wwPDB EM Validation Summary Report (i)

Sep 10, 2026 – 12:32 AM JST

PDB ID	:	6J3Z / pdb_00006j3z
EMDB ID	:	EMD-9776
Title	:	Structure of C2S1M1-type PSII-FCPII supercomplex from diatom
Authors	:	Nagao, R.; Kato, K.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on	:	2019-01-07
Resolution	:	3.60 Å(reported)
Based on initial models	:	3JCU, 3WU2

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

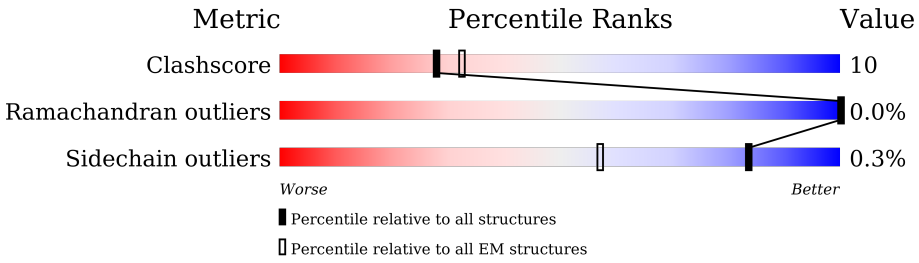
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

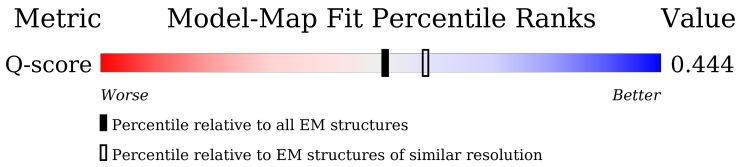
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	83% 14% .
1	a	344	84% 13% .
2	B	509	82% 13% 5%
2	b	509	81% 14% 5%

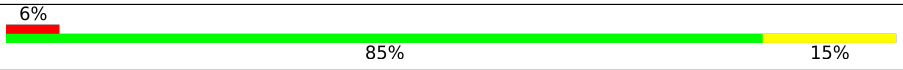
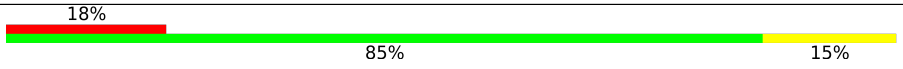
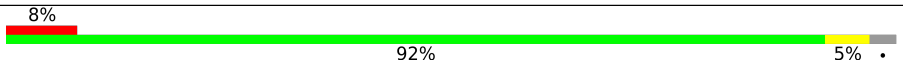
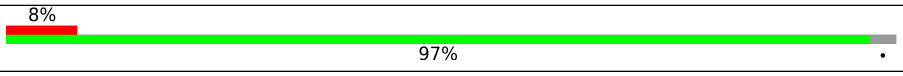
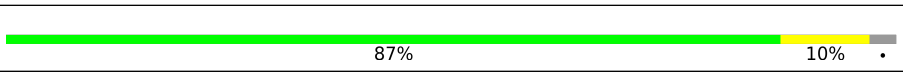
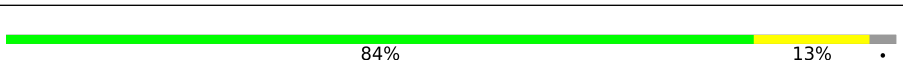
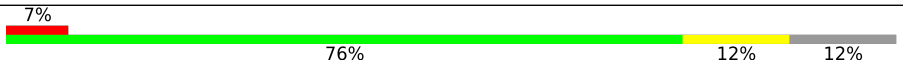
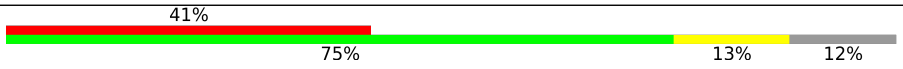
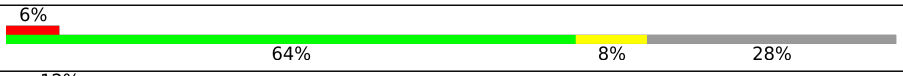
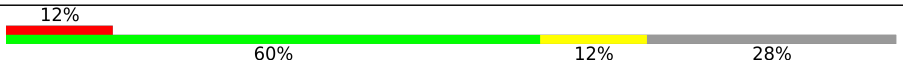
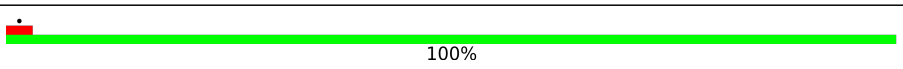
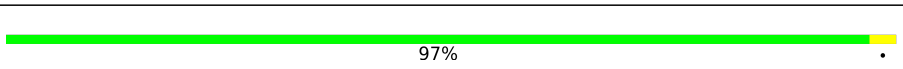
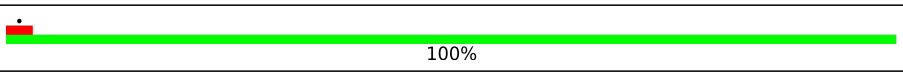
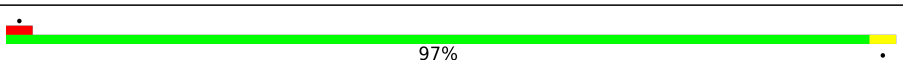
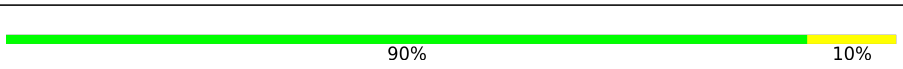
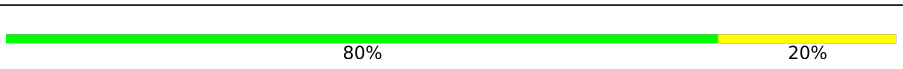
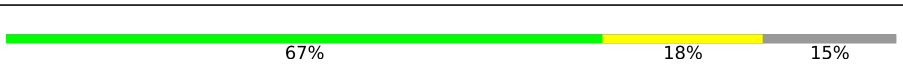
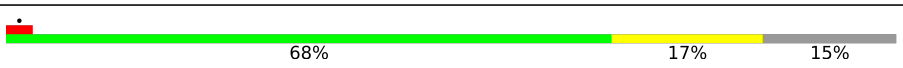
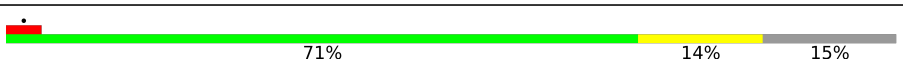
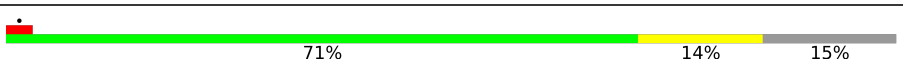
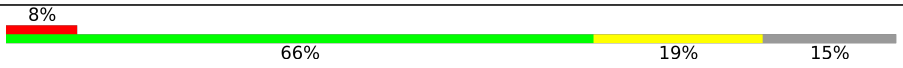
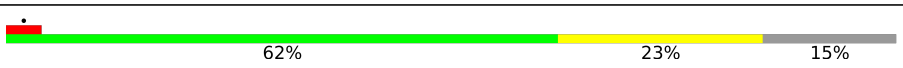
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	471	81% 15%
3	c	471	81% 15%
4	D	351	84% 13%
4	d	351	84% 13%
5	E	84	6% 83% 6% 11%
5	e	84	83% 6% 11%
6	F	43	51% 14% 35%
6	f	43	51% 14% 35%
7	H	67	88% 10%
7	h	67	90% 9%
8	I	38	76% 16% 8%
8	i	38	74% 18% 8%
9	J	39	72% 15% 13%
9	j	39	5% 79% 8% 13%
10	K	44	73% 11% 16%
10	k	44	5% 73% 11% 16%
11	L	38	5% 84% 16%
11	l	38	5% 84% 16%
12	M	131	28% 68%
12	m	131	30% 68%
13	O	248	5% 79% 20%
13	o	248	8% 78% 21%
14	T	31	81% 16%
14	t	31	10% 81% 16%
15	U	93	85% 15%

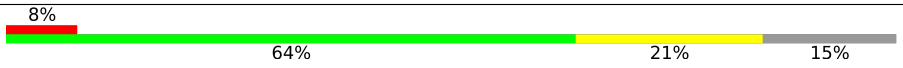
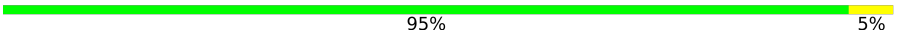
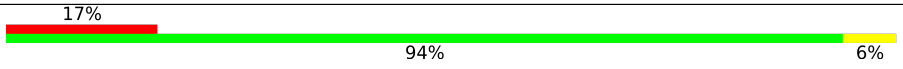
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	u	93	
16	V	137	
16	v	137	
17	Y	34	
17	y	34	
18	X	38	
18	x	38	
19	Z	61	
19	z	61	
20	Q	155	
20	q	155	
21	W	72	
21	w	72	
22	0	31	
22	5	31	
23	1	30	
23	6	30	
24	2	10	
24	7	10	
25	11	207	
25	12	207	
25	13	207	
25	14	207	
25	15	207	
25	16	207	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
25	17	207	
25	18	207	
26	19	215	
27	20	143	
28	21	155	

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	BCT	a	406	-	-	X	-

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 74619 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a protein called Unknown protein 0.

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

- Molecule 23 is a protein called Unknown protein 1.

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

- Molecule 24 is a protein called Unknown protein 2.

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
25	16	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	17	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	18	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

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

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

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

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

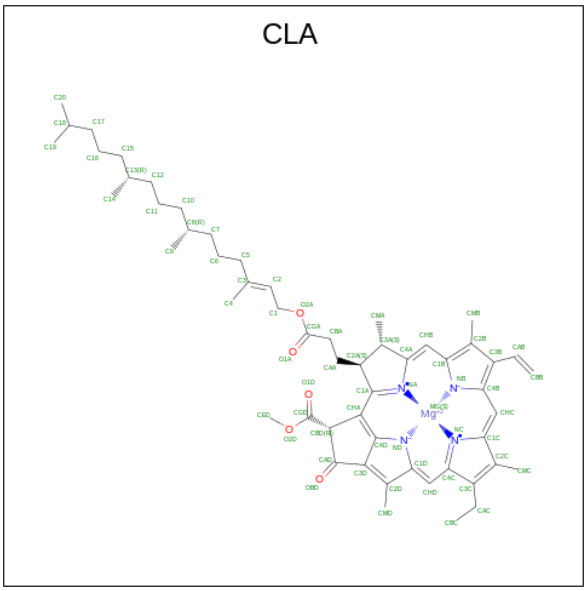
- Molecule 28 is a protein called Fucoxanthin chlorophyll a/c-binding protein monomer 3.

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

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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



Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	m	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	17	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	18	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

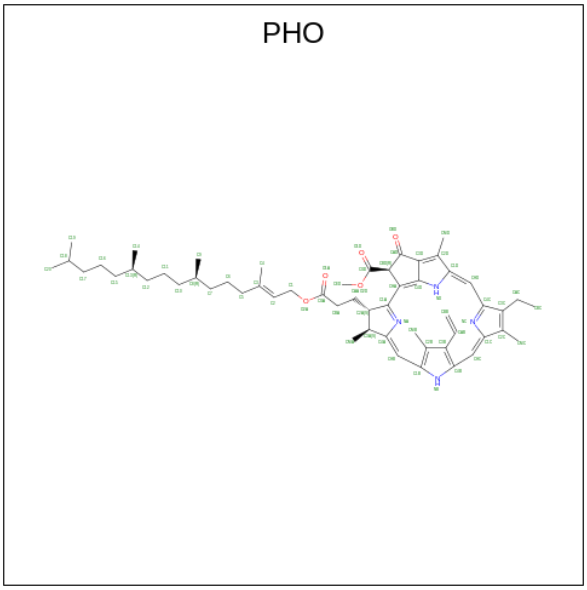
Mol	Chain	Residues	Atoms					AltConf
30	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	19	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	20	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

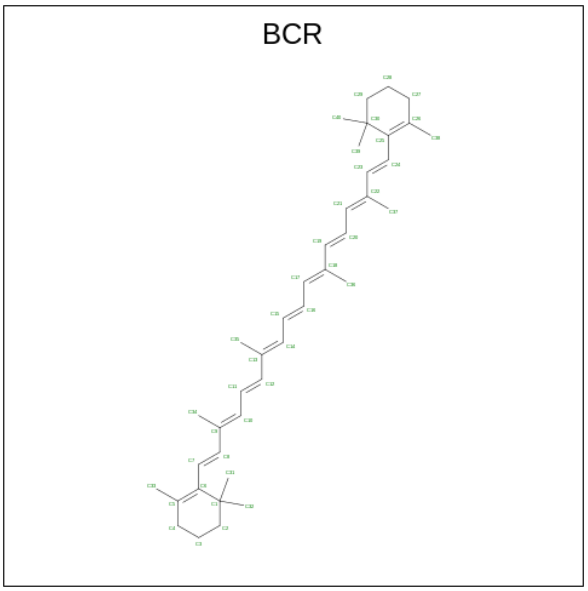
Mol	Chain	Residues	Atoms					AltConf
30	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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



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

- Molecule 32 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



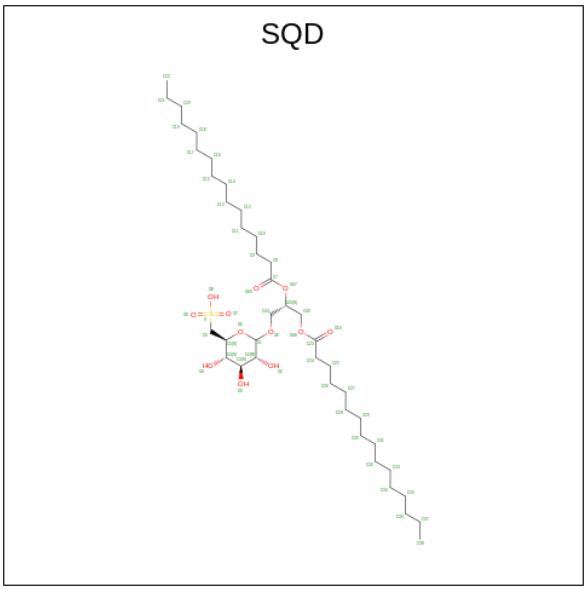
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	C	1	Total C 40 40	0
32	C	1	Total C 40 40	0
32	F	1	Total C 40 40	0
32	H	1	Total C 40 40	0
32	Y	1	Total C 40 40	0
32	Z	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	h	1	Total C 40 40	0
32	m	1	Total C 40 40	0

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



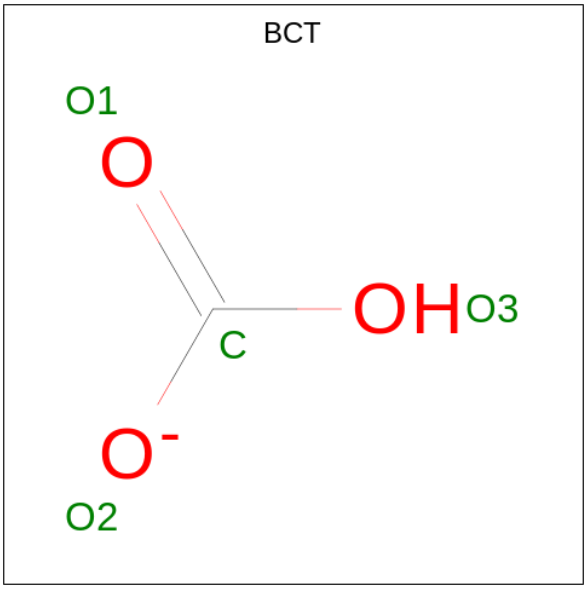
Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C O S 54 41 12 1	0

Continued on next page...

Continued from previous page...

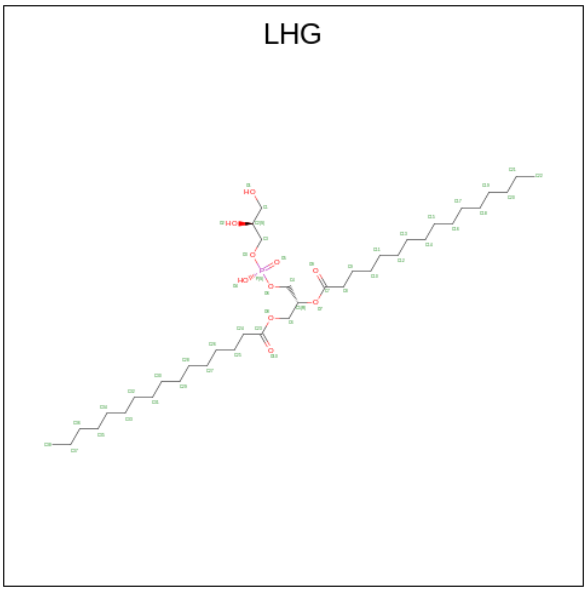
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O	S	0
			37	24	12	1	
33	L	1	Total	C	O	S	0
			54	41	12	1	
33	a	1	Total	C	O	S	0
			54	41	12	1	
33	b	1	Total	C	O	S	0
			37	24	12	1	
33	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



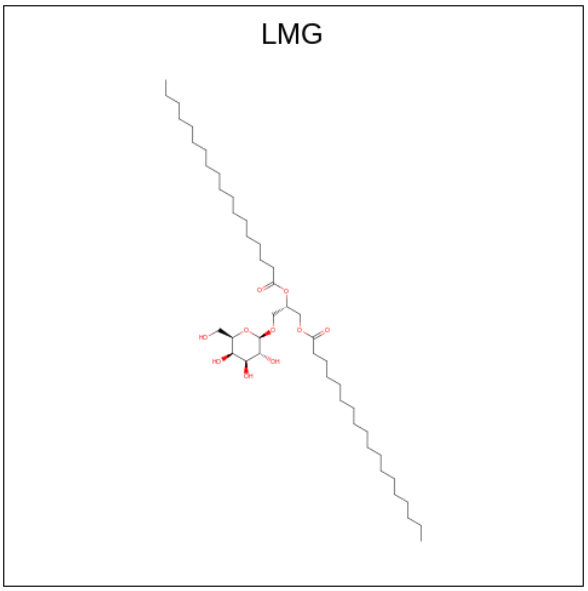
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			4	1	3	
34	a	1	Total	C	O	0
			4	1	3	

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



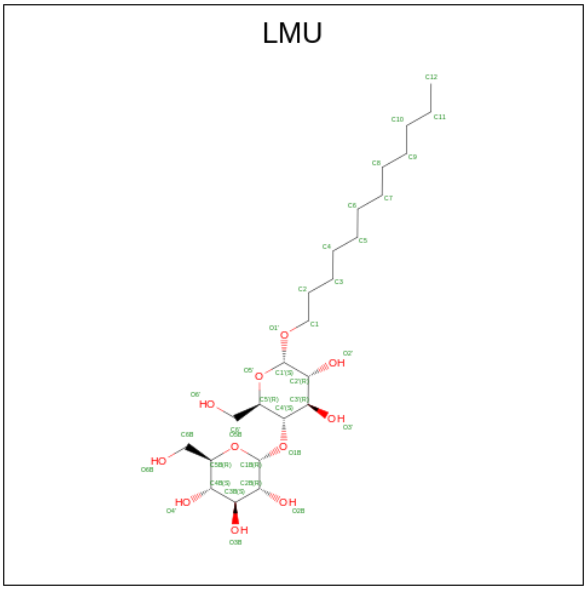
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	P	0
			46	35	10	1	
35	B	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	a	1	Total	C	O	P	0
			46	35	10	1	
35	b	1	Total	C	O	P	0
			49	38	10	1	
35	d	1	Total	C	O	P	0
			49	38	10	1	
35	l	1	Total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

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



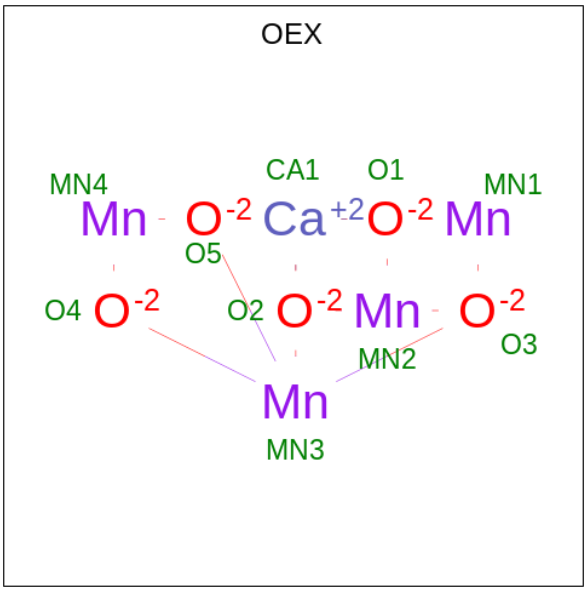
Mol	Chain	Residues	Atoms	AltConf
36	B	1	Total C O 51 41 10	0
36	B	1	Total C O 51 41 10	0
36	D	1	Total C O 51 41 10	0
36	M	1	Total C O 40 30 10	0
36	Q	1	Total C O 51 41 10	0
36	W	1	Total C O 51 41 10	0
36	1	1	Total C O 39 29 10	0
36	b	1	Total C O 51 41 10	0
36	b	1	Total C O 51 41 10	0
36	c	1	Total C O 51 41 10	0
36	d	1	Total C O 51 41 10	0
36	m	1	Total C O 40 30 10	0
36	w	1	Total C O 51 41 10	0
36	12	1	Total C O 39 29 10	0

- Molecule 37 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			32	21	11	
37	12	1	Total	C	O	0
			32	21	11	

- Molecule 38 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



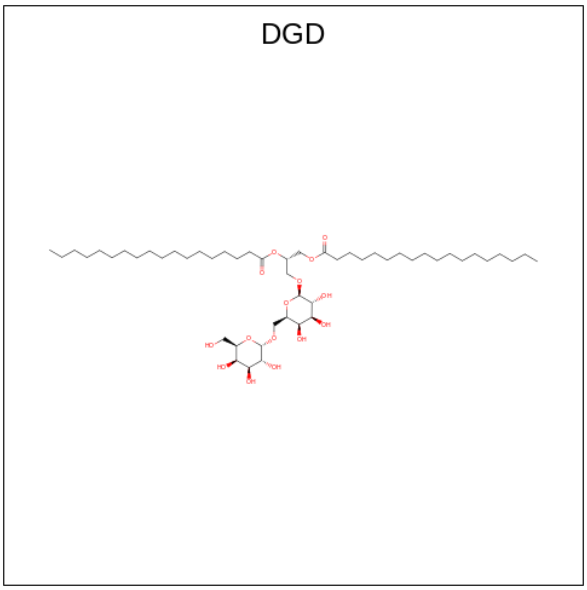
Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total	Ca	Mn	O	0
			10	1	4	5	

Continued on next page...

Continued from previous page...

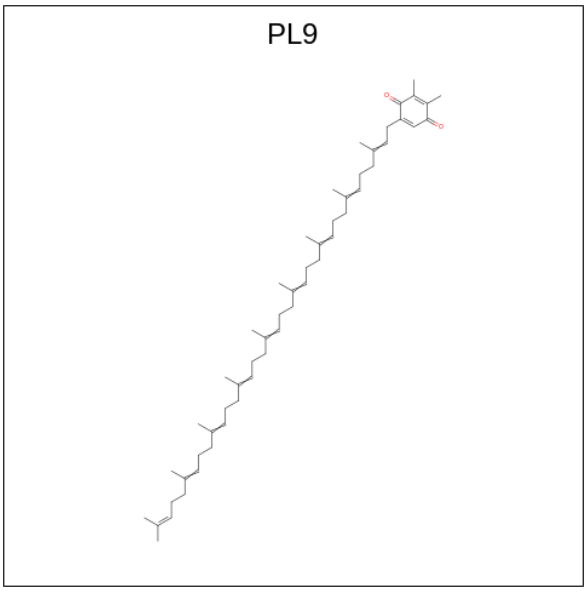
Mol	Chain	Residues	Atoms				AltConf
38	c	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



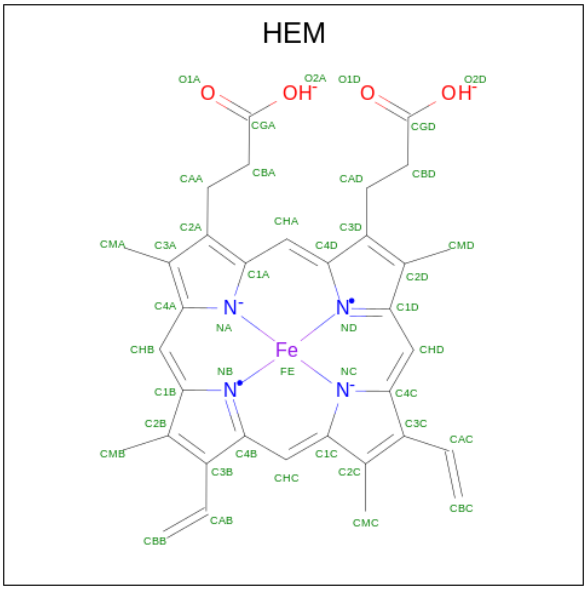
Mol	Chain	Residues	Atoms			AltConf
39	C	1	Total	C	O	0
			62	47	15	
39	C	1	Total	C	O	0
			62	47	15	
39	H	1	Total	C	O	0
			62	47	15	
39	J	1	Total	C	O	0
			62	47	15	
39	c	1	Total	C	O	0
			62	47	15	
39	c	1	Total	C	O	0
			62	47	15	
39	h	1	Total	C	O	0
			62	47	15	
39	j	1	Total	C	O	0
			62	47	15	

- Molecule 40 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



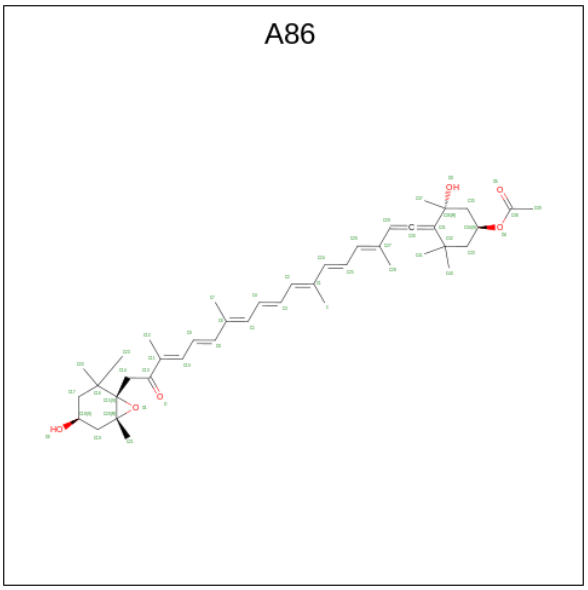
Mol	Chain	Residues	Atoms	AltConf
40	D	1	Total C O 55 53 2	0
40	D	1	Total C O 55 53 2	0
40	d	1	Total C O 55 53 2	0
40	d	1	Total C O 55 53 2	0

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
41	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 42 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: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms			AltConf
42	11	1	Total	C	O	0
			48	42	6	
42	11	1	Total	C	O	0
			48	42	6	
42	11	1	Total	C	O	0
			48	42	6	
42	11	1	Total	C	O	0
			48	42	6	
42	11	1	Total	C	O	0
			48	42	6	
42	11	1	Total	C	O	0
			48	42	6	
42	12	1	Total	C	O	0
			48	42	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
42	12	1	Total C O 48 42 6	0
42	12	1	Total C O 48 42 6	0
42	12	1	Total C O 48 42 6	0
42	12	1	Total C O 48 42 6	0
42	12	1	Total C O 48 42 6	0
42	13	1	Total C O 48 42 6	0
42	13	1	Total C O 48 42 6	0
42	13	1	Total C O 48 42 6	0
42	13	1	Total C O 48 42 6	0
42	13	1	Total C O 48 42 6	0
42	13	1	Total C O 48 42 6	0
42	14	1	Total C O 48 42 6	0
42	14	1	Total C O 48 42 6	0
42	14	1	Total C O 48 42 6	0
42	14	1	Total C O 48 42 6	0
42	14	1	Total C O 48 42 6	0
42	14	1	Total C O 48 42 6	0
42	15	1	Total C O 48 42 6	0
42	15	1	Total C O 48 42 6	0
42	15	1	Total C O 48 42 6	0
42	15	1	Total C O 48 42 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
42	15	1	Total C O 48 42 6	0
42	15	1	Total C O 48 42 6	0
42	15	1	Total C O 48 42 6	0
42	16	1	Total C O 48 42 6	0
42	16	1	Total C O 48 42 6	0
42	16	1	Total C O 48 42 6	0
42	16	1	Total C O 48 42 6	0
42	17	1	Total C O 48 42 6	0
42	17	1	Total C O 48 42 6	0
42	17	1	Total C O 48 42 6	0
42	17	1	Total C O 48 42 6	0
42	17	1	Total C O 48 42 6	0
42	17	1	Total C O 48 42 6	0
42	17	1	Total C O 48 42 6	0
42	18	1	Total C O 48 42 6	0
42	18	1	Total C O 48 42 6	0
42	18	1	Total C O 48 42 6	0
42	18	1	Total C O 48 42 6	0
42	19	1	Total C O 48 42 6	0
42	19	1	Total C O 48 42 6	0
42	19	1	Total C O 48 42 6	0

Continued on next page...

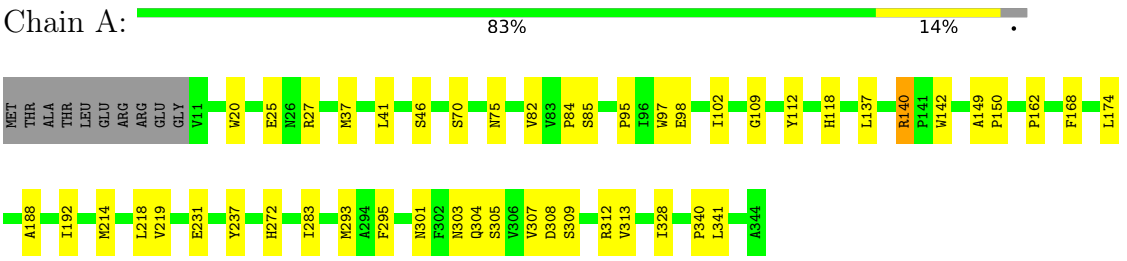
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
42	20	1	Total	C	O	0
			48	42	6	
42	20	1	Total	C	O	0
			48	42	6	
42	20	1	Total	C	O	0
			48	42	6	
42	20	1	Total	C	O	0
			48	42	6	
42	20	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	

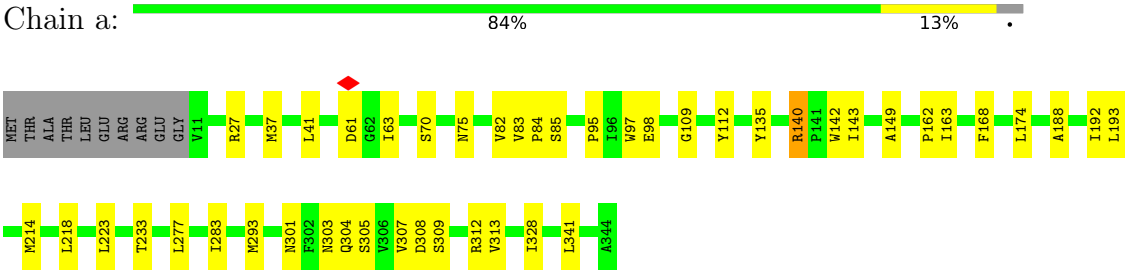
3 Residue-property plots

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

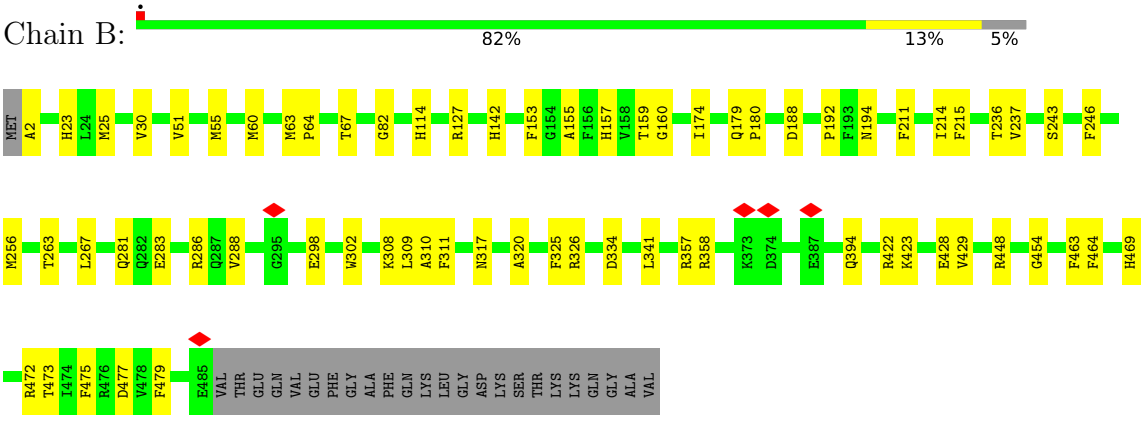
• Molecule 1: Photosystem II reaction center protein D1



• Molecule 1: Photosystem II reaction center protein D1

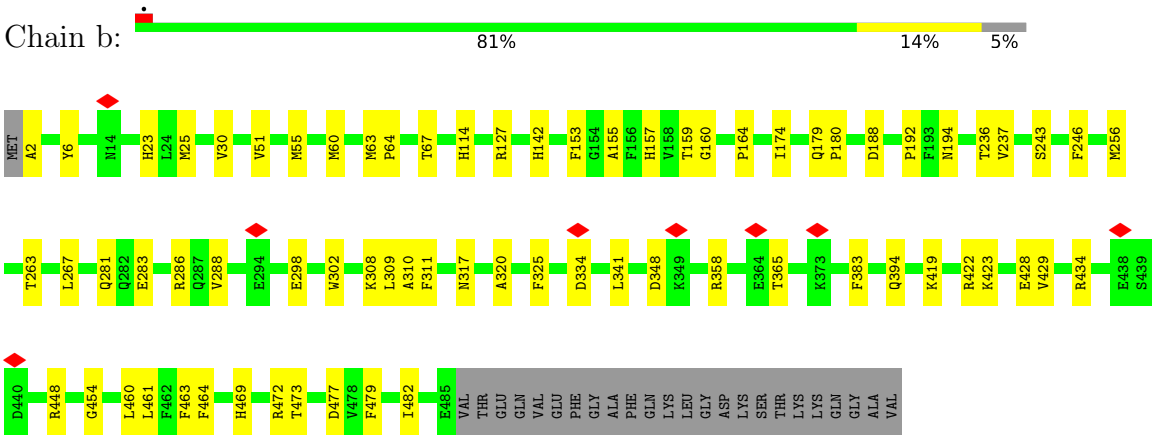


• Molecule 2: Photosystem II chlorophyll protein CP47



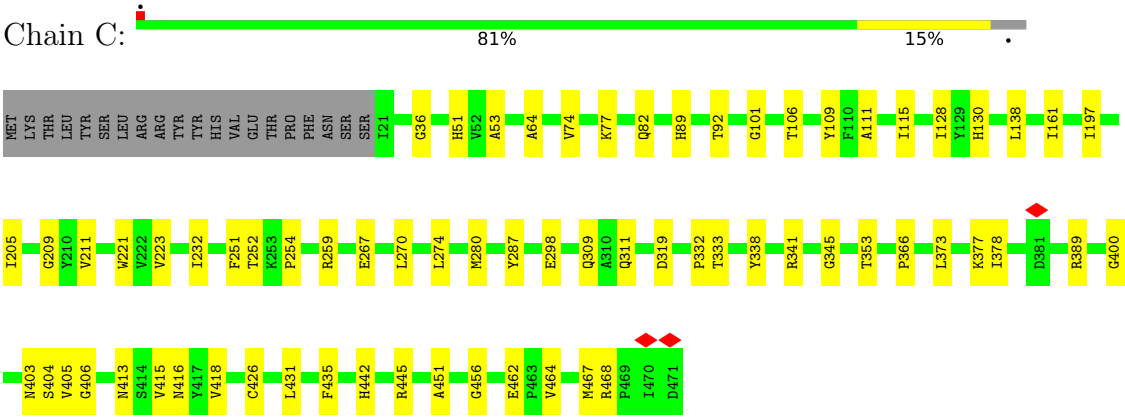
• Molecule 2: Photosystem II chlorophyll protein CP47

Chain b:



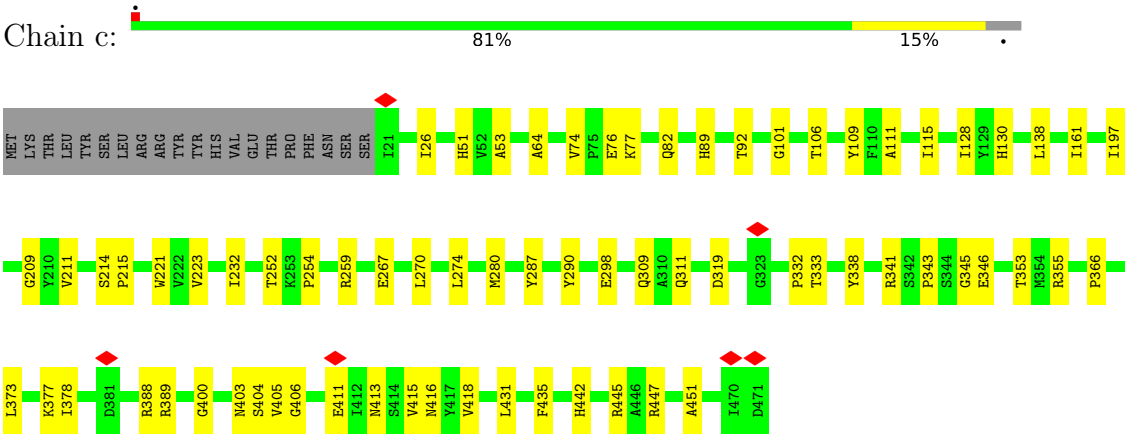
• Molecule 3: Photosystem II chlorophyll protein CP43

Chain C:



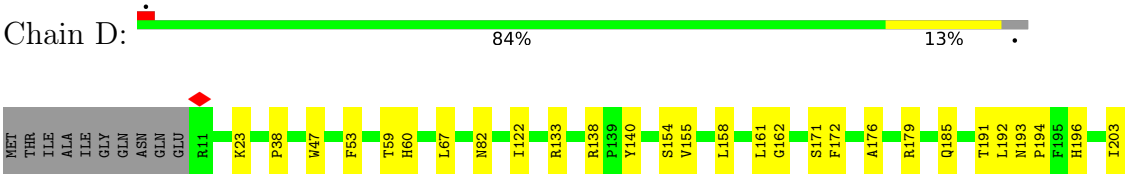
• Molecule 3: Photosystem II chlorophyll protein CP43

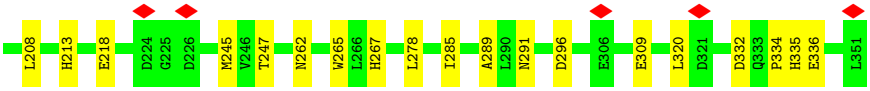
Chain c:



• Molecule 4: Photosystem II reaction center protein D2

Chain D:



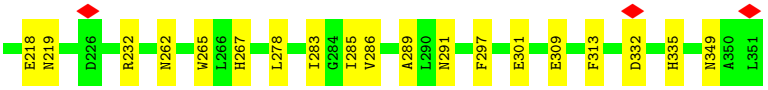


• Molecule 4: Photosystem II reaction center protein D2

Chain d:



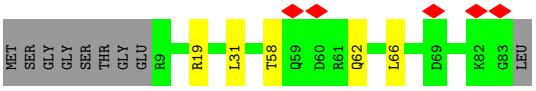




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:





• Molecule 5: Cytochrome b559 subunit alpha

Chain e:





• Molecule 6: Cytochrome b559 subunit beta

Chain F:

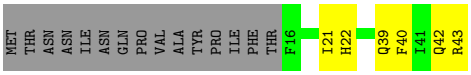




• Molecule 6: Cytochrome b559 subunit beta

Chain f:

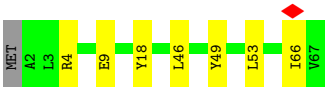




• Molecule 7: Photosystem II reaction center protein H

Chain H:

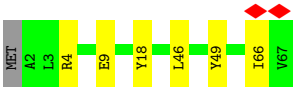




• Molecule 7: Photosystem II reaction center protein H

Chain h:





• Molecule 8: Photosystem II reaction center protein I

Chain I:

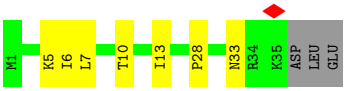




• Molecule 8: Photosystem II reaction center protein I

Chain i:

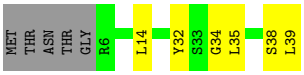




• Molecule 9: Photosystem II reaction center protein J

Chain J:

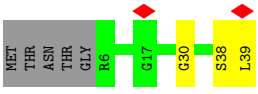




• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

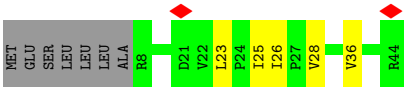




• Molecule 10: Photosystem II reaction center protein K

Chain k:

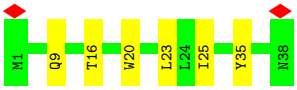




• Molecule 11: Photosystem II reaction center protein L

Chain L:

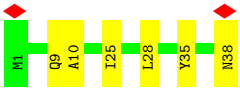




• Molecule 11: Photosystem II reaction center protein L

Chain l:

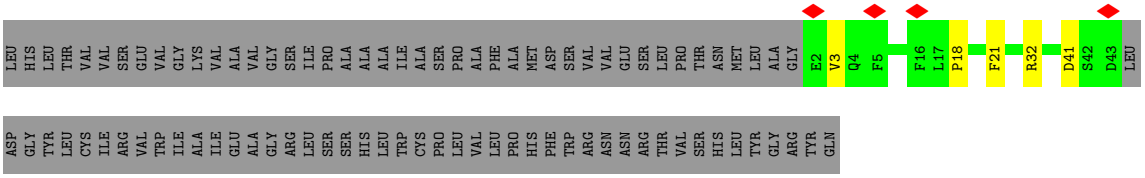




• Molecule 12: Photosystem II reaction center protein M

Chain M:

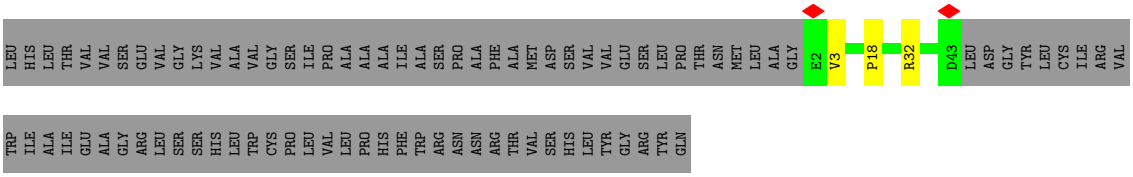




• Molecule 12: Photosystem II reaction center protein M

Chain m:

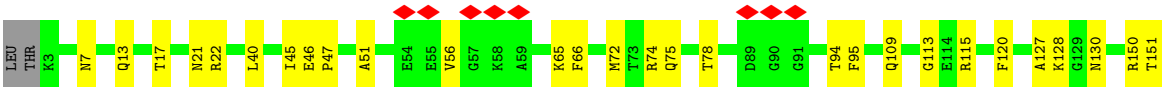


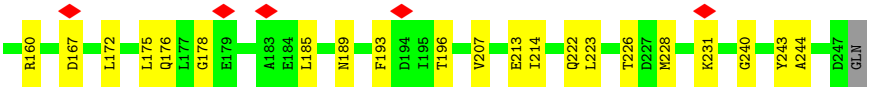


• Molecule 13: Extrinsic protein in photosystem II

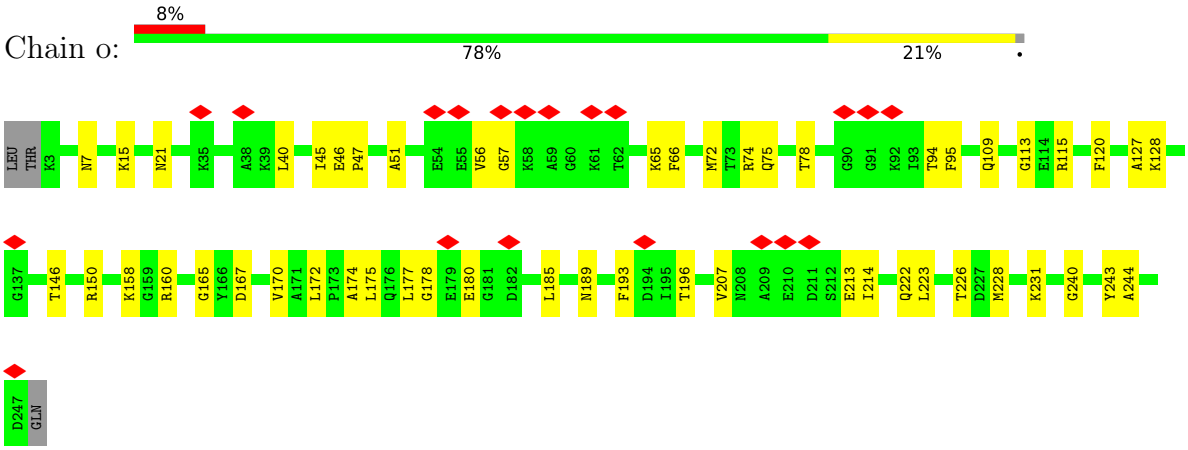
Chain O:



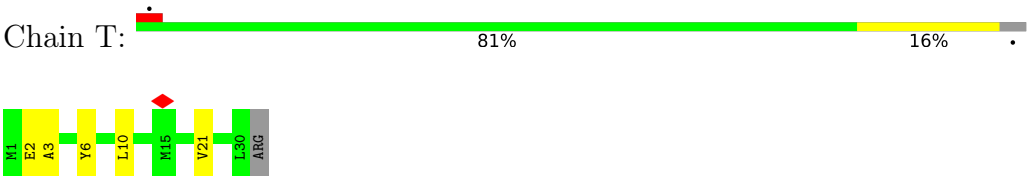




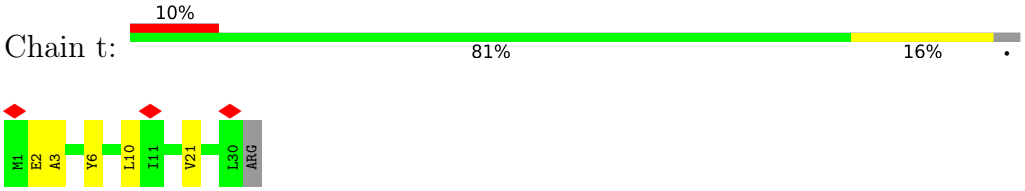
• Molecule 13: Extrinsic protein in photosystem II



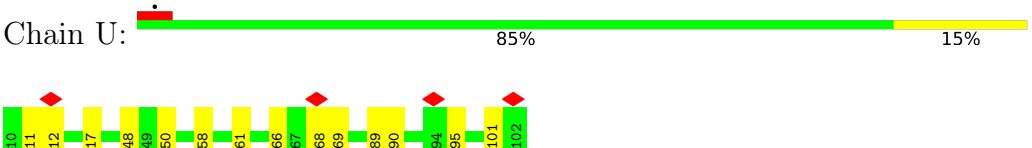
• Molecule 14: Photosystem II reaction center protein T



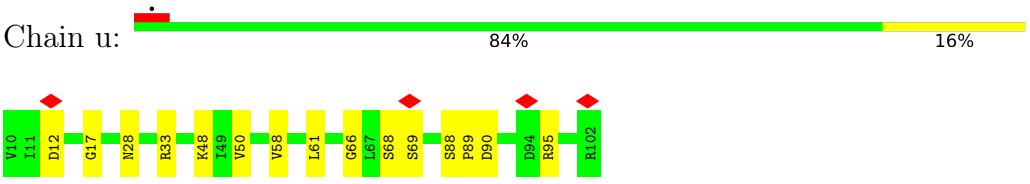
• Molecule 14: Photosystem II reaction center protein T



• Molecule 15: Extrinsic protein in photosystem II



• Molecule 15: Extrinsic protein in photosystem II



• Molecule 16: Cytochrome c-550

Chain V:

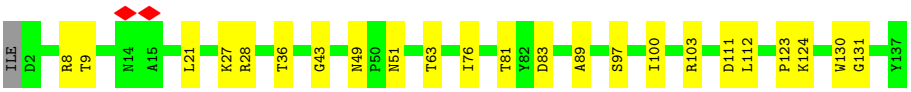




• Molecule 16: Cytochrome c-550

Chain v:

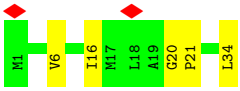




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:

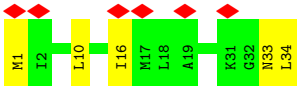




• Molecule 17: Photosystem II reaction center protein Ycf12

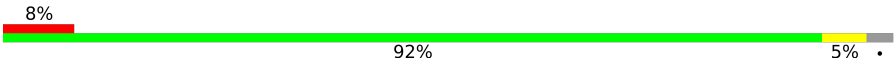
Chain y:

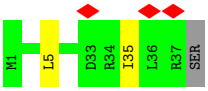




• Molecule 18: Photosystem II reaction center X protein

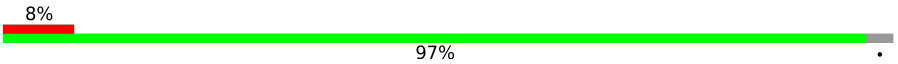
Chain X:

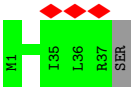




• Molecule 18: Photosystem II reaction center X protein

Chain x:

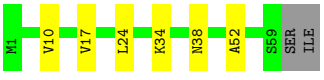




• Molecule 19: Photosystem II reaction center protein Z

Chain Z:

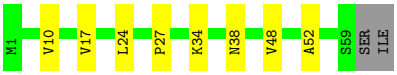




• Molecule 19: Photosystem II reaction center protein Z

Chain z:

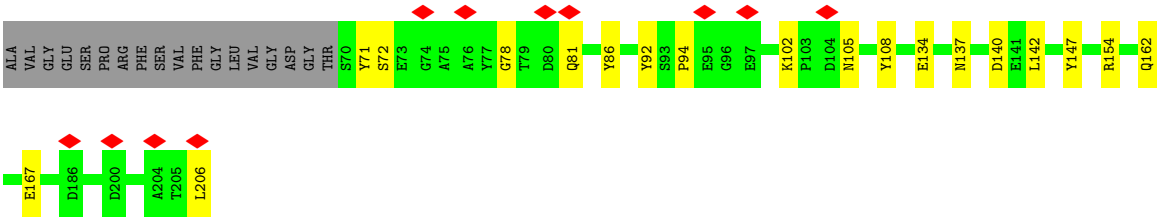




• Molecule 20: Extrinsic protein in photosystem II

Chain Q:

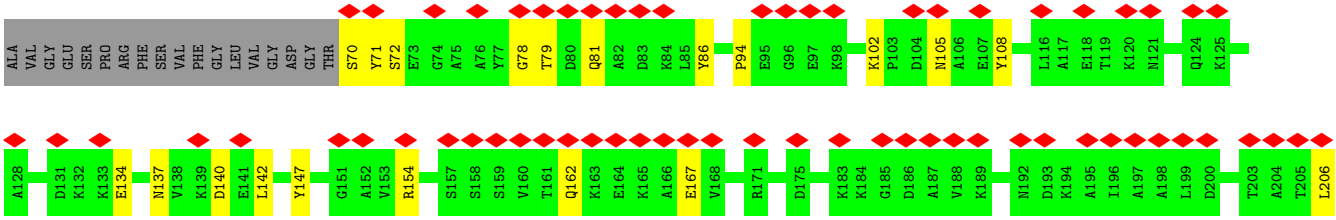




• Molecule 20: Extrinsic protein in photosystem II

Chain q:

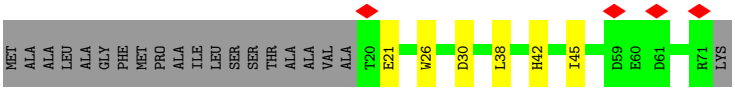




• Molecule 21: Photosystem II reaction center protein W

Chain W:

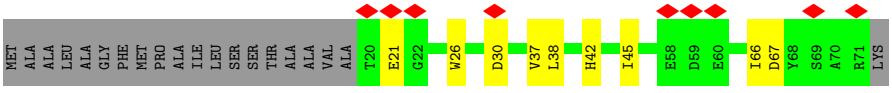




• Molecule 21: Photosystem II reaction center protein W

Chain w:





• Molecule 22: Unknown protein 0

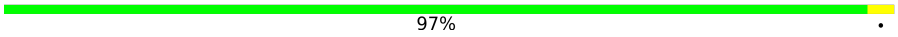
Chain 0:





• Molecule 22: Unknown protein 0

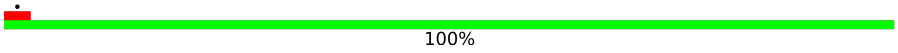
Chain 5:





• Molecule 23: Unknown protein 1

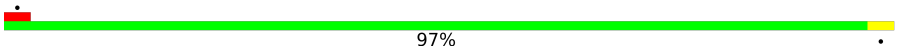
Chain 1:

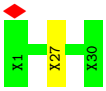




• Molecule 23: Unknown protein 1

Chain 6:





• Molecule 24: Unknown protein 2

Chain 2:





• Molecule 24: Unknown protein 2

Chain 7:

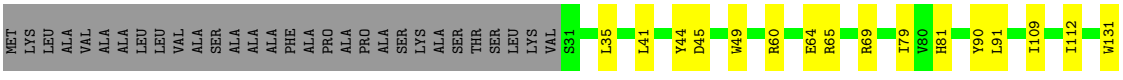


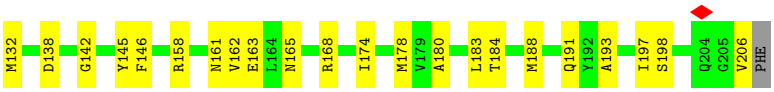


• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 11:

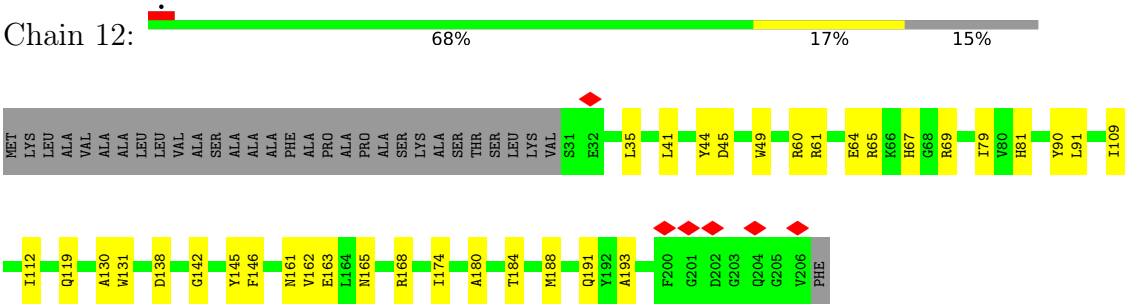






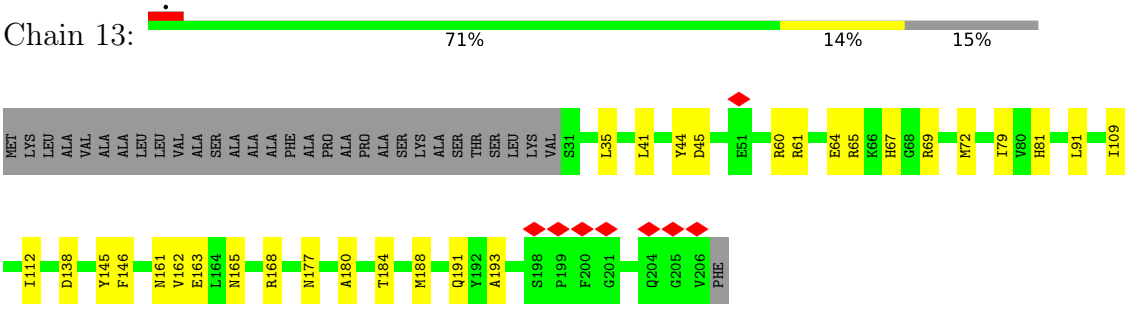
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 12:



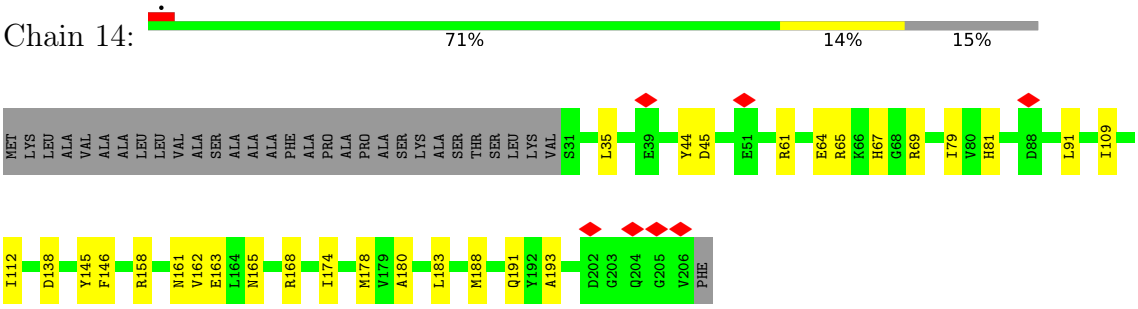
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 13:



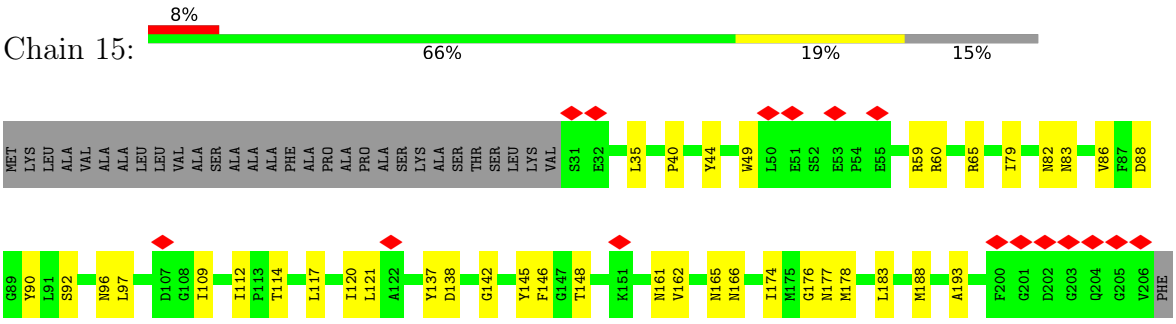
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 14:



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

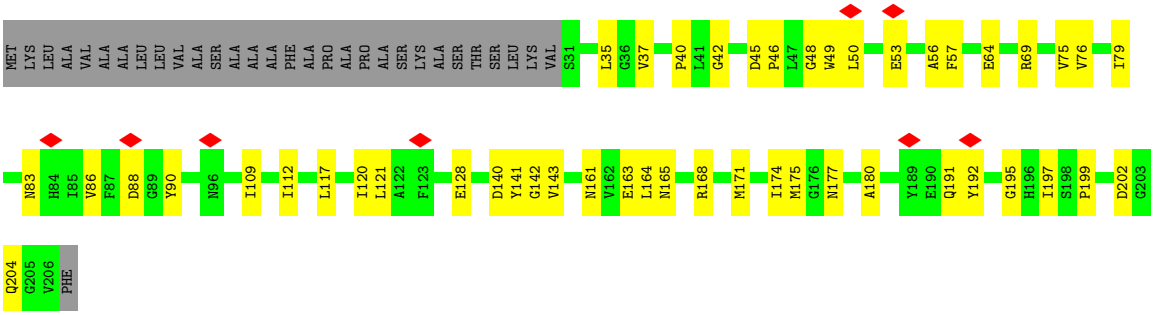
Chain 15:



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

Chain 16:

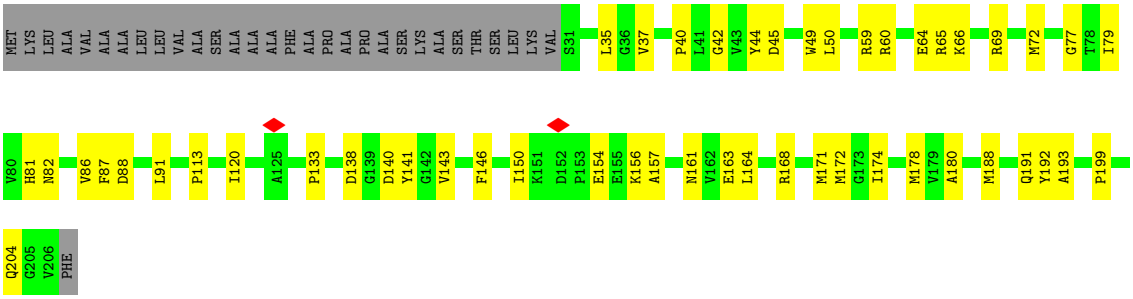




• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 17:

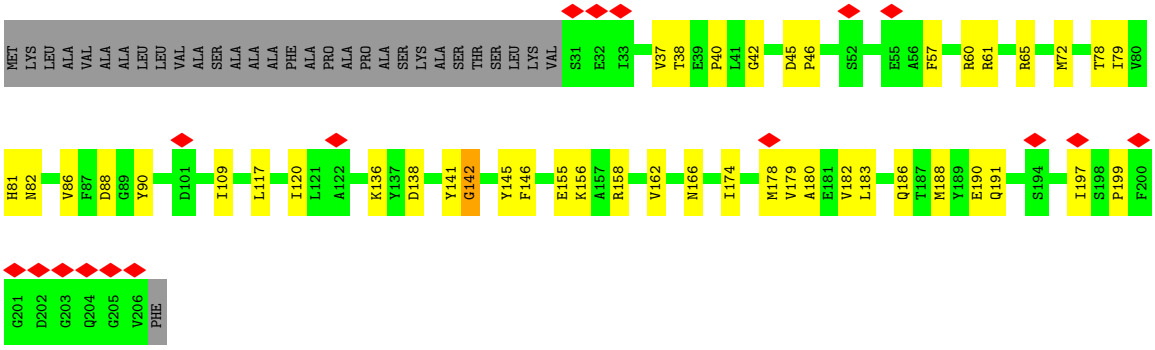




• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

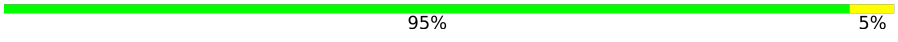
Chain 18:

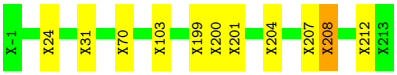




• Molecule 26: Fucoxanthin chlorophyll a/c-binding protein monomer 1

Chain 19:

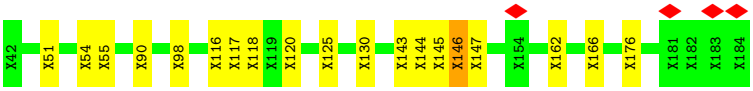




• Molecule 27: Fucoxanthin chlorophyll a/c-binding protein monomer 2

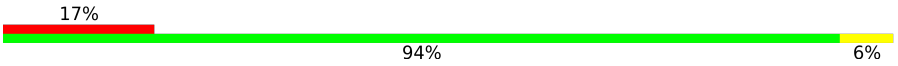
Chain 20:

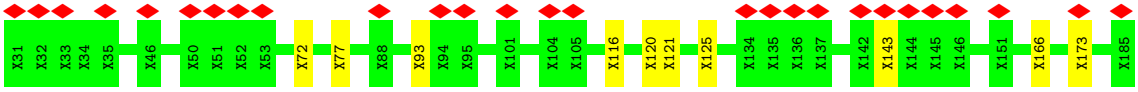




• Molecule 28: Fucoxanthin chlorophyll a/c-binding protein monomer 3

Chain 21:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	147981	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.164	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	573.44, 573.44, 573.44	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, LHG, OEX, A86, BCR, PL9, SQD, PHO, LMG, LMU, BCT, CLA, FE2, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.53	0/2701	0.61	0/3682
1	a	0.53	0/2701	0.61	0/3682
2	B	0.51	0/3942	0.60	1/5362 (0.0%)
2	b	0.52	0/3942	0.60	1/5362 (0.0%)
3	C	0.52	0/3620	0.63	2/4933 (0.0%)
3	c	0.52	0/3620	0.63	2/4933 (0.0%)
4	D	0.52	0/2789	0.61	0/3803
4	d	0.52	0/2789	0.61	0/3803
5	E	0.36	0/634	0.55	0/864
5	e	0.36	0/634	0.55	0/864
6	F	0.45	0/235	0.80	0/316
6	f	0.45	0/235	0.80	0/316
7	H	0.44	0/523	0.60	0/714
7	h	0.43	0/523	0.60	0/714
8	I	0.55	0/294	0.78	0/397
8	i	0.55	0/294	0.77	0/397
9	J	0.35	0/260	0.52	0/351
9	j	0.35	0/260	0.52	0/351
10	K	0.49	0/313	1.00	2/429 (0.5%)
10	k	0.49	0/313	1.00	2/429 (0.5%)
11	L	0.52	0/319	0.53	0/433
11	l	0.52	0/319	0.53	0/433
12	M	0.46	0/321	0.67	0/433
12	m	0.46	0/321	0.67	0/433
13	O	0.37	0/1875	0.61	2/2528 (0.1%)
13	o	0.37	0/1875	0.61	2/2528 (0.1%)
14	T	0.38	0/256	0.54	0/346
14	t	0.38	0/256	0.54	0/346
15	U	0.32	0/728	0.62	0/989
15	u	0.32	0/728	0.62	0/989
16	V	0.39	0/1056	0.57	0/1435
16	v	0.39	0/1056	0.57	0/1435

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
17	Y	0.29	0/252	0.54	0/341
17	y	0.29	0/252	0.54	0/341
18	X	0.29	0/263	0.52	0/355
18	x	0.29	0/263	0.51	0/355
19	Z	0.34	0/456	0.55	0/624
19	z	0.35	0/456	0.55	0/624
20	Q	0.30	0/1099	0.56	0/1482
20	q	0.30	0/1099	0.56	0/1482
21	W	0.49	0/434	0.66	0/590
21	w	0.49	0/434	0.66	0/590
25	11	0.36	0/1373	0.58	0/1861
25	12	0.36	0/1373	0.58	0/1861
25	13	0.36	0/1373	0.58	0/1861
25	14	0.36	0/1373	0.58	0/1861
25	15	0.24	0/1373	0.50	0/1861
25	16	0.36	0/1373	0.66	0/1861
25	17	0.33	0/1373	0.59	0/1861
25	18	0.26	0/1373	0.53	0/1861
All	All	0.45	0/55724	0.61	14/75702 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	a	0	1
16	V	0	1
16	v	0	1
25	18	0	1
26	19	0	4
27	20	0	3
All	All	0	12

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	k	25	ILE	CA-C-N	8.78	125.77	120.24
10	k	25	ILE	C-N-CA	8.78	125.77	120.24
10	K	25	ILE	CA-C-N	8.77	125.76	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	25	ILE	C-N-CA	8.77	125.76	120.24
3	C	252	THR	CA-C-N	6.62	137.17	122.67

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	18	142	GLY	Peptide
1	A	140	ARG	Peptide
16	V	63	THR	Peptide
1	a	140	ARG	Peptide
16	v	63	THR	Peptide

5.2 Too-close contacts (i)

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	2618	0	2520	45	0
1	a	2618	0	2520	37	0
2	B	3812	0	3690	55	0
2	b	3812	0	3690	57	0
3	C	3504	0	3409	61	0
3	c	3504	0	3410	59	0
4	D	2697	0	2596	41	0
4	d	2697	0	2596	40	0
5	E	616	0	602	3	0
5	e	616	0	602	3	0
6	F	228	0	234	11	0
6	f	228	0	234	9	0
7	H	513	0	541	7	0
7	h	513	0	541	6	0
8	I	287	0	306	8	0
8	i	287	0	306	6	0
9	J	254	0	266	6	0
9	j	254	0	266	3	0
10	K	302	0	316	4	0
10	k	302	0	316	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	L	310	0	313	8	0
11	l	310	0	313	8	0
12	M	316	0	319	7	0
12	m	316	0	319	4	0
13	O	1845	0	1841	38	0
13	o	1845	0	1841	37	0
14	T	250	0	268	4	0
14	t	250	0	268	4	0
15	U	713	0	715	14	0
15	u	713	0	715	11	0
16	V	1037	0	1033	16	0
16	v	1037	0	1033	13	0
17	Y	250	0	287	8	0
17	y	250	0	287	6	0
18	X	263	0	301	3	0
18	x	263	0	301	0	0
19	Z	447	0	489	6	0
19	z	447	0	490	8	0
20	Q	1079	0	1068	15	0
20	q	1079	0	1068	16	0
21	W	422	0	377	5	0
21	w	422	0	377	9	0
22	0	155	0	34	0	0
22	5	155	0	34	1	0
23	1	150	0	34	0	0
23	6	150	0	34	1	0
24	2	50	0	12	4	0
24	7	50	0	12	2	0
25	11	1343	0	1306	43	0
25	12	1343	0	1305	39	0
25	13	1343	0	1306	37	0
25	14	1343	0	1306	27	0
25	15	1343	0	1306	41	0
25	16	1343	0	1306	45	0
25	17	1343	0	1306	53	0
25	18	1343	0	1305	57	0
26	19	1075	0	224	21	0
27	20	715	0	148	16	0
28	21	775	0	157	10	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	11	530	0	486	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	12	595	0	555	38	0
30	13	465	0	414	21	0
30	14	530	0	486	24	0
30	15	465	0	414	25	0
30	16	465	0	412	32	0
30	17	485	0	451	39	0
30	18	595	0	558	50	0
30	19	465	0	413	9	0
30	20	420	0	378	15	0
30	21	485	0	452	31	0
30	A	130	0	144	13	0
30	B	1040	0	1152	41	0
30	C	975	0	1080	51	0
30	D	260	0	288	12	0
30	M	65	0	67	1	0
30	W	130	0	144	9	0
30	Z	65	0	68	9	0
30	a	130	0	144	7	0
30	b	1040	0	1152	45	0
30	c	845	0	936	36	0
30	d	260	0	288	10	0
30	m	65	0	68	2	0
30	w	130	0	144	5	0
30	z	65	0	72	4	0
31	A	64	0	74	1	0
31	D	64	0	74	2	0
31	d	128	0	148	2	0
32	A	80	0	112	3	0
32	B	160	0	224	10	0
32	C	80	0	112	5	0
32	F	40	0	56	2	0
32	H	40	0	56	5	0
32	Y	40	0	56	4	0
32	Z	40	0	56	1	0
32	a	80	0	112	2	0
32	b	120	0	168	7	0
32	c	160	0	224	8	0
32	f	40	0	56	1	0
32	h	40	0	56	3	0
32	m	40	0	56	3	0
33	A	54	0	77	0	0
33	B	37	0	37	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	L	54	0	77	3	0
33	a	54	0	78	0	0
33	b	37	0	37	2	0
33	l	54	0	77	3	0
34	A	4	0	0	1	0
34	a	4	0	0	2	0
35	A	46	0	65	4	0
35	B	49	0	74	1	0
35	L	98	0	148	6	0
35	a	46	0	65	6	0
35	b	49	0	74	2	0
35	d	49	0	74	3	0
35	l	49	0	74	3	0
36	1	39	0	48	0	0
36	12	39	0	46	8	0
36	B	102	0	143	5	0
36	D	51	0	72	2	0
36	M	40	0	50	5	0
36	Q	51	0	72	2	0
36	W	51	0	72	8	0
36	b	102	0	143	5	0
36	c	51	0	72	1	0
36	d	51	0	72	1	0
36	m	40	0	50	2	0
36	w	51	0	72	6	0
37	12	32	0	34	0	0
37	B	32	0	37	0	0
38	C	10	0	0	0	0
38	c	10	0	0	1	0
39	C	124	0	162	0	0
39	H	62	0	82	5	0
39	J	62	0	82	1	0
39	c	124	0	162	0	0
39	h	62	0	82	3	0
39	j	62	0	82	1	0
40	D	110	0	157	7	0
40	d	110	0	157	8	0
41	F	43	0	30	3	0
41	V	43	0	30	2	0
41	f	43	0	30	4	0
41	v	43	0	30	2	0
42	11	288	0	0	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	12	288	0	0	26	0
42	13	288	0	0	36	0
42	14	288	0	0	18	0
42	15	336	0	0	40	0
42	16	192	0	0	21	0
42	17	336	0	0	61	0
42	18	192	0	0	33	0
42	19	144	0	0	22	0
42	20	240	0	0	42	0
42	21	240	0	0	44	0
All	All	74619	0	69551	1379	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 10.

The worst 5 of 1379 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)
36:12:301:LMG:C16	30:12:308:CLA:CED	1.75	1.65
30:21:303:CLA:H11	42:21:314:A86:C4	1.35	1.55
30:18:303:CLA:H61	42:18:314:A86:C29	1.28	1.55
30:16:308:CLA:CAB	42:17:302:A86:C3	1.86	1.53
30:21:309:CLA:HAB	42:21:312:A86:C7	1.39	1.53

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	332/344 (96%)	322 (97%)	10 (3%)	0	100	100
1	a	332/344 (96%)	322 (97%)	10 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	482/509 (95%)	466 (97%)	16 (3%)	0	100	100
2	b	482/509 (95%)	466 (97%)	16 (3%)	0	100	100
3	C	449/471 (95%)	429 (96%)	20 (4%)	0	100	100
3	c	449/471 (95%)	429 (96%)	20 (4%)	0	100	100
4	D	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
4	d	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
5	E	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
5	e	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
6	F	26/43 (60%)	26 (100%)	0	0	100	100
6	f	26/43 (60%)	26 (100%)	0	0	100	100
7	H	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
7	h	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	32/39 (82%)	32 (100%)	0	0	100	100
9	j	32/39 (82%)	32 (100%)	0	0	100	100
10	K	35/44 (80%)	35 (100%)	0	0	100	100
10	k	35/44 (80%)	35 (100%)	0	0	100	100
11	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	M	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
12	m	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
13	O	243/248 (98%)	231 (95%)	12 (5%)	0	100	100
13	o	243/248 (98%)	231 (95%)	12 (5%)	0	100	100
14	T	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
14	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
15	U	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
15	u	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
16	V	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
16	v	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
17	Y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
18	X	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
18	x	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
19	Z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
19	z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
20	Q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
20	q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
21	W	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
21	w	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
25	11	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	12	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	13	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	14	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	15	174/207 (84%)	163 (94%)	11 (6%)	0	100	100
25	16	174/207 (84%)	159 (91%)	15 (9%)	0	100	100
25	17	174/207 (84%)	162 (93%)	12 (7%)	0	100	100
25	18	174/207 (84%)	165 (95%)	8 (5%)	1 (1%)	21	54
All	All	6884/7712 (89%)	6586 (96%)	297 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	18	142	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/280 (97%)	272 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	272/280 (97%)	272 (100%)	0	100	100
2	B	385/405 (95%)	385 (100%)	0	100	100
2	b	385/405 (95%)	385 (100%)	0	100	100
3	C	356/376 (95%)	354 (99%)	2 (1%)	78	79
3	c	356/376 (95%)	354 (99%)	2 (1%)	78	79
4	D	273/281 (97%)	273 (100%)	0	100	100
4	d	273/281 (97%)	273 (100%)	0	100	100
5	E	69/75 (92%)	68 (99%)	1 (1%)	59	71
5	e	69/75 (92%)	68 (99%)	1 (1%)	59	71
6	F	22/36 (61%)	22 (100%)	0	100	100
6	f	22/36 (61%)	22 (100%)	0	100	100
7	H	55/56 (98%)	55 (100%)	0	100	100
7	h	55/56 (98%)	55 (100%)	0	100	100
8	I	34/37 (92%)	34 (100%)	0	100	100
8	i	34/37 (92%)	34 (100%)	0	100	100
9	J	27/31 (87%)	27 (100%)	0	100	100
9	j	27/31 (87%)	27 (100%)	0	100	100
10	K	32/38 (84%)	32 (100%)	0	100	100
10	k	32/38 (84%)	32 (100%)	0	100	100
11	L	34/34 (100%)	34 (100%)	0	100	100
11	l	34/34 (100%)	34 (100%)	0	100	100
12	M	31/104 (30%)	31 (100%)	0	100	100
12	m	31/104 (30%)	31 (100%)	0	100	100
13	O	196/201 (98%)	196 (100%)	0	100	100
13	o	196/201 (98%)	196 (100%)	0	100	100
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	27 (100%)	0	100	100
15	U	77/77 (100%)	77 (100%)	0	100	100
15	u	77/77 (100%)	77 (100%)	0	100	100
16	V	114/115 (99%)	114 (100%)	0	100	100
16	v	114/115 (99%)	114 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	27/27 (100%)	27 (100%)	0	100	100
17	y	27/27 (100%)	27 (100%)	0	100	100
18	X	29/30 (97%)	29 (100%)	0	100	100
18	x	29/30 (97%)	29 (100%)	0	100	100
19	Z	48/50 (96%)	48 (100%)	0	100	100
19	z	48/50 (96%)	48 (100%)	0	100	100
20	Q	111/124 (90%)	110 (99%)	1 (1%)	70	76
20	q	111/124 (90%)	110 (99%)	1 (1%)	70	76
21	W	43/55 (78%)	42 (98%)	1 (2%)	44	64
21	w	43/55 (78%)	42 (98%)	1 (2%)	44	64
25	11	138/158 (87%)	137 (99%)	1 (1%)	76	78
25	12	138/158 (87%)	137 (99%)	1 (1%)	76	78
25	13	138/158 (87%)	137 (99%)	1 (1%)	76	78
25	14	138/158 (87%)	137 (99%)	1 (1%)	76	78
25	15	138/158 (87%)	138 (100%)	0	100	100
25	16	138/158 (87%)	137 (99%)	1 (1%)	76	78
25	17	138/158 (87%)	137 (99%)	1 (1%)	76	78
25	18	138/158 (87%)	138 (100%)	0	100	100
All	All	5628/6184 (91%)	5612 (100%)	16 (0%)	84	83

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	16	128	GLU
25	14	91	LEU
20	q	142	LEU
25	13	91	LEU
5	e	31	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
25	13	161	ASN
25	18	96	ASN
25	14	161	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	16	83	ASN
20	Q	105	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 323 ligands modelled in this entry, 2 are monoatomic - leaving 321 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	LMU	B	625	-	33,33,36	1.28	3 (9%)	44,44,47	1.57	8 (18%)
42	A86	12	316	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	16	309	-	49,53,73	1.49	11 (22%)	59,89,113	1.48	8 (13%)
32	BCR	B	618	-	41,41,41	1.24	2 (4%)	56,56,56	1.41	10 (17%)
30	CLA	c	512	3	69,73,73	1.32	11 (15%)	83,113,113	1.51	13 (15%)
30	CLA	B	603	2	69,73,73	1.26	10 (14%)	83,113,113	1.52	13 (15%)
30	CLA	20	202	-	69,73,73	1.24	9 (13%)	83,113,113	1.33	9 (10%)
36	LMG	W	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.40	7 (11%)
30	CLA	12	311	25	69,73,73	1.28	10 (14%)	83,113,113	1.44	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	17	310	-	49,53,73	1.46	10 (20%)	59,89,113	1.48	5 (8%)
40	PL9	d	408	-	55,55,55	2.32	14 (25%)	68,69,69	1.48	14 (20%)
30	CLA	18	301	25	69,73,73	1.25	10 (14%)	83,113,113	1.35	9 (10%)
30	CLA	19	308	-	49,53,73	1.47	11 (22%)	59,89,113	1.59	8 (13%)
42	A86	21	310	-	44,50,50	3.88	22 (50%)	51,76,76	7.42	21 (41%)
42	A86	15	316	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	21	301	28	69,73,73	1.25	10 (14%)	83,113,113	1.32	4 (4%)
42	A86	17	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
42	A86	18	313	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
33	SQD	B	621	-	36,37,54	1.20	6 (16%)	45,48,65	1.64	9 (20%)
30	CLA	18	310	25	69,73,73	1.27	9 (13%)	83,113,113	1.33	7 (8%)
30	CLA	b	605	2	69,73,73	1.26	10 (14%)	83,113,113	1.41	8 (9%)
42	A86	21	314	-	44,50,50	4.01	23 (52%)	51,76,76	7.82	18 (35%)
35	LHG	b	621	-	48,48,48	0.75	1 (2%)	51,54,54	1.29	6 (11%)
30	CLA	C	514	3,30	69,73,73	1.26	10 (14%)	83,113,113	1.47	8 (9%)
42	A86	18	315	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
39	DGD	H	102	-	63,63,67	0.93	3 (4%)	77,77,81	1.42	8 (10%)
30	CLA	B	614	2	69,73,73	1.24	11 (15%)	83,113,113	1.46	8 (9%)
30	CLA	C	502	3	69,73,73	1.26	11 (15%)	83,113,113	1.53	11 (13%)
30	CLA	16	303	25	49,53,73	1.47	11 (22%)	59,89,113	1.78	10 (16%)
32	BCR	Y	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.47	9 (16%)
42	A86	20	211	-	44,50,50	3.89	23 (52%)	51,76,76	7.50	15 (29%)
30	CLA	B	609	2	69,73,73	1.24	10 (14%)	83,113,113	1.43	8 (9%)
30	CLA	19	303	-	69,73,73	1.24	10 (14%)	83,113,113	1.46	8 (9%)
36	LMG	D	408	-	51,51,55	0.90	3 (5%)	59,59,63	1.42	7 (11%)
41	HEM	v	201	16	50,50,50	1.32	5 (10%)	66,82,82	1.29	7 (10%)
30	CLA	C	505	-	69,73,73	1.27	10 (14%)	83,113,113	1.57	10 (12%)
42	A86	21	313	-	44,50,50	3.90	23 (52%)	51,76,76	7.52	22 (43%)
32	BCR	C	515	-	41,41,41	1.30	4 (9%)	56,56,56	1.40	9 (16%)
30	CLA	17	303	25	69,73,73	1.26	10 (14%)	83,113,113	1.53	8 (9%)
39	DGD	C	516	-	63,63,67	1.05	7 (11%)	77,77,81	1.60	15 (19%)
30	CLA	15	303	25	69,73,73	1.22	9 (13%)	83,113,113	1.43	10 (12%)
32	BCR	A	405	-	41,41,41	1.28	2 (4%)	56,56,56	1.40	6 (10%)
42	A86	12	319	-	44,50,50	3.93	23 (52%)	51,76,76	7.96	18 (35%)
42	A86	21	312	-	44,50,50	3.82	21 (47%)	51,76,76	7.17	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	17	308	25	69,73,73	1.33	8 (11%)	83,113,113	1.45	11 (13%)
30	CLA	d	406	4	69,73,73	1.33	12 (17%)	83,113,113	1.46	12 (14%)
30	CLA	12	310	25	49,53,73	1.47	9 (18%)	59,89,113	1.70	8 (13%)
30	CLA	17	307	25	49,53,73	1.48	9 (18%)	59,89,113	1.65	13 (22%)
30	CLA	a	403	1	69,73,73	1.28	10 (14%)	83,113,113	1.50	8 (9%)
30	CLA	15	305	-	49,53,73	1.48	9 (18%)	59,89,113	1.52	5 (8%)
36	LMG	B	620	-	51,51,55	0.98	5 (9%)	59,59,63	1.44	8 (13%)
35	LHG	L	101	-	48,48,48	0.81	1 (2%)	51,54,54	1.27	5 (9%)
30	CLA	b	601	-	69,73,73	1.25	11 (15%)	83,113,113	1.42	7 (8%)
30	CLA	18	312	-	49,53,73	1.47	10 (20%)	59,89,113	1.47	6 (10%)
36	LMG	d	410	-	51,51,55	0.90	3 (5%)	59,59,63	1.42	7 (11%)
36	LMG	B	619	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	8 (13%)
42	A86	15	314	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	19 (37%)
42	A86	17	315	-	44,50,50	4.06	23 (52%)	51,76,76	8.44	16 (31%)
30	CLA	15	301	25	69,73,73	1.26	11 (15%)	83,113,113	1.52	10 (12%)
36	LMG	w	101	-	51,51,55	0.89	4 (7%)	59,59,63	1.40	7 (11%)
30	CLA	C	511	3	69,73,73	1.36	12 (17%)	83,113,113	1.45	12 (14%)
30	CLA	15	309	-	49,53,73	1.48	10 (20%)	59,89,113	1.47	6 (10%)
42	A86	20	212	-	44,50,50	4.17	23 (52%)	51,76,76	8.24	15 (29%)
32	BCR	B	617	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	9 (16%)
30	CLA	B	612	2	69,73,73	1.38	8 (11%)	83,113,113	1.67	11 (13%)
42	A86	14	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.97	18 (35%)
42	A86	12	318	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	C	519	-	69,73,73	1.28	11 (15%)	83,113,113	1.41	7 (8%)
32	BCR	c	521	-	41,41,41	1.27	2 (4%)	56,56,56	1.37	6 (10%)
42	A86	17	302	-	44,50,50	3.94	23 (52%)	51,76,76	8.13	21 (41%)
32	BCR	H	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.31	7 (12%)
30	CLA	c	508	-	69,73,73	1.30	10 (14%)	83,113,113	1.54	13 (15%)
41	HEM	V	201	16	50,50,50	1.32	5 (10%)	66,82,82	1.29	9 (13%)
30	CLA	15	306	25	49,53,73	1.47	9 (18%)	59,89,113	1.60	6 (10%)
36	LMG	12	301	-	39,39,55	1.00	4 (10%)	47,47,63	1.21	5 (10%)
30	CLA	20	208	-	49,53,73	1.48	8 (16%)	59,89,113	1.56	8 (13%)
30	CLA	w	102	21	69,73,73	1.24	11 (15%)	83,113,113	1.35	9 (10%)
30	CLA	11	304	25	49,53,73	1.51	10 (20%)	59,89,113	1.83	13 (22%)
30	CLA	21	304	-	49,53,73	1.44	9 (18%)	59,89,113	1.43	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	b	611	2	69,73,73	1.34	11 (15%)	83,113,113	1.50	11 (13%)
30	CLA	14	309	25	69,73,73	1.30	11 (15%)	83,113,113	1.44	12 (14%)
30	CLA	16	307	25	49,53,73	1.51	10 (20%)	59,89,113	1.75	9 (15%)
42	A86	15	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
30	CLA	16	308	25	49,53,73	1.48	10 (20%)	59,89,113	1.57	10 (16%)
42	A86	11	316	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	12	312	25	69,73,73	1.27	10 (14%)	83,113,113	1.39	6 (7%)
30	CLA	18	307	-	49,53,73	1.47	10 (20%)	59,89,113	1.50	7 (11%)
30	CLA	c	503	3	69,73,73	1.38	11 (15%)	83,113,113	1.46	12 (14%)
30	CLA	11	302	25	49,53,73	1.45	11 (22%)	59,89,113	1.60	7 (11%)
42	A86	18	314	-	44,50,50	3.98	23 (52%)	51,76,76	7.94	18 (35%)
30	CLA	b	614	2	69,73,73	1.25	12 (17%)	83,113,113	1.48	8 (9%)
32	BCR	m	103	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	8 (14%)
30	CLA	W	102	21	69,73,73	1.26	10 (14%)	83,113,113	1.35	9 (10%)
30	CLA	21	302	-	49,53,73	1.49	9 (18%)	59,89,113	1.57	9 (15%)
30	CLA	C	512	3	69,73,73	1.33	10 (14%)	83,113,113	1.52	11 (13%)
42	A86	19	310	-	44,50,50	3.88	23 (52%)	51,76,76	7.70	16 (31%)
30	CLA	11	305	-	49,53,73	1.46	10 (20%)	59,89,113	1.54	7 (11%)
30	CLA	12	308	25	49,53,73	1.51	10 (20%)	59,89,113	1.85	13 (22%)
35	LHG	B	622	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	6 (11%)
30	CLA	18	309	25	69,73,73	1.32	10 (14%)	83,113,113	1.49	11 (13%)
30	CLA	20	203	30	49,53,73	1.48	9 (18%)	59,89,113	1.59	7 (11%)
30	CLA	W	103	-	69,73,73	1.26	7 (10%)	83,113,113	1.30	7 (8%)
33	SQD	b	620	-	36,37,54	1.20	6 (16%)	45,48,65	1.64	9 (20%)
42	A86	16	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
30	CLA	13	302	25	69,73,73	1.27	10 (14%)	83,113,113	1.58	8 (9%)
30	CLA	11	315	25	69,73,73	1.27	11 (15%)	83,113,113	1.38	6 (7%)
30	CLA	b	609	2	69,73,73	1.24	10 (14%)	83,113,113	1.44	8 (9%)
30	CLA	C	509	3	69,73,73	1.33	10 (14%)	83,113,113	1.52	10 (12%)
42	A86	14	314	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
30	CLA	15	307	25	69,73,73	1.27	11 (15%)	83,113,113	1.52	12 (14%)
30	CLA	20	204	-	69,73,73	1.23	10 (14%)	83,113,113	1.43	9 (10%)
30	CLA	w	103	-	69,73,73	1.27	9 (13%)	83,113,113	1.30	7 (8%)
36	LMG	b	618	-	51,51,55	0.88	4 (7%)	59,59,63	1.43	9 (15%)
30	CLA	B	601	-	69,73,73	1.25	10 (14%)	83,113,113	1.42	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	z	101	-	69,73,73	1.28	11 (15%)	83,113,113	1.43	7 (8%)
30	CLA	17	301	25	69,73,73	1.29	11 (15%)	83,113,113	1.43	9 (10%)
30	CLA	d	401	-	69,73,73	1.33	9 (13%)	83,113,113	1.45	11 (13%)
37	LMU	12	302	25,30	33,33,36	1.30	3 (9%)	44,44,47	1.54	7 (15%)
35	LHG	L	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
30	CLA	b	615	2	69,73,73	1.33	11 (15%)	83,113,113	1.38	11 (13%)
30	CLA	A	402	1	69,73,73	1.29	11 (15%)	83,113,113	1.47	9 (10%)
42	A86	13	315	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
31	PHO	D	403	-	58,69,69	1.91	12 (20%)	56,99,99	1.77	8 (14%)
30	CLA	12	305	25	69,73,73	1.27	11 (15%)	83,113,113	1.57	8 (9%)
34	BCT	A	407	1,29	2,3,3	1.26	0	2,3,3	3.94	2 (100%)
30	CLA	14	305	25	69,73,73	1.22	11 (15%)	83,113,113	1.51	10 (12%)
30	CLA	14	310	25	49,53,73	1.50	10 (20%)	59,89,113	1.59	6 (10%)
30	CLA	17	305	25	69,73,73	1.24	11 (15%)	83,113,113	1.44	11 (13%)
30	CLA	19	302	-	49,53,73	1.49	11 (22%)	59,89,113	1.65	10 (16%)
36	LMG	b	619	-	51,51,55	0.99	5 (9%)	59,59,63	1.44	8 (13%)
30	CLA	b	622	-	69,73,73	1.29	10 (14%)	83,113,113	1.51	13 (15%)
32	BCR	c	515	-	41,41,41	1.34	3 (7%)	56,56,56	1.41	8 (14%)
32	BCR	b	623	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
42	A86	20	213	-	44,50,50	4.01	23 (52%)	51,76,76	7.82	18 (35%)
42	A86	14	315	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	c	507	3	69,73,73	1.30	10 (14%)	83,113,113	1.45	12 (14%)
34	BCT	a	406	1,29	2,3,3	1.27	0	2,3,3	3.96	2 (100%)
32	BCR	h	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.32	8 (14%)
30	CLA	13	304	25	69,73,73	1.23	11 (15%)	83,113,113	1.48	9 (10%)
30	CLA	19	306	-	49,53,73	1.48	11 (22%)	59,89,113	1.49	5 (8%)
30	CLA	21	306	-	69,73,73	1.28	10 (14%)	83,113,113	1.36	7 (8%)
30	CLA	m	101	12,2,36	69,73,73	1.24	10 (14%)	83,113,113	1.29	6 (7%)
30	CLA	c	506	3	69,73,73	1.26	9 (13%)	83,113,113	1.46	10 (12%)
30	CLA	21	308	-	49,53,73	1.48	8 (16%)	59,89,113	1.51	6 (10%)
35	LHG	d	409	-	48,48,48	0.81	1 (2%)	51,54,54	1.26	5 (9%)
30	CLA	d	407	4	69,73,73	1.25	11 (15%)	83,113,113	1.52	7 (8%)
30	CLA	D	405	4	69,73,73	1.33	12 (17%)	83,113,113	1.47	11 (13%)
30	CLA	c	502	3	69,73,73	1.26	11 (15%)	83,113,113	1.52	13 (15%)
42	A86	14	301	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	c	510	3	69,73,73	1.35	10 (14%)	83,113,113	1.60	12 (14%)
42	A86	19	312	-	44,50,50	4.00	21 (47%)	51,76,76	8.15	18 (35%)
30	CLA	19	305	-	49,53,73	1.47	11 (22%)	59,89,113	1.54	5 (8%)
32	BCR	c	516	-	41,41,41	1.31	4 (9%)	56,56,56	1.40	9 (16%)
42	A86	11	311	-	44,50,50	3.96	23 (52%)	51,76,76	7.93	18 (35%)
32	BCR	b	616	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	9 (16%)
30	CLA	19	309	-	49,53,73	1.45	9 (18%)	59,89,113	1.63	10 (16%)
30	CLA	16	306	25	49,53,73	1.48	9 (18%)	59,89,113	1.62	6 (10%)
42	A86	18	302	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	d	402	-	69,73,73	1.28	10 (14%)	83,113,113	1.42	7 (8%)
30	CLA	B	615	2	69,73,73	1.33	11 (15%)	83,113,113	1.38	11 (13%)
30	CLA	b	610	-	69,73,73	1.33	11 (15%)	83,113,113	1.43	7 (8%)
30	CLA	18	304	25	49,53,73	1.45	9 (18%)	59,89,113	1.65	6 (10%)
30	CLA	12	314	-	49,53,73	1.47	9 (18%)	59,89,113	1.53	5 (8%)
30	CLA	14	307	-	49,53,73	1.46	10 (20%)	59,89,113	1.53	7 (11%)
30	CLA	21	305	28	49,53,73	1.53	8 (16%)	59,89,113	1.62	10 (16%)
30	CLA	C	520	-	69,73,73	1.25	10 (14%)	83,113,113	1.57	12 (14%)
30	CLA	12	309	-	49,53,73	1.45	10 (20%)	59,89,113	1.54	7 (11%)
30	CLA	13	310	-	49,53,73	1.48	10 (20%)	59,89,113	1.53	6 (10%)
30	CLA	c	514	3	69,73,73	1.27	11 (15%)	83,113,113	1.46	8 (9%)
30	CLA	16	304	25	69,73,73	1.25	10 (14%)	83,113,113	1.39	8 (9%)
42	A86	19	311	-	44,50,50	4.09	21 (47%)	51,76,76	7.17	19 (37%)
30	CLA	14	303	25	69,73,73	1.27	10 (14%)	83,113,113	1.58	8 (9%)
30	CLA	11	307	25	69,73,73	1.28	10 (14%)	83,113,113	1.45	11 (13%)
30	CLA	12	313	25	49,53,73	1.49	11 (22%)	59,89,113	1.61	7 (11%)
42	A86	13	311	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
42	A86	16	310	-	44,50,50	3.97	23 (52%)	51,76,76	8.08	20 (39%)
30	CLA	c	504	3	69,73,73	1.28	11 (15%)	83,113,113	1.44	10 (12%)
30	CLA	b	612	2	69,73,73	1.39	9 (13%)	83,113,113	1.66	11 (13%)
30	CLA	13	309	25	49,53,73	1.49	11 (22%)	59,89,113	1.60	7 (11%)
30	CLA	11	309	-	49,53,73	1.48	10 (20%)	59,89,113	1.51	5 (8%)
30	CLA	14	304	25	49,53,73	1.45	11 (22%)	59,89,113	1.62	6 (10%)
30	CLA	c	511	3	69,73,73	1.36	12 (17%)	83,113,113	1.46	12 (14%)
42	A86	17	312	-	44,50,50	3.97	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	A	404	1	69,73,73	1.28	11 (15%)	83,113,113	1.50	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	A86	13	301	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
36	LMG	1	101	-	39,39,55	1.01	4 (10%)	47,47,63	1.18	4 (8%)
30	CLA	16	301	25	69,73,73	1.25	9 (13%)	83,113,113	1.36	7 (8%)
30	CLA	17	309	25	49,53,73	1.50	11 (22%)	59,89,113	1.91	11 (18%)
42	A86	13	313	-	44,50,50	4.05	23 (52%)	51,76,76	7.81	19 (37%)
30	CLA	13	306	-	49,53,73	1.45	10 (20%)	59,89,113	1.54	7 (11%)
30	CLA	b	604	2	69,73,73	1.34	10 (14%)	83,113,113	1.57	15 (18%)
32	BCR	B	616	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	8 (14%)
30	CLA	13	303	25	49,53,73	1.45	11 (22%)	59,89,113	1.63	7 (11%)
39	DGD	j	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
42	A86	12	304	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	21 (41%)
31	PHO	d	404	-	58,69,69	1.91	12 (20%)	56,99,99	1.77	8 (14%)
42	A86	11	312	-	44,50,50	4.04	23 (52%)	51,76,76	7.82	20 (39%)
38	OEX	c	501	3,1	0,14,14	-	-	-		
42	A86	13	312	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
35	LHG	l	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
30	CLA	B	610	-	69,73,73	1.33	11 (15%)	83,113,113	1.43	7 (8%)
42	A86	17	311	-	44,50,50	4.03	22 (50%)	51,76,76	8.34	19 (37%)
30	CLA	18	308	25	49,53,73	1.51	9 (18%)	59,89,113	1.57	6 (10%)
32	BCR	B	624	-	41,41,41	1.13	3 (7%)	56,56,56	1.30	7 (12%)
30	CLA	14	311	-	49,53,73	1.48	10 (20%)	59,89,113	1.53	6 (10%)
42	A86	15	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	C	510	3	69,73,73	1.35	10 (14%)	83,113,113	1.60	12 (14%)
30	CLA	19	307	-	69,73,73	1.24	11 (15%)	83,113,113	1.39	8 (9%)
42	A86	15	315	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
33	SQD	A	406	-	53,54,54	0.97	6 (11%)	62,65,65	1.58	11 (17%)
30	CLA	M	101	12,2,36	69,73,73	1.25	10 (14%)	83,113,113	1.29	6 (7%)
42	A86	16	312	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
30	CLA	16	305	25	49,53,73	1.46	9 (18%)	59,89,113	1.70	11 (18%)
30	CLA	D	402	-	69,73,73	1.27	10 (14%)	83,113,113	1.42	7 (8%)
30	CLA	c	509	3	69,73,73	1.33	10 (14%)	83,113,113	1.53	10 (12%)
41	HEM	f	102	6,5	50,50,50	1.35	4 (8%)	66,82,82	1.16	4 (6%)
42	A86	16	313	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	B	613	2	69,73,73	1.33	10 (14%)	83,113,113	1.46	11 (13%)
42	A86	12	315	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	13	307	25	49,53,73	1.46	9 (18%)	59,89,113	1.71	7 (11%)
30	CLA	21	309	-	49,53,73	1.50	10 (20%)	59,89,113	1.54	9 (15%)
42	A86	15	312	-	44,50,50	4.04	23 (52%)	51,76,76	7.82	20 (39%)
42	A86	17	313	-	44,50,50	4.05	24 (54%)	51,76,76	7.82	19 (37%)
30	CLA	18	305	25	69,73,73	1.22	10 (14%)	83,113,113	1.38	5 (6%)
39	DGD	J	101	-	63,63,67	1.11	10 (15%)	77,77,81	1.56	15 (19%)
40	PL9	D	407	-	55,55,55	2.32	15 (27%)	68,69,69	1.48	14 (20%)
30	CLA	B	604	2	69,73,73	1.34	10 (14%)	83,113,113	1.56	16 (19%)
35	LHG	a	407	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	7 (14%)
42	A86	14	312	-	44,50,50	3.93	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	11	301	25	69,73,73	1.28	11 (15%)	83,113,113	1.58	8 (9%)
32	BCR	f	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
42	A86	14	313	-	44,50,50	3.96	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	C	507	3	69,73,73	1.30	10 (14%)	83,113,113	1.45	11 (13%)
30	CLA	b	603	2	69,73,73	1.27	11 (15%)	83,113,113	1.52	13 (15%)
36	LMG	m	102	30	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
39	DGD	c	517	-	63,63,67	1.06	8 (12%)	77,77,81	1.60	15 (19%)
38	OEX	C	501	3,1	0,14,14	-	-	-		
42	A86	12	317	-	44,50,50	4.05	22 (50%)	51,76,76	7.80	19 (37%)
30	CLA	18	306	25	49,53,73	1.47	8 (16%)	59,89,113	1.66	10 (16%)
33	SQD	a	405	-	53,54,54	0.96	5 (9%)	62,65,65	1.59	11 (17%)
30	CLA	c	513	3	69,73,73	1.27	11 (15%)	83,113,113	1.38	7 (8%)
30	CLA	b	608	2	69,73,73	1.24	9 (13%)	83,113,113	1.39	7 (8%)
32	BCR	F	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
30	CLA	20	207	-	49,53,73	1.49	11 (22%)	59,89,113	1.59	8 (13%)
33	SQD	l	101	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
30	CLA	19	304	26	49,53,73	1.47	9 (18%)	59,89,113	1.67	12 (20%)
30	CLA	21	307	-	69,73,73	1.24	8 (11%)	83,113,113	1.33	6 (7%)
30	CLA	15	308	25	49,53,73	1.47	10 (20%)	59,89,113	1.61	9 (15%)
42	A86	21	311	-	44,50,50	3.89	23 (52%)	51,76,76	7.50	15 (29%)
42	A86	11	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	B	606	2	69,73,73	1.37	12 (17%)	83,113,113	1.50	13 (15%)
30	CLA	b	602	2	69,73,73	1.27	9 (13%)	83,113,113	1.41	10 (12%)
30	CLA	16	302	25	69,73,73	1.30	10 (14%)	83,113,113	1.79	17 (20%)
32	BCR	a	408	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	B	611	2	69,73,73	1.34	11 (15%)	83,113,113	1.50	11 (13%)
32	BCR	a	404	-	41,41,41	1.29	2 (4%)	56,56,56	1.39	6 (10%)
40	PL9	d	405	4	55,55,55	1.36	6 (10%)	68,69,69	1.50	14 (20%)
42	A86	11	314	-	44,50,50	3.93	23 (52%)	51,76,76	7.98	19 (37%)
35	LHG	A	408	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	7 (14%)
30	CLA	14	306	25	49,53,73	1.50	10 (20%)	59,89,113	1.86	13 (22%)
31	PHO	A	403	-	58,69,69	1.97	13 (22%)	56,99,99	1.83	10 (17%)
30	CLA	C	504	3	69,73,73	1.29	11 (15%)	83,113,113	1.45	10 (12%)
31	PHO	d	403	-	58,69,69	1.97	13 (22%)	56,99,99	1.83	10 (17%)
30	CLA	15	304	25	49,53,73	1.48	8 (16%)	59,89,113	1.61	11 (18%)
36	LMG	M	102	30	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
32	BCR	c	520	-	41,41,41	1.27	3 (7%)	56,56,56	1.47	10 (17%)
30	CLA	20	206	27	49,53,73	1.48	10 (20%)	59,89,113	1.64	7 (11%)
32	BCR	A	409	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	5 (8%)
32	BCR	C	518	-	41,41,41	1.28	2 (4%)	56,56,56	1.37	6 (10%)
30	CLA	14	302	25	69,73,73	1.27	10 (14%)	83,113,113	1.37	6 (7%)
30	CLA	12	306	25,37	49,53,73	1.45	11 (22%)	59,89,113	1.61	7 (11%)
30	CLA	15	302	25	49,53,73	1.45	8 (16%)	59,89,113	1.70	6 (10%)
30	CLA	b	607	-	69,73,73	1.27	10 (14%)	83,113,113	1.41	9 (10%)
30	CLA	14	308	25	49,53,73	1.45	8 (16%)	59,89,113	1.69	8 (13%)
30	CLA	20	205	-	49,53,73	1.47	9 (18%)	59,89,113	1.66	12 (20%)
30	CLA	C	503	3	69,73,73	1.38	11 (15%)	83,113,113	1.46	12 (14%)
30	CLA	17	306	25	49,53,73	1.48	9 (18%)	59,89,113	1.77	13 (22%)
42	A86	13	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	C	506	3	69,73,73	1.26	9 (13%)	83,113,113	1.46	11 (13%)
41	HEM	F	102	6,5	50,50,50	1.35	4 (8%)	66,82,82	1.15	4 (6%)
30	CLA	B	605	2	69,73,73	1.28	10 (14%)	83,113,113	1.41	8 (9%)
39	DGD	c	518	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	16 (20%)
30	CLA	17	304	25	49,53,73	1.45	12 (24%)	59,89,113	1.64	9 (15%)
42	A86	17	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	18 (35%)
30	CLA	C	508	-	69,73,73	1.30	10 (14%)	83,113,113	1.56	13 (15%)
30	CLA	18	303	25	69,73,73	1.26	10 (14%)	83,113,113	1.41	8 (9%)
30	CLA	20	209	30	69,73,73	1.26	10 (14%)	83,113,113	1.35	10 (12%)
30	CLA	11	308	25	49,53,73	1.48	11 (22%)	59,89,113	1.59	7 (11%)
30	CLA	12	307	25	69,73,73	1.25	11 (15%)	83,113,113	1.48	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	19	301	-	69,73,73	1.31	11 (15%)	83,113,113	1.39	10 (12%)
30	CLA	c	505	-	69,73,73	1.27	11 (15%)	83,113,113	1.57	10 (12%)
30	CLA	B	623	-	69,73,73	1.28	11 (15%)	83,113,113	1.50	13 (15%)
30	CLA	13	308	25	69,73,73	1.27	10 (14%)	83,113,113	1.45	12 (14%)
30	CLA	a	402	1	69,73,73	1.30	11 (15%)	83,113,113	1.46	8 (9%)
36	LMG	Q	301	-	51,51,55	0.96	5 (9%)	59,59,63	1.46	9 (15%)
30	CLA	b	613	2	69,73,73	1.34	10 (14%)	83,113,113	1.48	9 (10%)
30	CLA	B	602	2	69,73,73	1.27	9 (13%)	83,113,113	1.42	9 (10%)
30	CLA	Z	102	19,30	69,73,73	1.26	8 (11%)	83,113,113	1.33	8 (9%)
30	CLA	18	311	25	49,53,73	1.48	9 (18%)	59,89,113	1.65	9 (15%)
42	A86	20	210	-	44,50,50	4.07	23 (52%)	51,76,76	8.32	17 (33%)
42	A86	20	201	-	44,50,50	3.93	22 (50%)	51,76,76	7.88	19 (37%)
42	A86	15	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	12	303	25	69,73,73	1.27	10 (14%)	83,113,113	1.38	6 (7%)
30	CLA	D	401	-	69,73,73	1.33	10 (14%)	83,113,113	1.45	11 (13%)
39	DGD	h	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.42	8 (10%)
32	BCR	Z	101	-	41,41,41	1.32	3 (7%)	56,56,56	1.41	8 (14%)
42	A86	11	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
36	LMG	c	519	-	51,51,55	0.96	5 (9%)	59,59,63	1.46	9 (15%)
30	CLA	B	607	-	69,73,73	1.27	11 (15%)	83,113,113	1.42	9 (10%)
30	CLA	11	306	25	49,53,73	1.45	9 (18%)	59,89,113	1.71	7 (11%)
30	CLA	B	608	2	69,73,73	1.24	9 (13%)	83,113,113	1.39	7 (8%)
30	CLA	D	406	4	69,73,73	1.25	11 (15%)	83,113,113	1.52	7 (8%)
30	CLA	b	606	2	69,73,73	1.37	12 (17%)	83,113,113	1.48	13 (15%)
40	PL9	D	404	4	55,55,55	1.35	6 (10%)	68,69,69	1.49	15 (22%)
30	CLA	C	513	3	69,73,73	1.26	10 (14%)	83,113,113	1.38	7 (8%)
30	CLA	13	305	25	49,53,73	1.51	10 (20%)	59,89,113	1.84	13 (22%)
32	BCR	b	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.41	10 (17%)
30	CLA	11	303	25	69,73,73	1.23	11 (15%)	83,113,113	1.48	8 (9%)
33	SQD	L	103	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
30	CLA	21	303	-	69,73,73	1.24	8 (11%)	83,113,113	1.33	6 (7%)
39	DGD	C	517	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	16 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMU	B	625	-	-	7/18/58/61	0/2/2/2
42	A86	12	316	-	-	3/34/90/90	0/3/3/3
30	CLA	16	309	-	-	7/15/91/115	-
32	BCR	B	618	-	-	9/29/63/63	0/2/2/2
30	CLA	c	512	3	-	10/39/115/115	-
30	CLA	B	603	2	-	12/39/115/115	-
30	CLA	20	202	-	-	19/39/115/115	-
36	LMG	W	101	-	-	28/46/66/70	0/1/1/1
30	CLA	12	311	25	-	16/39/115/115	-
30	CLA	17	310	-	-	9/15/91/115	-
40	PL9	d	408	-	-	13/53/73/73	0/1/1/1
30	CLA	18	301	25	-	13/39/115/115	-
30	CLA	19	308	-	-	3/15/91/115	-
42	A86	21	310	-	-	9/34/90/90	0/3/3/3
42	A86	15	316	-	-	16/34/90/90	0/3/3/3
30	CLA	21	301	28	-	16/39/115/115	-
42	A86	17	314	-	-	10/34/90/90	0/3/3/3
42	A86	18	313	-	-	8/34/90/90	0/3/3/3
33	SQD	B	621	-	-	9/32/52/69	0/1/1/1
30	CLA	18	310	25	-	12/39/115/115	-
30	CLA	b	605	2	-	19/39/115/115	-
42	A86	21	314	-	-	12/34/90/90	0/3/3/3
35	LHG	b	621	-	-	20/53/53/53	-
30	CLA	C	514	3,30	-	13/39/115/115	-
42	A86	18	315	-	-	10/34/90/90	0/3/3/3
39	DGD	H	102	-	-	24/51/91/95	0/2/2/2
30	CLA	B	614	2	-	8/39/115/115	-
30	CLA	C	502	3	-	14/39/115/115	-
30	CLA	16	303	25	-	6/15/91/115	-
32	BCR	Y	101	-	-	16/29/63/63	0/2/2/2
42	A86	20	211	-	-	8/34/90/90	0/3/3/3
30	CLA	B	609	2	-	10/39/115/115	-
30	CLA	19	303	-	-	17/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMG	D	408	-	-	14/46/66/70	0/1/1/1
41	HEM	v	201	16	-	1/14/54/54	-
30	CLA	C	505	-	-	19/39/115/115	-
42	A86	21	313	-	-	16/34/90/90	0/3/3/3
32	BCR	C	515	-	-	10/29/63/63	0/2/2/2
30	CLA	17	303	25	-	15/39/115/115	-
39	DGD	C	516	-	-	19/51/91/95	0/2/2/2
30	CLA	15	303	25	-	17/39/115/115	-
32	BCR	A	405	-	-	12/29/63/63	0/2/2/2
42	A86	12	319	-	-	7/34/90/90	0/3/3/3
42	A86	21	312	-	-	7/34/90/90	0/3/3/3
30	CLA	17	308	25	-	19/39/115/115	-
30	CLA	d	406	4	-	8/39/115/115	-
30	CLA	12	310	25	-	10/15/91/115	-
30	CLA	17	307	25	-	9/15/91/115	-
30	CLA	a	403	1	-	12/39/115/115	-
30	CLA	15	305	-	-	10/15/91/115	-
36	LMG	B	620	-	-	20/46/66/70	0/1/1/1
35	LHG	L	101	-	-	29/53/53/53	-
30	CLA	b	601	-	-	20/39/115/115	-
30	CLA	18	312	-	-	6/15/91/115	-
36	LMG	d	410	-	-	14/46/66/70	0/1/1/1
36	LMG	B	619	-	-	18/46/66/70	0/1/1/1
42	A86	15	314	-	-	7/34/90/90	0/3/3/3
42	A86	17	315	-	-	13/34/90/90	0/3/3/3
30	CLA	15	301	25	-	12/39/115/115	-
36	LMG	w	101	-	-	28/46/66/70	0/1/1/1
30	CLA	C	511	3	-	12/39/115/115	-
30	CLA	15	309	-	-	6/15/91/115	-
42	A86	20	212	-	-	11/34/90/90	0/3/3/3
32	BCR	B	617	-	-	9/29/63/63	0/2/2/2
30	CLA	B	612	2	-	13/39/115/115	-
42	A86	14	316	-	-	7/34/90/90	0/3/3/3
42	A86	12	318	-	-	10/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	C	519	-	-	23/39/115/115	-
32	BCR	c	521	-	-	8/29/63/63	0/2/2/2
42	A86	17	302	-	-	16/34/90/90	1/3/3/3
32	BCR	H	101	-	-	7/29/63/63	0/2/2/2
30	CLA	c	508	-	-	18/39/115/115	-
41	HEM	V	201	16	-	1/14/54/54	-
30	CLA	15	306	25	-	10/15/91/115	-
36	LMG	12	301	-	-	17/34/54/70	0/1/1/1
30	CLA	20	208	-	-	8/15/91/115	-
30	CLA	w	102	21	-	16/39/115/115	-
30	CLA	11	304	25	-	9/15/91/115	-
30	CLA	21	304	-	-	8/15/91/115	-
30	CLA	b	611	2	-	14/39/115/115	-
30	CLA	14	309	25	-	16/39/115/115	-
30	CLA	16	307	25	-	9/15/91/115	-
42	A86	15	311	-	-	3/34/90/90	0/3/3/3
30	CLA	16	308	25	-	9/15/91/115	-
42	A86	11	316	-	-	16/34/90/90	0/3/3/3
30	CLA	12	312	25	-	13/39/115/115	-
30	CLA	18	307	-	-	8/15/91/115	-
30	CLA	c	503	3	-	13/39/115/115	-
30	CLA	11	302	25	-	5/15/91/115	-
42	A86	18	314	-	-	3/34/90/90	0/3/3/3
30	CLA	b	614	2	-	8/39/115/115	-
32	BCR	m	103	-	-	8/29/63/63	0/2/2/2
30	CLA	W	102	21	-	16/39/115/115	-
30	CLA	21	302	-	-	9/15/91/115	-
30	CLA	C	512	3	-	10/39/115/115	-
42	A86	19	310	-	-	11/34/90/90	0/3/3/3
30	CLA	11	305	-	-	10/15/91/115	-
30	CLA	12	308	25	-	9/15/91/115	-
35	LHG	B	622	-	-	20/53/53/53	-
30	CLA	18	309	25	-	17/39/115/115	-
30	CLA	20	203	30	-	7/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	W	103	-	-	21/39/115/115	-
33	SQD	b	620	-	-	9/32/52/69	0/1/1/1
42	A86	16	311	-	-	3/34/90/90	0/3/3/3
30	CLA	13	302	25	-	14/39/115/115	-
30	CLA	11	315	25	-	13/39/115/115	-
30	CLA	b	609	2	-	10/39/115/115	-
30	CLA	C	509	3	-	12/39/115/115	-
42	A86	14	314	-	-	8/34/90/90	0/3/3/3
30	CLA	15	307	25	-	13/39/115/115	-
30	CLA	20	204	-	-	15/39/115/115	-
30	CLA	w	103	-	-	21/39/115/115	-
36	LMG	b	618	-	-	18/46/66/70	0/1/1/1
30	CLA	B	601	-	-	20/39/115/115	-
30	CLA	z	101	-	-	23/39/115/115	-
30	CLA	17	301	25	-	16/39/115/115	-
30	CLA	d	401	-	-	14/39/115/115	-
37	LMU	12	302	25,30	-	7/18/58/61	0/2/2/2
35	LHG	L	102	-	-	22/53/53/53	-
30	CLA	b	615	2	-	13/39/115/115	-
30	CLA	A	402	1	-	7/39/115/115	-
42	A86	13	315	-	-	16/34/90/90	0/3/3/3
31	PHO	D	403	-	-	8/37/103/103	0/5/6/6
30	CLA	12	305	25	-	13/39/115/115	-
30	CLA	14	305	25	-	15/39/115/115	-
30	CLA	14	310	25	-	8/15/91/115	-
30	CLA	17	305	25	-	21/39/115/115	-
30	CLA	19	302	-	-	4/15/91/115	-
36	LMG	b	619	-	-	20/46/66/70	0/1/1/1
30	CLA	b	622	-	-	17/39/115/115	-
32	BCR	c	515	-	-	15/29/63/63	0/2/2/2
32	BCR	b	623	-	-	18/29/63/63	0/2/2/2
42	A86	20	213	-	-	12/34/90/90	0/3/3/3
42	A86	14	315	-	-	10/34/90/90	0/3/3/3
30	CLA	c	507	3	-	19/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	BCR	h	101	-	-	7/29/63/63	0/2/2/2
30	CLA	13	304	25	-	15/39/115/115	-
30	CLA	19	306	-	-	10/15/91/115	-
30	CLA	21	306	-	-	16/39/115/115	-
30	CLA	m	101	12,2,36	-	21/39/115/115	-
30	CLA	c	506	3	-	18/39/115/115	-
30	CLA	21	308	-	-	10/15/91/115	-
35	LHG	d	409	-	-	29/53/53/53	-
30	CLA	d	407	4	-	6/39/115/115	-
30	CLA	D	405	4	-	8/39/115/115	-
30	CLA	c	502	3	-	14/39/115/115	-
42	A86	14	301	-	-	7/34/90/90	0/3/3/3
30	CLA	c	510	3	-	12/39/115/115	-
42	A86	19	312	-	-	8/34/90/90	0/3/3/3
30	CLA	19	305	-	-	9/15/91/115	-
32	BCR	c	516	-	-	10/29/63/63	0/2/2/2
42	A86	11	311	-	-	3/34/90/90	0/3/3/3
32	BCR	b	616	-	-	9/29/63/63	0/2/2/2
30	CLA	19	309	-	-	10/15/91/115	-
30	CLA	16	306	25	-	9/15/91/115	-
42	A86	18	302	-	-	15/34/90/90	0/3/3/3
30	CLA	d	402	-	-	15/39/115/115	-
30	CLA	B	615	2	-	13/39/115/115	-
30	CLA	b	610	-	-	16/39/115/115	-
30	CLA	18	304	25	-	5/15/91/115	-
30	CLA	12	314	-	-	8/15/91/115	-
30	CLA	14	307	-	-	10/15/91/115	-
30	CLA	21	305	28	-	11/15/91/115	-
30	CLA	C	520	-	-	16/39/115/115	-
30	CLA	12	309	-	-	10/15/91/115	-
30	CLA	13	310	-	-	8/15/91/115	-
30	CLA	c	514	3	-	13/39/115/115	-
30	CLA	16	304	25	-	17/39/115/115	-
42	A86	19	311	-	-	17/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	14	303	25	-	14/39/115/115	-
30	CLA	11	307	25	-	16/39/115/115	-
30	CLA	12	313	25	-	8/15/91/115	-
42	A86	13	311	-	-	8/34/90/90	0/3/3/3
42	A86	16	310	-	-	12/34/90/90	0/3/3/3
30	CLA	c	504	3	-	19/39/115/115	-
30	CLA	b	612	2	-	13/39/115/115	-
30	CLA	13	309	25	-	8/15/91/115	-
30	CLA	11	309	-	-	8/15/91/115	-
30	CLA	14	304	25	-	4/15/91/115	-
30	CLA	c	511	3	-	12/39/115/115	-
42	A86	17	312	-	-	3/34/90/90	0/3/3/3
30	CLA	A	404	1	-	12/39/115/115	-
42	A86	13	301	-	-	15/34/90/90	0/3/3/3
36	LMG	1	101	-	-	14/34/54/70	0/1/1/1
30	CLA	16	301	25	-	12/39/115/115	-
30	CLA	17	309	25	-	4/15/91/115	-
42	A86	13	313	-	-	9/34/90/90	0/3/3/3
30	CLA	13	306	-	-	10/15/91/115	-
30	CLA	b	604	2	-	14/39/115/115	-
32	BCR	B	616	-	-	8/29/63/63	0/2/2/2
30	CLA	13	303	25	-	5/15/91/115	-
39	DGD	j	101	-	-	15/51/91/95	0/2/2/2
42	A86	12	304	-	-	16/34/90/90	0/3/3/3
31	PHO	d	404	-	-	8/37/103/103	0/5/6/6
42	A86	11	312	-	-	8/34/90/90	0/3/3/3
42	A86	13	312	-	-	3/34/90/90	0/3/3/3
35	LHG	l	102	-	-	22/53/53/53	-
30	CLA	B	610	-	-	16/39/115/115	-
42	A86	17	311	-	-	13/34/90/90	0/3/3/3
30	CLA	18	308	25	-	10/15/91/115	-
32	BCR	B	624	-	-	18/29/63/63	0/2/2/2
30	CLA	14	311	-	-	8/15/91/115	-
42	A86	15	310	-	-	8/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	C	510	3	-	12/39/115/115	-
30	CLA	19	307	-	-	17/39/115/115	-
42	A86	15	315	-	-	15/34/90/90	0/3/3/3
33	SQD	A	406	-	-	14/49/69/69	0/1/1/1
30	CLA	M	101	12,2,36	-	21/39/115/115	-
42	A86	16	312	-	-	8/34/90/90	0/3/3/3
30	CLA	16	305	25	-	8/15/91/115	-
30	CLA	D	402	-	-	15/39/115/115	-
30	CLA	c	509	3	-	12/39/115/115	-
41	HEM	f	102	6,5	-	7/14/54/54	-
42	A86	16	313	-	-	7/34/90/90	0/3/3/3
30	CLA	B	613	2	-	8/39/115/115	-
42	A86	12	315	-	-	8/34/90/90	0/3/3/3
30	CLA	13	307	25	-	10/15/91/115	-
30	CLA	21	309	-	-	8/15/91/115	-
42	A86	15	312	-	-	8/34/90/90	0/3/3/3
42	A86	17	313	-	-	9/34/90/90	0/3/3/3
30	CLA	18	305	25	-	21/39/115/115	-
39	DGD	J	101	-	-	15/51/91/95	0/2/2/2
40	PL9	D	407	-	-	13/53/73/73	0/1/1/1
30	CLA	B	604	2	-	14/39/115/115	-
35	LHG	a	407	-	-	23/50/50/53	-
42	A86	14	312	-	-	8/34/90/90	0/3/3/3
30	CLA	11	301	25	-	13/39/115/115	-
32	BCR	f	101	-	-	15/29/63/63	0/2/2/2
42	A86	14	313	-	-	3/34/90/90	0/3/3/3
30	CLA	C	507	3	-	19/39/115/115	-
30	CLA	b	603	2	-	12/39/115/115	-
36	LMG	m	102	30	-	10/35/55/70	0/1/1/1
39	DGD	c	517	-	-	19/51/91/95	0/2/2/2
42	A86	12	317	-	-	9/34/90/90	0/3/3/3
30	CLA	18	306	25	-	9/15/91/115	-
33	SQD	a	405	-	-	14/49/69/69	0/1/1/1
30	CLA	c	513	3	-	18/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	608	2	-	9/39/115/115	-
32	BCR	F	101	-	-	15/29/63/63	0/2/2/2
30	CLA	20	207	-	-	9/15/91/115	-
33	SQD	l	101	-	-	21/49/69/69	0/1/1/1
30	CLA	19	304	26	-	11/15/91/115	-
30	CLA	21	307	-	-	13/39/115/115	-
30	CLA	15	308	25	-	8/15/91/115	-
42	A86	21	311	-	-	8/34/90/90	0/3/3/3
42	A86	11	310	-	-	8/34/90/90	0/3/3/3
30	CLA	B	606	2	-	7/39/115/115	-
30	CLA	b	602	2	-	15/39/115/115	-
30	CLA	16	302	25	-	17/39/115/115	-
32	BCR	a	408	-	-	9/29/63/63	0/2/2/2
30	CLA	B	611	2	-	14/39/115/115	-
32	BCR	a	404	-	-	12/29/63/63	0/2/2/2
40	PL9	d	405	4	-	17/53/73/73	0/1/1/1
42	A86	11	314	-	-	7/34/90/90	0/3/3/3
35	LHG	A	408	-	-	23/50/50/53	-
30	CLA	14	306	25	-	9/15/91/115	-
31	PHO	A	403	-	-	12/37/103/103	0/5/6/6
30	CLA	C	504	3	-	19/39/115/115	-
31	PHO	d	403	-	-	12/37/103/103	0/5/6/6
30	CLA	15	304	25	-	7/15/91/115	-
36	LMG	M	102	30	-	10/35/55/70	0/1/1/1
32	BCR	c	520	-	-	16/29/63/63	0/2/2/2
30	CLA	20	206	27	-	9/15/91/115	-
32	BCR	A	409	-	-	9/29/63/63	0/2/2/2
32	BCR	C	518	-	-	8/29/63/63	0/2/2/2
30	CLA	14	302	25	-	13/39/115/115	-
30	CLA	12	306	25,37	-	4/15/91/115	-
30	CLA	15	302	25	-	10/15/91/115	-
30	CLA	b	607	-	-	12/39/115/115	-
30	CLA	14	308	25	-	10/15/91/115	-
30	CLA	20	205	-	-	11/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	C	503	3	-	13/39/115/115	-
30	CLA	17	306	25	-	8/15/91/115	-
42	A86	13	314	-	-	10/34/90/90	0/3/3/3
30	CLA	C	506	3	-	18/39/115/115	-
41	HEM	F	102	6,5	-	7/14/54/54	-
30	CLA	B	605	2	-	19/39/115/115	-
39	DGD	c	518	-	-	22/51/91/95	0/2/2/2
30	CLA	17	304	25	-	6/15/91/115	-
42	A86	17	316	-	-	7/34/90/90	0/3/3/3
30	CLA	C	508	-	-	18/39/115/115	-
30	CLA	18	303	25	-	16/39/115/115	-
30	CLA	20	209	30	-	13/39/115/115	-
30	CLA	11	308	25	-	8/15/91/115	-
30	CLA	12	307	25	-	15/39/115/115	-
30	CLA	19	301	-	-	14/39/115/115	-
30	CLA	c	505	-	-	19/39/115/115	-
30	CLA	B	623	-	-	17/39/115/115	-
30	CLA	13	308	25	-	16/39/115/115	-
30	CLA	a	402	1	-	7/39/115/115	-
36	LMG	Q	301	-	-	22/46/66/70	0/1/1/1
30	CLA	b	613	2	-	8/39/115/115	-
30	CLA	B	602	2	-	15/39/115/115	-
30	CLA	Z	102	19,30	-	17/39/115/115	-
30	CLA	18	311	25	-	10/15/91/115	-
42	A86	20	210	-	-	14/34/90/90	0/3/3/3
42	A86	20	201	-	-	12/34/90/90	0/3/3/3
42	A86	15	313	-	-	10/34/90/90	0/3/3/3
30	CLA	12	303	25	-	13/39/115/115	-
30	CLA	D	401	-	-	14/39/115/115	-
39	DGD	h	102	-	-	24/51/91/95	0/2/2/2
32	BCR	Z	101	-	-	15/29/63/63	0/2/2/2
42	A86	11	313	-	-	10/34/90/90	0/3/3/3
36	LMG	c	519	-	-	22/46/66/70	0/1/1/1
30	CLA	B	607	-	-	12/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	11	306	25	-	10/15/91/115	-
30	CLA	B	608	2	-	9/39/115/115	-
30	CLA	D	406	4	-	6/39/115/115	-
30	CLA	b	606	2	-	7/39/115/115	-
40	PL9	D	404	4	-	17/53/73/73	0/1/1/1
30	CLA	C	513	3	-	18/39/115/115	-
30	CLA	13	305	25	-	9/15/91/115	-
32	BCR	b	617	-	-	9/29/63/63	0/2/2/2
30	CLA	11	303	25	-	15/39/115/115	-
33	SQD	L	103	-	-	21/49/69/69	0/1/1/1
30	CLA	21	303	-	-	19/39/115/115	-
39	DGD	C	517	-	-	22/51/91/95	0/2/2/2

The worst 5 of 3538 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	19	311	A86	C14-C13	14.34	1.68	1.51
42	11	313	A86	C14-C13	14.10	1.68	1.51
42	12	318	A86	C14-C13	14.06	1.68	1.51
42	13	314	A86	C14-C13	14.04	1.68	1.51
42	18	315	A86	C14-C13	14.01	1.68	1.51

The worst 5 of 3400 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	17	311	A86	O1-C20-C19	55.34	154.95	113.38
42	17	315	A86	O1-C20-C19	55.32	154.94	113.38
42	18	313	A86	O1-C20-C19	55.08	154.75	113.38
42	20	210	A86	O1-C20-C19	55.05	154.74	113.38
42	11	310	A86	O1-C20-C19	55.03	154.72	113.38

There are no chirality outliers.

5 of 3923 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	A	402	CLA	CBD-CGD-O2D-CED
30	A	404	CLA	C2B-C3B-CAB-CBB
30	A	404	CLA	C4B-C3B-CAB-CBB
30	B	601	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	601	CLA	C2B-C3B-CAB-CBB

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	17	302	A86	C31-C32-C33-C34-C35-C36

284 monomers are involved in 862 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	12	316	A86	9	0
30	16	309	CLA	5	0
32	B	618	BCR	2	0
30	c	512	CLA	2	0
30	20	202	CLA	5	0
36	W	101	LMG	8	0
30	12	311	CLA	2	0
30	17	310	CLA	1	0
40	d	408	PL9	5	0
30	18	301	CLA	2	0
42	21	310	A86	10	0
42	15	316	A86	14	0
30	21	301	CLA	3	0
42	17	314	A86	2	0
42	18	313	A86	1	0
30	18	310	CLA	2	0
30	b	605	CLA	1	0
42	21	314	A86	19	0
35	b	621	LHG	2	0
30	C	514	CLA	10	0
42	18	315	A86	7	0
39	H	102	DGD	5	0
30	B	614	CLA	3	0
30	C	502	CLA	3	0
30	16	303	CLA	1	0
32	Y	101	BCR	4	0
42	20	211	A86	7	0
30	B	609	CLA	1	0
30	19	303	CLA	5	0
36	D	408	LMG	2	0
41	v	201	HEM	2	0
30	C	505	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	21	313	A86	2	0
32	C	515	BCR	2	0
30	17	303	CLA	11	0
30	15	303	CLA	1	0
32	A	405	BCR	1	0
42	12	319	A86	2	0
42	21	312	A86	4	0
30	17	308	CLA	5	0
30	d	406	CLA	5	0
30	12	310	CLA	3	0
30	17	307	CLA	1	0
30	a	403	CLA	6	0
30	15	305	CLA	1	0
36	B	620	LMG	2	0
35	L	101	LHG	5	0
30	b	601	CLA	4	0
30	18	312	CLA	19	0
36	d	410	LMG	1	0
36	B	619	LMG	3	0
42	15	314	A86	1	0
42	17	315	A86	19	0
30	15	301	CLA	8	0
36	w	101	LMG	6	0
30	C	511	CLA	4	0
30	15	309	CLA	1	0
42	20	212	A86	13	0
32	B	617	BCR	1	0
30	B	612	CLA	4	0
42	14	316	A86	2	0
42	12	318	A86	4	0
30	C	519	CLA	1	0
32	c	521	BCR	2	0
42	17	302	A86	18	0
32	H	101	BCR	5	0
30	c	508	CLA	3	0
41	V	201	HEM	2	0
30	15	306	CLA	3	0
36	12	301	LMG	8	0
30	w	102	CLA	3	0
30	11	304	CLA	2	0
30	21	304	CLA	5	0
30	b	611	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	14	309	CLA	2	0
30	16	307	CLA	7	0
42	15	311	A86	10	0
30	16	308	CLA	10	0
42	11	316	A86	10	0
30	12	312	CLA	3	0
30	c	503	CLA	3	0
30	11	302	CLA	1	0
42	18	314	A86	15	0
30	b	614	CLA	5	0
32	m	103	BCR	3	0
30	W	102	CLA	5	0
30	21	302	CLA	4	0
30	C	512	CLA	3	0
42	19	310	A86	6	0
30	11	305	CLA	2	0
30	12	308	CLA	7	0
35	B	622	LHG	1	0
30	18	309	CLA	4	0
30	20	203	CLA	6	0
30	W	103	CLA	4	0
33	b	620	SQD	2	0
42	16	311	A86	7	0
30	13	302	CLA	9	0
30	11	315	CLA	7	0
30	b	609	CLA	2	0
30	C	509	CLA	6	0
42	14	314	A86	1	0
30	15	307	CLA	3	0
30	w	103	CLA	2	0
36	b	618	LMG	4	0
30	B	601	CLA	4	0
30	z	101	CLA	4	0
30	17	301	CLA	3	0
30	d	401	CLA	3	0
35	L	102	LHG	1	0
30	b	615	CLA	3	0
30	A	402	CLA	2	0
42	13	315	A86	8	0
31	D	403	PHO	2	0
30	12	305	CLA	9	0
34	A	407	BCT	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	14	305	CLA	4	0
30	14	310	CLA	3	0
30	17	305	CLA	12	0
36	b	619	LMG	1	0
30	b	622	CLA	3	0
32	c	515	BCR	3	0
32	b	623	BCR	4	0
42	20	213	A86	1	0
42	14	315	A86	3	0
30	c	507	CLA	5	0
34	a	406	BCT	2	0
32	h	101	BCR	3	0
30	13	304	CLA	4	0
30	21	306	CLA	3	0
30	m	101	CLA	2	0
30	c	506	CLA	1	0
30	21	308	CLA	1	0
35	d	409	LHG	3	0
30	d	407	CLA	1	0
30	D	405	CLA	6	0
30	c	502	CLA	4	0
42	14	301	A86	2	0
30	c	510	CLA	2	0
42	19	312	A86	3	0
32	c	516	BCR	1	0
42	11	311	A86	9	0
32	b	616	BCR	1	0
30	19	309	CLA	1	0
30	16	306	CLA	1	0
42	18	302	A86	10	0
30	d	402	CLA	1	0
30	B	615	CLA	2	0
30	b	610	CLA	2	0
30	18	304	CLA	3	0
30	14	307	CLA	2	0
30	21	305	CLA	1	0
30	C	520	CLA	3	0
30	12	309	CLA	4	0
30	c	514	CLA	2	0
30	16	304	CLA	1	0
42	19	311	A86	13	0
30	14	303	CLA	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	11	307	CLA	2	0
30	12	313	CLA	1	0
42	13	311	A86	2	0
42	16	310	A86	7	0
30	c	504	CLA	4	0
30	b	612	CLA	4	0
30	13	309	CLA	1	0
30	14	304	CLA	3	0
30	c	511	CLA	5	0
42	17	312	A86	12	0
30	A	404	CLA	11	0
42	13	301	A86	9	0
30	16	301	CLA	3	0
30	17	309	CLA	1	0
42	13	313	A86	3	0
30	13	306	CLA	2	0
30	b	604	CLA	6	0
32	B	616	BCR	2	0
30	13	303	CLA	2	0
39	j	101	DGD	1	0
42	12	304	A86	7	0
31	d	404	PHO	2	0
42	11	312	A86	3	0
38	c	501	OEX	1	0
42	13	312	A86	11	0
35	l	102	LHG	3	0
30	B	610	CLA	2	0
42	17	311	A86	6	0
30	18	308	CLA	1	0
32	B	624	BCR	5	0
42	15	310	A86	2	0
30	C	510	CLA	2	0
42	15	315	A86	7	0
30	M	101	CLA	1	0
42	16	312	A86	5	0
30	D	402	CLA	1	0
30	c	509	CLA	6	0
41	f	102	HEM	4	0
42	16	313	A86	2	0
30	B	613	CLA	4	0
30	13	307	CLA	2	0
30	21	309	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	17	313	A86	1	0
30	18	305	CLA	2	0
39	J	101	DGD	1	0
40	D	407	PL9	4	0
30	B	604	CLA	6	0
35	a	407	LHG	6	0
30	11	301	CLA	8	0
32	f	101	BCR	1	0
42	14	313	A86	10	0
30	C	507	CLA	11	0
30	b	603	CLA	1	0
36	m	102	LMG	2	0
42	12	317	A86	4	0
30	c	513	CLA	4	0
30	b	608	CLA	3	0
32	F	101	BCR	2	0
30	20	207	CLA	2	0
33	l	101	SQD	3	0
30	21	307	CLA	1	0
30	15	308	CLA	6	0
42	21	311	A86	9	0
30	B	606	CLA	3	0
30	b	602	CLA	6	0
30	16	302	CLA	7	0
32	a	408	BCR	1	0
30	B	611	CLA	3	0
32	a	404	BCR	1	0
40	d	405	PL9	3	0
42	11	314	A86	3	0
35	A	408	LHG	4	0
31	A	403	PHO	1	0
30	C	504	CLA	4	0
36	M	102	LMG	5	0
32	c	520	BCR	2	0
32	A	409	BCR	2	0
32	C	518	BCR	3	0
30	14	302	CLA	2	0
30	12	306	CLA	2	0
30	15	302	CLA	3	0
30	b	607	CLA	2	0
30	14	308	CLA	1	0
30	C	503	CLA	3	0

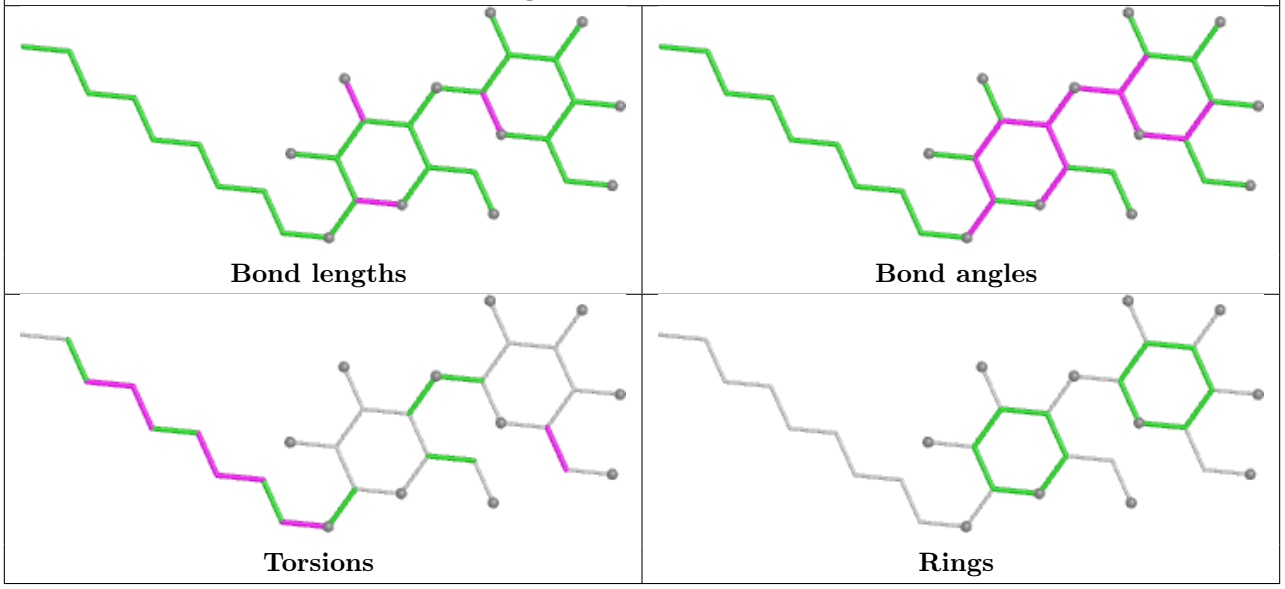
Continued on next page...

Continued from previous page...

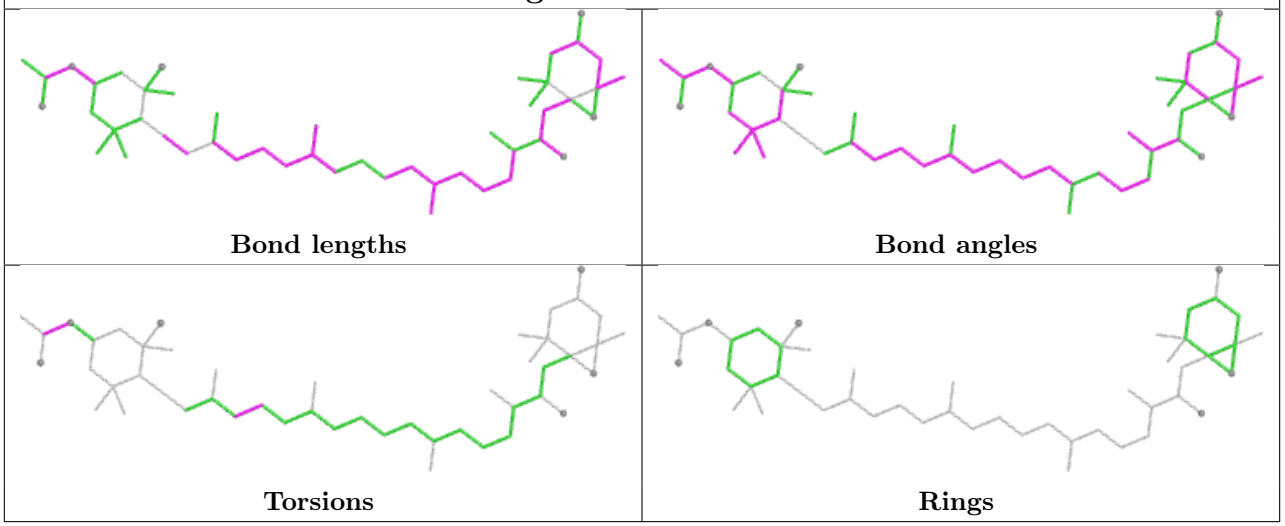
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	17	306	CLA	4	0
42	13	314	A86	3	0
30	C	506	CLA	4	0
41	F	102	HEM	3	0
30	B	605	CLA	2	0
30	17	304	CLA	2	0
42	17	316	A86	5	0
30	C	508	CLA	1	0
30	18	303	CLA	14	0
30	20	209	CLA	2	0
30	11	308	CLA	1	0
30	12	307	CLA	3	0
30	19	301	CLA	3	0
30	c	505	CLA	1	0
30	B	623	CLA	3	0
30	13	308	CLA	2	0
30	a	402	CLA	1	0
36	Q	301	LMG	2	0
30	b	613	CLA	3	0
30	B	602	CLA	6	0
30	Z	102	CLA	9	0
30	18	311	CLA	5	0
42	20	210	A86	10	0
42	20	201	A86	11	0
42	15	313	A86	6	0
30	12	303	CLA	6	0
30	D	401	CLA	4	0
39	h	102	DGD	3	0
32	Z	101	BCR	1	0
42	11	313	A86	6	0
36	c	519	LMG	1	0
30	B	607	CLA	2	0
30	11	306	CLA	1	0
30	B	608	CLA	2	0
30	D	406	CLA	1	0
30	b	606	CLA	4	0
40	D	404	PL9	3	0
30	C	513	CLA	2	0
32	b	617	BCR	2	0
30	11	303	CLA	3	0
33	L	103	SQD	3	0
30	21	303	CLA	11	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.

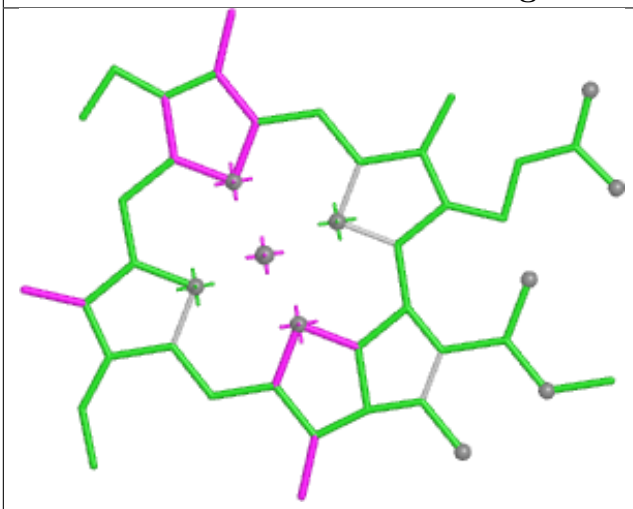
Ligand LMU B 625



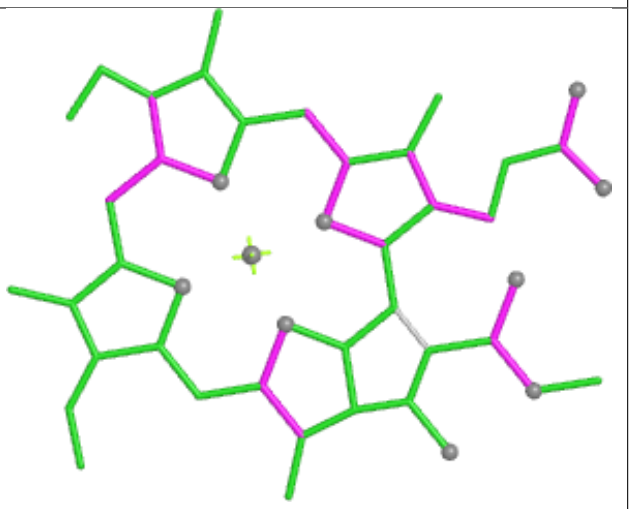
Ligand A86 12 316



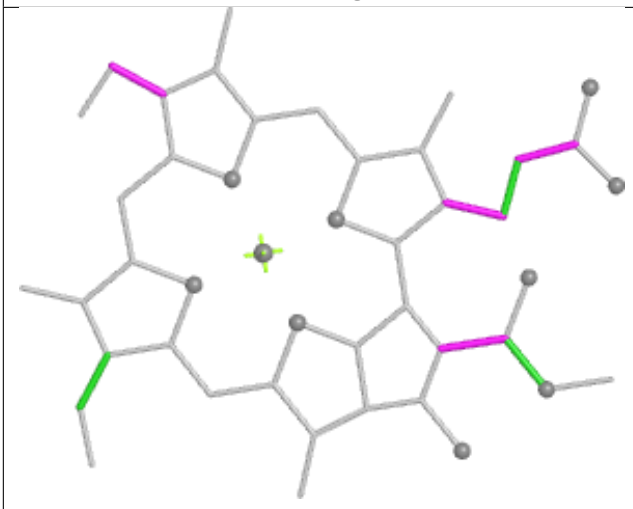
Ligand CLA 16 309



Bond lengths



Bond angles

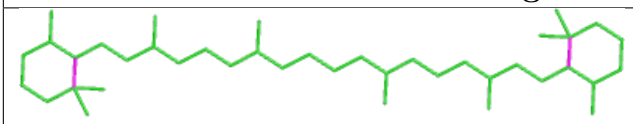


Torsions

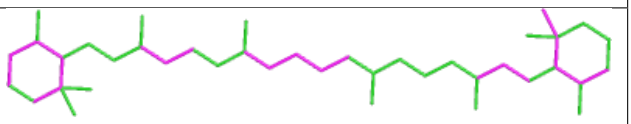


Rings

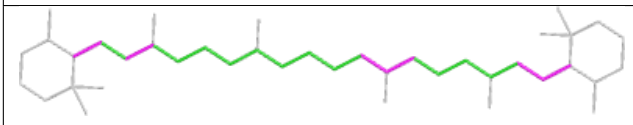
Ligand BCR B 618



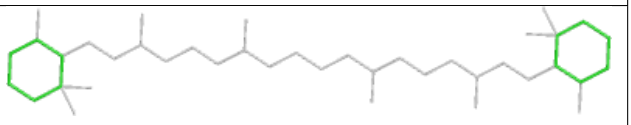
Bond lengths



Bond angles

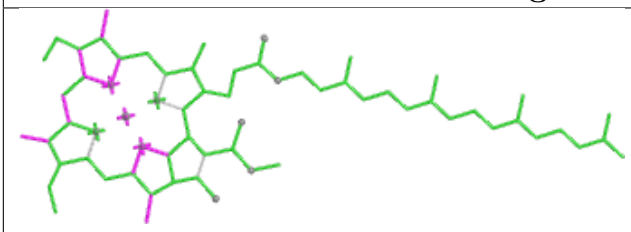


Torsions

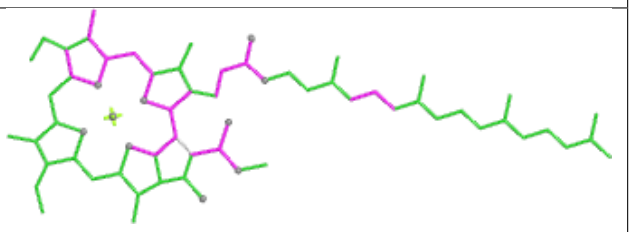


Rings

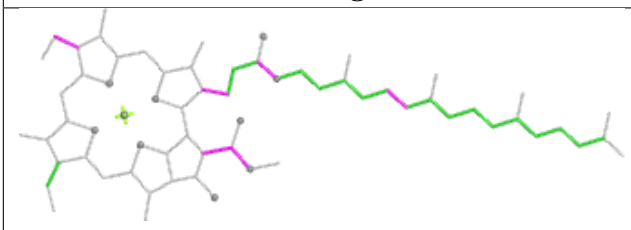
Ligand CLA c 512



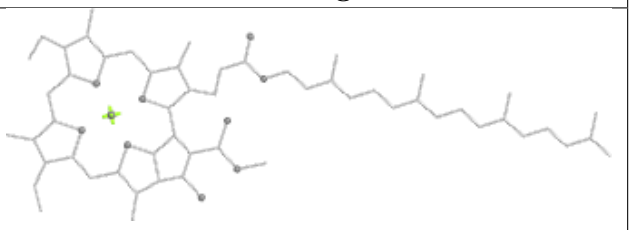
Bond lengths



Bond angles

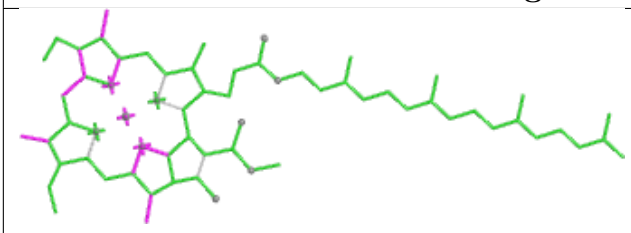


Torsions

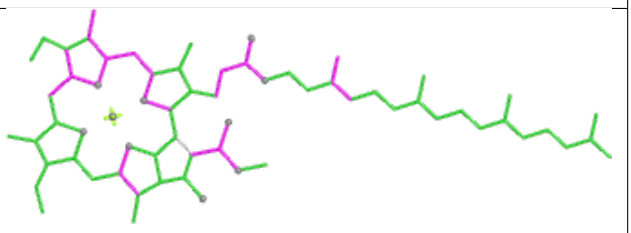


Rings

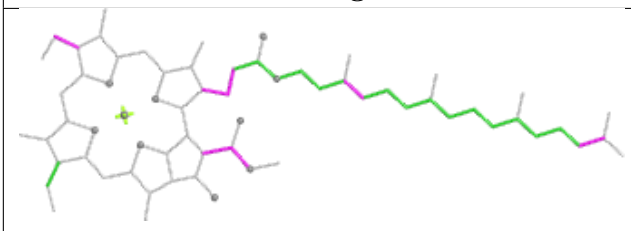
Ligand CLA B 603



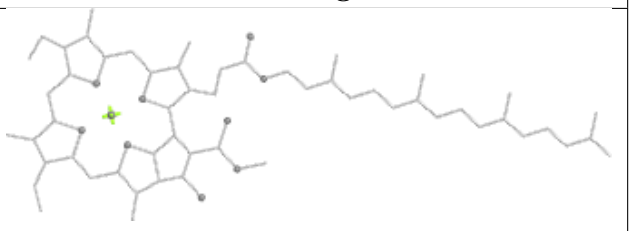
Bond lengths



Bond angles

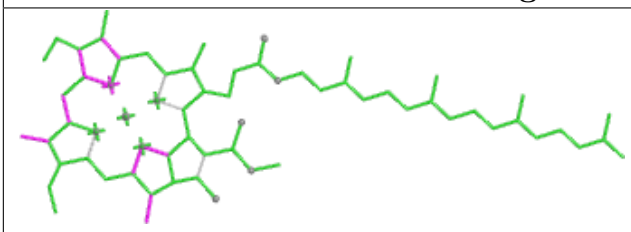


Torsions

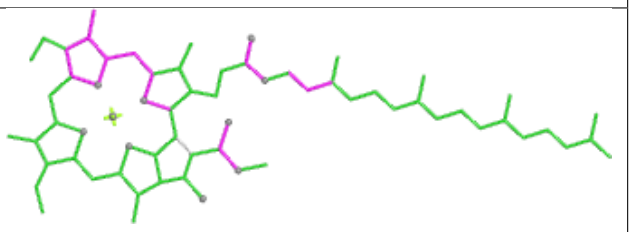


Rings

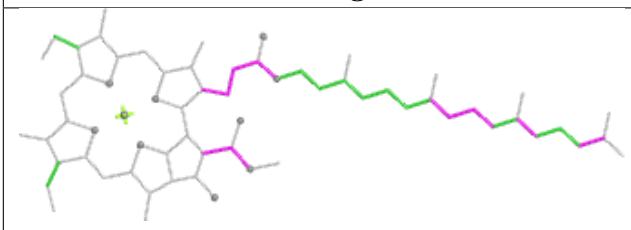
Ligand CLA 20 202



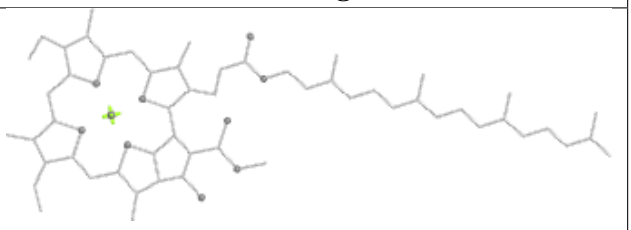
Bond lengths



Bond angles

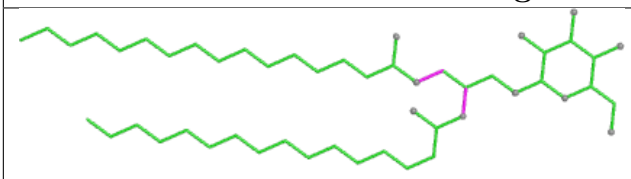


Torsions

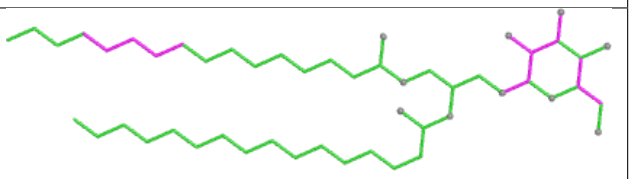


Rings

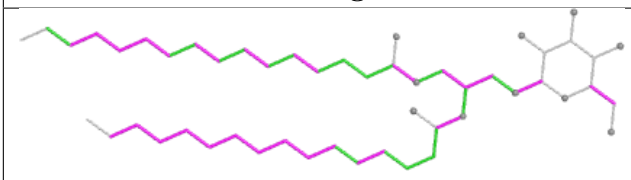
Ligand LMG W 101



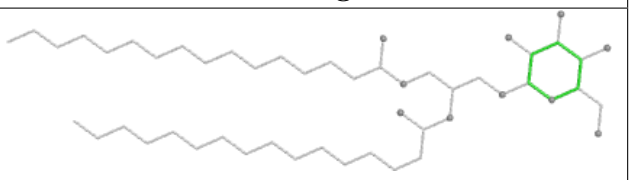
Bond lengths



Bond angles

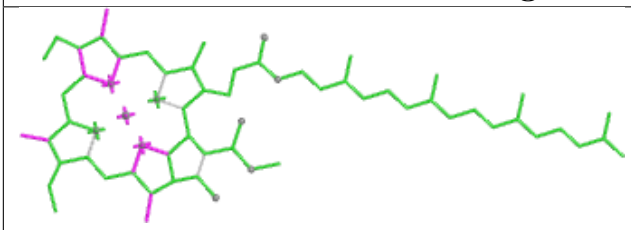


Torsions

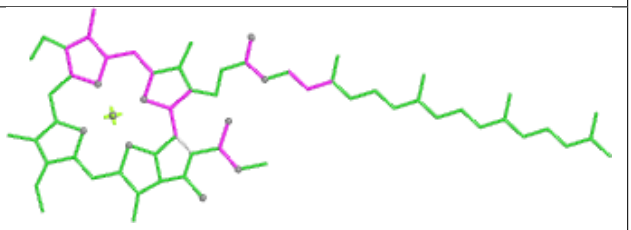


Rings

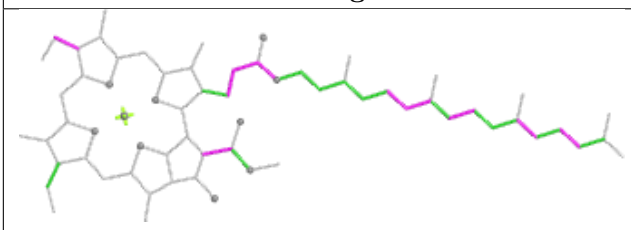
Ligand CLA 12 311



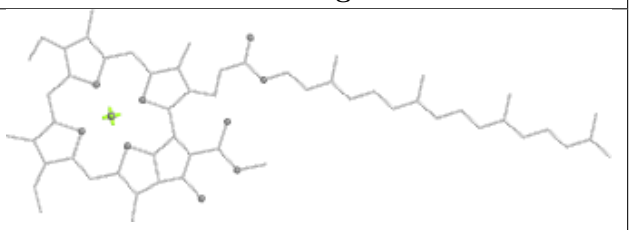
Bond lengths



Bond angles

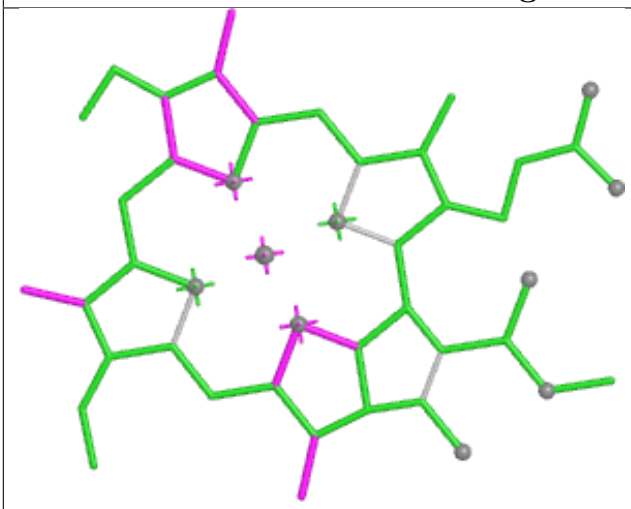


Torsions

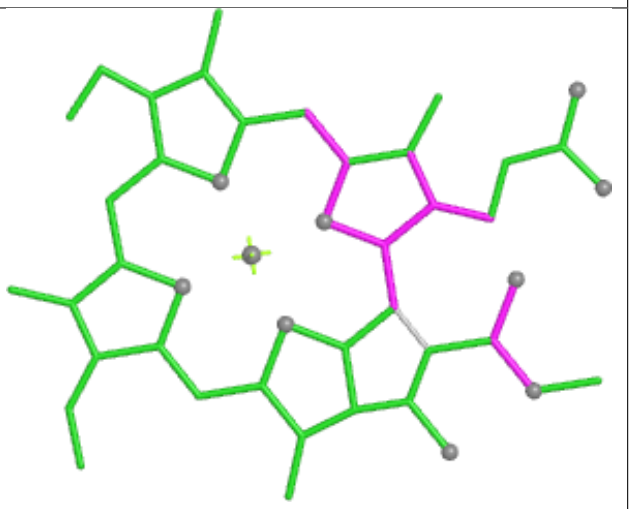


Rings

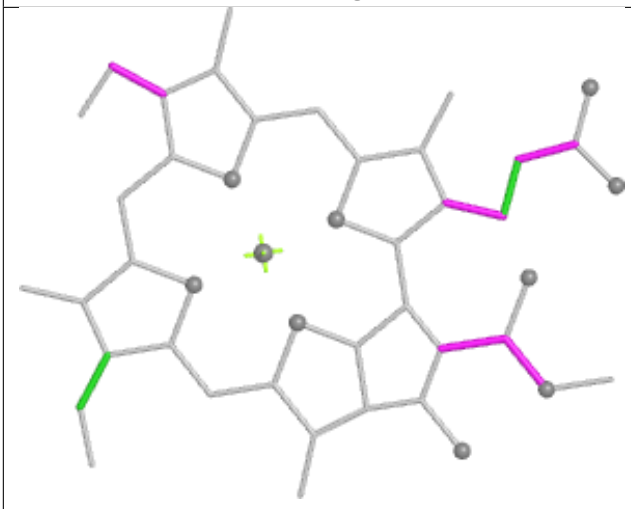
Ligand CLA 17 310



Bond lengths



Bond angles

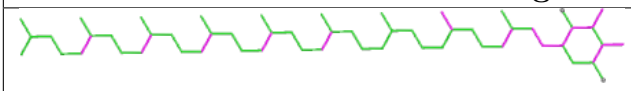


Torsions

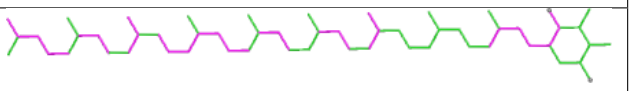


Rings

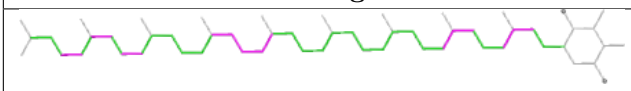
Ligand PL9 d 408



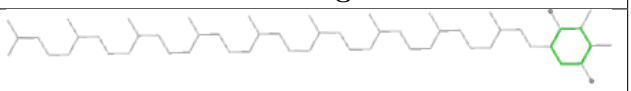
Bond lengths



Bond angles

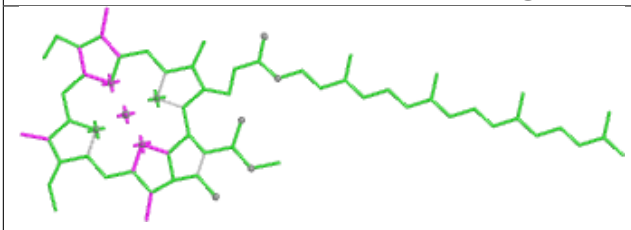


Torsions

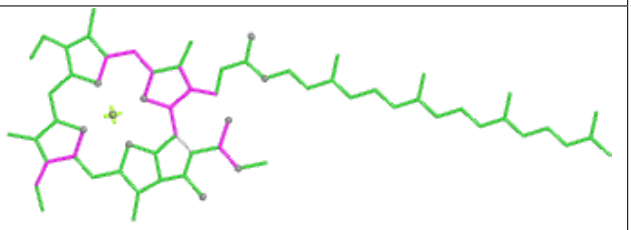


Rings

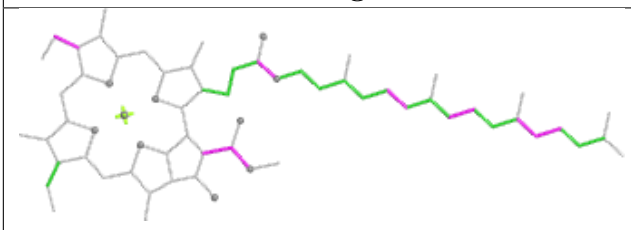
Ligand CLA 18 301



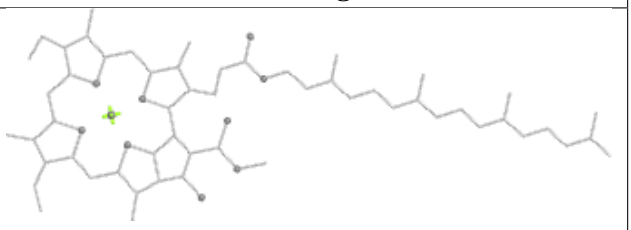
Bond lengths



Bond angles

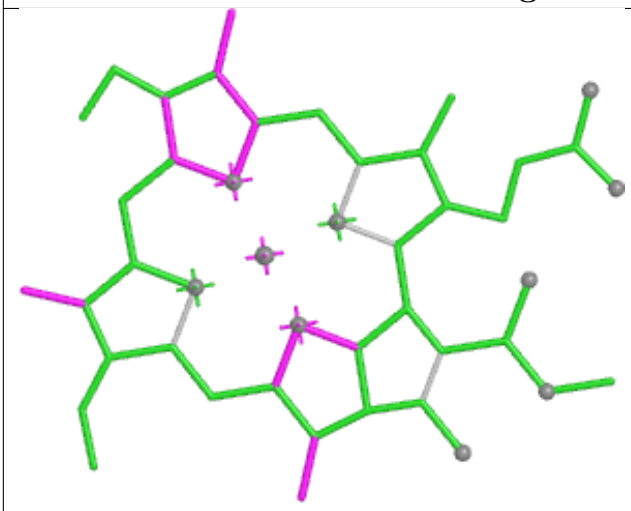


Torsions

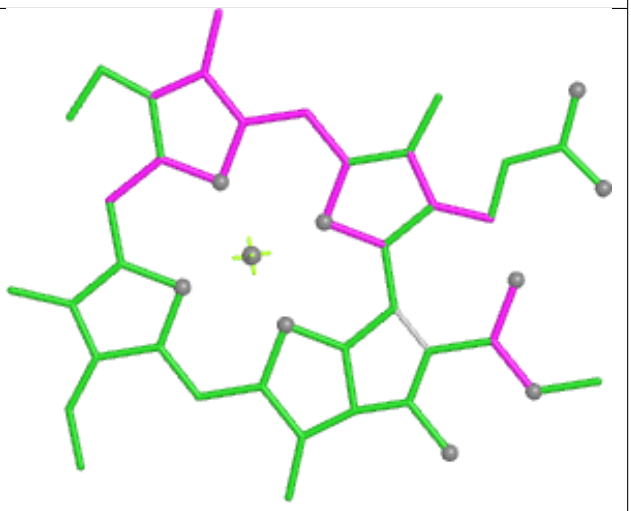


Rings

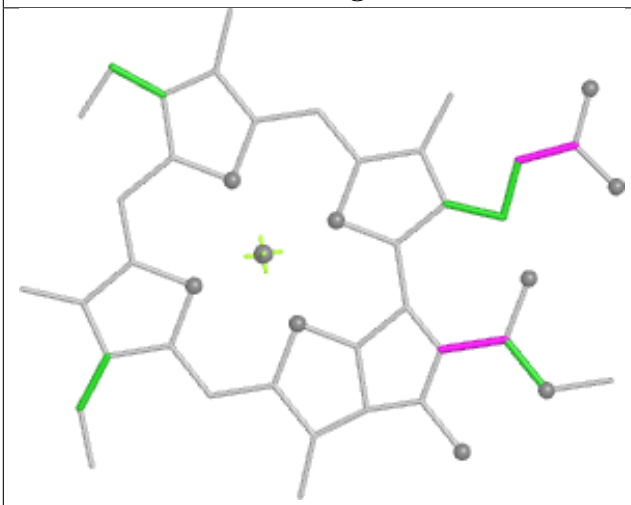
Ligand CLA 19 308



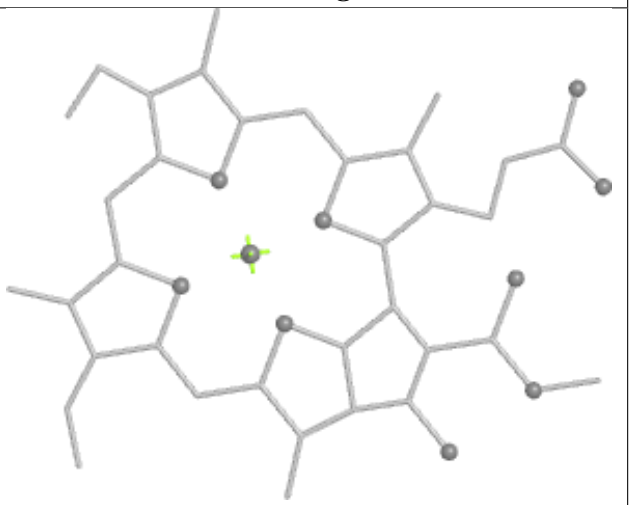
Bond lengths



Bond angles

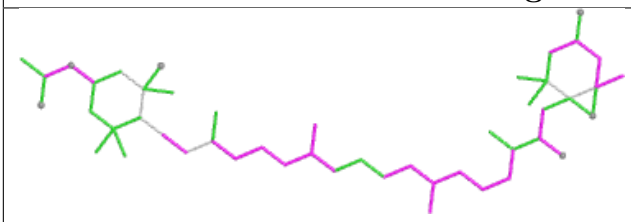


Torsions

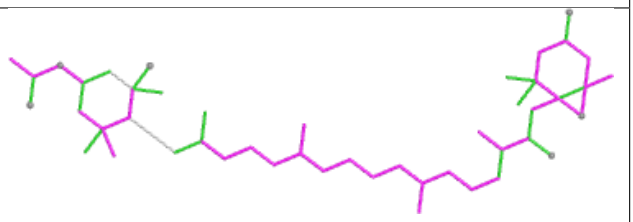


Rings

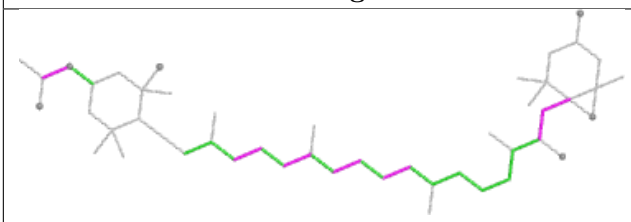
Ligand A86 21 310



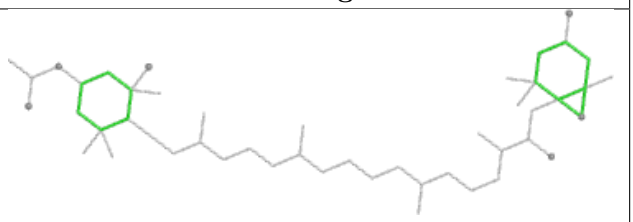
Bond lengths



Bond angles

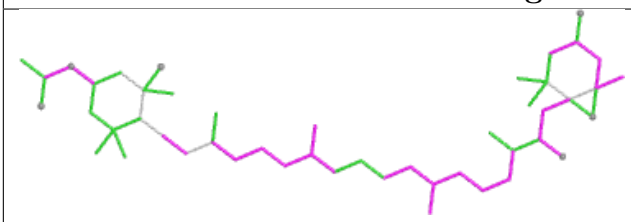


Torsions

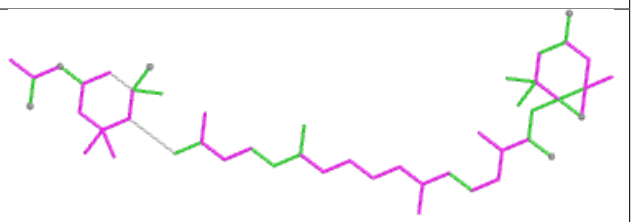


Rings

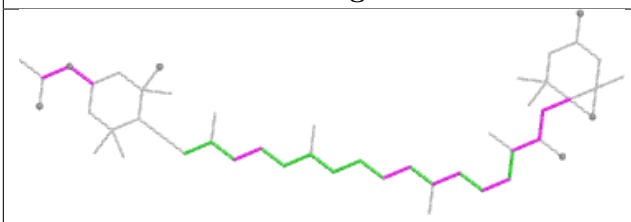
Ligand A86 15 316



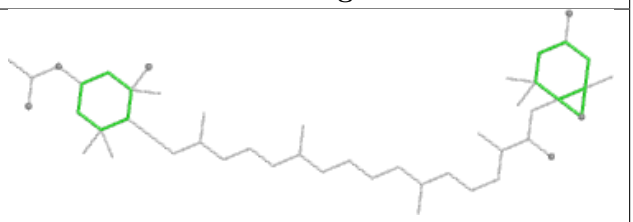
Bond lengths



Bond angles

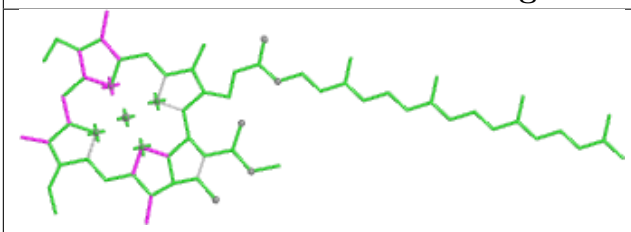


Torsions

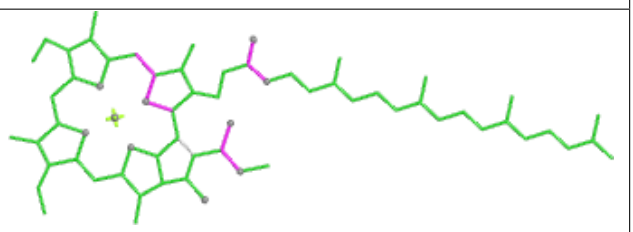


Rings

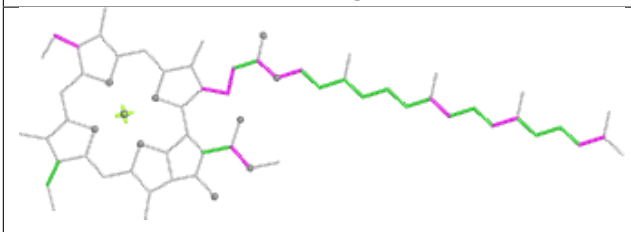
Ligand CLA 21 301



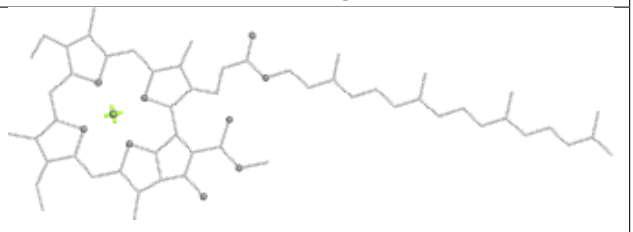
Bond lengths



Bond angles

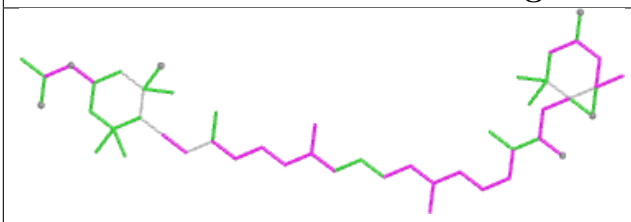


Torsions

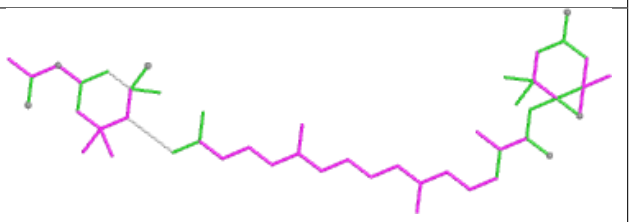


Rings

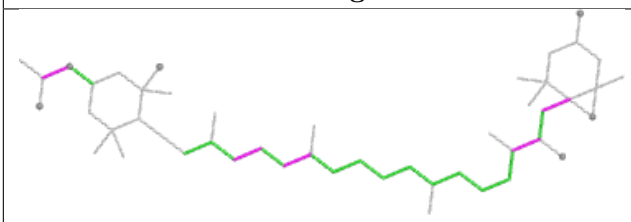
Ligand A86 17 314



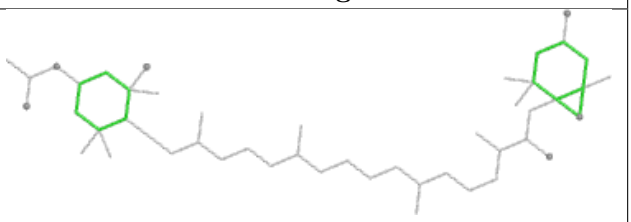
Bond lengths



Bond angles

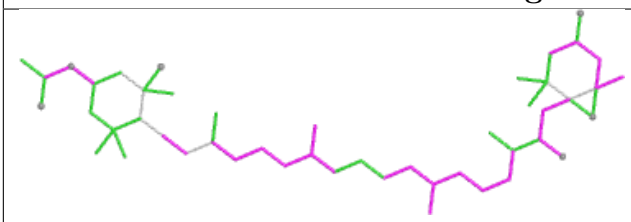


Torsions

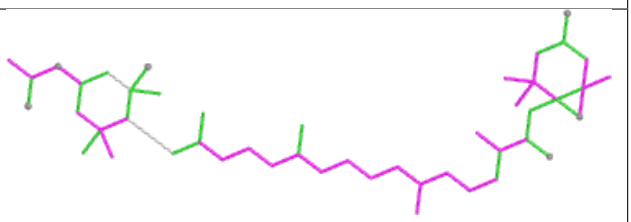


Rings

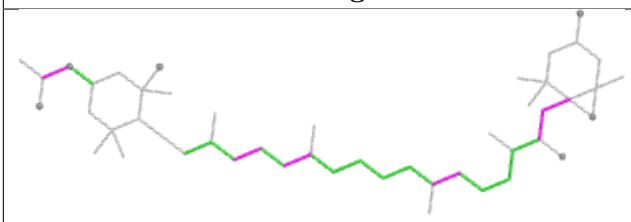
Ligand A86 18 313



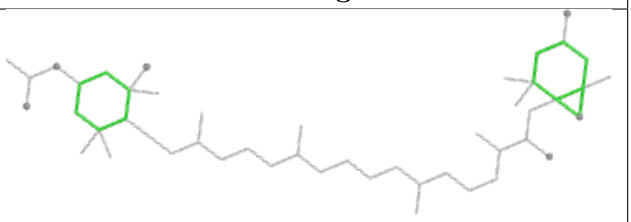
Bond lengths



Bond angles

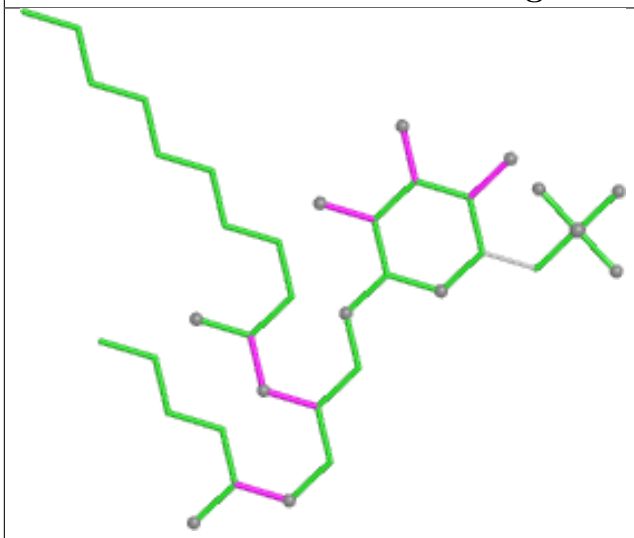


Torsions

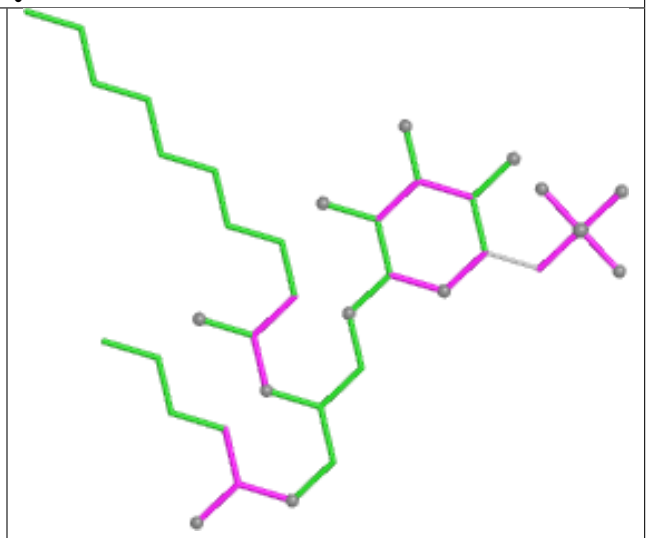


Rings

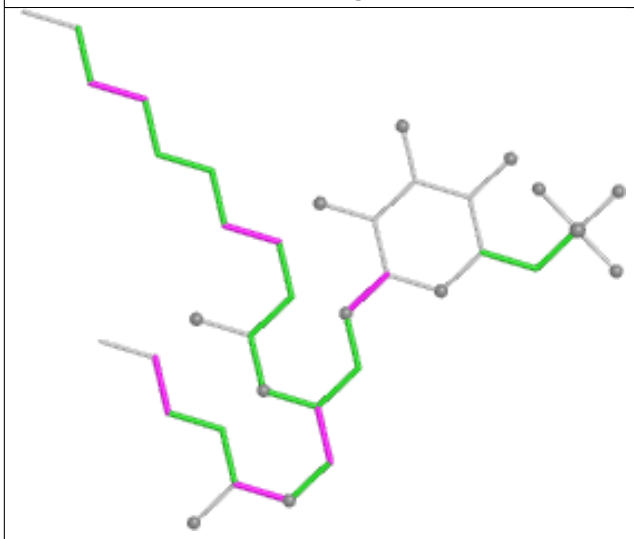
Ligand SQD B 621



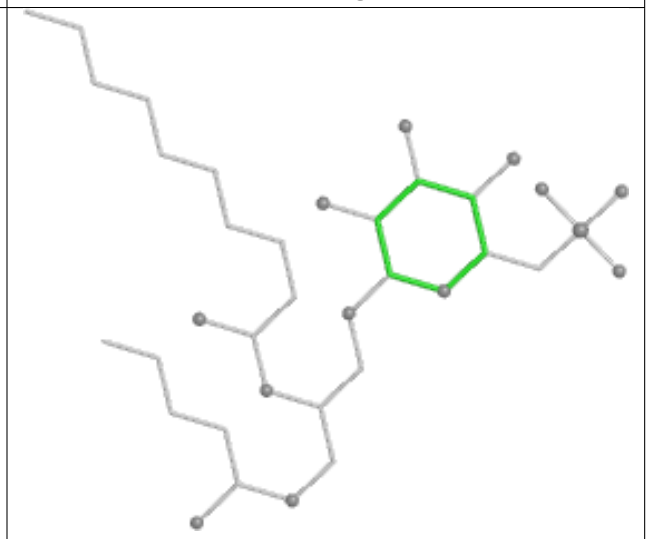
Bond lengths



Bond angles

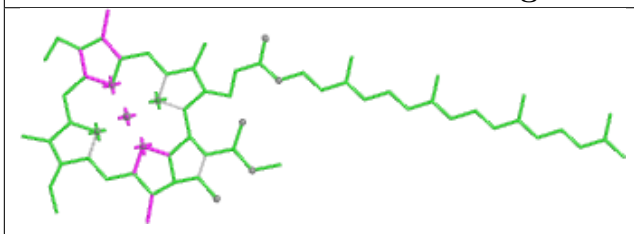


Torsions

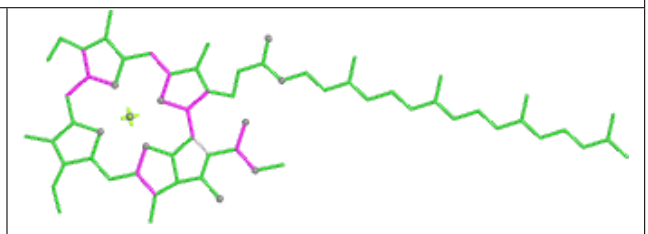


Rings

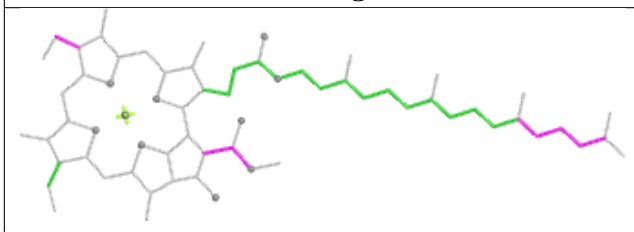
Ligand CLA 18 310



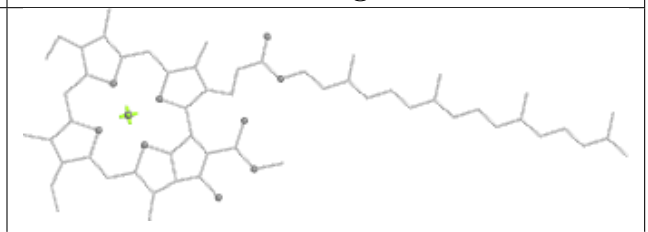
Bond lengths



Bond angles

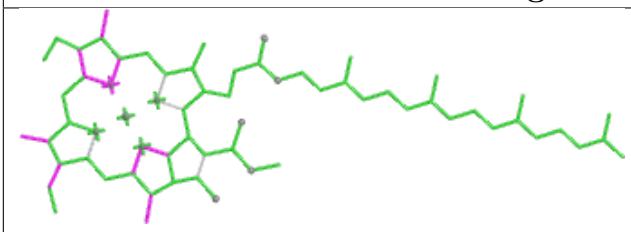


Torsions

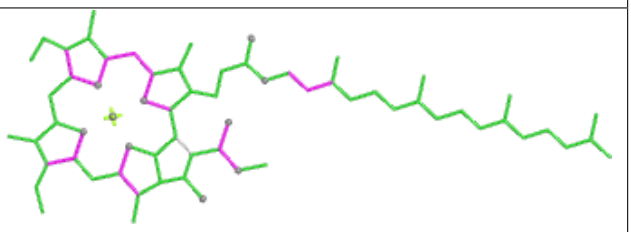


Rings

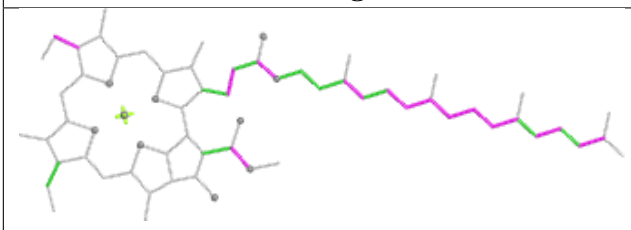
Ligand CLA b 605



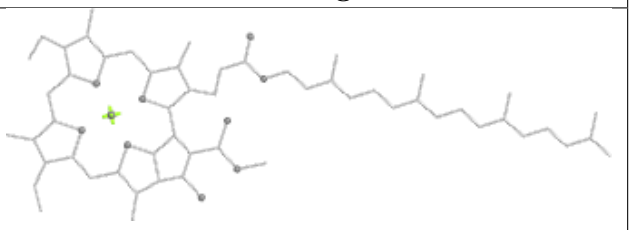
Bond lengths



Bond angles

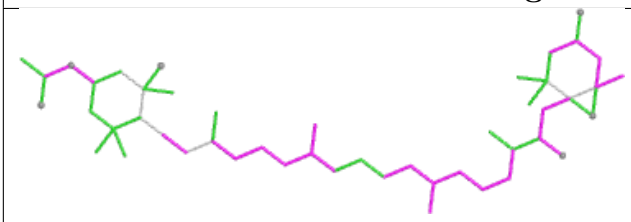


Torsions

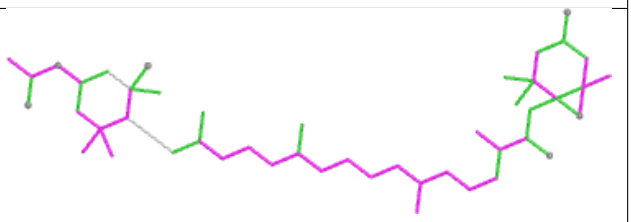


Rings

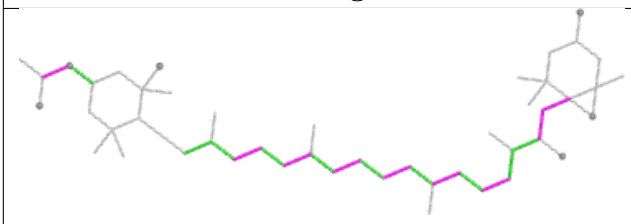
Ligand A86 21 314



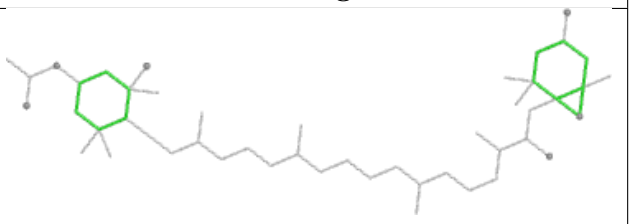
Bond lengths



Bond angles

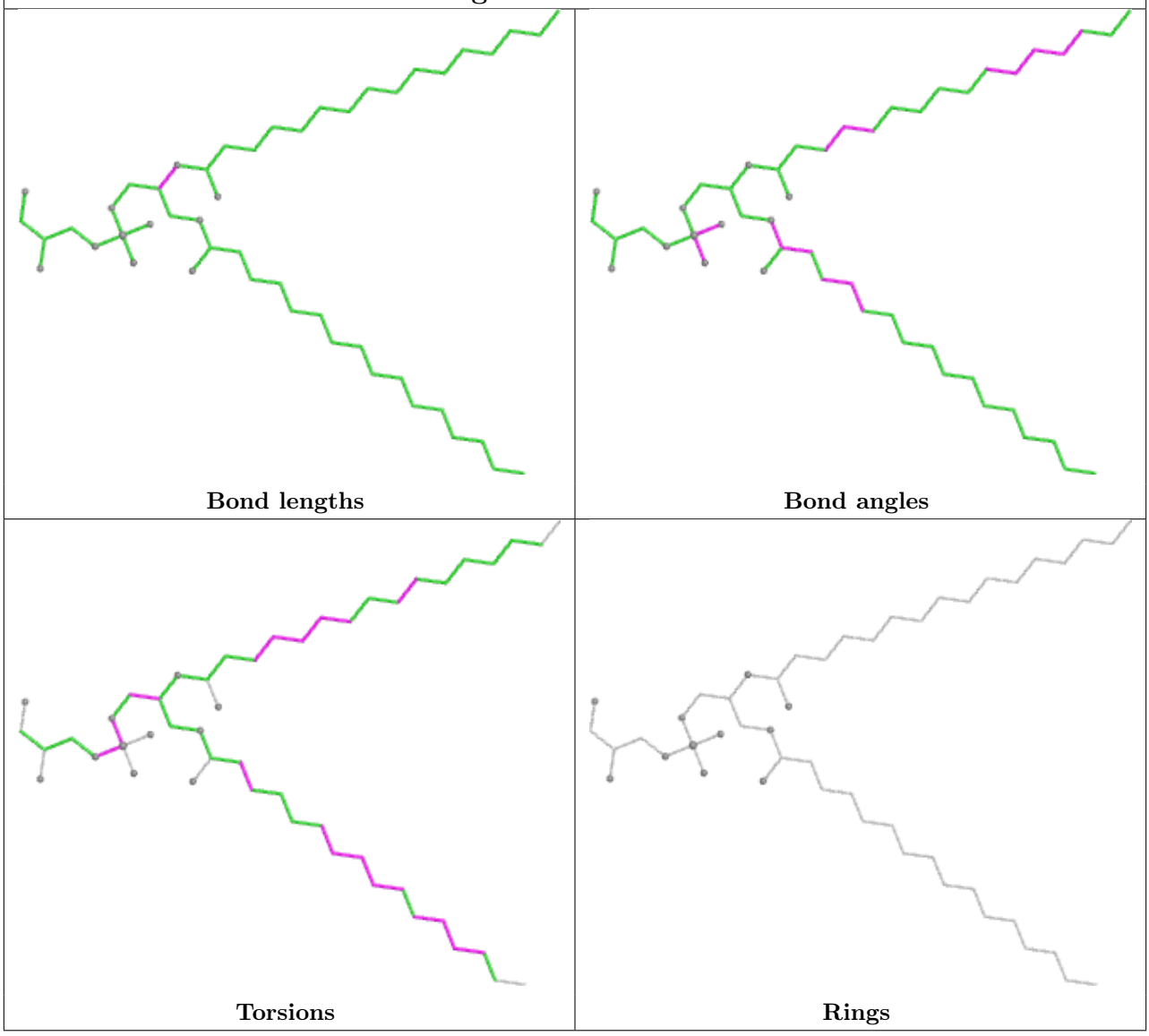


Torsions

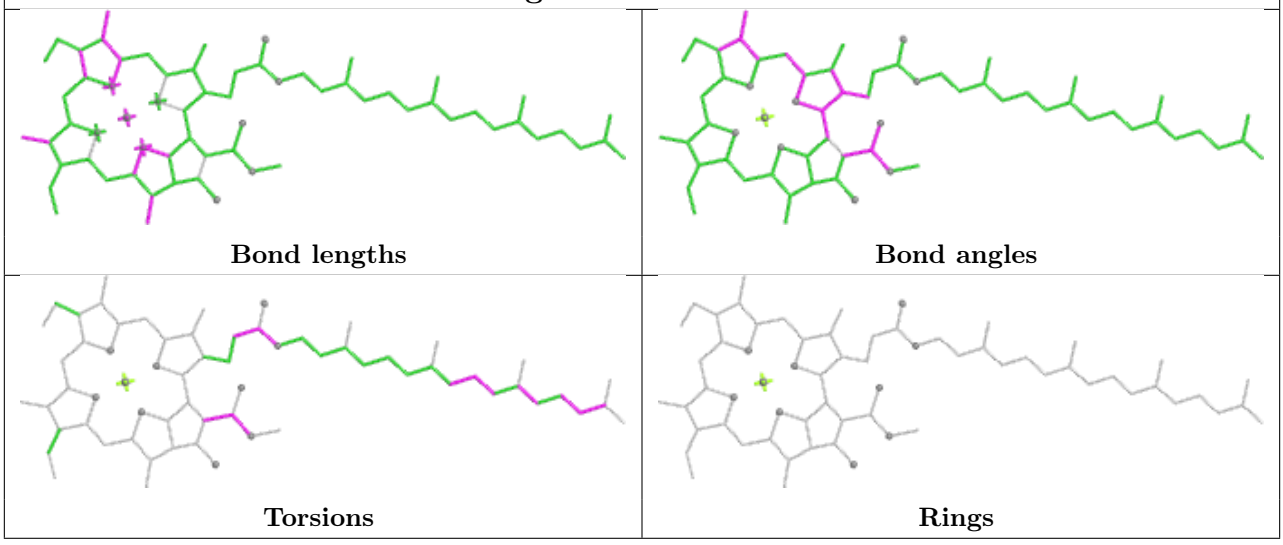


Rings

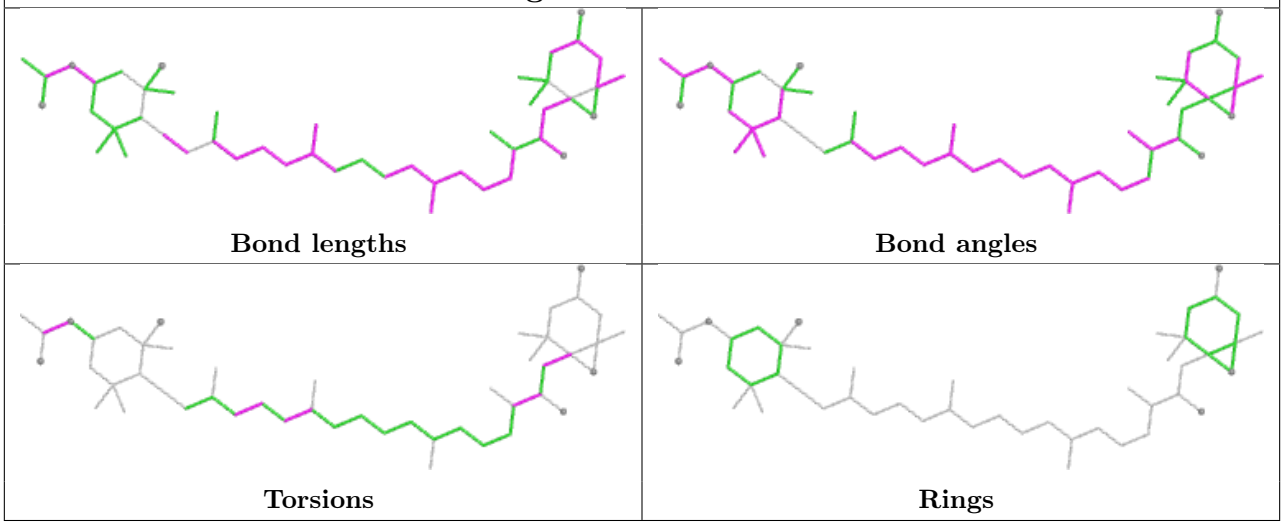
Ligand LHG b 621



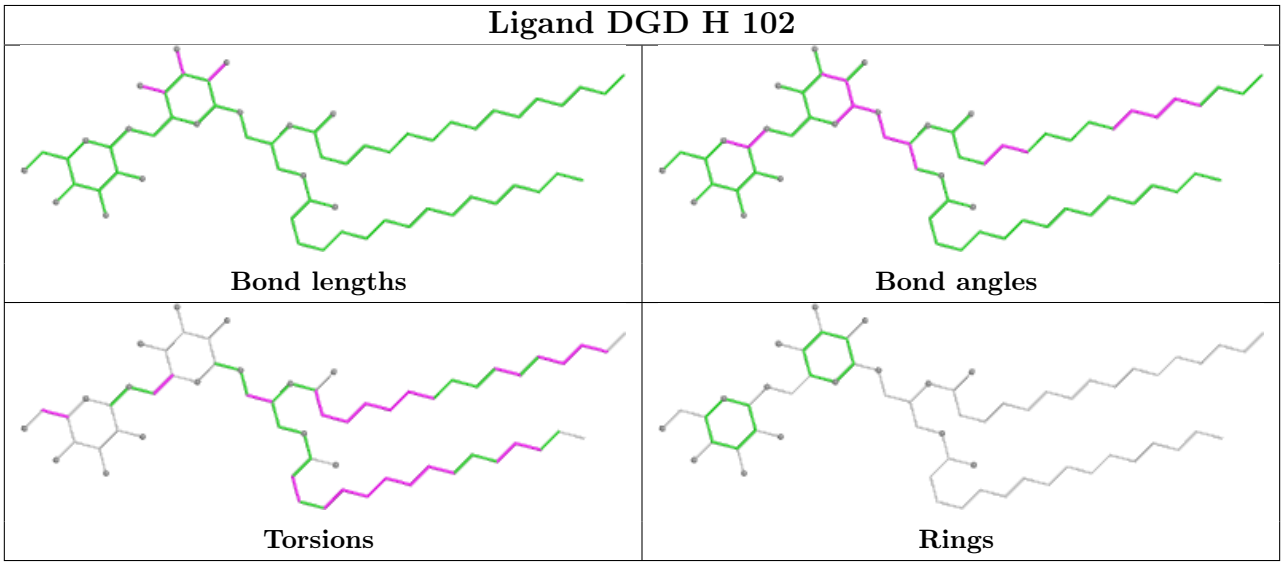
Ligand CLA C 514



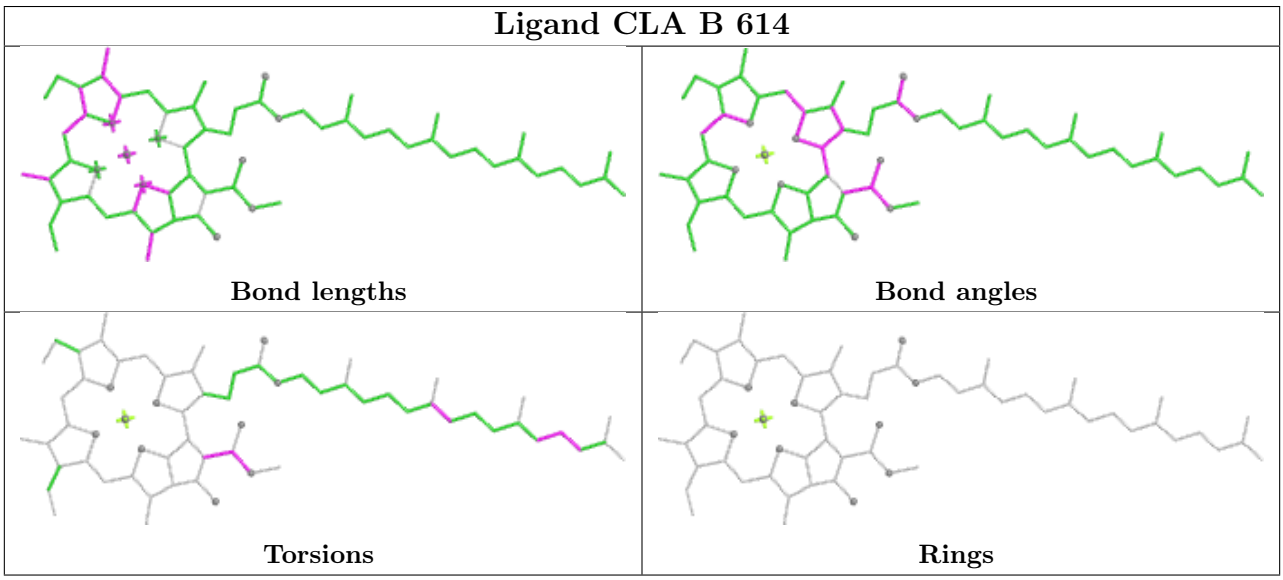
Ligand A86 18 315



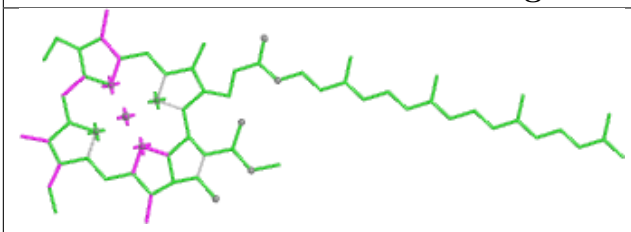
Ligand DGD H 102



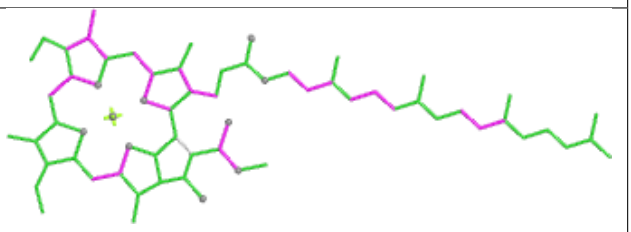
Ligand CLA B 614



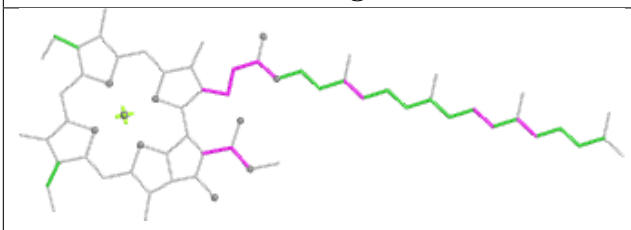
Ligand CLA C 502



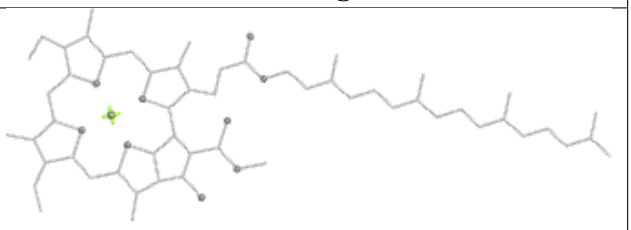
Bond lengths



Bond angles

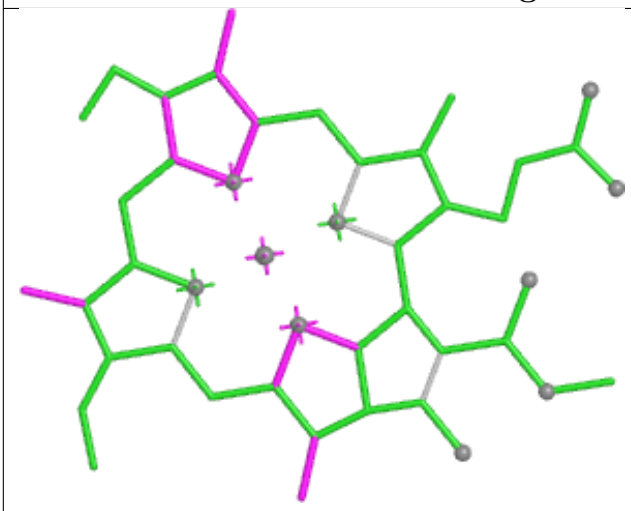


Torsions

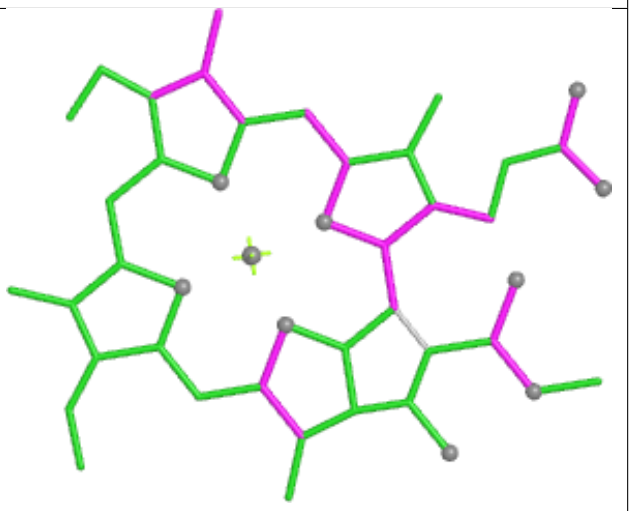


Rings

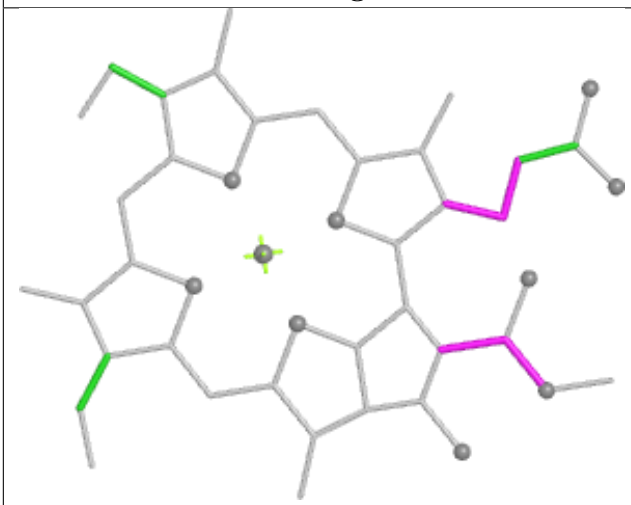
Ligand CLA 16 303



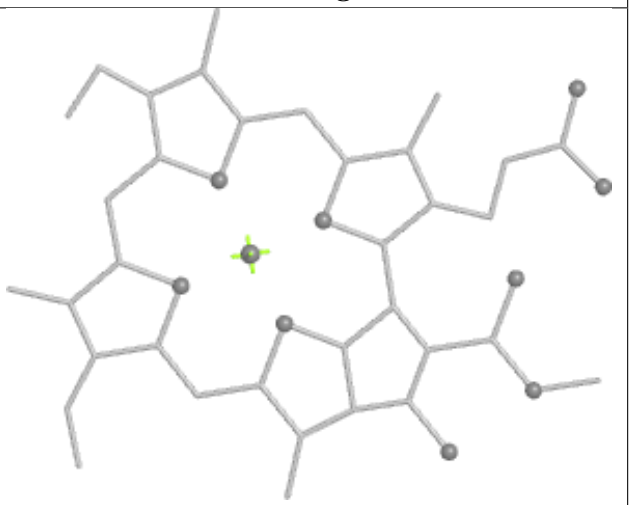
Bond lengths



Bond angles

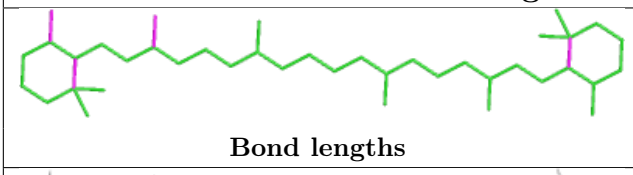


Torsions

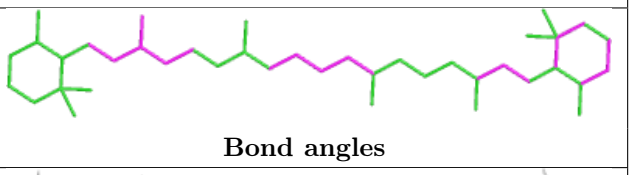


Rings

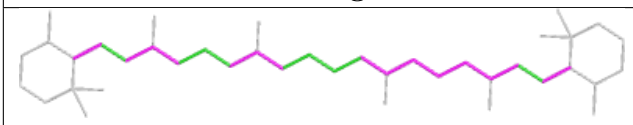
Ligand BCR Y 101



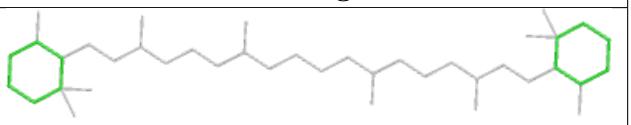
Bond lengths



Bond angles

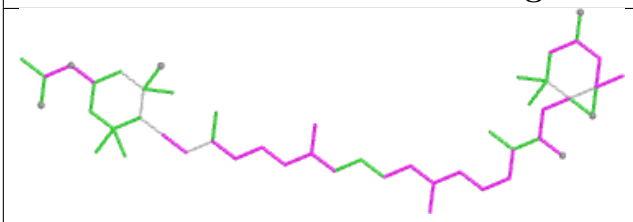


Torsions

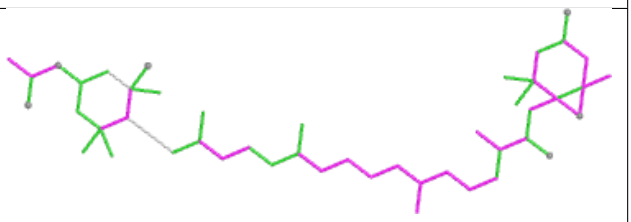


Rings

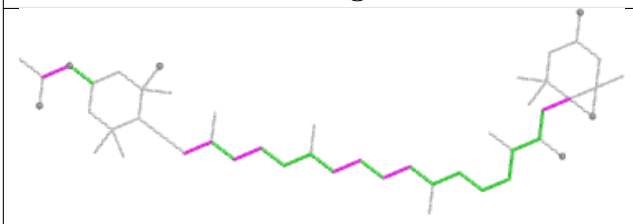
Ligand A86 20 211



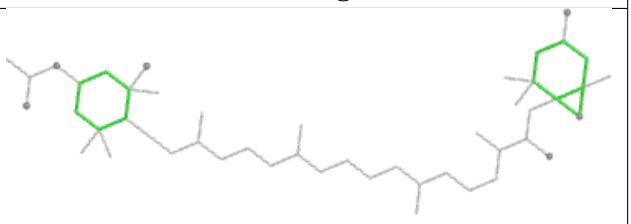
Bond lengths



Bond angles

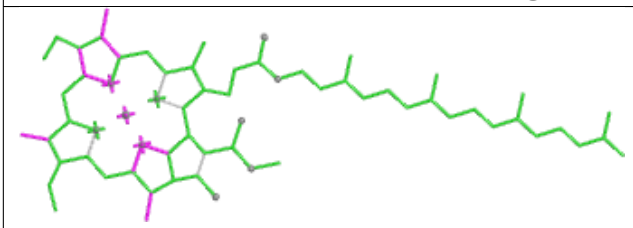


Torsions

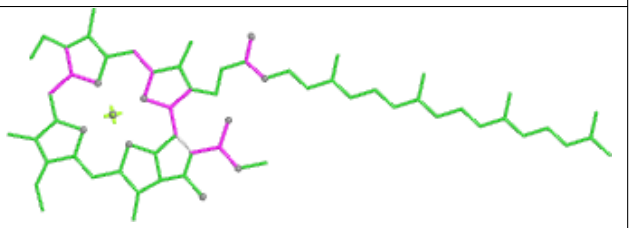


Rings

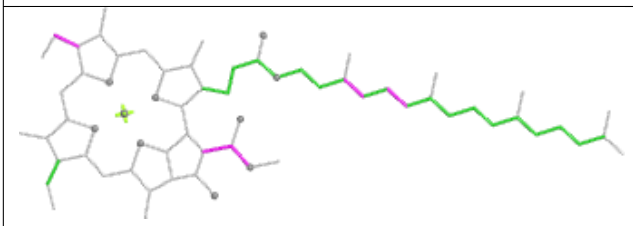
Ligand CLA B 609



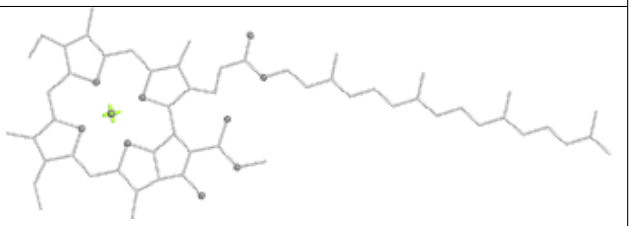
Bond lengths



Bond angles

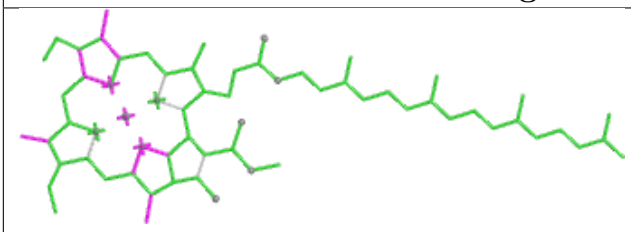


Torsions

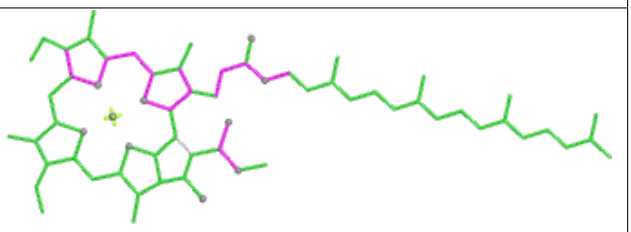


Rings

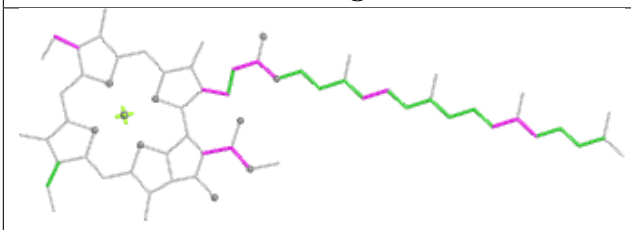
Ligand CLA 19 303



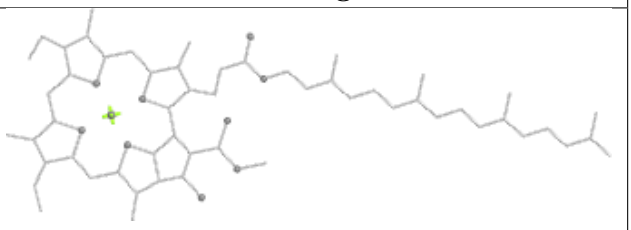
Bond lengths



Bond angles

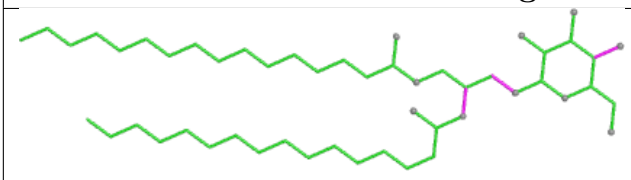


Torsions

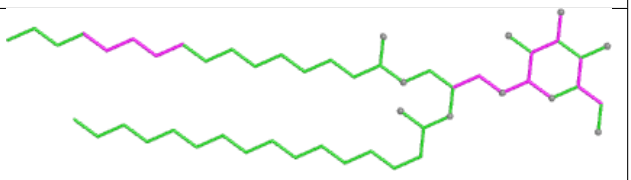


Rings

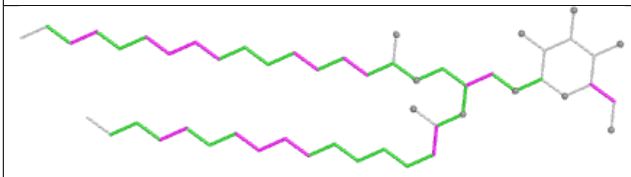
Ligand LMG D 408



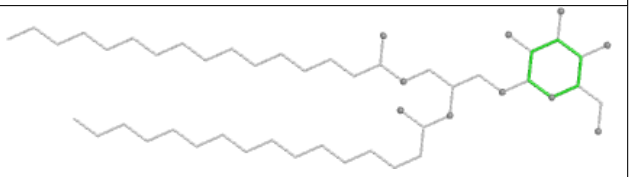
Bond lengths



Bond angles

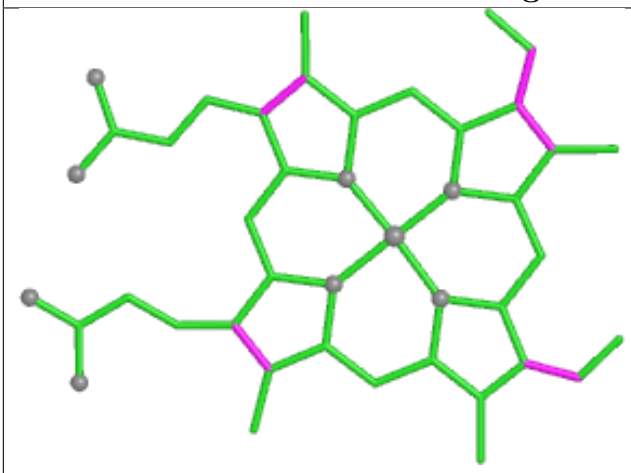


Torsions

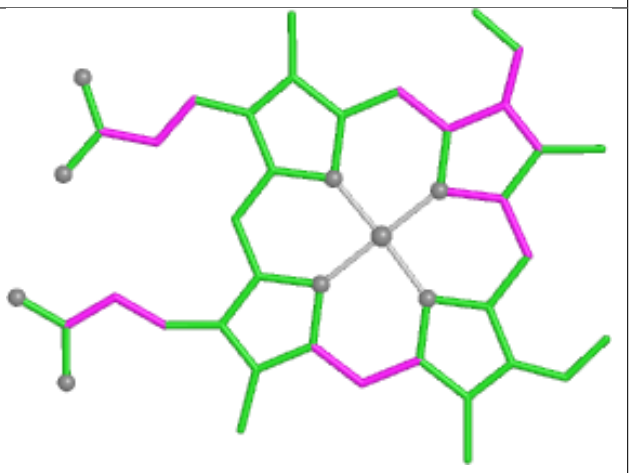


Rings

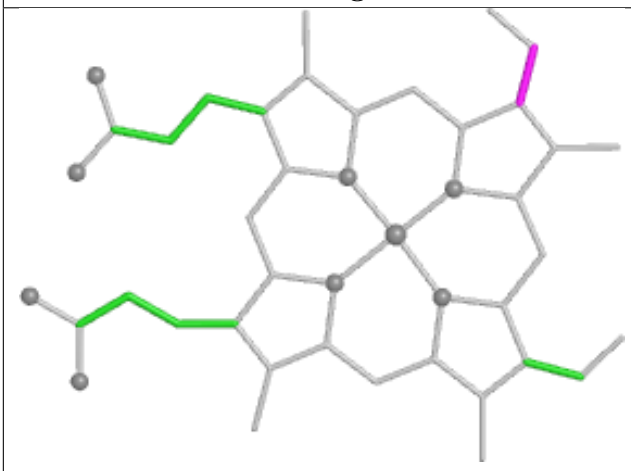
Ligand HEM v 201



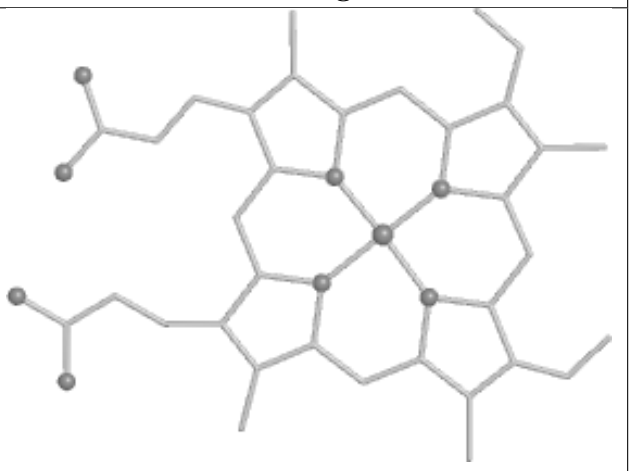
Bond lengths



Bond angles

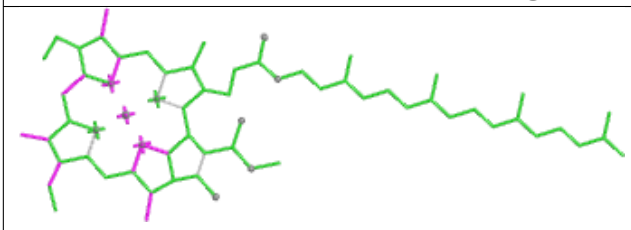


Torsions

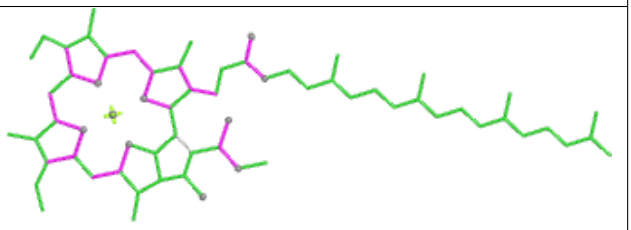


Rings

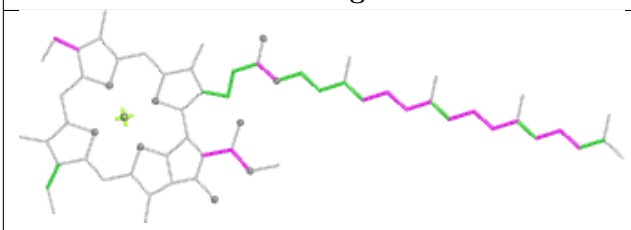
Ligand CLA C 505



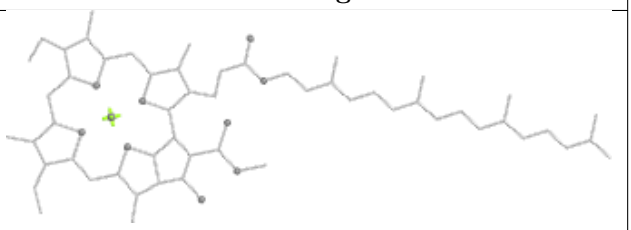
Bond lengths



Bond angles

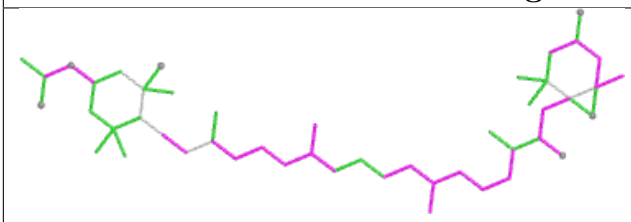


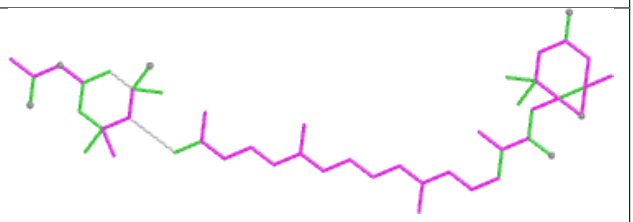
Torsions

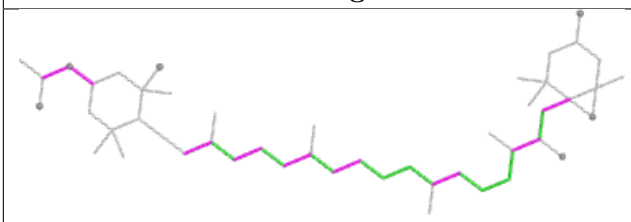


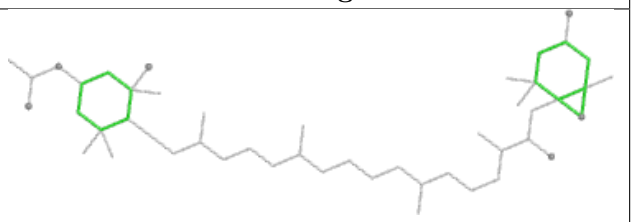
Rings

Ligand A86 21 313


Bond lengths

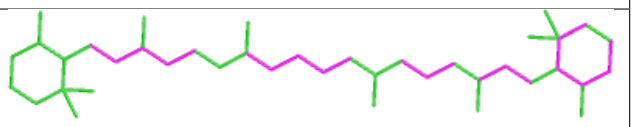

Bond angles

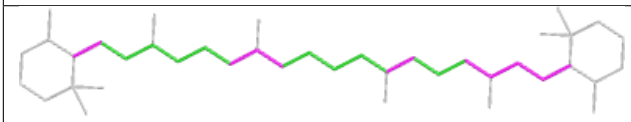

Torsions

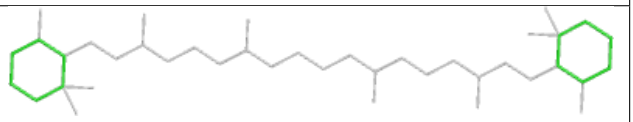

Rings

Ligand BCR C 515

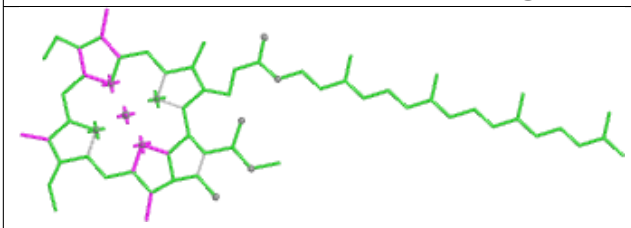

Bond lengths

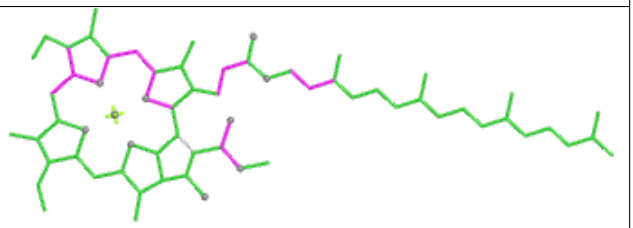

Bond angles

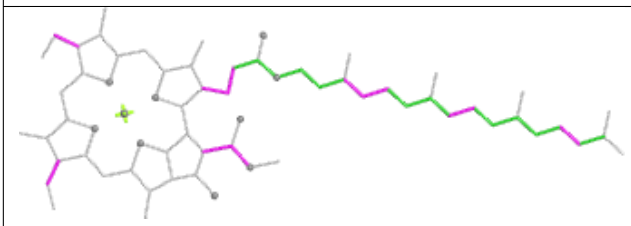

Torsions

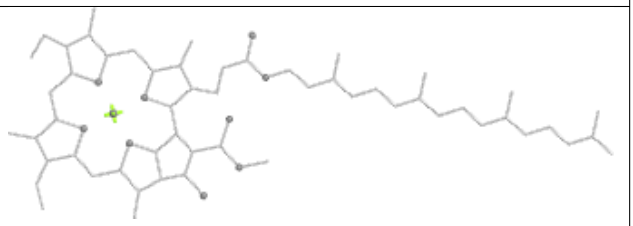

Rings

Ligand CLA 17 303

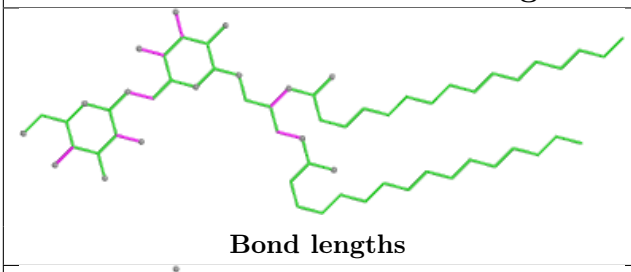

Bond lengths


Bond angles

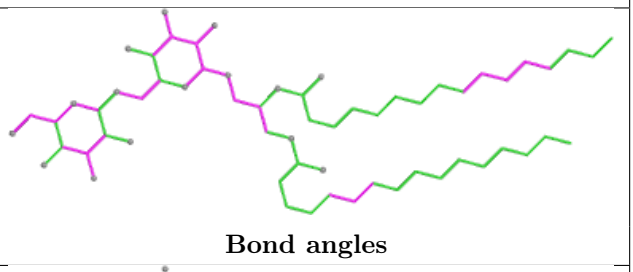

Torsions


Rings

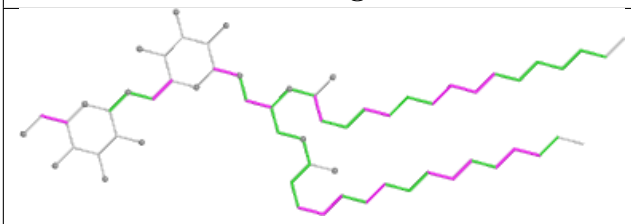
Ligand DGD C 516



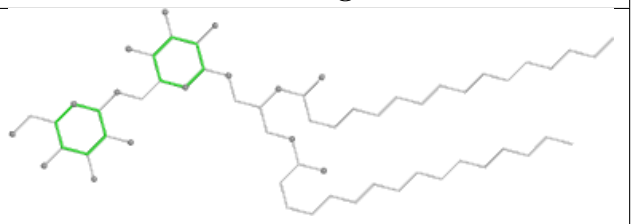
Bond lengths



Bond angles

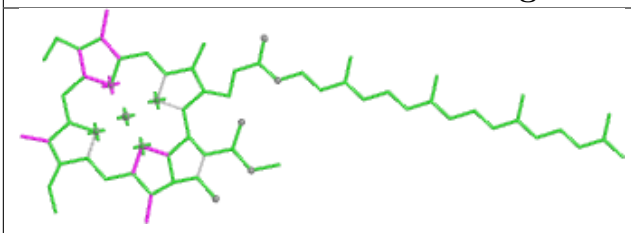


Torsions

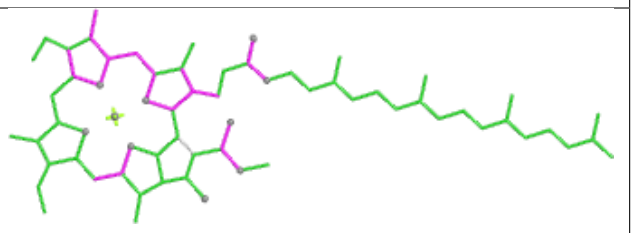


Rings

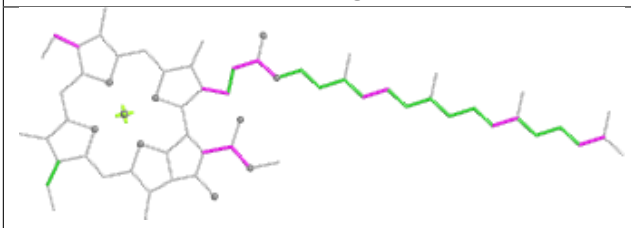
Ligand CLA 15 303



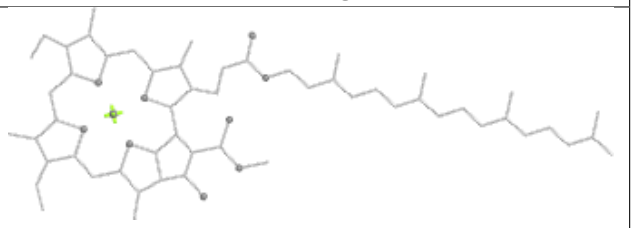
Bond lengths



Bond angles

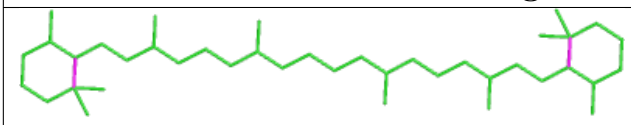


Torsions

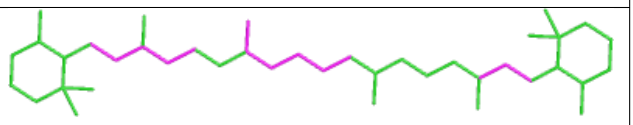


Rings

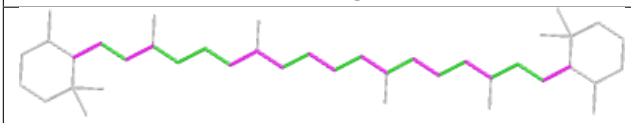
Ligand BCR A 405



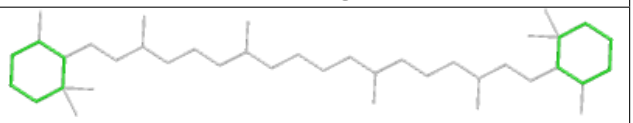
Bond lengths



Bond angles

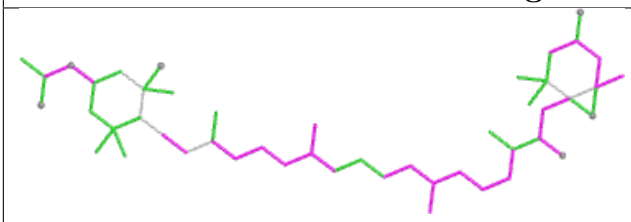


Torsions

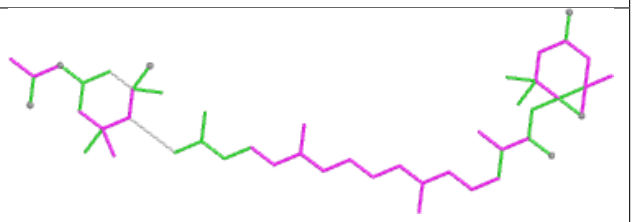


Rings

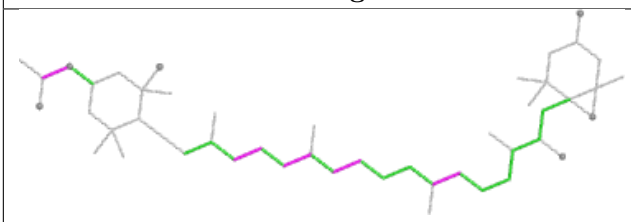
Ligand A86 12 319



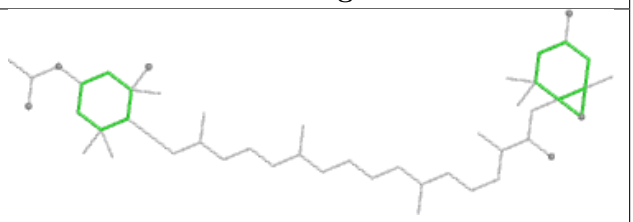
Bond lengths



Bond angles

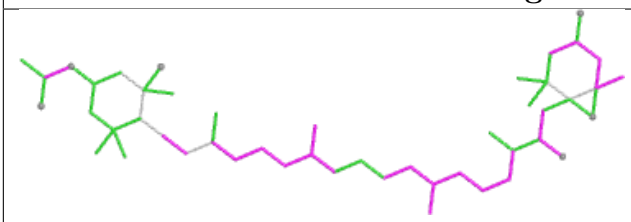


Torsions

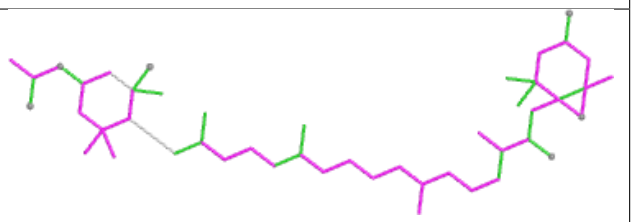


Rings

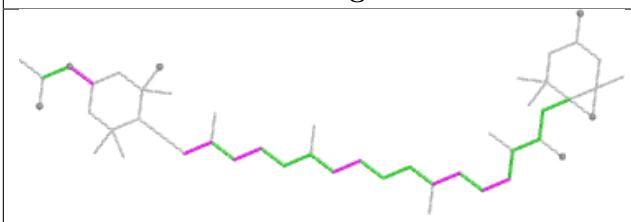
Ligand A86 21 312



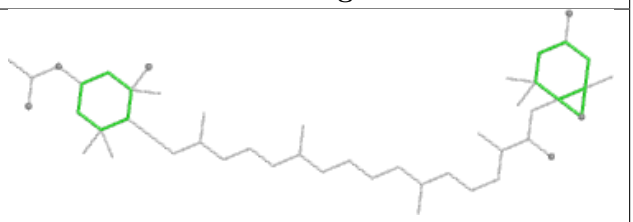
Bond lengths



Bond angles

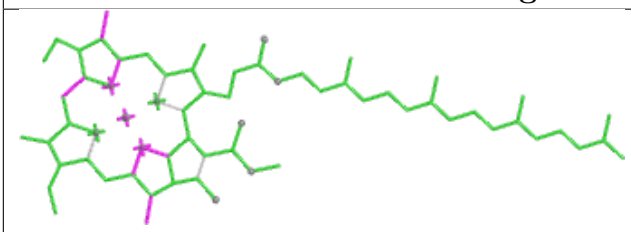


Torsions

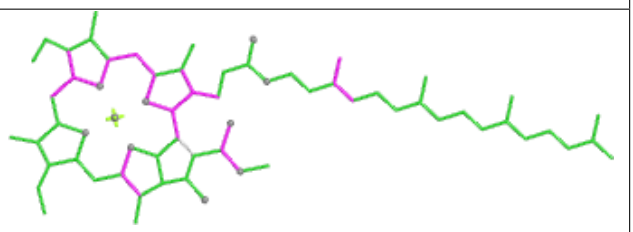


Rings

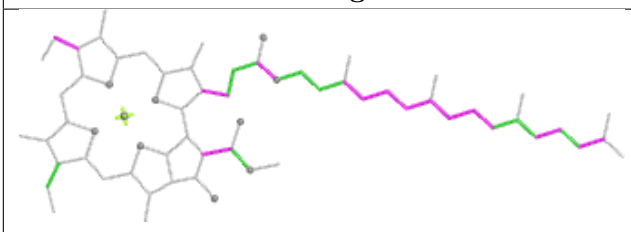
Ligand CLA 17 308



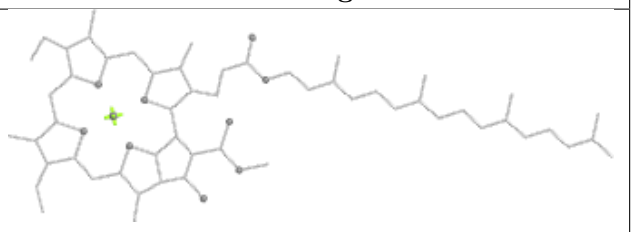
Bond lengths



Bond angles

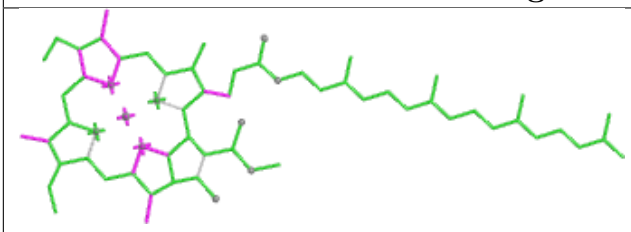


Torsions

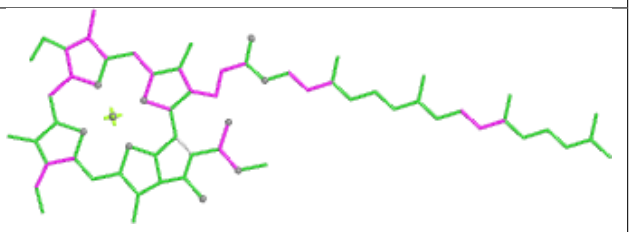


Rings

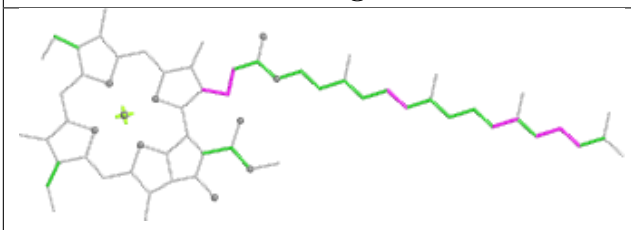
Ligand CLA d 406



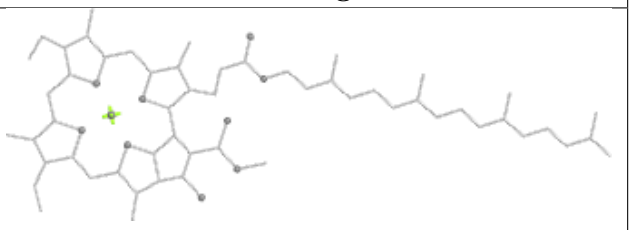
Bond lengths



Bond angles

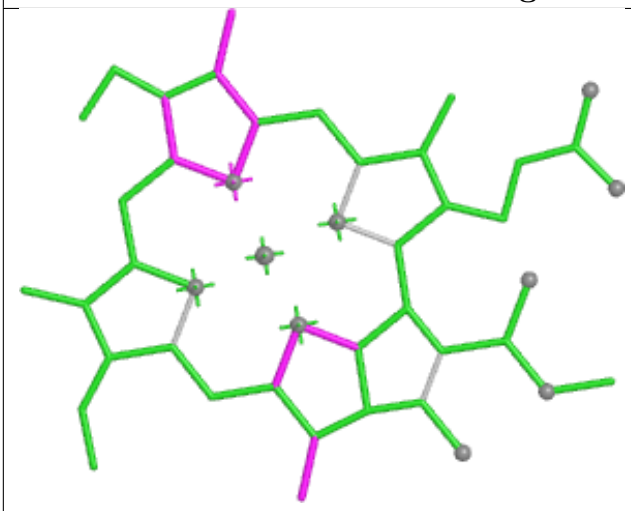


Torsions

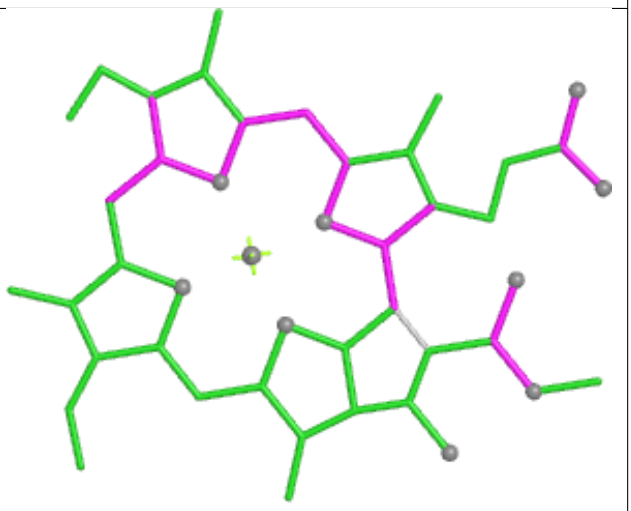


Rings

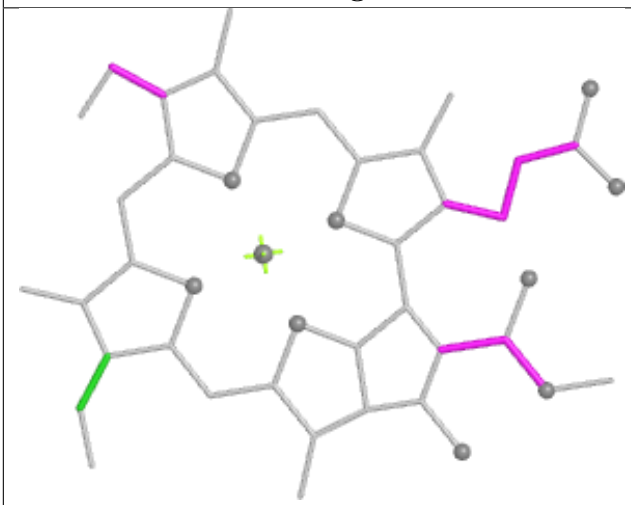
Ligand CLA 12 310



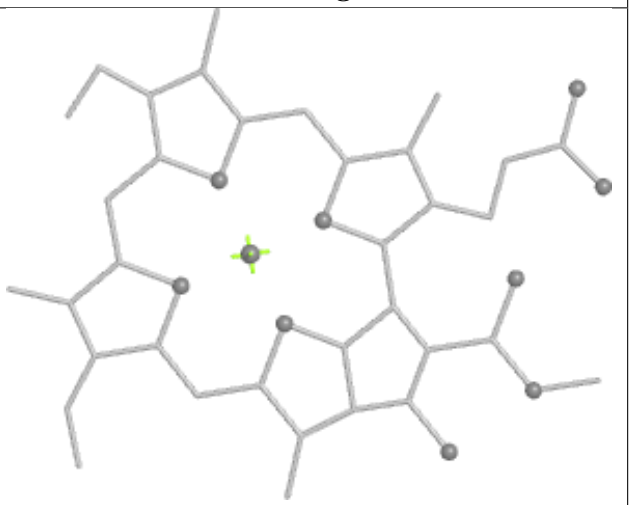
Bond lengths



Bond angles

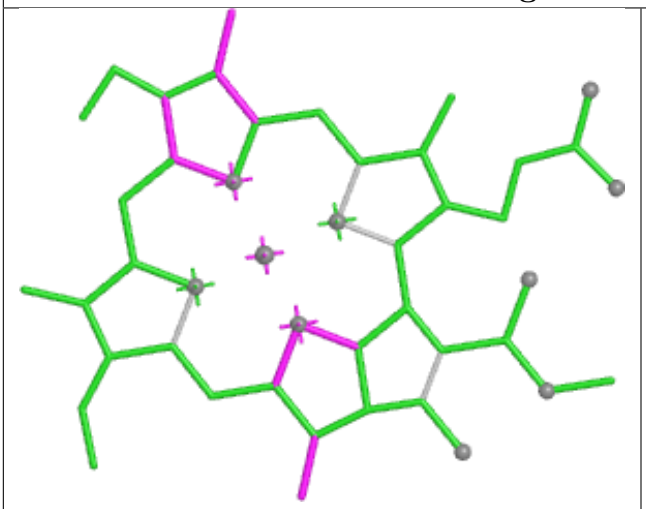


Torsions

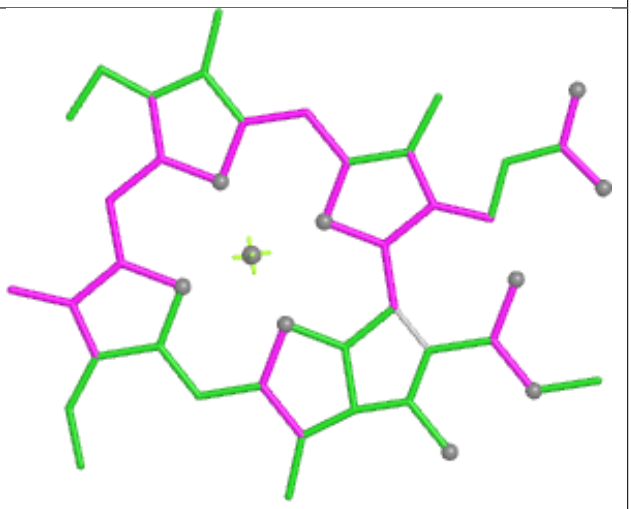


Rings

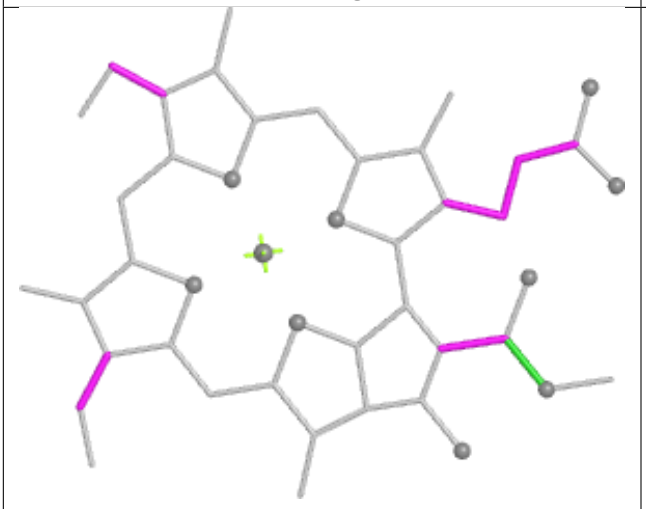
Ligand CLA 17 307



Bond lengths



Bond angles

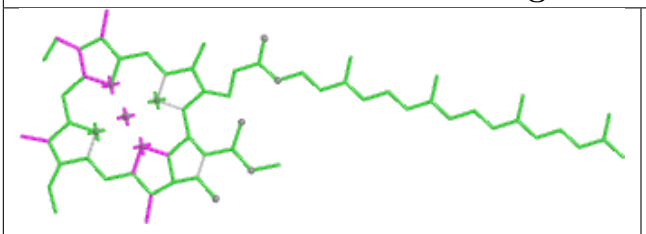


Torsions

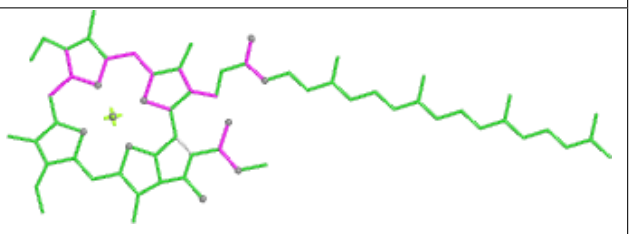


Rings

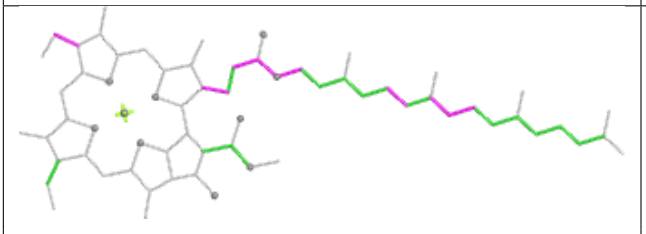
Ligand CLA a 403



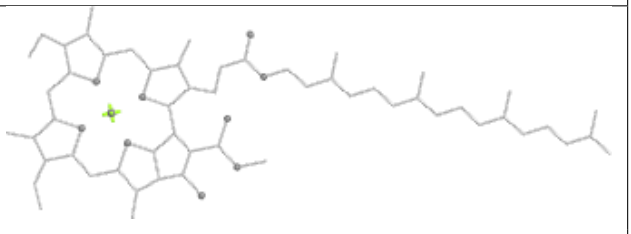
Bond lengths



Bond angles

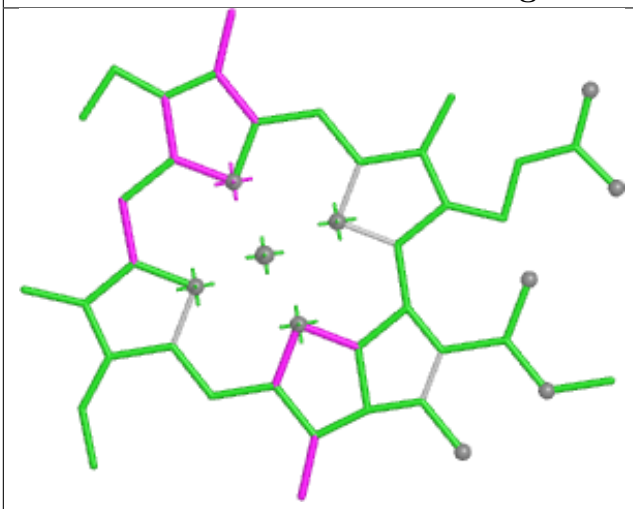


Torsions

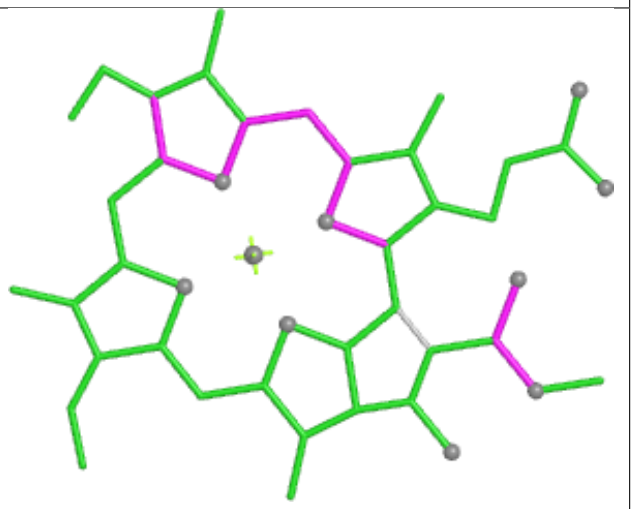


Rings

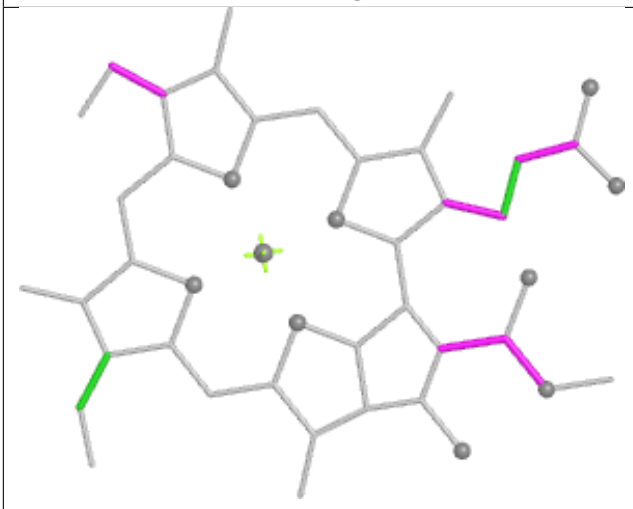
Ligand CLA 15 305



Bond lengths



Bond angles

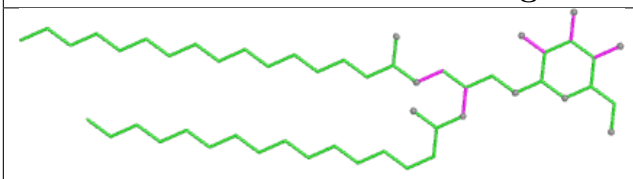


Torsions

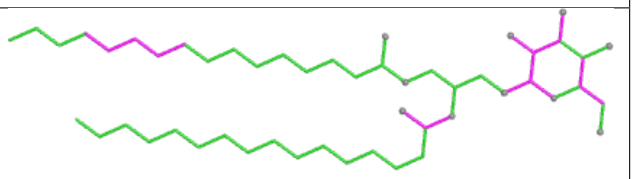


Rings

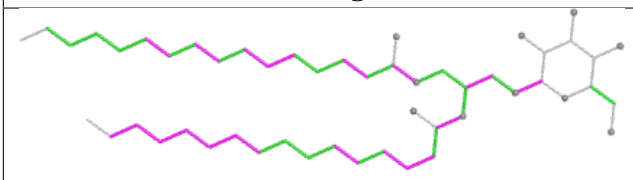
Ligand LMG B 620



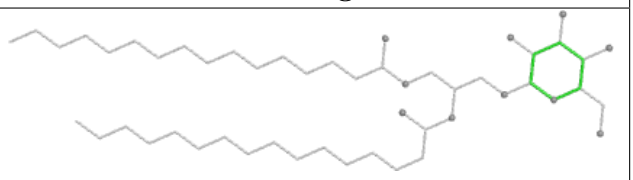
Bond lengths



Bond angles

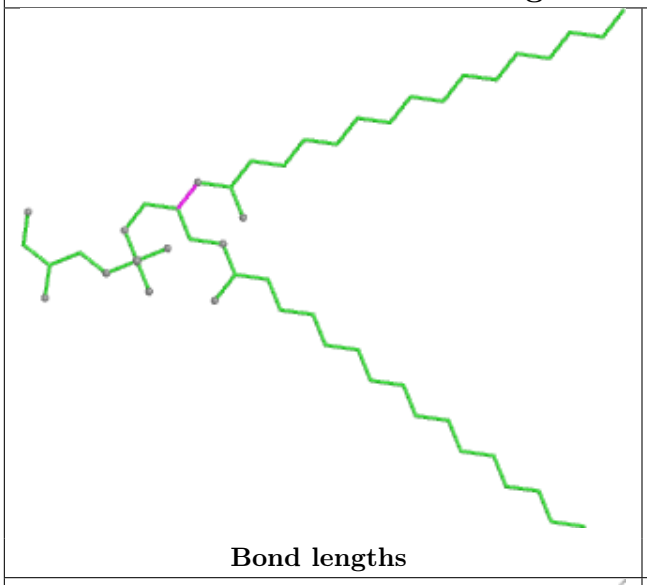


Torsions

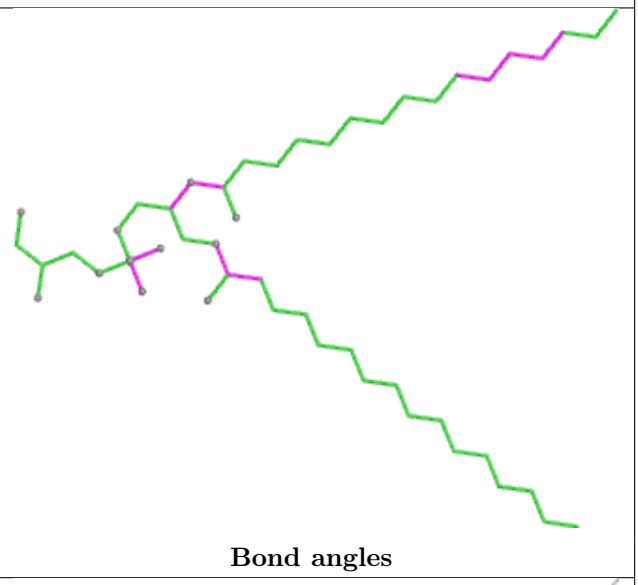


Rings

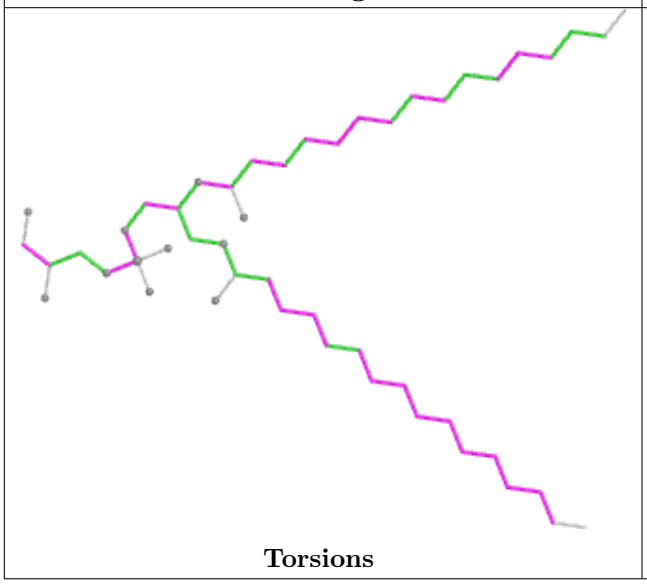
Ligand LHG L 101



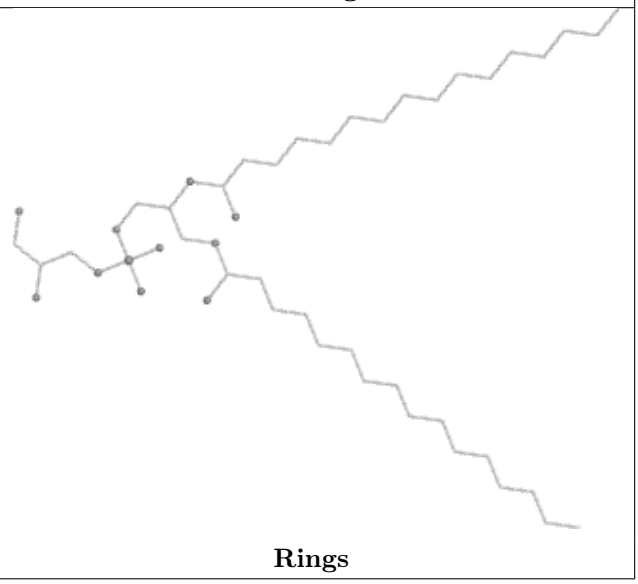
Bond lengths



Bond angles

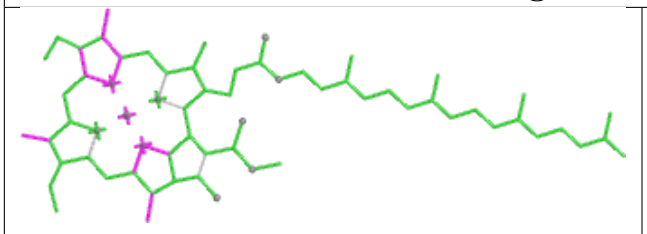


Torsions

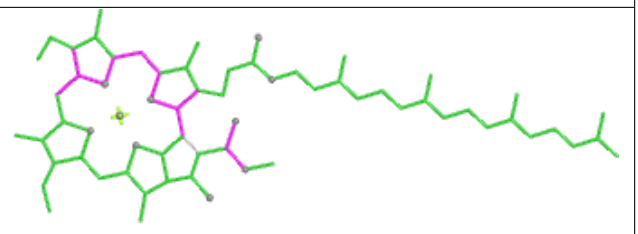


Rings

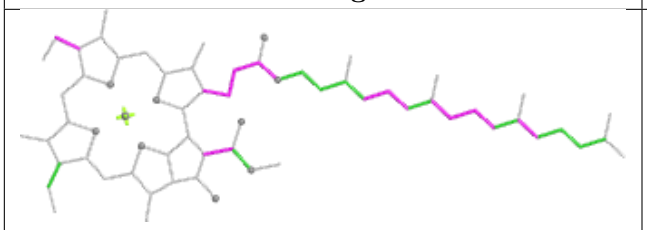
Ligand CLA b 601



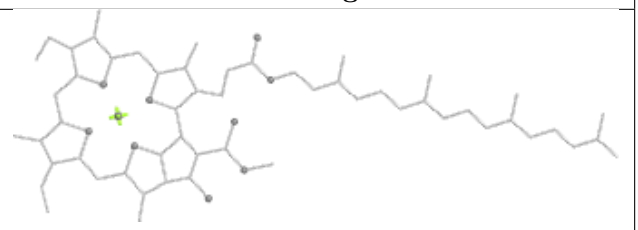
Bond lengths



Bond angles

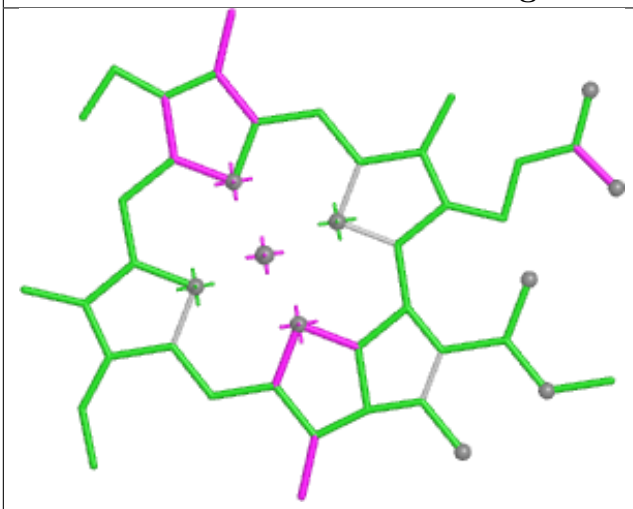


Torsions

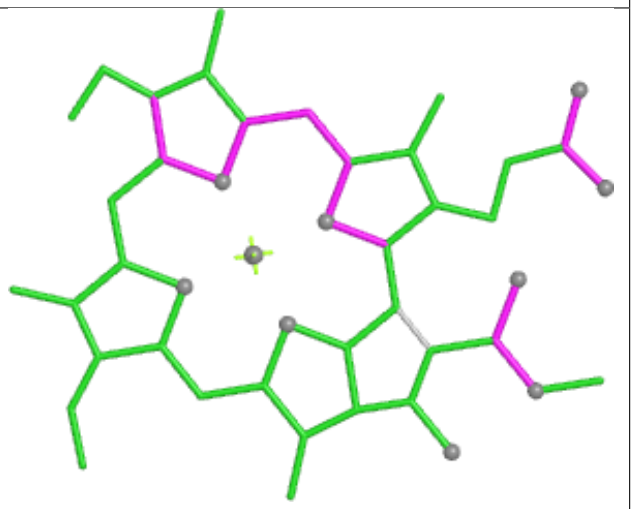


Rings

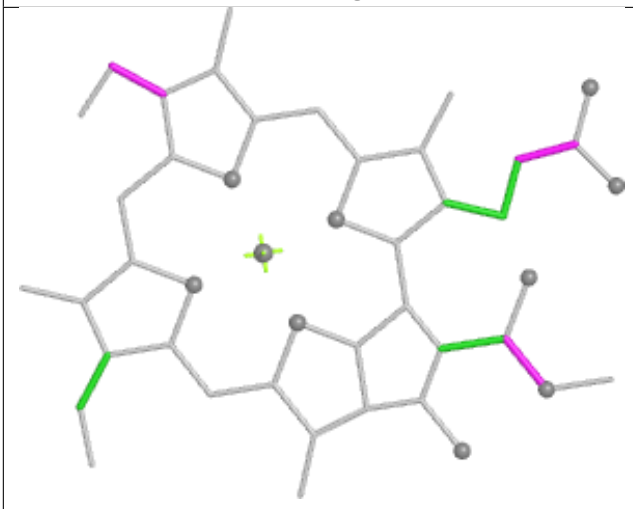
Ligand CLA 18 312



Bond lengths



Bond angles

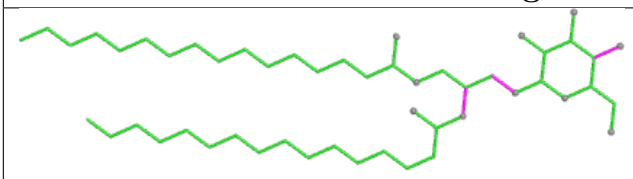


Torsions

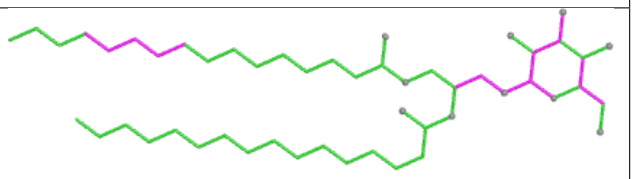


Rings

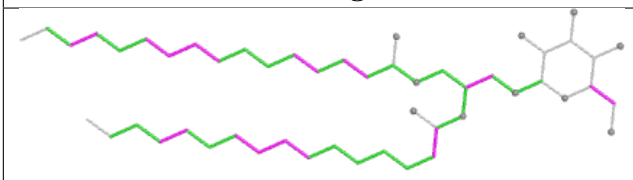
Ligand LMG d 410



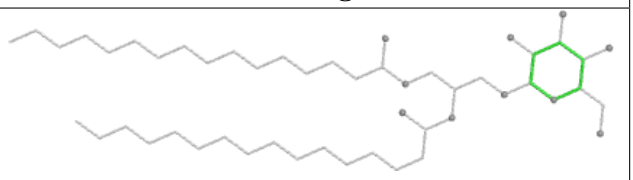
Bond lengths



Bond angles

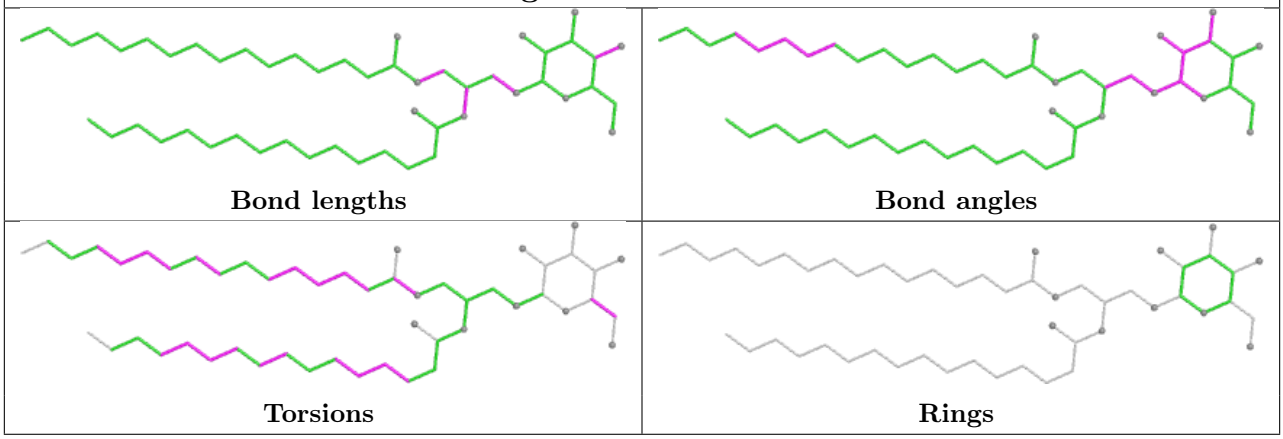


Torsions

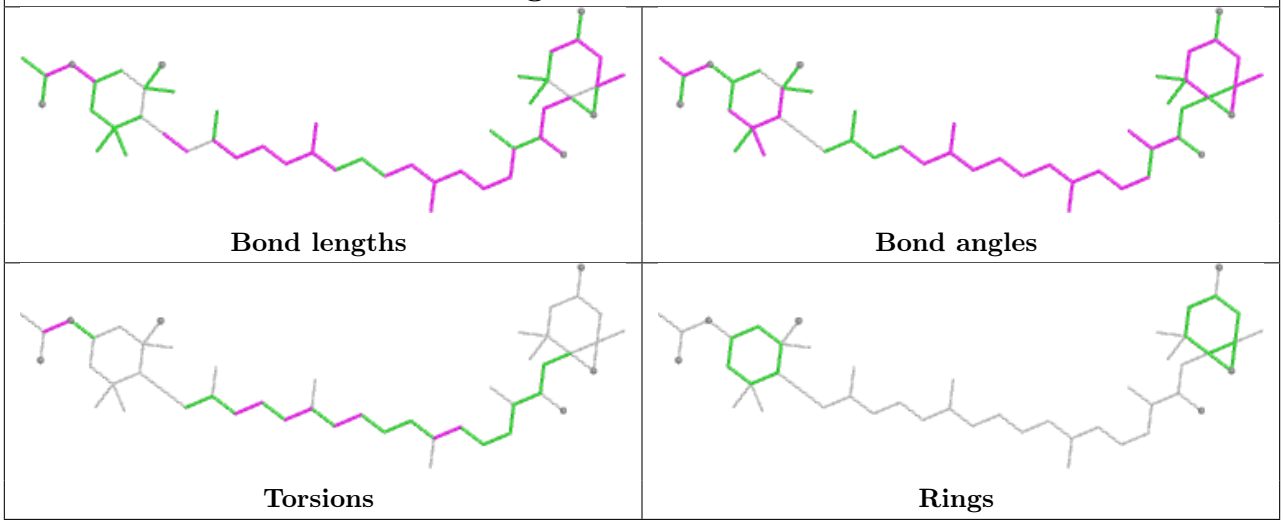


Rings

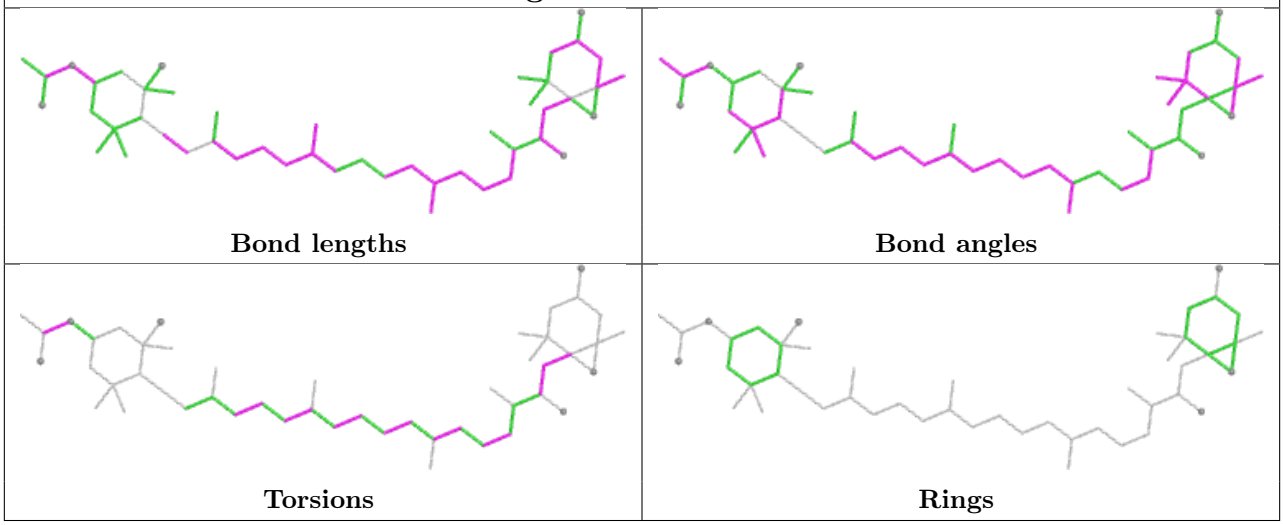
Ligand LMG B 619



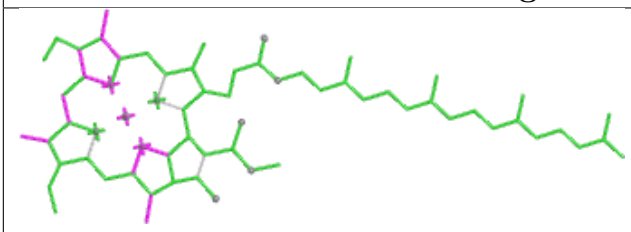
Ligand A86 15 314



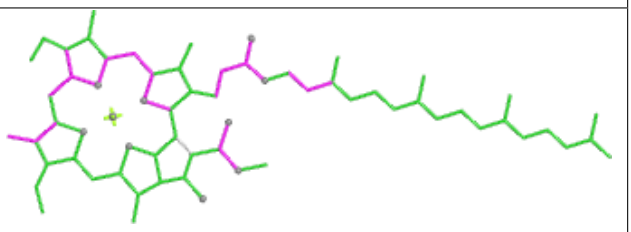
Ligand A86 17 315



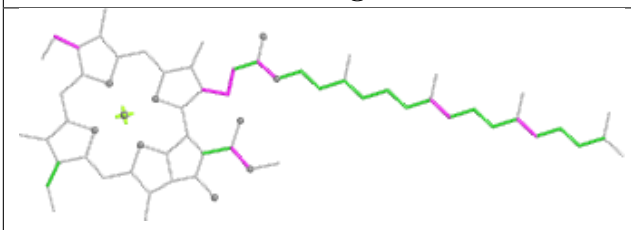
Ligand CLA 15 301



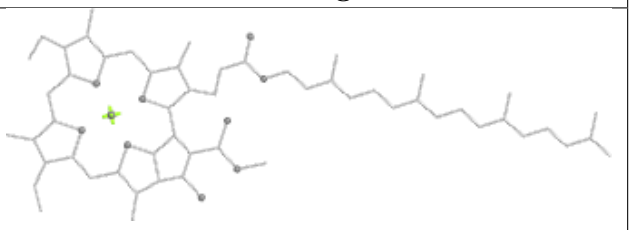
Bond lengths



Bond angles

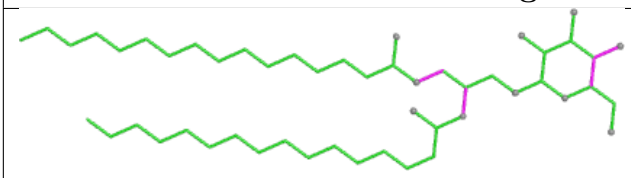


Torsions

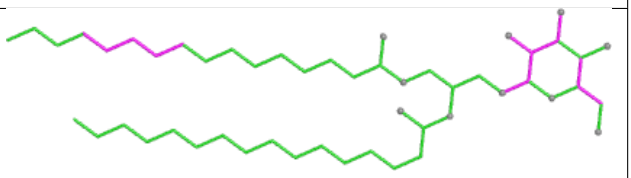


Rings

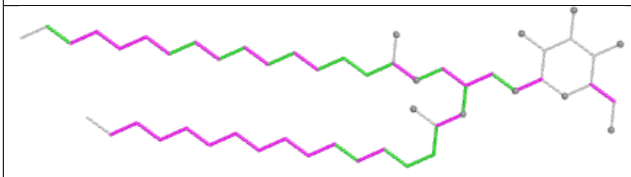
Ligand LMG w 101



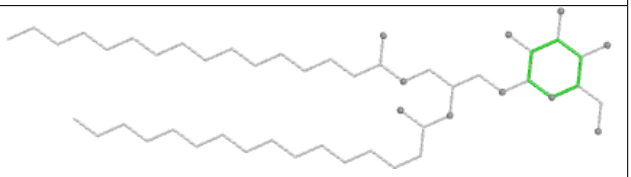
Bond lengths



Bond angles

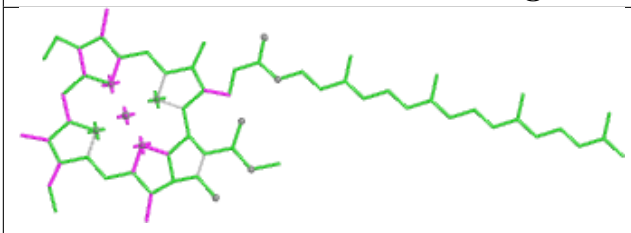


Torsions

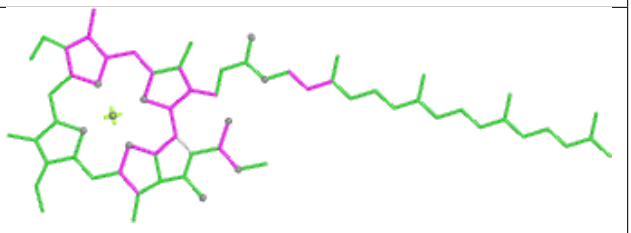


Rings

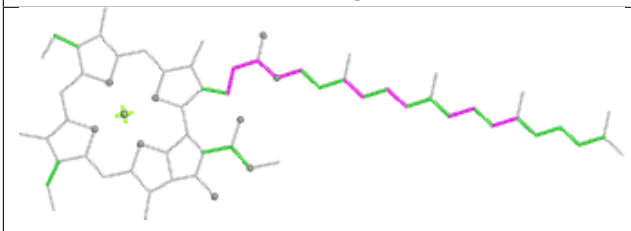
Ligand CLA C 511



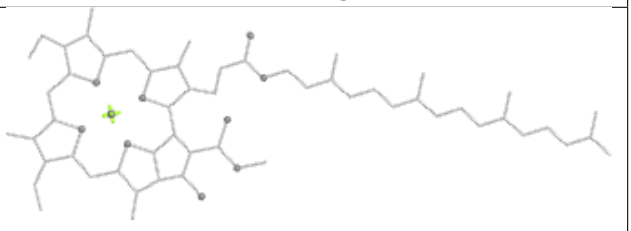
Bond lengths



Bond angles

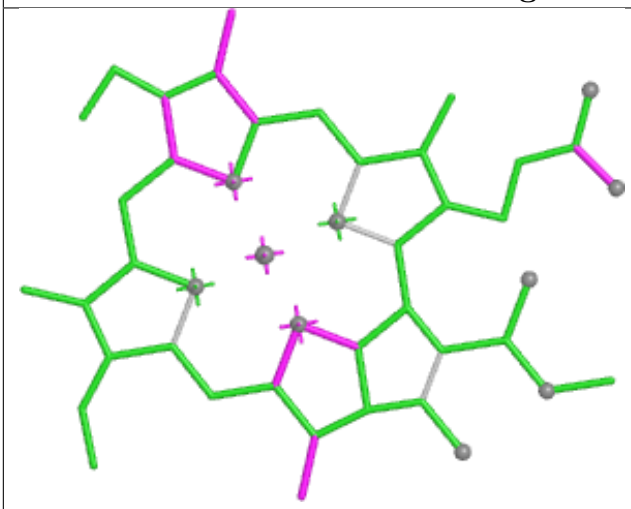


Torsions

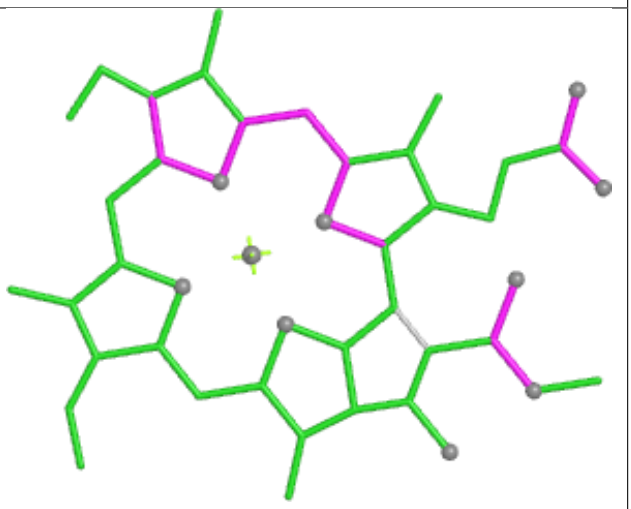


Rings

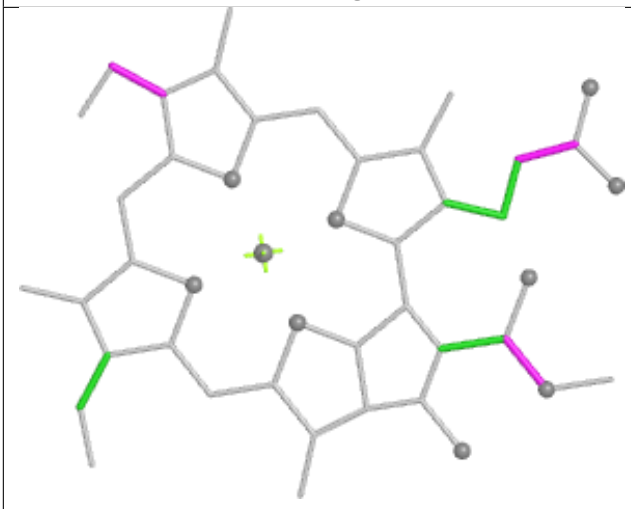
Ligand CLA 15 309



Bond lengths



Bond angles

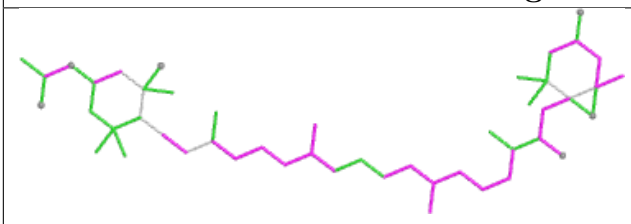


Torsions

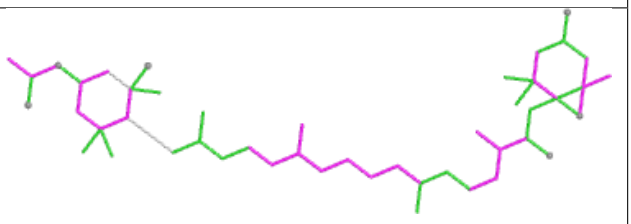


Rings

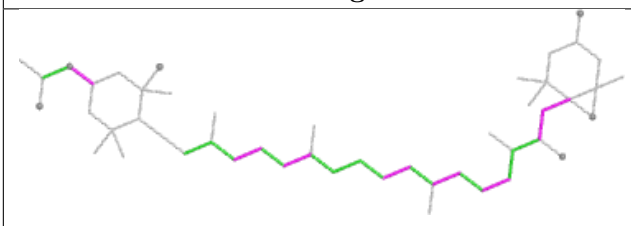
Ligand A86 20 212



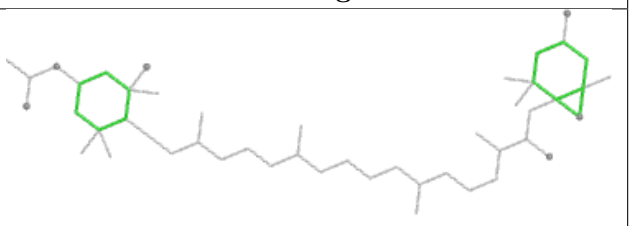
Bond lengths



Bond angles

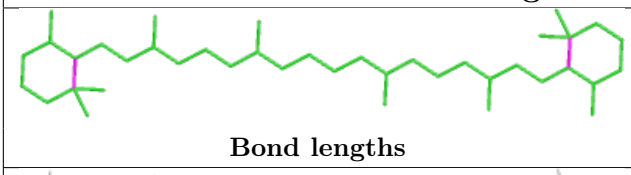


Torsions

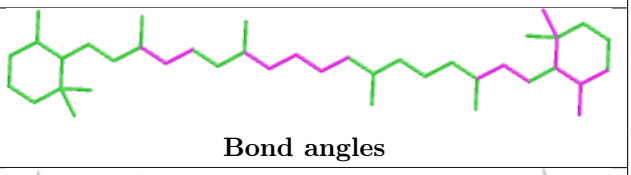


Rings

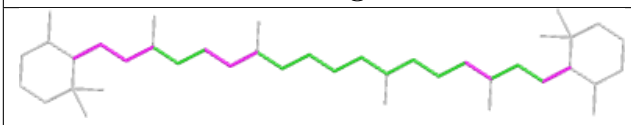
Ligand BCR B 617



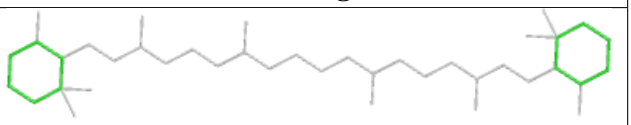
Bond lengths



Bond angles

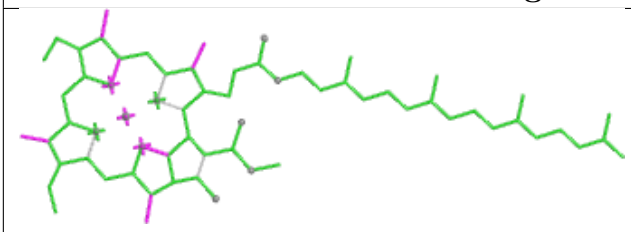


Torsions

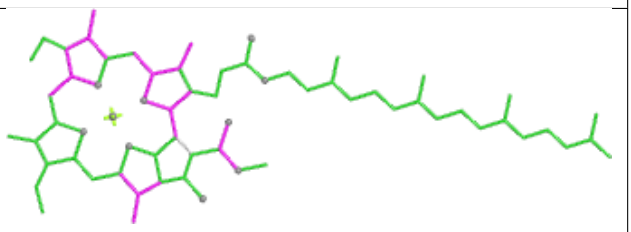


Rings

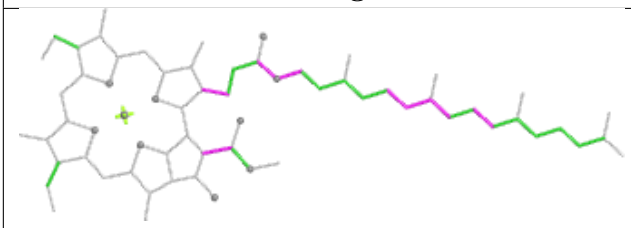
Ligand CLA B 612



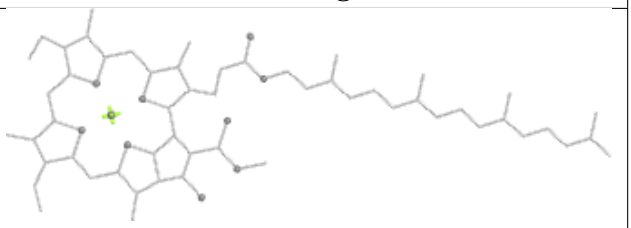
Bond lengths



Bond angles

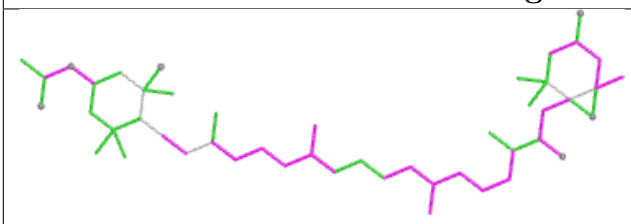


Torsions

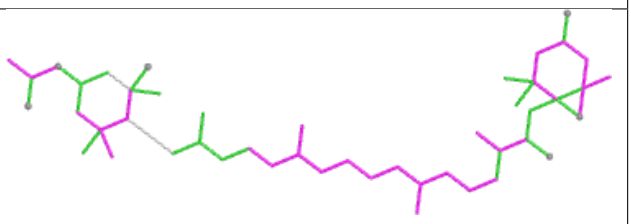


Rings

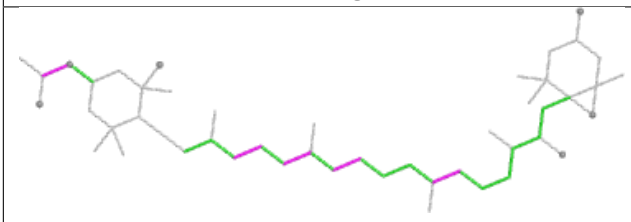
Ligand A86 14 316



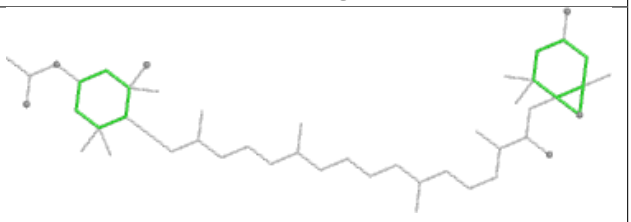
Bond lengths



Bond angles

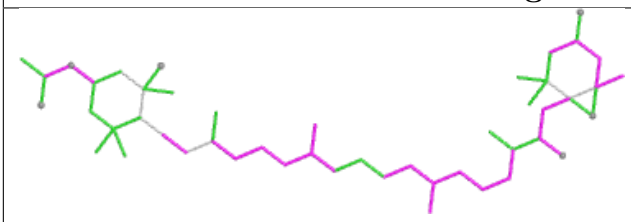


Torsions

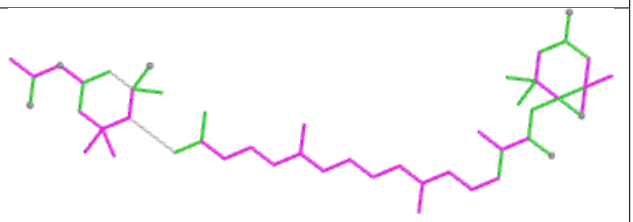


Rings

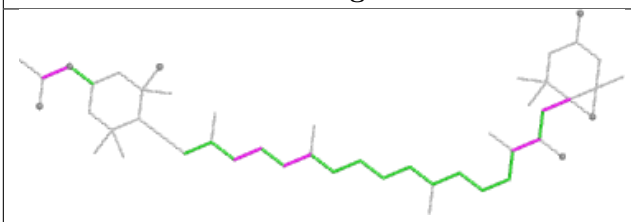
Ligand A86 12 318



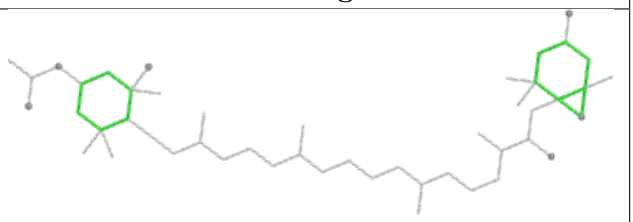
Bond lengths



Bond angles

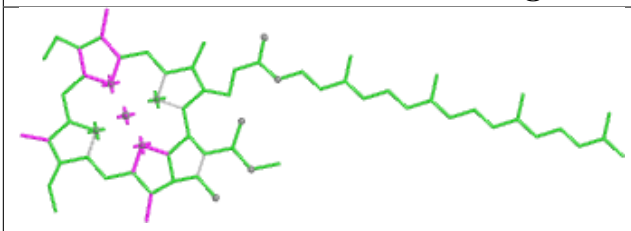


Torsions

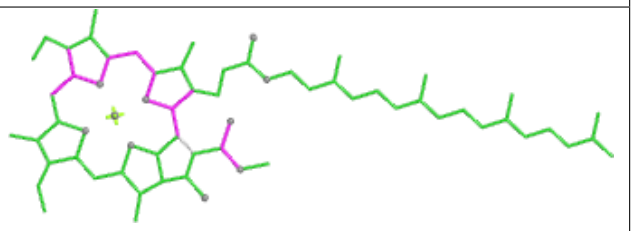


Rings

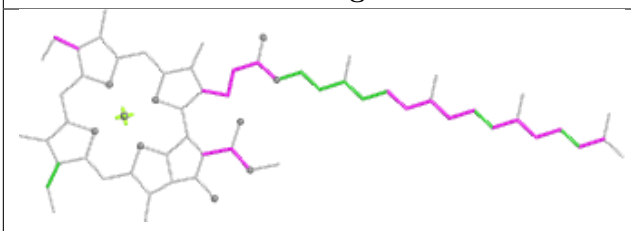
Ligand CLA C 519



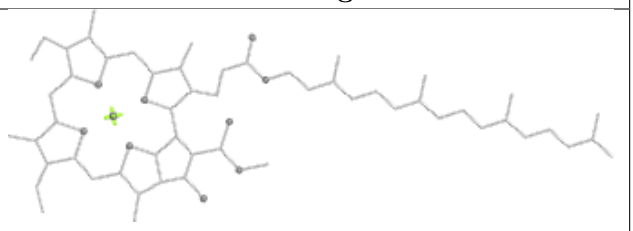
Bond lengths



Bond angles

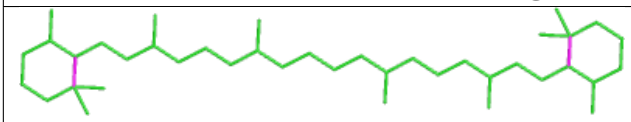


Torsions

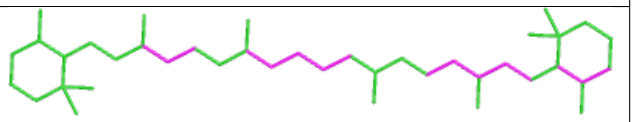


Rings

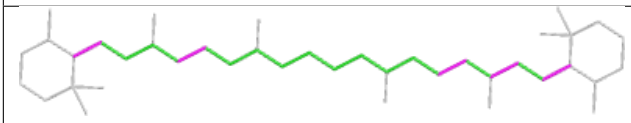
Ligand BCR c 521



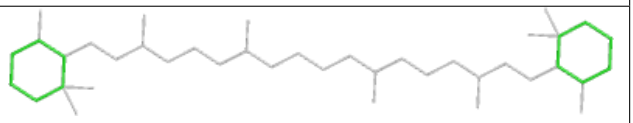
Bond lengths



Bond angles

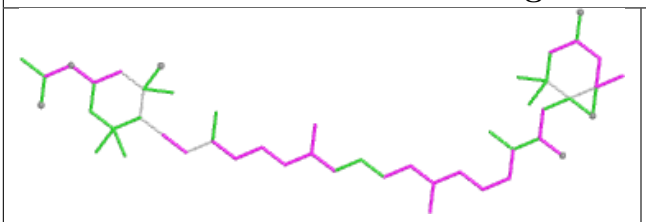


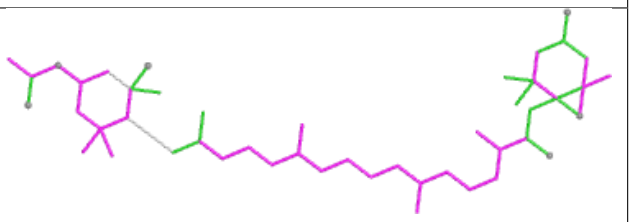
Torsions

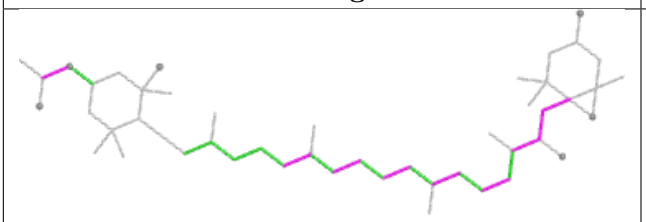


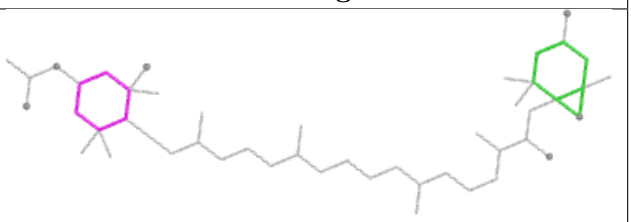
Rings

Ligand A86 17 302


Bond lengths

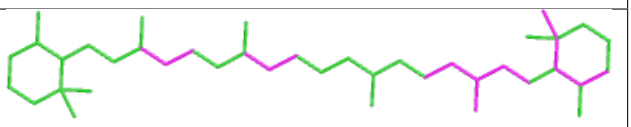

Bond angles

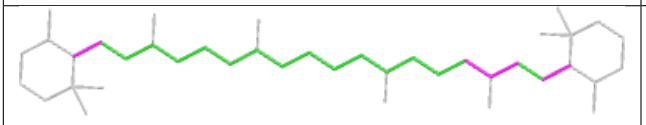

Torsions

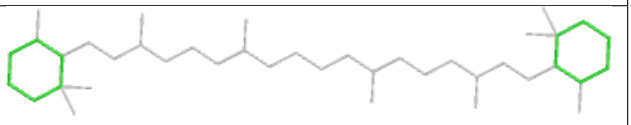

Rings

Ligand BCR H 101

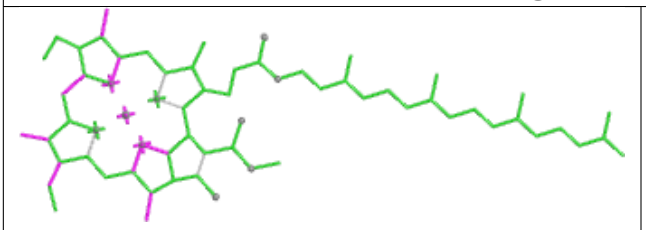

Bond lengths

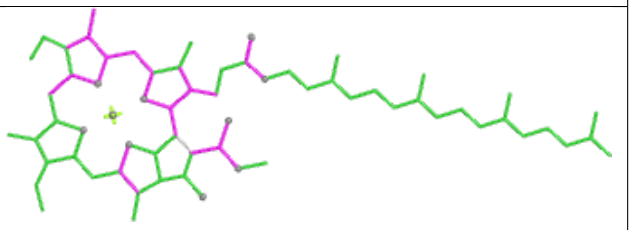

Bond angles

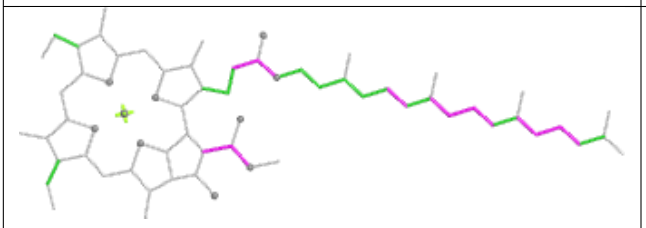

Torsions

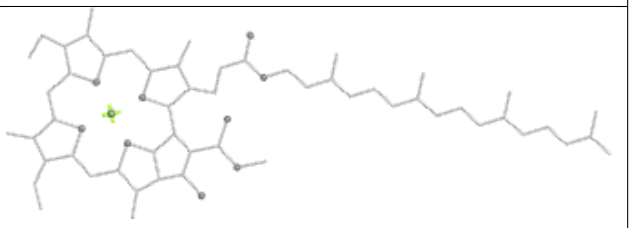

Rings

Ligand CLA c 508

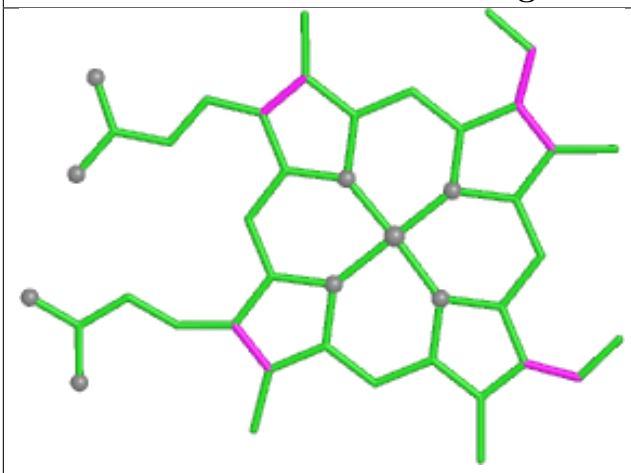

Bond lengths


Bond angles

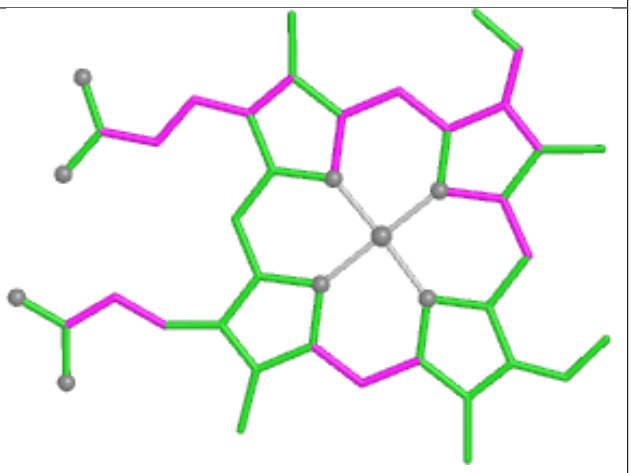

Torsions


Rings

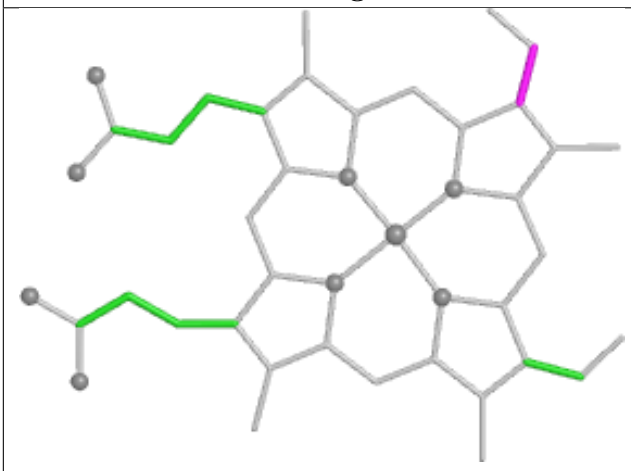
Ligand HEM V 201



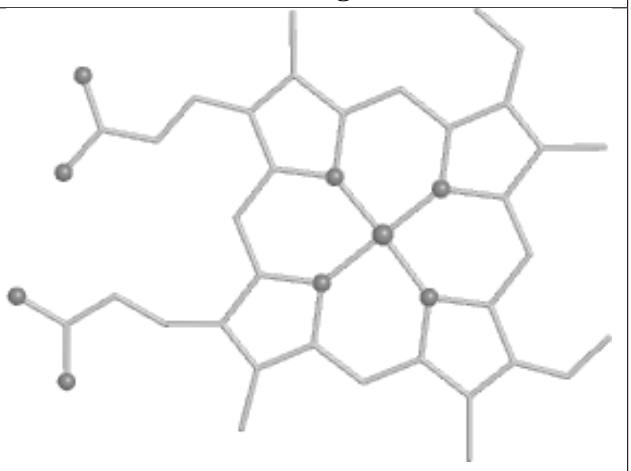
Bond lengths



Bond angles

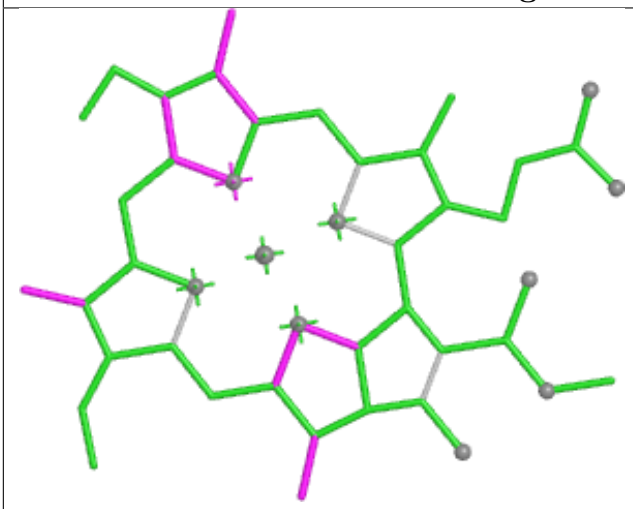


Torsions

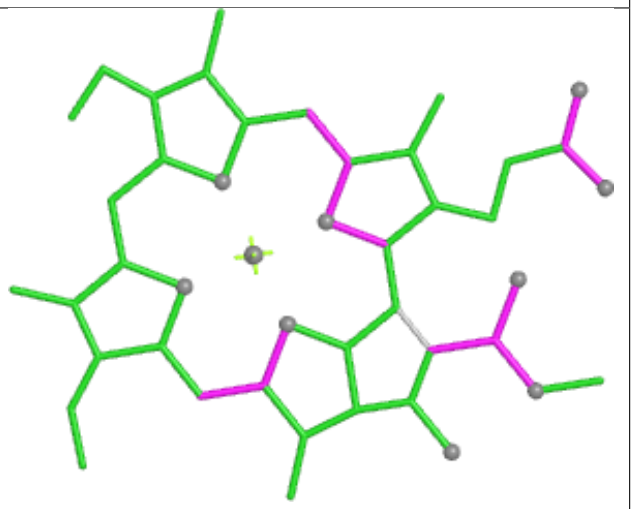


Rings

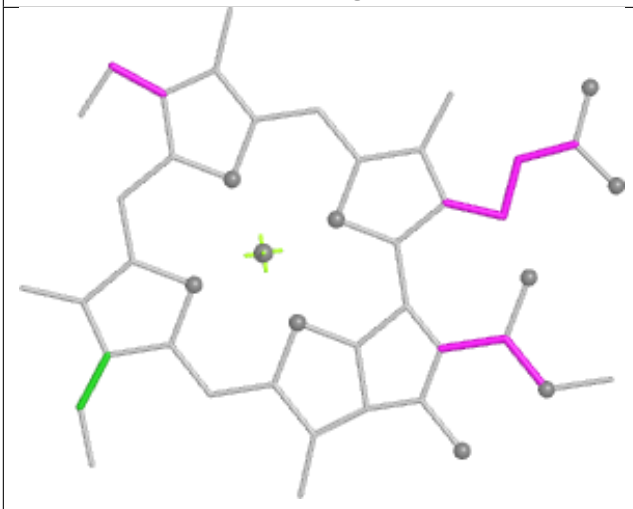
Ligand CLA 15 306



Bond lengths



Bond angles

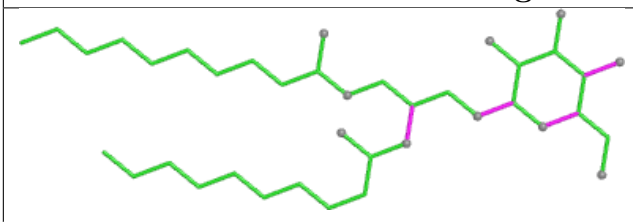


Torsions

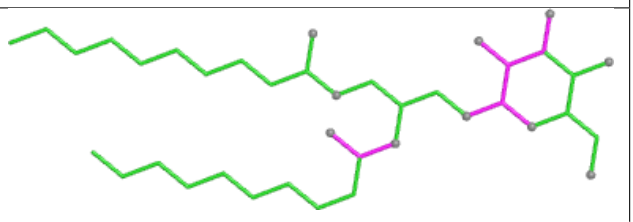


Rings

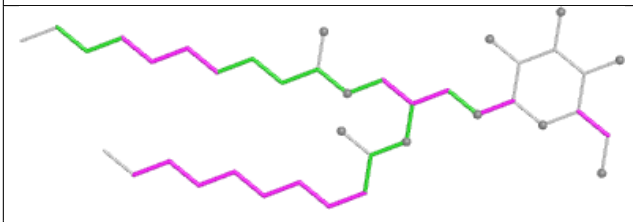
Ligand LMG 12 301



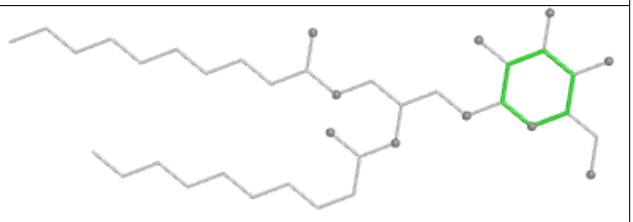
Bond lengths



Bond angles

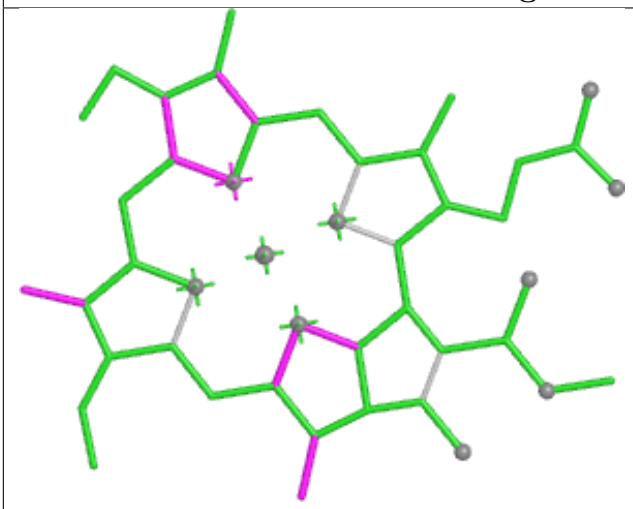


Torsions

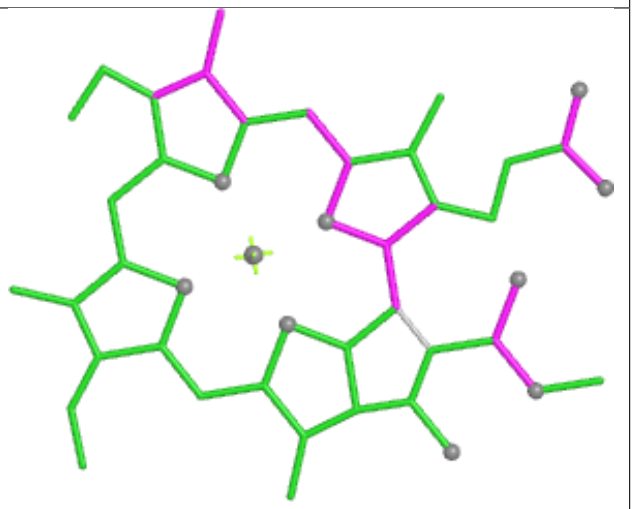


Rings

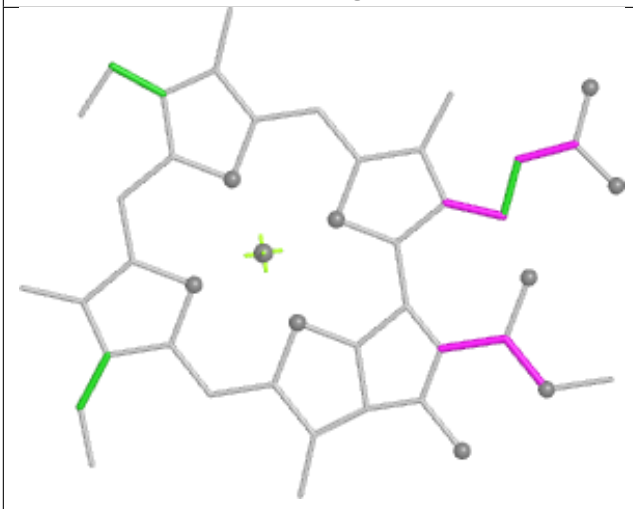
Ligand CLA 20 208



Bond lengths



Bond angles

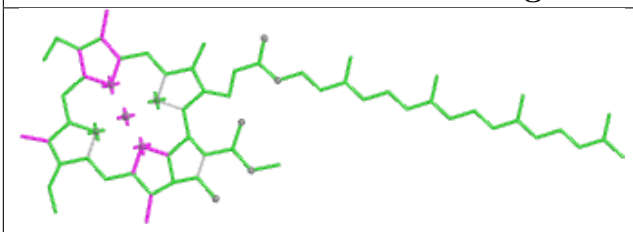


Torsions

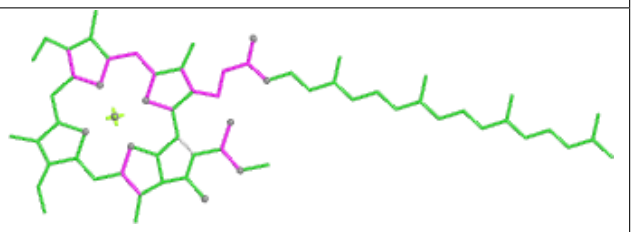


Rings

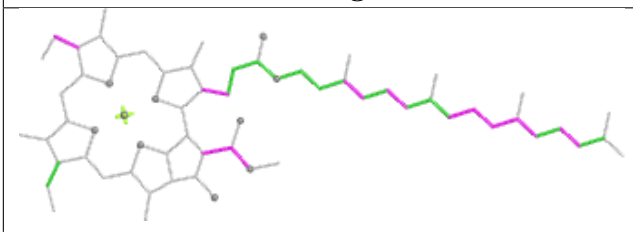
Ligand CLA w 102



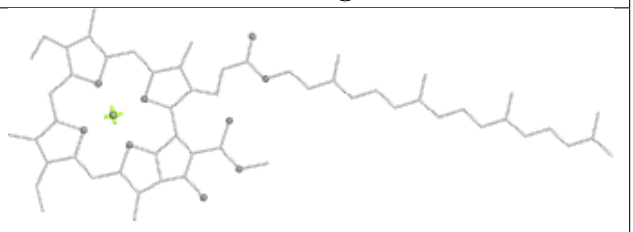
Bond lengths



Bond angles

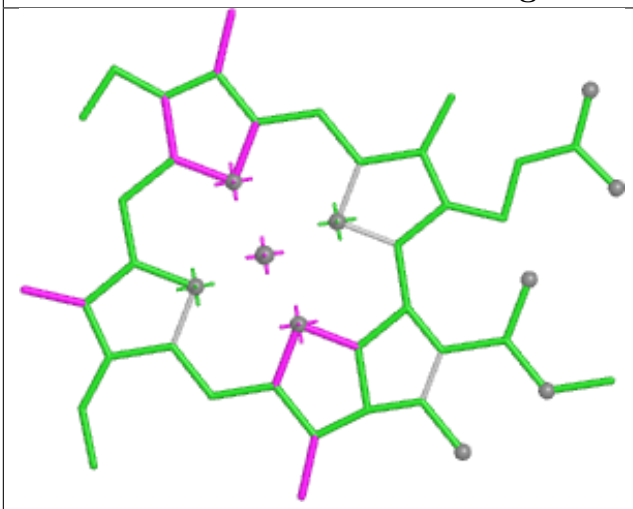


Torsions

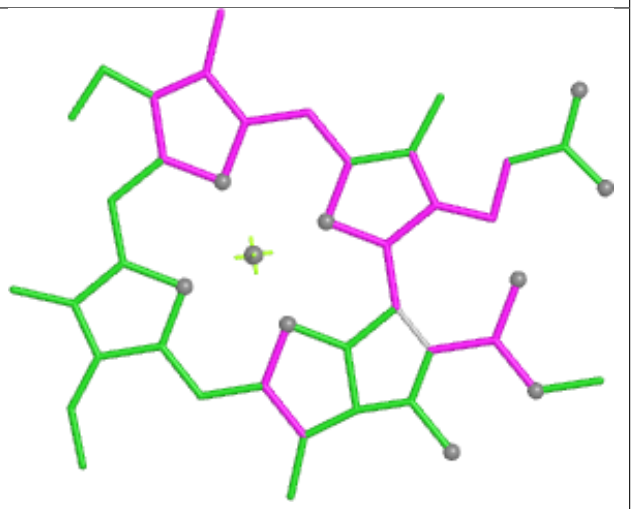


Rings

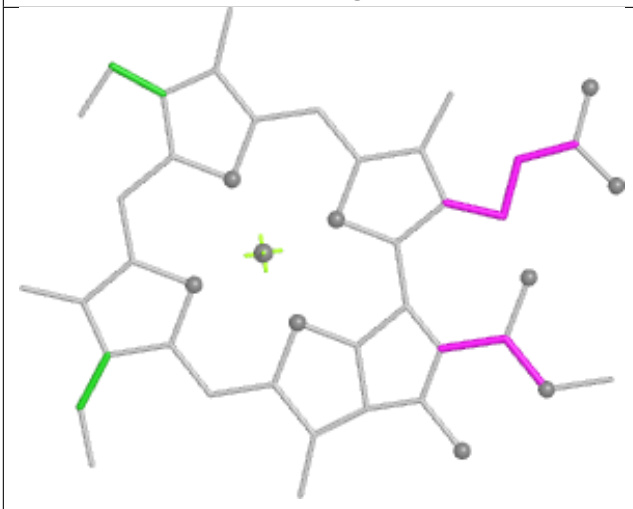
Ligand CLA 11 304



Bond lengths



Bond angles

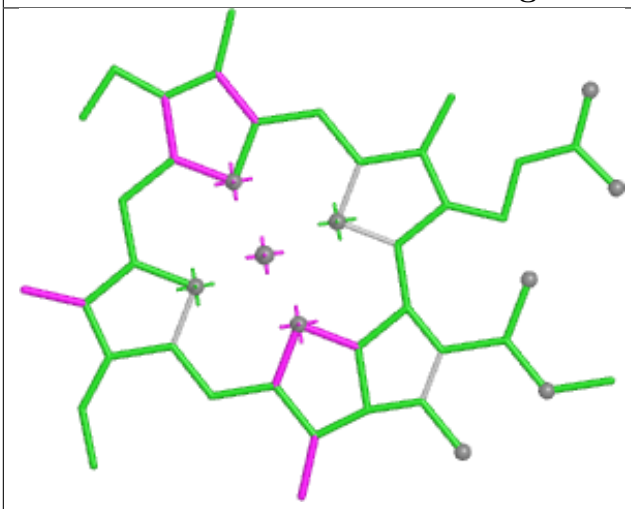


Torsions

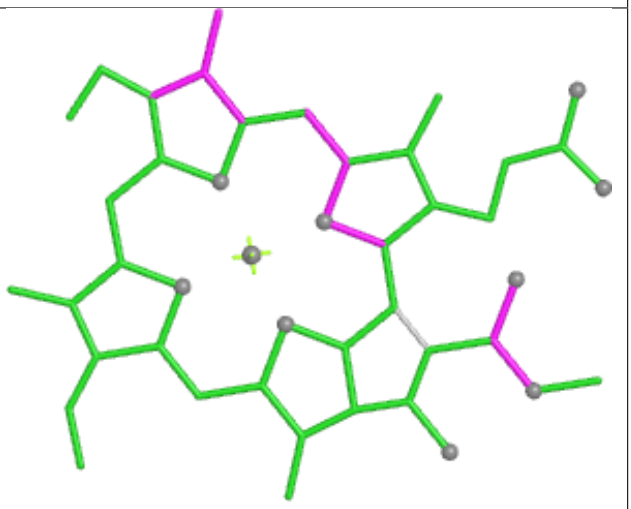


Rings

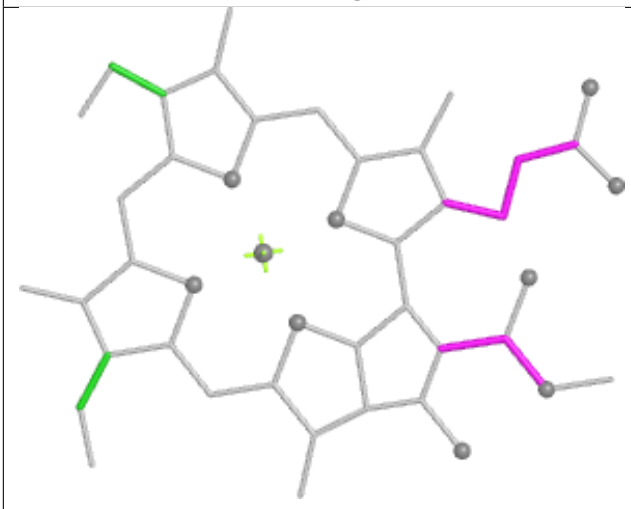
Ligand CLA 21 304



Bond lengths



Bond angles

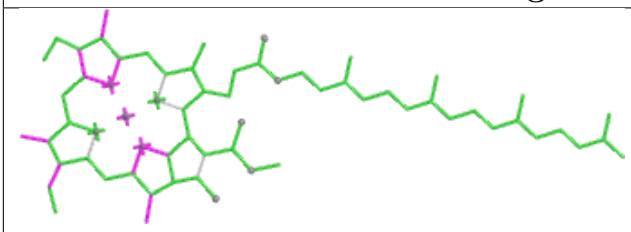


Torsions

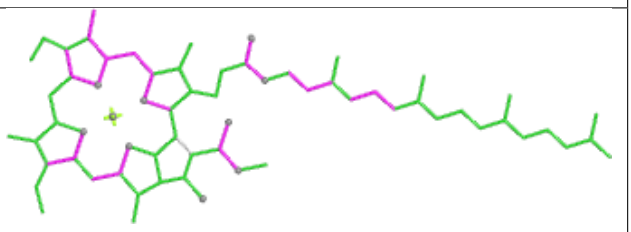


Rings

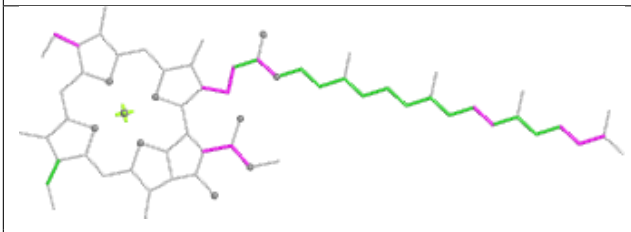
Ligand CLA b 611



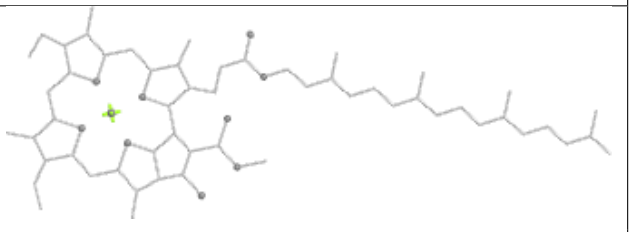
Bond lengths



Bond angles

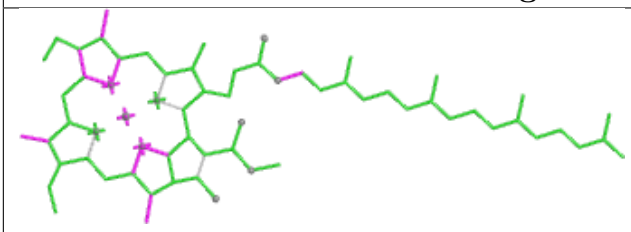


Torsions

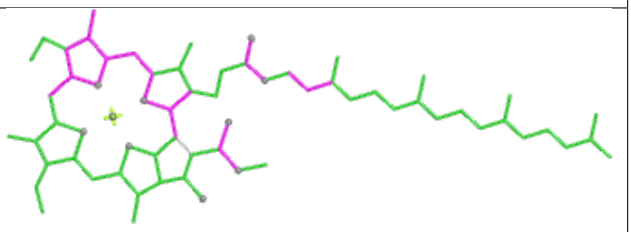


Rings

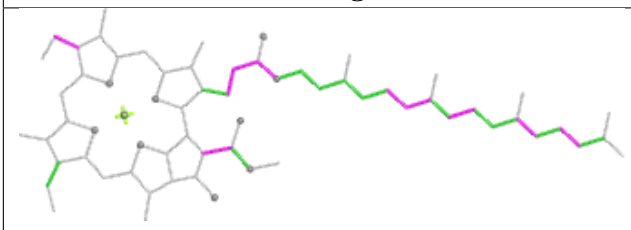
Ligand CLA 14 309



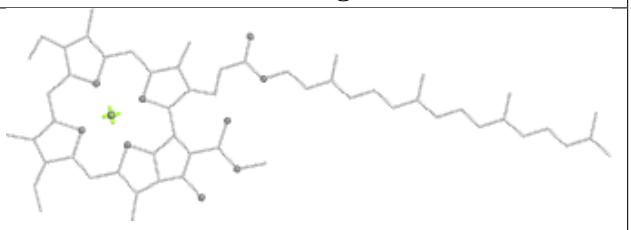
Bond lengths



Bond angles

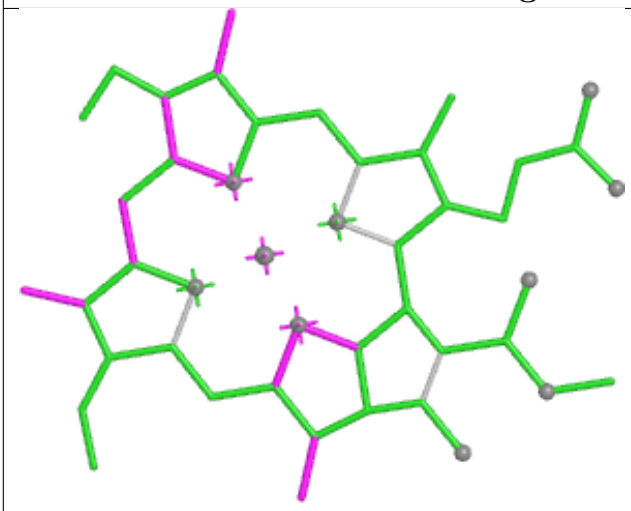


Torsions

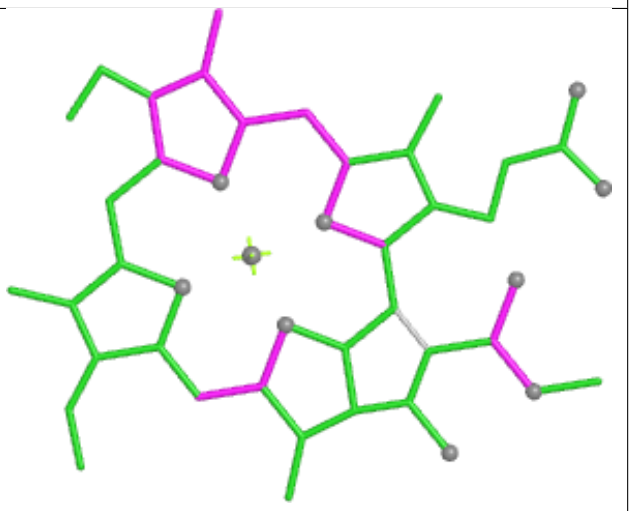


Rings

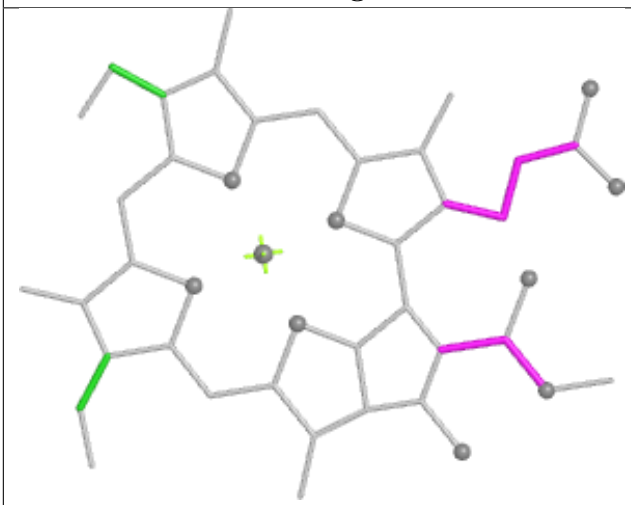
Ligand CLA 16 307



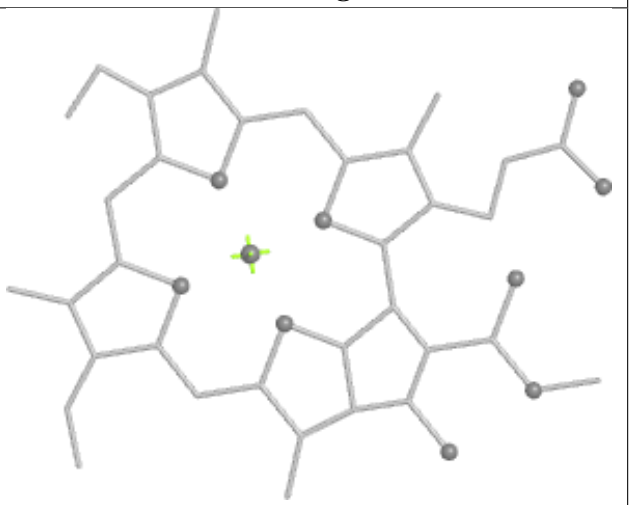
Bond lengths



Bond angles

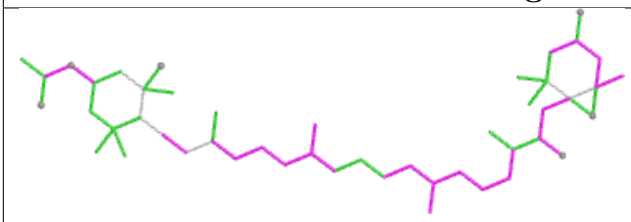


Torsions

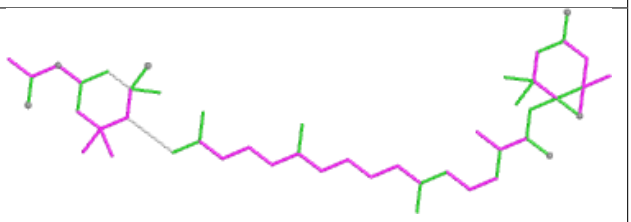


Rings

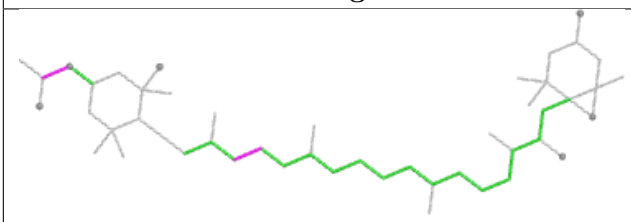
Ligand A86 15 311



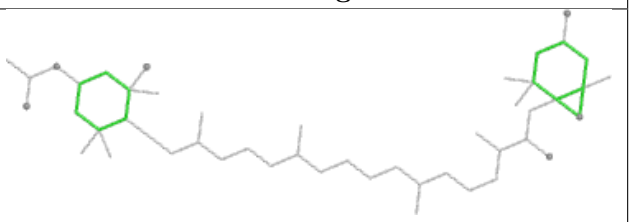
Bond lengths



Bond angles

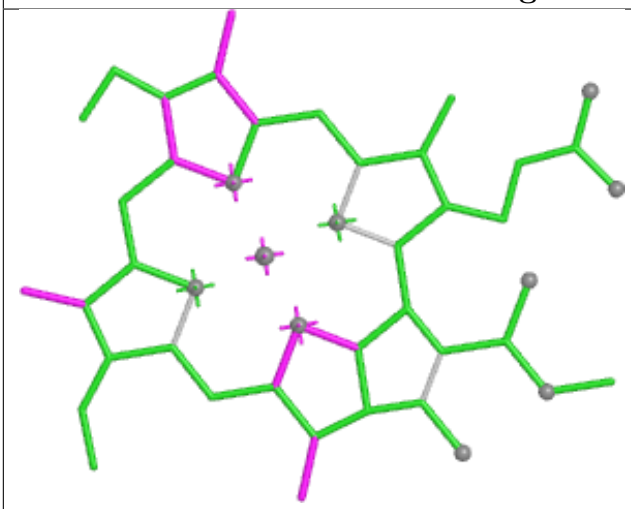


Torsions

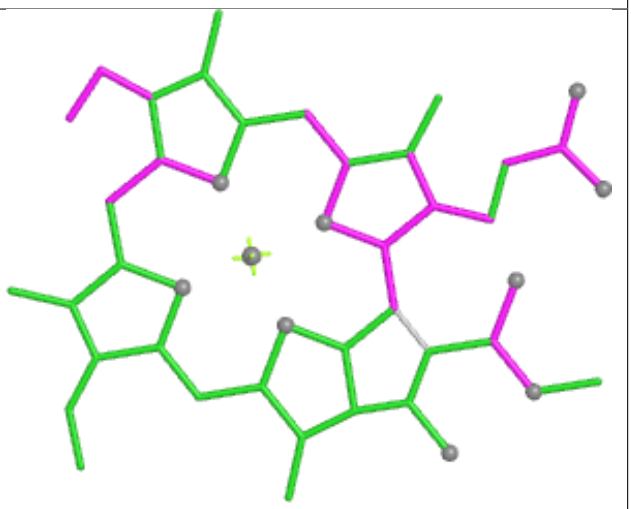


Rings

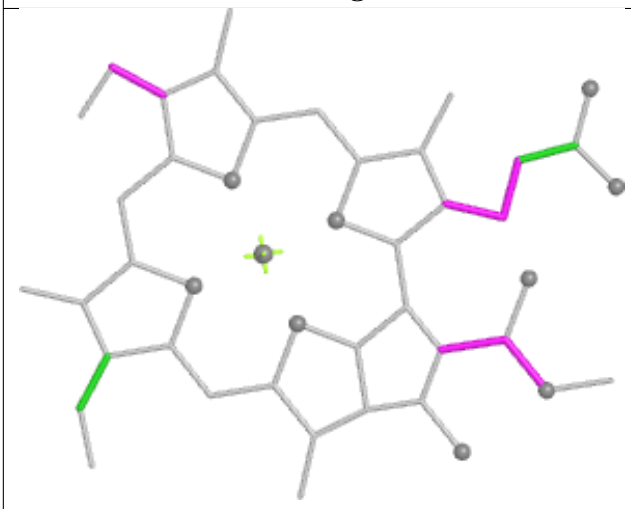
Ligand CLA 16 308



Bond lengths



Bond angles

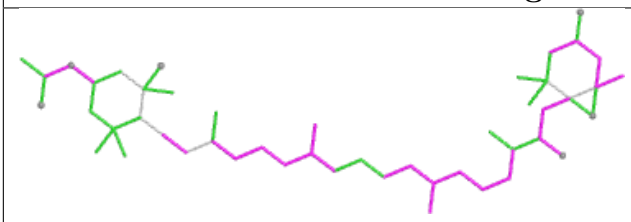


Torsions

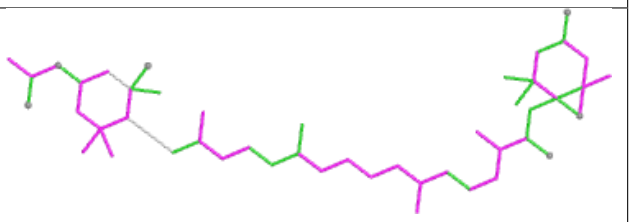


Rings

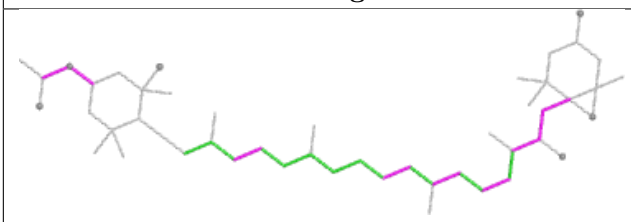
Ligand A86 11 316



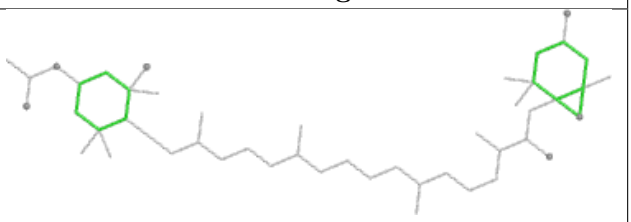
Bond lengths



Bond angles

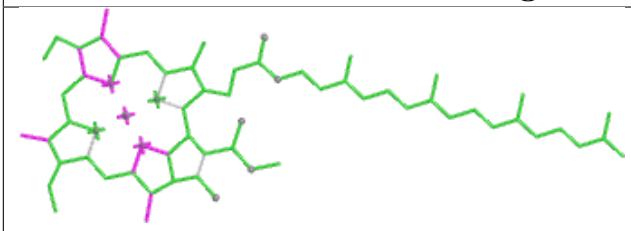


Torsions

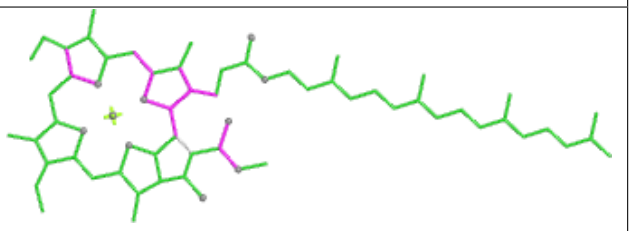


Rings

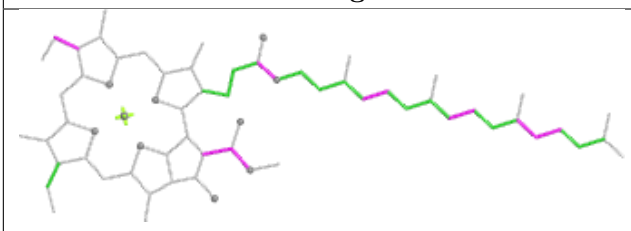
Ligand CLA 12 312



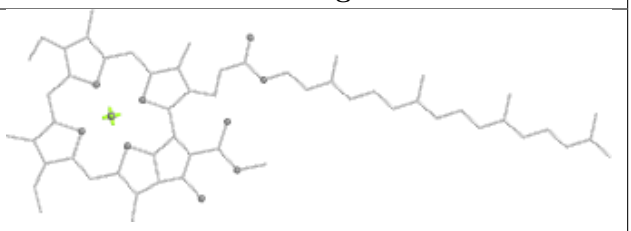
Bond lengths



Bond angles

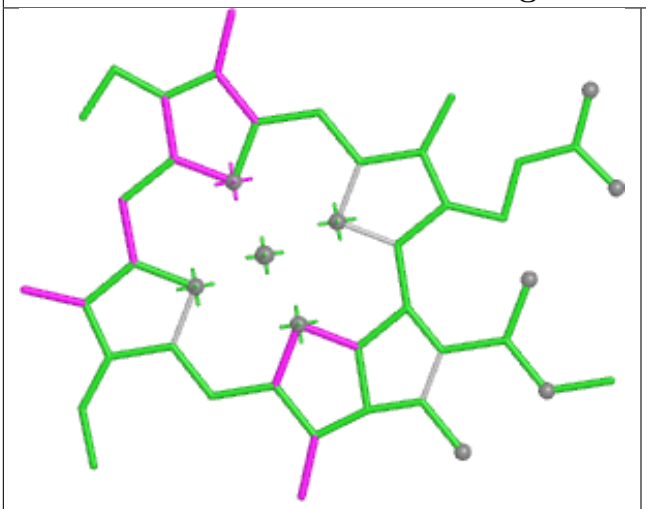


Torsions

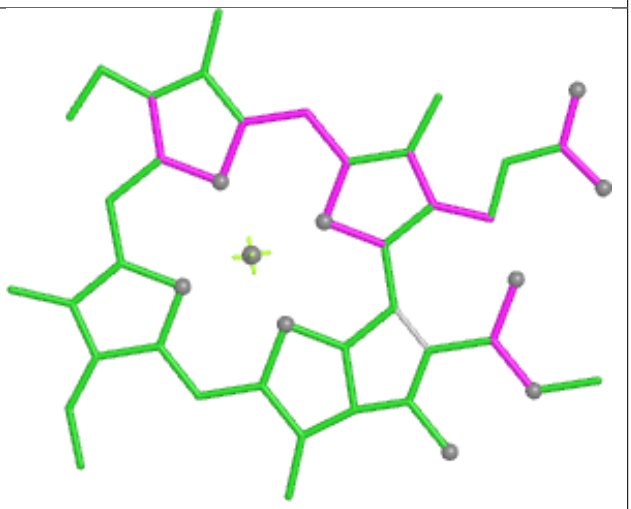


Rings

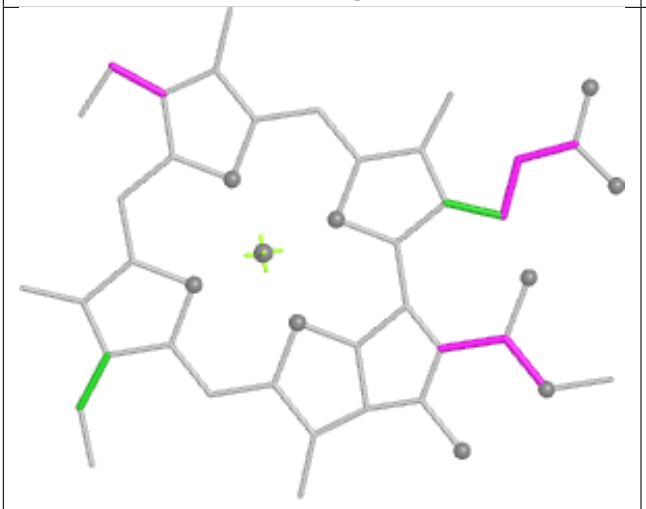
Ligand CLA 18 307



Bond lengths



Bond angles

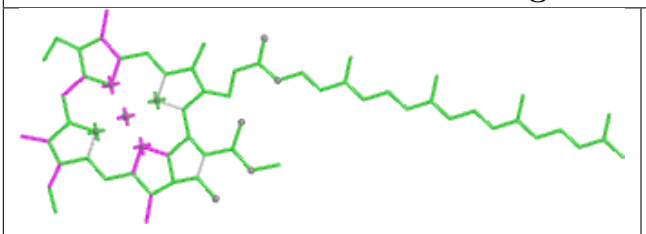


Torsions

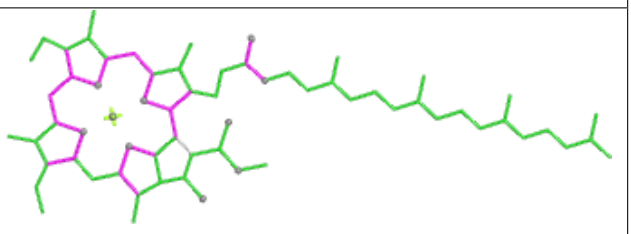


Rings

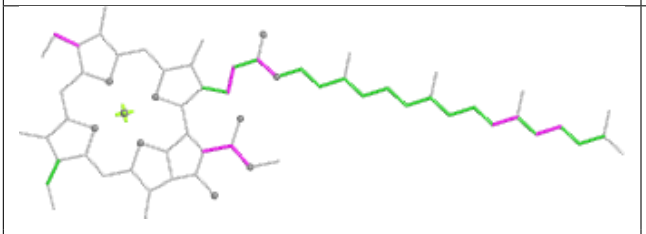
Ligand CLA c 503



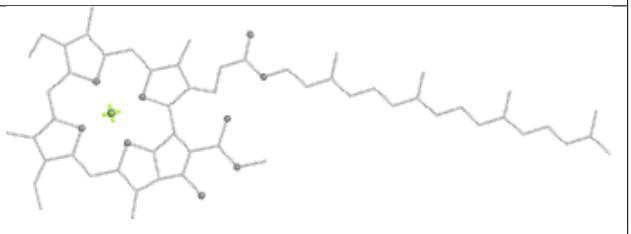
Bond lengths



Bond angles

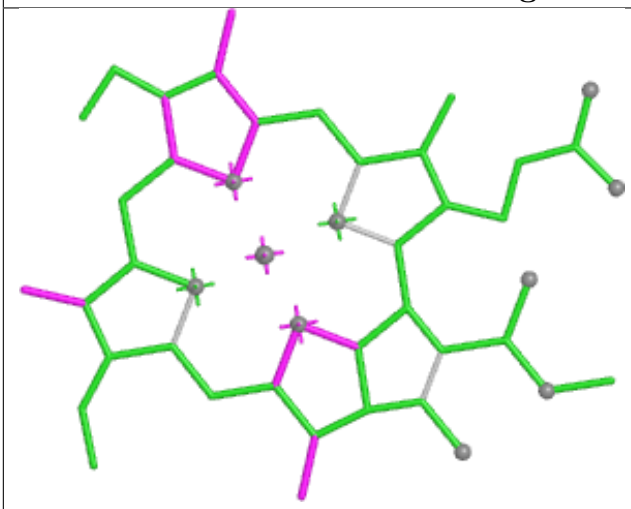


Torsions

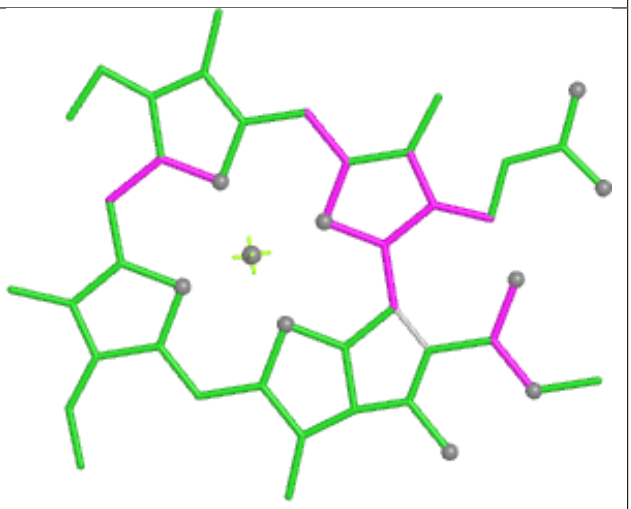


Rings

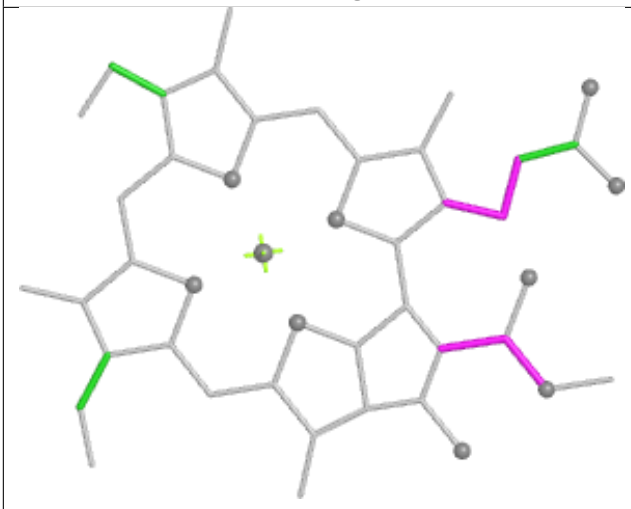
Ligand CLA 11 302



Bond lengths



Bond angles

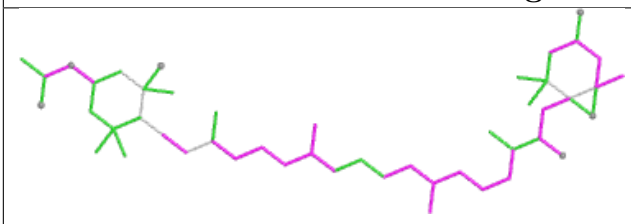


Torsions

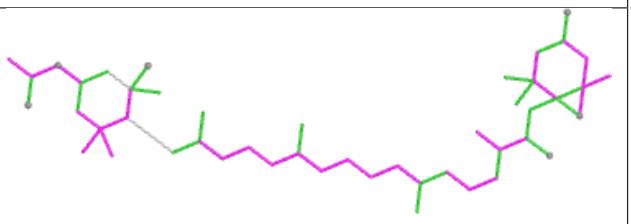


Rings

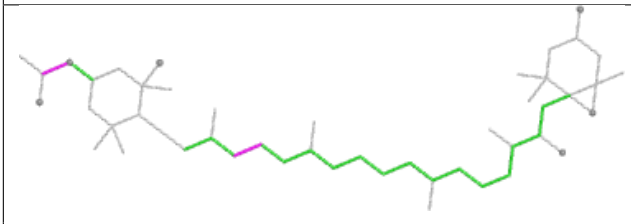
Ligand A86 18 314



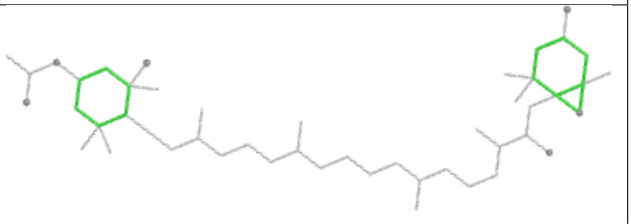
Bond lengths



Bond angles

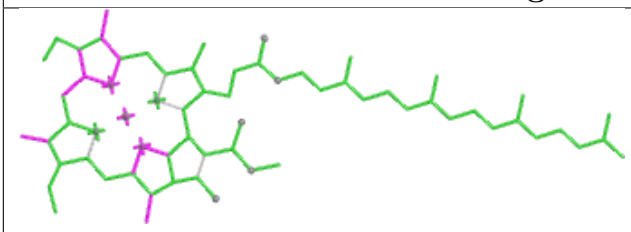


Torsions

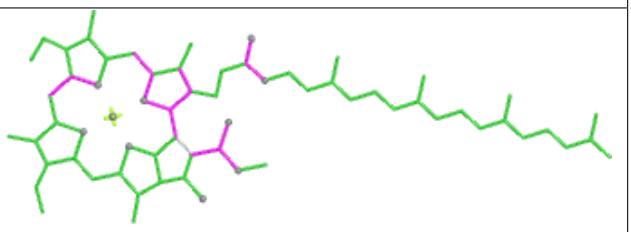


Rings

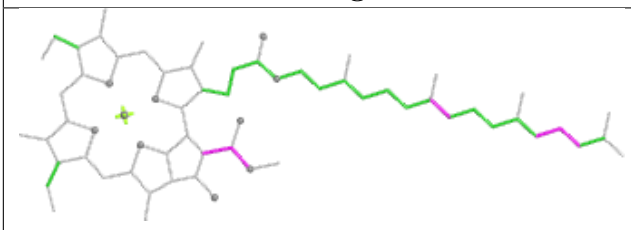
Ligand CLA b 614



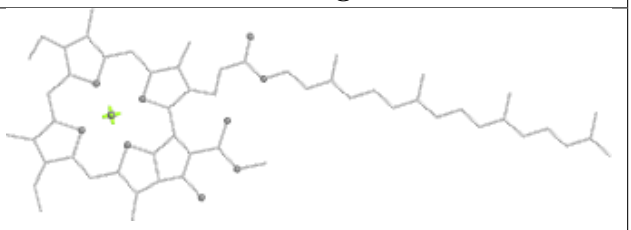
Bond lengths



Bond angles



Torsions

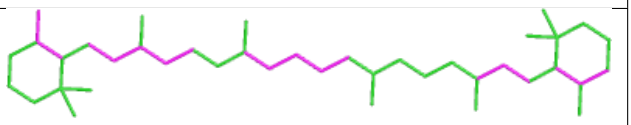


Rings

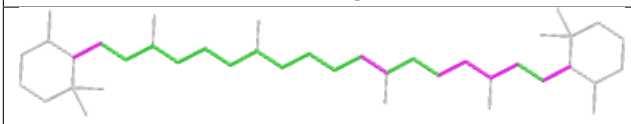
Ligand BCR m 103



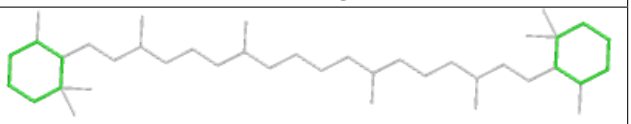
Bond lengths



Bond angles

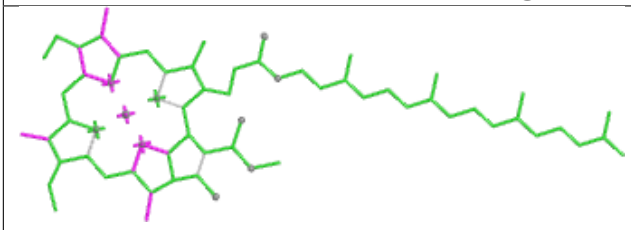


Torsions

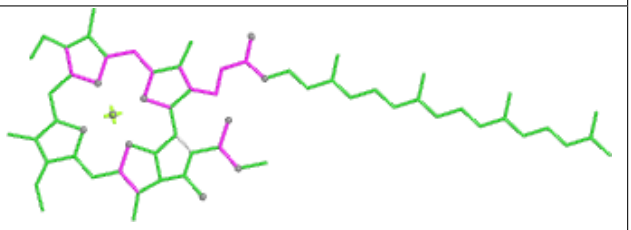


Rings

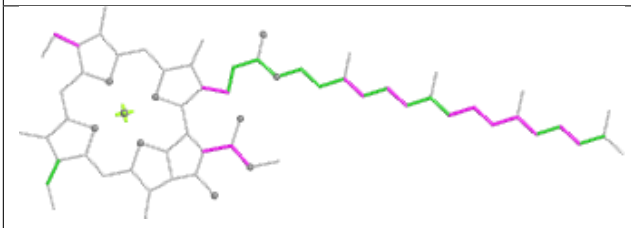
Ligand CLA W 102



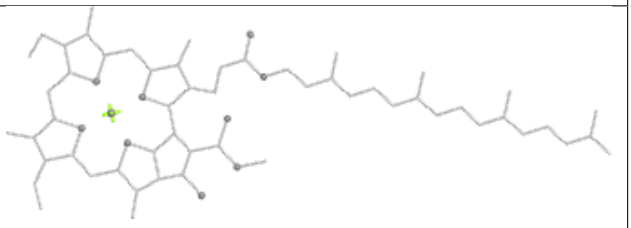
Bond lengths



Bond angles

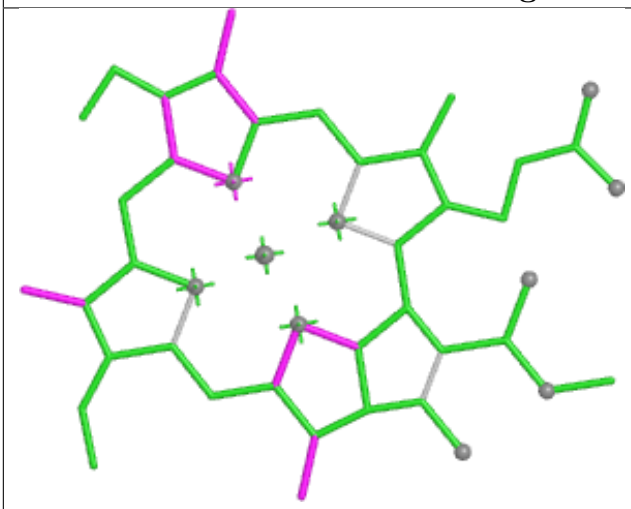


Torsions

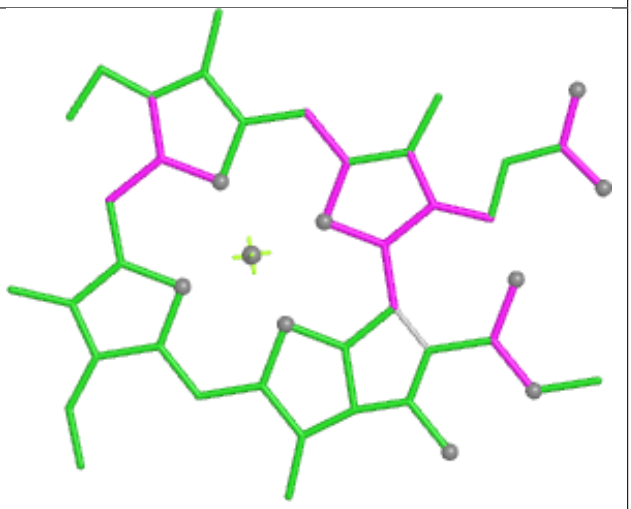


Rings

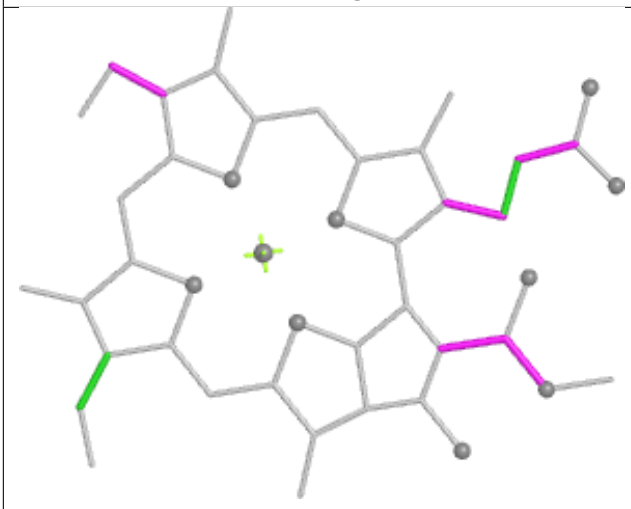
Ligand CLA 21 302



Bond lengths



Bond angles

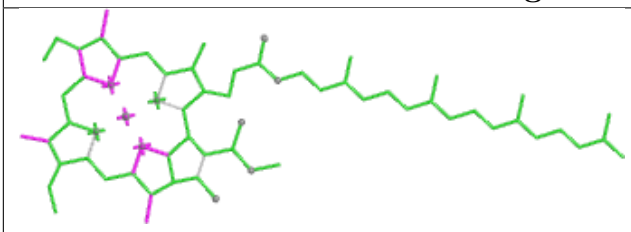


Torsions

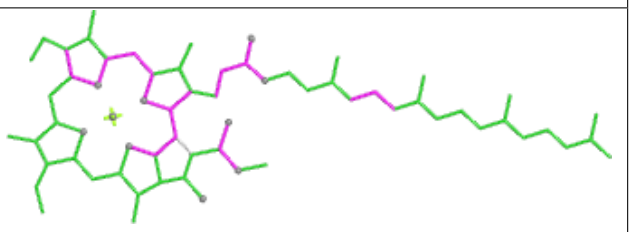


Rings

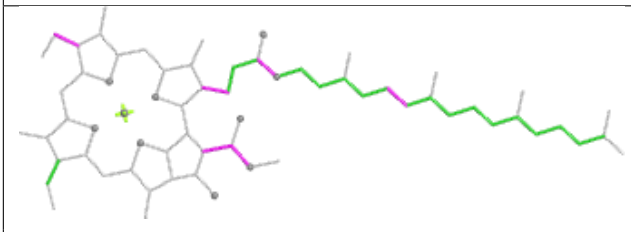
Ligand CLA C 512



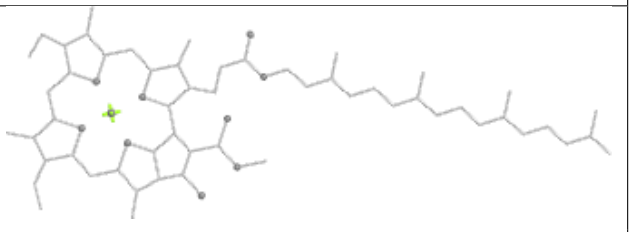
Bond lengths



Bond angles

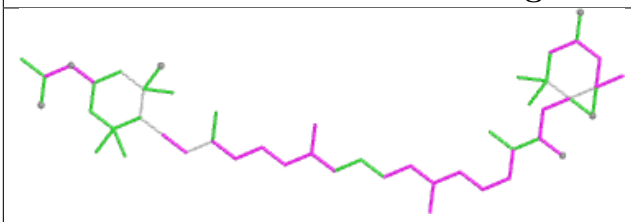


Torsions

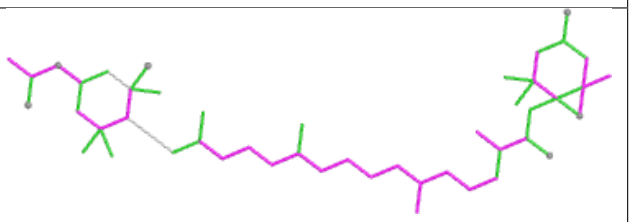


Rings

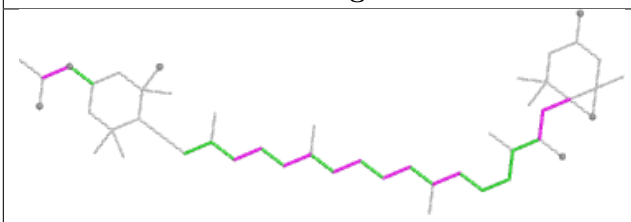
Ligand A86 19 310



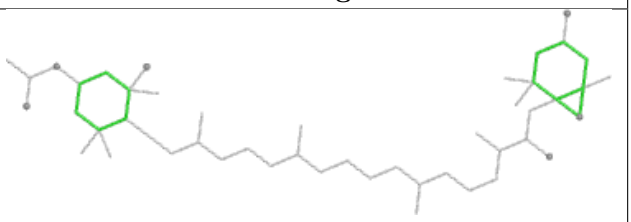
Bond lengths



Bond angles

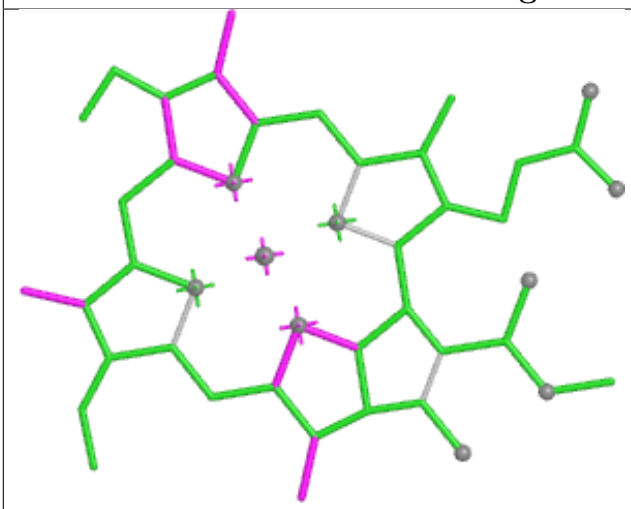


Torsions

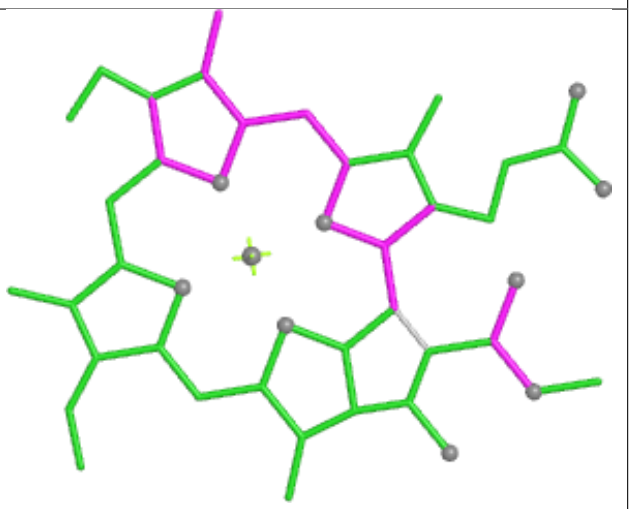


Rings

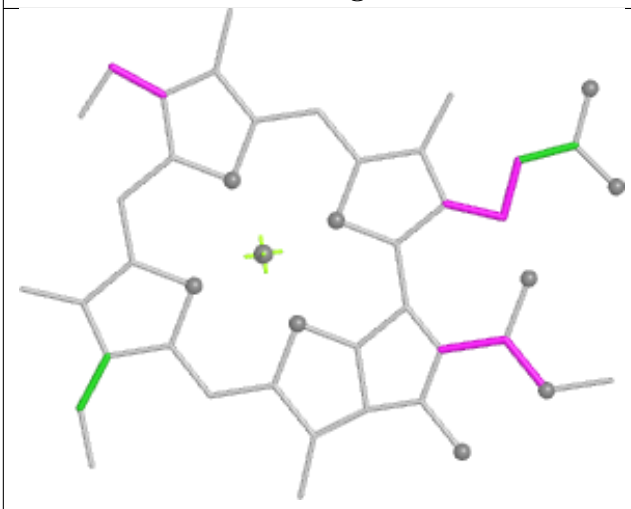
Ligand CLA 11 305



Bond lengths



Bond angles

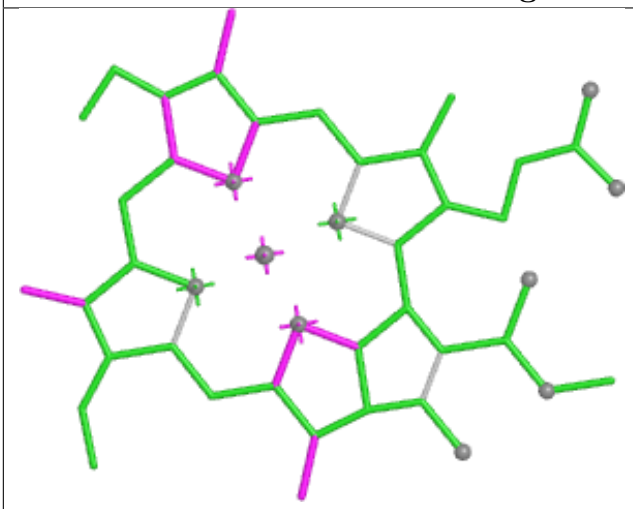


Torsions

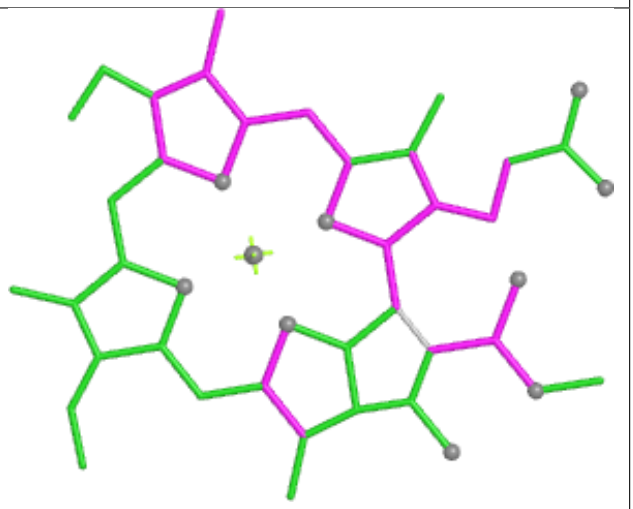


Rings

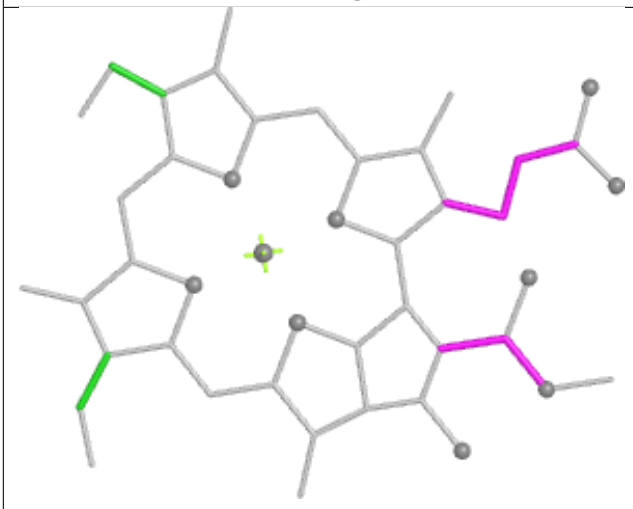
Ligand CLA 12 308



Bond lengths



Bond angles

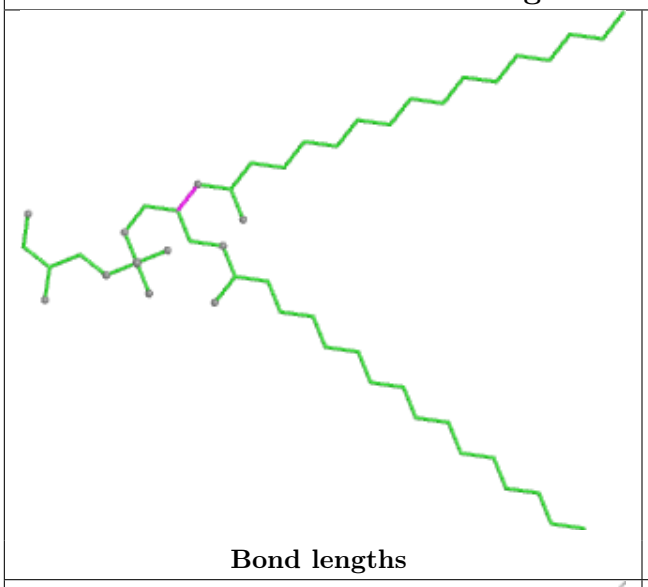


Torsions

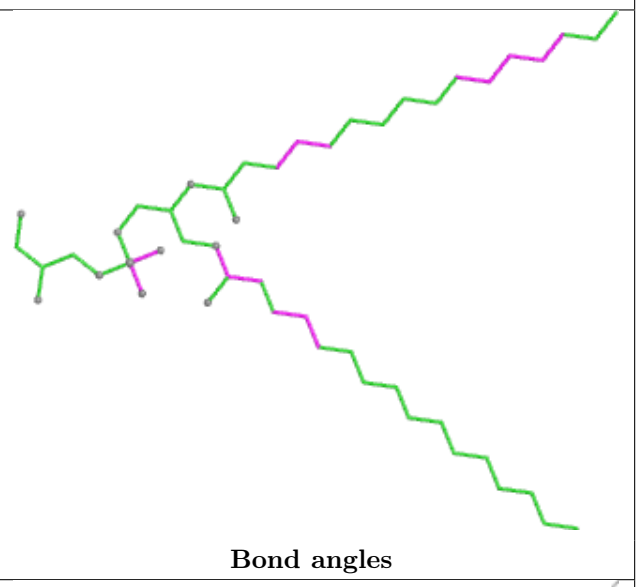


Rings

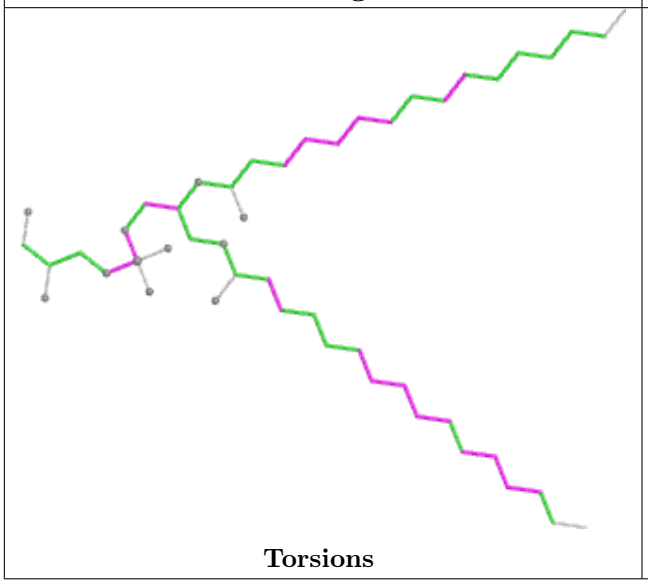
Ligand LHG B 622



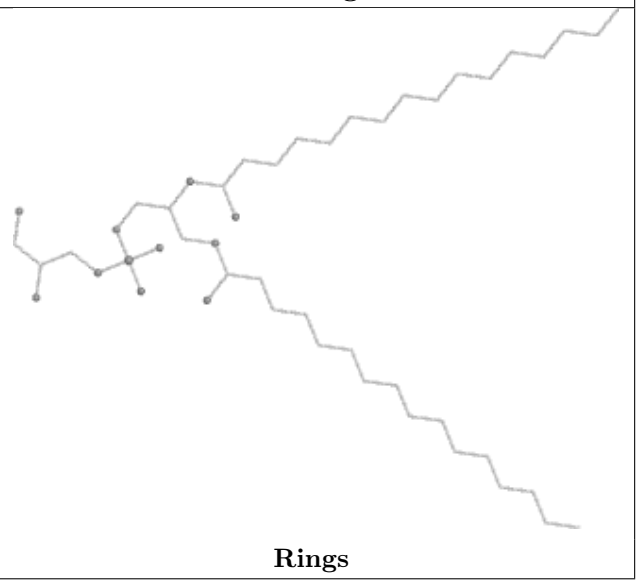
Bond lengths



Bond angles

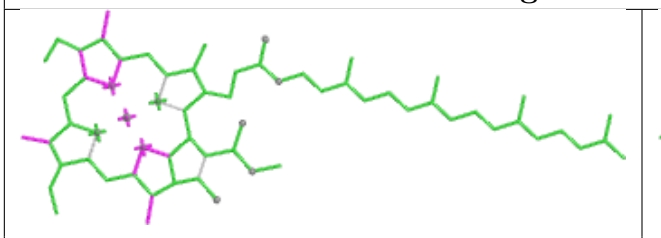


Torsions

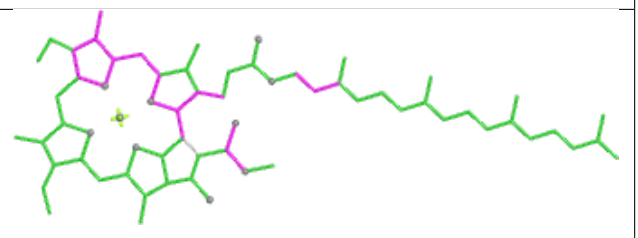


Rings

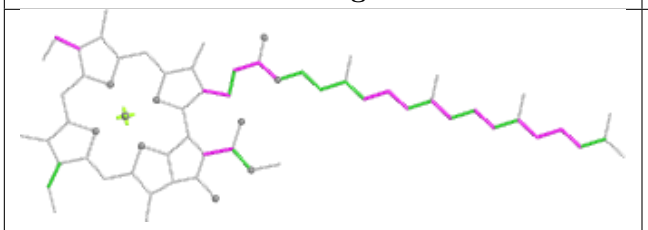
Ligand CLA 18 309



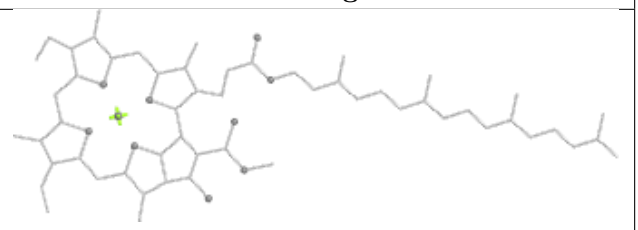
Bond lengths



Bond angles

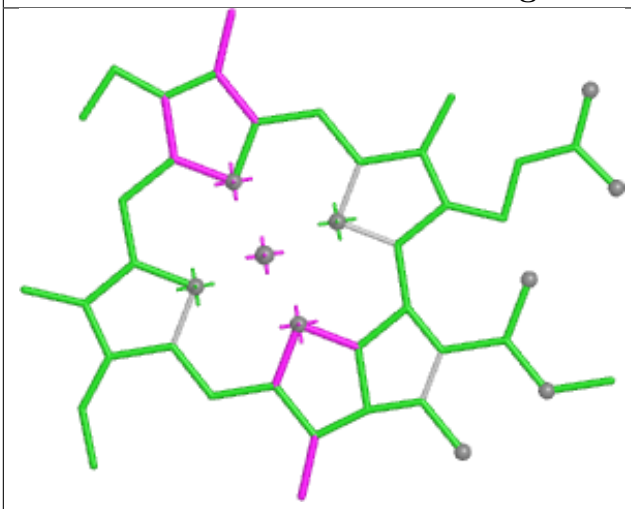


Torsions

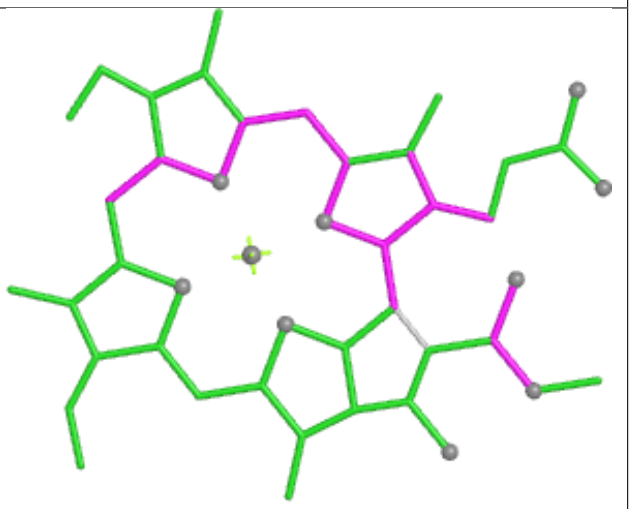


Rings

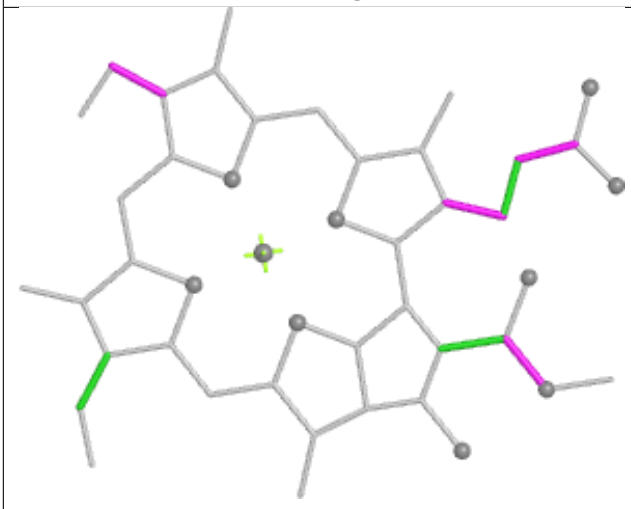
Ligand CLA 20 203



Bond lengths



Bond angles

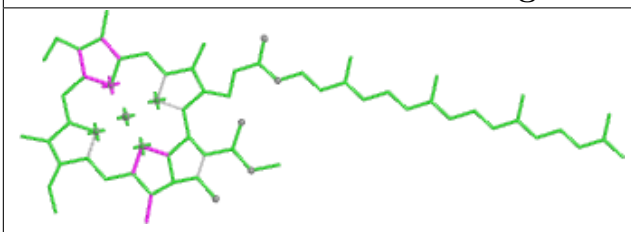


Torsions

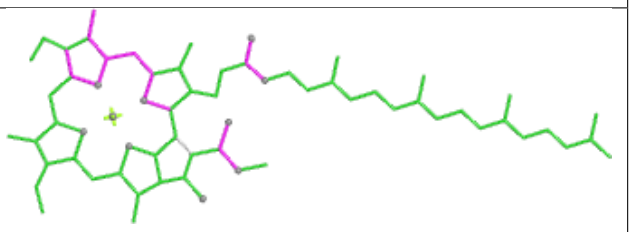


Rings

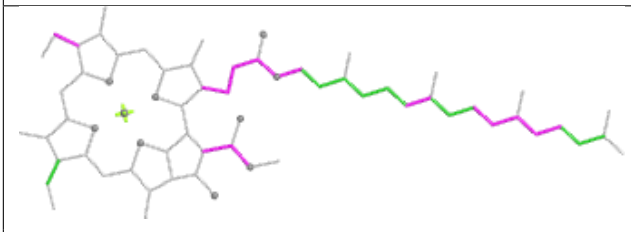
Ligand CLA W 103



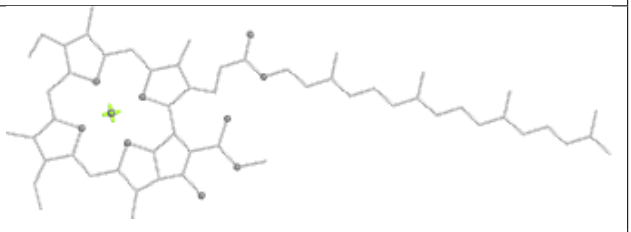
Bond lengths



Bond angles

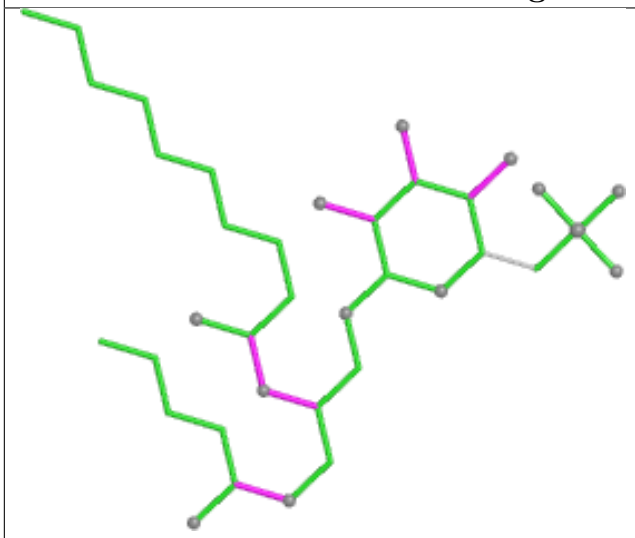


Torsions

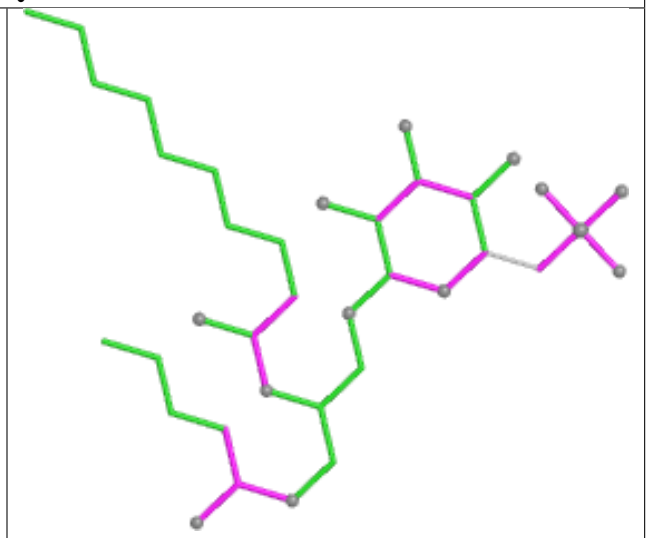


Rings

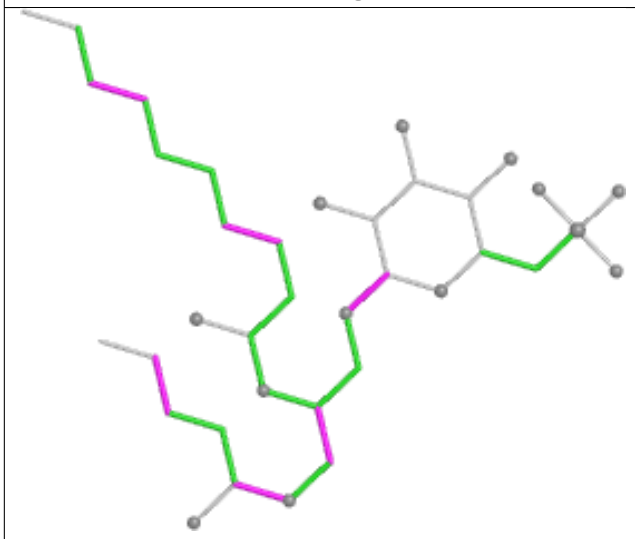
Ligand SQD b 620



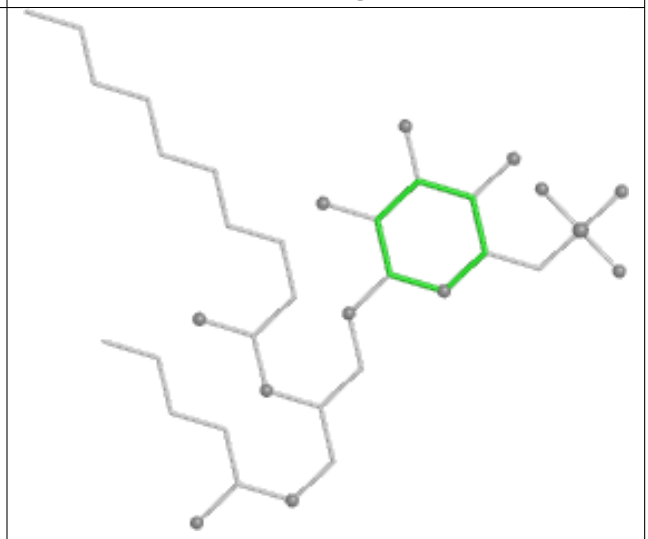
Bond lengths



Bond angles

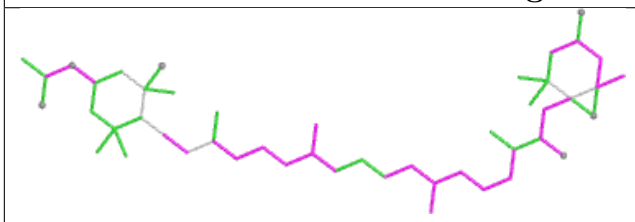


Torsions

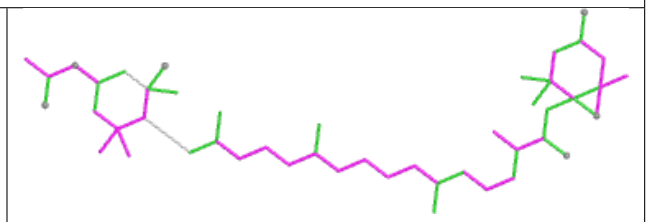


Rings

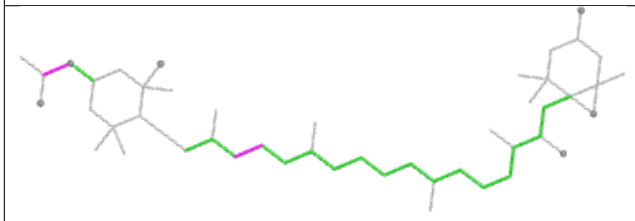
Ligand A86 16 311



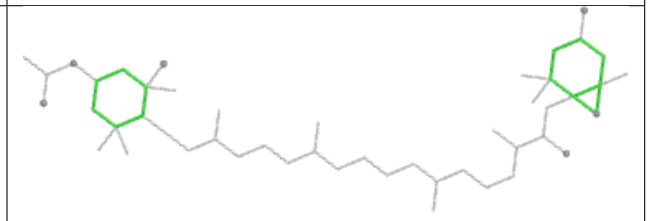
Bond lengths



Bond angles

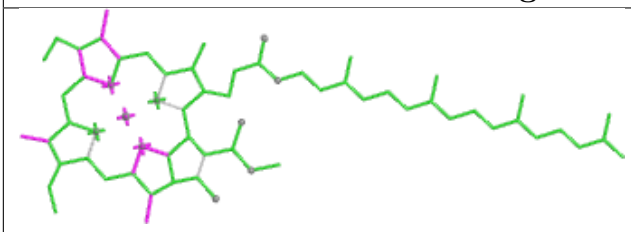


Torsions

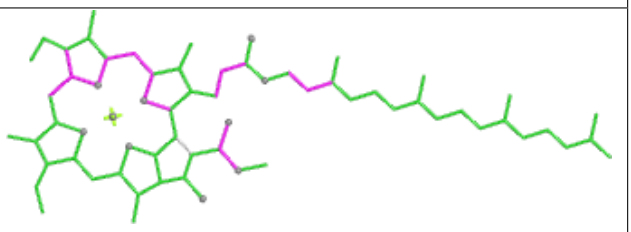


Rings

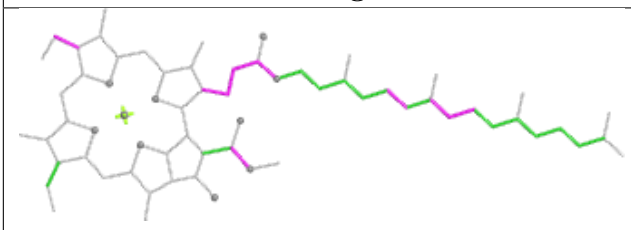
Ligand CLA 13 302



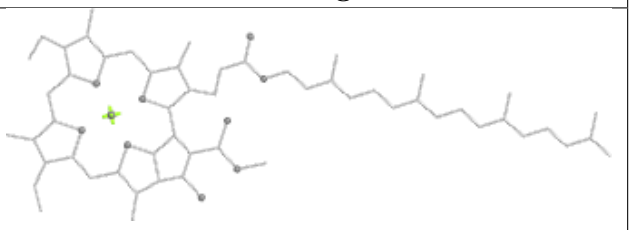
Bond lengths



Bond angles

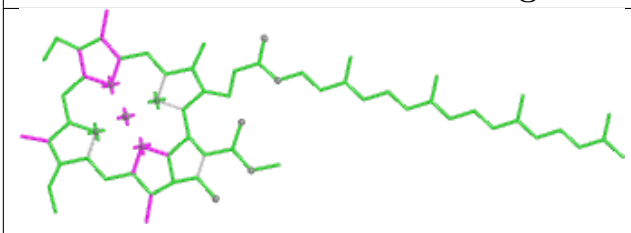


Torsions

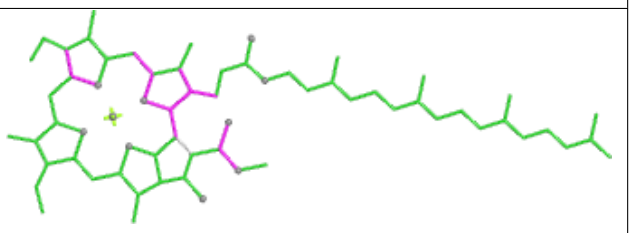


Rings

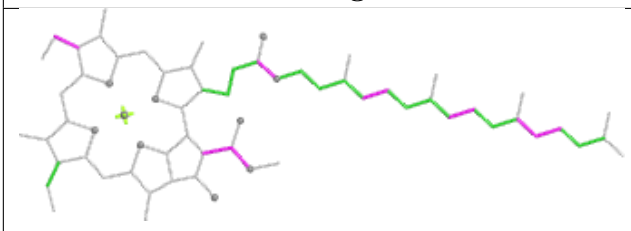
Ligand CLA 11 315



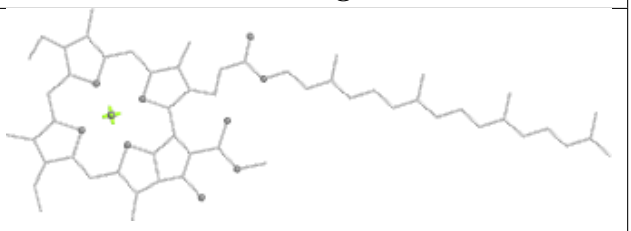
Bond lengths



Bond angles

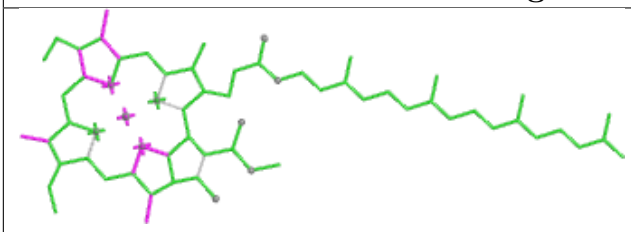


Torsions

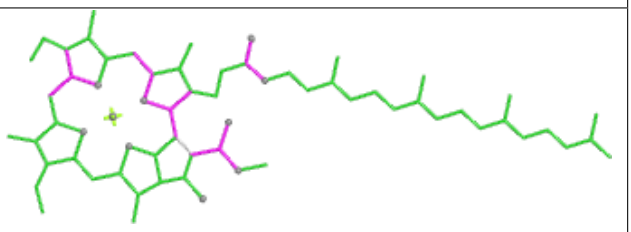


Rings

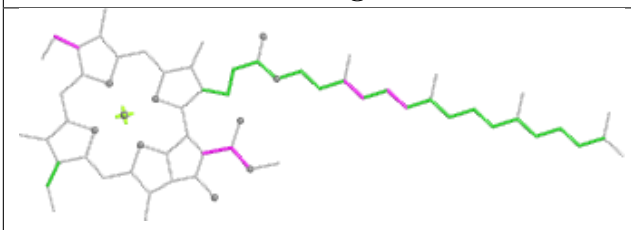
Ligand CLA b 609



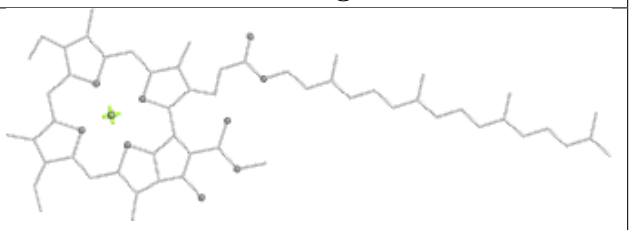
Bond lengths



Bond angles

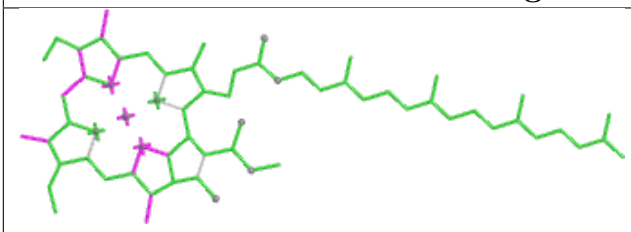


Torsions

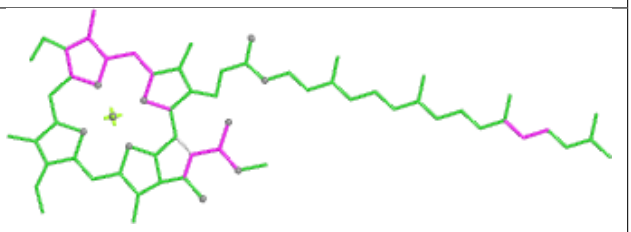


Rings

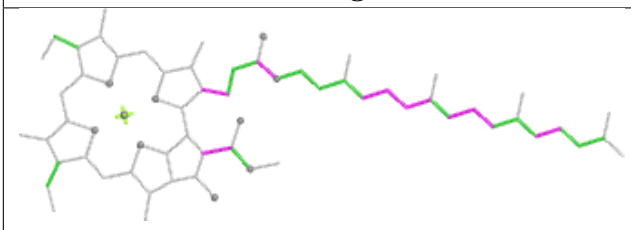
Ligand CLA C 509



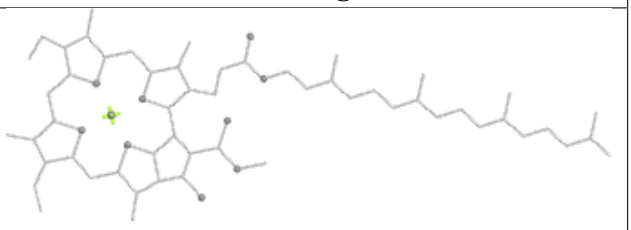
Bond lengths



Bond angles

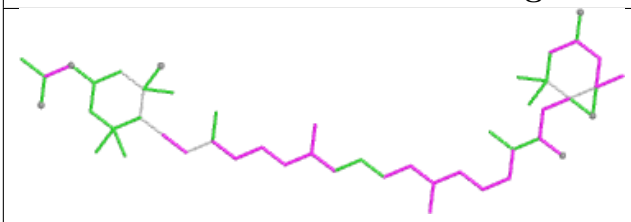


Torsions



Rings

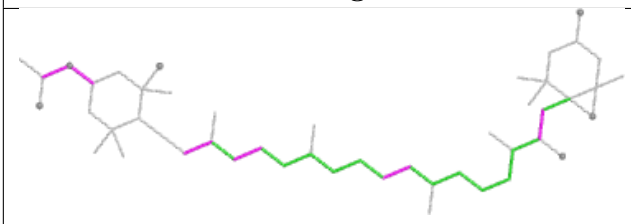
Ligand A86 14 314



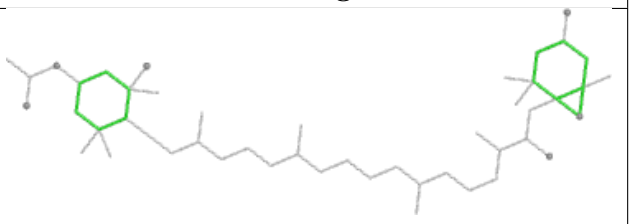
Bond lengths



Bond angles

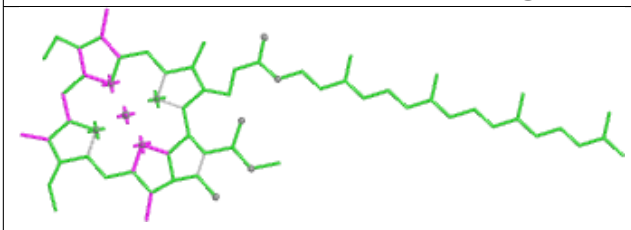


Torsions

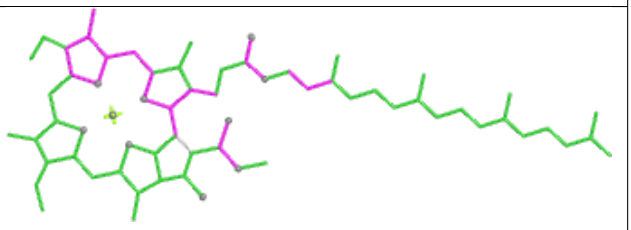


Rings

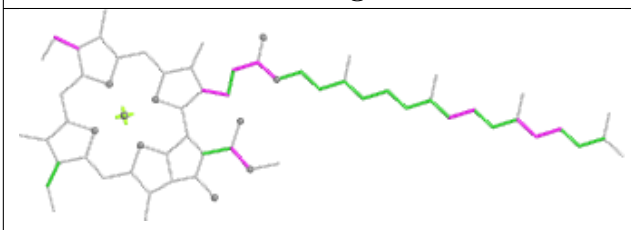
Ligand CLA 15 307



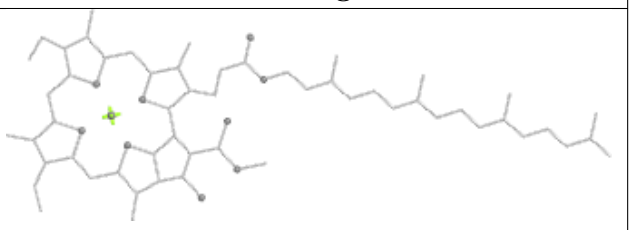
Bond lengths



Bond angles

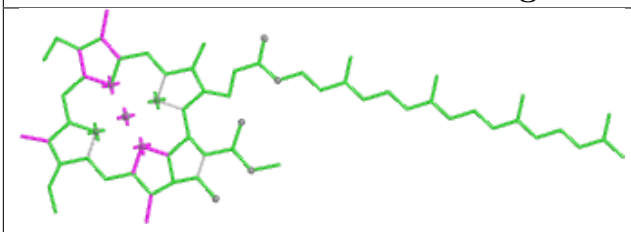


Torsions

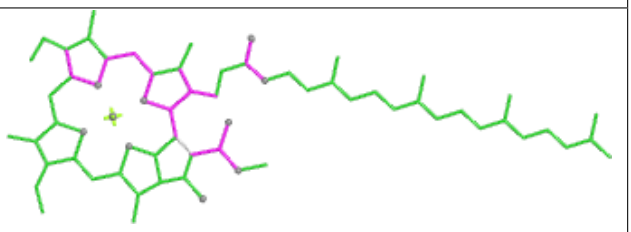


Rings

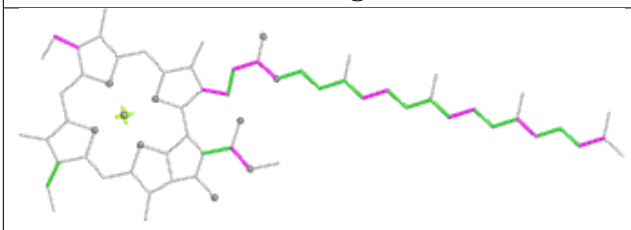
Ligand CLA 20 204



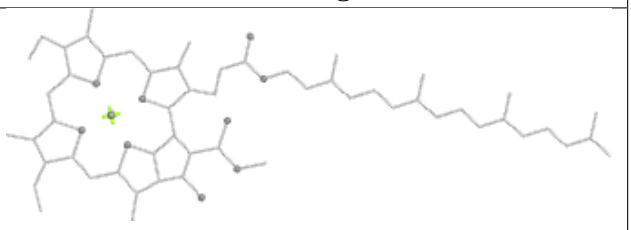
Bond lengths



Bond angles

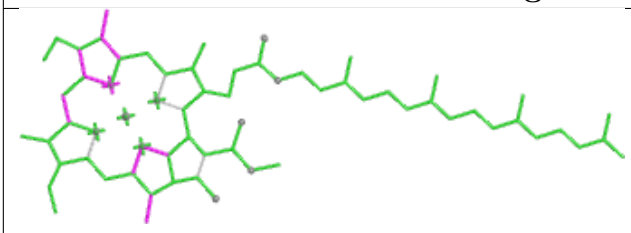


Torsions

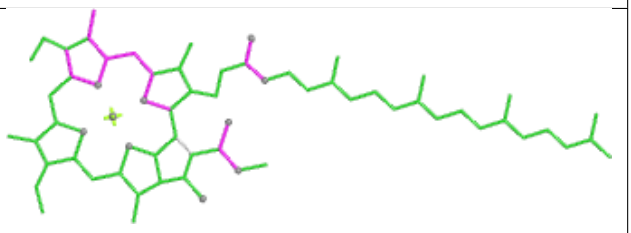


Rings

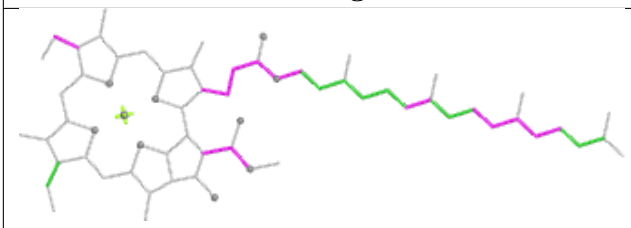
Ligand CLA w 103



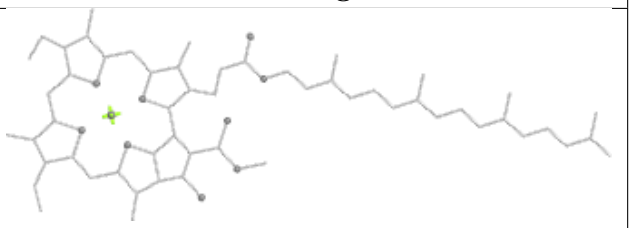
Bond lengths



Bond angles

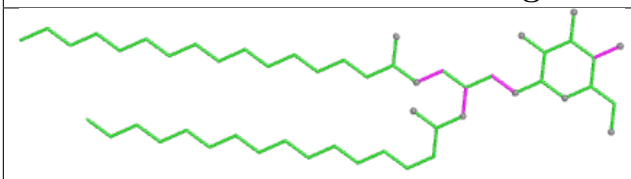


Torsions

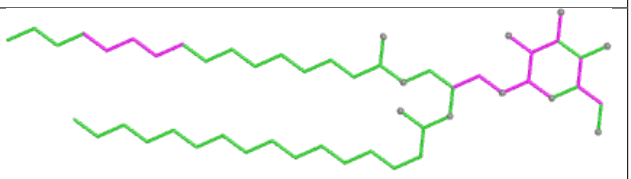


Rings

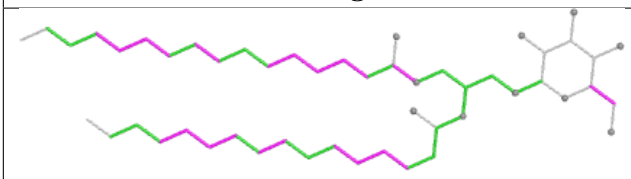
Ligand LMG b 618



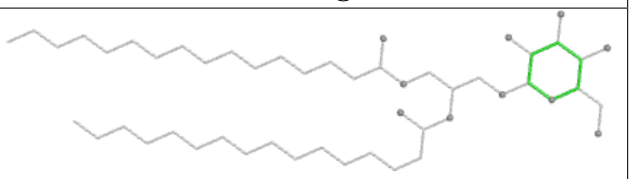
Bond lengths



Bond angles

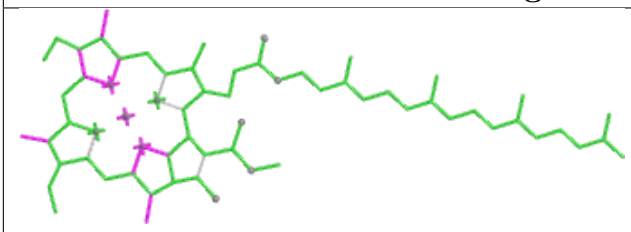


Torsions

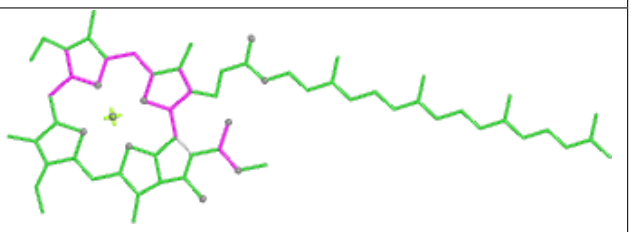


Rings

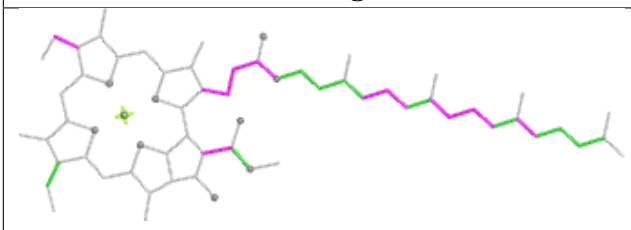
Ligand CLA B 601



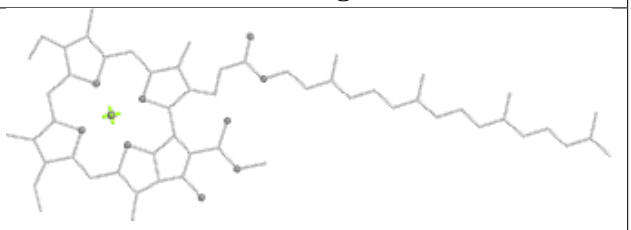
Bond lengths



Bond angles

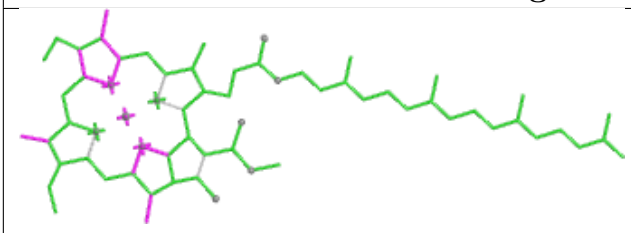


Torsions

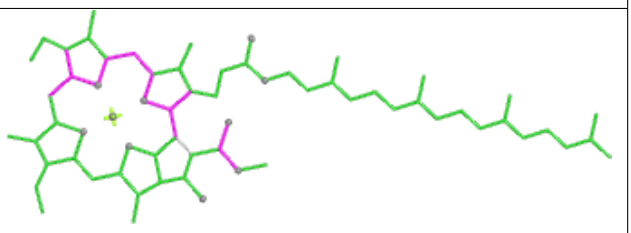


Rings

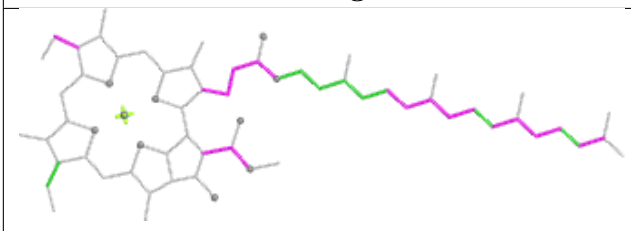
Ligand CLA z 101



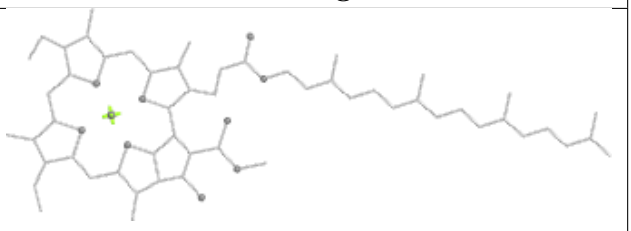
Bond lengths



Bond angles

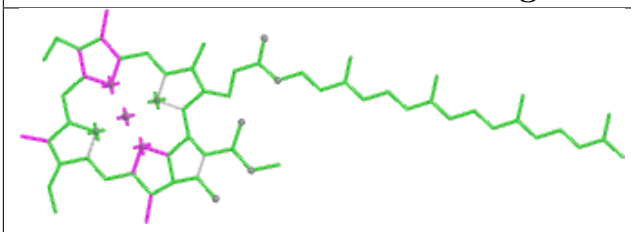


Torsions

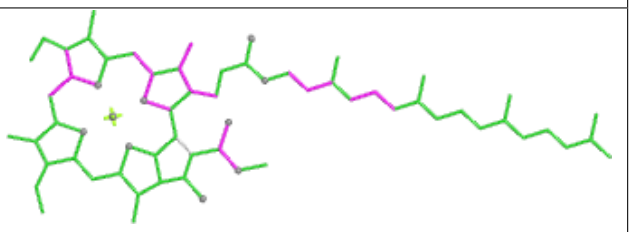


Rings

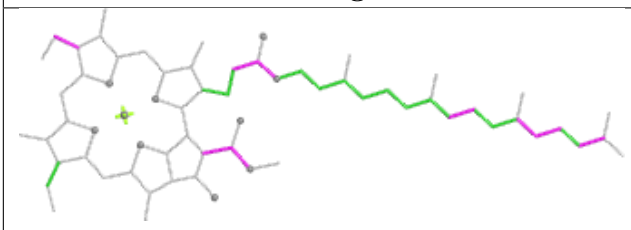
Ligand CLA 17 301



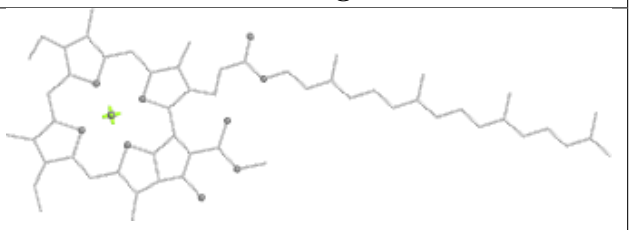
Bond lengths



Bond angles

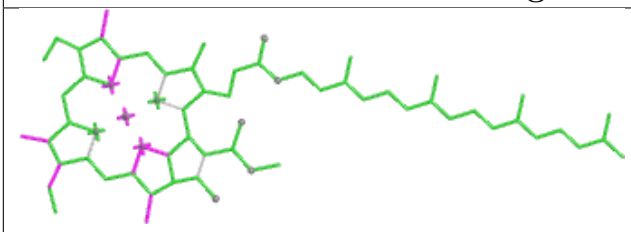


Torsions

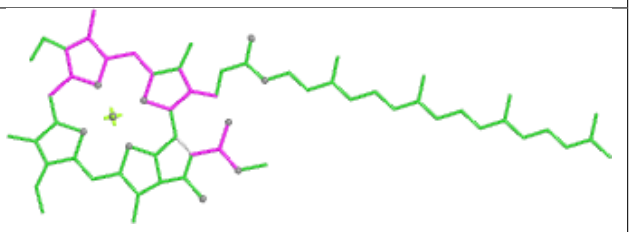


Rings

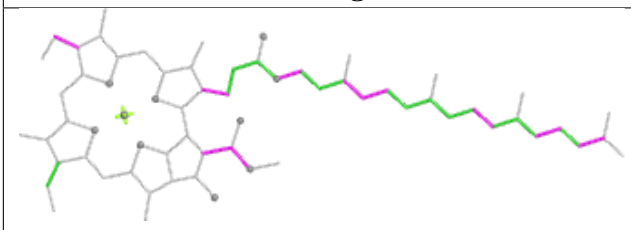
Ligand CLA d 401



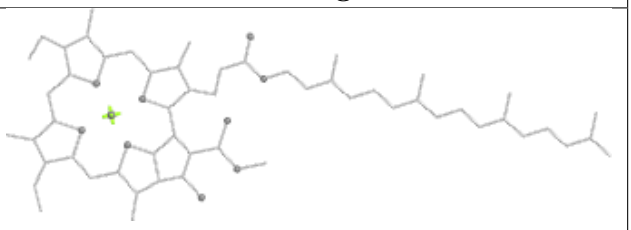
Bond lengths



Bond angles

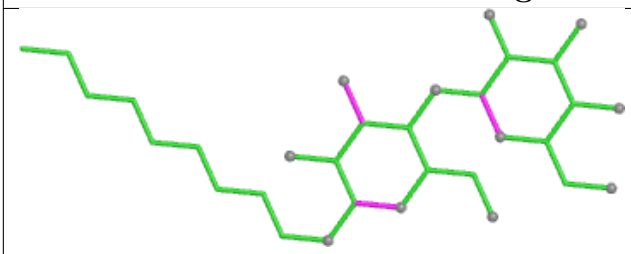


Torsions

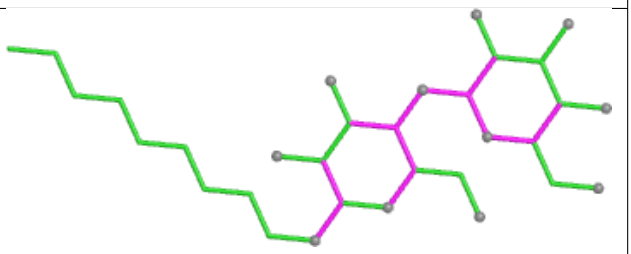


Rings

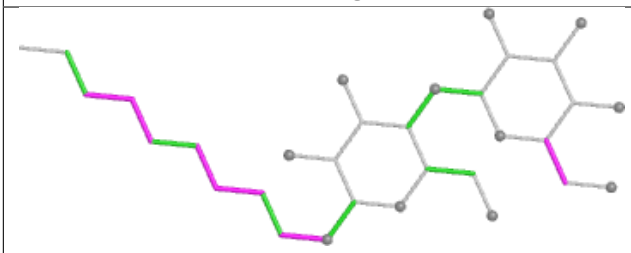
Ligand LMU 12 302



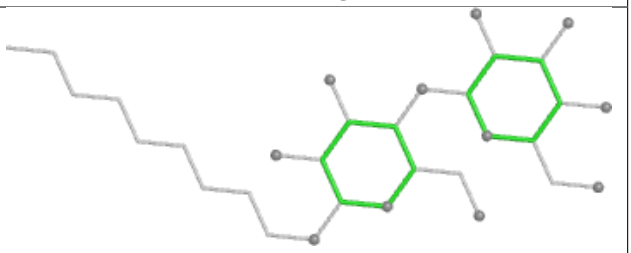
Bond lengths



Bond angles

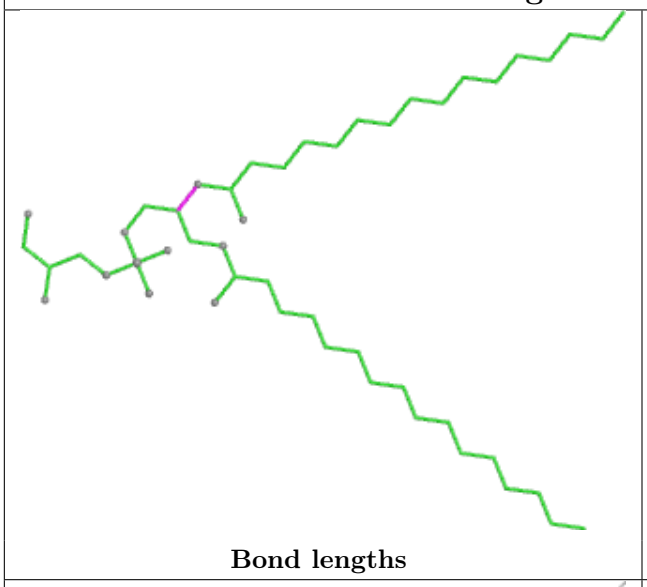


Torsions

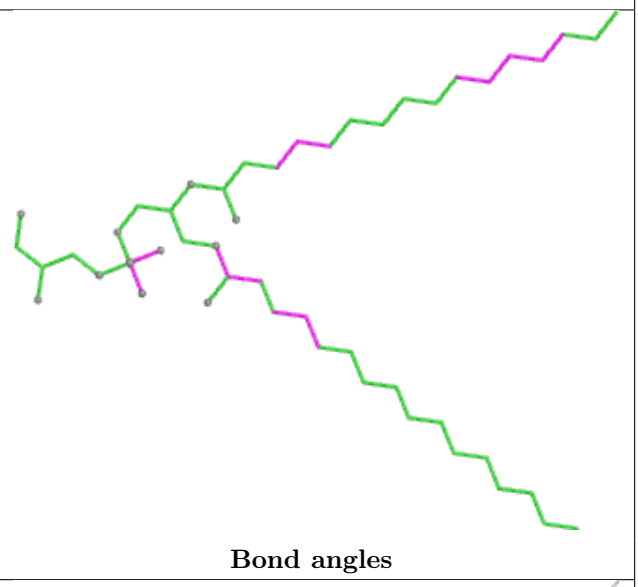


Rings

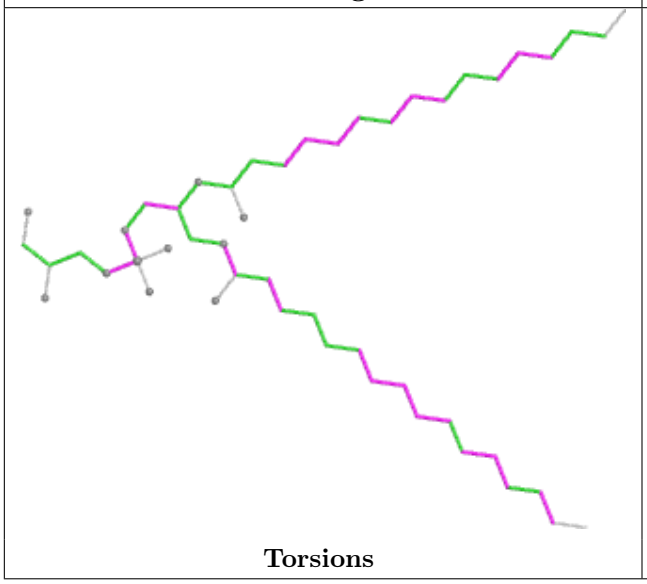
Ligand LHG L 102



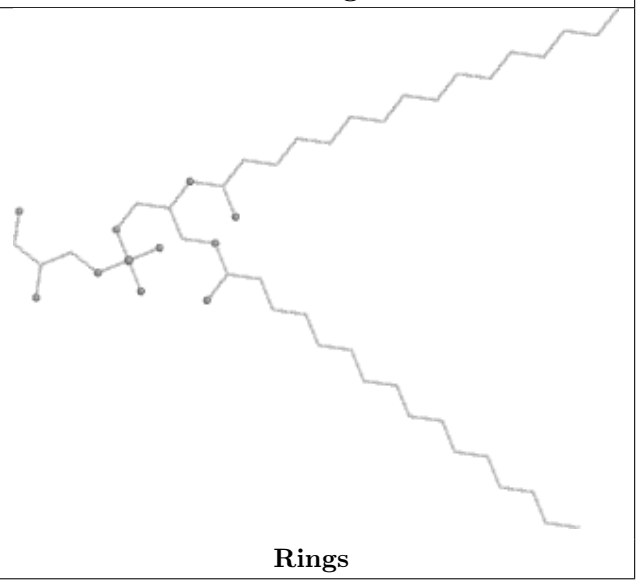
Bond lengths



Bond angles

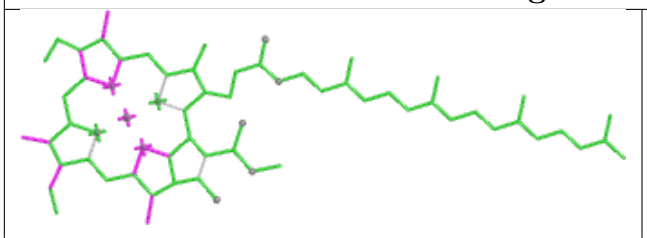


Torsions

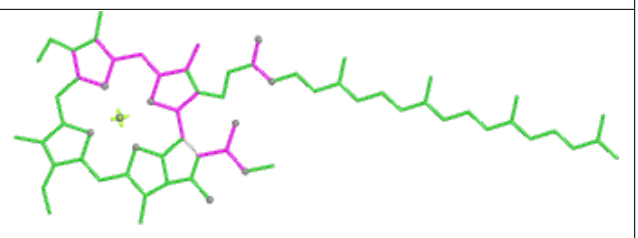


Rings

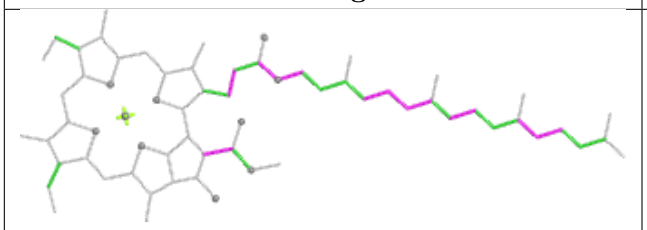
Ligand CLA b 615



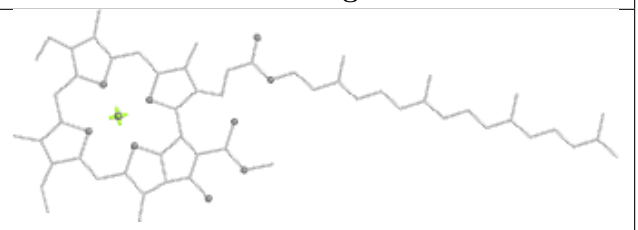
Bond lengths



Bond angles

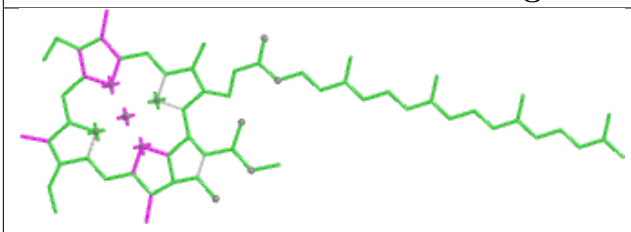


Torsions

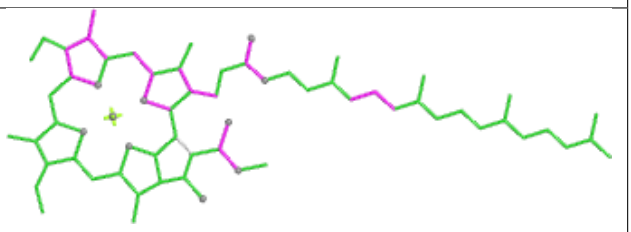


Rings

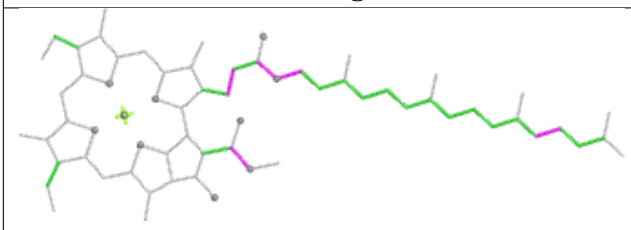
Ligand CLA A 402



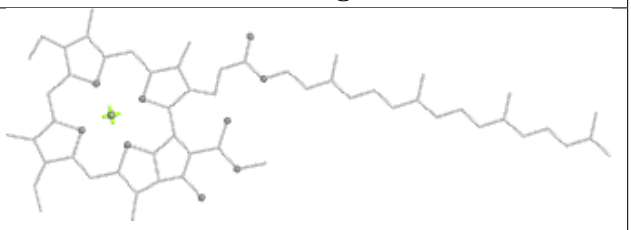
Bond lengths



Bond angles

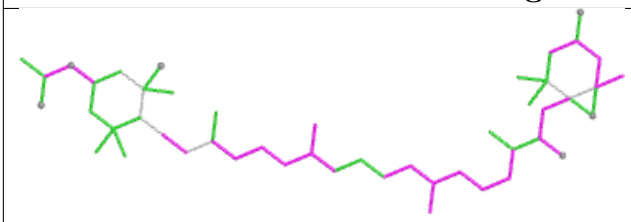


Torsions

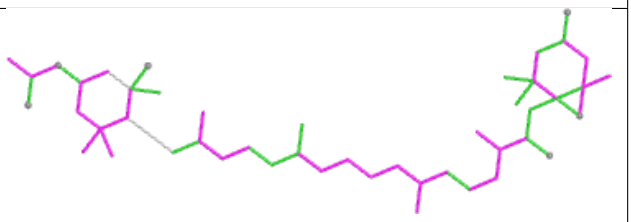


Rings

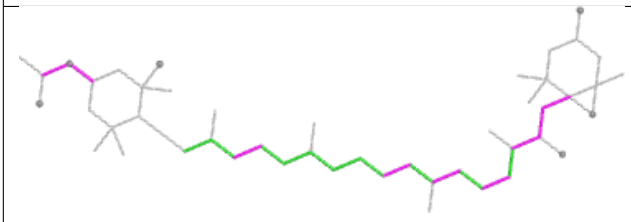
Ligand A86 13 315



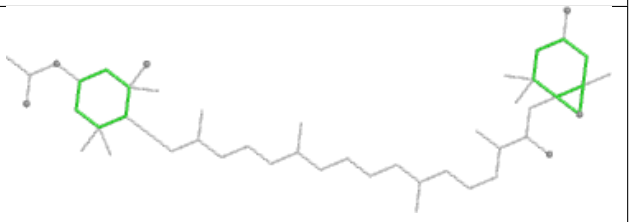
Bond lengths



Bond angles

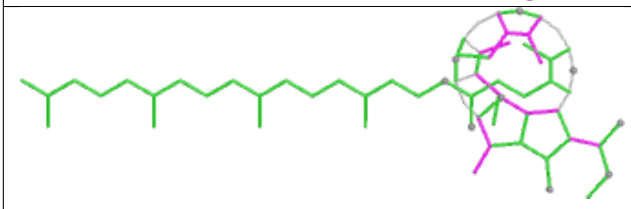


Torsions

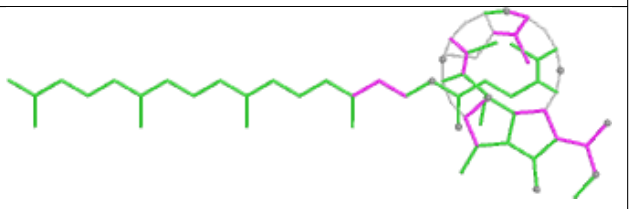


Rings

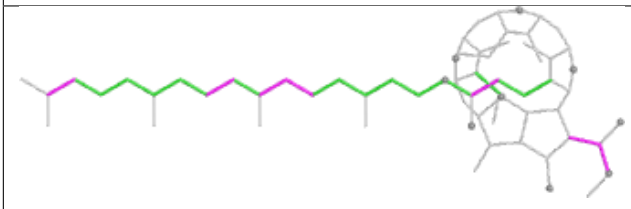
Ligand PHO D 403



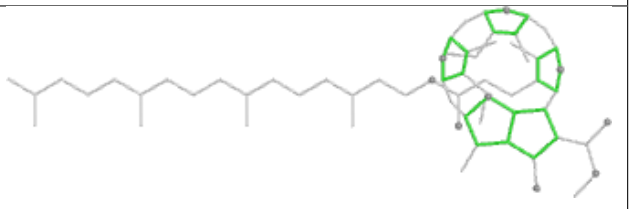
Bond lengths



Bond angles

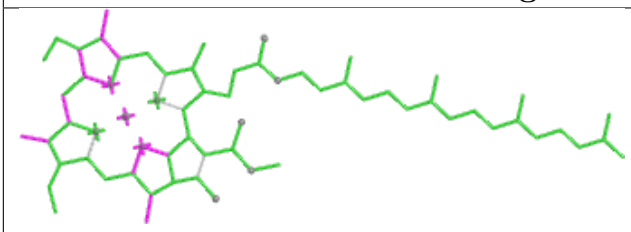


Torsions

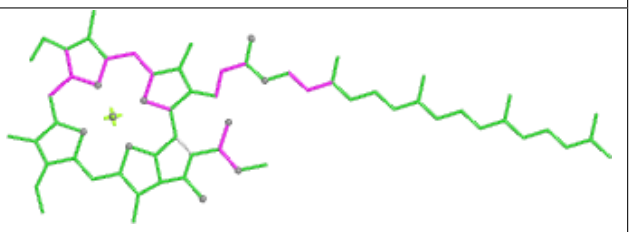


Rings

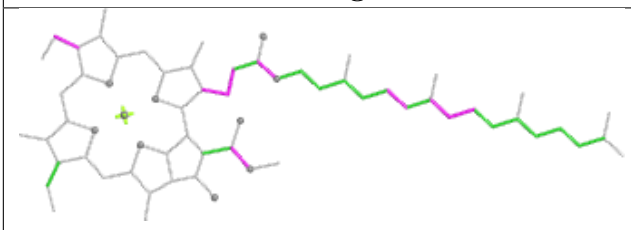
Ligand CLA 12 305



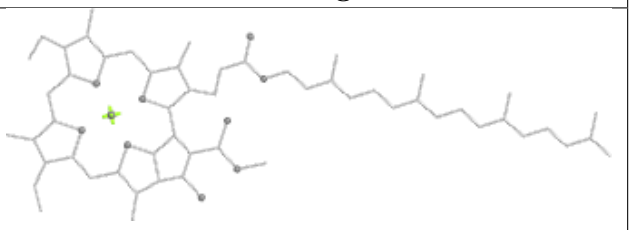
Bond lengths



Bond angles

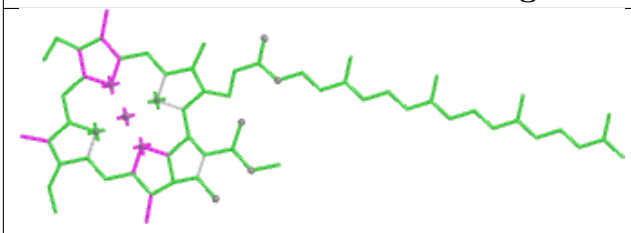


Torsions

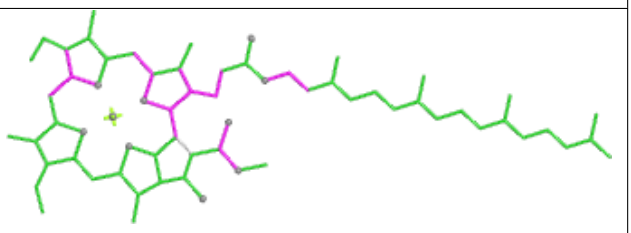


Rings

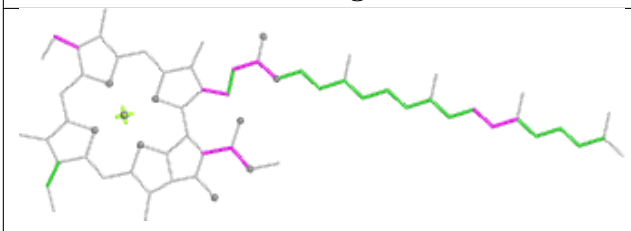
Ligand CLA 14 305



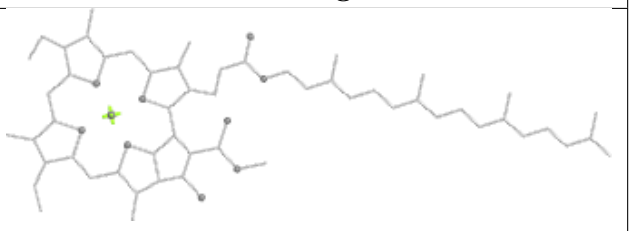
Bond lengths



Bond angles

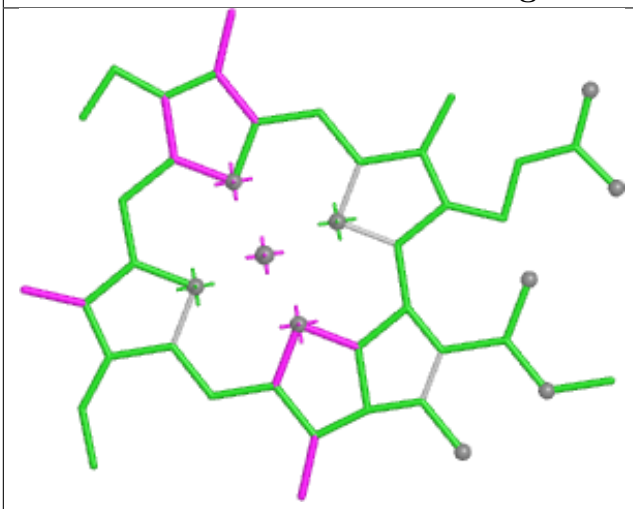


Torsions

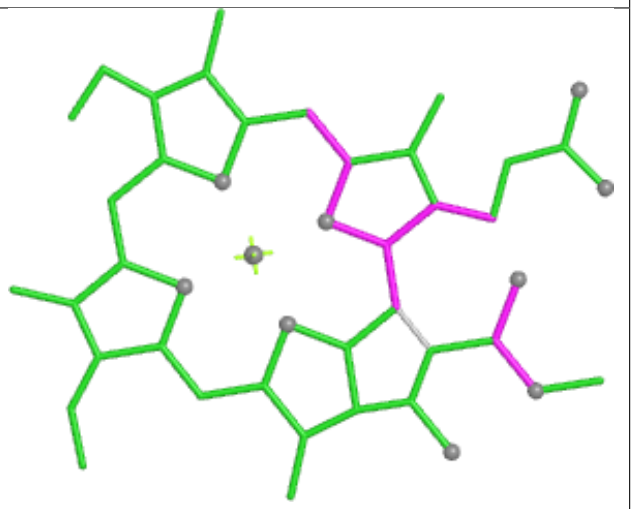


Rings

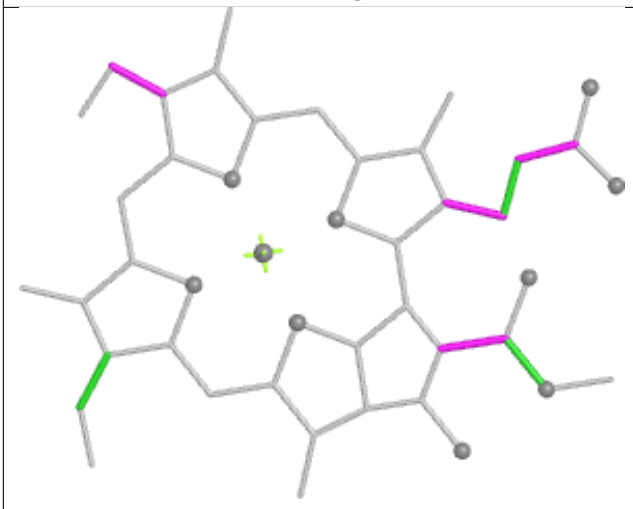
Ligand CLA 14 310



Bond lengths



Bond angles

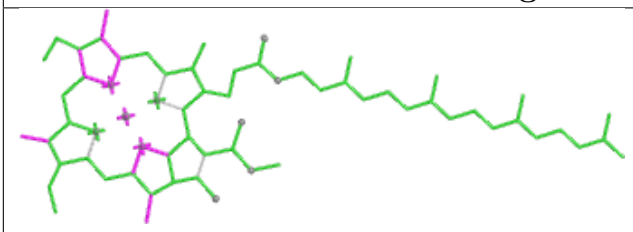


Torsions

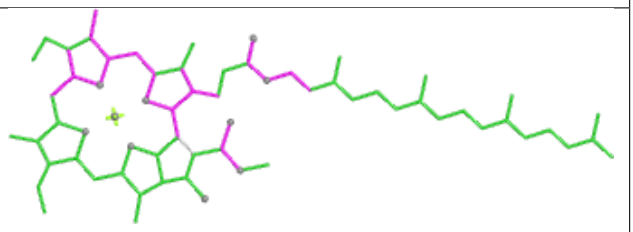


Rings

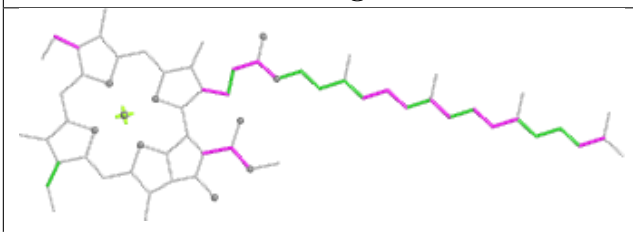
Ligand CLA 17 305



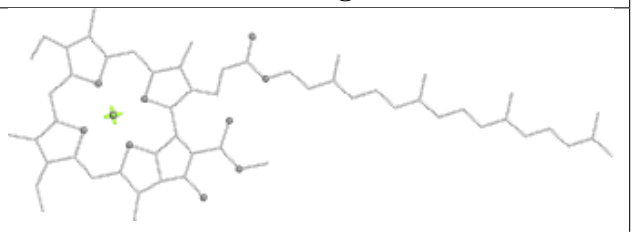
Bond lengths



Bond angles

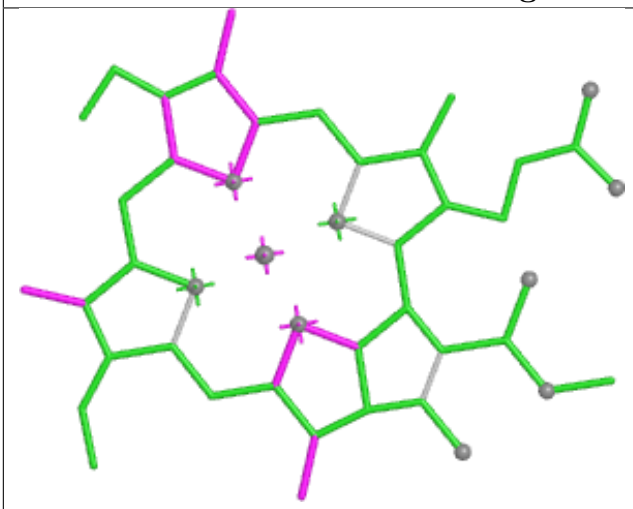


Torsions

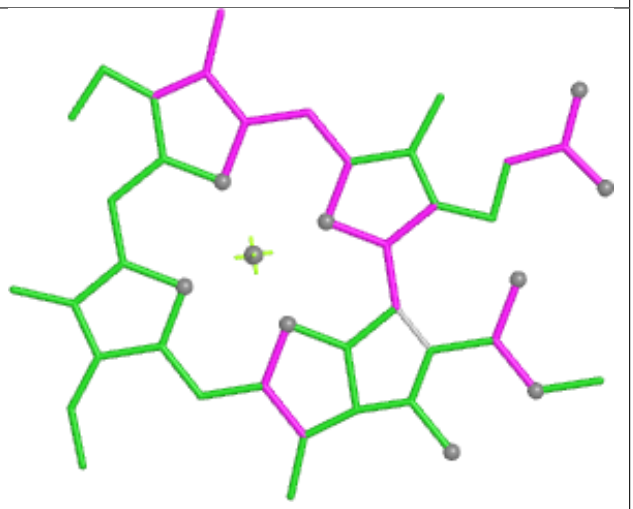


Rings

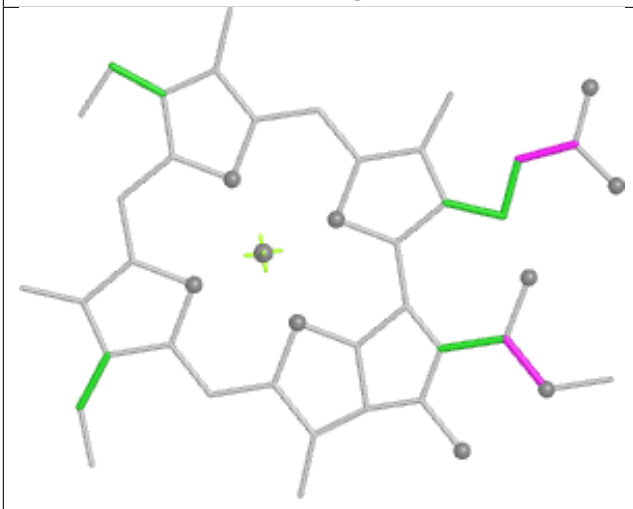
Ligand CLA 19 302



Bond lengths



Bond angles

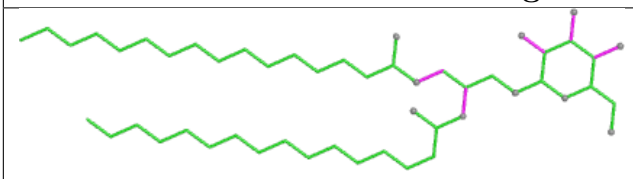


Torsions

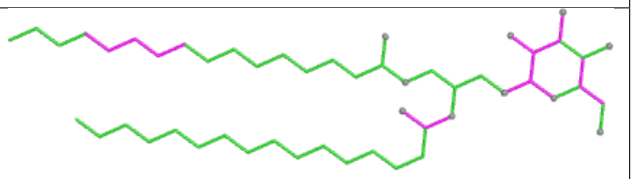


Rings

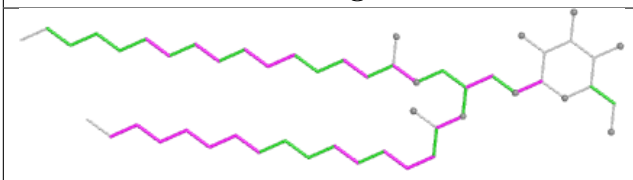
Ligand LMG b 619



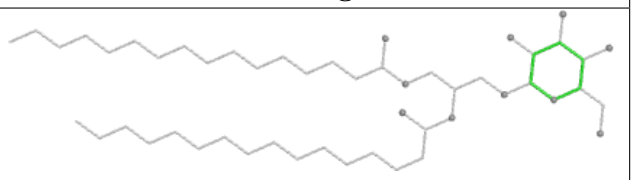
Bond lengths



Bond angles

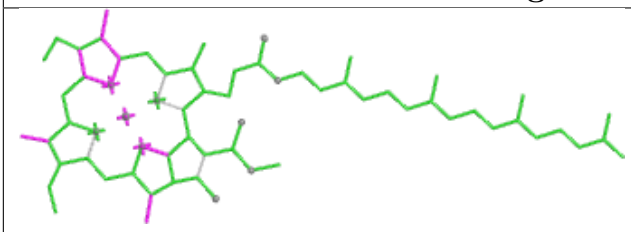


Torsions

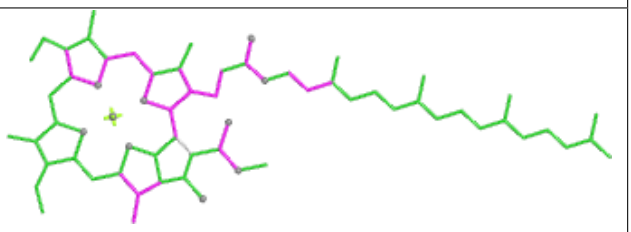


Rings

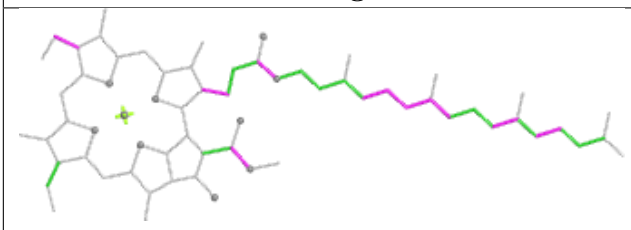
Ligand CLA b 622



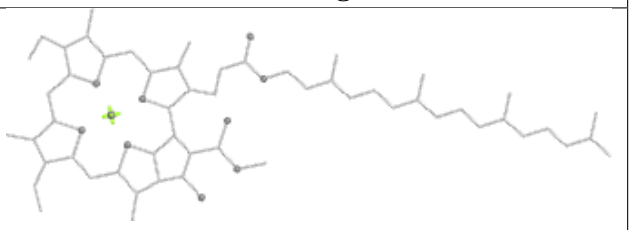
Bond lengths



Bond angles



Torsions

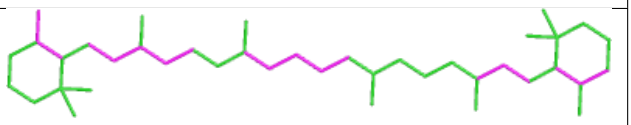


Rings

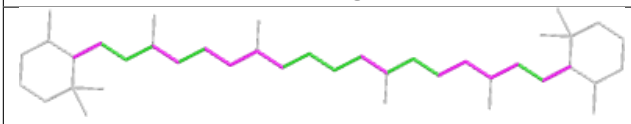
Ligand BCR c 515



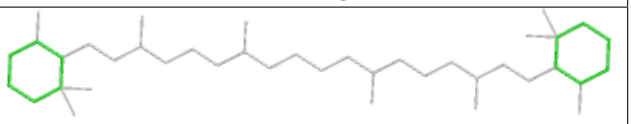
Bond lengths



Bond angles

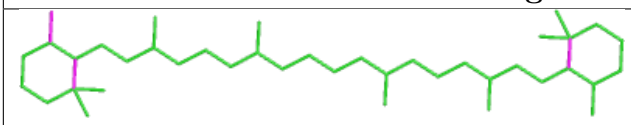


Torsions

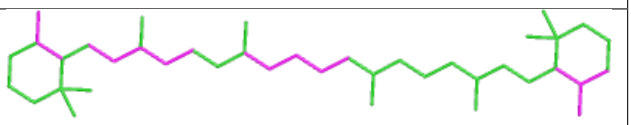


Rings

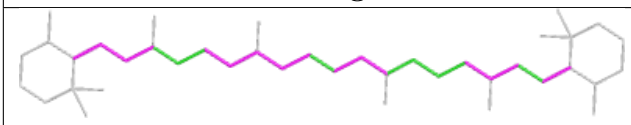
Ligand BCR b 623



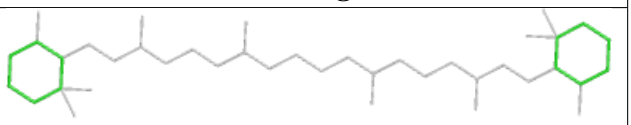
Bond lengths



Bond angles

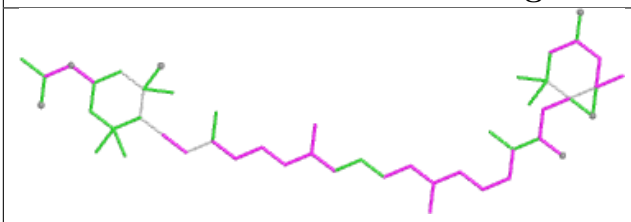


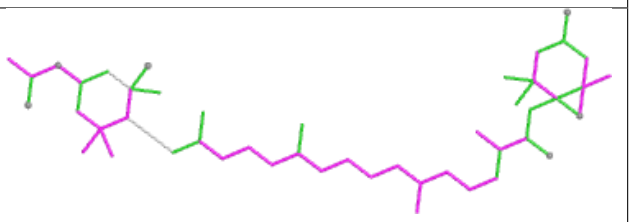
Torsions

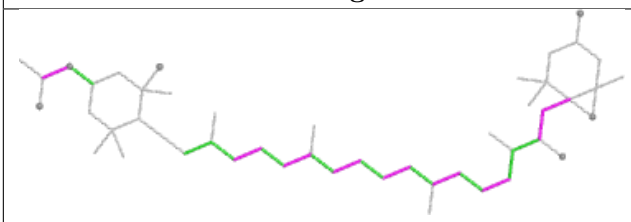


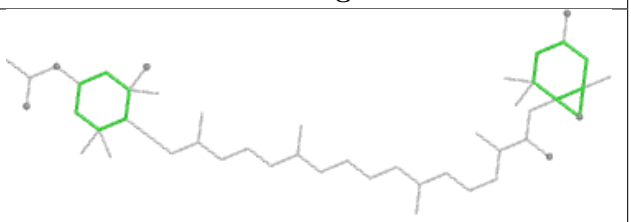
Rings

Ligand A86 20 213

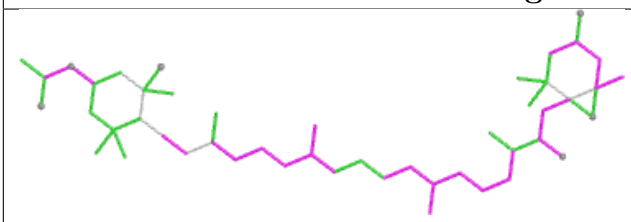

Bond lengths

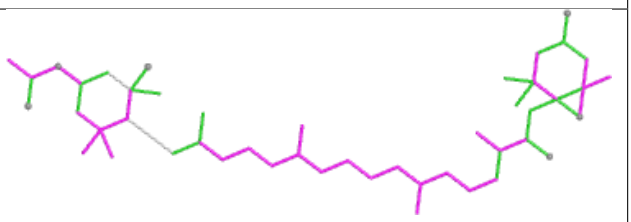

Bond angles

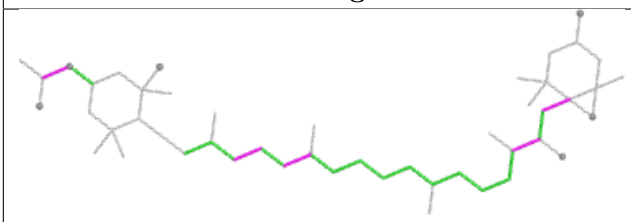

Torsions

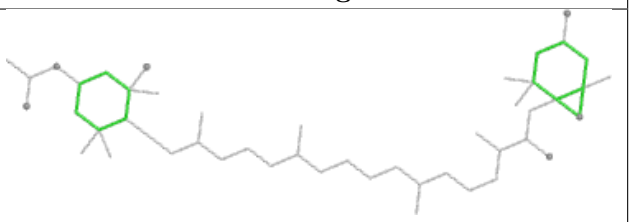

Rings

Ligand A86 14 315

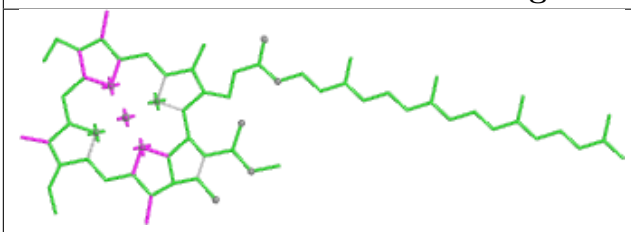

Bond lengths

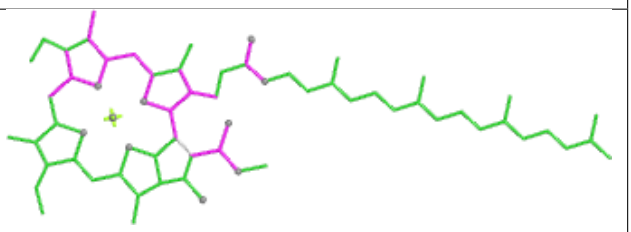

Bond angles

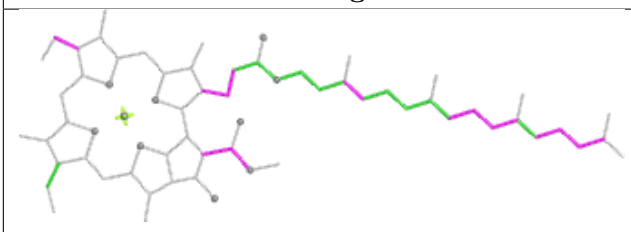

Torsions

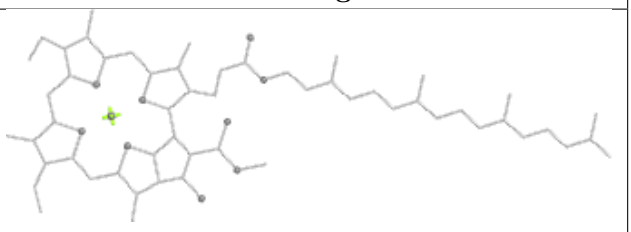

Rings

Ligand CLA c 507

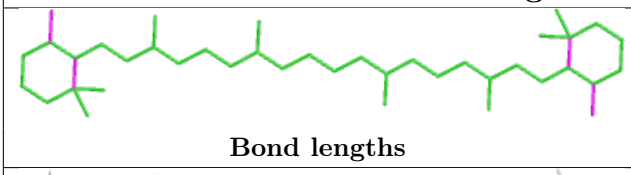

Bond lengths


Bond angles

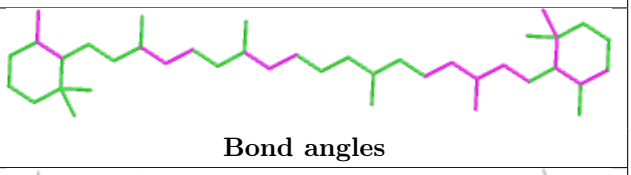

Torsions


Rings

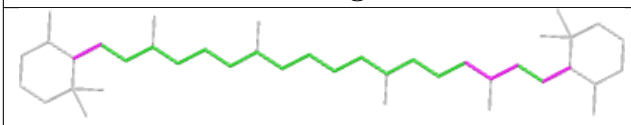
Ligand BCR h 101



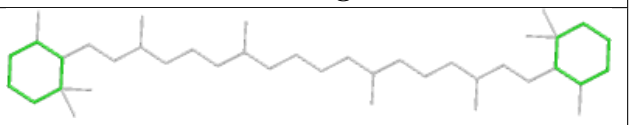
Bond lengths



Bond angles

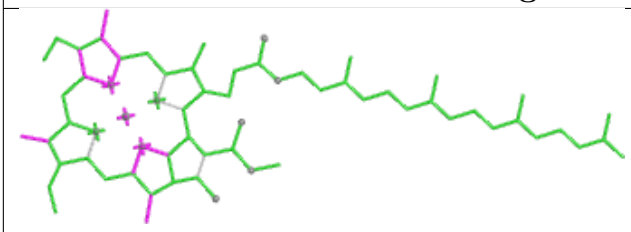


Torsions

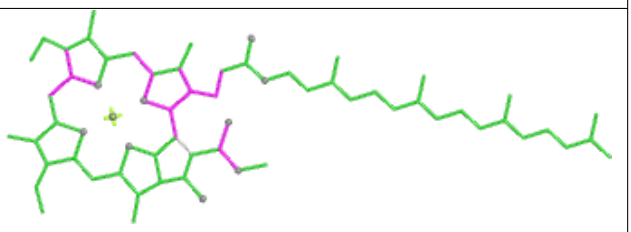


Rings

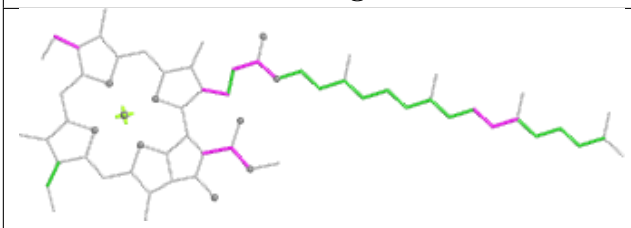
Ligand CLA 13 304



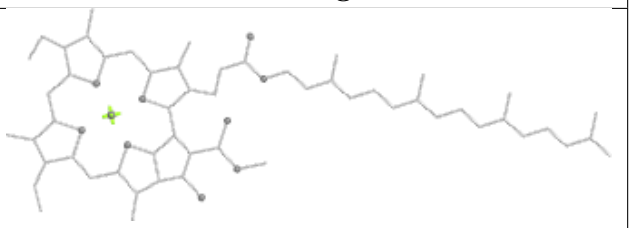
Bond lengths



Bond angles

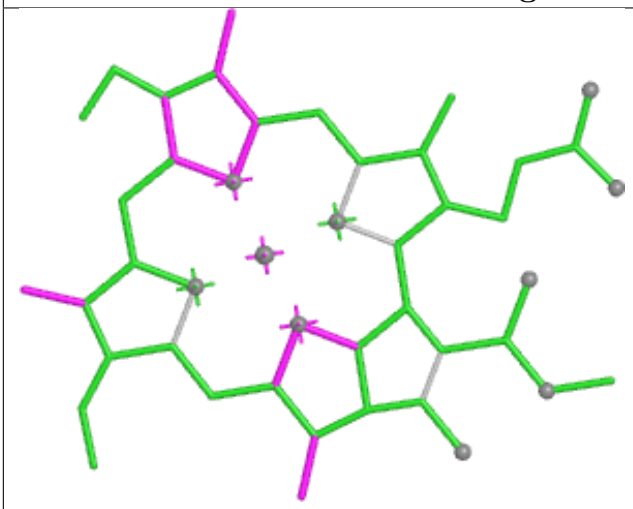


Torsions

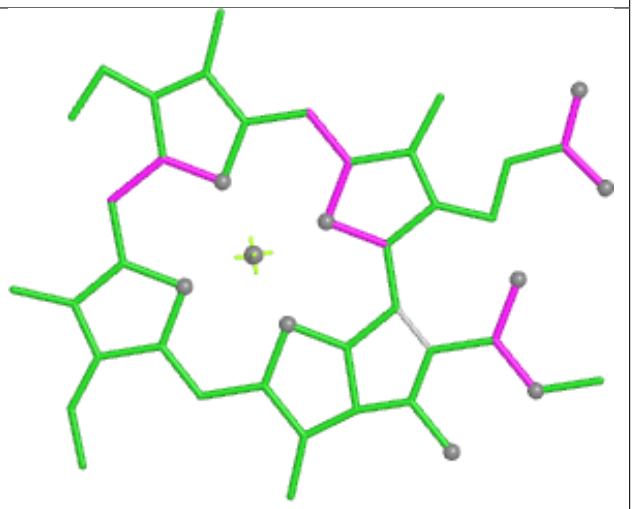


Rings

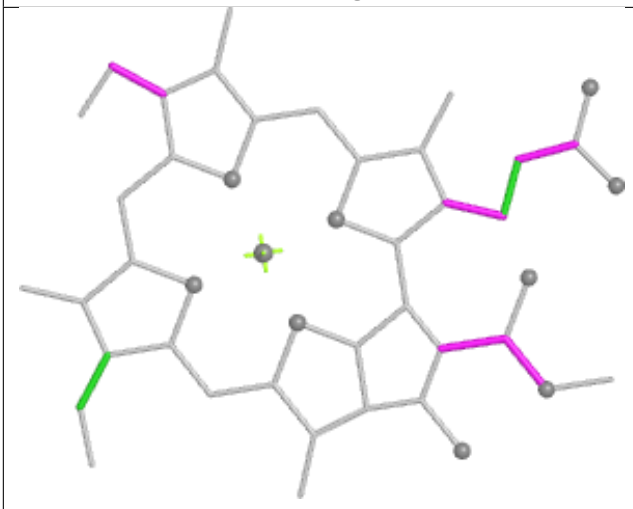
Ligand CLA 19 306



Bond lengths



Bond angles

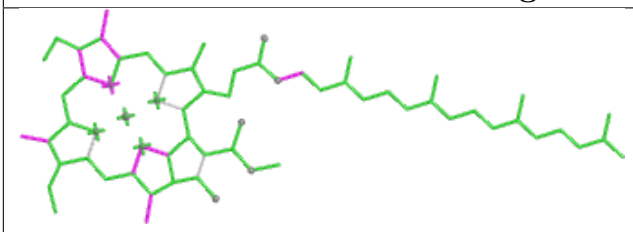


Torsions

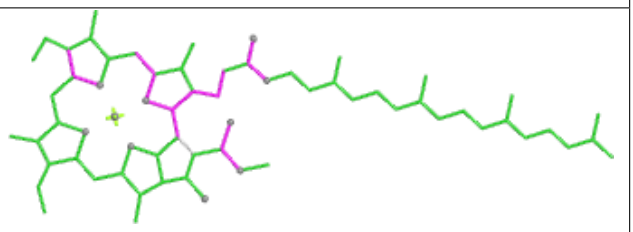


Rings

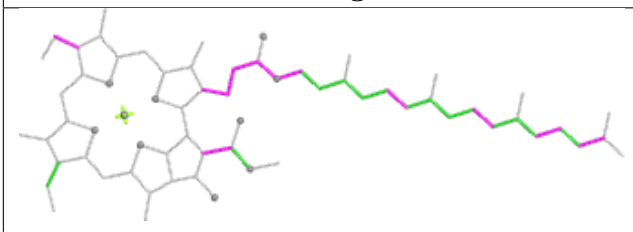
Ligand CLA 21 306



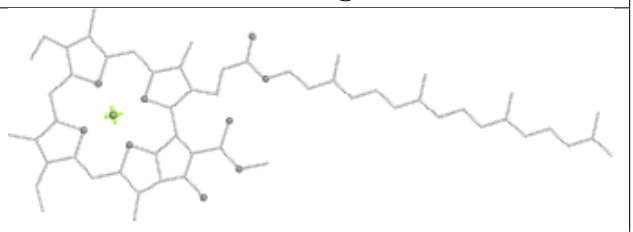
Bond lengths



Bond angles

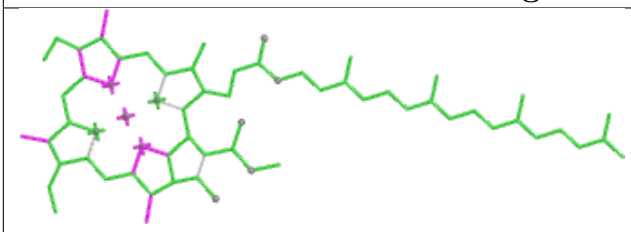


Torsions

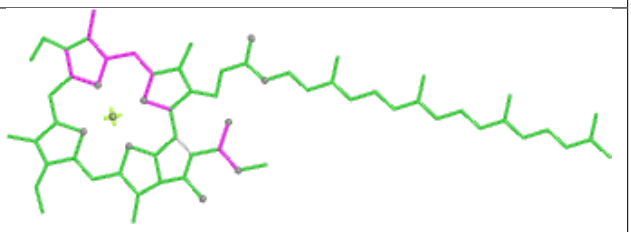


Rings

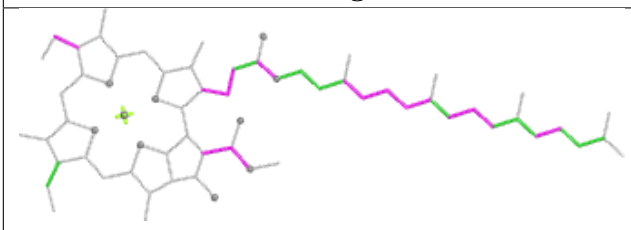
Ligand CLA m 101



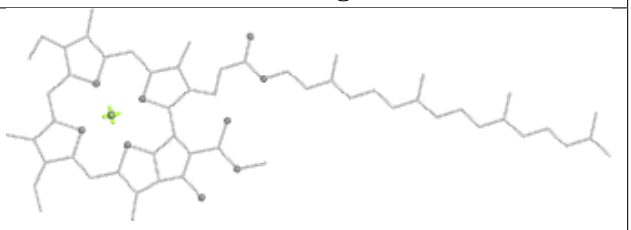
Bond lengths



Bond angles

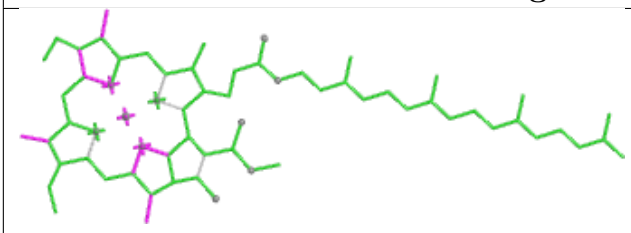


Torsions

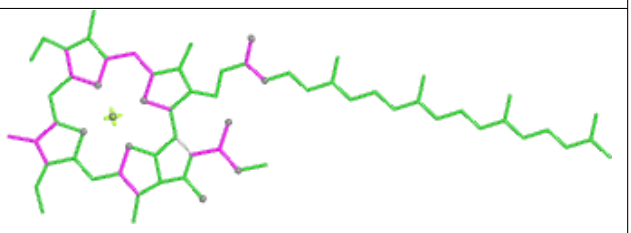


Rings

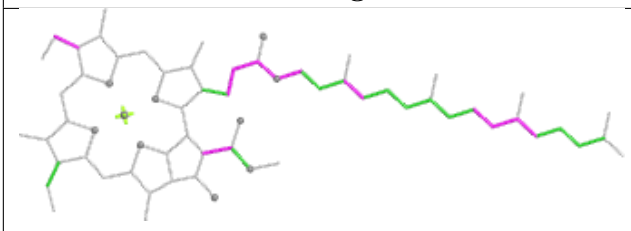
Ligand CLA c 506



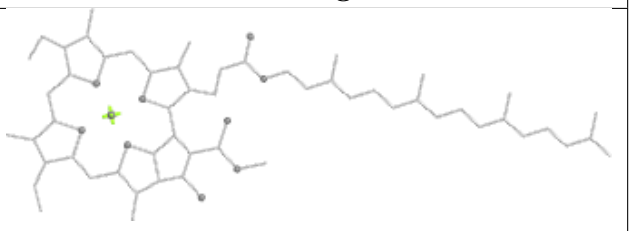
Bond lengths



Bond angles

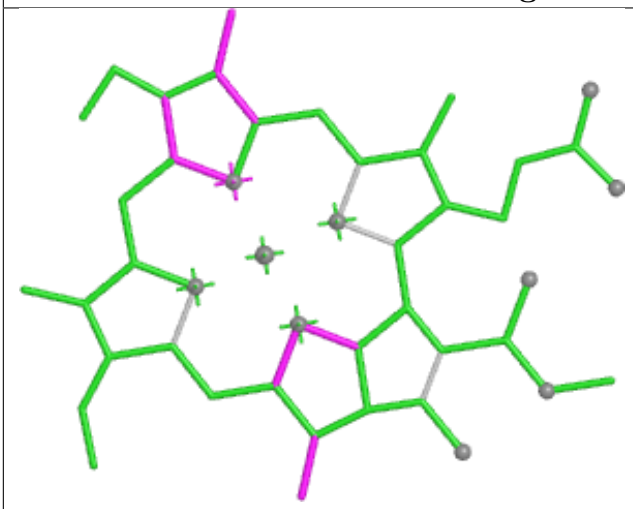


Torsions

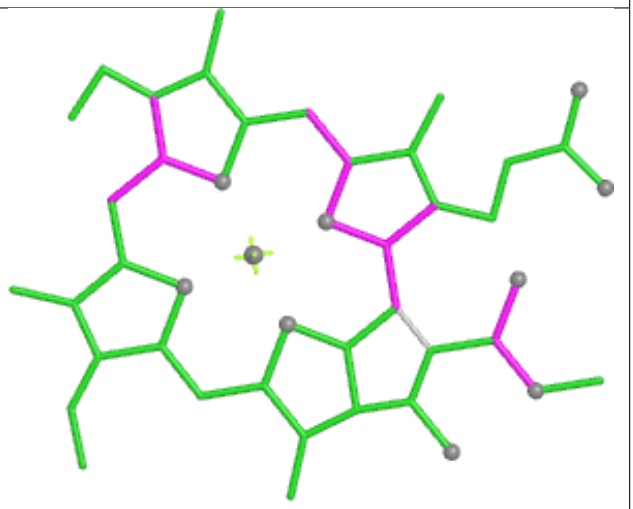


Rings

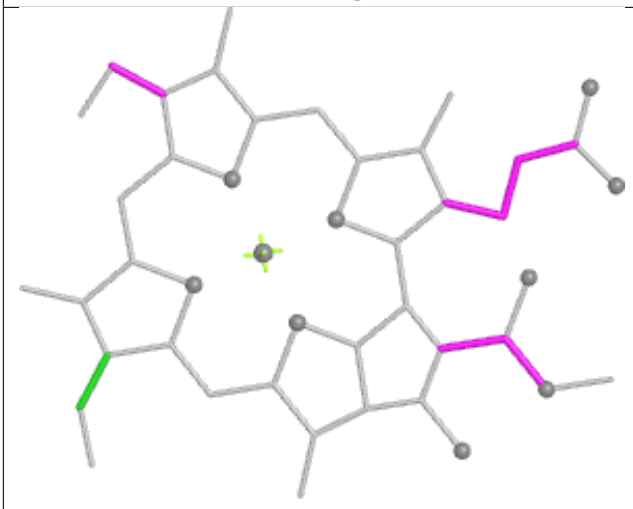
Ligand CLA 21 308



Bond lengths



Bond angles

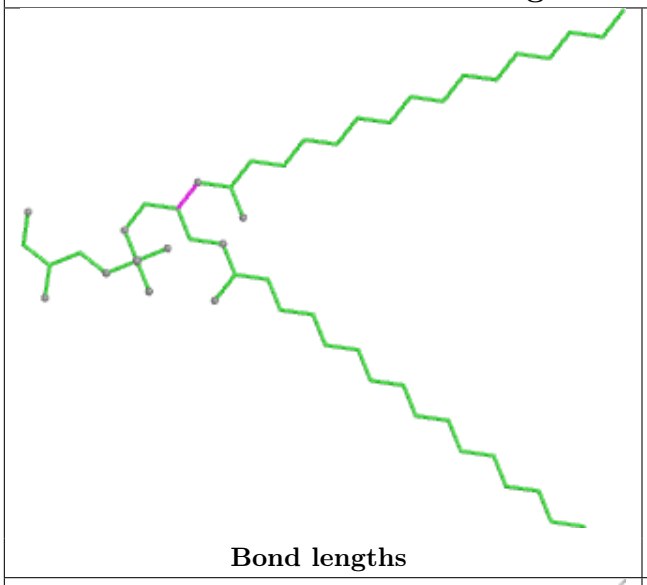


Torsions

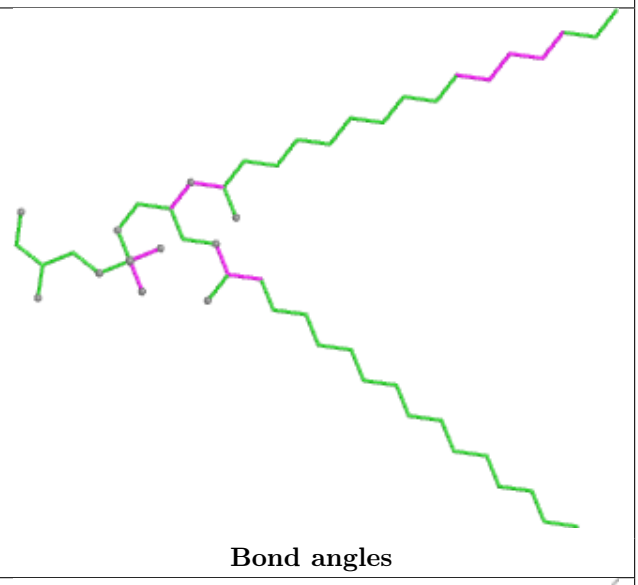


Rings

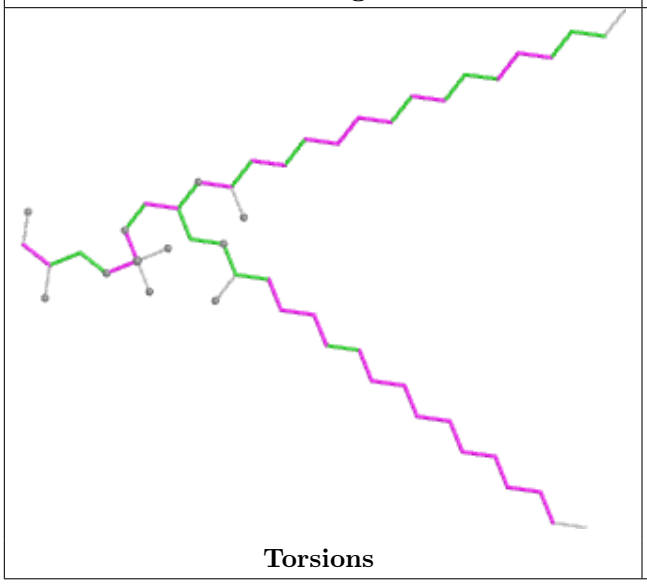
Ligand LHG d 409



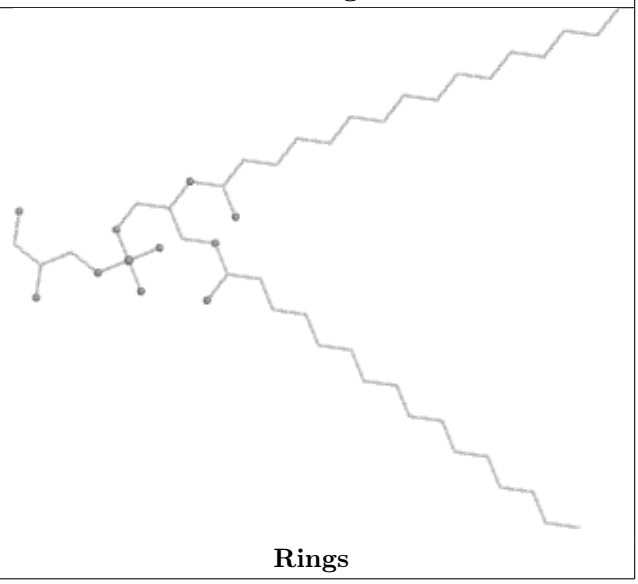
Bond lengths



Bond angles

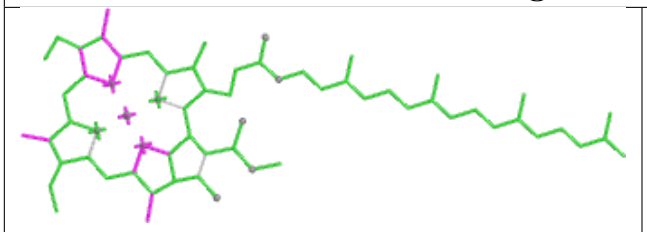


Torsions

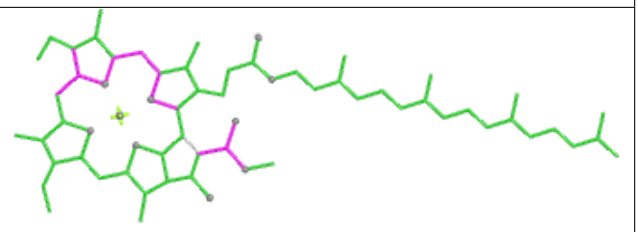


Rings

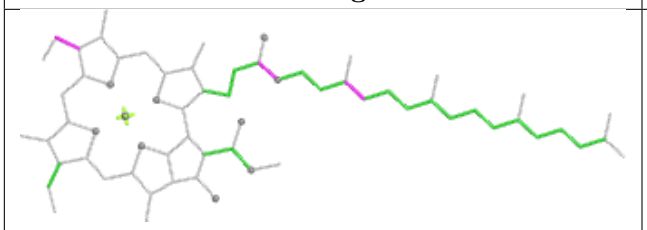
Ligand CLA d 407



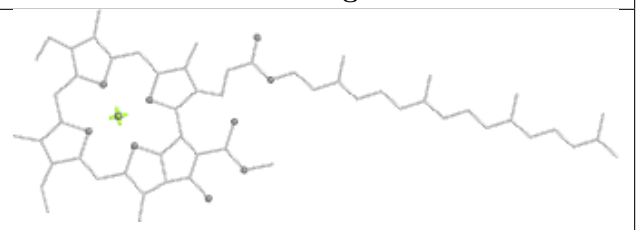
Bond lengths



Bond angles

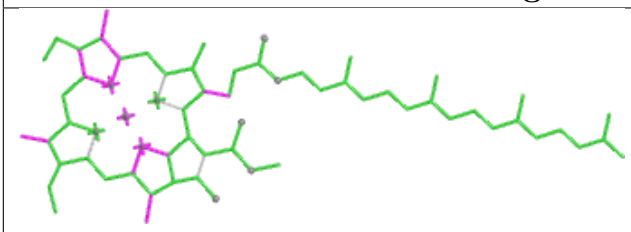


Torsions

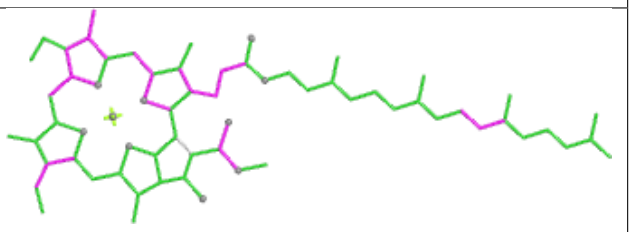


Rings

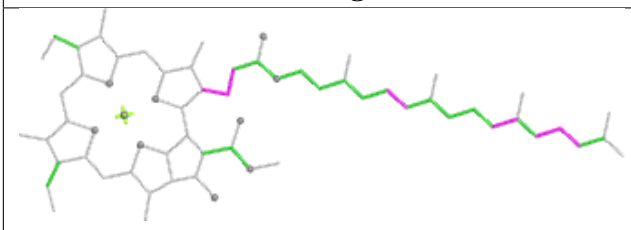
Ligand CLA D 405



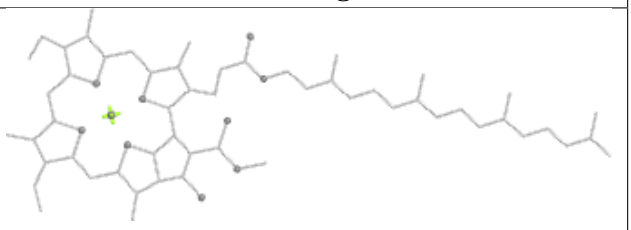
Bond lengths



Bond angles

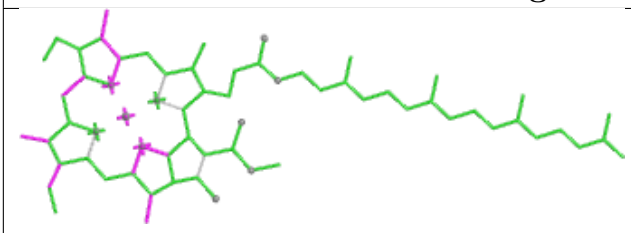


Torsions

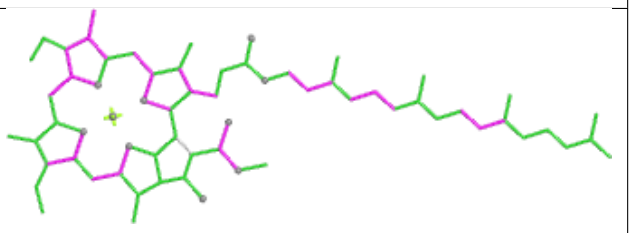


Rings

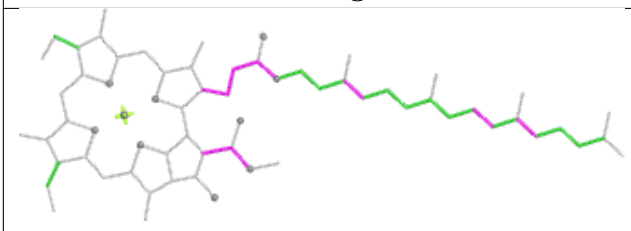
Ligand CLA c 502



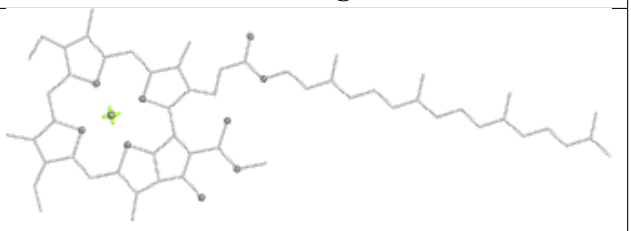
Bond lengths



Bond angles

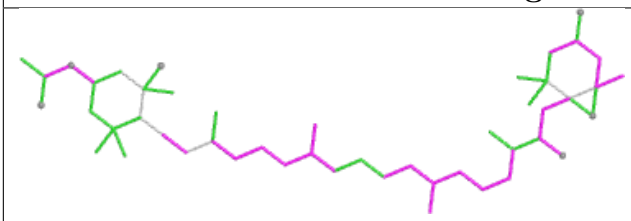


Torsions

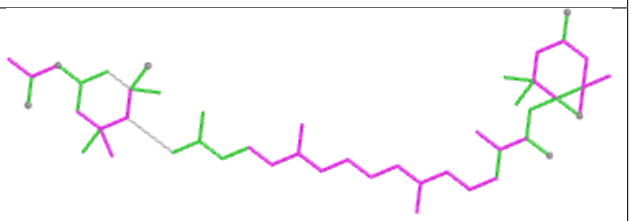


Rings

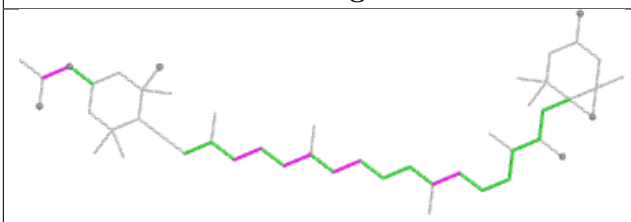
Ligand A86 14 301



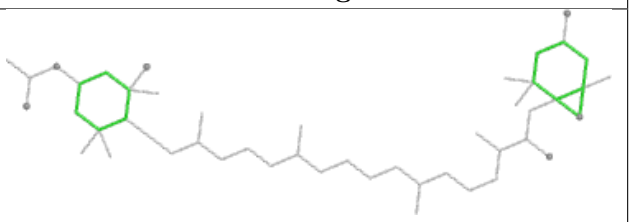
Bond lengths



Bond angles

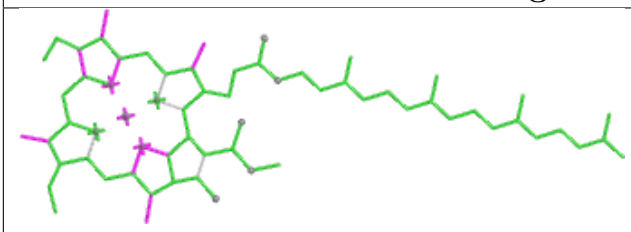


Torsions

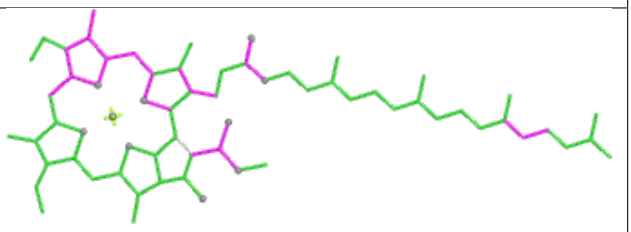


Rings

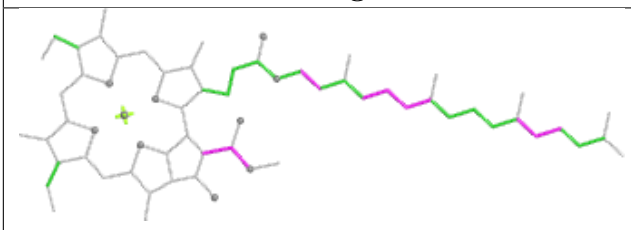
Ligand CLA c 510



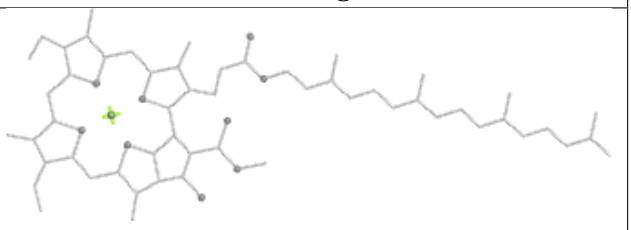
Bond lengths



Bond angles

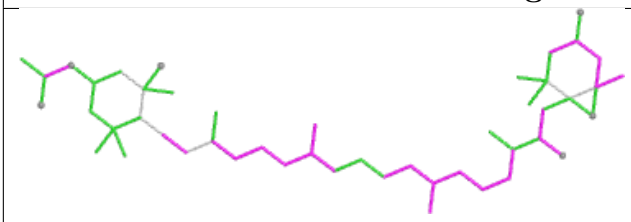


Torsions

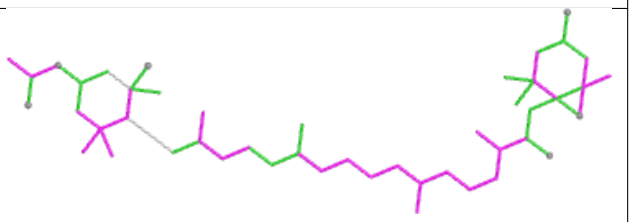


Rings

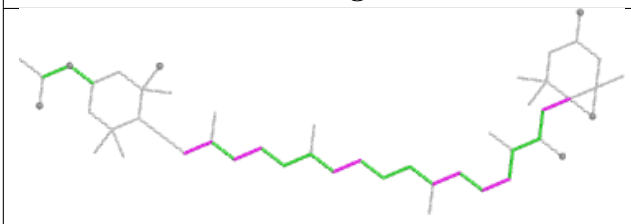
Ligand A86 19 312



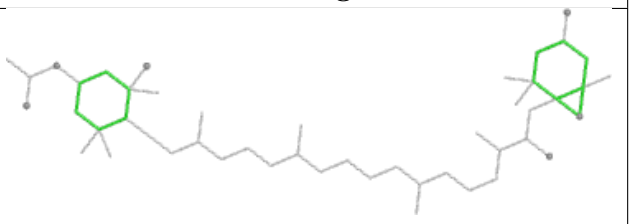
Bond lengths



Bond angles

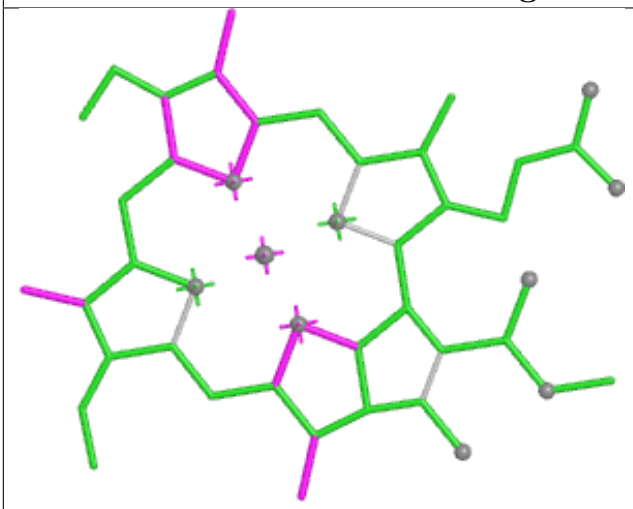


Torsions

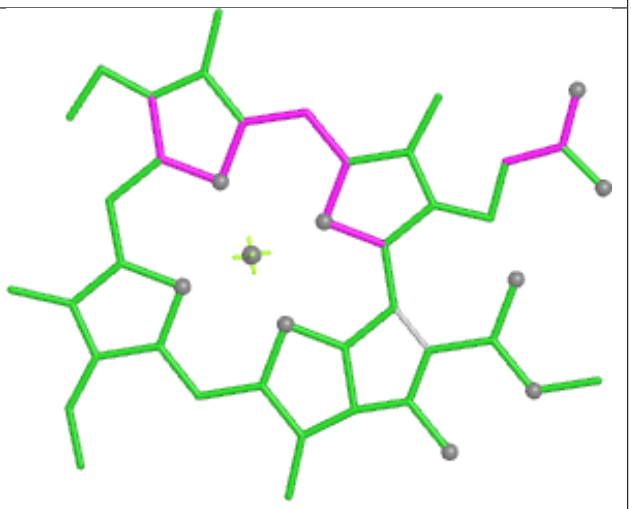


Rings

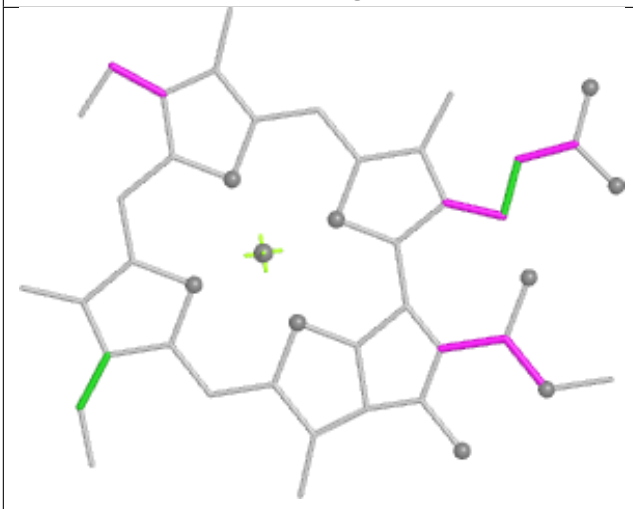
Ligand CLA 19 305



Bond lengths



Bond angles

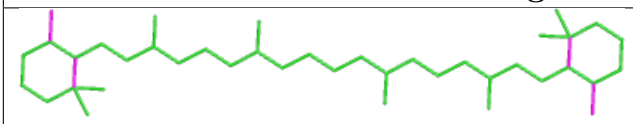


Torsions

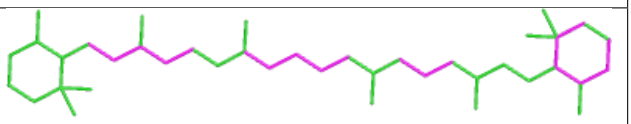


Rings

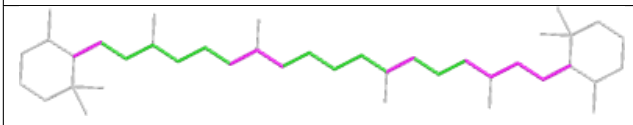
Ligand BCR c 516



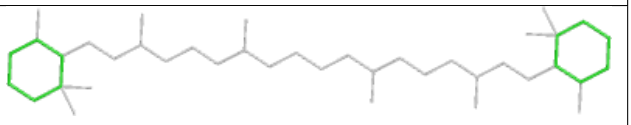
Bond lengths



Bond angles

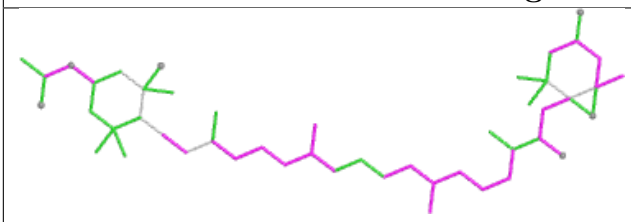


Torsions

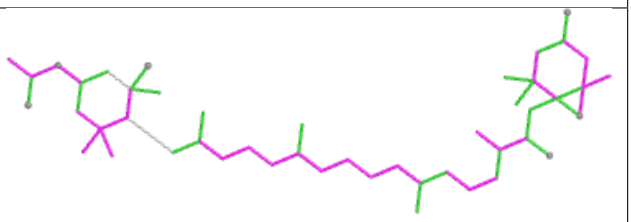


Rings

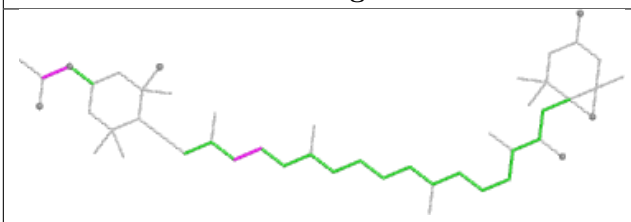
Ligand A86 11 311



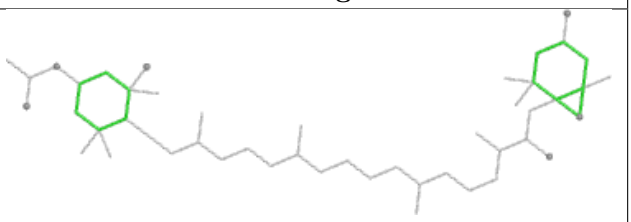
Bond lengths



Bond angles



Torsions

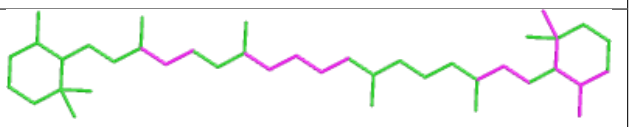


Rings

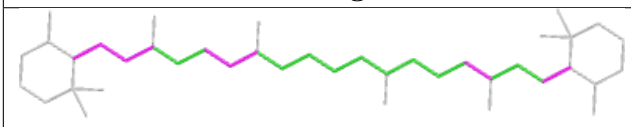
Ligand BCR b 616



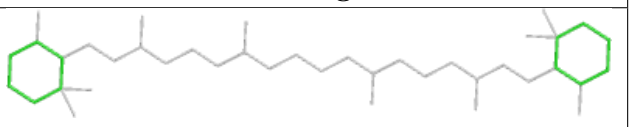
Bond lengths



Bond angles

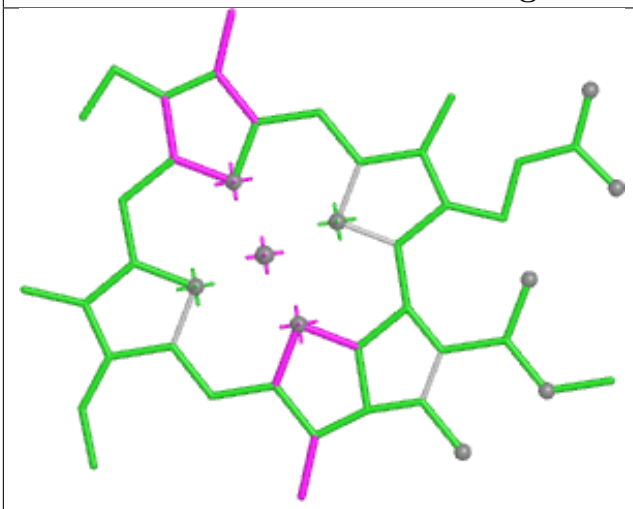


Torsions

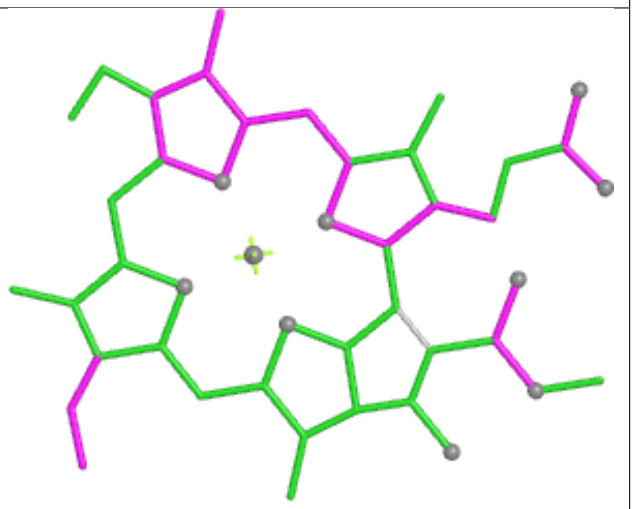


Rings

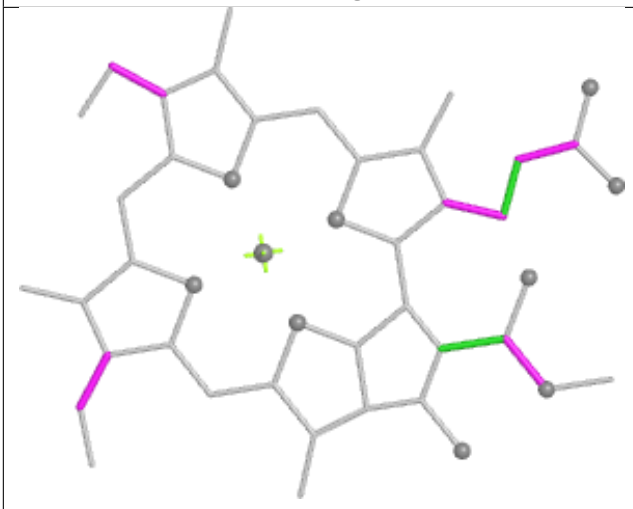
Ligand CLA 19 309



Bond lengths



Bond angles

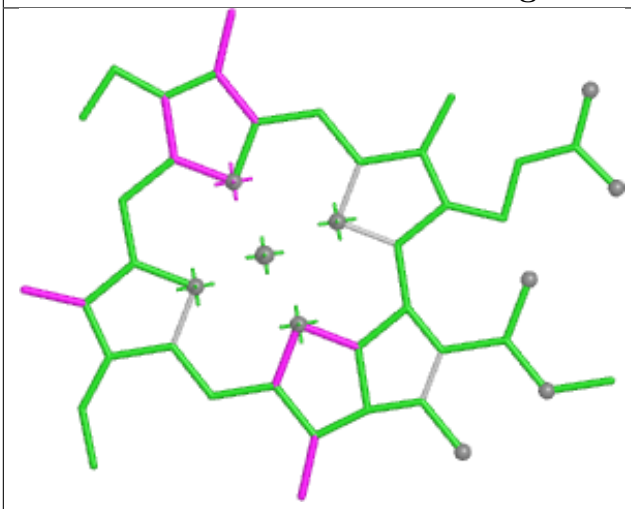


Torsions

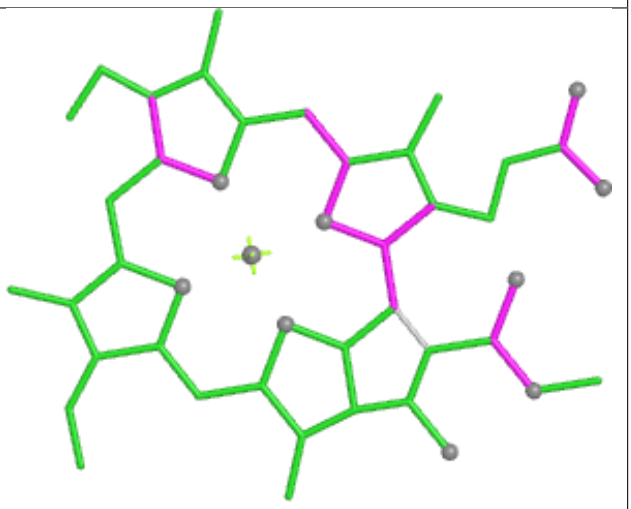


Rings

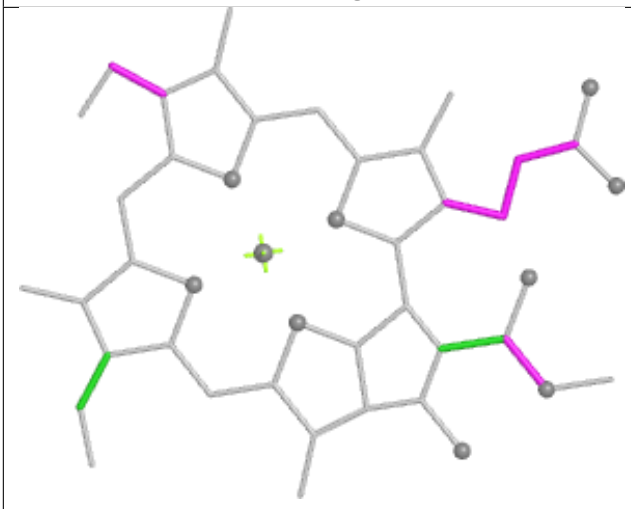
Ligand CLA 16 306



Bond lengths



Bond angles

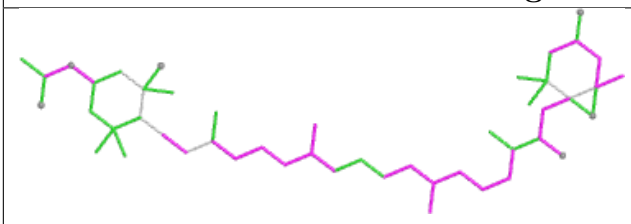


Torsions

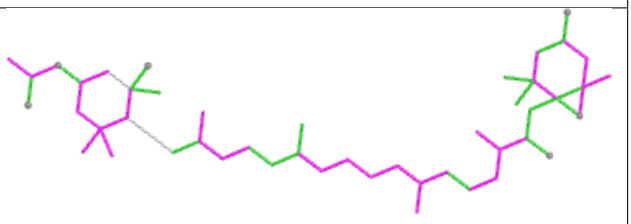


Rings

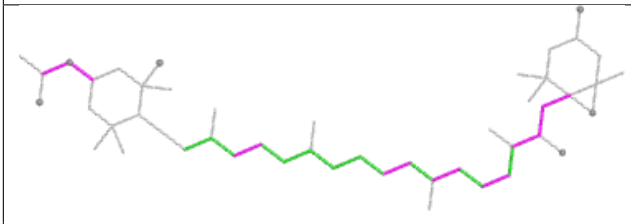
Ligand A86 18 302



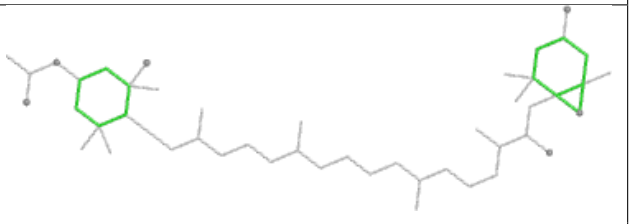
Bond lengths



Bond angles

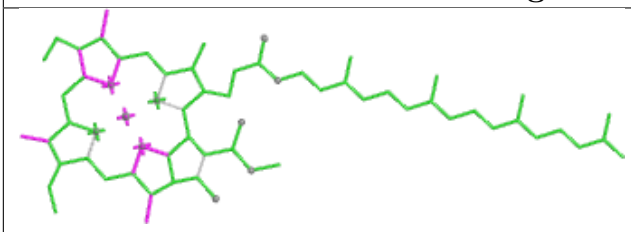


Torsions

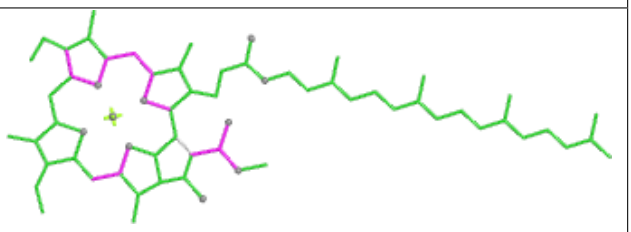


Rings

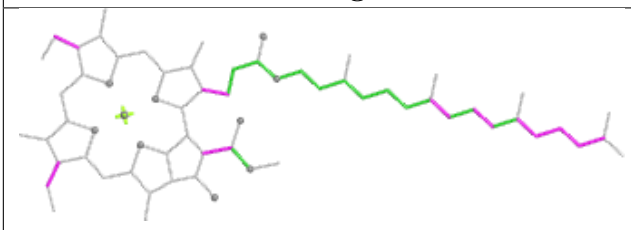
Ligand CLA d 402



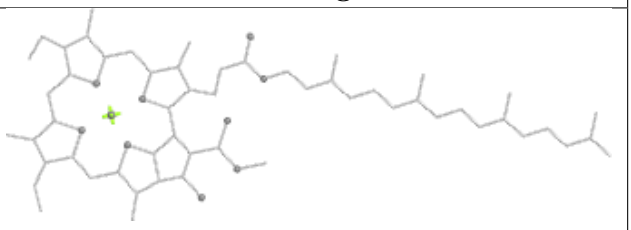
Bond lengths



Bond angles

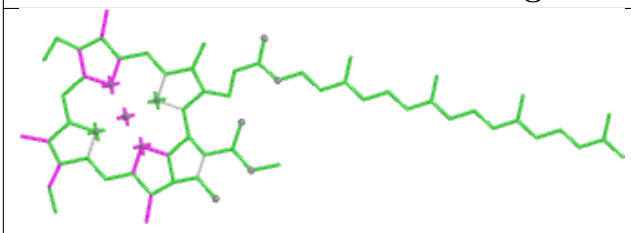


Torsions

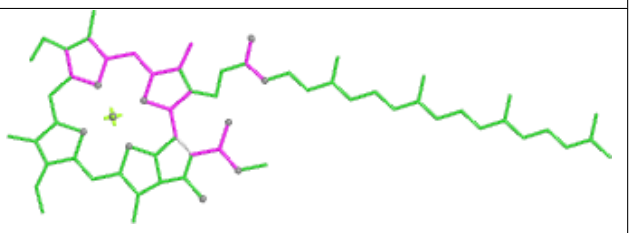


Rings

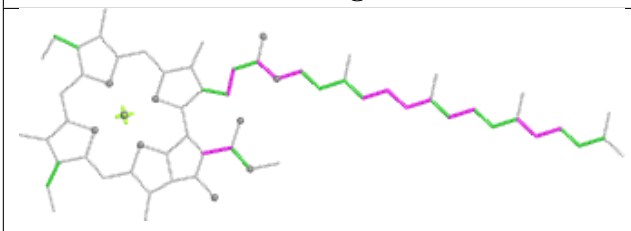
Ligand CLA B 615



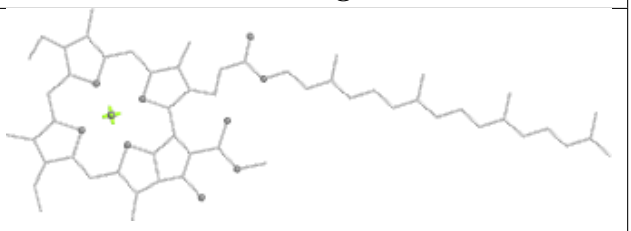
Bond lengths



Bond angles

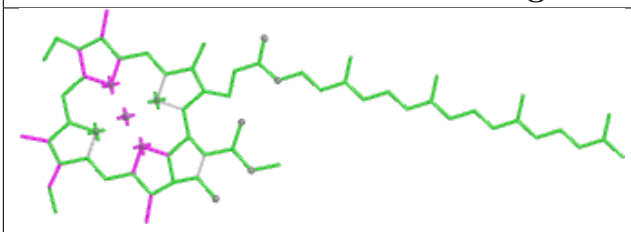


Torsions

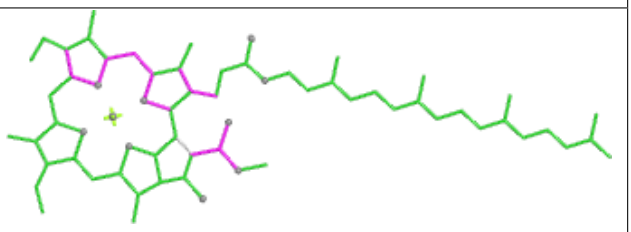


Rings

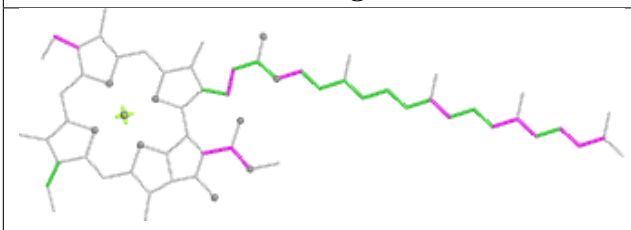
Ligand CLA b 610



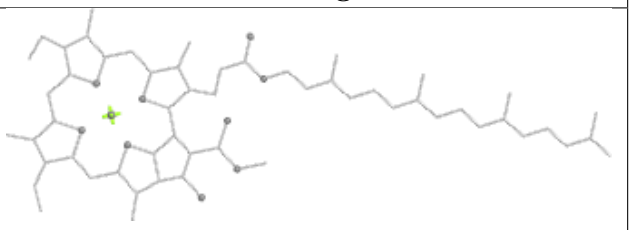
Bond lengths



Bond angles

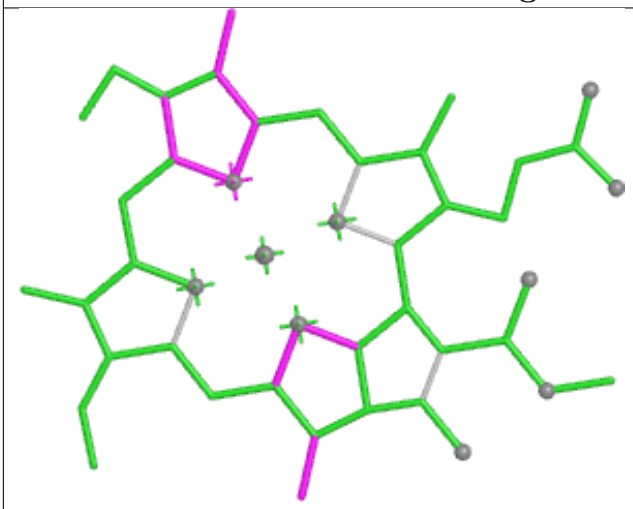


Torsions

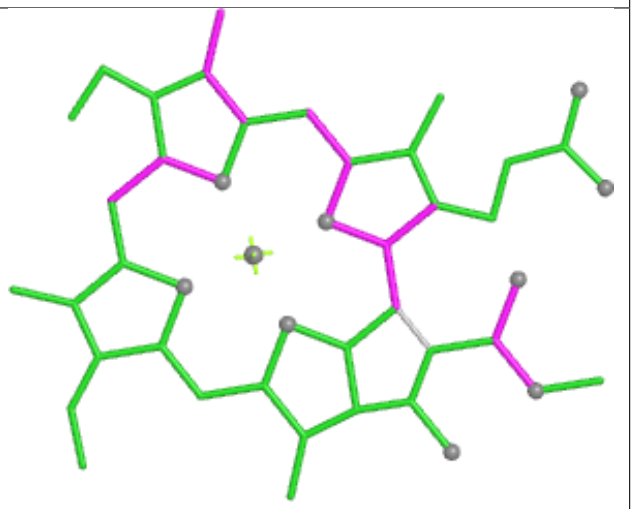


Rings

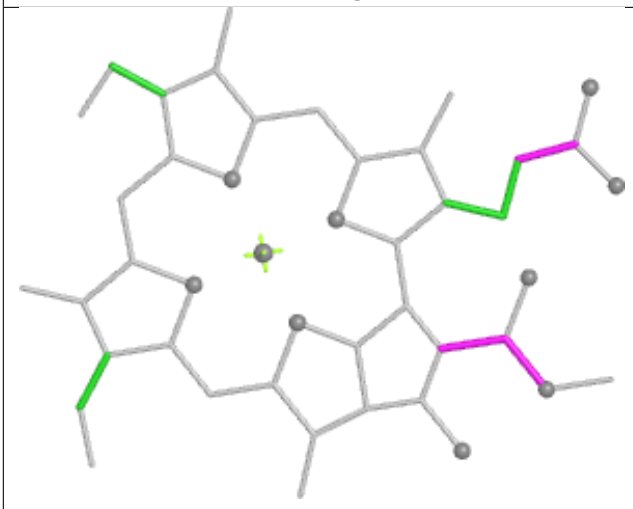
Ligand CLA 18 304



Bond lengths



Bond angles

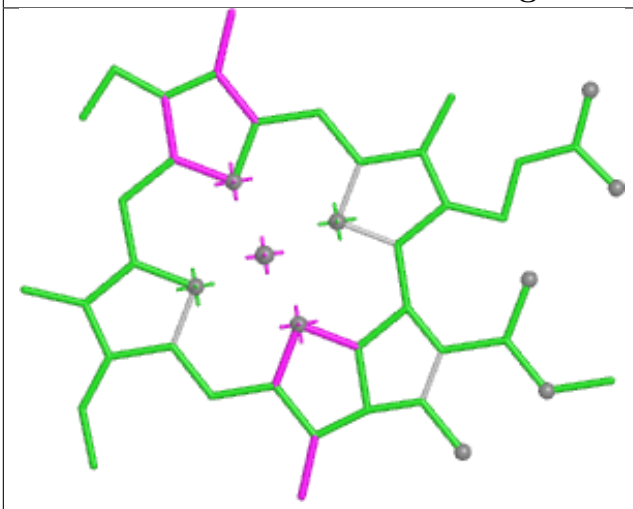


Torsions

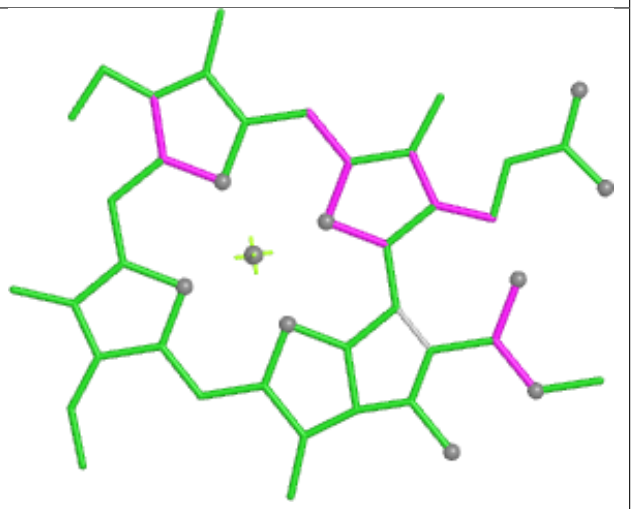


Rings

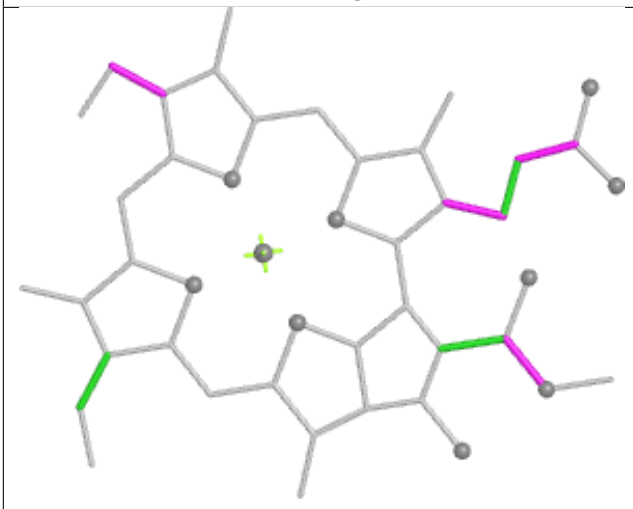
Ligand CLA 12 314



Bond lengths



Bond angles

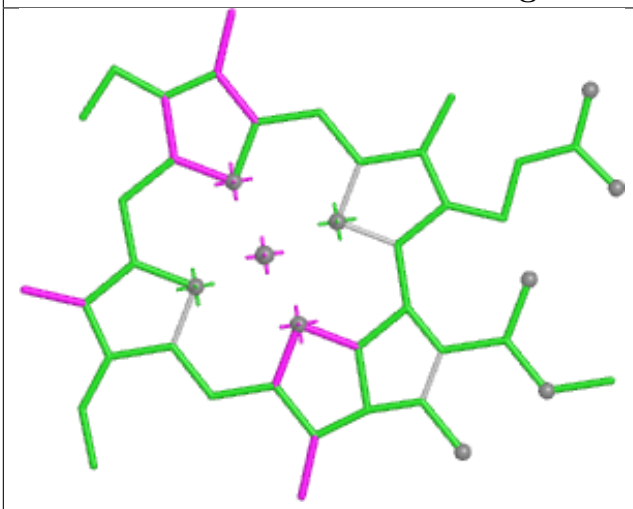


Torsions

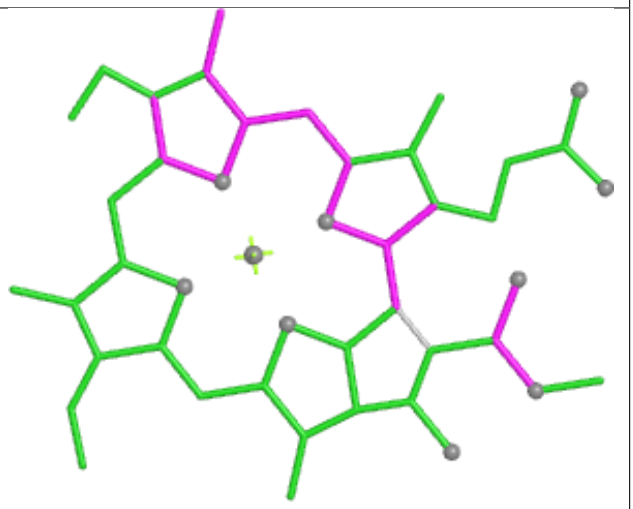


Rings

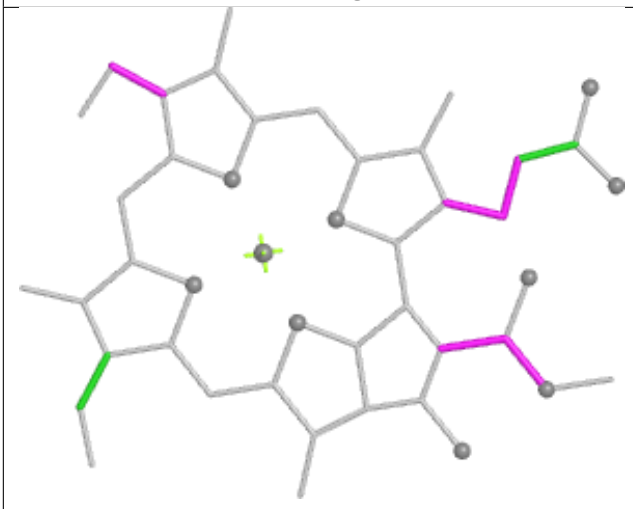
Ligand CLA 14 307



Bond lengths



Bond angles

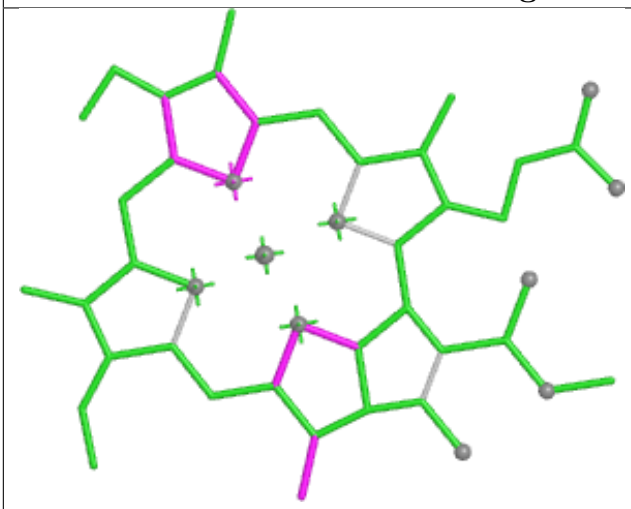


Torsions

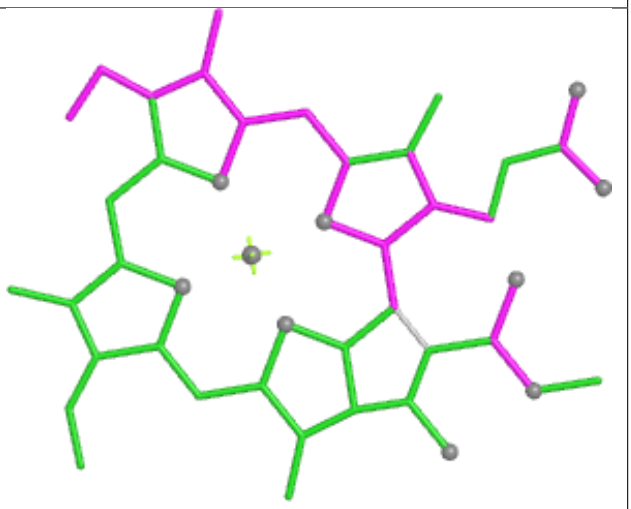


Rings

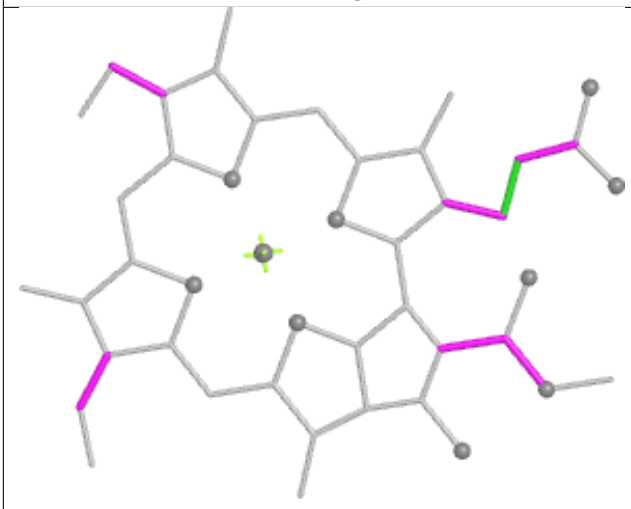
Ligand CLA 21 305



Bond lengths



Bond angles

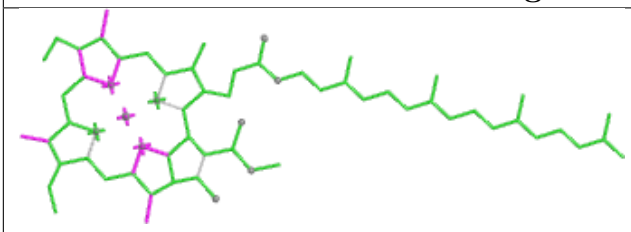


Torsions

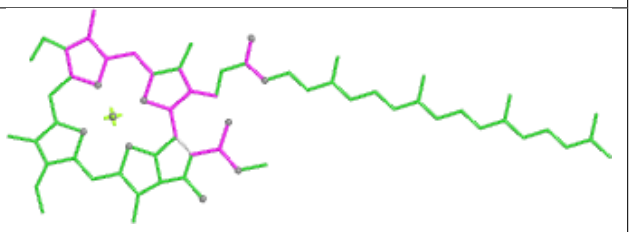


Rings

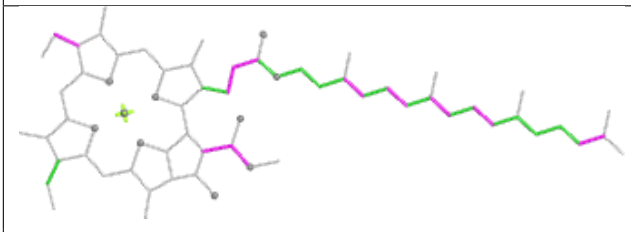
Ligand CLA C 520



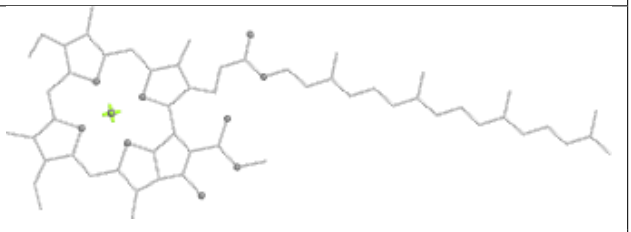
Bond lengths



Bond angles

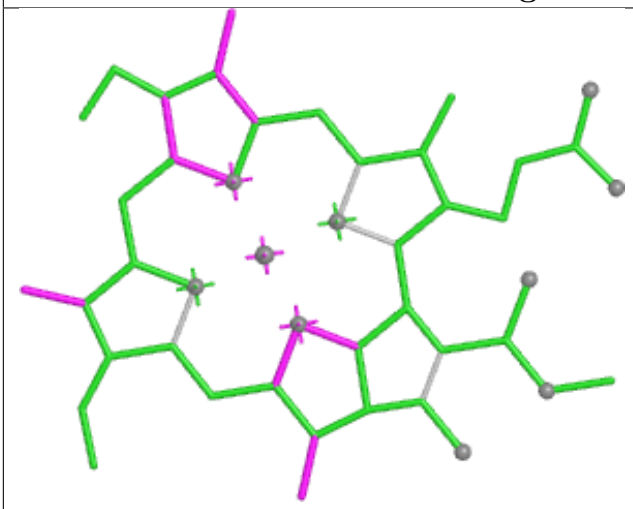


Torsions

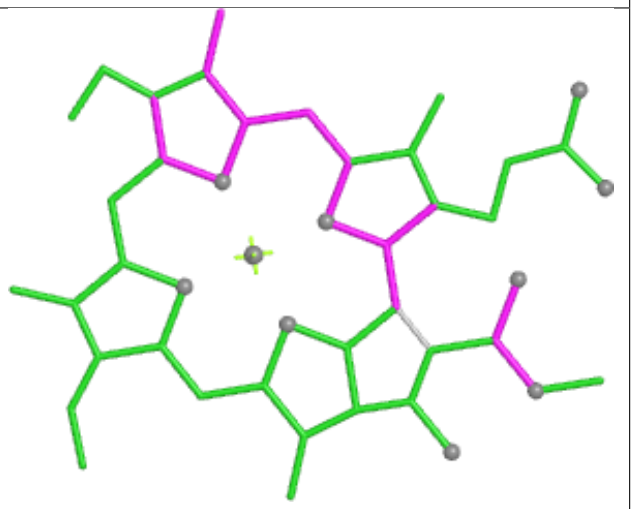


Rings

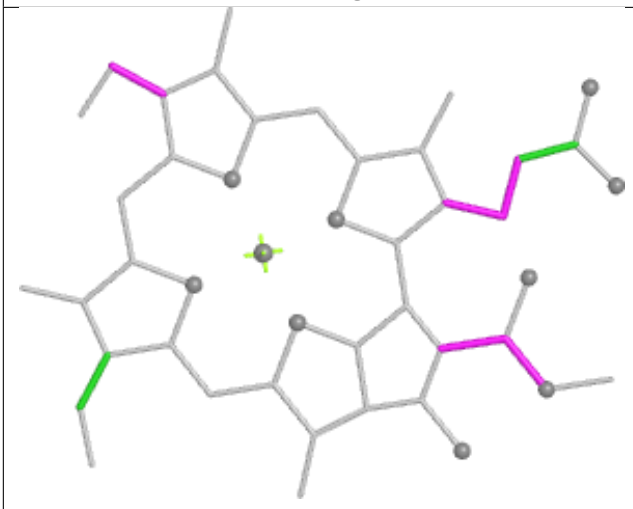
Ligand CLA 12 309



Bond lengths



Bond angles

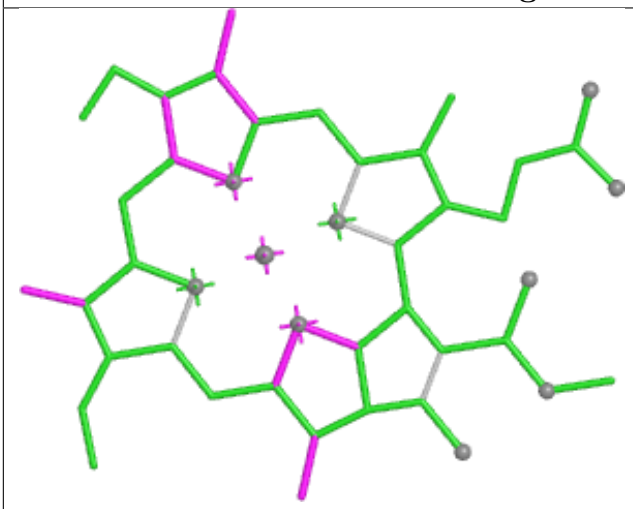


Torsions

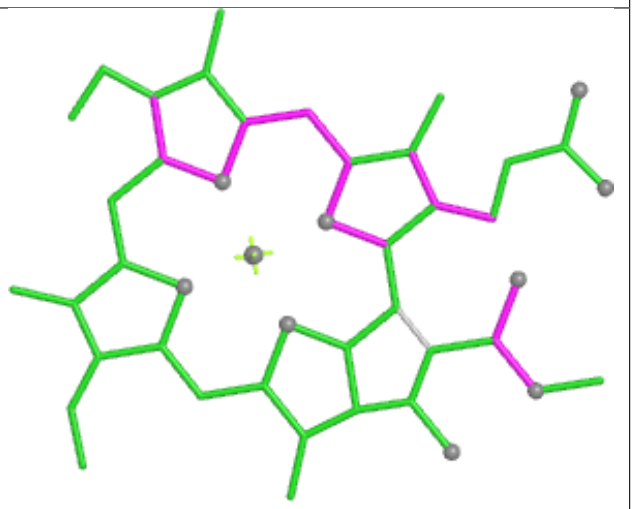


Rings

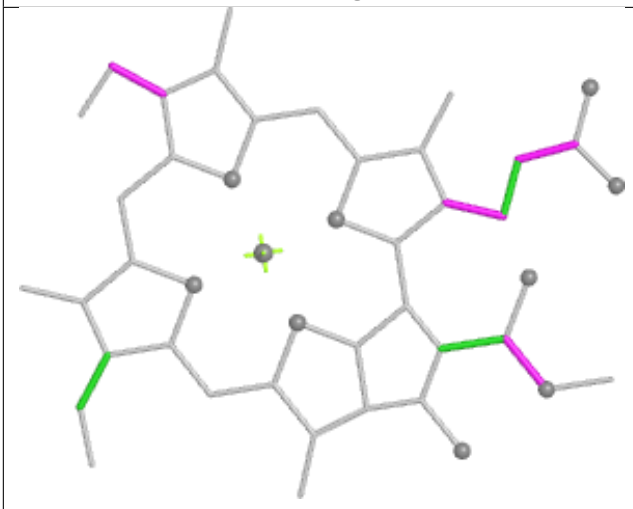
Ligand CLA 13 310



Bond lengths



Bond angles

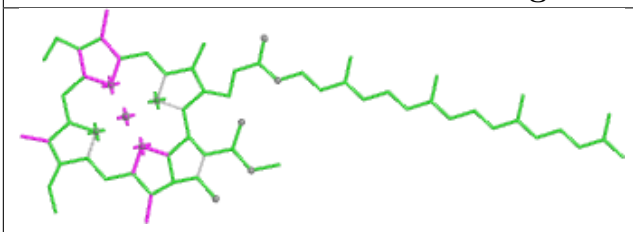


Torsions

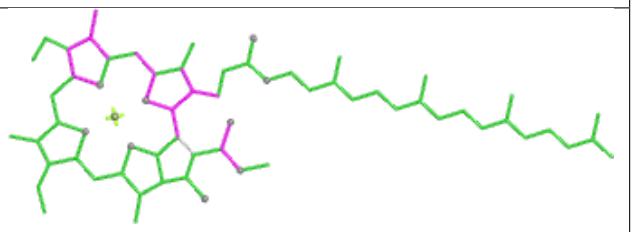


Rings

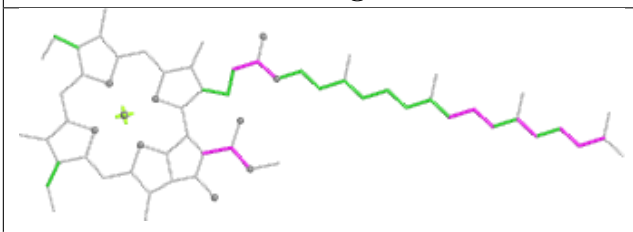
Ligand CLA c 514



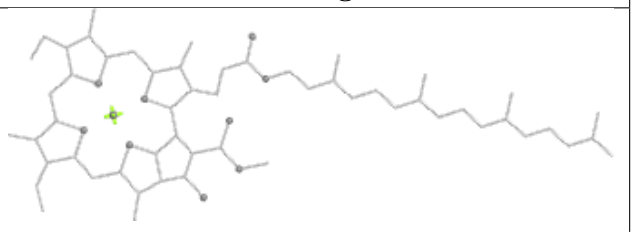
Bond lengths



Bond angles

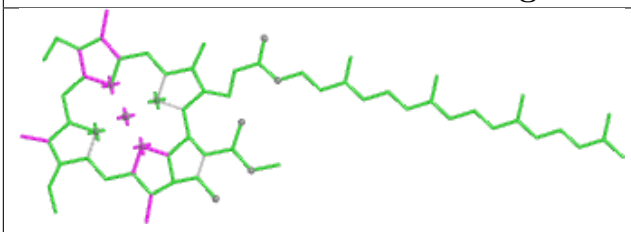


Torsions

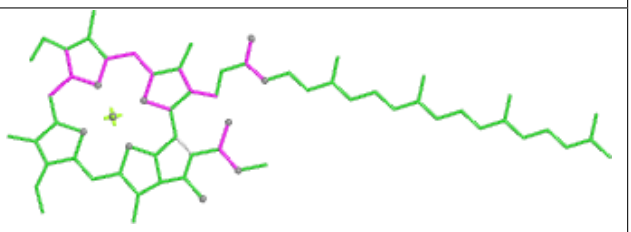


Rings

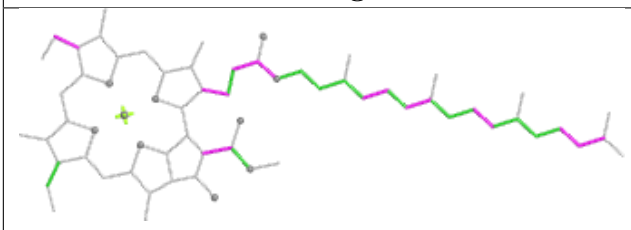
Ligand CLA 16 304



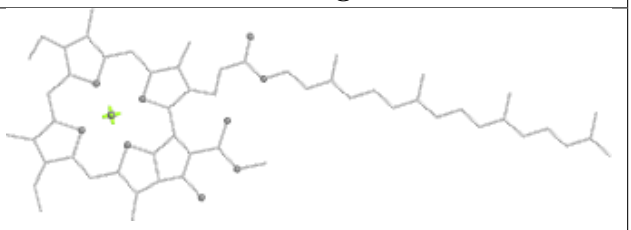
Bond lengths



Bond angles

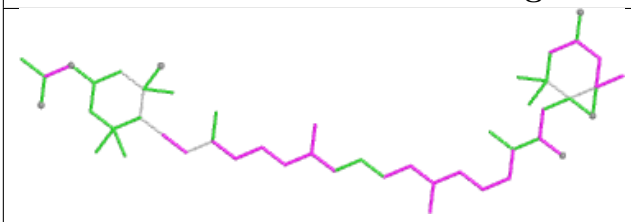


Torsions

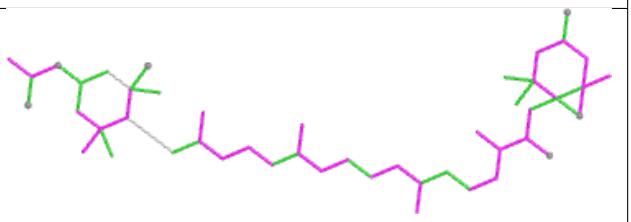


Rings

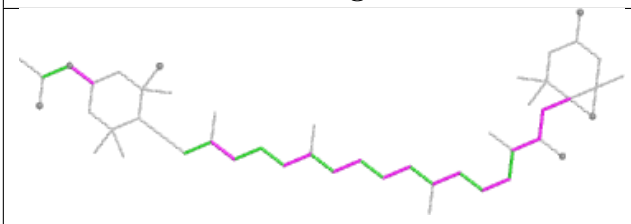
Ligand A86 19 311



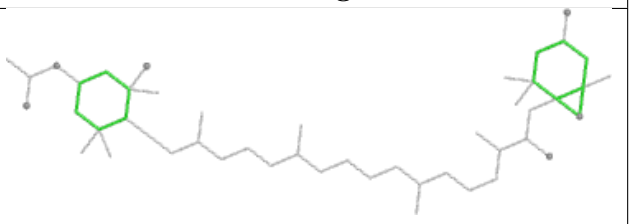
Bond lengths



Bond angles

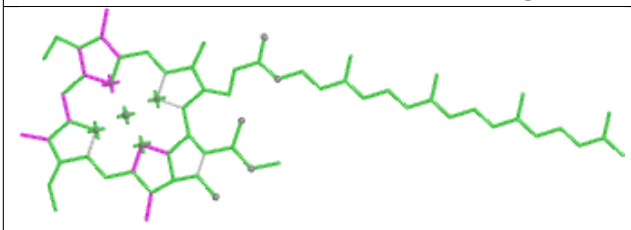


Torsions

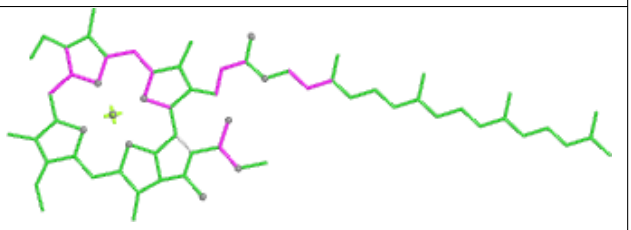


Rings

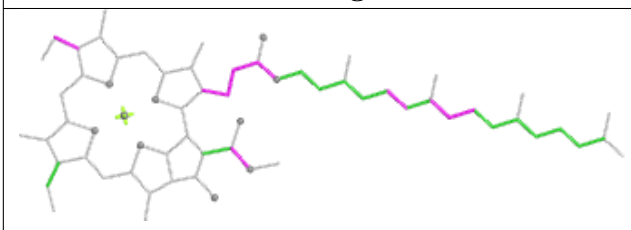
Ligand CLA 14 303



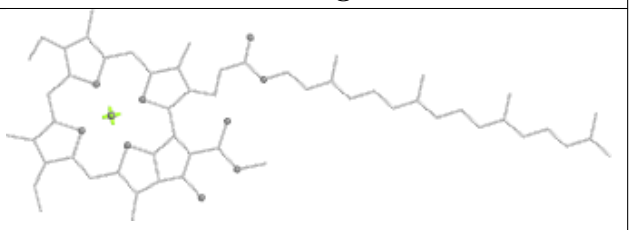
Bond lengths



Bond angles

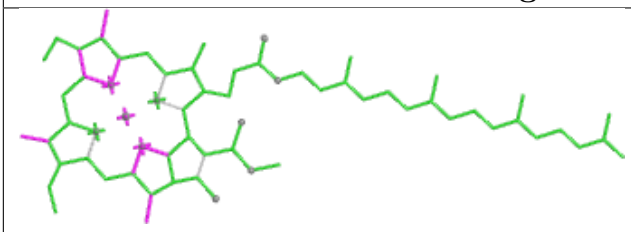


Torsions

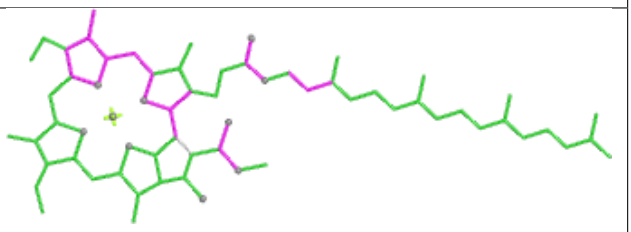


Rings

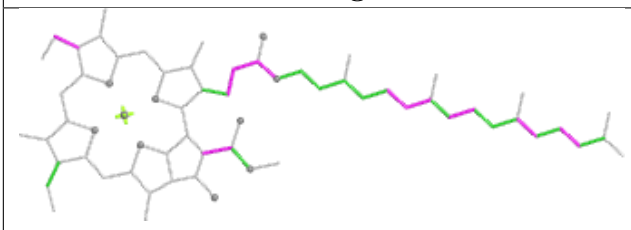
Ligand CLA 11 307



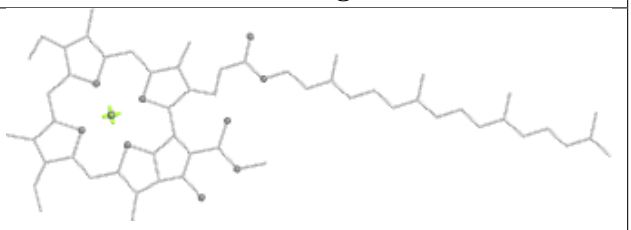
Bond lengths



Bond angles

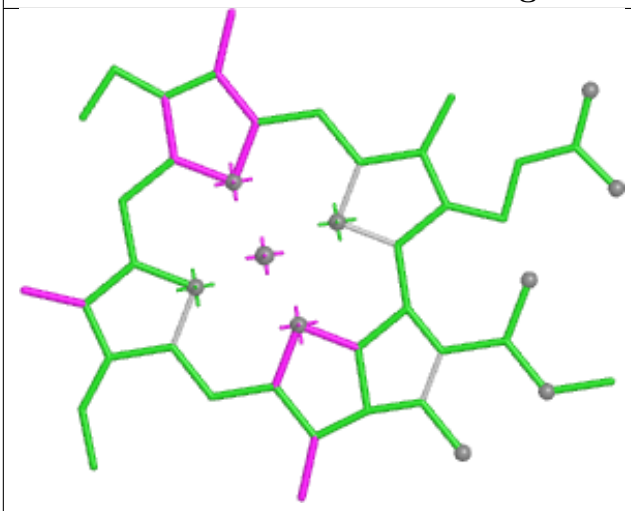


Torsions

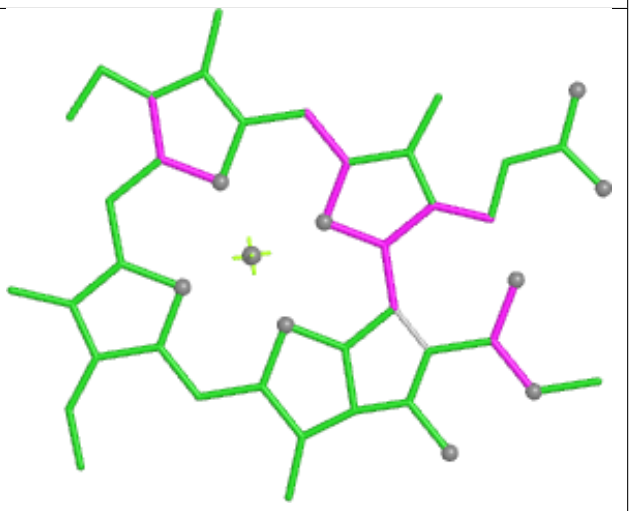


Rings

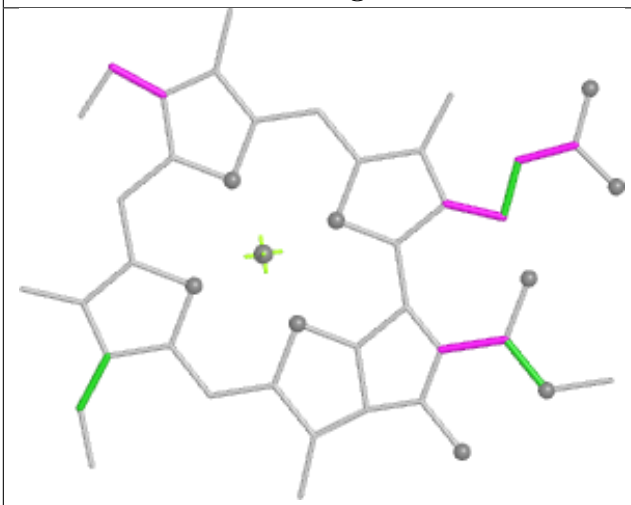
Ligand CLA 12 313



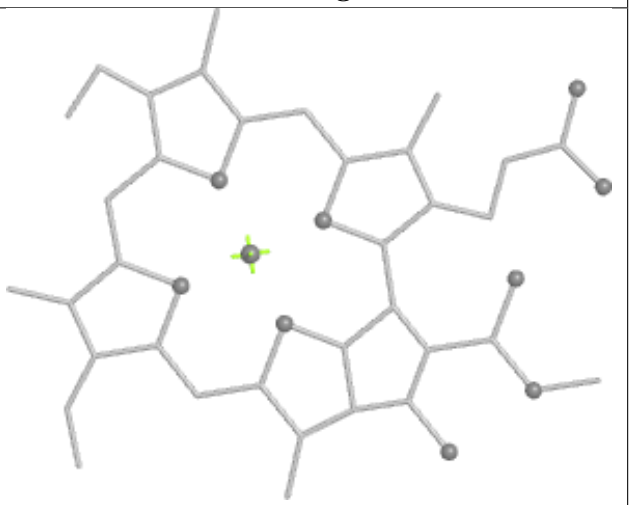
Bond lengths



Bond angles

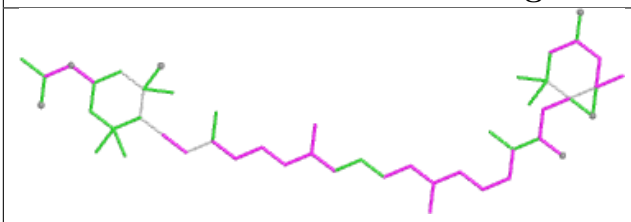


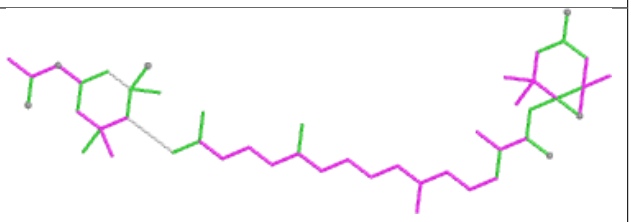
Torsions

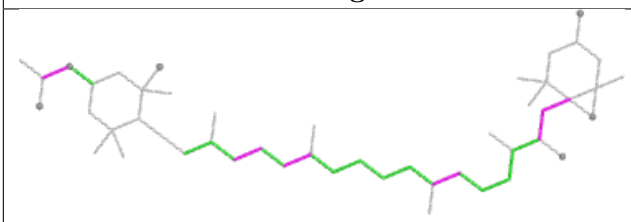


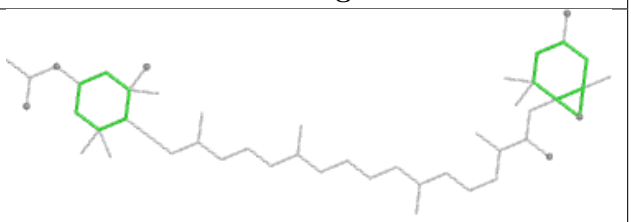
Rings

Ligand A86 13 311

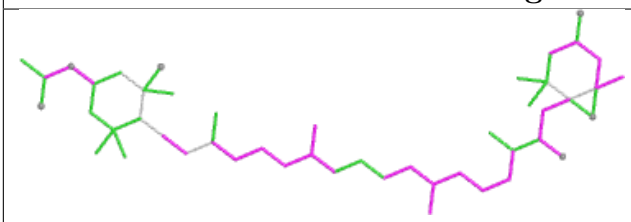

Bond lengths

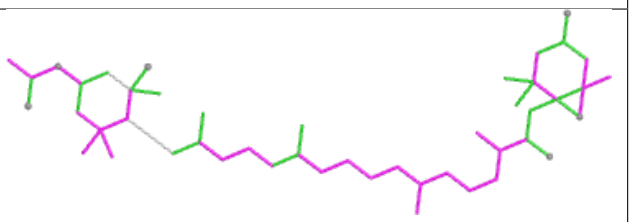

Bond angles

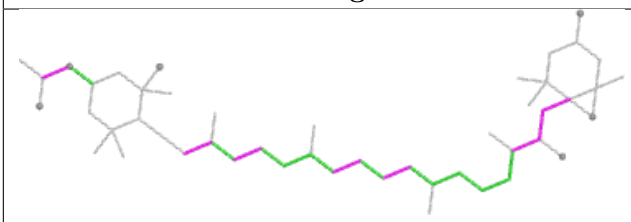

Torsions

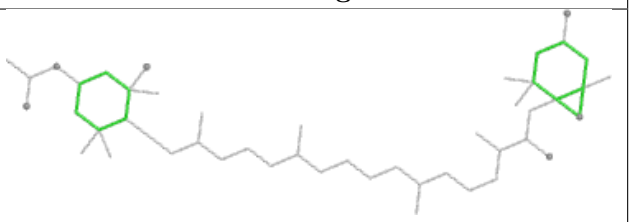

Rings

Ligand A86 16 310

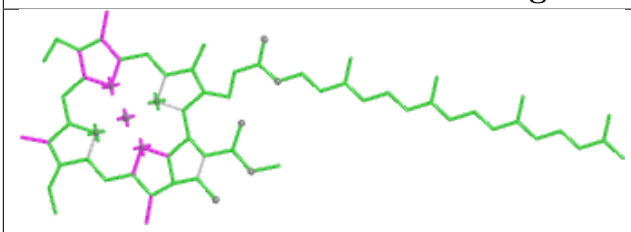

Bond lengths

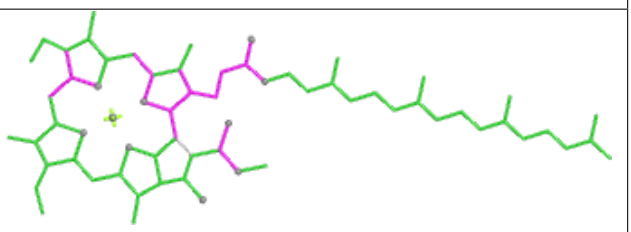

Bond angles

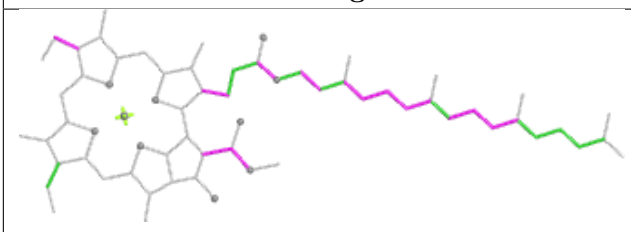

Torsions

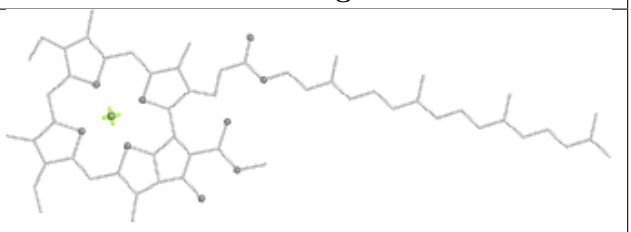

Rings

Ligand CLA c 504

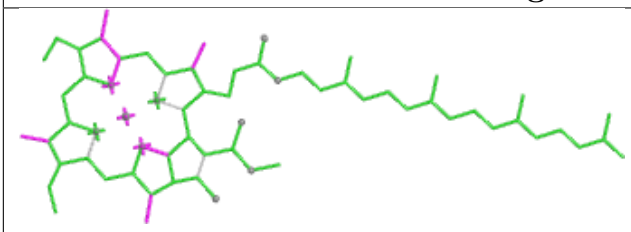

Bond lengths


Bond angles

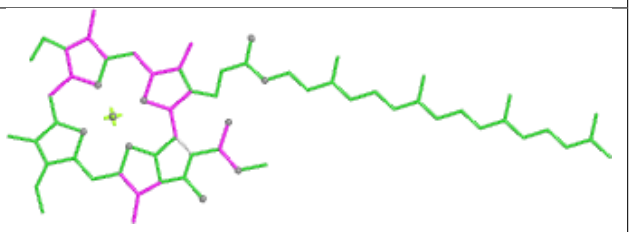

Torsions


Rings

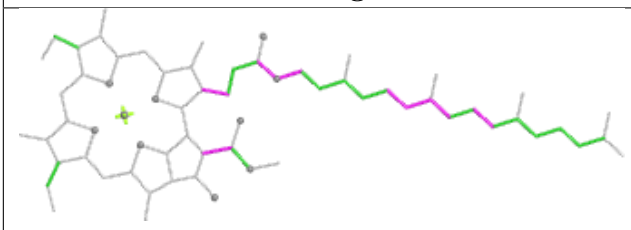
Ligand CLA b 612



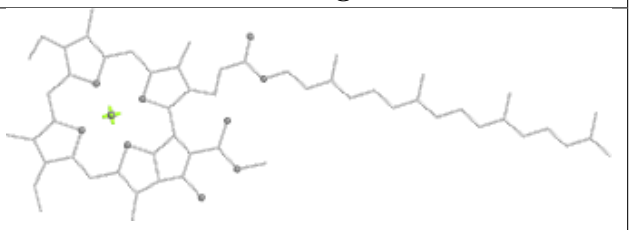
Bond lengths



Bond angles

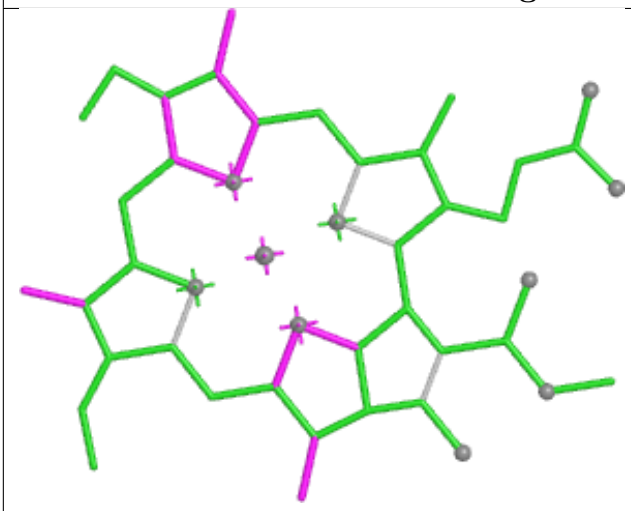


Torsions

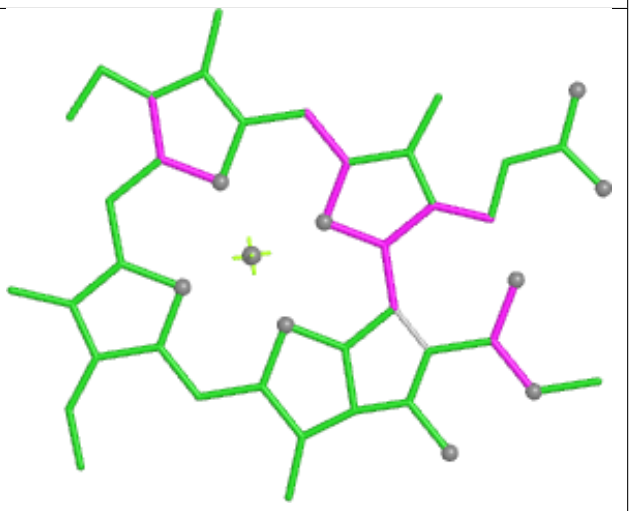


Rings

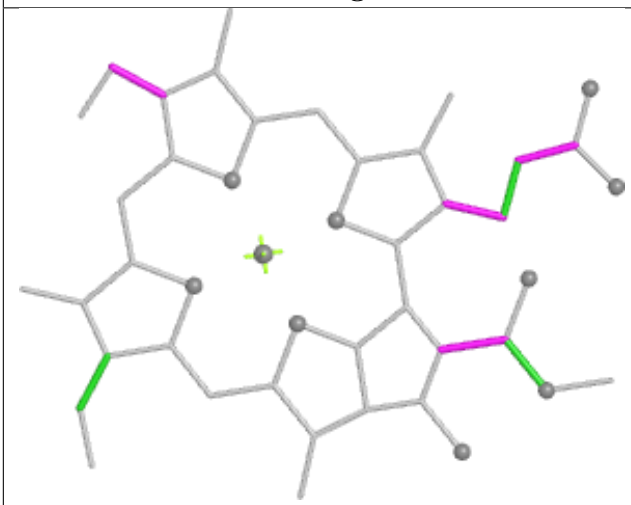
Ligand CLA 13 309



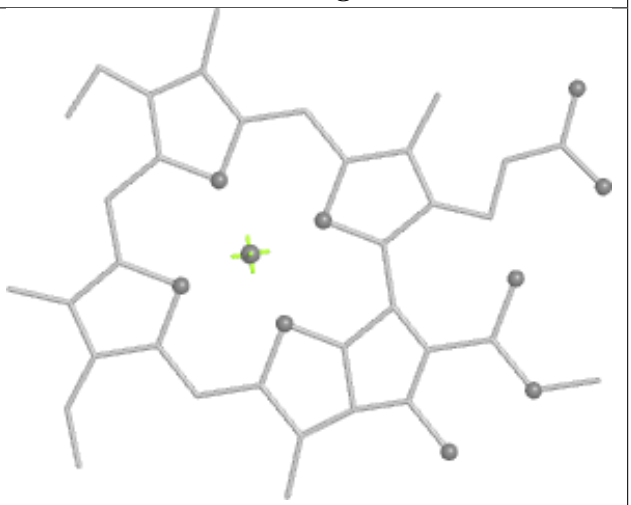
Bond lengths



Bond angles

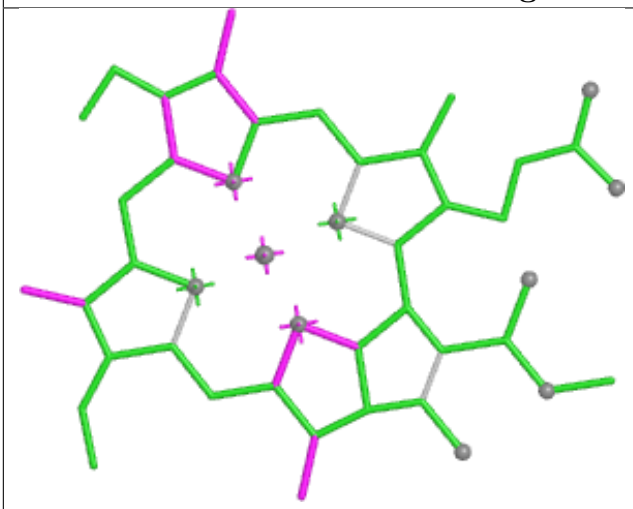


Torsions

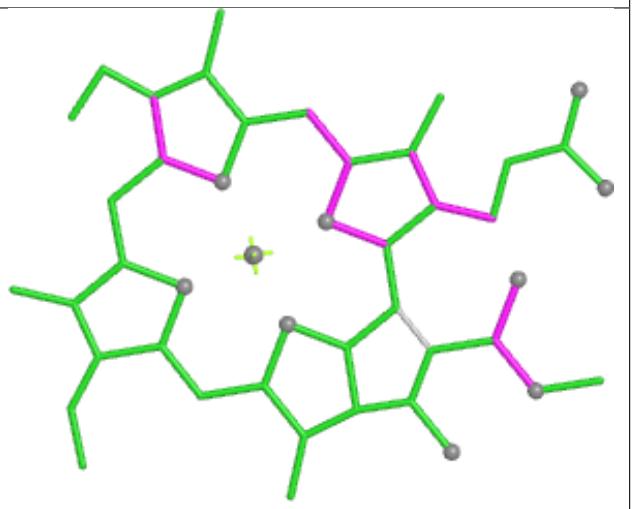


Rings

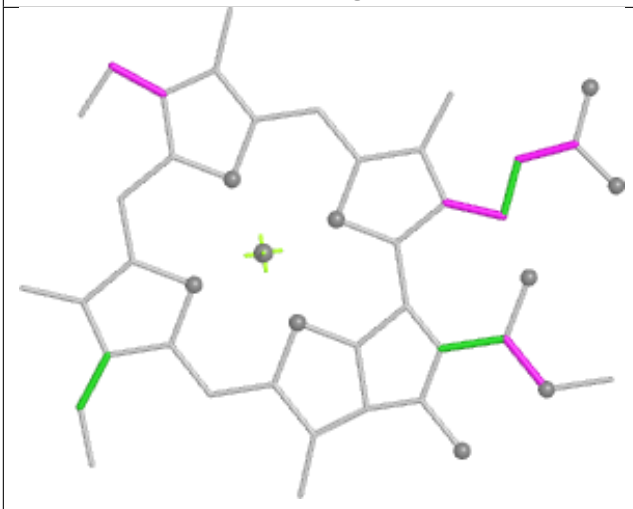
Ligand CLA 11 309



Bond lengths



Bond angles

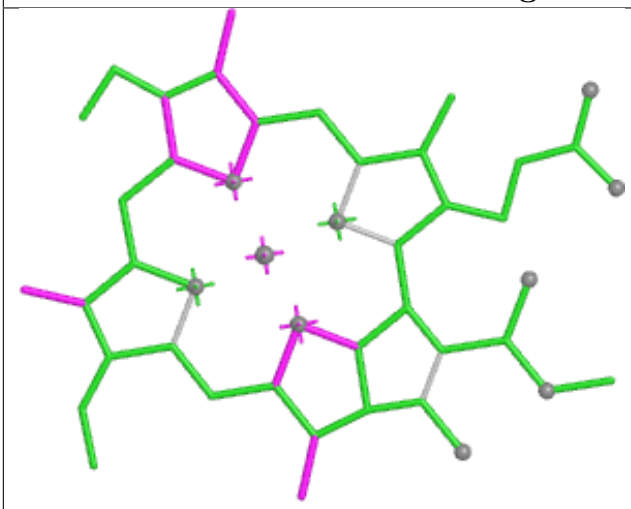


Torsions

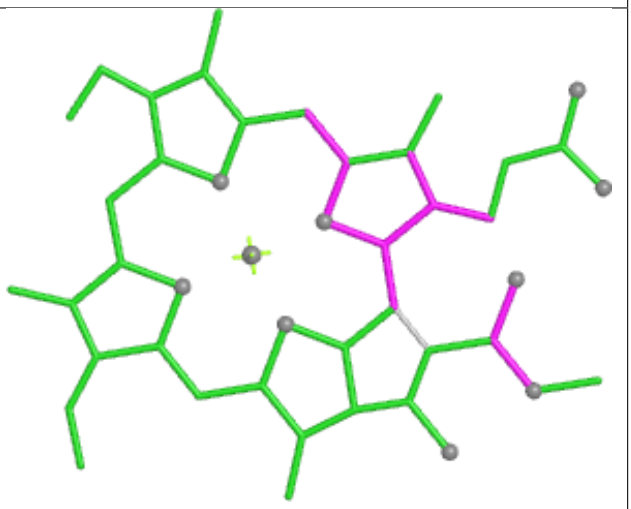


Rings

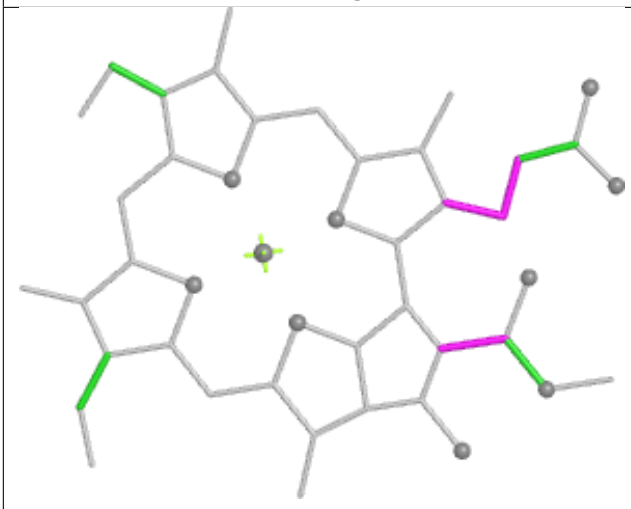
Ligand CLA 14 304



Bond lengths



Bond angles

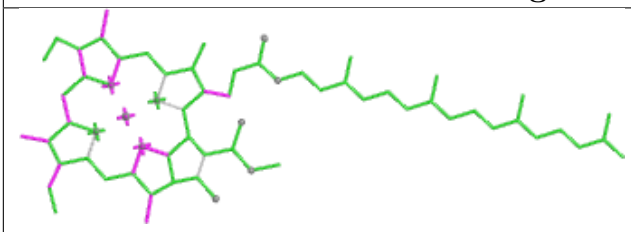


Torsions

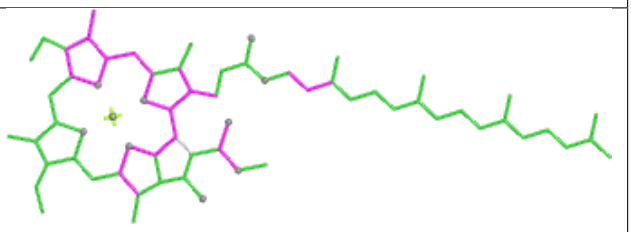


Rings

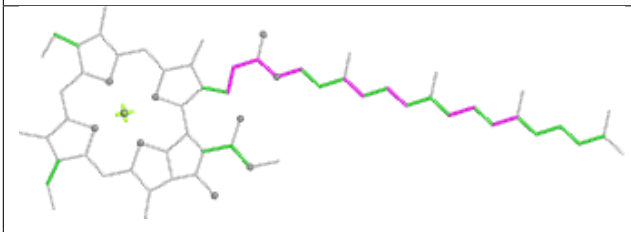
Ligand CLA c 511



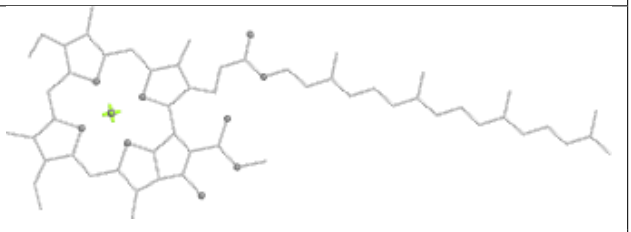
Bond lengths



Bond angles

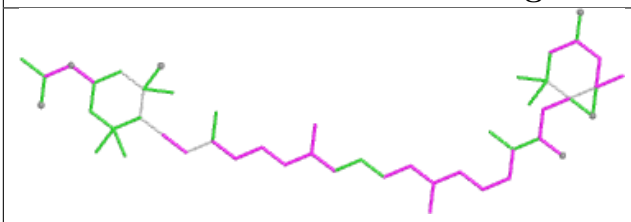


Torsions

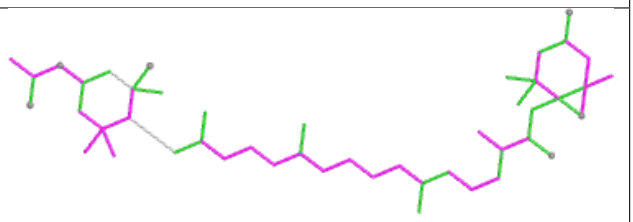


Rings

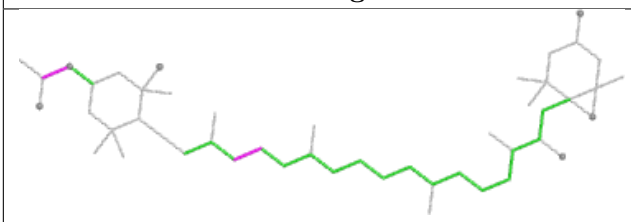
Ligand A86 17 312



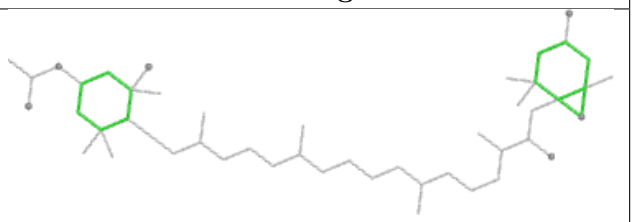
Bond lengths



Bond angles

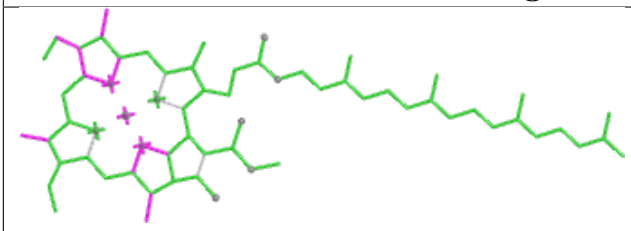


Torsions

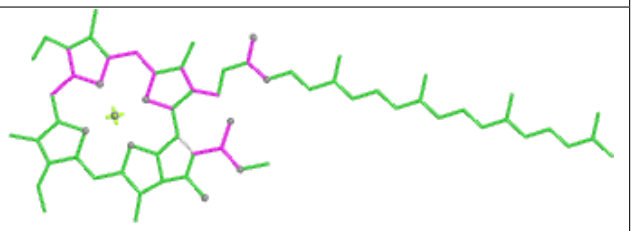


Rings

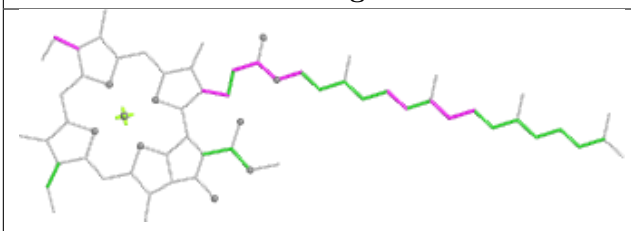
Ligand CLA A 404



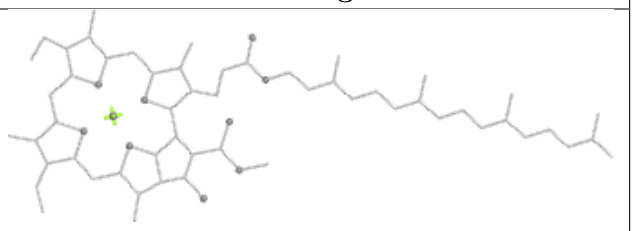
Bond lengths



Bond angles

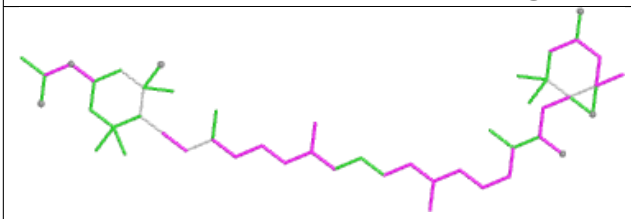


Torsions

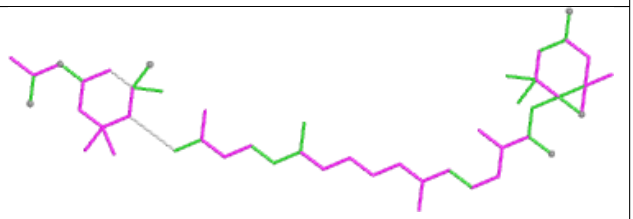


Rings

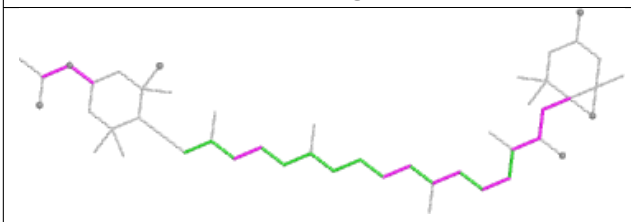
Ligand A86 13 301



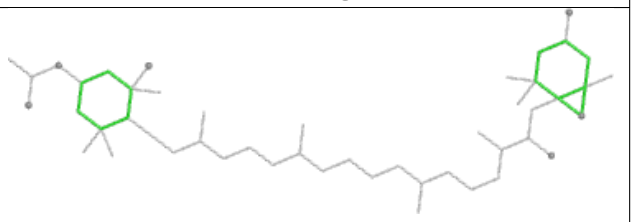
Bond lengths



Bond angles

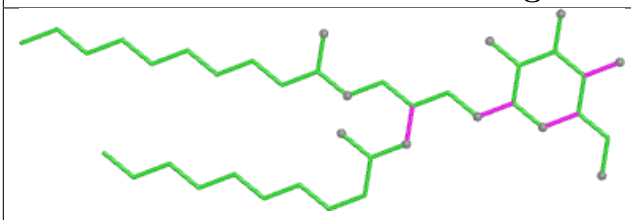


Torsions

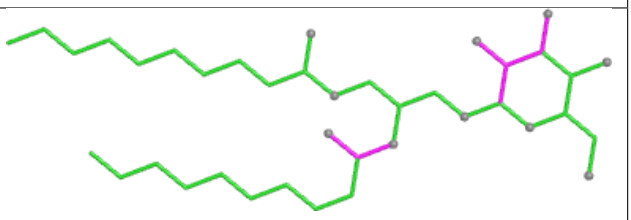


Rings

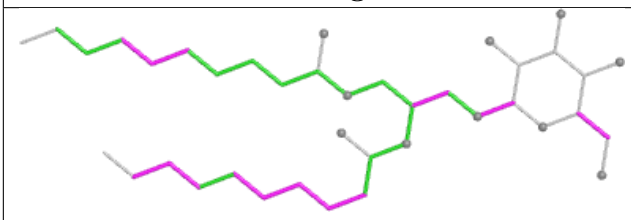
Ligand LMG 1 101



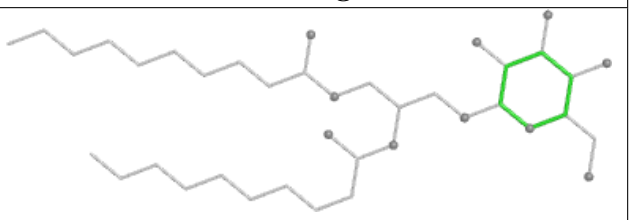
Bond lengths



Bond angles

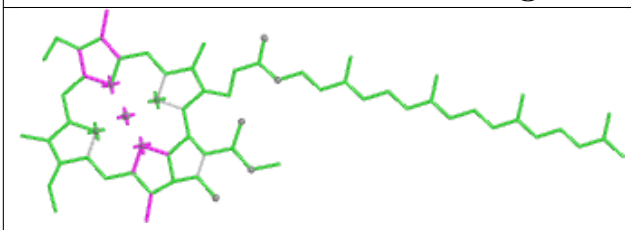


Torsions

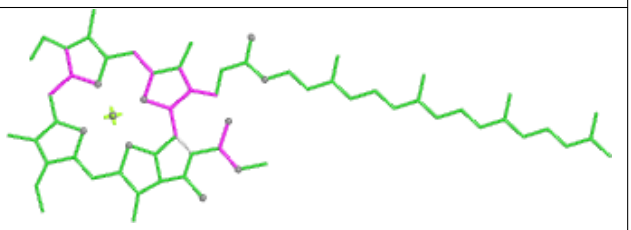


Rings

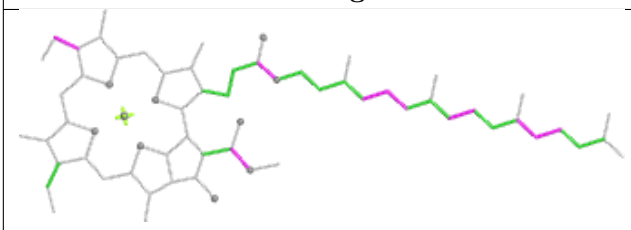
Ligand CLA 16 301



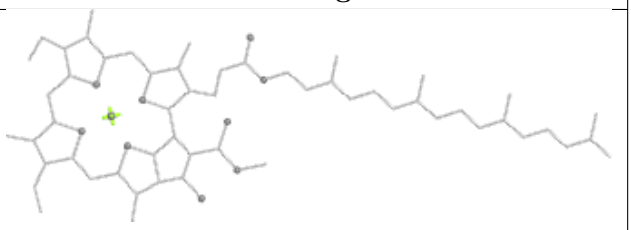
Bond lengths



Bond angles

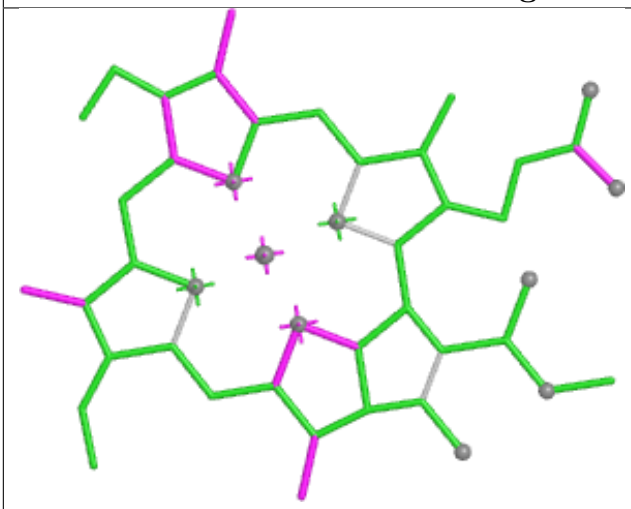


Torsions

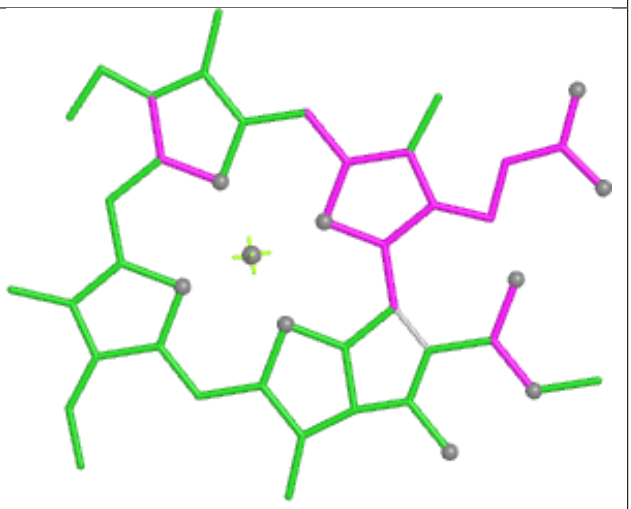


Rings

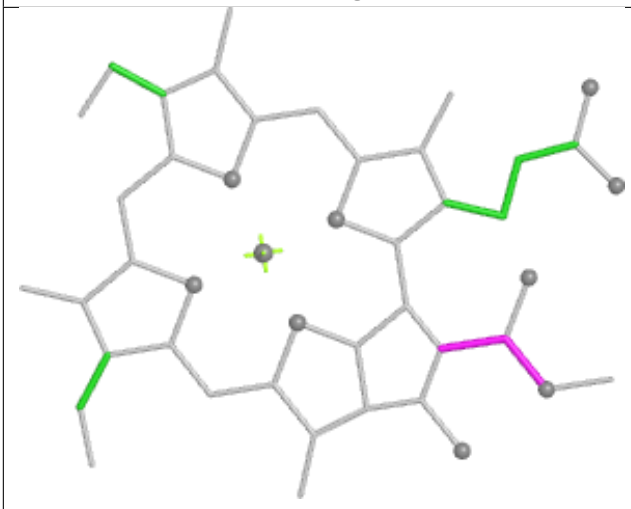
Ligand CLA 17 309



Bond lengths



Bond angles

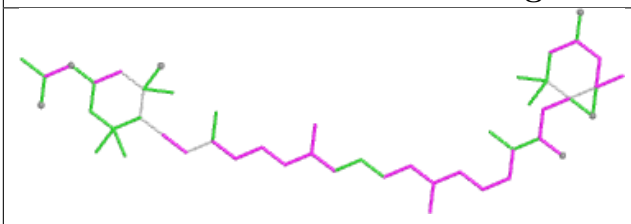


Torsions

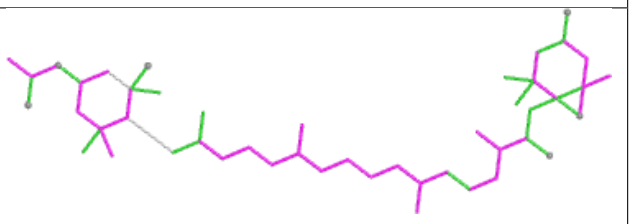


Rings

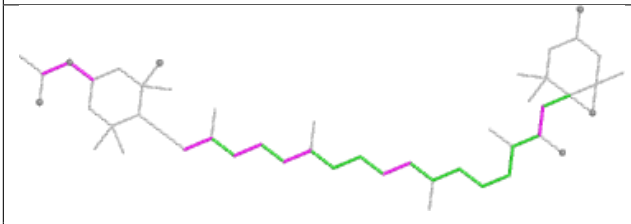
Ligand A86 13 313



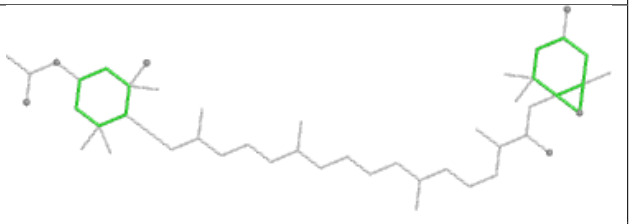
Bond lengths



Bond angles

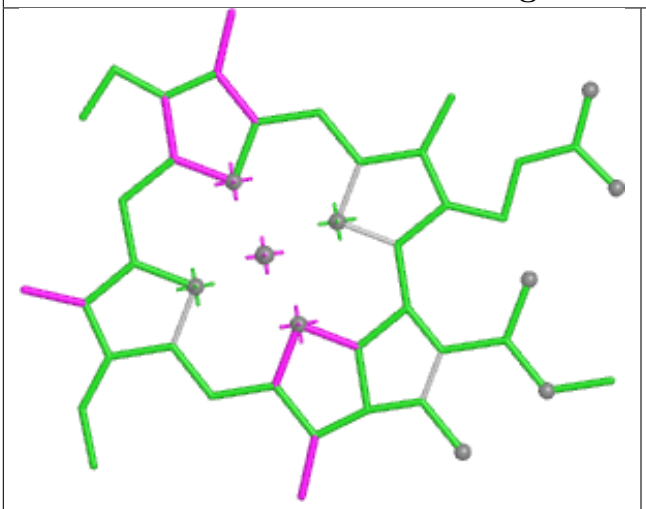


Torsions

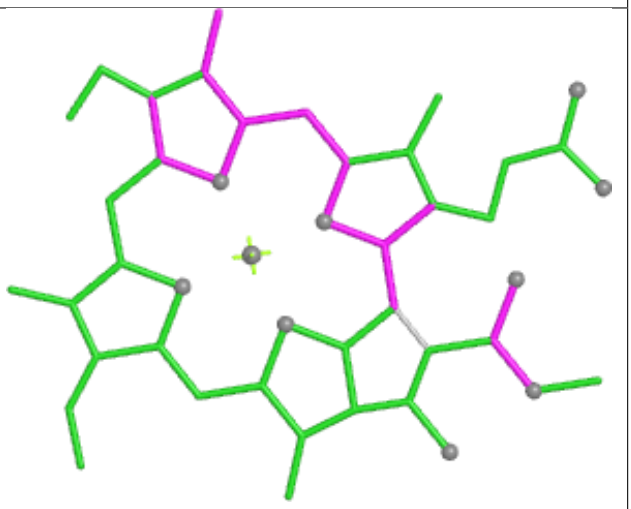


Rings

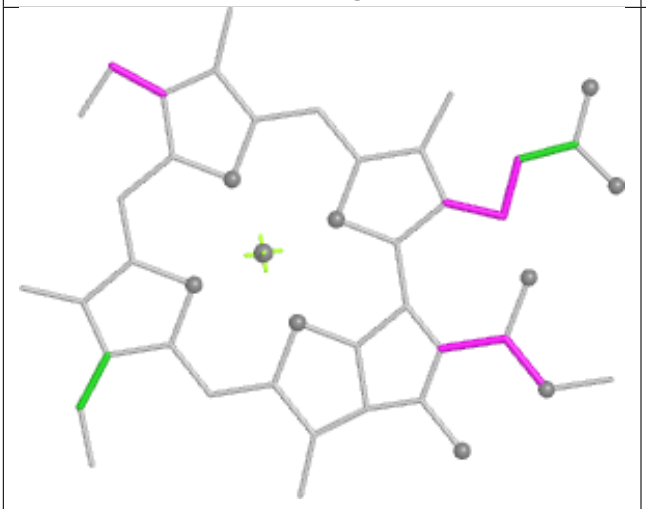
Ligand CLA 13 306



Bond lengths



Bond angles

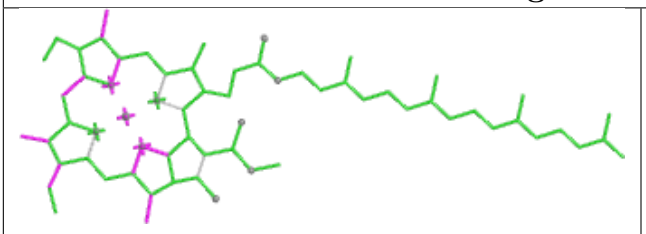


Torsions

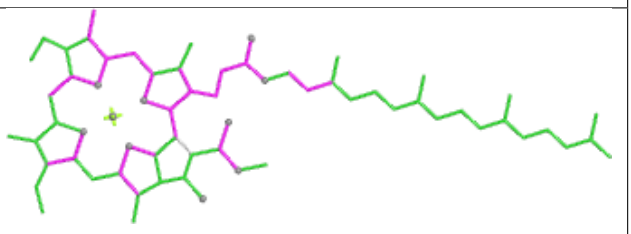


Rings

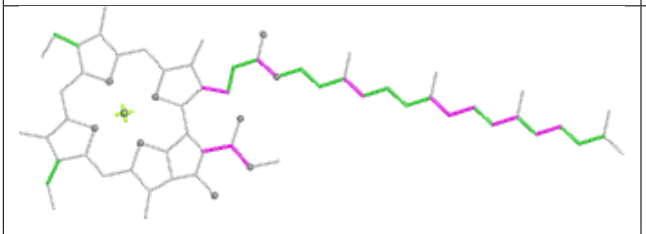
Ligand CLA b 604



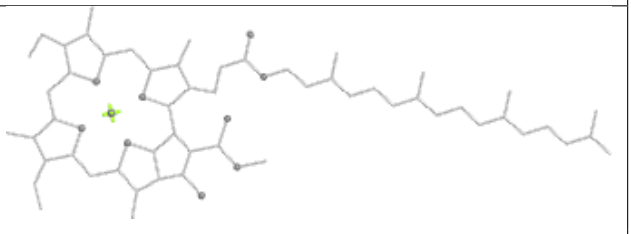
Bond lengths



Bond angles

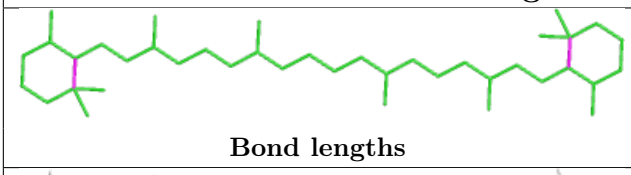


Torsions

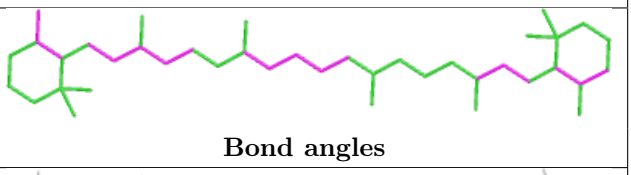


Rings

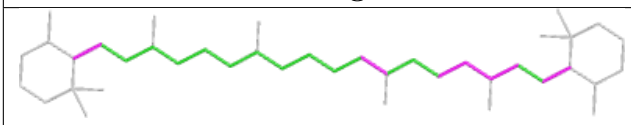
Ligand BCR B 616



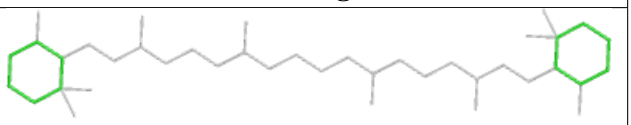
Bond lengths



Bond angles

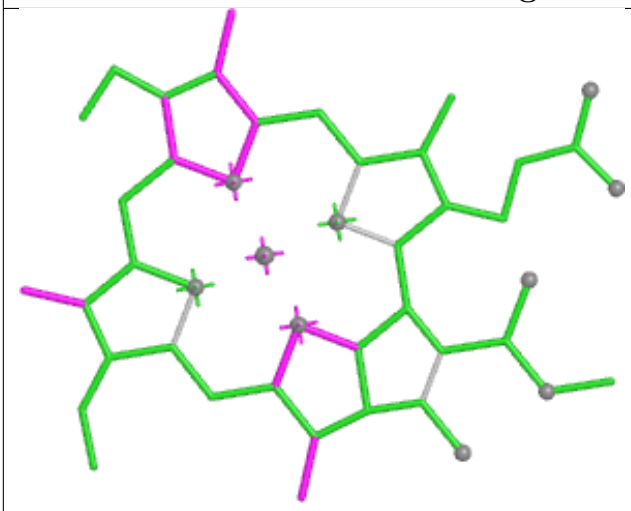


Torsions

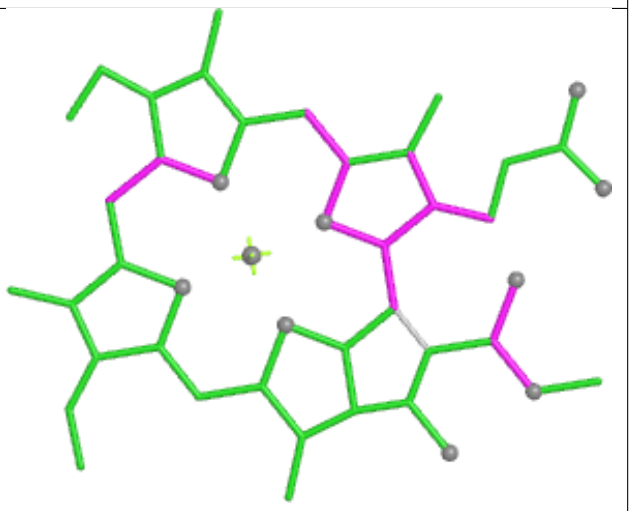


Rings

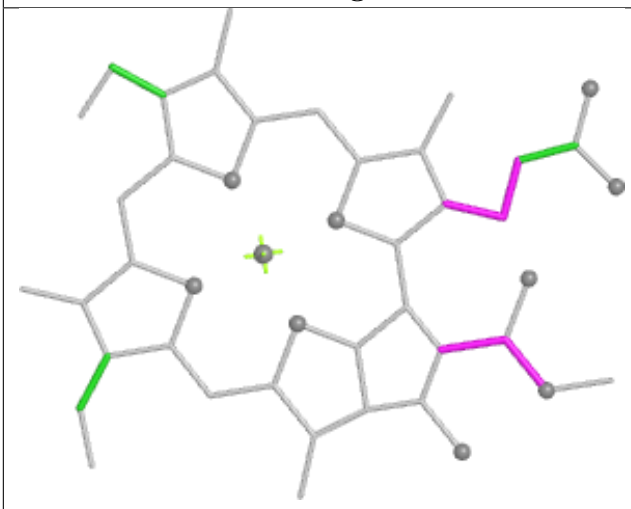
Ligand CLA 13 303



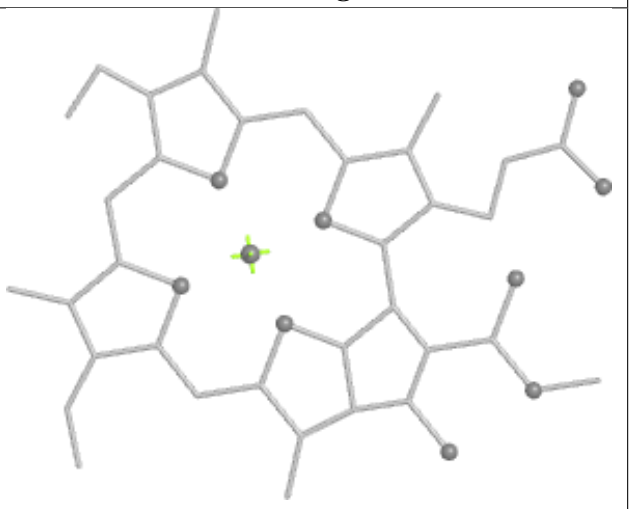
Bond lengths



Bond angles

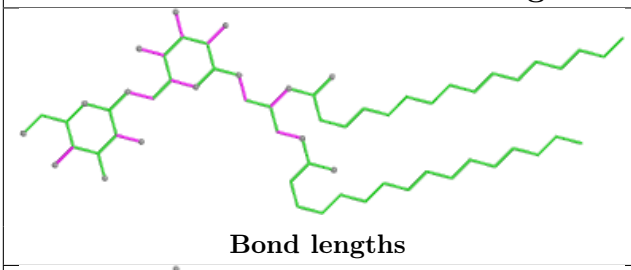


Torsions

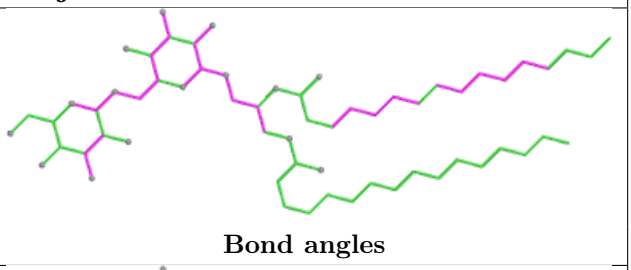


Rings

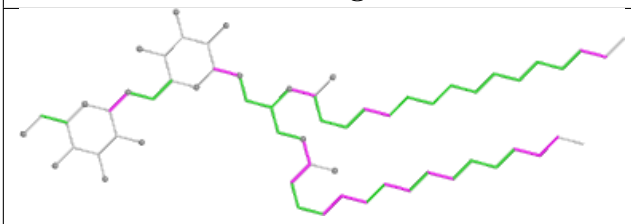
Ligand DGD j 101



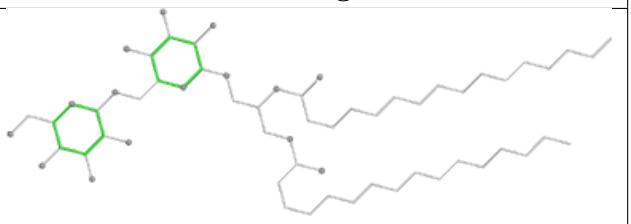
Bond lengths



Bond angles

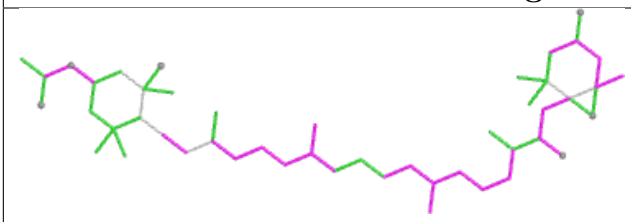


Torsions

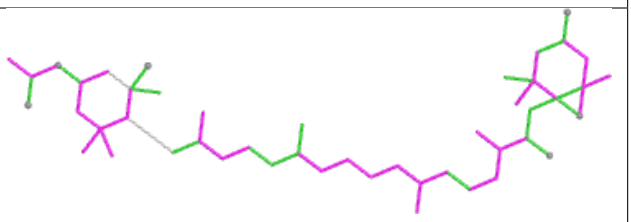


Rings

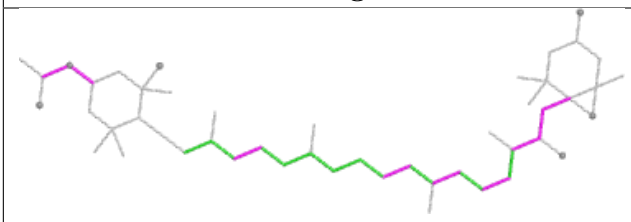
Ligand A86 12 304



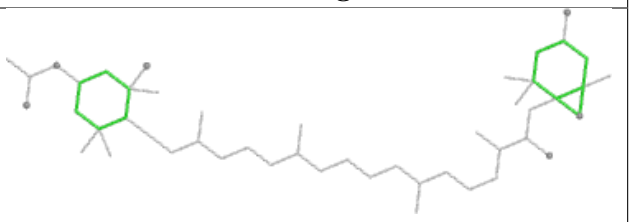
Bond lengths



Bond angles

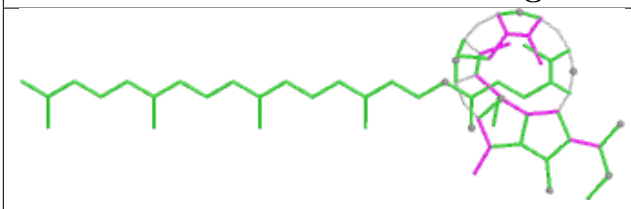


Torsions

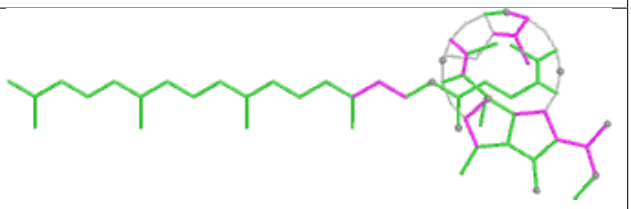


Rings

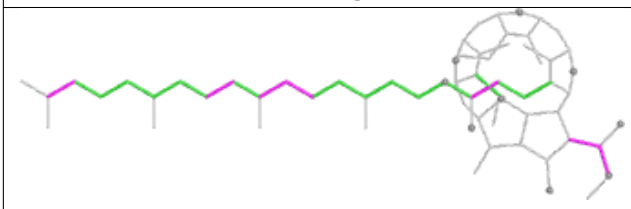
Ligand PHO d 404



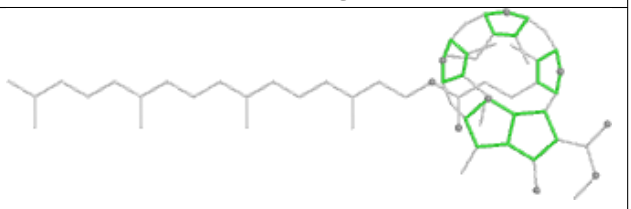
Bond lengths



Bond angles

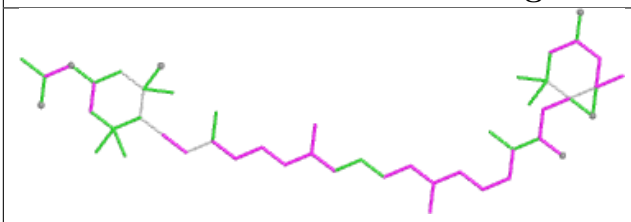


Torsions

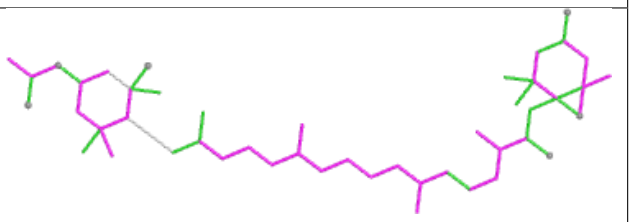


Rings

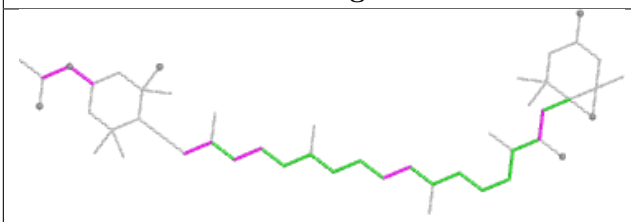
Ligand A86 11 312



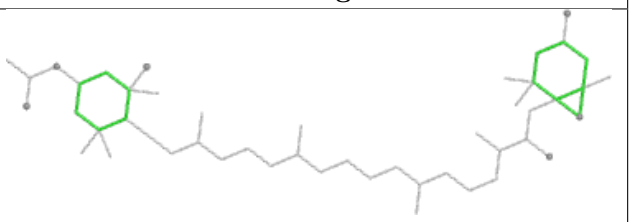
Bond lengths



Bond angles

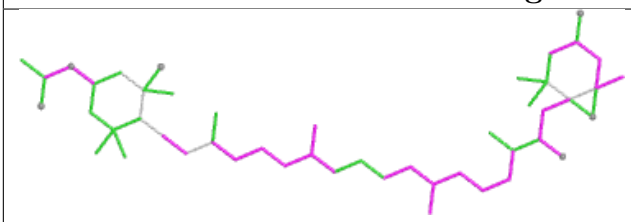


Torsions

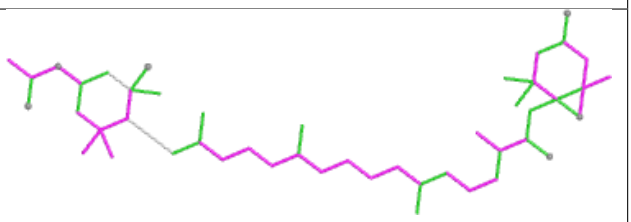


Rings

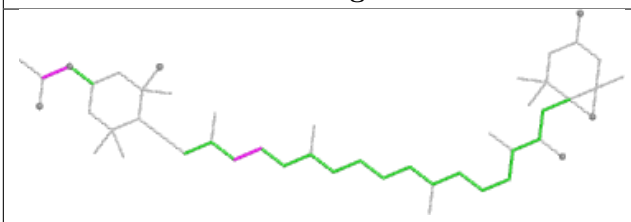
Ligand A86 13 312



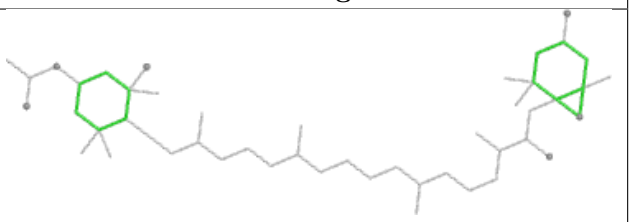
Bond lengths



Bond angles

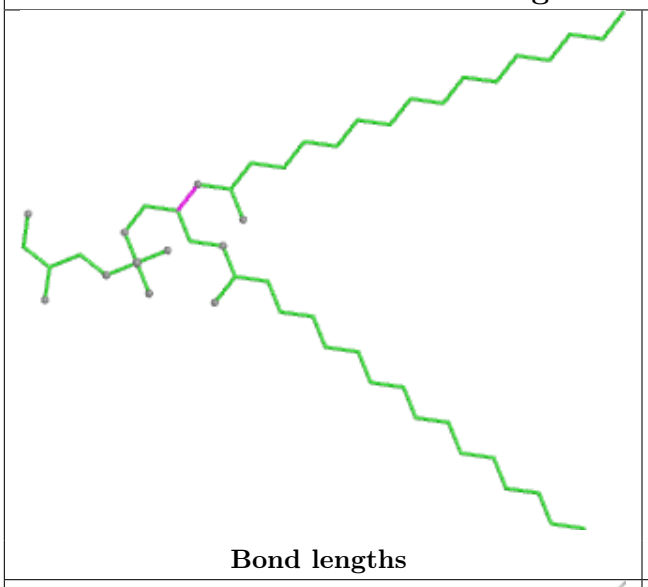


Torsions

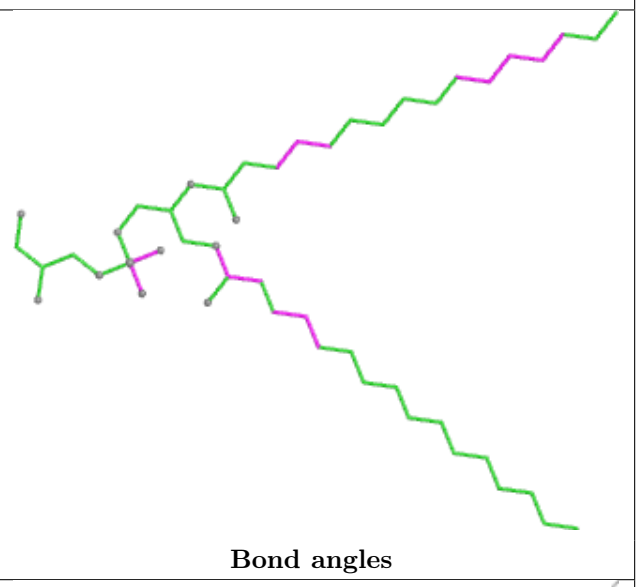


Rings

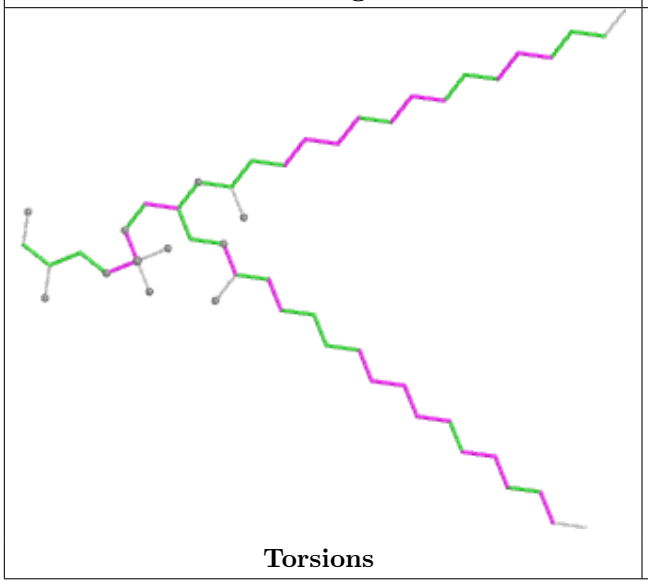
Ligand LHG l 102



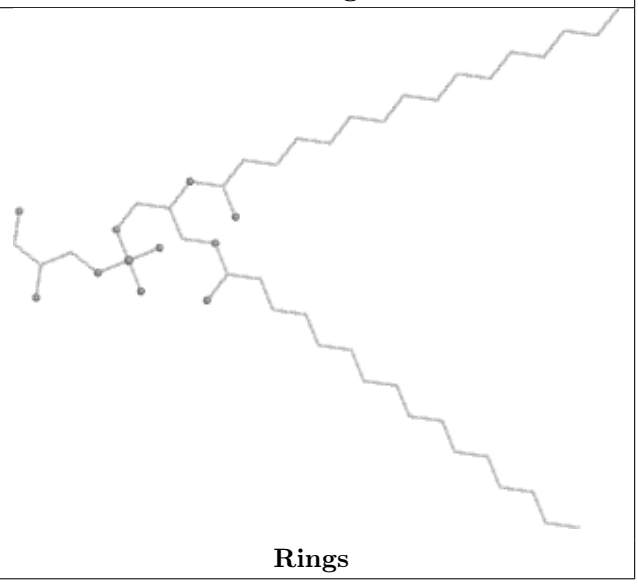
Bond lengths



Bond angles

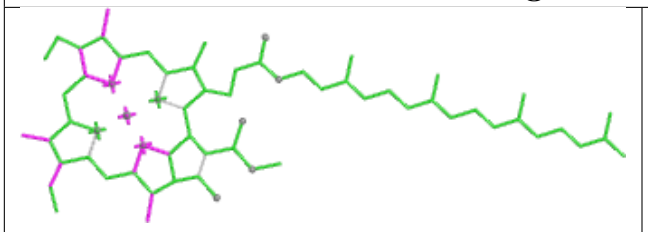


Torsions

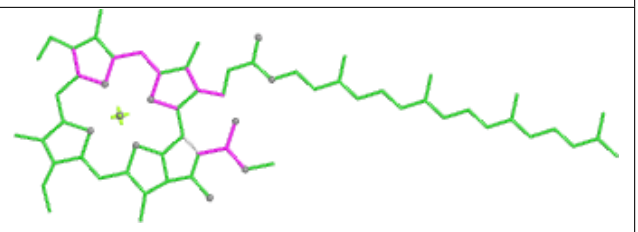


Rings

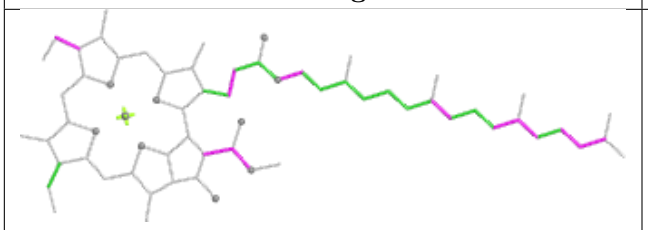
Ligand CLA B 610



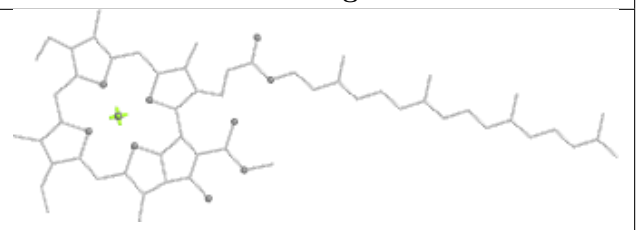
Bond lengths



Bond angles

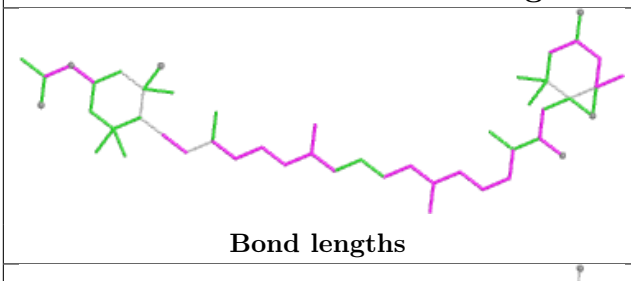


Torsions

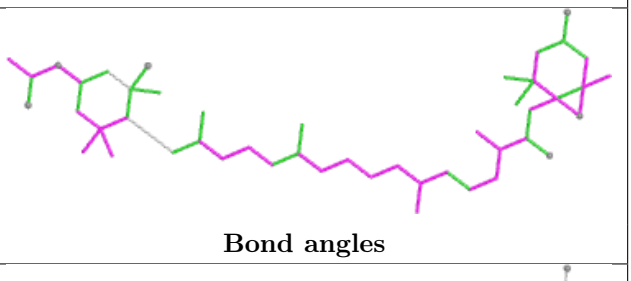


Rings

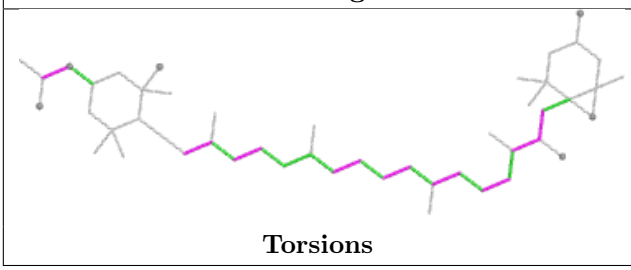
Ligand A86 17 311



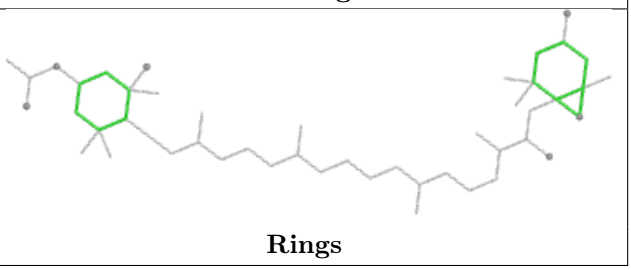
Bond lengths



Bond angles

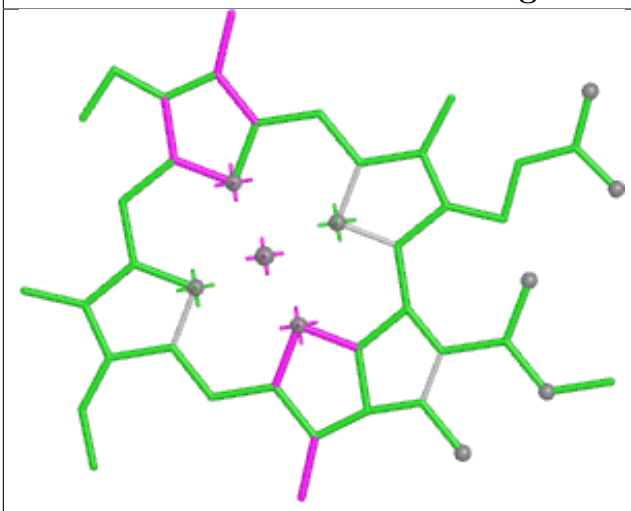


Torsions

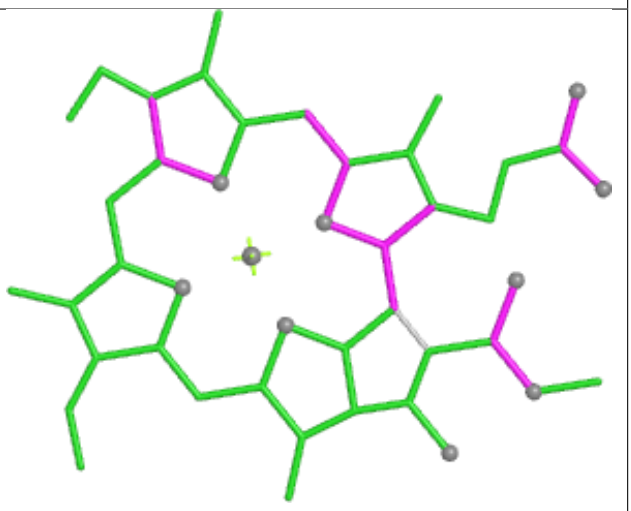


Rings

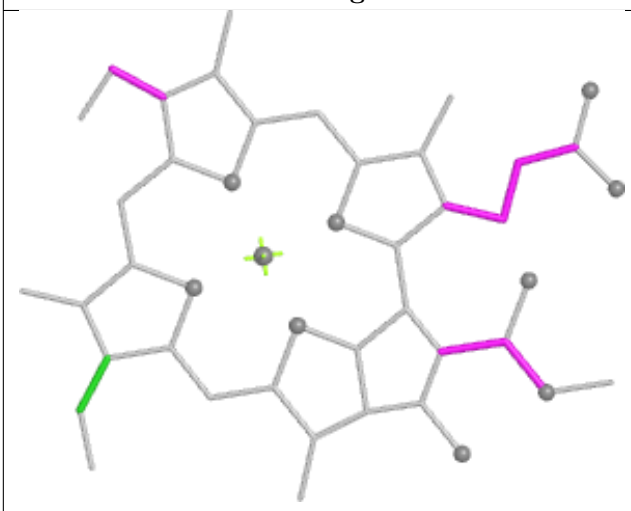
Ligand CLA 18 308



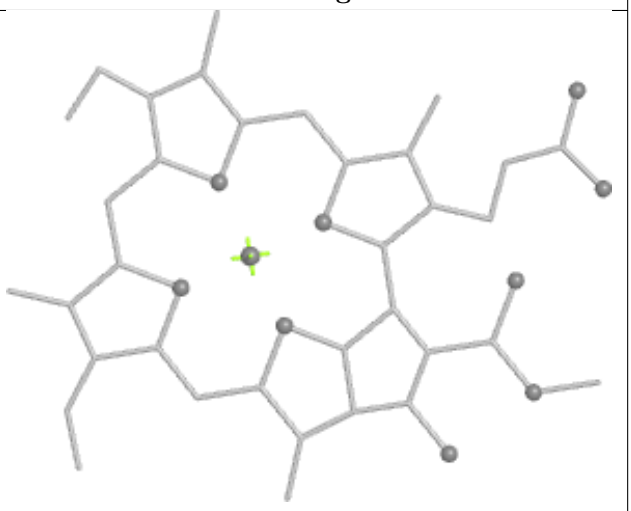
Bond lengths



Bond angles

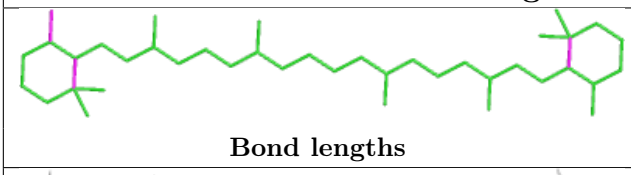


Torsions

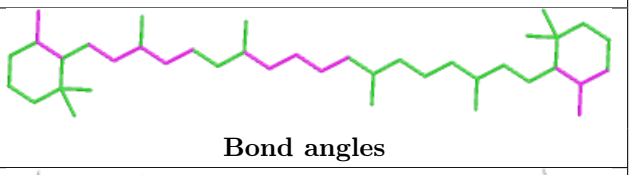


Rings

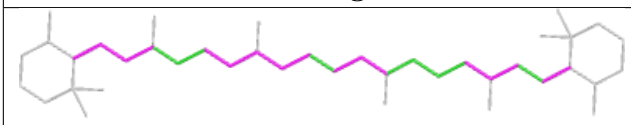
Ligand BCR B 624



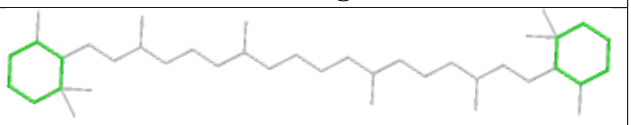
Bond lengths



Bond angles

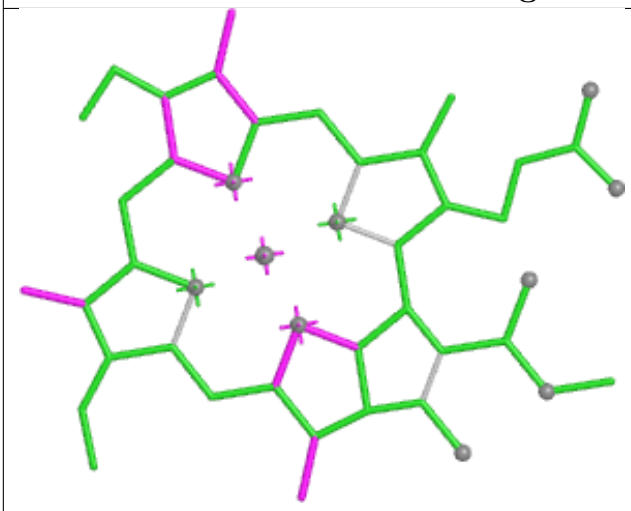


Torsions

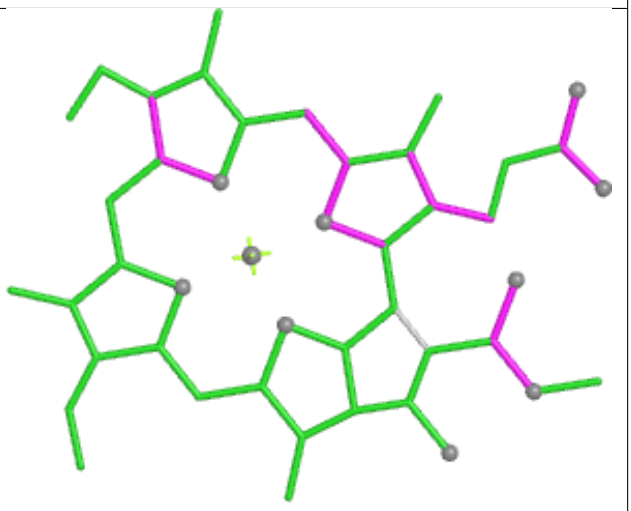


Rings

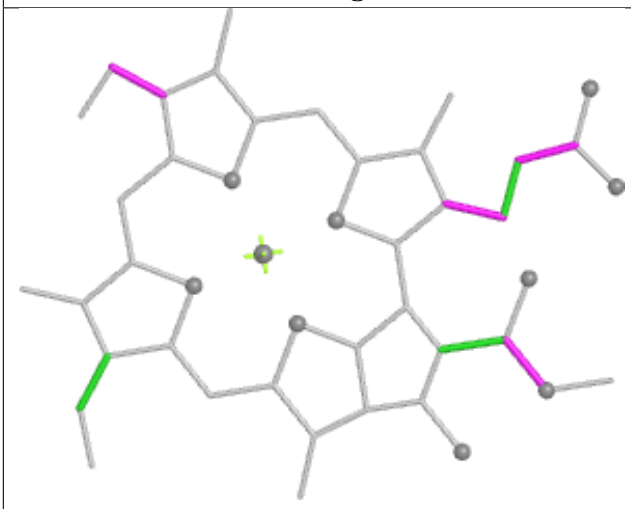
Ligand CLA 14 311



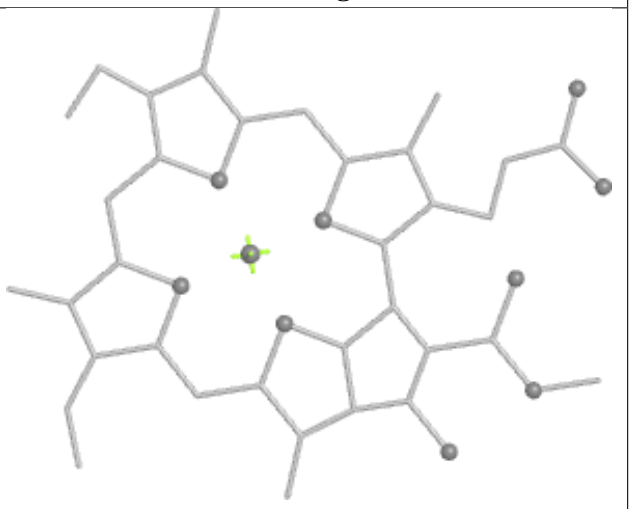
Bond lengths



Bond angles

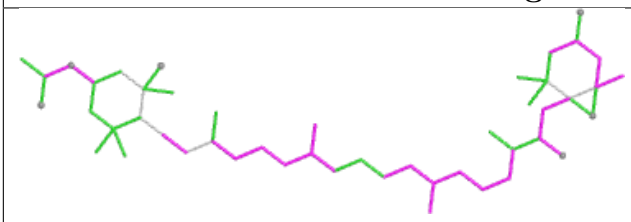


Torsions

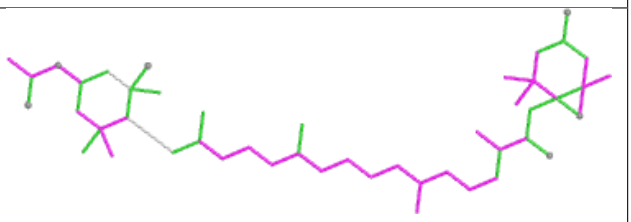


Rings

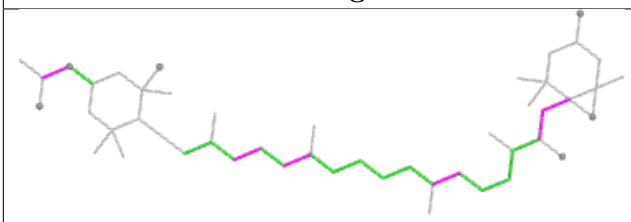
Ligand A86 15 310



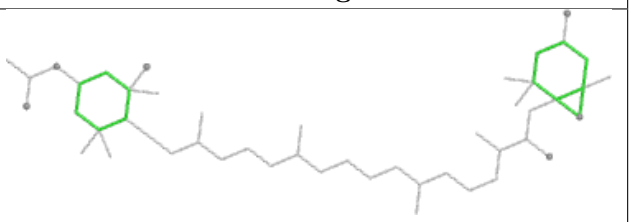
Bond lengths



Bond angles

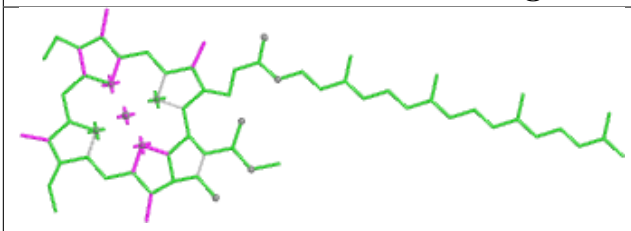


Torsions

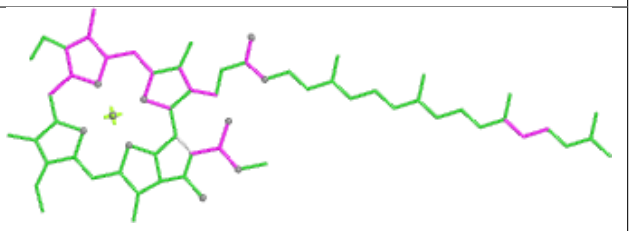


Rings

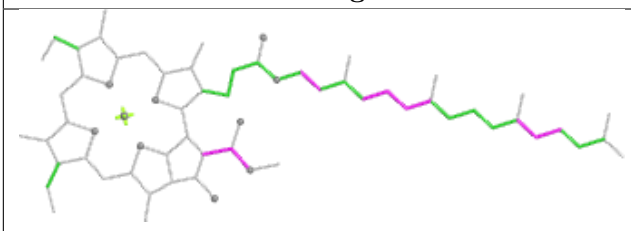
Ligand CLA C 510



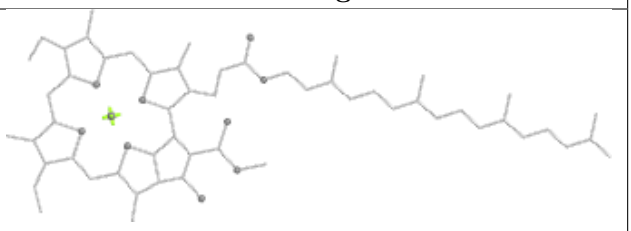
Bond lengths



Bond angles

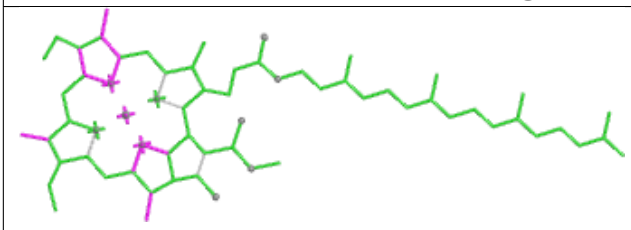


Torsions

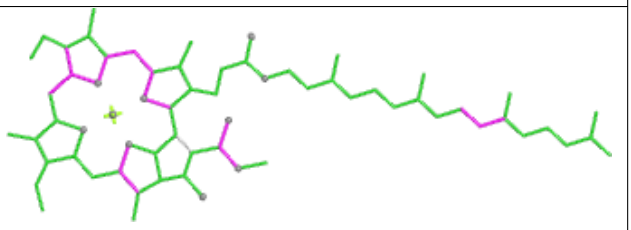


Rings

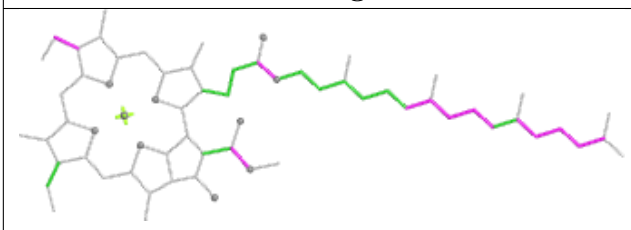
Ligand CLA 19 307



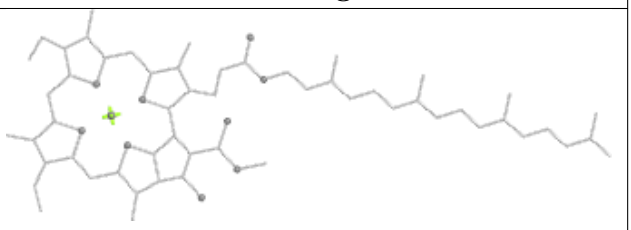
Bond lengths



Bond angles

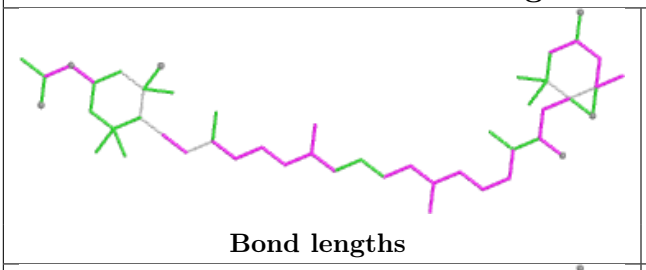


Torsions

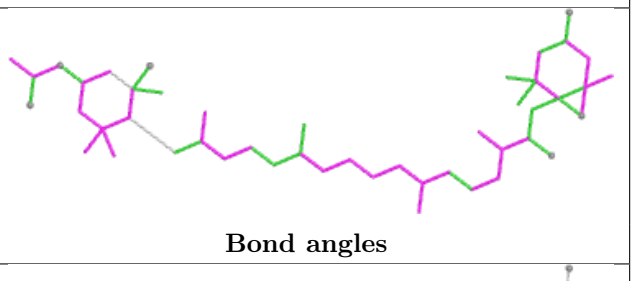


Rings

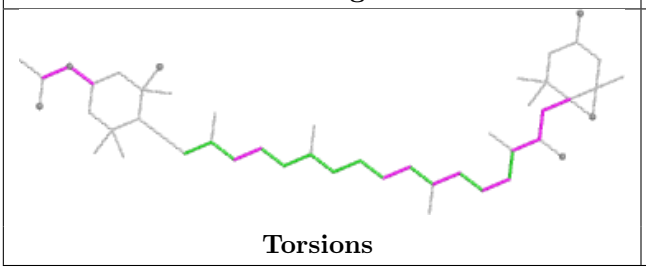
Ligand A86 15 315



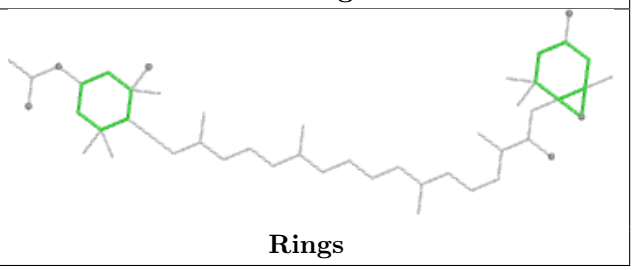
Bond lengths



Bond angles

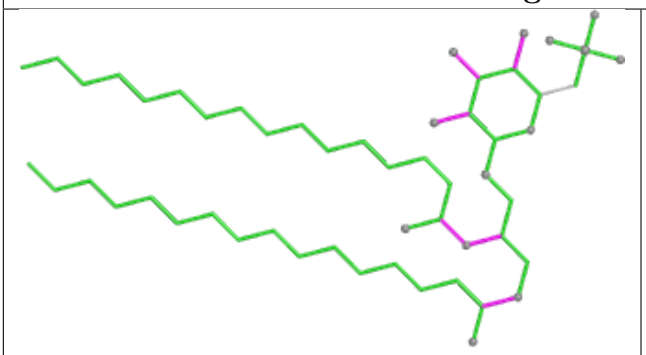


Torsions

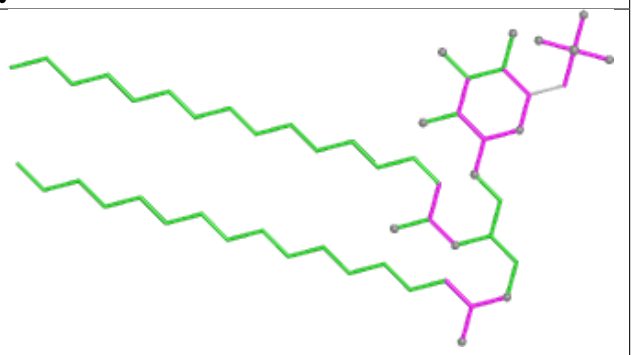


Rings

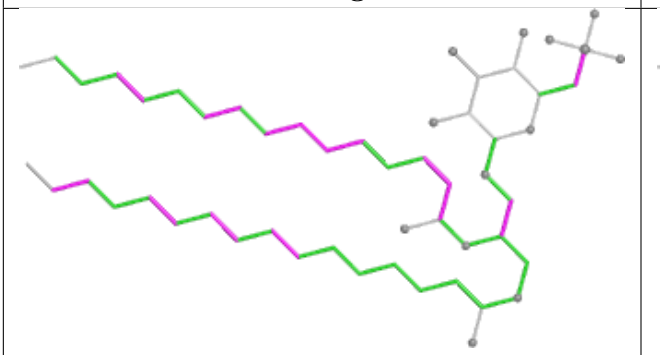
Ligand SQD A 406



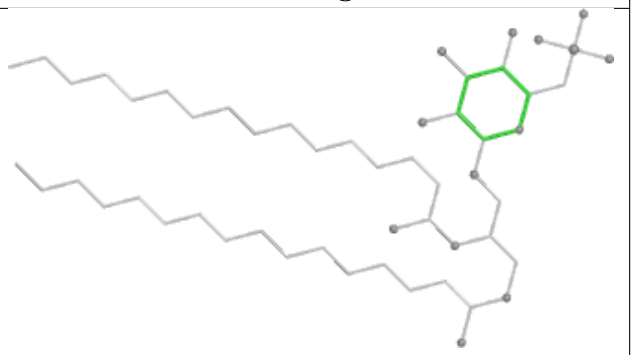
Bond lengths



Bond angles

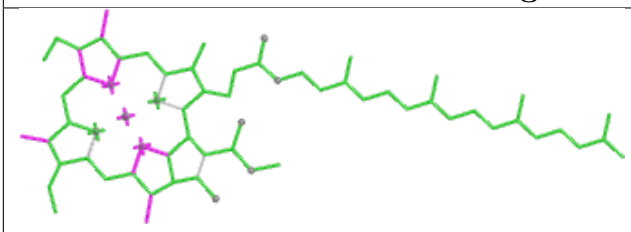


Torsions

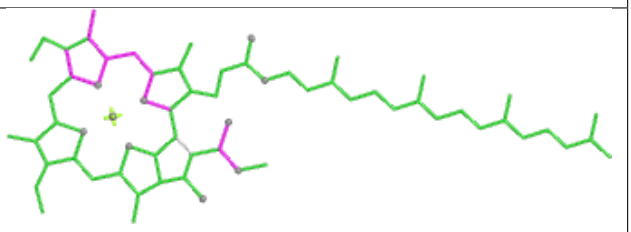


Rings

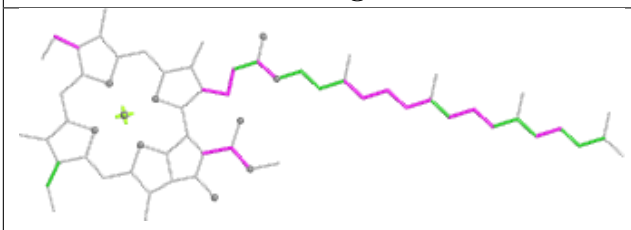
Ligand CLA M 101



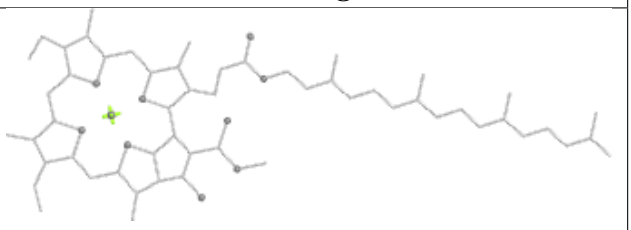
Bond lengths



Bond angles

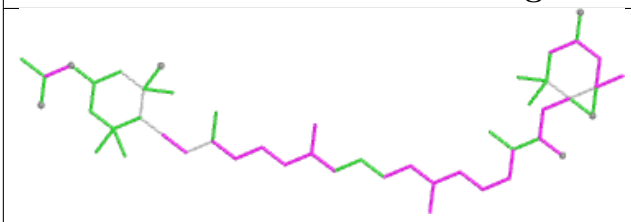


Torsions



Rings

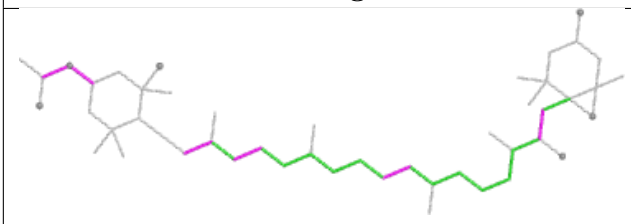
Ligand A86 16 312



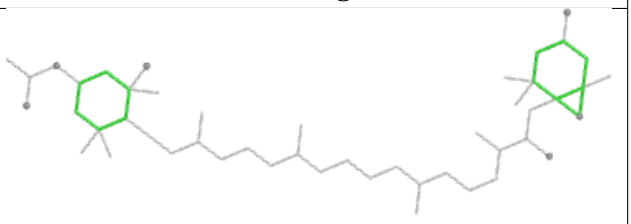
Bond lengths



Bond angles

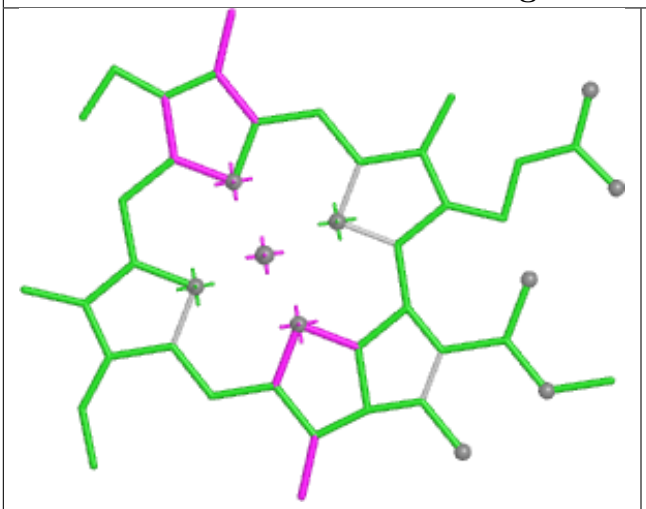


Torsions

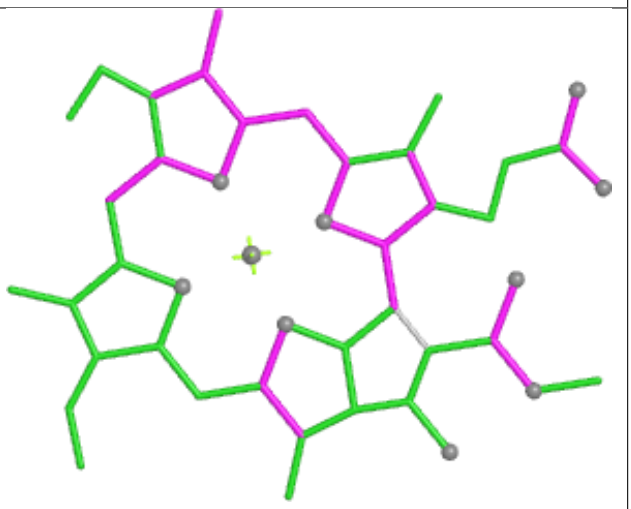


Rings

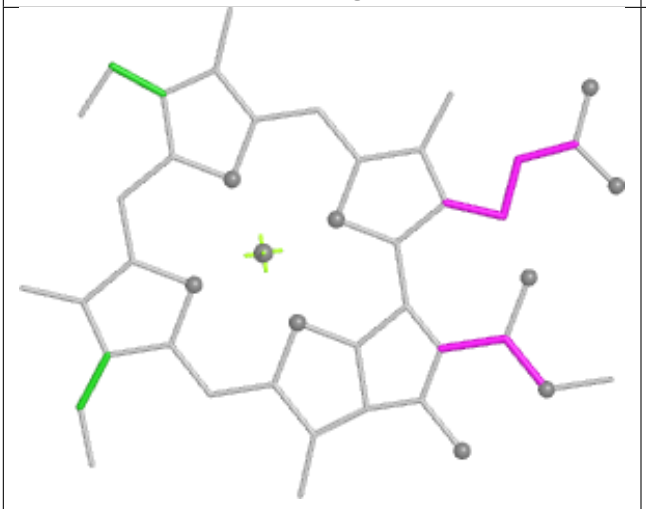
Ligand CLA 16 305



Bond lengths



Bond angles

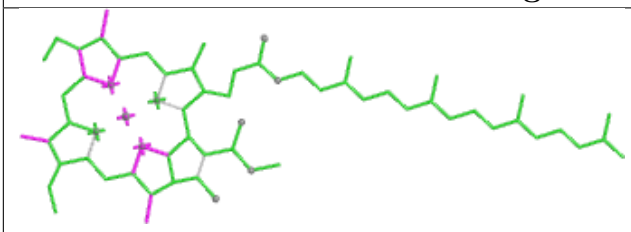


Torsions

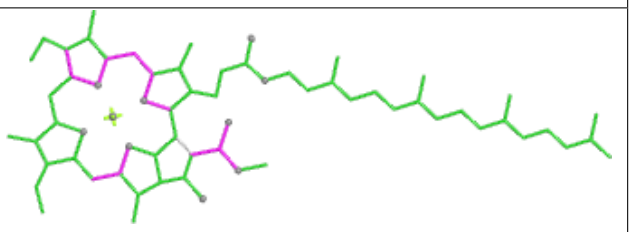


Rings

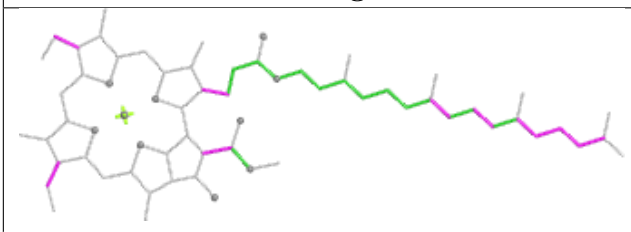
Ligand CLA D 402



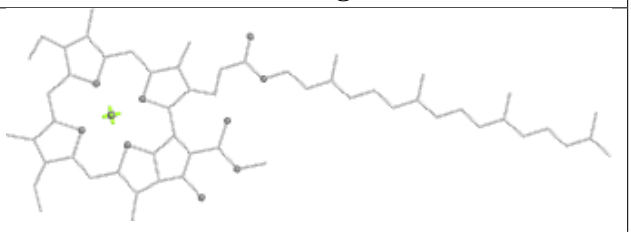
Bond lengths



Bond angles

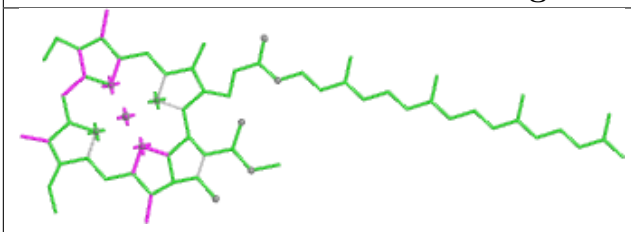


Torsions

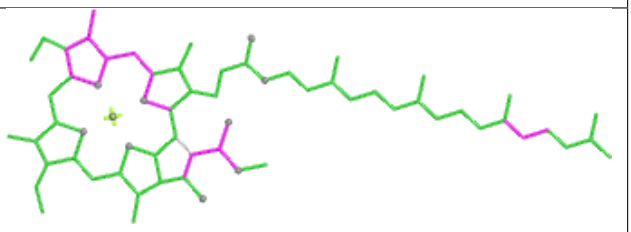


Rings

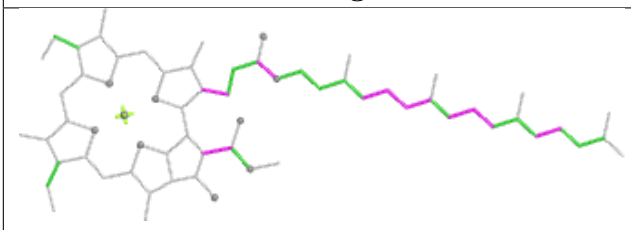
Ligand CLA c 509



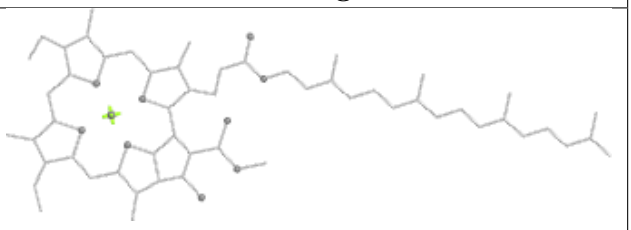
Bond lengths



Bond angles

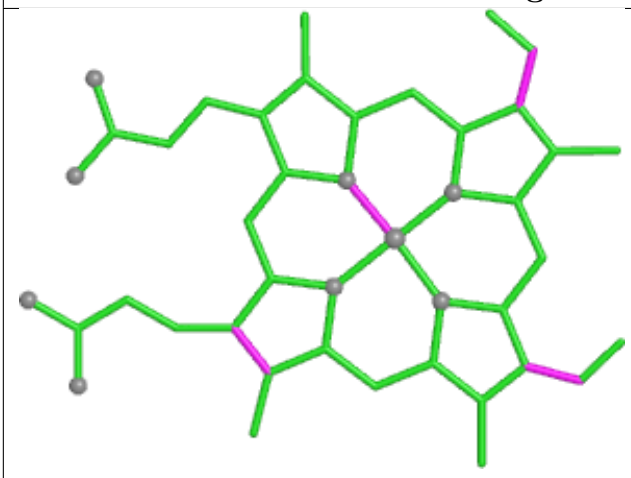


Torsions

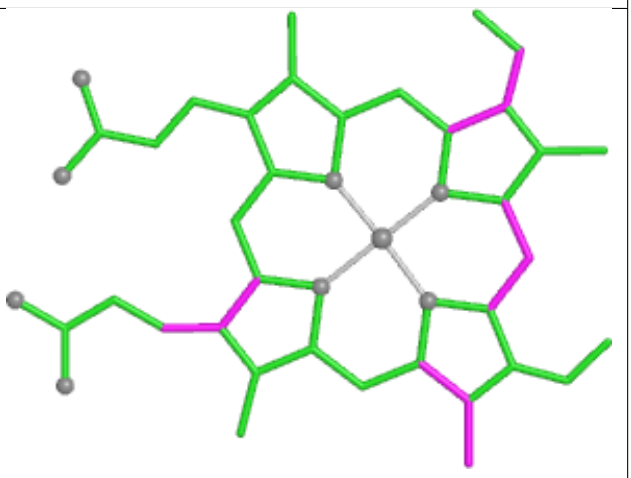


Rings

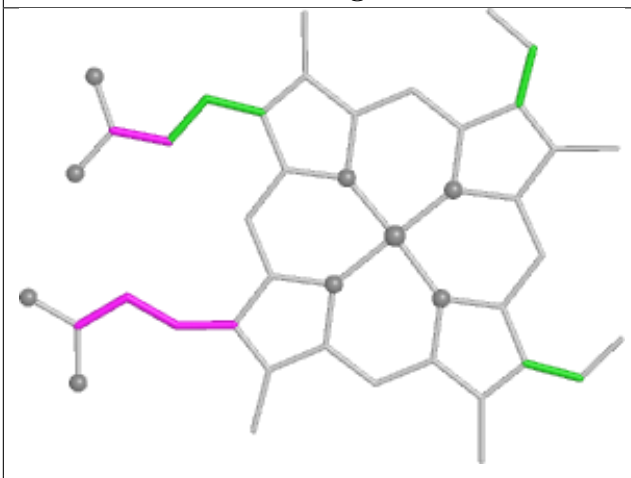
Ligand HEM f 102



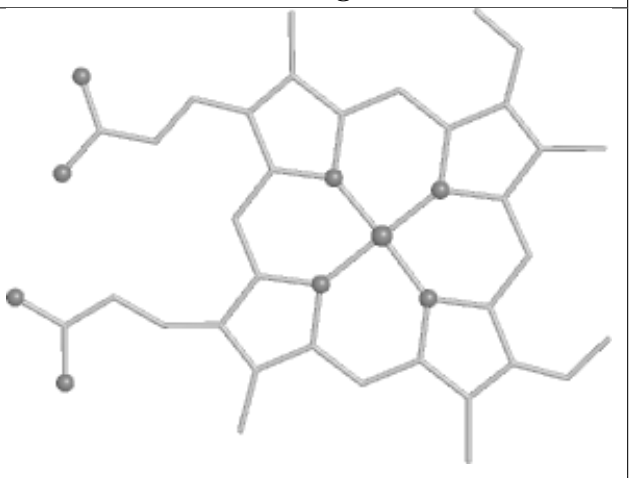
Bond lengths



Bond angles

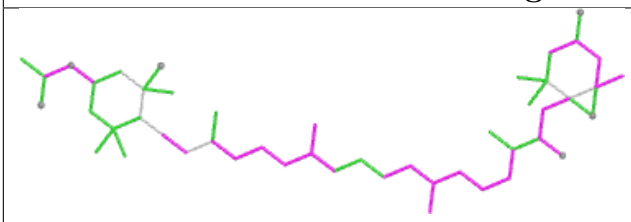


Torsions

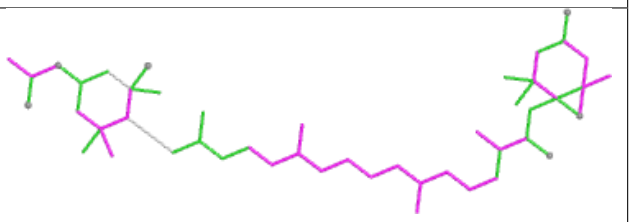


Rings

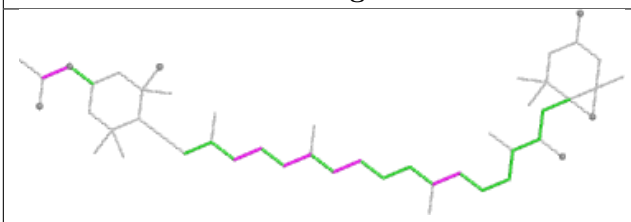
Ligand A86 16 313



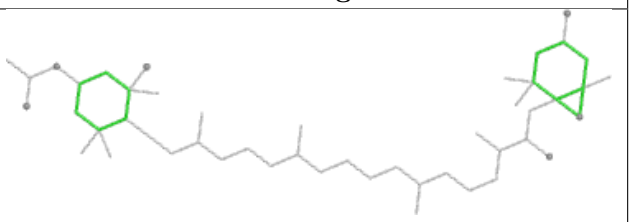
Bond lengths



Bond angles

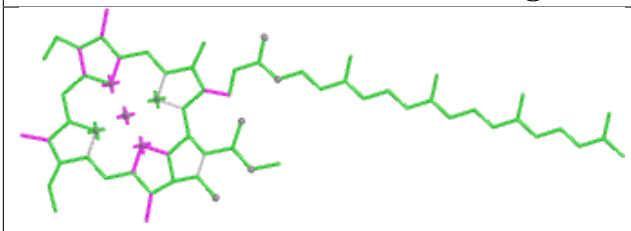


Torsions

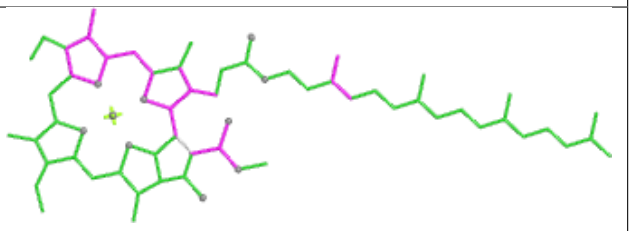


Rings

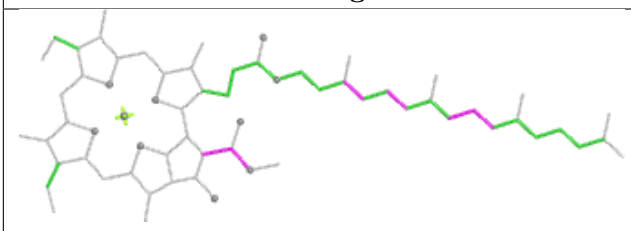
Ligand CLA B 613



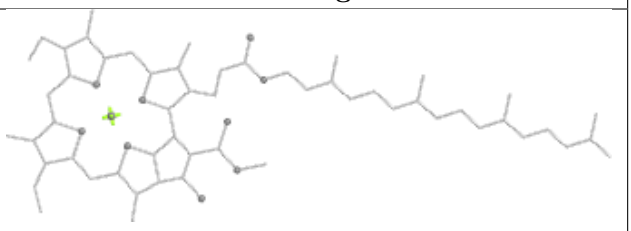
Bond lengths



Bond angles

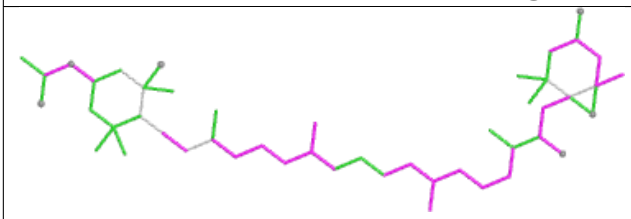


Torsions

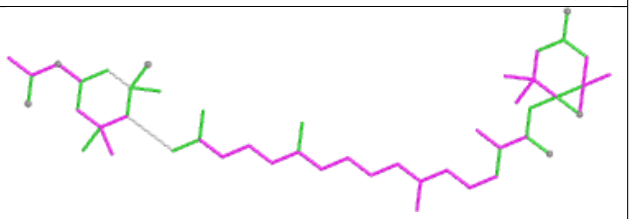


Rings

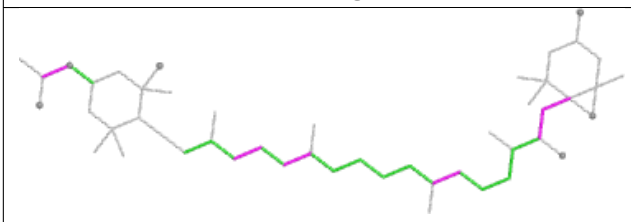
Ligand A86 12 315



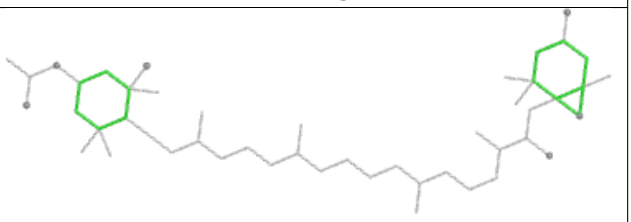
Bond lengths



Bond angles

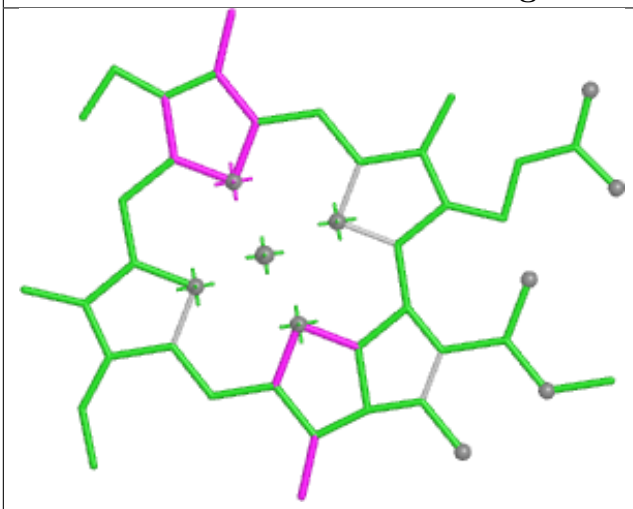


Torsions

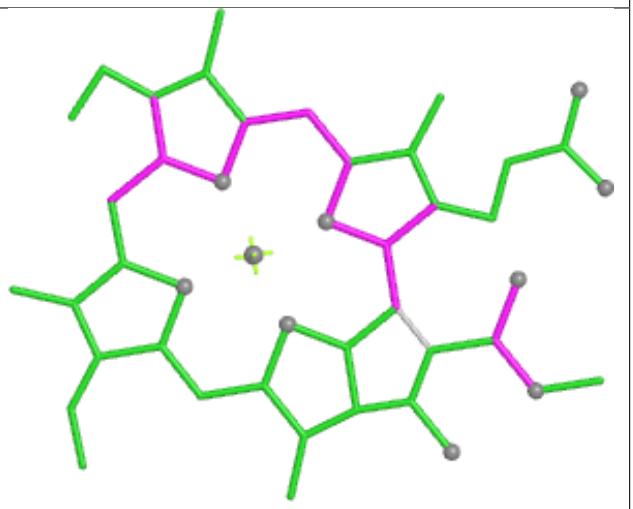


Rings

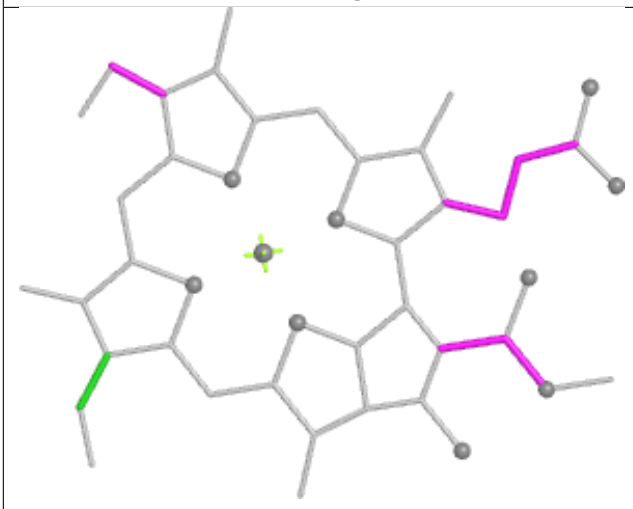
Ligand CLA 13 307



Bond lengths



Bond angles

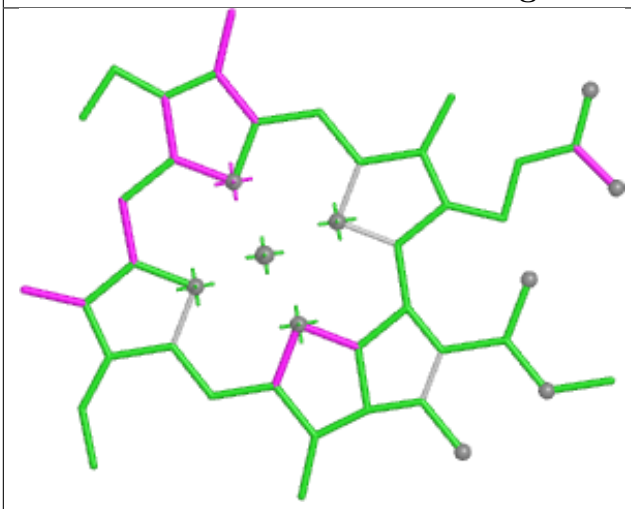


Torsions

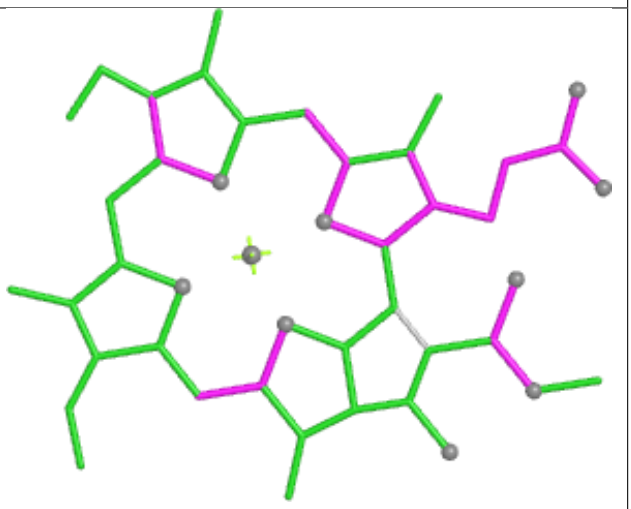


Rings

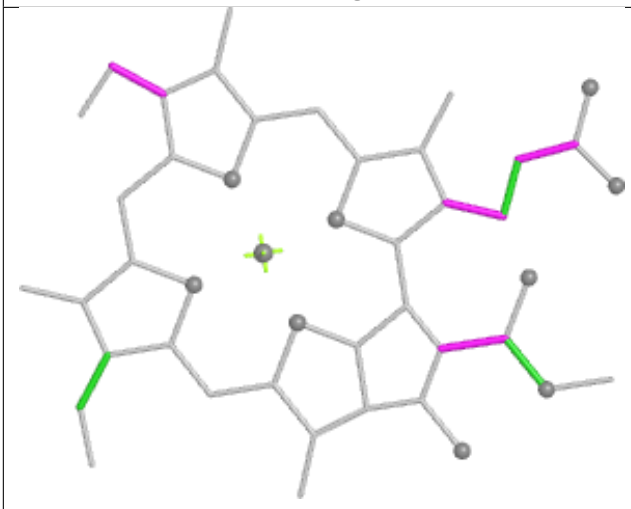
Ligand CLA 21 309



Bond lengths



Bond angles

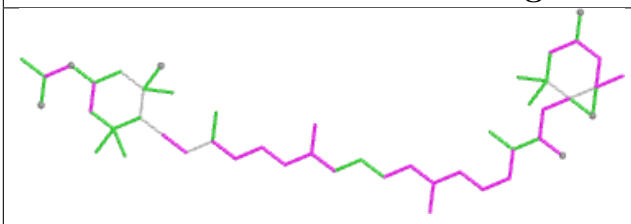


Torsions

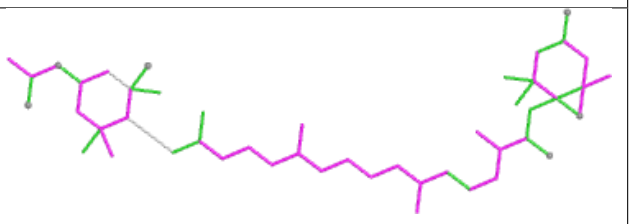


Rings

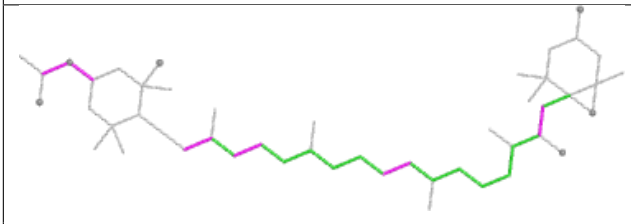
Ligand A86 15 312



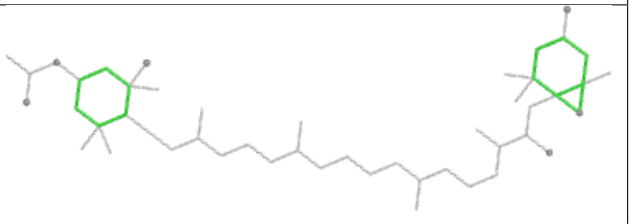
Bond lengths



Bond angles

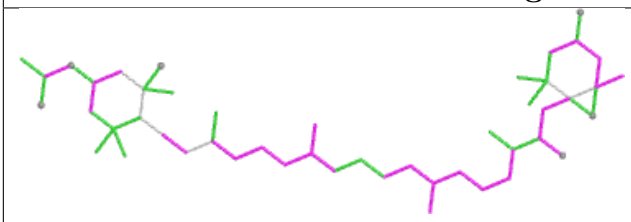


Torsions

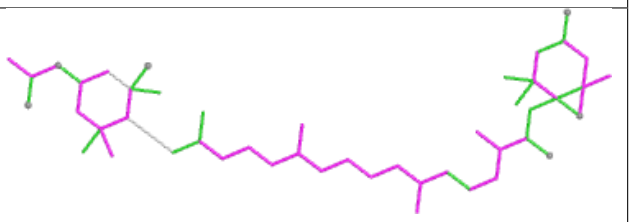


Rings

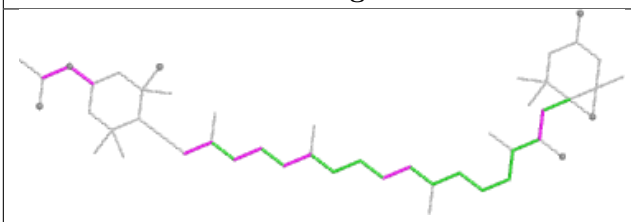
Ligand A86 17 313



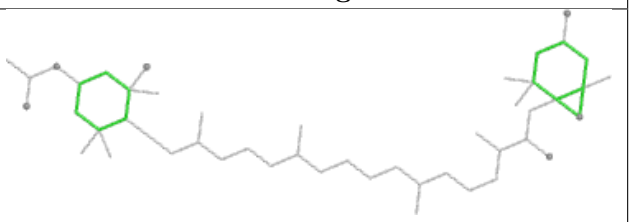
Bond lengths



Bond angles

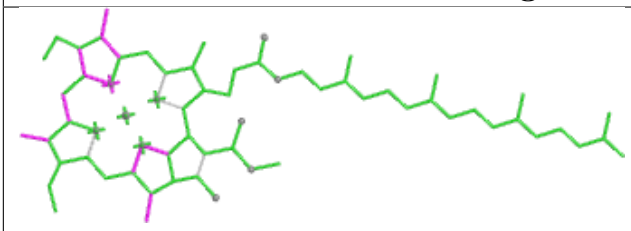


Torsions

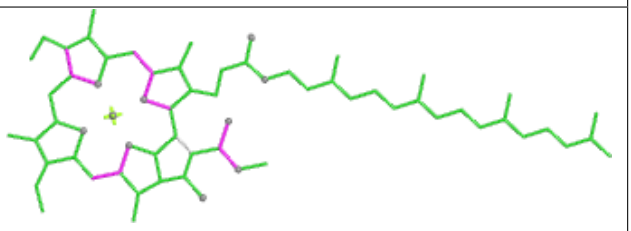


Rings

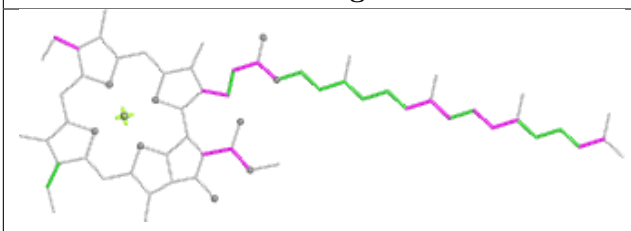
Ligand CLA 18 305



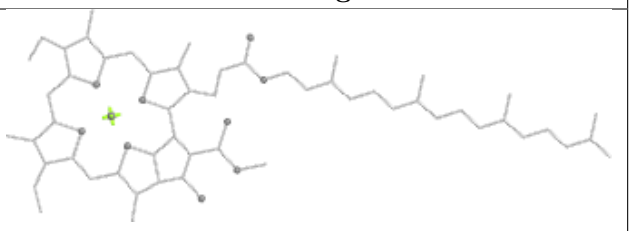
Bond lengths



Bond angles

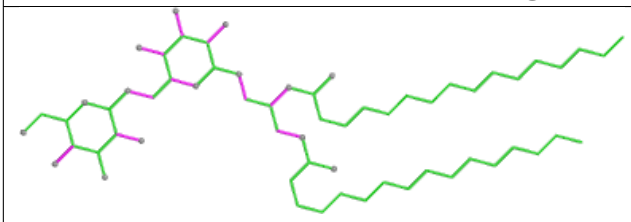


Torsions

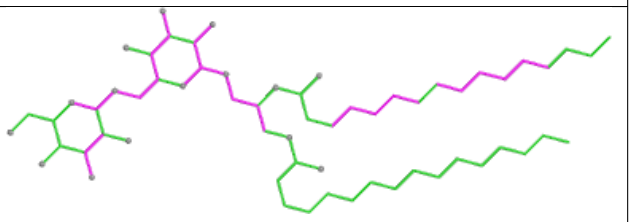


Rings

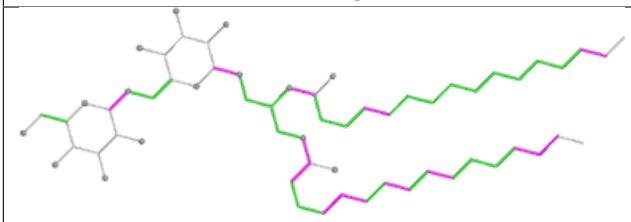
Ligand DGD J 101



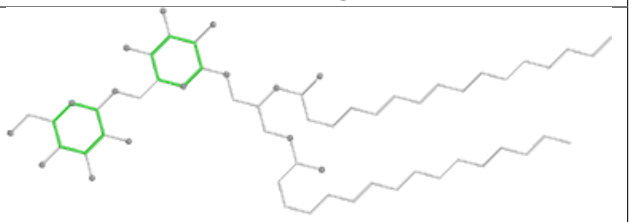
Bond lengths



Bond angles

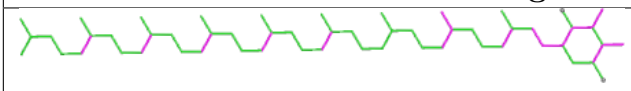


Torsions

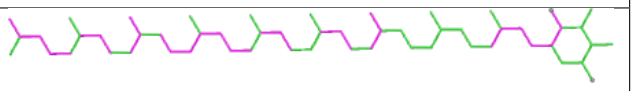


Rings

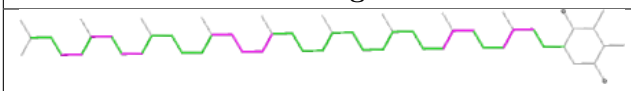
Ligand PL9 D 407



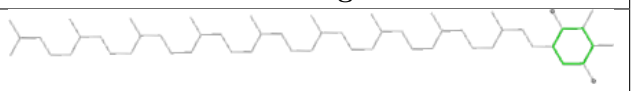
Bond lengths



Bond angles

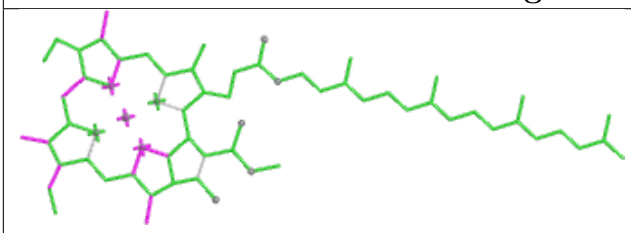


Torsions

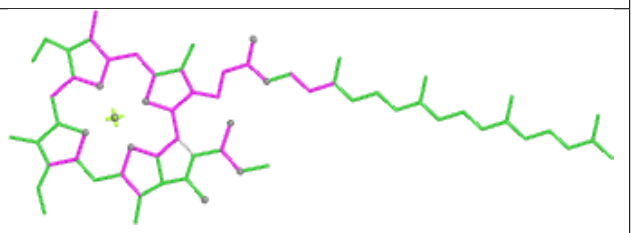


Rings

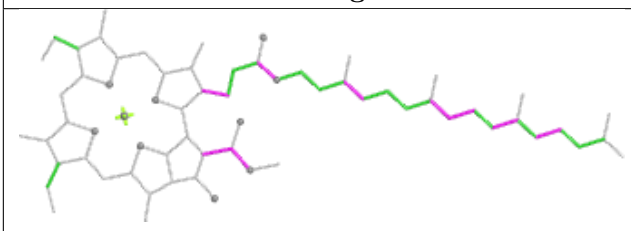
Ligand CLA B 604



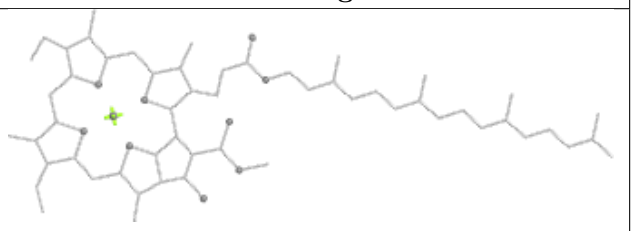
Bond lengths



Bond angles

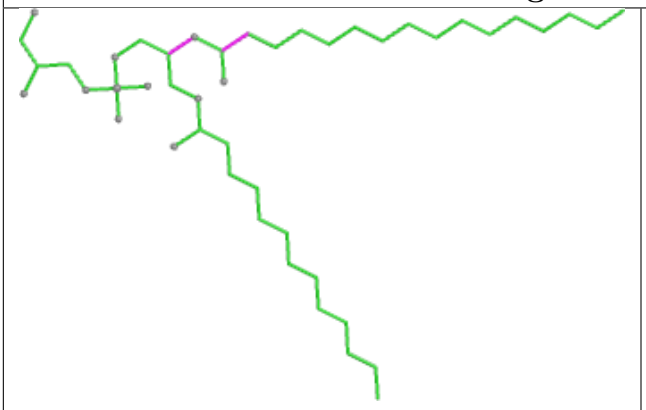


Torsions

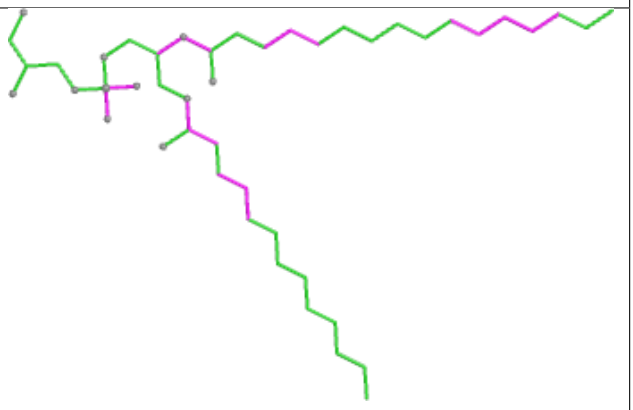


Rings

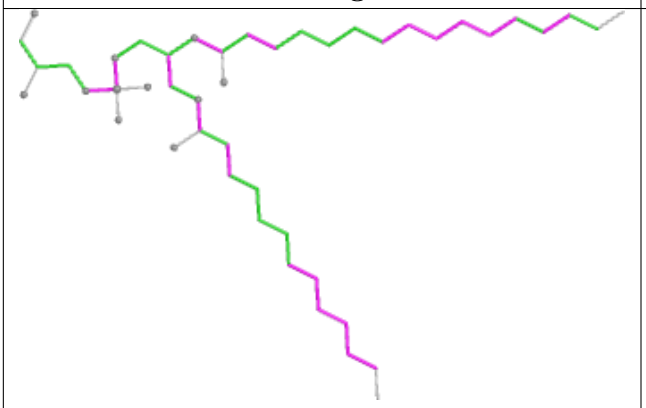
Ligand LHG a 407



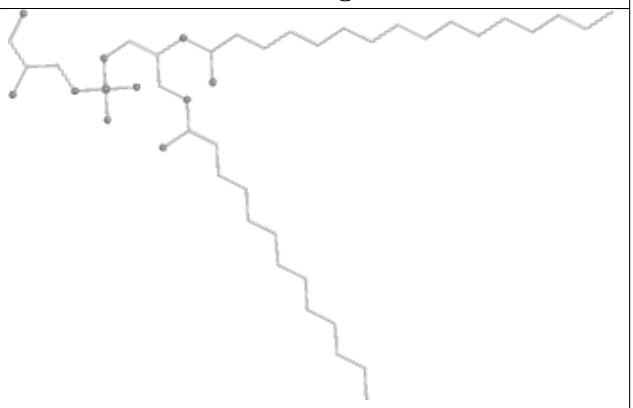
Bond lengths



Bond angles

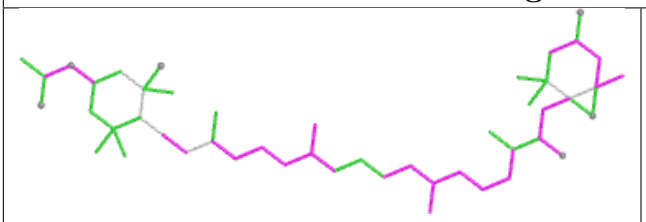


Torsions

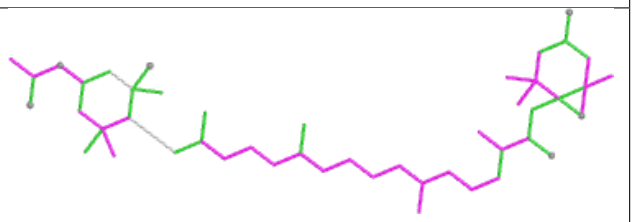


Rings

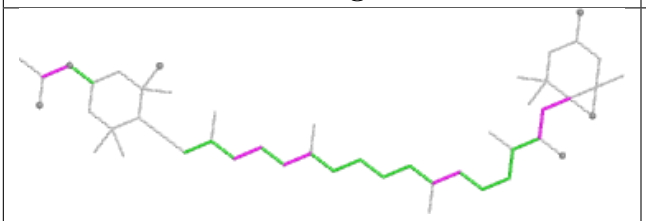
Ligand A86 14 312



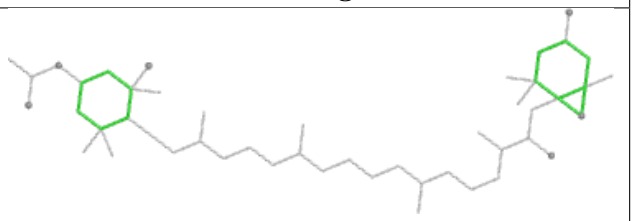
Bond lengths



Bond angles

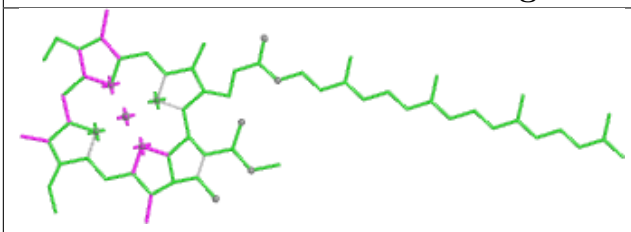


Torsions

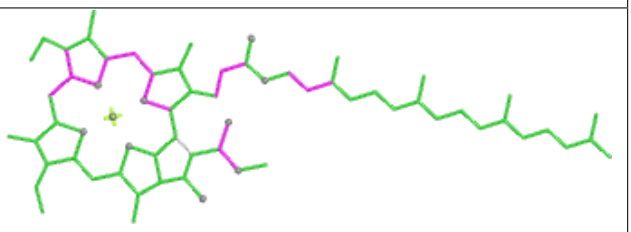


Rings

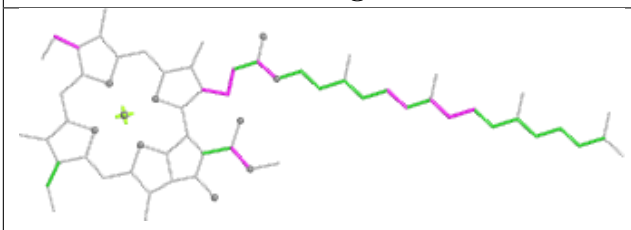
Ligand CLA 11 301



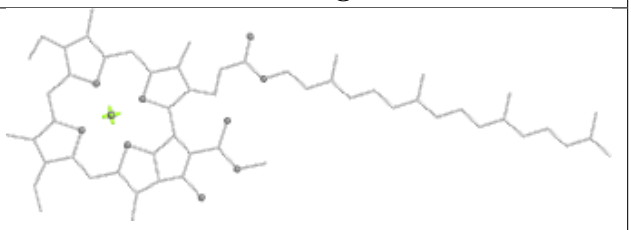
Bond lengths



Bond angles



Torsions

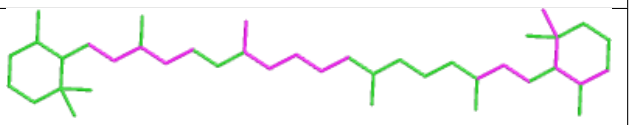


Rings

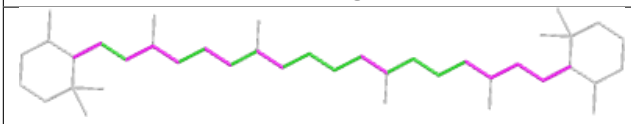
Ligand BCR f 101



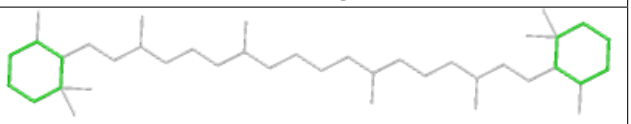
Bond lengths



Bond angles

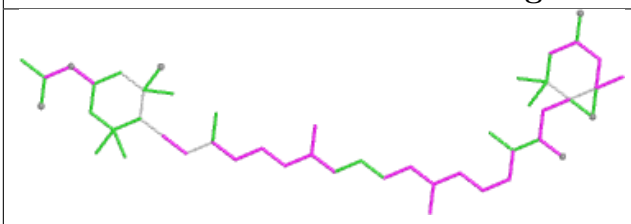


Torsions

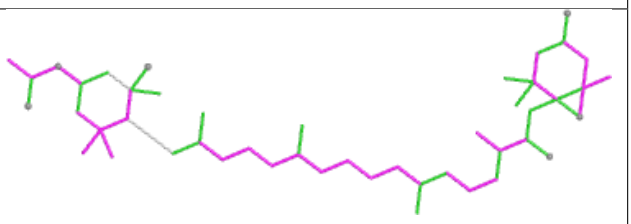


Rings

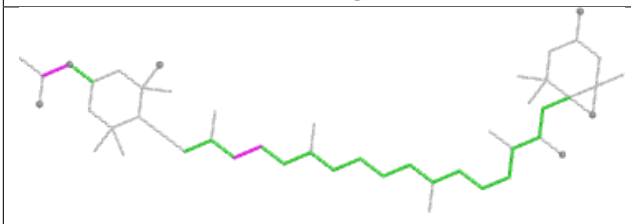
Ligand A86 14 313



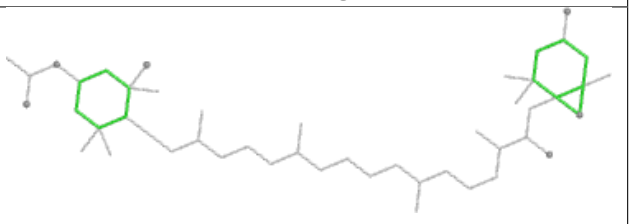
Bond lengths



Bond angles

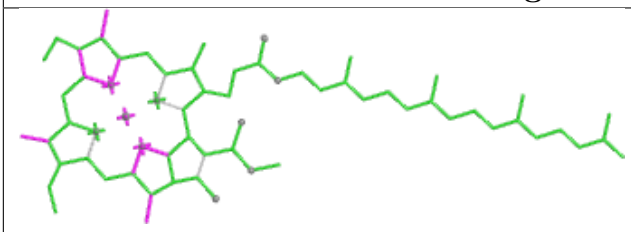


Torsions

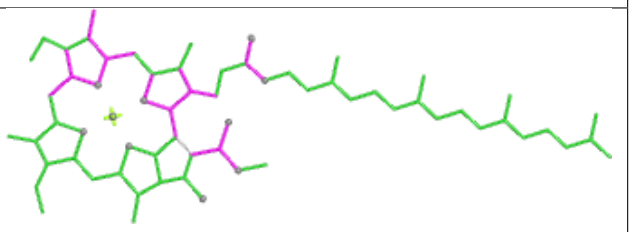


Rings

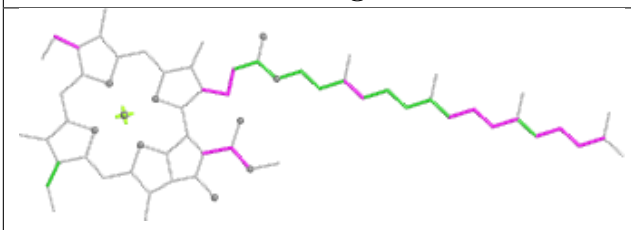
Ligand CLA C 507



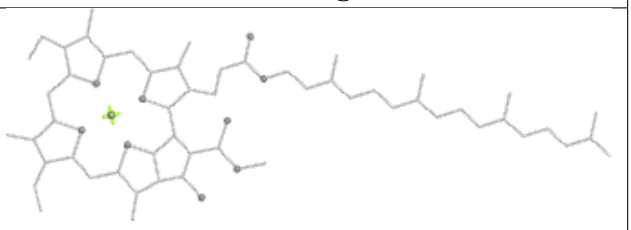
Bond lengths



Bond angles

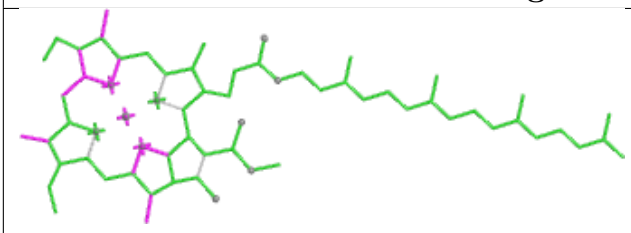


Torsions

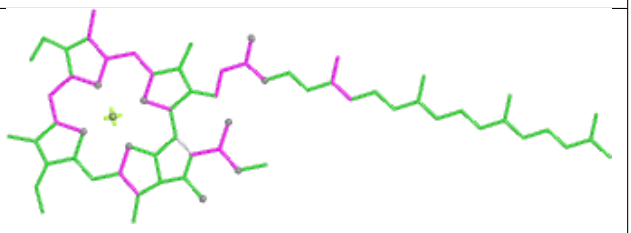


Rings

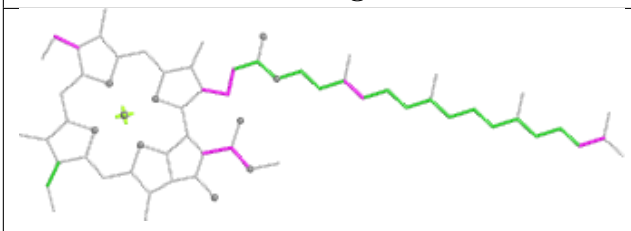
Ligand CLA b 603



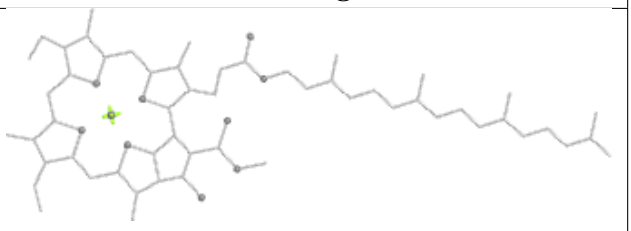
Bond lengths



Bond angles

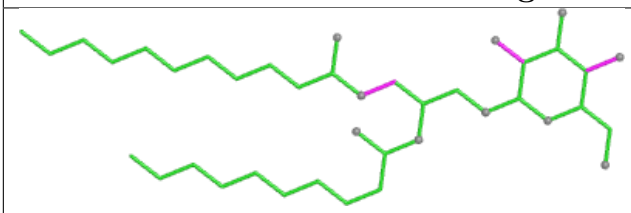


Torsions

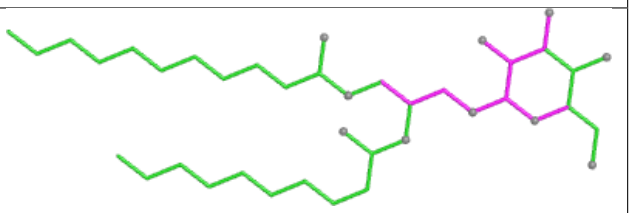


Rings

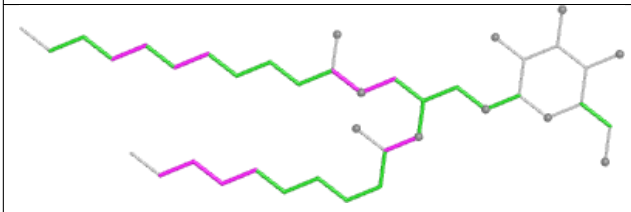
Ligand LMG m 102



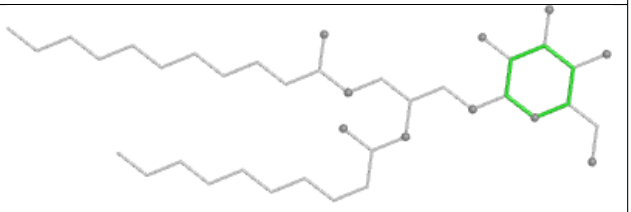
Bond lengths



Bond angles

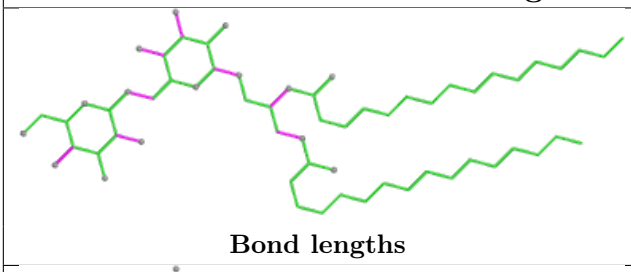


Torsions

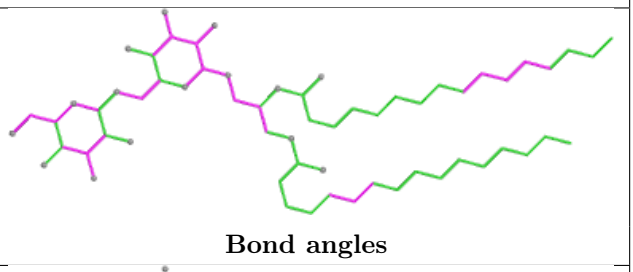


Rings

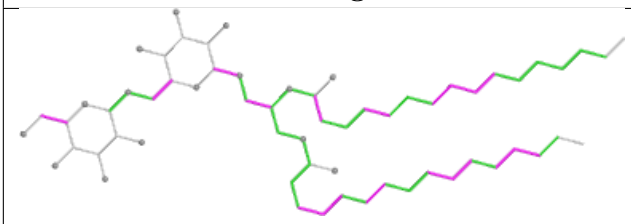
Ligand DGD c 517



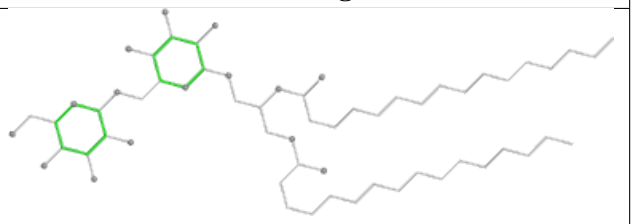
Bond lengths



Bond angles

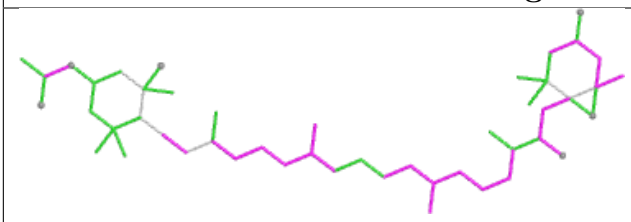


Torsions

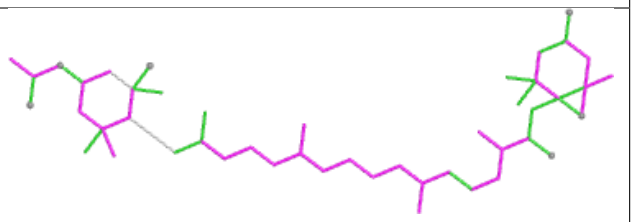


Rings

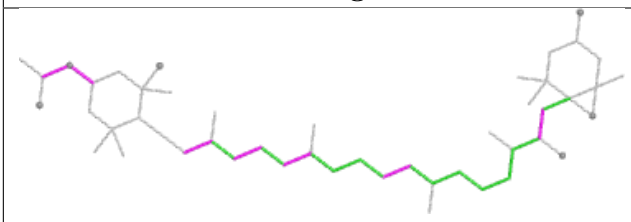
Ligand A86 12 317



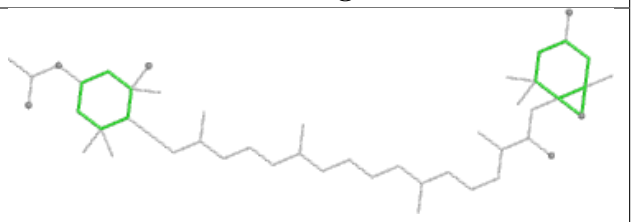
Bond lengths



Bond angles

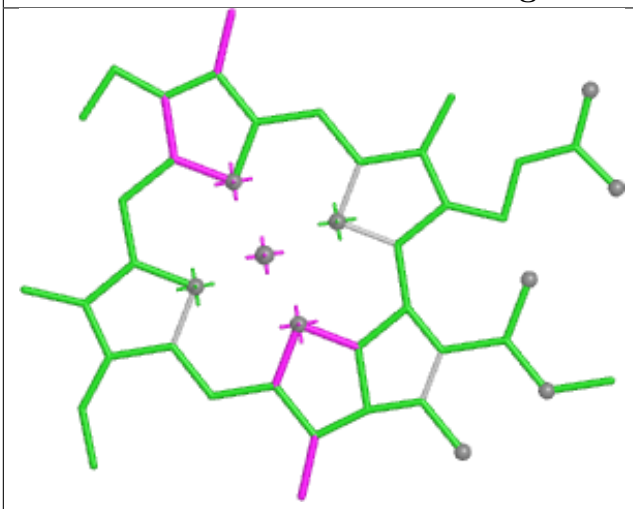


Torsions

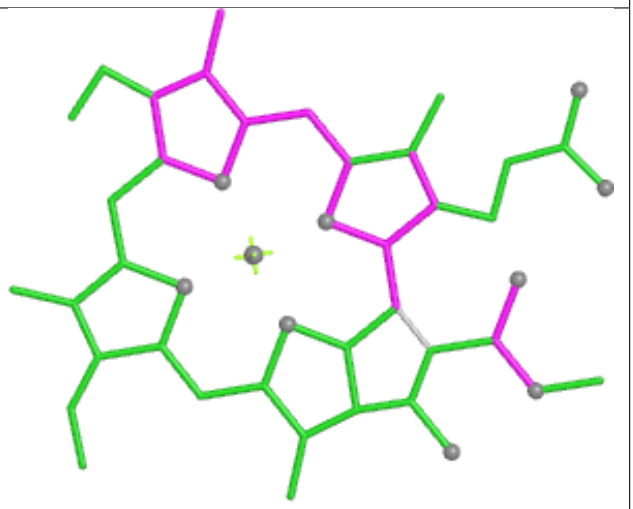


Rings

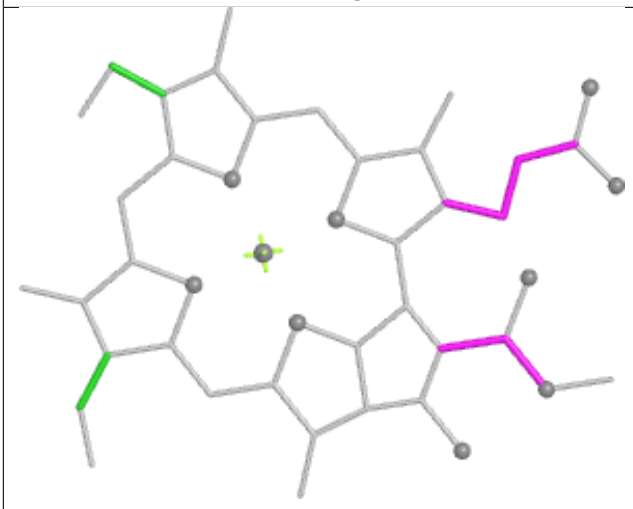
Ligand CLA 18 306



Bond lengths



Bond angles

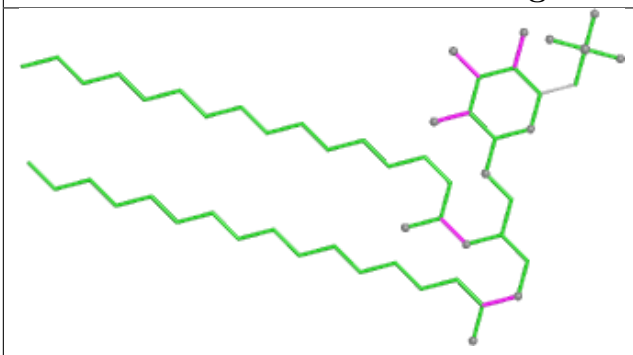


Torsions

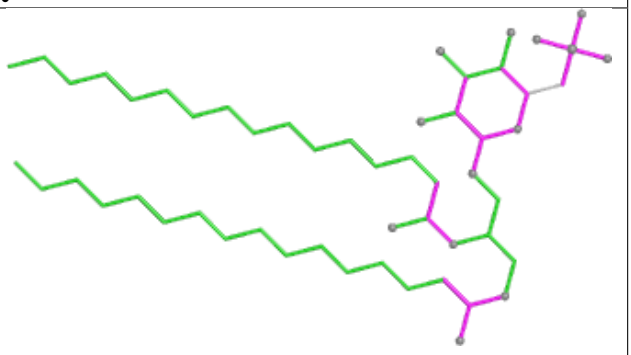


Rings

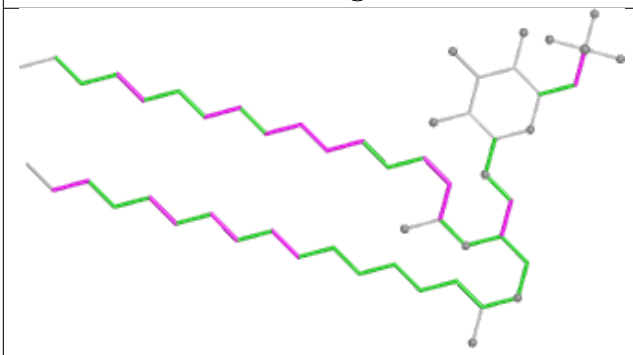
Ligand SQD a 405



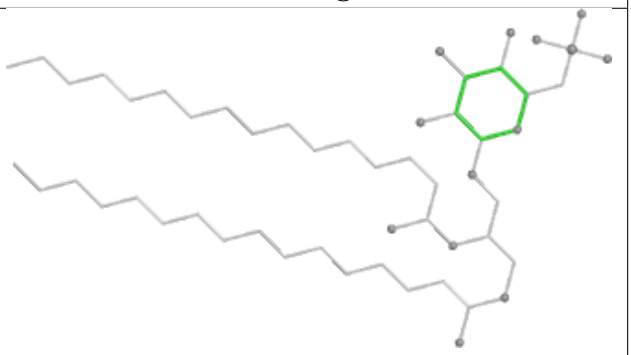
Bond lengths



Bond angles

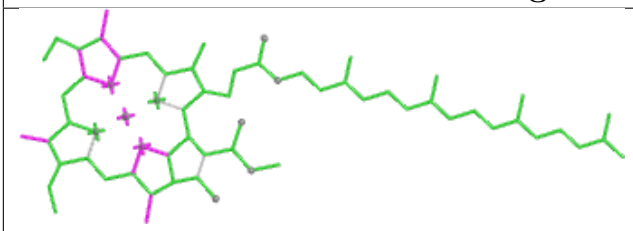


Torsions

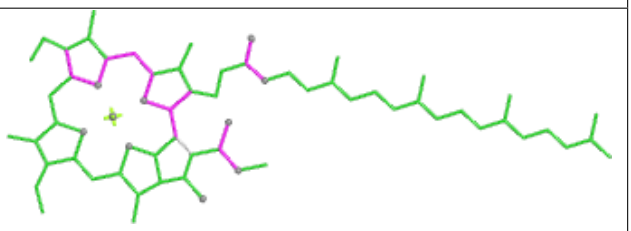


Rings

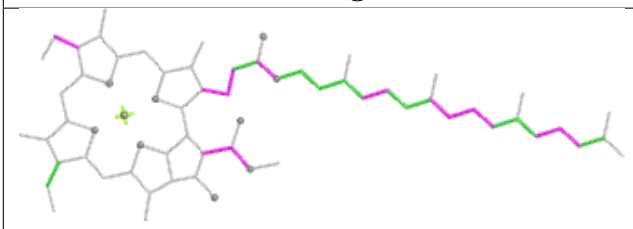
Ligand CLA c 513



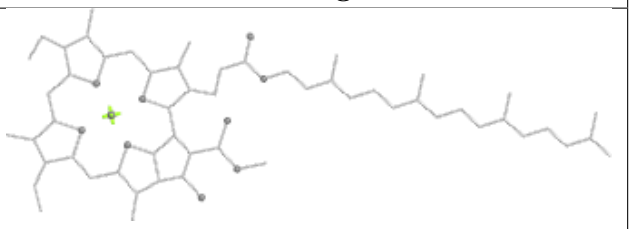
Bond lengths



Bond angles

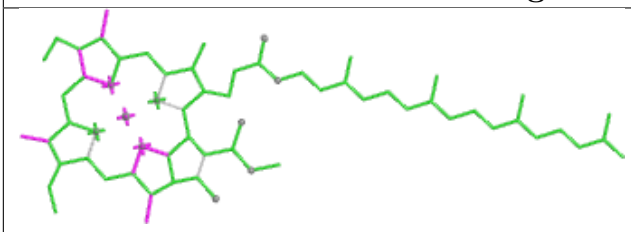


Torsions

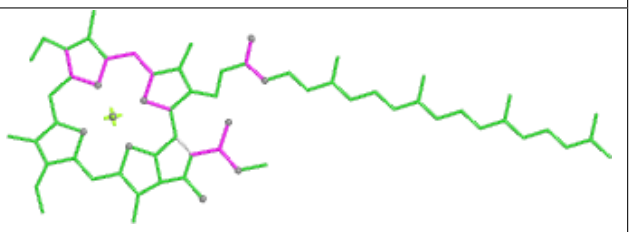


Rings

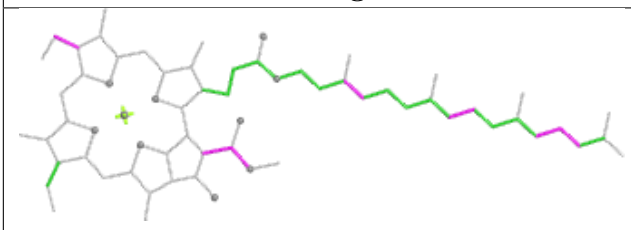
Ligand CLA b 608



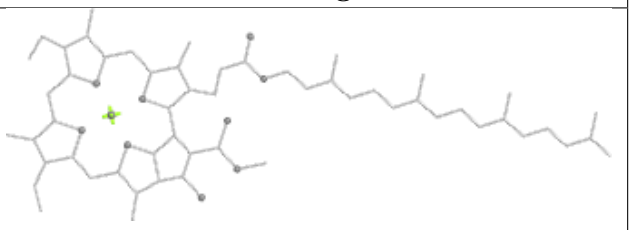
Bond lengths



Bond angles



Torsions

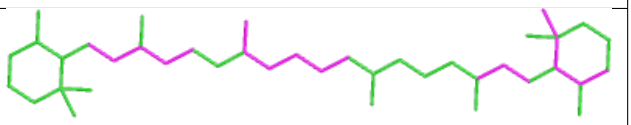


Rings

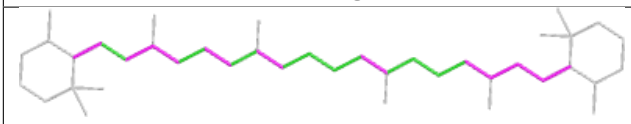
Ligand BCR F 101



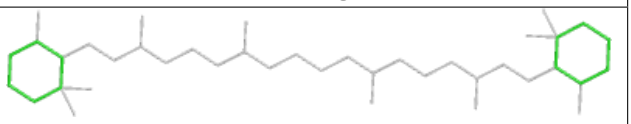
Bond lengths



Bond angles

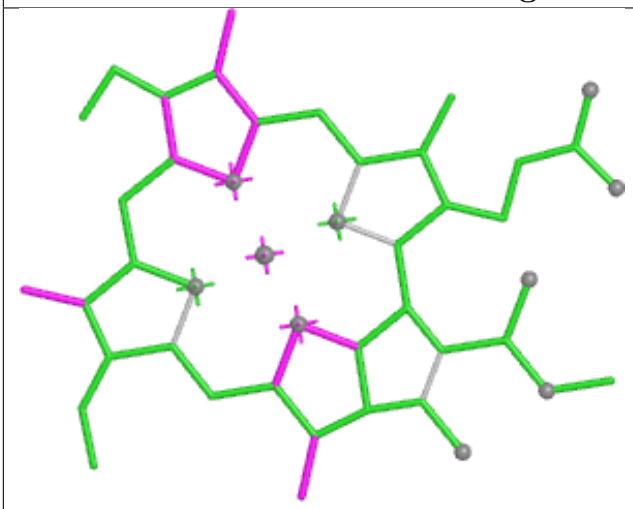


Torsions

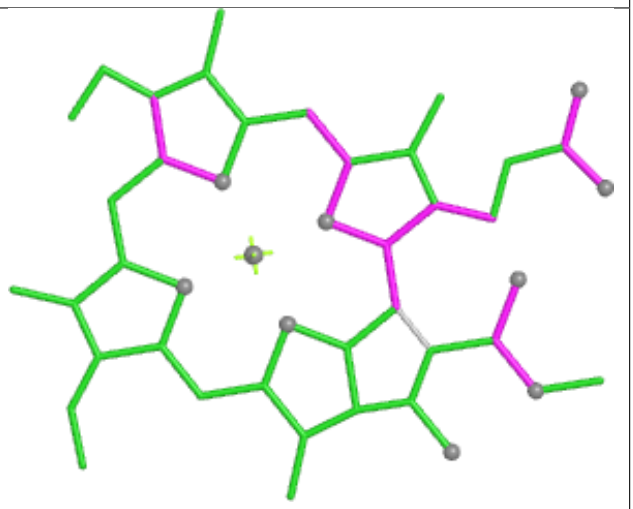


Rings

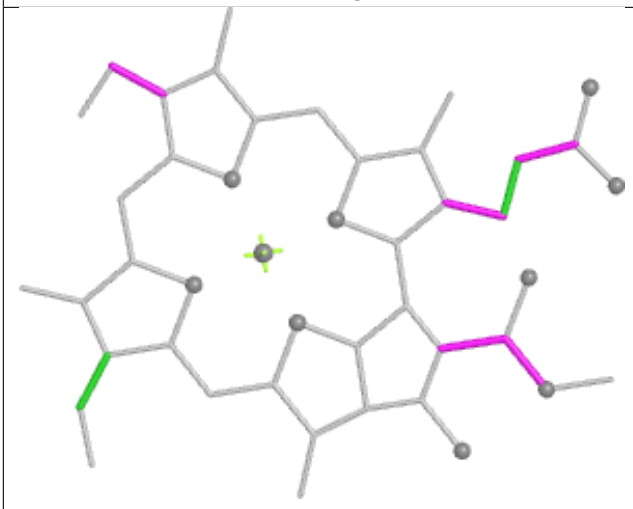
Ligand CLA 20 207



Bond lengths



Bond angles

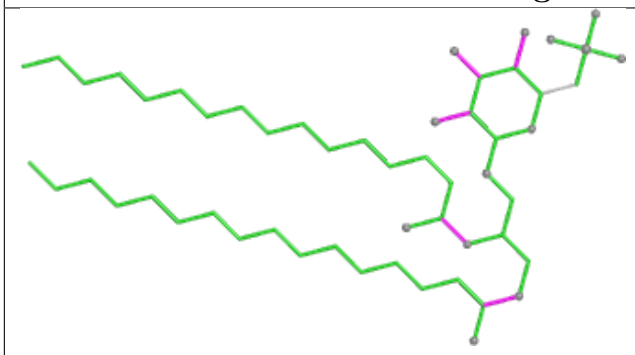


Torsions

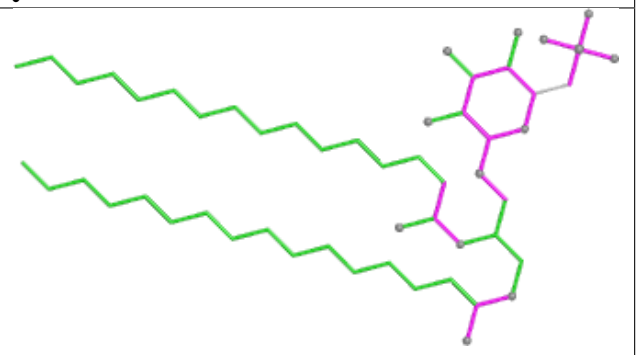


Rings

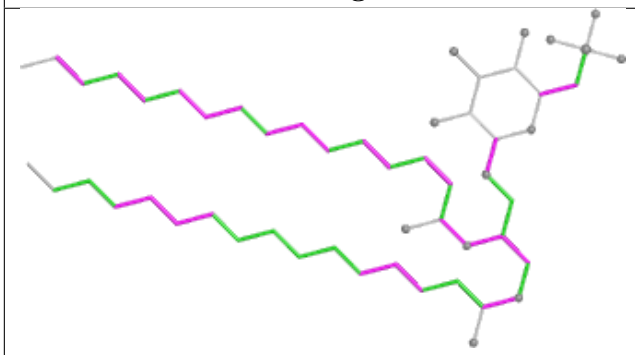
Ligand SQD l 101



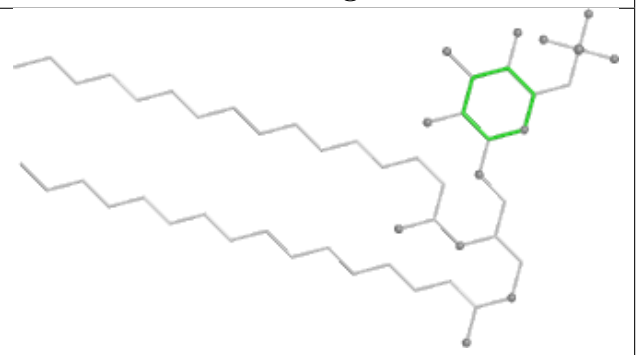
Bond lengths



Bond angles

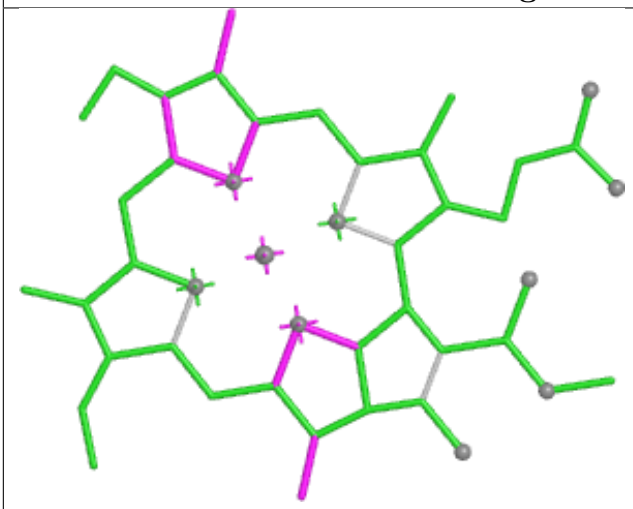


Torsions

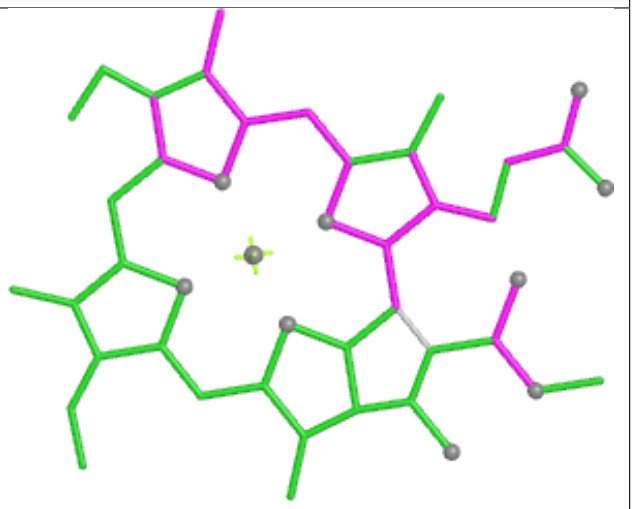


Rings

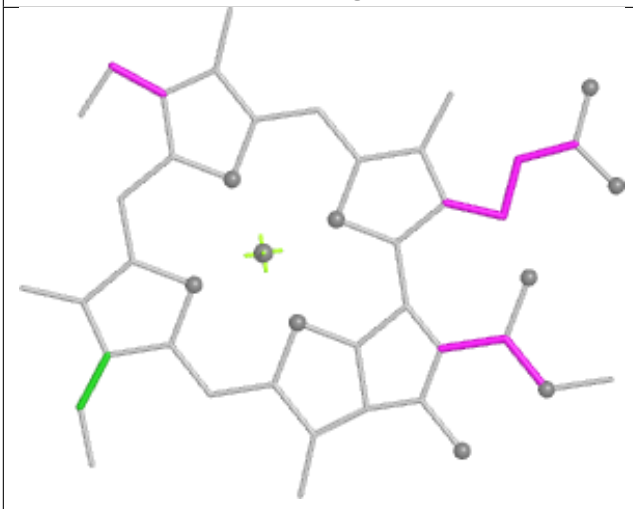
Ligand CLA 19 304



Bond lengths



Bond angles

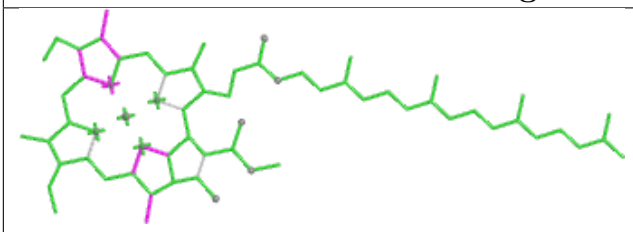


Torsions

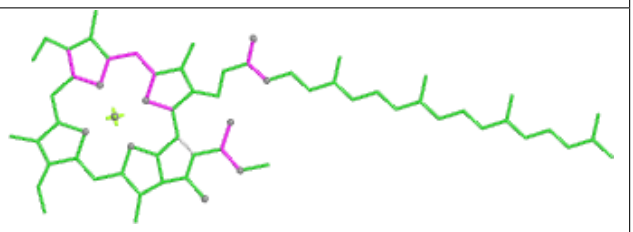


Rings

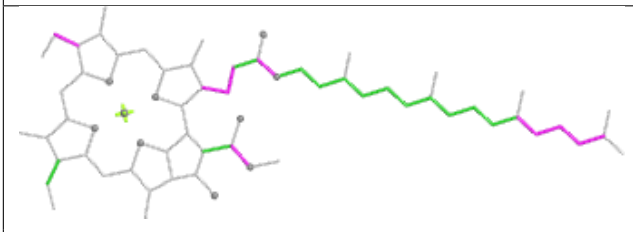
Ligand CLA 21 307



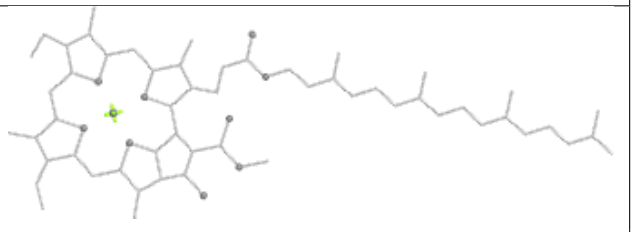
Bond lengths



Bond angles

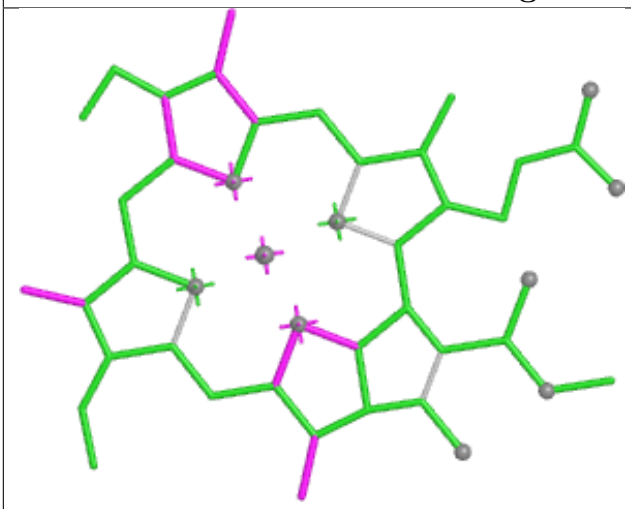


Torsions

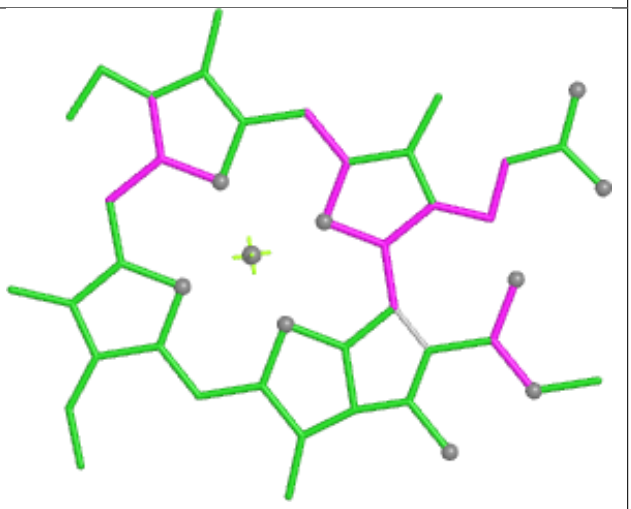


Rings

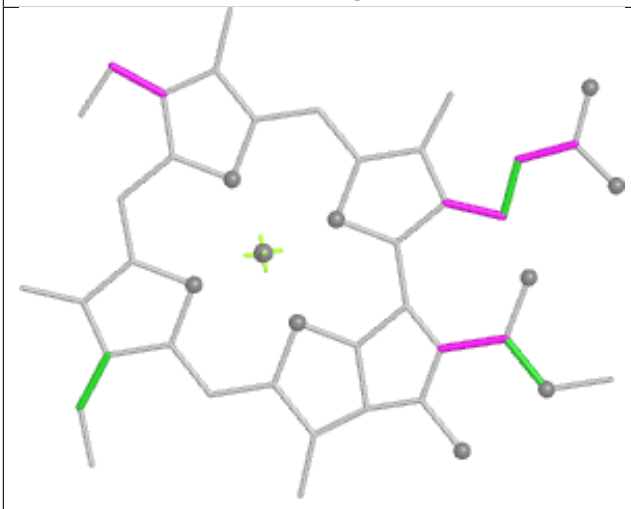
Ligand CLA 15 308



Bond lengths



Bond angles

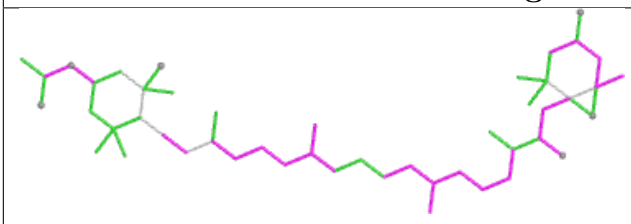


Torsions

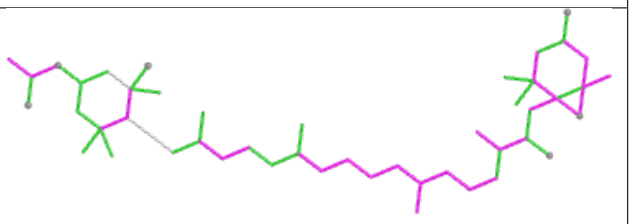


Rings

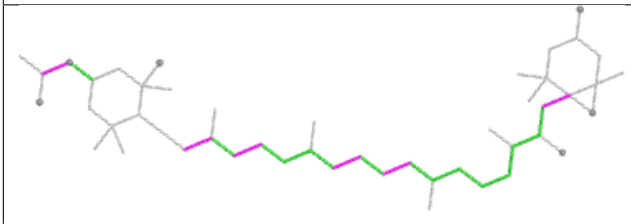
Ligand A86 21 311



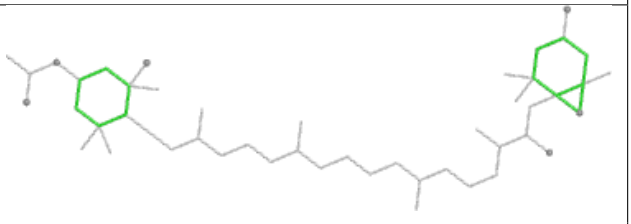
Bond lengths



Bond angles

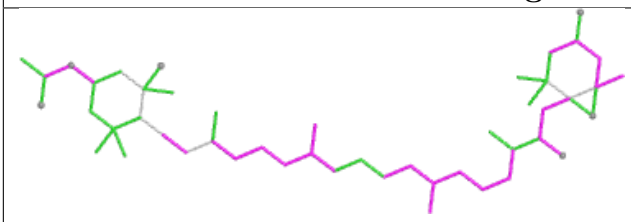


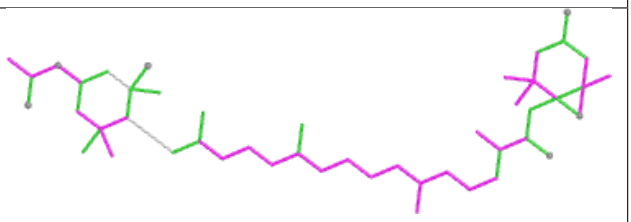
Torsions

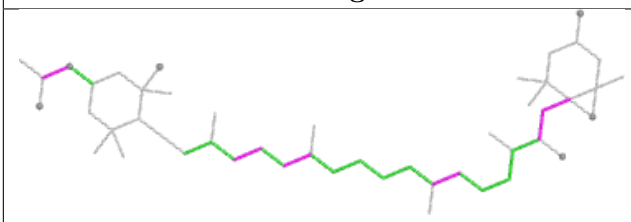


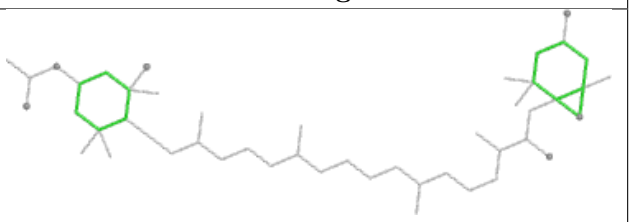
Rings

Ligand A86 11 310

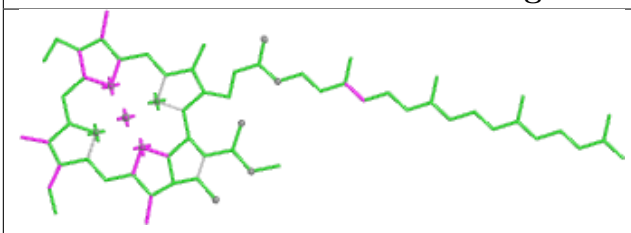

Bond lengths

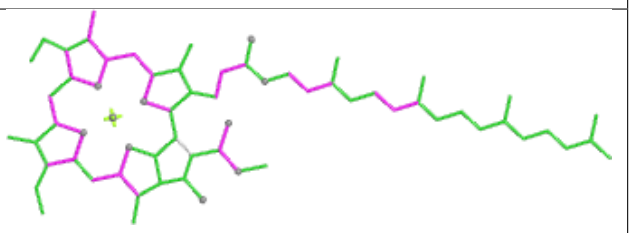

Bond angles

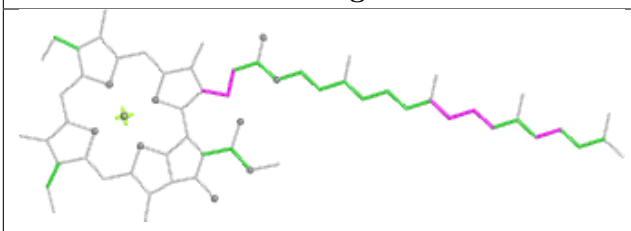

Torsions

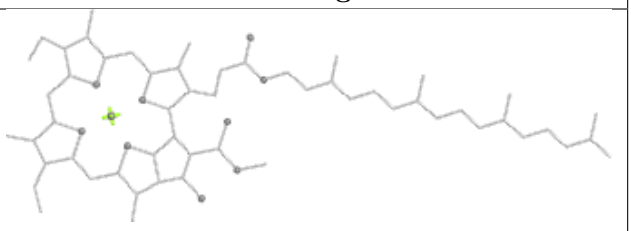

Rings

Ligand CLA B 606

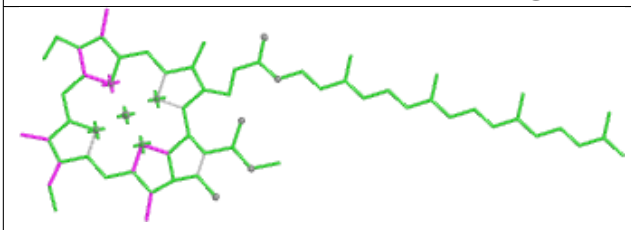

Bond lengths

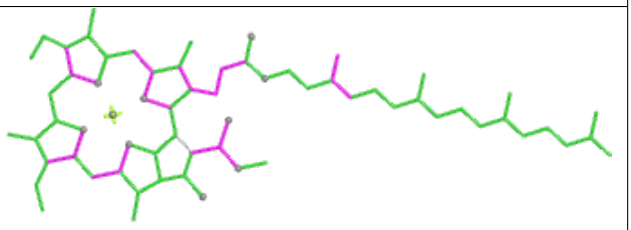

Bond angles

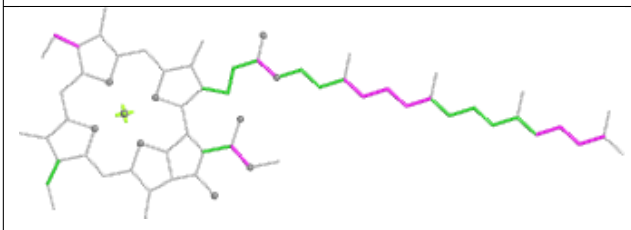

Torsions

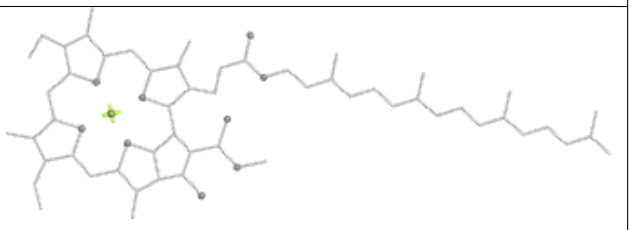

Rings

Ligand CLA b 602

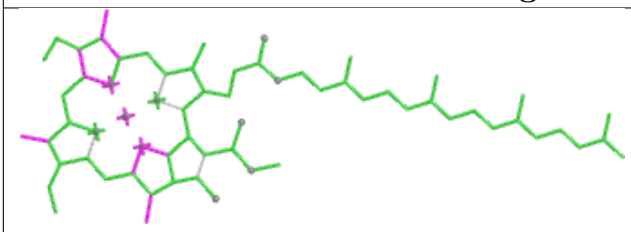

Bond lengths


Bond angles

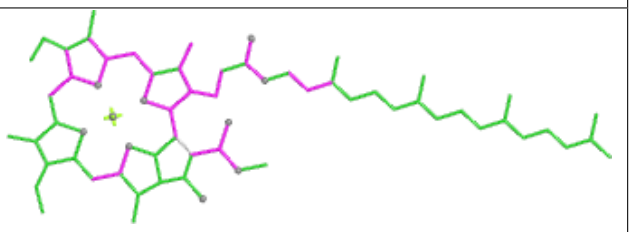

Torsions


Rings

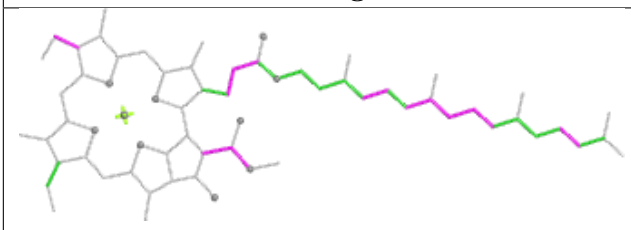
Ligand CLA 16 302



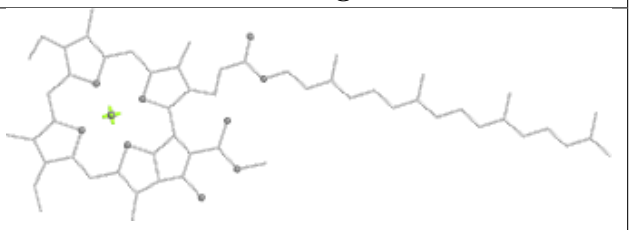
Bond lengths



Bond angles



Torsions

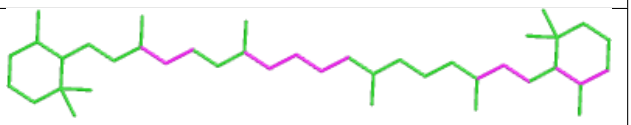


Rings

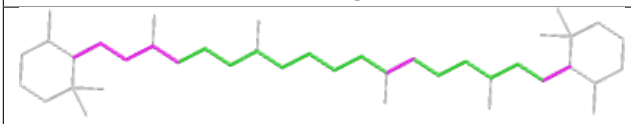
Ligand BCR a 408



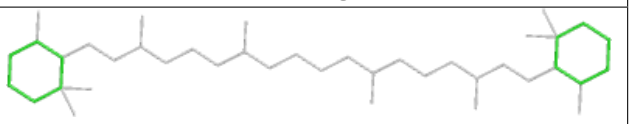
Bond lengths



Bond angles

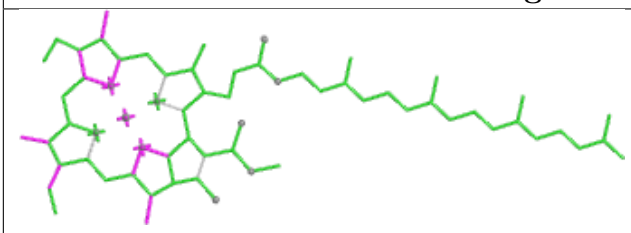


Torsions

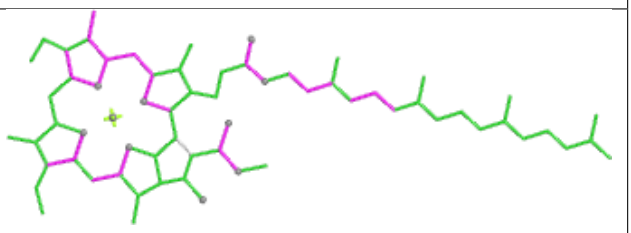


Rings

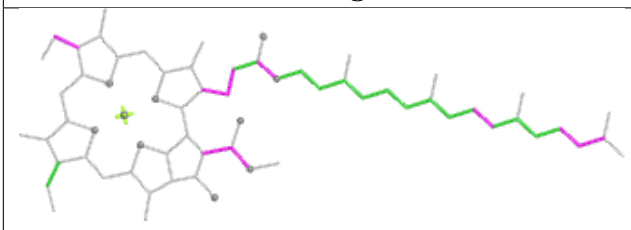
Ligand CLA B 611



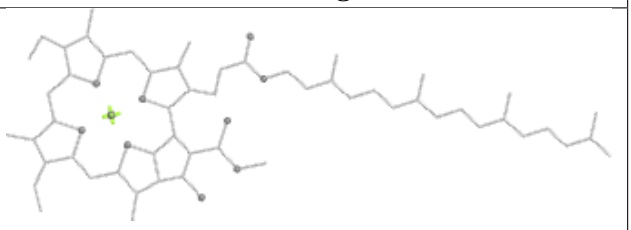
Bond lengths



Bond angles

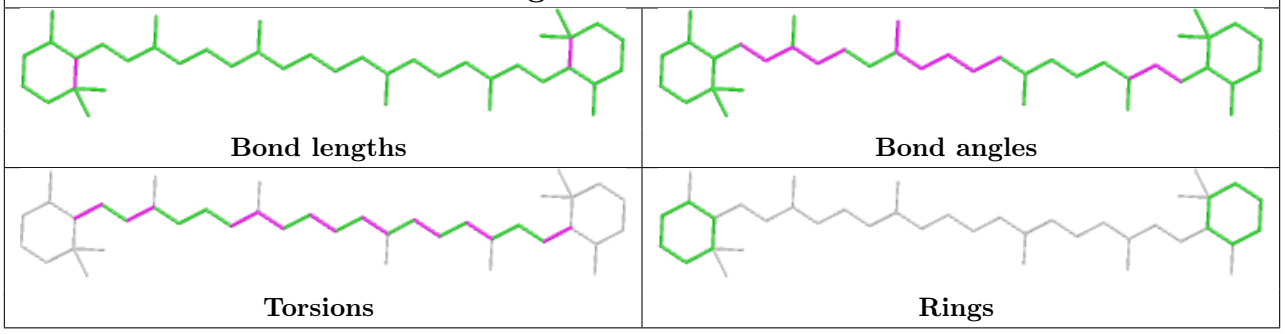


Torsions

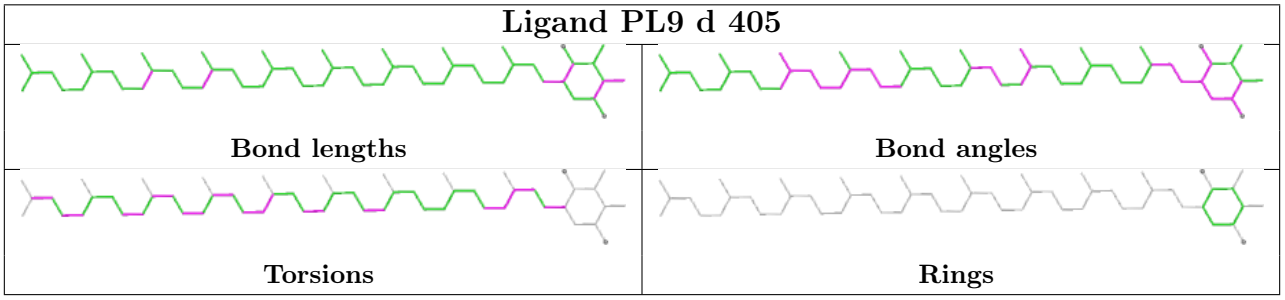


Rings

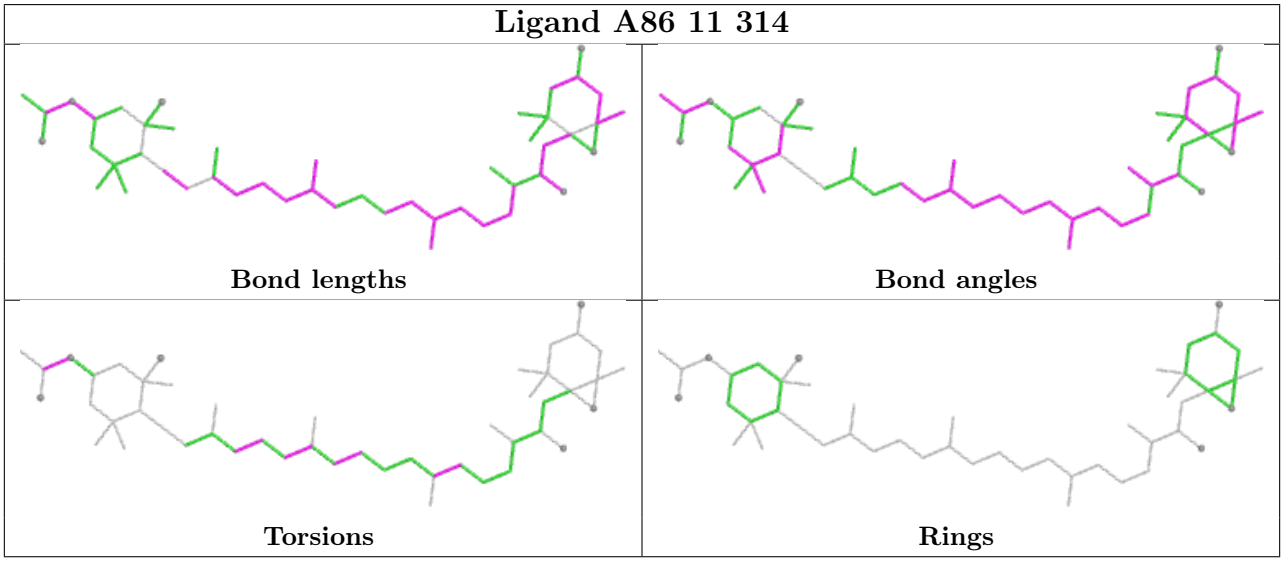
Ligand BCR a 404



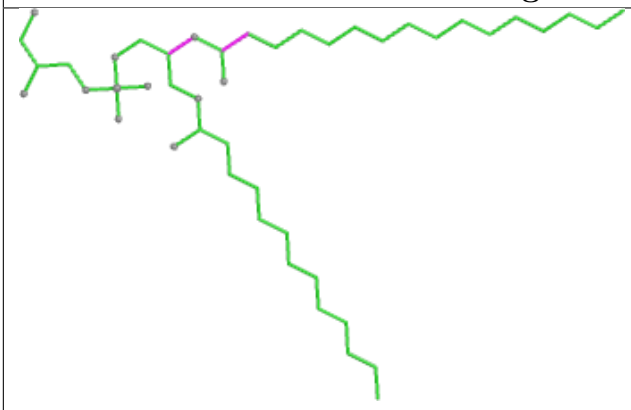
Ligand PL9 d 405



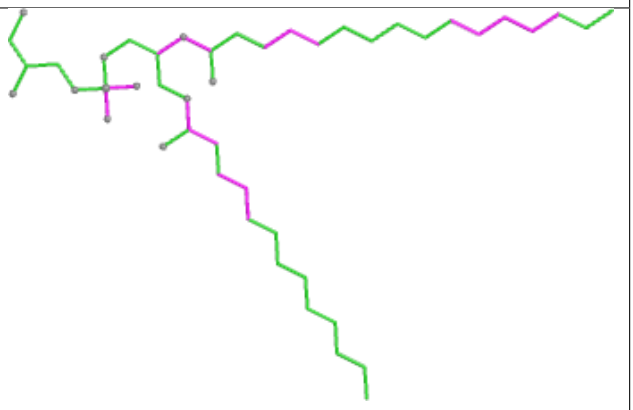
Ligand A86 11 314



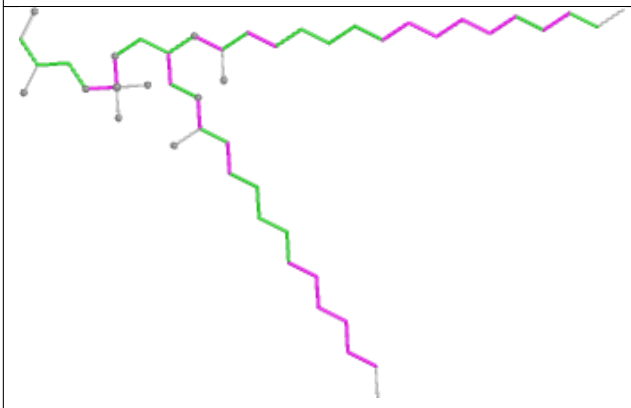
Ligand LHG A 408



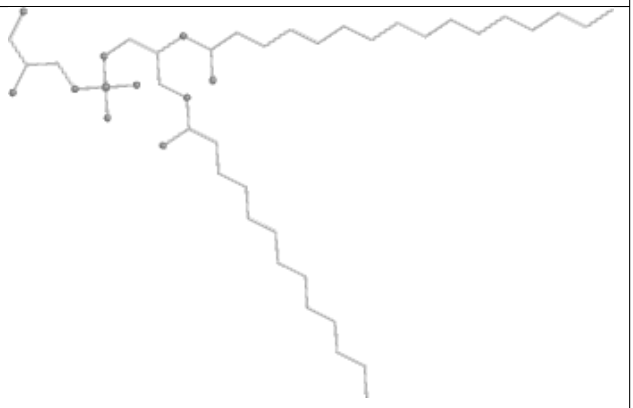
Bond lengths



Bond angles

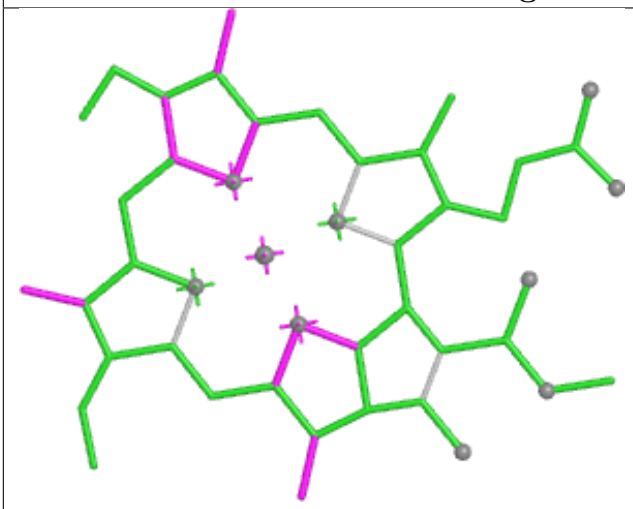


Torsions

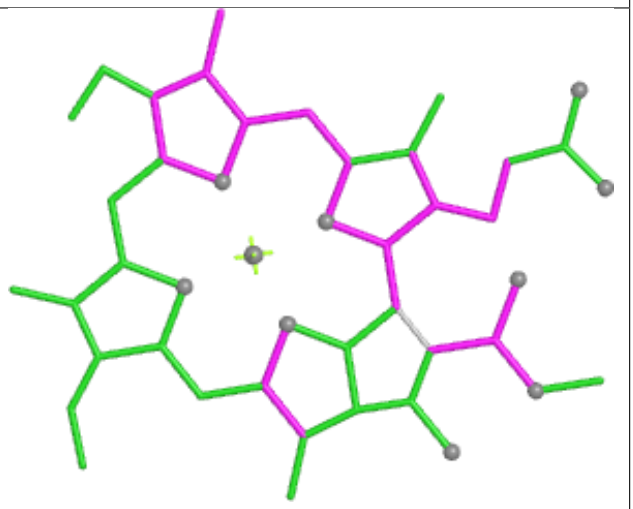


Rings

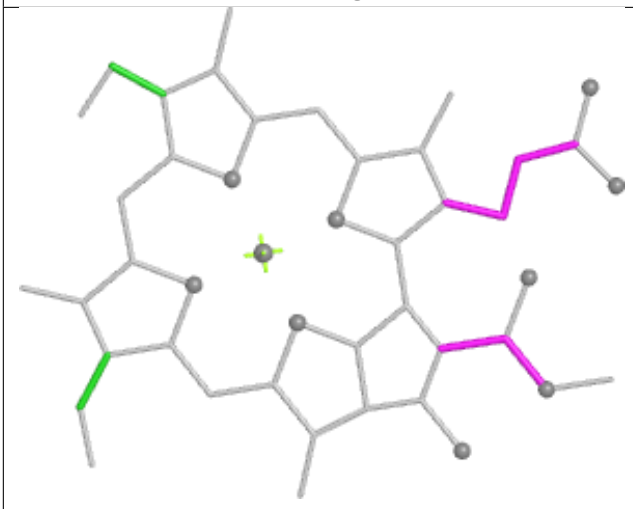
Ligand CLA 14 306



Bond lengths



Bond angles

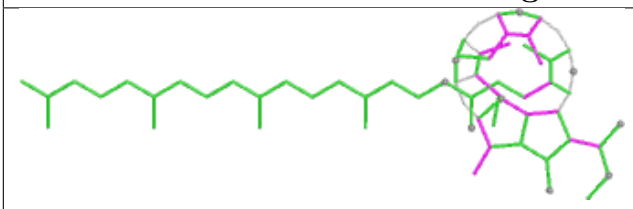


Torsions

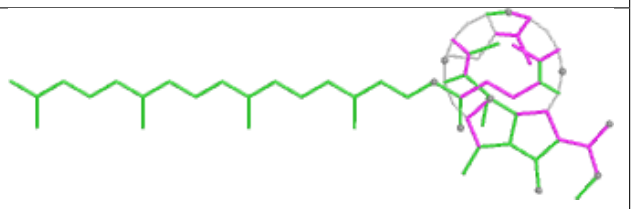


Rings

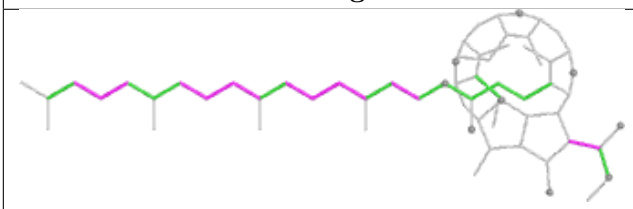
Ligand PHO A 403



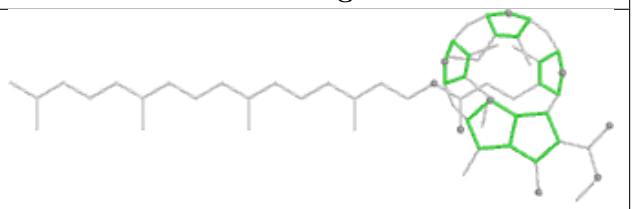
Bond lengths



Bond angles

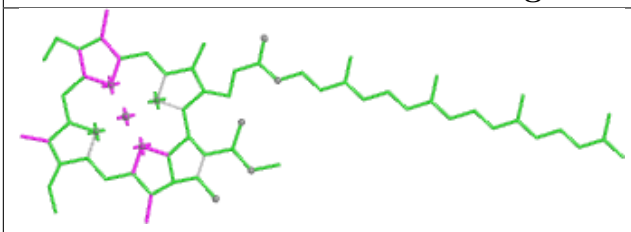


Torsions

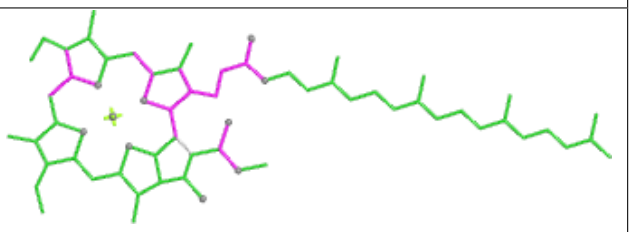


Rings

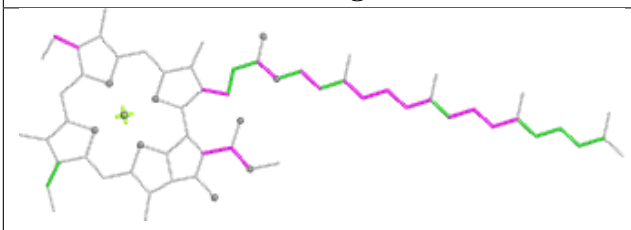
Ligand CLA C 504



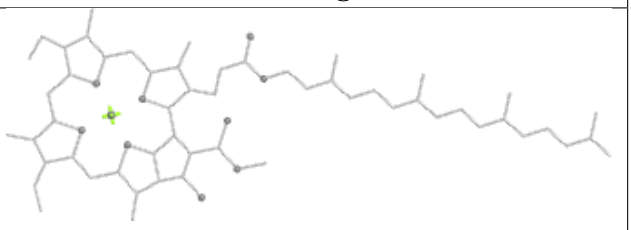
Bond lengths



Bond angles



Torsions



Rings

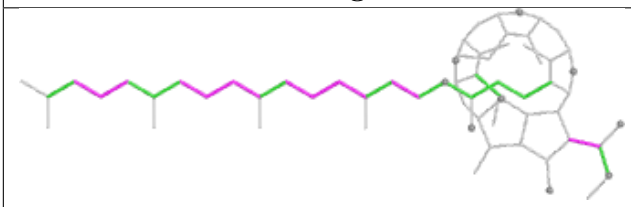
Ligand PHO d 403



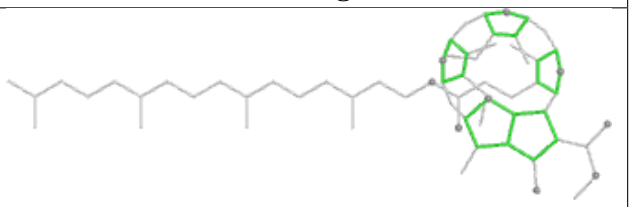
Bond lengths



Bond angles

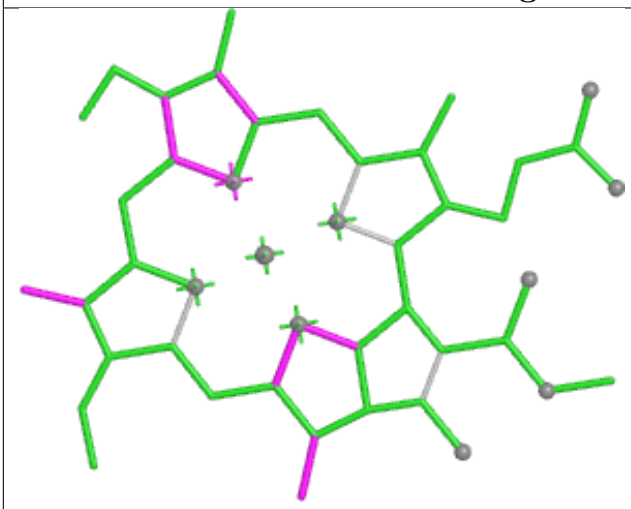


Torsions

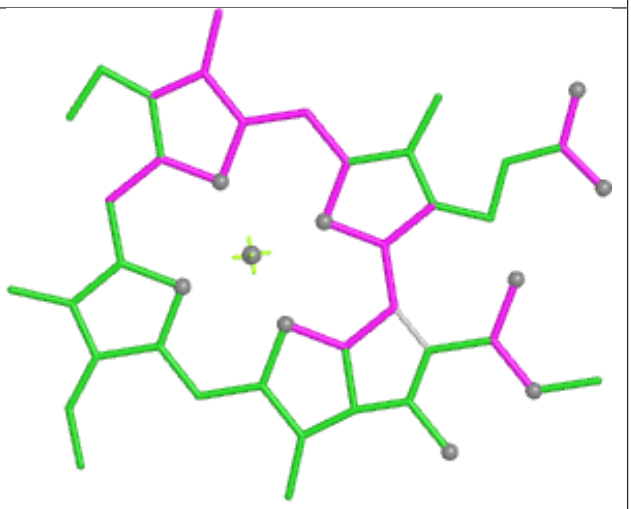


Rings

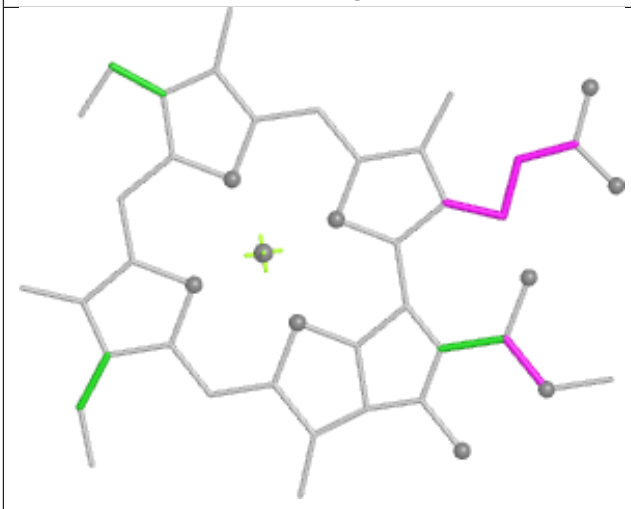
Ligand CLA 15 304



Bond lengths



Bond angles

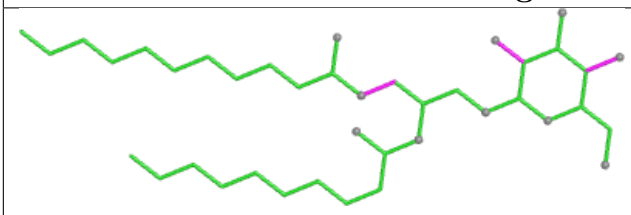


Torsions

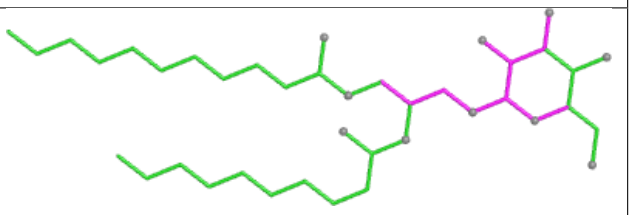


Rings

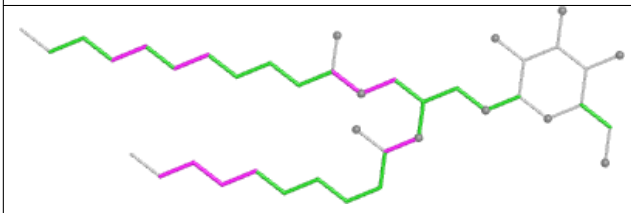
Ligand LMG M 102



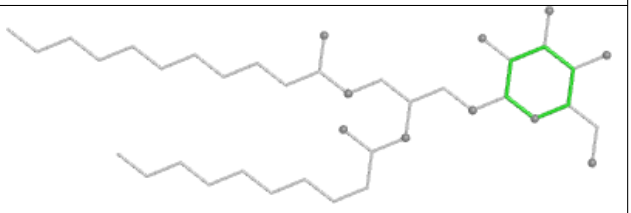
Bond lengths



Bond angles

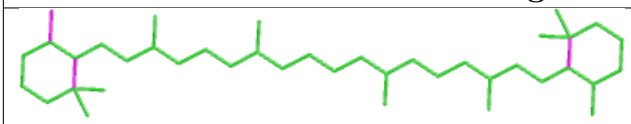


Torsions

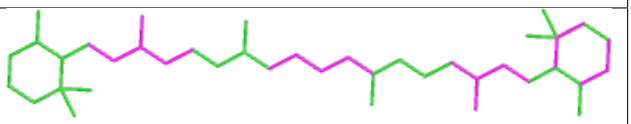


Rings

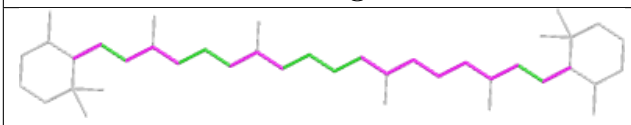
Ligand BCR c 520



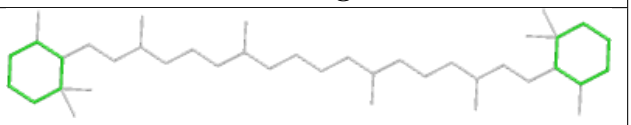
Bond lengths



Bond angles

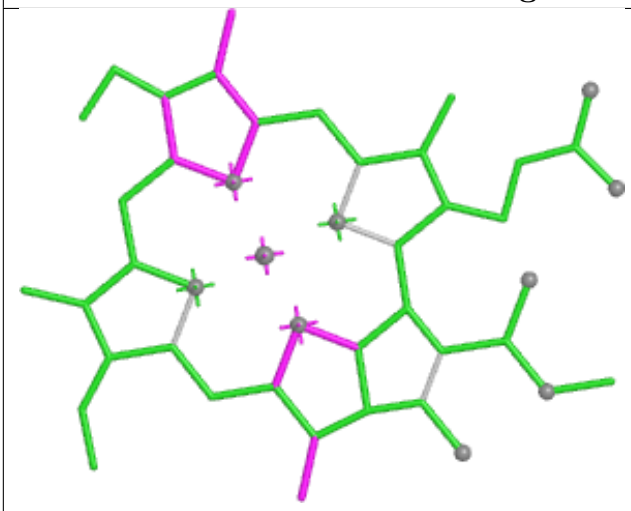


Torsions

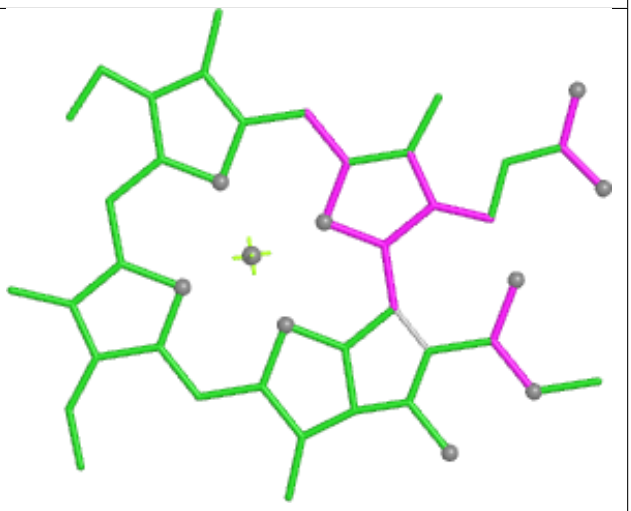


Rings

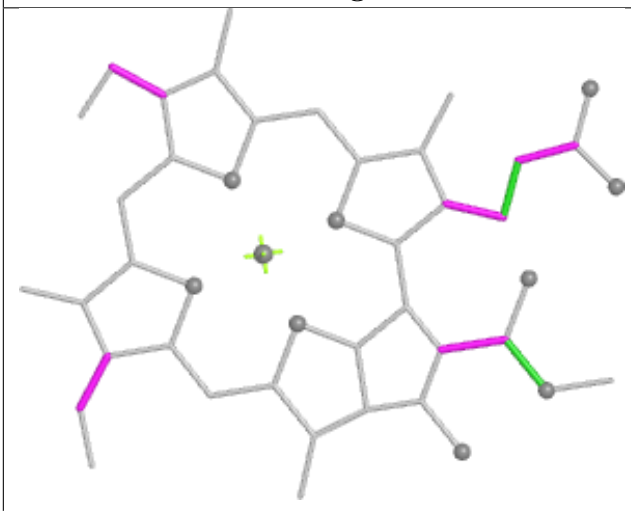
Ligand CLA 20 206



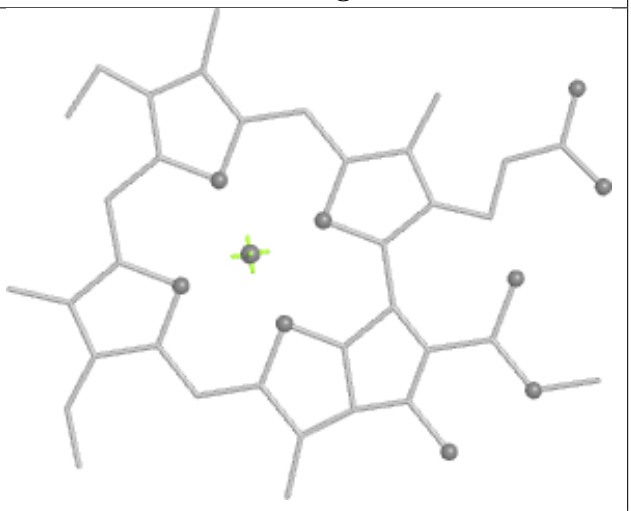
Bond lengths



Bond angles

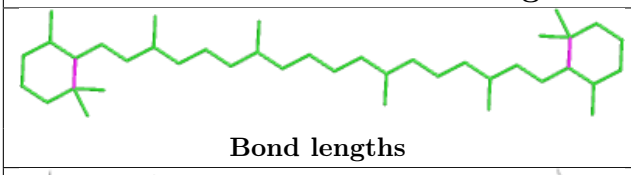


Torsions

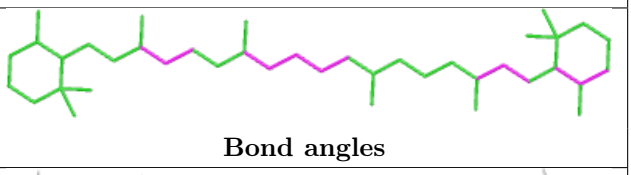


Rings

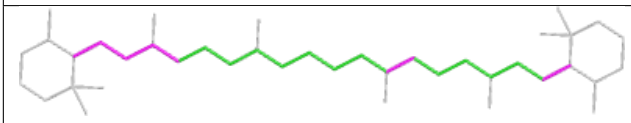
Ligand BCR A 409



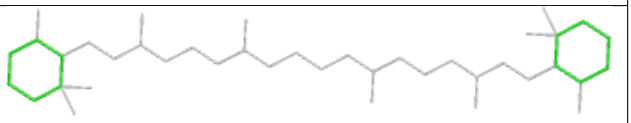
Bond lengths



Bond angles



Torsions

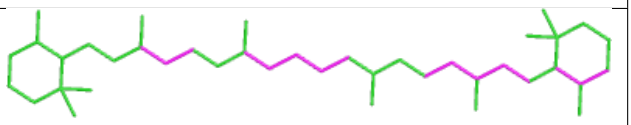


Rings

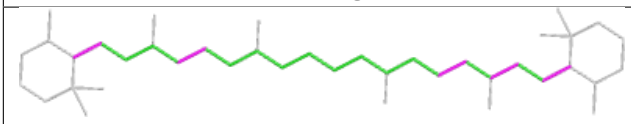
Ligand BCR C 518



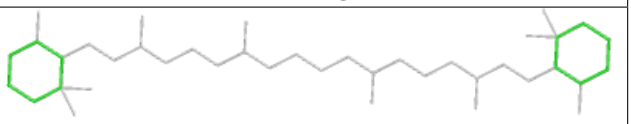
Bond lengths



Bond angles

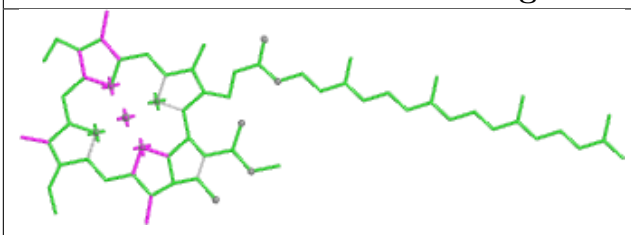


Torsions

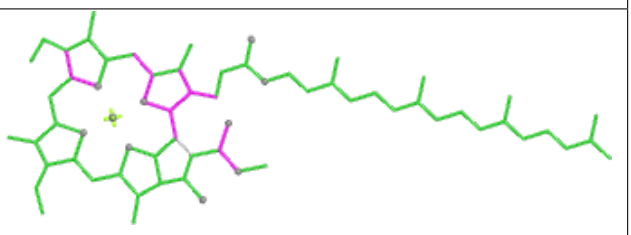


Rings

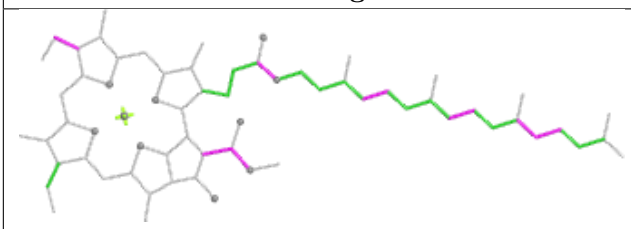
Ligand CLA 14 302



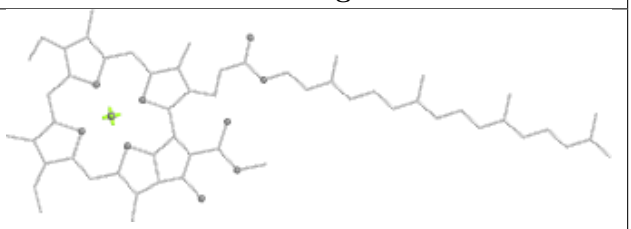
Bond lengths



Bond angles

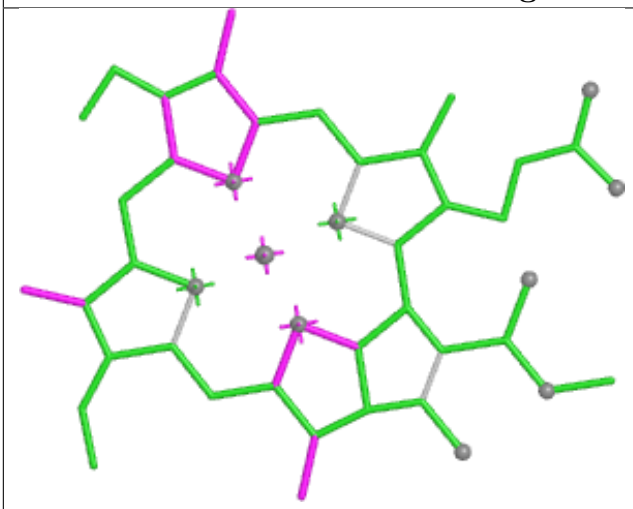


Torsions

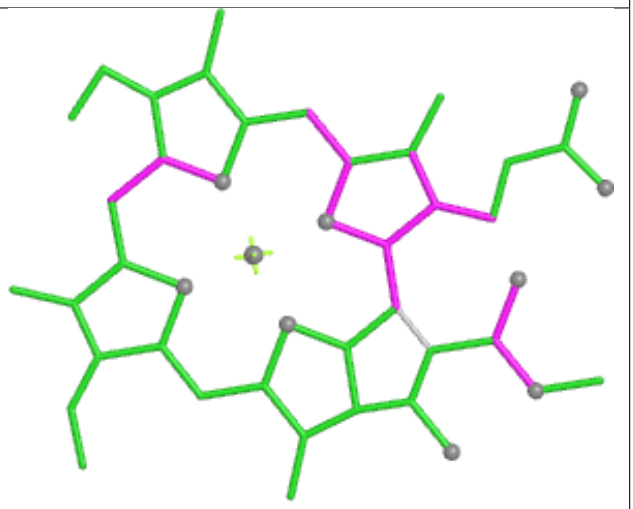


Rings

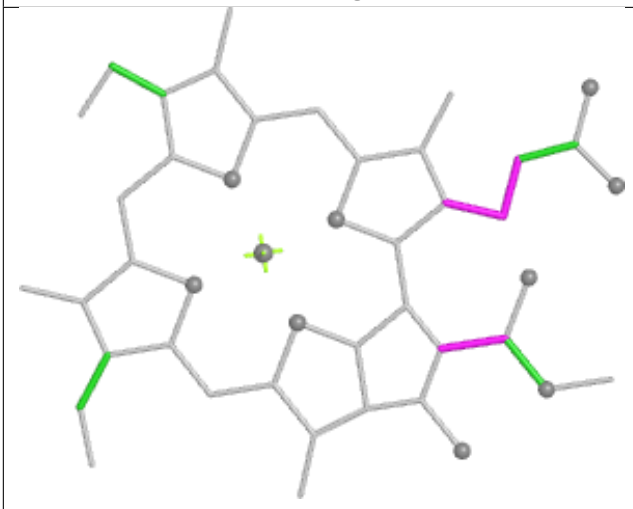
Ligand CLA 12 306



Bond lengths



Bond angles

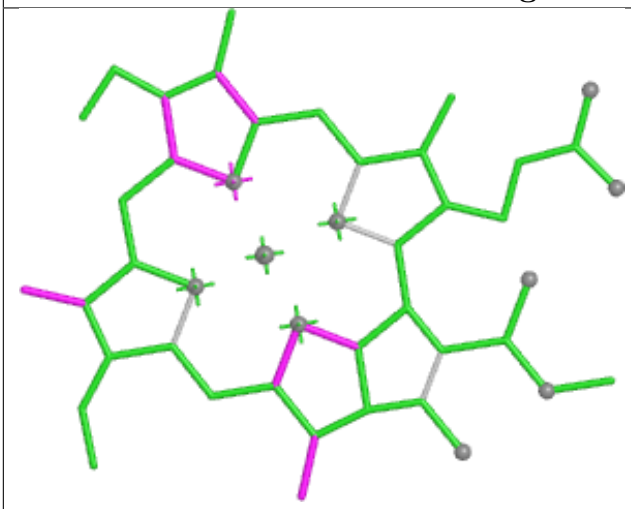


Torsions

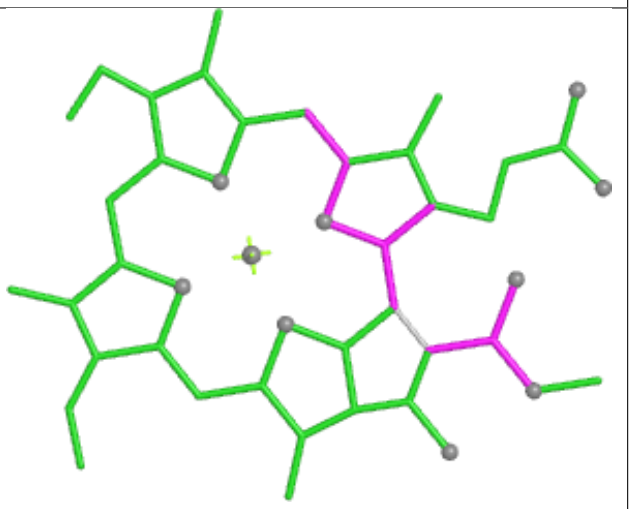


Rings

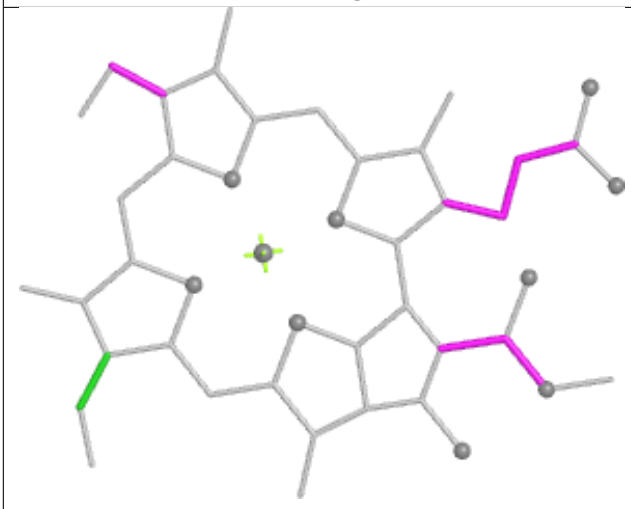
Ligand CLA 15 302



Bond lengths



Bond angles

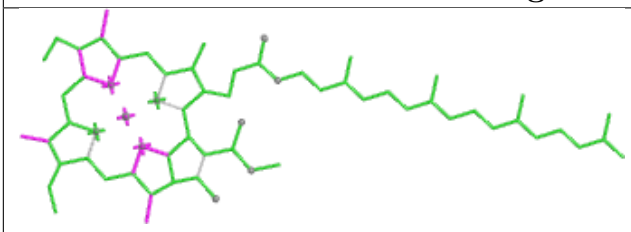


Torsions

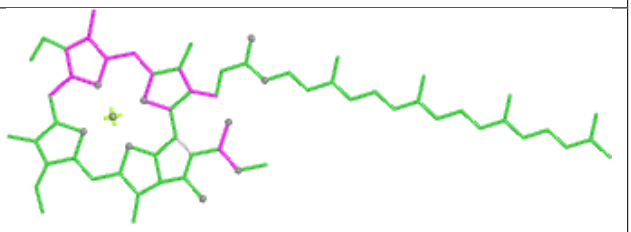


Rings

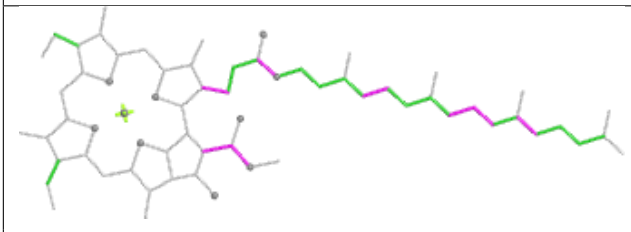
Ligand CLA b 607



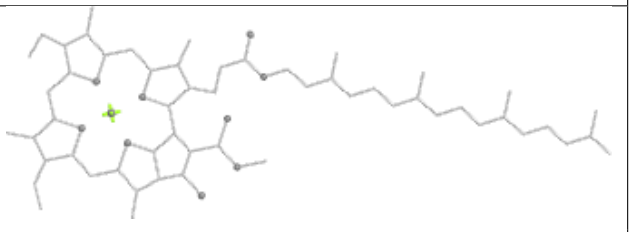
Bond lengths



Bond angles

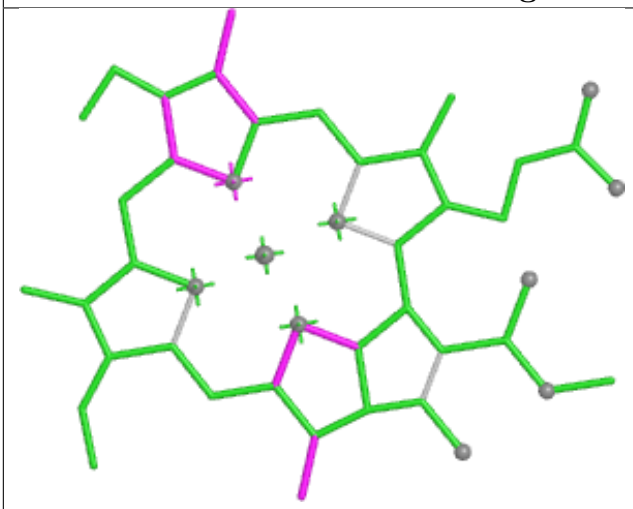


Torsions

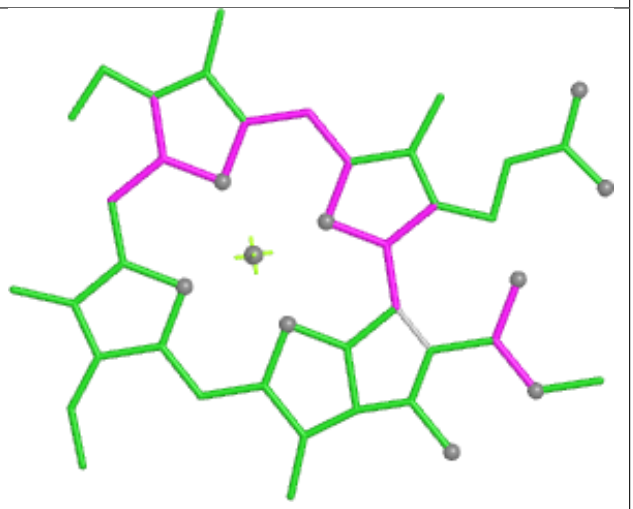


Rings

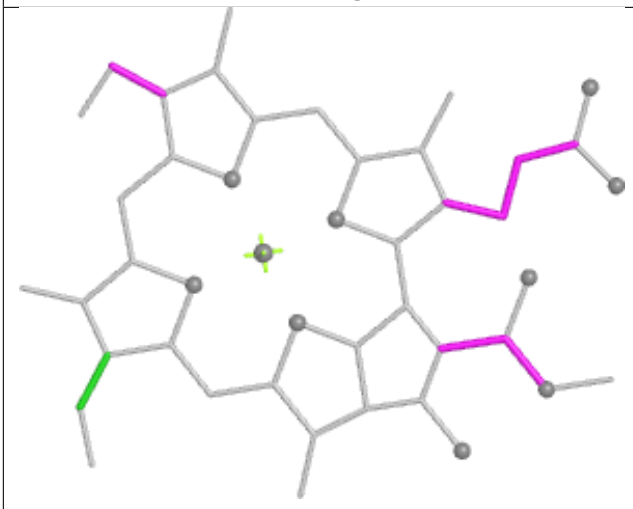
Ligand CLA 14 308



Bond lengths



Bond angles

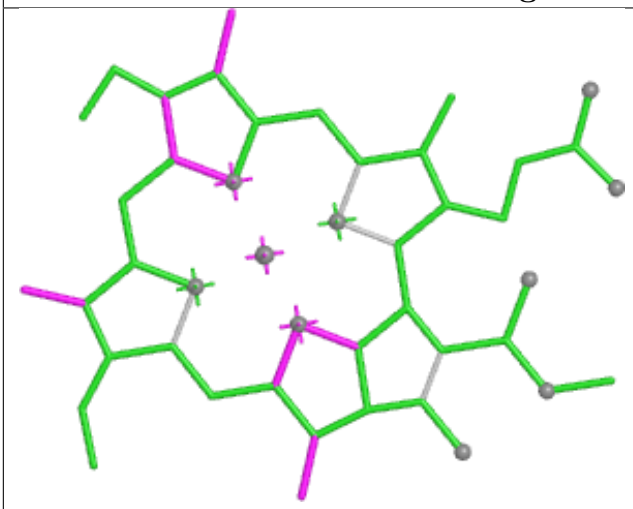


Torsions

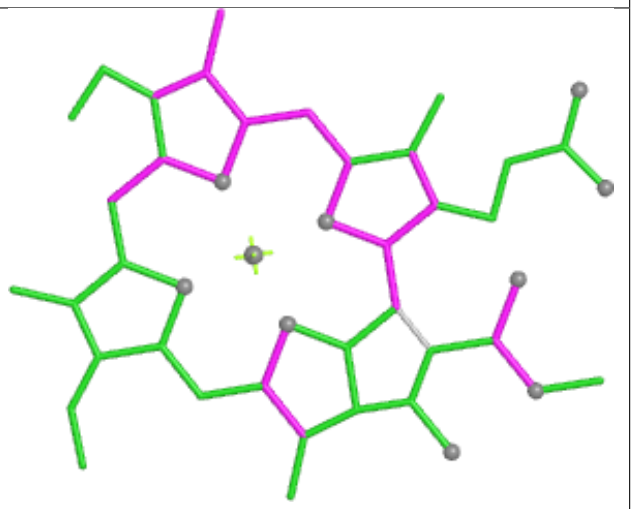


Rings

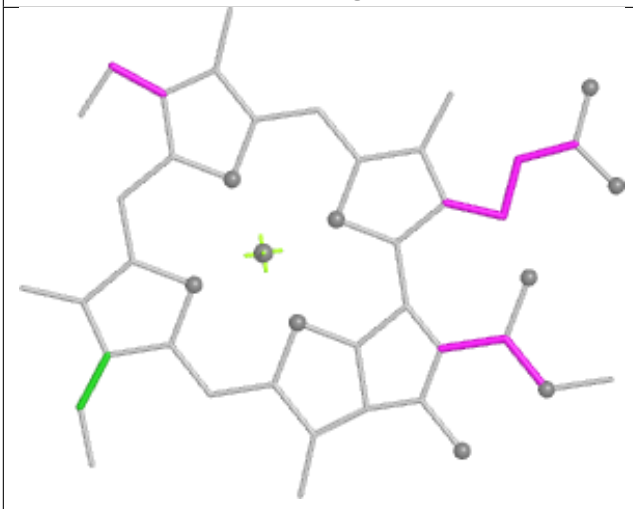
Ligand CLA 20 205



Bond lengths



Bond angles

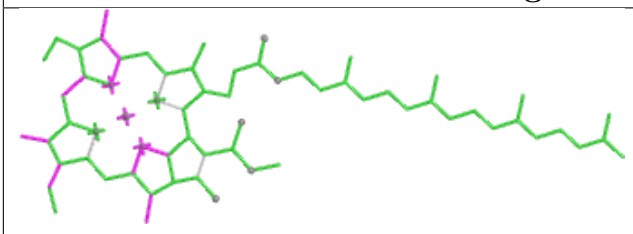


Torsions

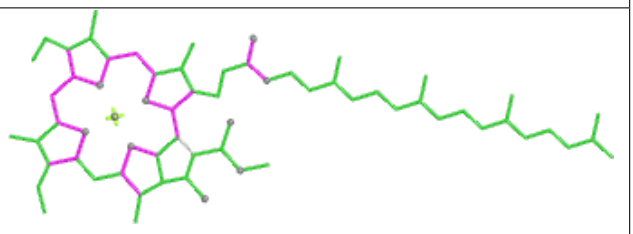


Rings

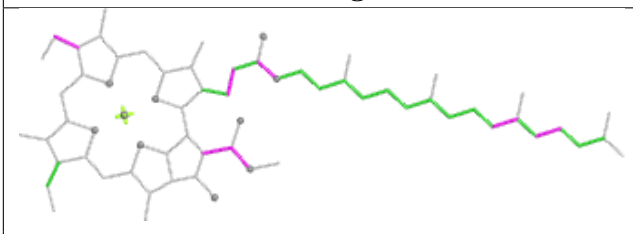
Ligand CLA C 503



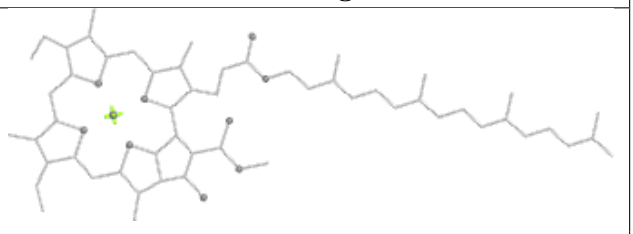
Bond lengths



Bond angles

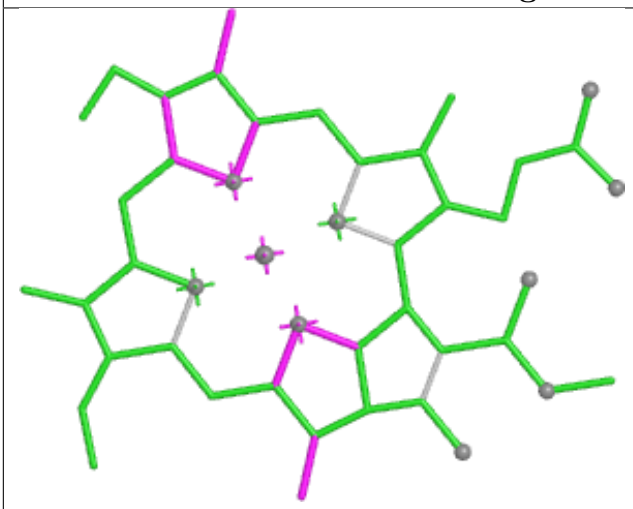


Torsions

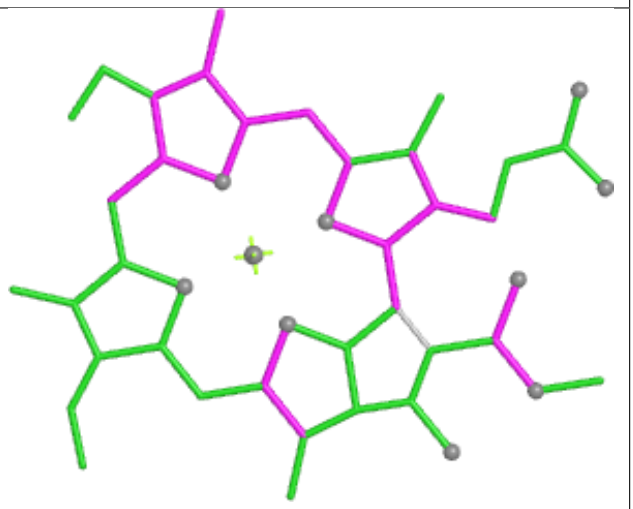


Rings

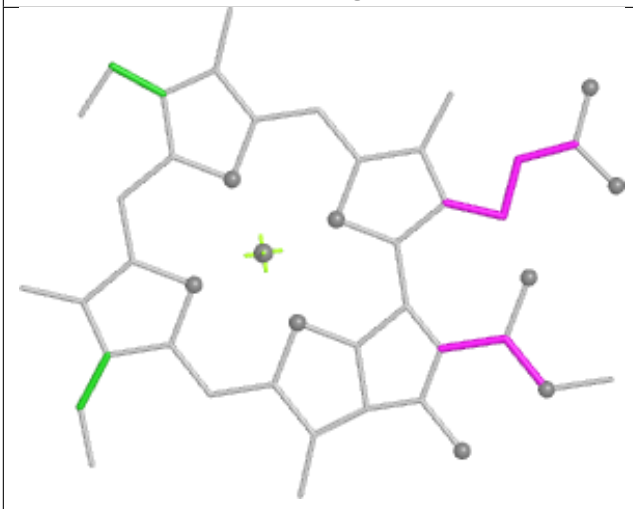
Ligand CLA 17 306



Bond lengths



Bond angles

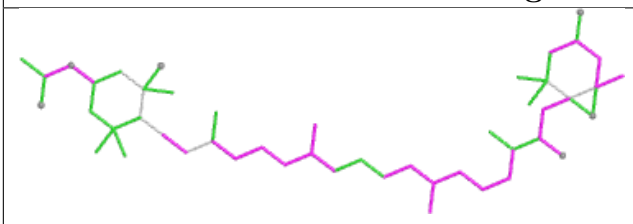


Torsions

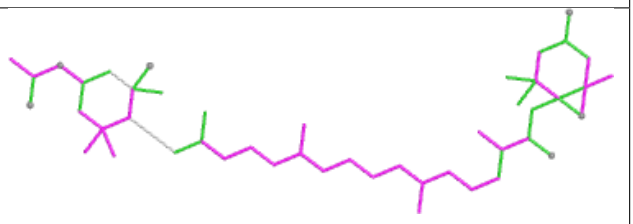


Rings

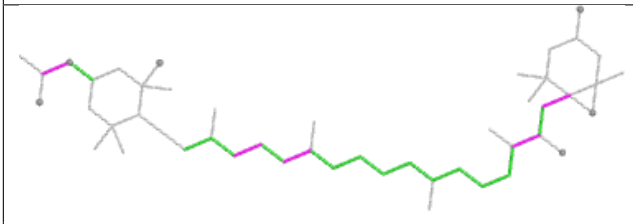
Ligand A86 13 314



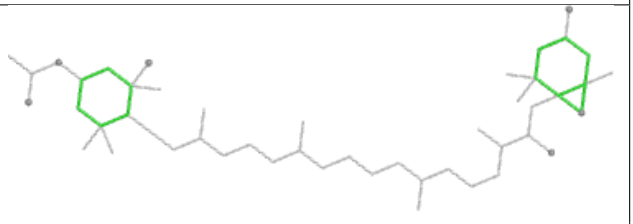
Bond lengths



Bond angles

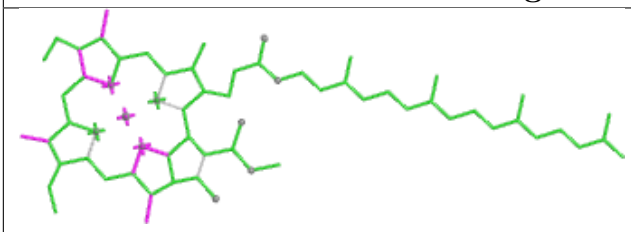


Torsions

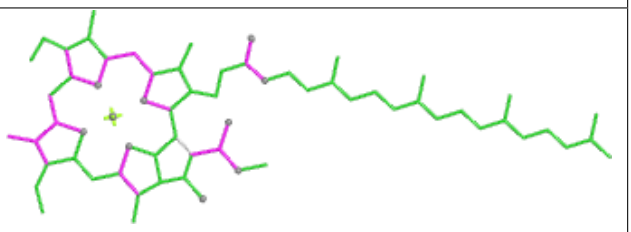


Rings

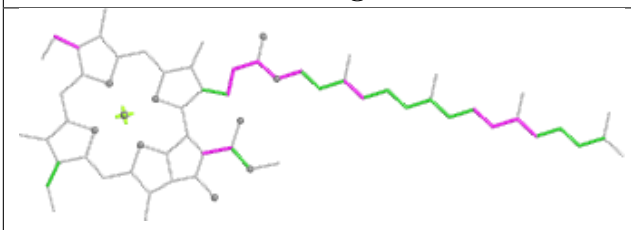
Ligand CLA C 506



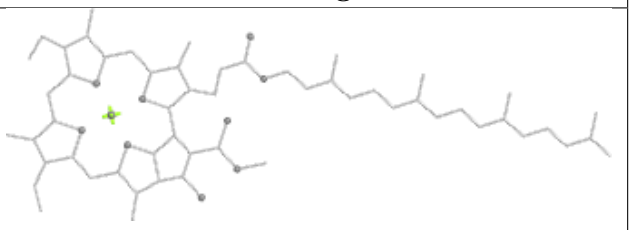
Bond lengths



Bond angles

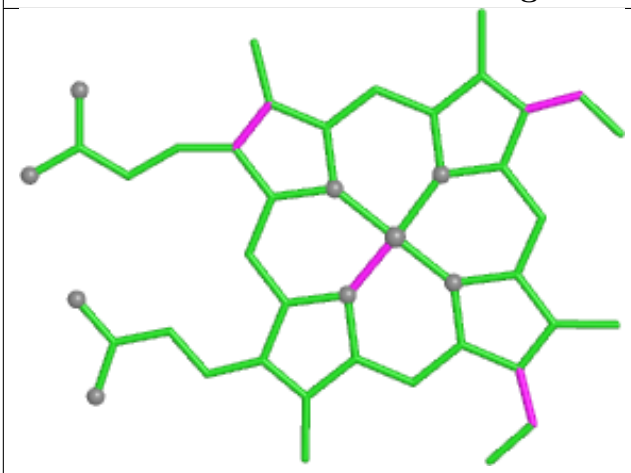


Torsions

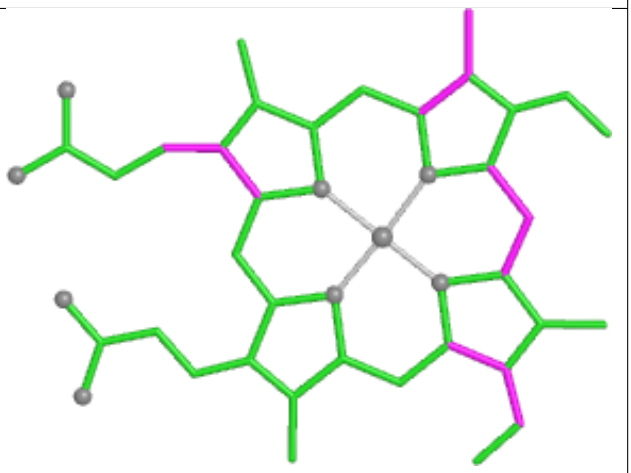


Rings

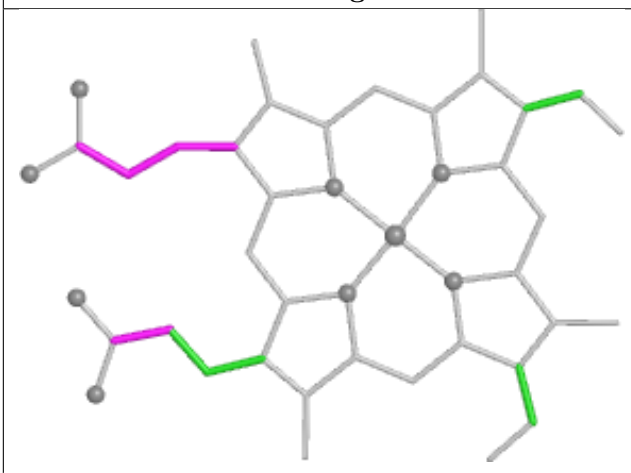
Ligand HEM F 102



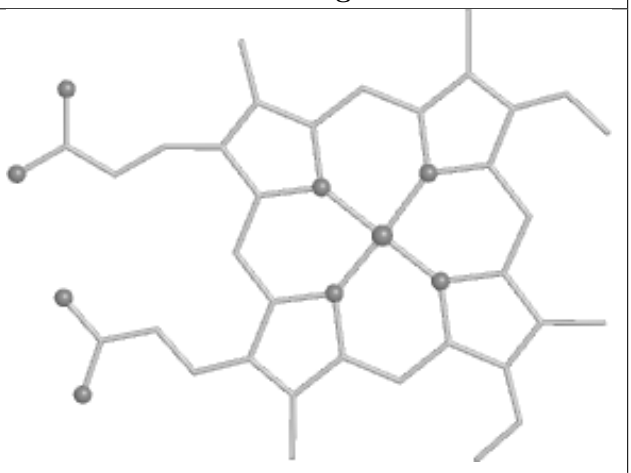
Bond lengths



Bond angles

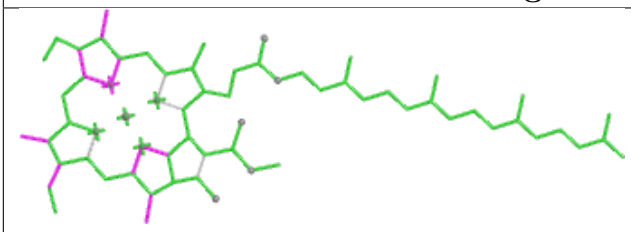


Torsions

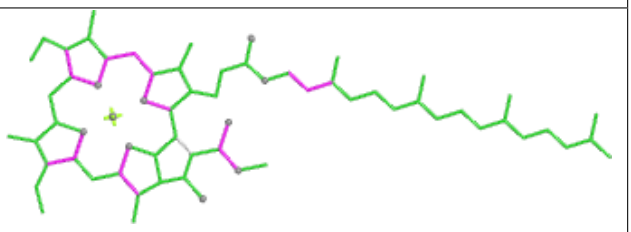


Rings

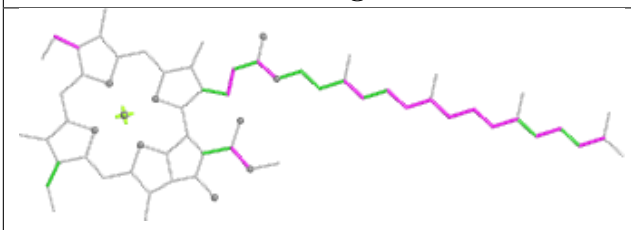
Ligand CLA B 605



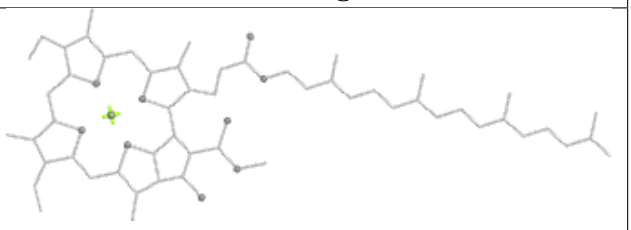
Bond lengths



Bond angles

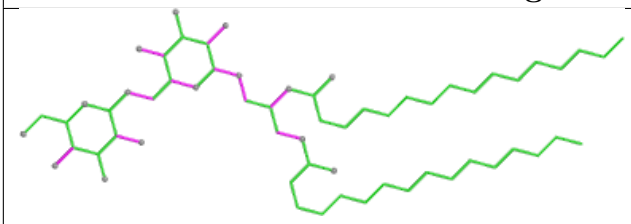


Torsions

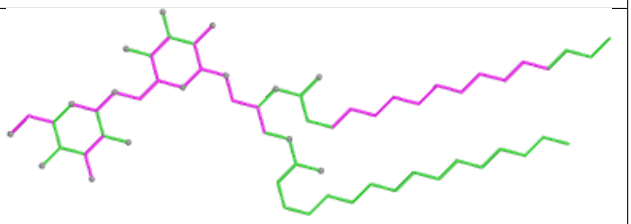


Rings

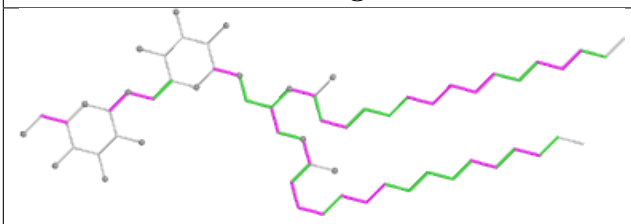
Ligand DGD c 518



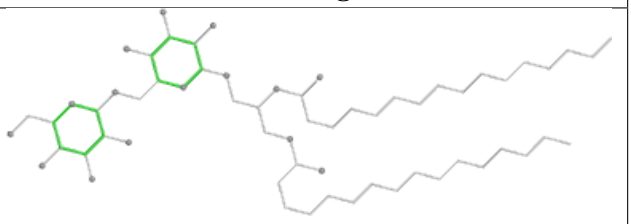
Bond lengths



Bond angles

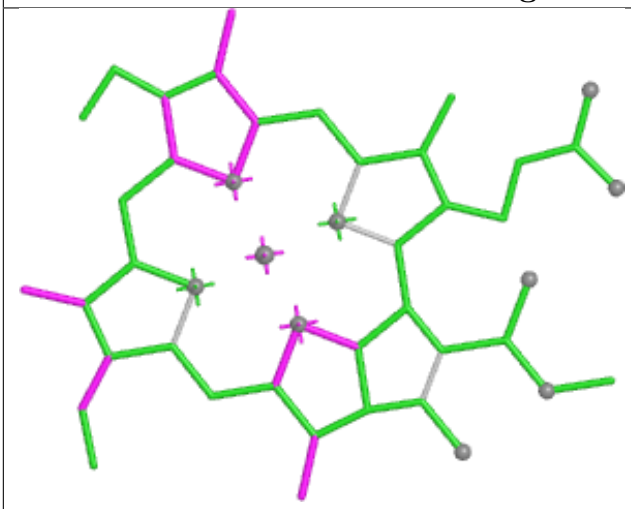


Torsions

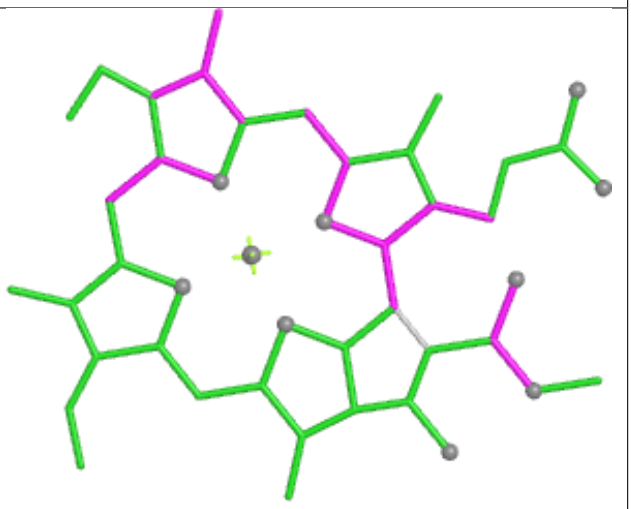


Rings

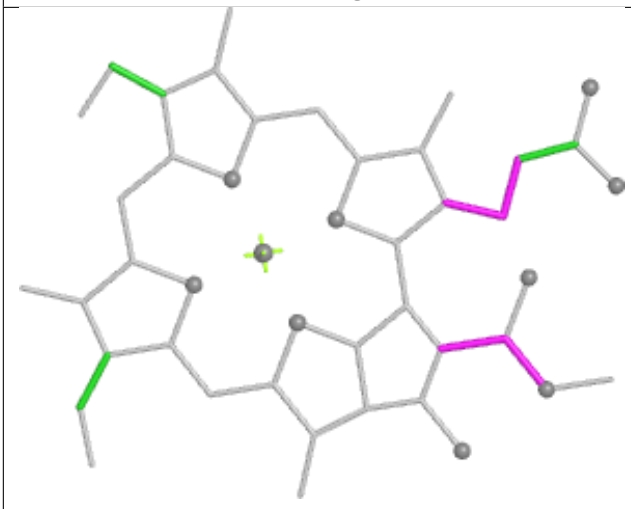
Ligand CLA 17 304



Bond lengths



Bond angles

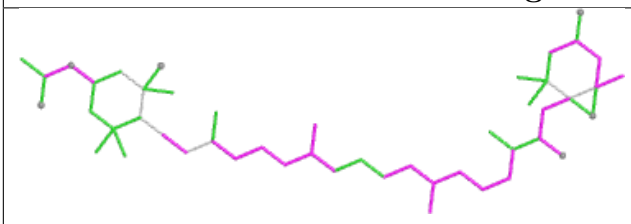


Torsions

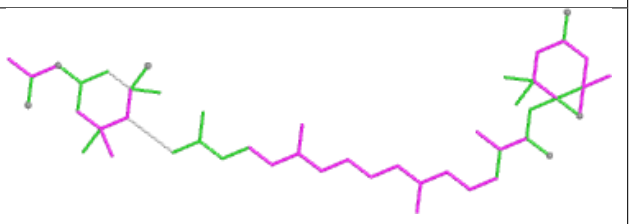


Rings

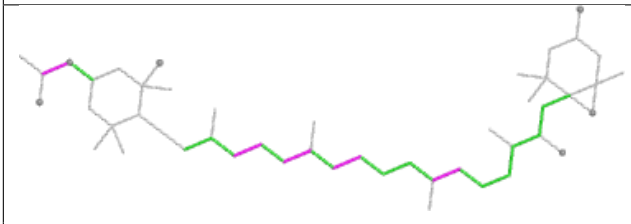
Ligand A86 17 316



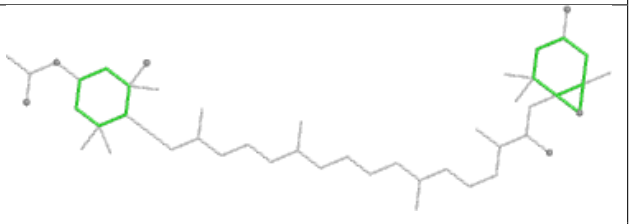
Bond lengths



Bond angles

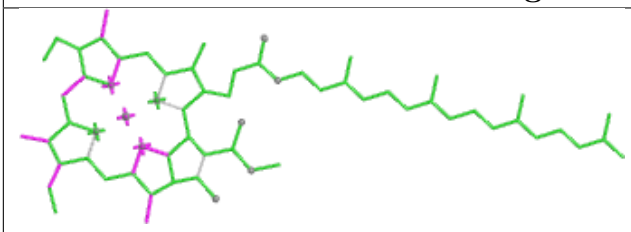


Torsions

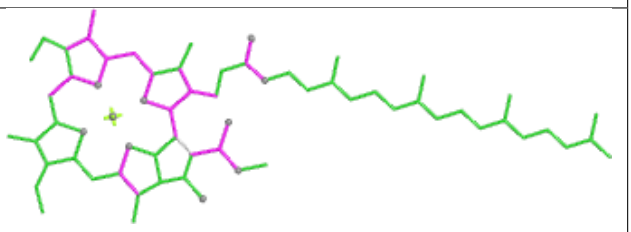


Rings

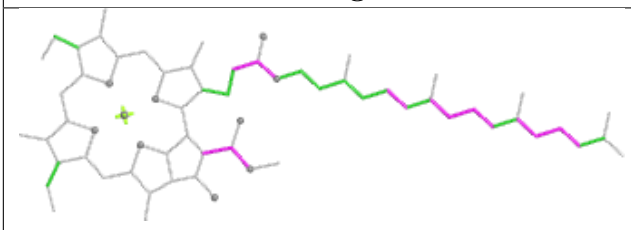
Ligand CLA C 508



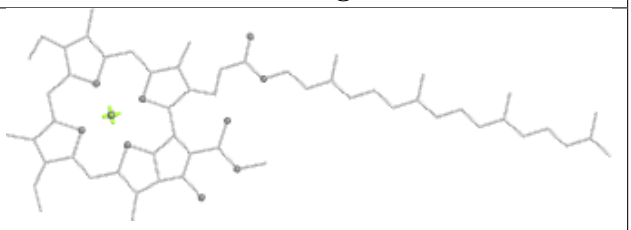
Bond lengths



Bond angles

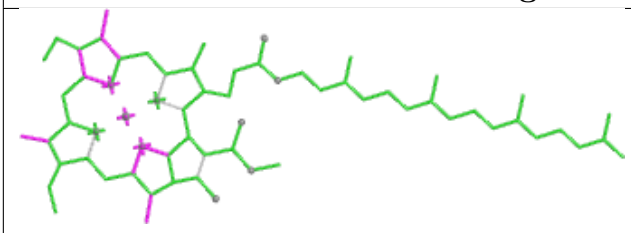


Torsions

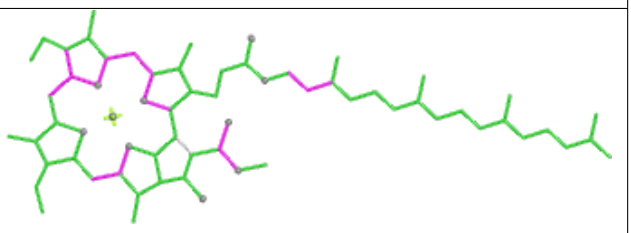


Rings

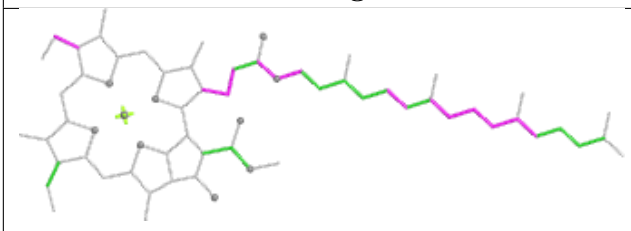
Ligand CLA 18 303



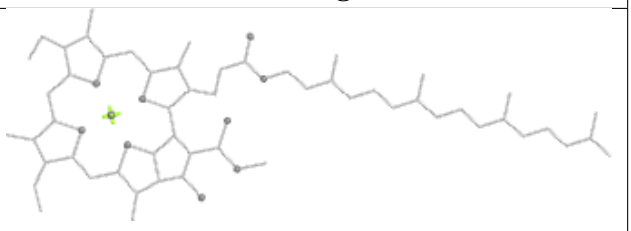
Bond lengths



Bond angles

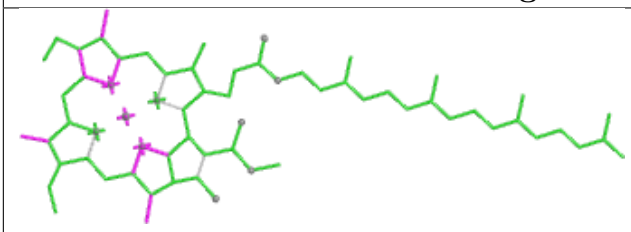


Torsions

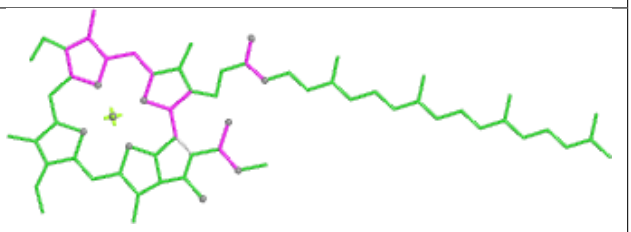


Rings

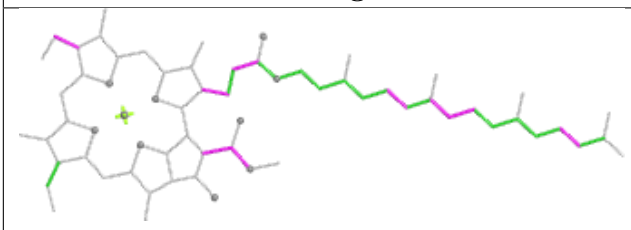
Ligand CLA 20 209



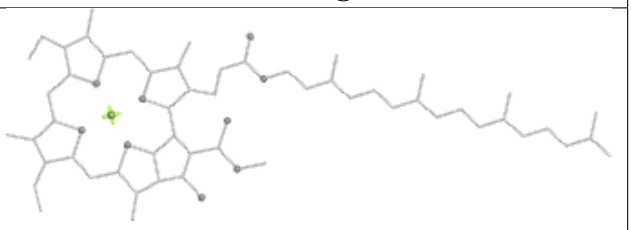
Bond lengths



Bond angles

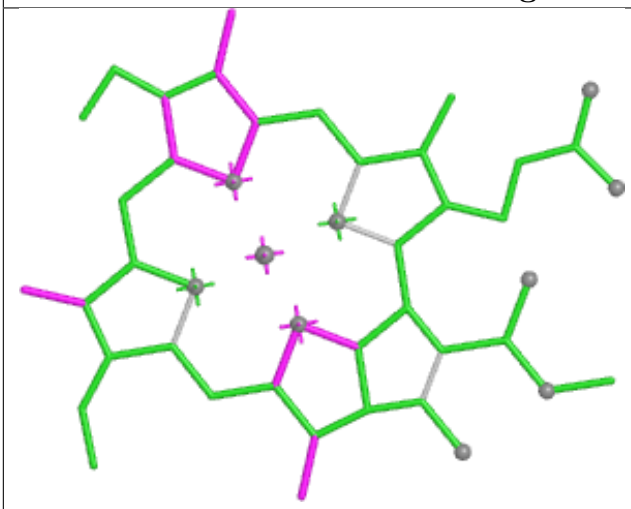


Torsions

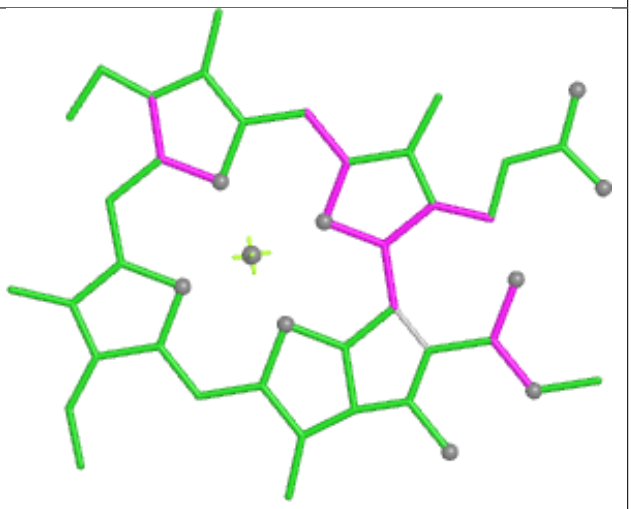


Rings

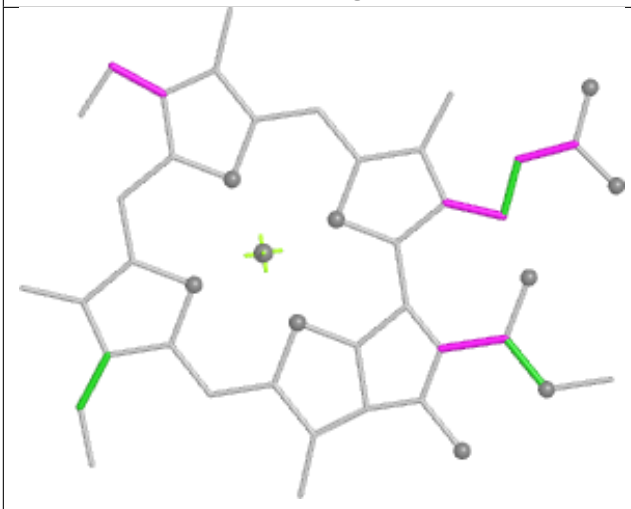
Ligand CLA 11 308



Bond lengths



Bond angles

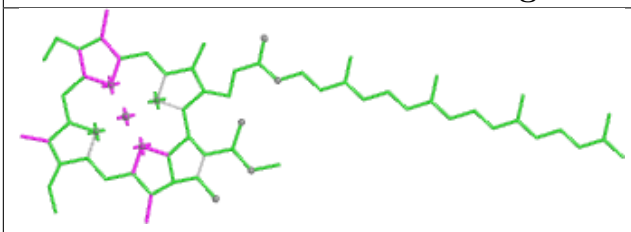


Torsions

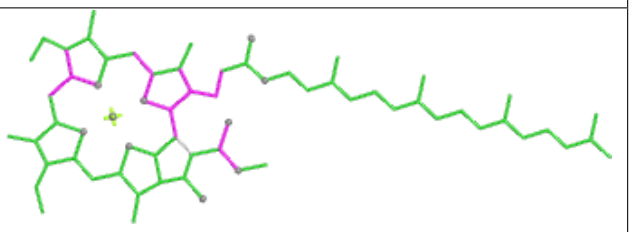


Rings

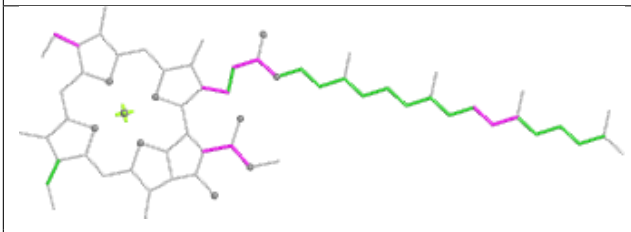
Ligand CLA 12 307



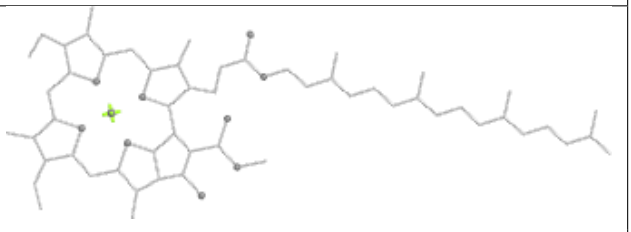
Bond lengths



Bond angles

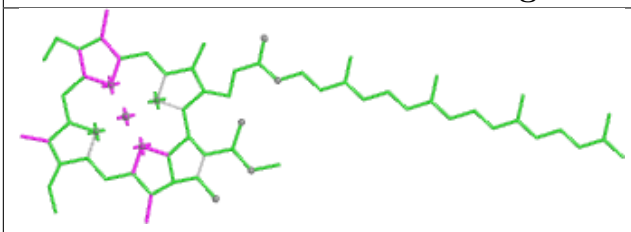


Torsions

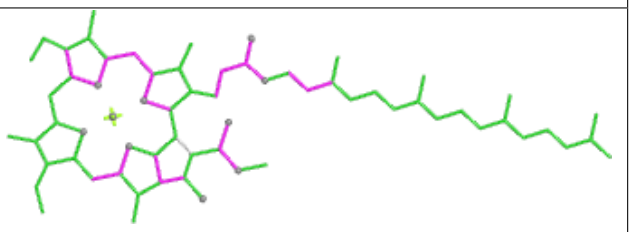


Rings

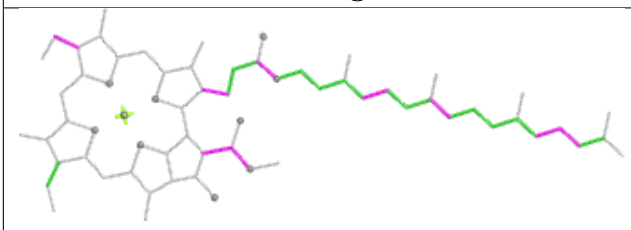
Ligand CLA 19 301



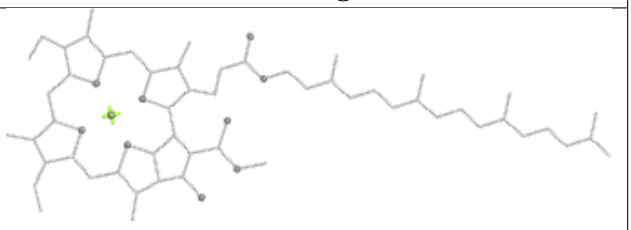
Bond lengths



Bond angles

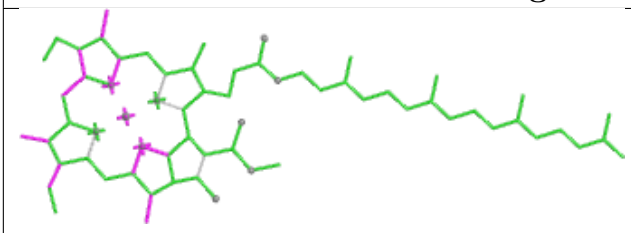


Torsions

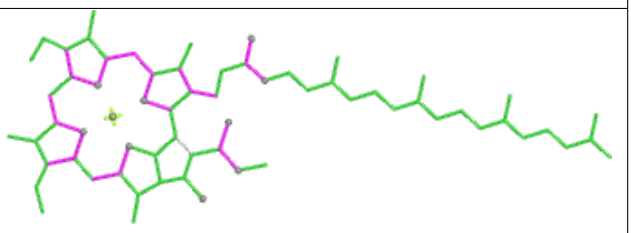


Rings

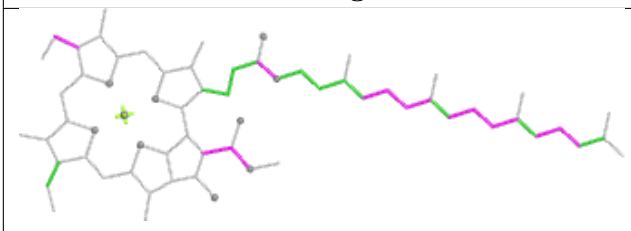
Ligand CLA c 505



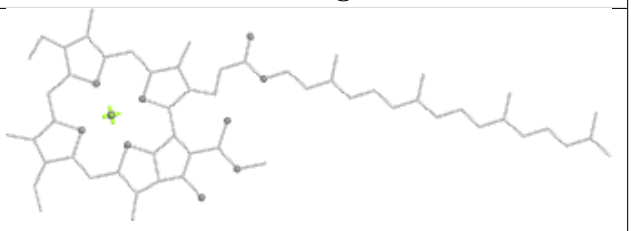
Bond lengths



Bond angles

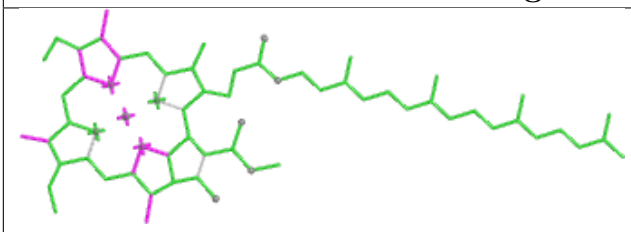


Torsions

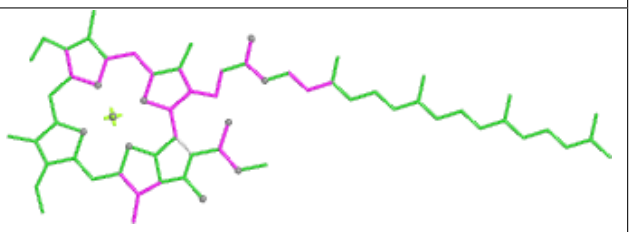


Rings

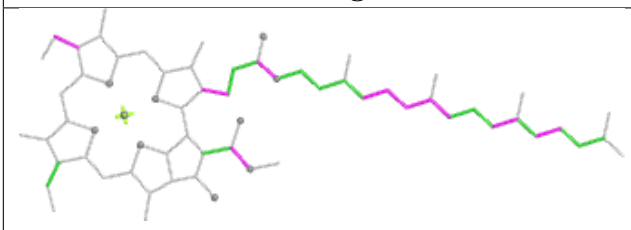
Ligand CLA B 623



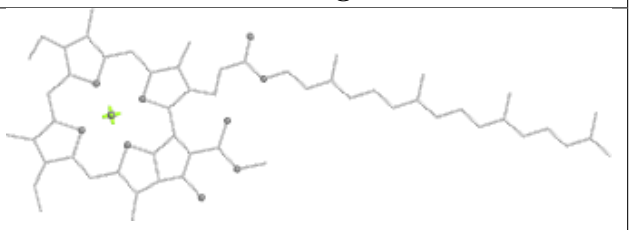
Bond lengths



Bond angles

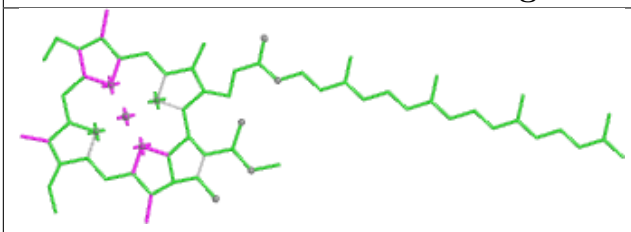


Torsions

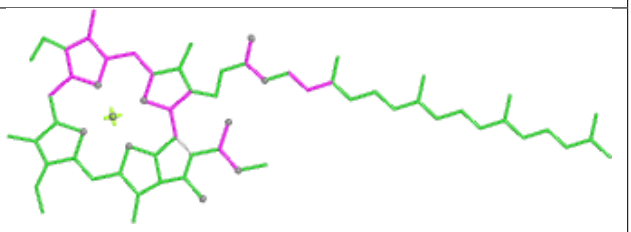


Rings

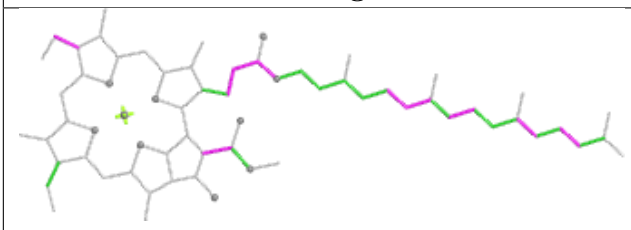
Ligand CLA 13 308



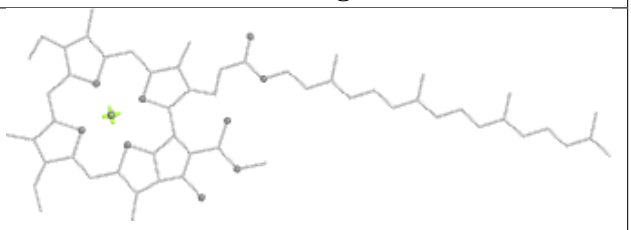
Bond lengths



Bond angles

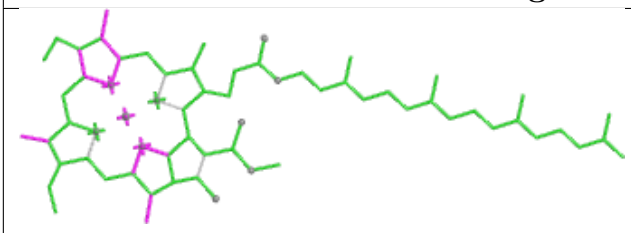


Torsions

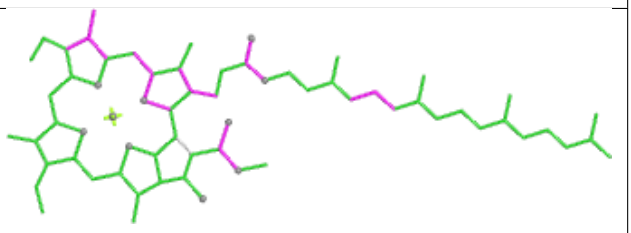


Rings

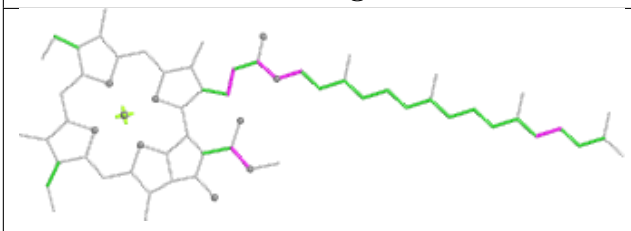
Ligand CLA a 402



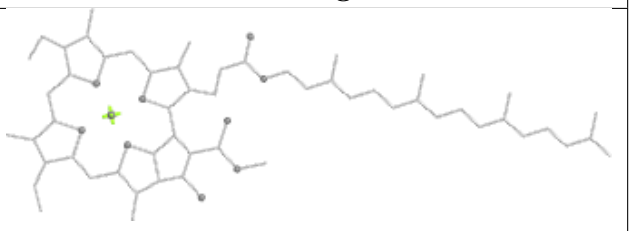
Bond lengths



Bond angles

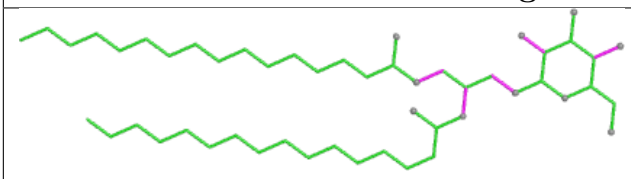


Torsions

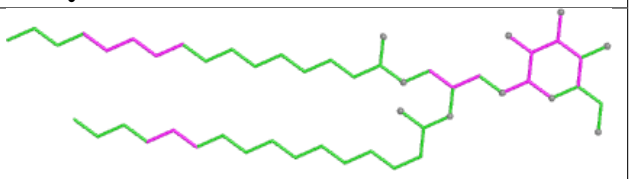


Rings

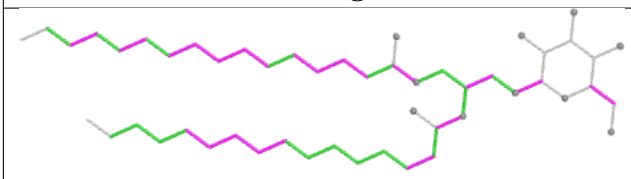
Ligand LMG Q 301



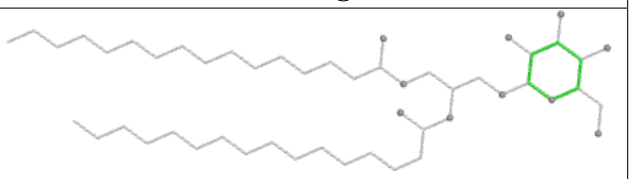
Bond lengths



Bond angles

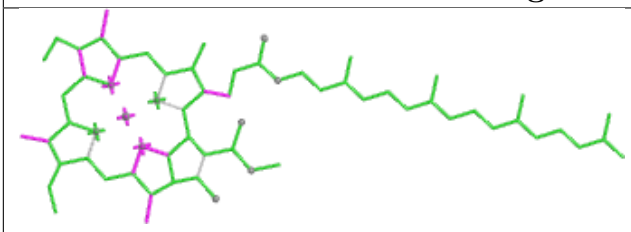


Torsions

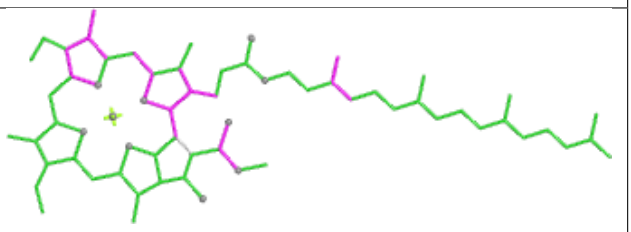


Rings

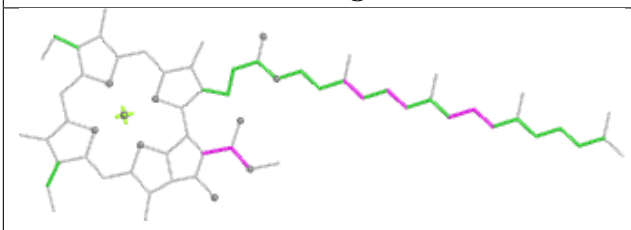
Ligand CLA b 613



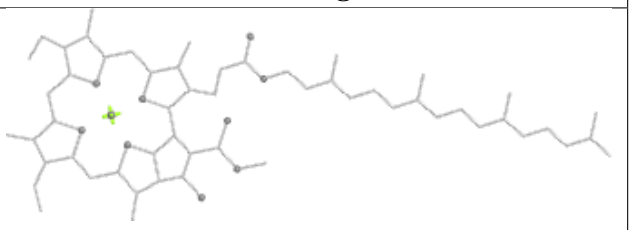
Bond lengths



Bond angles

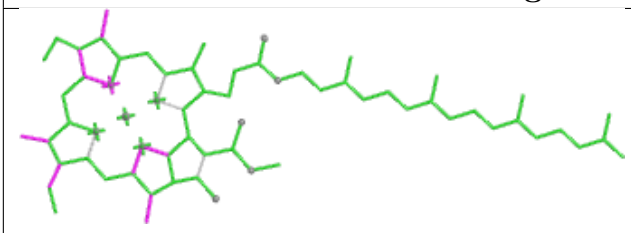


Torsions

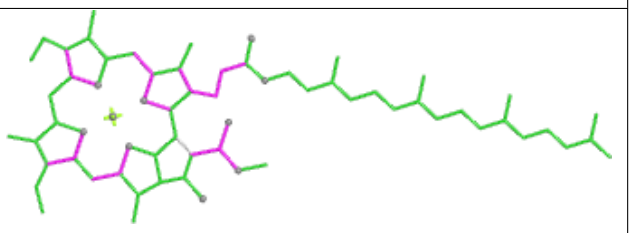


Rings

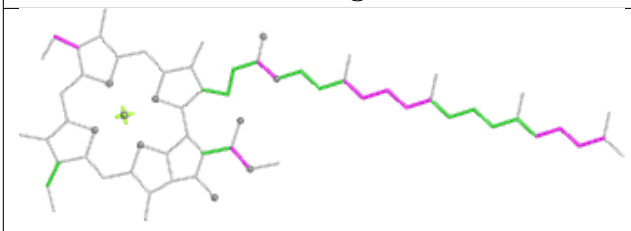
Ligand CLA B 602



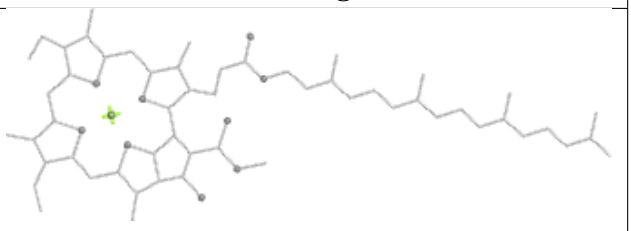
Bond lengths



Bond angles

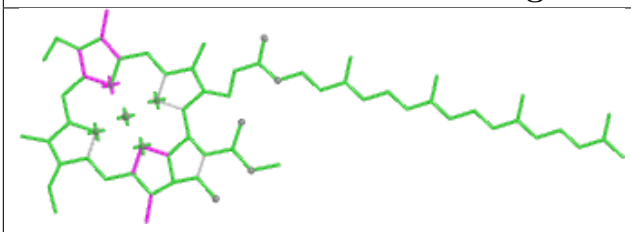


Torsions

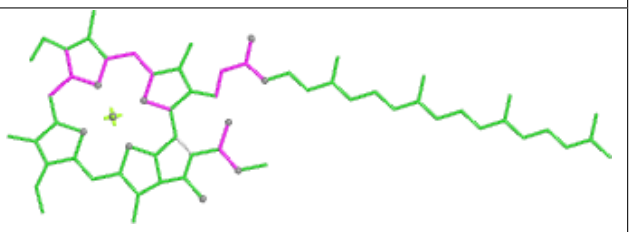


Rings

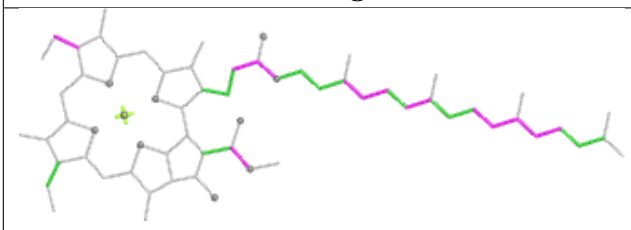
Ligand CLA Z 102



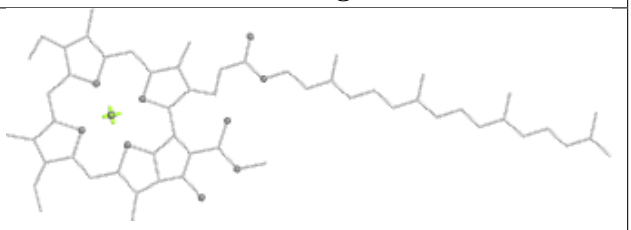
Bond lengths



Bond angles

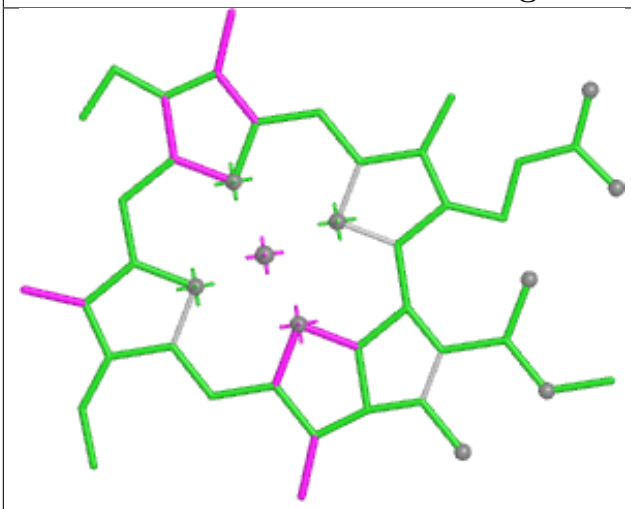


Torsions

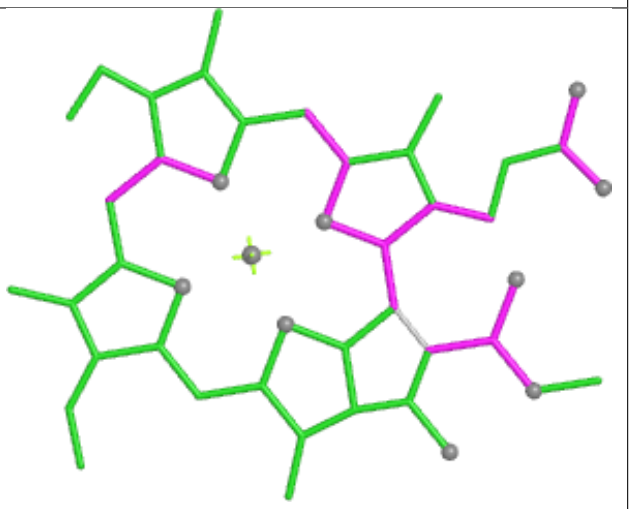


Rings

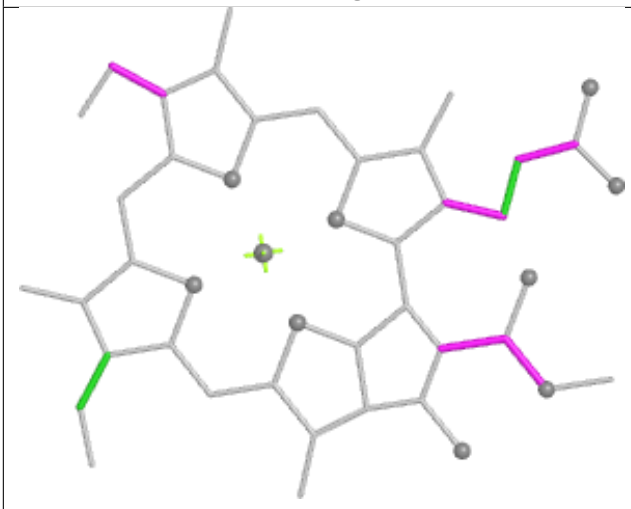
Ligand CLA 18 311



Bond lengths



Bond angles

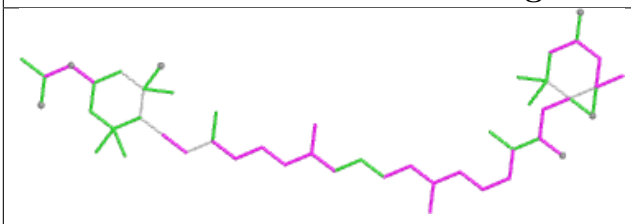


Torsions

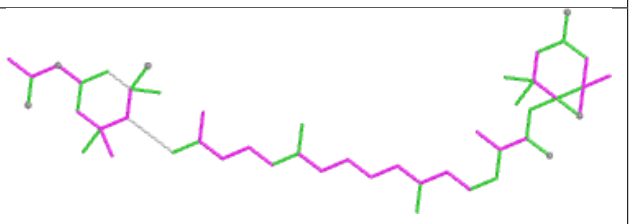


Rings

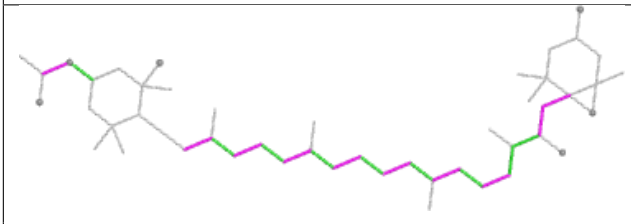
Ligand A86 20 210



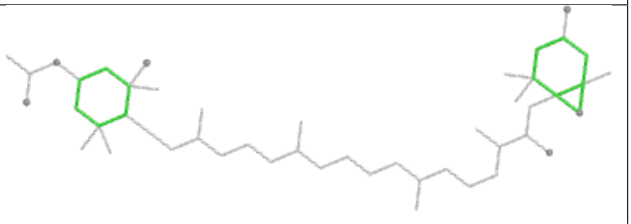
Bond lengths



Bond angles

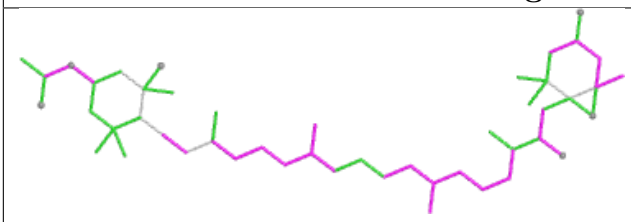


Torsions

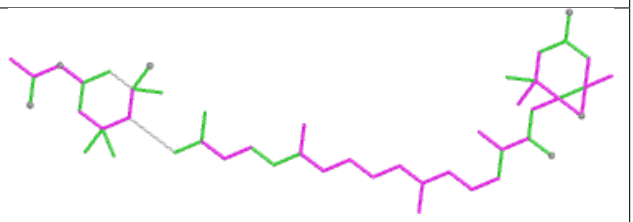


Rings

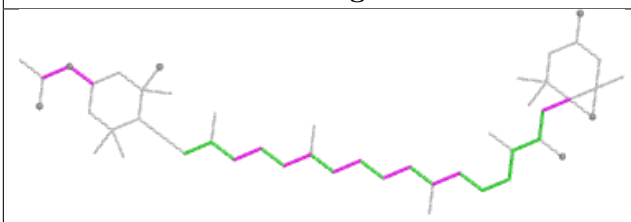
Ligand A86 20 201



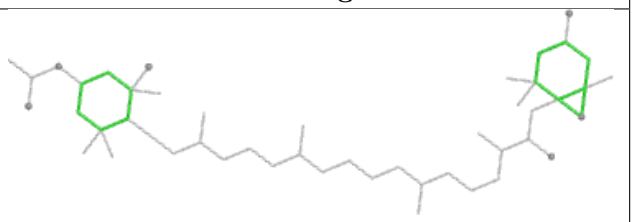
Bond lengths



Bond angles

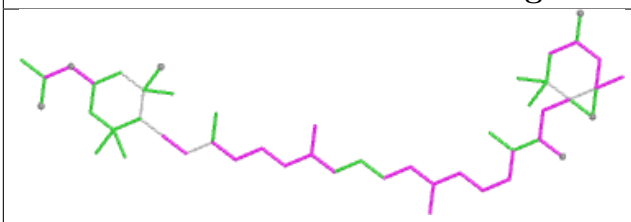


Torsions

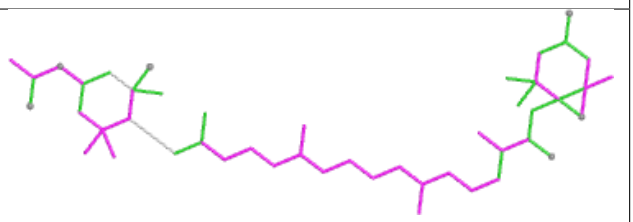


Rings

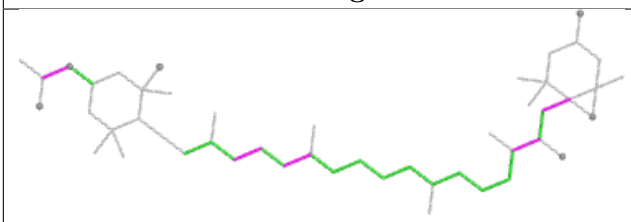
Ligand A86 15 313



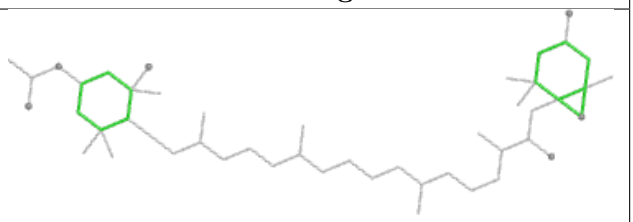
Bond lengths



Bond angles

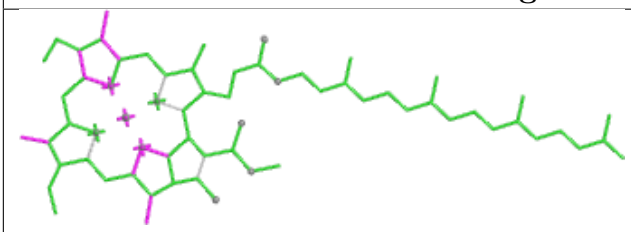


Torsions

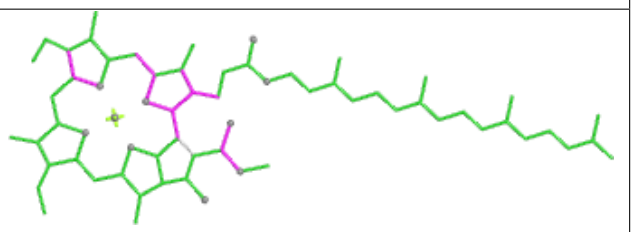


Rings

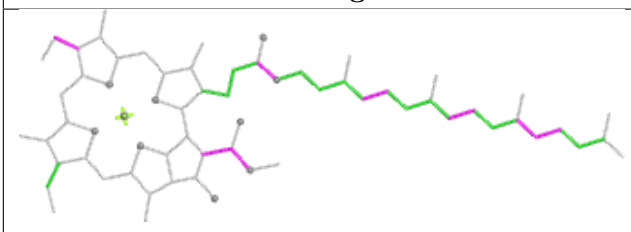
Ligand CLA 12 303



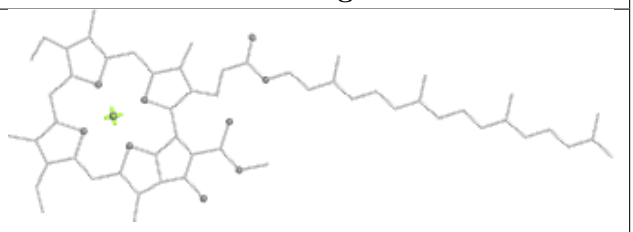
Bond lengths



Bond angles

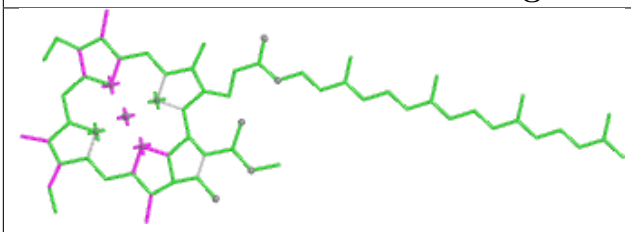


Torsions

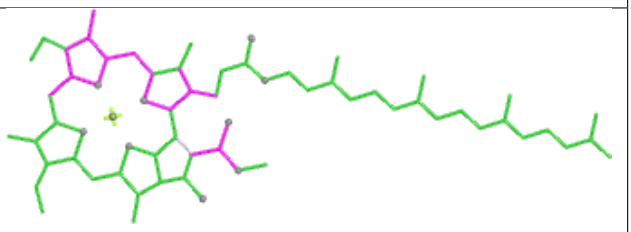


Rings

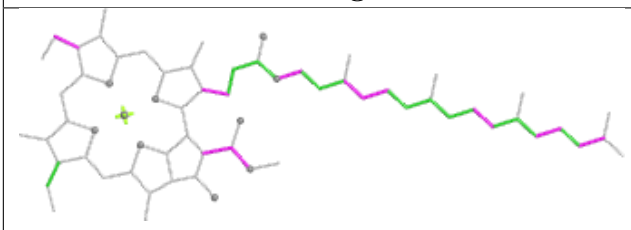
Ligand CLA D 401



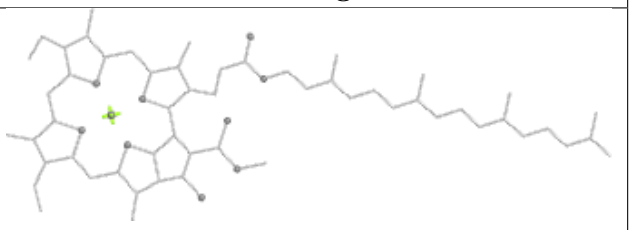
Bond lengths



Bond angles

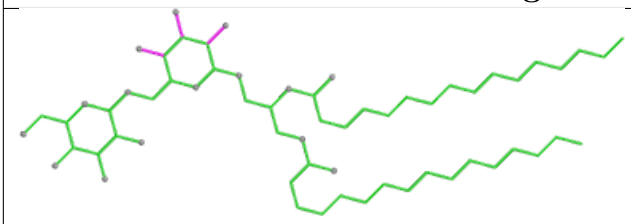


Torsions

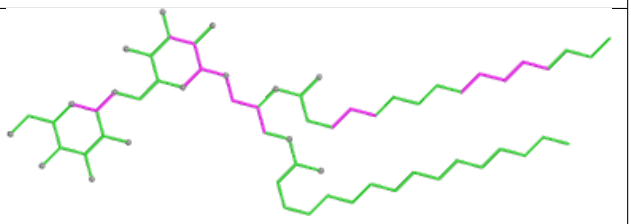


Rings

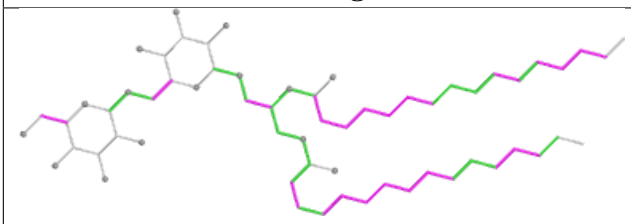
Ligand DGD h 102



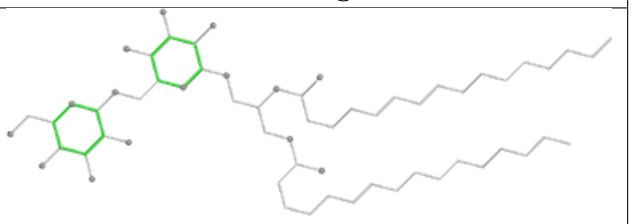
Bond lengths



Bond angles

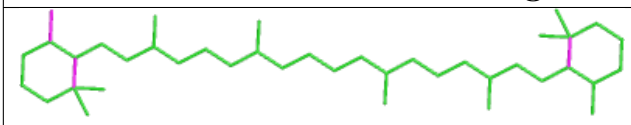


Torsions

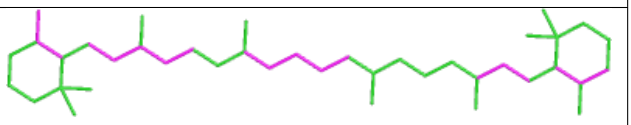


Rings

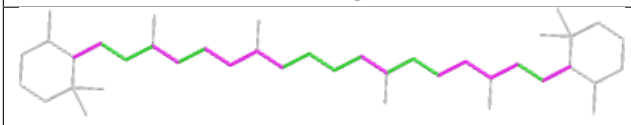
Ligand BCR Z 101



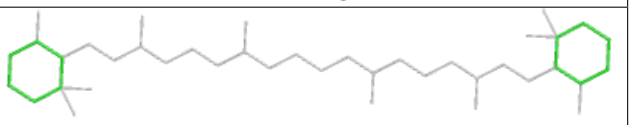
Bond lengths



Bond angles

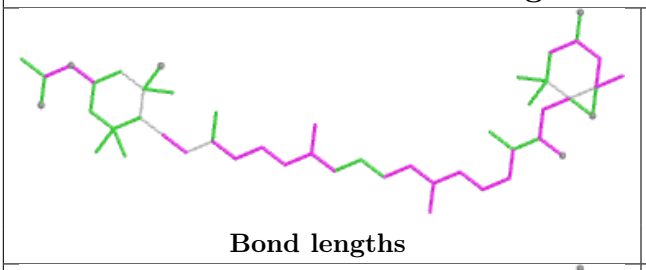


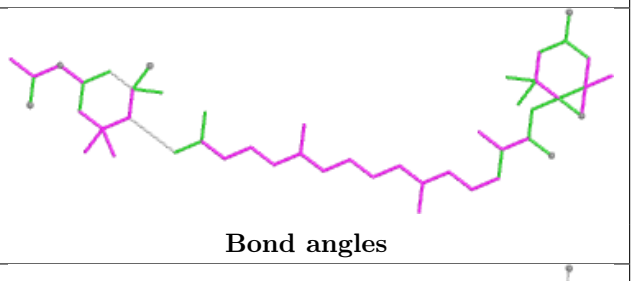
Torsions

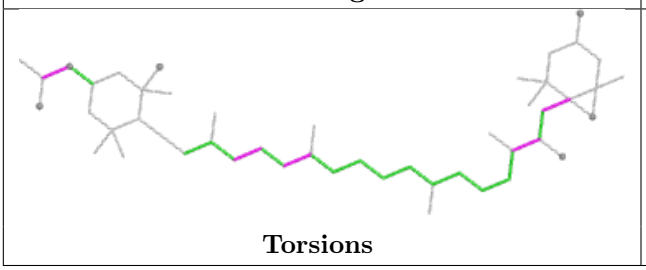


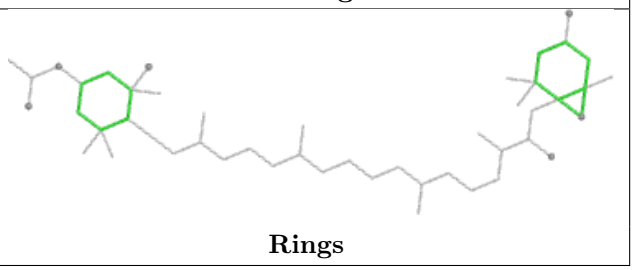
Rings

Ligand A86 11 313

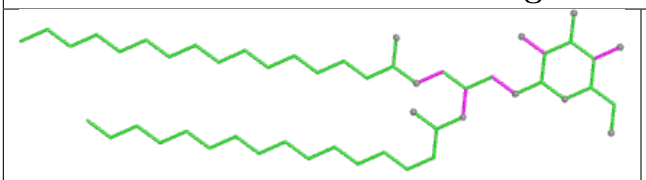

Bond lengths

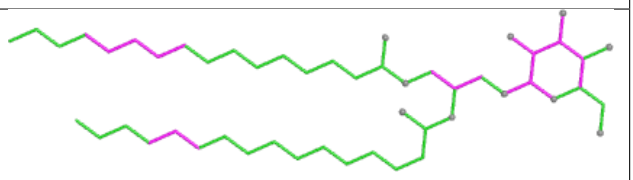

Bond angles

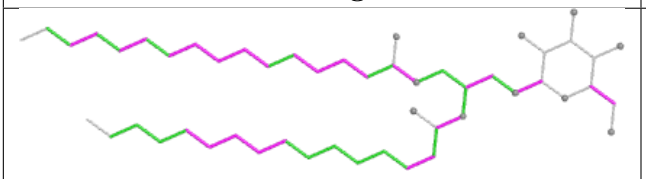

Torsions

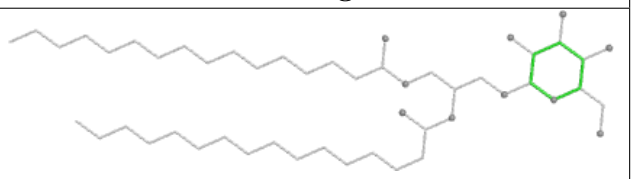

Rings

Ligand LMG c 519

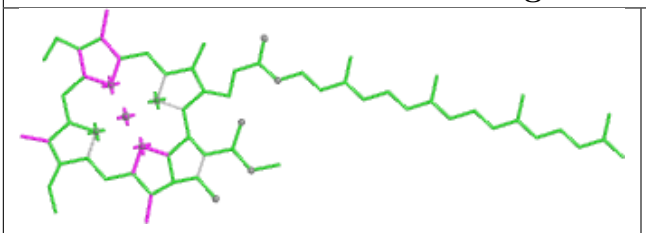

Bond lengths

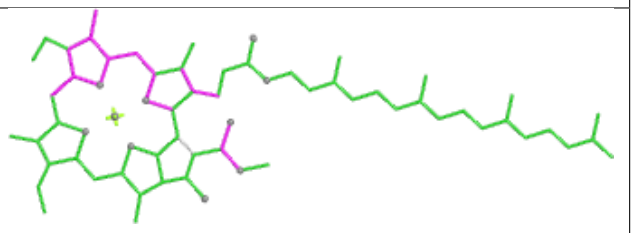

Bond angles

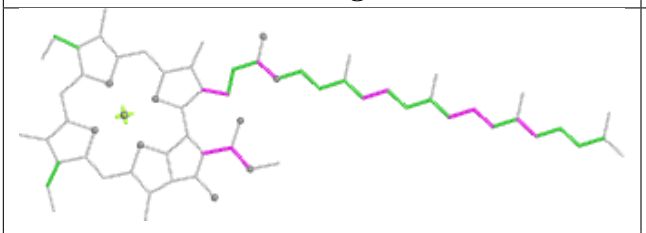

Torsions

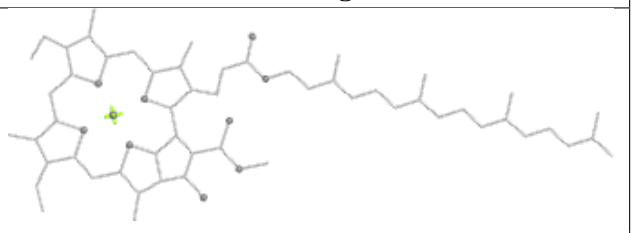

Rings

Ligand CLA B 607

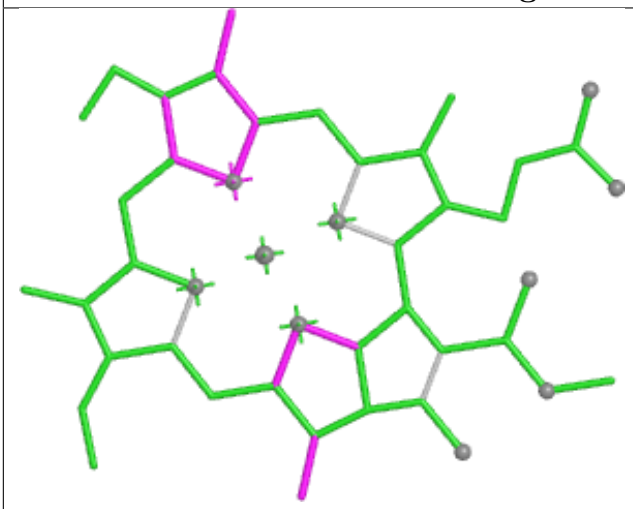

Bond lengths


Bond angles

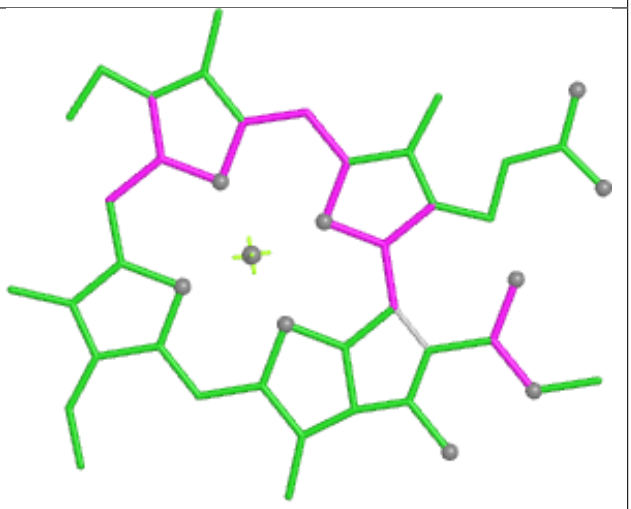

Torsions


Rings

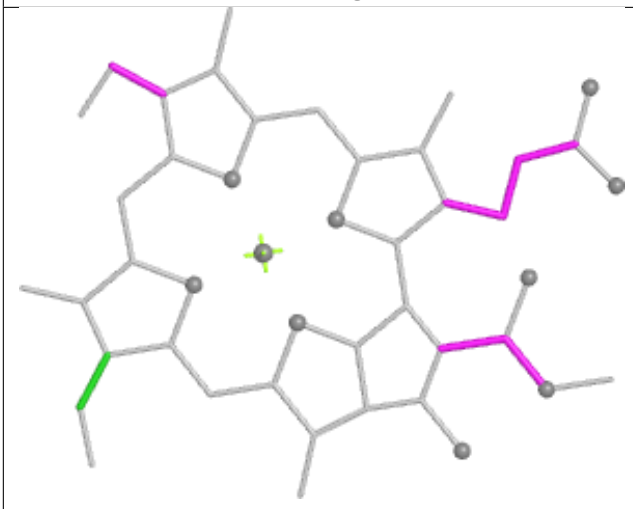
Ligand CLA 11 306



Bond lengths



Bond angles

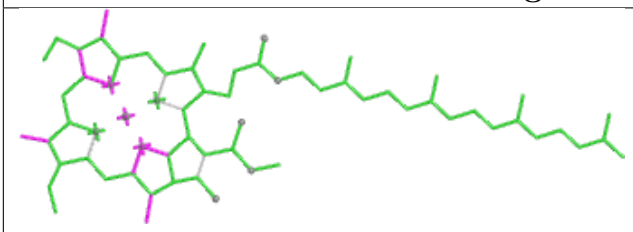


Torsions

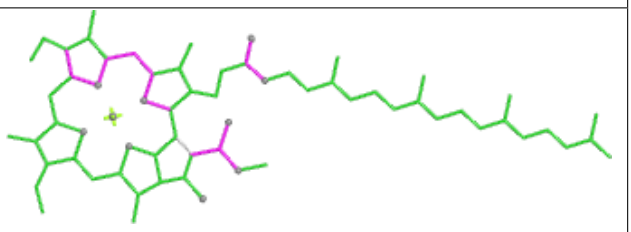


Rings

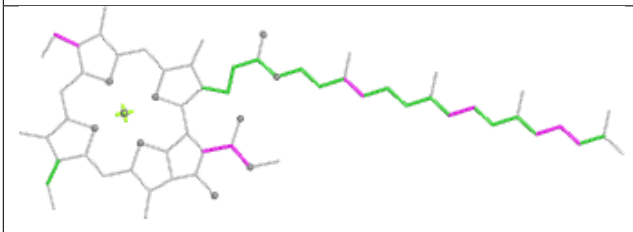
Ligand CLA B 608



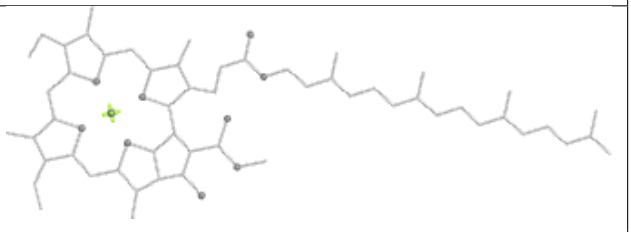
Bond lengths



Bond angles

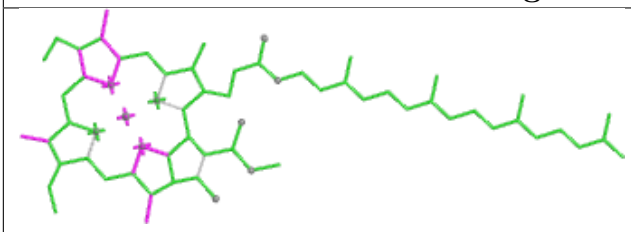


Torsions

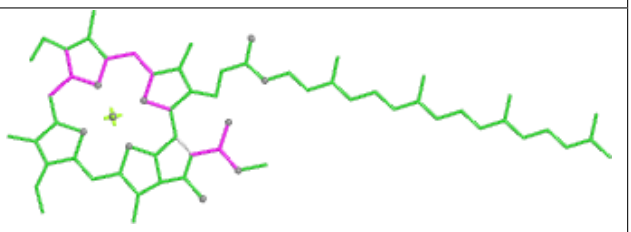


Rings

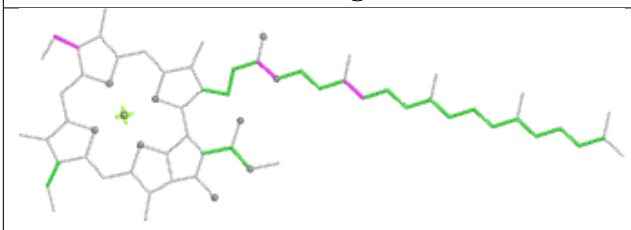
Ligand CLA D 406



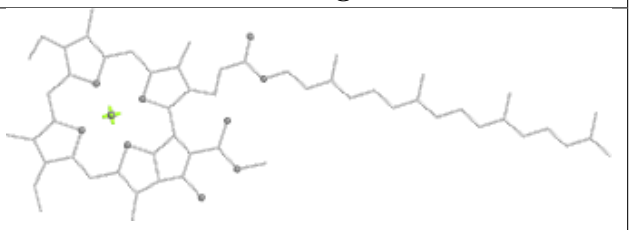
Bond lengths



Bond angles

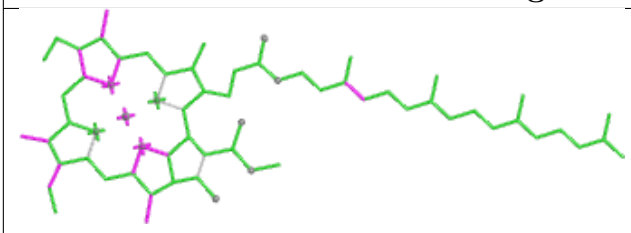


Torsions

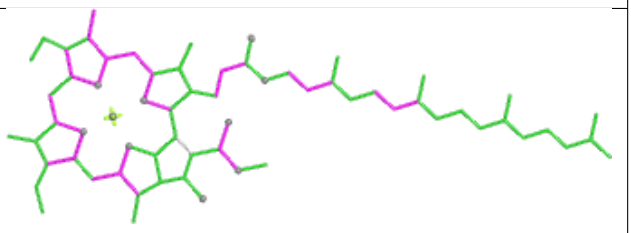


Rings

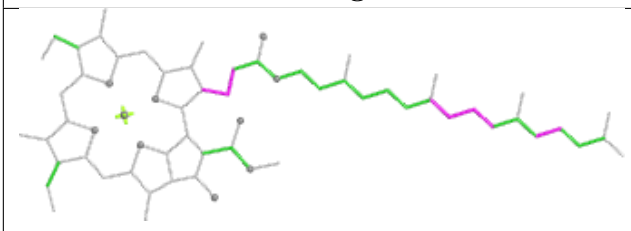
Ligand CLA b 606



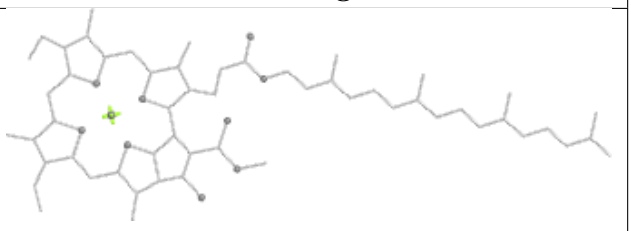
Bond lengths



Bond angles

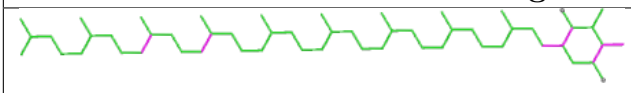


Torsions

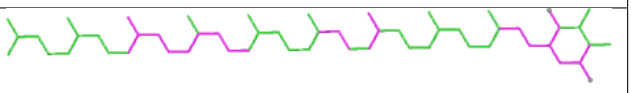


Rings

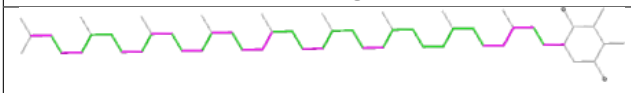
Ligand PL9 D 404



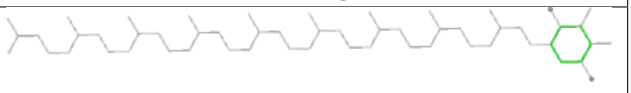
Bond lengths



Bond angles

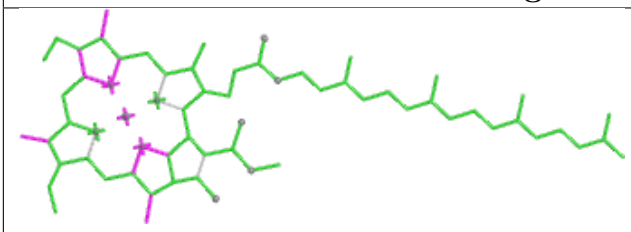


Torsions

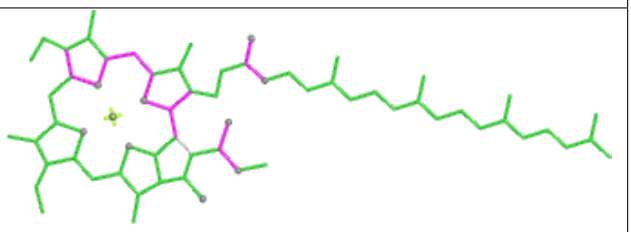


Rings

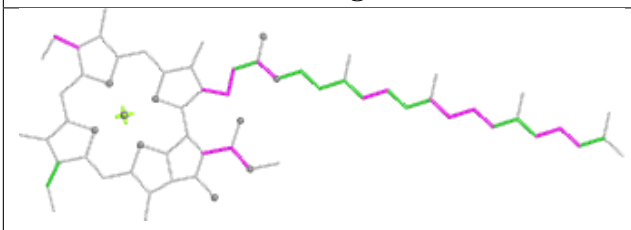
Ligand CLA C 513



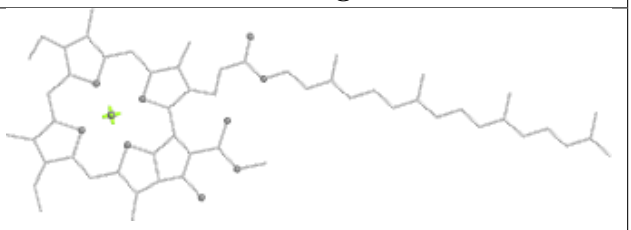
Bond lengths



Bond angles

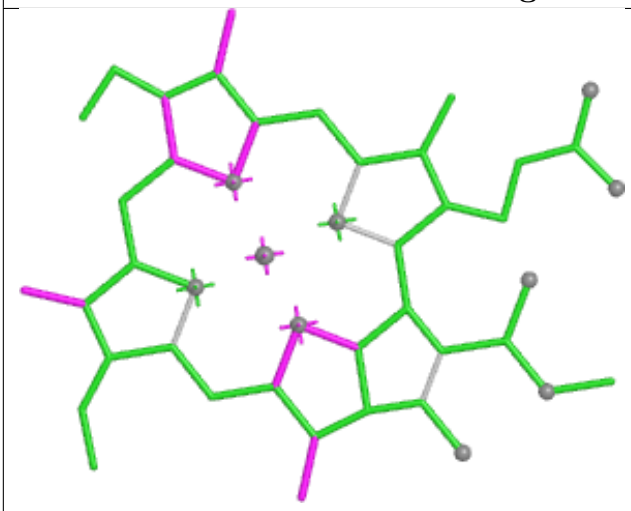


Torsions

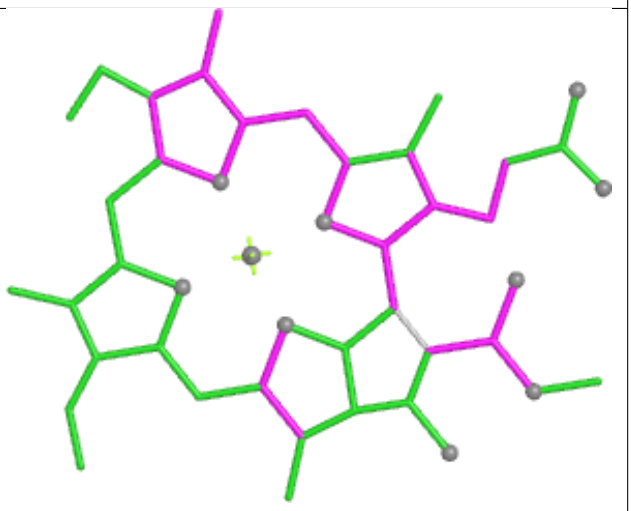


Rings

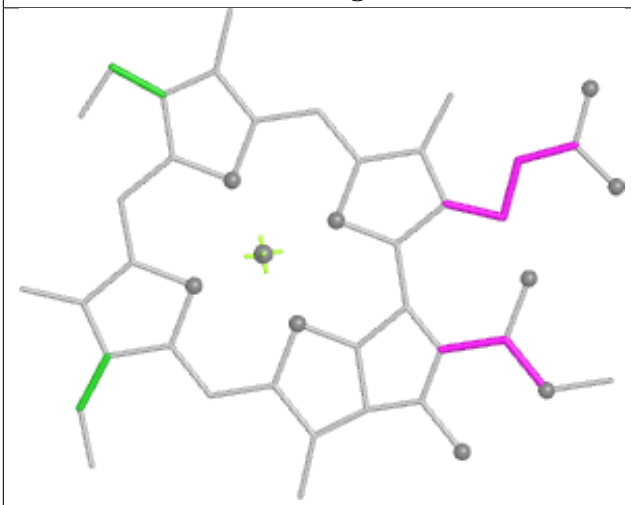
Ligand CLA 13 305



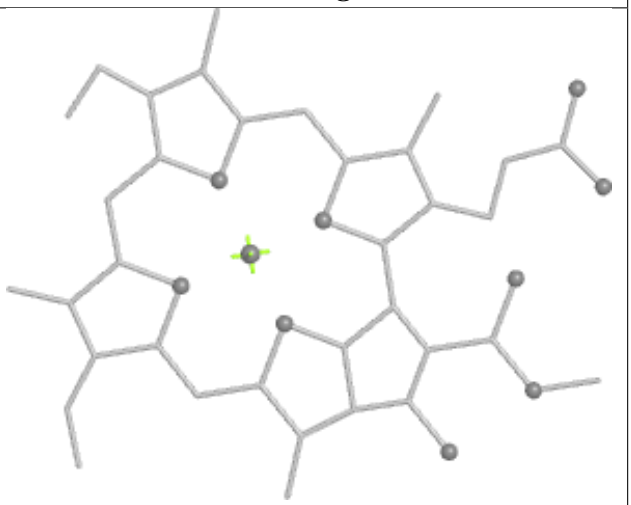
Bond lengths



Bond angles

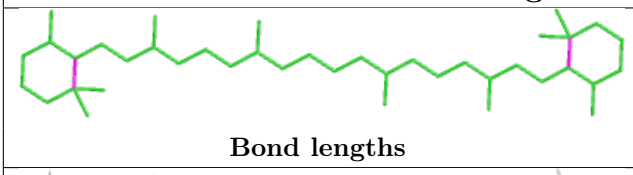


Torsions

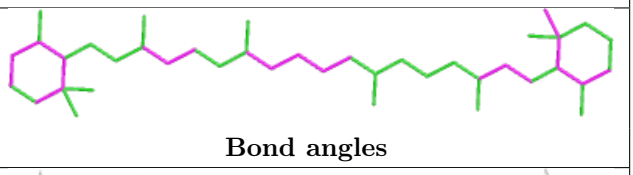


Rings

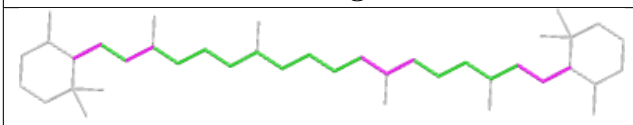
Ligand BCR b 617



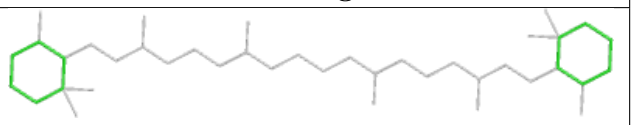
Bond lengths



Bond angles

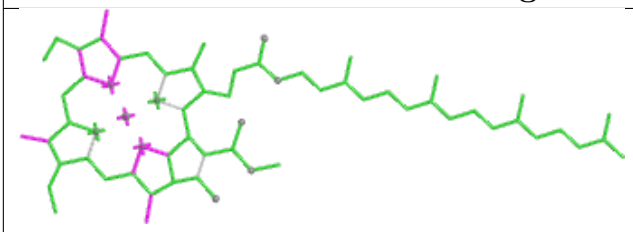


Torsions

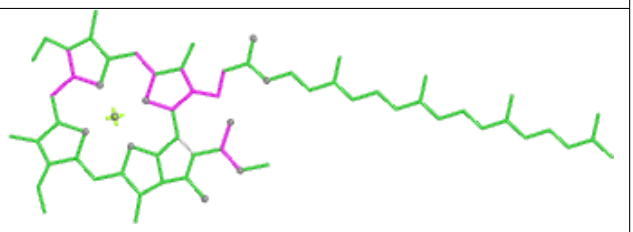


Rings

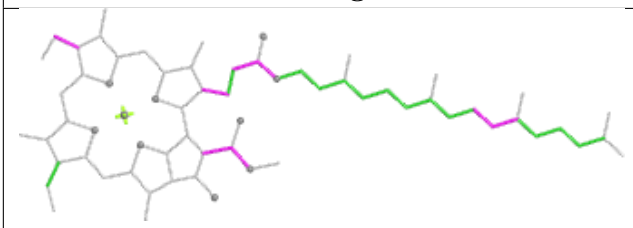
Ligand CLA 11 303



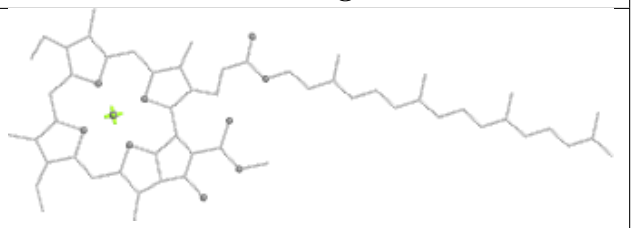
Bond lengths



Bond angles

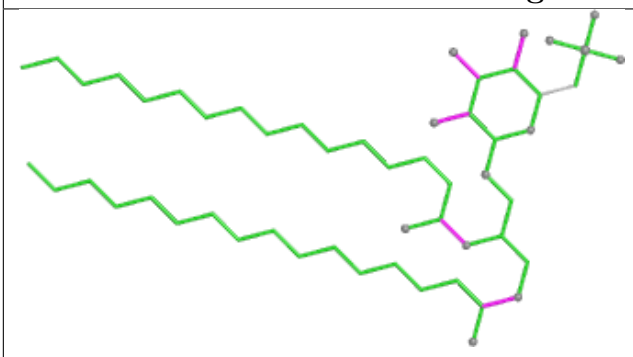


Torsions

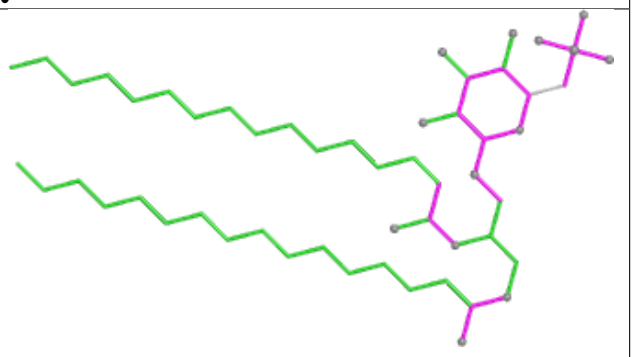


Rings

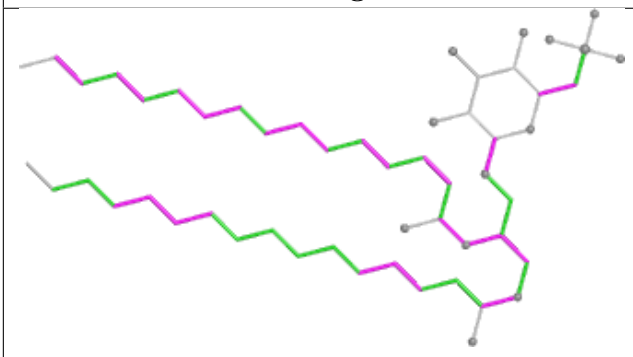
Ligand SQD L 103



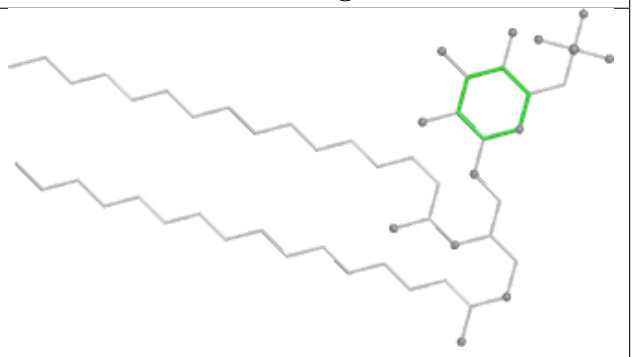
Bond lengths



Bond angles

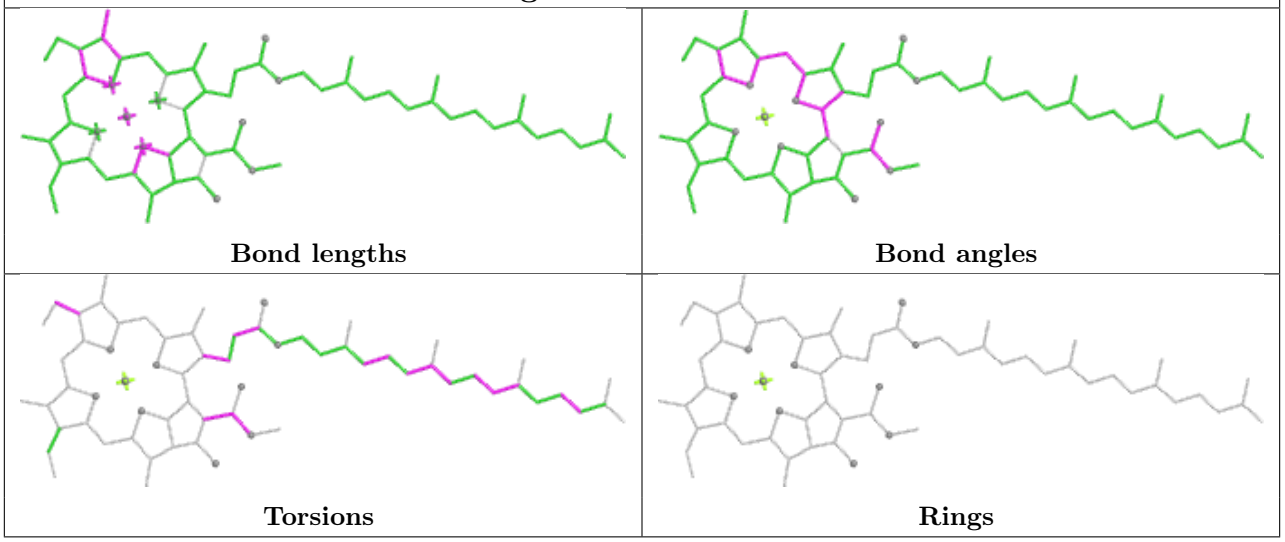


Torsions

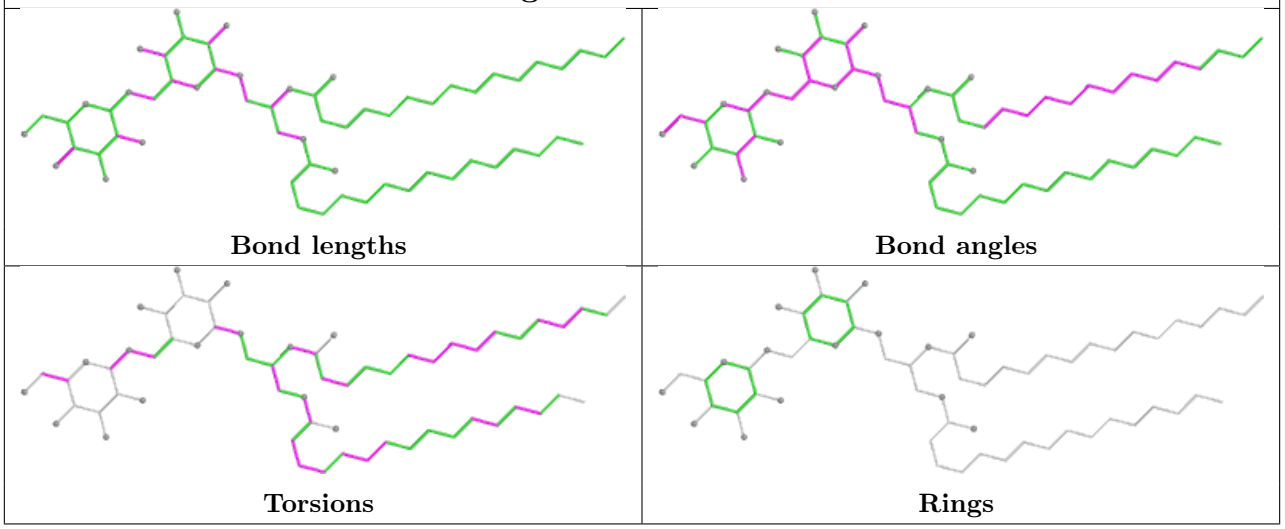


Rings

Ligand CLA 21 303



Ligand DGD C 517



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.

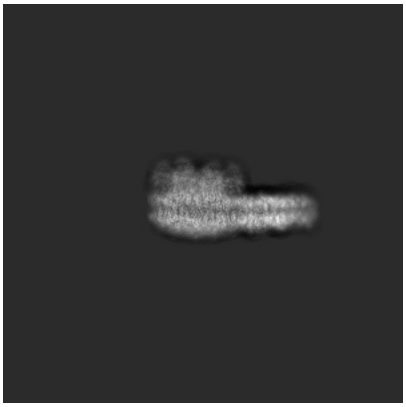
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9776. These allow visual inspection of the internal detail of the map and identification of artifacts.

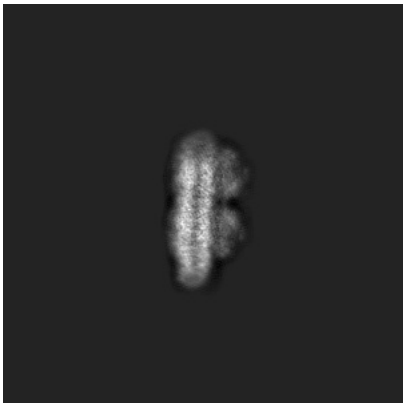
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

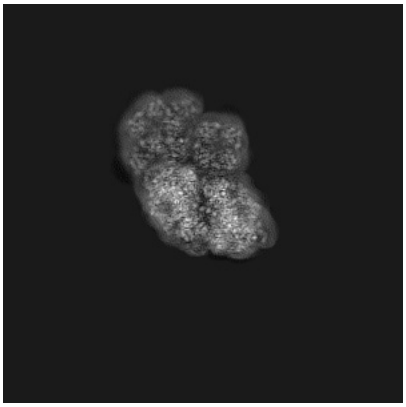
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

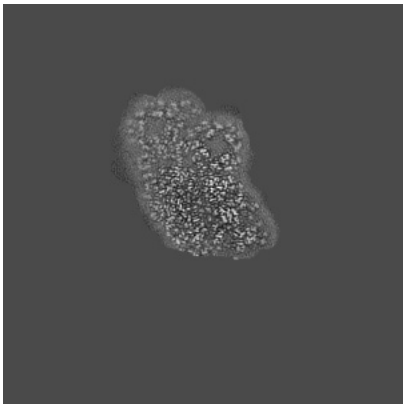
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

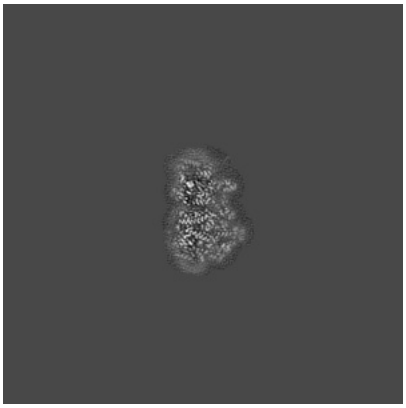
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

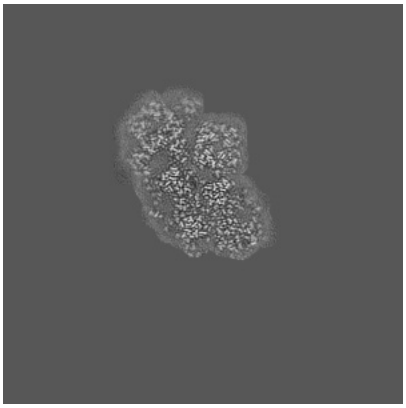
6.3.1 Primary map



X Index: 283



Y Index: 274

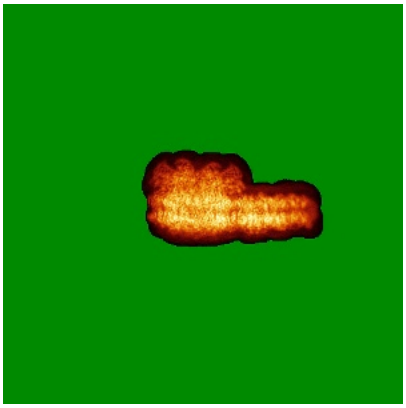


Z Index: 237

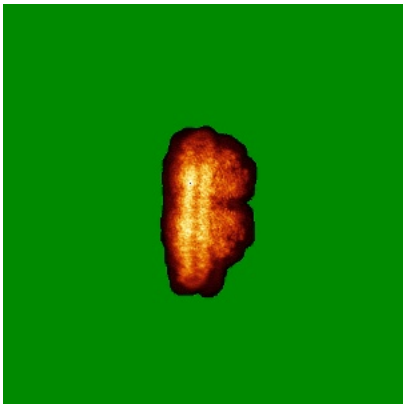
The images above show the largest variance slices of the map in three orthogonal directions.

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

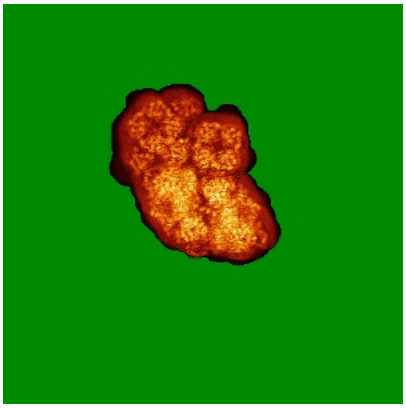
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

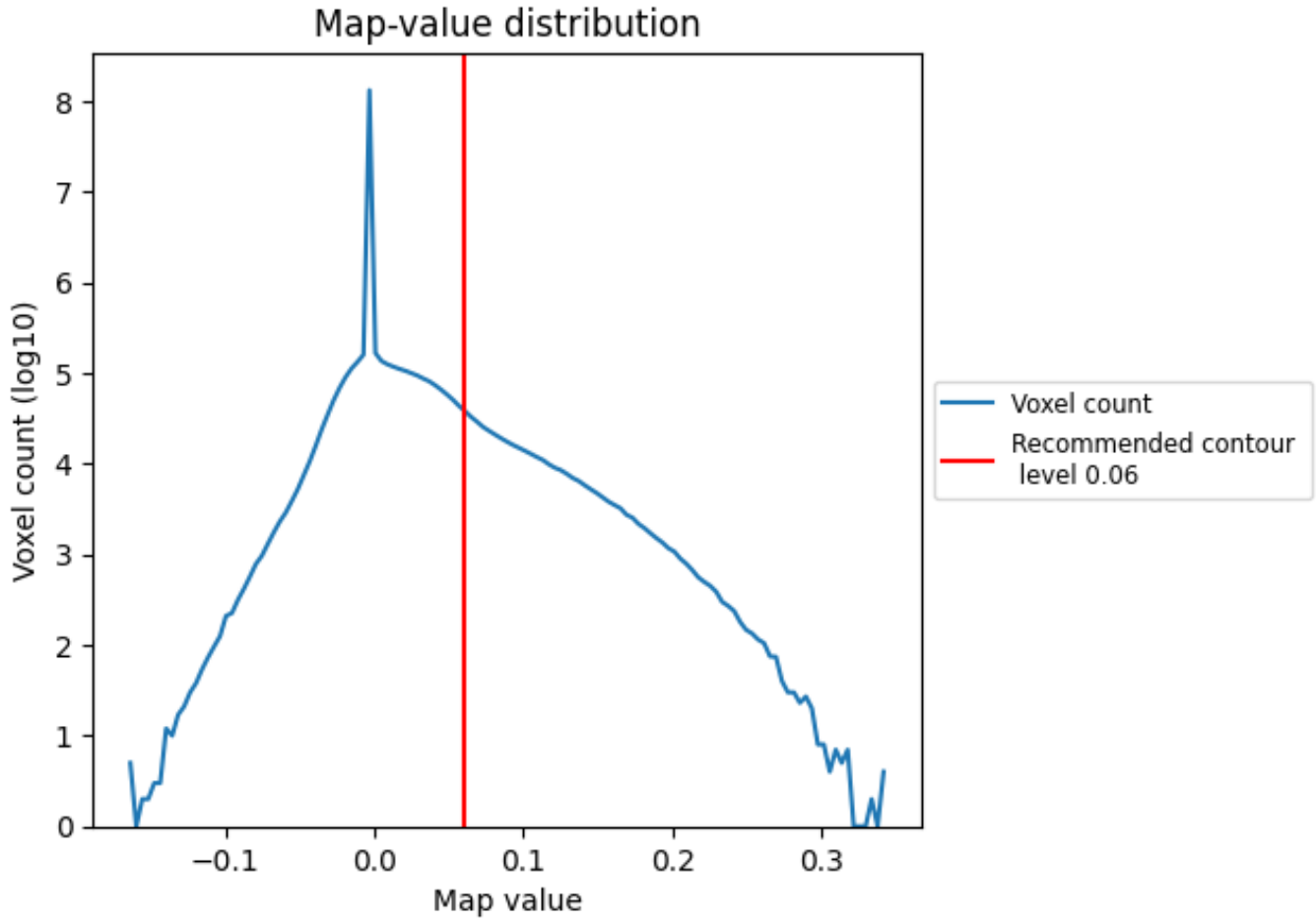
6.6 Mask visualisation (i)

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

7 Map analysis

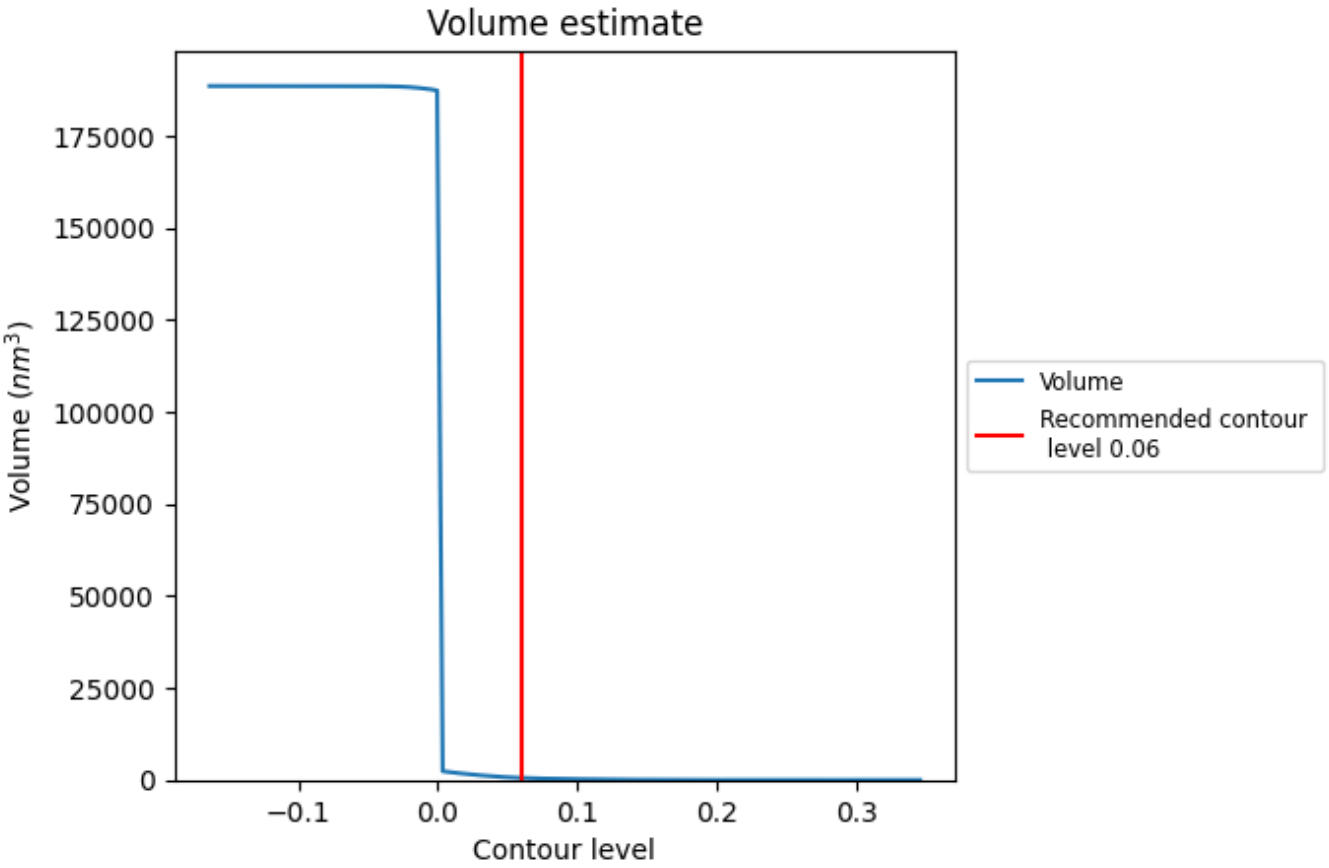
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

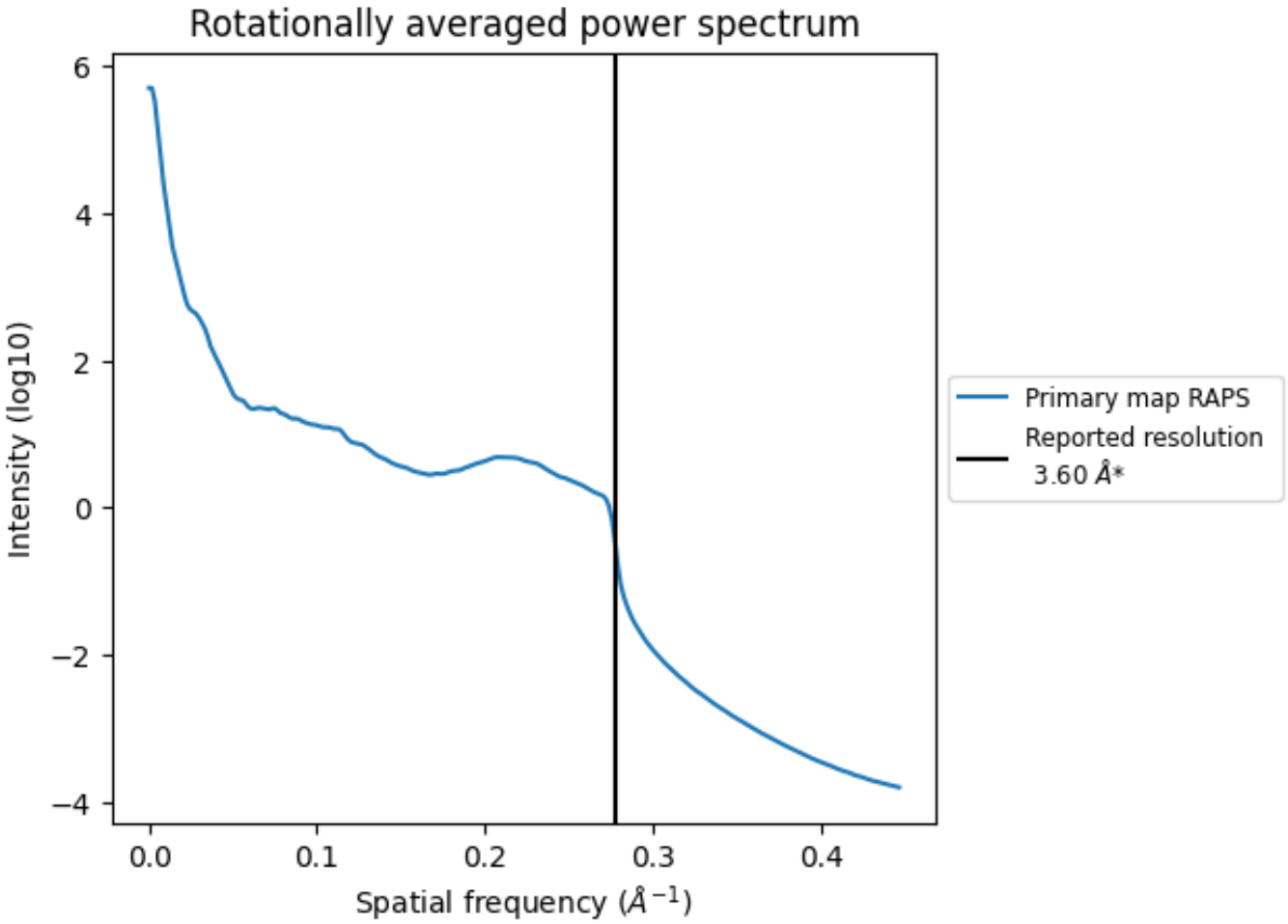
7.2 Volume estimate



The volume at the recommended contour level is 558 nm^3; this corresponds to an approximate mass of 504 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)

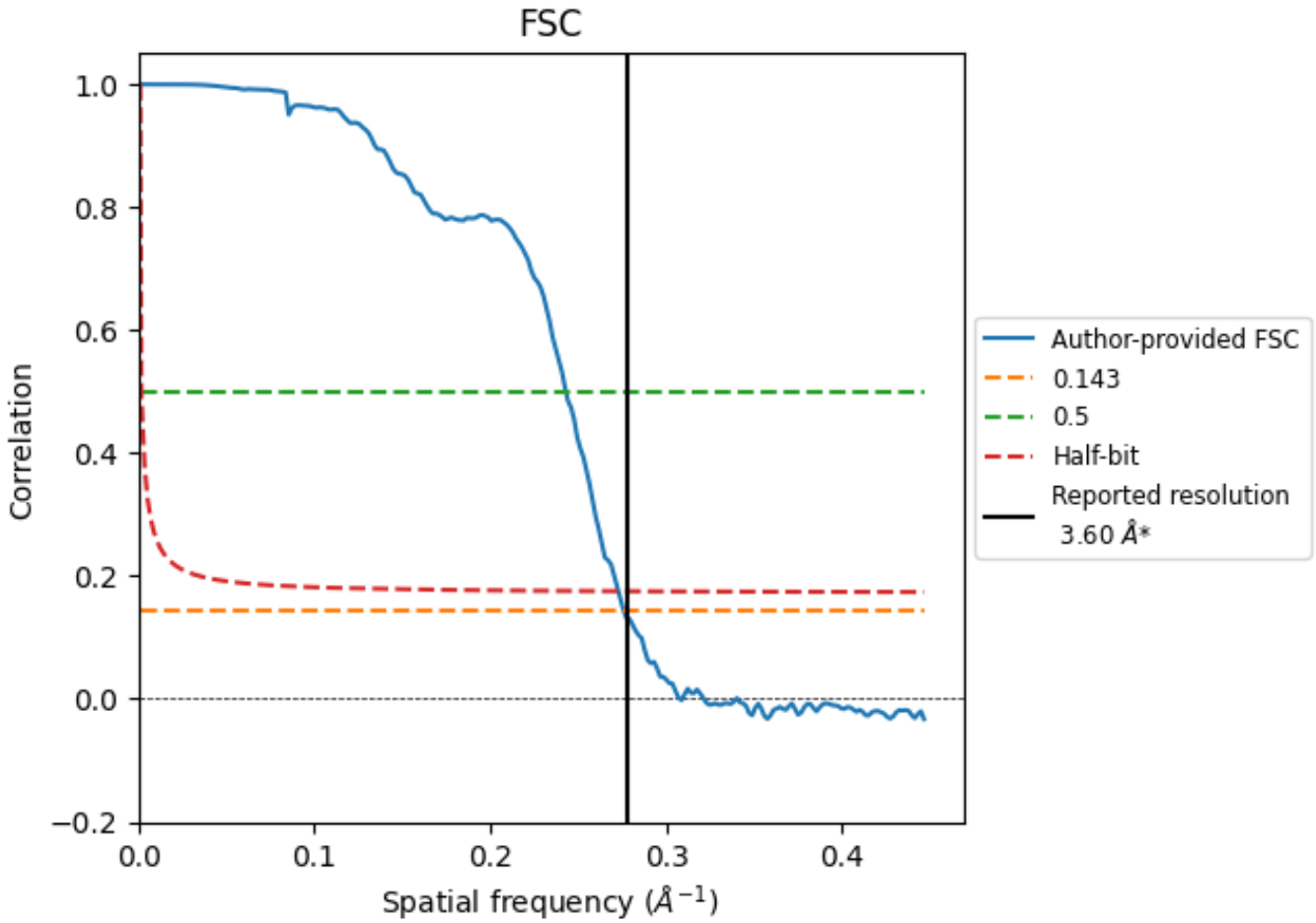


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

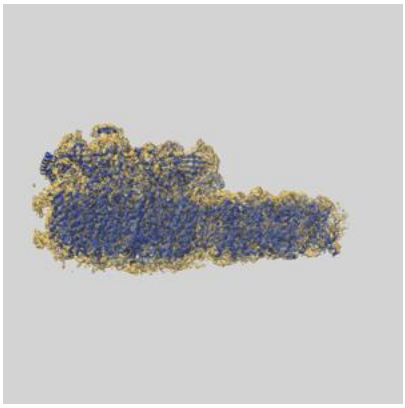
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.62	4.12	3.67
Unmasked-calculated*	-	-	-

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

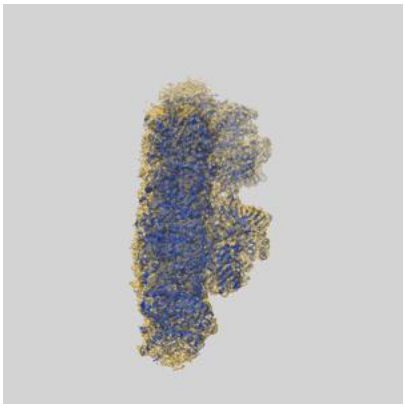
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9776 and PDB model 6J3Z. Per-residue inclusion information can be found in section 3 on page 34.

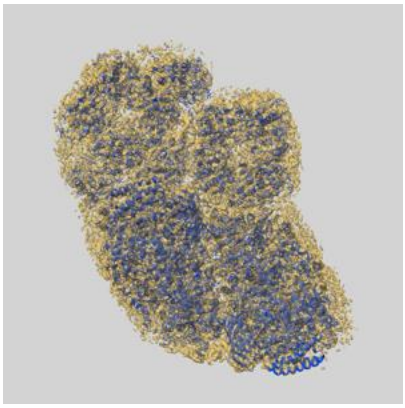
9.1 Map-model overlay



X



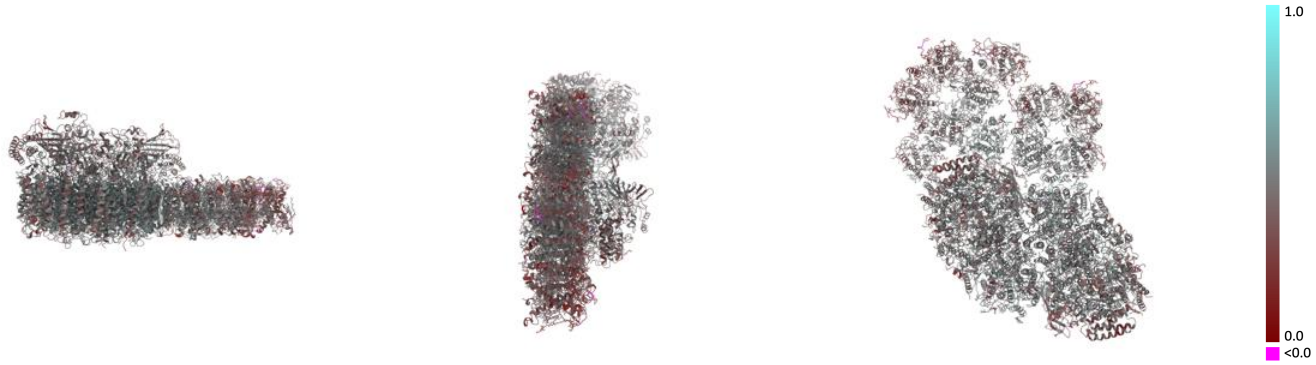
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

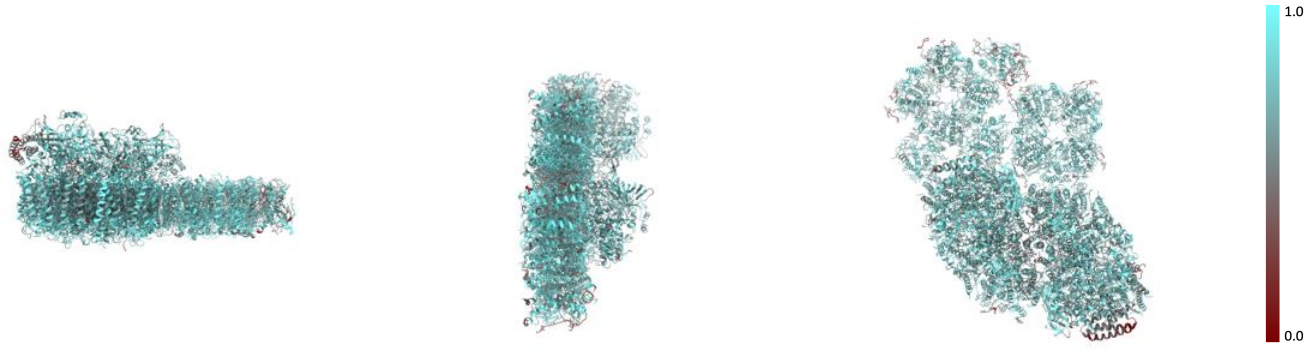
9.2 Q-score mapped to coordinate model



X Y Z

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

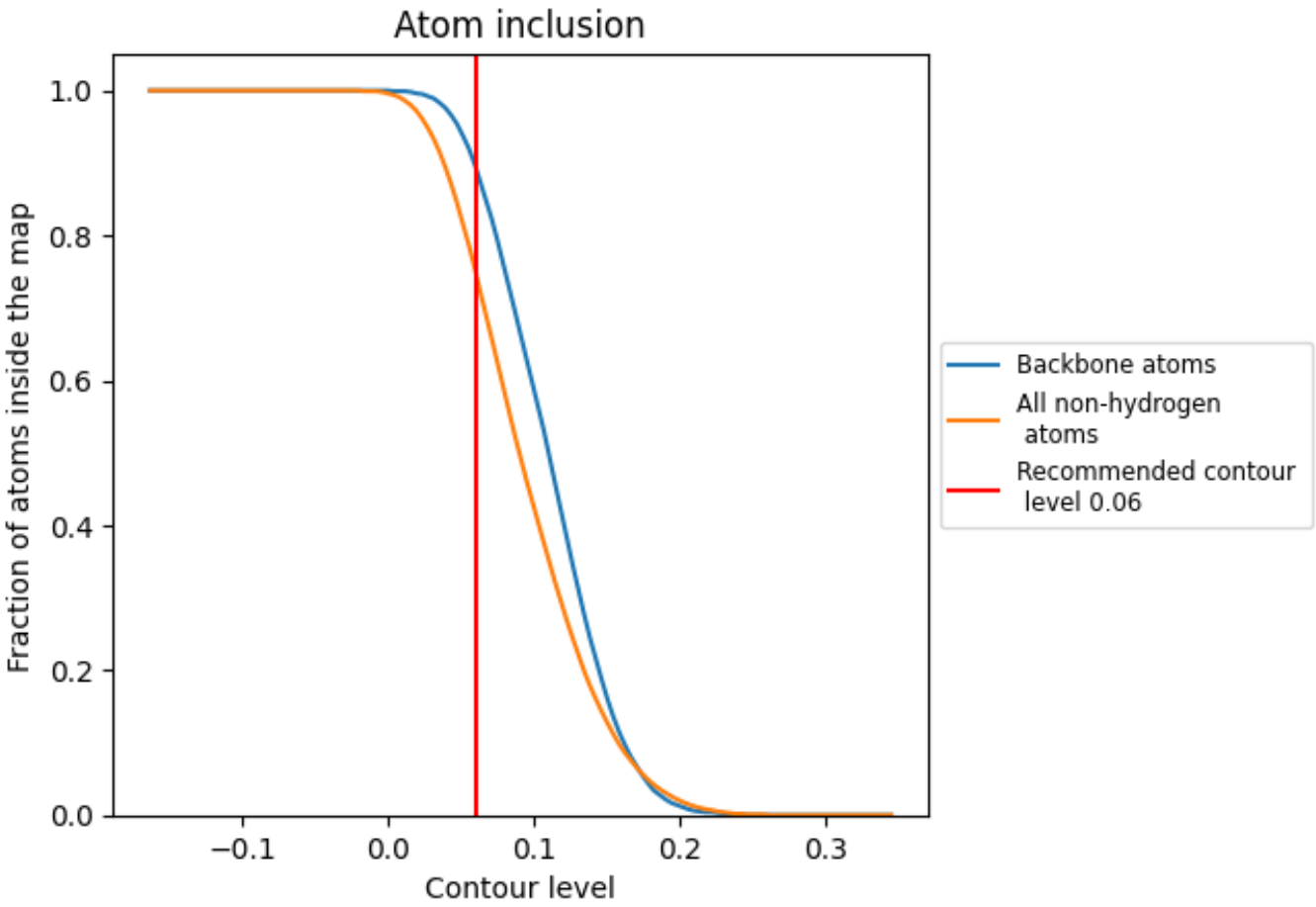
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 75% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7500	0.4440
0	0.8060	0.4800
1	0.7990	0.4560
11	0.8000	0.4590
12	0.7620	0.4290
13	0.7400	0.3620
14	0.7470	0.3900
15	0.6860	0.3320
16	0.7630	0.4130
17	0.7650	0.4300
18	0.7030	0.3440
19	0.8770	0.4910
2	0.9200	0.4440
20	0.7920	0.4140
21	0.6320	0.3220
5	0.8450	0.5000
6	0.9070	0.4900
7	0.7800	0.4160
A	0.7910	0.4950
B	0.7670	0.4850
C	0.7830	0.4850
D	0.7590	0.4850
E	0.7750	0.4020
F	0.7120	0.4340
H	0.7690	0.4620
I	0.7770	0.4740
J	0.7010	0.4580
K	0.7800	0.4690
L	0.6670	0.4870
M	0.6230	0.4450
O	0.7260	0.4240
Q	0.6860	0.3850
T	0.7180	0.4600
U	0.7340	0.4100
V	0.7720	0.4250



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
W	0.6360	0.4260
X	0.6760	0.3880
Y	0.6370	0.4140
Z	0.7210	0.4190
a	0.7940	0.4950
b	0.7950	0.4960
c	0.7700	0.4750
d	0.7600	0.4960
e	0.7800	0.4230
f	0.7420	0.4250
h	0.7720	0.4750
i	0.7870	0.4590
j	0.7040	0.4360
k	0.7500	0.4510
l	0.6620	0.4800
m	0.6540	0.4620
o	0.6960	0.4120
q	0.4380	0.3550
t	0.7060	0.4560
u	0.7360	0.4070
v	0.7780	0.4320
w	0.5870	0.3920
x	0.6910	0.3720
y	0.5980	0.3680
z	0.7000	0.3950