l	202	CLA	CHD-C1D-C2D	2.01	129.69	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	826	CLA	C2C-C1C-NC	2.01	111.85	109.97
32	O	309	CLA	CHD-C1D-C2D	2.01	129.69	125.48
32	N	312	CLA	CHD-C1D-C2D	2.00	129.69	125.48
32	W	312	CLA	CHD-C1D-C2D	2.00	129.69	125.48
32	a	834	CLA	CHD-C1D-C2D	2.00	129.69	125.48
32	O	308	CLA	CHA-C1A-NA	-2.00	121.81	126.40
32	b	801	CLA	CHC-C4B-NB	-2.00	122.14	124.26
32	Q	307	CLA	CHD-C1D-C2D	2.00	129.68	125.48
32	G	303	CLA	CBA-CAA-C2A	2.00	119.78	113.86
32	b	831	CLA	CHB-C4A-NA	2.00	127.28	124.51
32	H	310	CLA	CHD-C1D-C2D	2.00	129.68	125.48
32	S	305	CLA	C2C-C1C-NC	2.00	111.85	109.97
32	E	315	CLA	CAA-C2A-C1A	-2.00	105.41	111.97
32	P	304	CLA	CAA-C2A-C1A	-2.00	105.41	111.97
32	F	301	CLA	CHA-C1A-NA	-2.00	121.91	126.41
32	B	304	CLA	CHA-C1A-NA	-2.00	121.81	126.40
32	S	309	CLA	CHC-C4B-NB	-2.00	122.14	124.26
32	K	301	CLA	CHD-C1D-C2D	2.00	129.68	125.48
33	Q	302	KC2	CHC-C4B-NB	2.00	126.29	124.45

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	J	317	DD6	C20
34	K	315	DD6	C20
34	O	313	DD6	C20
34	S	321	DD6	C20
37	O	312	A86	C36

All (3346) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	304	CLA	C1A-C2A-CAA-CBA
32	A	304	CLA	C3A-C2A-CAA-CBA
32	A	305	CLA	C2B-C3B-CAB-CBB
32	A	305	CLA	C4B-C3B-CAB-CBB
32	A	309	CLA	CHA-CBD-CGD-O1D
32	A	309	CLA	CHA-CBD-CGD-O2D
32	A	311	CLA	C1A-C2A-CAA-CBA
32	A	311	CLA	C3A-C2A-CAA-CBA
32	B	302	CLA	CHA-CBD-CGD-O1D
32	B	302	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	B	304	CLA	C1A-C2A-CAA-CBA
32	B	306	CLA	CHA-CBD-CGD-O2D
32	B	309	CLA	O2A-C1-C2-C3
32	C	304	CLA	C1A-C2A-CAA-CBA
32	C	304	CLA	C3A-C2A-CAA-CBA
32	C	304	CLA	C2B-C3B-CAB-CBB
32	C	304	CLA	C4B-C3B-CAB-CBB
32	C	305	CLA	C1A-C2A-CAA-CBA
32	C	305	CLA	C2B-C3B-CAB-CBB
32	C	305	CLA	C4B-C3B-CAB-CBB
32	C	305	CLA	C2-C3-C5-C6
32	C	305	CLA	C4-C3-C5-C6
32	C	307	CLA	C3A-C2A-CAA-CBA
32	C	307	CLA	C2B-C3B-CAB-CBB
32	C	307	CLA	C4B-C3B-CAB-CBB
32	D	304	CLA	C2B-C3B-CAB-CBB
32	D	304	CLA	C4B-C3B-CAB-CBB
32	D	307	CLA	C2B-C3B-CAB-CBB
32	D	307	CLA	C4B-C3B-CAB-CBB
32	D	307	CLA	C4-C3-C5-C6
32	D	310	CLA	C3A-C2A-CAA-CBA
32	D	310	CLA	C2B-C3B-CAB-CBB
32	D	310	CLA	C4B-C3B-CAB-CBB
32	D	312	CLA	CHA-CBD-CGD-O1D
32	D	312	CLA	CHA-CBD-CGD-O2D
32	D	312	CLA	C2-C3-C5-C6
32	D	312	CLA	C4-C3-C5-C6
32	D	313	CLA	CHA-CBD-CGD-O1D
32	D	313	CLA	CHA-CBD-CGD-O2D
32	D	313	CLA	CAD-CBD-CGD-O1D
32	D	314	CLA	C4B-C3B-CAB-CBB
32	E	306	CLA	C2B-C3B-CAB-CBB
32	E	306	CLA	C4B-C3B-CAB-CBB
32	E	308	CLA	C1A-C2A-CAA-CBA
32	E	308	CLA	C3A-C2A-CAA-CBA
32	E	309	CLA	CHA-CBD-CGD-O1D
32	E	309	CLA	CHA-CBD-CGD-O2D
32	E	309	CLA	C2-C3-C5-C6
32	E	309	CLA	C4-C3-C5-C6
32	E	312	CLA	CHA-CBD-CGD-O1D
32	E	312	CLA	CHA-CBD-CGD-O2D
32	E	315	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	E	315	CLA	C2B-C3B-CAB-CBB
32	E	315	CLA	C4B-C3B-CAB-CBB
32	F	304	CLA	C2B-C3B-CAB-CBB
32	F	304	CLA	C4B-C3B-CAB-CBB
32	F	306	CLA	C2-C3-C5-C6
32	F	306	CLA	C4-C3-C5-C6
32	F	307	CLA	C2B-C3B-CAB-CBB
32	F	307	CLA	C4B-C3B-CAB-CBB
32	G	301	CLA	CHA-CBD-CGD-O1D
32	G	301	CLA	CHA-CBD-CGD-O2D
32	G	303	CLA	C1A-C2A-CAA-CBA
32	G	303	CLA	C3A-C2A-CAA-CBA
32	G	303	CLA	C2B-C3B-CAB-CBB
32	G	303	CLA	C4B-C3B-CAB-CBB
32	G	306	CLA	C2B-C3B-CAB-CBB
32	G	306	CLA	C4B-C3B-CAB-CBB
32	H	302	CLA	CHA-CBD-CGD-O2D
32	H	304	CLA	C1A-C2A-CAA-CBA
32	I	301	CLA	CHA-CBD-CGD-O1D
32	I	301	CLA	CHA-CBD-CGD-O2D
32	I	301	CLA	C2-C3-C5-C6
32	I	301	CLA	C4-C3-C5-C6
32	I	303	CLA	C2B-C3B-CAB-CBB
32	I	303	CLA	C4B-C3B-CAB-CBB
32	I	305	CLA	C1A-C2A-CAA-CBA
32	I	306	CLA	C2B-C3B-CAB-CBB
32	I	306	CLA	C4B-C3B-CAB-CBB
32	I	306	CLA	C14-C13-C15-C16
32	I	307	CLA	C3A-C2A-CAA-CBA
32	I	307	CLA	CHA-CBD-CGD-O1D
32	I	307	CLA	CHA-CBD-CGD-O2D
32	I	307	CLA	CAD-CBD-CGD-O1D
32	I	307	CLA	CAD-CBD-CGD-O2D
32	I	308	CLA	C1A-C2A-CAA-CBA
32	J	304	CLA	C2B-C3B-CAB-CBB
32	J	304	CLA	C4B-C3B-CAB-CBB
32	J	305	CLA	O2A-C1-C2-C3
32	J	307	CLA	C2B-C3B-CAB-CBB
32	J	307	CLA	C4B-C3B-CAB-CBB
32	J	307	CLA	CHA-CBD-CGD-O1D
32	J	307	CLA	CHA-CBD-CGD-O2D
32	J	308	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	J	308	CLA	CAD-CBD-CGD-O2D
32	J	312	CLA	C1A-C2A-CAA-CBA
32	J	312	CLA	C3A-C2A-CAA-CBA
32	K	301	CLA	CHA-CBD-CGD-O1D
32	K	306	CLA	C1A-C2A-CAA-CBA
32	K	306	CLA	C3A-C2A-CAA-CBA
32	K	307	CLA	CHA-CBD-CGD-O1D
32	K	307	CLA	CHA-CBD-CGD-O2D
32	K	308	CLA	C1A-C2A-CAA-CBA
32	K	308	CLA	C3A-C2A-CAA-CBA
32	K	310	CLA	CHA-CBD-CGD-O1D
32	L	301	CLA	CHA-CBD-CGD-O1D
32	L	301	CLA	CHA-CBD-CGD-O2D
32	L	309	CLA	C2B-C3B-CAB-CBB
32	L	309	CLA	C4B-C3B-CAB-CBB
32	L	310	CLA	C2B-C3B-CAB-CBB
32	L	310	CLA	C4B-C3B-CAB-CBB
32	L	310	CLA	CAD-CBD-CGD-O1D
32	L	310	CLA	CAD-CBD-CGD-O2D
32	L	314	CLA	C1A-C2A-CAA-CBA
32	L	314	CLA	C3A-C2A-CAA-CBA
32	M	308	CLA	C1A-C2A-CAA-CBA
32	M	308	CLA	C3A-C2A-CAA-CBA
32	M	308	CLA	C2B-C3B-CAB-CBB
32	M	308	CLA	C4B-C3B-CAB-CBB
32	M	311	CLA	CAD-CBD-CGD-O1D
32	M	311	CLA	CAD-CBD-CGD-O2D
32	N	310	CLA	C4-C3-C5-C6
32	N	311	CLA	C6-C7-C8-C9
32	N	312	CLA	CHA-CBD-CGD-O1D
32	N	312	CLA	CHA-CBD-CGD-O2D
32	N	312	CLA	CAD-CBD-CGD-O1D
32	N	312	CLA	CAD-CBD-CGD-O2D
32	N	313	CLA	CAD-CBD-CGD-O1D
32	N	313	CLA	CAD-CBD-CGD-O2D
32	O	308	CLA	C4B-C3B-CAB-CBB
32	P	309	CLA	CHA-CBD-CGD-O1D
32	P	311	CLA	CHA-CBD-CGD-O1D
32	P	311	CLA	CHA-CBD-CGD-O2D
32	Q	301	CLA	C1A-C2A-CAA-CBA
32	Q	303	CLA	C1A-C2A-CAA-CBA
32	Q	305	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	Q	305	CLA	C3A-C2A-CAA-CBA
32	Q	306	CLA	C2B-C3B-CAB-CBB
32	Q	306	CLA	C4B-C3B-CAB-CBB
32	Q	306	CLA	C2-C3-C5-C6
32	Q	306	CLA	C4-C3-C5-C6
32	Q	307	CLA	C2B-C3B-CAB-CBB
32	Q	307	CLA	C4B-C3B-CAB-CBB
32	Q	310	CLA	C1A-C2A-CAA-CBA
32	Q	310	CLA	C3A-C2A-CAA-CBA
32	R	308	CLA	C2B-C3B-CAB-CBB
32	R	308	CLA	C4B-C3B-CAB-CBB
32	R	310	CLA	CHA-CBD-CGD-O1D
32	R	310	CLA	CHA-CBD-CGD-O2D
32	R	310	CLA	CAD-CBD-CGD-O1D
32	S	301	CLA	C1A-C2A-CAA-CBA
32	S	305	CLA	C4B-C3B-CAB-CBB
32	S	309	CLA	C2B-C3B-CAB-CBB
32	S	309	CLA	C4B-C3B-CAB-CBB
32	S	309	CLA	C2-C3-C5-C6
32	S	309	CLA	C4-C3-C5-C6
32	S	311	CLA	CHA-CBD-CGD-O1D
32	S	311	CLA	CHA-CBD-CGD-O2D
32	S	311	CLA	CAD-CBD-CGD-O1D
32	S	311	CLA	CAD-CBD-CGD-O2D
32	S	313	CLA	C1A-C2A-CAA-CBA
32	S	313	CLA	C3A-C2A-CAA-CBA
32	T	305	CLA	CHA-CBD-CGD-O1D
32	T	305	CLA	CHA-CBD-CGD-O2D
32	T	305	CLA	CAD-CBD-CGD-O1D
32	T	305	CLA	CAD-CBD-CGD-O2D
32	T	308	CLA	C1A-C2A-CAA-CBA
32	T	308	CLA	C3A-C2A-CAA-CBA
32	T	309	CLA	C1A-C2A-CAA-CBA
32	T	310	CLA	CAD-CBD-CGD-O1D
32	T	310	CLA	CAD-CBD-CGD-O2D
32	U	305	CLA	CHA-CBD-CGD-O1D
32	U	305	CLA	CHA-CBD-CGD-O2D
32	U	305	CLA	CAD-CBD-CGD-O1D
32	U	306	CLA	CHA-CBD-CGD-O1D
32	U	306	CLA	CHA-CBD-CGD-O2D
32	V	201	CLA	C2B-C3B-CAB-CBB
32	V	201	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	V	203	CLA	CHA-CBD-CGD-O1D
32	V	203	CLA	CHA-CBD-CGD-O2D
32	W	306	CLA	C1A-C2A-CAA-CBA
32	W	310	CLA	C2B-C3B-CAB-CBB
32	W	310	CLA	C4B-C3B-CAB-CBB
32	W	311	CLA	CHA-CBD-CGD-O1D
32	W	311	CLA	CHA-CBD-CGD-O2D
32	W	311	CLA	CAD-CBD-CGD-O1D
32	a	803	CLA	C4-C3-C5-C6
32	a	804	CLA	C1A-C2A-CAA-CBA
32	a	804	CLA	C3A-C2A-CAA-CBA
32	a	808	CLA	C1A-C2A-CAA-CBA
32	a	808	CLA	C3A-C2A-CAA-CBA
32	a	808	CLA	C2A-CAA-CBA-CGA
32	a	810	CLA	C2B-C3B-CAB-CBB
32	a	810	CLA	C4B-C3B-CAB-CBB
32	a	812	CLA	C2B-C3B-CAB-CBB
32	a	812	CLA	C4B-C3B-CAB-CBB
32	a	814	CLA	C1A-C2A-CAA-CBA
32	a	814	CLA	C3A-C2A-CAA-CBA
32	a	817	CLA	C2-C3-C5-C6
32	a	817	CLA	C4-C3-C5-C6
32	a	818	CLA	C2B-C3B-CAB-CBB
32	a	818	CLA	C4B-C3B-CAB-CBB
32	a	821	CLA	CHA-CBD-CGD-O1D
32	a	821	CLA	CHA-CBD-CGD-O2D
32	a	821	CLA	CAD-CBD-CGD-O1D
32	a	824	CLA	O2A-C1-C2-C3
32	a	826	CLA	CHA-CBD-CGD-O1D
32	a	826	CLA	CHA-CBD-CGD-O2D
32	a	827	CLA	C1A-C2A-CAA-CBA
32	a	827	CLA	CHA-CBD-CGD-O1D
32	a	827	CLA	CHA-CBD-CGD-O2D
32	a	827	CLA	CAD-CBD-CGD-O1D
32	a	828	CLA	C3A-C2A-CAA-CBA
32	a	831	CLA	C2B-C3B-CAB-CBB
32	a	831	CLA	C4B-C3B-CAB-CBB
32	a	835	CLA	C2B-C3B-CAB-CBB
32	a	835	CLA	C4B-C3B-CAB-CBB
32	a	835	CLA	CHA-CBD-CGD-O1D
32	a	835	CLA	CHA-CBD-CGD-O2D
32	a	837	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	a	837	CLA	CHA-CBD-CGD-O2D
32	a	838	CLA	C2B-C3B-CAB-CBB
32	a	838	CLA	C4B-C3B-CAB-CBB
32	a	840	CLA	C2B-C3B-CAB-CBB
32	a	840	CLA	C4B-C3B-CAB-CBB
32	a	841	CLA	C2B-C3B-CAB-CBB
32	a	841	CLA	C4B-C3B-CAB-CBB
32	b	801	CLA	C3A-C2A-CAA-CBA
32	b	802	CLA	C1A-C2A-CAA-CBA
32	b	804	CLA	C1A-C2A-CAA-CBA
32	b	807	CLA	C1A-C2A-CAA-CBA
32	b	807	CLA	C2A-CAA-CBA-CGA
32	b	811	CLA	C2A-CAA-CBA-CGA
32	b	815	CLA	C3A-C2A-CAA-CBA
32	b	817	CLA	C1A-C2A-CAA-CBA
32	b	817	CLA	C2B-C3B-CAB-CBB
32	b	817	CLA	C4B-C3B-CAB-CBB
32	b	817	CLA	O2A-C1-C2-C3
32	b	822	CLA	C2B-C3B-CAB-CBB
32	b	822	CLA	C4B-C3B-CAB-CBB
32	b	823	CLA	CHA-CBD-CGD-O1D
32	b	823	CLA	CHA-CBD-CGD-O2D
32	b	825	CLA	CHA-CBD-CGD-O1D
32	b	825	CLA	CHA-CBD-CGD-O2D
32	b	827	CLA	C2B-C3B-CAB-CBB
32	b	827	CLA	C4B-C3B-CAB-CBB
32	b	828	CLA	C4B-C3B-CAB-CBB
32	b	830	CLA	C2-C1-O2A-CGA
32	b	831	CLA	CHA-CBD-CGD-O1D
32	b	831	CLA	CHA-CBD-CGD-O2D
32	b	831	CLA	CAD-CBD-CGD-O1D
32	b	831	CLA	CAD-CBD-CGD-O2D
32	b	837	CLA	C1A-C2A-CAA-CBA
32	b	837	CLA	CHA-CBD-CGD-O1D
32	b	837	CLA	CHA-CBD-CGD-O2D
32	b	837	CLA	CAD-CBD-CGD-O1D
32	b	839	CLA	C1A-C2A-CAA-CBA
32	b	839	CLA	C2B-C3B-CAB-CBB
32	b	839	CLA	C4B-C3B-CAB-CBB
32	f	201	CLA	CHA-CBD-CGD-O2D
32	k	202	CLA	C2B-C3B-CAB-CBB
32	k	202	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	k	202	CLA	C4-C3-C5-C6
32	l	203	CLA	C1A-C2A-CAA-CBA
32	r	201	CLA	C1A-C2A-CAA-CBA
32	r	201	CLA	C3A-C2A-CAA-CBA
33	A	310	KC2	C2B-C3B-CAB-CBB
33	A	310	KC2	C4B-C3B-CAB-CBB
33	C	303	KC2	C1A-C2A-CAA-CBA
33	E	313	KC2	C1A-C2A-CAA-CBA
33	E	313	KC2	C2B-C3B-CAB-CBB
33	E	313	KC2	C4B-C3B-CAB-CBB
33	F	302	KC2	C1A-C2A-CAA-CBA
33	F	310	KC2	C2B-C3B-CAB-CBB
33	F	310	KC2	C4B-C3B-CAB-CBB
33	G	302	KC2	C1A-C2A-CAA-CBA
33	G	302	KC2	C3A-C2A-CAA-CBA
33	G	309	KC2	C1A-C2A-CAA-CBA
33	G	309	KC2	C3A-C2A-CAA-CBA
33	G	309	KC2	C2B-C3B-CAB-CBB
33	G	309	KC2	C4B-C3B-CAB-CBB
33	G	309	KC2	C2C-C3C-CAC-CBC
33	G	309	KC2	C4C-C3C-CAC-CBC
33	G	309	KC2	CAA-CBA-CGA-O1A
33	G	309	KC2	CAA-CBA-CGA-O2A
33	H	303	KC2	C1A-C2A-CAA-CBA
33	I	309	KC2	C2B-C3B-CAB-CBB
33	I	309	KC2	C4B-C3B-CAB-CBB
33	I	309	KC2	C2C-C3C-CAC-CBC
33	I	309	KC2	C4C-C3C-CAC-CBC
33	I	309	KC2	CAA-CBA-CGA-O2A
33	I	316	KC2	C1A-C2A-CAA-CBA
33	I	316	KC2	C3A-C2A-CAA-CBA
33	I	316	KC2	C2B-C3B-CAB-CBB
33	J	303	KC2	C1A-C2A-CAA-CBA
33	J	303	KC2	C3A-C2A-CAA-CBA
33	J	310	KC2	C1A-C2A-CAA-CBA
33	J	310	KC2	C2B-C3B-CAB-CBB
33	J	310	KC2	C4B-C3B-CAB-CBB
33	J	310	KC2	C2C-C3C-CAC-CBC
33	J	310	KC2	C4C-C3C-CAC-CBC
33	K	302	KC2	C2C-C3C-CAC-CBC
33	K	302	KC2	CAA-CBA-CGA-O1A
33	K	302	KC2	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	K	303	KC2	C1A-C2A-CAA-CBA
33	K	303	KC2	C2B-C3B-CAB-CBB
33	K	303	KC2	C4B-C3B-CAB-CBB
33	K	303	KC2	CAA-CBA-CGA-O2A
33	K	305	KC2	C2C-C3C-CAC-CBC
33	K	309	KC2	C1A-C2A-CAA-CBA
33	K	309	KC2	C3A-C2A-CAA-CBA
33	K	309	KC2	C2B-C3B-CAB-CBB
33	K	309	KC2	C4B-C3B-CAB-CBB
33	L	302	KC2	C2C-C3C-CAC-CBC
33	L	302	KC2	C4C-C3C-CAC-CBC
33	L	305	KC2	C1A-C2A-CAA-CBA
33	L	305	KC2	C3A-C2A-CAA-CBA
33	L	305	KC2	C2C-C3C-CAC-CBC
33	L	305	KC2	C4C-C3C-CAC-CBC
33	L	305	KC2	CHA-CBD-CGD-O1D
33	L	305	KC2	CHA-CBD-CGD-O2D
33	L	306	KC2	C2B-C3B-CAB-CBB
33	L	306	KC2	C4B-C3B-CAB-CBB
33	L	313	KC2	C1A-C2A-CAA-CBA
33	M	302	KC2	C1A-C2A-CAA-CBA
33	M	303	KC2	C2C-C3C-CAC-CBC
33	M	303	KC2	C4C-C3C-CAC-CBC
33	M	304	KC2	C1A-C2A-CAA-CBA
33	M	304	KC2	CAA-CBA-CGA-O1A
33	M	304	KC2	CAA-CBA-CGA-O2A
33	M	304	KC2	CHA-CBD-CGD-O1D
33	M	304	KC2	CHA-CBD-CGD-O2D
33	M	307	KC2	C1A-C2A-CAA-CBA
33	M	313	KC2	C2B-C3B-CAB-CBB
33	M	313	KC2	C2C-C3C-CAC-CBC
33	M	313	KC2	C4C-C3C-CAC-CBC
33	M	321	KC2	C1A-C2A-CAA-CBA
33	M	321	KC2	C3A-C2A-CAA-CBA
33	M	321	KC2	C4B-C3B-CAB-CBB
33	N	302	KC2	C2B-C3B-CAB-CBB
33	N	302	KC2	C4B-C3B-CAB-CBB
33	N	303	KC2	C1A-C2A-CAA-CBA
33	N	303	KC2	C3A-C2A-CAA-CBA
33	N	303	KC2	CAA-CBA-CGA-O2A
33	N	304	KC2	C2B-C3B-CAB-CBB
33	N	304	KC2	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
33	N	304	KC2	C2C-C3C-CAC-CBC
33	N	304	KC2	C4C-C3C-CAC-CBC
33	N	306	KC2	C4B-C3B-CAB-CBB
33	N	306	KC2	C2C-C3C-CAC-CBC
33	N	306	KC2	C4C-C3C-CAC-CBC
33	N	308	KC2	C2B-C3B-CAB-CBB
33	N	314	KC2	C1A-C2A-CAA-CBA
33	N	314	KC2	C2B-C3B-CAB-CBB
33	N	314	KC2	C4B-C3B-CAB-CBB
33	O	302	KC2	C1A-C2A-CAA-CBA
33	O	302	KC2	C3A-C2A-CAA-CBA
33	O	302	KC2	C2B-C3B-CAB-CBB
33	O	302	KC2	C4B-C3B-CAB-CBB
33	O	303	KC2	C1A-C2A-CAA-CBA
33	O	303	KC2	C3A-C2A-CAA-CBA
33	O	303	KC2	C2B-C3B-CAB-CBB
33	O	303	KC2	C4B-C3B-CAB-CBB
33	O	310	KC2	C1A-C2A-CAA-CBA
33	O	310	KC2	C3A-C2A-CAA-CBA
33	O	310	KC2	C2B-C3B-CAB-CBB
33	O	310	KC2	C4B-C3B-CAB-CBB
33	P	301	KC2	C1A-C2A-CAA-CBA
33	P	301	KC2	C2B-C3B-CAB-CBB
33	P	301	KC2	C4B-C3B-CAB-CBB
33	P	302	KC2	C1A-C2A-CAA-CBA
33	P	302	KC2	C3A-C2A-CAA-CBA
33	P	302	KC2	C2C-C3C-CAC-CBC
33	P	302	KC2	C4C-C3C-CAC-CBC
33	P	306	KC2	C1A-C2A-CAA-CBA
33	P	306	KC2	C2C-C3C-CAC-CBC
33	P	306	KC2	C4C-C3C-CAC-CBC
33	Q	302	KC2	C1A-C2A-CAA-CBA
33	Q	302	KC2	C4B-C3B-CAB-CBB
33	Q	302	KC2	C2C-C3C-CAC-CBC
33	Q	302	KC2	C4C-C3C-CAC-CBC
33	Q	302	KC2	CAA-CBA-CGA-O1A
33	Q	317	KC2	C1A-C2A-CAA-CBA
33	Q	317	KC2	C3A-C2A-CAA-CBA
33	Q	317	KC2	CHA-CBD-CGD-O1D
33	Q	317	KC2	CHA-CBD-CGD-O2D
33	R	302	KC2	C1A-C2A-CAA-CBA
33	R	303	KC2	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
33	R	305	KC2	C1A-C2A-CAA-CBA
33	R	311	KC2	C1A-C2A-CAA-CBA
33	S	302	KC2	C1A-C2A-CAA-CBA
33	S	302	KC2	C3A-C2A-CAA-CBA
33	S	302	KC2	C2C-C3C-CAC-CBC
33	S	302	KC2	C4C-C3C-CAC-CBC
33	S	303	KC2	C1A-C2A-CAA-CBA
33	S	306	KC2	C1A-C2A-CAA-CBA
33	S	306	KC2	C2B-C3B-CAB-CBB
33	S	306	KC2	C4B-C3B-CAB-CBB
33	S	312	KC2	C2B-C3B-CAB-CBB
33	T	303	KC2	C2B-C3B-CAB-CBB
33	T	303	KC2	C4B-C3B-CAB-CBB
33	T	303	KC2	C2C-C3C-CAC-CBC
33	T	303	KC2	C4C-C3C-CAC-CBC
33	T	311	KC2	C1A-C2A-CAA-CBA
33	T	311	KC2	C2B-C3B-CAB-CBB
33	T	311	KC2	C4B-C3B-CAB-CBB
33	U	304	KC2	C1A-C2A-CAA-CBA
33	U	304	KC2	C3A-C2A-CAA-CBA
33	U	304	KC2	C2C-C3C-CAC-CBC
33	W	301	KC2	C1A-C2A-CAA-CBA
33	W	301	KC2	C2B-C3B-CAB-CBB
33	W	301	KC2	C4B-C3B-CAB-CBB
33	W	301	KC2	C2C-C3C-CAC-CBC
33	W	301	KC2	C4C-C3C-CAC-CBC
33	W	303	KC2	C2B-C3B-CAB-CBB
33	W	303	KC2	C2C-C3C-CAC-CBC
33	W	304	KC2	C1A-C2A-CAA-CBA
33	W	304	KC2	C3A-C2A-CAA-CBA
33	W	305	KC2	C2B-C3B-CAB-CBB
33	W	305	KC2	C4B-C3B-CAB-CBB
33	W	308	KC2	C2C-C3C-CAC-CBC
33	W	308	KC2	C4C-C3C-CAC-CBC
33	W	314	KC2	C2B-C3B-CAB-CBB
34	B	307	DD6	C13-C14-C15-C16
34	B	307	DD6	C13-C14-C15-C20
34	D	301	DD6	C13-C14-C15-O1
34	D	318	DD6	C13-C14-C15-O1
34	E	318	DD6	C27-C29-C30-C31
34	F	314	DD6	C13-C14-C15-C16
34	F	315	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
34	F	315	DD6	C12-C11-C13-C14
34	F	315	DD6	C13-C14-C15-O1
34	F	316	DD6	C-C1-C24-C25
34	F	316	DD6	C2-C1-C24-C25
34	F	316	DD6	C13-C14-C15-O1
34	G	312	DD6	C13-C14-C15-C16
34	H	312	DD6	C13-C14-C15-C20
34	H	313	DD6	C13-C14-C15-C20
34	J	314	DD6	C13-C14-C15-O1
34	K	315	DD6	C13-C14-C15-O1
34	L	319	DD6	C13-C14-C15-C16
34	N	319	DD6	C13-C14-C15-O1
34	N	321	DD6	C13-C14-C15-O1
34	Q	315	DD6	C13-C14-C15-O1
34	S	321	DD6	C13-C14-C15-C16
34	S	321	DD6	C13-C14-C15-C20
34	S	321	DD6	C13-C14-C15-O1
34	j	103	DD6	C13-C14-C15-O1
35	A	316	LHG	C4-O6-P-O5
35	A	316	LHG	O9-C7-O7-C5
35	A	316	LHG	C8-C7-O7-C5
35	B	308	LHG	C2-C3-O3-P
35	D	320	LHG	C1-C2-C3-O3
35	D	320	LHG	C3-O3-P-O4
35	D	320	LHG	C3-O3-P-O5
35	D	320	LHG	C4-O6-P-O5
35	D	320	LHG	C8-C7-O7-C5
35	E	301	LHG	O1-C1-C2-C3
35	E	301	LHG	C3-O3-P-O4
35	E	301	LHG	C3-O3-P-O5
35	E	301	LHG	C3-O3-P-O6
35	E	301	LHG	C4-O6-P-O5
35	E	321	LHG	O2-C2-C3-O3
35	E	321	LHG	C4-O6-P-O4
35	F	318	LHG	C3-O3-P-O4
35	F	318	LHG	C4-O6-P-O4
35	F	321	LHG	C4-O6-P-O4
35	I	314	LHG	C4-O6-P-O4
35	I	314	LHG	O9-C7-O7-C5
35	I	318	LHG	O1-C1-C2-C3
35	I	318	LHG	C4-O6-P-O3
35	I	318	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
35	I	318	LHG	C4-O6-P-O5
35	I	318	LHG	O9-C7-O7-C5
35	I	318	LHG	C8-C7-O7-C5
35	M	319	LHG	C4-O6-P-O3
35	M	319	LHG	C4-O6-P-O4
35	M	319	LHG	C4-O6-P-O5
35	P	317	LHG	C3-O3-P-O5
35	P	317	LHG	C4-C5-O7-C7
35	P	317	LHG	C8-C7-O7-C5
35	W	319	LHG	C3-O3-P-O5
35	W	319	LHG	C4-O6-P-O5
35	a	850	LHG	C3-O3-P-O4
35	a	850	LHG	C4-O6-P-O3
35	a	851	LHG	C4-O6-P-O3
35	a	851	LHG	O9-C7-O7-C5
35	f	205	LHG	C3-O3-P-O5
35	f	205	LHG	C4-O6-P-O4
35	f	205	LHG	O9-C7-O7-C5
35	f	205	LHG	C8-C7-O7-C5
36	A	317	LMG	C8-C9-O8-C28
36	A	318	LMG	C2-C1-O1-C7
36	A	318	LMG	O6-C1-O1-C7
36	D	302	LMG	O6-C1-O1-C7
36	E	302	LMG	C2-C1-O1-C7
36	E	320	LMG	O6-C1-O1-C7
36	E	320	LMG	O9-C10-O7-C8
36	E	322	LMG	O9-C10-O7-C8
36	E	322	LMG	C11-C10-O7-C8
36	E	322	LMG	O10-C28-O8-C9
36	E	322	LMG	C29-C28-O8-C9
36	F	320	LMG	C11-C10-O7-C8
36	L	320	LMG	O7-C8-C9-O8
36	L	320	LMG	C11-C10-O7-C8
36	M	320	LMG	C11-C10-O7-C8
36	N	301	LMG	O6-C1-O1-C7
36	P	318	LMG	C2-C1-O1-C7
36	P	318	LMG	O6-C1-O1-C7
36	S	322	LMG	C11-C10-O7-C8
36	T	301	LMG	C2-C1-O1-C7
36	T	301	LMG	O6-C1-O1-C7
36	T	301	LMG	C11-C10-O7-C8
36	j	104	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
36	l	201	LMG	C2-C1-O1-C7
36	l	201	LMG	O6-C1-O1-C7
36	l	201	LMG	O9-C10-O7-C8
36	l	201	LMG	C11-C10-O7-C8
37	C	311	A86	C12-C11-C13-C14
37	C	311	A86	C13-C14-C15-O1
37	C	312	A86	C-C1-C24-C25
37	C	312	A86	C2-C1-C24-C25
37	C	312	A86	C9-C10-C11-C12
37	C	312	A86	C9-C10-C11-C13
37	C	312	A86	C13-C14-C15-O1
37	D	323	A86	C26-C27-C29-C30
37	D	323	A86	C28-C27-C29-C30
37	F	317	A86	C9-C10-C11-C12
37	F	317	A86	C9-C10-C11-C13
37	F	317	A86	C26-C27-C29-C30
37	H	314	A86	C9-C10-C11-C12
37	H	314	A86	C9-C10-C11-C13
37	J	313	A86	C9-C10-C11-C12
37	J	313	A86	C9-C10-C11-C13
37	J	313	A86	C13-C14-C15-O1
37	K	311	A86	C12-C11-C13-C14
37	L	315	A86	C9-C10-C11-C13
37	L	316	A86	C28-C27-C29-C30
37	L	317	A86	C12-C11-C13-O
37	L	317	A86	C13-C14-C15-O1
37	L	317	A86	C28-C27-C29-C30
37	M	301	A86	C9-C10-C11-C12
37	M	301	A86	C9-C10-C11-C13
37	M	314	A86	C10-C11-C13-O
37	M	314	A86	C12-C11-C13-O
37	M	315	A86	C13-C14-C15-C16
37	M	315	A86	C13-C14-C15-O1
37	M	317	A86	C13-C14-C15-C16
37	M	317	A86	C13-C14-C15-O1
37	M	318	A86	C5-C6-C8-C9
37	M	318	A86	C7-C6-C8-C9
37	M	322	A86	C12-C11-C13-C14
37	N	316	A86	C12-C11-C13-C14
37	N	316	A86	C13-C14-C15-O1
37	N	316	A86	C28-C27-C29-C30
37	P	313	A86	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	P	313	A86	C9-C10-C11-C13
37	P	313	A86	C13-C14-C15-C16
37	P	313	A86	C13-C14-C15-O1
37	P	314	A86	C13-C14-C15-C16
37	P	316	A86	C13-C14-C15-O1
37	Q	311	A86	C13-C14-C15-C20
37	Q	316	A86	C12-C11-C13-O
37	Q	316	A86	C12-C11-C13-C14
37	R	313	A86	C13-C14-C15-O1
37	S	315	A86	C13-C14-C15-O1
37	S	317	A86	C9-C10-C11-C13
37	S	317	A86	C26-C27-C29-C30
37	S	318	A86	C9-C10-C11-C12
37	S	318	A86	C9-C10-C11-C13
37	S	319	A86	C9-C10-C11-C12
37	S	319	A86	C9-C10-C11-C13
37	S	319	A86	C12-C11-C13-C14
37	S	320	A86	C12-C11-C13-C14
37	T	313	A86	C9-C10-C11-C12
37	T	313	A86	C9-C10-C11-C13
37	W	315	A86	C12-C11-C13-O
37	W	315	A86	C13-C14-C15-O1
38	J	318	LMU	O5'-C1'-O1'-C1
38	j	105	LMU	C2'-C1'-O1'-C1
38	j	105	LMU	O5'-C1'-O1'-C1
39	H	315	SQD	C2-C1-O6-C44
39	H	315	SQD	O5-C1-O6-C44
39	k	206	SQD	O5-C1-O6-C44
39	k	206	SQD	C46-C45-O47-C7
39	k	206	SQD	C8-C7-O47-C45
39	k	206	SQD	O5-C5-C6-S
40	Q	318	DGD	O1B-C1B-O2G-C2G
40	Q	318	DGD	C2D-C1D-O3G-C3G
40	Q	318	DGD	O6D-C1D-O3G-C3G
40	b	846	DGD	C2G-C1G-O1G-C1A
41	U	310	BCR	C17-C18-C19-C20
41	a	843	BCR	C1-C6-C7-C8
41	a	843	BCR	C37-C22-C23-C24
41	a	845	BCR	C23-C24-C25-C26
41	b	844	BCR	C23-C24-C25-C30
41	b	845	BCR	C21-C22-C23-C24
41	b	845	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
41	f	202	BCR	C11-C12-C13-C14
41	j	102	BCR	C1-C6-C7-C8
41	j	102	BCR	C5-C6-C7-C8
41	j	102	BCR	C23-C24-C25-C26
41	l	205	BCR	C21-C22-C23-C24
41	l	205	BCR	C37-C22-C23-C24
41	l	205	BCR	C23-C24-C25-C26
38	I	315	LMU	C3'-C4'-O1B-C1B
32	W	310	CLA	CBD-CGD-O2D-CED
35	E	321	LHG	O10-C23-O8-C6
35	a	850	LHG	O10-C23-O8-C6
32	W	310	CLA	O1D-CGD-O2D-CED
35	E	321	LHG	C24-C23-O8-C6
35	P	317	LHG	C24-C23-O8-C6
35	M	319	LHG	O10-C23-O8-C6
35	P	317	LHG	O10-C23-O8-C6
36	D	303	LMG	O10-C28-O8-C9
36	N	301	LMG	O10-C28-O8-C9
33	K	303	KC2	CAA-CBA-CGA-O1A
33	N	303	KC2	CAA-CBA-CGA-O1A
33	Q	302	KC2	CAA-CBA-CGA-O2A
36	D	321	LMG	O6-C5-C6-O5
35	D	320	LHG	O9-C7-O7-C5
35	P	317	LHG	O9-C7-O7-C5
35	a	850	LHG	O9-C7-O7-C5
36	E	302	LMG	O9-C10-O7-C8
36	F	320	LMG	O9-C10-O7-C8
36	L	320	LMG	O9-C10-O7-C8
36	S	322	LMG	O9-C10-O7-C8
36	T	301	LMG	O9-C10-O7-C8
39	k	206	SQD	O49-C7-O47-C45
32	B	309	CLA	C3-C5-C6-C7
32	D	308	CLA	C3-C5-C6-C7
32	E	307	CLA	C3-C5-C6-C7
32	E	308	CLA	C3-C5-C6-C7
32	J	307	CLA	C3-C5-C6-C7
32	N	311	CLA	C3-C5-C6-C7
32	P	311	CLA	C3-C5-C6-C7
32	V	201	CLA	C3-C5-C6-C7
32	a	801	CLA	C3-C5-C6-C7
32	a	804	CLA	C3-C5-C6-C7
32	a	818	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	a	823	CLA	C3-C5-C6-C7
32	a	829	CLA	C3-C5-C6-C7
32	a	831	CLA	C3-C5-C6-C7
32	a	837	CLA	C3-C5-C6-C7
32	a	839	CLA	C3-C5-C6-C7
32	b	810	CLA	C3-C5-C6-C7
32	b	831	CLA	C3-C5-C6-C7
35	a	850	LHG	C24-C23-O8-C6
39	H	315	SQD	C24-C23-O48-C46
35	a	851	LHG	C8-C7-O7-C5
36	E	320	LMG	C11-C10-O7-C8
40	Q	318	DGD	C2B-C1B-O2G-C2G
37	J	313	A86	C39-C38-O4-C34
37	J	313	A86	O5-C38-O4-C34
37	S	314	A86	C39-C38-O4-C34
37	S	314	A86	O5-C38-O4-C34
36	L	320	LMG	O6-C5-C6-O5
36	D	302	LMG	C4-C5-C6-O5
33	F	310	KC2	CAA-CBA-CGA-O2A
33	I	309	KC2	CAA-CBA-CGA-O1A
33	I	316	KC2	CAA-CBA-CGA-O1A
33	I	316	KC2	CAA-CBA-CGA-O2A
33	L	313	KC2	CAA-CBA-CGA-O1A
33	L	313	KC2	CAA-CBA-CGA-O2A
33	M	313	KC2	CAA-CBA-CGA-O1A
33	M	313	KC2	CAA-CBA-CGA-O2A
33	W	304	KC2	CAA-CBA-CGA-O1A
33	W	304	KC2	CAA-CBA-CGA-O2A
32	D	307	CLA	C2-C3-C5-C6
32	N	310	CLA	C2-C3-C5-C6
32	b	804	CLA	C2-C3-C5-C6
32	k	202	CLA	C2-C3-C5-C6
32	G	306	CLA	C2A-CAA-CBA-CGA
32	O	307	CLA	C2A-CAA-CBA-CGA
32	a	810	CLA	C2A-CAA-CBA-CGA
32	a	830	CLA	C2A-CAA-CBA-CGA
32	b	828	CLA	C2A-CAA-CBA-CGA
32	A	302	CLA	C3-C5-C6-C7
32	P	309	CLA	C3-C5-C6-C7
43	b	847	PQN	C13-C15-C16-C17
35	B	308	LHG	C24-C23-O8-C6
35	I	318	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
36	D	303	LMG	C29-C28-O8-C9
36	N	301	LMG	C29-C28-O8-C9
36	P	318	LMG	C29-C28-O8-C9
36	W	320	LMG	C29-C28-O8-C9
36	E	302	LMG	O6-C5-C6-O5
36	M	320	LMG	O9-C10-O7-C8
36	P	318	LMG	O10-C28-O8-C9
36	W	320	LMG	O10-C28-O8-C9
39	H	315	SQD	O10-C23-O48-C46
37	P	316	A86	C39-C38-O4-C34
37	C	311	A86	C39-C38-O4-C34
37	D	322	A86	C39-C38-O4-C34
37	D	323	A86	C39-C38-O4-C34
37	F	312	A86	C39-C38-O4-C34
37	K	311	A86	C39-C38-O4-C34
37	K	312	A86	C39-C38-O4-C34
37	K	314	A86	C39-C38-O4-C34
37	L	318	A86	C39-C38-O4-C34
37	M	315	A86	C39-C38-O4-C34
37	M	317	A86	C39-C38-O4-C34
37	N	315	A86	C39-C38-O4-C34
37	N	316	A86	C39-C38-O4-C34
37	N	317	A86	C39-C38-O4-C34
37	O	312	A86	C39-C38-O4-C34
37	P	313	A86	C39-C38-O4-C34
37	P	314	A86	C39-C38-O4-C34
37	P	316	A86	O5-C38-O4-C34
37	Q	311	A86	C39-C38-O4-C34
37	S	316	A86	C39-C38-O4-C34
37	S	317	A86	C39-C38-O4-C34
37	S	318	A86	C39-C38-O4-C34
37	T	313	A86	C39-C38-O4-C34
37	U	308	A86	C39-C38-O4-C34
37	W	315	A86	C39-C38-O4-C34
37	W	316	A86	C39-C38-O4-C34
37	W	318	A86	C39-C38-O4-C34
37	r	204	A86	C39-C38-O4-C34
33	K	309	KC2	CAA-CBA-CGA-O1A
33	K	309	KC2	CAA-CBA-CGA-O2A
32	D	314	CLA	CBD-CGD-O2D-CED
32	P	311	CLA	CBD-CGD-O2D-CED
32	l	203	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	D	320	LHG	O2-C2-C3-O3
32	J	312	CLA	C3-C5-C6-C7
32	a	809	CLA	C3-C5-C6-C7
32	a	811	CLA	C3-C5-C6-C7
32	a	822	CLA	CBA-CGA-O2A-C1
35	M	319	LHG	C24-C23-O8-C6
35	a	849	LHG	C24-C23-O8-C6
36	E	320	LMG	C29-C28-O8-C9
40	Q	318	DGD	C2A-C1A-O1G-C1G
37	C	311	A86	O5-C38-O4-C34
37	D	322	A86	O5-C38-O4-C34
37	F	312	A86	O5-C38-O4-C34
37	K	314	A86	O5-C38-O4-C34
37	M	315	A86	O5-C38-O4-C34
37	M	317	A86	O5-C38-O4-C34
37	N	316	A86	O5-C38-O4-C34
37	O	312	A86	O5-C38-O4-C34
37	P	313	A86	O5-C38-O4-C34
37	S	316	A86	O5-C38-O4-C34
37	S	317	A86	O5-C38-O4-C34
37	W	316	A86	O5-C38-O4-C34
37	W	318	A86	O5-C38-O4-C34
37	r	204	A86	O5-C38-O4-C34
36	E	320	LMG	O6-C5-C6-O5
36	N	301	LMG	O6-C5-C6-O5
35	B	308	LHG	C8-C7-O7-C5
37	D	323	A86	O5-C38-O4-C34
37	K	311	A86	O5-C38-O4-C34
37	K	312	A86	O5-C38-O4-C34
37	L	318	A86	O5-C38-O4-C34
37	N	315	A86	O5-C38-O4-C34
37	N	317	A86	O5-C38-O4-C34
37	P	314	A86	O5-C38-O4-C34
37	Q	311	A86	O5-C38-O4-C34
37	S	318	A86	O5-C38-O4-C34
37	T	313	A86	O5-C38-O4-C34
37	U	308	A86	O5-C38-O4-C34
37	W	315	A86	O5-C38-O4-C34
35	a	849	LHG	C23-C24-C25-C26
32	T	305	CLA	CBD-CGD-O2D-CED
40	Q	318	DGD	O6E-C5E-C6E-O5E
37	L	315	A86	C33-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
36	E	320	LMG	O10-C28-O8-C9
36	F	319	LMG	C32-C33-C34-C35
39	H	315	SQD	C11-C12-C13-C14
36	D	302	LMG	O6-C5-C6-O5
32	E	312	CLA	C3-C5-C6-C7
32	F	304	CLA	C3-C5-C6-C7
32	a	812	CLA	C3-C5-C6-C7
32	b	840	CLA	C3-C5-C6-C7
35	I	314	LHG	C24-C23-O8-C6
36	j	104	LMG	O6-C5-C6-O5
33	F	302	KC2	CAA-CBA-CGA-O2A
33	N	302	KC2	CAA-CBA-CGA-O1A
33	Q	317	KC2	CAA-CBA-CGA-O2A
33	R	305	KC2	CAA-CBA-CGA-O1A
33	U	304	KC2	CAA-CBA-CGA-O2A
36	D	321	LMG	C4-C5-C6-O5
35	B	308	LHG	O10-C23-O8-C6
35	I	318	LHG	O10-C23-O8-C6
38	D	324	LMU	O5'-C5'-C6'-O6'
32	E	306	CLA	C4-C3-C5-C6
32	I	303	CLA	C4-C3-C5-C6
32	K	308	CLA	C4-C3-C5-C6
32	a	810	CLA	C4-C3-C5-C6
32	a	814	CLA	C4-C3-C5-C6
32	a	827	CLA	C4-C3-C5-C6
32	a	834	CLA	C4-C3-C5-C6
32	b	812	CLA	C4-C3-C5-C6
32	b	829	CLA	C4-C3-C5-C6
32	b	835	CLA	C4-C3-C5-C6
36	L	320	LMG	C4-C5-C6-O5
32	E	306	CLA	C2-C3-C5-C6
32	I	303	CLA	C2-C3-C5-C6
32	K	308	CLA	C2-C3-C5-C6
32	a	803	CLA	C2-C3-C5-C6
32	a	810	CLA	C2-C3-C5-C6
32	a	814	CLA	C2-C3-C5-C6
32	a	827	CLA	C2-C3-C5-C6
32	a	834	CLA	C2-C3-C5-C6
32	b	812	CLA	C2-C3-C5-C6
32	b	829	CLA	C2-C3-C5-C6
32	b	835	CLA	C2-C3-C5-C6
32	C	301	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
32	a	823	CLA	C2A-CAA-CBA-CGA
32	W	312	CLA	C3-C5-C6-C7
36	F	319	LMG	C11-C12-C13-C14
40	Q	318	DGD	O1A-C1A-O1G-C1G
33	F	310	KC2	CAA-CBA-CGA-O1A
33	L	305	KC2	CAA-CBA-CGA-O1A
33	N	308	KC2	CAA-CBA-CGA-O2A
33	Q	317	KC2	CAA-CBA-CGA-O1A
33	W	305	KC2	CAA-CBA-CGA-O1A
33	W	305	KC2	CAA-CBA-CGA-O2A
35	E	321	LHG	C8-C7-O7-C5
37	R	312	A86	C33-C34-O4-C38
36	E	302	LMG	C4-C5-C6-O5
35	B	308	LHG	O9-C7-O7-C5
38	D	324	LMU	C4'-C5'-C6'-O6'
35	a	849	LHG	O10-C23-O8-C6
32	C	306	CLA	C3-C5-C6-C7
32	E	307	CLA	CBA-CGA-O2A-C1
32	H	307	CLA	CBA-CGA-O2A-C1
32	Q	307	CLA	CBA-CGA-O2A-C1
32	a	805	CLA	CBA-CGA-O2A-C1
32	b	812	CLA	CBA-CGA-O2A-C1
32	b	817	CLA	CBA-CGA-O2A-C1
32	b	825	CLA	CBA-CGA-O2A-C1
32	k	203	CLA	CBA-CGA-O2A-C1
35	F	321	LHG	C24-C23-O8-C6
36	D	321	LMG	C29-C28-O8-C9
36	T	301	LMG	C29-C28-O8-C9
39	k	206	SQD	C24-C23-O48-C46
37	L	317	A86	C35-C34-O4-C38
33	F	302	KC2	CAA-CBA-CGA-O1A
33	L	305	KC2	CAA-CBA-CGA-O2A
33	U	304	KC2	CAA-CBA-CGA-O1A
32	I	306	CLA	C10-C11-C12-C13
32	P	309	CLA	C8-C10-C11-C12
32	a	814	CLA	C13-C15-C16-C17
36	P	318	LMG	C28-C29-C30-C31
36	j	104	LMG	C2-C1-O1-C7
39	k	206	SQD	C2-C1-O6-C44
35	A	316	LHG	O7-C5-C6-O8
32	a	822	CLA	O1A-CGA-O2A-C1
32	I	308	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	D	305	CLA	C6-C7-C8-C9
32	D	307	CLA	C6-C7-C8-C9
32	F	303	CLA	C11-C10-C8-C9
32	F	322	CLA	C11-C10-C8-C9
32	Q	303	CLA	C11-C10-C8-C9
32	Q	307	CLA	C11-C10-C8-C9
32	W	309	CLA	C11-C10-C8-C9
32	a	802	CLA	C6-C7-C8-C9
32	a	841	CLA	C11-C10-C8-C9
32	b	807	CLA	C11-C10-C8-C9
32	b	838	CLA	C14-C13-C15-C16
32	a	830	CLA	C8-C10-C11-C12
32	U	305	CLA	C2A-CAA-CBA-CGA
32	b	806	CLA	C2A-CAA-CBA-CGA
34	S	321	DD6	C12-C11-C13-C14
34	V	202	DD6	C12-C11-C13-C14
37	D	323	A86	C-C1-C24-C25
37	L	316	A86	C7-C6-C8-C9
41	a	845	BCR	C37-C22-C23-C24
41	b	842	BCR	C7-C8-C9-C34
41	r	203	BCR	C7-C8-C9-C34
41	r	203	BCR	C11-C12-C13-C35
34	S	321	DD6	C10-C11-C13-C14
34	V	202	DD6	C10-C11-C13-C14
41	b	842	BCR	C7-C8-C9-C10
41	r	203	BCR	C7-C8-C9-C10
36	M	320	LMG	O6-C5-C6-O5
36	E	322	LMG	C11-C12-C13-C14
36	N	301	LMG	C4-C5-C6-O5
39	k	206	SQD	O10-C23-O48-C46
40	Q	318	DGD	C4D-C5D-C6D-O5D
33	C	303	KC2	CAA-CBA-CGA-O2A
33	N	302	KC2	CAA-CBA-CGA-O2A
33	N	308	KC2	CAA-CBA-CGA-O1A
33	P	302	KC2	CAA-CBA-CGA-O1A
33	R	305	KC2	CAA-CBA-CGA-O2A
32	A	307	CLA	C3-C5-C6-C7
32	b	823	CLA	C3-C5-C6-C7
32	Q	306	CLA	C8-C10-C11-C12
32	a	819	CLA	C5-C6-C7-C8
36	E	302	LMG	C28-C29-C30-C31
36	j	104	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
32	A	309	CLA	C8-C10-C11-C12
32	E	306	CLA	C8-C10-C11-C12
32	H	307	CLA	C10-C11-C12-C13
32	I	306	CLA	C15-C16-C17-C18
32	R	310	CLA	C5-C6-C7-C8
32	W	310	CLA	C10-C11-C12-C13
32	a	801	CLA	C13-C15-C16-C17
32	b	821	CLA	C5-C6-C7-C8
32	a	805	CLA	O1A-CGA-O2A-C1
35	a	850	LHG	C23-C24-C25-C26
36	A	318	LMG	C28-C29-C30-C31
36	l	201	LMG	C10-C11-C12-C13
32	a	835	CLA	C8-C10-C11-C12
32	b	828	CLA	C5-C6-C7-C8
32	b	836	CLA	C10-C11-C12-C13
32	S	309	CLA	CBA-CGA-O2A-C1
32	a	820	CLA	CBA-CGA-O2A-C1
35	E	321	LHG	O9-C7-O7-C5
36	A	317	LMG	O9-C10-O7-C8
33	C	303	KC2	CAA-CBA-CGA-O1A
33	P	302	KC2	CAA-CBA-CGA-O2A
38	j	105	LMU	O1'-C1-C2-C3
32	C	307	CLA	C8-C10-C11-C12
32	I	303	CLA	C5-C6-C7-C8
32	a	814	CLA	C5-C6-C7-C8
32	b	807	CLA	C5-C6-C7-C8
35	E	301	LHG	C2-C3-O3-P
36	M	320	LMG	C28-C29-C30-C31
39	H	315	SQD	C7-C8-C9-C10
40	Q	318	DGD	C1B-C2B-C3B-C4B
36	E	320	LMG	C4-C5-C6-O5
36	A	317	LMG	C11-C10-O7-C8
32	a	812	CLA	C5-C6-C7-C8
32	a	823	CLA	C5-C6-C7-C8
32	l	204	CLA	C10-C11-C12-C13
32	Q	301	CLA	C11-C10-C8-C7
32	a	830	CLA	C11-C12-C13-C15
32	b	804	CLA	C3-C5-C6-C7
32	E	307	CLA	O1A-CGA-O2A-C1
32	b	812	CLA	O1A-CGA-O2A-C1
32	b	817	CLA	O1A-CGA-O2A-C1
32	b	825	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	E	315	CLA	C2A-CAA-CBA-CGA
32	a	801	CLA	C2A-CAA-CBA-CGA
32	C	306	CLA	C5-C6-C7-C8
32	b	816	CLA	C5-C6-C7-C8
32	b	835	CLA	C8-C10-C11-C12
36	T	301	LMG	C4-C5-C6-O5
35	F	318	LHG	O10-C23-O8-C6
32	T	306	CLA	C5-C6-C7-C8
36	D	321	LMG	C10-C11-C12-C13
36	D	321	LMG	C28-C29-C30-C31
39	H	315	SQD	C23-C24-C25-C26
36	l	201	LMG	O6-C5-C6-O5
35	I	314	LHG	O2-C2-C3-O3
32	F	303	CLA	C3-C5-C6-C7
32	M	306	CLA	C3-C5-C6-C7
32	A	306	CLA	C13-C15-C16-C17
32	K	308	CLA	C8-C10-C11-C12
32	b	837	CLA	C13-C15-C16-C17
32	k	203	CLA	O1A-CGA-O2A-C1
36	D	321	LMG	O10-C28-O8-C9
35	f	205	LHG	C7-C8-C9-C10
32	D	304	CLA	C10-C11-C12-C13
32	L	307	CLA	C5-C6-C7-C8
32	a	831	CLA	C10-C11-C12-C13
32	a	833	CLA	C15-C16-C17-C18
32	b	823	CLA	C10-C11-C12-C13
36	E	302	LMG	C11-C10-O7-C8
32	D	311	CLA	C8-C10-C11-C12
32	D	311	CLA	C10-C11-C12-C13
32	I	317	CLA	C13-C15-C16-C17
32	Q	306	CLA	C5-C6-C7-C8
32	a	827	CLA	C15-C16-C17-C18
32	b	815	CLA	C13-C15-C16-C17
35	A	316	LHG	C3-O3-P-O6
35	A	316	LHG	C4-O6-P-O3
35	B	308	LHG	C3-O3-P-O6
35	B	308	LHG	C4-O6-P-O3
35	D	320	LHG	C3-O3-P-O6
35	D	320	LHG	C4-O6-P-O3
35	E	301	LHG	C4-O6-P-O3
35	E	321	LHG	C3-O3-P-O6
35	F	318	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
35	F	321	LHG	C3-O3-P-O6
35	I	314	LHG	C3-O3-P-O6
35	I	314	LHG	C4-O6-P-O3
35	a	849	LHG	C3-O3-P-O6
35	a	850	LHG	C3-O3-P-O6
35	f	205	LHG	C4-O6-P-O3
32	O	309	CLA	C3-C5-C6-C7
32	Q	303	CLA	C3-C5-C6-C7
32	b	832	CLA	CBA-CGA-O2A-C1
36	F	319	LMG	C10-C11-C12-C13
35	E	321	LHG	C1-C2-C3-O3
35	I	314	LHG	C1-C2-C3-O3
32	D	314	CLA	C4-C3-C5-C6
32	b	804	CLA	C4-C3-C5-C6
32	M	312	CLA	C8-C10-C11-C12
32	B	309	CLA	C2A-CAA-CBA-CGA
32	L	301	CLA	C2A-CAA-CBA-CGA
32	a	838	CLA	C2A-CAA-CBA-CGA
32	b	818	CLA	C16-C17-C18-C19
32	r	201	CLA	C11-C12-C13-C15
33	G	302	KC2	CAA-CBA-CGA-O2A
33	J	310	KC2	CAA-CBA-CGA-O2A
36	F	319	LMG	C29-C28-O8-C9
40	Q	318	DGD	O6D-C5D-C6D-O5D
32	Q	307	CLA	C10-C11-C12-C13
40	Q	318	DGD	C4E-C5E-C6E-O5E
35	F	318	LHG	C8-C7-O7-C5
35	I	314	LHG	C8-C7-O7-C5
36	D	325	LMG	C11-C10-O7-C8
36	j	104	LMG	C11-C10-O7-C8
32	C	305	CLA	C8-C10-C11-C12
32	E	308	CLA	C8-C10-C11-C12
32	a	852	CLA	C13-C15-C16-C17
36	E	302	LMG	C32-C33-C34-C35
36	E	322	LMG	C32-C33-C34-C35
36	F	319	LMG	C30-C31-C32-C33
40	Q	318	DGD	C4B-C5B-C6B-C7B
40	b	846	DGD	C8A-C9A-CAA-CBA
37	L	315	A86	C9-C10-C11-C12
37	S	317	A86	C9-C10-C11-C12
32	b	839	CLA	C16-C17-C18-C19
40	b	846	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
35	W	319	LHG	C10-C11-C12-C13
36	S	322	LMG	C11-C12-C13-C14
36	A	317	LMG	C7-C8-O7-C10
36	D	303	LMG	C9-C8-O7-C10
36	D	321	LMG	O9-C10-O7-C8
36	D	325	LMG	O9-C10-O7-C8
36	j	104	LMG	O9-C10-O7-C8
32	a	807	CLA	C5-C6-C7-C8
36	j	104	LMG	C10-C11-C12-C13
36	l	201	LMG	C33-C34-C35-C36
40	Q	318	DGD	CDB-CEB-CFB-CGB
40	b	846	DGD	C3A-C4A-C5A-C6A
36	F	320	LMG	C12-C13-C14-C15
36	N	301	LMG	C30-C31-C32-C33
35	B	308	LHG	O2-C2-C3-O3
35	E	321	LHG	C16-C17-C18-C19
35	P	317	LHG	C15-C16-C17-C18
36	E	320	LMG	C2-C1-O1-C7
35	f	205	LHG	C34-C35-C36-C37
36	E	320	LMG	C11-C12-C13-C14
39	H	315	SQD	C11-C10-C9-C8
32	a	835	CLA	C5-C6-C7-C8
32	a	837	CLA	C6-C7-C8-C10
32	a	852	CLA	C16-C17-C18-C20
32	b	829	CLA	C6-C7-C8-C10
32	I	317	CLA	C4-C3-C5-C6
32	k	201	CLA	C4-C3-C5-C6
36	l	201	LMG	C22-C23-C24-C25
40	Q	318	DGD	C6B-C7B-C8B-C9B
32	I	308	CLA	C2-C3-C5-C6
32	I	317	CLA	C2-C3-C5-C6
32	D	305	CLA	C11-C10-C8-C9
32	a	819	CLA	C14-C13-C15-C16
32	b	808	CLA	C11-C12-C13-C14
32	b	833	CLA	C6-C7-C8-C9
32	b	833	CLA	C13-C15-C16-C17
36	N	301	LMG	C28-C29-C30-C31
35	a	850	LHG	C24-C25-C26-C27
38	V	205	LMU	C2-C3-C4-C5
38	V	205	LMU	C4-C5-C6-C7
40	b	846	DGD	C5A-C6A-C7A-C8A
32	a	823	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	G	302	KC2	CAA-CBA-CGA-O1A
32	Q	307	CLA	O1A-CGA-O2A-C1
41	l	206	BCR	C7-C8-C9-C34
36	D	303	LMG	C32-C33-C34-C35
35	I	314	LHG	O1-C1-C2-C3
35	P	317	LHG	O1-C1-C2-C3
35	a	849	LHG	O1-C1-C2-C3
35	f	205	LHG	O1-C1-C2-C3
41	l	206	BCR	C7-C8-C9-C10
32	O	307	CLA	C3-C5-C6-C7
32	k	201	CLA	C3-C5-C6-C7
35	F	321	LHG	O9-C7-O7-C5
35	a	849	LHG	O9-C7-O7-C5
32	a	819	CLA	C8-C10-C11-C12
32	b	823	CLA	C15-C16-C17-C18
35	a	850	LHG	C8-C7-O7-C5
35	f	205	LHG	C29-C30-C31-C32
36	D	303	LMG	C29-C30-C31-C32
36	j	104	LMG	C30-C31-C32-C33
38	D	324	LMU	C7-C8-C9-C10
35	a	849	LHG	C7-C8-C9-C10
35	I	318	LHG	C24-C25-C26-C27
36	A	317	LMG	C30-C31-C32-C33
36	D	321	LMG	C31-C32-C33-C34
36	N	301	LMG	C11-C12-C13-C14
36	P	318	LMG	C36-C37-C38-C39
40	b	846	DGD	C2B-C3B-C4B-C5B
32	A	304	CLA	C4B-C3B-CAB-CBB
32	F	308	CLA	C4B-C3B-CAB-CBB
32	G	301	CLA	C4B-C3B-CAB-CBB
32	H	302	CLA	C4B-C3B-CAB-CBB
32	H	309	CLA	C4B-C3B-CAB-CBB
32	I	301	CLA	C4B-C3B-CAB-CBB
32	J	312	CLA	C4B-C3B-CAB-CBB
32	L	301	CLA	C4B-C3B-CAB-CBB
32	P	309	CLA	C4B-C3B-CAB-CBB
32	Q	301	CLA	C4B-C3B-CAB-CBB
32	Q	310	CLA	C4B-C3B-CAB-CBB
32	S	304	CLA	C4B-C3B-CAB-CBB
32	S	313	CLA	C4B-C3B-CAB-CBB
32	T	302	CLA	C4B-C3B-CAB-CBB
32	T	307	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	U	302	CLA	C4B-C3B-CAB-CBB
32	W	306	CLA	C4B-C3B-CAB-CBB
32	W	307	CLA	C4B-C3B-CAB-CBB
32	W	311	CLA	C4B-C3B-CAB-CBB
32	W	312	CLA	C4B-C3B-CAB-CBB
32	a	816	CLA	C4B-C3B-CAB-CBB
32	a	826	CLA	C4B-C3B-CAB-CBB
32	a	836	CLA	C4B-C3B-CAB-CBB
32	a	839	CLA	C4B-C3B-CAB-CBB
32	b	808	CLA	C4B-C3B-CAB-CBB
32	b	838	CLA	C4B-C3B-CAB-CBB
32	b	840	CLA	C4B-C3B-CAB-CBB
32	j	101	CLA	C4B-C3B-CAB-CBB
32	k	203	CLA	C4B-C3B-CAB-CBB
32	a	829	CLA	C11-C12-C13-C15
32	a	852	CLA	C16-C17-C18-C19
32	I	301	CLA	C13-C15-C16-C17
36	F	319	LMG	C13-C14-C15-C16
36	P	318	LMG	C16-C17-C18-C19
36	j	104	LMG	C29-C30-C31-C32
35	P	317	LHG	C28-C29-C30-C31
36	A	317	LMG	C31-C32-C33-C34
36	N	301	LMG	C31-C32-C33-C34
36	P	318	LMG	C31-C32-C33-C34
36	S	322	LMG	C14-C15-C16-C17
38	I	315	LMU	C5-C6-C7-C8
35	D	320	LHG	C7-C8-C9-C10
32	E	304	CLA	C5-C6-C7-C8
32	E	304	CLA	C10-C11-C12-C13
32	T	306	CLA	C8-C10-C11-C12
32	b	831	CLA	C8-C10-C11-C12
33	J	310	KC2	CAA-CBA-CGA-O1A
35	I	314	LHG	O10-C23-O8-C6
36	l	201	LMG	C35-C36-C37-C38
40	b	846	DGD	C7B-C8B-C9B-CAB
32	b	837	CLA	CBA-CGA-O2A-C1
40	b	846	DGD	C9B-CAB-CBB-CCB
32	D	314	CLA	O1D-CGD-O2D-CED
32	A	303	CLA	C3A-C2A-CAA-CBA
32	A	306	CLA	C3A-C2A-CAA-CBA
32	B	304	CLA	C3A-C2A-CAA-CBA
32	C	305	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	D	306	CLA	C3A-C2A-CAA-CBA
32	E	315	CLA	C3A-C2A-CAA-CBA
32	F	303	CLA	C3A-C2A-CAA-CBA
32	H	304	CLA	C3A-C2A-CAA-CBA
32	I	302	CLA	C3A-C2A-CAA-CBA
32	I	305	CLA	C3A-C2A-CAA-CBA
32	I	308	CLA	C3A-C2A-CAA-CBA
32	J	306	CLA	C3A-C2A-CAA-CBA
32	K	304	CLA	C3A-C2A-CAA-CBA
32	M	309	CLA	C3A-C2A-CAA-CBA
32	N	305	CLA	C3A-C2A-CAA-CBA
32	P	304	CLA	C3A-C2A-CAA-CBA
32	Q	301	CLA	C3A-C2A-CAA-CBA
32	Q	303	CLA	C3A-C2A-CAA-CBA
32	S	307	CLA	C3A-C2A-CAA-CBA
32	T	302	CLA	C3A-C2A-CAA-CBA
32	T	305	CLA	C3A-C2A-CAA-CBA
32	T	309	CLA	C3A-C2A-CAA-CBA
32	W	306	CLA	C3A-C2A-CAA-CBA
32	W	310	CLA	C3A-C2A-CAA-CBA
32	a	803	CLA	C3A-C2A-CAA-CBA
32	a	806	CLA	C3A-C2A-CAA-CBA
32	a	811	CLA	C3A-C2A-CAA-CBA
32	a	813	CLA	C3A-C2A-CAA-CBA
32	a	822	CLA	C3A-C2A-CAA-CBA
32	a	827	CLA	C3A-C2A-CAA-CBA
32	a	829	CLA	C3A-C2A-CAA-CBA
32	b	802	CLA	C3A-C2A-CAA-CBA
32	b	804	CLA	C3A-C2A-CAA-CBA
32	b	837	CLA	C3A-C2A-CAA-CBA
32	b	839	CLA	C3A-C2A-CAA-CBA
32	l	203	CLA	C3A-C2A-CAA-CBA
32	J	304	CLA	C5-C6-C7-C8
32	b	819	CLA	C10-C11-C12-C13
38	V	205	LMU	C2-C1-O1'-C1'
38	j	105	LMU	C2-C1-O1'-C1'
35	E	301	LHG	C27-C28-C29-C30
35	W	319	LHG	C28-C29-C30-C31
37	G	310	A86	C35-C34-O4-C38
37	L	316	A86	C33-C34-O4-C38
36	M	320	LMG	C4-C5-C6-O5
32	H	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	b	818	CLA	C16-C17-C18-C20
36	P	318	LMG	C30-C31-C32-C33
40	b	846	DGD	C5B-C6B-C7B-C8B
36	E	302	LMG	O1-C7-C8-C9
36	N	301	LMG	O1-C7-C8-C9
36	S	322	LMG	C7-C8-C9-O8
32	F	303	CLA	O2A-C1-C2-C3
37	D	323	A86	C9-C10-C11-C13
37	F	313	A86	C9-C10-C11-C13
37	G	310	A86	C9-C10-C11-C13
37	O	311	A86	C9-C10-C11-C13
37	T	312	A86	C9-C10-C11-C13
35	P	317	LHG	C23-C24-C25-C26
40	Q	318	DGD	CBB-CCB-CDB-CEB
36	T	301	LMG	O10-C28-O8-C9
32	A	309	CLA	C4-C3-C5-C6
32	a	842	CLA	C4-C3-C5-C6
32	a	853	CLA	C4-C3-C5-C6
32	a	829	CLA	CBA-CGA-O2A-C1
32	J	304	CLA	C2-C3-C5-C6
32	a	842	CLA	C2-C3-C5-C6
32	a	853	CLA	C2-C3-C5-C6
32	b	824	CLA	C2-C3-C5-C6
32	k	201	CLA	C2-C3-C5-C6
36	N	301	LMG	C11-C10-O7-C8
36	W	320	LMG	C11-C10-O7-C8
35	W	319	LHG	C15-C16-C17-C18
36	j	104	LMG	C11-C12-C13-C14
37	J	313	A86	C35-C34-O4-C38
32	H	310	CLA	C2A-CAA-CBA-CGA
32	Q	309	CLA	C2A-CAA-CBA-CGA
32	a	822	CLA	C8-C10-C11-C12
35	M	319	LHG	C28-C29-C30-C31
36	E	302	LMG	C29-C30-C31-C32
36	N	301	LMG	C29-C30-C31-C32
39	H	315	SQD	C14-C15-C16-C17
40	b	846	DGD	O1A-C1A-O1G-C1G
32	A	301	CLA	C2B-C3B-CAB-CBB
32	A	304	CLA	C2B-C3B-CAB-CBB
32	B	305	CLA	C2B-C3B-CAB-CBB
32	B	309	CLA	C2B-C3B-CAB-CBB
32	D	314	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	E	307	CLA	C2B-C3B-CAB-CBB
32	E	309	CLA	C2B-C3B-CAB-CBB
32	F	308	CLA	C2B-C3B-CAB-CBB
32	G	301	CLA	C2B-C3B-CAB-CBB
32	H	302	CLA	C2B-C3B-CAB-CBB
32	H	309	CLA	C2B-C3B-CAB-CBB
32	I	301	CLA	C2B-C3B-CAB-CBB
32	J	312	CLA	C2B-C3B-CAB-CBB
32	K	301	CLA	C2B-C3B-CAB-CBB
32	L	301	CLA	C2B-C3B-CAB-CBB
32	O	308	CLA	C2B-C3B-CAB-CBB
32	P	309	CLA	C2B-C3B-CAB-CBB
32	P	311	CLA	C2B-C3B-CAB-CBB
32	Q	301	CLA	C2B-C3B-CAB-CBB
32	Q	310	CLA	C2B-C3B-CAB-CBB
32	R	301	CLA	C2B-C3B-CAB-CBB
32	S	304	CLA	C2B-C3B-CAB-CBB
32	S	305	CLA	C2B-C3B-CAB-CBB
32	S	313	CLA	C2B-C3B-CAB-CBB
32	T	302	CLA	C2B-C3B-CAB-CBB
32	T	307	CLA	C2B-C3B-CAB-CBB
32	T	309	CLA	C2B-C3B-CAB-CBB
32	U	302	CLA	C2B-C3B-CAB-CBB
32	U	303	CLA	C2B-C3B-CAB-CBB
32	V	203	CLA	C2B-C3B-CAB-CBB
32	W	306	CLA	C2B-C3B-CAB-CBB
32	W	307	CLA	C2B-C3B-CAB-CBB
32	W	311	CLA	C2B-C3B-CAB-CBB
32	W	312	CLA	C2B-C3B-CAB-CBB
32	a	816	CLA	C2B-C3B-CAB-CBB
32	a	826	CLA	C2B-C3B-CAB-CBB
32	a	836	CLA	C2B-C3B-CAB-CBB
32	a	839	CLA	C2B-C3B-CAB-CBB
32	b	808	CLA	C2B-C3B-CAB-CBB
32	b	828	CLA	C2B-C3B-CAB-CBB
32	b	840	CLA	C2B-C3B-CAB-CBB
32	f	203	CLA	C2B-C3B-CAB-CBB
32	j	101	CLA	C2B-C3B-CAB-CBB
32	k	203	CLA	C2B-C3B-CAB-CBB
35	f	205	LHG	O2-C2-C3-O3
32	R	308	CLA	C3-C5-C6-C7
32	a	820	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	a	818	CLA	CBA-CGA-O2A-C1
32	S	309	CLA	O1A-CGA-O2A-C1
32	a	820	CLA	O1A-CGA-O2A-C1
36	F	319	LMG	O10-C28-O8-C9
35	B	308	LHG	C1-C2-C3-O3
36	D	303	LMG	O9-C10-O7-C8
36	N	301	LMG	O9-C10-O7-C8
36	W	320	LMG	O9-C10-O7-C8
32	C	307	CLA	C2-C1-O2A-CGA
32	a	805	CLA	C2-C1-O2A-CGA
36	F	319	LMG	C34-C35-C36-C37
36	T	301	LMG	C30-C31-C32-C33
36	l	201	LMG	C17-C18-C19-C20
32	b	838	CLA	C10-C11-C12-C13
40	Q	318	DGD	C2B-C3B-C4B-C5B
41	a	845	BCR	C23-C24-C25-C30
41	a	846	BCR	C23-C24-C25-C26
41	a	846	BCR	C23-C24-C25-C30
41	b	842	BCR	C1-C6-C7-C8
41	b	842	BCR	C5-C6-C7-C8
41	b	844	BCR	C1-C6-C7-C8
41	b	844	BCR	C23-C24-C25-C26
41	j	102	BCR	C23-C24-C25-C30
41	l	205	BCR	C23-C24-C25-C30
41	r	205	BCR	C23-C24-C25-C26
41	r	205	BCR	C23-C24-C25-C30
32	D	312	CLA	CBA-CGA-O2A-C1
37	R	312	A86	C35-C34-O4-C38
32	A	309	CLA	C5-C6-C7-C8
36	D	321	LMG	C11-C10-O7-C8
36	P	318	LMG	C38-C39-C40-C41
36	l	201	LMG	C15-C16-C17-C18
38	j	105	LMU	O5B-C5B-C6B-O6B
36	j	104	LMG	C32-C33-C34-C35
32	b	818	CLA	C15-C16-C17-C18
33	T	303	KC2	CAA-CBA-CGA-O1A
35	D	320	LHG	C11-C12-C13-C14
36	D	321	LMG	C15-C16-C17-C18
40	Q	318	DGD	C8B-C9B-CAB-CBB
32	a	805	CLA	C4-C3-C5-C6
32	b	824	CLA	C4-C3-C5-C6
32	A	309	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	E	308	CLA	C6-C7-C8-C10
32	K	308	CLA	C12-C13-C15-C16
32	M	312	CLA	C2-C3-C5-C6
32	N	313	CLA	C2-C3-C5-C6
32	O	305	CLA	C6-C7-C8-C10
32	T	306	CLA	C6-C7-C8-C10
32	a	805	CLA	C2-C3-C5-C6
32	a	810	CLA	C6-C7-C8-C10
32	a	834	CLA	C11-C10-C8-C7
32	a	841	CLA	C6-C7-C8-C10
32	a	841	CLA	C12-C13-C15-C16
32	b	808	CLA	C11-C12-C13-C15
32	b	836	CLA	C6-C7-C8-C10
32	b	839	CLA	C6-C7-C8-C10
32	l	203	CLA	C11-C12-C13-C15
35	W	319	LHG	O10-C23-O8-C6
32	F	306	CLA	C5-C6-C7-C8
32	a	837	CLA	C6-C7-C8-C9
32	b	839	CLA	C16-C17-C18-C20
32	k	203	CLA	C6-C7-C8-C10
43	a	848	PQN	C26-C27-C28-C29
35	B	308	LHG	C23-C24-C25-C26
32	C	307	CLA	CBA-CGA-O2A-C1
32	D	306	CLA	CBA-CGA-O2A-C1
32	b	833	CLA	CBA-CGA-O2A-C1
35	D	320	LHG	C29-C30-C31-C32
38	j	105	LMU	C5-C6-C7-C8
39	H	315	SQD	C26-C27-C28-C29
32	C	308	CLA	C2A-CAA-CBA-CGA
32	F	322	CLA	C2A-CAA-CBA-CGA
32	Q	306	CLA	C2A-CAA-CBA-CGA
32	b	803	CLA	C2A-CAA-CBA-CGA
32	b	813	CLA	C2A-CAA-CBA-CGA
35	M	319	LHG	C16-C17-C18-C19
36	F	319	LMG	O6-C5-C6-O5
35	B	308	LHG	C26-C27-C28-C29
35	F	321	LHG	C23-C24-C25-C26
36	P	318	LMG	O6-C5-C6-O5
36	S	322	LMG	C12-C13-C14-C15
36	l	201	LMG	C32-C33-C34-C35
33	C	303	KC2	C2B-C3B-CAB-CBB
33	C	303	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
33	F	302	KC2	C2B-C3B-CAB-CBB
33	G	302	KC2	C2C-C3C-CAC-CBC
33	H	303	KC2	C2B-C3B-CAB-CBB
33	H	303	KC2	C2C-C3C-CAC-CBC
33	K	309	KC2	C2C-C3C-CAC-CBC
33	L	305	KC2	C2B-C3B-CAB-CBB
33	L	306	KC2	C2C-C3C-CAC-CBC
33	M	321	KC2	C2B-C3B-CAB-CBB
33	N	306	KC2	C2B-C3B-CAB-CBB
33	N	307	KC2	C2B-C3B-CAB-CBB
33	P	302	KC2	C2B-C3B-CAB-CBB
33	P	312	KC2	C2C-C3C-CAC-CBC
33	Q	302	KC2	C2B-C3B-CAB-CBB
33	R	302	KC2	C2C-C3C-CAC-CBC
33	R	305	KC2	C2B-C3B-CAB-CBB
33	S	303	KC2	C2B-C3B-CAB-CBB
33	W	308	KC2	C2B-C3B-CAB-CBB
33	W	314	KC2	C2C-C3C-CAC-CBC
32	b	833	CLA	C3-C5-C6-C7
35	F	318	LHG	C29-C30-C31-C32
32	l	204	CLA	C5-C6-C7-C8
35	F	318	LHG	C11-C12-C13-C14
36	D	321	LMG	C12-C13-C14-C15
36	D	321	LMG	C16-C17-C18-C19
36	D	302	LMG	C10-C11-C12-C13
35	F	321	LHG	C8-C7-O7-C5
35	a	849	LHG	C8-C7-O7-C5
36	D	303	LMG	C11-C10-O7-C8
40	b	846	DGD	C2B-C1B-O2G-C2G
36	T	301	LMG	O6-C5-C6-O5
33	C	303	KC2	C4B-C3B-CAB-CBB
33	C	303	KC2	C4C-C3C-CAC-CBC
33	G	302	KC2	C4C-C3C-CAC-CBC
33	H	303	KC2	C4B-C3B-CAB-CBB
33	H	303	KC2	C4C-C3C-CAC-CBC
33	I	316	KC2	C4B-C3B-CAB-CBB
33	J	303	KC2	C4B-C3B-CAB-CBB
33	K	302	KC2	C4C-C3C-CAC-CBC
33	K	305	KC2	C4B-C3B-CAB-CBB
33	K	305	KC2	C4C-C3C-CAC-CBC
33	K	309	KC2	C4C-C3C-CAC-CBC
33	L	306	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
33	M	313	KC2	C4B-C3B-CAB-CBB
33	N	307	KC2	C4B-C3B-CAB-CBB
33	N	308	KC2	C4B-C3B-CAB-CBB
33	P	302	KC2	C4B-C3B-CAB-CBB
33	P	312	KC2	C4C-C3C-CAC-CBC
33	R	302	KC2	C4C-C3C-CAC-CBC
33	R	305	KC2	C4B-C3B-CAB-CBB
33	S	312	KC2	C4B-C3B-CAB-CBB
33	T	304	KC2	C4C-C3C-CAC-CBC
33	U	304	KC2	C4C-C3C-CAC-CBC
33	W	303	KC2	C4B-C3B-CAB-CBB
33	W	303	KC2	C4C-C3C-CAC-CBC
33	W	308	KC2	C4B-C3B-CAB-CBB
33	W	314	KC2	C4B-C3B-CAB-CBB
33	W	314	KC2	C4C-C3C-CAC-CBC
32	a	823	CLA	C10-C11-C12-C13
32	b	824	CLA	C5-C6-C7-C8
36	E	320	LMG	C13-C14-C15-C16
32	a	838	CLA	C3-C5-C6-C7
36	T	301	LMG	C28-C29-C30-C31
36	E	320	LMG	O7-C8-C9-O8
36	l	201	LMG	O1-C7-C8-O7
40	b	846	DGD	O2G-C2G-C3G-O3G
35	E	301	LHG	C10-C11-C12-C13
35	E	321	LHG	C30-C31-C32-C33
36	E	302	LMG	C30-C31-C32-C33
33	W	314	KC2	CAA-CBA-CGA-O1A
35	B	308	LHG	C11-C10-C9-C8
36	W	320	LMG	C13-C14-C15-C16
32	J	304	CLA	C4-C3-C5-C6
32	M	312	CLA	C4-C3-C5-C6
32	N	313	CLA	C4-C3-C5-C6
32	a	830	CLA	C4-C3-C5-C6
32	D	314	CLA	C2-C3-C5-C6
32	E	312	CLA	C2-C3-C5-C6
34	A	314	DD6	C27-C29-C30-C31
34	D	318	DD6	C27-C29-C30-C31
34	M	316	DD6	C27-C29-C30-C31
34	W	317	DD6	C27-C29-C30-C31
38	D	324	LMU	C6-C7-C8-C9
32	E	308	CLA	C6-C7-C8-C9
32	J	312	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
32	K	308	CLA	C6-C7-C8-C9
32	K	308	CLA	C14-C13-C15-C16
32	O	305	CLA	C6-C7-C8-C9
32	T	306	CLA	C6-C7-C8-C9
32	a	810	CLA	C6-C7-C8-C9
32	a	830	CLA	C11-C12-C13-C14
32	a	834	CLA	C11-C10-C8-C9
32	a	841	CLA	C6-C7-C8-C9
32	a	841	CLA	C14-C13-C15-C16
32	b	836	CLA	C6-C7-C8-C9
32	b	839	CLA	C6-C7-C8-C9
32	b	840	CLA	C6-C7-C8-C9
32	l	203	CLA	C11-C12-C13-C14
36	D	303	LMG	O6-C5-C6-O5
32	b	835	CLA	C3-C5-C6-C7
32	P	311	CLA	O1D-CGD-O2D-CED
32	L	314	CLA	C2A-CAA-CBA-CGA
32	b	830	CLA	C2A-CAA-CBA-CGA
36	D	303	LMG	C31-C32-C33-C34
38	I	315	LMU	O5B-C5B-C6B-O6B
32	a	807	CLA	C8-C10-C11-C12
32	b	822	CLA	C8-C10-C11-C12
39	H	315	SQD	C12-C13-C14-C15
37	D	323	A86	C2-C1-C24-C25
37	L	316	A86	C2-C1-C24-C25
41	a	843	BCR	C21-C22-C23-C24
38	D	324	LMU	C1-C2-C3-C4
32	b	832	CLA	O1A-CGA-O2A-C1
32	A	303	CLA	C1A-C2A-CAA-CBA
32	A	306	CLA	C1A-C2A-CAA-CBA
32	C	307	CLA	C1A-C2A-CAA-CBA
32	D	305	CLA	C1A-C2A-CAA-CBA
32	D	306	CLA	C1A-C2A-CAA-CBA
32	D	308	CLA	C1A-C2A-CAA-CBA
32	D	310	CLA	C1A-C2A-CAA-CBA
32	E	310	CLA	C1A-C2A-CAA-CBA
32	E	311	CLA	C1A-C2A-CAA-CBA
32	F	303	CLA	C1A-C2A-CAA-CBA
32	I	302	CLA	C1A-C2A-CAA-CBA
32	I	307	CLA	C1A-C2A-CAA-CBA
32	J	306	CLA	C1A-C2A-CAA-CBA
32	J	309	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	K	304	CLA	C1A-C2A-CAA-CBA
32	M	309	CLA	C1A-C2A-CAA-CBA
32	N	305	CLA	C1A-C2A-CAA-CBA
32	O	305	CLA	C1A-C2A-CAA-CBA
32	P	304	CLA	C1A-C2A-CAA-CBA
32	R	306	CLA	C1A-C2A-CAA-CBA
32	S	307	CLA	C1A-C2A-CAA-CBA
32	S	310	CLA	C1A-C2A-CAA-CBA
32	T	302	CLA	C1A-C2A-CAA-CBA
32	T	305	CLA	C1A-C2A-CAA-CBA
32	U	306	CLA	C1A-C2A-CAA-CBA
32	W	310	CLA	C1A-C2A-CAA-CBA
32	W	312	CLA	C1A-C2A-CAA-CBA
32	a	803	CLA	C1A-C2A-CAA-CBA
32	a	805	CLA	C1A-C2A-CAA-CBA
32	a	806	CLA	C1A-C2A-CAA-CBA
32	a	811	CLA	C1A-C2A-CAA-CBA
32	a	813	CLA	C1A-C2A-CAA-CBA
32	a	816	CLA	C1A-C2A-CAA-CBA
32	a	820	CLA	C1A-C2A-CAA-CBA
32	a	822	CLA	C1A-C2A-CAA-CBA
32	a	828	CLA	C1A-C2A-CAA-CBA
32	a	829	CLA	C1A-C2A-CAA-CBA
32	a	840	CLA	C1A-C2A-CAA-CBA
32	b	801	CLA	C1A-C2A-CAA-CBA
32	b	815	CLA	C1A-C2A-CAA-CBA
32	b	818	CLA	C1A-C2A-CAA-CBA
32	b	822	CLA	C1A-C2A-CAA-CBA
32	b	824	CLA	C1A-C2A-CAA-CBA
32	b	830	CLA	C1A-C2A-CAA-CBA
32	b	836	CLA	C1A-C2A-CAA-CBA
32	k	203	CLA	C1A-C2A-CAA-CBA
32	a	829	CLA	C11-C12-C13-C14
32	b	829	CLA	C6-C7-C8-C9
32	r	201	CLA	C11-C12-C13-C14
43	a	848	PQN	C26-C27-C28-C30
40	b	846	DGD	O1B-C1B-O2G-C2G
33	O	310	KC2	CAA-CBA-CGA-O1A
35	I	318	LHG	C25-C26-C27-C28
35	a	849	LHG	C15-C16-C17-C18
32	a	853	CLA	C13-C15-C16-C17
32	b	807	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	G	310	A86	C33-C34-O4-C38
35	P	317	LHG	C3-O3-P-O6
35	a	849	LHG	C33-C34-C35-C36
35	A	316	LHG	C2-C3-O3-P
32	A	303	CLA	C8-C10-C11-C12
32	b	810	CLA	C10-C11-C12-C13
35	f	205	LHG	O6-C4-C5-C6
36	E	322	LMG	C31-C32-C33-C34
36	D	325	LMG	O6-C5-C6-O5
32	b	828	CLA	C8-C10-C11-C12
35	E	301	LHG	C13-C14-C15-C16
35	E	301	LHG	C25-C26-C27-C28
35	f	205	LHG	C11-C12-C13-C14
33	O	302	KC2	CAA-CBA-CGA-O1A
33	O	310	KC2	CAA-CBA-CGA-O2A
33	T	303	KC2	CAA-CBA-CGA-O2A
33	W	314	KC2	CAA-CBA-CGA-O2A
36	L	320	LMG	C30-C31-C32-C33
38	I	315	LMU	C2-C3-C4-C5
35	A	316	LHG	C1-C2-C3-O3
36	A	317	LMG	C33-C34-C35-C36
38	D	324	LMU	C5-C6-C7-C8
32	b	803	CLA	C15-C16-C17-C18
36	E	302	LMG	C14-C15-C16-C17
36	N	301	LMG	C32-C33-C34-C35
36	S	322	LMG	C13-C14-C15-C16
38	j	105	LMU	C4-C5-C6-C7
38	j	105	LMU	C3-C4-C5-C6
32	l	203	CLA	O1D-CGD-O2D-CED
35	F	321	LHG	C4-C5-C6-O8
35	I	314	LHG	C4-C5-C6-O8
36	A	318	LMG	C7-C8-C9-O8
36	F	319	LMG	C7-C8-C9-O8
39	k	206	SQD	O6-C44-C45-C46
40	Q	318	DGD	C3A-C4A-C5A-C6A
33	W	303	KC2	CAA-CBA-CGA-O1A
35	F	318	LHG	C24-C23-O8-C6
32	a	802	CLA	C8-C10-C11-C12
32	b	837	CLA	O1A-CGA-O2A-C1
36	A	317	LMG	C8-C7-O1-C1
36	D	325	LMG	C8-C7-O1-C1
36	j	104	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
32	H	304	CLA	C2C-C3C-CAC-CBC
35	I	318	LHG	C11-C10-C9-C8
35	W	319	LHG	C32-C33-C34-C35
36	E	322	LMG	C29-C30-C31-C32
39	H	315	SQD	C17-C18-C19-C20
32	C	309	CLA	C2A-CAA-CBA-CGA
32	a	826	CLA	C13-C15-C16-C17
35	W	319	LHG	C19-C20-C21-C22
36	l	201	LMG	C24-C25-C26-C27
38	J	318	LMU	O5'-C5'-C6'-O6'
36	T	301	LMG	C16-C17-C18-C19
36	W	320	LMG	O6-C5-C6-O5
32	W	312	CLA	C5-C6-C7-C8
36	P	318	LMG	C11-C10-O7-C8
32	E	312	CLA	C5-C6-C7-C8
32	a	853	CLA	C15-C16-C17-C18
32	b	804	CLA	C10-C11-C12-C13
36	F	320	LMG	O6-C5-C6-O5
38	I	315	LMU	O5'-C5'-C6'-O6'
32	E	312	CLA	C4-C3-C5-C6
32	O	309	CLA	C4-C3-C5-C6
32	a	819	CLA	C4-C3-C5-C6
36	W	320	LMG	C15-C16-C17-C18
37	O	311	A86	C9-C10-C11-C12
37	T	312	A86	C9-C10-C11-C12
35	F	318	LHG	C7-C8-C9-C10
32	b	829	CLA	CBA-CGA-O2A-C1
35	A	316	LHG	C12-C13-C14-C15
32	M	312	CLA	C10-C11-C12-C13
33	P	312	KC2	CAA-CBA-CGA-O2A
32	A	304	CLA	C15-C16-C17-C18
32	b	804	CLA	C2-C1-O2A-CGA
38	V	205	LMU	C3'-C4'-O1B-C1B
36	S	322	LMG	C15-C16-C17-C18
32	A	305	CLA	C10-C11-C12-C13
32	a	826	CLA	C10-C11-C12-C13
32	G	308	CLA	C6-C7-C8-C9
32	K	306	CLA	CBA-CGA-O2A-C1
32	T	308	CLA	CBA-CGA-O2A-C1
32	a	826	CLA	CBA-CGA-O2A-C1
35	F	321	LHG	O10-C23-O8-C6
35	D	320	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
32	a	810	CLA	C13-C15-C16-C17
32	D	307	CLA	C8-C10-C11-C12
32	O	305	CLA	C15-C16-C17-C18
32	a	826	CLA	C15-C16-C17-C18
32	a	830	CLA	C10-C11-C12-C13
32	l	203	CLA	C5-C6-C7-C8
32	D	312	CLA	O1A-CGA-O2A-C1
32	a	816	CLA	CBD-CGD-O2D-CED
33	O	302	KC2	CAA-CBA-CGA-O2A
33	W	303	KC2	CAA-CBA-CGA-O2A
32	A	308	CLA	C5-C6-C7-C8
32	Q	303	CLA	C10-C11-C12-C13
36	N	301	LMG	C2-C1-O1-C7
38	D	324	LMU	C2'-C1'-O1'-C1
38	V	205	LMU	C5'-C4'-O1B-C1B
36	F	319	LMG	O7-C8-C9-O8
39	H	315	SQD	O47-C45-C46-O48
37	L	316	A86	C35-C34-O4-C38
32	a	818	CLA	O1A-CGA-O2A-C1
32	a	829	CLA	O1A-CGA-O2A-C1
38	I	315	LMU	C9-C10-C11-C12
32	a	802	CLA	C4-C3-C5-C6
32	A	304	CLA	C11-C12-C13-C15
32	D	305	CLA	C6-C7-C8-C10
32	F	303	CLA	C11-C10-C8-C7
32	F	322	CLA	C11-C10-C8-C7
32	I	306	CLA	C12-C13-C15-C16
32	J	312	CLA	C11-C10-C8-C7
32	K	308	CLA	C6-C7-C8-C10
32	L	312	CLA	C11-C10-C8-C7
32	a	809	CLA	C6-C7-C8-C10
32	a	818	CLA	C11-C10-C8-C7
32	a	819	CLA	C2-C3-C5-C6
32	a	830	CLA	C2-C3-C5-C6
32	a	841	CLA	C11-C10-C8-C7
32	b	806	CLA	C11-C10-C8-C7
32	b	820	CLA	C11-C12-C13-C15
32	b	840	CLA	C6-C7-C8-C10
32	l	203	CLA	C11-C10-C8-C7
32	W	309	CLA	C3-C5-C6-C7
32	a	824	CLA	C3-C5-C6-C7
35	A	316	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	A	304	CLA	C11-C12-C13-C14
32	D	304	CLA	C6-C7-C8-C9
32	D	306	CLA	C11-C10-C8-C9
32	L	312	CLA	C11-C10-C8-C9
32	a	818	CLA	C11-C10-C8-C9
32	b	831	CLA	C6-C7-C8-C9
32	l	203	CLA	C11-C10-C8-C9
32	l	204	CLA	C6-C7-C8-C9
36	E	322	LMG	C17-C18-C19-C20
36	F	319	LMG	C14-C15-C16-C17
32	b	830	CLA	CBA-CGA-O2A-C1
32	C	307	CLA	O1A-CGA-O2A-C1
34	N	318	DD6	C12-C11-C13-C14
37	L	316	A86	C-C1-C24-C25
32	A	309	CLA	C10-C11-C12-C13
32	I	301	CLA	C15-C16-C17-C18
35	E	301	LHG	C32-C33-C34-C35
36	D	303	LMG	C34-C35-C36-C37
36	S	322	LMG	C16-C17-C18-C19
38	J	318	LMU	C9-C10-C11-C12
32	W	311	CLA	C3-C5-C6-C7
32	a	806	CLA	C5-C6-C7-C8
35	D	320	LHG	C14-C15-C16-C17
36	L	320	LMG	C16-C17-C18-C19
32	F	322	CLA	CBA-CGA-O2A-C1
32	Q	304	CLA	CBA-CGA-O2A-C1
32	W	311	CLA	CBA-CGA-O2A-C1
35	f	205	LHG	C24-C23-O8-C6
35	A	316	LHG	C7-C8-C9-C10
35	W	319	LHG	C7-C8-C9-C10
36	A	317	LMG	C10-C11-C12-C13
32	A	306	CLA	C5-C6-C7-C8
32	J	312	CLA	C5-C6-C7-C8
33	P	312	KC2	CAA-CBA-CGA-O1A
35	I	314	LHG	C30-C31-C32-C33
39	H	315	SQD	C10-C11-C12-C13
32	A	301	CLA	C4B-C3B-CAB-CBB
32	A	302	CLA	C4B-C3B-CAB-CBB
32	B	301	CLA	C4B-C3B-CAB-CBB
32	B	302	CLA	C4B-C3B-CAB-CBB
32	B	305	CLA	C4B-C3B-CAB-CBB
32	B	309	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	C	309	CLA	C4B-C3B-CAB-CBB
32	E	303	CLA	C4B-C3B-CAB-CBB
32	E	307	CLA	C4B-C3B-CAB-CBB
32	E	309	CLA	C4B-C3B-CAB-CBB
32	F	301	CLA	C4B-C3B-CAB-CBB
32	G	304	CLA	C4B-C3B-CAB-CBB
32	G	305	CLA	C4B-C3B-CAB-CBB
32	G	307	CLA	C4B-C3B-CAB-CBB
32	H	304	CLA	C4B-C3B-CAB-CBB
32	H	310	CLA	C4B-C3B-CAB-CBB
32	J	302	CLA	C4B-C3B-CAB-CBB
32	K	301	CLA	C4B-C3B-CAB-CBB
32	L	304	CLA	C4B-C3B-CAB-CBB
32	L	311	CLA	C4B-C3B-CAB-CBB
32	M	305	CLA	C4B-C3B-CAB-CBB
32	M	309	CLA	C4B-C3B-CAB-CBB
32	M	310	CLA	C4B-C3B-CAB-CBB
32	M	311	CLA	C4B-C3B-CAB-CBB
32	N	305	CLA	C4B-C3B-CAB-CBB
32	N	310	CLA	C4B-C3B-CAB-CBB
32	N	311	CLA	C4B-C3B-CAB-CBB
32	N	312	CLA	C4B-C3B-CAB-CBB
32	O	301	CLA	C4B-C3B-CAB-CBB
32	P	304	CLA	C4B-C3B-CAB-CBB
32	P	305	CLA	C4B-C3B-CAB-CBB
32	P	310	CLA	C4B-C3B-CAB-CBB
32	P	311	CLA	C4B-C3B-CAB-CBB
32	Q	308	CLA	C4B-C3B-CAB-CBB
32	R	301	CLA	C4B-C3B-CAB-CBB
32	S	301	CLA	C4B-C3B-CAB-CBB
32	T	309	CLA	C4B-C3B-CAB-CBB
32	U	301	CLA	C4B-C3B-CAB-CBB
32	U	303	CLA	C4B-C3B-CAB-CBB
32	U	306	CLA	C4B-C3B-CAB-CBB
32	V	203	CLA	C4B-C3B-CAB-CBB
32	a	807	CLA	C4B-C3B-CAB-CBB
32	a	819	CLA	C4B-C3B-CAB-CBB
32	a	820	CLA	C4B-C3B-CAB-CBB
32	a	828	CLA	C4B-C3B-CAB-CBB
32	a	832	CLA	C4B-C3B-CAB-CBB
32	a	853	CLA	C4B-C3B-CAB-CBB
32	b	803	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	b	812	CLA	C4B-C3B-CAB-CBB
32	b	823	CLA	C4B-C3B-CAB-CBB
32	f	203	CLA	C4B-C3B-CAB-CBB
32	k	201	CLA	C4B-C3B-CAB-CBB
32	l	203	CLA	C4B-C3B-CAB-CBB
32	l	204	CLA	C4B-C3B-CAB-CBB
32	b	803	CLA	C5-C6-C7-C8
35	W	319	LHG	O6-C4-C5-C6
36	E	302	LMG	C10-C11-C12-C13
32	D	313	CLA	C5-C6-C7-C8
32	a	839	CLA	C5-C6-C7-C8
32	b	806	CLA	C8-C10-C11-C12
43	a	848	PQN	C23-C25-C26-C27
32	F	309	CLA	C4-C3-C5-C6
32	I	305	CLA	C4-C3-C5-C6
32	b	823	CLA	C4-C3-C5-C6
32	F	309	CLA	C2-C3-C5-C6
32	I	305	CLA	C2-C3-C5-C6
32	O	309	CLA	C2-C3-C5-C6
32	a	802	CLA	C2-C3-C5-C6
32	b	823	CLA	C2-C3-C5-C6
38	D	324	LMU	C9-C10-C11-C12
32	b	808	CLA	C8-C10-C11-C12
32	b	801	CLA	CBA-CGA-O2A-C1
36	l	201	LMG	C29-C28-O8-C9
35	B	308	LHG	C5-C4-O6-P
32	H	305	CLA	CBD-CGD-O2D-CED
32	J	308	CLA	C3A-C2A-CAA-CBA
32	b	822	CLA	C3A-C2A-CAA-CBA
32	b	826	CLA	C3A-C2A-CAA-CBA
32	b	830	CLA	C3A-C2A-CAA-CBA
32	b	832	CLA	C3A-C2A-CAA-CBA
36	F	319	LMG	C29-C30-C31-C32
36	P	318	LMG	C13-C14-C15-C16
37	H	314	A86	O-C13-C14-C15
37	K	311	A86	O-C13-C14-C15
37	K	312	A86	O-C13-C14-C15
37	L	317	A86	O-C13-C14-C15
37	N	316	A86	O-C13-C14-C15
37	R	313	A86	O-C13-C14-C15
37	S	320	A86	O-C13-C14-C15
37	T	312	A86	O-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
37	T	313	A86	O-C13-C14-C15
37	T	315	A86	O-C13-C14-C15
37	r	204	A86	O-C13-C14-C15
38	J	318	LMU	C2-C1-O1'-C1'
35	I	314	LHG	C14-C15-C16-C17
32	k	203	CLA	C6-C7-C8-C9
32	P	311	CLA	CBA-CGA-O2A-C1
32	Q	306	CLA	CBA-CGA-O2A-C1
32	a	828	CLA	C5-C6-C7-C8
35	A	316	LHG	C4-C5-C6-O8
36	E	320	LMG	C7-C8-C9-O8
36	L	320	LMG	C7-C8-C9-O8
36	W	320	LMG	C7-C8-C9-O8
36	j	104	LMG	O1-C7-C8-C9
36	l	201	LMG	O1-C7-C8-C9
39	H	315	SQD	C44-C45-C46-O48
40	b	846	DGD	C1G-C2G-C3G-O3G
35	F	318	LHG	O9-C7-O7-C5
32	D	305	CLA	O2A-C1-C2-C3
37	L	315	A86	C35-C34-O4-C38
32	Q	306	CLA	C3-C5-C6-C7
37	K	312	A86	C9-C10-C11-C13
37	N	316	A86	C9-C10-C11-C13
37	N	317	A86	C9-C10-C11-C13
37	Q	311	A86	C9-C10-C11-C13
37	S	315	A86	C9-C10-C11-C13
32	M	308	CLA	C5-C6-C7-C8
32	a	822	CLA	C10-C11-C12-C13
32	b	818	CLA	C4-C3-C5-C6
35	a	849	LHG	C24-C25-C26-C27
32	A	303	CLA	C5-C6-C7-C8
35	W	319	LHG	C3-O3-P-O6
32	D	306	CLA	O1A-CGA-O2A-C1
35	W	319	LHG	C26-C27-C28-C29
32	b	804	CLA	C2A-CAA-CBA-CGA
32	b	827	CLA	C2A-CAA-CBA-CGA
35	I	314	LHG	O1-C1-C2-O2
35	a	849	LHG	O1-C1-C2-O2
35	W	319	LHG	O6-C4-C5-O7
32	a	819	CLA	CBA-CGA-O2A-C1
36	E	302	LMG	C17-C18-C19-C20
36	P	318	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	b	830	CLA	O1A-CGA-O2A-C1
32	b	833	CLA	O1A-CGA-O2A-C1
35	E	301	LHG	C23-C24-C25-C26
32	A	302	CLA	C2B-C3B-CAB-CBB
32	E	303	CLA	C2B-C3B-CAB-CBB
32	G	305	CLA	C2B-C3B-CAB-CBB
32	G	307	CLA	C2B-C3B-CAB-CBB
32	H	310	CLA	C2B-C3B-CAB-CBB
32	J	302	CLA	C2B-C3B-CAB-CBB
32	L	304	CLA	C2B-C3B-CAB-CBB
32	L	311	CLA	C2B-C3B-CAB-CBB
32	N	310	CLA	C2B-C3B-CAB-CBB
32	N	312	CLA	C2B-C3B-CAB-CBB
32	O	307	CLA	C2B-C3B-CAB-CBB
32	P	305	CLA	C2B-C3B-CAB-CBB
32	P	310	CLA	C2B-C3B-CAB-CBB
32	S	301	CLA	C2B-C3B-CAB-CBB
32	U	301	CLA	C2B-C3B-CAB-CBB
32	U	306	CLA	C2B-C3B-CAB-CBB
32	a	819	CLA	C2B-C3B-CAB-CBB
32	a	832	CLA	C2B-C3B-CAB-CBB
32	b	803	CLA	C2B-C3B-CAB-CBB
32	b	838	CLA	C2B-C3B-CAB-CBB
32	k	201	CLA	C2B-C3B-CAB-CBB
32	l	203	CLA	C2B-C3B-CAB-CBB
32	l	204	CLA	C2B-C3B-CAB-CBB
36	F	319	LMG	C15-C16-C17-C18
36	W	320	LMG	C29-C30-C31-C32
35	F	321	LHG	O7-C5-C6-O8
36	D	302	LMG	O1-C7-C8-O7
36	j	104	LMG	O1-C7-C8-O7
36	P	318	LMG	C34-C35-C36-C37
37	L	317	A86	C33-C34-O4-C38
32	P	305	CLA	C11-C12-C13-C14
38	D	324	LMU	O5'-C1'-O1'-C1
37	G	311	A86	C10-C11-C13-C14
37	K	311	A86	C10-C11-C13-C14
37	S	320	A86	C10-C11-C13-C14
37	T	313	A86	C10-C11-C13-C14
35	E	301	LHG	C15-C16-C17-C18
35	f	205	LHG	C32-C33-C34-C35
36	l	201	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
36	P	318	LMG	O9-C10-O7-C8
32	a	819	CLA	C2-C1-O2A-CGA
32	a	824	CLA	C2-C1-O2A-CGA
32	b	812	CLA	C2-C1-O2A-CGA
32	b	835	CLA	C2-C1-O2A-CGA
32	b	837	CLA	C2-C1-O2A-CGA
35	M	319	LHG	C14-C15-C16-C17
32	a	811	CLA	C5-C6-C7-C8
32	Q	301	CLA	C11-C10-C8-C9
32	W	312	CLA	C6-C7-C8-C9
32	a	809	CLA	C6-C7-C8-C9
32	b	819	CLA	C11-C10-C8-C9
32	b	833	CLA	C11-C12-C13-C14
32	b	838	CLA	C11-C10-C8-C9
35	E	321	LHG	C17-C18-C19-C20
32	I	302	CLA	C5-C6-C7-C8
33	F	310	KC2	C1A-C2A-CAA-CBA
33	T	304	KC2	C1A-C2A-CAA-CBA
35	W	319	LHG	C2-C3-O3-P
35	a	851	LHG	C2-C3-O3-P
36	M	320	LMG	C14-C15-C16-C17
39	H	315	SQD	C16-C17-C18-C19
32	a	835	CLA	C2A-CAA-CBA-CGA
32	b	812	CLA	C2A-CAA-CBA-CGA
41	k	204	BCR	C23-C24-C25-C30
32	a	810	CLA	C8-C10-C11-C12
32	a	830	CLA	C15-C16-C17-C18
39	H	315	SQD	C13-C14-C15-C16
37	N	316	A86	C-C1-C24-C25
37	H	314	A86	C5-C6-C8-C9
37	L	316	A86	C5-C6-C8-C9
37	N	316	A86	C2-C1-C24-C25
41	k	204	BCR	C17-C18-C19-C20
32	b	828	CLA	C10-C11-C12-C13
35	M	319	LHG	C32-C33-C34-C35
36	l	201	LMG	C19-C20-C21-C22
32	b	806	CLA	C16-C17-C18-C20
35	D	320	LHG	O6-C4-C5-C6
35	A	316	LHG	O2-C2-C3-O3
35	f	205	LHG	C9-C10-C11-C12
32	A	305	CLA	C6-C7-C8-C10
32	A	306	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
32	D	304	CLA	C6-C7-C8-C10
32	D	305	CLA	C2-C3-C5-C6
32	D	306	CLA	C11-C10-C8-C7
32	D	310	CLA	C11-C12-C13-C15
32	I	301	CLA	C6-C7-C8-C10
32	N	311	CLA	C6-C7-C8-C10
32	N	313	CLA	C6-C7-C8-C10
32	W	309	CLA	C11-C10-C8-C7
32	a	819	CLA	C12-C13-C15-C16
32	b	803	CLA	C11-C10-C8-C7
32	b	818	CLA	C2-C3-C5-C6
32	b	824	CLA	C6-C7-C8-C10
32	b	840	CLA	C11-C12-C13-C15
32	l	204	CLA	C6-C7-C8-C10
32	I	308	CLA	C6-C7-C8-C9
40	b	846	DGD	C3B-C4B-C5B-C6B
32	a	822	CLA	C2A-CAA-CBA-CGA
36	D	302	LMG	C29-C30-C31-C32
32	a	802	CLA	C3-C5-C6-C7
35	a	849	LHG	C10-C11-C12-C13
37	D	323	A86	C9-C10-C11-C12
37	F	313	A86	C9-C10-C11-C12
37	G	310	A86	C9-C10-C11-C12
32	F	303	CLA	C5-C6-C7-C8
32	a	836	CLA	CBA-CGA-O2A-C1
32	b	811	CLA	CBA-CGA-O2A-C1
32	l	204	CLA	CBA-CGA-O2A-C1
40	Q	318	DGD	CAB-CBB-CCB-CDB
35	a	849	LHG	C18-C19-C20-C21
32	A	311	CLA	CAD-CBD-CGD-O2D
32	B	303	CLA	CAD-CBD-CGD-O2D
32	E	303	CLA	CAD-CBD-CGD-O2D
32	E	305	CLA	CAD-CBD-CGD-O2D
32	E	314	CLA	CAD-CBD-CGD-O2D
32	G	305	CLA	CAD-CBD-CGD-O2D
32	I	303	CLA	CAD-CBD-CGD-O2D
32	K	304	CLA	CAD-CBD-CGD-O2D
32	M	309	CLA	CAD-CBD-CGD-O2D
32	N	305	CLA	CAD-CBD-CGD-O2D
32	N	309	CLA	CAD-CBD-CGD-O2D
32	P	310	CLA	CAD-CBD-CGD-O2D
32	R	304	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	T	306	CLA	CAD-CBD-CGD-O2D
32	W	311	CLA	CAD-CBD-CGD-O2D
32	a	804	CLA	CAD-CBD-CGD-O2D
32	a	809	CLA	CAD-CBD-CGD-O2D
32	a	811	CLA	CAD-CBD-CGD-O2D
32	a	819	CLA	CAD-CBD-CGD-O2D
32	a	821	CLA	CAD-CBD-CGD-O2D
32	b	803	CLA	CAD-CBD-CGD-O2D
32	b	804	CLA	CAD-CBD-CGD-O2D
32	b	814	CLA	CAD-CBD-CGD-O2D
32	b	826	CLA	CAD-CBD-CGD-O2D
32	b	827	CLA	CAD-CBD-CGD-O2D
32	b	837	CLA	CAD-CBD-CGD-O2D
32	b	840	CLA	CAD-CBD-CGD-O2D
32	k	203	CLA	CAD-CBD-CGD-O2D
32	l	203	CLA	CAD-CBD-CGD-O2D
33	A	310	KC2	C2C-C3C-CAC-CBC
33	E	313	KC2	C2C-C3C-CAC-CBC
33	F	302	KC2	C2C-C3C-CAC-CBC
33	F	310	KC2	C2C-C3C-CAC-CBC
33	I	316	KC2	CAD-CBD-CGD-O2D
33	J	303	KC2	C2B-C3B-CAB-CBB
33	J	303	KC2	C2C-C3C-CAC-CBC
33	K	302	KC2	C2B-C3B-CAB-CBB
33	K	303	KC2	C2C-C3C-CAC-CBC
33	L	303	KC2	C2B-C3B-CAB-CBB
33	L	313	KC2	C2B-C3B-CAB-CBB
33	M	302	KC2	C2B-C3B-CAB-CBB
33	N	303	KC2	C2C-C3C-CAC-CBC
33	N	307	KC2	C2C-C3C-CAC-CBC
33	N	308	KC2	CAD-CBD-CGD-O2D
33	O	302	KC2	C2C-C3C-CAC-CBC
33	P	301	KC2	C2C-C3C-CAC-CBC
33	P	301	KC2	CAD-CBD-CGD-O2D
33	P	302	KC2	CAD-CBD-CGD-O2D
33	P	306	KC2	C2B-C3B-CAB-CBB
33	P	312	KC2	C2B-C3B-CAB-CBB
33	Q	317	KC2	C2B-C3B-CAB-CBB
33	R	302	KC2	C2B-C3B-CAB-CBB
33	R	303	KC2	C2B-C3B-CAB-CBB
33	R	311	KC2	C2B-C3B-CAB-CBB
33	S	306	KC2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
33	S	306	KC2	CAD-CBD-CGD-O2D
33	S	312	KC2	C2C-C3C-CAC-CBC
33	T	303	KC2	CAD-CBD-CGD-O2D
33	T	304	KC2	C2C-C3C-CAC-CBC
33	T	311	KC2	CAD-CBD-CGD-O2D
33	W	308	KC2	CAD-CBD-CGD-O2D
33	W	314	KC2	CAD-CBD-CGD-O2D
36	E	302	LMG	C9-C8-O7-C10
32	a	852	CLA	C10-C11-C12-C13
32	G	303	CLA	CBA-CGA-O2A-C1
32	a	824	CLA	CBA-CGA-O2A-C1
32	C	306	CLA	C4-C3-C5-C6
32	D	304	CLA	C4-C3-C5-C6
32	D	305	CLA	C4-C3-C5-C6
36	A	317	LMG	O6-C1-O1-C7
36	D	321	LMG	O6-C1-O1-C7
40	Q	318	DGD	O6E-C1E-O5D-C6D
32	C	306	CLA	C2-C3-C5-C6
37	F	313	A86	C12-C11-C13-O
37	G	311	A86	C12-C11-C13-O
37	K	311	A86	C12-C11-C13-O
37	K	312	A86	C12-C11-C13-O
37	K	314	A86	C12-C11-C13-O
37	M	322	A86	C12-C11-C13-O
37	N	316	A86	C12-C11-C13-O
37	N	317	A86	C12-C11-C13-O
37	P	319	A86	C12-C11-C13-O
37	S	314	A86	C12-C11-C13-O
37	S	319	A86	C12-C11-C13-O
37	S	320	A86	C12-C11-C13-O
37	T	313	A86	C12-C11-C13-O
32	K	306	CLA	O1A-CGA-O2A-C1
35	M	319	LHG	C8-C7-O7-C5
36	T	301	LMG	C11-C12-C13-C14
35	M	319	LHG	O6-C4-C5-O7
32	L	312	CLA	C5-C6-C7-C8
32	a	814	CLA	C10-C11-C12-C13
32	a	852	CLA	C3-C5-C6-C7
33	F	302	KC2	C4B-C3B-CAB-CBB
33	L	305	KC2	C4B-C3B-CAB-CBB
33	O	302	KC2	C4C-C3C-CAC-CBC
33	R	303	KC2	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
32	a	826	CLA	C2A-CAA-CBA-CGA
32	a	835	CLA	C16-C17-C18-C20
32	B	306	CLA	CHA-CBD-CGD-O1D
32	E	310	CLA	CHA-CBD-CGD-O1D
32	E	310	CLA	CHA-CBD-CGD-O2D
32	E	311	CLA	CHA-CBD-CGD-O1D
32	E	311	CLA	CHA-CBD-CGD-O2D
32	G	306	CLA	CHA-CBD-CGD-O1D
32	G	306	CLA	CHA-CBD-CGD-O2D
32	H	301	CLA	CHA-CBD-CGD-O1D
32	H	302	CLA	CHA-CBD-CGD-O1D
32	H	307	CLA	CHA-CBD-CGD-O2D
32	H	308	CLA	CHA-CBD-CGD-O1D
32	H	308	CLA	CHA-CBD-CGD-O2D
32	H	309	CLA	CHA-CBD-CGD-O1D
32	H	309	CLA	CHA-CBD-CGD-O2D
32	I	308	CLA	CHA-CBD-CGD-O1D
32	I	308	CLA	CHA-CBD-CGD-O2D
32	K	301	CLA	CHA-CBD-CGD-O2D
32	K	308	CLA	CHA-CBD-CGD-O1D
32	K	308	CLA	CHA-CBD-CGD-O2D
32	K	310	CLA	CHA-CBD-CGD-O2D
32	O	306	CLA	CHA-CBD-CGD-O1D
32	O	306	CLA	CHA-CBD-CGD-O2D
32	O	309	CLA	CHA-CBD-CGD-O1D
32	O	309	CLA	CHA-CBD-CGD-O2D
32	P	305	CLA	CHA-CBD-CGD-O1D
32	P	305	CLA	CHA-CBD-CGD-O2D
32	P	309	CLA	CHA-CBD-CGD-O2D
32	S	309	CLA	CHA-CBD-CGD-O1D
32	U	301	CLA	CHA-CBD-CGD-O1D
32	V	204	CLA	CHA-CBD-CGD-O1D
32	V	204	CLA	CHA-CBD-CGD-O2D
32	W	307	CLA	CHA-CBD-CGD-O1D
32	W	310	CLA	CHA-CBD-CGD-O1D
32	W	312	CLA	CHA-CBD-CGD-O1D
32	W	312	CLA	CHA-CBD-CGD-O2D
32	W	313	CLA	CHA-CBD-CGD-O1D
32	W	313	CLA	CHA-CBD-CGD-O2D
32	a	802	CLA	CHA-CBD-CGD-O1D
32	a	802	CLA	CHA-CBD-CGD-O2D
32	a	803	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	a	803	CLA	CHA-CBD-CGD-O2D
32	a	805	CLA	CHA-CBD-CGD-O1D
32	a	806	CLA	CHA-CBD-CGD-O1D
32	a	806	CLA	CHA-CBD-CGD-O2D
32	a	813	CLA	CHA-CBD-CGD-O1D
32	a	813	CLA	CHA-CBD-CGD-O2D
32	a	816	CLA	CHA-CBD-CGD-O1D
32	a	816	CLA	CHA-CBD-CGD-O2D
32	a	817	CLA	CHA-CBD-CGD-O1D
32	a	825	CLA	CHA-CBD-CGD-O1D
32	a	825	CLA	CHA-CBD-CGD-O2D
32	a	830	CLA	CHA-CBD-CGD-O1D
32	a	836	CLA	CHA-CBD-CGD-O1D
32	a	836	CLA	CHA-CBD-CGD-O2D
32	a	840	CLA	CHA-CBD-CGD-O1D
32	a	840	CLA	CHA-CBD-CGD-O2D
32	a	842	CLA	CHA-CBD-CGD-O1D
32	a	842	CLA	CHA-CBD-CGD-O2D
32	b	807	CLA	CHA-CBD-CGD-O1D
32	b	807	CLA	CHA-CBD-CGD-O2D
32	b	816	CLA	CHA-CBD-CGD-O1D
32	b	817	CLA	CHA-CBD-CGD-O1D
32	b	817	CLA	CHA-CBD-CGD-O2D
32	b	838	CLA	CHA-CBD-CGD-O1D
32	f	201	CLA	CHA-CBD-CGD-O1D
32	l	202	CLA	CHA-CBD-CGD-O1D
32	l	202	CLA	CHA-CBD-CGD-O2D
32	l	204	CLA	CHA-CBD-CGD-O1D
32	l	204	CLA	CHA-CBD-CGD-O2D
33	C	303	KC2	CHA-CBD-CGD-O1D
33	H	303	KC2	CHA-CBD-CGD-O1D
33	H	303	KC2	CHA-CBD-CGD-O2D
33	L	303	KC2	CHA-CBD-CGD-O1D
33	L	303	KC2	CHA-CBD-CGD-O2D
33	L	313	KC2	CHA-CBD-CGD-O1D
33	L	313	KC2	CHA-CBD-CGD-O2D
32	a	821	CLA	C3-C5-C6-C7
32	a	828	CLA	C3-C5-C6-C7
32	a	834	CLA	C3-C5-C6-C7
32	T	308	CLA	O1A-CGA-O2A-C1
32	a	826	CLA	O1A-CGA-O2A-C1
36	l	201	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
35	f	205	LHG	C13-C14-C15-C16
36	A	317	LMG	C2-C1-O1-C7
36	A	318	LMG	O7-C8-C9-O8
36	N	301	LMG	O1-C7-C8-O7
36	W	320	LMG	O7-C8-C9-O8
40	Q	318	DGD	O1G-C1G-C2G-O2G
33	O	303	KC2	CAA-CBA-CGA-O1A
33	O	303	KC2	CAA-CBA-CGA-O2A
32	b	829	CLA	O1A-CGA-O2A-C1
36	M	320	LMG	C34-C35-C36-C37
35	E	301	LHG	O1-C1-C2-O2
35	I	318	LHG	O1-C1-C2-O2
35	f	205	LHG	O1-C1-C2-O2
37	C	311	A86	C10-C11-C13-O
37	D	323	A86	C13-C14-C15-O1
37	F	313	A86	C10-C11-C13-O
37	F	317	A86	C13-C14-C15-O1
37	G	310	A86	C13-C14-C15-O1
37	G	311	A86	C10-C11-C13-O
37	H	314	A86	C13-C14-C15-O1
37	K	311	A86	C10-C11-C13-O
37	K	311	A86	C13-C14-C15-O1
37	K	312	A86	C10-C11-C13-O
37	K	314	A86	C10-C11-C13-O
37	M	322	A86	C10-C11-C13-O
37	N	317	A86	C13-C14-C15-O1
37	P	314	A86	C13-C14-C15-O1
37	P	319	A86	C10-C11-C13-O
37	P	319	A86	C13-C14-C15-O1
37	Q	311	A86	C13-C14-C15-O1
37	Q	316	A86	C10-C11-C13-O
37	S	314	A86	C10-C11-C13-O
37	S	319	A86	C13-C14-C15-O1
37	S	320	A86	C10-C11-C13-O
37	S	320	A86	C13-C14-C15-O1
37	T	312	A86	C13-C14-C15-O1
37	T	313	A86	C10-C11-C13-O
37	T	313	A86	C13-C14-C15-O1
37	W	302	A86	C13-C14-C15-O1
37	W	315	A86	C10-C11-C13-O
37	W	316	A86	C10-C11-C13-O
37	W	318	A86	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
37	r	204	A86	C10-C11-C13-O
37	r	204	A86	C13-C14-C15-O1
36	W	320	LMG	C12-C13-C14-C15
40	b	846	DGD	C7A-C8A-C9A-CAA
32	W	310	CLA	C3-C5-C6-C7
32	a	826	CLA	C8-C10-C11-C12
36	A	318	LMG	C11-C10-O7-C8
34	A	313	DD6	C27-C29-C30-C31
34	A	315	DD6	C27-C29-C30-C31
34	D	301	DD6	C27-C29-C30-C31
34	D	316	DD6	C27-C29-C30-C31
34	I	311	DD6	C27-C29-C30-C31
34	J	314	DD6	C27-C29-C30-C31
34	V	202	DD6	C27-C29-C30-C31
36	P	318	LMG	C18-C19-C20-C21
32	C	306	CLA	C14-C13-C15-C16
32	D	310	CLA	C11-C12-C13-C14
32	a	822	CLA	C11-C12-C13-C14
32	b	803	CLA	C11-C10-C8-C9
32	F	322	CLA	O1A-CGA-O2A-C1
32	Q	304	CLA	O1A-CGA-O2A-C1
36	E	302	LMG	C16-C17-C18-C19
32	b	814	CLA	C2A-CAA-CBA-CGA
34	A	313	DD6	C12-C11-C13-C14
41	k	204	BCR	C36-C18-C19-C20
35	F	321	LHG	C24-C25-C26-C27
40	b	846	DGD	C6B-C7B-C8B-C9B
34	N	318	DD6	C10-C11-C13-C14
37	S	317	A86	C2-C1-C24-C25
41	a	845	BCR	C21-C22-C23-C24
41	l	206	BCR	C11-C12-C13-C14
41	m	101	BCR	C17-C18-C19-C20
32	H	307	CLA	C1A-C2A-CAA-CBA
32	J	308	CLA	C1A-C2A-CAA-CBA
32	b	810	CLA	C1A-C2A-CAA-CBA
35	F	321	LHG	C11-C12-C13-C14
32	T	308	CLA	C2-C1-O2A-CGA
32	E	309	CLA	CBA-CGA-O2A-C1
35	E	321	LHG	C4-O6-P-O3
35	f	205	LHG	C3-O3-P-O6
35	D	320	LHG	C32-C33-C34-C35
32	A	303	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	b	834	CLA	C4-C3-C5-C6
32	O	305	CLA	C5-C6-C7-C8
35	F	321	LHG	C2-C3-O3-P
35	I	314	LHG	C2-C3-O3-P
32	E	308	CLA	C2-C3-C5-C6
38	j	105	LMU	C5'-C4'-O1B-C1B
32	P	311	CLA	O1A-CGA-O2A-C1
32	C	306	CLA	C4B-C3B-CAB-CBB
32	D	308	CLA	C4B-C3B-CAB-CBB
32	D	315	CLA	C4B-C3B-CAB-CBB
32	E	304	CLA	C4B-C3B-CAB-CBB
32	G	308	CLA	C4B-C3B-CAB-CBB
32	H	301	CLA	C4B-C3B-CAB-CBB
32	H	305	CLA	C4B-C3B-CAB-CBB
32	I	304	CLA	C4B-C3B-CAB-CBB
32	J	305	CLA	C4B-C3B-CAB-CBB
32	L	314	CLA	C4B-C3B-CAB-CBB
32	O	304	CLA	C4B-C3B-CAB-CBB
32	S	310	CLA	C4B-C3B-CAB-CBB
32	T	305	CLA	C4B-C3B-CAB-CBB
32	W	309	CLA	C4B-C3B-CAB-CBB
32	a	827	CLA	C4B-C3B-CAB-CBB
32	a	837	CLA	C4B-C3B-CAB-CBB
32	a	842	CLA	C4B-C3B-CAB-CBB
32	b	804	CLA	C4B-C3B-CAB-CBB
32	b	811	CLA	C4B-C3B-CAB-CBB
32	b	831	CLA	C4B-C3B-CAB-CBB
32	f	201	CLA	C4B-C3B-CAB-CBB
32	f	204	CLA	C4B-C3B-CAB-CBB
35	A	316	LHG	C3-O3-P-O5
35	A	316	LHG	C4-O6-P-O4
35	B	308	LHG	C3-O3-P-O5
35	B	308	LHG	C4-O6-P-O5
35	D	320	LHG	C4-O6-P-O4
35	E	321	LHG	C4-O6-P-O5
35	F	321	LHG	C3-O3-P-O5
35	I	314	LHG	C3-O3-P-O5
35	a	849	LHG	C3-O3-P-O5
35	a	850	LHG	C4-O6-P-O5
35	a	851	LHG	C4-O6-P-O4
32	b	832	CLA	C16-C17-C18-C19
36	D	302	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
36	j	104	LMG	C12-C13-C14-C15
32	Q	304	CLA	C2A-CAA-CBA-CGA
32	a	818	CLA	C2A-CAA-CBA-CGA
32	W	313	CLA	C3-C5-C6-C7
32	a	805	CLA	C10-C11-C12-C13
32	T	305	CLA	O1D-CGD-O2D-CED
32	E	310	CLA	CAD-CBD-CGD-O1D
32	G	306	CLA	CAD-CBD-CGD-O1D
32	H	301	CLA	CAD-CBD-CGD-O1D
32	H	309	CLA	CAD-CBD-CGD-O1D
32	I	308	CLA	CAD-CBD-CGD-O1D
32	O	306	CLA	CAD-CBD-CGD-O1D
32	O	309	CLA	CAD-CBD-CGD-O1D
32	S	309	CLA	CAD-CBD-CGD-O1D
32	U	306	CLA	CAD-CBD-CGD-O1D
32	V	204	CLA	CAD-CBD-CGD-O1D
32	W	307	CLA	CAD-CBD-CGD-O1D
32	W	310	CLA	CAD-CBD-CGD-O1D
32	W	312	CLA	CAD-CBD-CGD-O1D
32	a	802	CLA	CAD-CBD-CGD-O1D
32	a	805	CLA	CAD-CBD-CGD-O1D
32	a	806	CLA	CAD-CBD-CGD-O1D
32	a	813	CLA	CAD-CBD-CGD-O1D
32	a	816	CLA	CAD-CBD-CGD-O1D
32	a	817	CLA	CAD-CBD-CGD-O1D
32	a	842	CLA	CAD-CBD-CGD-O1D
32	b	816	CLA	CAD-CBD-CGD-O1D
32	b	817	CLA	CAD-CBD-CGD-O1D
32	b	838	CLA	CAD-CBD-CGD-O1D
32	l	202	CLA	CAD-CBD-CGD-O1D
32	l	204	CLA	CAD-CBD-CGD-O1D
33	G	302	KC2	CAD-CBD-CGD-O1D
37	L	316	A86	C26-C27-C29-C30
37	L	317	A86	C26-C27-C29-C30
37	N	316	A86	C26-C27-C29-C30
35	E	321	LHG	C7-C8-C9-C10
32	J	312	CLA	CBA-CGA-O2A-C1
38	D	324	LMU	O1'-C1-C2-C3
39	H	315	SQD	C15-C16-C17-C18
32	a	814	CLA	C16-C17-C18-C19
32	E	308	CLA	C4-C3-C5-C6
32	A	309	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
32	D	313	CLA	C6-C7-C8-C10
32	E	309	CLA	C11-C10-C8-C7
32	H	301	CLA	C3A-C2A-CAA-CBA
32	M	308	CLA	C6-C7-C8-C10
32	O	307	CLA	C6-C7-C8-C10
32	S	309	CLA	C6-C7-C8-C10
32	V	201	CLA	C6-C7-C8-C10
32	a	817	CLA	C11-C10-C8-C7
32	a	826	CLA	C11-C10-C8-C7
32	a	826	CLA	C12-C13-C15-C16
32	a	852	CLA	C6-C7-C8-C10
32	b	804	CLA	C12-C13-C15-C16
32	b	805	CLA	C6-C7-C8-C10
32	b	809	CLA	C3A-C2A-CAA-CBA
32	b	810	CLA	C3A-C2A-CAA-CBA
32	b	819	CLA	C11-C10-C8-C7
35	a	849	LHG	O6-C4-C5-O7
35	f	205	LHG	O6-C4-C5-O7
35	I	318	LHG	C33-C34-C35-C36
32	C	306	CLA	C8-C10-C11-C12
32	F	303	CLA	C10-C11-C12-C13
32	a	841	CLA	C15-C16-C17-C18
32	b	805	CLA	C15-C16-C17-C18
32	M	305	CLA	C2A-CAA-CBA-CGA
36	D	302	LMG	O1-C7-C8-C9
36	D	303	LMG	C7-C8-C9-O8
36	D	325	LMG	O1-C7-C8-C9
36	l	201	LMG	C34-C35-C36-C37
35	I	314	LHG	O7-C5-C6-O8
35	M	319	LHG	O7-C5-C6-O8
36	D	325	LMG	O1-C7-C8-O7
36	E	302	LMG	O1-C7-C8-O7
36	S	322	LMG	O7-C8-C9-O8
36	T	301	LMG	O7-C8-C9-O8
39	k	206	SQD	O6-C44-C45-O47
40	b	846	DGD	O1G-C1G-C2G-O2G
36	P	318	LMG	C35-C36-C37-C38
40	Q	318	DGD	C2A-C3A-C4A-C5A
35	E	301	LHG	C17-C18-C19-C20
35	F	321	LHG	C11-C10-C9-C8
36	L	320	LMG	C14-C15-C16-C17
35	f	205	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
36	M	320	LMG	C29-C30-C31-C32
36	S	322	LMG	C8-C7-O1-C1
36	T	301	LMG	C8-C7-O1-C1
39	H	315	SQD	C45-C44-O6-C1
32	A	309	CLA	C16-C17-C18-C20
35	a	850	LHG	C27-C28-C29-C30
35	W	319	LHG	C23-C24-C25-C26
35	I	314	LHG	C9-C10-C11-C12
32	b	801	CLA	O1A-CGA-O2A-C1
33	P	301	KC2	CAA-CBA-CGA-O1A
33	P	301	KC2	CAA-CBA-CGA-O2A
37	C	311	A86	C13-C14-C15-C20
37	C	312	A86	C13-C14-C15-C20
37	J	313	A86	C13-C14-C15-C20
37	P	316	A86	C13-C14-C15-C20
37	S	315	A86	C13-C14-C15-C20
37	W	315	A86	C13-C14-C15-C20
35	I	314	LHG	C15-C16-C17-C18
39	k	206	SQD	C11-C12-C13-C14
32	A	306	CLA	C11-C12-C13-C14
32	a	852	CLA	C6-C7-C8-C9
32	b	805	CLA	C6-C7-C8-C9
32	b	806	CLA	C11-C10-C8-C9
32	b	815	CLA	C14-C13-C15-C16
32	b	824	CLA	C6-C7-C8-C9
32	b	839	CLA	C14-C13-C15-C16
32	b	840	CLA	C11-C12-C13-C14
32	W	311	CLA	O1A-CGA-O2A-C1
36	F	319	LMG	C12-C13-C14-C15
37	S	314	A86	C35-C34-O4-C38
32	a	819	CLA	O1A-CGA-O2A-C1
35	P	317	LHG	C27-C28-C29-C30
41	f	202	BCR	C11-C12-C13-C35
43	a	848	PQN	C25-C26-C27-C28
35	A	316	LHG	C13-C14-C15-C16
35	P	317	LHG	C13-C14-C15-C16
34	D	319	DD6	C5-C6-C8-C9
34	N	321	DD6	C2-C1-C24-C25
32	A	311	CLA	C2B-C3B-CAB-CBB
32	B	301	CLA	C2B-C3B-CAB-CBB
32	B	302	CLA	C2B-C3B-CAB-CBB
32	C	309	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	D	311	CLA	C2B-C3B-CAB-CBB
32	D	313	CLA	C2B-C3B-CAB-CBB
32	E	310	CLA	C2B-C3B-CAB-CBB
32	E	312	CLA	C2B-C3B-CAB-CBB
32	F	301	CLA	C2B-C3B-CAB-CBB
32	F	309	CLA	C2B-C3B-CAB-CBB
32	G	304	CLA	C2B-C3B-CAB-CBB
32	H	304	CLA	C2B-C3B-CAB-CBB
32	H	306	CLA	C2B-C3B-CAB-CBB
32	I	302	CLA	C2B-C3B-CAB-CBB
32	K	304	CLA	C2B-C3B-CAB-CBB
32	K	307	CLA	C2B-C3B-CAB-CBB
32	L	314	CLA	C2B-C3B-CAB-CBB
32	M	305	CLA	C2B-C3B-CAB-CBB
32	M	309	CLA	C2B-C3B-CAB-CBB
32	M	310	CLA	C2B-C3B-CAB-CBB
32	M	311	CLA	C2B-C3B-CAB-CBB
32	N	305	CLA	C2B-C3B-CAB-CBB
32	N	311	CLA	C2B-C3B-CAB-CBB
32	O	301	CLA	C2B-C3B-CAB-CBB
32	O	304	CLA	C2B-C3B-CAB-CBB
32	P	304	CLA	C2B-C3B-CAB-CBB
32	Q	308	CLA	C2B-C3B-CAB-CBB
32	R	309	CLA	C2B-C3B-CAB-CBB
32	S	310	CLA	C2B-C3B-CAB-CBB
32	T	305	CLA	C2B-C3B-CAB-CBB
32	T	308	CLA	C2B-C3B-CAB-CBB
32	W	309	CLA	C2B-C3B-CAB-CBB
32	a	807	CLA	C2B-C3B-CAB-CBB
32	a	820	CLA	C2B-C3B-CAB-CBB
32	a	842	CLA	C2B-C3B-CAB-CBB
32	a	853	CLA	C2B-C3B-CAB-CBB
32	b	812	CLA	C2B-C3B-CAB-CBB
32	b	823	CLA	C2B-C3B-CAB-CBB
32	b	831	CLA	C2B-C3B-CAB-CBB
32	b	832	CLA	C2B-C3B-CAB-CBB
32	b	837	CLA	C2B-C3B-CAB-CBB
32	r	201	CLA	C2B-C3B-CAB-CBB
32	K	308	CLA	C15-C16-C17-C18
32	Q	306	CLA	O1A-CGA-O2A-C1
32	D	304	CLA	C2-C3-C5-C6
37	K	312	A86	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	N	317	A86	C9-C10-C11-C12
32	P	305	CLA	C11-C12-C13-C15
38	V	205	LMU	O5B-C5B-C6B-O6B
32	b	826	CLA	C1-C2-C3-C4
35	D	320	LHG	O10-C23-O8-C6
35	M	319	LHG	C27-C28-C29-C30
35	a	850	LHG	C6-C5-O7-C7
39	H	315	SQD	C46-C45-O47-C7
32	K	306	CLA	C2A-CAA-CBA-CGA
36	A	318	LMG	O9-C10-O7-C8
36	S	322	LMG	C8-C9-O8-C28
32	A	306	CLA	C2-C1-O2A-CGA
32	P	311	CLA	C2-C1-O2A-CGA
32	Q	305	CLA	C2-C1-O2A-CGA
32	a	810	CLA	C2-C1-O2A-CGA
32	a	836	CLA	C2-C1-O2A-CGA
32	b	803	CLA	C2-C1-O2A-CGA
32	b	829	CLA	C2-C1-O2A-CGA
32	b	836	CLA	C2-C1-O2A-CGA
37	P	316	A86	C35-C34-O4-C38
39	k	206	SQD	C9-C10-C11-C12
36	l	201	LMG	C4-C5-C6-O5
35	W	319	LHG	C5-C4-O6-P
37	F	317	A86	C12-C11-C13-C14
37	G	310	A86	C12-C11-C13-C14
37	G	311	A86	C12-C11-C13-C14
37	L	317	A86	C12-C11-C13-C14
37	M	314	A86	C12-C11-C13-C14
37	M	317	A86	C12-C11-C13-C14
37	N	317	A86	C12-C11-C13-C14
37	W	315	A86	C12-C11-C13-C14
37	W	318	A86	C12-C11-C13-C14
32	a	836	CLA	O1A-CGA-O2A-C1
32	l	204	CLA	O1A-CGA-O2A-C1
35	f	205	LHG	C10-C11-C12-C13
33	P	303	KC2	CAA-CBA-CGA-O1A
32	Q	306	CLA	C10-C11-C12-C13
32	H	307	CLA	C4-C3-C5-C6
38	j	105	LMU	C3'-C4'-O1B-C1B
41	U	310	BCR	C23-C24-C25-C30
41	a	843	BCR	C5-C6-C7-C8
41	a	844	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
41	a	844	BCR	C23-C24-C25-C30
41	b	844	BCR	C5-C6-C7-C8
41	k	204	BCR	C23-C24-C25-C26
41	r	203	BCR	C23-C24-C25-C30
32	a	824	CLA	O1A-CGA-O2A-C1
35	I	318	LHG	C26-C27-C28-C29
32	b	807	CLA	CBA-CGA-O2A-C1
32	a	817	CLA	C8-C10-C11-C12
36	j	104	LMG	C14-C15-C16-C17
33	P	303	KC2	CAA-CBA-CGA-O2A
36	S	322	LMG	C10-C11-C12-C13
32	a	803	CLA	C2A-CAA-CBA-CGA
40	Q	318	DGD	C2E-C1E-O5D-C6D
36	E	322	LMG	O7-C8-C9-O8
35	P	317	LHG	C4-O6-P-O3
35	W	319	LHG	C4-O6-P-O3
35	M	319	LHG	C4-C5-C6-O8
40	Q	318	DGD	O1G-C1G-C2G-C3G
32	l	204	CLA	C4-C3-C5-C6
35	a	851	LHG	C27-C28-C29-C30
32	b	830	CLA	C5-C6-C7-C8
32	D	305	CLA	C11-C10-C8-C7
32	H	307	CLA	C2-C3-C5-C6
32	b	804	CLA	C11-C10-C8-C7
32	A	308	CLA	C3-C5-C6-C7
36	E	302	LMG	C13-C14-C15-C16
32	A	305	CLA	C6-C7-C8-C9
32	A	309	CLA	C14-C13-C15-C16
32	I	301	CLA	C6-C7-C8-C9
32	N	313	CLA	C6-C7-C8-C9
32	a	810	CLA	C11-C12-C13-C14
32	a	817	CLA	C11-C10-C8-C9
32	b	820	CLA	C11-C12-C13-C14
32	a	801	CLA	C16-C17-C18-C20
32	b	805	CLA	C16-C17-C18-C20
32	b	832	CLA	C16-C17-C18-C20
32	a	834	CLA	C13-C15-C16-C17
36	D	303	LMG	C28-C29-C30-C31
35	M	319	LHG	C15-C16-C17-C18
34	D	319	DD6	C7-C6-C8-C9
41	j	102	BCR	C7-C8-C9-C34
32	M	312	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	b	806	CLA	C16-C17-C18-C19
35	D	320	LHG	C24-C25-C26-C27
32	k	202	CLA	CBA-CGA-O2A-C1
35	E	321	LHG	C2-C3-O3-P
36	P	318	LMG	C15-C16-C17-C18
32	a	835	CLA	C4-C3-C5-C6
35	P	317	LHG	O1-C1-C2-O2
32	b	815	CLA	CBA-CGA-O2A-C1
35	D	320	LHG	C24-C23-O8-C6
35	W	319	LHG	C24-C23-O8-C6
36	F	320	LMG	C15-C16-C17-C18
33	M	302	KC2	C2C-C3C-CAC-CBC
33	N	314	KC2	C2C-C3C-CAC-CBC
32	b	808	CLA	C15-C16-C17-C18
32	L	308	CLA	CAA-CBA-CGA-O1A
33	E	313	KC2	CAA-CBA-CGA-O1A
32	b	810	CLA	CAA-CBA-CGA-O2A
36	N	301	LMG	C34-C35-C36-C37
32	O	309	CLA	C5-C6-C7-C8
32	A	311	CLA	C4B-C3B-CAB-CBB
32	D	311	CLA	C4B-C3B-CAB-CBB
32	D	313	CLA	C4B-C3B-CAB-CBB
32	E	310	CLA	C4B-C3B-CAB-CBB
32	E	312	CLA	C4B-C3B-CAB-CBB
32	F	309	CLA	C4B-C3B-CAB-CBB
32	H	306	CLA	C4B-C3B-CAB-CBB
32	H	307	CLA	C4B-C3B-CAB-CBB
32	I	302	CLA	C4B-C3B-CAB-CBB
32	K	304	CLA	C4B-C3B-CAB-CBB
32	K	307	CLA	C4B-C3B-CAB-CBB
32	L	308	CLA	C4B-C3B-CAB-CBB
32	O	307	CLA	C4B-C3B-CAB-CBB
32	R	309	CLA	C4B-C3B-CAB-CBB
32	T	308	CLA	C4B-C3B-CAB-CBB
32	b	805	CLA	C4B-C3B-CAB-CBB
32	b	809	CLA	C4B-C3B-CAB-CBB
32	b	814	CLA	C4B-C3B-CAB-CBB
32	b	832	CLA	C4B-C3B-CAB-CBB
32	r	201	CLA	C4B-C3B-CAB-CBB
32	a	814	CLA	C16-C17-C18-C20
32	M	309	CLA	CAA-CBA-CGA-O2A
35	E	301	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
32	b	823	CLA	C5-C6-C7-C8
32	D	309	CLA	CAA-CBA-CGA-O2A
32	J	312	CLA	O1A-CGA-O2A-C1
32	b	811	CLA	O1A-CGA-O2A-C1
36	j	104	LMG	O10-C28-O8-C9
33	A	310	KC2	C4C-C3C-CAC-CBC
33	E	313	KC2	C4C-C3C-CAC-CBC
33	F	302	KC2	C4C-C3C-CAC-CBC
33	F	310	KC2	C4C-C3C-CAC-CBC
33	I	316	KC2	C4C-C3C-CAC-CBC
33	J	303	KC2	C4C-C3C-CAC-CBC
33	M	302	KC2	C4B-C3B-CAB-CBB
33	N	307	KC2	C4C-C3C-CAC-CBC
33	P	312	KC2	C4B-C3B-CAB-CBB
33	R	303	KC2	C4B-C3B-CAB-CBB
33	S	303	KC2	C4B-C3B-CAB-CBB
35	A	316	LHG	C11-C10-C9-C8
32	C	308	CLA	CAA-CBA-CGA-O1A
32	H	309	CLA	CAA-CBA-CGA-O1A
32	S	310	CLA	CAA-CBA-CGA-O2A
32	W	307	CLA	CAA-CBA-CGA-O2A
32	E	309	CLA	O1A-CGA-O2A-C1
32	B	305	CLA	CAA-CBA-CGA-O2A
32	J	301	CLA	CAA-CBA-CGA-O1A
32	P	304	CLA	CAA-CBA-CGA-O2A
32	a	830	CLA	C2-C1-O2A-CGA
32	b	806	CLA	C13-C15-C16-C17
32	H	307	CLA	C2A-CAA-CBA-CGA
32	J	301	CLA	C2A-CAA-CBA-CGA
32	a	852	CLA	C2A-CAA-CBA-CGA
36	A	317	LMG	O7-C8-C9-O8
32	E	307	CLA	C3A-C2A-CAA-CBA
32	M	311	CLA	C3A-C2A-CAA-CBA
32	O	301	CLA	C3A-C2A-CAA-CBA
32	S	308	CLA	C3A-C2A-CAA-CBA
32	a	805	CLA	C3A-C2A-CAA-CBA
32	a	810	CLA	C3A-C2A-CAA-CBA
32	a	818	CLA	C3A-C2A-CAA-CBA
32	b	807	CLA	C3A-C2A-CAA-CBA
32	b	833	CLA	C3A-C2A-CAA-CBA
32	O	301	CLA	CAA-CBA-CGA-O1A
32	S	310	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	j	101	CLA	CAA-CBA-CGA-O1A
32	E	307	CLA	C6-C7-C8-C10
37	G	310	A86	O-C13-C14-C15
37	N	317	A86	O-C13-C14-C15
37	P	319	A86	O-C13-C14-C15
35	a	849	LHG	C27-C28-C29-C30
32	C	301	CLA	CAA-CBA-CGA-O2A
32	H	309	CLA	CAA-CBA-CGA-O2A
32	K	310	CLA	CAA-CBA-CGA-O1A
32	M	309	CLA	CAA-CBA-CGA-O1A
32	P	304	CLA	CAA-CBA-CGA-O1A
32	a	824	CLA	C4-C3-C5-C6
36	L	320	LMG	C28-C29-C30-C31
32	b	834	CLA	C2-C3-C5-C6
34	J	315	DD6	C27-C29-C30-C31
32	A	304	CLA	C6-C7-C8-C9
32	A	306	CLA	C6-C7-C8-C9
32	E	306	CLA	C6-C7-C8-C9
32	S	309	CLA	C6-C7-C8-C9
32	a	817	CLA	C11-C12-C13-C14
32	a	826	CLA	C11-C12-C13-C14
36	D	321	LMG	C30-C31-C32-C33
32	U	306	CLA	CAA-CBA-CGA-O1A
32	j	101	CLA	CAA-CBA-CGA-O2A
32	E	308	CLA	C5-C6-C7-C8
35	E	321	LHG	C11-C10-C9-C8
32	b	831	CLA	C10-C11-C12-C13
35	a	850	LHG	C4-C5-C6-O8
36	D	303	LMG	O1-C7-C8-C9
41	a	854	BCR	C35-C13-C14-C15
41	b	842	BCR	C20-C21-C22-C37
41	l	206	BCR	C11-C10-C9-C34
32	J	311	CLA	CAA-CBA-CGA-O1A
32	M	311	CLA	CAA-CBA-CGA-O1A
32	O	308	CLA	CAA-CBA-CGA-O1A
32	N	309	CLA	O2A-C1-C2-C3
32	r	201	CLA	O2A-C1-C2-C3
32	b	806	CLA	CBA-CGA-O2A-C1
36	F	319	LMG	O6-C1-O1-C7
32	C	308	CLA	CAA-CBA-CGA-O2A
32	G	301	CLA	CAA-CBA-CGA-O1A
32	P	308	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	S	313	CLA	CAA-CBA-CGA-O1A
41	U	310	BCR	C36-C18-C19-C20
35	F	318	LHG	C12-C13-C14-C15
32	I	304	CLA	CAA-CBA-CGA-O2A
32	R	306	CLA	CAA-CBA-CGA-O1A
32	U	305	CLA	CAA-CBA-CGA-O1A
32	b	813	CLA	CAA-CBA-CGA-O2A
35	f	205	LHG	C4-C5-O7-C7
32	b	806	CLA	C15-C16-C17-C18
32	b	837	CLA	C4-C3-C5-C6
32	E	303	CLA	C1A-C2A-CAA-CBA
32	H	301	CLA	C1A-C2A-CAA-CBA
32	R	301	CLA	C1A-C2A-CAA-CBA
32	S	308	CLA	C1A-C2A-CAA-CBA
32	U	307	CLA	C1A-C2A-CAA-CBA
32	W	309	CLA	C1A-C2A-CAA-CBA
32	b	809	CLA	C1A-C2A-CAA-CBA
32	b	826	CLA	C1A-C2A-CAA-CBA
32	b	832	CLA	C1A-C2A-CAA-CBA
32	A	302	CLA	C6-C7-C8-C10
32	W	312	CLA	C6-C7-C8-C10
32	a	801	CLA	C11-C12-C13-C15
32	b	808	CLA	C6-C7-C8-C10
32	b	816	CLA	C11-C10-C8-C7
32	b	831	CLA	C11-C10-C8-C7
32	b	836	CLA	C11-C10-C8-C7
32	I	304	CLA	CAA-CBA-CGA-O1A
32	K	310	CLA	CAA-CBA-CGA-O2A
32	b	813	CLA	CAA-CBA-CGA-O1A
35	P	317	LHG	C12-C13-C14-C15
37	S	314	A86	C33-C34-O4-C38
32	G	303	CLA	O1A-CGA-O2A-C1
32	A	311	CLA	CAA-CBA-CGA-O1A
32	J	311	CLA	CAA-CBA-CGA-O2A
32	a	807	CLA	C16-C17-C18-C20
32	G	303	CLA	C2A-CAA-CBA-CGA
32	H	301	CLA	C2A-CAA-CBA-CGA
32	J	307	CLA	C2A-CAA-CBA-CGA
32	P	305	CLA	C2A-CAA-CBA-CGA
32	P	311	CLA	C2A-CAA-CBA-CGA
33	E	313	KC2	CAA-CBA-CGA-O2A
35	F	321	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
32	D	311	CLA	C13-C15-C16-C17
32	I	301	CLA	C10-C11-C12-C13
35	D	320	LHG	C27-C28-C29-C30
32	R	304	CLA	CAA-CBA-CGA-O1A
32	U	306	CLA	CAA-CBA-CGA-O2A
32	a	842	CLA	C5-C6-C7-C8
33	E	313	KC2	C3A-C2A-CAA-CBA
33	F	302	KC2	C3A-C2A-CAA-CBA
33	H	303	KC2	C3A-C2A-CAA-CBA
33	J	310	KC2	C3A-C2A-CAA-CBA
33	K	303	KC2	C3A-C2A-CAA-CBA
33	L	313	KC2	C3A-C2A-CAA-CBA
33	M	304	KC2	C3A-C2A-CAA-CBA
33	M	307	KC2	C3A-C2A-CAA-CBA
33	N	314	KC2	C3A-C2A-CAA-CBA
33	P	301	KC2	C3A-C2A-CAA-CBA
33	R	303	KC2	C3A-C2A-CAA-CBA
33	R	311	KC2	C3A-C2A-CAA-CBA
33	S	303	KC2	C3A-C2A-CAA-CBA
35	f	205	LHG	C16-C17-C18-C19
32	B	305	CLA	CAA-CBA-CGA-O1A
32	L	308	CLA	CAA-CBA-CGA-O2A
32	M	311	CLA	CAA-CBA-CGA-O2A
32	O	308	CLA	CAA-CBA-CGA-O2A
32	a	809	CLA	C4-C3-C5-C6
43	a	848	PQN	C14-C13-C15-C16
39	H	315	SQD	C24-C25-C26-C27
32	A	303	CLA	C2B-C3B-CAB-CBB
32	B	304	CLA	C2B-C3B-CAB-CBB
32	C	306	CLA	C2B-C3B-CAB-CBB
32	D	308	CLA	C2B-C3B-CAB-CBB
32	D	315	CLA	C2B-C3B-CAB-CBB
32	E	304	CLA	C2B-C3B-CAB-CBB
32	F	305	CLA	C2B-C3B-CAB-CBB
32	G	308	CLA	C2B-C3B-CAB-CBB
32	H	301	CLA	C2B-C3B-CAB-CBB
32	H	305	CLA	C2B-C3B-CAB-CBB
32	H	307	CLA	C2B-C3B-CAB-CBB
32	I	304	CLA	C2B-C3B-CAB-CBB
32	J	305	CLA	C2B-C3B-CAB-CBB
32	K	306	CLA	C2B-C3B-CAB-CBB
32	L	308	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	a	827	CLA	C2B-C3B-CAB-CBB
32	a	828	CLA	C2B-C3B-CAB-CBB
32	a	837	CLA	C2B-C3B-CAB-CBB
32	b	804	CLA	C2B-C3B-CAB-CBB
32	b	811	CLA	C2B-C3B-CAB-CBB
32	b	814	CLA	C2B-C3B-CAB-CBB
32	f	201	CLA	C2B-C3B-CAB-CBB
36	j	104	LMG	C29-C28-O8-C9
32	O	301	CLA	CAA-CBA-CGA-O2A
32	P	308	CLA	CAA-CBA-CGA-O2A
32	S	308	CLA	CAA-CBA-CGA-O1A
32	T	305	CLA	CAA-CBA-CGA-O2A
35	F	318	LHG	C25-C26-C27-C28
32	a	805	CLA	C5-C6-C7-C8
32	b	838	CLA	C16-C17-C18-C20
37	D	323	A86	C13-C14-C15-C16
37	G	310	A86	C13-C14-C15-C16
37	N	316	A86	C13-C14-C15-C16
41	a	854	BCR	C12-C13-C14-C15
41	b	842	BCR	C20-C21-C22-C23
41	l	206	BCR	C11-C10-C9-C8
32	A	311	CLA	CAA-CBA-CGA-O2A
32	B	303	CLA	CAA-CBA-CGA-O1A
32	Q	308	CLA	CAA-CBA-CGA-O1A
32	k	201	CLA	CBA-CGA-O2A-C1
35	B	308	LHG	C7-C8-C9-C10
32	G	301	CLA	CAA-CBA-CGA-O2A
32	S	308	CLA	CAA-CBA-CGA-O2A
32	l	203	CLA	C16-C17-C18-C19
32	N	305	CLA	CBD-CGD-O2D-CED
37	C	311	A86	C10-C11-C13-C14
37	M	301	A86	C10-C11-C13-C14
37	M	322	A86	C10-C11-C13-C14
37	N	316	A86	C10-C11-C13-C14
37	Q	311	A86	C10-C11-C13-C14
37	Q	316	A86	C10-C11-C13-C14
37	S	319	A86	C10-C11-C13-C14
37	T	315	A86	C10-C11-C13-C14
32	C	301	CLA	CAA-CBA-CGA-O1A
32	Q	308	CLA	CAA-CBA-CGA-O2A
32	W	307	CLA	CAA-CBA-CGA-O1A
36	j	104	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
32	b	802	CLA	C2-C1-O2A-CGA
32	b	839	CLA	C2-C1-O2A-CGA
32	a	824	CLA	C2-C3-C5-C6
32	b	837	CLA	C2-C3-C5-C6
32	D	309	CLA	CAA-CBA-CGA-O1A
32	J	301	CLA	CAA-CBA-CGA-O2A
32	R	304	CLA	CAA-CBA-CGA-O2A
32	W	313	CLA	CAA-CBA-CGA-O2A
32	b	820	CLA	C11-C10-C8-C9
32	b	836	CLA	C11-C12-C13-C14
35	M	319	LHG	C12-C13-C14-C15
33	I	309	KC2	C1A-C2A-CAA-CBA
33	K	305	KC2	C1A-C2A-CAA-CBA
33	L	306	KC2	C1A-C2A-CAA-CBA
33	P	312	KC2	C1A-C2A-CAA-CBA
33	T	303	KC2	C1A-C2A-CAA-CBA
33	W	308	KC2	C1A-C2A-CAA-CBA
35	I	314	LHG	C26-C27-C28-C29
35	a	849	LHG	C25-C26-C27-C28
35	P	317	LHG	C11-C10-C9-C8
32	B	303	CLA	CAA-CBA-CGA-O2A
41	U	310	BCR	C23-C24-C25-C26
41	a	854	BCR	C23-C24-C25-C30
41	b	843	BCR	C23-C24-C25-C30
41	i	101	BCR	C1-C6-C7-C8
41	i	101	BCR	C23-C24-C25-C30
41	r	203	BCR	C23-C24-C25-C26
32	H	304	CLA	CAA-CBA-CGA-O2A
32	b	824	CLA	CBA-CGA-O2A-C1
35	A	316	LHG	C24-C23-O8-C6
32	J	312	CLA	C4-C3-C5-C6
32	L	312	CLA	C4-C3-C5-C6
32	P	305	CLA	C4-C3-C5-C6
32	R	310	CLA	C4-C3-C5-C6
32	a	820	CLA	C4-C3-C5-C6
34	Q	312	DD6	C5-C6-C8-C9
37	M	301	A86	C5-C6-C8-C9
41	i	101	BCR	C17-C18-C19-C20
32	V	201	CLA	C5-C6-C7-C8
35	E	321	LHG	C27-C28-C29-C30
32	A	303	CLA	C2-C3-C5-C6
32	l	204	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	L	301	CLA	CAA-CBA-CGA-O2A
32	R	306	CLA	CAA-CBA-CGA-O2A
36	F	320	LMG	C8-C7-O1-C1
39	k	206	SQD	C45-C44-O6-C1
35	I	318	LHG	C29-C30-C31-C32
32	G	305	CLA	CAA-CBA-CGA-O2A
32	L	314	CLA	CAA-CBA-CGA-O2A
32	U	307	CLA	CAA-CBA-CGA-O2A
36	A	318	LMG	C34-C35-C36-C37
36	l	201	LMG	C29-C30-C31-C32
32	a	832	CLA	C10-C11-C12-C13
35	I	318	LHG	O6-C4-C5-O7
32	L	314	CLA	CAA-CBA-CGA-O1A
32	O	306	CLA	CAA-CBA-CGA-O2A
32	T	305	CLA	CAA-CBA-CGA-O1A
32	a	807	CLA	C2A-CAA-CBA-CGA
32	C	306	CLA	C15-C16-C17-C18
32	F	322	CLA	C3-C5-C6-C7
32	S	313	CLA	CAA-CBA-CGA-O2A
32	B	304	CLA	C4B-C3B-CAB-CBB
32	F	322	CLA	C4B-C3B-CAB-CBB
32	R	304	CLA	C4B-C3B-CAB-CBB
32	b	818	CLA	C4B-C3B-CAB-CBB
32	F	322	CLA	CAA-CBA-CGA-O2A
32	A	306	CLA	C4-C3-C5-C6
32	A	308	CLA	C4-C3-C5-C6
32	b	825	CLA	C4-C3-C5-C6
32	C	306	CLA	C12-C13-C15-C16
32	Q	303	CLA	C11-C10-C8-C7
32	a	853	CLA	C11-C10-C8-C7
32	L	309	CLA	CAA-CBA-CGA-O2A
35	D	320	LHG	O1-C1-C2-O2
36	D	321	LMG	O7-C10-C11-C12
32	a	809	CLA	C11-C12-C13-C15
32	U	302	CLA	CAA-CBA-CGA-O1A
35	M	319	LHG	C13-C14-C15-C16
35	F	318	LHG	O7-C5-C6-O8
35	f	205	LHG	O7-C5-C6-O8
32	b	831	CLA	CBA-CGA-O2A-C1
32	a	807	CLA	C15-C16-C17-C18
32	a	832	CLA	C8-C10-C11-C12
32	b	840	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	O	306	CLA	CAA-CBA-CGA-O1A
32	U	302	CLA	CAA-CBA-CGA-O2A
32	B	304	CLA	CAA-CBA-CGA-O2A
32	a	805	CLA	CAA-CBA-CGA-O2A
32	a	812	CLA	CAA-CBA-CGA-O2A
32	a	805	CLA	C8-C10-C11-C12
32	b	839	CLA	C10-C11-C12-C13
32	A	309	CLA	C16-C17-C18-C19
32	l	203	CLA	C16-C17-C18-C20
33	N	304	KC2	CAA-CBA-CGA-O1A
32	J	308	CLA	CAA-CBA-CGA-O1A
32	U	307	CLA	CAA-CBA-CGA-O1A
32	b	839	CLA	CBA-CGA-O2A-C1
36	A	317	LMG	C29-C28-O8-C9
32	A	303	CLA	CAA-CBA-CGA-O2A
32	K	306	CLA	CAA-CBA-CGA-O2A
36	D	325	LMG	O7-C10-C11-C12
36	W	320	LMG	O7-C10-C11-C12
32	G	308	CLA	C4-C3-C5-C6
32	M	306	CLA	C4-C3-C5-C6
32	W	311	CLA	C4-C3-C5-C6
32	W	312	CLA	C4-C3-C5-C6
32	b	820	CLA	C4-C3-C5-C6
32	k	203	CLA	C4-C3-C5-C6
32	A	304	CLA	C13-C15-C16-C17
37	P	316	A86	C33-C34-O4-C38
35	I	314	LHG	C18-C19-C20-C21
36	M	320	LMG	C13-C14-C15-C16
32	A	301	CLA	CAA-CBA-CGA-O1A
32	B	302	CLA	CAA-CBA-CGA-O2A
32	Q	309	CLA	CAA-CBA-CGA-O2A
32	b	815	CLA	O1A-CGA-O2A-C1
32	J	312	CLA	C2-C3-C5-C6
32	a	835	CLA	C2-C3-C5-C6
32	b	825	CLA	C2-C3-C5-C6
43	a	848	PQN	C12-C13-C15-C16
37	D	322	A86	C9-C10-C11-C12
37	Q	311	A86	C9-C10-C11-C12
32	a	821	CLA	CAA-CBA-CGA-O2A
40	Q	318	DGD	O2G-C1B-C2B-C3B
40	b	846	DGD	O6D-C5D-C6D-O5D
32	E	309	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
32	M	308	CLA	C6-C7-C8-C9
32	O	307	CLA	C6-C7-C8-C9
32	V	201	CLA	C6-C7-C8-C9
32	a	826	CLA	C14-C13-C15-C16
32	b	804	CLA	C11-C10-C8-C9
32	b	804	CLA	C14-C13-C15-C16
32	O	305	CLA	C3A-C2A-CAA-CBA
32	P	305	CLA	C3A-C2A-CAA-CBA
32	S	309	CLA	C3A-C2A-CAA-CBA
32	b	817	CLA	C3A-C2A-CAA-CBA
32	b	821	CLA	C3A-C2A-CAA-CBA
32	I	302	CLA	CAA-CBA-CGA-O2A
32	S	309	CLA	CAA-CBA-CGA-O2A
32	H	302	CLA	CBD-CGD-O2D-CED
35	E	301	LHG	C30-C31-C32-C33
36	l	201	LMG	C36-C37-C38-C39
32	A	303	CLA	CAD-CBD-CGD-O2D
32	B	301	CLA	CAD-CBD-CGD-O2D
32	B	305	CLA	CAD-CBD-CGD-O2D
32	C	306	CLA	CAD-CBD-CGD-O2D
32	C	308	CLA	CAD-CBD-CGD-O2D
32	D	306	CLA	CAD-CBD-CGD-O2D
32	D	311	CLA	CAD-CBD-CGD-O2D
32	D	313	CLA	CAD-CBD-CGD-O2D
32	G	303	CLA	CAD-CBD-CGD-O2D
32	H	308	CLA	CAD-CBD-CGD-O2D
32	I	302	CLA	CAD-CBD-CGD-O2D
32	J	309	CLA	CAD-CBD-CGD-O2D
32	K	306	CLA	CAD-CBD-CGD-O2D
32	L	312	CLA	CAD-CBD-CGD-O2D
32	N	310	CLA	CAD-CBD-CGD-O2D
32	Q	306	CLA	CAD-CBD-CGD-O2D
32	Q	308	CLA	CAD-CBD-CGD-O2D
32	R	306	CLA	CAD-CBD-CGD-O2D
32	R	309	CLA	CAD-CBD-CGD-O2D
32	U	305	CLA	CAD-CBD-CGD-O2D
32	U	307	CLA	CAD-CBD-CGD-O2D
32	W	313	CLA	CAD-CBD-CGD-O2D
32	a	815	CLA	CAD-CBD-CGD-O2D
32	a	818	CLA	CAD-CBD-CGD-O2D
32	a	822	CLA	CAD-CBD-CGD-O2D
32	a	827	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	a	833	CLA	CAD-CBD-CGD-O2D
32	a	838	CLA	CAD-CBD-CGD-O2D
32	a	839	CLA	CAD-CBD-CGD-O2D
32	a	841	CLA	CAD-CBD-CGD-O2D
32	b	801	CLA	CAD-CBD-CGD-O2D
32	b	806	CLA	CAD-CBD-CGD-O2D
32	b	809	CLA	CAD-CBD-CGD-O2D
32	b	811	CLA	CAD-CBD-CGD-O2D
32	b	824	CLA	CAD-CBD-CGD-O2D
32	r	201	CLA	CAD-CBD-CGD-O2D
32	r	202	CLA	CAD-CBD-CGD-O2D
33	A	310	KC2	CAD-CBD-CGD-O2D
33	F	310	KC2	CAD-CBD-CGD-O2D
33	G	309	KC2	CAD-CBD-CGD-O2D
33	I	309	KC2	CAD-CBD-CGD-O2D
33	L	302	KC2	C2B-C3B-CAB-CBB
33	L	306	KC2	CAD-CBD-CGD-O2D
33	M	302	KC2	CAD-CBD-CGD-O2D
33	M	313	KC2	CAD-CBD-CGD-O2D
33	M	321	KC2	CAD-CBD-CGD-O2D
33	N	302	KC2	CAD-CBD-CGD-O2D
33	N	303	KC2	C2B-C3B-CAB-CBB
33	N	314	KC2	CAD-CBD-CGD-O2D
35	f	205	LHG	C6-C5-O7-C7
36	A	318	LMG	C9-C8-O7-C10
32	a	806	CLA	CBA-CGA-O2A-C1
32	S	310	CLA	C2A-CAA-CBA-CGA
32	b	833	CLA	CBD-CGD-O2D-CED
32	J	306	CLA	C2-C1-O2A-CGA
32	U	305	CLA	CAA-CBA-CGA-O2A
32	S	305	CLA	CAA-CBA-CGA-O2A
32	G	306	CLA	C4-C3-C5-C6
32	B	306	CLA	CAA-CBA-CGA-O2A
32	a	852	CLA	C8-C10-C11-C12
32	G	306	CLA	C2-C3-C5-C6
32	L	312	CLA	C2-C3-C5-C6
32	R	310	CLA	C2-C3-C5-C6
32	W	312	CLA	C2-C3-C5-C6
32	F	303	CLA	CAA-CBA-CGA-O2A
32	M	310	CLA	CAA-CBA-CGA-O2A
32	P	311	CLA	CAA-CBA-CGA-O2A
32	Q	306	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	b	804	CLA	CAA-CBA-CGA-O2A
35	B	308	LHG	O8-C23-C24-C25
34	I	310	DD6	C2-C1-C24-C25
34	T	314	DD6	C10-C11-C13-C14
34	V	202	DD6	C5-C6-C8-C9
37	J	313	A86	C5-C6-C8-C9
37	P	313	A86	C2-C1-C24-C25
37	P	316	A86	C2-C1-C24-C25
34	A	315	DD6	C13-C14-C15-O1
34	H	312	DD6	C13-C14-C15-O1
34	H	313	DD6	C13-C14-C15-O1
34	L	319	DD6	C13-C14-C15-O1
35	P	317	LHG	C2-C3-O3-P
37	C	311	A86	C12-C11-C13-O
37	F	317	A86	C12-C11-C13-O
37	G	310	A86	C12-C11-C13-O
37	L	318	A86	C12-C11-C13-O
37	M	301	A86	C12-C11-C13-O
37	M	317	A86	C12-C11-C13-O
37	M	318	A86	C12-C11-C13-O
37	O	311	A86	C12-C11-C13-O
37	O	312	A86	C12-C11-C13-O
37	Q	311	A86	C12-C11-C13-O
37	R	313	A86	C12-C11-C13-O
37	T	315	A86	C12-C11-C13-O
37	W	316	A86	C12-C11-C13-O
37	W	318	A86	C12-C11-C13-O
37	r	204	A86	C12-C11-C13-O
40	b	846	DGD	O1G-C1G-C2G-C3G
32	G	305	CLA	CAA-CBA-CGA-O1A
32	L	309	CLA	CAA-CBA-CGA-O1A
36	D	303	LMG	C11-C12-C13-C14
35	a	851	LHG	O6-C4-C5-O7
32	O	305	CLA	C8-C10-C11-C12
32	M	308	CLA	CAA-CBA-CGA-O2A
32	a	852	CLA	CAA-CBA-CGA-O2A
32	L	301	CLA	CAA-CBA-CGA-O1A
35	A	316	LHG	C27-C28-C29-C30
35	F	318	LHG	C9-C10-C11-C12
38	D	324	LMU	C2-C3-C4-C5
32	A	307	CLA	O2A-C1-C2-C3
32	D	314	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	E	314	CLA	O2A-C1-C2-C3
32	I	301	CLA	O2A-C1-C2-C3
32	a	805	CLA	O2A-C1-C2-C3
32	a	832	CLA	O2A-C1-C2-C3
32	a	839	CLA	O2A-C1-C2-C3
32	b	801	CLA	O2A-C1-C2-C3
32	b	805	CLA	O2A-C1-C2-C3
32	b	828	CLA	O2A-C1-C2-C3
32	k	202	CLA	O1A-CGA-O2A-C1
36	A	317	LMG	C34-C35-C36-C37
33	K	302	KC2	C4B-C3B-CAB-CBB
33	K	303	KC2	C4C-C3C-CAC-CBC
33	L	302	KC2	C4B-C3B-CAB-CBB
33	L	303	KC2	C4B-C3B-CAB-CBB
33	L	313	KC2	C4B-C3B-CAB-CBB
33	M	302	KC2	C4C-C3C-CAC-CBC
33	M	307	KC2	C4B-C3B-CAB-CBB
33	N	303	KC2	C4B-C3B-CAB-CBB
33	P	301	KC2	C4C-C3C-CAC-CBC
33	P	306	KC2	C4B-C3B-CAB-CBB
33	Q	317	KC2	C4B-C3B-CAB-CBB
33	R	302	KC2	C4B-C3B-CAB-CBB
33	R	311	KC2	C4B-C3B-CAB-CBB
33	S	303	KC2	C4C-C3C-CAC-CBC
33	S	306	KC2	C4C-C3C-CAC-CBC
33	S	312	KC2	C4C-C3C-CAC-CBC
33	T	311	KC2	C4C-C3C-CAC-CBC
33	W	304	KC2	C4B-C3B-CAB-CBB
36	D	325	LMG	C29-C28-O8-C9
32	C	307	CLA	C10-C11-C12-C13
32	b	804	CLA	C5-C6-C7-C8
32	G	303	CLA	CAA-CBA-CGA-O2A
32	a	803	CLA	CAA-CBA-CGA-O2A
32	D	315	CLA	CAA-CBA-CGA-O1A
32	H	304	CLA	CAA-CBA-CGA-O1A
36	F	320	LMG	C14-C15-C16-C17
37	D	322	A86	C9-C10-C11-C13
37	L	317	A86	C9-C10-C11-C13
32	A	304	CLA	CHA-CBD-CGD-O2D
32	E	306	CLA	CHA-CBD-CGD-O2D
32	G	308	CLA	CHA-CBD-CGD-O1D
32	G	308	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	H	301	CLA	CHA-CBD-CGD-O2D
32	H	307	CLA	CHA-CBD-CGD-O1D
32	J	306	CLA	CHA-CBD-CGD-O1D
32	J	306	CLA	CHA-CBD-CGD-O2D
32	M	312	CLA	CHA-CBD-CGD-O1D
32	M	312	CLA	CHA-CBD-CGD-O2D
32	N	313	CLA	CHA-CBD-CGD-O1D
32	N	313	CLA	CHA-CBD-CGD-O2D
32	O	308	CLA	CHA-CBD-CGD-O1D
32	O	308	CLA	CHA-CBD-CGD-O2D
32	S	309	CLA	CHA-CBD-CGD-O2D
32	S	310	CLA	CHA-CBD-CGD-O1D
32	S	310	CLA	CHA-CBD-CGD-O2D
32	T	310	CLA	CHA-CBD-CGD-O1D
32	T	310	CLA	CHA-CBD-CGD-O2D
32	W	307	CLA	CHA-CBD-CGD-O2D
32	W	310	CLA	CHA-CBD-CGD-O2D
32	a	805	CLA	CHA-CBD-CGD-O2D
32	a	807	CLA	CHA-CBD-CGD-O2D
32	a	814	CLA	CHA-CBD-CGD-O2D
32	a	817	CLA	CHA-CBD-CGD-O2D
32	a	820	CLA	CHA-CBD-CGD-O2D
32	a	830	CLA	CHA-CBD-CGD-O2D
32	a	853	CLA	CHA-CBD-CGD-O1D
32	a	853	CLA	CHA-CBD-CGD-O2D
32	b	812	CLA	CHA-CBD-CGD-O1D
32	b	812	CLA	CHA-CBD-CGD-O2D
32	b	813	CLA	CHA-CBD-CGD-O2D
32	b	820	CLA	CHA-CBD-CGD-O2D
32	b	834	CLA	CHA-CBD-CGD-O2D
32	b	835	CLA	CHA-CBD-CGD-O1D
32	b	835	CLA	CHA-CBD-CGD-O2D
32	k	201	CLA	CHA-CBD-CGD-O2D
32	k	202	CLA	CHA-CBD-CGD-O1D
32	k	202	CLA	CHA-CBD-CGD-O2D
33	C	303	KC2	CHA-CBD-CGD-O2D
33	G	302	KC2	CHA-CBD-CGD-O1D
33	G	302	KC2	CHA-CBD-CGD-O2D
33	N	304	KC2	CHA-CBD-CGD-O1D
33	N	304	KC2	CHA-CBD-CGD-O2D
33	P	303	KC2	CHA-CBD-CGD-O2D
33	S	303	KC2	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	b	836	CLA	C4-C3-C5-C6
32	k	201	CLA	CAA-CBA-CGA-O2A
35	a	849	LHG	O8-C23-C24-C25
32	M	306	CLA	C2-C3-C5-C6
32	a	820	CLA	C2-C3-C5-C6
33	N	304	KC2	CAA-CBA-CGA-O2A
32	G	304	CLA	C5-C6-C7-C8
35	M	319	LHG	O6-C4-C5-C6
35	a	849	LHG	O6-C4-C5-C6
32	H	305	CLA	CAA-CBA-CGA-O2A
32	I	305	CLA	CAA-CBA-CGA-O2A
36	j	104	LMG	O7-C10-C11-C12
32	b	822	CLA	C3-C5-C6-C7
32	D	315	CLA	CAA-CBA-CGA-O2A
36	E	320	LMG	C12-C13-C14-C15
32	H	307	CLA	C8-C10-C11-C12
32	D	304	CLA	CAA-CBA-CGA-O2A
32	F	306	CLA	CAA-CBA-CGA-O2A
32	P	305	CLA	CAA-CBA-CGA-O2A
32	Q	305	CLA	CAA-CBA-CGA-O2A
32	a	836	CLA	CAA-CBA-CGA-O2A
32	b	825	CLA	CAA-CBA-CGA-O2A
32	A	301	CLA	C2A-CAA-CBA-CGA
32	F	309	CLA	C2A-CAA-CBA-CGA
32	W	310	CLA	C2A-CAA-CBA-CGA
32	B	306	CLA	CAA-CBA-CGA-O1A
37	F	313	A86	C13-C14-C15-O1
37	F	317	A86	C10-C11-C13-O
37	G	310	A86	C10-C11-C13-O
37	L	317	A86	C10-C11-C13-O
37	L	318	A86	C10-C11-C13-O
37	M	301	A86	C10-C11-C13-O
37	M	314	A86	C13-C14-C15-O1
37	M	317	A86	C10-C11-C13-O
37	M	318	A86	C10-C11-C13-O
37	N	316	A86	C10-C11-C13-O
37	O	311	A86	C13-C14-C15-O1
37	O	312	A86	C10-C11-C13-O
37	Q	316	A86	C13-C14-C15-O1
37	R	312	A86	C13-C14-C15-O1
37	R	313	A86	C10-C11-C13-O
37	S	319	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
37	T	315	A86	C10-C11-C13-O
37	W	318	A86	C10-C11-C13-O
32	L	307	CLA	C3-C5-C6-C7
32	S	305	CLA	C3-C5-C6-C7
32	N	310	CLA	CAA-CBA-CGA-O2A
32	a	822	CLA	CAA-CBA-CGA-O2A
32	b	816	CLA	CAA-CBA-CGA-O2A
32	a	802	CLA	C6-C7-C8-C10
32	a	809	CLA	C2-C3-C5-C6
32	a	820	CLA	C12-C13-C15-C16
32	a	841	CLA	C2-C3-C5-C6
32	b	820	CLA	C2-C3-C5-C6
43	a	848	PQN	C16-C17-C18-C20
36	D	303	LMG	C13-C14-C15-C16
36	N	301	LMG	C17-C18-C19-C20
32	A	301	CLA	CAA-CBA-CGA-O2A
32	J	308	CLA	CAA-CBA-CGA-O2A
35	a	849	LHG	C26-C27-C28-C29
36	D	303	LMG	C33-C34-C35-C36
32	D	313	CLA	C6-C7-C8-C9
32	O	307	CLA	C11-C10-C8-C9
32	a	826	CLA	C11-C10-C8-C9
32	b	804	CLA	CAA-CBA-CGA-O1A
32	R	304	CLA	C2B-C3B-CAB-CBB
32	B	302	CLA	CAA-CBA-CGA-O1A
32	W	311	CLA	C10-C11-C12-C13
32	W	311	CLA	CAA-CBA-CGA-O2A
32	l	203	CLA	CAA-CBA-CGA-O2A
35	B	308	LHG	O10-C23-C24-C25
32	b	807	CLA	O1A-CGA-O2A-C1
32	C	305	CLA	C5-C6-C7-C8
32	Q	309	CLA	CAA-CBA-CGA-O1A
32	D	313	CLA	C2A-CAA-CBA-CGA
32	M	308	CLA	CAA-CBA-CGA-O1A
36	W	320	LMG	O9-C10-C11-C12
36	N	301	LMG	C12-C13-C14-C15
32	R	307	CLA	CAA-CBA-CGA-O2A
32	N	313	CLA	C3-C5-C6-C7
32	S	305	CLA	CAA-CBA-CGA-O1A
35	D	320	LHG	O1-C1-C2-C3
35	F	321	LHG	O1-C1-C2-C3
32	F	303	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	G	303	CLA	CAA-CBA-CGA-O1A
32	I	302	CLA	CAA-CBA-CGA-O1A
32	Q	306	CLA	CAA-CBA-CGA-O1A
32	a	812	CLA	CAA-CBA-CGA-O1A
36	E	302	LMG	O10-C28-C29-C30
34	A	313	DD6	C10-C11-C13-C14
34	A	315	DD6	C2-C1-C24-C25
32	E	307	CLA	C1A-C2A-CAA-CBA
32	G	306	CLA	C1A-C2A-CAA-CBA
32	K	310	CLA	C1A-C2A-CAA-CBA
32	P	305	CLA	C1A-C2A-CAA-CBA
32	S	309	CLA	C1A-C2A-CAA-CBA
32	W	311	CLA	C1A-C2A-CAA-CBA
32	a	810	CLA	C1A-C2A-CAA-CBA
32	b	816	CLA	C1A-C2A-CAA-CBA
32	b	833	CLA	C1A-C2A-CAA-CBA
32	b	838	CLA	C1A-C2A-CAA-CBA
32	B	304	CLA	CAA-CBA-CGA-O1A
32	a	821	CLA	CAA-CBA-CGA-O1A
32	H	305	CLA	CAA-CBA-CGA-O1A
32	C	306	CLA	C2-C1-O2A-CGA
32	a	812	CLA	C2-C1-O2A-CGA
32	b	817	CLA	C2-C1-O2A-CGA
32	D	305	CLA	C5-C6-C7-C8
32	K	306	CLA	CAA-CBA-CGA-O1A
32	b	825	CLA	CAA-CBA-CGA-O1A
35	A	316	LHG	O9-C7-C8-C9
36	D	325	LMG	O9-C10-C11-C12
40	Q	318	DGD	O1B-C1B-C2B-C3B
32	b	814	CLA	CAA-CBA-CGA-O2A
36	E	322	LMG	C7-C8-C9-O8
32	L	312	CLA	CAA-CBA-CGA-O2A
38	j	105	LMU	C11-C10-C9-C8
32	A	309	CLA	C2A-CAA-CBA-CGA
32	A	303	CLA	CAA-CBA-CGA-O1A
32	l	202	CLA	CAA-CBA-CGA-O2A
33	J	303	KC2	CAA-CBA-CGA-O2A
32	N	311	CLA	CAA-CBA-CGA-O2A
32	W	306	CLA	CAA-CBA-CGA-O2A
32	l	204	CLA	CAA-CBA-CGA-O2A
32	I	306	CLA	C13-C15-C16-C17
32	A	303	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	P	311	CLA	CAA-CBA-CGA-O1A
32	a	836	CLA	CAA-CBA-CGA-O1A
32	b	816	CLA	CAA-CBA-CGA-O1A
36	D	302	LMG	C2-C1-O1-C7
36	D	321	LMG	C2-C1-O1-C7
32	D	306	CLA	C4B-C3B-CAB-CBB
32	K	306	CLA	C4B-C3B-CAB-CBB
32	N	309	CLA	C4B-C3B-CAB-CBB
35	E	321	LHG	C3-O3-P-O5
35	P	317	LHG	C4-O6-P-O5
32	k	201	CLA	CAA-CBA-CGA-O1A
35	a	849	LHG	O10-C23-C24-C25
36	L	320	LMG	O9-C10-C11-C12
32	S	311	CLA	CAA-CBA-CGA-O2A
36	L	320	LMG	C13-C14-C15-C16
40	Q	318	DGD	C5B-C6B-C7B-C8B
33	J	303	KC2	CAA-CBA-CGA-O1A
41	a	854	BCR	C1-C6-C7-C8
41	a	854	BCR	C23-C24-C25-C26
41	b	843	BCR	C1-C6-C7-C8
32	F	306	CLA	CAA-CBA-CGA-O1A
32	a	852	CLA	CAA-CBA-CGA-O1A
36	A	317	LMG	O10-C28-O8-C9
32	D	313	CLA	CAA-CBA-CGA-O2A
32	O	305	CLA	C16-C17-C18-C19
32	b	822	CLA	C2A-CAA-CBA-CGA
32	M	310	CLA	CAA-CBA-CGA-O1A
35	P	317	LHG	C29-C30-C31-C32
32	T	302	CLA	CAA-CBA-CGA-O2A
32	T	307	CLA	CAA-CBA-CGA-O2A
32	k	202	CLA	CAA-CBA-CGA-O2A
32	b	832	CLA	C15-C16-C17-C18
35	I	314	LHG	C7-C8-C9-C10
32	D	304	CLA	CAA-CBA-CGA-O1A
32	Q	305	CLA	CAA-CBA-CGA-O1A
36	P	318	LMG	C37-C38-C39-C40
32	A	307	CLA	CAD-CBD-CGD-O1D
32	B	304	CLA	CAD-CBD-CGD-O1D
32	F	308	CLA	CAD-CBD-CGD-O1D
32	F	322	CLA	CAD-CBD-CGD-O1D
32	S	310	CLA	CAD-CBD-CGD-O1D
32	a	834	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	b	818	CLA	CAD-CBD-CGD-O1D
32	b	829	CLA	CAD-CBD-CGD-O1D
33	L	305	KC2	CAD-CBD-CGD-O1D
39	H	315	SQD	O5-C5-C6-S
32	P	305	CLA	CAA-CBA-CGA-O1A
32	S	309	CLA	CAA-CBA-CGA-O1A
32	W	306	CLA	CAA-CBA-CGA-O1A
36	E	302	LMG	O8-C28-C29-C30
32	A	305	CLA	C8-C10-C11-C12
32	a	833	CLA	C14-C13-C15-C16
32	a	835	CLA	C11-C10-C8-C9
32	a	853	CLA	C14-C13-C15-C16
32	b	831	CLA	C11-C10-C8-C9
32	b	836	CLA	C11-C10-C8-C9
32	E	310	CLA	CAA-CBA-CGA-O2A
32	A	307	CLA	CAA-CBA-CGA-O2A
32	C	306	CLA	CAA-CBA-CGA-O2A
32	F	307	CLA	CAA-CBA-CGA-O2A
32	G	306	CLA	CAA-CBA-CGA-O2A
36	L	320	LMG	O7-C10-C11-C12
32	R	307	CLA	CAA-CBA-CGA-O1A
32	I	305	CLA	CAA-CBA-CGA-O1A
32	D	306	CLA	CAA-CBA-CGA-O2A
32	E	308	CLA	CAA-CBA-CGA-O2A
32	J	306	CLA	CAA-CBA-CGA-O2A
32	M	312	CLA	CAA-CBA-CGA-O2A
32	a	802	CLA	CAA-CBA-CGA-O2A
32	a	819	CLA	CAA-CBA-CGA-O2A
32	b	821	CLA	CAA-CBA-CGA-O2A
35	f	205	LHG	C1-C2-C3-O3
32	a	809	CLA	C5-C6-C7-C8
32	U	303	CLA	CAA-CBA-CGA-O2A
32	b	809	CLA	CAA-CBA-CGA-O2A
39	H	315	SQD	C25-C26-C27-C28
32	k	202	CLA	CAA-CBA-CGA-O1A
32	l	204	CLA	CAA-CBA-CGA-O1A
32	F	307	CLA	C4-C3-C5-C6
32	G	304	CLA	C4-C3-C5-C6
32	a	828	CLA	C4-C3-C5-C6
32	b	833	CLA	C4-C3-C5-C6
37	r	204	A86	C7-C6-C8-C9
32	F	322	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	I	304	CLA	C3A-C2A-CAA-CBA
32	K	310	CLA	C3A-C2A-CAA-CBA
32	M	312	CLA	C6-C7-C8-C10
32	N	309	CLA	C3A-C2A-CAA-CBA
32	R	301	CLA	C3A-C2A-CAA-CBA
32	U	307	CLA	C3A-C2A-CAA-CBA
32	a	810	CLA	C11-C12-C13-C15
32	a	840	CLA	C11-C12-C13-C15
32	b	812	CLA	C6-C7-C8-C10
32	b	815	CLA	C12-C13-C15-C16
32	b	818	CLA	C12-C13-C15-C16
32	b	820	CLA	C11-C10-C8-C7
32	b	838	CLA	C3A-C2A-CAA-CBA
32	L	312	CLA	CAA-CBA-CGA-O1A
36	j	104	LMG	O9-C10-C11-C12
32	T	302	CLA	CAA-CBA-CGA-O1A
32	b	808	CLA	CAA-CBA-CGA-O2A
35	F	318	LHG	O7-C7-C8-C9
32	b	819	CLA	C13-C15-C16-C17
32	P	309	CLA	C10-C11-C12-C13
34	Q	314	DD6	C10-C11-C13-C14
34	k	205	DD6	C2-C1-C24-C25
37	W	316	A86	C2-C1-C24-C25
37	r	204	A86	C5-C6-C8-C9
32	N	310	CLA	CAA-CBA-CGA-O1A
32	T	307	CLA	CAA-CBA-CGA-O1A
32	b	808	CLA	CAA-CBA-CGA-O1A
32	a	813	CLA	CAA-CBA-CGA-O2A
37	Q	316	A86	O-C13-C14-C15
35	A	316	LHG	O7-C7-C8-C9
32	E	308	CLA	CAA-CBA-CGA-O1A
32	G	306	CLA	CAA-CBA-CGA-O1A
32	J	306	CLA	CAA-CBA-CGA-O1A
32	N	311	CLA	CAA-CBA-CGA-O1A
32	Q	307	CLA	CAA-CBA-CGA-O1A
32	b	804	CLA	CBA-CGA-O2A-C1
32	b	814	CLA	CAA-CBA-CGA-O1A
32	l	202	CLA	CAA-CBA-CGA-O1A
36	E	322	LMG	O6-C5-C6-O5
32	H	306	CLA	CAA-CBA-CGA-O2A
32	a	839	CLA	CAA-CBA-CGA-O2A
32	a	840	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
40	b	846	DGD	O1G-C1A-C2A-C3A
38	j	105	LMU	C6-C7-C8-C9
32	F	307	CLA	CAA-CBA-CGA-O1A
32	M	312	CLA	CAA-CBA-CGA-O1A
32	l	203	CLA	CAA-CBA-CGA-O1A
32	D	304	CLA	C2A-CAA-CBA-CGA
32	L	309	CLA	C2A-CAA-CBA-CGA
32	S	305	CLA	C2A-CAA-CBA-CGA
32	a	807	CLA	C16-C17-C18-C19
32	b	816	CLA	C4C-C3C-CAC-CBC
32	a	819	CLA	C13-C15-C16-C17
32	a	833	CLA	C13-C15-C16-C17
43	a	848	PQN	C15-C16-C17-C18
32	A	307	CLA	CAA-CBA-CGA-O1A
32	C	306	CLA	CAA-CBA-CGA-O1A
32	b	831	CLA	C4-C3-C5-C6
32	Q	307	CLA	CAA-CBA-CGA-O2A
35	a	851	LHG	O8-C23-C24-C25

All (6) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	M	314	A86	C31-C32-C33-C34-C35-C36
37	M	317	A86	C31-C32-C33-C34-C35-C36
37	S	315	A86	C31-C32-C33-C34-C35-C36
37	U	308	A86	C31-C32-C33-C34-C35-C36
37	G	311	A86	C31-C32-C33-C34-C35-C36
37	P	313	A86	C31-C32-C33-C34-C35-C36

163 monomers are involved in 261 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	P	311	CLA	2	0
39	H	315	SQD	16	0
37	T	313	A86	1	0
36	P	318	LMG	7	0
37	P	316	A86	1	0
33	O	302	KC2	1	0
41	a	843	BCR	1	0
33	W	314	KC2	1	0
34	I	312	DD6	1	0
32	R	308	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	c	101	SF4	1	0
32	k	203	CLA	6	0
37	Q	316	A86	2	0
32	W	306	CLA	1	0
33	K	309	KC2	2	0
32	a	810	CLA	1	0
41	k	204	BCR	1	0
36	l	201	LMG	5	0
32	b	835	CLA	1	0
32	H	309	CLA	1	0
37	D	322	A86	1	0
32	a	836	CLA	1	0
32	U	305	CLA	2	0
32	L	309	CLA	2	0
36	W	320	LMG	11	0
32	C	305	CLA	2	0
32	a	833	CLA	1	0
33	I	309	KC2	4	0
35	F	321	LHG	1	0
34	M	316	DD6	3	0
35	a	851	LHG	7	0
32	Q	303	CLA	1	0
32	J	312	CLA	4	0
32	K	301	CLA	2	0
36	A	318	LMG	1	0
32	H	306	CLA	1	0
37	W	316	A86	1	0
32	L	311	CLA	3	0
32	a	832	CLA	2	0
35	F	318	LHG	1	0
33	A	310	KC2	2	0
32	a	817	CLA	1	0
32	b	828	CLA	1	0
32	a	820	CLA	1	0
37	M	315	A86	1	0
33	R	311	KC2	1	0
32	K	304	CLA	1	0
32	a	852	CLA	1	0
32	a	822	CLA	1	0
32	I	303	CLA	1	0
37	R	313	A86	1	0
32	H	301	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	a	823	CLA	2	0
38	D	324	LMU	2	0
36	S	322	LMG	8	0
35	B	308	LHG	2	0
37	H	314	A86	1	0
33	K	303	KC2	1	0
32	U	306	CLA	1	0
36	A	317	LMG	1	0
33	M	313	KC2	1	0
37	L	316	A86	1	0
32	a	814	CLA	1	0
32	D	315	CLA	2	0
32	W	312	CLA	7	0
33	N	303	KC2	1	0
32	a	838	CLA	1	0
32	b	817	CLA	2	0
32	b	814	CLA	1	0
36	M	320	LMG	9	0
32	N	311	CLA	1	0
32	D	314	CLA	1	0
37	M	317	A86	3	0
32	W	310	CLA	5	0
33	P	312	KC2	2	0
34	S	321	DD6	2	0
32	F	304	CLA	2	0
32	b	833	CLA	4	0
32	a	828	CLA	3	0
32	a	802	CLA	1	0
34	D	316	DD6	1	0
35	P	317	LHG	1	0
41	b	841	BCR	1	0
38	J	318	LMU	3	0
32	A	307	CLA	1	0
36	j	104	LMG	1	0
36	T	301	LMG	2	0
32	a	803	CLA	1	0
36	N	301	LMG	5	0
32	H	305	CLA	2	0
32	I	301	CLA	2	0
34	A	313	DD6	2	0
37	M	318	A86	1	0
33	G	309	KC2	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	M	309	CLA	1	0
36	D	325	LMG	1	0
32	j	101	CLA	1	0
33	F	302	KC2	1	0
32	b	816	CLA	1	0
32	A	309	CLA	2	0
32	D	308	CLA	1	0
33	F	310	KC2	1	0
32	F	307	CLA	2	0
34	D	318	DD6	1	0
32	W	309	CLA	1	0
32	b	827	CLA	1	0
37	R	312	A86	1	0
39	k	206	SQD	6	0
34	L	319	DD6	1	0
32	D	307	CLA	1	0
32	O	304	CLA	4	0
32	b	811	CLA	1	0
32	a	834	CLA	1	0
32	b	831	CLA	1	0
41	b	845	BCR	3	0
32	a	807	CLA	1	0
32	W	311	CLA	1	0
34	I	311	DD6	1	0
32	A	301	CLA	3	0
41	b	843	BCR	2	0
32	A	303	CLA	1	0
32	b	826	CLA	2	0
40	Q	318	DGD	3	0
32	b	822	CLA	1	0
32	M	311	CLA	3	0
32	S	305	CLA	1	0
32	T	302	CLA	1	0
37	S	315	A86	2	0
33	S	312	KC2	5	0
32	b	830	CLA	1	0
37	W	302	A86	1	0
35	f	205	LHG	1	0
32	N	312	CLA	4	0
32	D	304	CLA	1	0
36	F	319	LMG	5	0
32	b	834	CLA	1	0

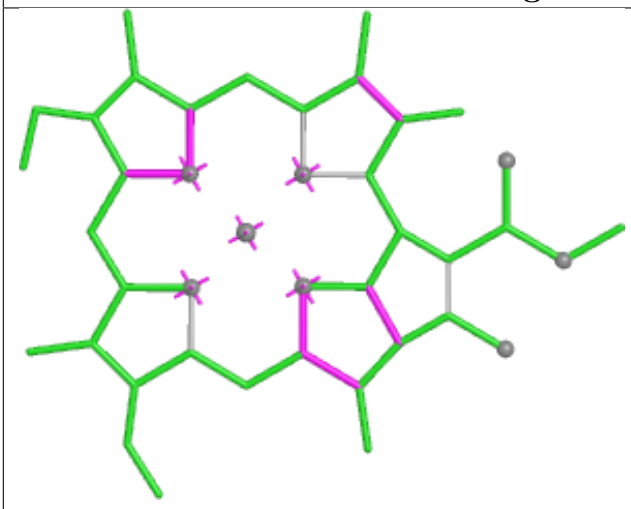
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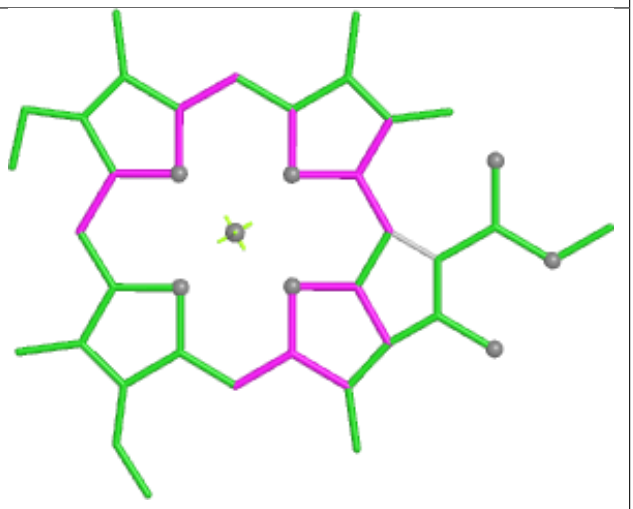
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	N	310	CLA	1	0
32	M	310	CLA	1	0
36	F	320	LMG	13	0
38	I	315	LMU	3	0
38	V	205	LMU	3	0
37	F	313	A86	1	0
32	a	805	CLA	1	0
37	M	301	A86	1	0
41	l	206	BCR	1	0
32	C	308	CLA	1	0
32	a	821	CLA	1	0
34	J	317	DD6	1	0
32	L	310	CLA	5	0
33	N	314	KC2	1	0
32	b	807	CLA	1	0
37	L	315	A86	3	0
32	P	307	CLA	1	0
41	U	310	BCR	1	0
32	k	201	CLA	1	0
37	F	312	A86	1	0
34	W	317	DD6	1	0
41	a	846	BCR	1	0
32	T	307	CLA	1	0
34	U	309	DD6	1	0
32	K	306	CLA	1	0
34	k	205	DD6	1	0
32	a	824	CLA	1	0

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

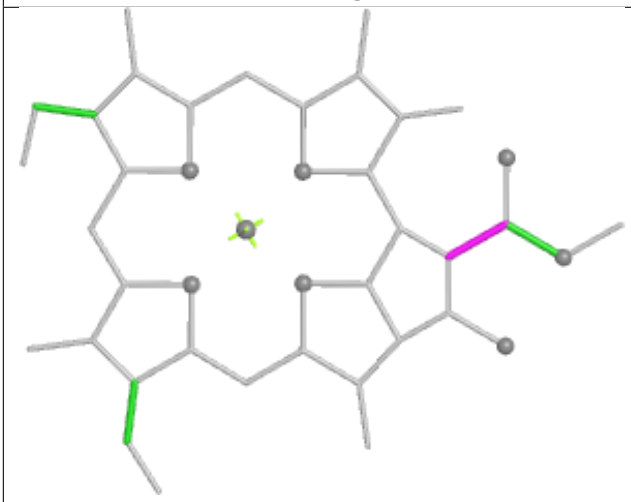
Ligand CLA H 308



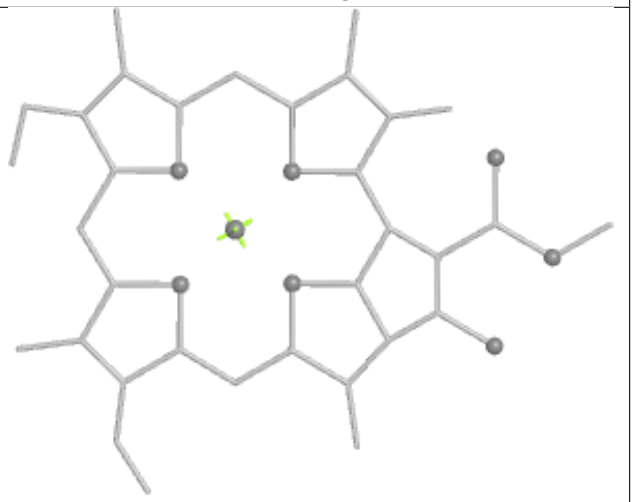
Bond lengths



Bond angles

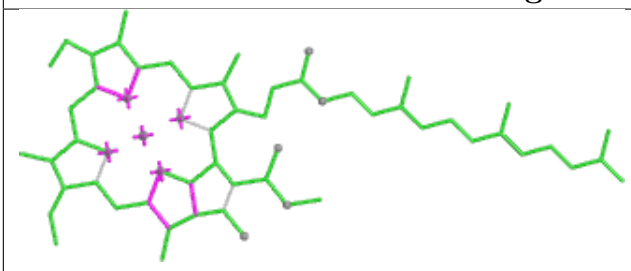


Torsions

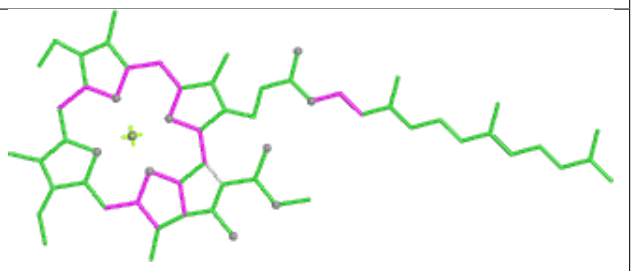


Rings

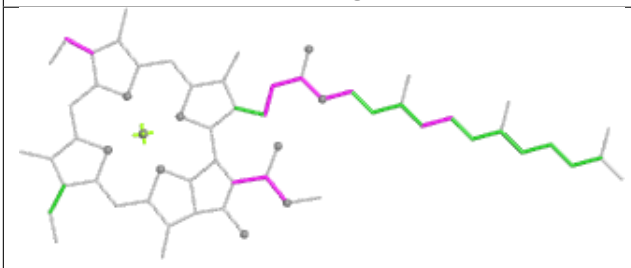
Ligand CLA P 311



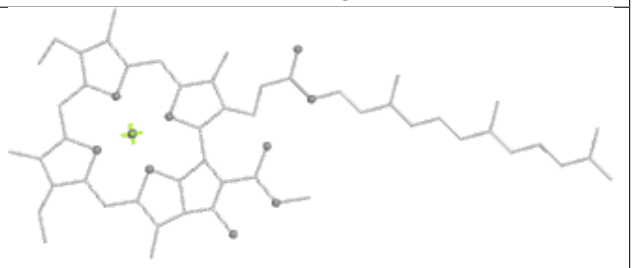
Bond lengths



Bond angles

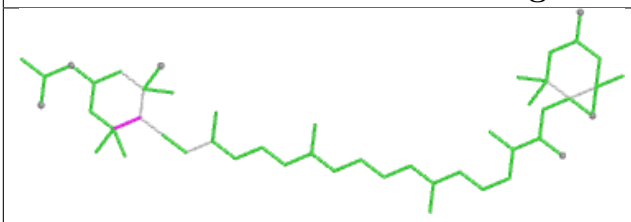


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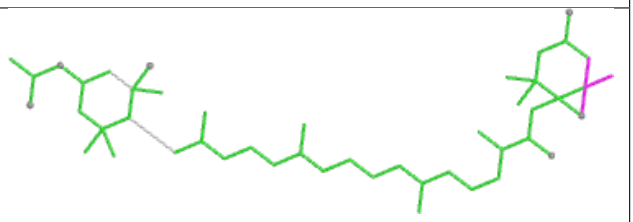


Rings

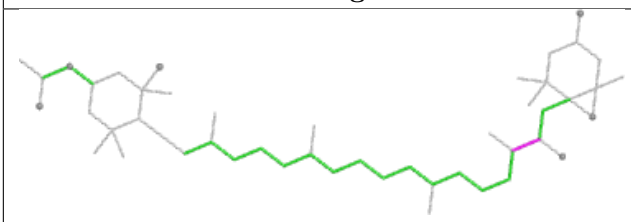
Ligand A86 G 311



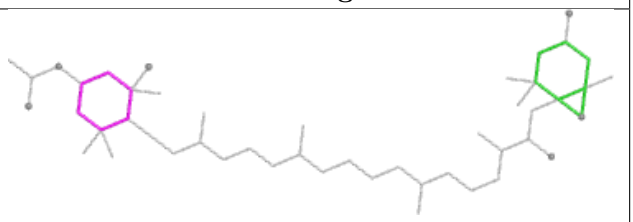
Bond lengths



Bond angles

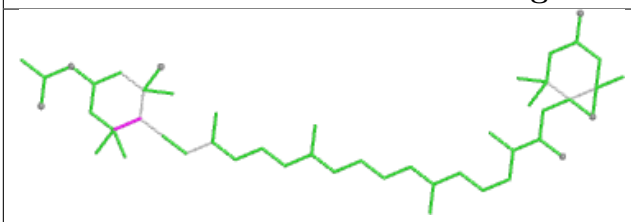


Torsions

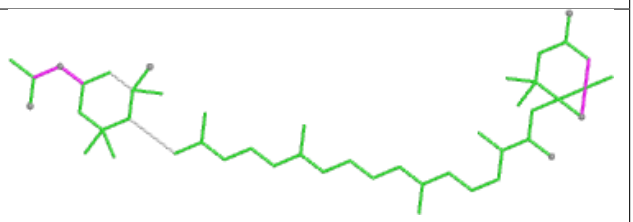


Rings

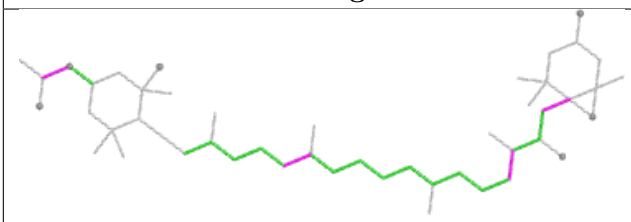
Ligand A86 P 313



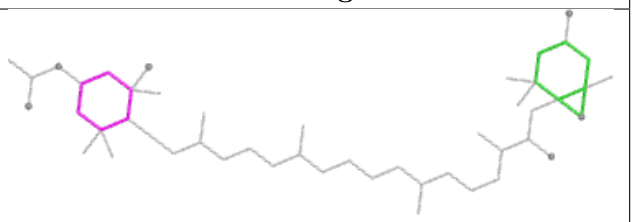
Bond lengths



Bond angles

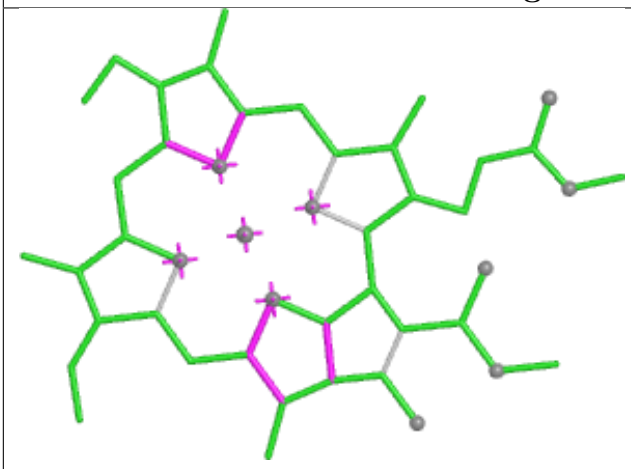


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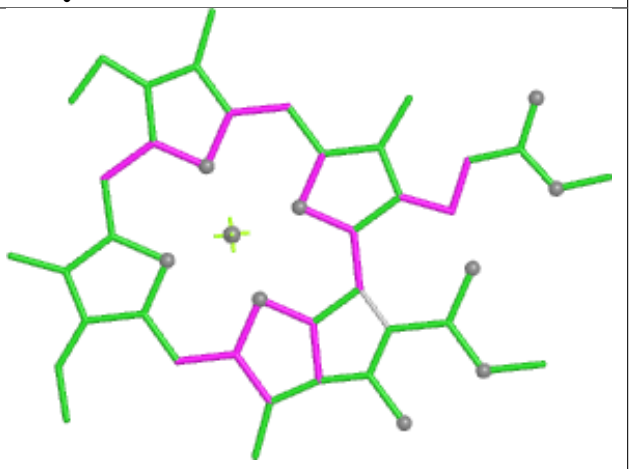


Rings

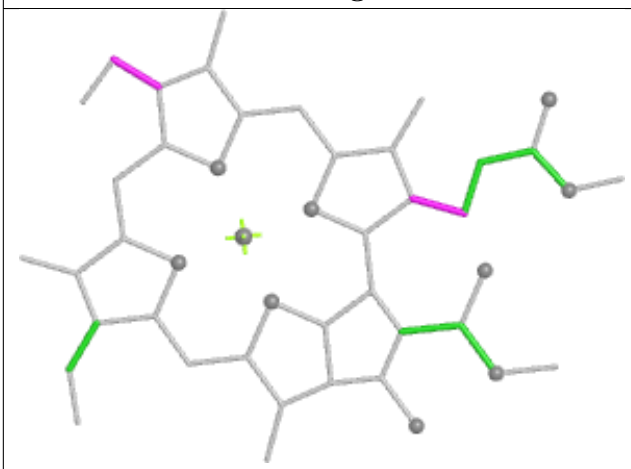
Ligand CLA Q 310



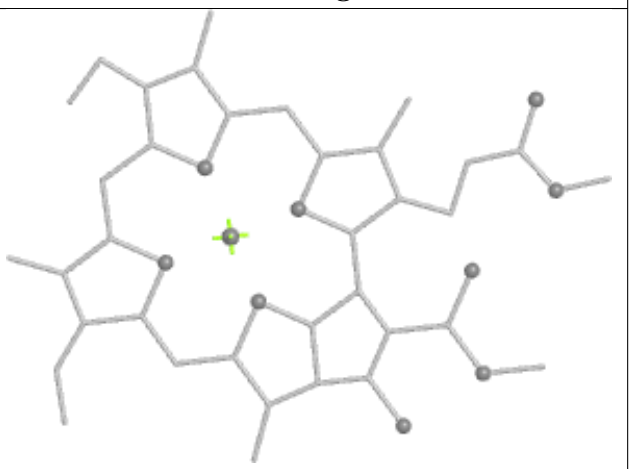
Bond lengths



Bond angles

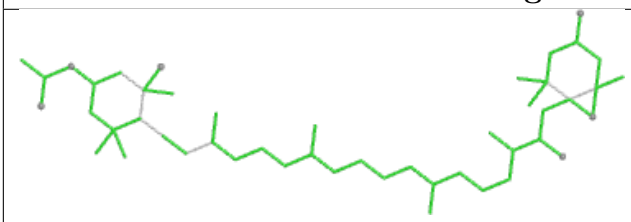


Torsions

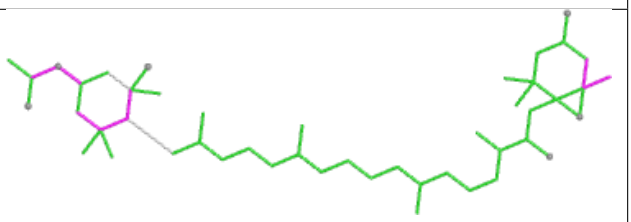


Rings

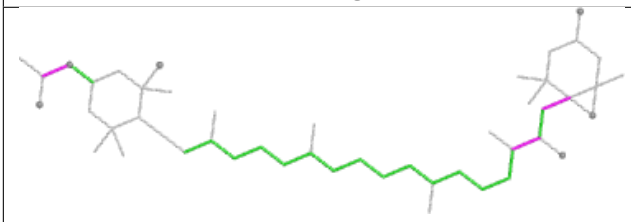
Ligand A86 W 318



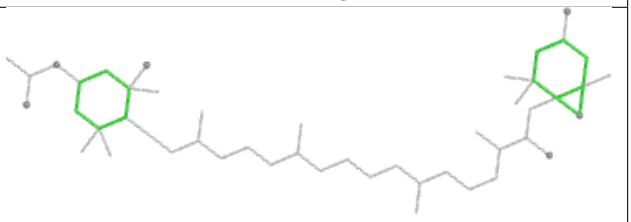
Bond lengths



Bond angles

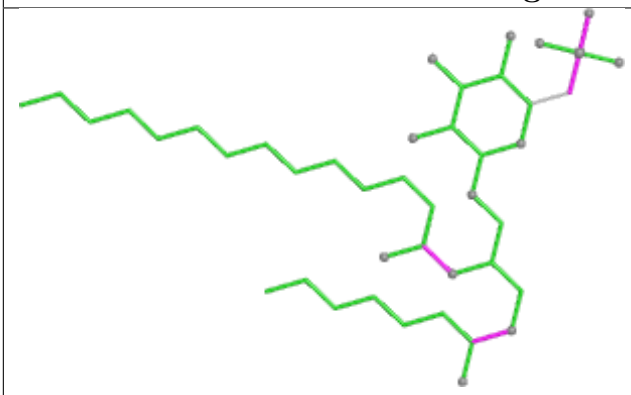


Torsions

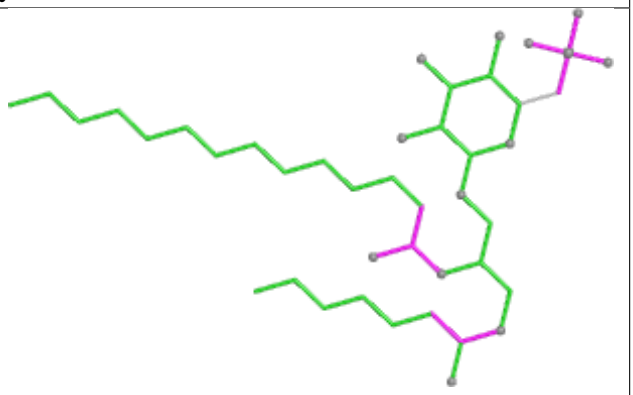


Rings

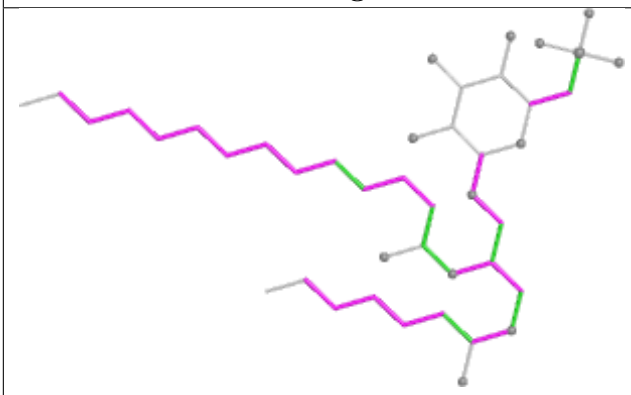
Ligand SQD H 315



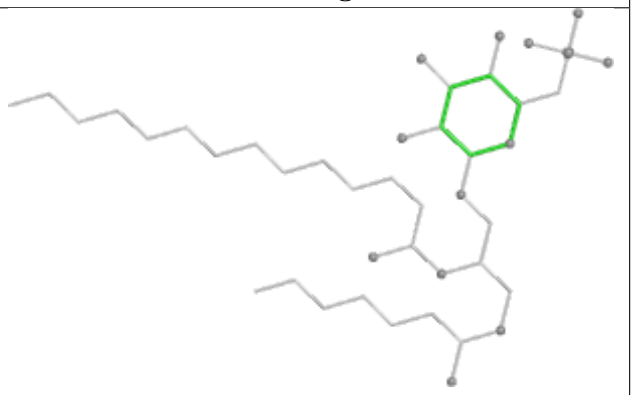
Bond lengths



Bond angles

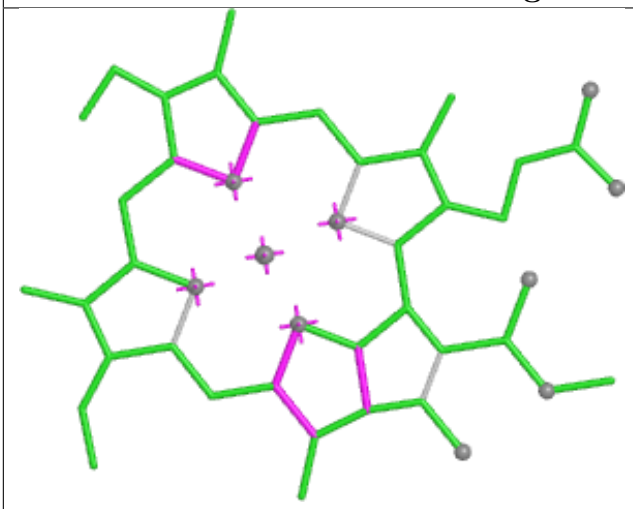


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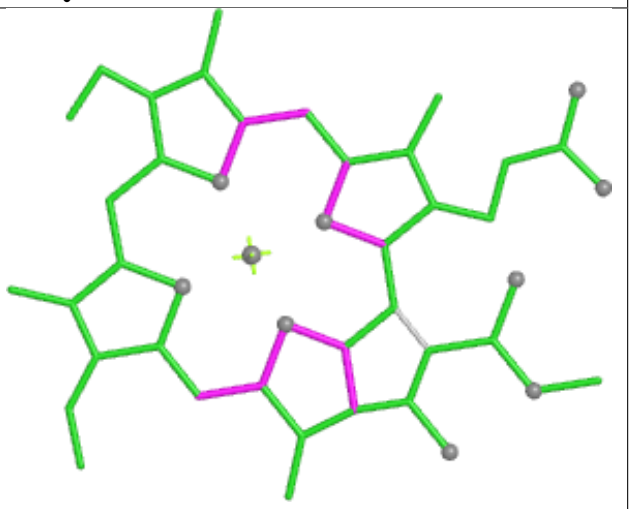


Rings

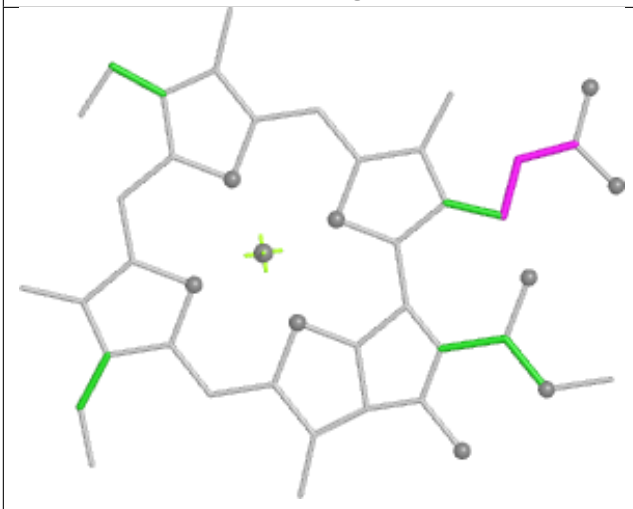
Ligand CLA Q 309



Bond lengths



Bond angles

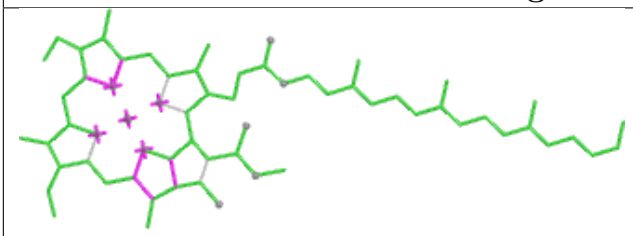


Torsions

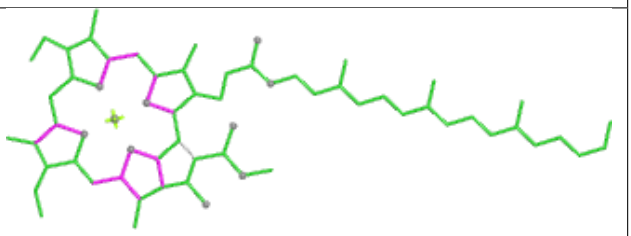


Rings

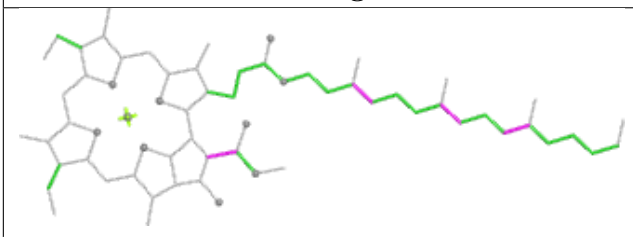
Ligand CLA b 820



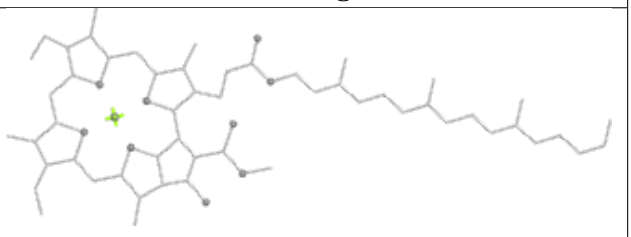
Bond lengths



Bond angles

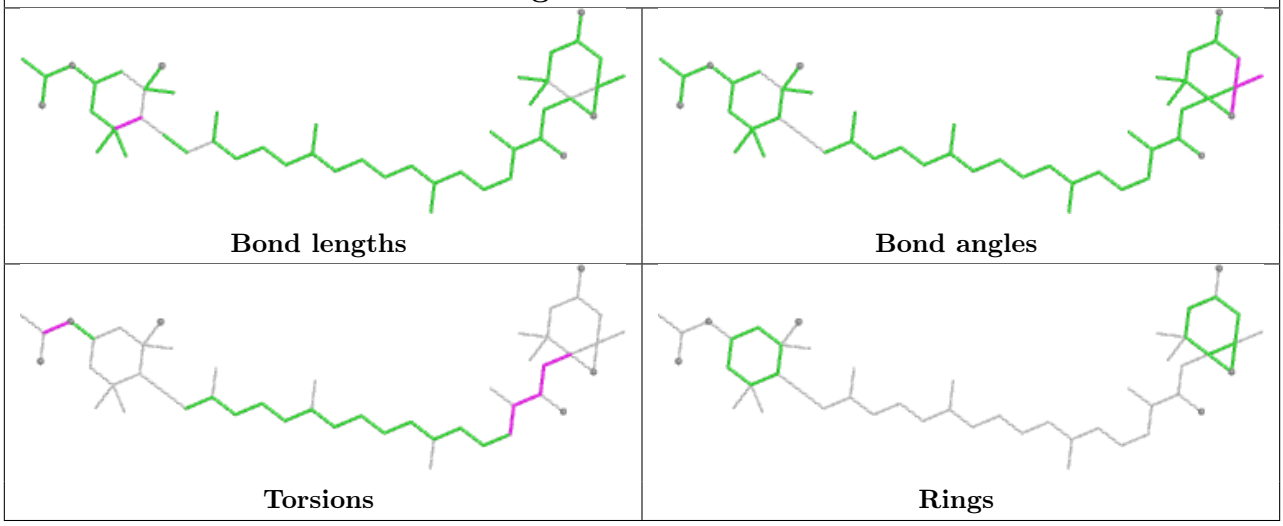


Torsions

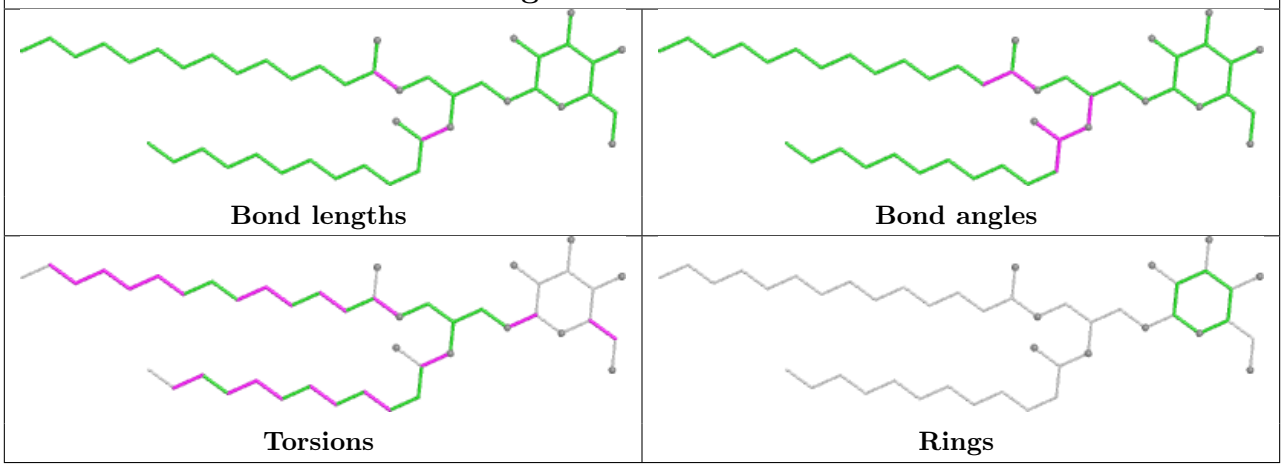


Rings

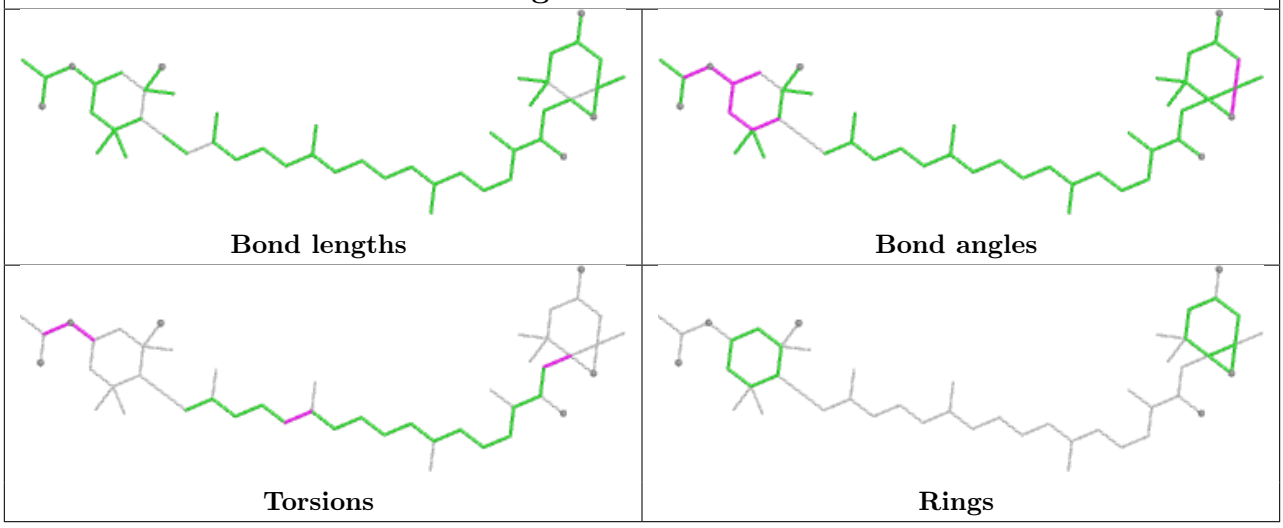
Ligand A86 T 313



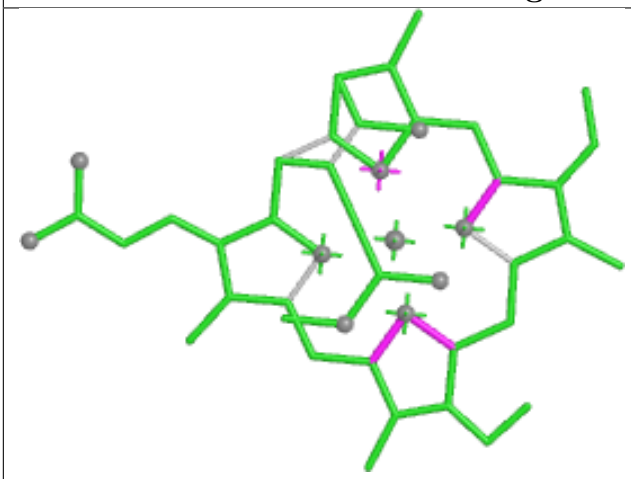
Ligand LMG P 318



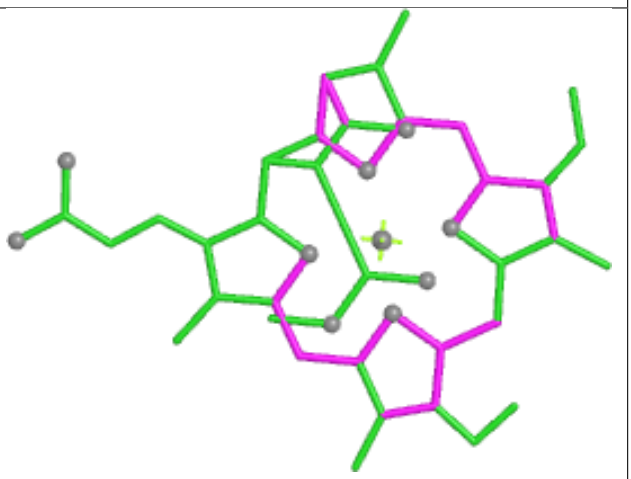
Ligand A86 P 316



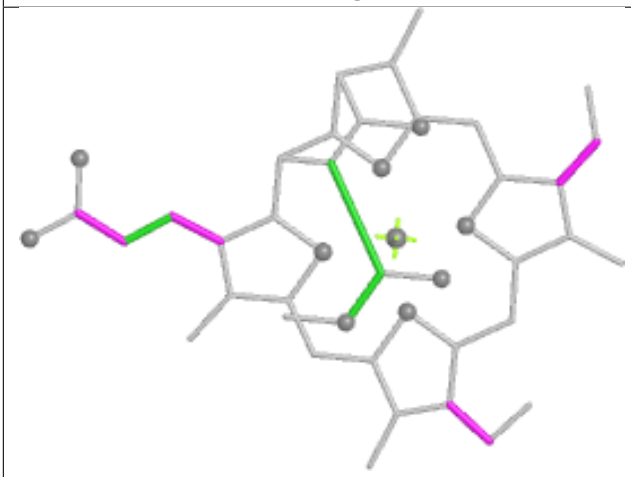
Ligand KC2 O 302



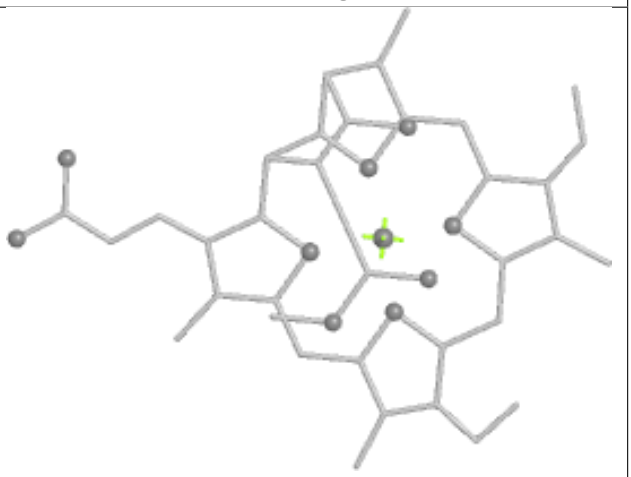
Bond lengths



Bond angles

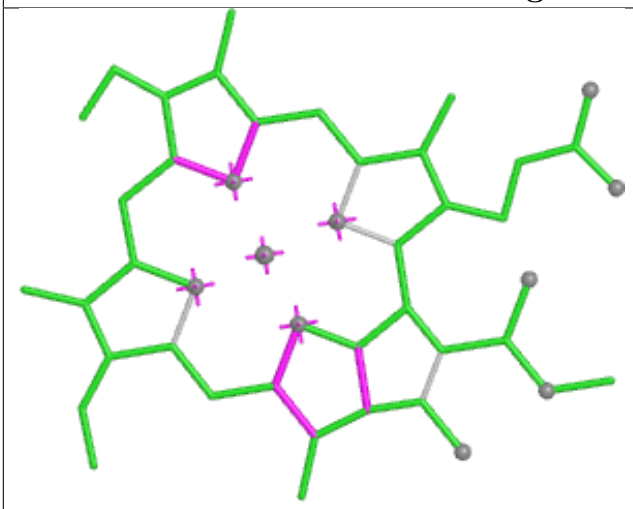


Torsions

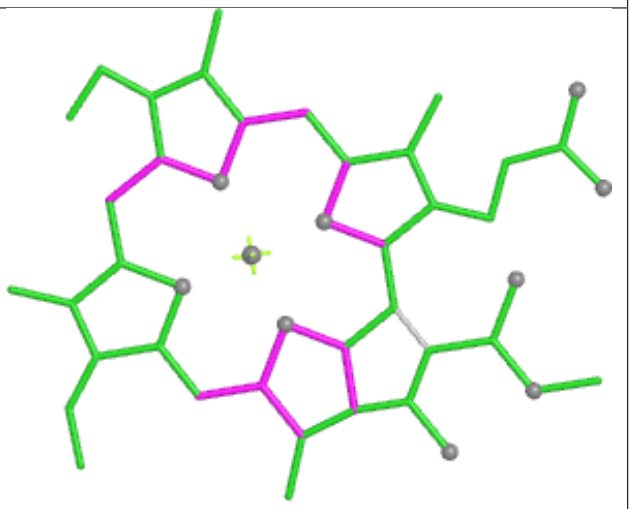


Rings

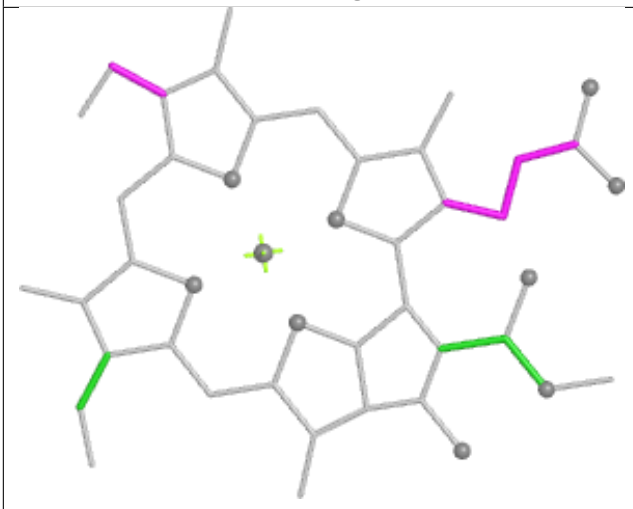
Ligand CLA L 314



Bond lengths



Bond angles

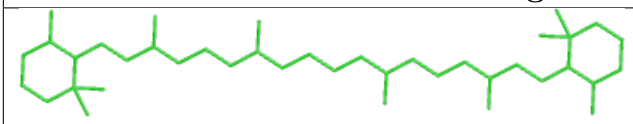


Torsions

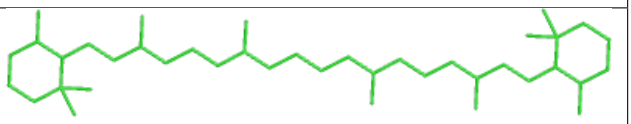


Rings

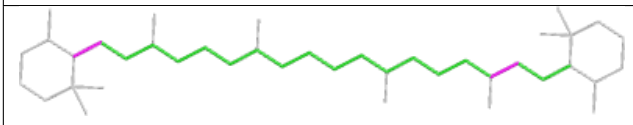
Ligand BCR a 843



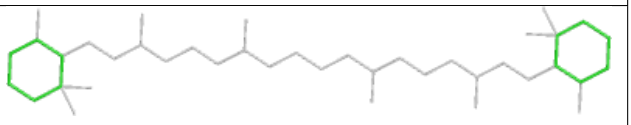
Bond lengths



Bond angles

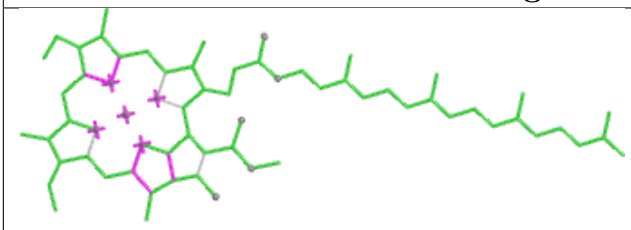


Torsions

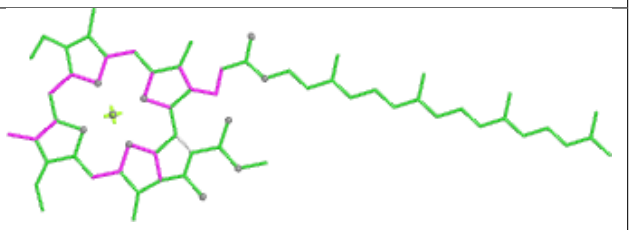


Rings

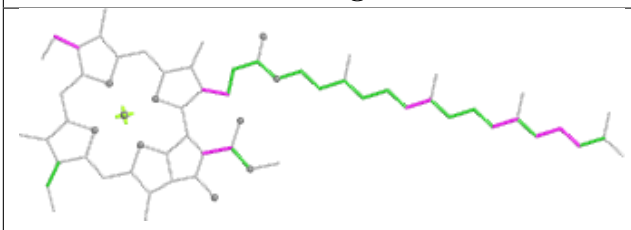
Ligand CLA A 304



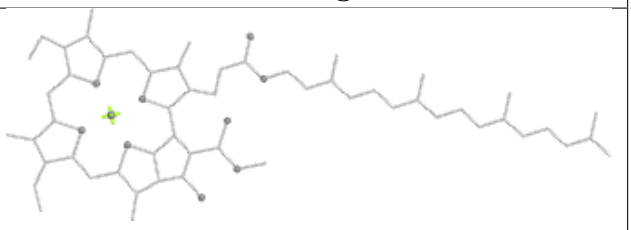
Bond lengths



Bond angles

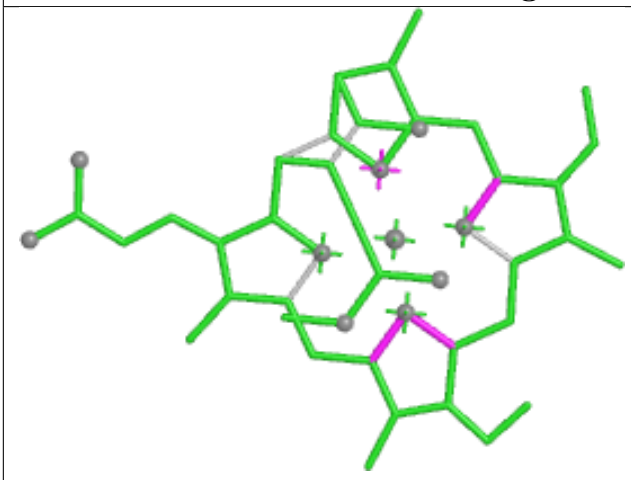


Torsions

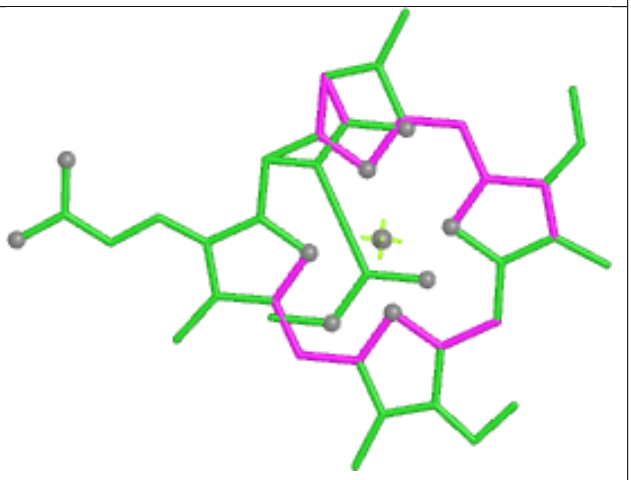


Rings

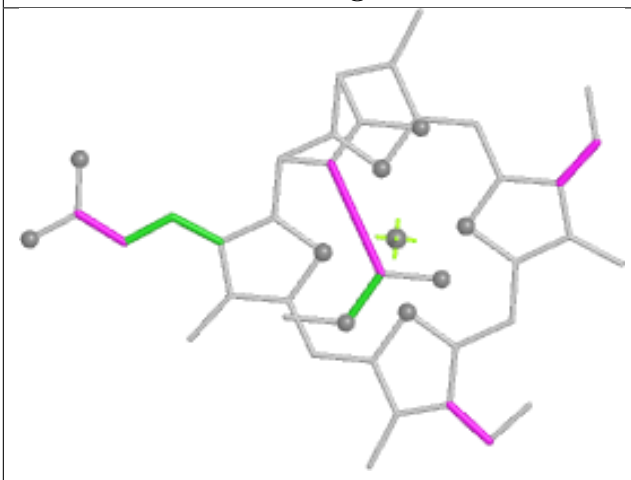
Ligand KC2 W 314



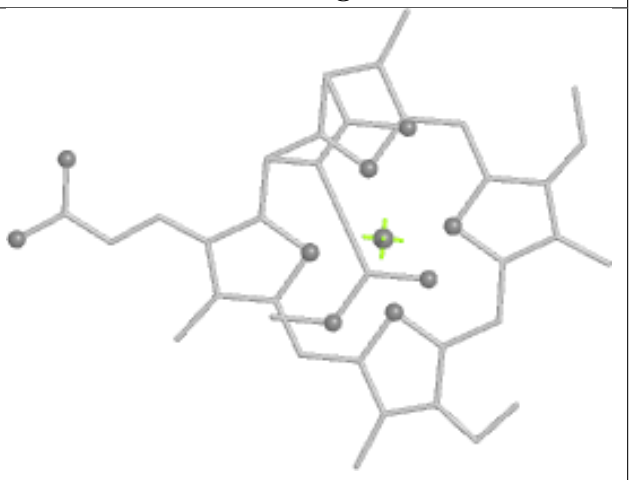
Bond lengths



Bond angles

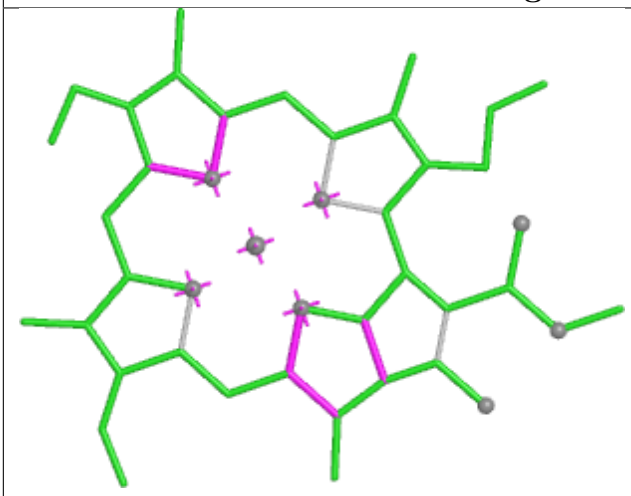


Torsions

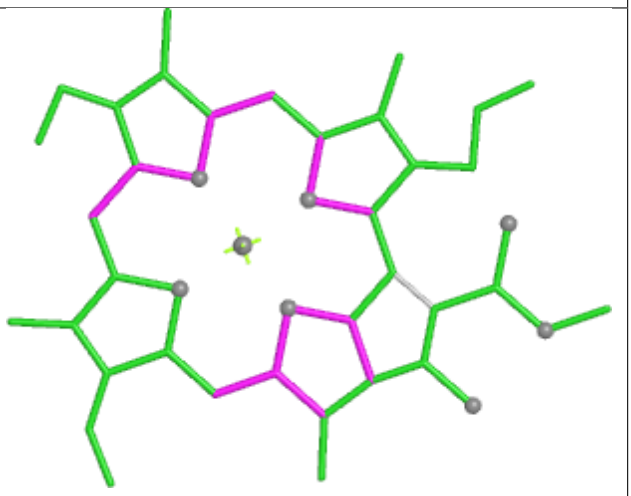


Rings

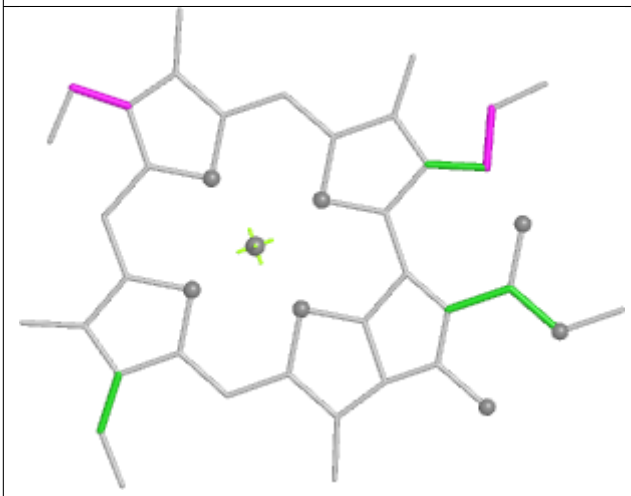
Ligand CLA C 309



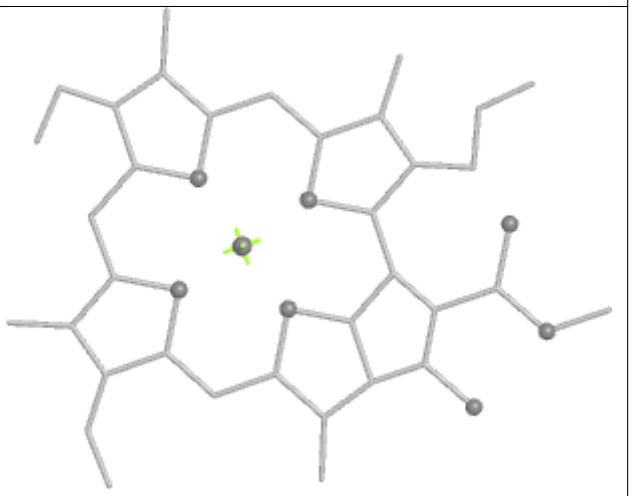
Bond lengths



Bond angles

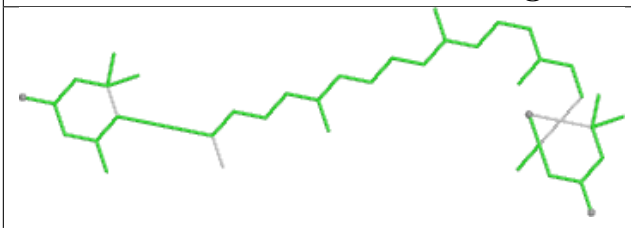


Torsions

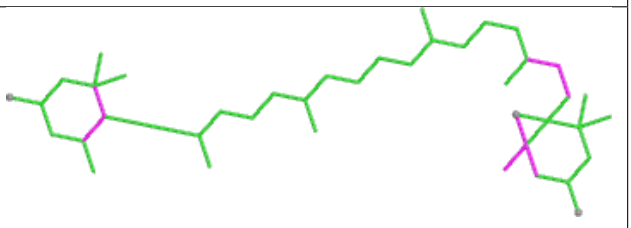


Rings

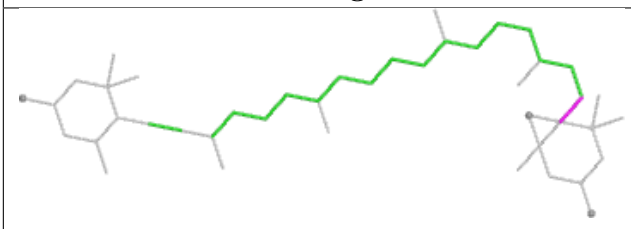
Ligand DD6 H 313



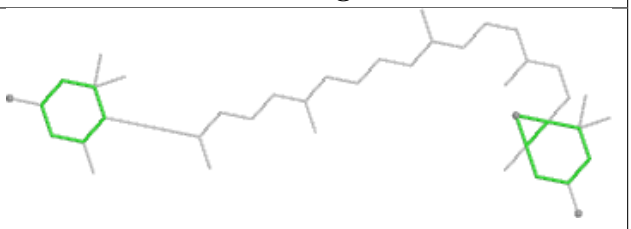
Bond lengths



Bond angles

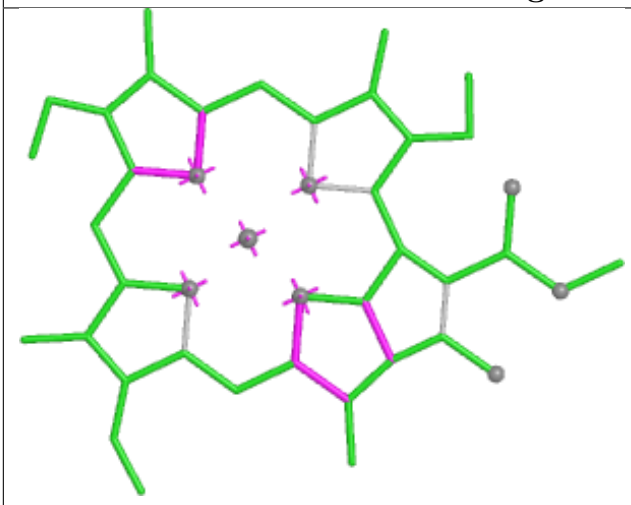


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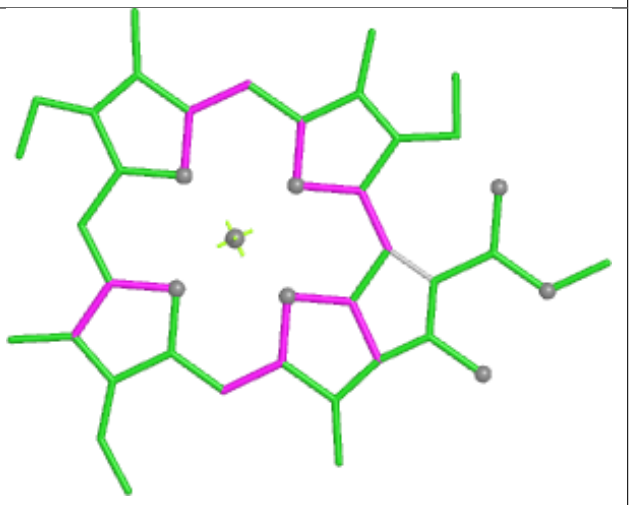


Rings

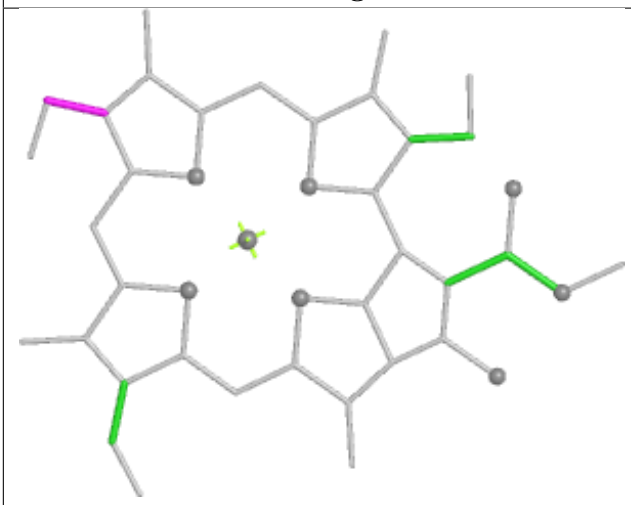
Ligand CLA S 304



Bond lengths



Bond angles

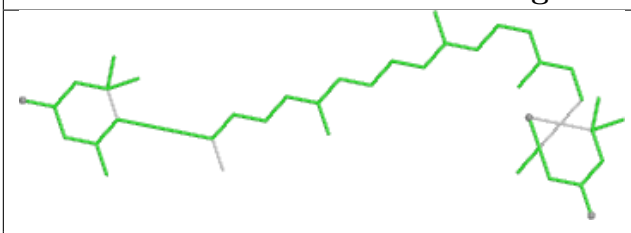


Torsions



Rings

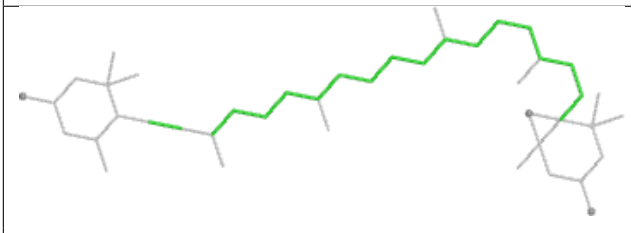
Ligand DD6 I 312



Bond lengths



Bond angles

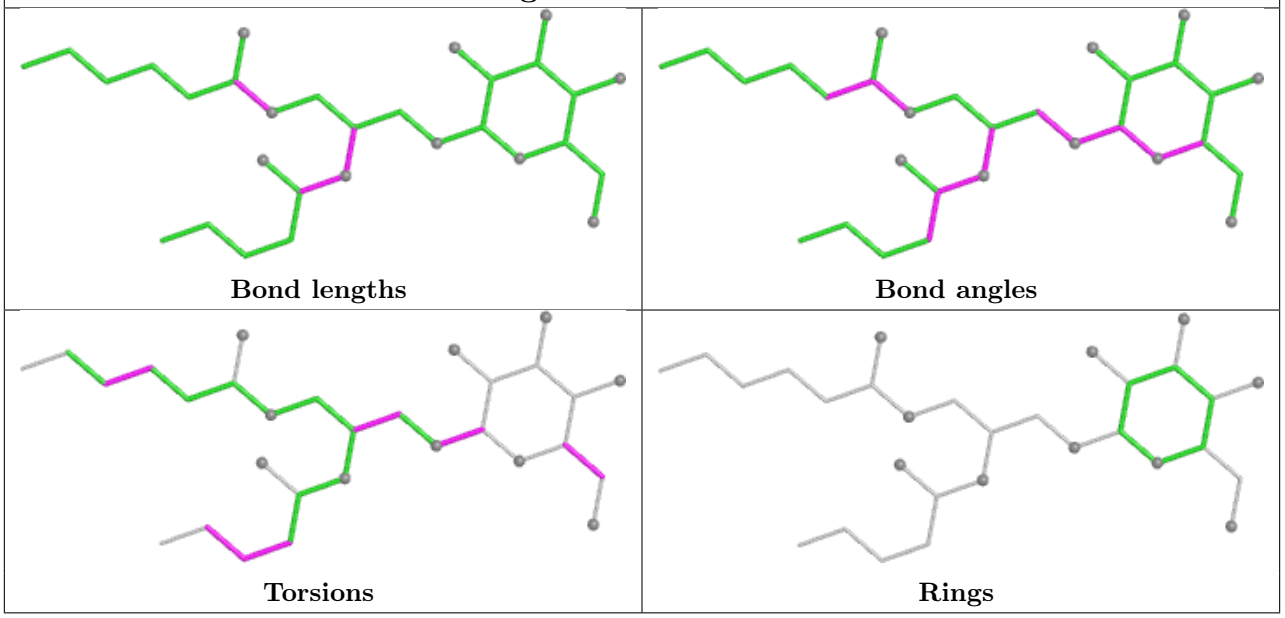


Torsions

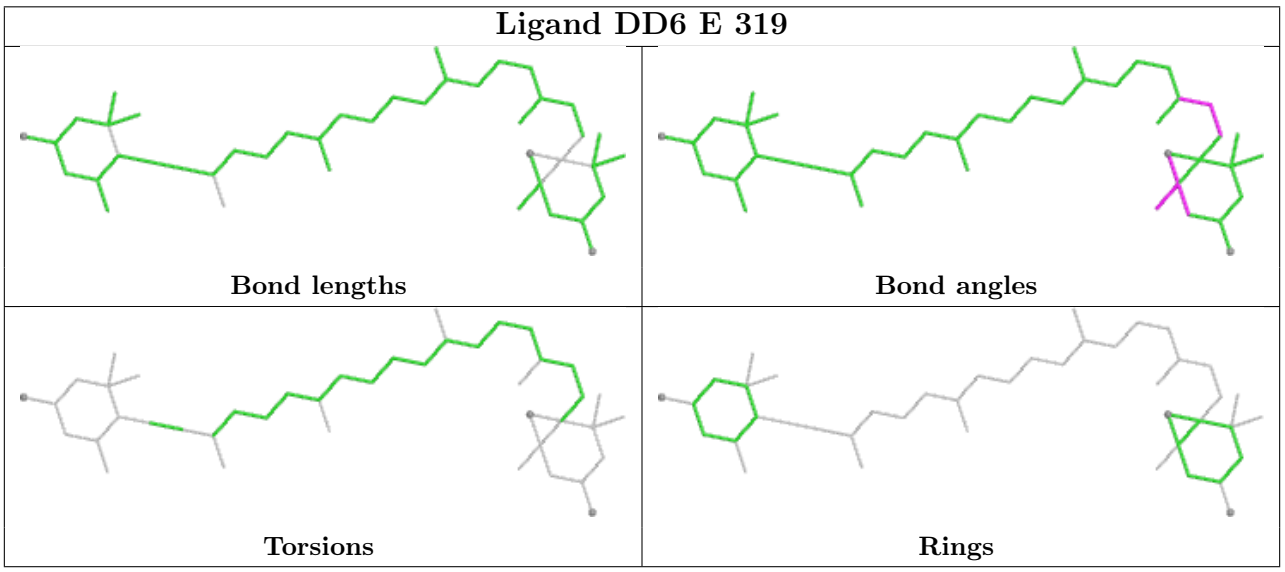


Rings

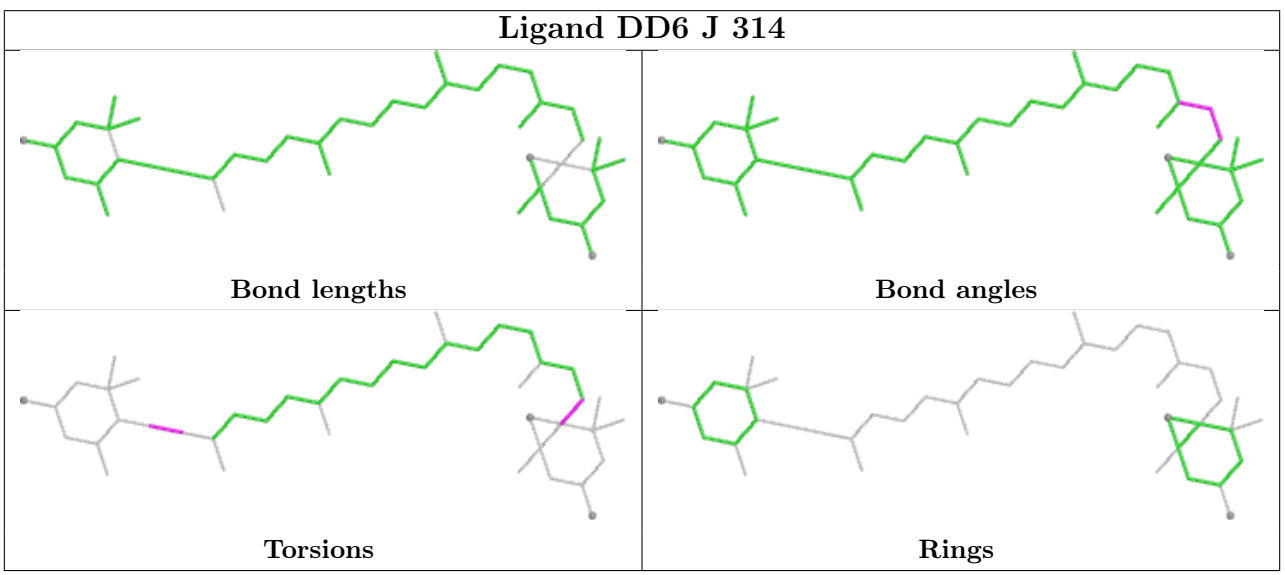
Ligand LMG D 302

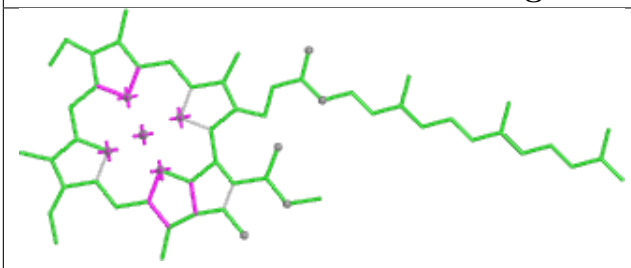
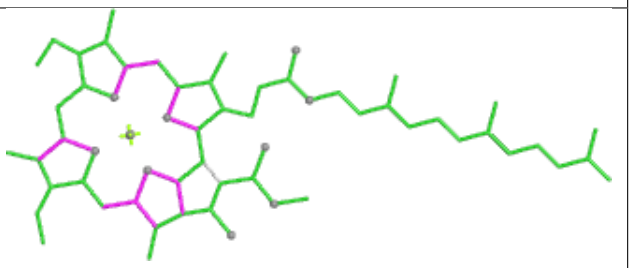
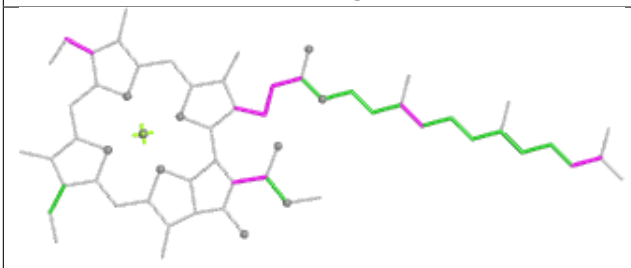
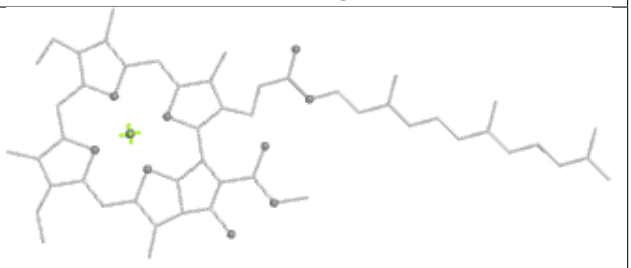


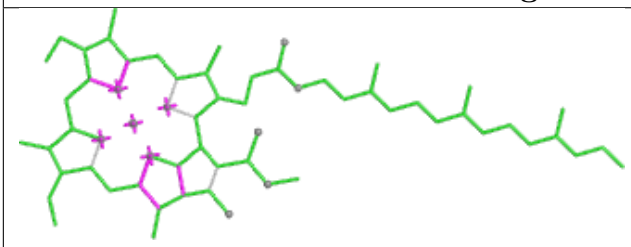
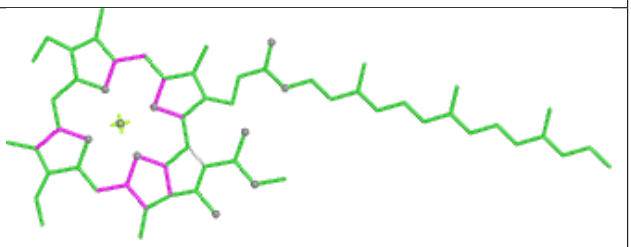
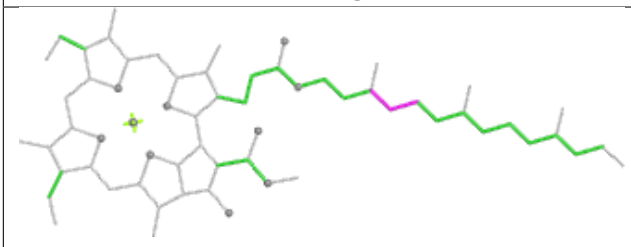
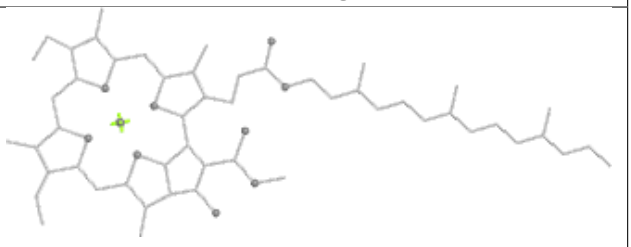
Ligand DD6 E 319



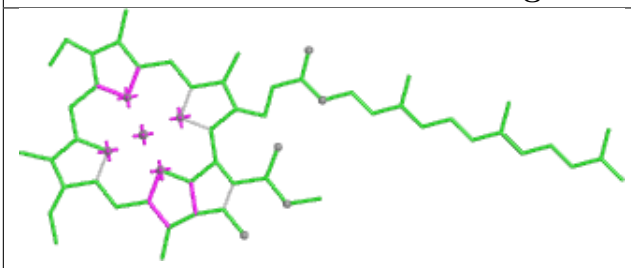
Ligand DD6 J 314



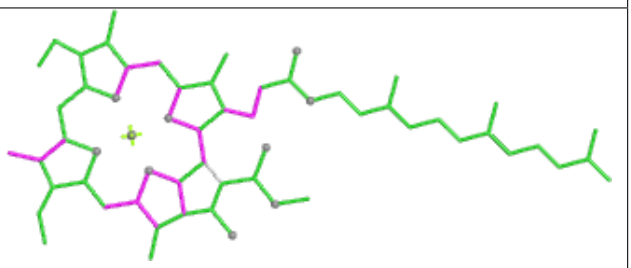
Ligand CLA P 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA M 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

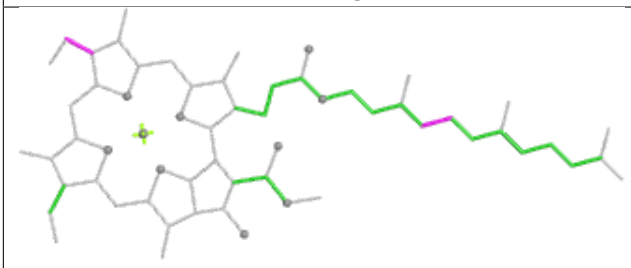
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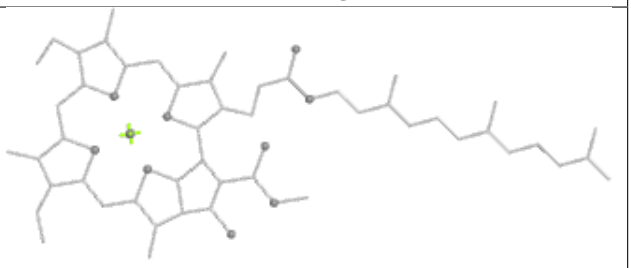
Bond lengths



Bond angles

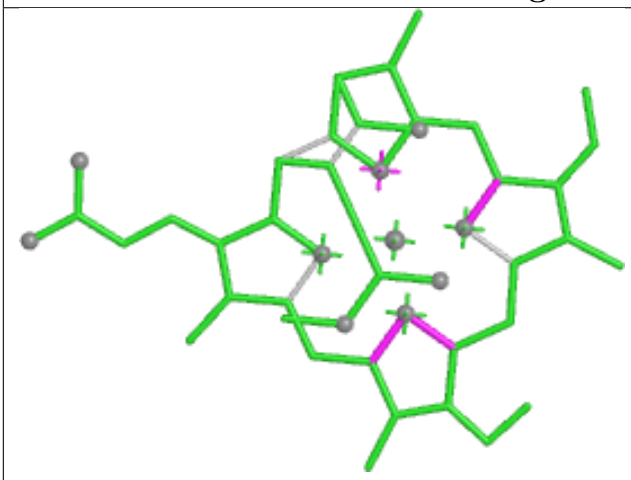


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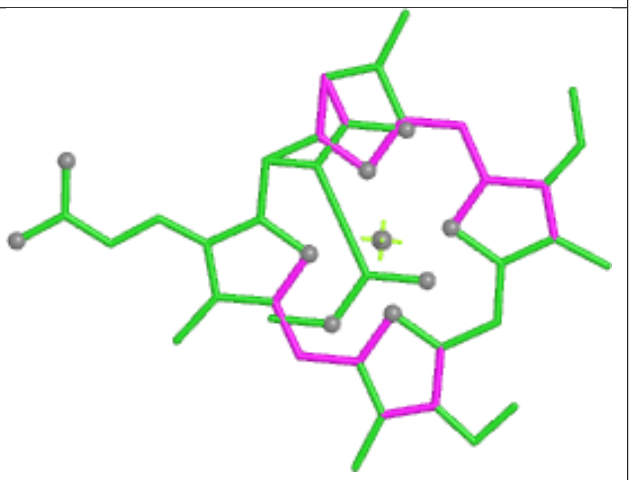


Rings

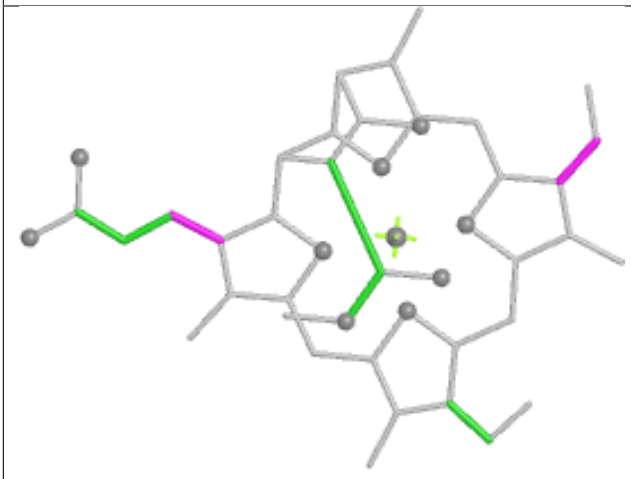
Ligand KC2 S 302



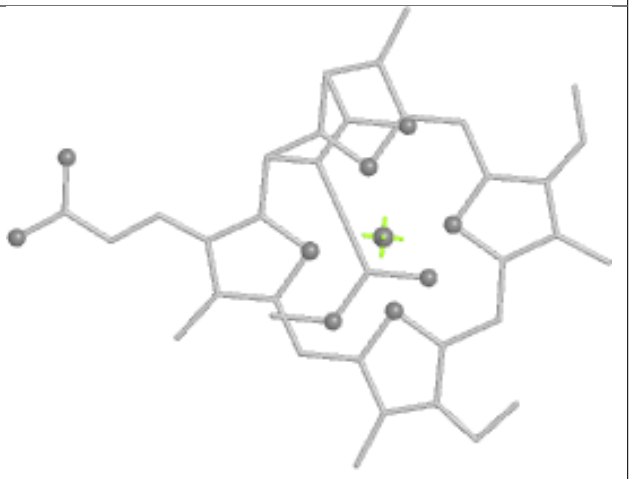
Bond lengths



Bond angles

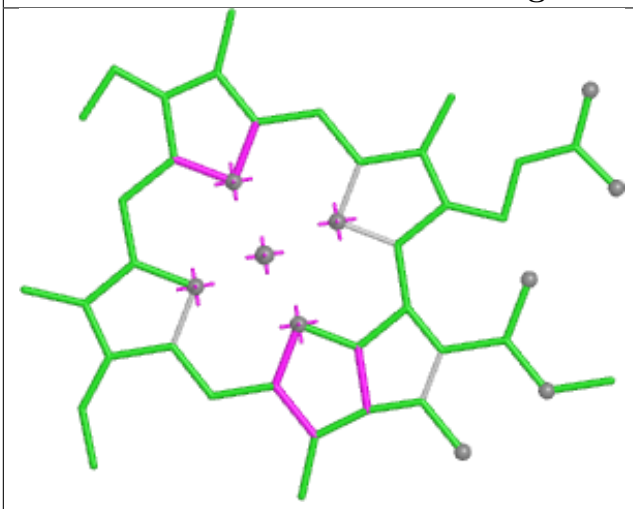


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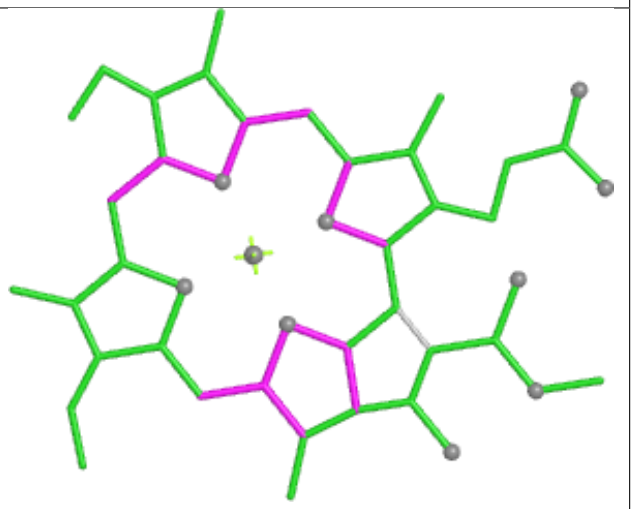


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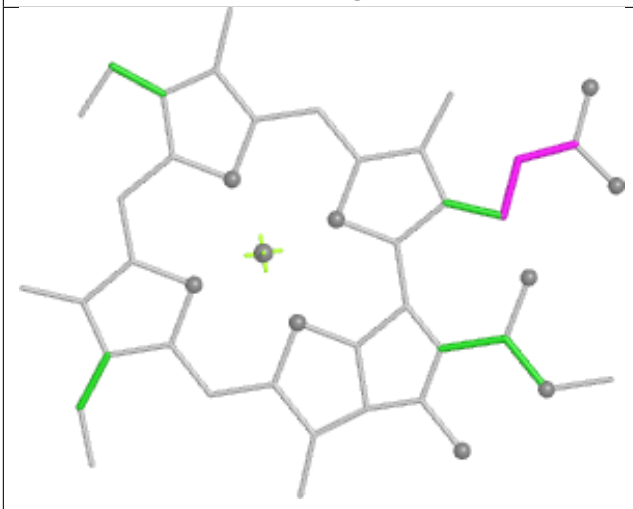
Ligand CLA J 301



Bond lengths



Bond angles

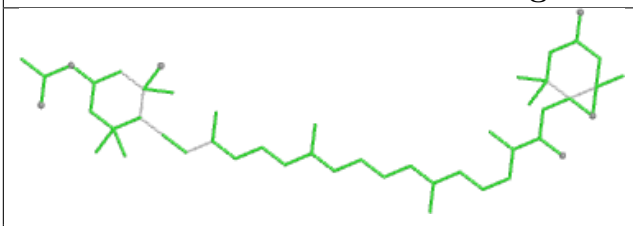


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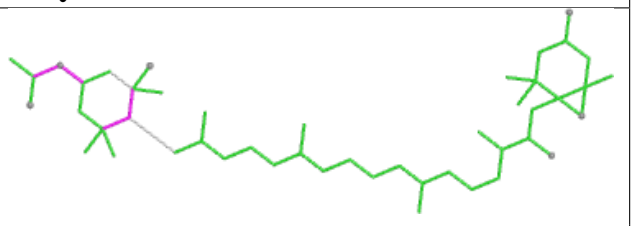


Rings

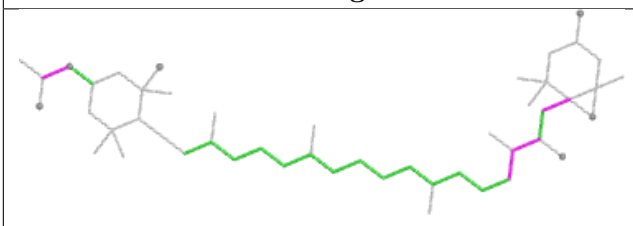
Ligand A86 Q 311



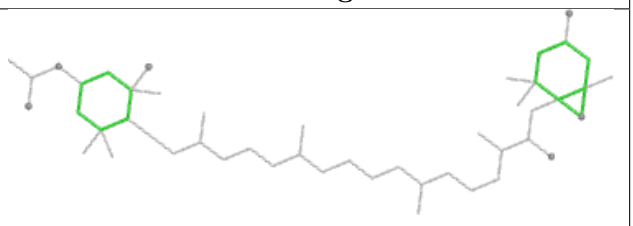
Bond lengths



Bond angles

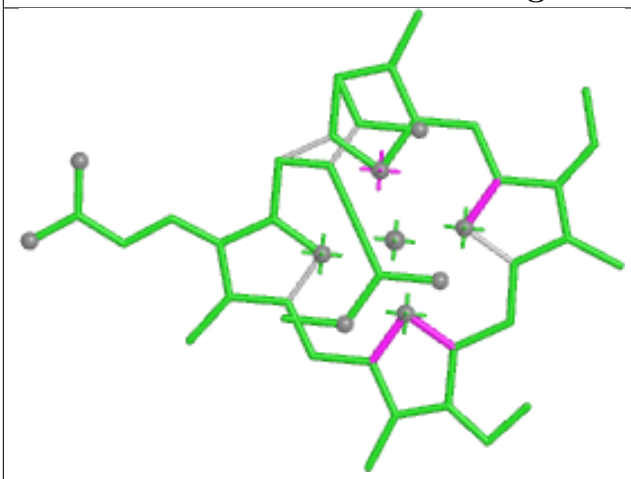


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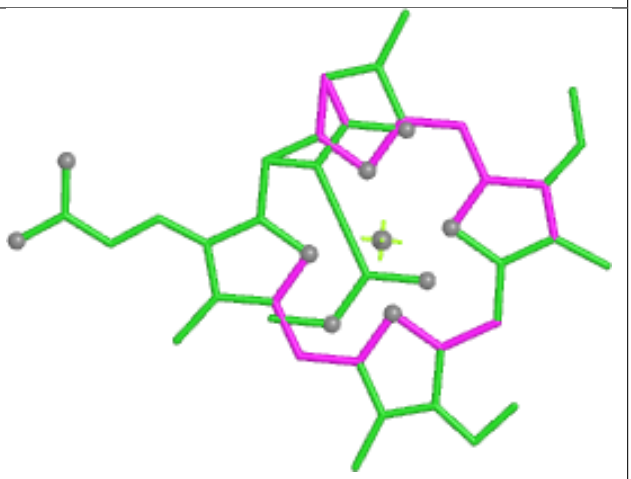


Rings

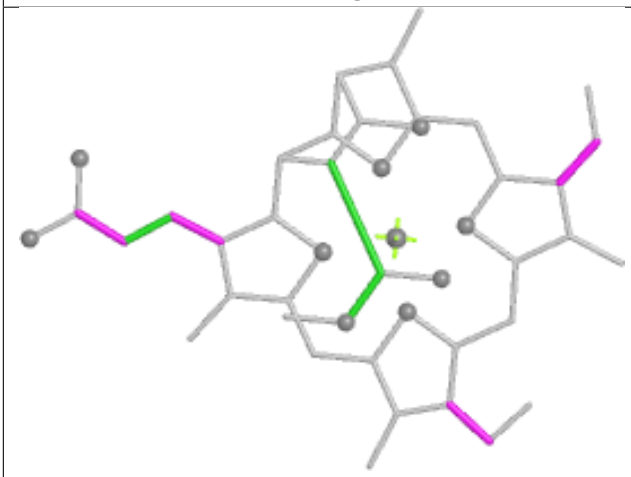
Ligand KC2 E 313



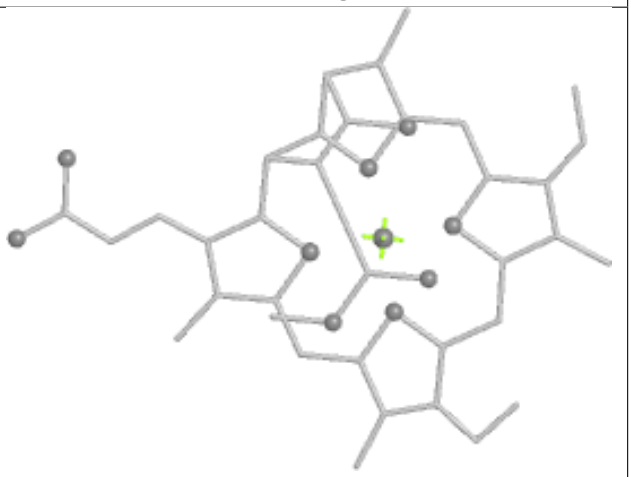
Bond lengths



Bond angles



Torsions



Rings

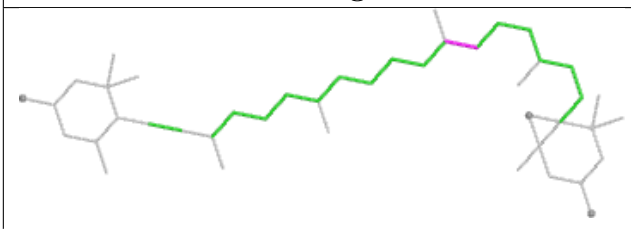
Ligand DD6 Q 312



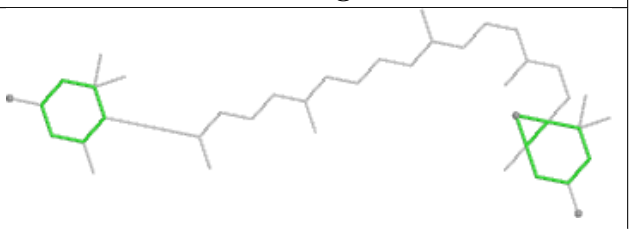
Bond lengths



Bond angles

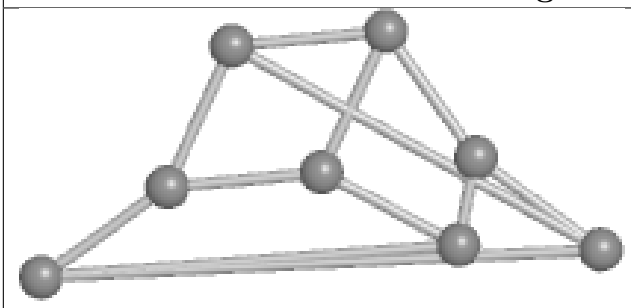


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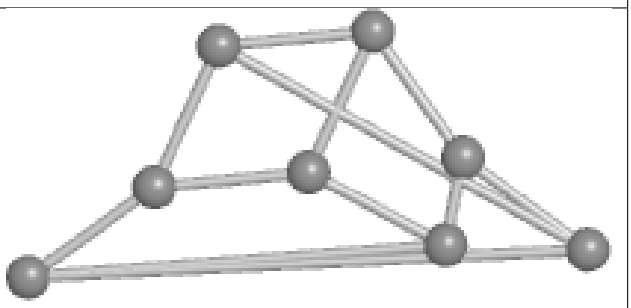


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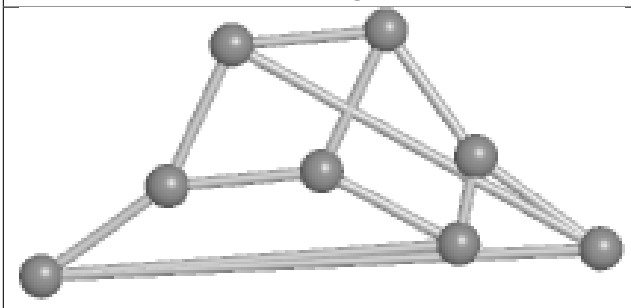
Ligand SF4 c 101



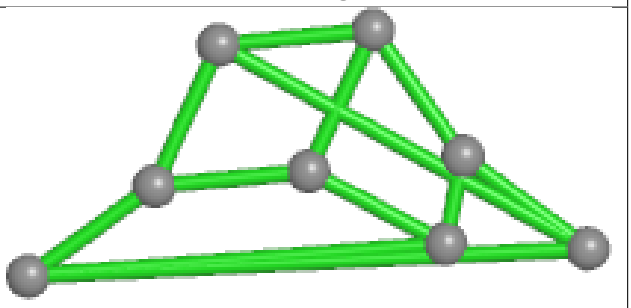
Bond lengths



Bond angles

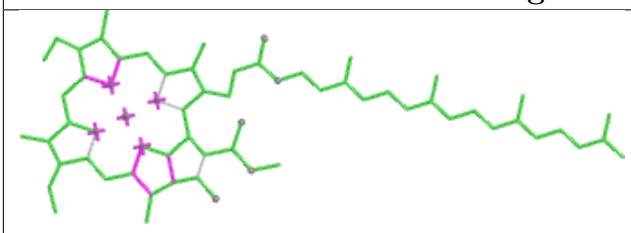


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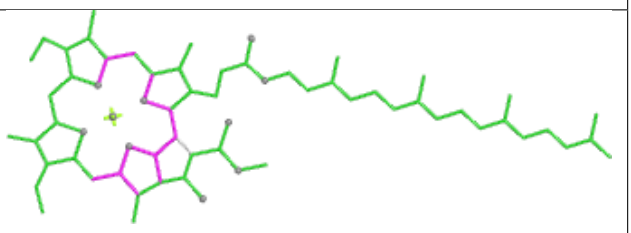


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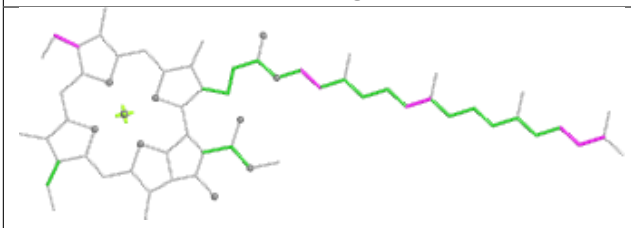
Ligand CLA b 805



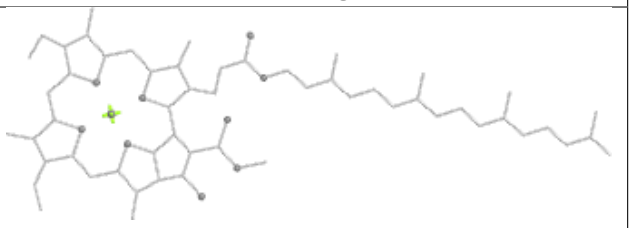
Bond lengths



Bond angles

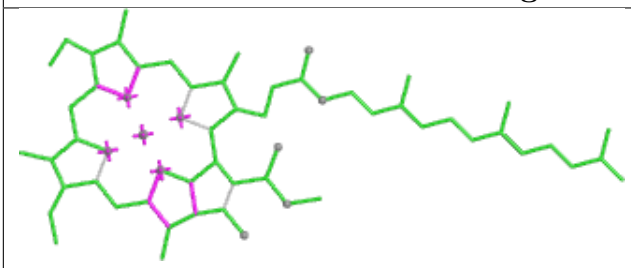


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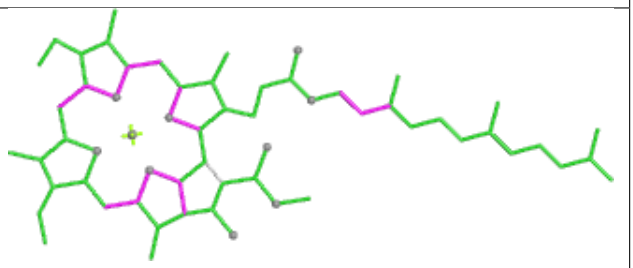


Rings

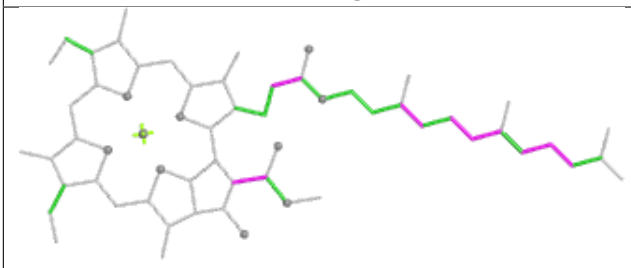
Ligand CLA M 312



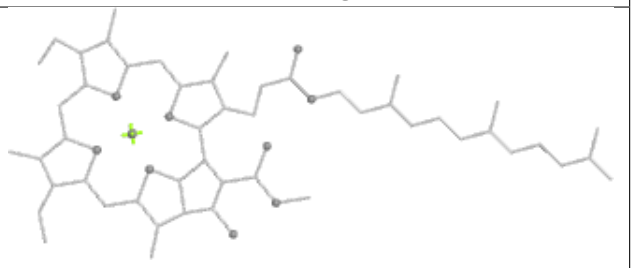
Bond lengths



Bond angles

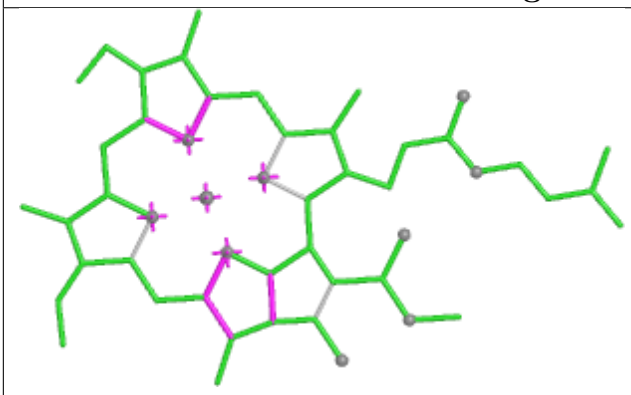


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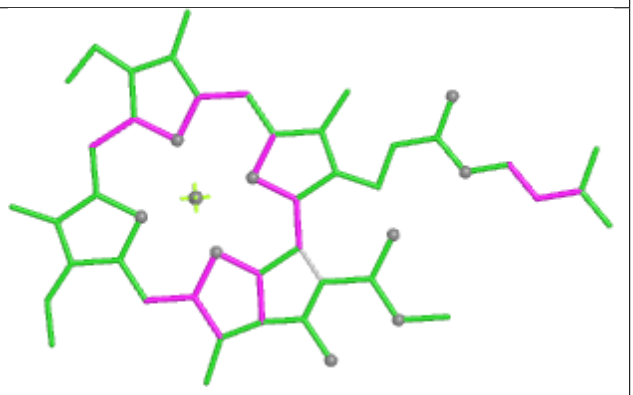


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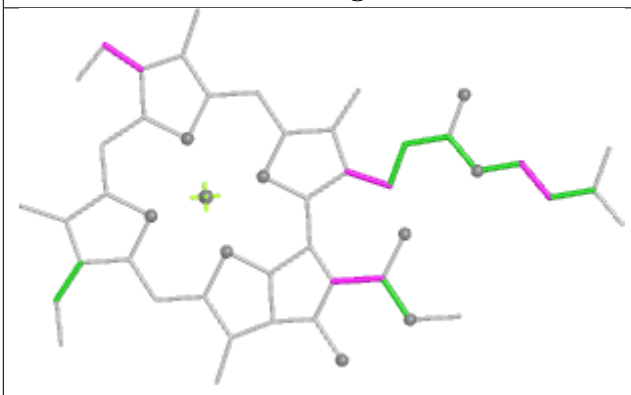
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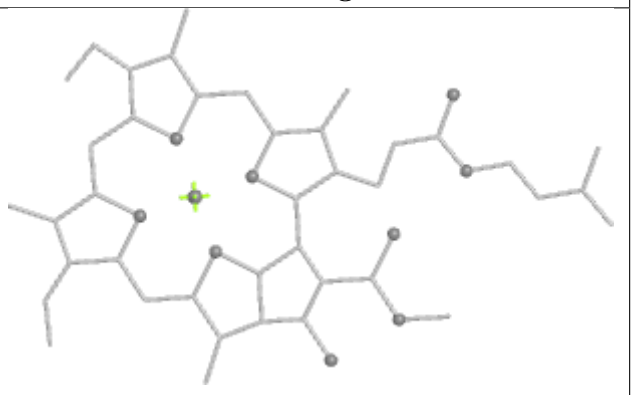
Bond lengths



Bond angles

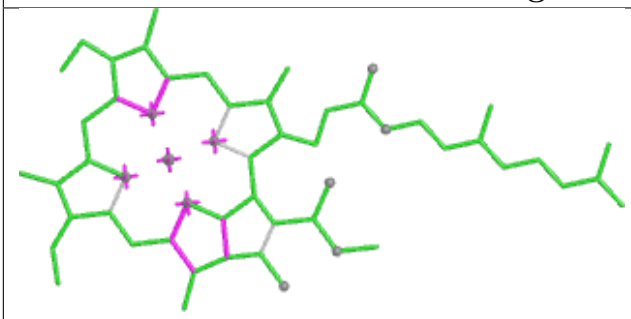


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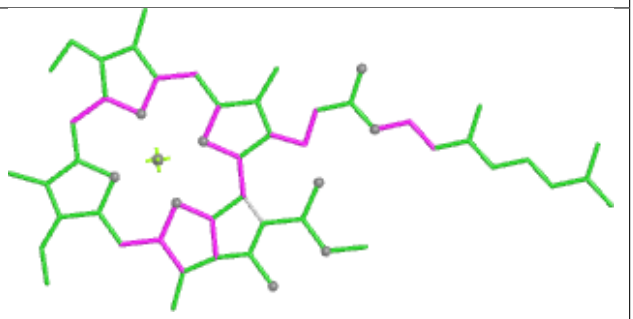


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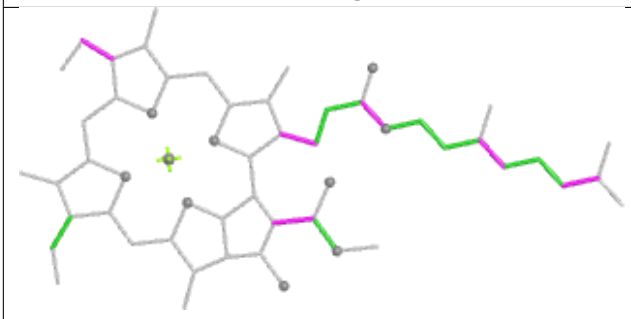
Ligand CLA k 203



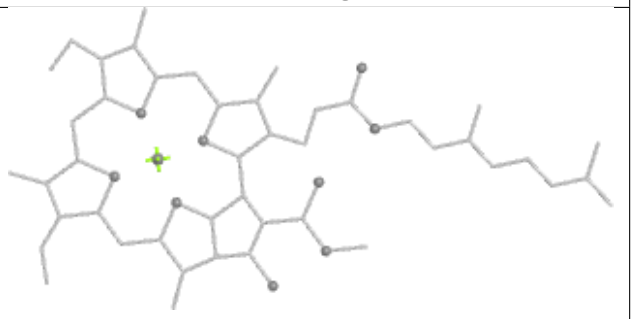
Bond lengths



Bond angles

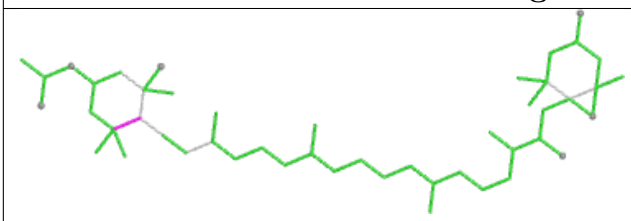


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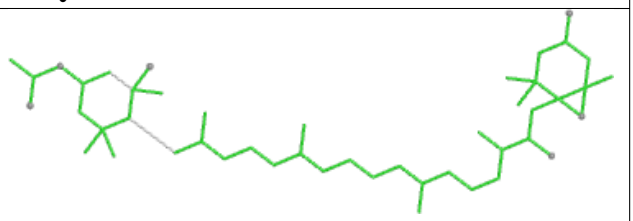


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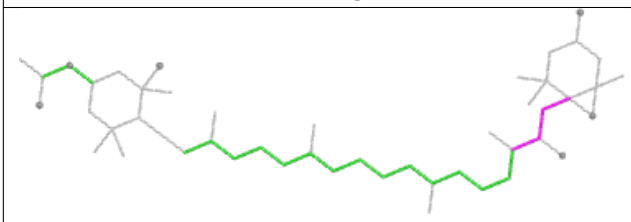
Ligand A86 Q 316



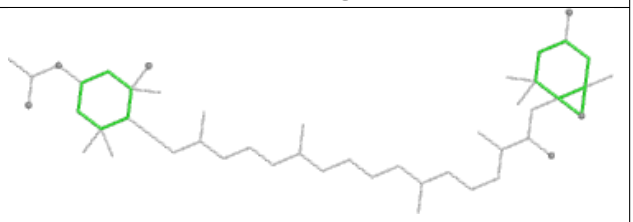
Bond lengths



Bond angles

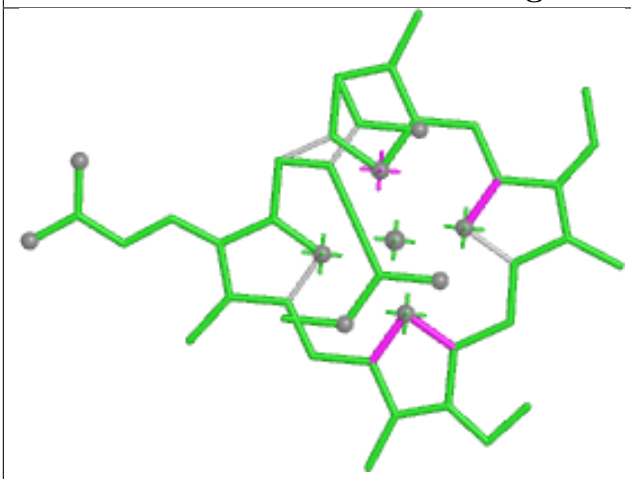


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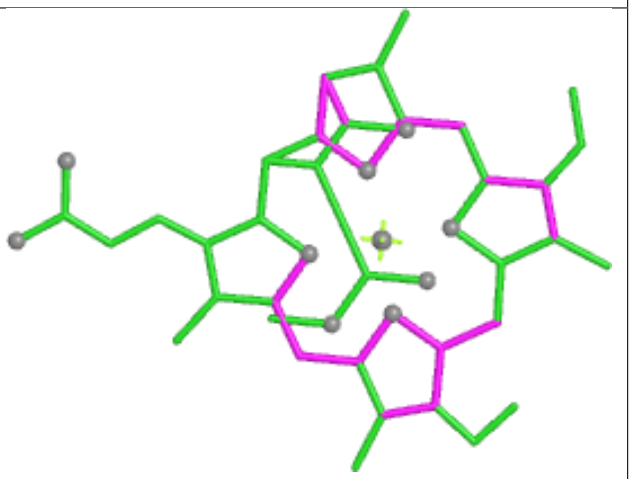


Rings

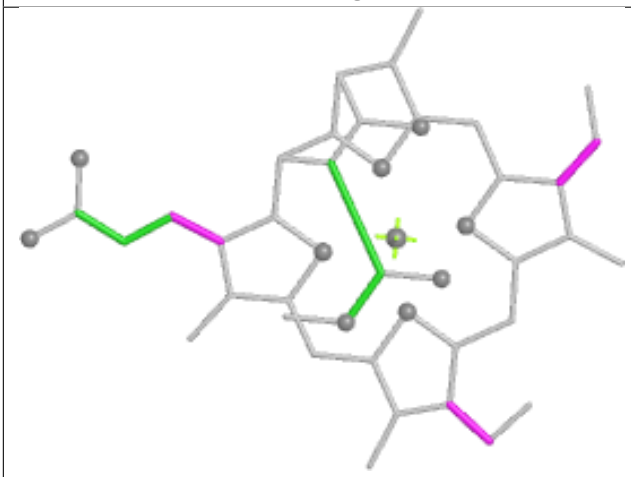
Ligand KC2 R 303



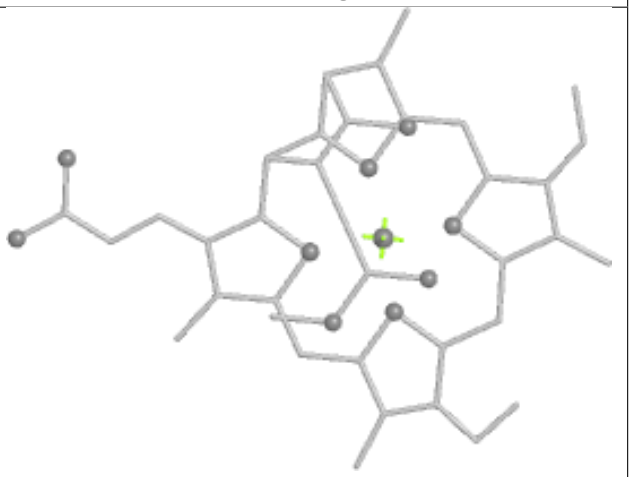
Bond lengths



Bond angles

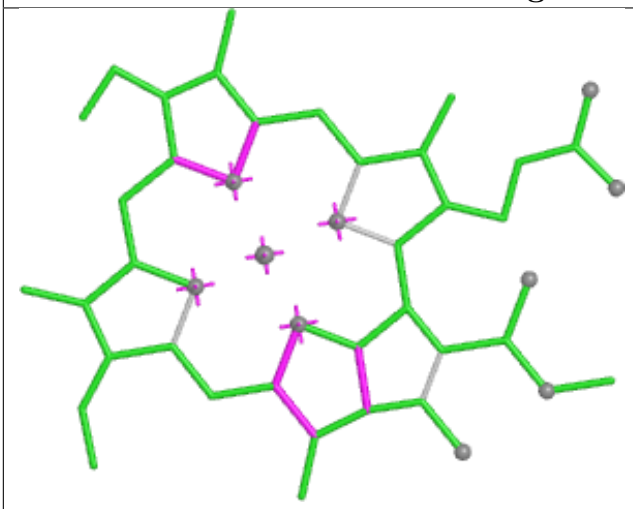


Torsions

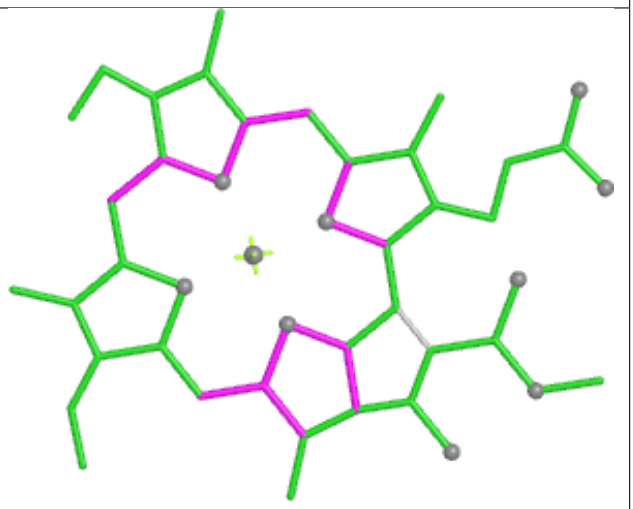


Rings

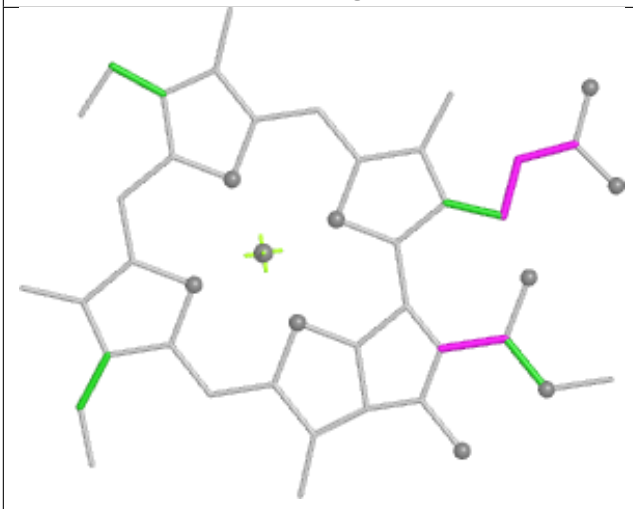
Ligand CLA b 813



Bond lengths



Bond angles

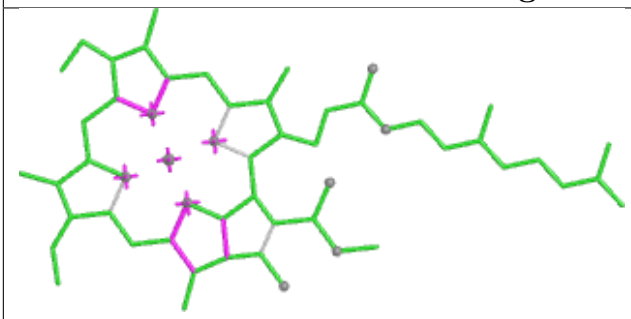


Torsions

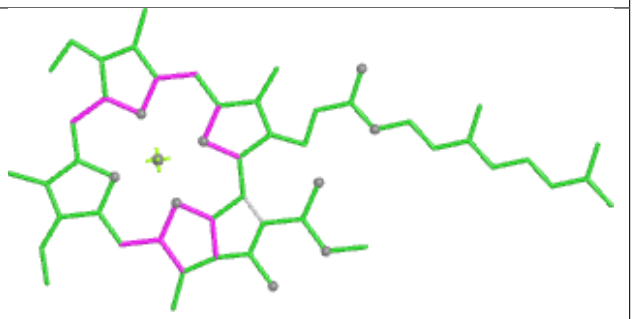


Rings

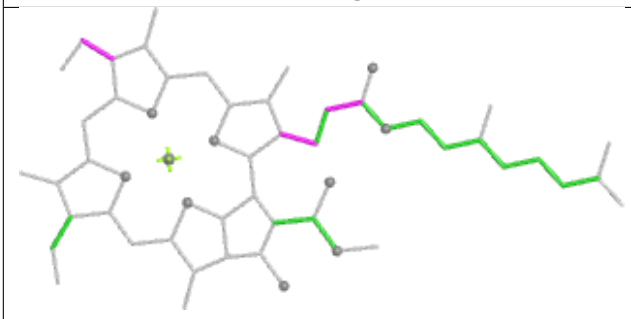
Ligand CLA W 306



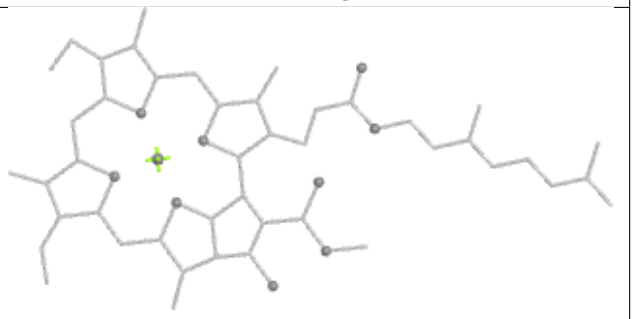
Bond lengths



Bond angles

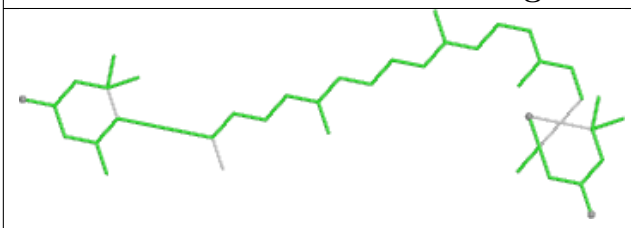


Torsions

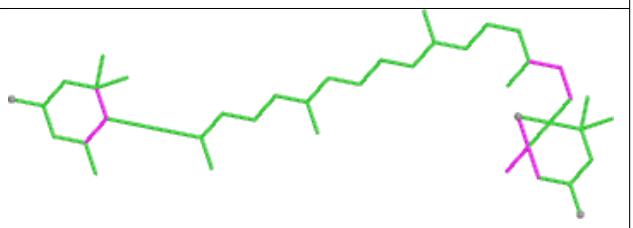


Rings

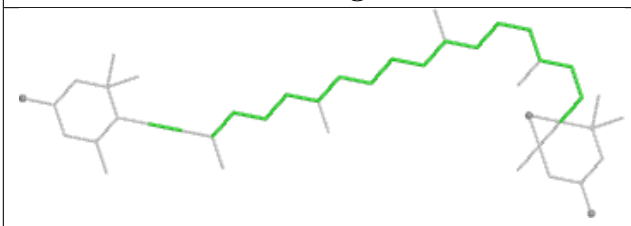
Ligand DD6 H 311



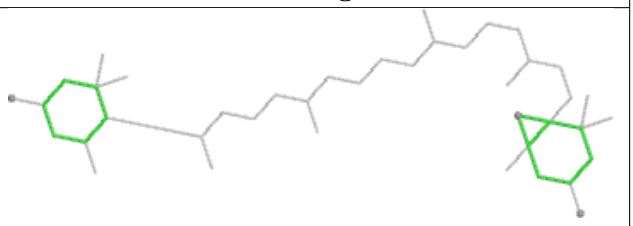
Bond lengths



Bond angles

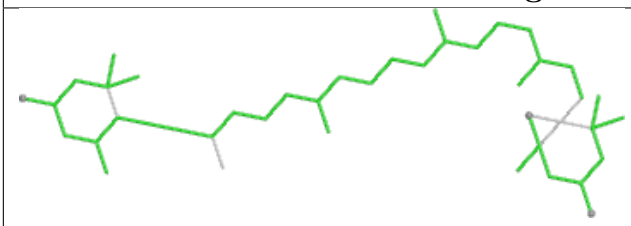


Torsions

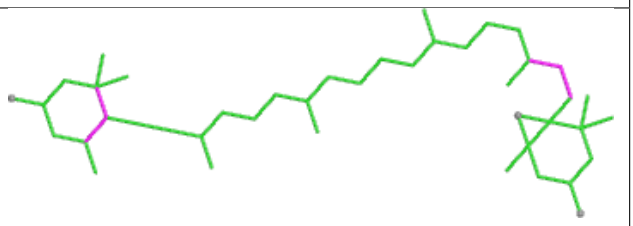


Rings

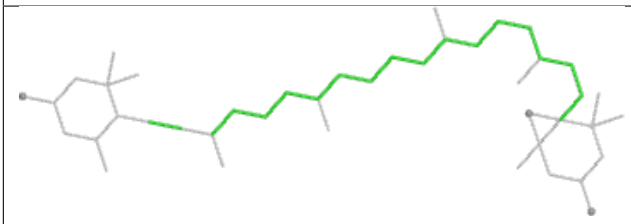
Ligand DD6 C 310



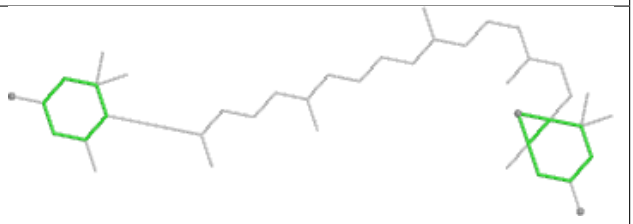
Bond lengths



Bond angles

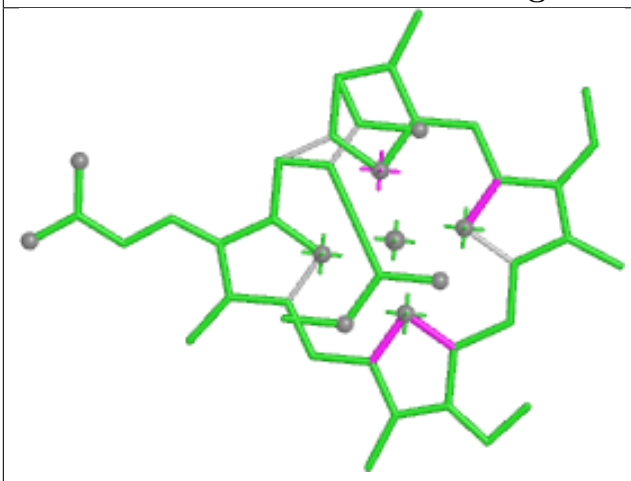


Torsions

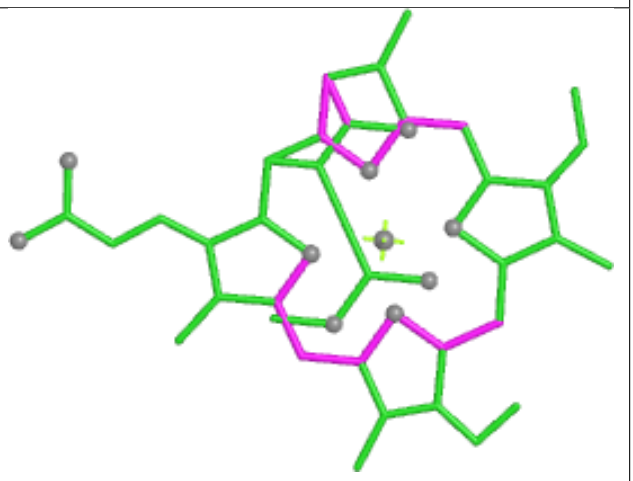


Rings

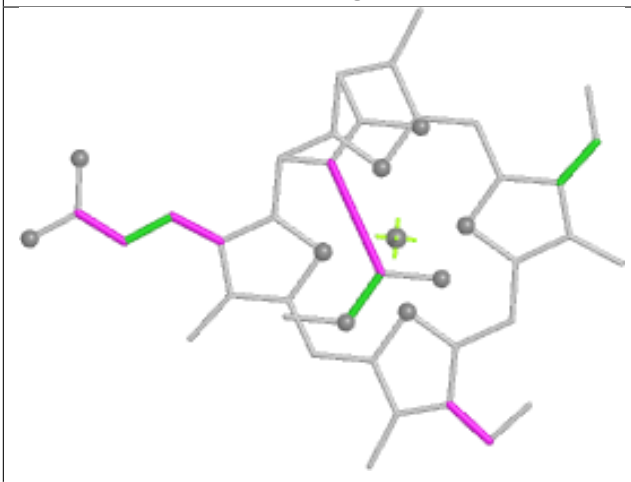
Ligand KC2 L 313



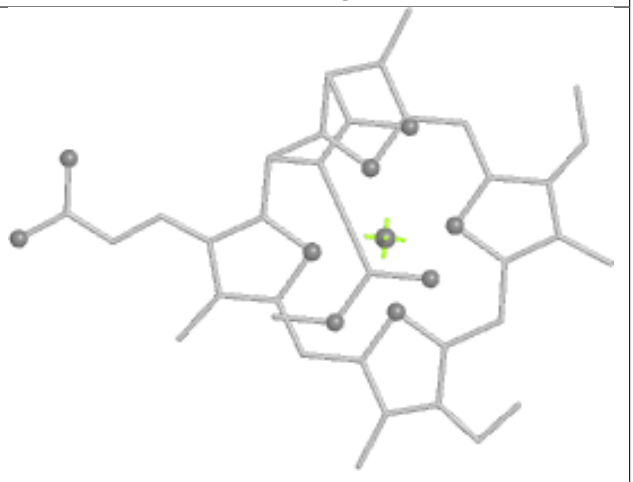
Bond lengths



Bond angles

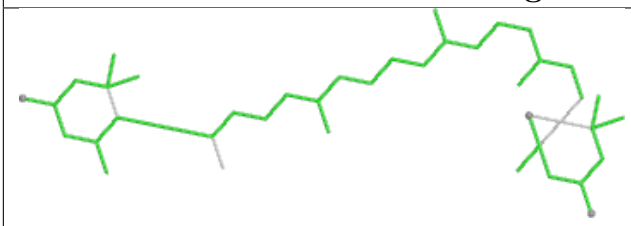


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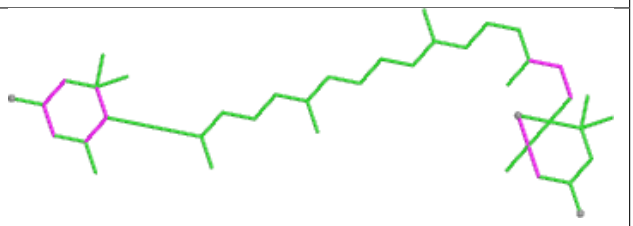


Rings

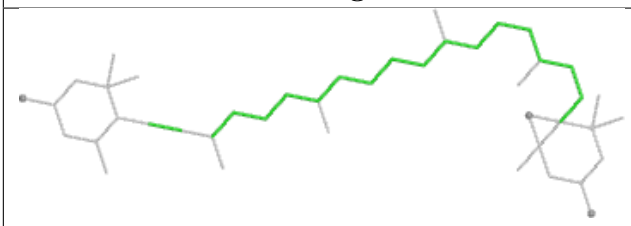
Ligand DD6 O 313



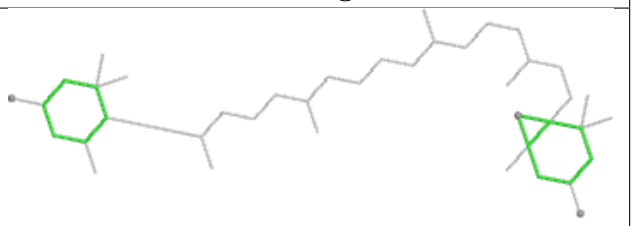
Bond lengths



Bond angles

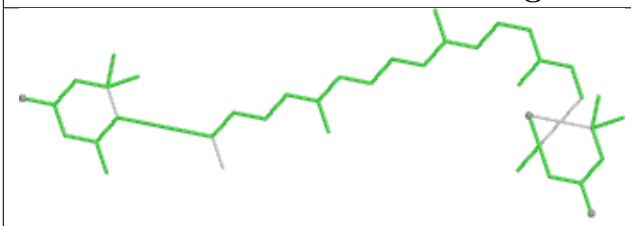


Torsions

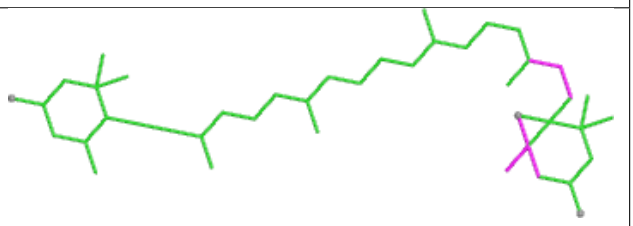


Rings

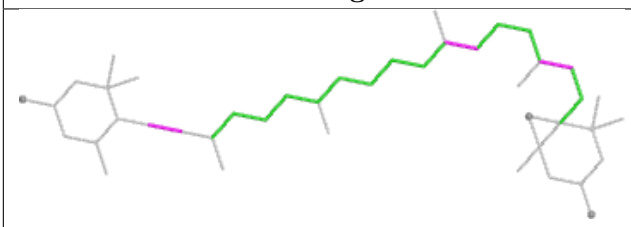
Ligand DD6 V 202



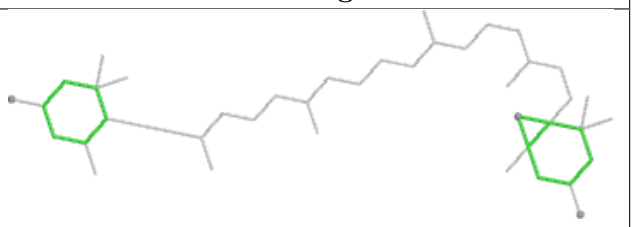
Bond lengths



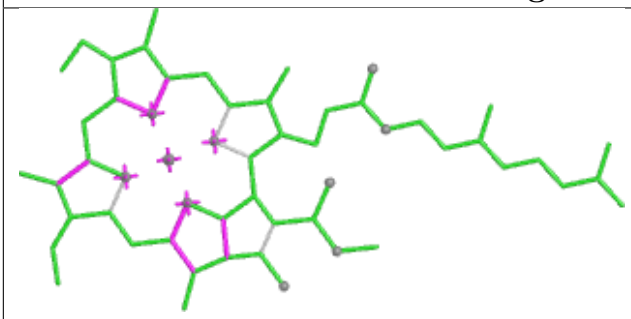
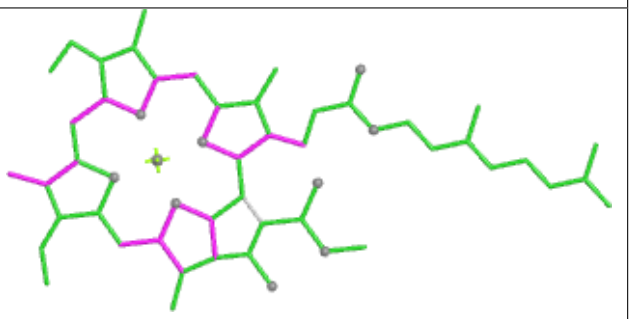
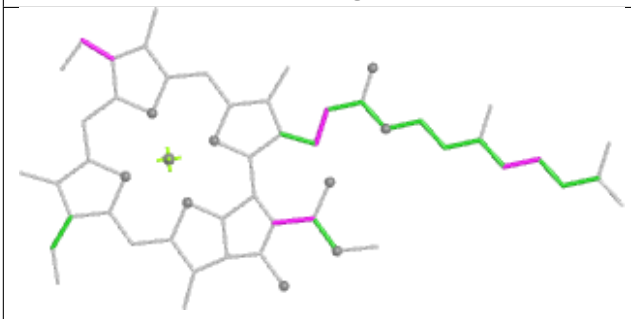
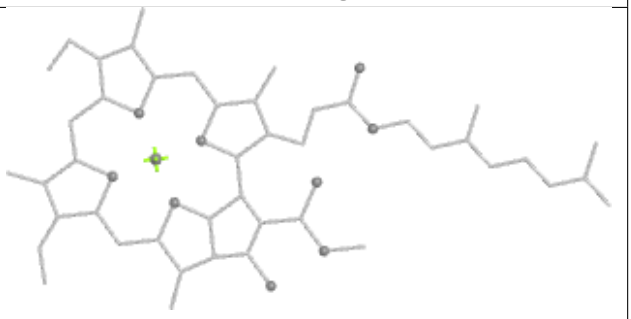
Bond angles

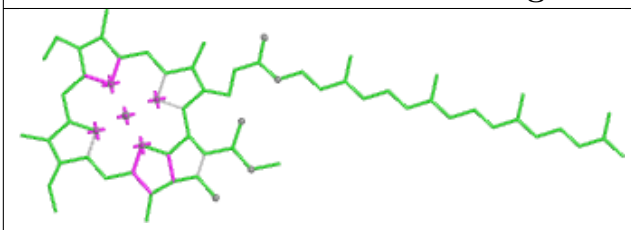
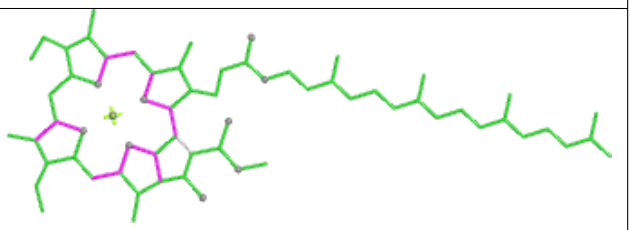
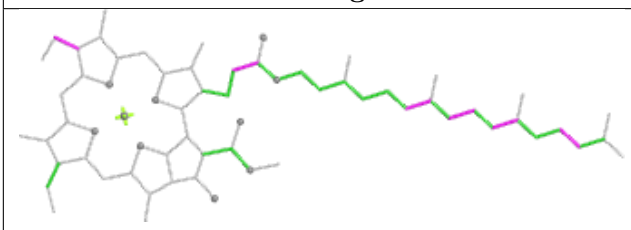
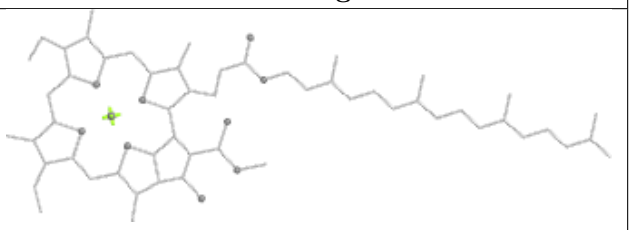


Torsions

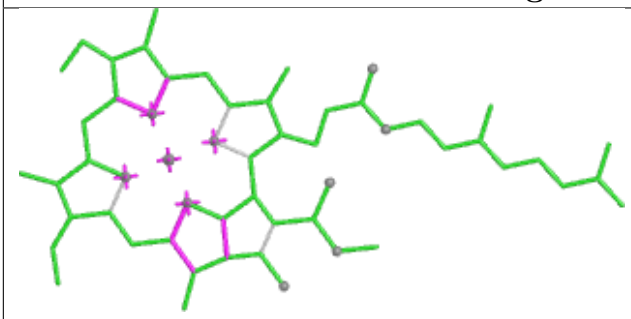


Rings

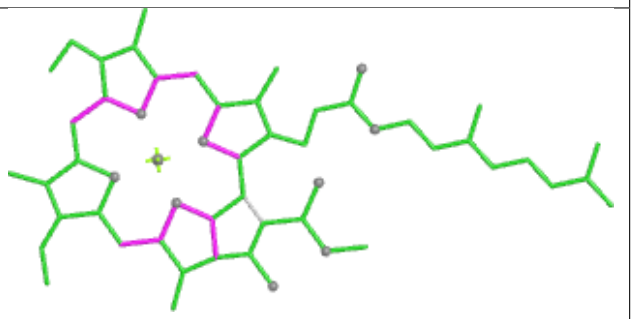
Ligand CLA J 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

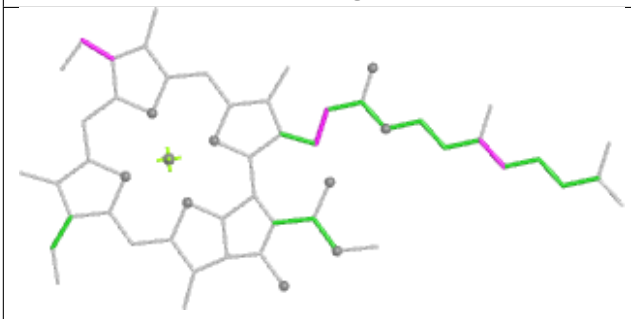
Ligand CLA F 309



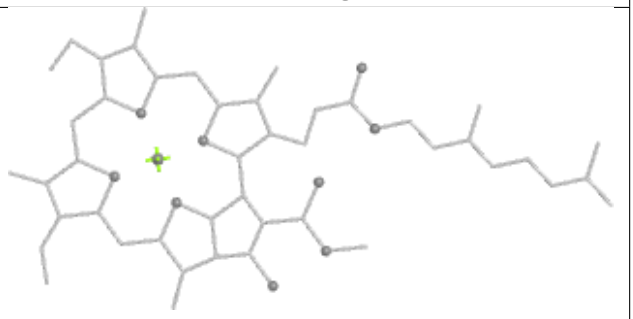
Bond lengths



Bond angles

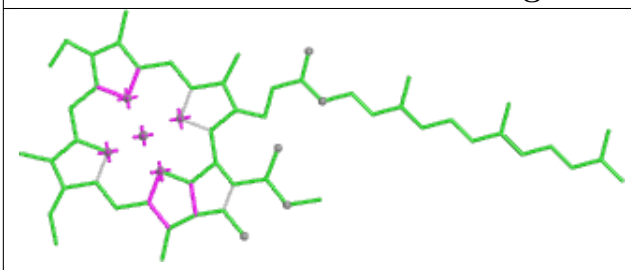


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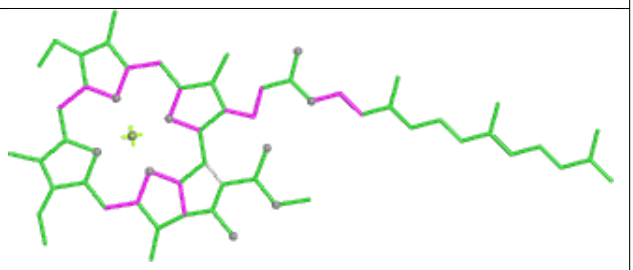


Rings

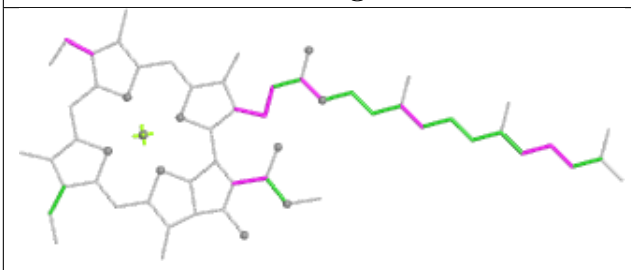
Ligand CLA H 307



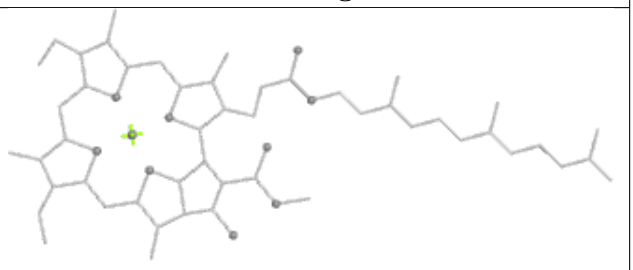
Bond lengths



Bond angles

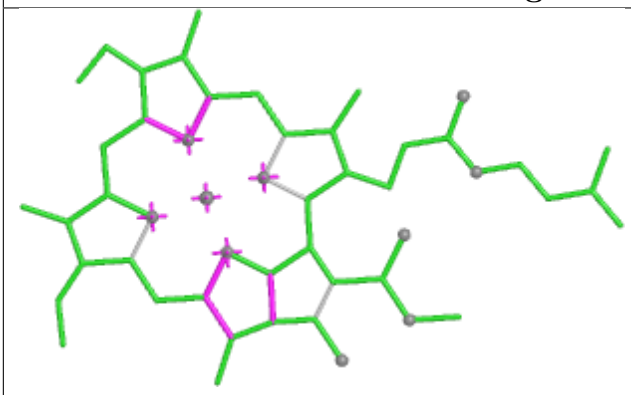


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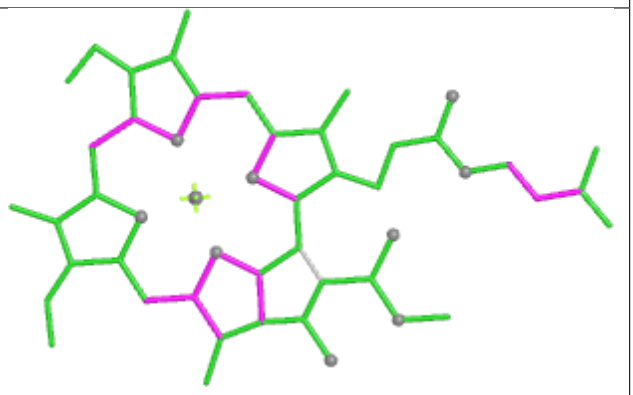


Rings

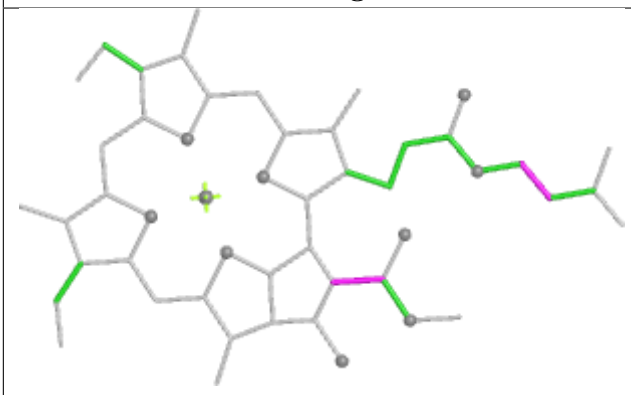
Ligand CLA E 314



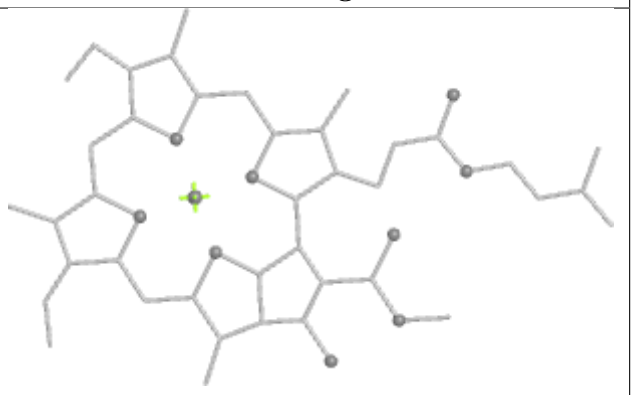
Bond lengths



Bond angles

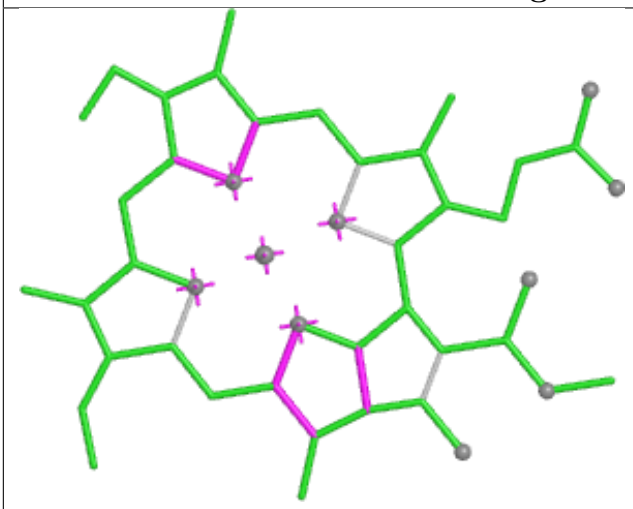


Torsions

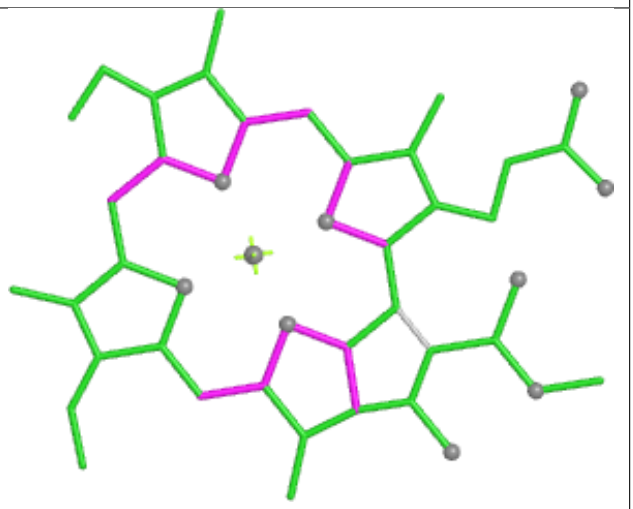


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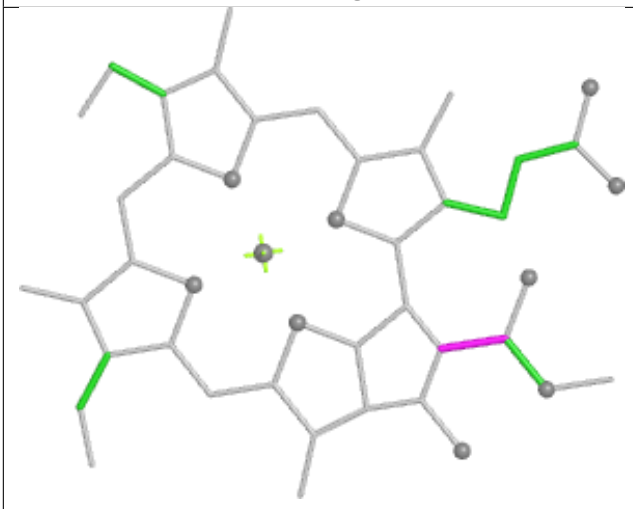
Ligand CLA r 202



Bond lengths



Bond angles

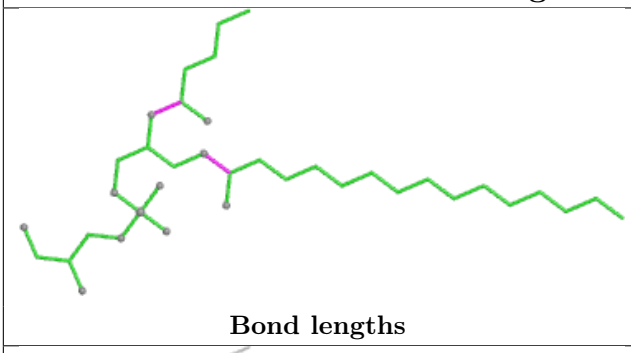


Torsions

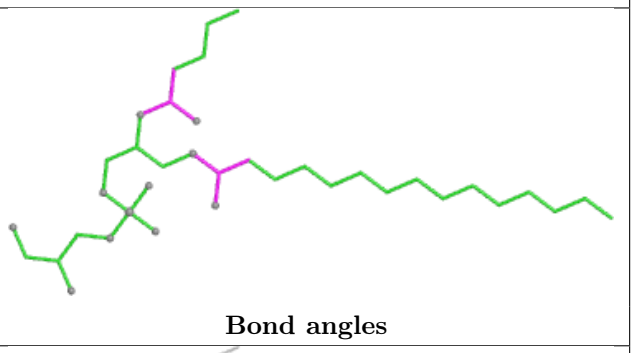


Rings

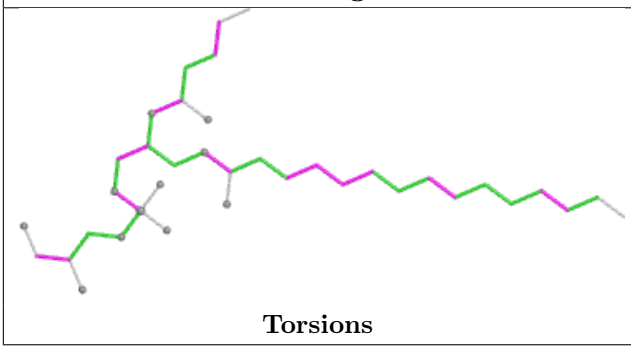
Ligand LHG I 318



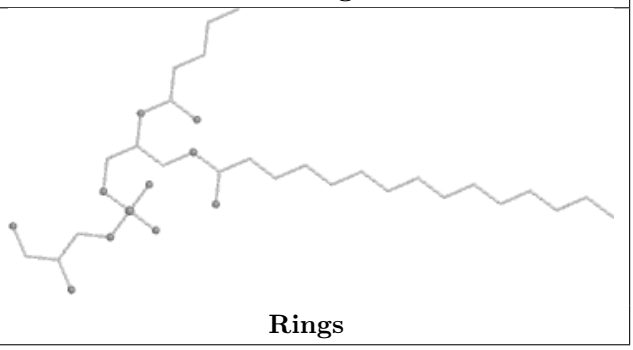
Bond lengths



Bond angles

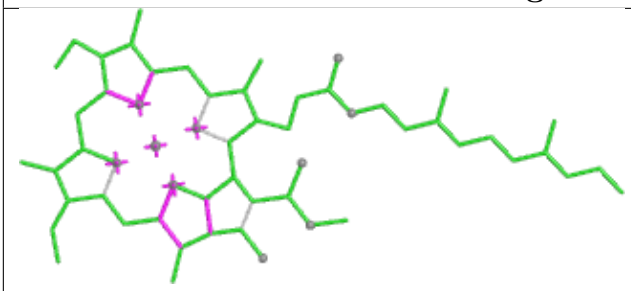


Torsions

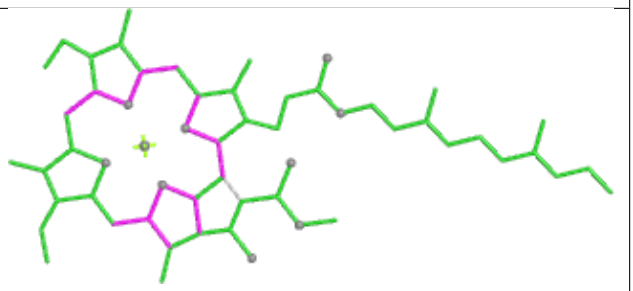


Rings

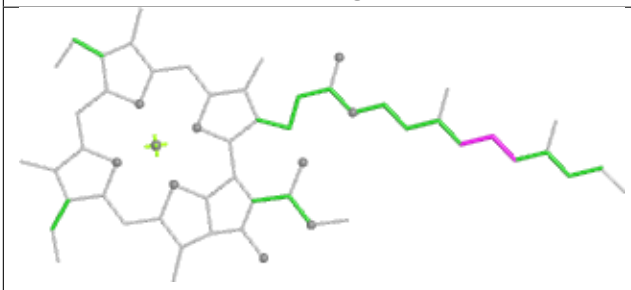
Ligand CLA L 307



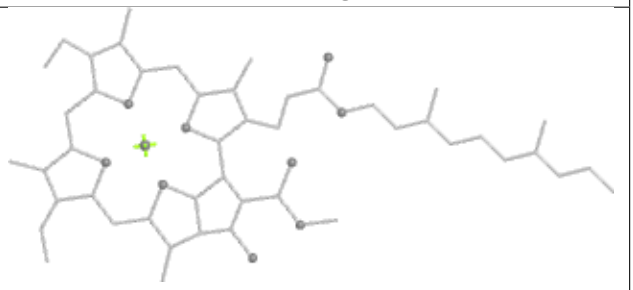
Bond lengths



Bond angles

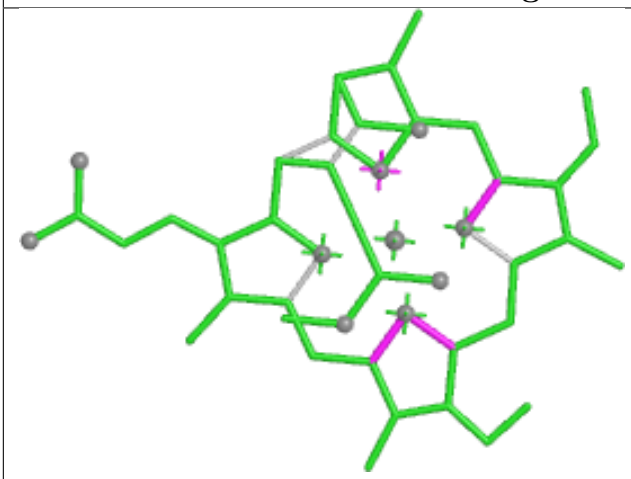


Torsions

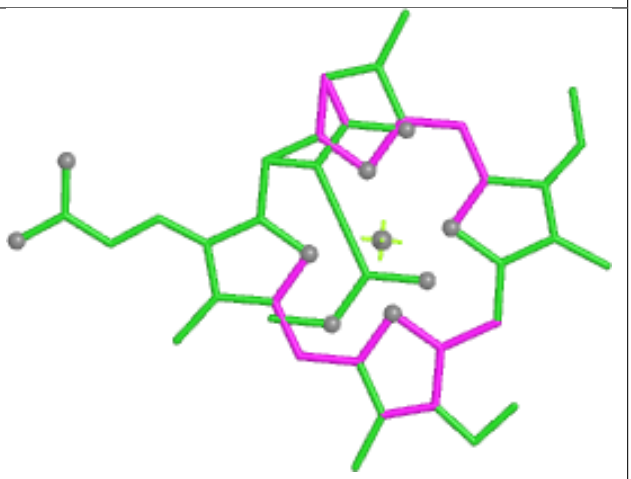


Rings

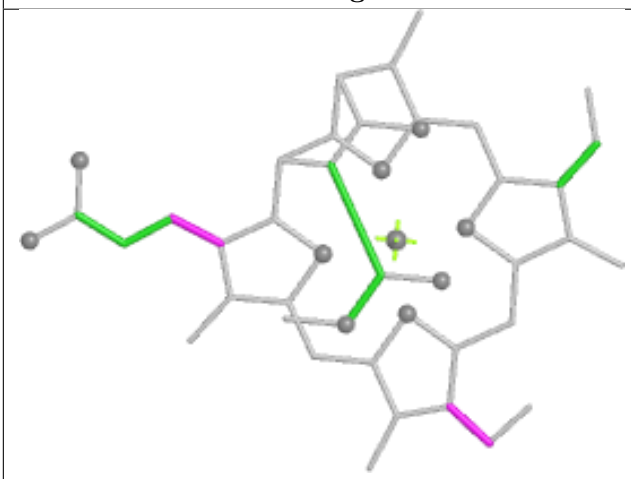
Ligand KC2 M 307



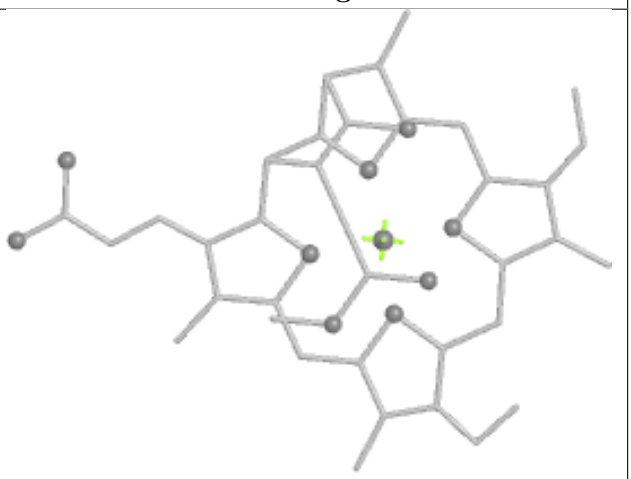
Bond lengths



Bond angles

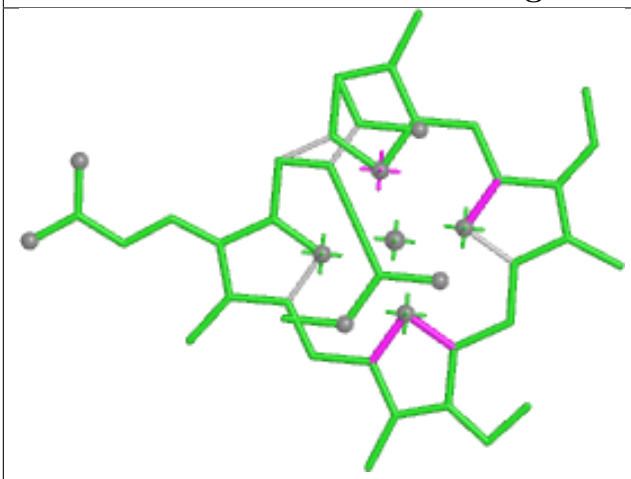


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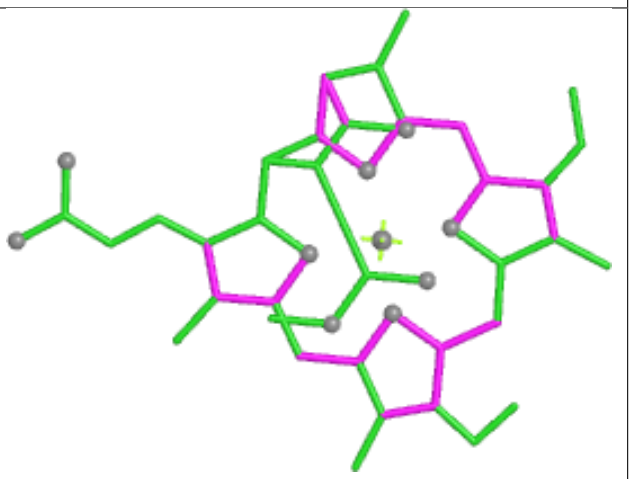


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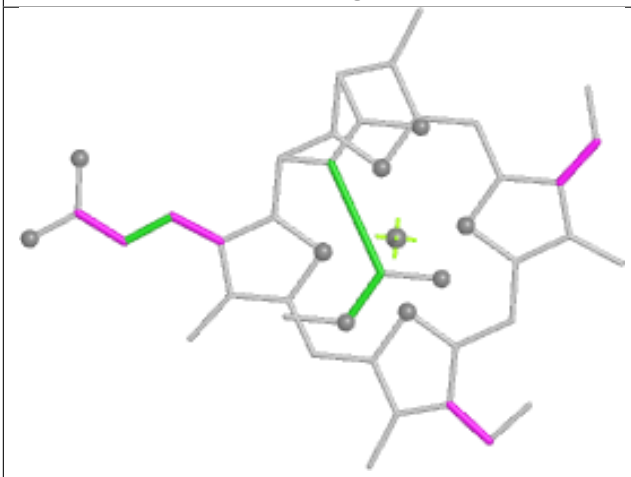
Ligand KC2 K 309



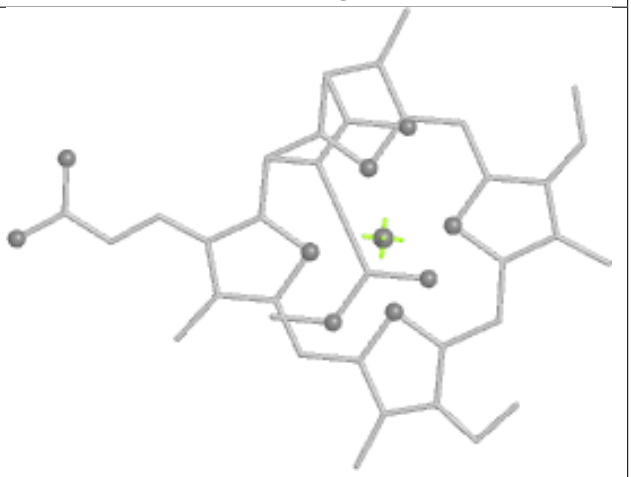
Bond lengths



Bond angles

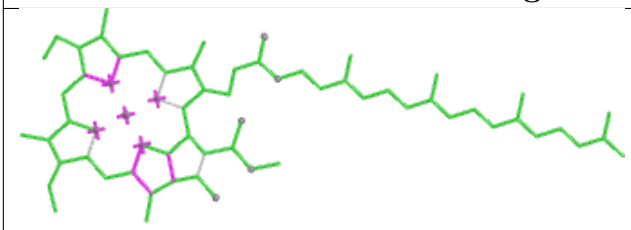


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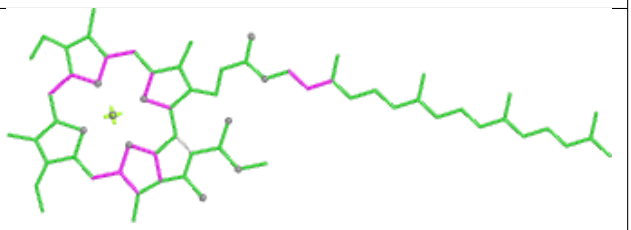


Rings

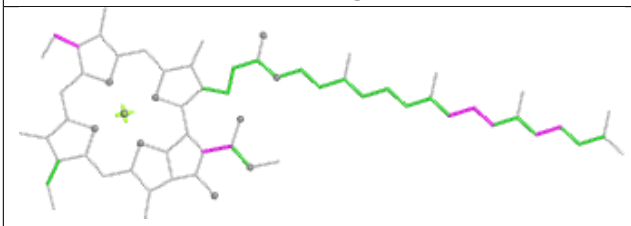
Ligand CLA D 311



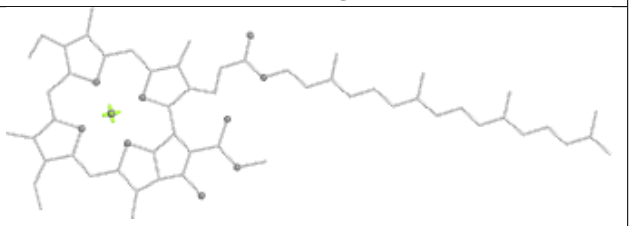
Bond lengths



Bond angles

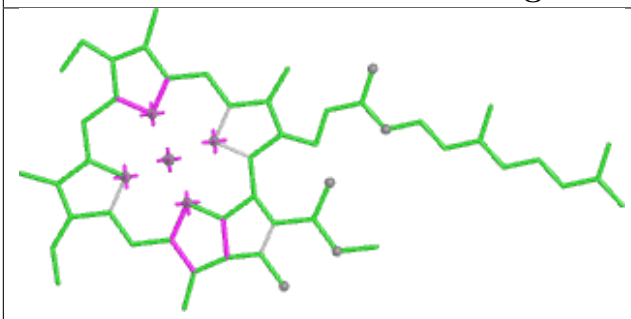


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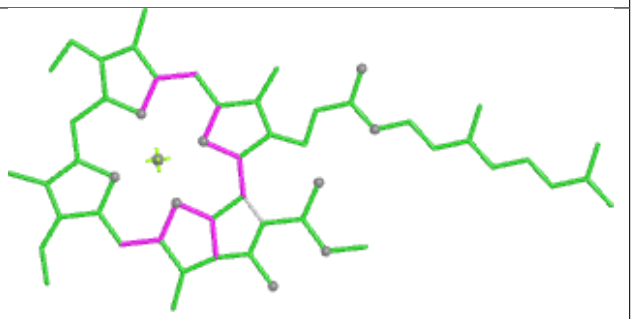


Rings

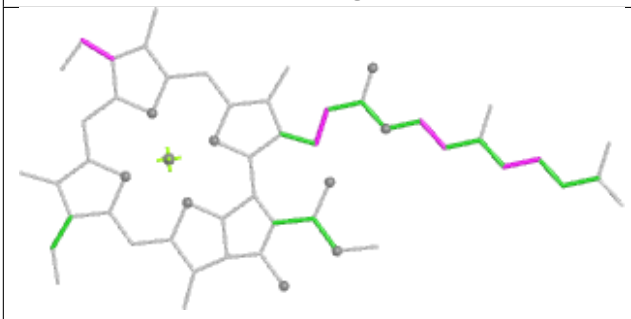
Ligand CLA B 309



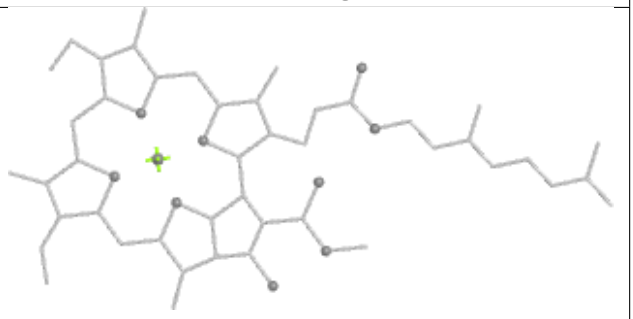
Bond lengths



Bond angles

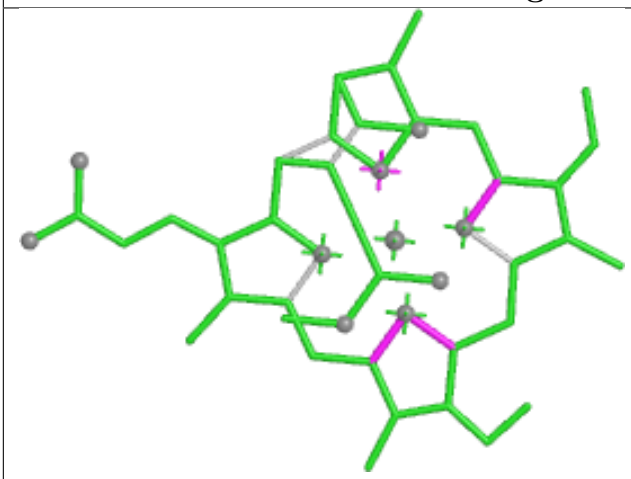


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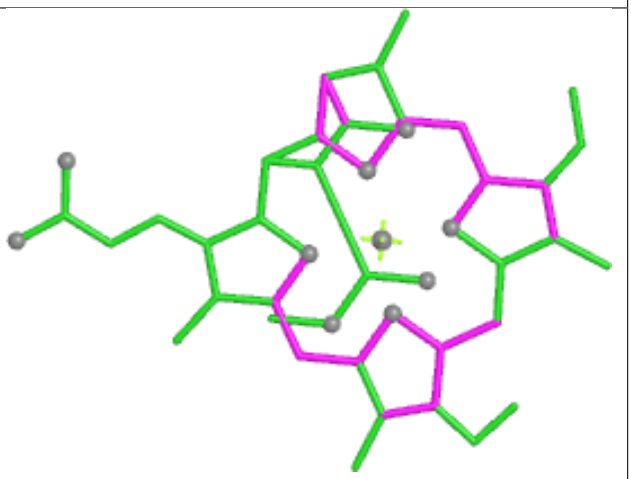


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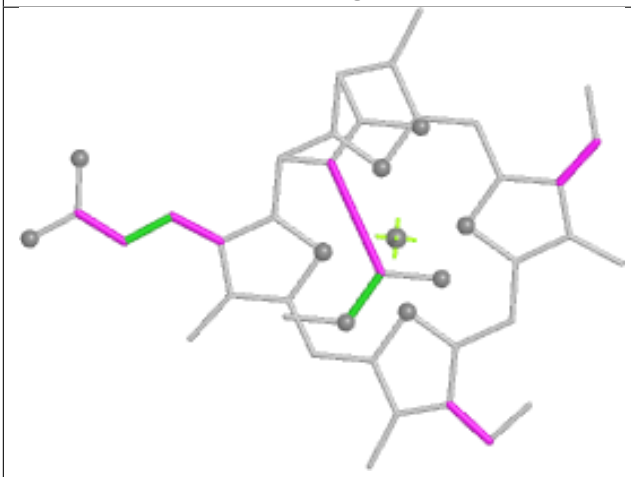
Ligand KC2 P 301



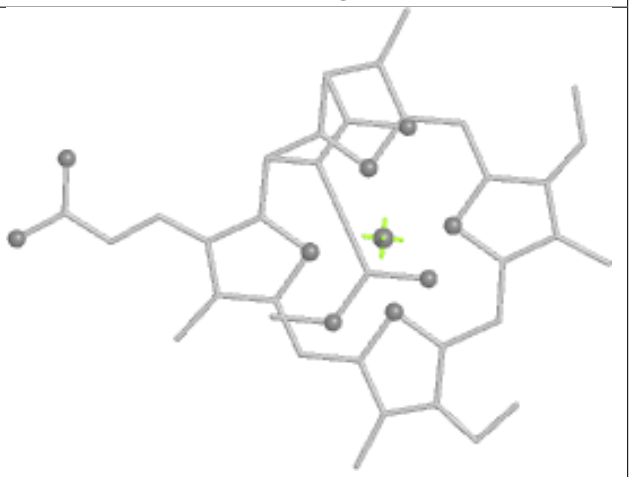
Bond lengths



Bond angles

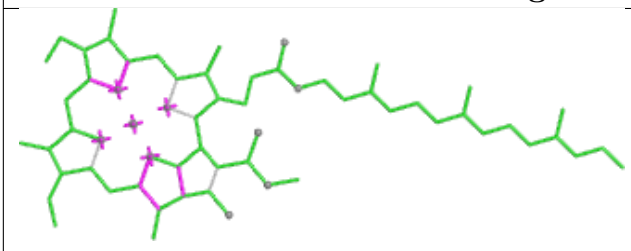


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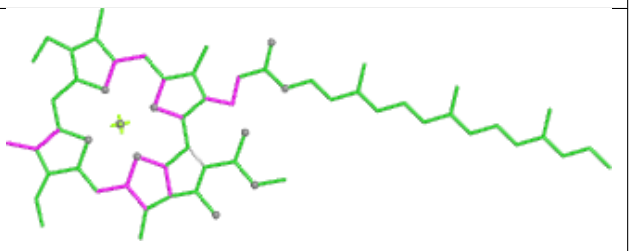


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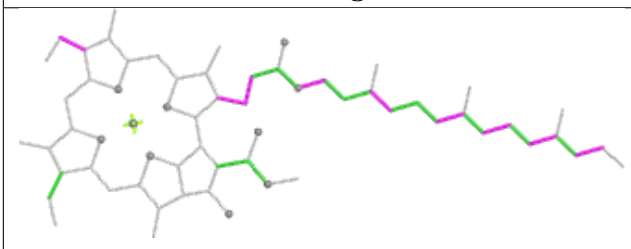
Ligand CLA a 810



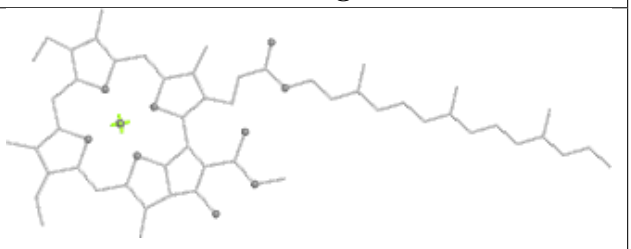
Bond lengths



Bond angles

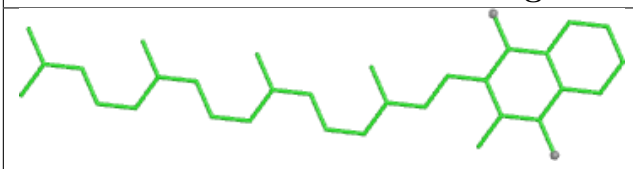


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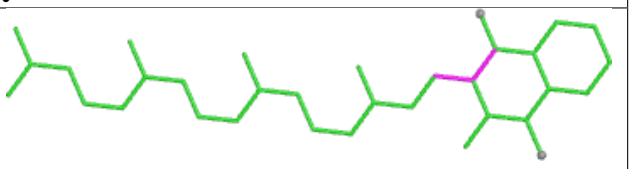


Rings

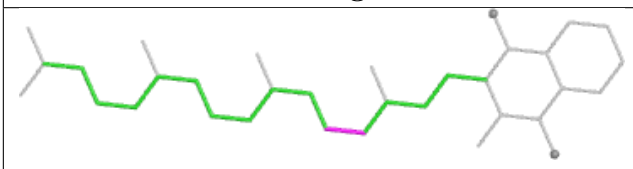
Ligand PQN b 847



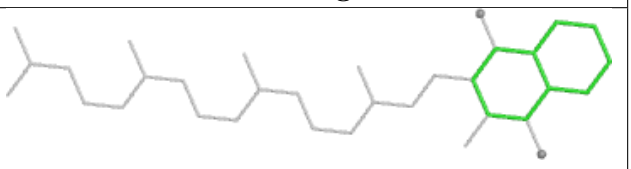
Bond lengths



Bond angles



Torsions

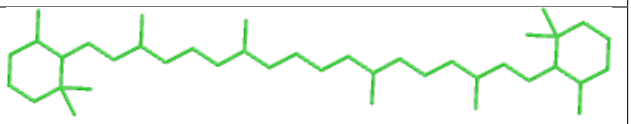


Rings

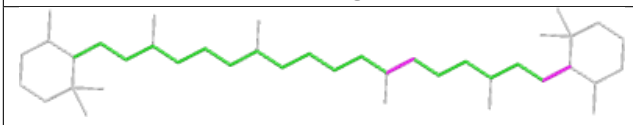
Ligand BCR k 204



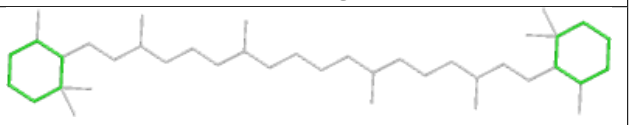
Bond lengths



Bond angles

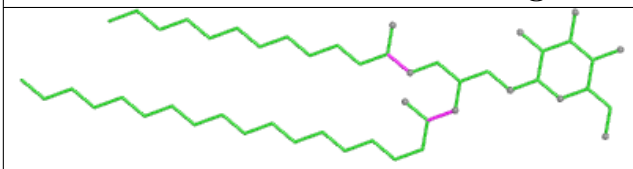


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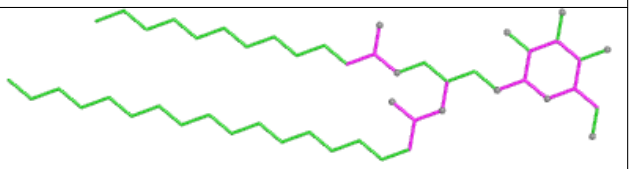


Rings

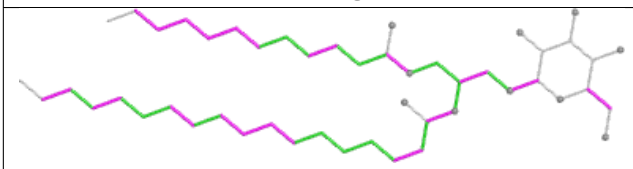
Ligand LMG l 201



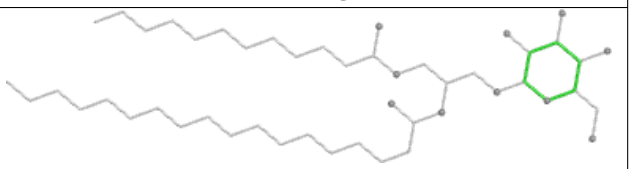
Bond lengths



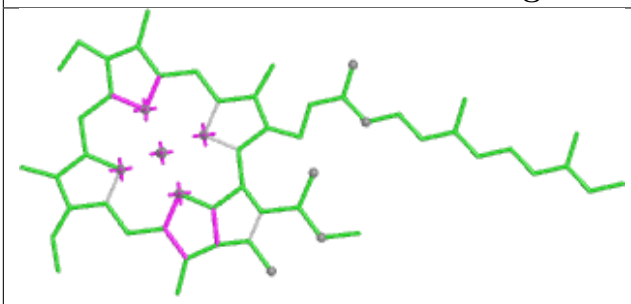
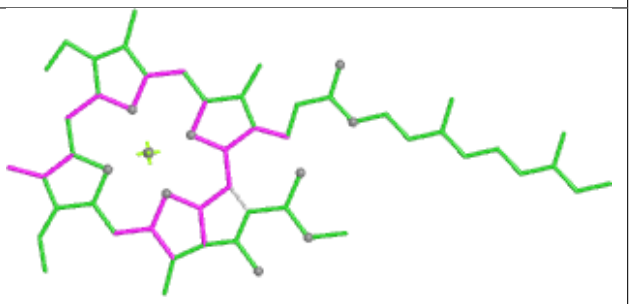
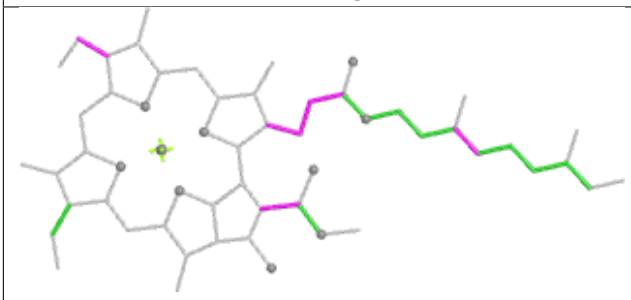
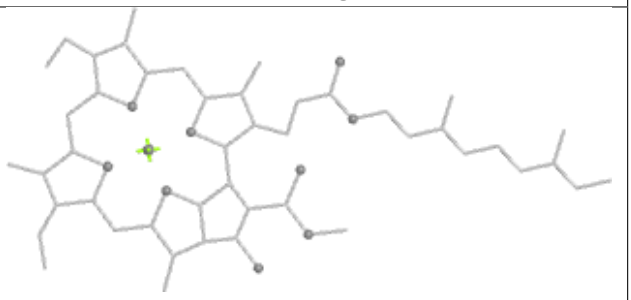
Bond angles

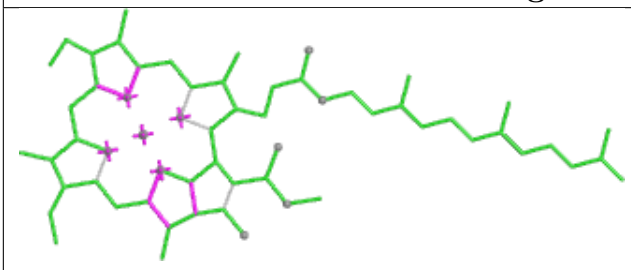
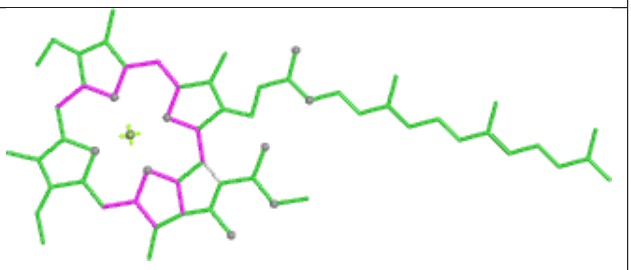
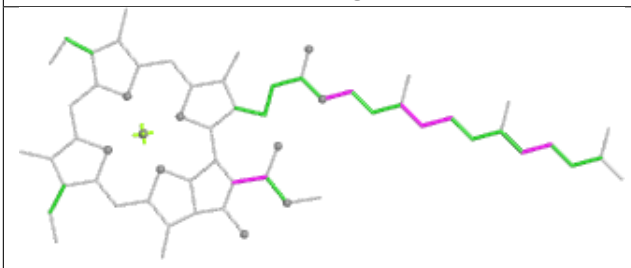
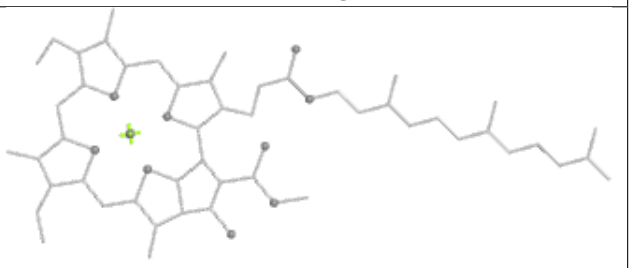


Torsions

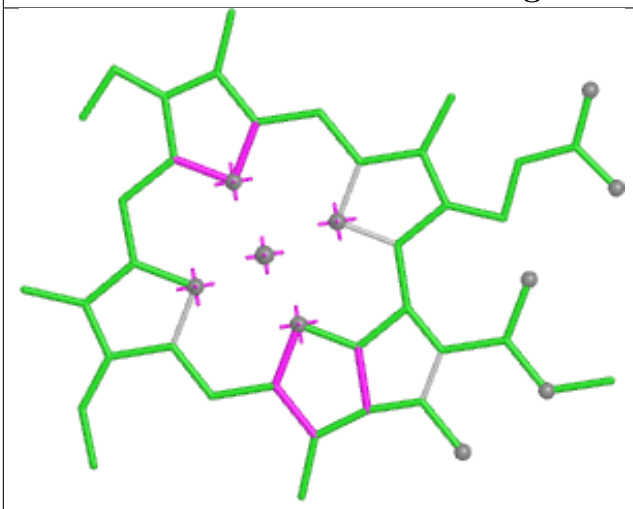


Rings

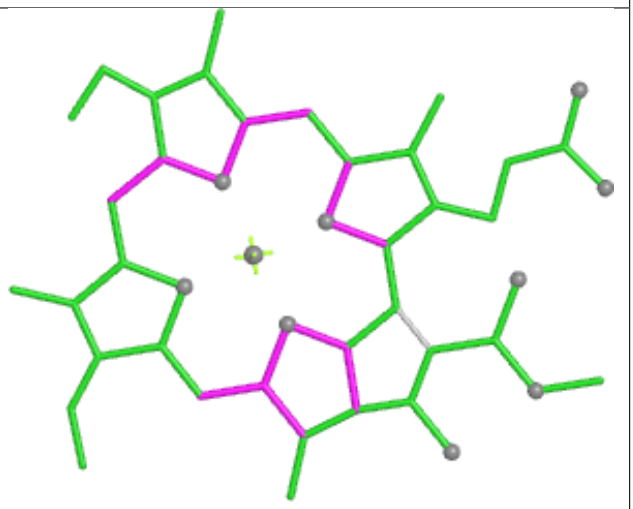
Ligand CLA G 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 835	
	
Bond lengths	Bond angles
	
Torsions	Rings

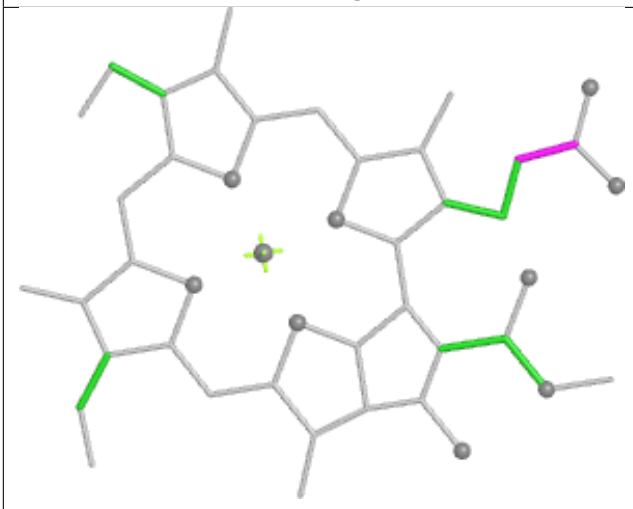
Ligand CLA D 309



Bond lengths



Bond angles

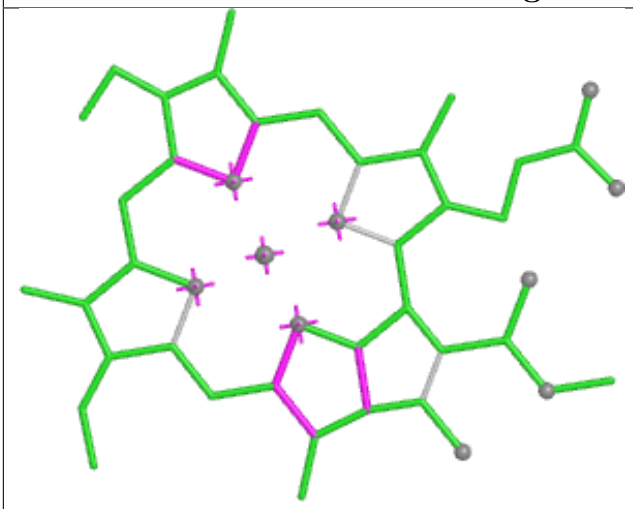


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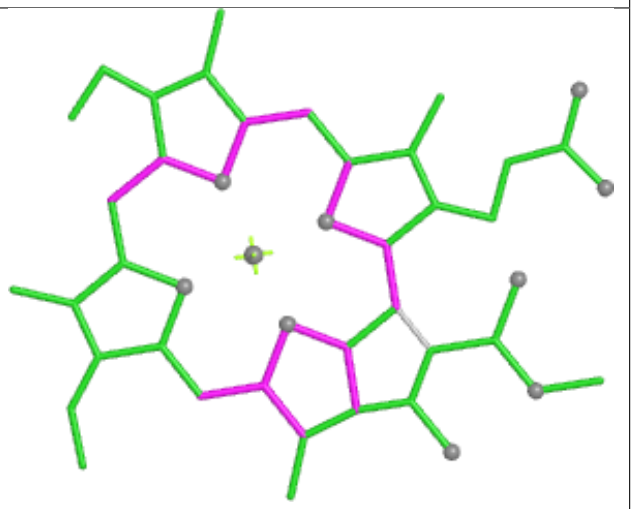


Rings

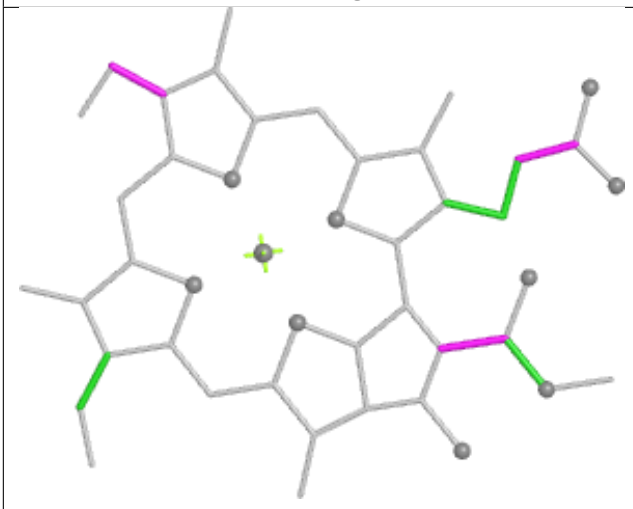
Ligand CLA H 309



Bond lengths



Bond angles

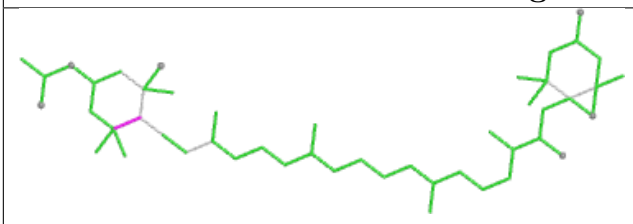


Torsions

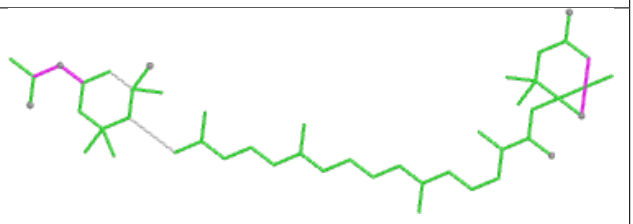


Rings

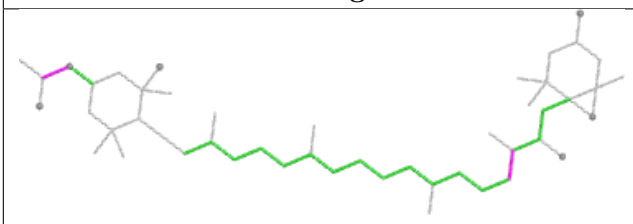
Ligand A86 D 322



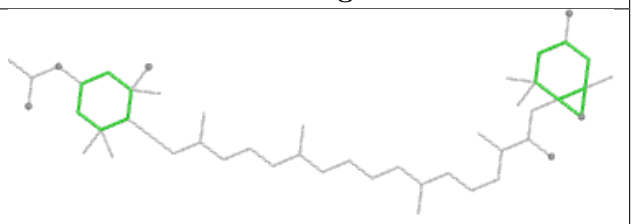
Bond lengths



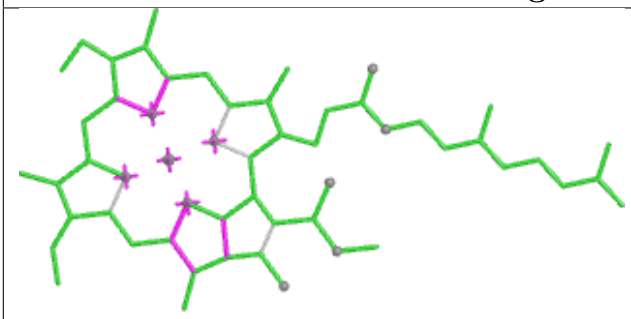
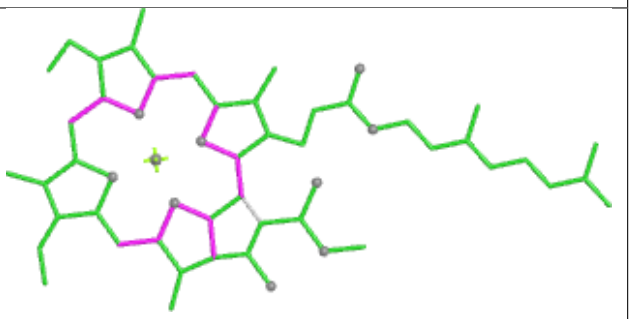
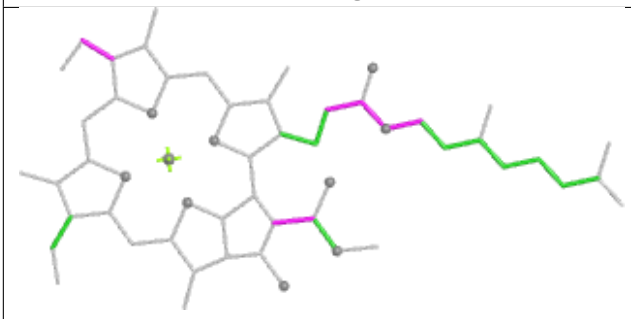
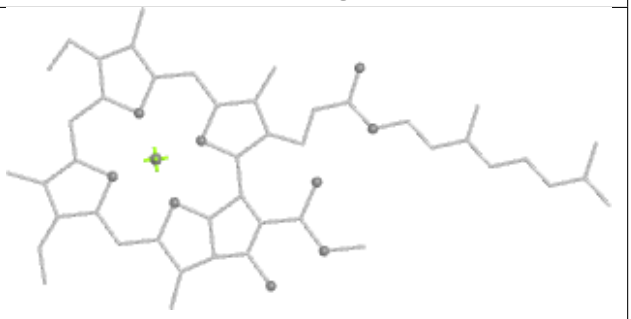
Bond angles

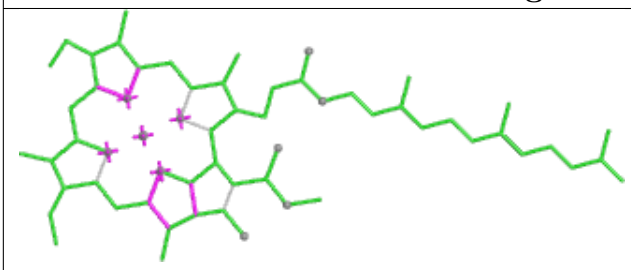
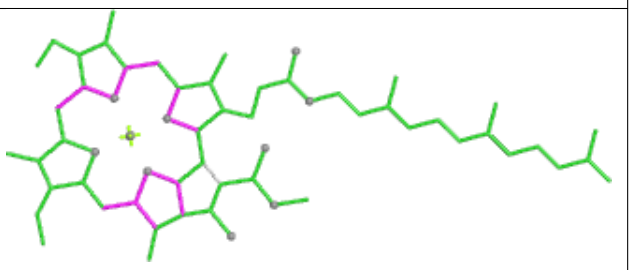
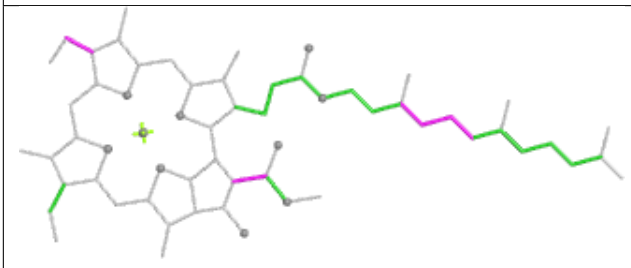
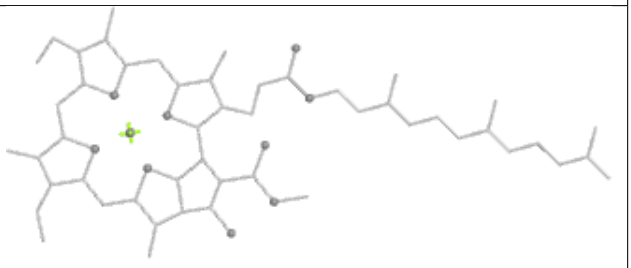


Torsions

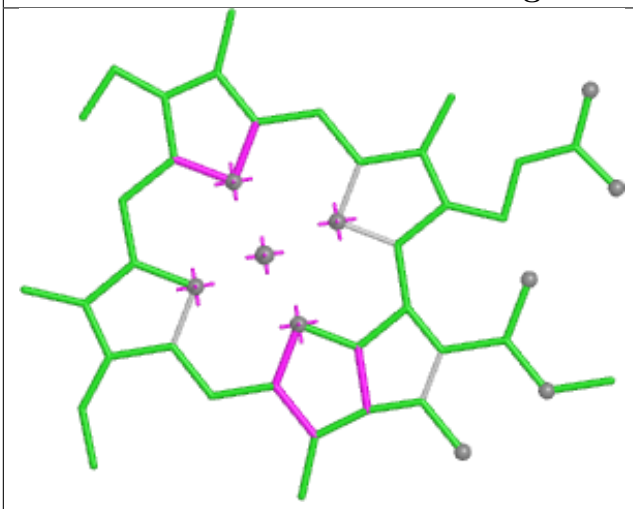


Rings

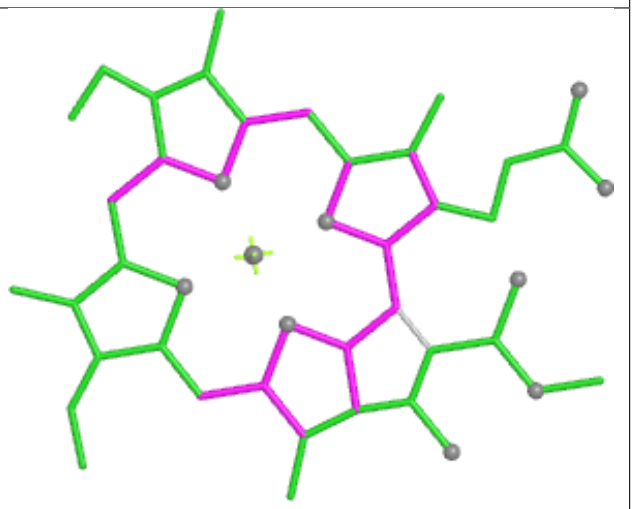
Ligand CLA a 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA E 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

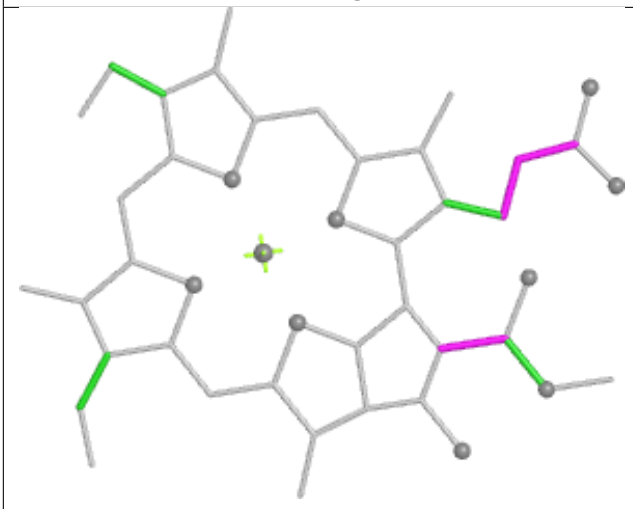
Ligand CLA U 305



Bond lengths



Bond angles

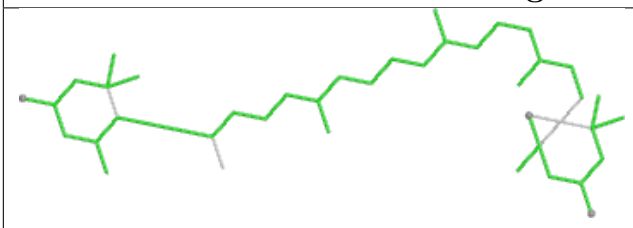


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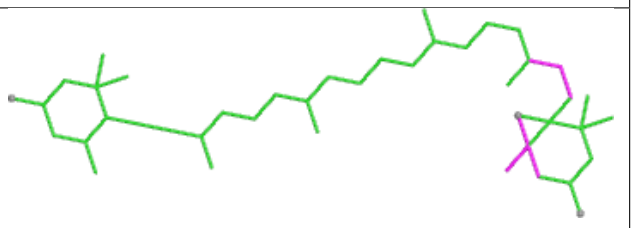


Rings

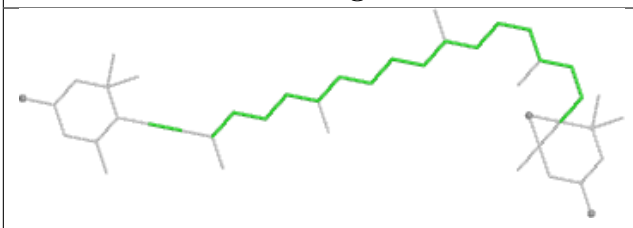
Ligand DD6 E 317



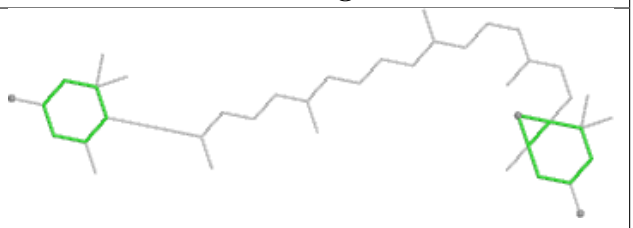
Bond lengths



Bond angles

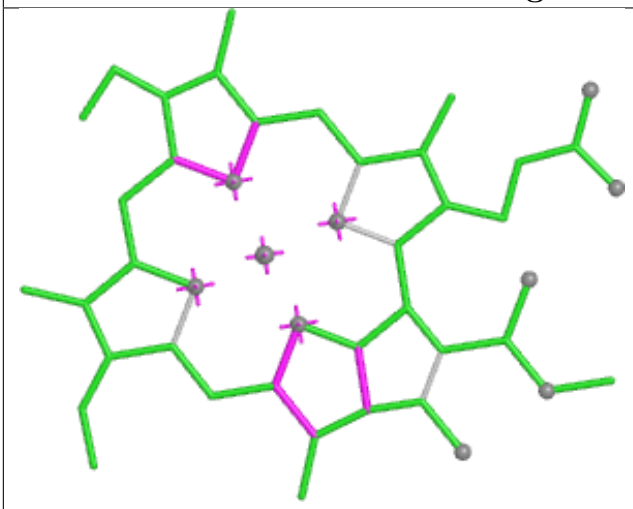


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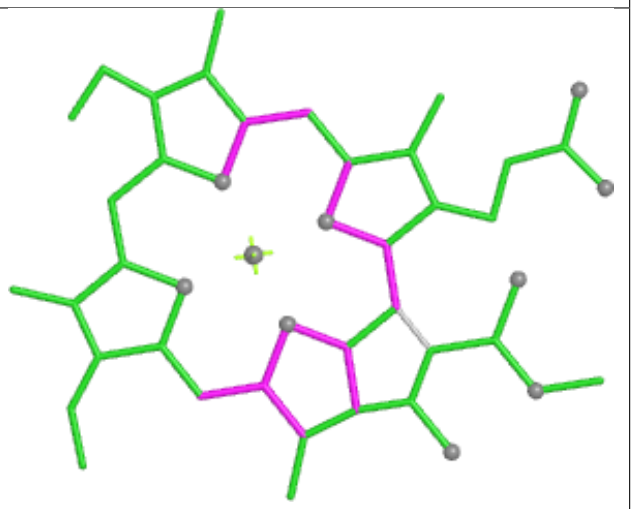


Rings

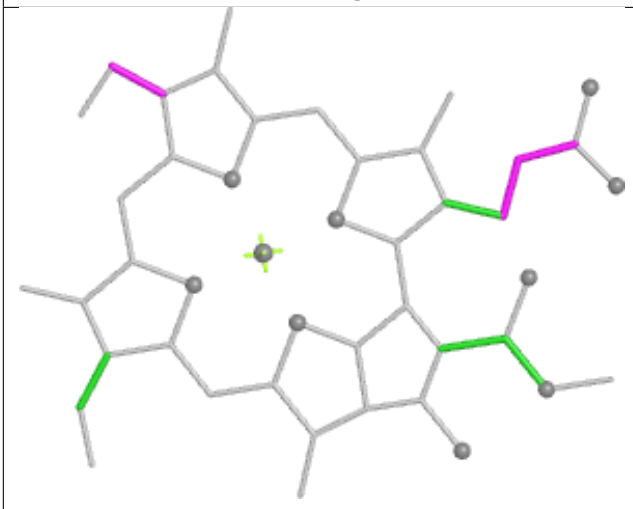
Ligand CLA L 309



Bond lengths



Bond angles

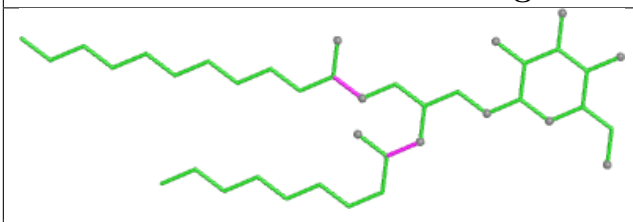


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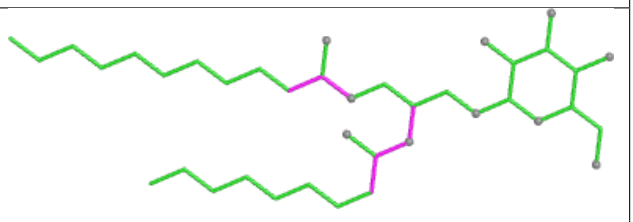


Rings

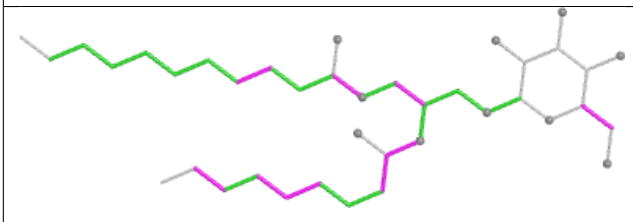
Ligand LMG W 320



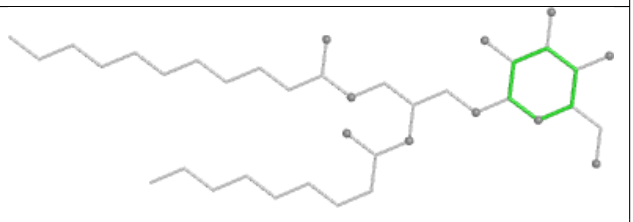
Bond lengths



Bond angles

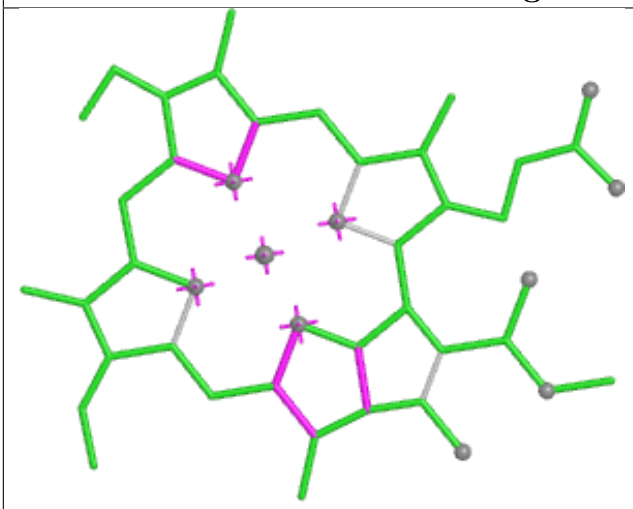


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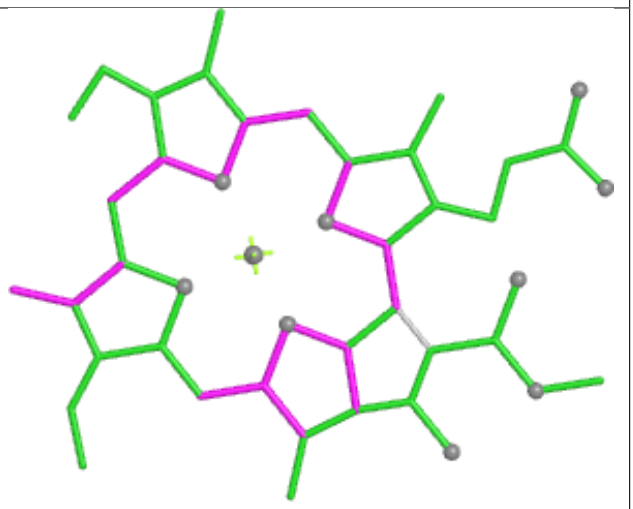


Rings

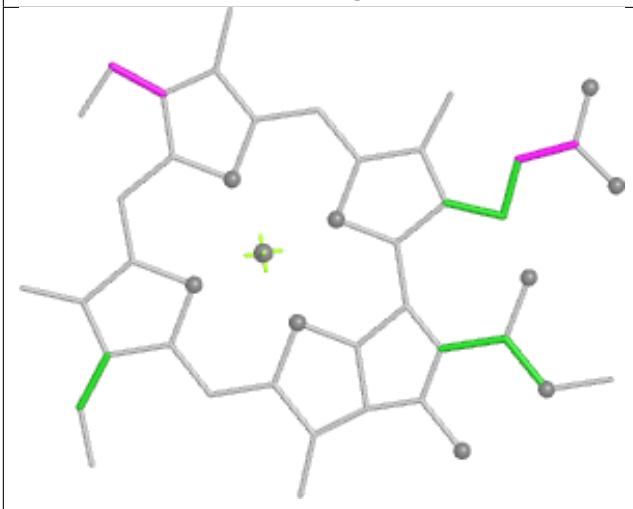
Ligand CLA U 302



Bond lengths



Bond angles

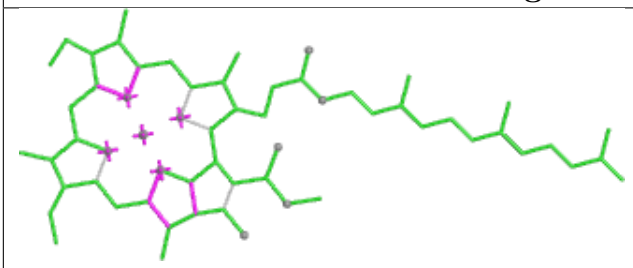


Torsions

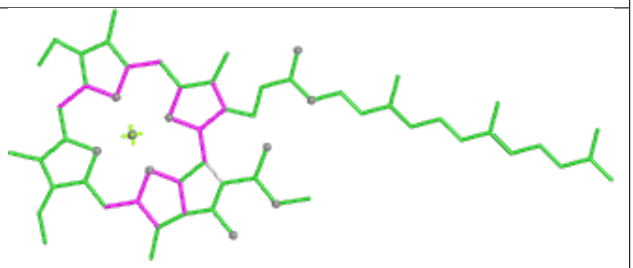


Rings

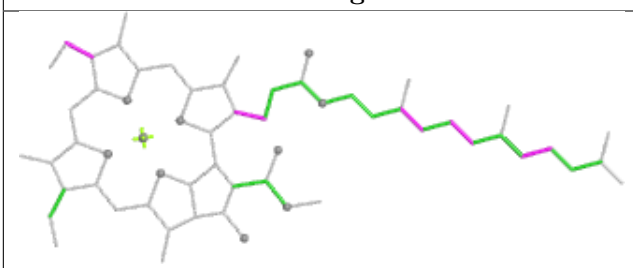
Ligand CLA C 305



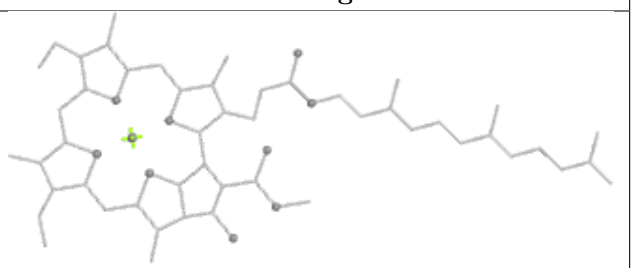
Bond lengths



Bond angles

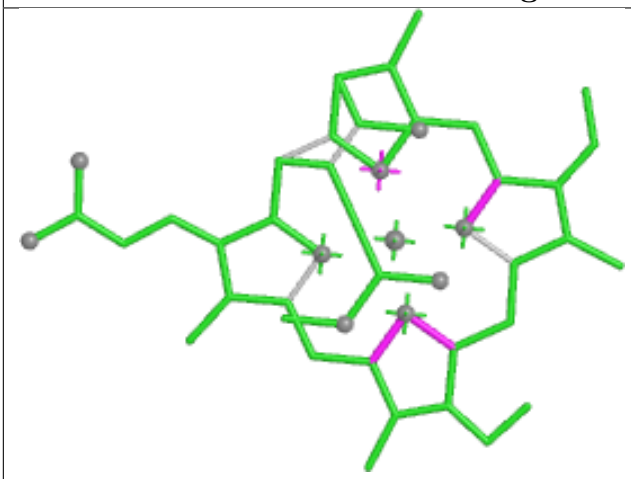


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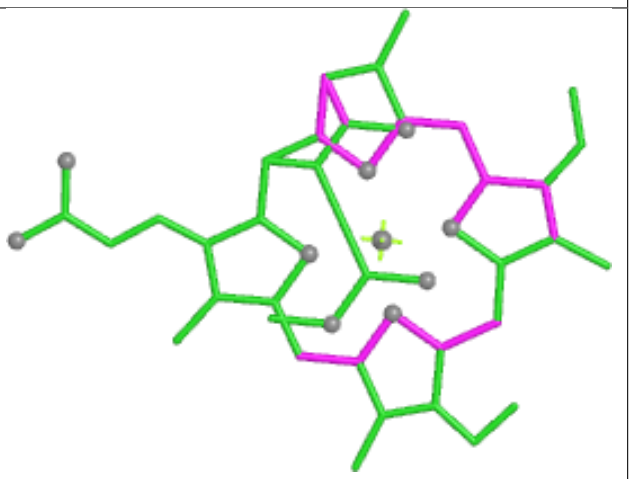


Rings

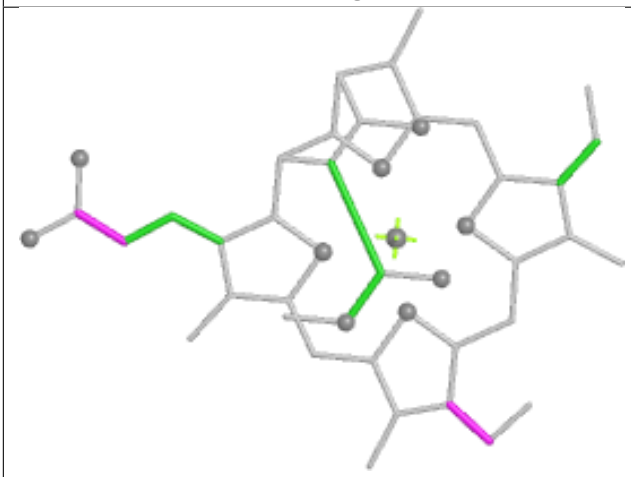
Ligand KC2 W 305



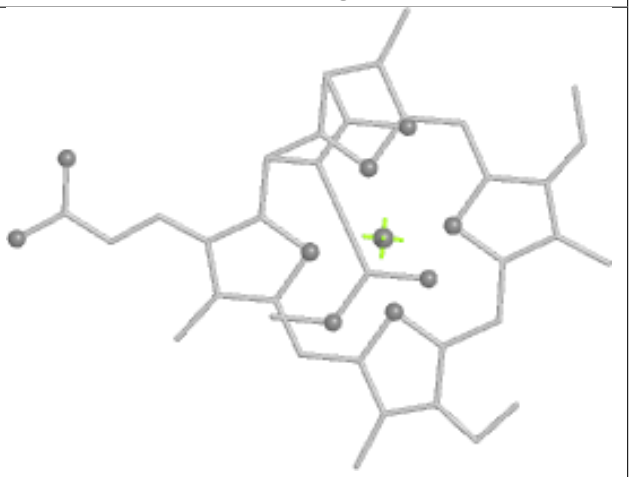
Bond lengths



Bond angles

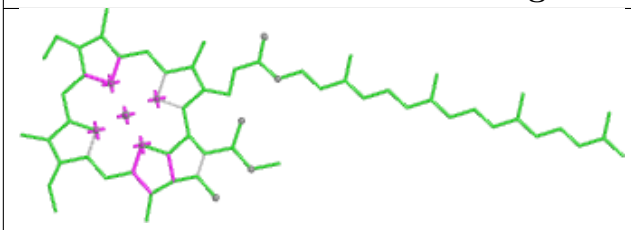


Torsions

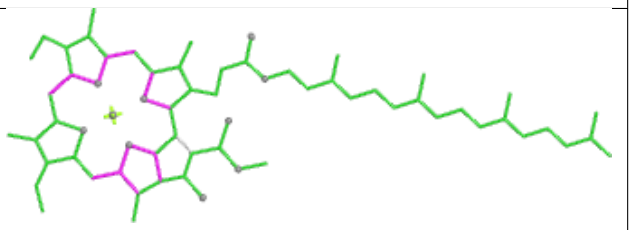


Rings

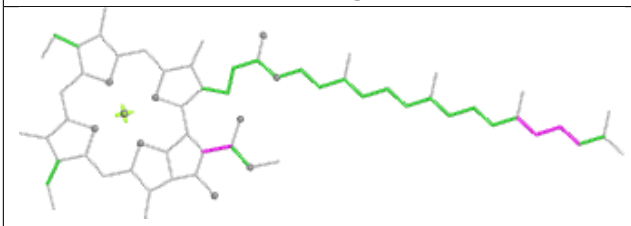
Ligand CLA a 833



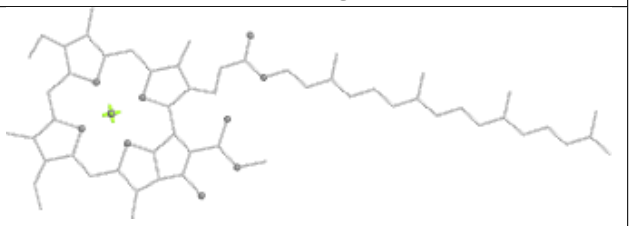
Bond lengths



Bond angles

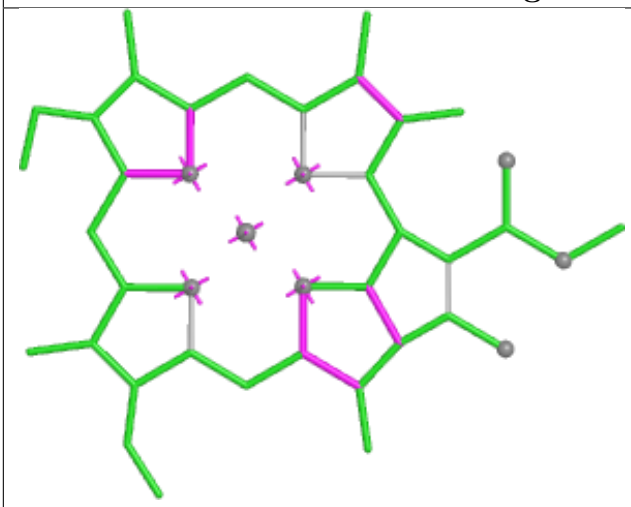


Torsions

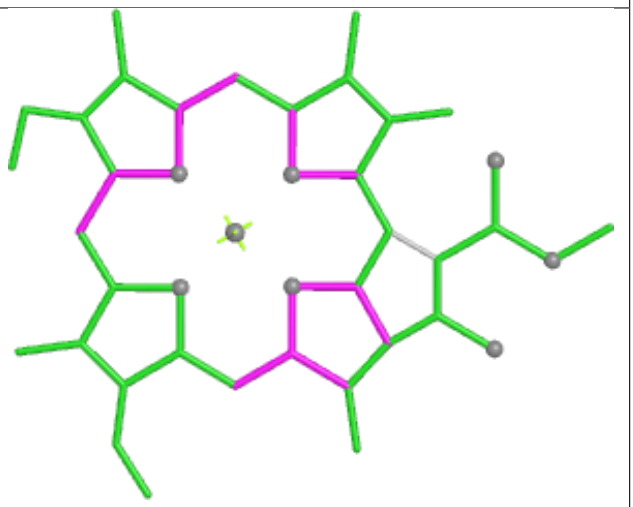


Rings

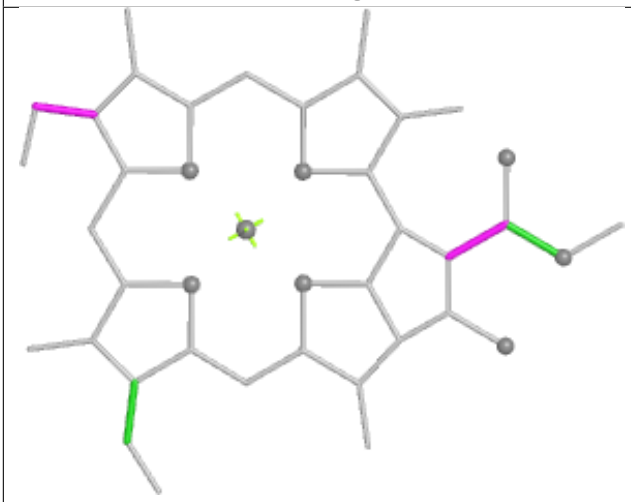
Ligand CLA R 309



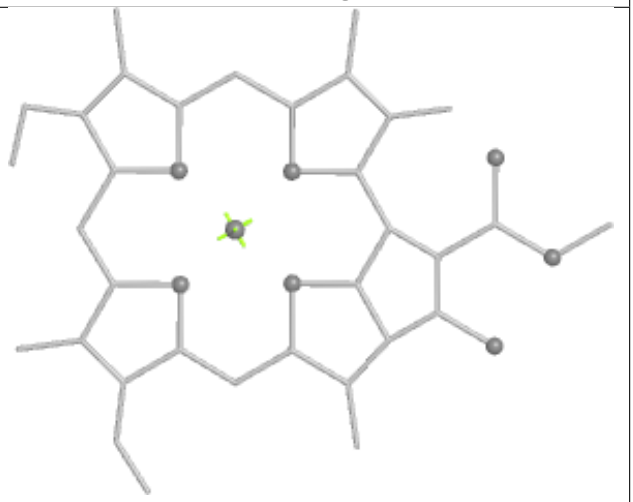
Bond lengths



Bond angles

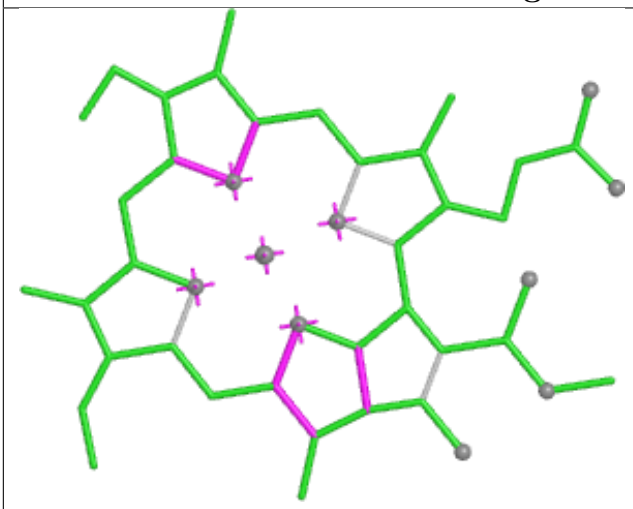


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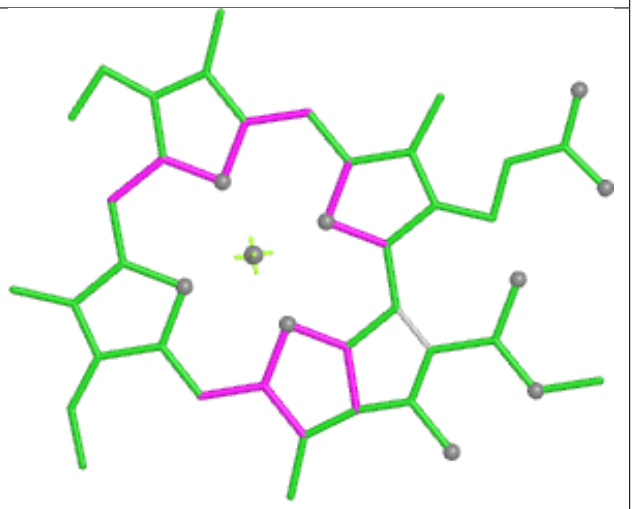


Rings

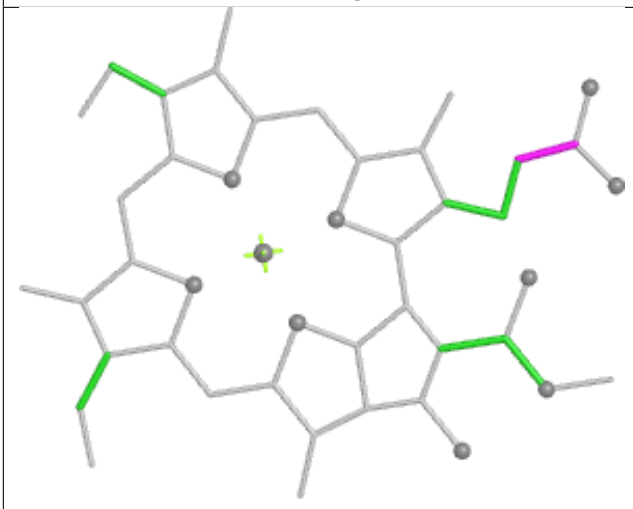
Ligand CLA R 307



Bond lengths



Bond angles

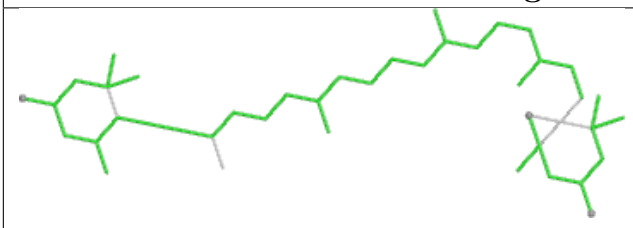


Torsions

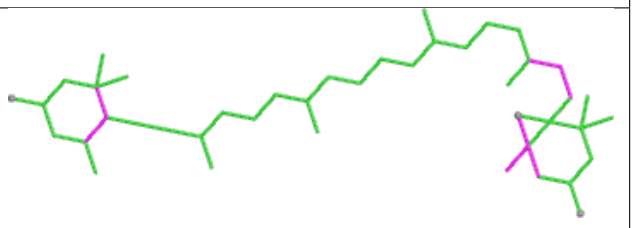


Rings

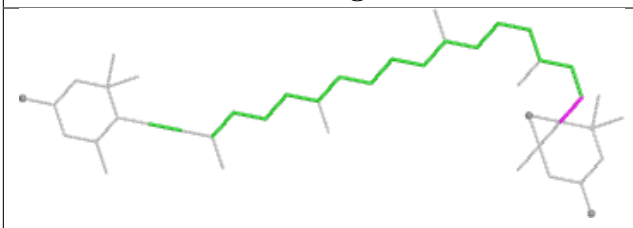
Ligand DD6 G 312



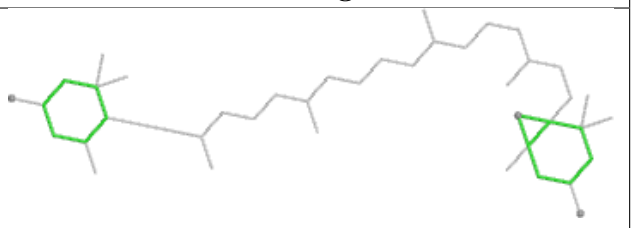
Bond lengths



Bond angles

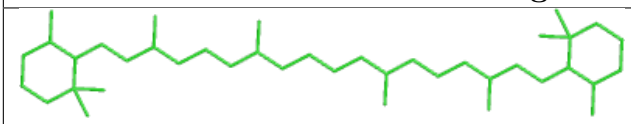


Torsions

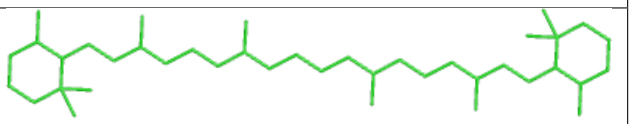


Rings

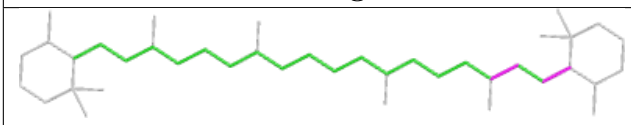
Ligand BCR l 205



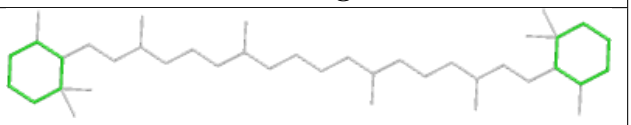
Bond lengths



Bond angles

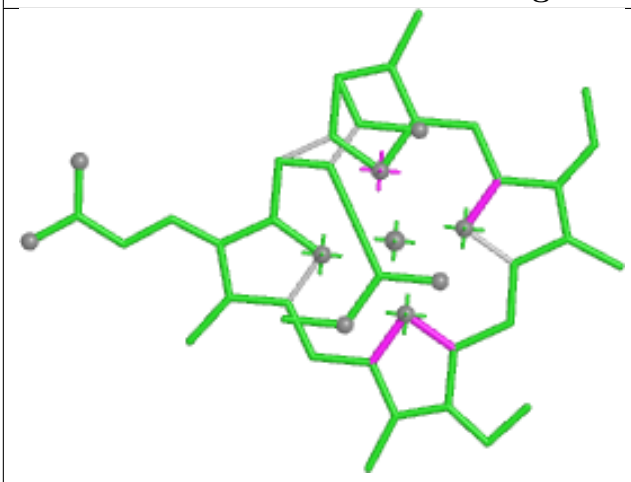


Torsions

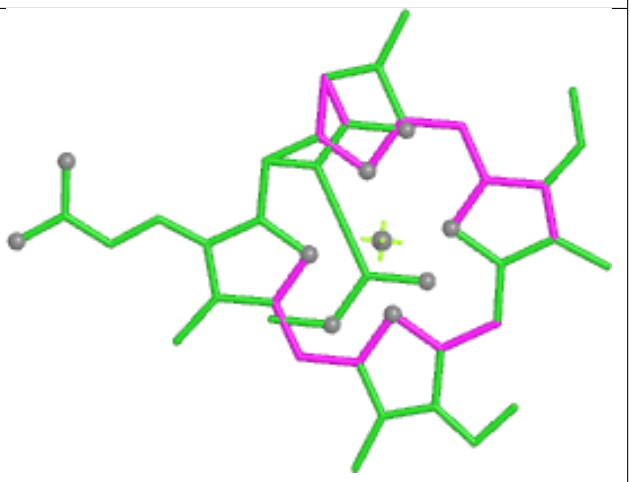


Rings

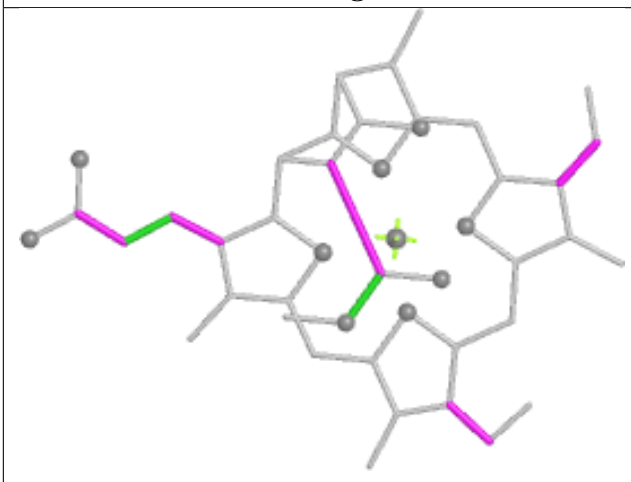
Ligand KC2 I 309



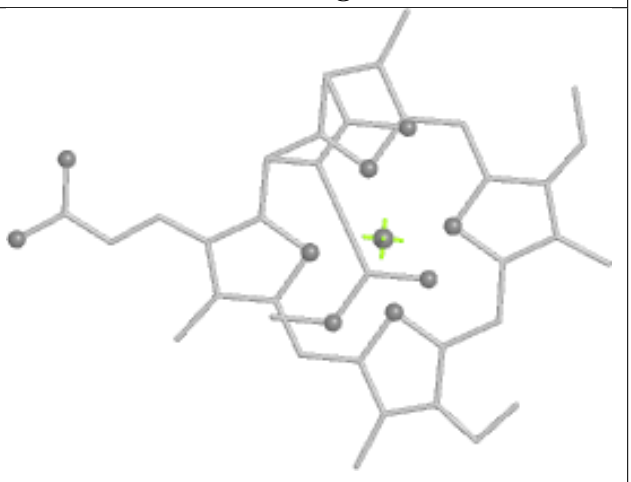
Bond lengths



Bond angles

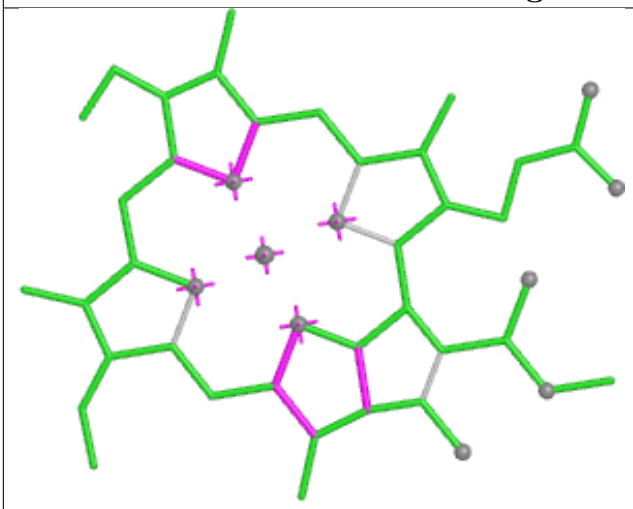


Torsions

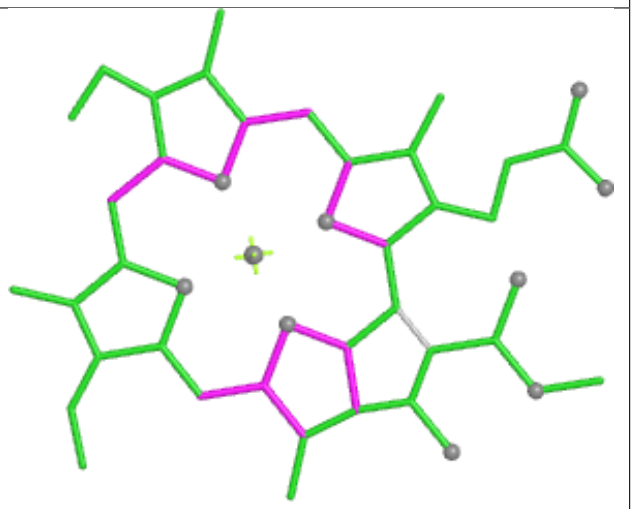


Rings

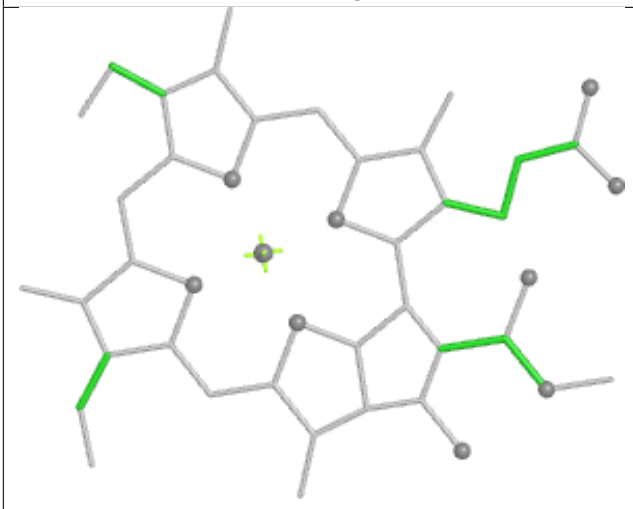
Ligand CLA F 311



Bond lengths



Bond angles

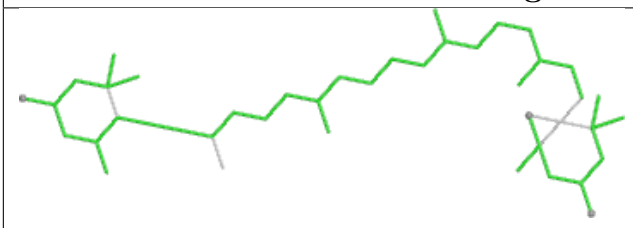


Torsions

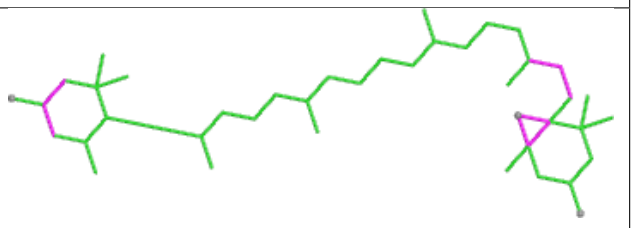


Rings

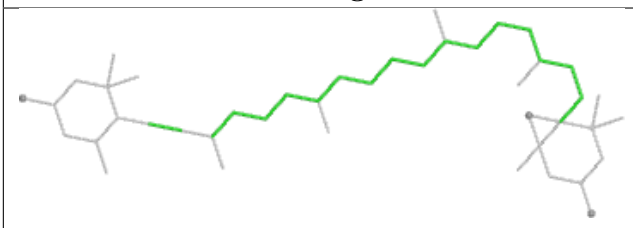
Ligand DD6 D 317



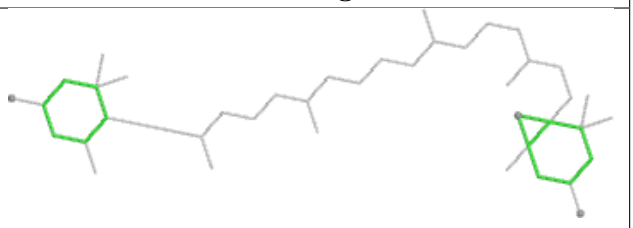
Bond lengths



Bond angles

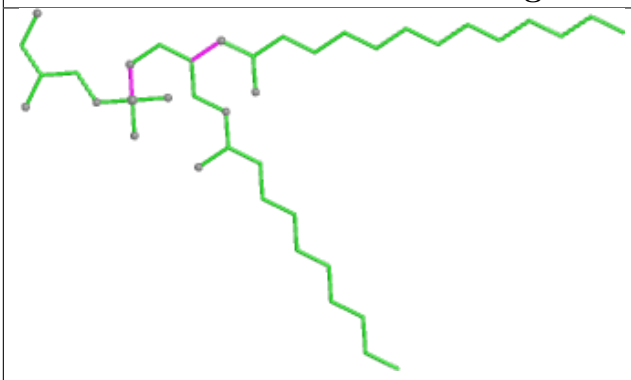


Torsions



Rings

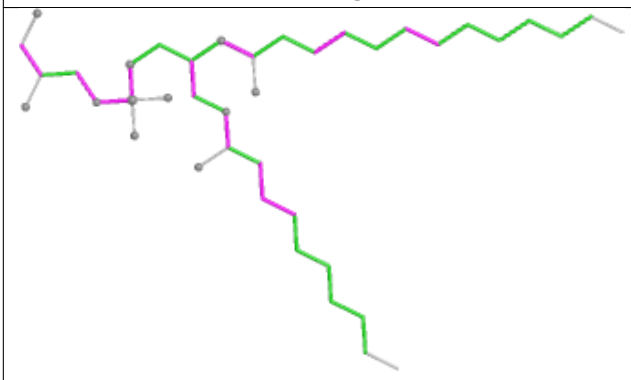
Ligand LHG F 321



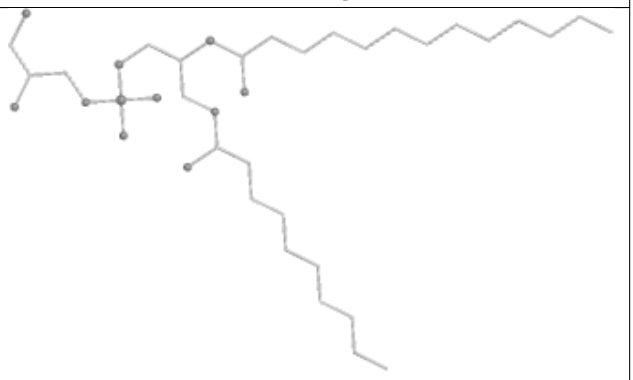
Bond lengths



Bond angles

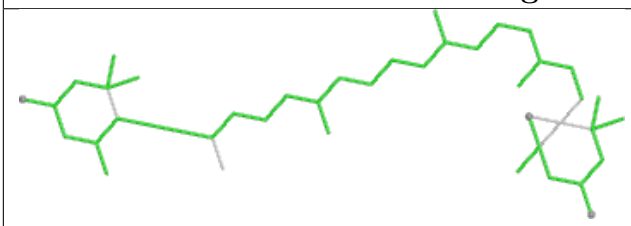


Torsions

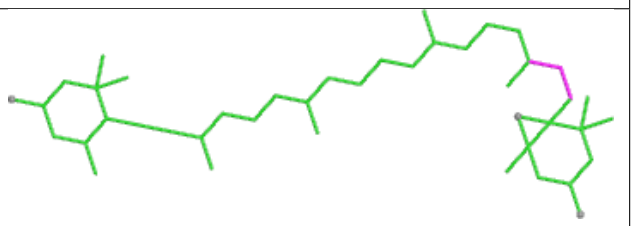


Rings

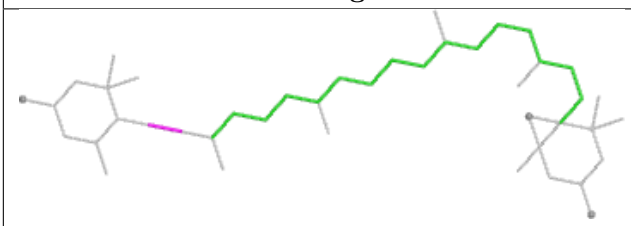
Ligand DD6 M 316



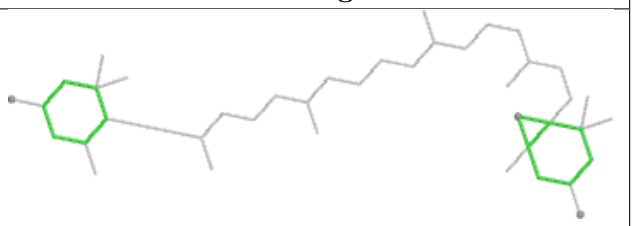
Bond lengths



Bond angles

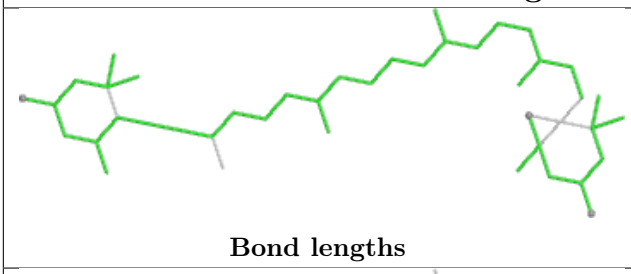


Torsions

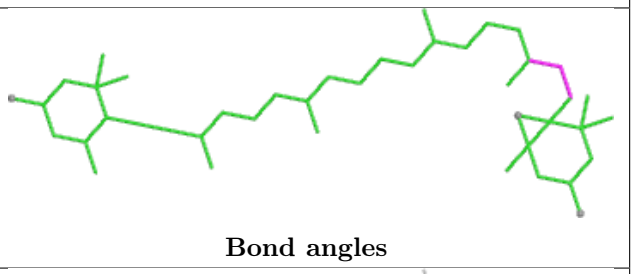


Rings

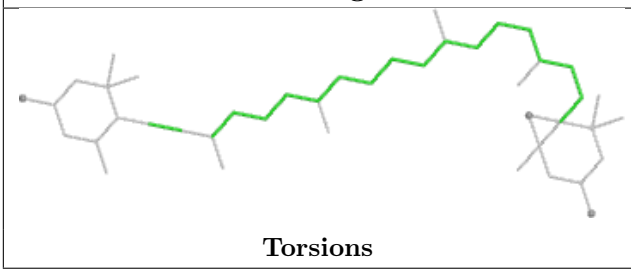
Ligand DD6 R 314



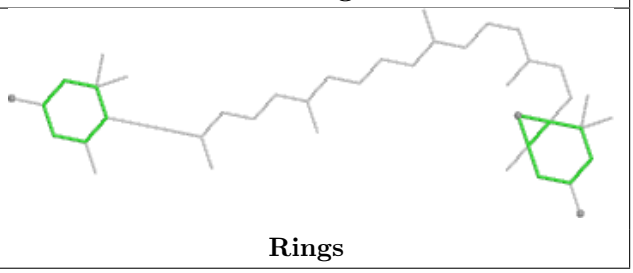
Bond lengths



Bond angles

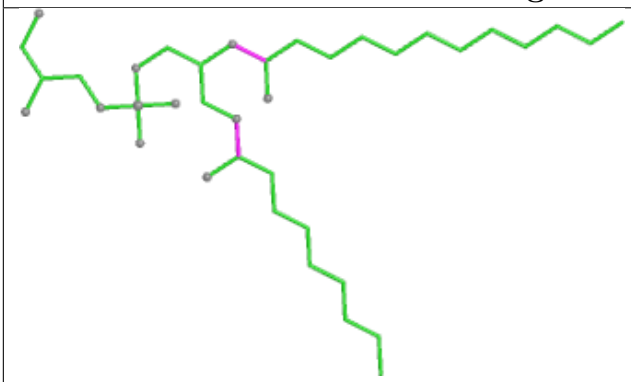


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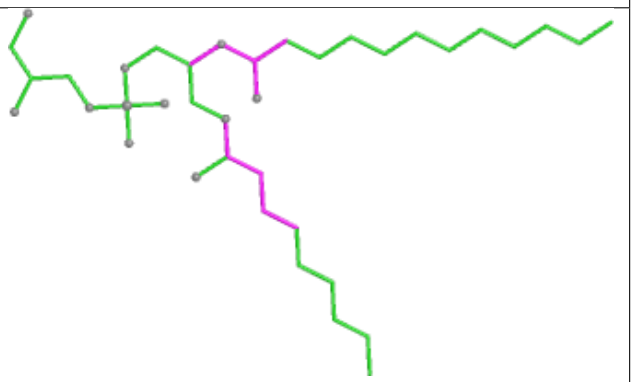


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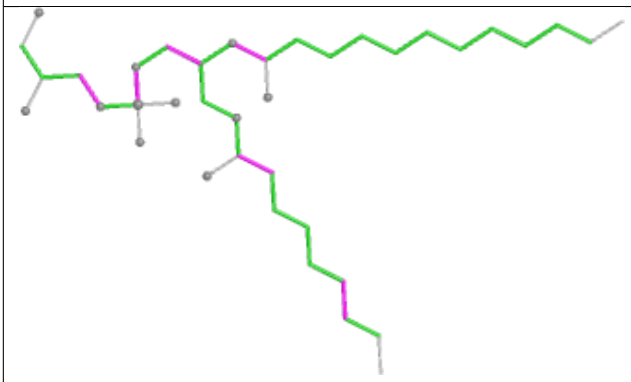
Ligand LHG a 851



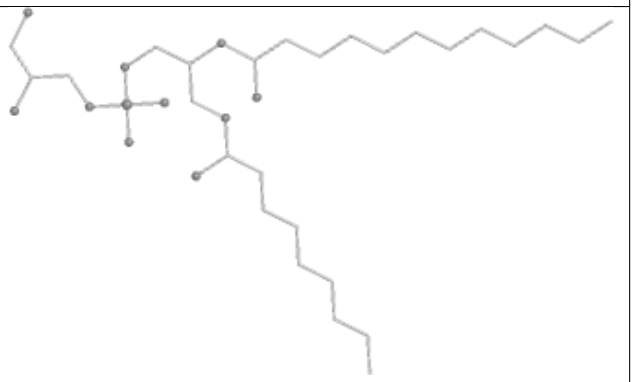
Bond lengths



Bond angles

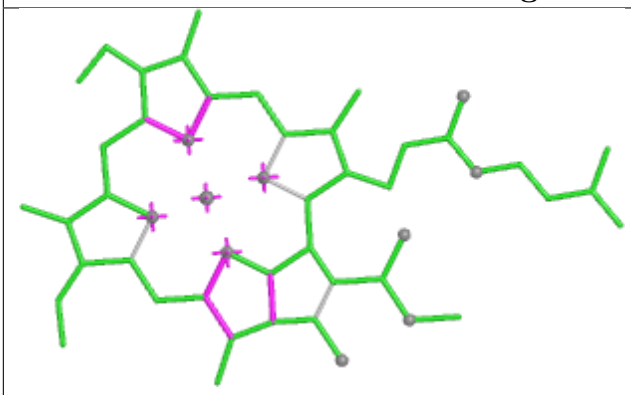


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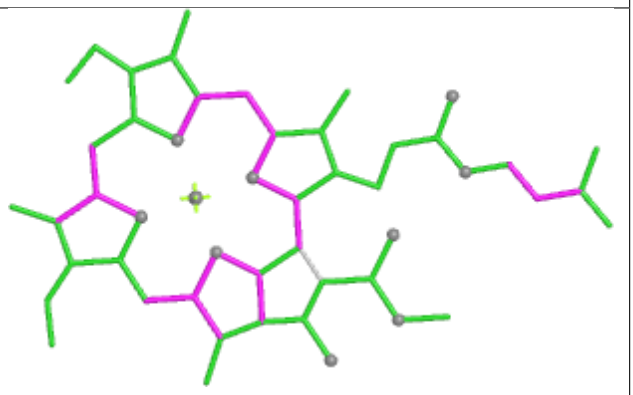


Rings

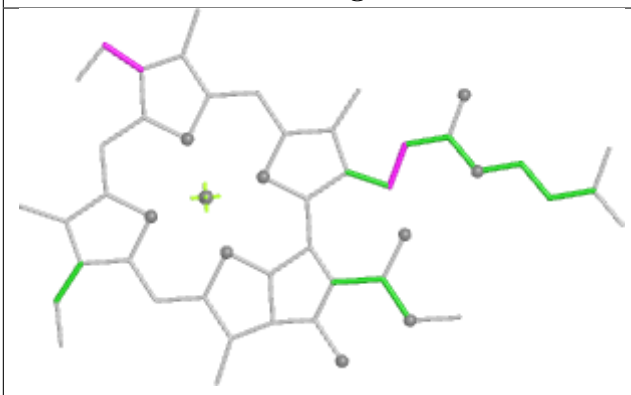
Ligand CLA M 305



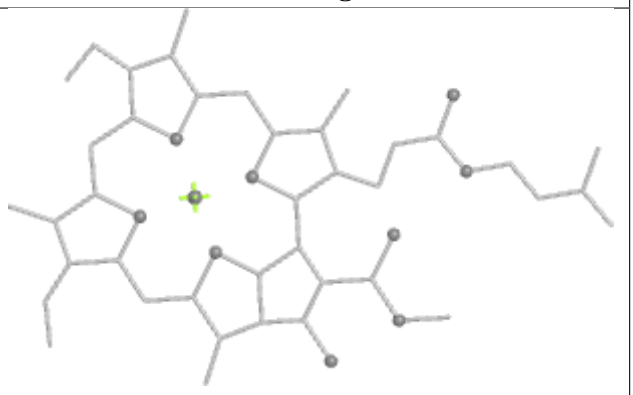
Bond lengths



Bond angles

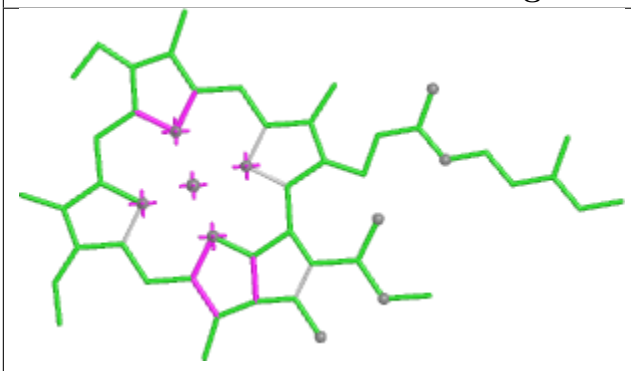


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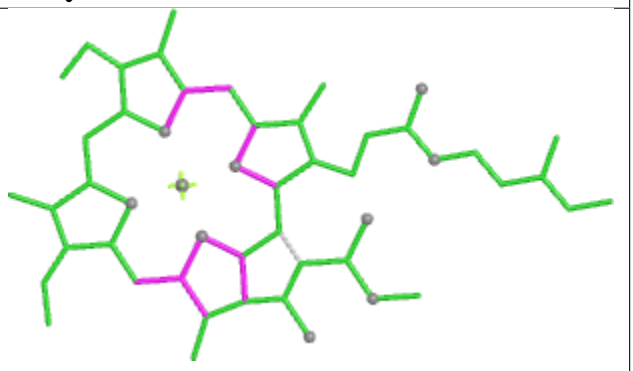


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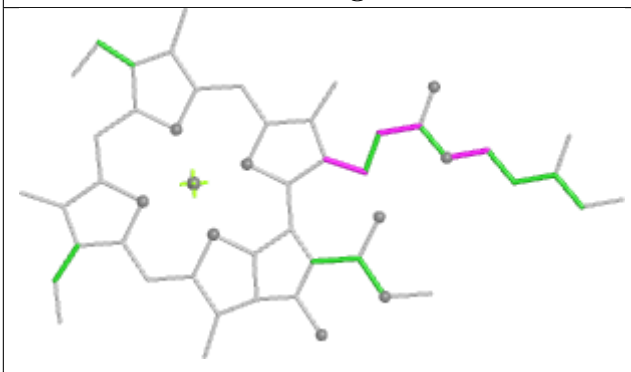
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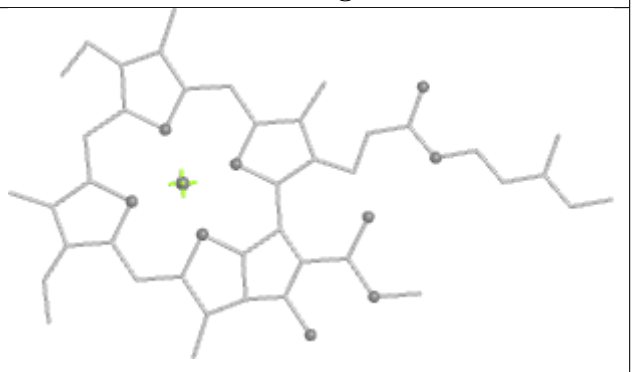
Bond lengths



Bond angles

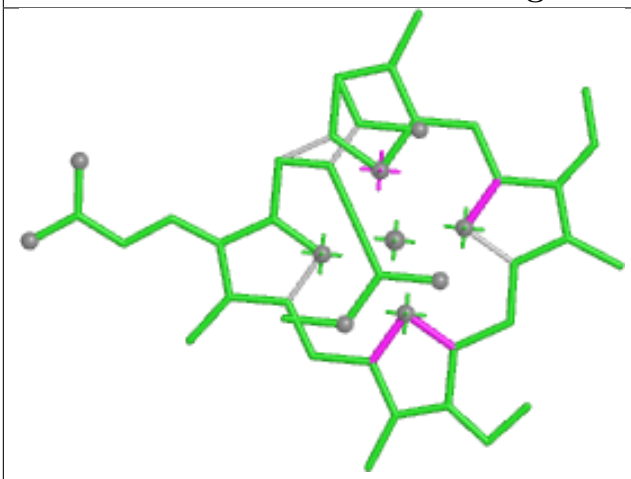


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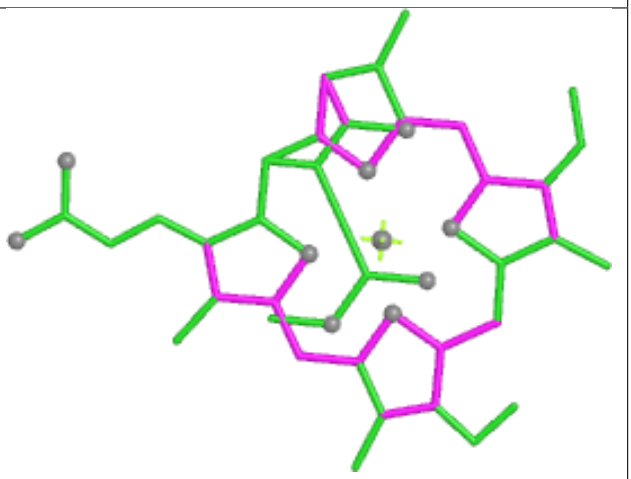


Rings

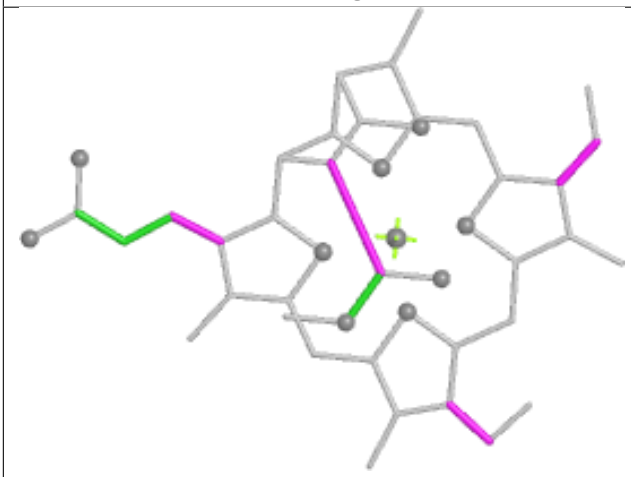
Ligand KC2 T 311



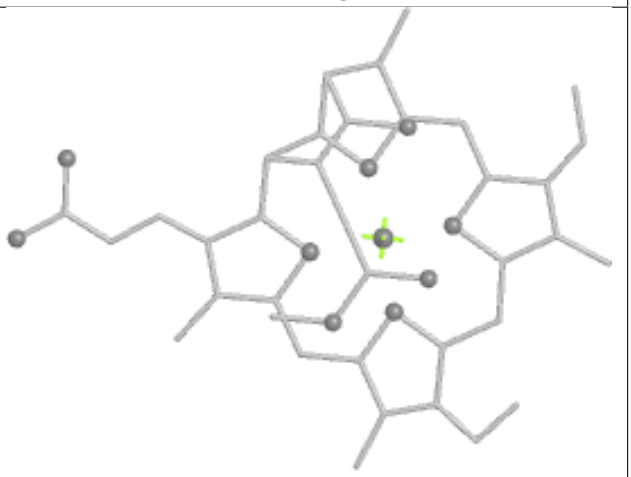
Bond lengths



Bond angles

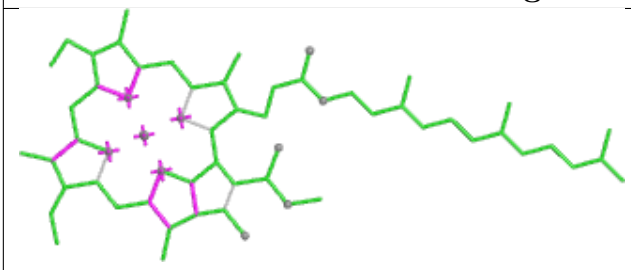


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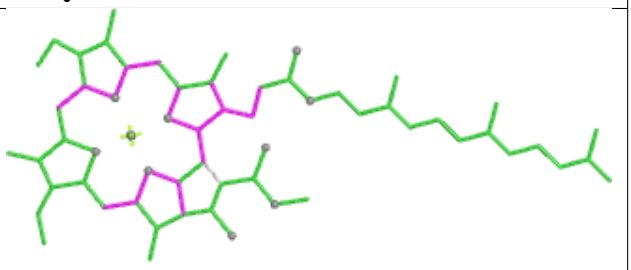


Rings

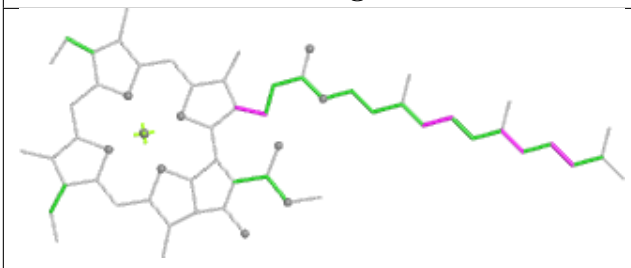
Ligand CLA Q 303



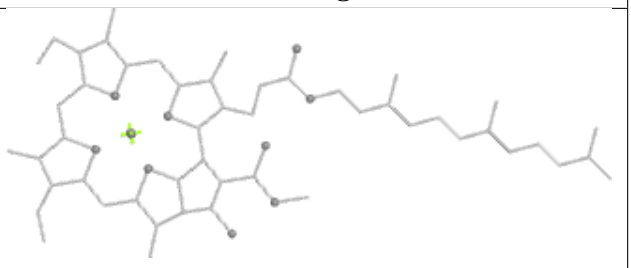
Bond lengths



Bond angles

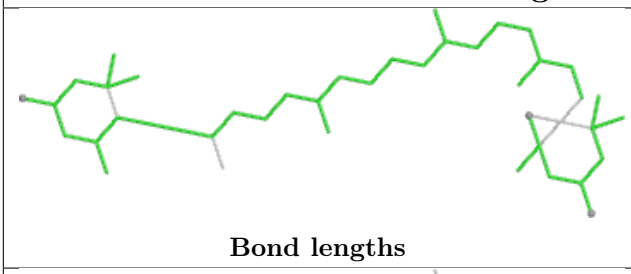


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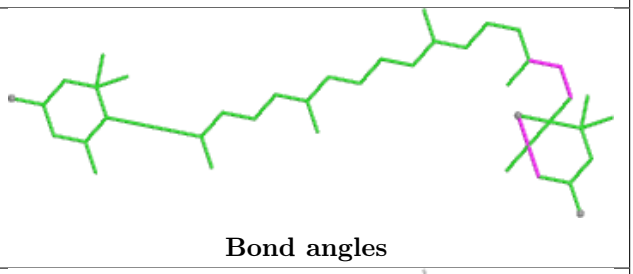


Rings

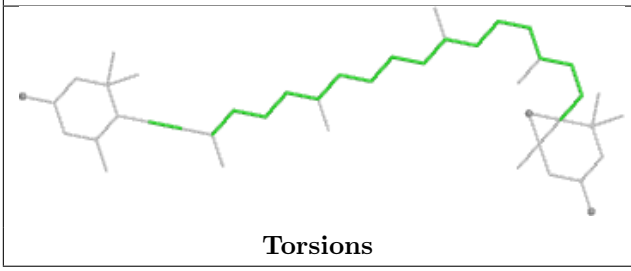
Ligand DD6 I 313



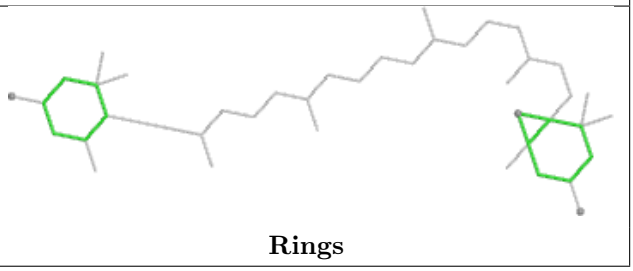
Bond lengths



Bond angles

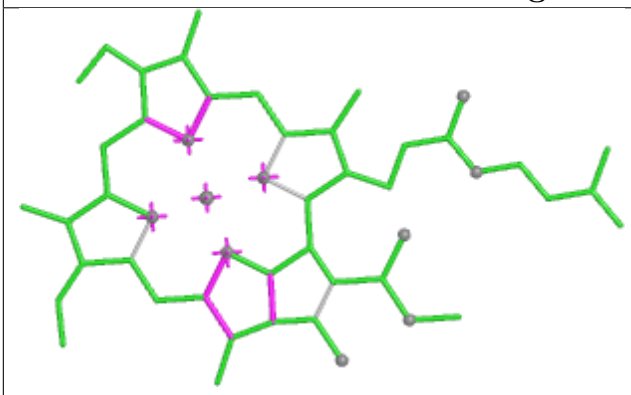


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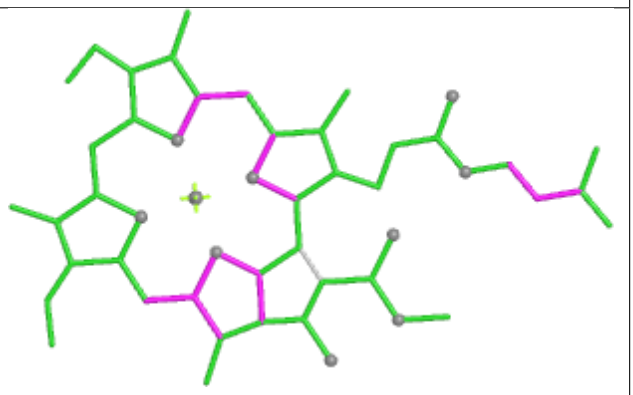


Rings

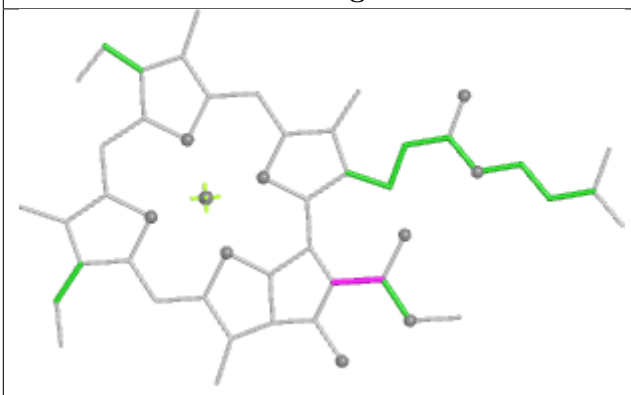
Ligand CLA a 815



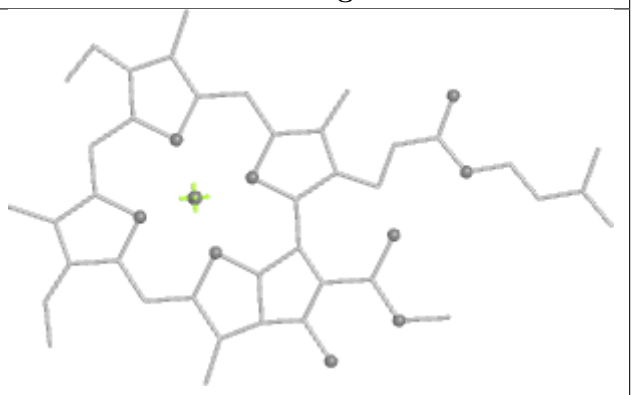
Bond lengths



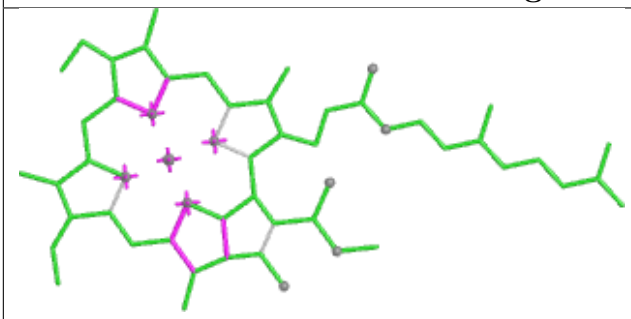
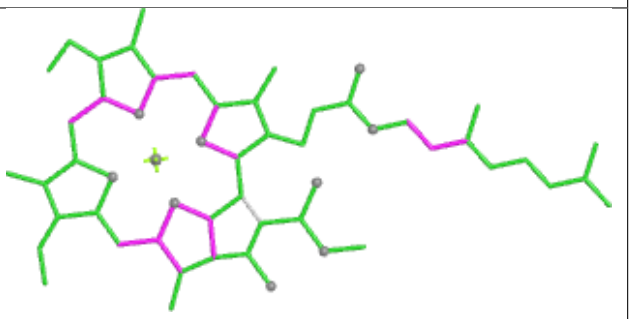
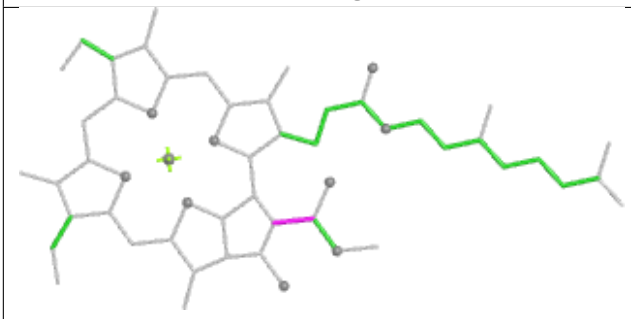
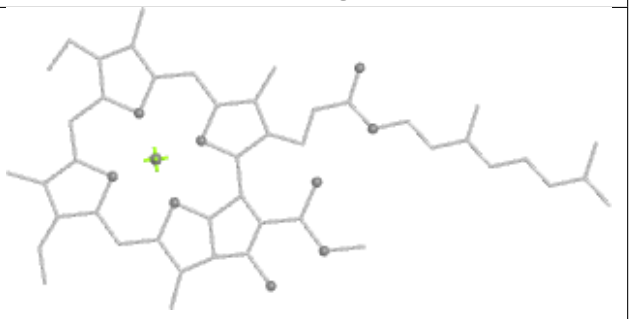
Bond angles

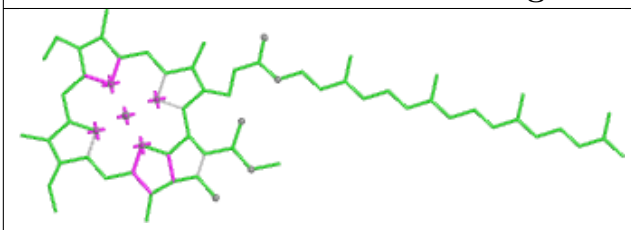
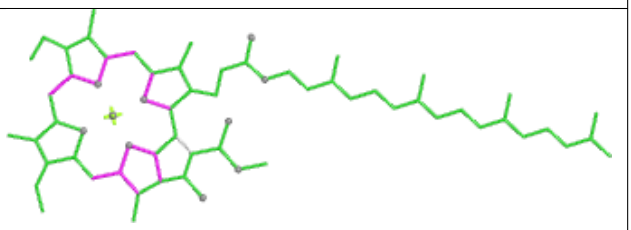
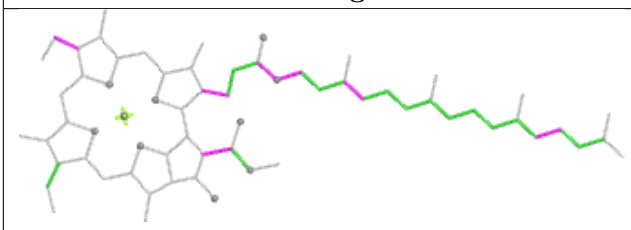
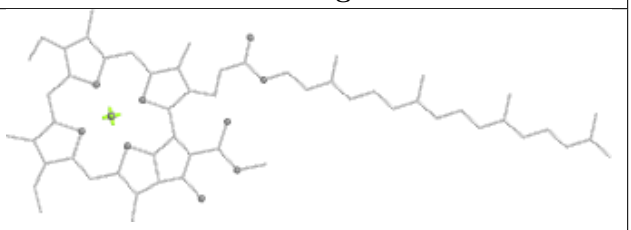


Torsions

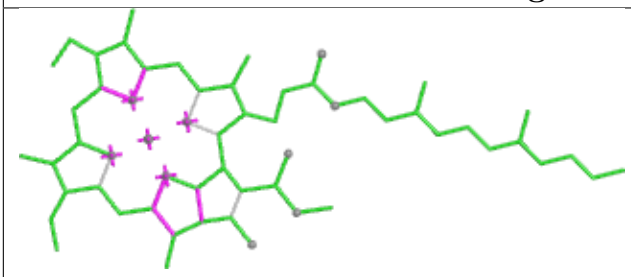


Rings

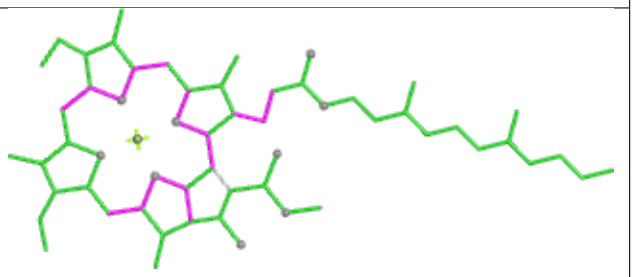
Ligand CLA T 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

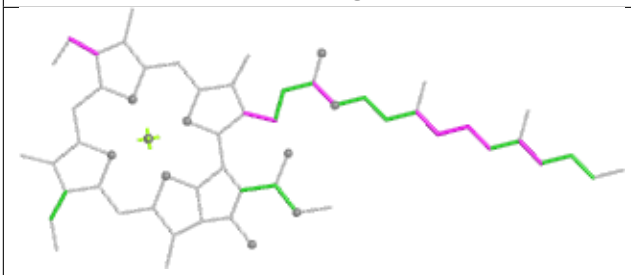
Ligand CLA J 312



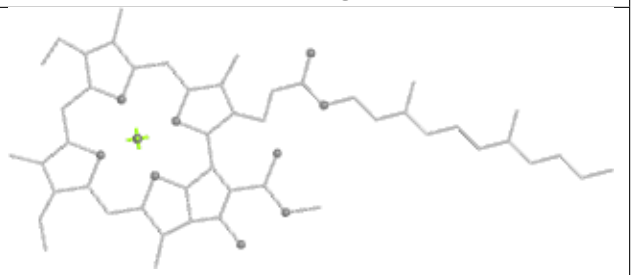
Bond lengths



Bond angles

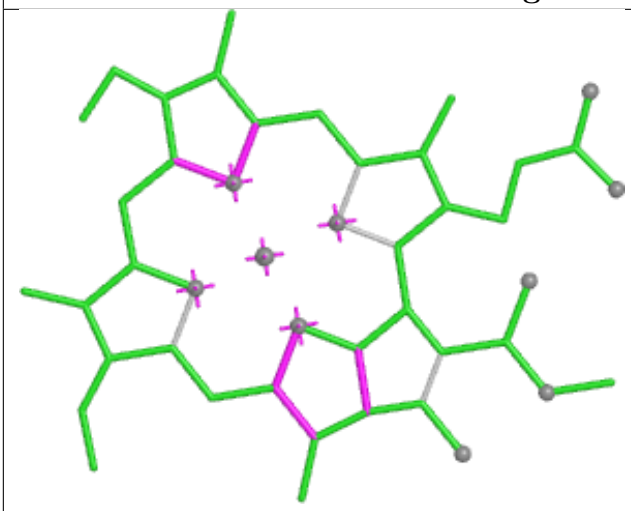


Torsions

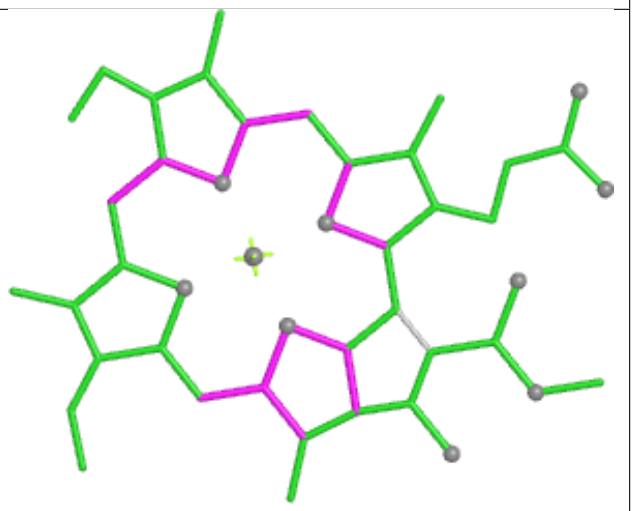


Rings

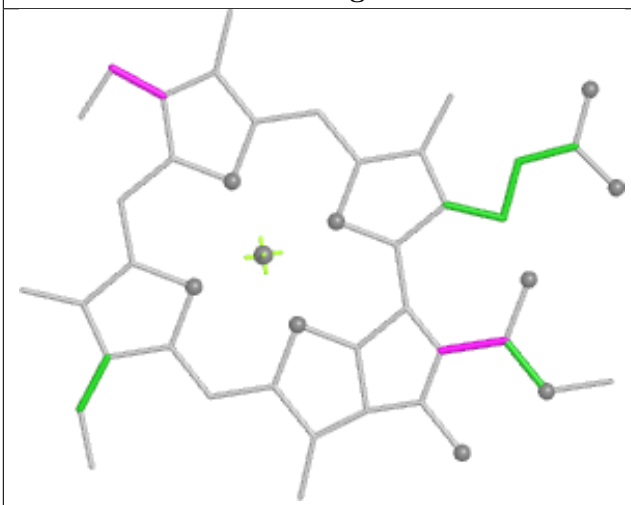
Ligand CLA K 301



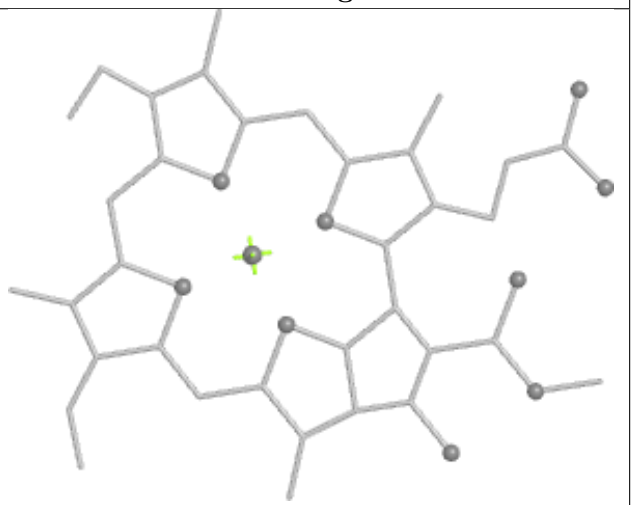
Bond lengths



Bond angles

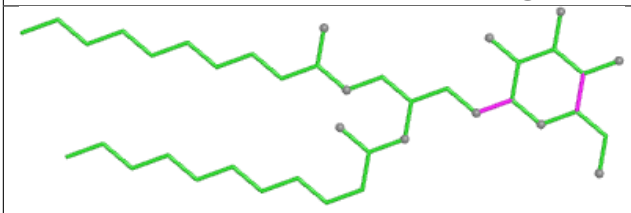


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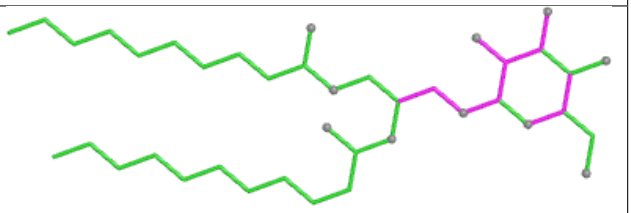


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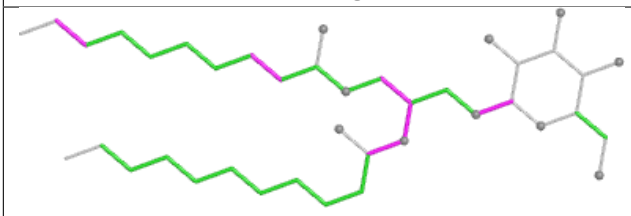
Ligand LMG A 318



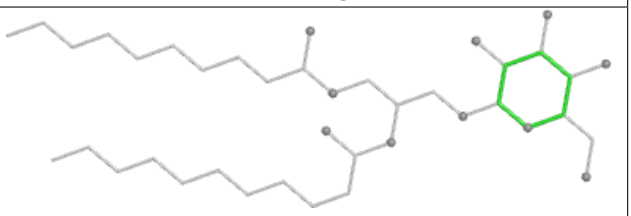
Bond lengths



Bond angles

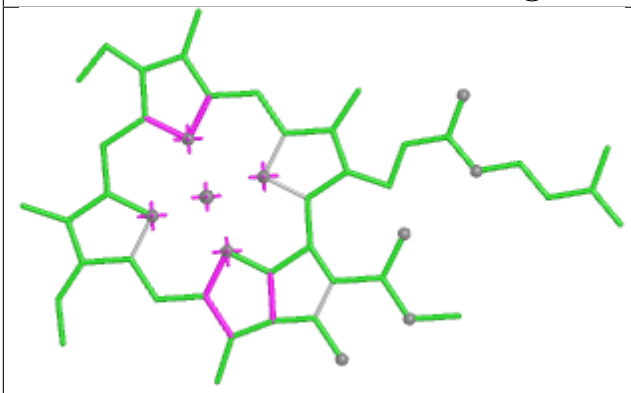


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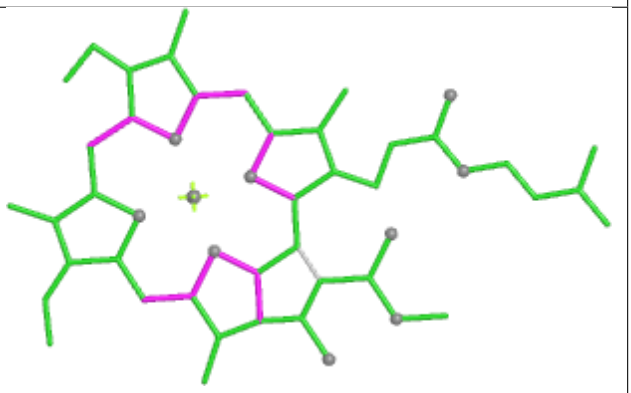


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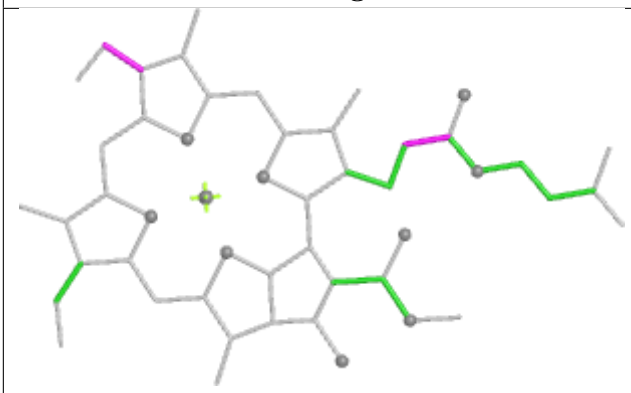
Ligand CLA H 306



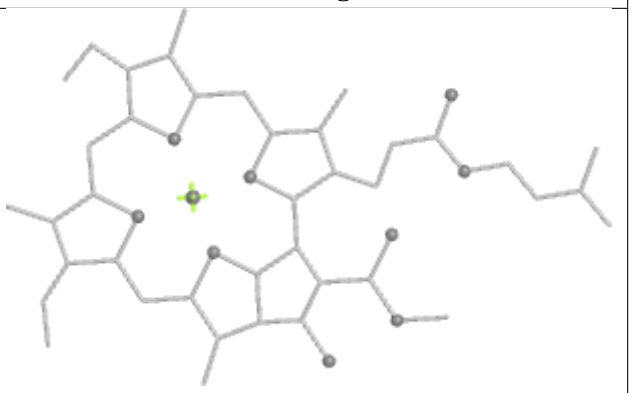
Bond lengths



Bond angles

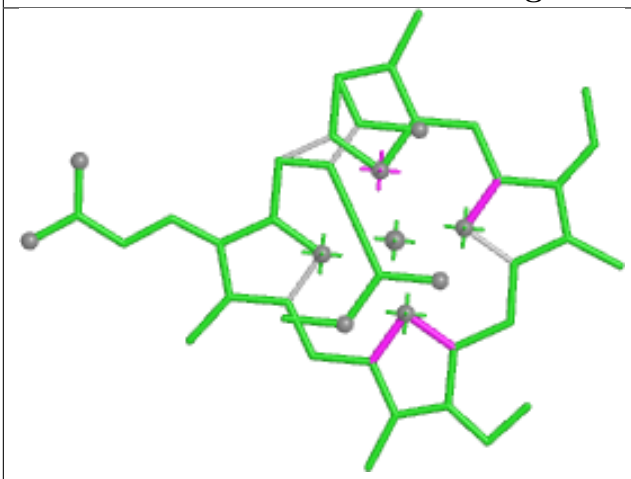


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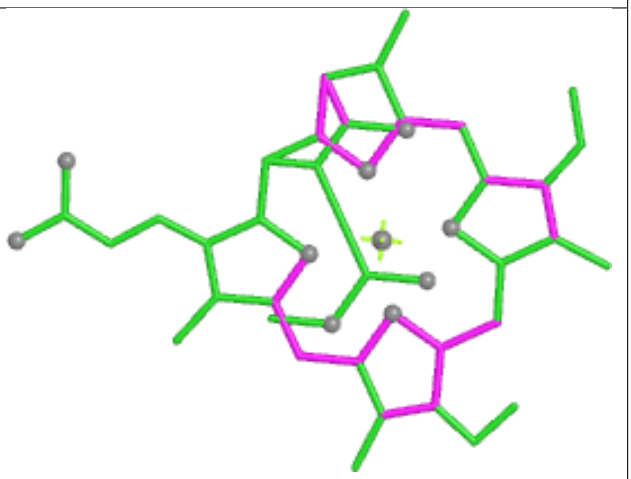


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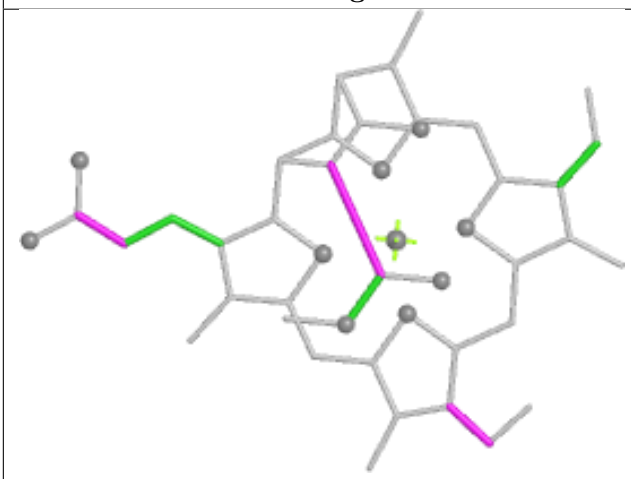
Ligand KC2 N 302



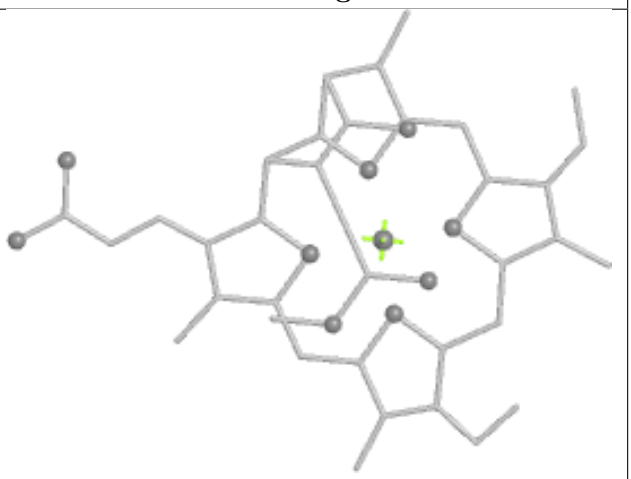
Bond lengths



Bond angles

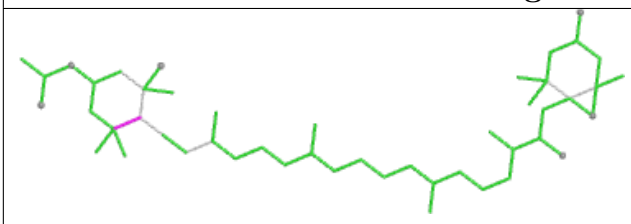


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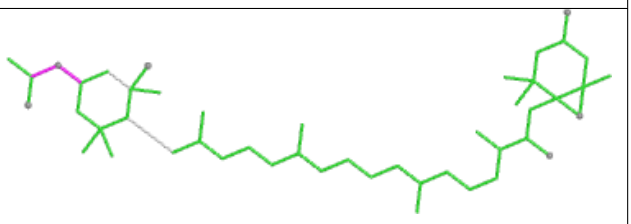


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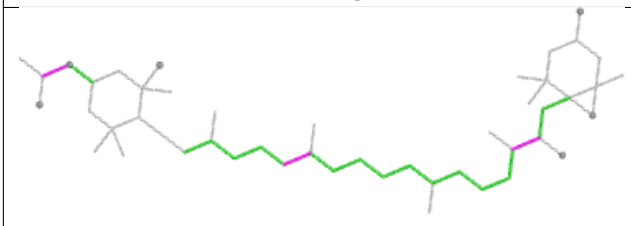
Ligand A86 W 316



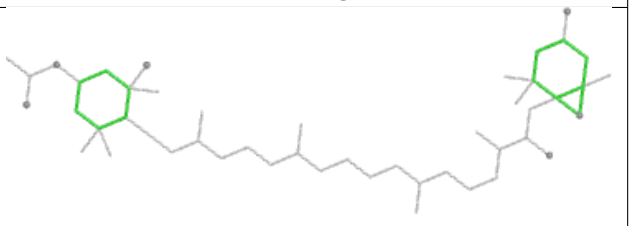
Bond lengths



Bond angles

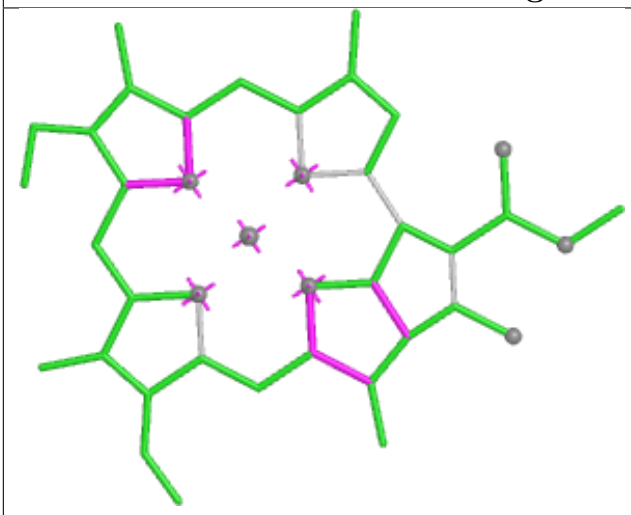


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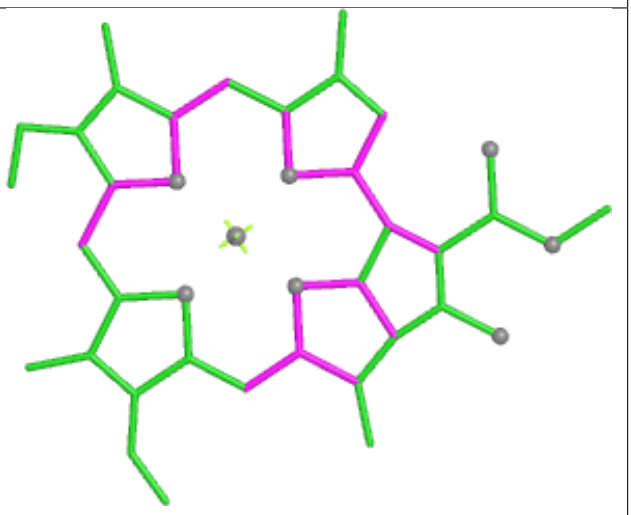


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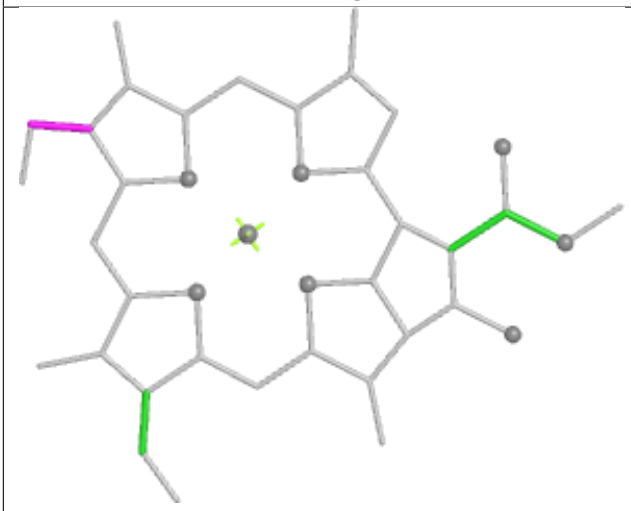
Ligand CLA L 311



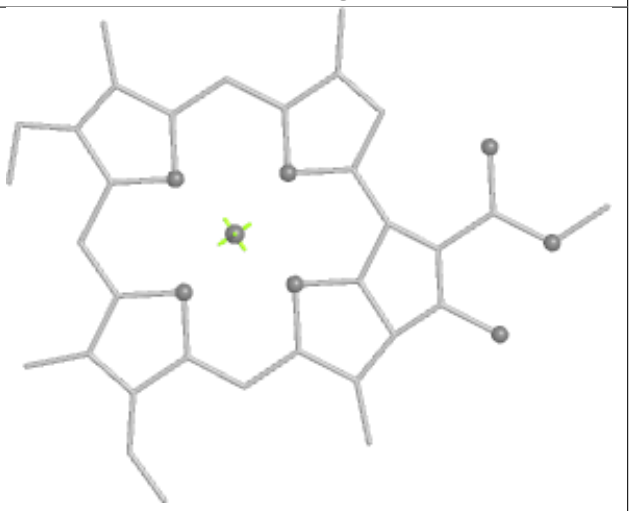
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Bond angles

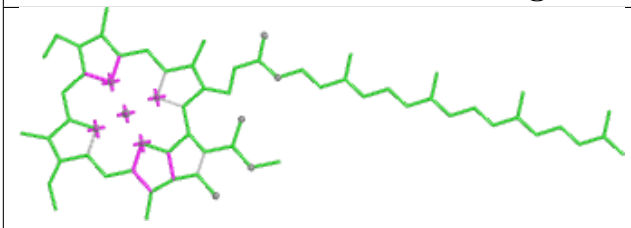


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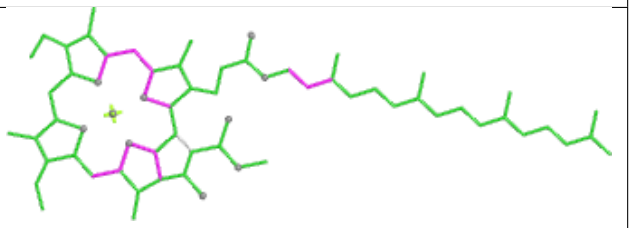


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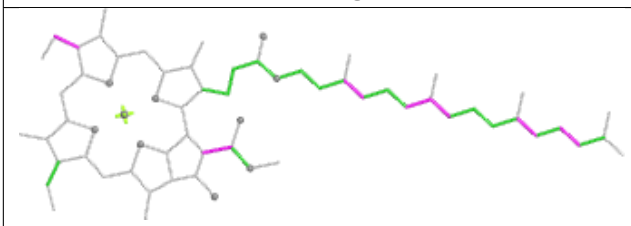
Ligand CLA a 841



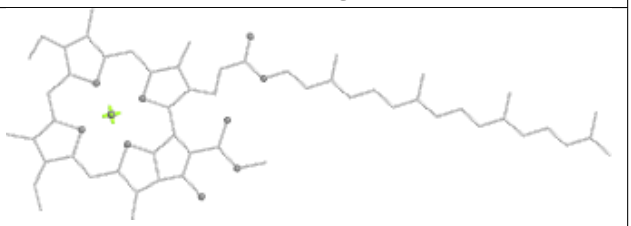
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Bond angles

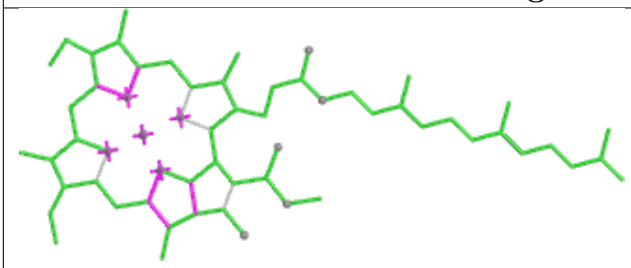


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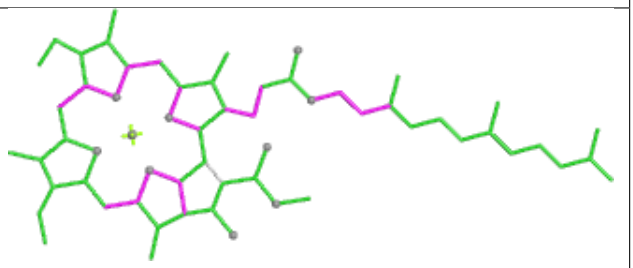


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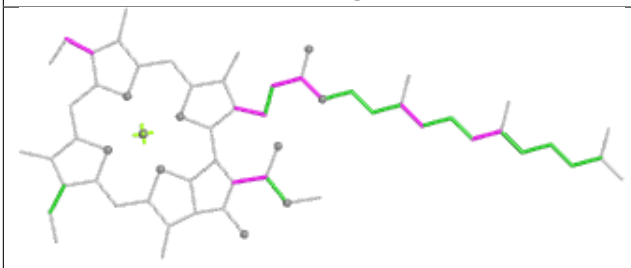
Ligand CLA S 309



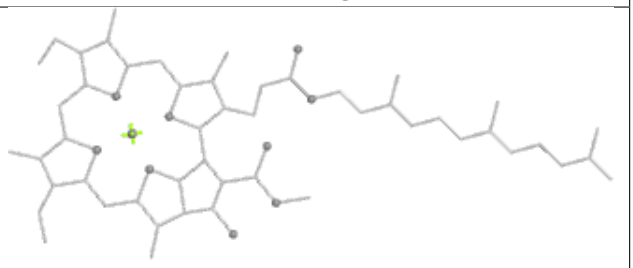
Bond lengths



Bond angles

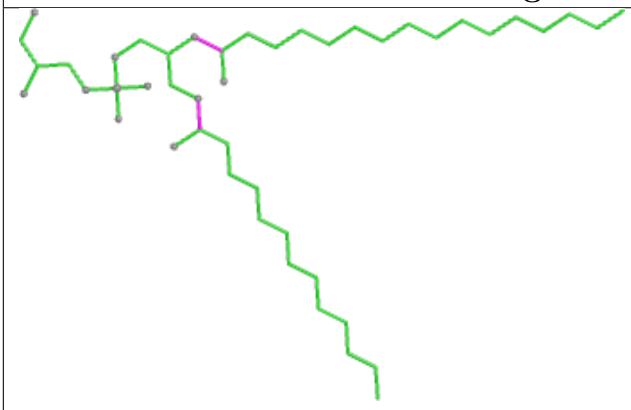


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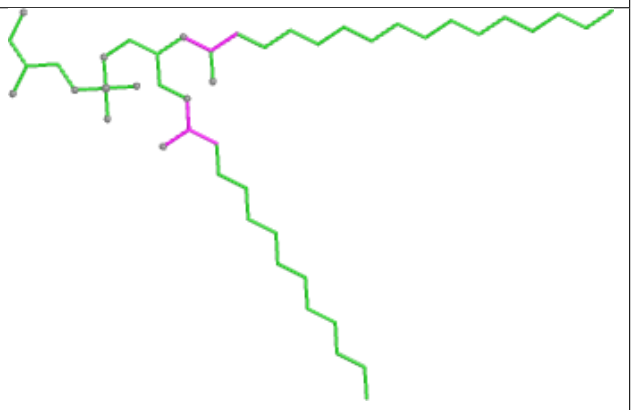


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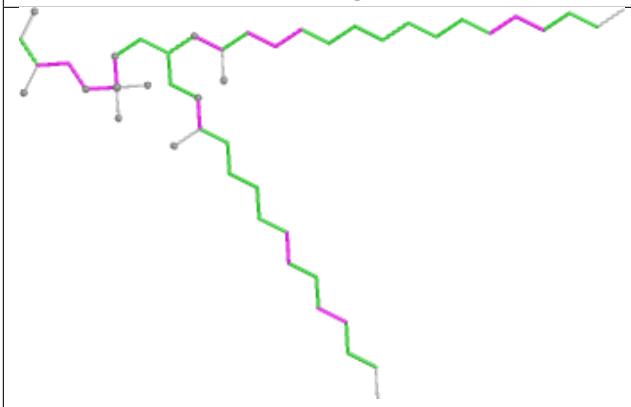
Ligand LHG E 321



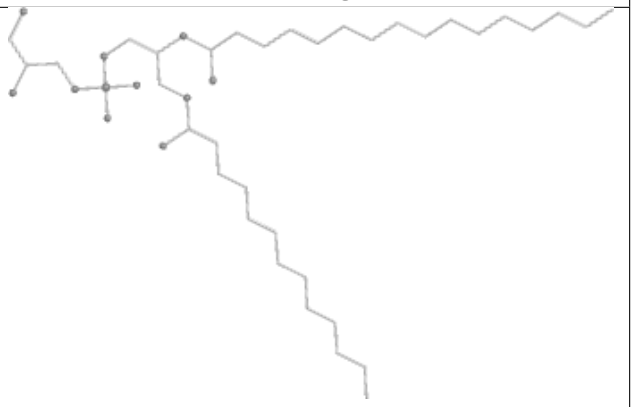
Bond lengths



Bond angles

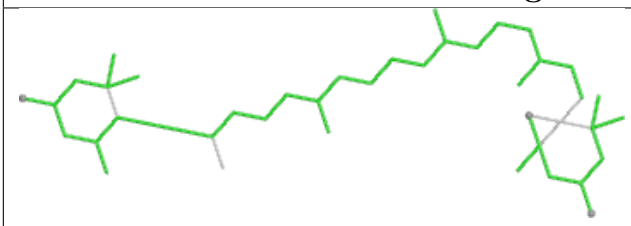


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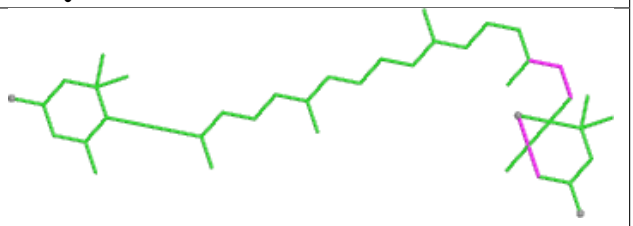


Rings

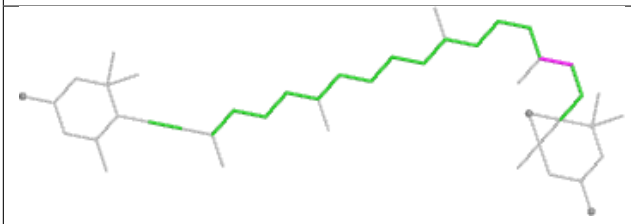
Ligand DD6 Q 314



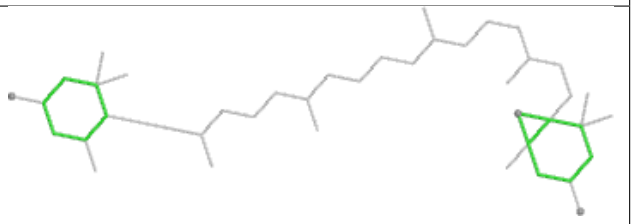
Bond lengths



Bond angles

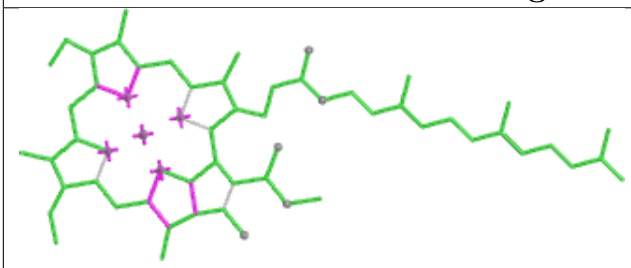


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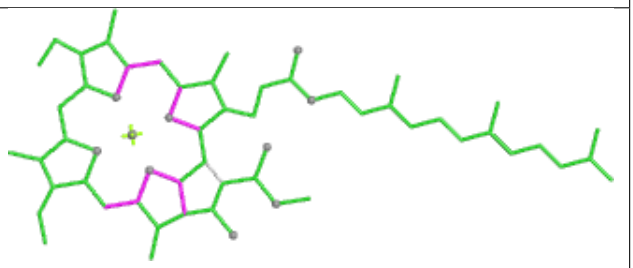


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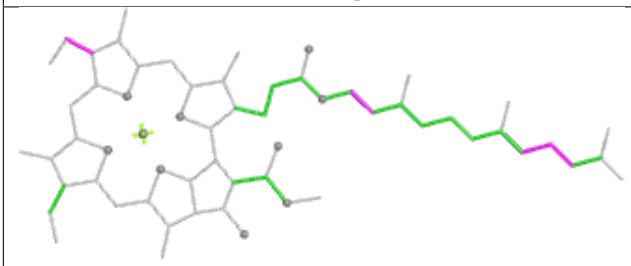
Ligand CLA a 832



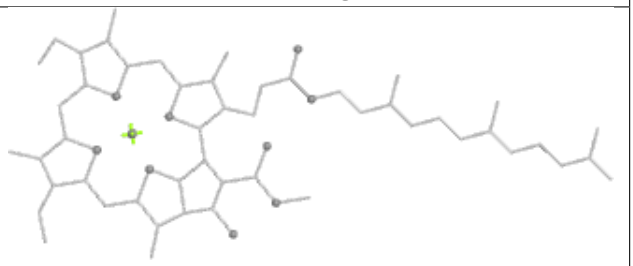
Bond lengths



Bond angles

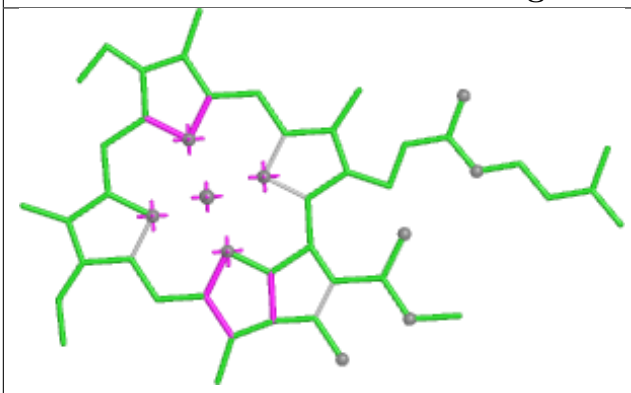


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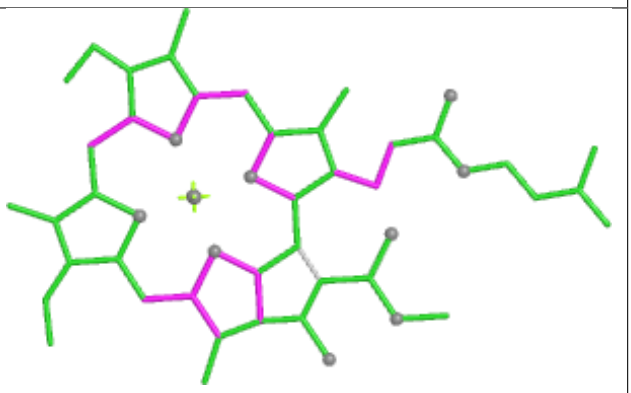


Rings

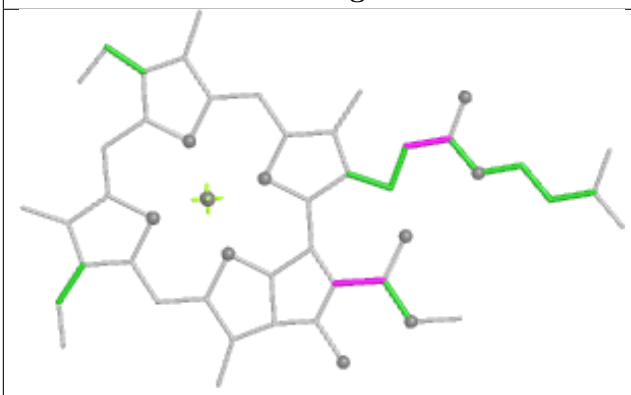
Ligand CLA S 311



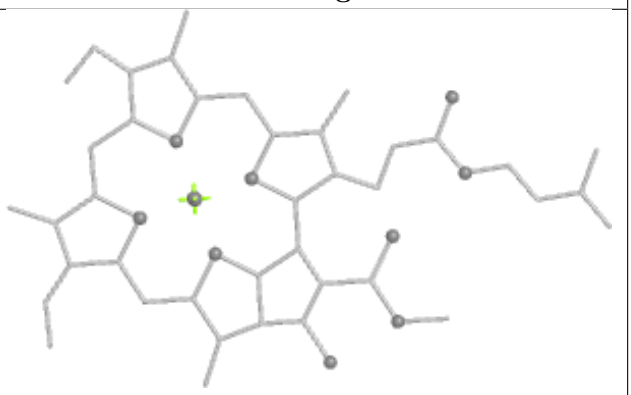
Bond lengths



Bond angles

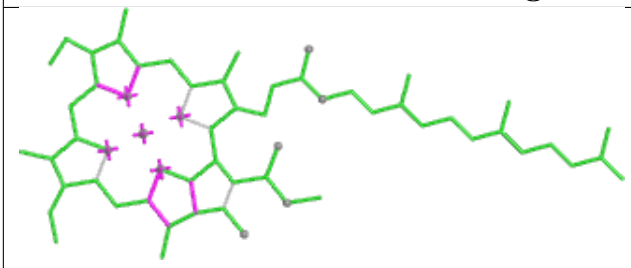


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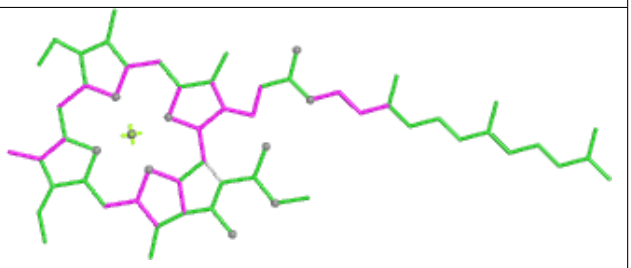


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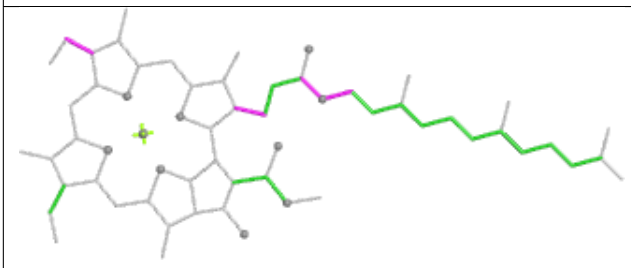
Ligand CLA T 308



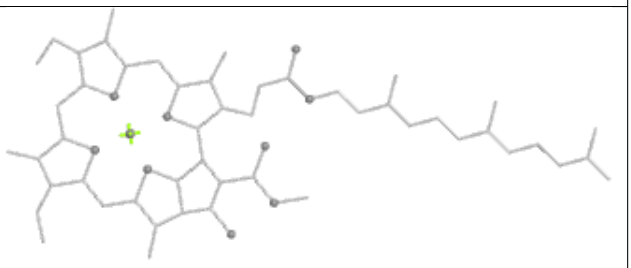
Bond lengths



Bond angles

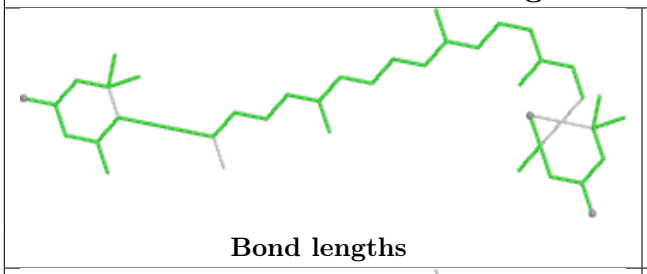


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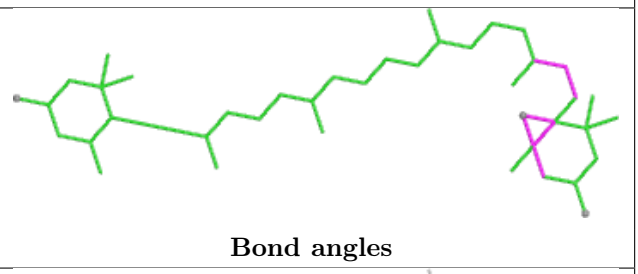


Rings

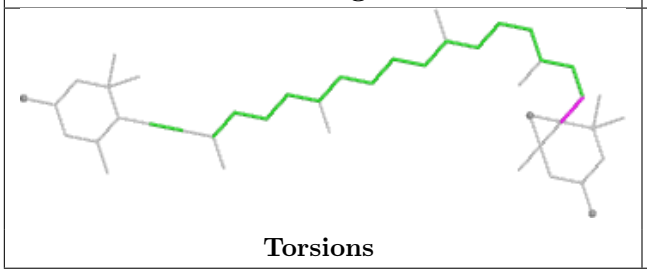
Ligand DD6 K 315



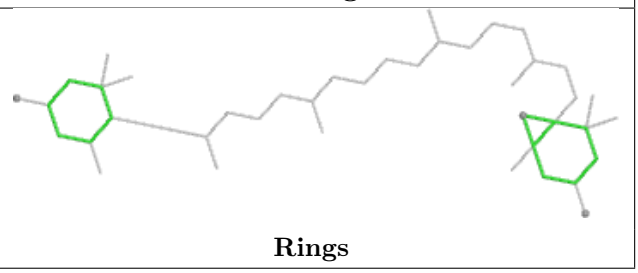
Bond lengths



Bond angles

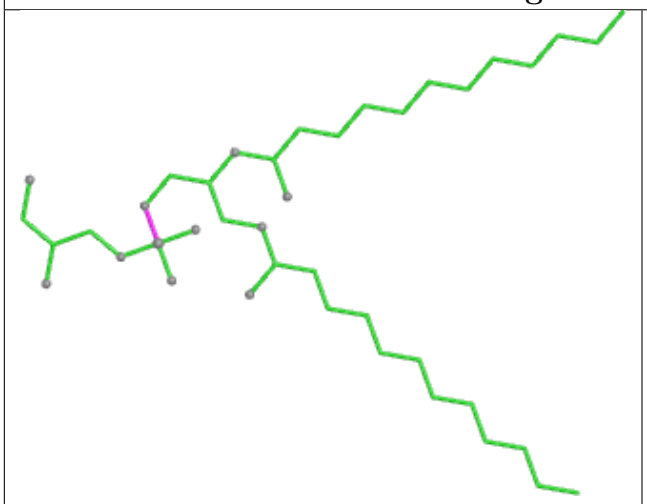


Torsions

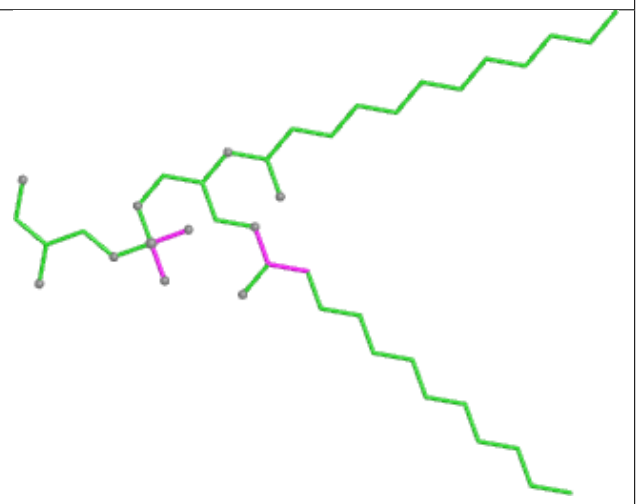


Rings

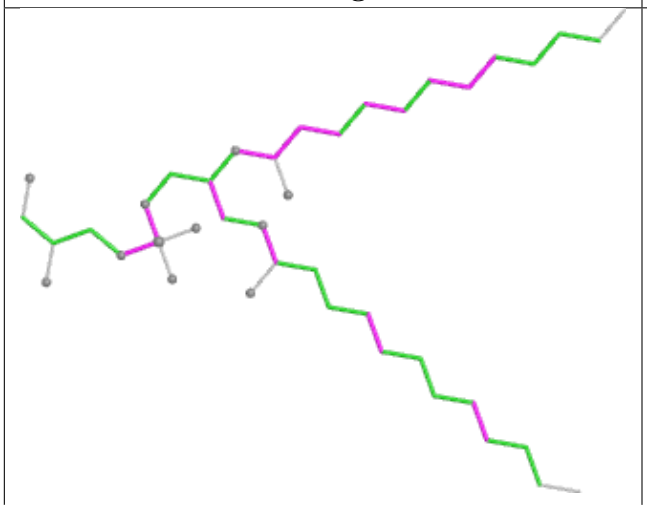
Ligand LHG F 318



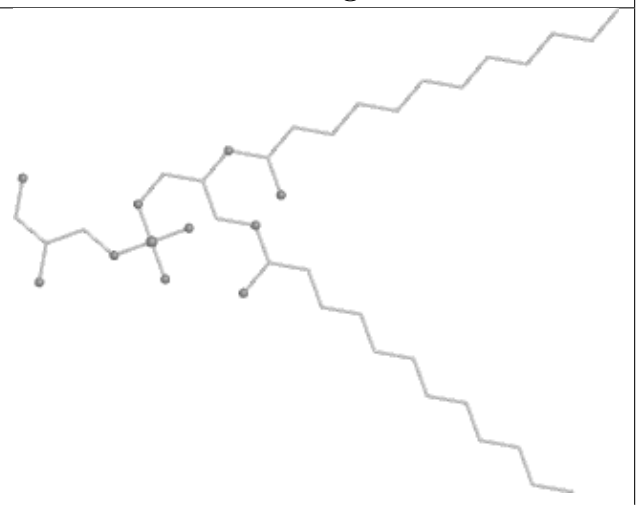
Bond lengths



Bond angles

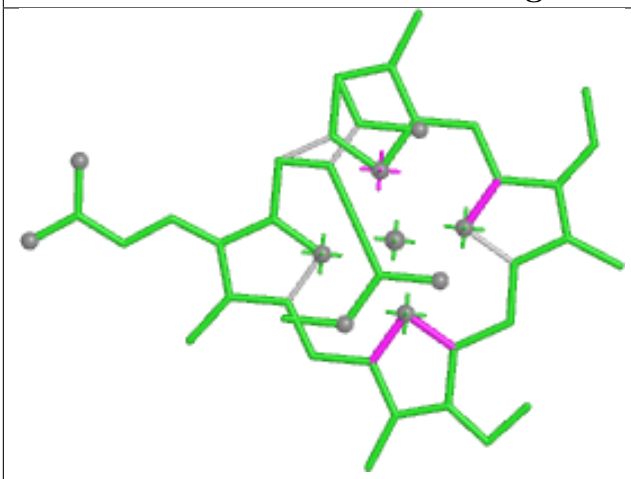


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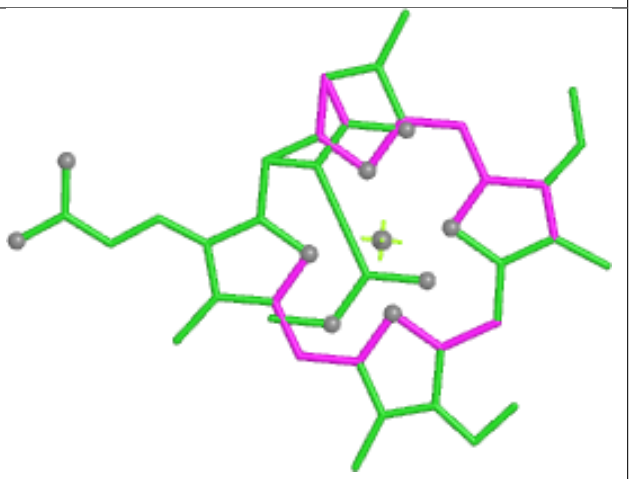


Rings

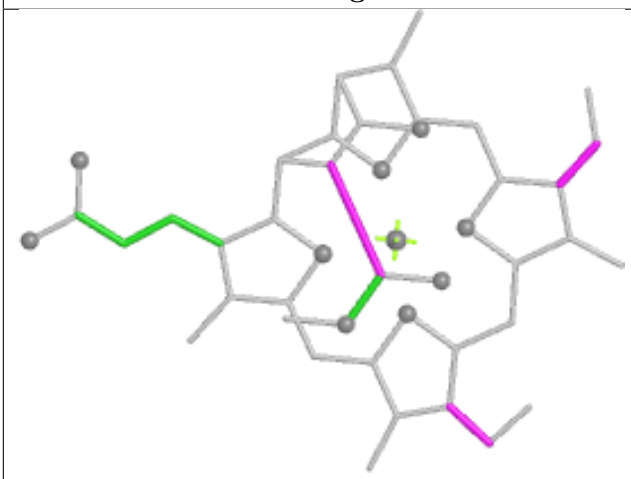
Ligand KC2 A 310



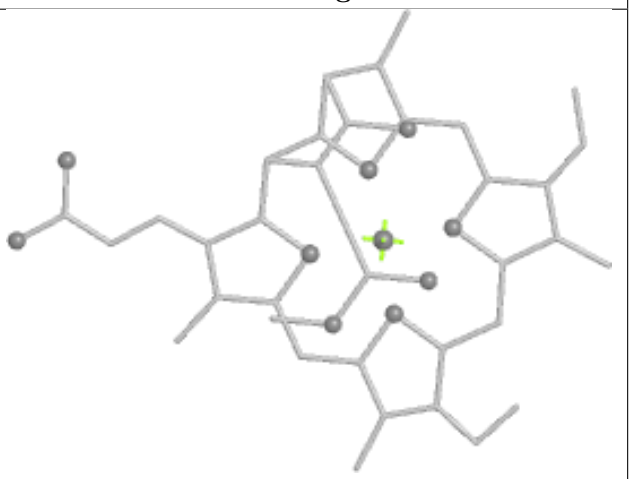
Bond lengths



Bond angles

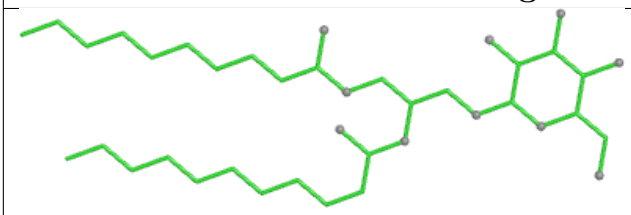


Torsions

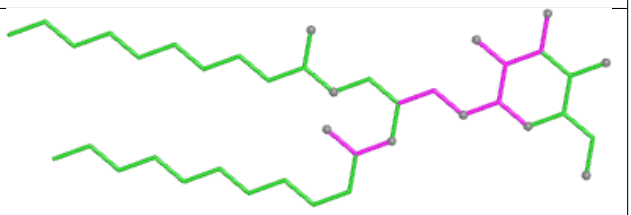


Rings

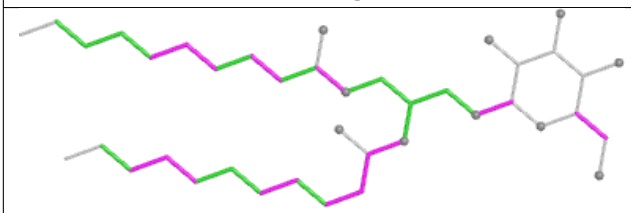
Ligand LMG D 321



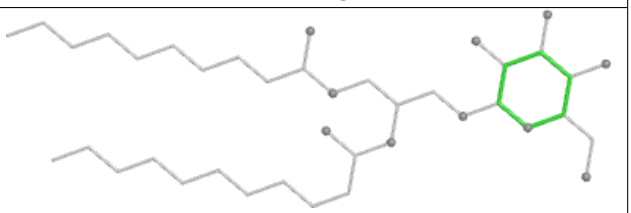
Bond lengths



Bond angles

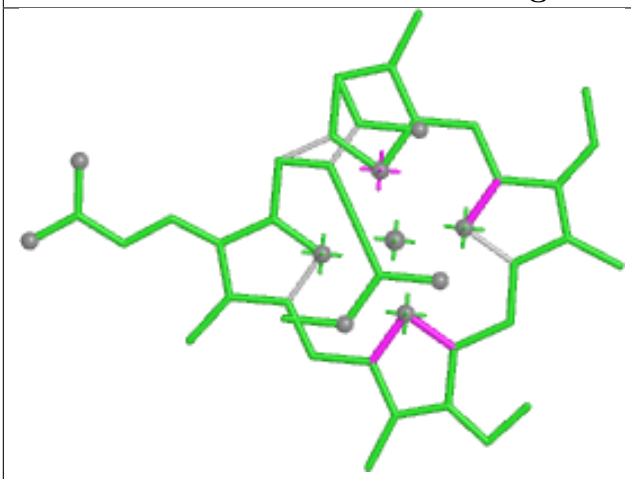


Torsions

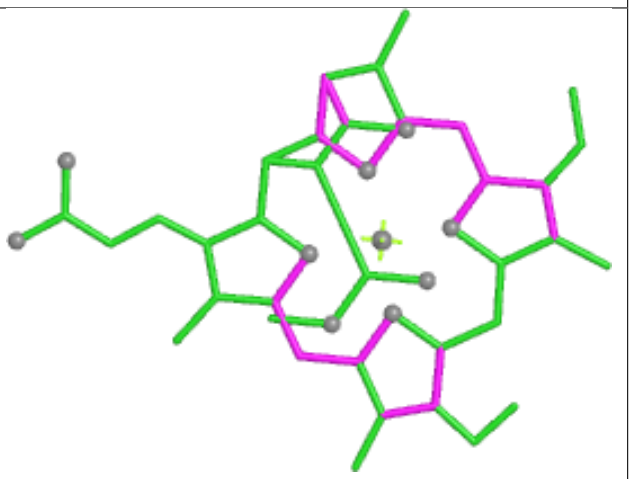


Rings

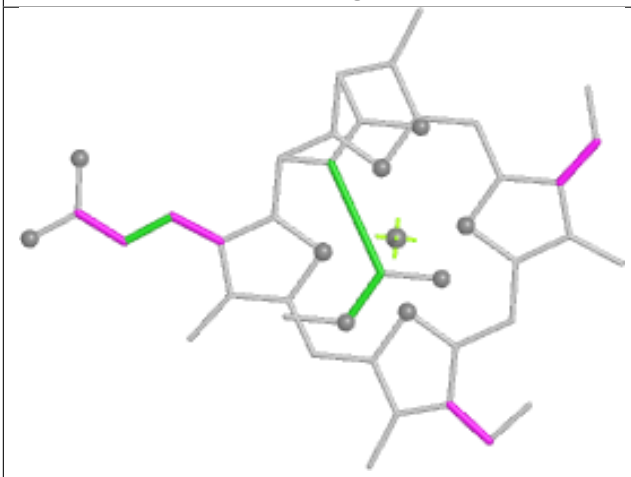
Ligand KC2 J 310



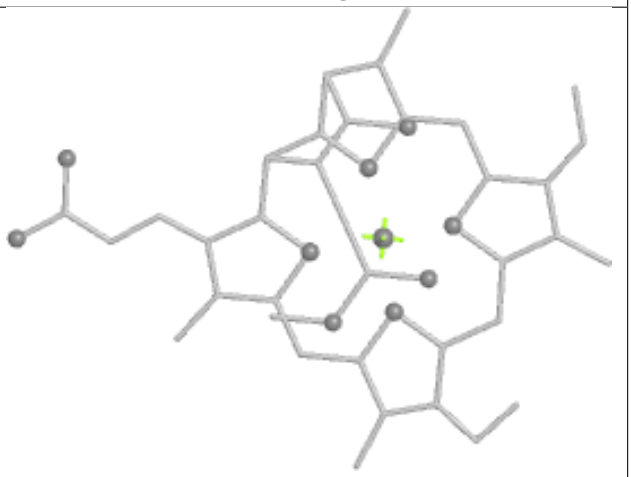
Bond lengths



Bond angles



Torsions



Rings

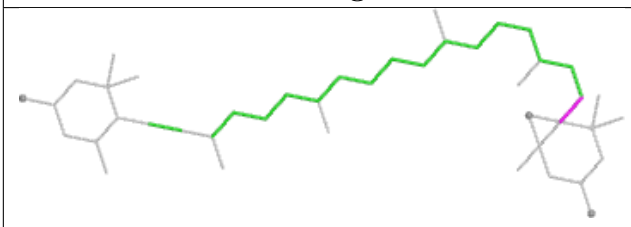
Ligand DD6 H 312



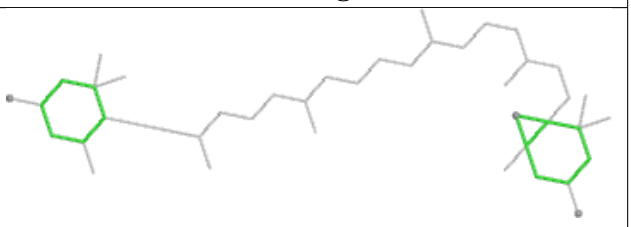
Bond lengths



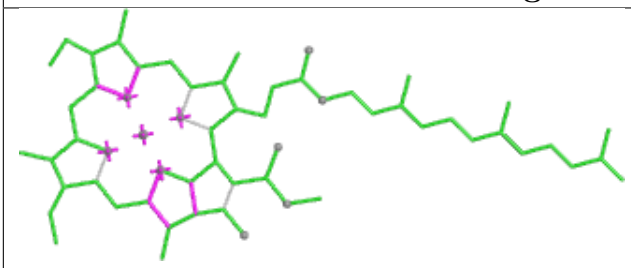
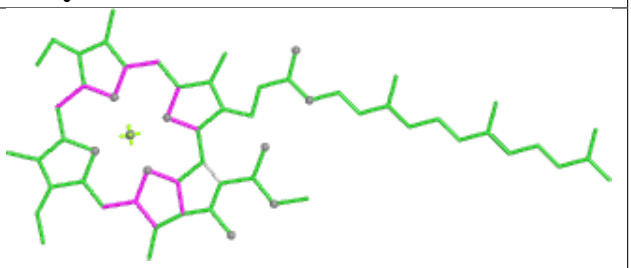
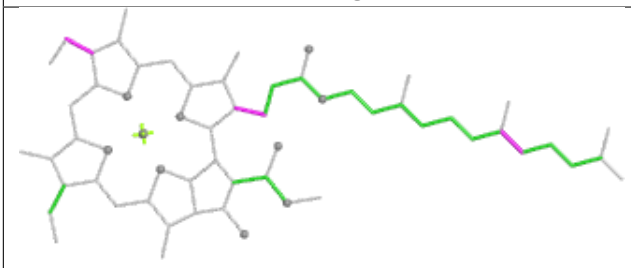
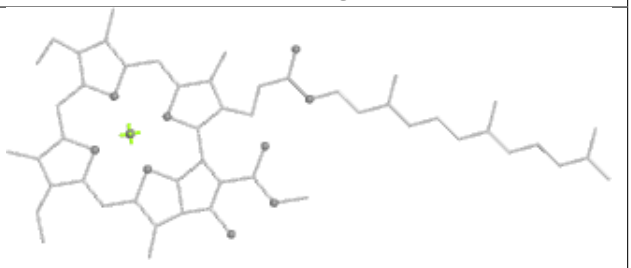
Bond angles

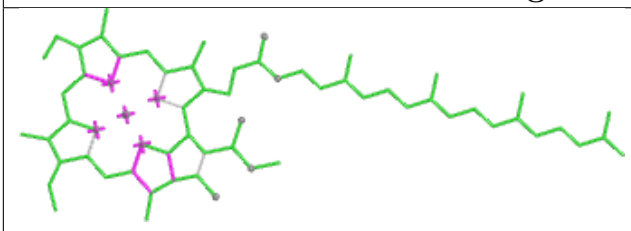
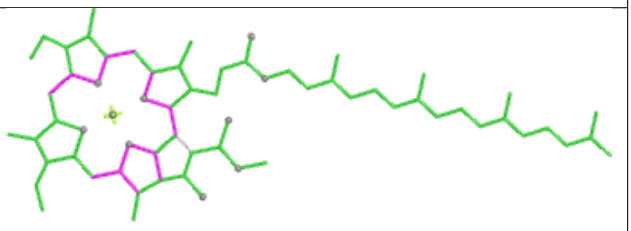
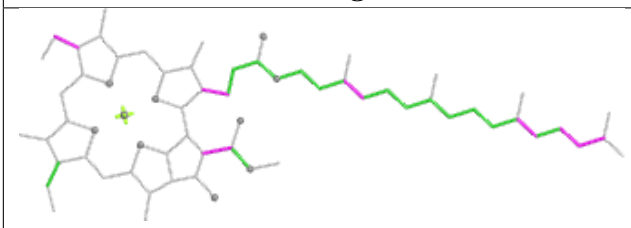
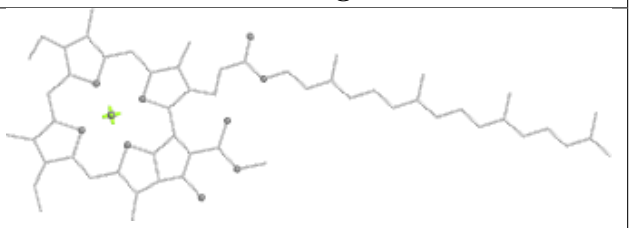


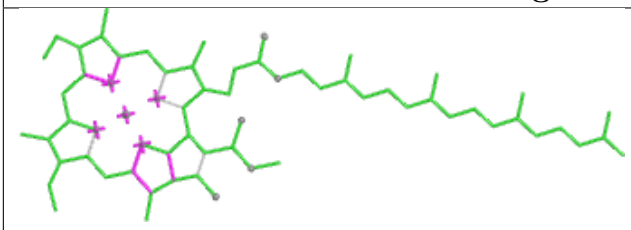
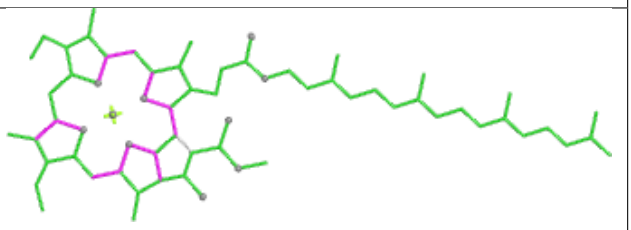
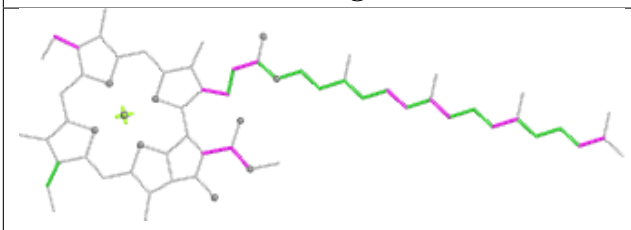
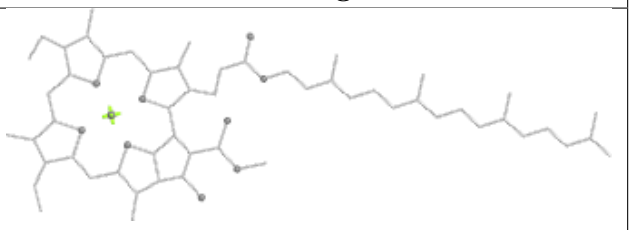
Torsions

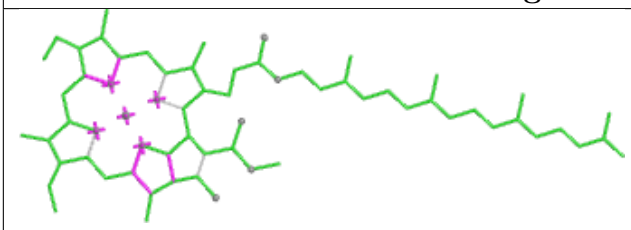
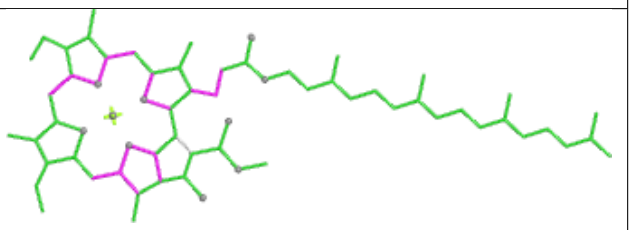
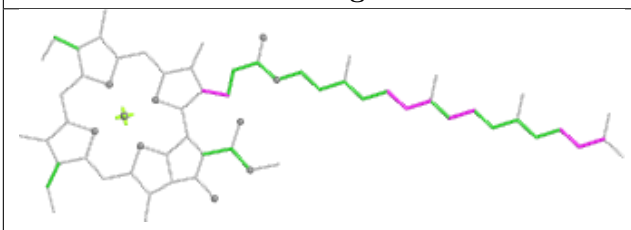
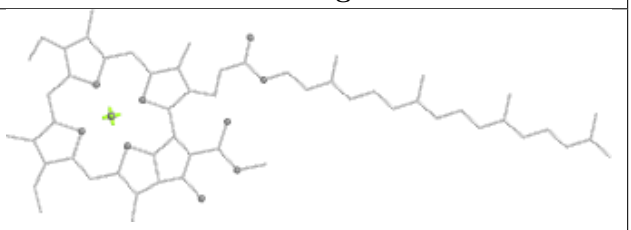


Rings

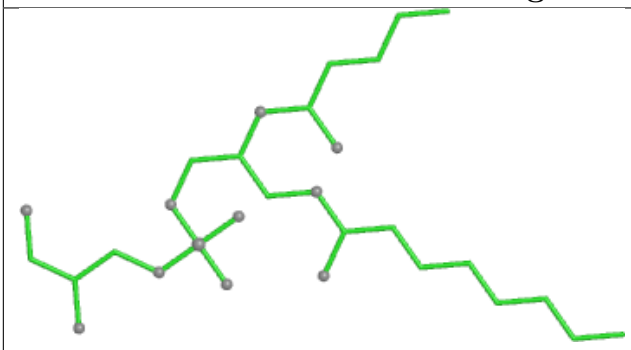
Ligand CLA Q 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

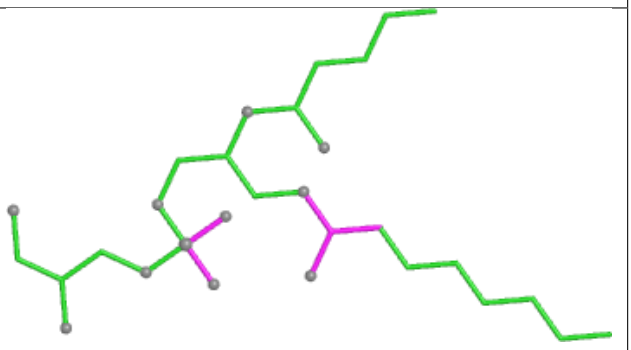
Ligand CLA l 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA O 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

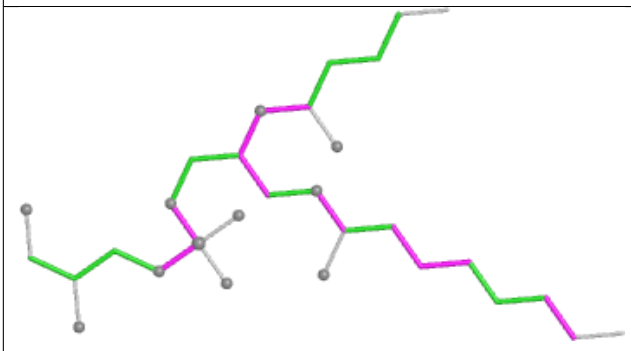
Ligand LHG a 850



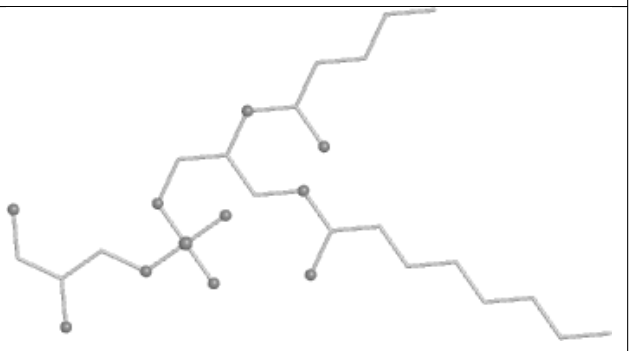
Bond lengths



Bond angles

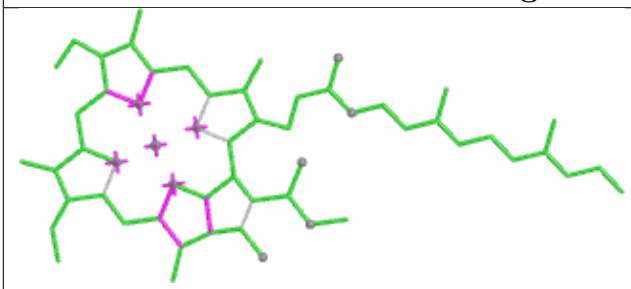


Torsions

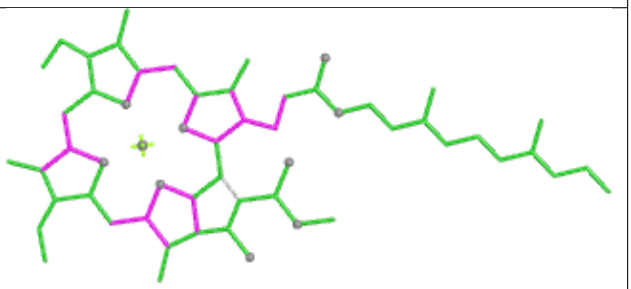


Rings

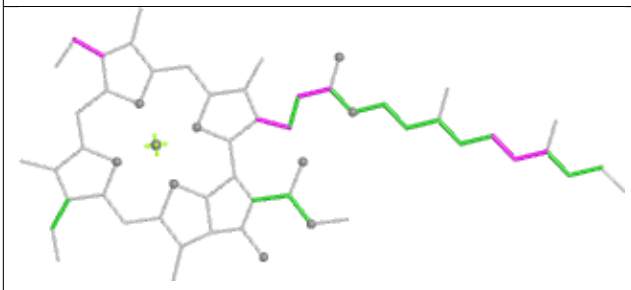
Ligand CLA M 308



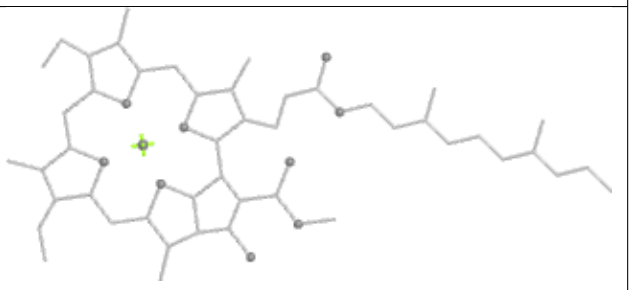
Bond lengths



Bond angles

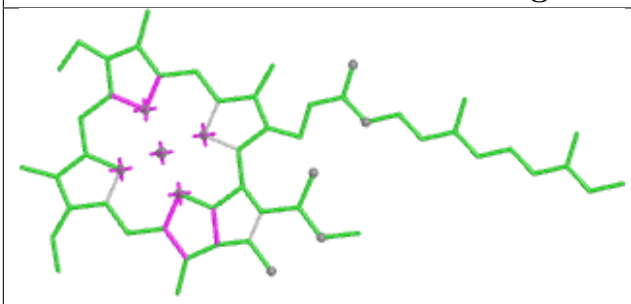


Torsions

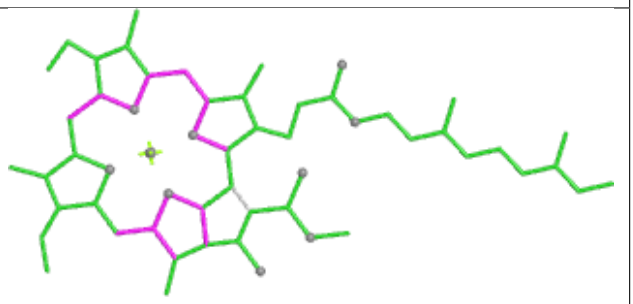


Rings

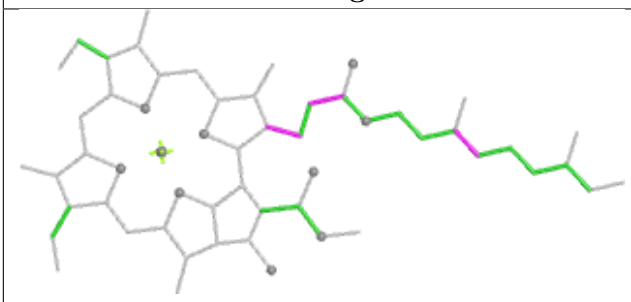
Ligand CLA I 305



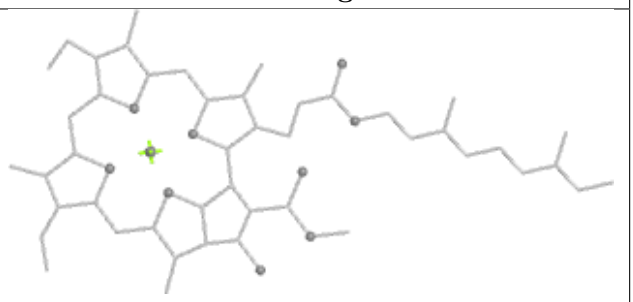
Bond lengths



Bond angles

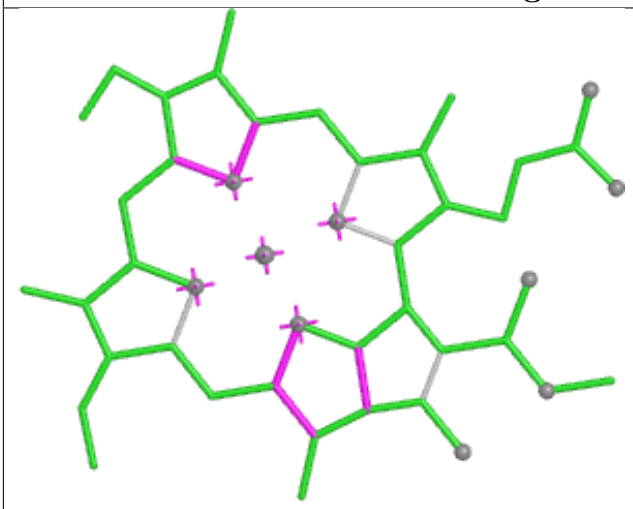


Torsions

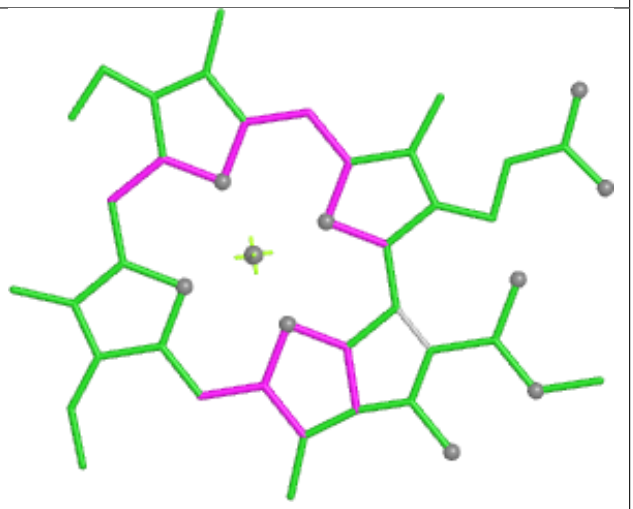


Rings

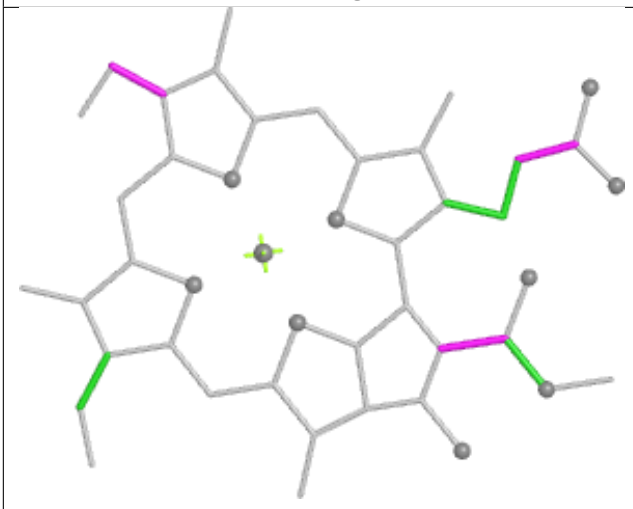
Ligand CLA R 304



Bond lengths



Bond angles

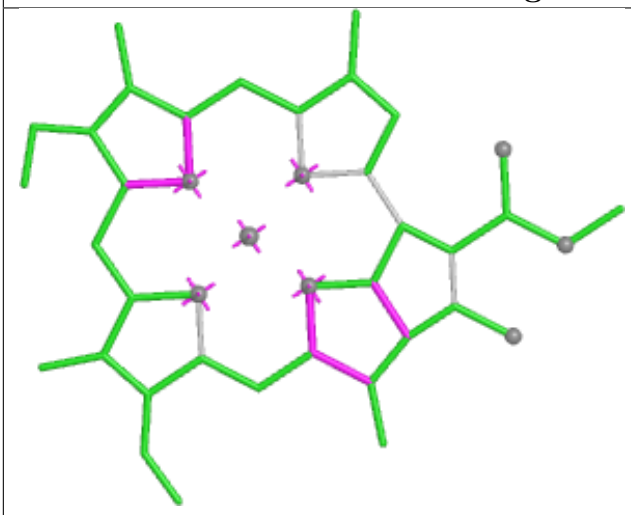


Torsions

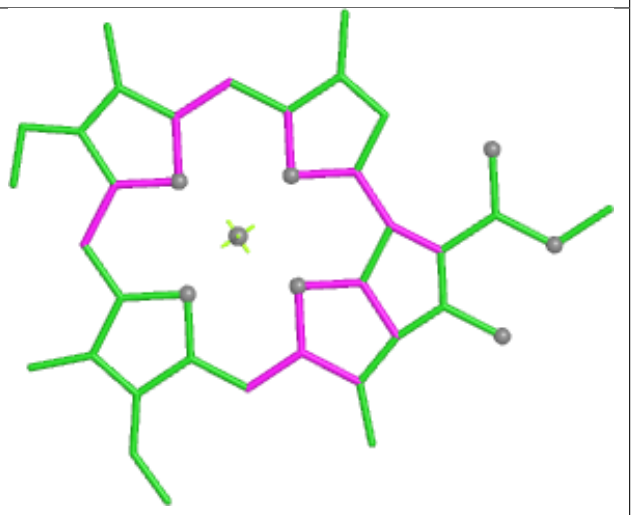


Rings

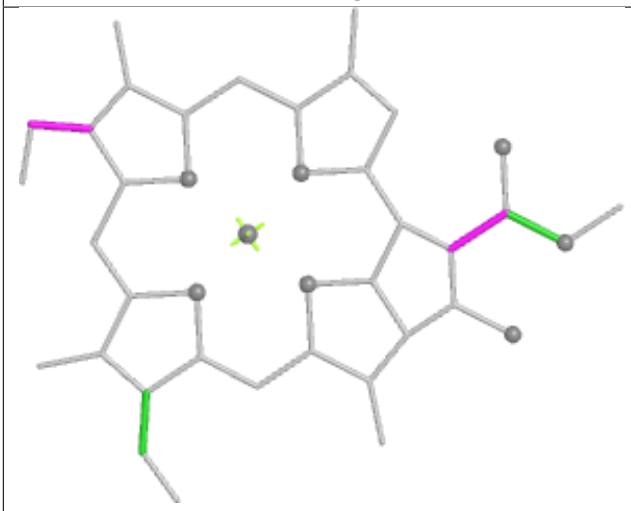
Ligand CLA B 301



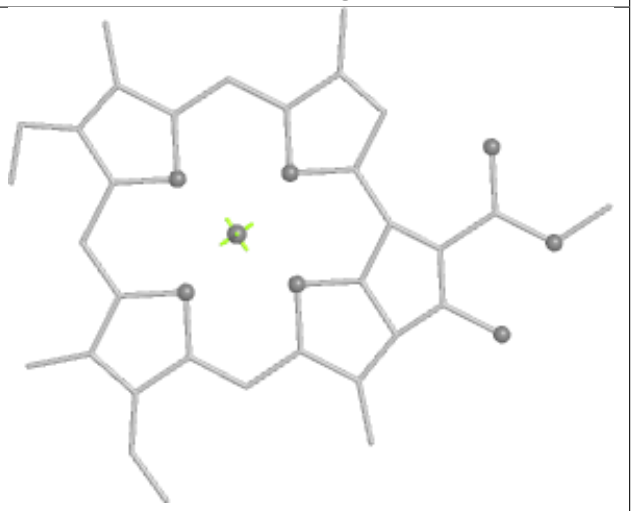
Bond lengths



Bond angles

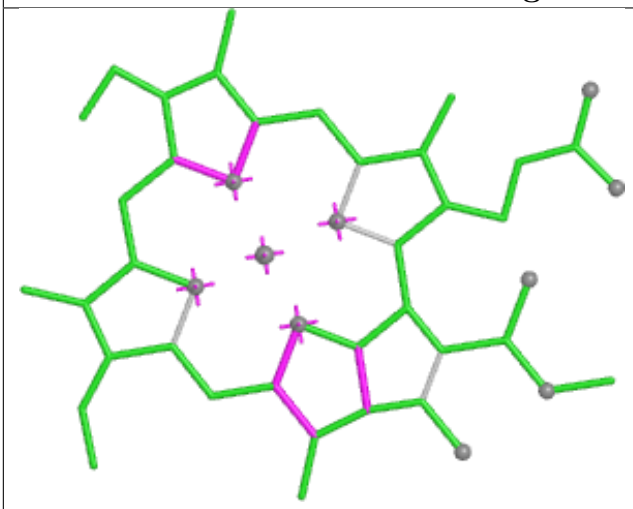


Torsions

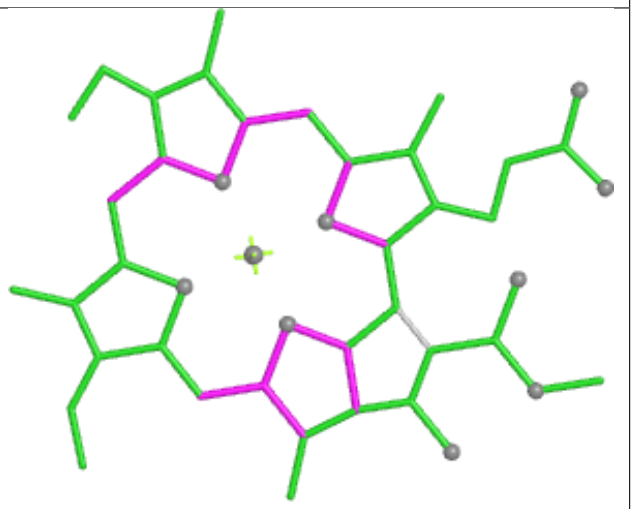


Rings

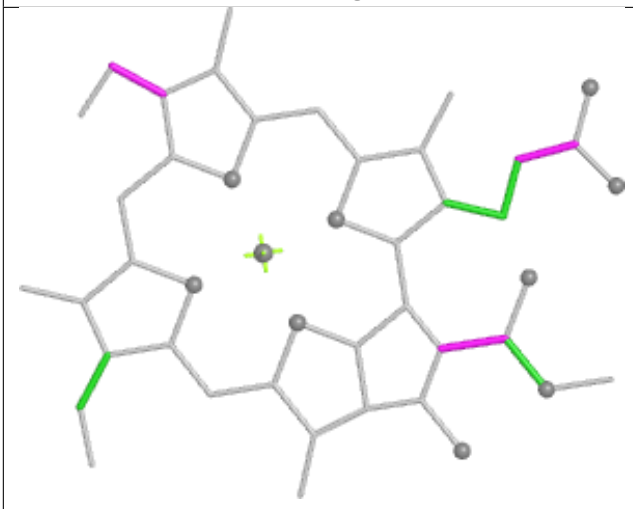
Ligand CLA G 301



Bond lengths



Bond angles

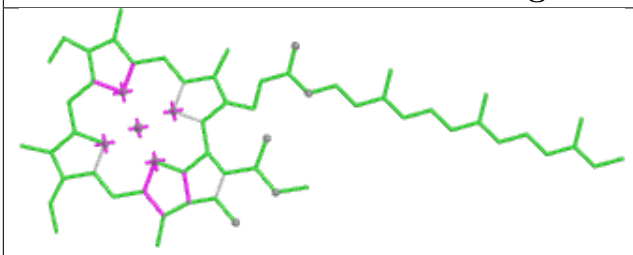


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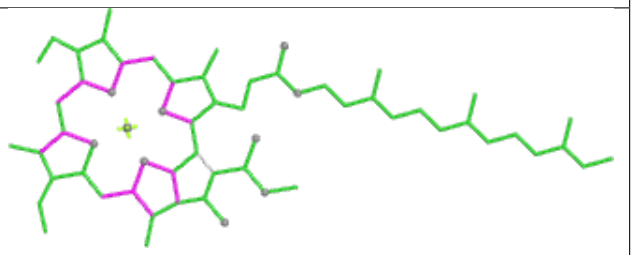


Rings

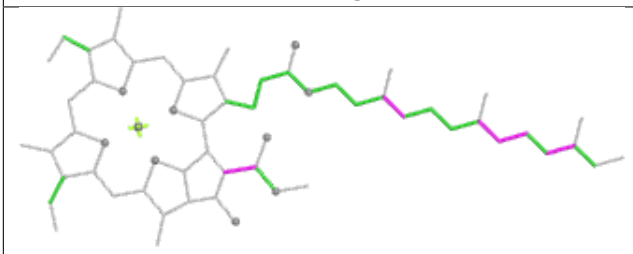
Ligand CLA a 817



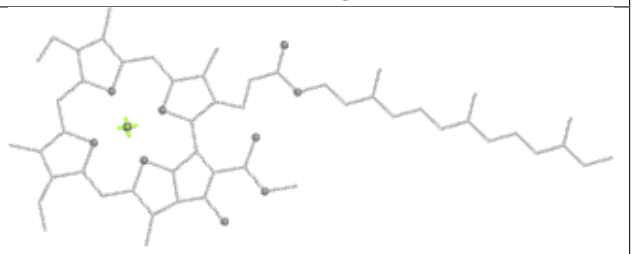
Bond lengths



Bond angles

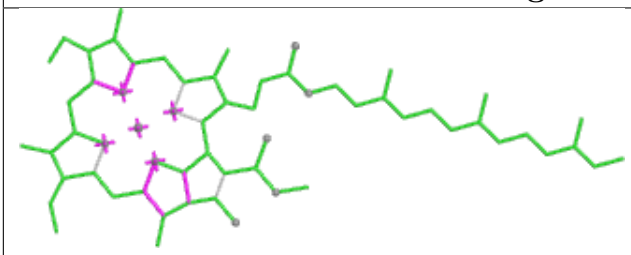


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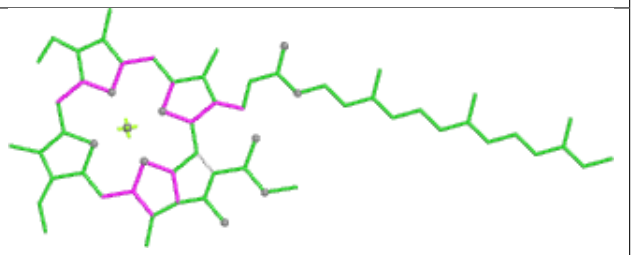


Rings

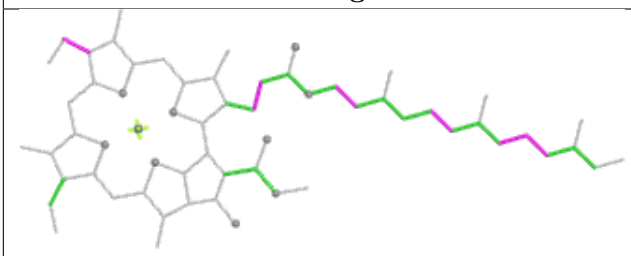
Ligand CLA b 828



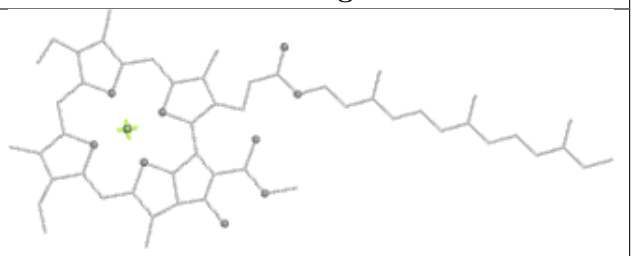
Bond lengths



Bond angles

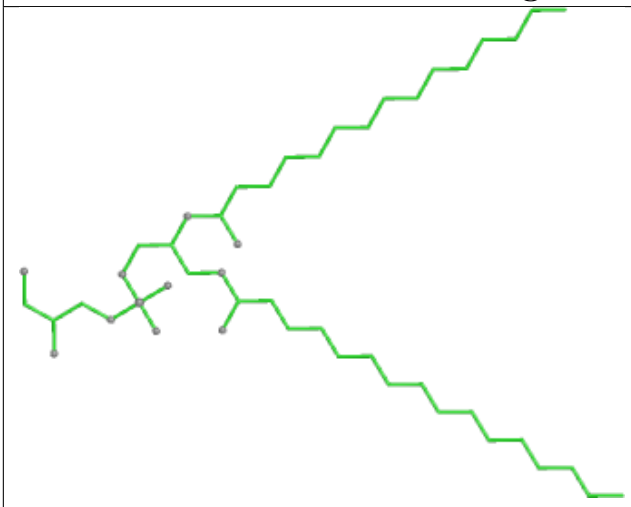


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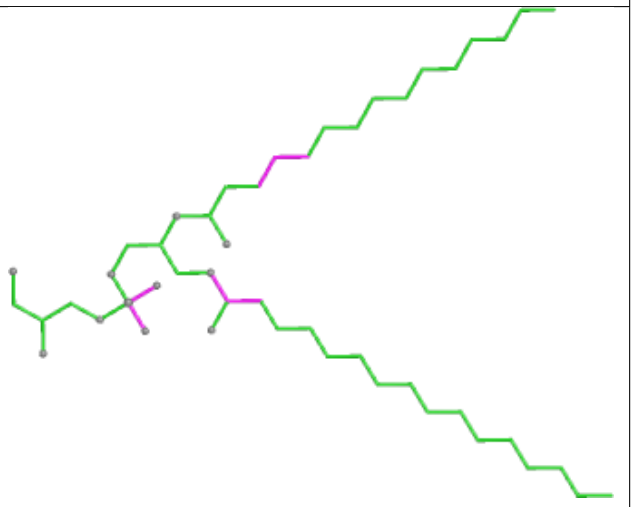


Rings

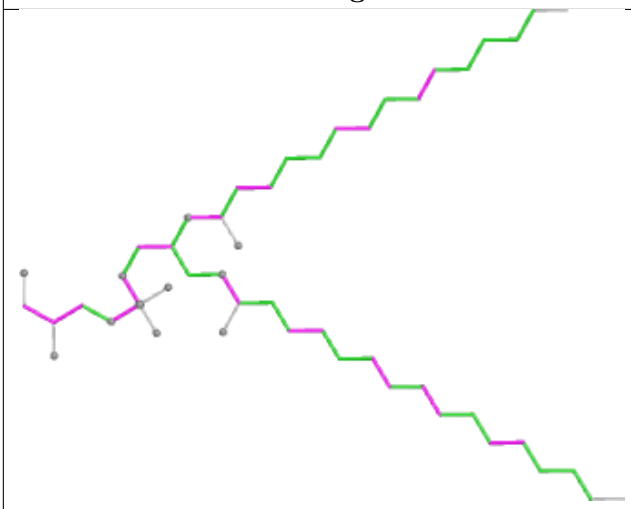
Ligand LHG D 320



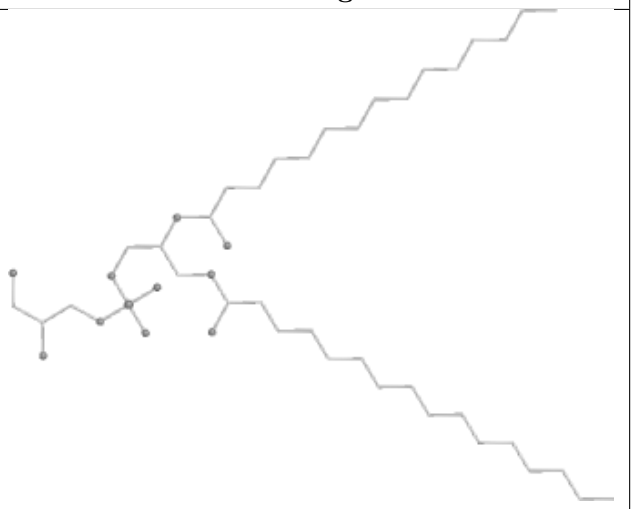
Bond lengths



Bond angles

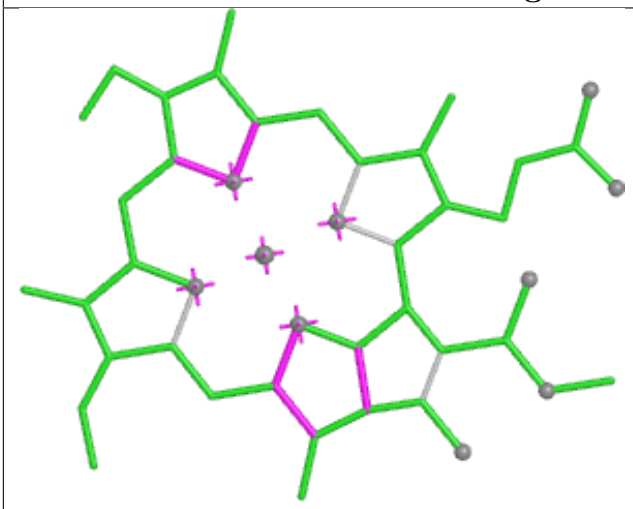


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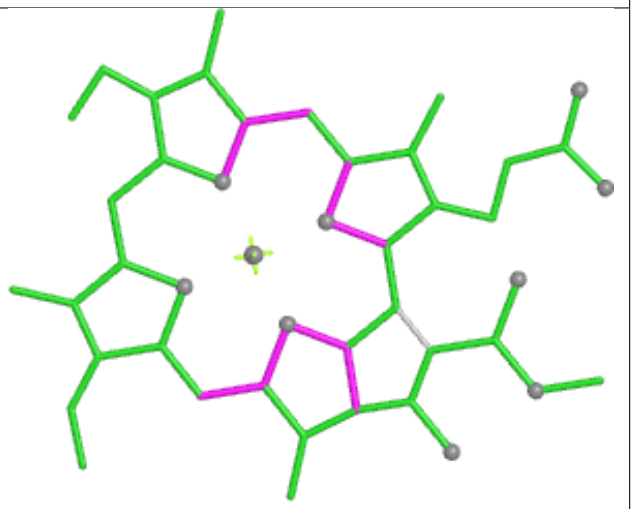


Rings

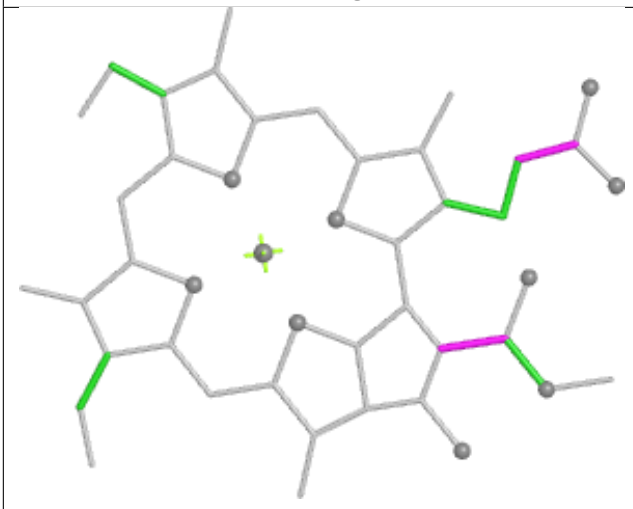
Ligand CLA B 303



Bond lengths



Bond angles

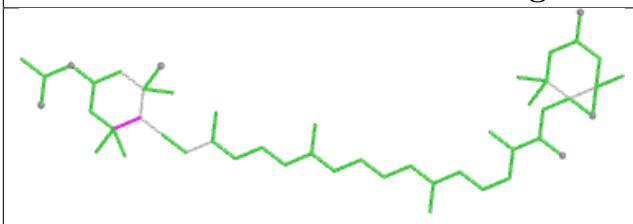


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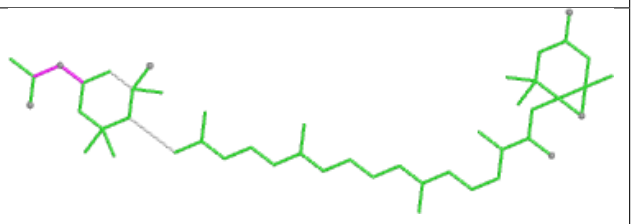


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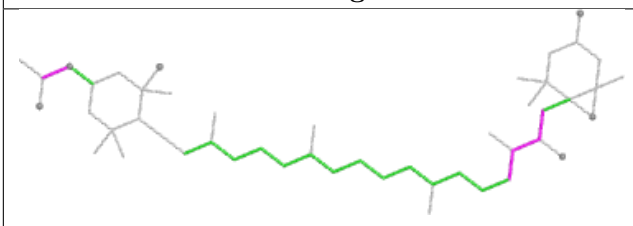
Ligand A86 K 312



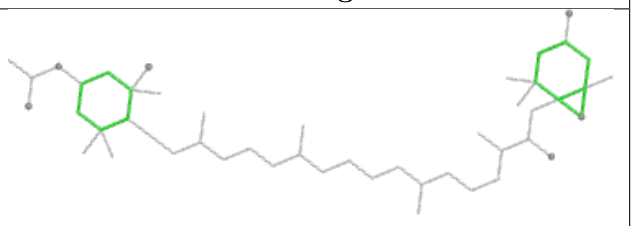
Bond lengths



Bond angles

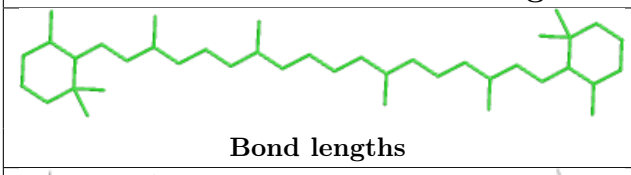


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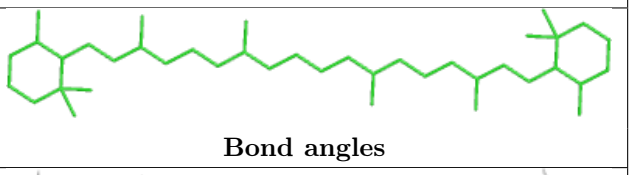


Rings

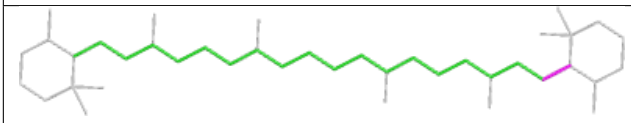
Ligand BCR a 844



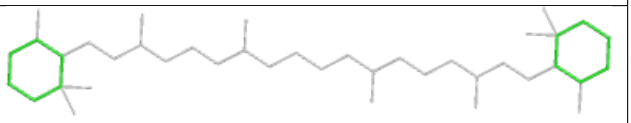
Bond lengths



Bond angles

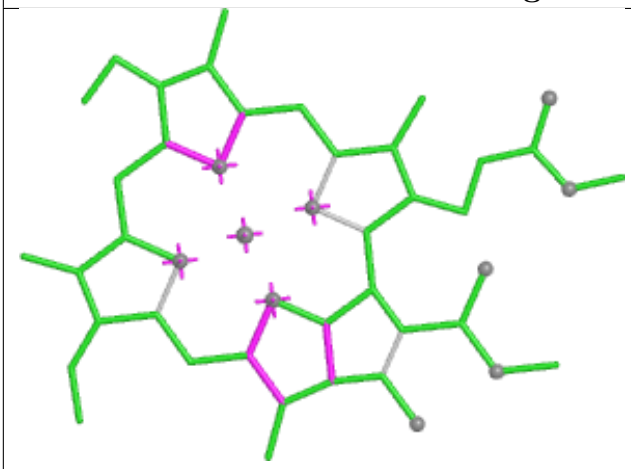


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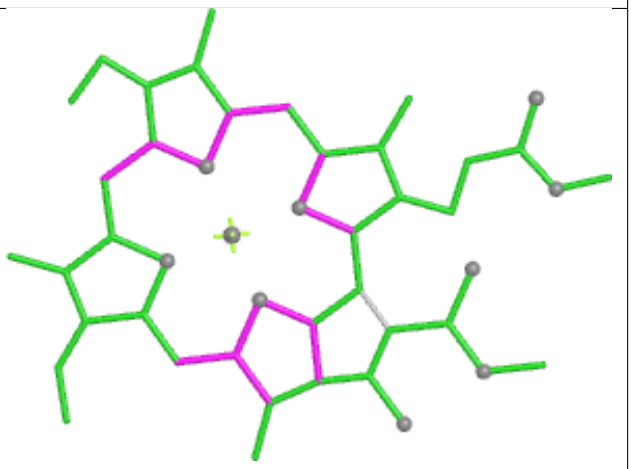


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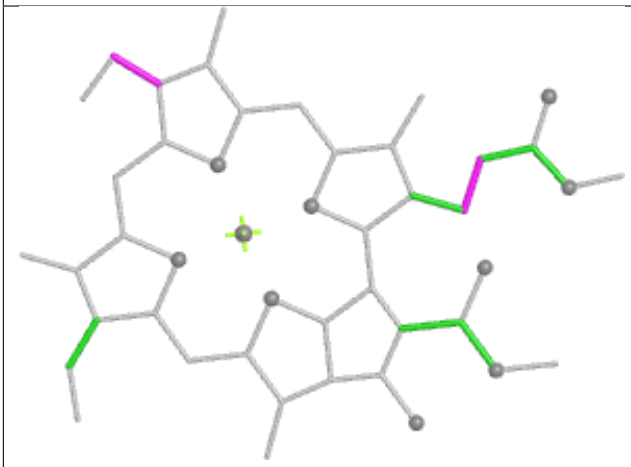
Ligand CLA H 310



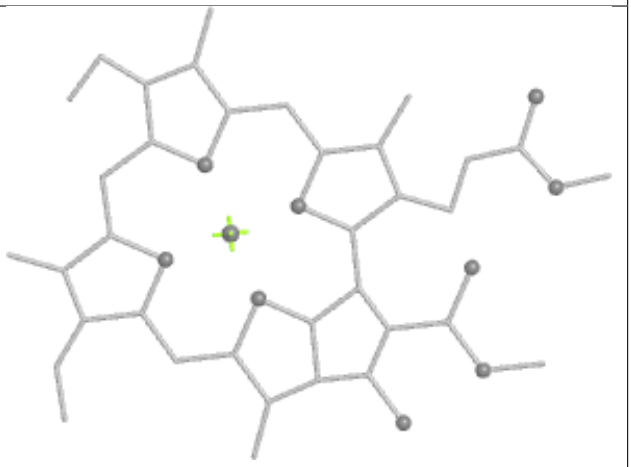
Bond lengths



Bond angles

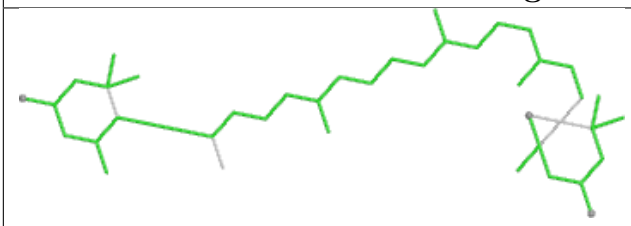


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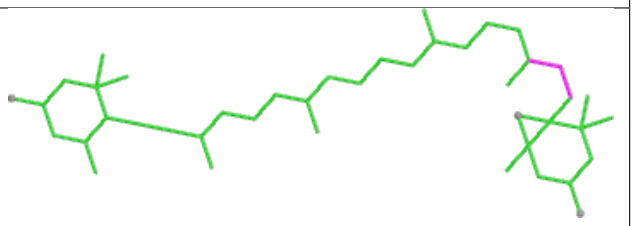


Rings

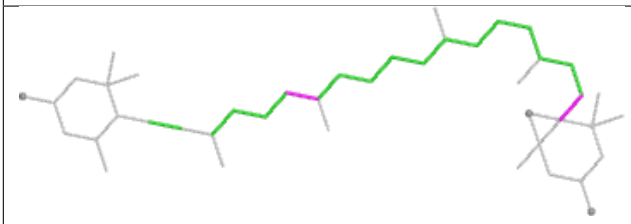
Ligand DD6 N 321



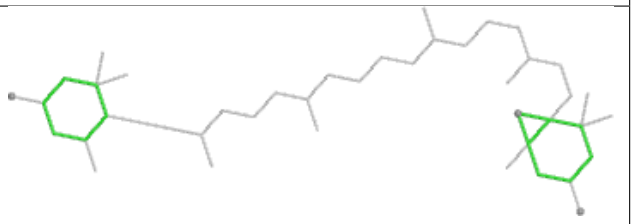
Bond lengths



Bond angles

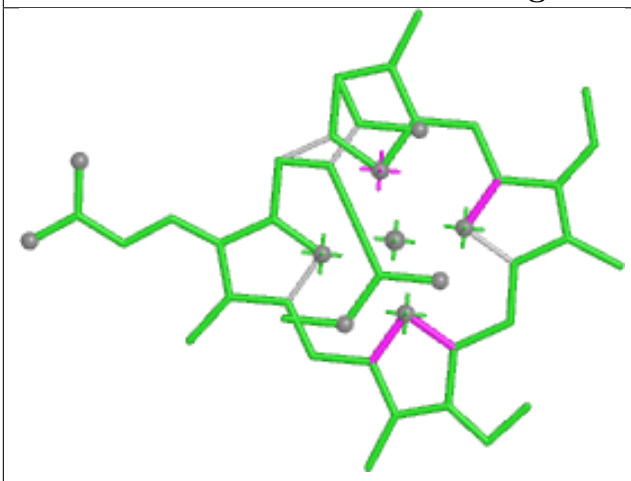


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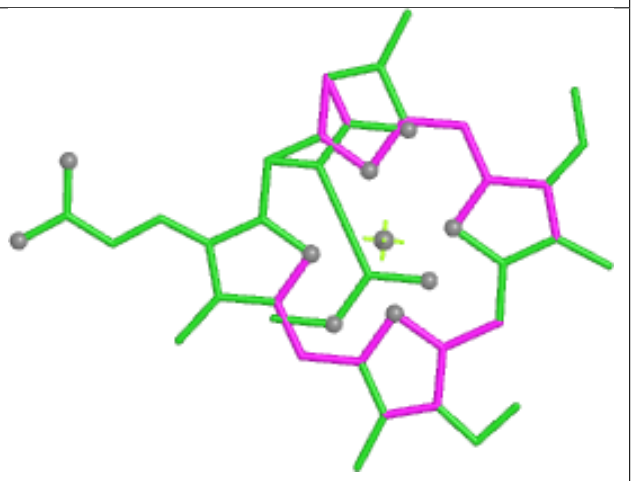


Rings

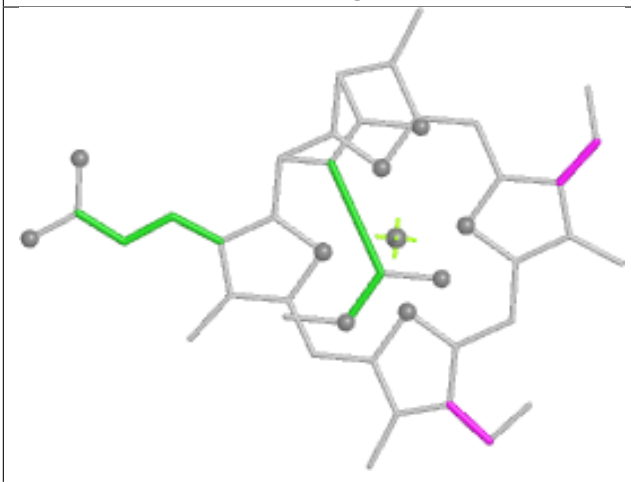
Ligand KC2 L 302



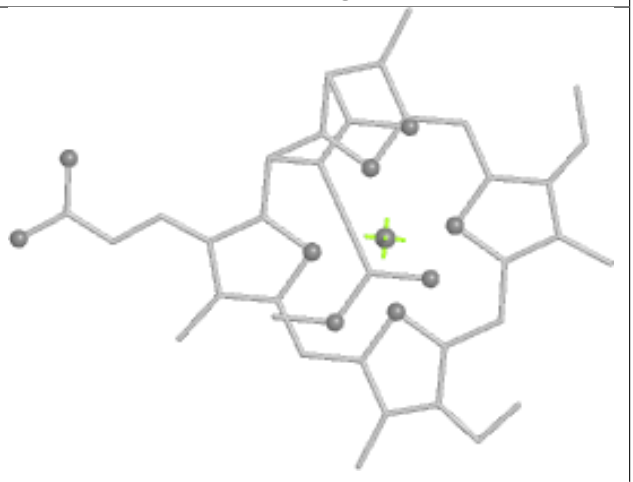
Bond lengths



Bond angles

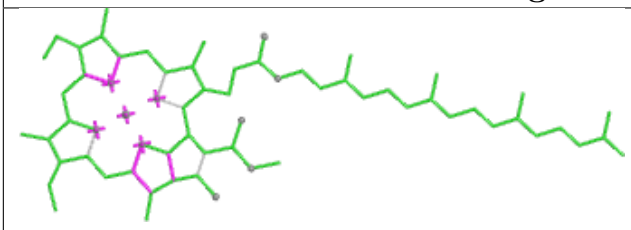


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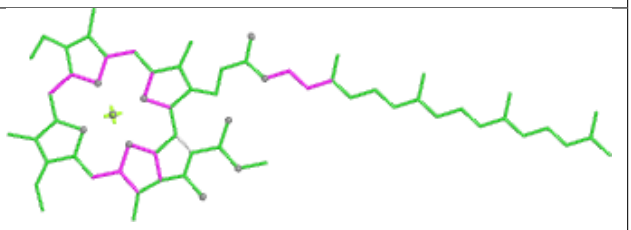


Rings

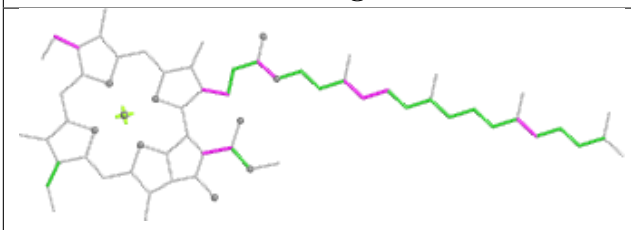
Ligand CLA a 820



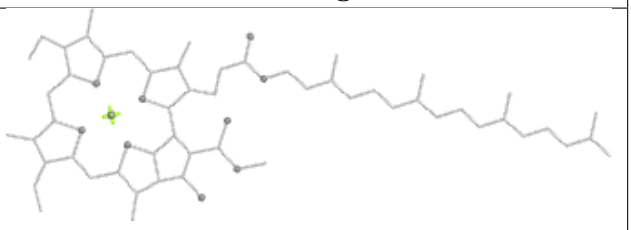
Bond lengths



Bond angles

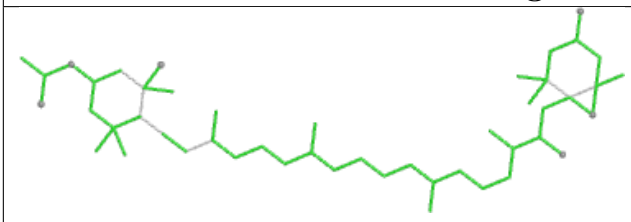


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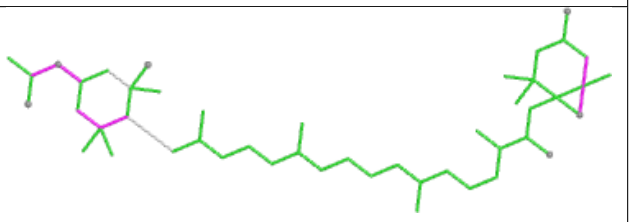


Rings

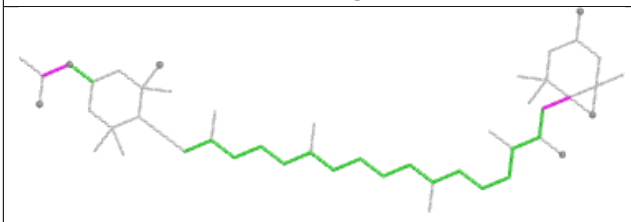
Ligand A86 M 315



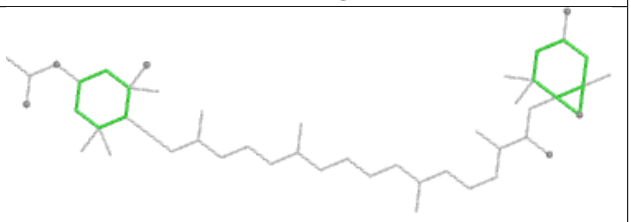
Bond lengths



Bond angles

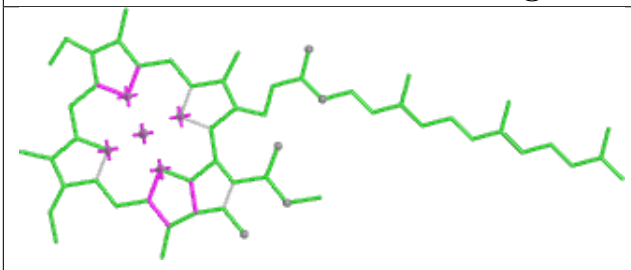


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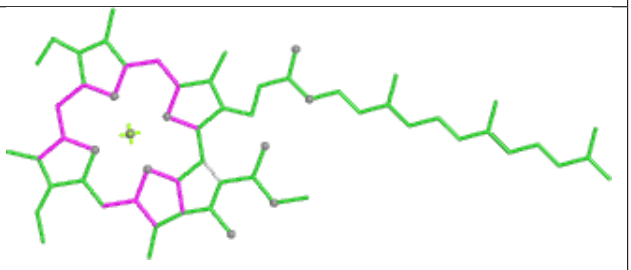


Rings

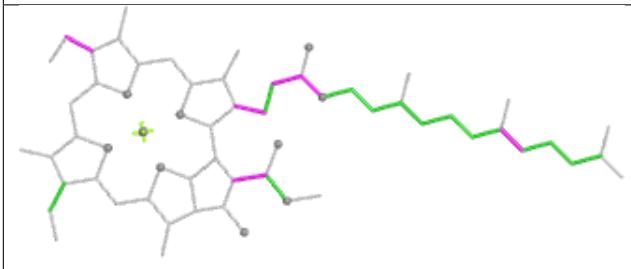
Ligand CLA D 306



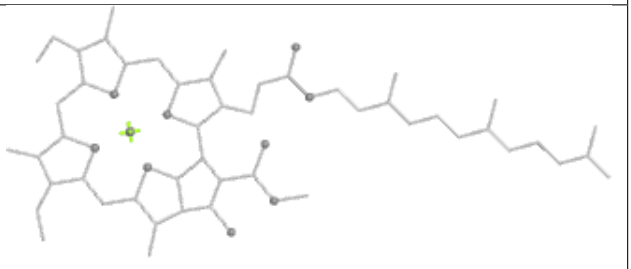
Bond lengths



Bond angles

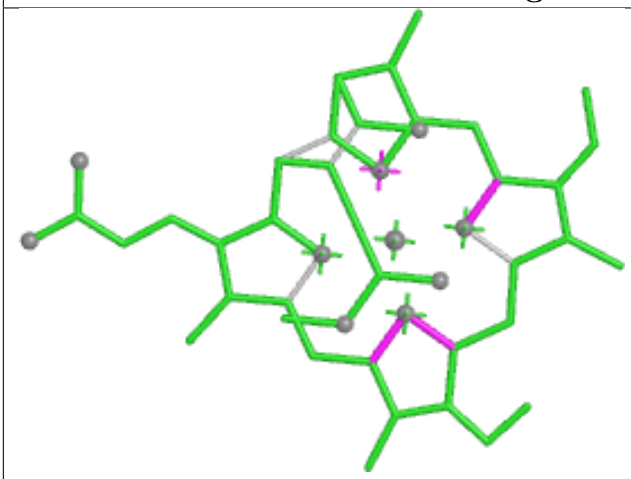


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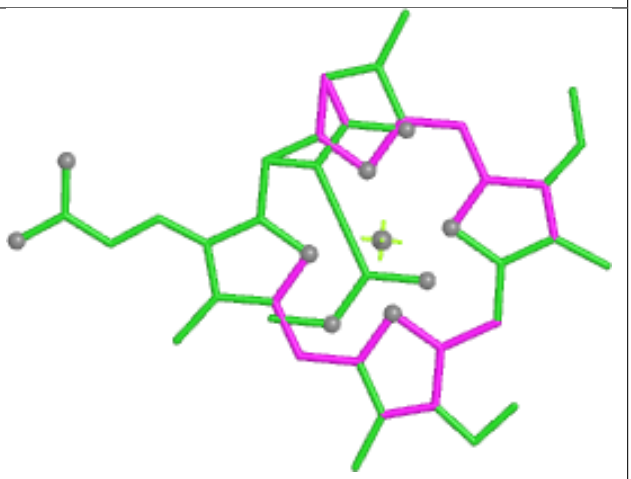


Rings

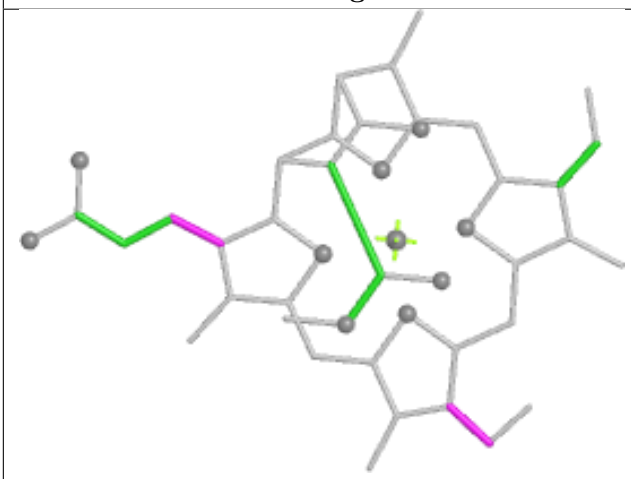
Ligand KC2 R 311



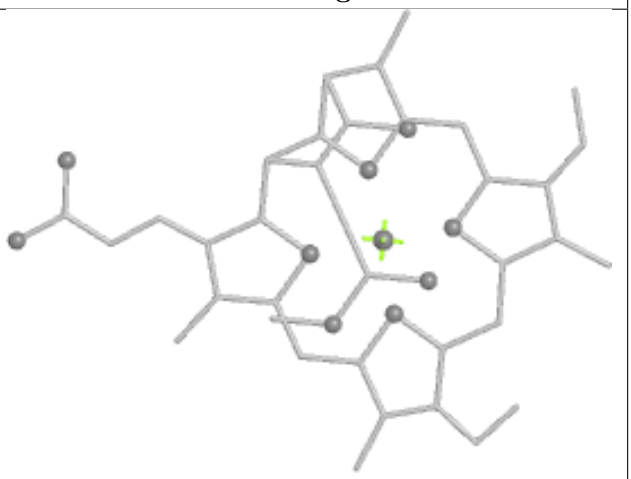
Bond lengths



Bond angles

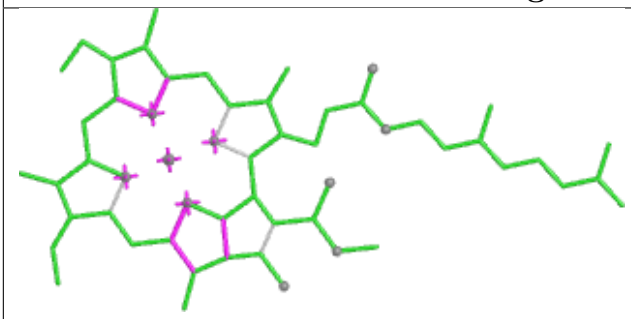


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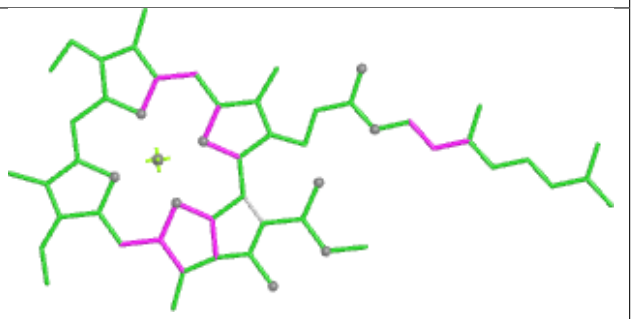


Rings

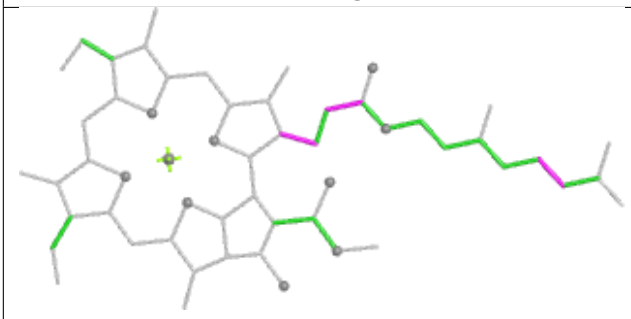
Ligand CLA b 821



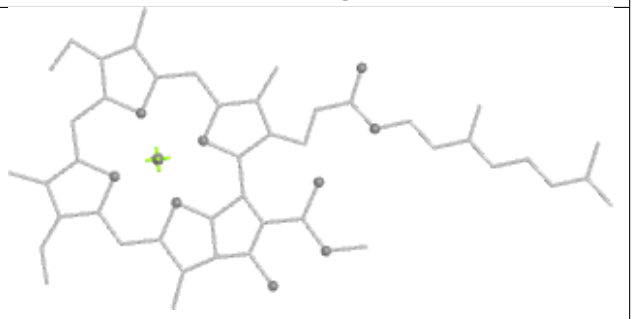
Bond lengths



Bond angles

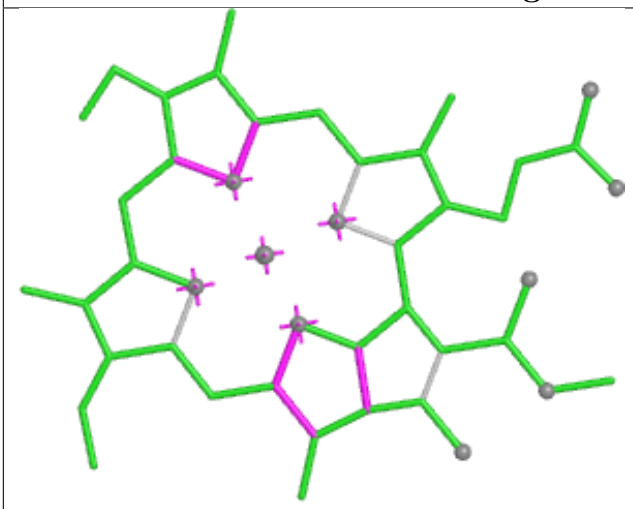


Torsions

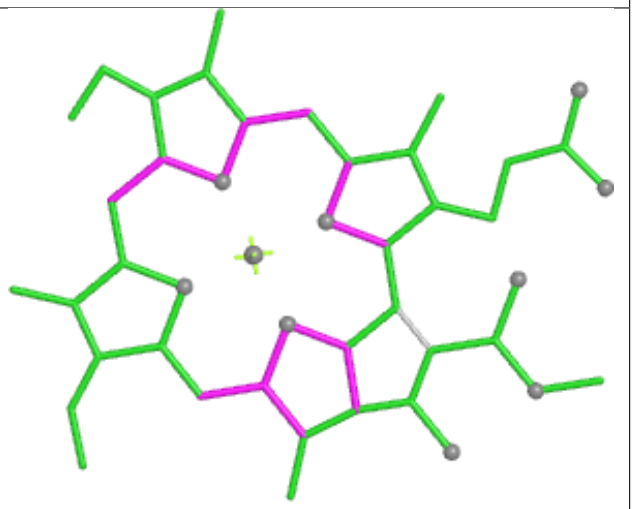


Rings

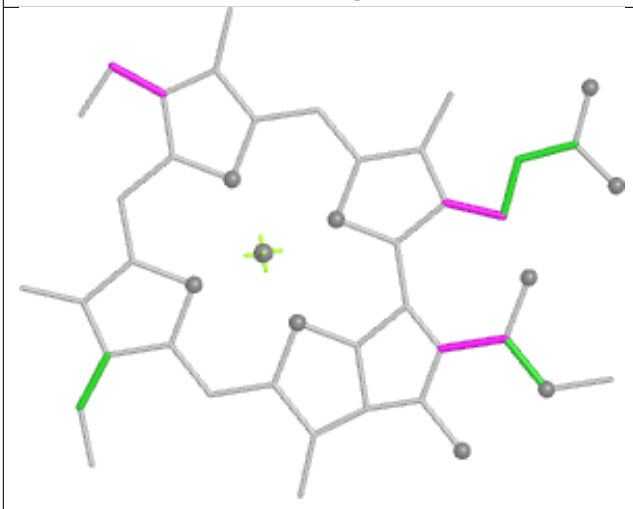
Ligand CLA K 304



Bond lengths



Bond angles

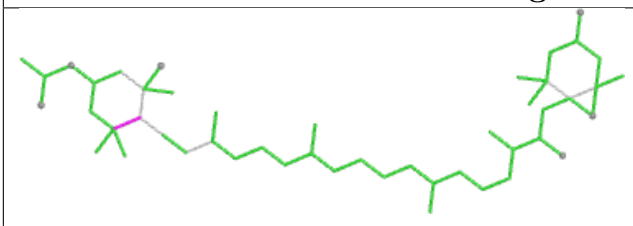


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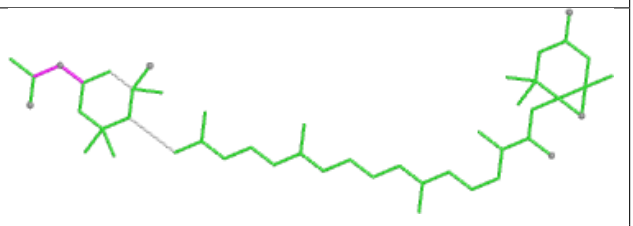


Rings

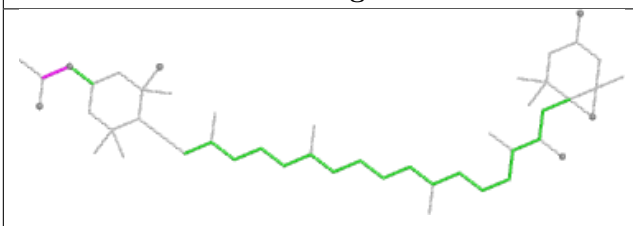
Ligand A86 N 315



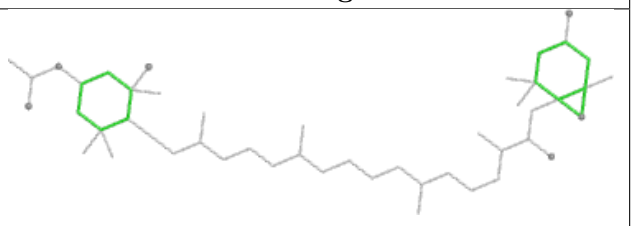
Bond lengths



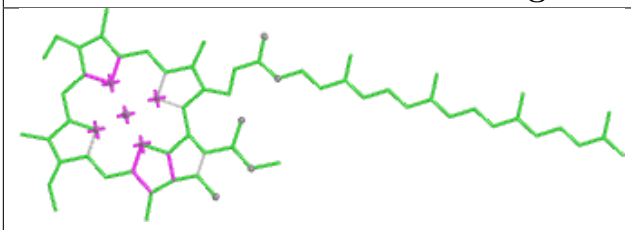
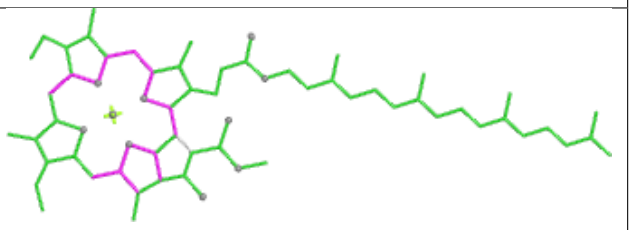
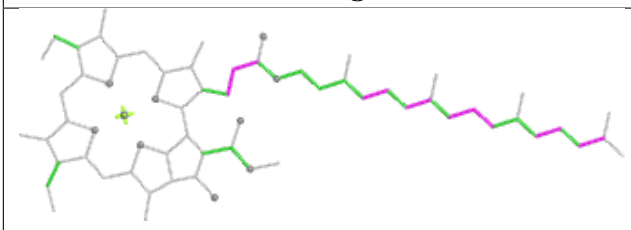
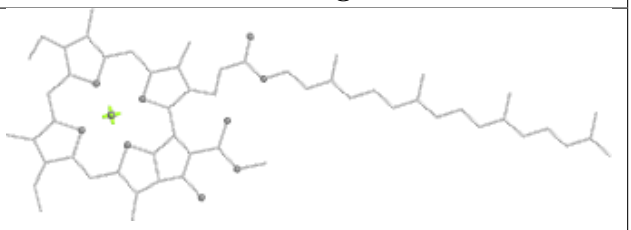
Bond angles

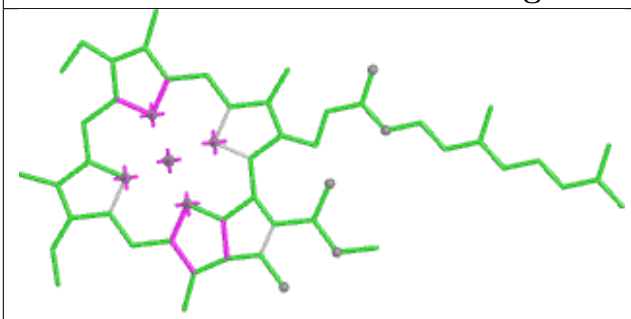
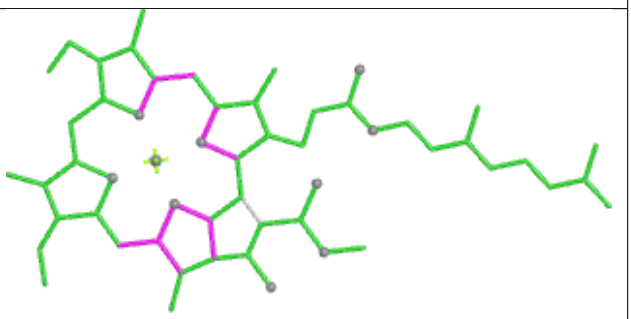
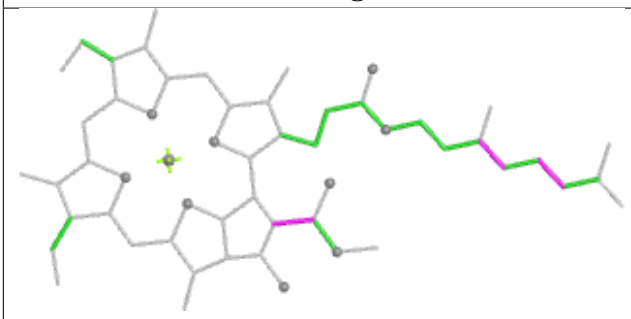
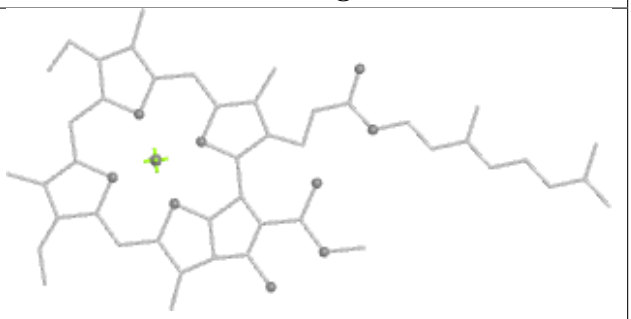


Torsions

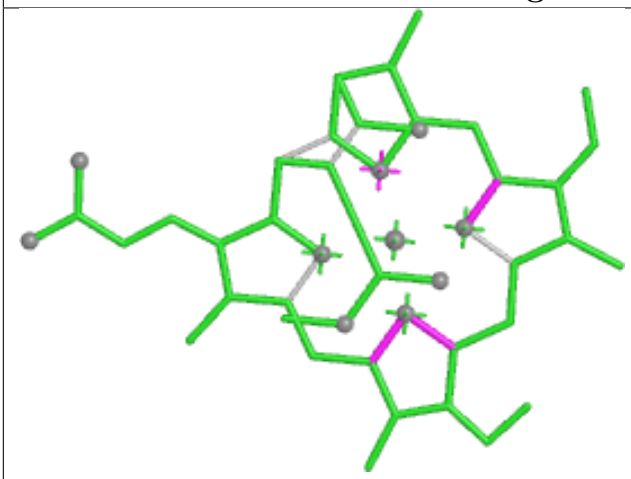


Rings

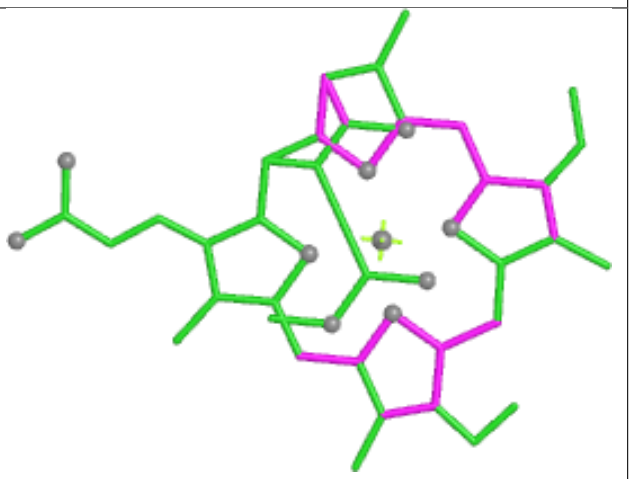
Ligand CLA a 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

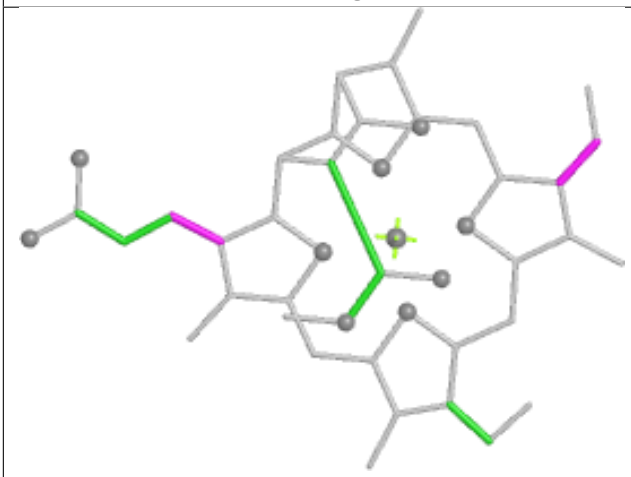
Ligand KC2 T 304



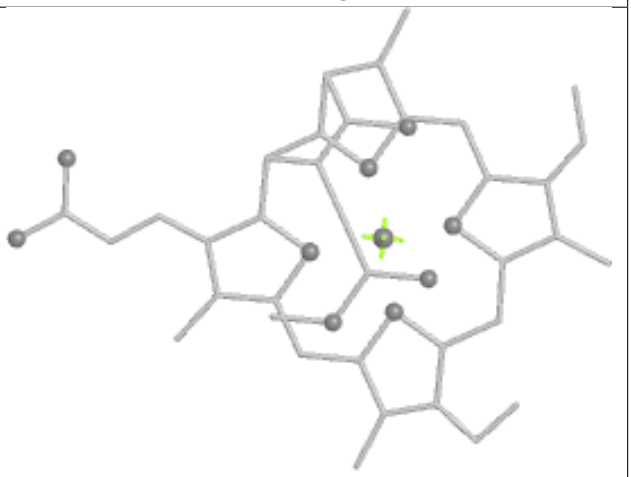
Bond lengths



Bond angles

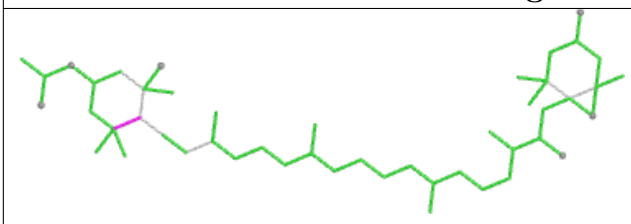


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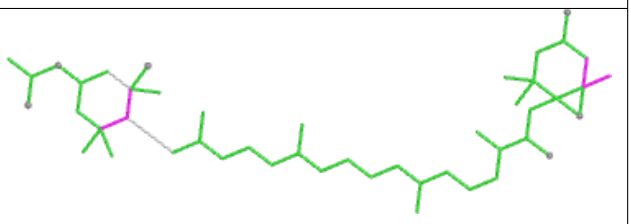


Rings

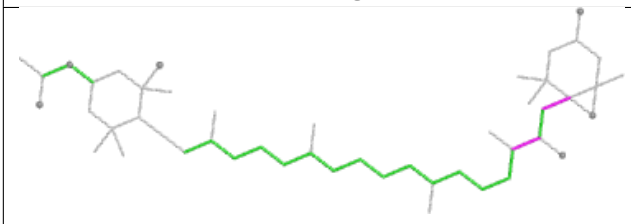
Ligand A86 M 314



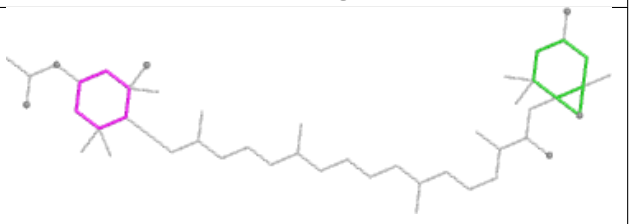
Bond lengths



Bond angles

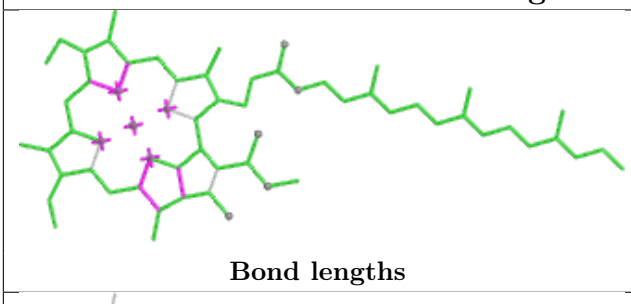


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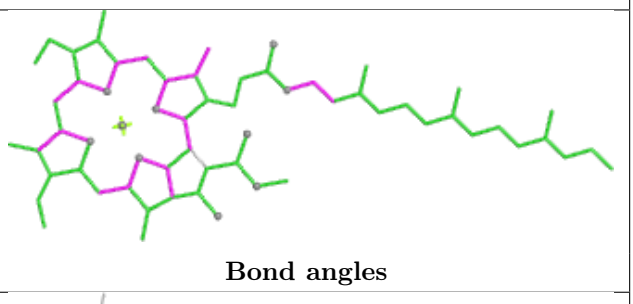


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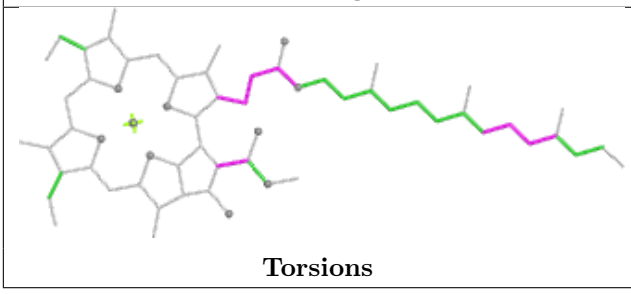
Ligand CLA a 822



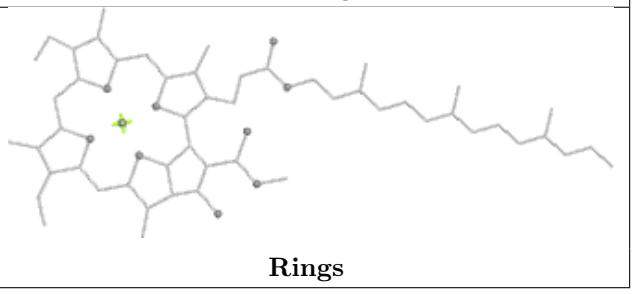
Bond lengths



Bond angles

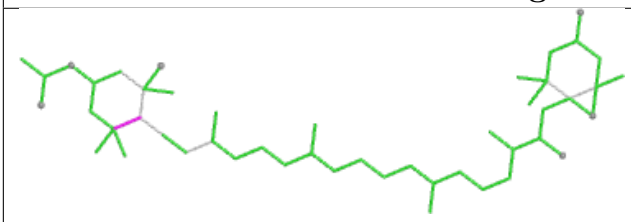


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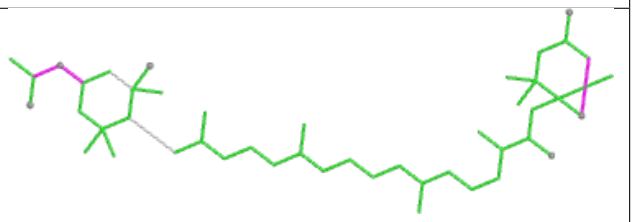


Rings

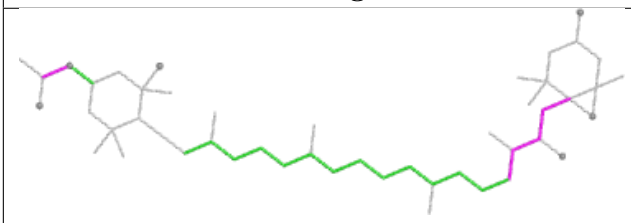
Ligand A86 N 317



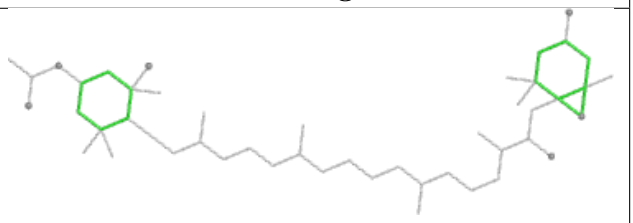
Bond lengths



Bond angles

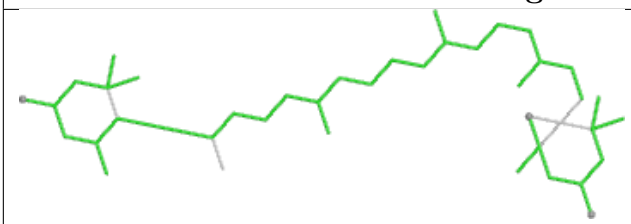


Torsions



Rings

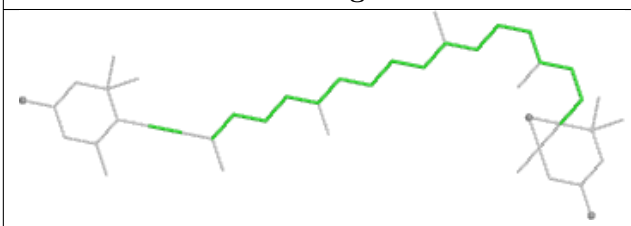
Ligand DD6 P 315



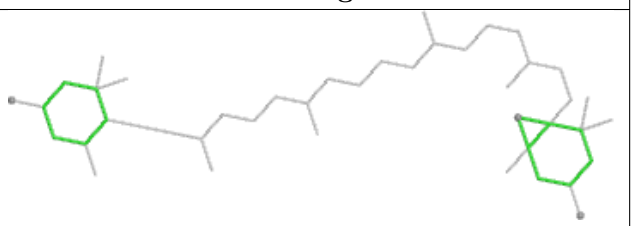
Bond lengths



Bond angles

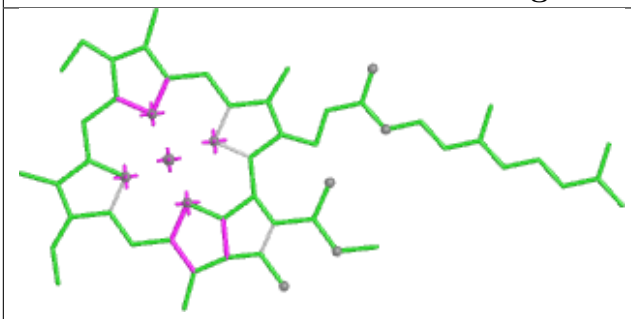


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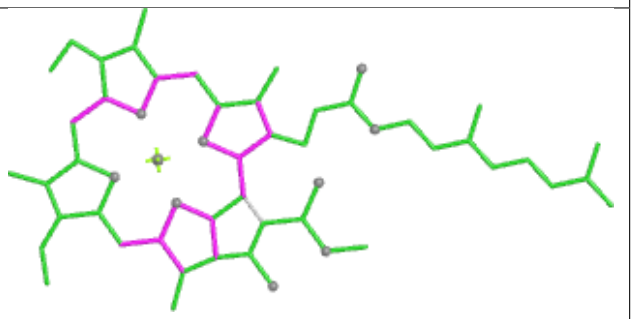


Rings

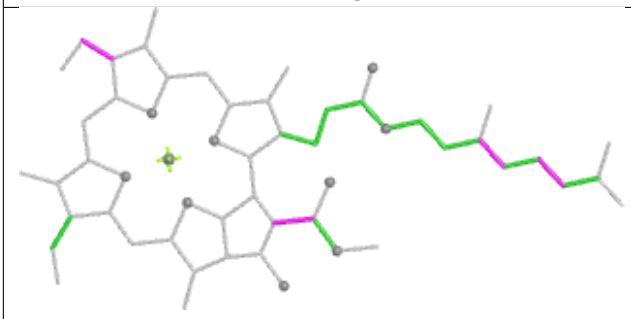
Ligand CLA I 303



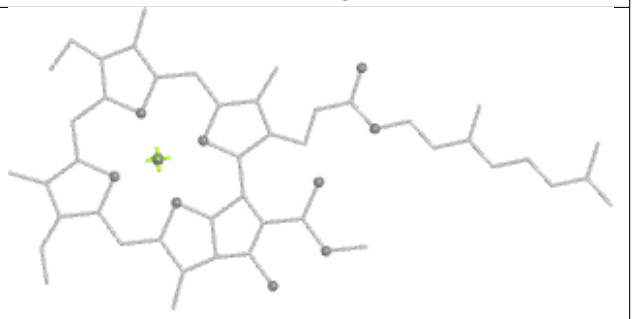
Bond lengths



Bond angles

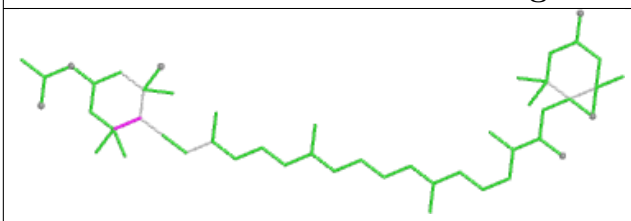


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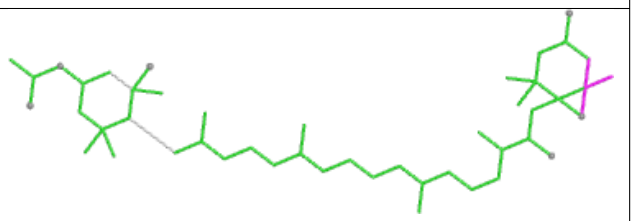


Rings

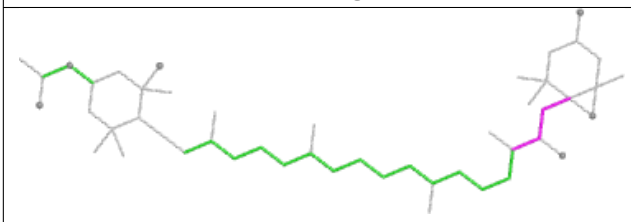
Ligand A86 R 313



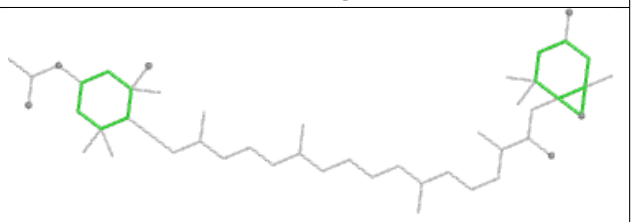
Bond lengths



Bond angles

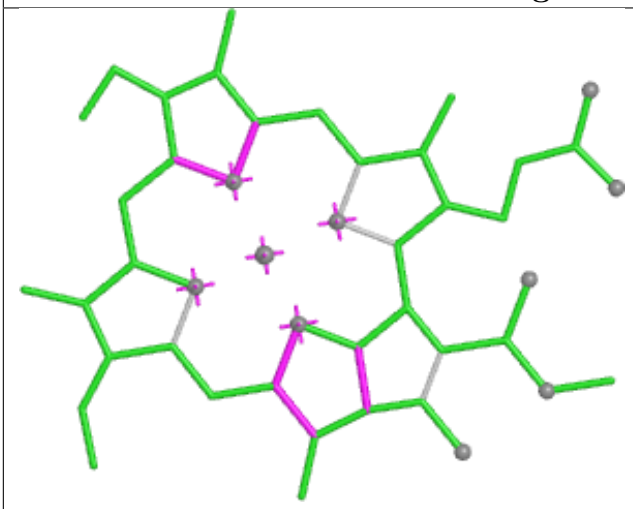


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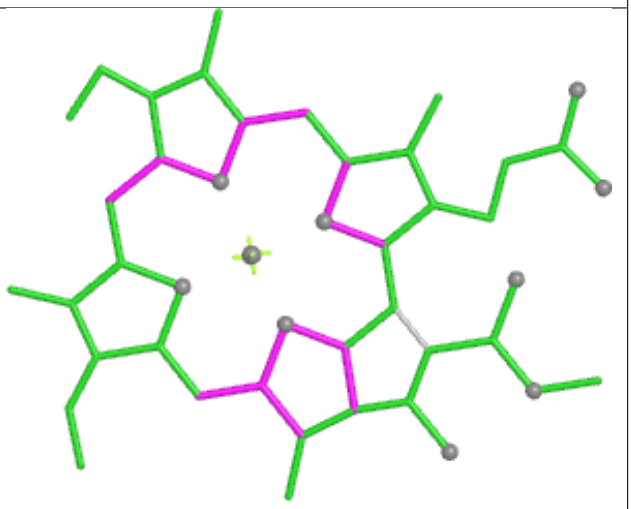


Rings

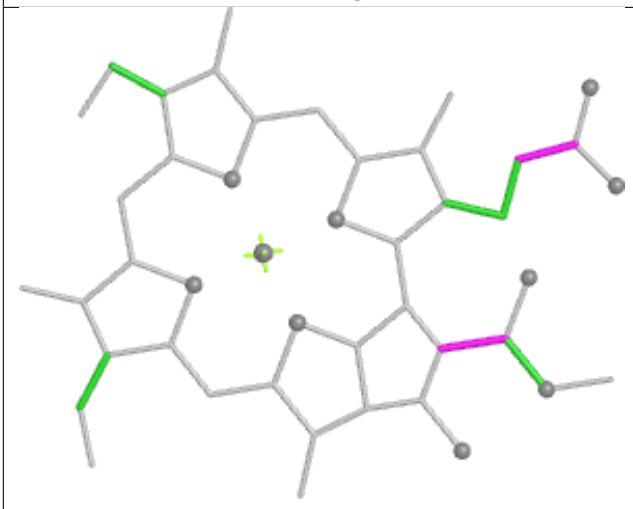
Ligand CLA l 202



Bond lengths



Bond angles

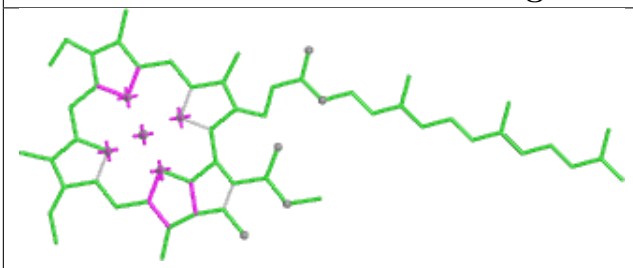


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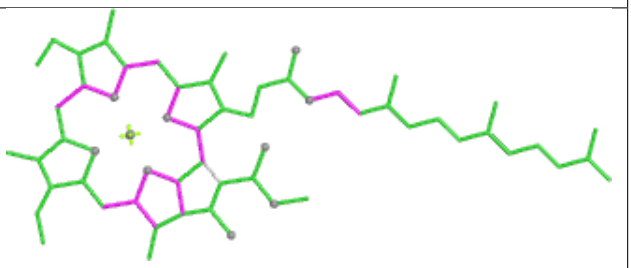


Rings

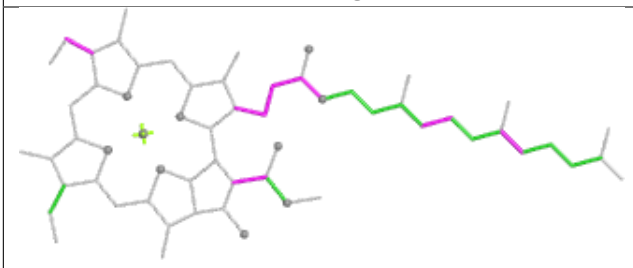
Ligand CLA F 322



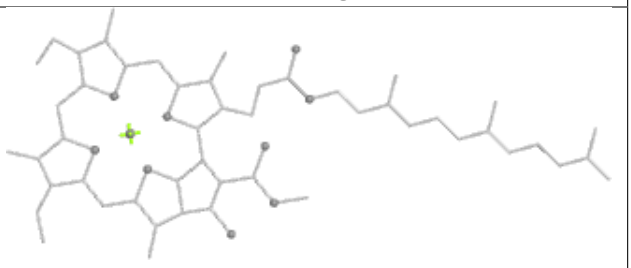
Bond lengths



Bond angles

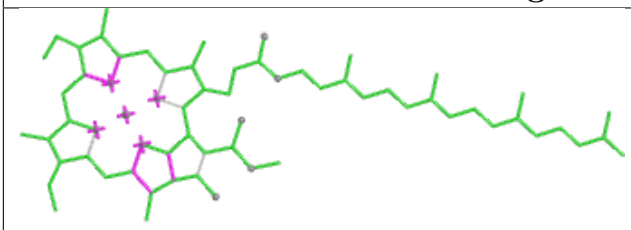


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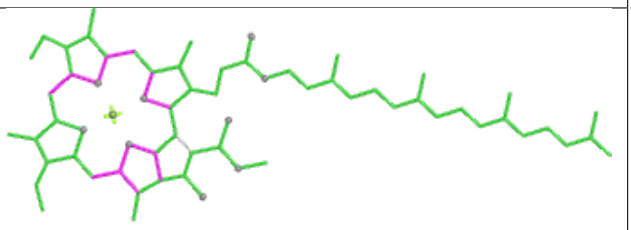


Rings

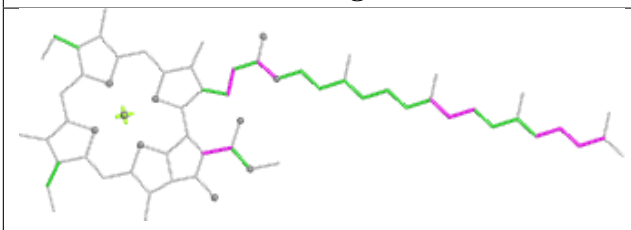
Ligand CLA b 806



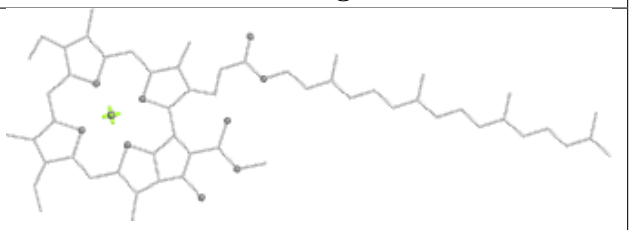
Bond lengths



Bond angles

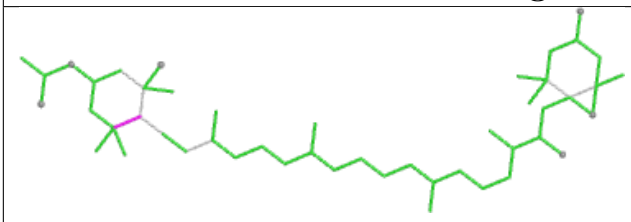


Torsions

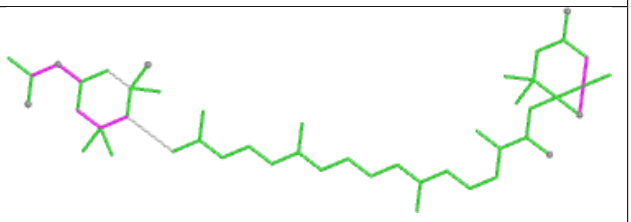


Rings

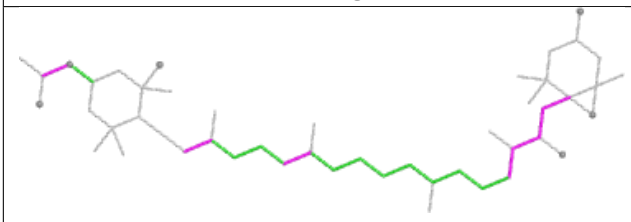
Ligand A86 N 316



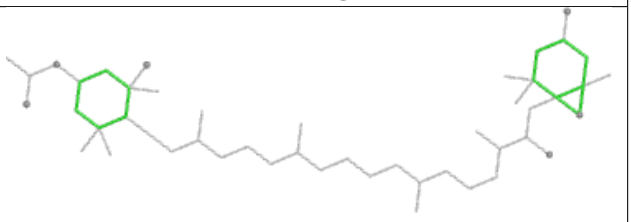
Bond lengths



Bond angles

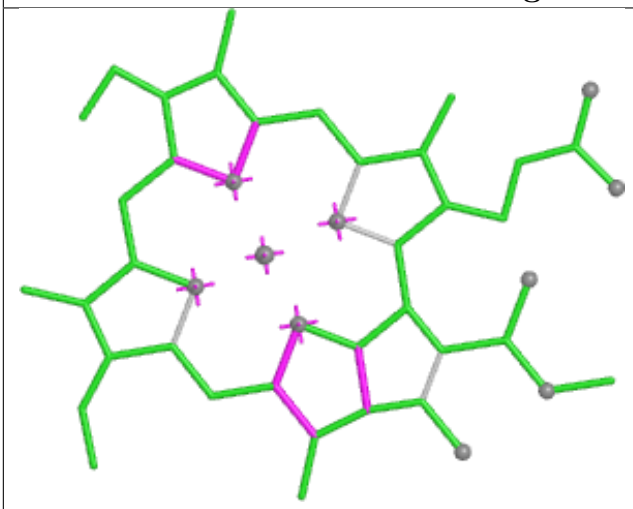


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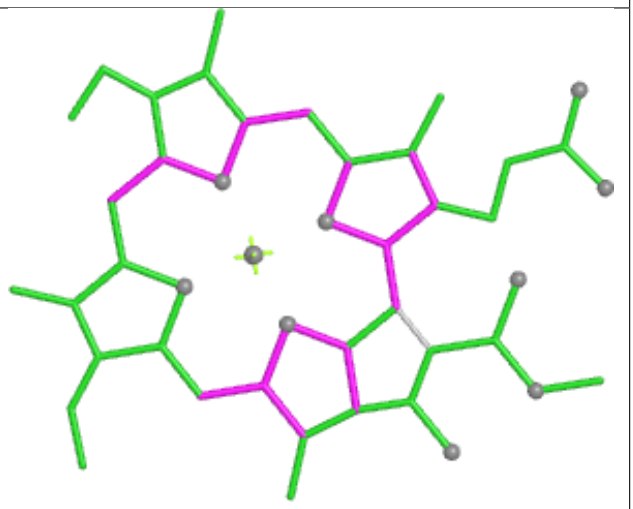


Rings

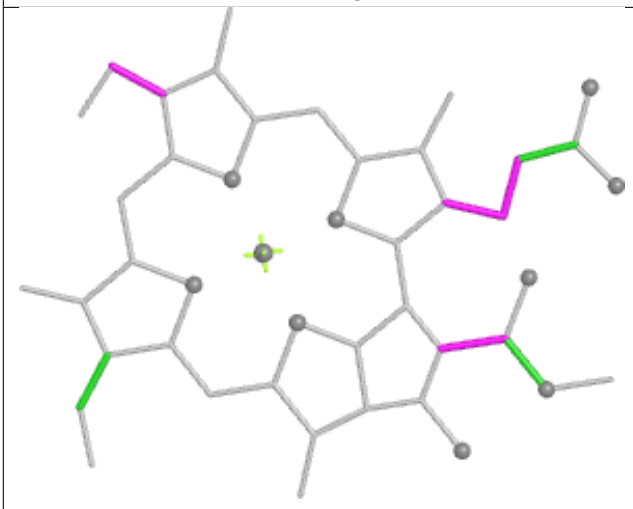
Ligand CLA H 301



Bond lengths



Bond angles

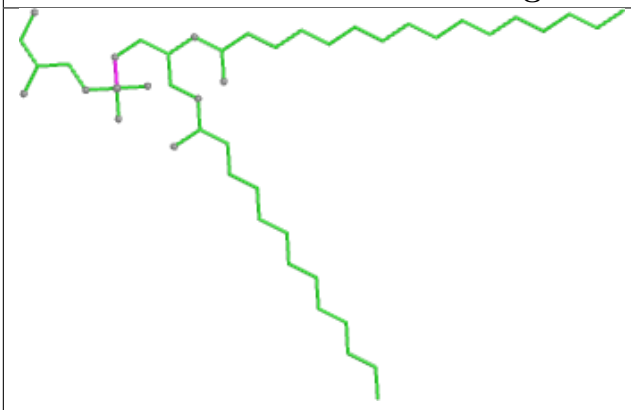


Torsions

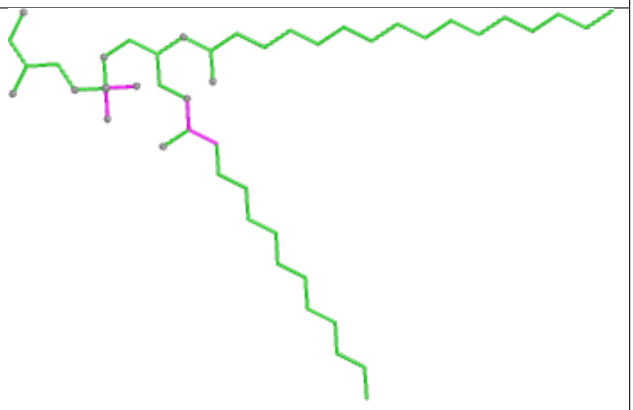


Rings

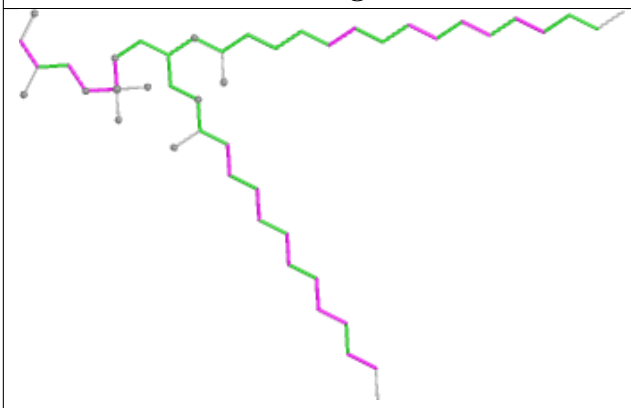
Ligand LHG E 301



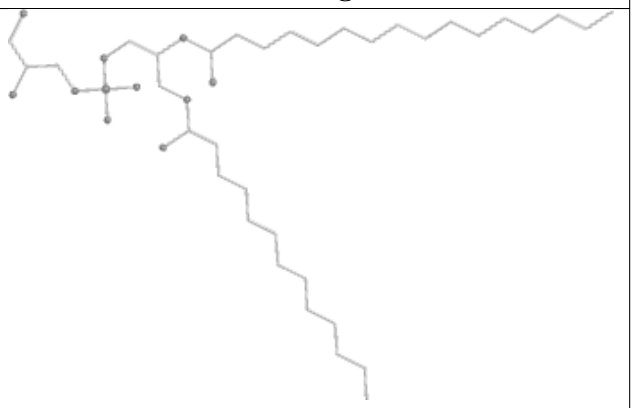
Bond lengths



Bond angles

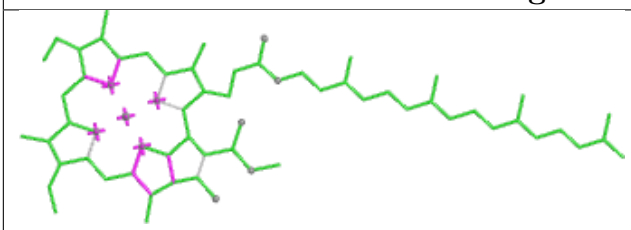


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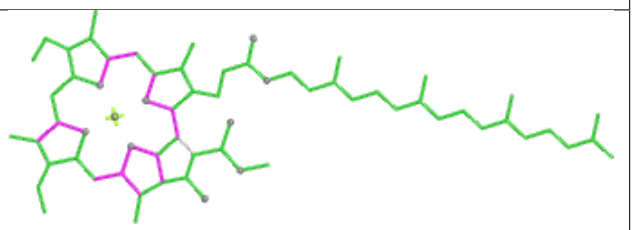


Rings

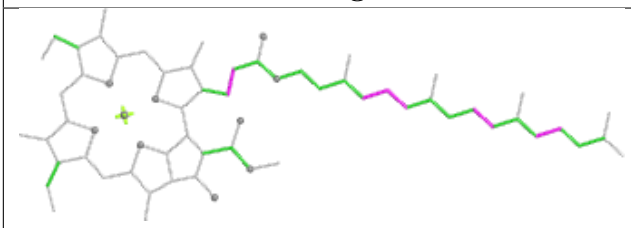
Ligand CLA a 823



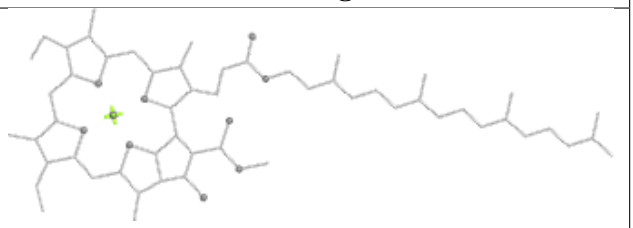
Bond lengths



Bond angles

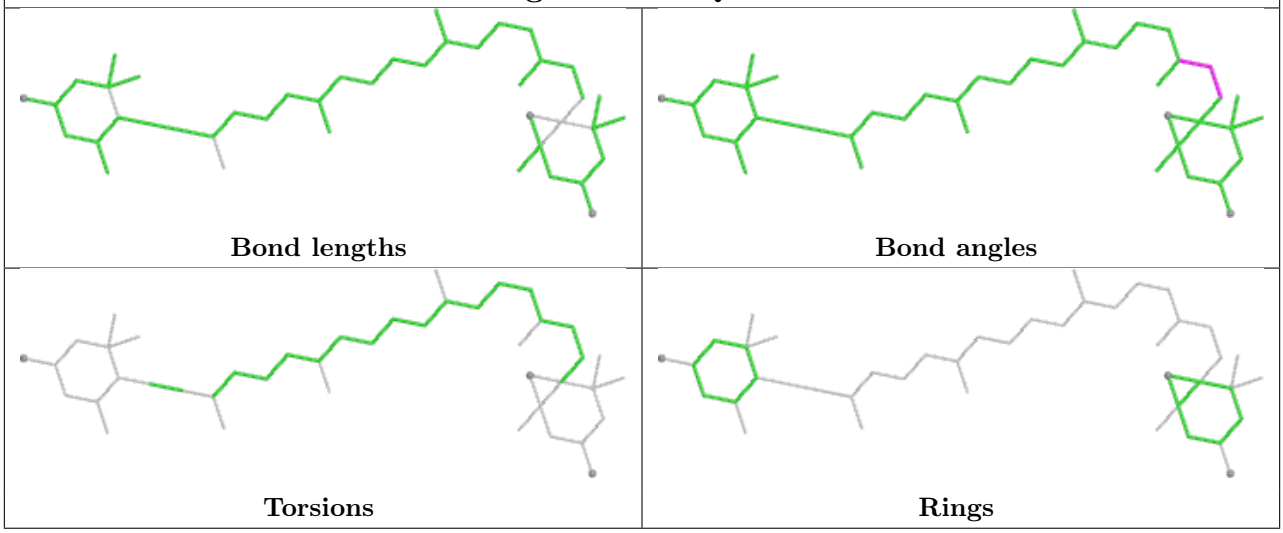


Torsions

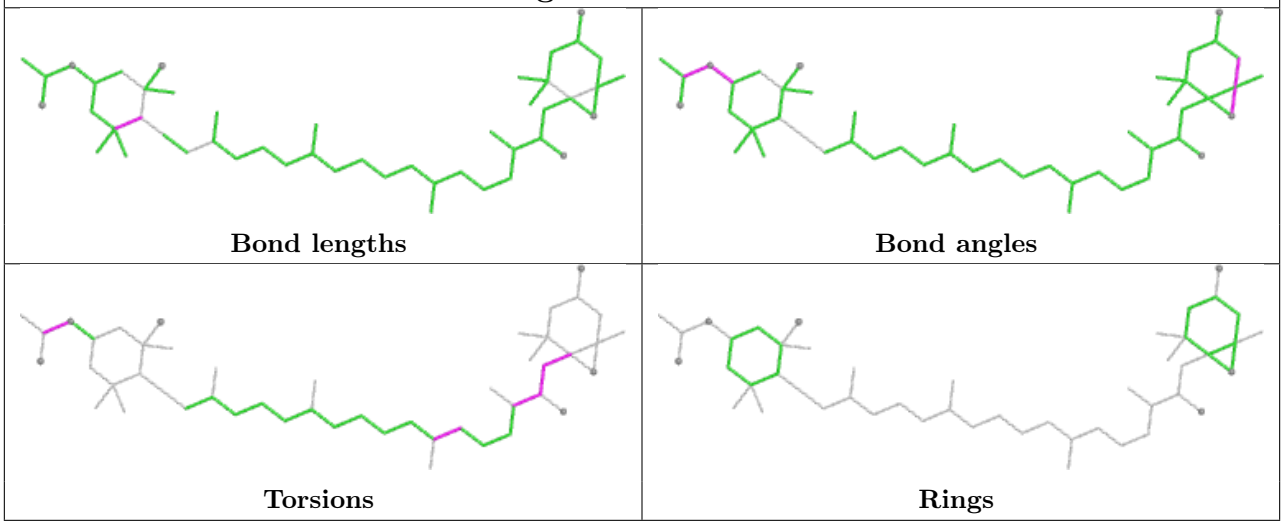


Rings

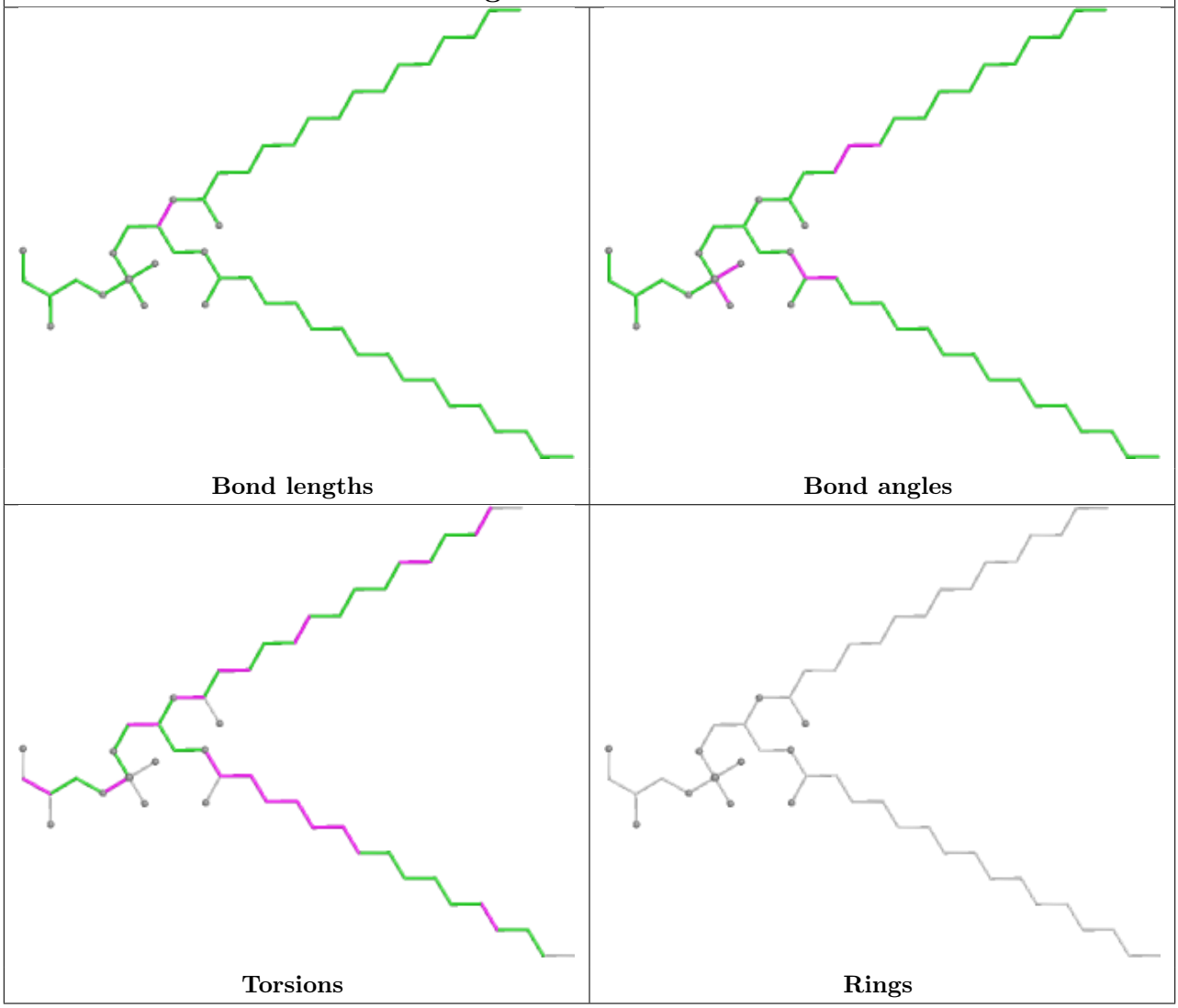
Ligand DD6 Q 313



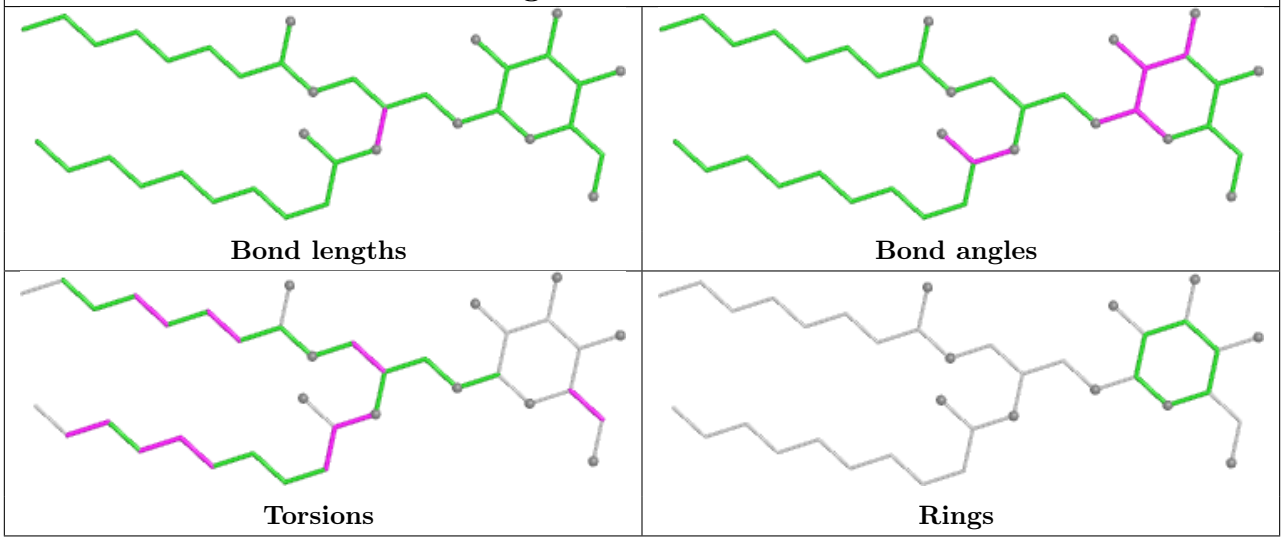
Ligand A86 r 204



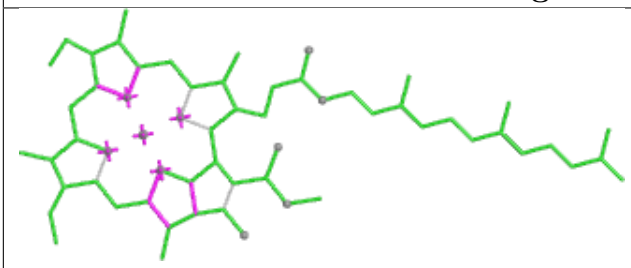
Ligand LHG a 849



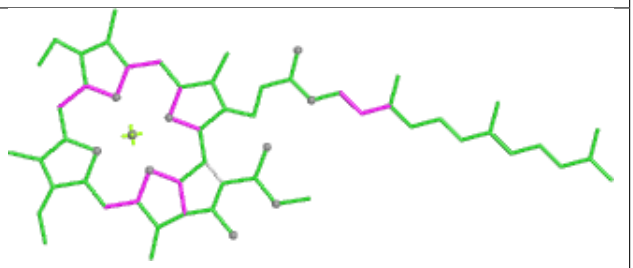
Ligand LMG L 320



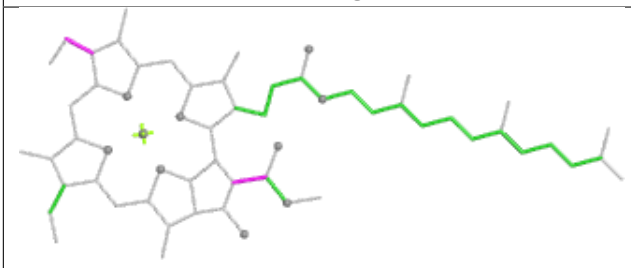
Ligand CLA f 201



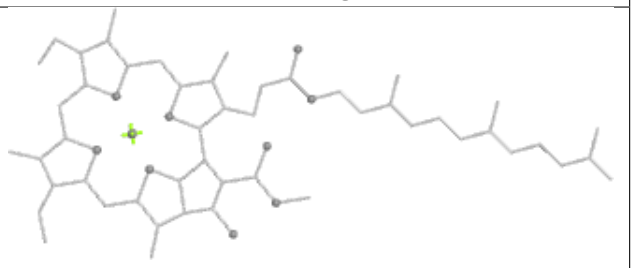
Bond lengths



Bond angles

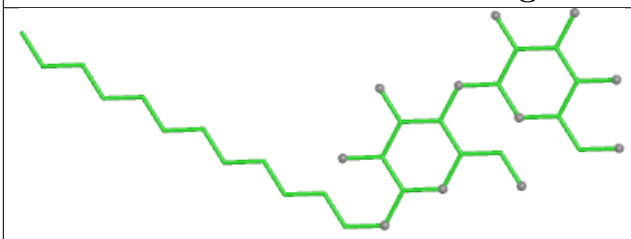


Torsions

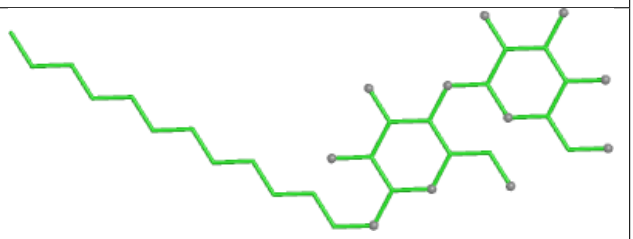


Rings

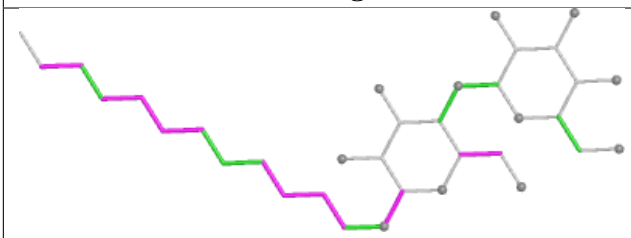
Ligand LMU D 324



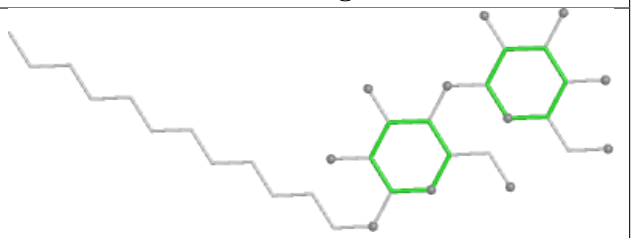
Bond lengths



Bond angles

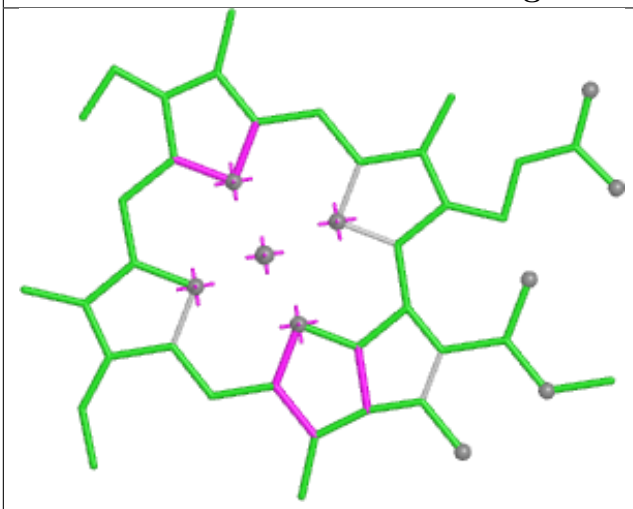


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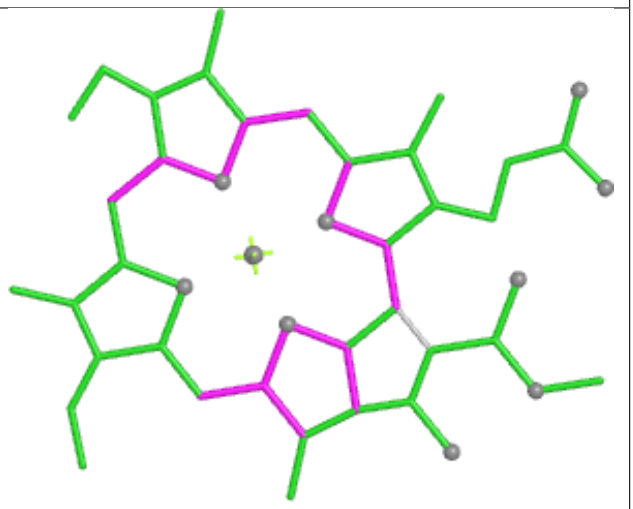


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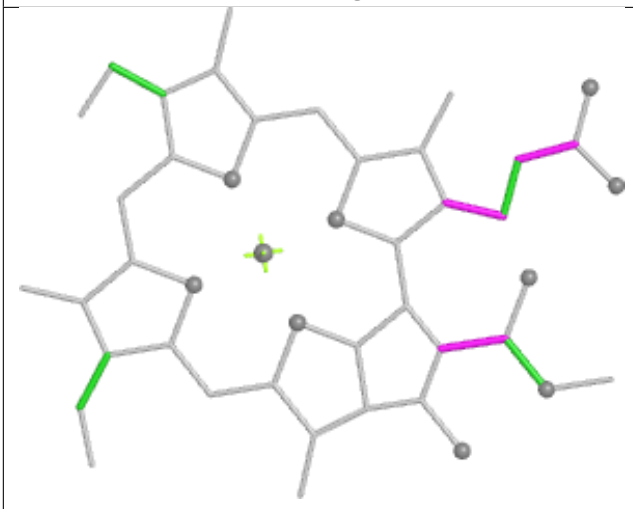
Ligand CLA U 307



Bond lengths



Bond angles

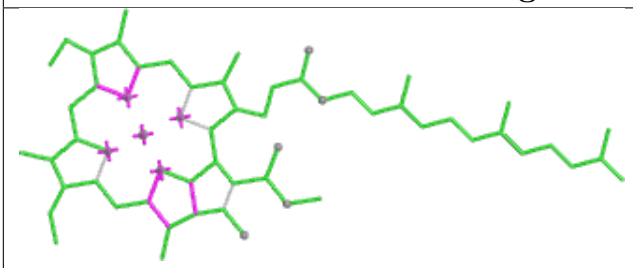


Torsions

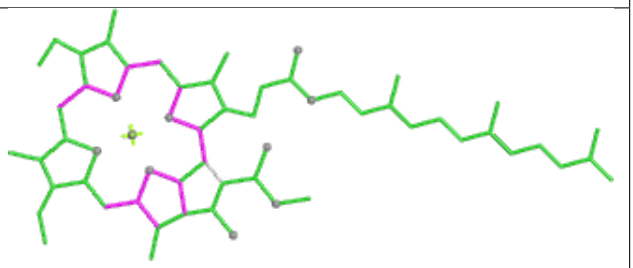


Rings

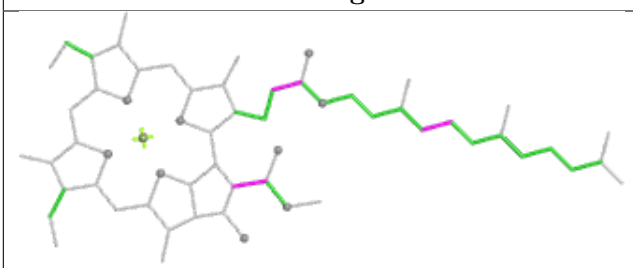
Ligand CLA W 313



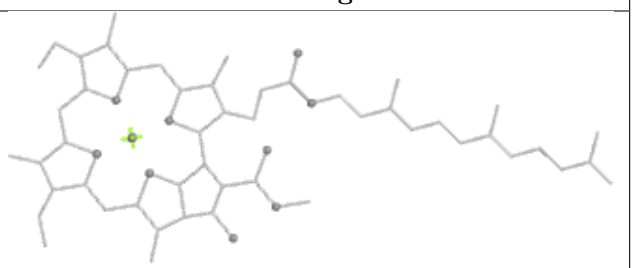
Bond lengths



Bond angles

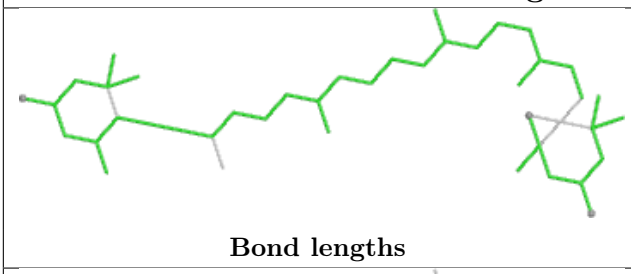


Torsions

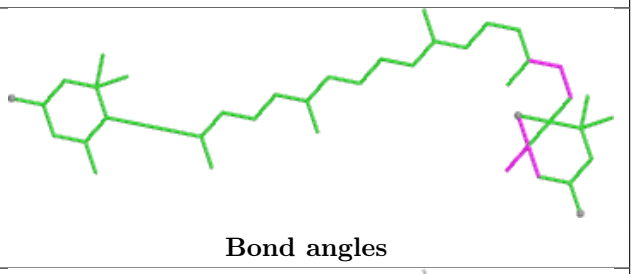


Rings

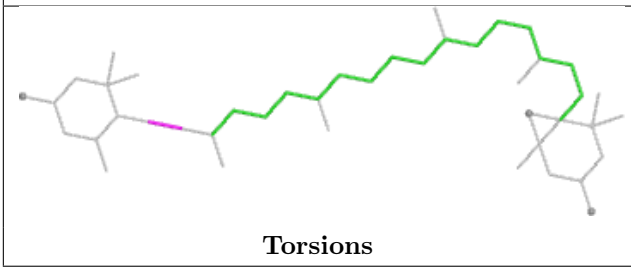
Ligand DD6 E 318



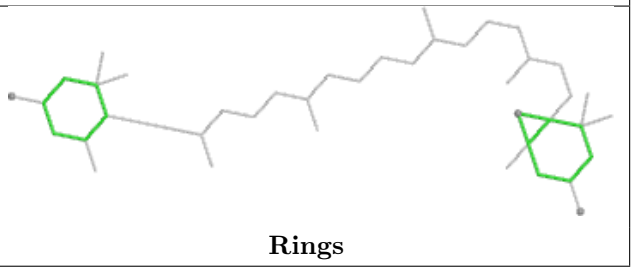
Bond lengths



Bond angles

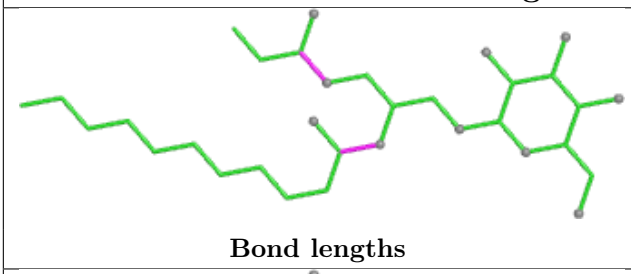


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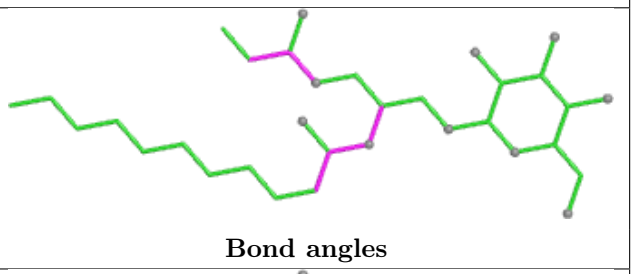


Rings

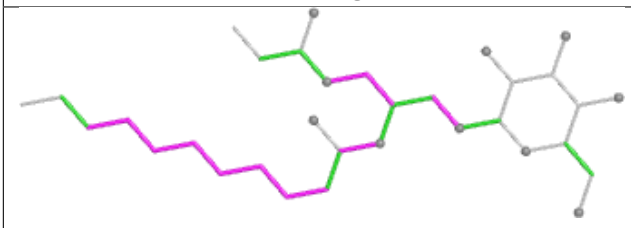
Ligand LMG S 322



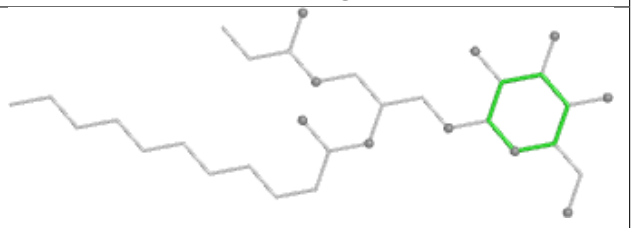
Bond lengths



Bond angles

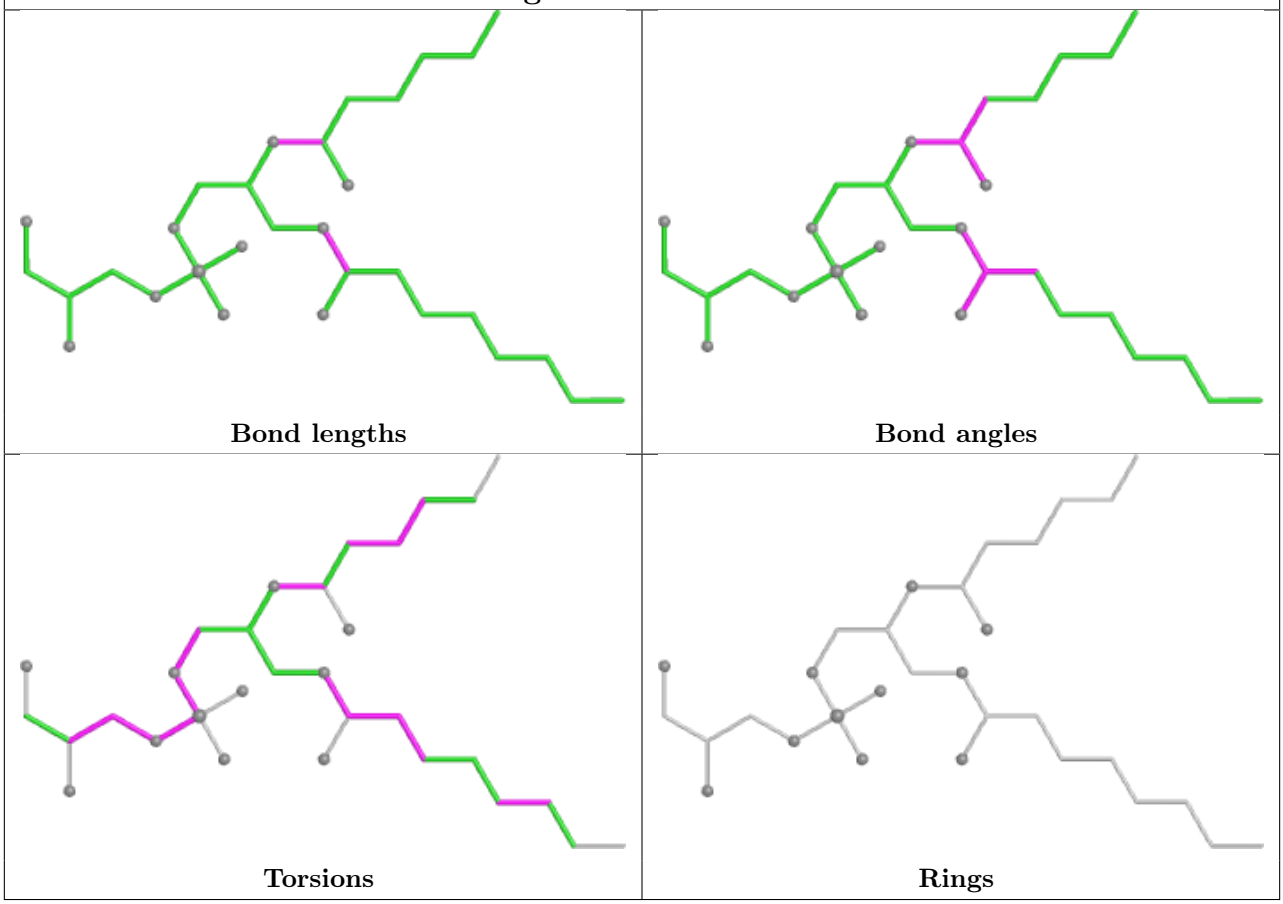


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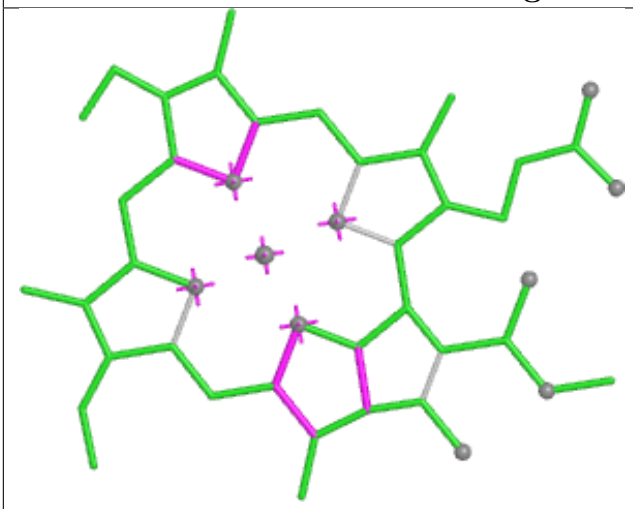


Rings

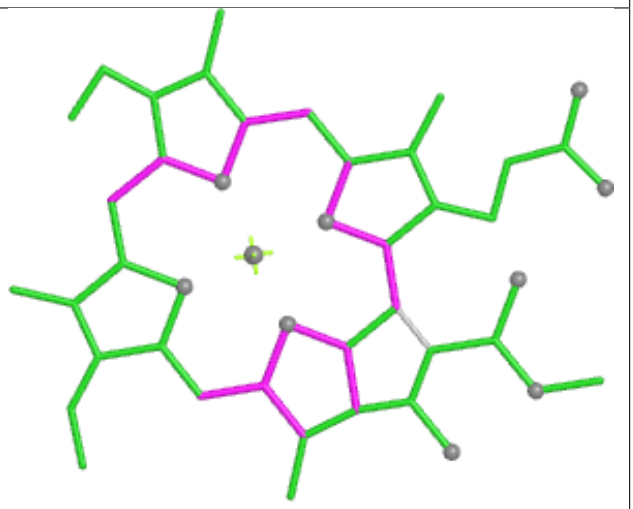
Ligand LHG B 308



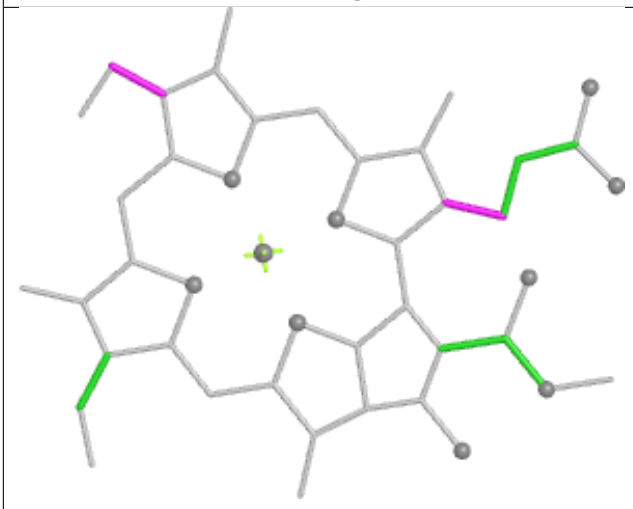
Ligand CLA R 301



Bond lengths



Bond angles

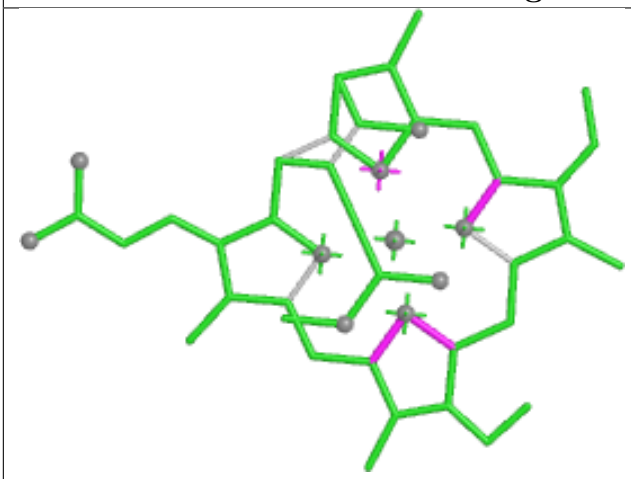


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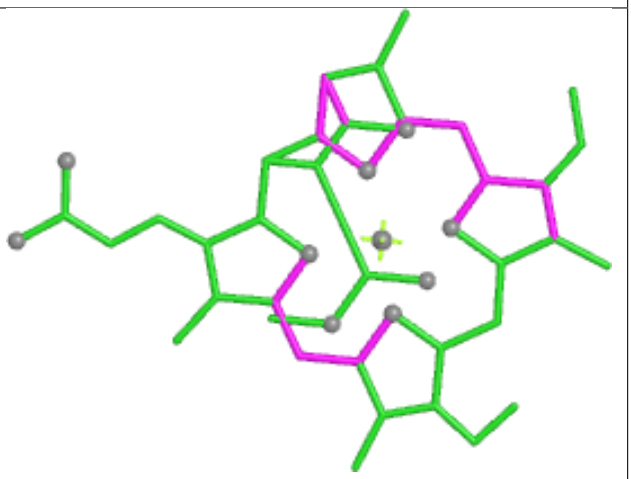


Rings

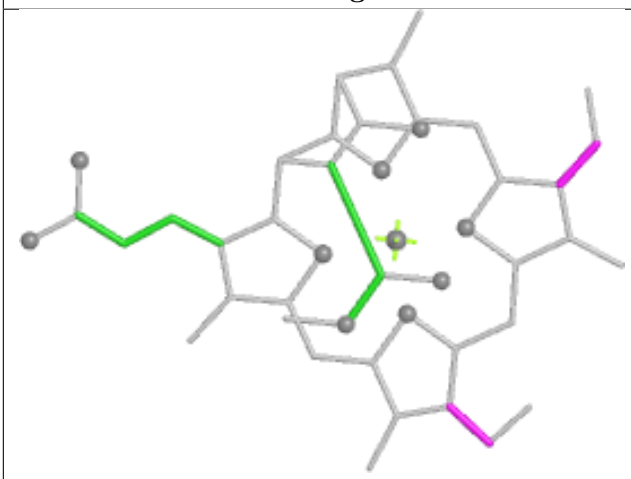
Ligand KC2 N 307



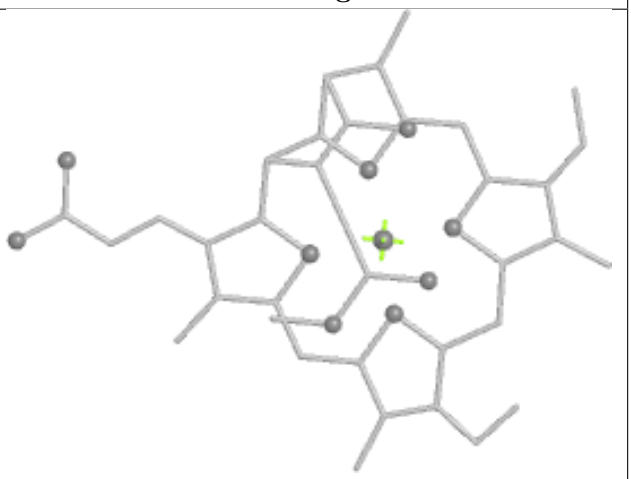
Bond lengths



Bond angles

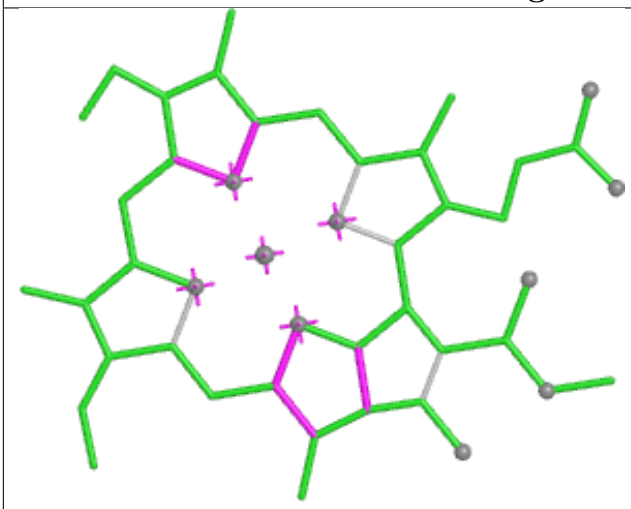


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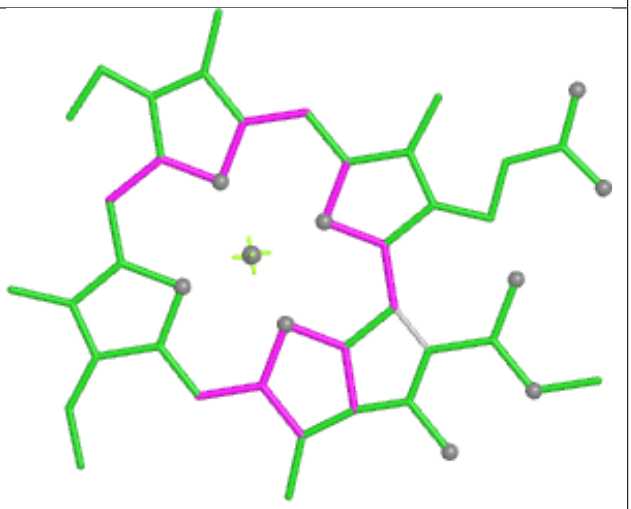


Rings

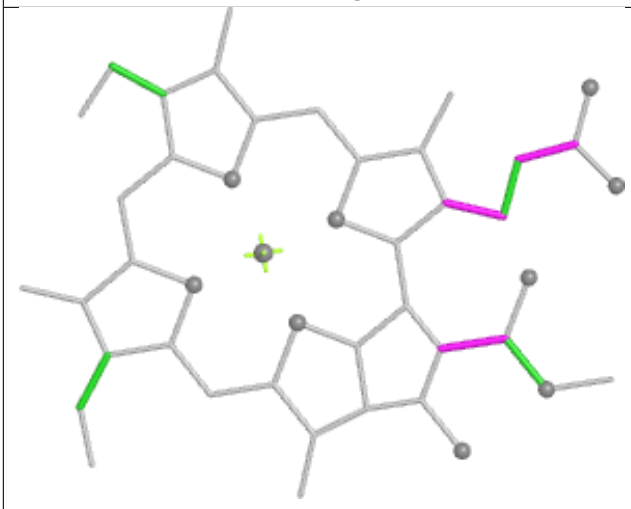
Ligand CLA J 308



Bond lengths



Bond angles

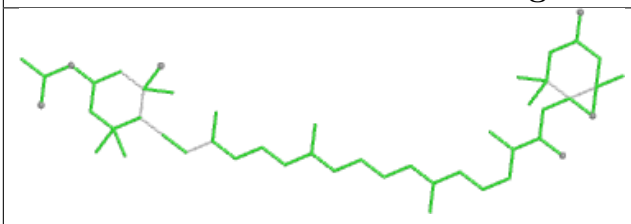


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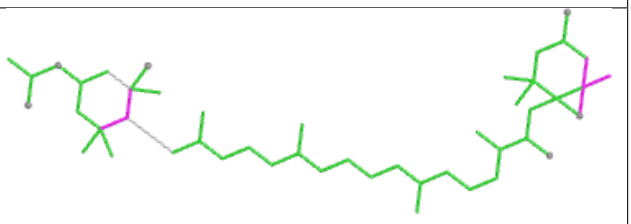


Rings

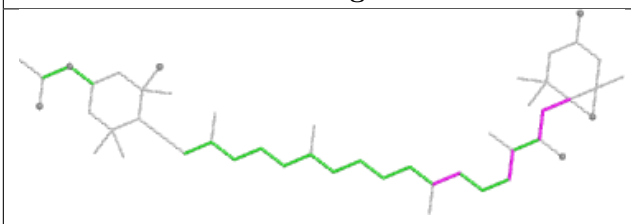
Ligand A86 H 314



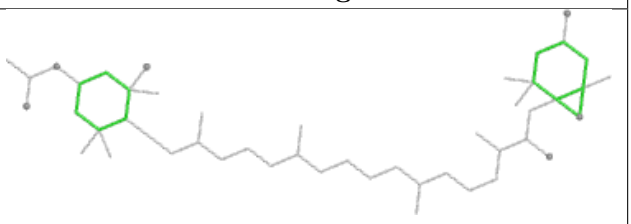
Bond lengths



Bond angles

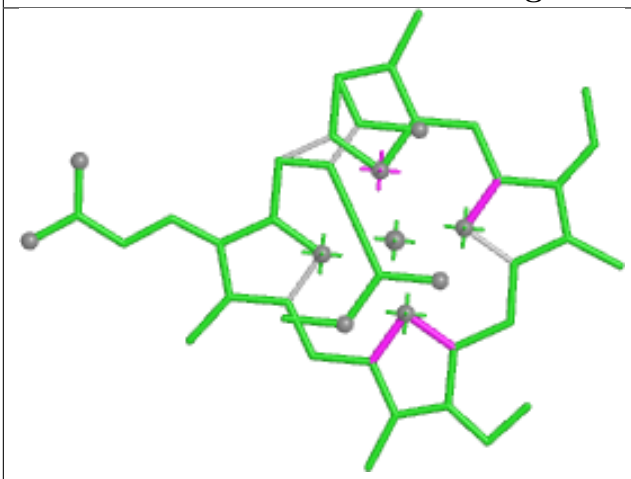


Torsions

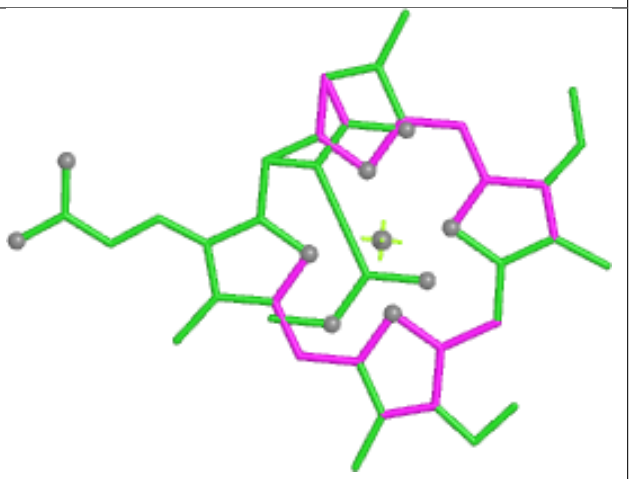


Rings

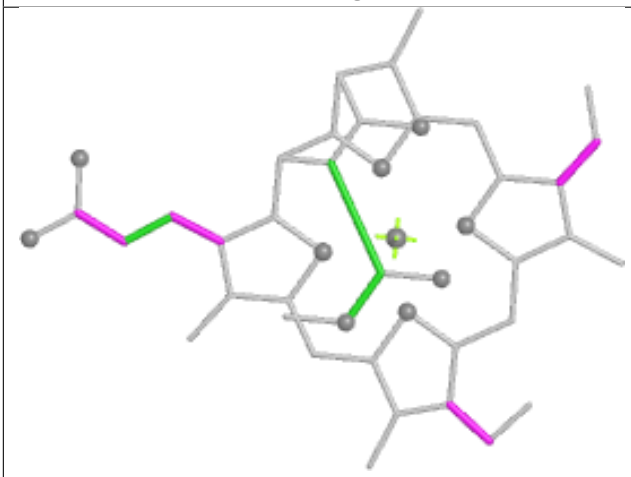
Ligand KC2 K 303



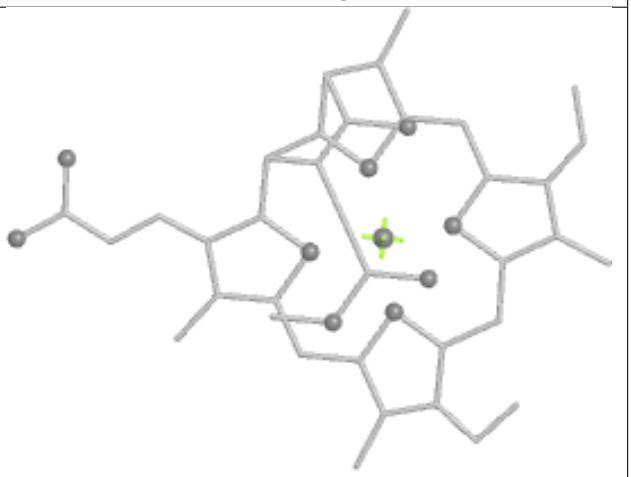
Bond lengths



Bond angles

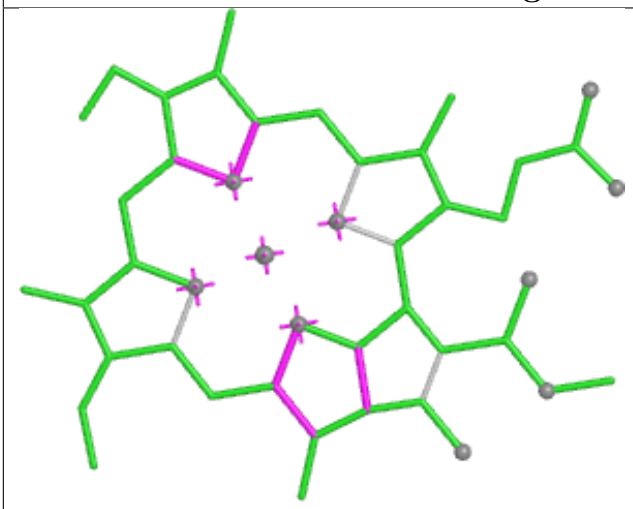


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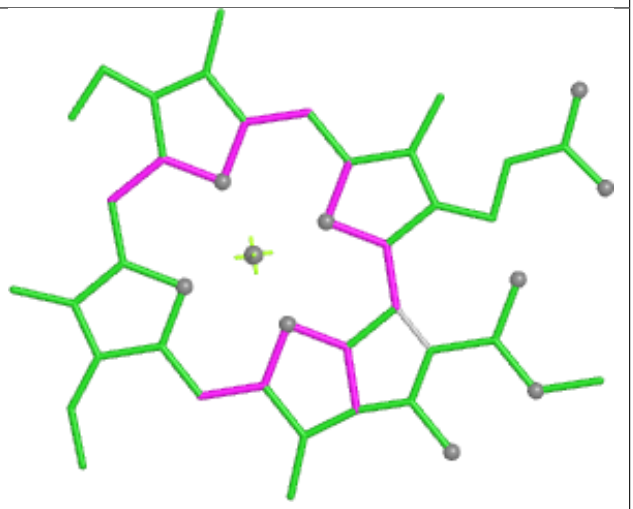


Rings

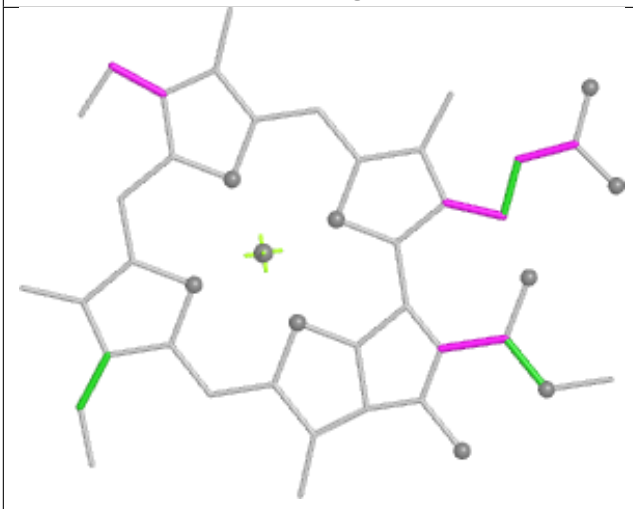
Ligand CLA U 306



Bond lengths



Bond angles

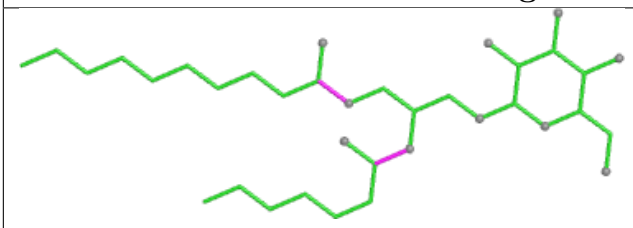


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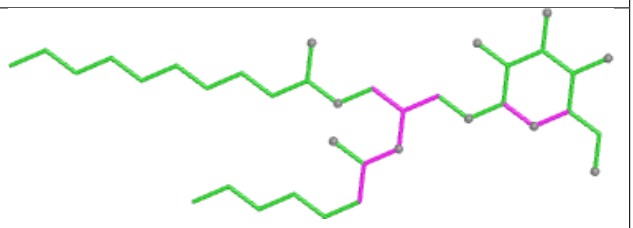


Rings

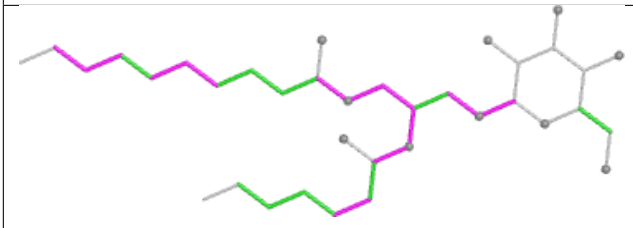
Ligand LMG A 317



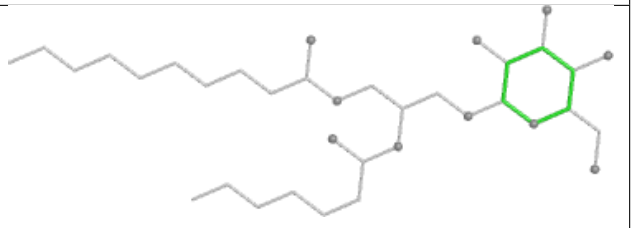
Bond lengths



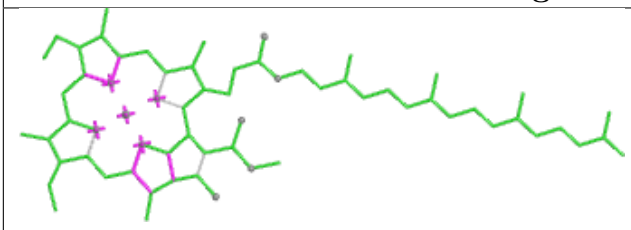
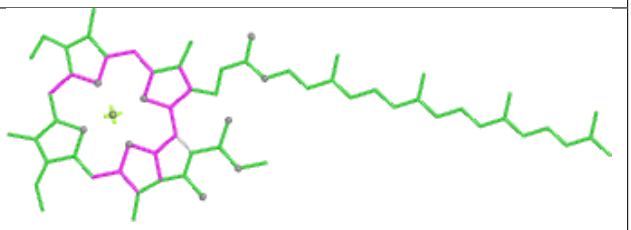
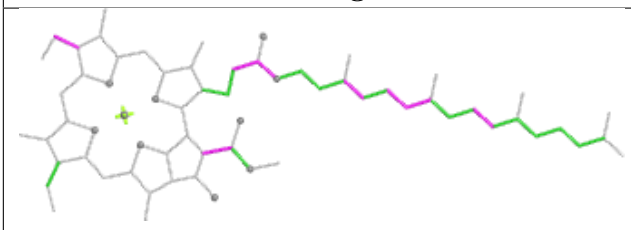
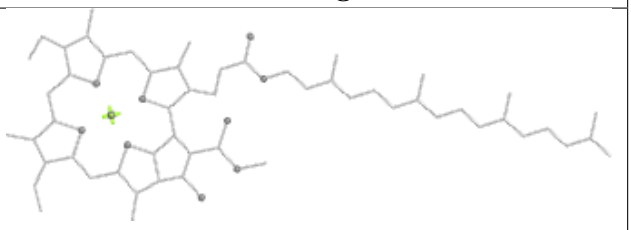
Bond angles

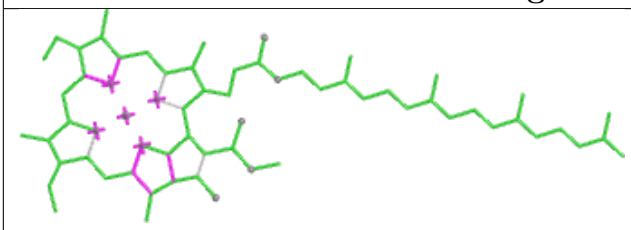
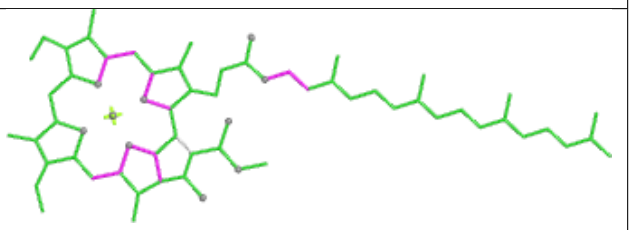
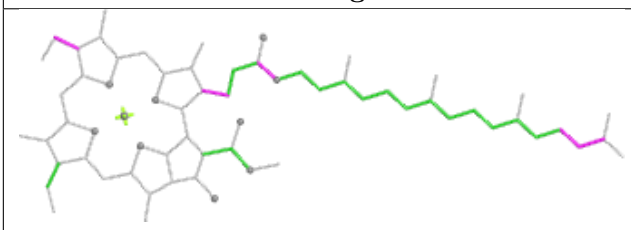
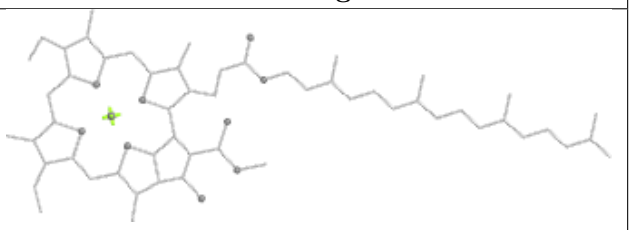


Torsions

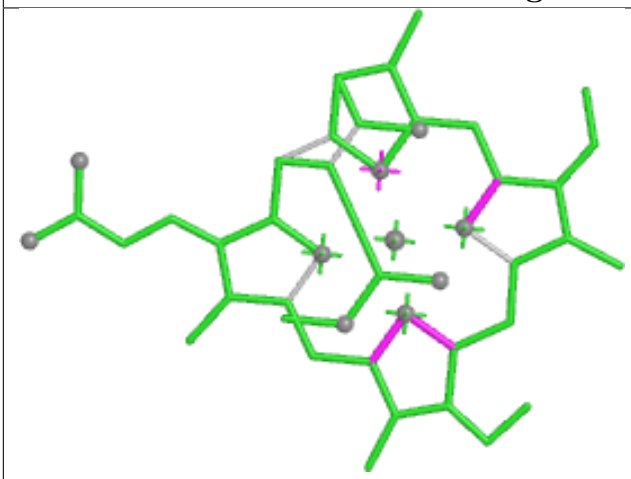


Rings

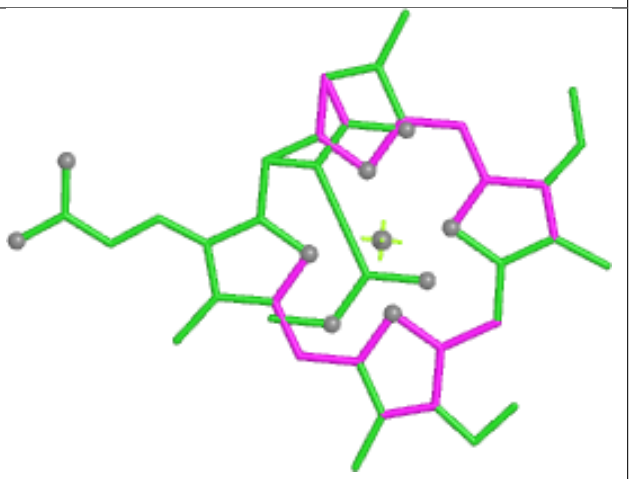
Ligand CLA l 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 832	
	
Bond lengths	Bond angles
	
Torsions	Rings

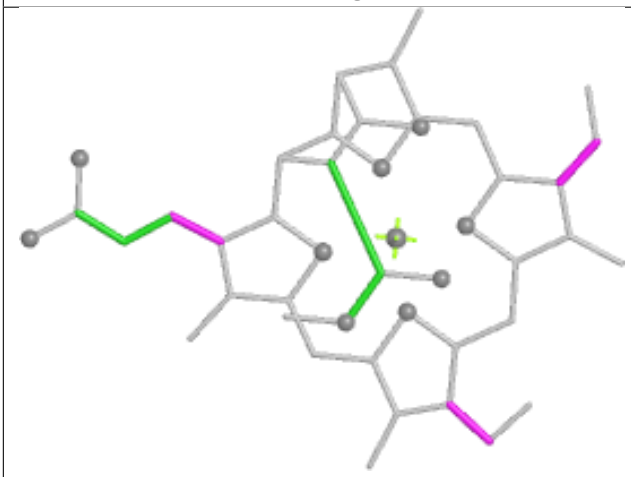
Ligand KC2 R 302



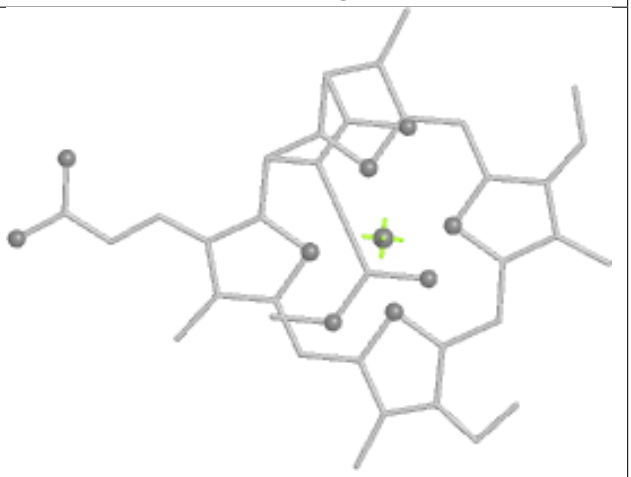
Bond lengths



Bond angles

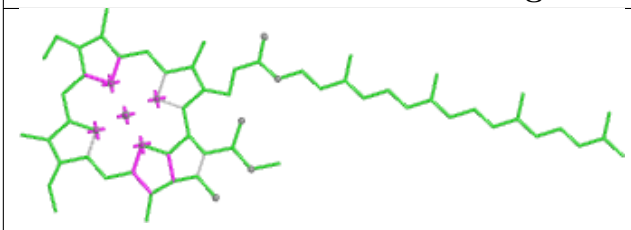


Torsions

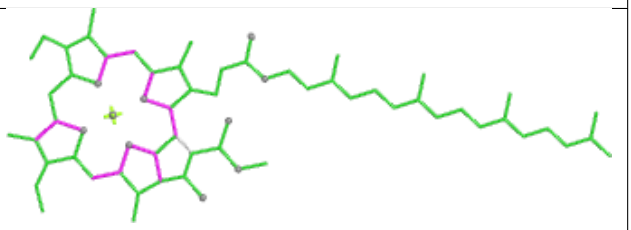


Rings

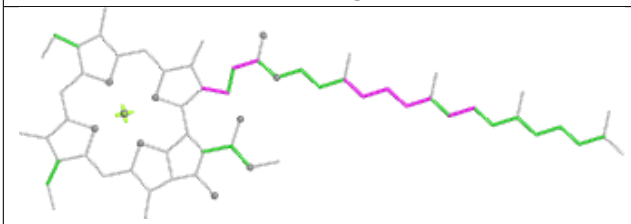
Ligand CLA E 308



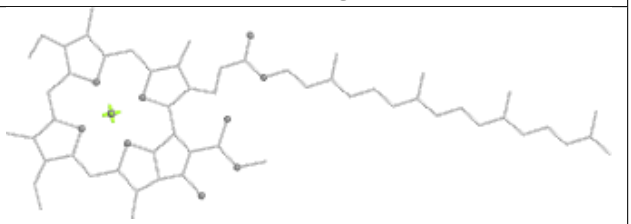
Bond lengths



Bond angles

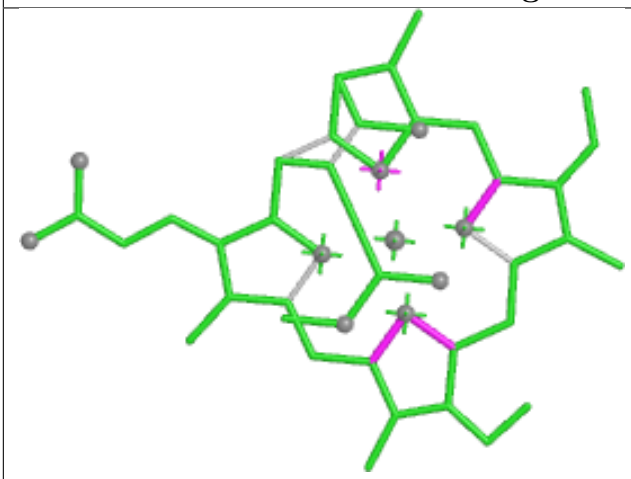


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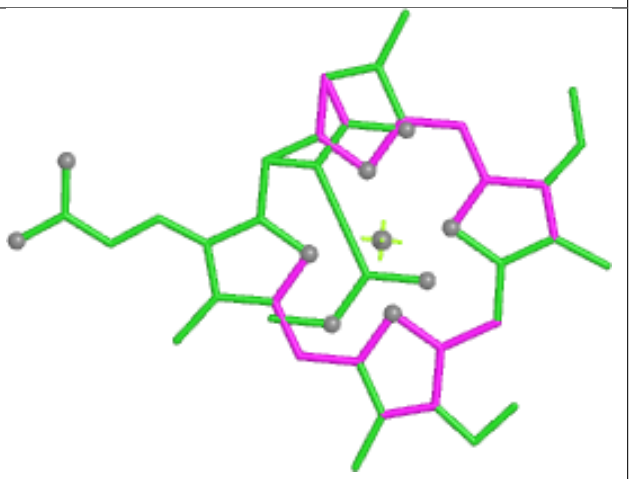


Rings

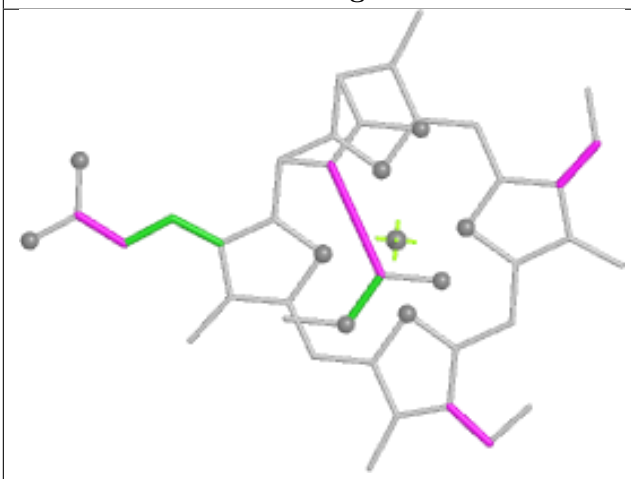
Ligand KC2 M 313



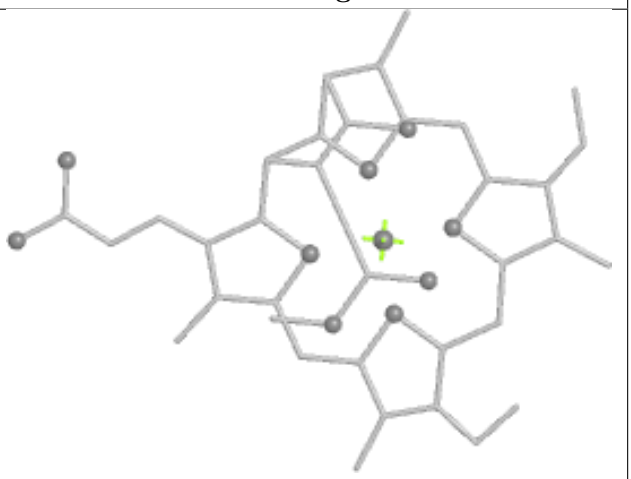
Bond lengths



Bond angles

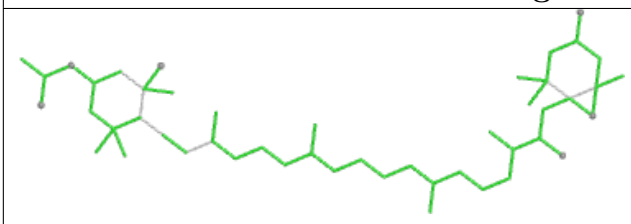


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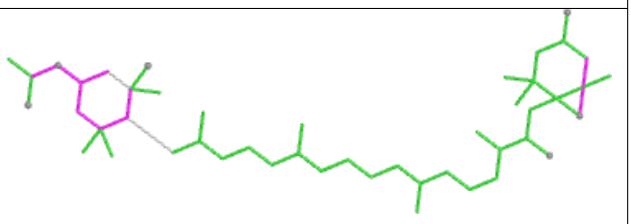


Rings

Ligand A86 S 314



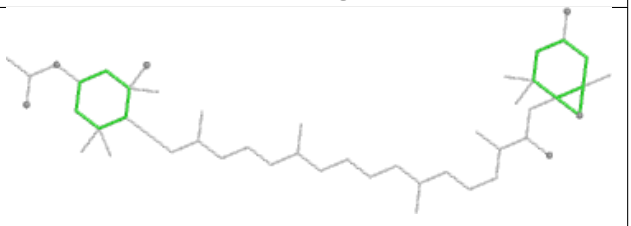
Bond lengths



Bond angles

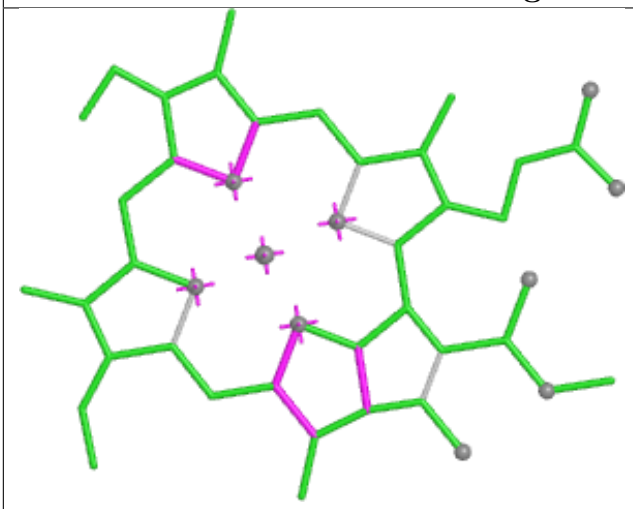


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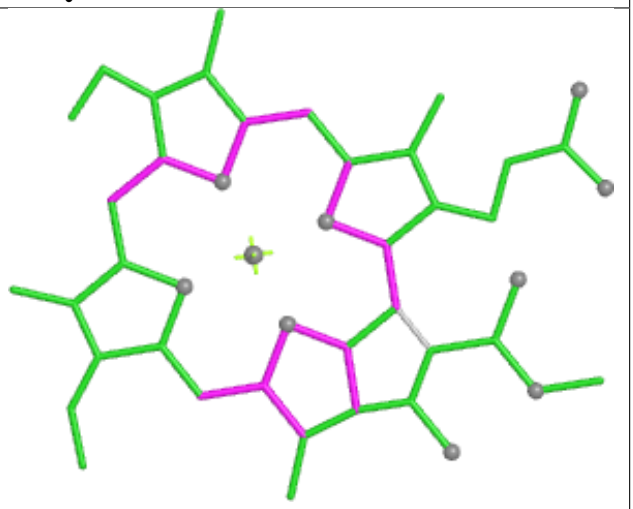


Rings

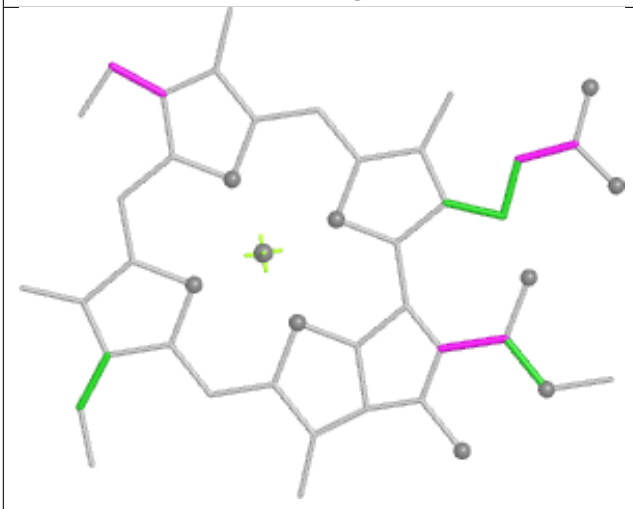
Ligand CLA Q 308



Bond lengths



Bond angles

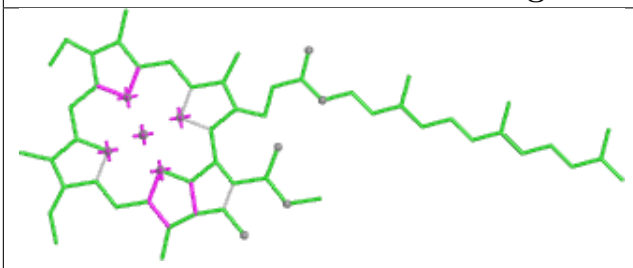


Torsions

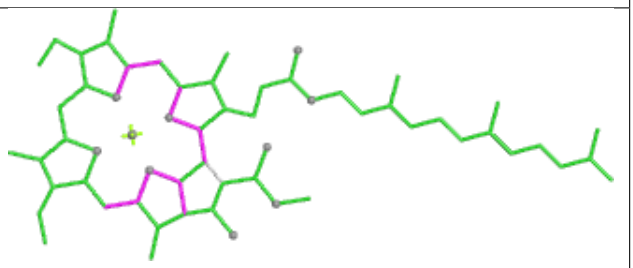


Rings

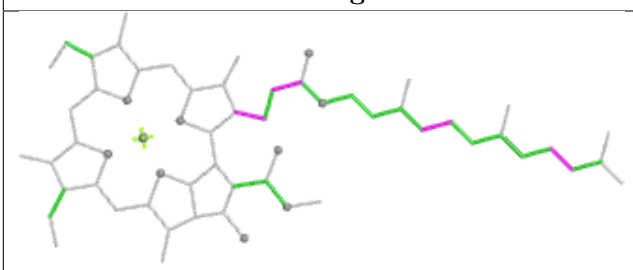
Ligand CLA b 810



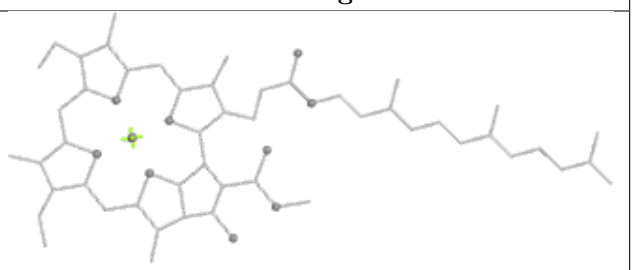
Bond lengths



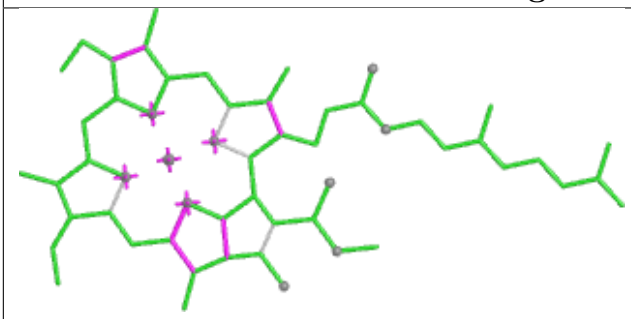
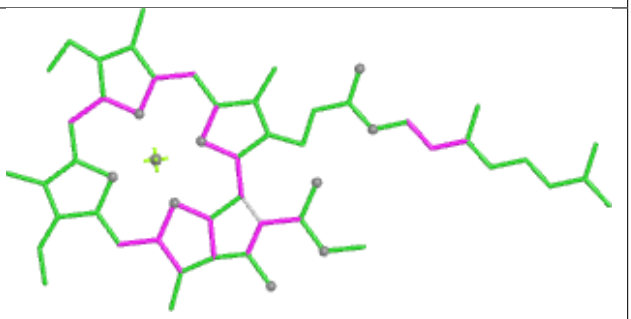
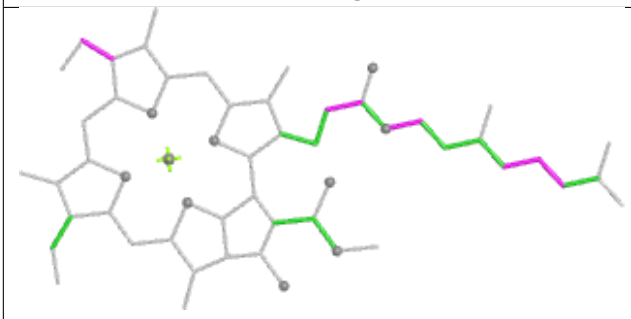
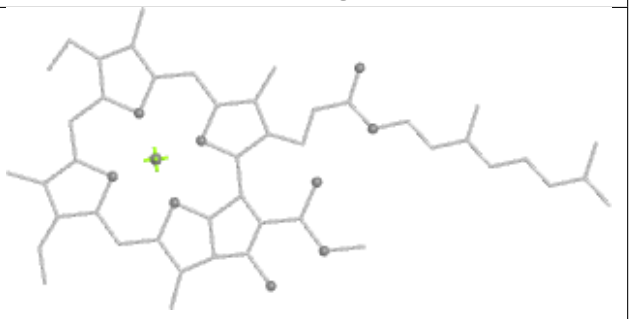
Bond angles

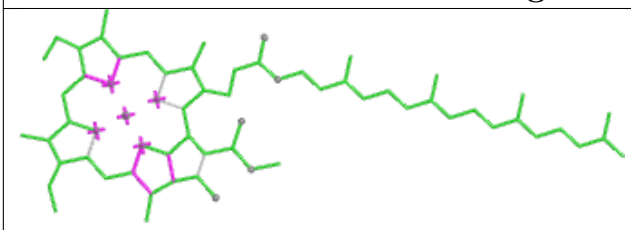
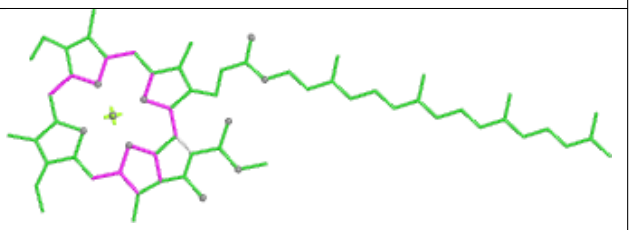
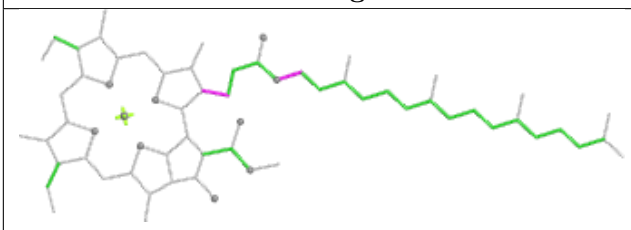
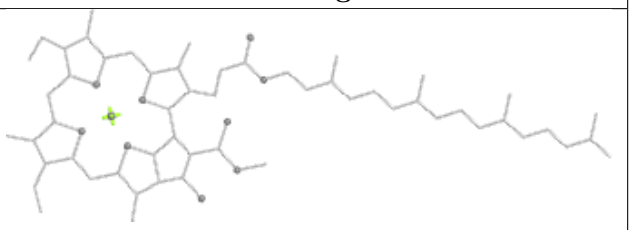


Torsions

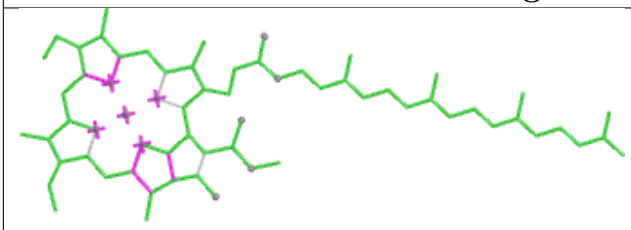


Rings

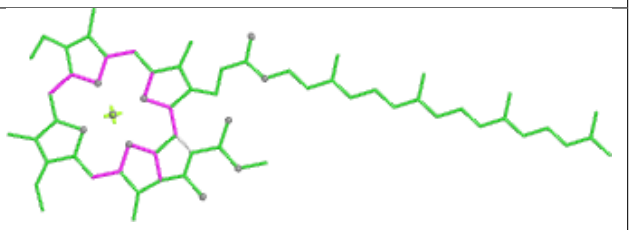
Ligand CLA a 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

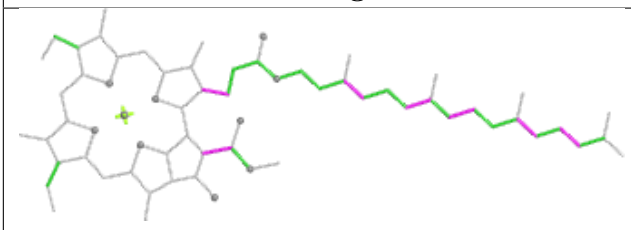
Ligand CLA K 308



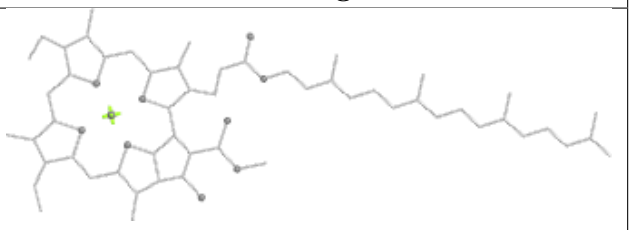
Bond lengths



Bond angles

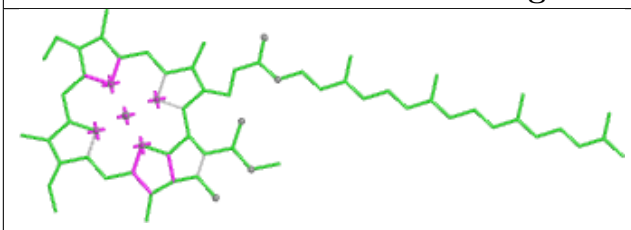


Torsions

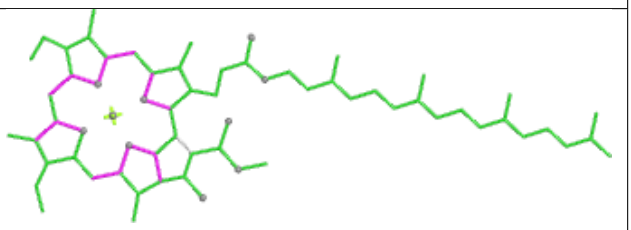


Rings

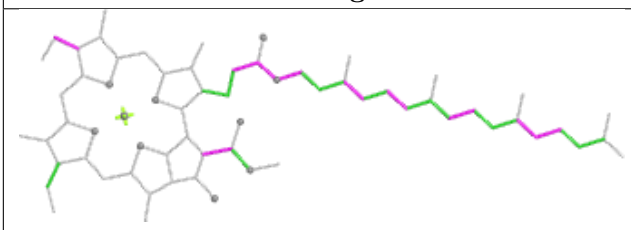
Ligand CLA a 819



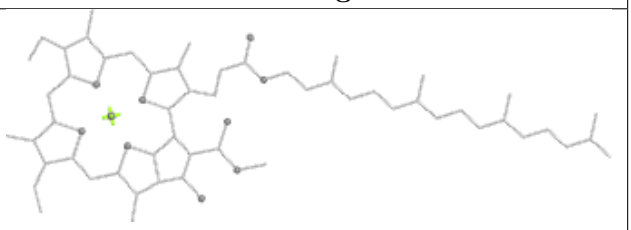
Bond lengths



Bond angles

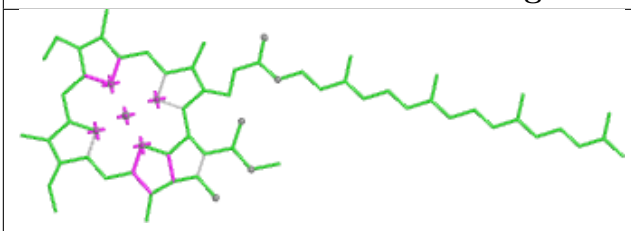


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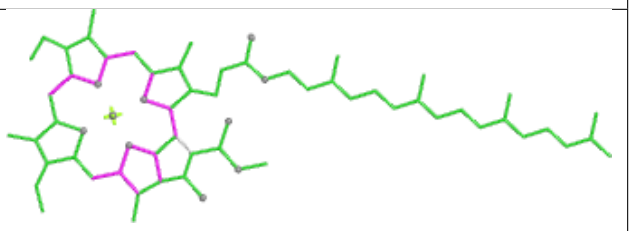


Rings

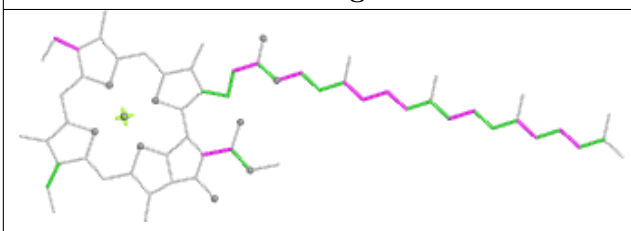
Ligand CLA C 306



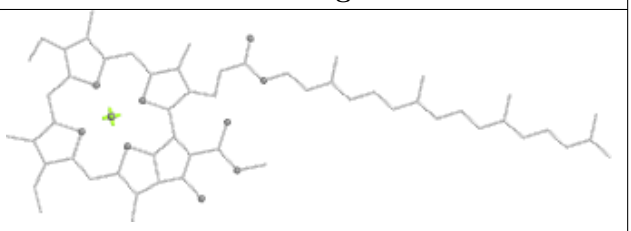
Bond lengths



Bond angles

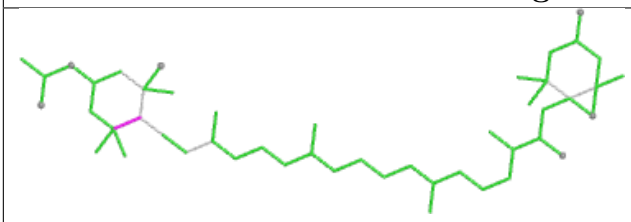


Torsions

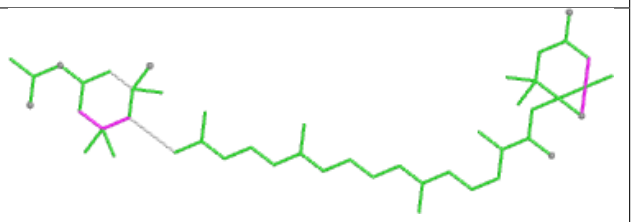


Rings

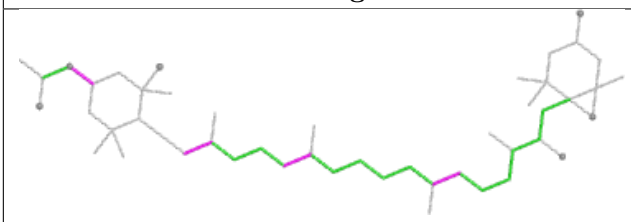
Ligand A86 L 316



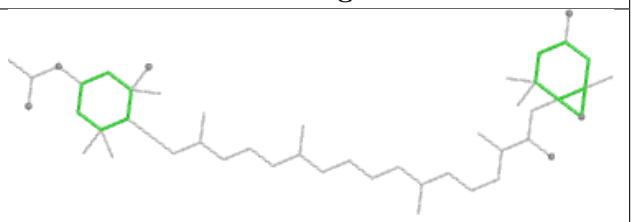
Bond lengths



Bond angles

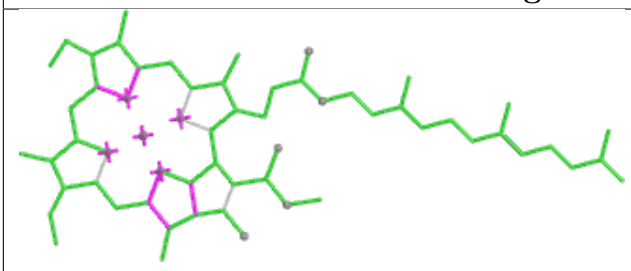


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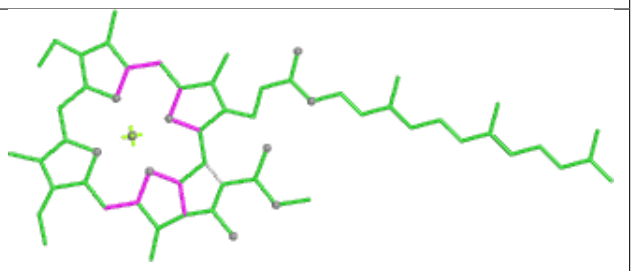


Rings

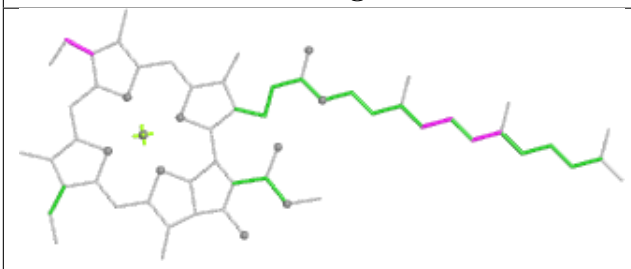
Ligand CLA A 302



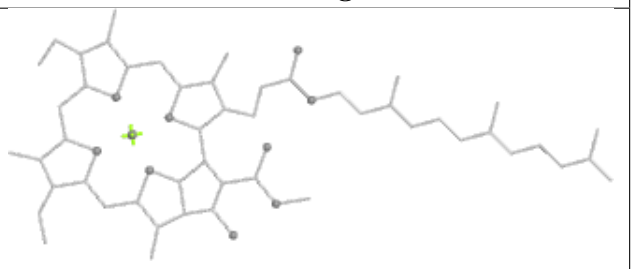
Bond lengths



Bond angles

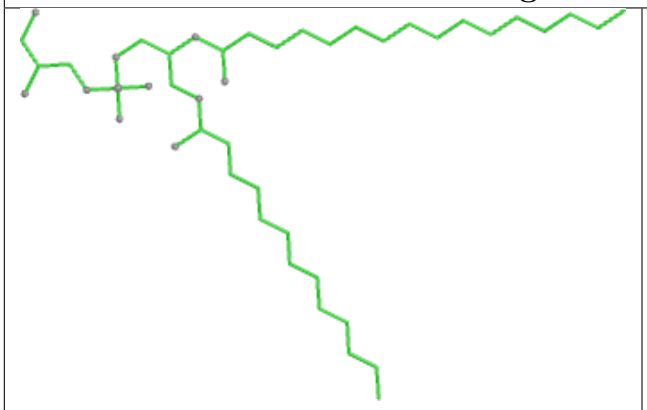


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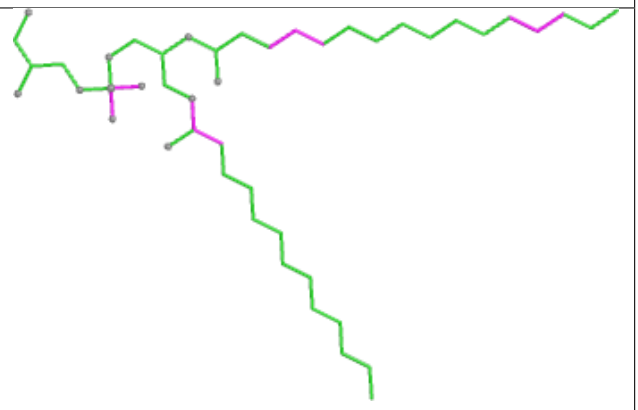


Rings

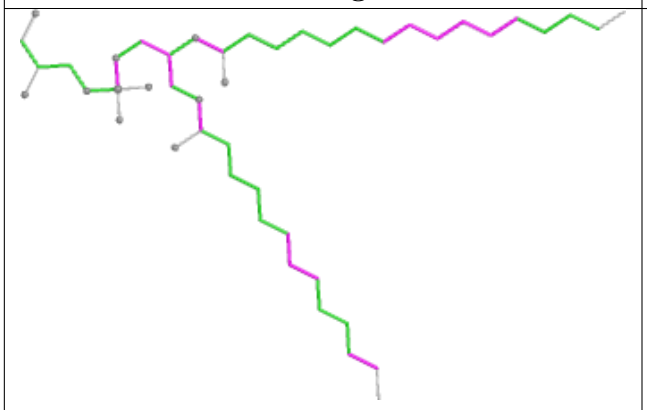
Ligand LHG M 319



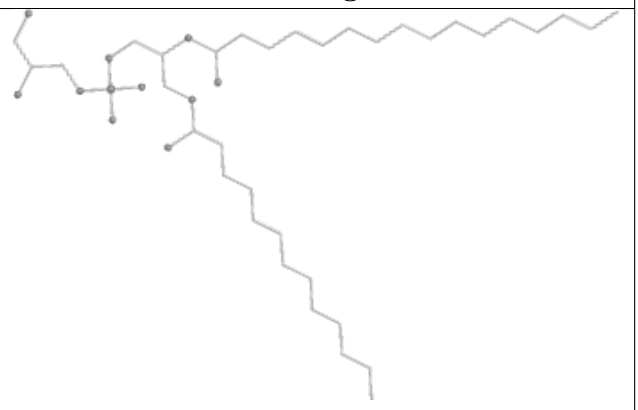
Bond lengths



Bond angles

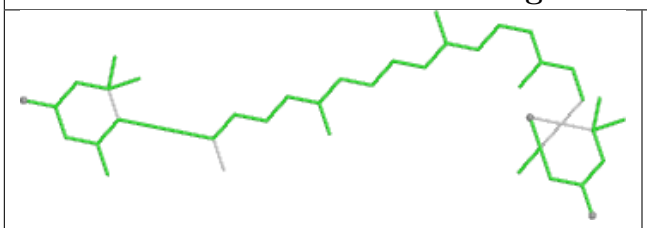


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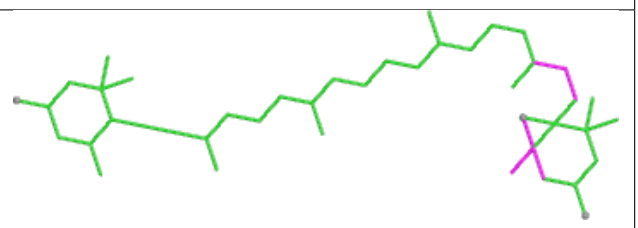


Rings

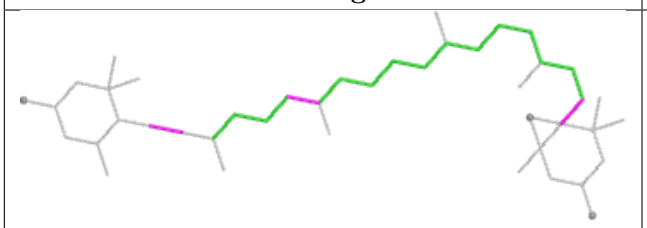
Ligand DD6 A 315



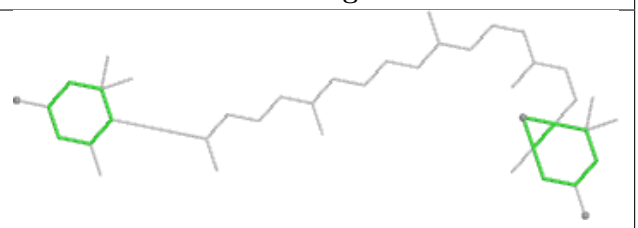
Bond lengths



Bond angles

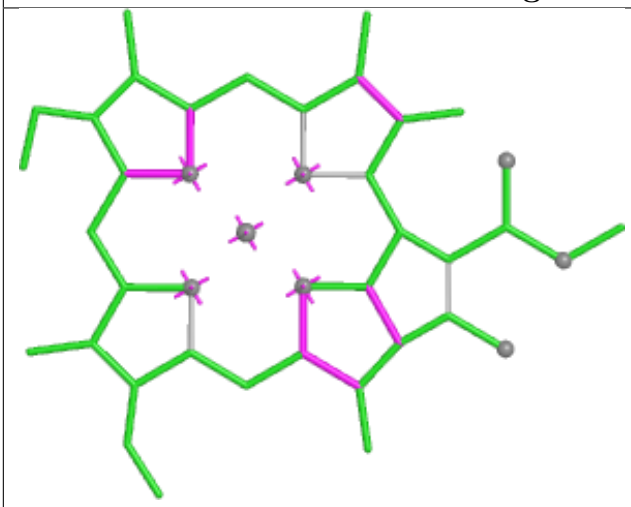


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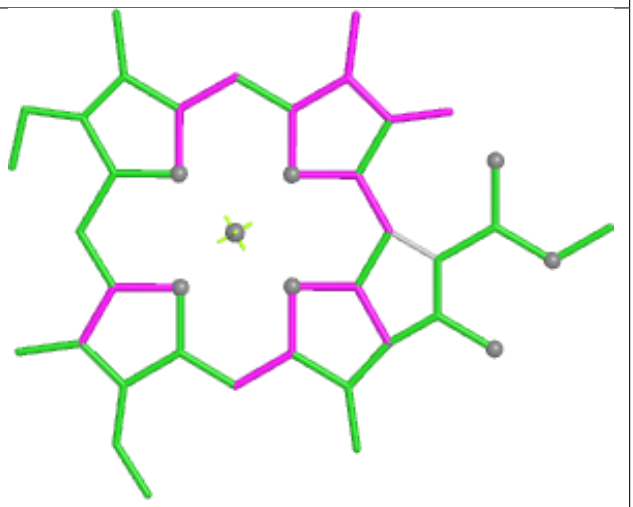


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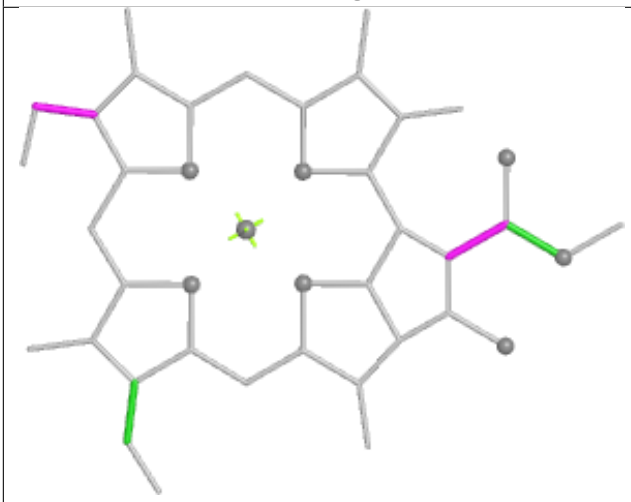
Ligand CLA K 307



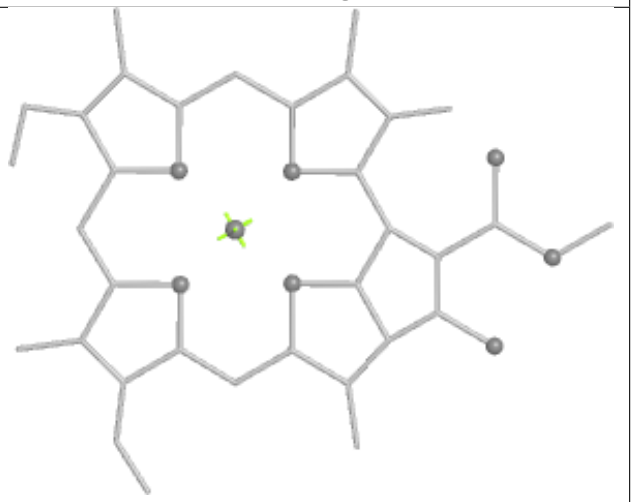
Bond lengths



Bond angles

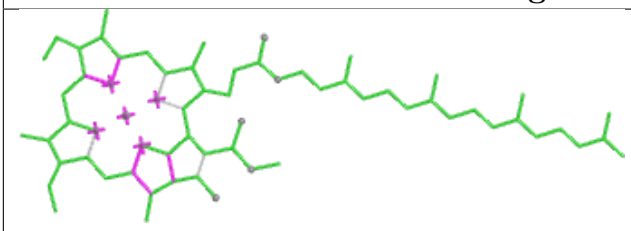


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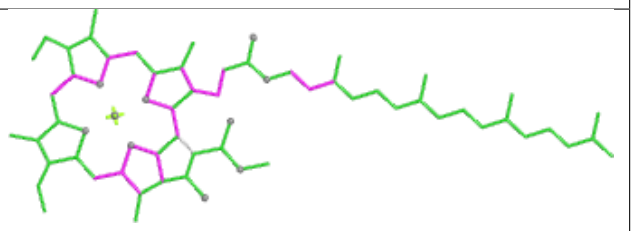


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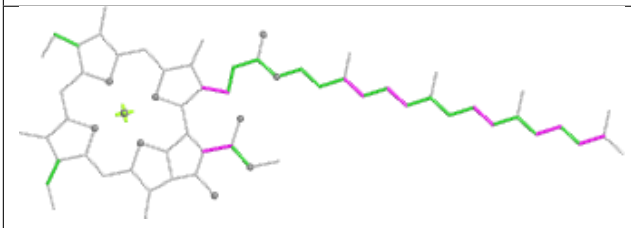
Ligand CLA a 814



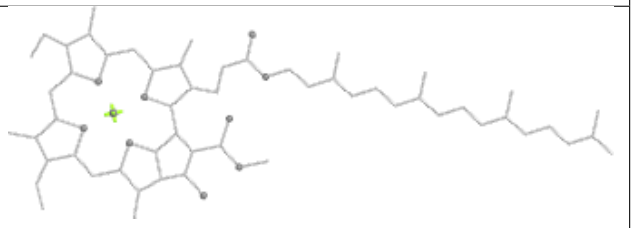
Bond lengths



Bond angles

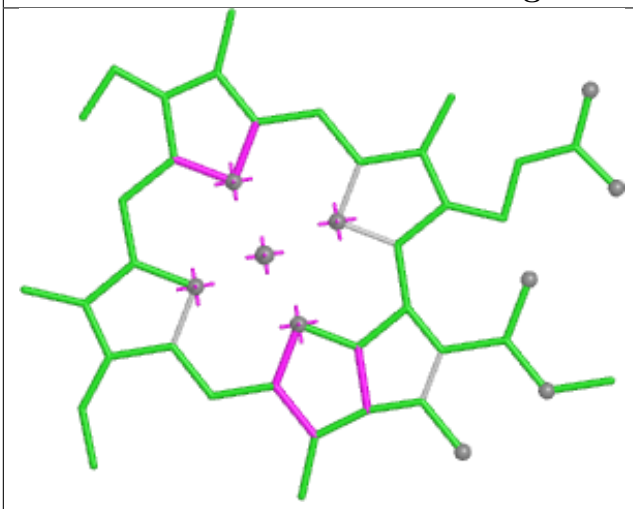


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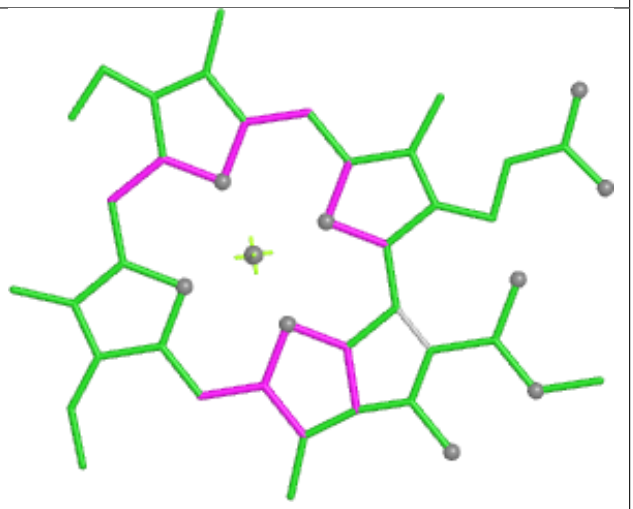


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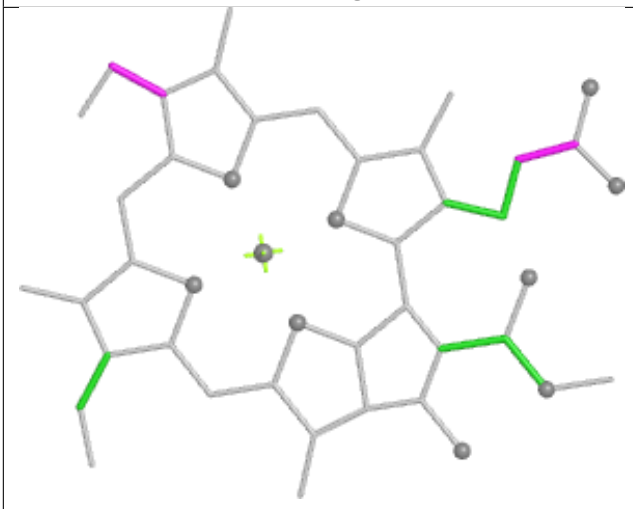
Ligand CLA D 315



Bond lengths



Bond angles

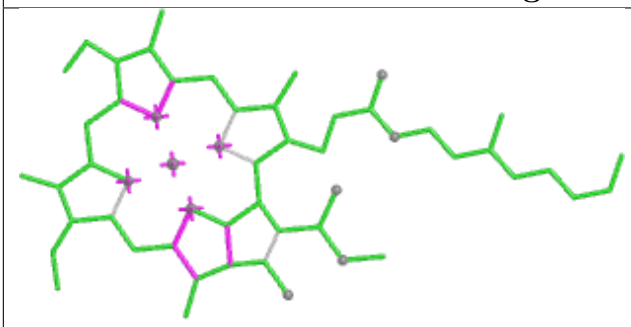


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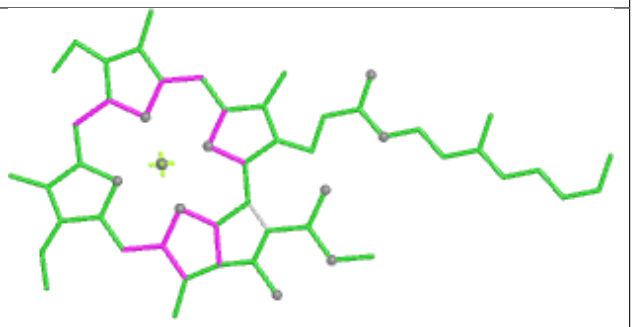


Rings

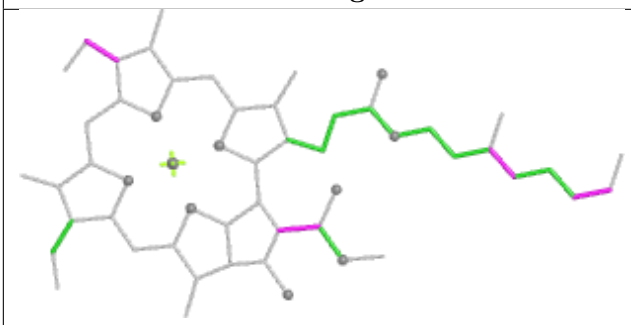
Ligand CLA G 308



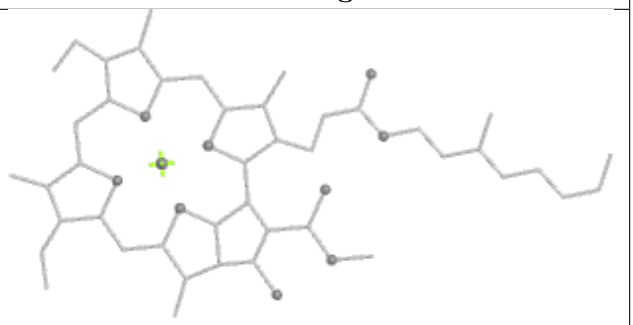
Bond lengths



Bond angles

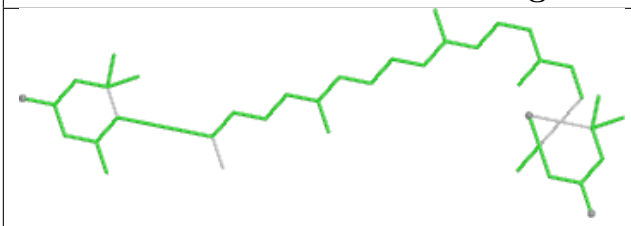


Torsions



Rings

Ligand DD6 J 315



Bond lengths



Bond angles

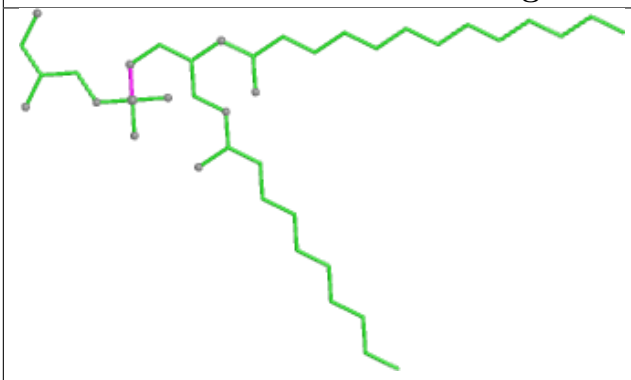


Torsions



Rings

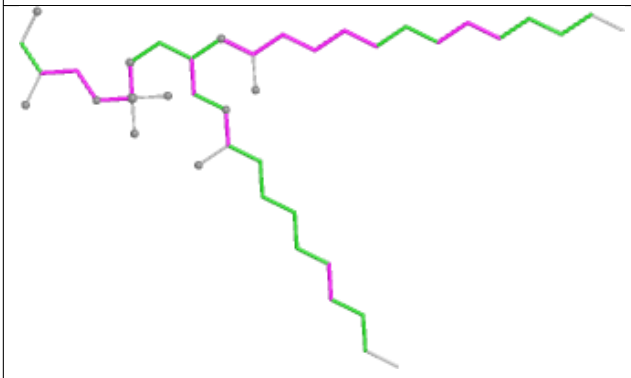
Ligand LHG A 316



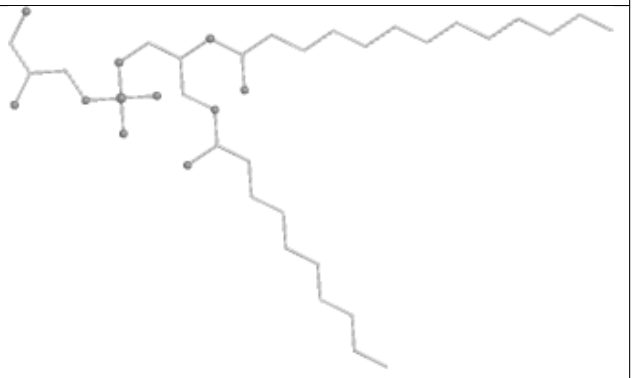
Bond lengths



Bond angles

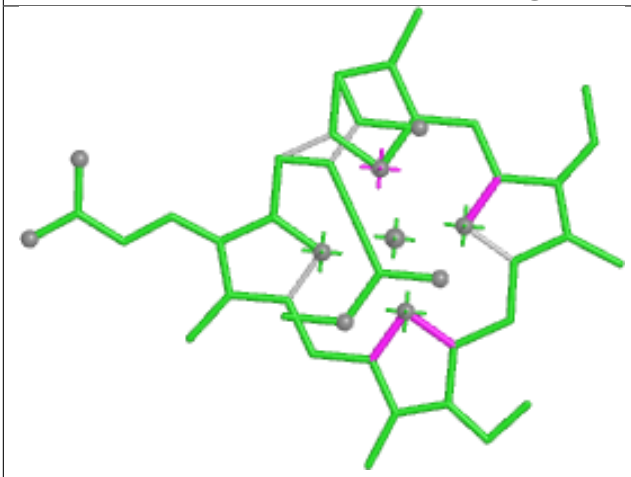


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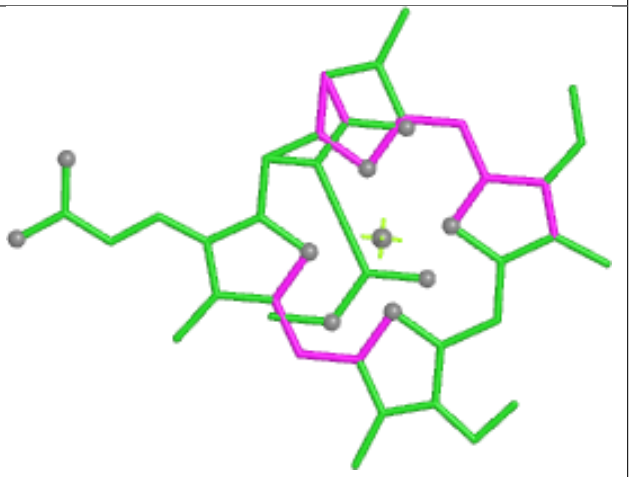


Rings

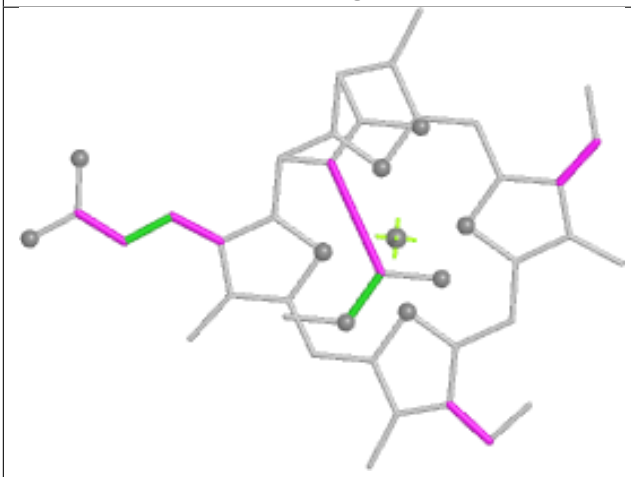
Ligand KC2 C 303



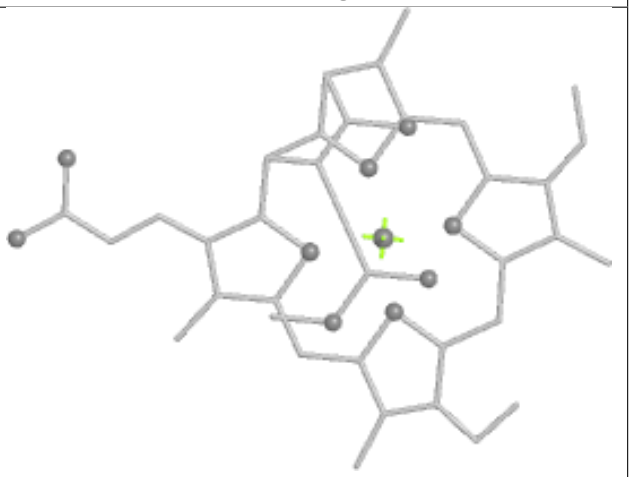
Bond lengths



Bond angles

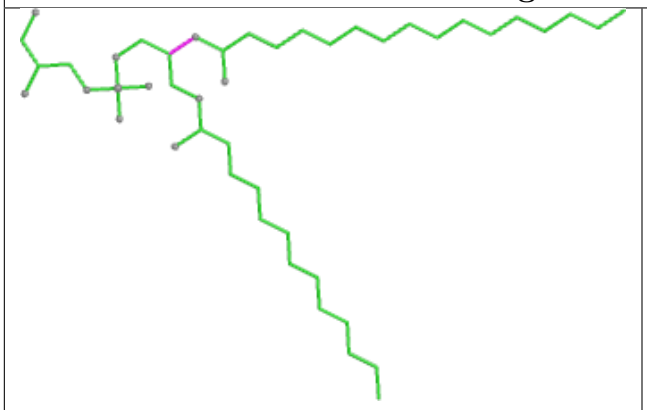


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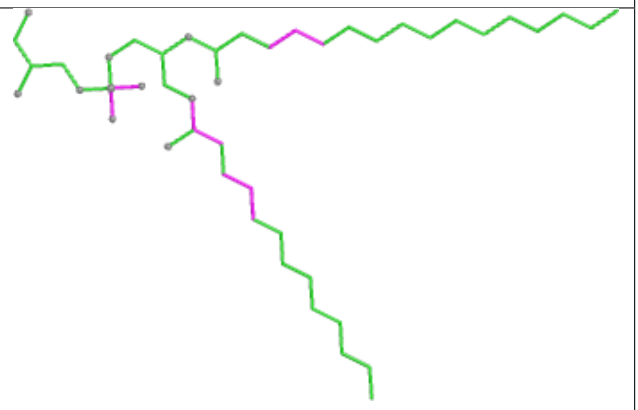


Rings

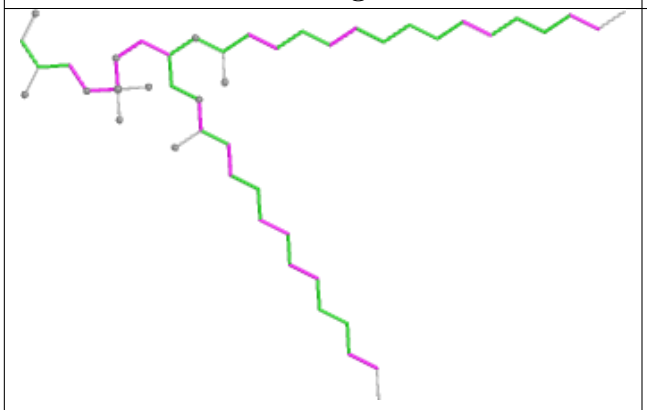
Ligand LHG W 319



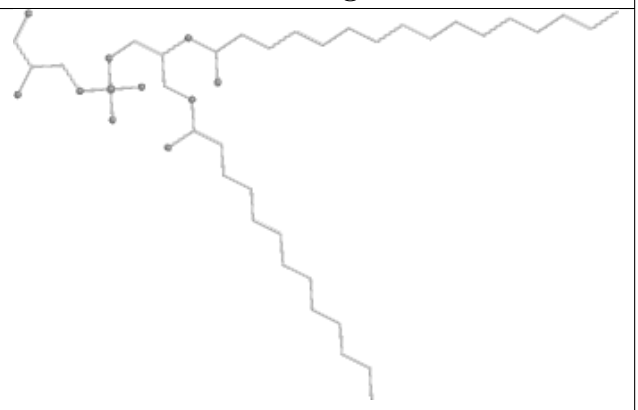
Bond lengths



Bond angles

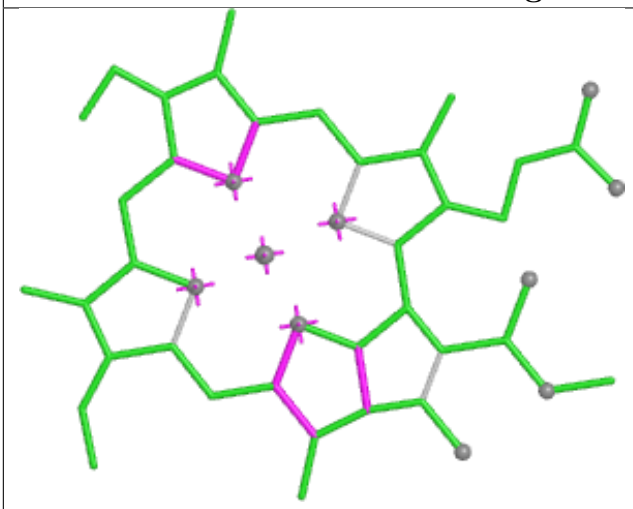


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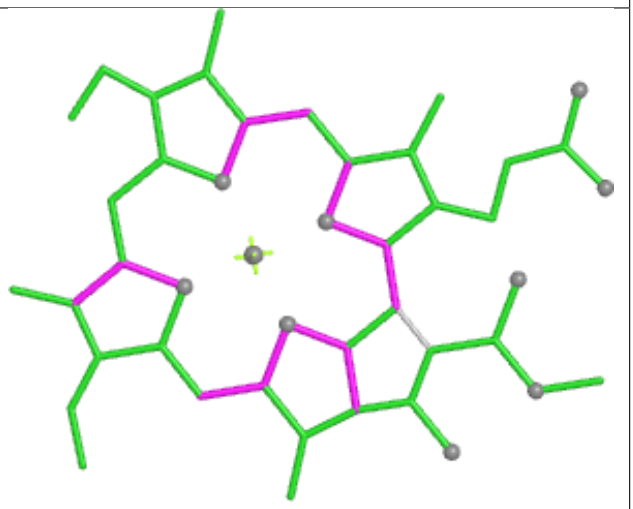


Rings

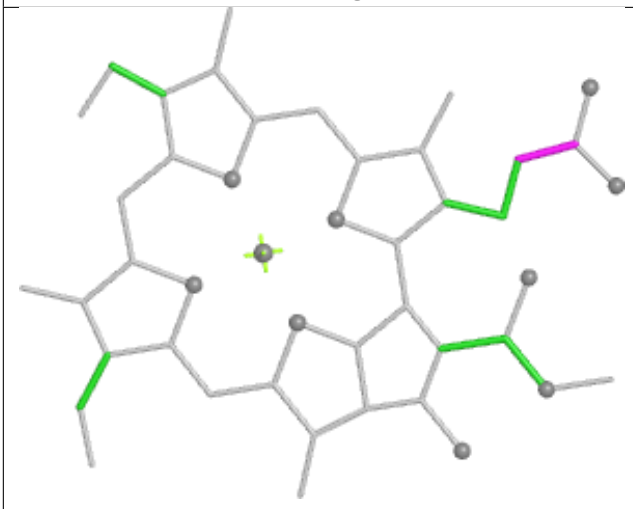
Ligand CLA P 308



Bond lengths



Bond angles

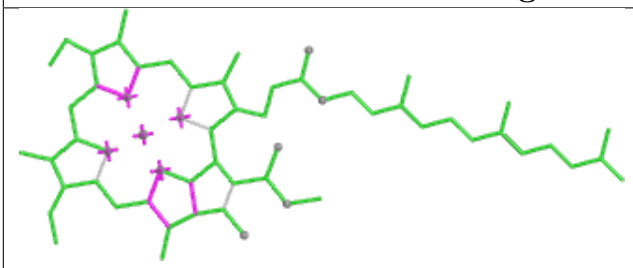


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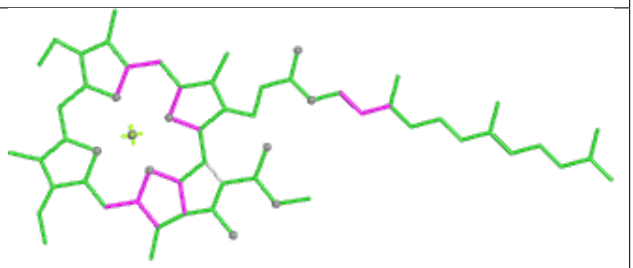


Rings

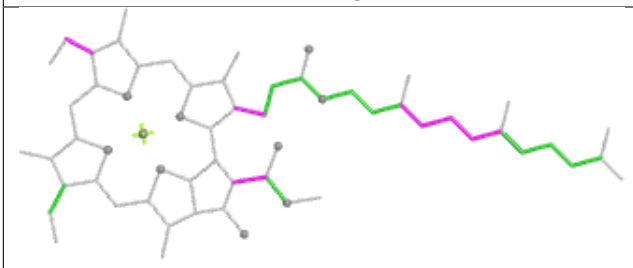
Ligand CLA W 312



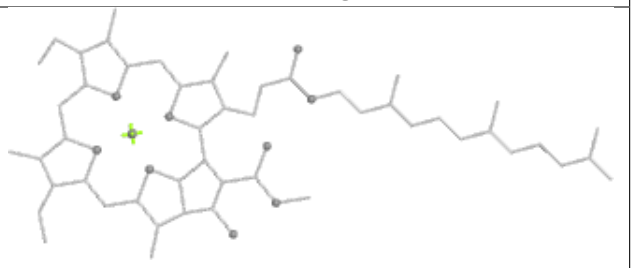
Bond lengths



Bond angles

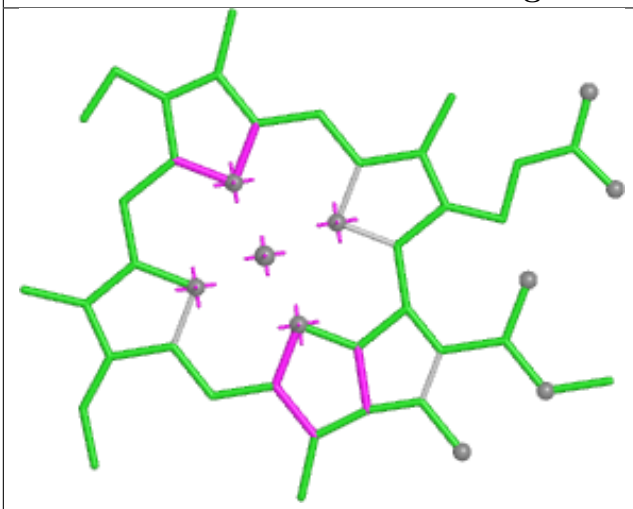


Torsions

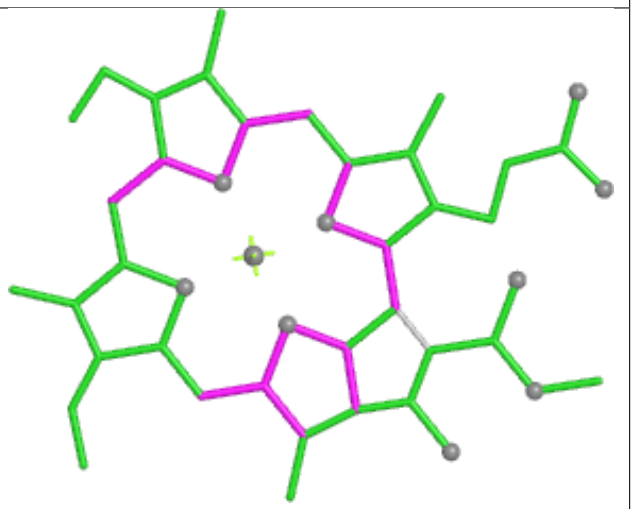


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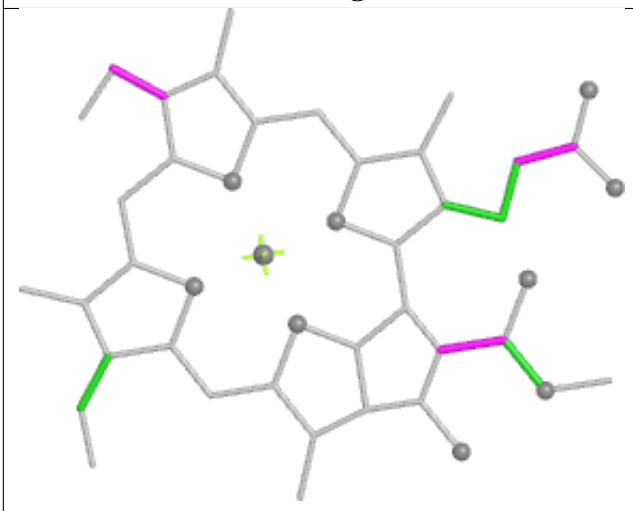
Ligand CLA O 308



Bond lengths



Bond angles

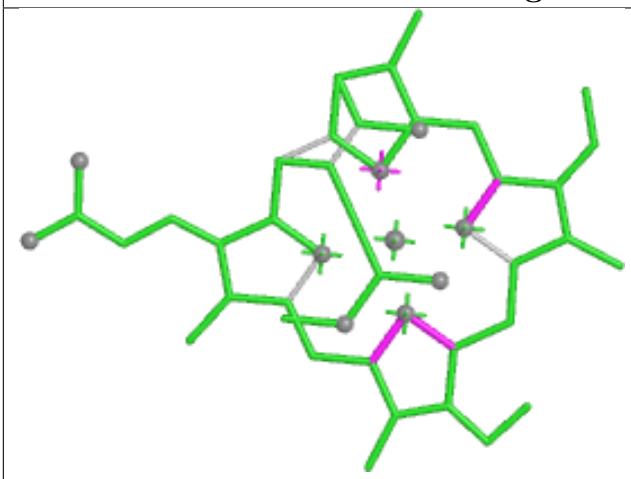


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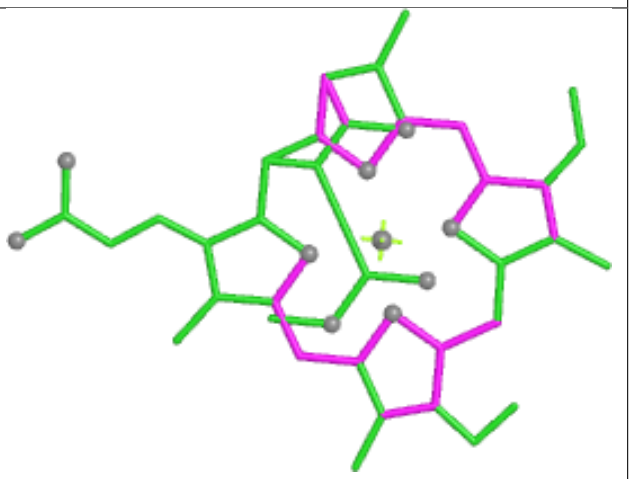


Rings

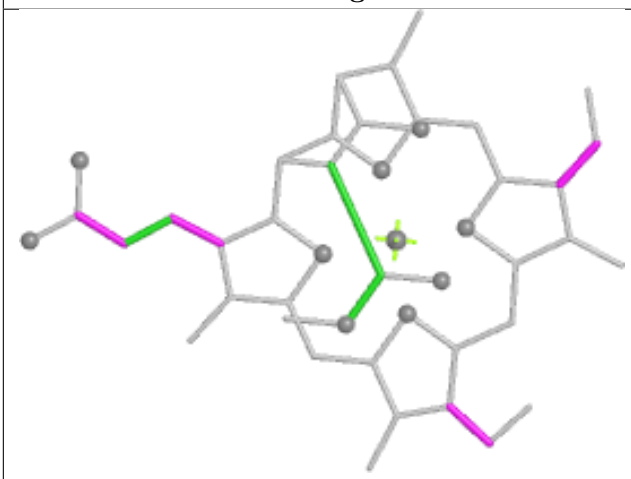
Ligand KC2 N 303



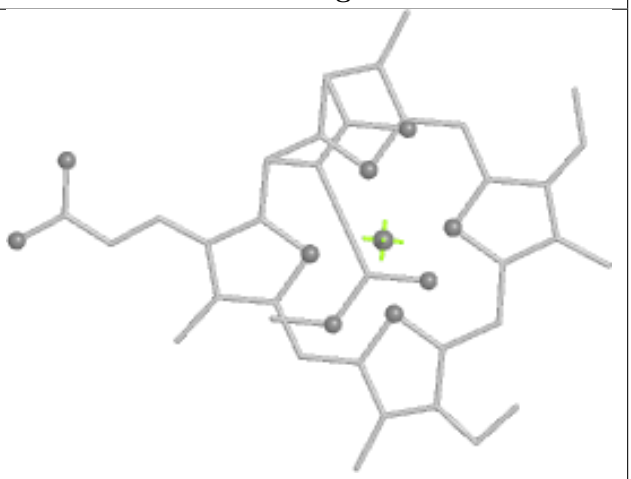
Bond lengths



Bond angles

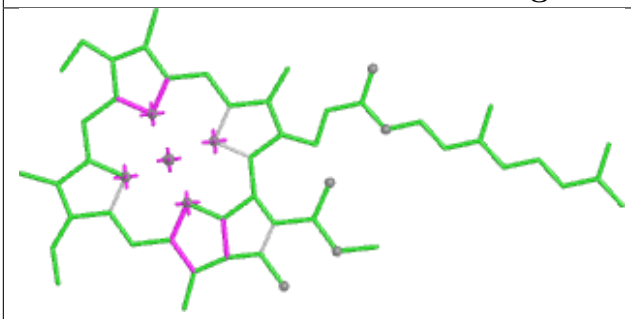


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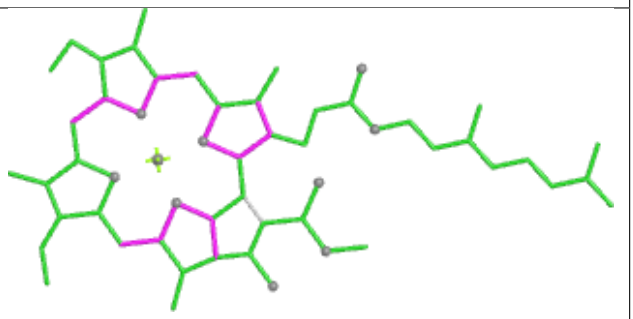


Rings

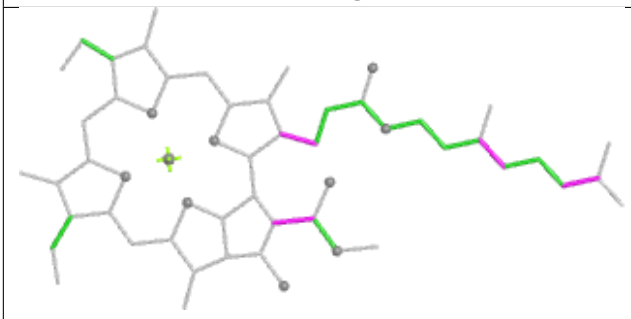
Ligand CLA I 308



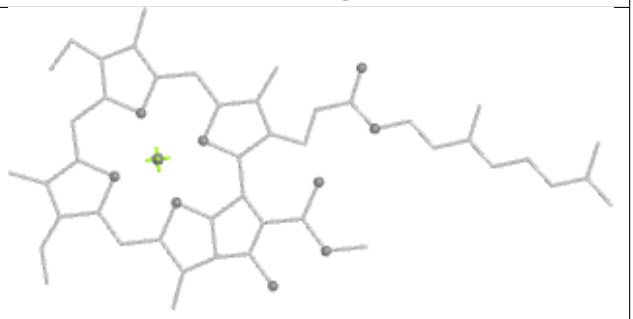
Bond lengths



Bond angles

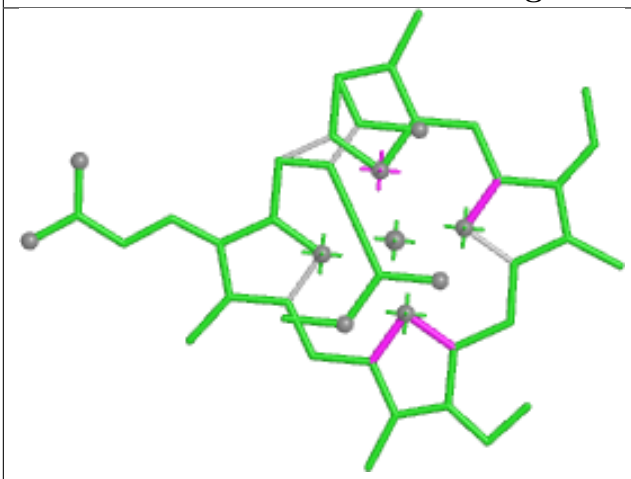


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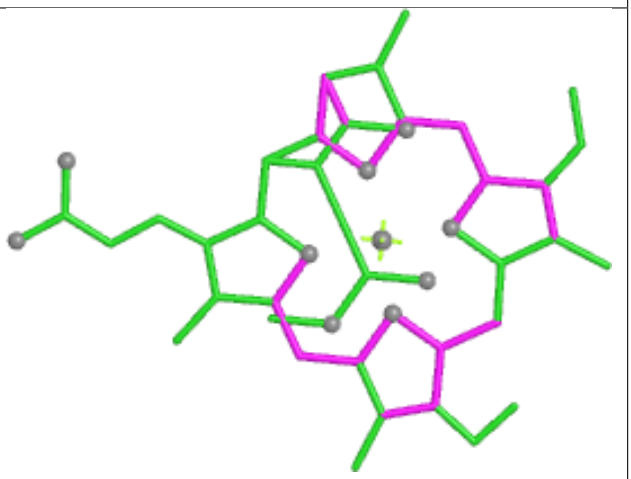


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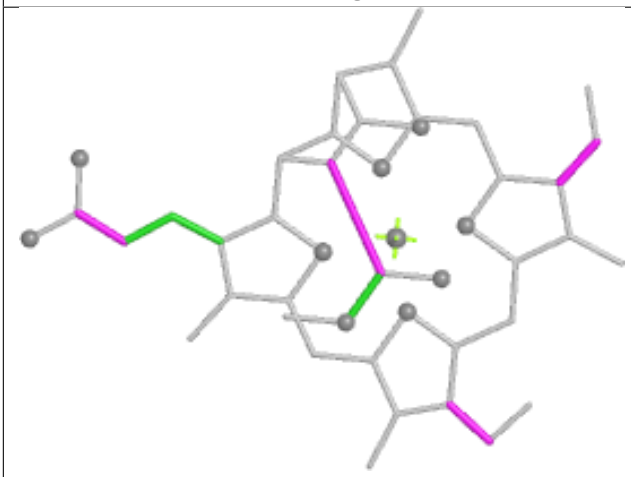
Ligand KC2 N 304



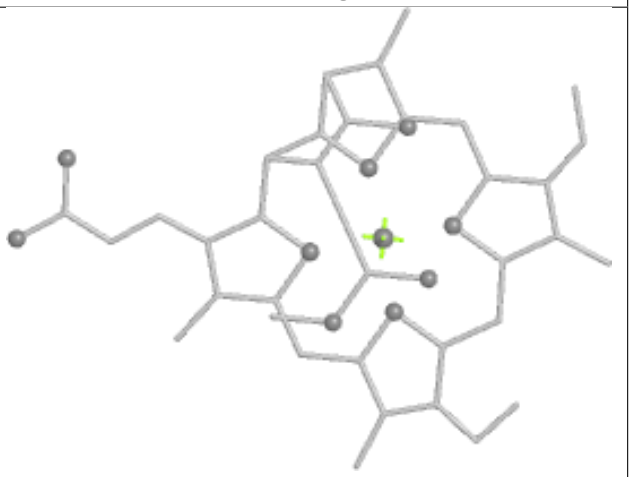
Bond lengths



Bond angles

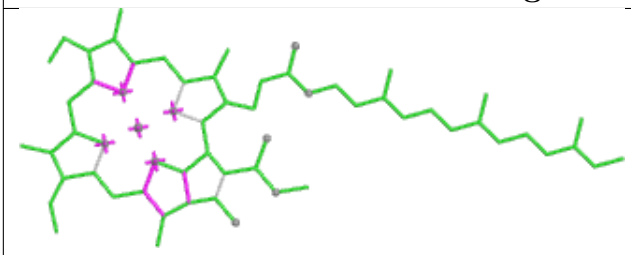


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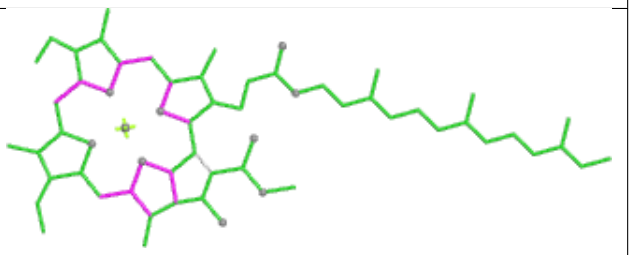


Rings

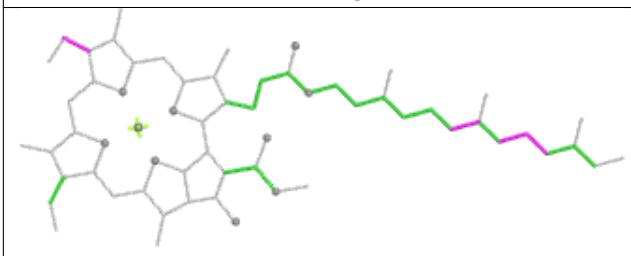
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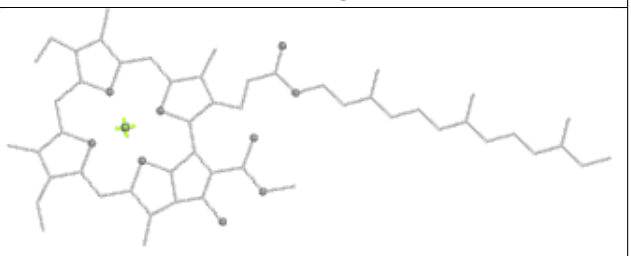
Bond lengths



Bond angles

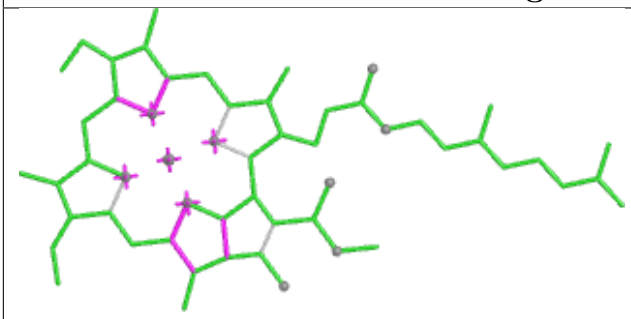


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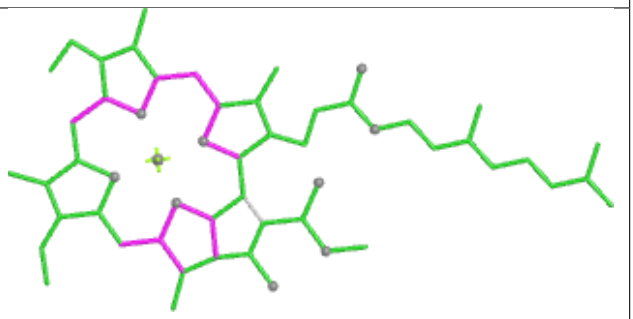


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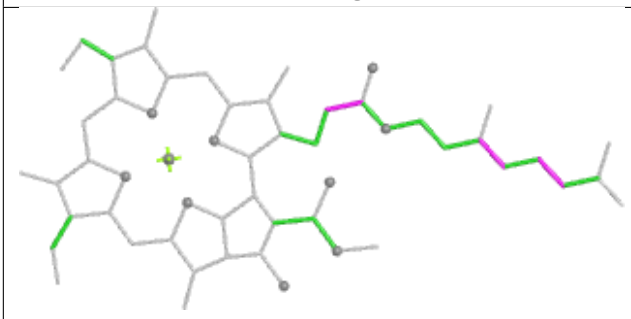
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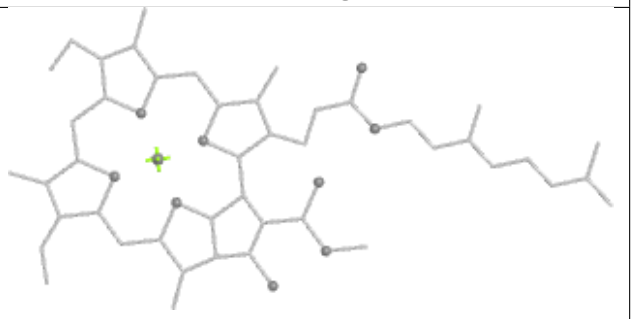
Bond lengths



Bond angles

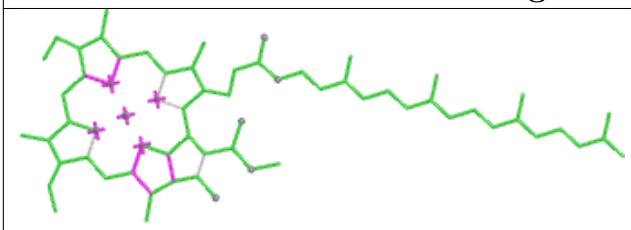


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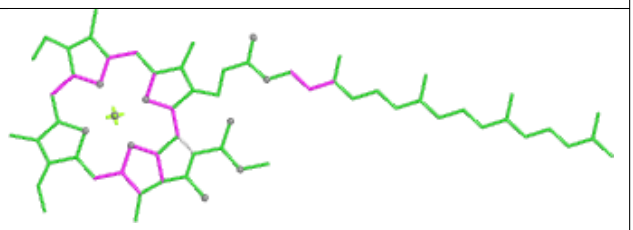


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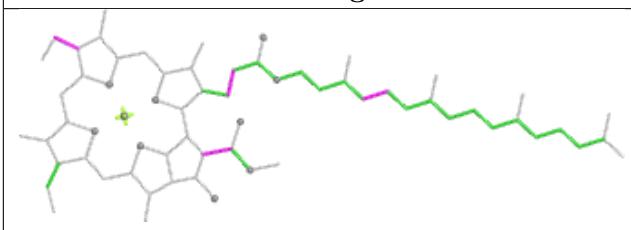
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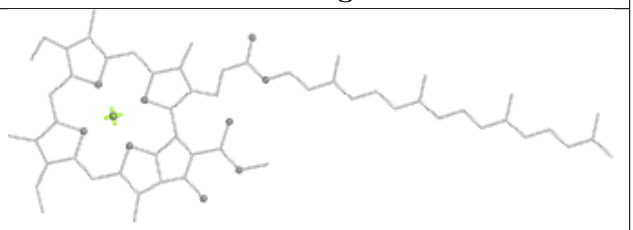
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Bond angles

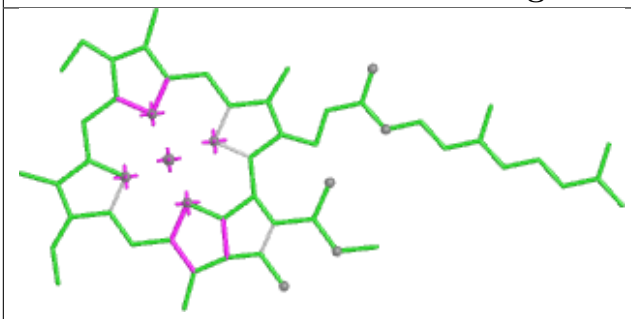


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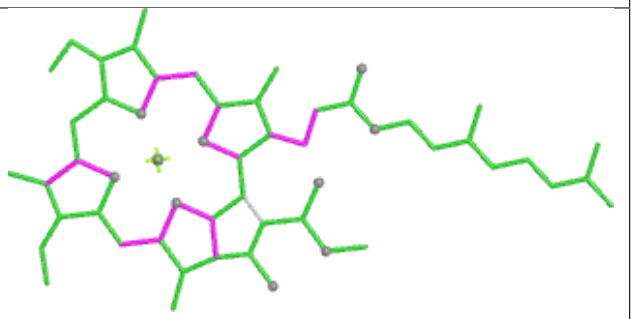


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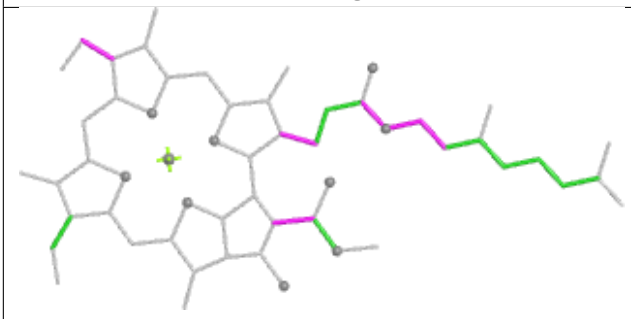
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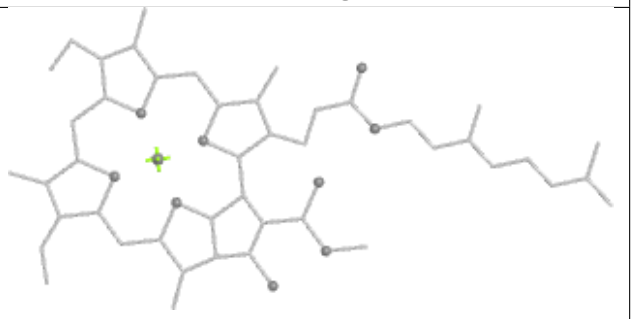
Bond lengths



Bond angles

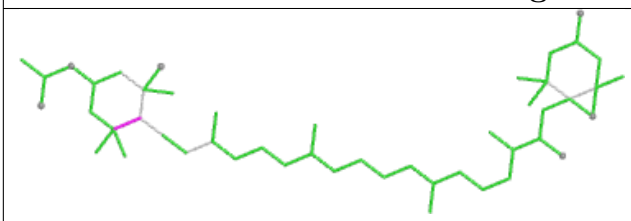


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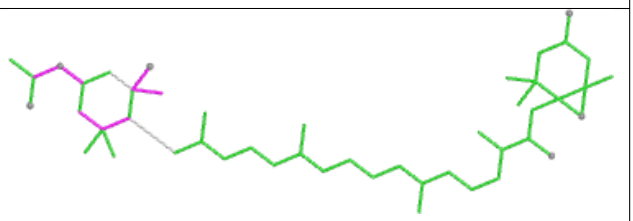


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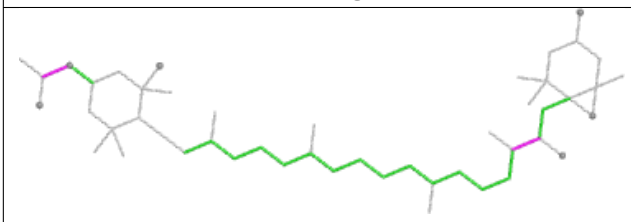
Ligand A86 O 312



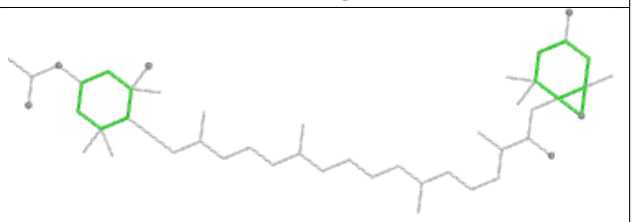
Bond lengths



Bond angles

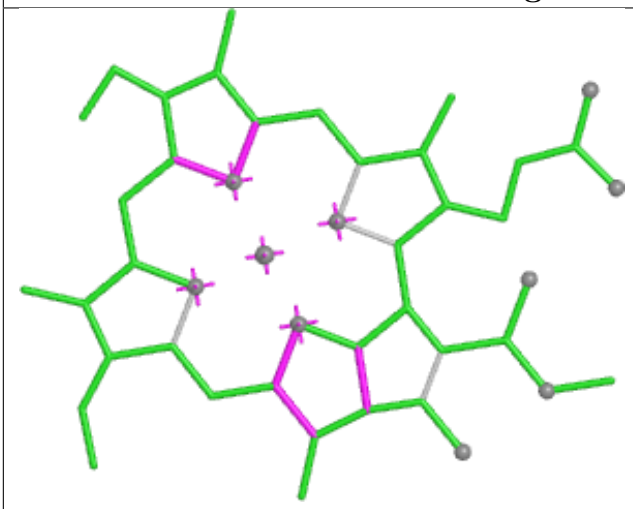


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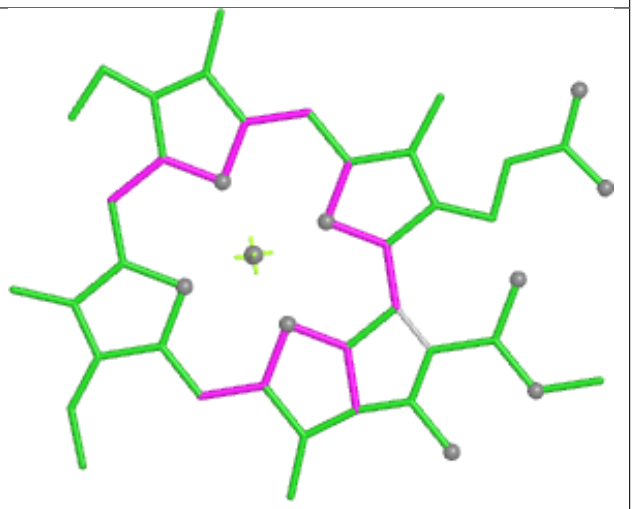


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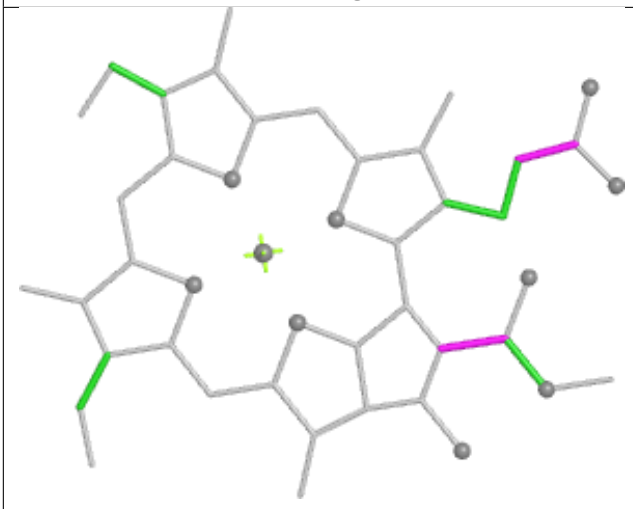
Ligand CLA B 306



Bond lengths



Bond angles

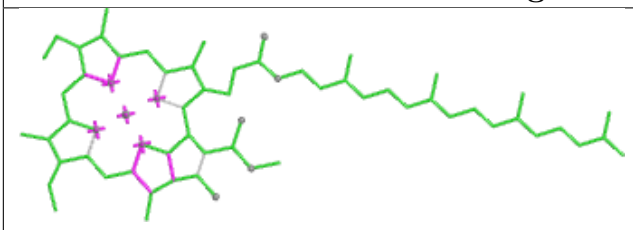


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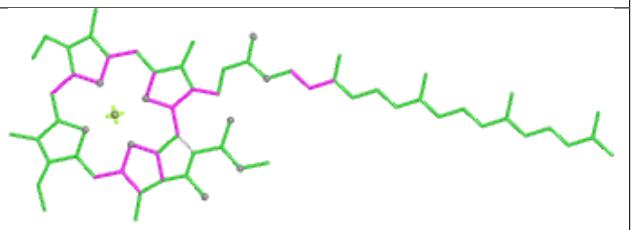


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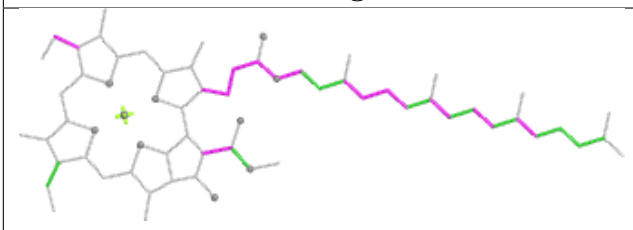
Ligand CLA b 804



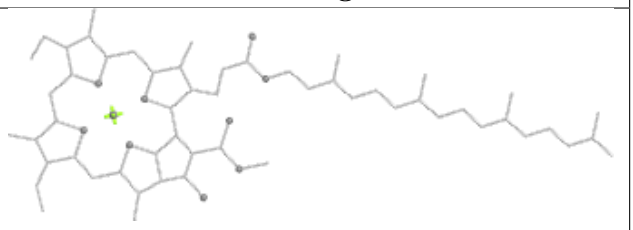
Bond lengths



Bond angles

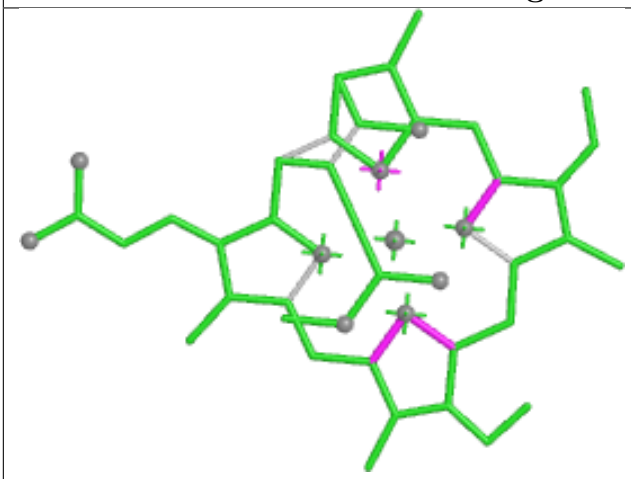


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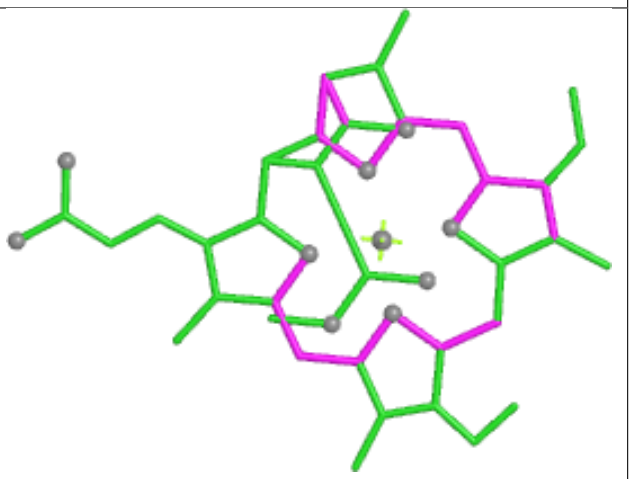


Rings

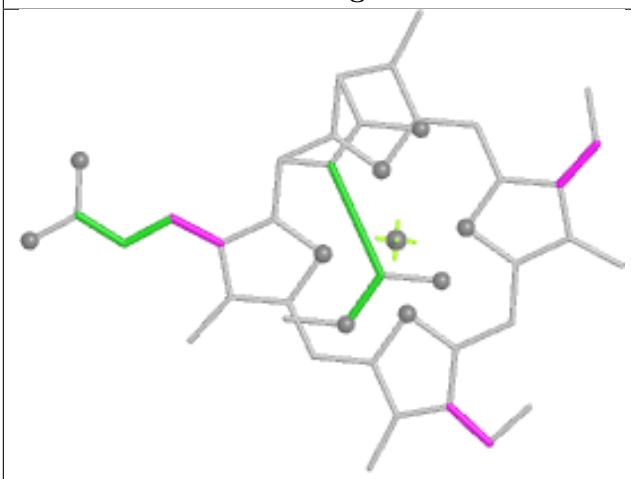
Ligand KC2 P 306



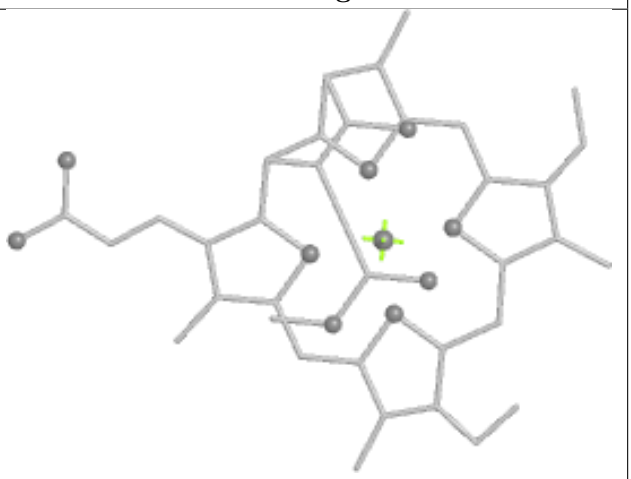
Bond lengths



Bond angles

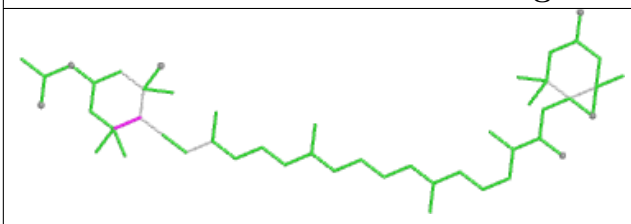


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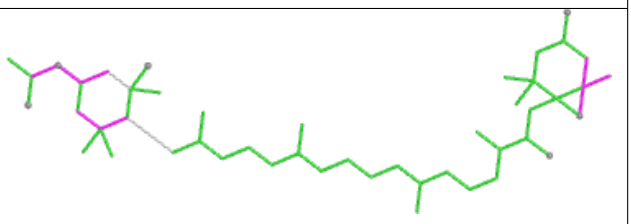


Rings

Ligand A86 J 313



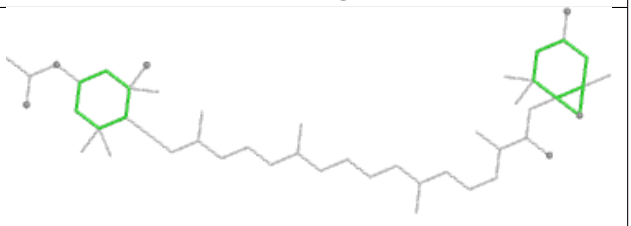
Bond lengths



Bond angles

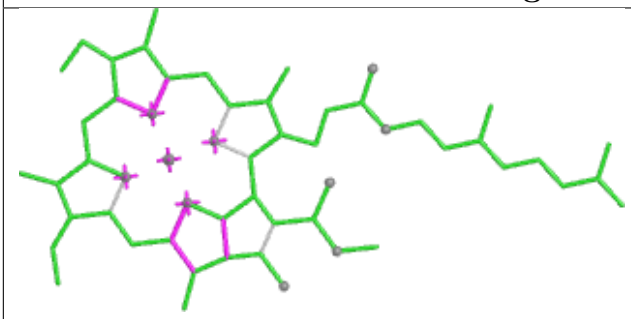


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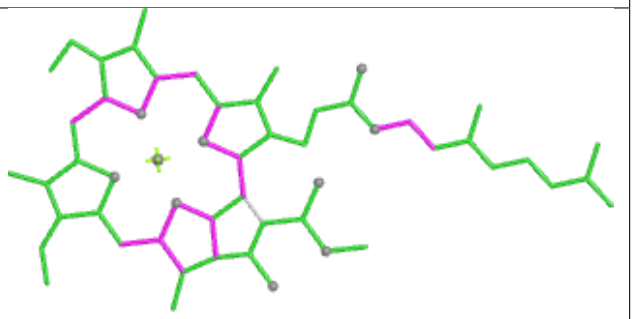


Rings

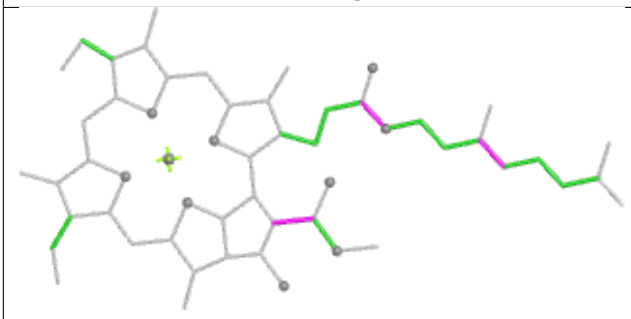
Ligand CLA D 312



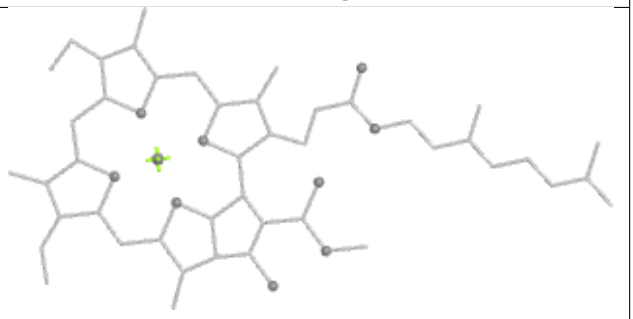
Bond lengths



Bond angles

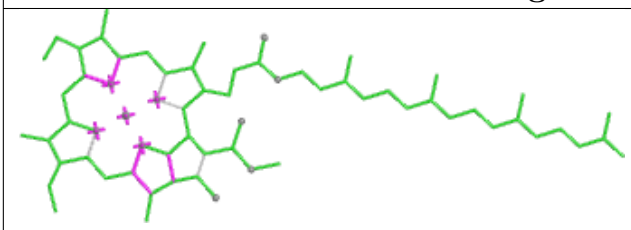


Torsions

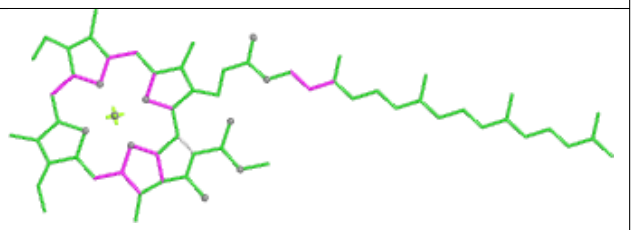


Rings

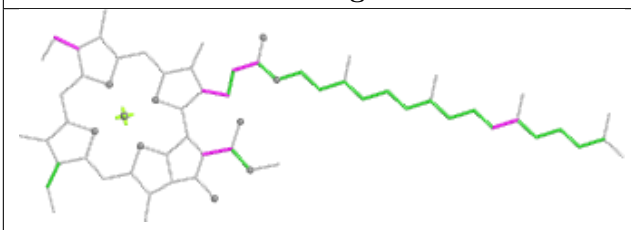
Ligand CLA a 840



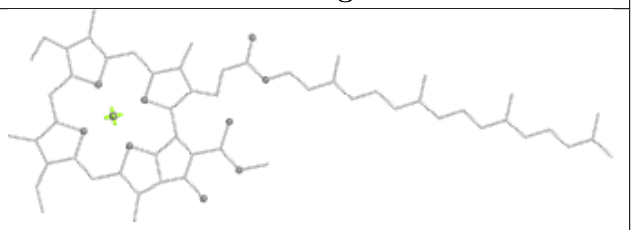
Bond lengths



Bond angles

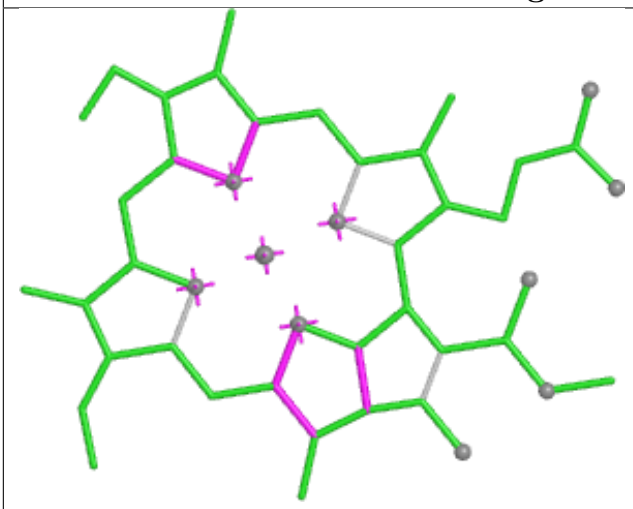


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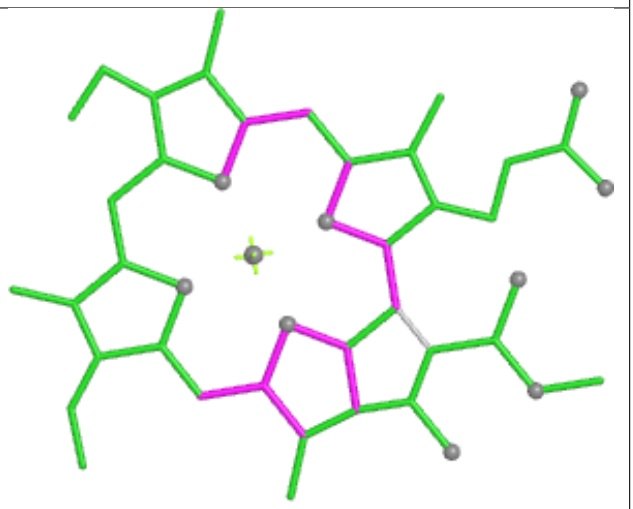


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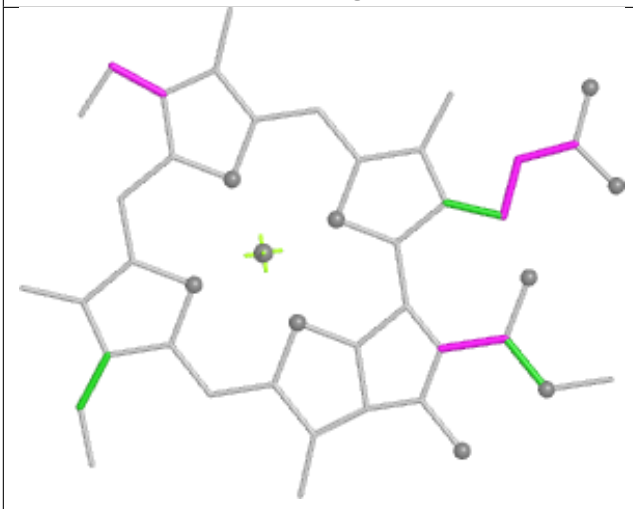
Ligand CLA b 814



Bond lengths



Bond angles

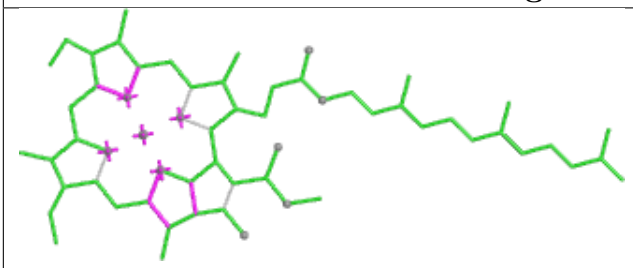


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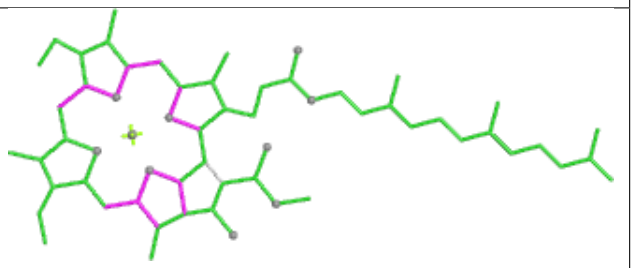


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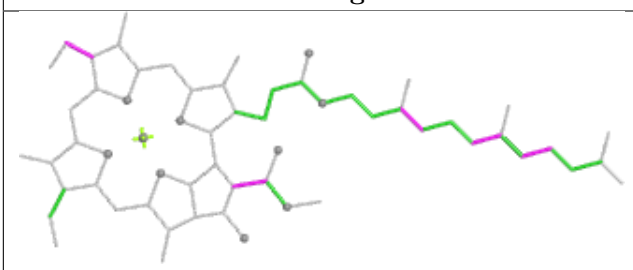
Ligand CLA E 306



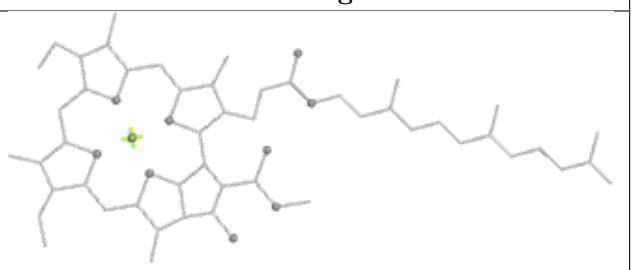
Bond lengths



Bond angles

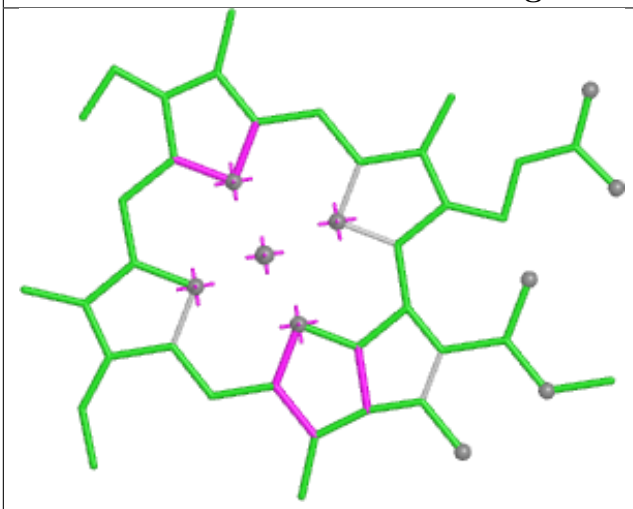


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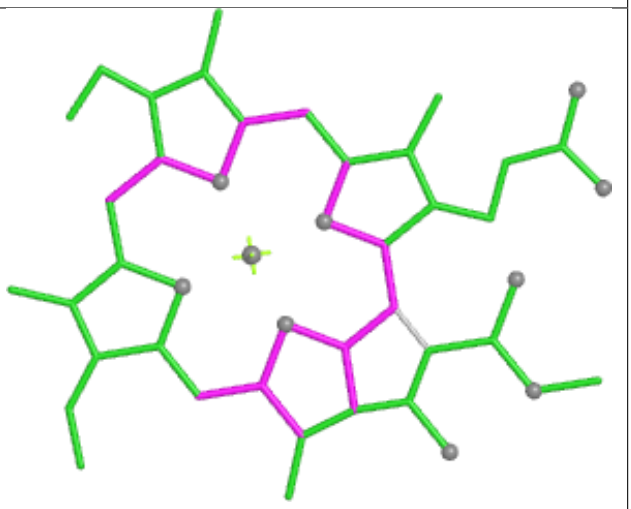


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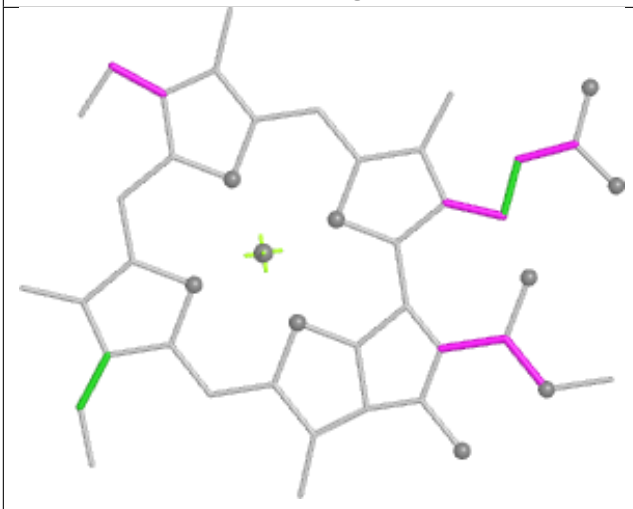
Ligand CLA T 305



Bond lengths



Bond angles

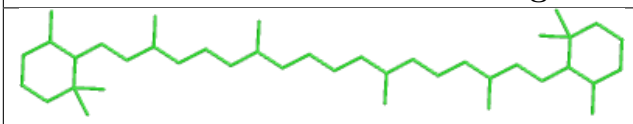


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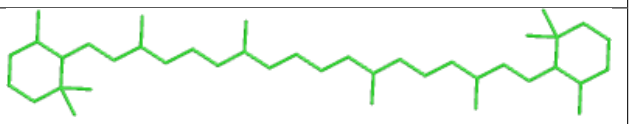


Rings

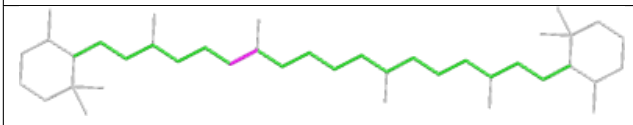
Ligand BCR f 202



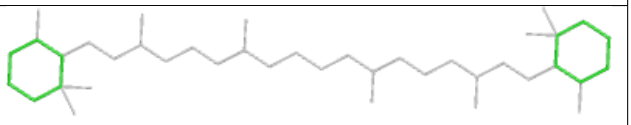
Bond lengths



Bond angles

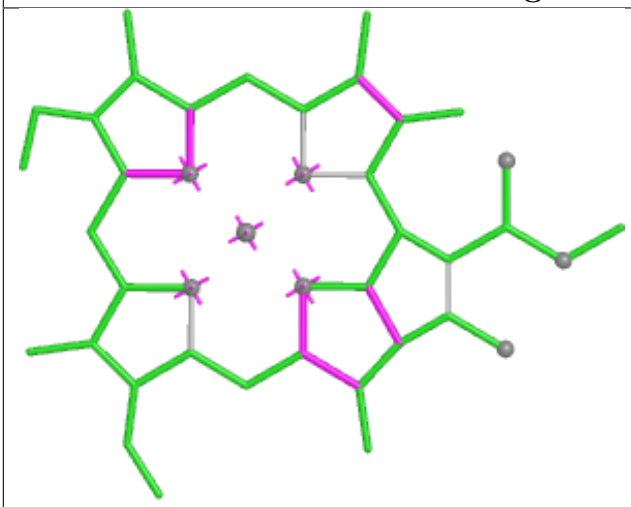


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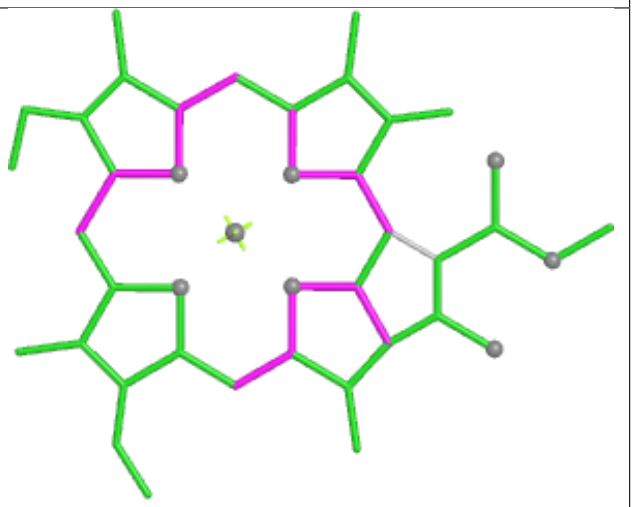


Rings

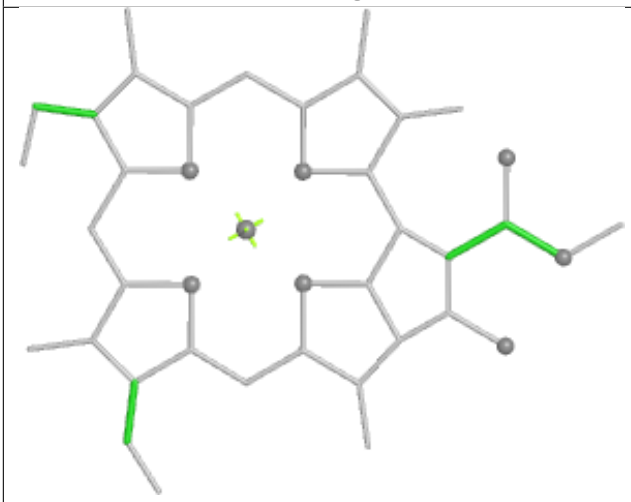
Ligand CLA C 302



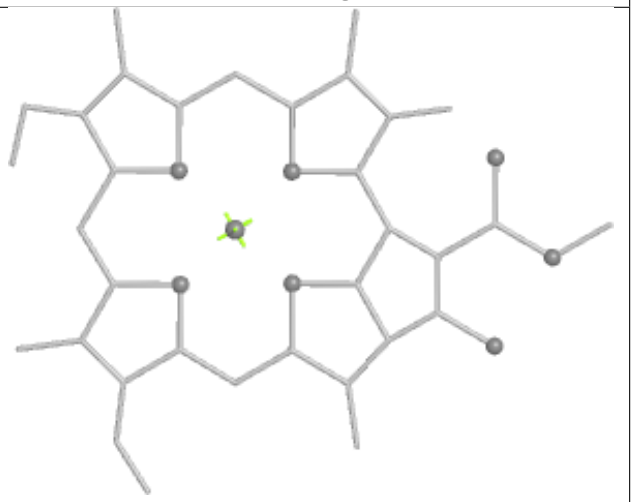
Bond lengths



Bond angles

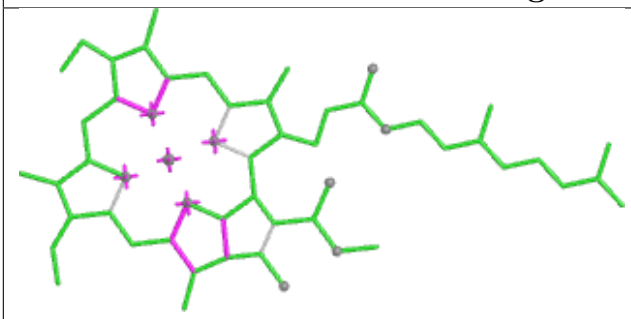


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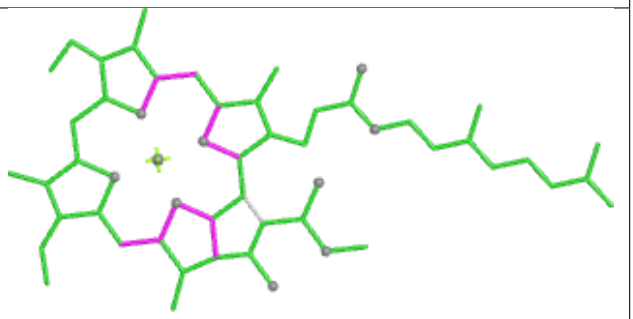


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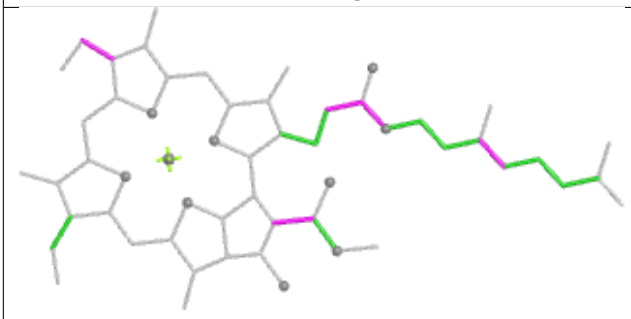
Ligand CLA k 202



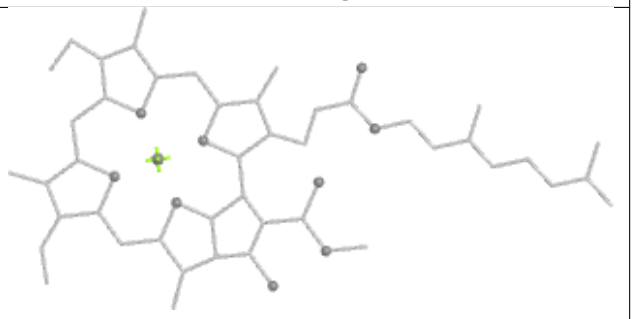
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Bond angles

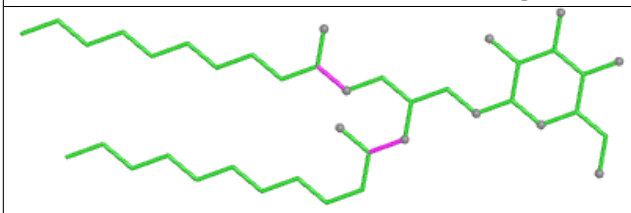


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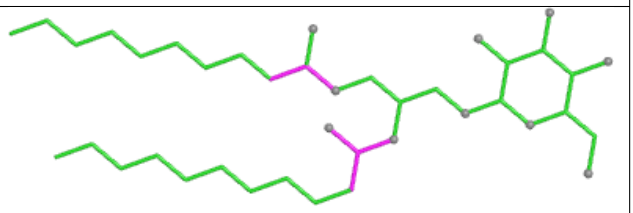


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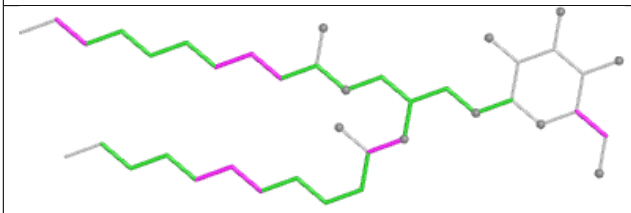
Ligand LMG M 320



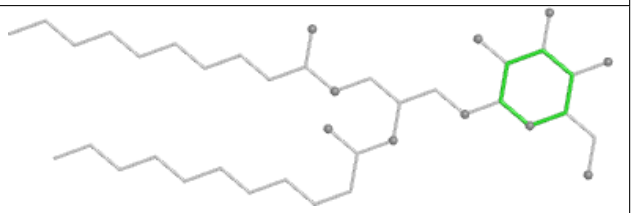
Bond lengths



Bond angles

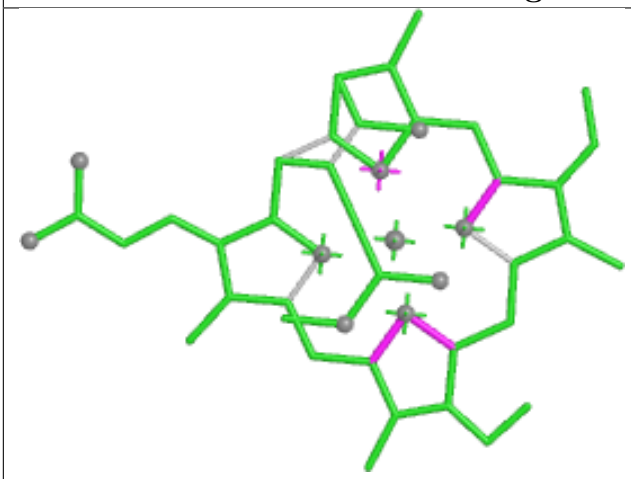


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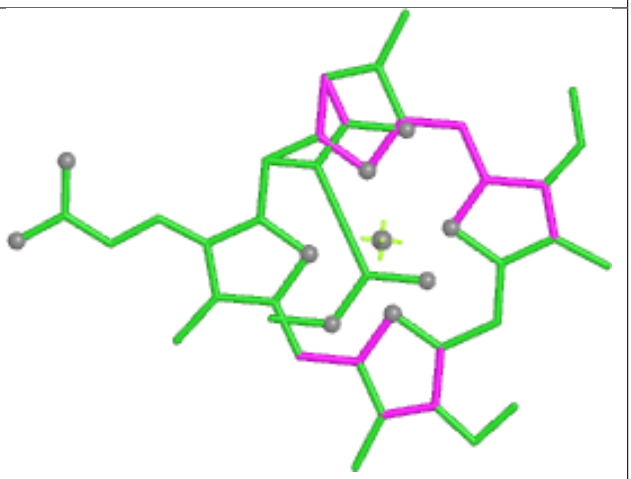


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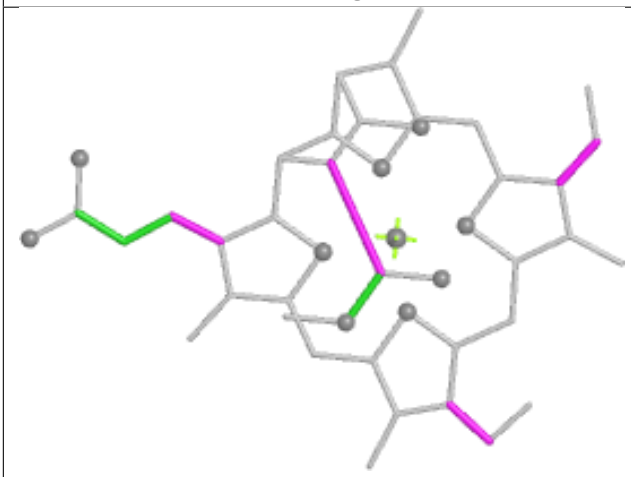
Ligand KC2 H 303



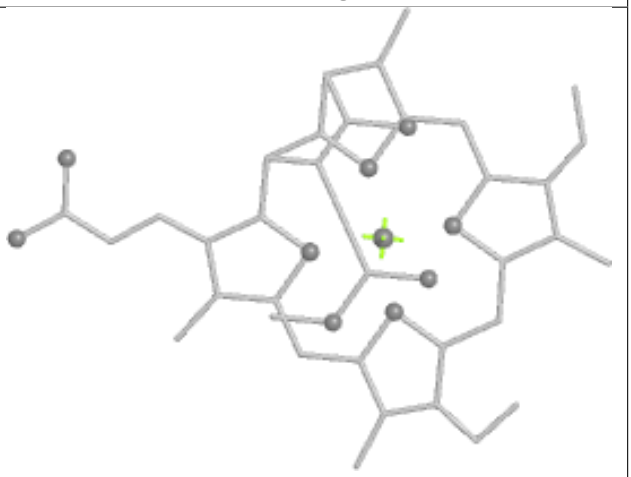
Bond lengths



Bond angles

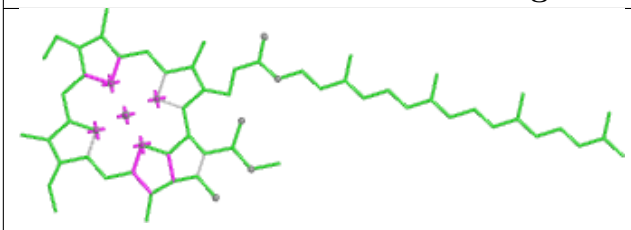


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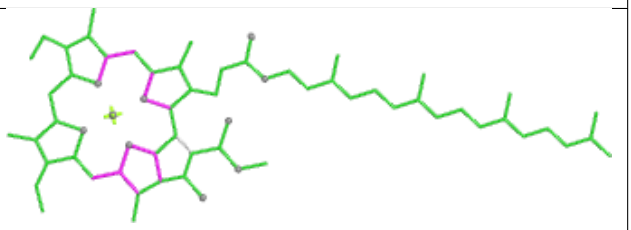


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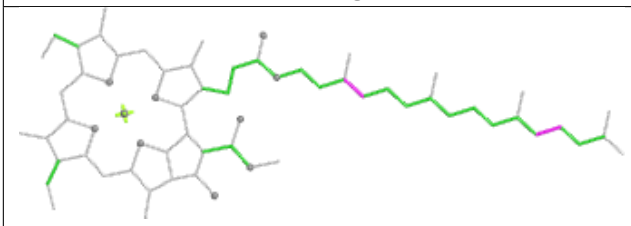
Ligand CLA I 317



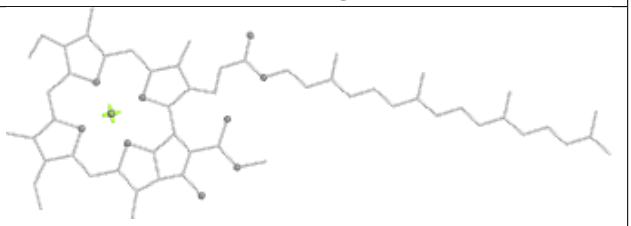
Bond lengths



Bond angles

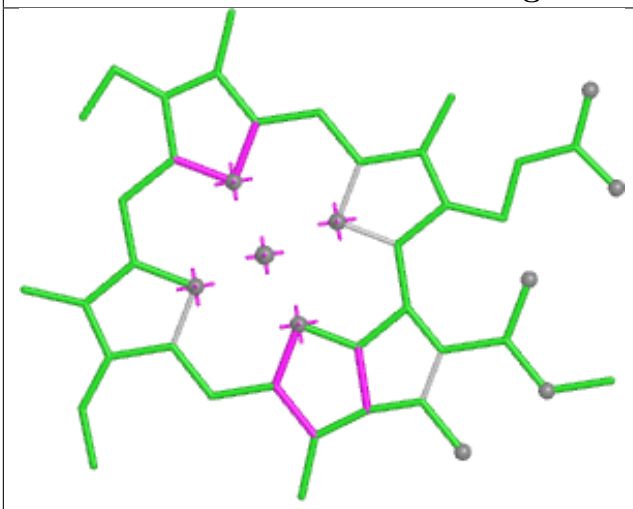


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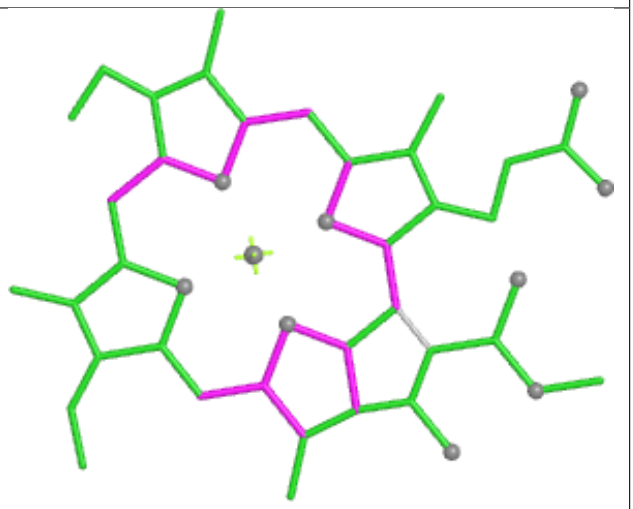


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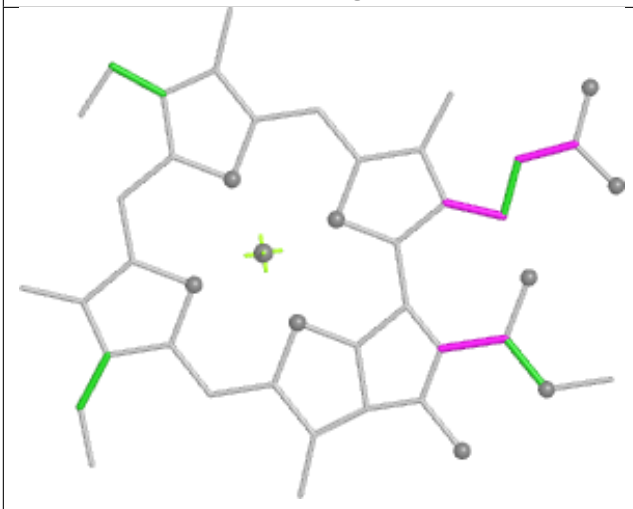
Ligand CLA K 310



Bond lengths



Bond angles

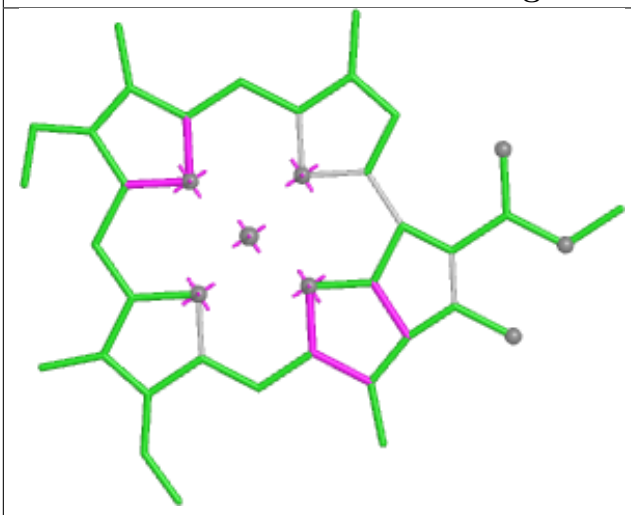


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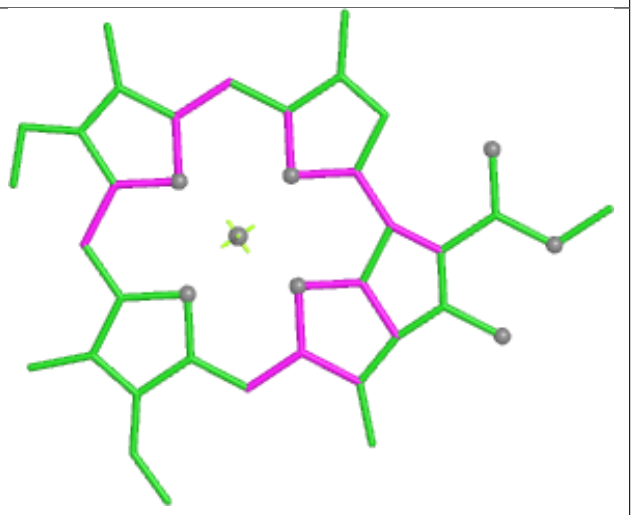


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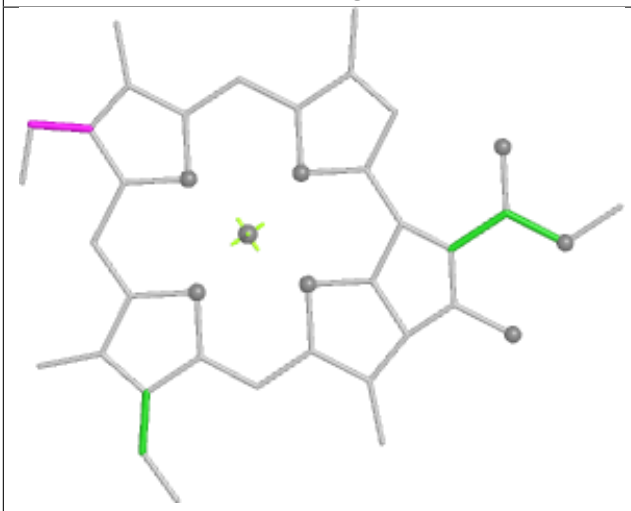
Ligand CLA G 307



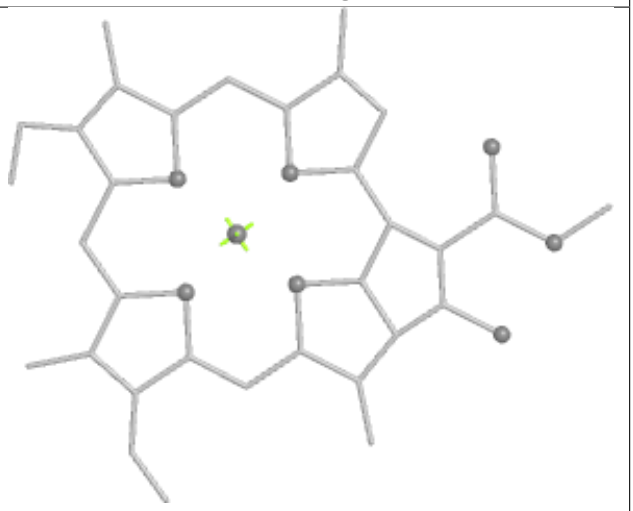
Bond lengths



Bond angles

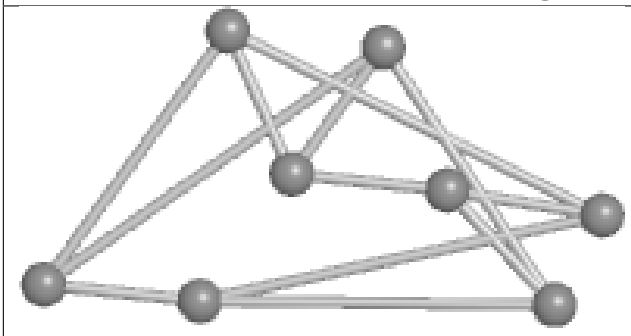


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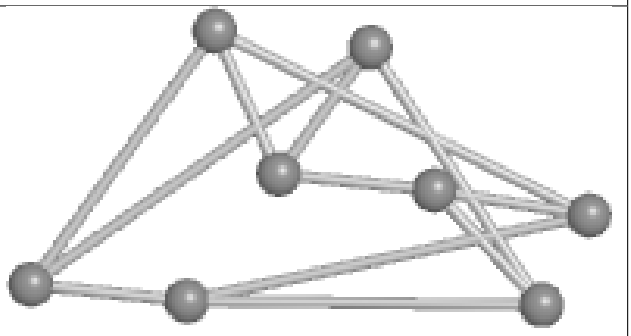


Rings

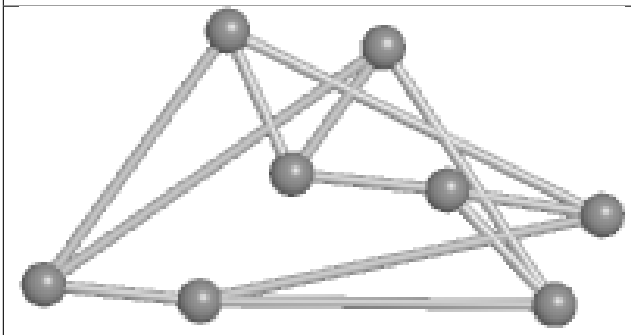
Ligand SF4 c 102



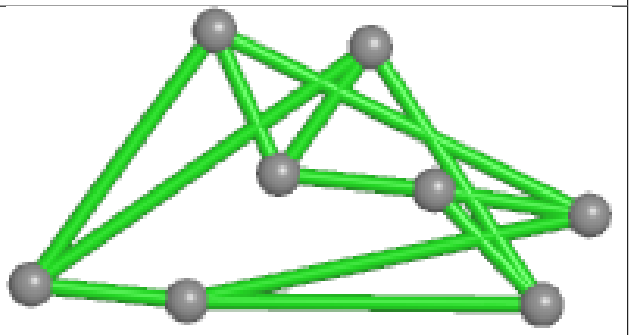
Bond lengths



Bond angles

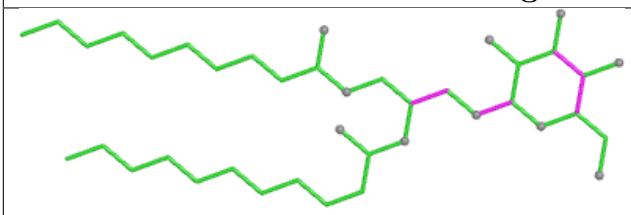


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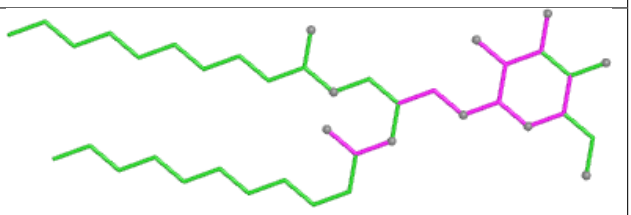


Rings

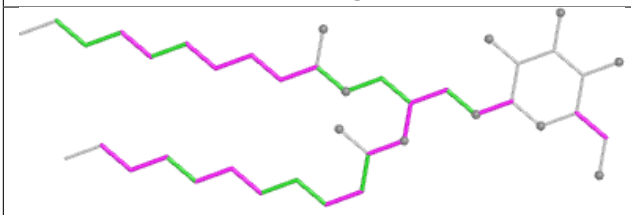
Ligand LMG E 302



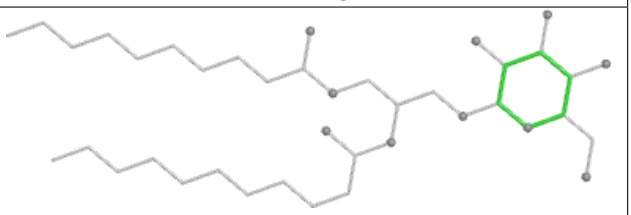
Bond lengths



Bond angles

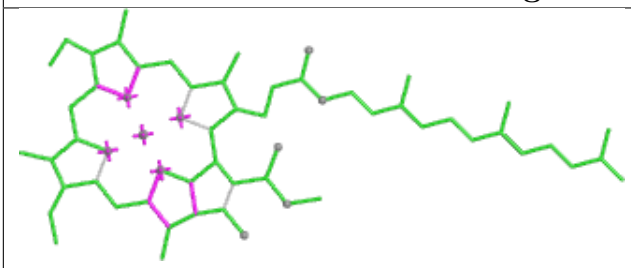


Torsions

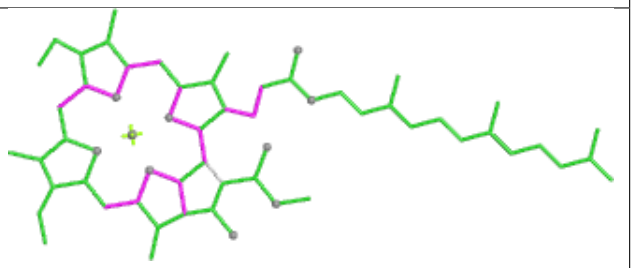


Rings

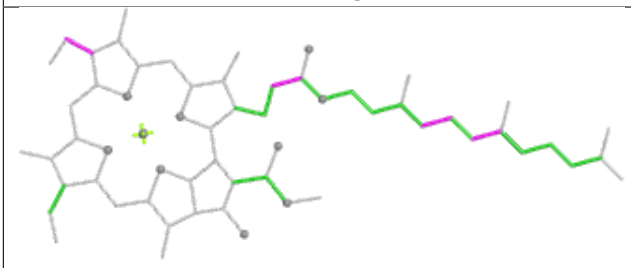
Ligand CLA N 311



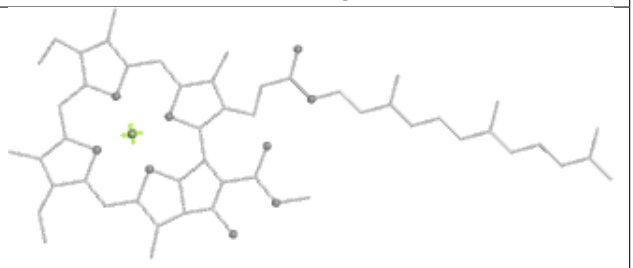
Bond lengths



Bond angles

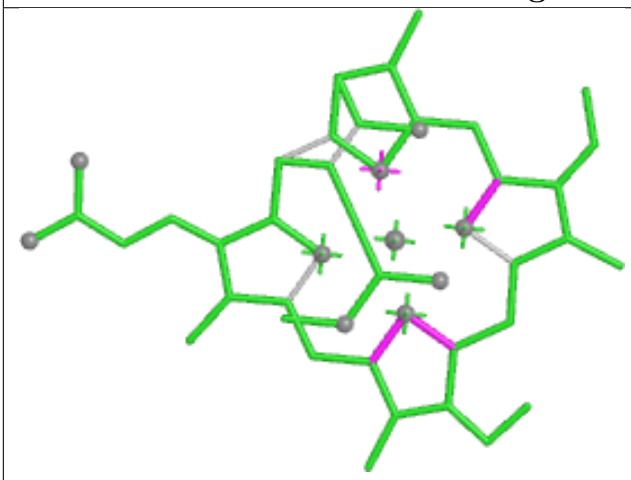


Torsions

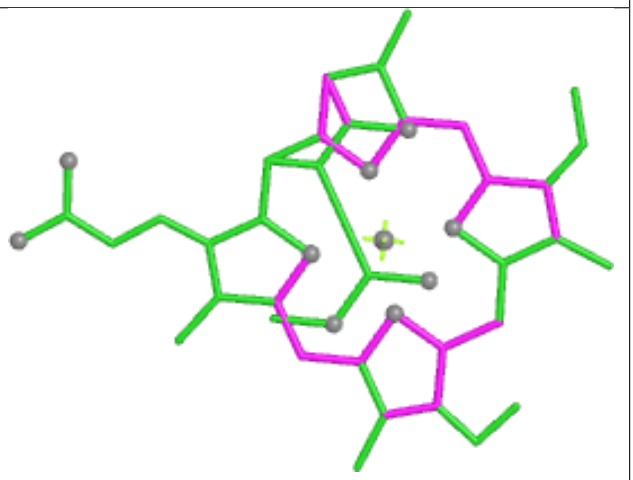


Rings

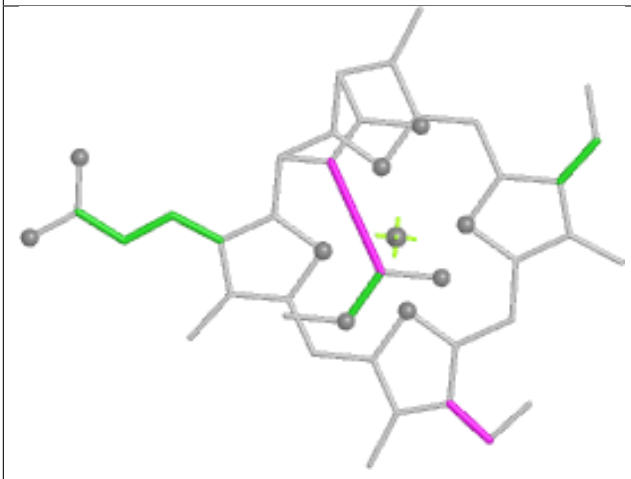
Ligand KC2 L 303



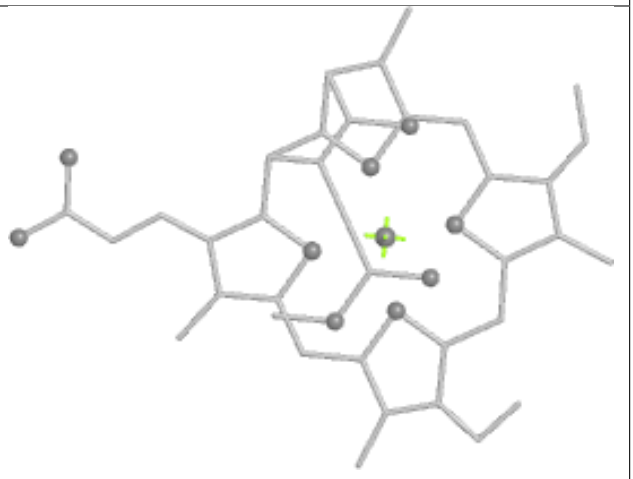
Bond lengths



Bond angles

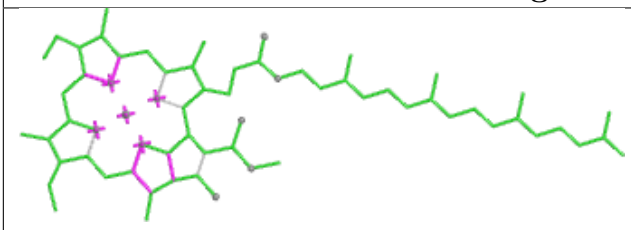


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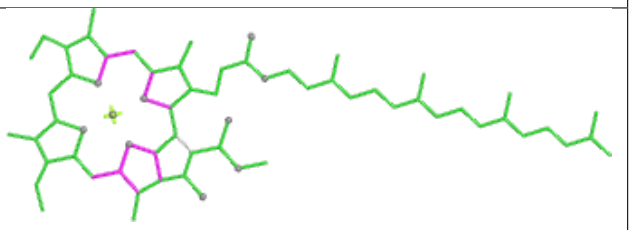


Rings

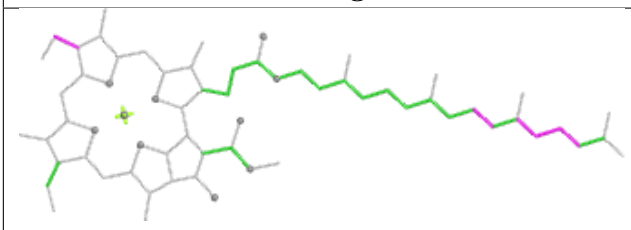
Ligand CLA I 306



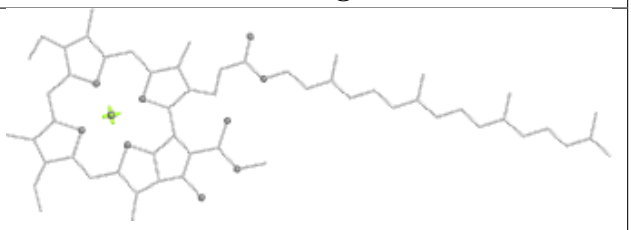
Bond lengths



Bond angles

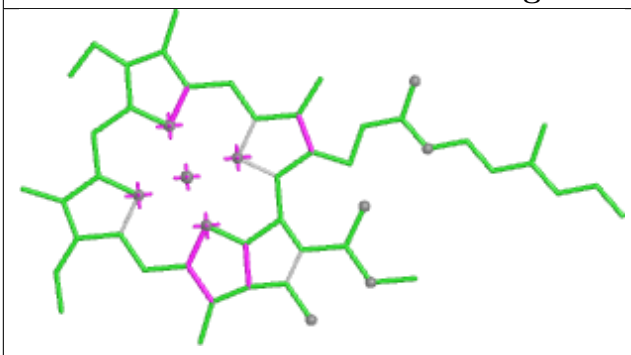


Torsions

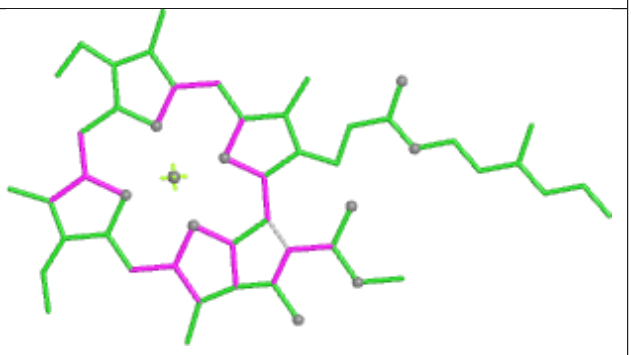


Rings

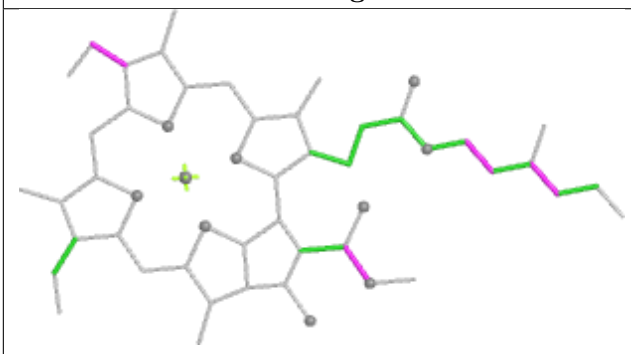
Ligand CLA D 314



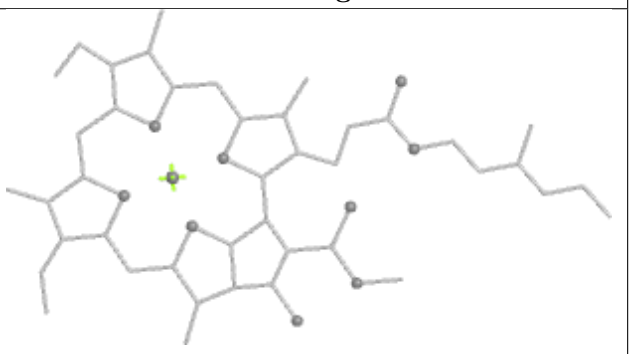
Bond lengths



Bond angles

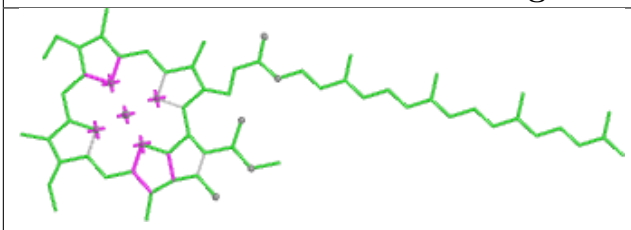


Torsions

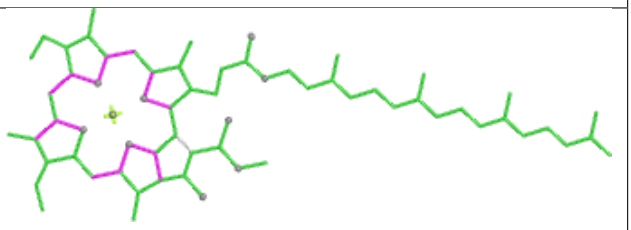


Rings

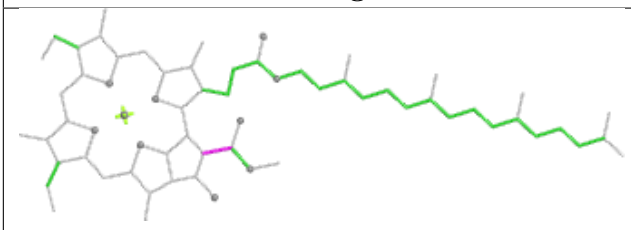
Ligand CLA a 825



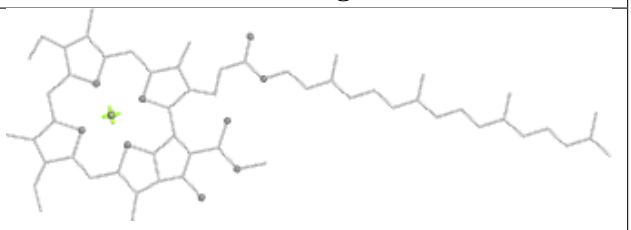
Bond lengths



Bond angles

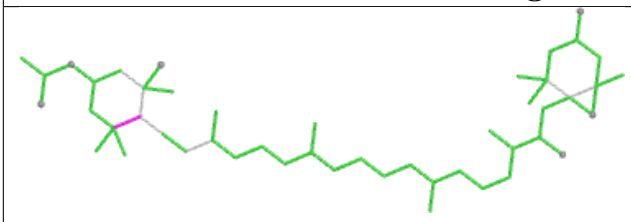


Torsions

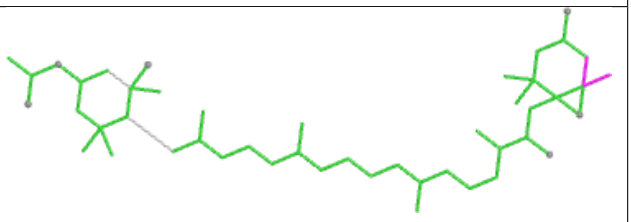


Rings

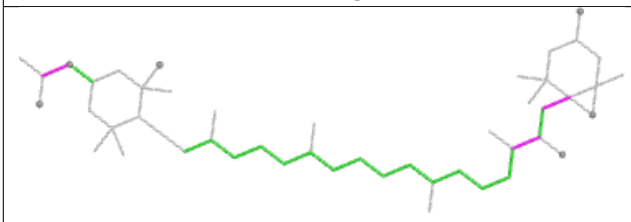
Ligand A86 M 317



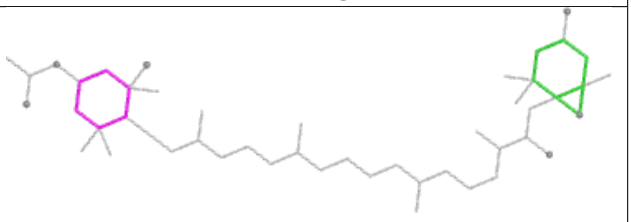
Bond lengths



Bond angles

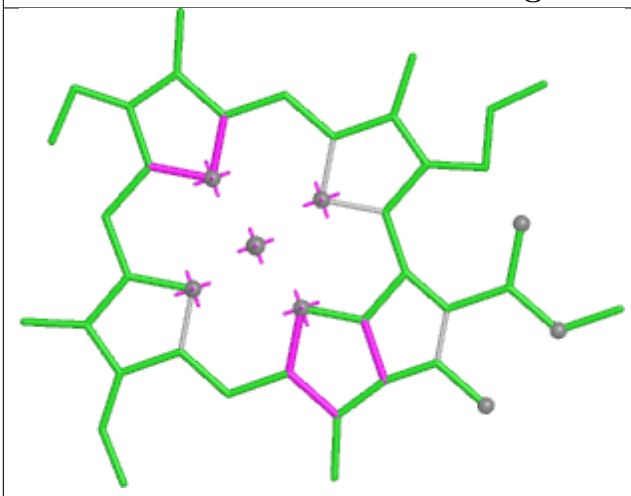


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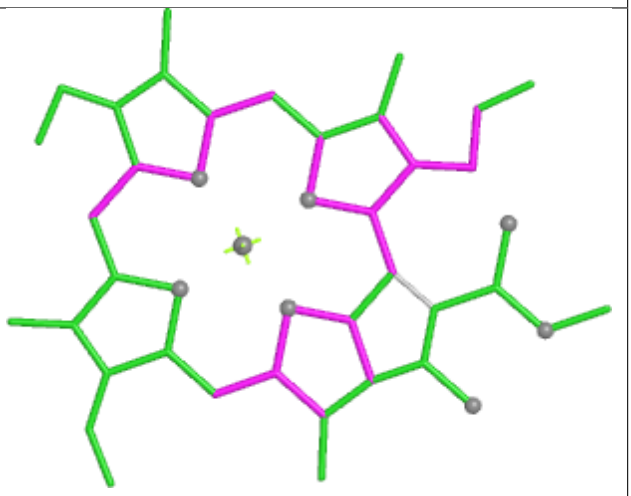


Rings

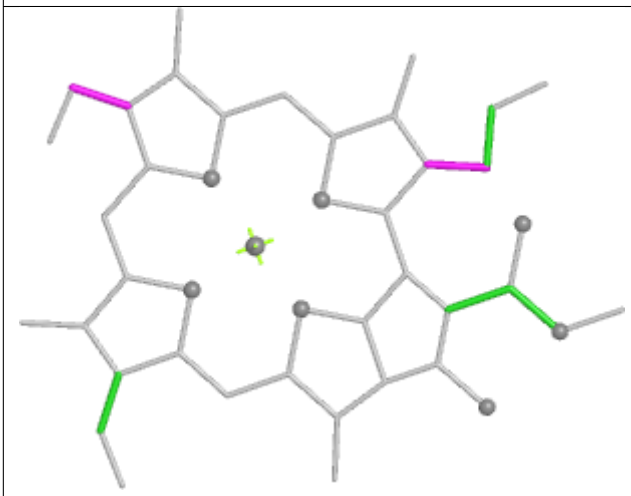
Ligand CLA C 304



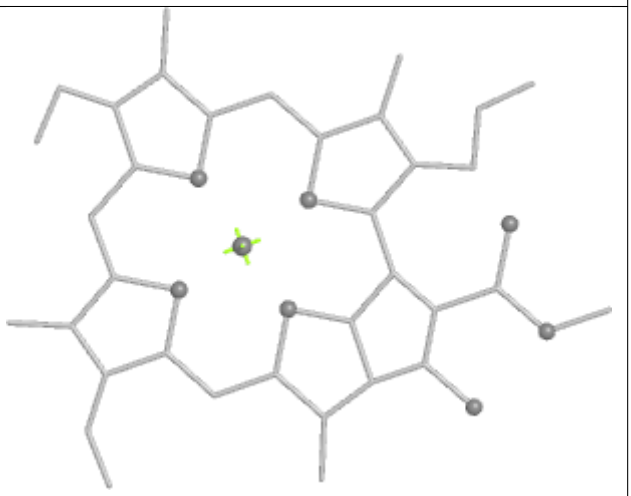
Bond lengths



Bond angles

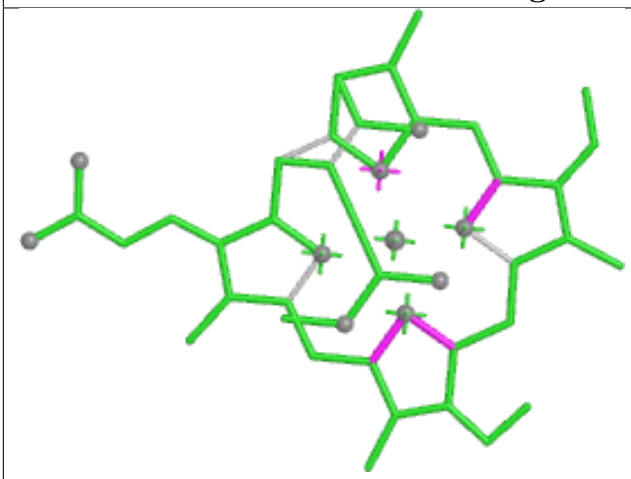


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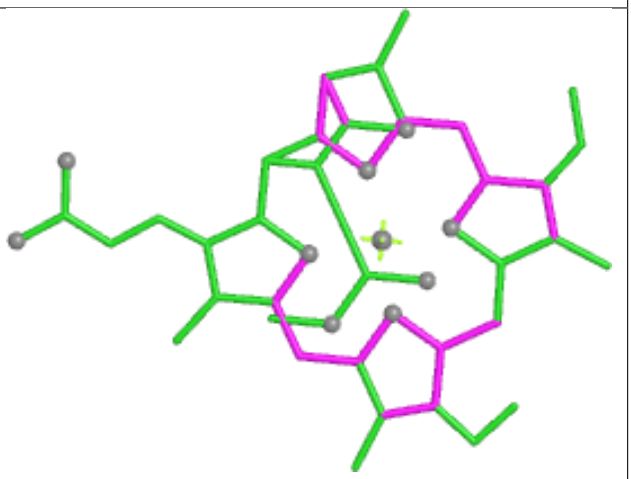


Rings

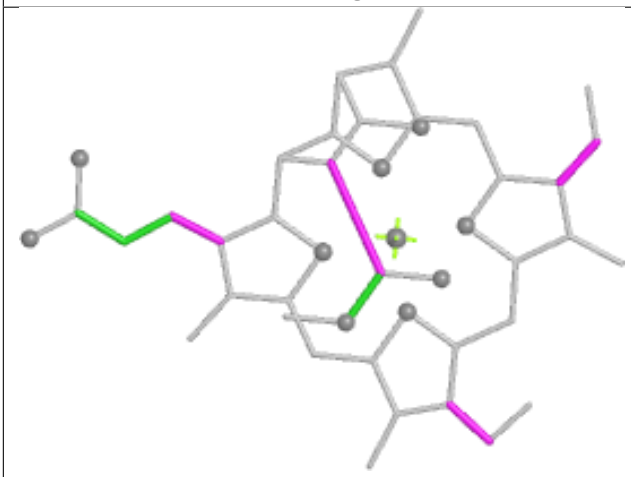
Ligand KC2 S 303



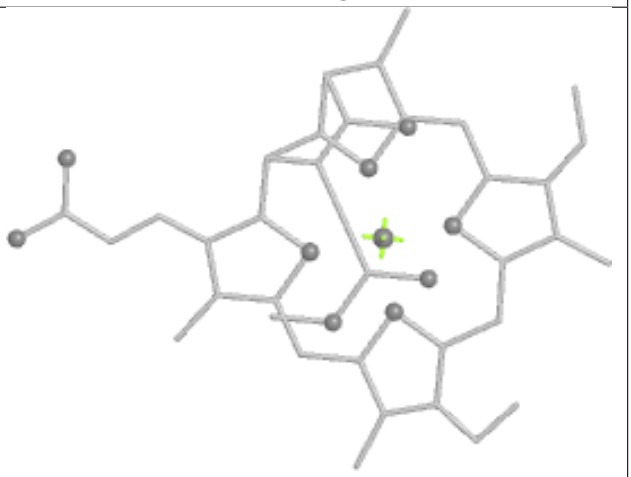
Bond lengths



Bond angles



Torsions



Rings

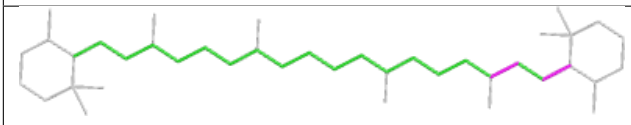
Ligand BCR a 845



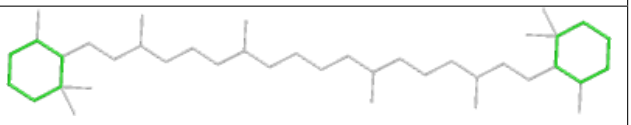
Bond lengths



Bond angles

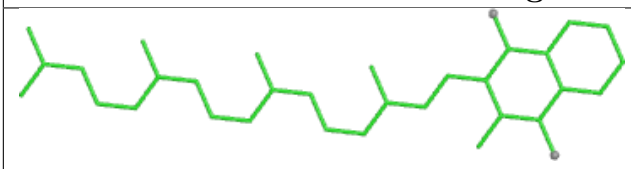


Torsions

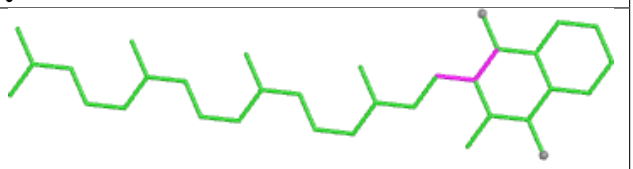


Rings

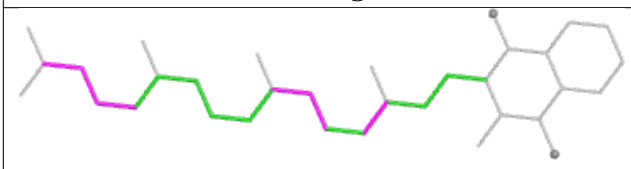
Ligand PQN a 848



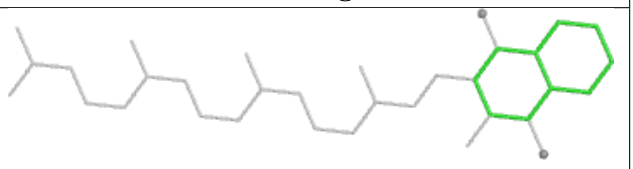
Bond lengths



Bond angles

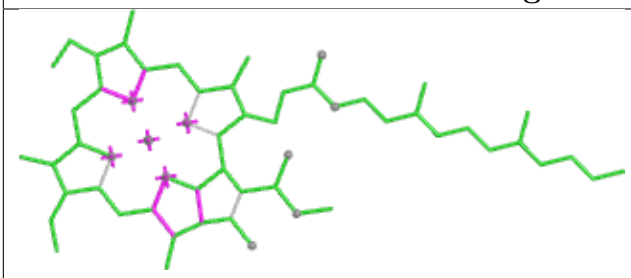


Torsions

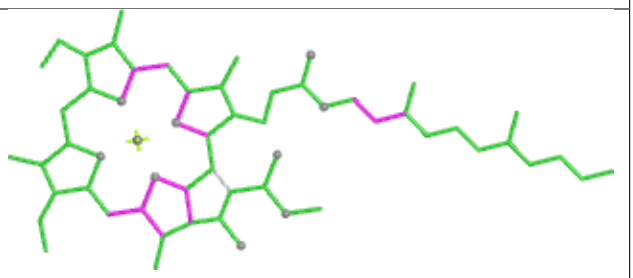


Rings

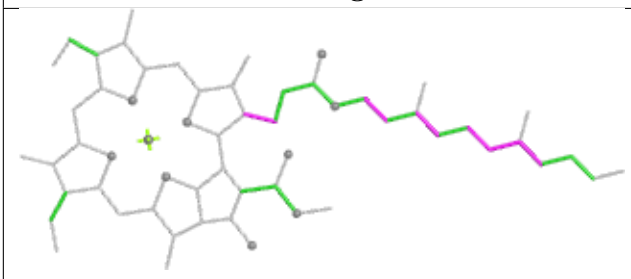
Ligand CLA D 305



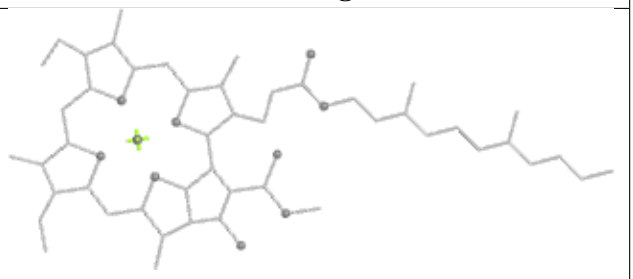
Bond lengths



Bond angles

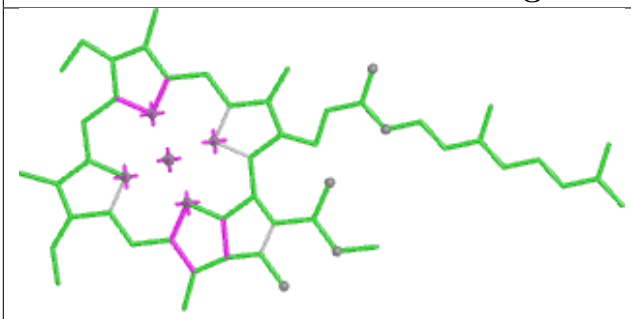


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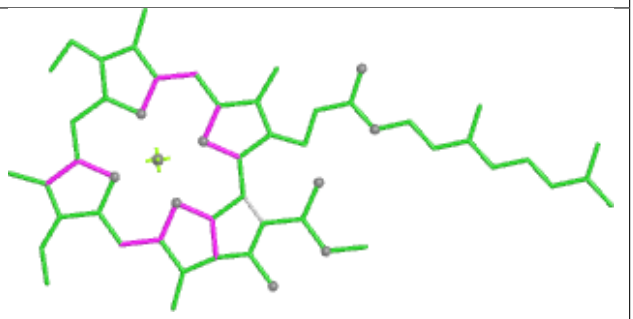


Rings

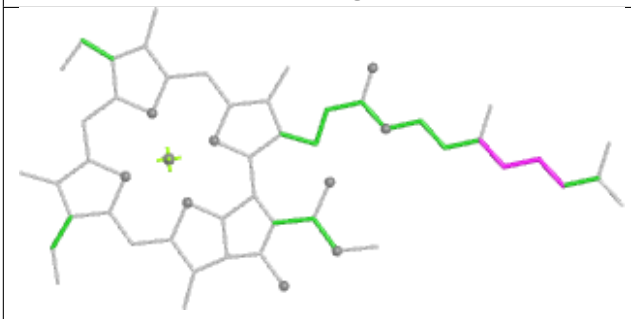
Ligand CLA A 308



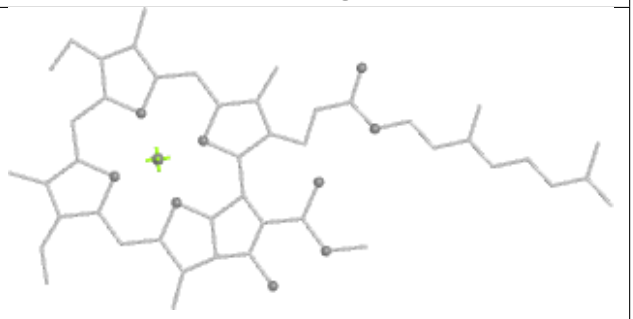
Bond lengths



Bond angles

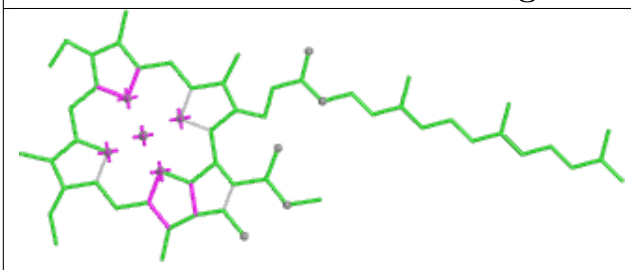


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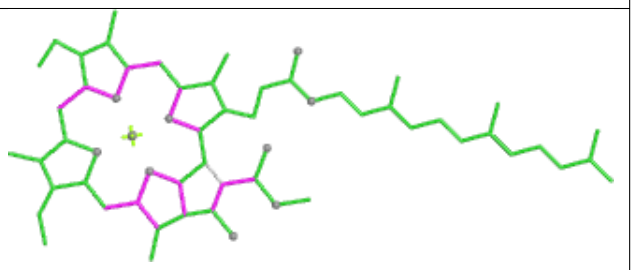


Rings

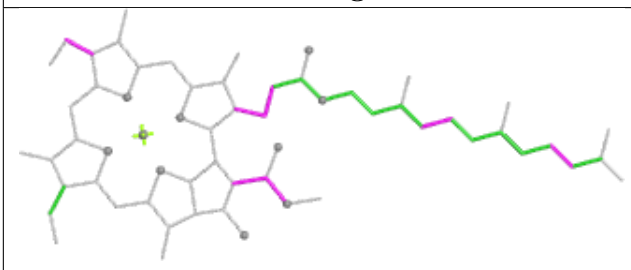
Ligand CLA W 310



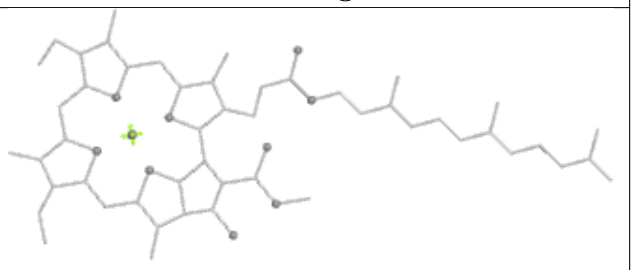
Bond lengths



Bond angles

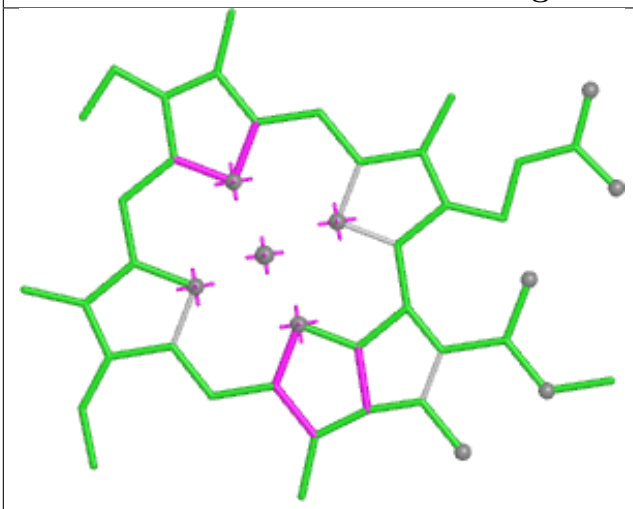


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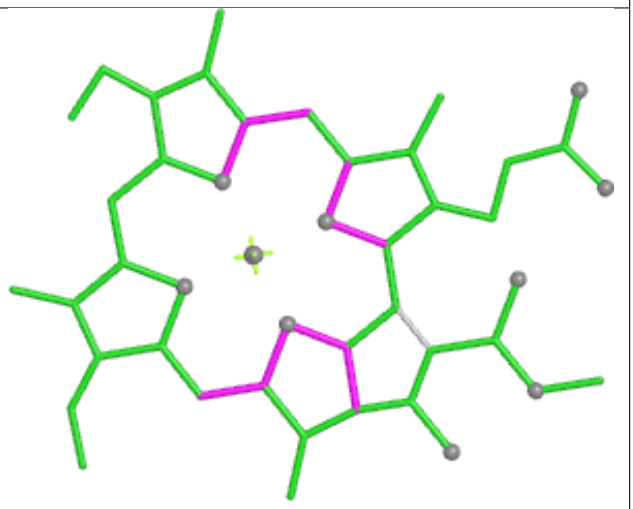


Rings

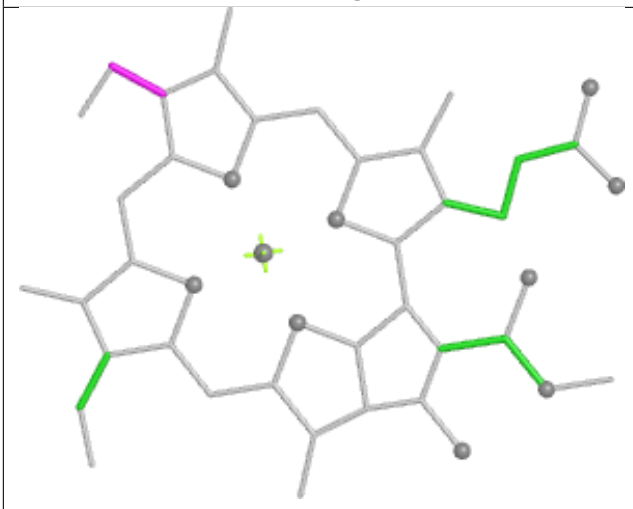
Ligand CLA f 203



Bond lengths



Bond angles

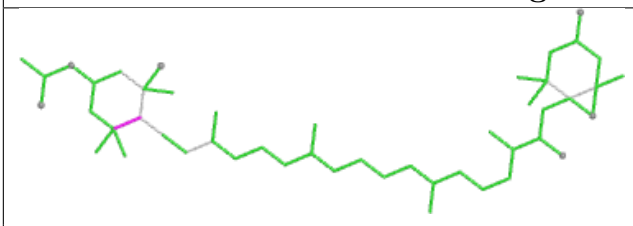


Torsions

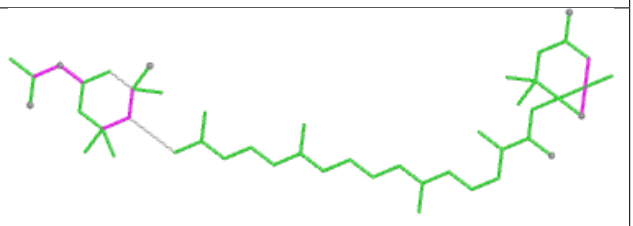


Rings

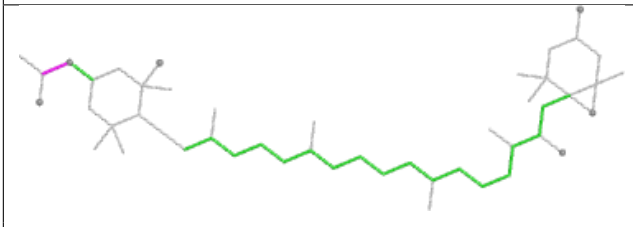
Ligand A86 U 308



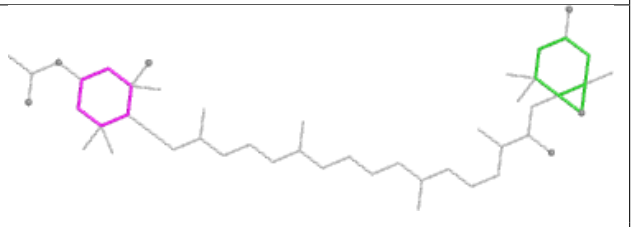
Bond lengths



Bond angles

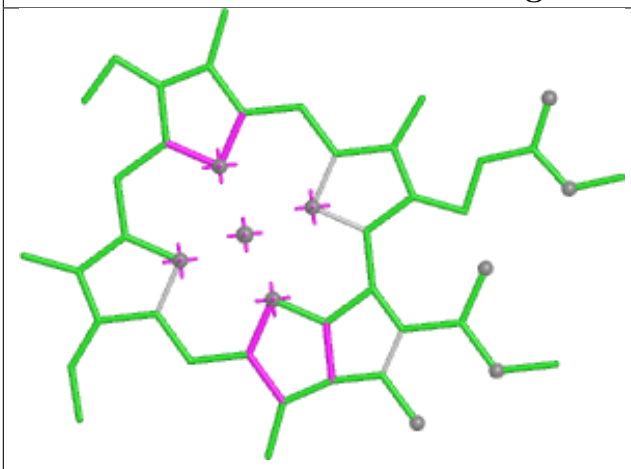


Torsions

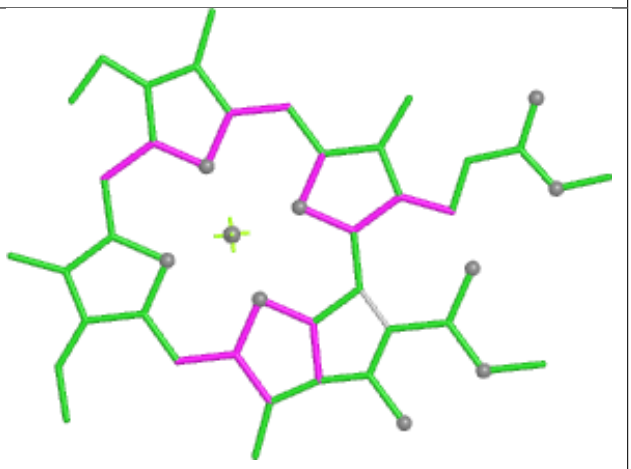


Rings

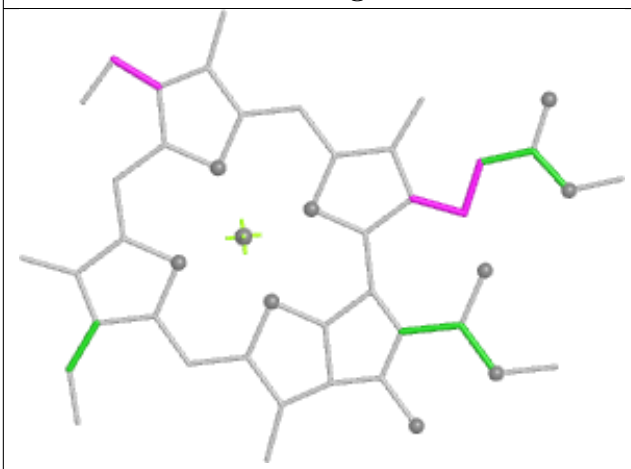
Ligand CLA E 315



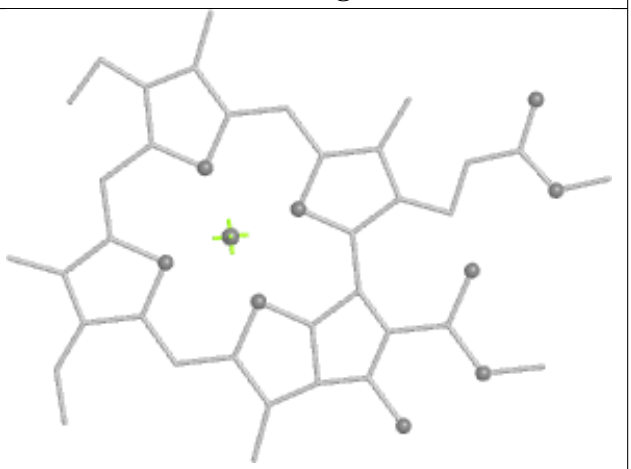
Bond lengths



Bond angles

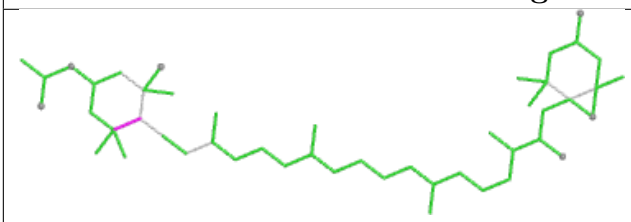


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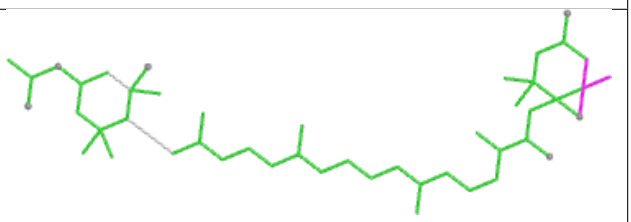


Rings

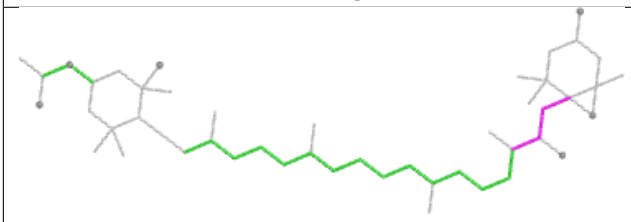
Ligand A86 P 319



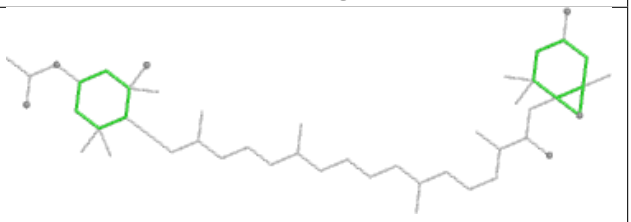
Bond lengths



Bond angles

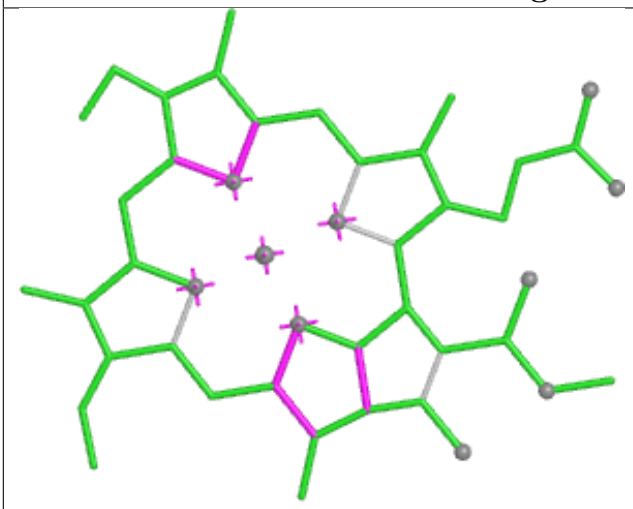


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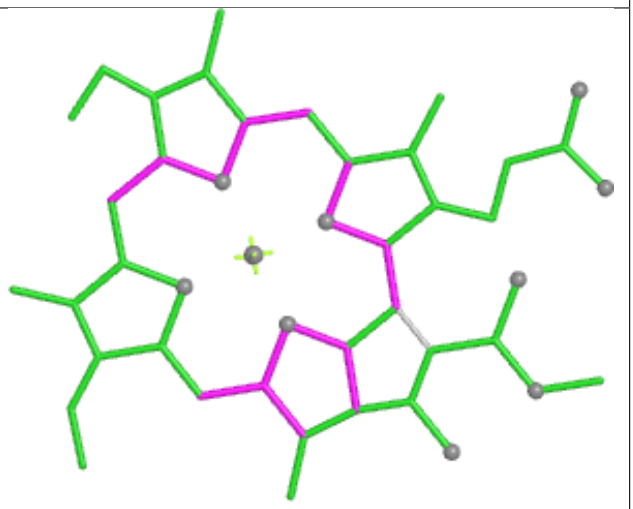


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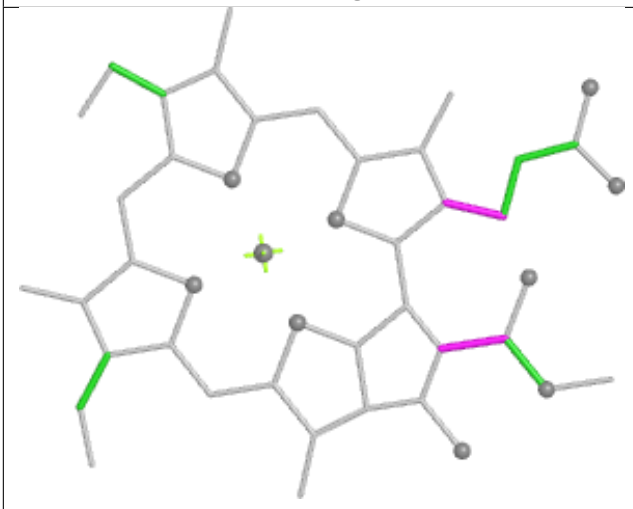
Ligand CLA I 307



Bond lengths



Bond angles

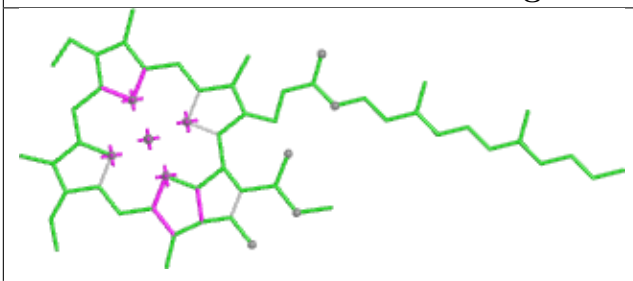


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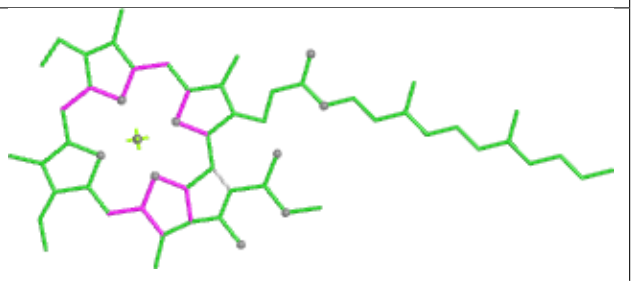


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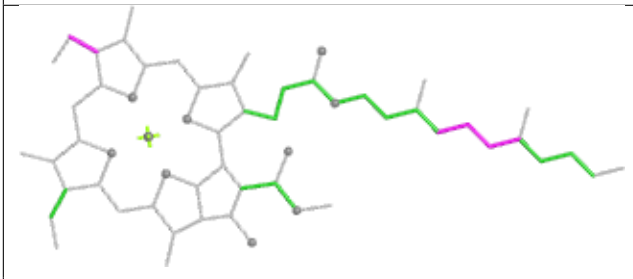
Ligand CLA V 201



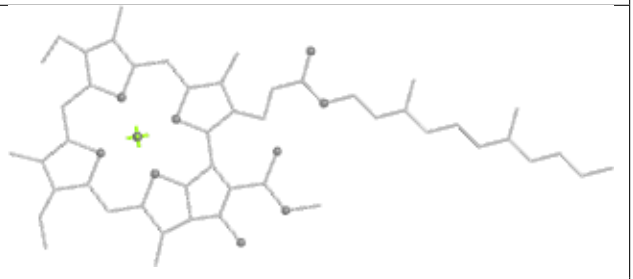
Bond lengths



Bond angles

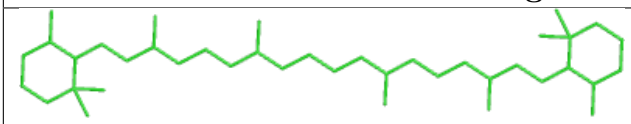


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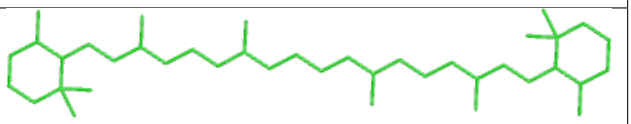


Rings

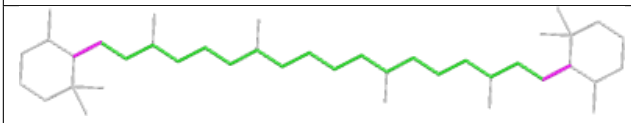
Ligand BCR b 844



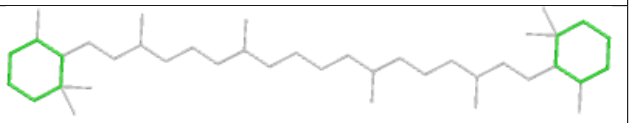
Bond lengths



Bond angles

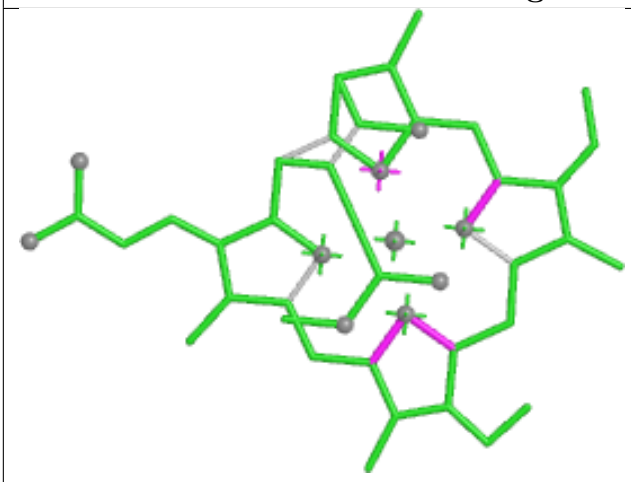


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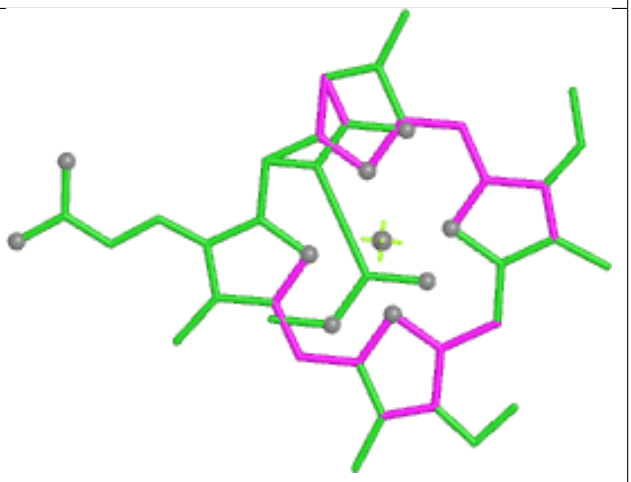


Rings

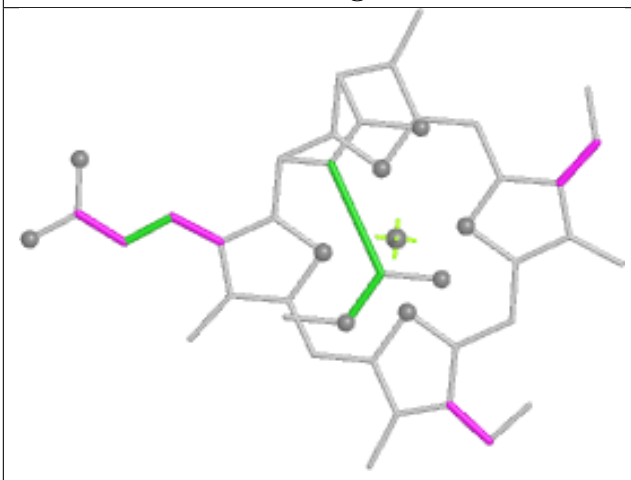
Ligand KC2 P 312



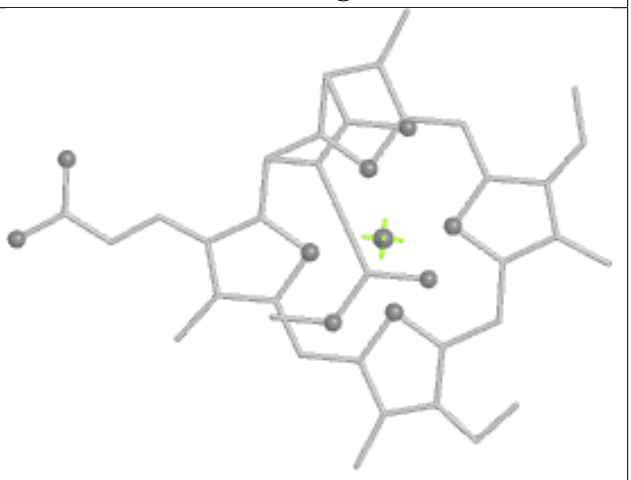
Bond lengths



Bond angles

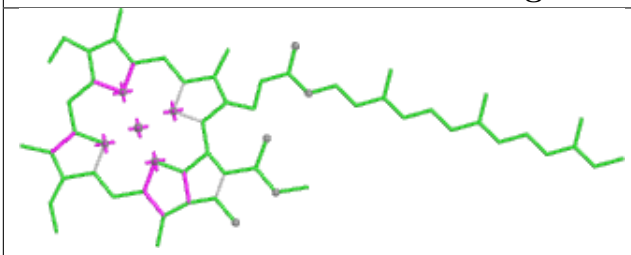


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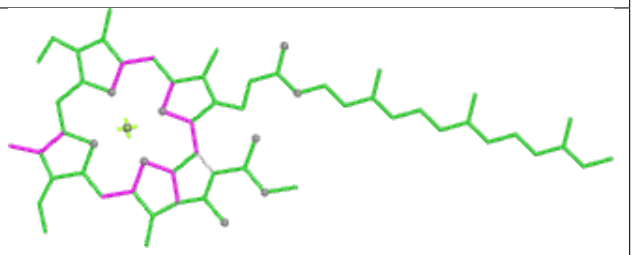


Rings

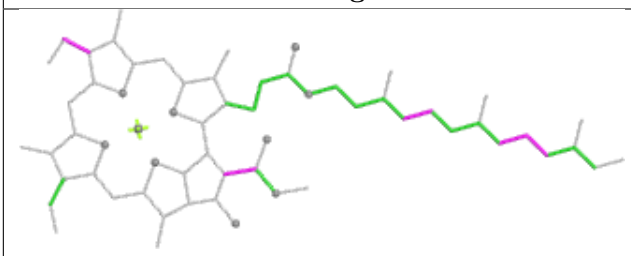
Ligand CLA P 309



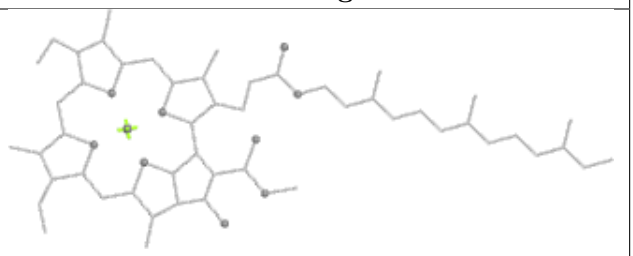
Bond lengths



Bond angles

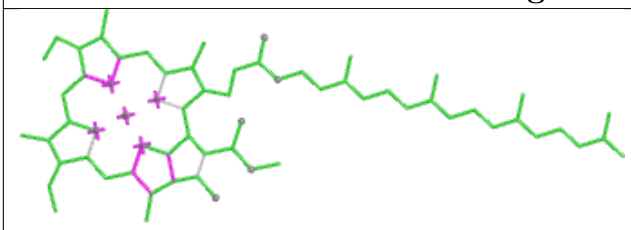


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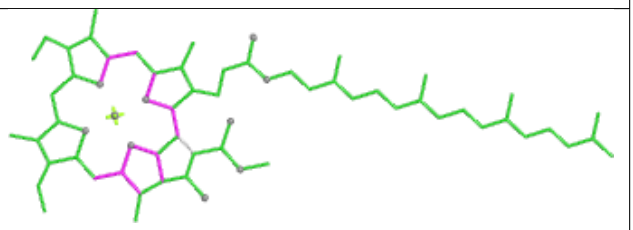


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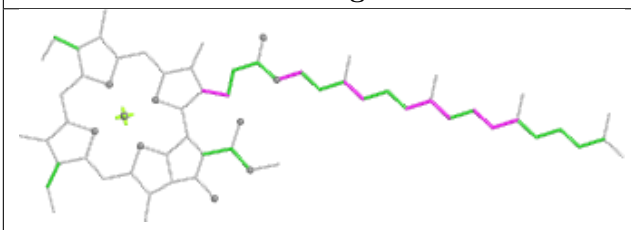
Ligand CLA b 836



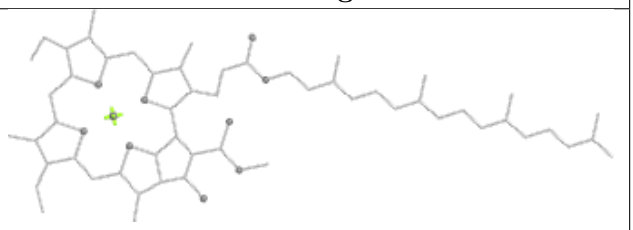
Bond lengths



Bond angles

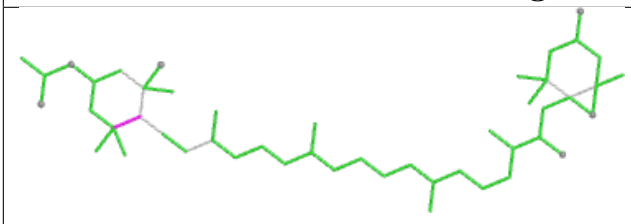


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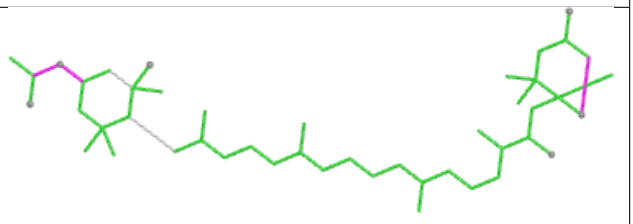


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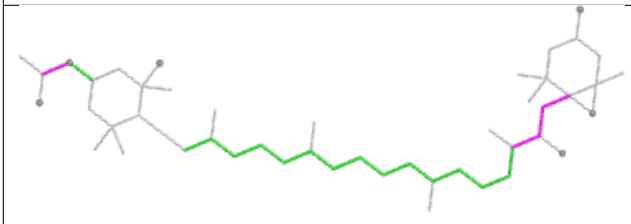
Ligand A86 K 311



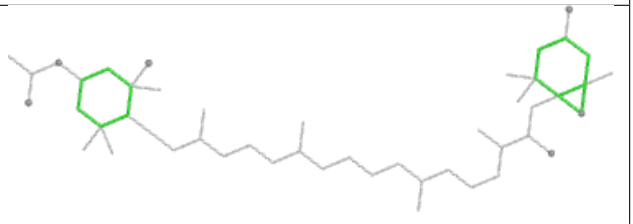
Bond lengths



Bond angles

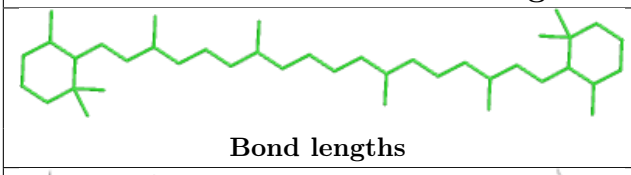


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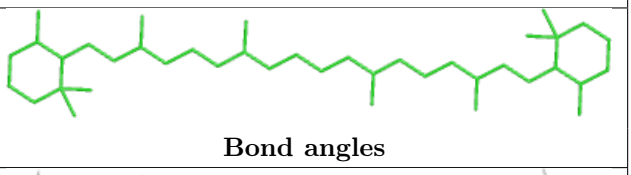


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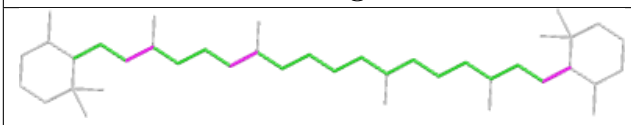
Ligand BCR r 203



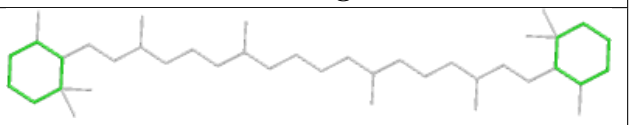
Bond lengths



Bond angles

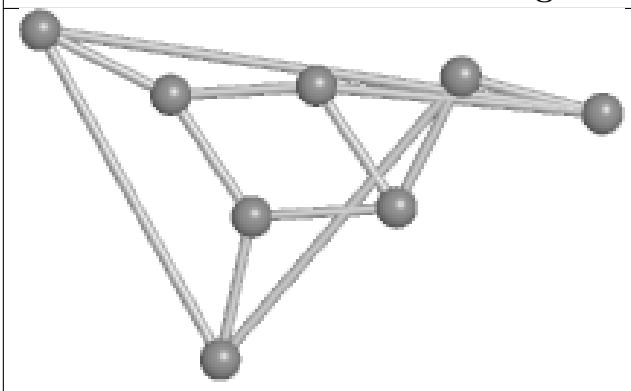


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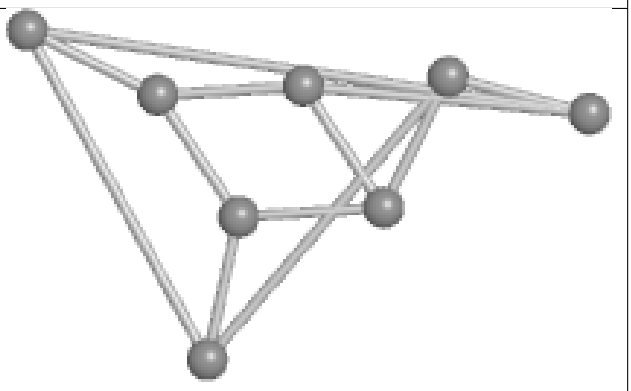


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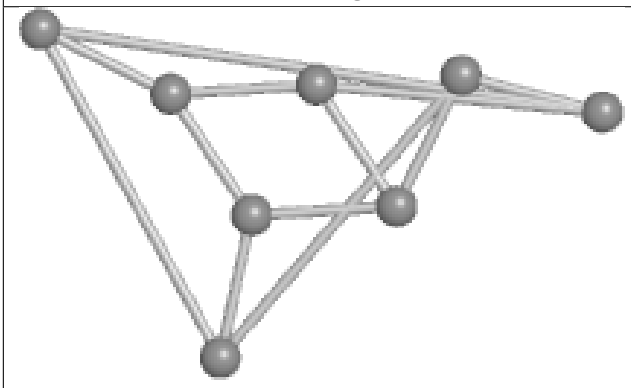
Ligand SF4 a 847



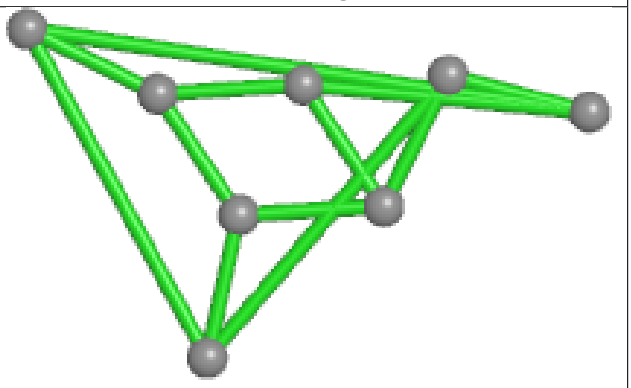
Bond lengths



Bond angles

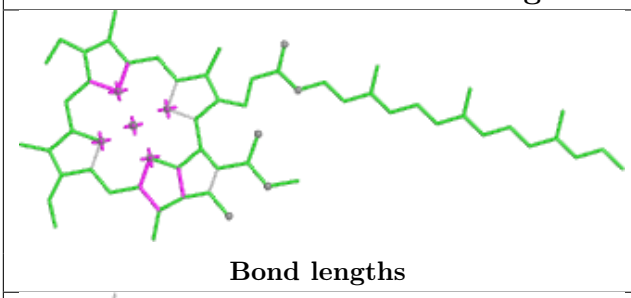


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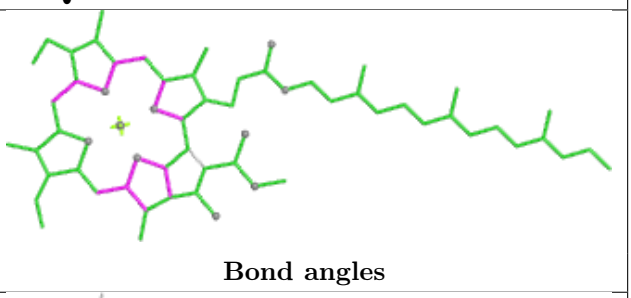


Rings

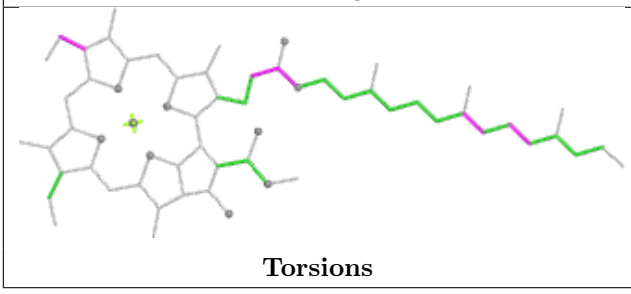
Ligand CLA Q 307



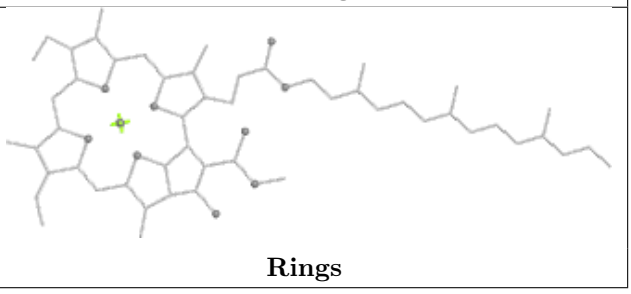
Bond lengths



Bond angles

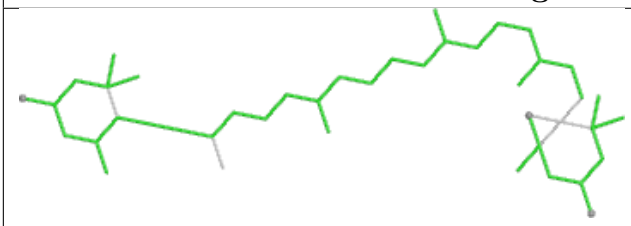


Torsions



Rings

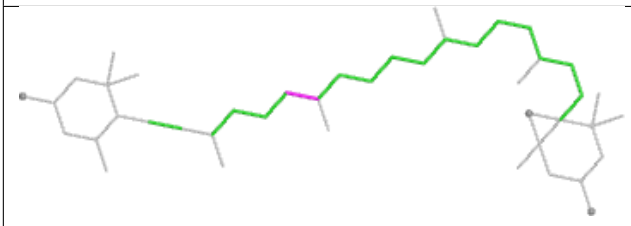
Ligand DD6 I 310



Bond lengths



Bond angles

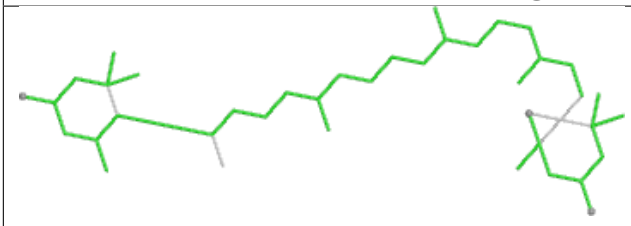


Torsions



Rings

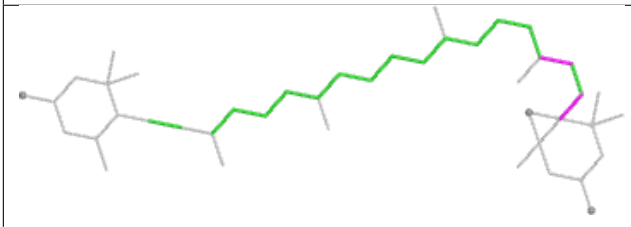
Ligand DD6 S 321



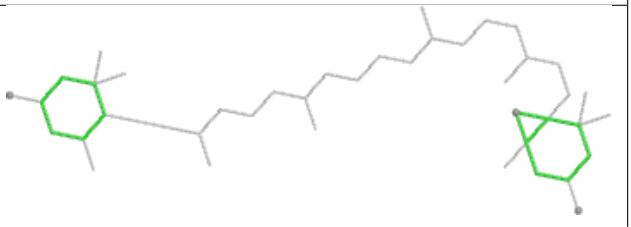
Bond lengths



Bond angles

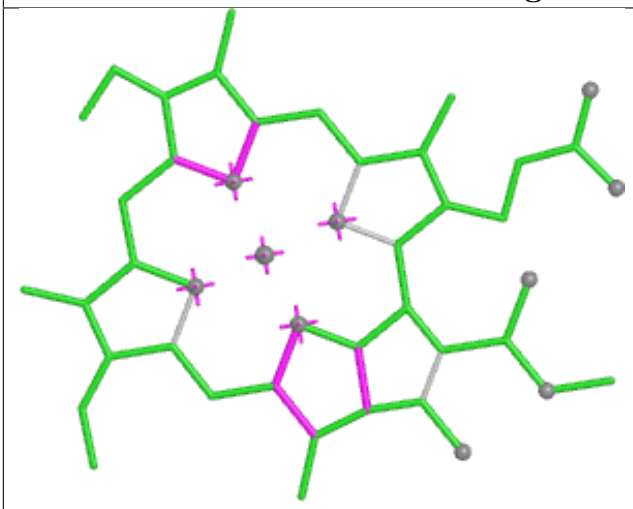


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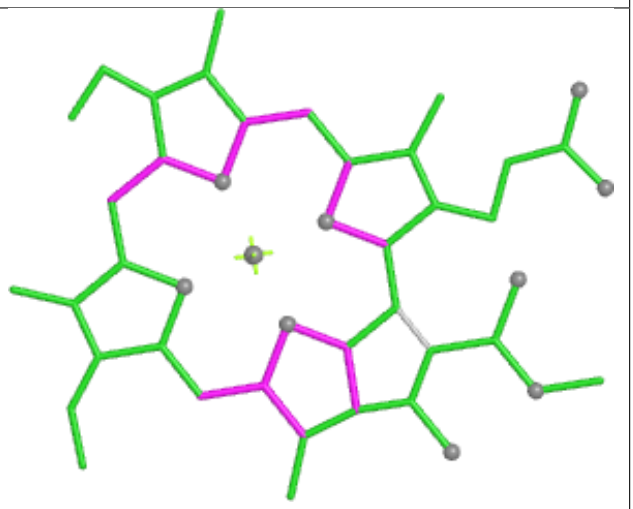


Rings

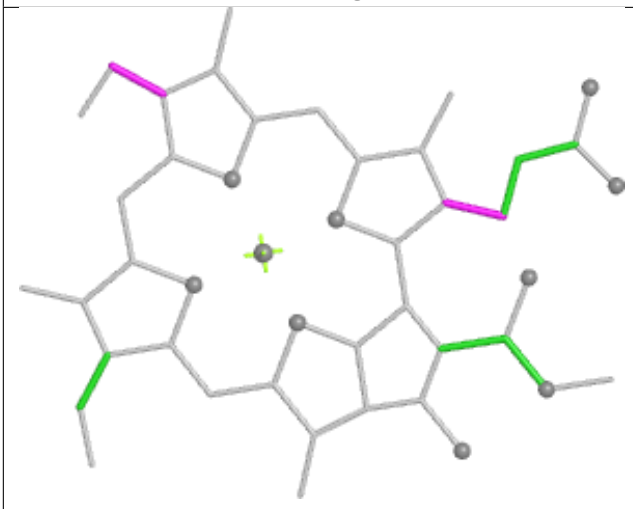
Ligand CLA T 309



Bond lengths



Bond angles

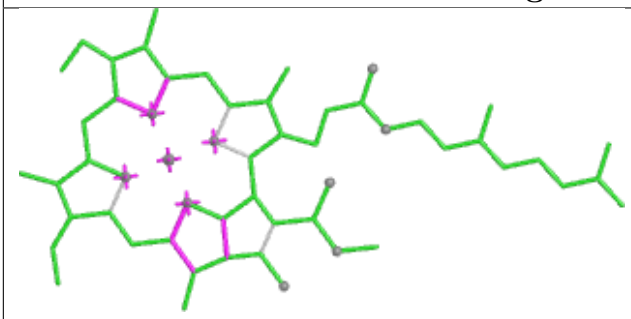


Torsions

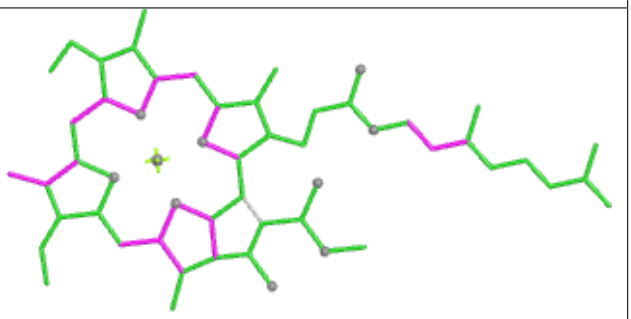


Rings

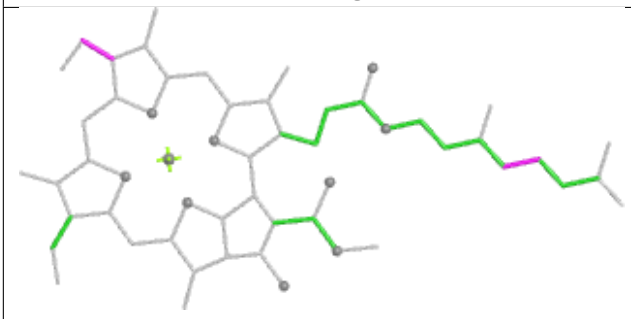
Ligand CLA F 304



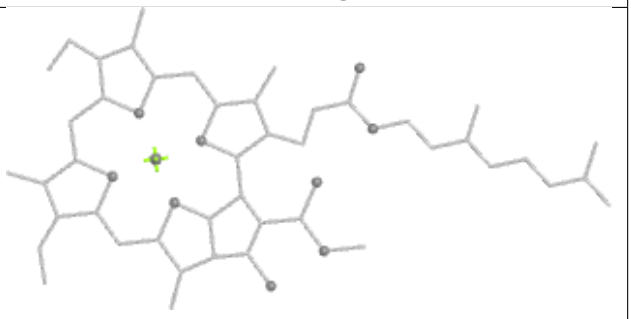
Bond lengths



Bond angles

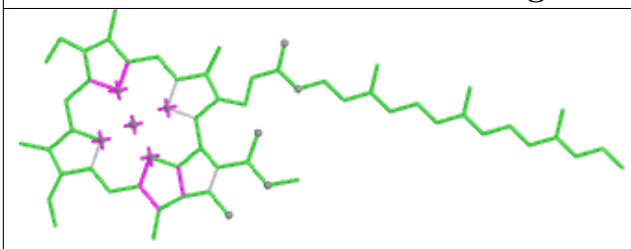


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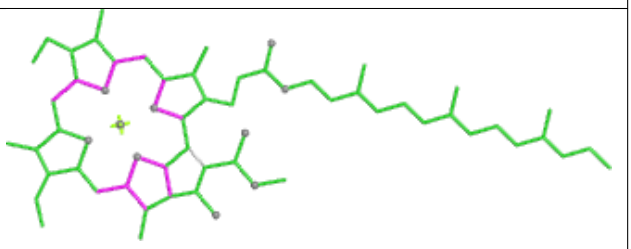


Rings

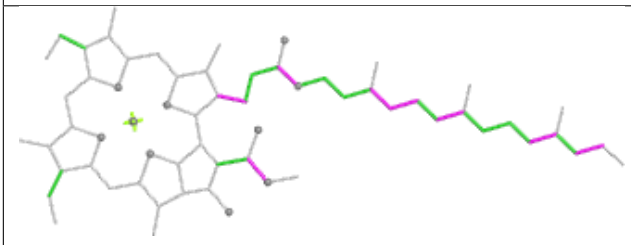
Ligand CLA b 833



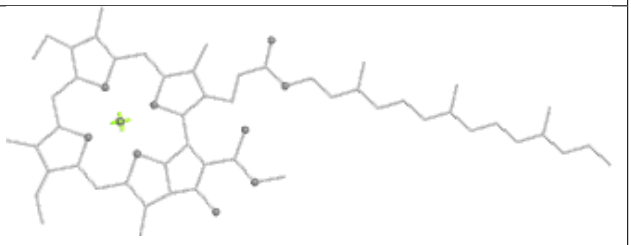
Bond lengths



Bond angles

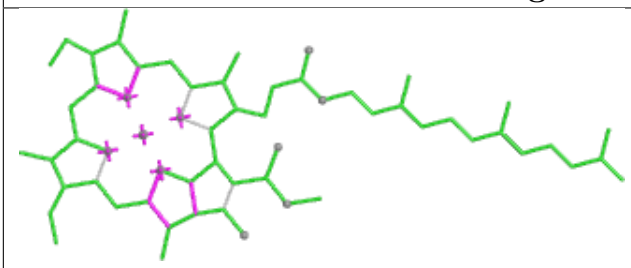


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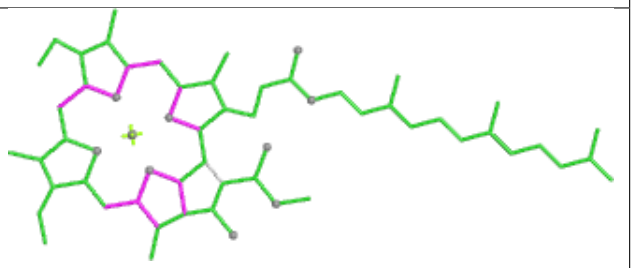


Rings

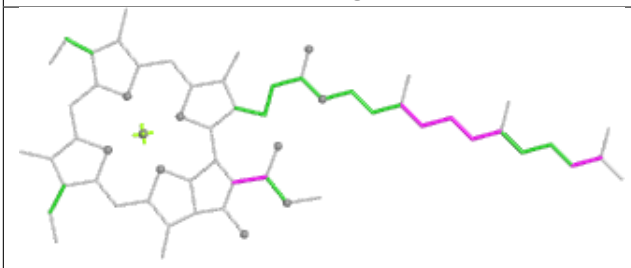
Ligand CLA a 809



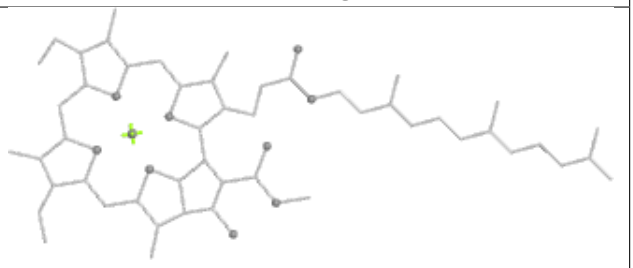
Bond lengths



Bond angles

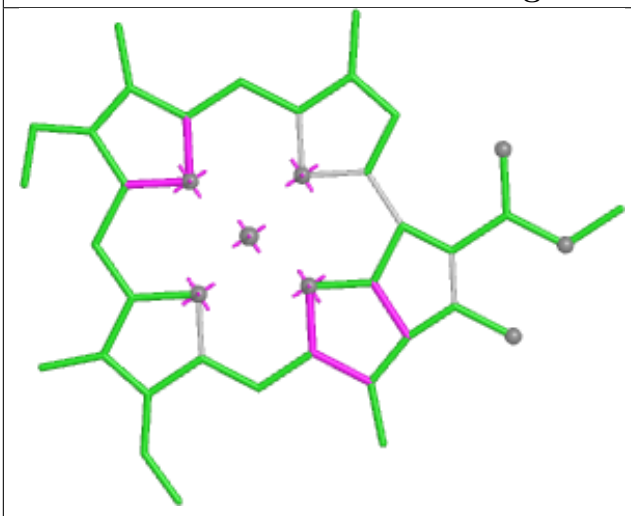


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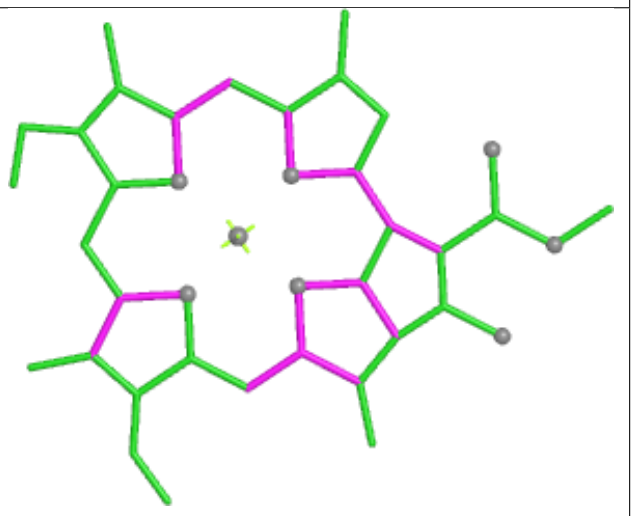


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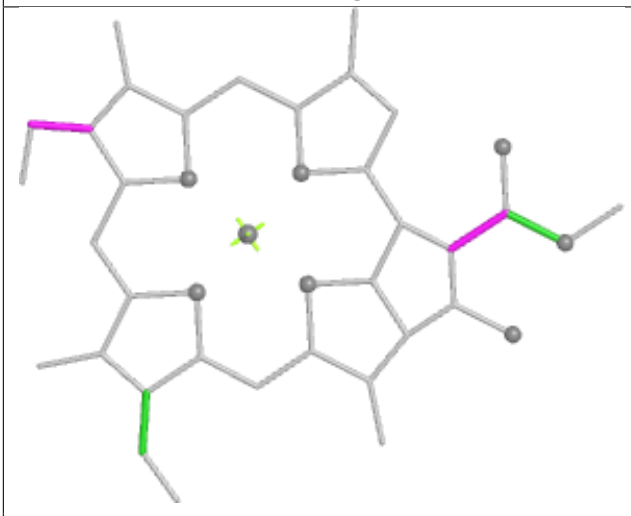
Ligand CLA U 301



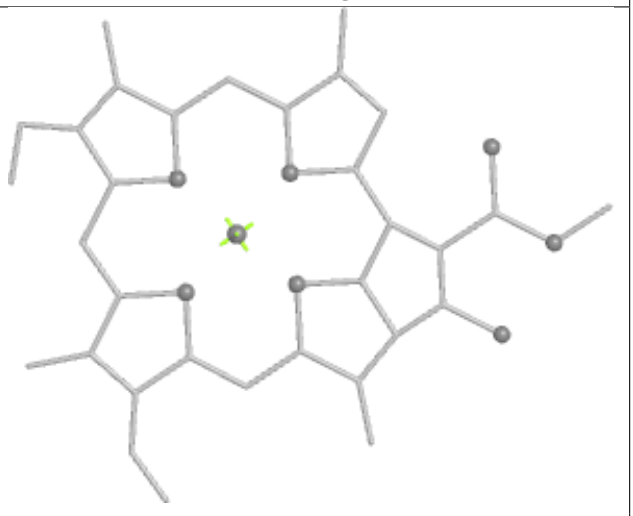
Bond lengths



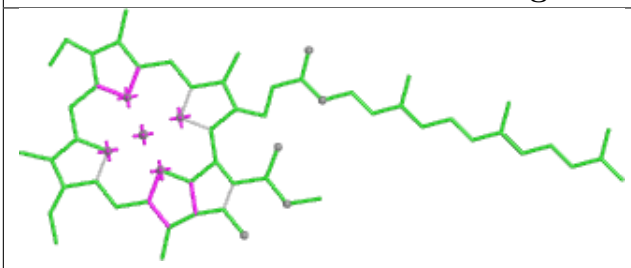
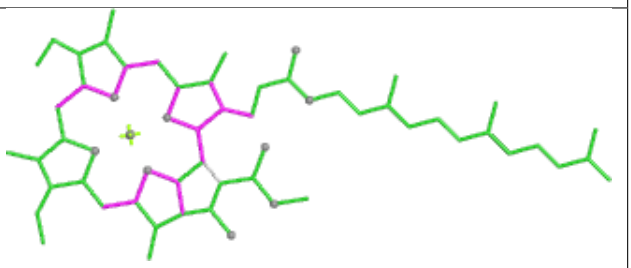
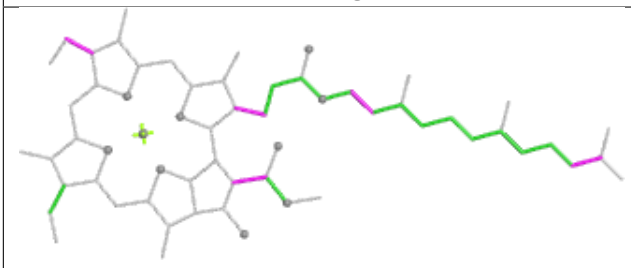
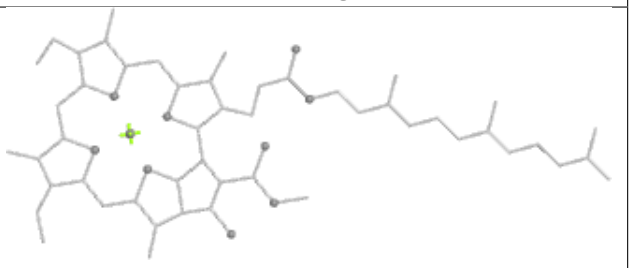
Bond angles

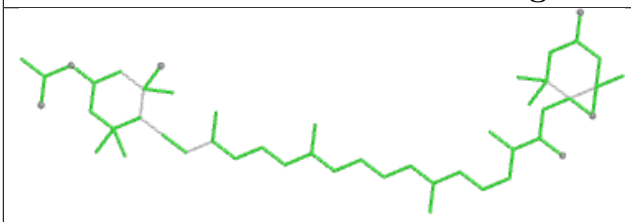
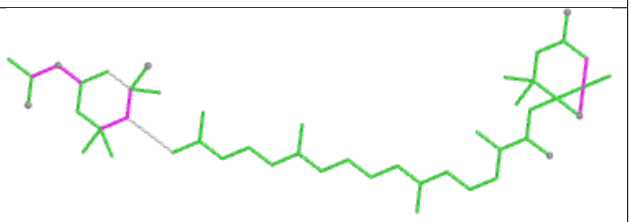
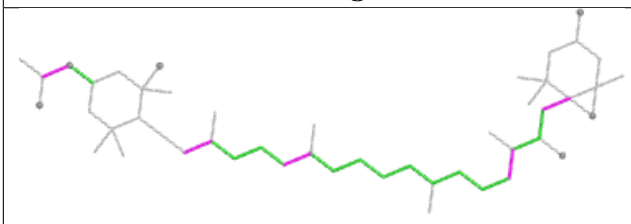
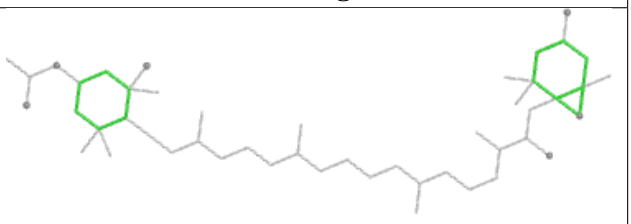


Torsions

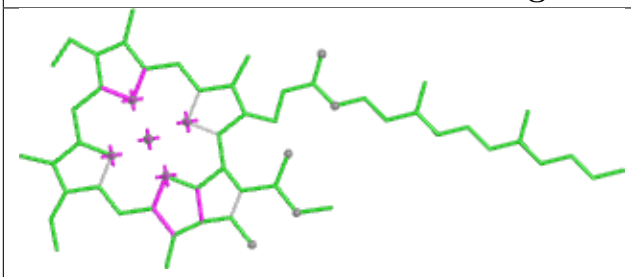


Rings

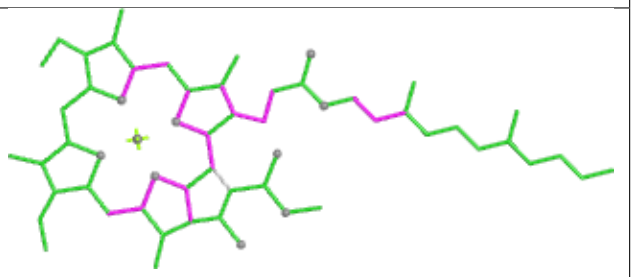
Ligand CLA r 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A86 D 323	
	
Bond lengths	Bond angles
	
Torsions	Rings

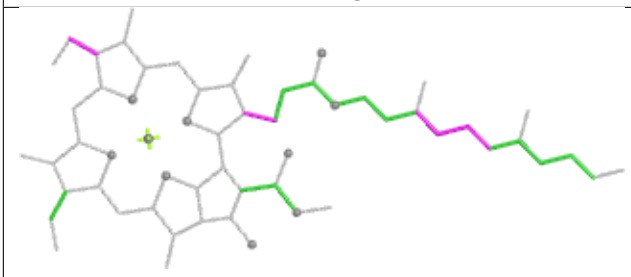
Ligand CLA a 828



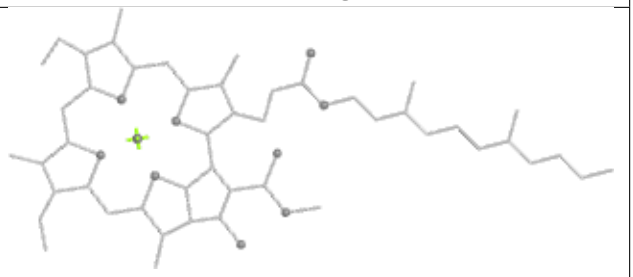
Bond lengths



Bond angles

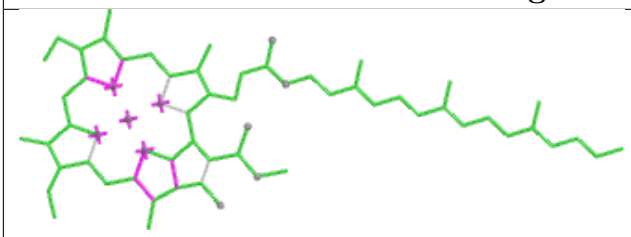


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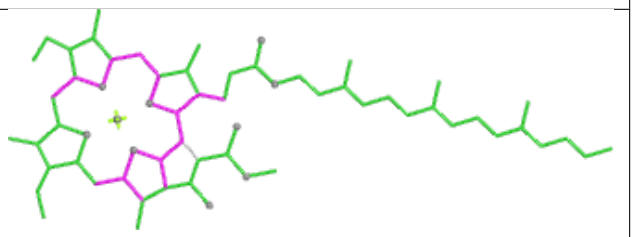


Rings

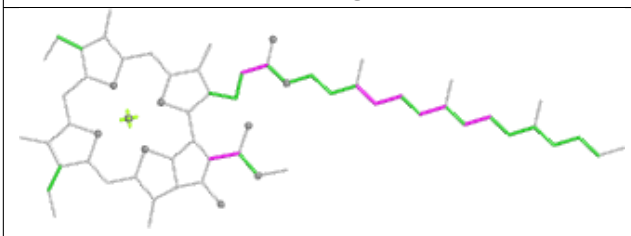
Ligand CLA a 802



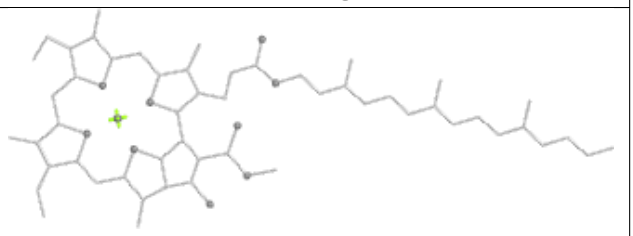
Bond lengths



Bond angles

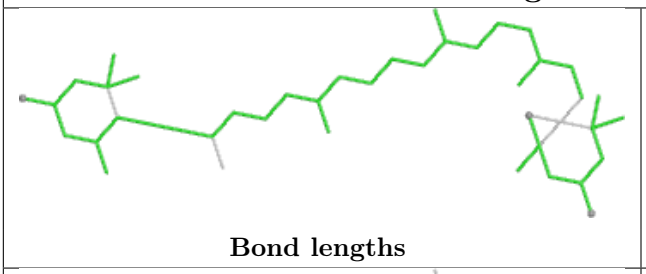


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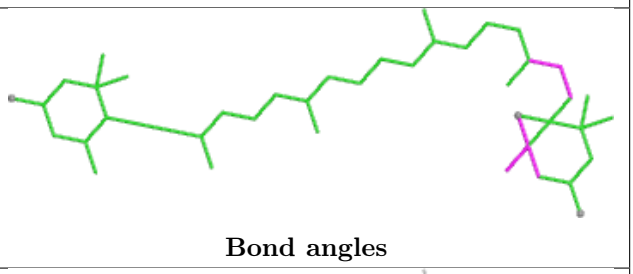


Rings

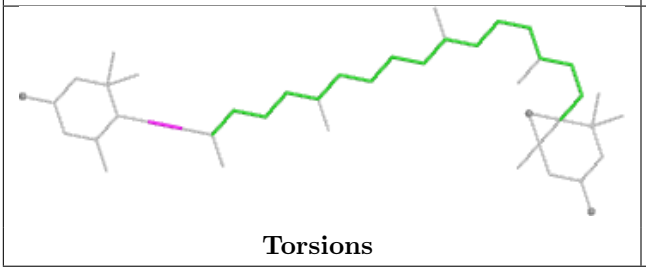
Ligand DD6 D 316



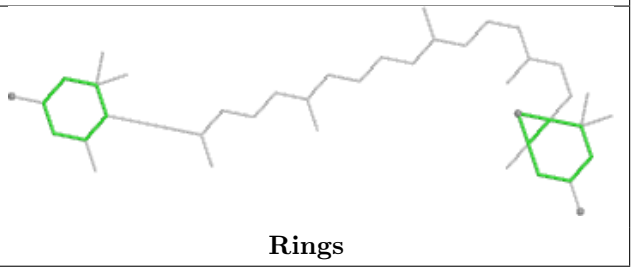
Bond lengths



Bond angles

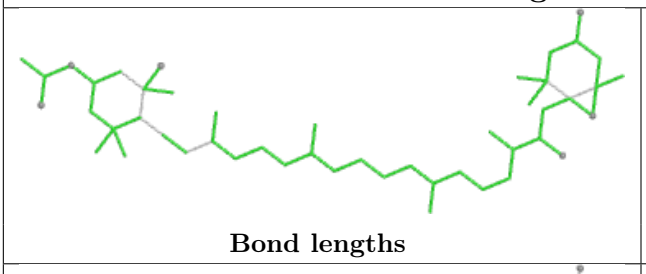


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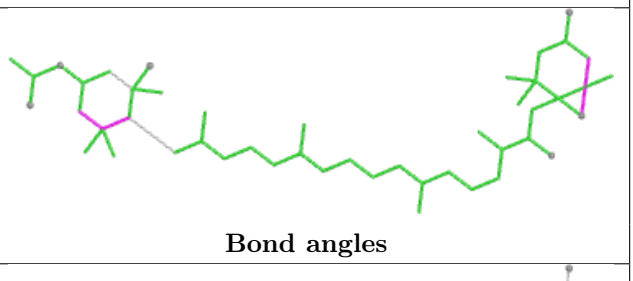


Rings

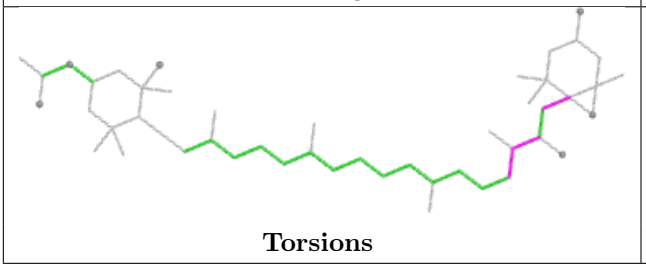
Ligand A86 O 311



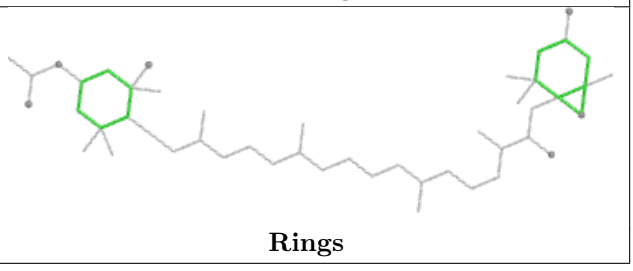
Bond lengths



Bond angles

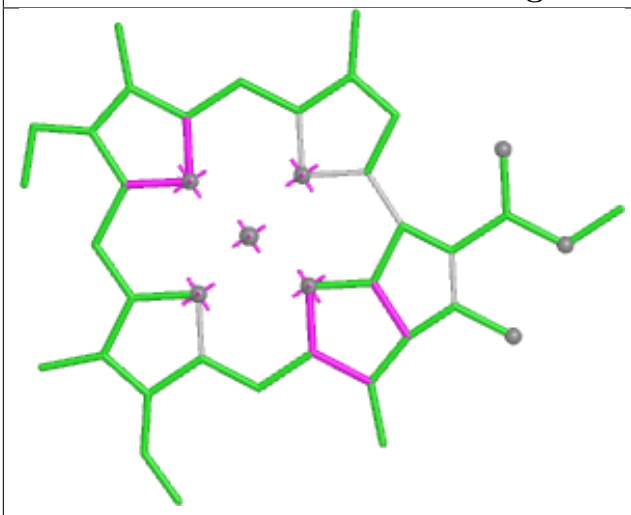


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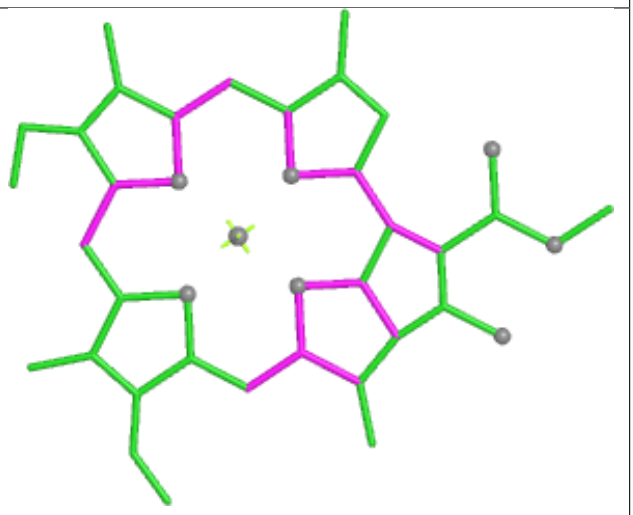


Rings

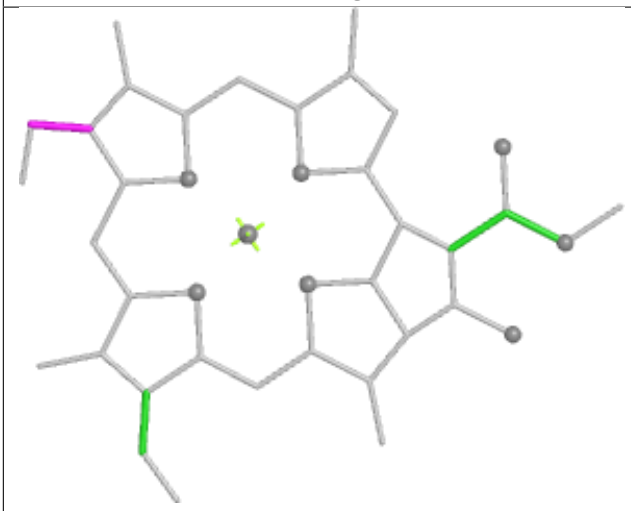
Ligand CLA F 301



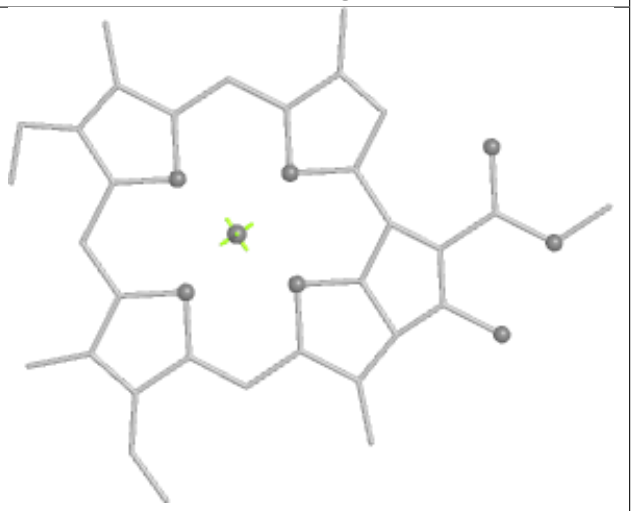
Bond lengths



Bond angles

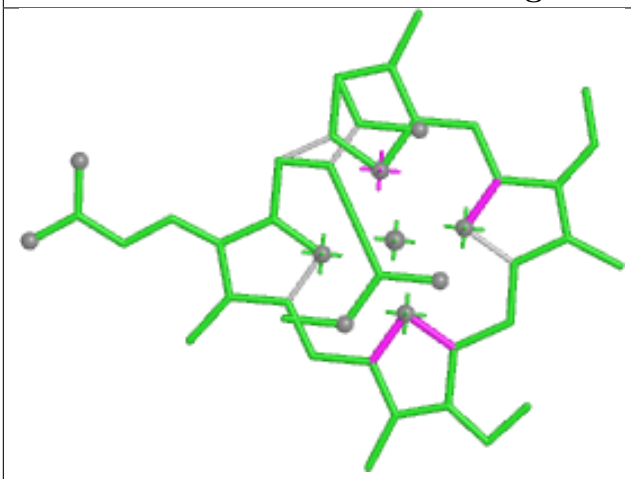


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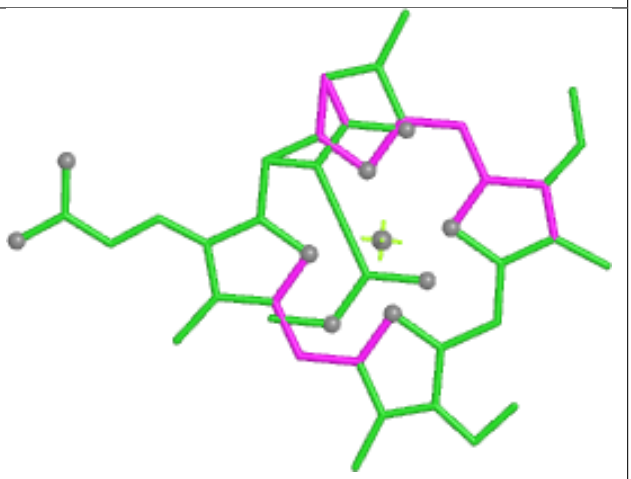


Rings

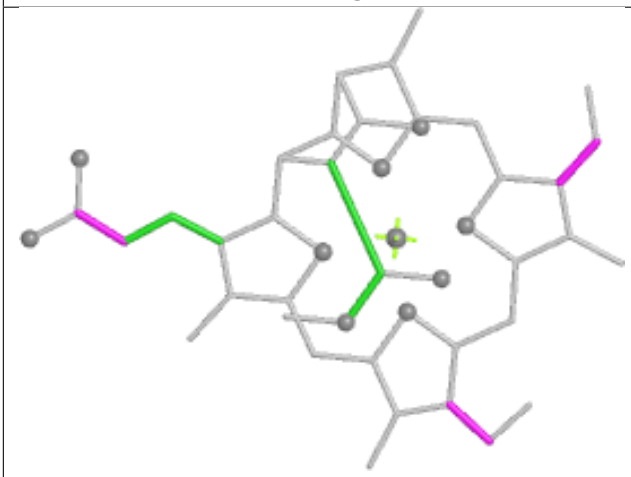
Ligand KC2 K 302



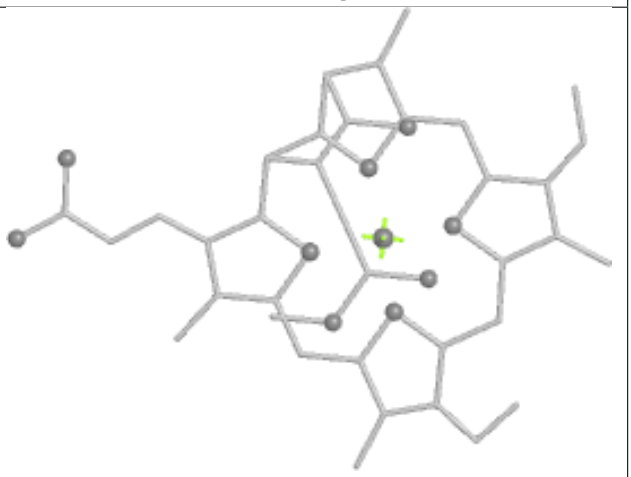
Bond lengths



Bond angles

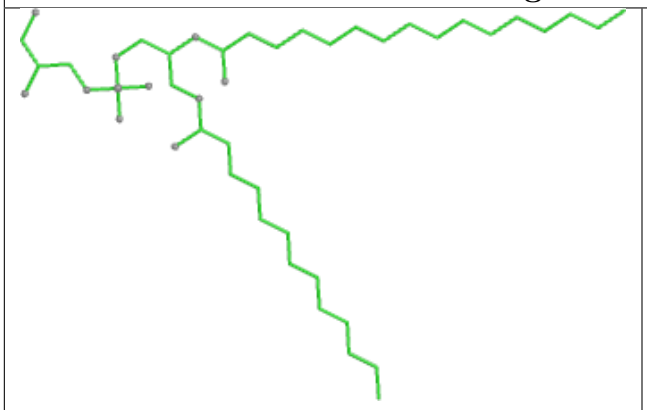


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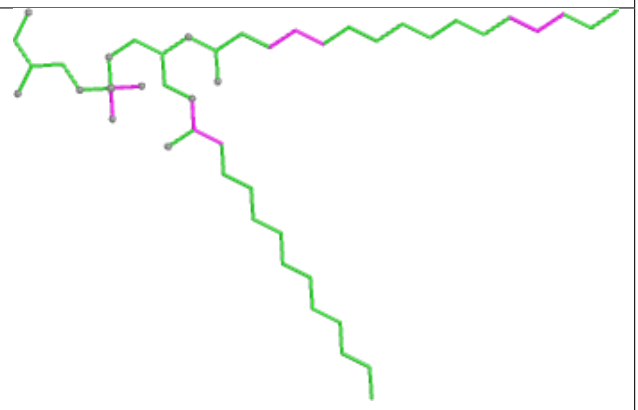


Rings

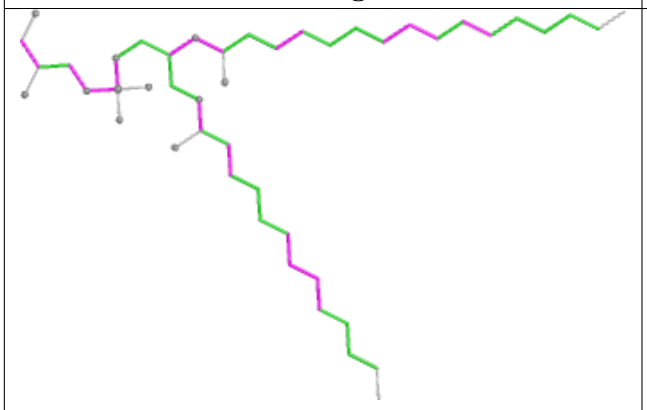
Ligand LHG P 317



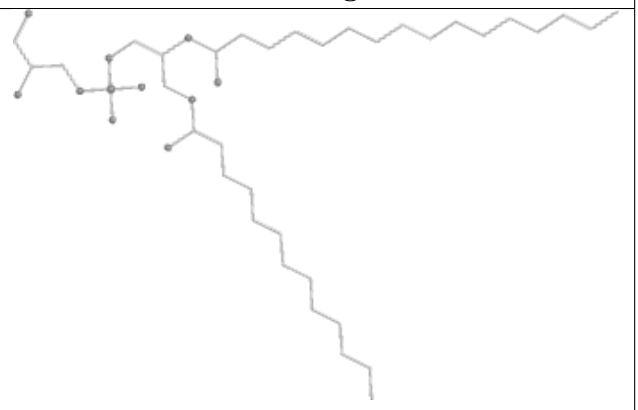
Bond lengths



Bond angles

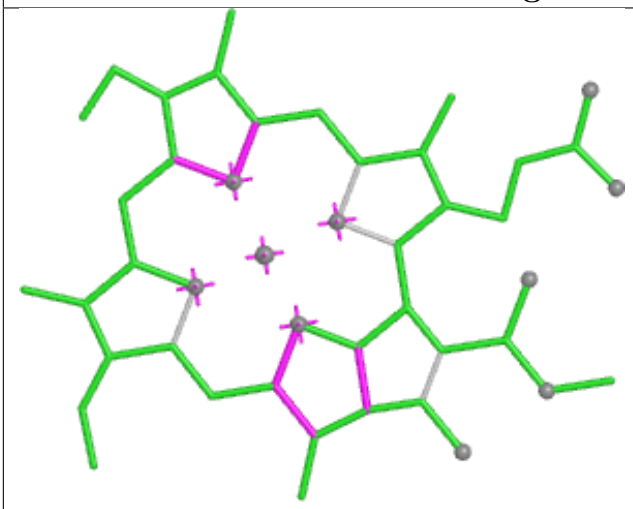


Torsions

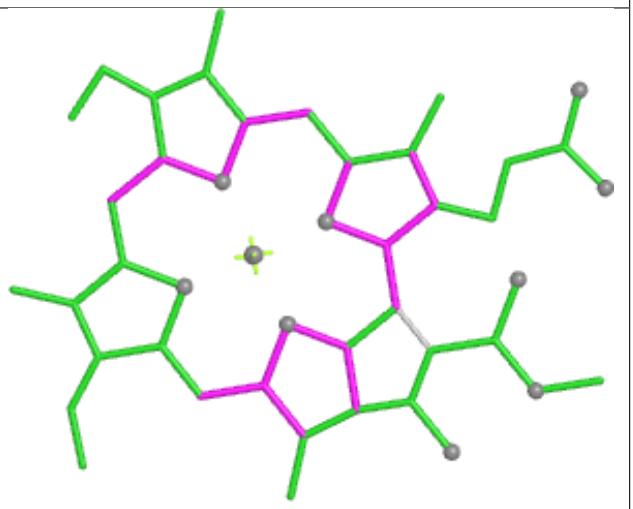


Rings

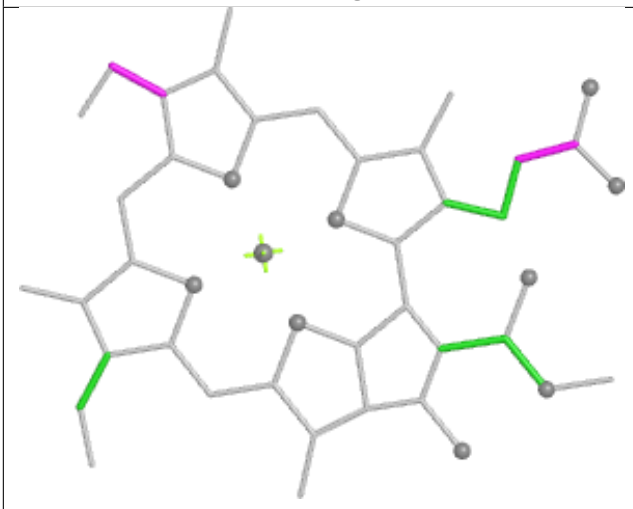
Ligand CLA U 303



Bond lengths



Bond angles

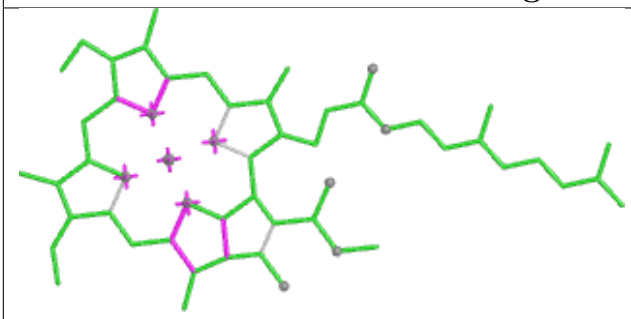


Torsions

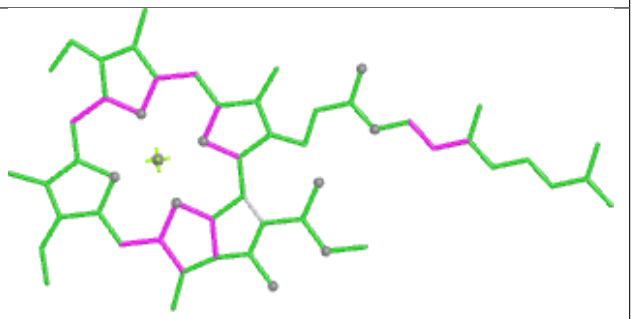


Rings

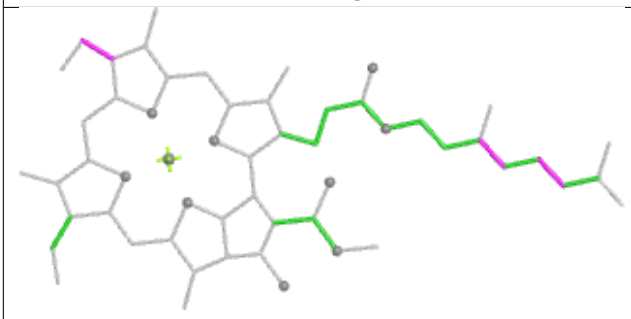
Ligand CLA G 304



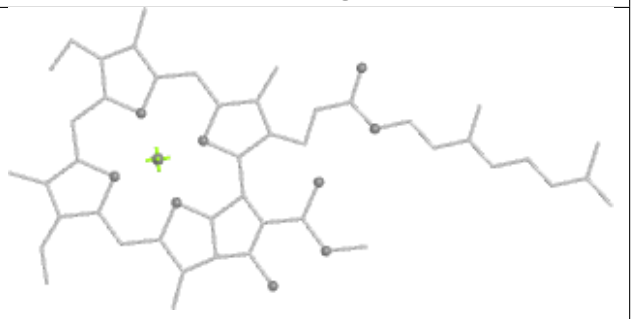
Bond lengths



Bond angles

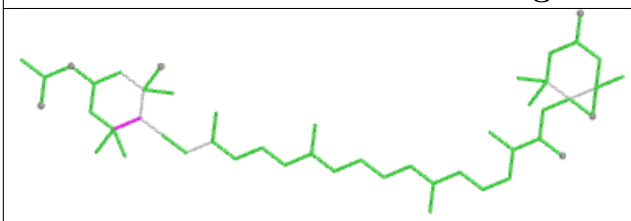


Torsions

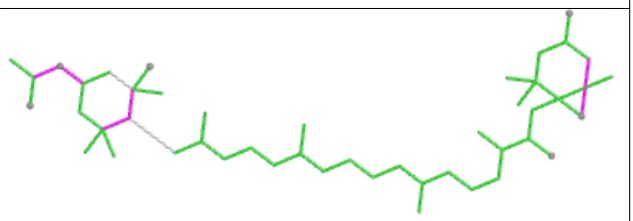


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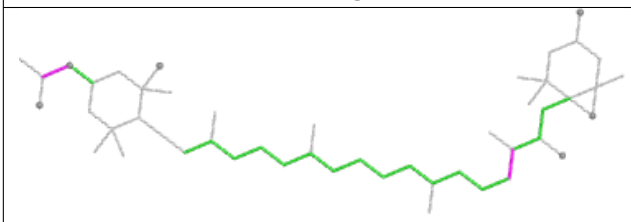
Ligand A86 S 318



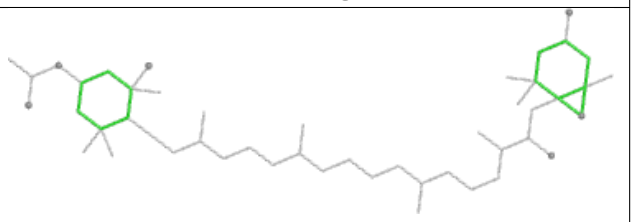
Bond lengths



Bond angles

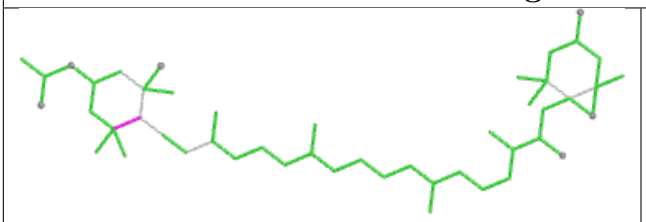


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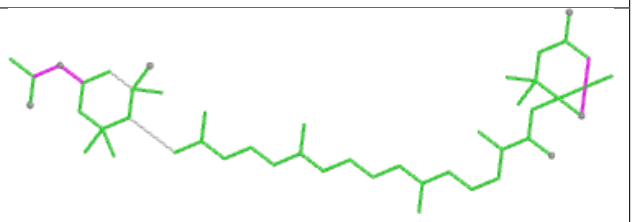


Rings

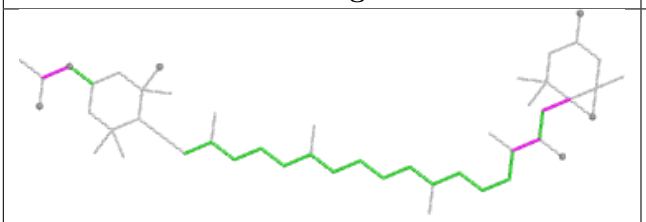
Ligand A86 W 315



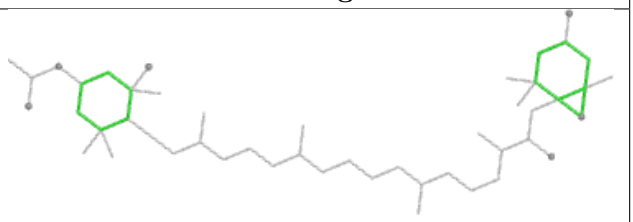
Bond lengths



Bond angles

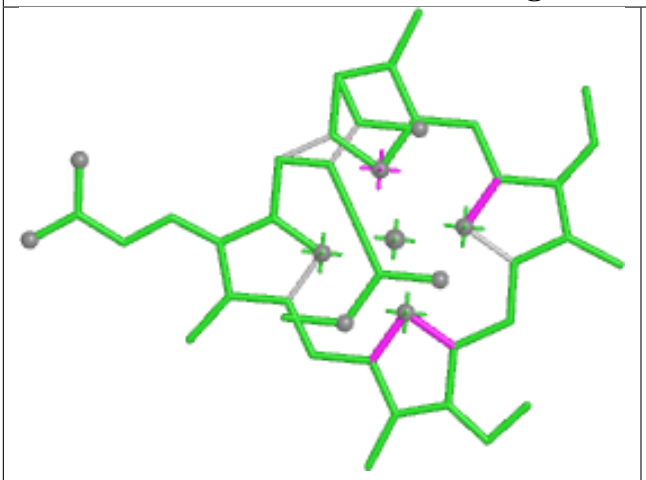


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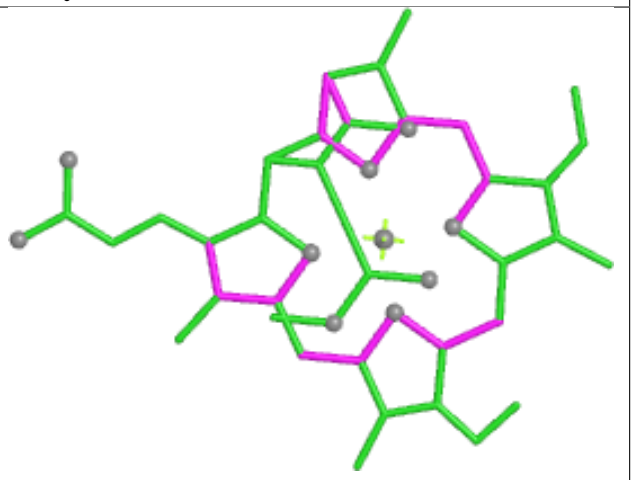


Rings

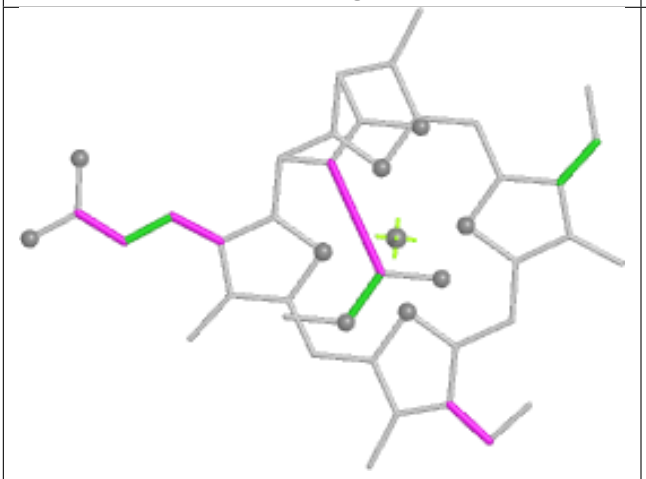
Ligand KC2 Q 317



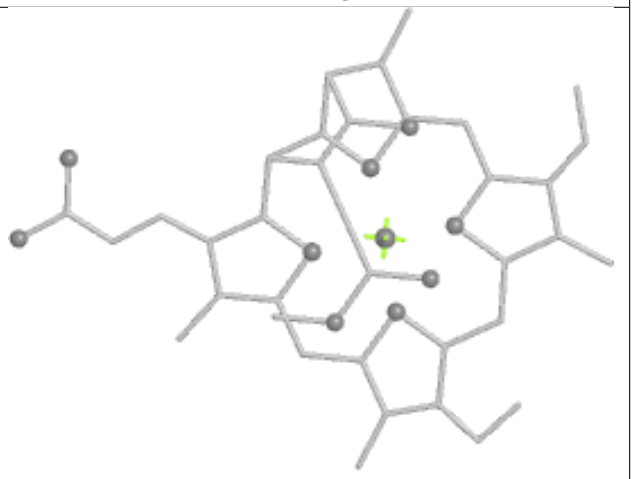
Bond lengths



Bond angles

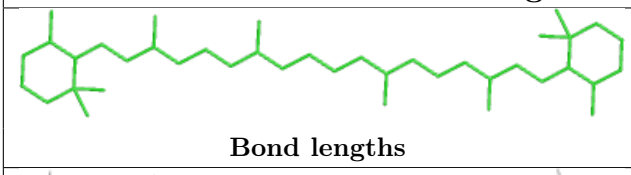


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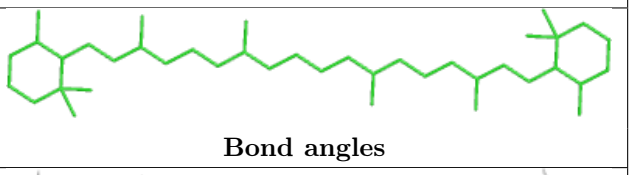


Rings

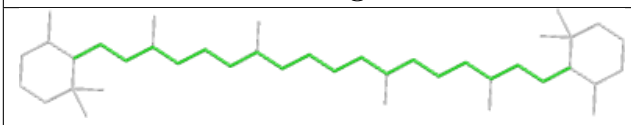
Ligand BCR b 841



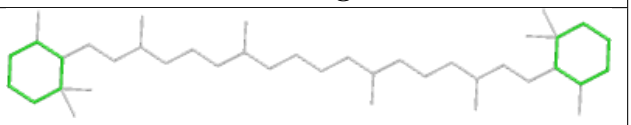
Bond lengths



Bond angles

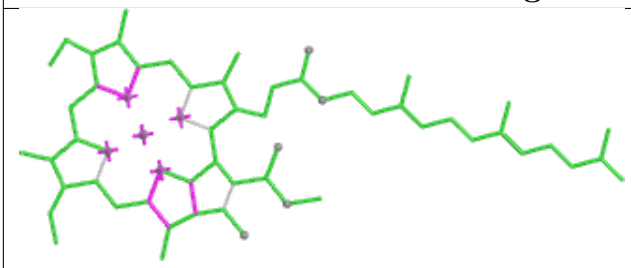


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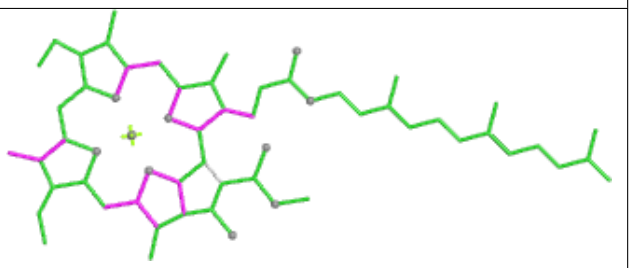


Rings

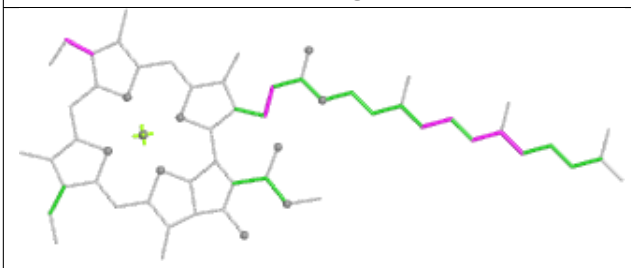
Ligand CLA O 307



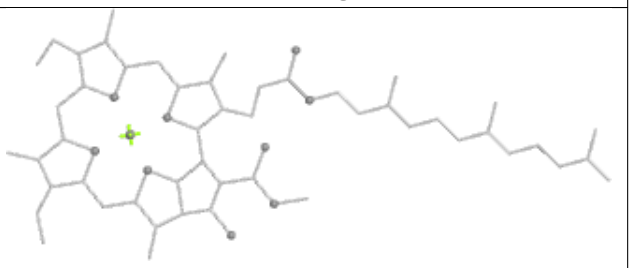
Bond lengths



Bond angles

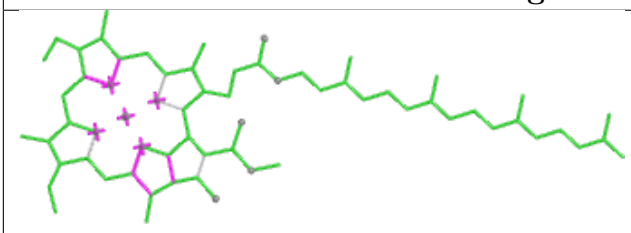


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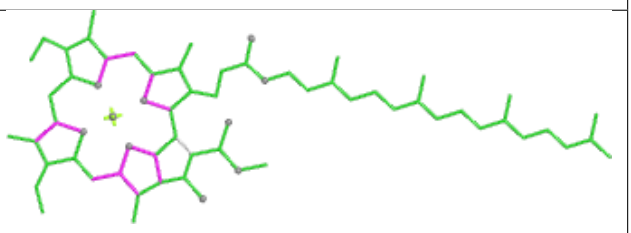


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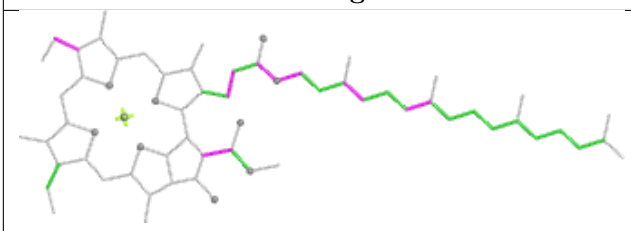
Ligand CLA b 812



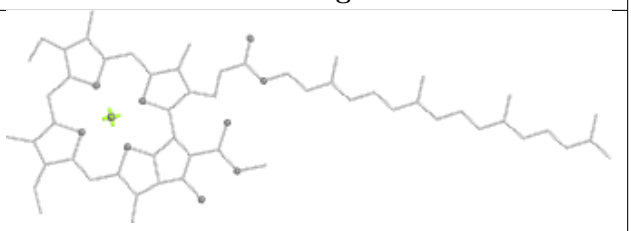
Bond lengths



Bond angles

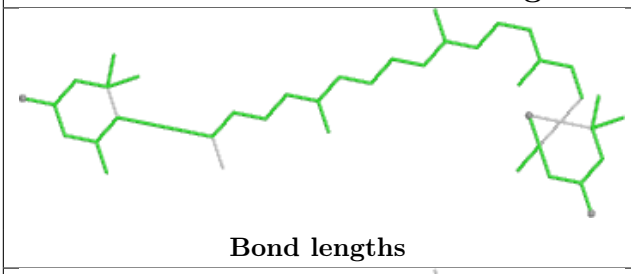


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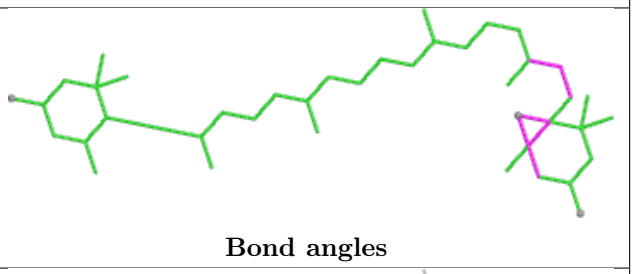


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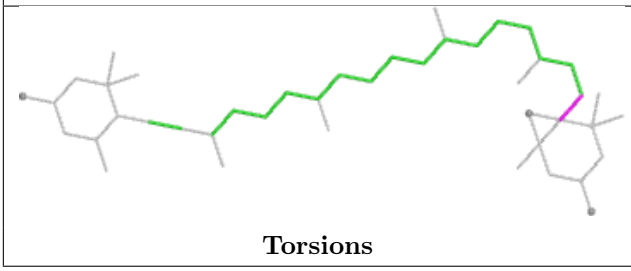
Ligand DD6 N 319



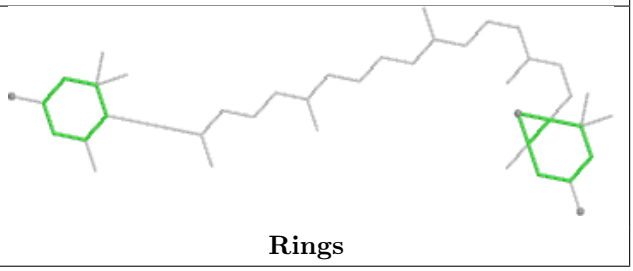
Bond lengths



Bond angles

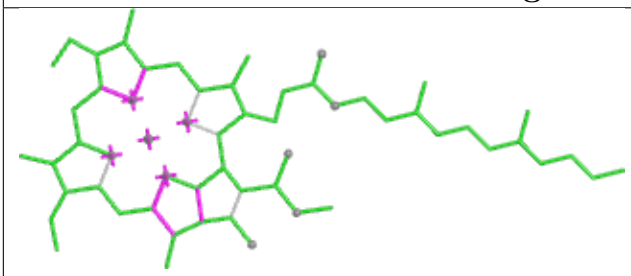


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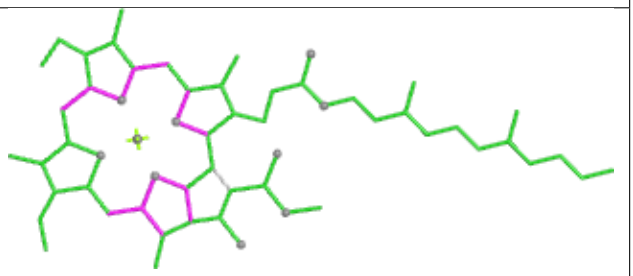


Rings

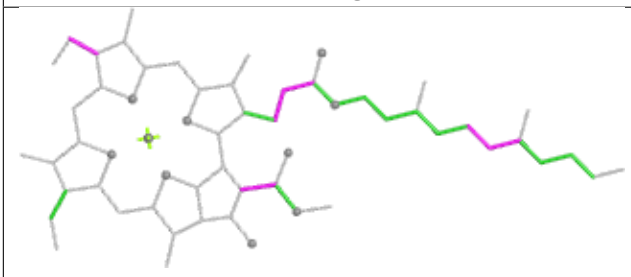
Ligand CLA D 313



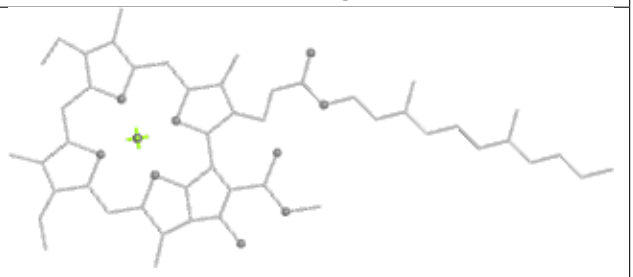
Bond lengths



Bond angles

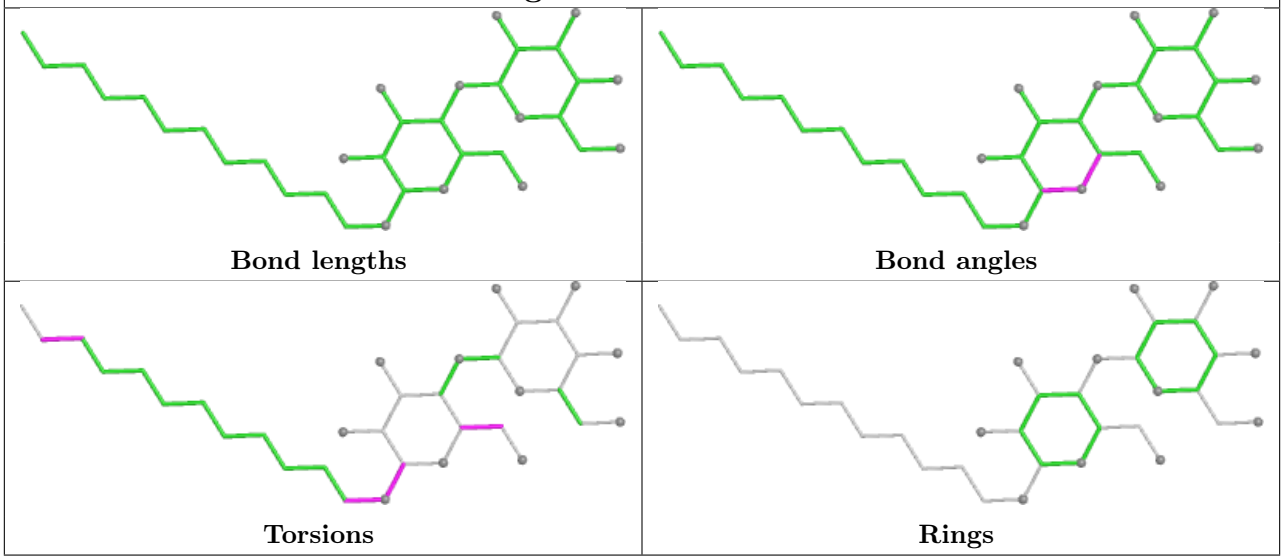


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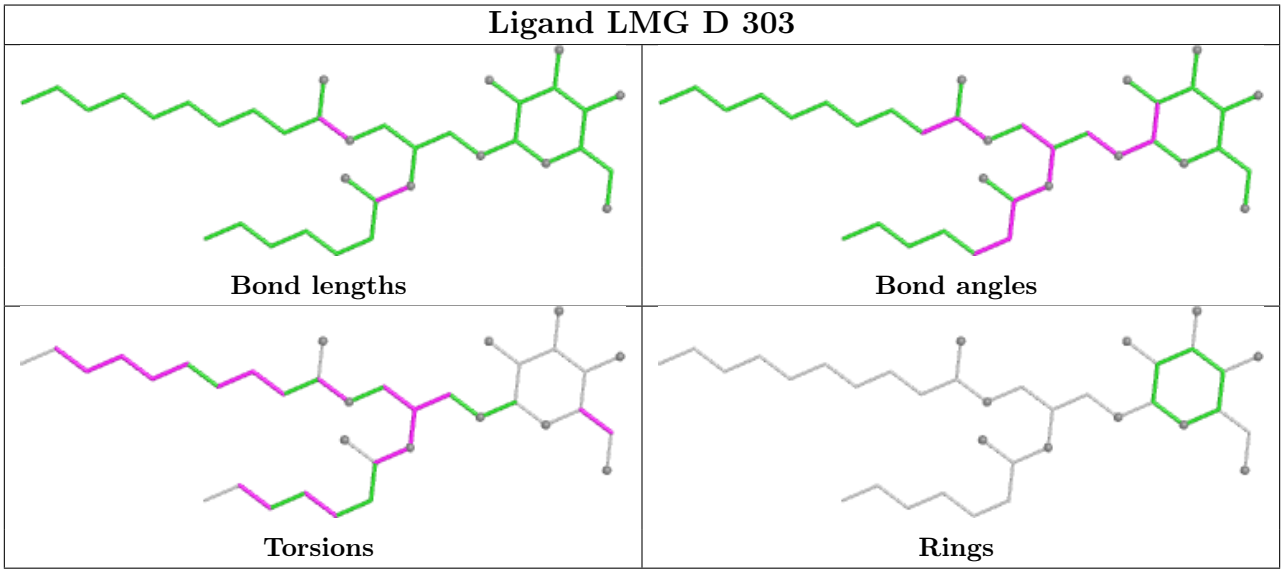


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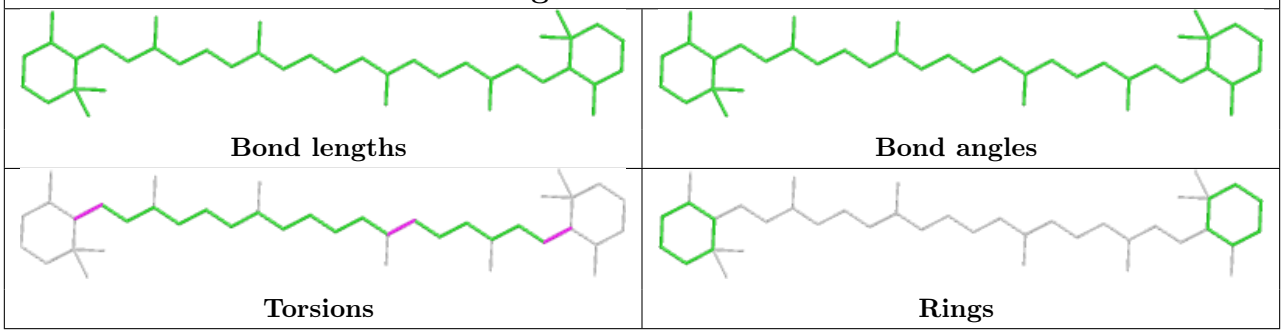
Ligand LMU J 318



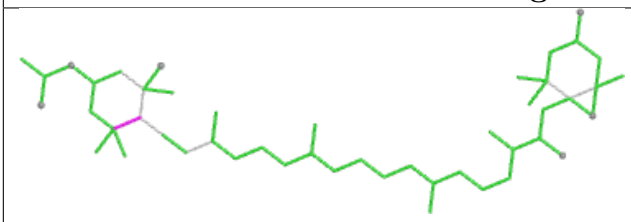
Ligand LMG D 303



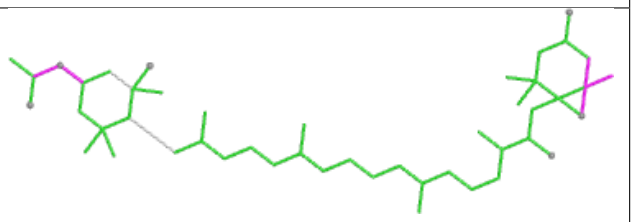
Ligand BCR i 101



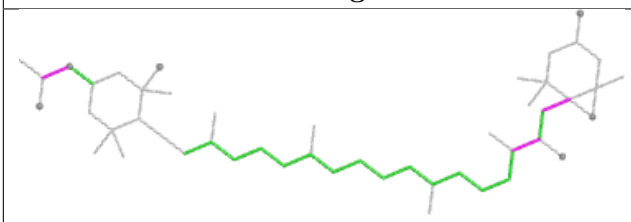
Ligand A86 C 311



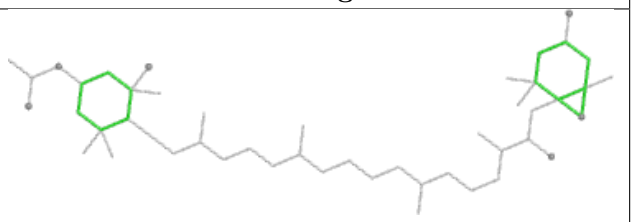
Bond lengths



Bond angles

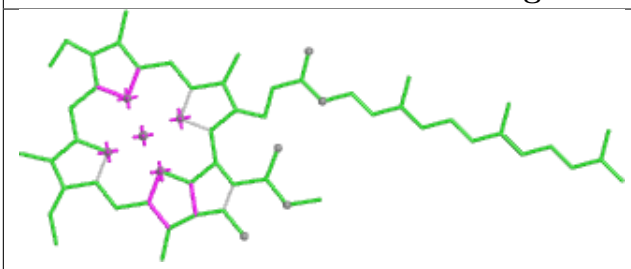


Torsions

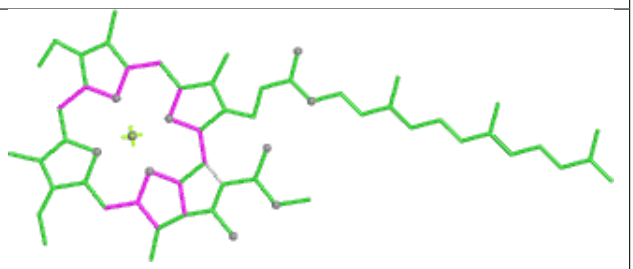


Rings

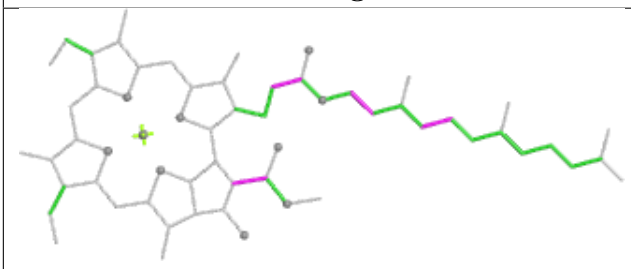
Ligand CLA A 307



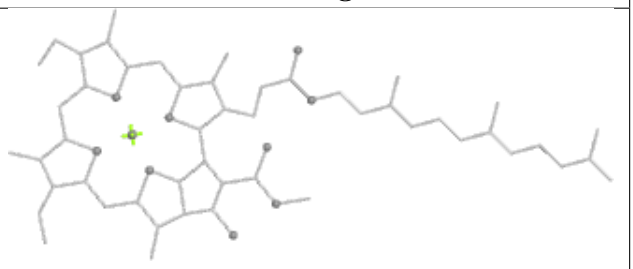
Bond lengths



Bond angles

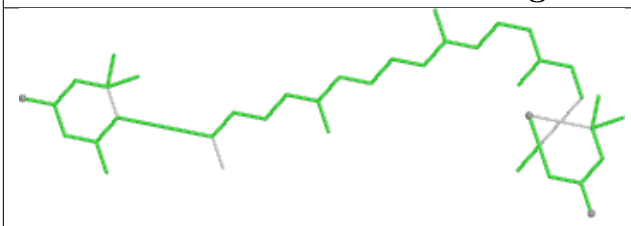


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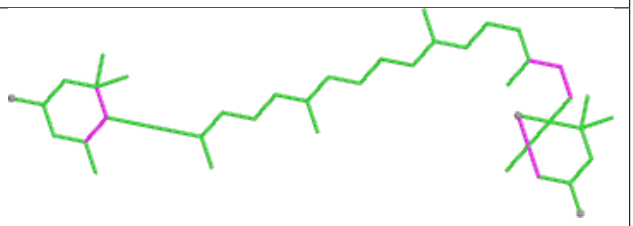


Rings

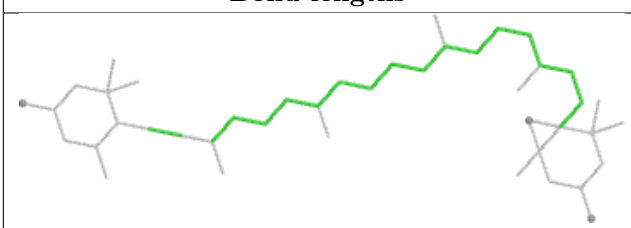
Ligand DD6 J 316



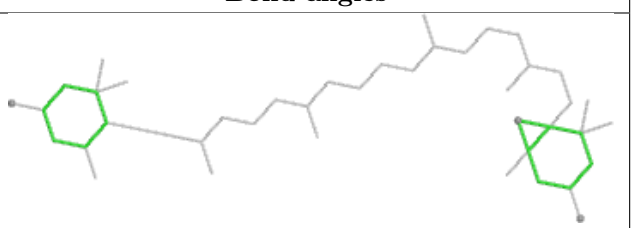
Bond lengths



Bond angles

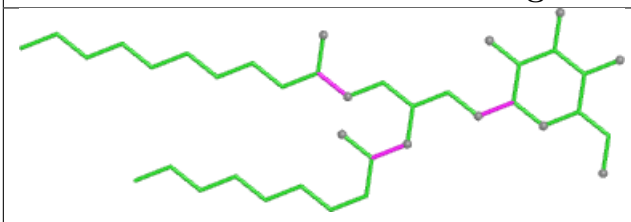


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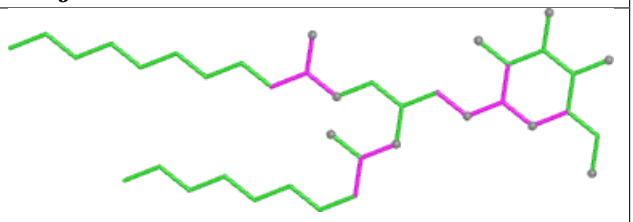


Rings

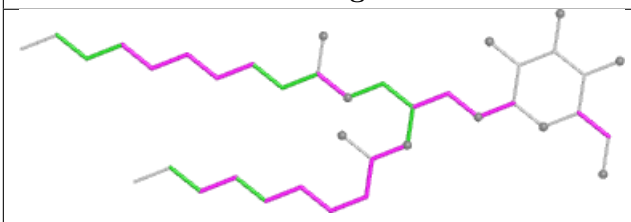
Ligand LMG j 104



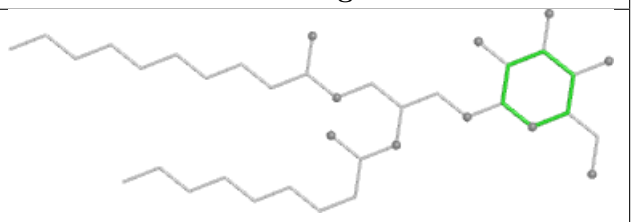
Bond lengths



Bond angles

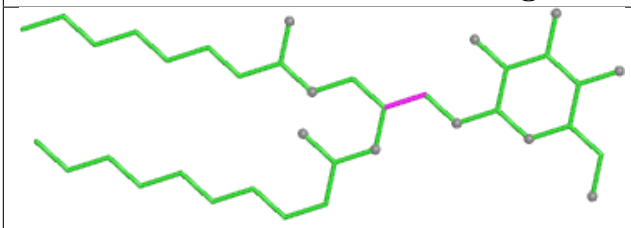


Torsions

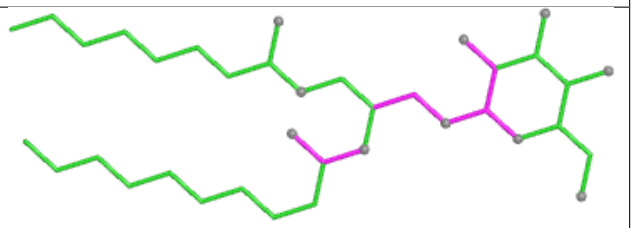


Rings

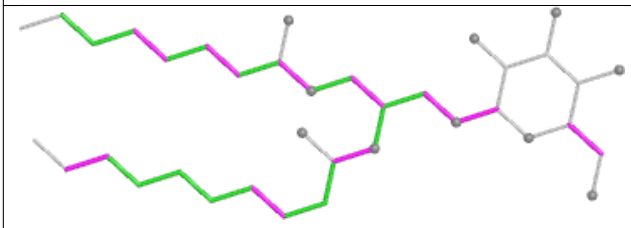
Ligand LMG T 301



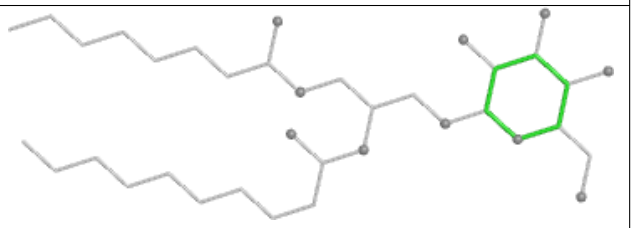
Bond lengths



Bond angles

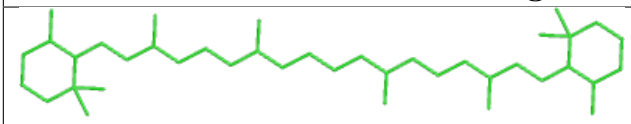


Torsions

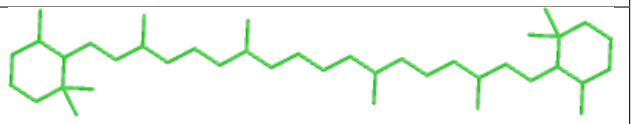


Rings

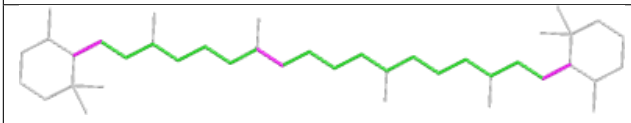
Ligand BCR a 854



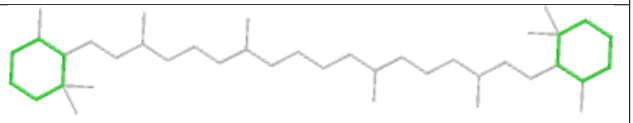
Bond lengths



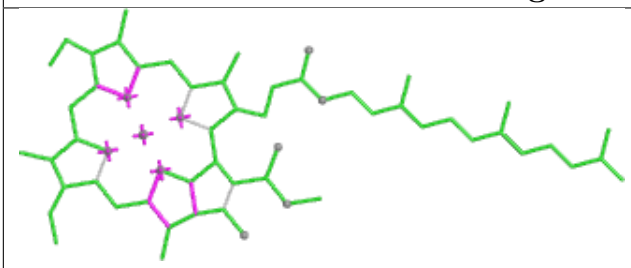
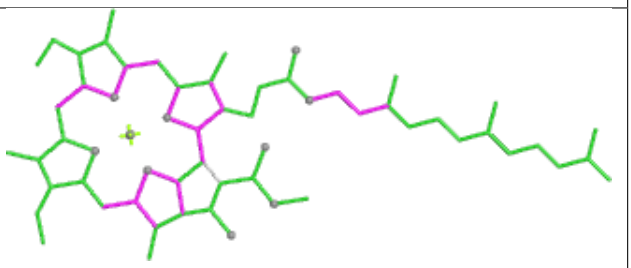
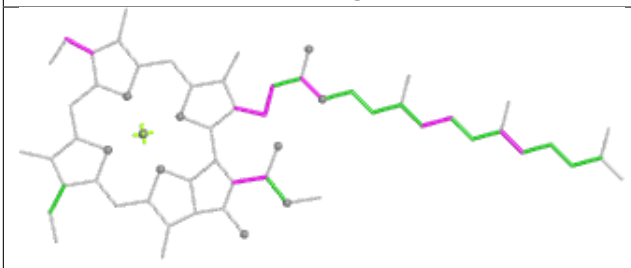
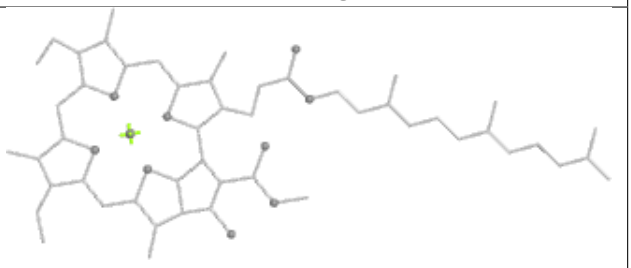
Bond angles

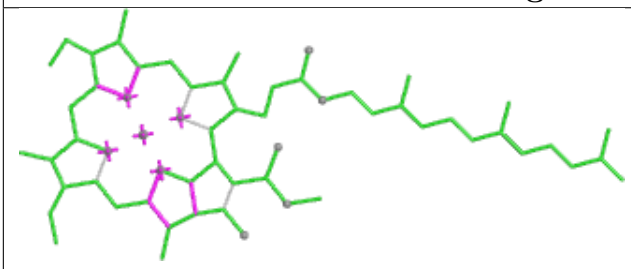
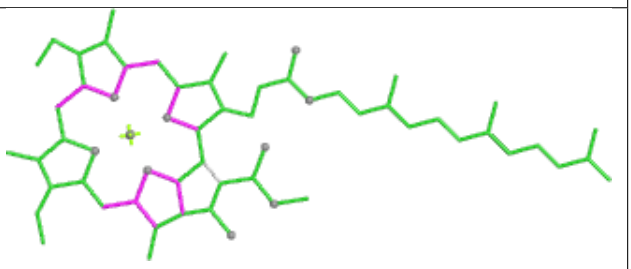
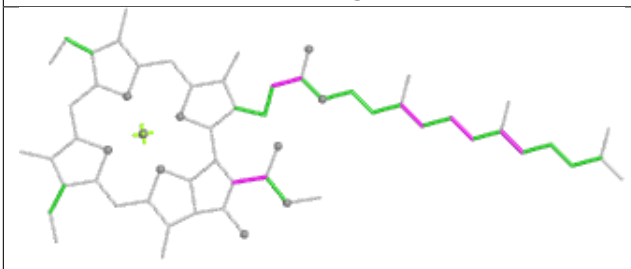
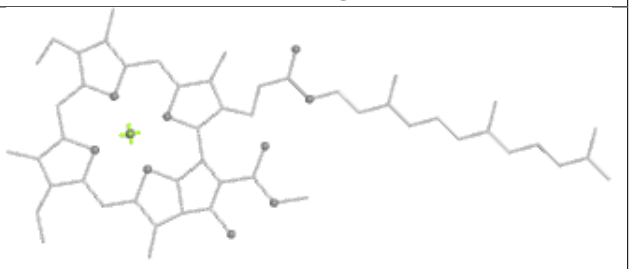


Torsions

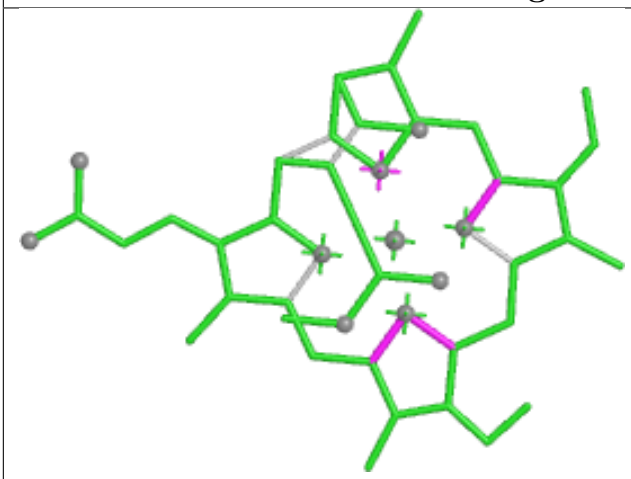


Rings

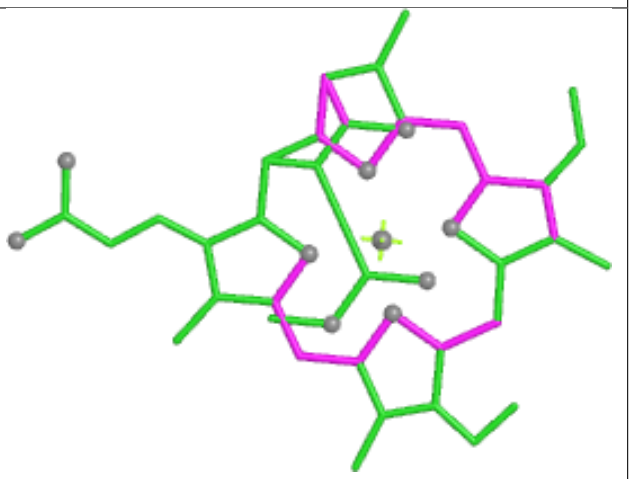
Ligand CLA a 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

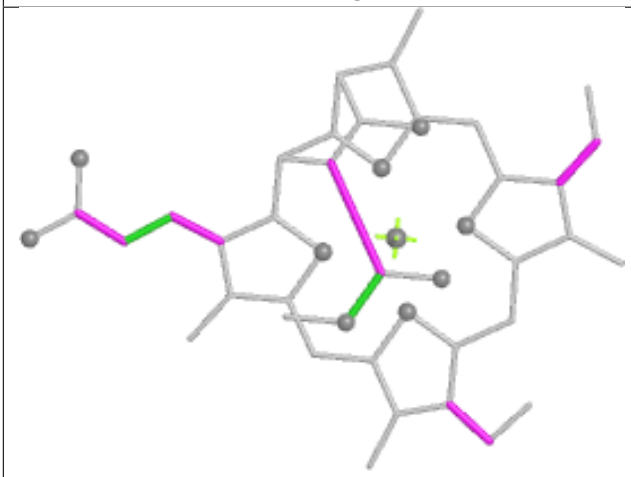
Ligand KC2 L 305



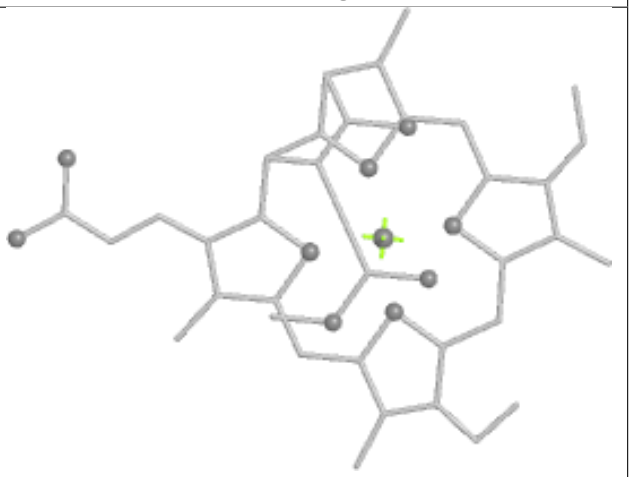
Bond lengths



Bond angles

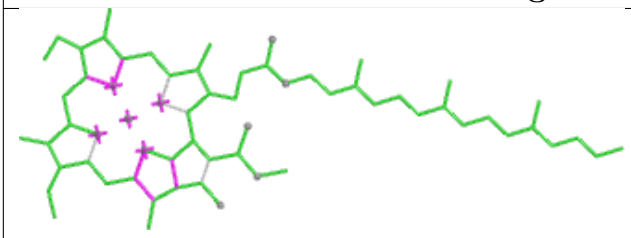


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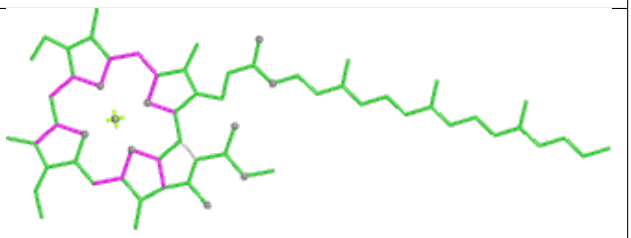


Rings

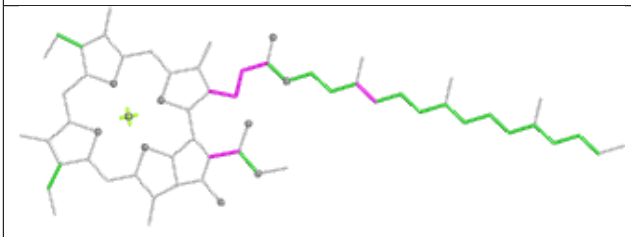
Ligand CLA a 803



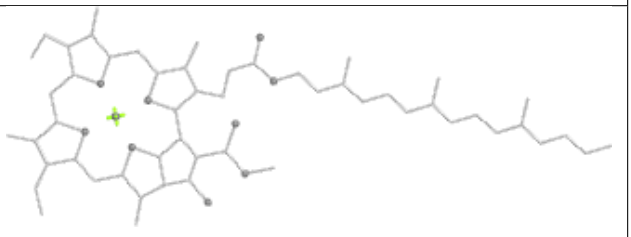
Bond lengths



Bond angles

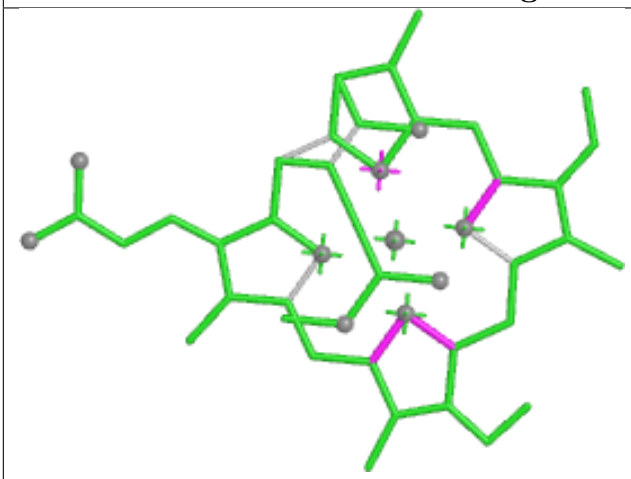


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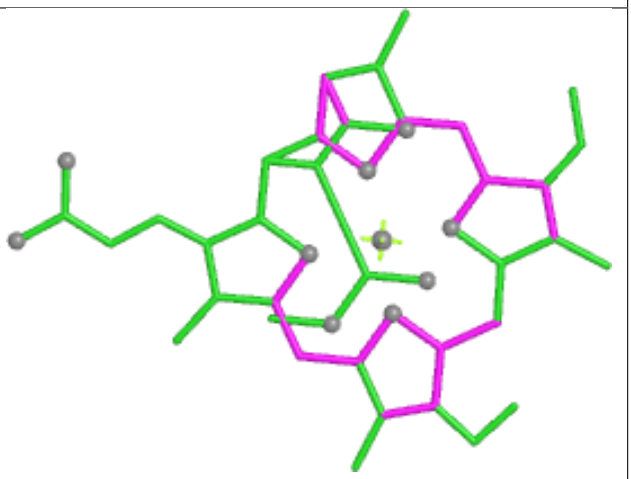


Rings

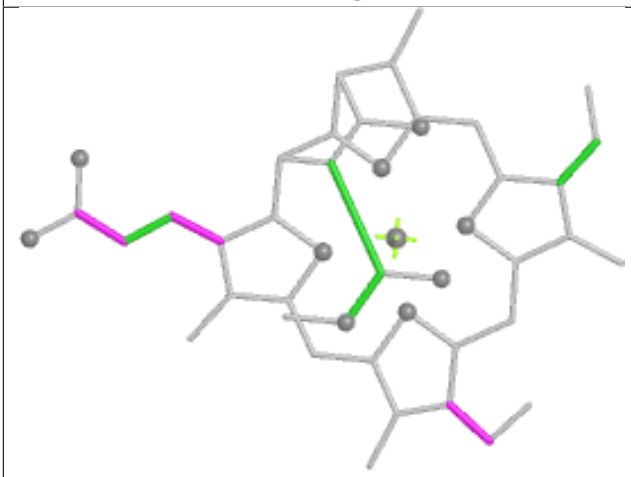
Ligand KC2 W 304



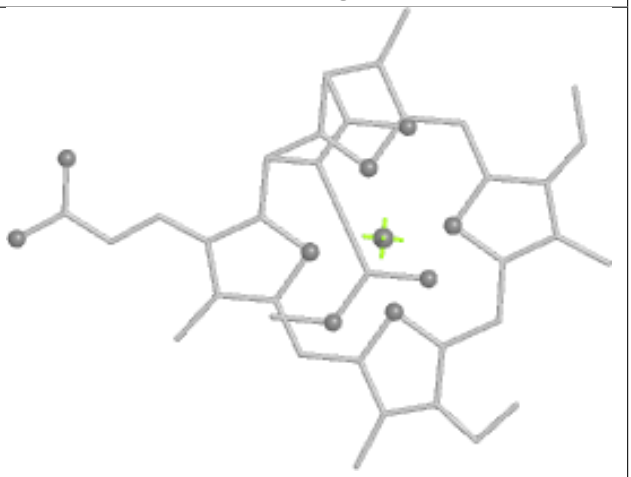
Bond lengths



Bond angles

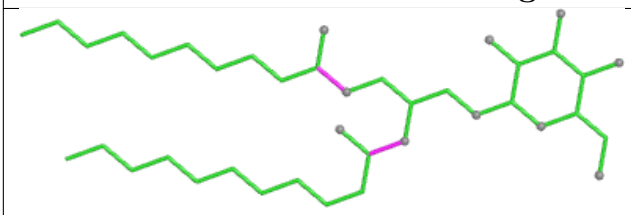


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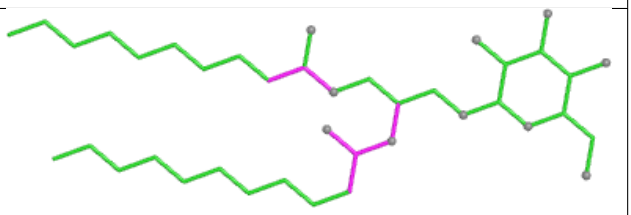


Rings

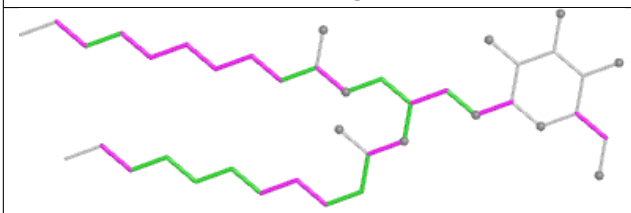
Ligand LMG N 301



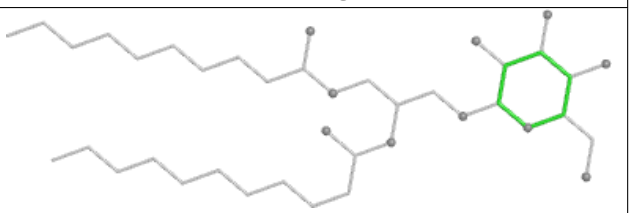
Bond lengths



Bond angles

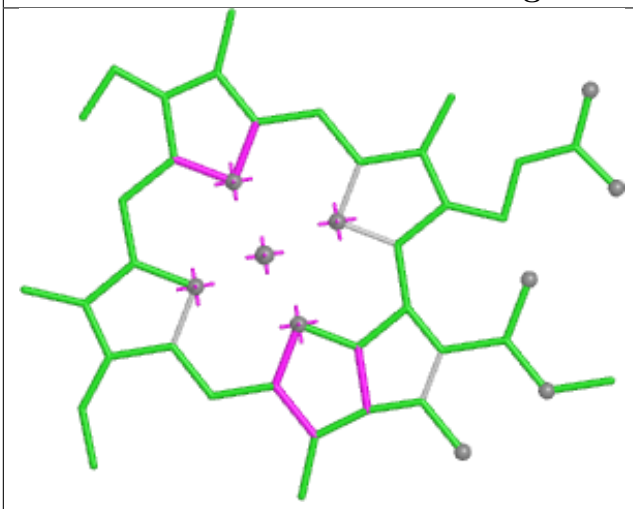


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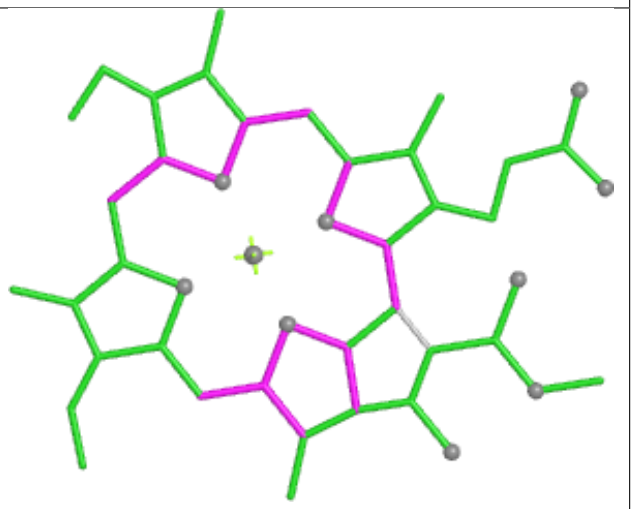


Rings

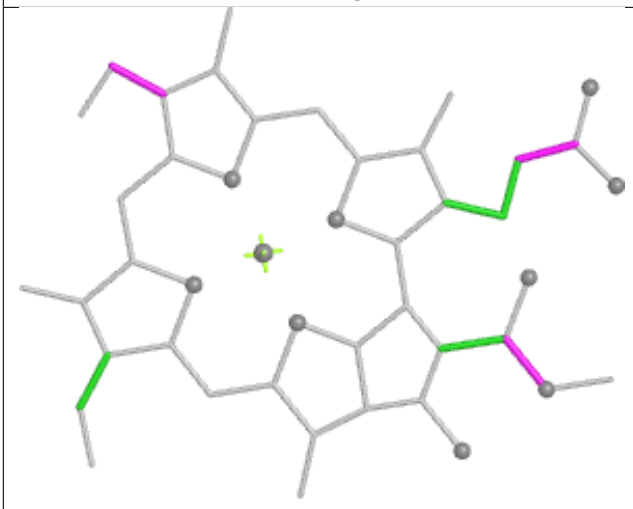
Ligand CLA H 305



Bond lengths



Bond angles

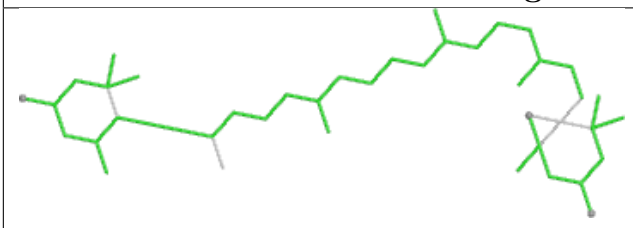


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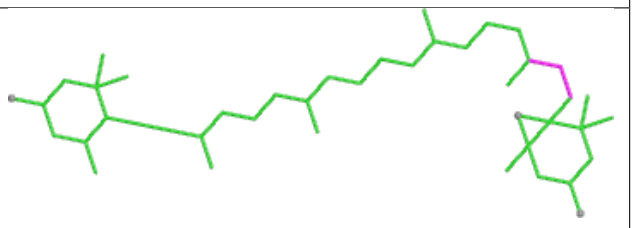


Rings

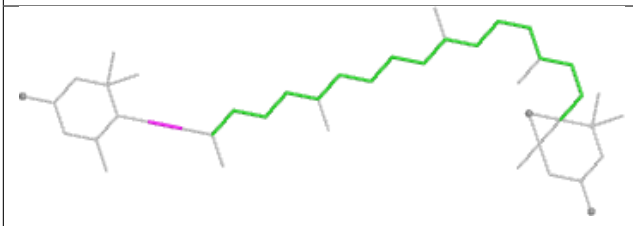
Ligand DD6 A 314



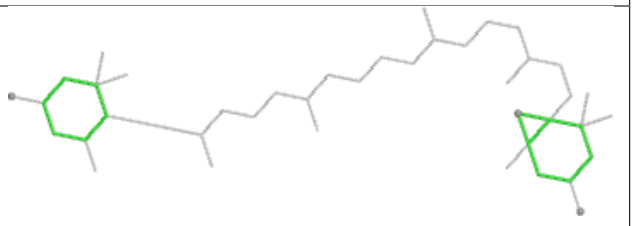
Bond lengths



Bond angles

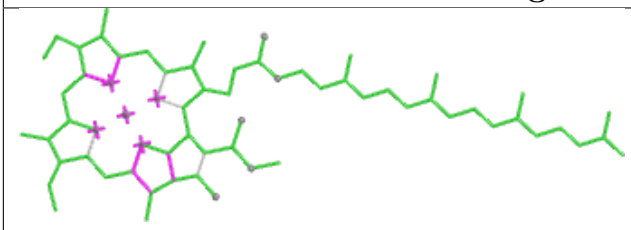


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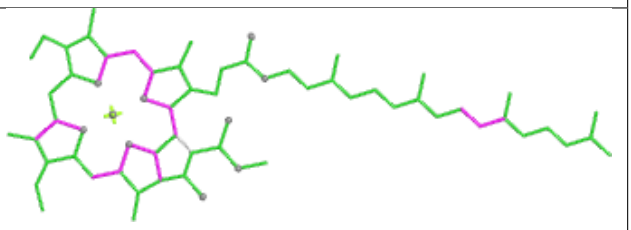


Rings

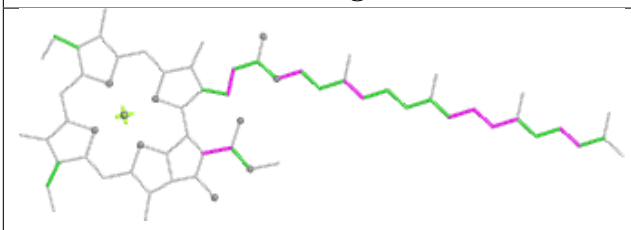
Ligand CLA a 830



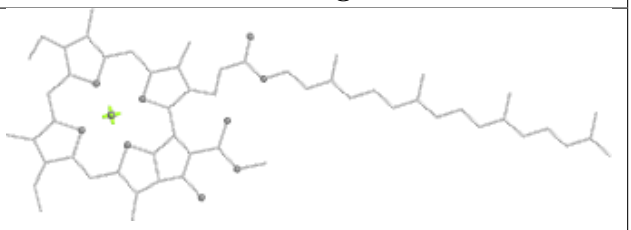
Bond lengths



Bond angles

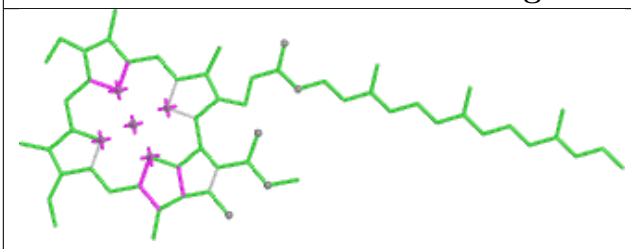


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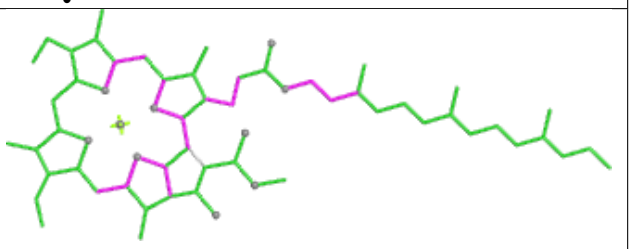


Rings

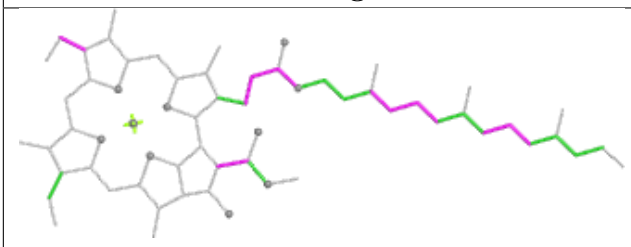
Ligand CLA Q 306



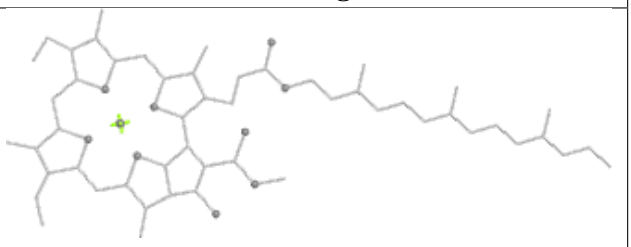
Bond lengths



Bond angles

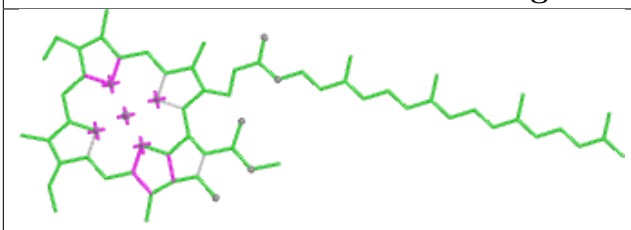


Torsions

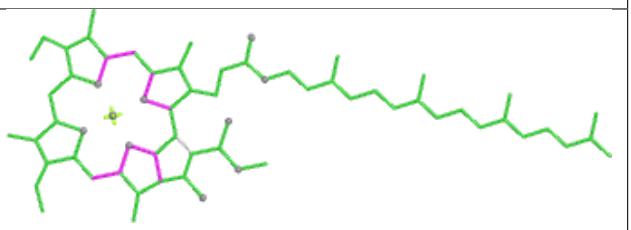


Rings

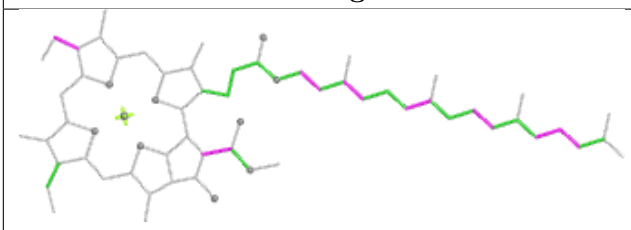
Ligand CLA I 301



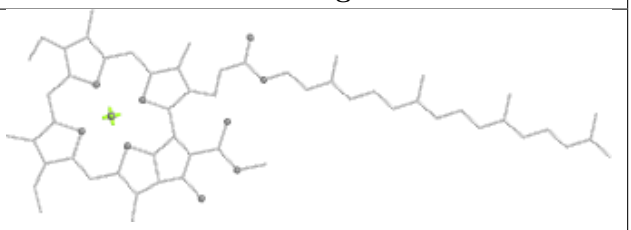
Bond lengths



Bond angles

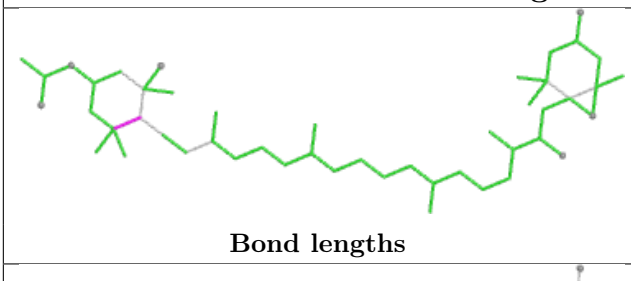


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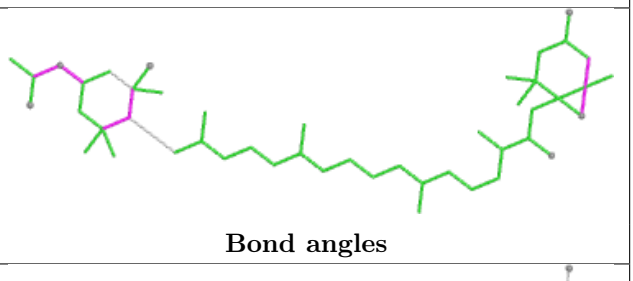


Rings

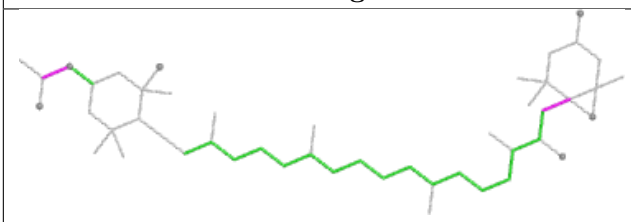
Ligand A86 P 314



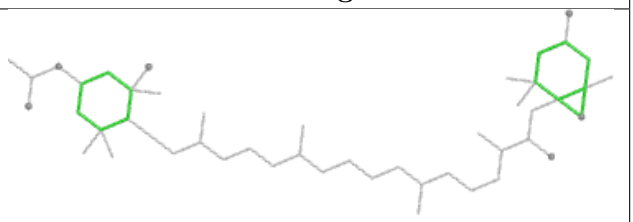
Bond lengths



Bond angles

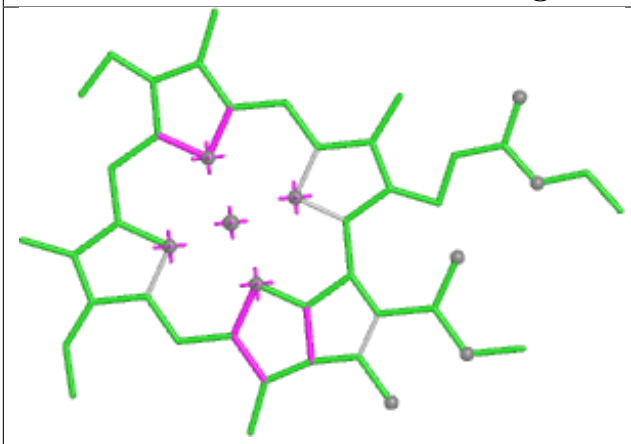


Torsions

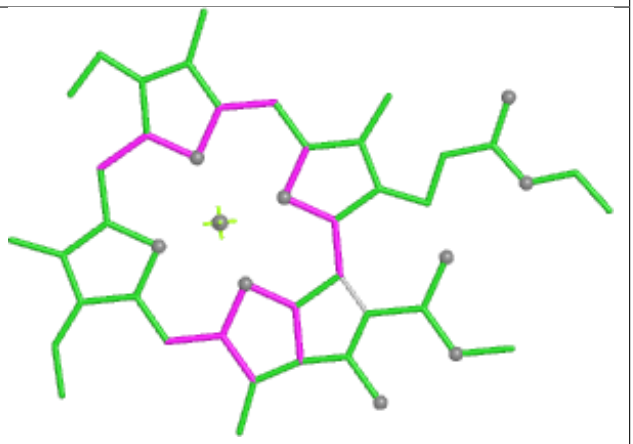


Rings

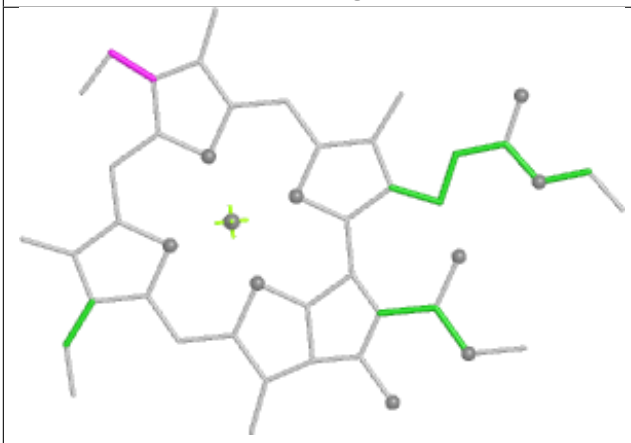
Ligand CLA f 204



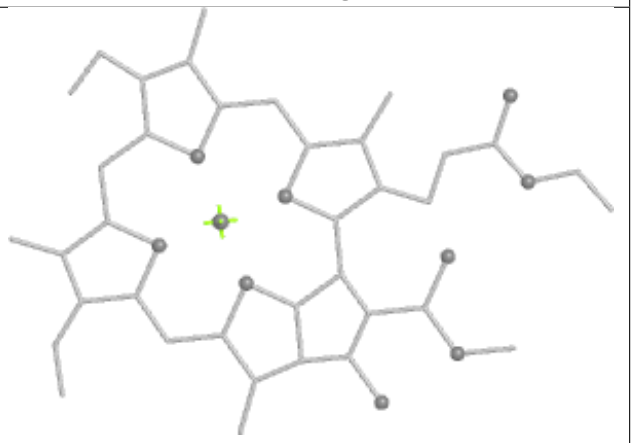
Bond lengths



Bond angles

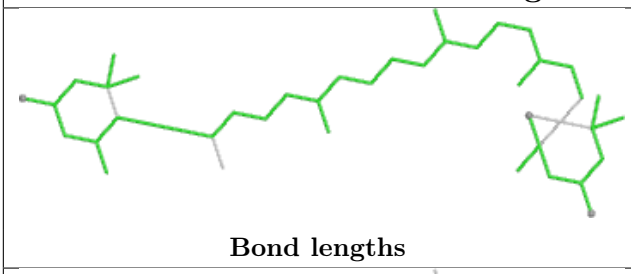


Torsions

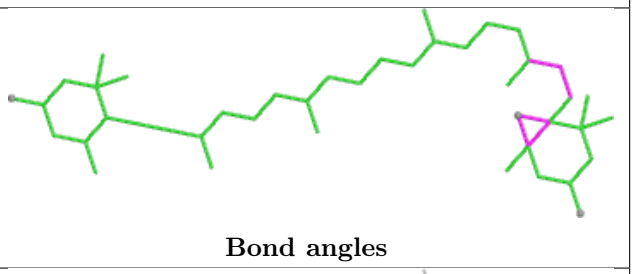


Rings

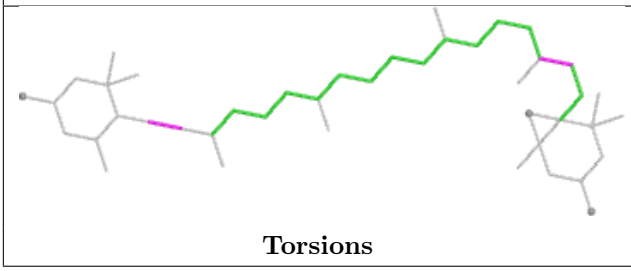
Ligand DD6 A 313



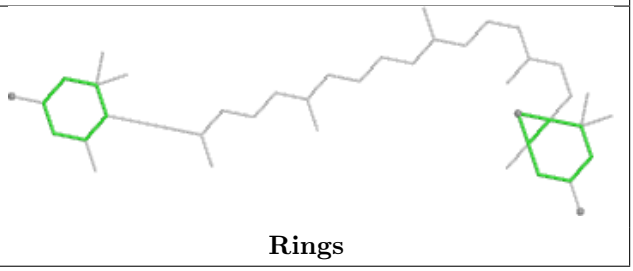
Bond lengths



Bond angles

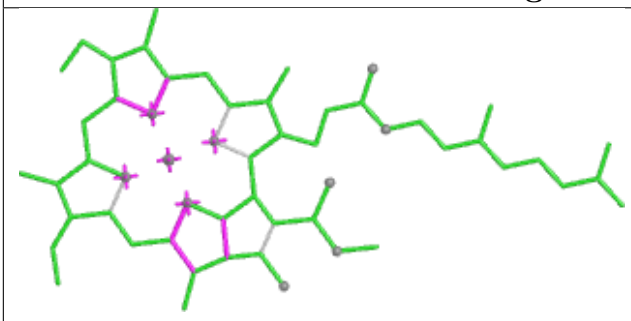


Torsions

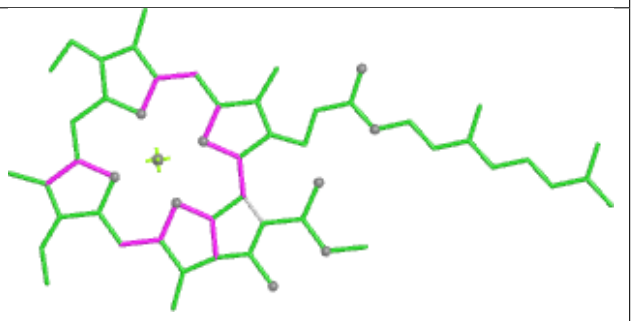


Rings

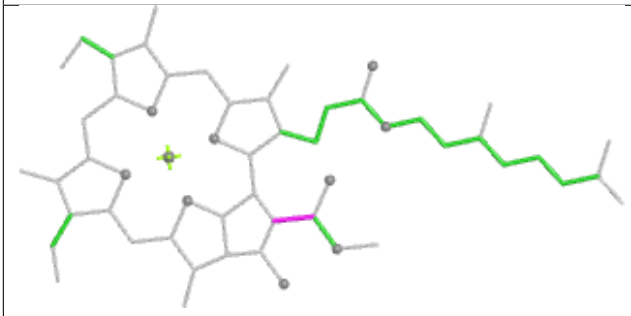
Ligand CLA E 305



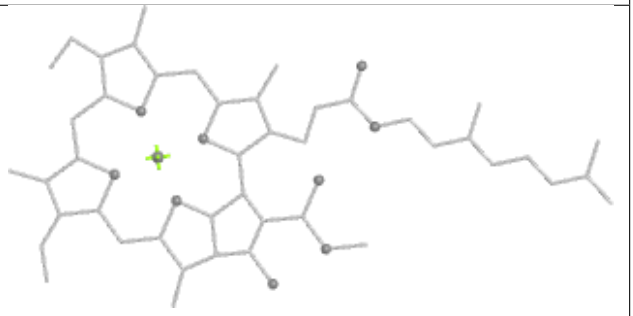
Bond lengths



Bond angles

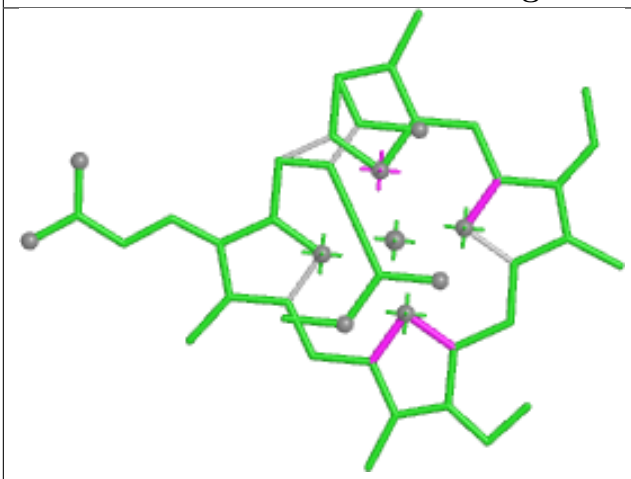


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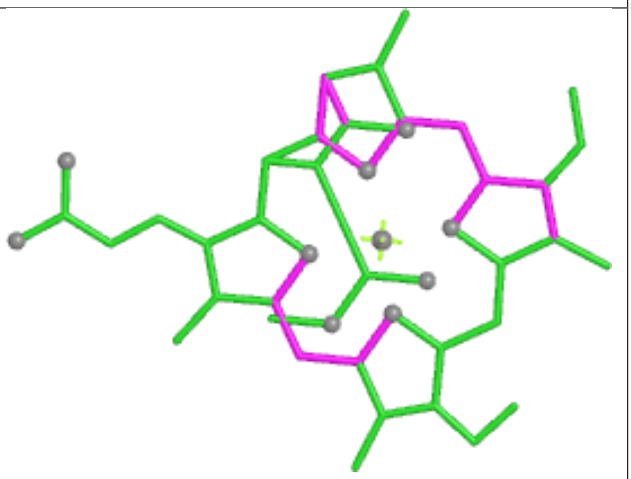


Rings

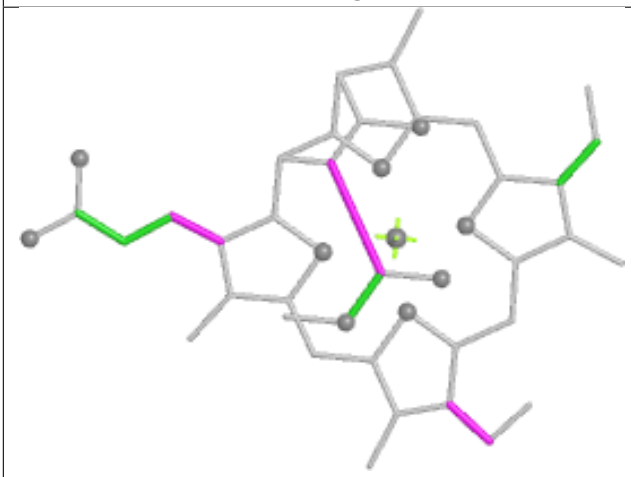
Ligand KC2 M 321



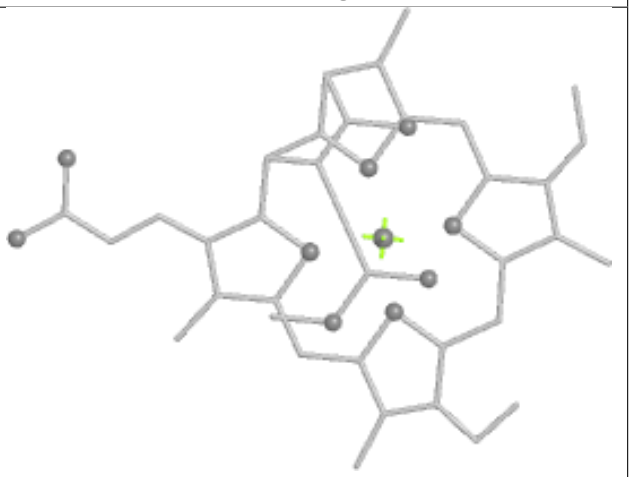
Bond lengths



Bond angles

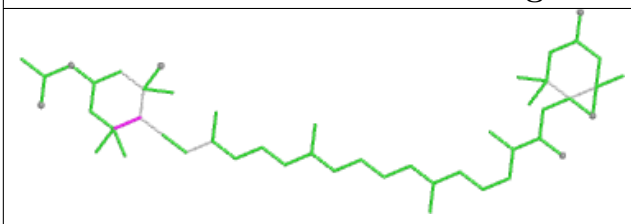


Torsions

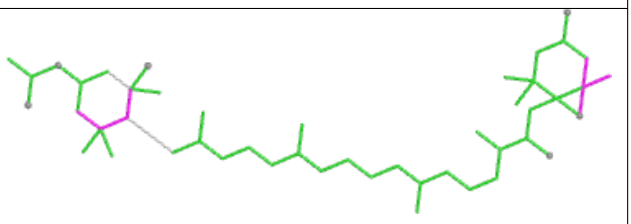


Rings

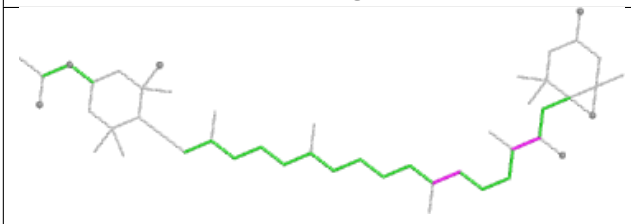
Ligand A86 M 318



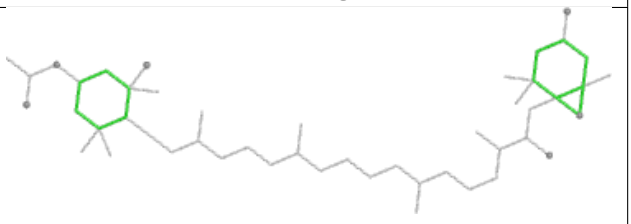
Bond lengths



Bond angles

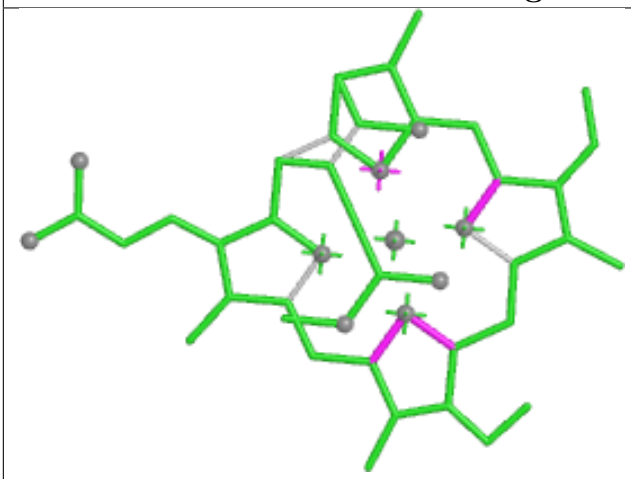


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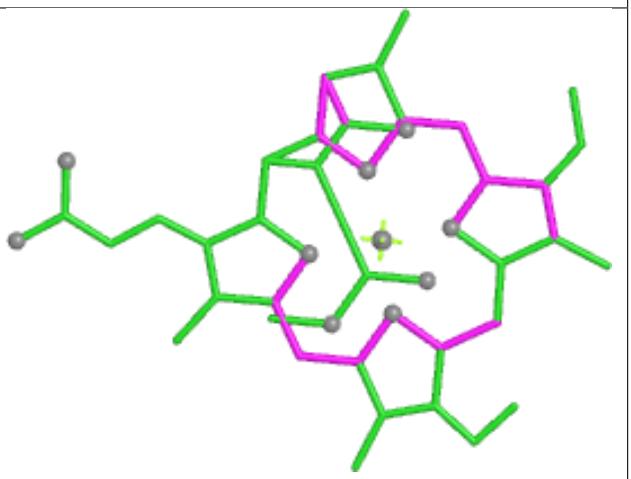


Rings

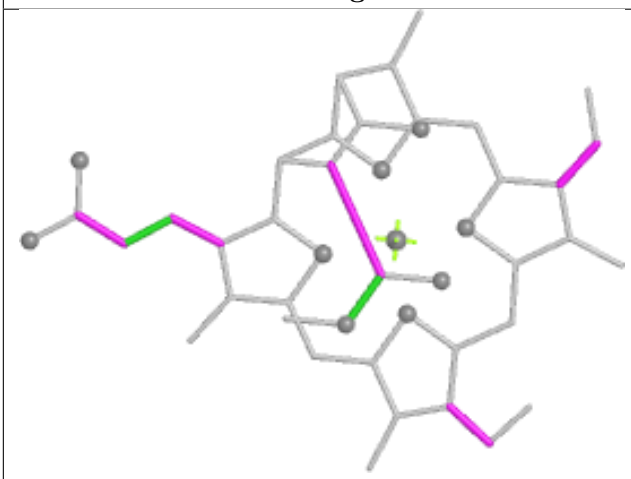
Ligand KC2 G 309



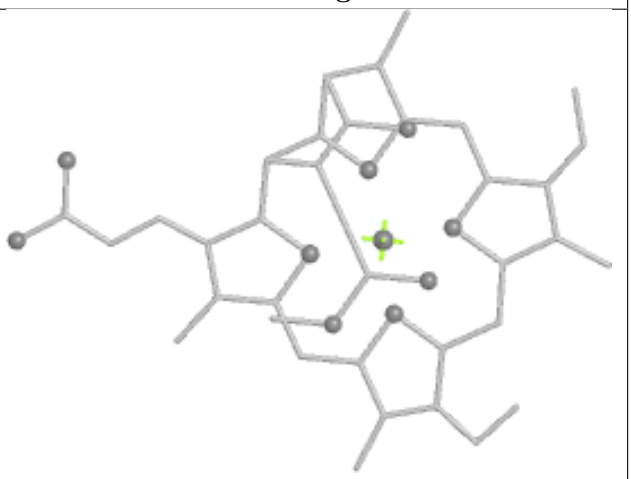
Bond lengths



Bond angles

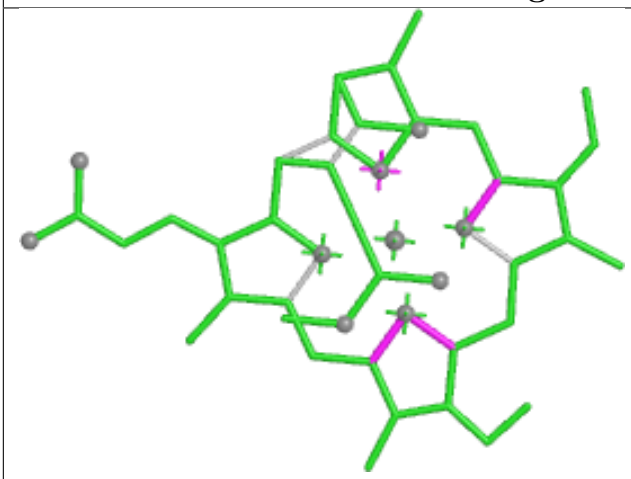


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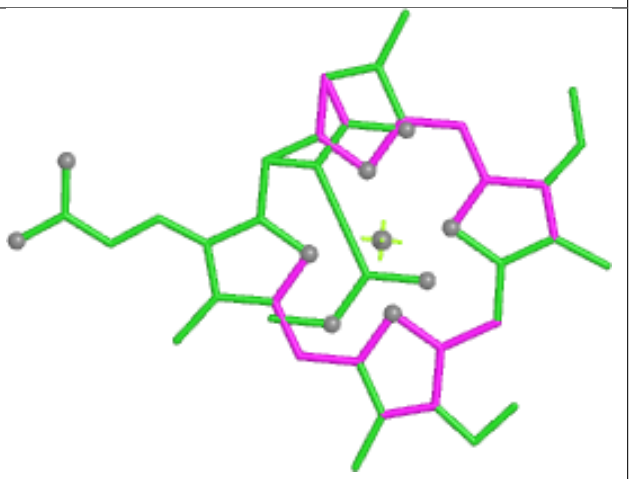


Rings

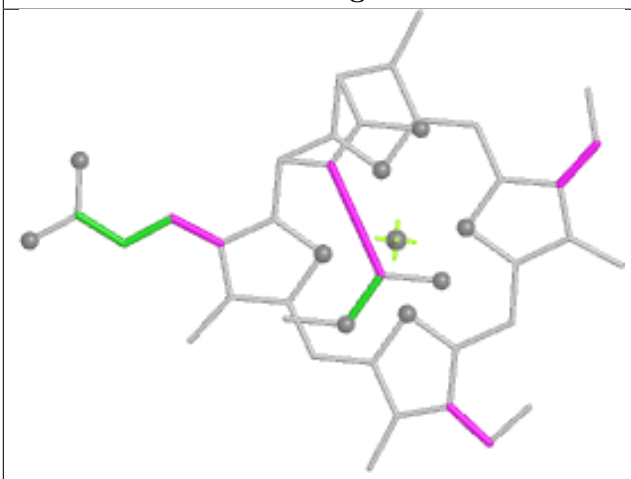
Ligand KC2 L 306



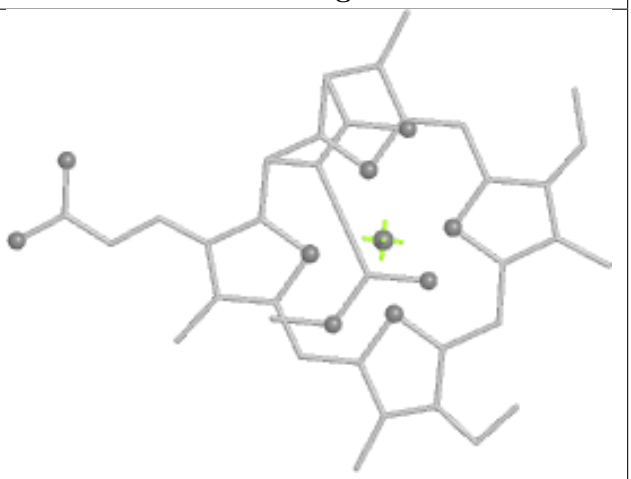
Bond lengths



Bond angles



Torsions



Rings

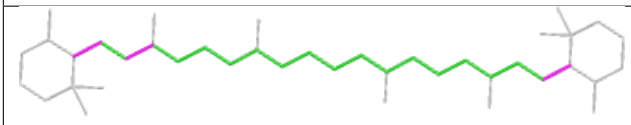
Ligand BCR j 102



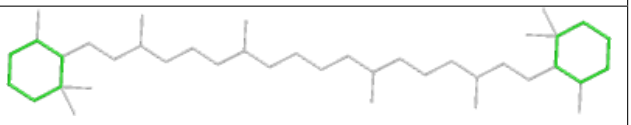
Bond lengths



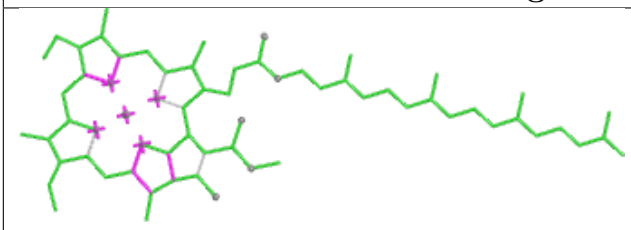
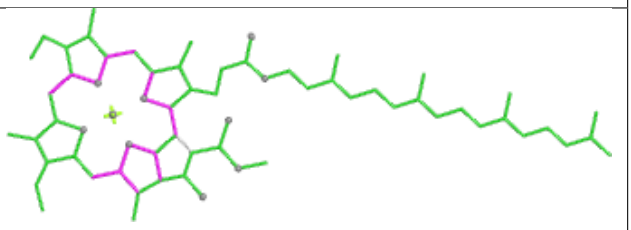
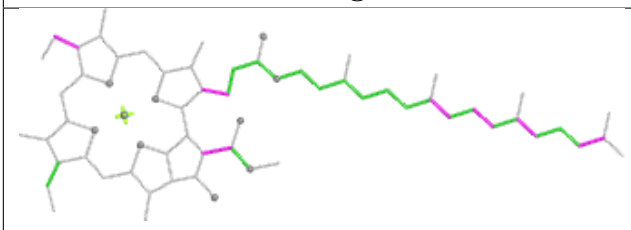
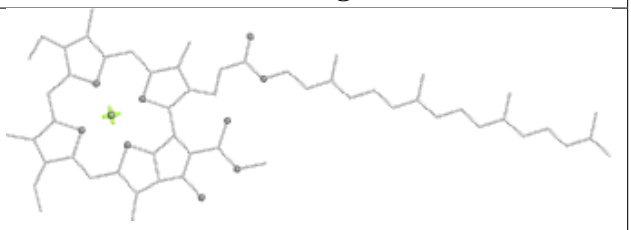
Bond angles

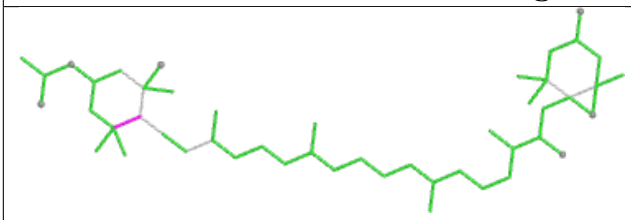
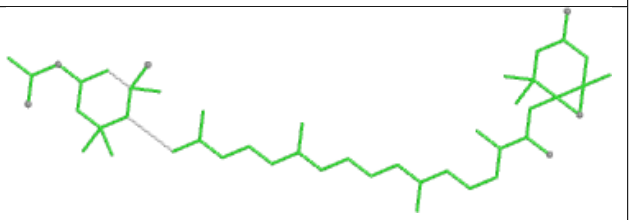
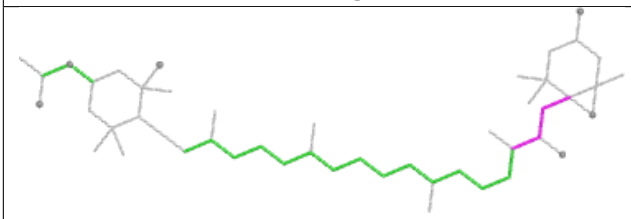
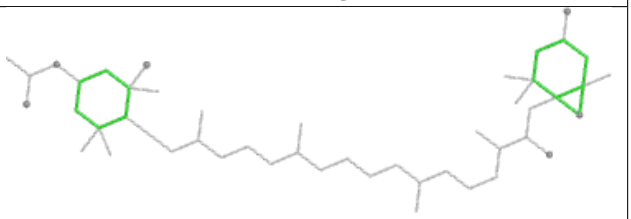


Torsions

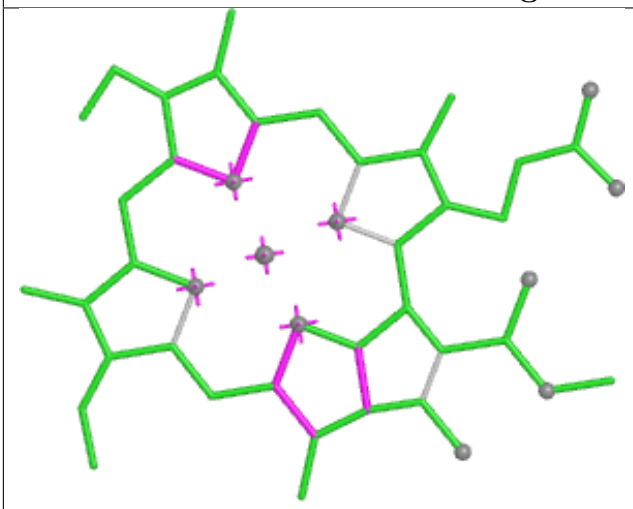


Rings

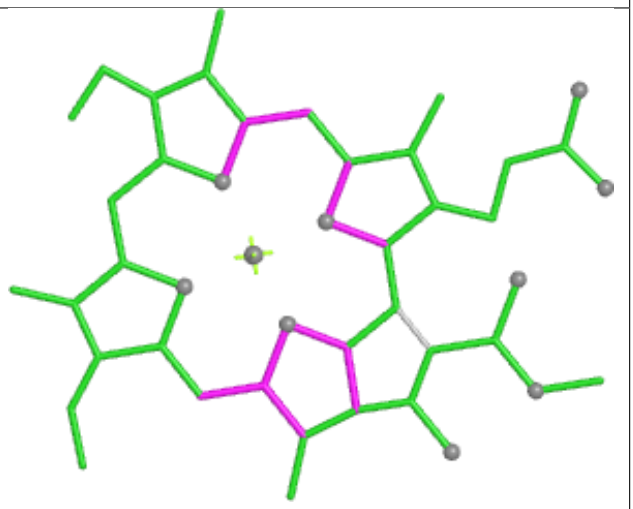
Ligand CLA b 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A86 S 320	
	
Bond lengths	Bond angles
	
Torsions	Rings

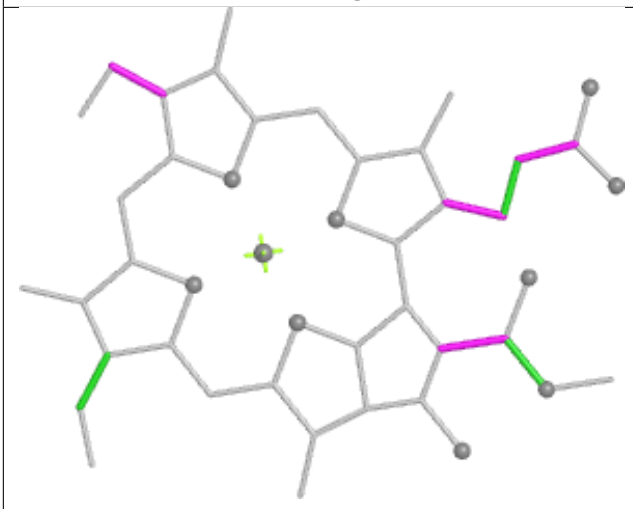
Ligand CLA M 309



Bond lengths



Bond angles

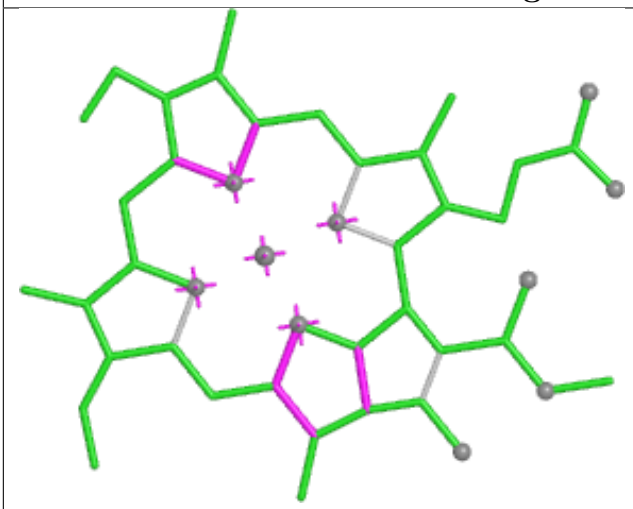


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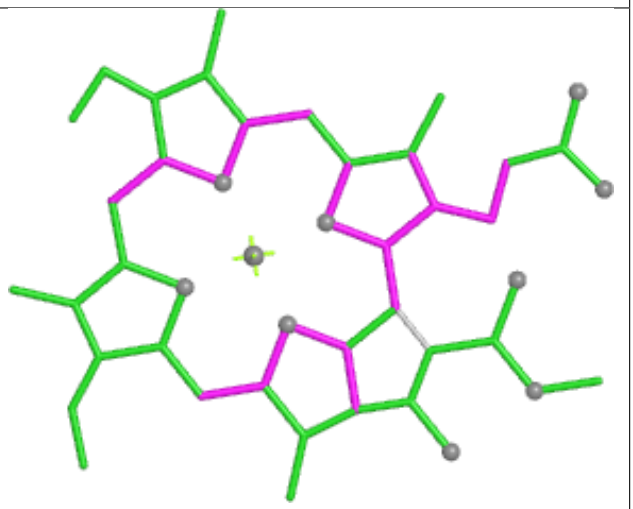


Rings

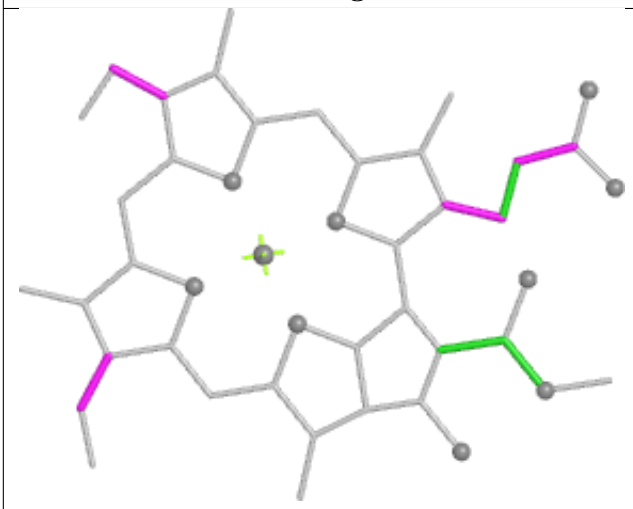
Ligand CLA H 304



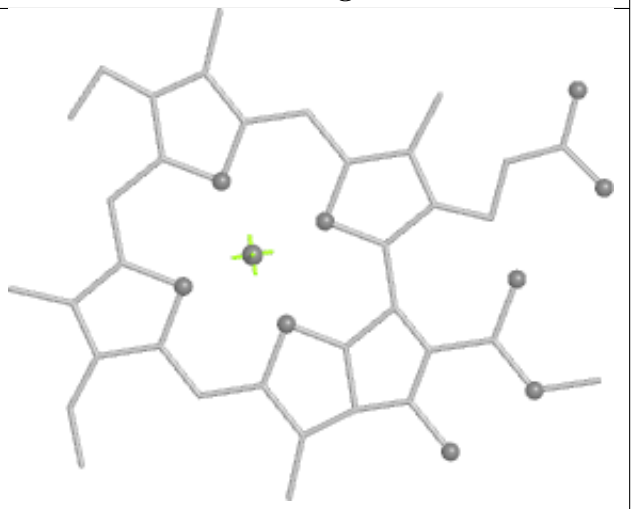
Bond lengths



Bond angles

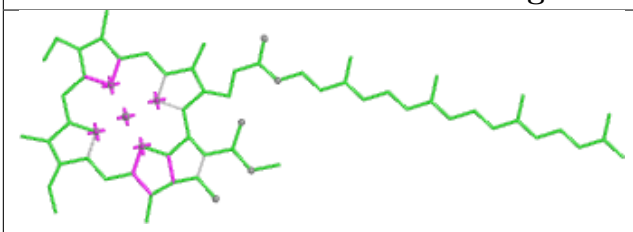


Torsions

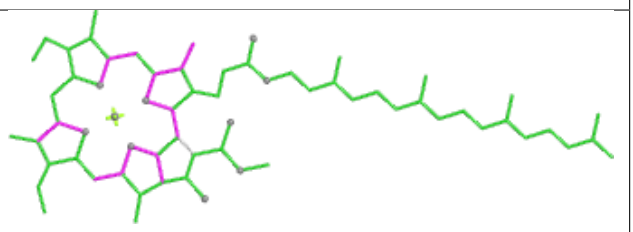


Rings

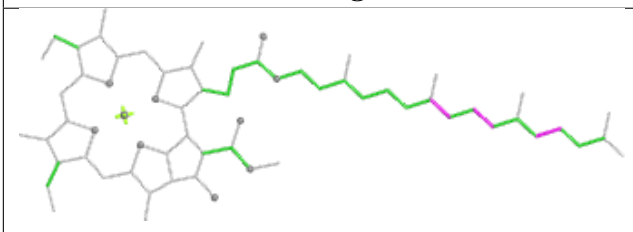
Ligand CLA b 819



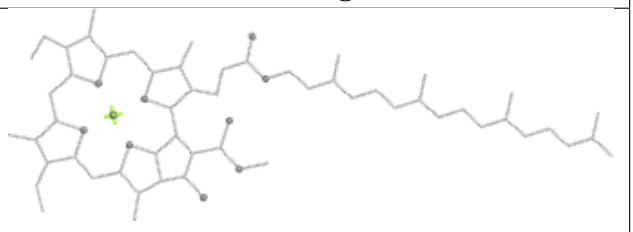
Bond lengths



Bond angles

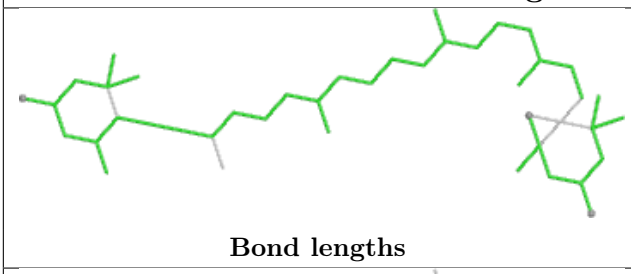


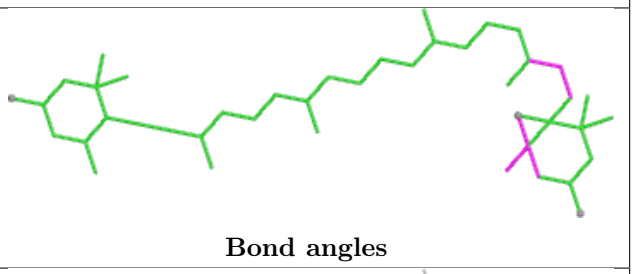
Torsions

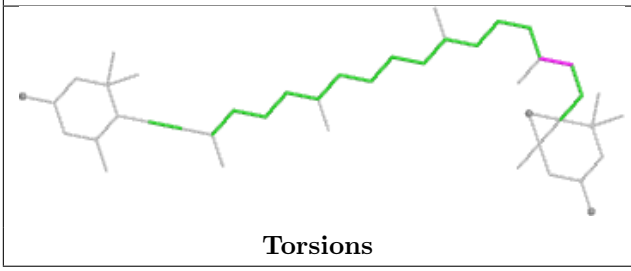


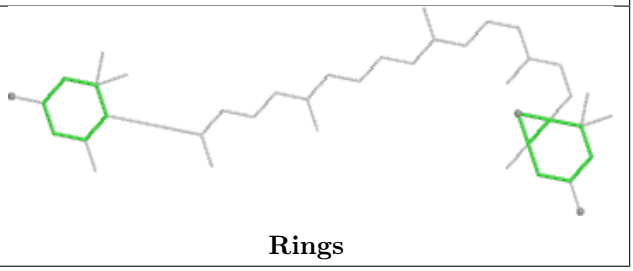
Rings

Ligand DD6 T 314

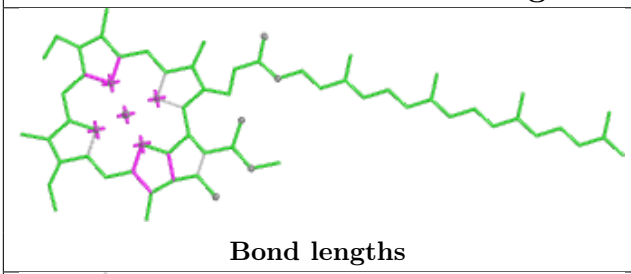

Bond lengths

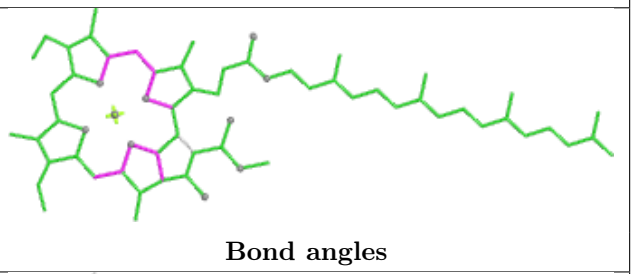

Bond angles

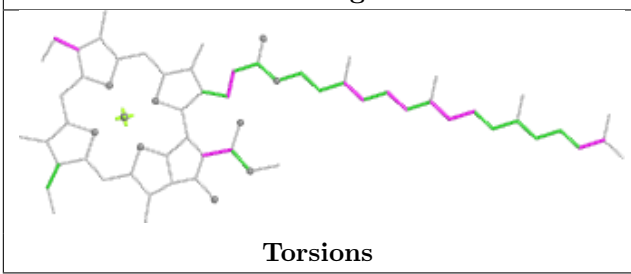

Torsions

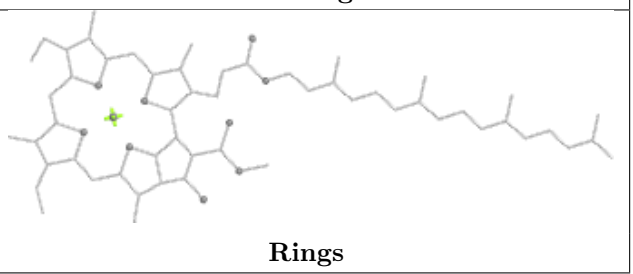

Rings

Ligand CLA a 835

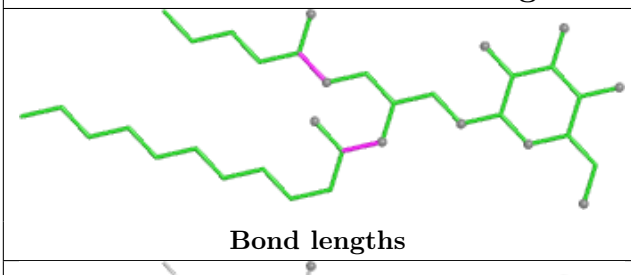

Bond lengths

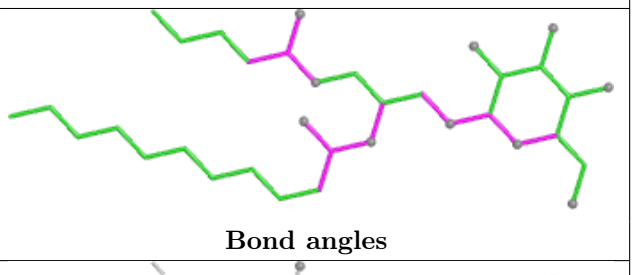

Bond angles

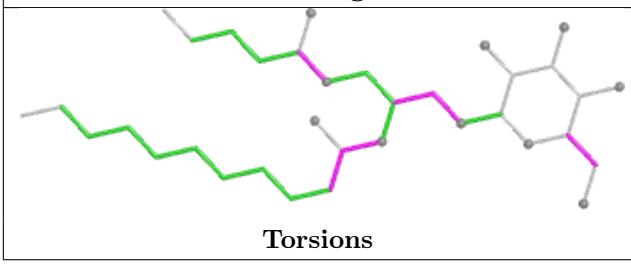

Torsions

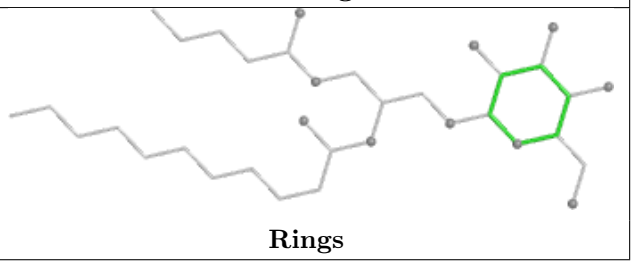

Rings

Ligand LMG D 325

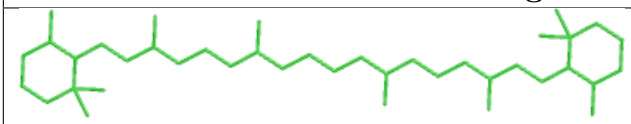

Bond lengths


Bond angles

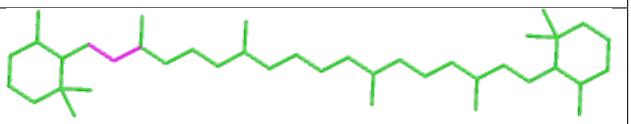

Torsions


Rings

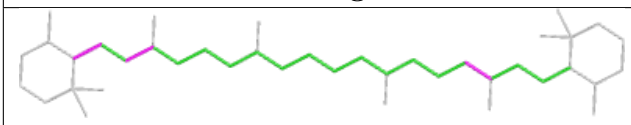
Ligand BCR b 842



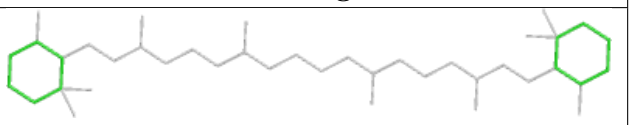
Bond lengths



Bond angles

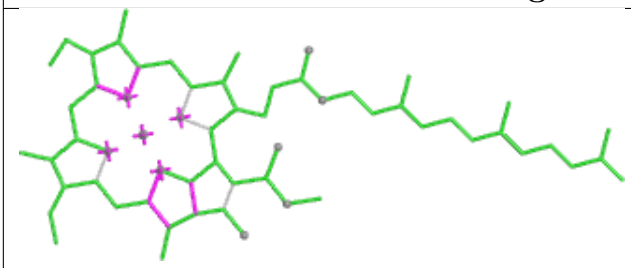


Torsions

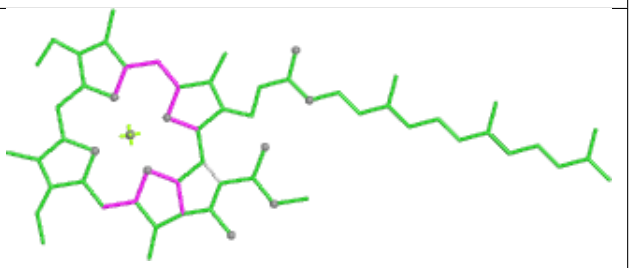


Rings

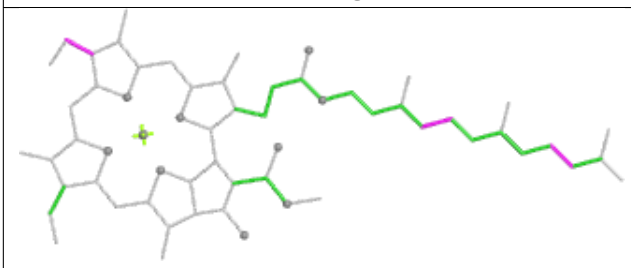
Ligand CLA a 831



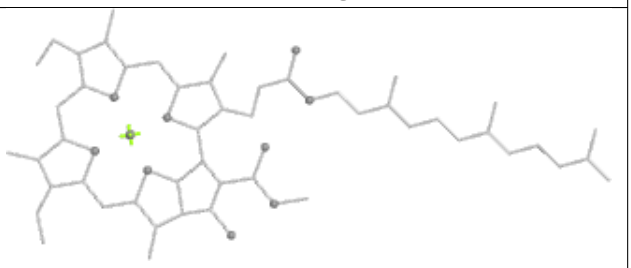
Bond lengths



Bond angles

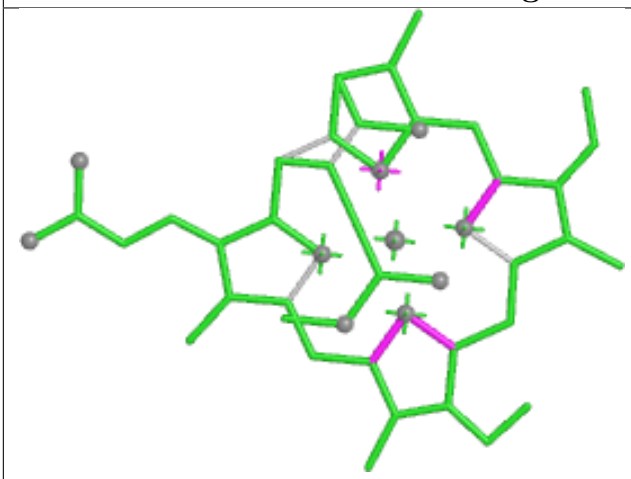


Torsions

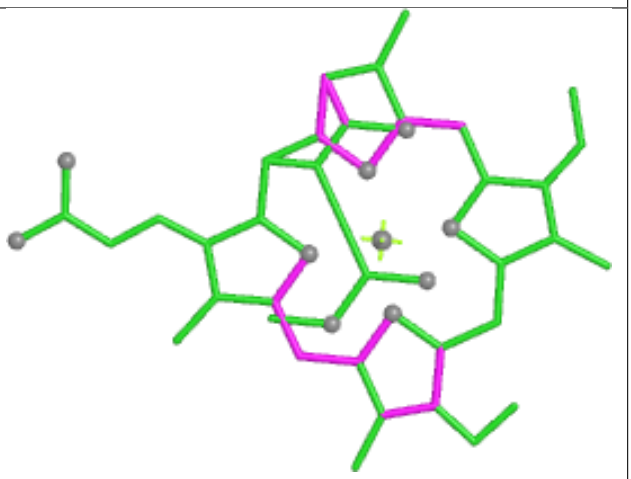


Rings

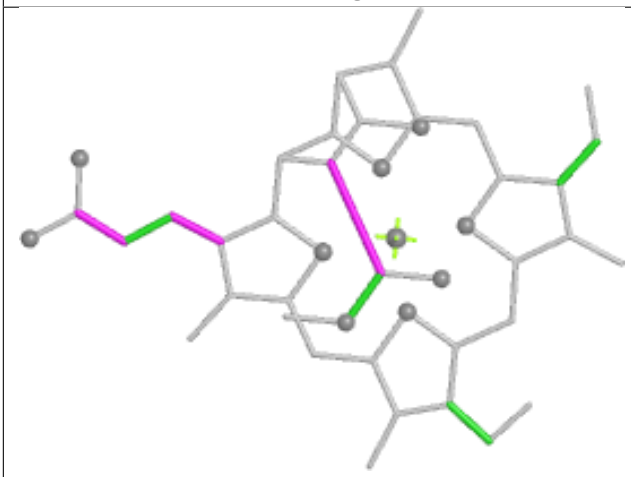
Ligand KC2 M 304



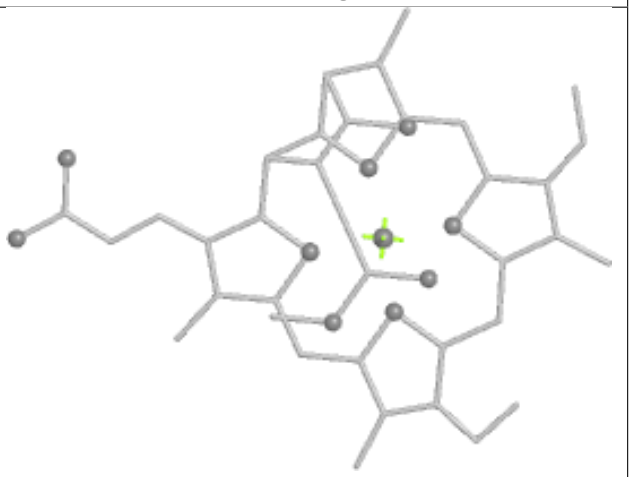
Bond lengths



Bond angles

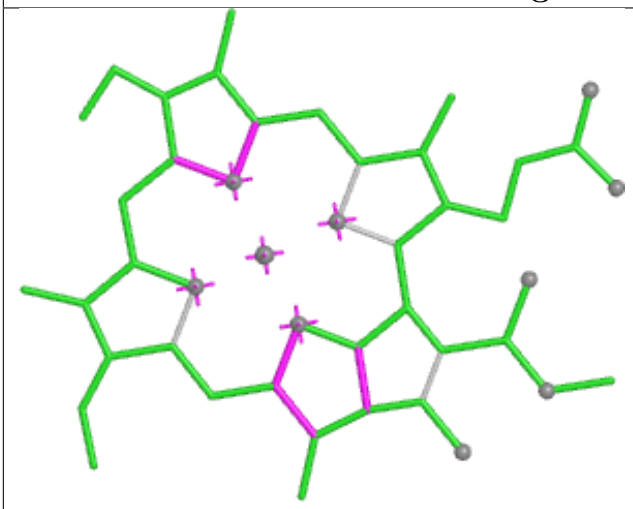


Torsions

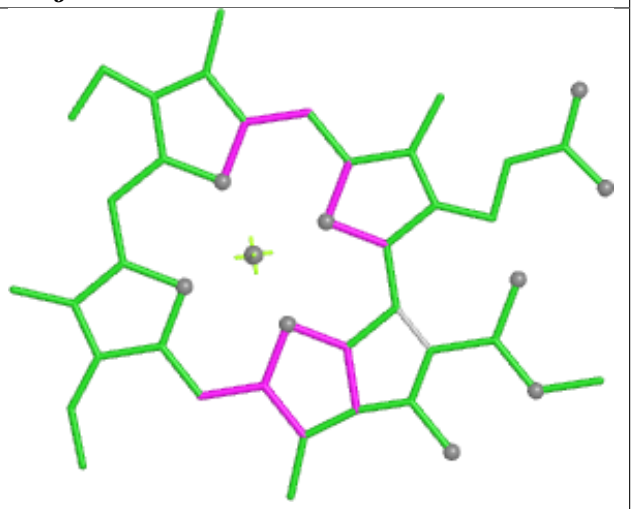


Rings

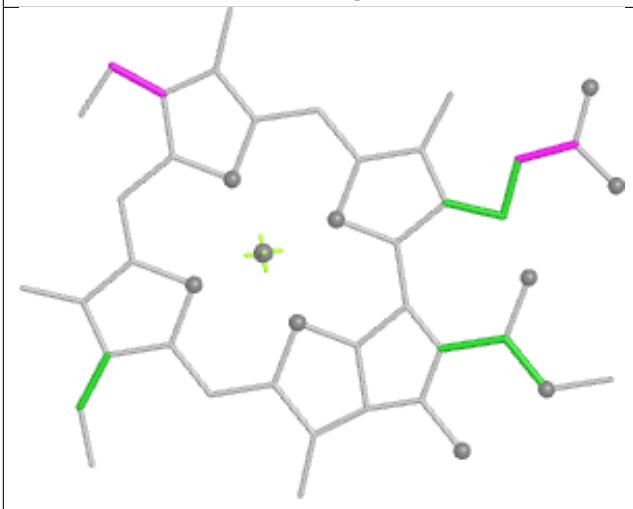
Ligand CLA j 101



Bond lengths



Bond angles

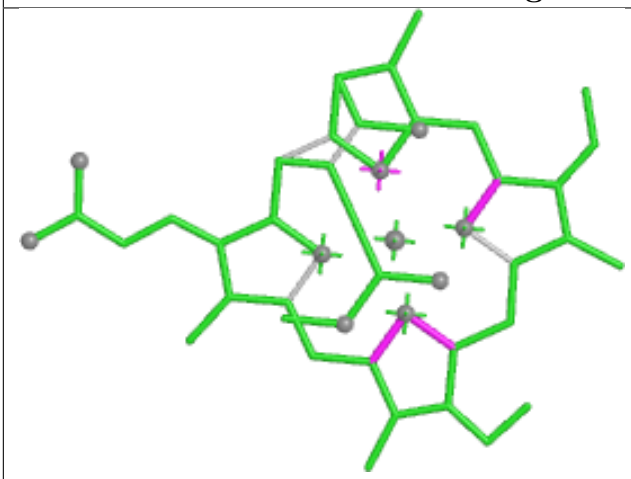


Torsions

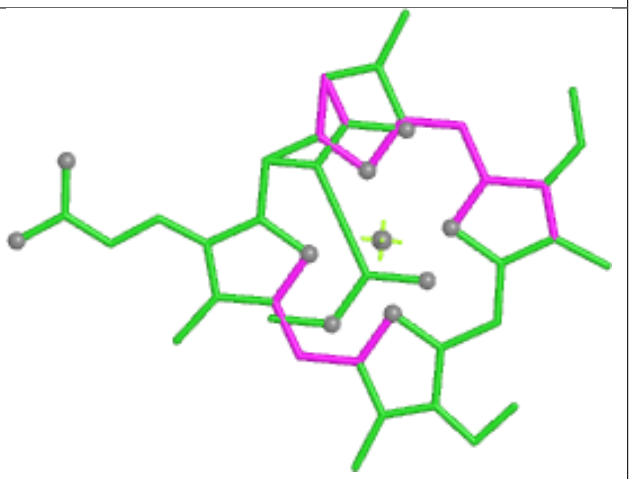


Rings

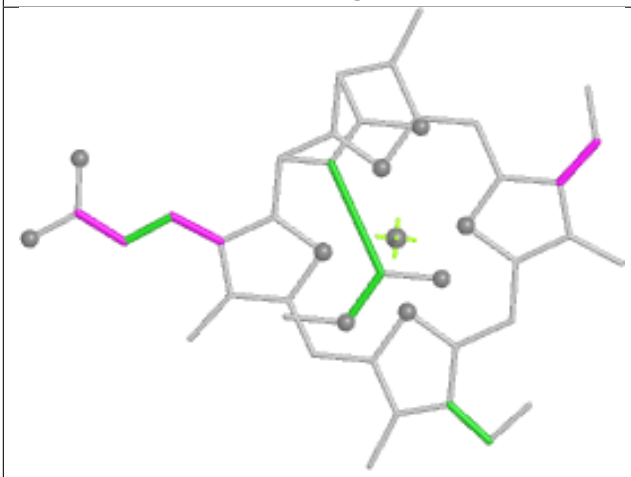
Ligand KC2 U 304



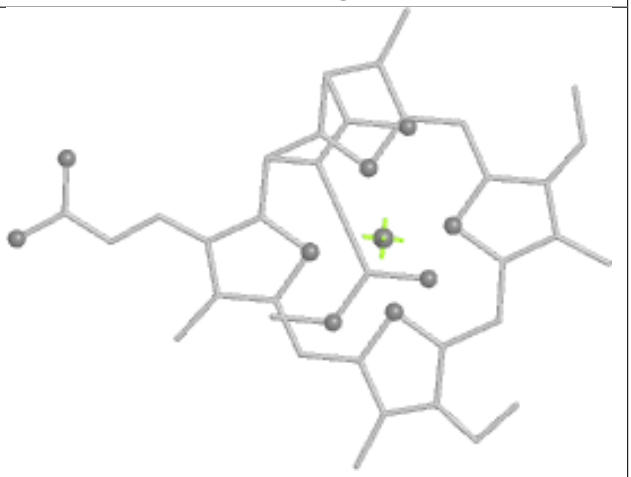
Bond lengths



Bond angles

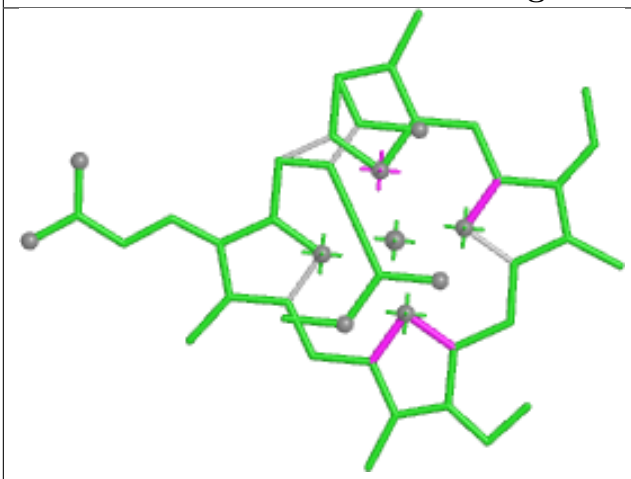


Torsions

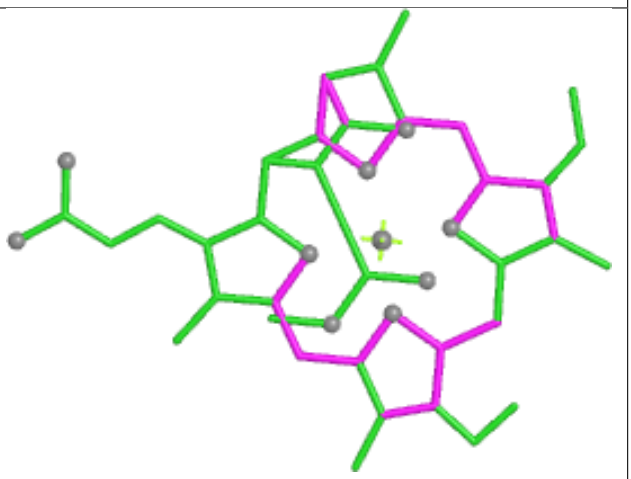


Rings

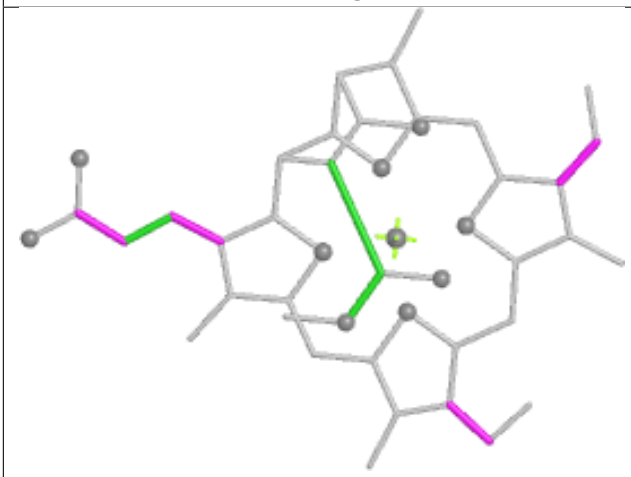
Ligand KC2 F 302



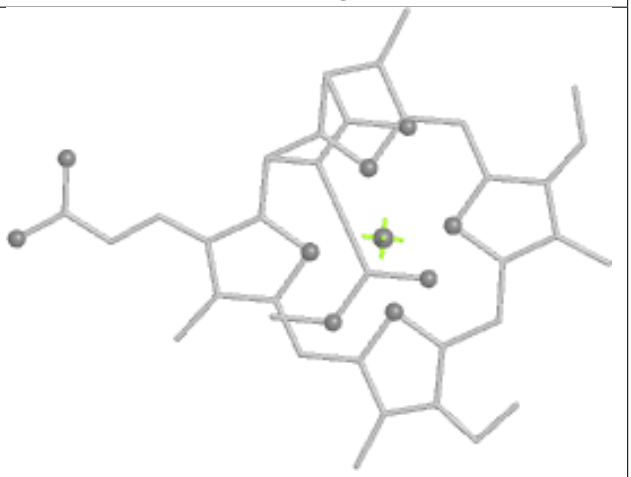
Bond lengths



Bond angles

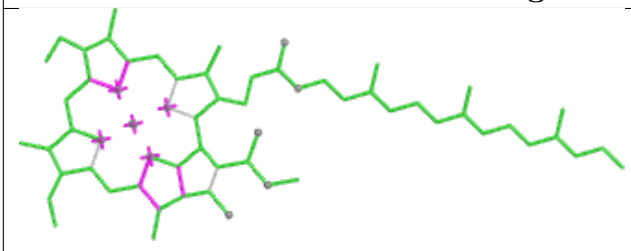


Torsions

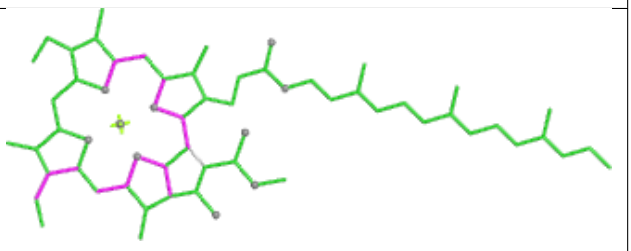


Rings

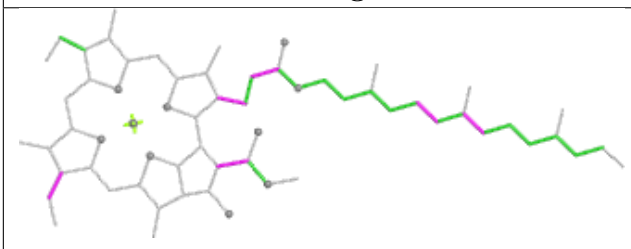
Ligand CLA b 816



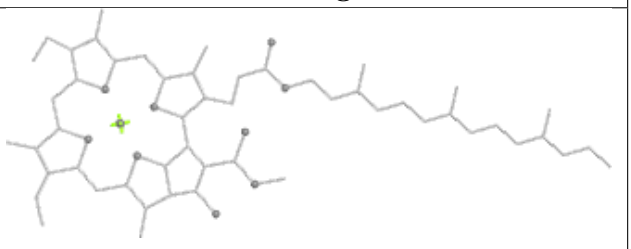
Bond lengths



Bond angles

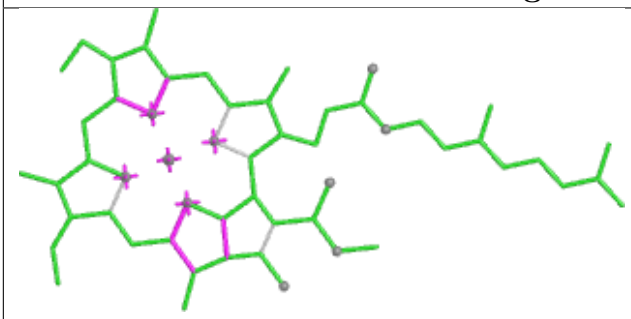


Torsions

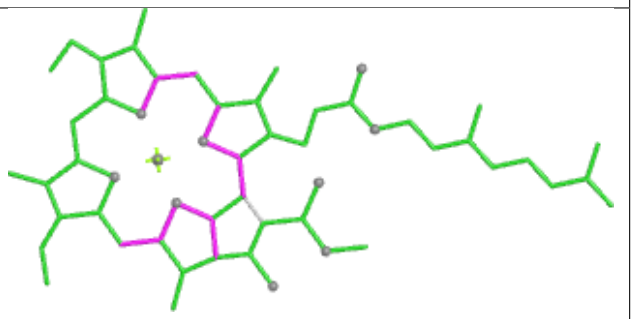


Rings

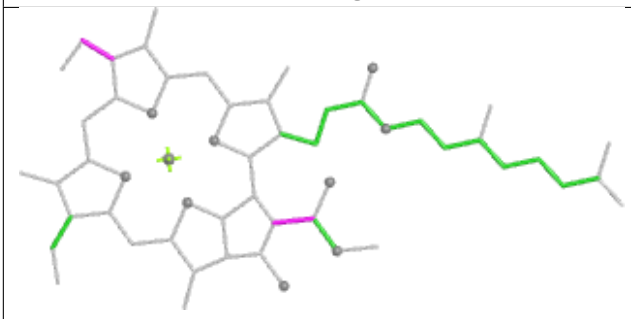
Ligand CLA V 203



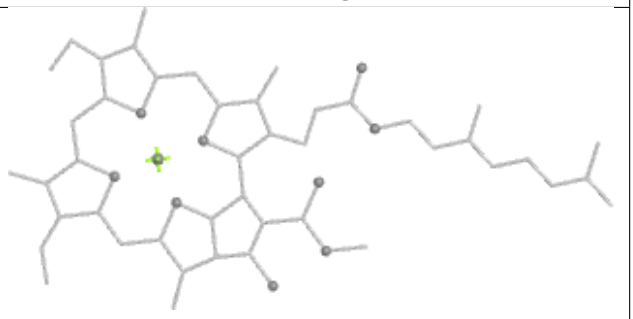
Bond lengths



Bond angles

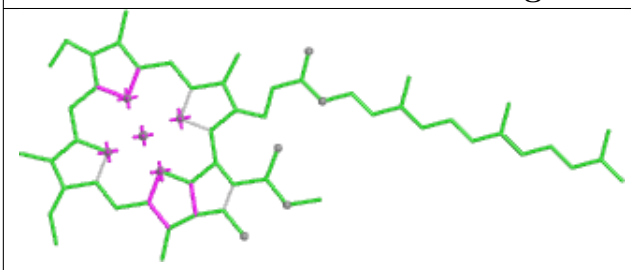


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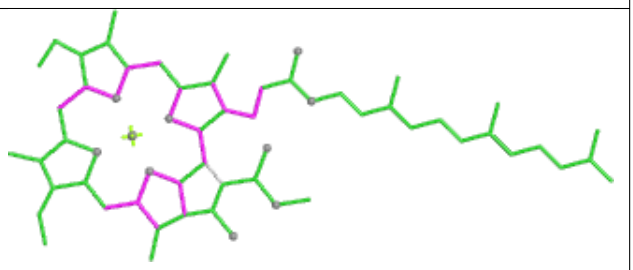


Rings

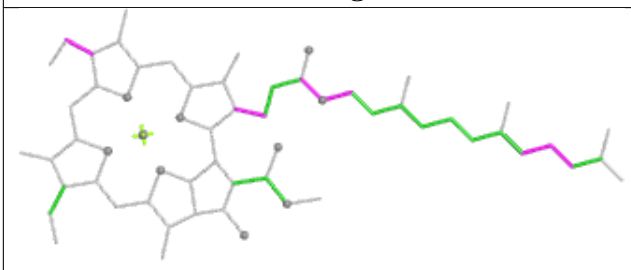
Ligand CLA C 307



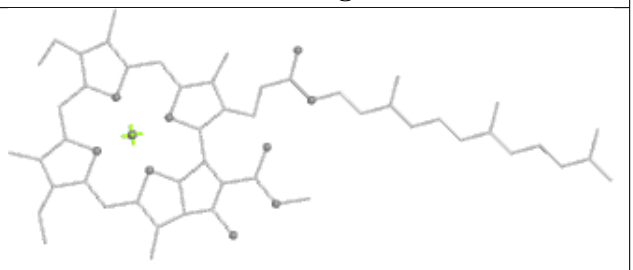
Bond lengths



Bond angles

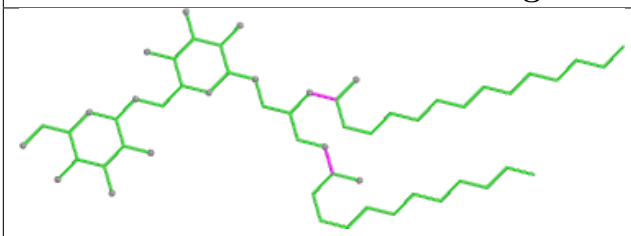


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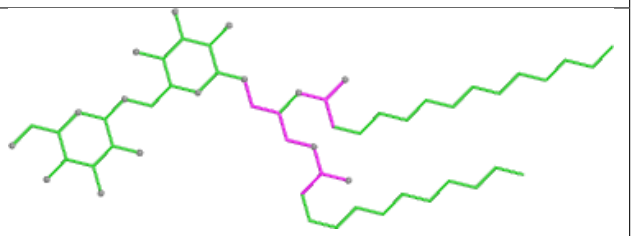


Rings

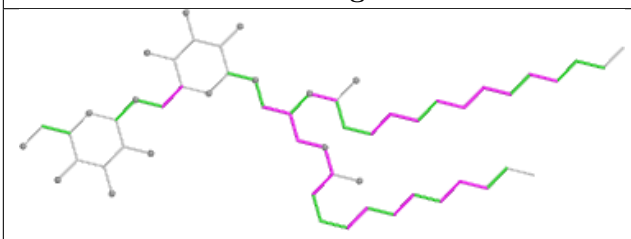
Ligand DGD b 846



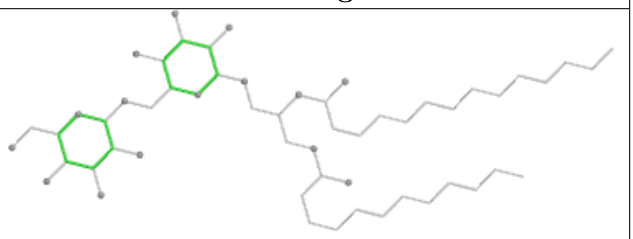
Bond lengths



Bond angles

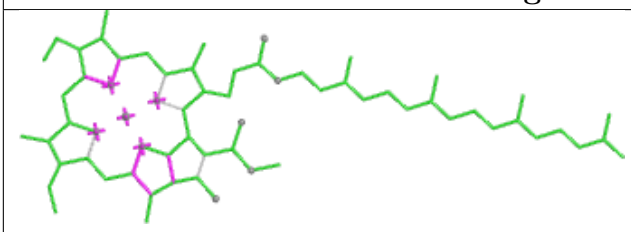


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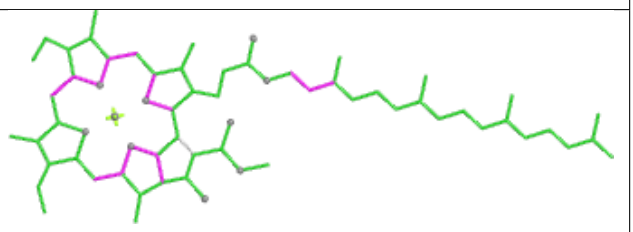


Rings

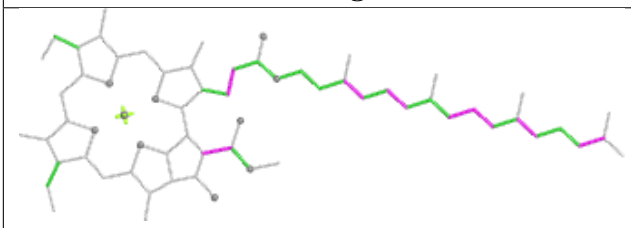
Ligand CLA A 309



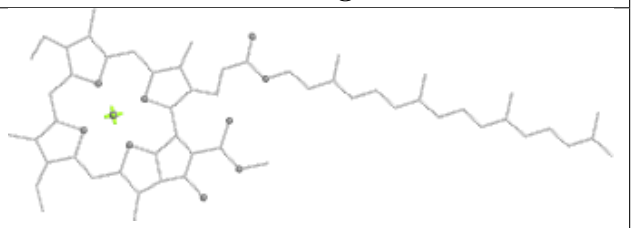
Bond lengths



Bond angles

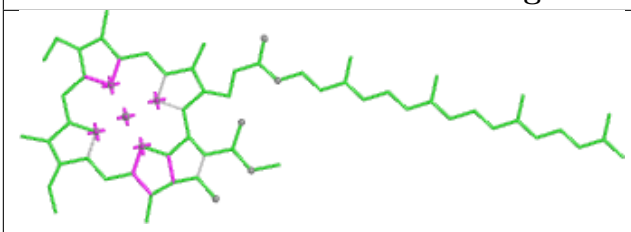


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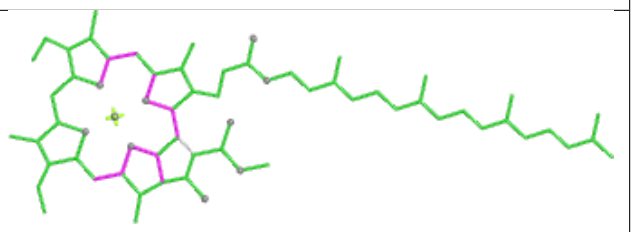


Rings

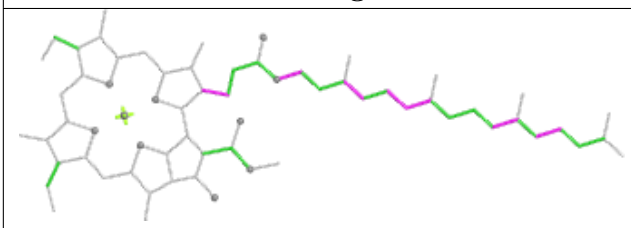
Ligand CLA A 306



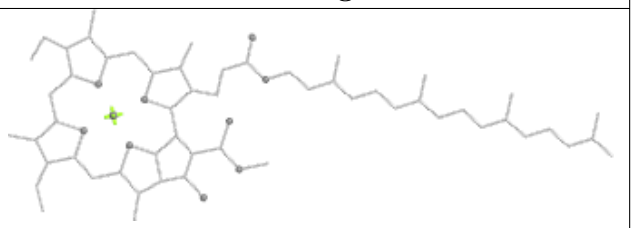
Bond lengths



Bond angles

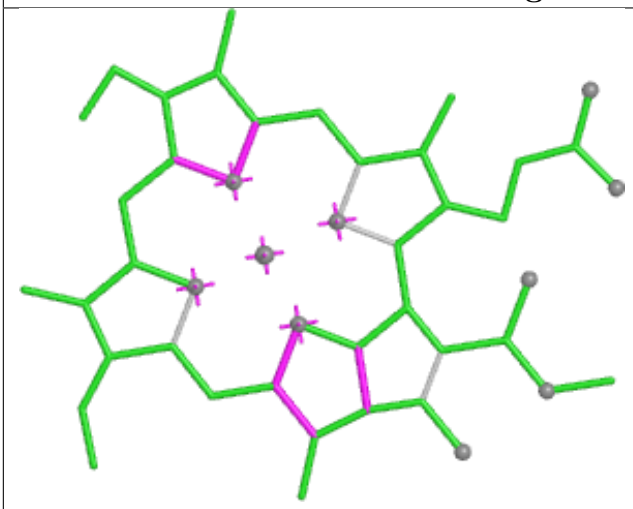


Torsions

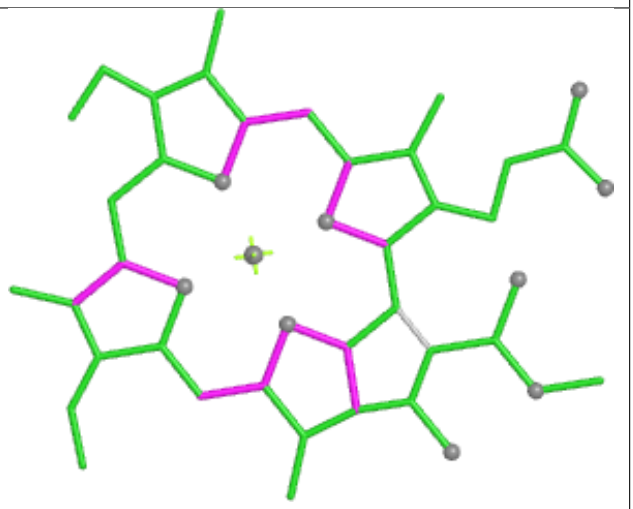


Rings

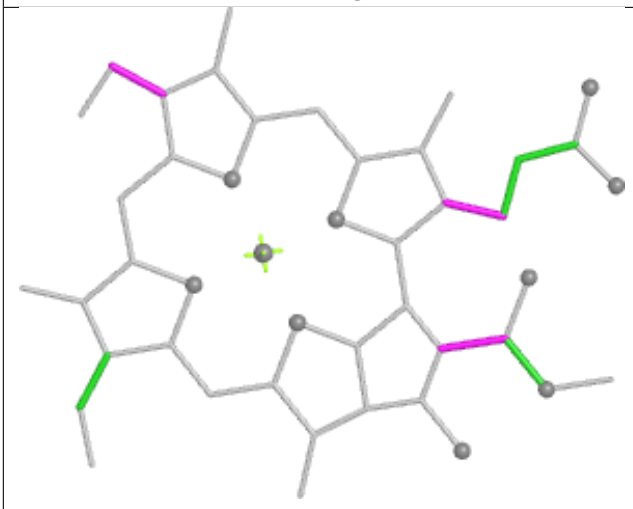
Ligand CLA E 303



Bond lengths



Bond angles

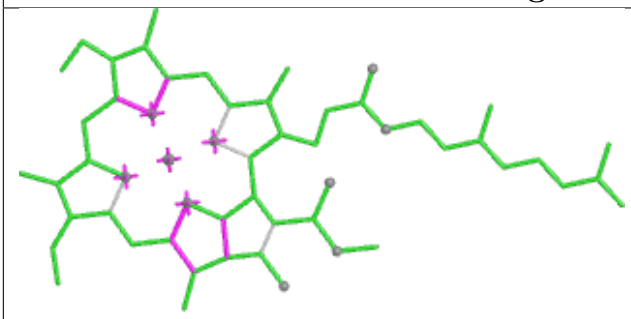


Torsions

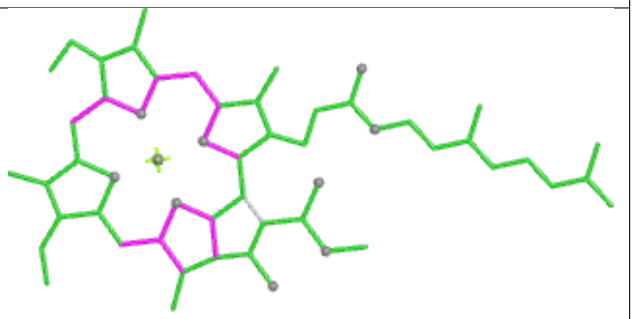


Rings

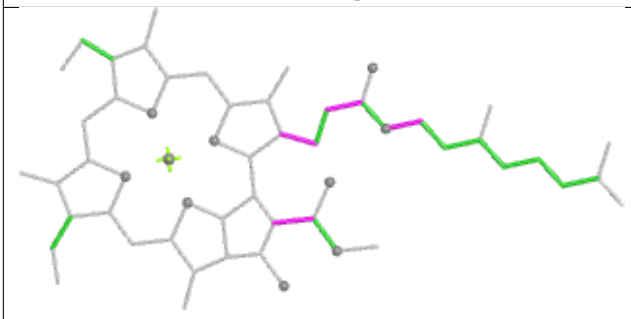
Ligand CLA J 306



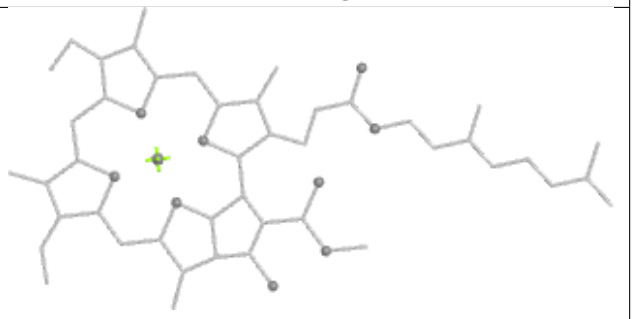
Bond lengths



Bond angles

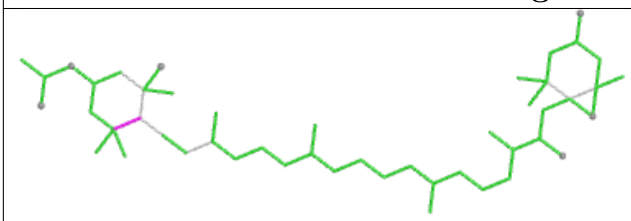


Torsions

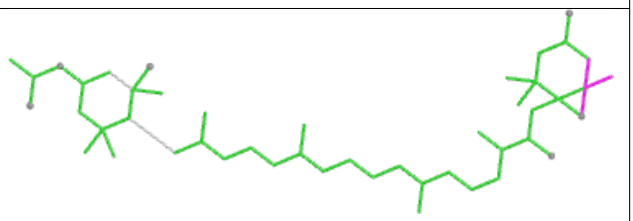


Rings

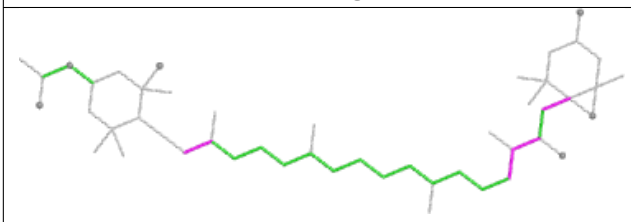
Ligand A86 F 317



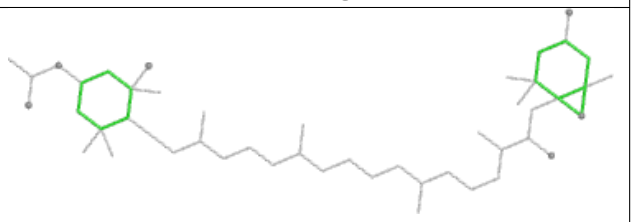
Bond lengths



Bond angles

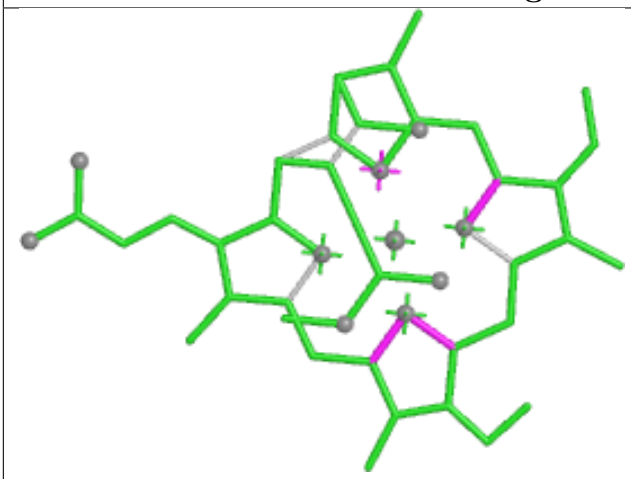


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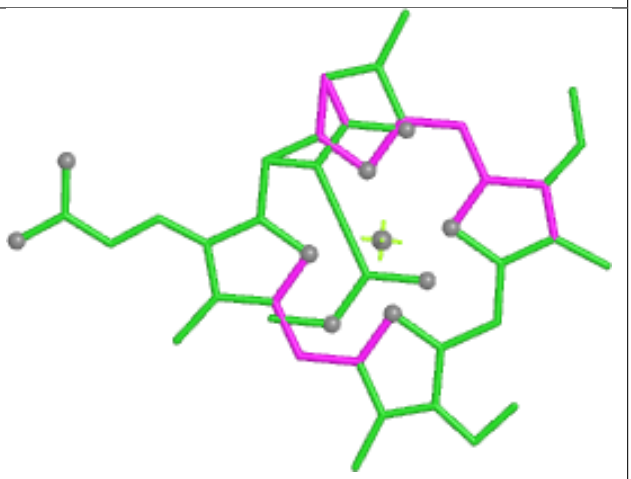


Rings

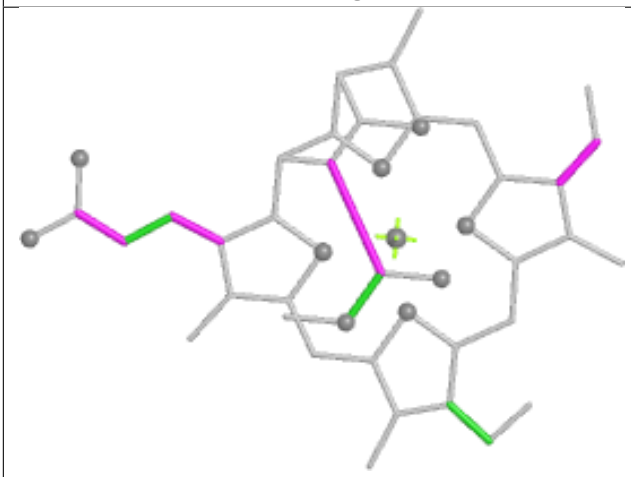
Ligand KC2 G 302



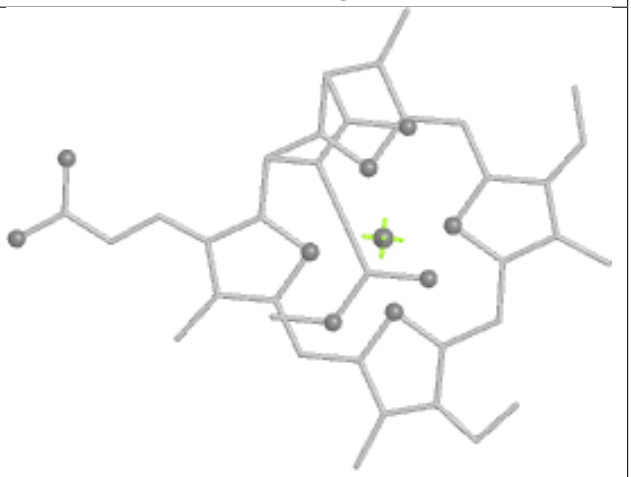
Bond lengths



Bond angles

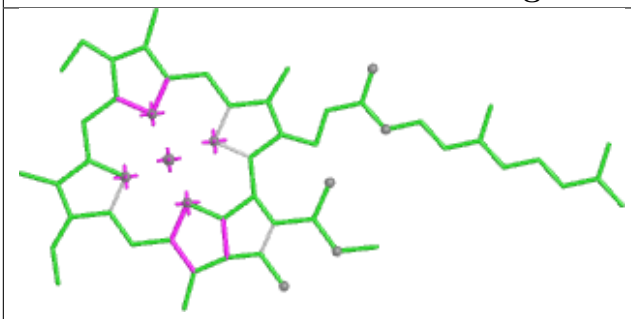


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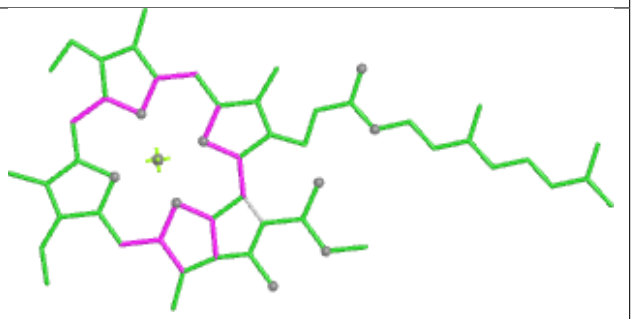


Rings

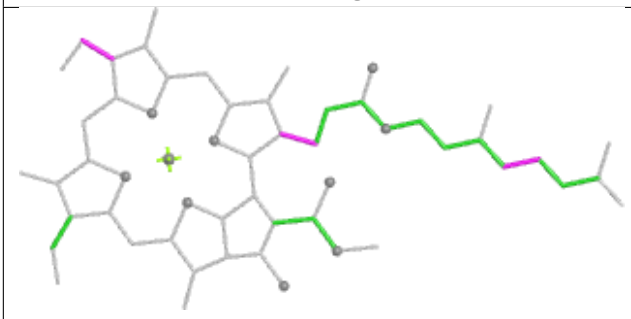
Ligand CLA D 308



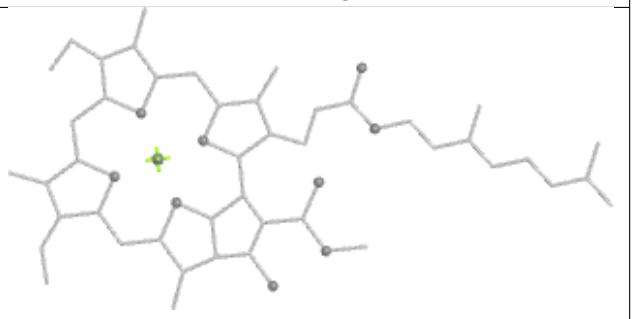
Bond lengths



Bond angles

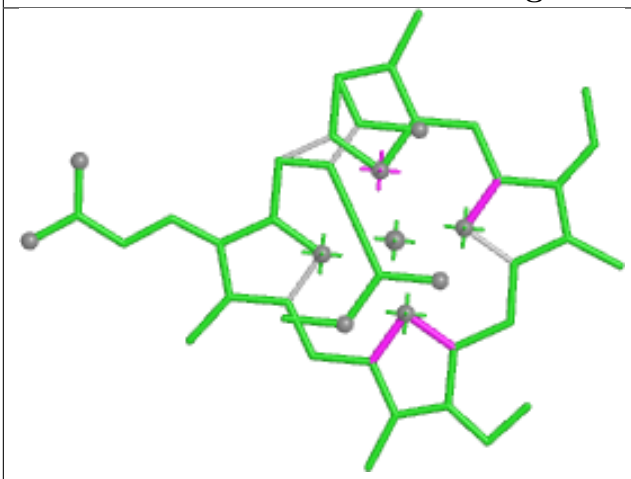


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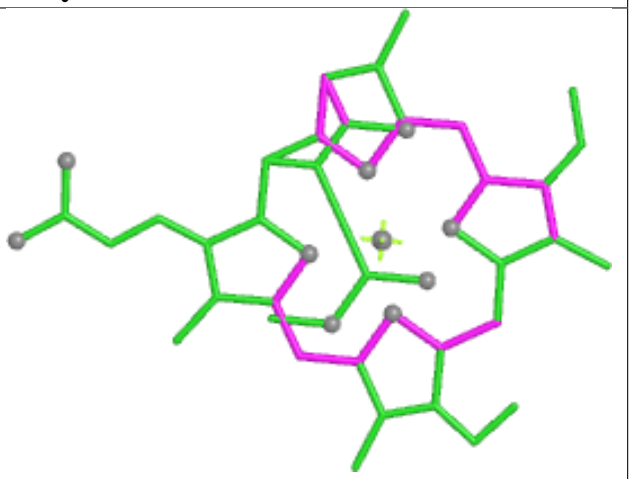


Rings

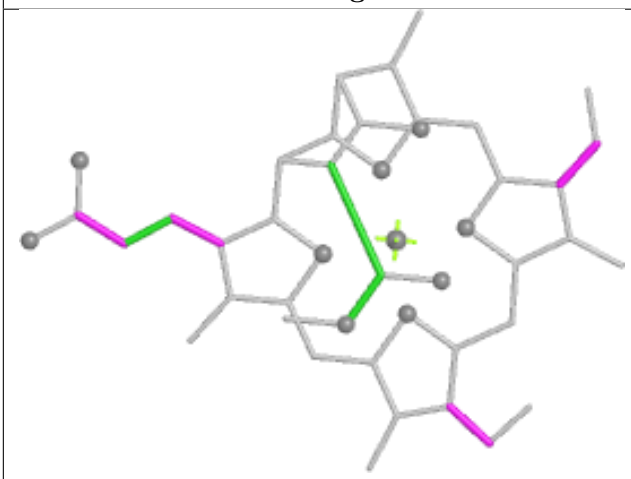
Ligand KC2 Q 302



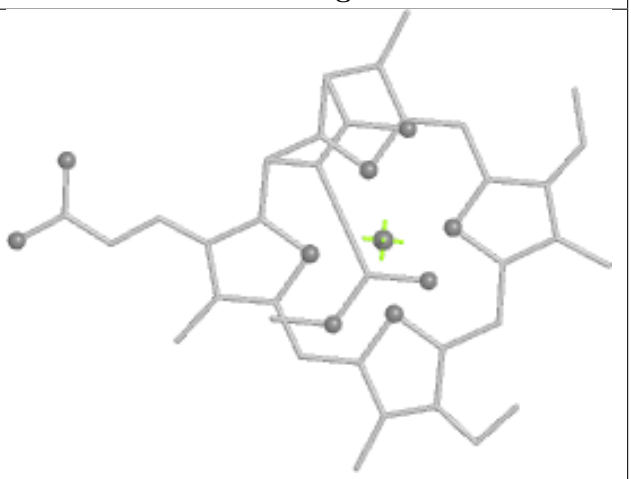
Bond lengths



Bond angles

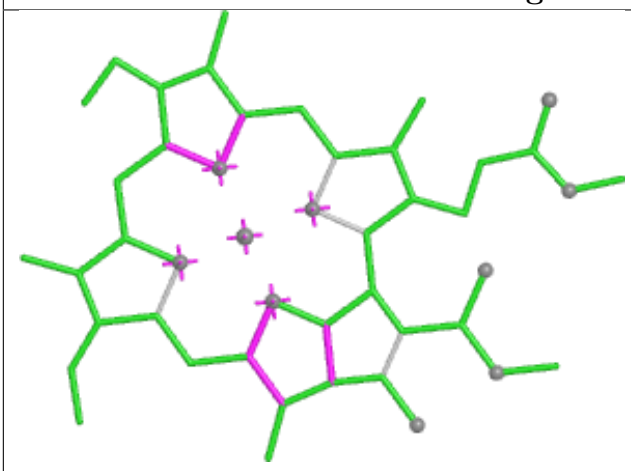


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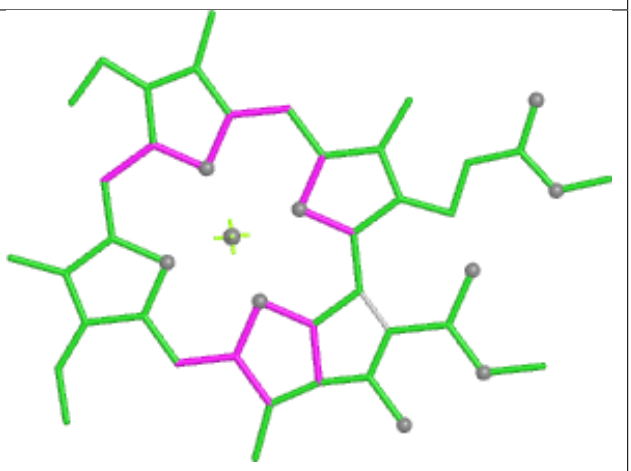


Rings

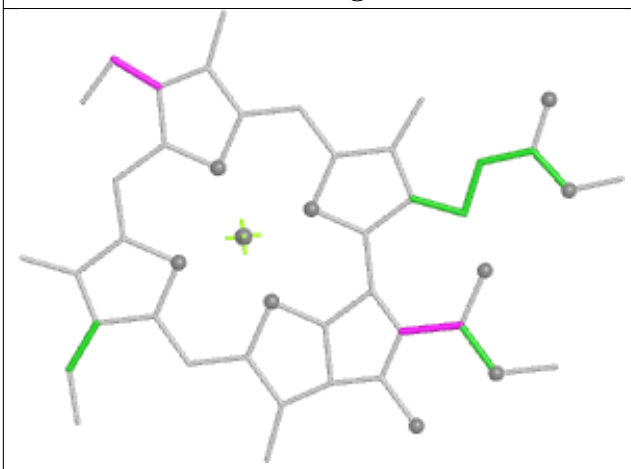
Ligand CLA F 308



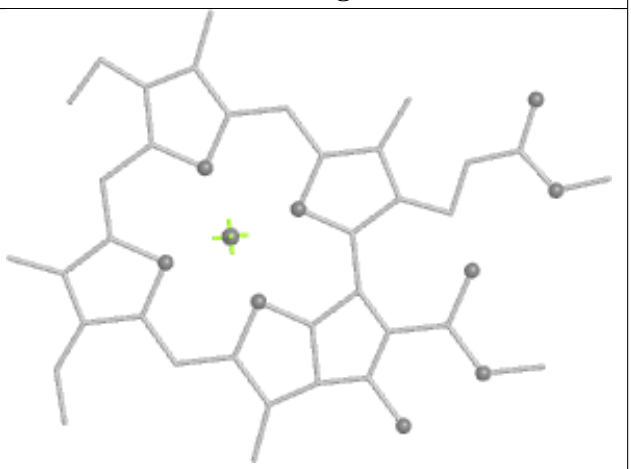
Bond lengths



Bond angles

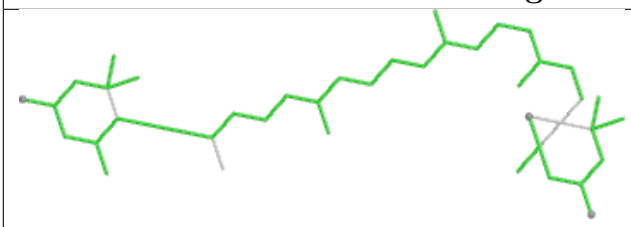


Torsions



Rings

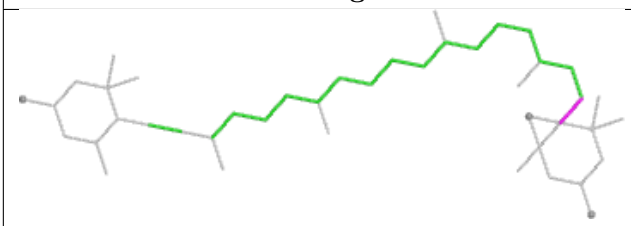
Ligand DD6 B 307



Bond lengths



Bond angles

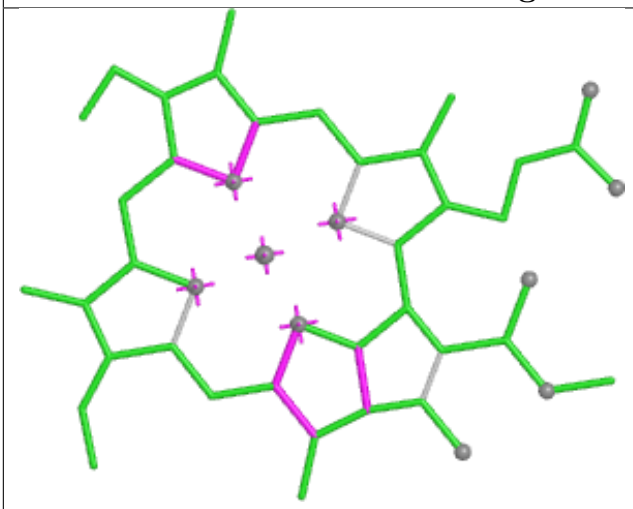


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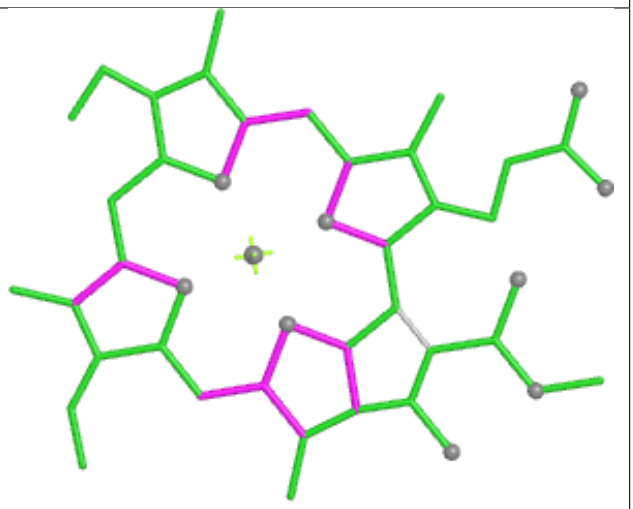


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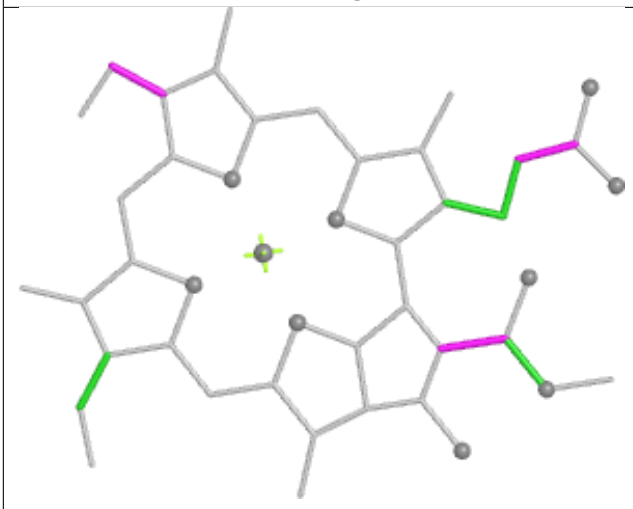
Ligand CLA W 307



Bond lengths



Bond angles

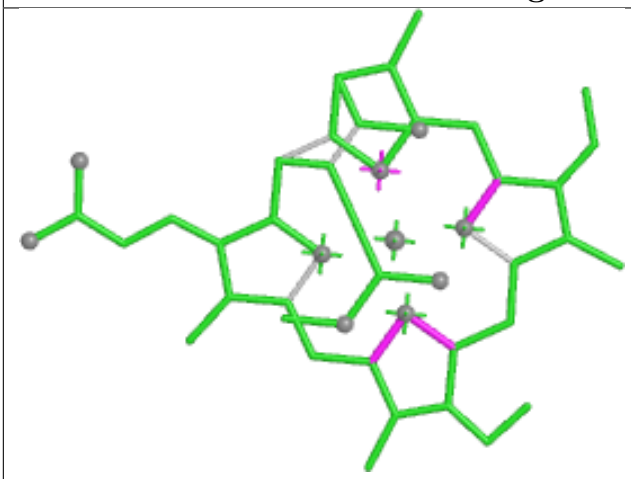


Torsions

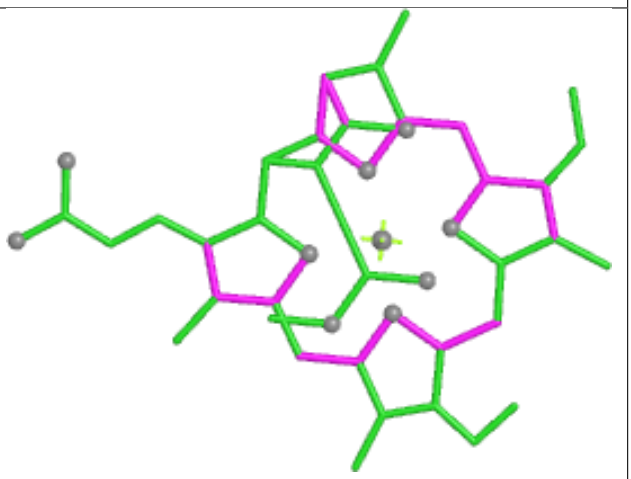


Rings

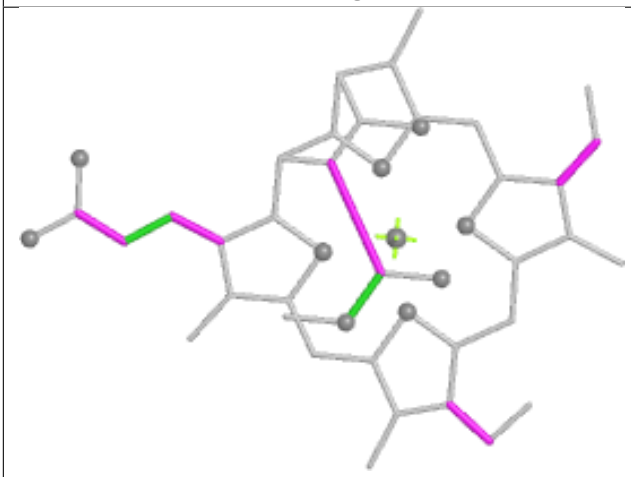
Ligand KC2 F 310



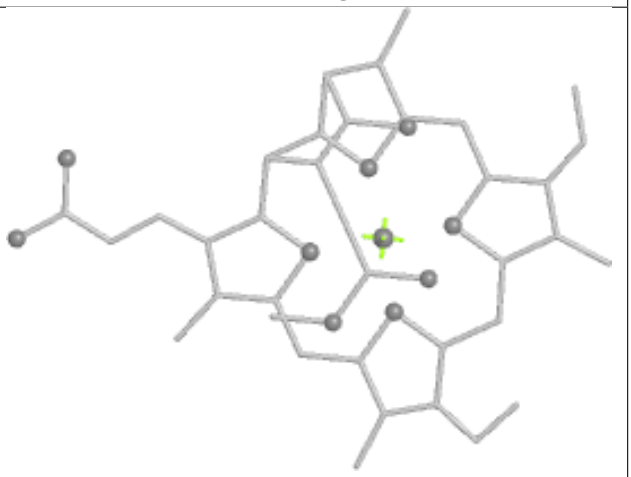
Bond lengths



Bond angles



Torsions



Rings

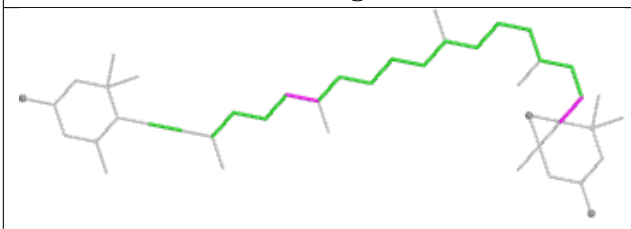
Ligand DD6 F 316



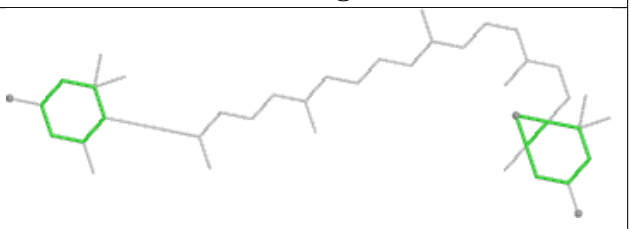
Bond lengths



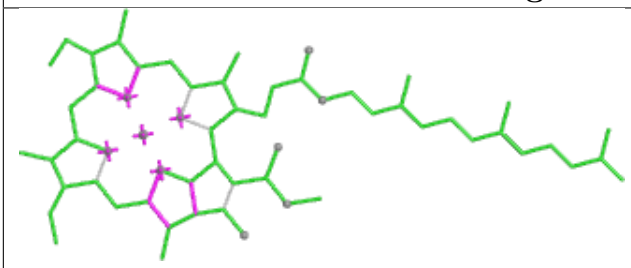
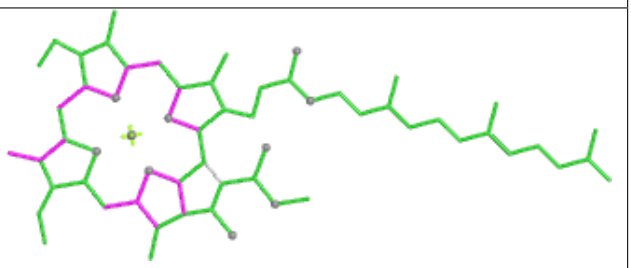
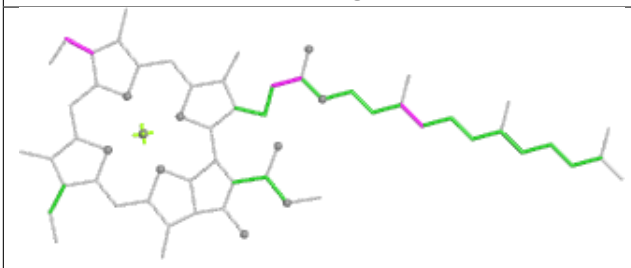
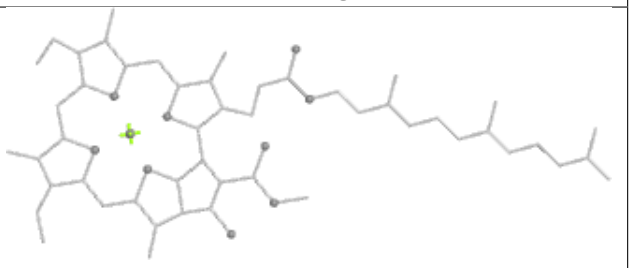
Bond angles

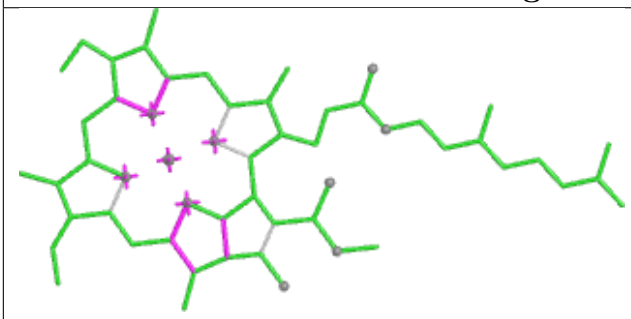
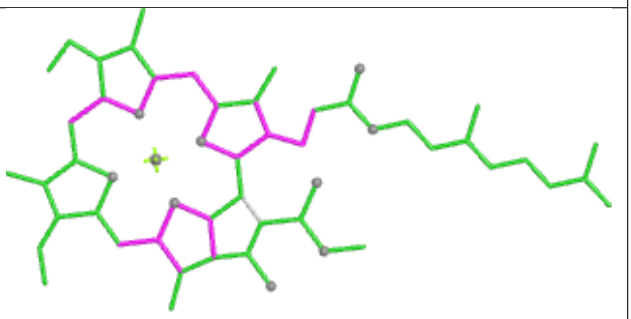
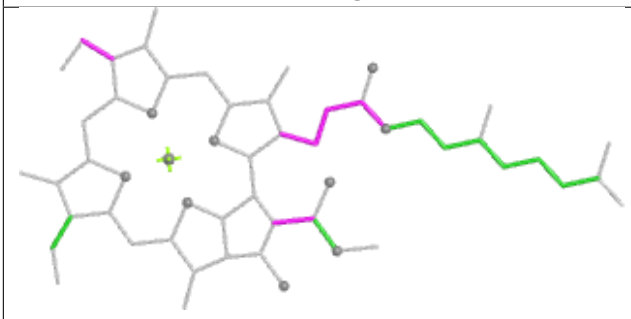
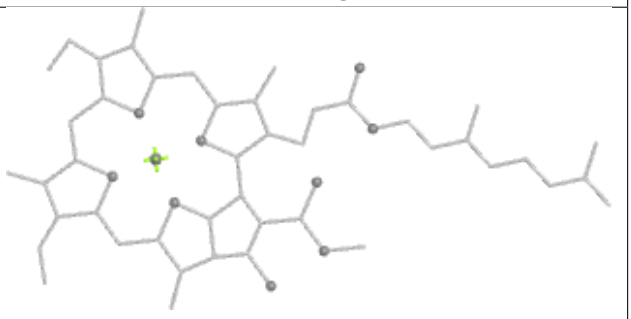


Torsions

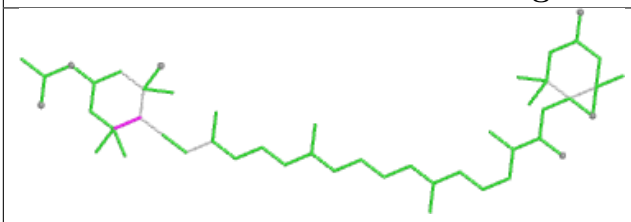


Rings

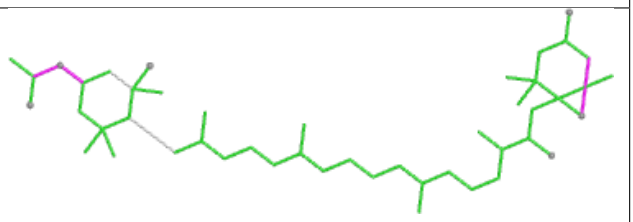
Ligand CLA F 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

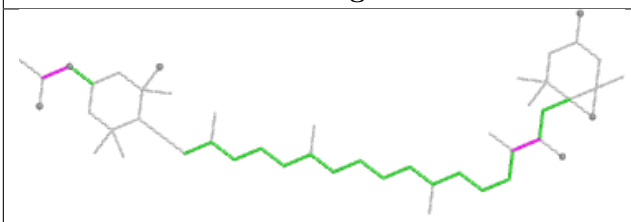
Ligand A86 L 318



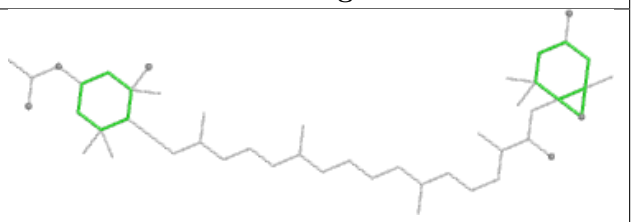
Bond lengths



Bond angles

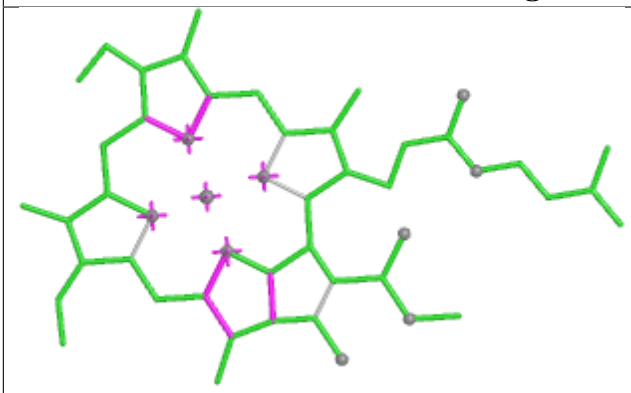


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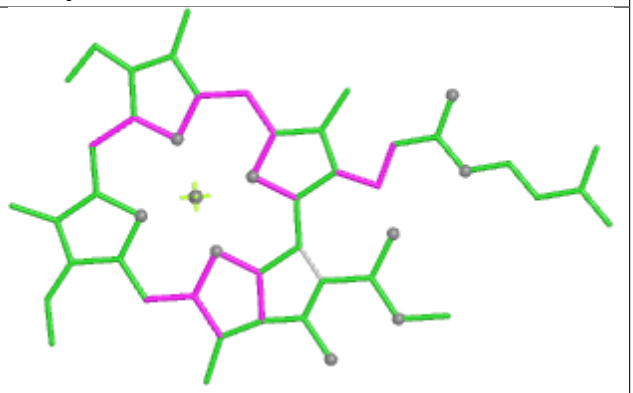


Rings

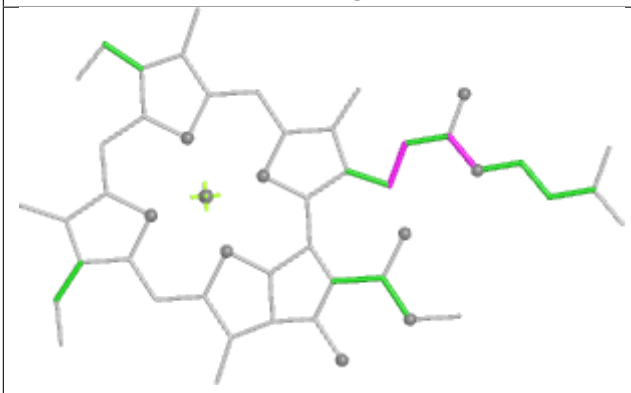
Ligand CLA Q 304



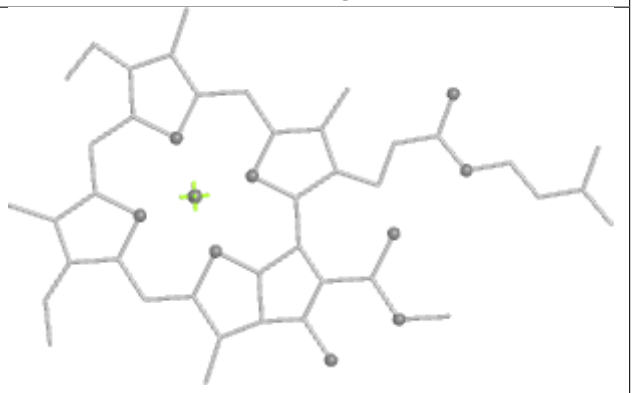
Bond lengths



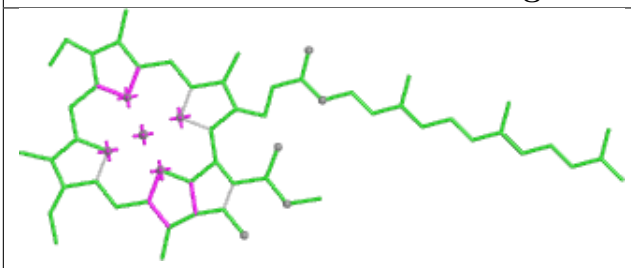
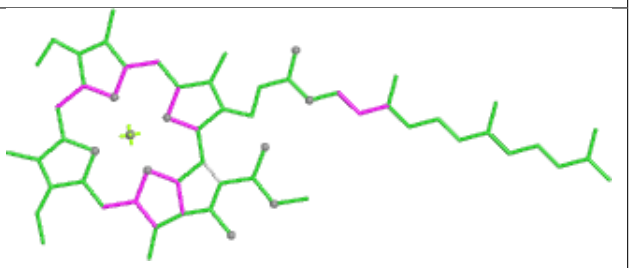
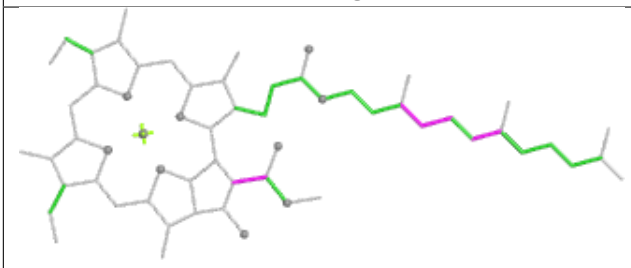
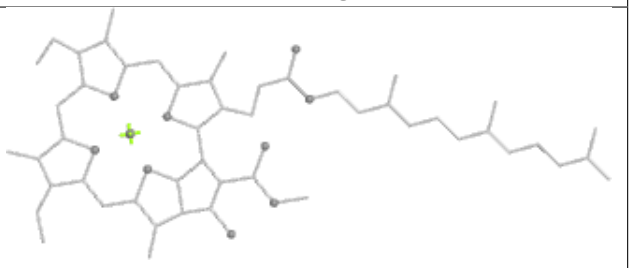
Bond angles

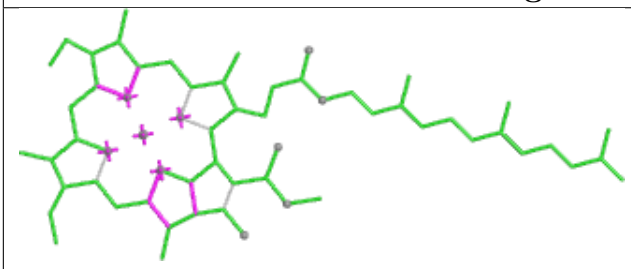
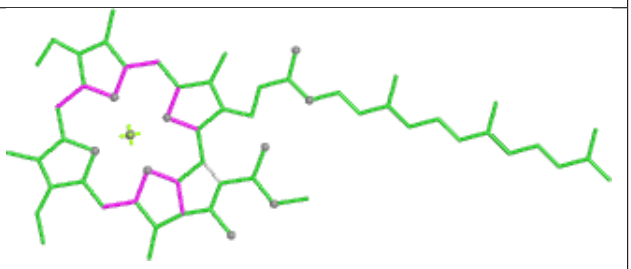
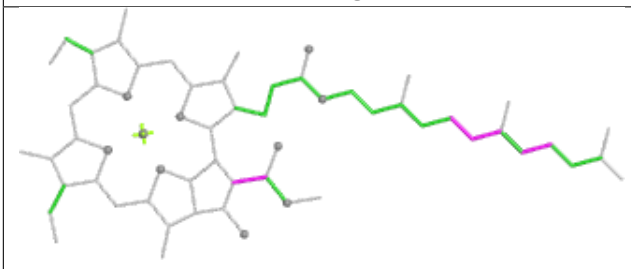
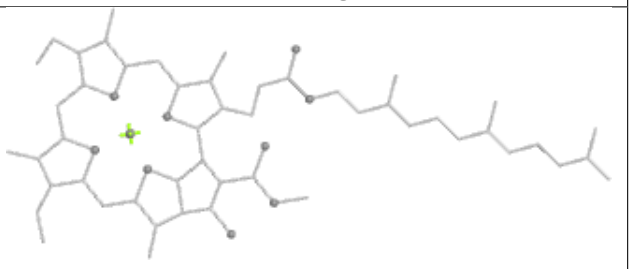


Torsions

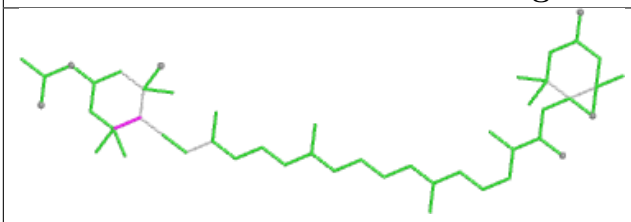


Rings

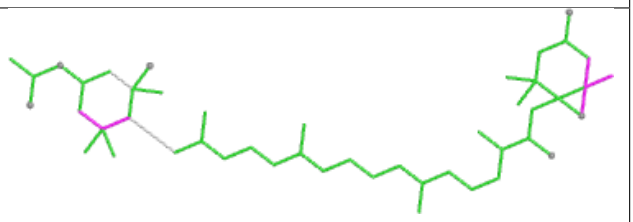
Ligand CLA N 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA T 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

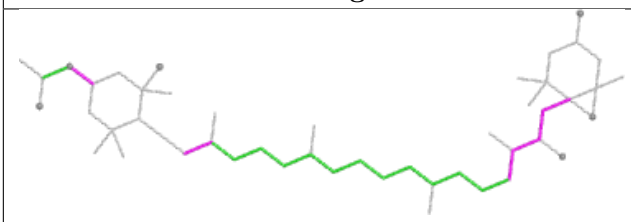
Ligand A86 L 317



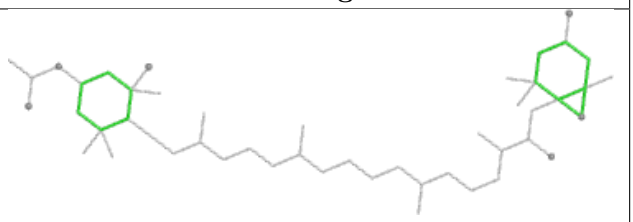
Bond lengths



Bond angles

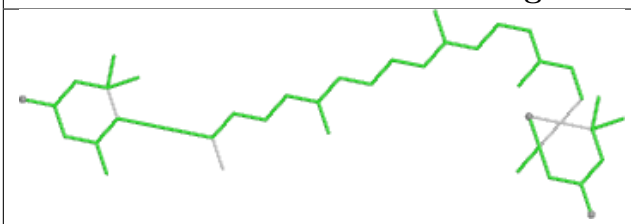


Torsions

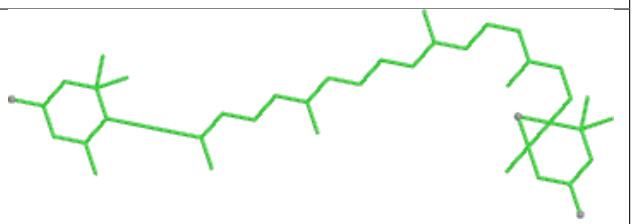


Rings

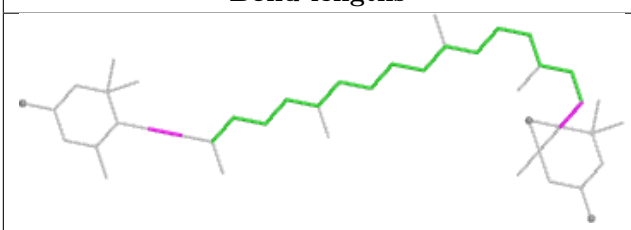
Ligand DD6 D 318



Bond lengths



Bond angles

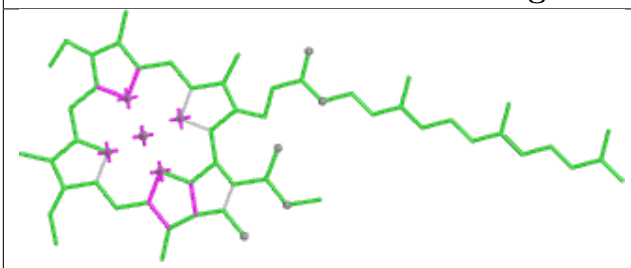


Torsions

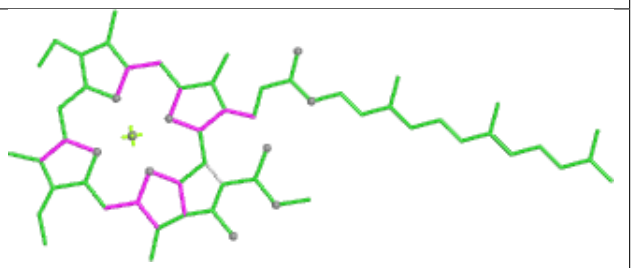


Rings

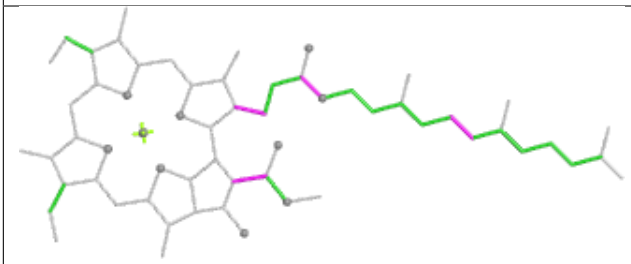
Ligand CLA a 806



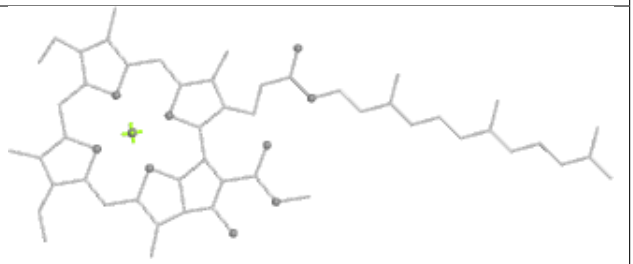
Bond lengths



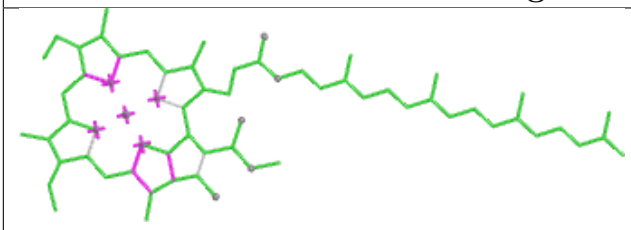
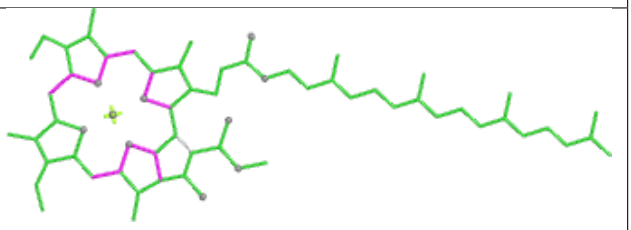
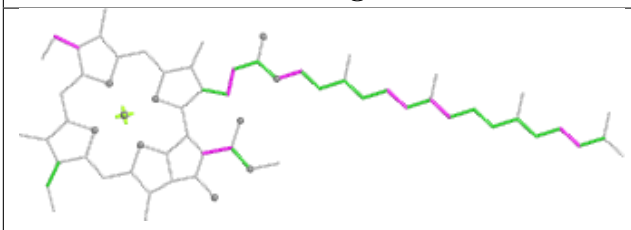
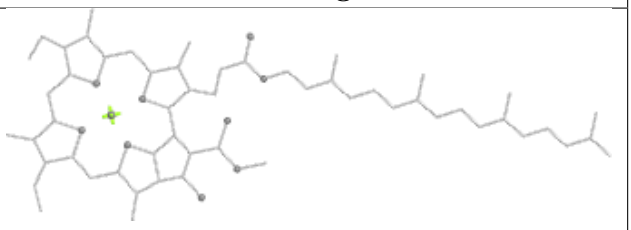
Bond angles

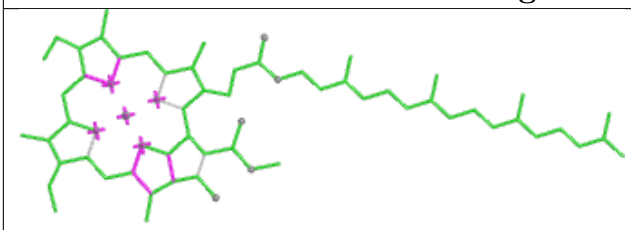
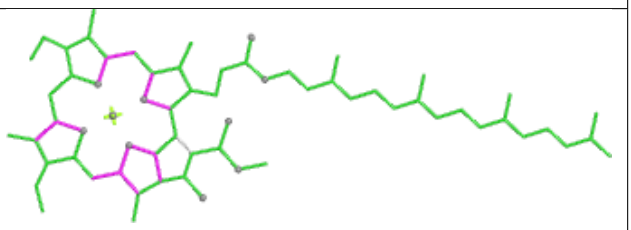
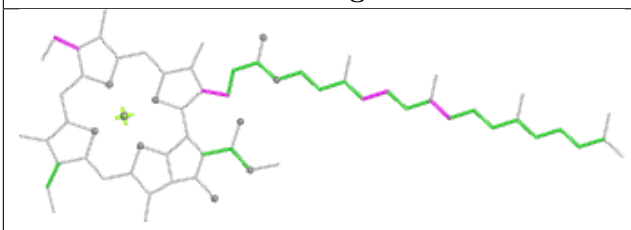
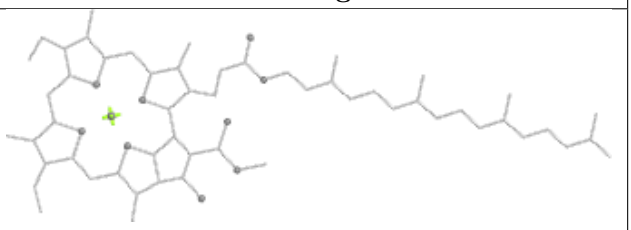


Torsions

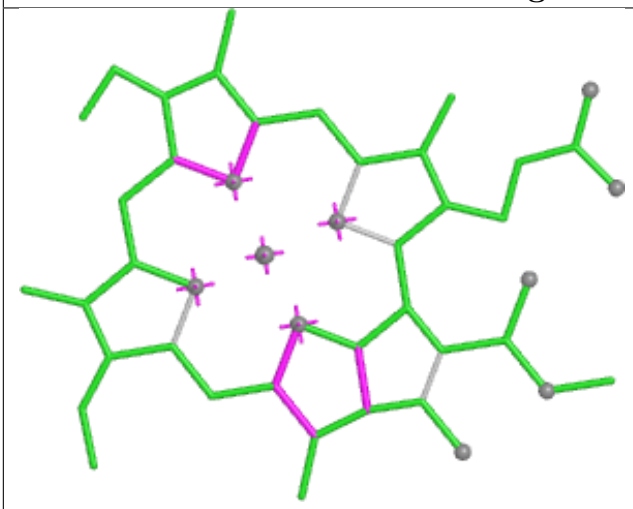


Rings

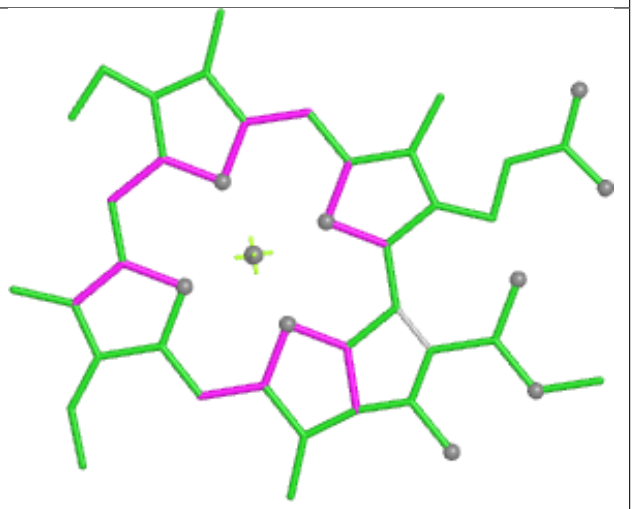
Ligand CLA b 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA W 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

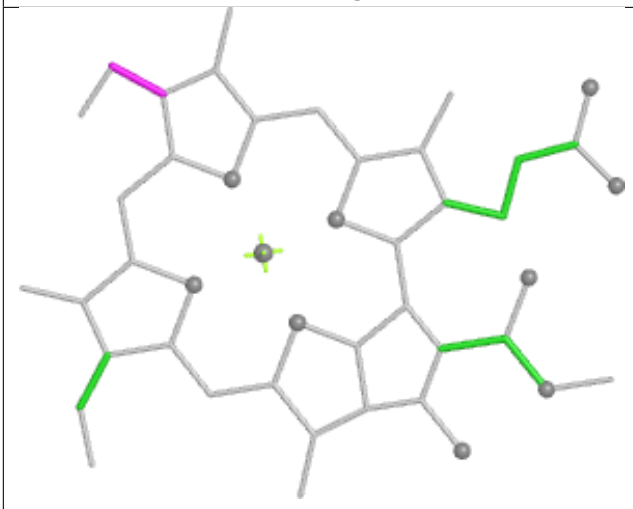
Ligand CLA J 302



Bond lengths



Bond angles

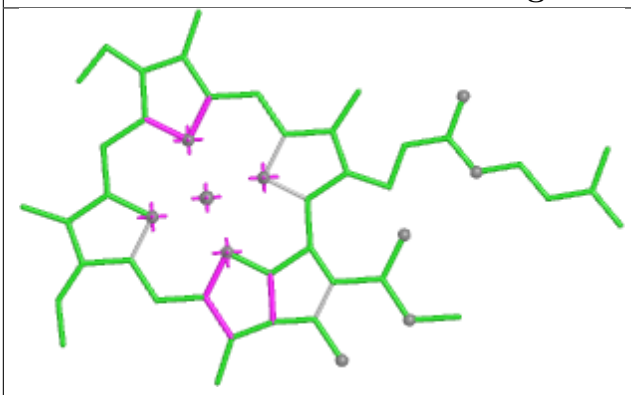


Torsions

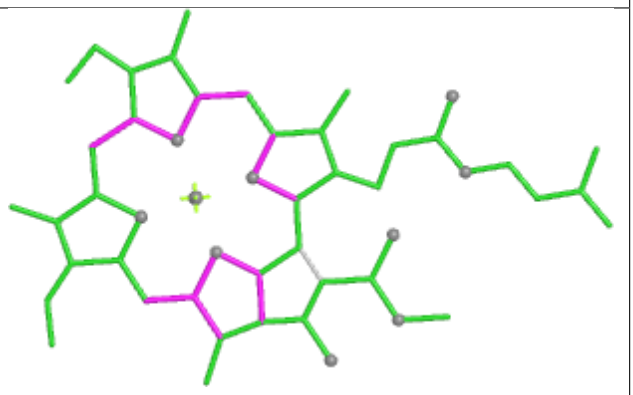


Rings

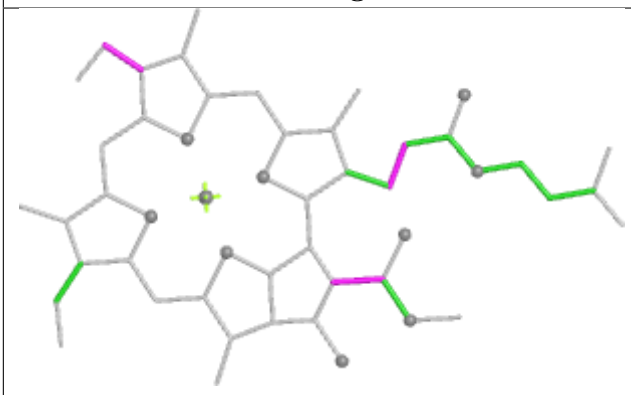
Ligand CLA b 827



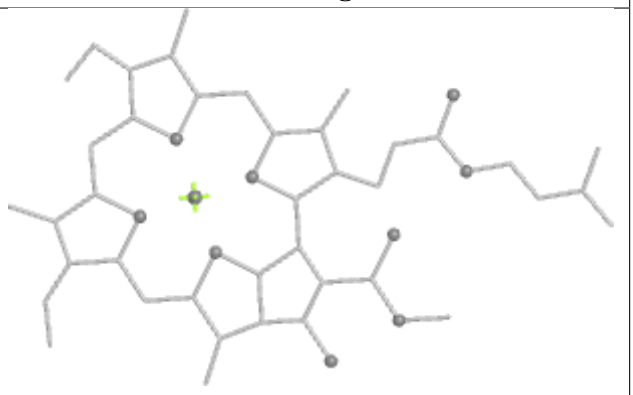
Bond lengths



Bond angles

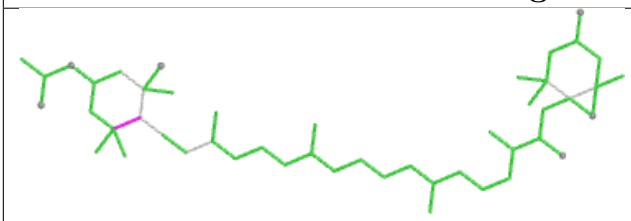


Torsions

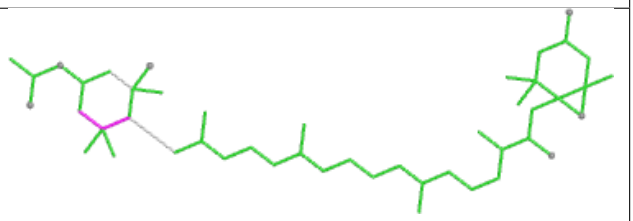


Rings

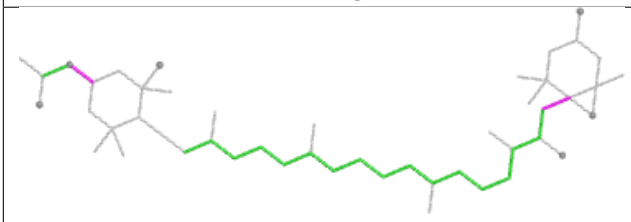
Ligand A86 R 312



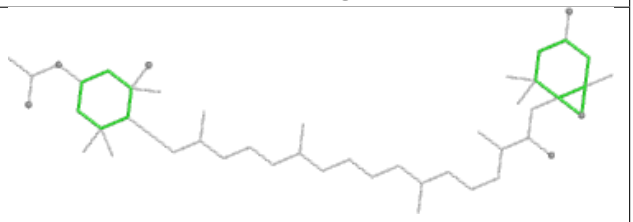
Bond lengths



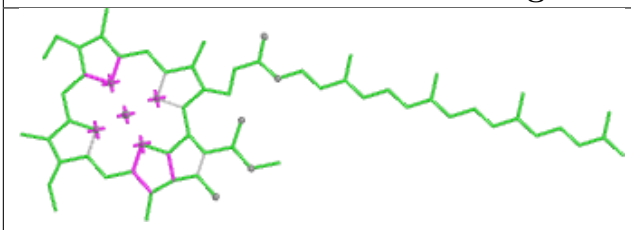
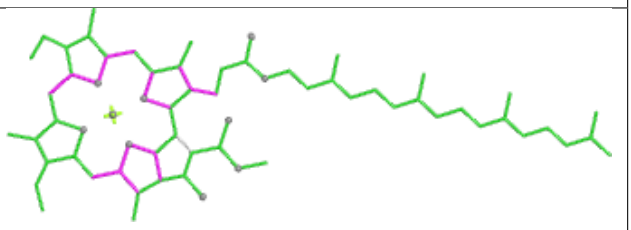
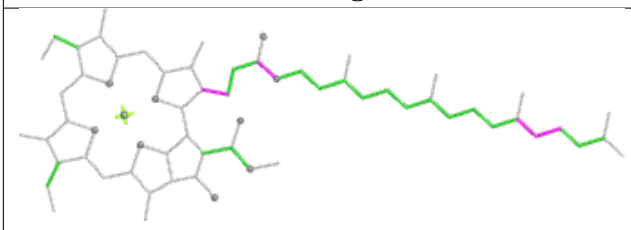
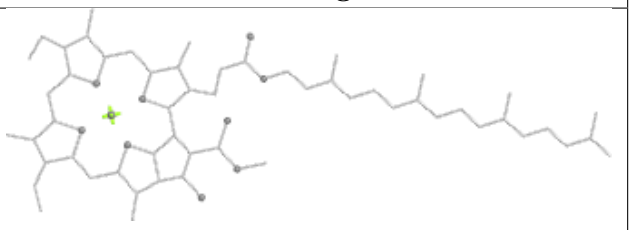
Bond angles



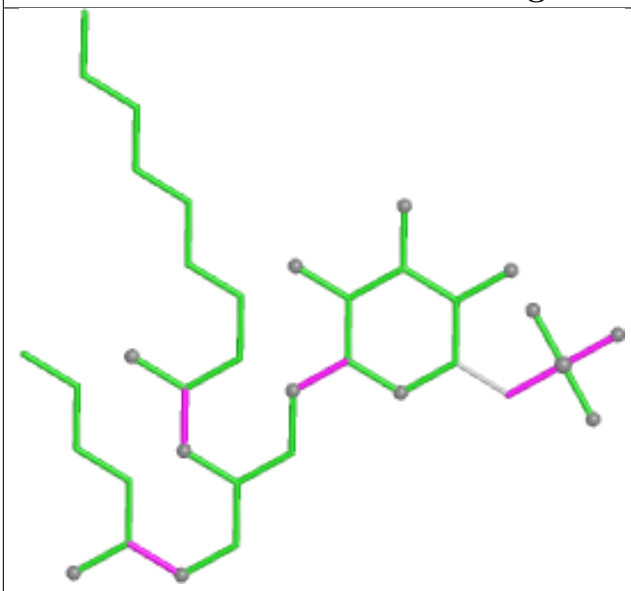
Torsions



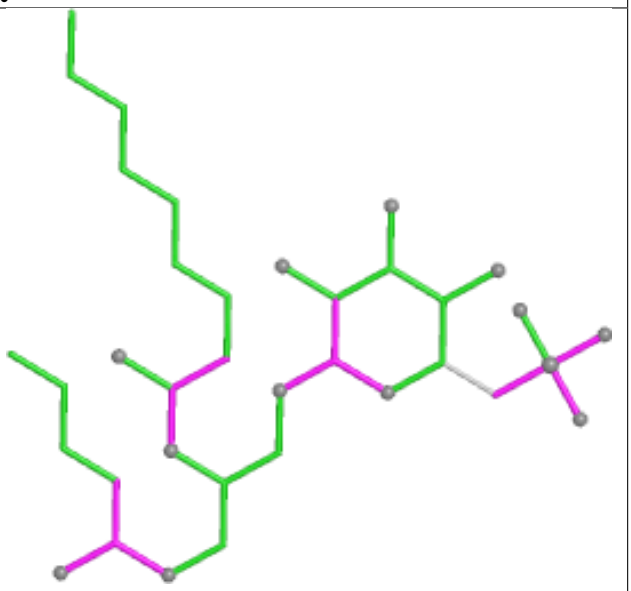
Rings

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

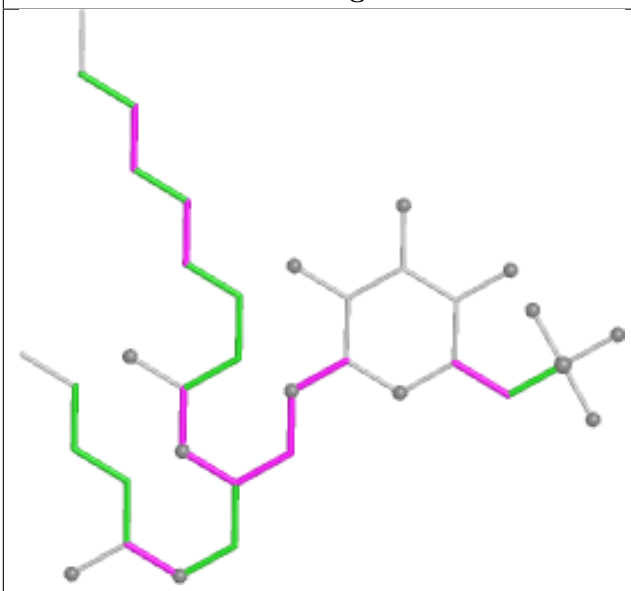
Ligand SQD k 206



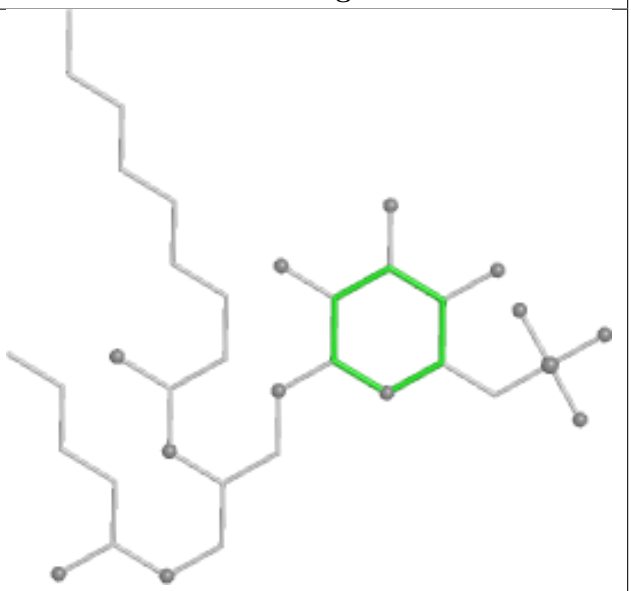
Bond lengths



Bond angles

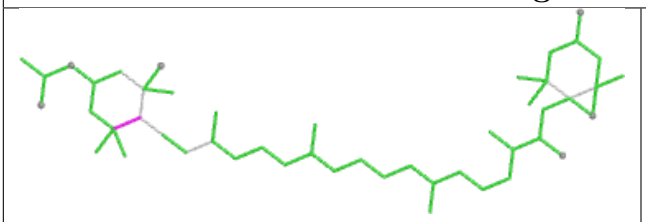


Torsions

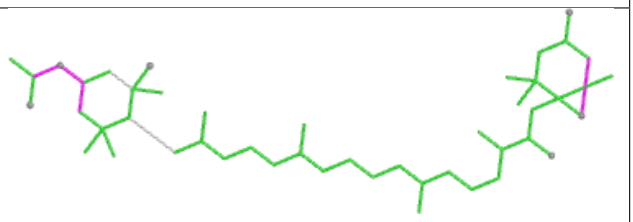


Rings

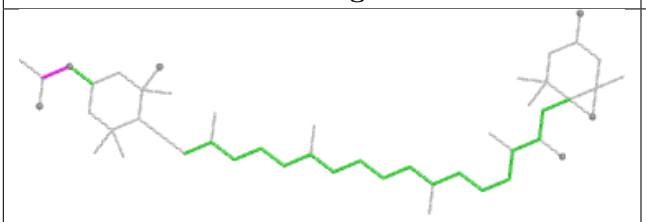
Ligand A86 S 316



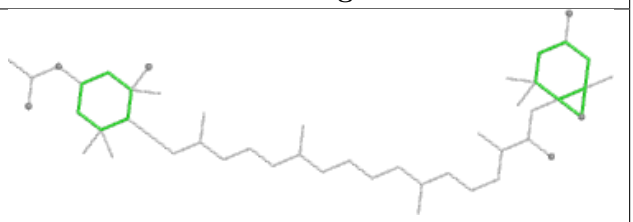
Bond lengths



Bond angles

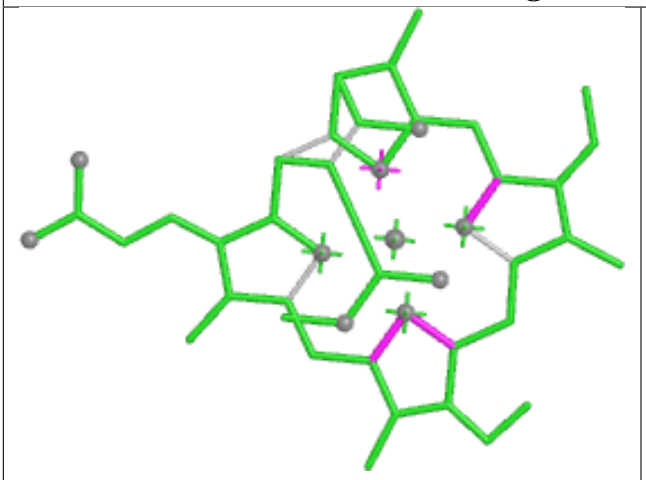


Torsions

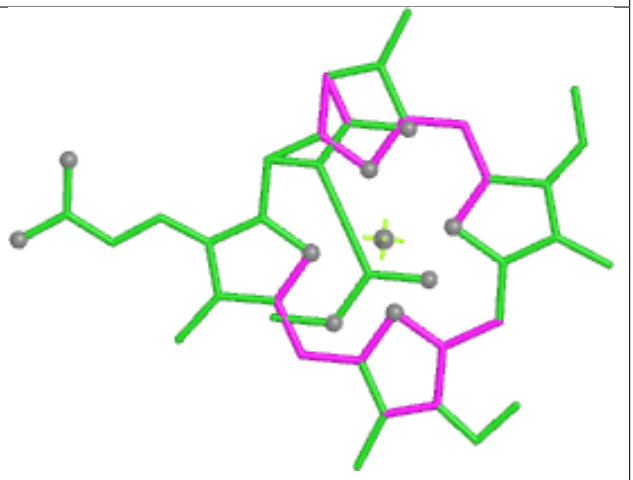


Rings

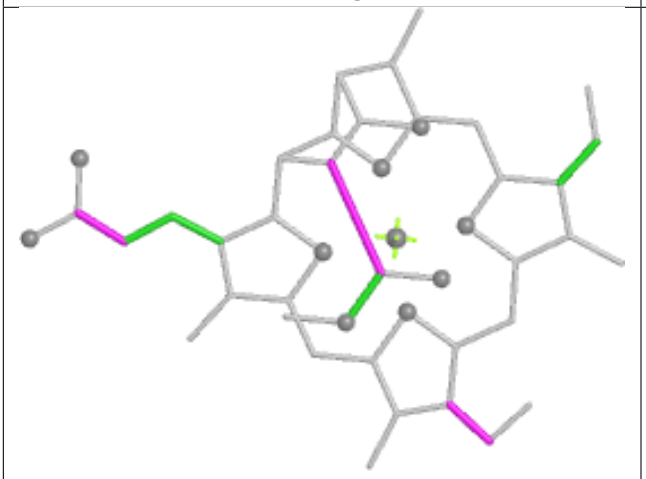
Ligand KC2 N 308



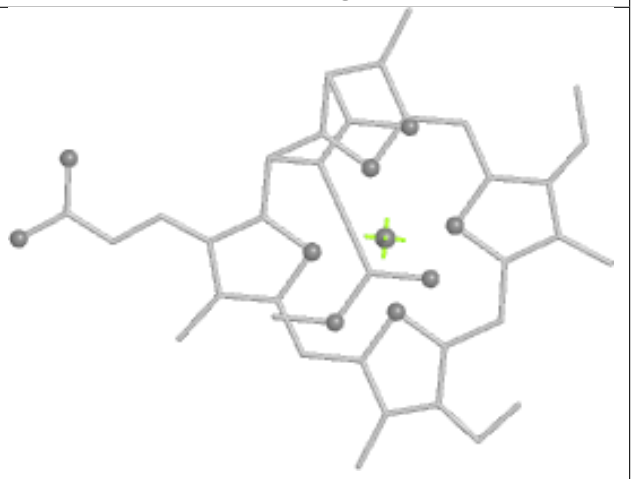
Bond lengths



Bond angles

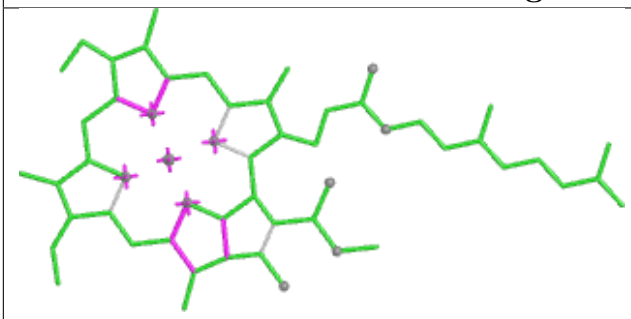


Torsions

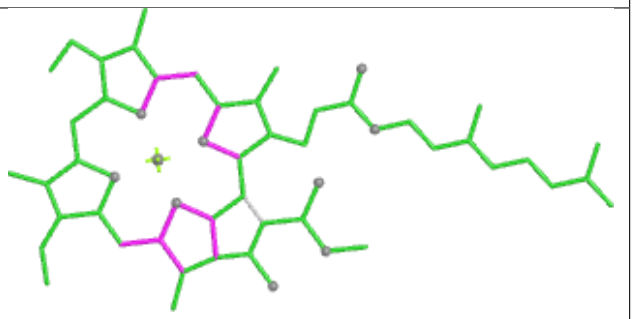


Rings

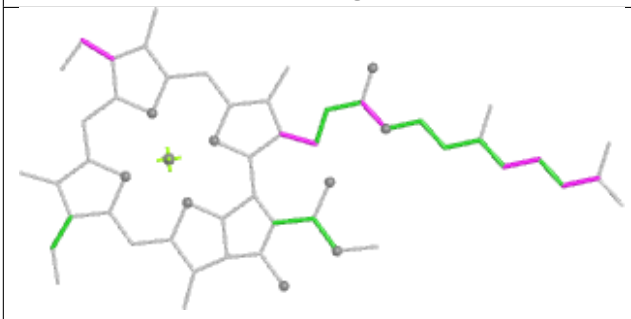
Ligand CLA E 307



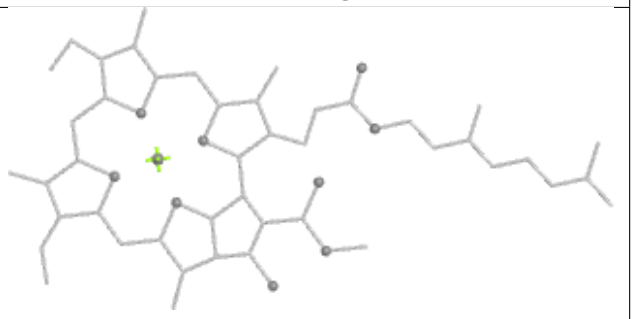
Bond lengths



Bond angles

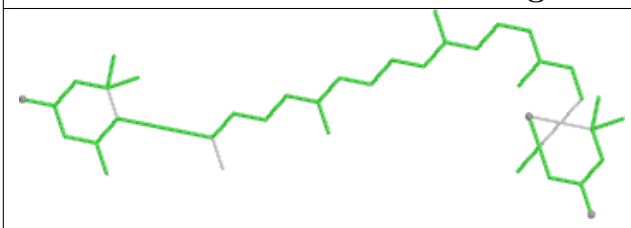


Torsions

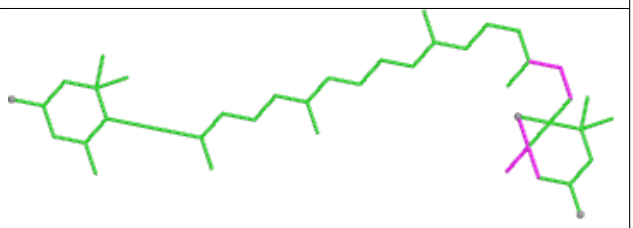


Rings

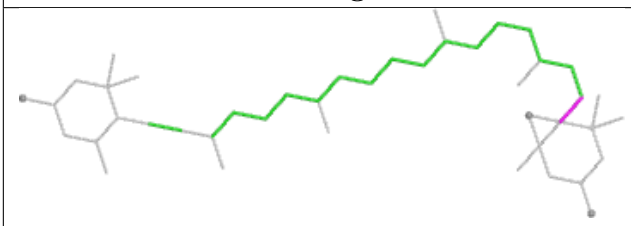
Ligand DD6 L 319



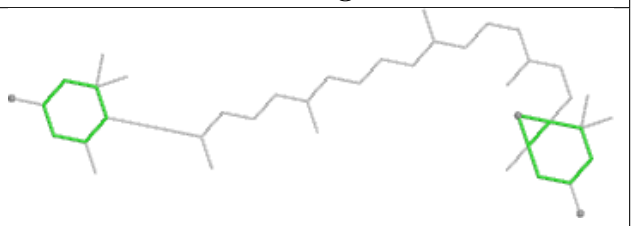
Bond lengths



Bond angles

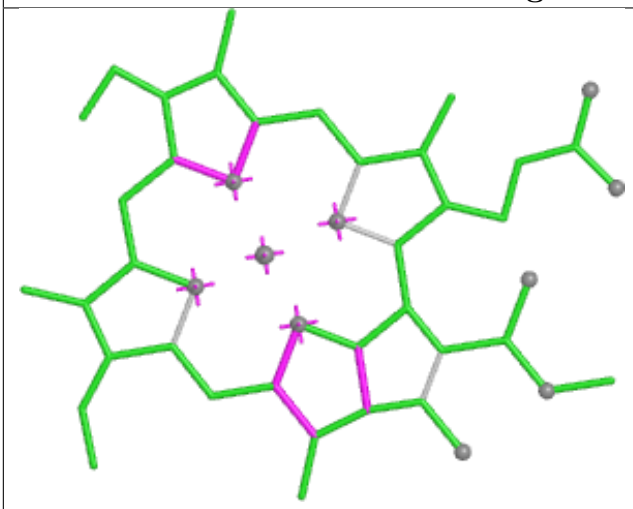


Torsions

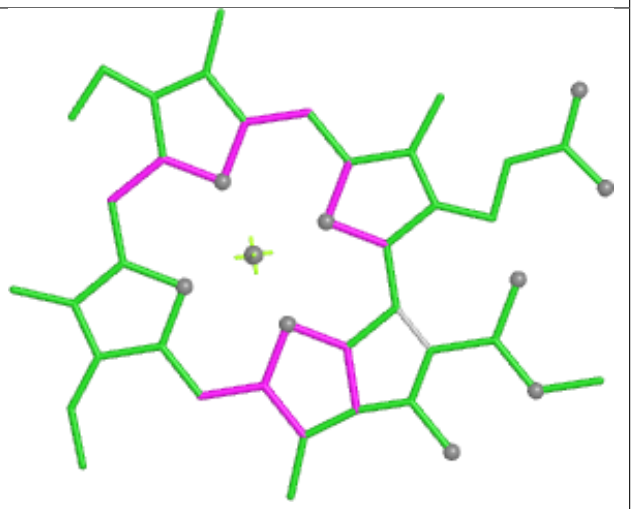


Rings

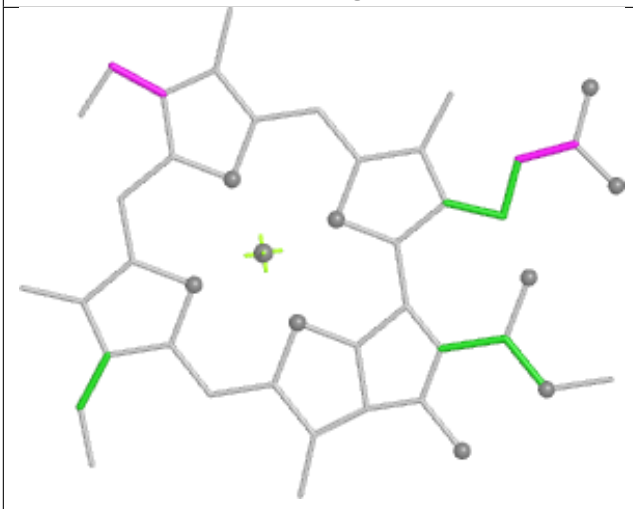
Ligand CLA L 308



Bond lengths



Bond angles

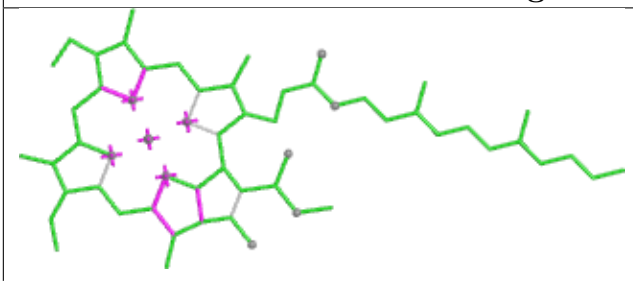


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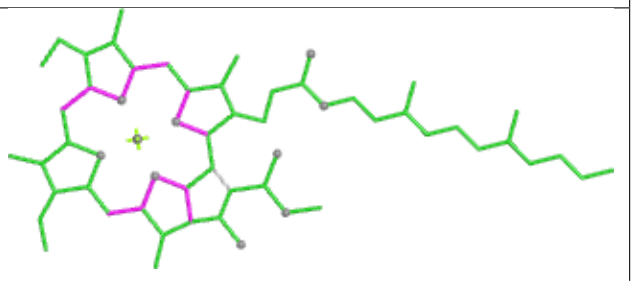


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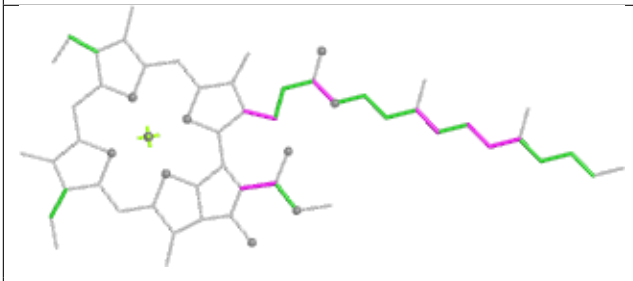
Ligand CLA b 824



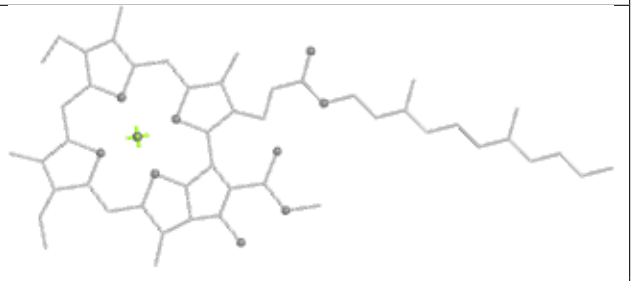
Bond lengths



Bond angles

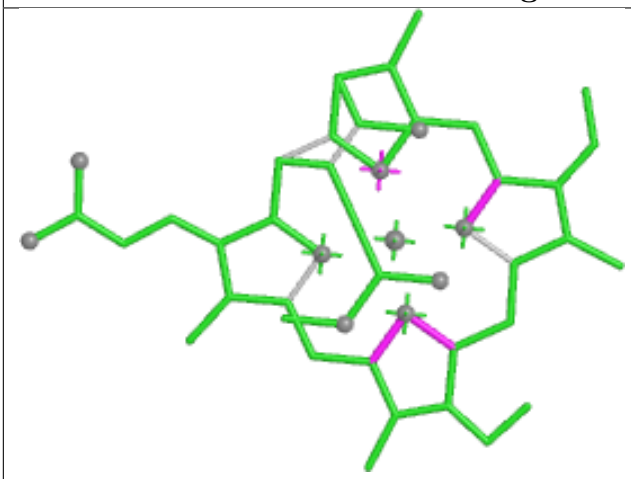


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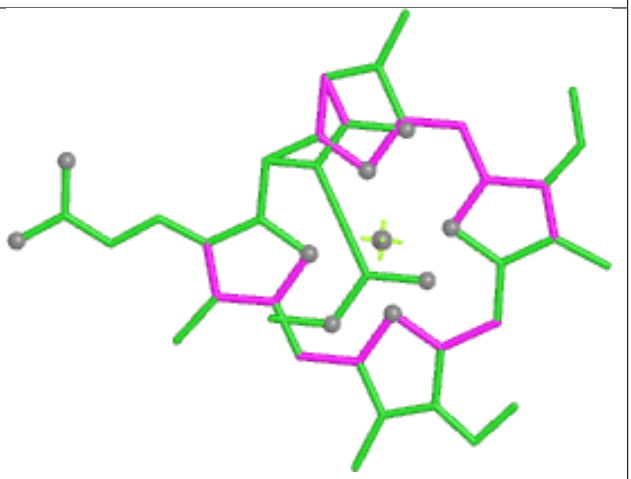


Rings

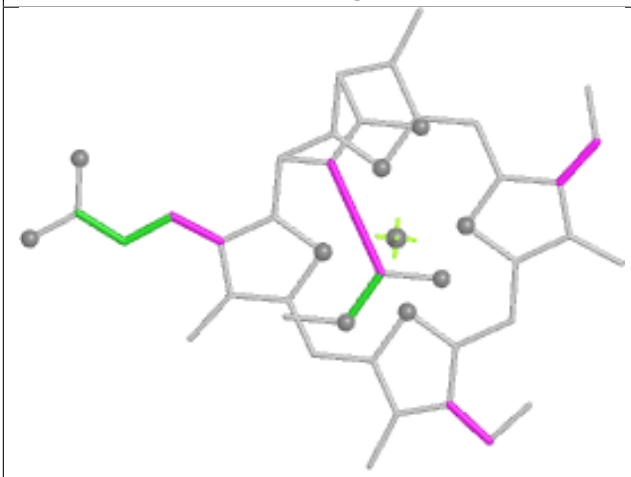
Ligand KC2 W 308



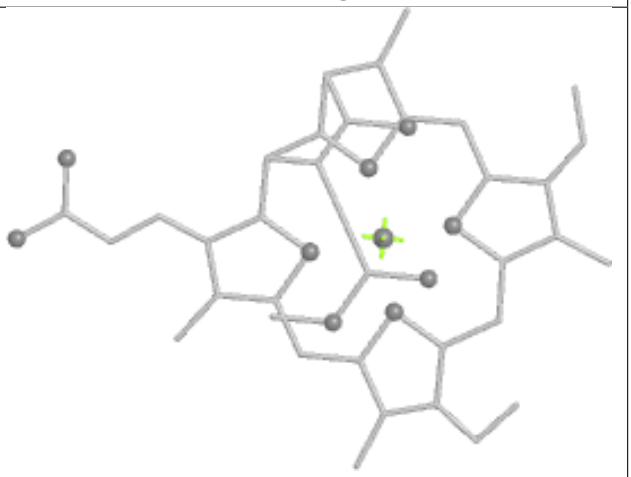
Bond lengths



Bond angles

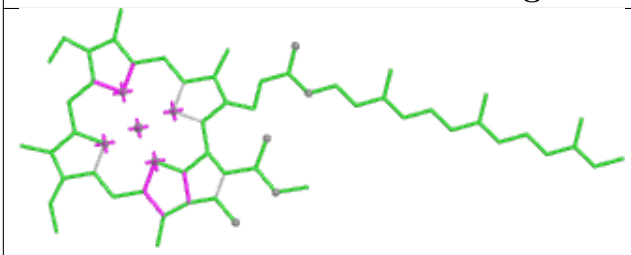


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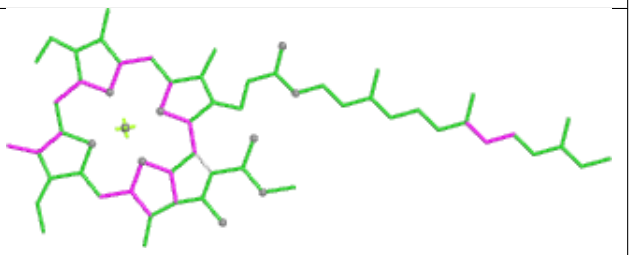


Rings

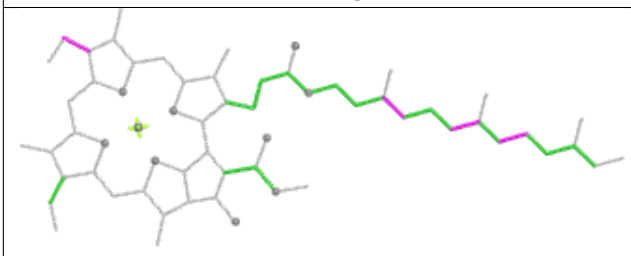
Ligand CLA D 307



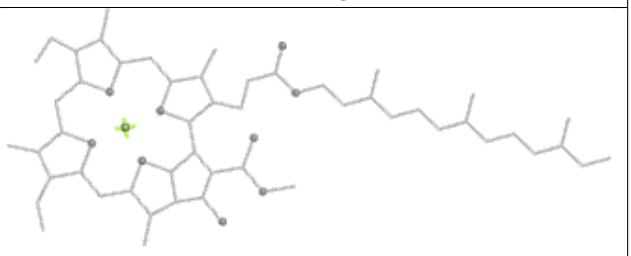
Bond lengths



Bond angles

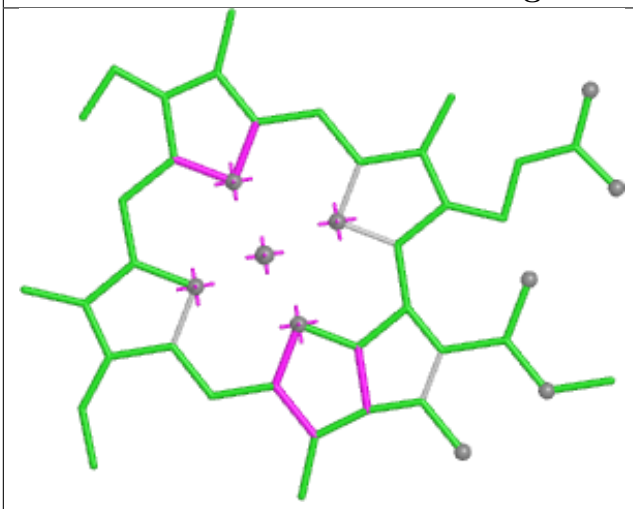


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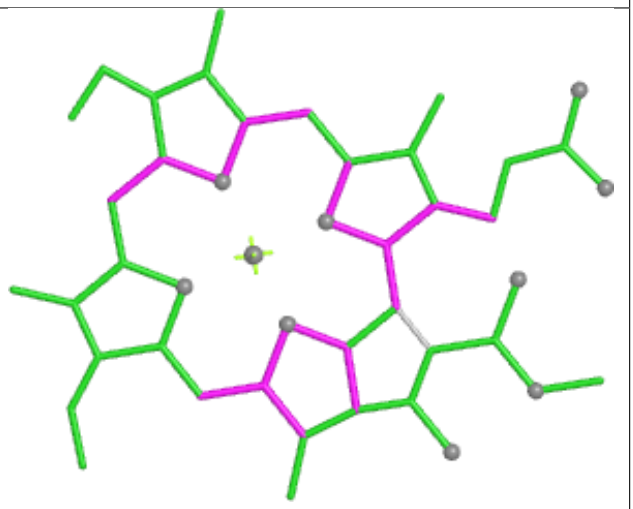


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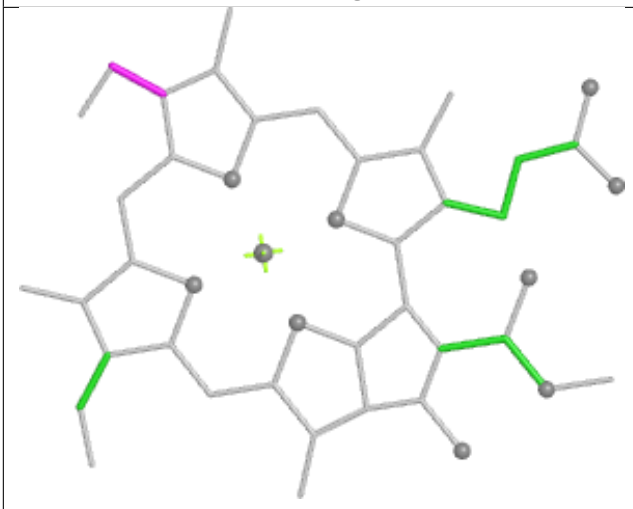
Ligand CLA O 304



Bond lengths



Bond angles

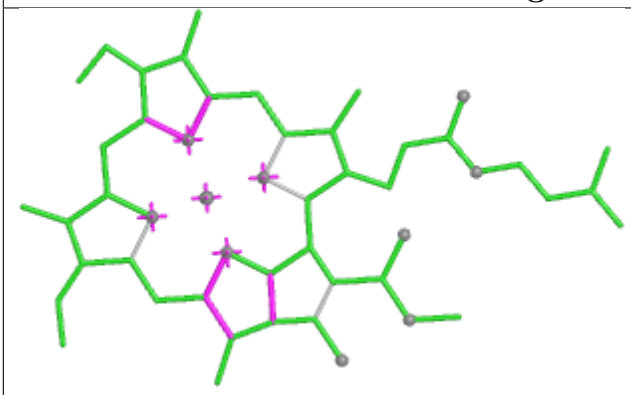


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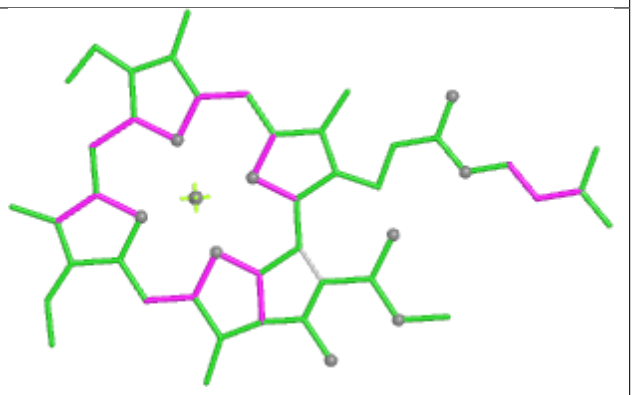


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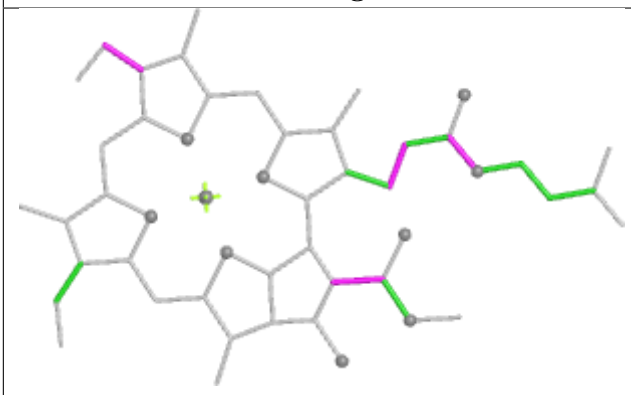
Ligand CLA b 811



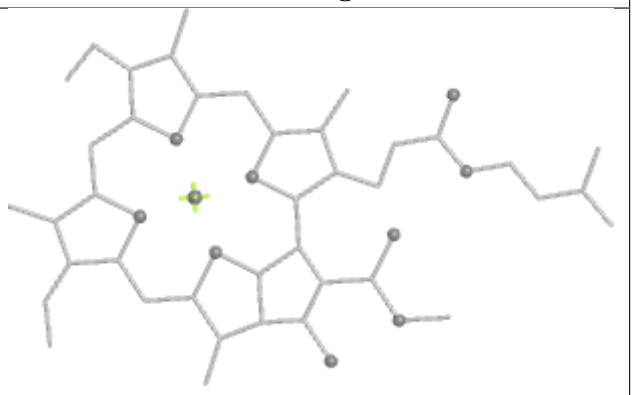
Bond lengths



Bond angles

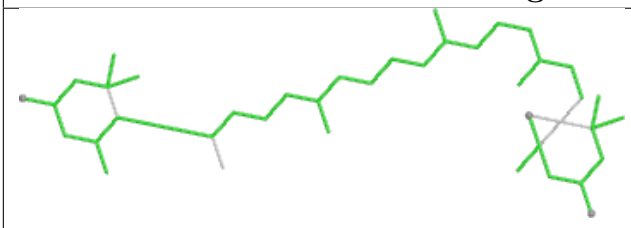


Torsions



Rings

Ligand DD6 F 314



Bond lengths



Bond angles

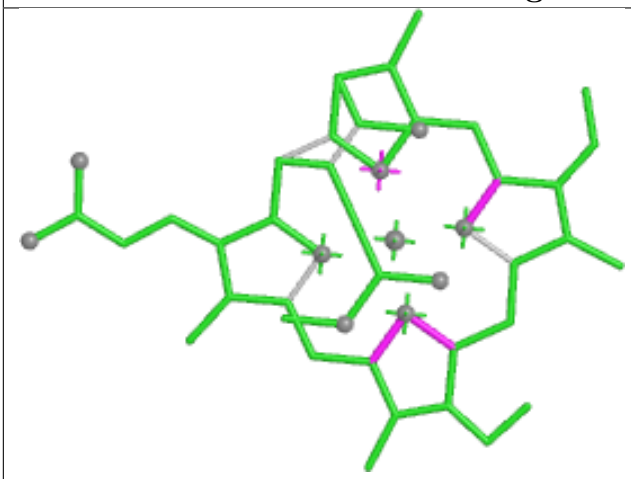


Torsions

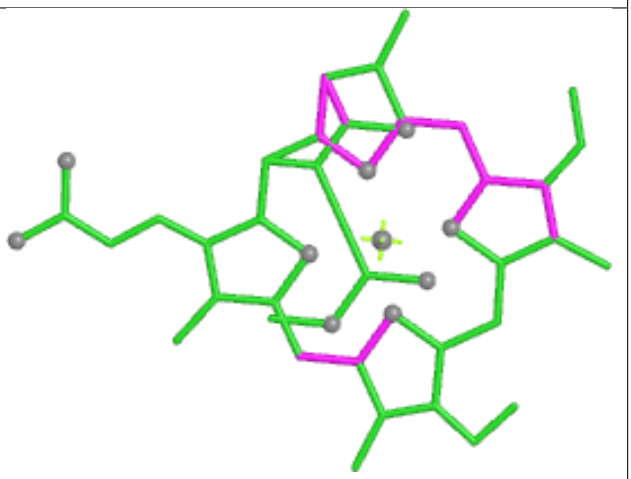


Rings

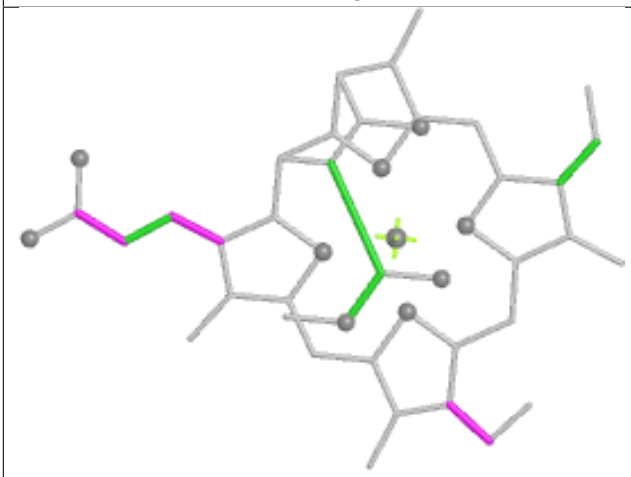
Ligand KC2 R 305



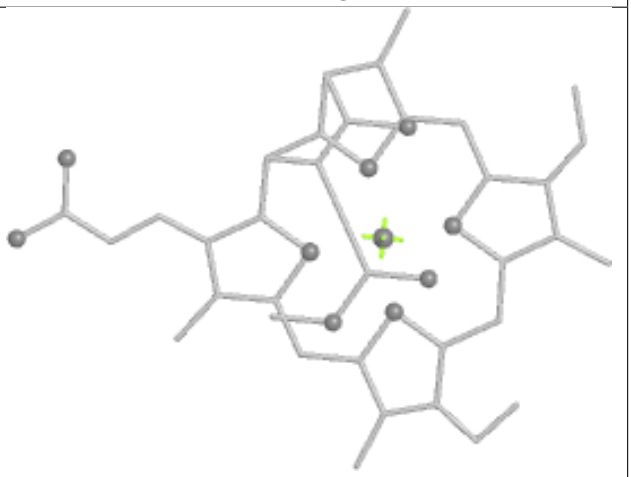
Bond lengths



Bond angles

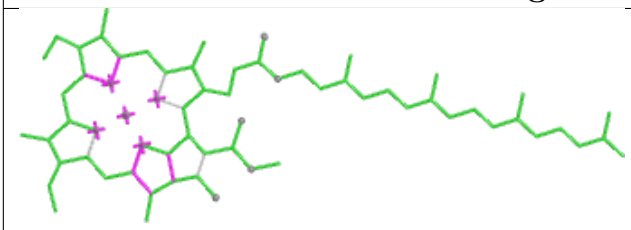


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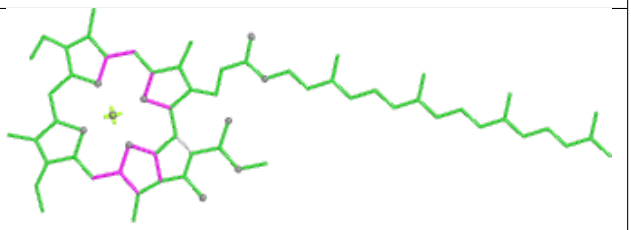


Rings

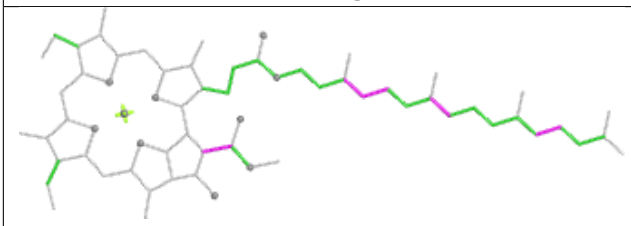
Ligand CLA a 834



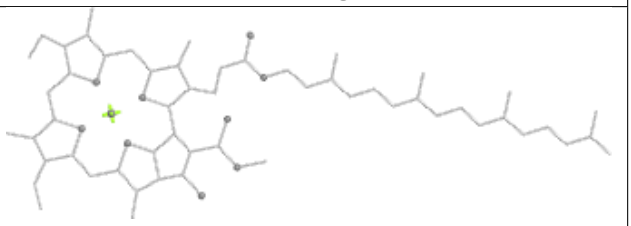
Bond lengths



Bond angles

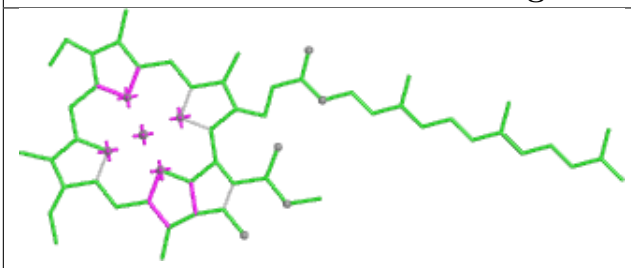


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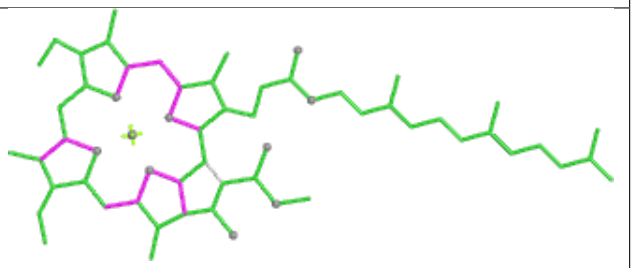


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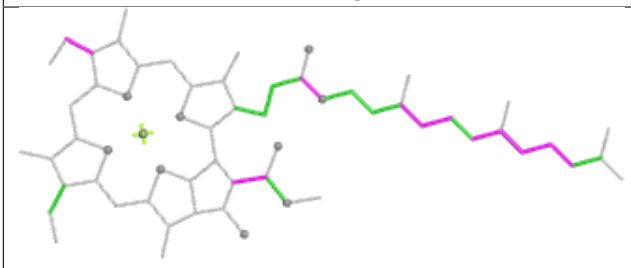
Ligand CLA b 831



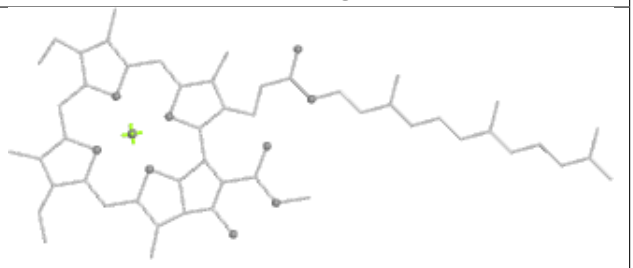
Bond lengths



Bond angles

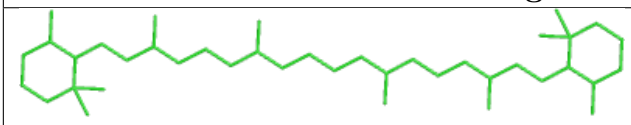


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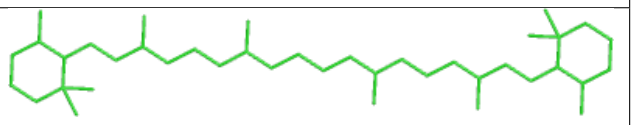


Rings

Ligand BCR b 845



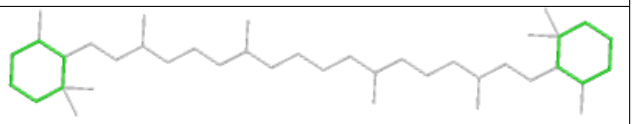
Bond lengths



Bond angles

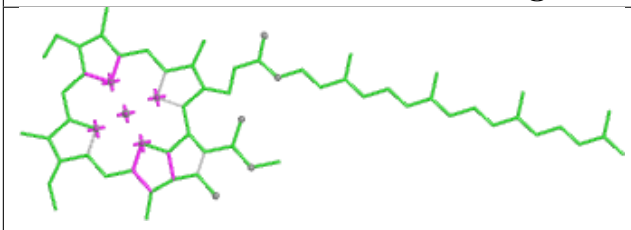


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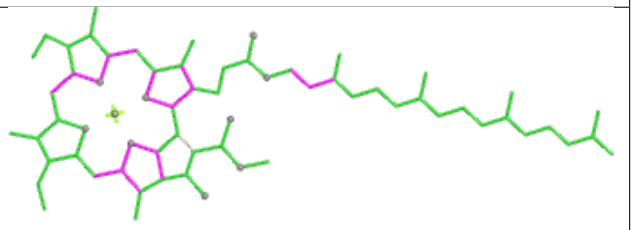


Rings

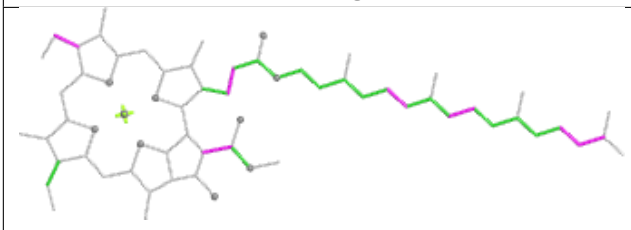
Ligand CLA a 807



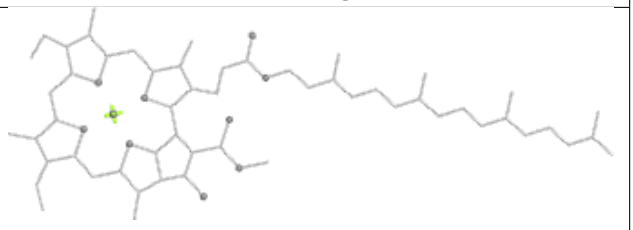
Bond lengths



Bond angles

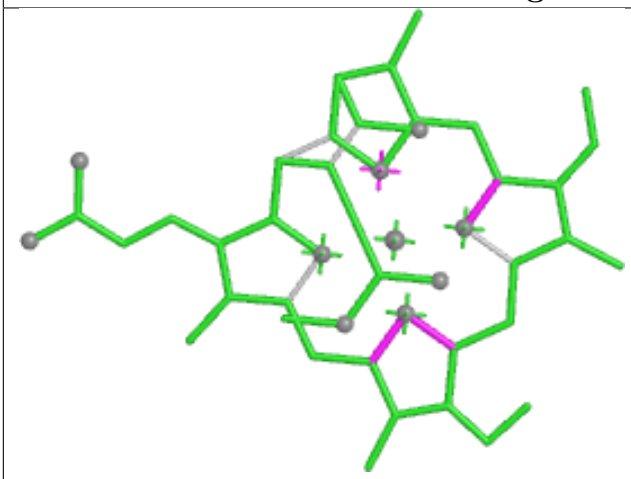


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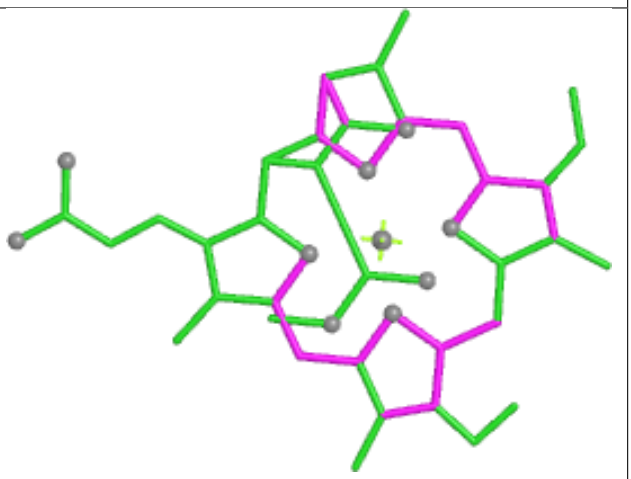


Rings

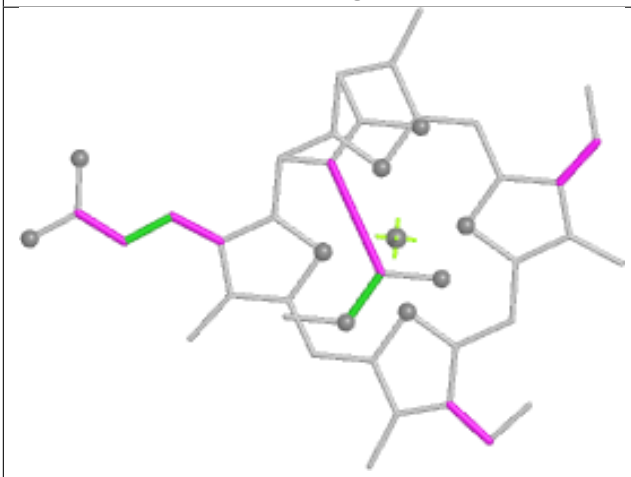
Ligand KC2 P 302



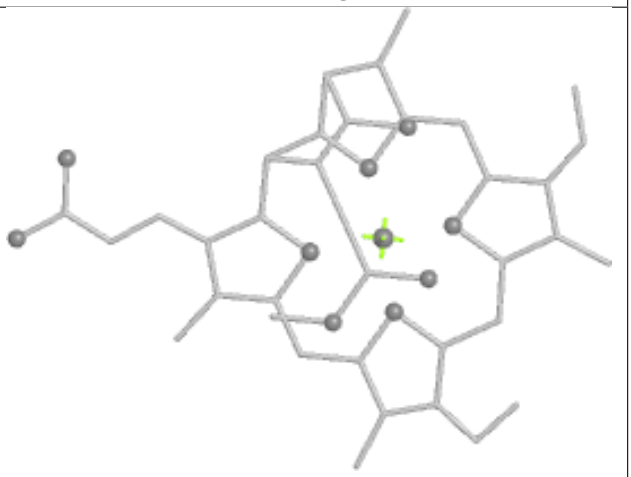
Bond lengths



Bond angles

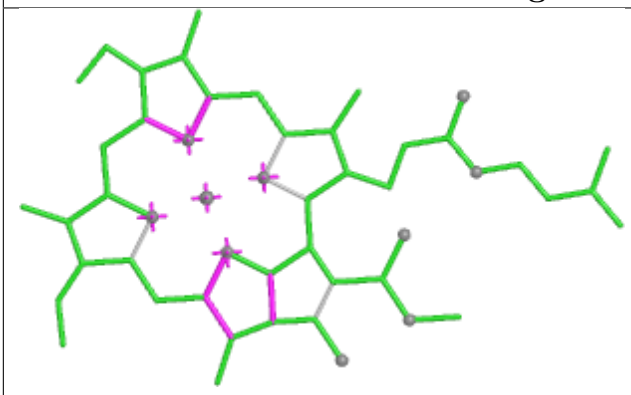


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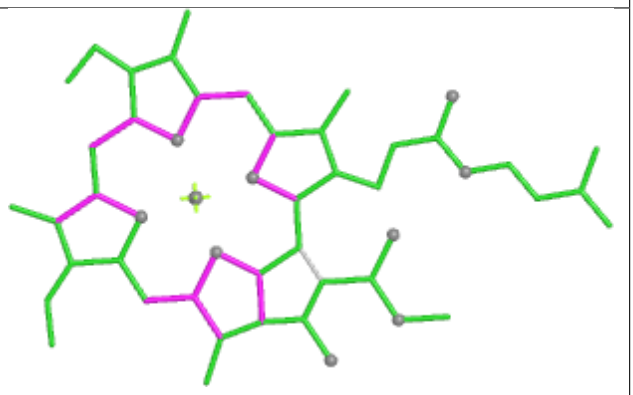


Rings

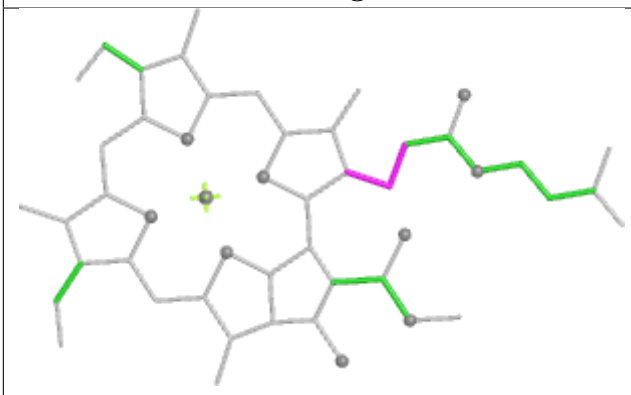
Ligand CLA a 808



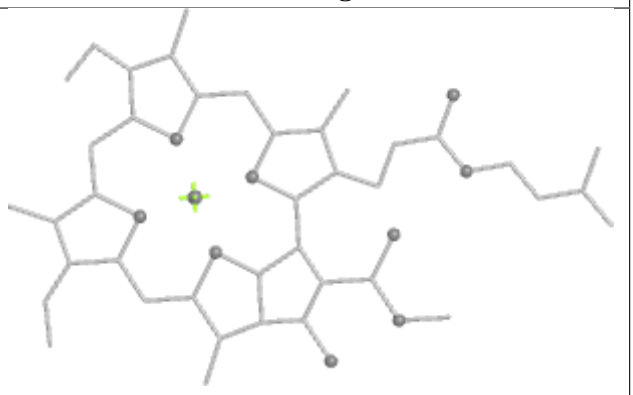
Bond lengths



Bond angles

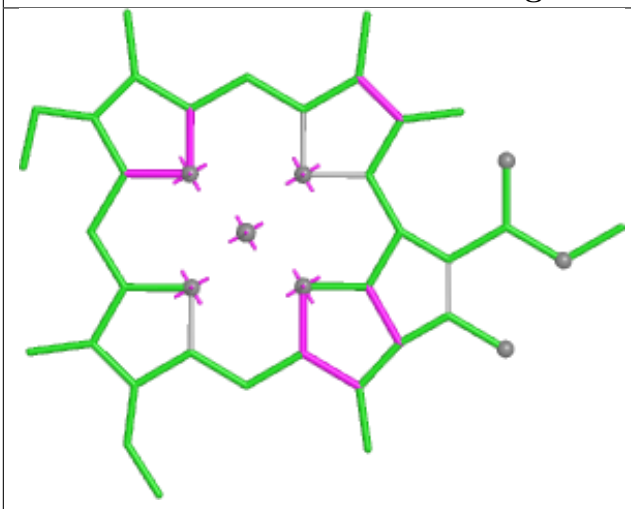


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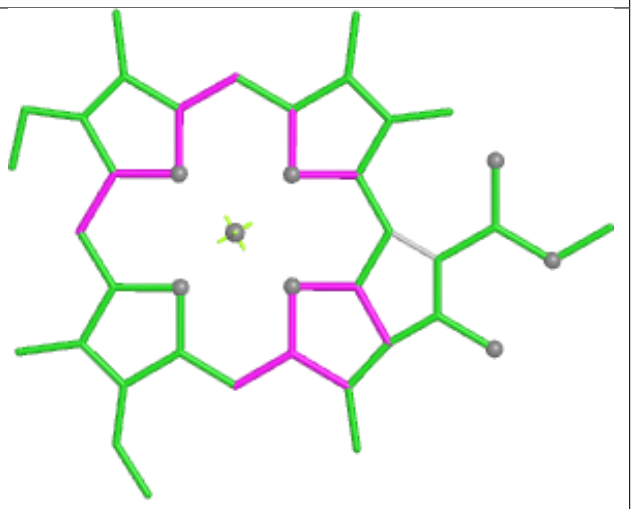


Rings

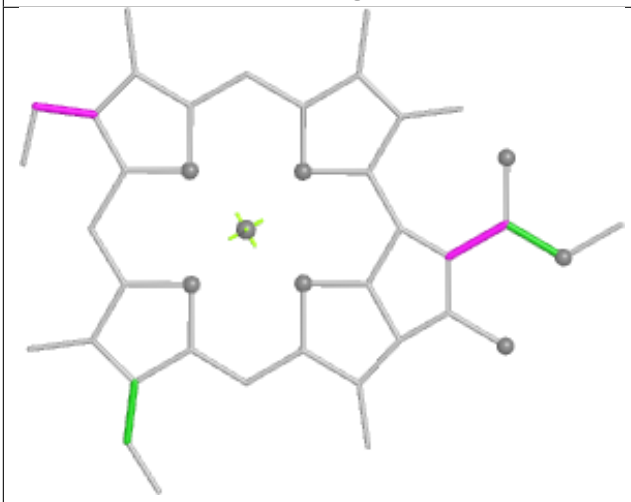
Ligand CLA P 310



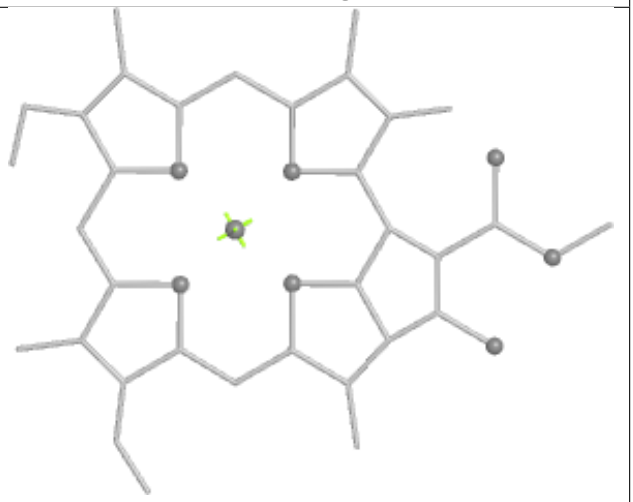
Bond lengths



Bond angles

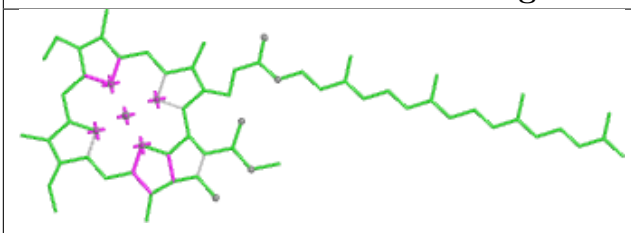


Torsions

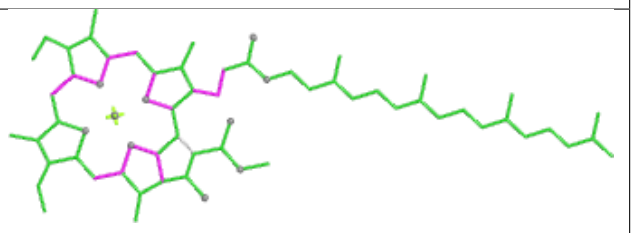


Rings

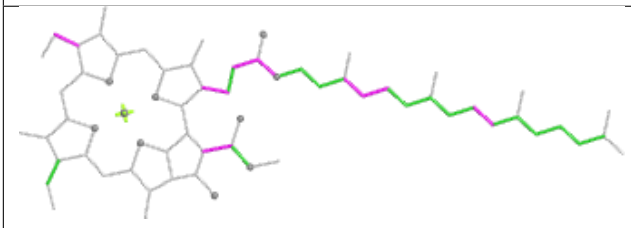
Ligand CLA W 311



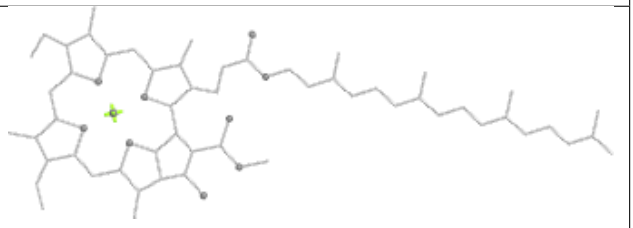
Bond lengths



Bond angles

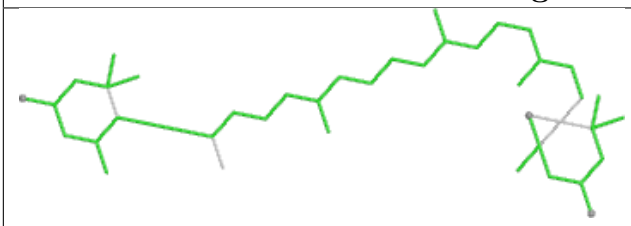


Torsions

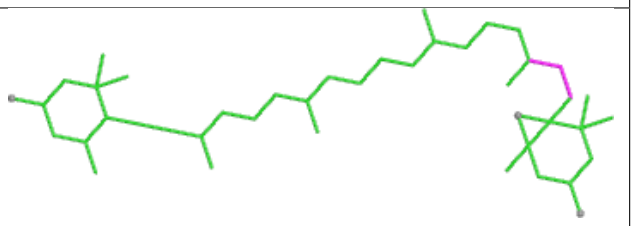


Rings

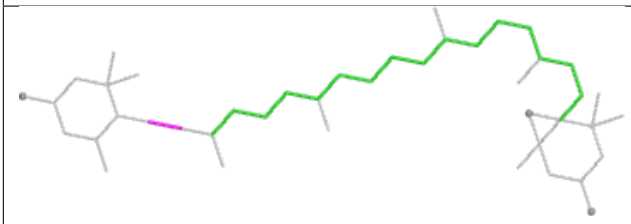
Ligand DD6 I 311



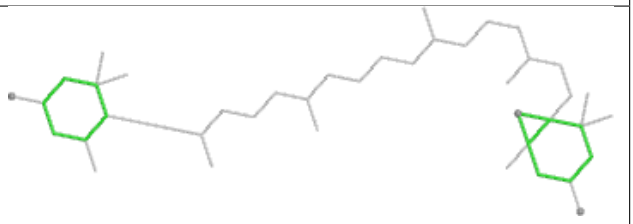
Bond lengths



Bond angles

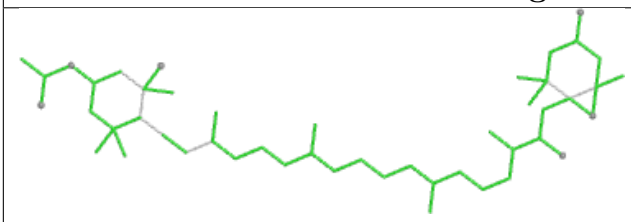


Torsions

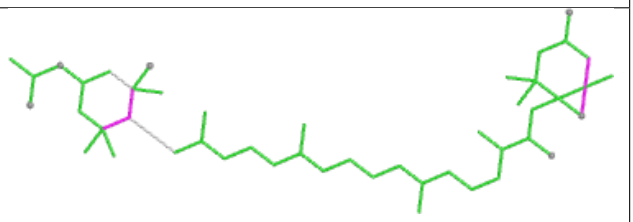


Rings

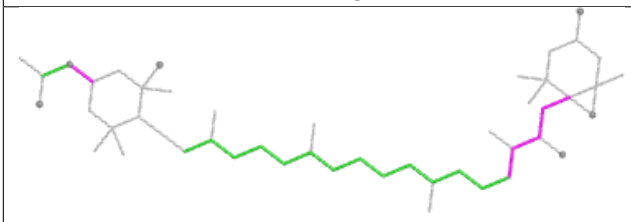
Ligand A86 G 310



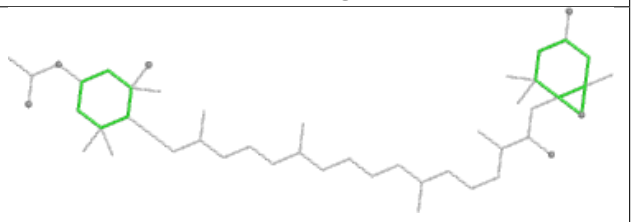
Bond lengths



Bond angles

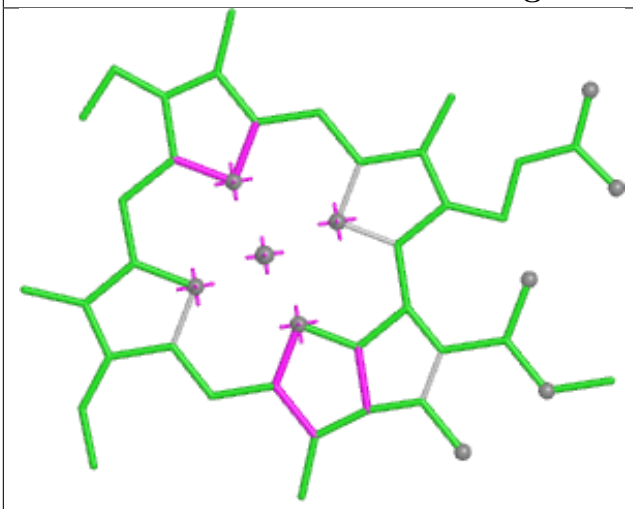


Torsions

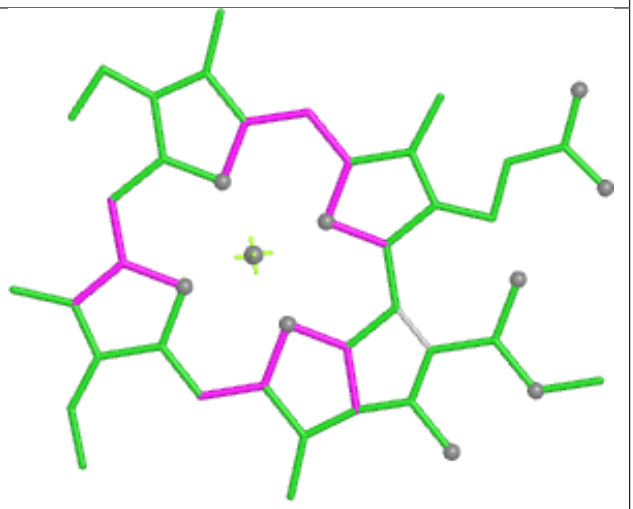


Rings

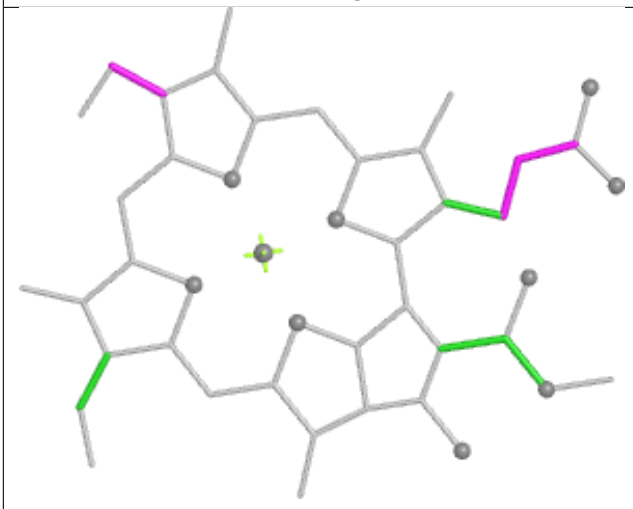
Ligand CLA A 301



Bond lengths



Bond angles

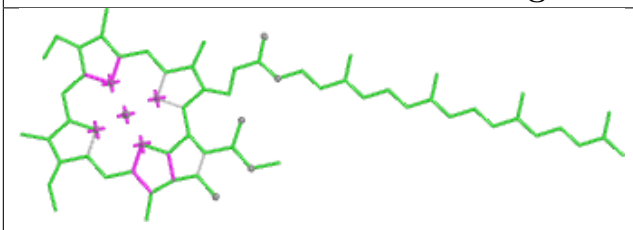


Torsions

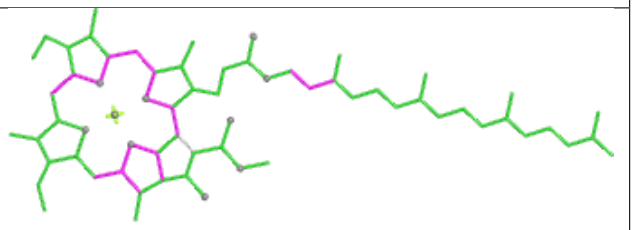


Rings

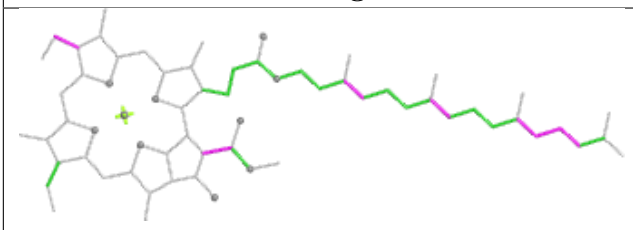
Ligand CLA a 853



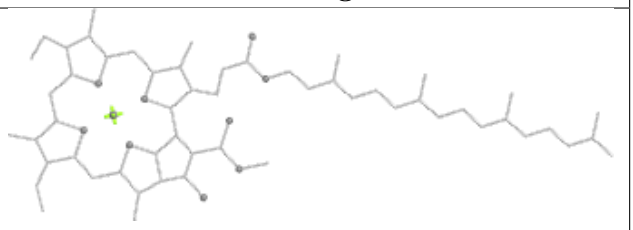
Bond lengths



Bond angles

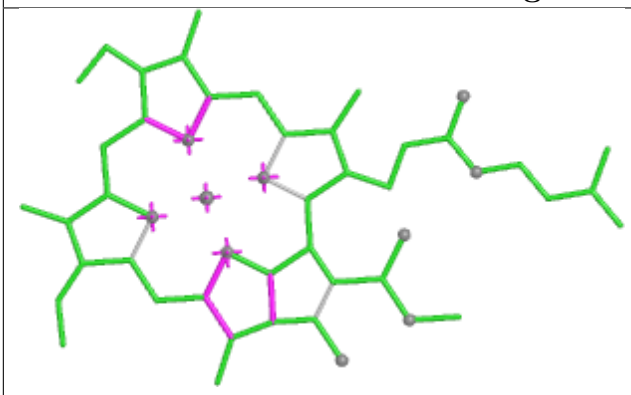


Torsions

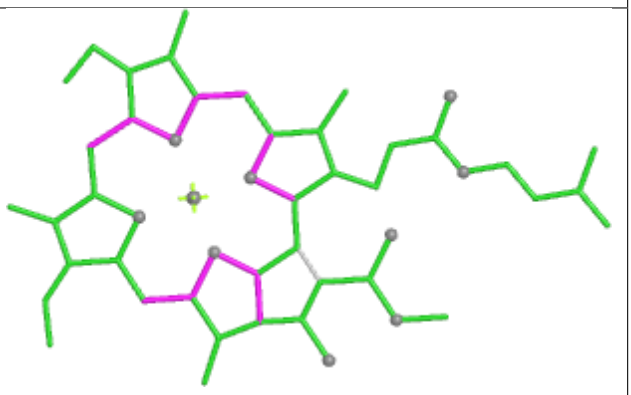


Rings

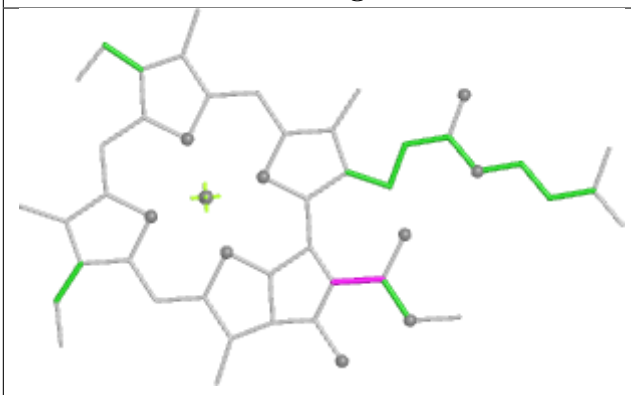
Ligand CLA V 204



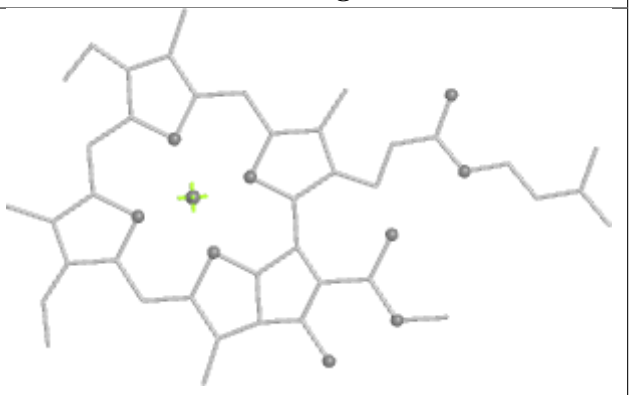
Bond lengths



Bond angles

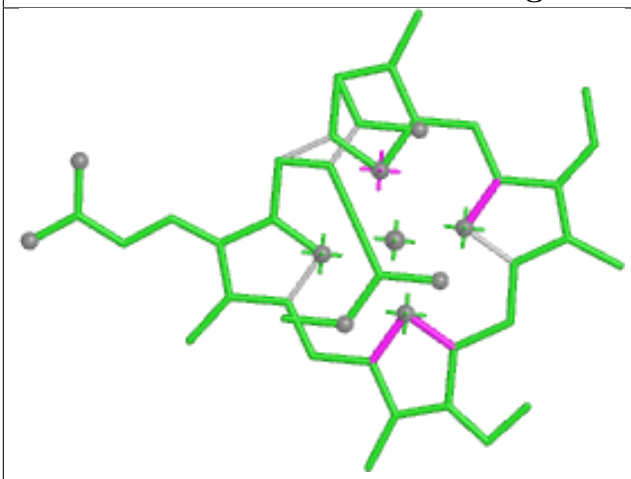


Torsions

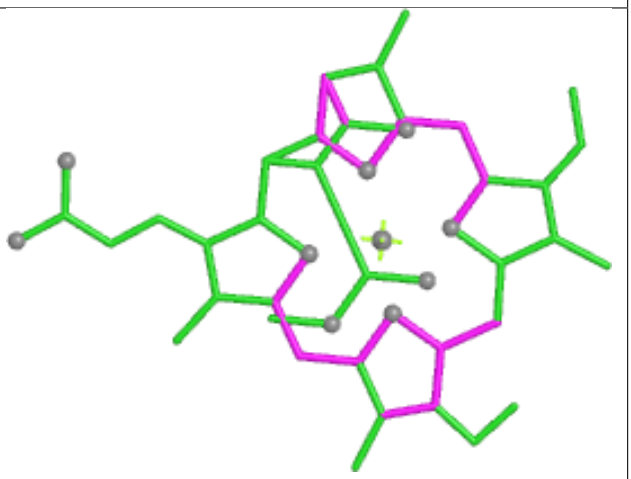


Rings

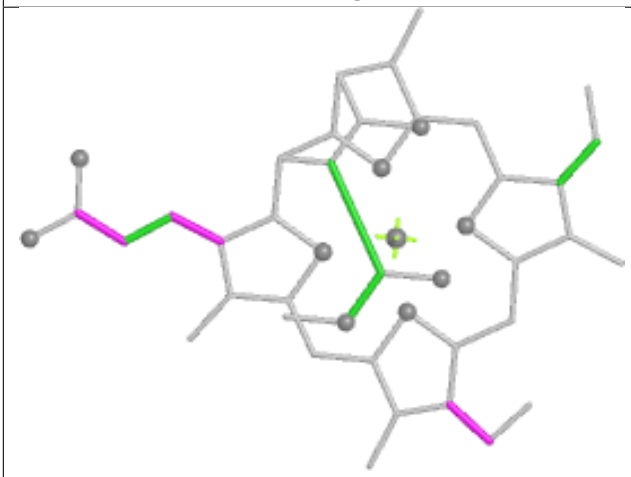
Ligand KC2 O 303



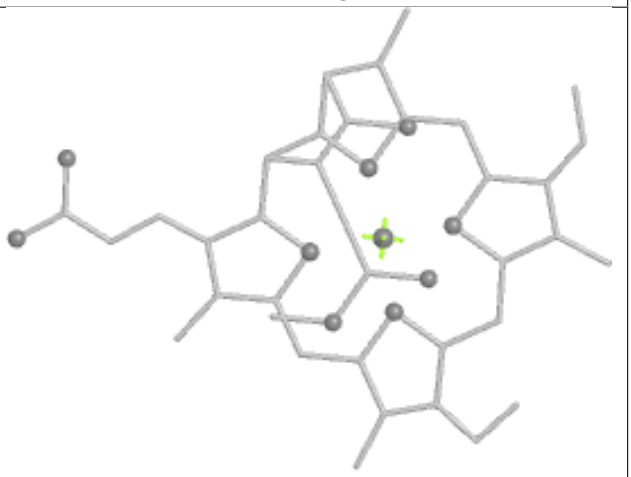
Bond lengths



Bond angles



Torsions



Rings

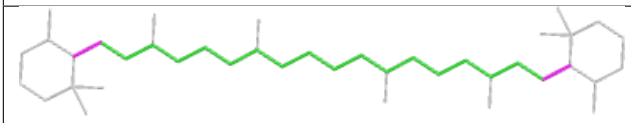
Ligand BCR b 843



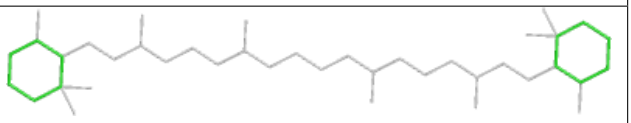
Bond lengths



Bond angles

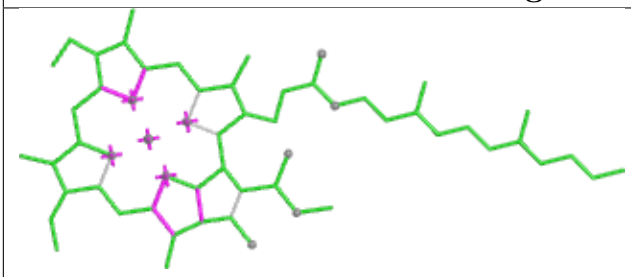


Torsions

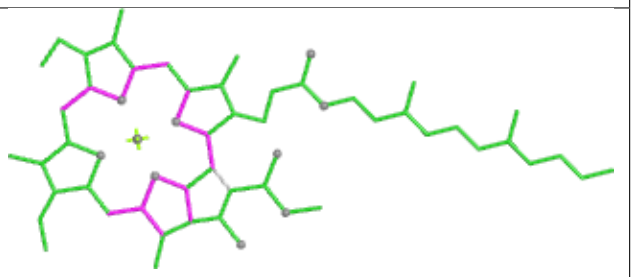


Rings

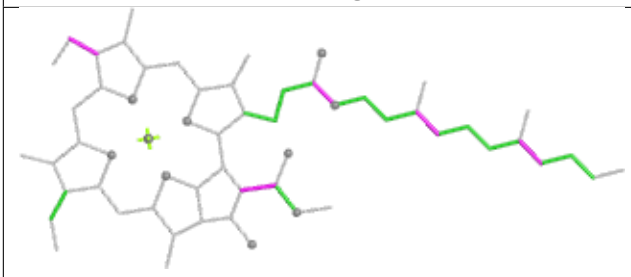
Ligand CLA E 309



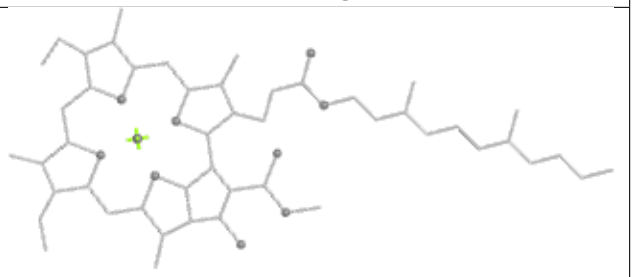
Bond lengths



Bond angles

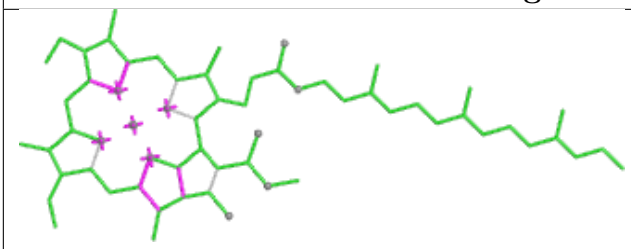


Torsions

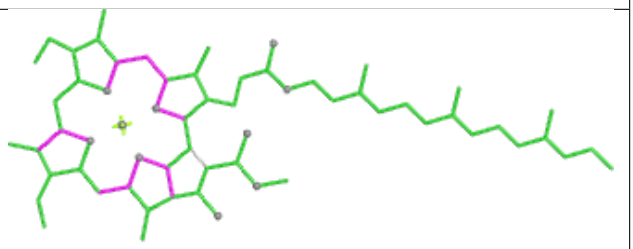


Rings

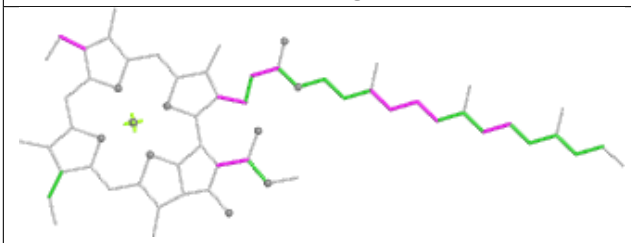
Ligand CLA A 303



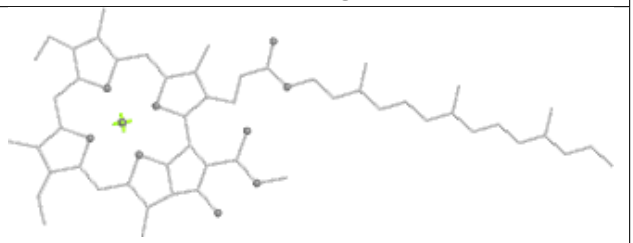
Bond lengths



Bond angles

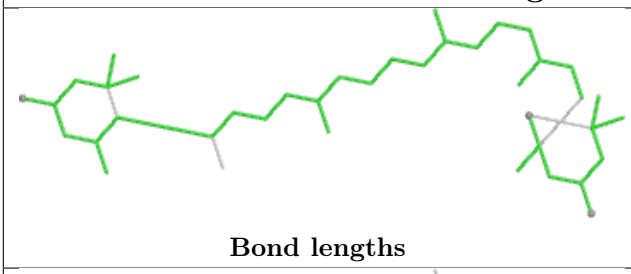


Torsions

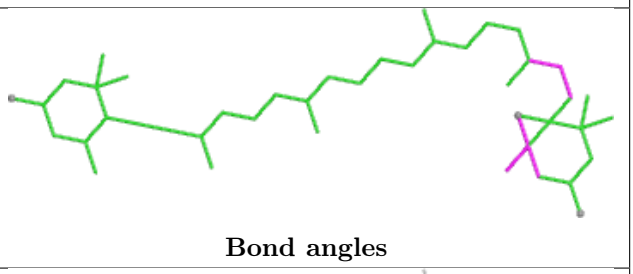


Rings

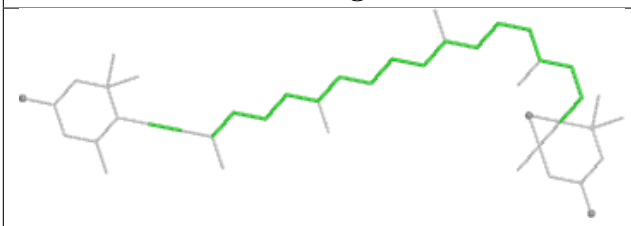
Ligand DD6 E 316



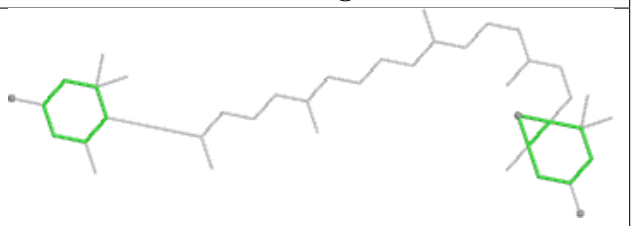
Bond lengths



Bond angles

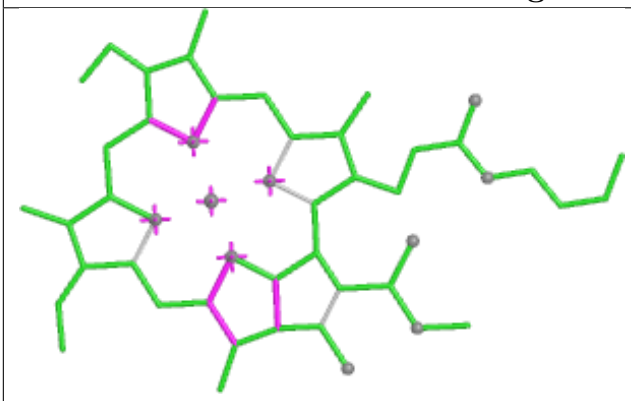


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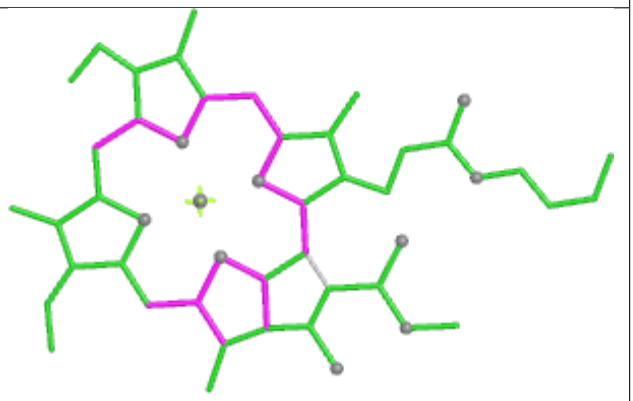


Rings

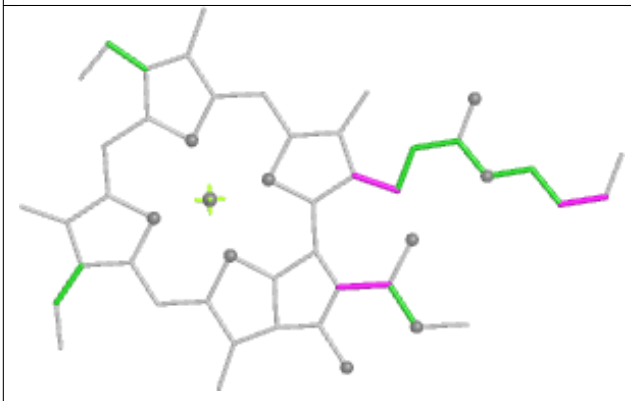
Ligand CLA b 826



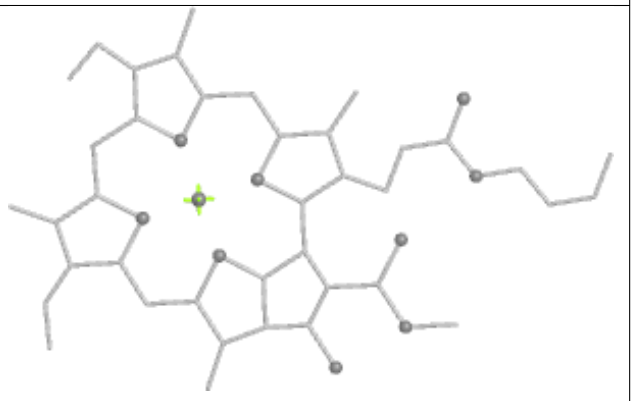
Bond lengths



Bond angles

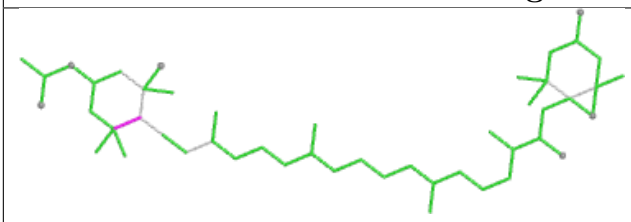


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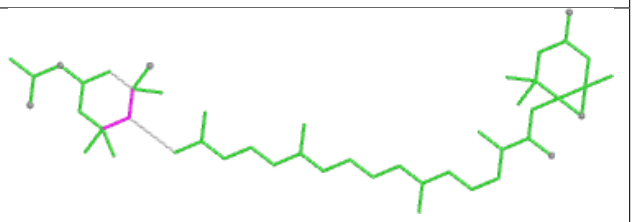


Rings

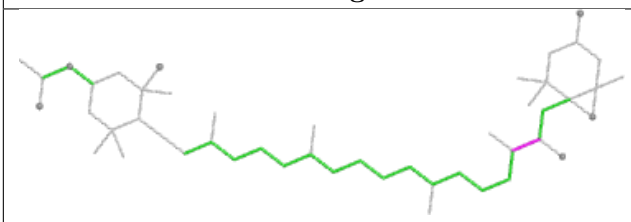
Ligand A86 M 322



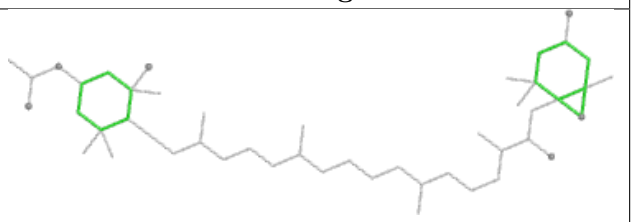
Bond lengths



Bond angles

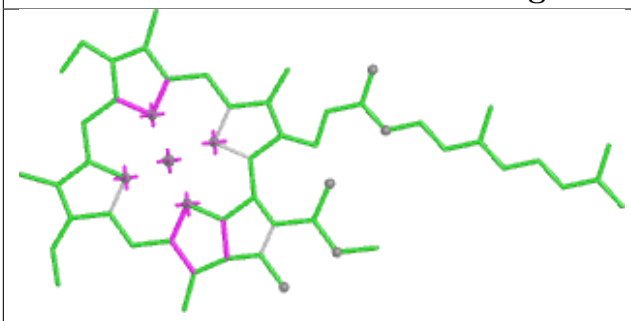


Torsions

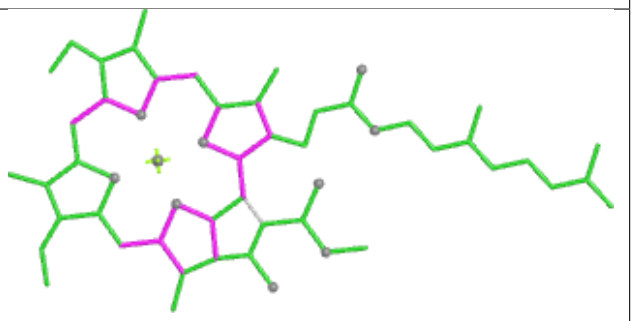


Rings

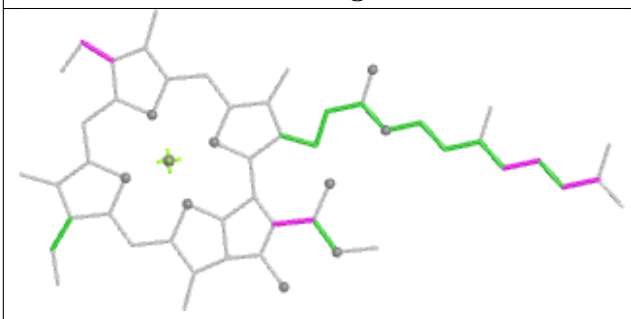
Ligand CLA a 837



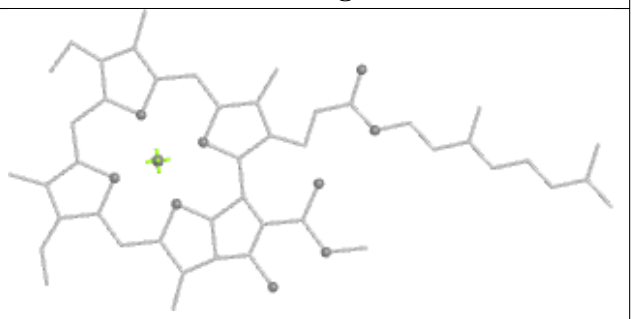
Bond lengths



Bond angles

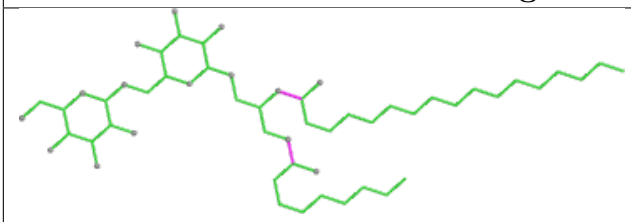


Torsions

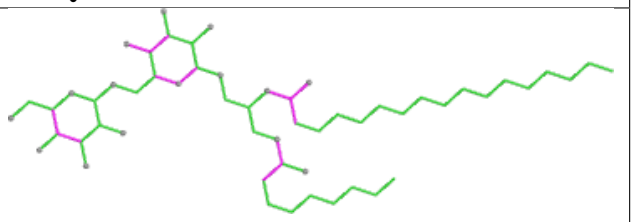


Rings

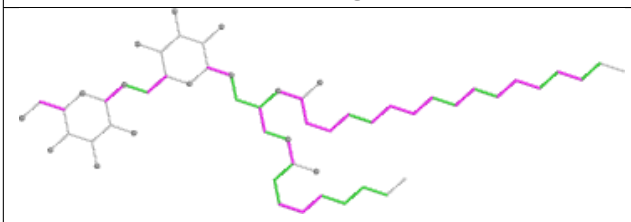
Ligand DGD Q 318



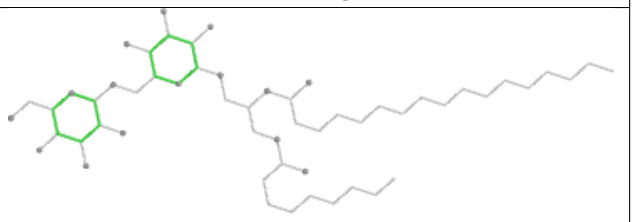
Bond lengths



Bond angles

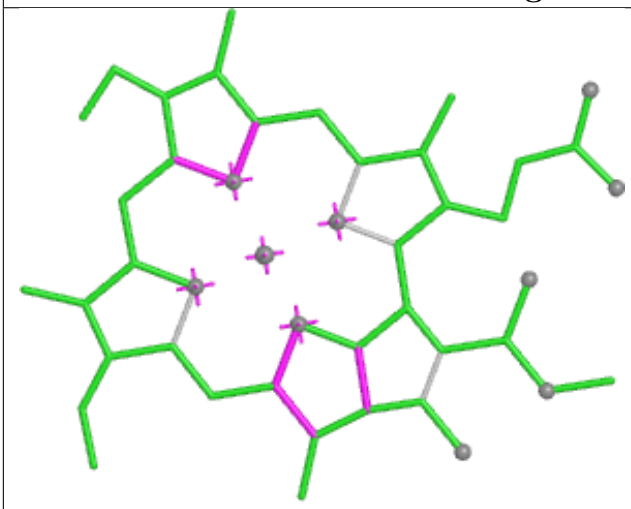


Torsions

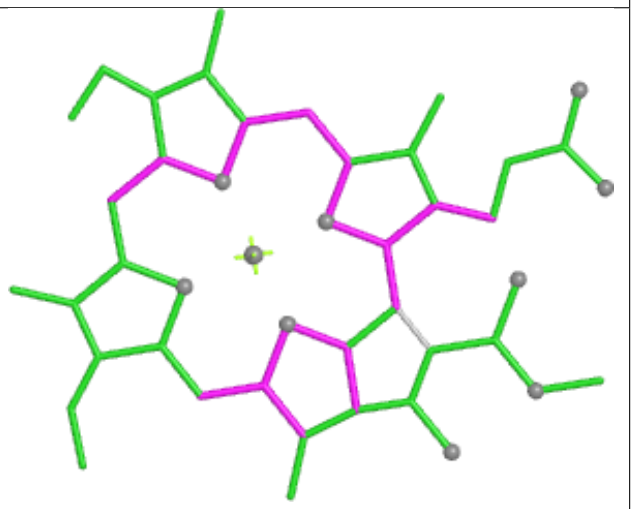


Rings

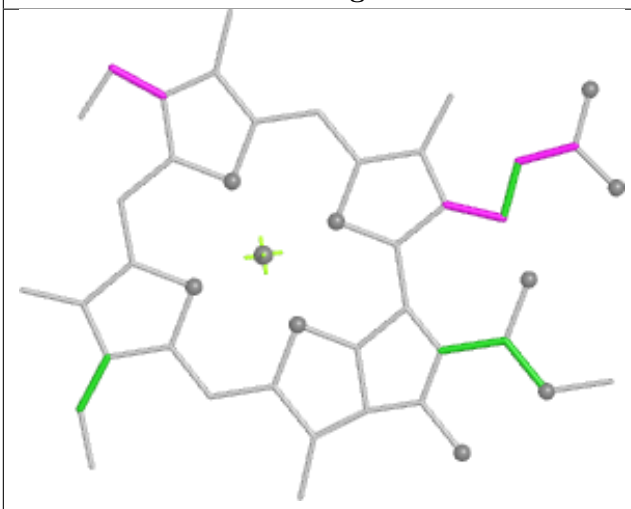
Ligand CLA P 304



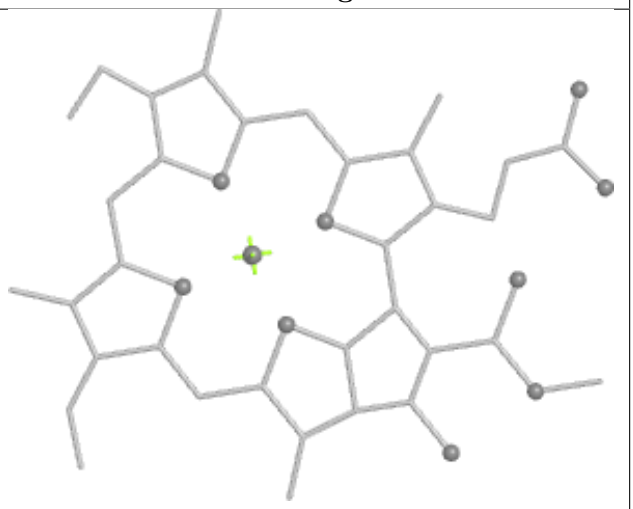
Bond lengths



Bond angles

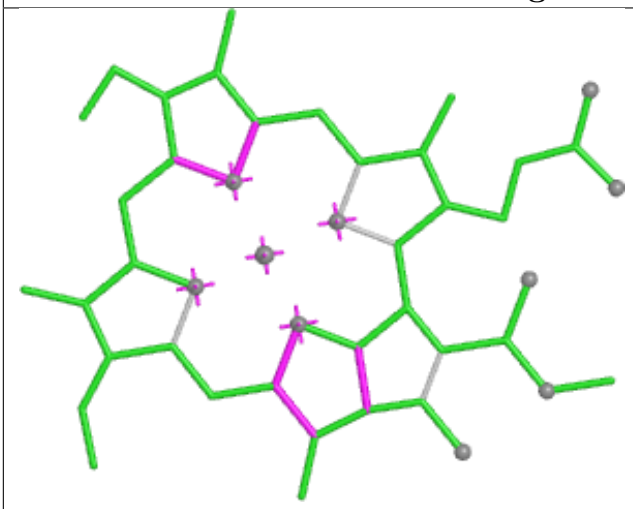


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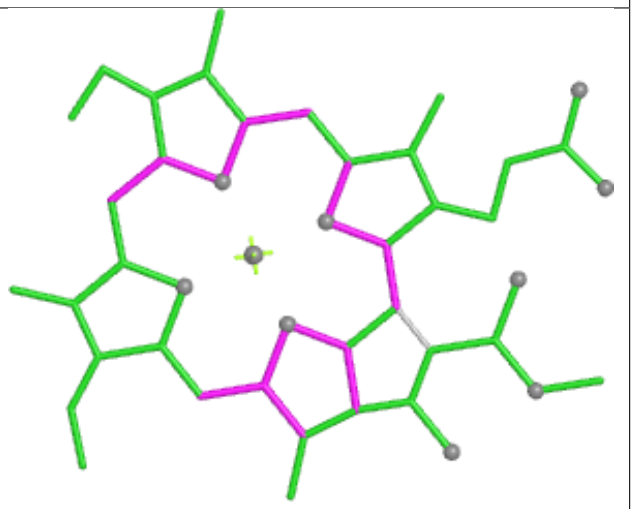


Rings

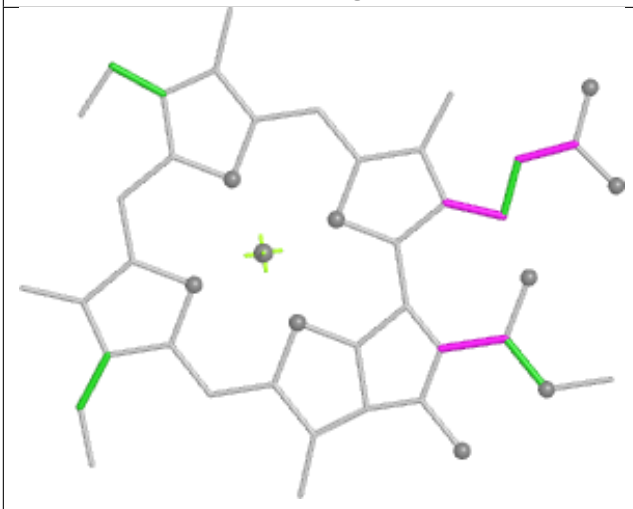
Ligand CLA a 813



Bond lengths



Bond angles

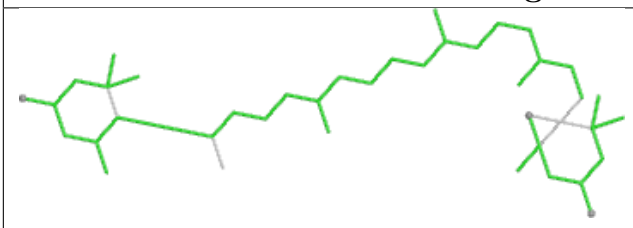


Torsions

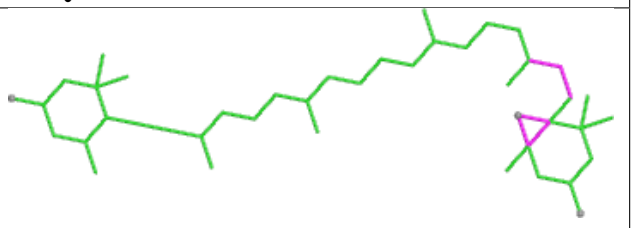


Rings

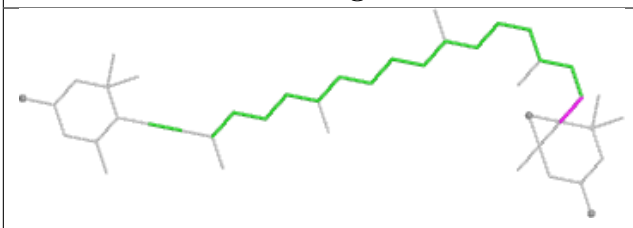
Ligand DD6 Q 315



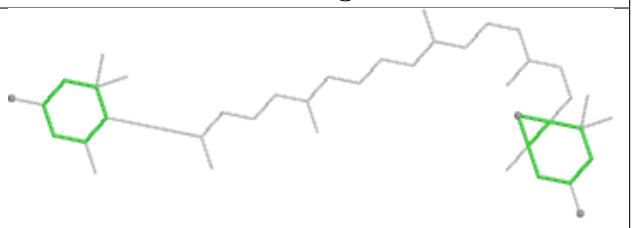
Bond lengths



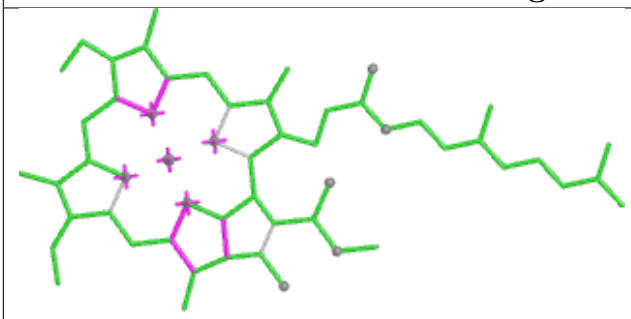
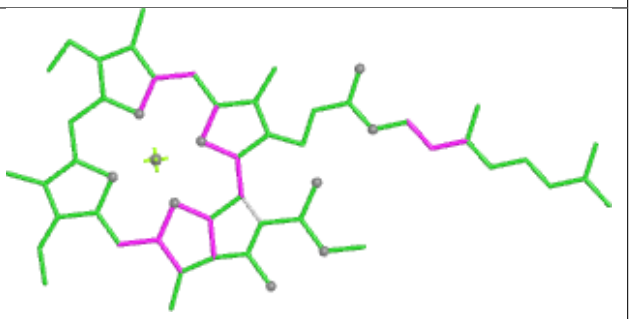
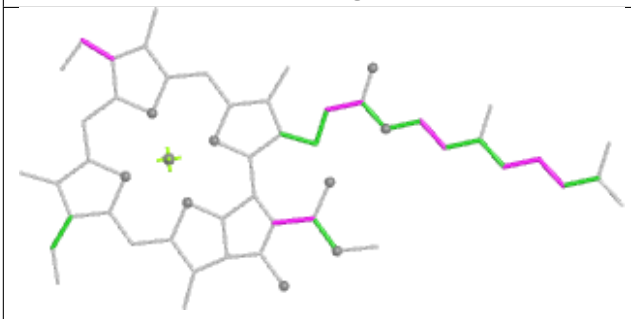
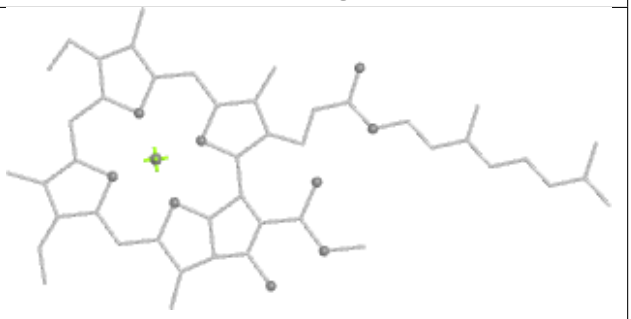
Bond angles

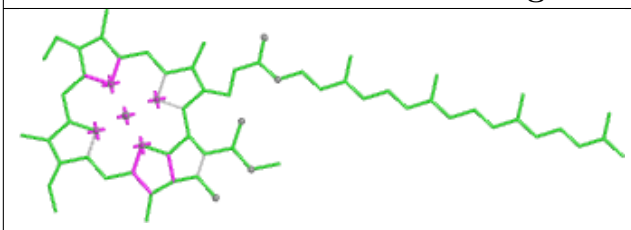
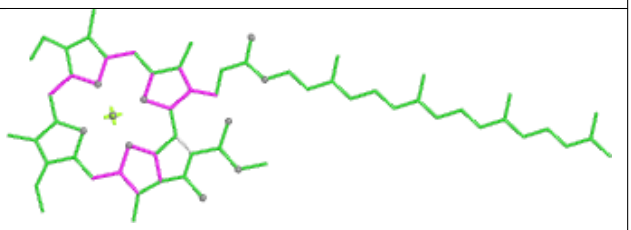
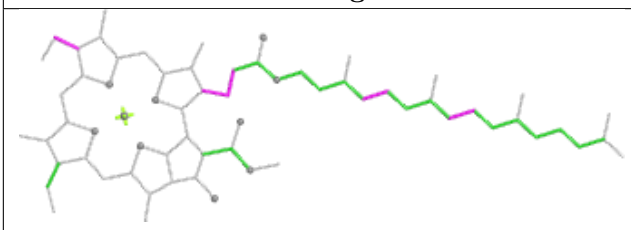
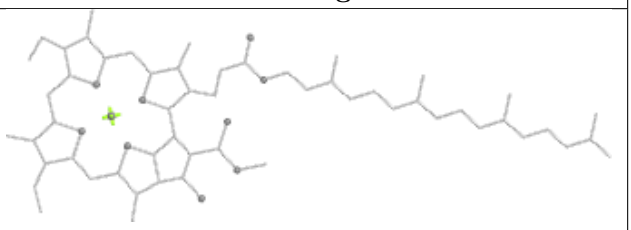


Torsions

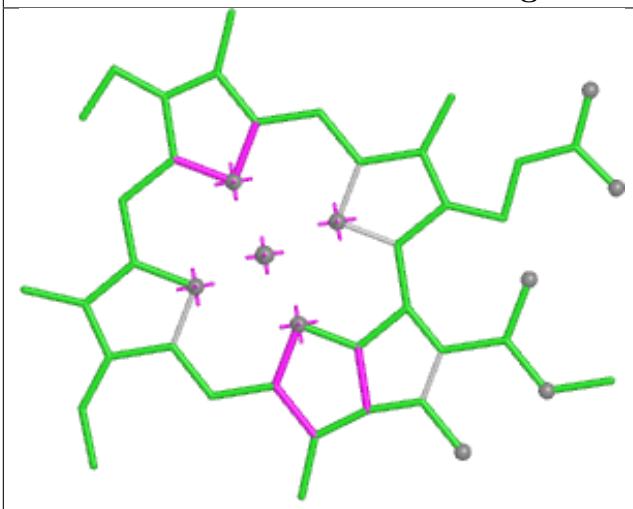


Rings

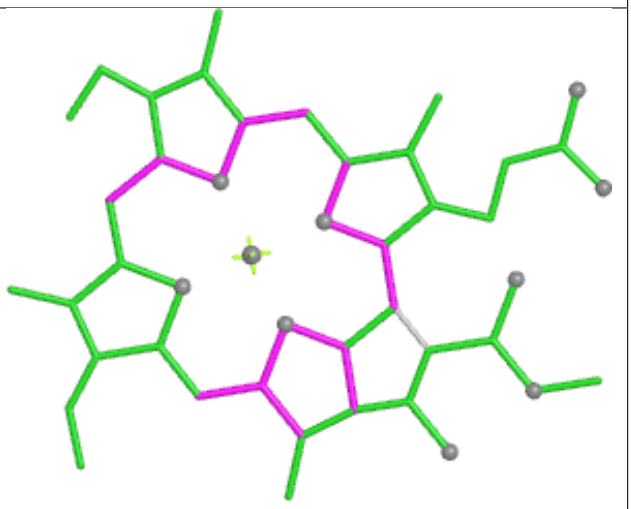
Ligand CLA a 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

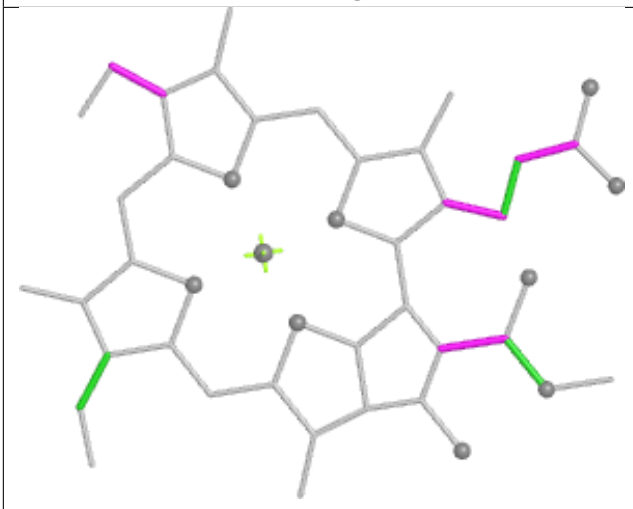
Ligand CLA M 311



Bond lengths



Bond angles

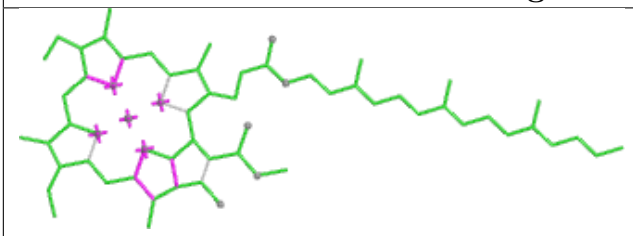


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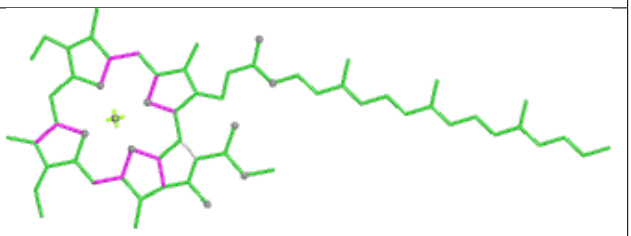


Rings

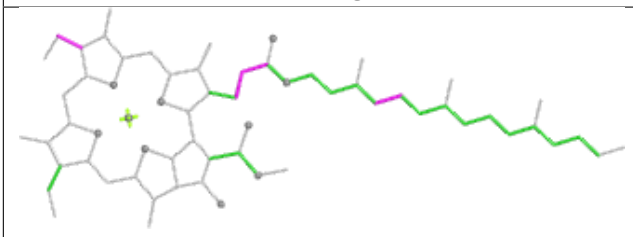
Ligand CLA S 305



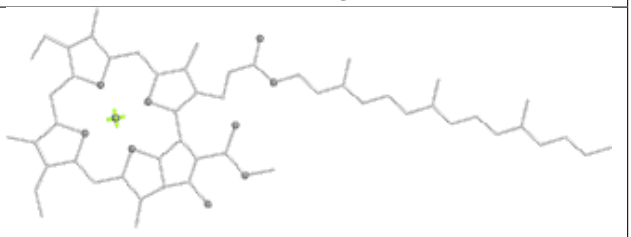
Bond lengths



Bond angles

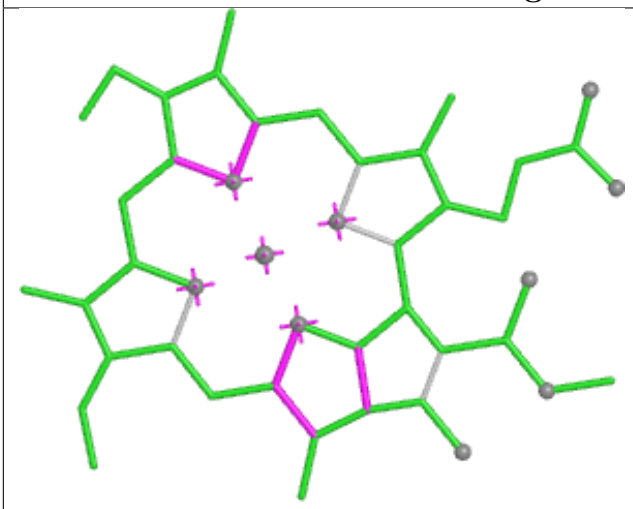


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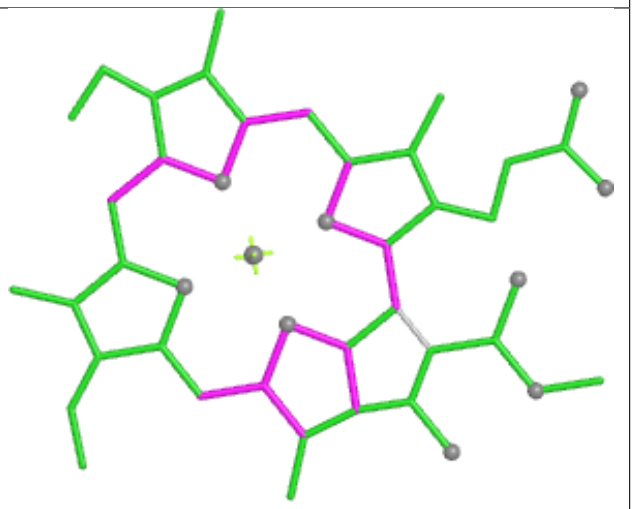


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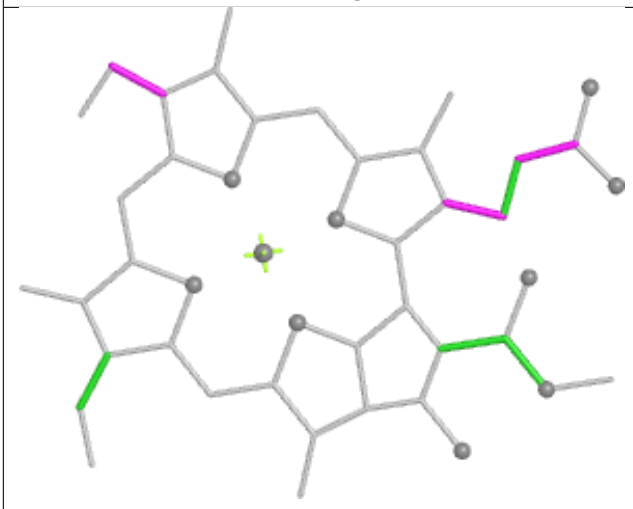
Ligand CLA T 302



Bond lengths



Bond angles

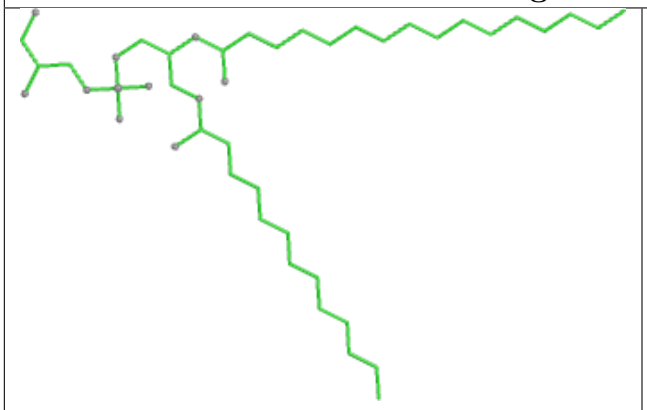


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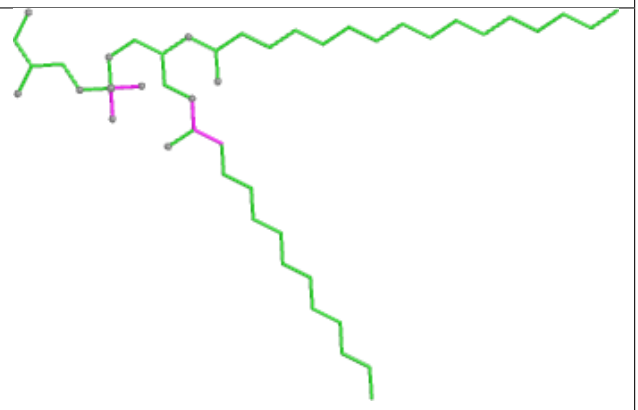


Rings

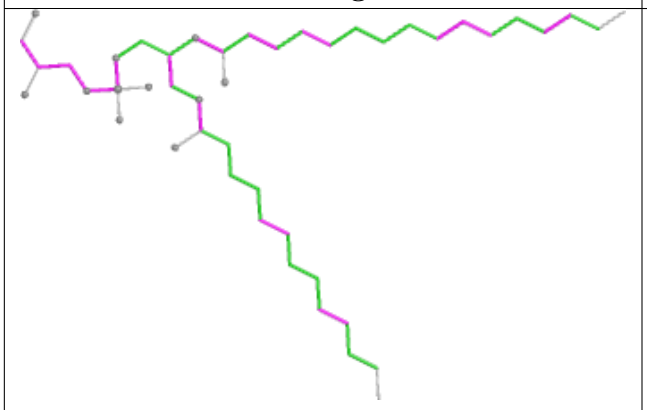
Ligand LHG I 314



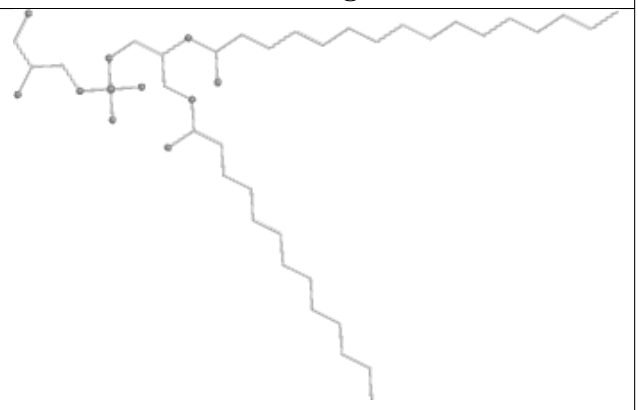
Bond lengths



Bond angles

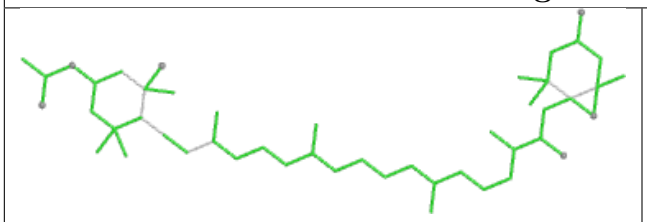


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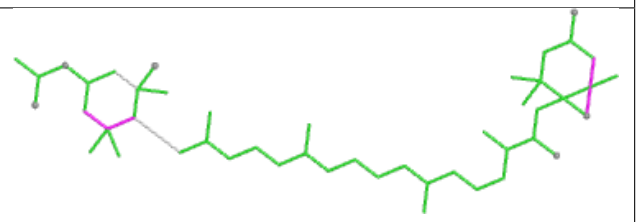


Rings

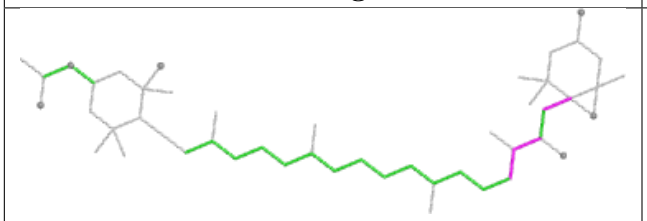
Ligand A86 S 319



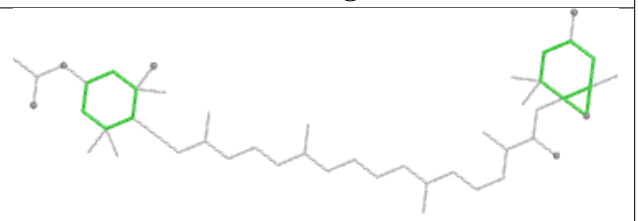
Bond lengths



Bond angles

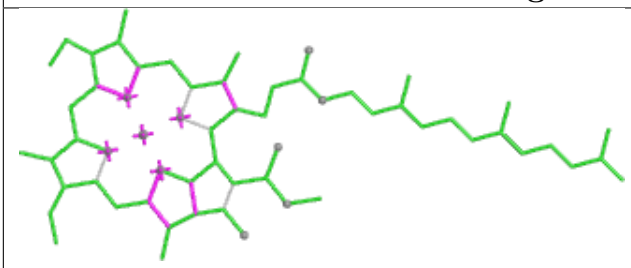


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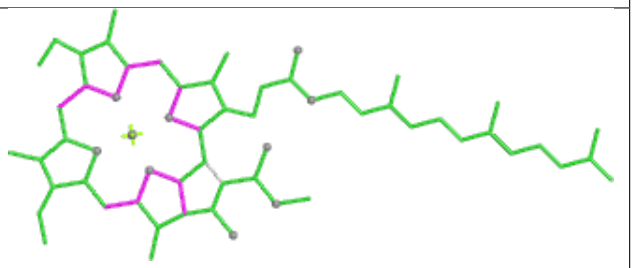


Rings

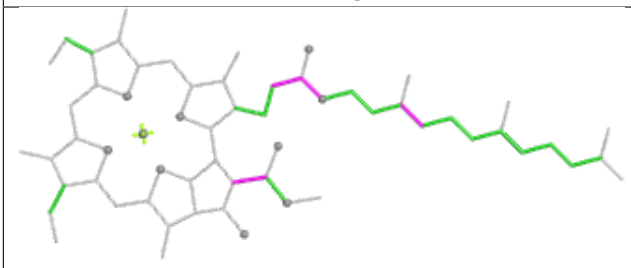
Ligand CLA b 825



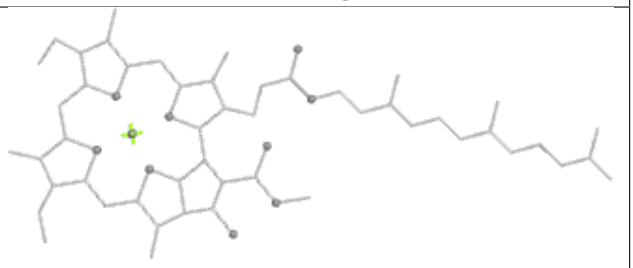
Bond lengths



Bond angles

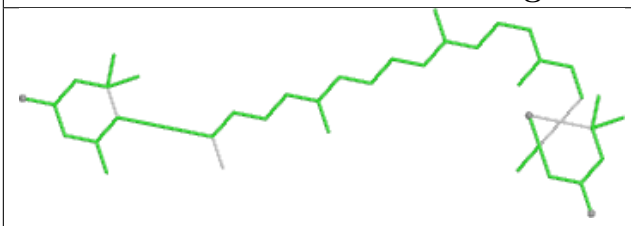


Torsions

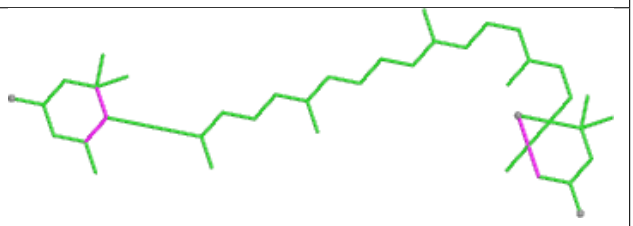


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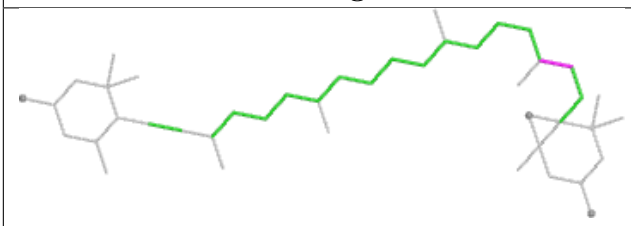
Ligand DD6 N 318



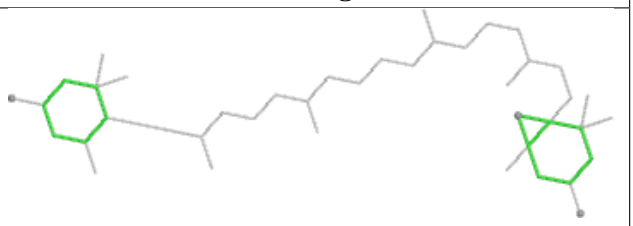
Bond lengths



Bond angles

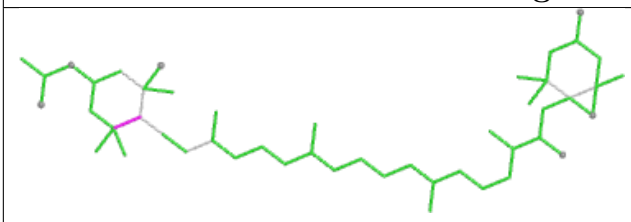


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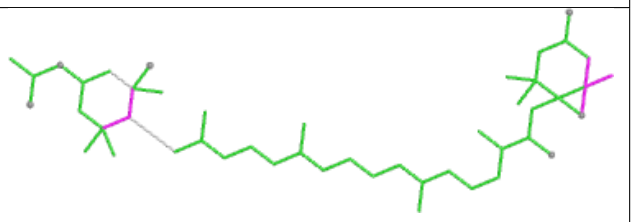


Rings

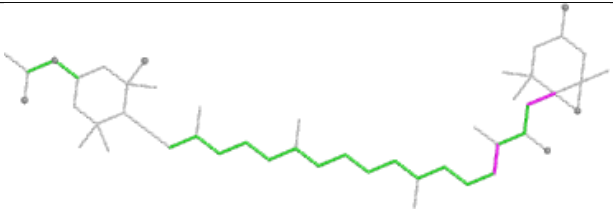
Ligand A86 S 315



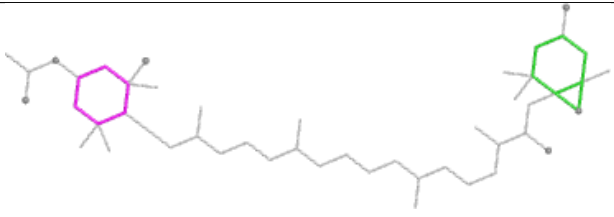
Bond lengths



Bond angles

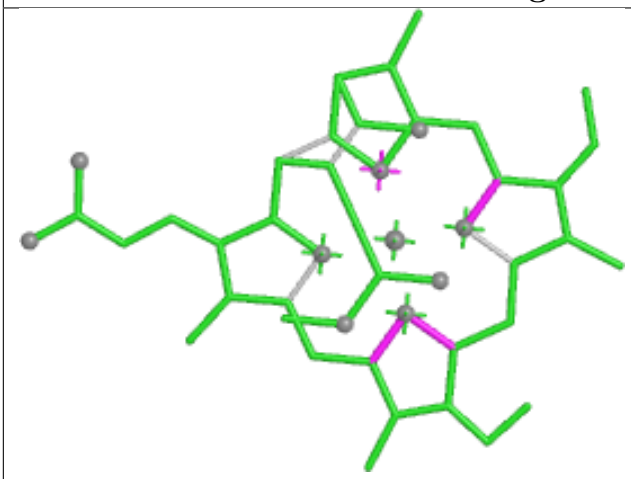


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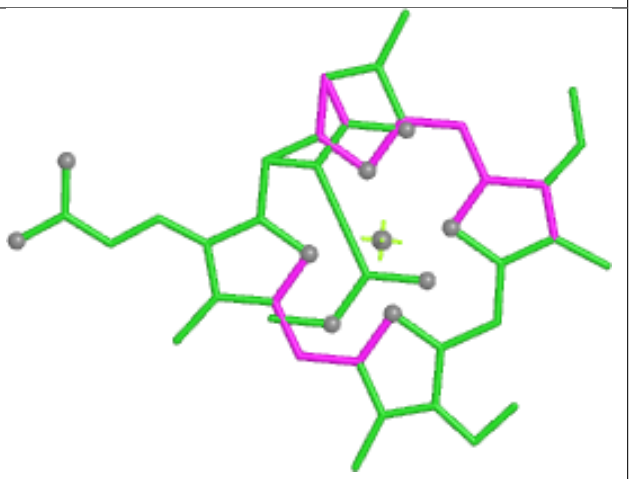


Rings

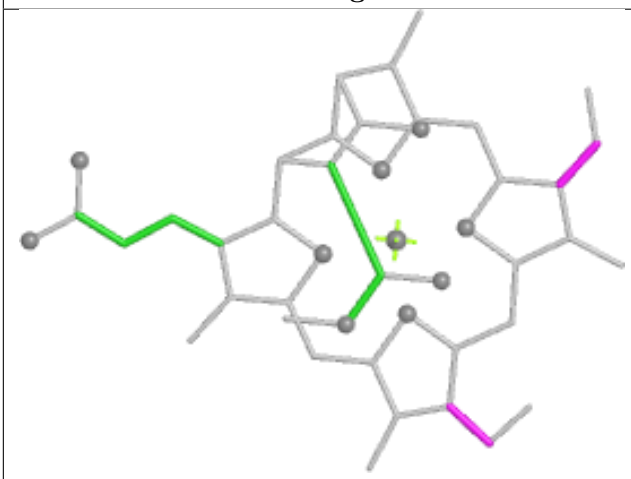
Ligand KC2 S 312



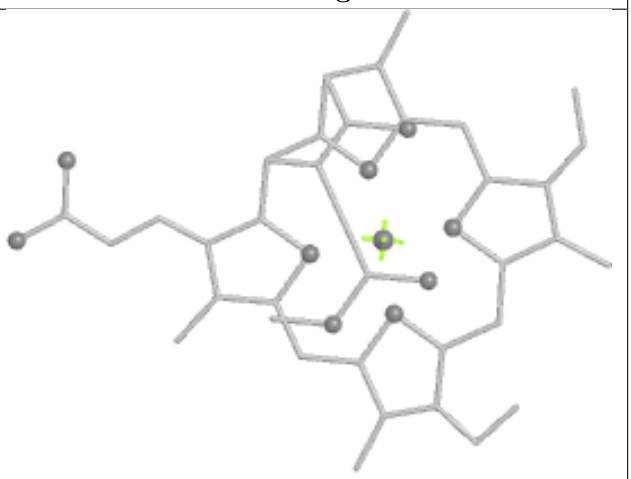
Bond lengths



Bond angles

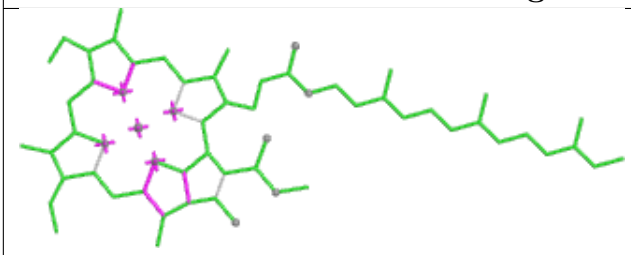


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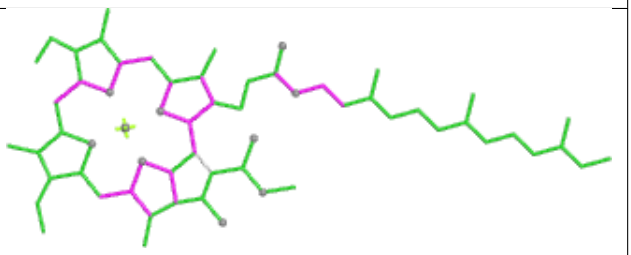


Rings

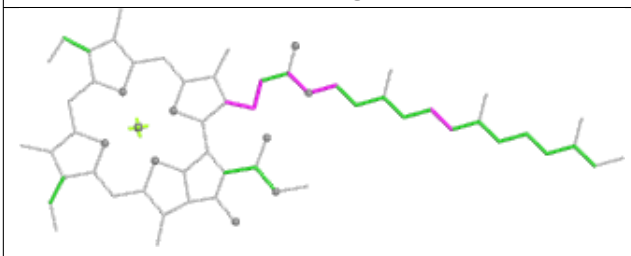
Ligand CLA b 830



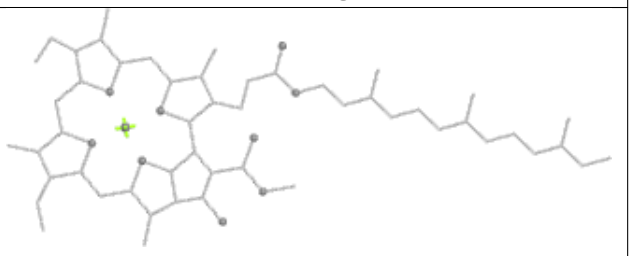
Bond lengths



Bond angles

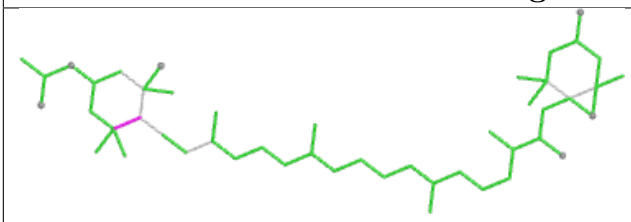


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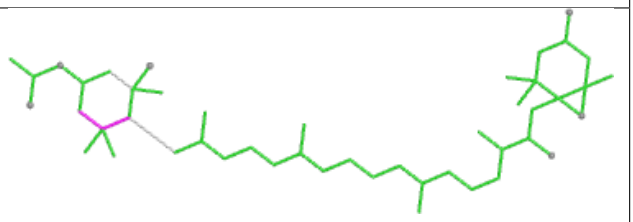


Rings

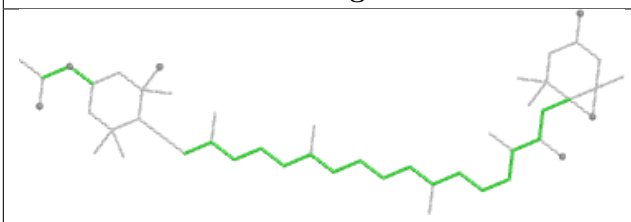
Ligand A86 N 320



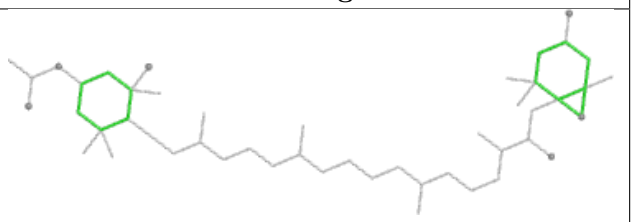
Bond lengths



Bond angles

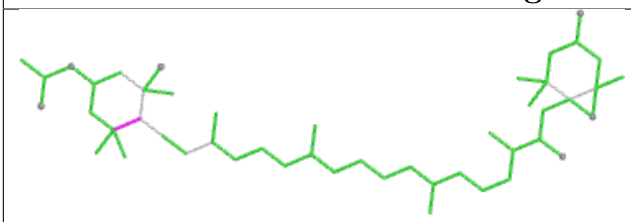


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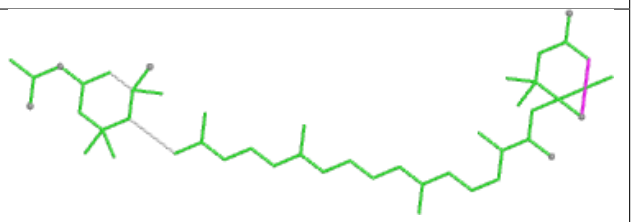


Rings

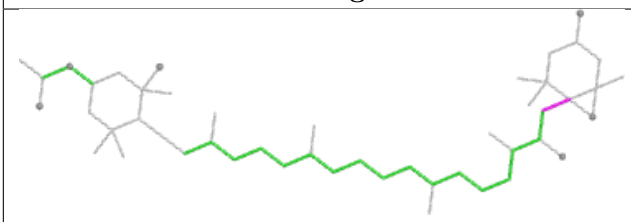
Ligand A86 W 302



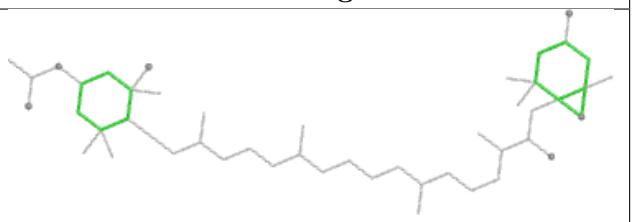
Bond lengths



Bond angles

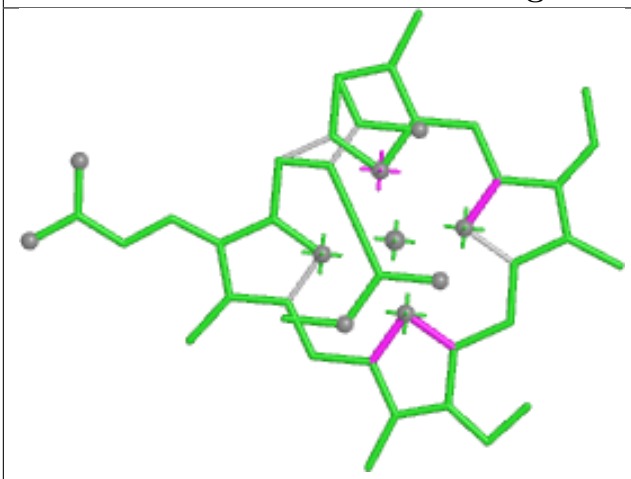


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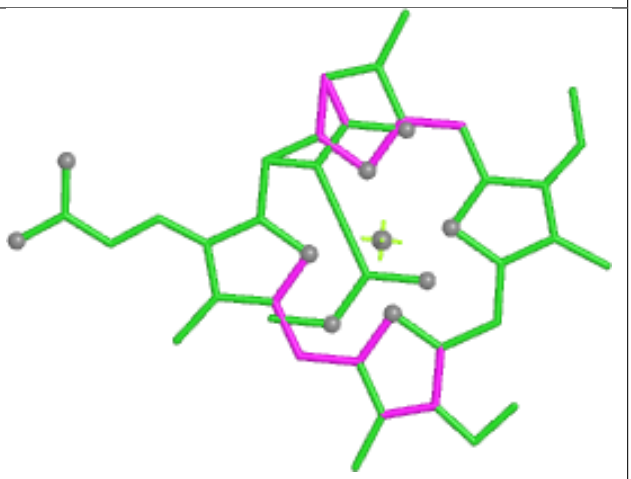


Rings

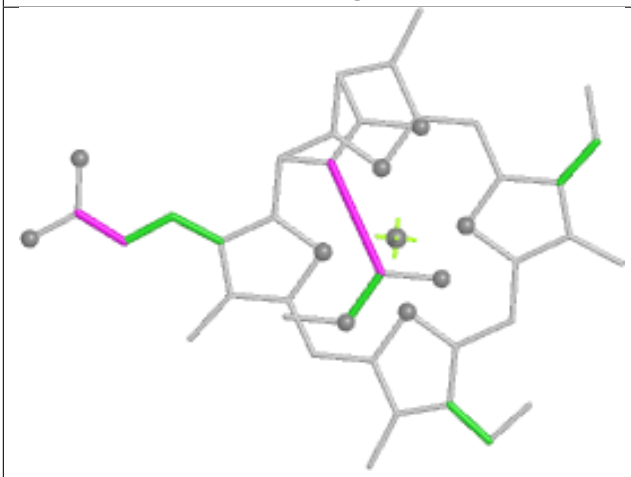
Ligand KC2 P 303



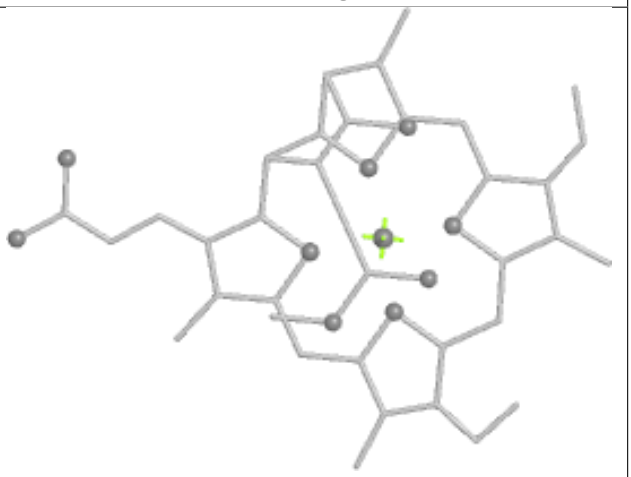
Bond lengths



Bond angles

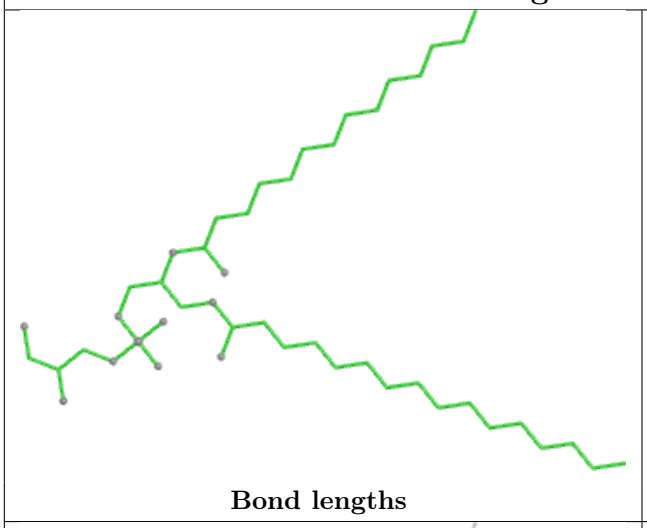


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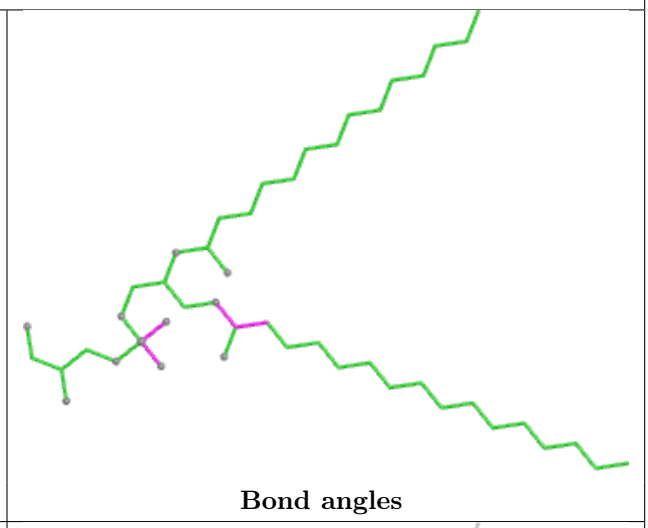


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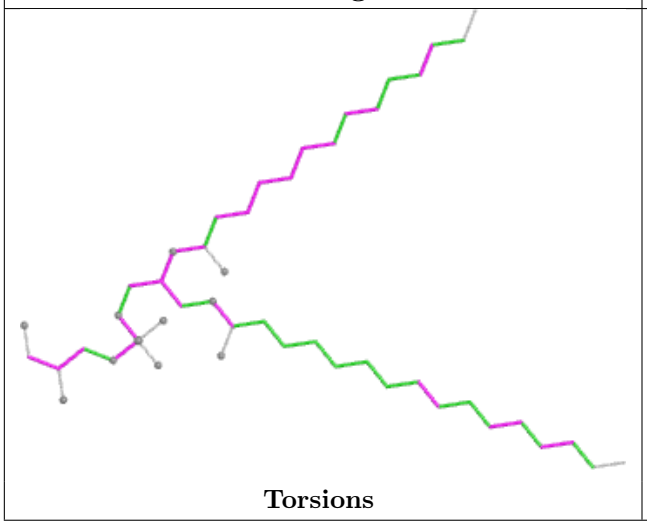
Ligand LHG f 205



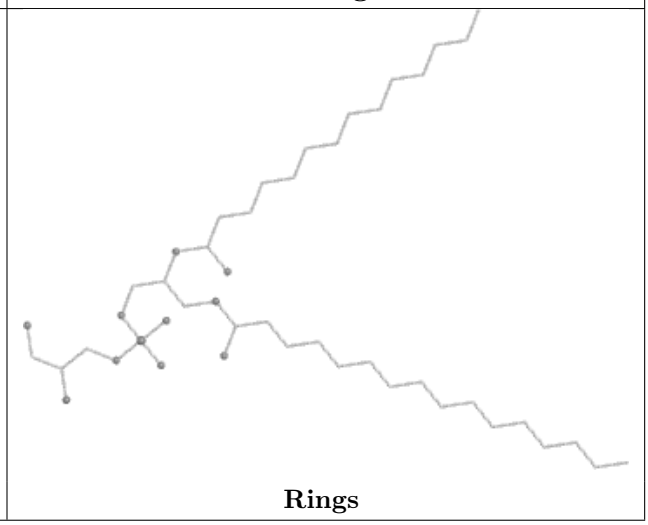
Bond lengths



Bond angles

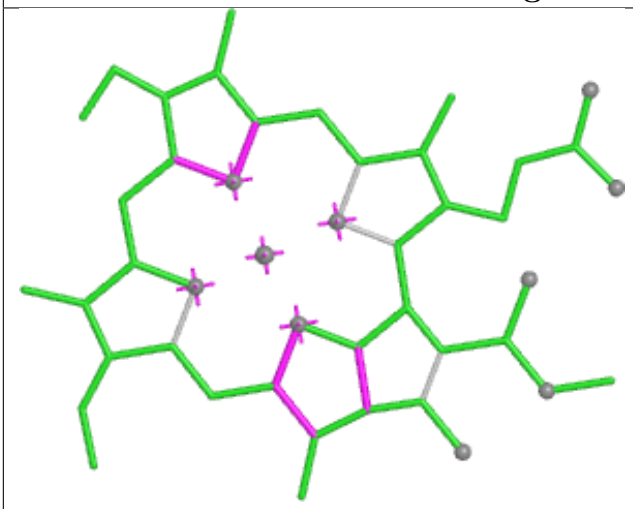


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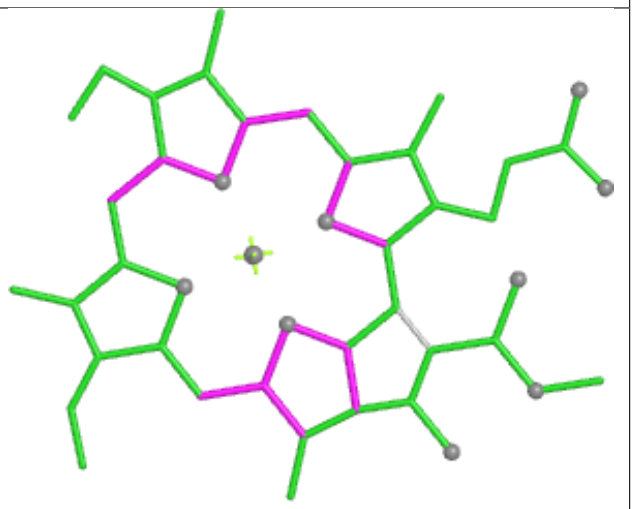


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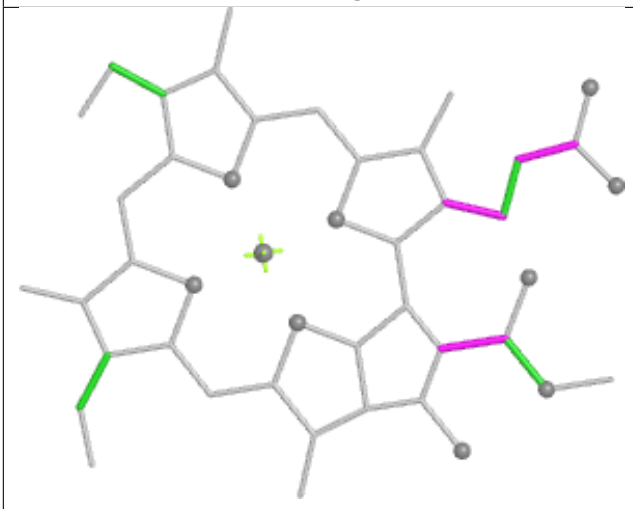
Ligand CLA R 306



Bond lengths



Bond angles

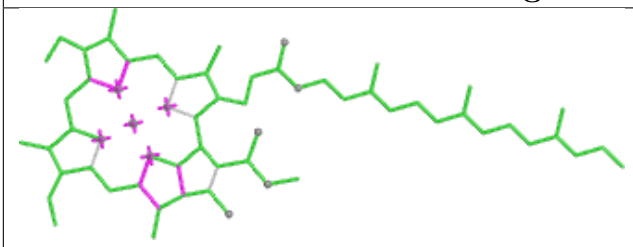


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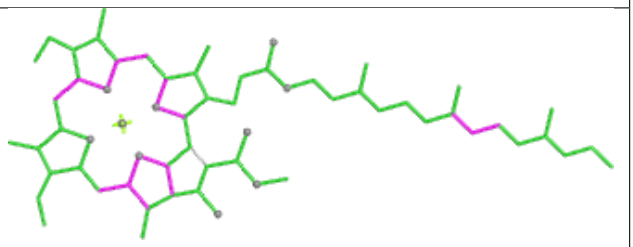


Rings

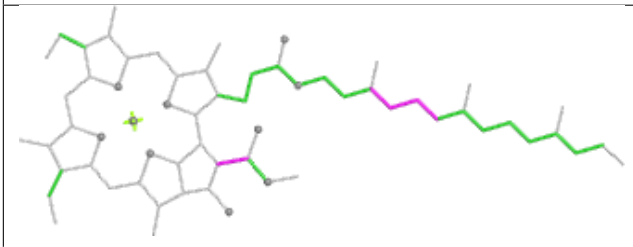
Ligand CLA O 309



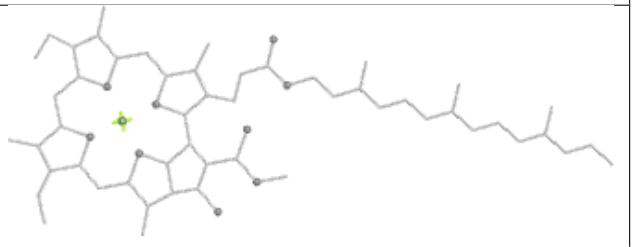
Bond lengths



Bond angles

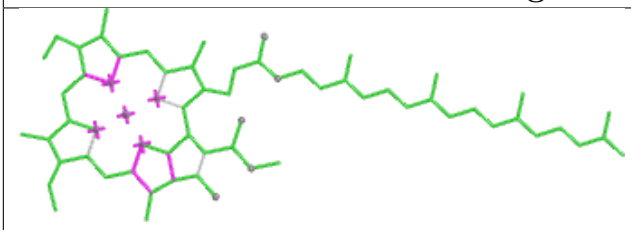


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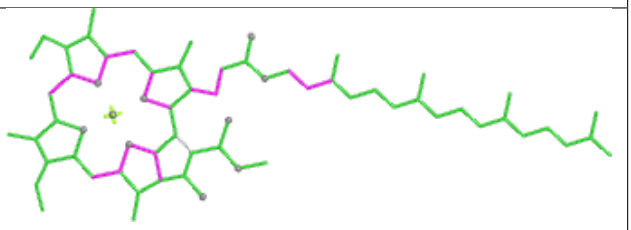


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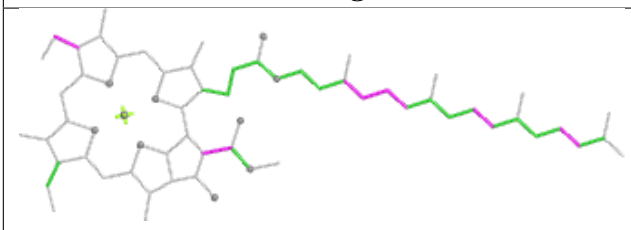
Ligand CLA b 823



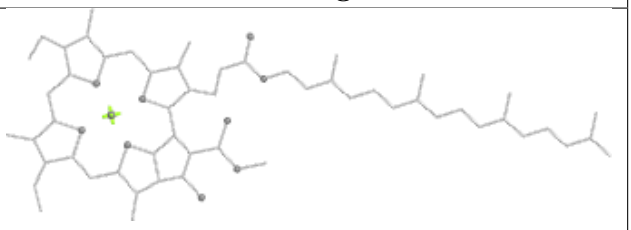
Bond lengths



Bond angles

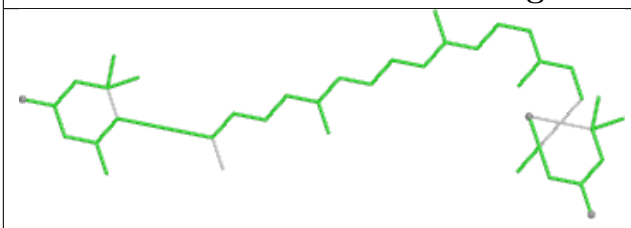


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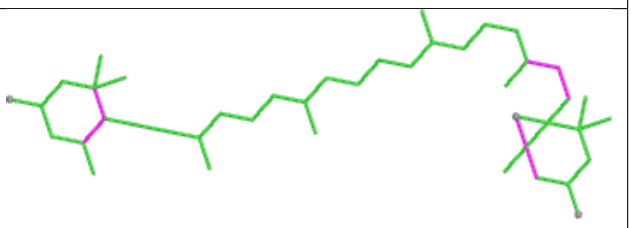


Rings

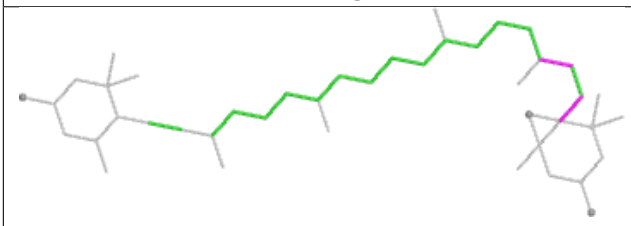
Ligand DD6 F 315



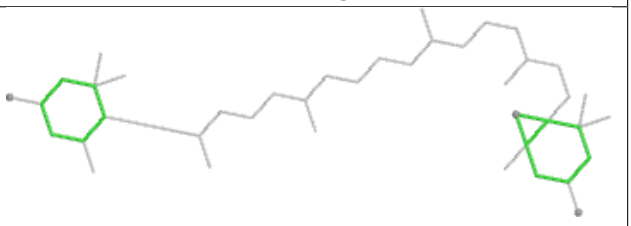
Bond lengths



Bond angles

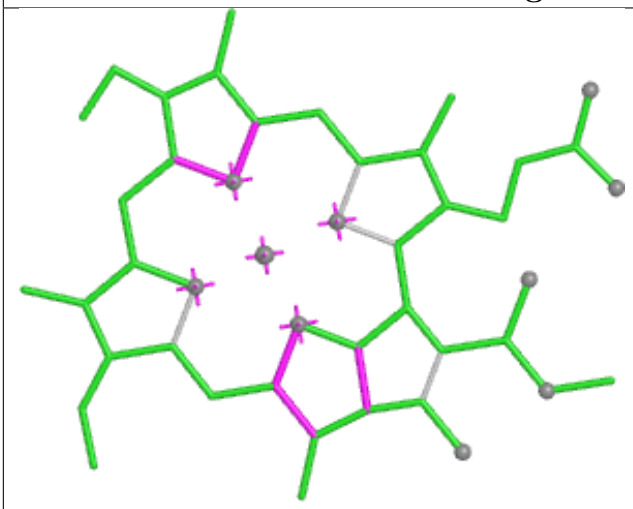


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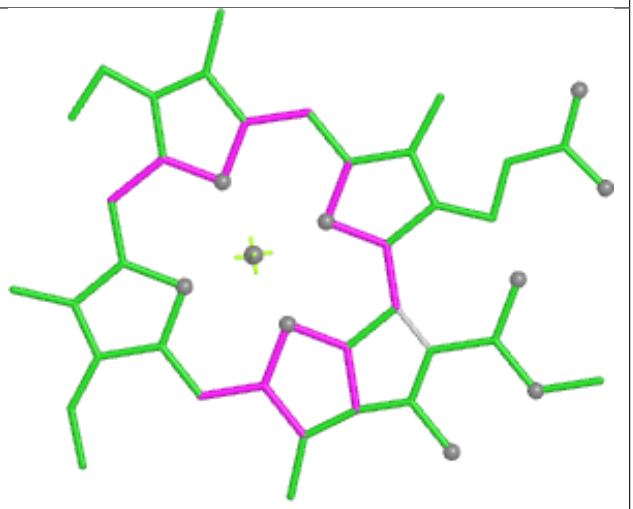


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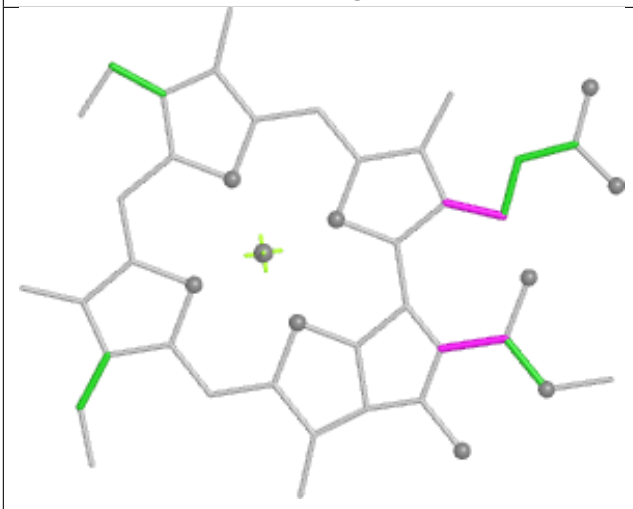
Ligand CLA E 311



Bond lengths



Bond angles

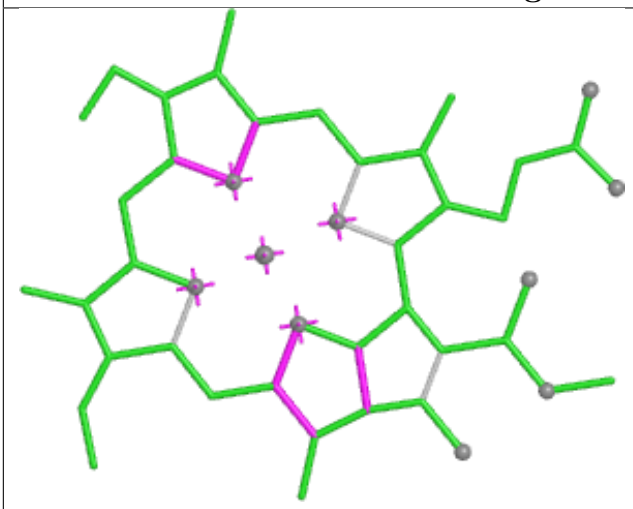


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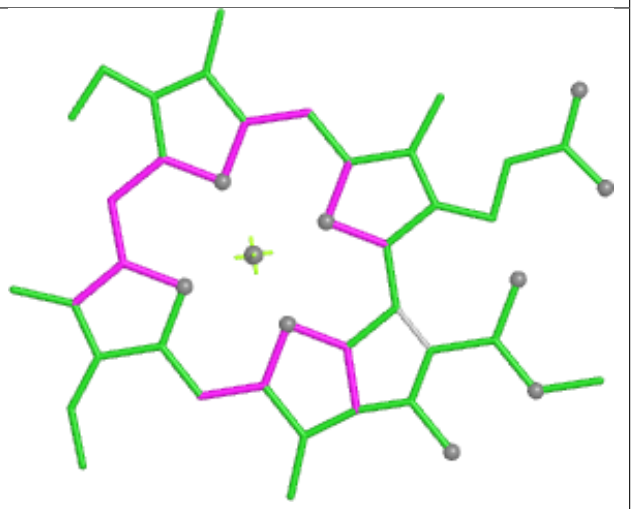


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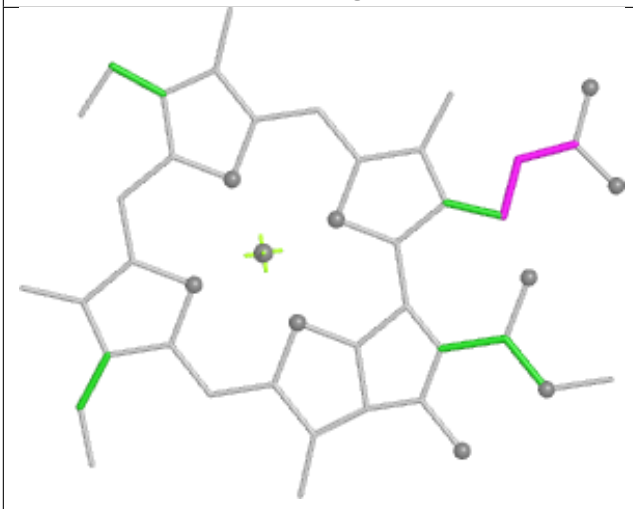
Ligand CLA C 301



Bond lengths



Bond angles

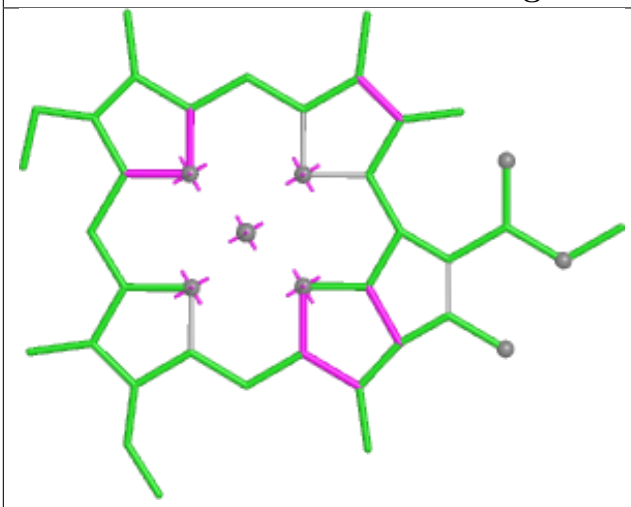


Torsions

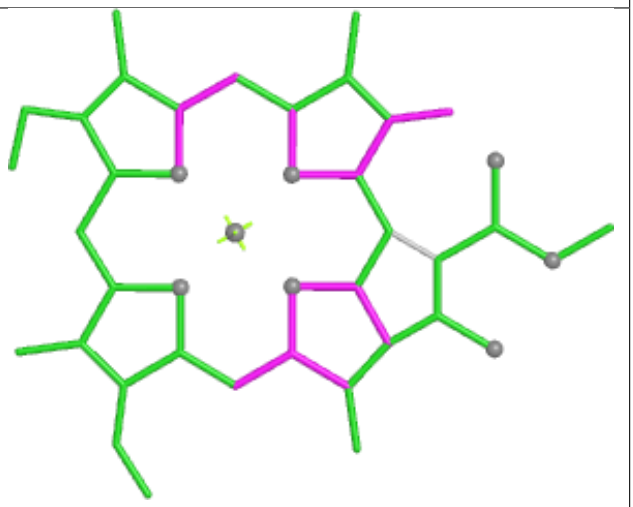


Rings

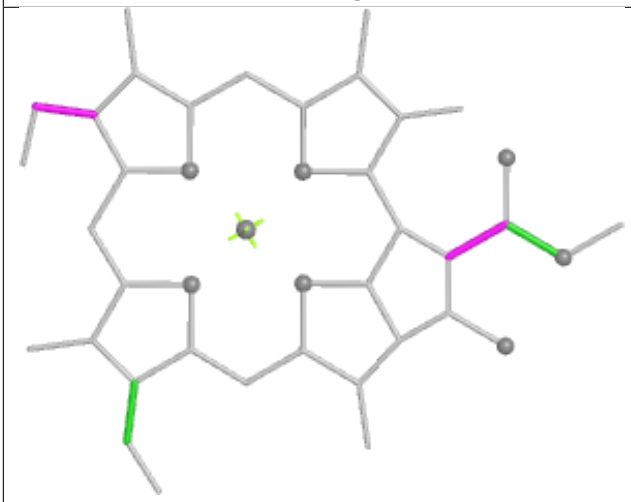
Ligand CLA N 312



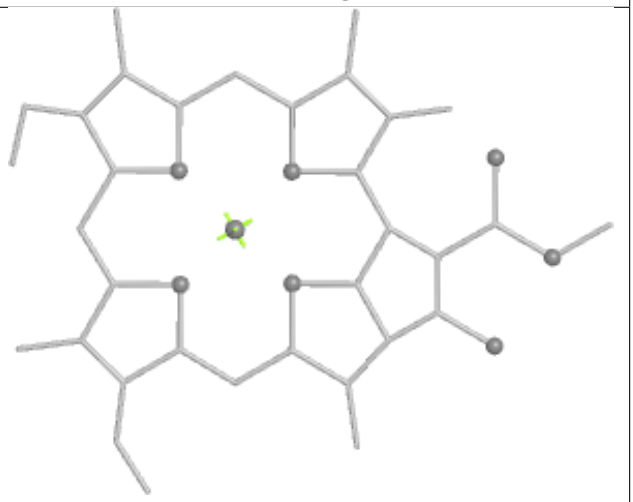
Bond lengths



Bond angles

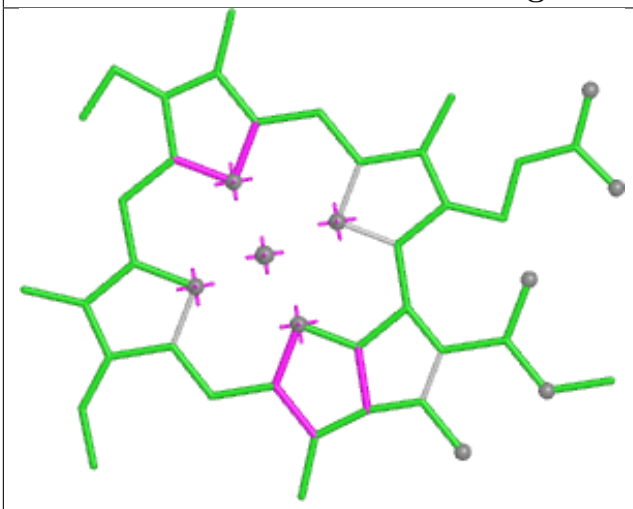


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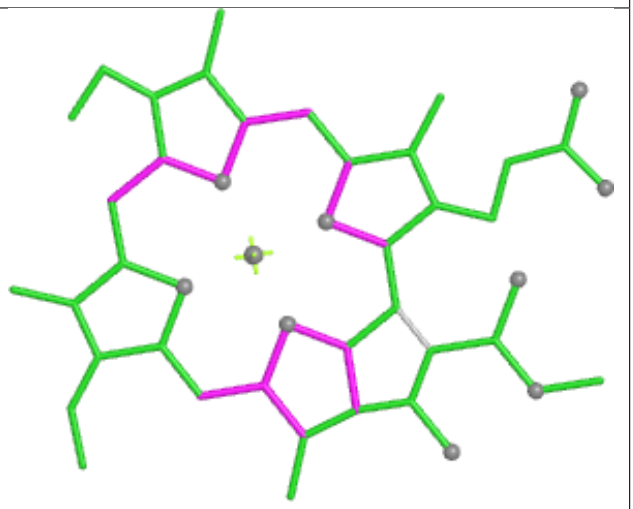


Rings

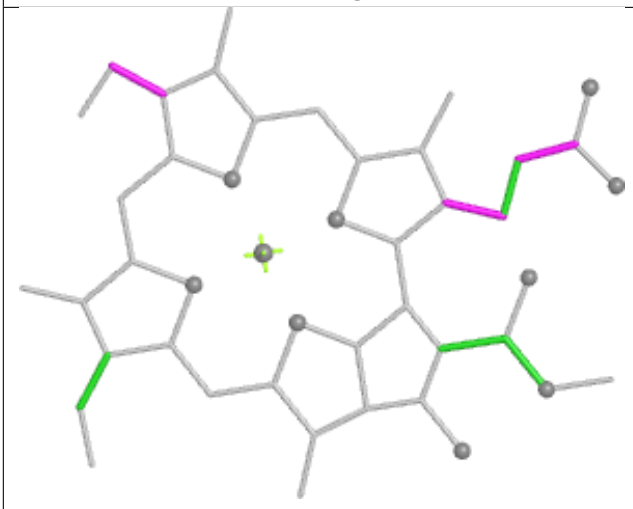
Ligand CLA S 313



Bond lengths



Bond angles

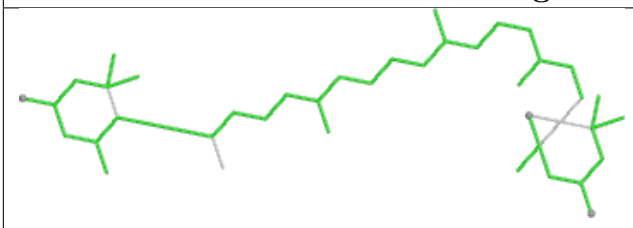


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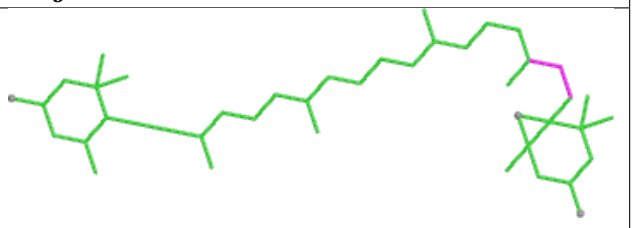


Rings

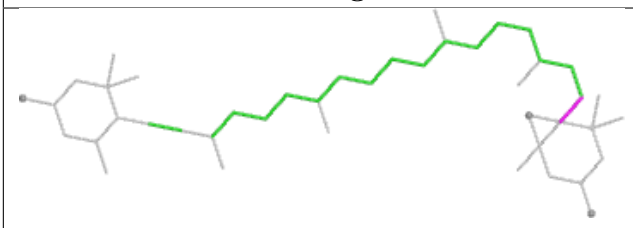
Ligand DD6 j 103



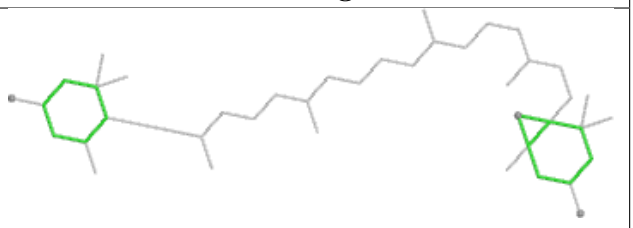
Bond lengths



Bond angles

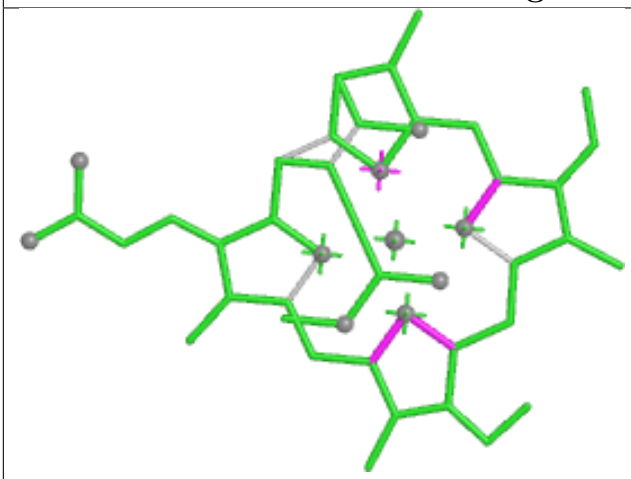


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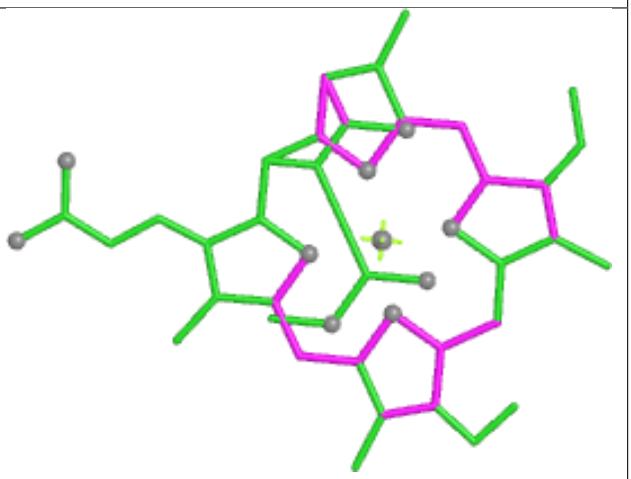


Rings

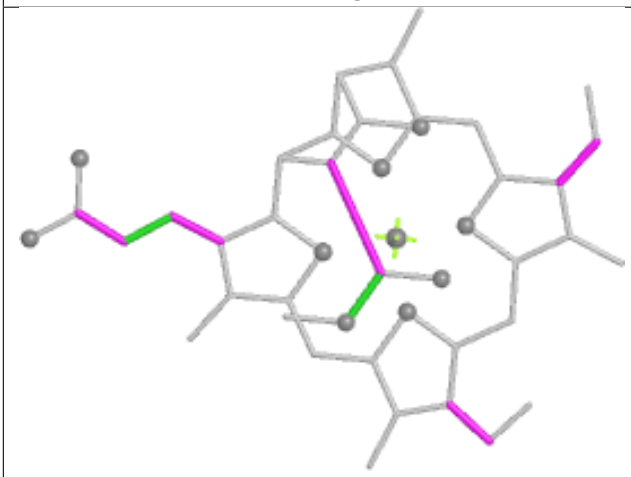
Ligand KC2 T 303



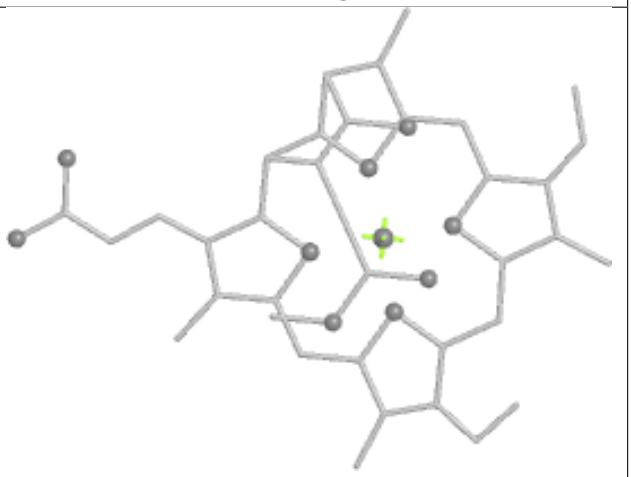
Bond lengths



Bond angles

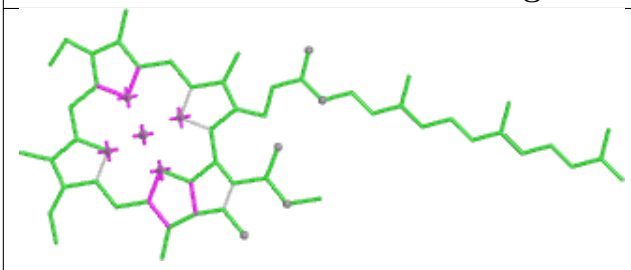


Torsions

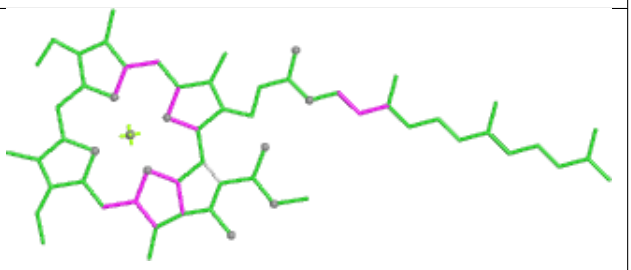


Rings

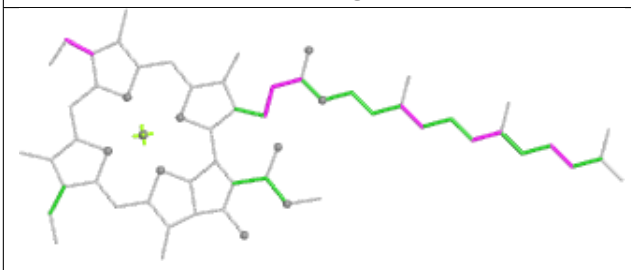
Ligand CLA D 304



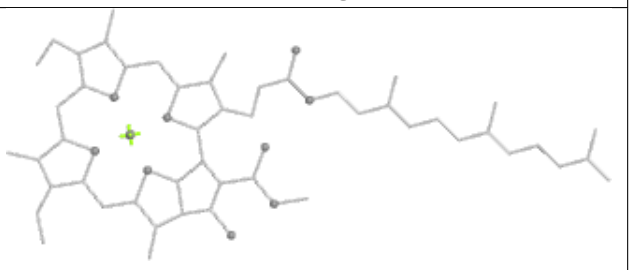
Bond lengths



Bond angles

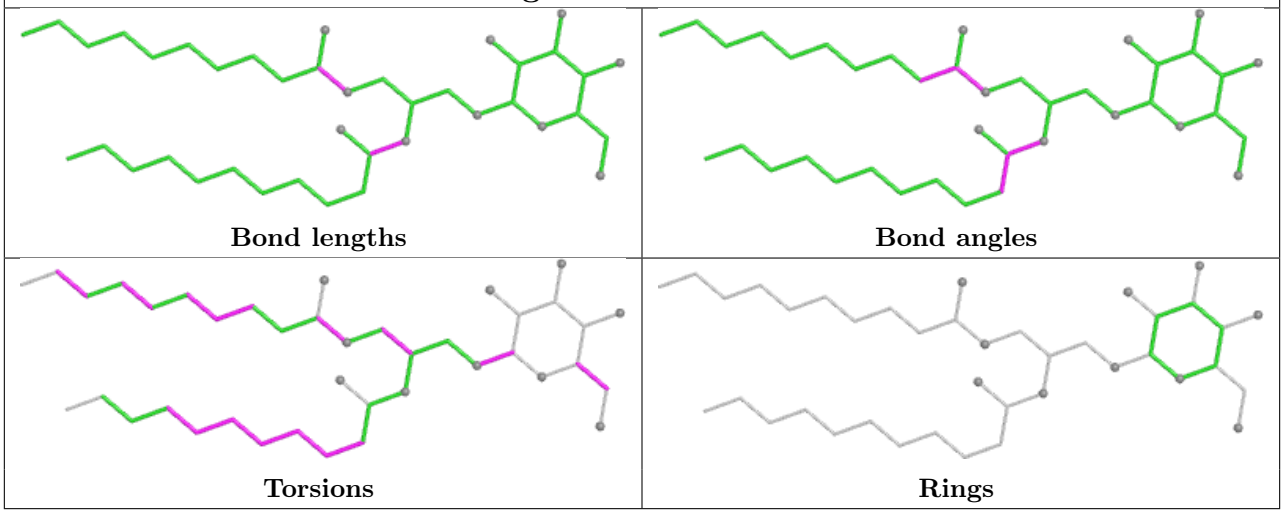


Torsions

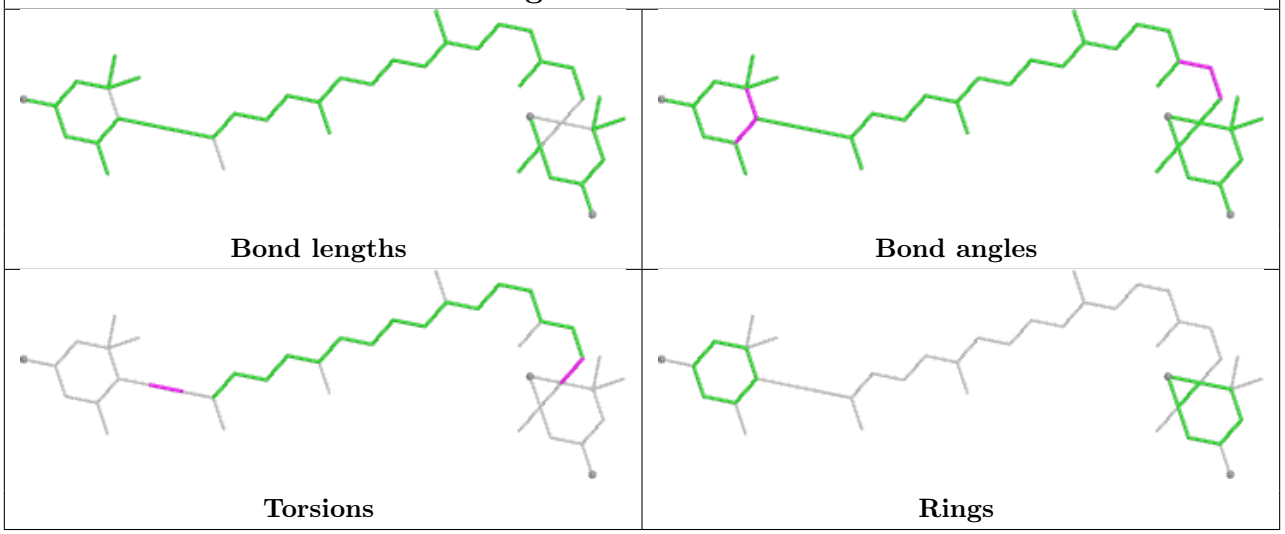


Rings

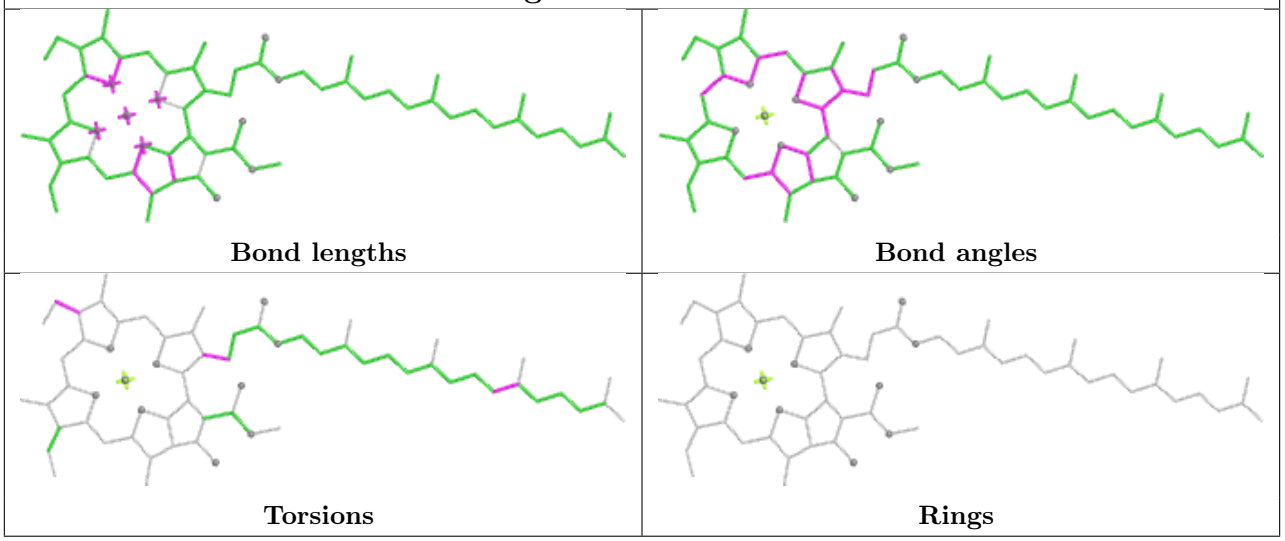
Ligand LMG F 319



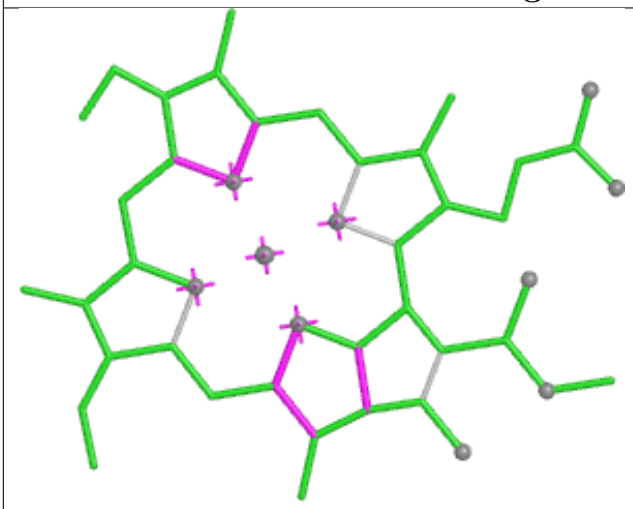
Ligand DD6 D 301



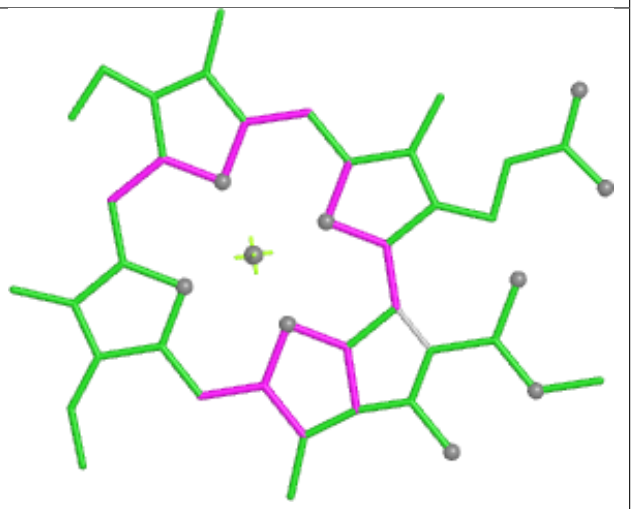
Ligand CLA D 310



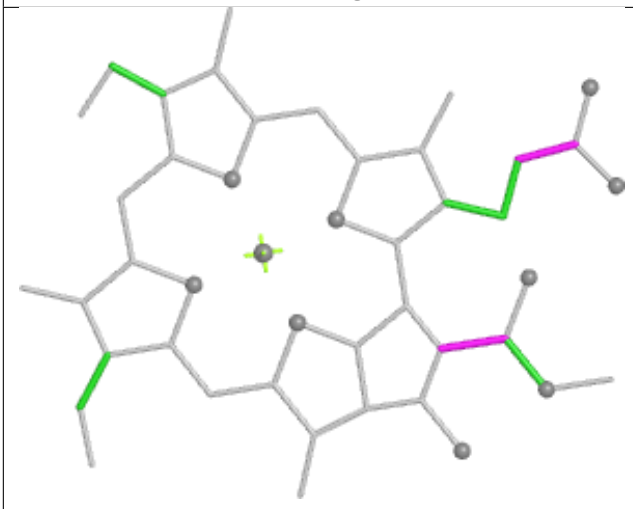
Ligand CLA O 306



Bond lengths



Bond angles

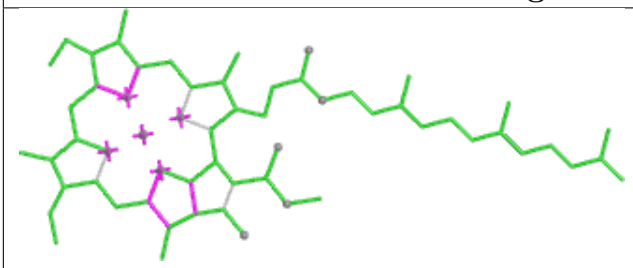


Torsions

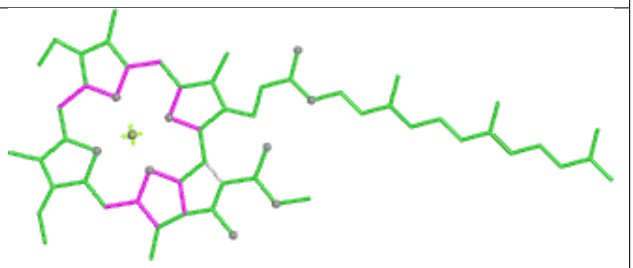


Rings

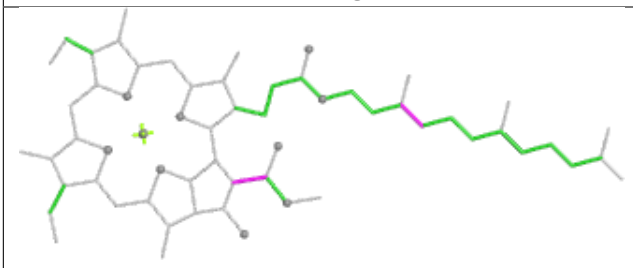
Ligand CLA b 834



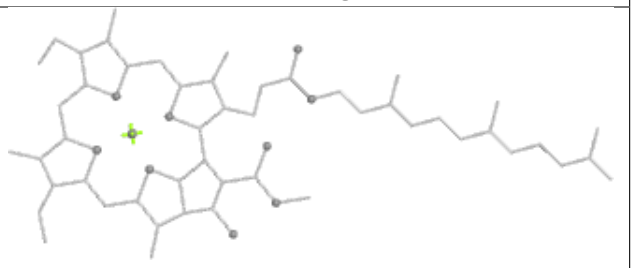
Bond lengths



Bond angles

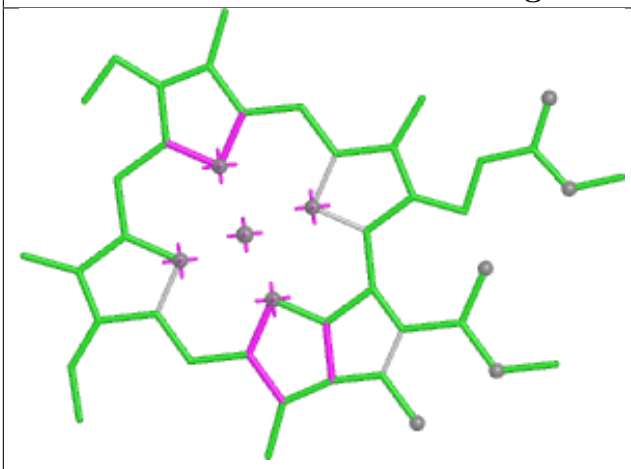


Torsions

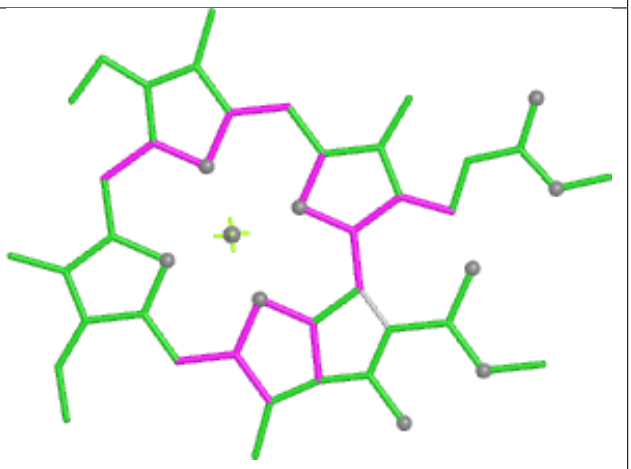


Rings

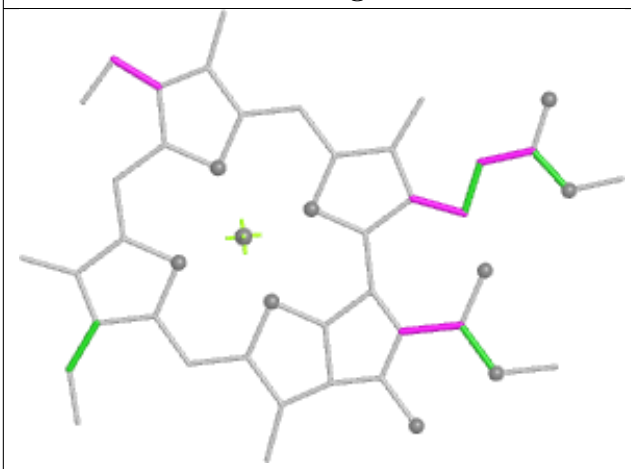
Ligand CLA B 304



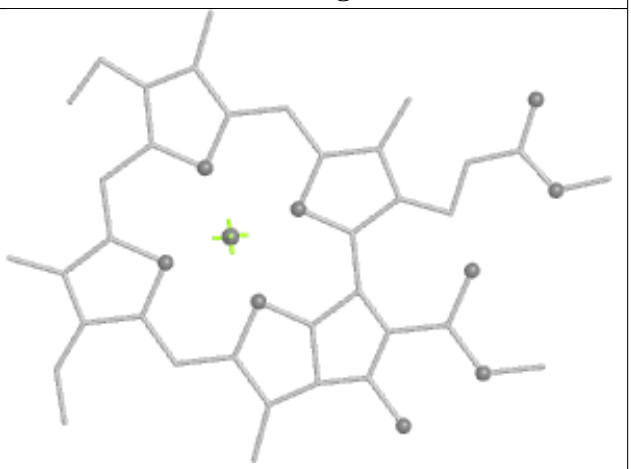
Bond lengths



Bond angles

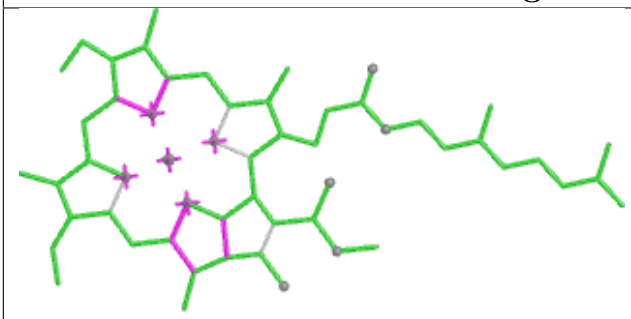


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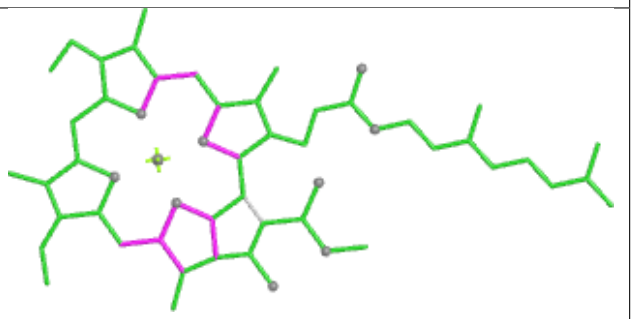


Rings

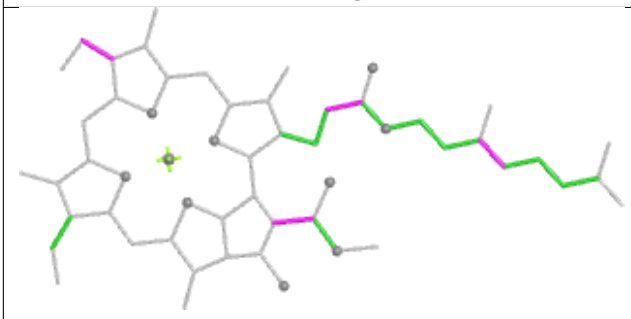
Ligand CLA N 310



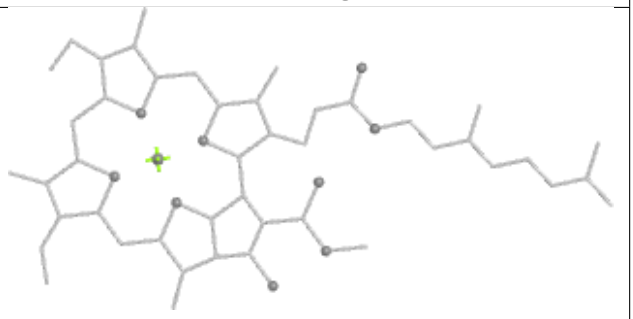
Bond lengths



Bond angles

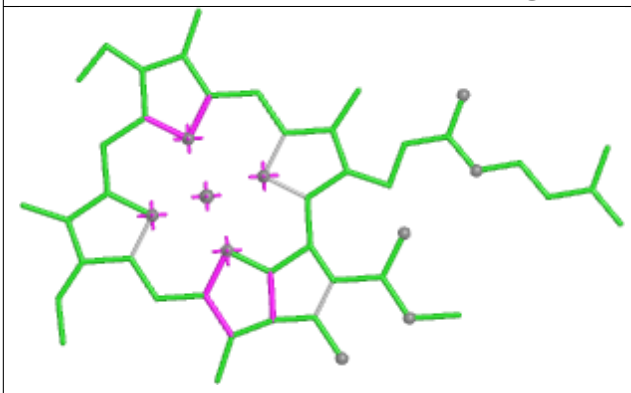


Torsions

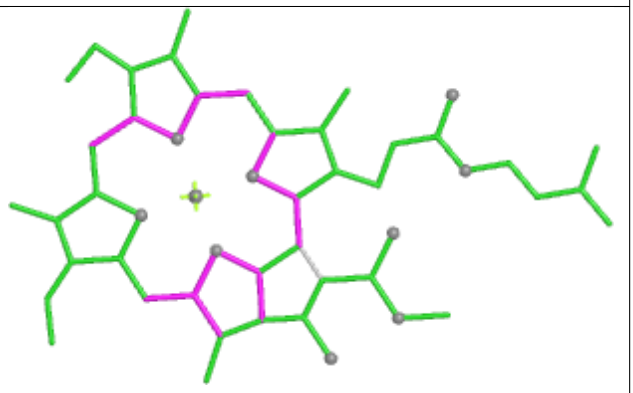


Rings

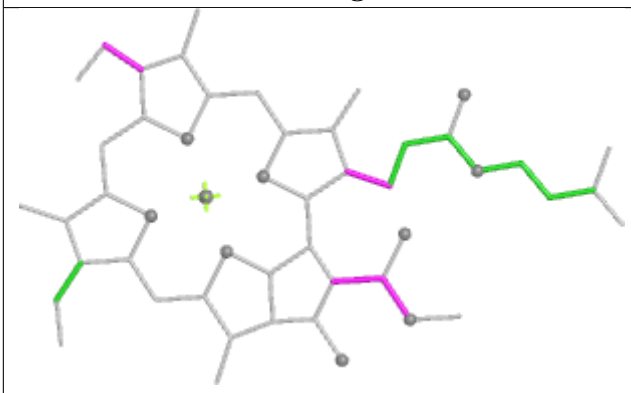
Ligand CLA N 305



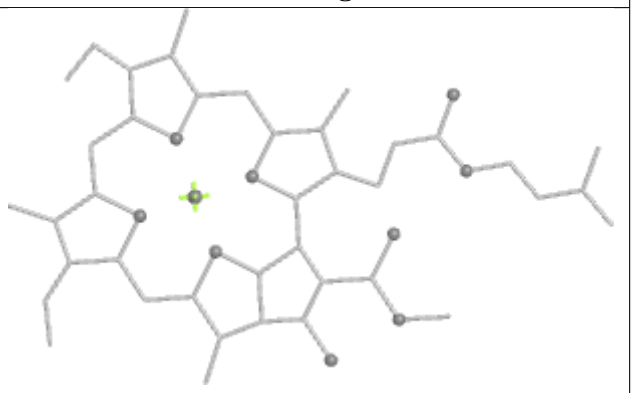
Bond lengths



Bond angles

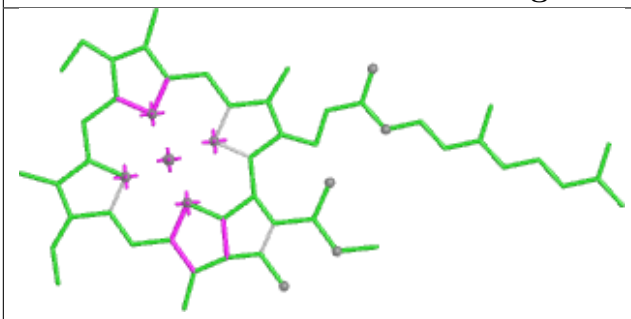


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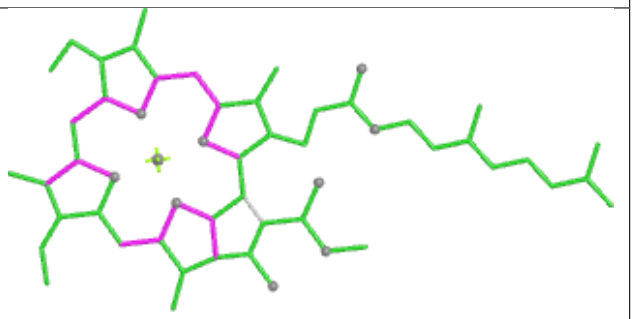


Rings

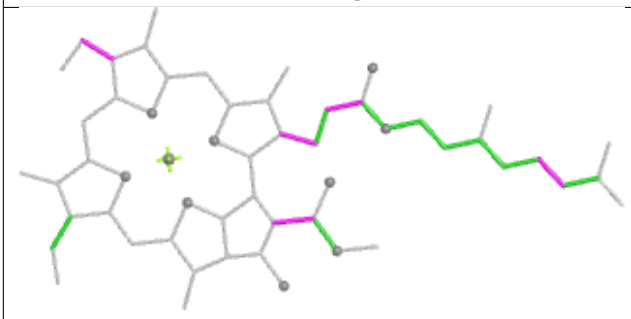
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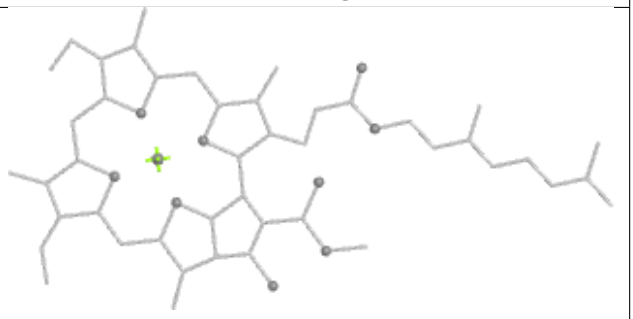
Bond lengths



Bond angles

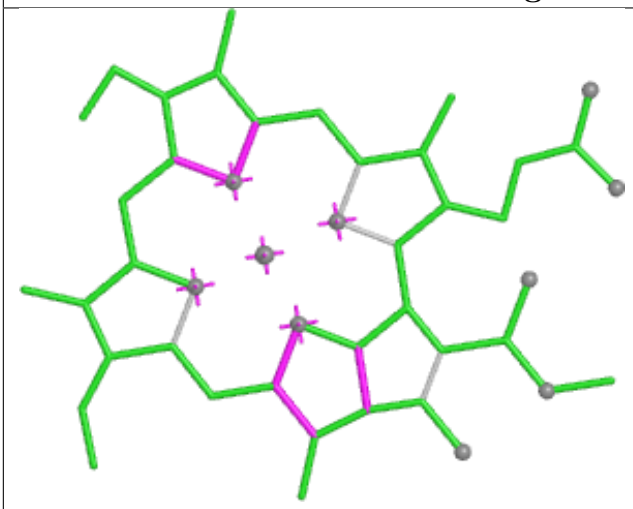


Torsions

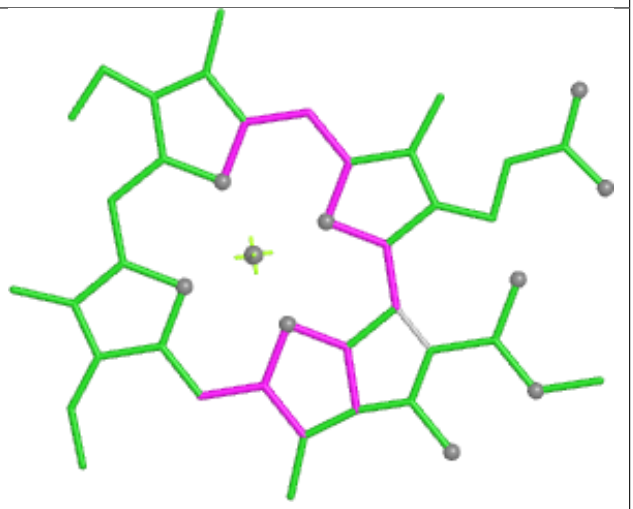


Rings

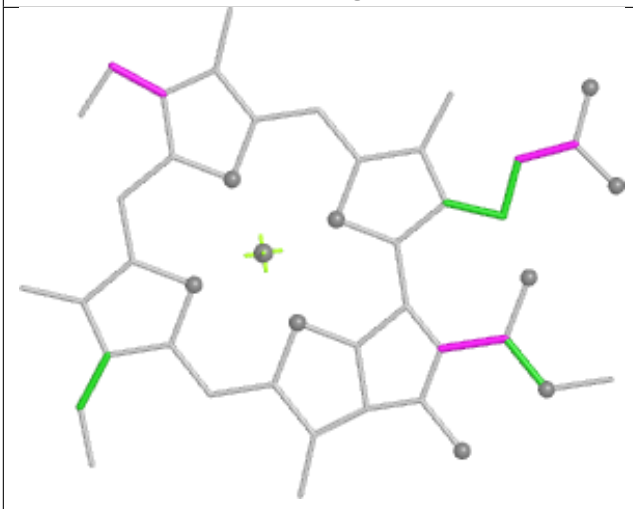
Ligand CLA B 302



Bond lengths



Bond angles

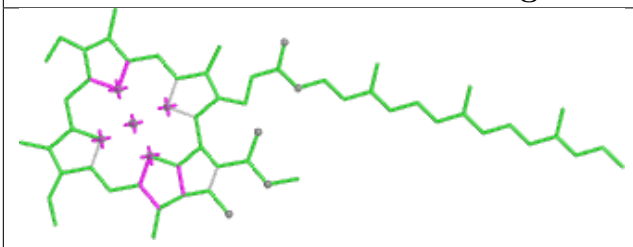


Torsions

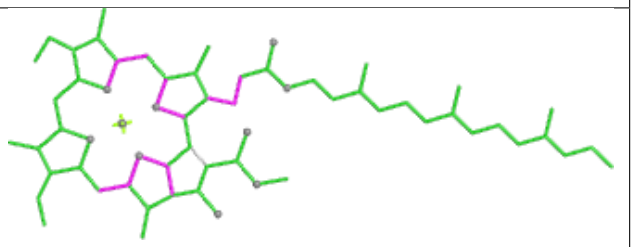


Rings

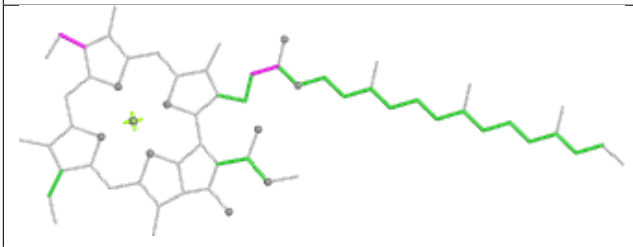
Ligand CLA M 310



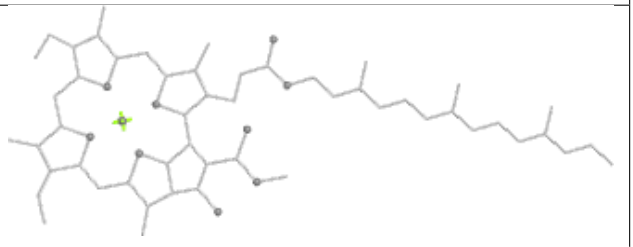
Bond lengths



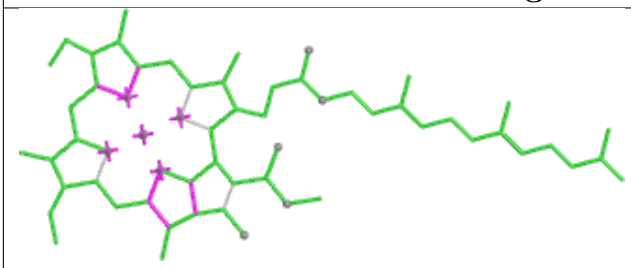
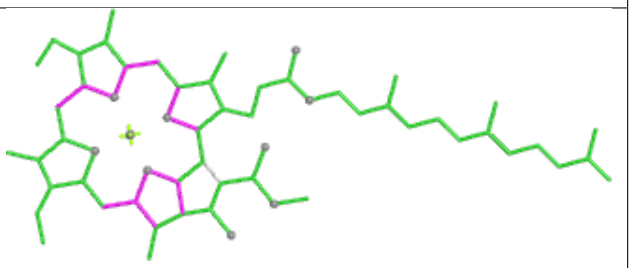
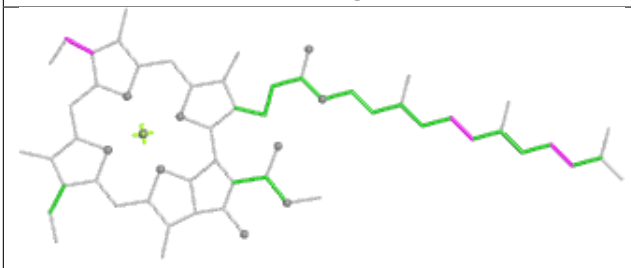
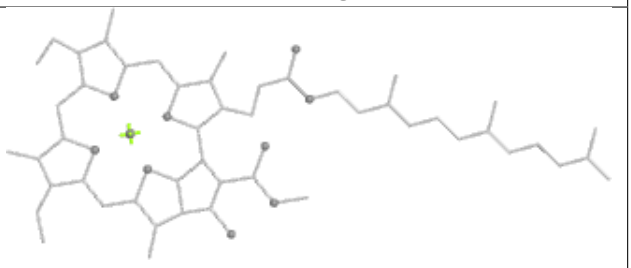
Bond angles

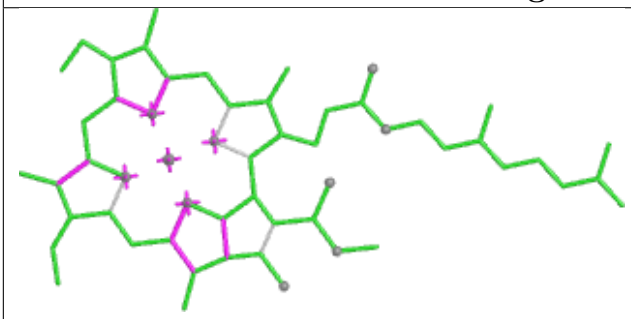
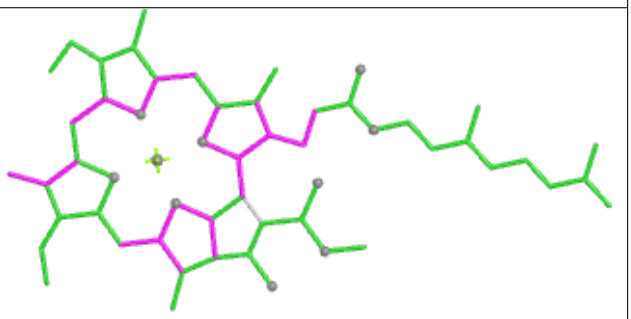
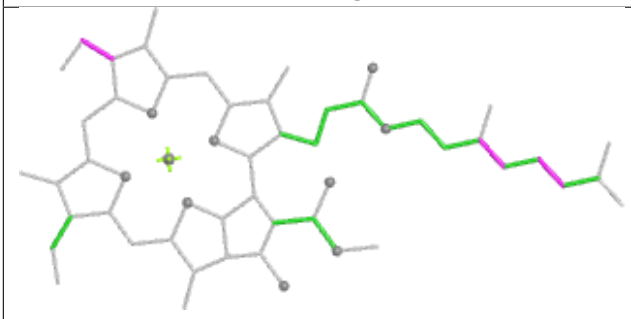
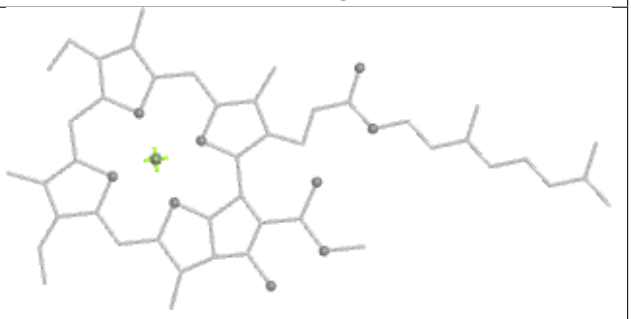


Torsions

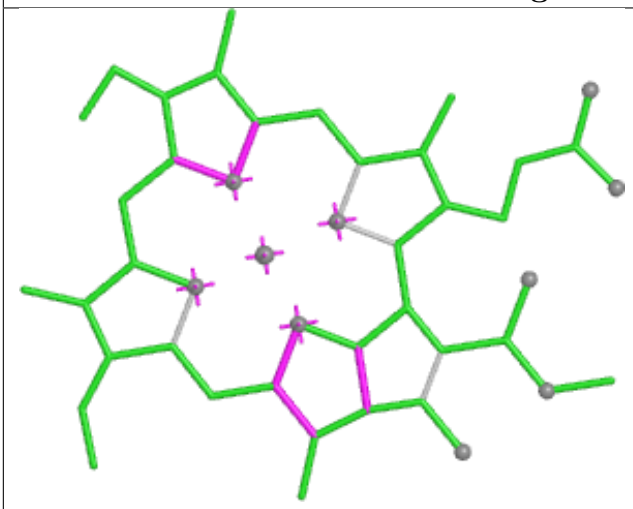


Rings

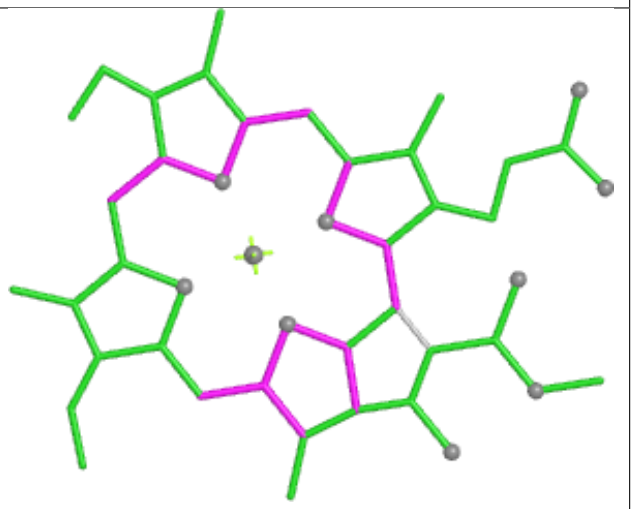
Ligand CLA E 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA J 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

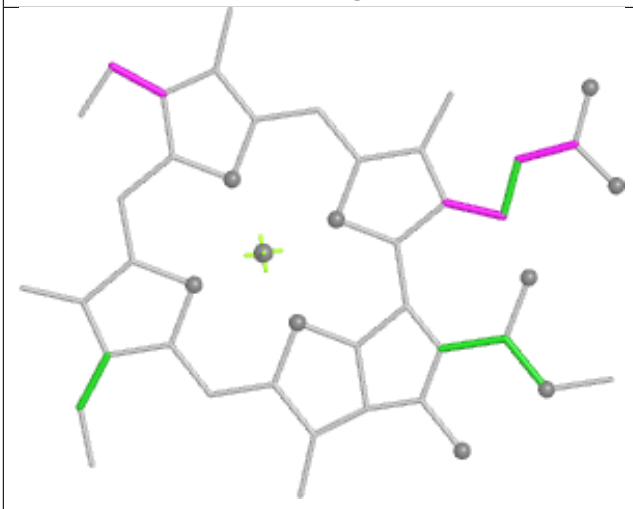
Ligand CLA I 304



Bond lengths



Bond angles

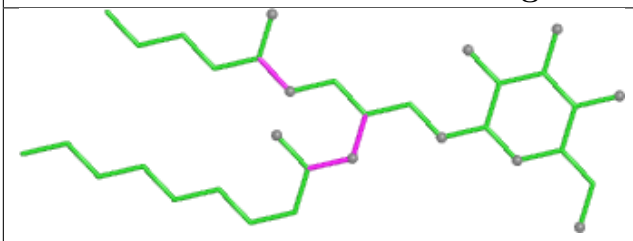


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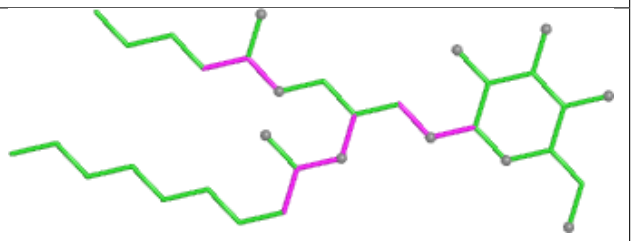


Rings

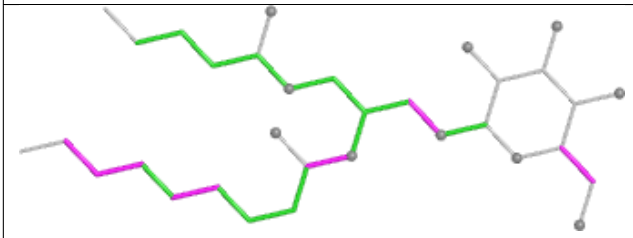
Ligand LMG F 320



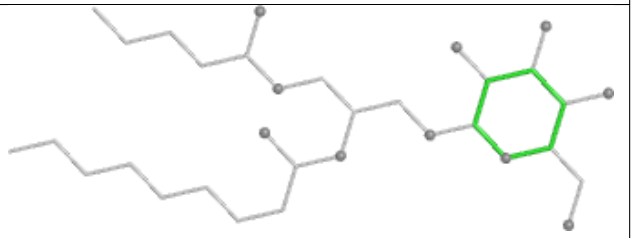
Bond lengths



Bond angles

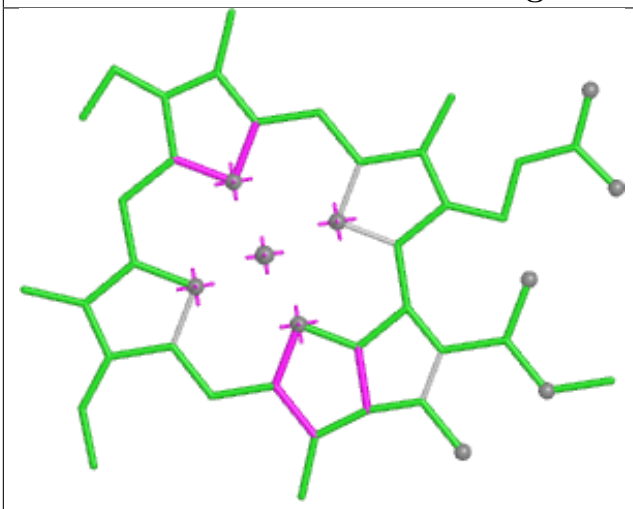


Torsions

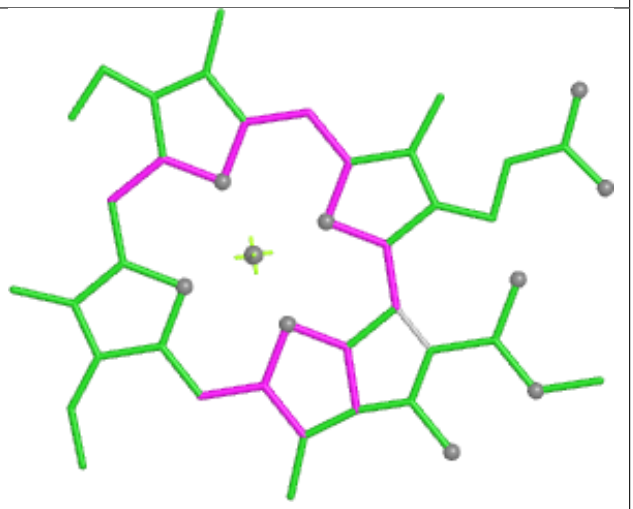


Rings

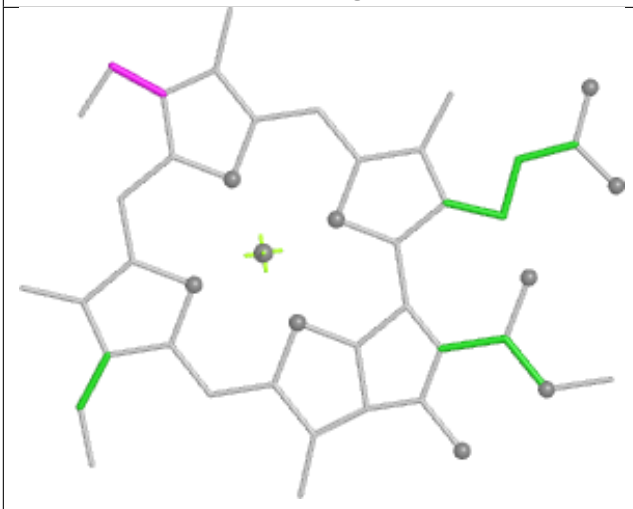
Ligand CLA L 304



Bond lengths



Bond angles

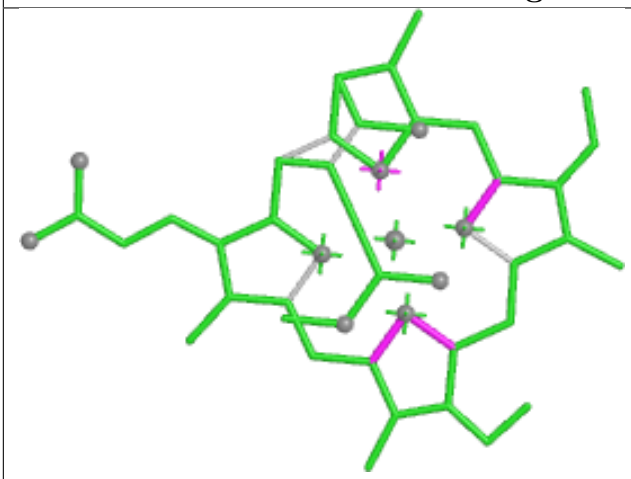


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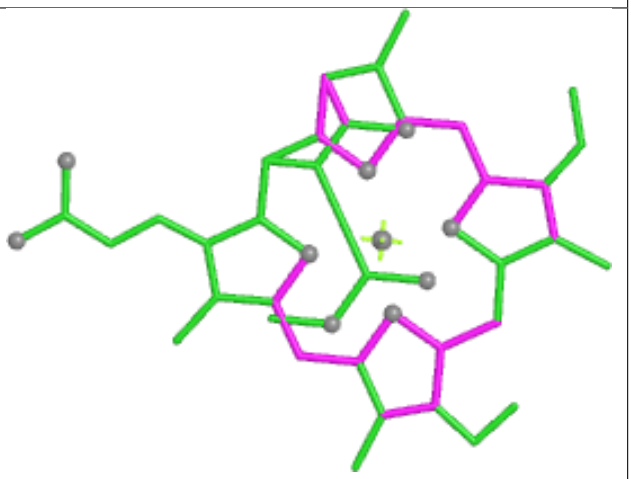


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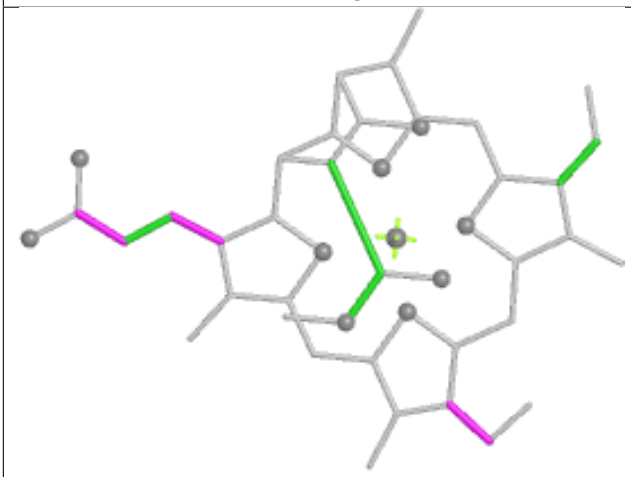
Ligand KC2 O 310



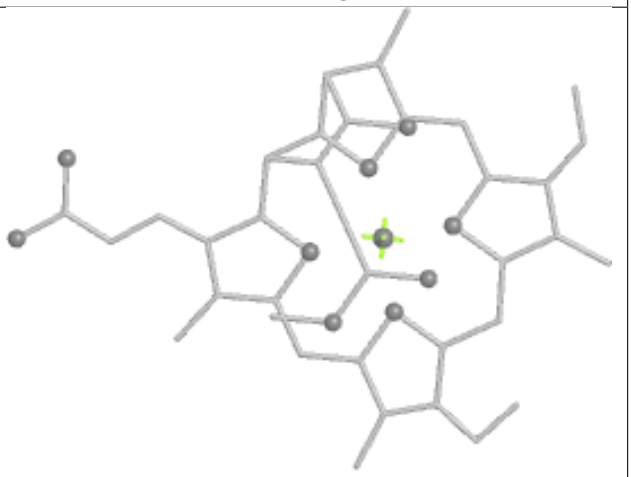
Bond lengths



Bond angles

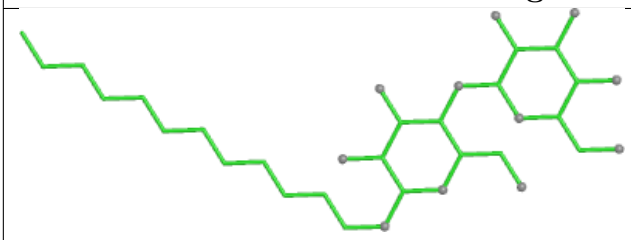


Torsions



Rings

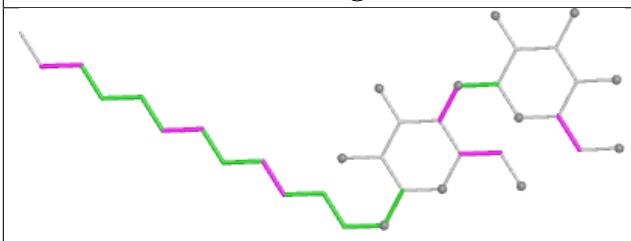
Ligand LMU I 315



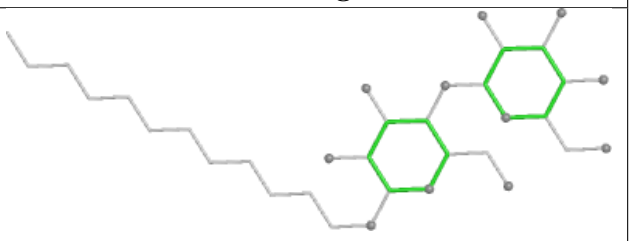
Bond lengths



Bond angles

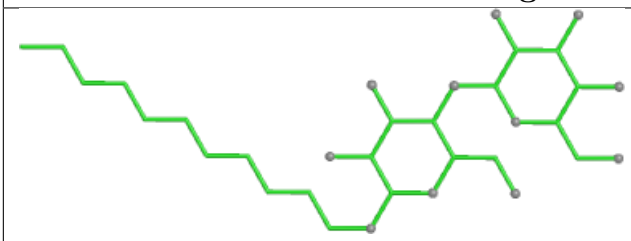


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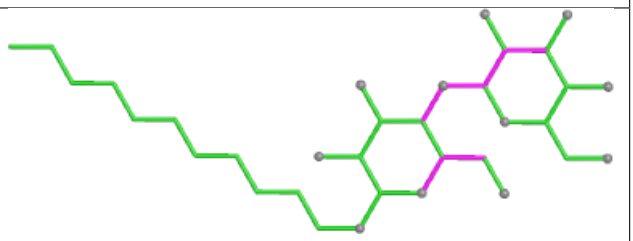


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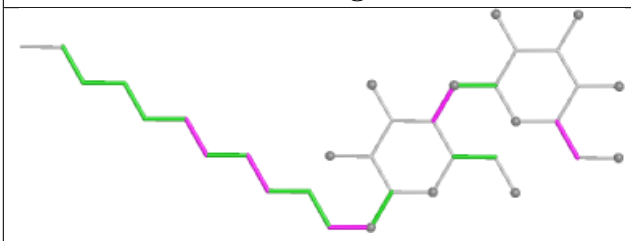
Ligand LMU V 205



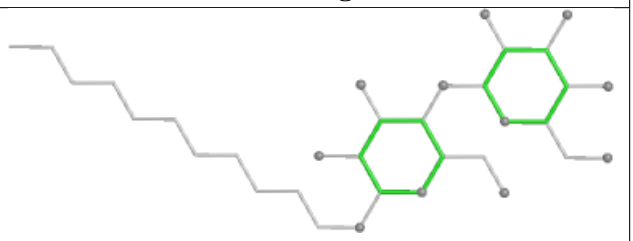
Bond lengths



Bond angles

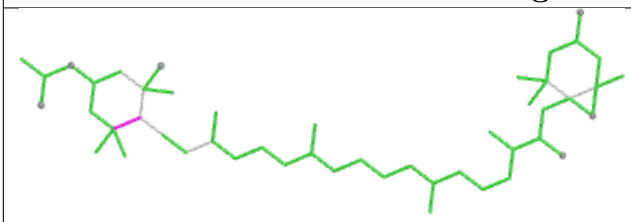


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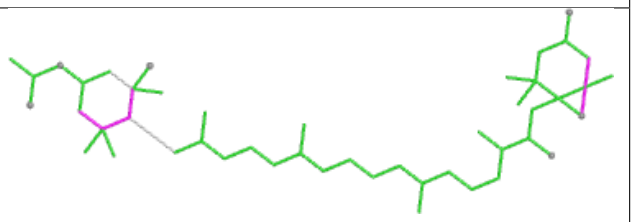


Rings

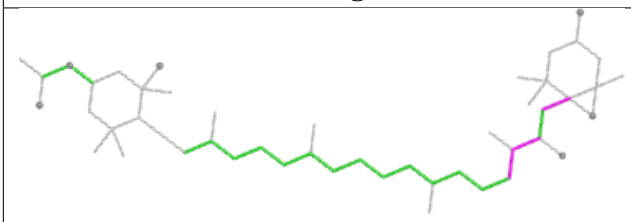
Ligand A86 F 313



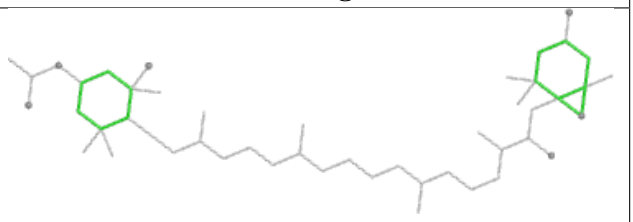
Bond lengths



Bond angles

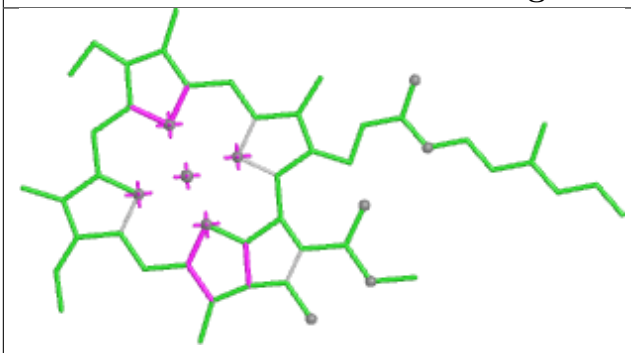


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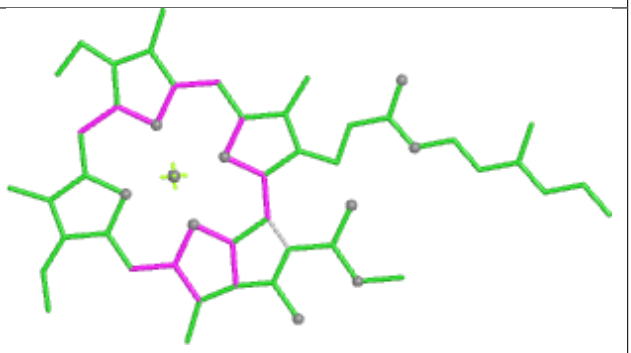


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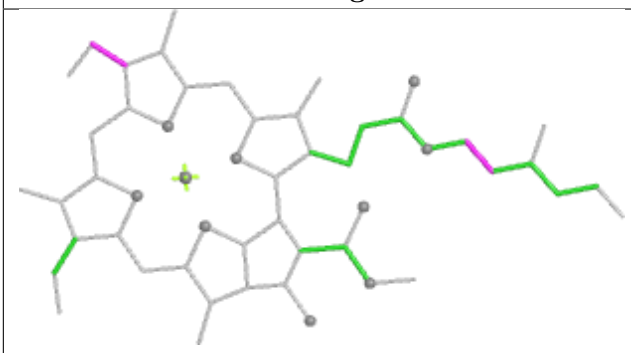
Ligand CLA J 305



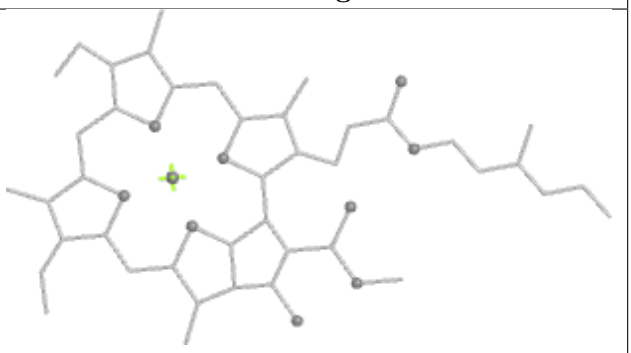
Bond lengths



Bond angles

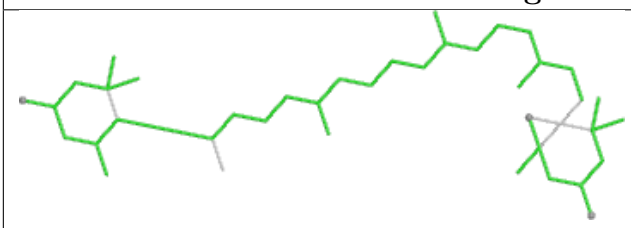


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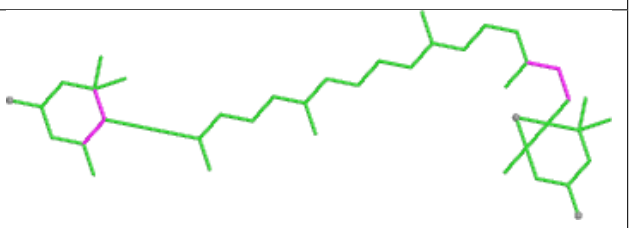


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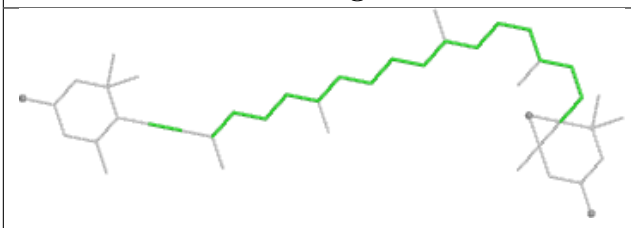
Ligand DD6 K 313



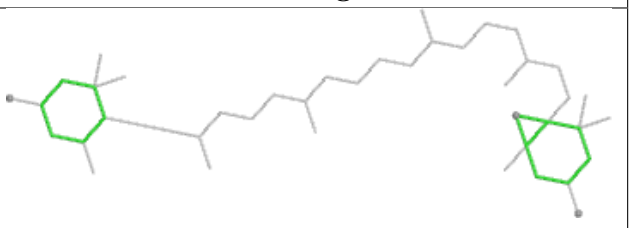
Bond lengths



Bond angles

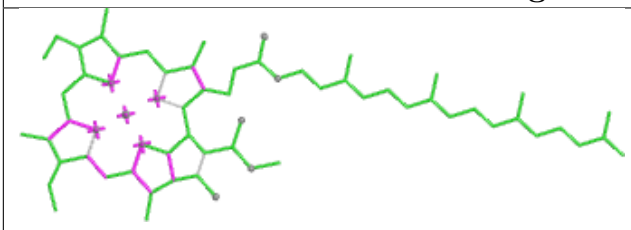


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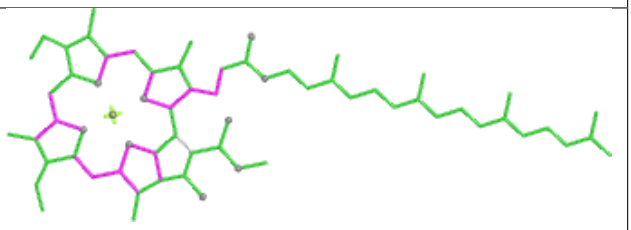


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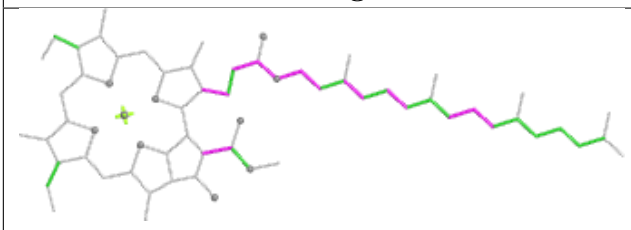
Ligand CLA a 805



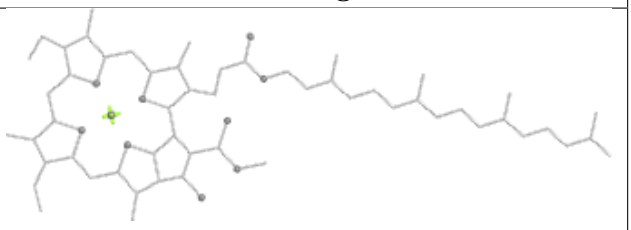
Bond lengths



Bond angles

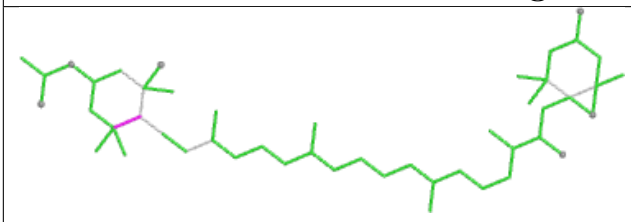


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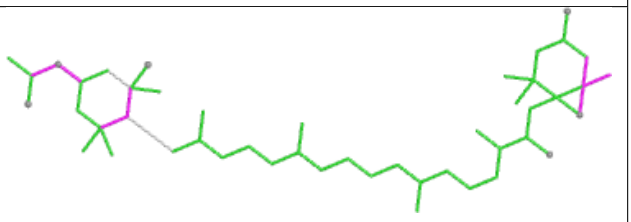


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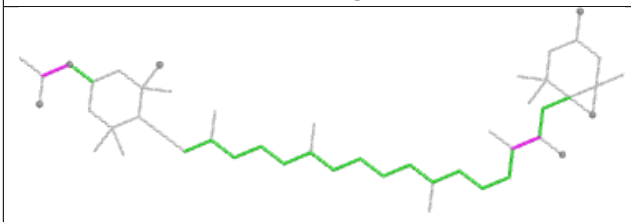
Ligand A86 K 314



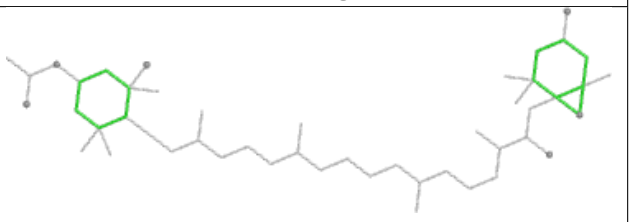
Bond lengths



Bond angles

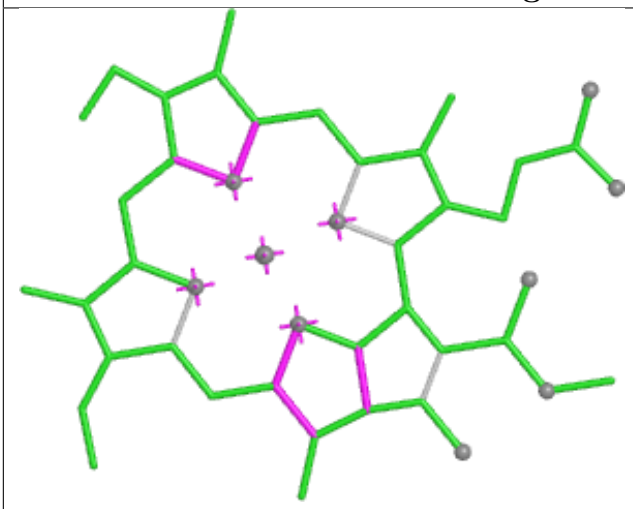


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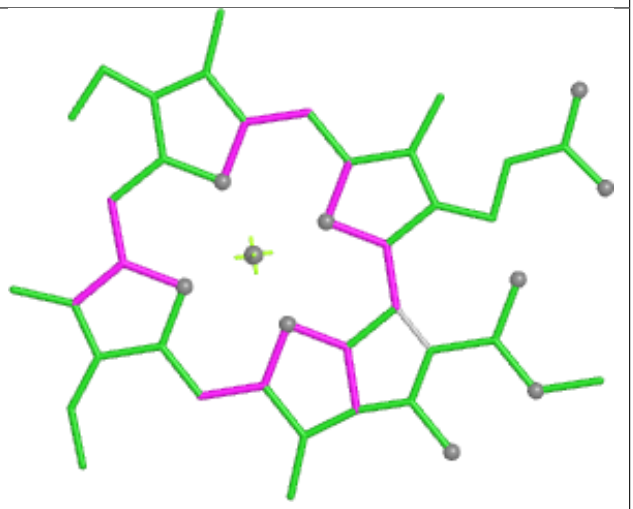


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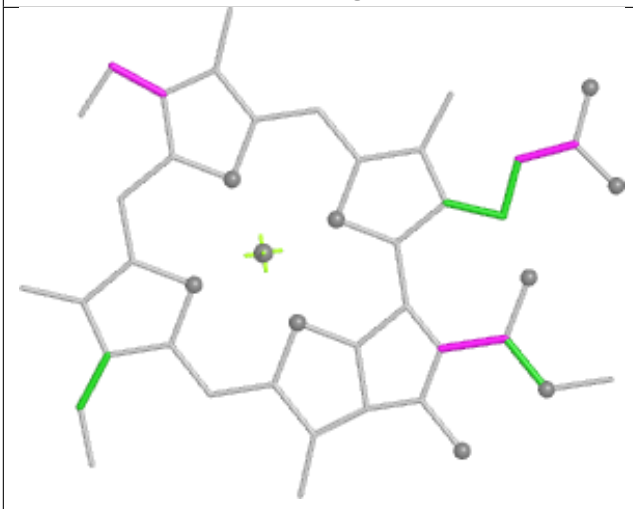
Ligand CLA G 305



Bond lengths



Bond angles

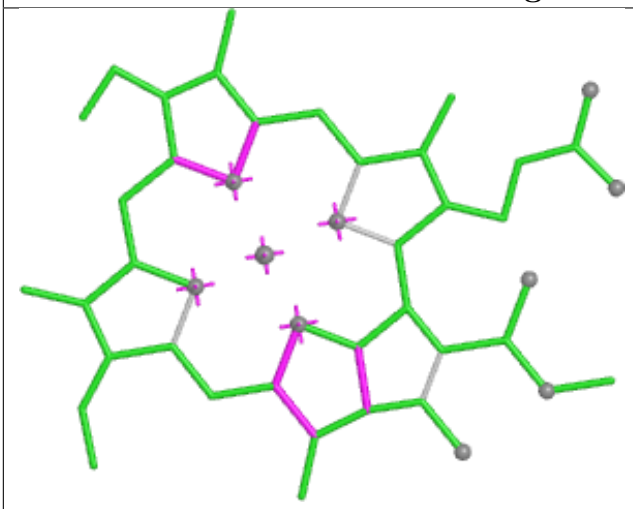


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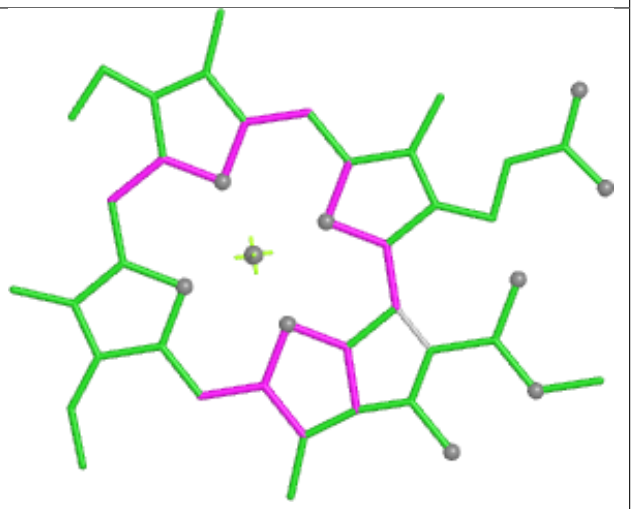


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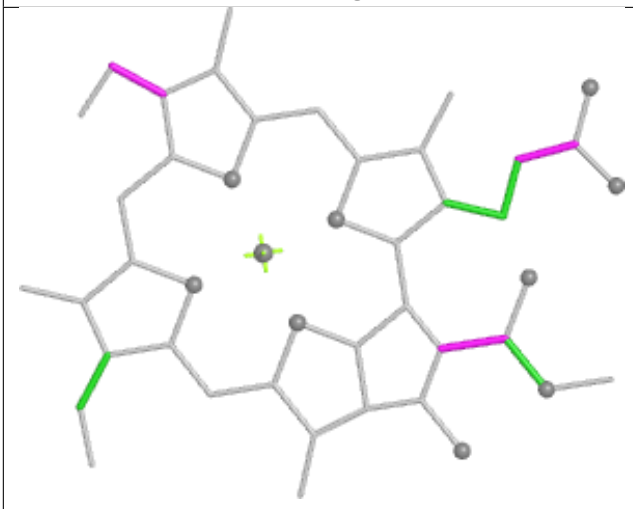
Ligand CLA B 305



Bond lengths



Bond angles

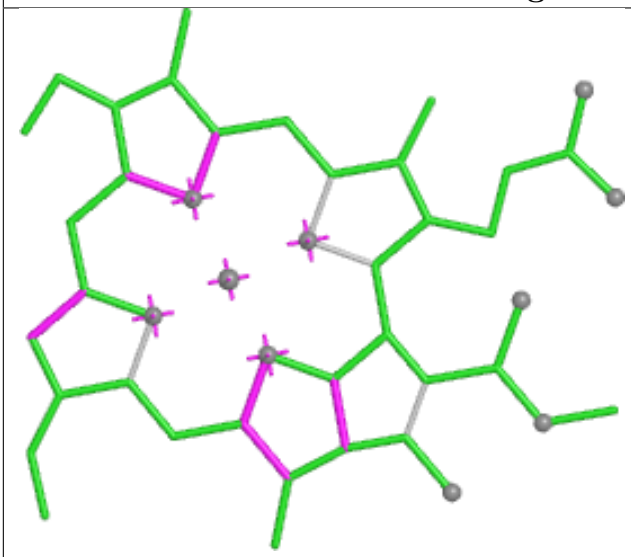


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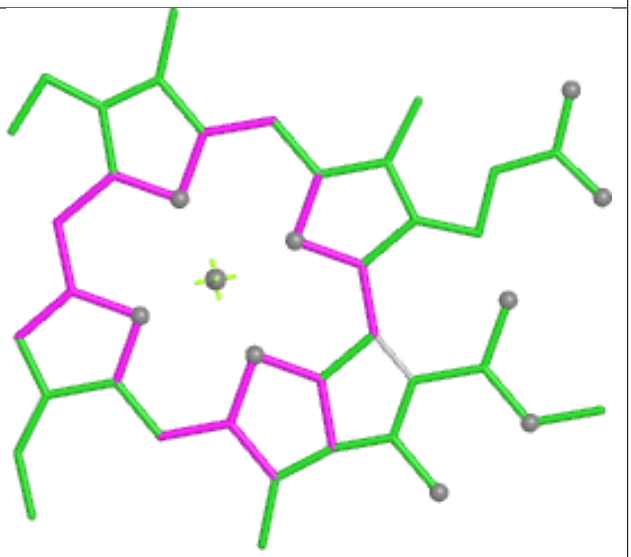


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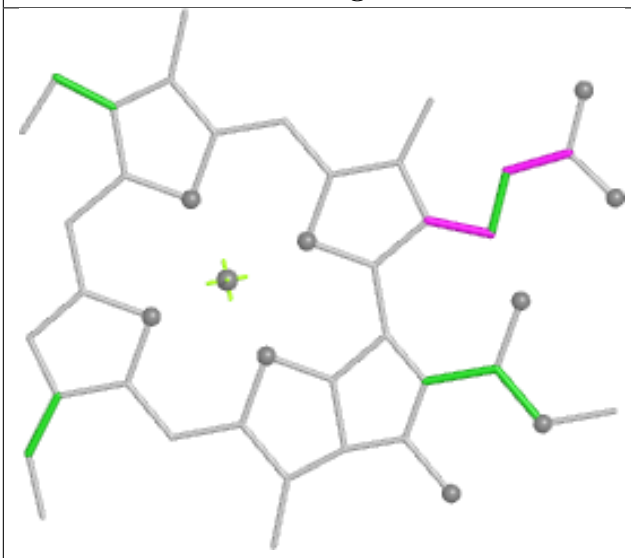
Ligand CLA S 308



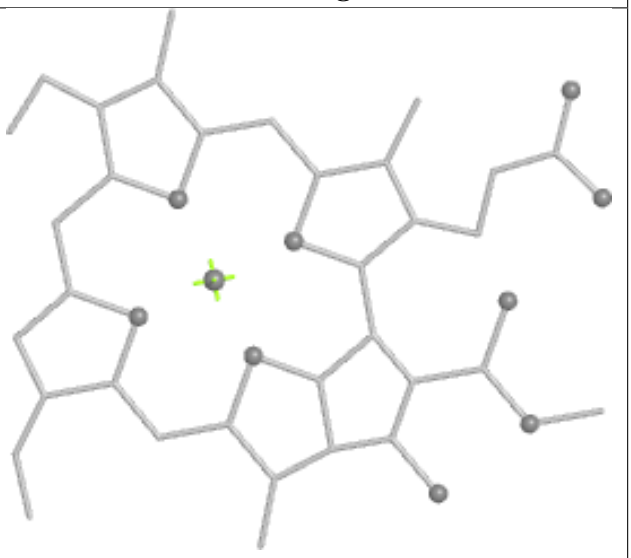
Bond lengths



Bond angles

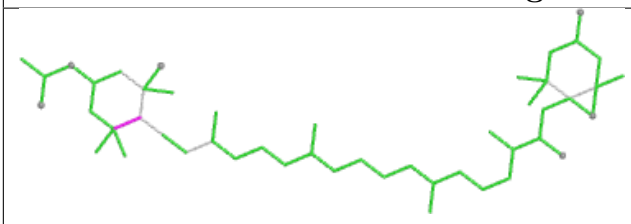


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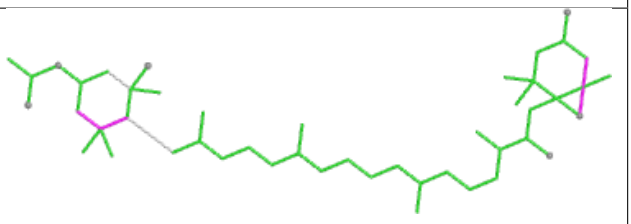


Rings

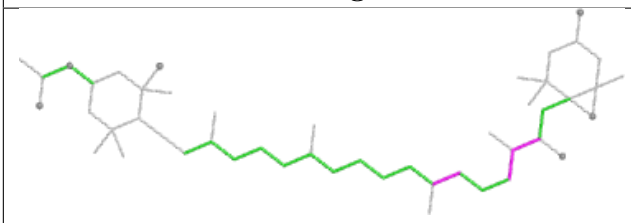
Ligand A86 M 301



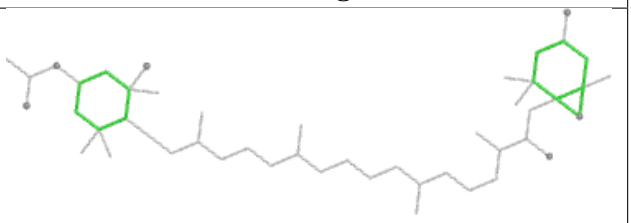
Bond lengths



Bond angles

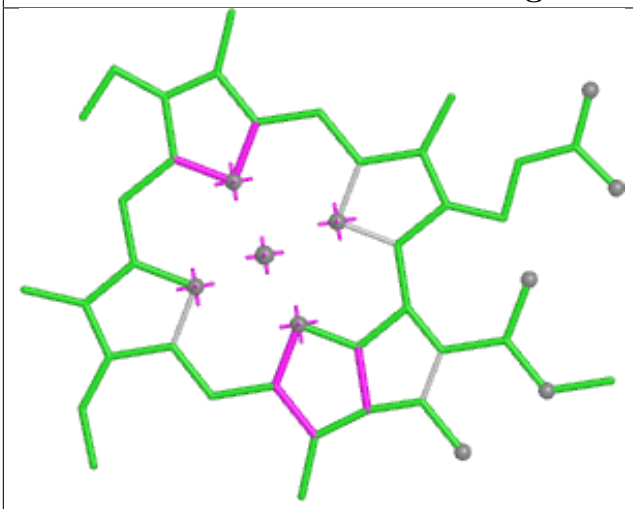


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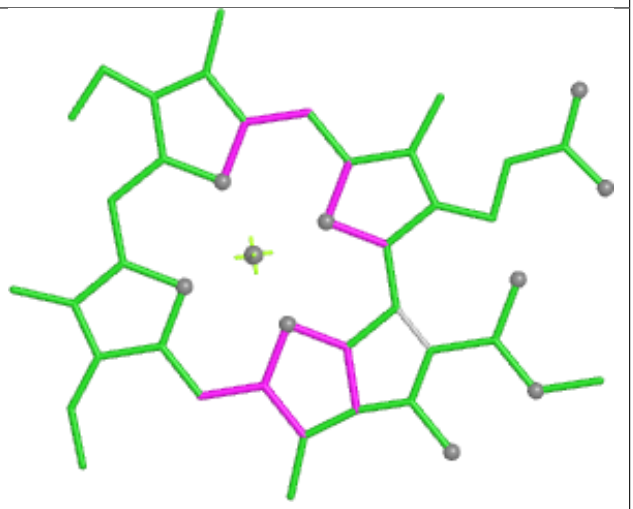


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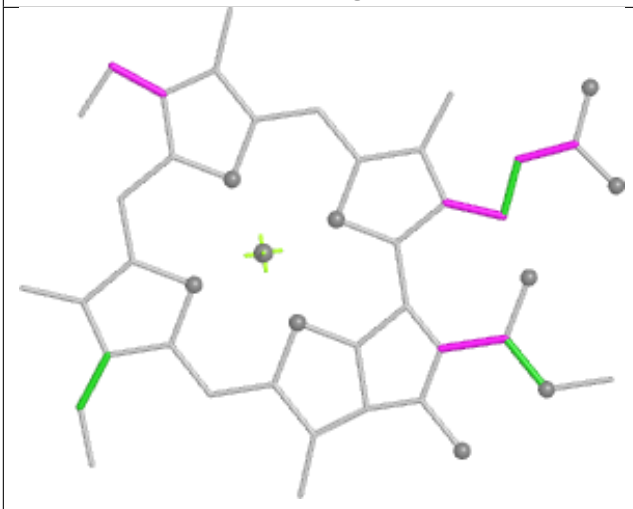
Ligand CLA E 310



Bond lengths



Bond angles

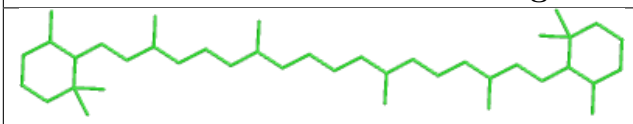


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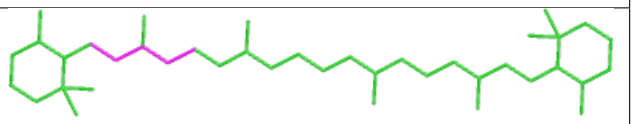


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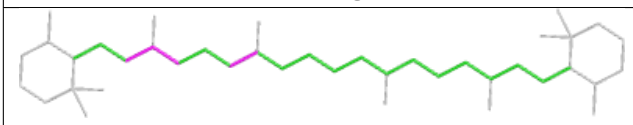
Ligand BCR l 206



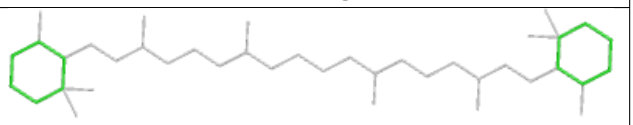
Bond lengths



Bond angles

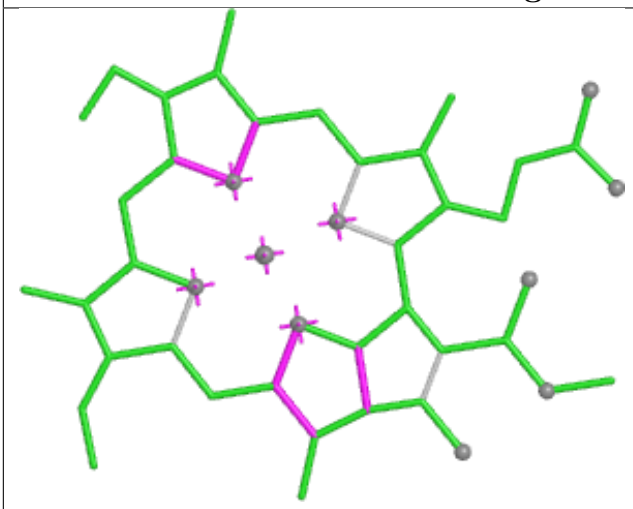


Torsions

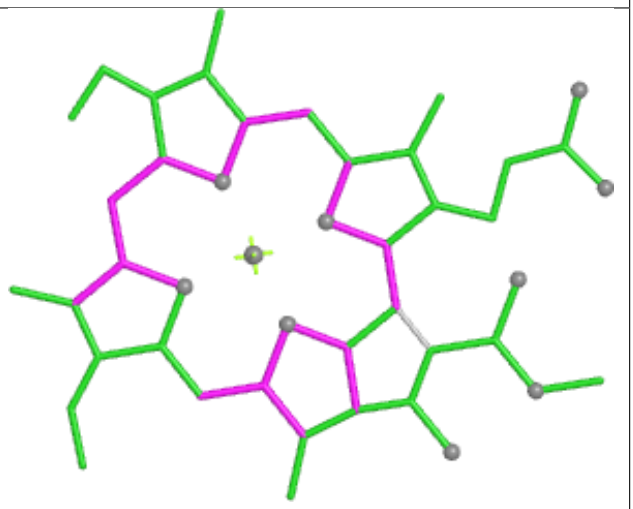


Rings

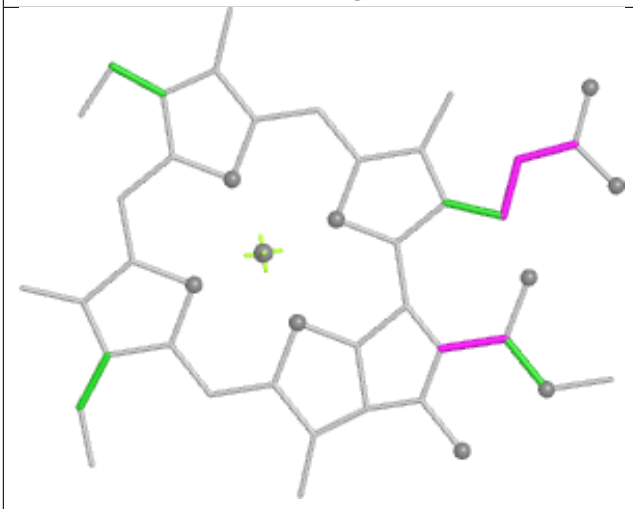
Ligand CLA C 308



Bond lengths



Bond angles

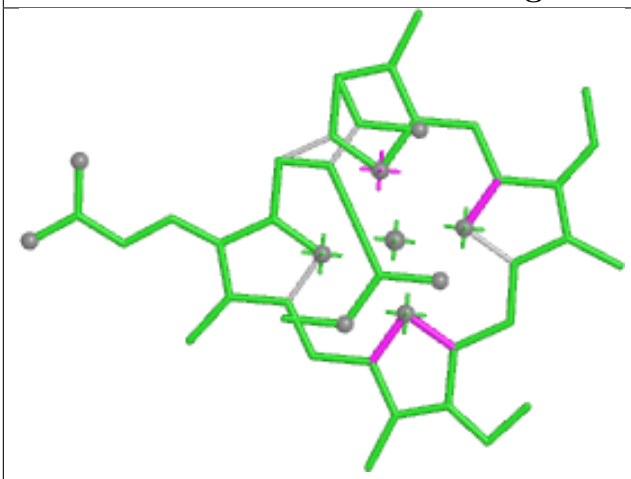


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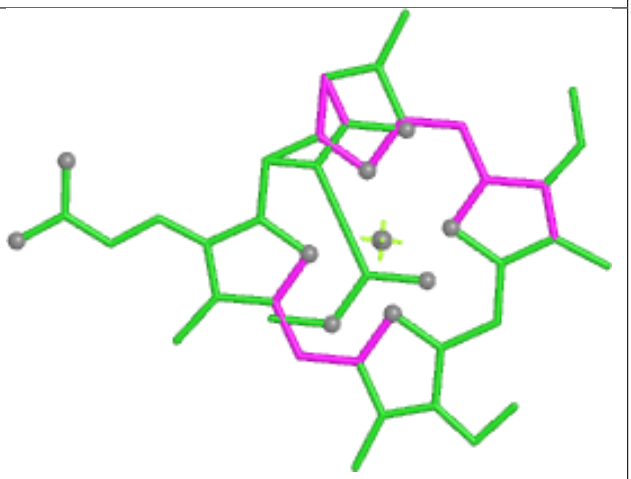


Rings

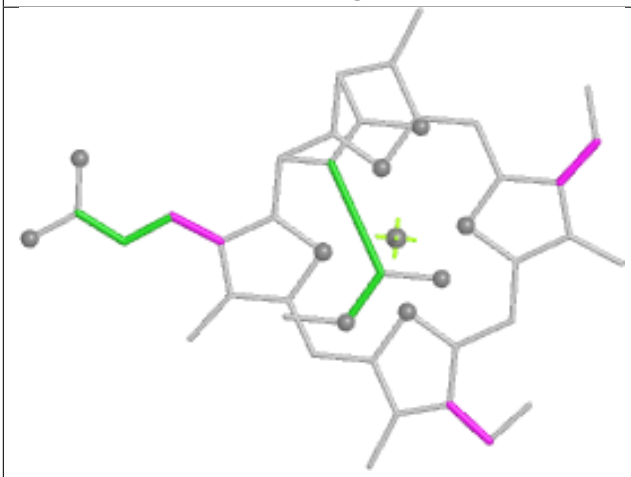
Ligand KC2 K 305



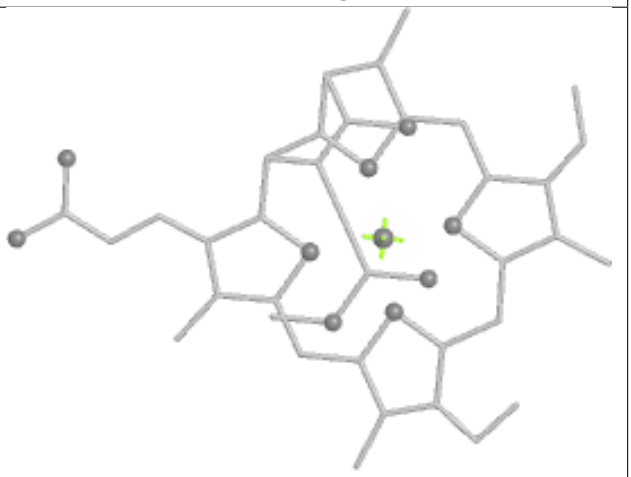
Bond lengths



Bond angles

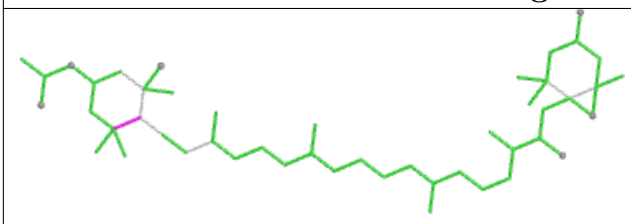


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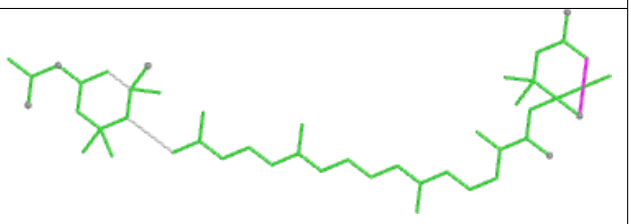


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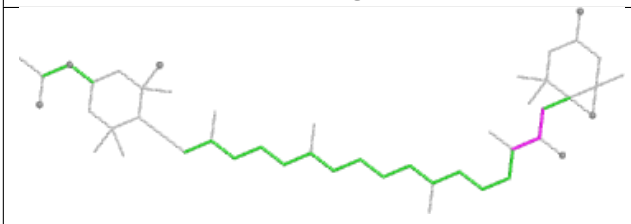
Ligand A86 T 315



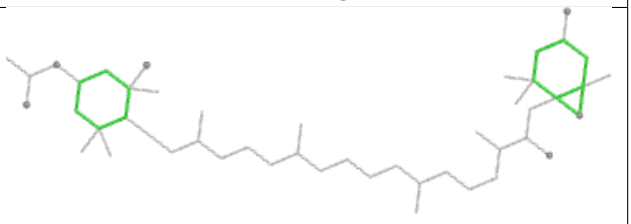
Bond lengths



Bond angles

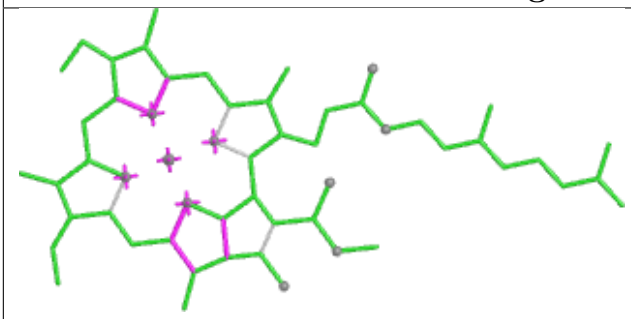


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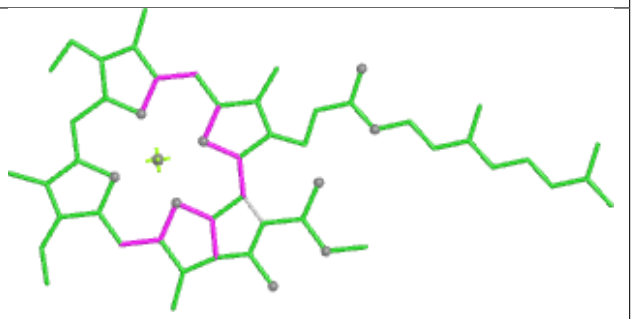


Rings

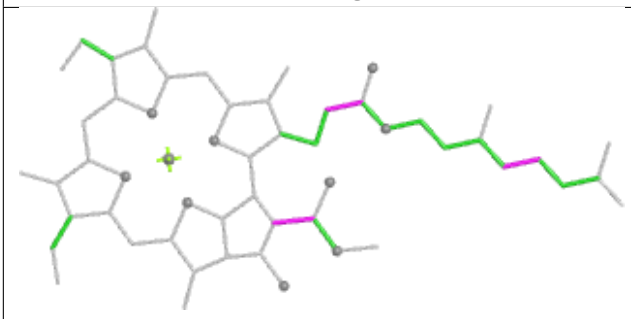
Ligand CLA a 821



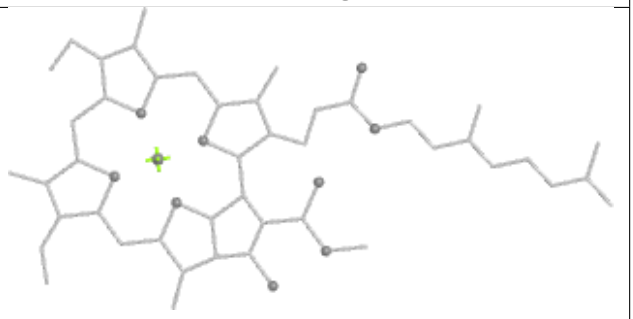
Bond lengths



Bond angles

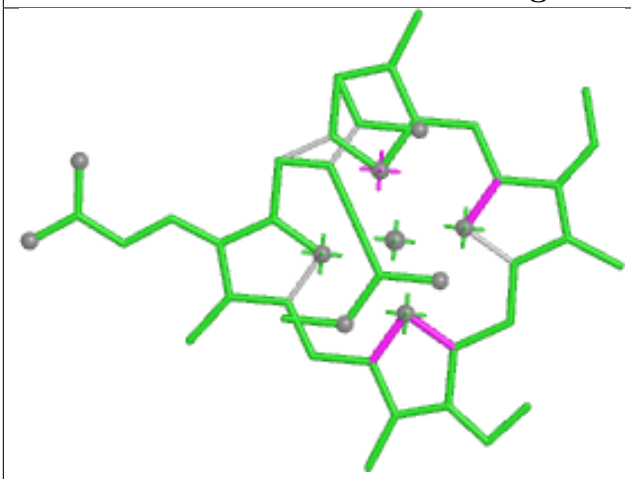


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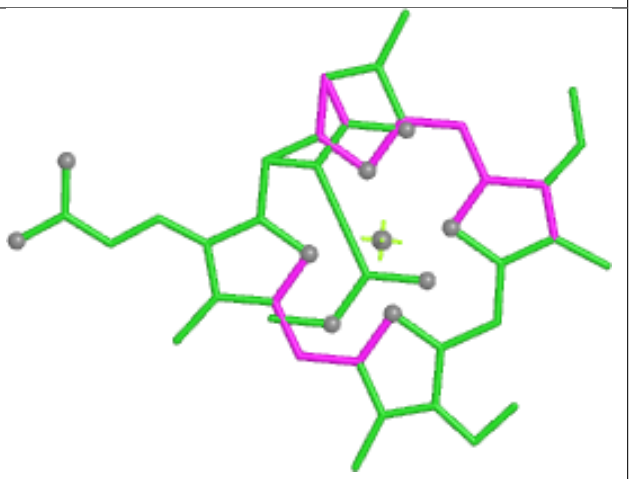


Rings

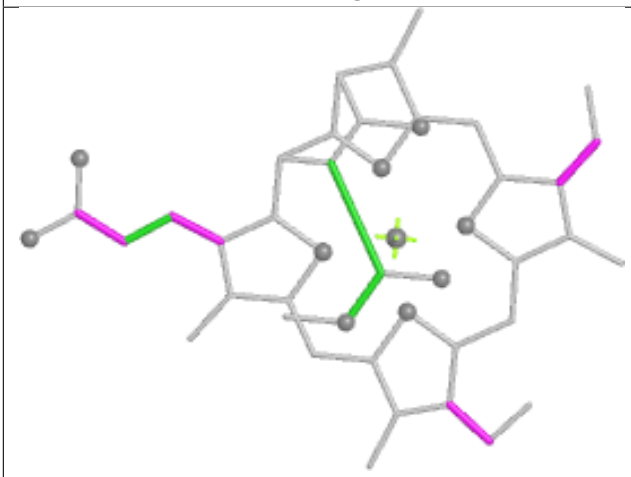
Ligand KC2 J 303



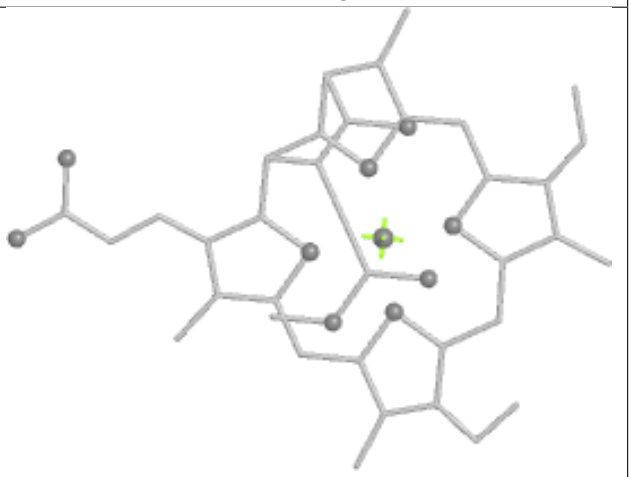
Bond lengths



Bond angles

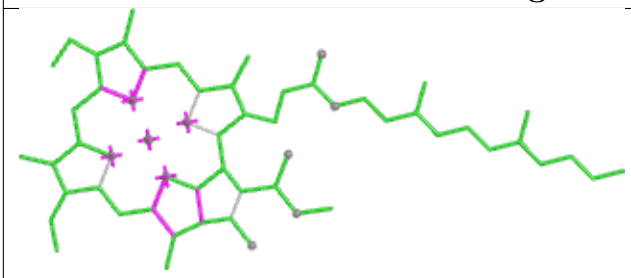


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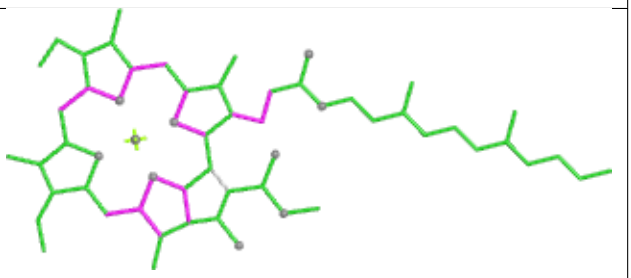


Rings

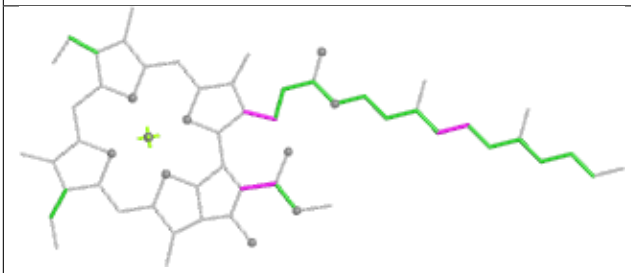
Ligand CLA a 804



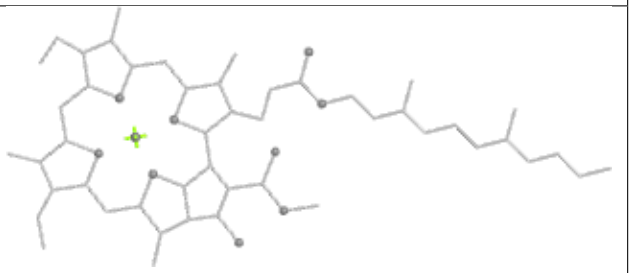
Bond lengths



Bond angles

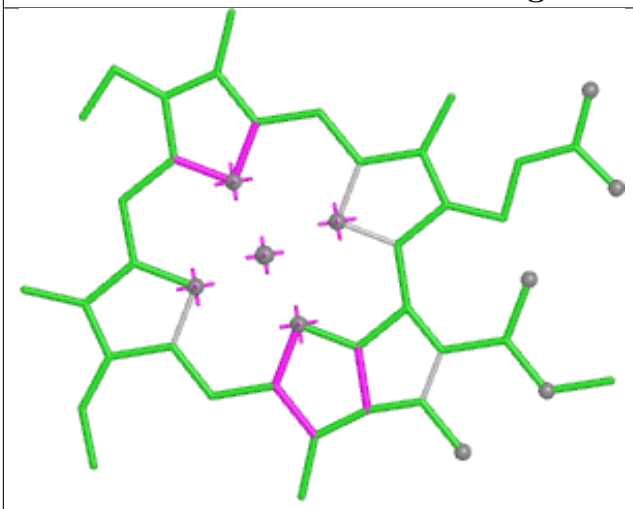


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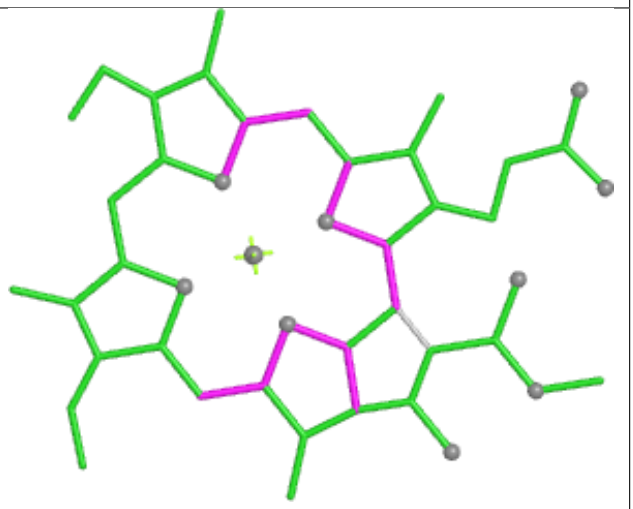


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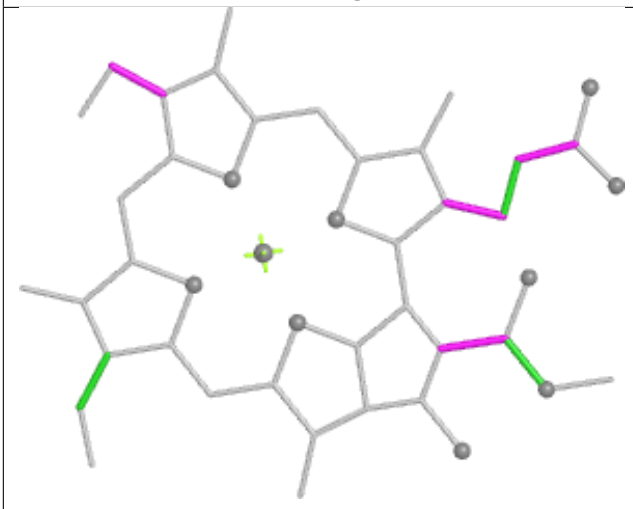
Ligand CLA b 809



Bond lengths



Bond angles

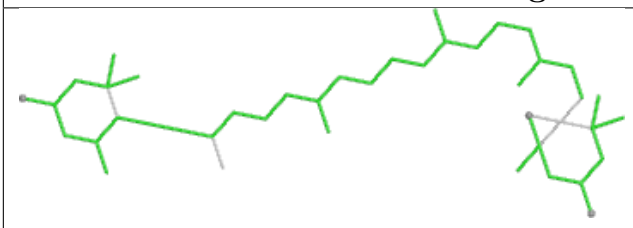


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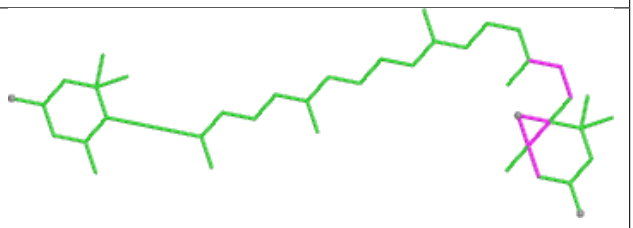


Rings

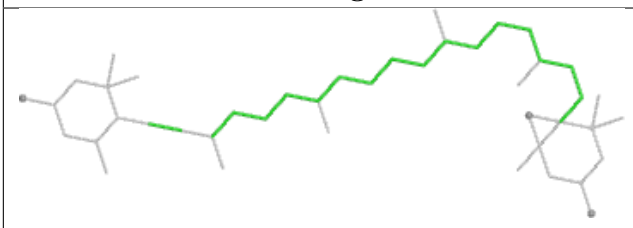
Ligand DD6 J 317



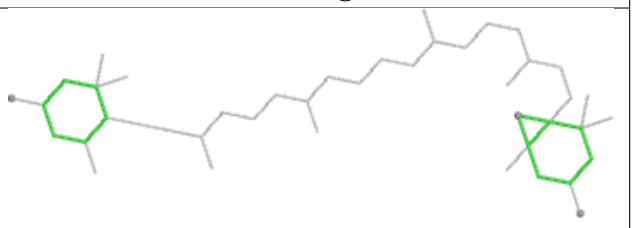
Bond lengths



Bond angles

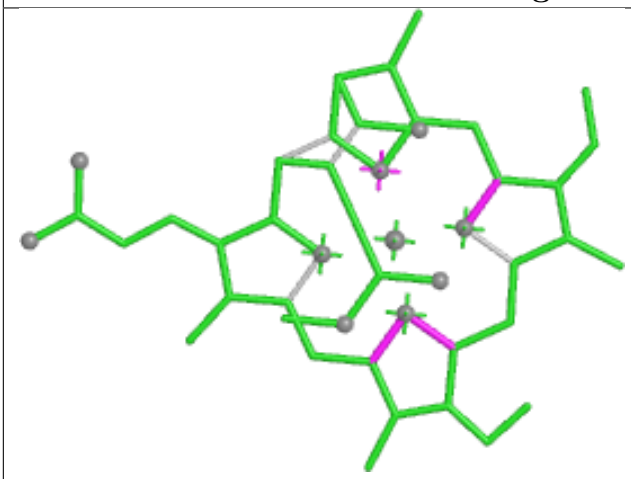


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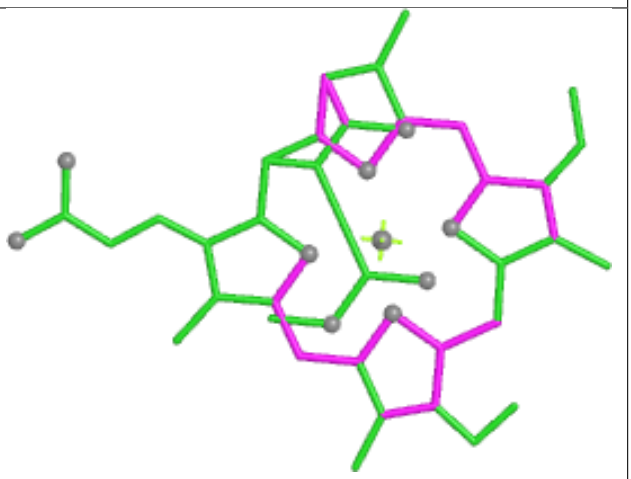


Rings

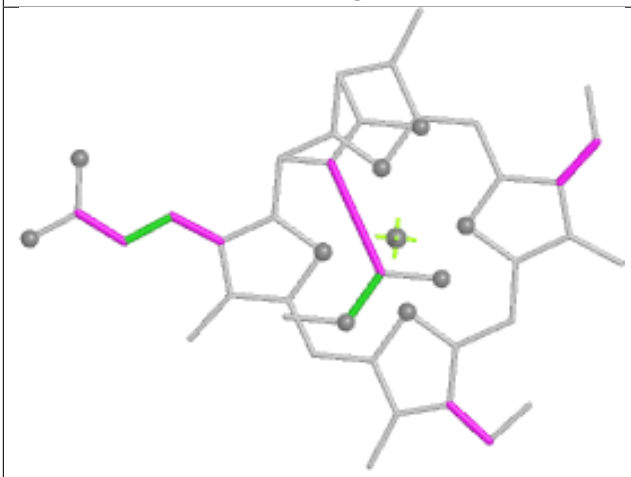
Ligand KC2 I 316



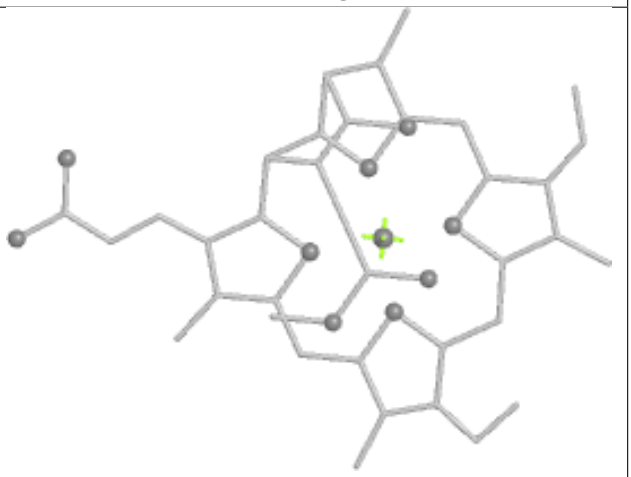
Bond lengths



Bond angles



Torsions



Rings

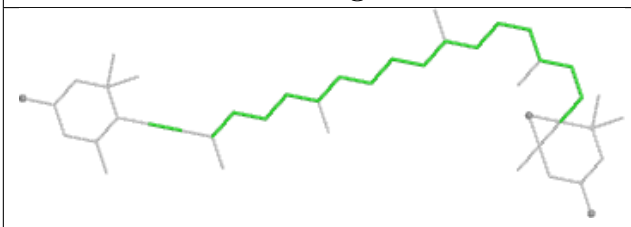
Ligand DD6 A 312



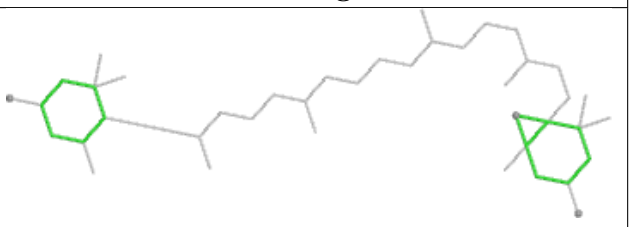
Bond lengths



Bond angles

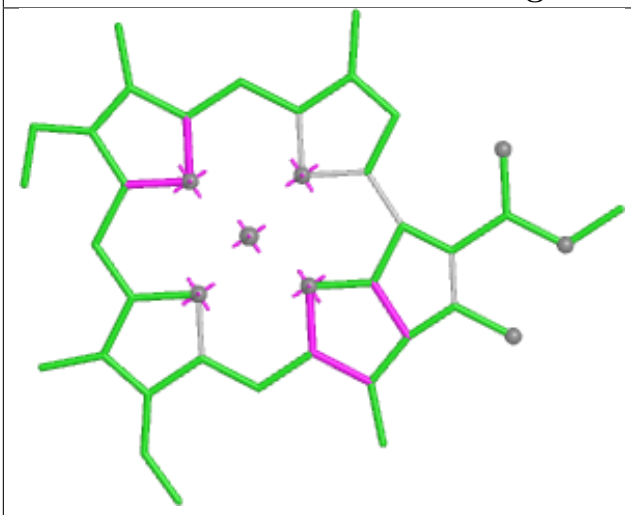


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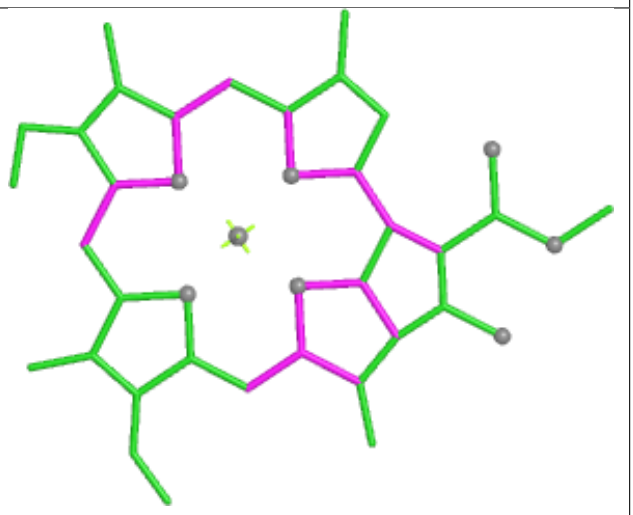


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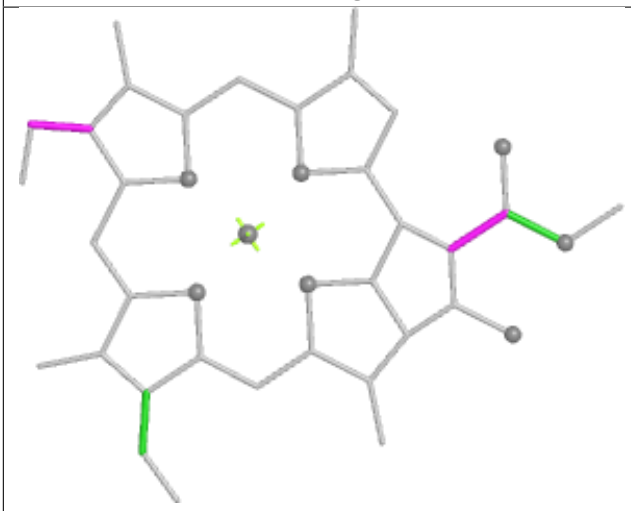
Ligand CLA L 310



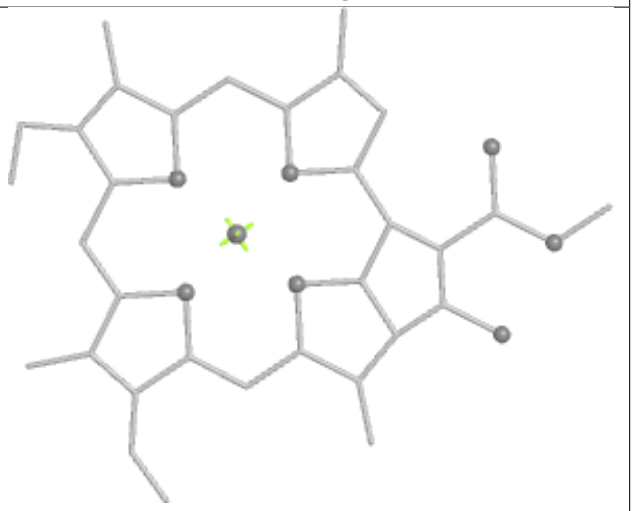
Bond lengths



Bond angles

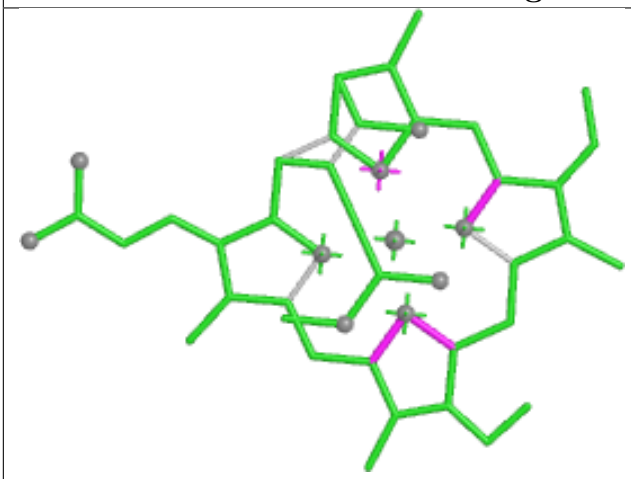


Torsions

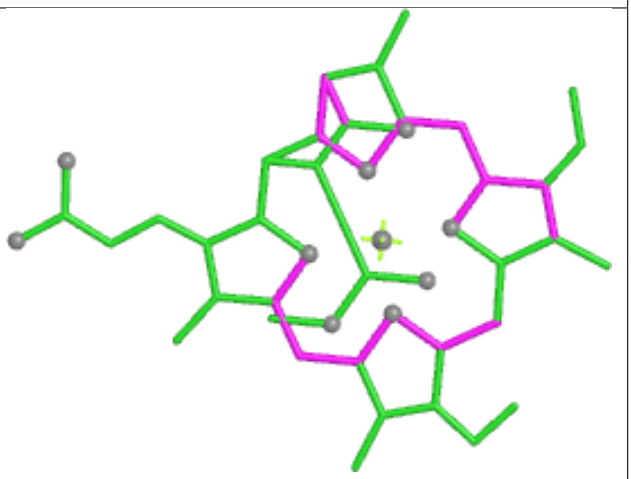


Rings

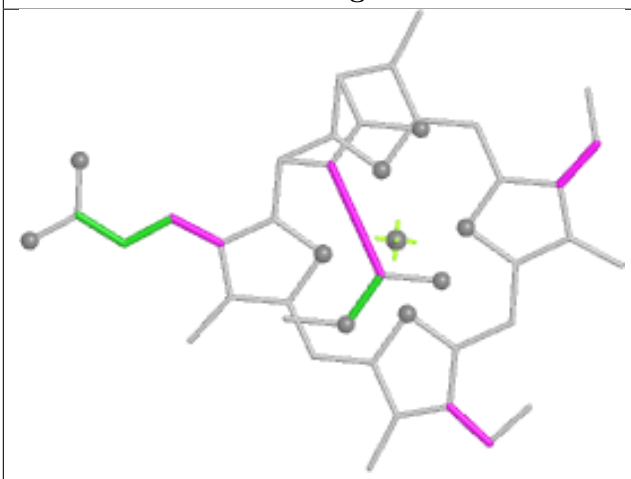
Ligand KC2 N 314



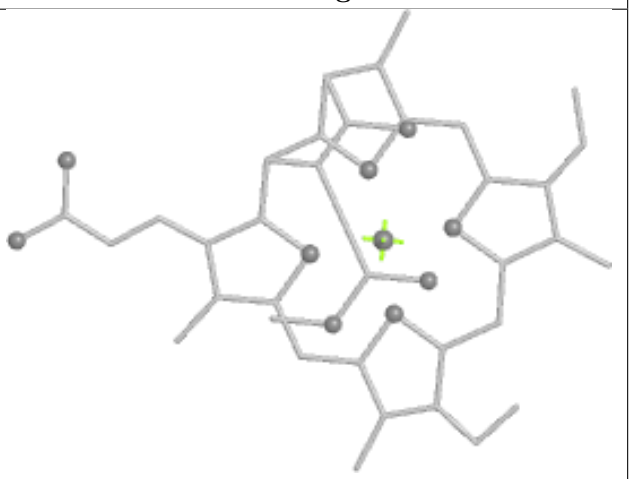
Bond lengths



Bond angles

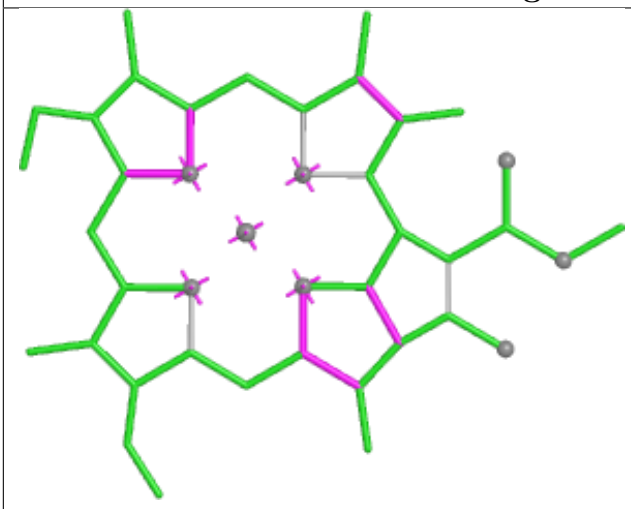


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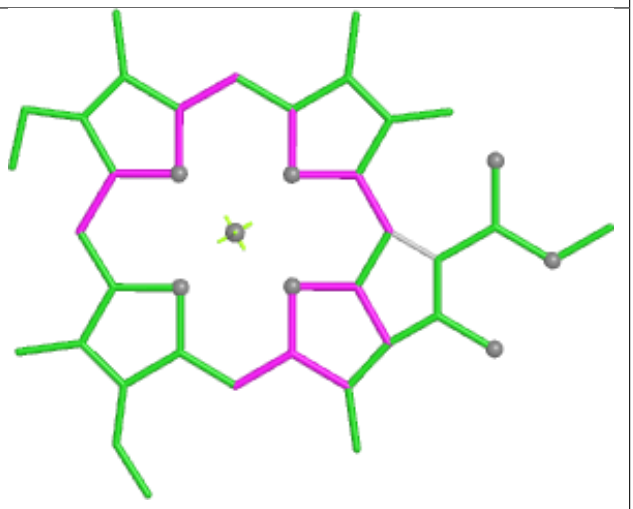


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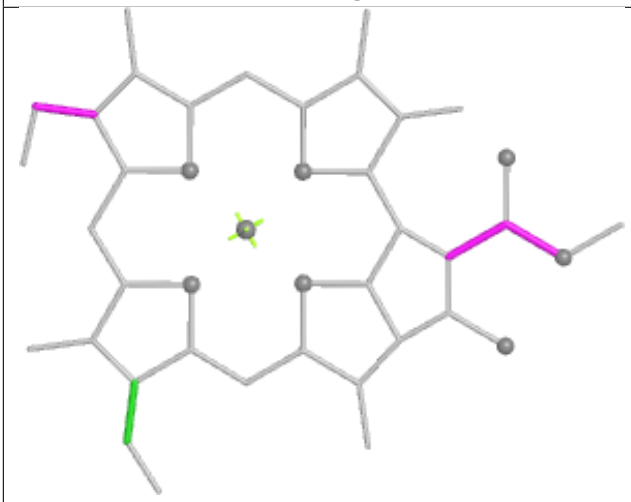
Ligand CLA H 302



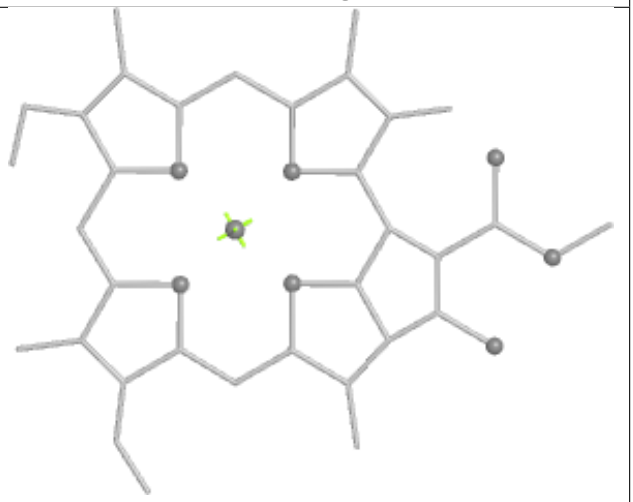
Bond lengths



Bond angles

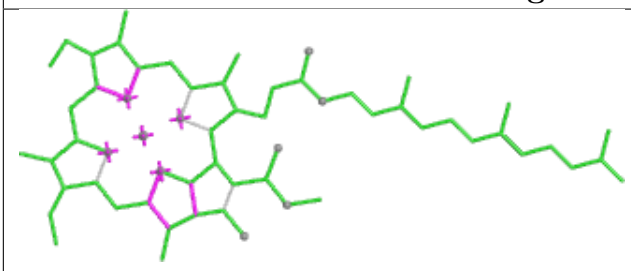


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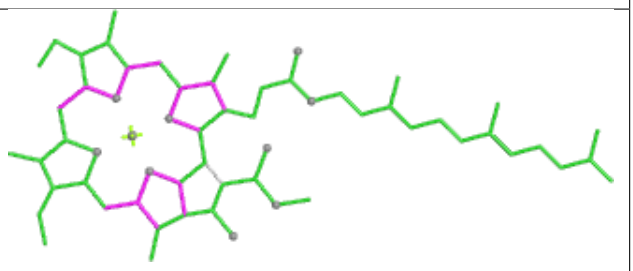


Rings

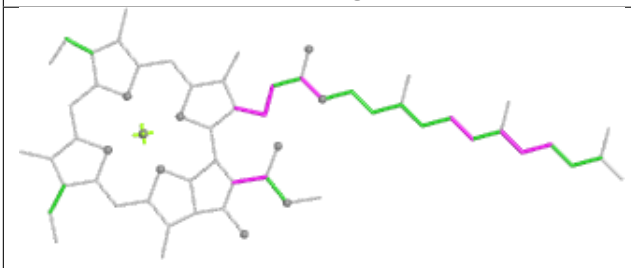
Ligand CLA b 807



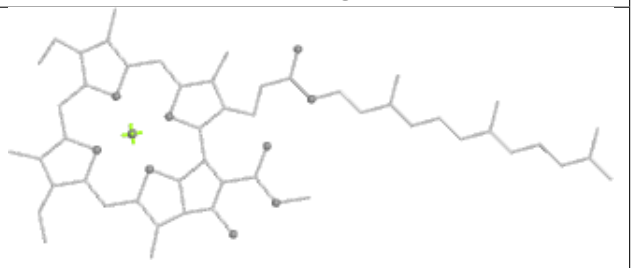
Bond lengths



Bond angles

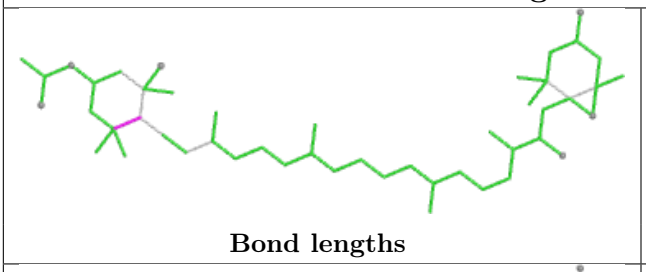


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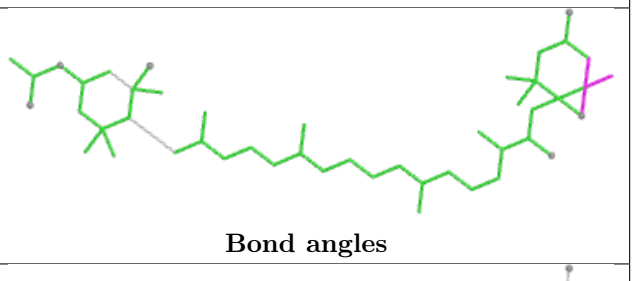


Rings

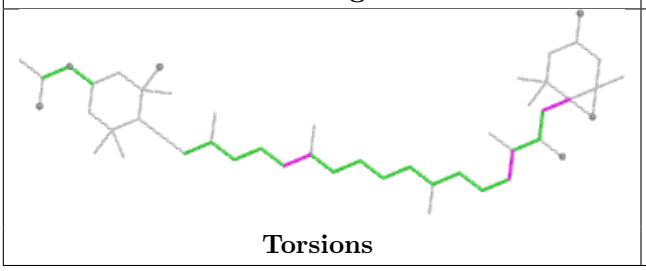
Ligand A86 C 312



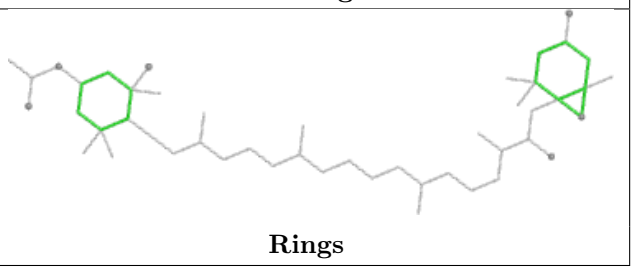
Bond lengths



Bond angles

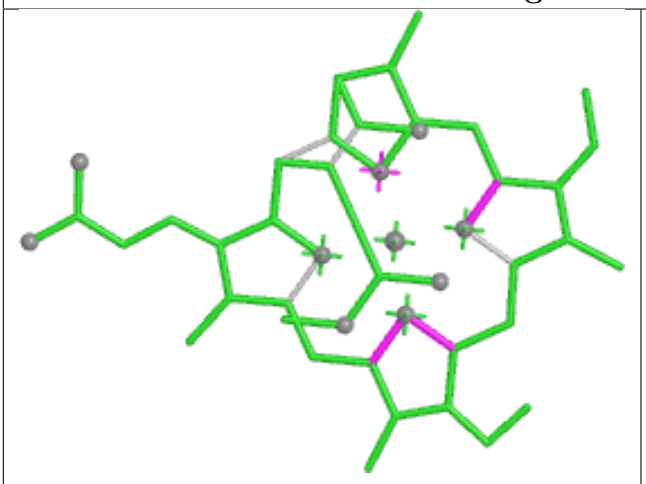


Torsions

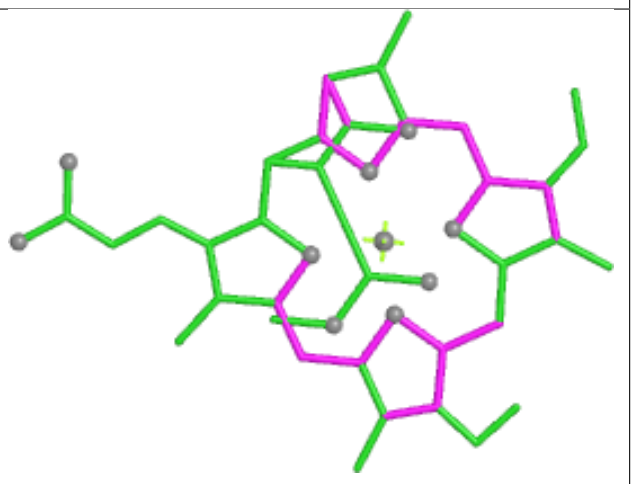


Rings

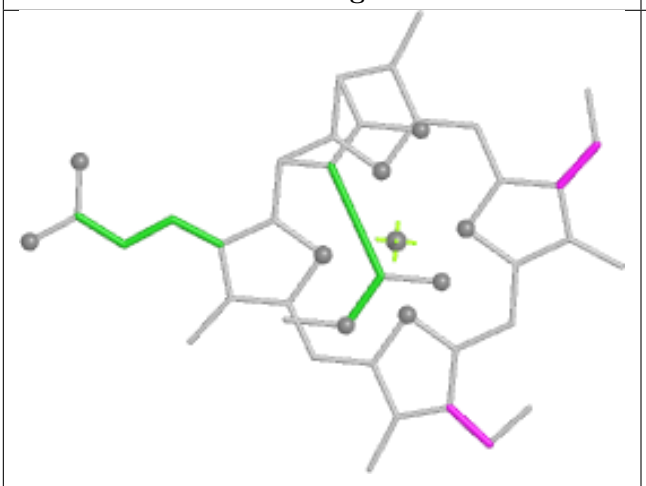
Ligand KC2 N 306



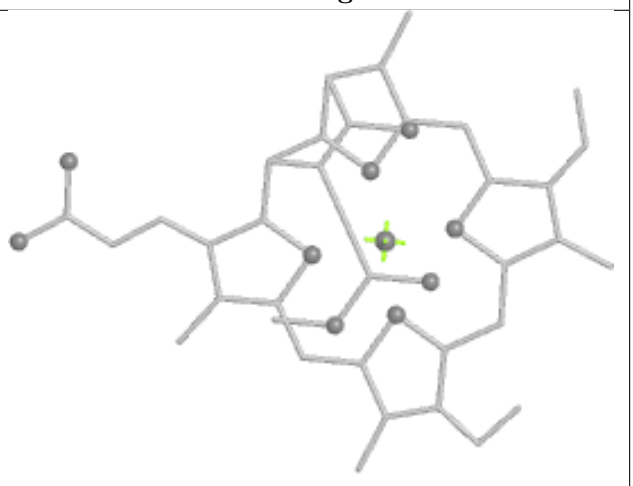
Bond lengths



Bond angles

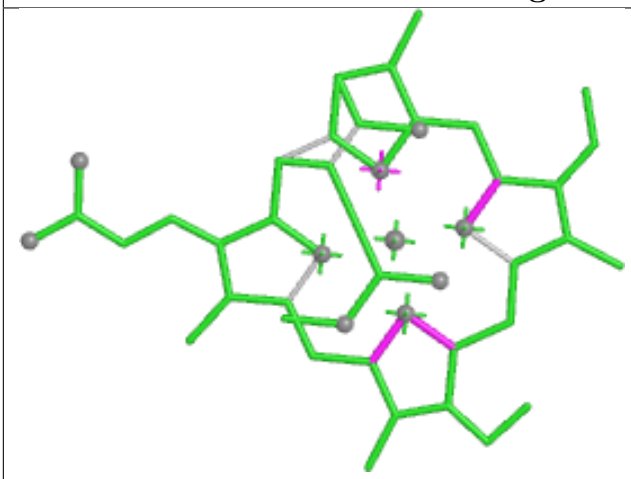


Torsions

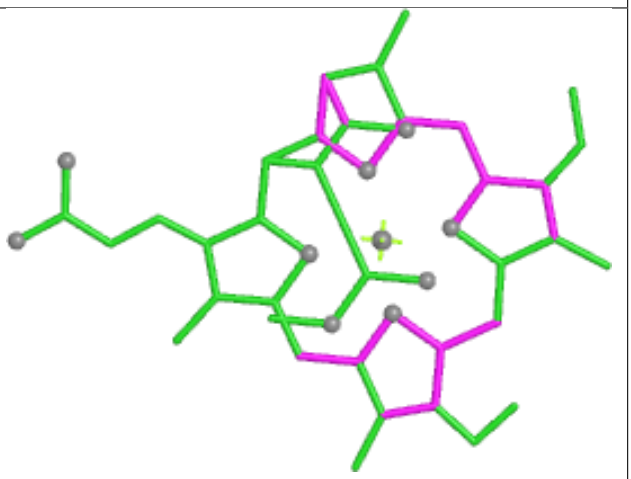


Rings

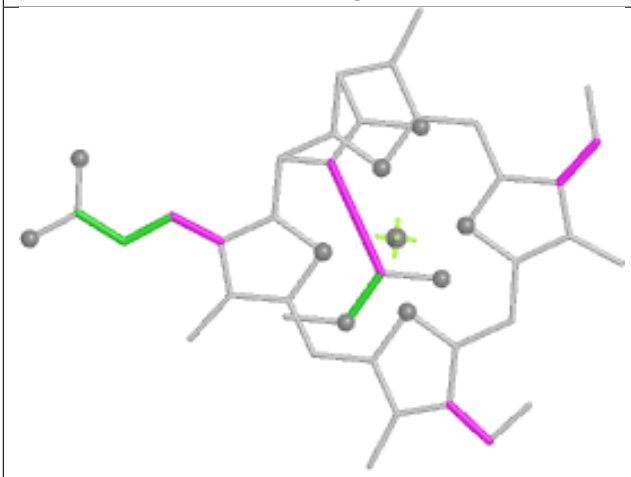
Ligand KC2 S 306



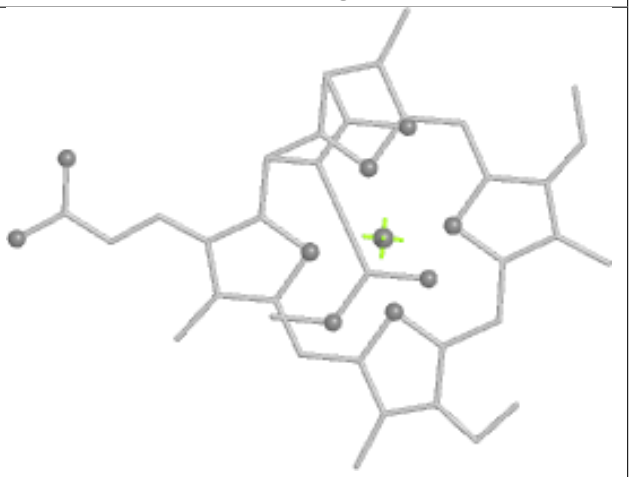
Bond lengths



Bond angles

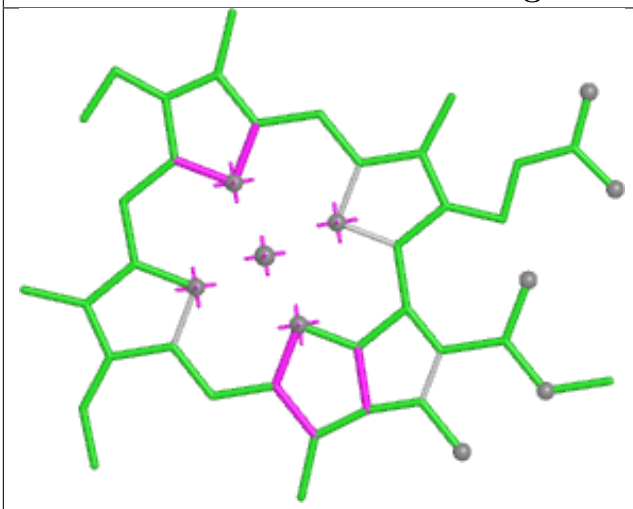


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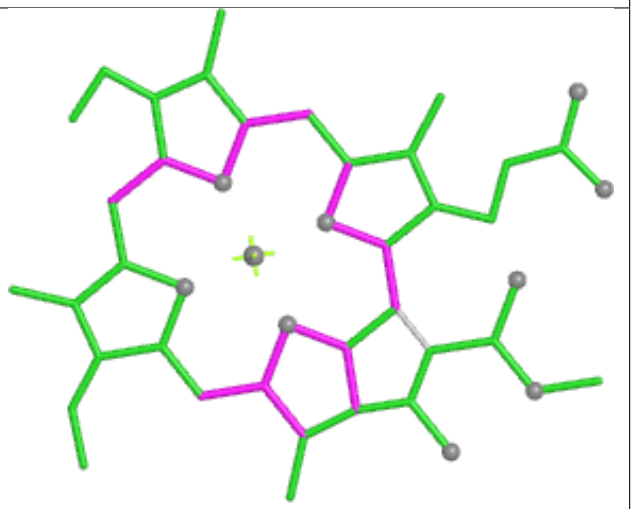


Rings

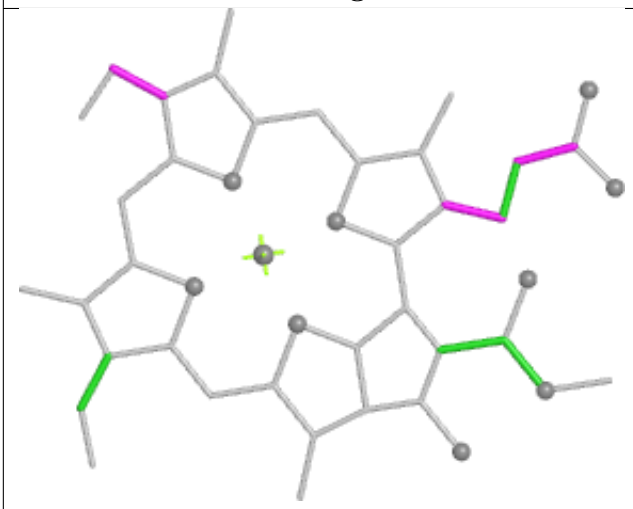
Ligand CLA O 301



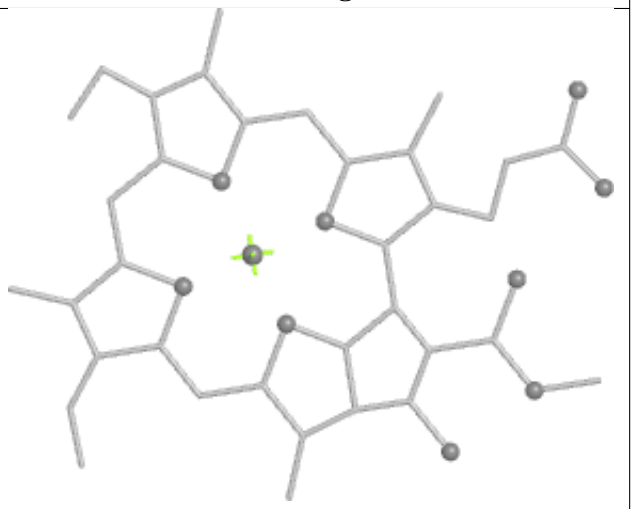
Bond lengths



Bond angles

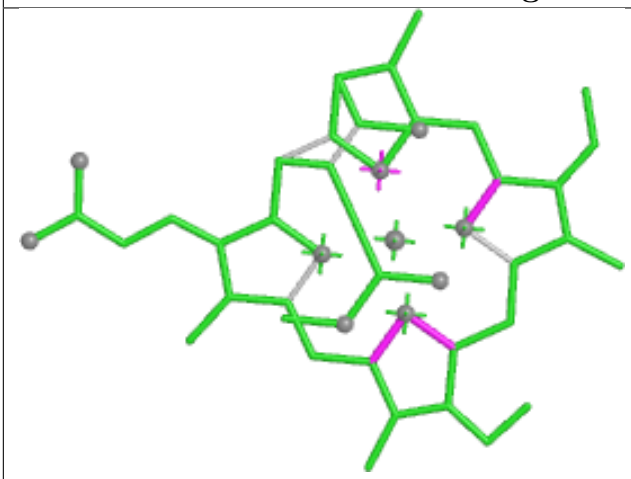


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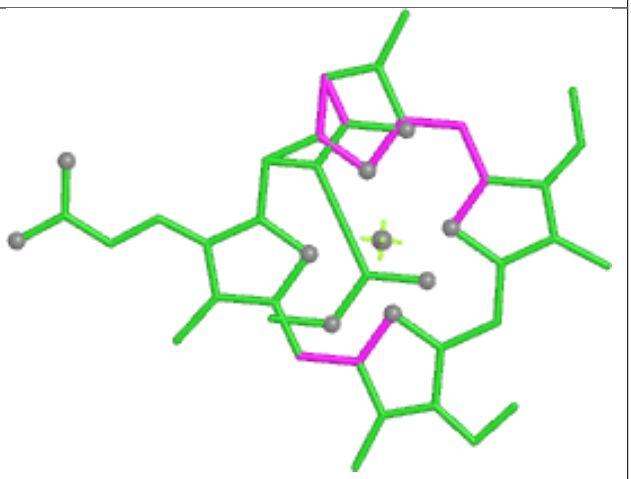


Rings

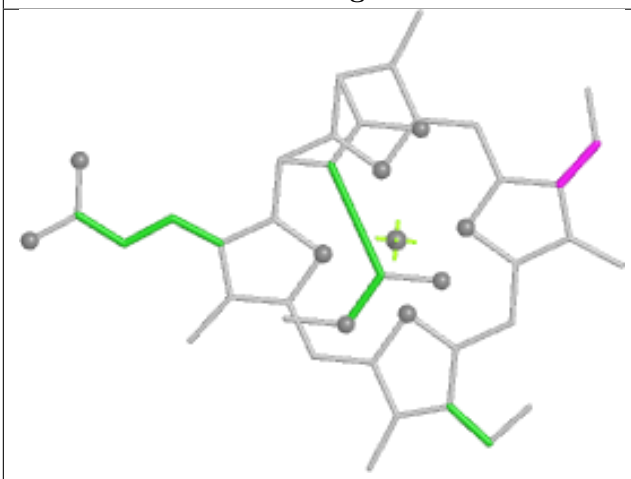
Ligand KC2 M 303



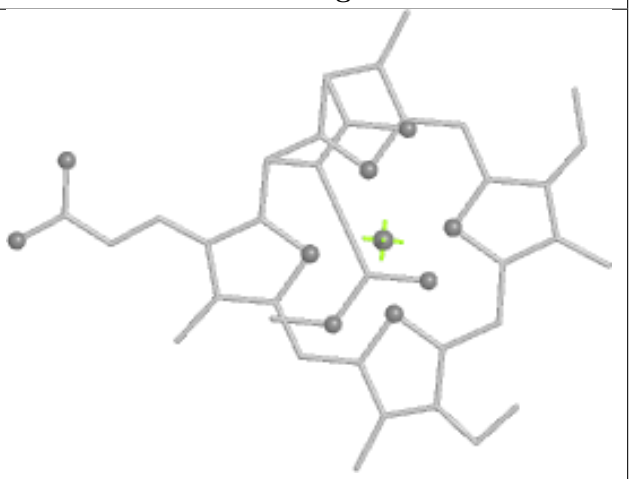
Bond lengths



Bond angles

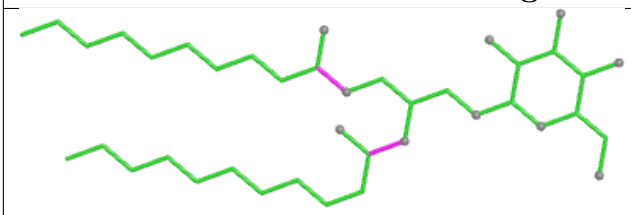


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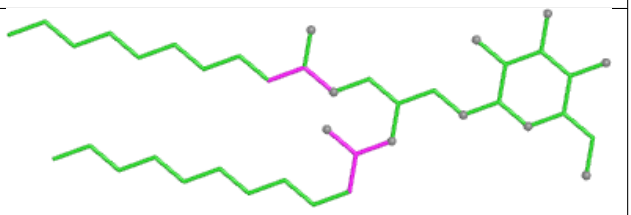


Rings

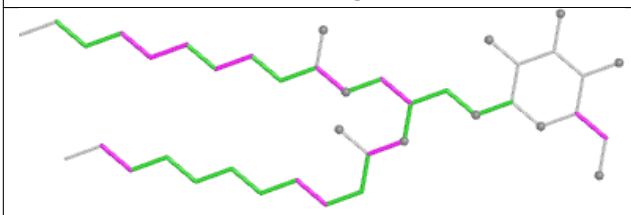
Ligand LMG E 322



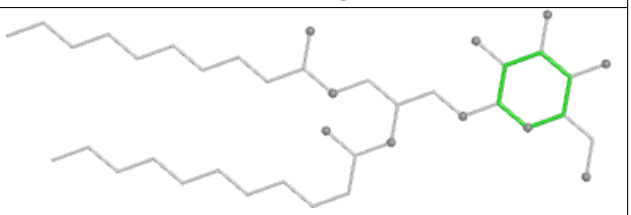
Bond lengths



Bond angles

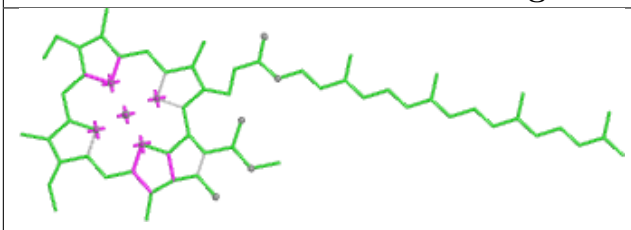


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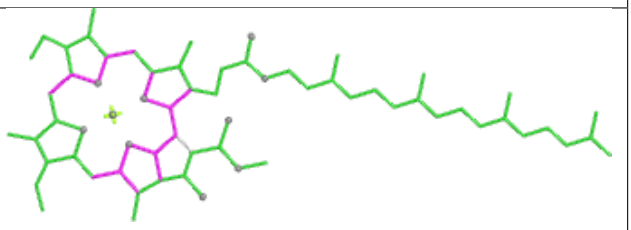


Rings

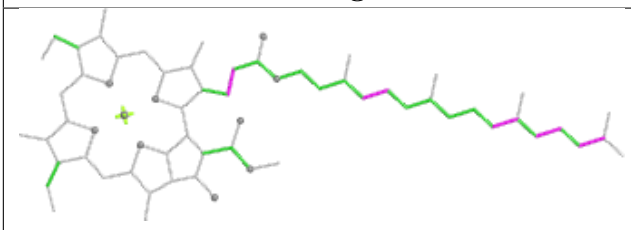
Ligand CLA a 801



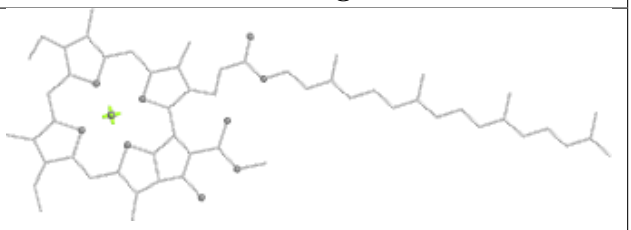
Bond lengths



Bond angles

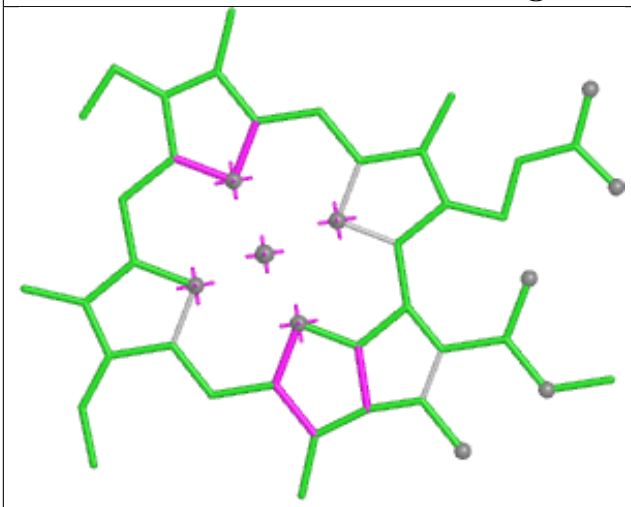


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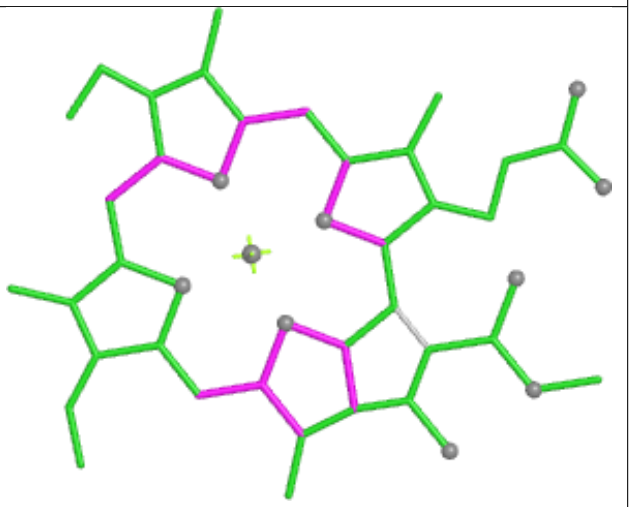


Rings

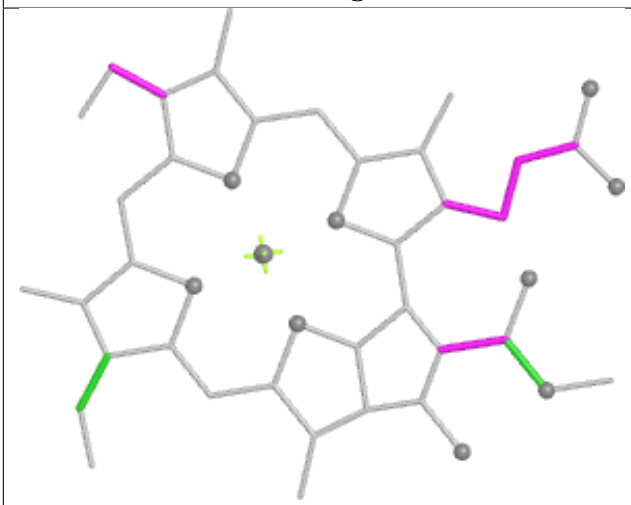
Ligand CLA S 310



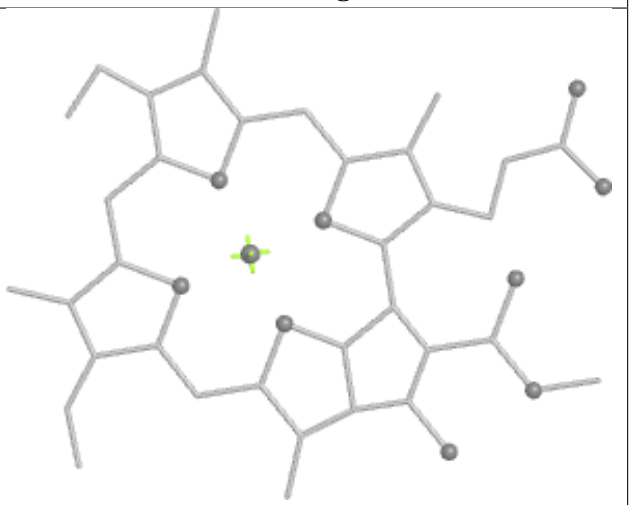
Bond lengths



Bond angles

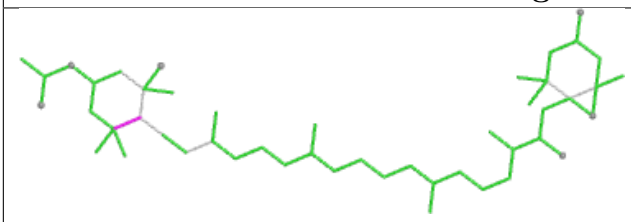


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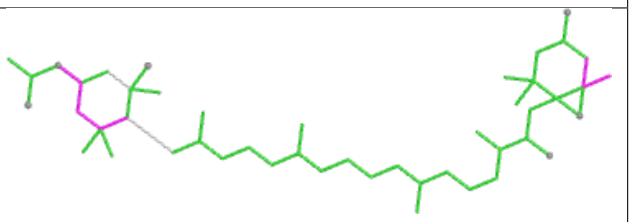


Rings

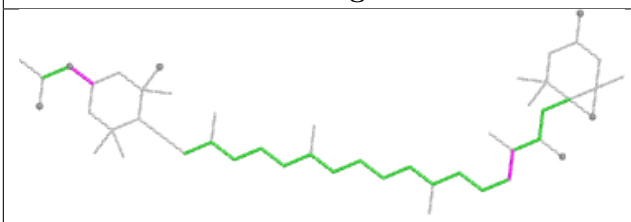
Ligand A86 L 315



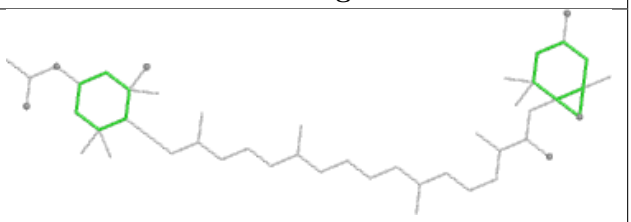
Bond lengths



Bond angles

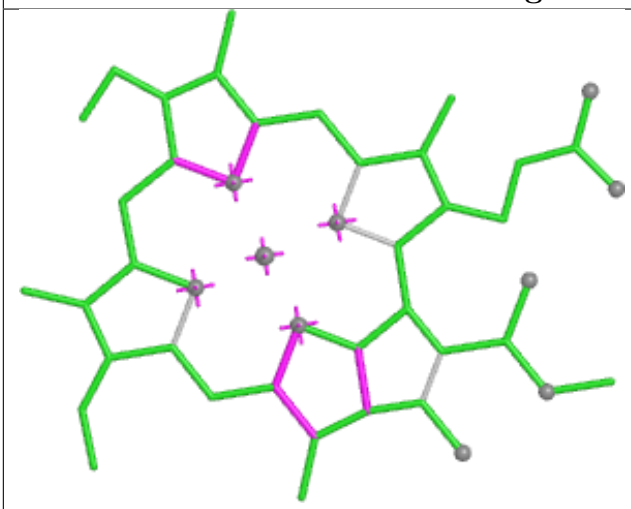


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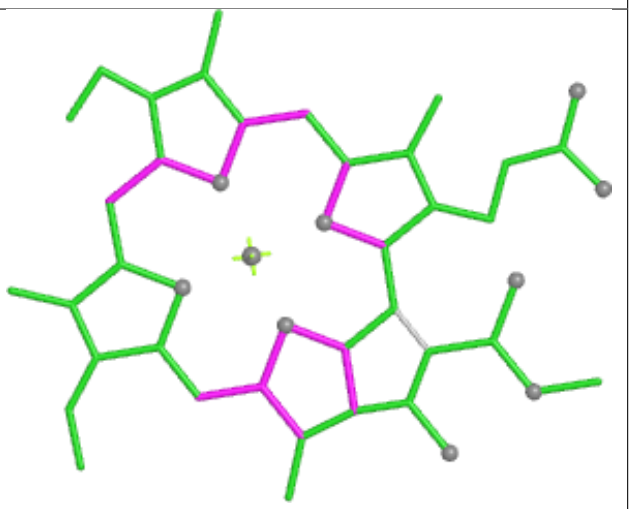


Rings

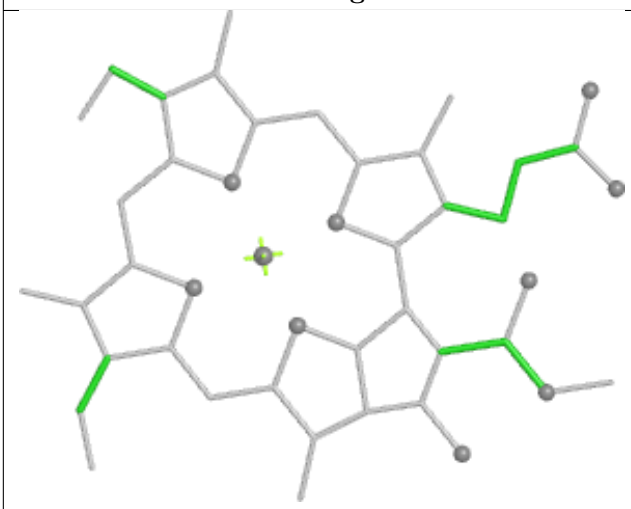
Ligand CLA P 307



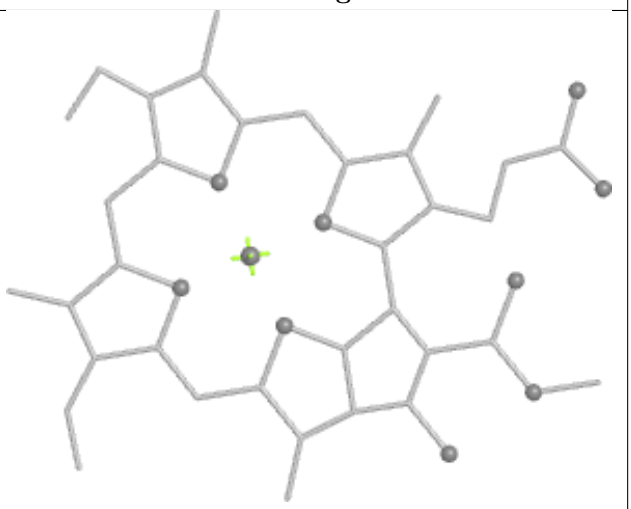
Bond lengths



Bond angles

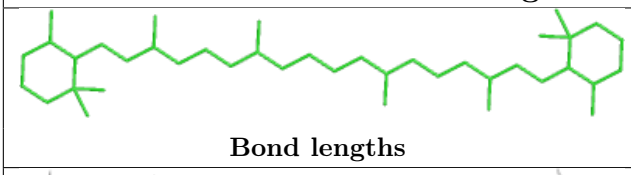


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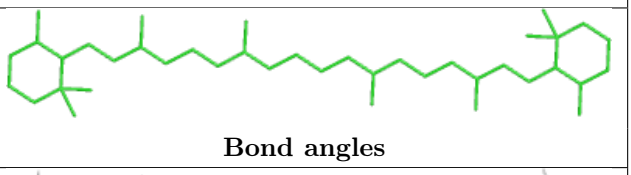


Rings

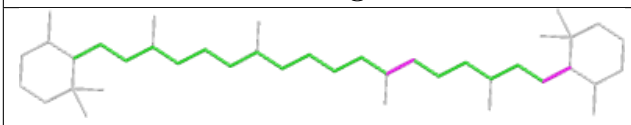
Ligand BCR U 310



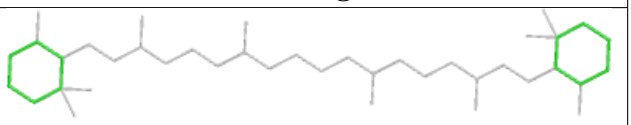
Bond lengths



Bond angles

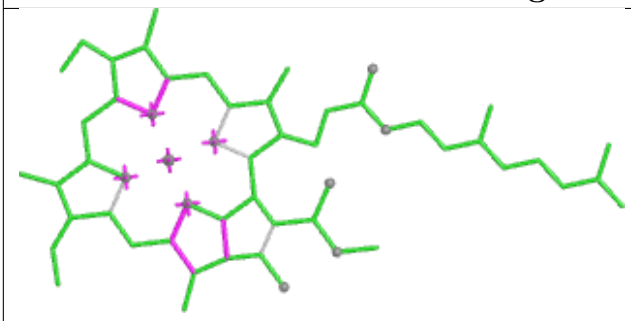


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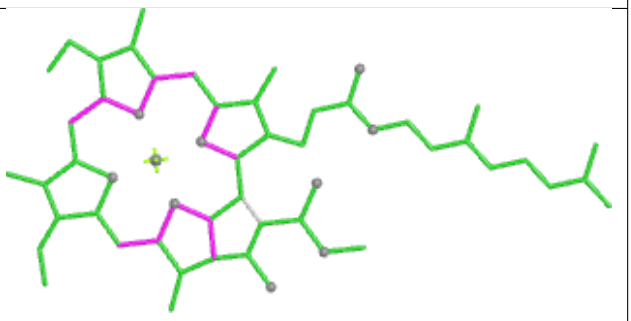


Rings

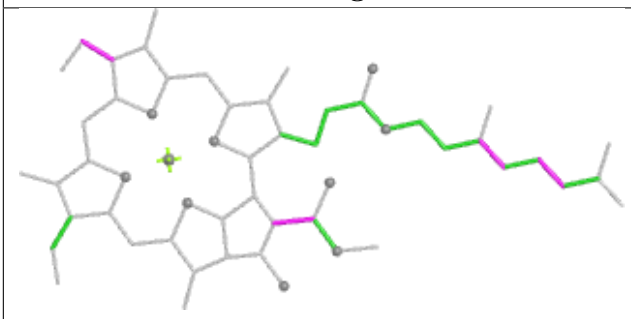
Ligand CLA a 842



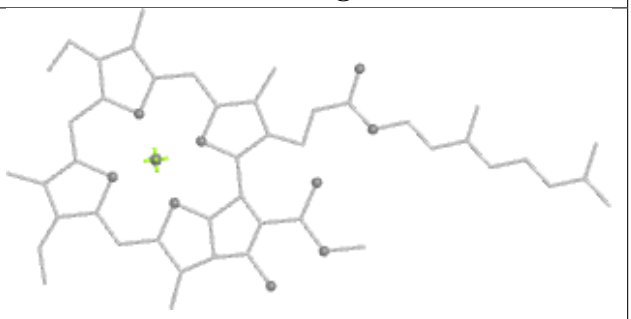
Bond lengths



Bond angles

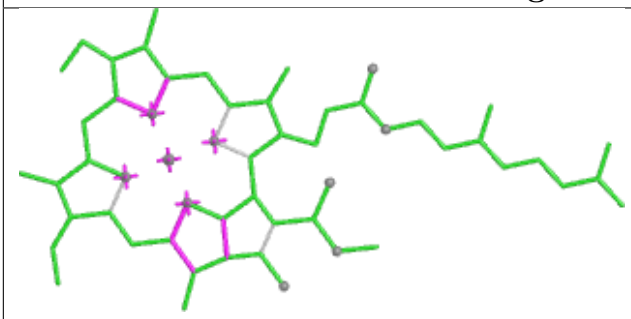


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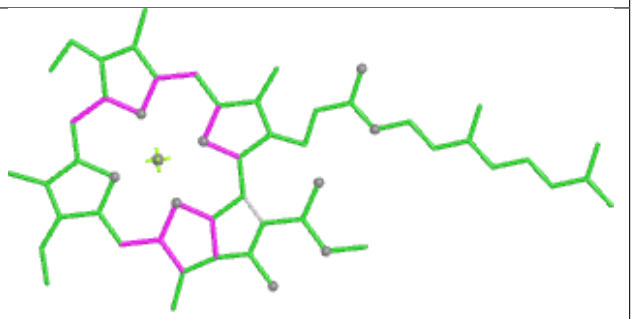


Rings

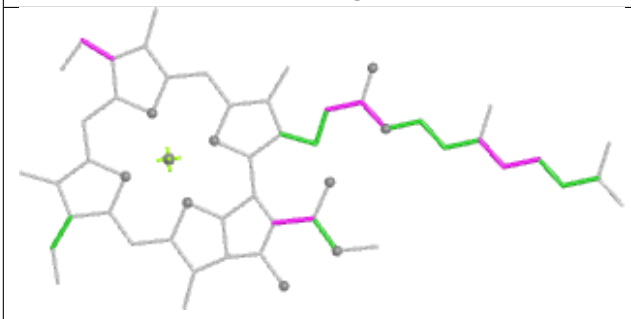
Ligand CLA k 201



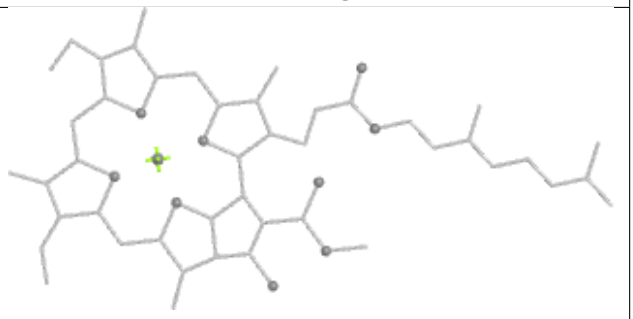
Bond lengths



Bond angles

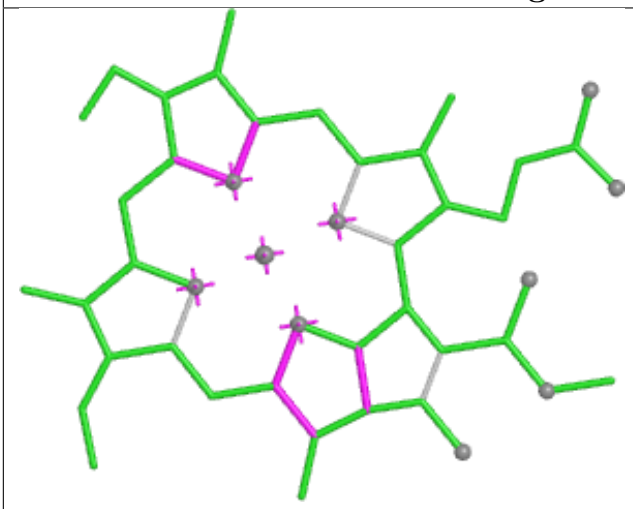


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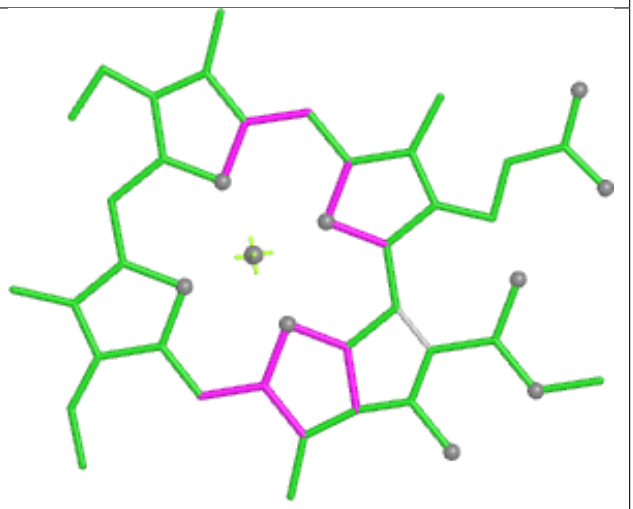


Rings

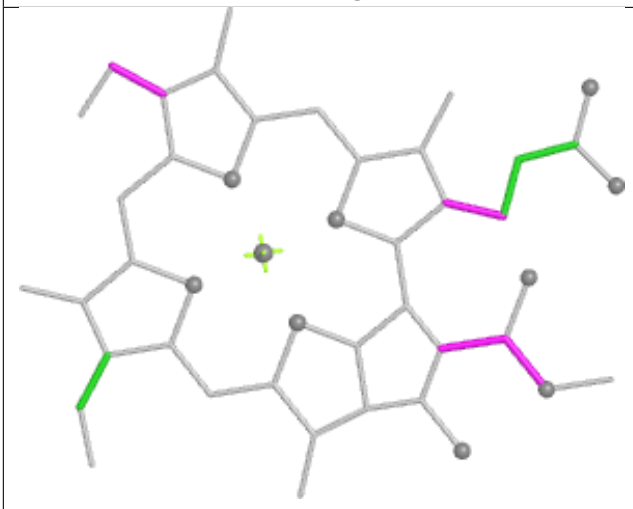
Ligand CLA a 816



Bond lengths



Bond angles

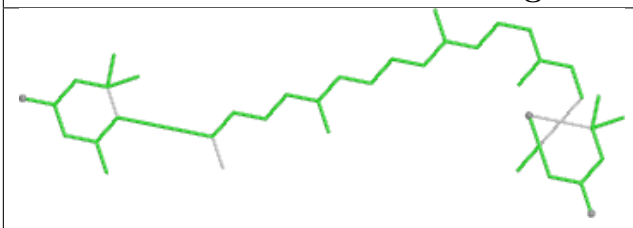


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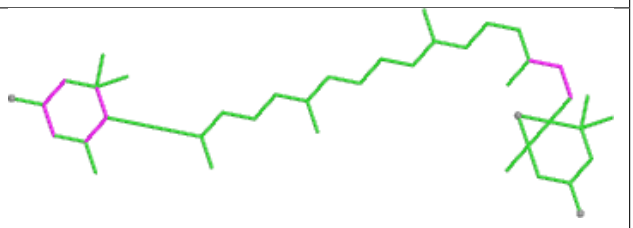


Rings

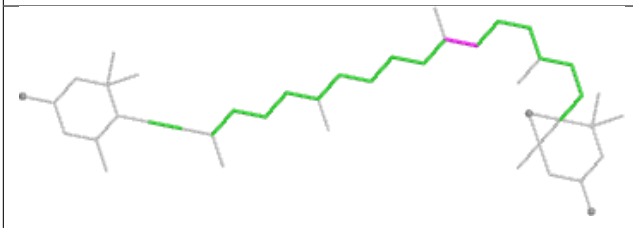
Ligand DD6 D 319



Bond lengths



Bond angles

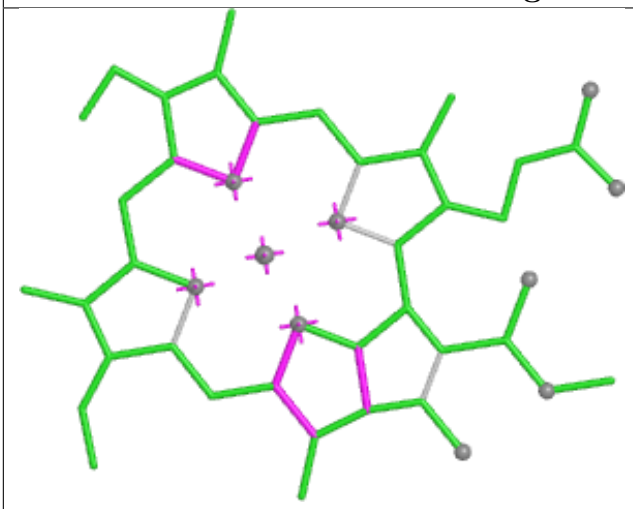


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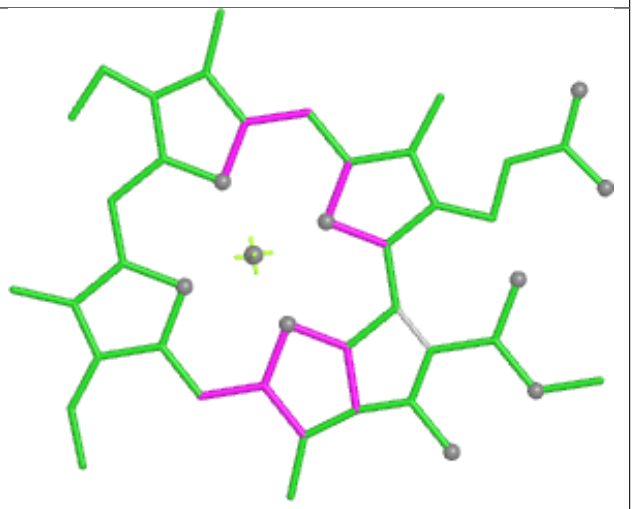


Rings

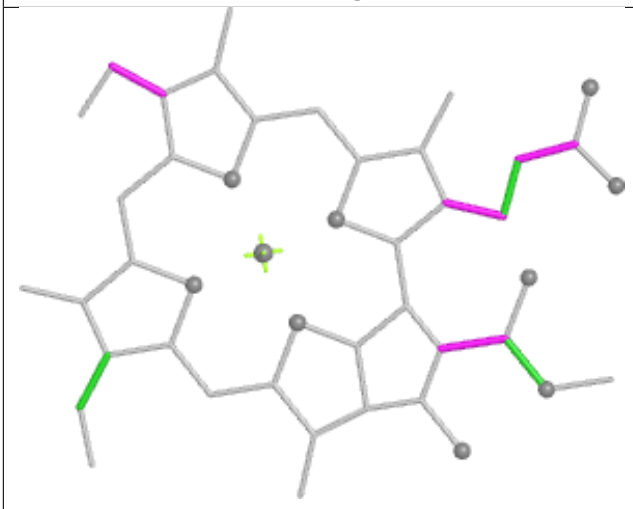
Ligand CLA A 311



Bond lengths



Bond angles

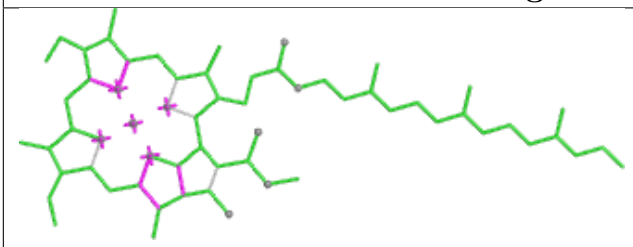


Torsions

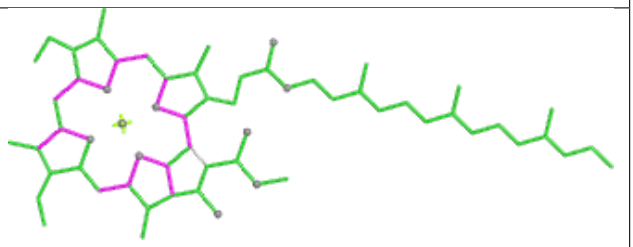


Rings

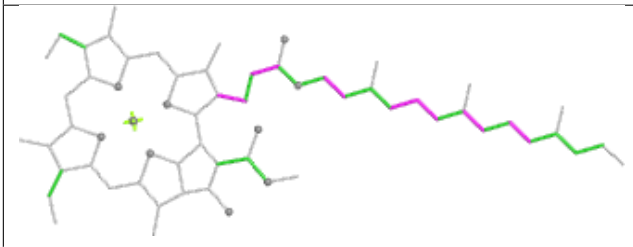
Ligand CLA F 303



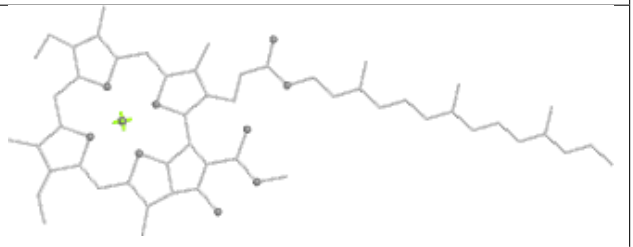
Bond lengths



Bond angles

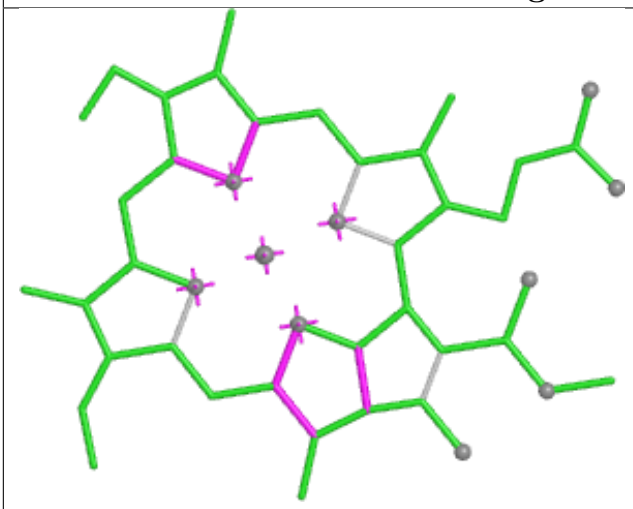


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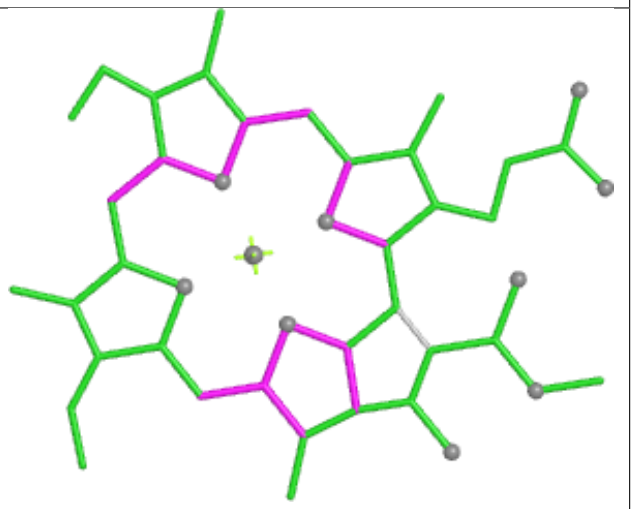


Rings

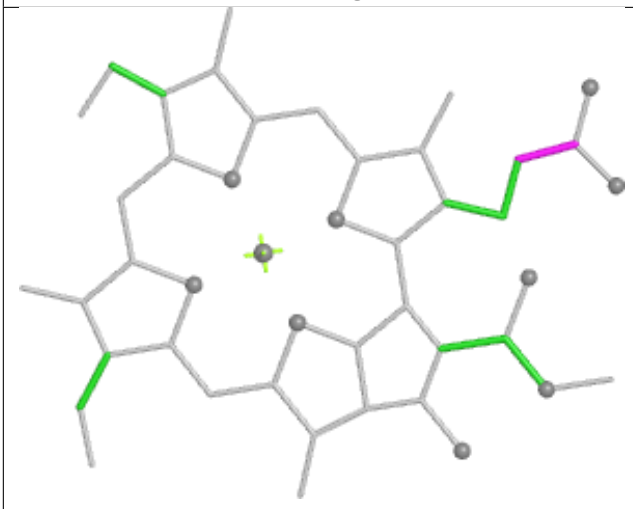
Ligand CLA J 311



Bond lengths



Bond angles

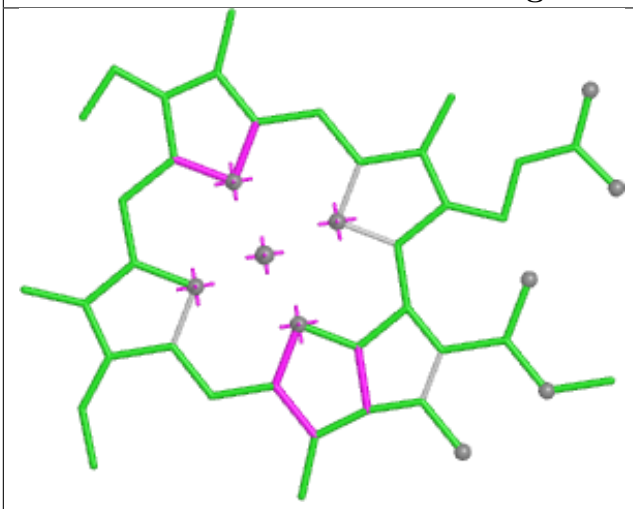


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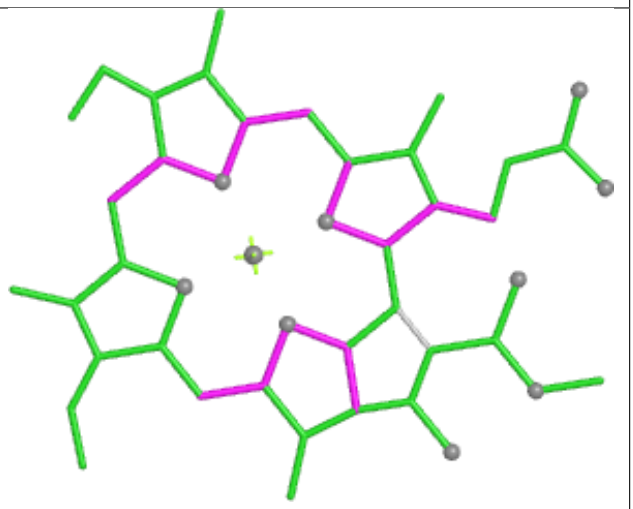


Rings

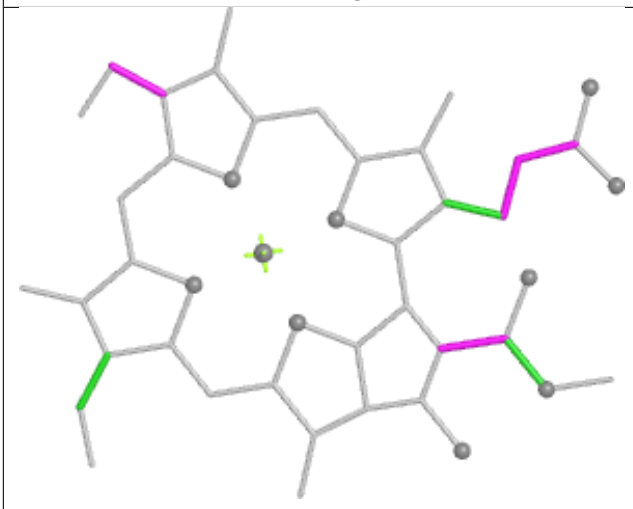
Ligand CLA L 301



Bond lengths



Bond angles

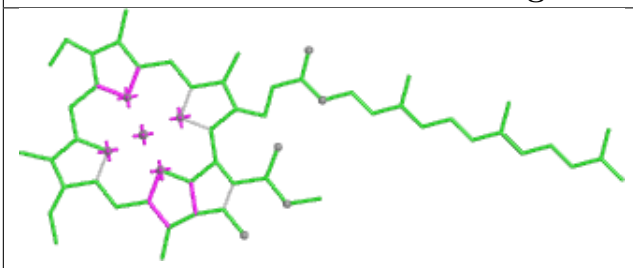


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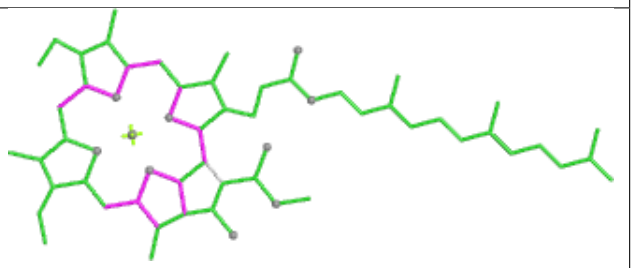


Rings

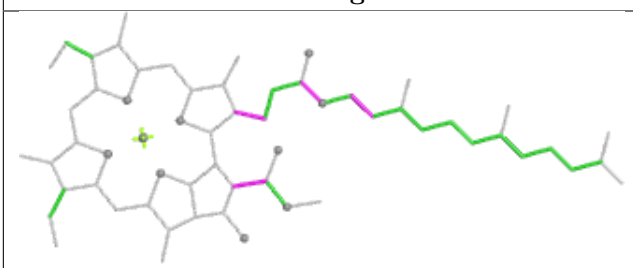
Ligand CLA b 801



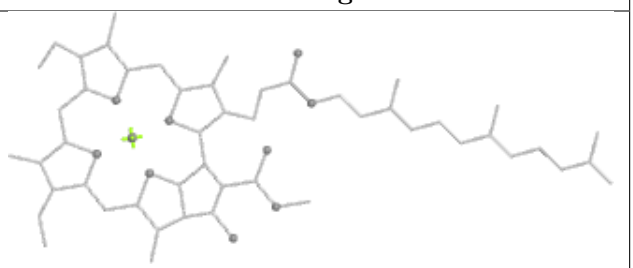
Bond lengths



Bond angles

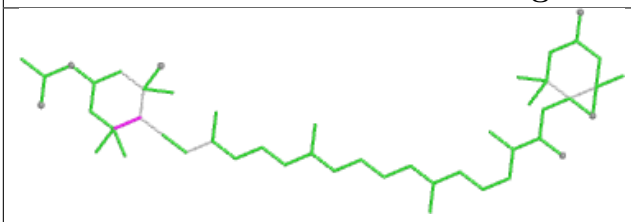


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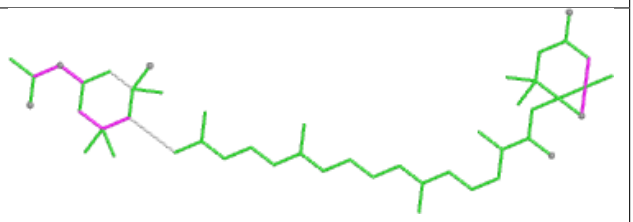


Rings

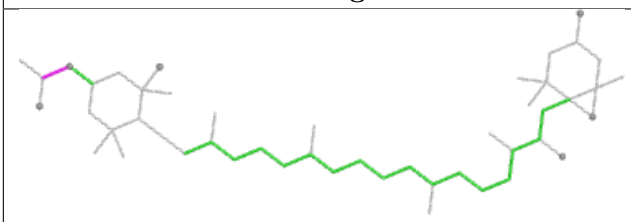
Ligand A86 F 312



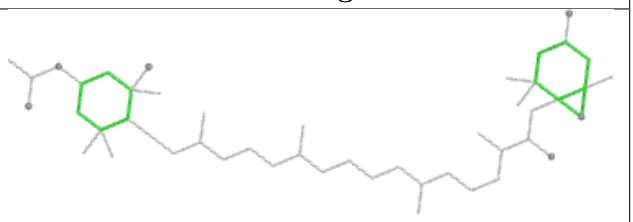
Bond lengths



Bond angles

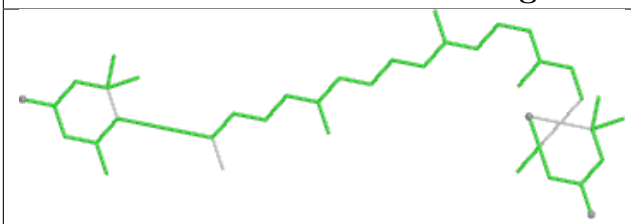


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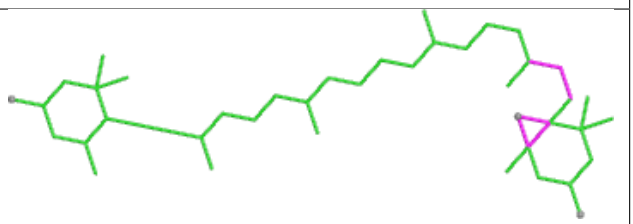


Rings

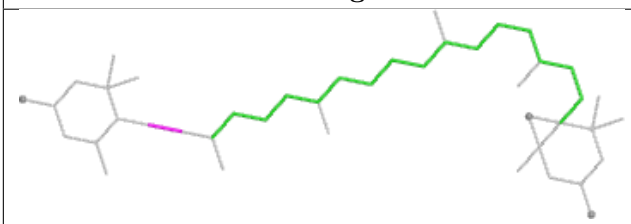
Ligand DD6 W 317



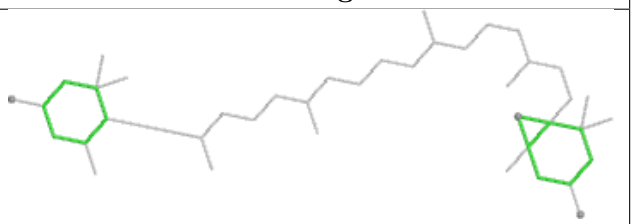
Bond lengths



Bond angles

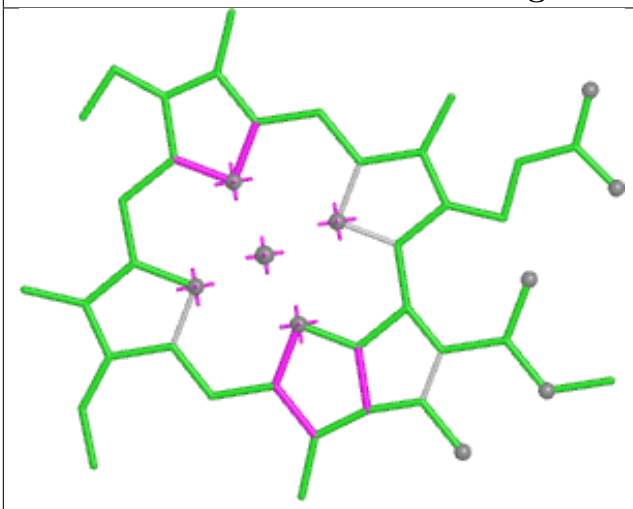


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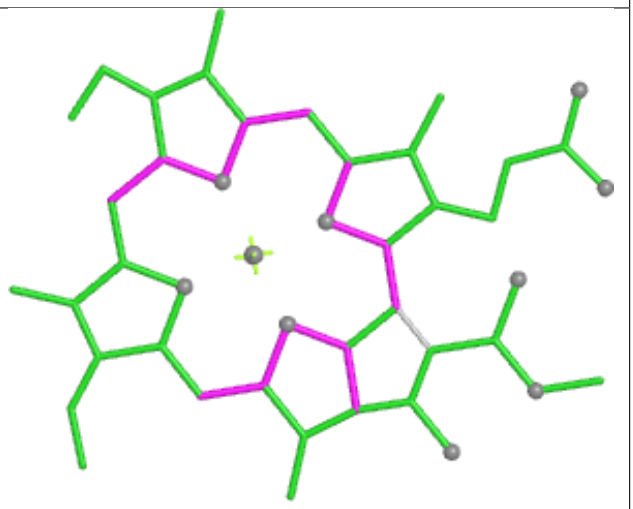


Rings

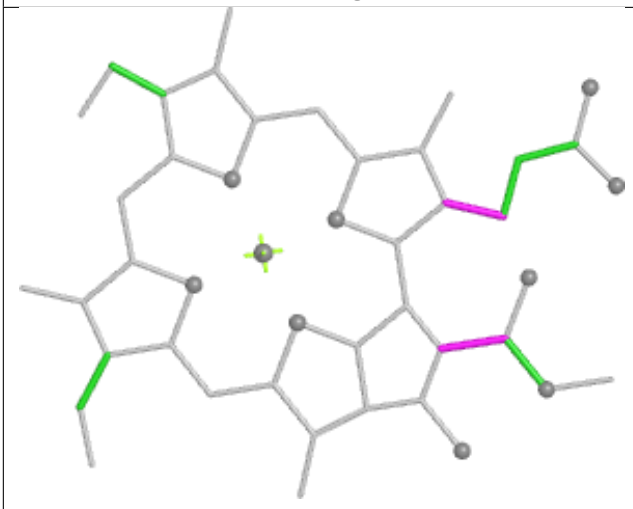
Ligand CLA J 309



Bond lengths



Bond angles

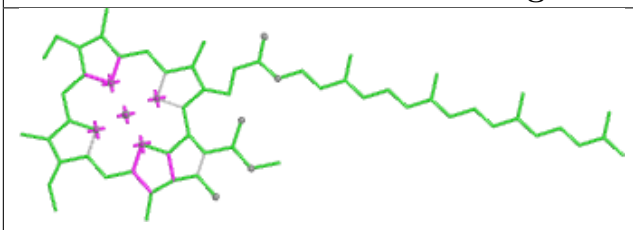


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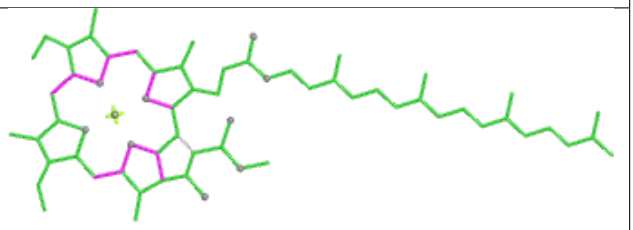


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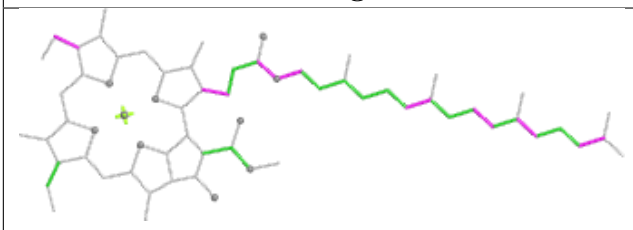
Ligand CLA b 839



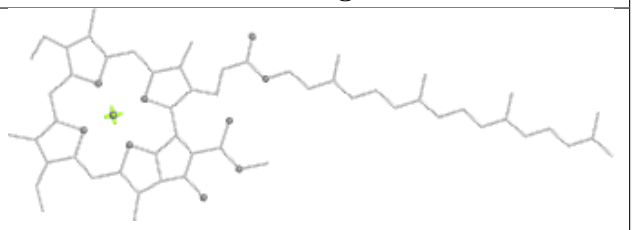
Bond lengths



Bond angles

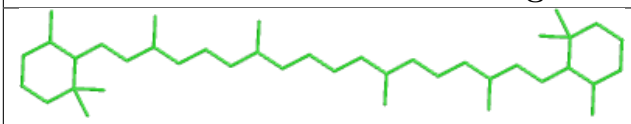


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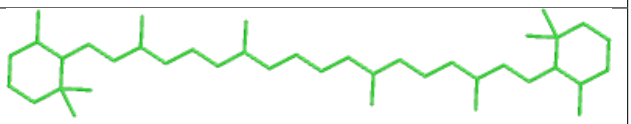


Rings

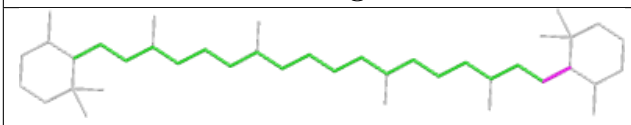
Ligand BCR a 846



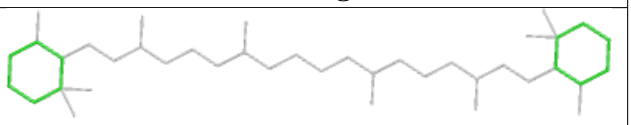
Bond lengths



Bond angles

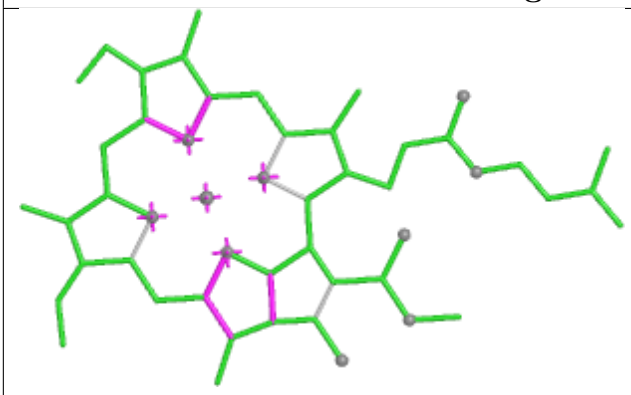


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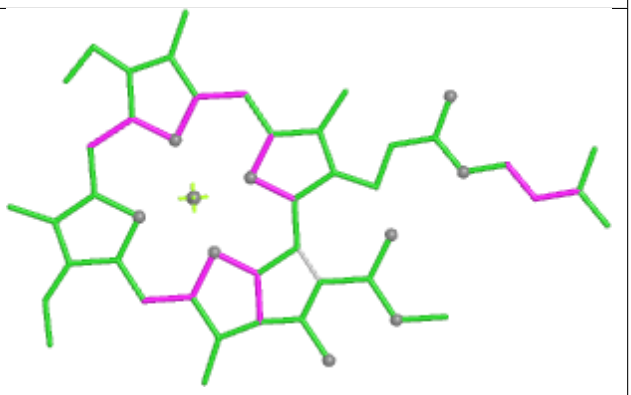


Rings

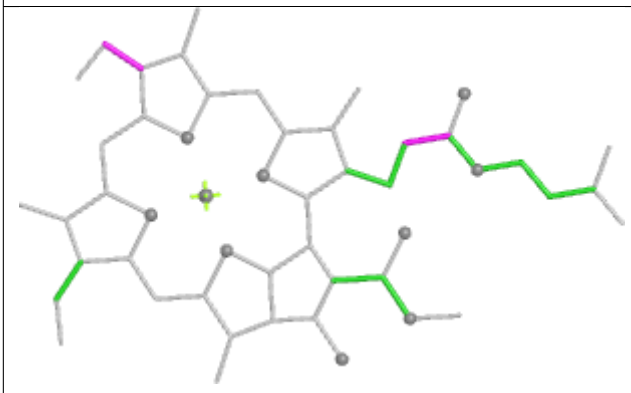
Ligand CLA T 307



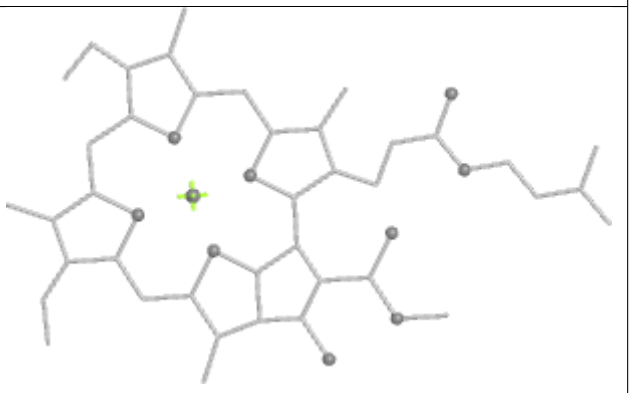
Bond lengths



Bond angles

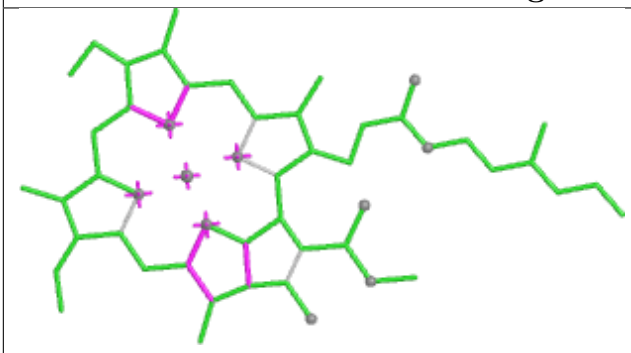


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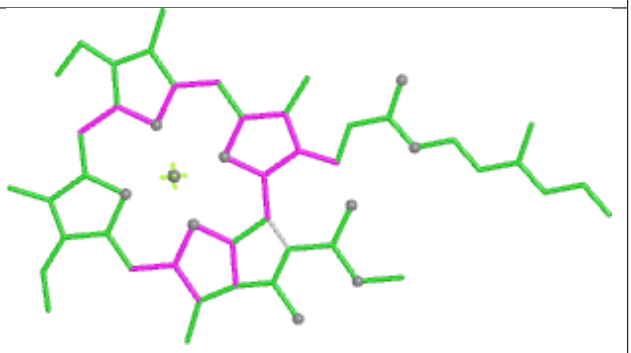


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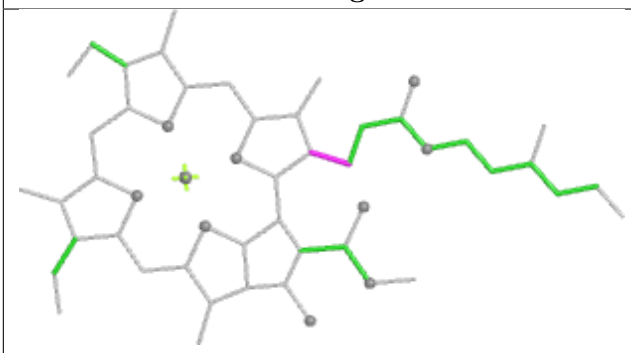
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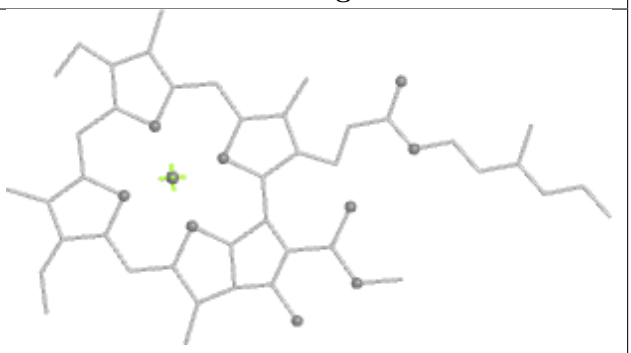
Bond lengths



Bond angles

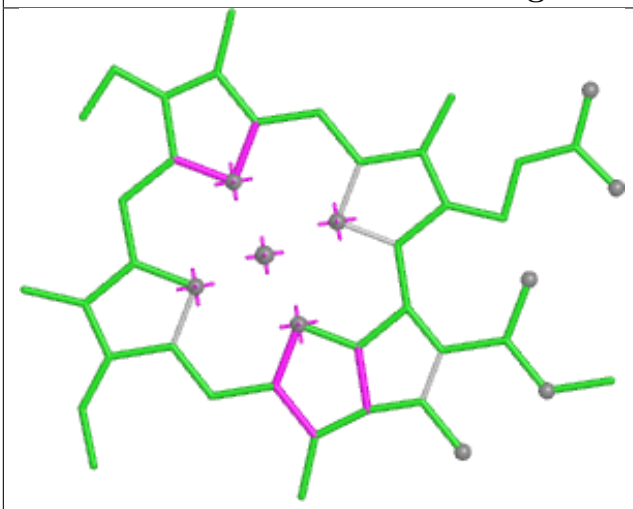


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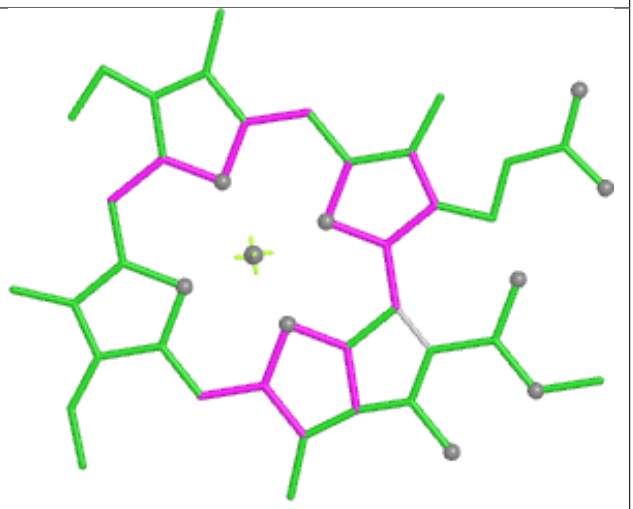


Rings

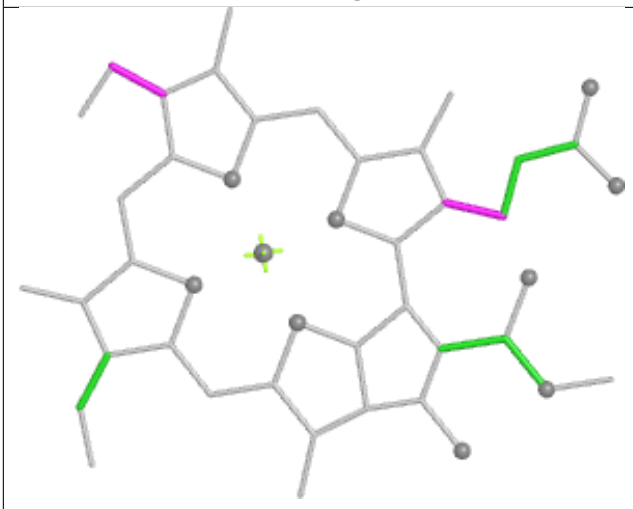
Ligand CLA S 301



Bond lengths



Bond angles

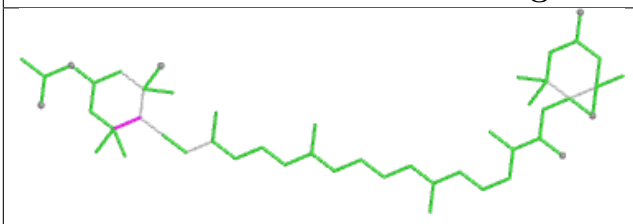


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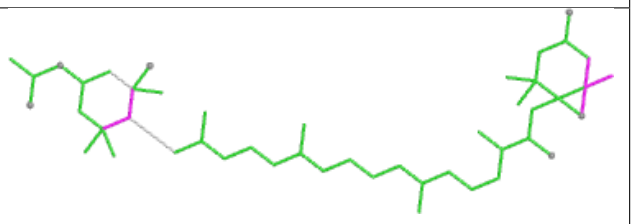


Rings

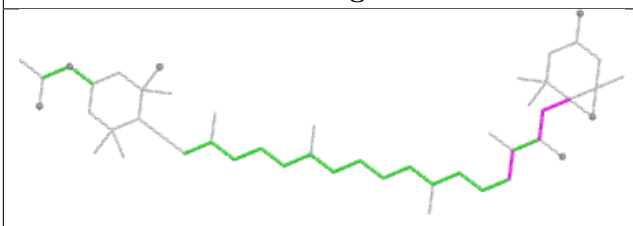
Ligand A86 T 312



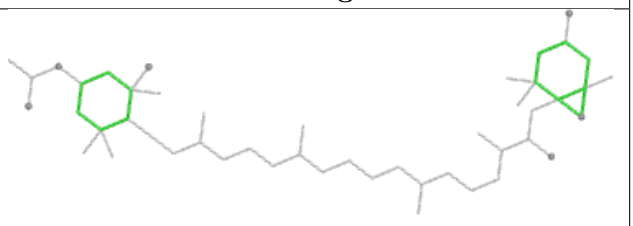
Bond lengths



Bond angles

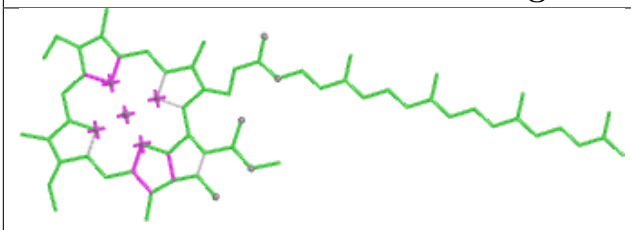


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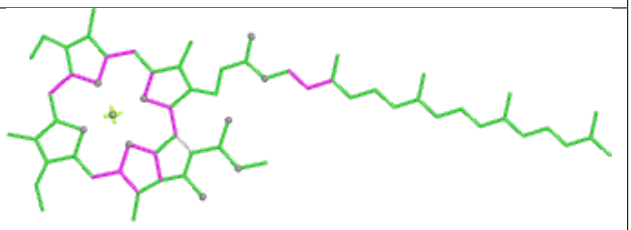


Rings

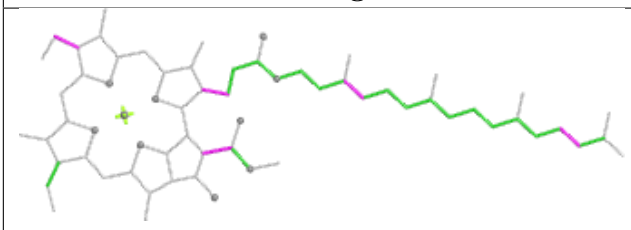
Ligand CLA a 827



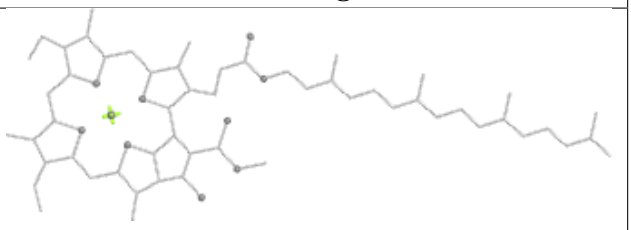
Bond lengths



Bond angles

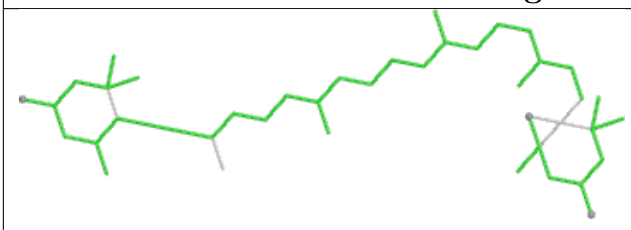


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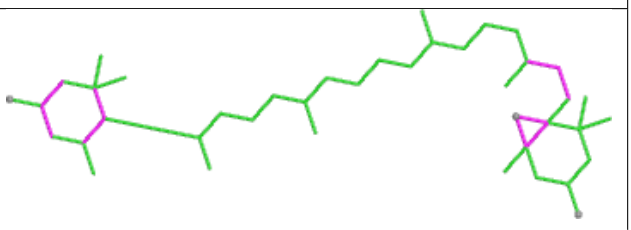


Rings

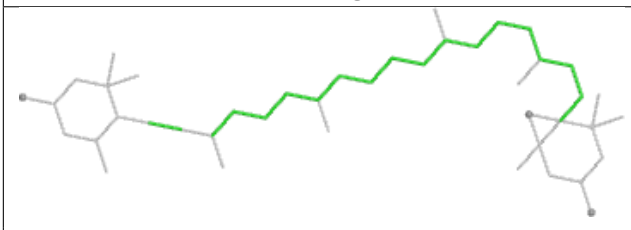
Ligand DD6 U 309



Bond lengths



Bond angles

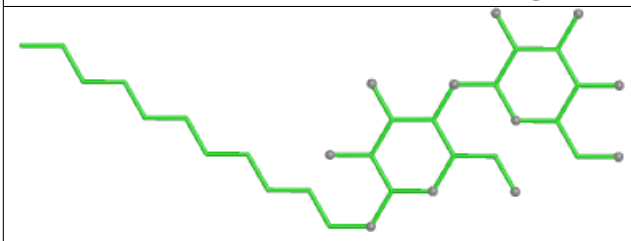


Torsions

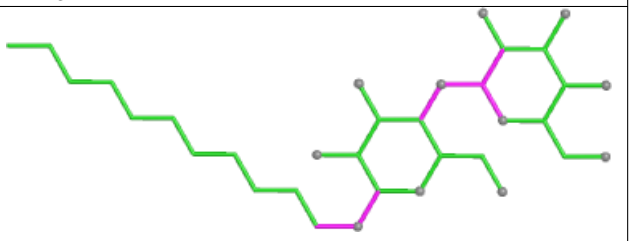


Rings

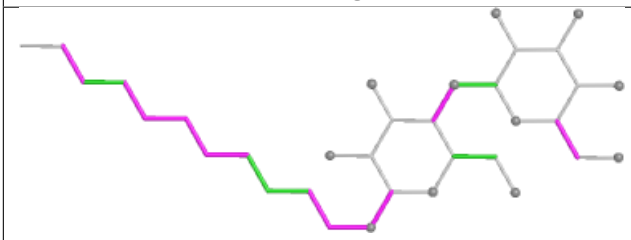
Ligand LMU j 105



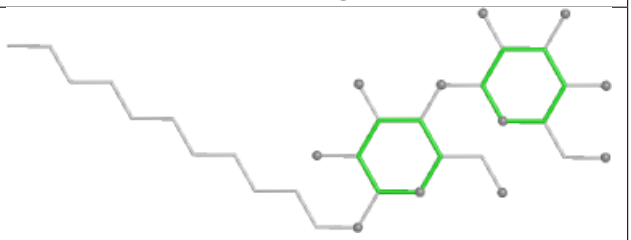
Bond lengths



Bond angles

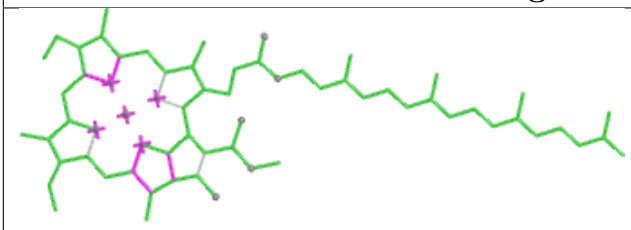


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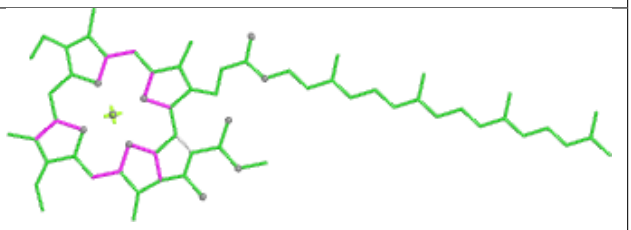


Rings

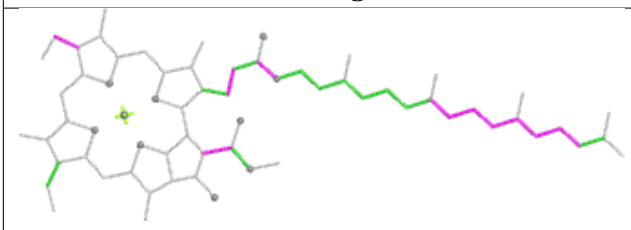
Ligand CLA a 826



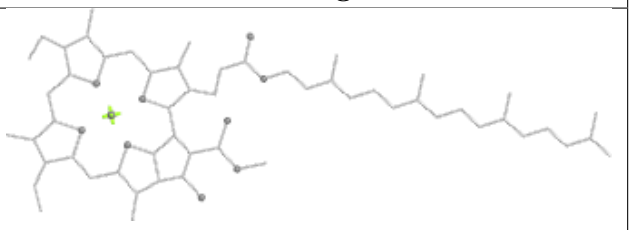
Bond lengths



Bond angles

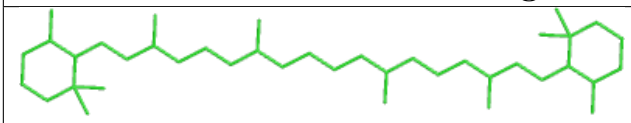


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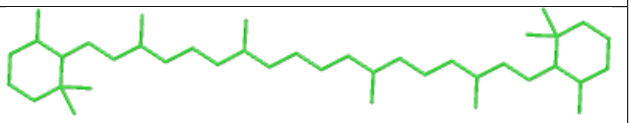


Rings

Ligand BCR m 101



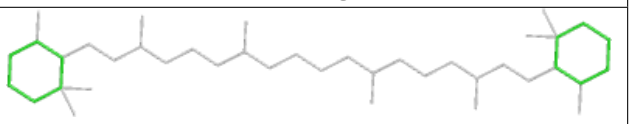
Bond lengths



Bond angles

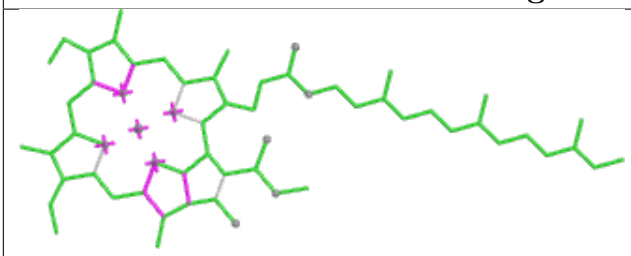


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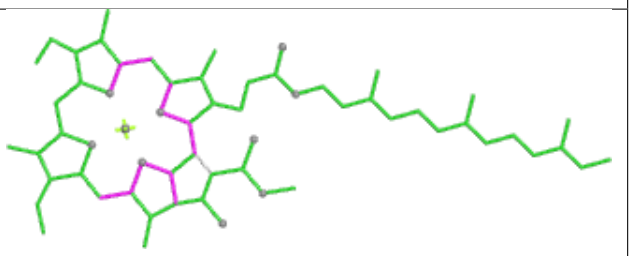


Rings

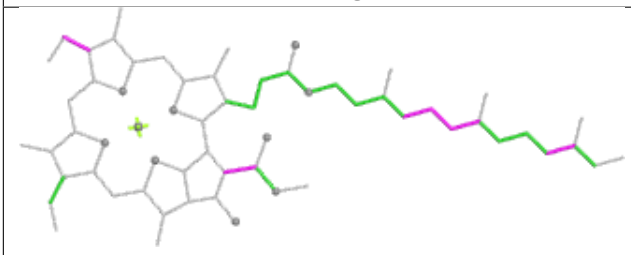
Ligand CLA b 840



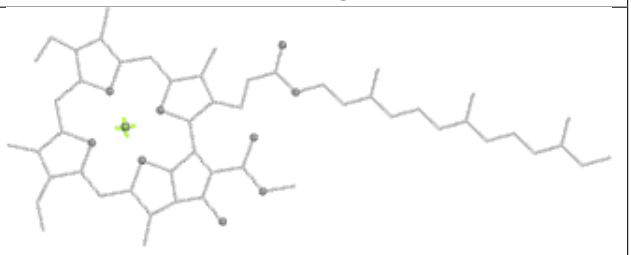
Bond lengths



Bond angles

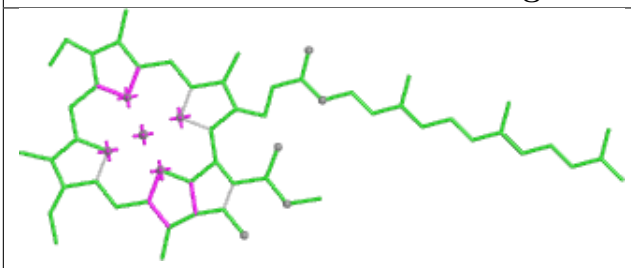


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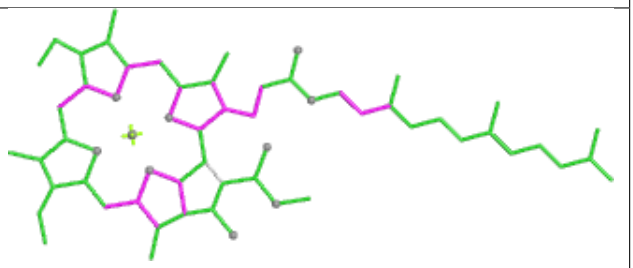


Rings

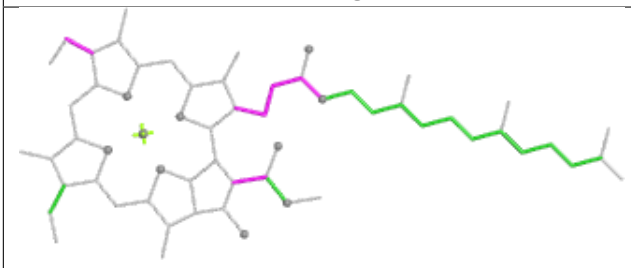
Ligand CLA K 306



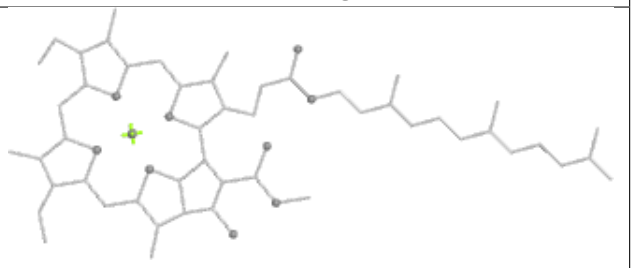
Bond lengths



Bond angles

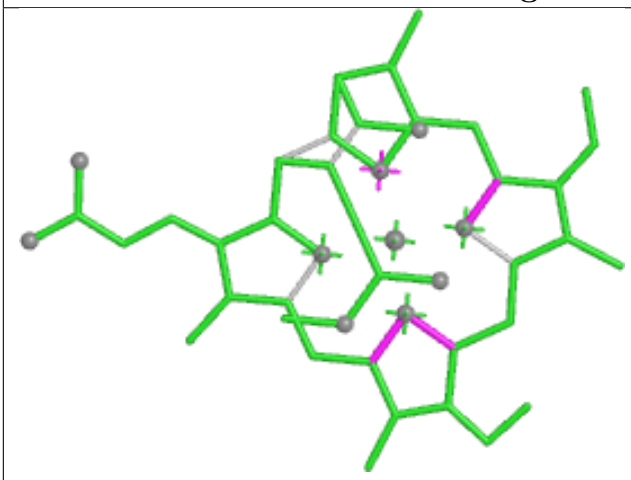


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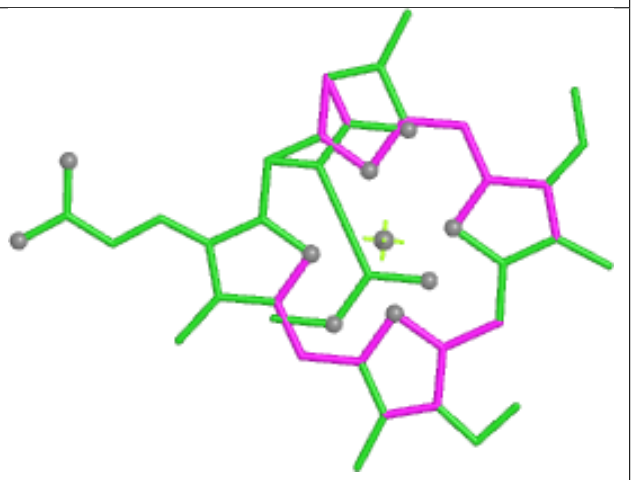


Rings

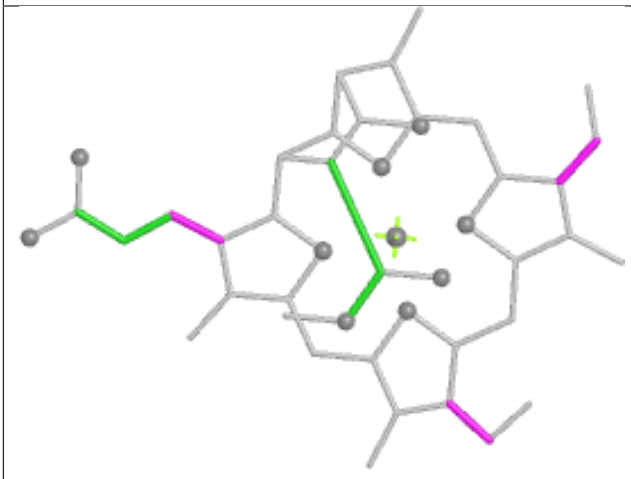
Ligand KC2 W 301



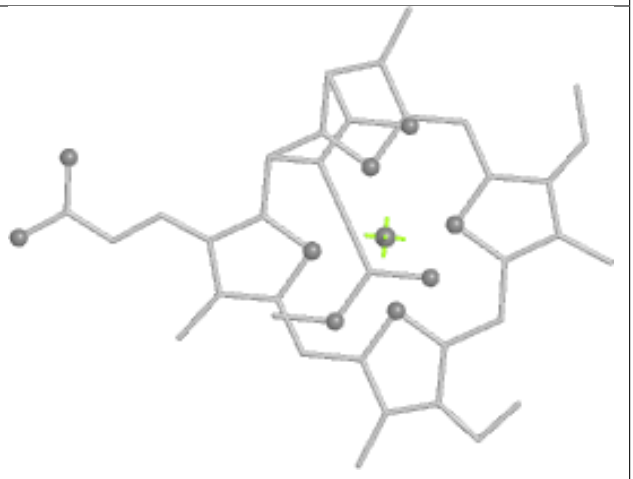
Bond lengths



Bond angles

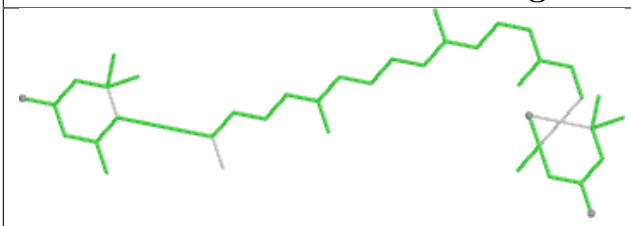


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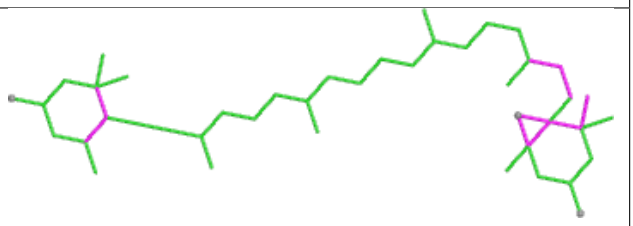


Rings

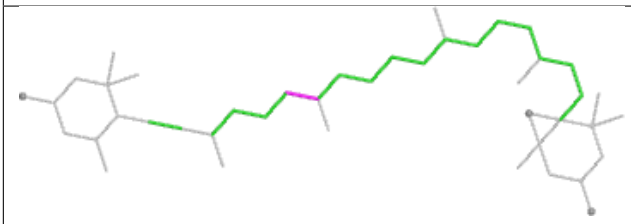
Ligand DD6 k 205



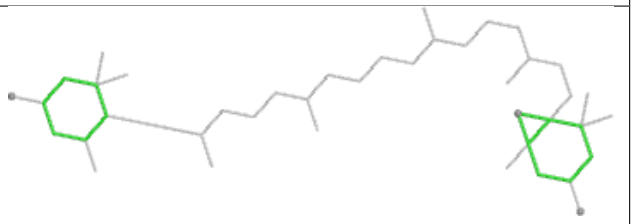
Bond lengths



Bond angles

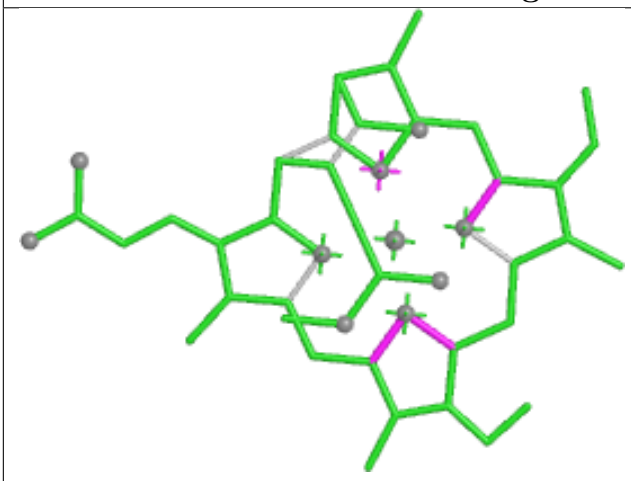


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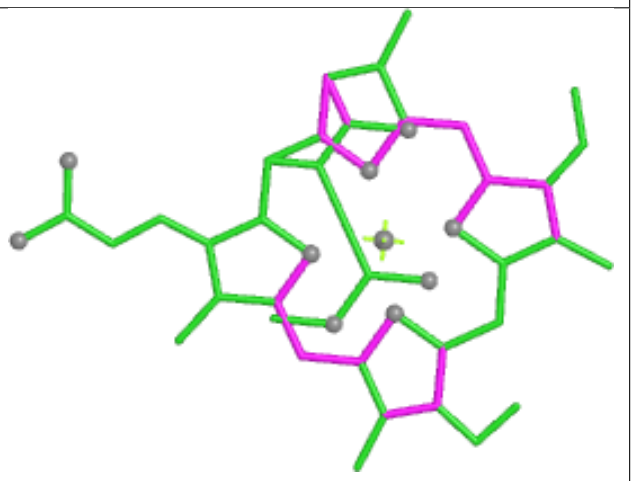


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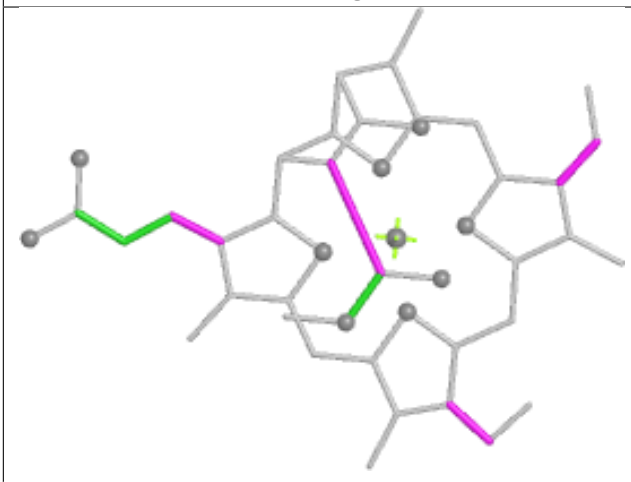
Ligand KC2 M 302



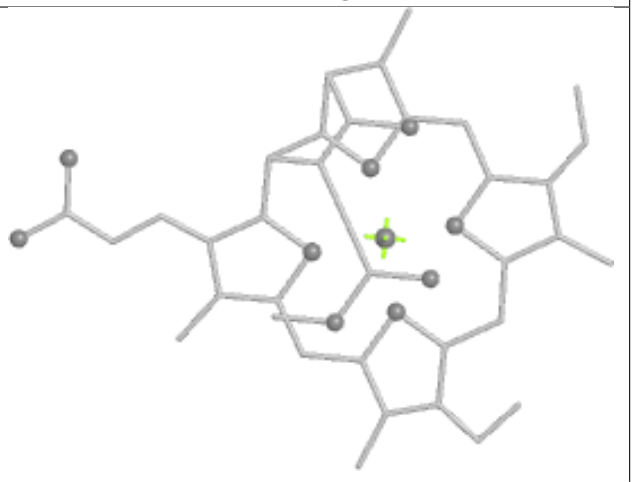
Bond lengths



Bond angles

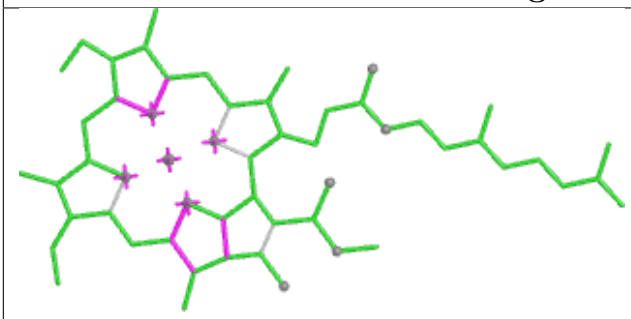


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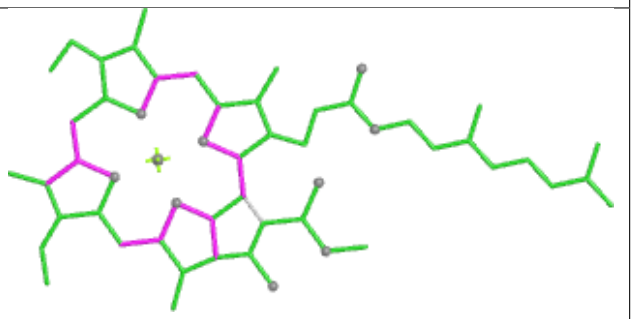


Rings

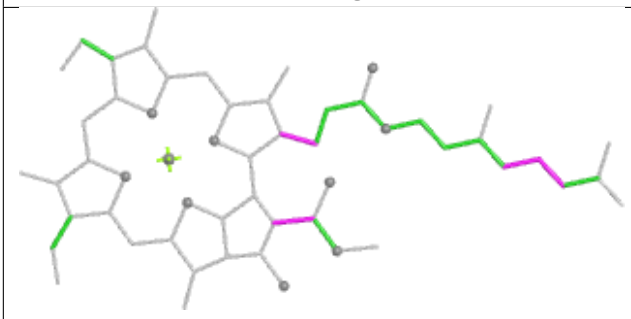
Ligand CLA a 811



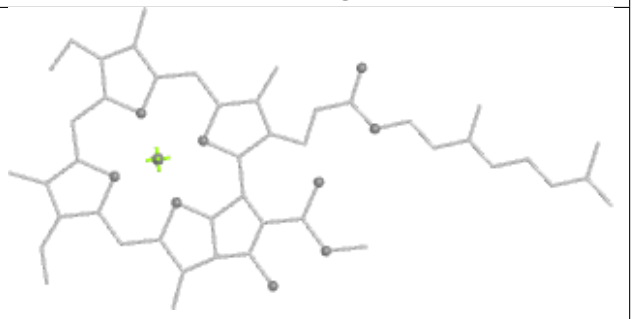
Bond lengths



Bond angles

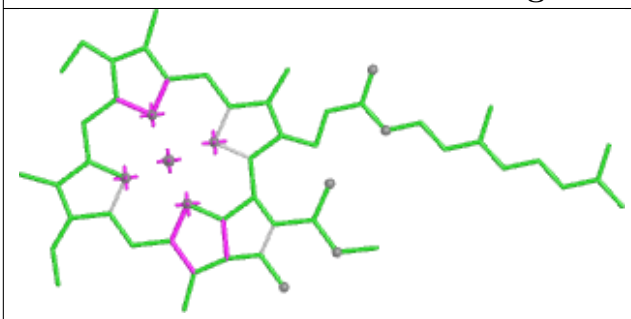


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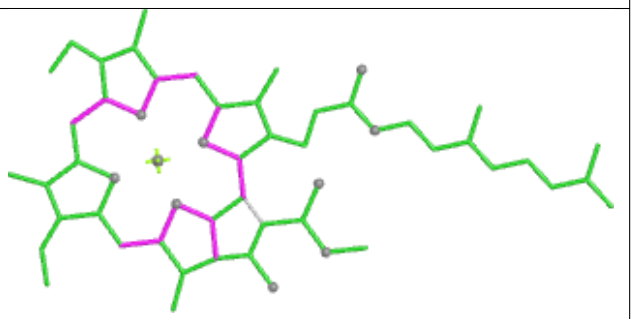


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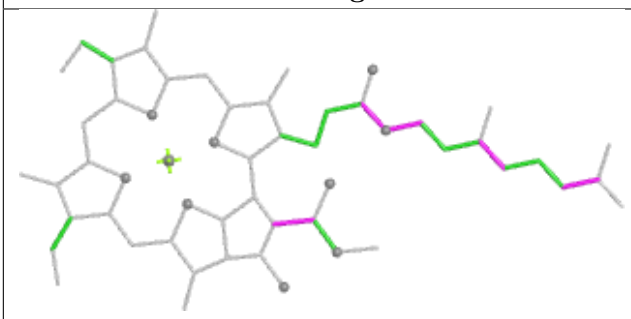
Ligand CLA b 829



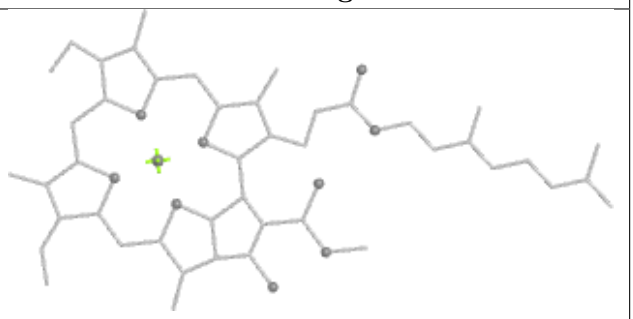
Bond lengths



Bond angles

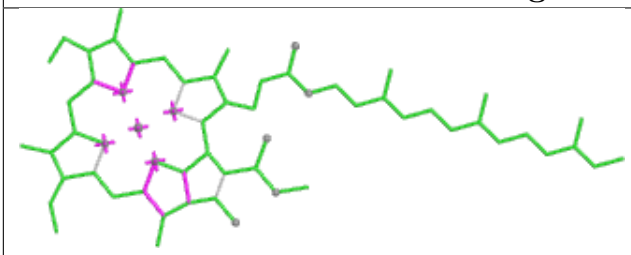


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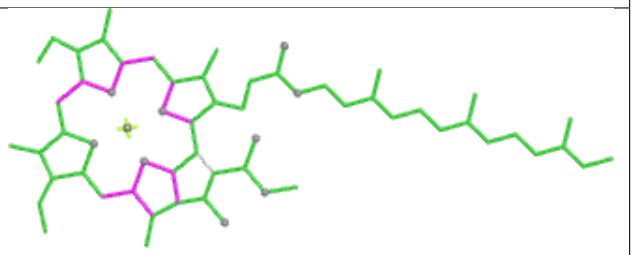


Rings

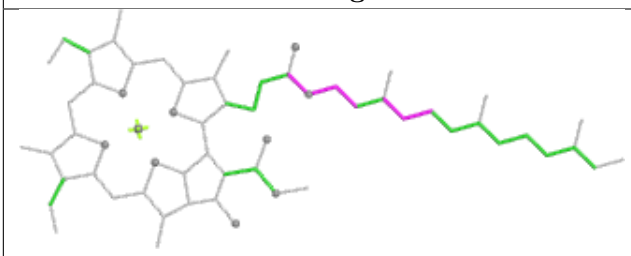
Ligand CLA a 824



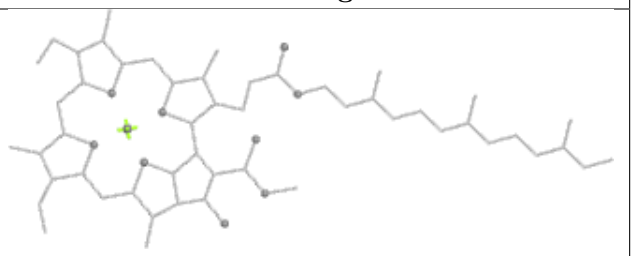
Bond lengths



Bond angles

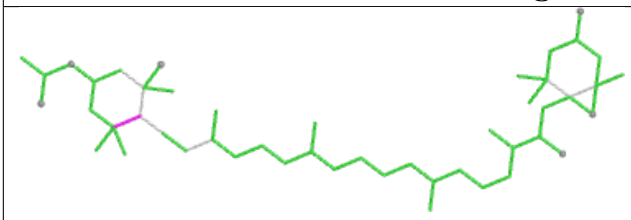


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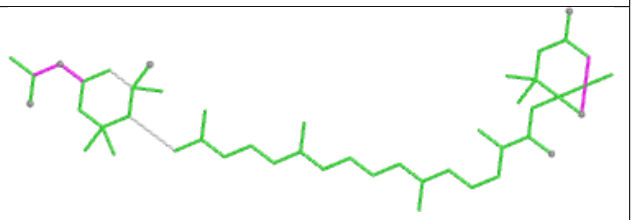


Rings

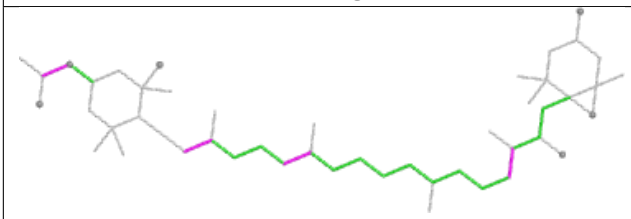
Ligand A86 S 317



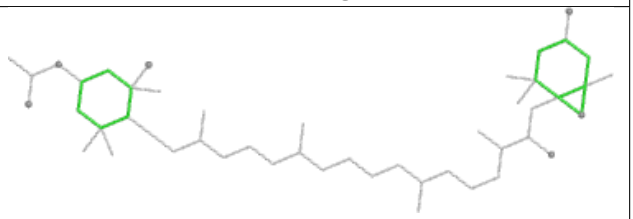
Bond lengths



Bond angles

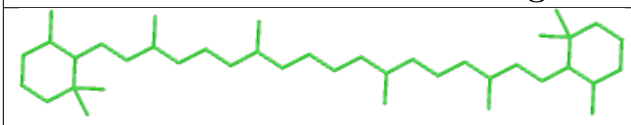


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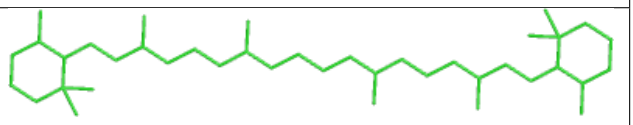


Rings

Ligand BCR r 205



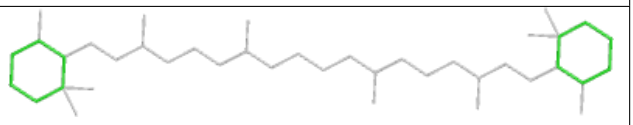
Bond lengths



Bond angles

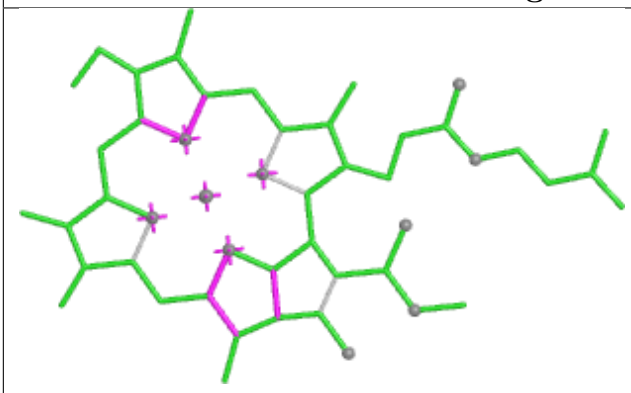


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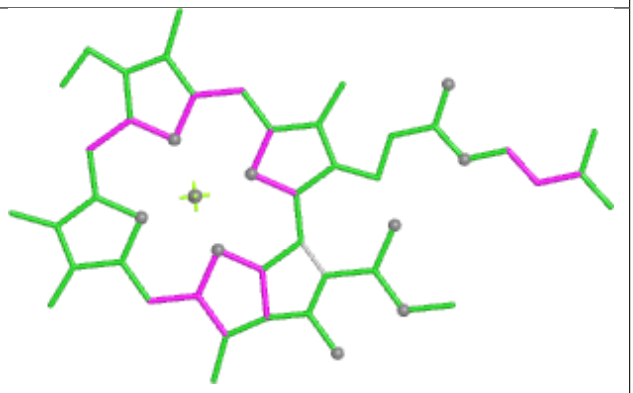


Rings

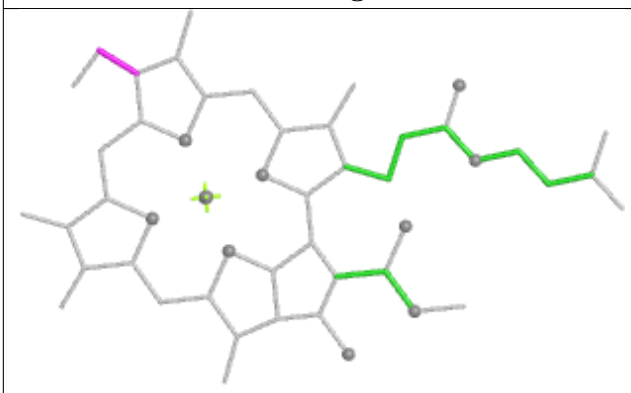
Ligand CLA F 305



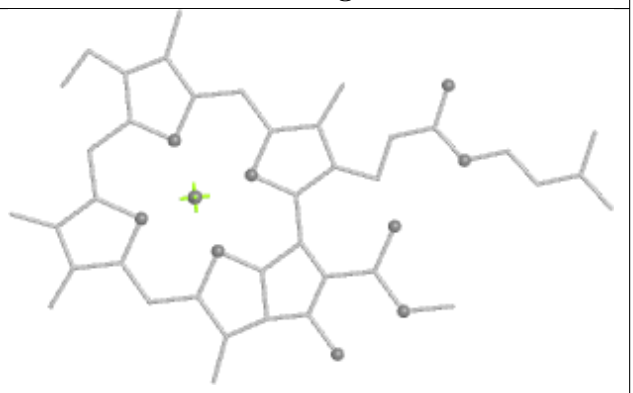
Bond lengths



Bond angles

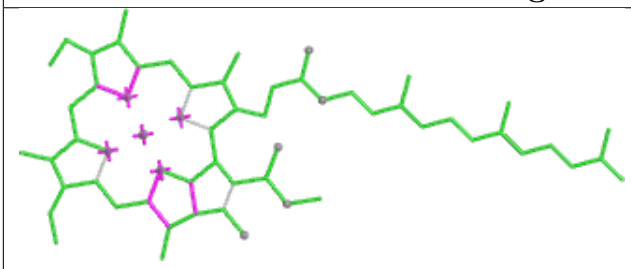


Torsions

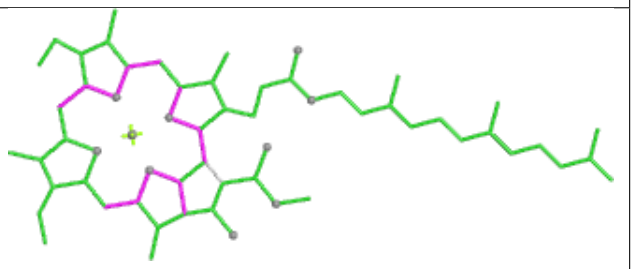


Rings

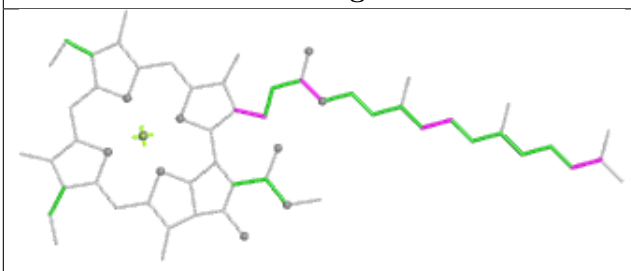
Ligand CLA a 829



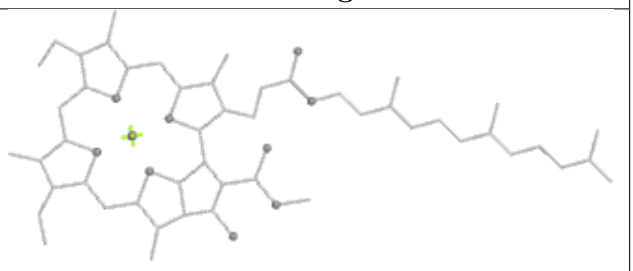
Bond lengths



Bond angles

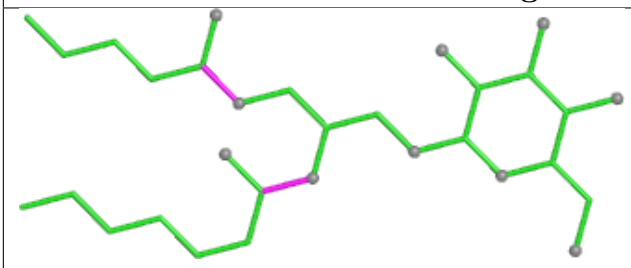


Torsions

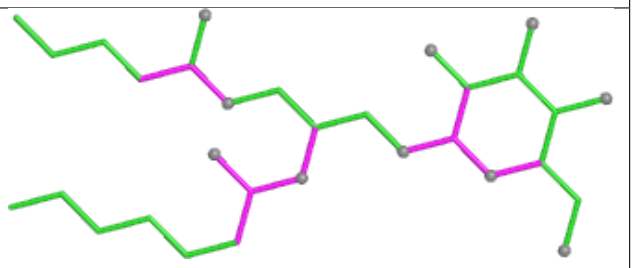


Rings

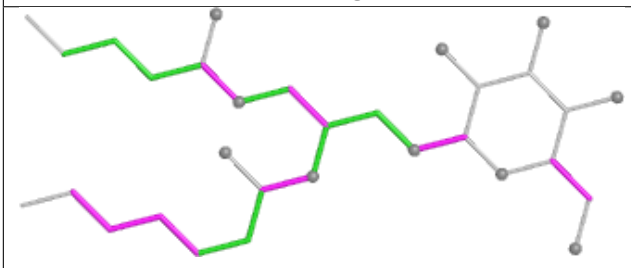
Ligand LMG E 320



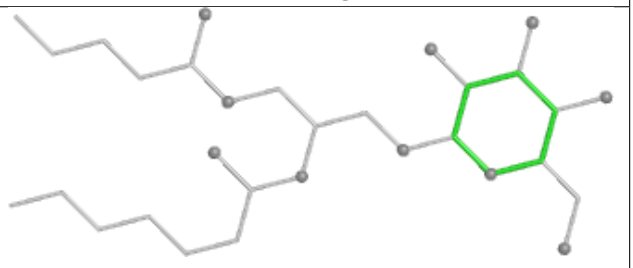
Bond lengths



Bond angles

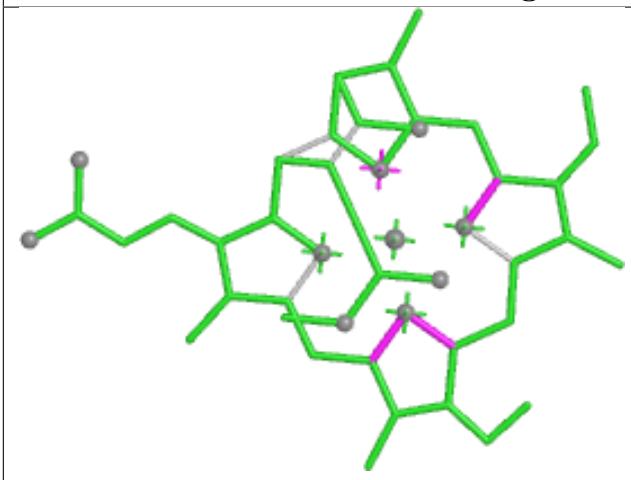


Torsions

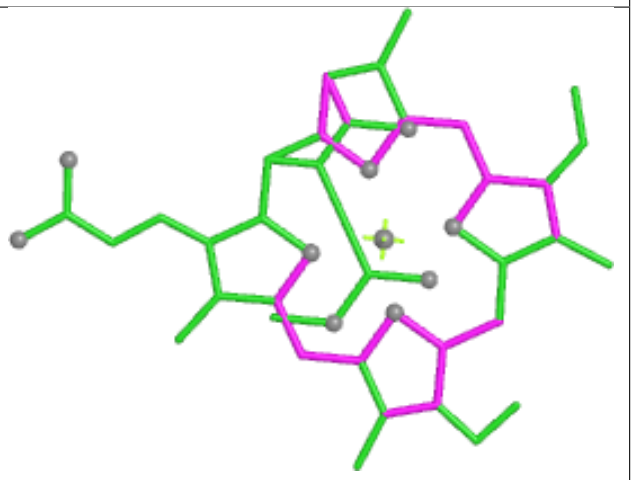


Rings

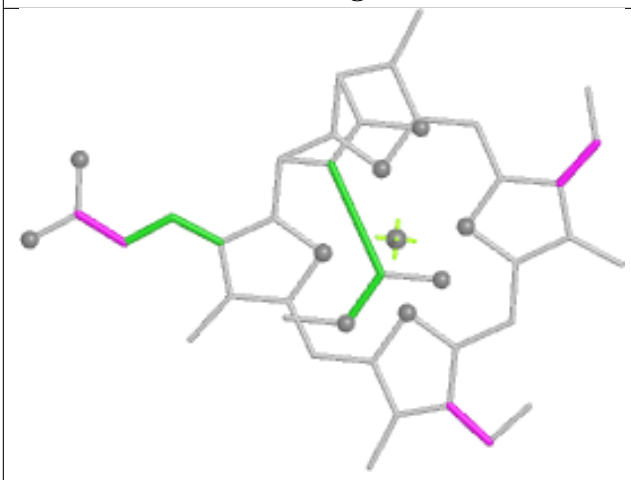
Ligand KC2 W 303



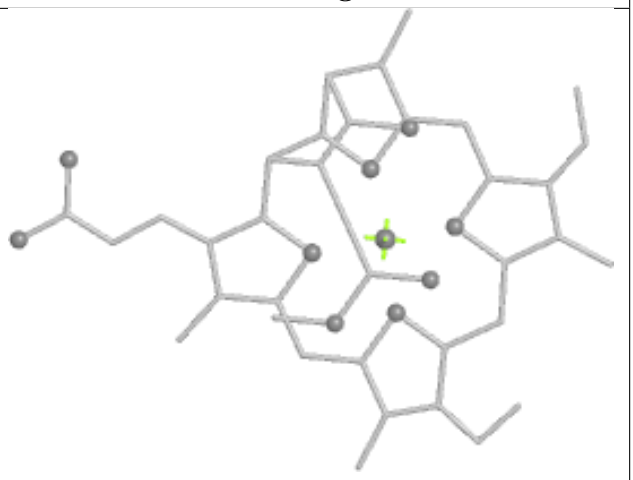
Bond lengths



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.

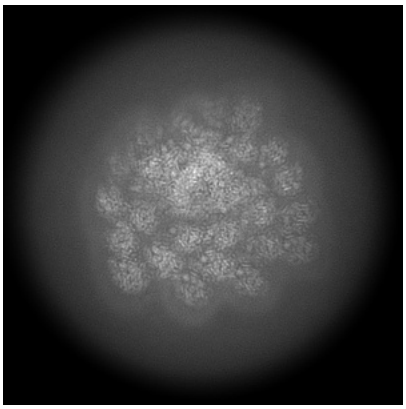
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39717. These allow visual inspection of the internal detail of the map and identification of artifacts.

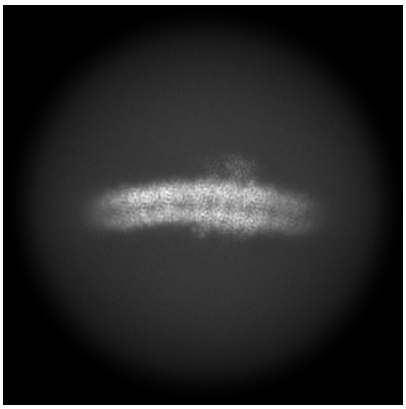
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

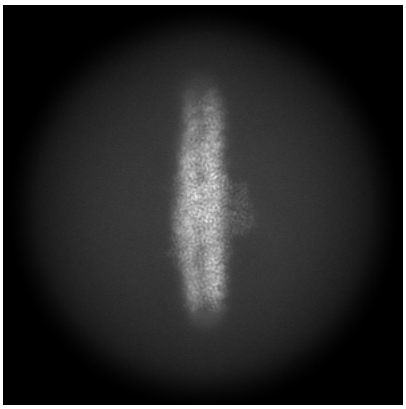
6.1.1 Primary map



X

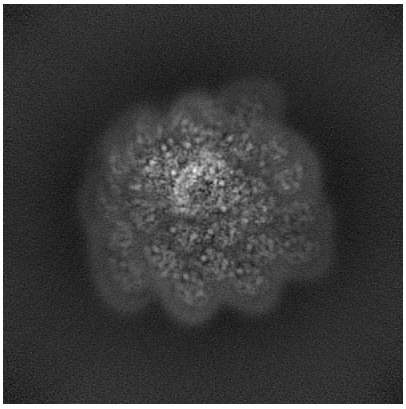


Y

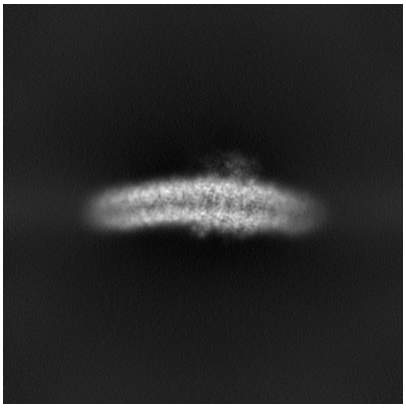


Z

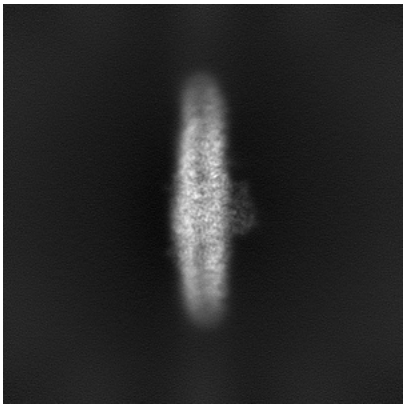
6.1.2 Raw map



X



Y

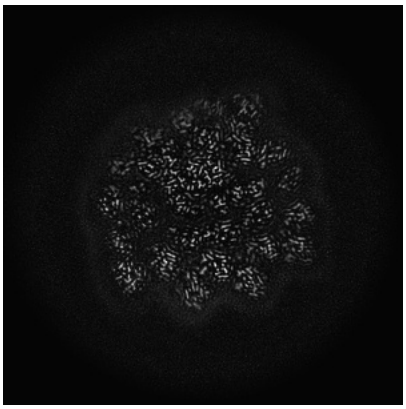


Z

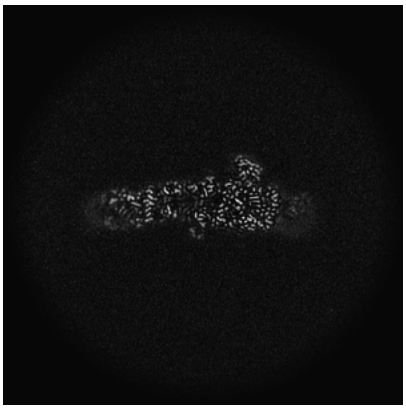
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

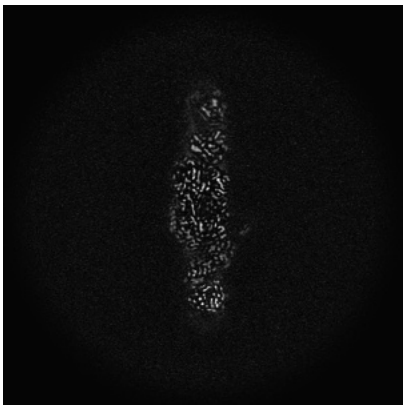
6.2.1 Primary map



X Index: 200

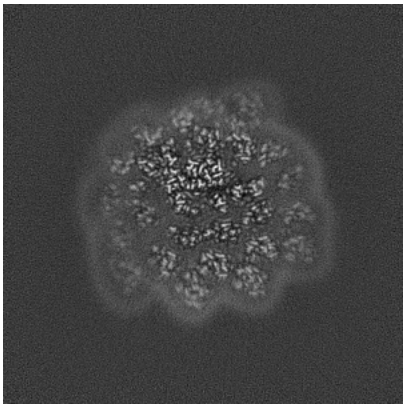


Y Index: 200

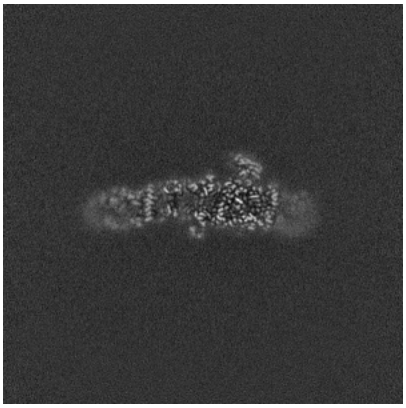


Z Index: 200

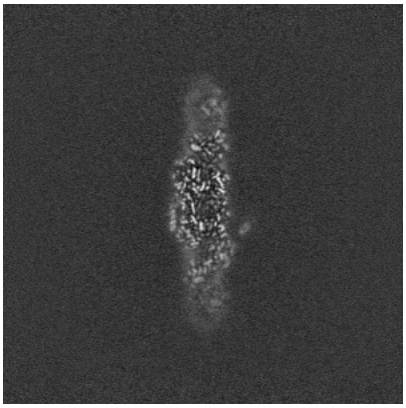
6.2.2 Raw map



X Index: 200



Y Index: 200

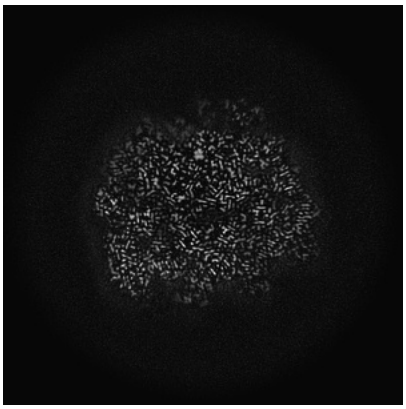


Z Index: 200

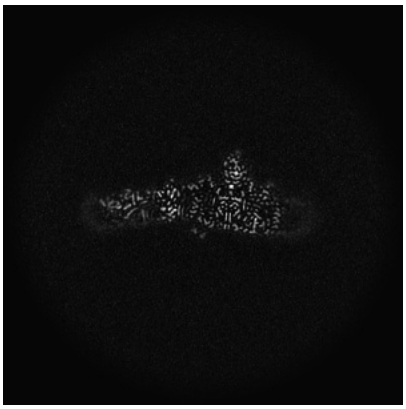
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 210

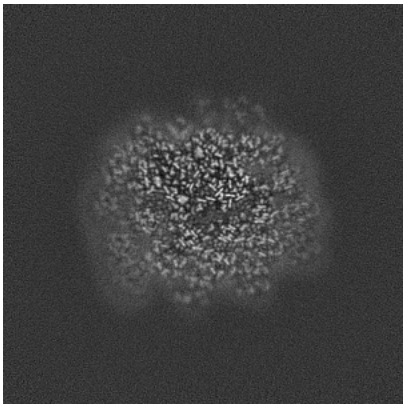


Y Index: 191

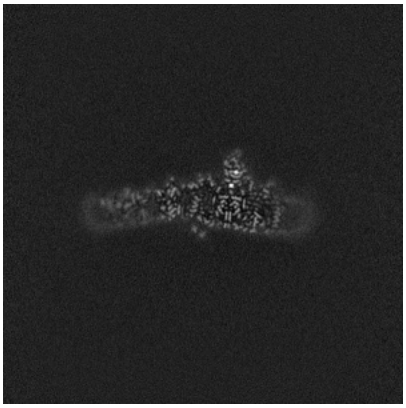


Z Index: 232

6.3.2 Raw map



X Index: 211



Y Index: 191

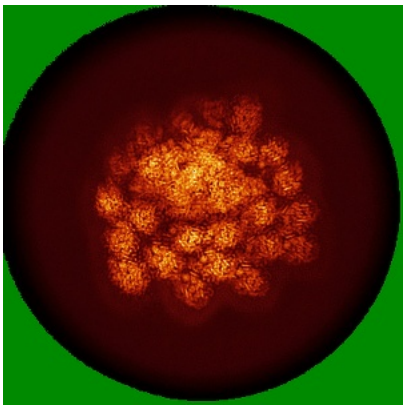


Z Index: 232

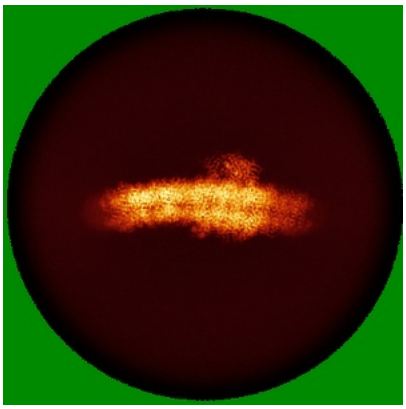
The images above show the largest variance slices of the map in three orthogonal directions.

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

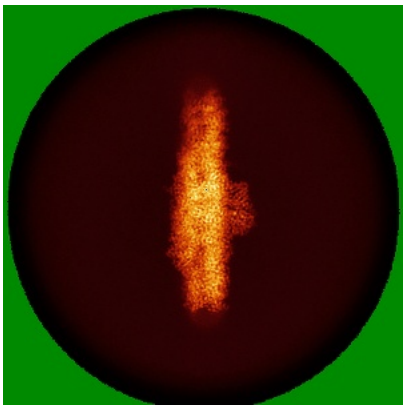
6.4.1 Primary map



X

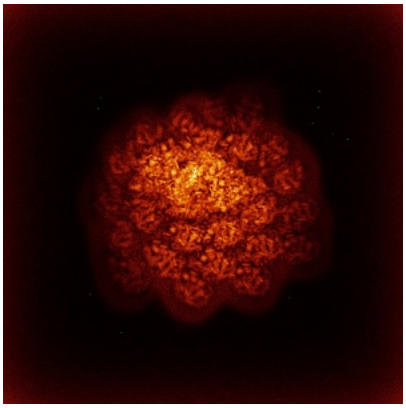


Y

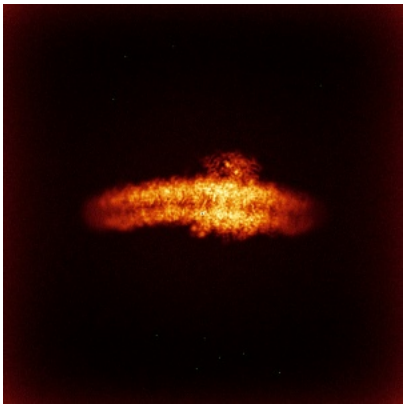


Z

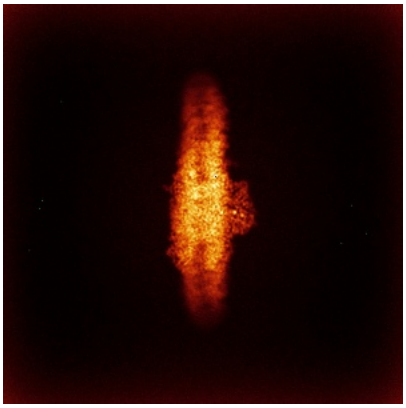
6.4.2 Raw map



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

6.5.2 Raw map



X Y Z

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

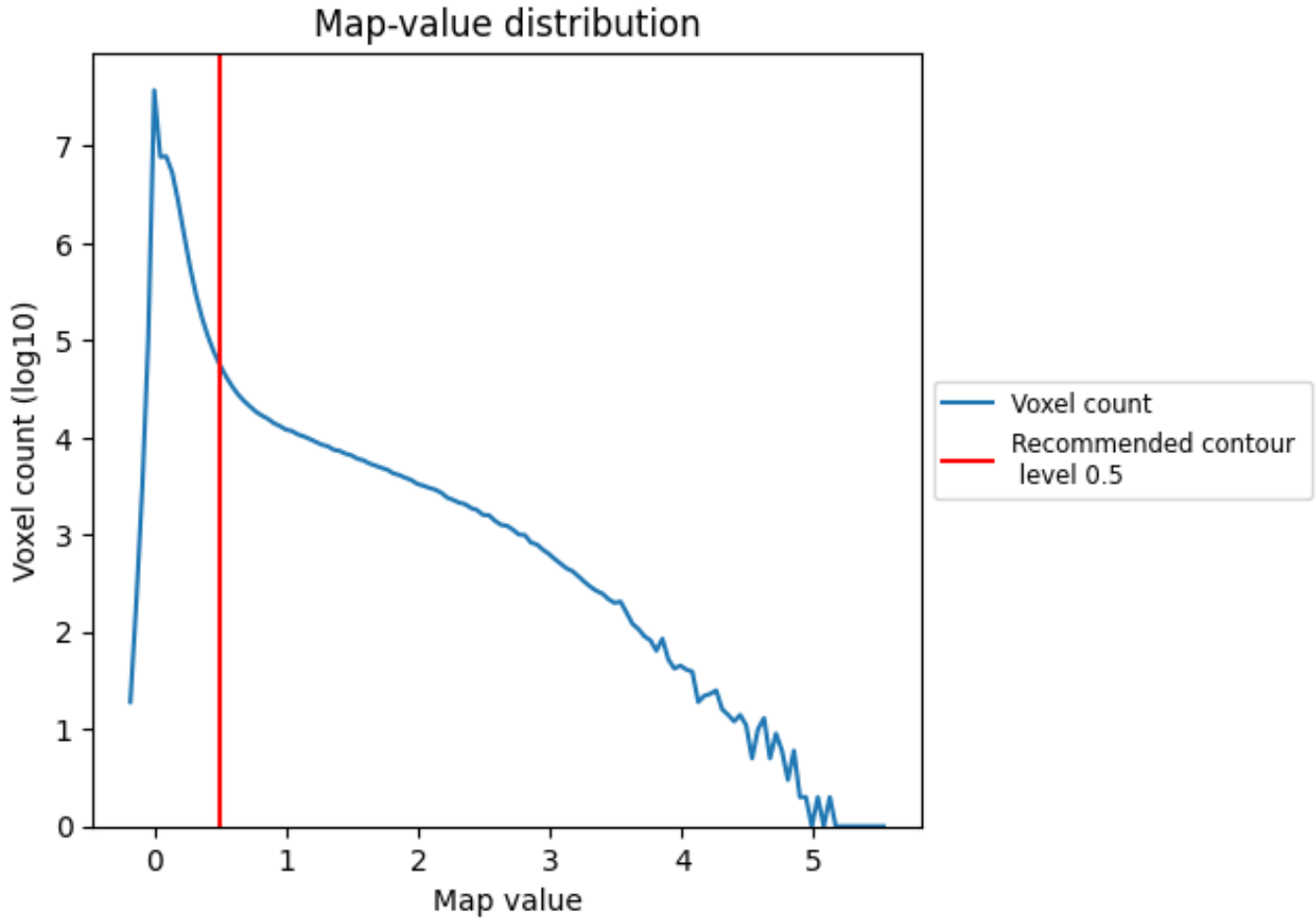
6.6 Mask visualisation (i)

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

7 Map analysis

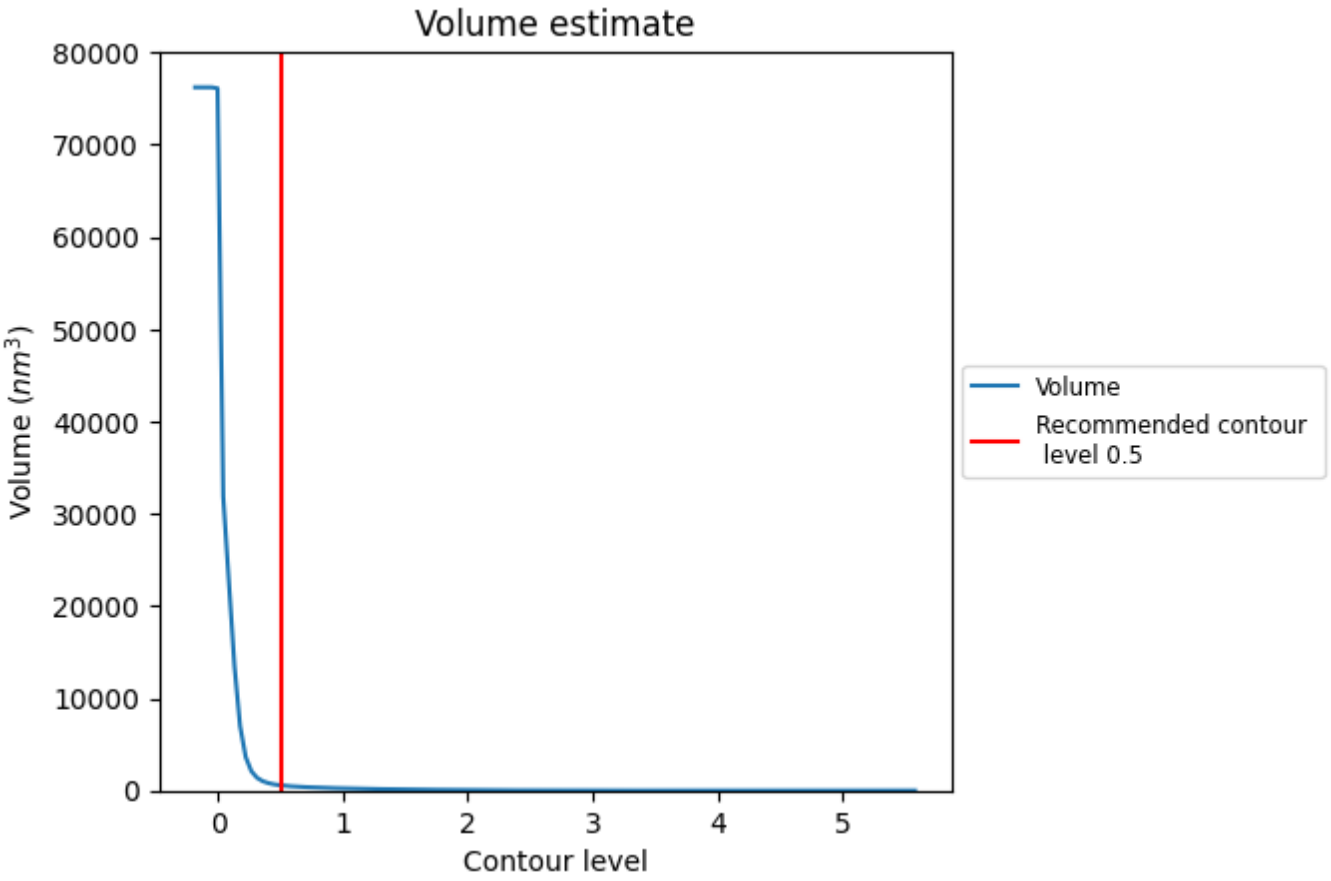
This section contains the results of statistical analysis of the map.

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.

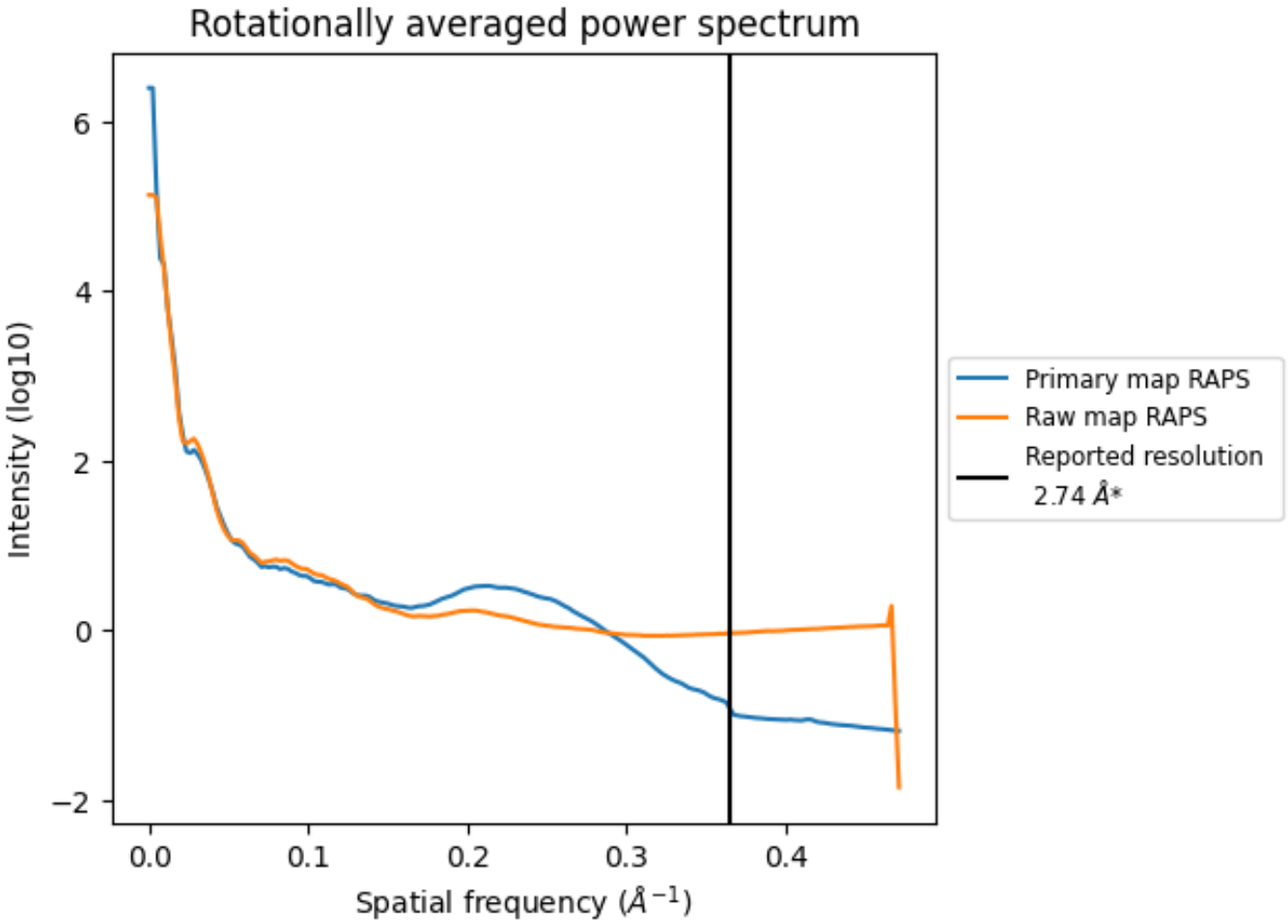
7.2 Volume estimate



The volume at the recommended contour level is 575 nm^3; this corresponds to an approximate mass of 519 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)

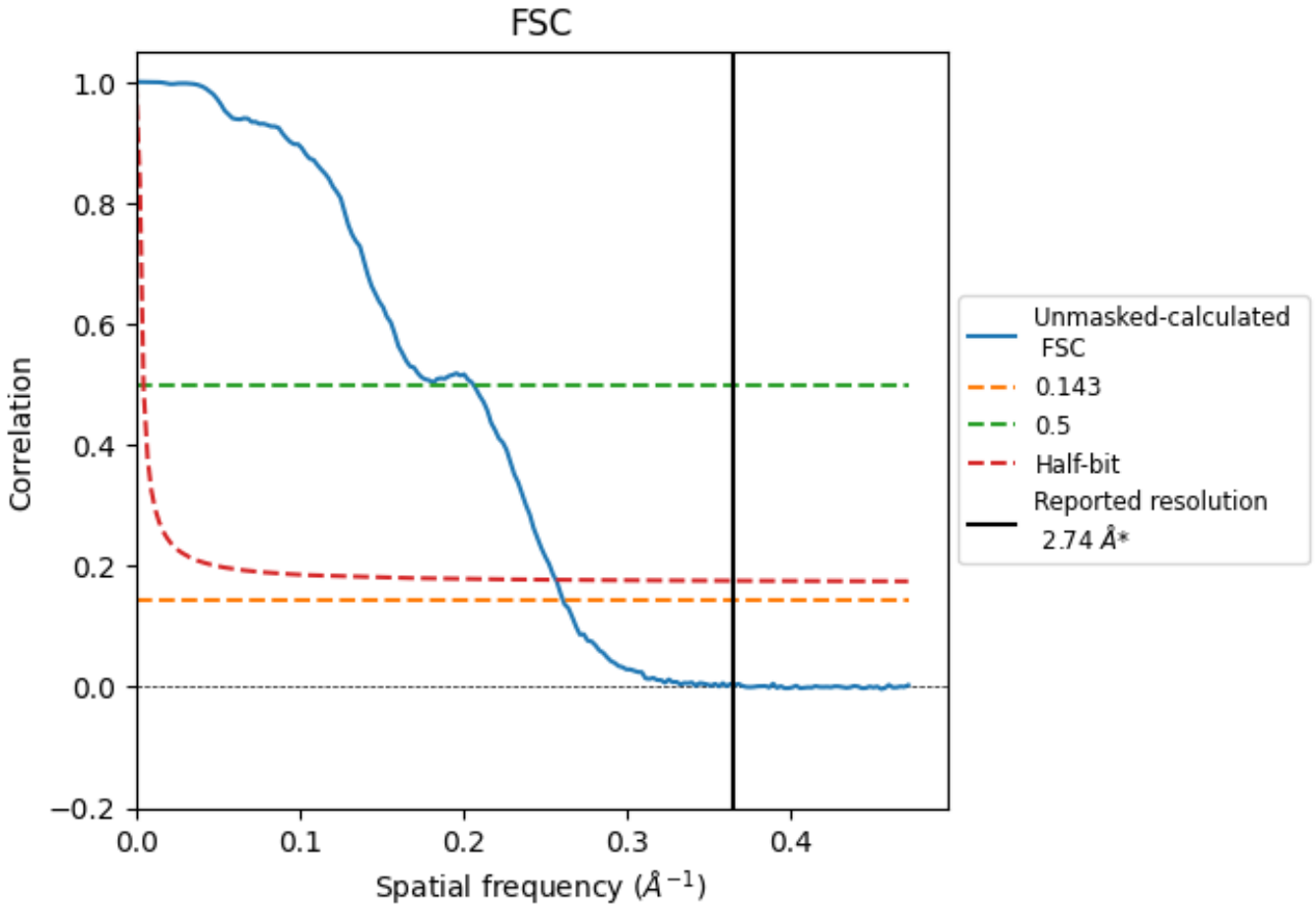


*Reported resolution corresponds to spatial frequency of 0.365 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.365 Å^{-1}

8.2 Resolution estimates (i)

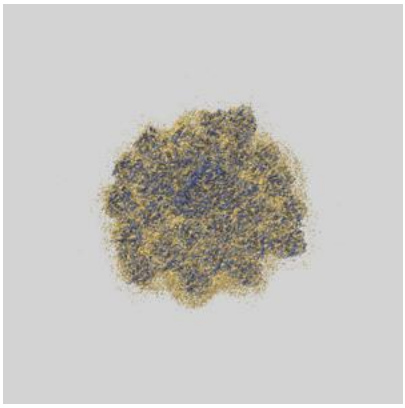
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	4.85	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 2.74 by more than 10 %

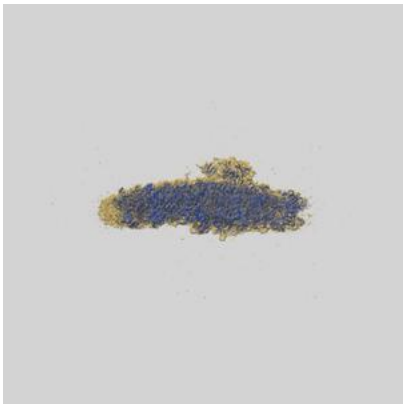
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39717 and PDB model 8Z11. Per-residue inclusion information can be found in section 3 on page 41.

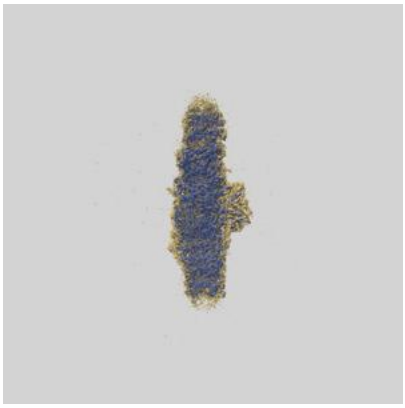
9.1 Map-model overlay



X



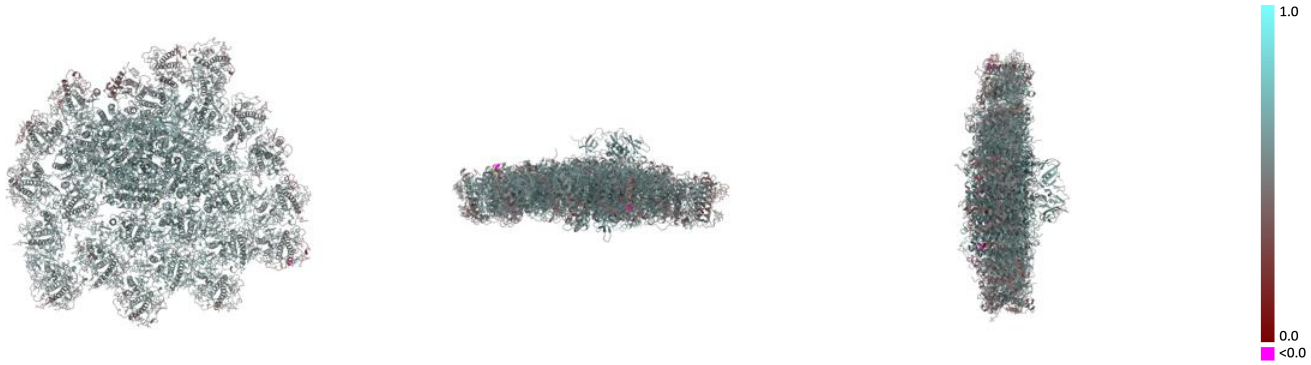
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

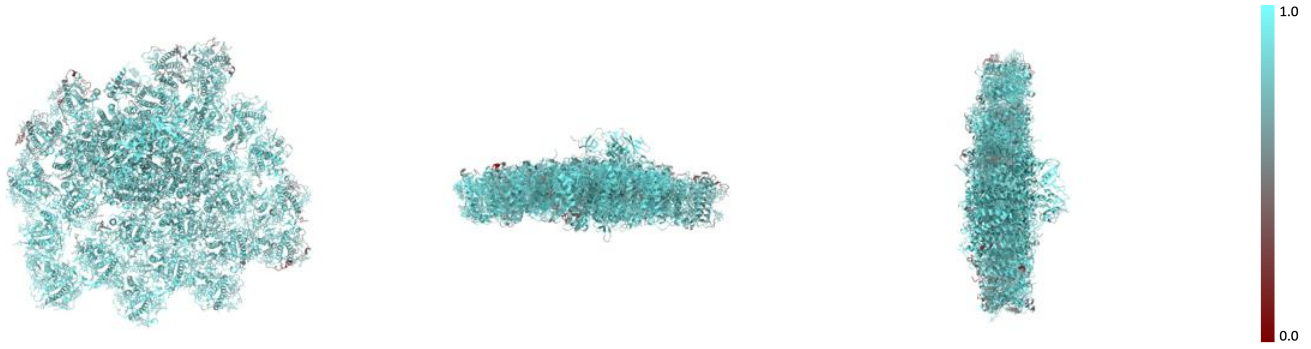
9.2 Q-score mapped to coordinate model (i)



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.

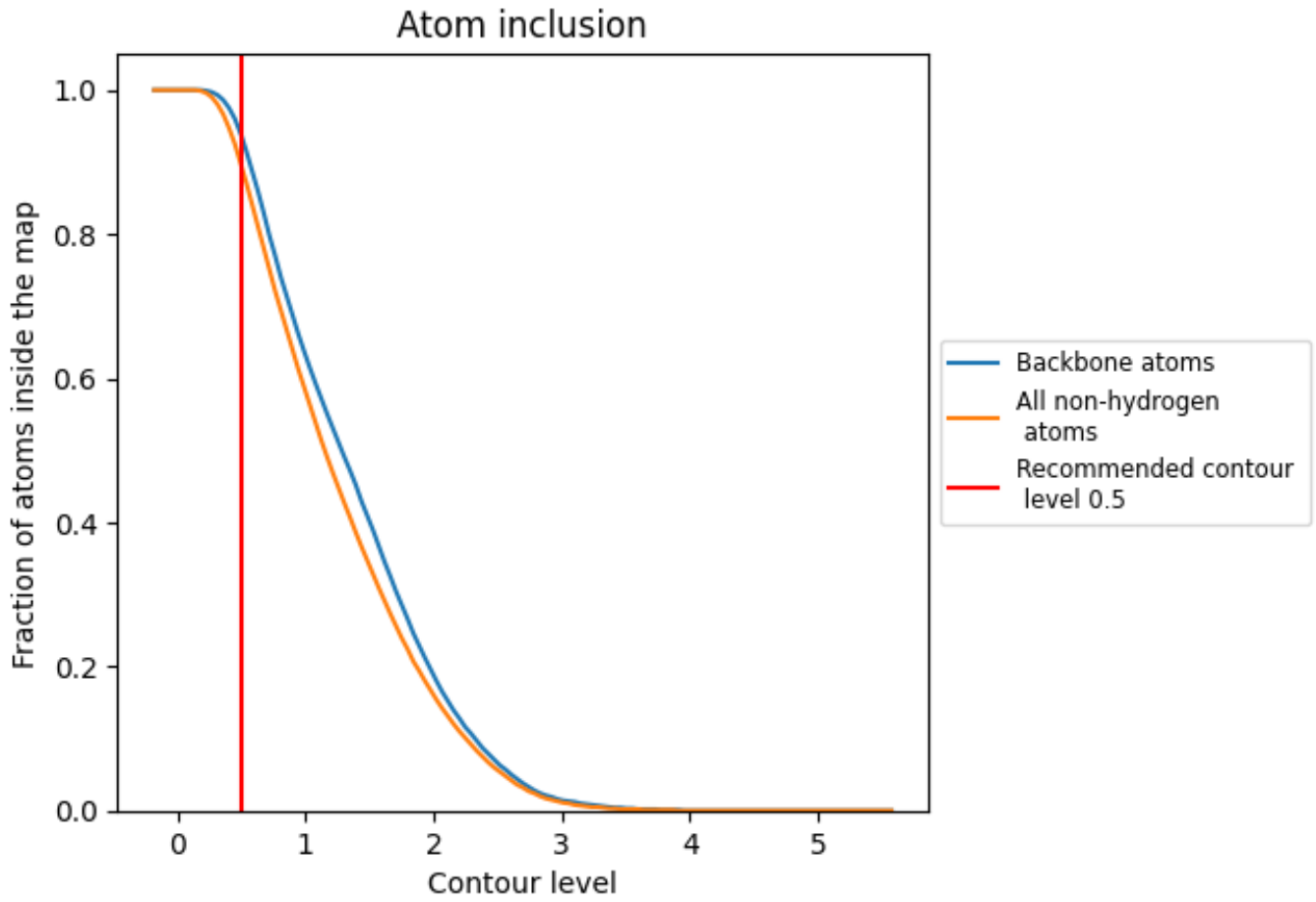
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.5540
A	0.9310	0.5850
B	0.8270	0.4560
C	0.7020	0.4480
D	0.9360	0.5930
E	0.9290	0.5770
F	0.9270	0.5630
G	0.8590	0.5040
H	0.7340	0.4810
I	0.9360	0.5770
J	0.8740	0.5120
K	0.8540	0.4960
L	0.7800	0.5020
M	0.8860	0.5630
N	0.9480	0.5340
O	0.8590	0.5240
P	0.7880	0.5110
Q	0.9360	0.5540
R	0.7400	0.4820
S	0.8870	0.5170
T	0.8950	0.5000
U	0.7030	0.4630
V	0.9140	0.5920
W	0.9540	0.5780
a	0.9600	0.6160
b	0.9620	0.6110
c	0.9680	0.5860
d	0.9330	0.5640
e	0.8630	0.5660
f	0.9020	0.5840
i	0.9090	0.5680
j	0.9090	0.5940
k	0.9480	0.5680
l	0.9540	0.5790
m	0.9100	0.5640
r	0.8910	0.5630

