wwPDB EM Validation Summary Report

Sep 29, 2026 – 05:00 PM JST

PDB ID	:	8JZE / pdb_00008jze
EMDB ID	:	EMD-36742
Title	:	PSI-AcpPCI supercomplex from Symbiodinium
Authors	:	Li, Z.H.; Li, X.Y.; Wang, W.D.
Deposited on	:	2023-07-05
Resolution	:	2.99 Å(reported)

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:

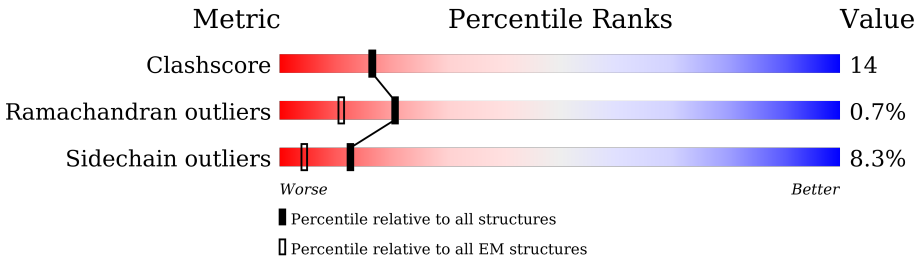
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

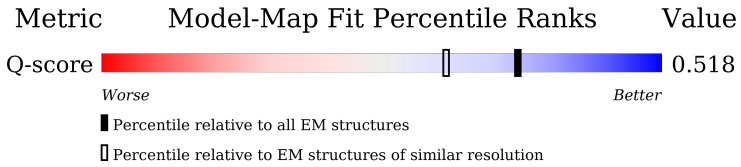
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.99 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	13287 (2.49 - 3.49)

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	I	200	6%, 71%, 26%
2	K	177	67%, 31%
3	z	78	92%, 8%
4	y	131	97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	G	224	65% 29%
6	A	189	73% 22%
7	c	86	72% 28%
8	d	218	76% 22%
9	e	73	75% 25%
10	f	184	79% 20%
11	h	131	69% 31%
12	i	119	73% 27%
13	j	98	74% 24%
14	l	250	69% 28%
15	m	79	76% 24%
16	a	670	70% 27%
17	b	663	70% 29%
18	B	192	65% 32%
19	D	165	57% 32% 8%
20	F	176	6% 64% 26% 5%
21	H	160	66% 61% 34% 5%
22	J	220	72% 25%
23	L	185	63% 30% 7%
24	M	173	62% 28% 8%
25	N	160	36% 55% 32% 8%
26	O	161	7% 66% 30%
27	P	160	59% 28% 12%

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 55927 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 Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	I	200	1480	961	250	259	10	0	0

- Molecule 2 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	K	177	1349	872	227	238	12	0	0

- Molecule 3 is a protein called Photosystem I unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	z	78	390	234	78	78	0	0

- Molecule 4 is a protein called Photosystem I unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	y	131	655	393	131	131	0	0

- Molecule 5 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	217	1572	1004	269	289	10	0	0

- Molecule 6 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	186	Total	C	N	O	S	0	0
			1346	870	225	242	9		

- Molecule 7 is a protein called Photosystem I PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	86	Total	C	N	O	S	0	0
			653	403	109	132	9		

- Molecule 8 is a protein called Photosystem I PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	218	Total	C	N	O	S	0	0
			1731	1096	307	315	13		

- Molecule 9 is a protein called Photosystem I PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	e	73	Total	C	N	O	0	0
			587	384	99	104		

- Molecule 10 is a protein called Photosystem I PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	184	Total	C	N	O	S	0	0
			1450	930	252	260	8		

- Molecule 11 is a protein called Photosystem I PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	h	131	Total	C	N	O	S	0	0
			1066	704	165	193	4		

- Molecule 12 is a protein called Photosystem I PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	i	119	Total	C	N	O	S	0	0
			964	620	167	175	2		

- Molecule 13 is a protein called Photosystem I PsaJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	j	98	Total 783	C 505	N 125	O 153	0	0

- Molecule 14 is a protein called Photosystem I PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	l	250	Total 1943	C 1267	N 312	O 354	S 10	0	0

- Molecule 15 is a protein called Photosystem I PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	m	79	Total 582	C 373	N 100	O 107	S 2	0	0

- Molecule 16 is a protein called Photosystem I PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	670	Total 5194	C 3393	N 875	O 910	S 16	0	0

- Molecule 17 is a protein called Photosystem I PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	663	Total 5199	C 3408	N 851	O 928	S 12	0	0

- Molecule 18 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	192	Total 1452	C 934	N 241	O 265	S 12	0	0

- Molecule 19 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D	160	Total 1158	C 728	N 195	O 228	S 7	0	0

- Molecule 20 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2,

acpPCI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	169	Total	C	N	O	S	0	0
			1237	777	209	239	12		

- Molecule 21 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	160	Total	C	N	O	S	0	0
			1202	769	198	228	7		

- Molecule 22 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	J	220	Total	C	N	O	S	0	0
			1496	938	261	290	7		

- Molecule 23 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	185	Total	C	N	O	S	0	0
			1427	924	239	258	6		

- Molecule 24 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	168	Total	C	N	O	S	0	0
			1211	773	208	225	5		

- Molecule 25 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	153	Total	C	N	O	S	0	0
			993	607	179	202	5		

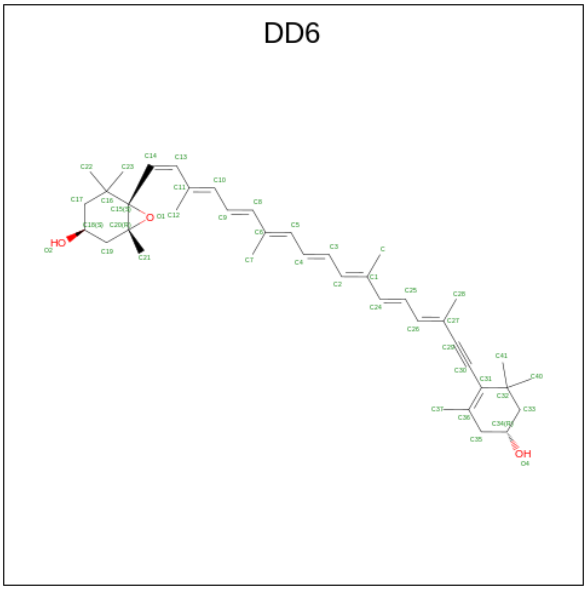
- Molecule 26 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	161	Total	C	N	O	S	0	0
			1073	670	189	207	7		

- Molecule 27 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	159	Total	C	N	O	S	0	0
			1113	693	191	223	6		

- Molecule 28 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	I	1	Total	C	O		0
			43	40	3		
28	I	1	Total	C	O		0
			43	40	3		
28	I	1	Total	C	O		0
			43	40	3		
28	I	1	Total	C	O		0
			43	40	3		
28	K	1	Total	C	O		0
			43	40	3		
28	K	1	Total	C	O		0
			43	40	3		

Continued on next page...

Continued from previous page...

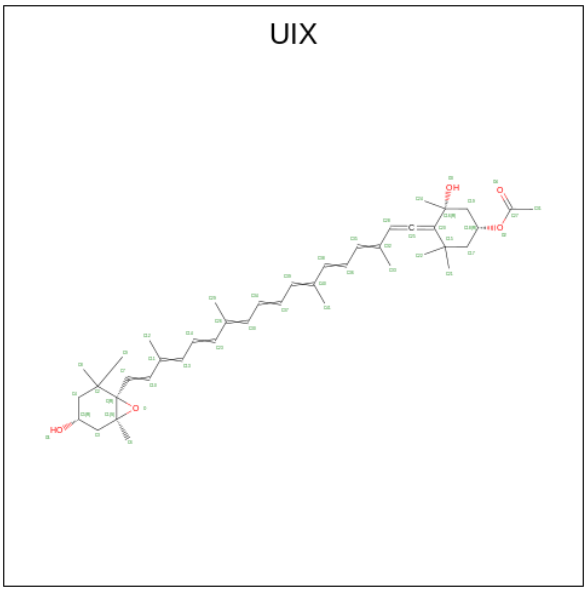
Mol	Chain	Residues	Atoms	AltConf
28	K	1	Total C O 43 40 3	0
28	K	1	Total C O 43 40 3	0
28	K	1	Total C O 43 40 3	0
28	G	1	Total C O 43 40 3	0
28	G	1	Total C O 43 40 3	0
28	G	1	Total C O 43 40 3	0
28	G	1	Total C O 43 40 3	0
28	A	1	Total C O 43 40 3	0
28	A	1	Total C O 43 40 3	0
28	A	1	Total C O 43 40 3	0
28	A	1	Total C O 43 40 3	0
28	h	1	Total C O 43 40 3	0
28	b	1	Total C O 43 40 3	0
28	B	1	Total C O 42 39 3	0
28	B	1	Total C O 43 40 3	0
28	B	1	Total C O 43 40 3	0
28	B	1	Total C O 43 40 3	0
28	D	1	Total C O 43 40 3	0
28	F	1	Total C O 43 40 3	0
28	F	1	Total C O 43 40 3	0
28	H	1	Total C O 43 40 3	0

Continued on next page...

Continued from previous page...

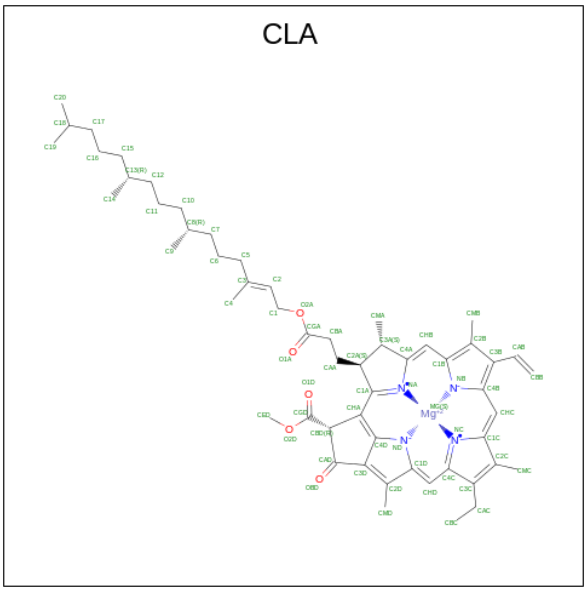
Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			43	40	3	
28	J	1	Total	C	O	0
			43	40	3	
28	J	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	N	1	Total	C	O	0
			43	40	3	
28	O	1	Total	C	O	0
			43	40	3	
28	P	1	Total	C	O	0
			43	40	3	

- Molecule 29 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]cyclohexyl] ethanoate (CCD ID: UIX) (formula: $C_{42}H_{58}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
29	I	1	Total C O 47 42 5	0
29	K	1	Total C O 47 42 5	0
29	G	1	Total C O 47 42 5	0
29	A	1	Total C O 47 42 5	0
29	h	1	Total C O 47 42 5	0
29	B	1	Total C O 47 42 5	0
29	J	1	Total C O 47 42 5	0
29	O	1	Total C O 47 42 5	0
29	P	1	Total C O 47 42 5	0

- Molecule 30 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
30	I	1	Total 49	C 39	Mg 1	N 4	O 5	0
30	I	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	I	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	I	1	Total 48	C 38	Mg 1	N 4	O 5	0
30	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	I	1	Total 52	C 42	Mg 1	N 4	O 5	0
30	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	I	1	Total 52	C 42	Mg 1	N 4	O 5	0
30	K	1	Total 49	C 39	Mg 1	N 4	O 5	0
30	K	1	Total 46	C 36	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	K	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			55	45	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
			46	36	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	f	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	f	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
30	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	l	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	l	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	l	1	Total	C	N	O		0
			45	36	4	5		
30	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	m	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			45	35	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
			55	45	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
			55	45	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			58	48	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
			51	41	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
			55	45	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			62	52	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
			58	48	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	a	1	Total	C	Mg	N	O	0
			61	51	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
			46	36	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			56	46	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	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			46	36	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
			48	38	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
			60	50	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			54	44	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
			46	36	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			50	40	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
			51	41	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			46	36	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
			50	40	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
			47	37	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
			60	50	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			45	35	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
			55	45	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
			51	41	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
			41	33	1	4	3	
30	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	D	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	H	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

Continued on next page...

Continued from previous page...

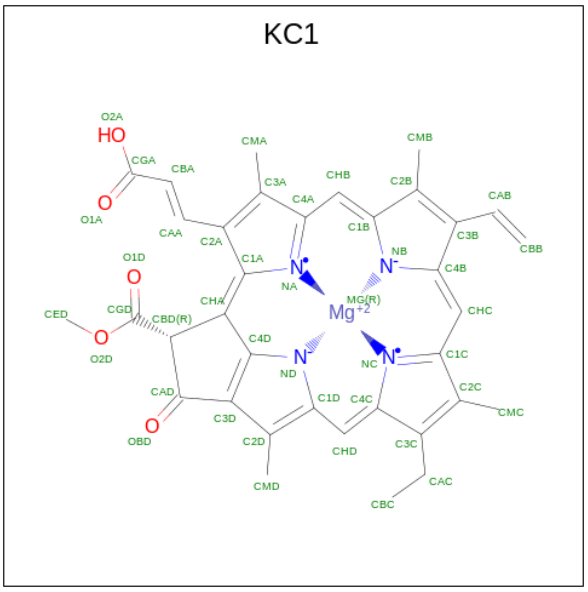
Mol	Chain	Residues	Atoms					AltConf
30	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			47	39	1	4	3	
30	L	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	M	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 31 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



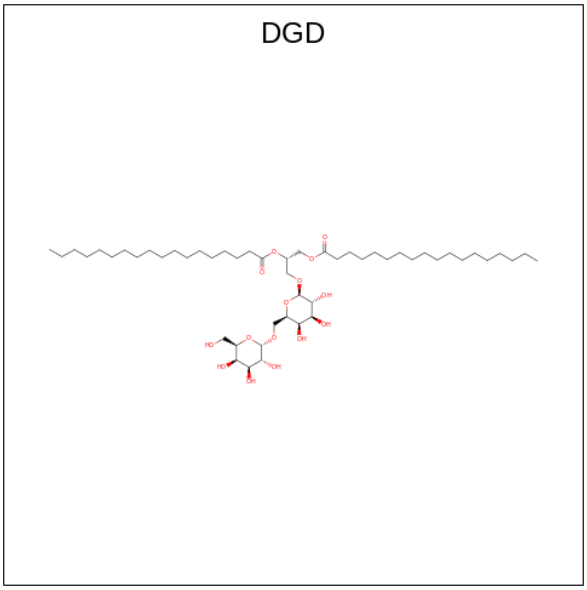
Mol	Chain	Residues	Atoms					AltConf
31	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

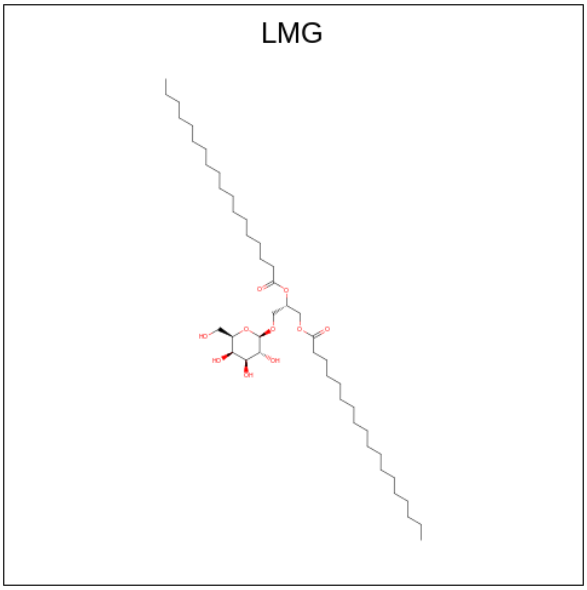
Mol	Chain	Residues	Atoms					AltConf
31	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	O	1	Total	C	Mg	N	O	0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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
32	I	1	Total C O 39 24 15	0
32	y	1	Total C O 54 39 15	0
32	G	1	Total C O 45 30 15	0
32	G	1	Total C O 44 29 15	0
32	j	1	Total C O 41 26 15	0
32	l	1	Total C O 50 35 15	0
32	L	1	Total C O 38 23 15	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



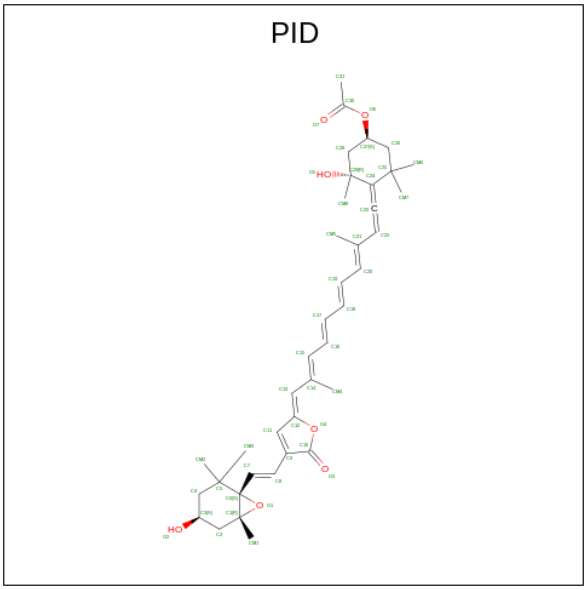
Mol	Chain	Residues	Atoms	AltConf
33	I	1	Total C O 36 26 10	0
33	I	1	Total C O 38 28 10	0
33	K	1	Total C O 43 33 10	0
33	j	1	Total C O 35 25 10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
33	b	1	Total C O 44 34 10	0
33	b	1	Total C O 31 21 10	0
33	B	1	Total C O 37 27 10	0
33	D	1	Total C O 49 39 10	0
33	P	1	Total C O 27 17 10	0

- Molecule 34 is PERIDININ (CCD ID: PID) (formula: $C_{39}H_{50}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
34	G	1	Total C O 46 39 7	0
34	G	1	Total C O 46 39 7	0
34	j	1	Total C O 46 39 7	0
34	D	1	Total C O 46 39 7	0
34	D	1	Total C O 46 39 7	0
34	D	1	Total C O 46 39 7	0

Continued on next page...

Continued from previous page...

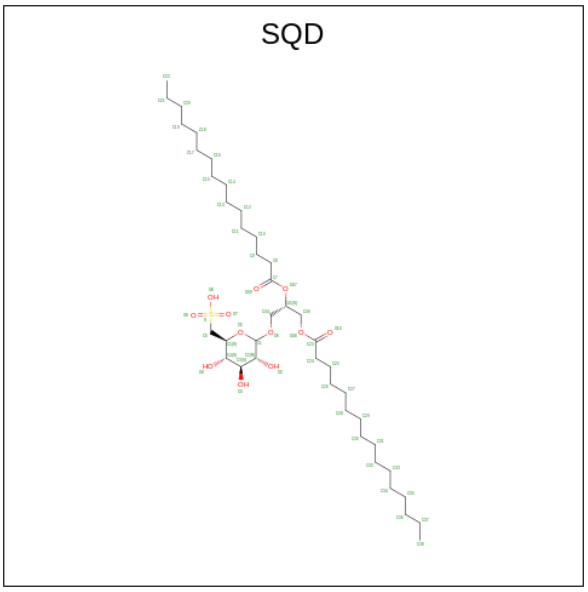
Mol	Chain	Residues	Atoms	AltConf
34	D	1	Total C O 46 39 7	0
34	D	1	Total C O 46 39 7	0
34	D	1	Total C O 46 39 7	0
34	F	1	Total C O 46 39 7	0
34	F	1	Total C O 46 39 7	0
34	F	1	Total C O 46 39 7	0
34	F	1	Total C O 46 39 7	0
34	H	1	Total C O 46 39 7	0
34	H	1	Total C O 46 39 7	0
34	M	1	Total C O 46 39 7	0
34	N	1	Total C O 46 39 7	0
34	N	1	Total C O 46 39 7	0
34	O	1	Total C O 46 39 7	0
34	O	1	Total C O 46 39 7	0
34	O	1	Total C O 46 39 7	0
34	O	1	Total C O 46 39 7	0
34	O	1	Total C O 46 39 7	0
34	P	1	Total C O 46 39 7	0
34	P	1	Total C O 46 39 7	0
34	P	1	Total C O 46 39 7	0
34	P	1	Total C O 46 39 7	0

Continued on next page...

Continued from previous page...

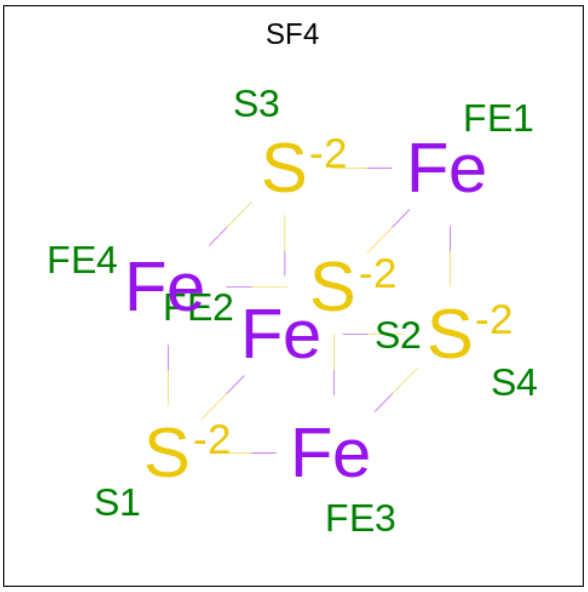
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	P	1	46	39	7	0

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



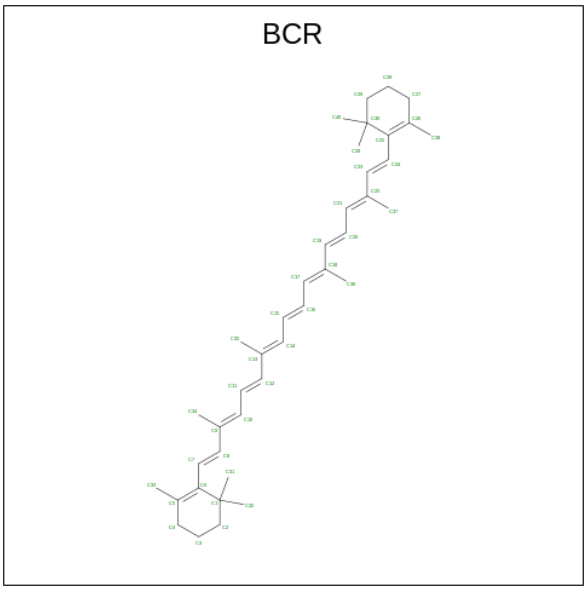
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
35	A	1	50	37	12	1	0

- Molecule 36 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 37 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



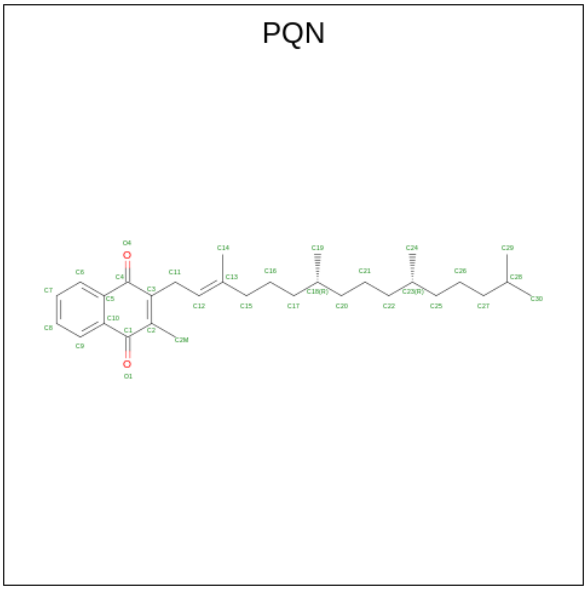
Mol	Chain	Residues	Atoms	AltConf
37	f	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

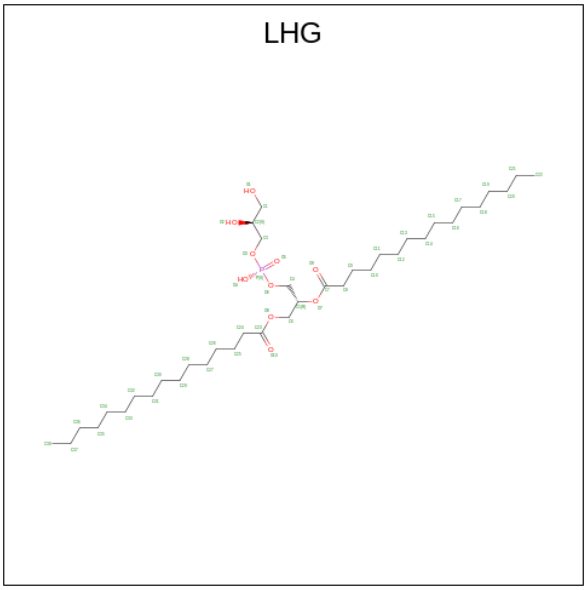
Mol	Chain	Residues	Atoms	AltConf
37	i	1	Total C 40 40	0
37	j	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	m	1	Total C 40 40	0
37	a	1	Total C 40 40	0
37	a	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	b	1	Total C 40 40	0

- Molecule 38 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 39 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

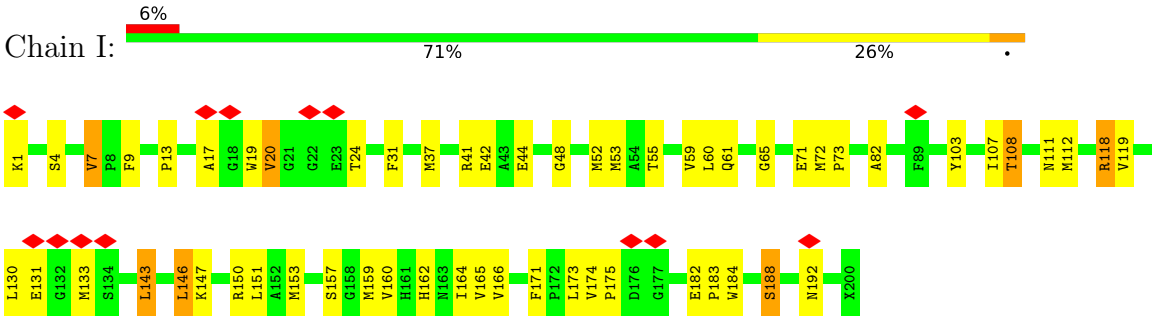


Mol	Chain	Residues	Atoms				AltConf
39	a	1	Total 48	C 37	O 10	P 1	0

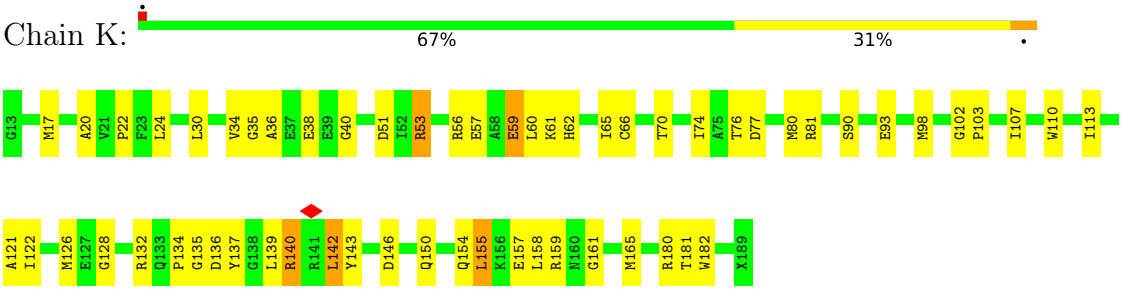
3 Residue-property plots (i)

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

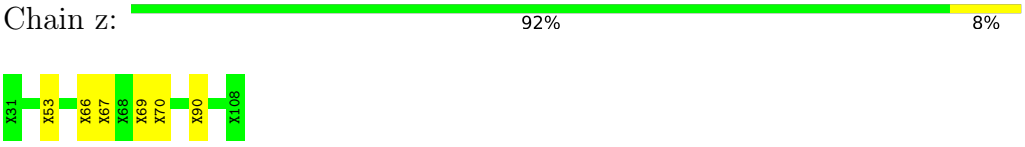
• Molecule 1: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7



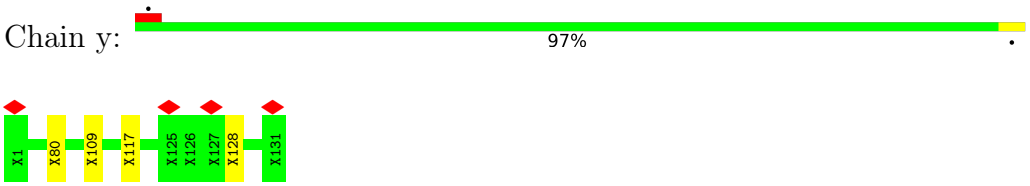
• Molecule 2: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6



• Molecule 3: Photosystem I unk

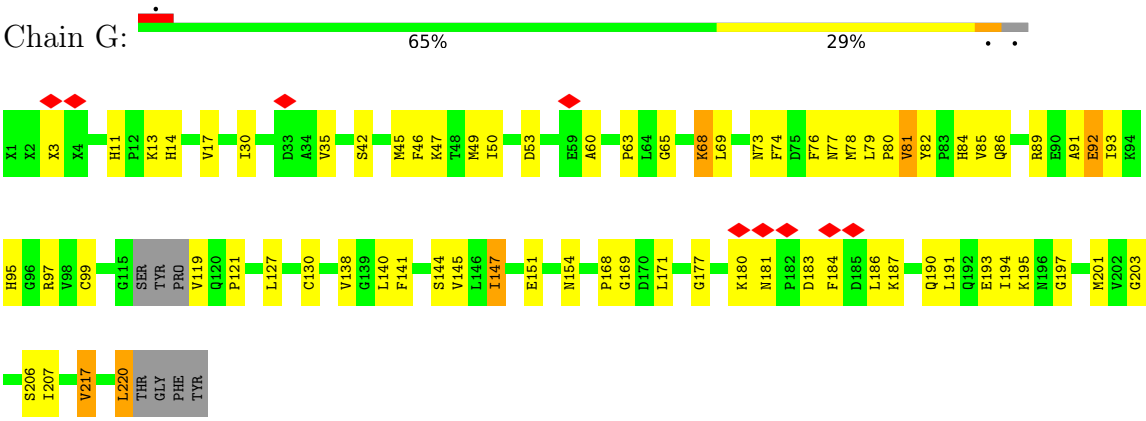


• Molecule 4: Photosystem I unk



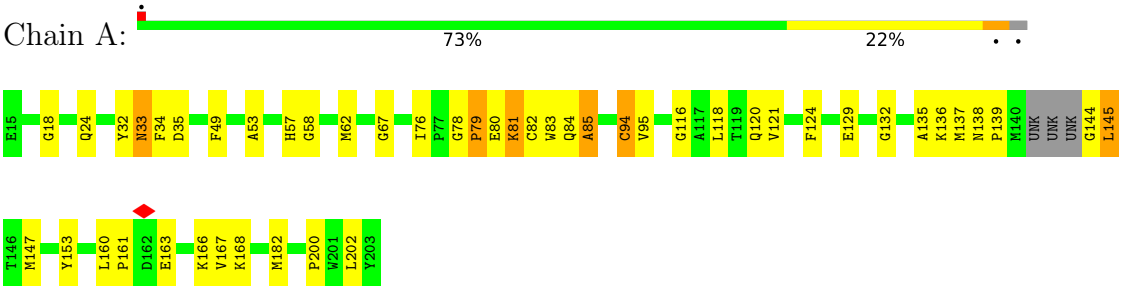
• Molecule 5: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8

Chain G:



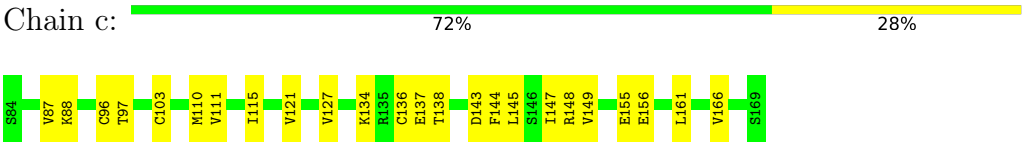
• Molecule 6: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10

Chain A:



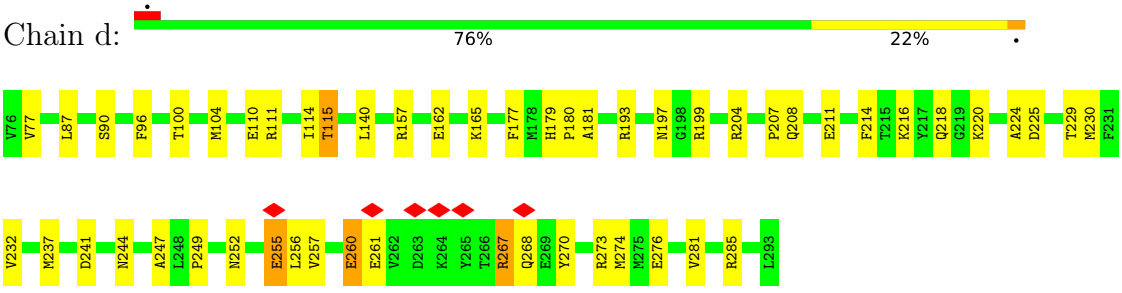
• Molecule 7: Photosystem I PsaC

Chain c:



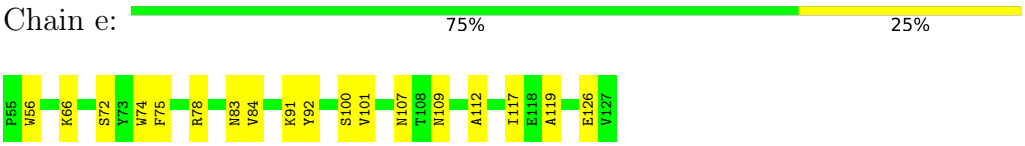
• Molecule 8: Photosystem I PsaD

Chain d:



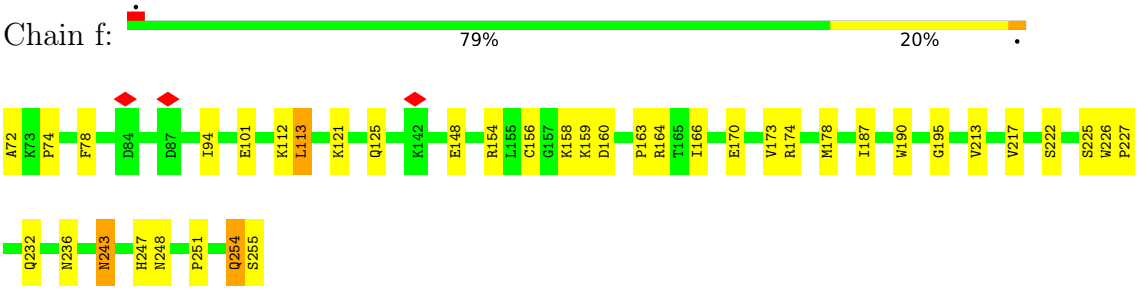
• Molecule 9: Photosystem I PsaE

Chain e:



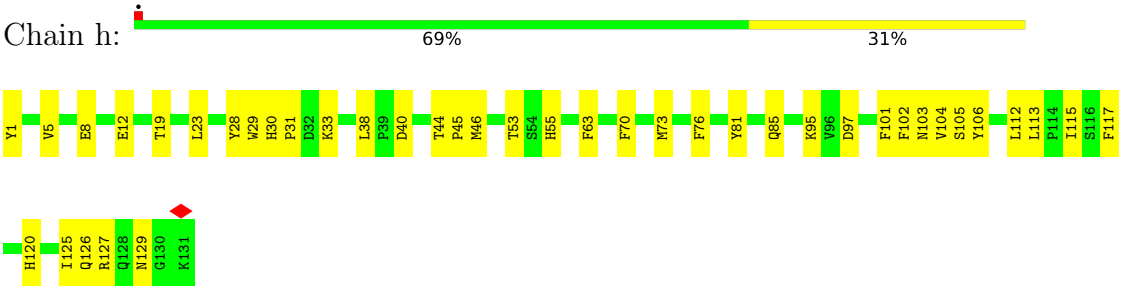
• Molecule 10: Photosystem I PsaF

Chain f:



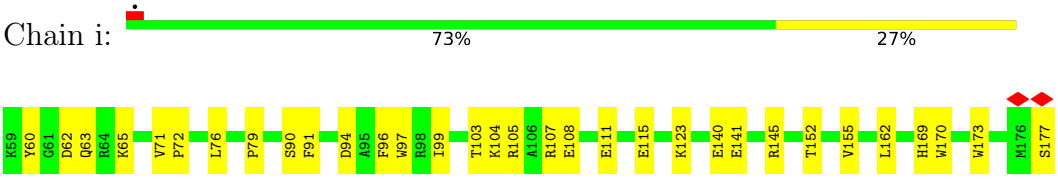
• Molecule 11: Photosystem I PsaR

Chain h:



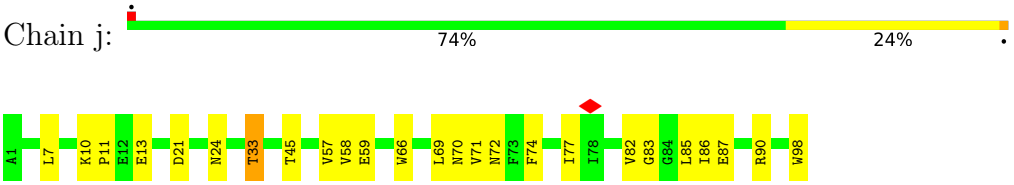
• Molecule 12: Photosystem I PsaI

Chain i:



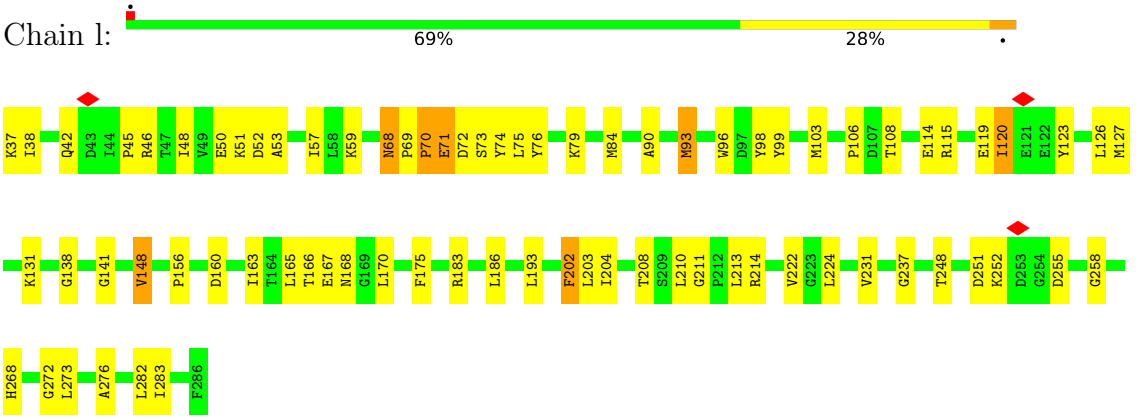
• Molecule 13: Photosystem I PsaJ

Chain j:



• Molecule 14: Photosystem I PsaL

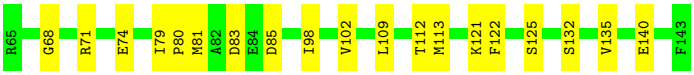
Chain l:



• Molecule 15: Photosystem I PsaM

Chain m:

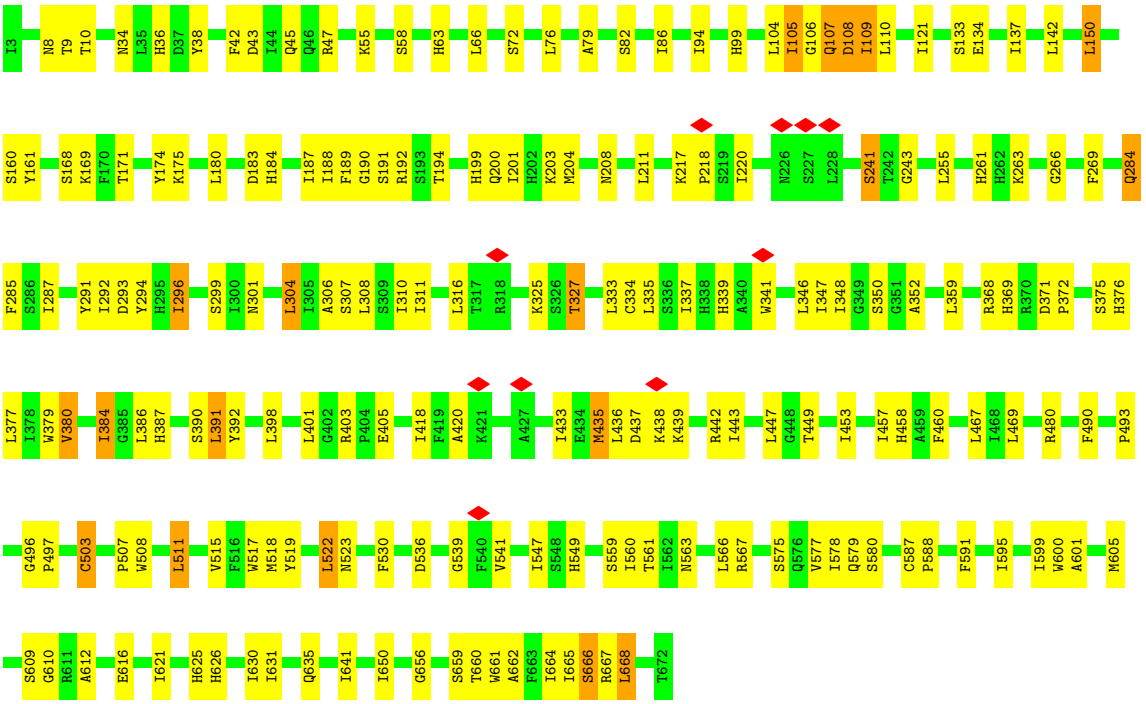




• Molecule 16: Photosystem I PsaA

Chain a:

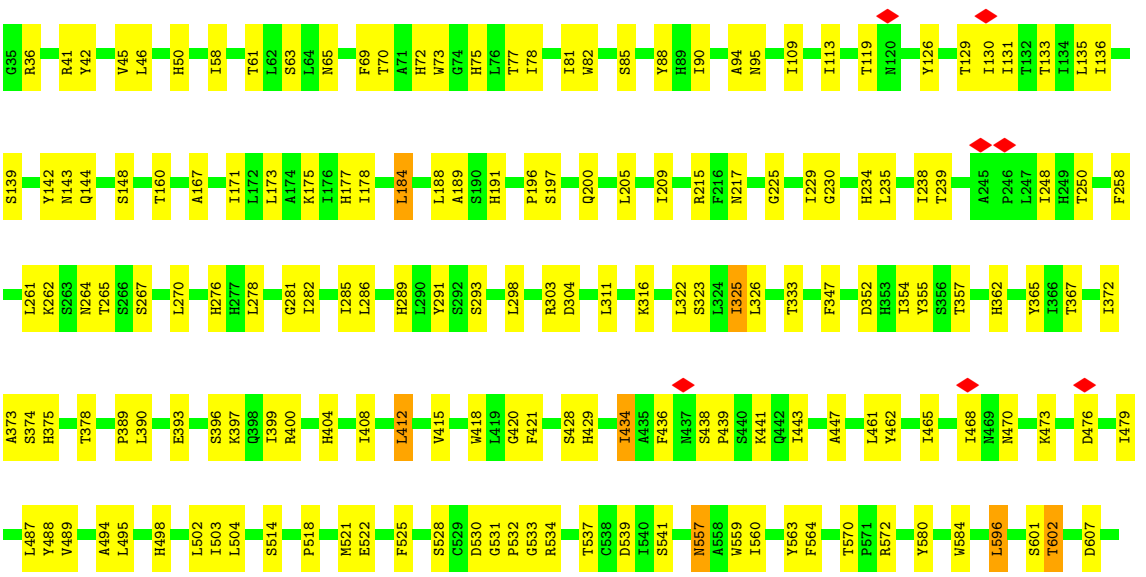




• Molecule 17: Photosystem I PsaB

Chain b:



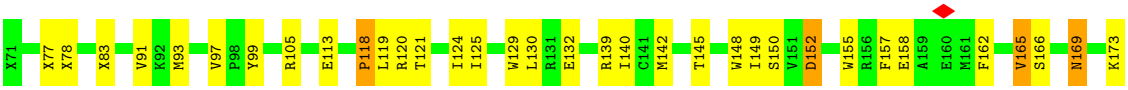




• Molecule 18: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11

Chain B:



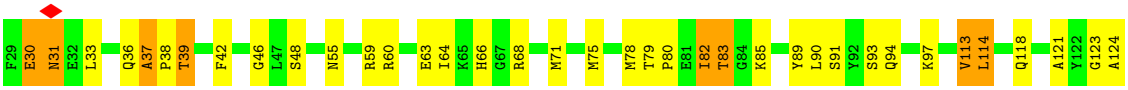


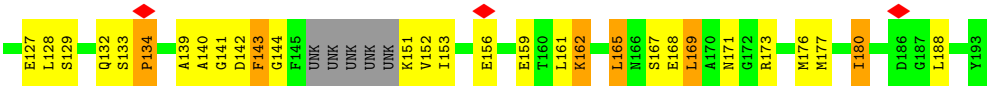


• Molecule 19: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9

Chain D:



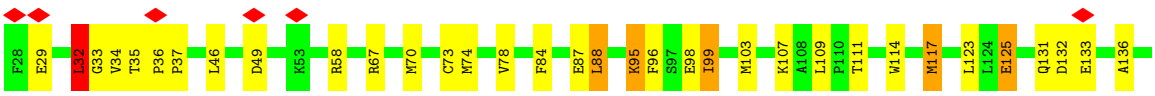


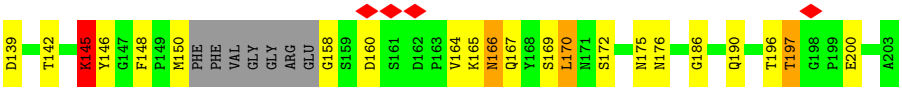


• Molecule 20: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2

Chain F:



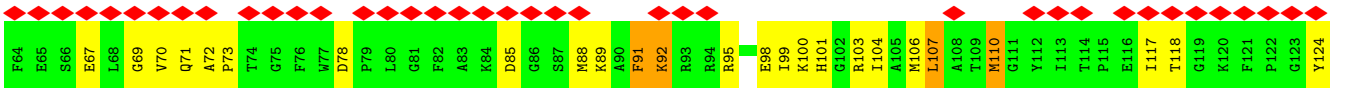


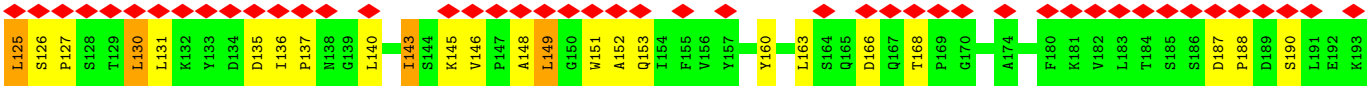


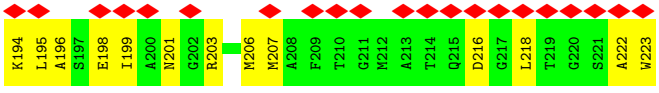
• Molecule 21: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12

Chain H:



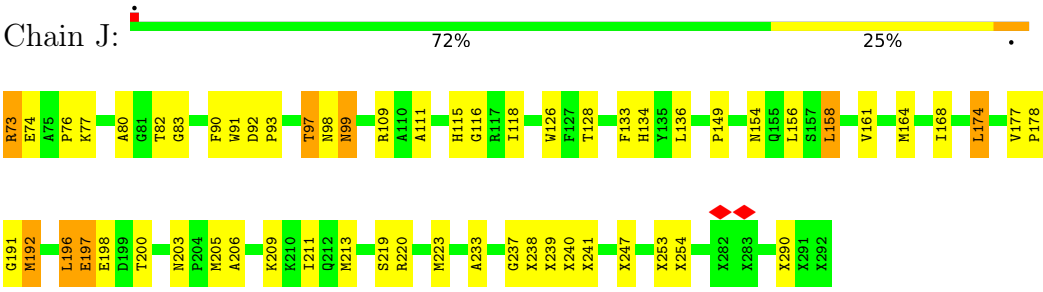






• Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3

Chain J:



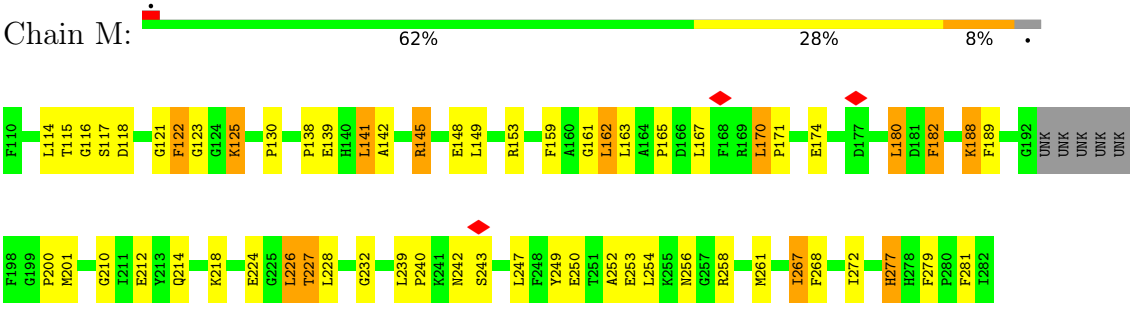
• Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5

Chain L:



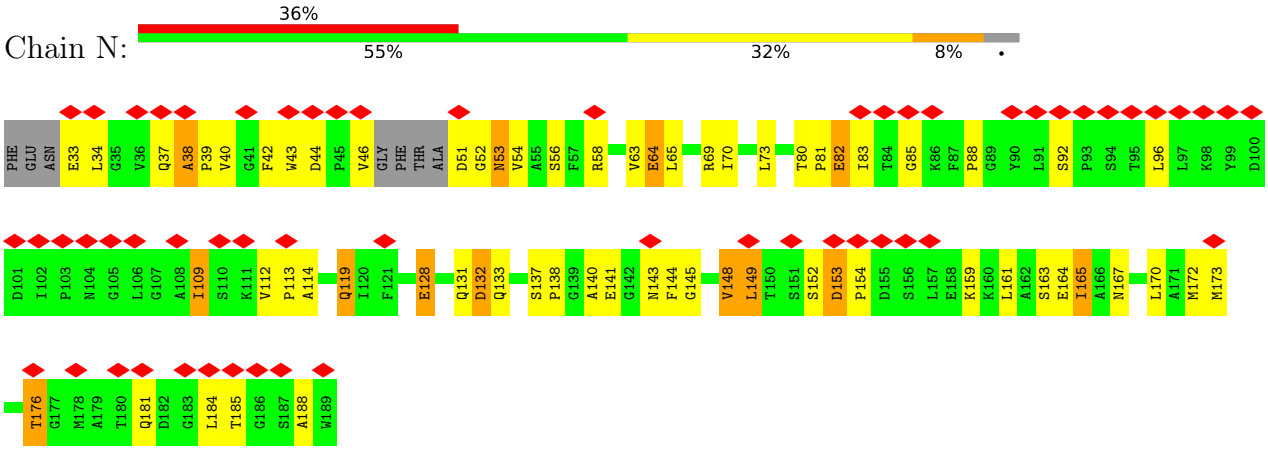
• Molecule 24: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4

Chain M:



• Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13

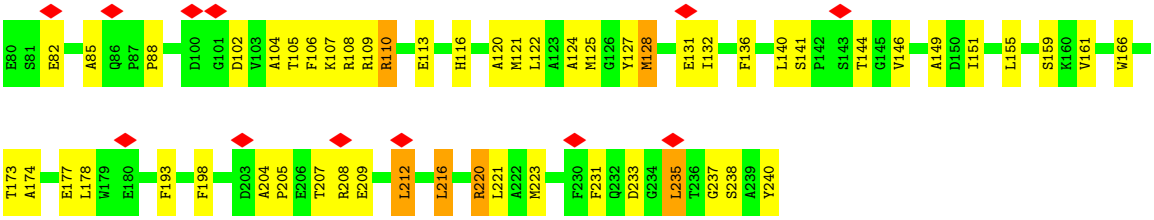
Chain N:



• Molecule 26: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15

Chain O:

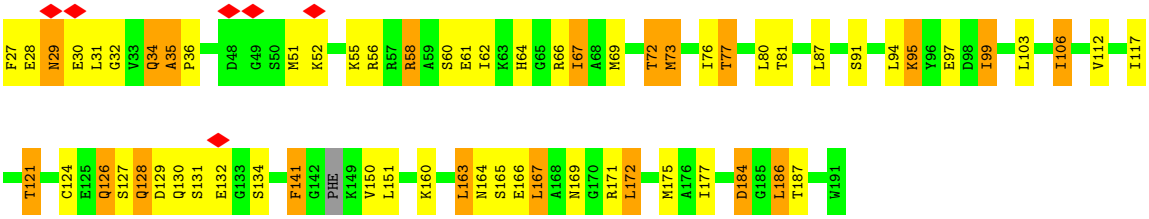




• Molecule 27: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14

Chain P:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46321	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.690	Depositor
Minimum map value	-0.344	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.235	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PID, SQD, LHG, DD6, PQN, UIX, DGD, LMG, CLA, KC1, SF4, BCR

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	I	0.13	0/1484	0.33	0/2019
2	K	0.14	0/1357	0.33	1/1838 (0.1%)
5	G	0.35	0/1562	0.52	1/2122 (0.0%)
6	A	0.37	0/1276	0.53	0/1725
7	c	0.12	0/663	0.31	0/902
8	d	0.11	0/1767	0.30	0/2375
9	e	0.24	0/608	0.29	0/833
10	f	0.16	0/1489	0.33	0/2016
11	h	0.12	0/1101	0.27	0/1493
12	i	0.17	0/992	0.32	0/1346
13	j	0.14	0/801	0.31	0/1092
14	l	0.20	0/1998	0.35	0/2706
15	m	0.13	0/590	0.29	0/793
16	a	0.26	0/5344	0.41	2/7280 (0.0%)
17	b	0.19	0/5362	0.33	0/7335
18	B	0.17	0/1382	0.36	1/1862 (0.1%)
19	D	0.25	0/1178	0.47	0/1592
20	F	0.24	0/1263	0.54	4/1708 (0.2%)
21	H	0.19	0/1232	0.42	1/1665 (0.1%)
22	J	0.17	0/1246	0.39	0/1699
23	L	0.24	0/1462	0.43	0/1985
24	M	0.20	0/1241	0.35	0/1681
25	N	0.23	0/1005	0.51	0/1370
26	O	0.12	0/1091	0.40	0/1491
27	P	0.28	0/1128	0.45	0/1523
All	All	0.22	0/38622	0.39	10/52451 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	145	LYS	N-CA-C	8.92	123.26	112.38
16	a	391	LEU	N-CA-C	-6.93	103.78	111.82
21	H	110	MET	N-CA-C	-6.54	104.15	111.28
20	F	148	PHE	CA-C-N	-6.02	113.74	119.76
20	F	148	PHE	C-N-CA	-6.02	113.74	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1480	0	1381	53	0
2	K	1349	0	1323	54	0
3	z	390	0	87	4	0
4	y	655	0	136	3	0
5	G	1572	0	1440	51	0
6	A	1346	0	1242	40	0
7	c	653	0	629	22	0
8	d	1731	0	1741	42	0
9	e	587	0	575	17	0
10	f	1450	0	1437	30	0
11	h	1066	0	1018	33	0
12	i	964	0	941	25	0
13	j	783	0	774	22	0
14	l	1943	0	1919	65	0
15	m	582	0	603	15	0
16	a	5194	0	5023	159	0
17	b	5199	0	5053	172	0
18	B	1452	0	1368	40	0
19	D	1158	0	1114	53	0
20	F	1237	0	1188	37	0
21	H	1202	0	1182	47	0
22	J	1496	0	1233	47	0
23	L	1427	0	1392	51	0
24	M	1211	0	1090	43	0
25	N	993	0	844	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	O	1073	0	956	37	0
27	P	1113	0	1050	49	0
28	A	172	0	0	2	0
28	B	171	0	0	1	0
28	D	43	0	0	0	0
28	F	86	0	0	1	0
28	G	172	0	0	5	0
28	H	43	0	0	1	0
28	I	172	0	0	2	0
28	J	129	0	0	5	0
28	K	215	0	0	0	0
28	L	215	0	0	2	0
28	M	215	0	0	2	0
28	N	43	0	0	0	0
28	O	43	0	0	0	0
28	P	43	0	0	0	0
28	b	43	0	0	0	0
28	h	43	0	0	0	0
29	A	47	0	0	1	0
29	B	47	0	0	0	0
29	G	47	0	0	0	0
29	I	47	0	0	2	0
29	J	47	0	0	1	0
29	K	47	0	0	1	0
29	O	47	0	0	0	0
29	P	47	0	0	0	0
29	h	47	0	0	0	0
30	A	597	0	493	23	0
30	B	587	0	532	20	0
30	D	317	0	229	18	0
30	F	317	0	227	22	0
30	G	592	0	530	22	0
30	H	343	0	278	15	0
30	I	637	0	554	31	0
30	J	552	0	456	29	0
30	K	496	0	398	18	0
30	L	503	0	411	21	0
30	M	481	0	370	19	0
30	N	256	0	216	10	0
30	O	297	0	245	14	0
30	P	297	0	245	18	0
30	a	1870	0	1786	110	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	b	1563	0	1526	106	0
30	f	147	0	115	10	0
30	h	55	0	49	0	0
30	j	113	0	104	8	0
30	l	493	0	471	25	0
30	m	60	0	59	2	0
31	A	90	0	0	0	0
31	B	45	0	0	0	0
31	D	90	0	0	1	0
31	F	90	0	0	2	0
31	G	45	0	0	0	0
31	H	90	0	0	1	0
31	I	45	0	0	0	0
31	J	45	0	0	0	0
31	K	45	0	0	0	0
31	L	90	0	0	0	0
31	M	90	0	0	1	0
31	N	135	0	0	1	0
31	O	135	0	0	4	0
31	P	135	0	0	1	0
32	G	89	0	94	2	0
32	I	39	0	36	0	0
32	L	38	0	34	2	0
32	j	41	0	40	3	0
32	l	50	0	58	0	0
32	y	54	0	66	1	0
33	B	37	0	44	1	0
33	D	49	0	64	5	0
33	I	74	0	88	2	0
33	K	43	0	56	0	0
33	P	27	0	24	0	0
33	b	75	0	90	5	0
33	j	35	0	40	4	0
34	D	276	0	300	12	0
34	F	184	0	200	13	0
34	G	92	0	100	6	0
34	H	92	0	100	8	0
34	M	46	0	50	1	0
34	N	92	0	100	4	0
34	O	230	0	250	23	0
34	P	230	0	250	17	0
34	j	46	0	50	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	50	0	64	8	0
36	a	8	0	0	1	0
36	c	16	0	0	2	0
37	a	80	0	112	5	0
37	b	120	0	168	15	0
37	f	40	0	56	4	0
37	i	40	0	56	7	0
37	j	40	0	56	5	0
37	l	120	0	168	10	0
37	m	40	0	56	4	0
38	a	33	0	46	5	0
38	b	33	0	46	4	0
39	a	48	0	69	3	0
All	All	55927	0	49064	1485	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 14.

The worst 5 of 1485 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)
10:f:72:ALA:N	17:b:462:TYR:HH	1.46	1.12
30:K:308:CLA:H2A	30:K:308:CLA:HED3	1.53	0.88
17:b:468:ILE:HG22	17:b:470:ASN:H	1.36	0.87
30:b:712:CLA:H12	18:B:124:ILE:HD11	1.56	0.87
26:O:221:LEU:HG	34:O:305:PID:H13	1.56	0.87

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	I	191/200 (96%)	163 (85%)	28 (15%)	0	100	100
2	K	171/177 (97%)	160 (94%)	11 (6%)	0	100	100
5	G	204/224 (91%)	175 (86%)	27 (13%)	2 (1%)	12	45
6	A	162/189 (86%)	144 (89%)	14 (9%)	4 (2%)	4	23
7	c	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
8	d	216/218 (99%)	197 (91%)	19 (9%)	0	100	100
9	e	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	f	182/184 (99%)	177 (97%)	4 (2%)	1 (0%)	24	60
11	h	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
12	i	117/119 (98%)	105 (90%)	12 (10%)	0	100	100
13	j	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
14	l	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	30	65
15	m	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
16	a	668/670 (100%)	622 (93%)	43 (6%)	3 (0%)	30	65
17	b	661/663 (100%)	613 (93%)	47 (7%)	1 (0%)	43	76
18	B	171/192 (89%)	153 (90%)	15 (9%)	3 (2%)	6	31
19	D	156/165 (94%)	131 (84%)	22 (14%)	3 (2%)	6	30
20	F	165/176 (94%)	153 (93%)	10 (6%)	2 (1%)	10	40
21	H	158/160 (99%)	140 (89%)	16 (10%)	2 (1%)	9	38
22	J	164/220 (74%)	146 (89%)	17 (10%)	1 (1%)	21	56
23	L	183/185 (99%)	161 (88%)	22 (12%)	0	100	100
24	M	164/173 (95%)	151 (92%)	13 (8%)	0	100	100
25	N	149/160 (93%)	119 (80%)	24 (16%)	6 (4%)	2	14
26	O	159/161 (99%)	130 (82%)	25 (16%)	4 (2%)	4	23
27	P	155/160 (97%)	135 (87%)	19 (12%)	1 (1%)	21	56
All	All	4901/5113 (96%)	4446 (91%)	421 (9%)	34 (1%)	20	53

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	121	PRO
6	A	85	ALA
14	l	70	PRO
16	a	47	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	a	218	PRO

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	I	139/155 (90%)	131 (94%)	8 (6%)	18 51
2	K	133/138 (96%)	126 (95%)	7 (5%)	20 54
5	G	147/171 (86%)	136 (92%)	11 (8%)	12 41
6	A	122/129 (95%)	117 (96%)	5 (4%)	27 61
7	c	76/76 (100%)	75 (99%)	1 (1%)	61 81
8	d	182/184 (99%)	176 (97%)	6 (3%)	33 67
9	e	63/63 (100%)	63 (100%)	0	100 100
10	f	148/148 (100%)	145 (98%)	3 (2%)	48 76
11	h	112/114 (98%)	111 (99%)	1 (1%)	70 85
12	i	100/101 (99%)	99 (99%)	1 (1%)	68 84
13	j	88/89 (99%)	84 (96%)	4 (4%)	24 59
14	l	199/201 (99%)	189 (95%)	10 (5%)	22 56
15	m	60/63 (95%)	59 (98%)	1 (2%)	53 78
16	a	540/592 (91%)	517 (96%)	23 (4%)	26 60
17	b	557/581 (96%)	540 (97%)	17 (3%)	35 68
18	B	142/146 (97%)	123 (87%)	19 (13%)	4 18
19	D	116/123 (94%)	91 (78%)	25 (22%)	1 6
20	F	126/140 (90%)	106 (84%)	20 (16%)	2 13
21	H	123/123 (100%)	111 (90%)	12 (10%)	7 30
22	J	124/136 (91%)	107 (86%)	17 (14%)	3 17
23	L	140/145 (97%)	115 (82%)	25 (18%)	2 10
24	M	106/128 (83%)	86 (81%)	20 (19%)	1 9
25	N	80/124 (64%)	52 (65%)	28 (35%)	0 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	O	89/124 (72%)	70 (79%)	19 (21%)	1 6
27	P	105/123 (85%)	72 (69%)	33 (31%)	0 1
All	All	3817/4117 (93%)	3501 (92%)	316 (8%)	12 37

5 of 316 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	M	227	THR
27	P	31	LEU
25	N	37	GLN
25	N	173	MET
27	P	121	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
20	F	166	ASN
20	F	191	ASN
23	L	268	GLN
14	l	280	HIS
13	j	72	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)

342 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	CLA	K	307	-	50,54,73	1.44	6 (12%)	60,90,113	1.44	6 (10%)
30	CLA	O	314	-	51,55,73	1.45	7 (13%)	61,91,113	1.49	6 (9%)
34	PID	F	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.77	7 (14%)
34	PID	O	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.31	6 (12%)
30	CLA	F	307	-	50,54,73	1.46	8 (16%)	60,90,113	1.46	5 (8%)
30	CLA	M	311	-	50,54,73	1.47	9 (18%)	60,90,113	1.40	5 (8%)
28	DD6	B	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.89	11 (21%)
30	CLA	b	720	17	57,61,73	1.37	6 (10%)	68,98,113	1.34	6 (8%)
28	DD6	A	303	-	39,45,45	1.94	2 (5%)	52,67,67	1.87	13 (25%)
39	LHG	a	733	-	47,47,48	0.27	0	50,53,54	0.33	0
30	CLA	a	702	-	69,73,73	1.30	11 (15%)	83,113,113	1.34	6 (7%)
28	DD6	L	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.95	12 (23%)
30	CLA	a	701	-	49,53,73	1.49	8 (16%)	59,89,113	1.45	5 (8%)
30	CLA	I	306	1	53,57,73	1.42	6 (11%)	62,93,113	1.45	6 (9%)
30	CLA	G	510	-	69,73,73	1.25	6 (8%)	83,113,113	1.30	7 (8%)
30	CLA	G	509	5	55,59,73	1.41	6 (10%)	66,96,113	1.39	6 (9%)
30	CLA	M	313	-	50,54,73	1.48	6 (12%)	60,90,113	1.39	5 (8%)
30	CLA	l	312	-	50,54,73	1.46	7 (14%)	60,90,113	1.36	5 (8%)
30	CLA	a	723	16	69,73,73	1.26	7 (10%)	83,113,113	1.23	6 (7%)
30	CLA	K	308	2	58,62,73	1.37	6 (10%)	69,99,113	1.35	6 (8%)
30	CLA	A	313	-	59,63,73	1.36	6 (10%)	71,101,113	1.34	7 (9%)
30	CLA	a	713	16	64,68,73	1.30	8 (12%)	77,107,113	1.30	8 (10%)
32	DGD	G	501	-	46,46,67	1.02	2 (4%)	60,60,81	1.01	3 (5%)
30	CLA	H	312	-	50,54,73	1.48	7 (14%)	60,90,113	1.41	5 (8%)
30	CLA	a	731	16	69,73,73	1.27	7 (10%)	83,113,113	1.28	7 (8%)
33	LMG	K	317	-	43,43,55	0.81	1 (2%)	51,51,63	1.31	6 (11%)
34	PID	O	307	-	41,49,49	1.34	4 (9%)	49,76,76	1.32	5 (10%)
30	CLA	b	705	-	69,73,73	1.26	6 (8%)	83,113,113	1.27	6 (7%)
30	CLA	P	217	27	45,49,73	1.53	9 (20%)	54,84,113	1.51	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	KC1	L	315	23	49,53,53	1.39	6 (12%)	63,89,89	2.01	14 (22%)
33	LMG	b	733	-	44,44,55	0.81	1 (2%)	52,52,63	1.30	6 (11%)
30	CLA	I	311	1	59,63,73	1.37	7 (11%)	71,101,113	1.35	8 (11%)
30	CLA	b	721	17,28	50,54,73	1.47	9 (18%)	60,90,113	1.35	4 (6%)
30	CLA	J	316	-	50,54,73	1.48	6 (12%)	60,90,113	1.38	5 (8%)
30	CLA	a	738	22	50,54,73	1.47	6 (12%)	60,90,113	1.45	5 (8%)
34	PID	O	305	-	41,49,49	1.35	4 (9%)	49,76,76	1.58	8 (16%)
30	CLA	b	710	-	56,60,73	1.41	9 (16%)	67,97,113	1.39	7 (10%)
30	CLA	H	309	-	51,55,73	1.45	8 (15%)	61,91,113	1.42	6 (9%)
38	PQN	a	732	-	34,34,34	1.58	2 (5%)	42,45,45	1.10	4 (9%)
30	CLA	b	708	17	69,73,73	1.26	6 (8%)	83,113,113	1.26	7 (8%)
30	CLA	L	314	-	57,61,73	1.38	7 (12%)	68,98,113	1.37	7 (10%)
30	CLA	J	309	-	60,64,73	1.34	7 (11%)	72,102,113	1.42	7 (9%)
28	DD6	F	301	-	39,45,45	1.99	2 (5%)	52,67,67	2.34	18 (34%)
29	UIX	A	304	-	41,49,49	1.23	3 (7%)	52,74,74	2.44	20 (38%)
30	CLA	I	313	-	59,63,73	1.35	6 (10%)	71,101,113	1.36	7 (9%)
30	CLA	a	719	-	51,55,73	1.46	9 (17%)	61,91,113	1.37	5 (8%)
31	KC1	I	314	1	49,53,53	1.37	6 (12%)	63,89,89	2.03	16 (25%)
34	PID	D	306	-	41,49,49	1.34	4 (9%)	49,76,76	1.44	5 (10%)
28	DD6	h	203	-	39,45,45	2.02	3 (7%)	52,67,67	1.87	13 (25%)
28	DD6	b	731	30	39,45,45	2.11	3 (7%)	52,67,67	1.96	15 (28%)
28	DD6	O	303	-	39,45,45	2.01	3 (7%)	52,67,67	2.01	14 (26%)
30	CLA	I	315	-	56,60,73	1.40	6 (10%)	67,97,113	1.38	7 (10%)
30	CLA	b	717	17	69,73,73	1.26	9 (13%)	83,113,113	1.24	6 (7%)
31	KC1	P	216	27	49,53,53	1.37	6 (12%)	63,89,89	1.98	13 (20%)
28	DD6	K	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.90	13 (25%)
30	CLA	b	714	-	50,54,73	1.46	6 (12%)	60,90,113	1.43	6 (10%)
28	DD6	I	303	-	39,45,45	2.22	5 (12%)	52,67,67	2.03	17 (32%)
31	KC1	B	314	18	49,53,53	1.37	6 (12%)	63,89,89	1.98	14 (22%)
29	UIX	P	207	-	41,49,49	1.28	4 (9%)	52,74,74	2.78	20 (38%)
30	CLA	J	308	22	50,54,73	1.47	9 (18%)	60,90,113	1.43	7 (11%)
30	CLA	G	520	17	53,57,73	1.42	8 (15%)	62,93,113	1.37	7 (11%)
30	CLA	l	313	14	69,73,73	1.27	7 (10%)	83,113,113	1.30	6 (7%)
37	BCR	b	730	-	41,41,41	0.75	0	56,56,56	2.25	20 (35%)
31	KC1	F	309	20	49,53,53	1.39	6 (12%)	63,89,89	2.08	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	a	711	16	49,53,73	1.48	7 (14%)	59,89,113	1.48	8 (13%)
28	DD6	I	301	-	39,45,45	2.06	3 (7%)	52,67,67	2.20	20 (38%)
30	CLA	j	106	17	62,66,73	1.33	8 (12%)	74,104,113	1.34	7 (9%)
30	CLA	J	306	-	50,54,73	1.46	8 (16%)	60,90,113	1.44	4 (6%)
31	KC1	P	211	27	49,53,53	1.37	6 (12%)	63,89,89	2.00	14 (22%)
30	CLA	l	309	-	45,49,73	1.53	6 (13%)	54,84,113	1.50	6 (11%)
30	CLA	B	315	-	45,49,73	1.52	7 (15%)	54,84,113	1.54	5 (9%)
30	CLA	I	321	30	56,60,73	1.40	6 (10%)	67,97,113	1.47	7 (10%)
34	PID	D	305	-	41,49,49	1.35	4 (9%)	49,76,76	1.46	7 (14%)
30	CLA	F	310	-	50,54,73	1.46	7 (14%)	60,90,113	1.48	6 (10%)
30	CLA	b	716	-	54,58,73	1.42	6 (11%)	65,95,113	1.42	6 (9%)
30	CLA	a	720	-	66,70,73	1.29	6 (9%)	79,109,113	1.31	6 (7%)
30	CLA	N	305	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	5 (6%)
32	DGD	G	521	-	45,45,67	1.03	2 (4%)	59,59,81	1.46	8 (13%)
29	UIX	O	306	-	41,49,49	1.28	3 (7%)	52,74,74	2.86	23 (44%)
30	CLA	P	210	-	69,73,73	1.25	7 (10%)	83,113,113	1.32	7 (8%)
32	DGD	I	317	-	40,40,67	1.10	2 (5%)	54,54,81	1.02	4 (7%)
30	CLA	a	717	16	61,65,73	1.35	8 (13%)	73,103,113	1.32	7 (9%)
30	CLA	L	308	31	50,55,73	1.46	6 (12%)	62,91,113	1.41	8 (12%)
37	BCR	b	702	-	41,41,41	0.73	0	56,56,56	2.17	17 (30%)
30	CLA	B	316	18	50,54,73	1.47	7 (14%)	60,90,113	1.37	5 (8%)
30	CLA	K	311	-	56,60,73	1.40	8 (14%)	67,97,113	1.36	5 (7%)
29	UIX	G	503	-	41,49,49	1.23	3 (7%)	52,74,74	2.34	16 (30%)
28	DD6	M	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.89	14 (26%)
30	CLA	b	703	17	69,73,73	1.25	7 (10%)	83,113,113	1.22	6 (7%)
28	DD6	K	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.98	15 (28%)
34	PID	P	202	-	41,49,49	1.33	4 (9%)	49,76,76	1.60	7 (14%)
34	PID	N	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.68	9 (18%)
30	CLA	A	307	31	49,53,73	1.51	6 (12%)	59,89,113	1.46	4 (6%)
30	CLA	H	307	-	55,59,73	1.41	6 (10%)	66,96,113	1.41	6 (9%)
30	CLA	F	315	-	45,49,73	1.53	6 (13%)	54,84,113	1.55	6 (11%)
30	CLA	A	308	-	59,63,73	1.36	6 (10%)	71,101,113	1.34	7 (9%)
30	CLA	a	705	16,30	59,63,73	1.37	6 (10%)	71,101,113	1.39	7 (9%)
30	CLA	M	308	31	57,61,73	1.38	6 (10%)	68,98,113	1.40	6 (8%)
30	CLA	l	303	14	69,73,73	1.27	7 (10%)	83,113,113	1.27	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	KC1	K	314	2	49,53,53	1.37	6 (12%)	63,89,89	1.99	13 (20%)
31	KC1	G	515	5	49,53,53	1.38	6 (12%)	63,89,89	1.96	15 (23%)
36	SF4	a	737	17,16	0,12,12	-	-	-		
28	DD6	A	302	-	39,45,45	2.01	3 (7%)	52,67,67	2.13	16 (30%)
30	CLA	L	311	-	59,63,73	1.36	7 (11%)	71,101,113	1.36	6 (8%)
30	CLA	b	723	-	54,58,73	1.42	8 (14%)	65,95,113	1.40	8 (12%)
30	CLA	G	511	5	59,63,73	1.37	7 (11%)	71,101,113	1.34	5 (7%)
30	CLA	a	708	16	55,59,73	1.41	6 (10%)	66,96,113	1.40	6 (9%)
32	DGD	l	301	-	51,51,67	0.95	2 (3%)	65,65,81	0.89	2 (3%)
35	SQD	A	318	-	49,50,54	0.40	1 (2%)	58,61,65	0.59	0
28	DD6	K	303	-	39,45,45	1.99	3 (7%)	52,67,67	1.69	10 (19%)
30	CLA	M	317	-	50,54,73	1.46	6 (12%)	60,90,113	1.45	5 (8%)
31	KC1	N	306	25	49,53,53	1.37	6 (12%)	63,89,89	2.00	14 (22%)
28	DD6	D	303	-	39,45,45	1.96	2 (5%)	52,67,67	1.88	13 (25%)
30	CLA	a	704	-	69,73,73	1.27	7 (10%)	83,113,113	1.19	3 (3%)
34	PID	H	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.65	6 (12%)
37	BCR	b	732	-	41,41,41	0.80	0	56,56,56	1.88	20 (35%)
30	CLA	h	202	-	59,63,73	1.37	6 (10%)	71,101,113	1.35	6 (8%)
30	CLA	L	310	23	59,63,73	1.36	7 (11%)	71,101,113	1.34	6 (8%)
33	LMG	P	201	-	27,27,55	1.00	0	35,35,63	1.19	4 (11%)
31	KC1	D	315	19	49,53,53	1.36	6 (12%)	63,89,89	2.00	15 (23%)
34	PID	P	208	-	41,49,49	1.34	4 (9%)	49,76,76	1.46	6 (12%)
30	CLA	b	725	17	69,73,73	1.26	6 (8%)	83,113,113	1.26	6 (7%)
28	DD6	B	302	-	38,44,45	2.18	3 (7%)	50,65,67	2.12	20 (40%)
30	CLA	l	310	-	39,50,73	2.74	11 (28%)	33,76,113	1.74	8 (24%)
28	DD6	A	301	-	39,45,45	1.99	2 (5%)	52,67,67	2.13	14 (26%)
28	DD6	K	318	-	39,45,45	2.02	3 (7%)	52,67,67	2.07	12 (23%)
31	KC1	M	314	24	49,53,53	1.38	6 (12%)	63,89,89	2.00	14 (22%)
30	CLA	P	214	-	50,54,73	1.43	8 (16%)	60,90,113	1.36	4 (6%)
29	UIX	B	305	-	41,49,49	1.25	3 (7%)	52,74,74	2.45	16 (30%)
30	CLA	A	309	6	59,63,73	1.36	7 (11%)	71,101,113	1.34	7 (9%)
30	CLA	b	727	-	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
28	DD6	P	204	-	39,45,45	2.00	3 (7%)	52,67,67	2.06	14 (26%)
28	DD6	G	508	-	39,45,45	2.04	3 (7%)	52,67,67	2.02	13 (25%)
30	CLA	H	305	-	69,73,73	1.26	6 (8%)	83,113,113	1.31	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	KC1	H	310	-	49,53,53	1.39	6 (12%)	63,89,89	2.00	13 (20%)
30	CLA	b	701	-	69,73,73	1.26	9 (13%)	83,113,113	1.30	6 (7%)
30	CLA	H	308	-	50,54,73	1.47	8 (16%)	60,90,113	1.41	4 (6%)
30	CLA	D	309	-	50,54,73	1.45	7 (14%)	60,90,113	1.44	5 (8%)
30	CLA	O	316	-	45,49,73	1.54	6 (13%)	54,84,113	1.52	5 (9%)
30	CLA	b	728	17	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
37	BCR	f	304	-	41,41,41	0.72	0	56,56,56	2.07	17 (30%)
30	CLA	b	711	17	59,63,73	1.37	6 (10%)	71,101,113	1.32	6 (8%)
30	CLA	J	301	-	64,68,73	1.31	7 (10%)	77,107,113	1.30	6 (7%)
30	CLA	I	310	-	52,56,73	1.43	6 (11%)	62,92,113	1.44	6 (9%)
30	CLA	A	320	-	50,54,73	1.47	8 (16%)	60,90,113	1.42	5 (8%)
31	KC1	L	307	30	49,53,53	1.37	6 (12%)	63,89,89	2.01	17 (26%)
31	KC1	N	308	-	49,53,53	1.46	6 (12%)	63,89,89	2.31	16 (25%)
30	CLA	J	311	22	51,55,73	1.46	6 (11%)	61,91,113	1.43	7 (11%)
30	CLA	A	311	6	50,54,73	1.47	6 (12%)	60,90,113	1.40	5 (8%)
30	CLA	G	516	5	45,49,73	1.54	6 (13%)	54,84,113	1.50	5 (9%)
30	CLA	I	308	-	64,68,73	1.31	8 (12%)	77,107,113	1.30	8 (10%)
30	CLA	L	318	-	50,54,73	1.47	9 (18%)	60,90,113	1.44	5 (8%)
30	CLA	a	707	16	69,73,73	1.27	6 (8%)	83,113,113	1.23	6 (7%)
37	BCR	m	201	-	41,41,41	0.71	0	56,56,56	2.33	16 (28%)
34	PID	F	305	-	41,49,49	1.38	5 (12%)	49,76,76	1.87	9 (18%)
30	CLA	l	311	16	69,73,73	1.27	6 (8%)	83,113,113	1.28	7 (8%)
33	LMG	j	101	-	35,35,55	0.88	0	43,43,63	1.23	4 (9%)
30	CLA	N	304	-	51,55,73	1.46	6 (11%)	61,91,113	1.42	6 (9%)
30	CLA	A	319	-	50,54,73	1.46	7 (14%)	60,90,113	1.36	5 (8%)
28	DD6	B	306	-	39,45,45	2.03	3 (7%)	52,67,67	1.95	19 (36%)
30	CLA	I	307	-	50,54,73	1.46	6 (12%)	60,90,113	1.41	4 (6%)
30	CLA	a	728	-	59,63,73	1.36	7 (11%)	71,101,113	1.35	7 (9%)
28	DD6	J	302	-	39,45,45	2.02	2 (5%)	52,67,67	2.11	15 (28%)
34	PID	G	506	-	41,49,49	1.34	4 (9%)	49,76,76	1.38	6 (12%)
30	CLA	B	309	18	69,73,73	1.26	6 (8%)	83,113,113	1.28	6 (7%)
28	DD6	N	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.09	16 (30%)
28	DD6	H	303	-	39,45,45	1.97	3 (7%)	52,67,67	1.90	12 (23%)
28	DD6	G	504	-	39,45,45	2.24	5 (12%)	52,67,67	2.19	19 (36%)
30	CLA	a	714	16	49,53,73	1.50	6 (12%)	59,89,113	1.45	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DD6	A	305	31	39,45,45	1.99	2 (5%)	52,67,67	1.96	14 (26%)
30	CLA	D	311	-	50,54,73	1.46	6 (12%)	60,90,113	1.43	5 (8%)
28	DD6	L	303	-	39,45,45	1.98	2 (5%)	52,67,67	1.99	14 (26%)
34	PID	O	301	-	41,49,49	1.32	4 (9%)	49,76,76	1.53	5 (10%)
30	CLA	D	308	-	51,55,73	1.45	6 (11%)	61,91,113	1.39	5 (8%)
30	CLA	a	710	16	59,63,73	1.37	8 (13%)	71,101,113	1.37	7 (9%)
30	CLA	I	312	-	69,73,73	1.26	9 (13%)	83,113,113	1.23	6 (7%)
30	CLA	D	316	-	45,49,73	1.53	7 (15%)	54,84,113	1.49	6 (11%)
30	CLA	O	311	-	55,59,73	1.41	7 (12%)	66,96,113	1.35	6 (9%)
30	CLA	a	706	16	62,66,73	1.32	7 (11%)	74,104,113	1.33	5 (6%)
32	DGD	L	301	-	39,39,67	0.95	2 (5%)	53,53,81	0.98	2 (3%)
30	CLA	b	704	-	69,73,73	1.27	11 (15%)	83,113,113	1.35	7 (8%)
30	CLA	L	317	23	56,60,73	1.41	8 (14%)	67,97,113	1.38	7 (10%)
38	PQN	b	729	-	34,34,34	1.55	2 (5%)	42,45,45	1.23	4 (9%)
30	CLA	a	709	-	69,73,73	1.26	8 (11%)	83,113,113	1.27	6 (7%)
28	DD6	G	505	-	39,45,45	2.26	4 (10%)	52,67,67	2.31	21 (40%)
30	CLA	l	304	14	64,68,73	1.30	6 (9%)	77,107,113	1.35	5 (6%)
30	CLA	L	312	23	50,54,73	1.46	7 (14%)	60,90,113	1.41	5 (8%)
30	CLA	O	309	-	69,73,73	1.26	8 (11%)	83,113,113	1.32	7 (8%)
37	BCR	l	302	-	41,41,41	0.73	0	56,56,56	2.19	21 (37%)
30	CLA	J	314	22	45,49,73	1.54	6 (13%)	54,84,113	1.50	6 (11%)
29	UIX	K	302	-	41,49,49	1.26	3 (7%)	52,74,74	2.71	23 (44%)
30	CLA	P	215	-	51,55,73	1.46	8 (15%)	61,91,113	1.53	6 (9%)
30	CLA	b	713	-	69,73,73	1.27	9 (13%)	83,113,113	1.25	6 (7%)
31	KC1	O	315	26	49,53,53	1.38	5 (10%)	63,89,89	1.94	13 (20%)
30	CLA	b	712	17	58,62,73	1.42	10 (17%)	73,100,113	1.44	10 (13%)
30	CLA	B	307	18	53,57,73	1.44	6 (11%)	62,93,113	1.39	7 (11%)
28	DD6	J	304	-	39,45,45	2.20	5 (12%)	52,67,67	2.12	18 (34%)
37	BCR	a	734	-	41,41,41	0.71	0	56,56,56	2.07	19 (33%)
30	CLA	a	725	16	65,69,73	1.30	6 (9%)	78,108,113	1.31	7 (8%)
30	CLA	b	715	17	64,68,73	1.31	6 (9%)	77,107,113	1.32	6 (7%)
30	CLA	P	212	-	55,59,73	1.41	8 (14%)	66,96,113	1.38	5 (7%)
34	PID	P	205	-	41,49,49	1.32	4 (9%)	49,76,76	1.70	6 (12%)
31	KC1	O	312	-	49,53,53	1.37	6 (12%)	63,89,89	2.02	15 (23%)
34	PID	D	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.78	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	PID	j	105	-	41,49,49	1.41	4 (9%)	49,76,76	1.48	10 (20%)
30	CLA	B	308	-	49,53,73	1.49	6 (12%)	59,89,113	1.46	6 (10%)
30	CLA	K	315	-	45,49,73	1.53	7 (15%)	54,84,113	1.52	8 (14%)
34	PID	D	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.51	6 (12%)
30	CLA	b	709	17	64,68,73	1.31	8 (12%)	77,107,113	1.32	8 (10%)
31	KC1	J	313	22	49,53,53	1.38	6 (12%)	63,89,89	1.96	12 (19%)
28	DD6	I	302	-	39,45,45	2.05	3 (7%)	52,67,67	2.16	17 (32%)
30	CLA	A	312	-	59,63,73	1.36	6 (10%)	71,101,113	1.31	6 (8%)
30	CLA	M	312	-	52,56,73	1.45	8 (15%)	62,92,113	1.43	8 (12%)
30	CLA	K	312	-	52,56,73	1.44	8 (15%)	62,92,113	1.40	5 (8%)
31	KC1	P	213	-	49,53,53	1.37	6 (12%)	63,89,89	2.02	15 (23%)
30	CLA	H	304	-	51,55,73	1.47	7 (13%)	61,91,113	1.39	6 (9%)
36	SF4	c	202	7	0,12,12	-	-	-		
30	CLA	I	309	1	59,63,73	1.38	7 (11%)	71,101,113	1.34	7 (9%)
30	CLA	A	317	-	45,49,73	1.53	6 (13%)	54,84,113	1.50	8 (14%)
30	CLA	G	514	-	57,61,73	1.38	7 (12%)	68,98,113	1.39	7 (10%)
30	CLA	B	301	-	64,68,73	1.32	7 (10%)	77,107,113	1.28	6 (7%)
30	CLA	a	712	30	64,68,73	1.30	8 (12%)	77,107,113	1.32	7 (9%)
34	PID	P	206	-	41,49,49	1.33	4 (9%)	49,76,76	1.86	9 (18%)
30	CLA	J	307	-	69,73,73	1.25	8 (11%)	83,113,113	1.32	4 (4%)
28	DD6	M	302	-	39,45,45	2.17	4 (10%)	52,67,67	2.24	16 (30%)
28	DD6	F	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.01	14 (26%)
37	BCR	l	306	-	41,41,41	0.73	0	56,56,56	1.91	13 (23%)
28	DD6	M	304	-	39,45,45	2.04	3 (7%)	52,67,67	1.91	14 (26%)
30	CLA	K	316	2	50,54,73	1.47	8 (16%)	60,90,113	1.43	6 (10%)
28	DD6	M	303	-	39,45,45	2.20	4 (10%)	52,67,67	2.20	19 (36%)
33	LMG	I	318	-	36,36,55	0.90	1 (2%)	44,44,63	1.24	3 (6%)
30	CLA	a	703	-	59,63,73	1.37	11 (18%)	71,101,113	1.46	8 (11%)
31	KC1	D	310	19	49,53,53	1.38	6 (12%)	63,89,89	2.04	14 (22%)
30	CLA	F	312	-	50,54,73	1.43	10 (20%)	60,90,113	1.40	6 (10%)
30	CLA	b	718	17	55,59,73	1.42	8 (14%)	66,96,113	1.42	5 (7%)
30	CLA	l	308	-	45,49,73	1.53	6 (13%)	54,84,113	1.47	6 (11%)
31	KC1	M	307	30	49,53,53	1.40	6 (12%)	63,89,89	2.04	15 (23%)
30	CLA	b	726	17	51,55,73	1.46	7 (13%)	61,91,113	1.38	6 (9%)
30	CLA	O	308	-	51,55,73	1.46	6 (11%)	61,91,113	1.41	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	b	719	-	50,54,73	1.47	8 (16%)	60,90,113	1.47	6 (10%)
30	CLA	a	718	-	50,54,73	1.46	6 (12%)	60,90,113	1.43	5 (8%)
30	CLA	K	310	-	59,63,73	1.36	8 (13%)	71,101,113	1.34	7 (9%)
30	CLA	D	312	19	50,54,73	1.47	7 (14%)	60,90,113	1.37	4 (6%)
30	CLA	N	307	-	55,59,73	1.43	8 (14%)	66,96,113	1.37	6 (9%)
37	BCR	a	736	-	41,41,41	0.74	0	56,56,56	2.03	18 (32%)
30	CLA	f	302	-	50,54,73	1.47	7 (14%)	60,90,113	1.41	6 (10%)
30	CLA	M	309	24	59,63,73	1.37	6 (10%)	71,101,113	1.33	6 (8%)
30	CLA	I	319	30	49,53,73	1.48	8 (16%)	59,89,113	1.48	6 (10%)
31	KC1	A	306	28,30	49,53,53	1.38	6 (12%)	63,89,89	1.98	14 (22%)
32	DGD	j	103	-	42,42,67	1.05	2 (4%)	56,56,81	1.00	3 (5%)
30	CLA	b	722	17	69,73,73	1.27	9 (13%)	83,113,113	1.33	8 (9%)
28	DD6	I	305	-	39,45,45	2.28	6 (15%)	52,67,67	2.29	17 (32%)
30	CLA	G	513	5	69,73,73	1.26	7 (10%)	83,113,113	1.29	7 (8%)
28	DD6	J	303	-	39,45,45	2.31	4 (10%)	52,67,67	2.44	18 (34%)
28	DD6	G	502	-	39,45,45	1.99	2 (5%)	52,67,67	1.94	16 (30%)
34	PID	O	304	-	41,49,49	1.32	4 (9%)	49,76,76	1.73	8 (16%)
28	DD6	L	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.82	12 (23%)
30	CLA	K	306	2	53,57,73	1.44	6 (11%)	62,93,113	1.43	7 (11%)
31	KC1	N	311	25	49,53,53	1.37	5 (10%)	63,89,89	1.99	14 (22%)
30	CLA	a	715	-	49,53,73	1.49	8 (16%)	59,89,113	1.47	5 (8%)
30	CLA	D	314	-	50,54,73	1.50	8 (16%)	60,90,113	1.47	8 (13%)
30	CLA	b	724	17	69,73,73	1.26	8 (11%)	83,113,113	1.25	6 (7%)
28	DD6	M	306	-	39,45,45	2.17	3 (7%)	52,67,67	2.24	18 (34%)
30	CLA	B	317	-	49,53,73	1.50	9 (18%)	59,89,113	1.46	5 (8%)
30	CLA	P	209	-	51,55,73	1.47	7 (13%)	61,91,113	1.41	6 (9%)
30	CLA	J	310	-	50,54,73	1.48	9 (18%)	60,90,113	1.39	5 (8%)
31	KC1	H	306	21	49,53,53	1.37	6 (12%)	63,89,89	2.01	14 (22%)
30	CLA	G	519	-	63,67,73	1.32	6 (9%)	75,105,113	1.32	5 (6%)
30	CLA	a	730	16	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
30	CLA	F	311	-	50,54,73	1.47	7 (14%)	60,90,113	1.47	6 (10%)
37	BCR	j	102	-	41,41,41	0.71	0	56,56,56	2.02	16 (28%)
30	CLA	A	315	6	45,49,73	1.52	7 (15%)	54,84,113	1.50	6 (11%)
30	CLA	J	315	-	50,54,73	1.47	6 (12%)	60,90,113	1.43	5 (8%)
30	CLA	l	305	-	69,73,73	1.27	8 (11%)	83,113,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CLA	L	316	-	45,49,73	1.54	6 (13%)	54,84,113	1.51	7 (12%)
34	PID	P	203	-	41,49,49	1.33	4 (9%)	49,76,76	1.37	5 (10%)
31	KC1	A	314	6	49,53,53	1.37	6 (12%)	63,89,89	2.01	15 (23%)
30	CLA	F	313	-	50,54,73	1.47	7 (14%)	60,90,113	1.49	5 (8%)
34	PID	F	306	-	41,49,49	1.33	4 (9%)	49,76,76	1.49	5 (10%)
34	PID	M	301	-	41,49,49	1.33	4 (9%)	49,76,76	1.74	8 (16%)
30	CLA	D	313	19	49,53,73	1.49	8 (16%)	59,89,113	1.41	5 (8%)
30	CLA	J	312	-	57,61,73	1.37	8 (14%)	68,98,113	1.43	7 (10%)
30	CLA	M	318	-	50,54,73	1.48	7 (14%)	60,90,113	1.40	6 (10%)
33	LMG	b	734	-	31,31,55	0.99	0	39,39,63	1.17	3 (7%)
28	DD6	L	302	-	39,45,45	1.94	2 (5%)	52,67,67	2.00	14 (26%)
33	LMG	D	317	-	48,48,55	0.76	1 (2%)	55,55,63	1.28	5 (9%)
30	CLA	a	735	-	69,73,73	1.26	6 (8%)	83,113,113	1.23	5 (6%)
34	PID	D	302	-	41,49,49	1.35	4 (9%)	49,76,76	1.44	7 (14%)
30	CLA	K	309	2	54,58,73	1.41	7 (12%)	65,95,113	1.42	7 (10%)
33	LMG	I	320	-	38,38,55	0.81	0	46,46,63	1.29	6 (13%)
34	PID	G	507	-	41,49,49	1.33	4 (9%)	49,76,76	1.40	7 (14%)
30	CLA	a	729	16	60,64,73	1.34	7 (11%)	72,102,113	1.32	6 (8%)
30	CLA	a	727	16	50,54,73	1.48	7 (14%)	60,90,113	1.40	5 (8%)
31	KC1	O	310	-	49,53,53	1.37	6 (12%)	63,89,89	1.99	15 (23%)
30	CLA	B	310	18	59,63,73	1.37	7 (11%)	71,101,113	1.34	9 (12%)
30	CLA	B	311	-	69,73,73	1.26	8 (11%)	83,113,113	1.23	5 (6%)
30	CLA	M	315	-	45,49,73	1.52	6 (13%)	54,84,113	1.57	8 (14%)
37	BCR	i	201	-	41,41,41	0.82	2 (4%)	56,56,56	2.11	20 (35%)
29	UIX	I	304	-	41,49,49	1.32	4 (9%)	52,74,74	2.59	14 (26%)
30	CLA	G	517	-	50,54,73	1.46	7 (14%)	60,90,113	1.40	5 (8%)
34	PID	N	301	-	41,49,49	1.35	4 (9%)	49,76,76	1.50	6 (12%)
28	DD6	L	306	-	39,45,45	2.00	3 (7%)	52,67,67	2.04	15 (28%)
30	CLA	b	706	17	52,56,73	1.46	7 (13%)	62,92,113	1.40	6 (9%)
30	CLA	H	311	-	45,49,73	1.54	7 (15%)	54,84,113	1.48	7 (12%)
30	CLA	A	316	6	51,55,73	1.45	7 (13%)	61,91,113	1.41	5 (8%)
32	DGD	y	201	-	55,55,67	0.92	2 (3%)	69,69,81	0.97	3 (4%)
30	CLA	N	310	-	51,55,73	1.46	6 (11%)	61,91,113	1.52	6 (9%)
30	CLA	M	316	24	56,60,73	1.41	9 (16%)	67,97,113	1.36	5 (7%)
30	CLA	K	313	-	59,63,73	1.36	6 (10%)	71,101,113	1.35	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	PID	F	302	-	41,49,49	1.33	4 (9%)	49,76,76	1.66	6 (12%)
31	KC1	F	314	20	49,53,53	1.39	6 (12%)	63,89,89	2.00	14 (22%)
30	CLA	f	301	-	59,63,73	1.36	8 (13%)	71,101,113	1.34	6 (8%)
30	CLA	b	707	17	69,73,73	1.27	6 (8%)	83,113,113	1.29	7 (8%)
30	CLA	a	726	16	69,73,73	1.26	7 (10%)	83,113,113	1.31	8 (9%)
30	CLA	A	310	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	6 (7%)
30	CLA	L	309	-	57,61,73	1.38	6 (10%)	68,98,113	1.38	7 (10%)
30	CLA	a	716	16	51,55,73	1.46	6 (11%)	61,91,113	1.42	6 (9%)
29	UIX	J	305	-	41,49,49	1.25	3 (7%)	52,74,74	2.46	17 (32%)
30	CLA	G	518	-	50,54,73	1.48	8 (16%)	60,90,113	1.45	7 (11%)
34	PID	D	307	-	41,49,49	1.34	4 (9%)	49,76,76	1.41	5 (10%)
30	CLA	M	310	24	52,56,73	1.45	7 (13%)	62,92,113	1.41	6 (9%)
30	CLA	G	512	-	64,68,73	1.31	8 (12%)	77,107,113	1.33	6 (7%)
33	LMG	B	318	-	37,37,55	0.85	0	45,45,63	1.32	6 (13%)
28	DD6	B	303	-	39,45,45	2.00	2 (5%)	52,67,67	2.00	17 (32%)
30	CLA	B	312	-	55,59,73	1.41	6 (10%)	66,96,113	1.37	6 (9%)
30	CLA	F	308	-	50,54,73	1.45	7 (14%)	60,90,113	1.42	5 (8%)
30	CLA	a	721	-	69,73,73	1.26	7 (10%)	83,113,113	1.26	7 (8%)
30	CLA	L	313	-	59,63,73	1.37	7 (11%)	71,101,113	1.32	7 (9%)
30	CLA	I	316	1	59,63,73	1.34	6 (10%)	71,101,113	1.35	7 (9%)
30	CLA	f	303	10	50,54,73	1.47	7 (14%)	60,90,113	1.41	5 (8%)
34	PID	H	302	-	41,49,49	1.38	4 (9%)	49,76,76	1.37	6 (12%)
30	CLA	j	104	16	59,63,73	1.38	6 (10%)	71,101,113	1.32	8 (11%)
28	DD6	K	305	-	39,45,45	1.98	3 (7%)	52,67,67	1.85	13 (25%)
30	CLA	N	309	25	50,54,73	1.45	8 (16%)	60,90,113	1.43	4 (6%)
30	CLA	a	724	16	69,73,73	1.27	9 (13%)	83,113,113	1.32	9 (10%)
30	CLA	m	202	-	64,68,73	1.30	7 (10%)	77,107,113	1.35	7 (9%)
29	UIX	h	201	-	41,49,49	1.28	3 (7%)	52,74,74	2.48	19 (36%)
37	BCR	l	307	-	41,41,41	0.72	0	56,56,56	2.01	19 (33%)
30	CLA	B	313	18	69,73,73	1.26	6 (8%)	83,113,113	1.29	5 (6%)
30	CLA	O	313	-	50,54,73	1.44	7 (14%)	60,90,113	1.38	5 (8%)
30	CLA	a	722	16	62,66,73	1.32	7 (11%)	74,104,113	1.31	7 (9%)
36	SF4	c	201	7	0,12,12	-	-	-		

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
30	CLA	K	307	-	-	2/17/93/115	-
30	CLA	O	314	-	-	9/18/94/115	-
34	PID	F	304	-	-	3/24/93/93	0/4/4/4
34	PID	O	302	-	-	2/24/93/93	0/4/4/4
30	CLA	F	307	-	-	6/17/93/115	-
30	CLA	M	311	-	-	6/17/93/115	-
28	DD6	B	304	-	-	0/26/80/80	0/3/3/3
30	CLA	b	720	17	-	9/25/101/115	-
28	DD6	A	303	-	-	1/26/80/80	0/3/3/3
39	LHG	a	733	-	-	18/52/52/53	-
30	CLA	a	702	-	-	14/39/115/115	-
28	DD6	L	305	-	-	3/26/80/80	0/3/3/3
30	CLA	a	701	-	-	2/15/91/115	-
30	CLA	I	306	1	-	9/20/96/115	-
30	CLA	G	510	-	-	14/39/115/115	-
30	CLA	G	509	5	-	4/23/99/115	-
30	CLA	M	313	-	-	4/17/93/115	-
30	CLA	l	312	-	-	8/17/93/115	-
30	CLA	a	723	16	-	16/39/115/115	-
30	CLA	K	308	2	-	13/26/102/115	-
30	CLA	A	313	-	-	10/27/103/115	-
30	CLA	a	713	16	-	12/33/109/115	-
32	DGD	G	501	-	-	10/34/74/95	0/2/2/2
30	CLA	H	312	-	-	10/17/93/115	-
30	CLA	a	731	16	-	13/39/115/115	-
33	LMG	K	317	-	-	18/38/58/70	0/1/1/1
34	PID	O	307	-	-	3/24/93/93	0/4/4/4
30	CLA	b	705	-	-	15/39/115/115	-
30	CLA	P	217	27	-	5/10/86/115	-
31	KC1	L	315	23	-	8/15/71/71	-
33	LMG	b	733	-	-	19/39/59/70	0/1/1/1
30	CLA	I	311	1	-	10/27/103/115	-
30	CLA	b	721	17,28	-	5/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	J	316	-	-	3/17/93/115	-
30	CLA	a	738	22	-	4/17/93/115	-
34	PID	O	305	-	-	16/24/93/93	0/4/4/4
30	CLA	b	710	-	-	7/24/100/115	-
30	CLA	H	309	-	-	9/18/94/115	-
38	PQN	a	732	-	-	8/23/43/43	0/2/2/2
30	CLA	b	708	17	-	11/39/115/115	-
30	CLA	L	314	-	-	6/25/101/115	-
30	CLA	J	309	-	-	10/29/105/115	-
28	DD6	F	301	-	-	2/26/80/80	0/3/3/3
29	UIX	A	304	-	-	0/31/87/87	0/3/3/3
30	CLA	I	313	-	-	12/27/103/115	-
30	CLA	a	719	-	-	6/18/94/115	-
31	KC1	I	314	1	-	8/15/71/71	-
34	PID	D	306	-	-	8/24/93/93	0/4/4/4
28	DD6	h	203	-	-	1/26/80/80	0/3/3/3
28	DD6	b	731	30	-	3/26/80/80	0/3/3/3
28	DD6	O	303	-	-	0/26/80/80	0/3/3/3
30	CLA	I	315	-	-	9/24/100/115	-
30	CLA	b	717	17	-	18/39/115/115	-
31	KC1	P	216	27	-	8/15/71/71	-
28	DD6	K	301	-	-	5/26/80/80	0/3/3/3
30	CLA	b	714	-	-	5/17/93/115	-
28	DD6	I	303	-	-	2/26/80/80	0/3/3/3
31	KC1	B	314	18	-	7/15/71/71	-
29	UIX	P	207	-	-	8/31/87/87	0/3/3/3
30	CLA	J	308	22	-	11/17/93/115	-
30	CLA	G	520	17	-	6/20/96/115	-
30	CLA	l	313	14	-	21/39/115/115	-
37	BCR	b	730	-	-	8/29/63/63	0/2/2/2
31	KC1	F	309	20	-	8/15/71/71	-
30	CLA	a	711	16	-	6/15/91/115	-
28	DD6	I	301	-	-	3/26/80/80	0/3/3/3
30	CLA	j	106	17	-	12/31/107/115	-
30	CLA	J	306	-	-	6/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	KC1	P	211	27	-	11/15/71/71	-
30	CLA	l	309	-	-	5/10/86/115	-
30	CLA	B	315	-	-	6/10/86/115	-
30	CLA	I	321	30	-	9/24/100/115	-
34	PID	D	305	-	-	2/24/93/93	0/4/4/4
30	CLA	F	310	-	-	8/17/93/115	-
30	CLA	b	716	-	-	7/21/97/115	-
30	CLA	a	720	-	-	6/36/112/115	-
30	CLA	N	305	-	-	11/39/115/115	-
32	DGD	G	521	-	-	18/33/73/95	0/2/2/2
29	UIX	O	306	-	-	4/31/87/87	0/3/3/3
30	CLA	P	210	-	-	15/39/115/115	-
32	DGD	I	317	-	-	3/28/68/95	0/2/2/2
30	CLA	a	717	16	-	13/30/106/115	-
30	CLA	L	308	31	-	9/15/91/115	-
37	BCR	b	702	-	-	2/29/63/63	0/2/2/2
30	CLA	B	316	18	-	9/17/93/115	-
30	CLA	K	311	-	-	11/24/100/115	-
29	UIX	G	503	-	-	4/31/87/87	0/3/3/3
28	DD6	M	305	-	-	1/26/80/80	0/3/3/3
30	CLA	b	703	17	-	14/39/115/115	-
28	DD6	K	304	-	-	1/26/80/80	0/3/3/3
34	PID	P	202	-	-	3/24/93/93	0/4/4/4
34	PID	N	302	-	-	2/24/93/93	0/4/4/4
30	CLA	A	307	31	-	3/15/91/115	-
30	CLA	H	307	-	-	7/23/99/115	-
30	CLA	F	315	-	-	4/10/86/115	-
30	CLA	A	308	-	-	5/27/103/115	-
30	CLA	a	705	16,30	-	9/27/103/115	-
30	CLA	M	308	31	-	10/25/101/115	-
30	CLA	l	303	14	-	16/39/115/115	-
31	KC1	K	314	2	-	8/15/71/71	-
31	KC1	G	515	5	-	8/15/71/71	-
36	SF4	a	737	17,16	-	-	0/6/5/5
28	DD6	A	302	-	-	3/26/80/80	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	L	311	-	-	4/27/103/115	-
30	CLA	b	723	-	-	9/21/97/115	-
30	CLA	G	511	5	-	4/27/103/115	-
30	CLA	a	708	16	-	6/23/99/115	-
32	DGD	l	301	-	-	7/39/79/95	0/2/2/2
35	SQD	A	318	-	-	6/45/65/69	0/1/1/1
28	DD6	K	303	-	-	0/26/80/80	0/3/3/3
30	CLA	M	317	-	-	8/17/93/115	-
31	KC1	N	306	25	-	6/15/71/71	-
28	DD6	D	303	-	-	6/26/80/80	0/3/3/3
30	CLA	a	704	-	-	6/39/115/115	-
34	PID	H	301	-	-	4/24/93/93	0/4/4/4
37	BCR	b	732	-	-	2/29/63/63	0/2/2/2
30	CLA	h	202	-	-	9/27/103/115	-
30	CLA	L	310	23	-	2/27/103/115	-
33	LMG	P	201	-	-	8/22/42/70	0/1/1/1
31	KC1	D	315	19	-	3/15/71/71	-
34	PID	P	208	-	-	2/24/93/93	0/4/4/4
30	CLA	b	725	17	-	13/39/115/115	-
28	DD6	B	302	-	-	3/24/78/80	0/3/3/3
30	CLA	l	310	-	-	9/15/65/115	0/5/5/9
28	DD6	A	301	-	-	3/26/80/80	0/3/3/3
28	DD6	K	318	-	-	4/26/80/80	0/3/3/3
31	KC1	M	314	24	-	9/15/71/71	-
30	CLA	P	214	-	-	3/17/93/115	-
29	UIX	B	305	-	-	2/31/87/87	0/3/3/3
30	CLA	A	309	6	-	7/27/103/115	-
30	CLA	b	727	-	-	10/39/115/115	-
28	DD6	P	204	-	-	1/26/80/80	0/3/3/3
28	DD6	G	508	-	-	1/26/80/80	0/3/3/3
30	CLA	H	305	-	-	8/39/115/115	-
31	KC1	H	310	-	-	6/15/71/71	-
30	CLA	b	701	-	-	15/39/115/115	-
30	CLA	H	308	-	-	4/17/93/115	-
30	CLA	D	309	-	-	7/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	O	316	-	-	4/10/86/115	-
30	CLA	b	728	17	-	9/39/115/115	-
37	BCR	f	304	-	-	3/29/63/63	0/2/2/2
30	CLA	b	711	17	-	12/27/103/115	-
30	CLA	J	301	-	-	13/33/109/115	-
30	CLA	I	310	-	-	10/19/95/115	-
30	CLA	A	320	-	-	6/17/93/115	-
31	KC1	L	307	30	-	6/15/71/71	-
31	KC1	N	308	-	-	8/15/71/71	-
30	CLA	J	311	22	-	8/18/94/115	-
30	CLA	A	311	6	-	6/17/93/115	-
30	CLA	G	516	5	-	6/10/86/115	-
30	CLA	I	308	-	-	12/33/109/115	-
30	CLA	L	318	-	-	10/17/93/115	-
30	CLA	a	707	16	-	18/39/115/115	-
37	BCR	m	201	-	-	5/29/63/63	0/2/2/2
34	PID	F	305	-	-	8/24/93/93	0/4/4/4
30	CLA	l	311	16	-	17/39/115/115	-
33	LMG	j	101	-	-	14/30/50/70	0/1/1/1
30	CLA	N	304	-	-	5/18/94/115	-
30	CLA	A	319	-	-	10/17/93/115	-
28	DD6	B	306	-	-	2/26/80/80	0/3/3/3
30	CLA	I	307	-	-	8/17/93/115	-
30	CLA	a	728	-	-	8/27/103/115	-
28	DD6	J	302	-	-	3/26/80/80	0/3/3/3
34	PID	G	506	-	-	3/24/93/93	0/4/4/4
30	CLA	B	309	18	-	22/39/115/115	-
28	DD6	N	303	-	-	0/26/80/80	0/3/3/3
28	DD6	H	303	-	-	1/26/80/80	0/3/3/3
28	DD6	G	504	-	-	5/26/80/80	0/3/3/3
30	CLA	a	714	16	-	4/15/91/115	-
28	DD6	A	305	31	-	1/26/80/80	0/3/3/3
30	CLA	D	311	-	-	4/17/93/115	-
28	DD6	L	303	-	-	0/26/80/80	0/3/3/3
34	PID	O	301	-	-	4/24/93/93	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	D	308	-	-	6/18/94/115	-
30	CLA	a	710	16	-	6/27/103/115	-
30	CLA	I	312	-	-	16/39/115/115	-
30	CLA	D	316	-	-	0/10/86/115	-
30	CLA	O	311	-	-	5/23/99/115	-
30	CLA	a	706	16	-	17/31/107/115	-
32	DGD	L	301	-	-	2/26/66/95	0/2/2/2
30	CLA	b	704	-	-	20/39/115/115	-
30	CLA	L	317	23	-	11/24/100/115	-
38	PQN	b	729	-	-	4/23/43/43	0/2/2/2
30	CLA	a	709	-	-	17/39/115/115	-
28	DD6	G	505	-	-	4/26/80/80	0/3/3/3
30	CLA	l	304	14	-	11/33/109/115	-
30	CLA	L	312	23	-	7/17/93/115	-
30	CLA	O	309	-	-	2/39/115/115	-
37	BCR	l	302	-	-	4/29/63/63	0/2/2/2
30	CLA	J	314	22	-	4/10/86/115	-
29	UIX	K	302	-	-	4/31/87/87	0/3/3/3
30	CLA	P	215	-	-	7/18/94/115	-
30	CLA	b	713	-	-	11/39/115/115	-
31	KC1	O	315	26	-	5/15/71/71	-
30	CLA	b	712	17	-	9/25/101/115	-
30	CLA	B	307	18	-	3/20/96/115	-
28	DD6	J	304	-	-	2/26/80/80	0/3/3/3
37	BCR	a	734	-	-	4/29/63/63	0/2/2/2
30	CLA	a	725	16	-	13/35/111/115	-
30	CLA	b	715	17	-	14/33/109/115	-
30	CLA	P	212	-	-	9/23/99/115	-
34	PID	P	205	-	-	2/24/93/93	0/4/4/4
31	KC1	O	312	-	-	8/15/71/71	-
34	PID	D	304	-	-	3/24/93/93	0/4/4/4
34	PID	j	105	-	-	4/24/93/93	0/4/4/4
30	CLA	B	308	-	-	5/15/91/115	-
30	CLA	K	315	-	-	3/10/86/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PID	D	301	-	-	2/24/93/93	0/4/4/4
30	CLA	b	709	17	-	8/33/109/115	-
31	KC1	J	313	22	-	6/15/71/71	-
28	DD6	I	302	-	-	5/26/80/80	0/3/3/3
30	CLA	A	312	-	-	6/27/103/115	-
30	CLA	M	312	-	-	6/19/95/115	-
30	CLA	K	312	-	-	6/19/95/115	-
31	KC1	P	213	-	-	8/15/71/71	-
30	CLA	H	304	-	-	8/18/94/115	-
36	SF4	c	202	7	-	-	0/6/5/5
30	CLA	I	309	1	-	8/27/103/115	-
30	CLA	A	317	-	-	0/10/86/115	-
30	CLA	G	514	-	-	11/25/101/115	-
30	CLA	B	301	-	-	11/33/109/115	-
30	CLA	a	712	30	-	10/33/109/115	-
34	PID	P	206	-	-	2/24/93/93	0/4/4/4
30	CLA	J	307	-	-	21/39/115/115	-
28	DD6	M	302	-	-	3/26/80/80	0/3/3/3
28	DD6	F	303	-	-	2/26/80/80	0/3/3/3
37	BCR	l	306	-	-	7/29/63/63	0/2/2/2
28	DD6	M	304	-	-	0/26/80/80	0/3/3/3
30	CLA	K	316	2	-	3/17/93/115	-
28	DD6	M	303	-	-	2/26/80/80	0/3/3/3
33	LMG	I	318	-	-	21/31/51/70	0/1/1/1
30	CLA	a	703	-	-	9/27/103/115	-
31	KC1	D	310	19	-	10/15/71/71	-
30	CLA	F	312	-	-	4/17/93/115	-
30	CLA	b	718	17	-	3/23/99/115	-
30	CLA	l	308	-	-	3/10/86/115	-
31	KC1	M	307	30	-	7/15/71/71	-
30	CLA	b	726	17	-	3/18/94/115	-
30	CLA	O	308	-	-	7/18/94/115	-
30	CLA	b	719	-	-	12/17/93/115	-
30	CLA	a	718	-	-	10/17/93/115	-
30	CLA	K	310	-	-	6/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	D	312	19	-	8/17/93/115	-
30	CLA	N	307	-	-	7/23/99/115	-
37	BCR	a	736	-	-	3/29/63/63	0/2/2/2
30	CLA	f	302	-	-	6/17/93/115	-
30	CLA	M	309	24	-	5/27/103/115	-
30	CLA	I	319	30	-	8/15/91/115	-
31	KC1	A	306	28,30	-	6/15/71/71	-
32	DGD	j	103	-	-	7/30/70/95	0/2/2/2
30	CLA	b	722	17	-	8/39/115/115	-
28	DD6	I	305	-	-	5/26/80/80	0/3/3/3
30	CLA	G	513	5	-	10/39/115/115	-
28	DD6	J	303	-	-	2/26/80/80	0/3/3/3
28	DD6	G	502	-	-	6/26/80/80	0/3/3/3
34	PID	O	304	-	-	3/24/93/93	0/4/4/4
28	DD6	L	304	-	-	0/26/80/80	0/3/3/3
30	CLA	K	306	2	-	6/20/96/115	-
31	KC1	N	311	25	-	7/15/71/71	-
30	CLA	a	715	-	-	7/15/91/115	-
30	CLA	D	314	-	-	8/17/93/115	-
30	CLA	b	724	17	-	16/39/115/115	-
28	DD6	M	306	-	-	5/26/80/80	0/3/3/3
30	CLA	B	317	-	-	7/15/91/115	-
30	CLA	P	209	-	-	6/18/94/115	-
30	CLA	J	310	-	-	8/17/93/115	-
31	KC1	H	306	21	-	4/15/71/71	-
30	CLA	G	519	-	-	13/32/108/115	-
30	CLA	a	730	16	-	4/39/115/115	-
30	CLA	F	311	-	-	6/17/93/115	-
37	BCR	j	102	-	-	6/29/63/63	0/2/2/2
30	CLA	A	315	6	-	6/10/86/115	-
30	CLA	J	315	-	-	4/17/93/115	-
30	CLA	l	305	-	-	13/39/115/115	-
30	CLA	L	316	-	-	6/10/86/115	-
34	PID	P	203	-	-	2/24/93/93	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	KC1	A	314	6	-	7/15/71/71	-
30	CLA	F	313	-	-	5/17/93/115	-
34	PID	F	306	-	-	0/24/93/93	0/4/4/4
34	PID	M	301	-	-	1/24/93/93	0/4/4/4
30	CLA	D	313	19	-	3/15/91/115	-
30	CLA	J	312	-	-	8/25/101/115	-
30	CLA	M	318	-	-	11/17/93/115	-
33	LMG	b	734	-	-	12/26/46/70	0/1/1/1
28	DD6	L	302	-	-	4/26/80/80	0/3/3/3
33	LMG	D	317	-	-	17/41/61/70	0/1/1/1
30	CLA	a	735	-	-	20/39/115/115	-
34	PID	D	302	-	-	2/24/93/93	0/4/4/4
30	CLA	K	309	2	-	2/21/97/115	-
33	LMG	I	320	-	-	14/33/53/70	0/1/1/1
34	PID	G	507	-	-	0/24/93/93	1/4/4/4
30	CLA	a	729	16	-	9/29/105/115	-
30	CLA	a	727	16	-	9/17/93/115	-
31	KC1	O	310	-	-	8/15/71/71	-
30	CLA	B	310	18	-	8/27/103/115	-
30	CLA	B	311	-	-	23/39/115/115	-
30	CLA	M	315	-	-	5/10/86/115	-
37	BCR	i	201	-	-	8/29/63/63	0/2/2/2
29	UIX	I	304	-	-	4/31/87/87	0/3/3/3
30	CLA	G	517	-	-	4/17/93/115	-
34	PID	N	301	-	-	6/24/93/93	0/4/4/4
28	DD6	L	306	-	-	3/26/80/80	0/3/3/3
30	CLA	b	706	17	-	4/19/95/115	-
30	CLA	H	311	-	-	8/10/86/115	-
30	CLA	A	316	6	-	4/18/94/115	-
32	DGD	y	201	-	-	7/43/83/95	0/2/2/2
30	CLA	N	310	-	-	11/18/94/115	-
30	CLA	M	316	24	-	11/24/100/115	-
30	CLA	K	313	-	-	7/27/103/115	-
34	PID	F	302	-	-	2/24/93/93	0/4/4/4
31	KC1	F	314	20	-	8/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	f	301	-	-	11/27/103/115	-
30	CLA	b	707	17	-	17/39/115/115	-
30	CLA	a	726	16	-	13/39/115/115	-
30	CLA	A	310	-	-	15/39/115/115	-
30	CLA	L	309	-	-	11/25/101/115	-
30	CLA	a	716	16	-	6/18/94/115	-
29	UIX	J	305	-	-	11/31/87/87	0/3/3/3
30	CLA	G	518	-	-	9/17/93/115	-
34	PID	D	307	-	-	4/24/93/93	0/4/4/4
30	CLA	M	310	24	-	7/19/95/115	-
30	CLA	G	512	-	-	13/33/109/115	-
33	LMG	B	318	-	-	15/32/52/70	0/1/1/1
28	DD6	B	303	-	-	2/26/80/80	0/3/3/3
30	CLA	B	312	-	-	4/23/99/115	-
30	CLA	F	308	-	-	3/17/93/115	-
30	CLA	a	721	-	-	20/39/115/115	-
30	CLA	L	313	-	-	11/27/103/115	-
30	CLA	I	316	1	-	14/27/103/115	-
30	CLA	f	303	10	-	10/17/93/115	-
34	PID	H	302	-	-	2/24/93/93	0/4/4/4
30	CLA	j	104	16	-	6/27/103/115	-
28	DD6	K	305	-	-	4/26/80/80	0/3/3/3
30	CLA	N	309	25	-	5/17/93/115	-
30	CLA	a	724	16	-	15/39/115/115	-
30	CLA	m	202	-	-	10/33/109/115	-
29	UIX	h	201	-	-	2/31/87/87	0/3/3/3
37	BCR	l	307	-	-	0/29/63/63	0/2/2/2
30	CLA	B	313	18	-	11/39/115/115	-
30	CLA	O	313	-	-	4/17/93/115	-
30	CLA	a	722	16	-	10/31/107/115	-
36	SF4	c	201	7	-	-	0/6/5/5

The worst 5 of 1889 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	I	305	DD6	C29-C27	-9.13	1.25	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	303	DD6	C29-C27	-9.10	1.25	1.42
28	M	303	DD6	C29-C27	-9.07	1.25	1.42
30	l	310	CLA	C1B-C2B	9.05	1.49	1.39
28	b	731	DD6	C29-C27	-9.03	1.25	1.42

The worst 5 of 2901 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	304	UIX	O-C1-C3	9.22	120.31	113.38
29	J	305	UIX	O-C1-C3	8.93	120.09	113.38
29	I	304	UIX	C6-C1-C	-8.91	107.33	122.26
29	B	305	UIX	O-C1-C3	8.34	119.65	113.38
37	m	201	BCR	C7-C8-C9	-8.14	113.94	126.23

There are no chirality outliers.

5 of 2447 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	I	302	DD6	C27-C29-C30-C31
28	K	301	DD6	C12-C11-C13-C14
28	G	502	DD6	C-C1-C24-C25
28	G	502	DD6	C2-C1-C24-C25
28	G	504	DD6	C10-C11-C13-C14

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	G	507	PID	C24-C25-C26-C27-C28-C29

264 monomers are involved in 671 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	K	307	CLA	1	0
30	O	314	CLA	5	0
34	F	304	PID	6	0
34	O	302	PID	2	0
30	F	307	CLA	1	0
30	b	720	CLA	8	0
28	A	303	DD6	1	0
39	a	733	LHG	3	0
30	a	702	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	L	305	DD6	1	0
30	I	306	CLA	2	0
30	G	510	CLA	4	0
30	G	509	CLA	1	0
30	M	313	CLA	3	0
30	l	312	CLA	3	0
30	a	723	CLA	7	0
30	K	308	CLA	3	0
30	A	313	CLA	4	0
30	a	713	CLA	3	0
32	G	501	DGD	2	0
30	H	312	CLA	1	0
30	a	731	CLA	6	0
34	O	307	PID	5	0
30	b	705	CLA	4	0
30	P	217	CLA	3	0
33	b	733	LMG	2	0
30	I	311	CLA	5	0
30	b	721	CLA	2	0
30	J	316	CLA	4	0
30	a	738	CLA	1	0
34	O	305	PID	14	0
30	b	710	CLA	6	0
30	H	309	CLA	2	0
38	a	732	PQN	5	0
30	b	708	CLA	2	0
30	L	314	CLA	4	0
30	J	309	CLA	3	0
28	F	301	DD6	1	0
29	A	304	UIX	1	0
30	I	313	CLA	3	0
30	a	719	CLA	4	0
34	D	306	PID	1	0
30	I	315	CLA	1	0
30	b	717	CLA	6	0
30	b	714	CLA	1	0
30	J	308	CLA	3	0
30	G	520	CLA	3	0
30	l	313	CLA	6	0
37	b	730	BCR	5	0
31	F	309	KC1	2	0
30	a	711	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	I	301	DD6	1	0
30	j	106	CLA	3	0
30	J	306	CLA	1	0
30	B	315	CLA	2	0
30	I	321	CLA	3	0
34	D	305	PID	3	0
30	F	310	CLA	5	0
30	b	716	CLA	4	0
30	a	720	CLA	2	0
30	N	305	CLA	2	0
30	P	210	CLA	4	0
30	a	717	CLA	4	0
30	L	308	CLA	2	0
37	b	702	BCR	6	0
30	B	316	CLA	1	0
30	K	311	CLA	2	0
30	b	703	CLA	6	0
34	P	202	PID	5	0
34	N	302	PID	3	0
30	H	307	CLA	1	0
30	F	315	CLA	1	0
30	A	308	CLA	3	0
30	a	705	CLA	2	0
30	M	308	CLA	2	0
30	l	303	CLA	5	0
36	a	737	SF4	1	0
30	b	723	CLA	3	0
30	G	511	CLA	2	0
30	a	708	CLA	2	0
35	A	318	SQD	8	0
30	M	317	CLA	2	0
30	a	704	CLA	5	0
34	H	301	PID	3	0
37	b	732	BCR	4	0
34	P	208	PID	2	0
30	b	725	CLA	4	0
28	B	302	DD6	1	0
30	l	310	CLA	1	0
30	P	214	CLA	3	0
30	A	309	CLA	2	0
30	b	727	CLA	6	0
28	G	508	DD6	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	H	305	CLA	4	0
31	H	310	KC1	1	0
30	b	701	CLA	7	0
30	H	308	CLA	2	0
30	D	309	CLA	2	0
30	O	316	CLA	2	0
30	b	728	CLA	3	0
37	f	304	BCR	4	0
30	J	301	CLA	5	0
30	I	310	CLA	4	0
30	A	320	CLA	3	0
31	N	308	KC1	1	0
30	J	311	CLA	2	0
30	A	311	CLA	1	0
30	I	308	CLA	4	0
30	a	707	CLA	7	0
37	m	201	BCR	4	0
34	F	305	PID	3	0
30	l	311	CLA	4	0
33	j	101	LMG	4	0
30	A	319	CLA	2	0
30	I	307	CLA	2	0
30	a	728	CLA	3	0
34	G	506	PID	2	0
30	B	309	CLA	4	0
28	H	303	DD6	1	0
28	G	504	DD6	3	0
30	a	714	CLA	3	0
28	A	305	DD6	1	0
30	D	311	CLA	2	0
34	O	301	PID	1	0
30	D	308	CLA	1	0
30	a	710	CLA	4	0
30	I	312	CLA	2	0
30	O	311	CLA	1	0
30	a	706	CLA	7	0
32	L	301	DGD	2	0
30	b	704	CLA	14	0
30	L	317	CLA	5	0
38	b	729	PQN	4	0
30	a	709	CLA	5	0
28	G	505	DD6	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	l	304	CLA	3	0
30	L	312	CLA	1	0
30	O	309	CLA	3	0
37	l	302	BCR	3	0
29	K	302	UIX	1	0
30	P	215	CLA	6	0
30	b	713	CLA	6	0
31	O	315	KC1	3	0
30	b	712	CLA	4	0
30	B	307	CLA	1	0
28	J	304	DD6	3	0
37	a	734	BCR	3	0
30	a	725	CLA	5	0
30	b	715	CLA	5	0
34	P	205	PID	2	0
31	O	312	KC1	1	0
34	D	304	PID	2	0
34	j	105	PID	4	0
30	B	308	CLA	1	0
34	D	301	PID	4	0
30	b	709	CLA	7	0
30	A	312	CLA	3	0
30	M	312	CLA	1	0
30	K	312	CLA	2	0
31	P	213	KC1	1	0
30	H	304	CLA	3	0
36	c	202	SF4	1	0
30	I	309	CLA	1	0
30	A	317	CLA	2	0
30	G	514	CLA	3	0
30	B	301	CLA	3	0
30	a	712	CLA	1	0
34	P	206	PID	4	0
30	J	307	CLA	11	0
37	l	306	BCR	4	0
30	K	316	CLA	1	0
28	M	303	DD6	2	0
30	a	703	CLA	5	0
31	D	310	KC1	1	0
30	F	312	CLA	5	0
30	b	718	CLA	4	0
30	l	308	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	M	307	KC1	1	0
30	b	726	CLA	1	0
30	O	308	CLA	1	0
30	a	718	CLA	1	0
30	K	310	CLA	1	0
30	D	312	CLA	2	0
30	N	307	CLA	1	0
37	a	736	BCR	2	0
30	f	302	CLA	4	0
30	M	309	CLA	8	0
30	I	319	CLA	2	0
32	j	103	DGD	3	0
30	b	722	CLA	4	0
28	I	305	DD6	1	0
30	G	513	CLA	4	0
28	J	303	DD6	2	0
34	O	304	PID	1	0
28	L	304	DD6	1	0
30	K	306	CLA	1	0
30	D	314	CLA	10	0
30	b	724	CLA	4	0
30	B	317	CLA	2	0
30	P	209	CLA	2	0
30	J	310	CLA	3	0
30	G	519	CLA	1	0
30	a	730	CLA	6	0
30	F	311	CLA	1	0
37	j	102	BCR	5	0
30	A	315	CLA	1	0
30	l	305	CLA	3	0
30	L	316	CLA	1	0
34	P	203	PID	5	0
30	F	313	CLA	8	0
34	F	306	PID	2	0
34	M	301	PID	1	0
30	D	313	CLA	1	0
30	J	312	CLA	2	0
30	M	318	CLA	1	0
33	b	734	LMG	3	0
33	D	317	LMG	5	0
30	a	735	CLA	5	0
34	D	302	PID	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	K	309	CLA	2	0
33	I	320	LMG	2	0
34	G	507	PID	5	0
30	a	729	CLA	3	0
30	a	727	CLA	1	0
30	B	310	CLA	1	0
30	B	311	CLA	2	0
30	M	315	CLA	2	0
37	i	201	BCR	7	0
29	I	304	UIX	2	0
30	G	517	CLA	6	0
34	N	301	PID	1	0
30	b	706	CLA	3	0
30	H	311	CLA	2	0
30	A	316	CLA	1	0
32	y	201	DGD	1	0
30	N	310	CLA	3	0
30	M	316	CLA	1	0
30	K	313	CLA	5	0
34	F	302	PID	2	0
30	f	301	CLA	5	0
30	b	707	CLA	5	0
30	a	726	CLA	6	0
30	A	310	CLA	4	0
30	L	309	CLA	1	0
30	a	716	CLA	3	0
29	J	305	UIX	1	0
30	G	518	CLA	1	0
30	M	310	CLA	2	0
33	B	318	LMG	1	0
30	F	308	CLA	1	0
30	a	721	CLA	6	0
30	L	313	CLA	7	0
30	I	316	CLA	3	0
30	f	303	CLA	1	0
34	H	302	PID	5	0
30	j	104	CLA	5	0
30	N	309	CLA	4	0
30	a	724	CLA	3	0
30	m	202	CLA	2	0
37	l	307	BCR	3	0
30	B	313	CLA	4	0

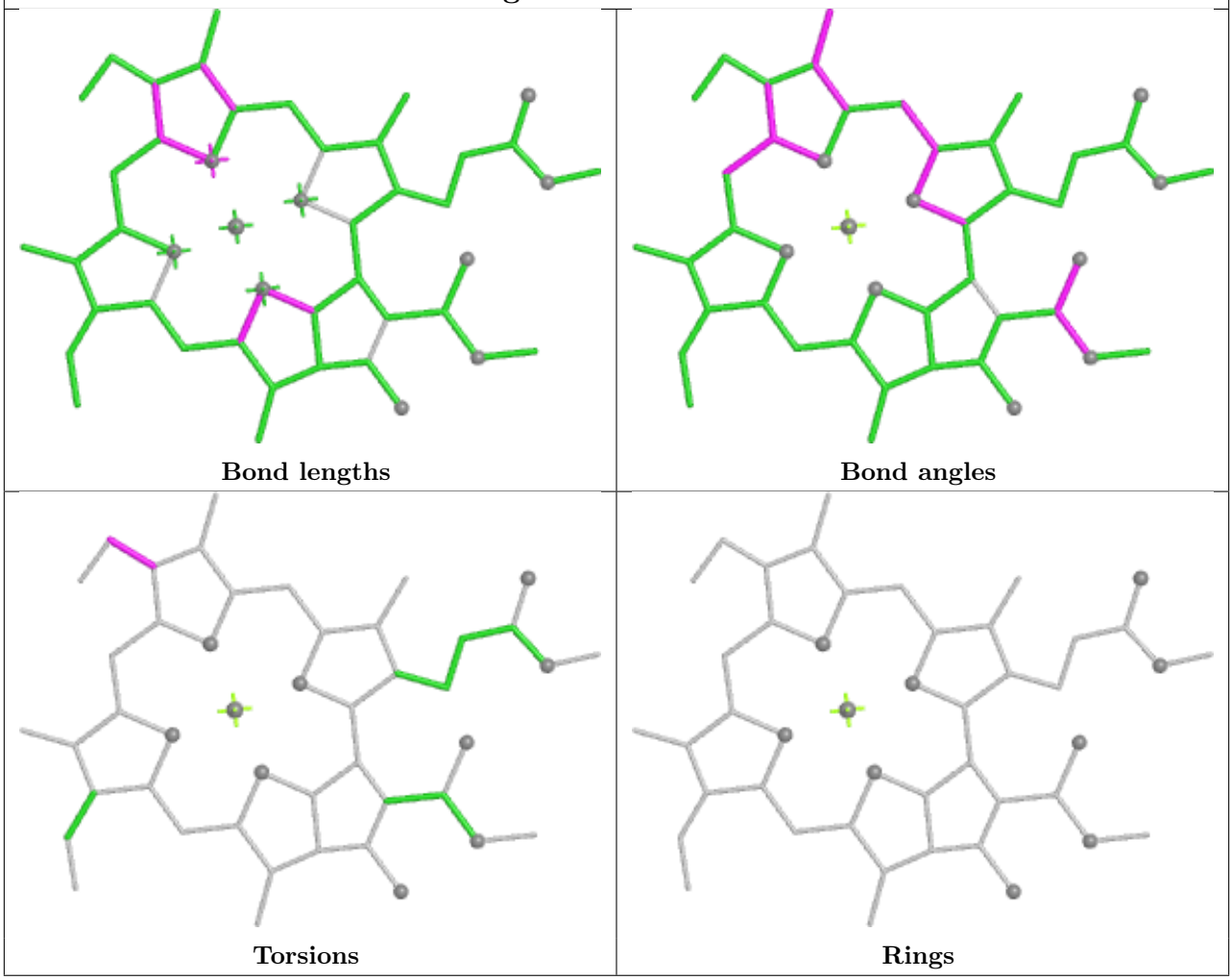
Continued on next page...

Continued from previous page...

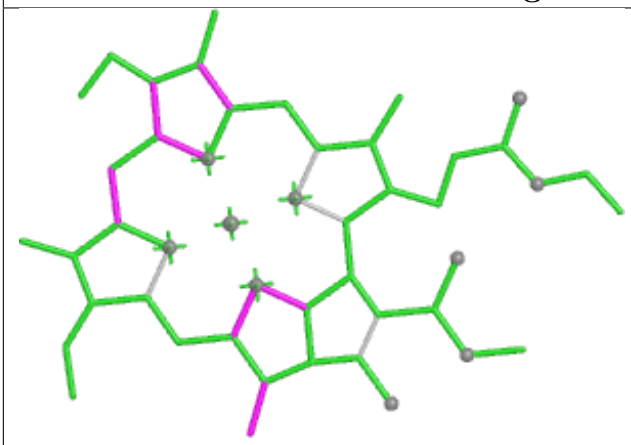
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	O	313	CLA	2	0
30	a	722	CLA	5	0
36	c	201	SF4	1	0

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

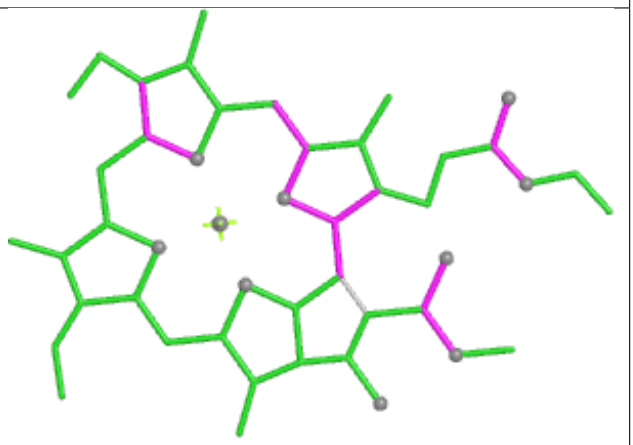
Ligand CLA K 307



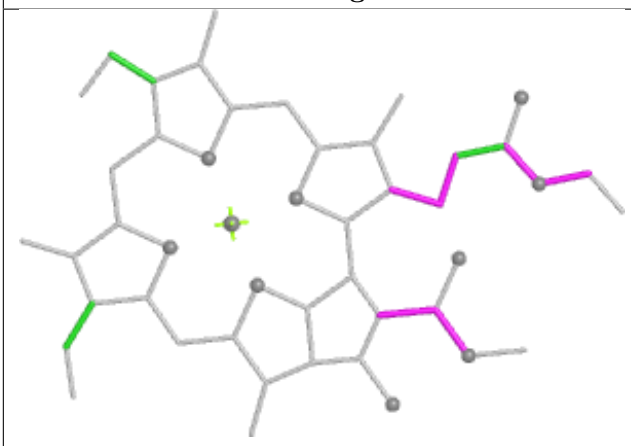
Ligand CLA O 314



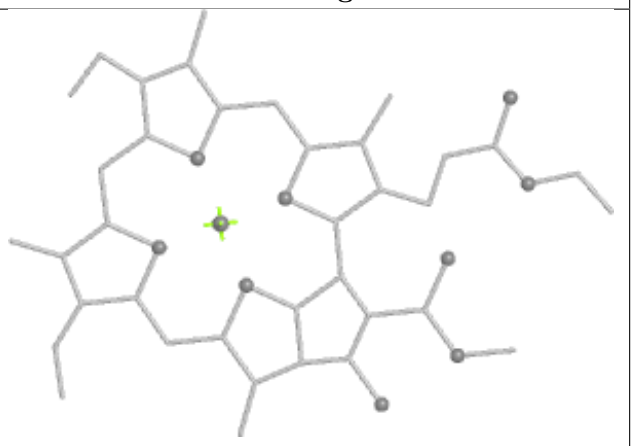
Bond lengths



Bond angles

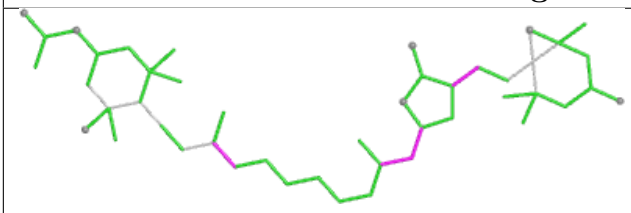


Torsions

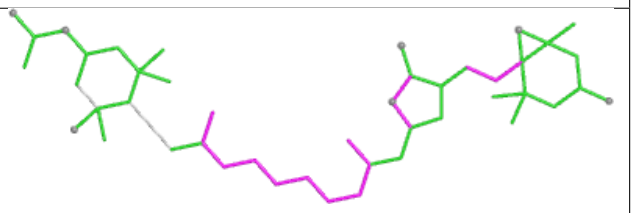


Rings

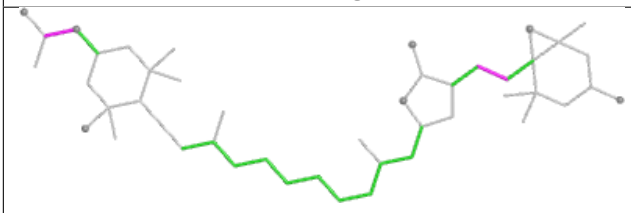
Ligand PID F 304



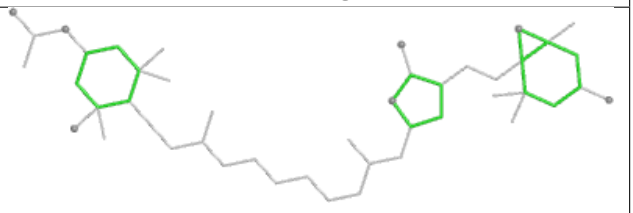
Bond lengths



Bond angles

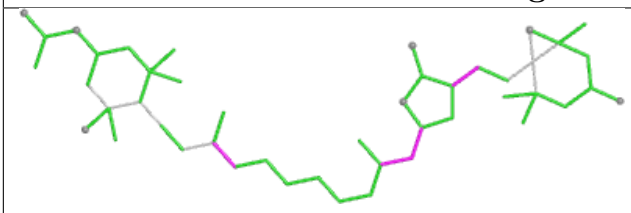


Torsions

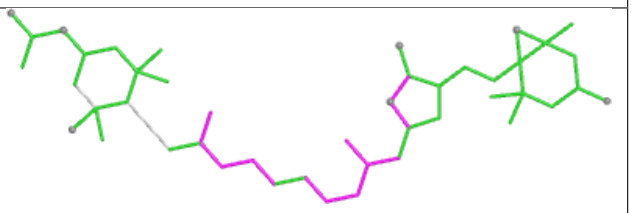


Rings

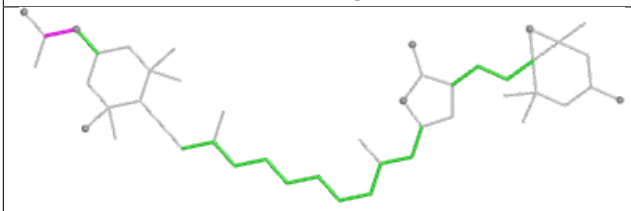
Ligand PID O 302



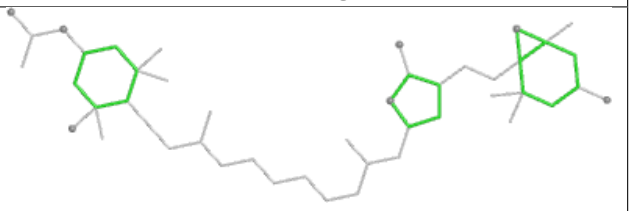
Bond lengths



Bond angles

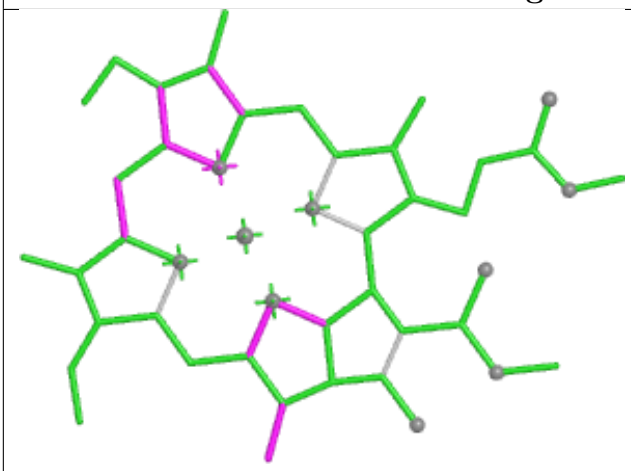


Torsions

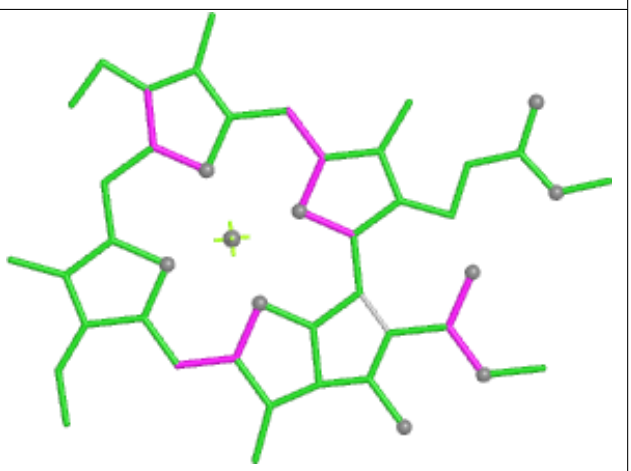


Rings

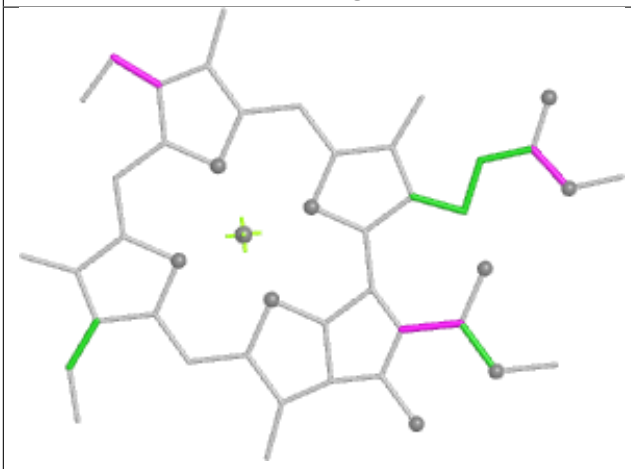
Ligand CLA F 307



Bond lengths



Bond angles

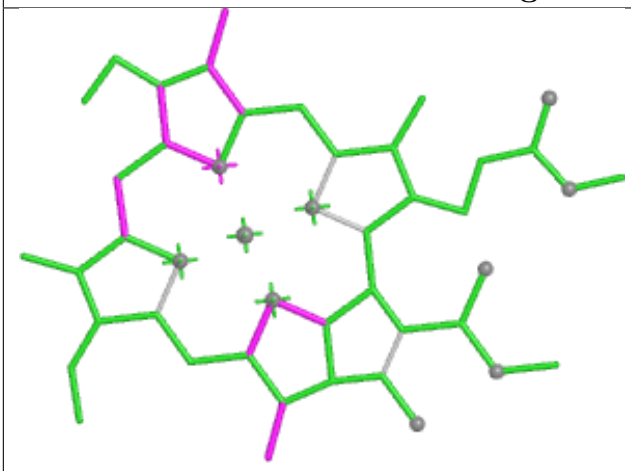


Torsions

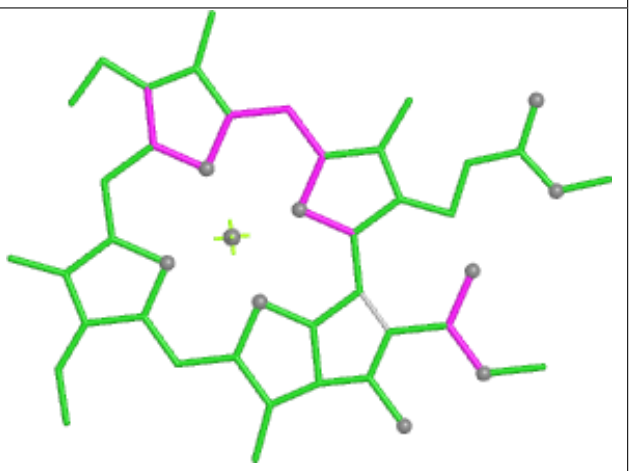


Rings

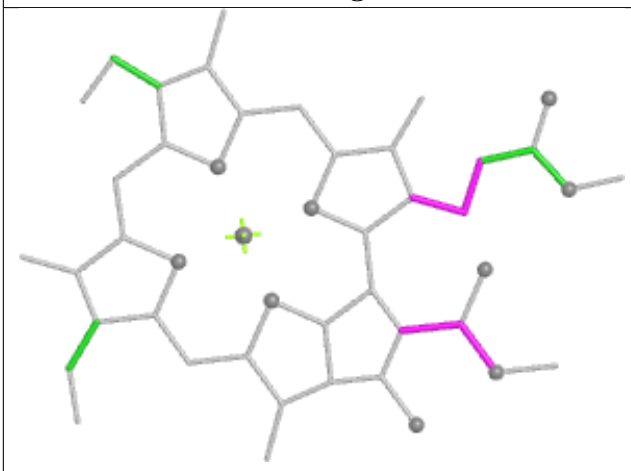
Ligand CLA M 311



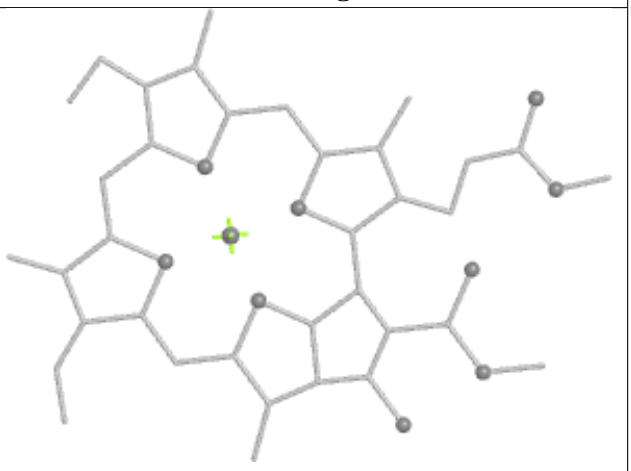
Bond lengths



Bond angles

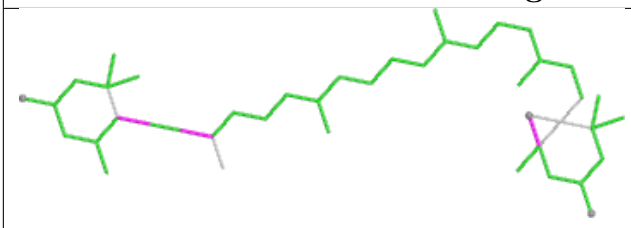


Torsions

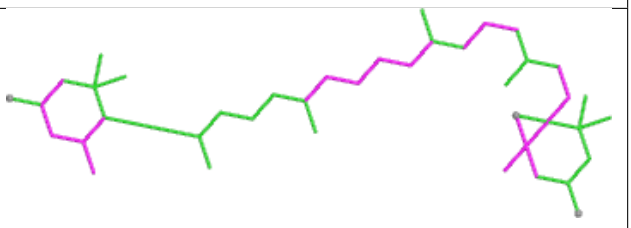


Rings

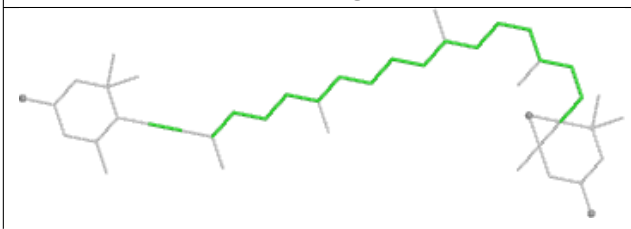
Ligand DD6 B 304



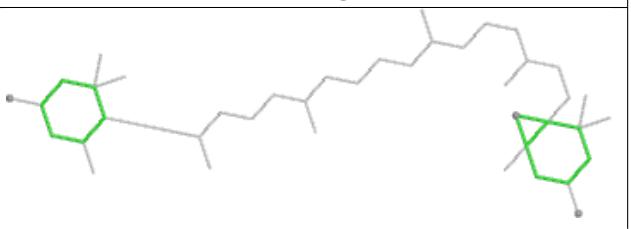
Bond lengths



Bond angles

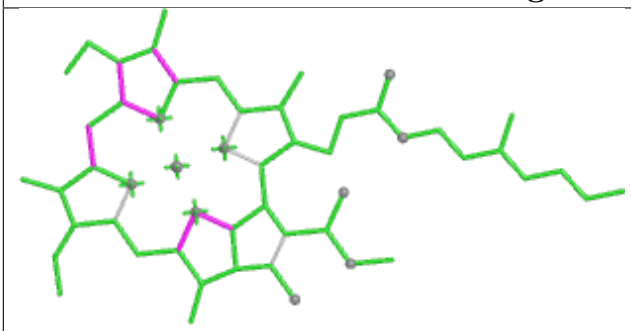


Torsions

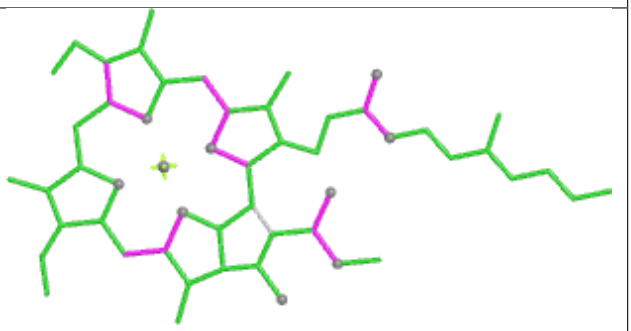


Rings

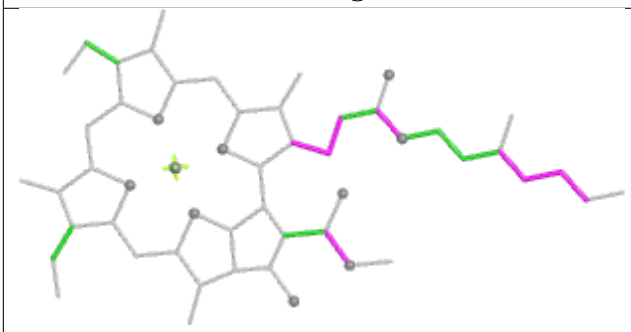
Ligand CLA b 720



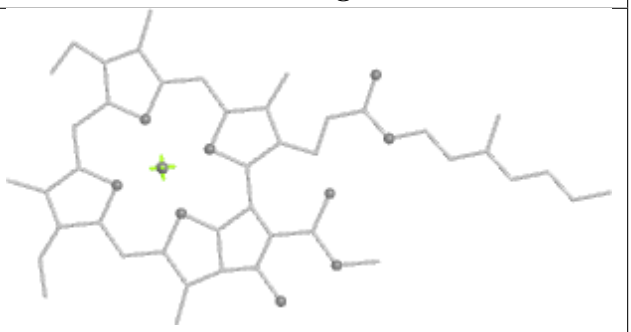
Bond lengths



Bond angles

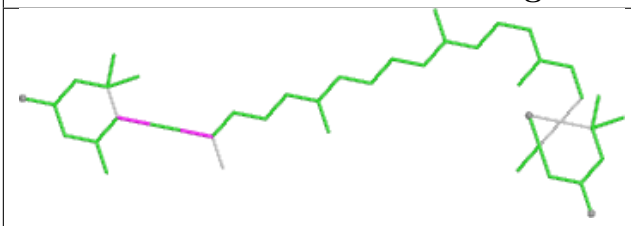


Torsions

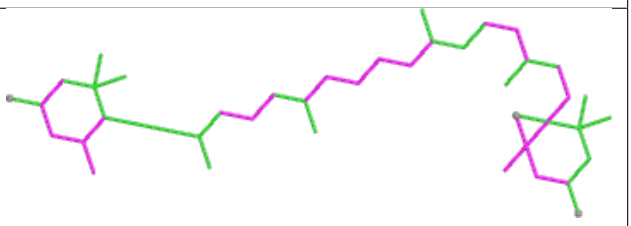


Rings

Ligand DD6 A 303



Bond lengths



Bond angles

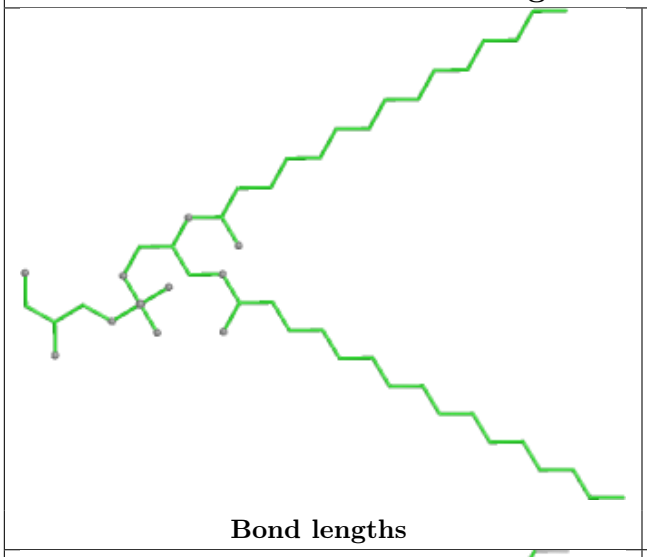


Torsions

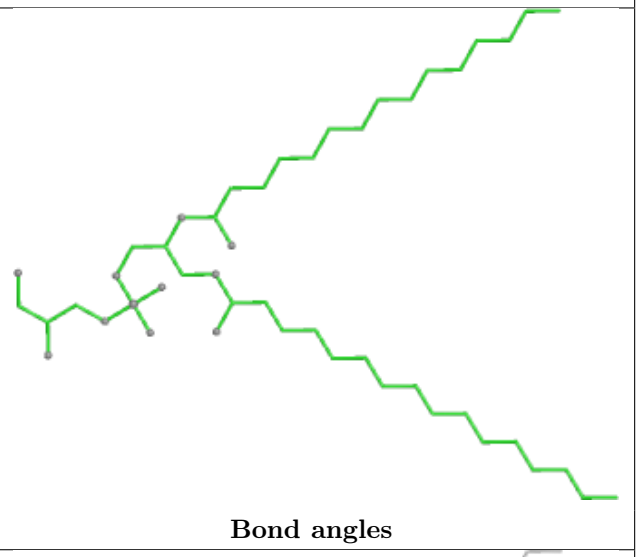


Rings

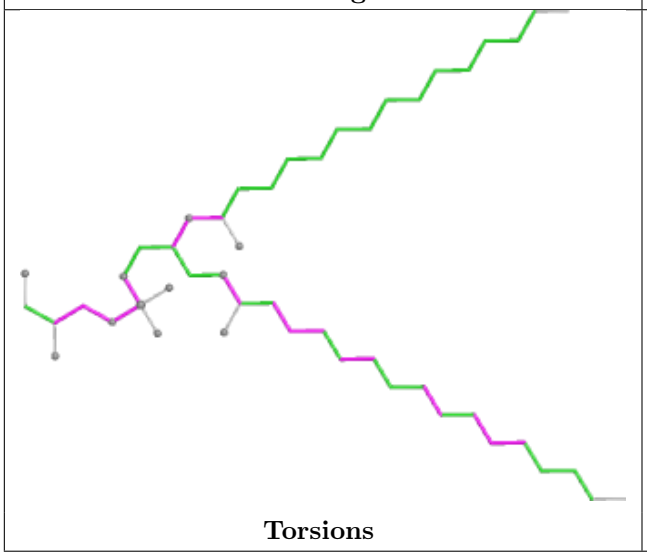
Ligand LHG a 733



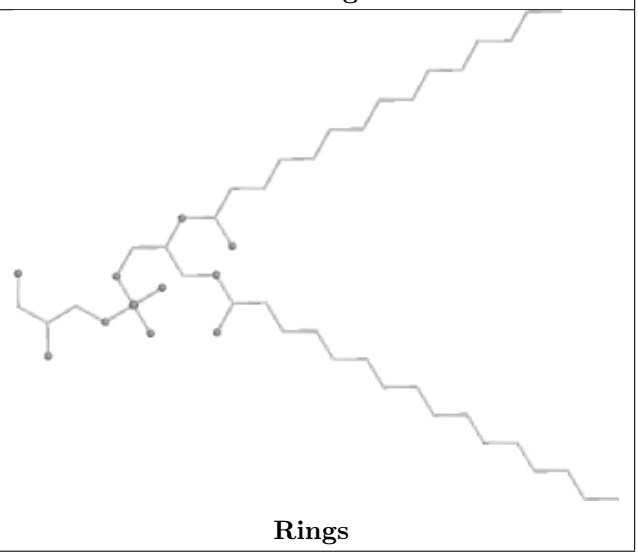
Bond lengths



Bond angles

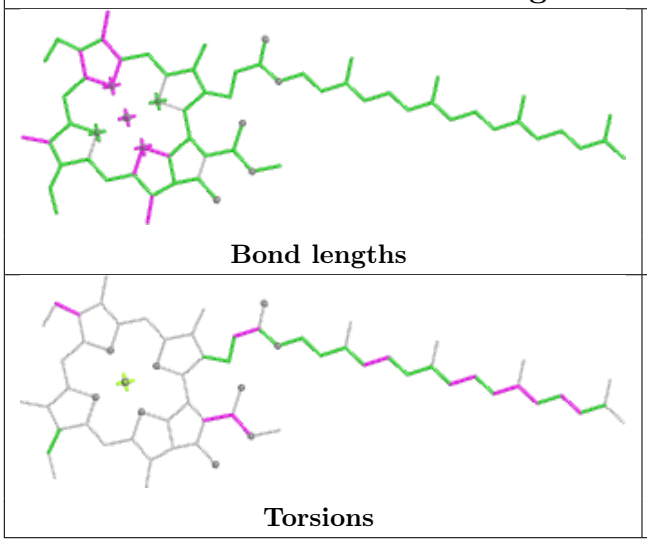


Torsions

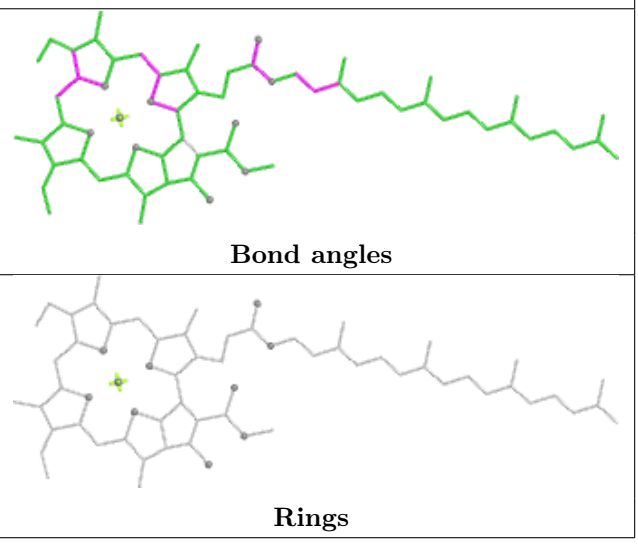


Rings

Ligand CLA a 702



Bond lengths

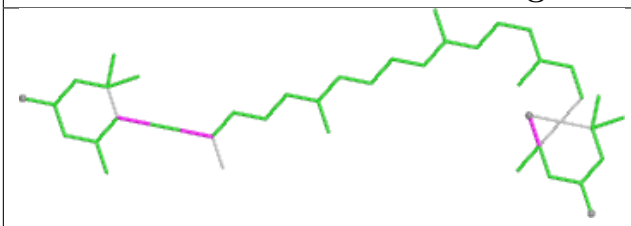


Bond angles

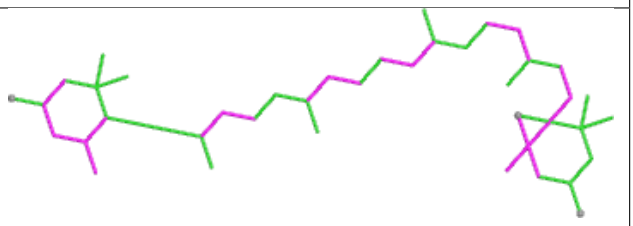
Torsions

Rings

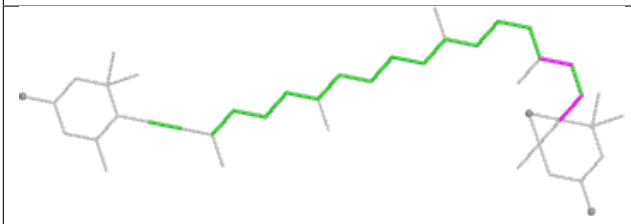
Ligand DD6 L 305



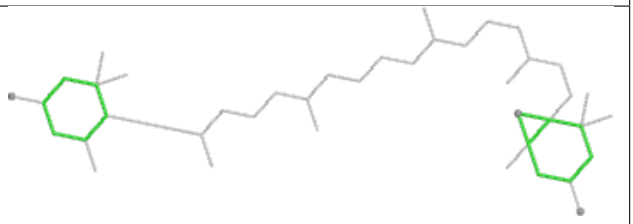
Bond lengths



Bond angles

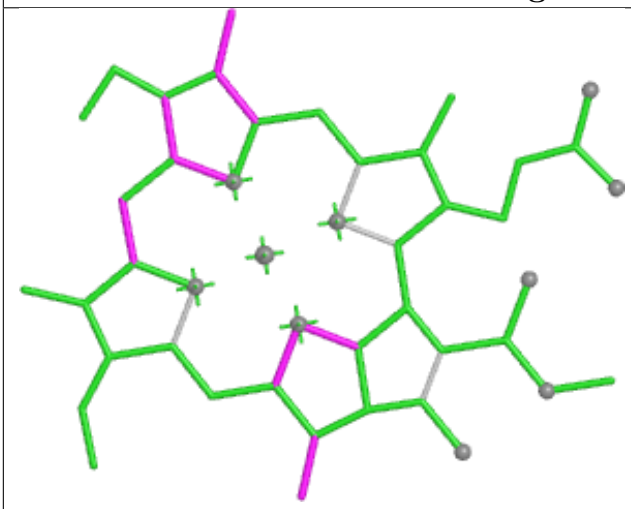


Torsions

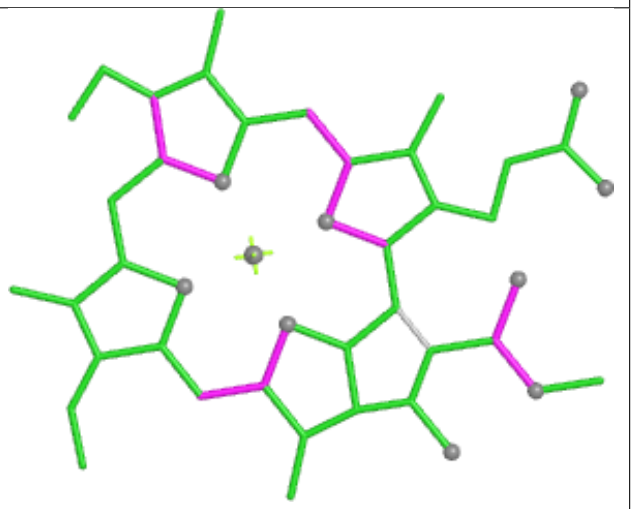


Rings

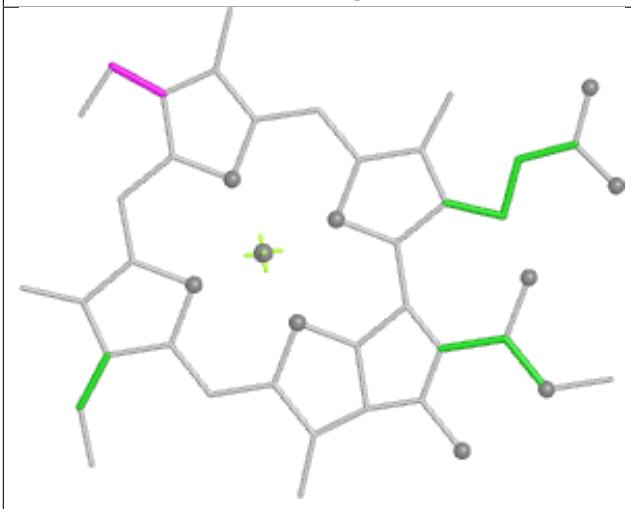
Ligand CLA a 701



Bond lengths



Bond angles

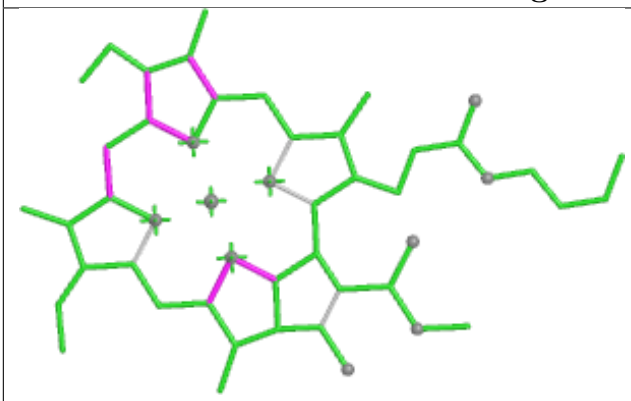


Torsions

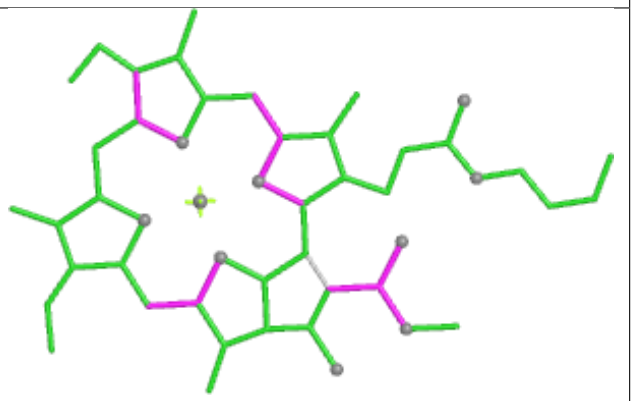


Rings

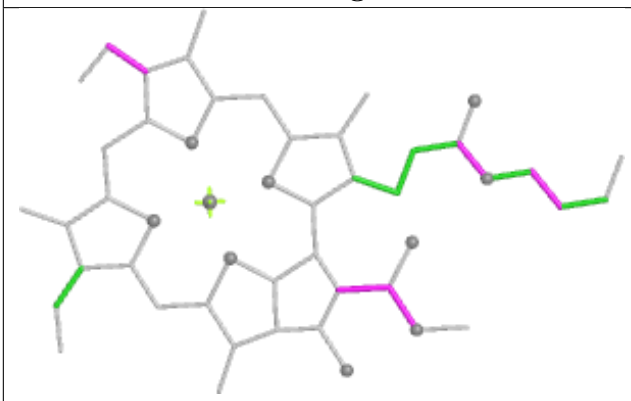
Ligand CLA I 306



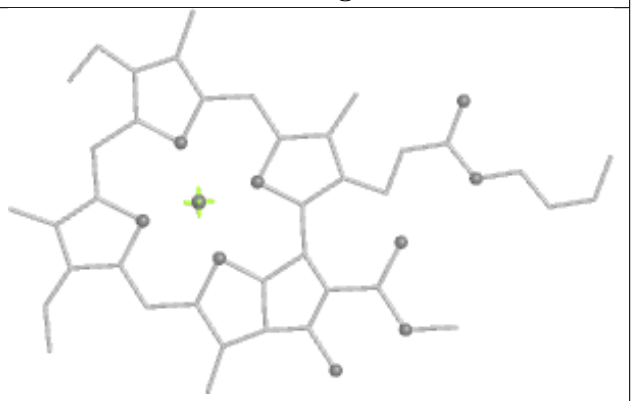
Bond lengths



Bond angles

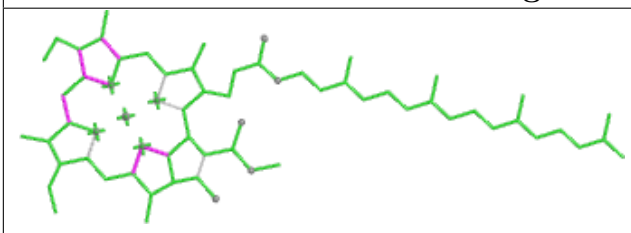


Torsions

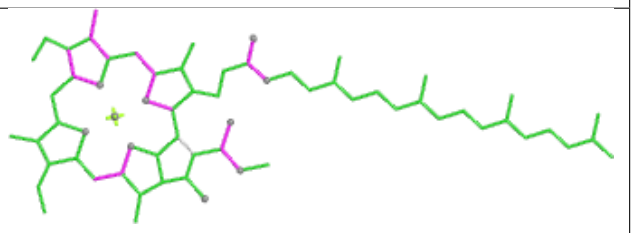


Rings

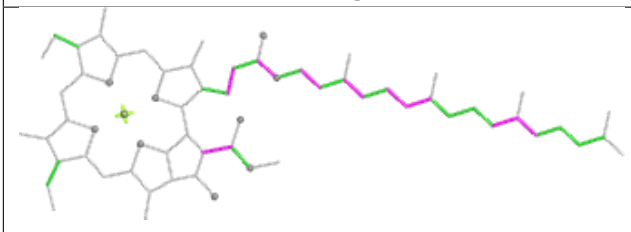
Ligand CLA G 510



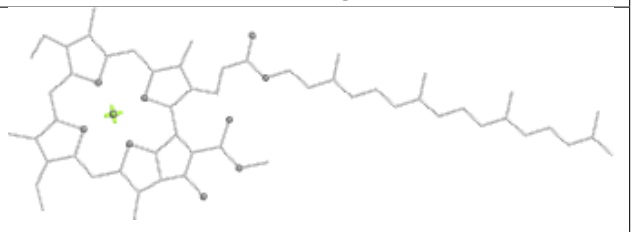
Bond lengths



Bond angles

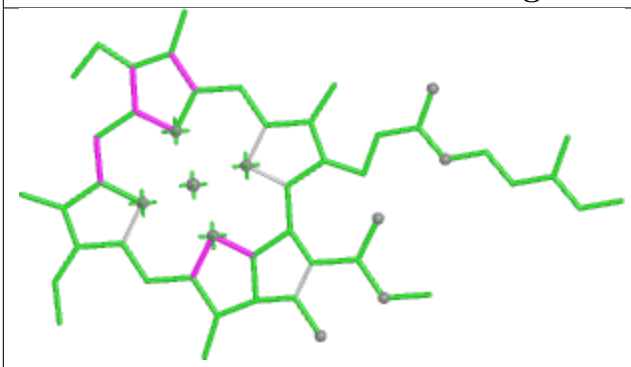


Torsions

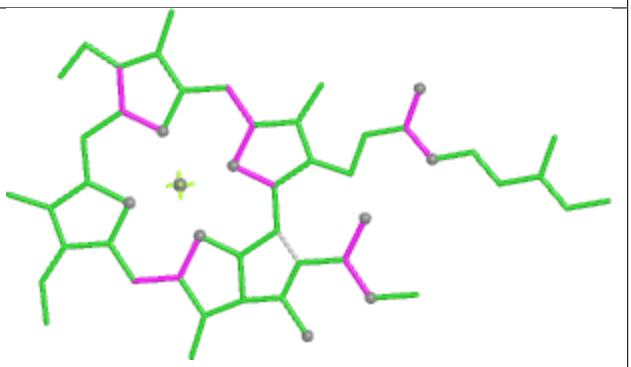


Rings

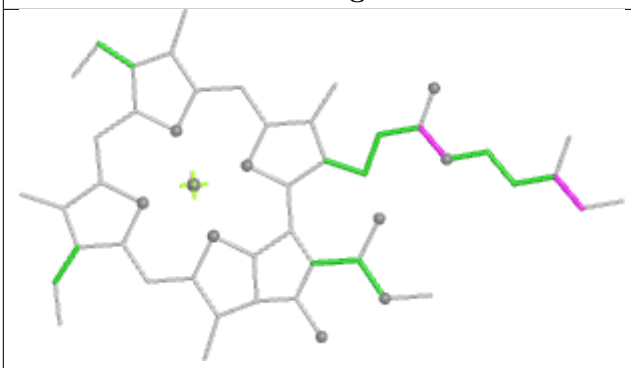
Ligand CLA G 509



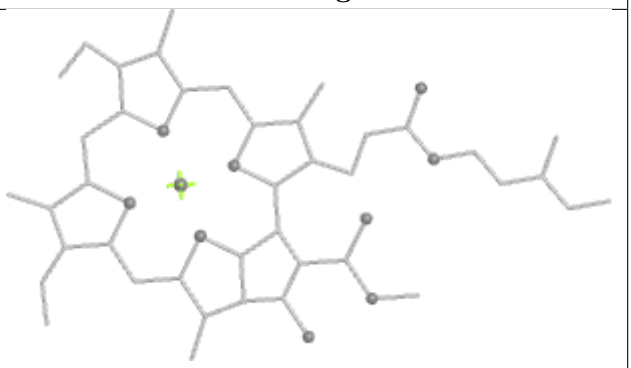
Bond lengths



Bond angles

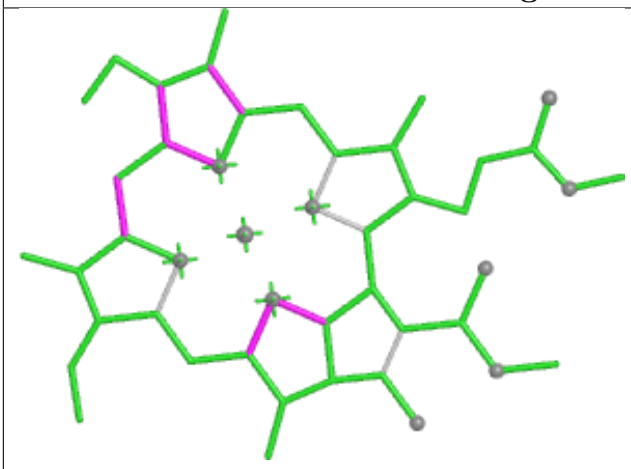


Torsions

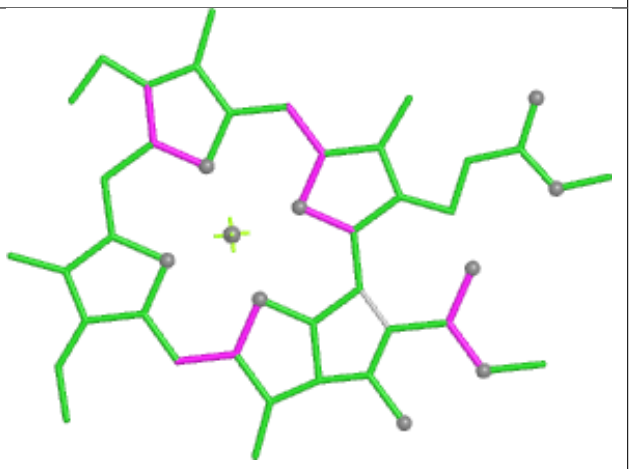


Rings

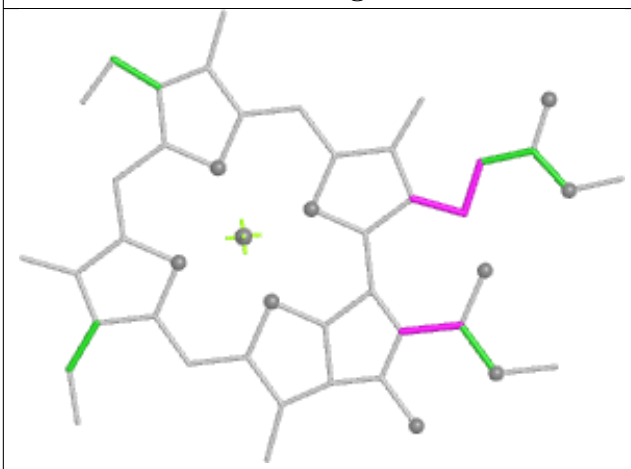
Ligand CLA M 313



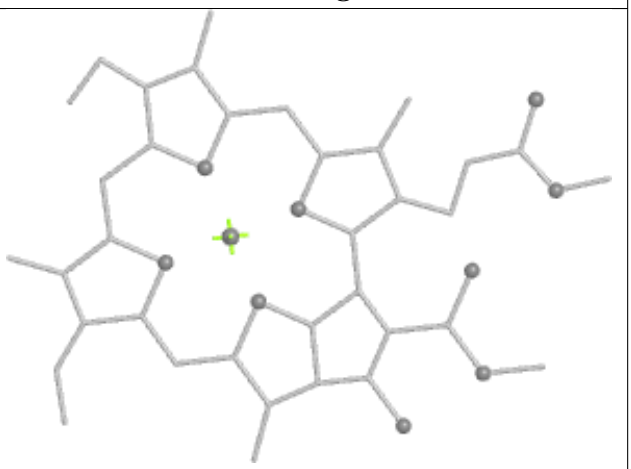
Bond lengths



Bond angles

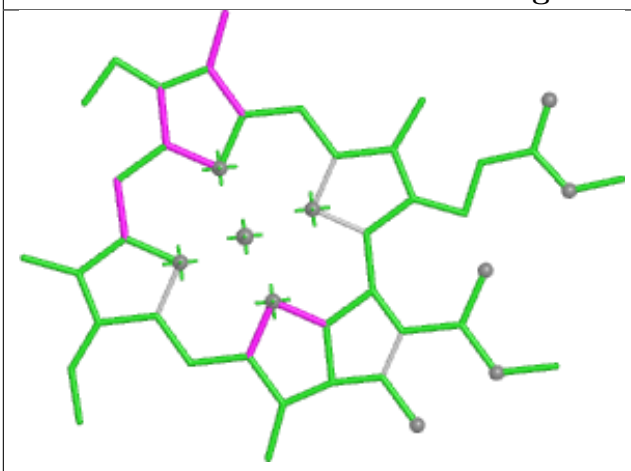


Torsions

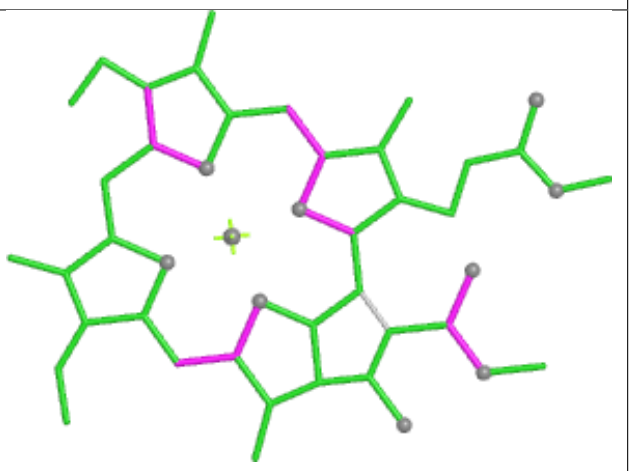


Rings

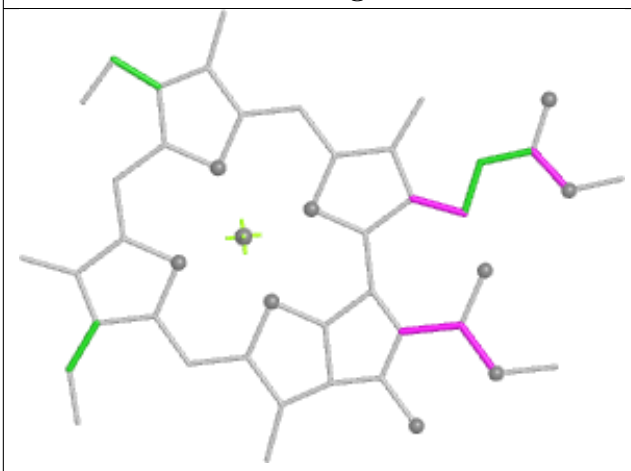
Ligand CLA l 312



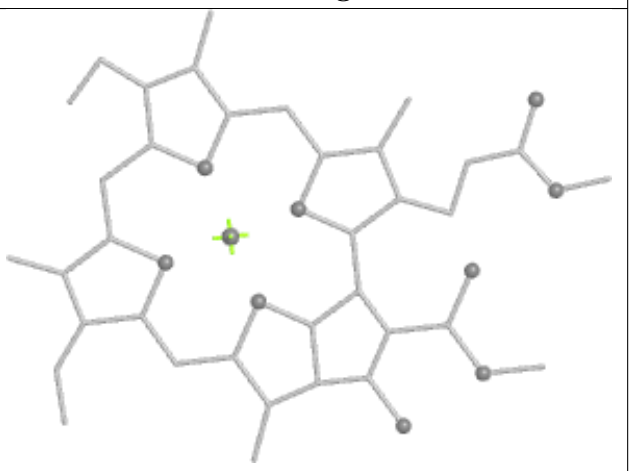
Bond lengths



Bond angles

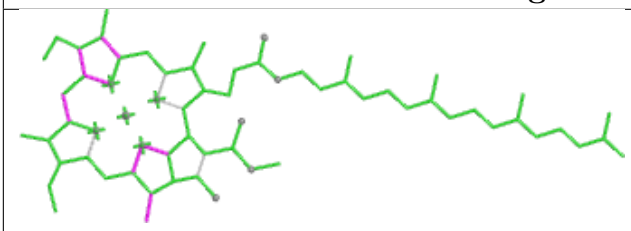


Torsions

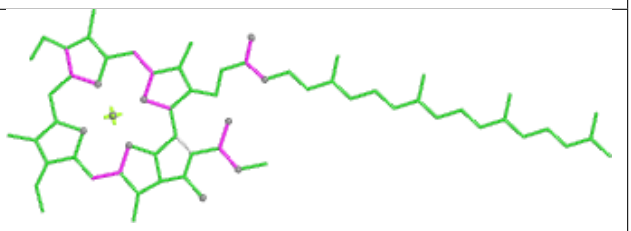


Rings

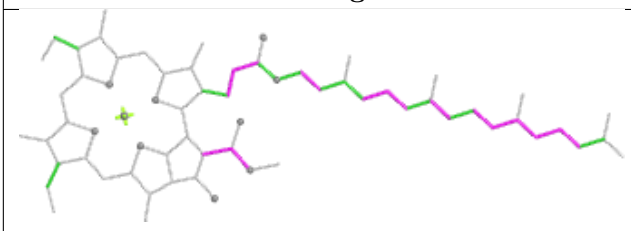
Ligand CLA a 723



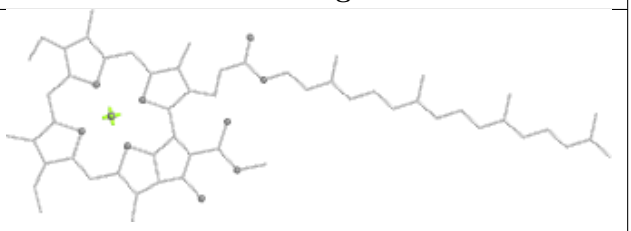
Bond lengths



Bond angles

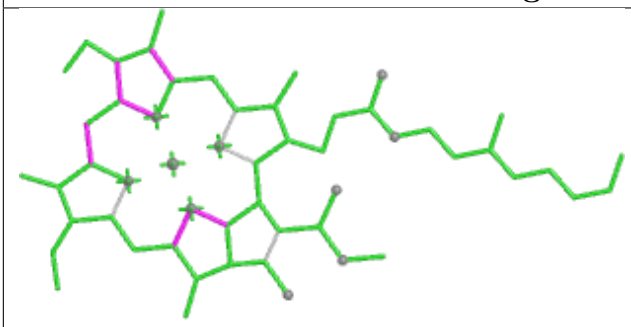


Torsions

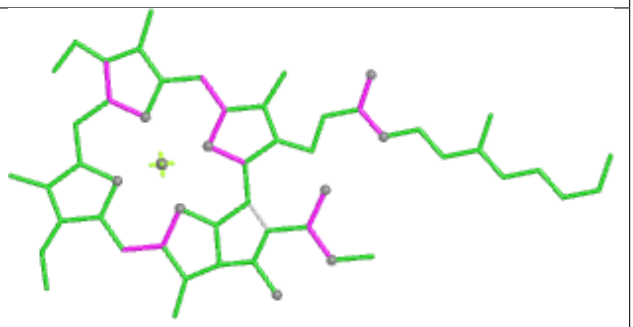


Rings

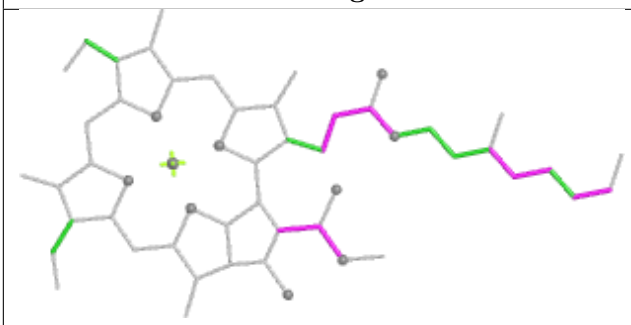
Ligand CLA K 308



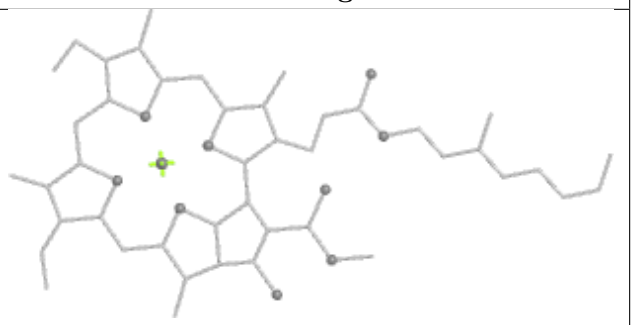
Bond lengths



Bond angles

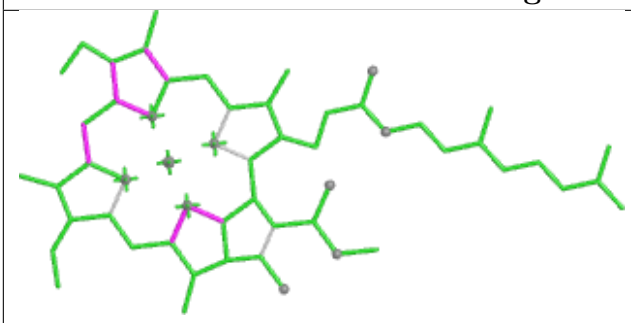


Torsions

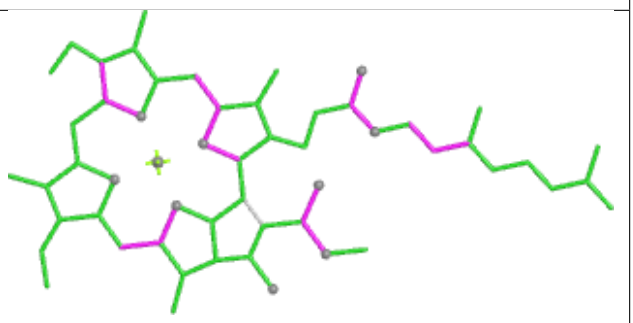


Rings

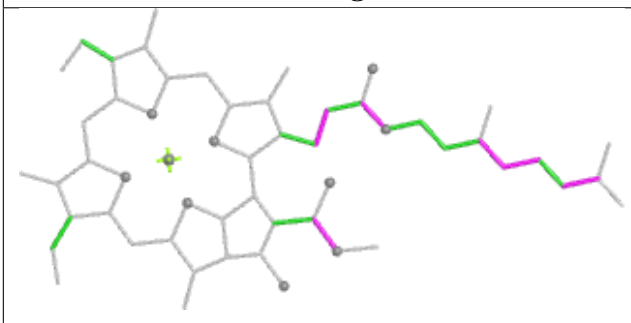
Ligand CLA A 313



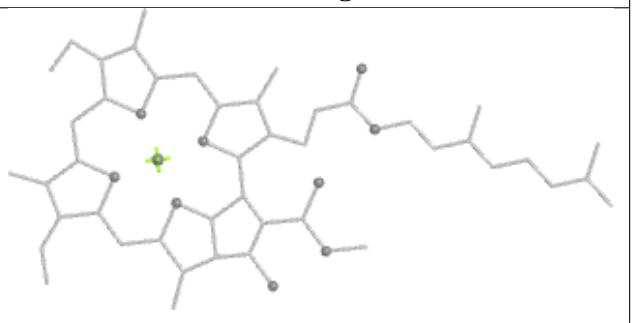
Bond lengths



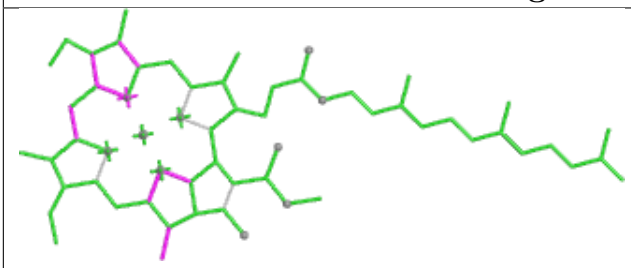
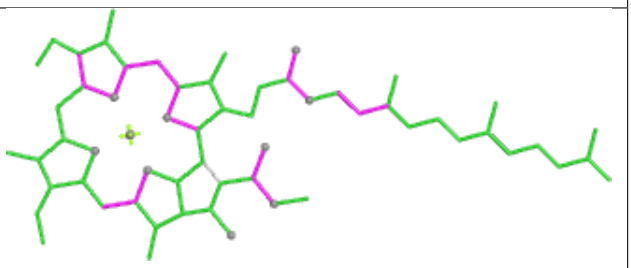
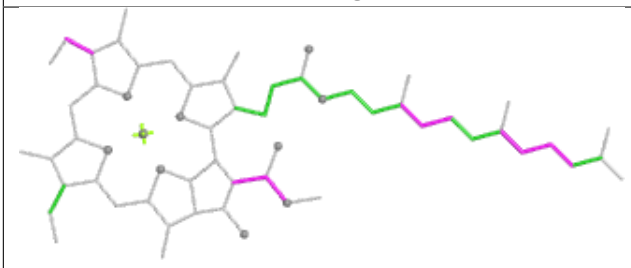
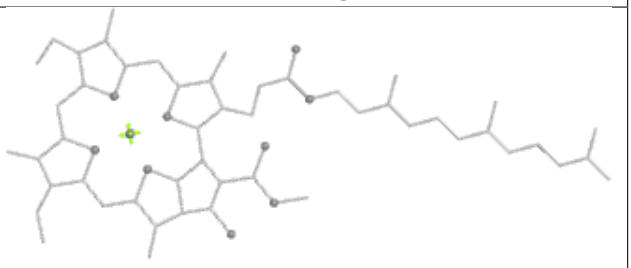
Bond angles

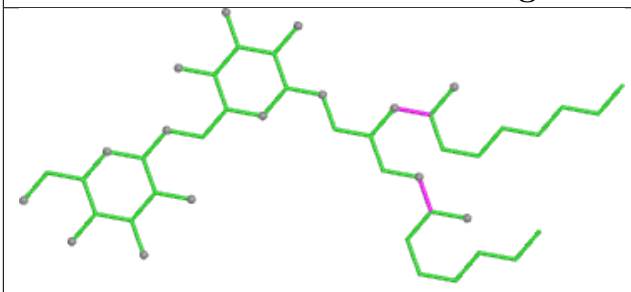
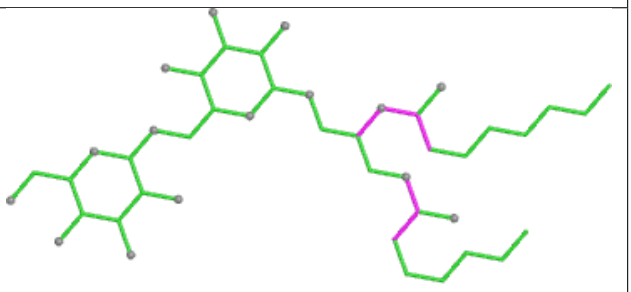
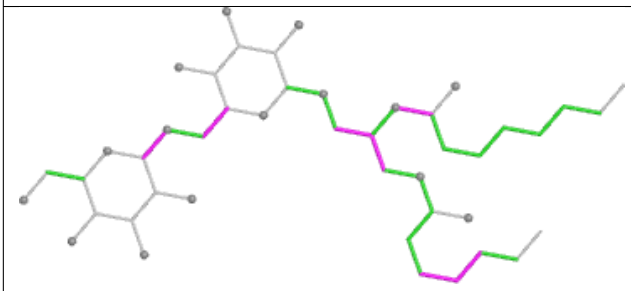
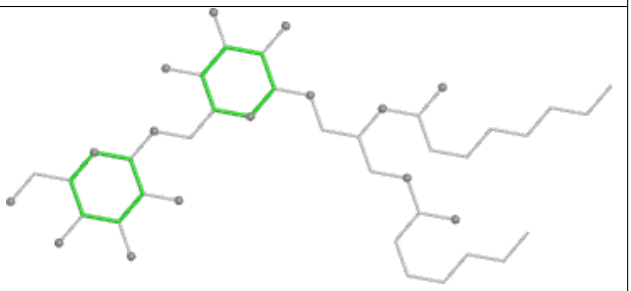


Torsions

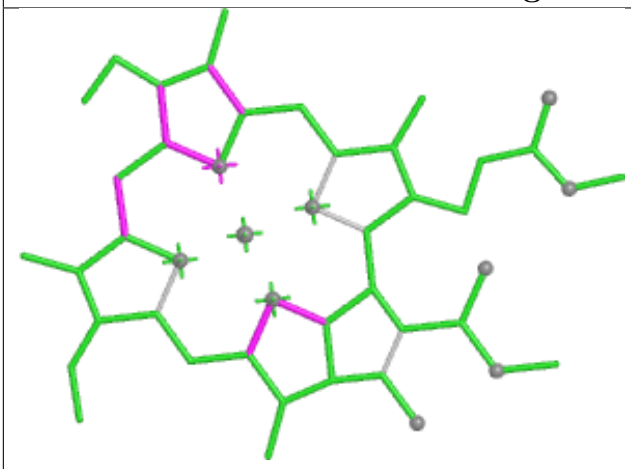


Rings

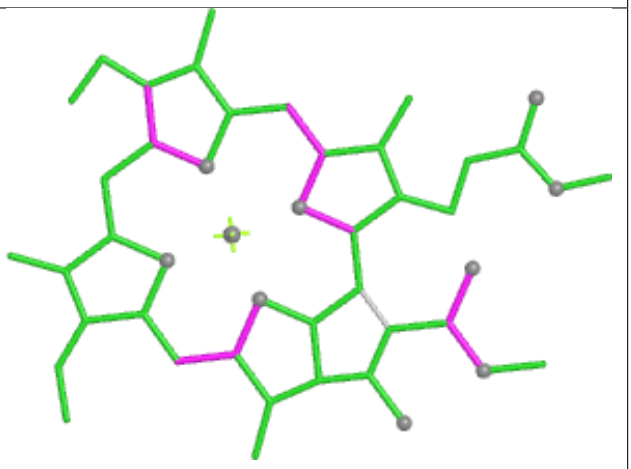
Ligand CLA a 713	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD G 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

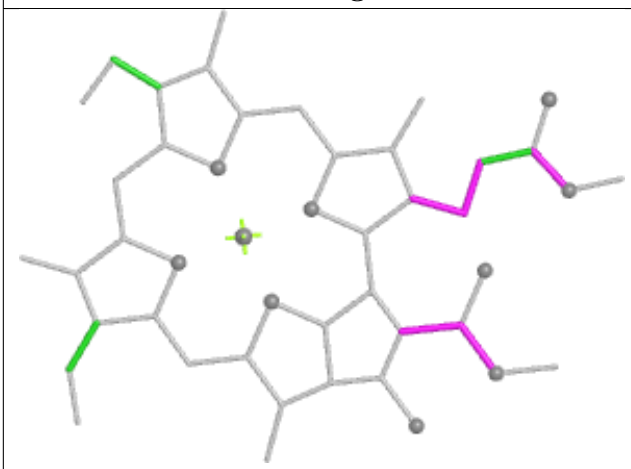
Ligand CLA H 312



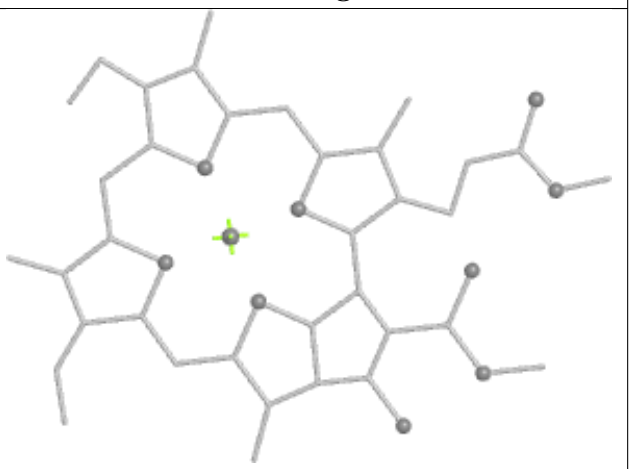
Bond lengths



Bond angles

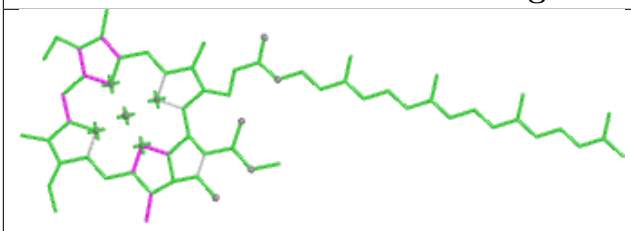


Torsions

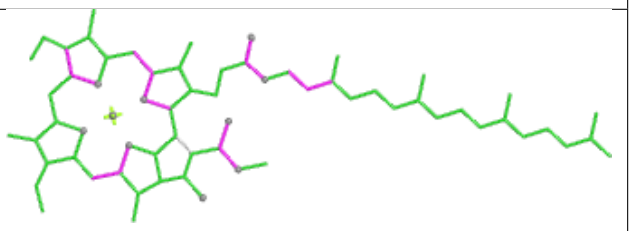


Rings

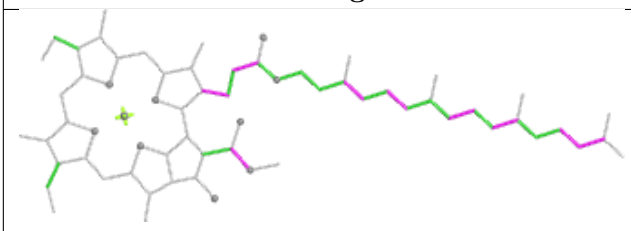
Ligand CLA a 731



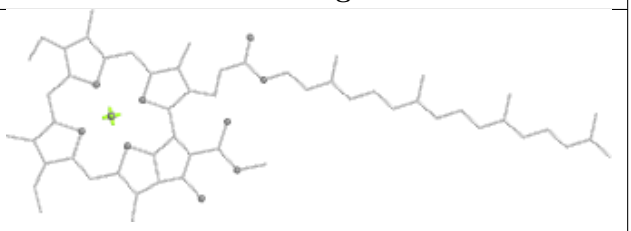
Bond lengths



Bond angles

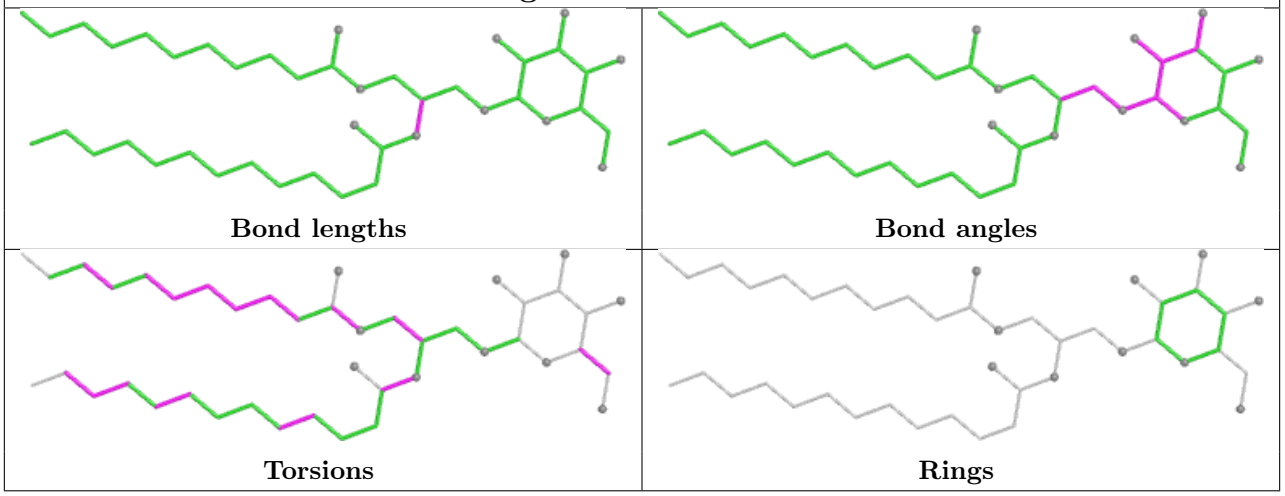


Torsions

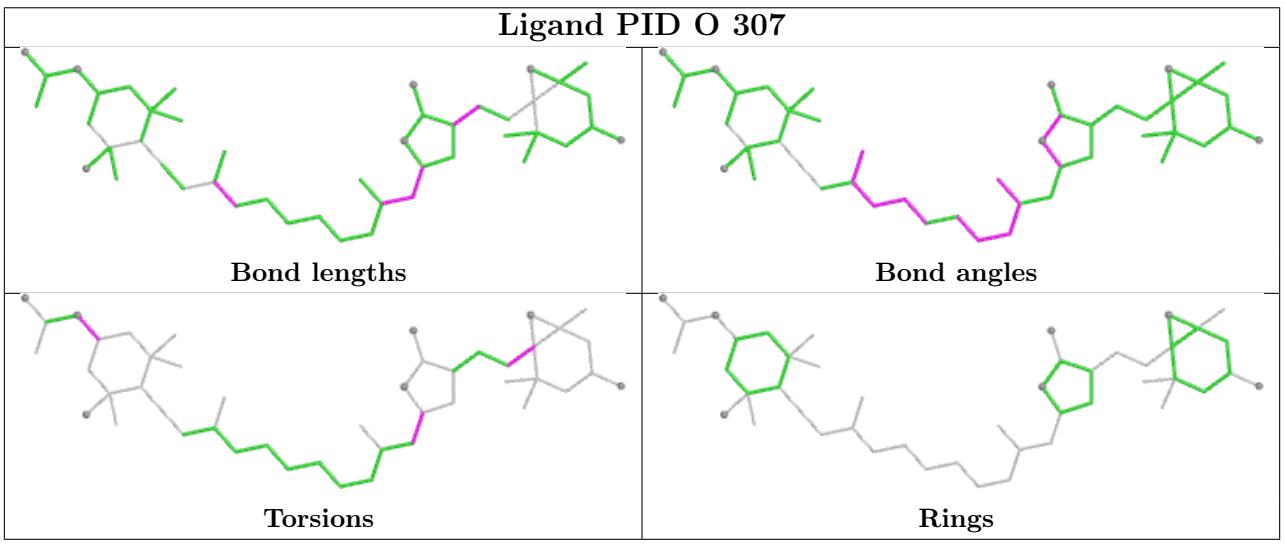


Rings

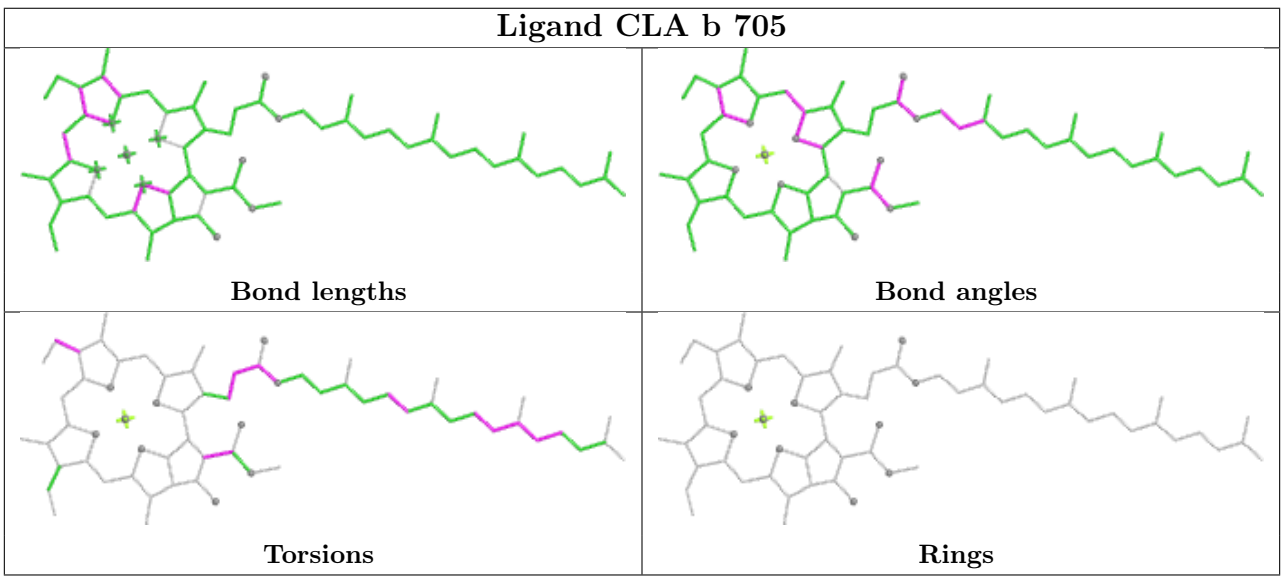
Ligand LMG K 317



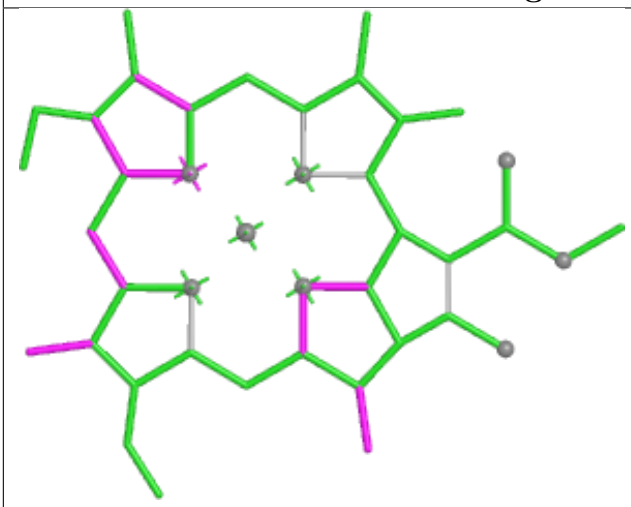
Ligand PID O 307



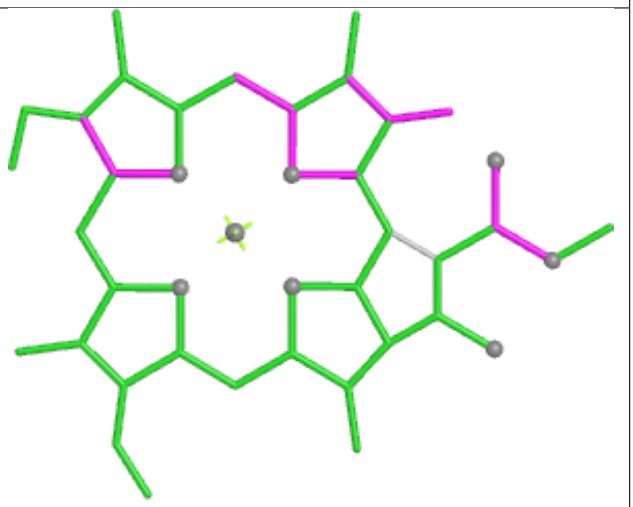
Ligand CLA b 705



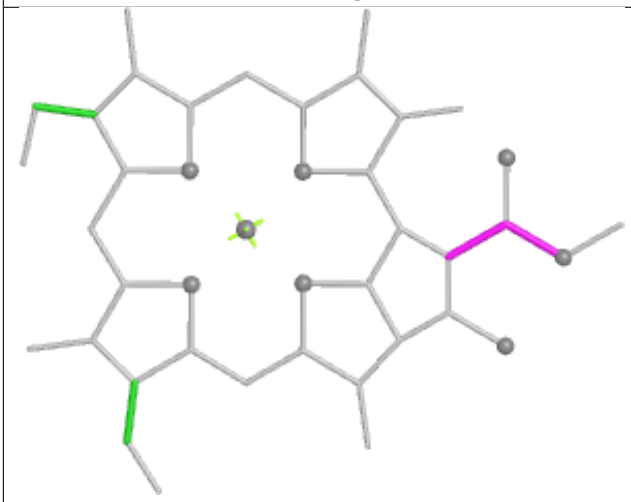
Ligand CLA P 217



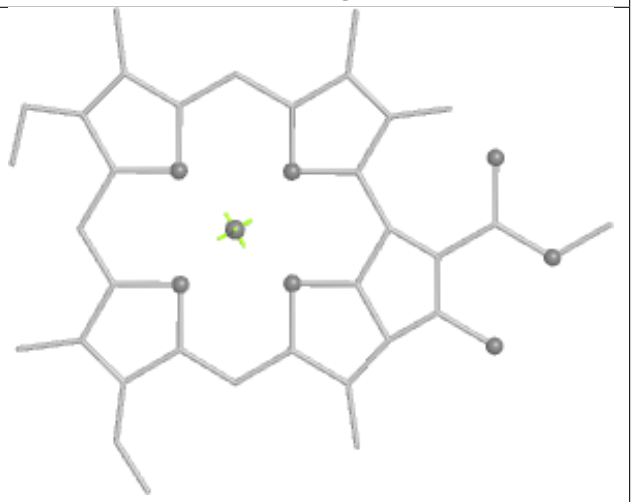
Bond lengths



Bond angles

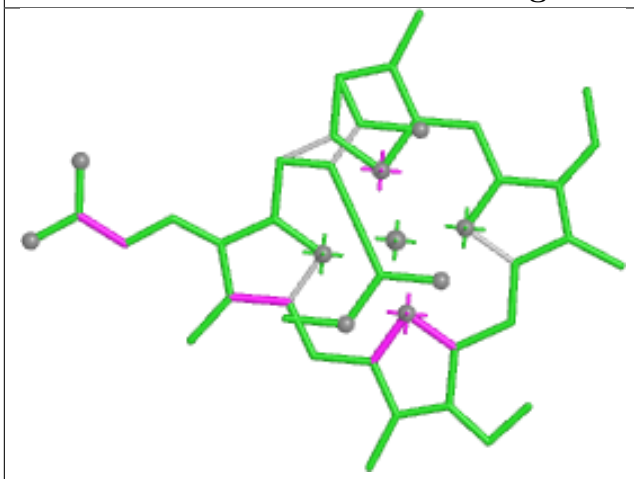


Torsions

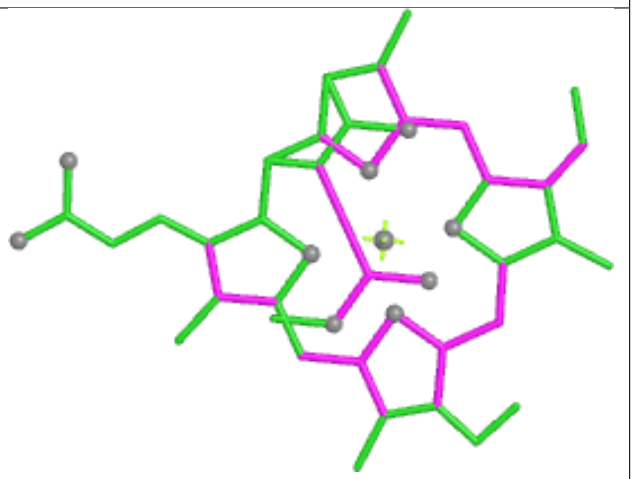


Rings

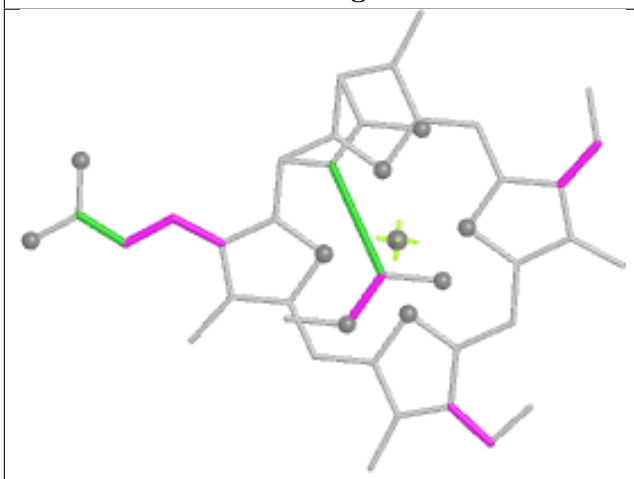
Ligand KC1 L 315



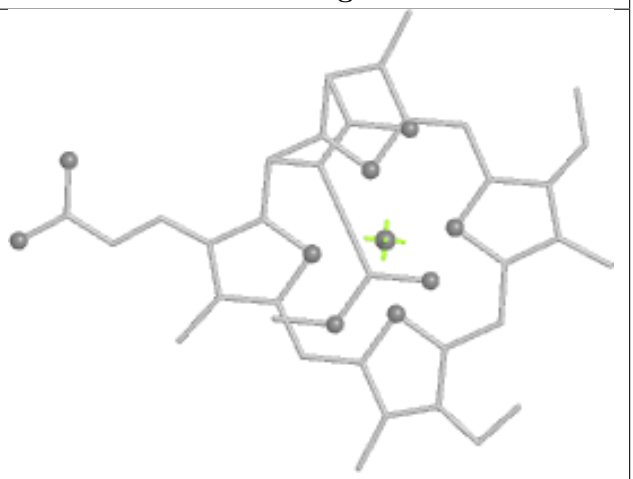
Bond lengths



Bond angles

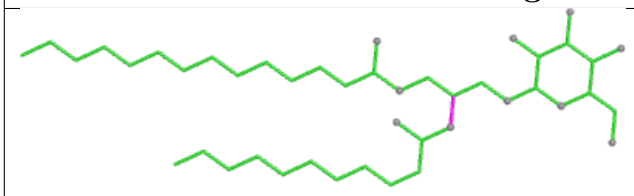


Torsions



Rings

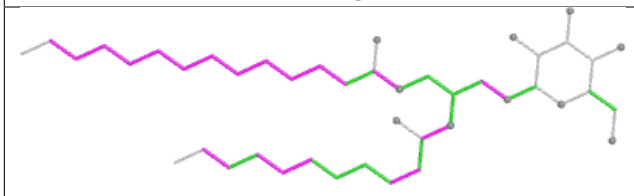
Ligand LMG b 733



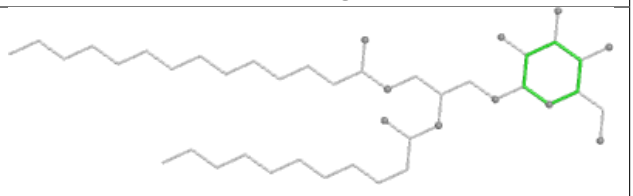
Bond lengths



Bond angles

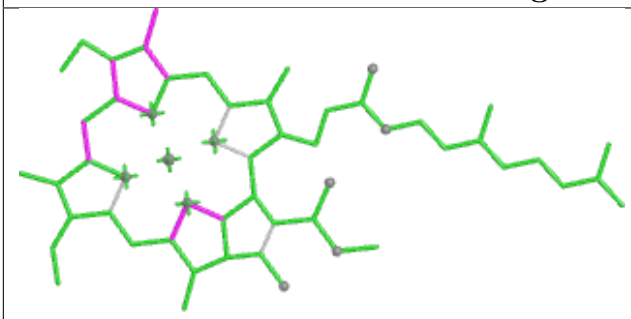


Torsions

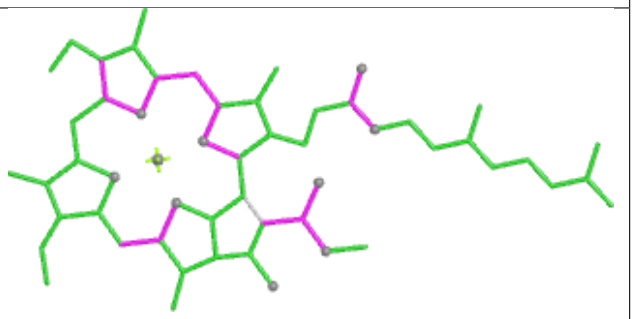


Rings

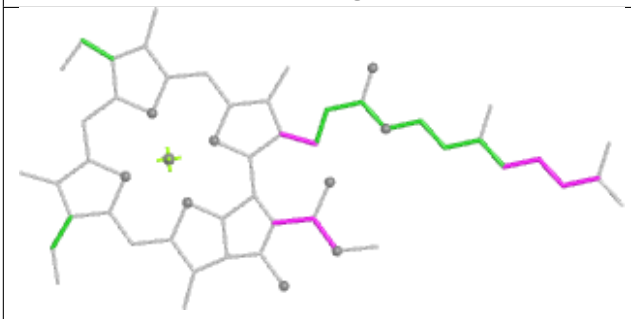
Ligand CLA I 311



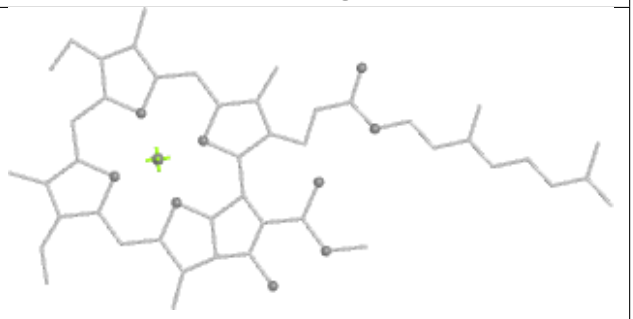
Bond lengths



Bond angles

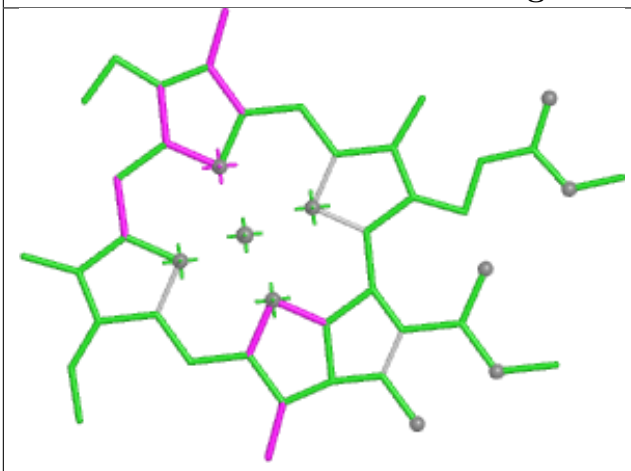


Torsions

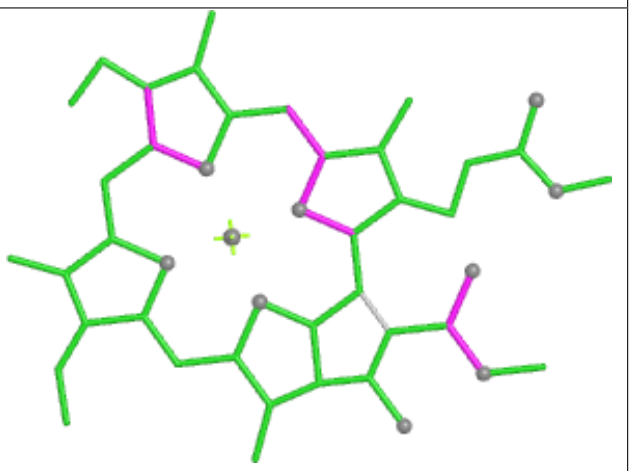


Rings

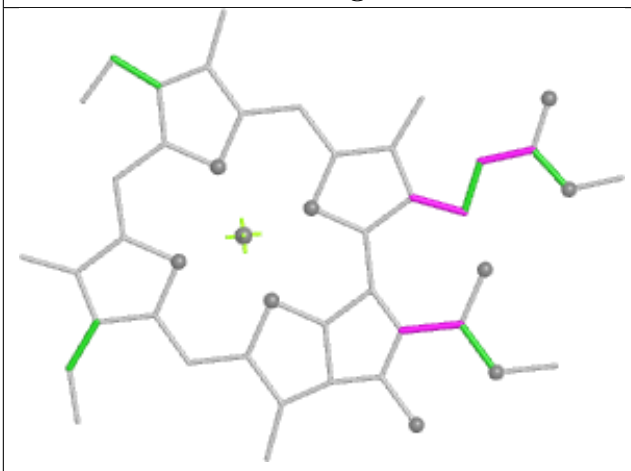
Ligand CLA b 721



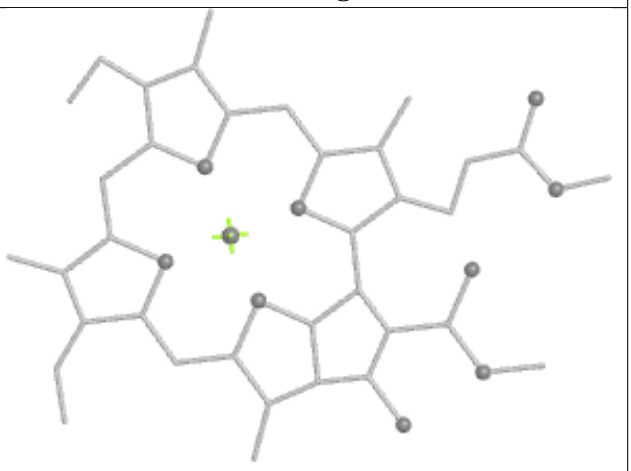
Bond lengths



Bond angles

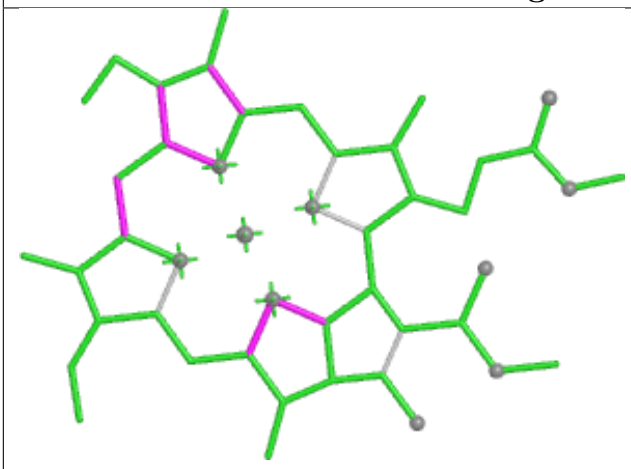


Torsions

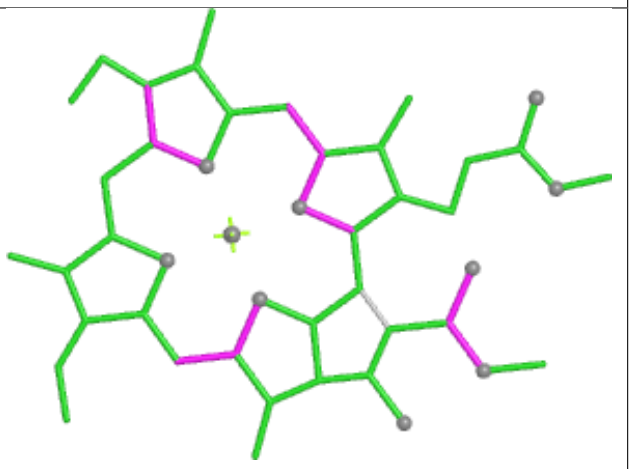


Rings

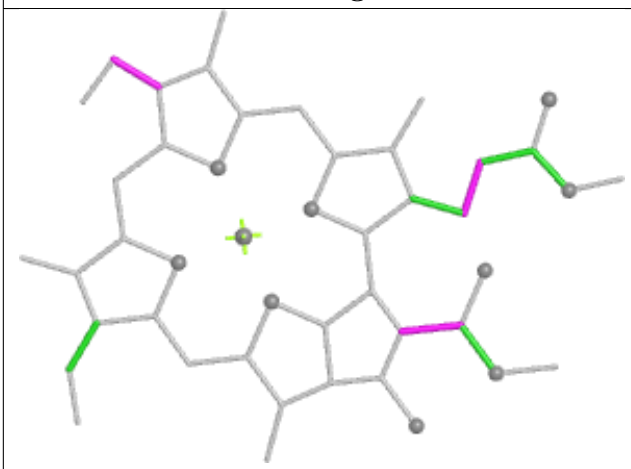
Ligand CLA J 316



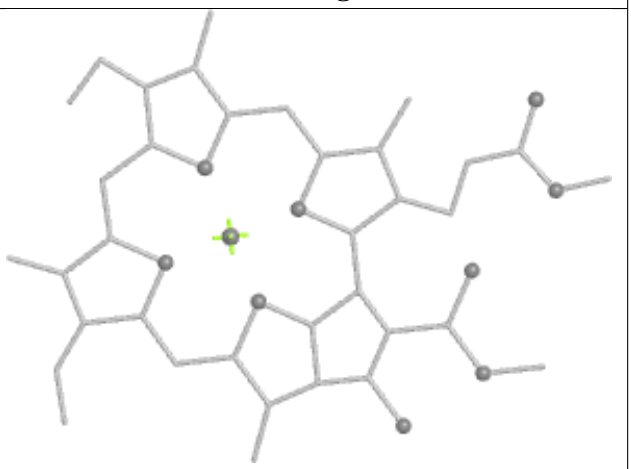
Bond lengths



Bond angles

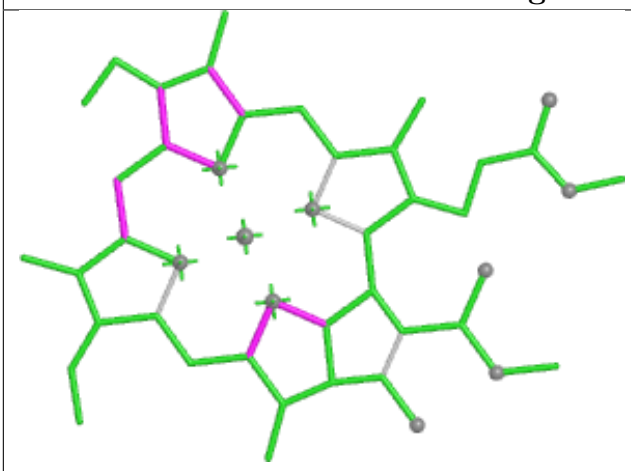


Torsions

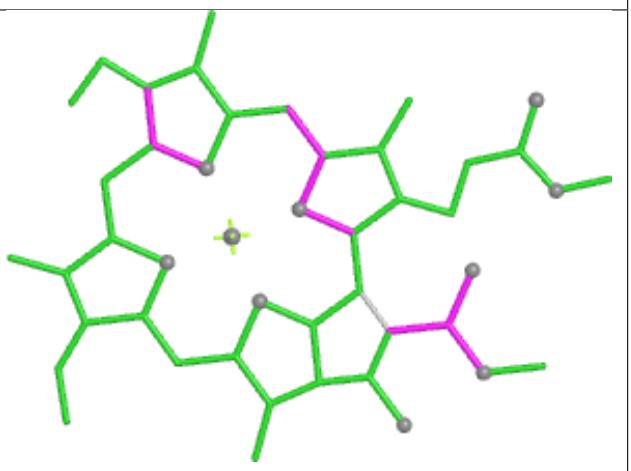


Rings

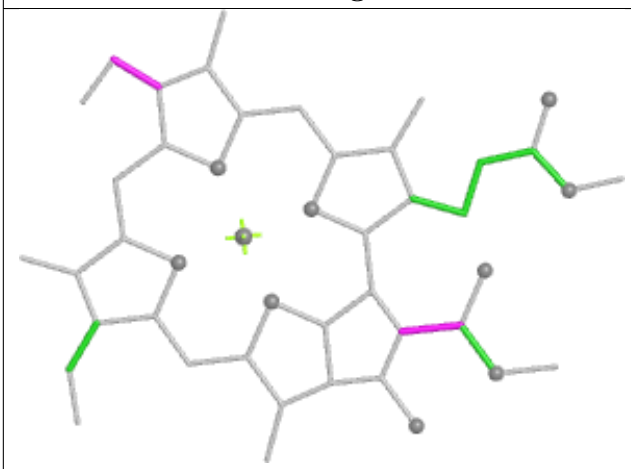
Ligand CLA a 738



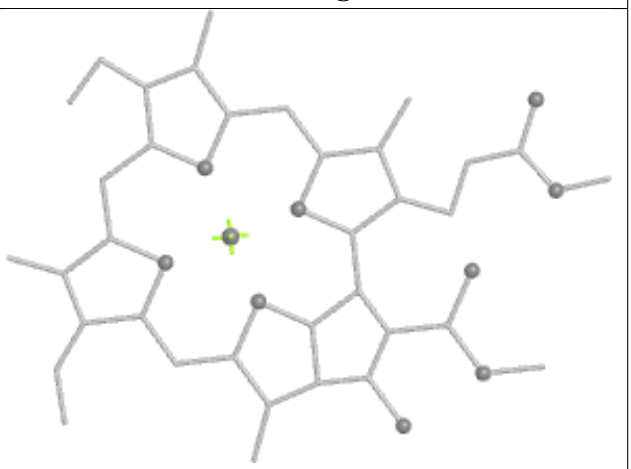
Bond lengths



Bond angles

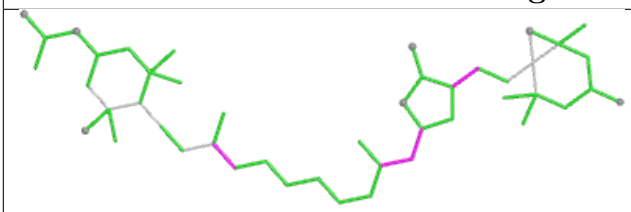


Torsions

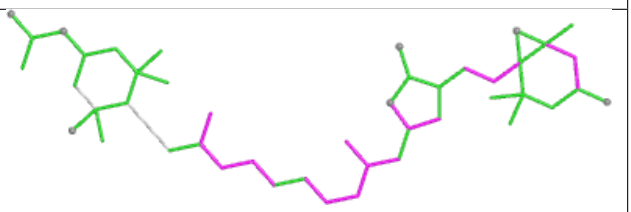


Rings

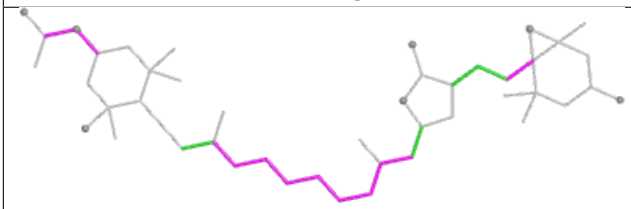
Ligand PID O 305



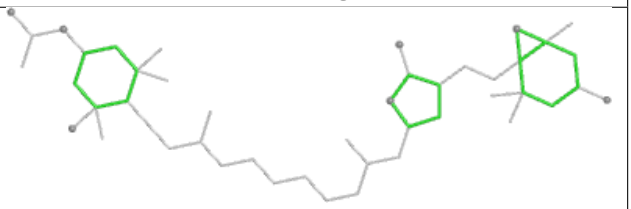
Bond lengths



Bond angles

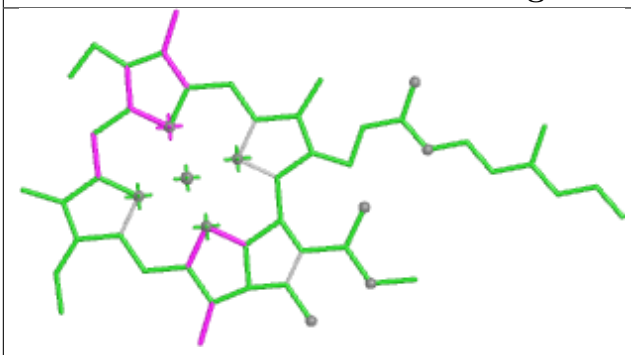


Torsions

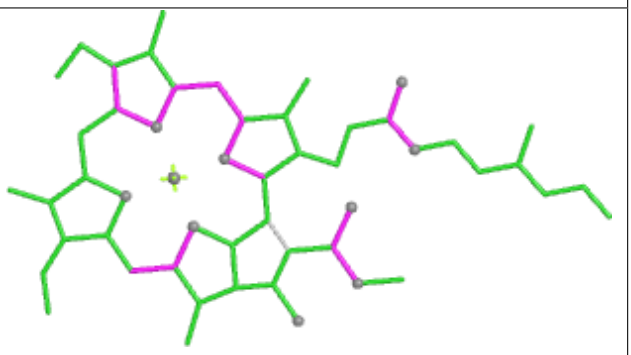


Rings

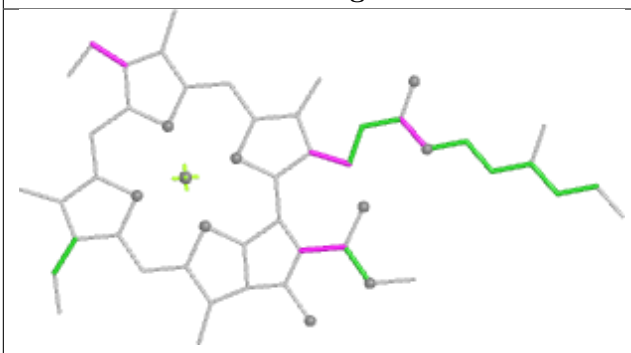
Ligand CLA b 710



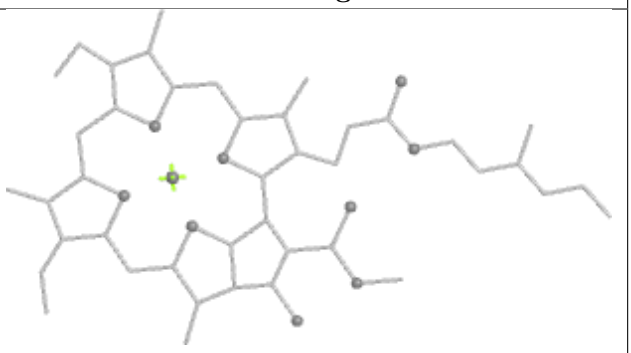
Bond lengths



Bond angles

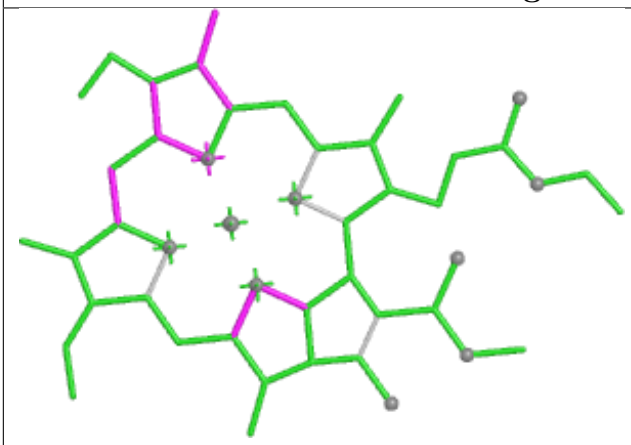


Torsions

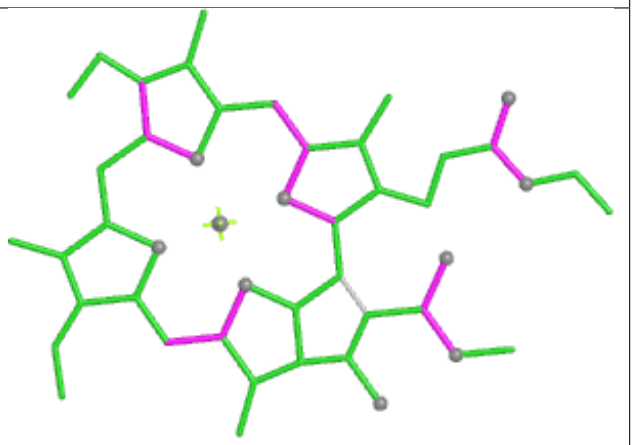


Rings

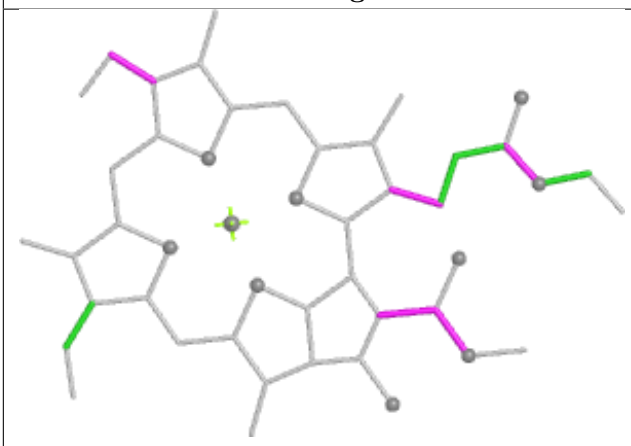
Ligand CLA H 309



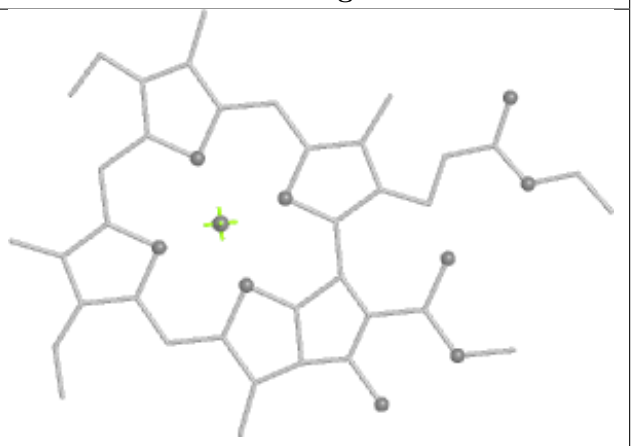
Bond lengths



Bond angles

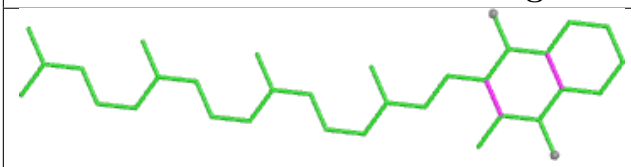


Torsions

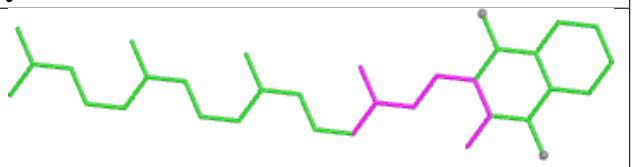


Rings

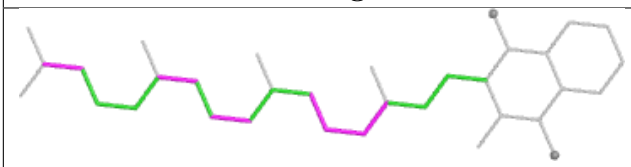
Ligand PQN a 732



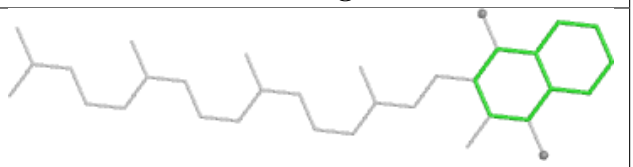
Bond lengths



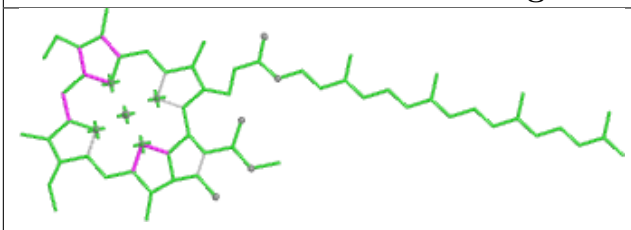
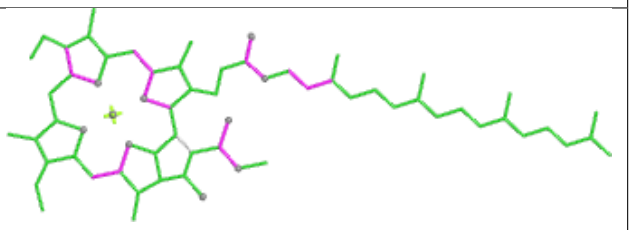
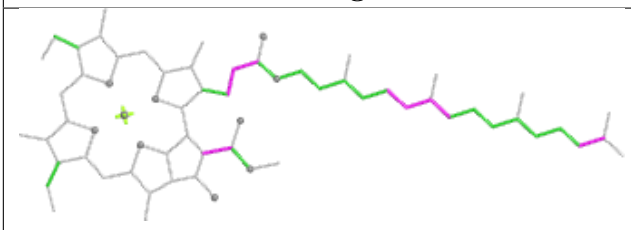
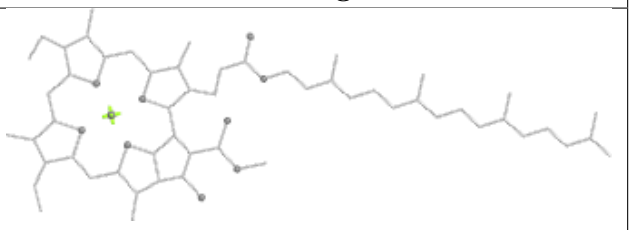
Bond angles

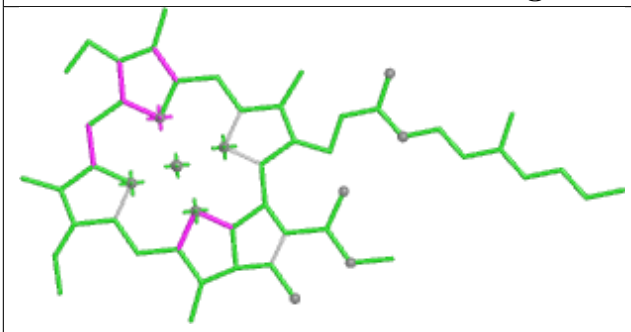
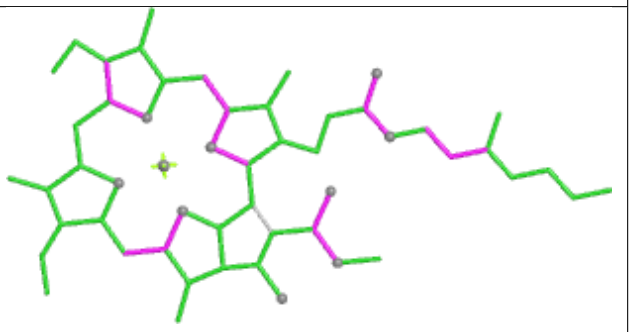
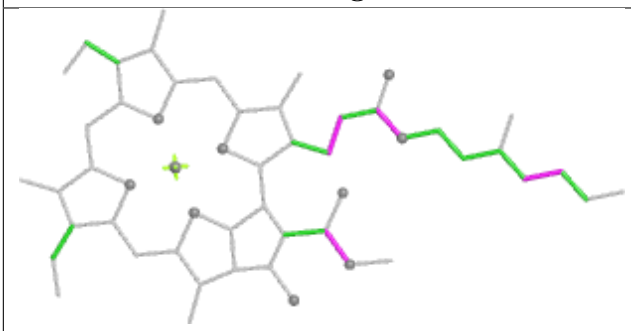
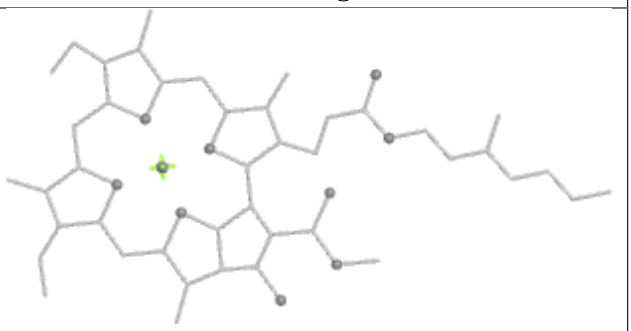


Torsions

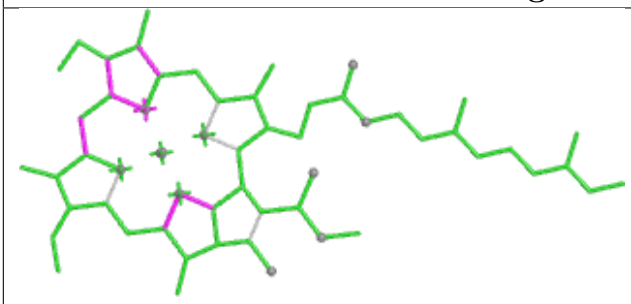


Rings

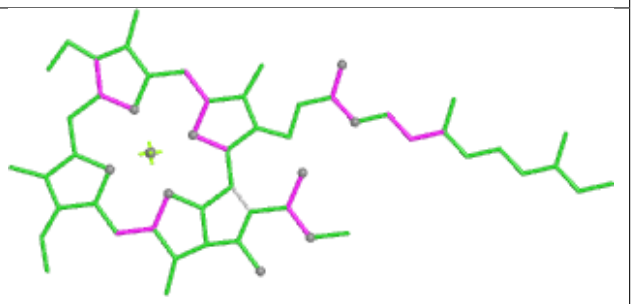
Ligand CLA b 708	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

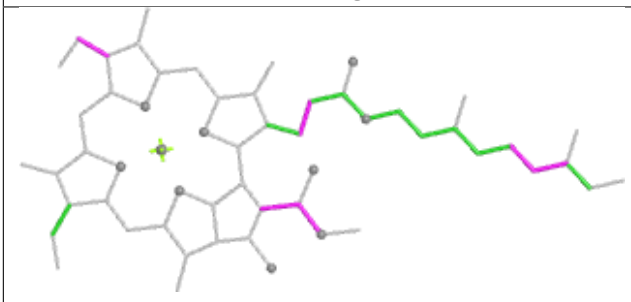
Ligand CLA J 309



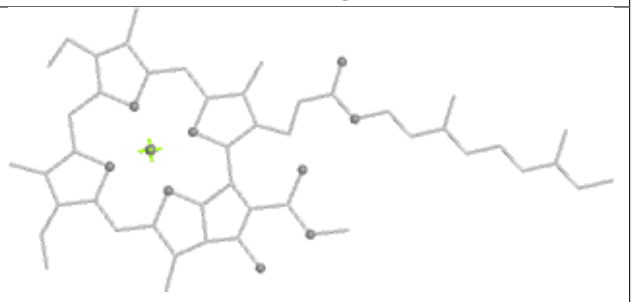
Bond lengths



Bond angles

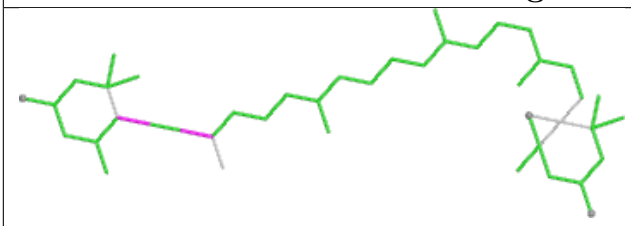


Torsions

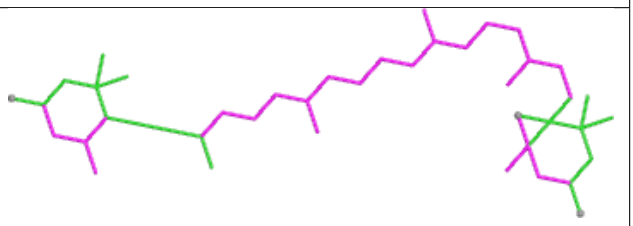


Rings

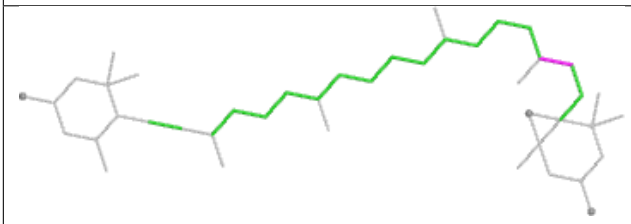
Ligand DD6 F 301



Bond lengths



Bond angles

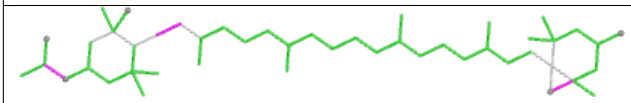


Torsions

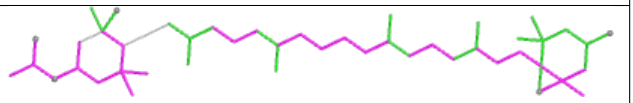


Rings

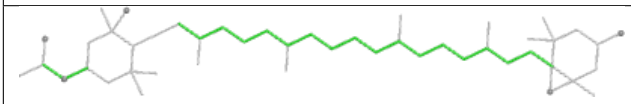
Ligand UIX A 304



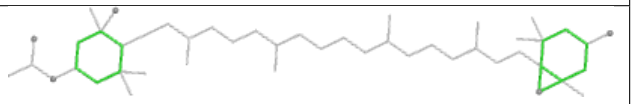
Bond lengths



Bond angles

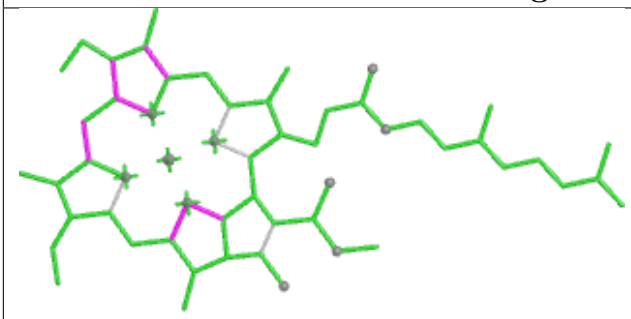


Torsions

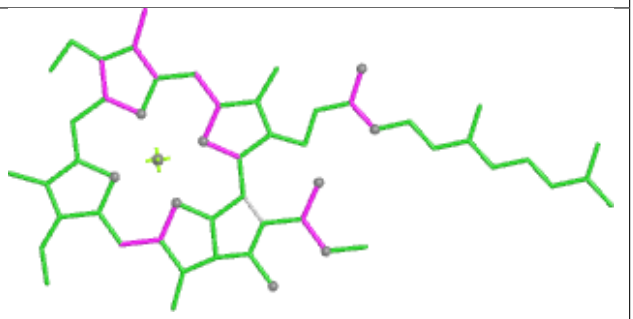


Rings

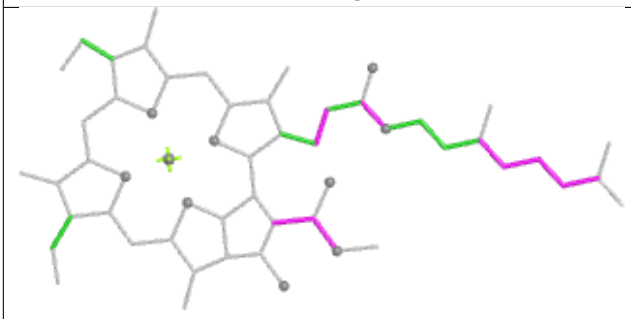
Ligand CLA I 313



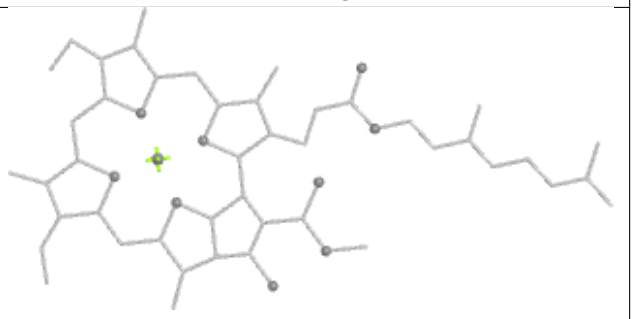
Bond lengths



Bond angles

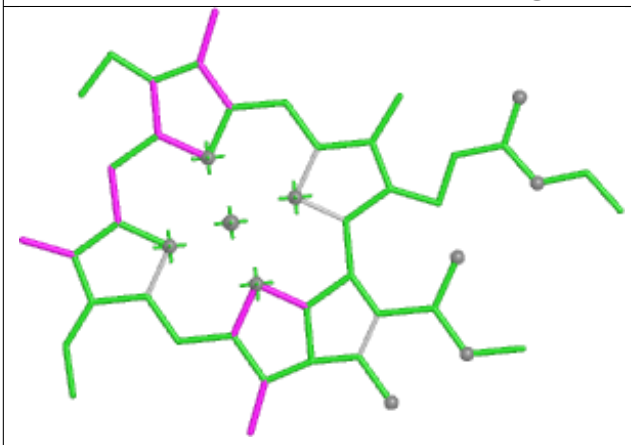


Torsions

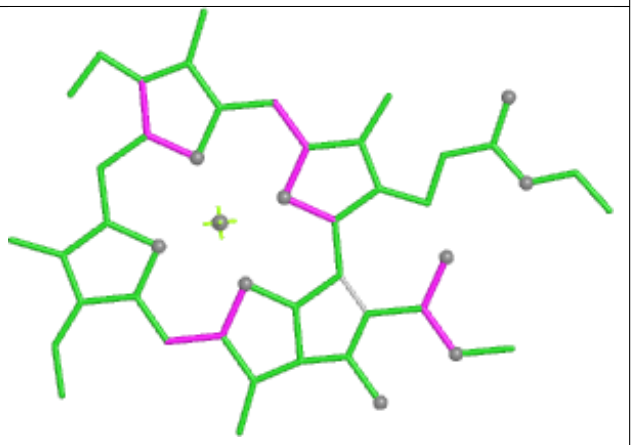


Rings

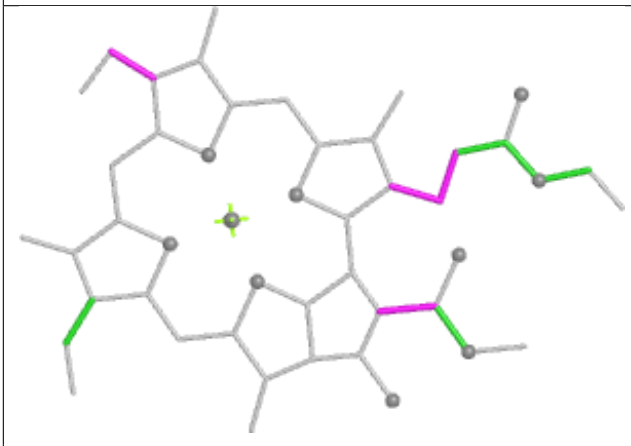
Ligand CLA a 719



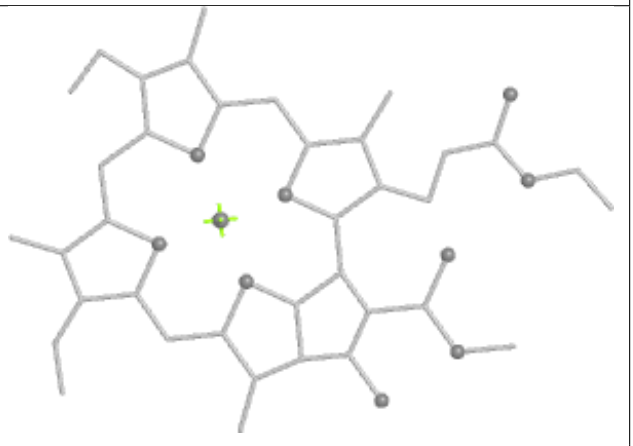
Bond lengths



Bond angles

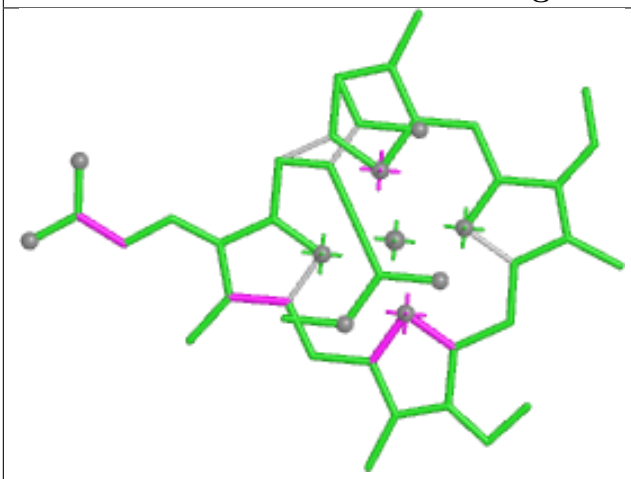


Torsions

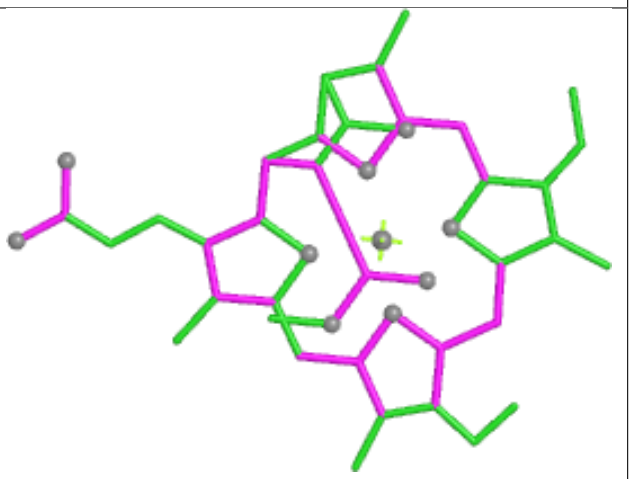


Rings

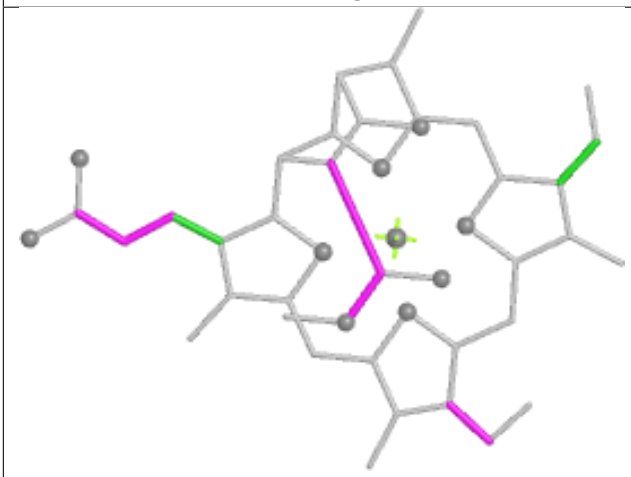
Ligand KC1 I 314



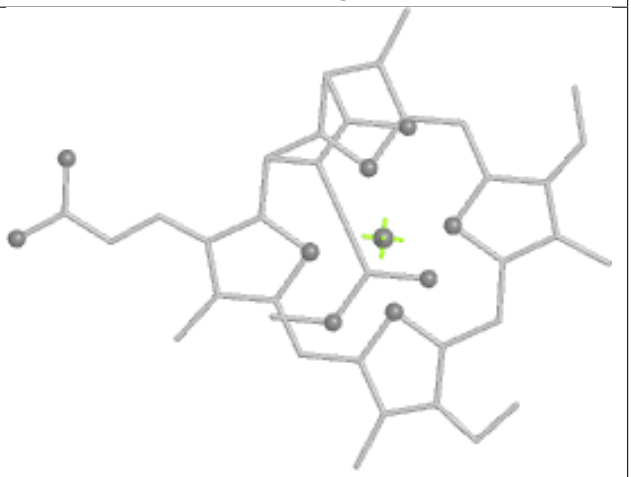
Bond lengths



Bond angles

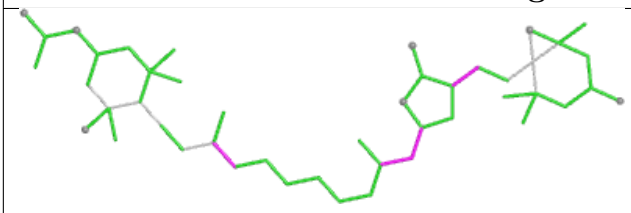


Torsions

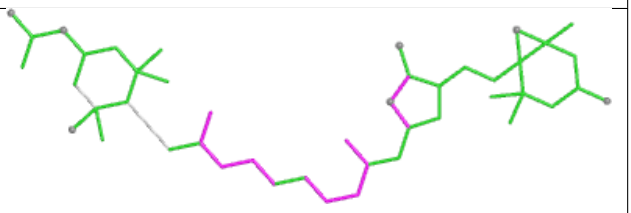


Rings

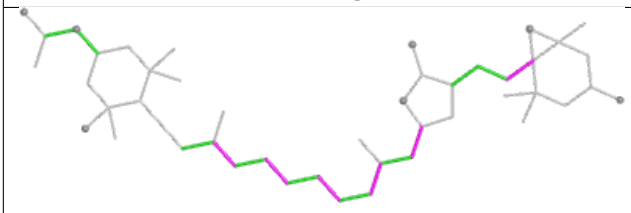
Ligand PID D 306



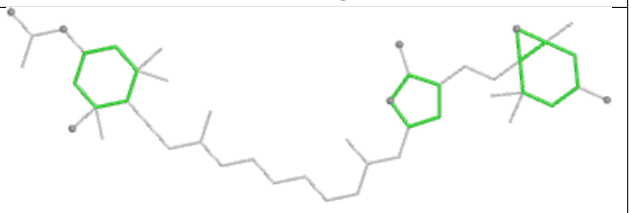
Bond lengths



Bond angles

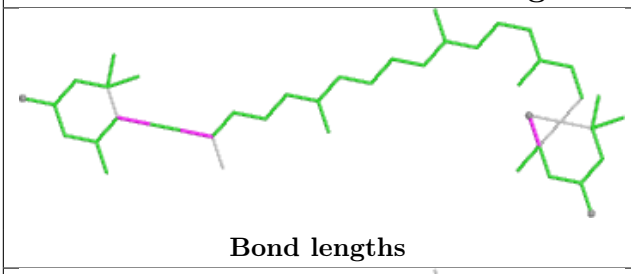


Torsions

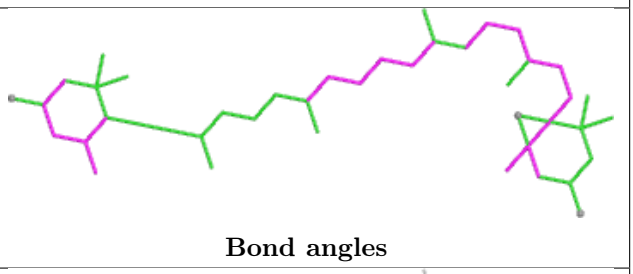


Rings

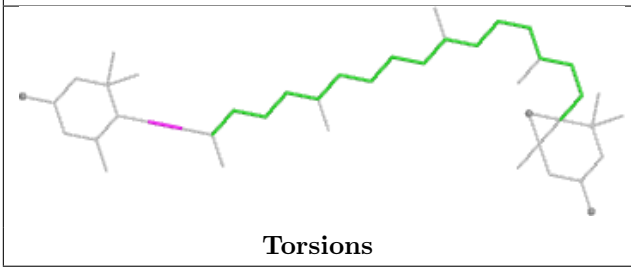
Ligand DD6 h 203



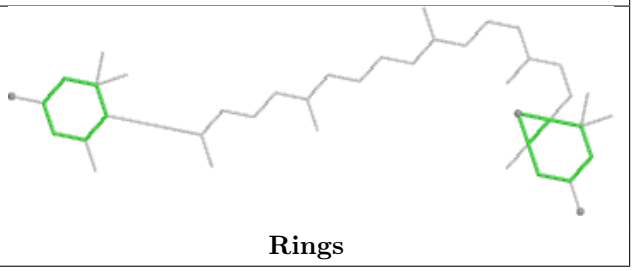
Bond lengths



Bond angles

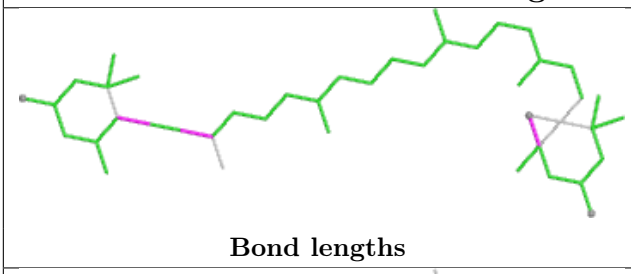


Torsions

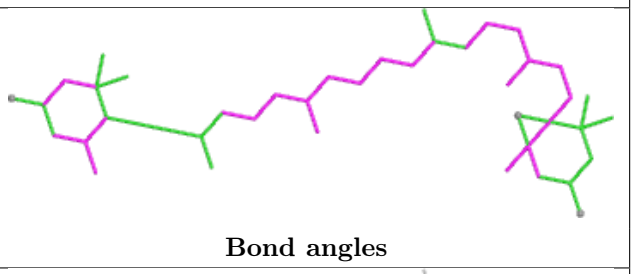


Rings

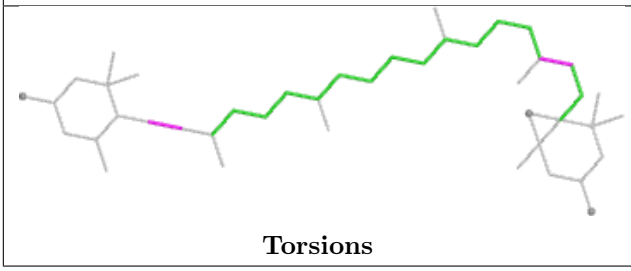
Ligand DD6 b 731



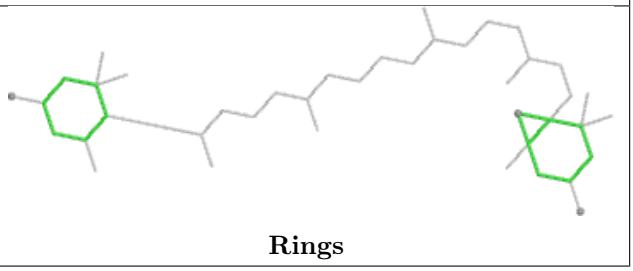
Bond lengths



Bond angles

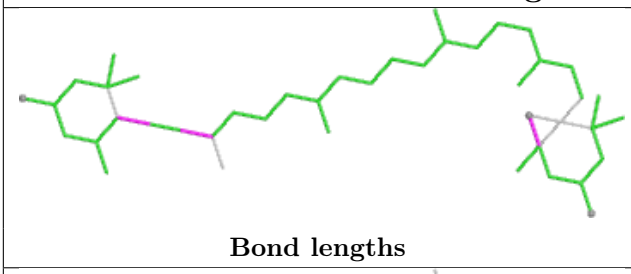


Torsions

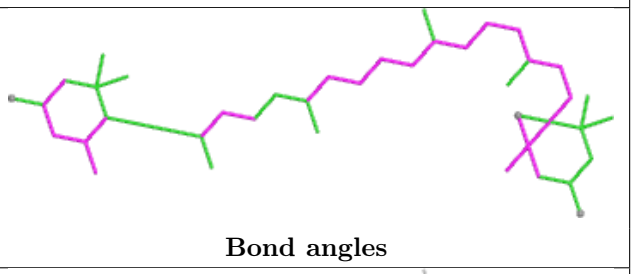


Rings

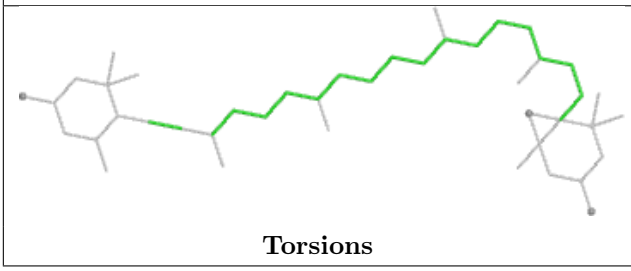
Ligand DD6 O 303



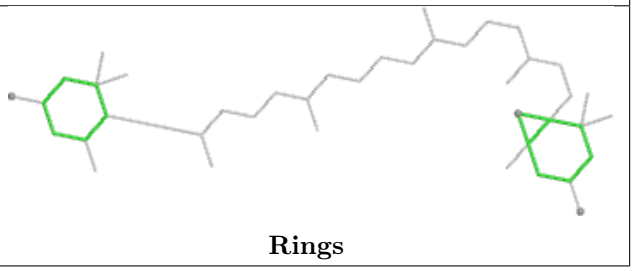
Bond lengths



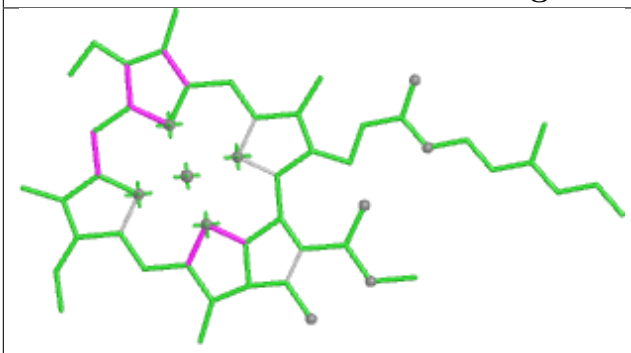
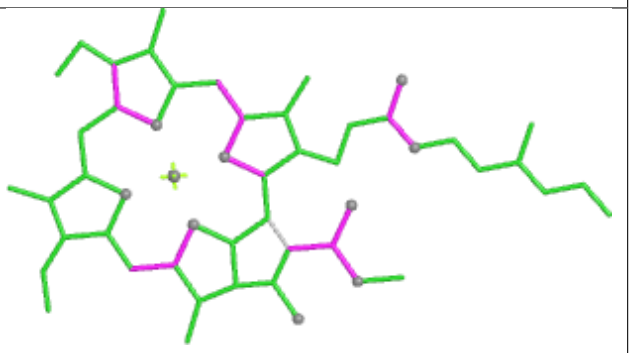
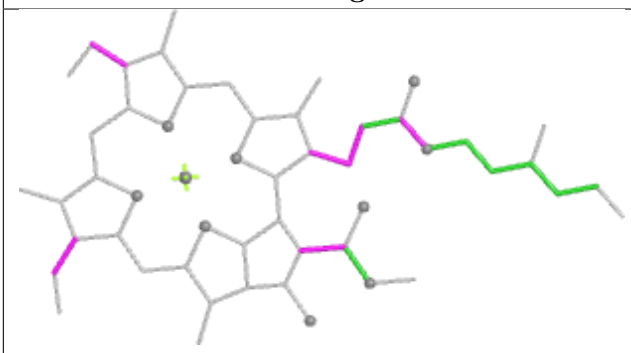
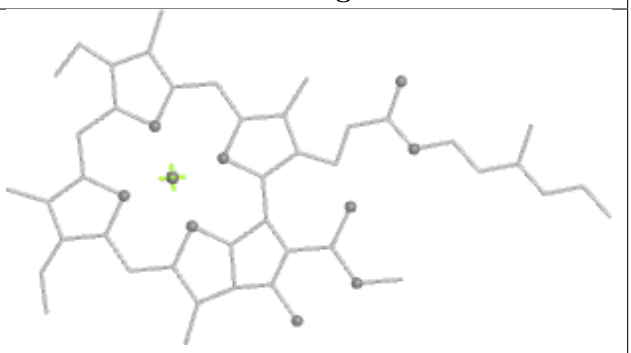
Bond angles

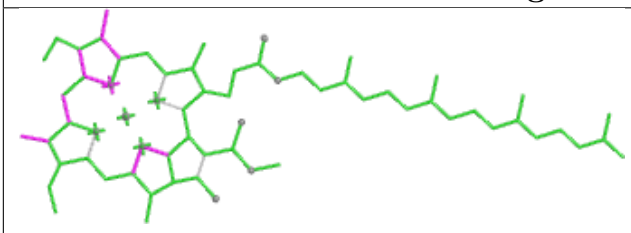
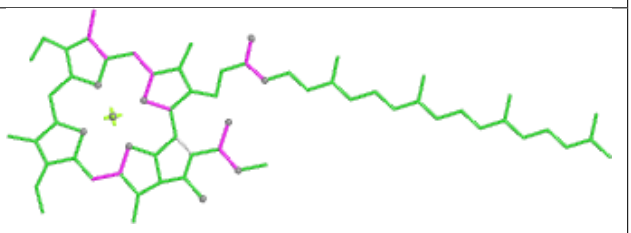
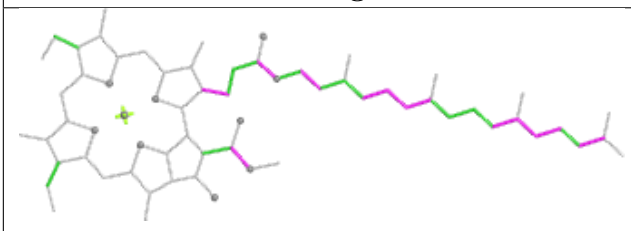
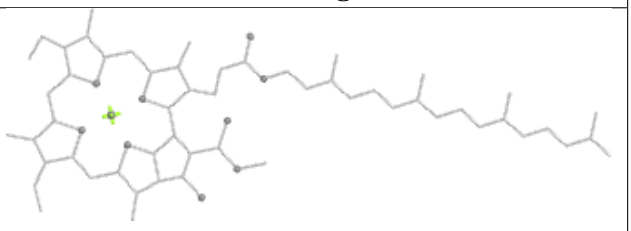


Torsions

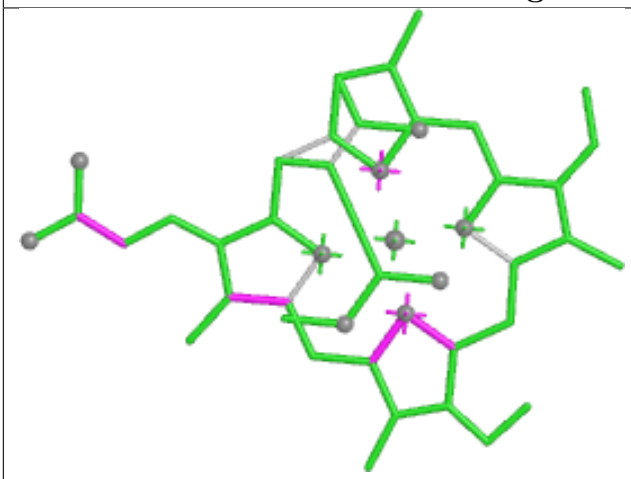


Rings

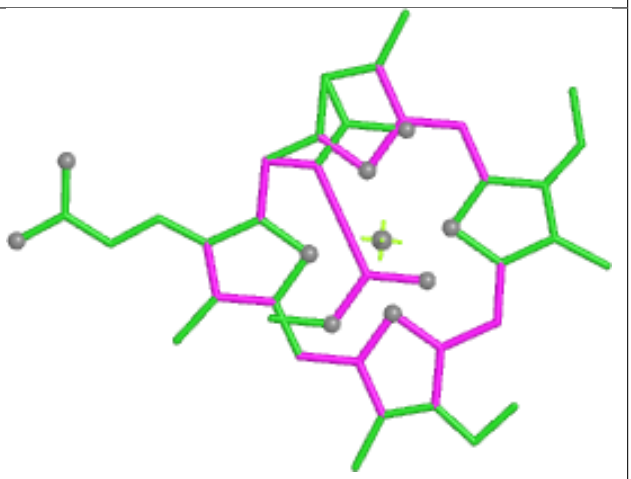
Ligand CLA I 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 717	
	
Bond lengths	Bond angles
	
Torsions	Rings

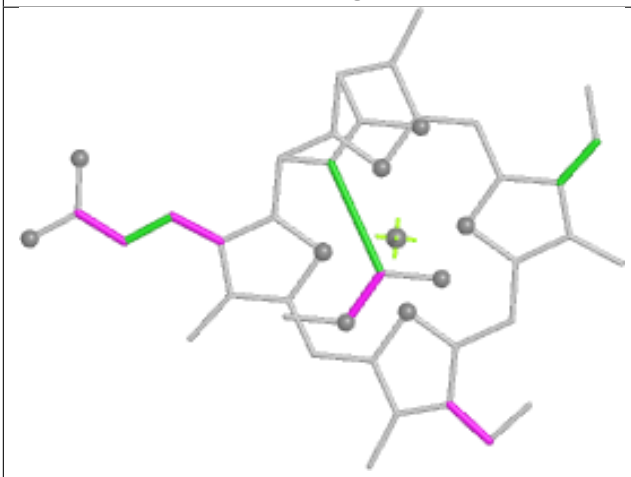
Ligand KC1 P 216



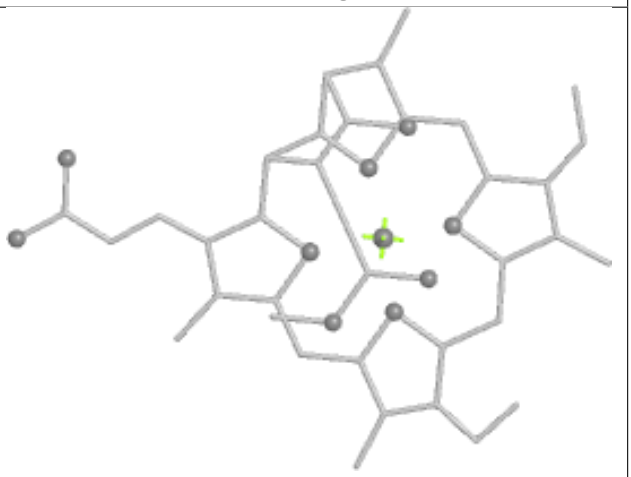
Bond lengths



Bond angles



Torsions

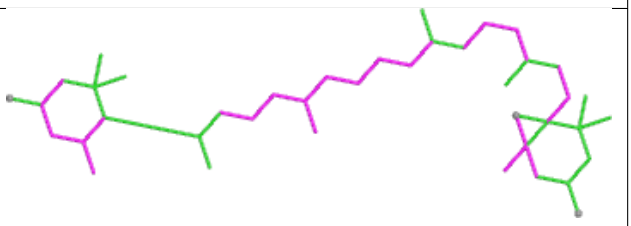


Rings

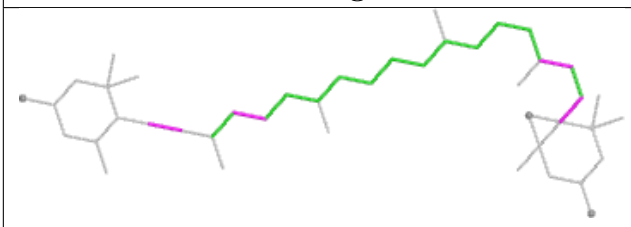
Ligand DD6 K 301



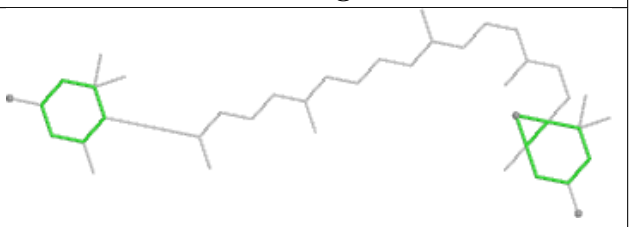
Bond lengths



Bond angles

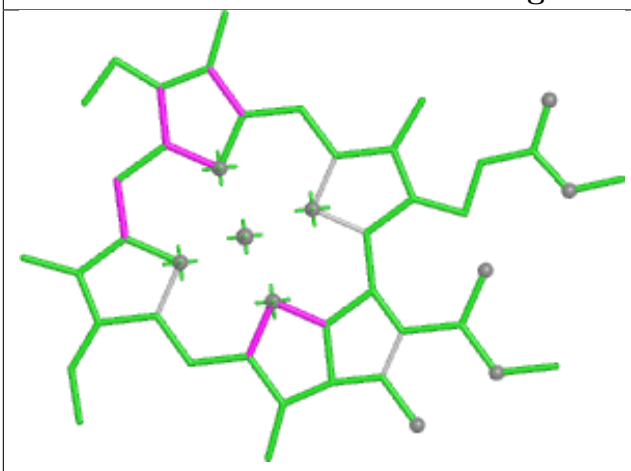


Torsions

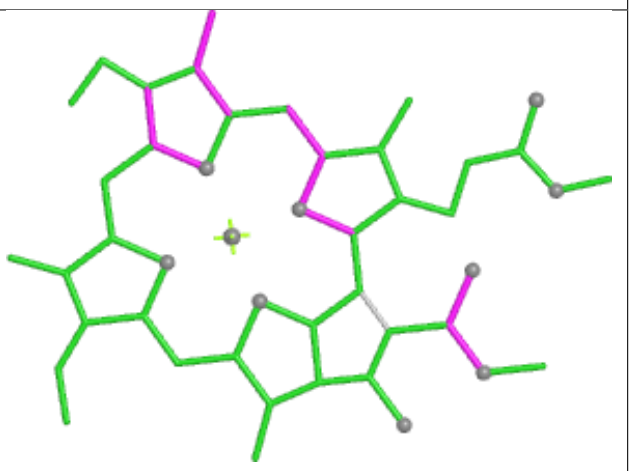


Rings

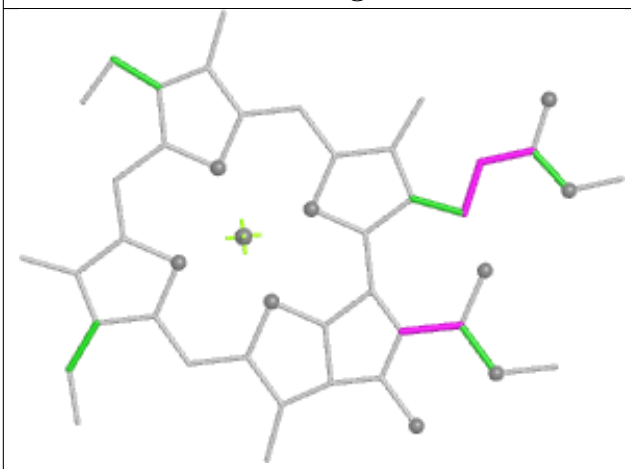
Ligand CLA b 714



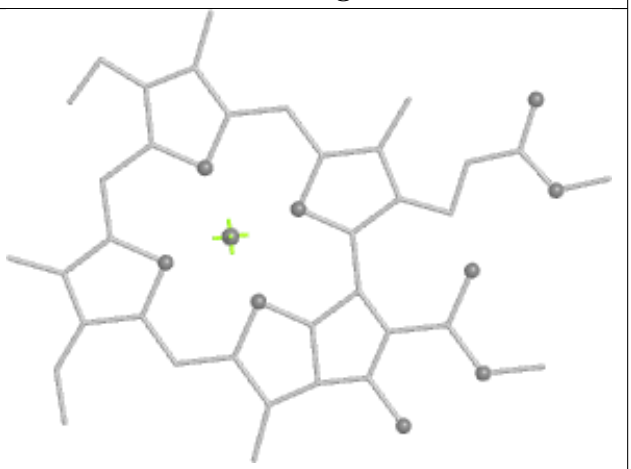
Bond lengths



Bond angles

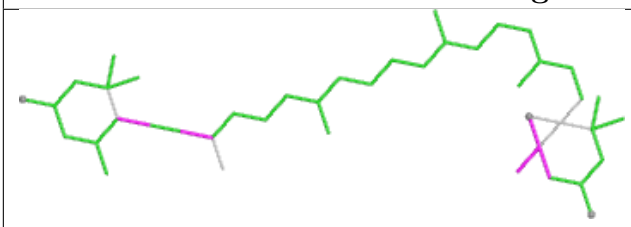


Torsions

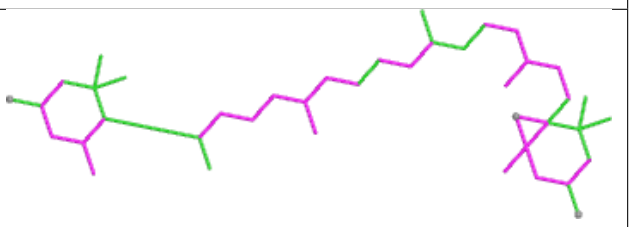


Rings

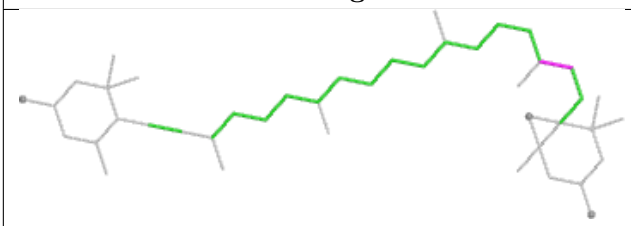
Ligand DD6 I 303



Bond lengths



Bond angles

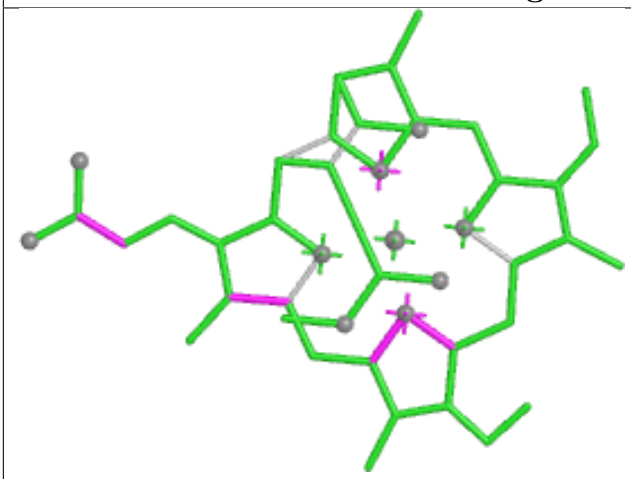


Torsions

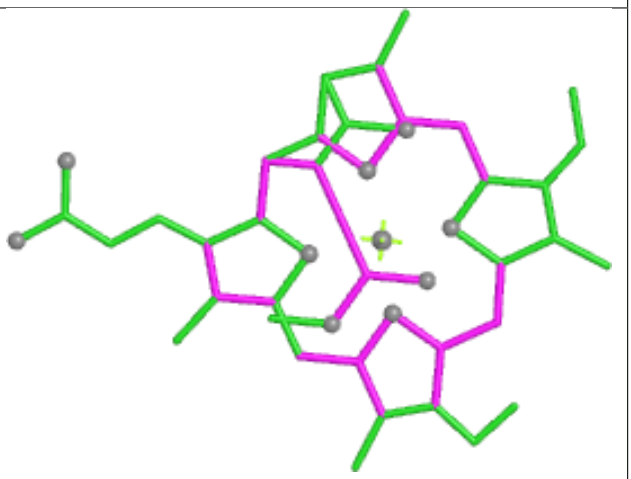


Rings

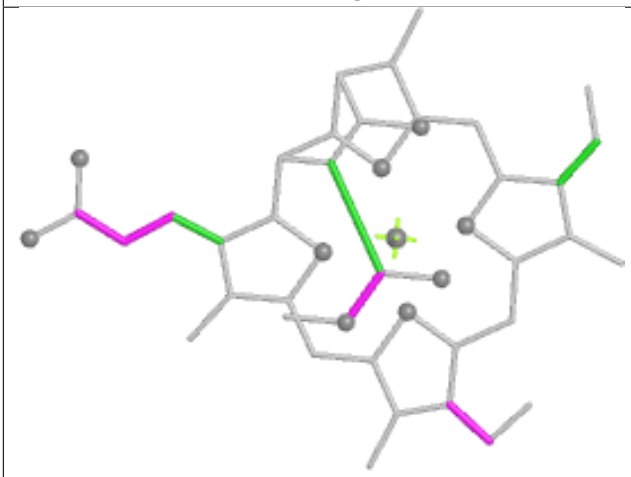
Ligand KC1 B 314



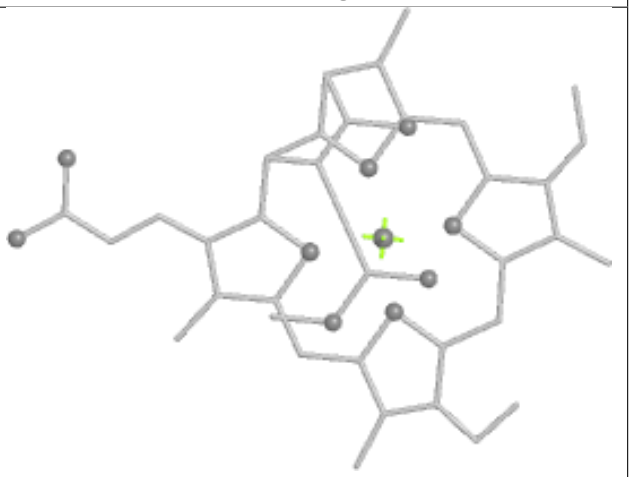
Bond lengths



Bond angles



Torsions



Rings

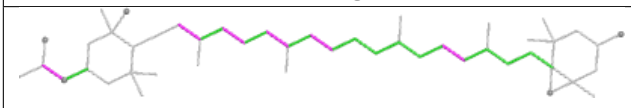
Ligand UIX P 207



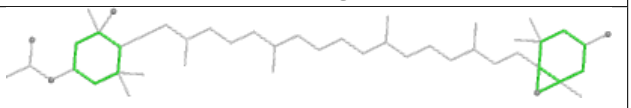
Bond lengths



Bond angles

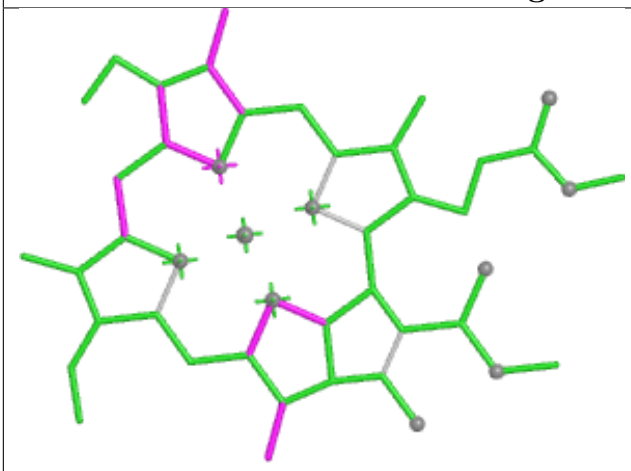


Torsions

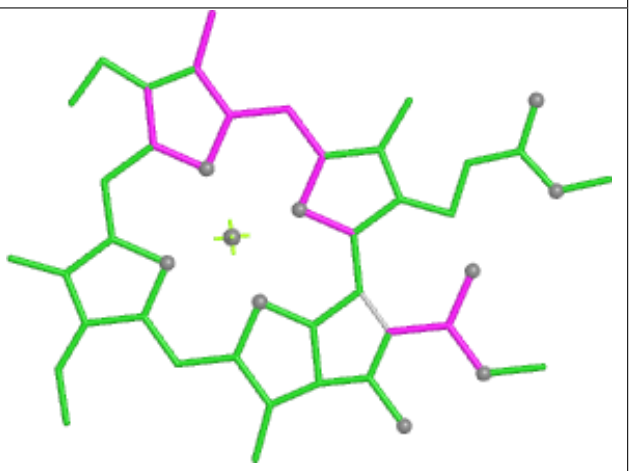


Rings

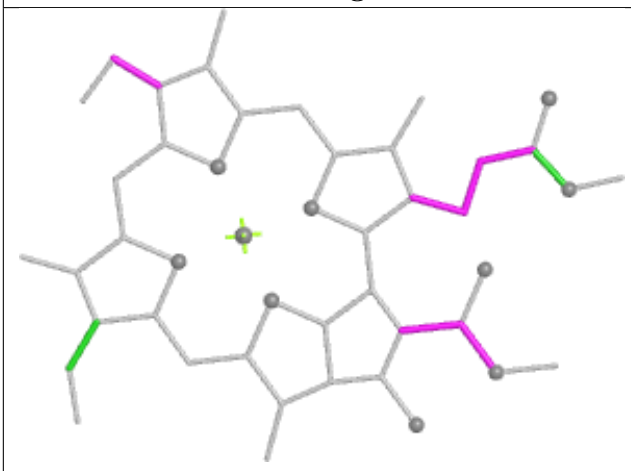
Ligand CLA J 308



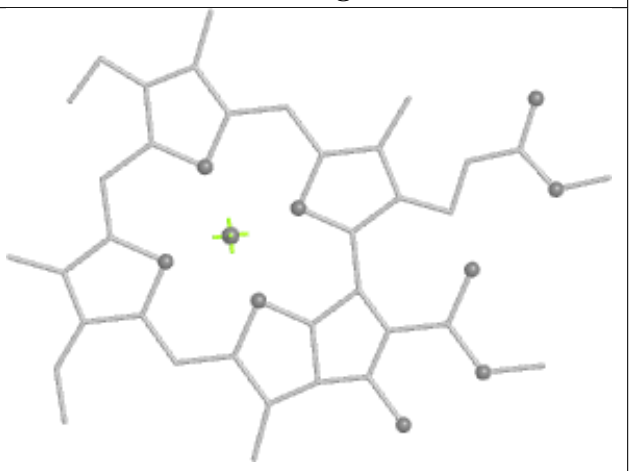
Bond lengths



Bond angles

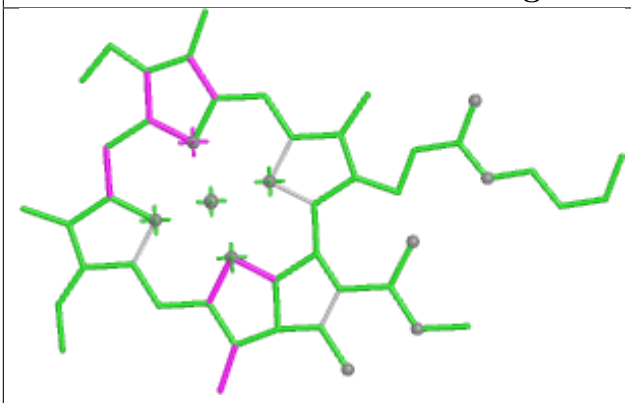


Torsions

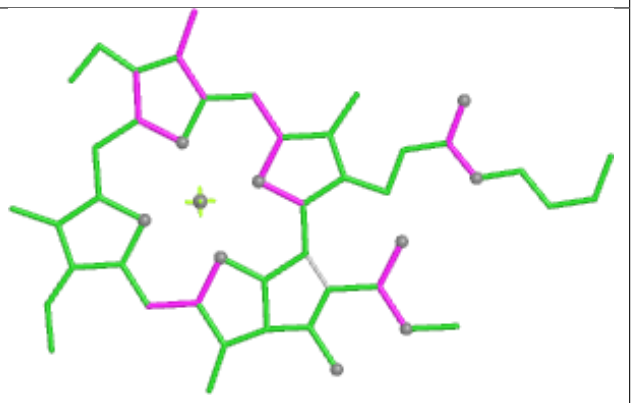


Rings

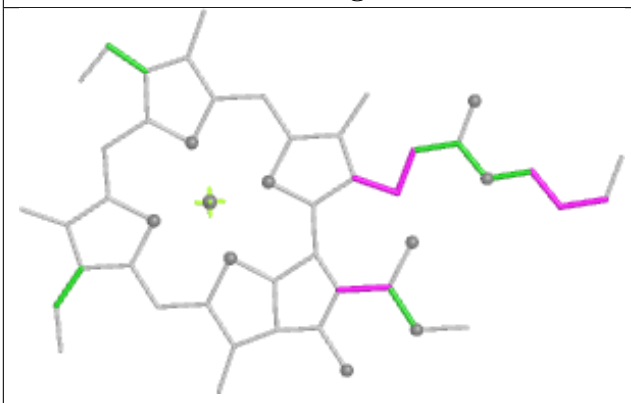
Ligand CLA G 520



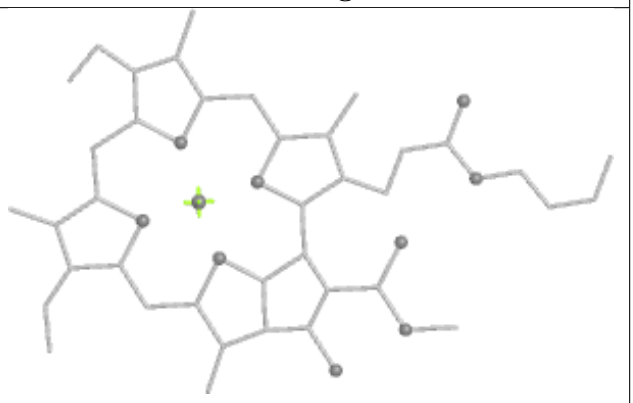
Bond lengths



Bond angles

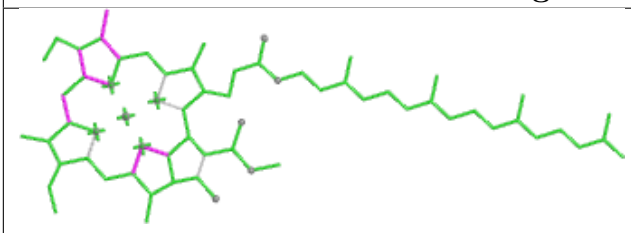


Torsions

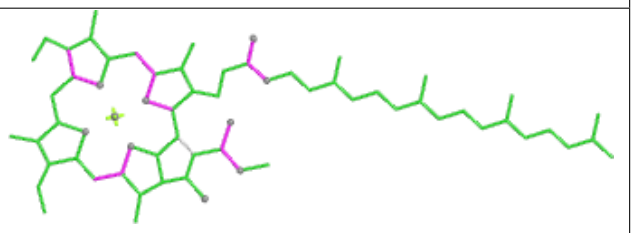


Rings

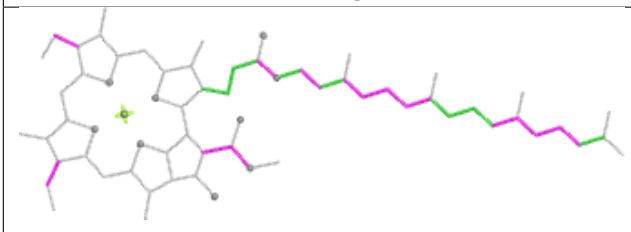
Ligand CLA l 313



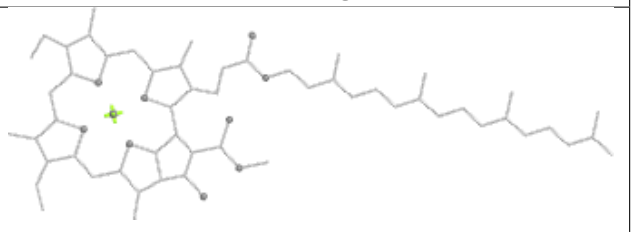
Bond lengths



Bond angles

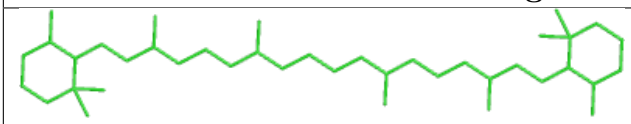


Torsions

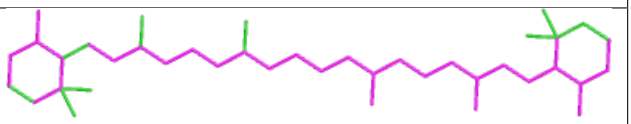


Rings

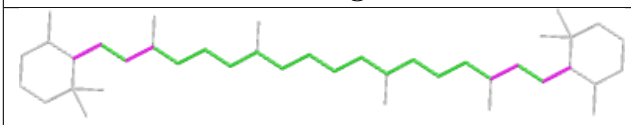
Ligand BCR b 730



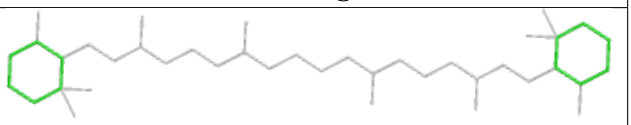
Bond lengths



Bond angles

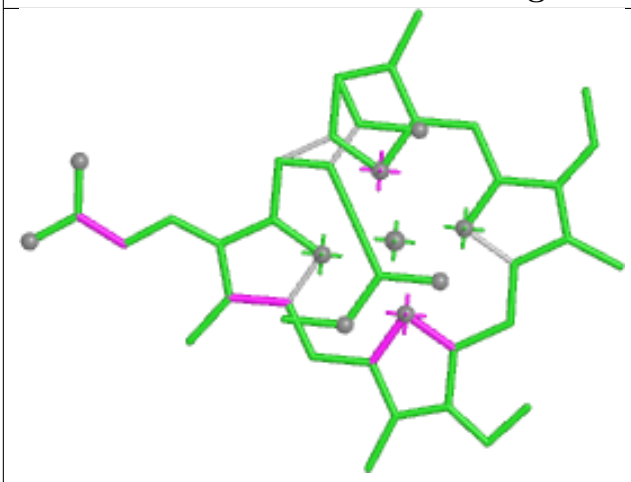


Torsions

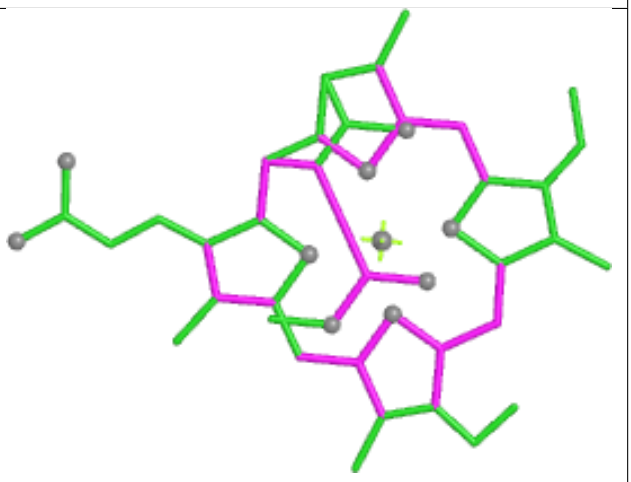


Rings

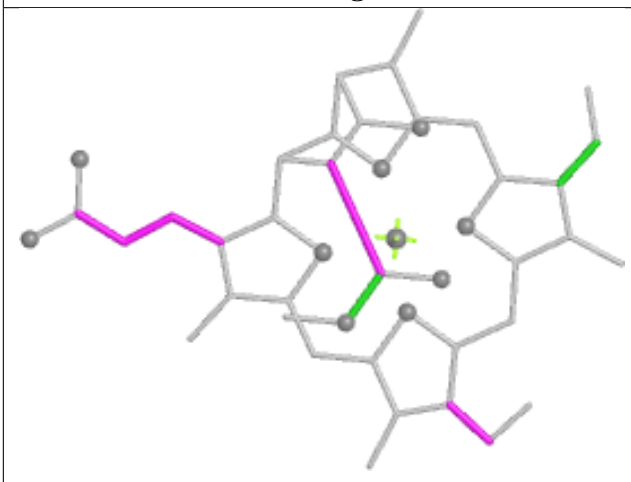
Ligand KC1 F 309



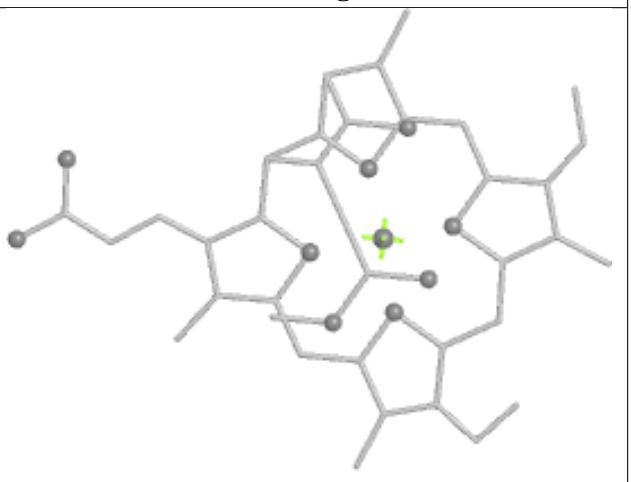
Bond lengths



Bond angles

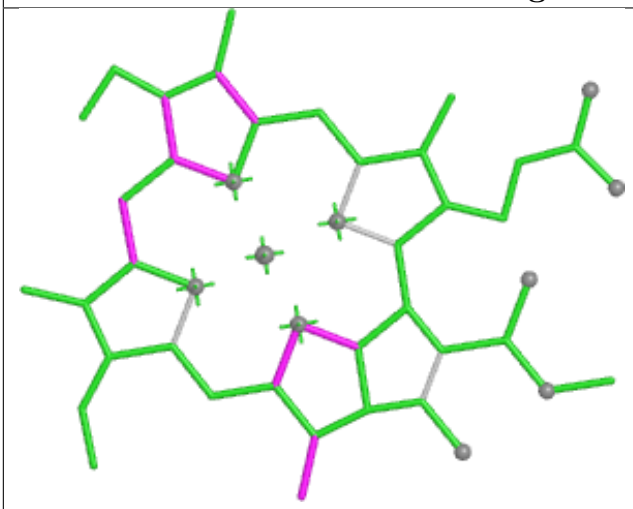


Torsions

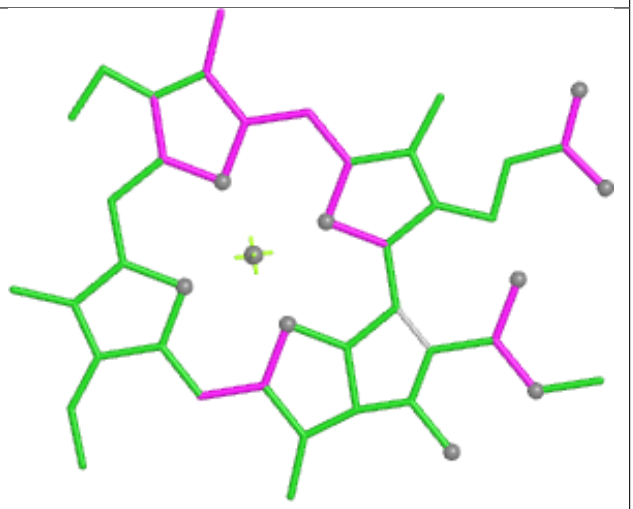


Rings

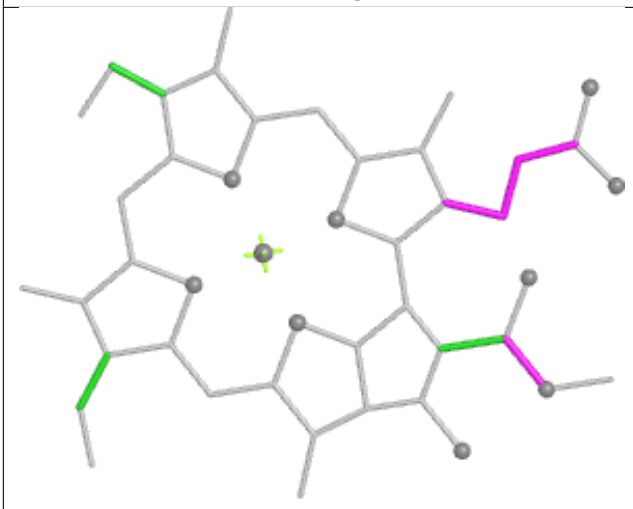
Ligand CLA a 711



Bond lengths



Bond angles

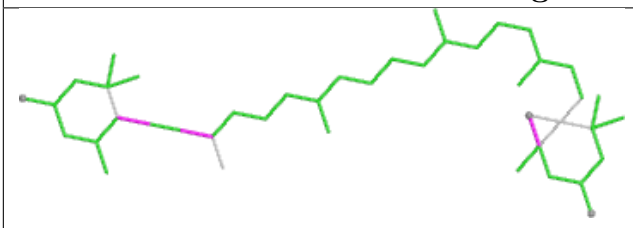


Torsions

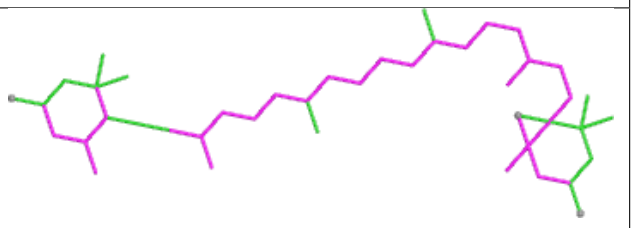


Rings

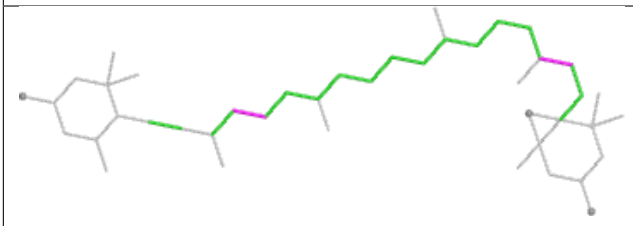
Ligand DD6 I 301



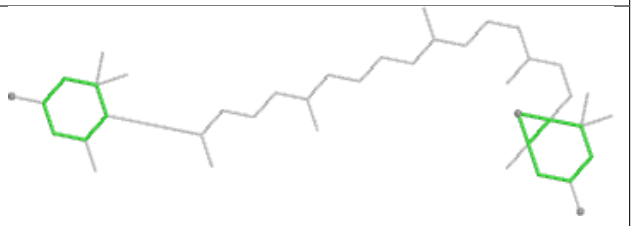
Bond lengths



Bond angles

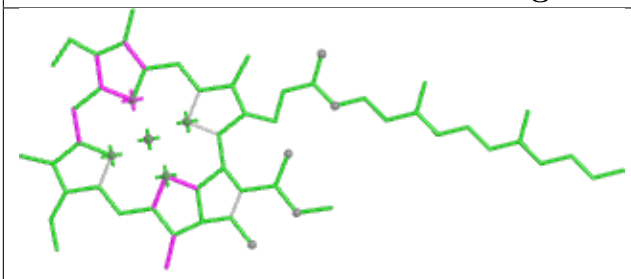


Torsions

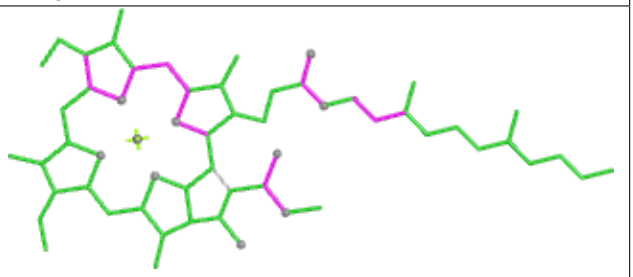


Rings

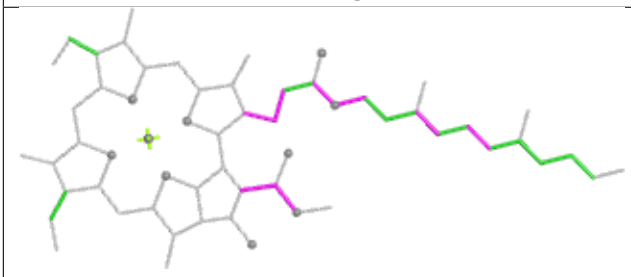
Ligand CLA j 106



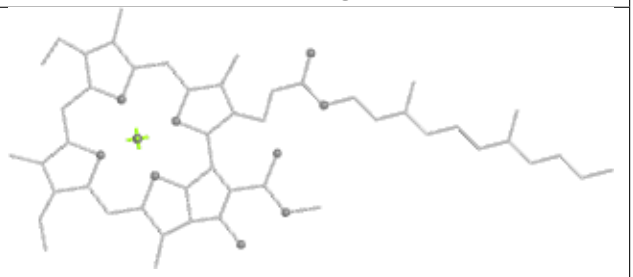
Bond lengths



Bond angles

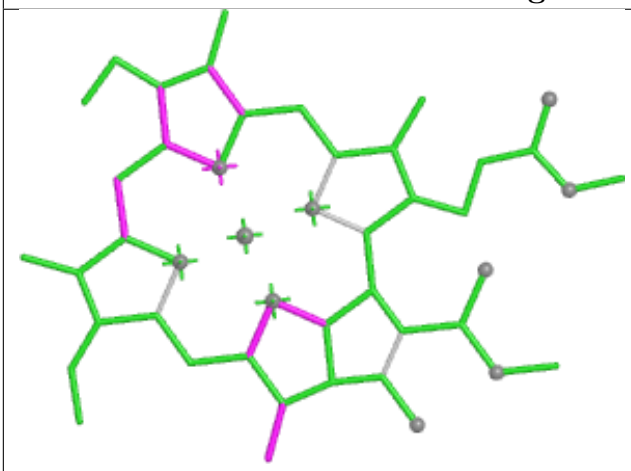


Torsions

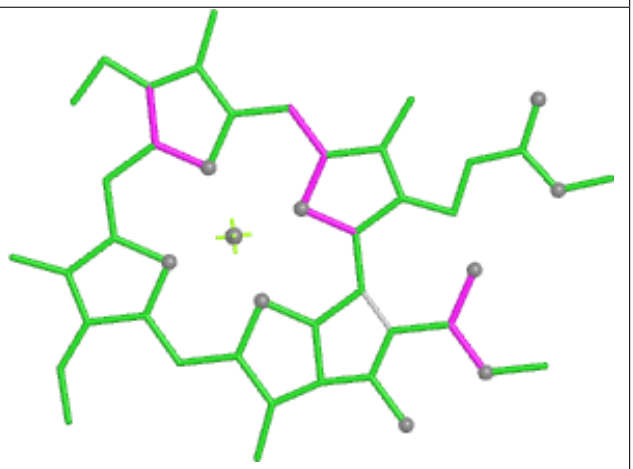


Rings

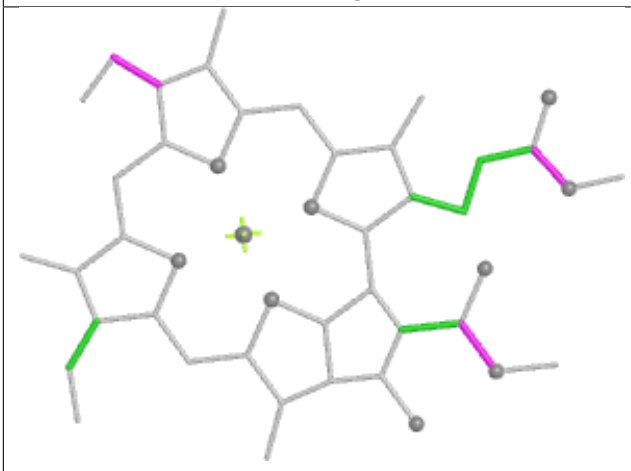
Ligand CLA J 306



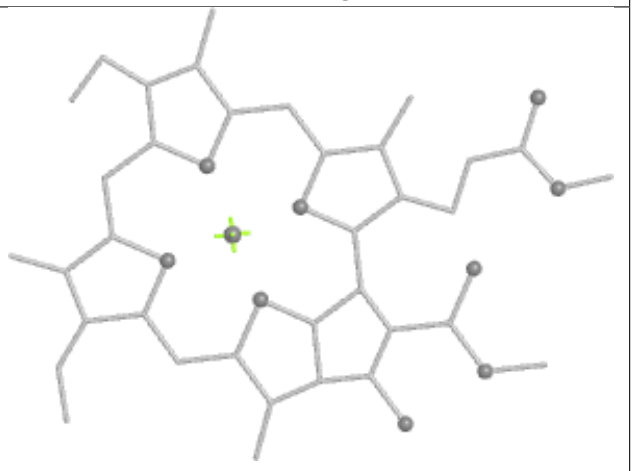
Bond lengths



Bond angles

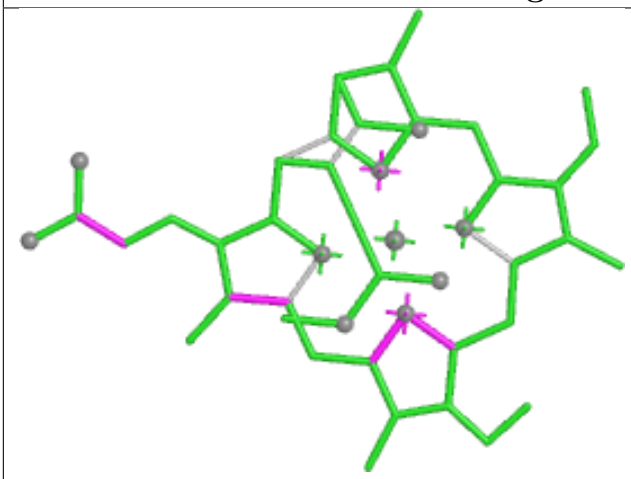


Torsions

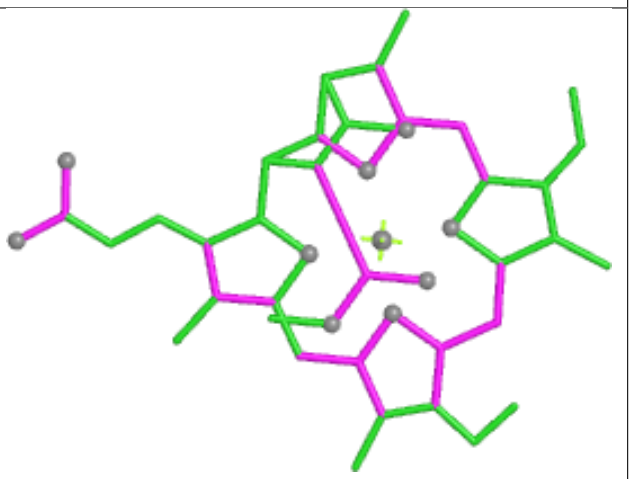


Rings

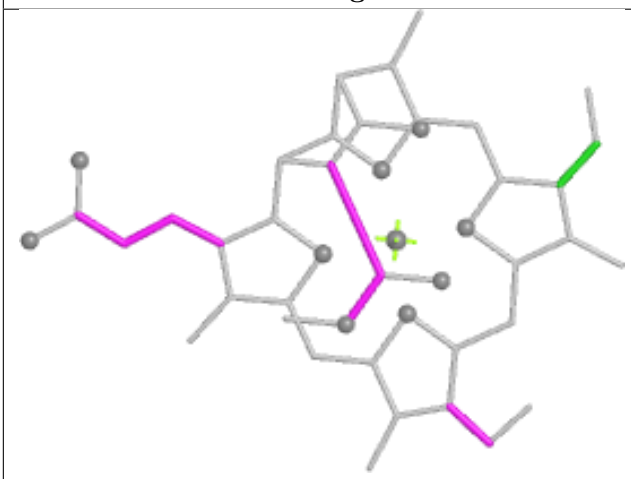
Ligand KC1 P 211



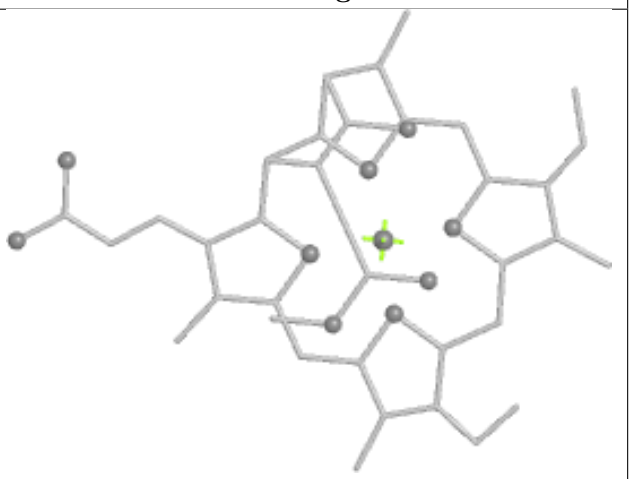
Bond lengths



Bond angles

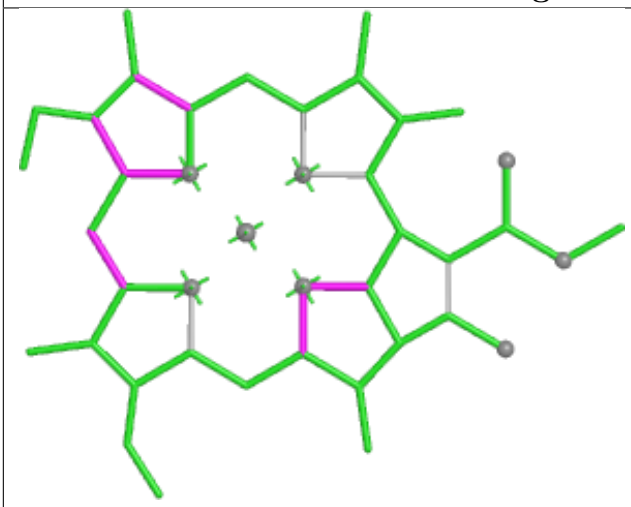


Torsions

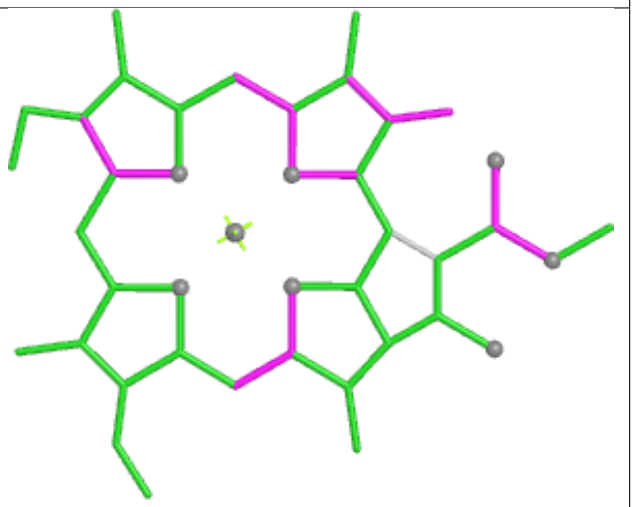


Rings

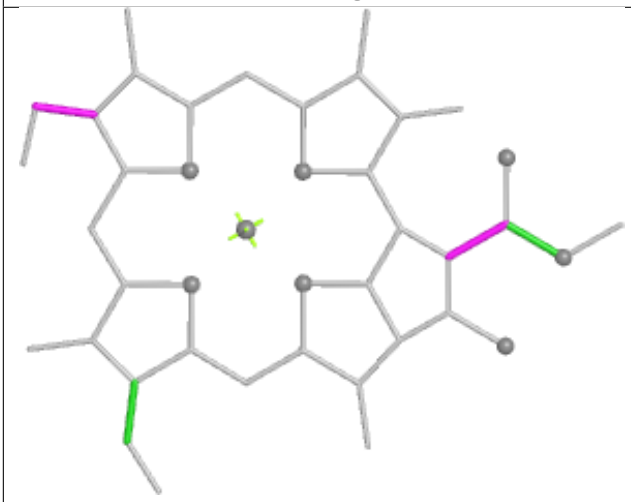
Ligand CLA l 309



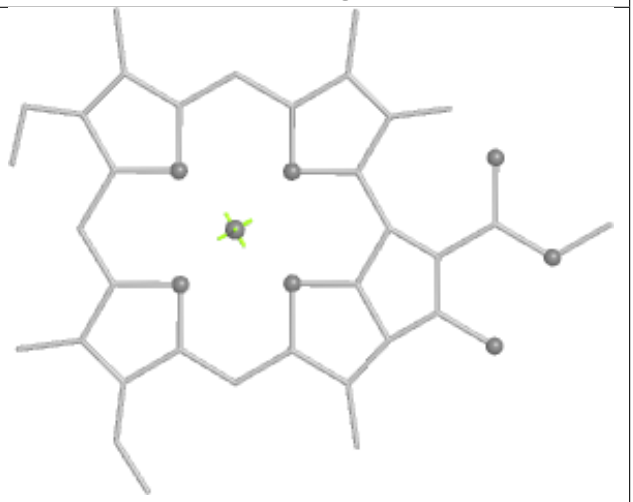
Bond lengths



Bond angles

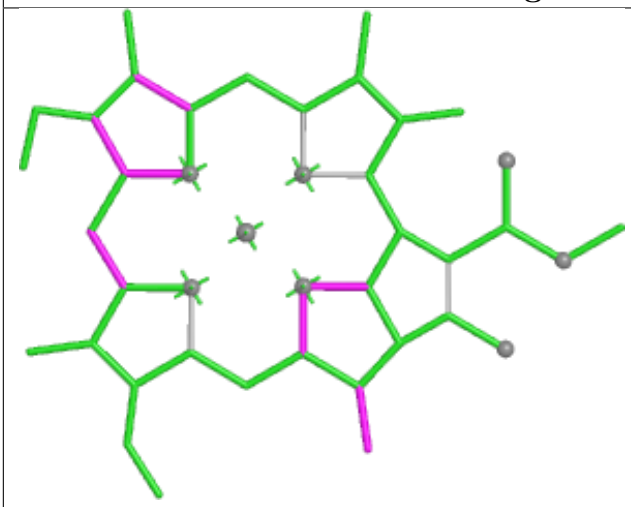


Torsions

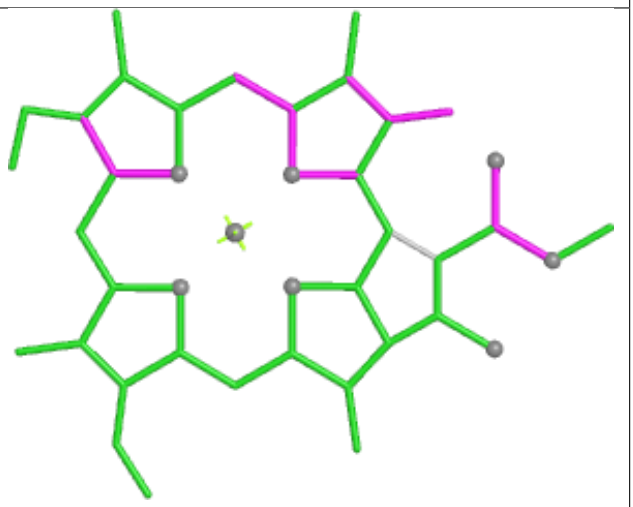


Rings

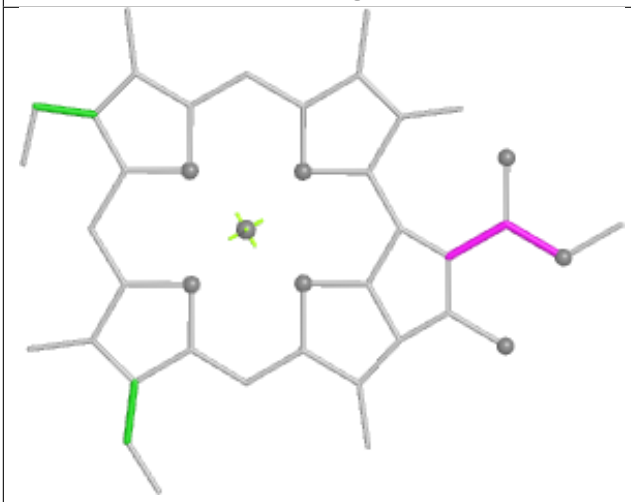
Ligand CLA B 315



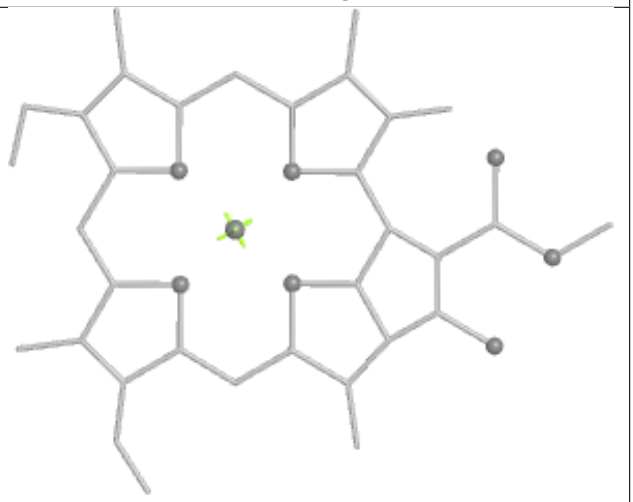
Bond lengths



Bond angles

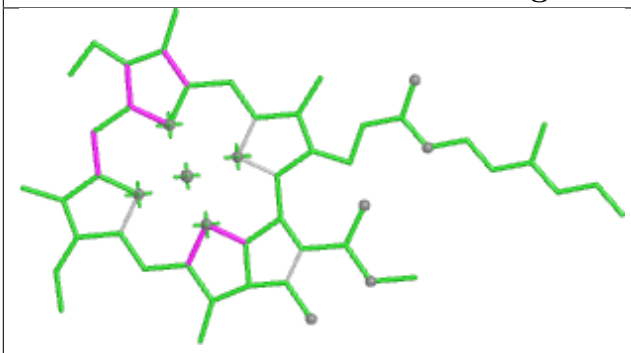


Torsions

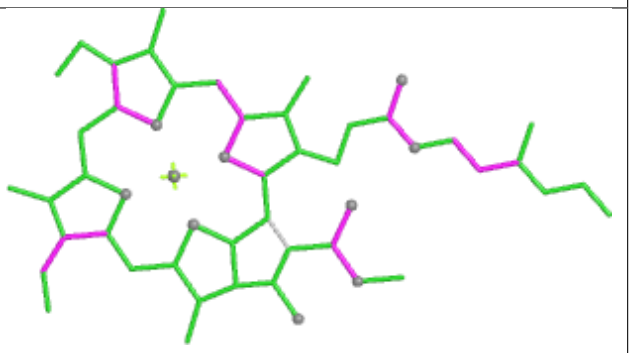


Rings

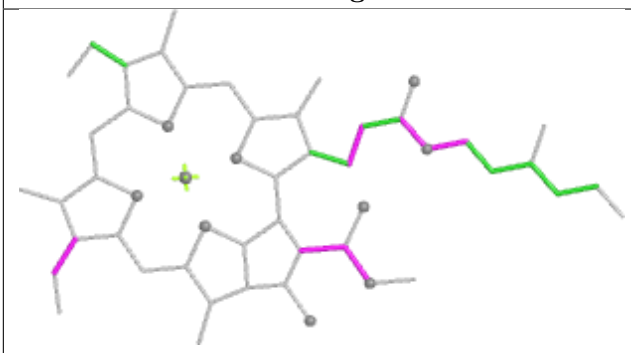
Ligand CLA I 321



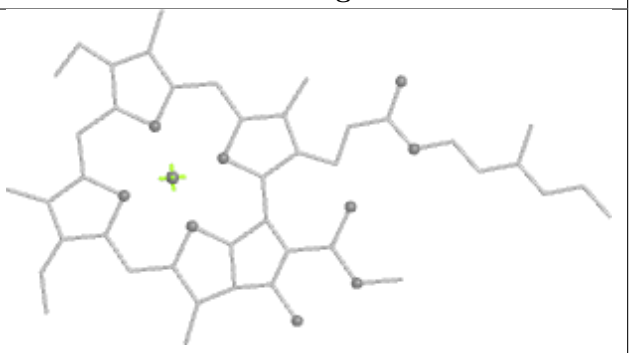
Bond lengths



Bond angles

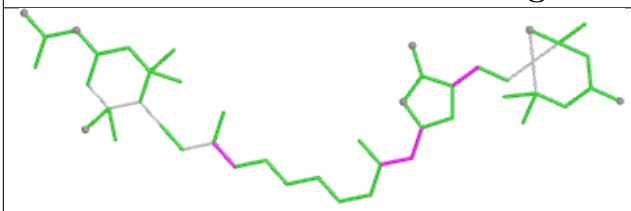


Torsions

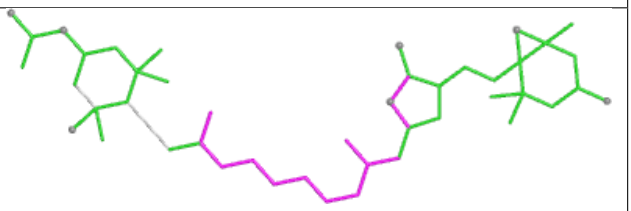


Rings

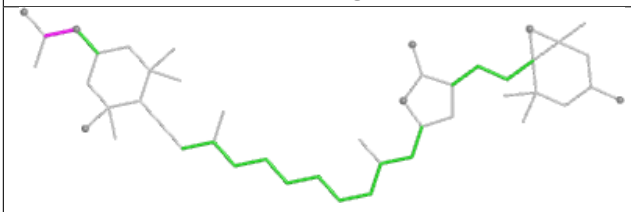
Ligand PID D 305



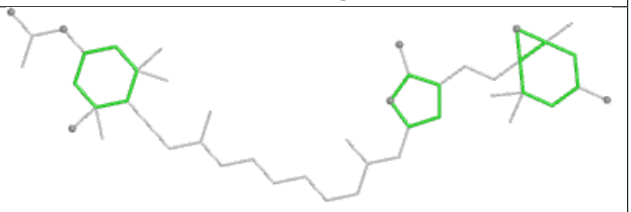
Bond lengths



Bond angles

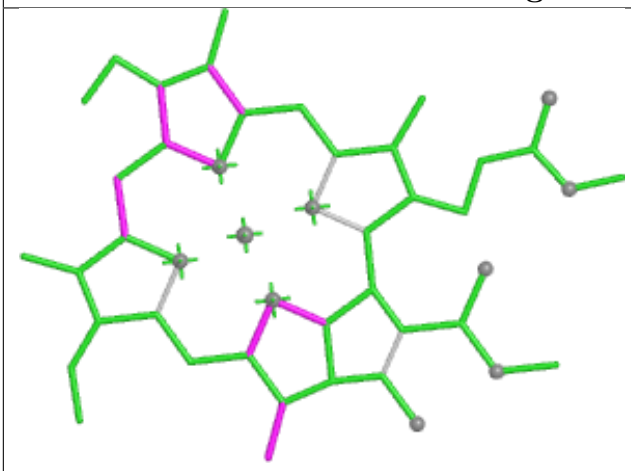


Torsions

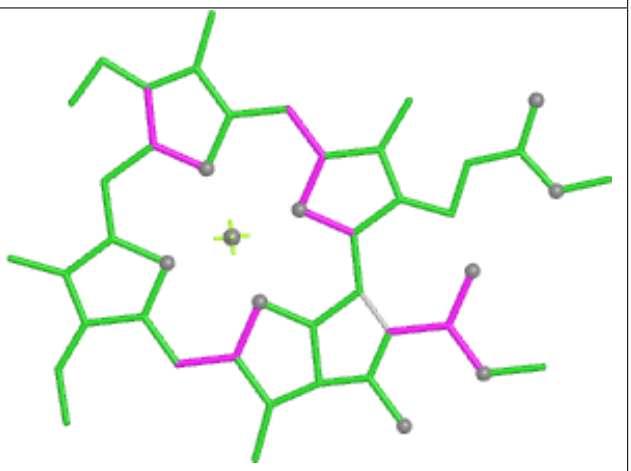


Rings

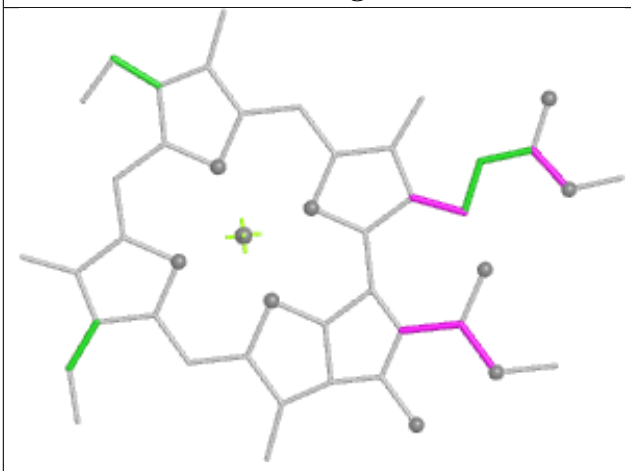
Ligand CLA F 310



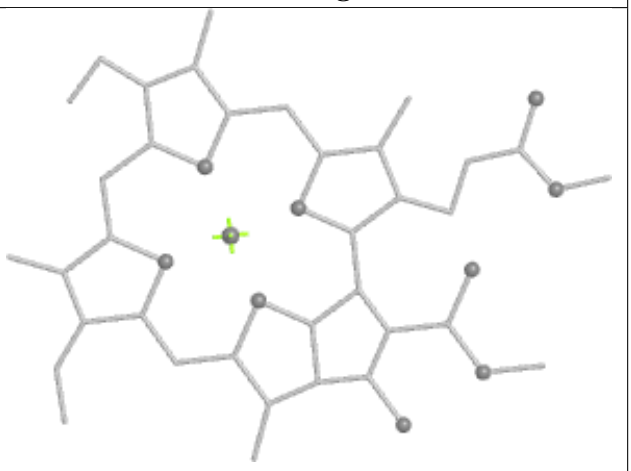
Bond lengths



Bond angles

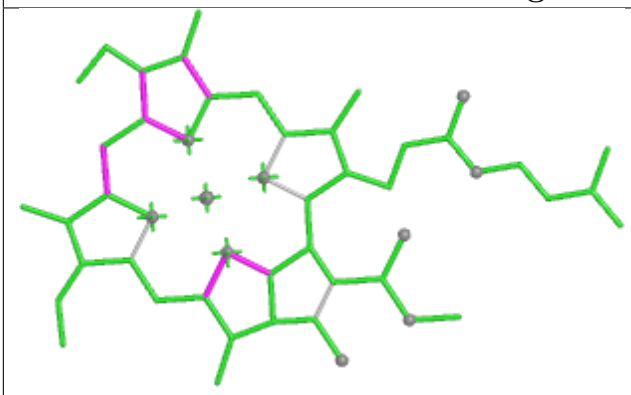


Torsions

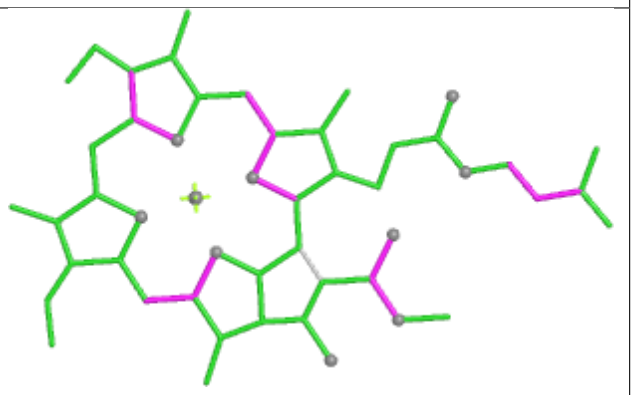


Rings

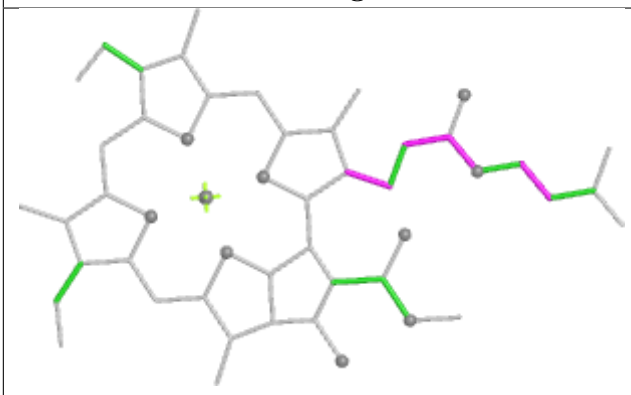
Ligand CLA b 716



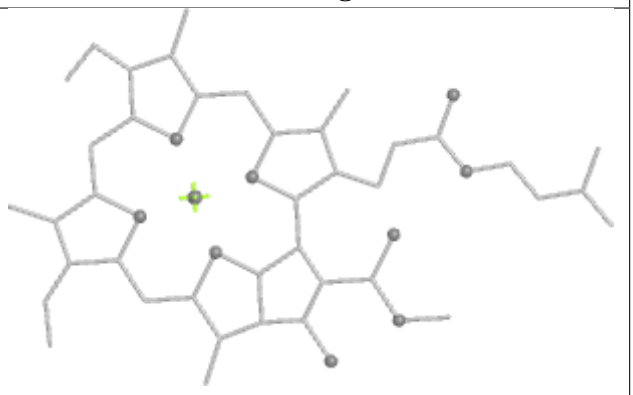
Bond lengths



Bond angles

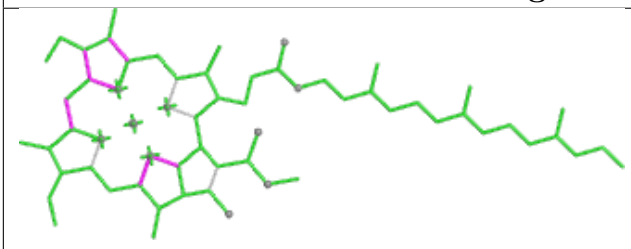


Torsions

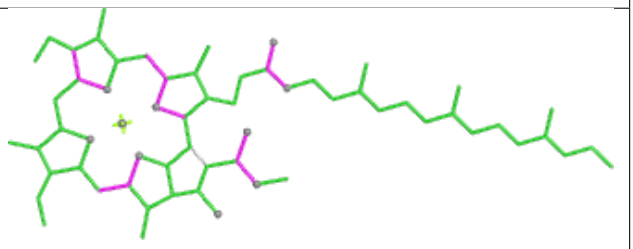


Rings

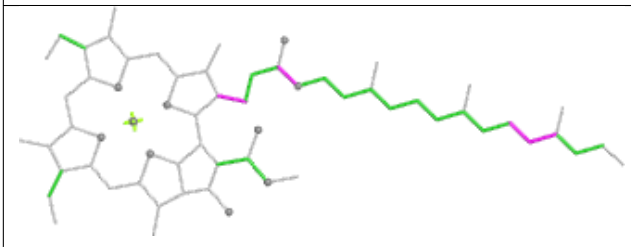
Ligand CLA a 720



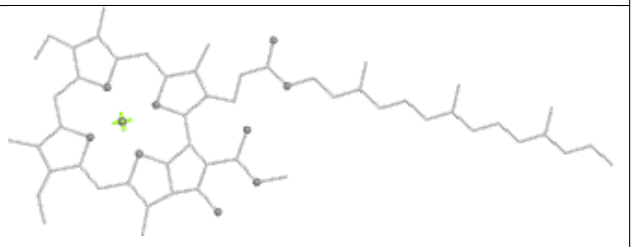
Bond lengths



Bond angles

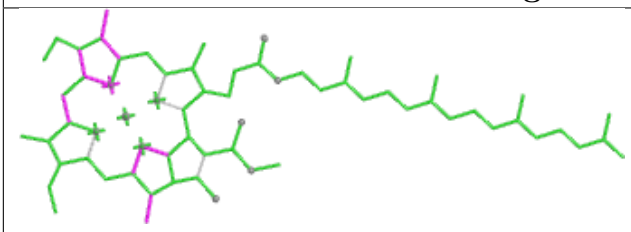


Torsions

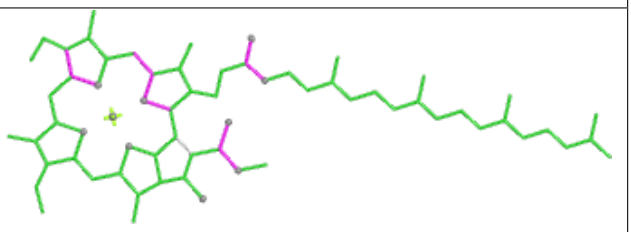


Rings

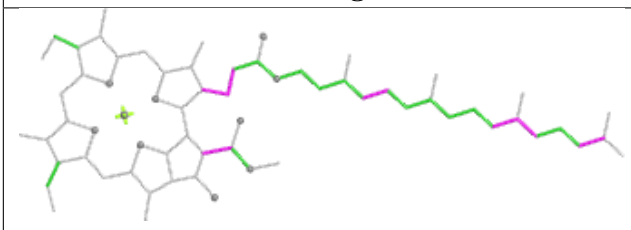
Ligand CLA N 305



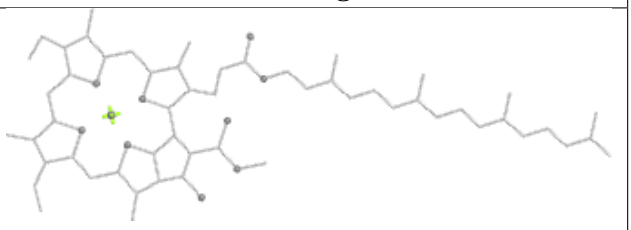
Bond lengths



Bond angles

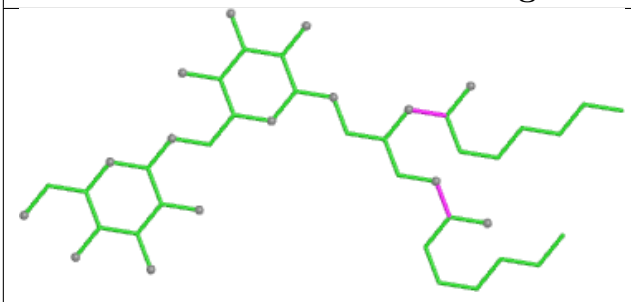


Torsions

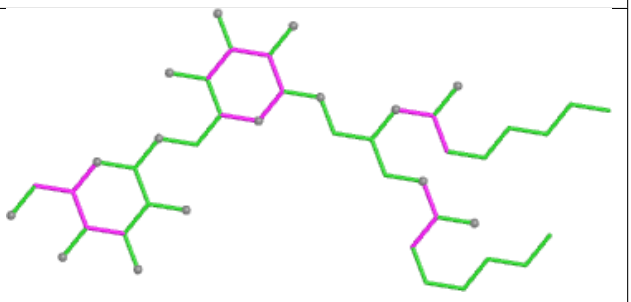


Rings

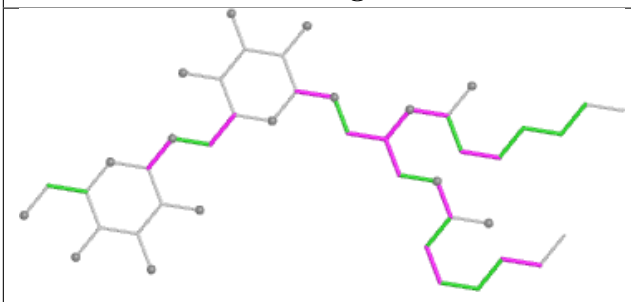
Ligand DGD G 521



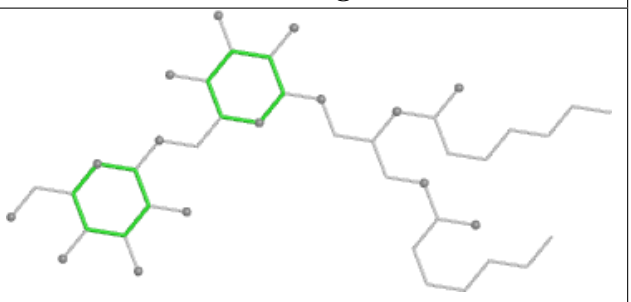
Bond lengths



Bond angles



Torsions

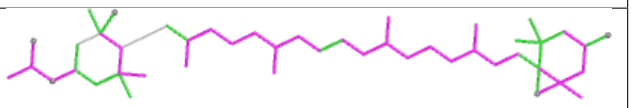


Rings

Ligand UIX O 306



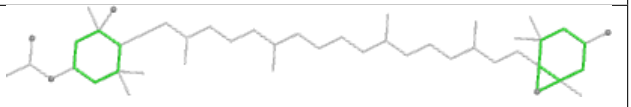
Bond lengths



Bond angles

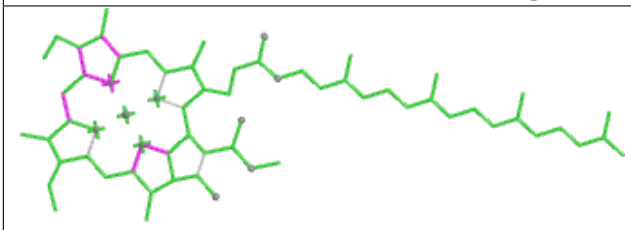


Torsions

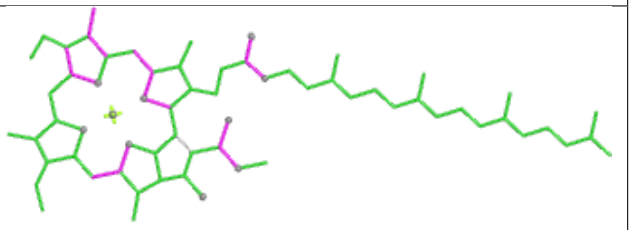


Rings

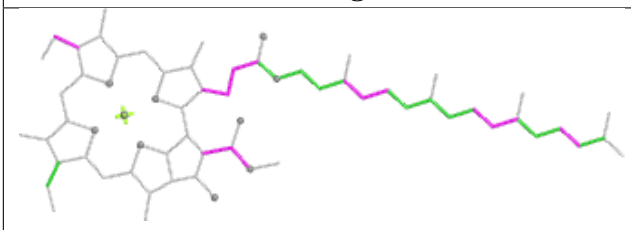
Ligand CLA P 210



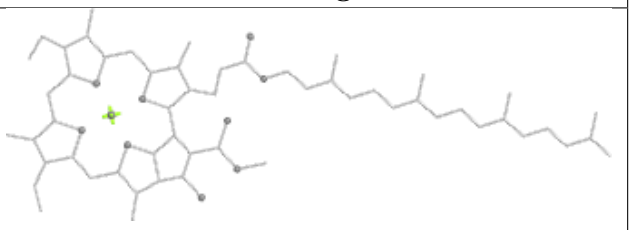
Bond lengths



Bond angles

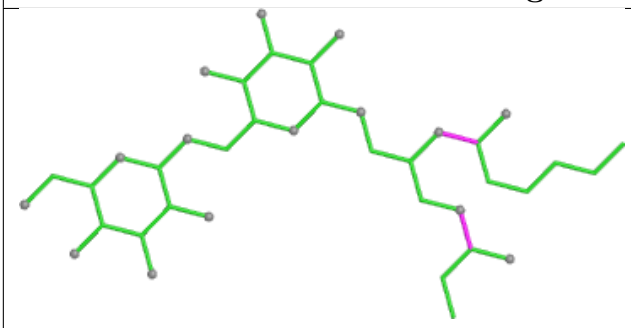


Torsions

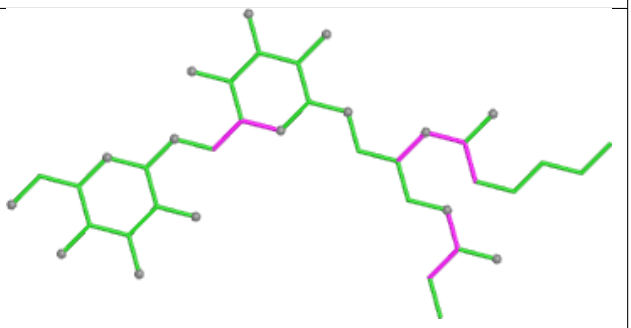


Rings

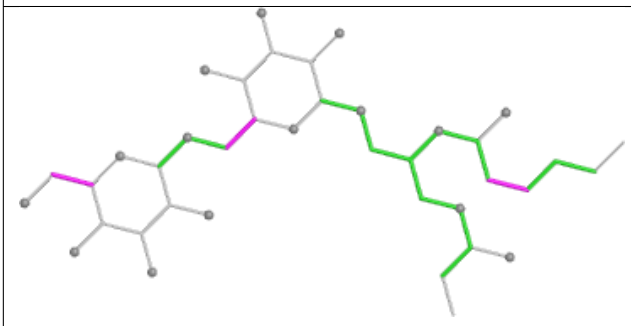
Ligand DGD I 317



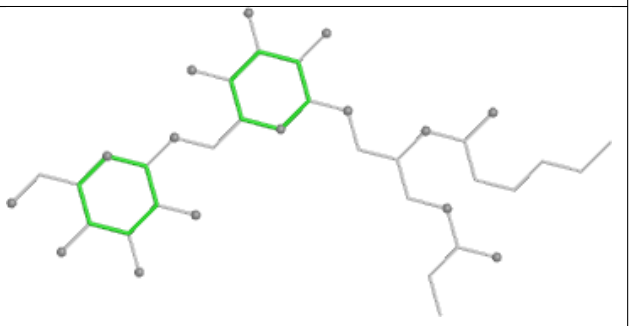
Bond lengths



Bond angles

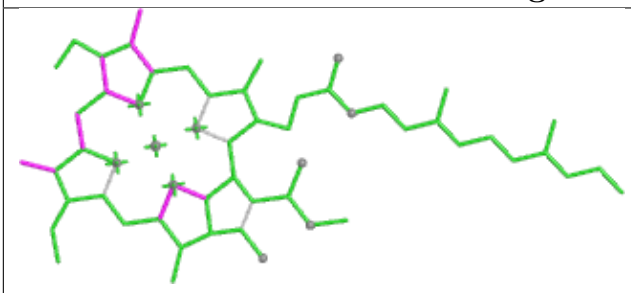


Torsions

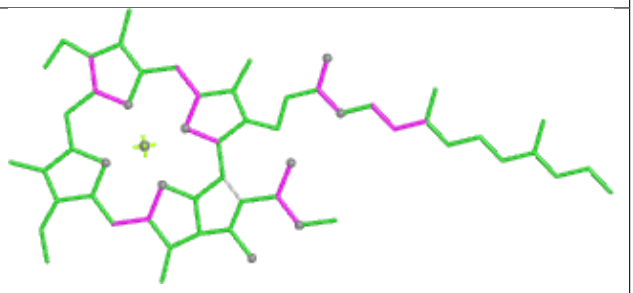


Rings

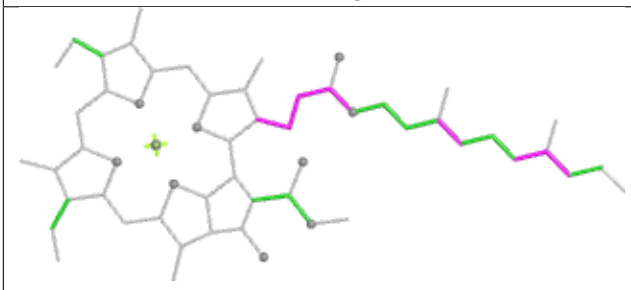
Ligand CLA a 717



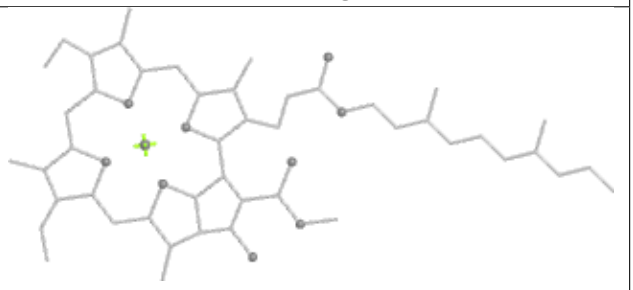
Bond lengths



Bond angles

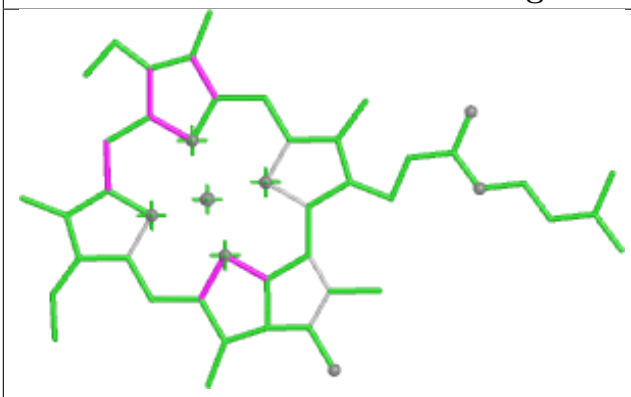


Torsions

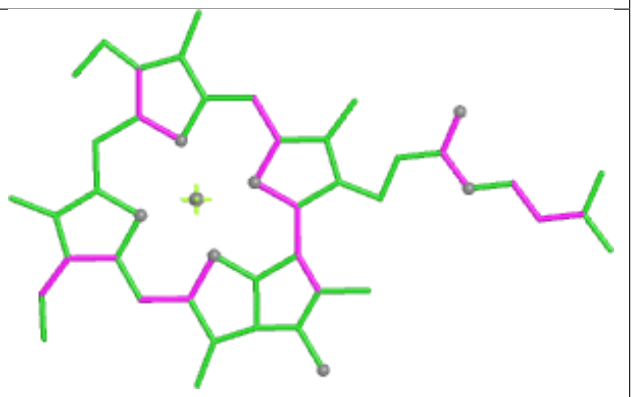


Rings

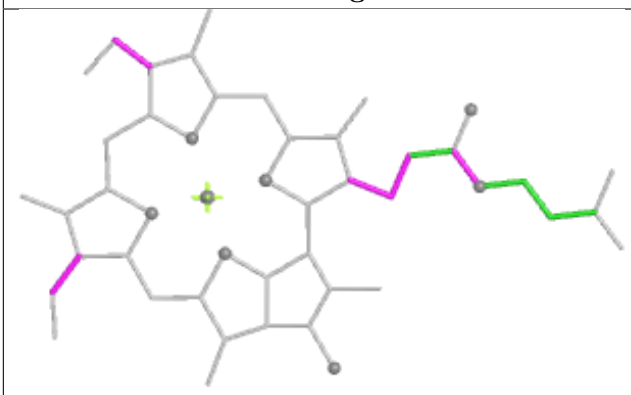
Ligand CLA L 308



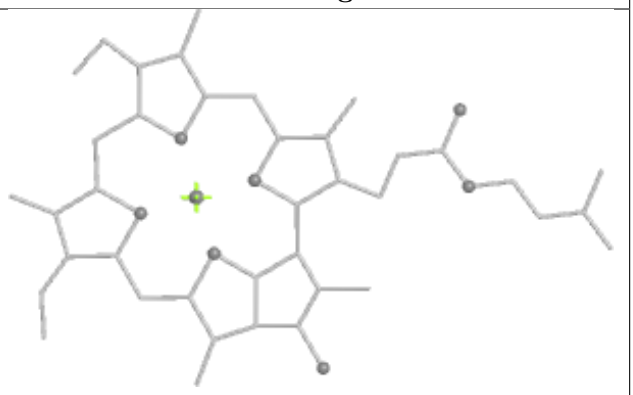
Bond lengths



Bond angles

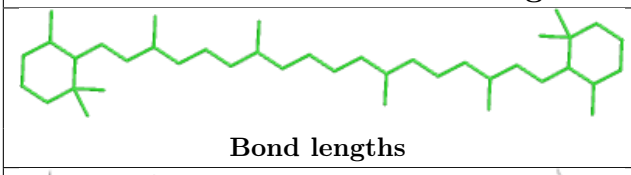


Torsions

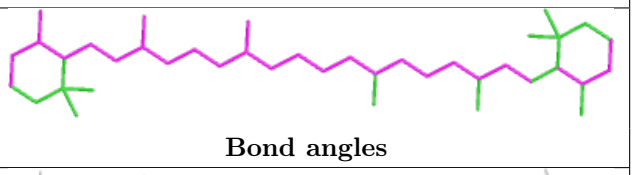


Rings

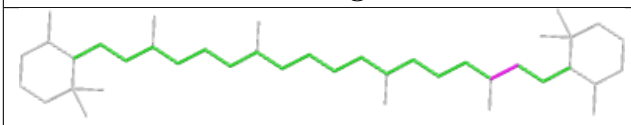
Ligand BCR b 702



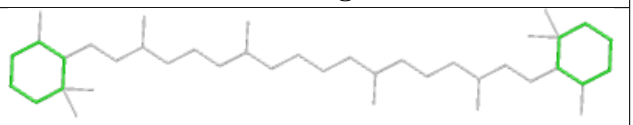
Bond lengths



Bond angles

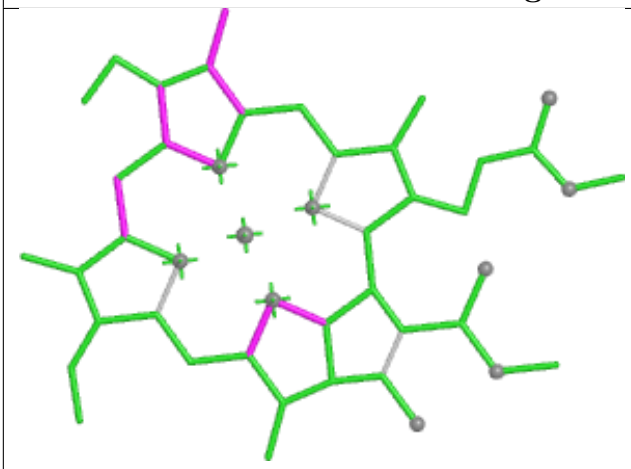


Torsions

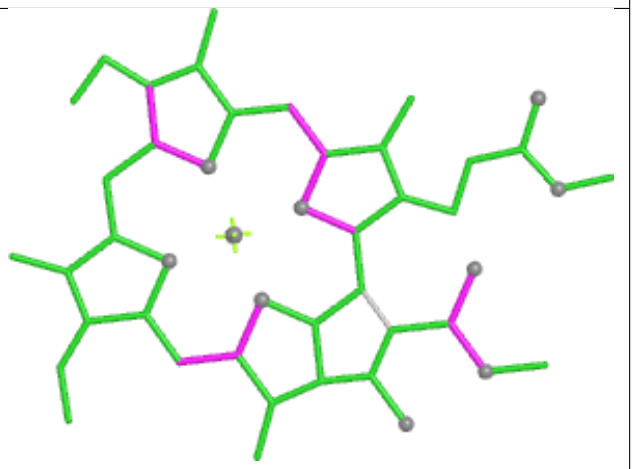


Rings

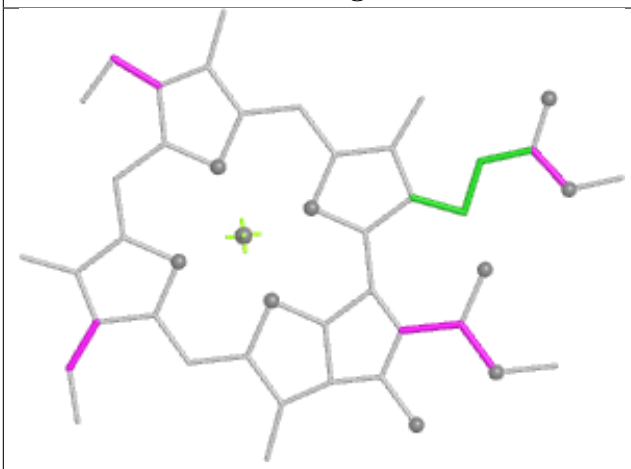
Ligand CLA B 316



Bond lengths



Bond angles

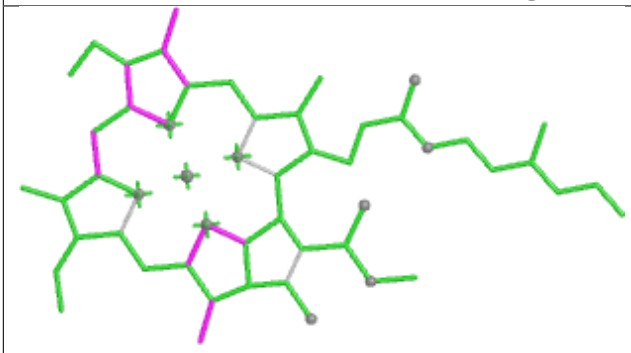


Torsions

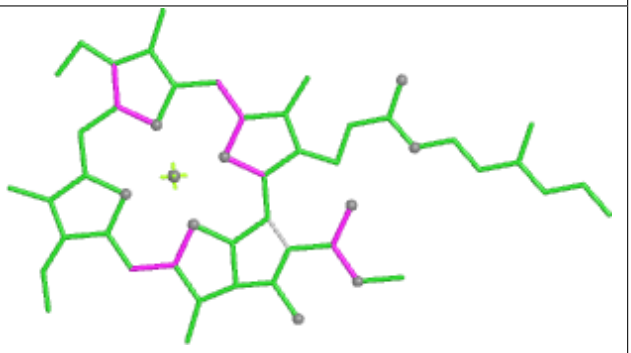


Rings

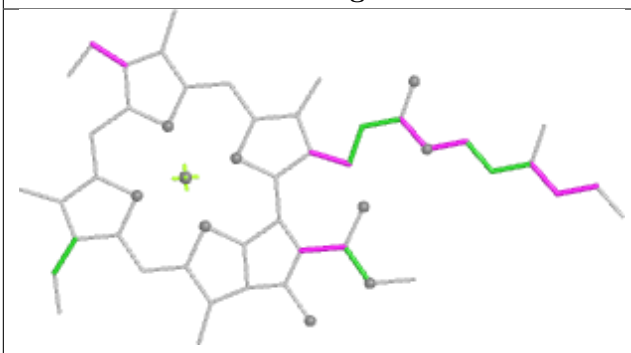
Ligand CLA K 311



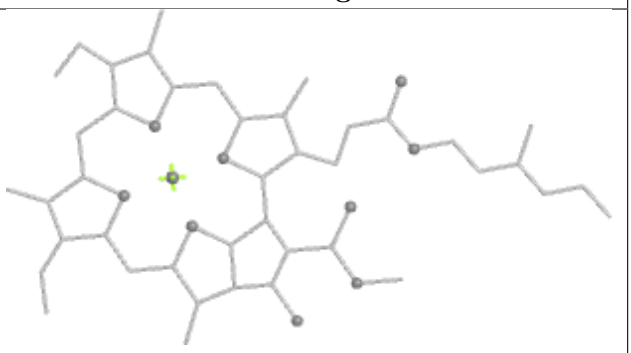
Bond lengths



Bond angles

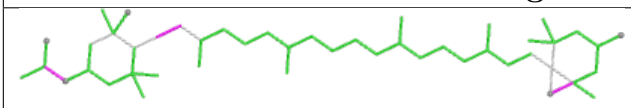


Torsions

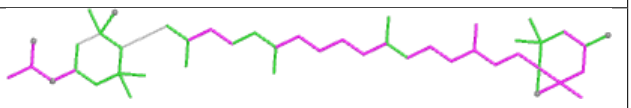


Rings

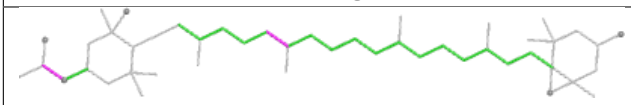
Ligand UIX G 503



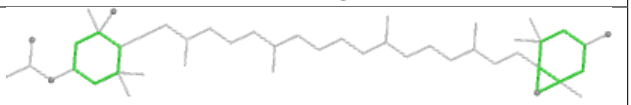
Bond lengths



Bond angles

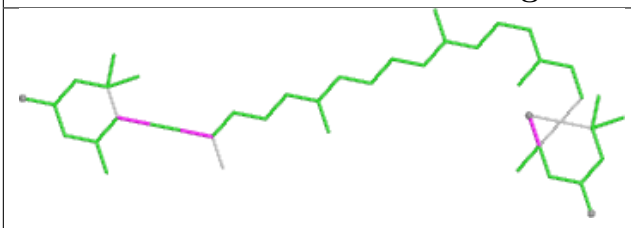


Torsions

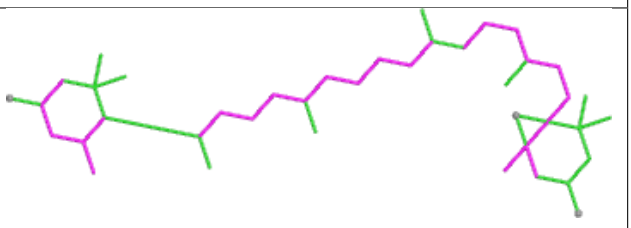


Rings

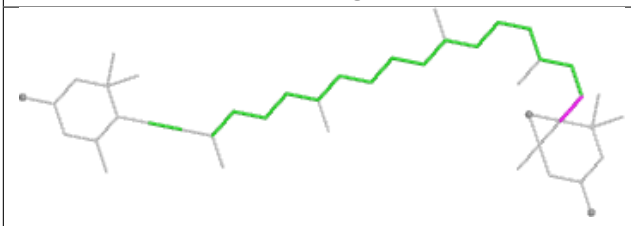
Ligand DD6 M 305



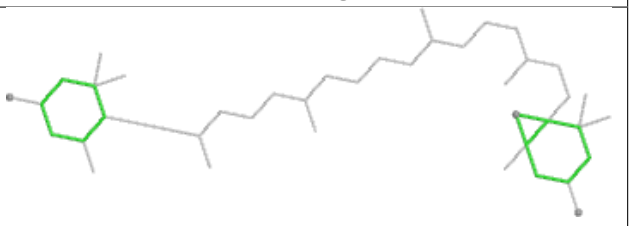
Bond lengths



Bond angles

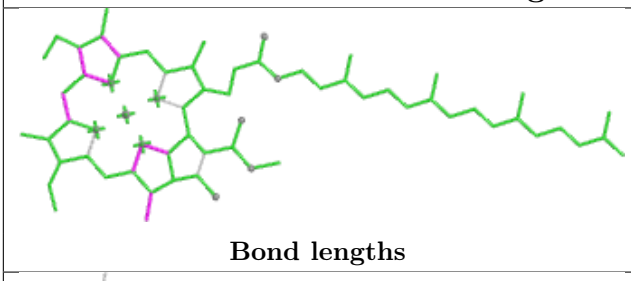


Torsions

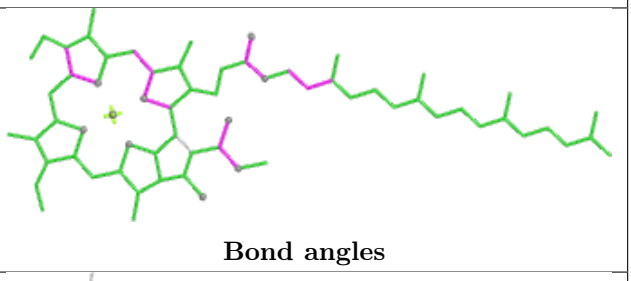


Rings

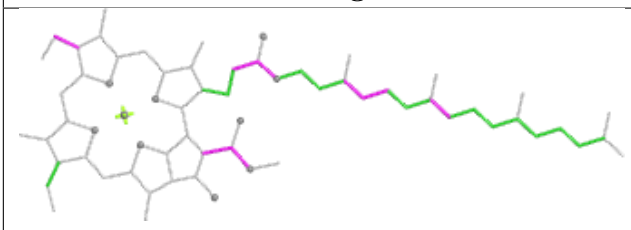
Ligand CLA b 703



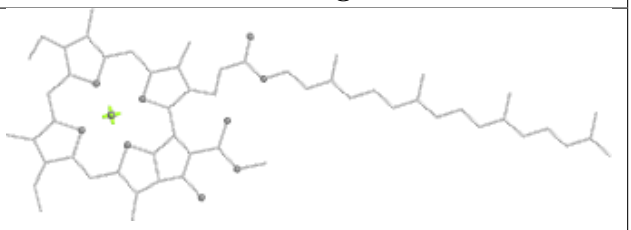
Bond lengths



Bond angles

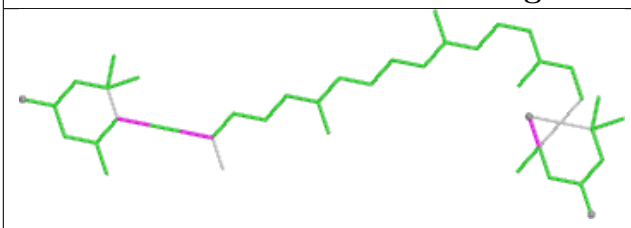


Torsions

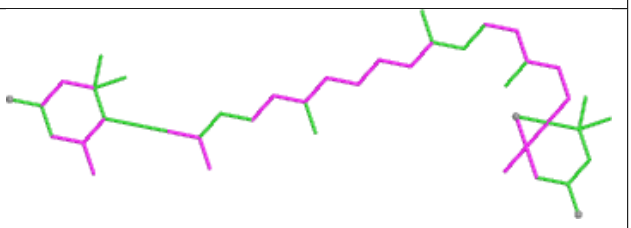


Rings

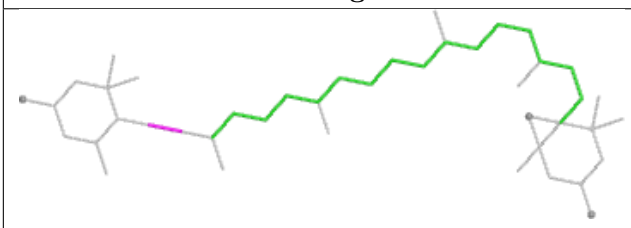
Ligand DD6 K 304



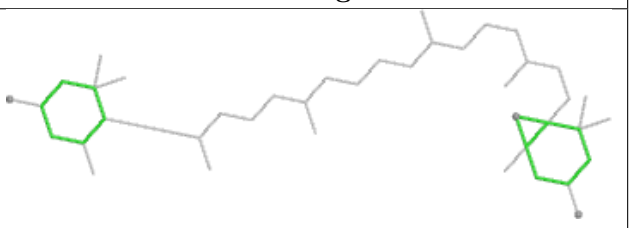
Bond lengths



Bond angles

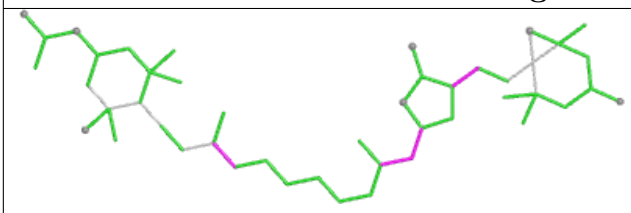


Torsions

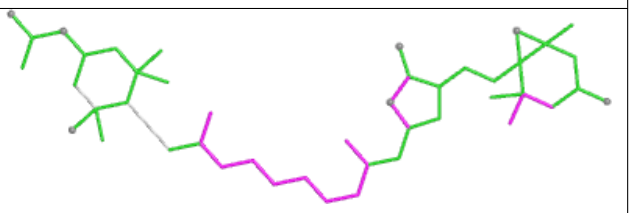


Rings

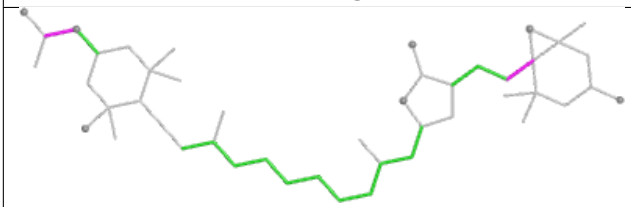
Ligand PID P 202



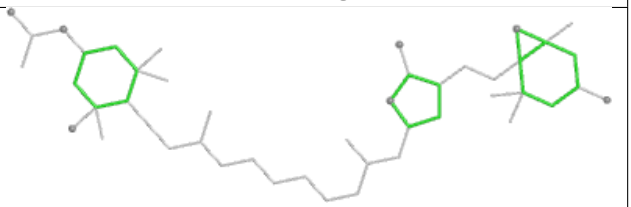
Bond lengths



Bond angles

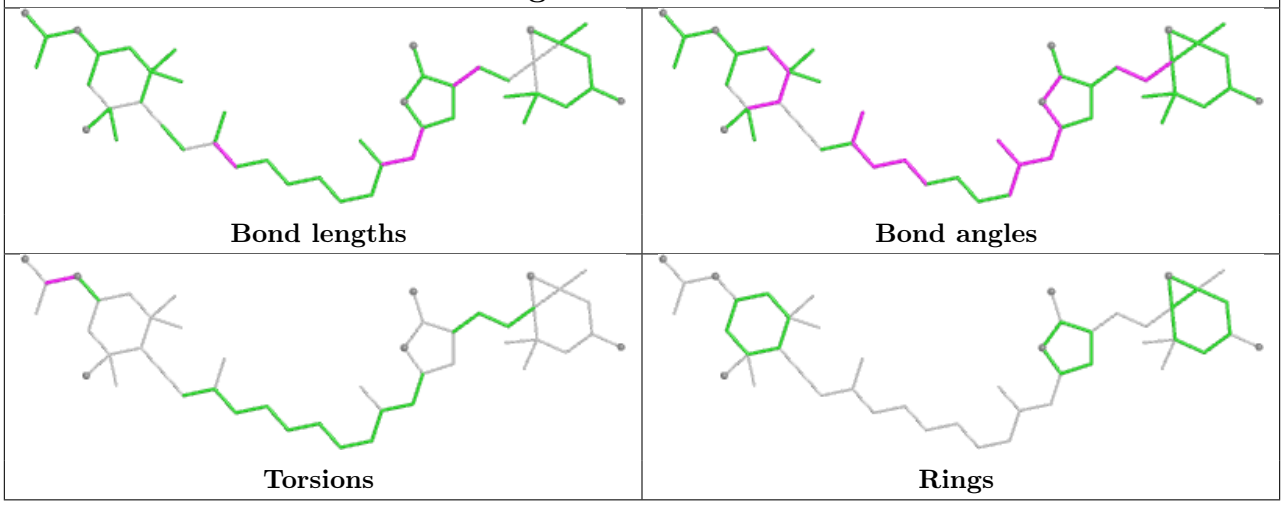


Torsions

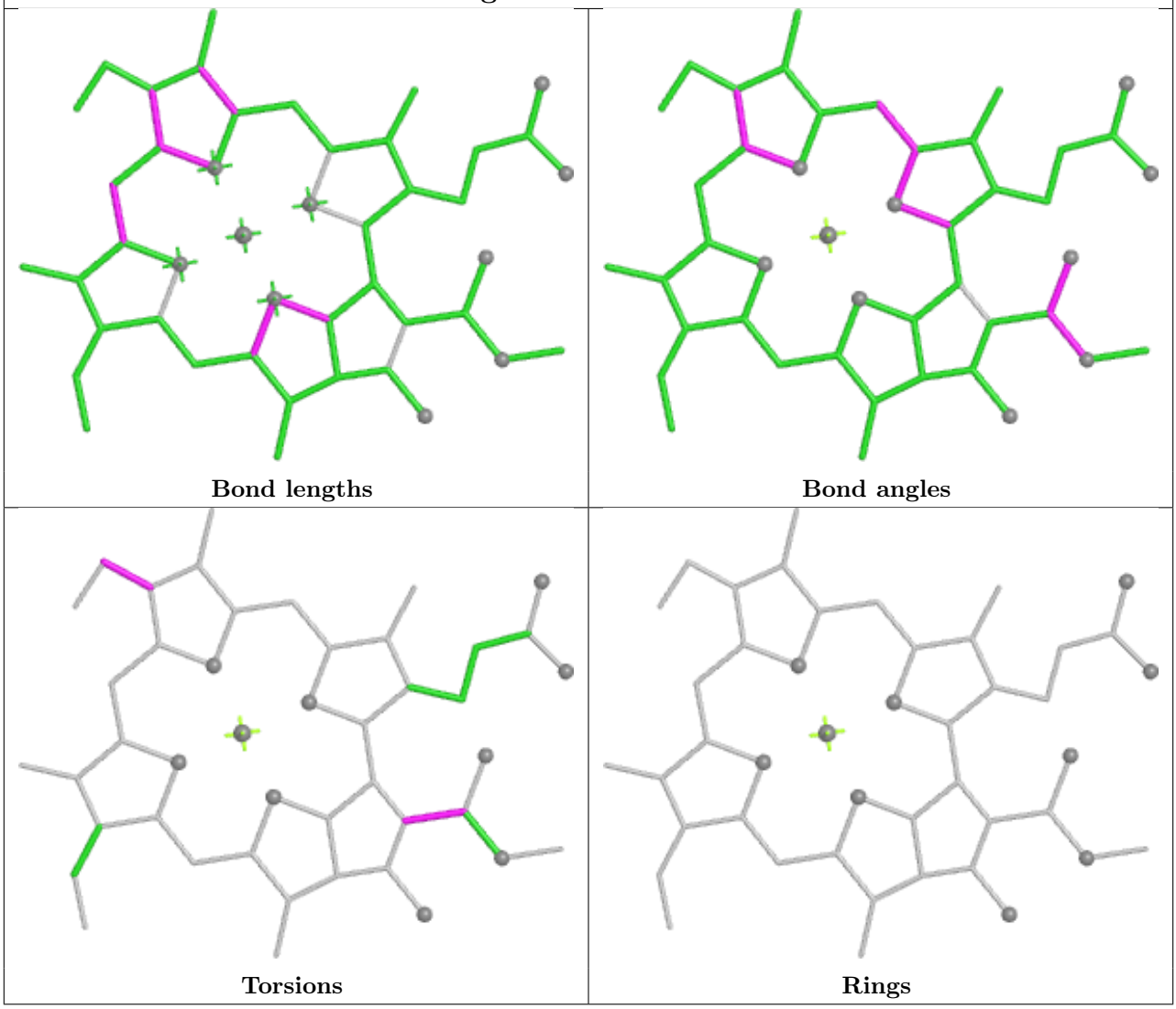


Rings

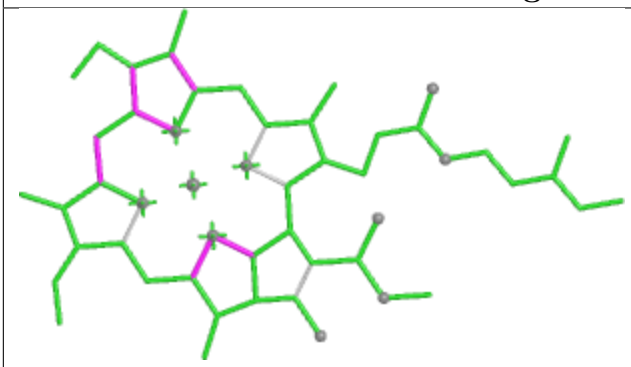
Ligand PID N 302



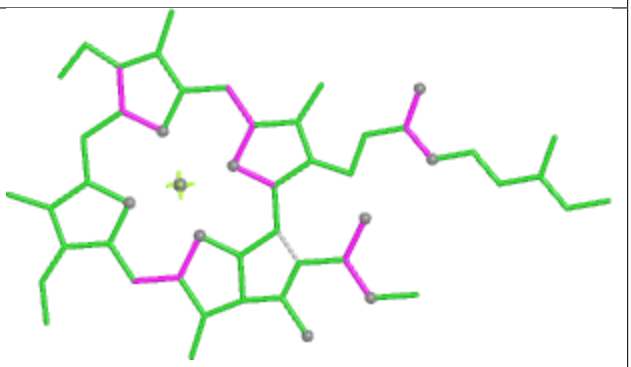
Ligand CLA A 307



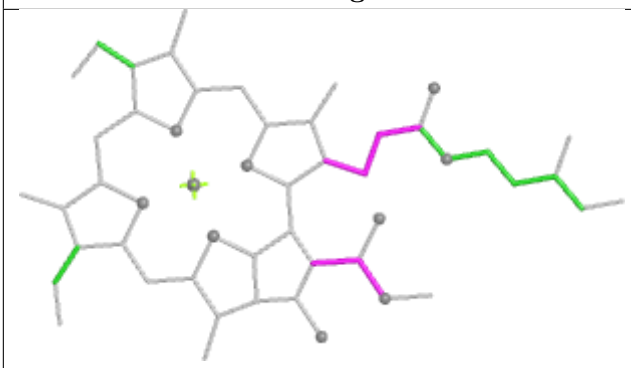
Ligand CLA H 307



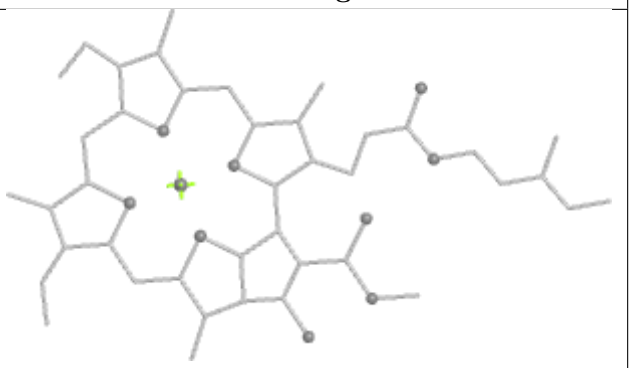
Bond lengths



Bond angles

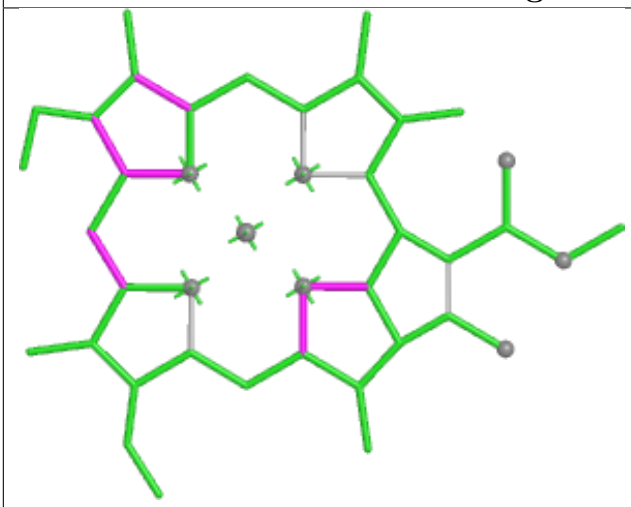


Torsions

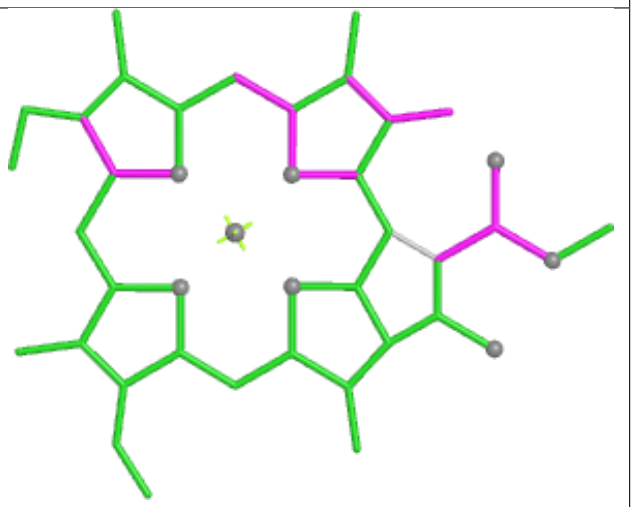


Rings

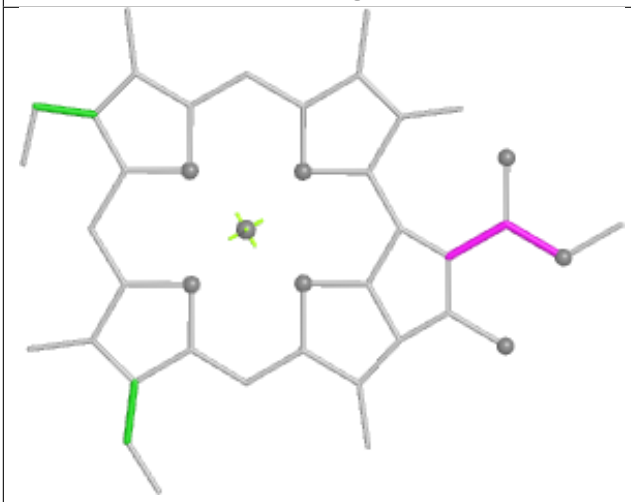
Ligand CLA F 315



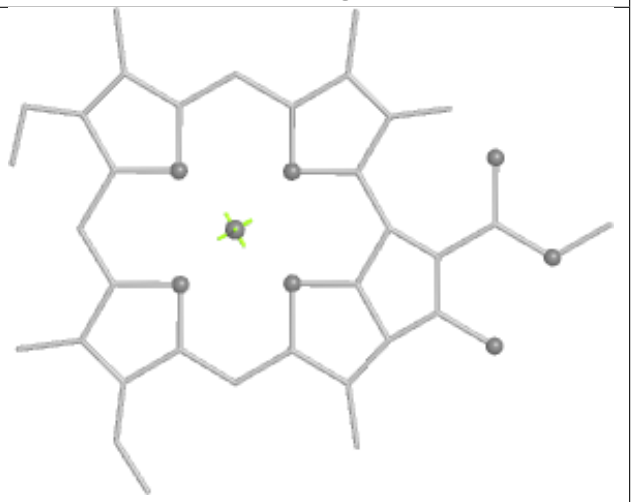
Bond lengths



Bond angles

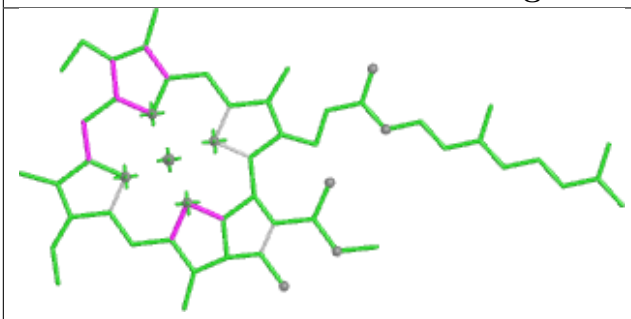


Torsions

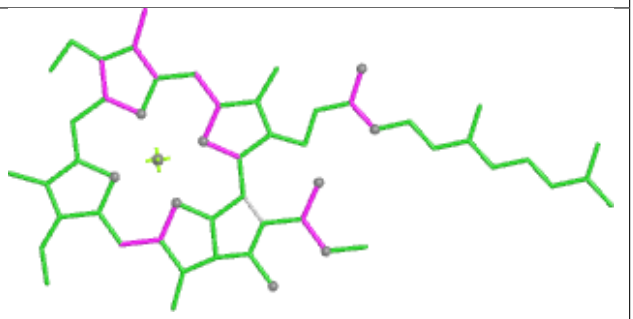


Rings

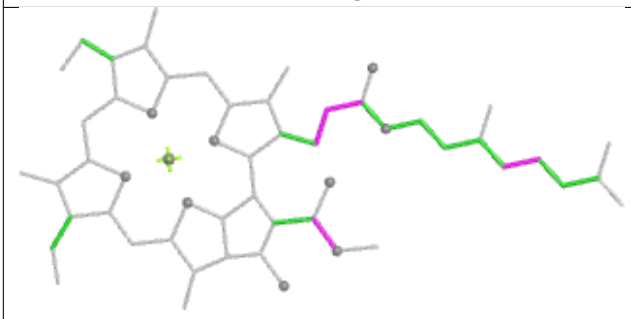
Ligand CLA A 308



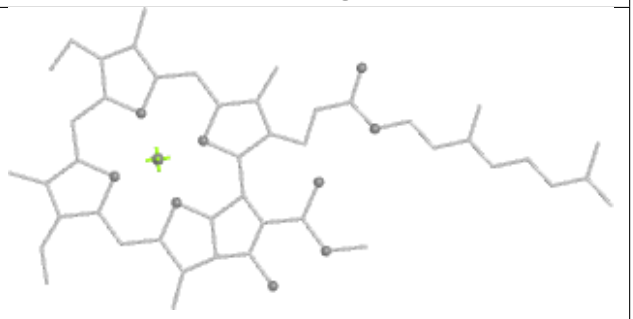
Bond lengths



Bond angles

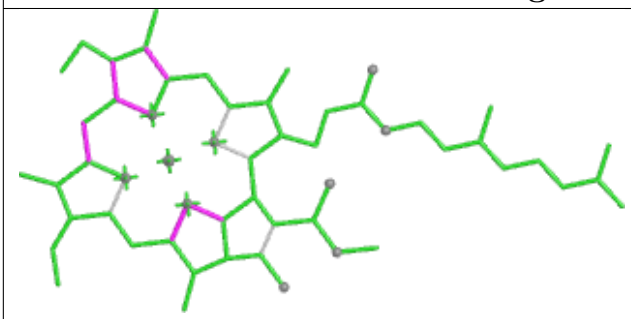


Torsions

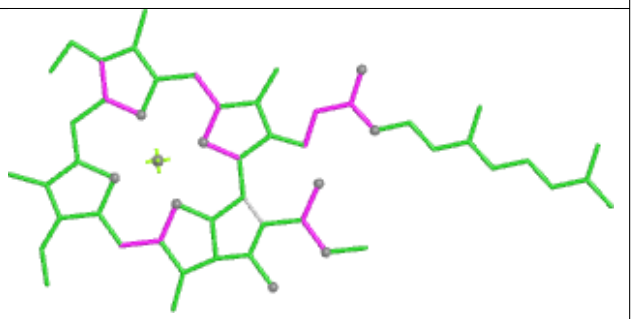


Rings

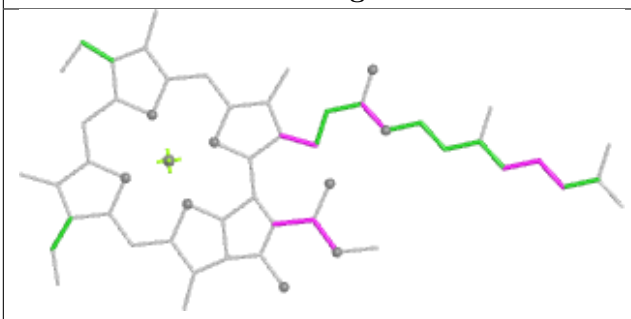
Ligand CLA a 705



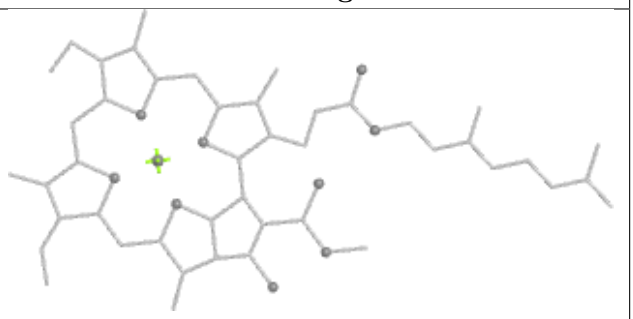
Bond lengths



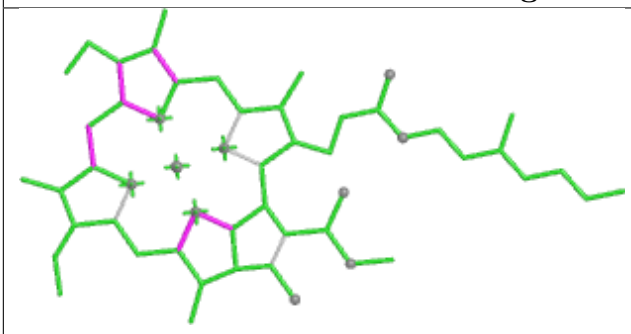
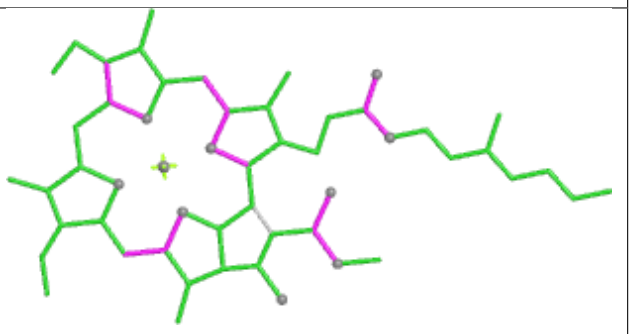
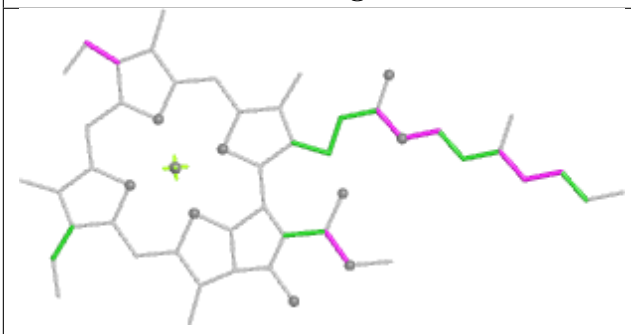
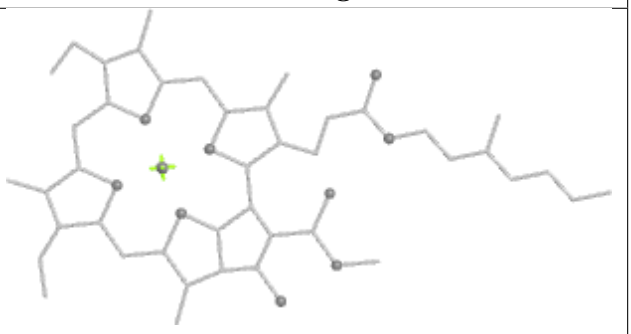
Bond angles

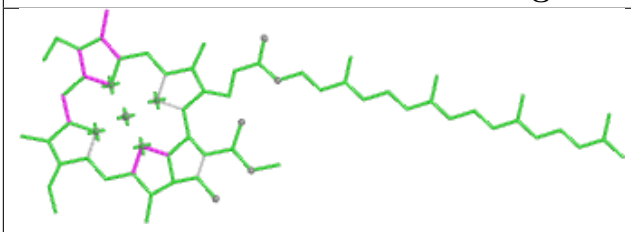
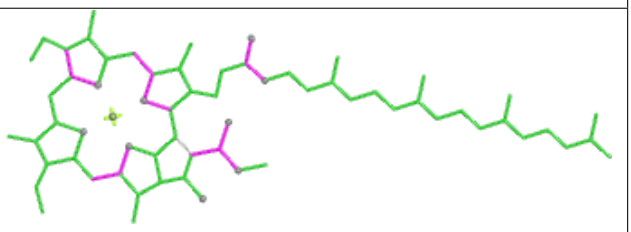
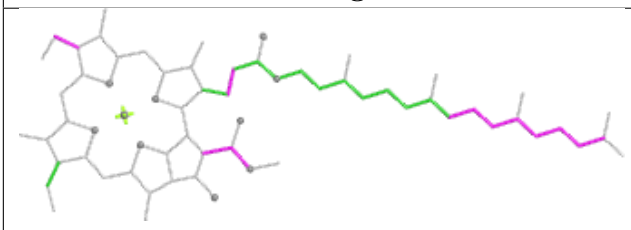
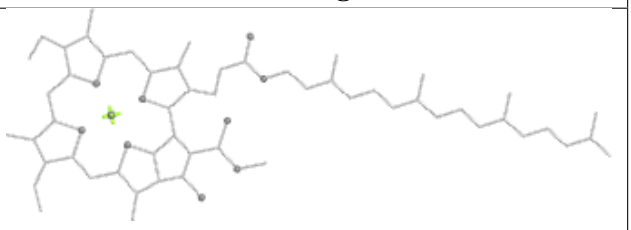


Torsions

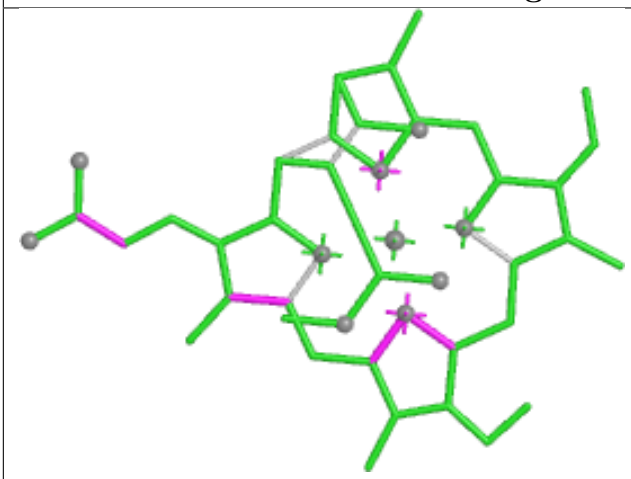


Rings

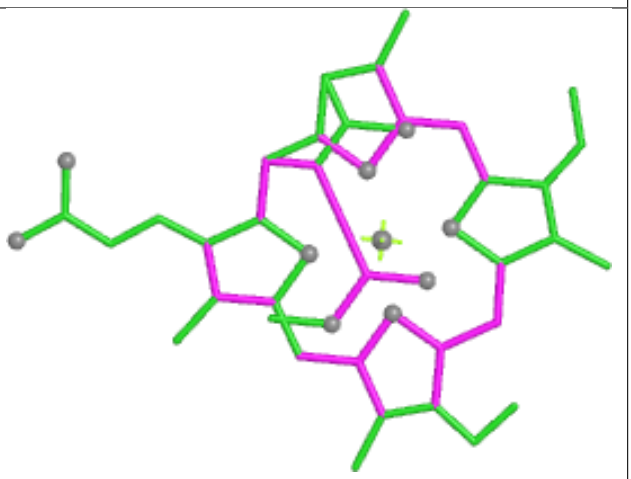
Ligand CLA M 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA l 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

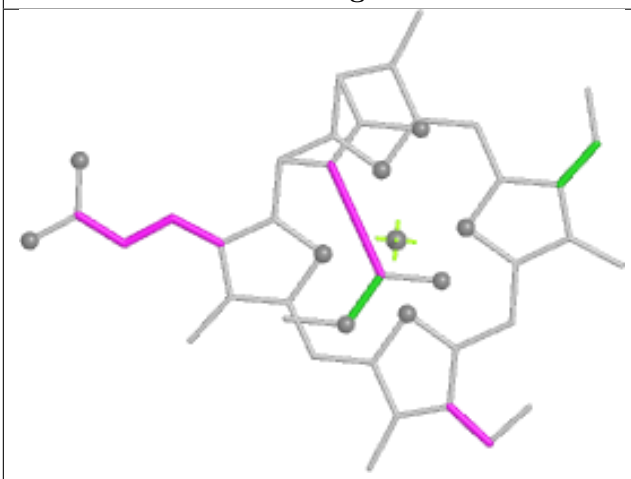
Ligand KC1 K 314



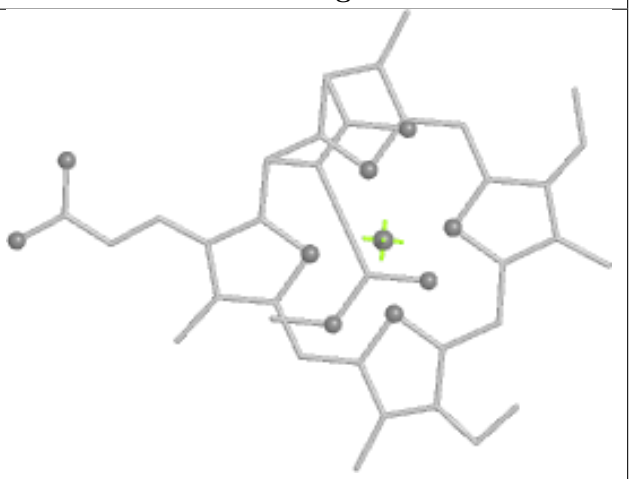
Bond lengths



Bond angles

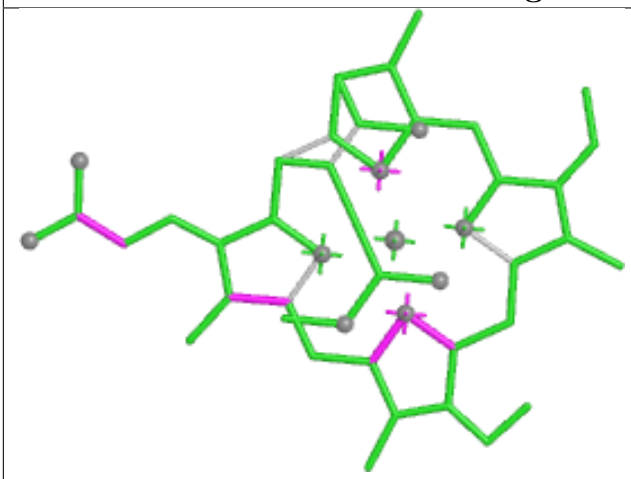


Torsions

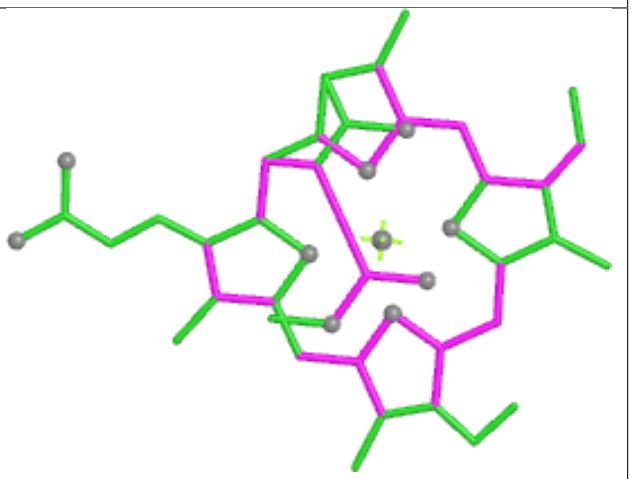


Rings

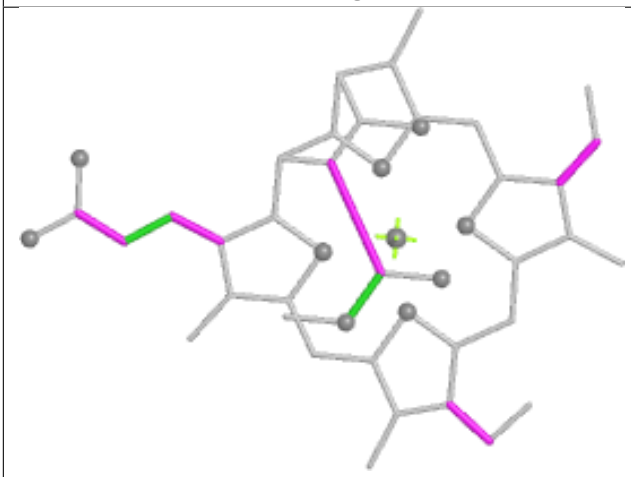
Ligand KC1 G 515



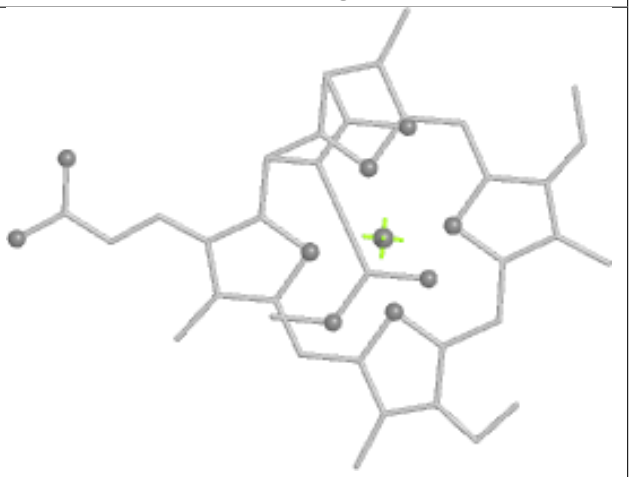
Bond lengths



Bond angles

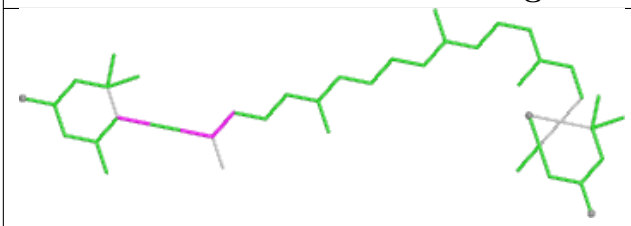


Torsions

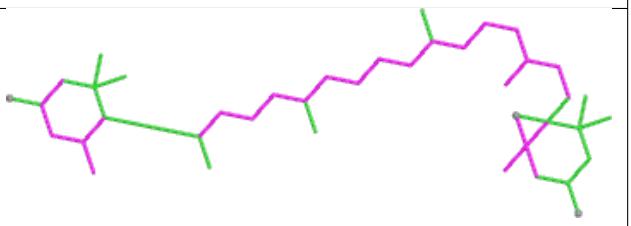


Rings

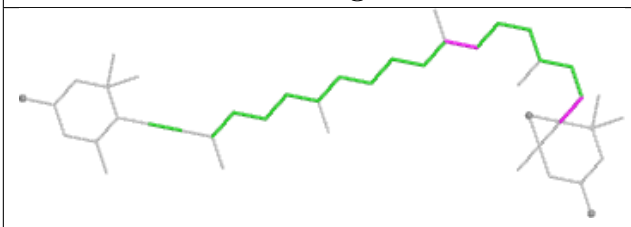
Ligand DD6 A 302



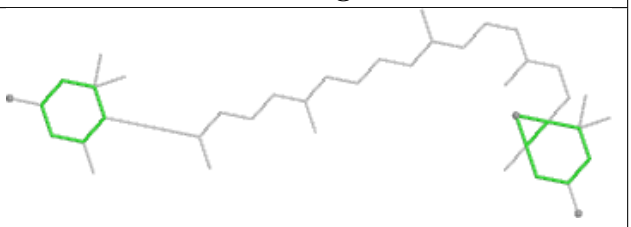
Bond lengths



Bond angles

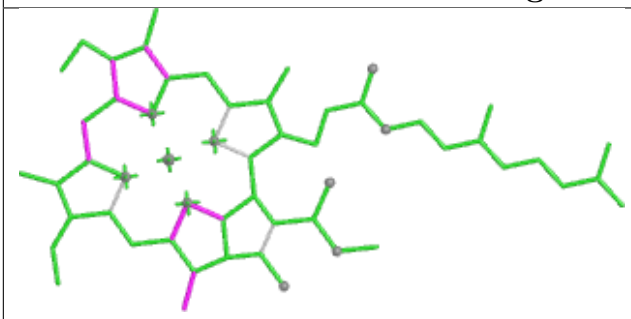


Torsions

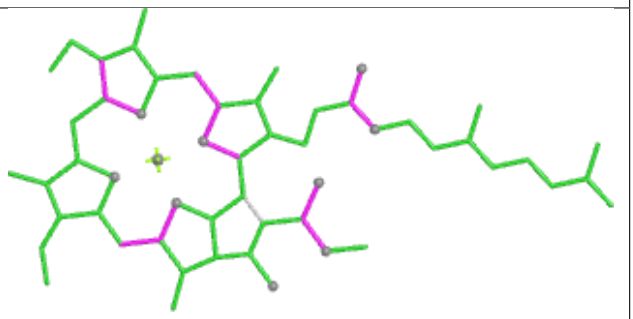


Rings

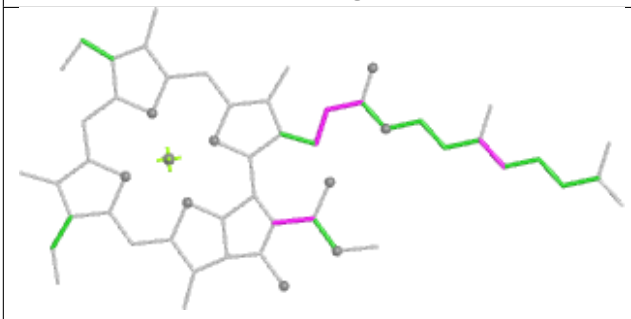
Ligand CLA L 311



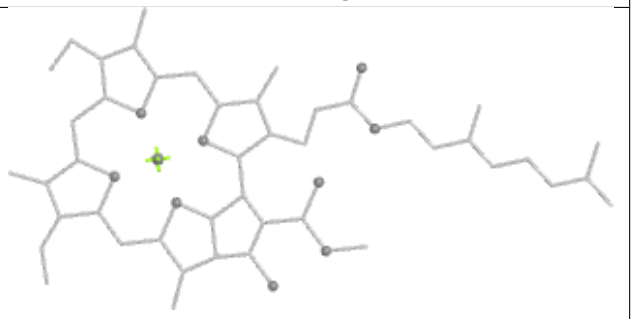
Bond lengths



Bond angles

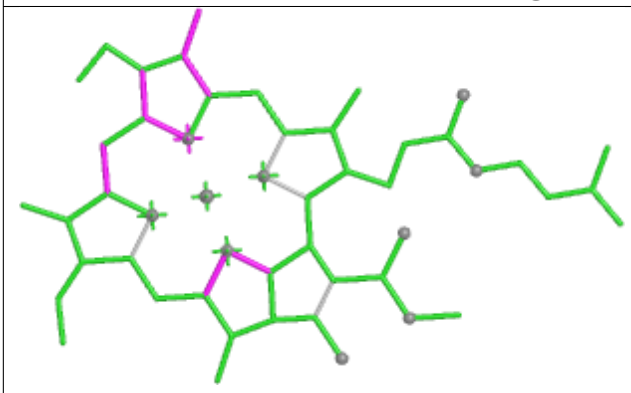


Torsions

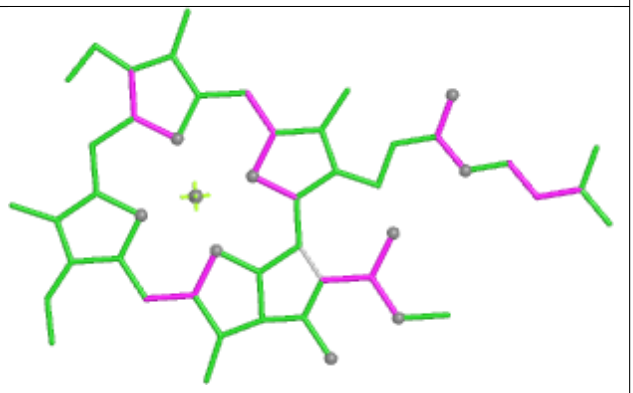


Rings

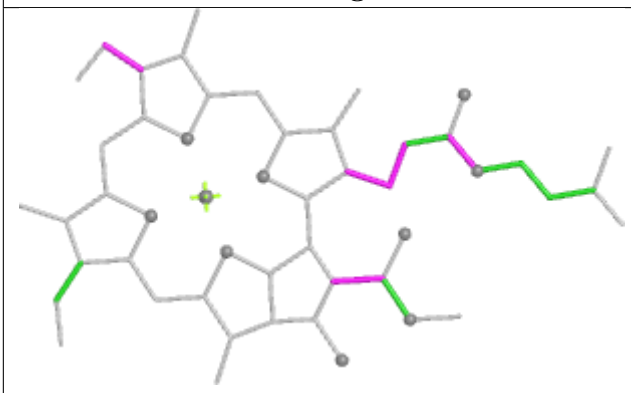
Ligand CLA b 723



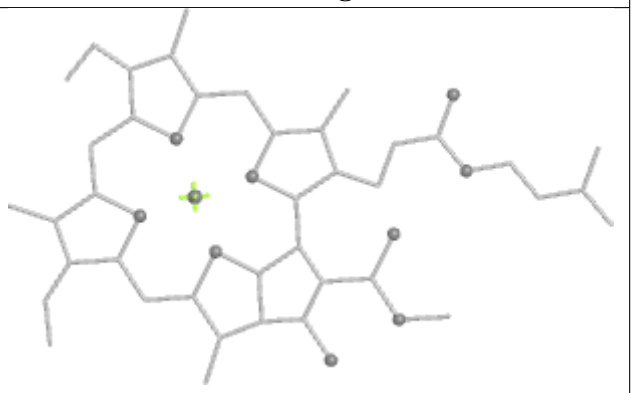
Bond lengths



Bond angles

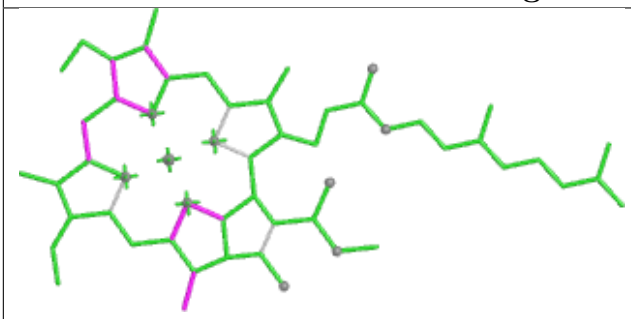


Torsions

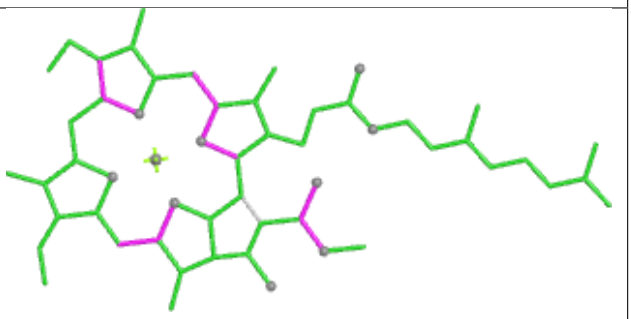


Rings

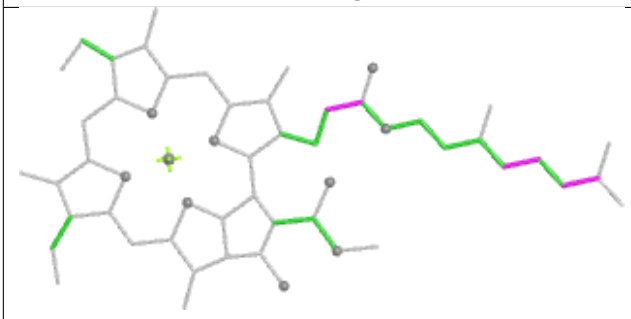
Ligand CLA G 511



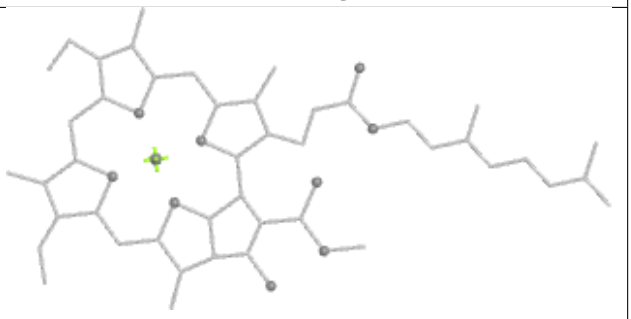
Bond lengths



Bond angles

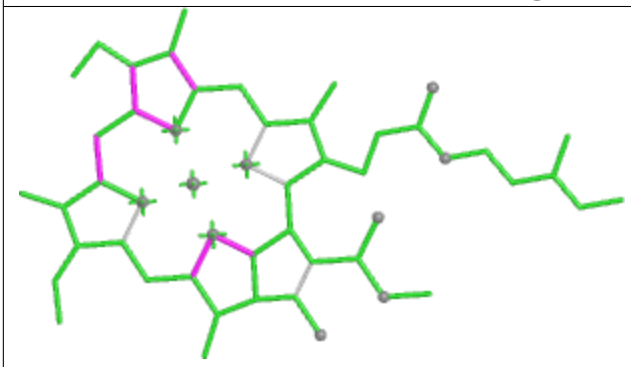


Torsions

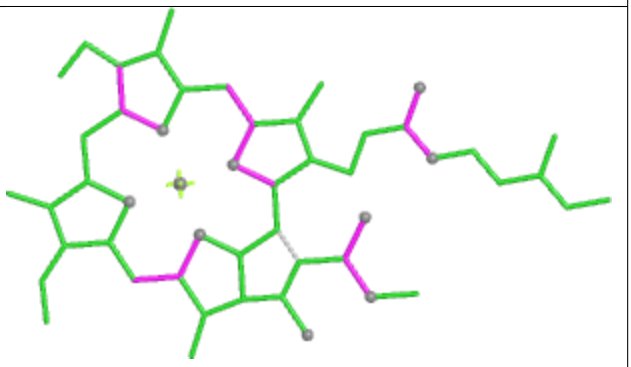


Rings

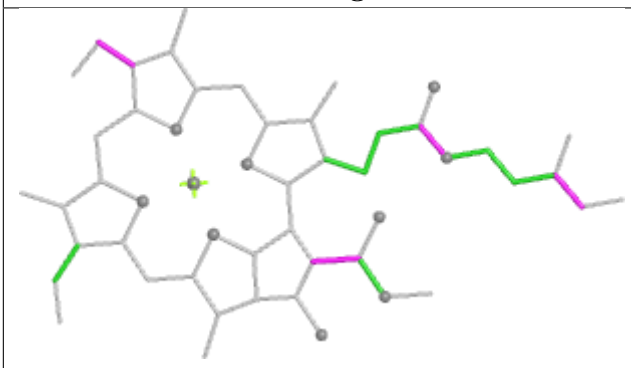
Ligand CLA a 708



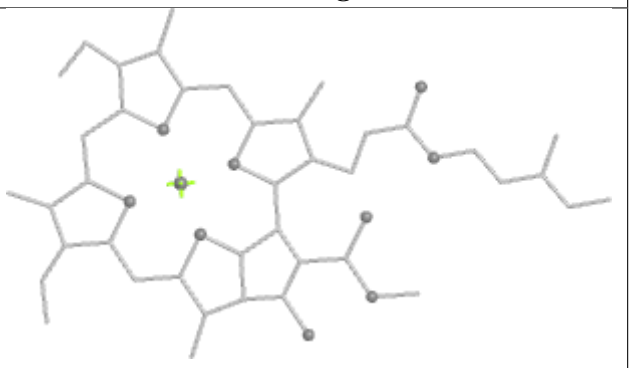
Bond lengths



Bond angles

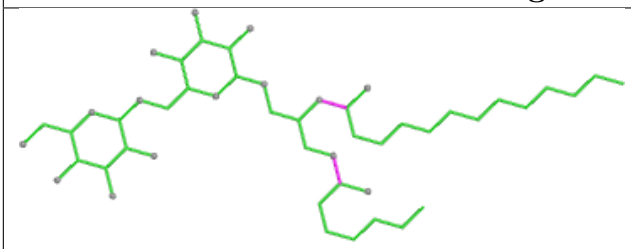


Torsions

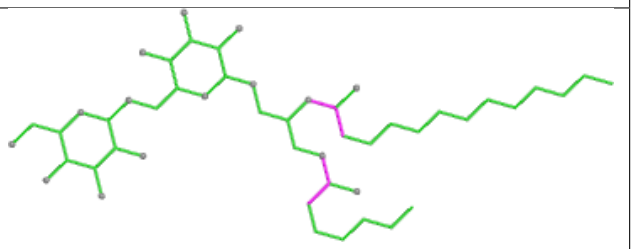


Rings

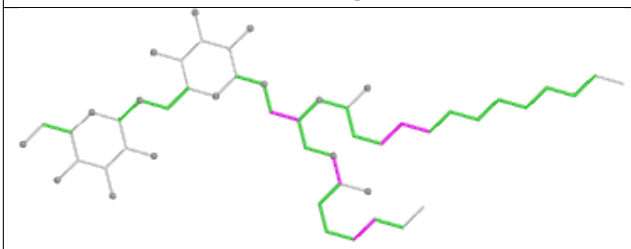
Ligand DGD l 301



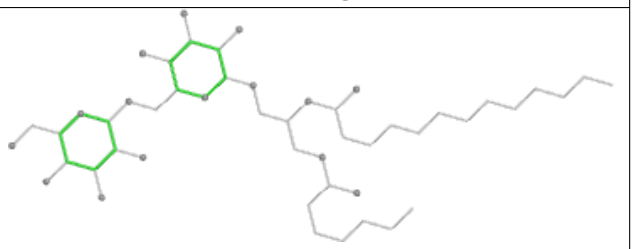
Bond lengths



Bond angles

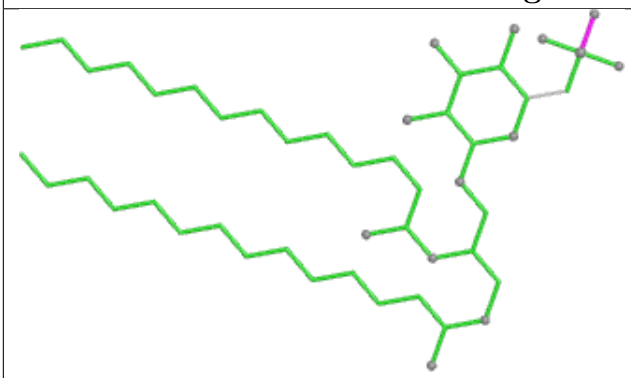


Torsions

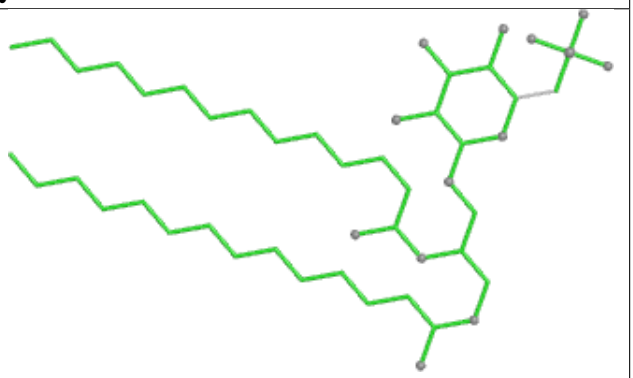


Rings

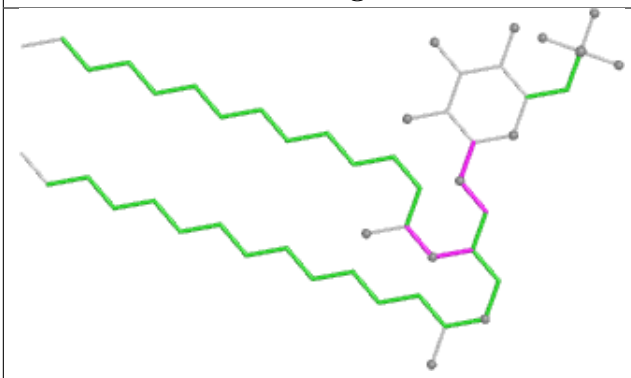
Ligand SQD A 318



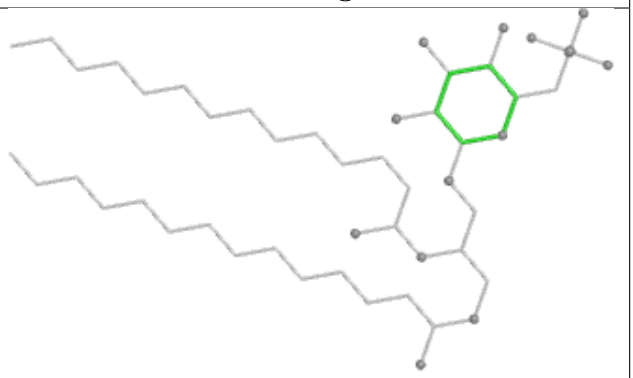
Bond lengths



Bond angles

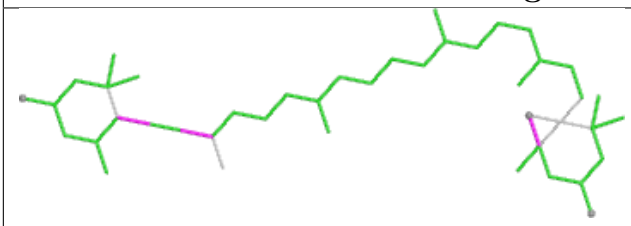


Torsions

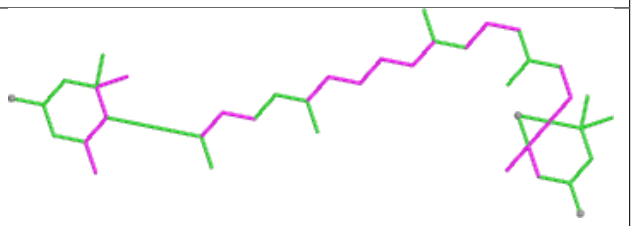


Rings

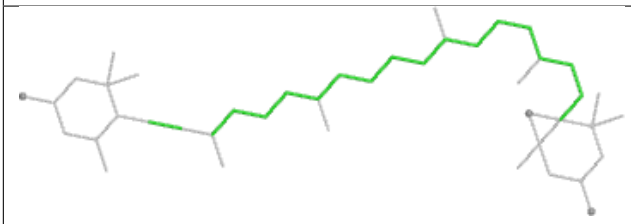
Ligand DD6 K 303



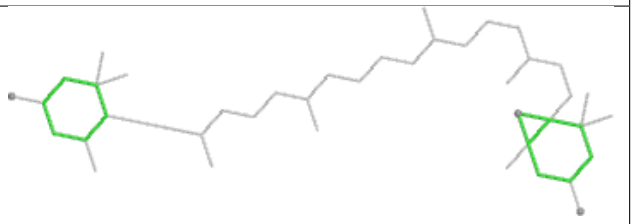
Bond lengths



Bond angles

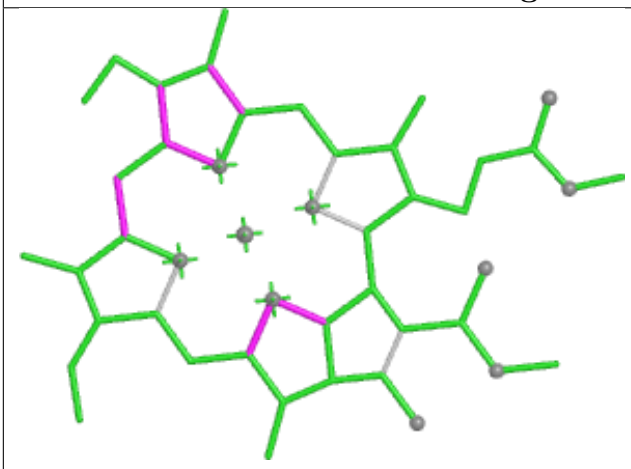


Torsions

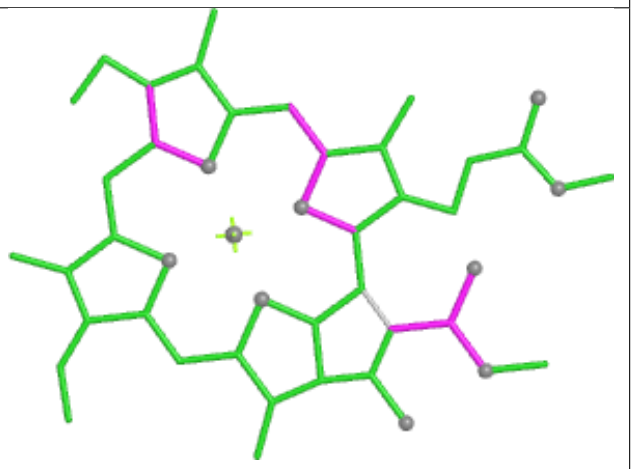


Rings

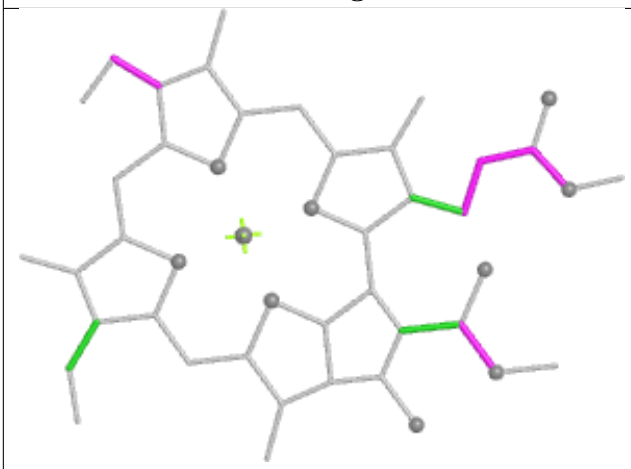
Ligand CLA M 317



Bond lengths



Bond angles

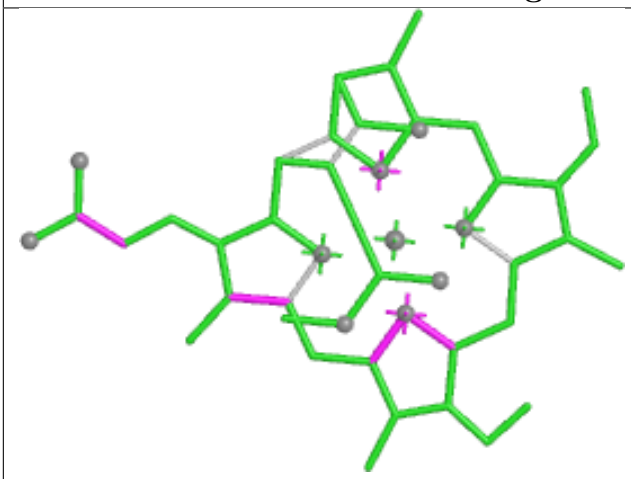


Torsions

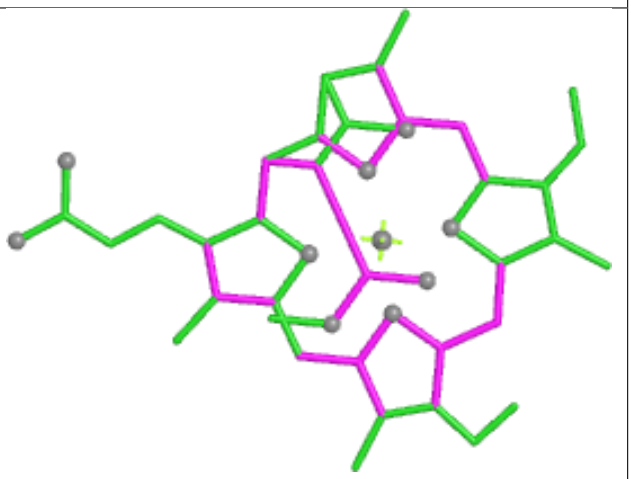


Rings

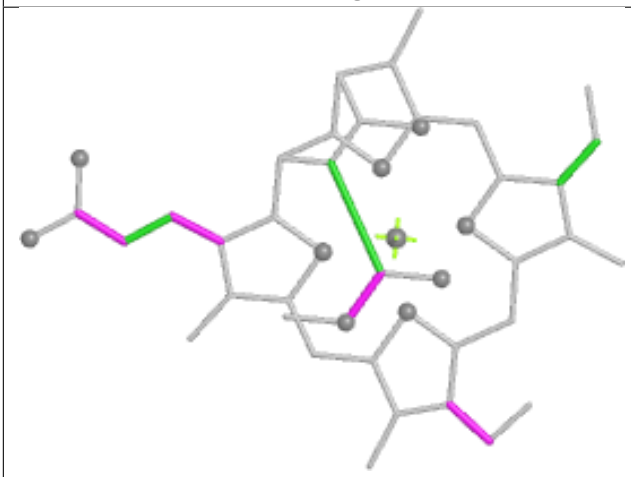
Ligand KC1 N 306



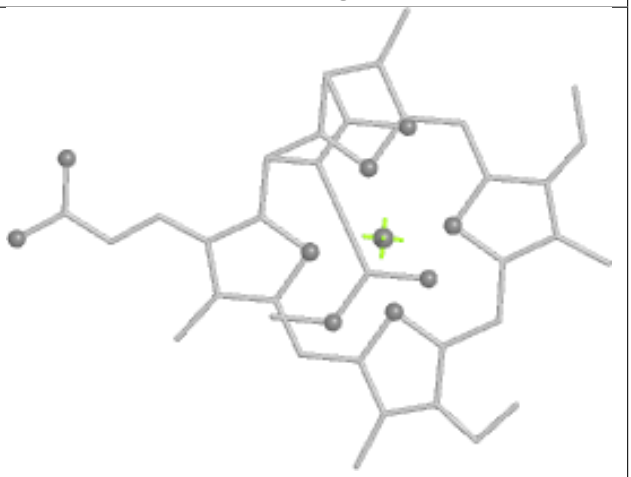
Bond lengths



Bond angles



Torsions

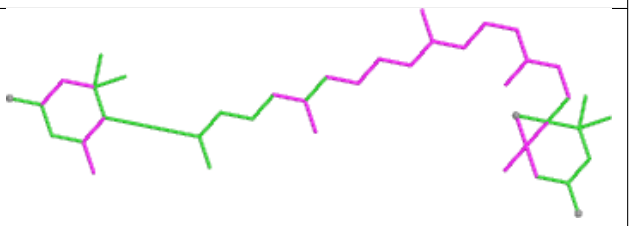


Rings

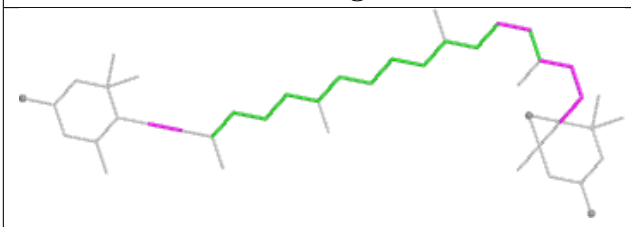
Ligand DD6 D 303



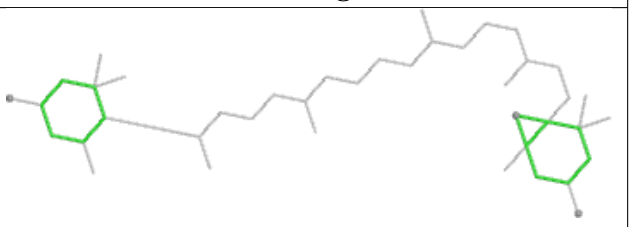
Bond lengths



Bond angles

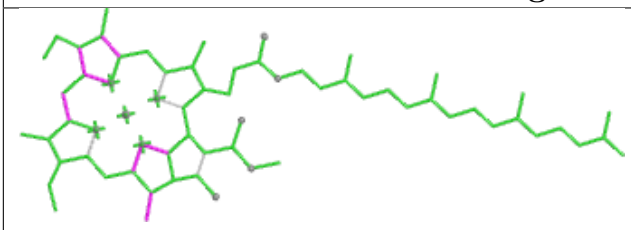


Torsions

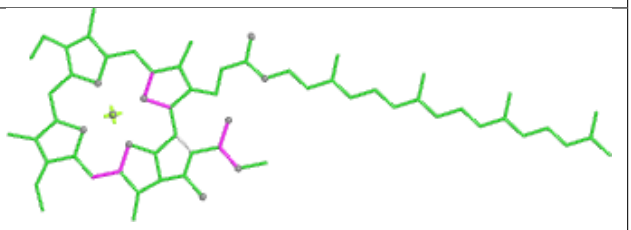


Rings

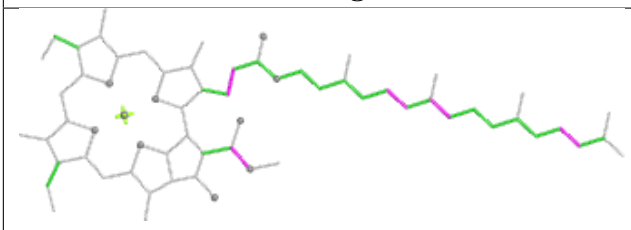
Ligand CLA a 704



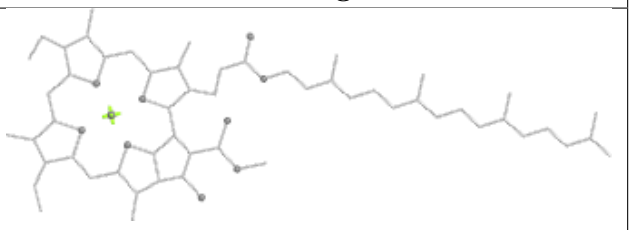
Bond lengths



Bond angles

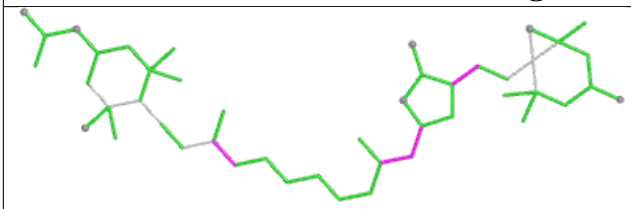


Torsions

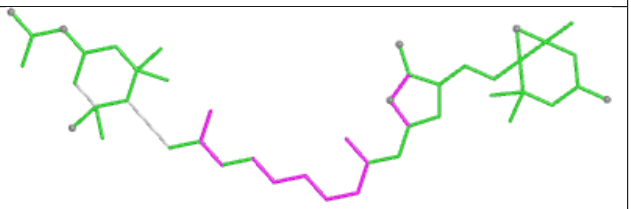


Rings

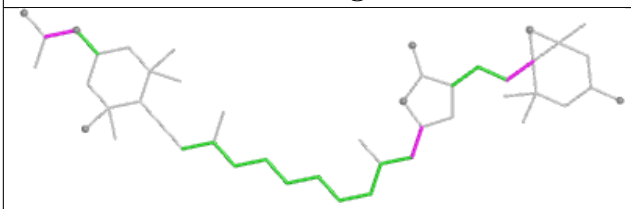
Ligand PID H 301



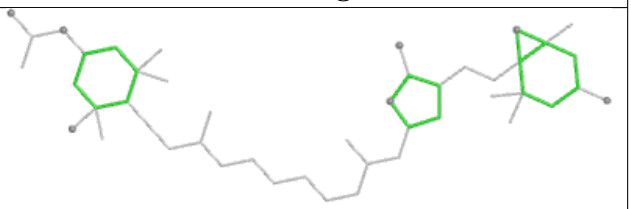
Bond lengths



Bond angles



Torsions

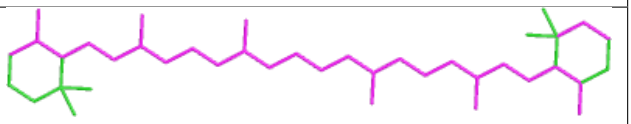


Rings

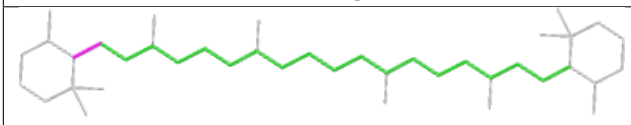
Ligand BCR b 732



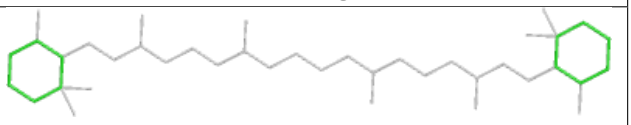
Bond lengths



Bond angles

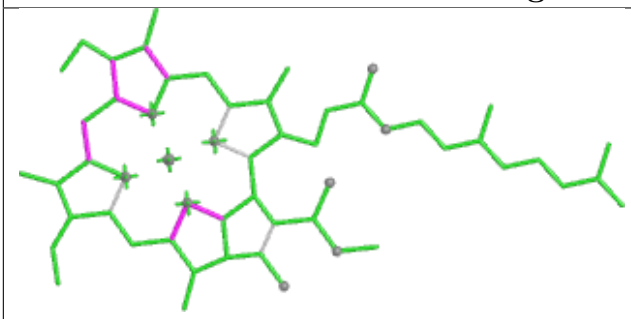


Torsions

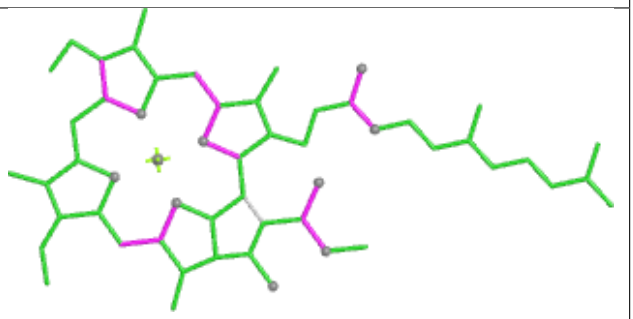


Rings

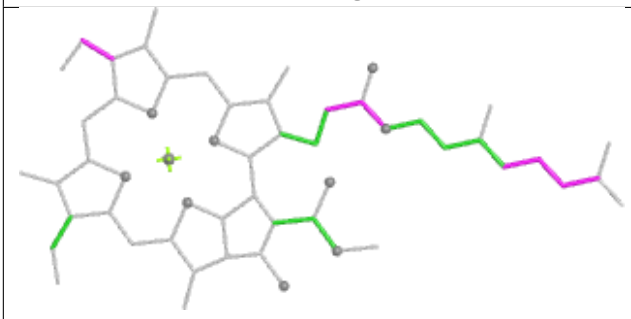
Ligand CLA h 202



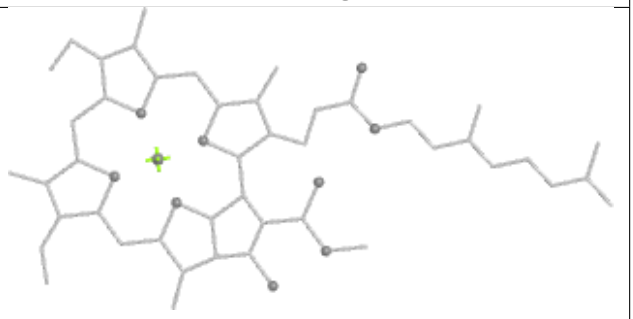
Bond lengths



Bond angles

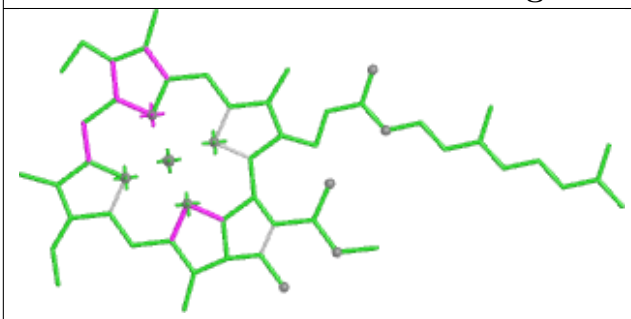


Torsions

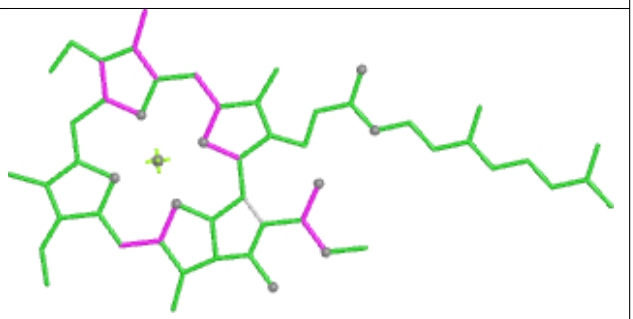


Rings

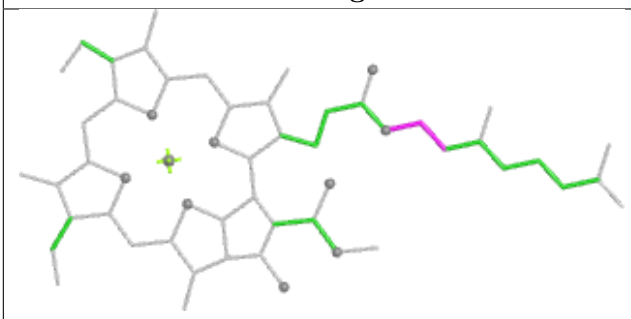
Ligand CLA L 310



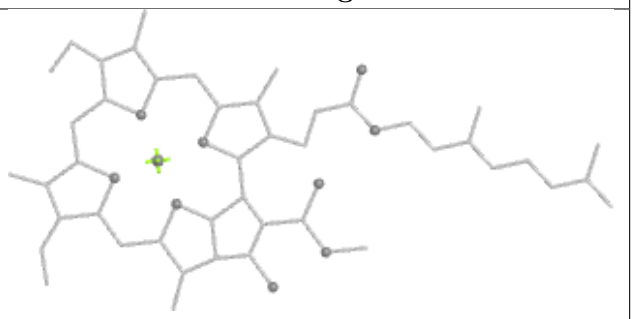
Bond lengths



Bond angles

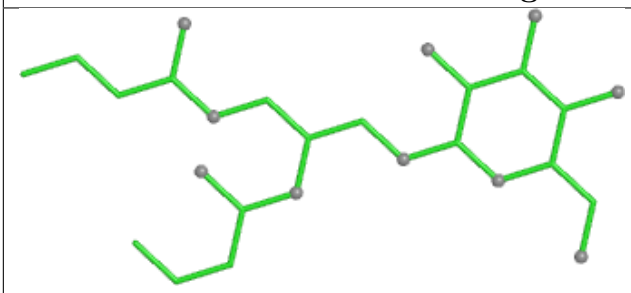


Torsions

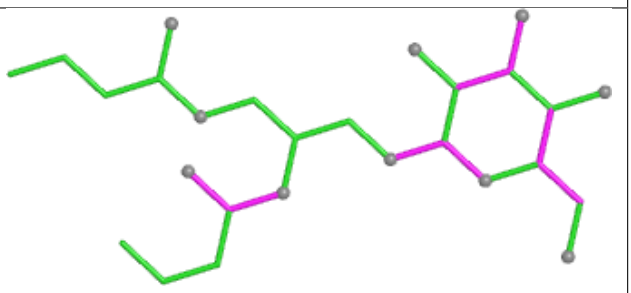


Rings

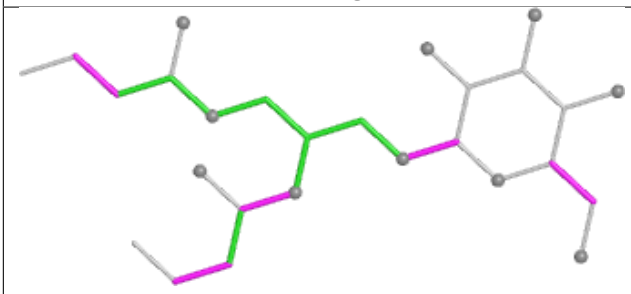
Ligand LMG P 201



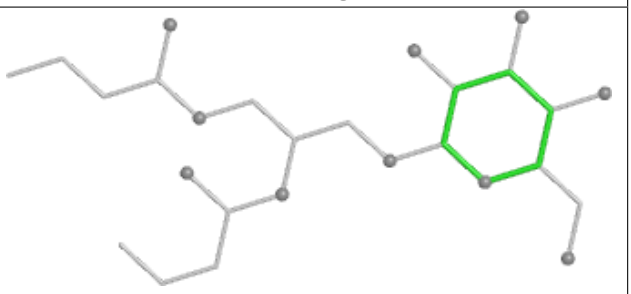
Bond lengths



Bond angles

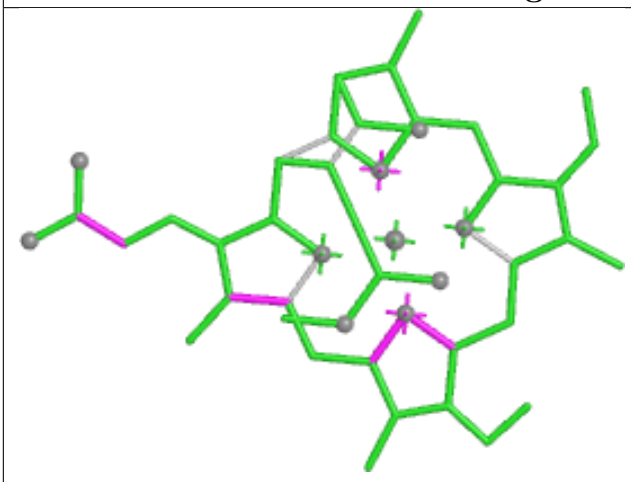


Torsions

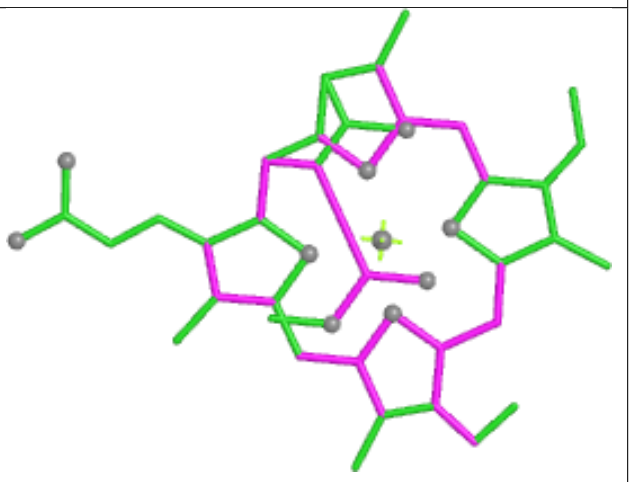


Rings

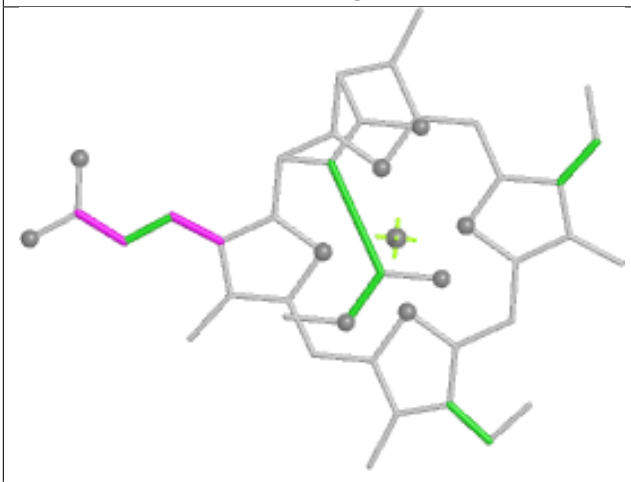
Ligand KC1 D 315



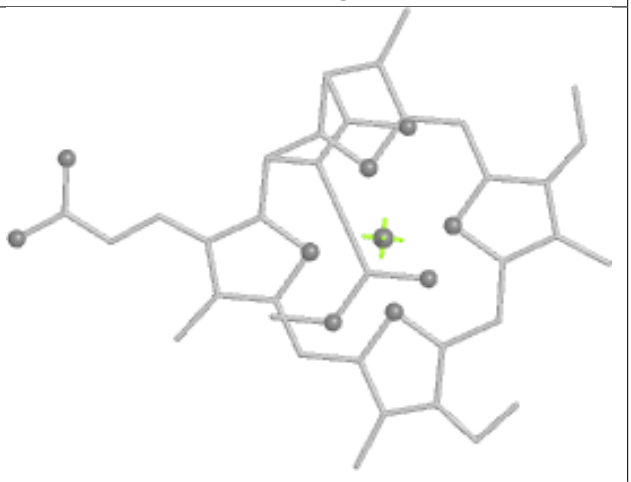
Bond lengths



Bond angles

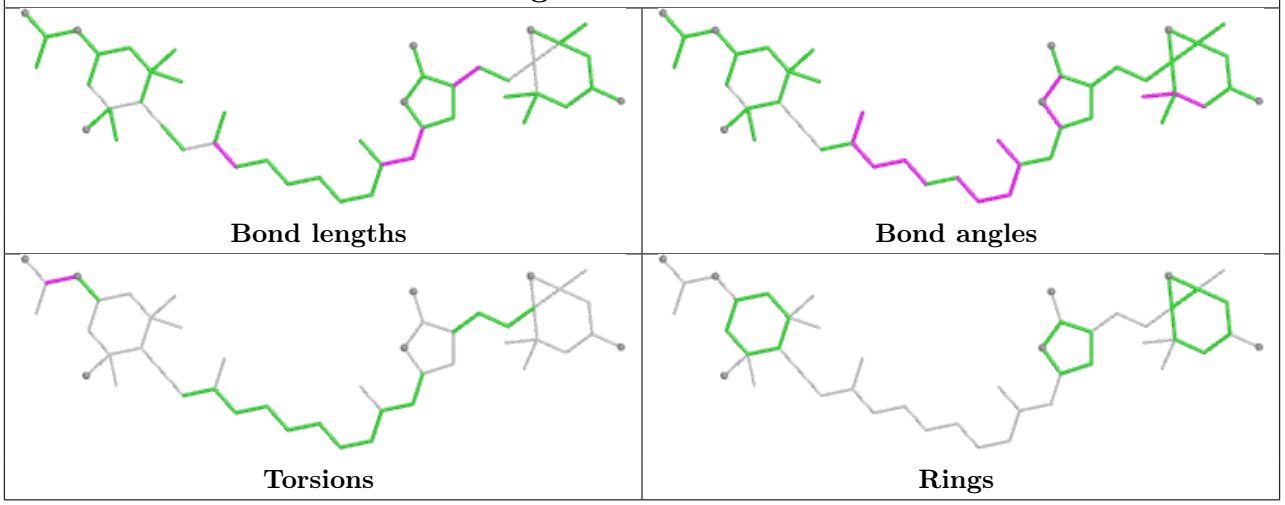


Torsions

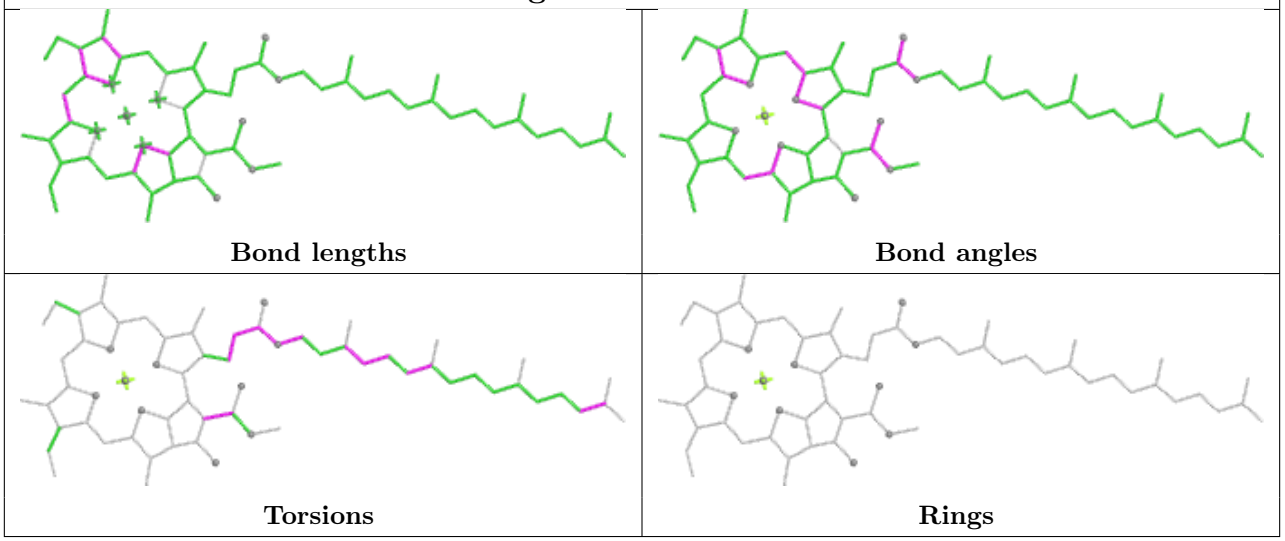


Rings

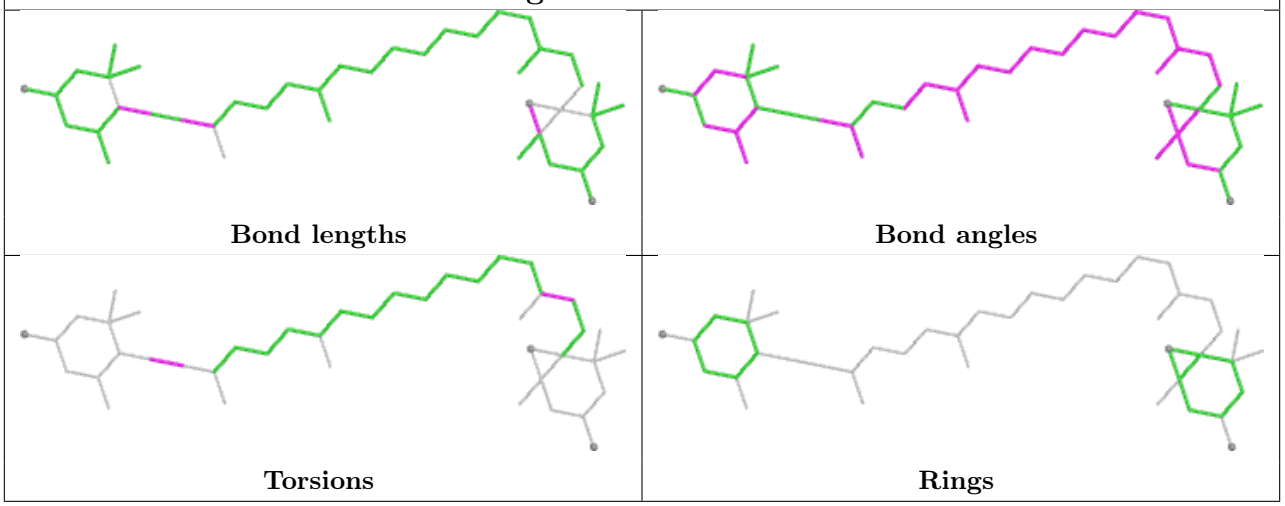
Ligand PID P 208



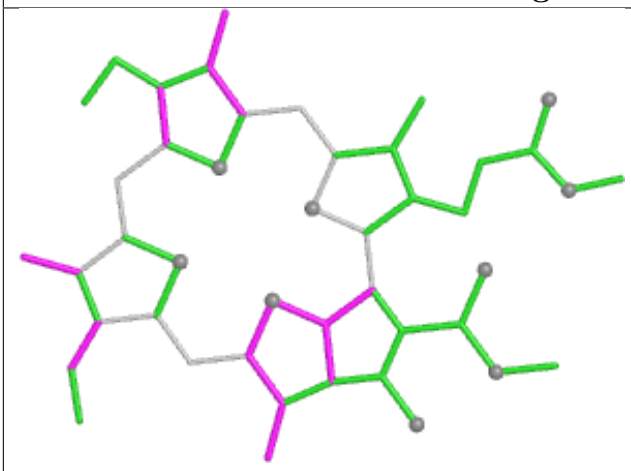
Ligand CLA b 725



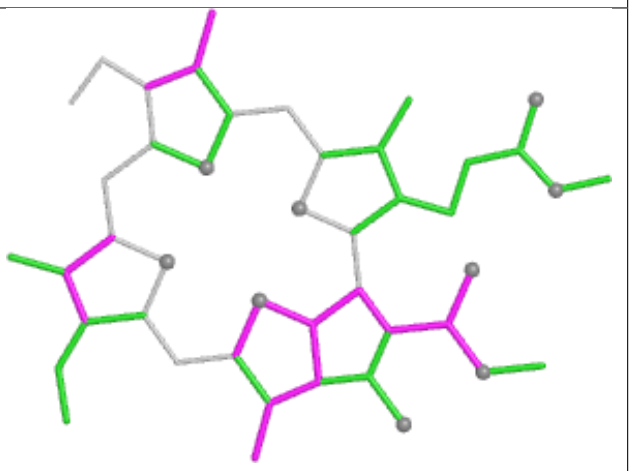
Ligand DD6 B 302



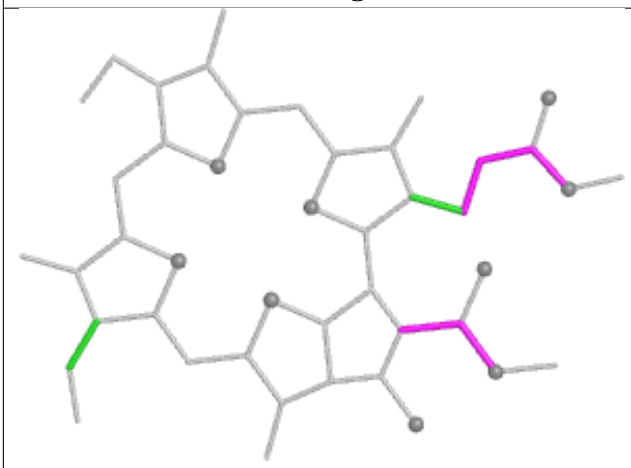
Ligand CLA l 310



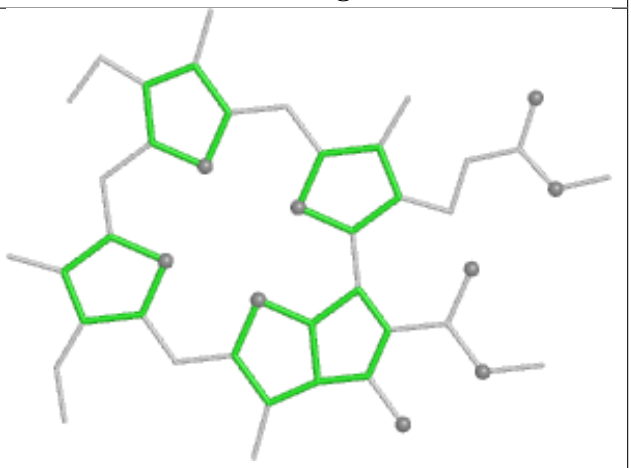
Bond lengths



Bond angles

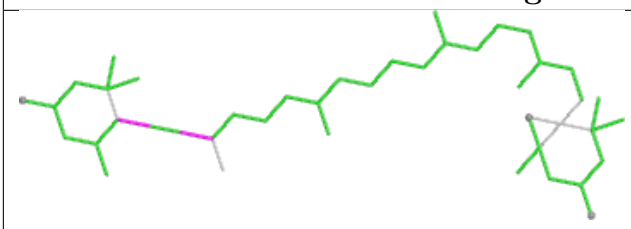


Torsions

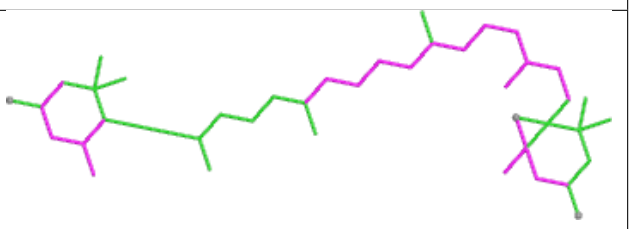


Rings

Ligand DD6 A 301



Bond lengths



Bond angles

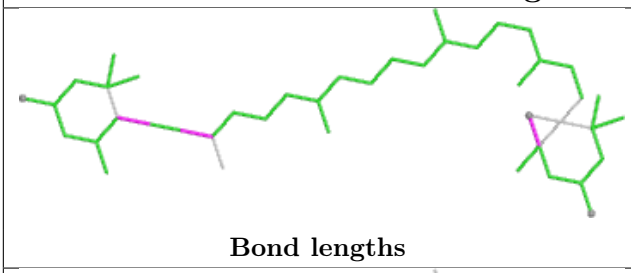


Torsions

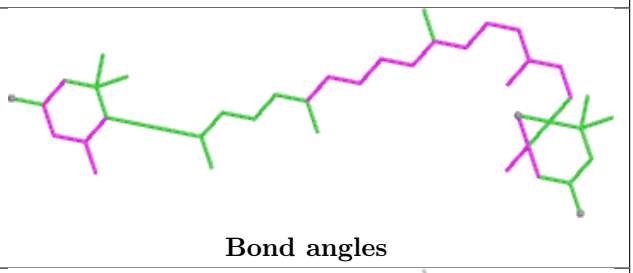


Rings

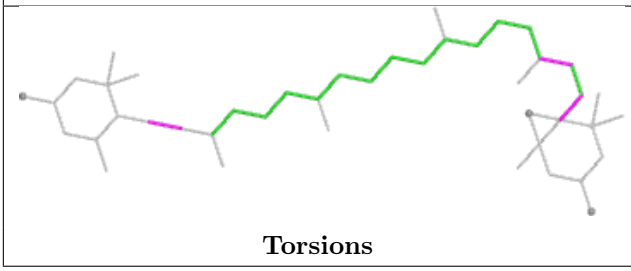
Ligand DD6 K 318



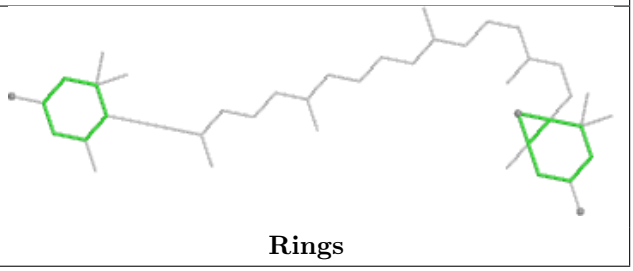
Bond lengths



Bond angles

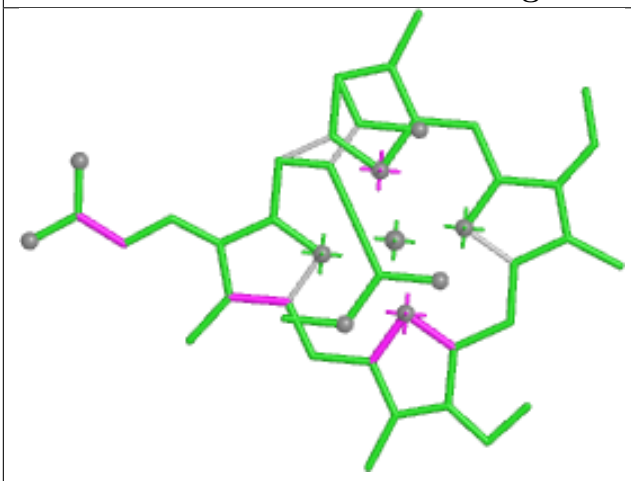


Torsions

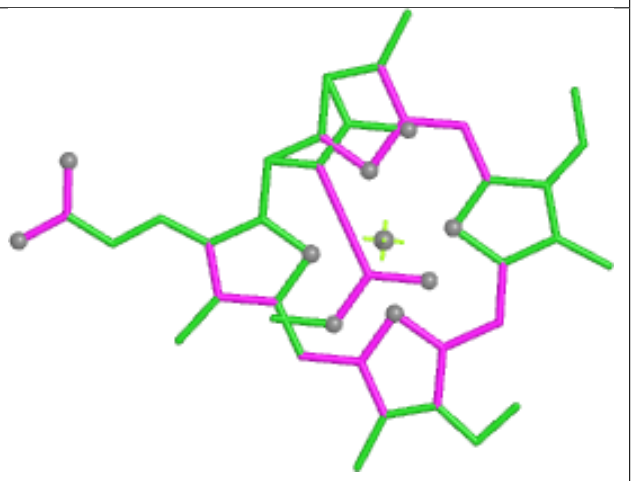


Rings

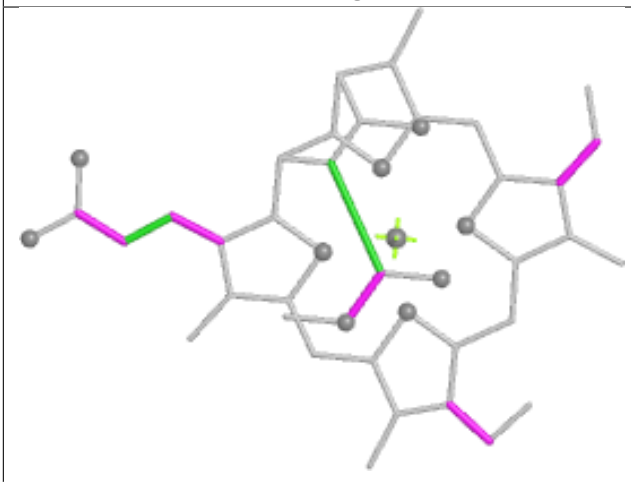
Ligand KC1 M 314



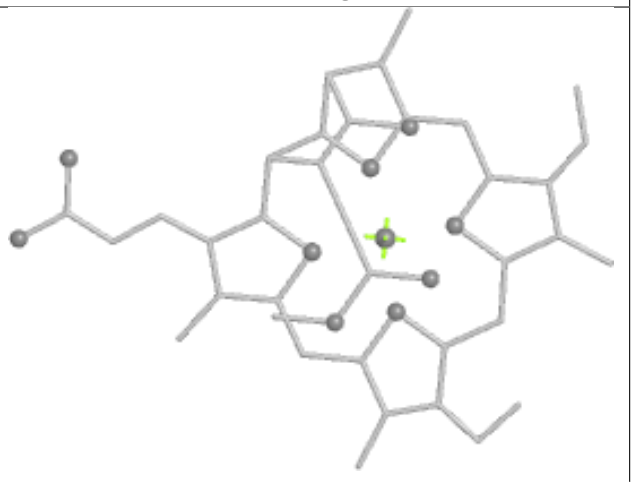
Bond lengths



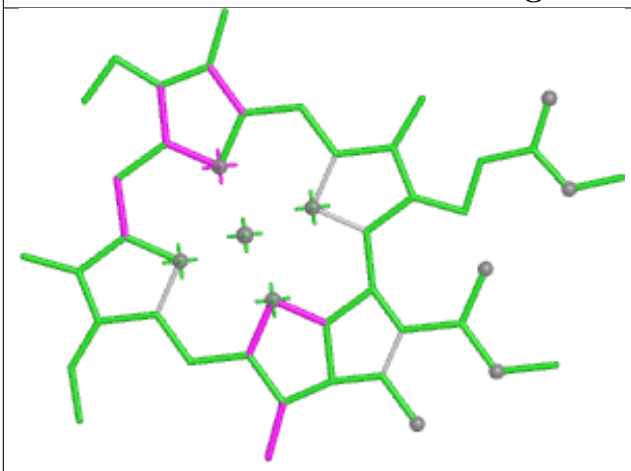
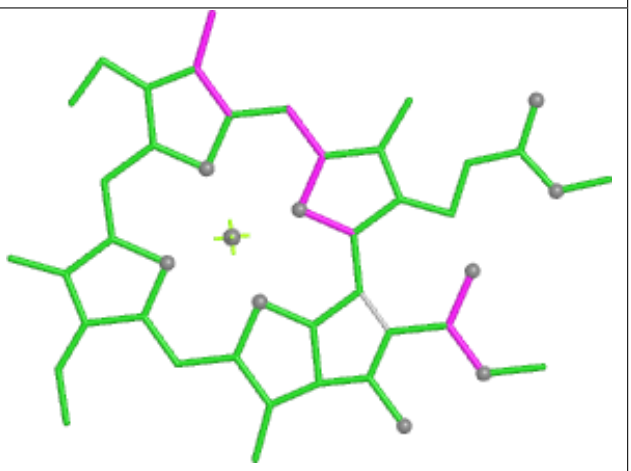
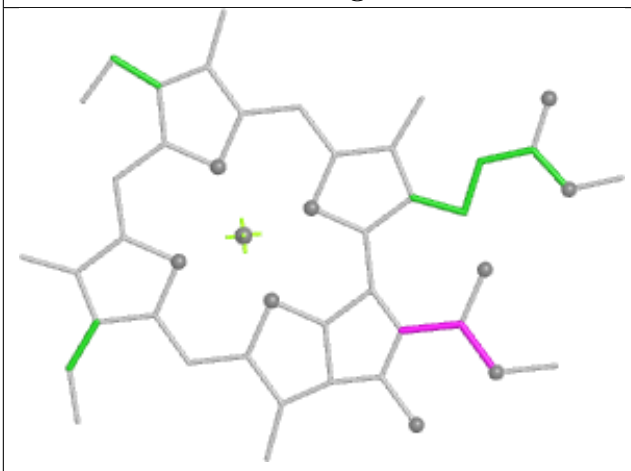
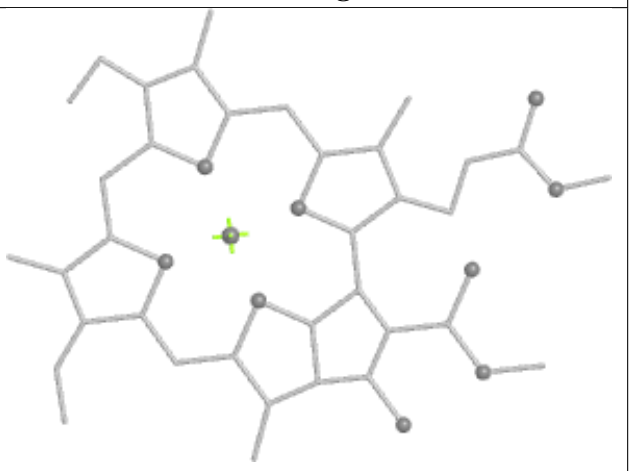
Bond angles

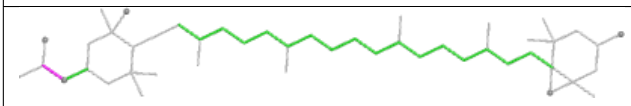
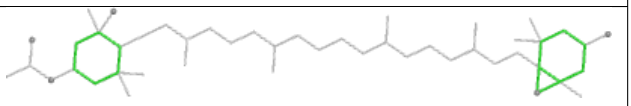


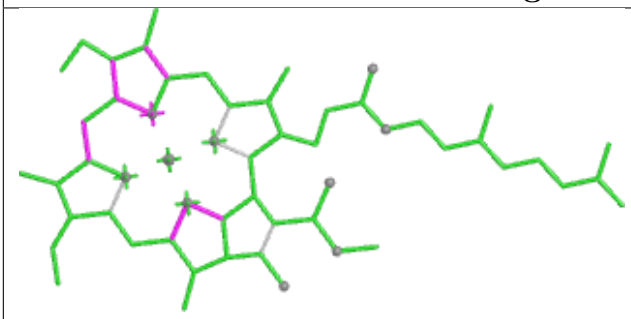
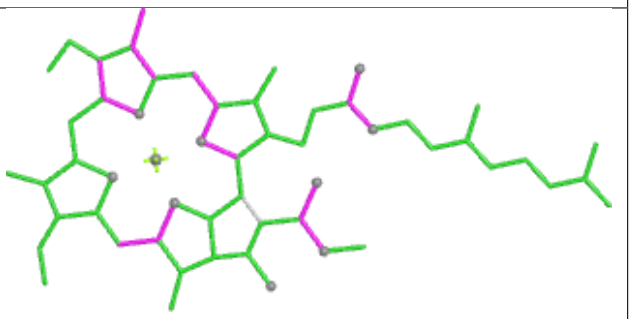
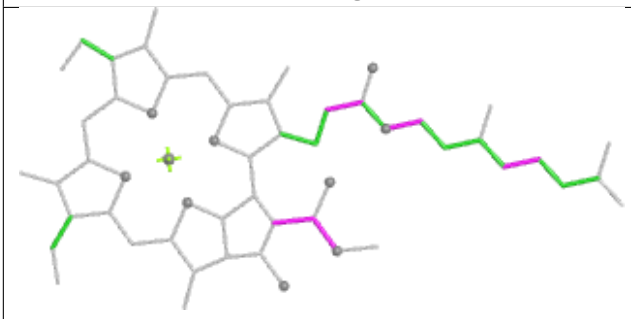
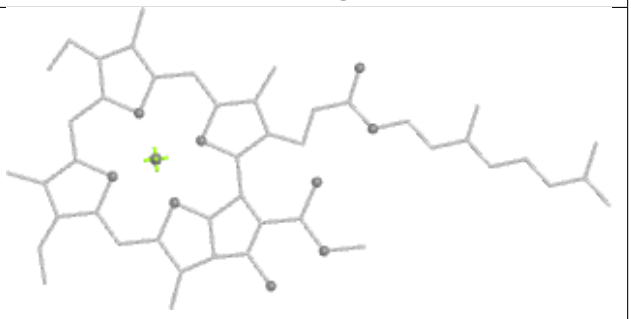
Torsions

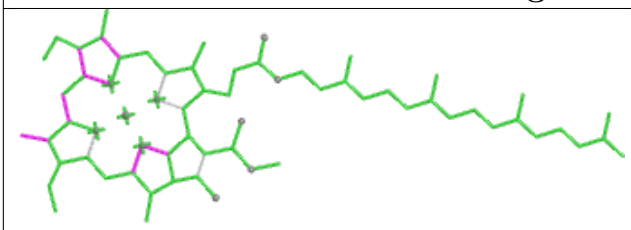
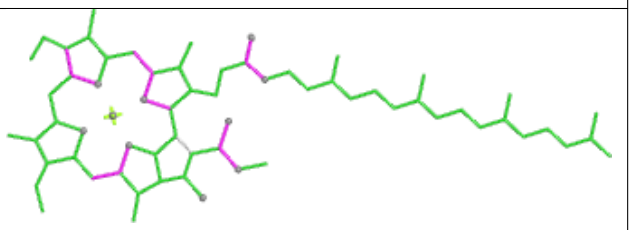
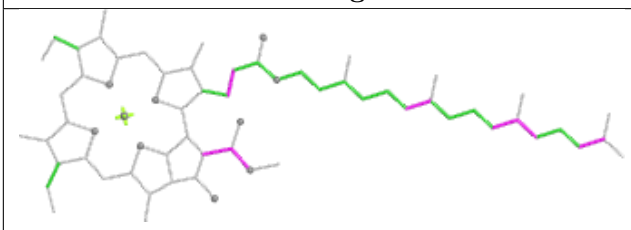
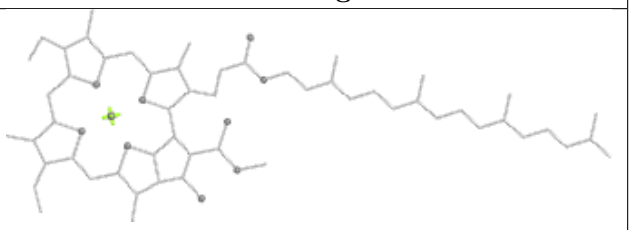


Rings

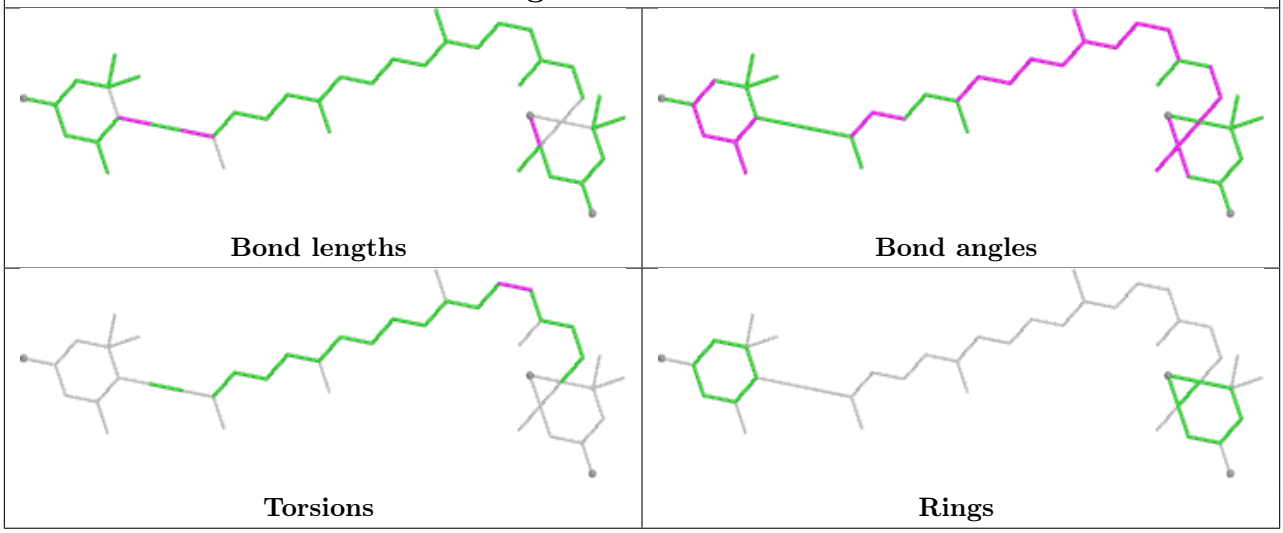
Ligand CLA P 214	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UIX B 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

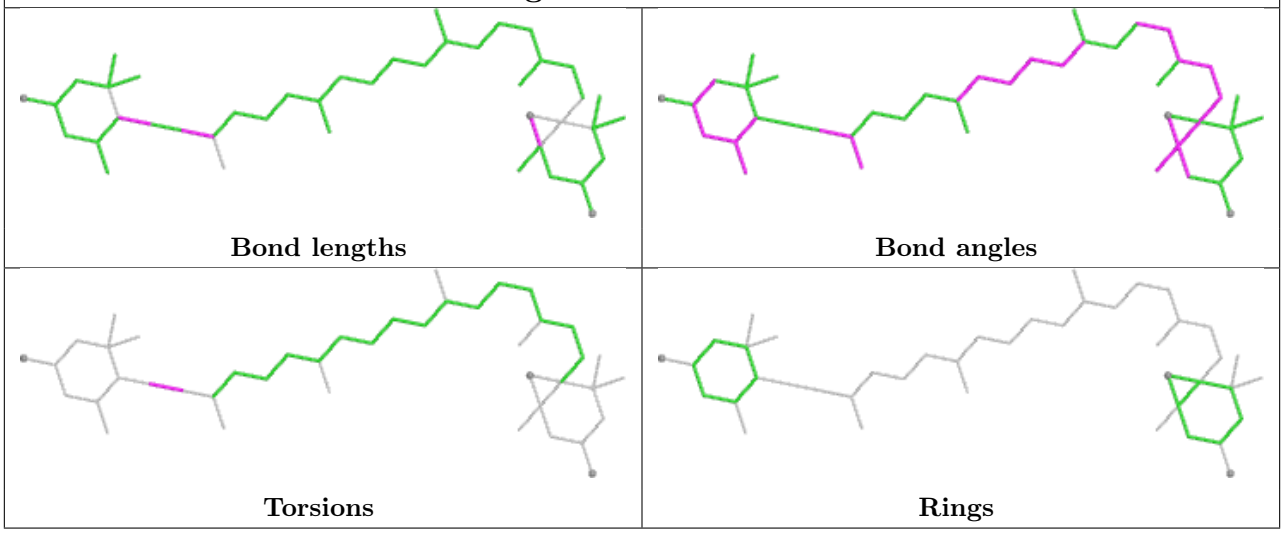
Ligand CLA A 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 727	
	
Bond lengths	Bond angles
	
Torsions	Rings

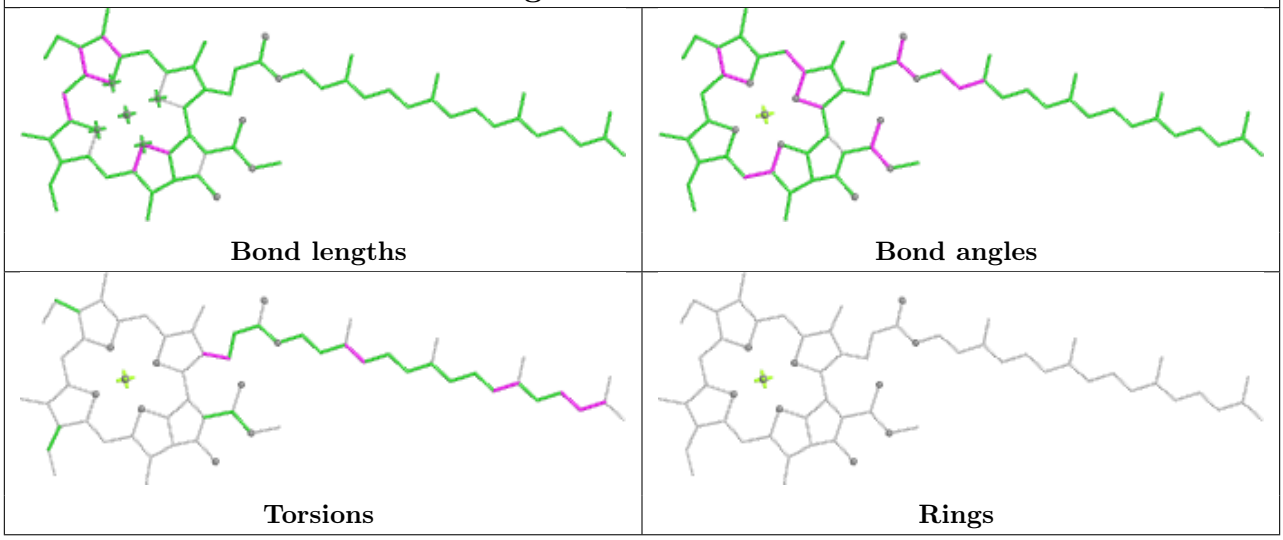
Ligand DD6 P 204



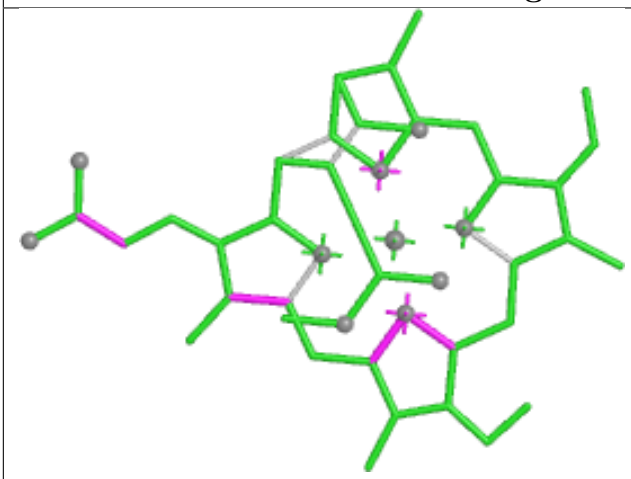
Ligand DD6 G 508



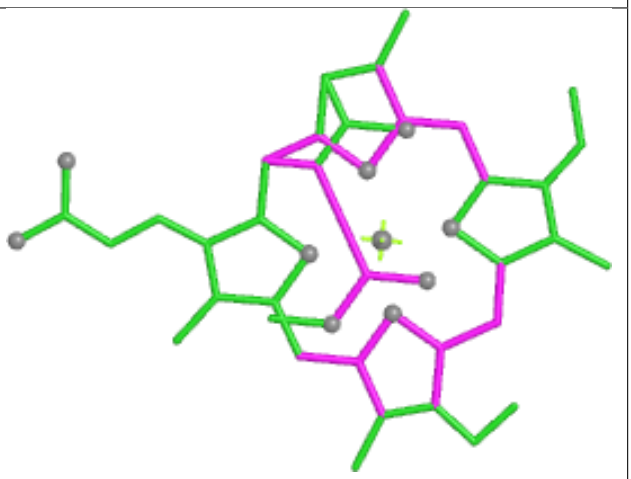
Ligand CLA H 305



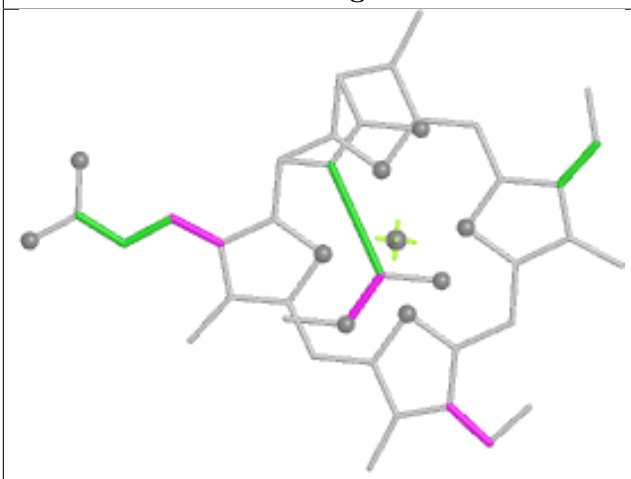
Ligand KC1 H 310



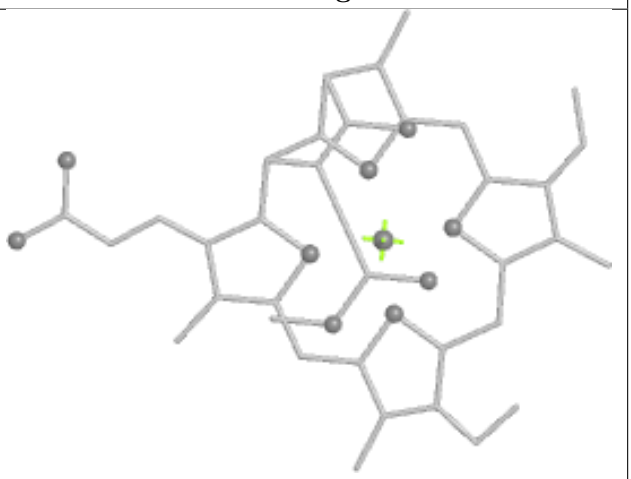
Bond lengths



Bond angles

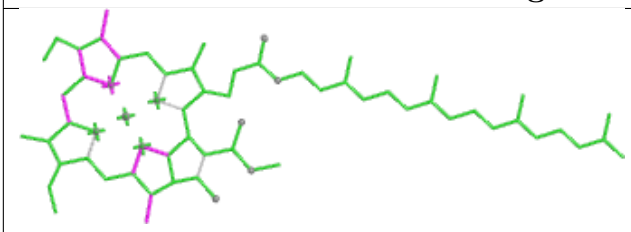


Torsions

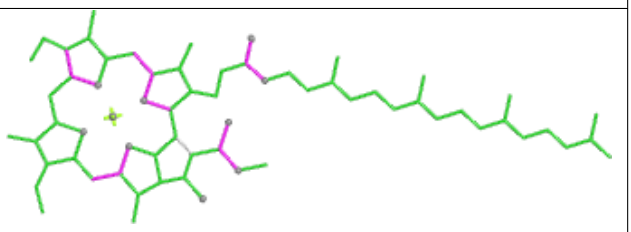


Rings

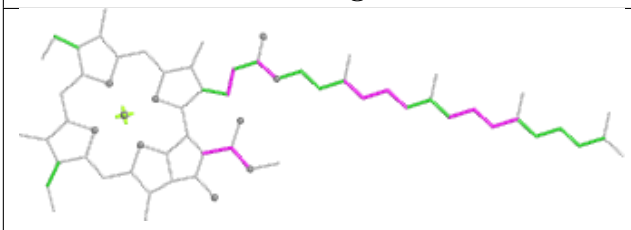
Ligand CLA b 701



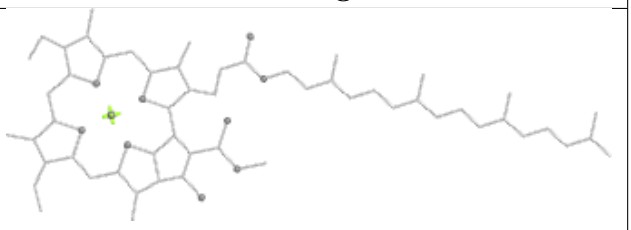
Bond lengths



Bond angles

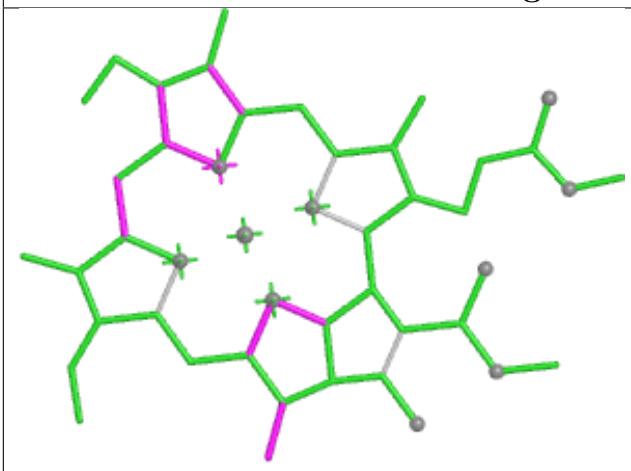


Torsions

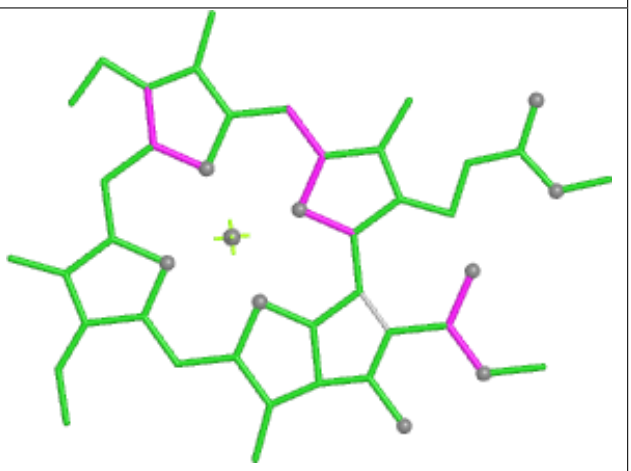


Rings

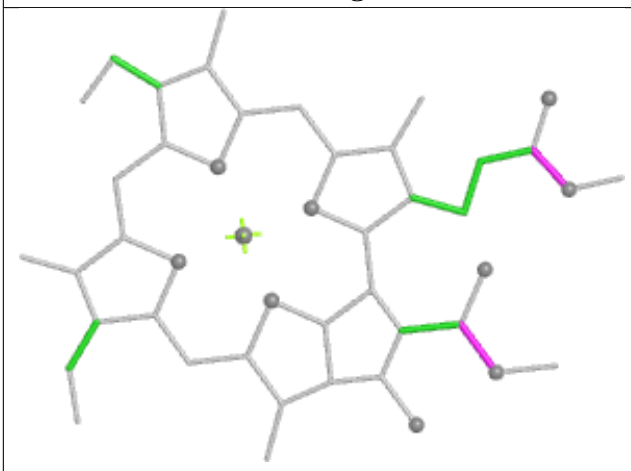
Ligand CLA H 308



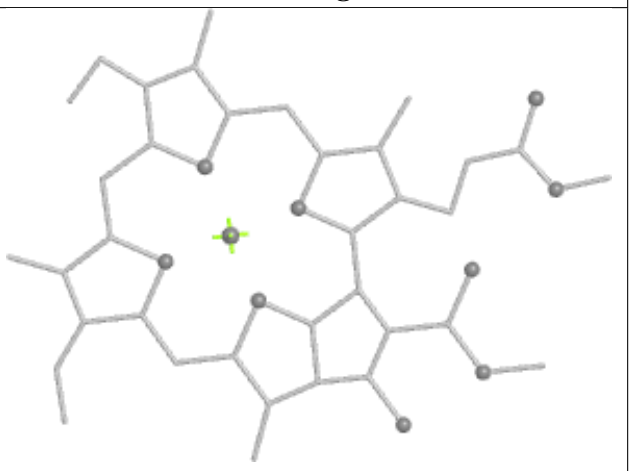
Bond lengths



Bond angles

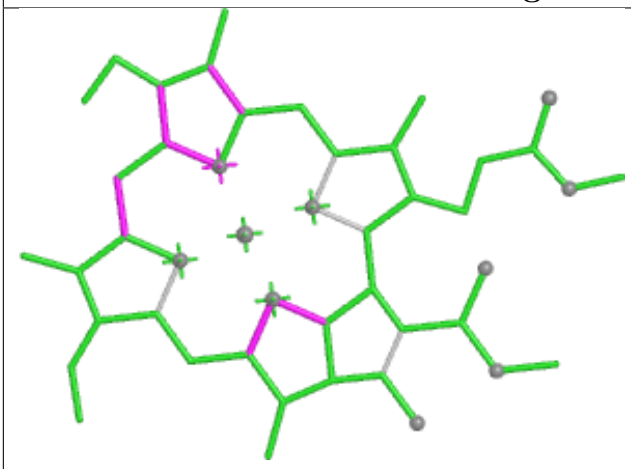


Torsions

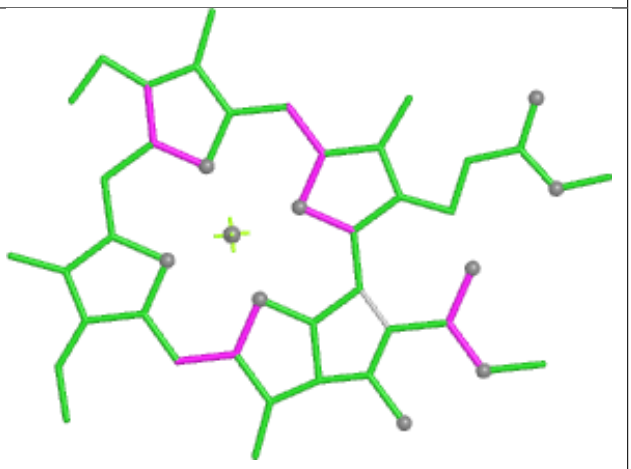


Rings

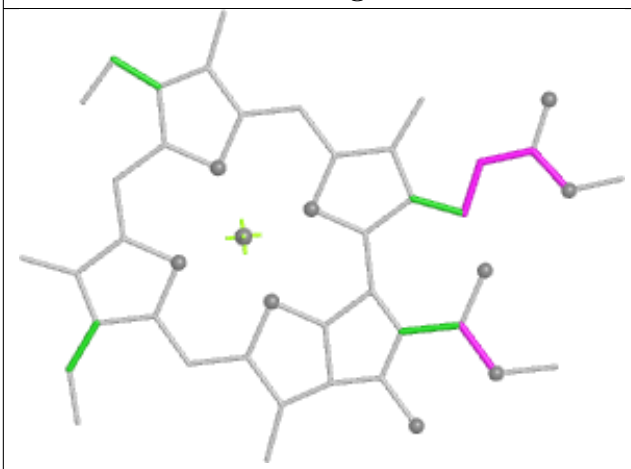
Ligand CLA D 309



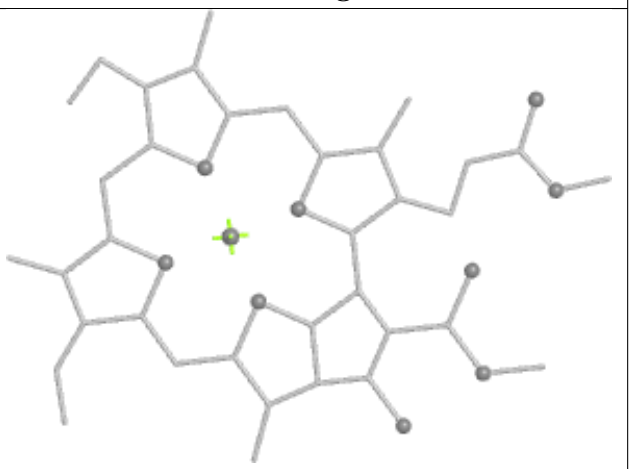
Bond lengths



Bond angles

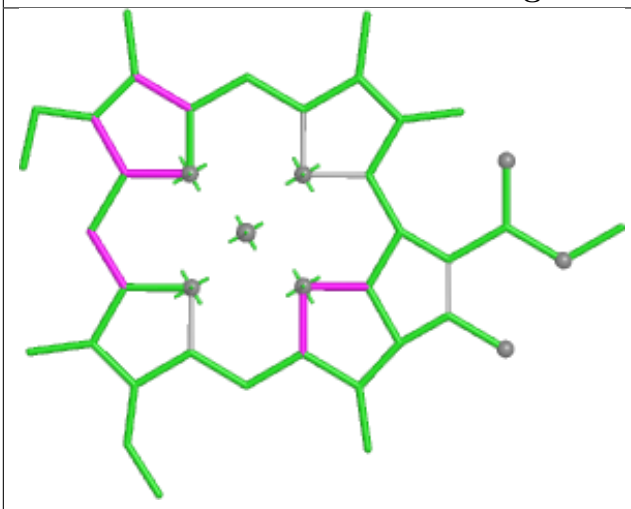


Torsions

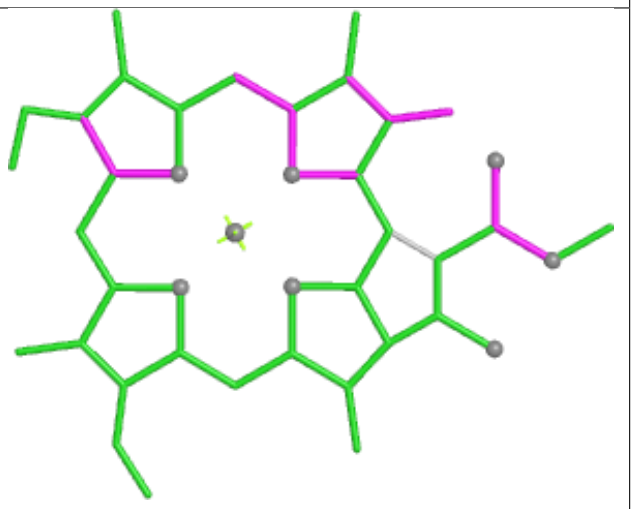


Rings

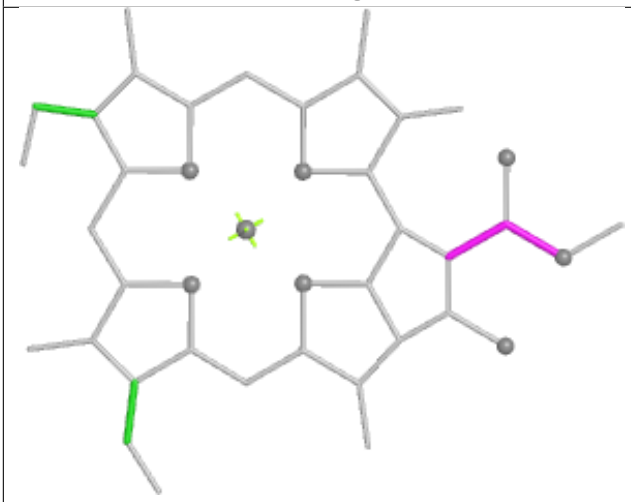
Ligand CLA O 316



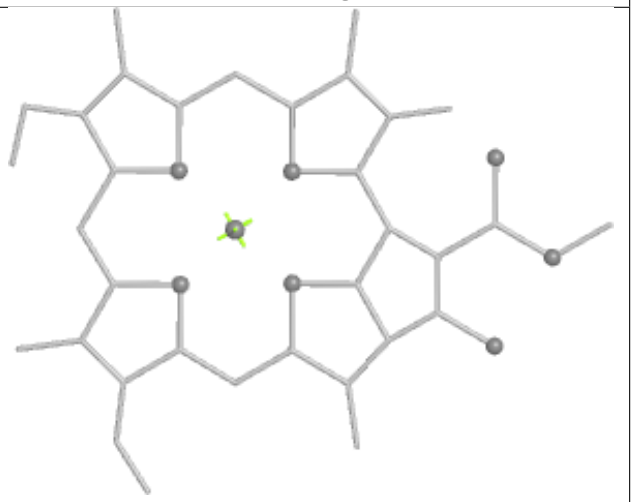
Bond lengths



Bond angles

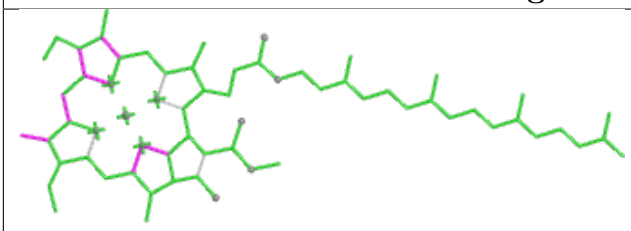


Torsions

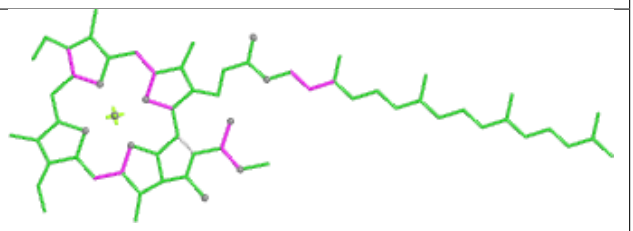


Rings

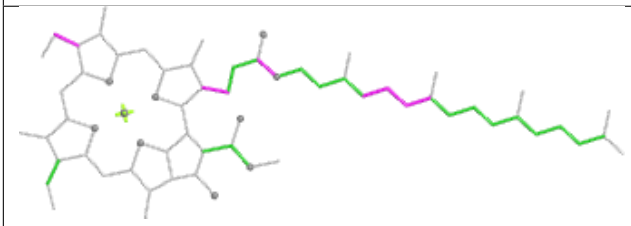
Ligand CLA b 728



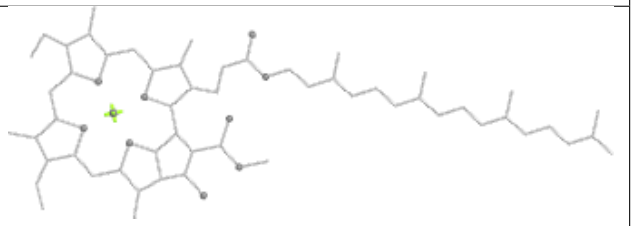
Bond lengths



Bond angles

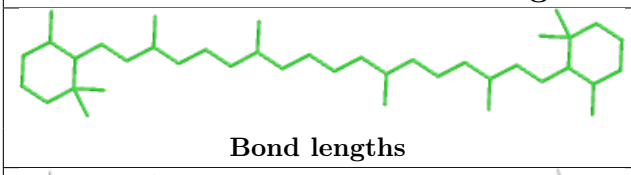


Torsions

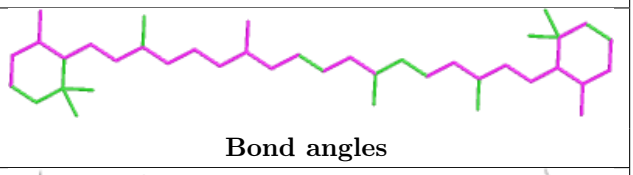


Rings

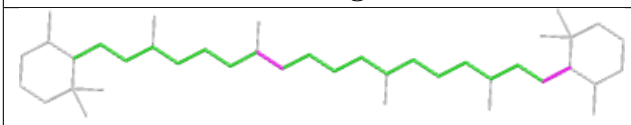
Ligand BCR f 304



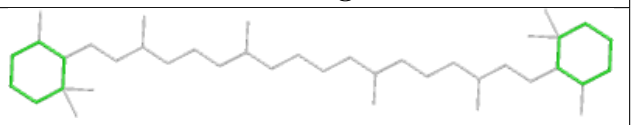
Bond lengths



Bond angles

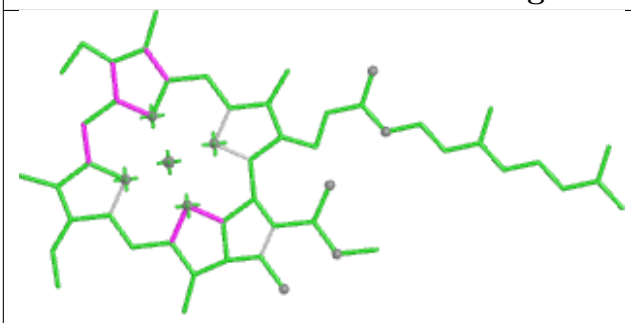


Torsions

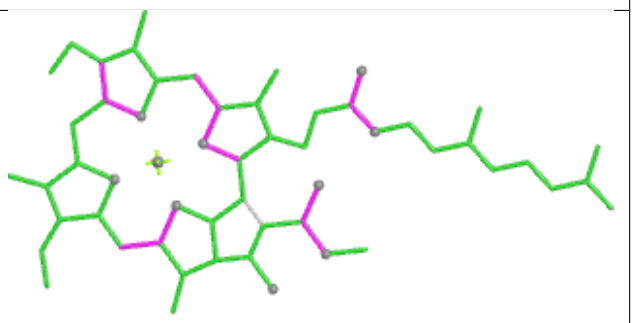


Rings

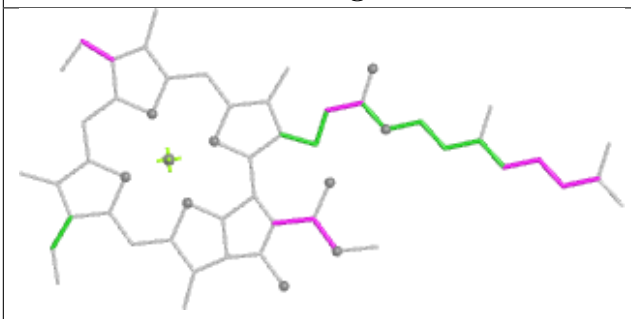
Ligand CLA b 711



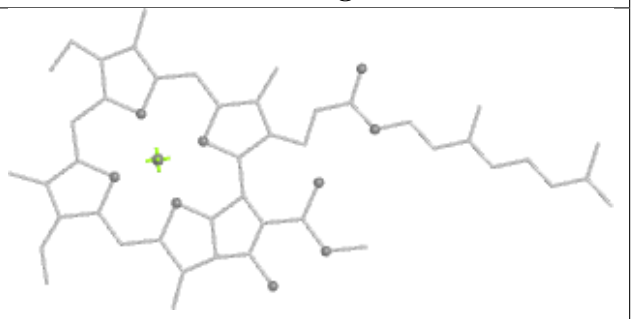
Bond lengths



Bond angles

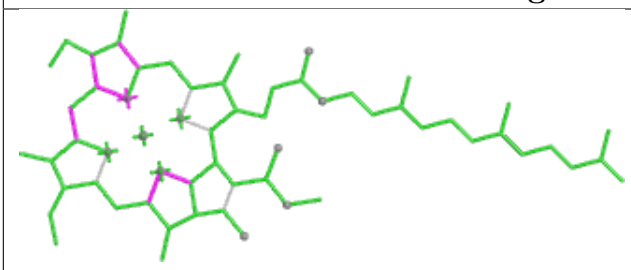


Torsions

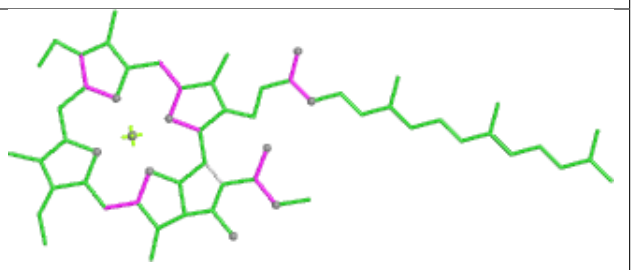


Rings

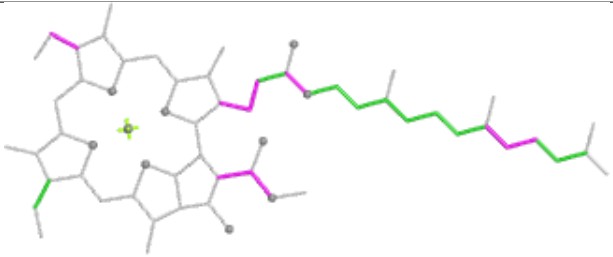
Ligand CLA J 301



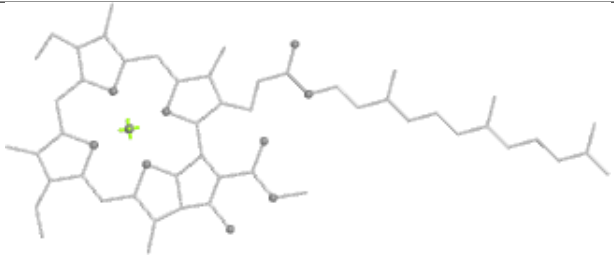
Bond lengths



Bond angles

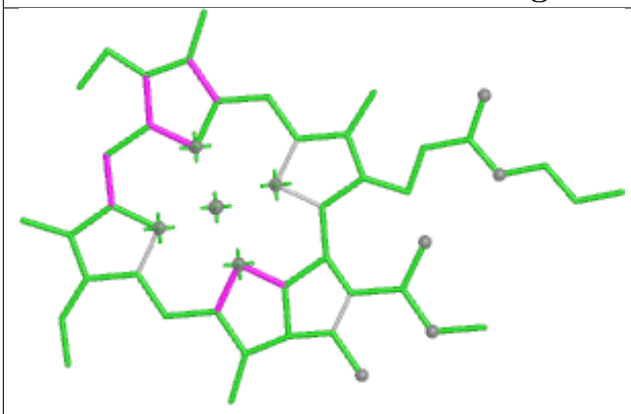


Torsions

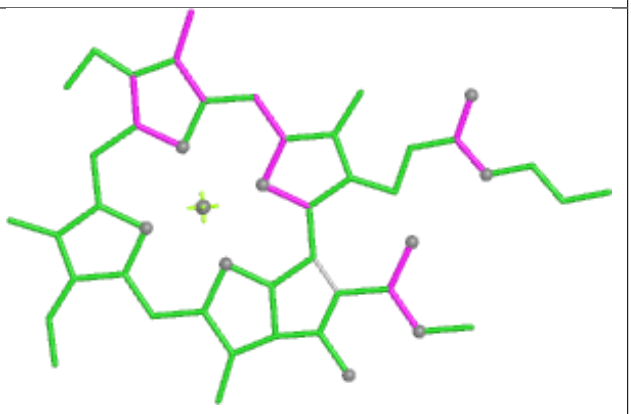


Rings

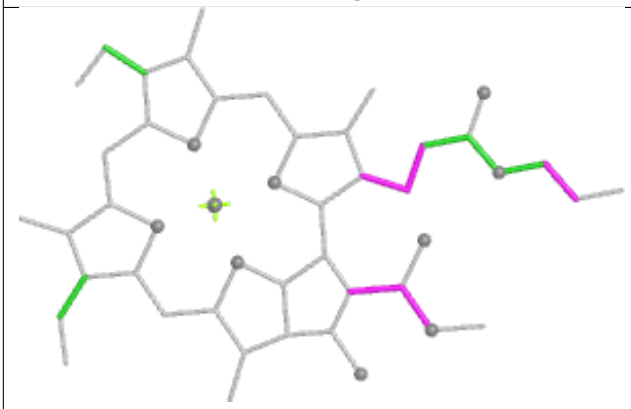
Ligand CLA I 310



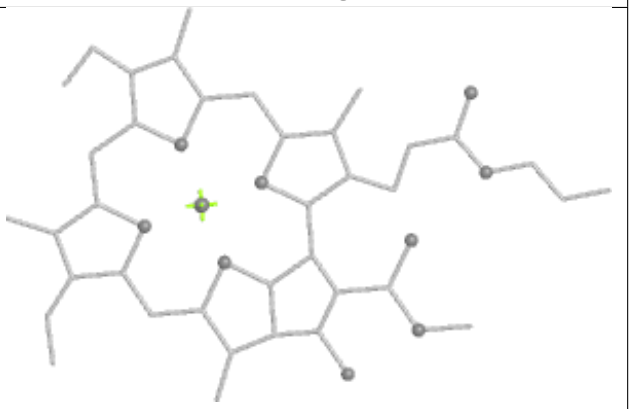
Bond lengths



Bond angles

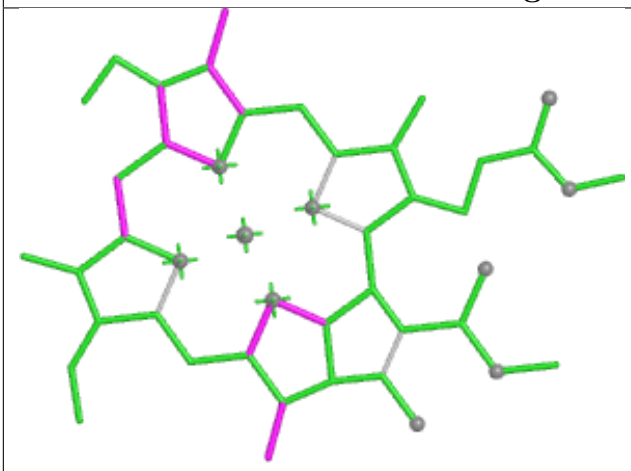


Torsions

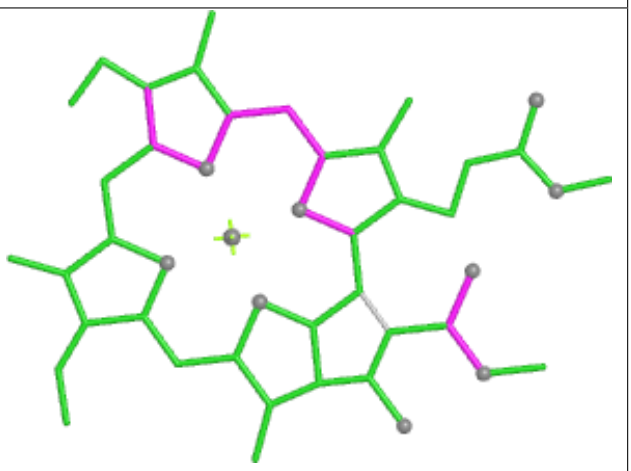


Rings

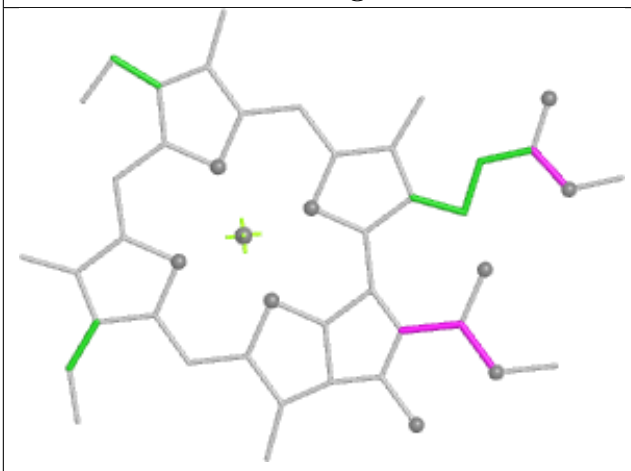
Ligand CLA A 320



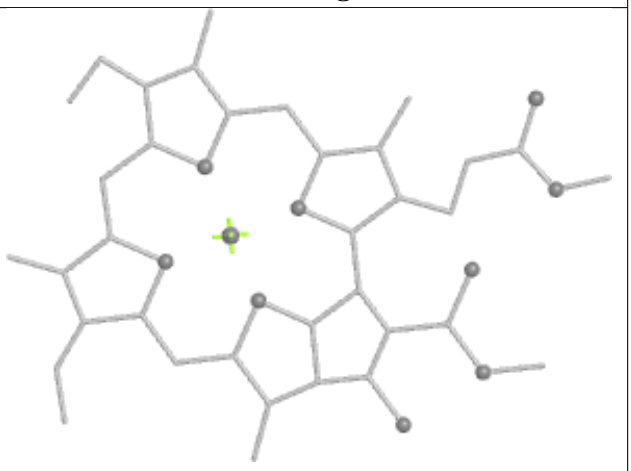
Bond lengths



Bond angles

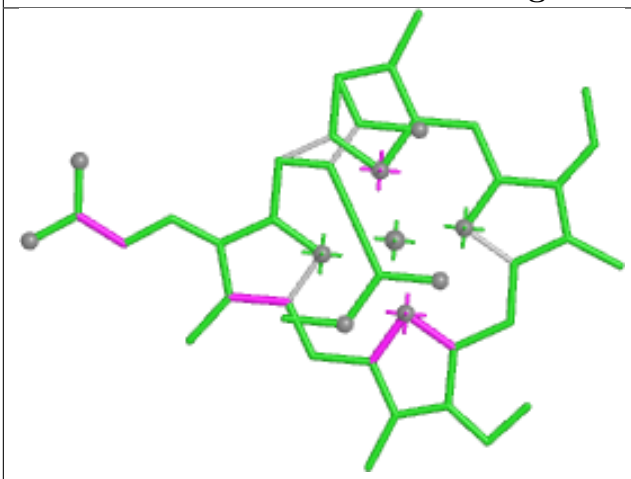


Torsions

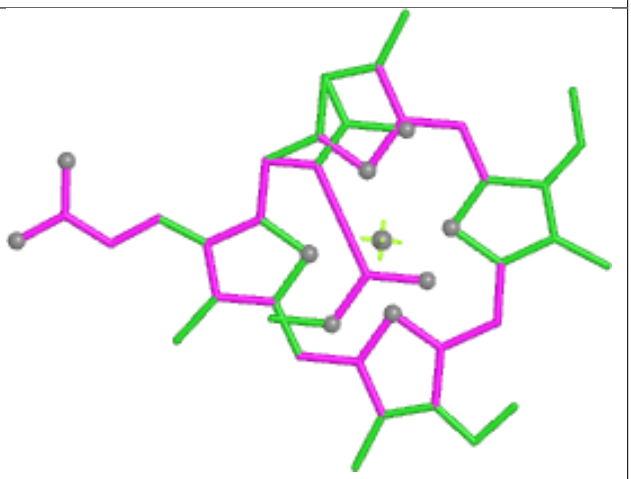


Rings

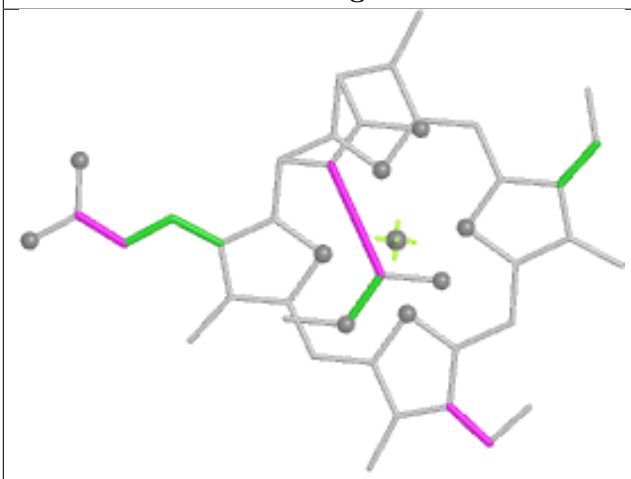
Ligand KC1 L 307



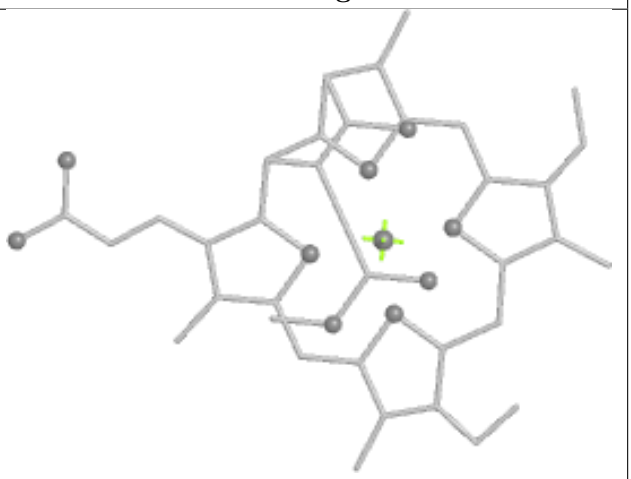
Bond lengths



Bond angles

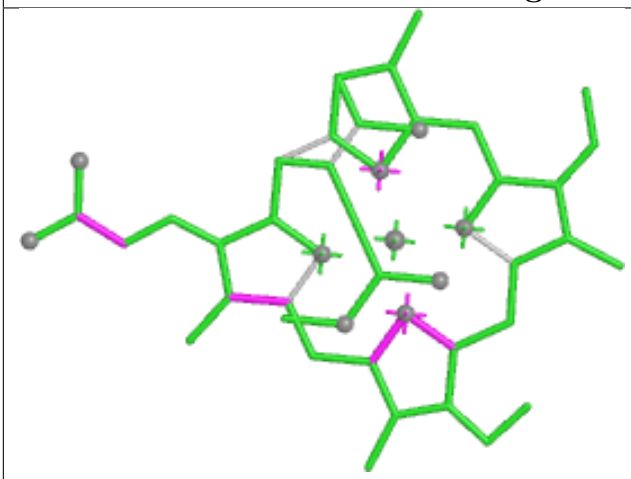


Torsions

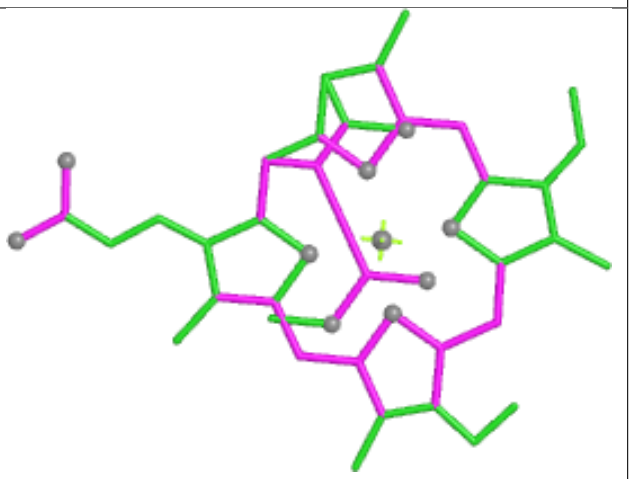


Rings

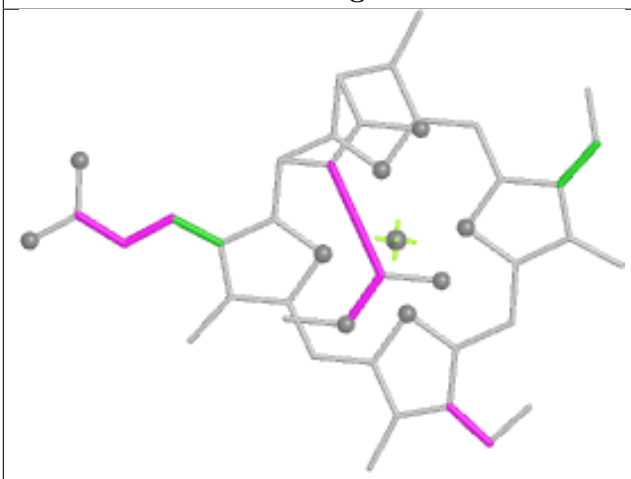
Ligand KC1 N 308



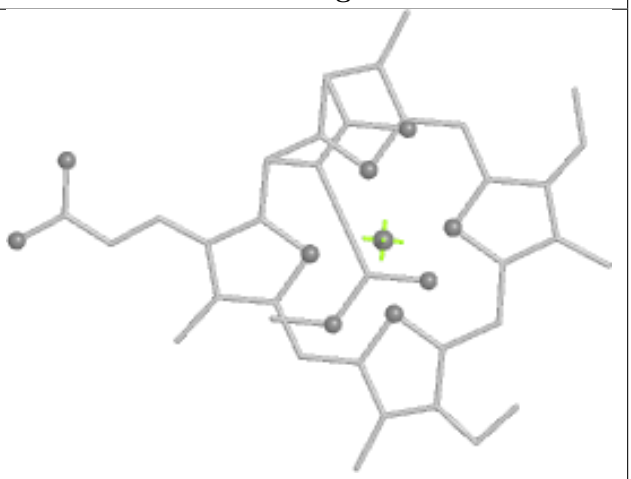
Bond lengths



Bond angles

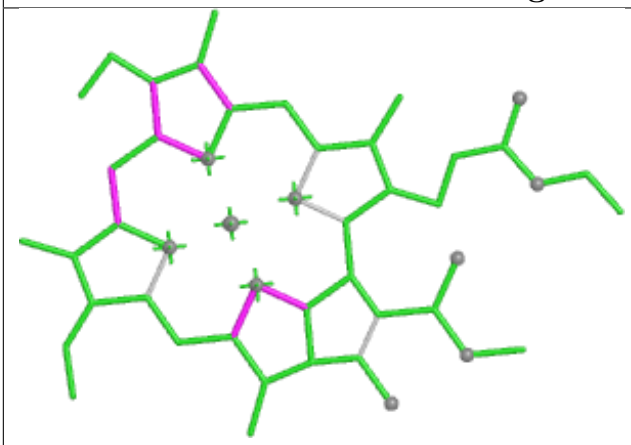


Torsions

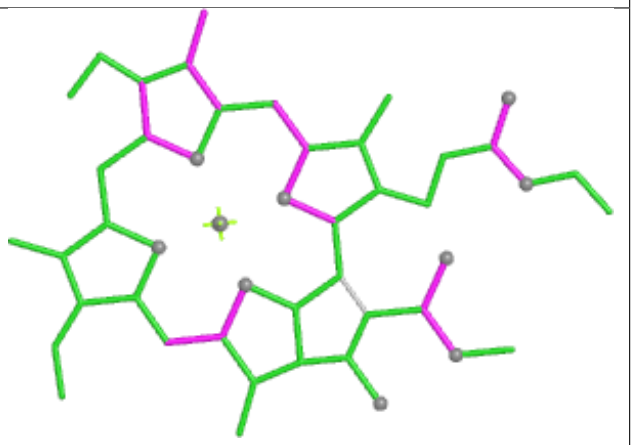


Rings

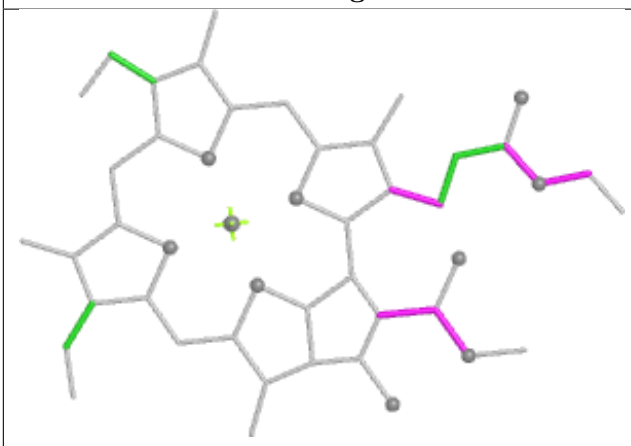
Ligand CLA J 311



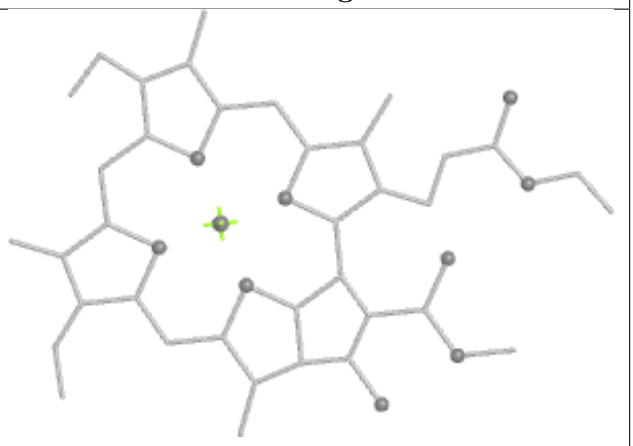
Bond lengths



Bond angles

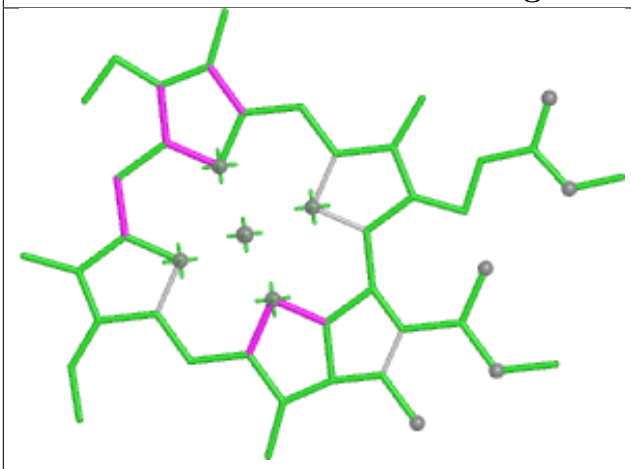


Torsions

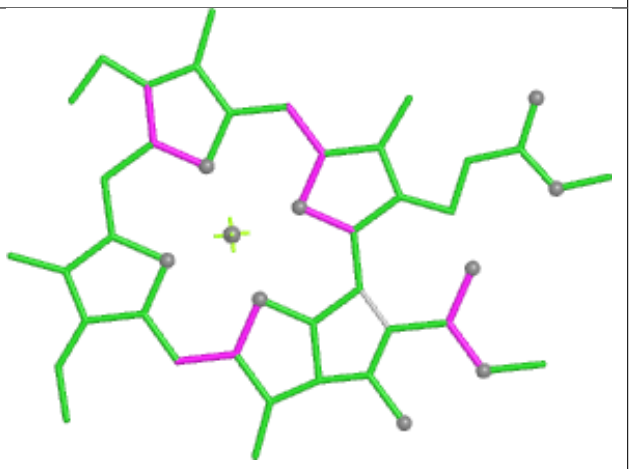


Rings

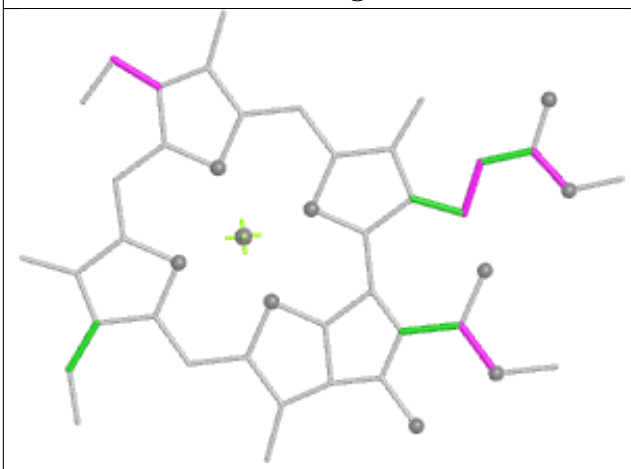
Ligand CLA A 311



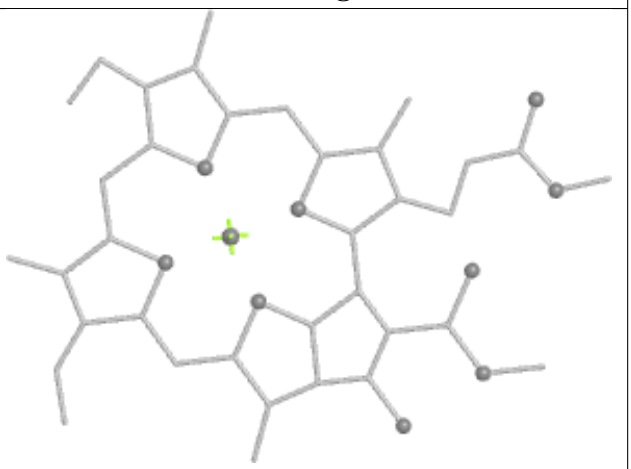
Bond lengths



Bond angles

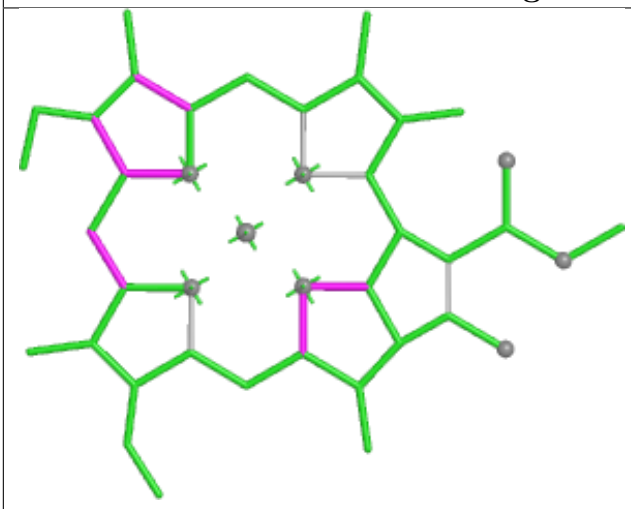


Torsions

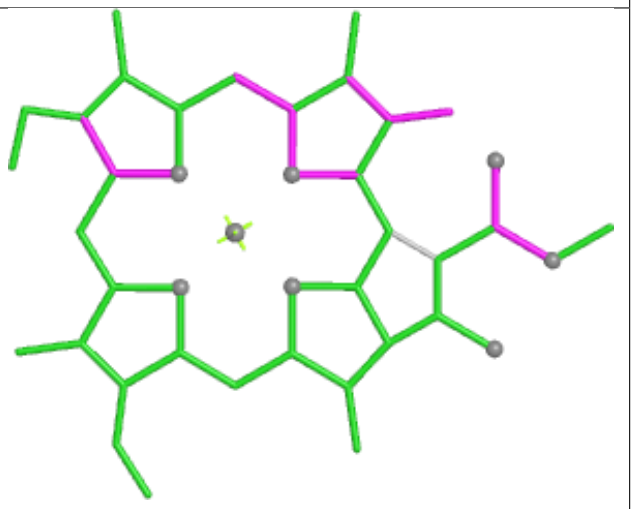


Rings

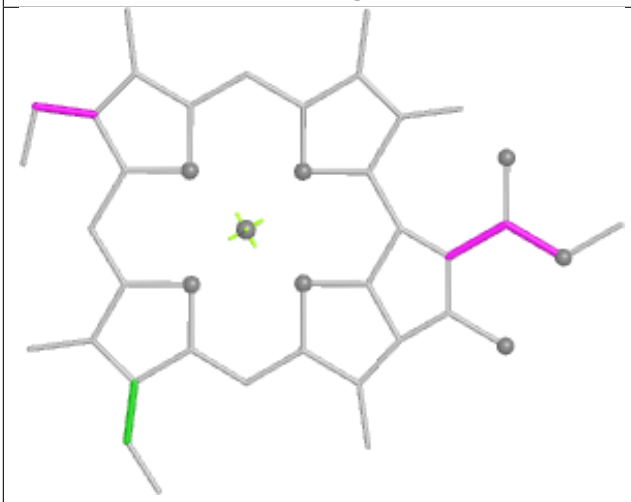
Ligand CLA G 516



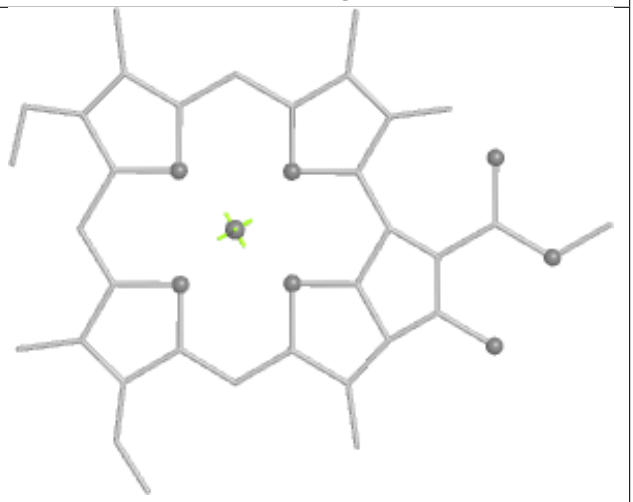
Bond lengths



Bond angles

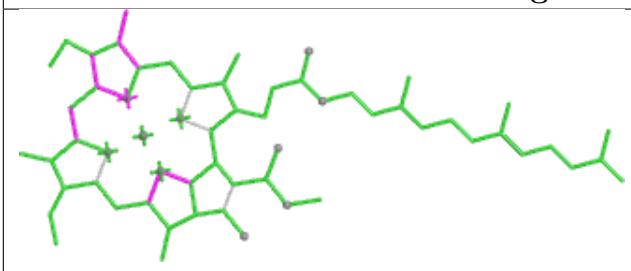


Torsions

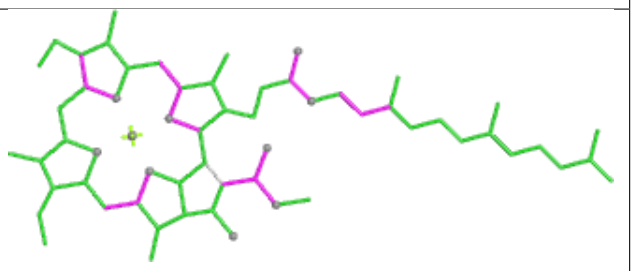


Rings

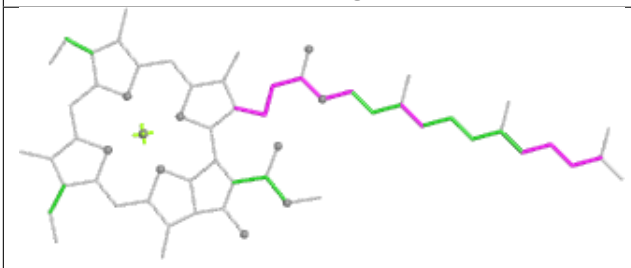
Ligand CLA I 308



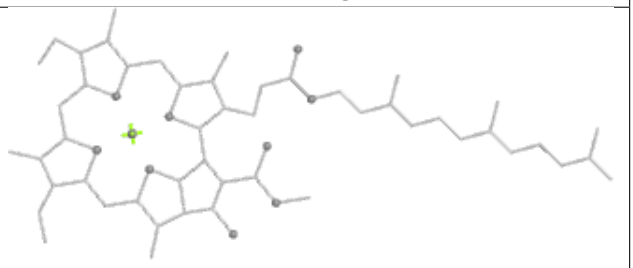
Bond lengths



Bond angles

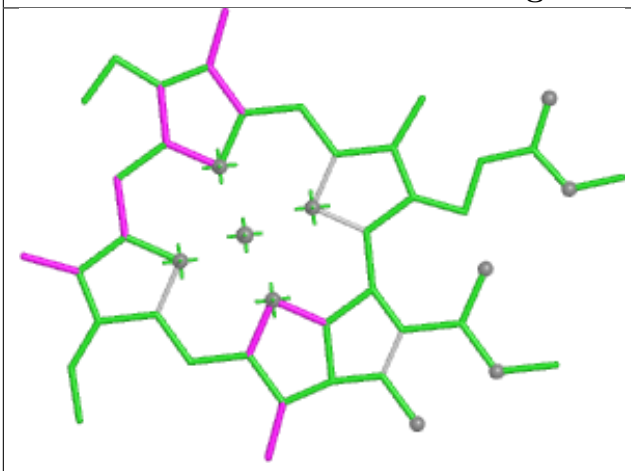


Torsions

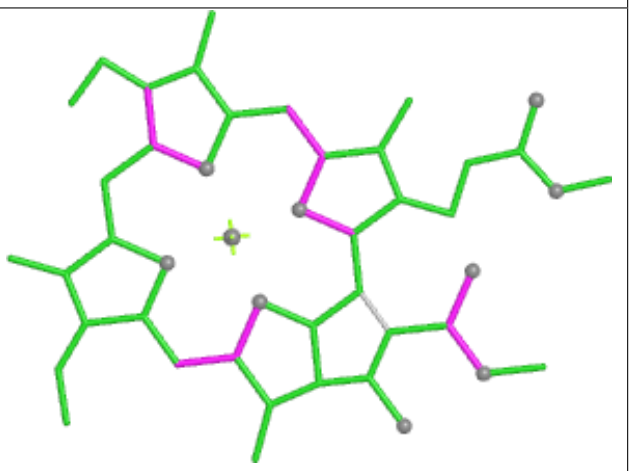


Rings

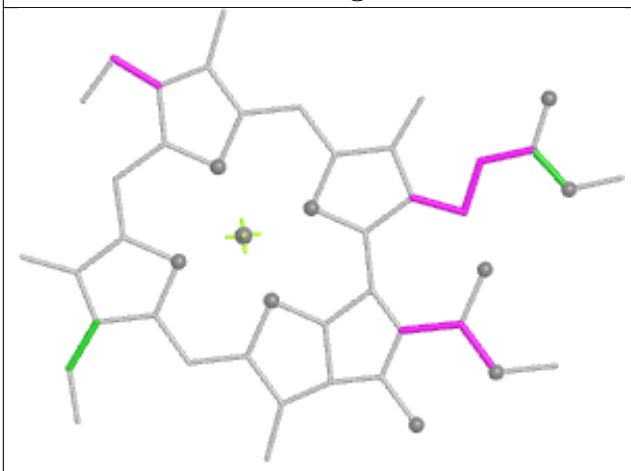
Ligand CLA L 318



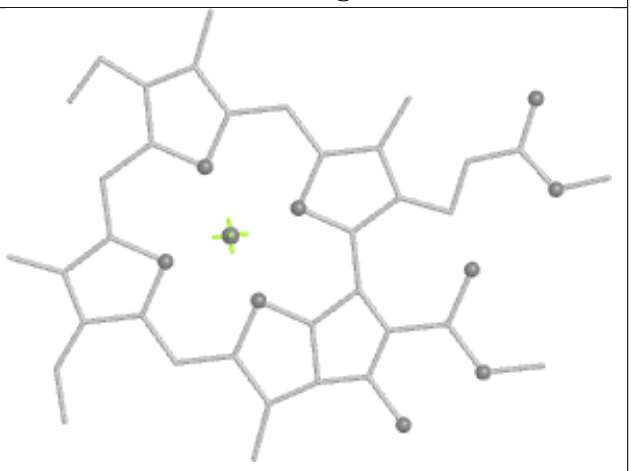
Bond lengths



Bond angles

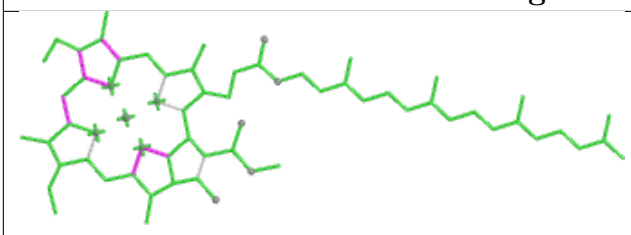


Torsions

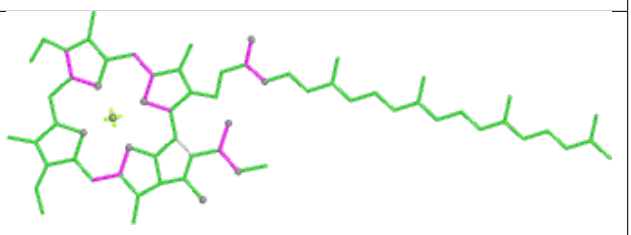


Rings

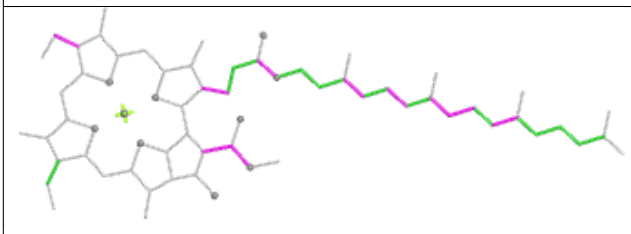
Ligand CLA a 707



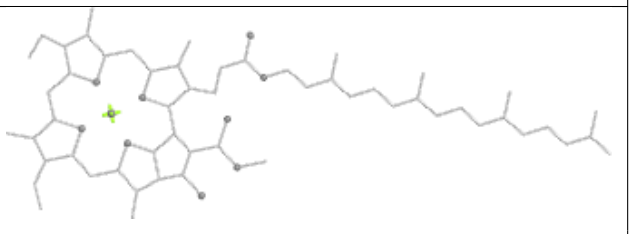
Bond lengths



Bond angles

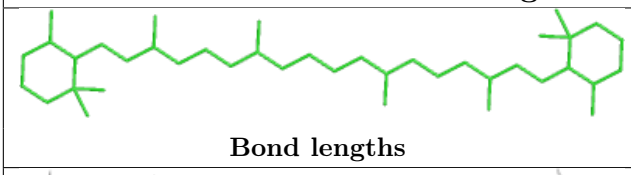


Torsions

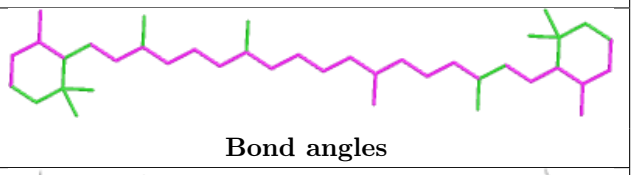


Rings

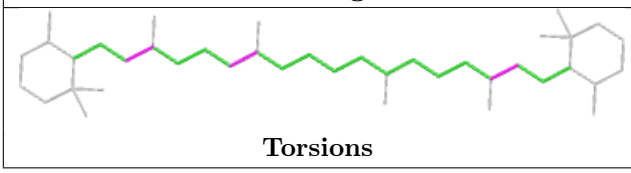
Ligand BCR m 201



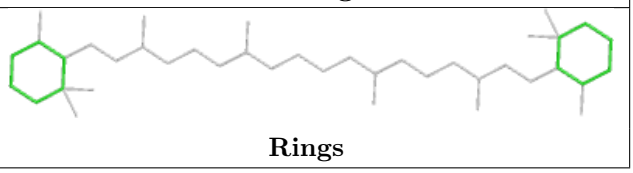
Bond lengths



Bond angles

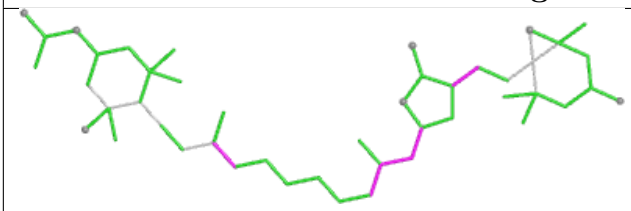


Torsions

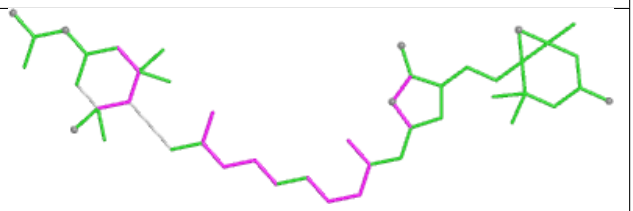


Rings

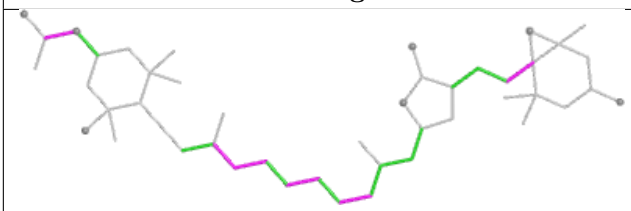
Ligand PID F 305



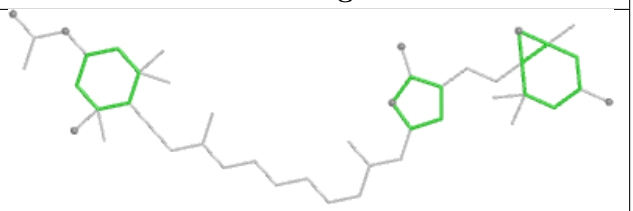
Bond lengths



Bond angles

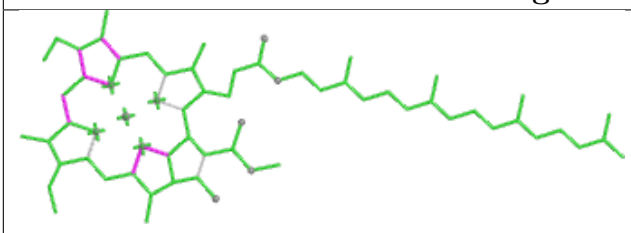


Torsions

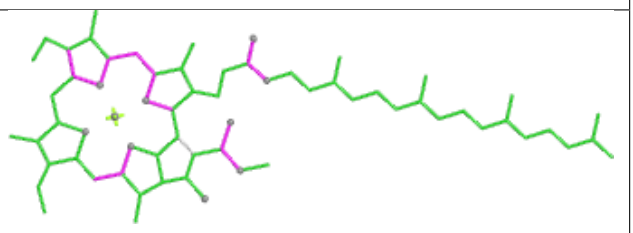


Rings

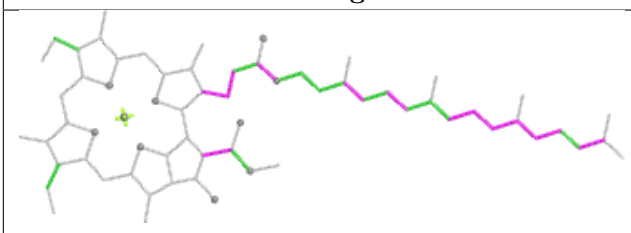
Ligand CLA l 311



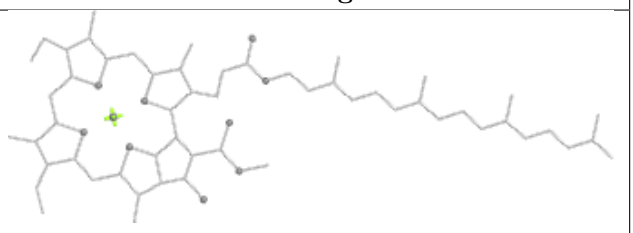
Bond lengths



Bond angles

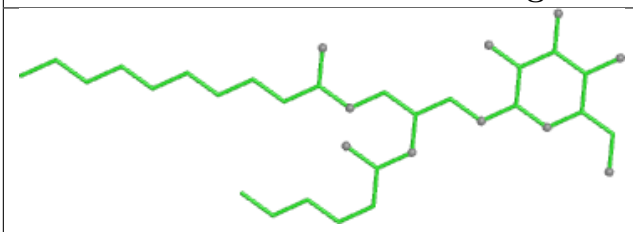


Torsions

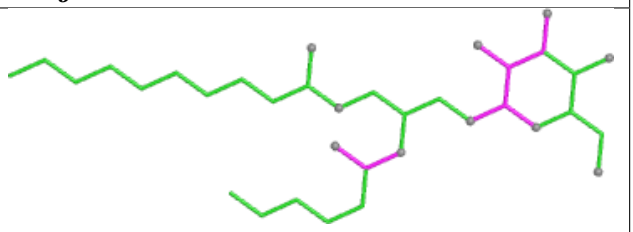


Rings

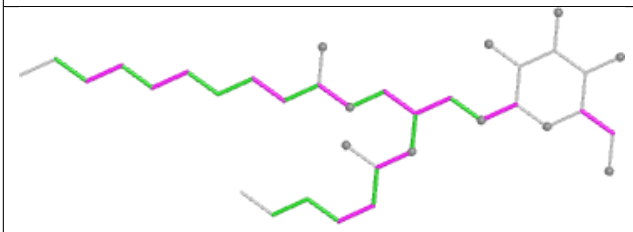
Ligand LMG j 101



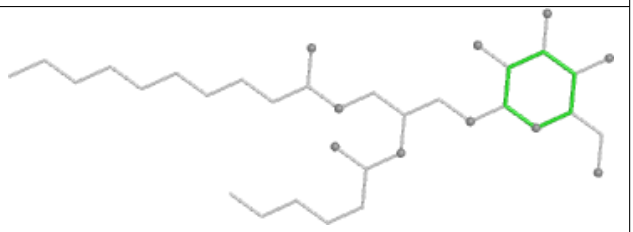
Bond lengths



Bond angles

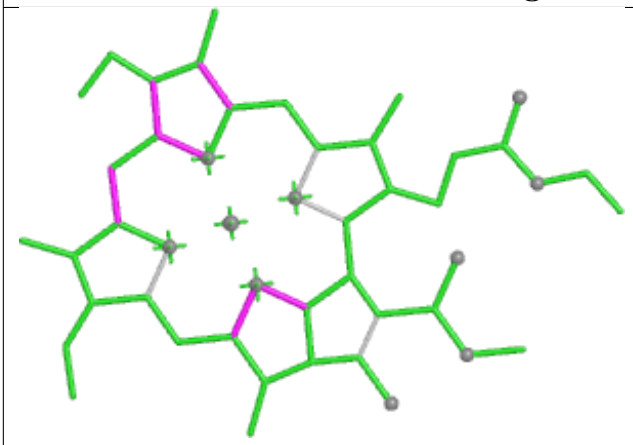


Torsions

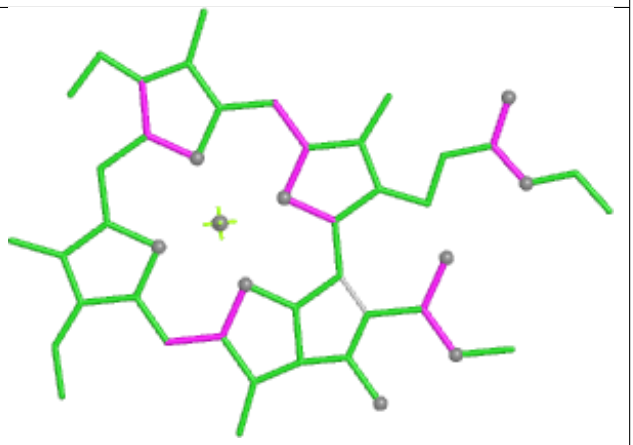


Rings

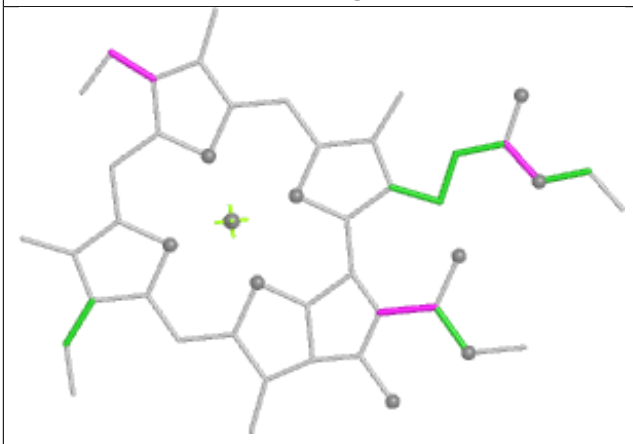
Ligand CLA N 304



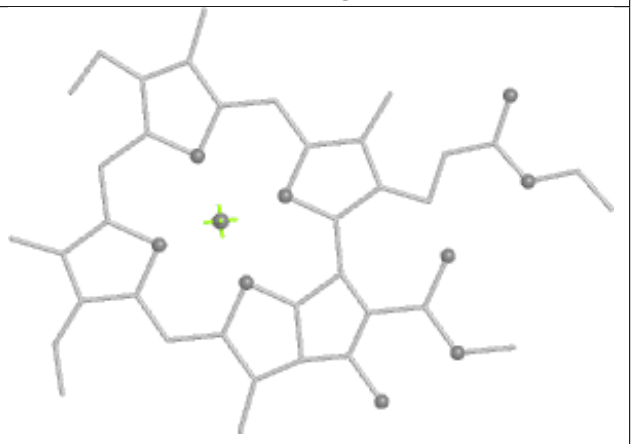
Bond lengths



Bond angles

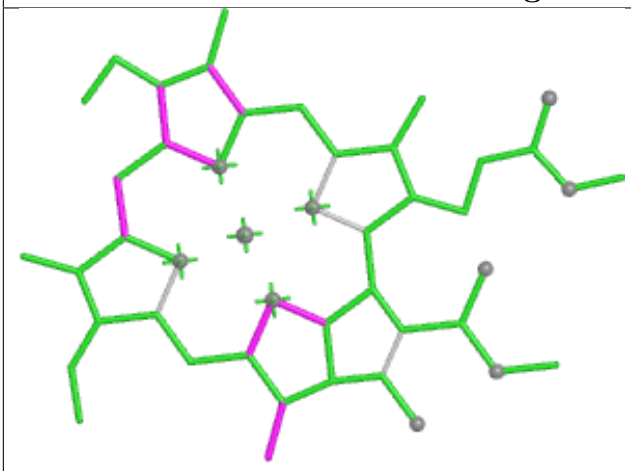


Torsions

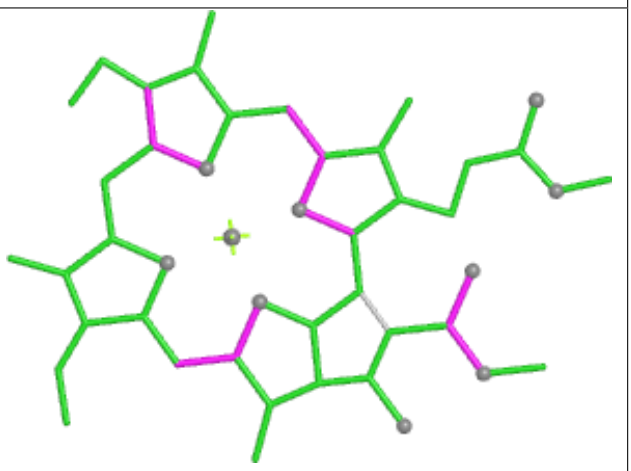


Rings

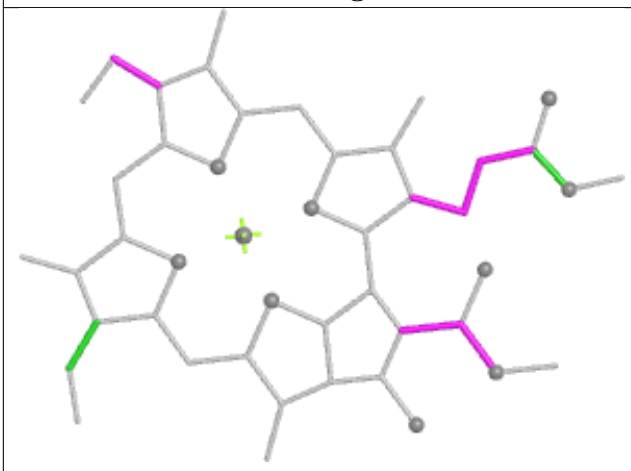
Ligand CLA A 319



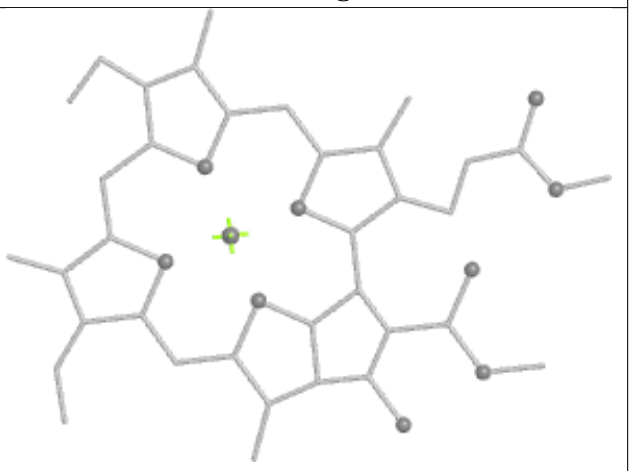
Bond lengths



Bond angles

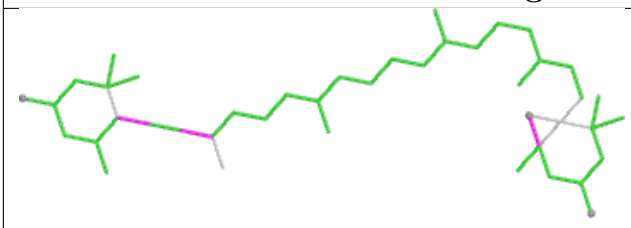


Torsions

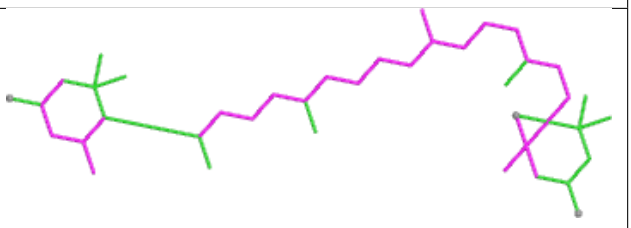


Rings

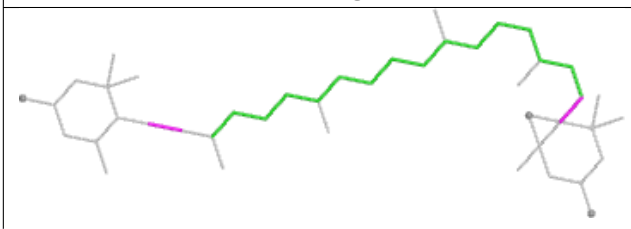
Ligand DD6 B 306



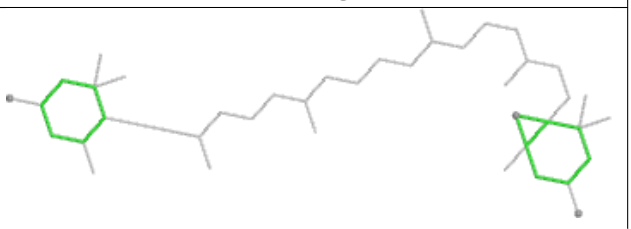
Bond lengths



Bond angles

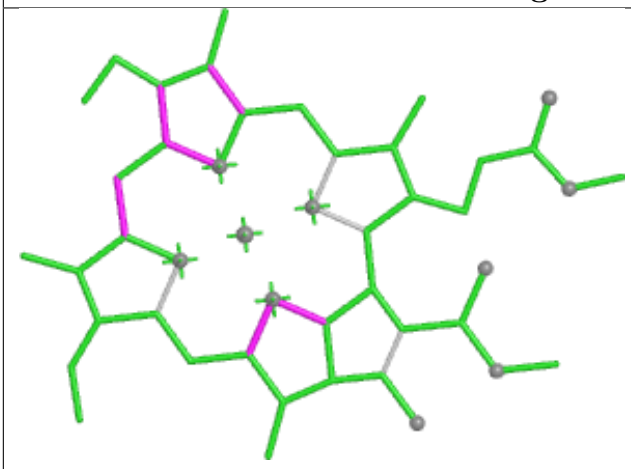


Torsions

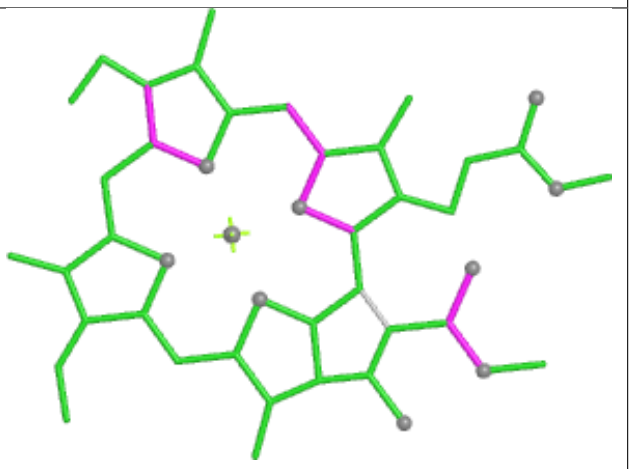


Rings

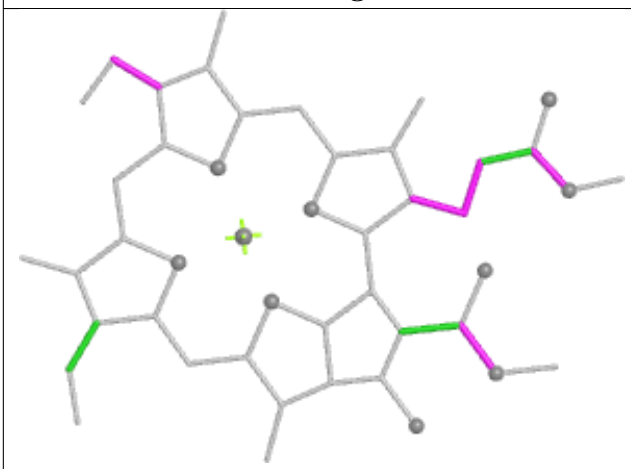
Ligand CLA I 307



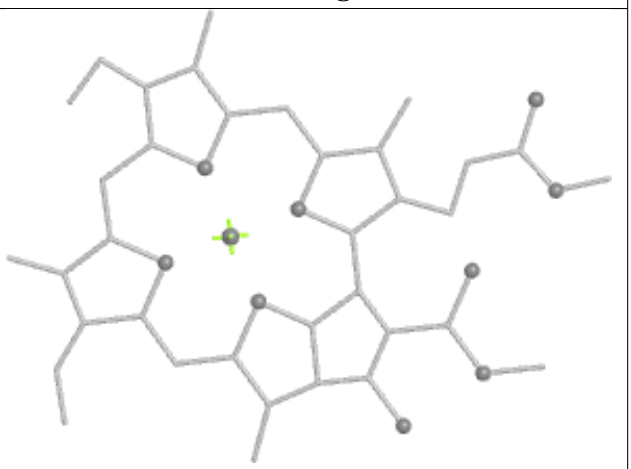
Bond lengths



Bond angles

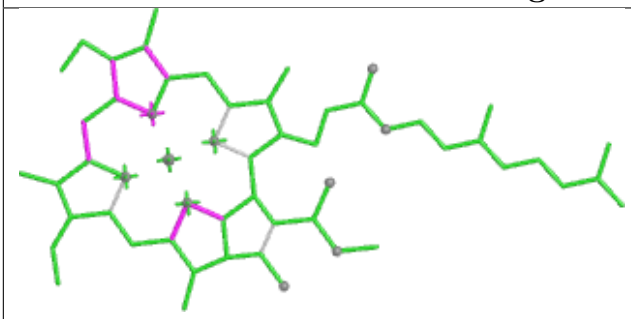


Torsions

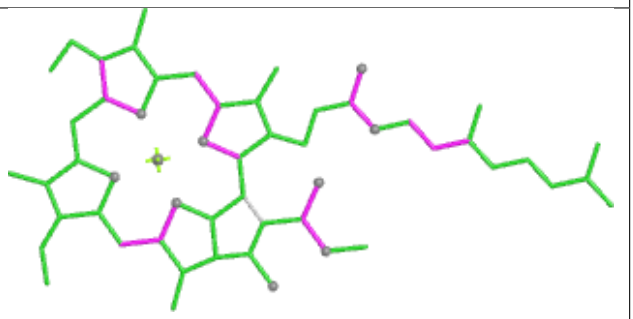


Rings

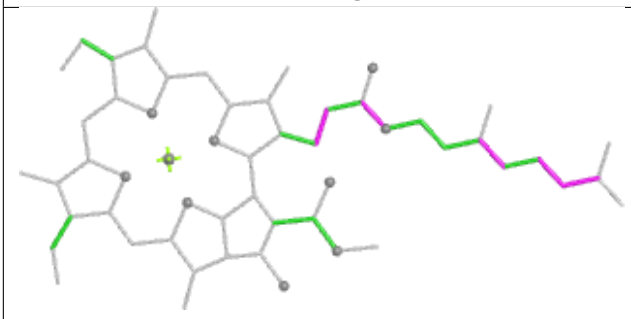
Ligand CLA a 728



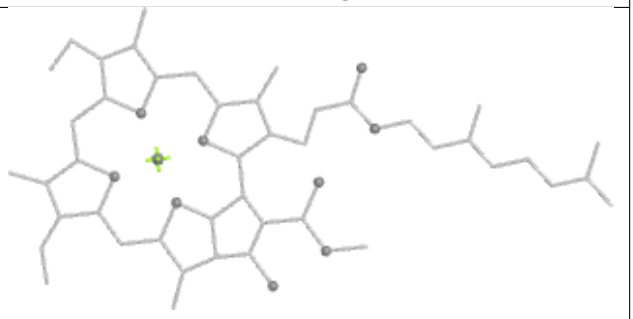
Bond lengths



Bond angles

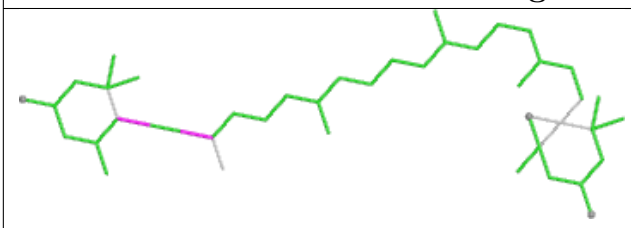


Torsions

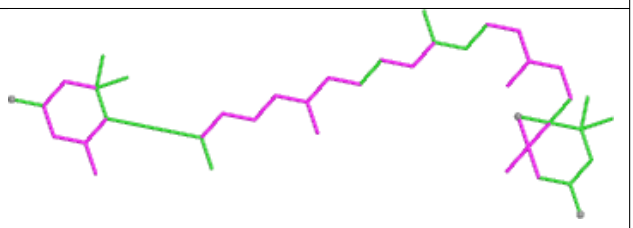


Rings

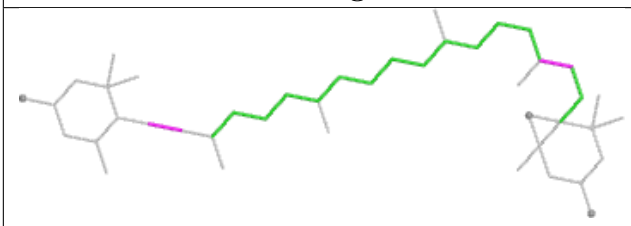
Ligand DD6 J 302



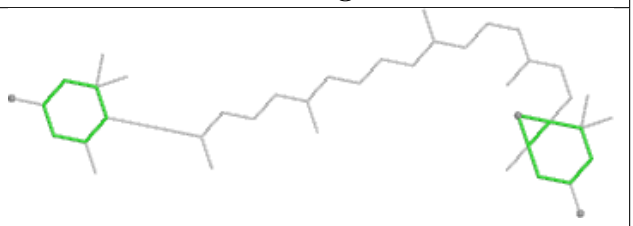
Bond lengths



Bond angles

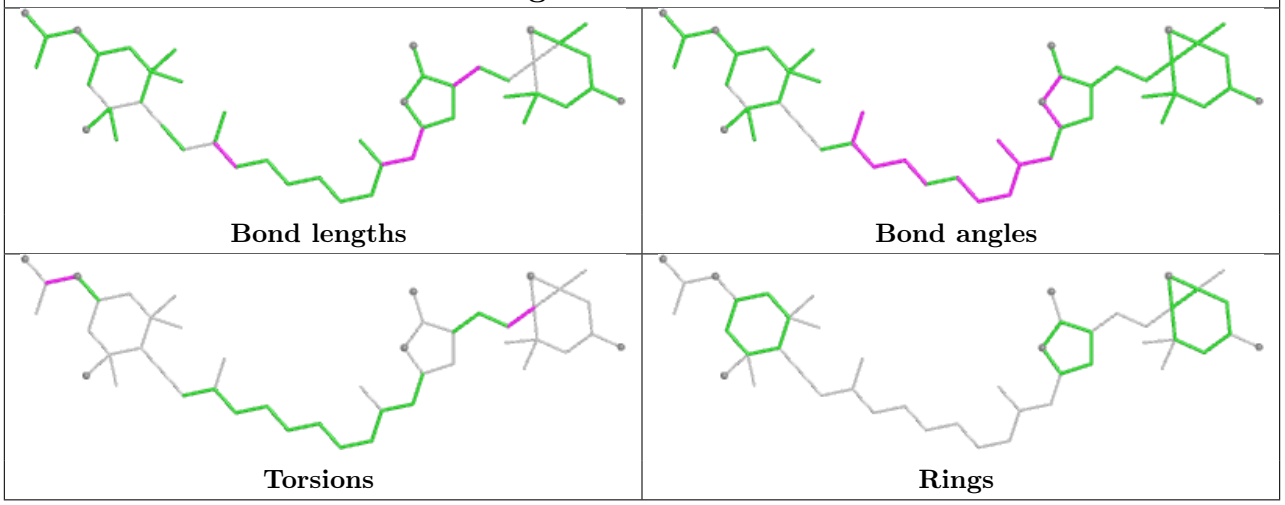


Torsions

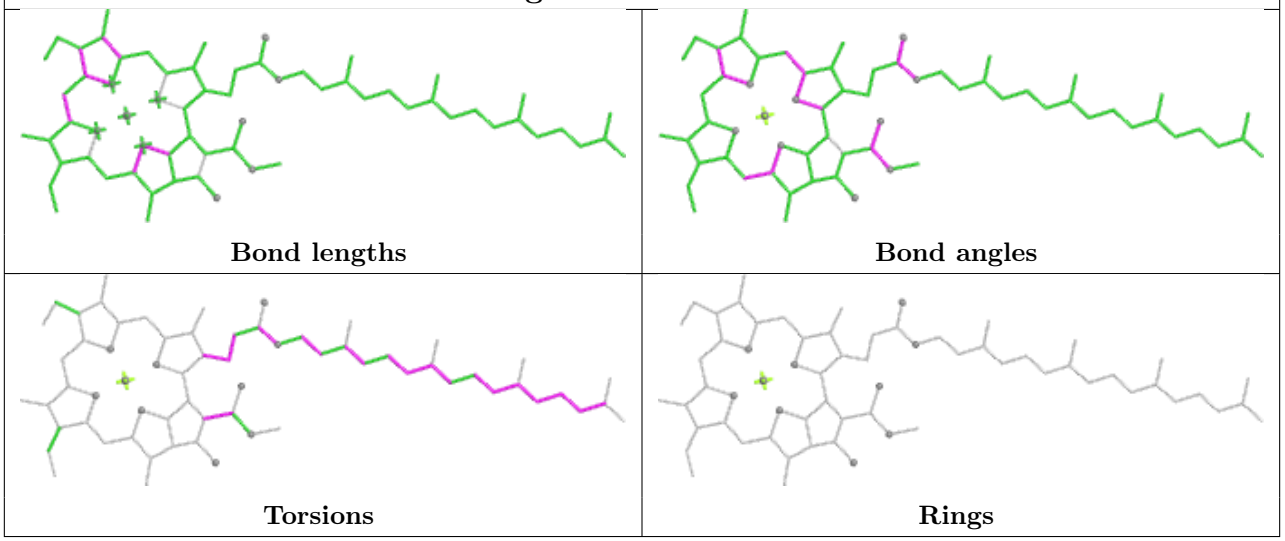


Rings

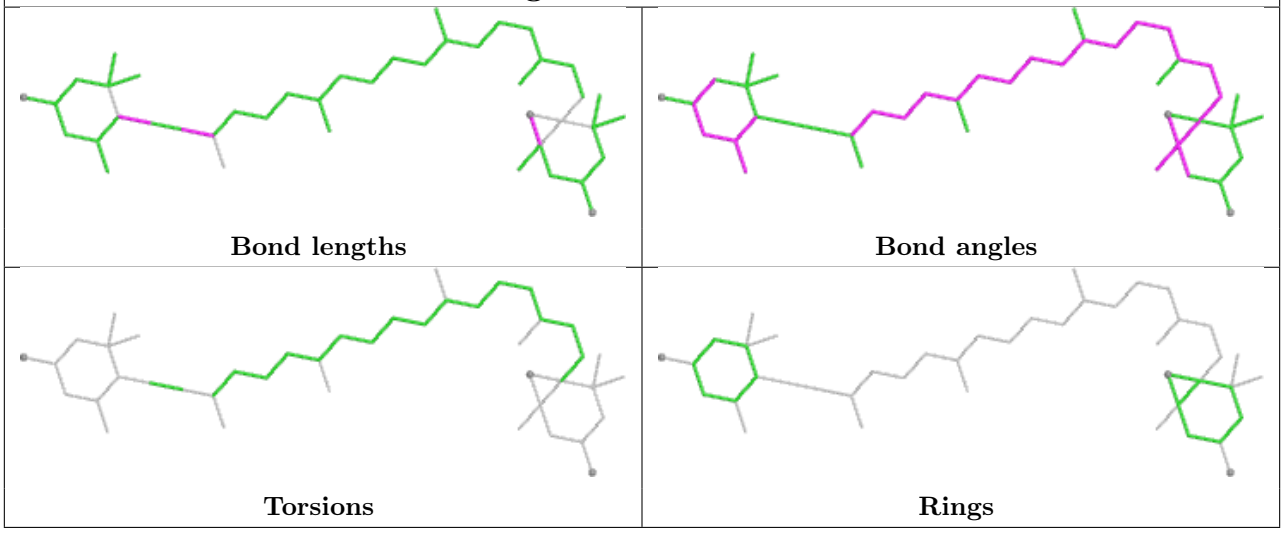
Ligand PID G 506



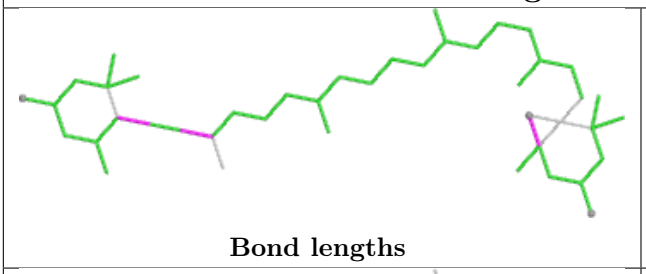
Ligand CLA B 309



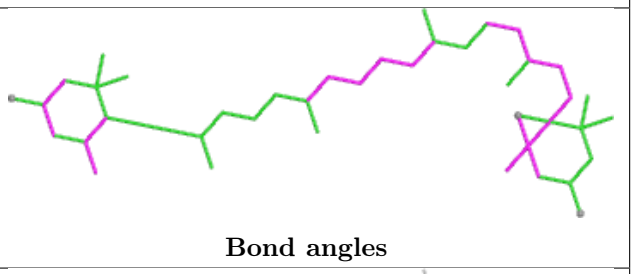
Ligand DD6 N 303



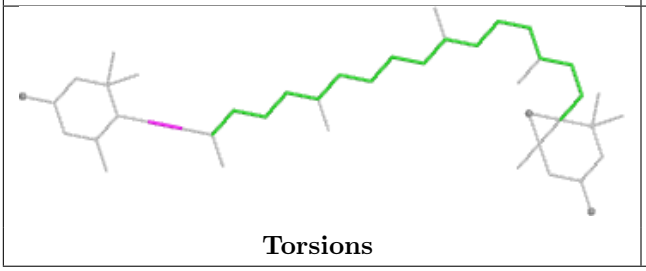
Ligand DD6 H 303



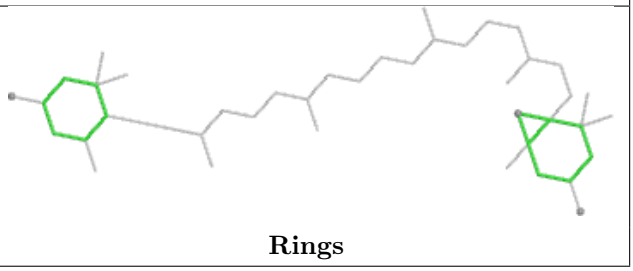
Bond lengths



Bond angles

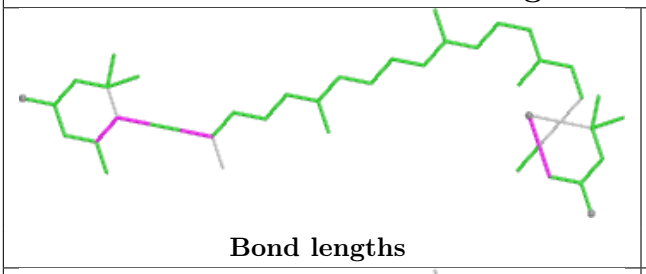


Torsions

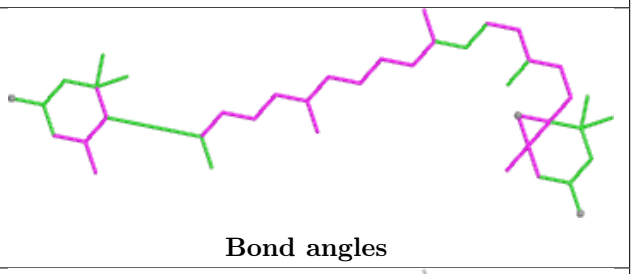


Rings

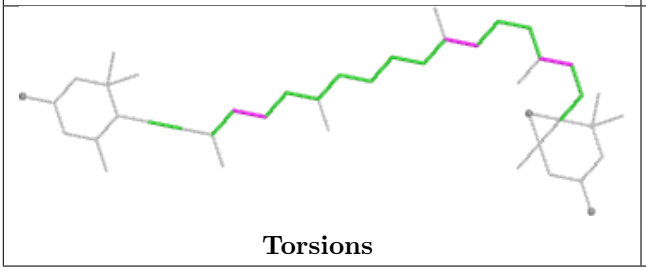
Ligand DD6 G 504



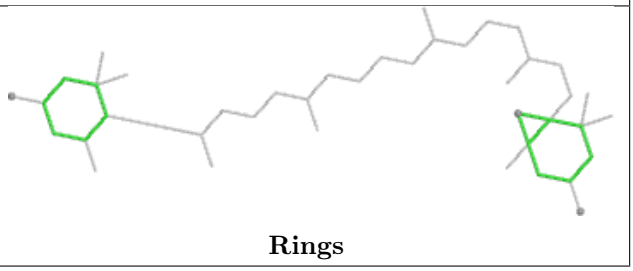
Bond lengths



Bond angles

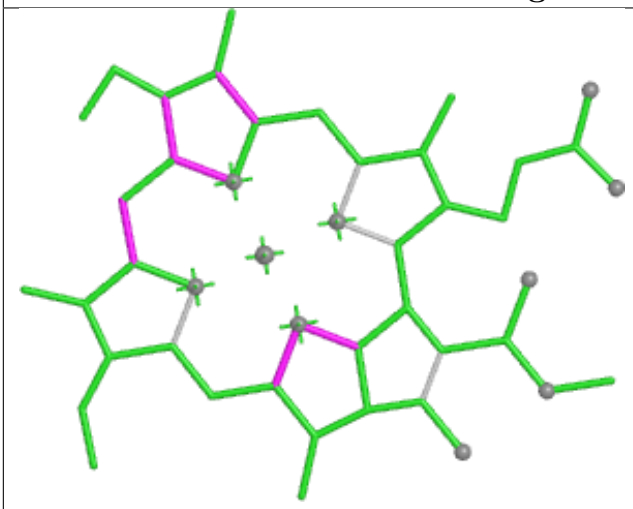


Torsions

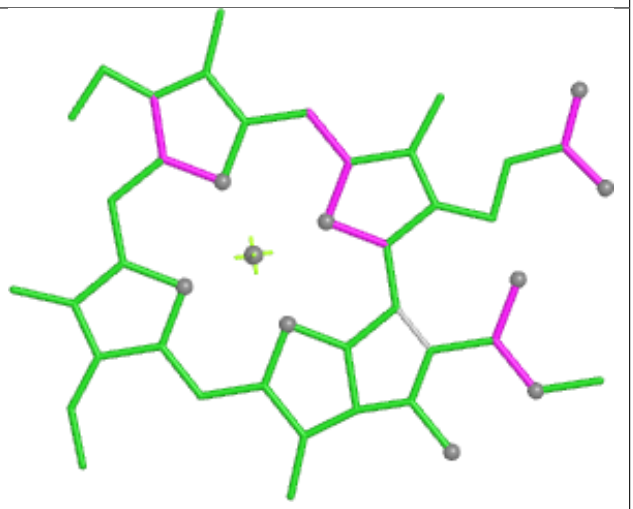


Rings

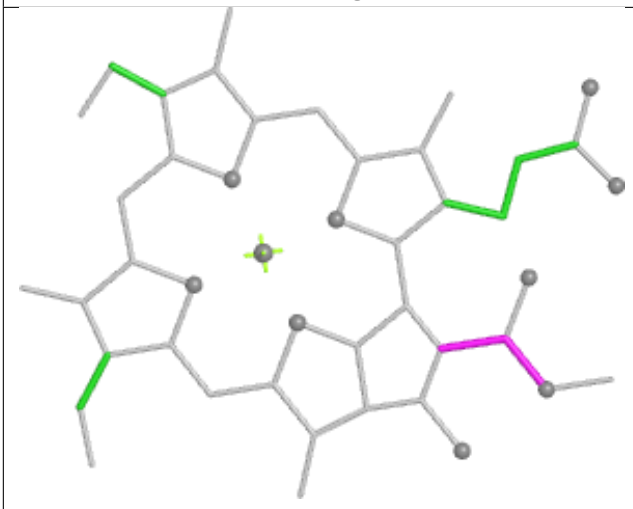
Ligand CLA a 714



Bond lengths



Bond angles

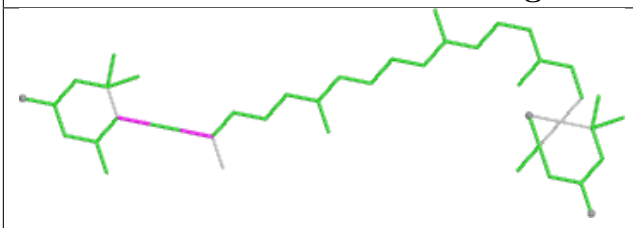


Torsions

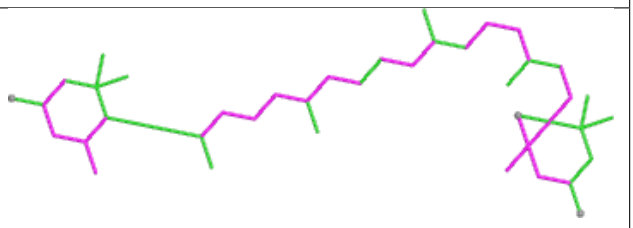


Rings

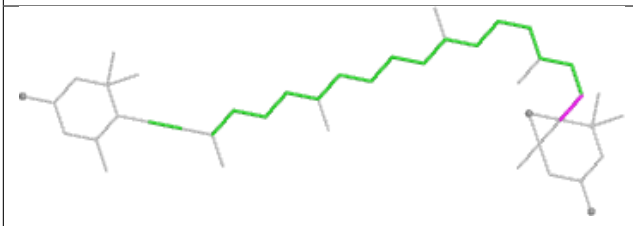
Ligand DD6 A 305



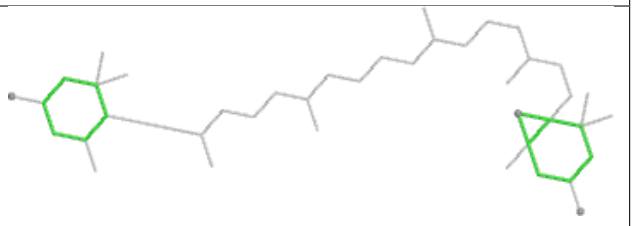
Bond lengths



Bond angles

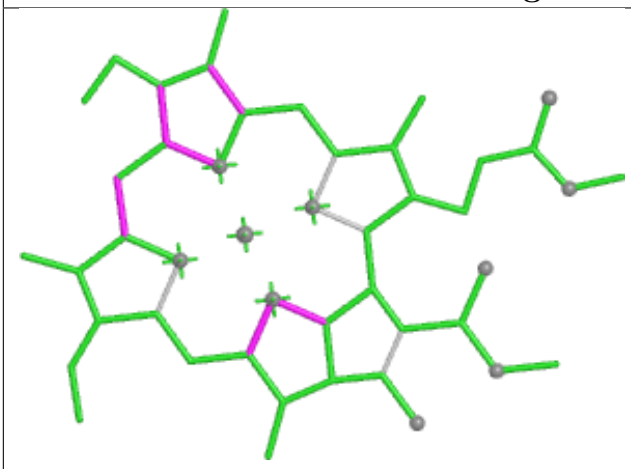


Torsions

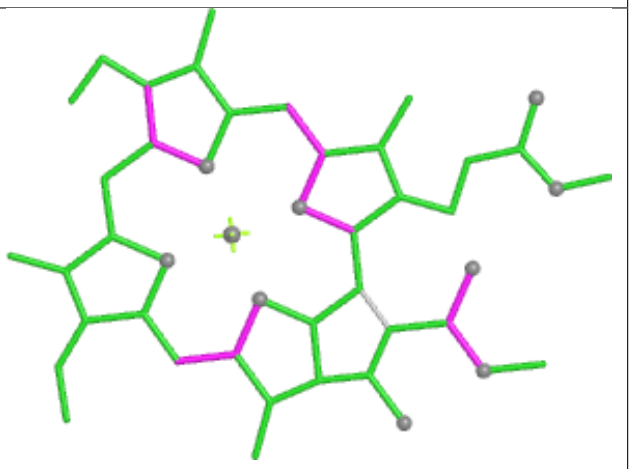


Rings

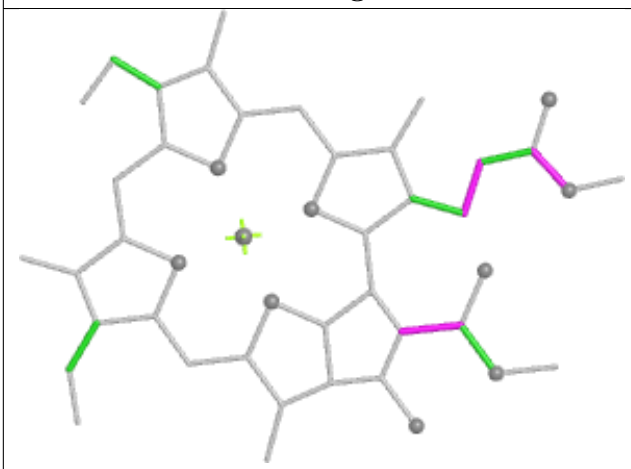
Ligand CLA D 311



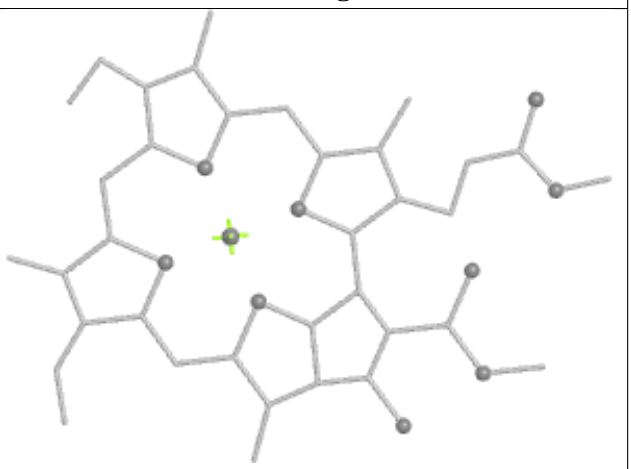
Bond lengths



Bond angles

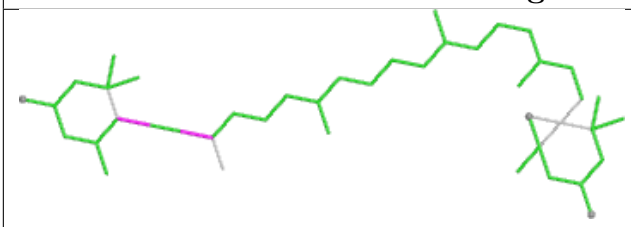


Torsions

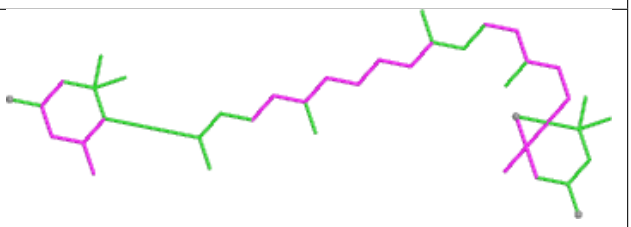


Rings

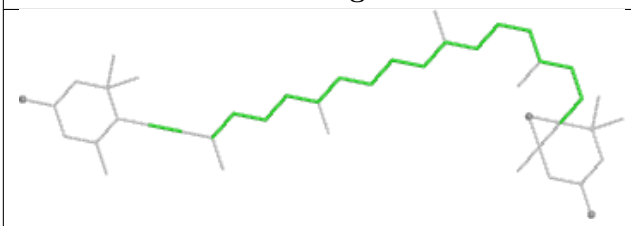
Ligand DD6 L 303



Bond lengths



Bond angles

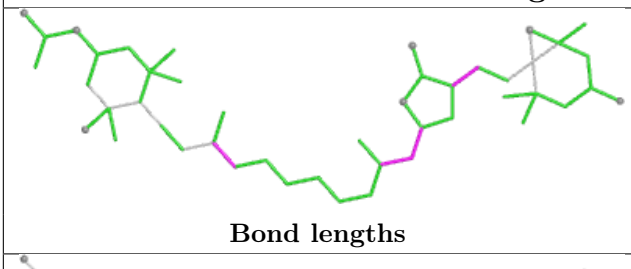


Torsions

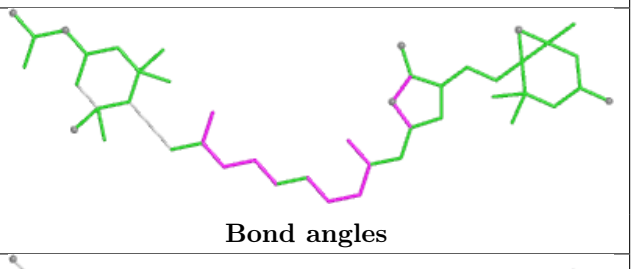


Rings

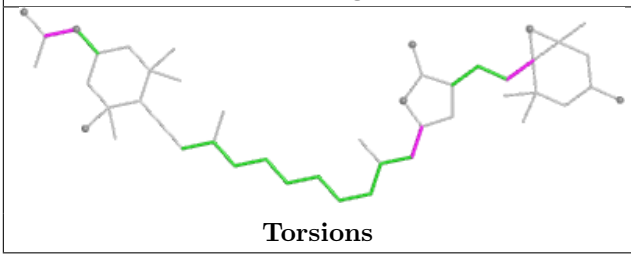
Ligand PID O 301



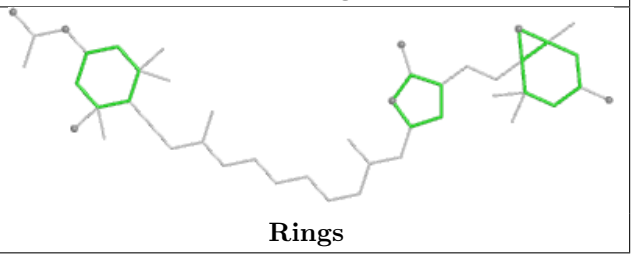
Bond lengths



Bond angles

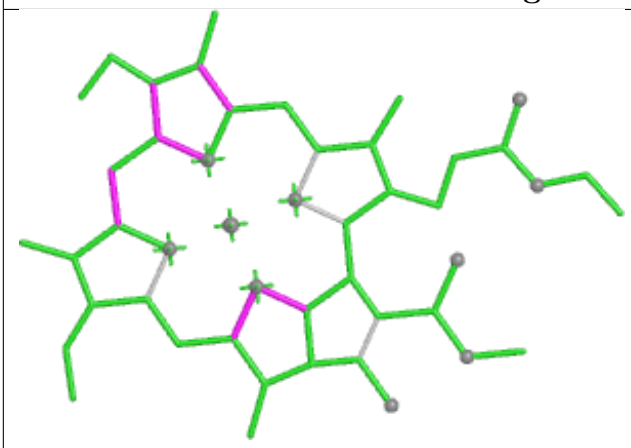


Torsions

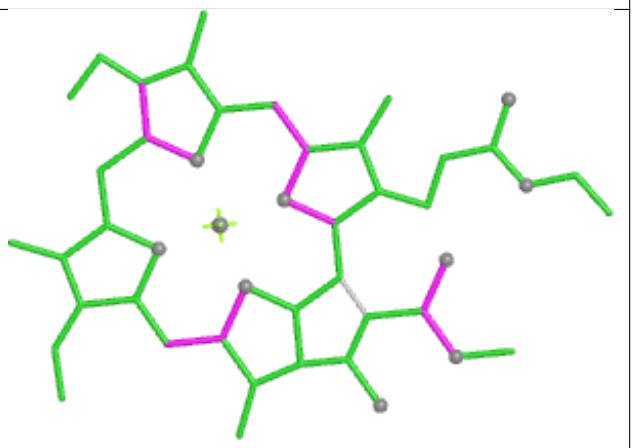


Rings

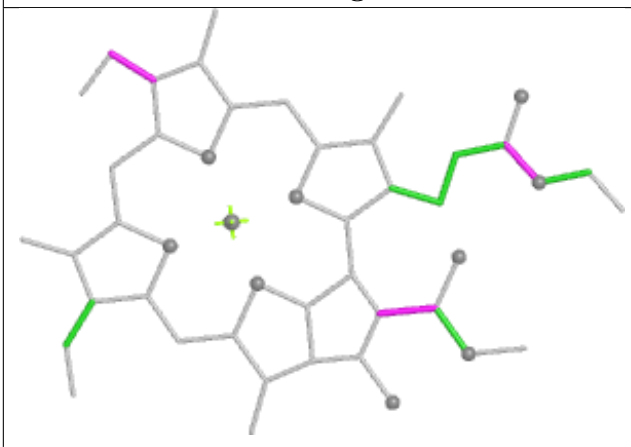
Ligand CLA D 308



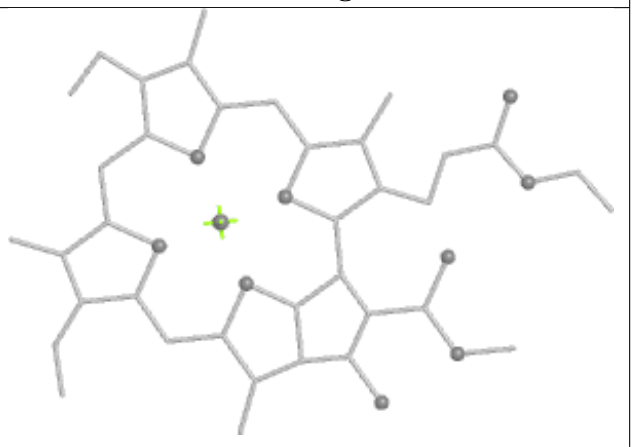
Bond lengths



Bond angles

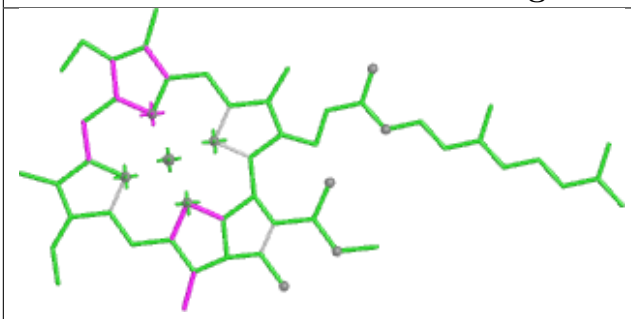


Torsions

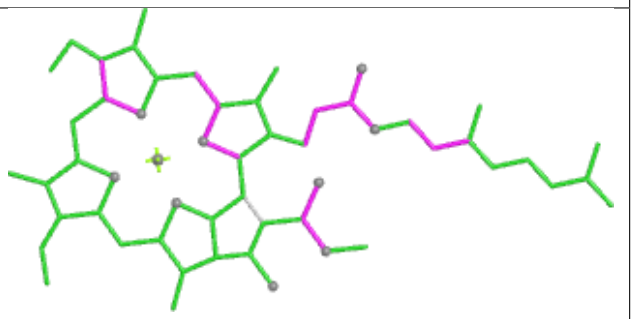


Rings

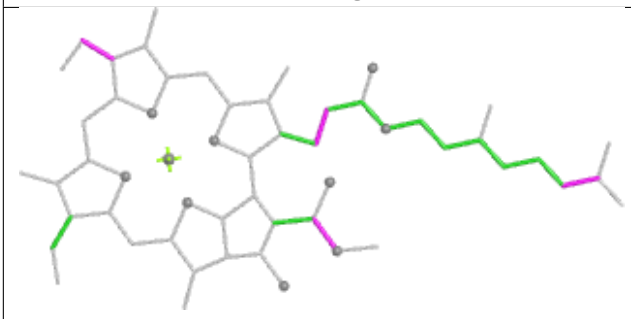
Ligand CLA a 710



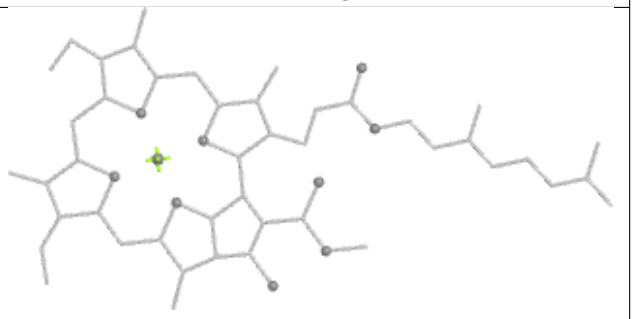
Bond lengths



Bond angles

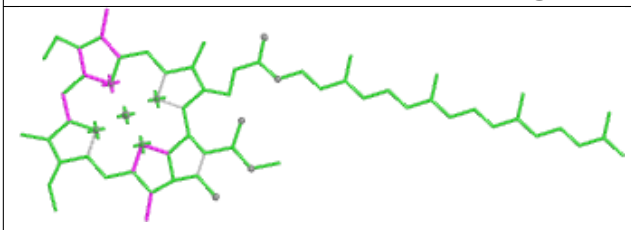


Torsions

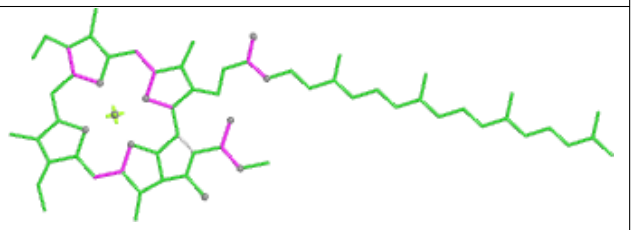


Rings

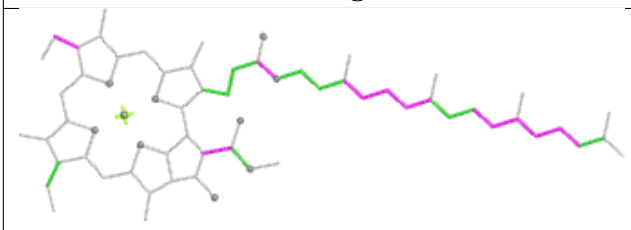
Ligand CLA I 312



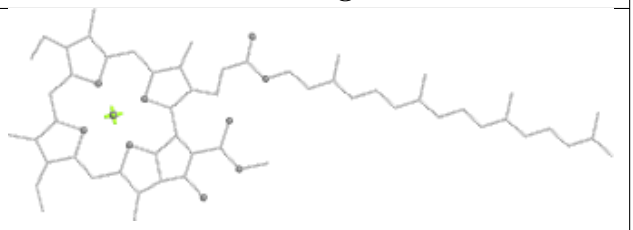
Bond lengths



Bond angles

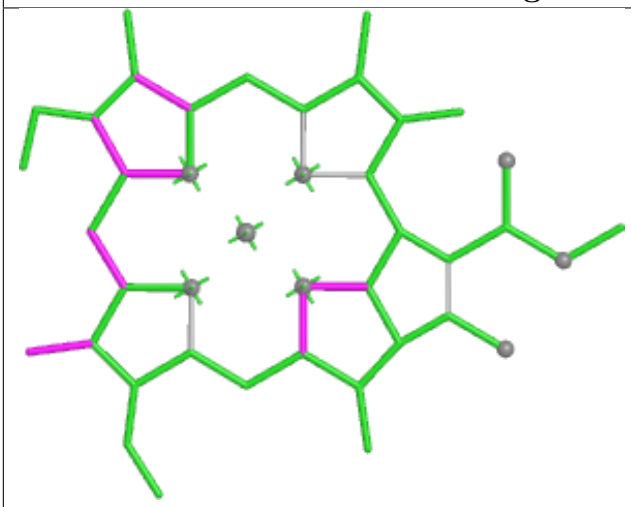


Torsions

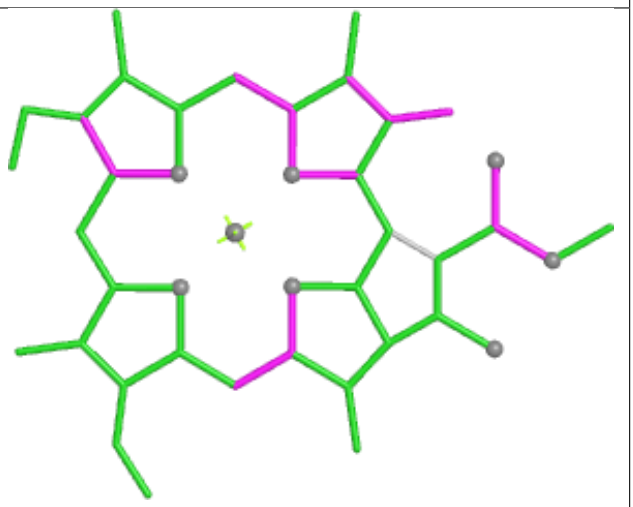


Rings

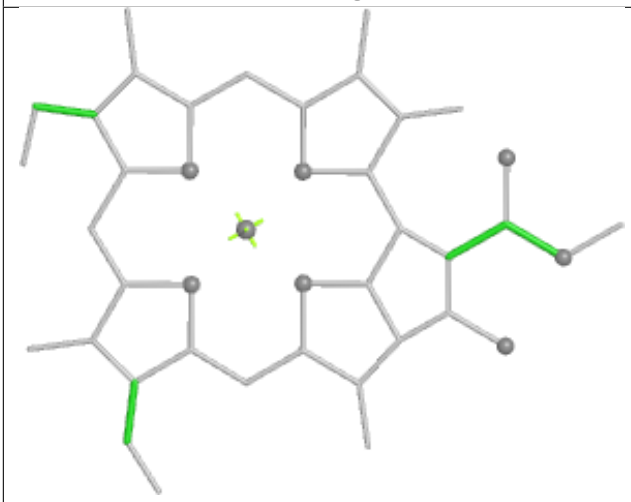
Ligand CLA D 316



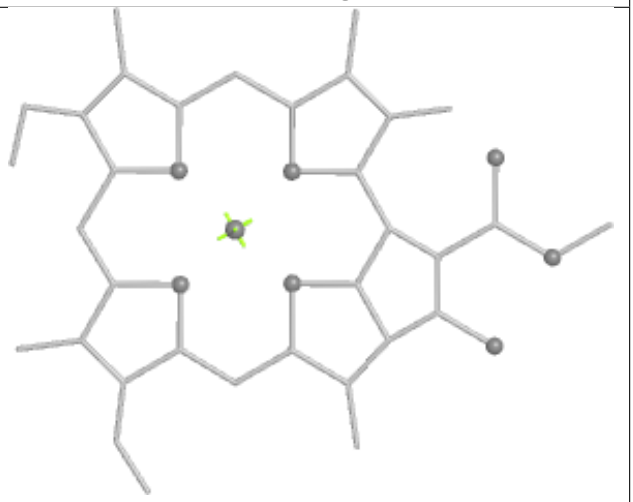
Bond lengths



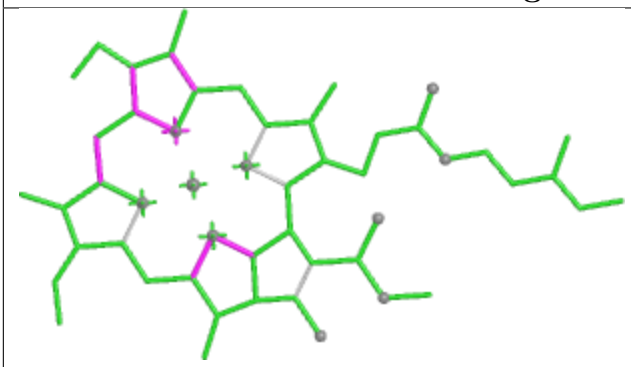
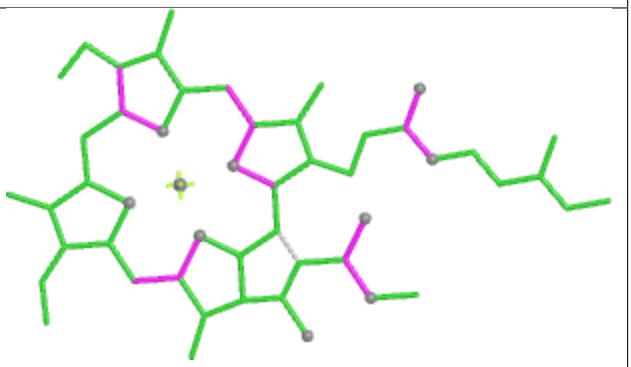
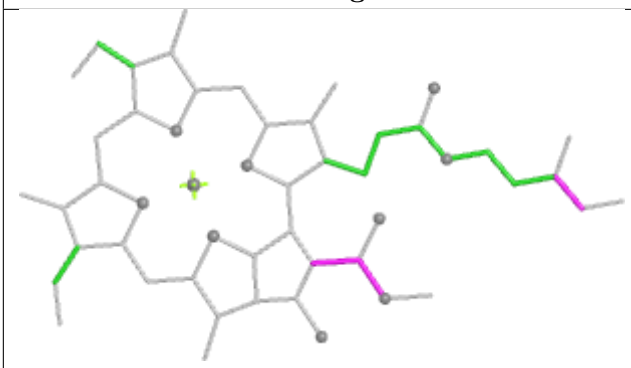
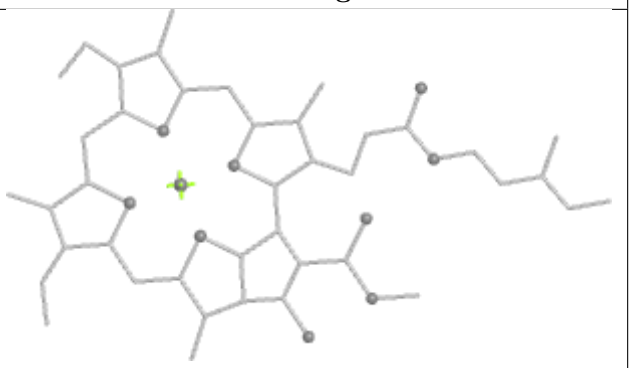
Bond angles

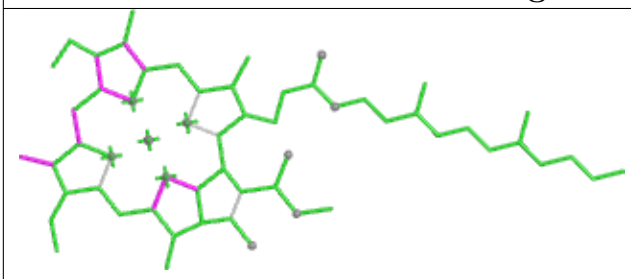
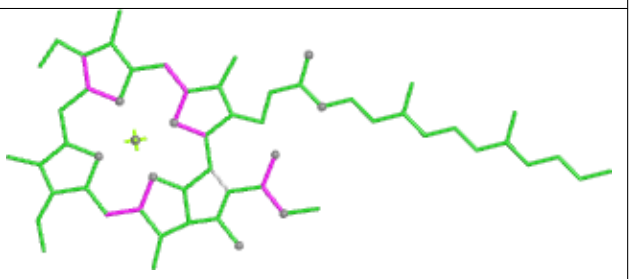
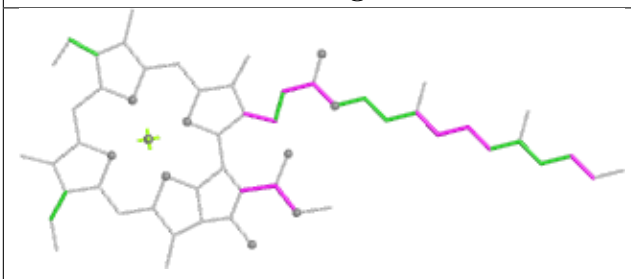
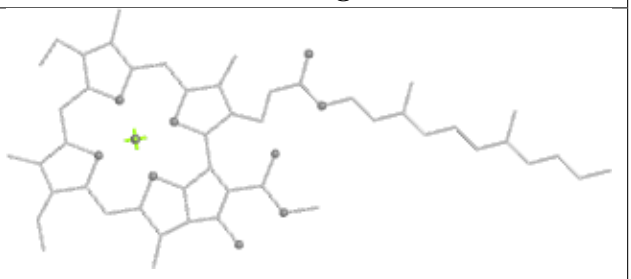


Torsions

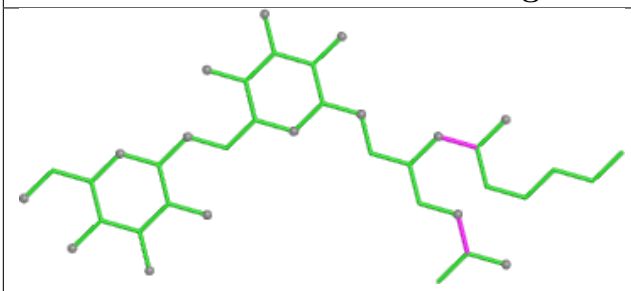


Rings

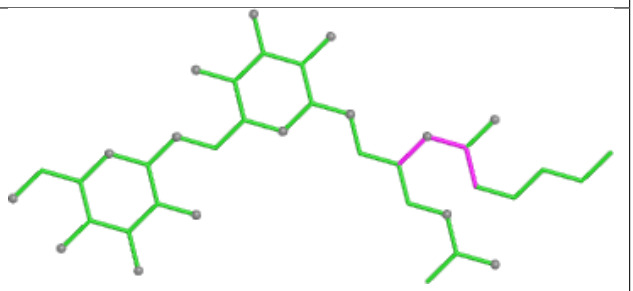
Ligand CLA O 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 706	
 Bond lengths	 Bond angles
 Torsions	 Rings

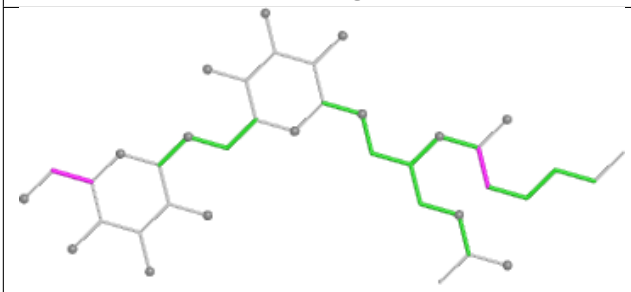
Ligand DGD L 301



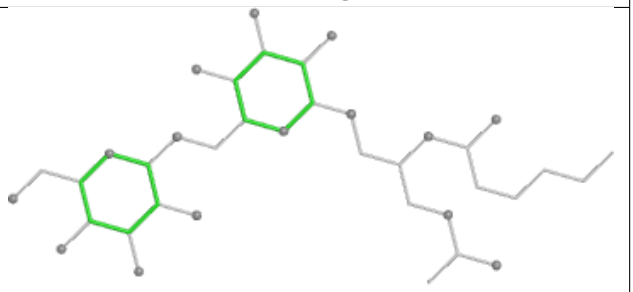
Bond lengths



Bond angles

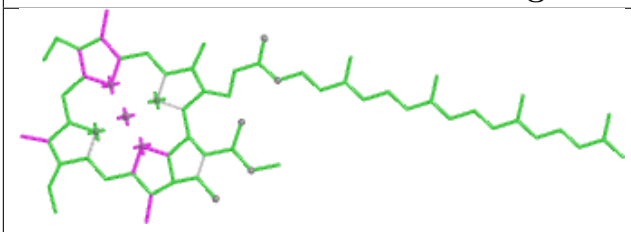


Torsions

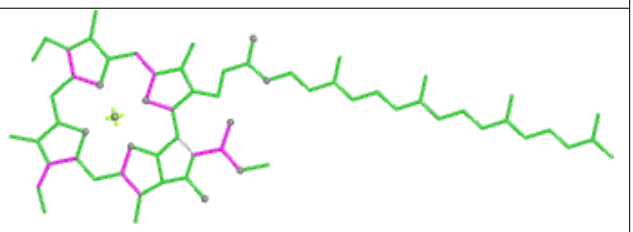


Rings

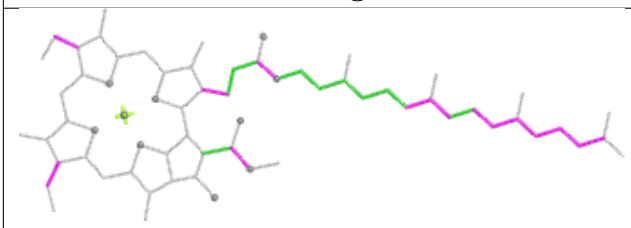
Ligand CLA b 704



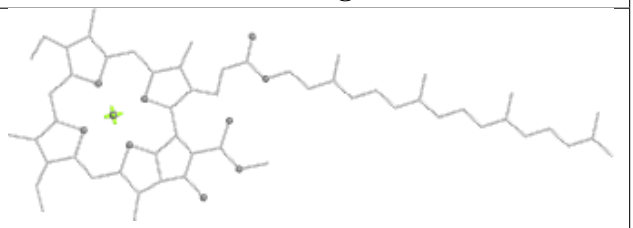
Bond lengths



Bond angles

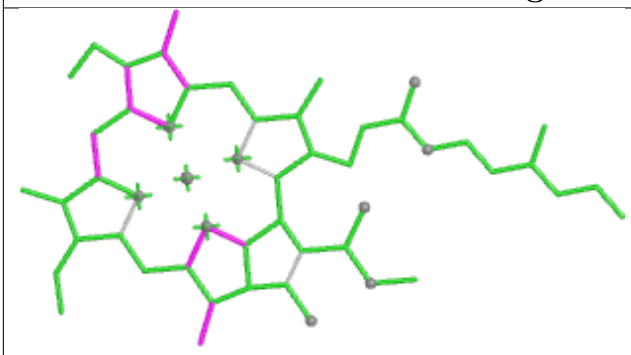


Torsions

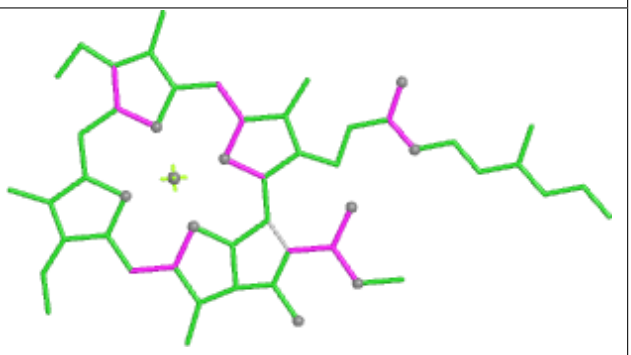


Rings

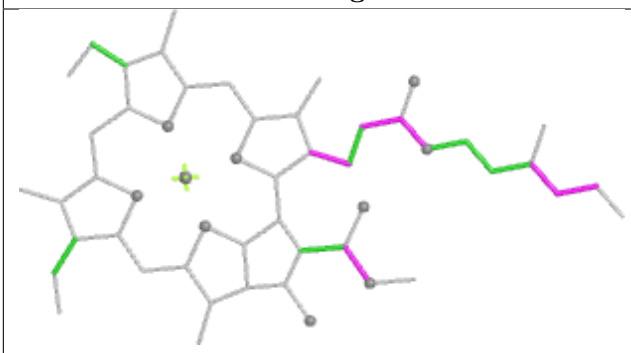
Ligand CLA L 317



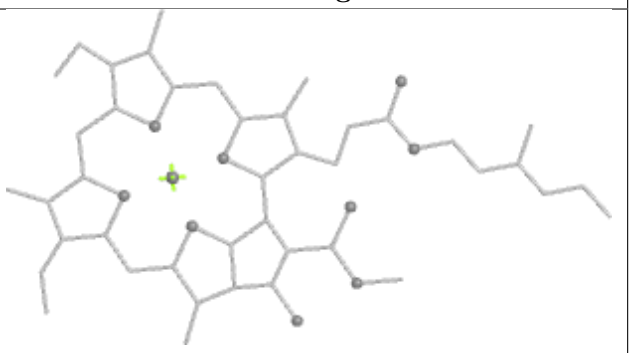
Bond lengths



Bond angles

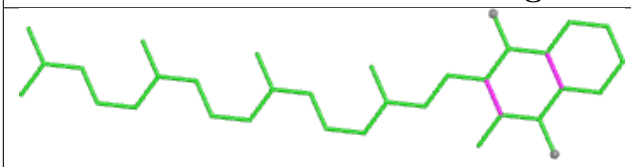


Torsions

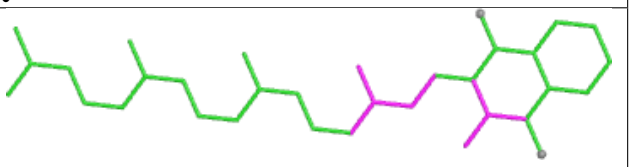


Rings

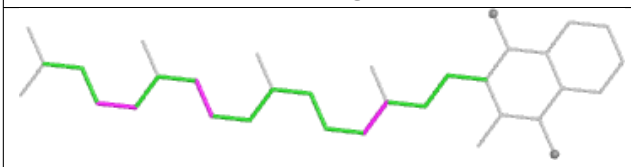
Ligand PQN b 729



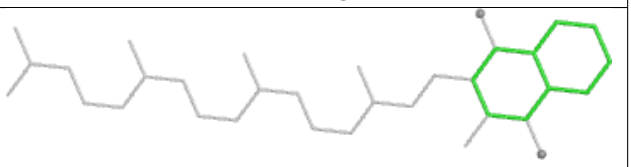
Bond lengths



Bond angles

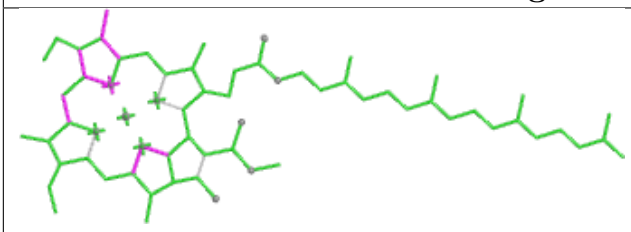


Torsions

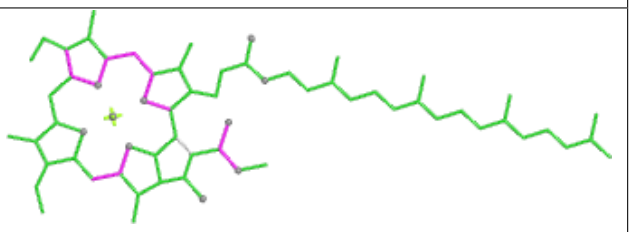


Rings

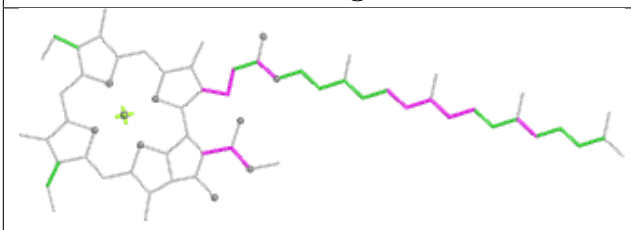
Ligand CLA a 709



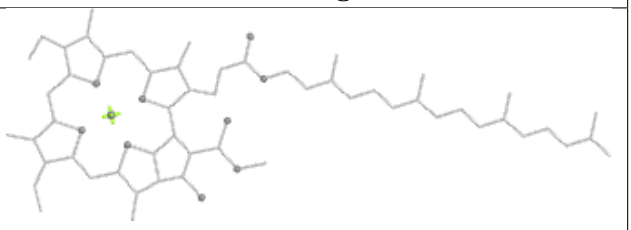
Bond lengths



Bond angles

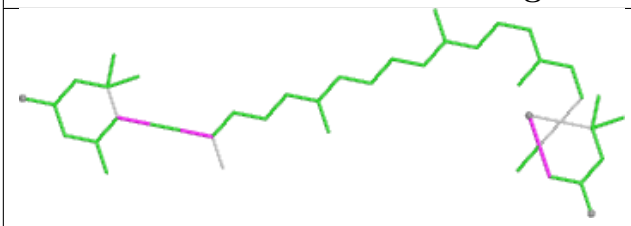


Torsions

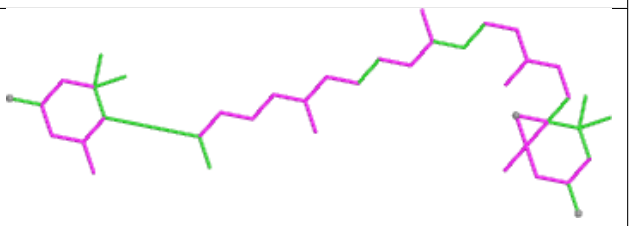


Rings

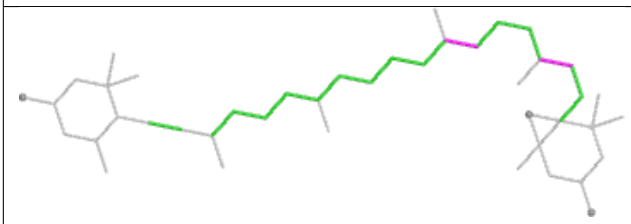
Ligand DD6 G 505



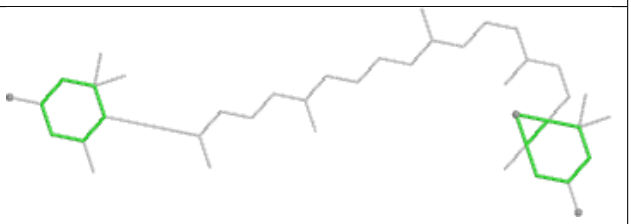
Bond lengths



Bond angles

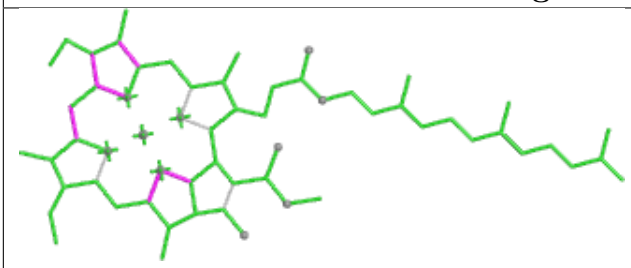


Torsions

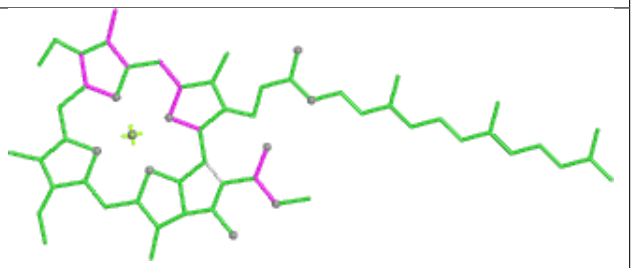


Rings

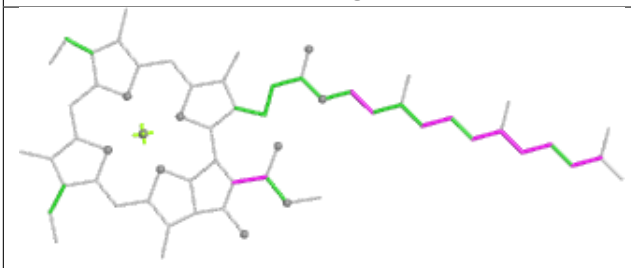
Ligand CLA l 304



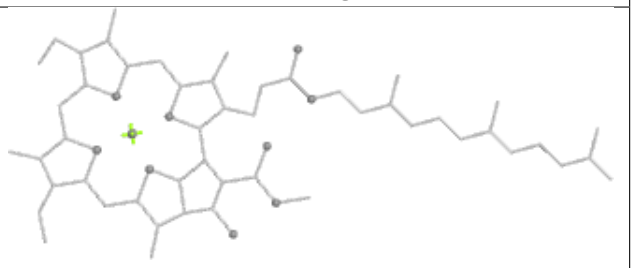
Bond lengths



Bond angles

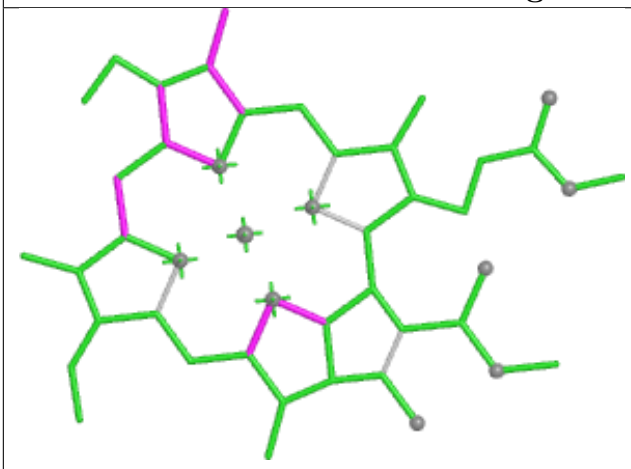


Torsions

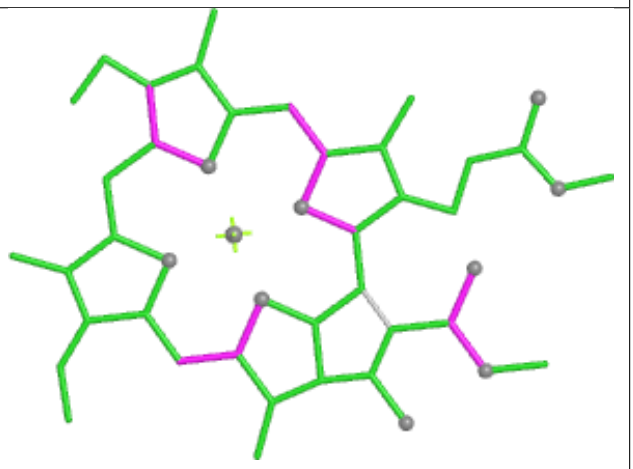


Rings

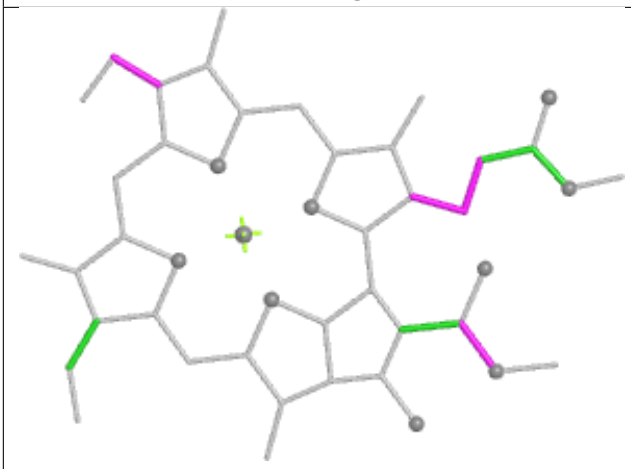
Ligand CLA L 312



Bond lengths



Bond angles

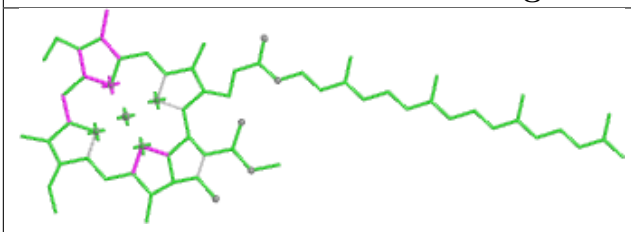


Torsions

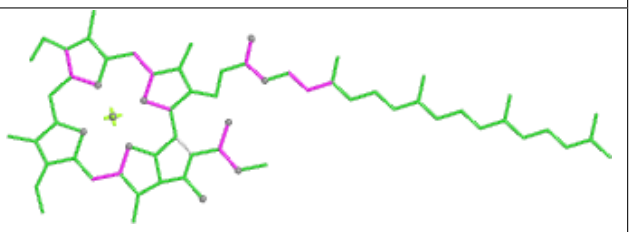


Rings

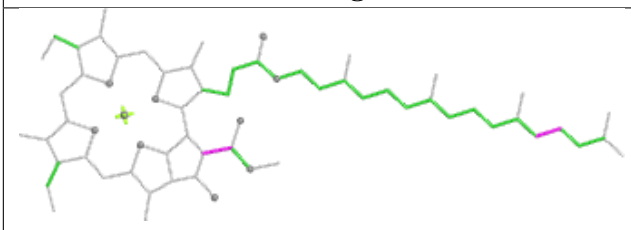
Ligand CLA O 309



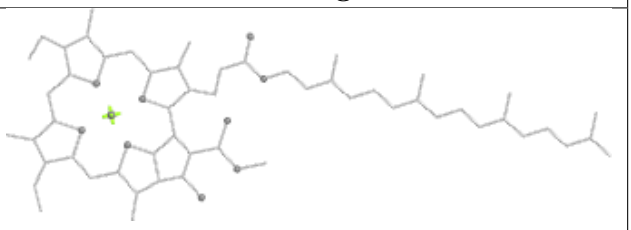
Bond lengths



Bond angles



Torsions

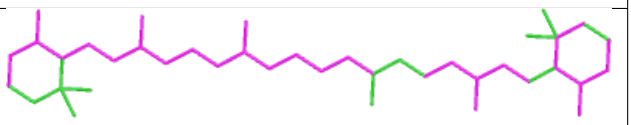


Rings

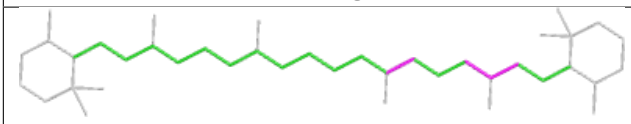
Ligand BCR l 302



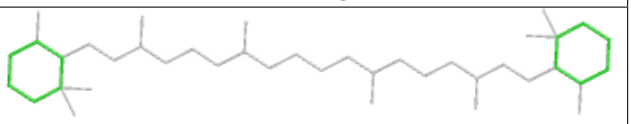
Bond lengths



Bond angles

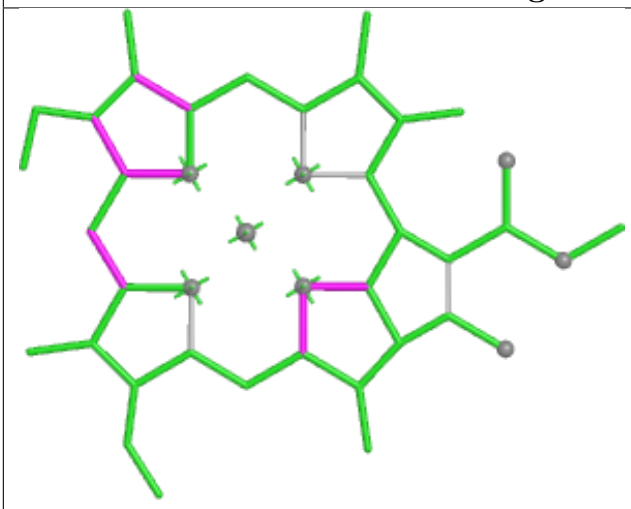


Torsions

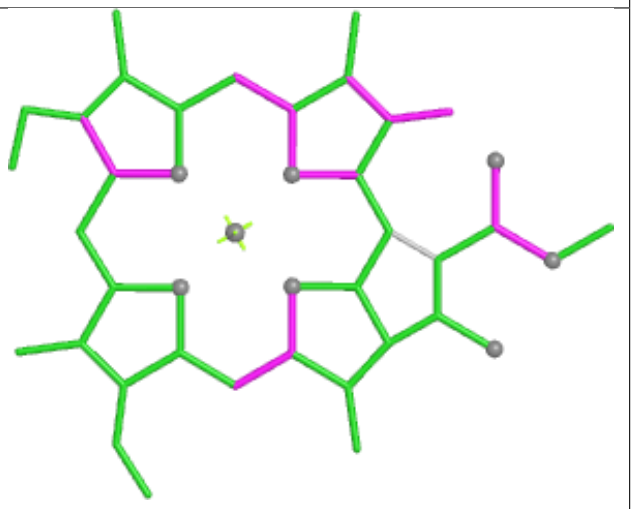


Rings

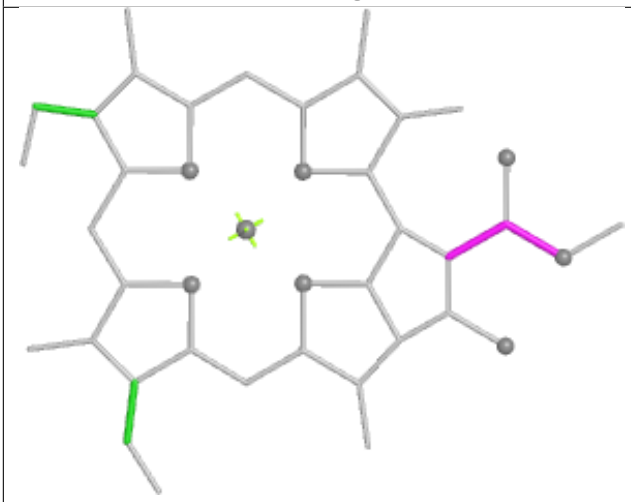
Ligand CLA J 314



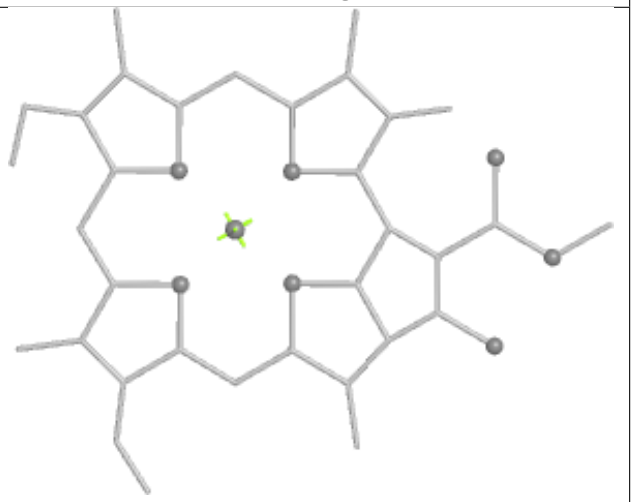
Bond lengths



Bond angles



Torsions

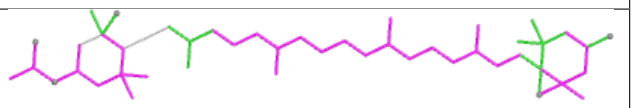


Rings

Ligand UIX K 302



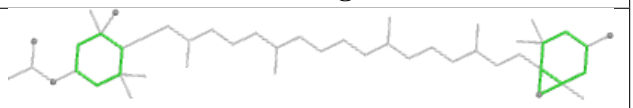
Bond lengths



Bond angles

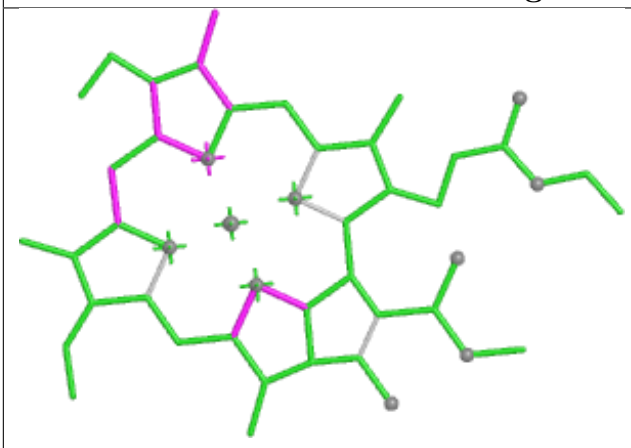


Torsions

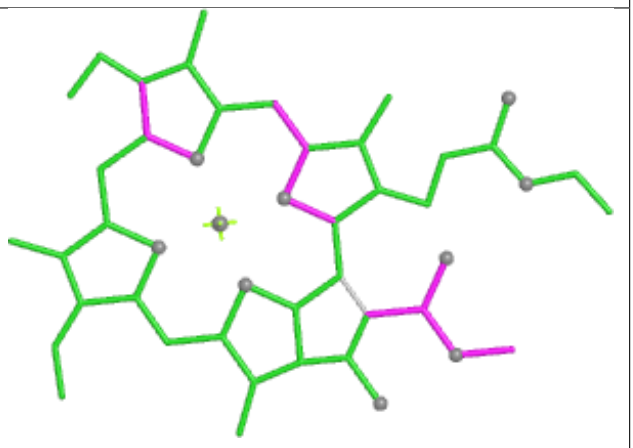


Rings

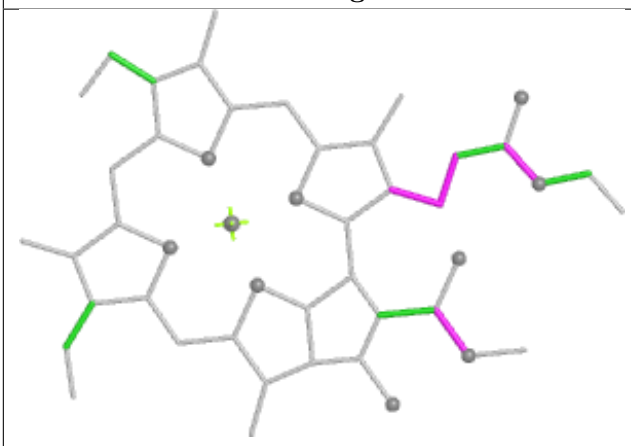
Ligand CLA P 215



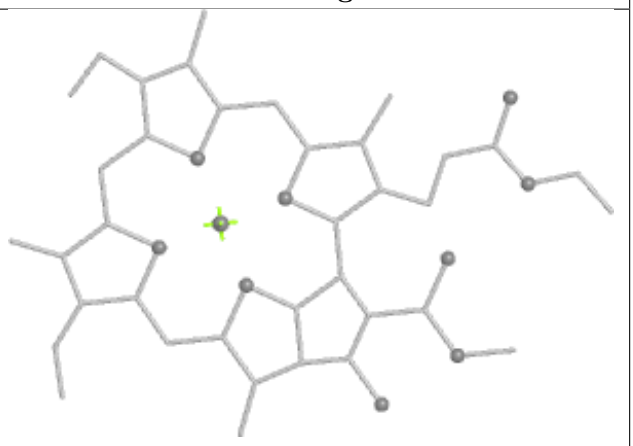
Bond lengths



Bond angles

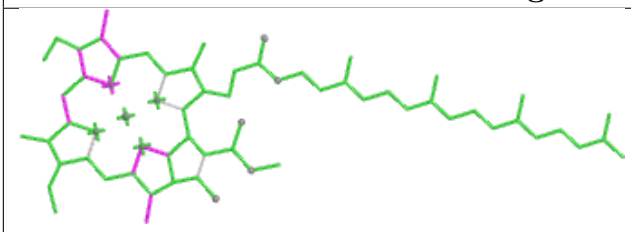


Torsions

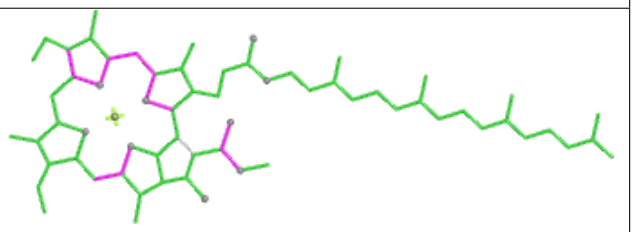


Rings

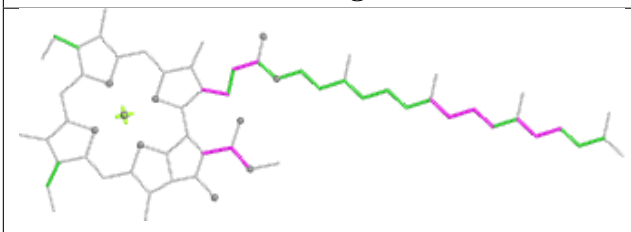
Ligand CLA b 713



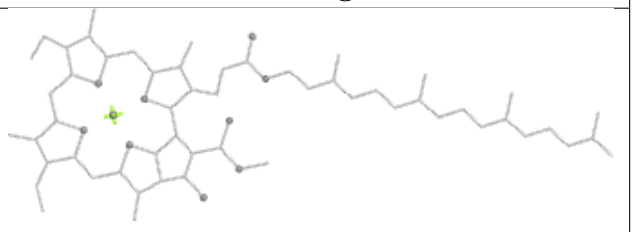
Bond lengths



Bond angles

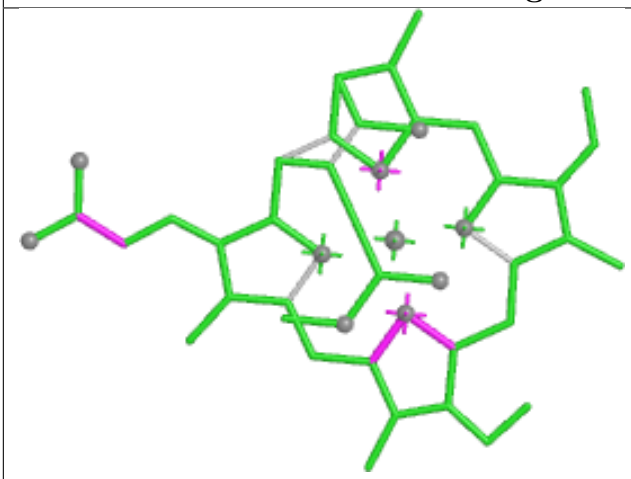


Torsions

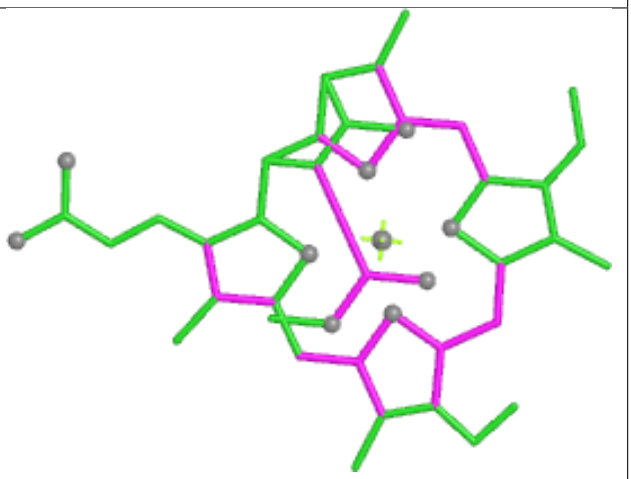


Rings

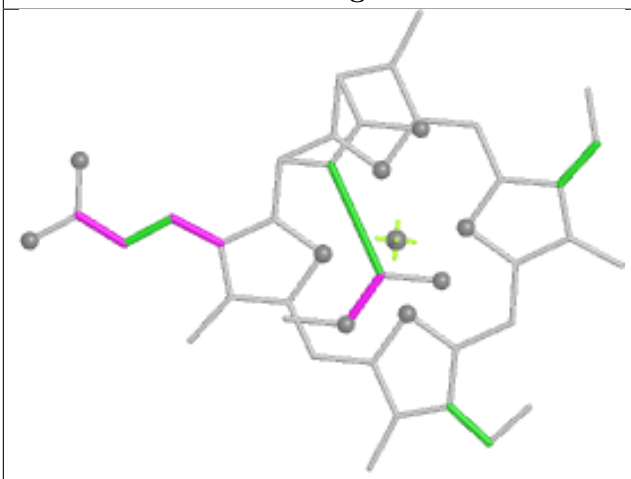
Ligand KC1 O 315



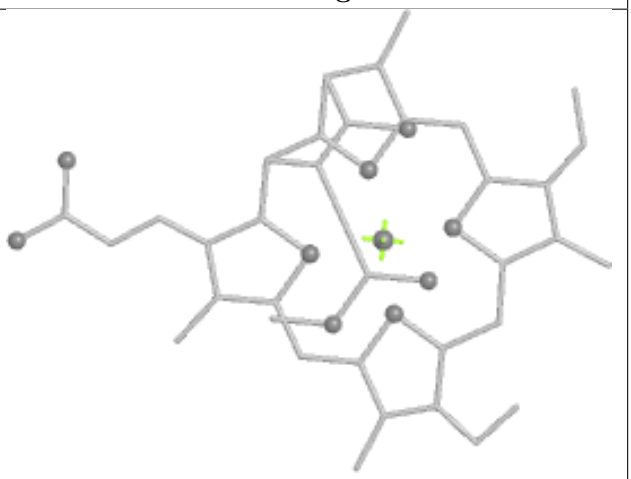
Bond lengths



Bond angles

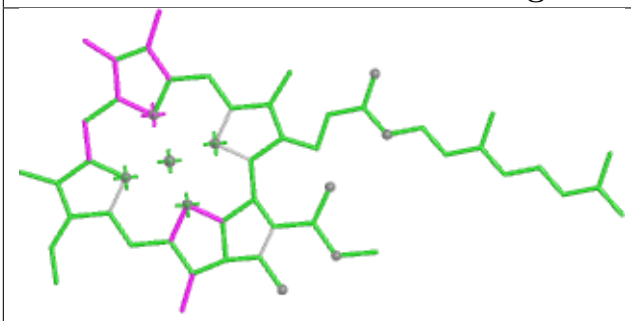


Torsions

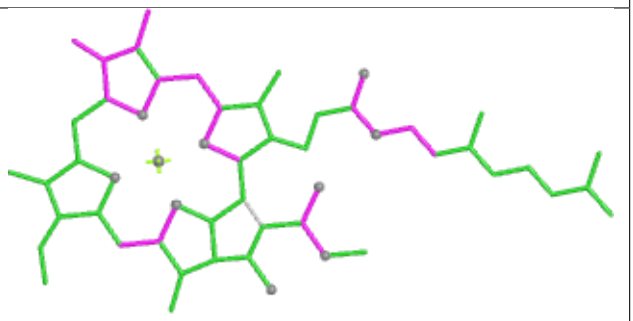


Rings

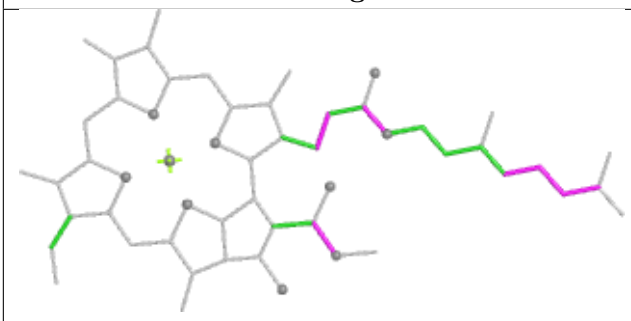
Ligand CLA b 712



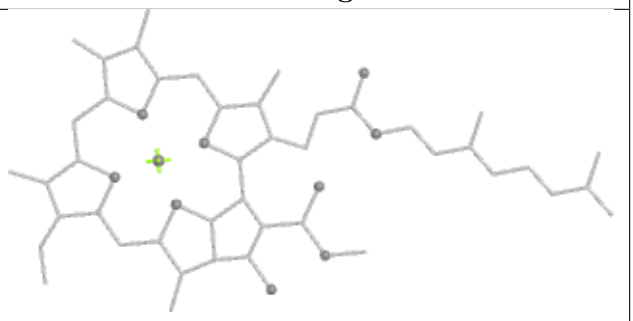
Bond lengths



Bond angles

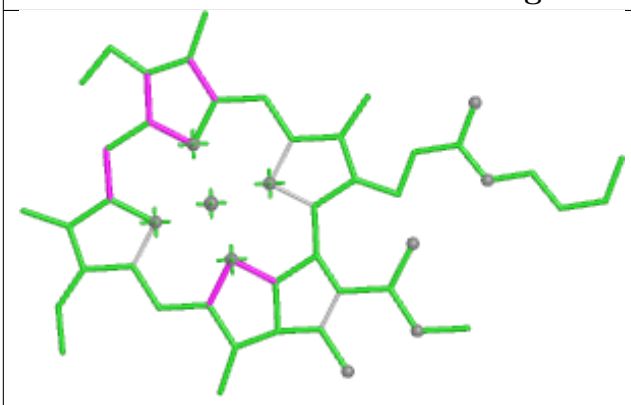


Torsions

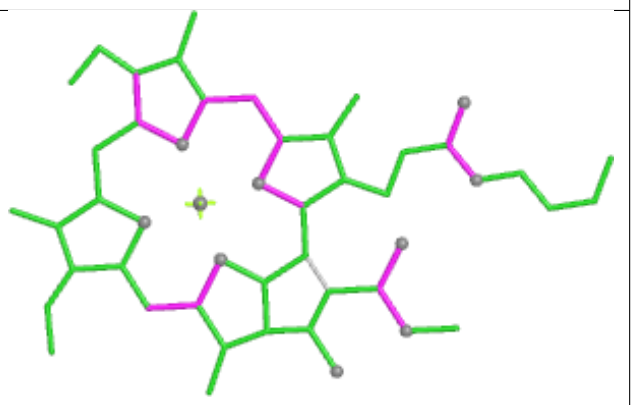


Rings

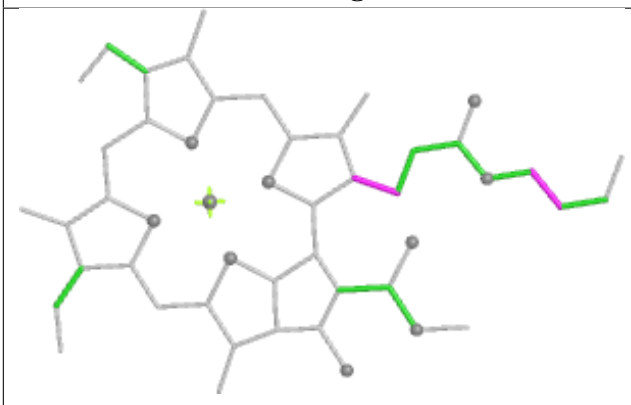
Ligand CLA B 307



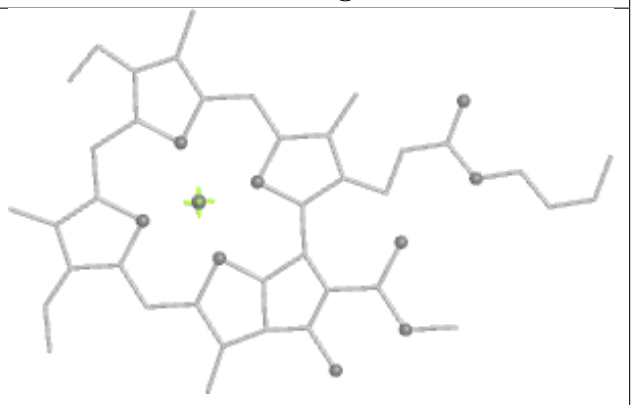
Bond lengths



Bond angles

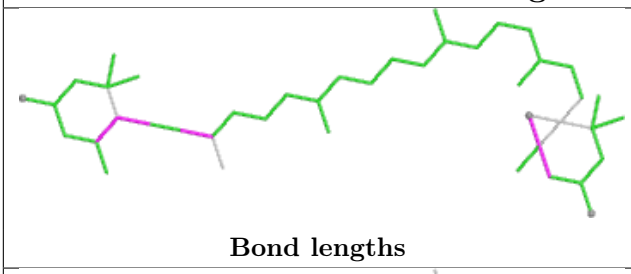


Torsions

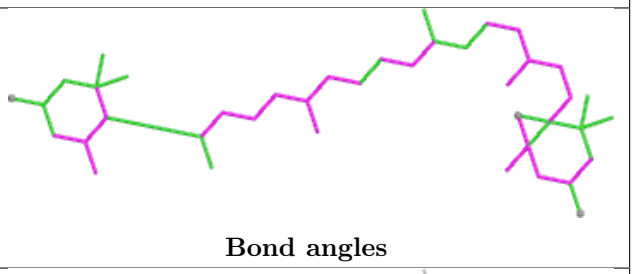


Rings

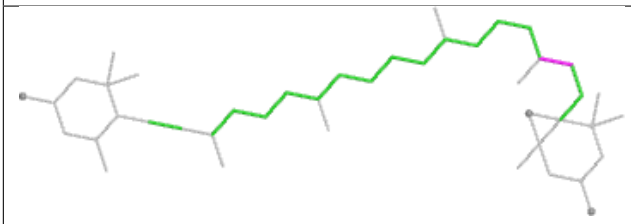
Ligand DD6 J 304



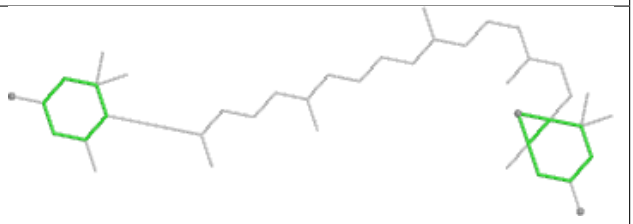
Bond lengths



Bond angles

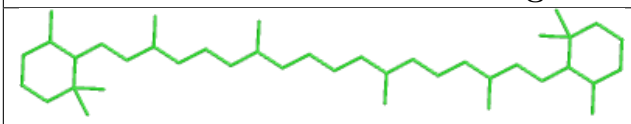


Torsions

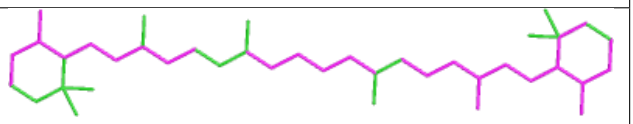


Rings

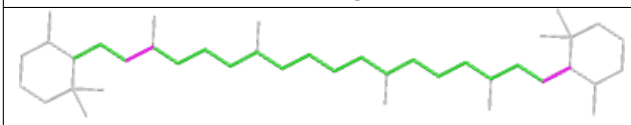
Ligand BCR a 734



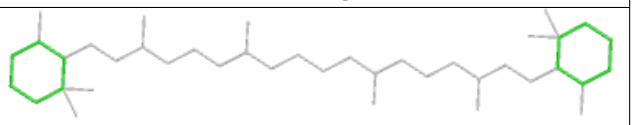
Bond lengths



Bond angles

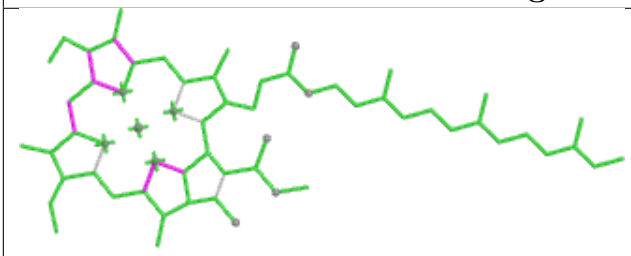


Torsions

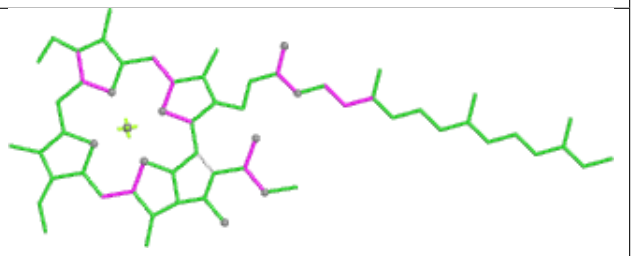


Rings

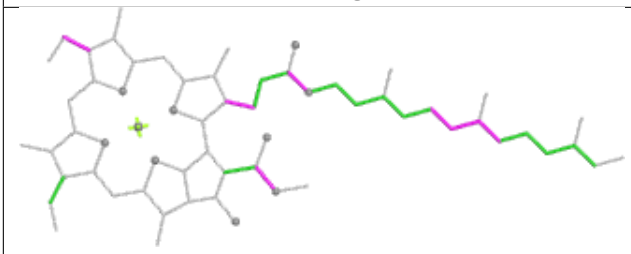
Ligand CLA a 725



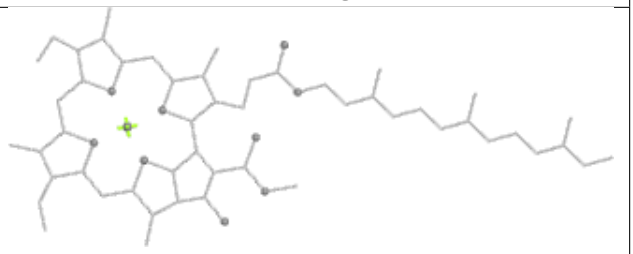
Bond lengths



Bond angles

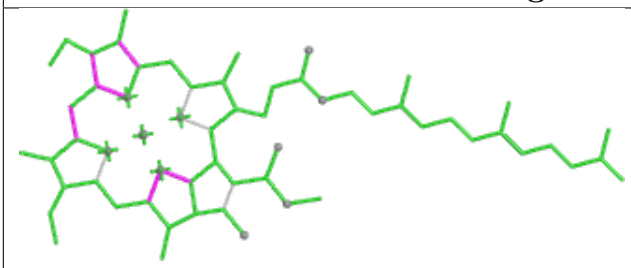


Torsions

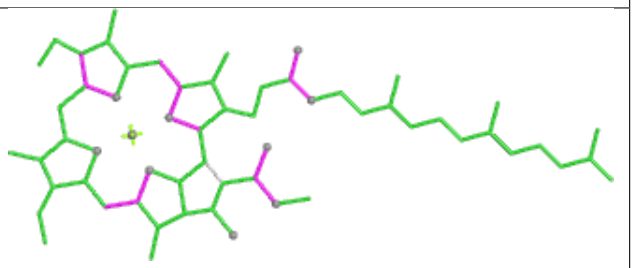


Rings

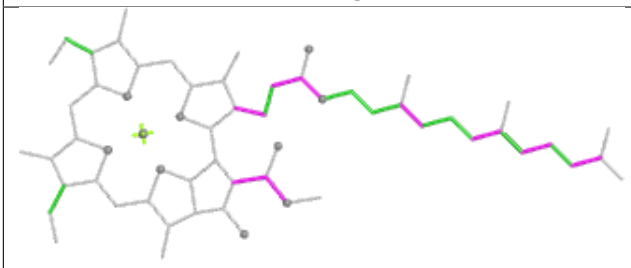
Ligand CLA b 715



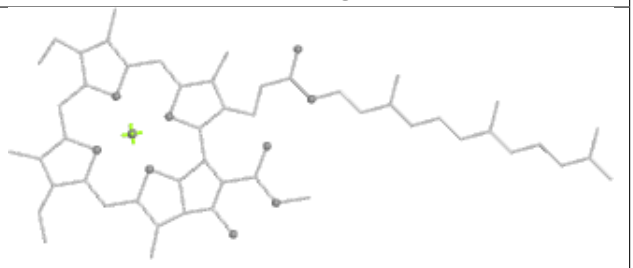
Bond lengths



Bond angles

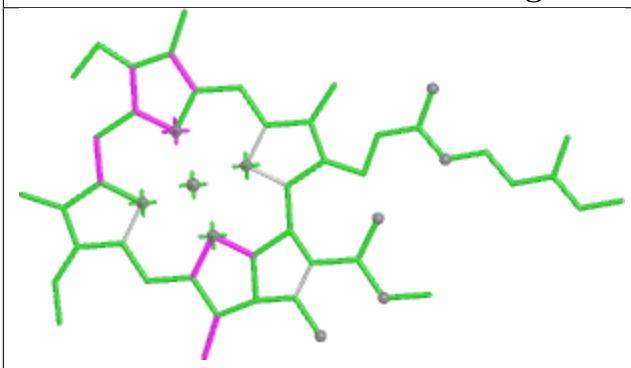


Torsions

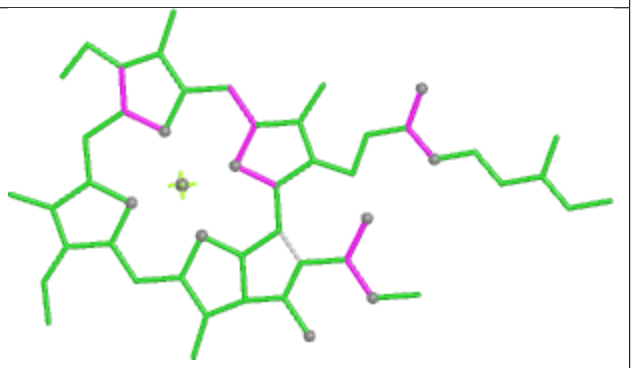


Rings

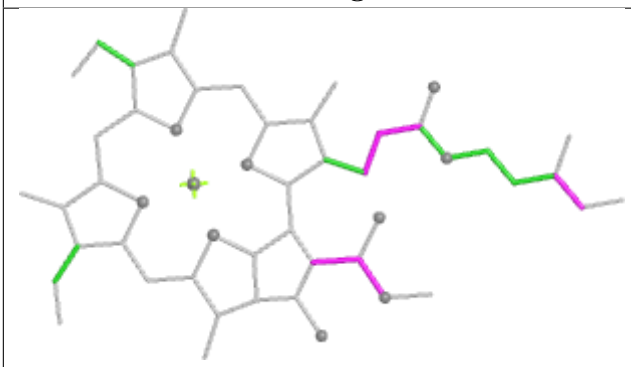
Ligand CLA P 212



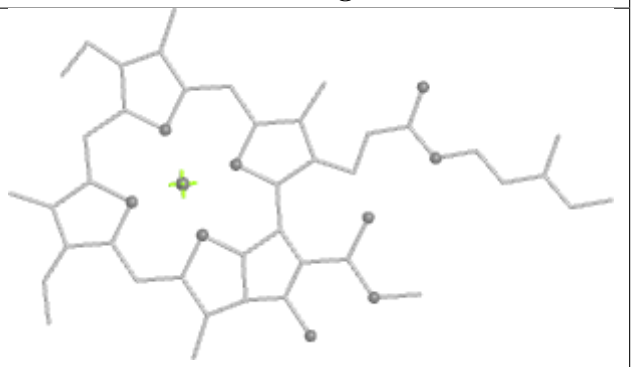
Bond lengths



Bond angles

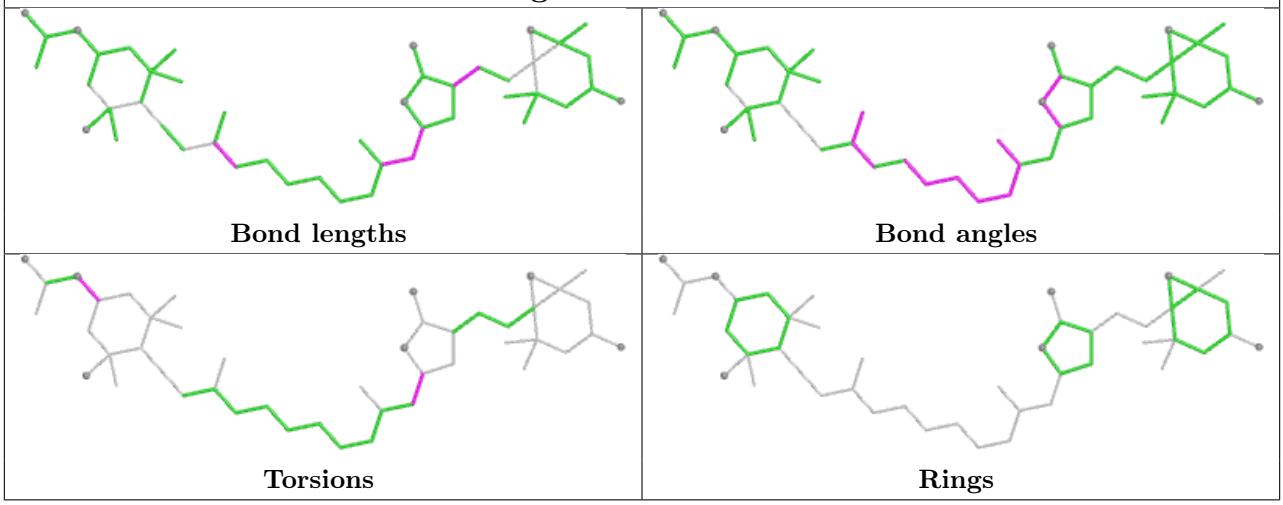


Torsions

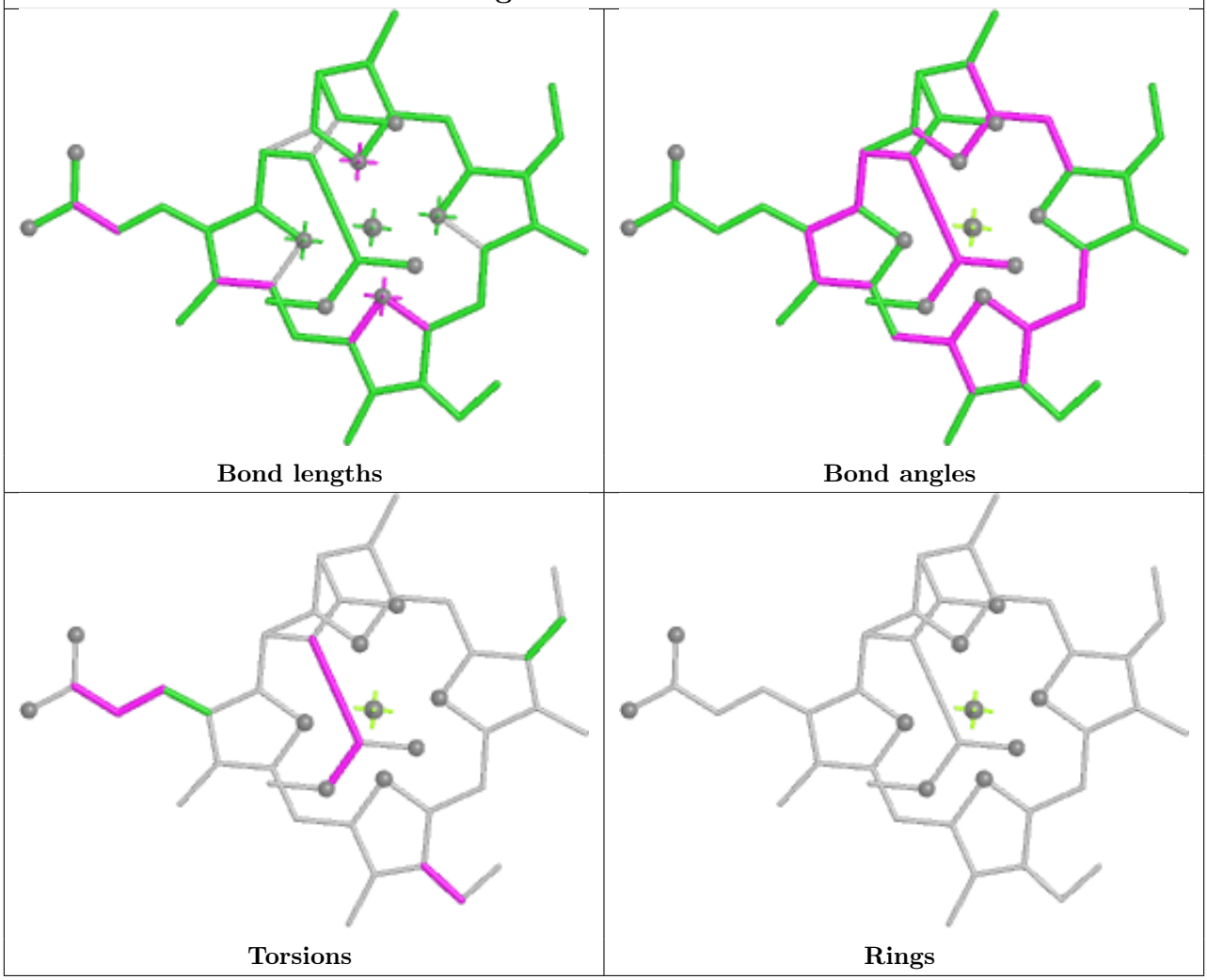


Rings

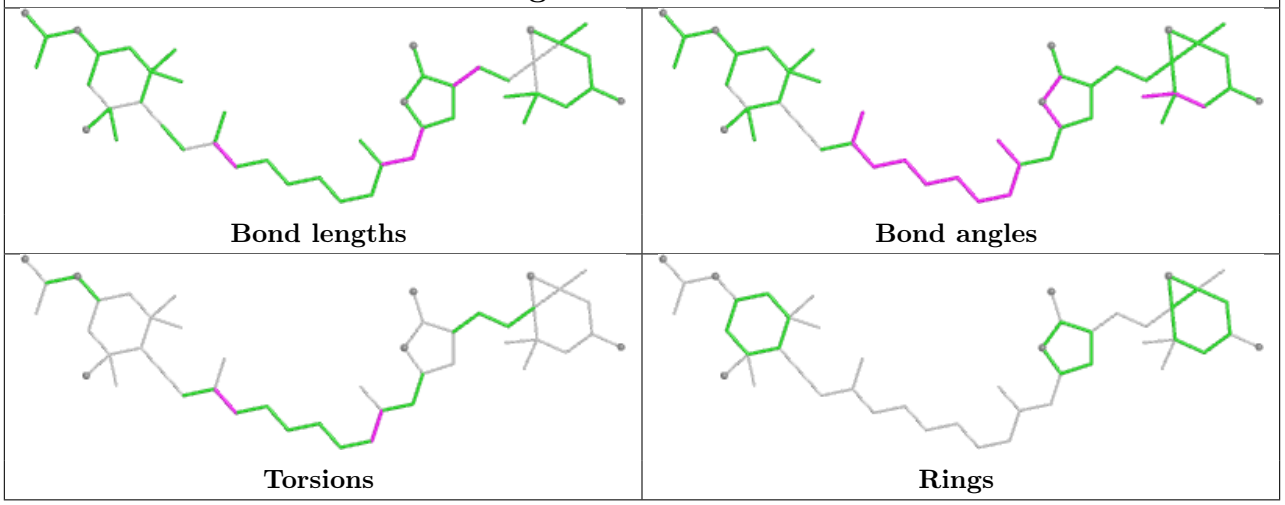
Ligand PID P 205



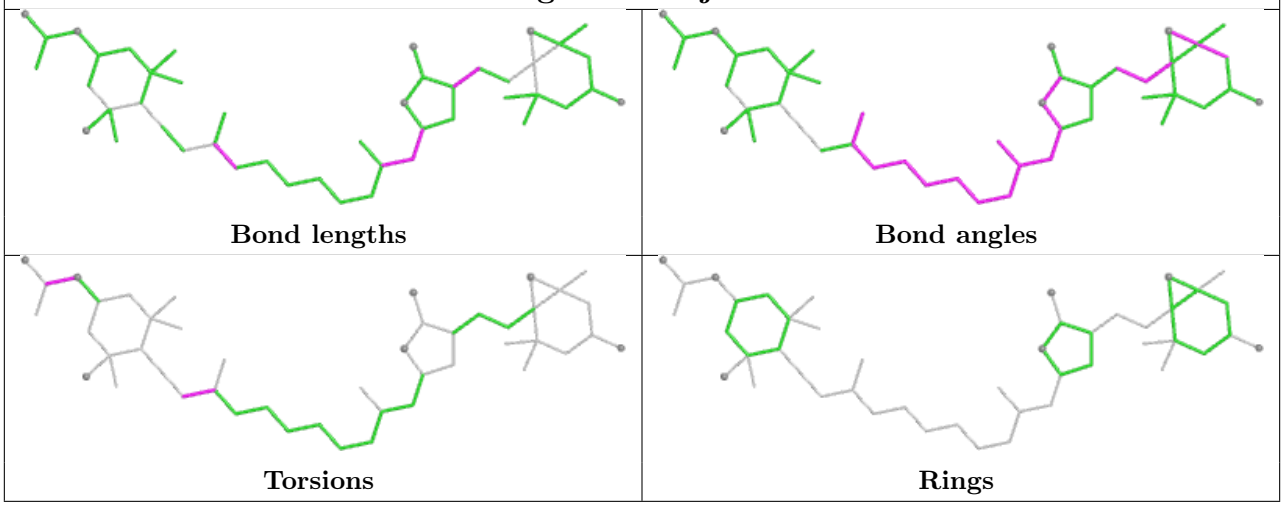
Ligand KC1 O 312



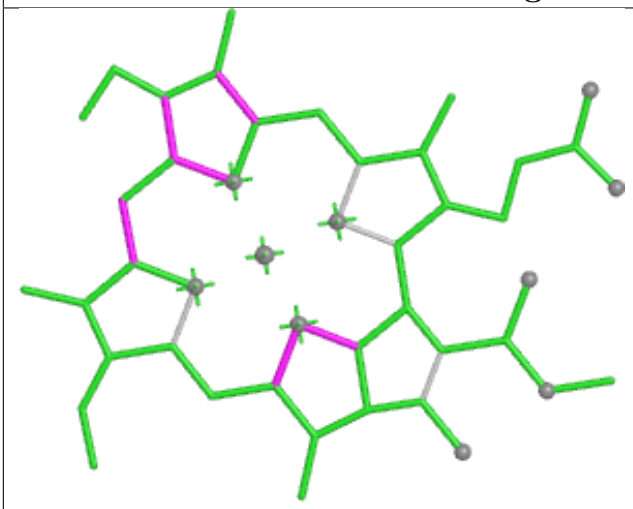
Ligand PID D 304



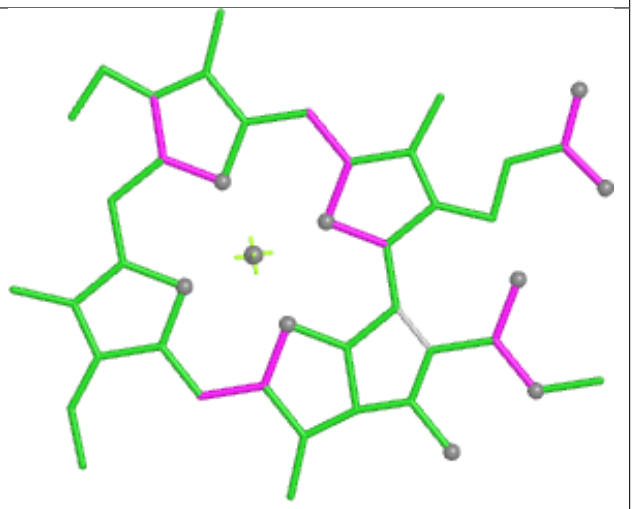
Ligand PID j 105



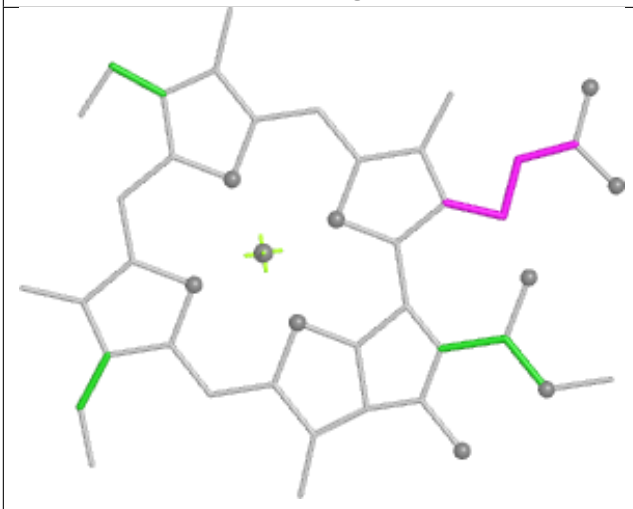
Ligand CLA B 308



Bond lengths



Bond angles

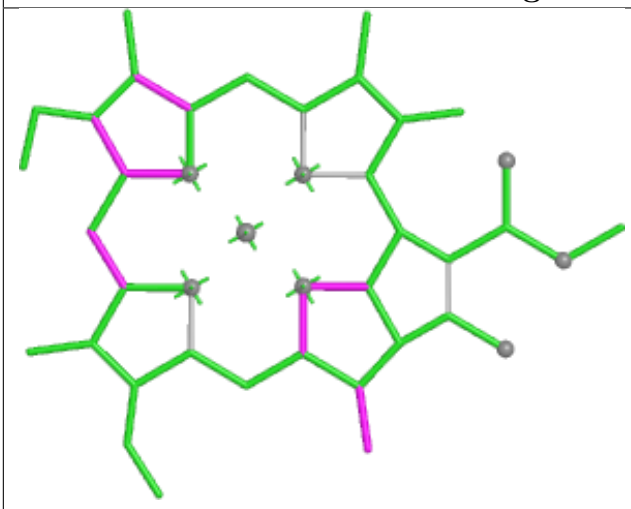


Torsions

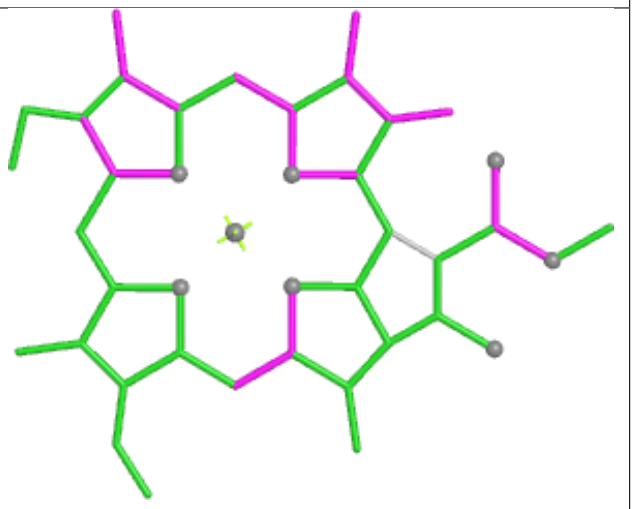


Rings

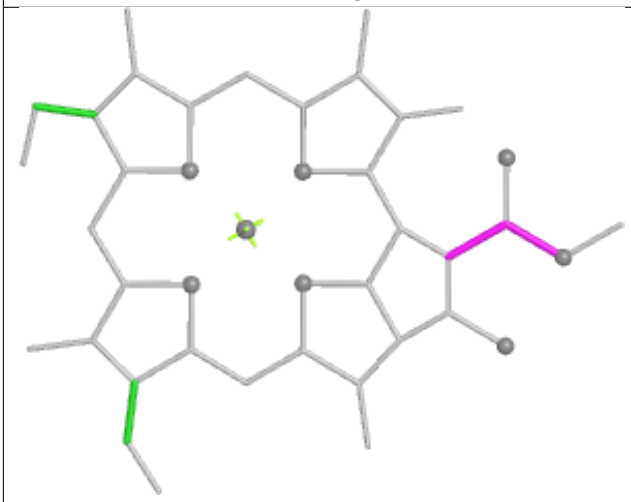
Ligand CLA K 315



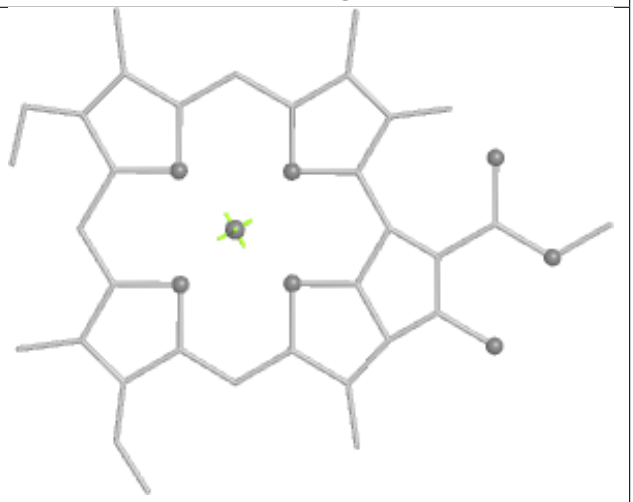
Bond lengths



Bond angles

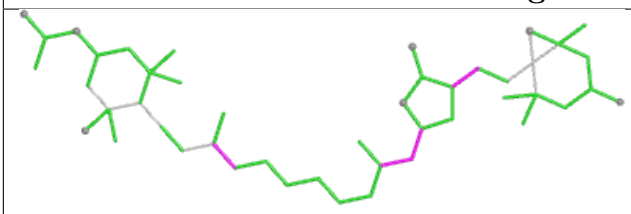


Torsions

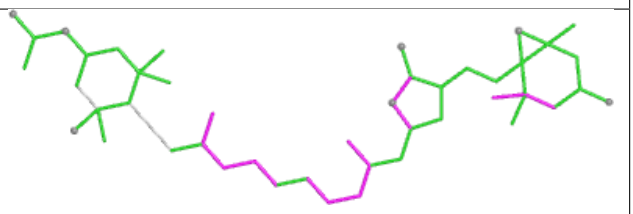


Rings

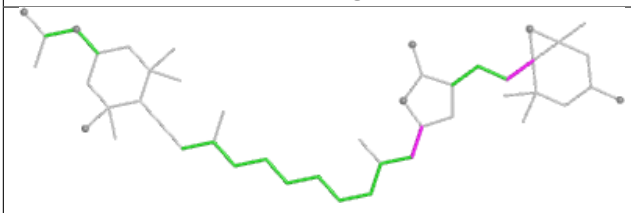
Ligand PID D 301



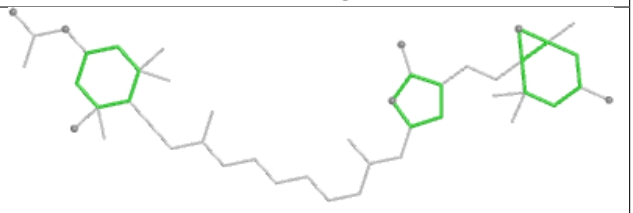
Bond lengths



Bond angles

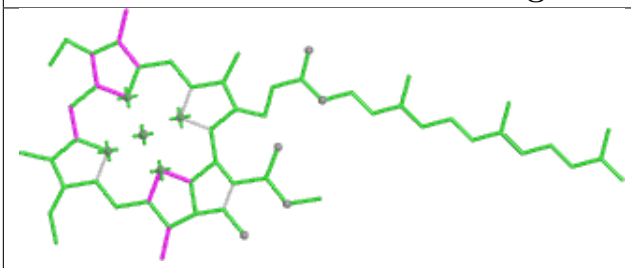


Torsions

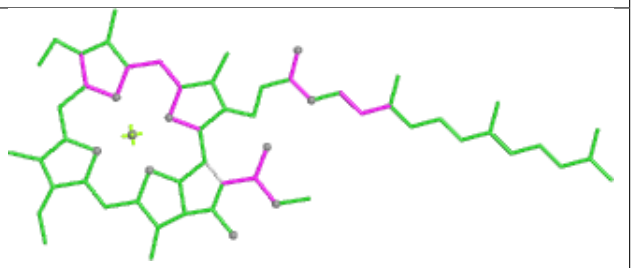


Rings

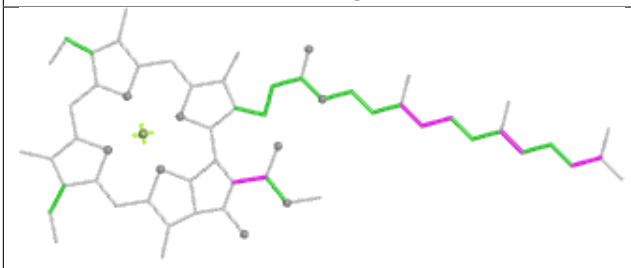
Ligand CLA b 709



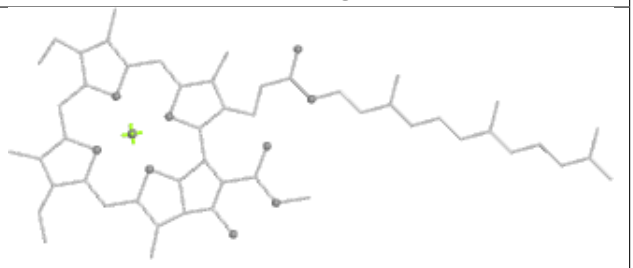
Bond lengths



Bond angles

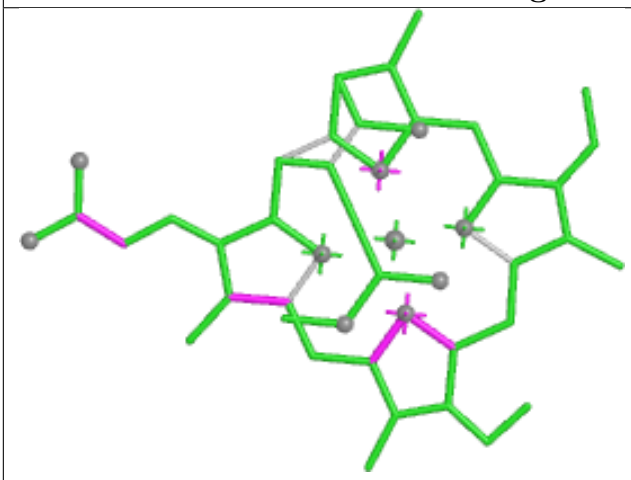


Torsions

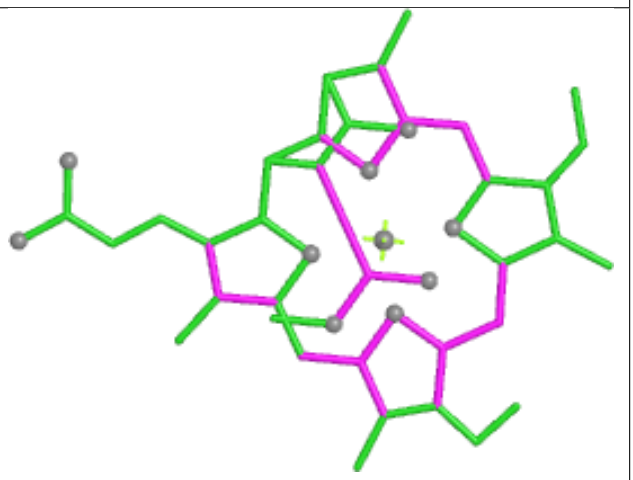


Rings

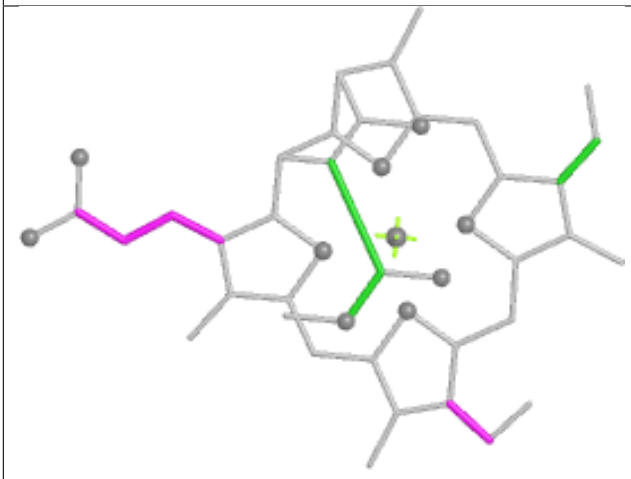
Ligand KC1 J 313



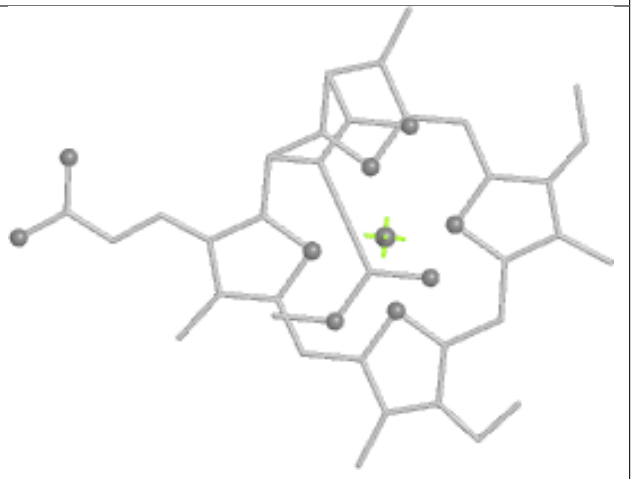
Bond lengths



Bond angles

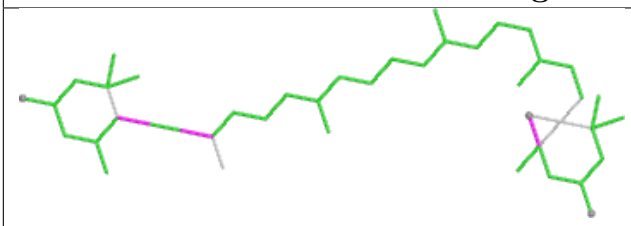


Torsions

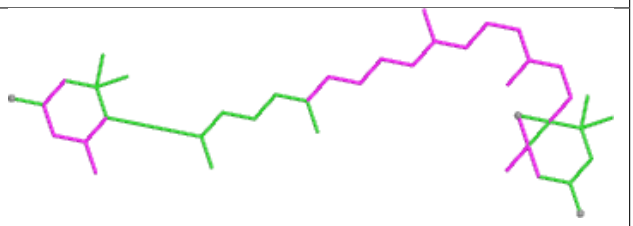


Rings

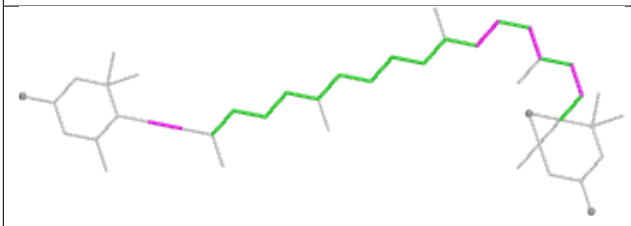
Ligand DD6 I 302



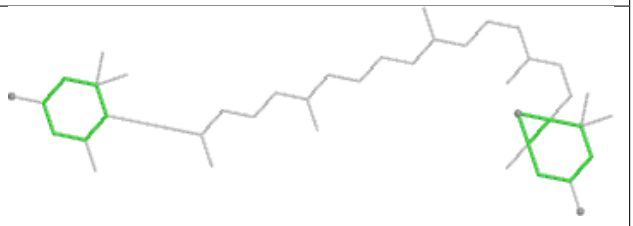
Bond lengths



Bond angles

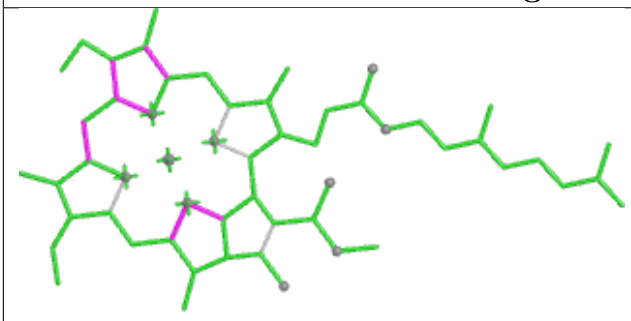


Torsions

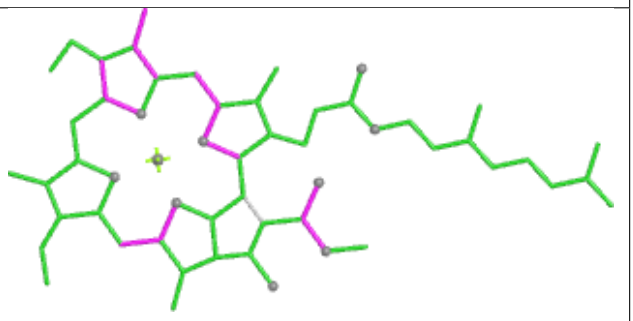


Rings

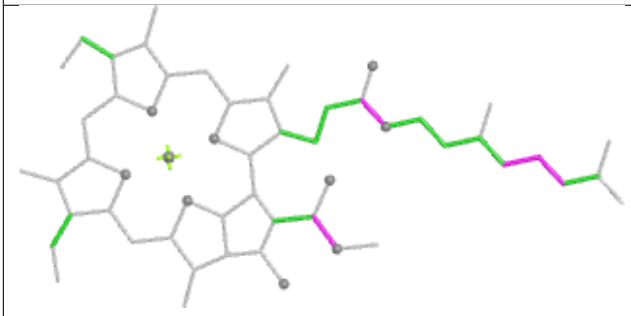
Ligand CLA A 312



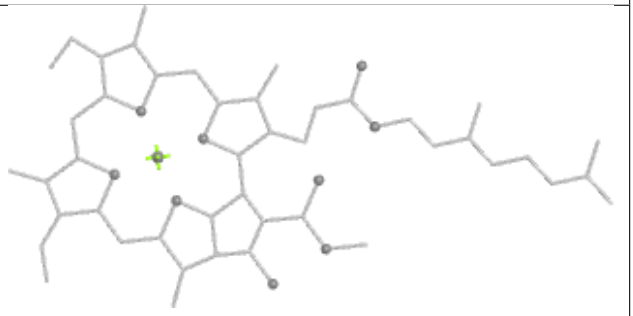
Bond lengths



Bond angles

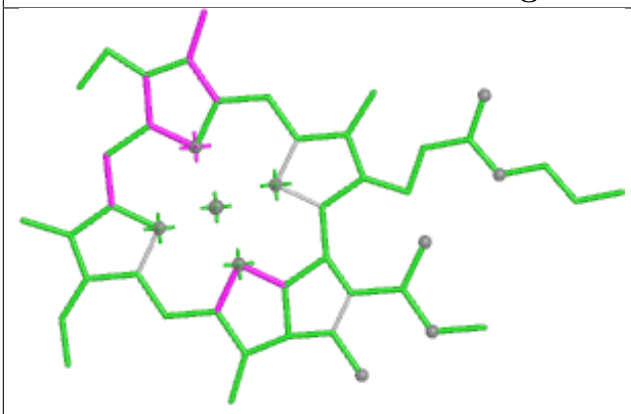


Torsions

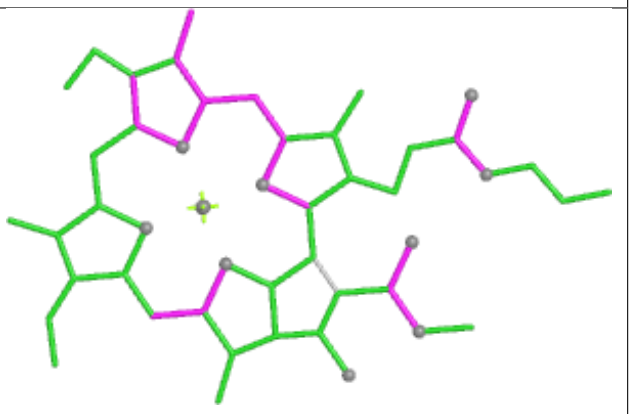


Rings

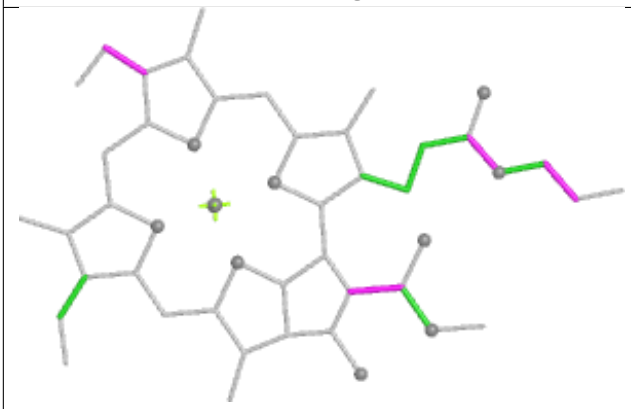
Ligand CLA M 312



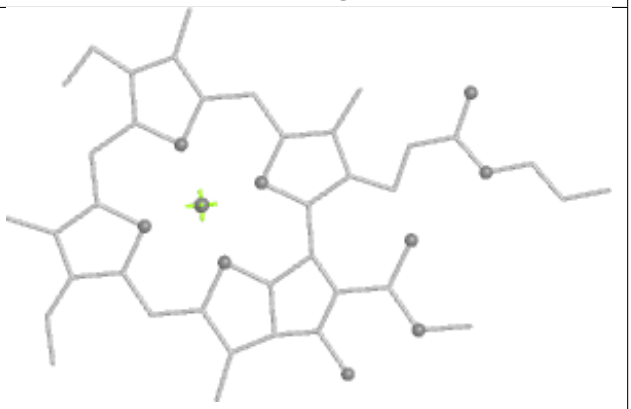
Bond lengths



Bond angles

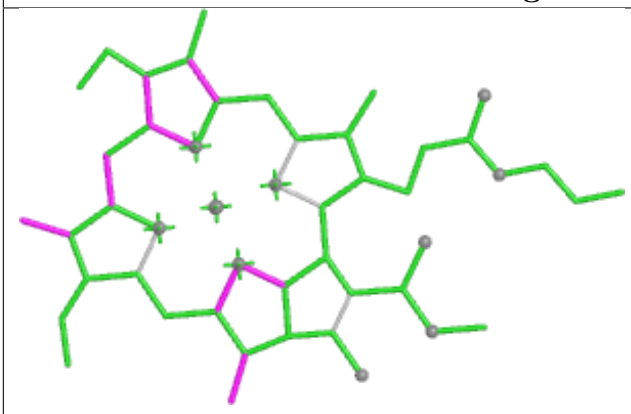


Torsions

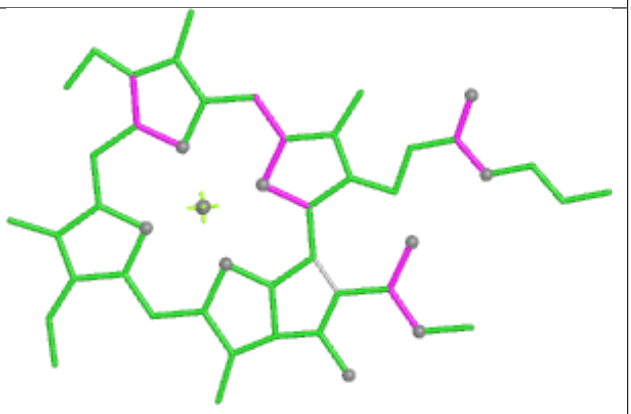


Rings

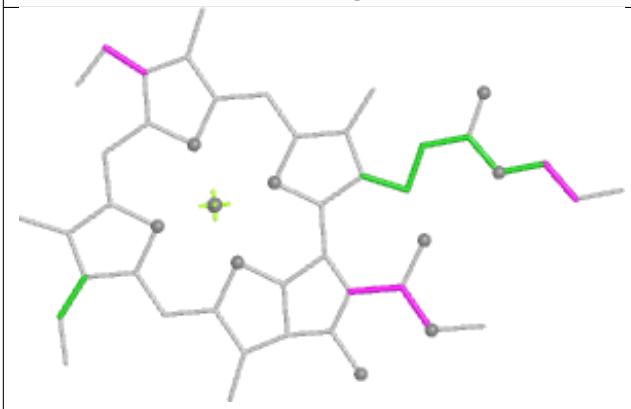
Ligand CLA K 312



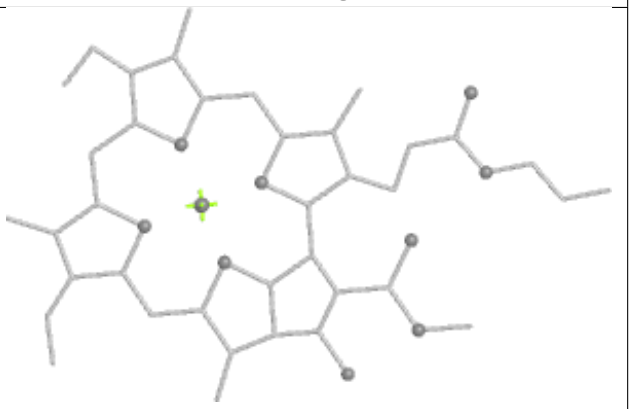
Bond lengths



Bond angles

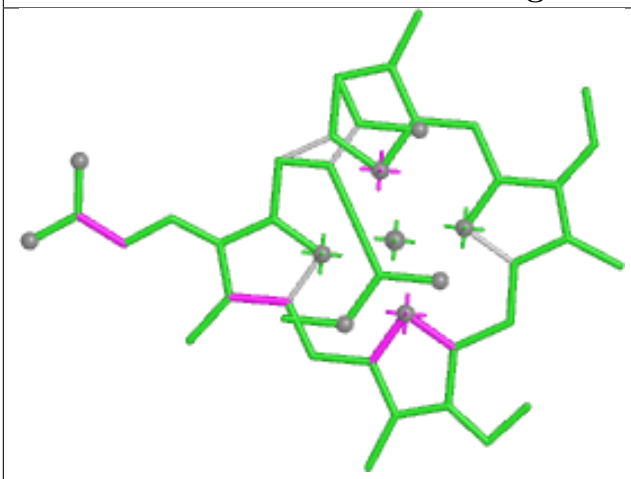


Torsions

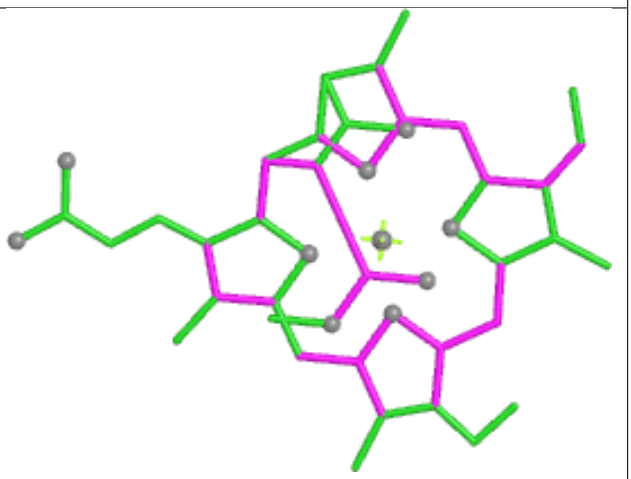


Rings

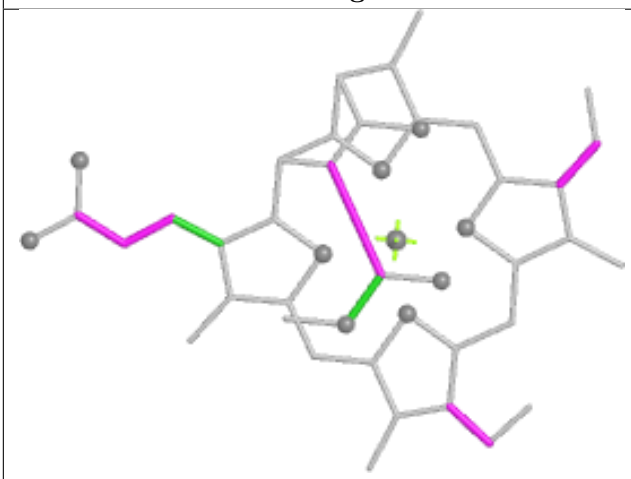
Ligand KC1 P 213



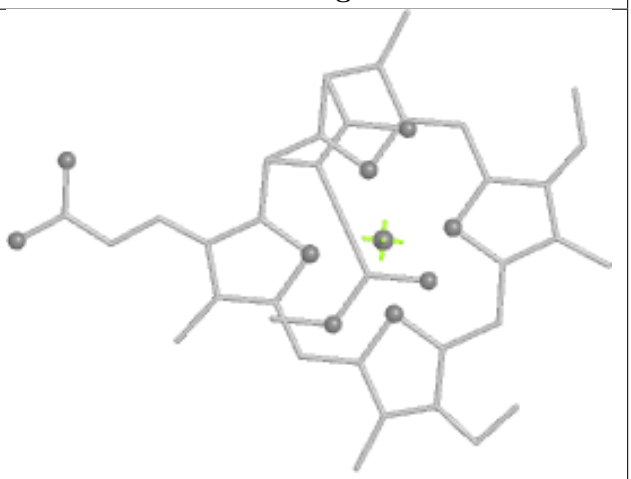
Bond lengths



Bond angles

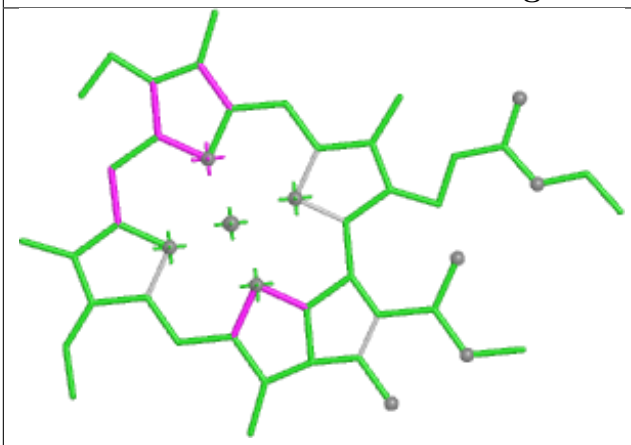


Torsions

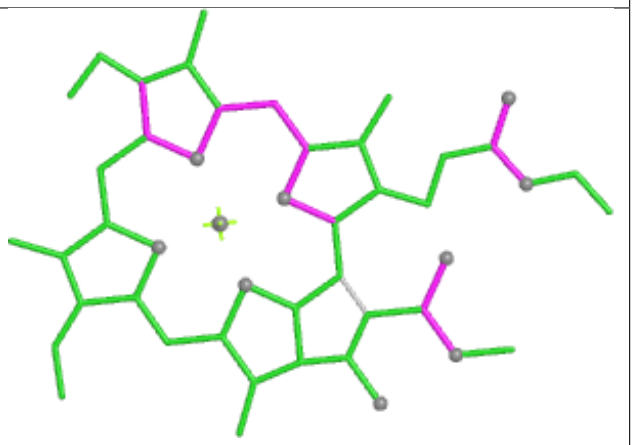


Rings

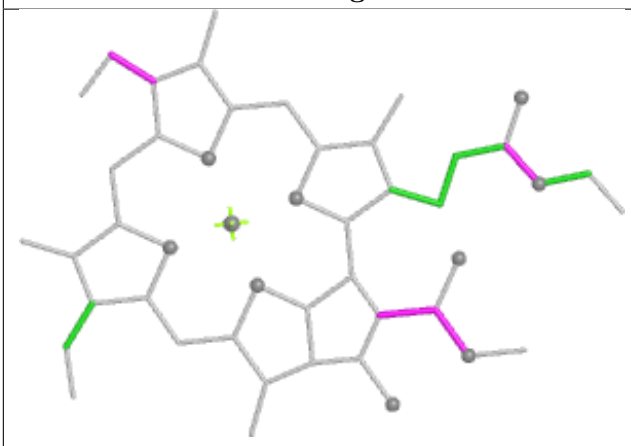
Ligand CLA H 304



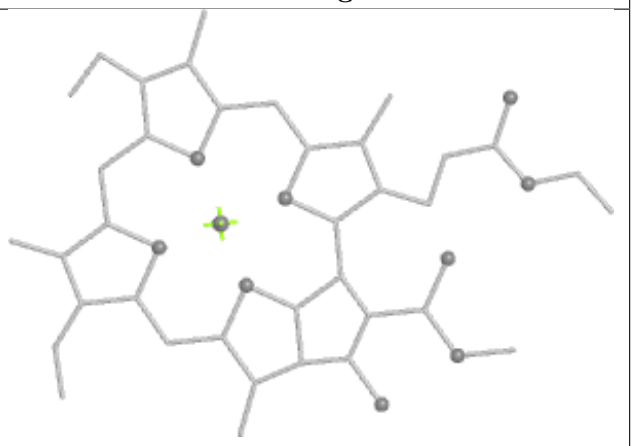
Bond lengths



Bond angles

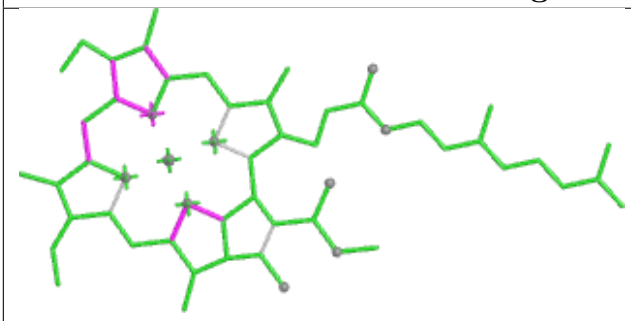


Torsions

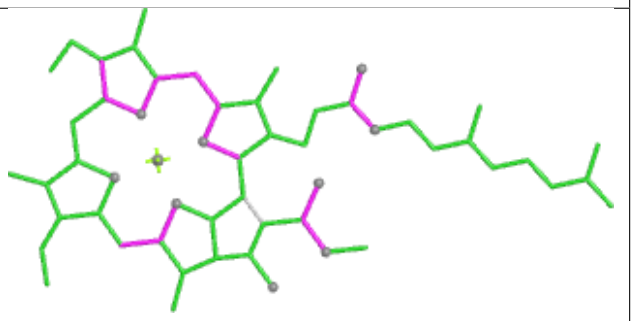


Rings

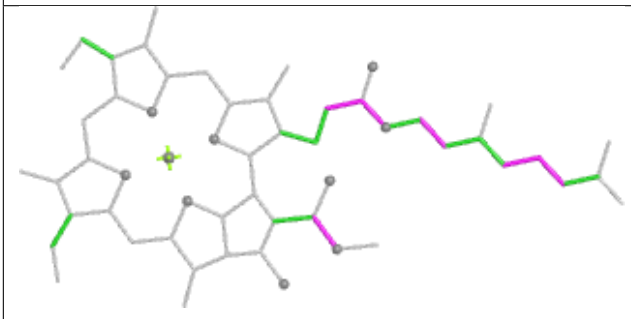
Ligand CLA I 309



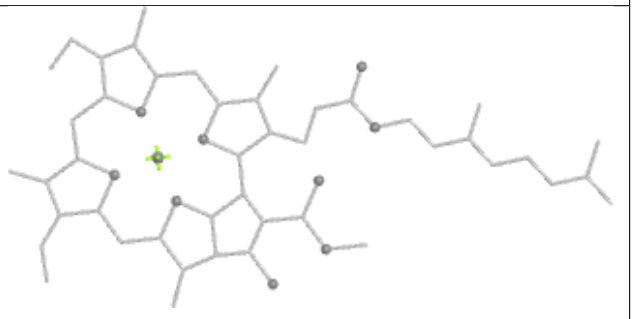
Bond lengths



Bond angles

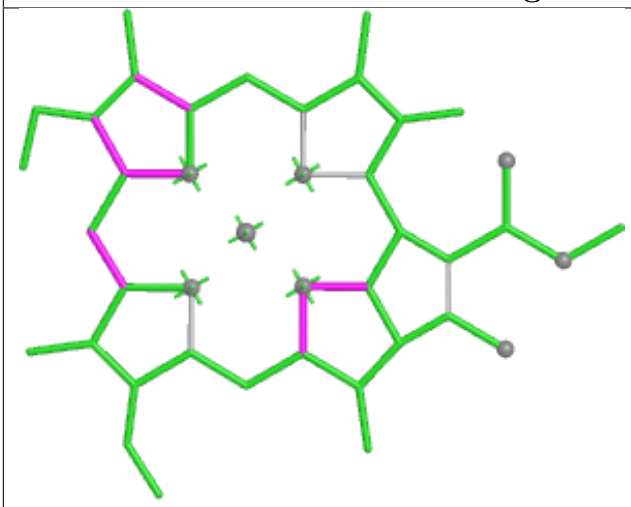


Torsions

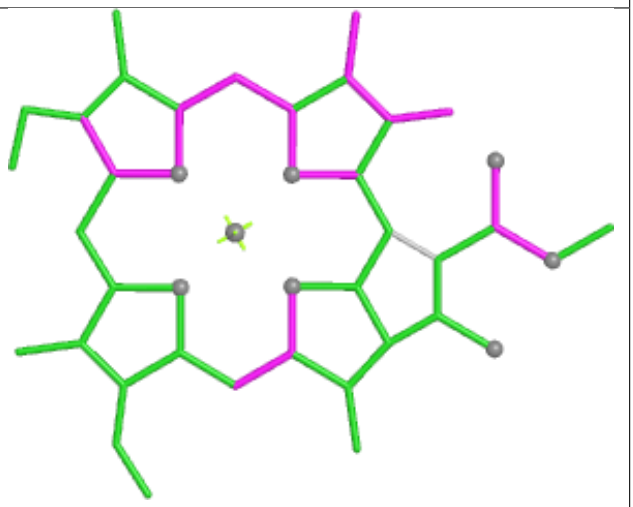


Rings

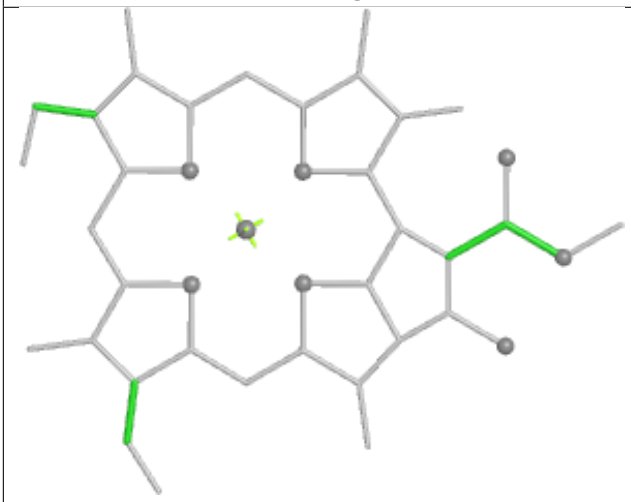
Ligand CLA A 317



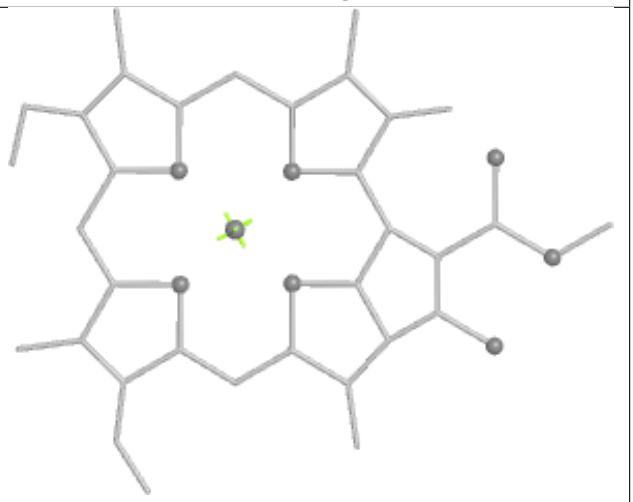
Bond lengths



Bond angles

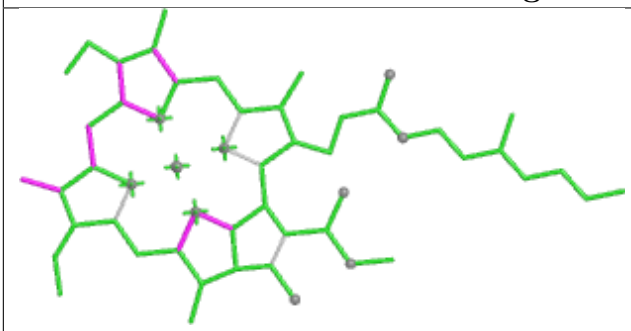


Torsions

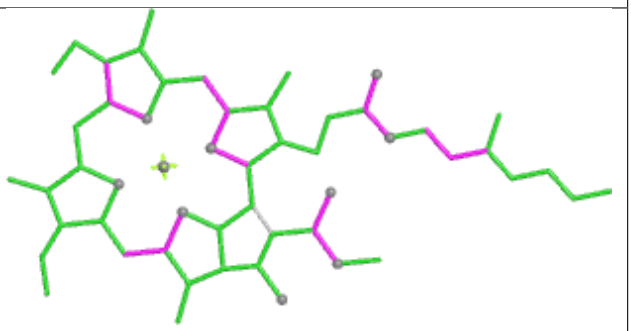


Rings

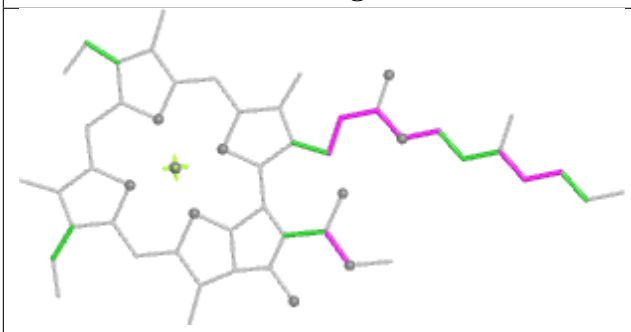
Ligand CLA G 514



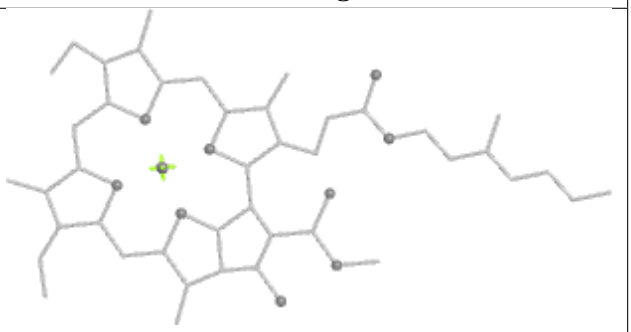
Bond lengths



Bond angles

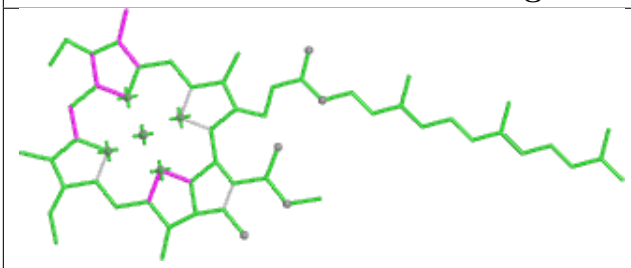


Torsions

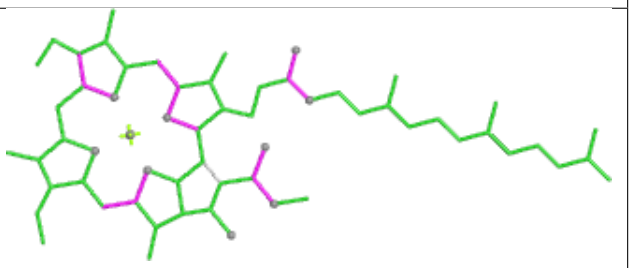


Rings

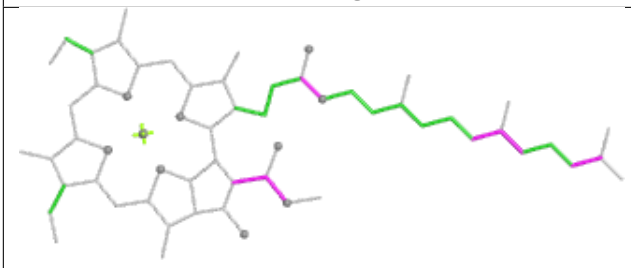
Ligand CLA B 301



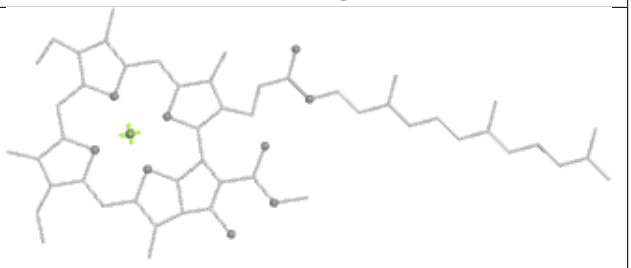
Bond lengths



Bond angles

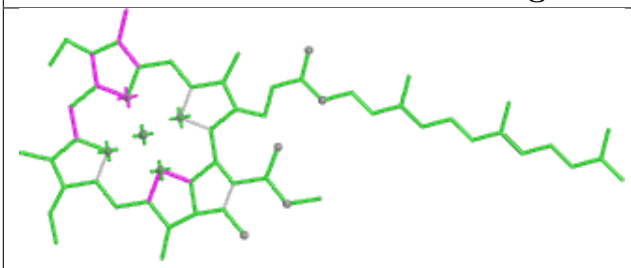


Torsions

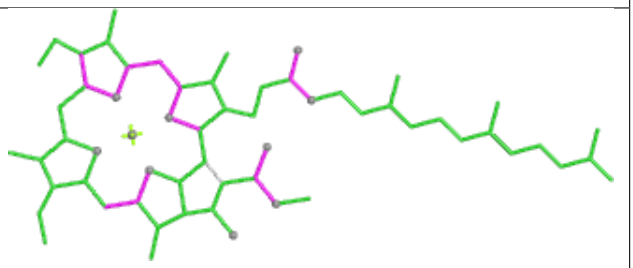


Rings

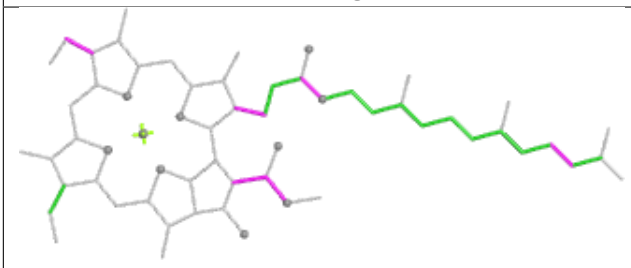
Ligand CLA a 712



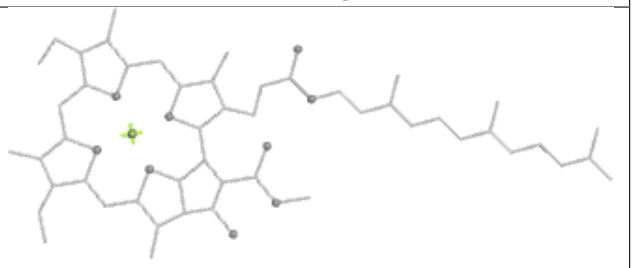
Bond lengths



Bond angles

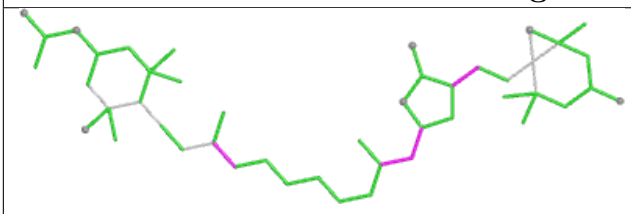


Torsions

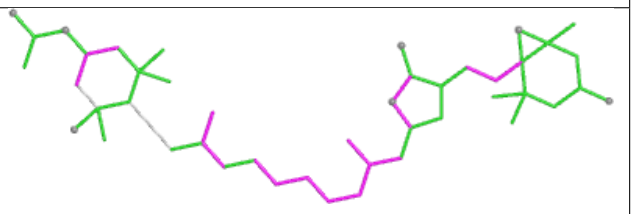


Rings

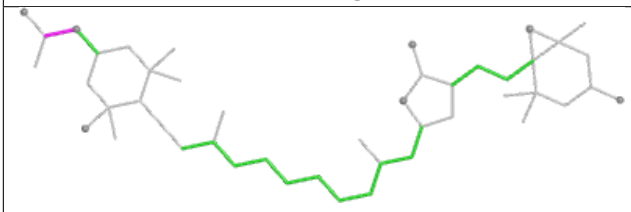
Ligand PID P 206



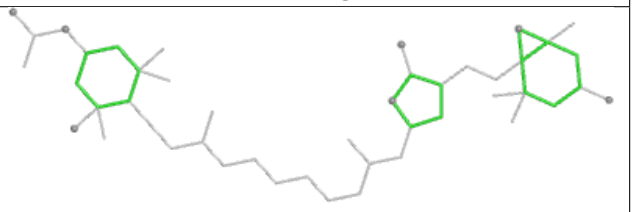
Bond lengths



Bond angles

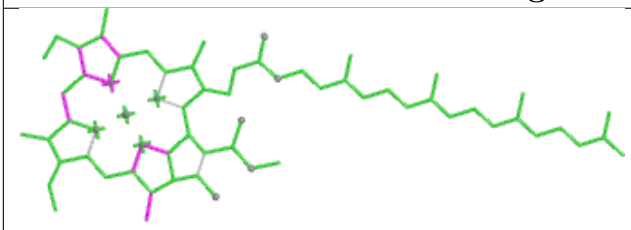


Torsions

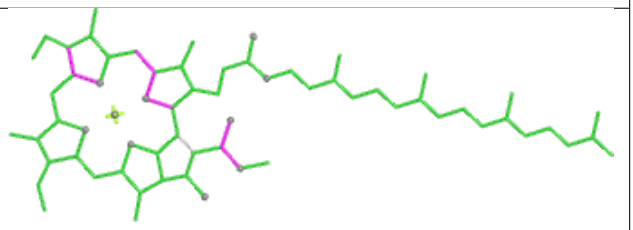


Rings

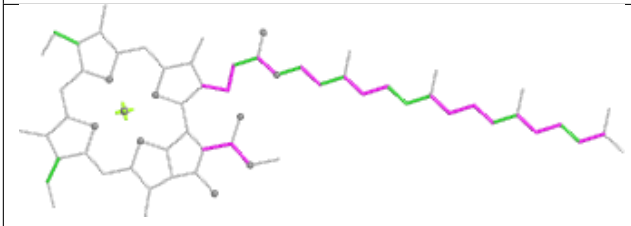
Ligand CLA J 307



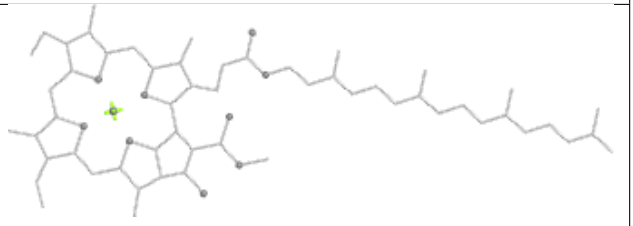
Bond lengths



Bond angles

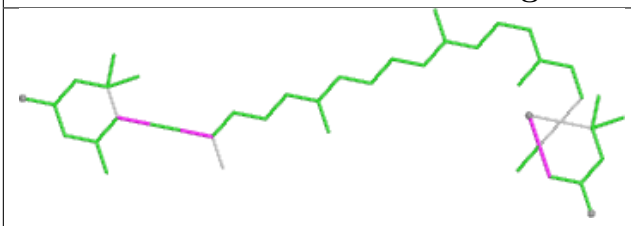


Torsions

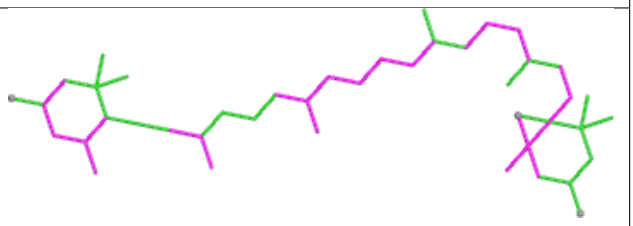


Rings

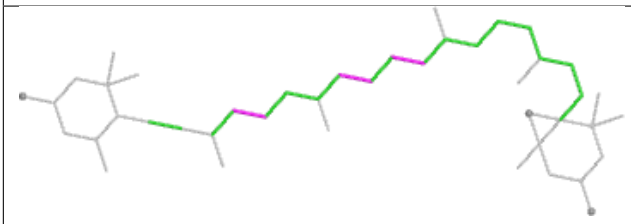
Ligand DD6 M 302



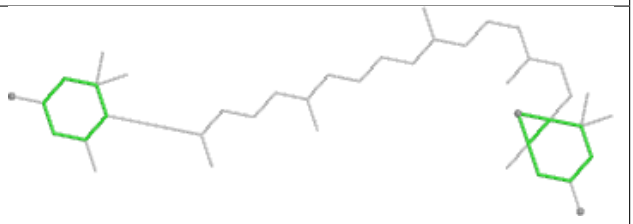
Bond lengths



Bond angles

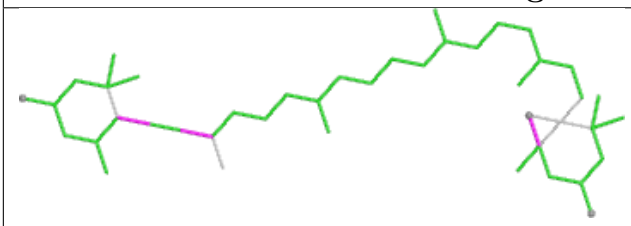


Torsions

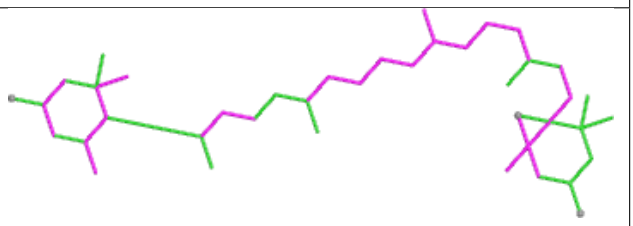


Rings

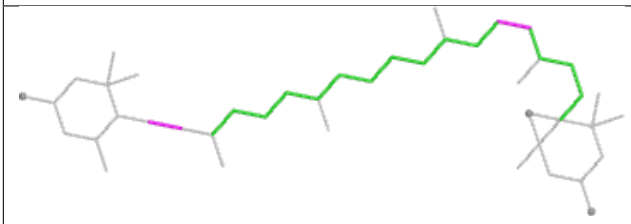
Ligand DD6 F 303



Bond lengths



Bond angles

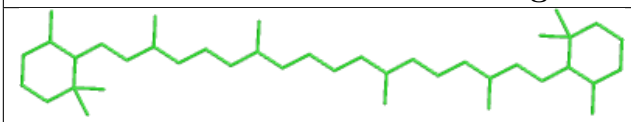


Torsions

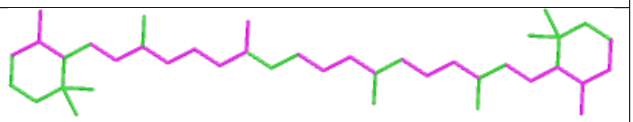


Rings

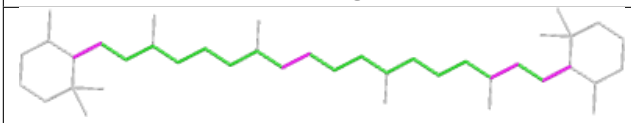
Ligand BCR l 306



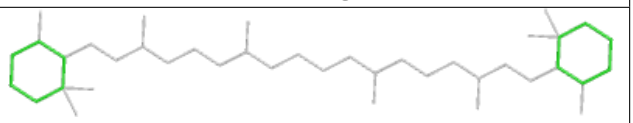
Bond lengths



Bond angles

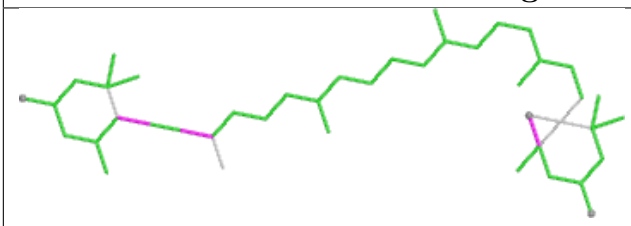


Torsions

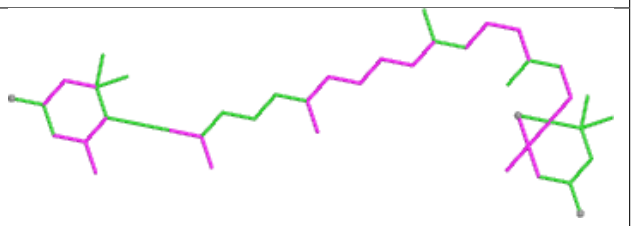


Rings

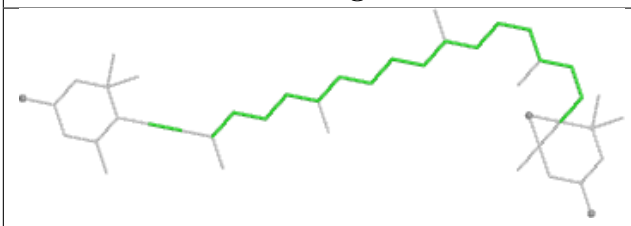
Ligand DD6 M 304



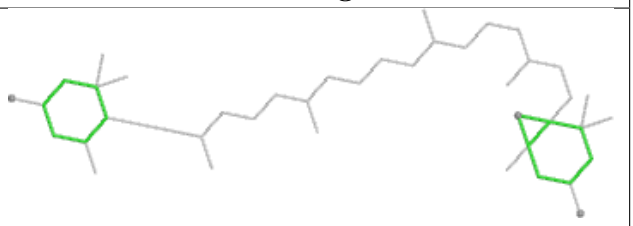
Bond lengths



Bond angles

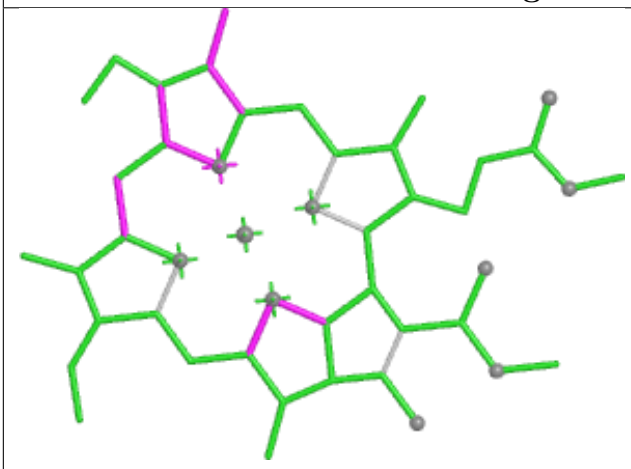


Torsions

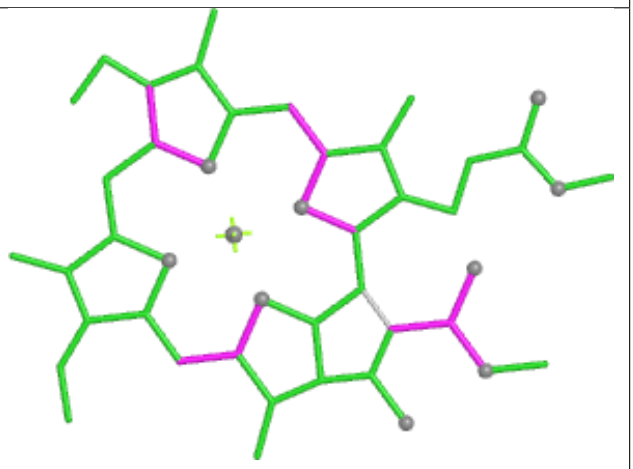


Rings

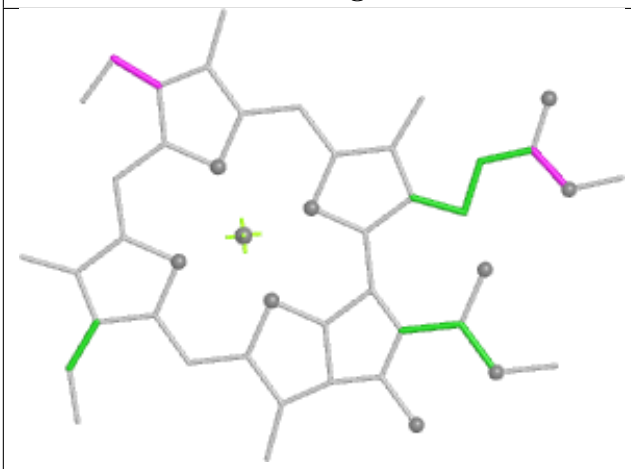
Ligand CLA K 316



Bond lengths



Bond angles

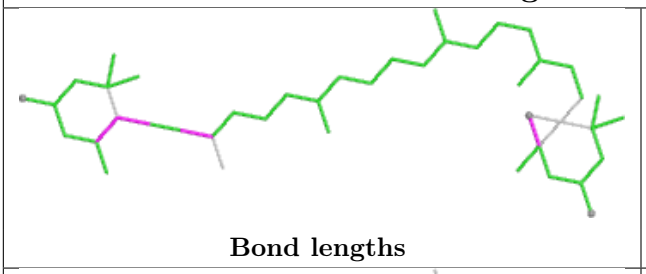


Torsions

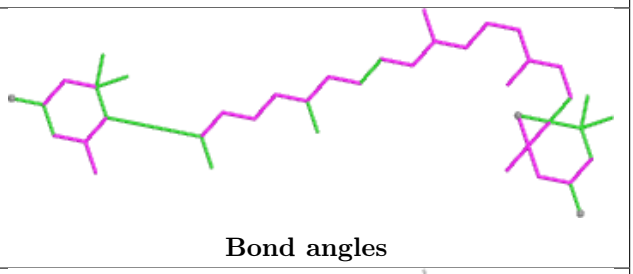


Rings

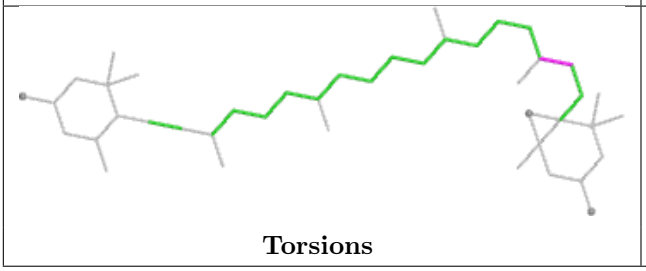
Ligand DD6 M 303



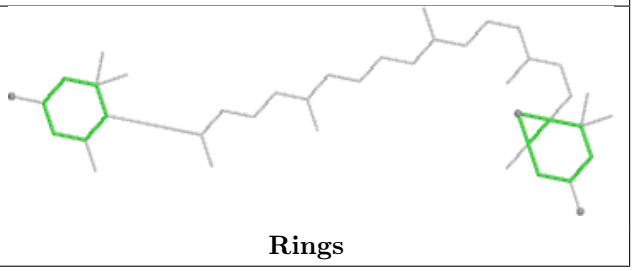
Bond lengths



Bond angles

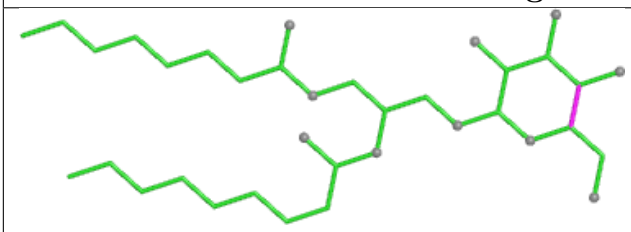


Torsions

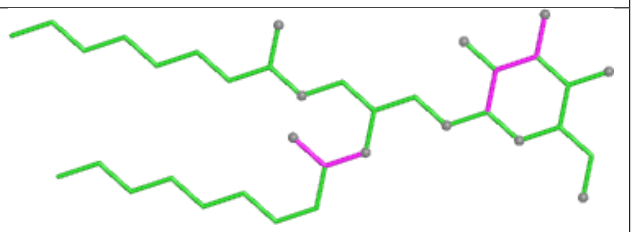


Rings

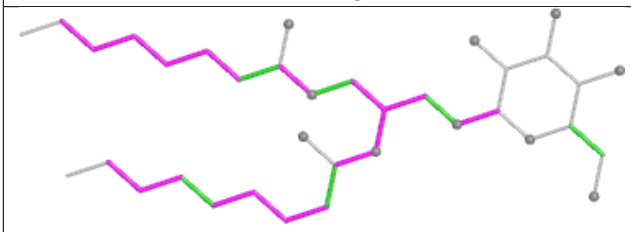
Ligand LMG I 318



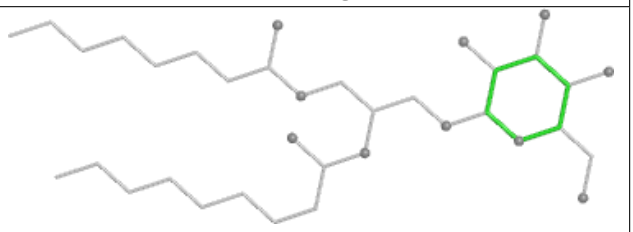
Bond lengths



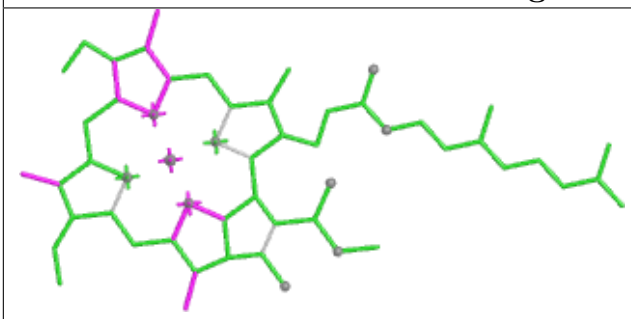
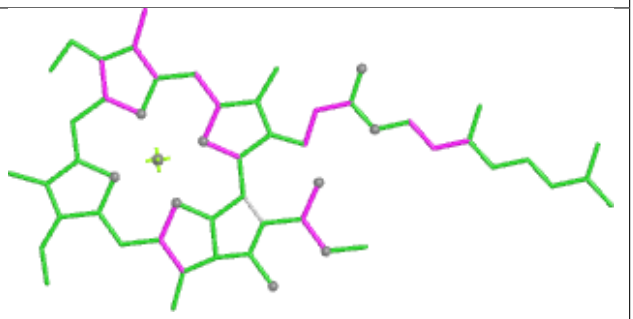
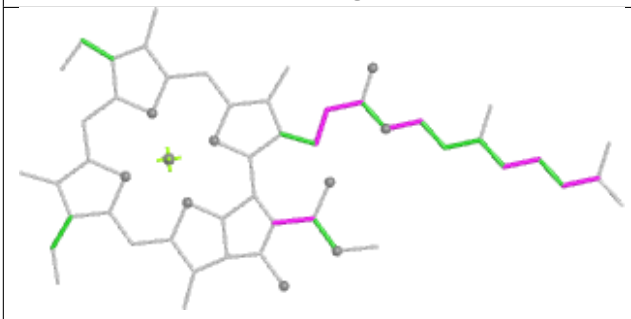
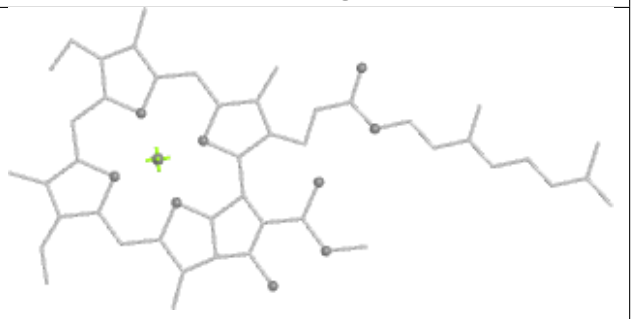
Bond angles



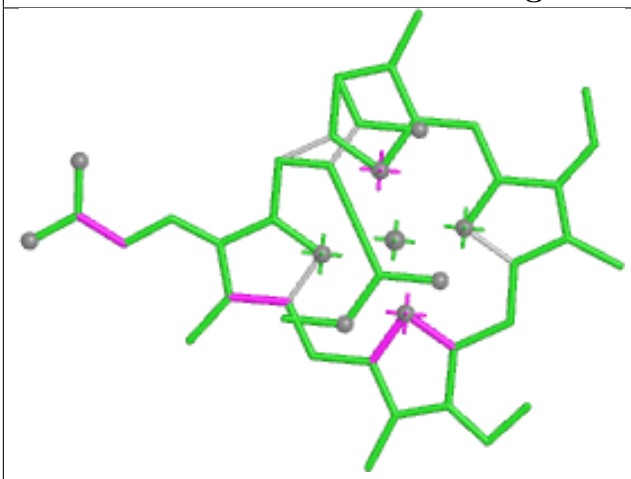
Torsions



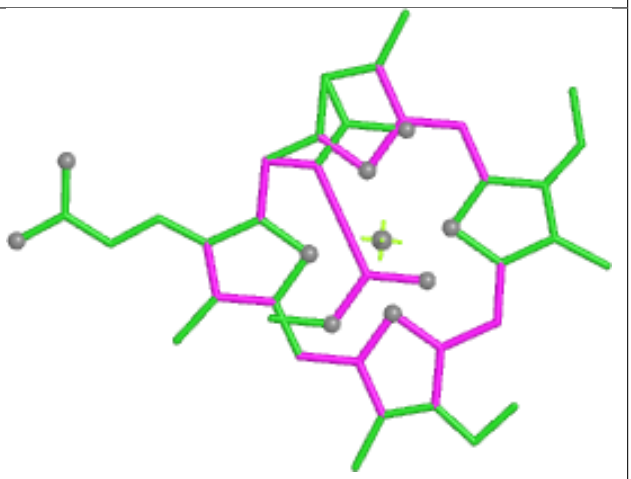
Rings

Ligand CLA a 703	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

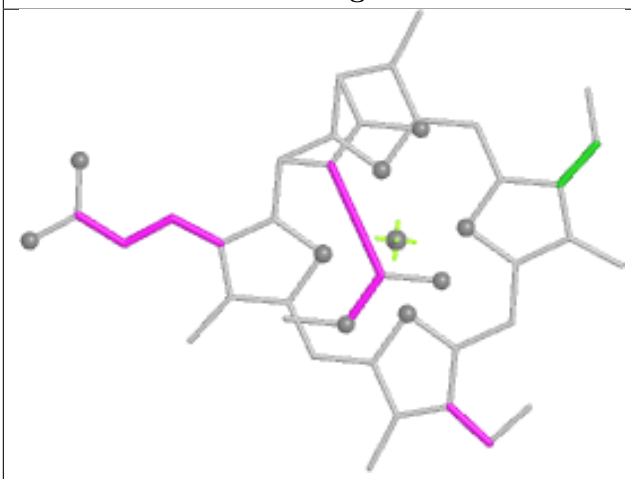
Ligand KC1 D 310



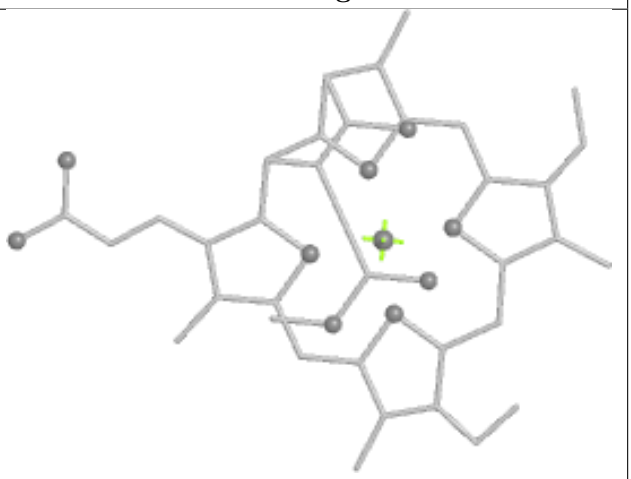
Bond lengths



Bond angles

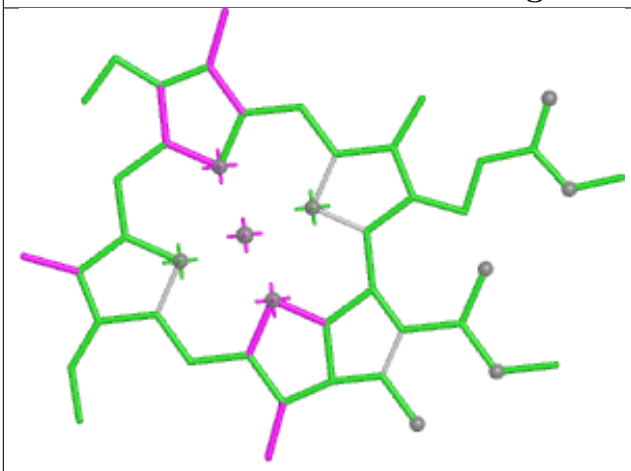


Torsions

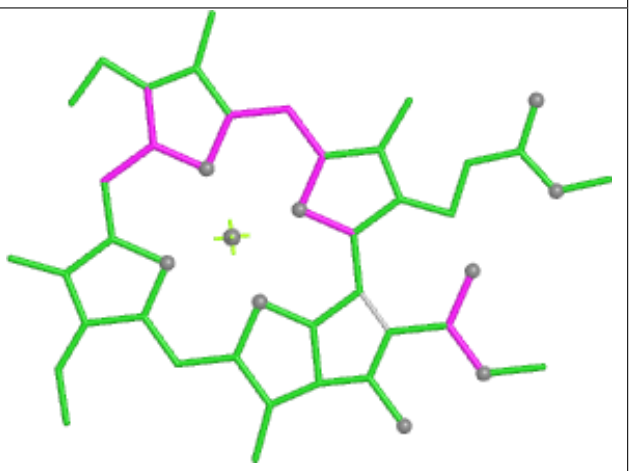


Rings

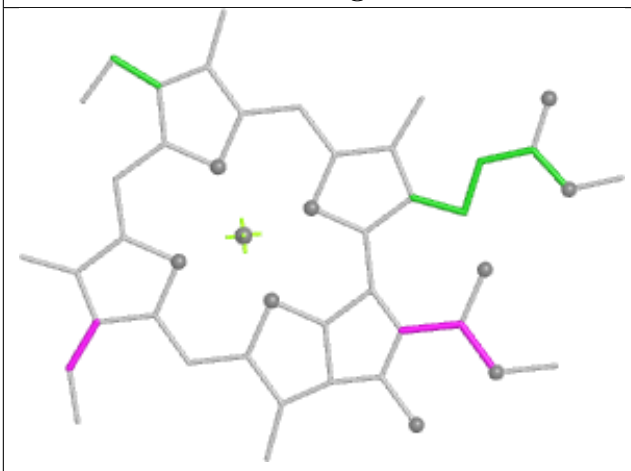
Ligand CLA F 312



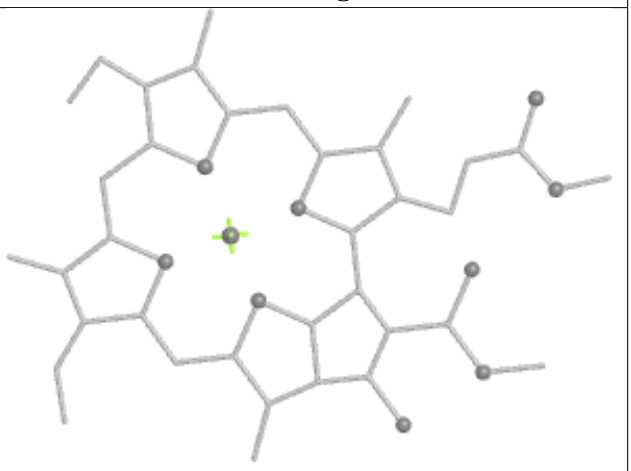
Bond lengths



Bond angles

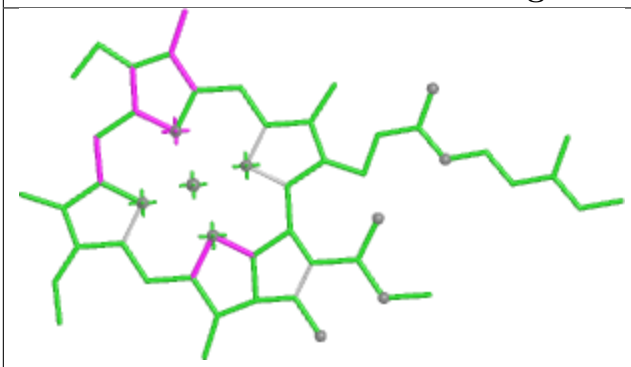


Torsions

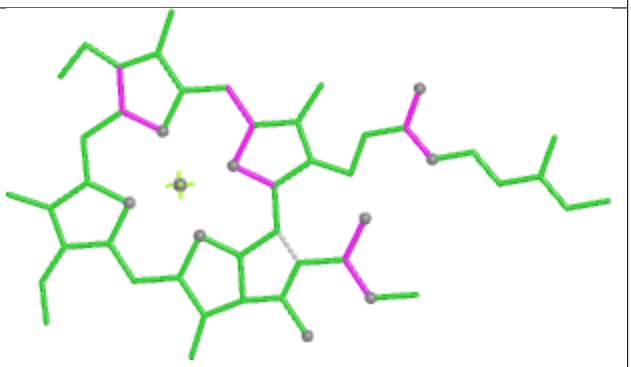


Rings

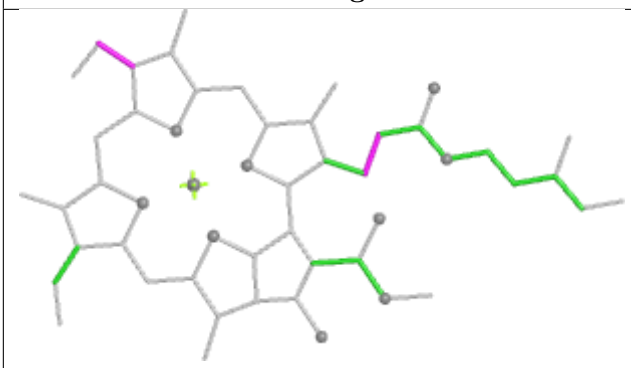
Ligand CLA b 718



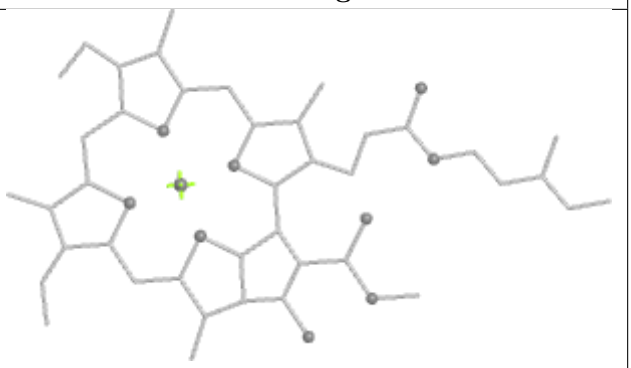
Bond lengths



Bond angles

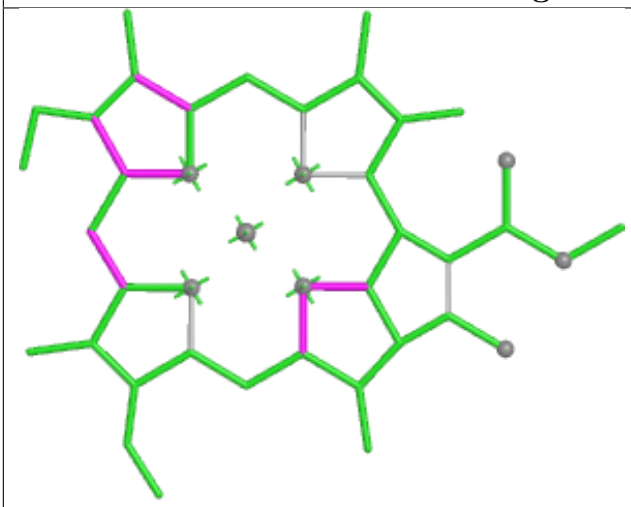


Torsions

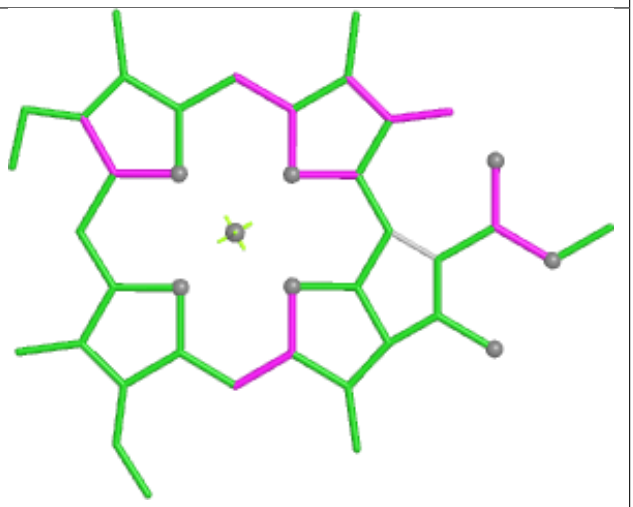


Rings

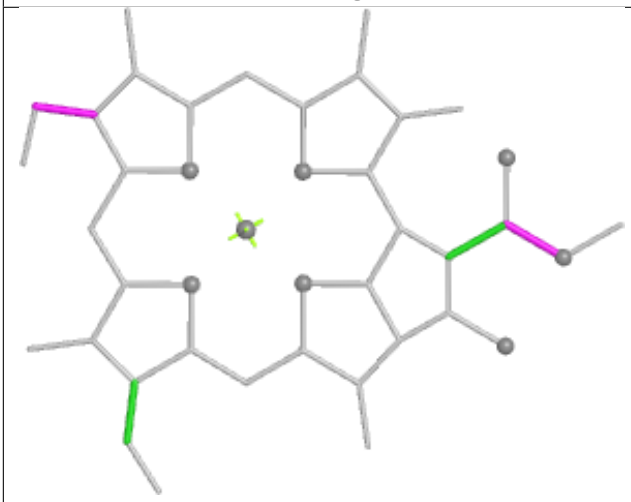
Ligand CLA l 308



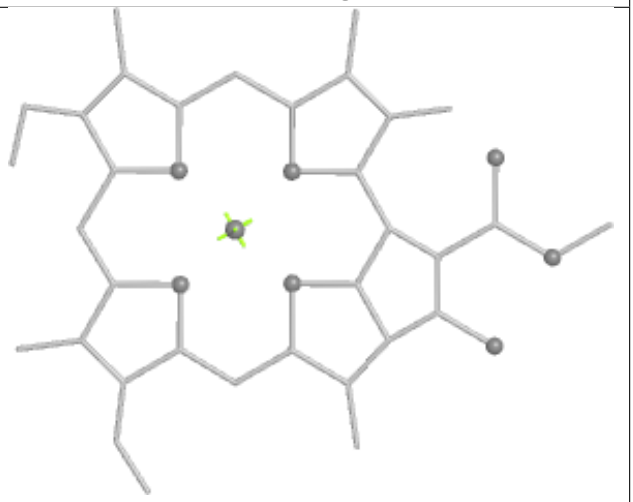
Bond lengths



Bond angles

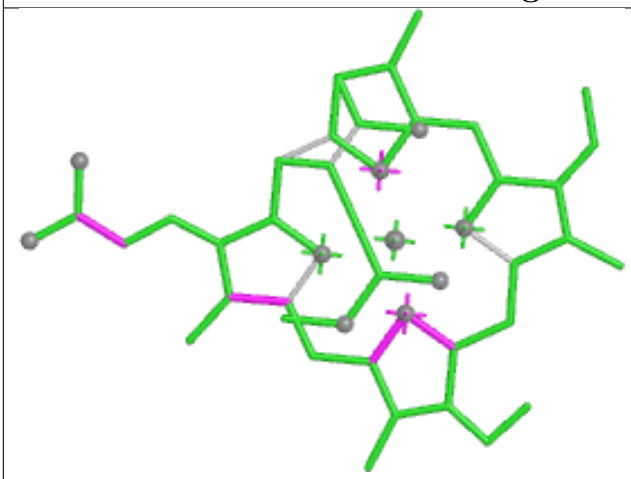


Torsions

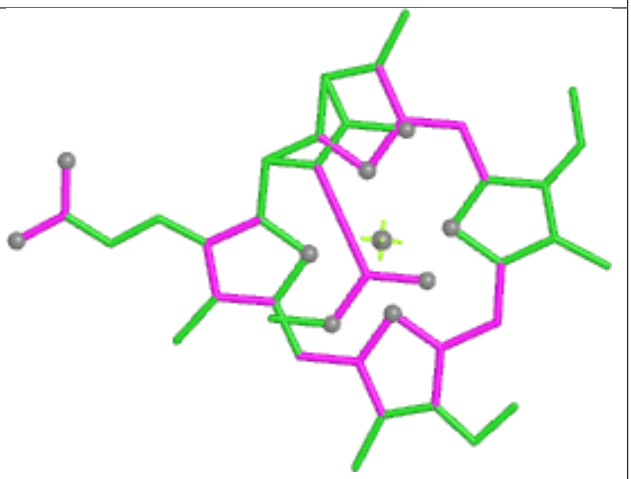


Rings

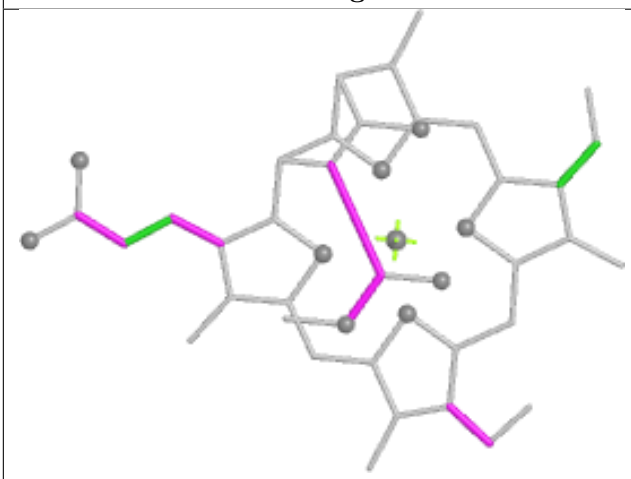
Ligand KC1 M 307



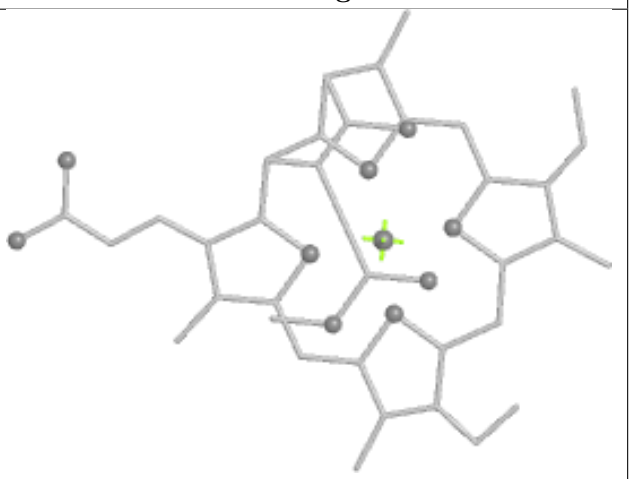
Bond lengths



Bond angles

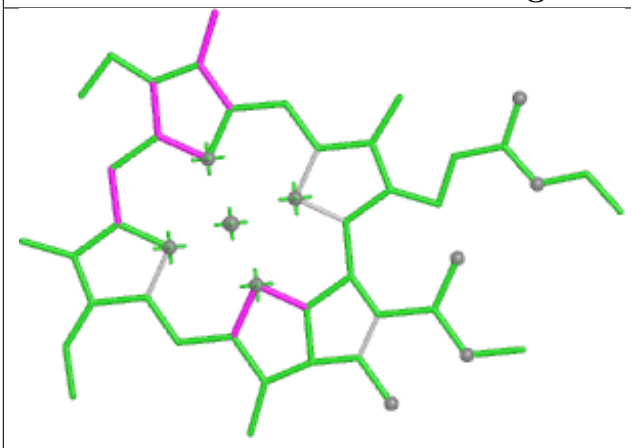


Torsions

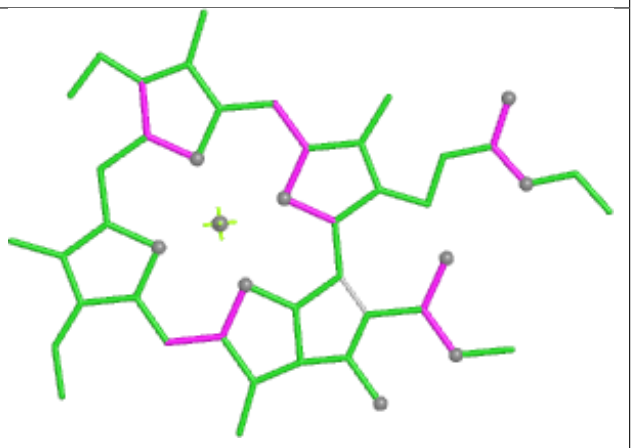


Rings

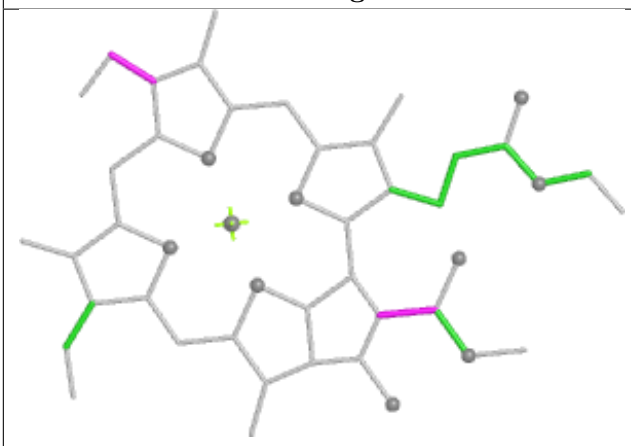
Ligand CLA b 726



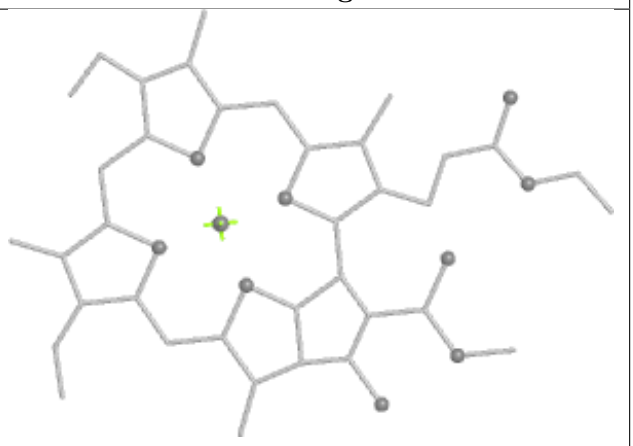
Bond lengths



Bond angles

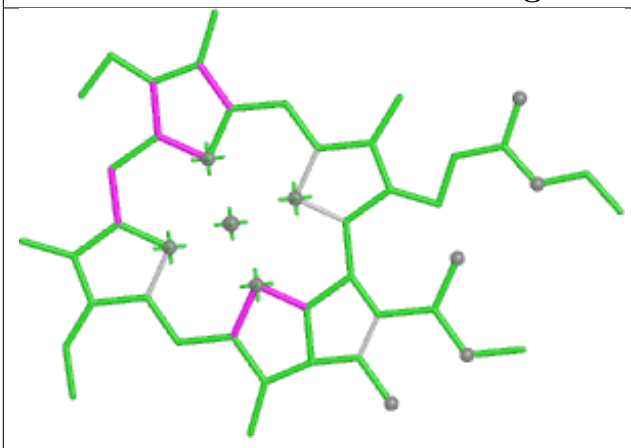


Torsions

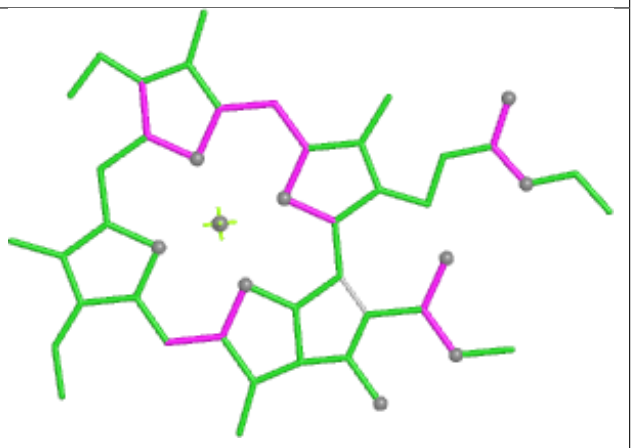


Rings

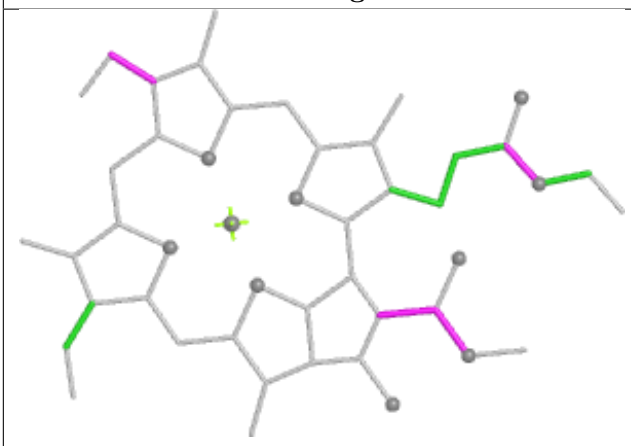
Ligand CLA O 308



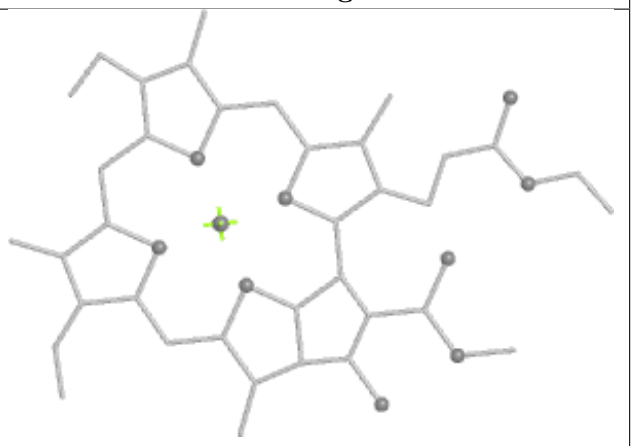
Bond lengths



Bond angles

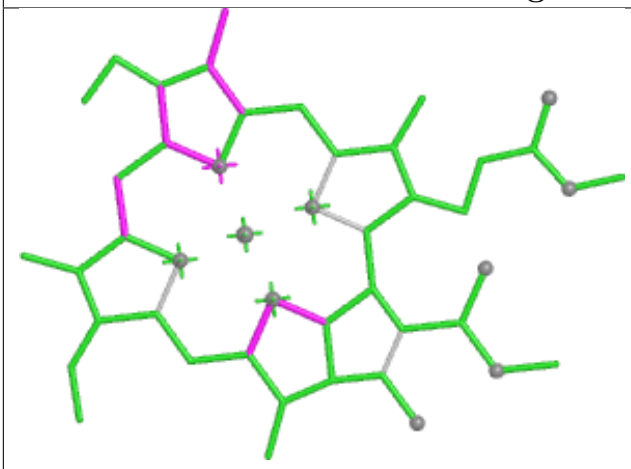


Torsions

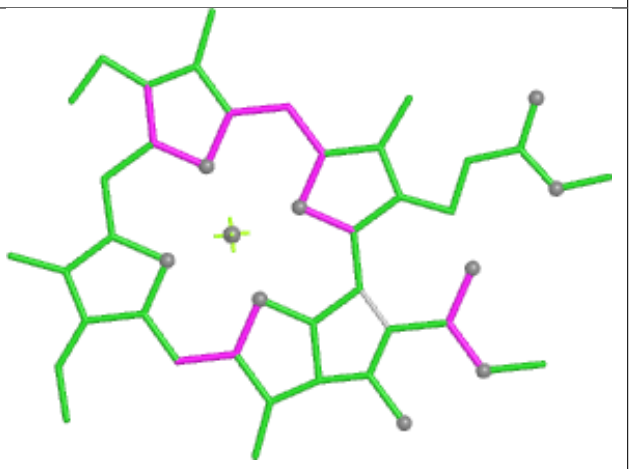


Rings

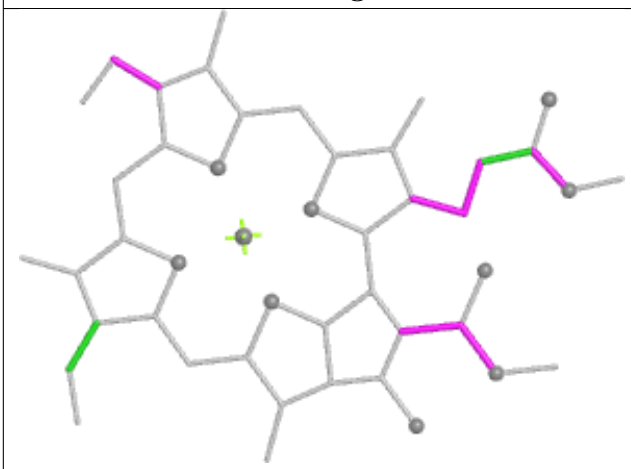
Ligand CLA b 719



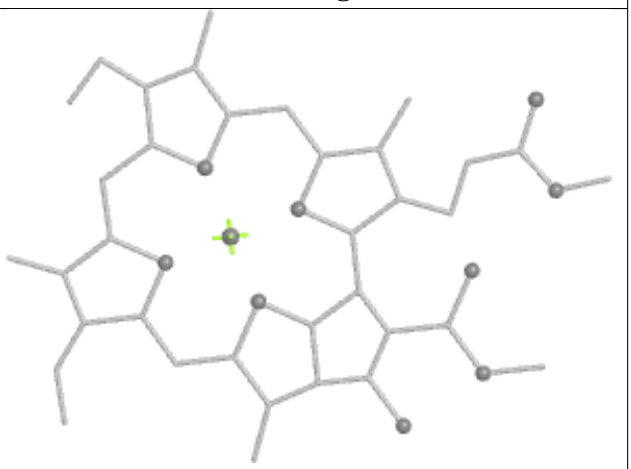
Bond lengths



Bond angles

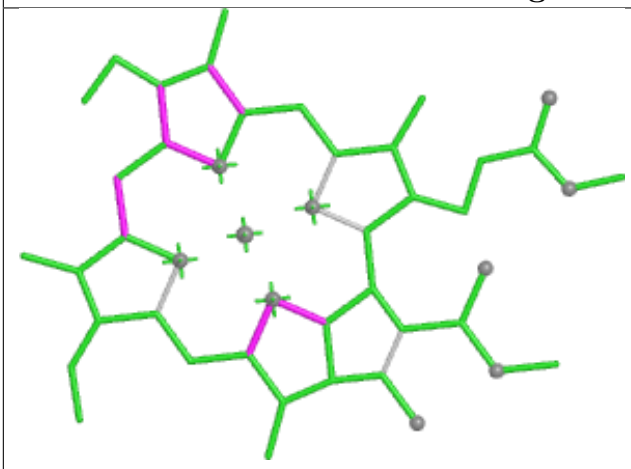


Torsions

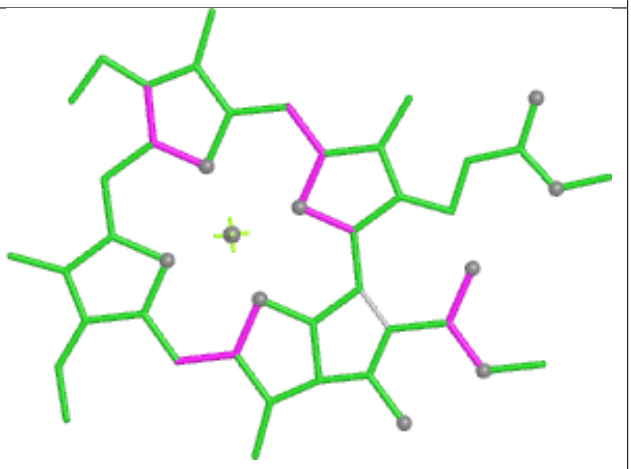


Rings

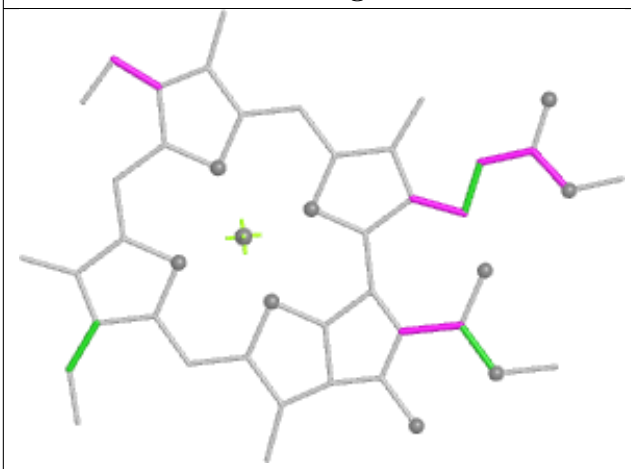
Ligand CLA a 718



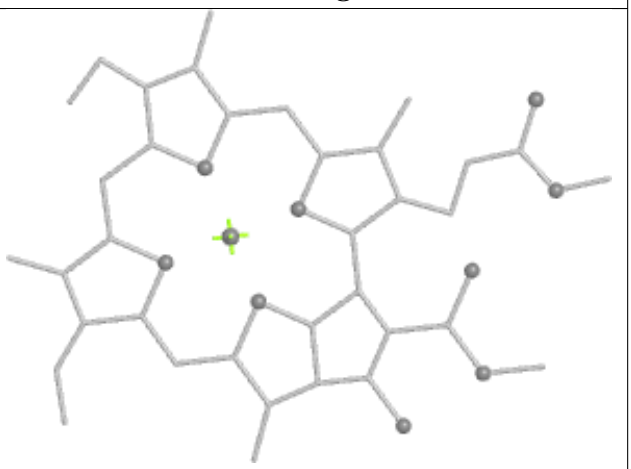
Bond lengths



Bond angles

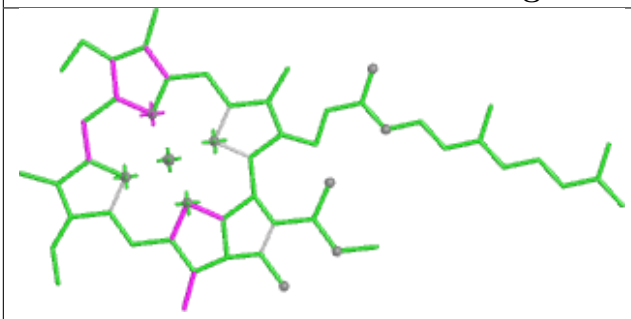


Torsions

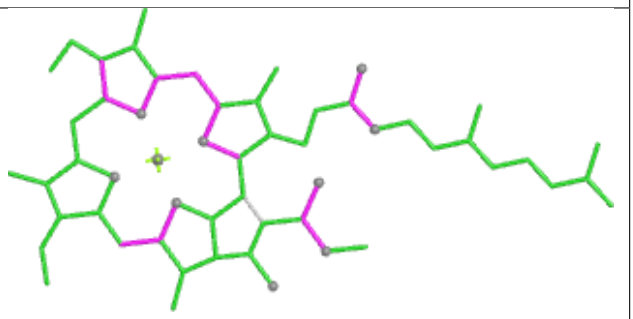


Rings

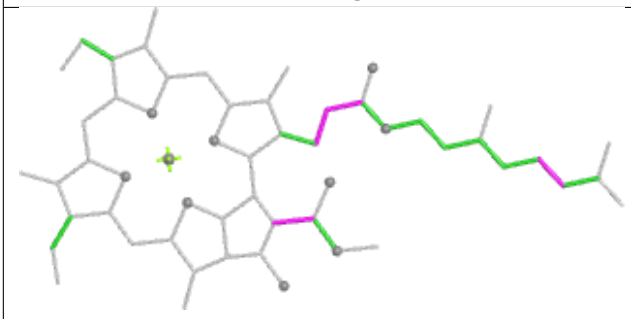
Ligand CLA K 310



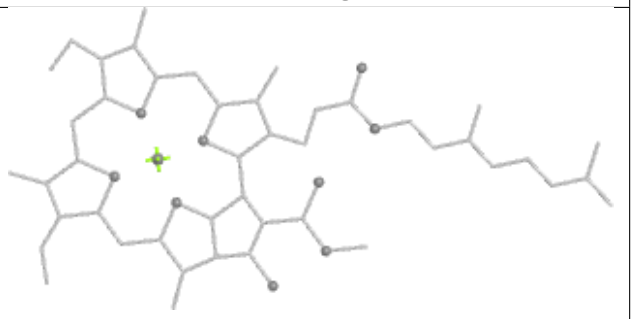
Bond lengths



Bond angles

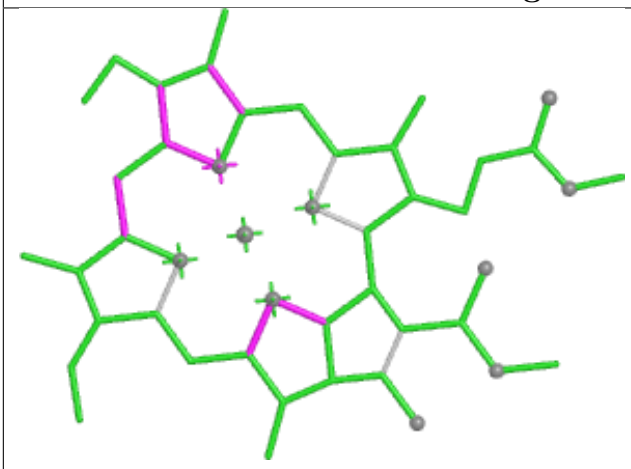


Torsions

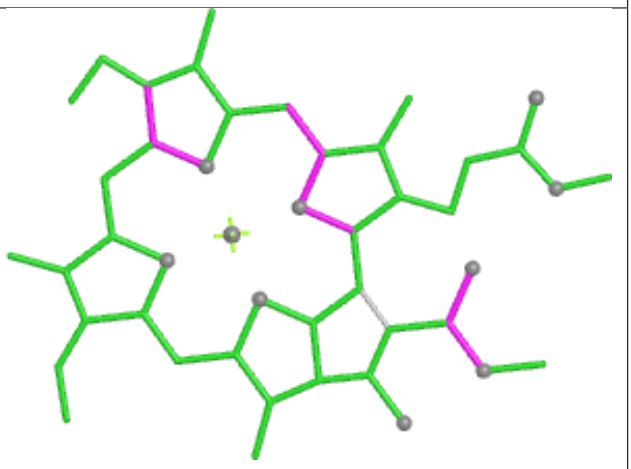


Rings

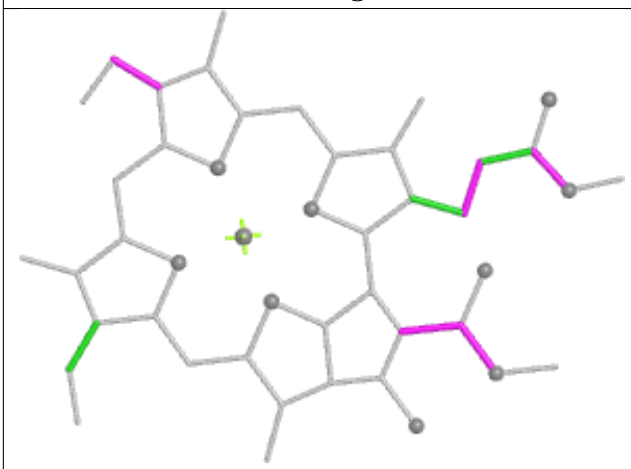
Ligand CLA D 312



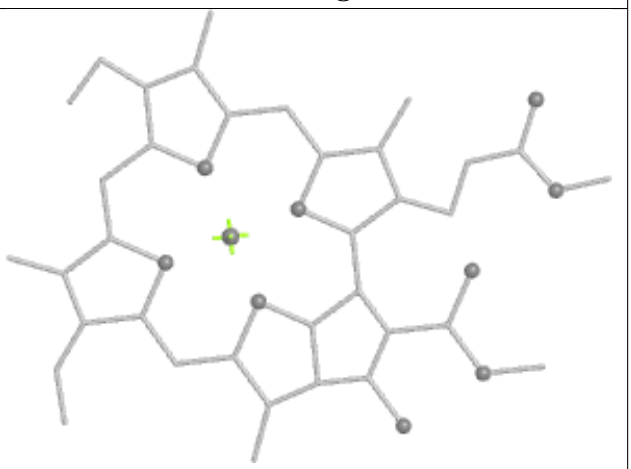
Bond lengths



Bond angles

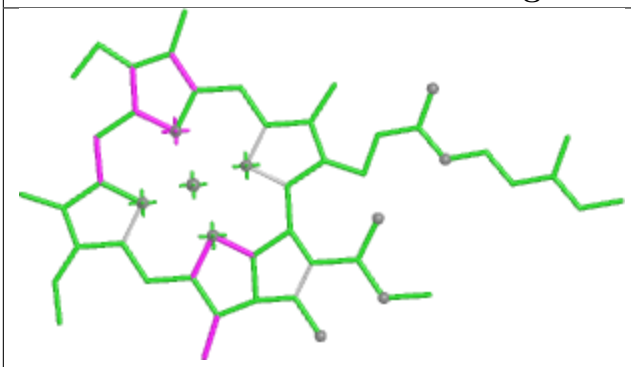


Torsions

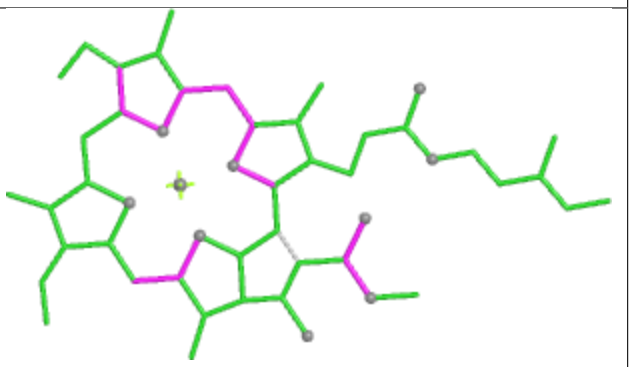


Rings

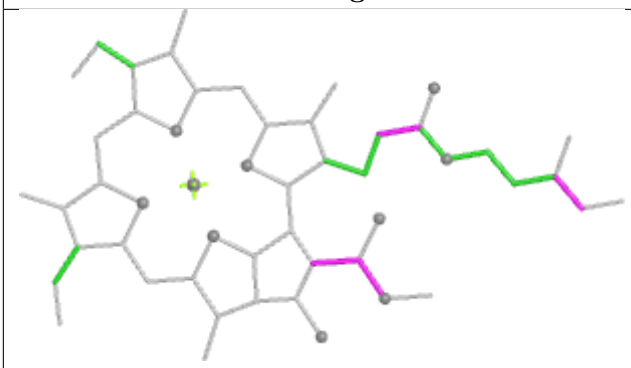
Ligand CLA N 307



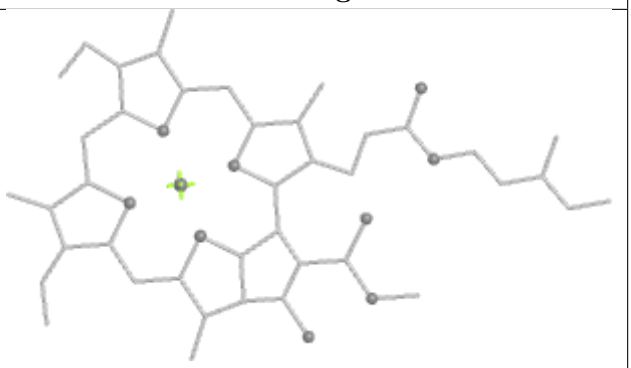
Bond lengths



Bond angles

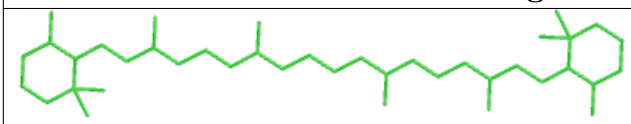


Torsions

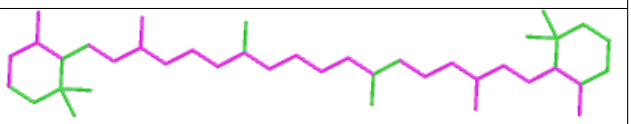


Rings

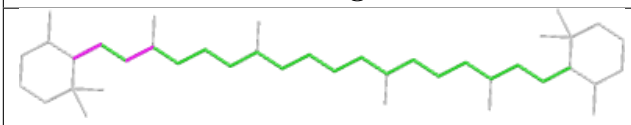
Ligand BCR a 736



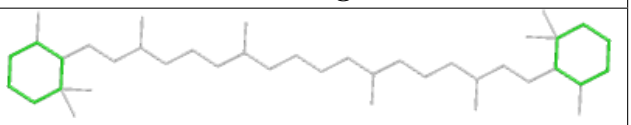
Bond lengths



Bond angles

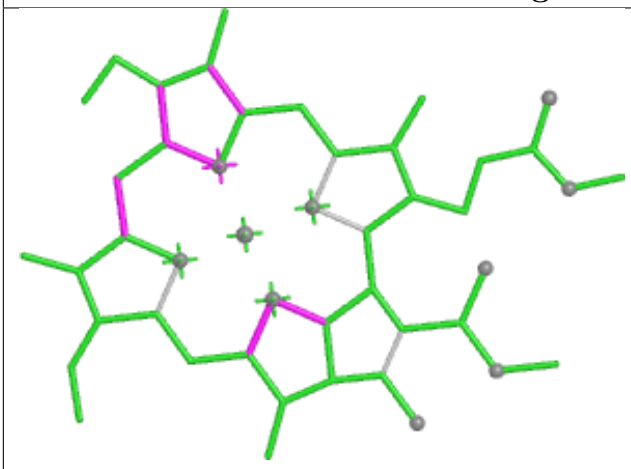


Torsions

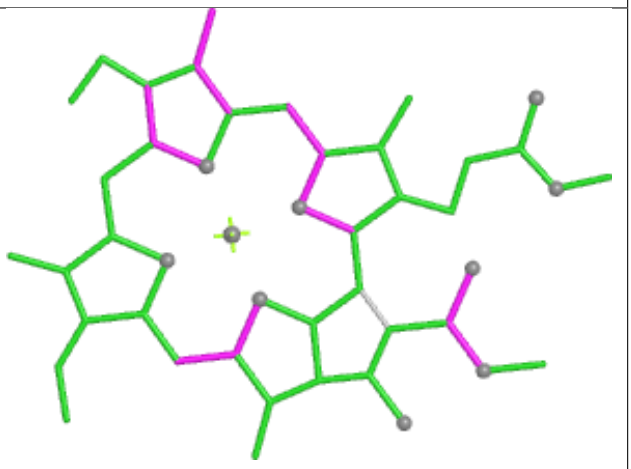


Rings

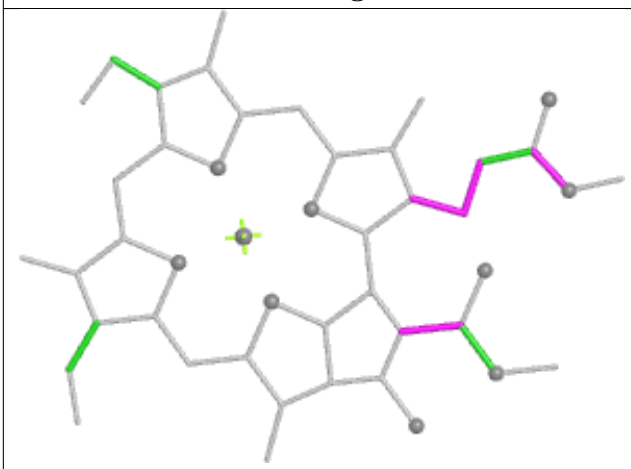
Ligand CLA f 302



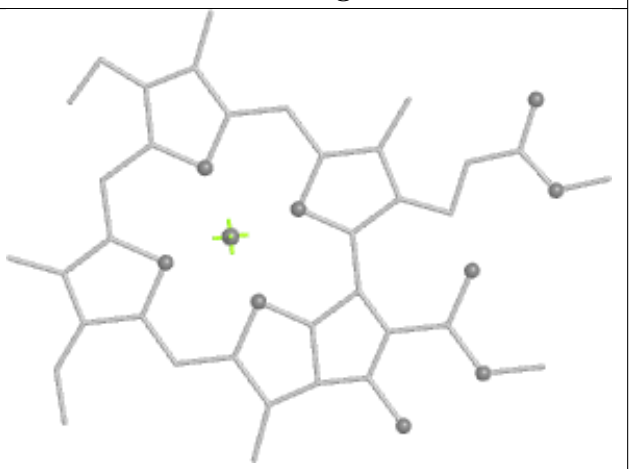
Bond lengths



Bond angles

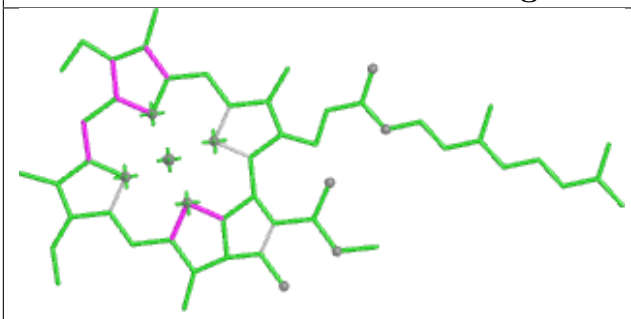


Torsions

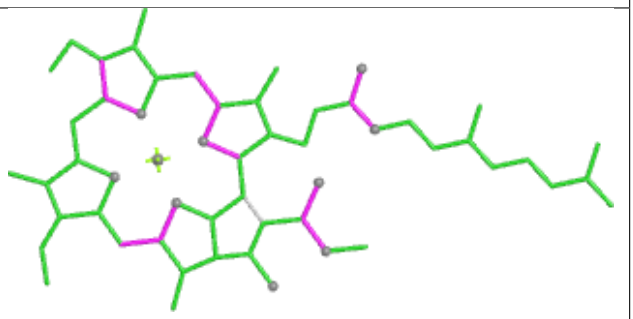


Rings

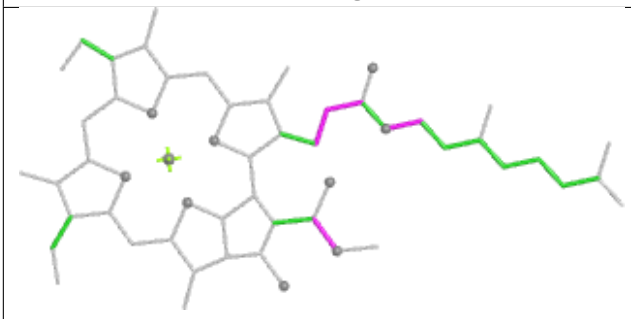
Ligand CLA M 309



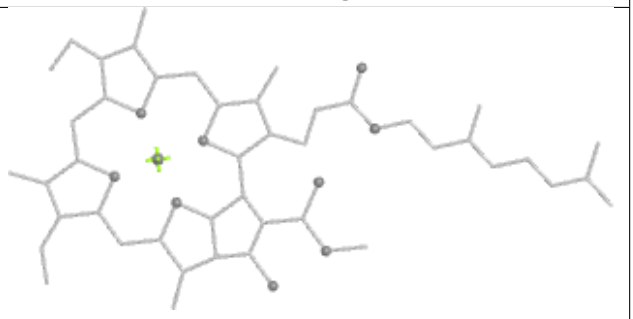
Bond lengths



Bond angles

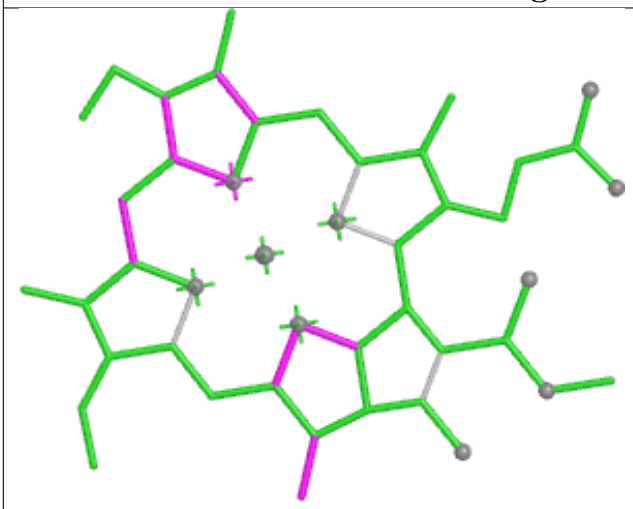


Torsions

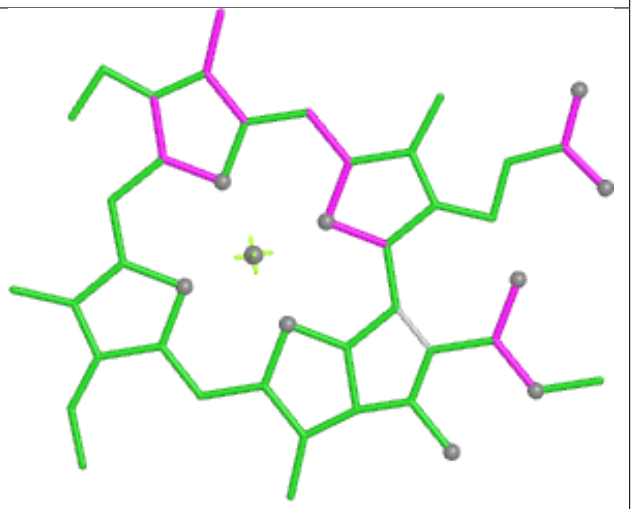


Rings

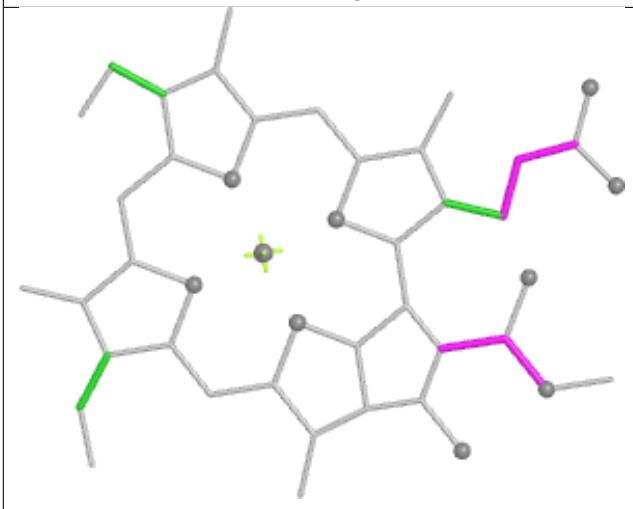
Ligand CLA I 319



Bond lengths



Bond angles

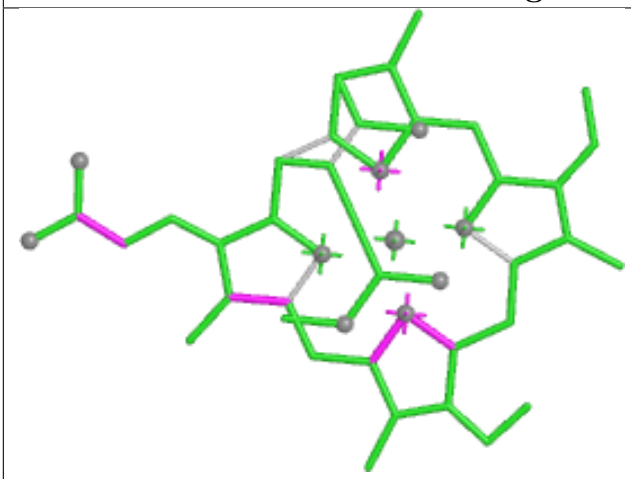


Torsions

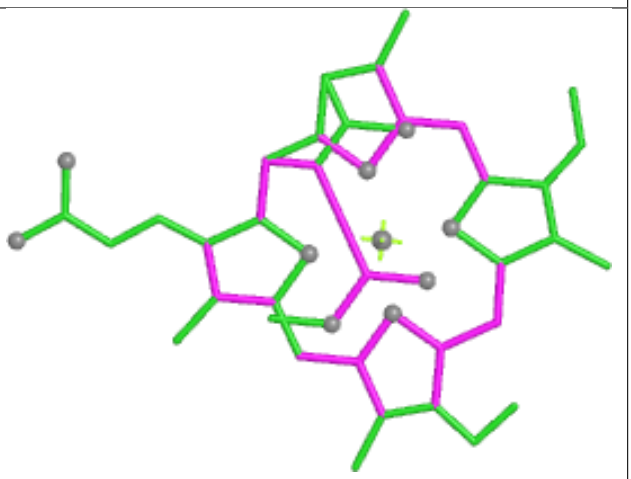


Rings

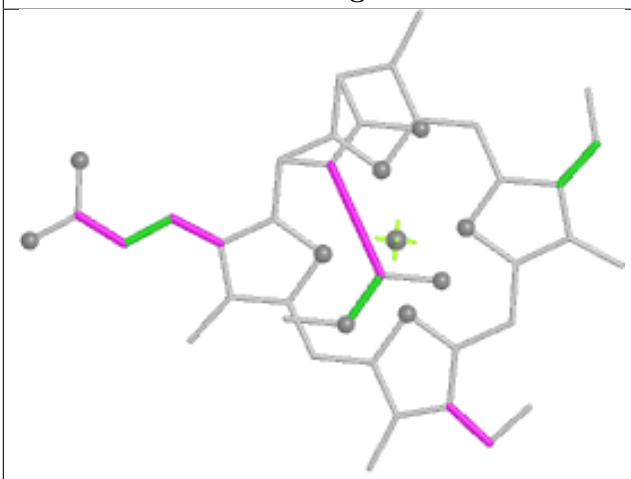
Ligand KC1 A 306



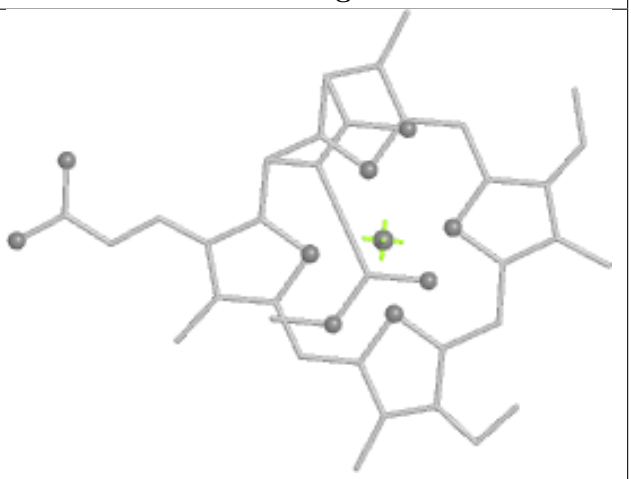
Bond lengths



Bond angles

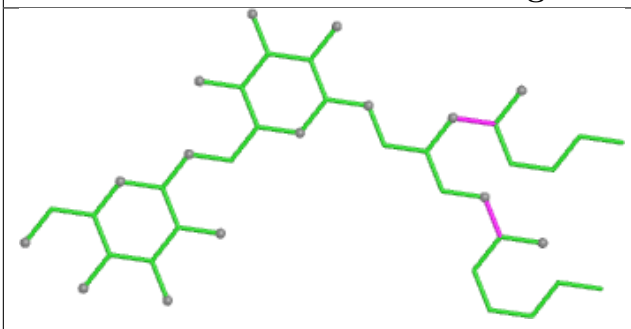


Torsions

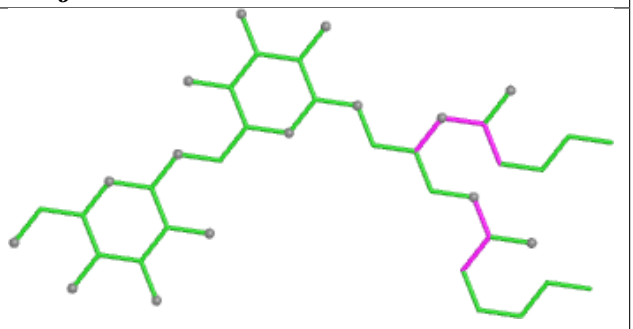


Rings

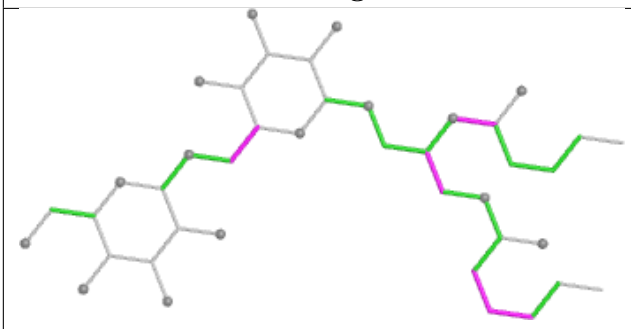
Ligand DGD j 103



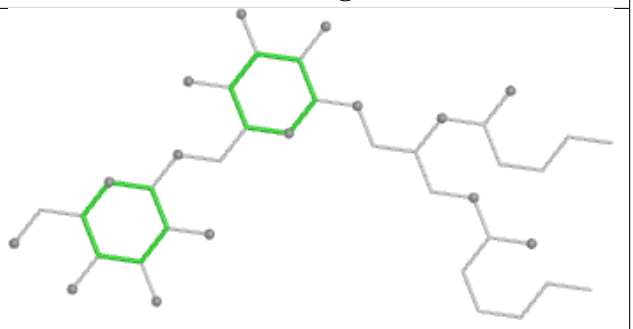
Bond lengths



Bond angles

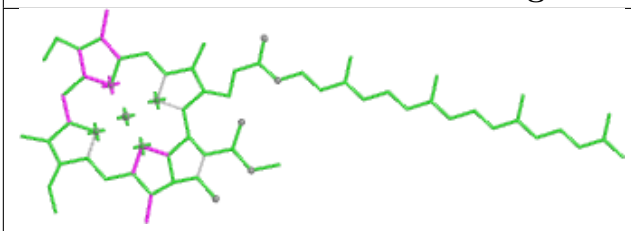


Torsions

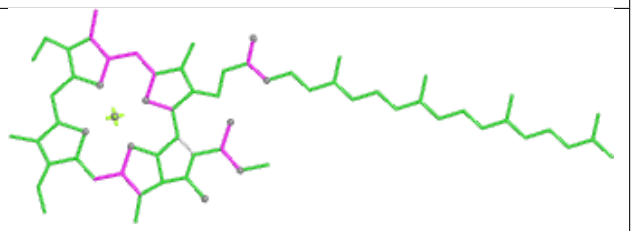


Rings

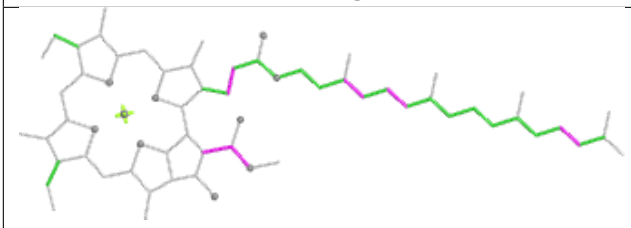
Ligand CLA b 722



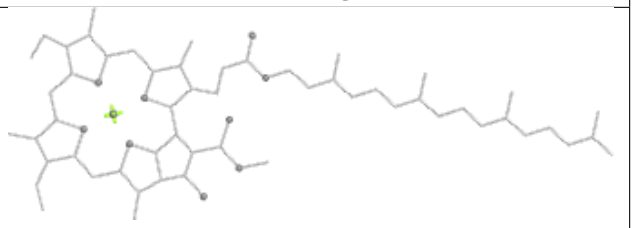
Bond lengths



Bond angles

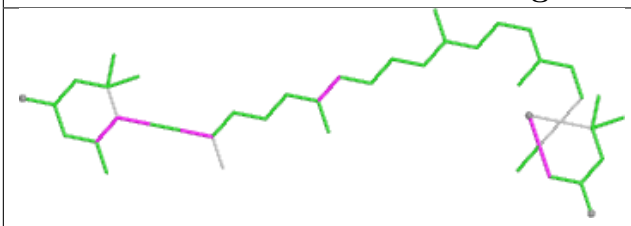


Torsions

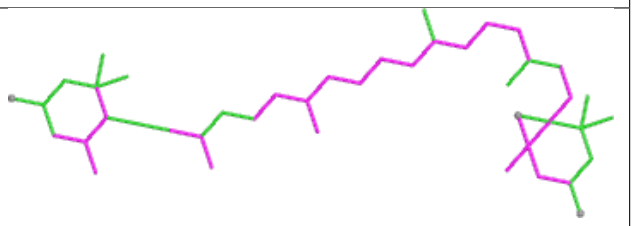


Rings

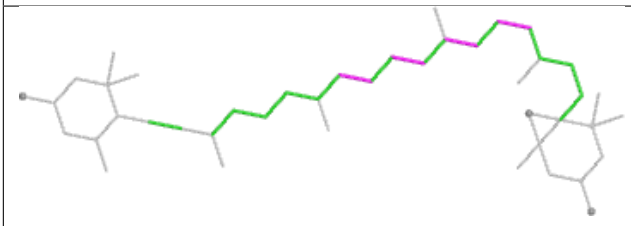
Ligand DD6 I 305



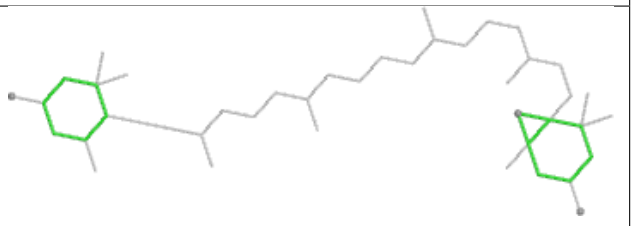
Bond lengths



Bond angles

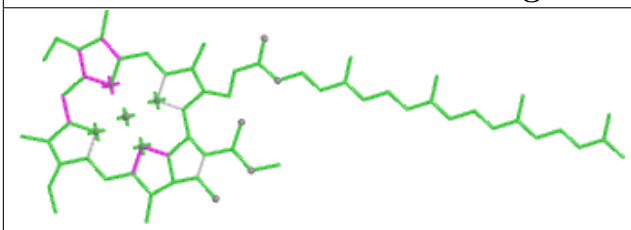


Torsions

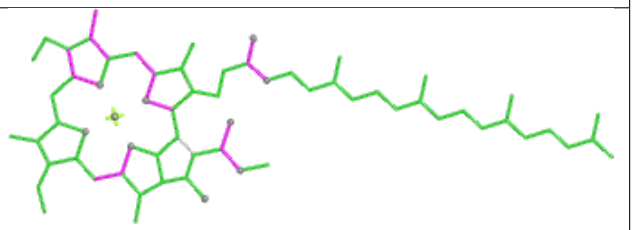


Rings

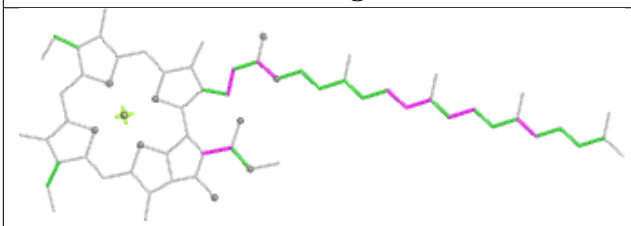
Ligand CLA G 513



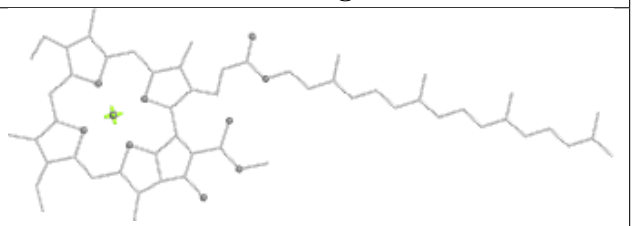
Bond lengths



Bond angles

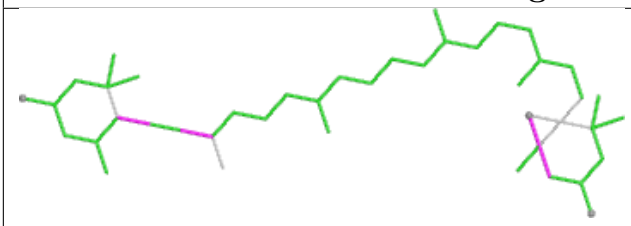


Torsions

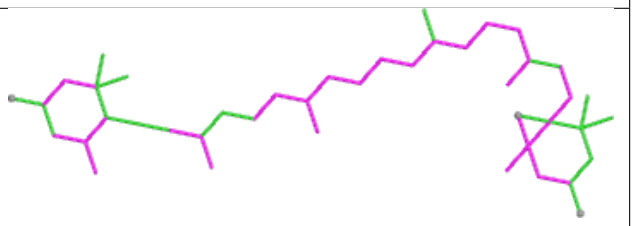


Rings

Ligand DD6 J 303



Bond lengths



Bond angles

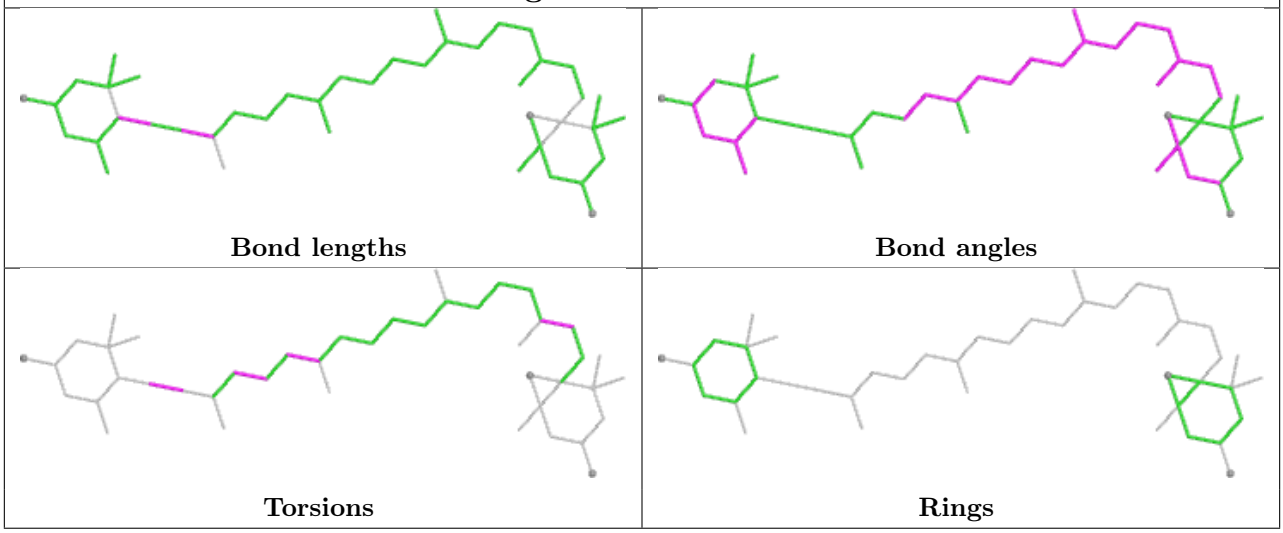


Torsions

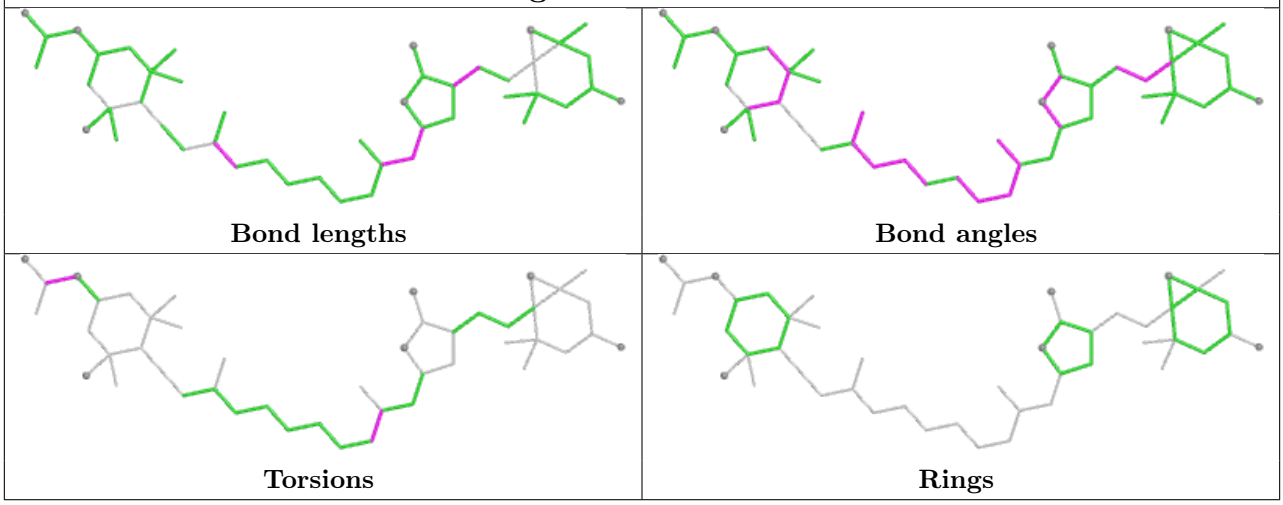


Rings

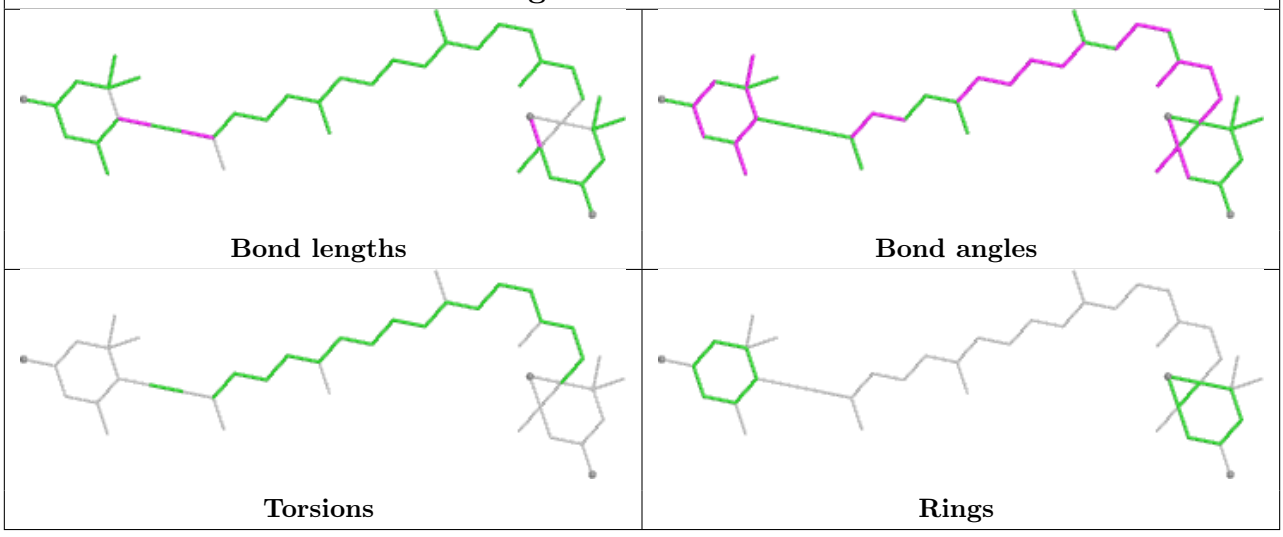
Ligand DD6 G 502



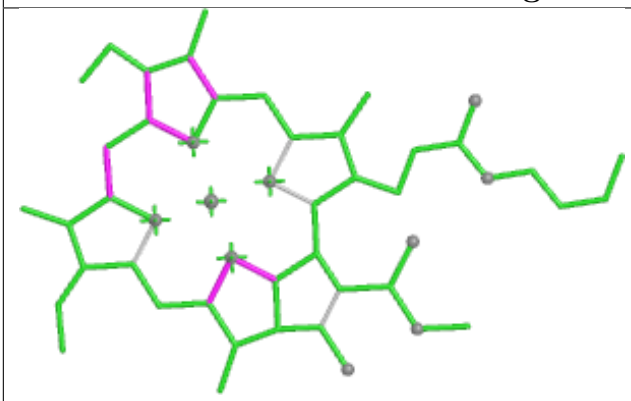
Ligand PID O 304



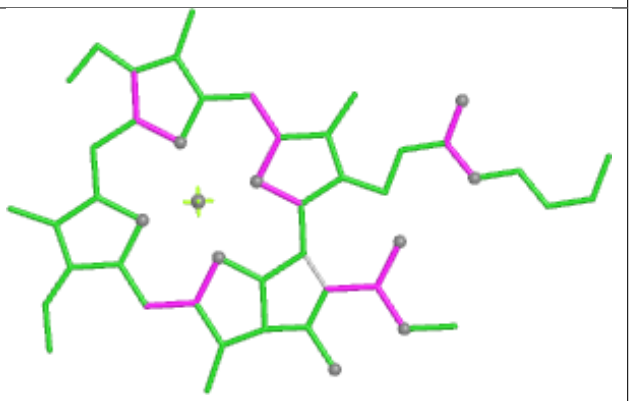
Ligand DD6 L 304



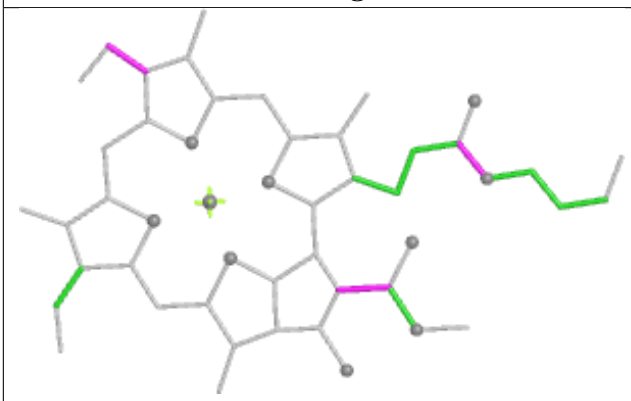
Ligand CLA K 306



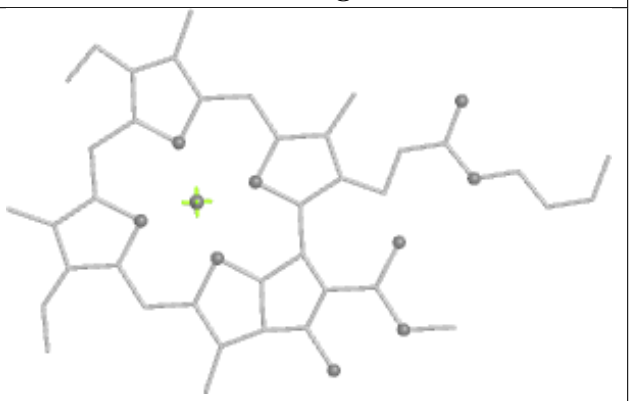
Bond lengths



Bond angles

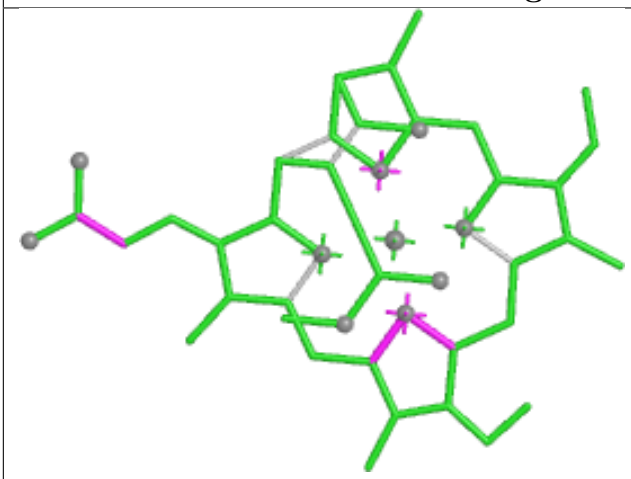


Torsions

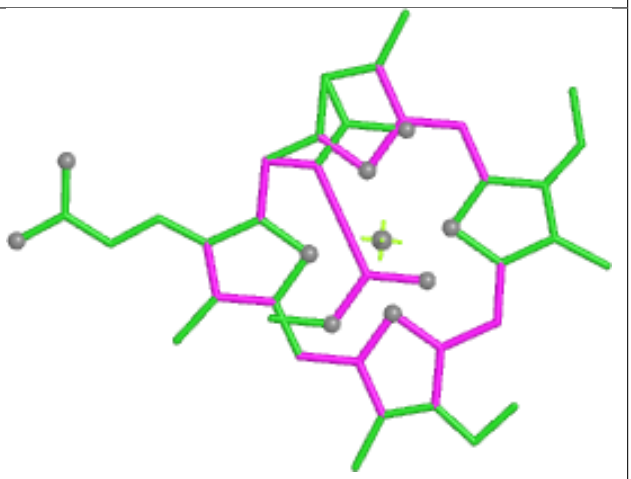


Rings

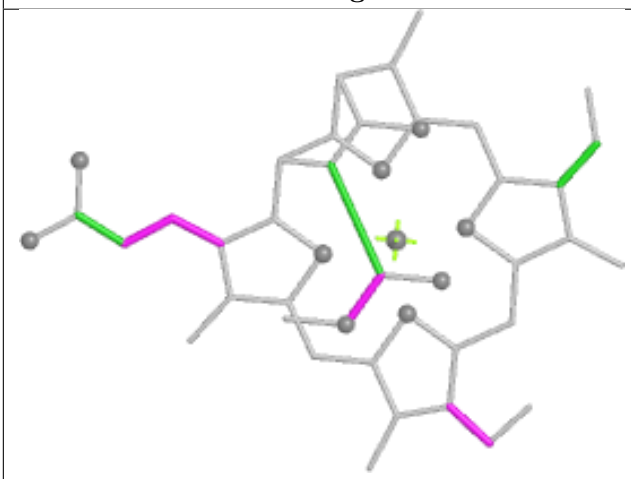
Ligand KC1 N 311



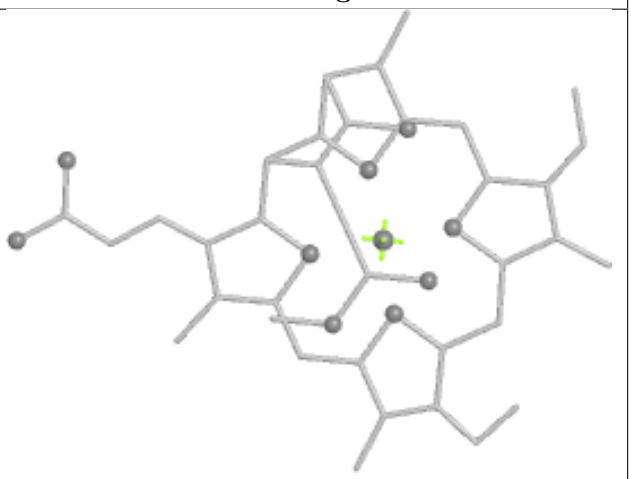
Bond lengths



Bond angles

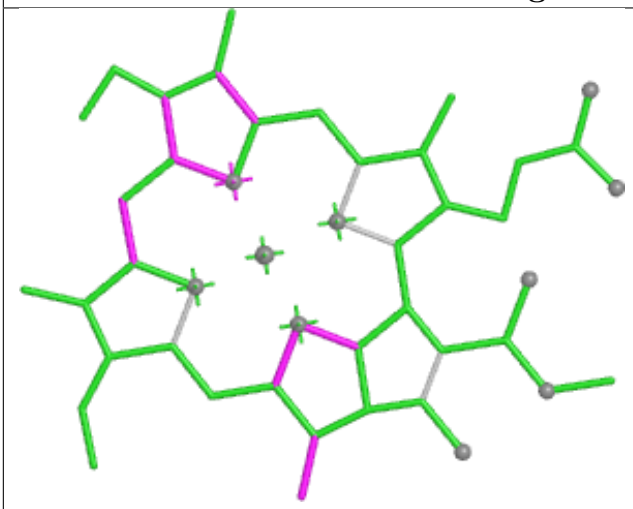


Torsions

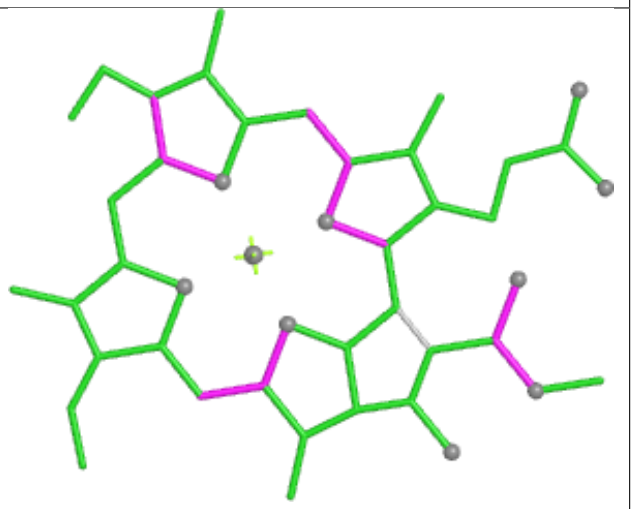


Rings

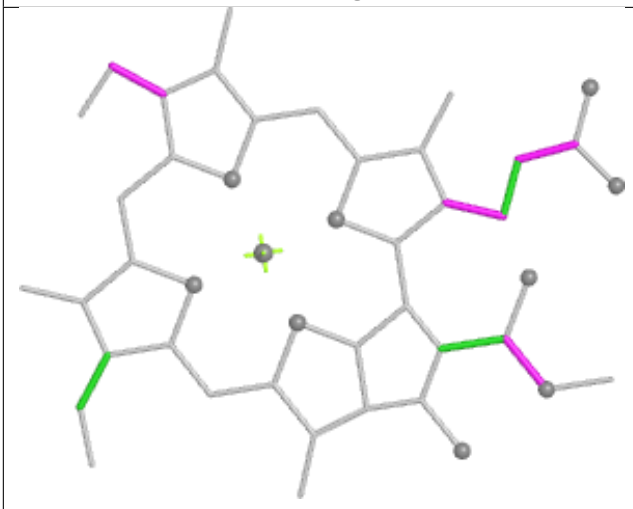
Ligand CLA a 715



Bond lengths



Bond angles

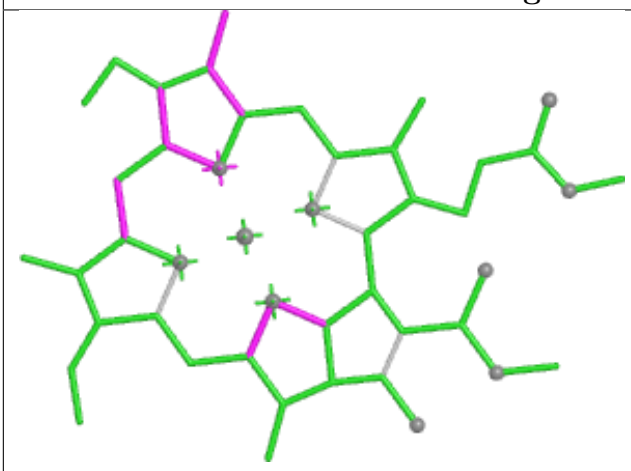


Torsions

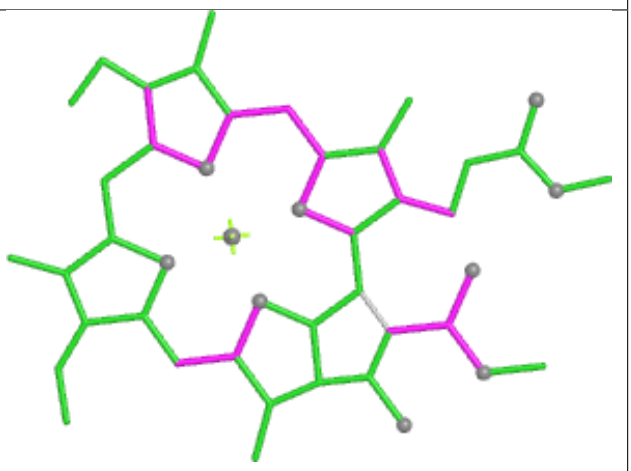


Rings

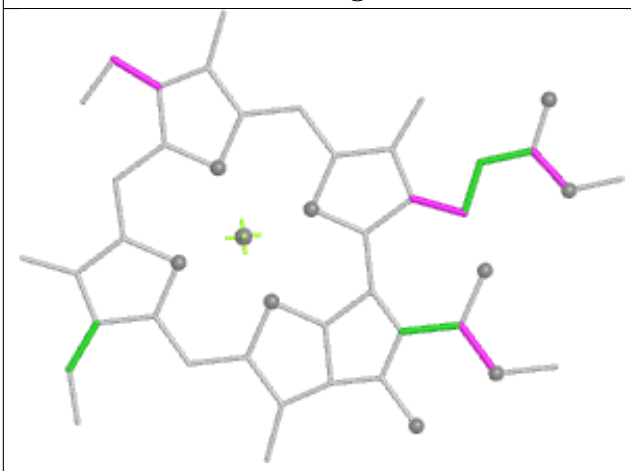
Ligand CLA D 314



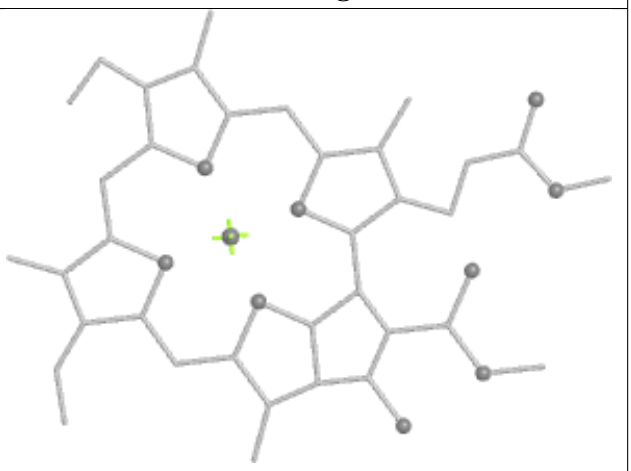
Bond lengths



Bond angles

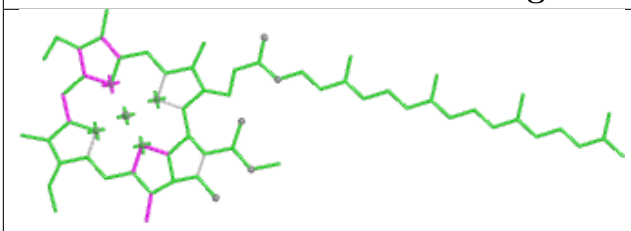


Torsions

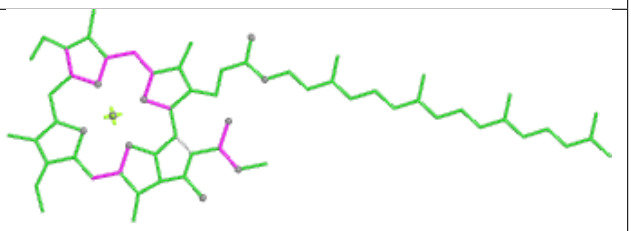


Rings

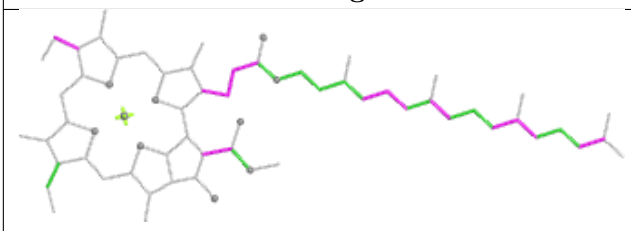
Ligand CLA b 724



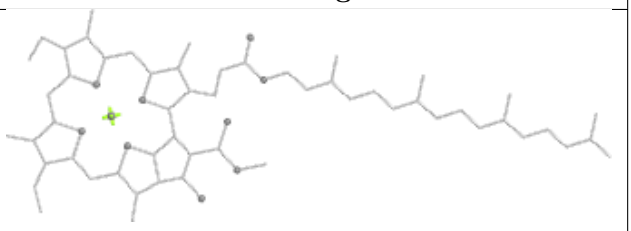
Bond lengths



Bond angles

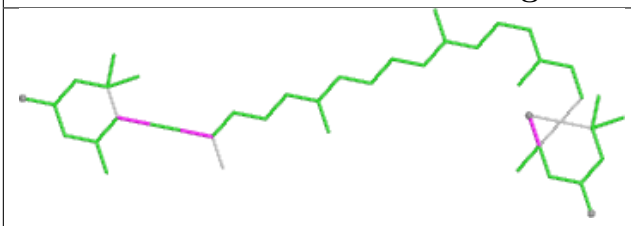


Torsions

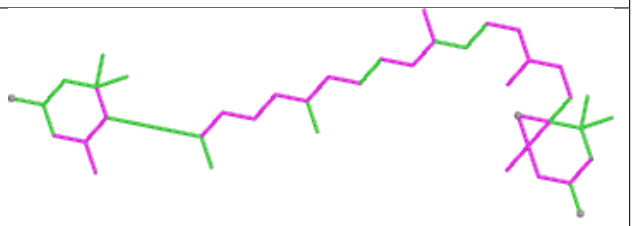


Rings

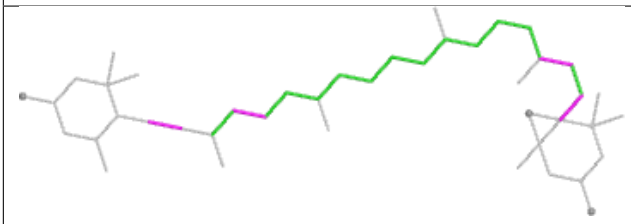
Ligand DD6 M 306



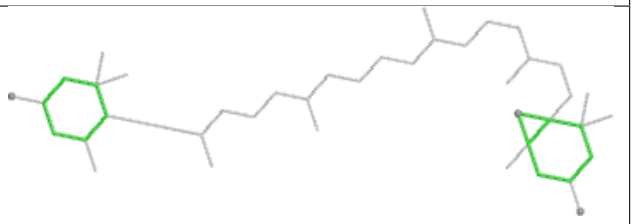
Bond lengths



Bond angles

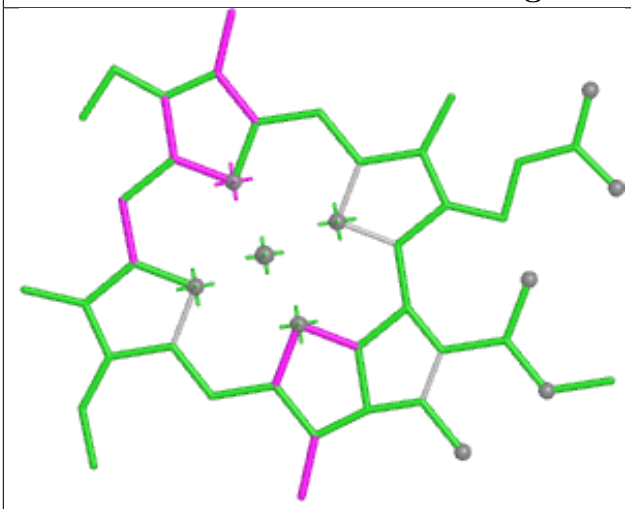


Torsions

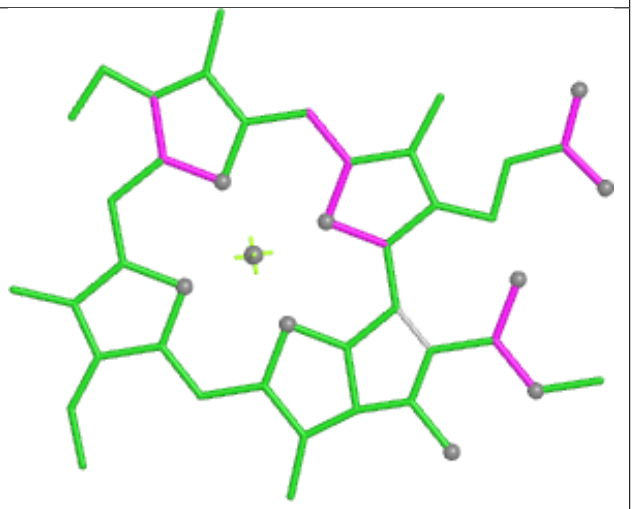


Rings

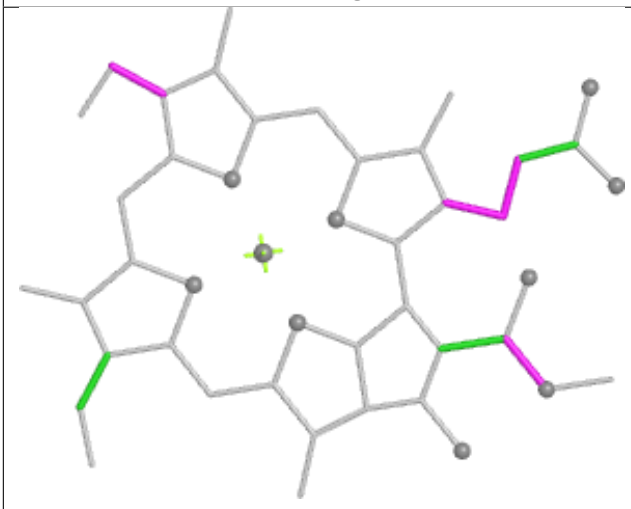
Ligand CLA B 317



Bond lengths



Bond angles

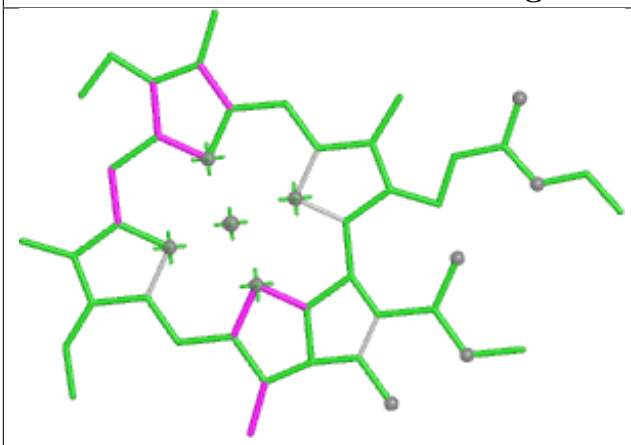


Torsions

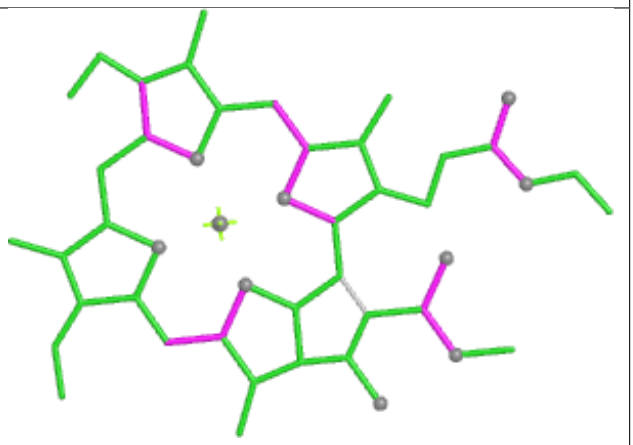


Rings

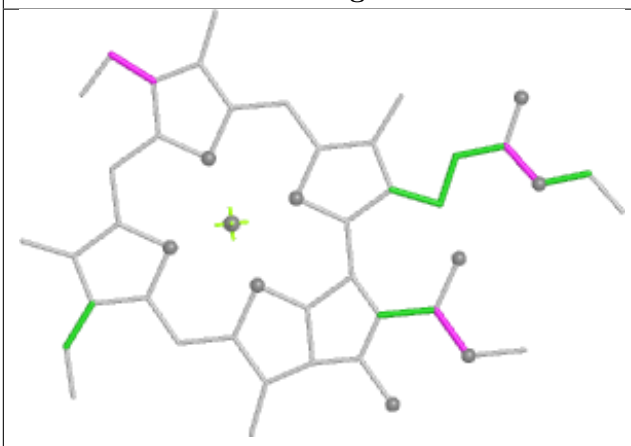
Ligand CLA P 209



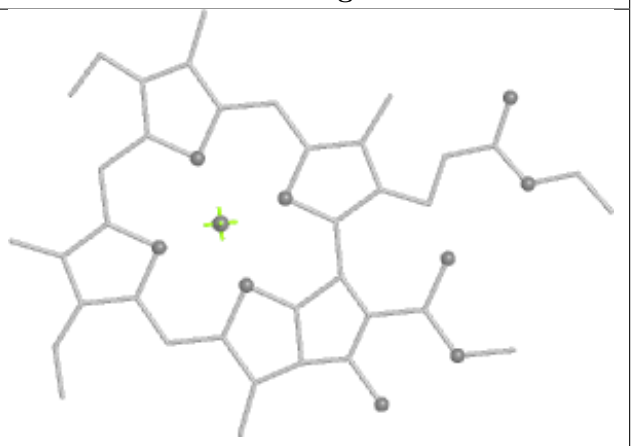
Bond lengths



Bond angles

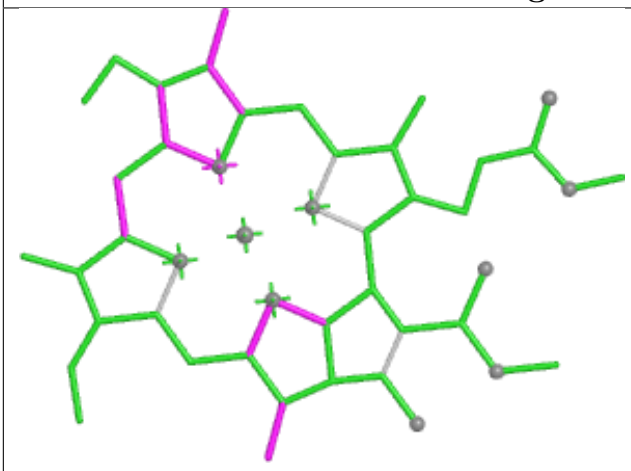


Torsions

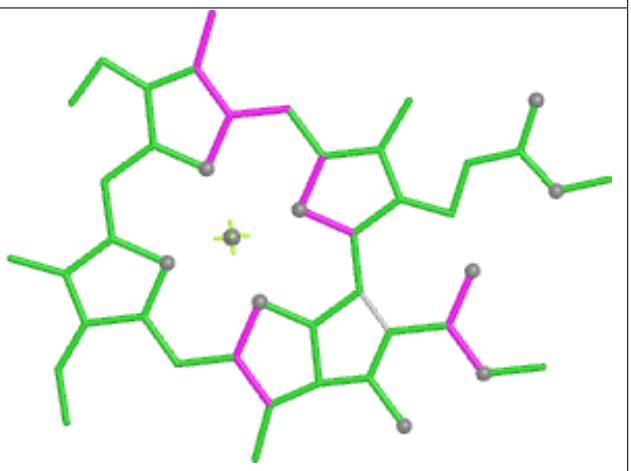


Rings

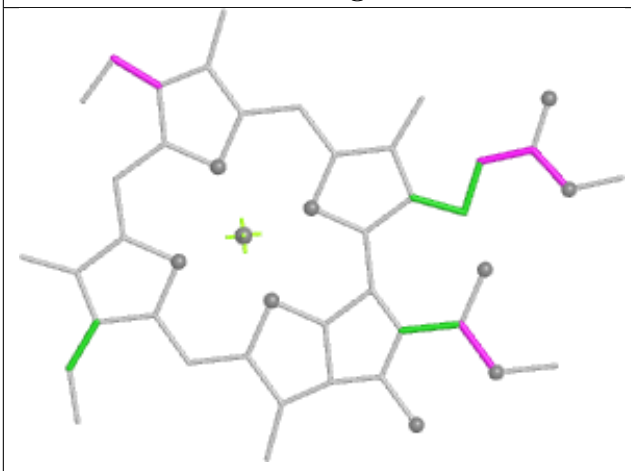
Ligand CLA J 310



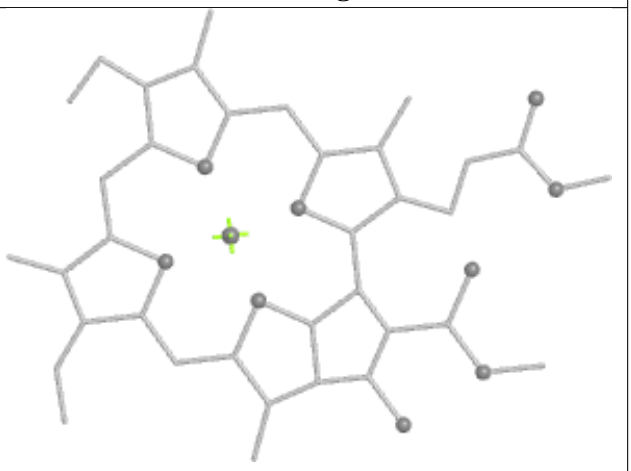
Bond lengths



Bond angles

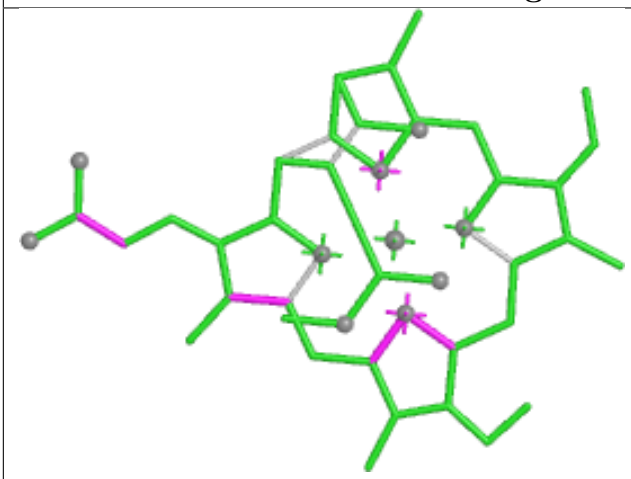


Torsions

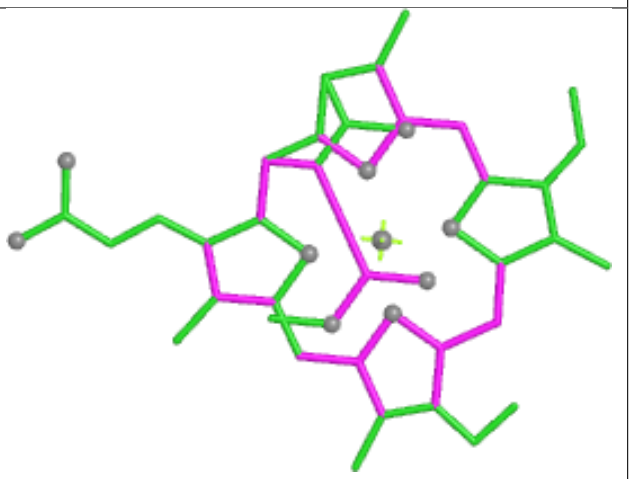


Rings

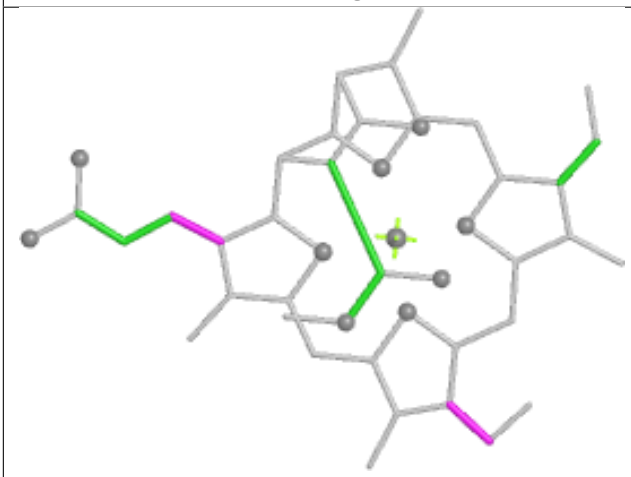
Ligand KC1 H 306



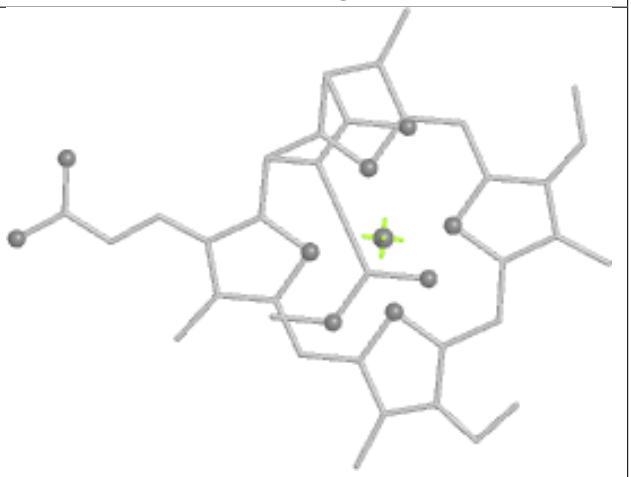
Bond lengths



Bond angles

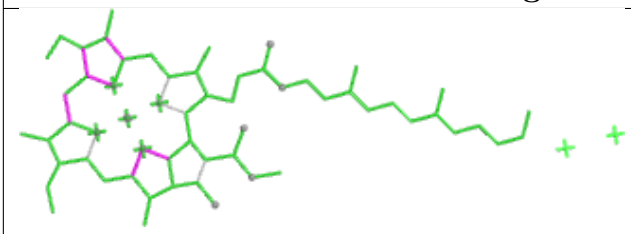


Torsions

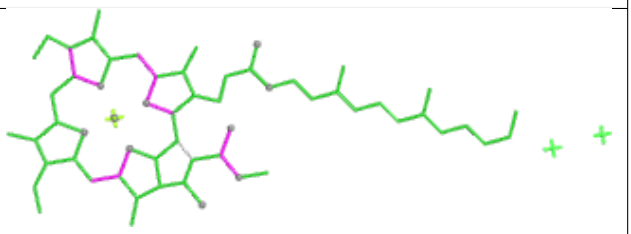


Rings

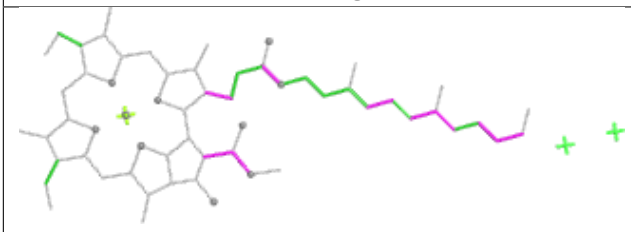
Ligand CLA G 519



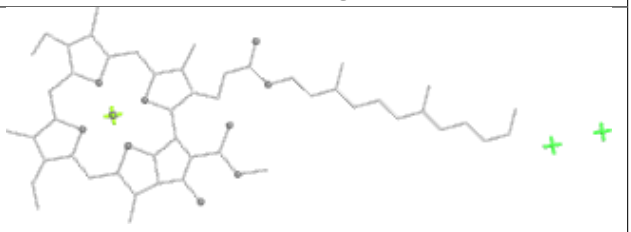
Bond lengths



Bond angles

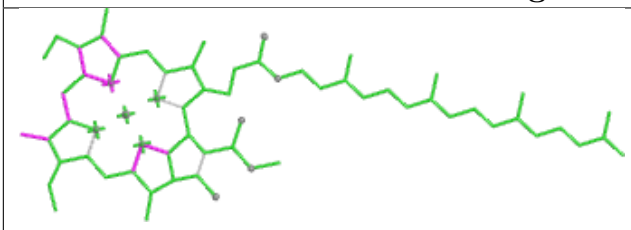


Torsions

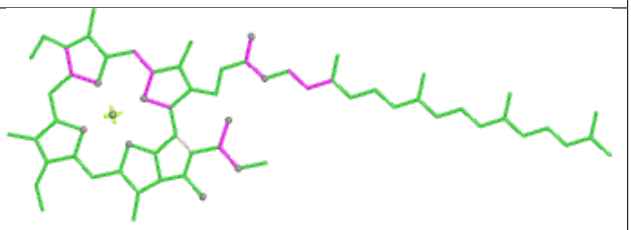


Rings

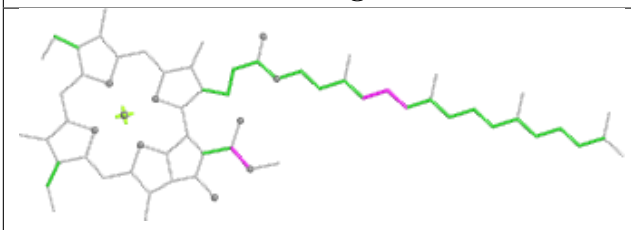
Ligand CLA a 730



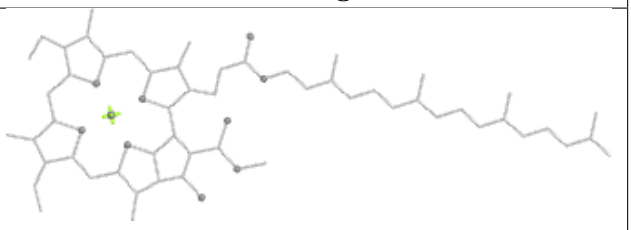
Bond lengths



Bond angles

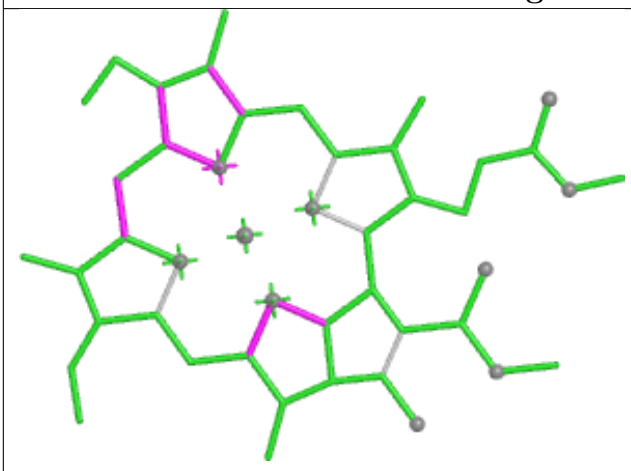


Torsions

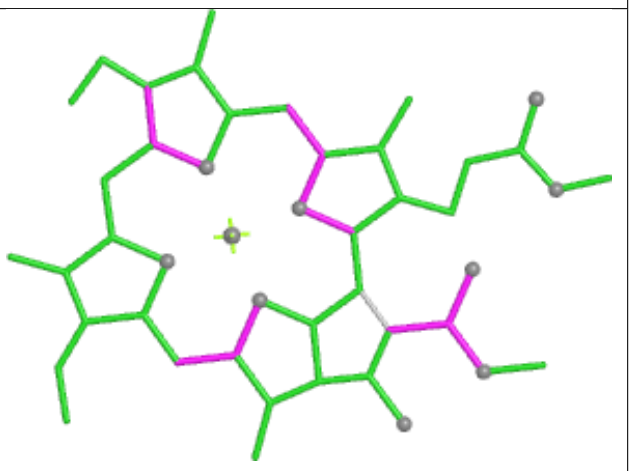


Rings

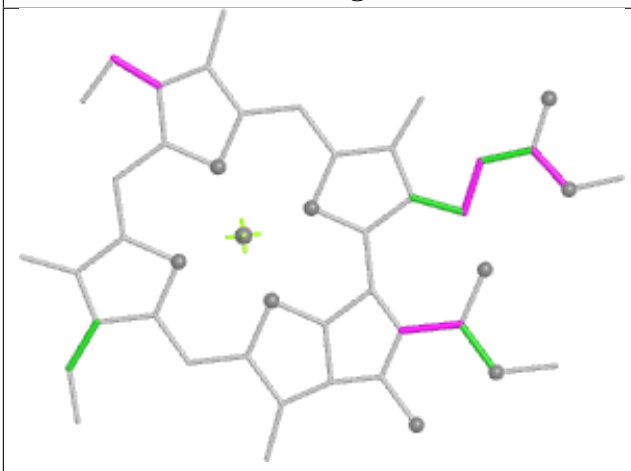
Ligand CLA F 311



Bond lengths



Bond angles

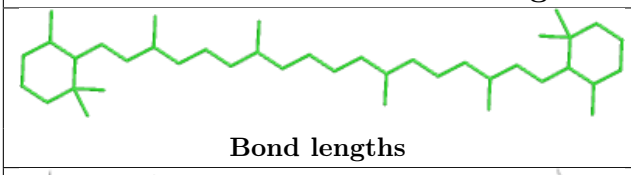


Torsions

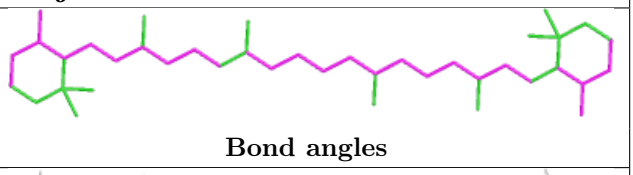


Rings

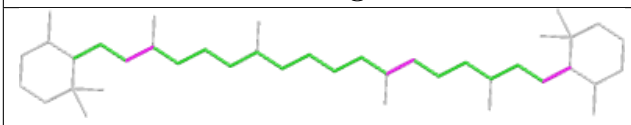
Ligand BCR j 102



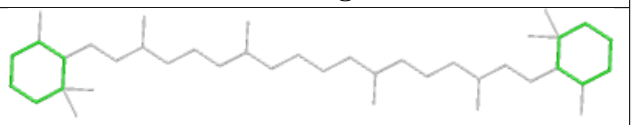
Bond lengths



Bond angles

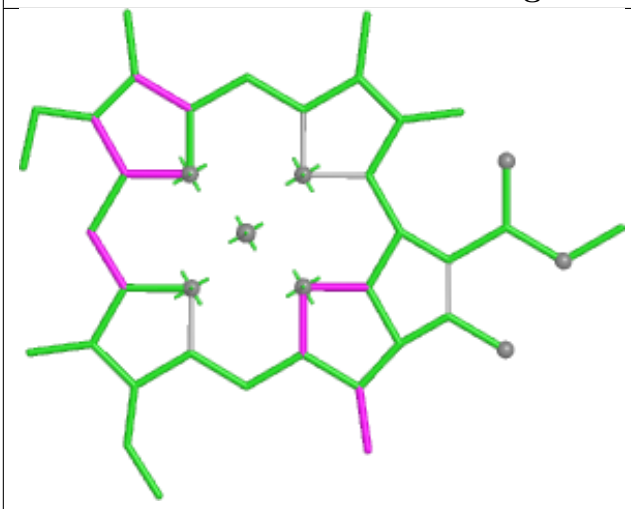


Torsions

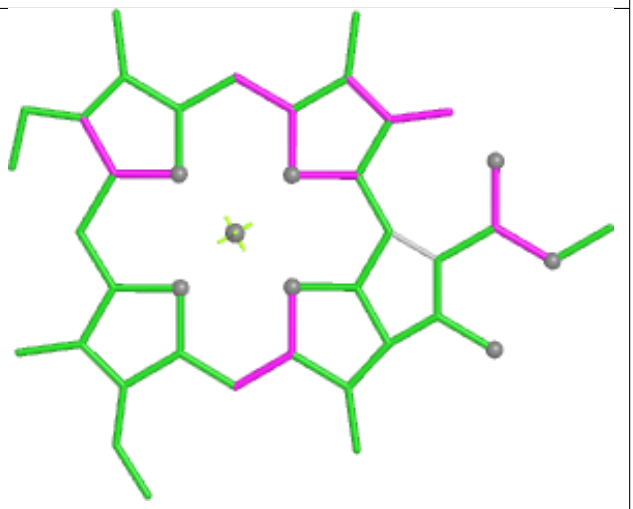


Rings

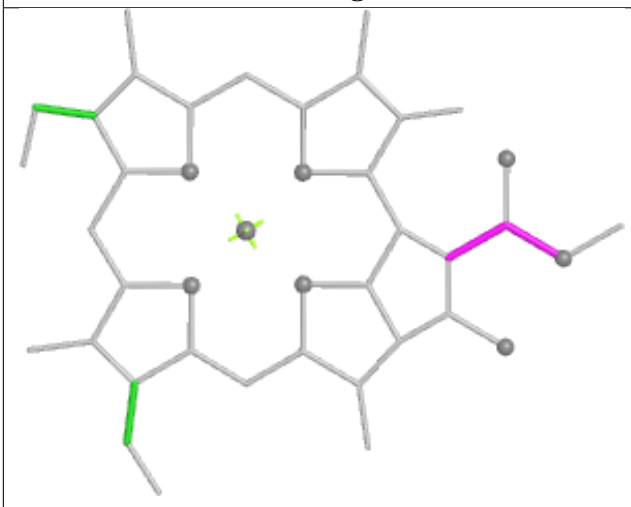
Ligand CLA A 315



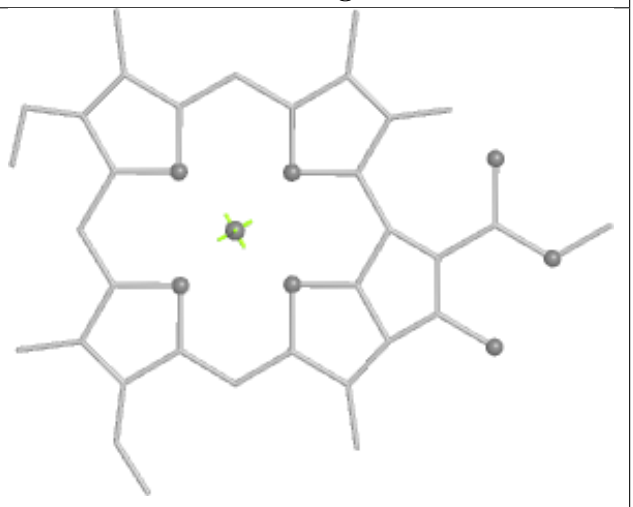
Bond lengths



Bond angles

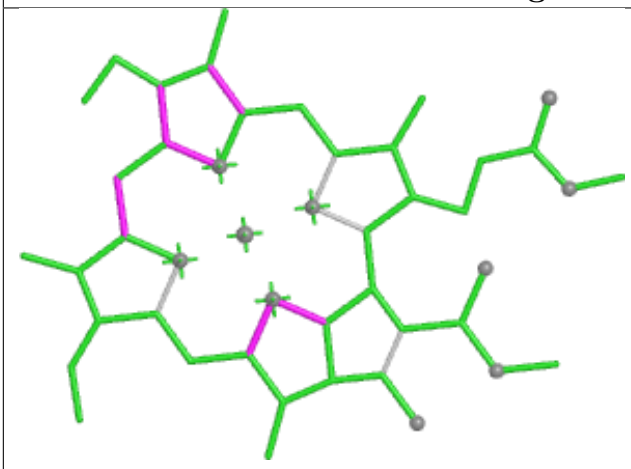


Torsions

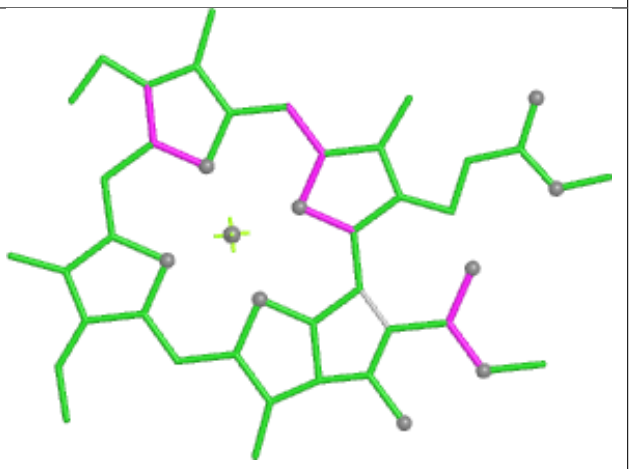


Rings

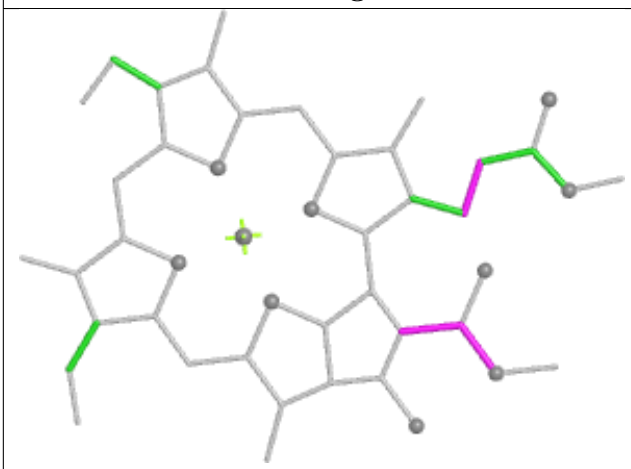
Ligand CLA J 315



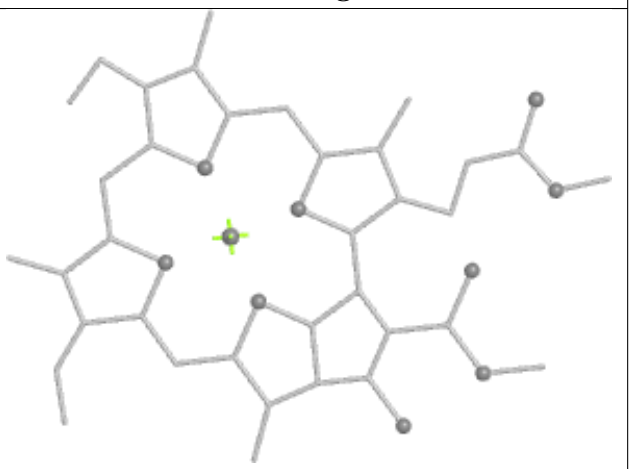
Bond lengths



Bond angles

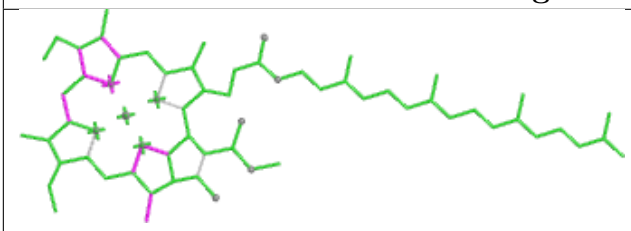


Torsions

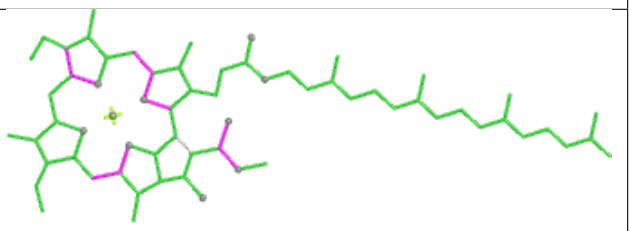


Rings

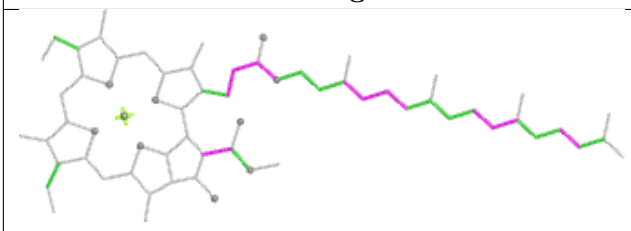
Ligand CLA l 305



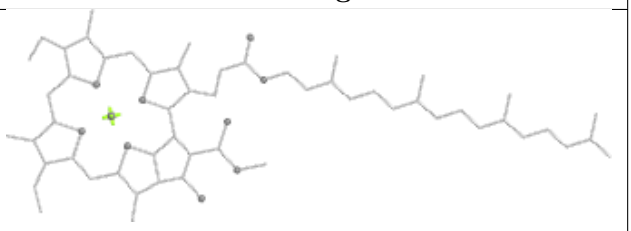
Bond lengths



Bond angles

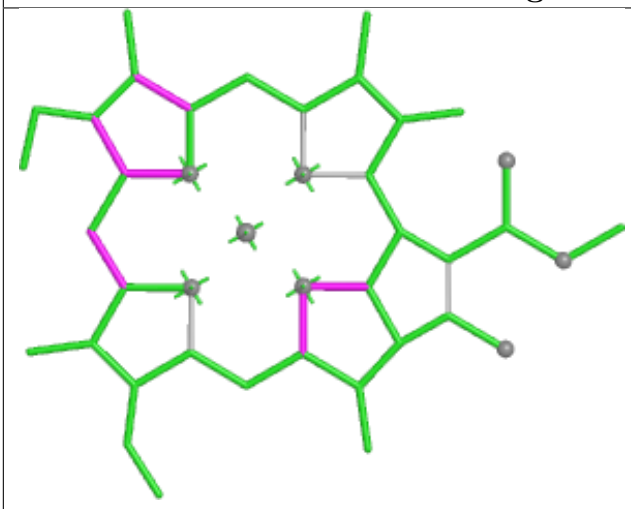


Torsions

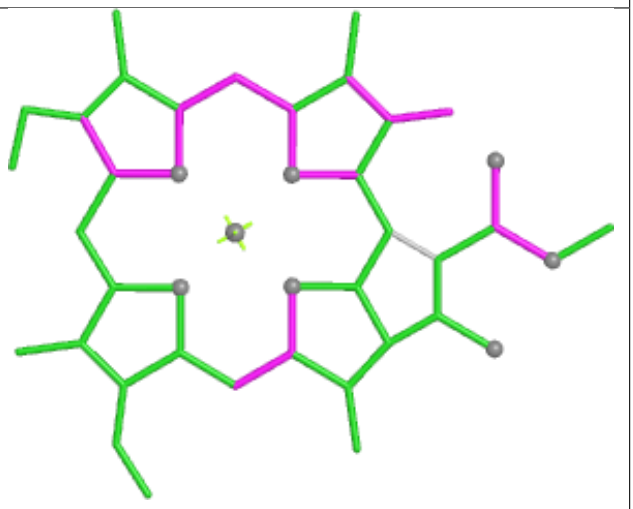


Rings

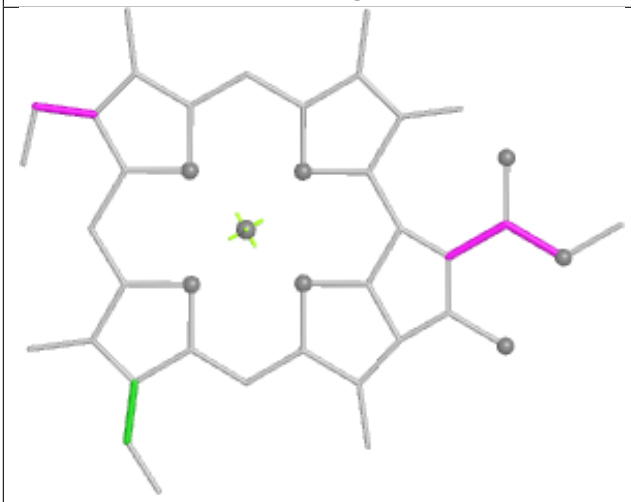
Ligand CLA L 316



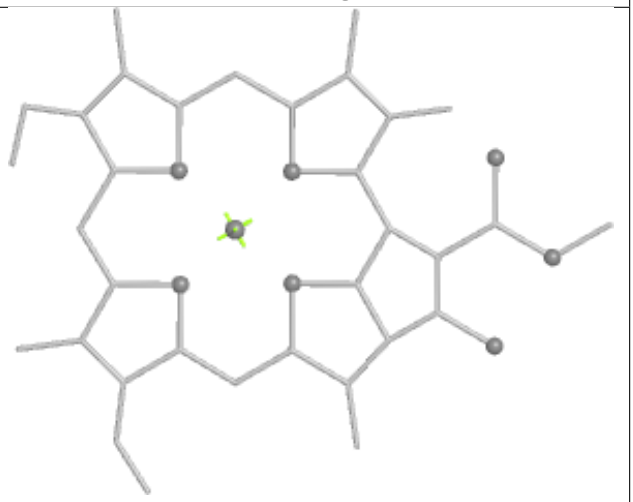
Bond lengths



Bond angles

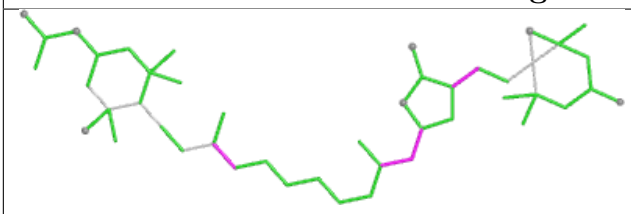


Torsions

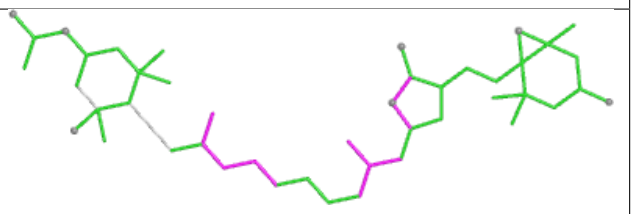


Rings

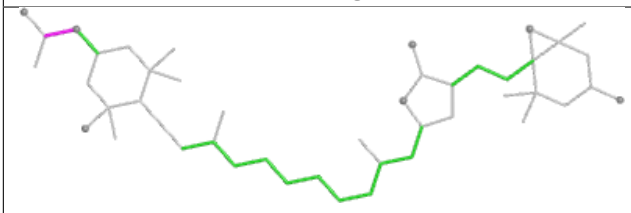
Ligand PID P 203



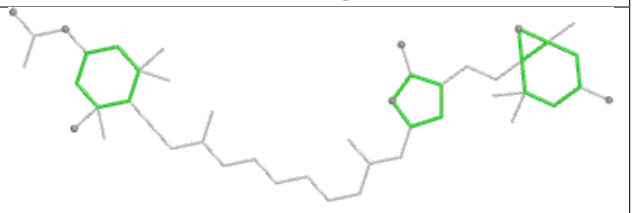
Bond lengths



Bond angles

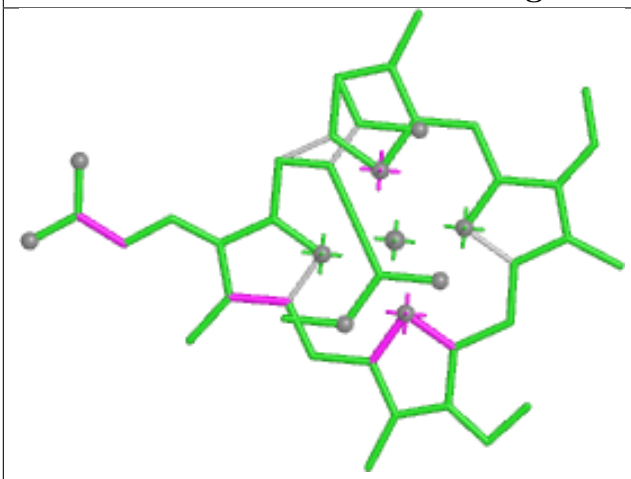


Torsions

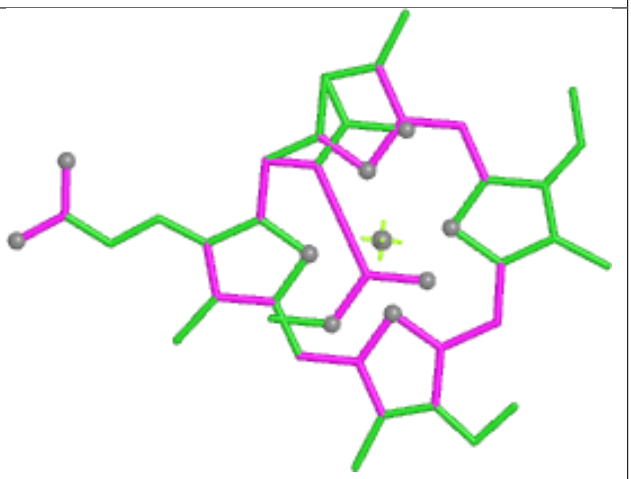


Rings

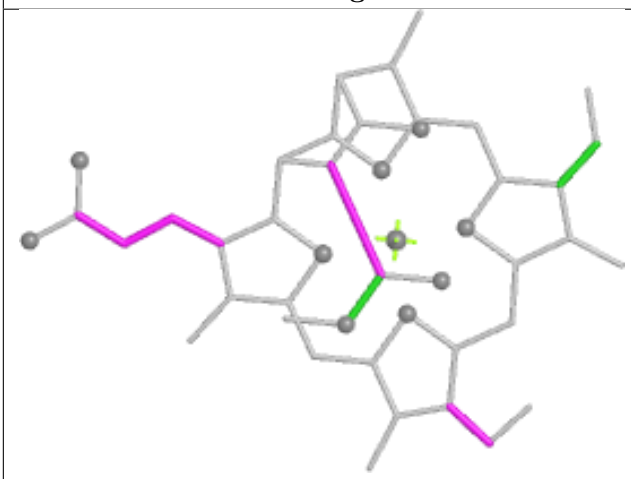
Ligand KC1 A 314



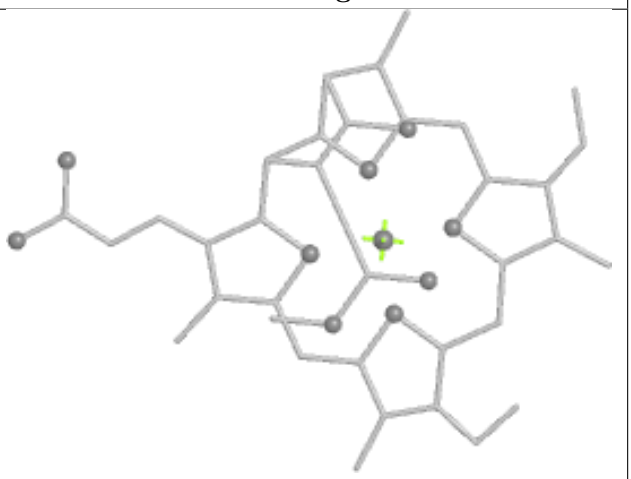
Bond lengths



Bond angles

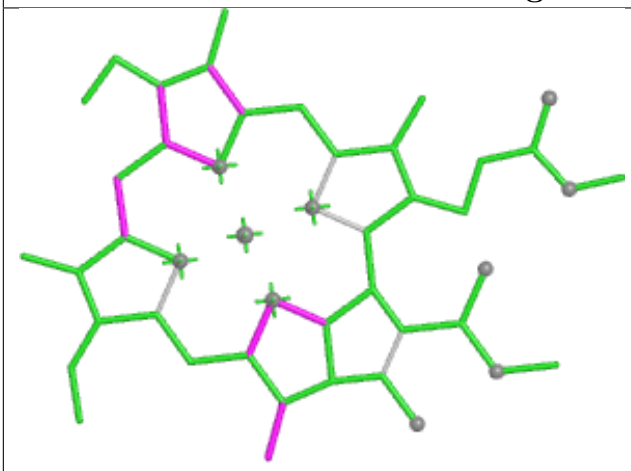


Torsions

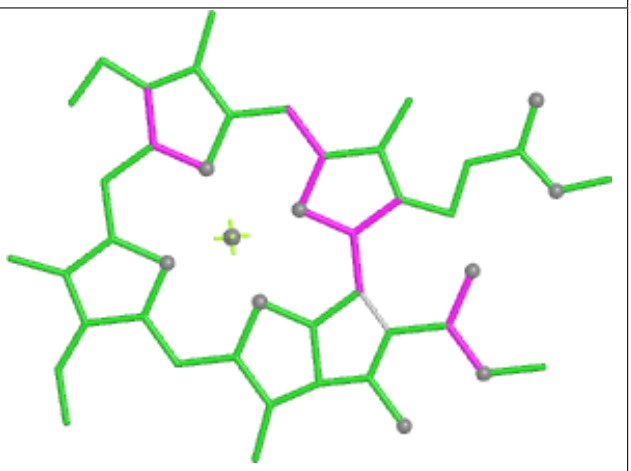


Rings

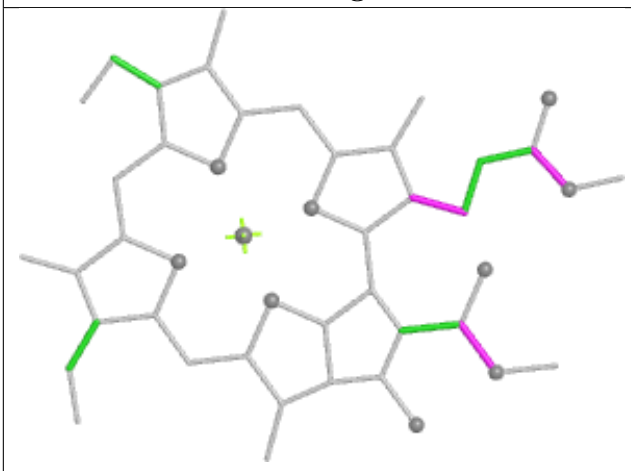
Ligand CLA F 313



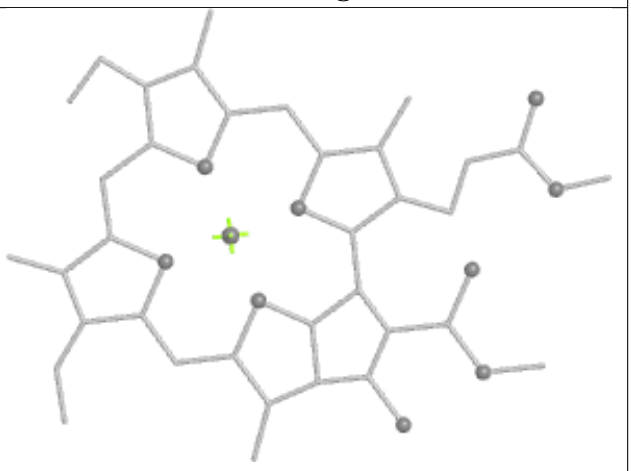
Bond lengths



Bond angles

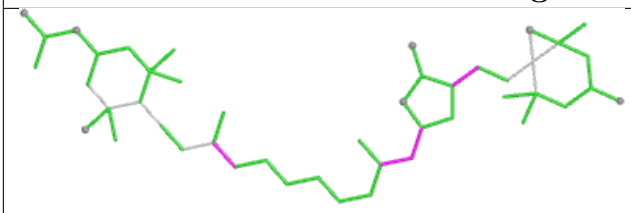


Torsions

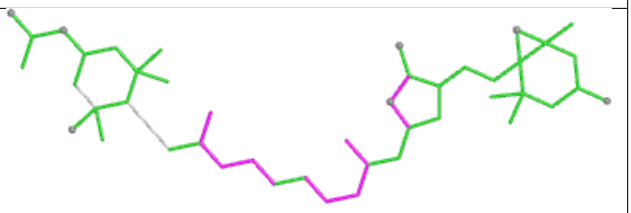


Rings

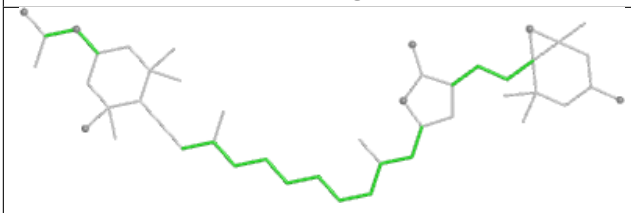
Ligand PID F 306



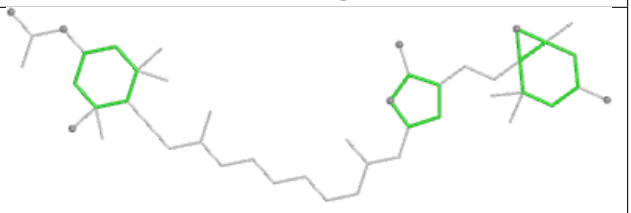
Bond lengths



Bond angles

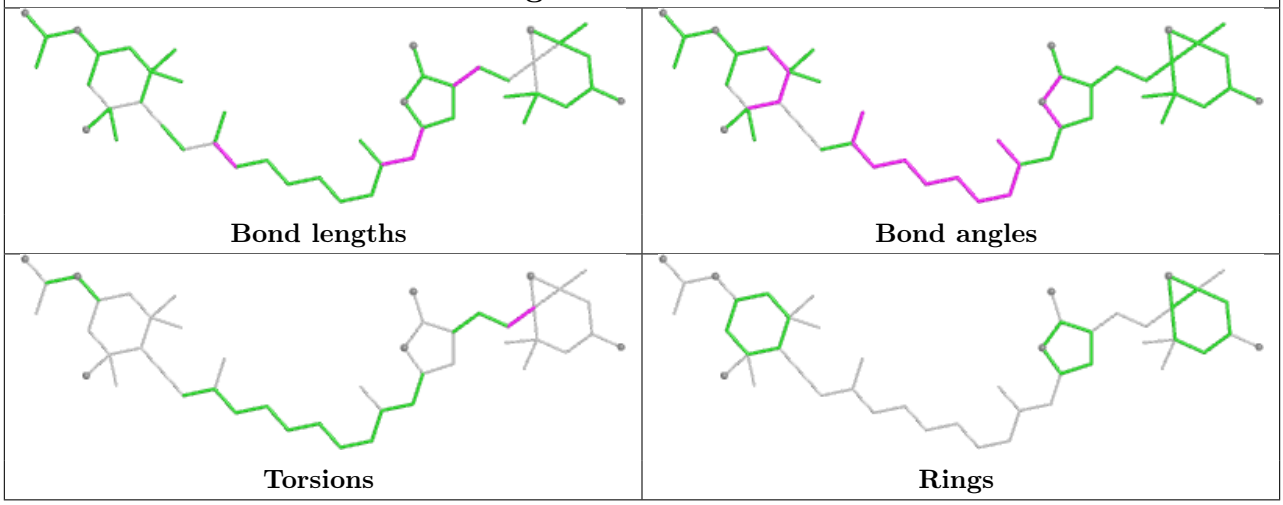


Torsions

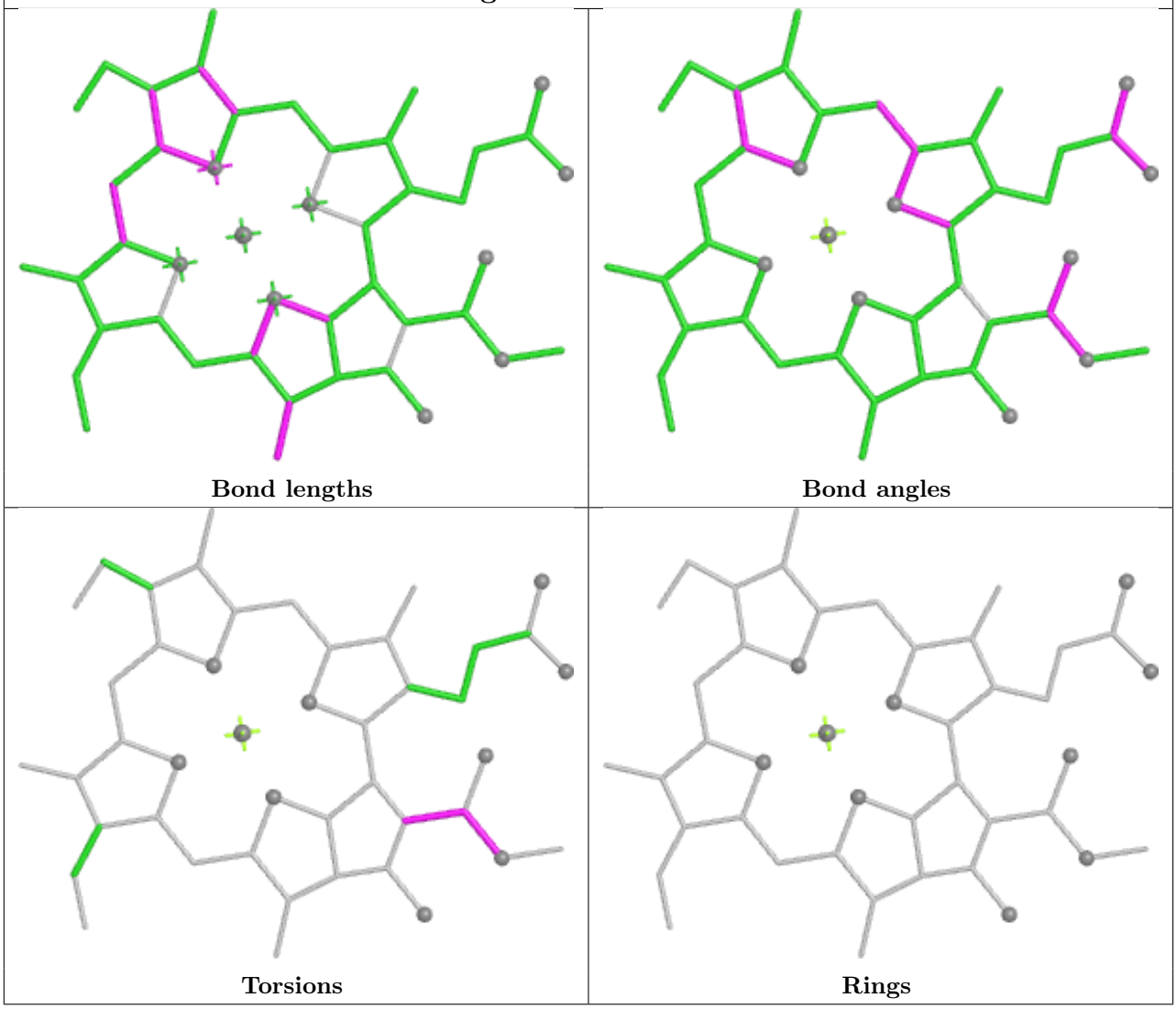


Rings

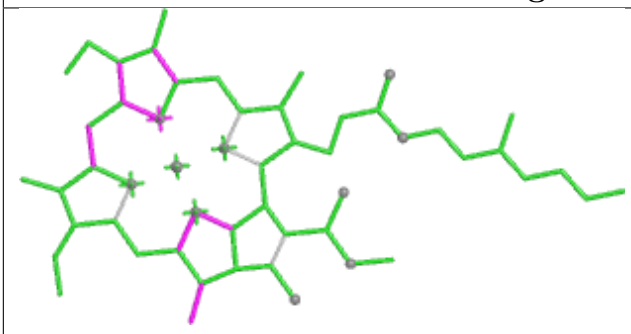
Ligand PID M 301



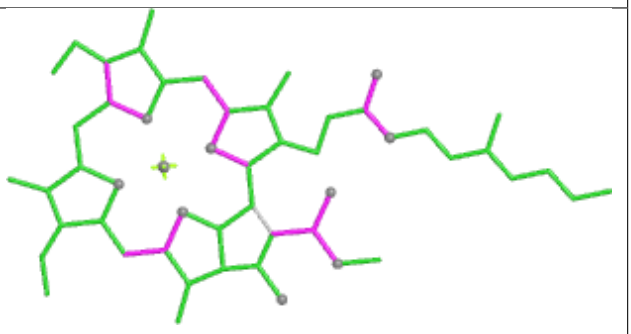
Ligand CLA D 313



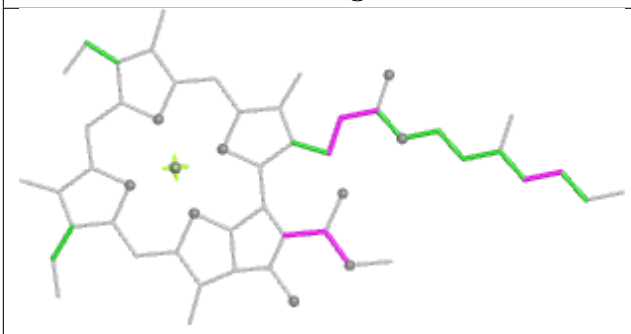
Ligand CLA J 312



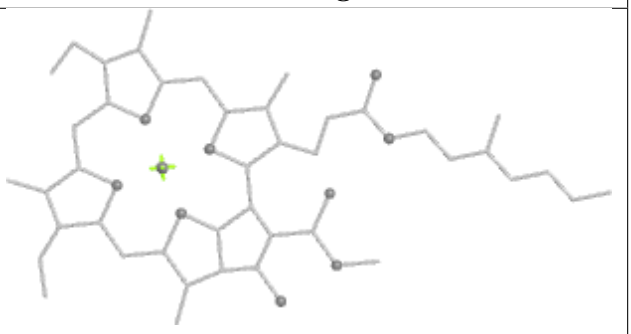
Bond lengths



Bond angles

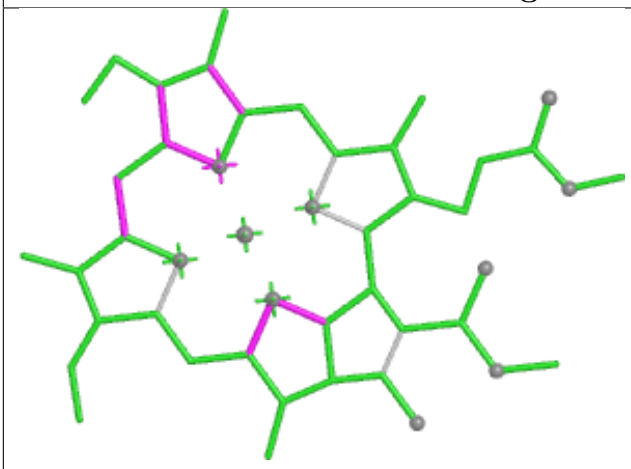


Torsions

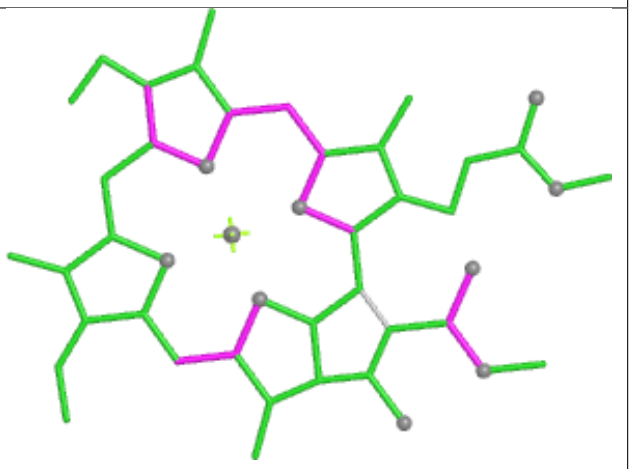


Rings

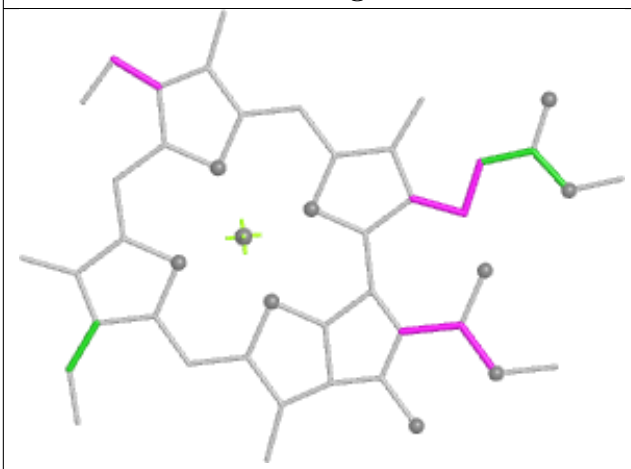
Ligand CLA M 318



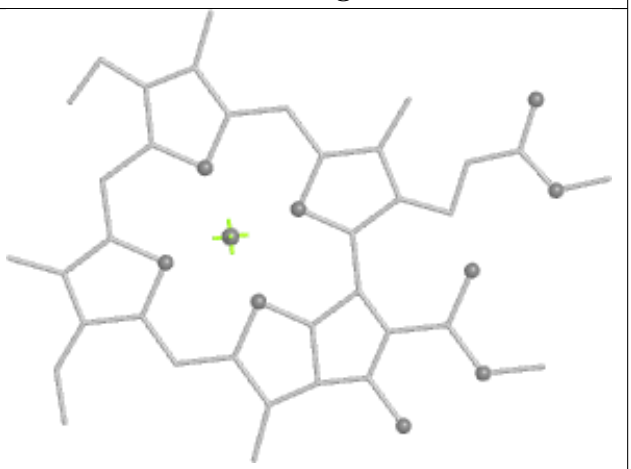
Bond lengths



Bond angles

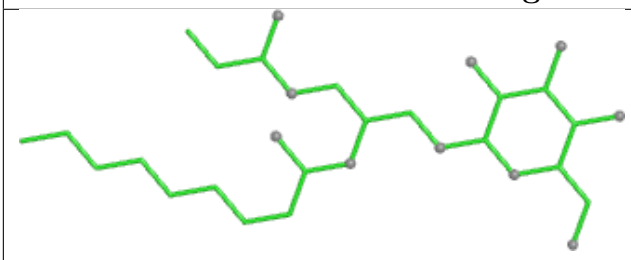


Torsions

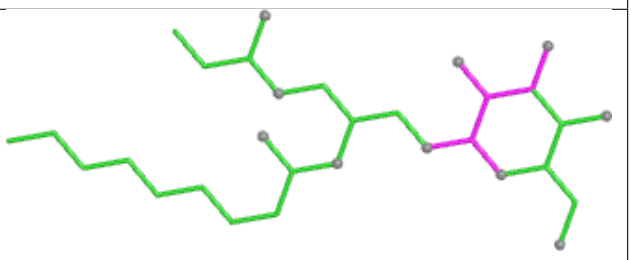


Rings

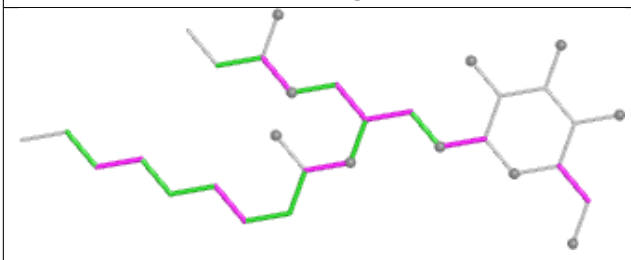
Ligand LMG b 734



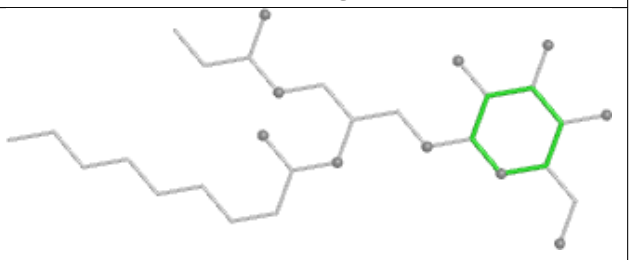
Bond lengths



Bond angles

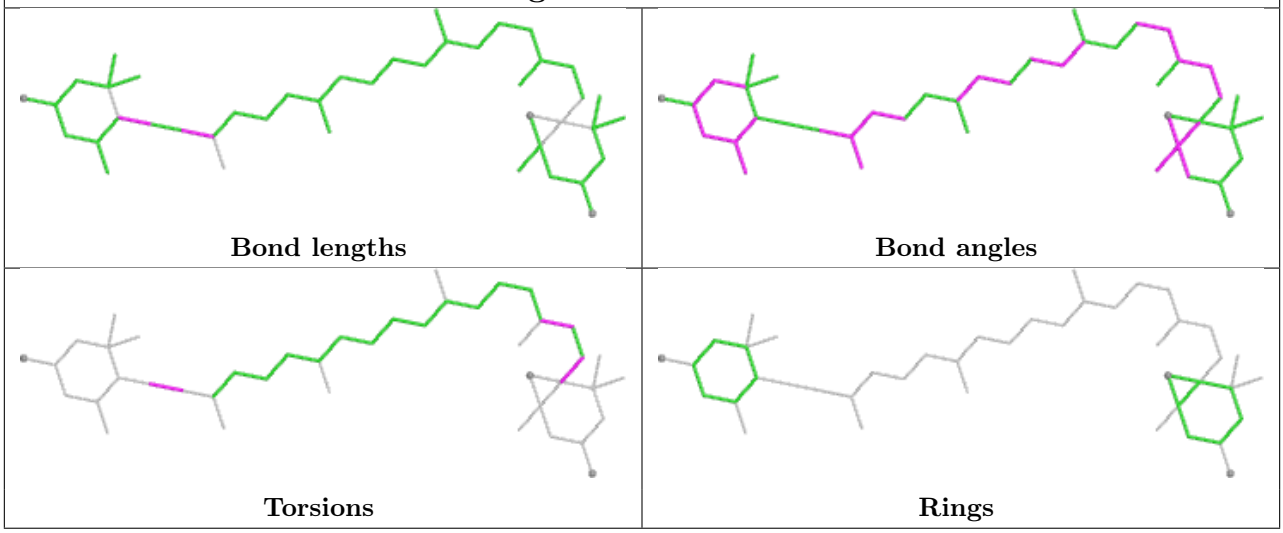


Torsions

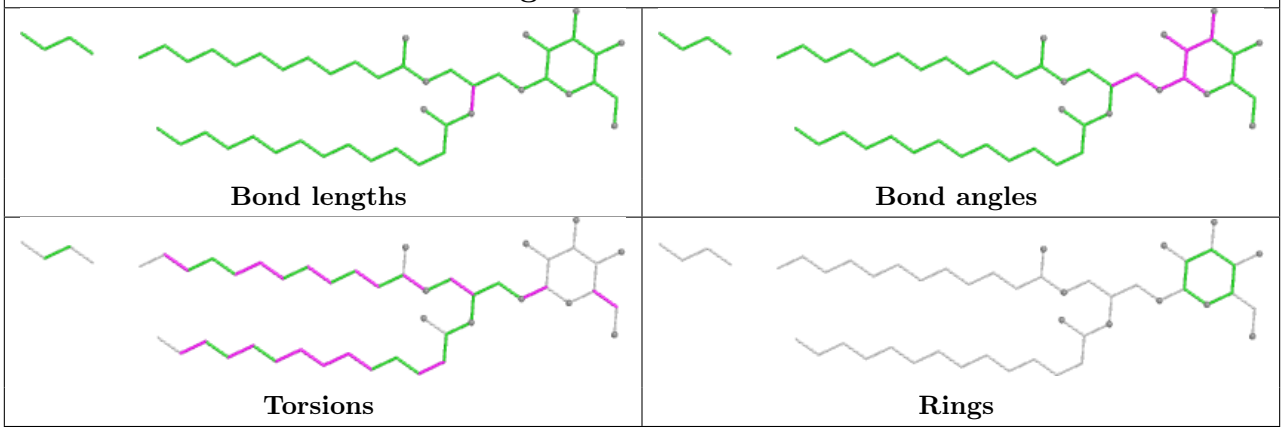


Rings

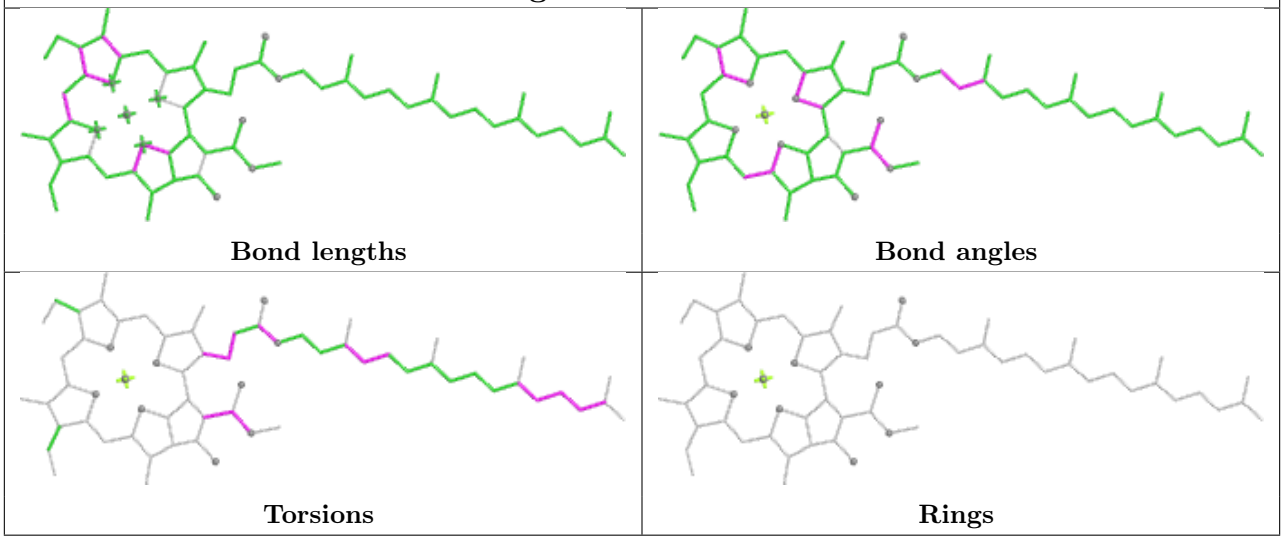
Ligand DD6 L 302



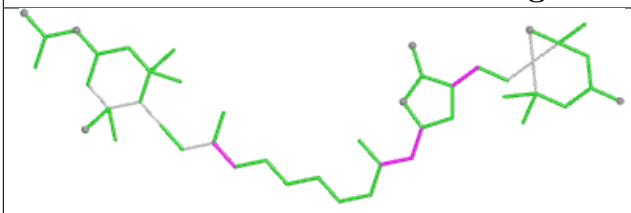
Ligand LMG D 317



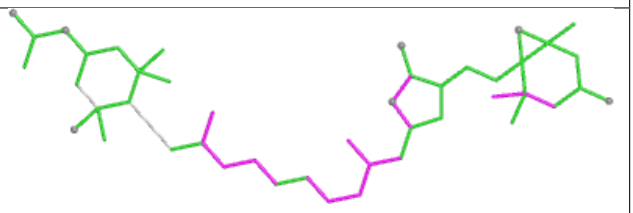
Ligand CLA a 735



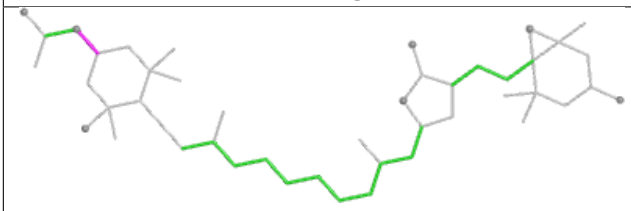
Ligand PID D 302



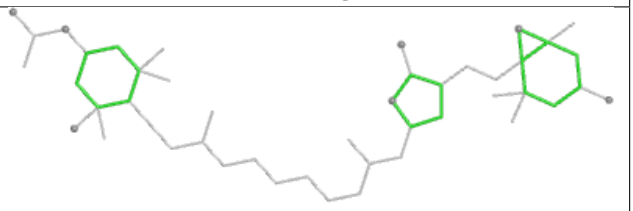
Bond lengths



Bond angles

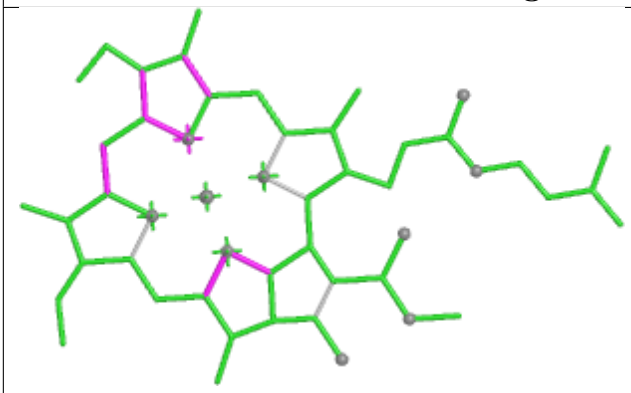


Torsions

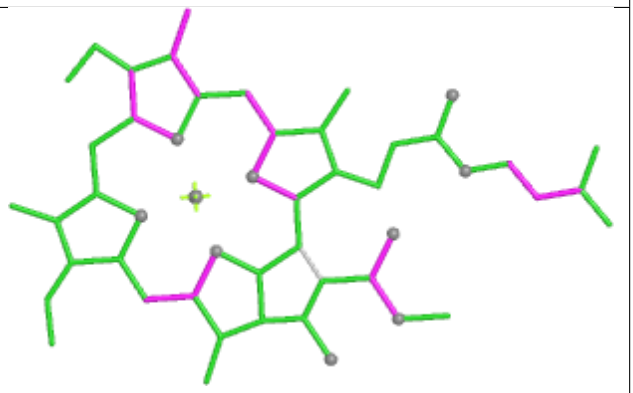


Rings

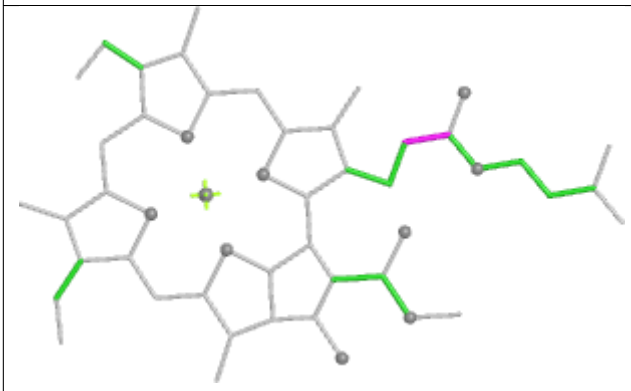
Ligand CLA K 309



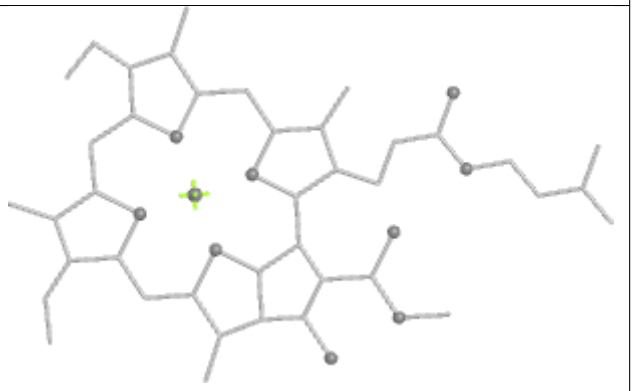
Bond lengths



Bond angles

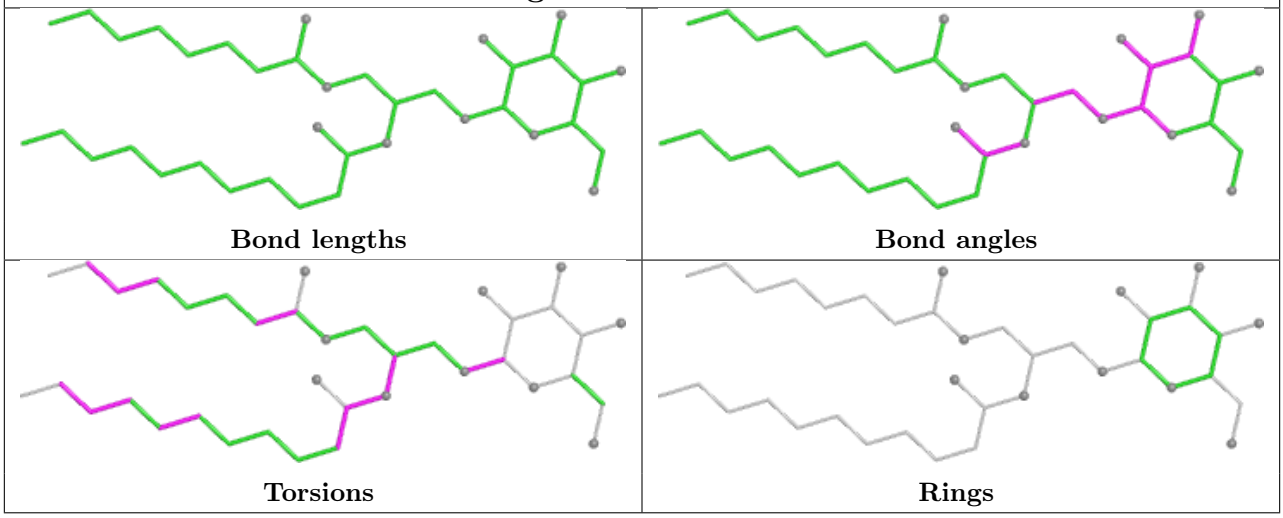


Torsions

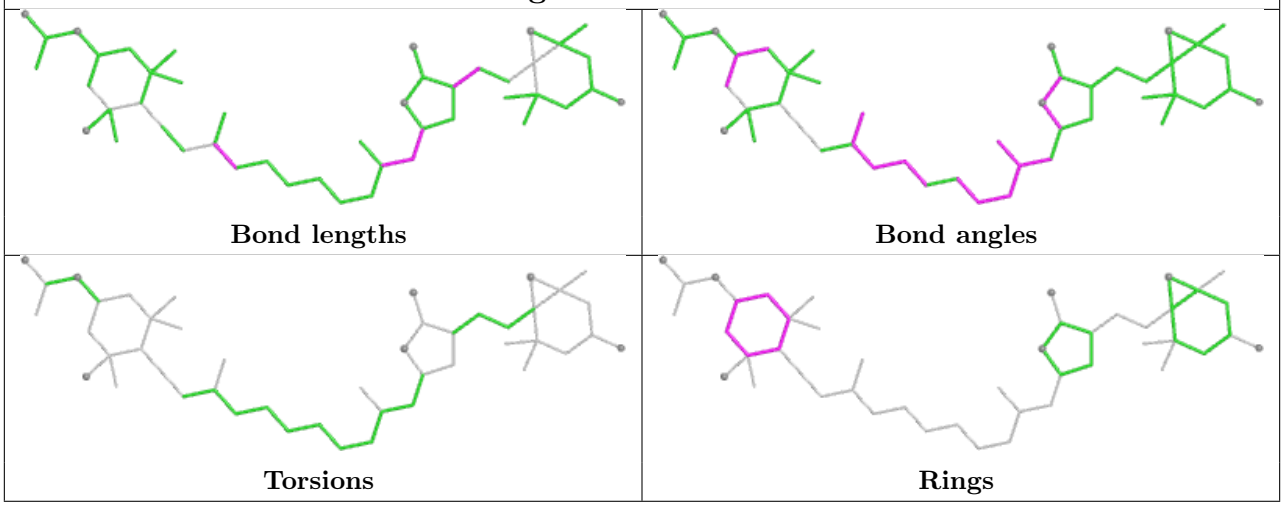


Rings

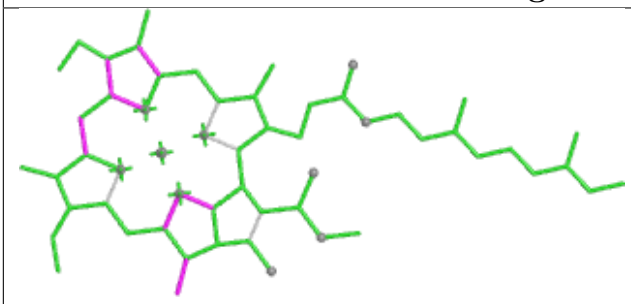
Ligand LMG I 320



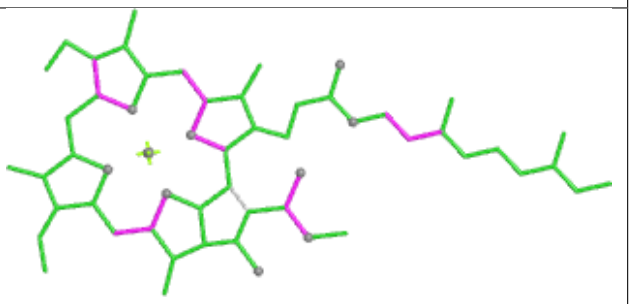
Ligand PID G 507



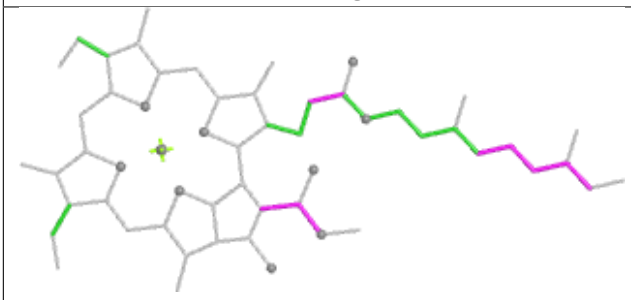
Ligand CLA a 729



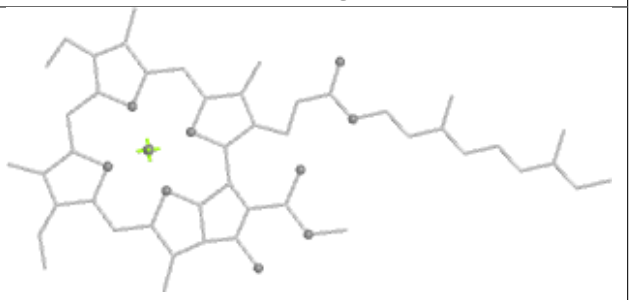
Bond lengths



Bond angles

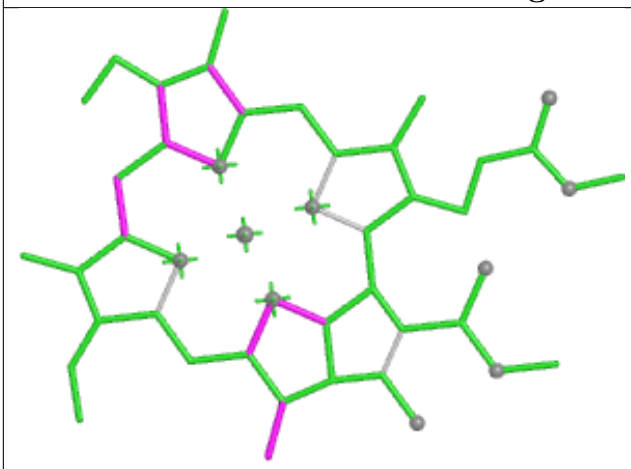


Torsions

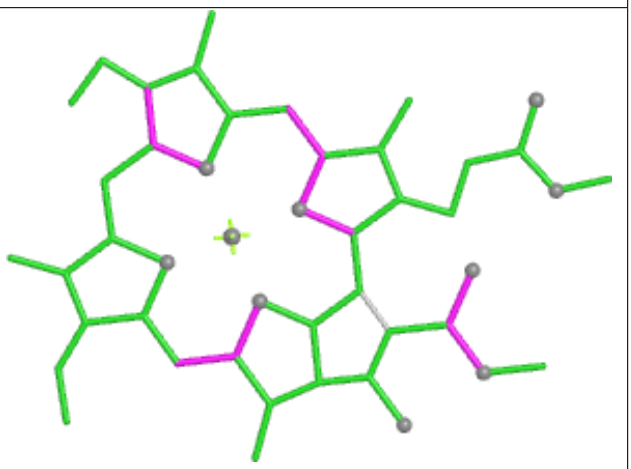


Rings

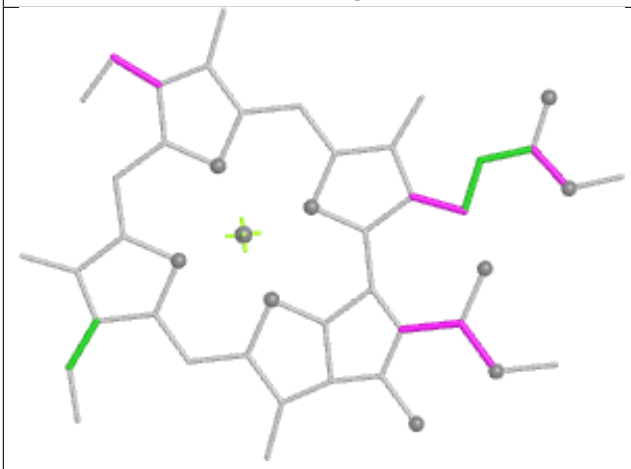
Ligand CLA a 727



Bond lengths



Bond angles

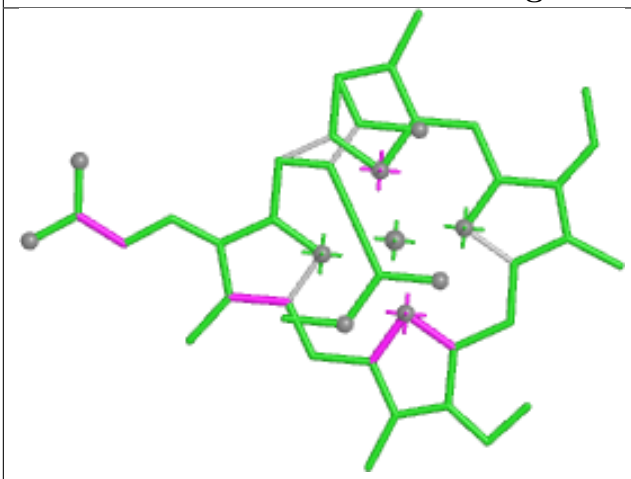


Torsions

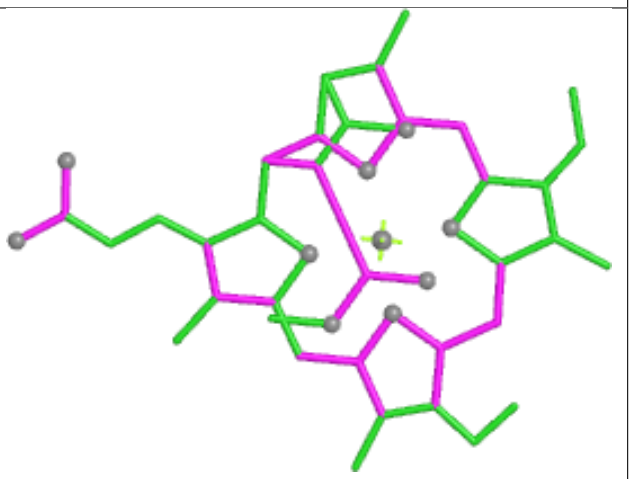


Rings

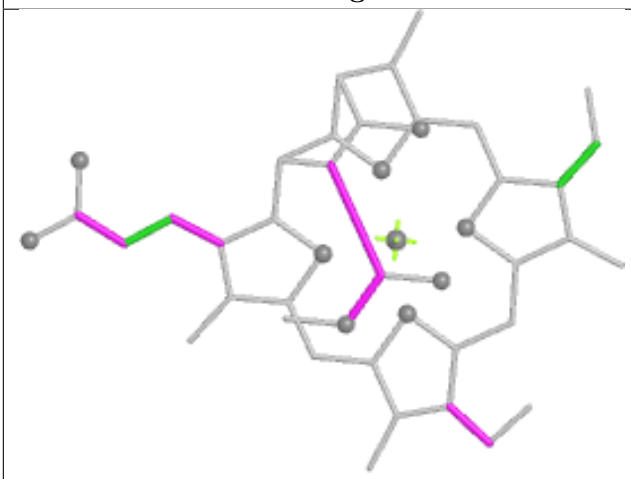
Ligand KC1 O 310



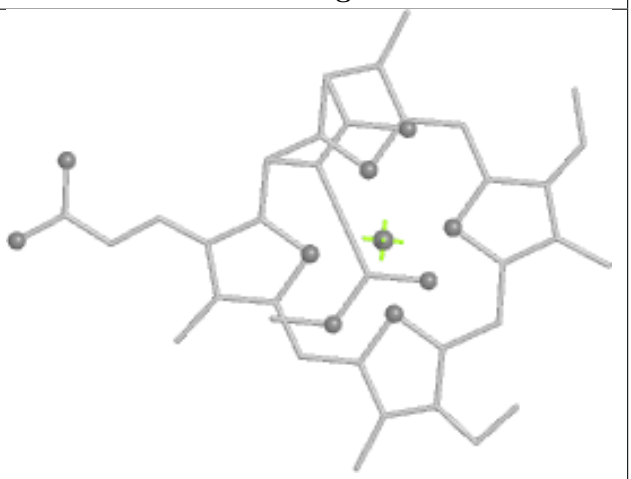
Bond lengths



Bond angles

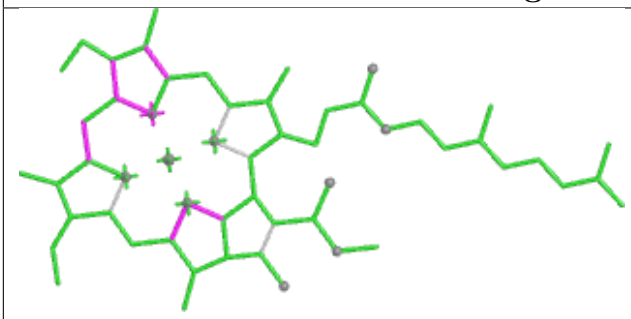


Torsions

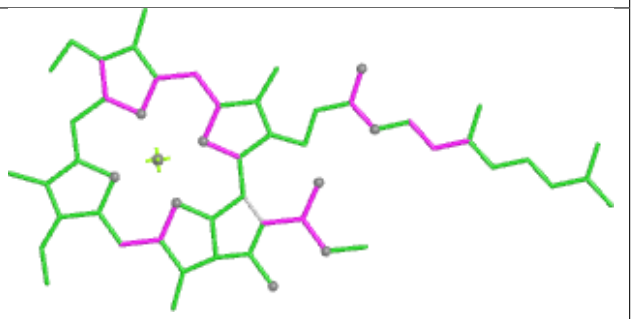


Rings

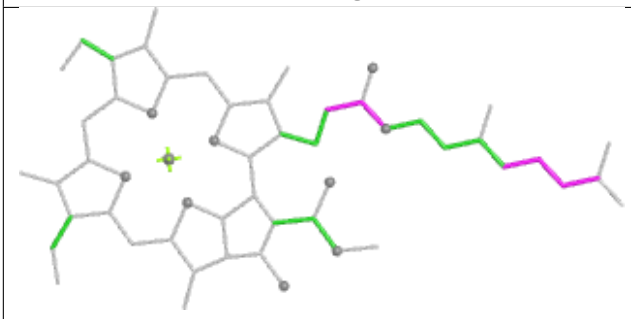
Ligand CLA B 310



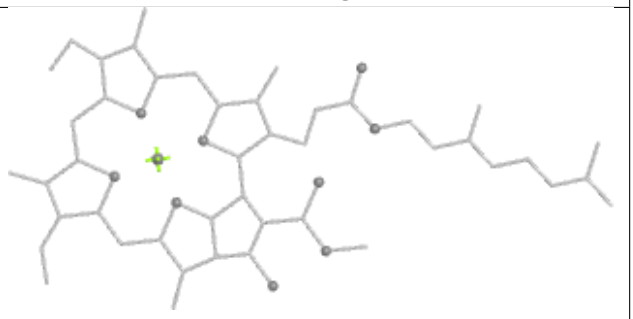
Bond lengths



Bond angles

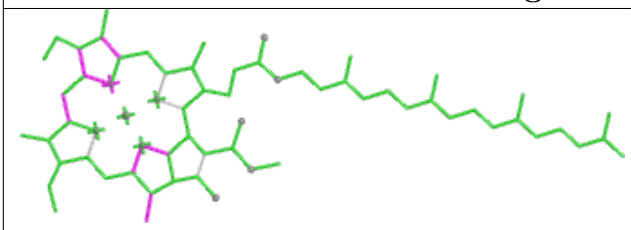


Torsions

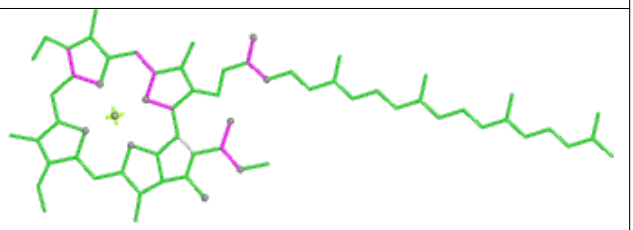


Rings

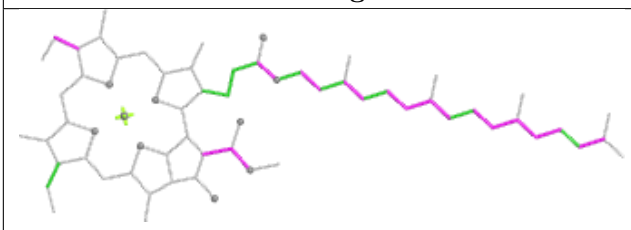
Ligand CLA B 311



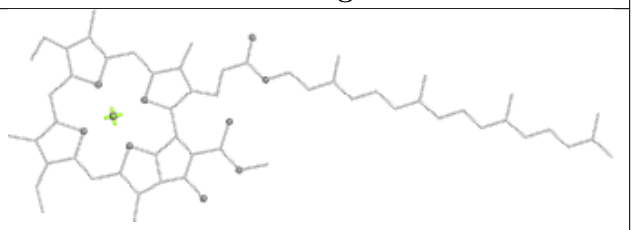
Bond lengths



Bond angles

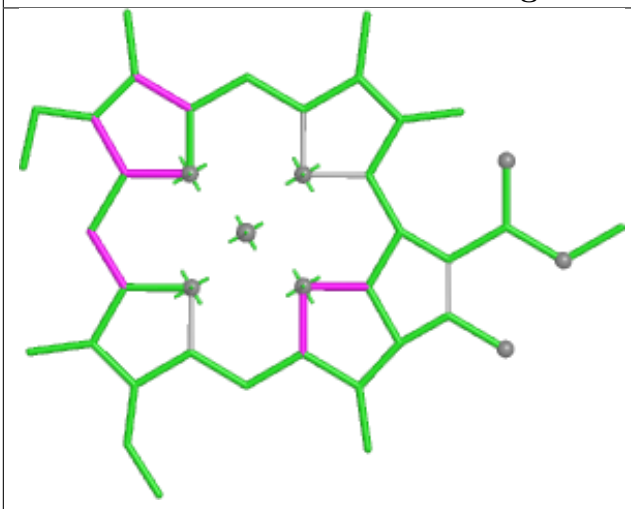


Torsions

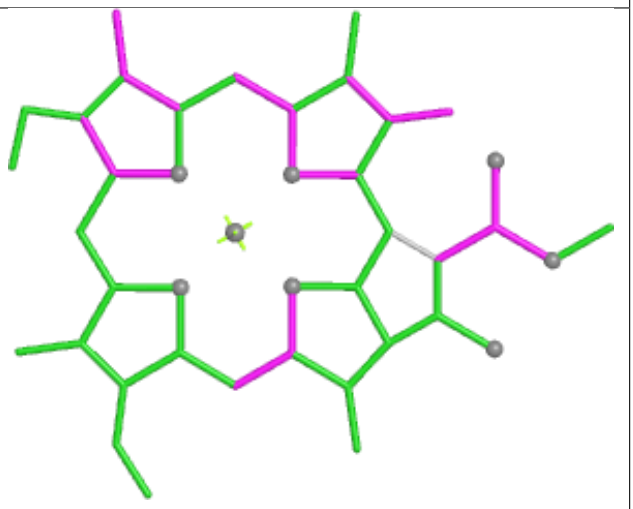


Rings

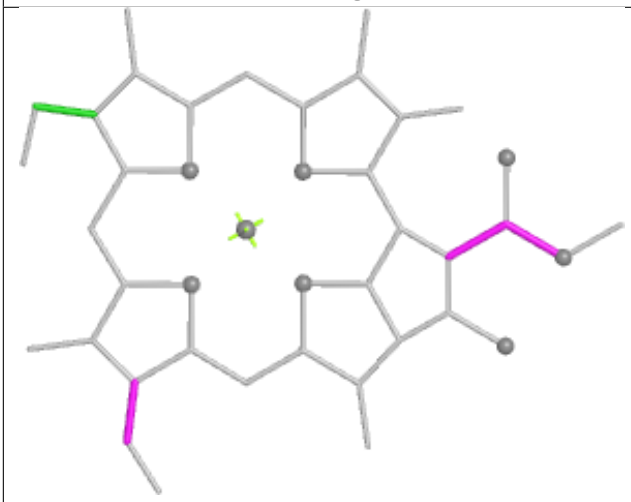
Ligand CLA M 315



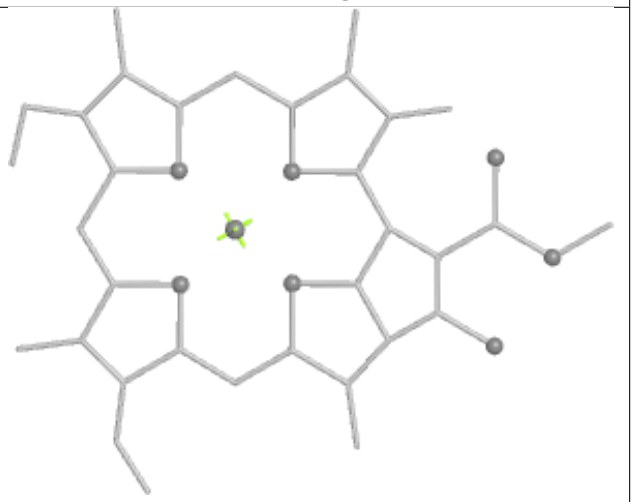
Bond lengths



Bond angles



Torsions

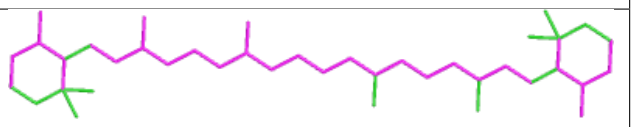


Rings

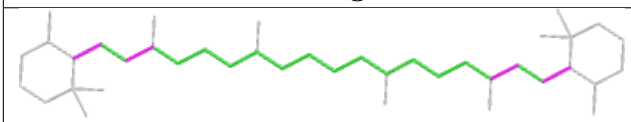
Ligand BCR i 201



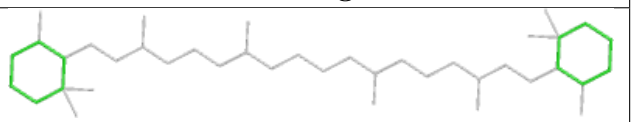
Bond lengths



Bond angles

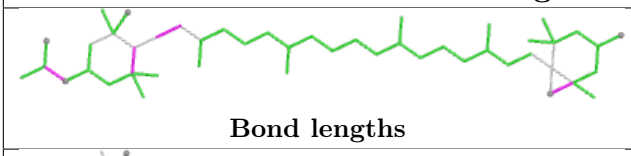


Torsions

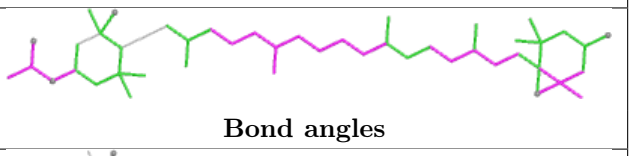


Rings

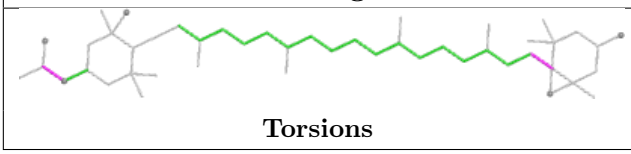
Ligand UIX I 304



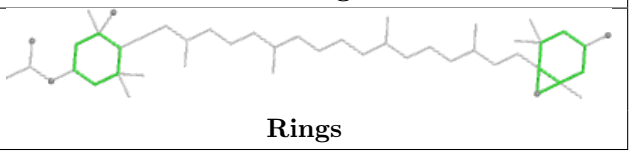
Bond lengths



Bond angles

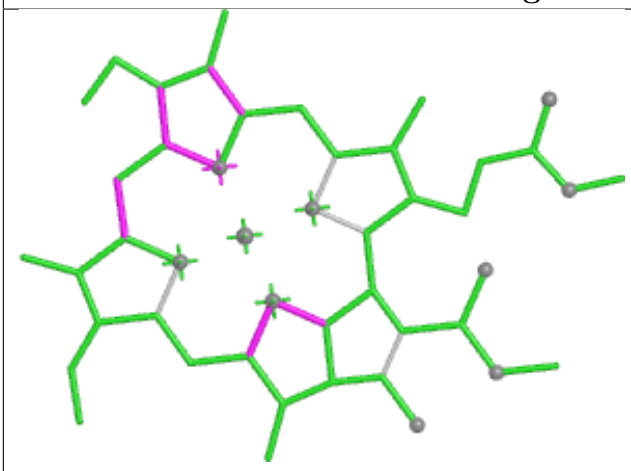


Torsions

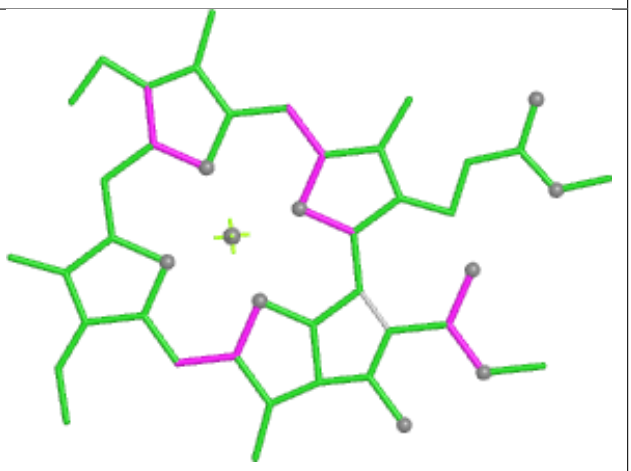


Rings

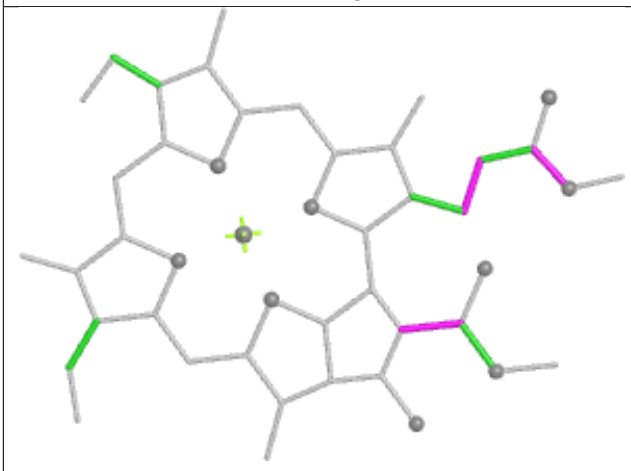
Ligand CLA G 517



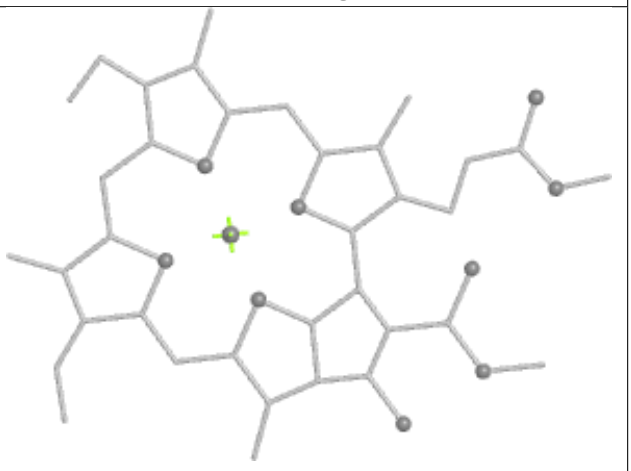
Bond lengths



Bond angles

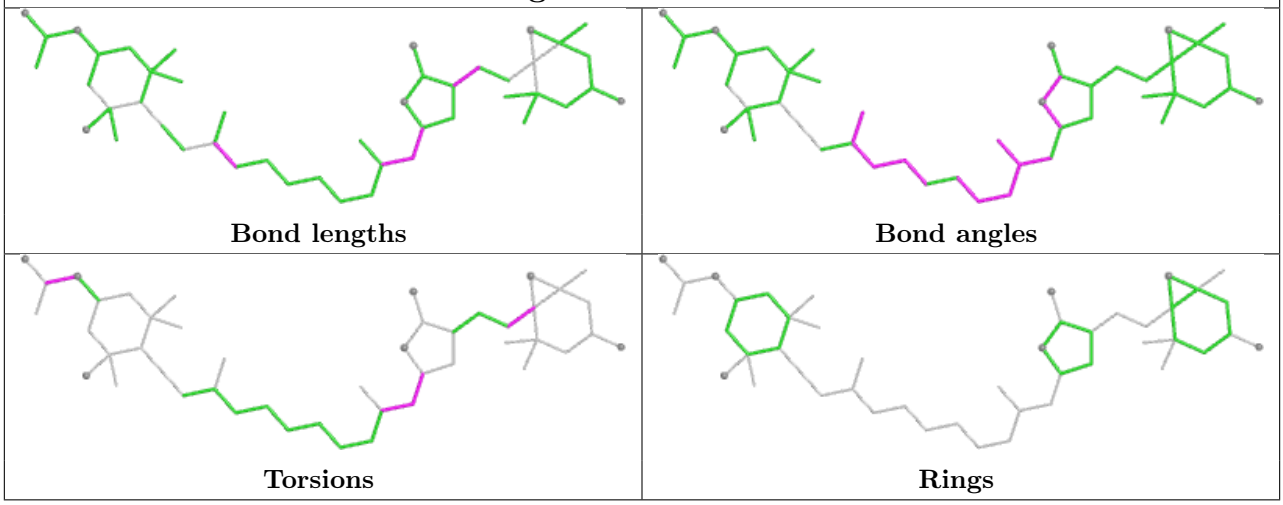


Torsions

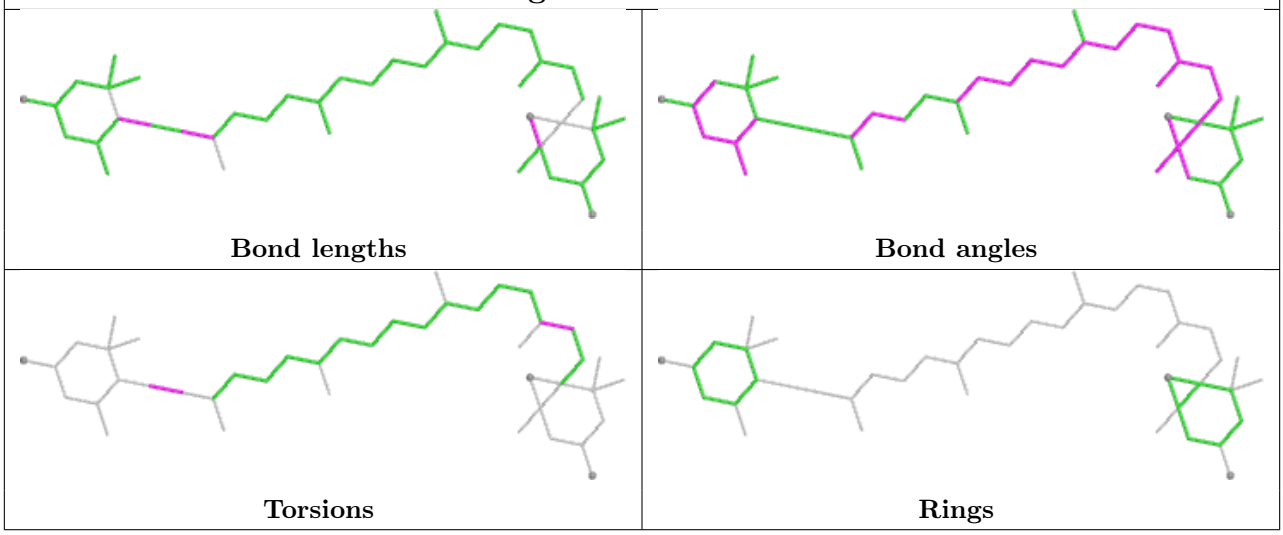


Rings

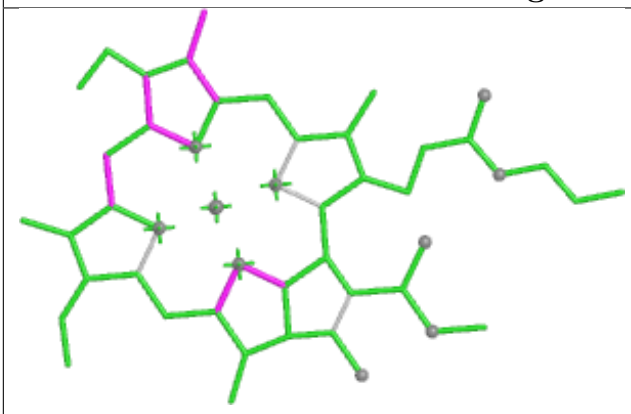
Ligand PID N 301



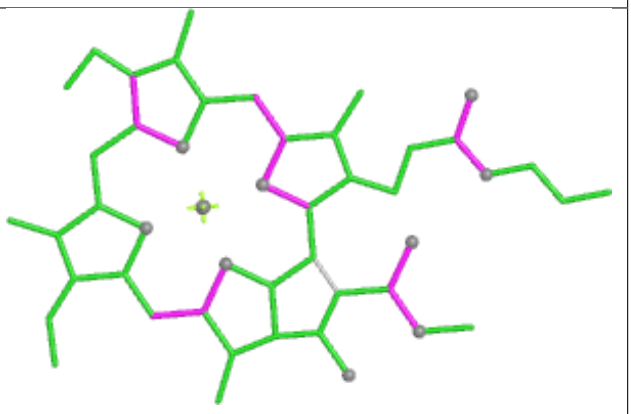
Ligand DD6 L 306



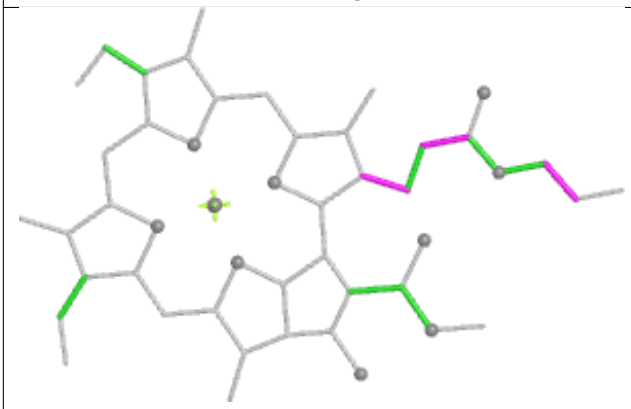
Ligand CLA b 706



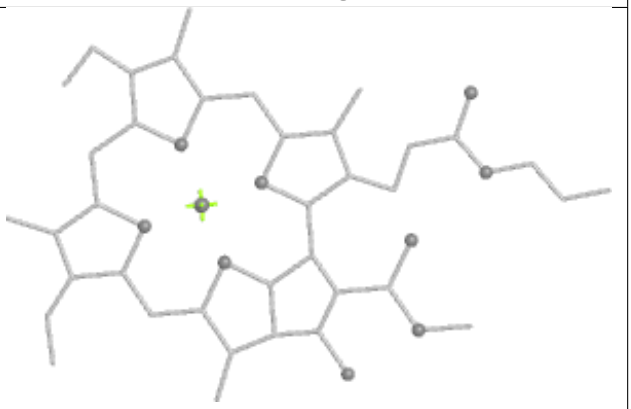
Bond lengths



Bond angles

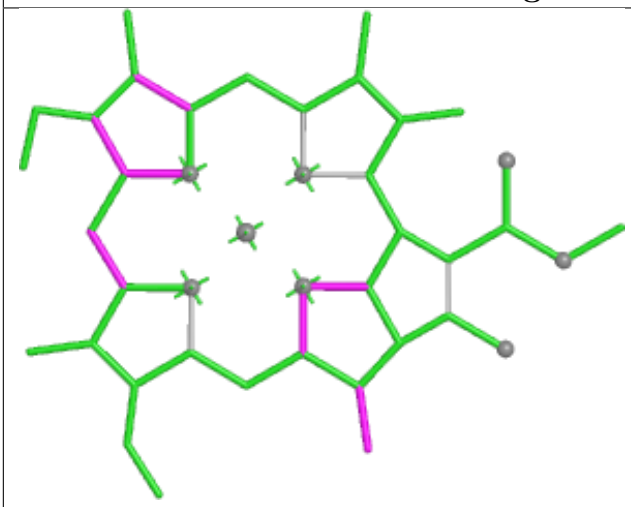


Torsions

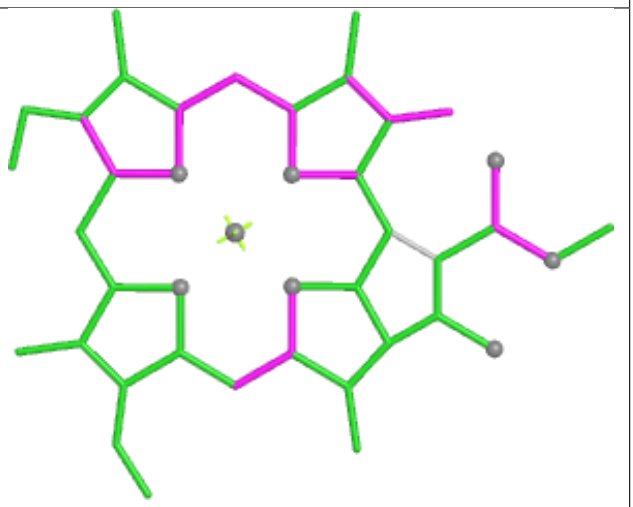


Rings

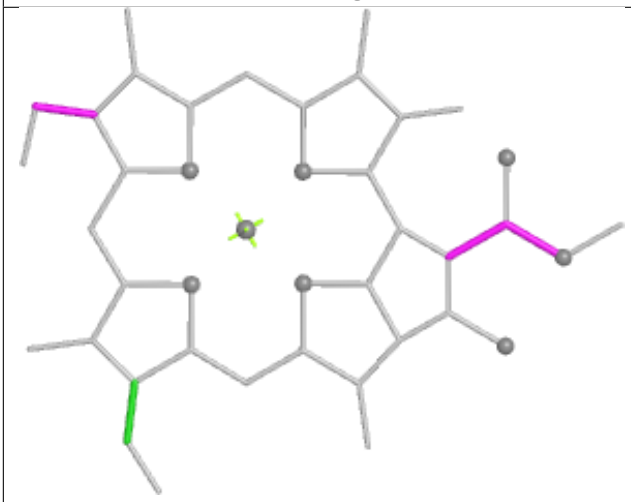
Ligand CLA H 311



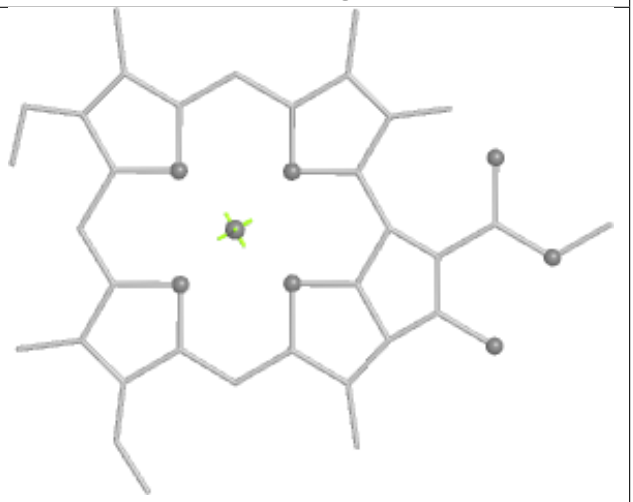
Bond lengths



Bond angles

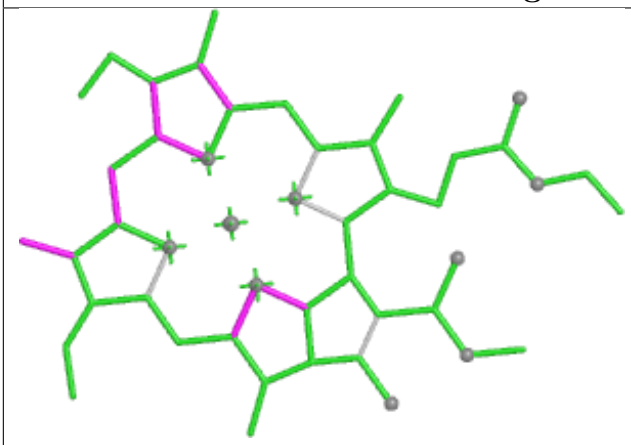


Torsions

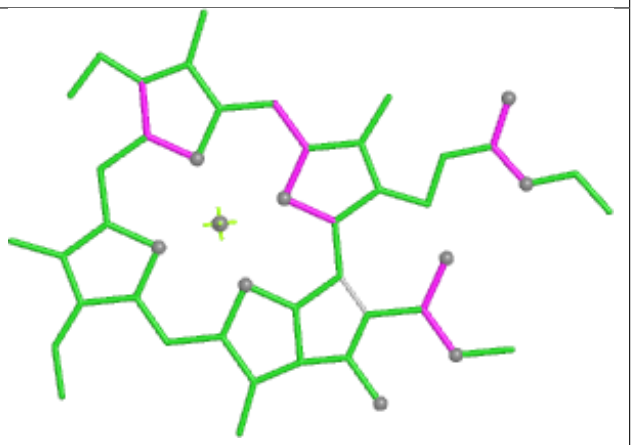


Rings

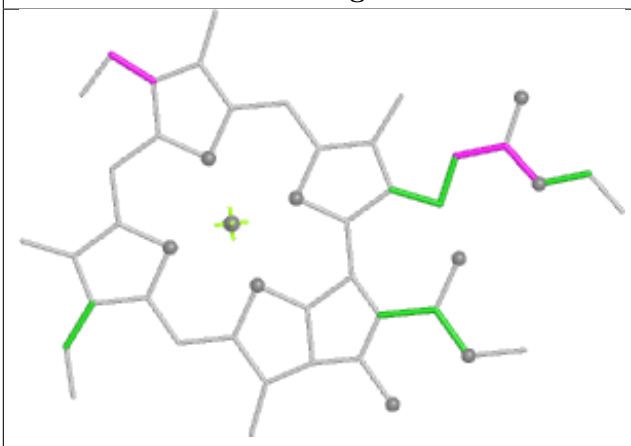
Ligand CLA A 316



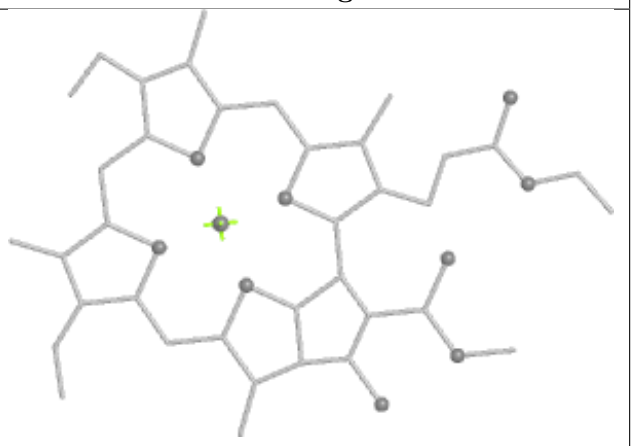
Bond lengths



Bond angles

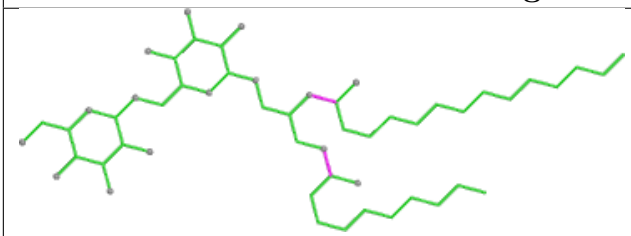


Torsions

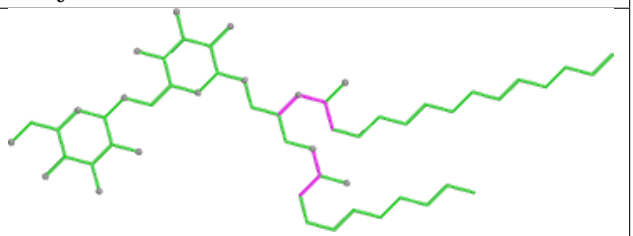


Rings

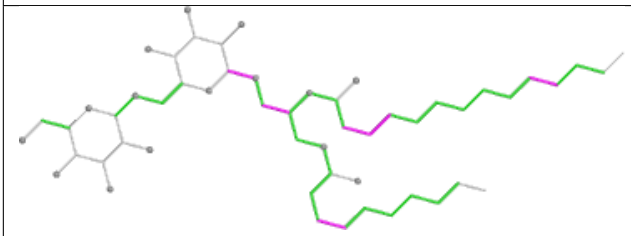
Ligand DGD y 201



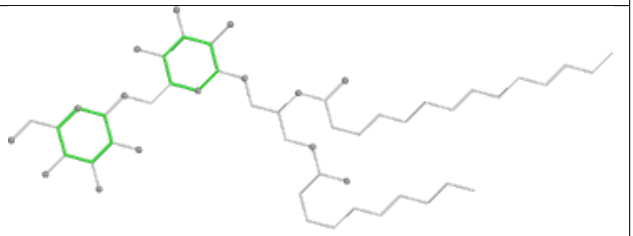
Bond lengths



Bond angles

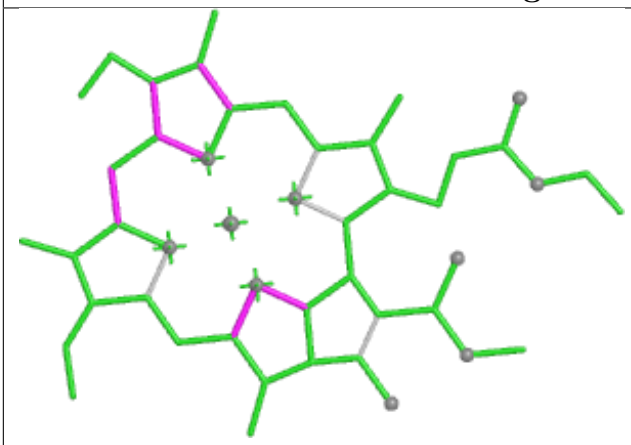


Torsions

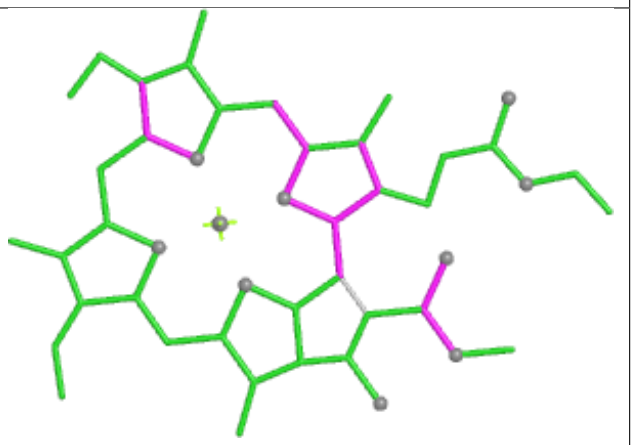


Rings

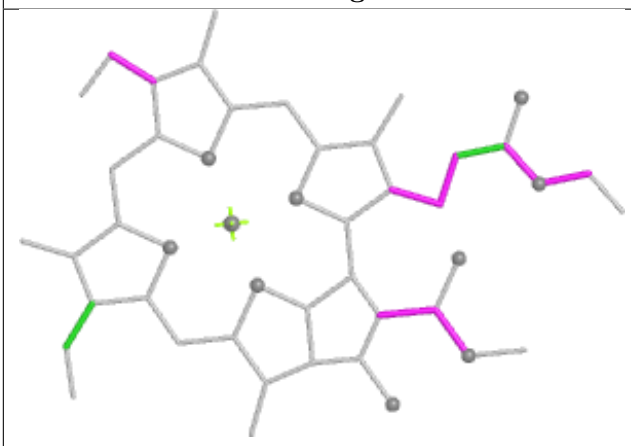
Ligand CLA N 310



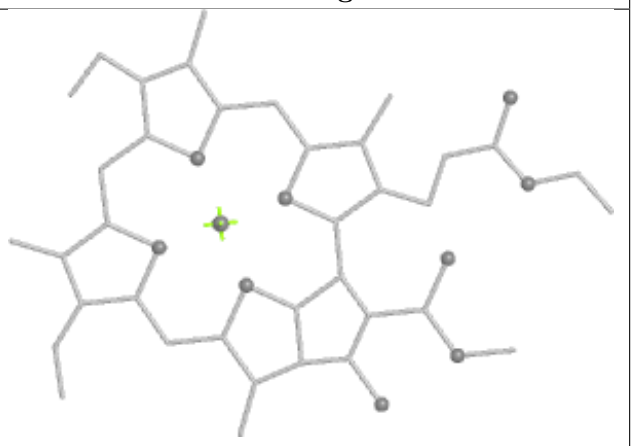
Bond lengths



Bond angles

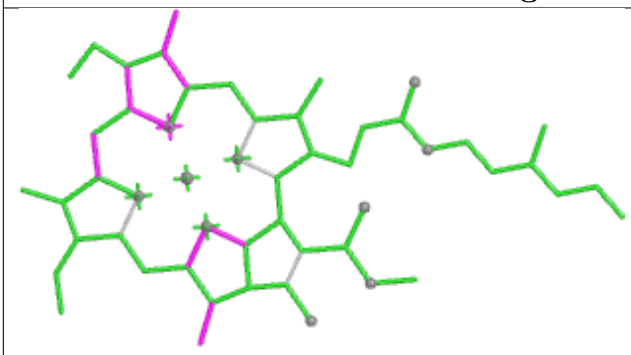


Torsions

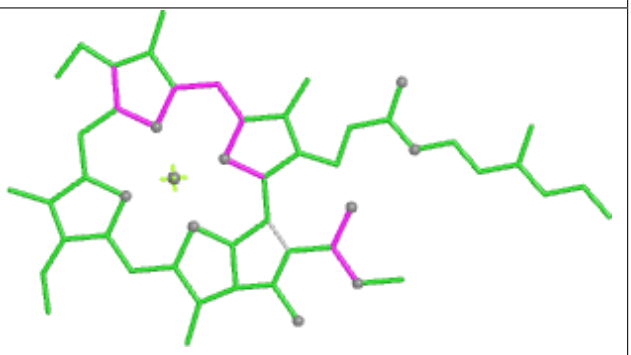


Rings

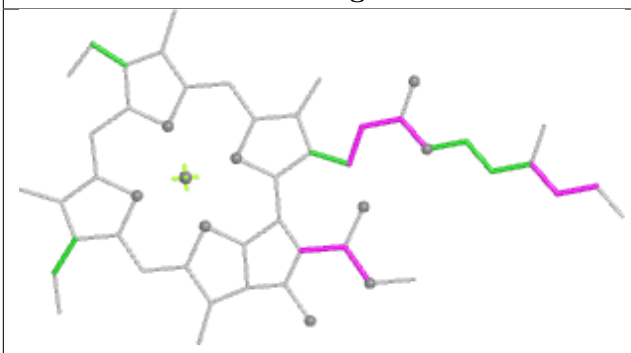
Ligand CLA M 316



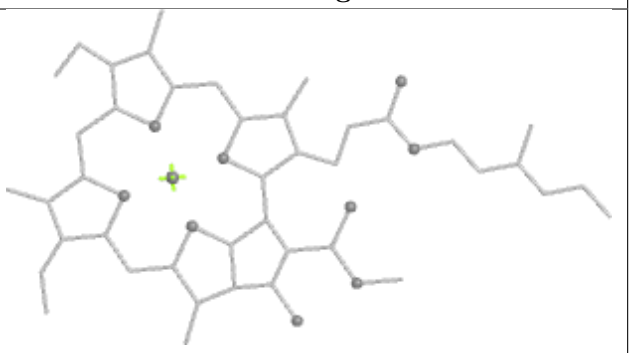
Bond lengths



Bond angles

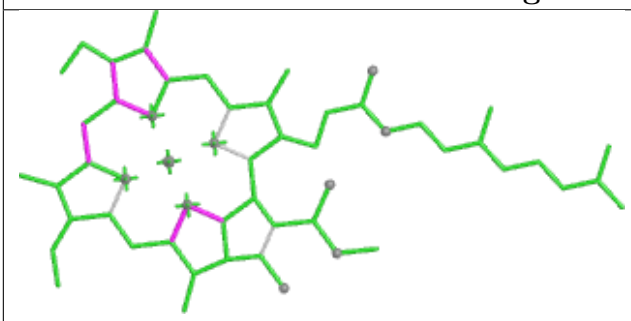


Torsions

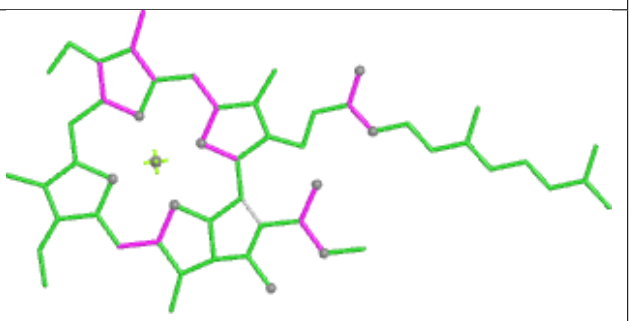


Rings

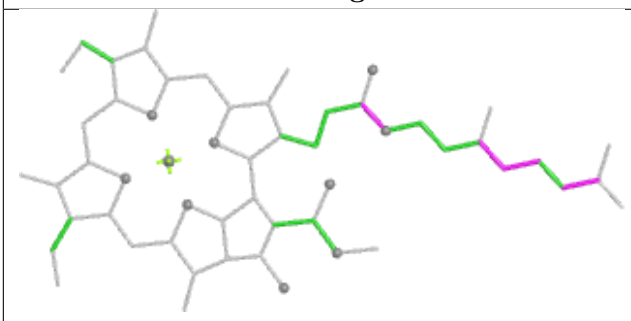
Ligand CLA K 313



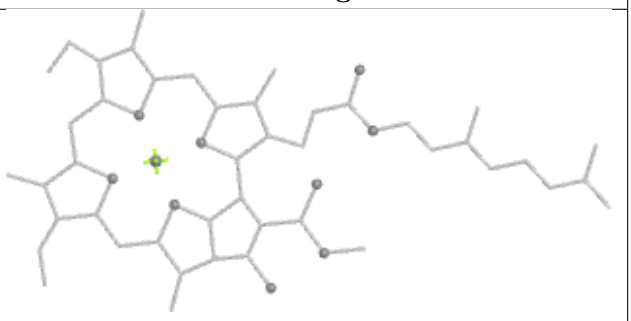
Bond lengths



Bond angles

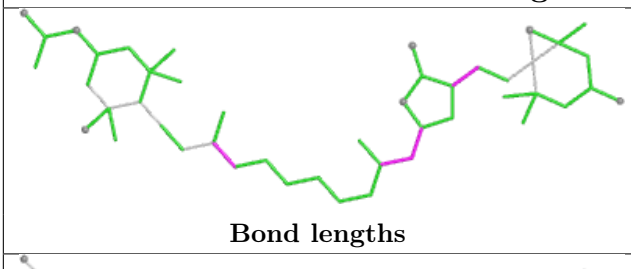


Torsions

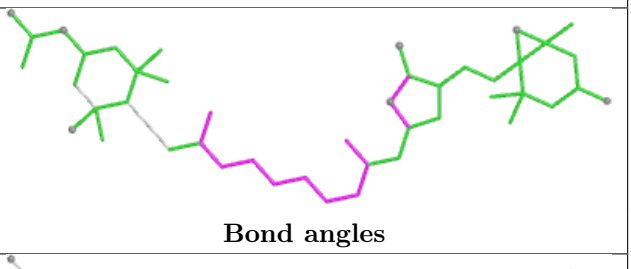


Rings

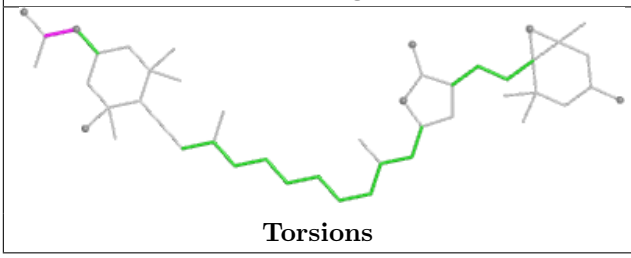
Ligand PID F 302



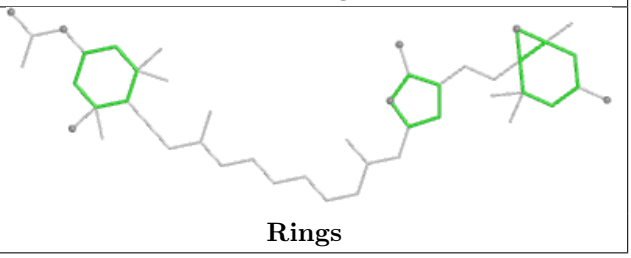
Bond lengths



Bond angles

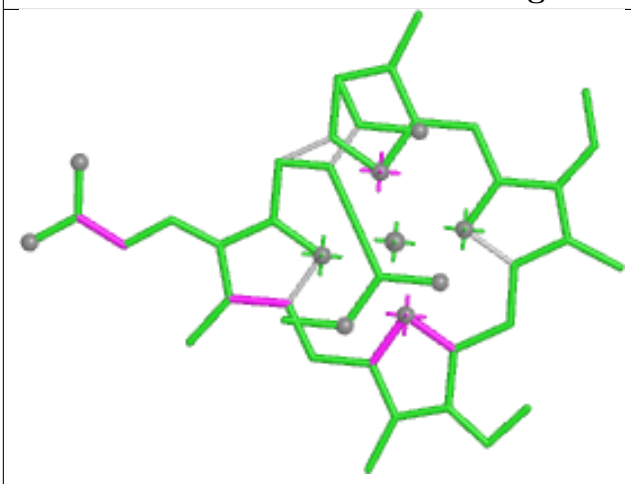


Torsions

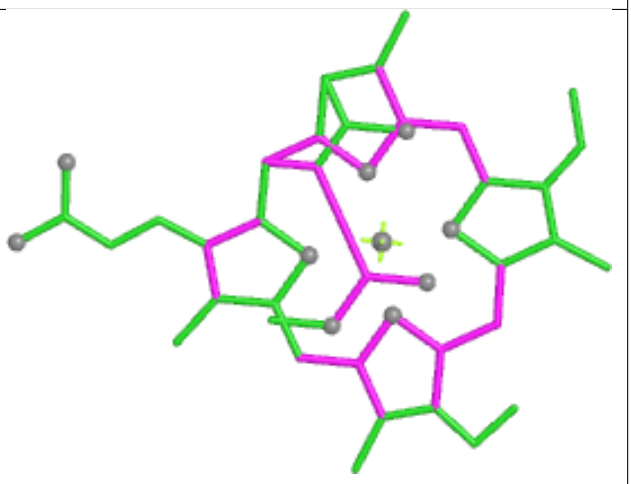


Rings

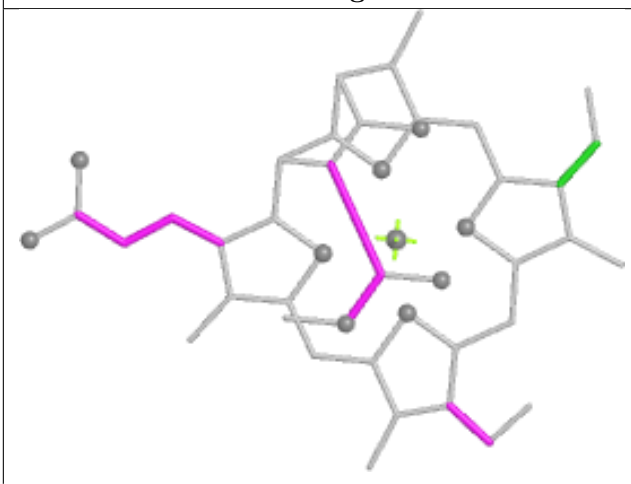
Ligand KC1 F 314



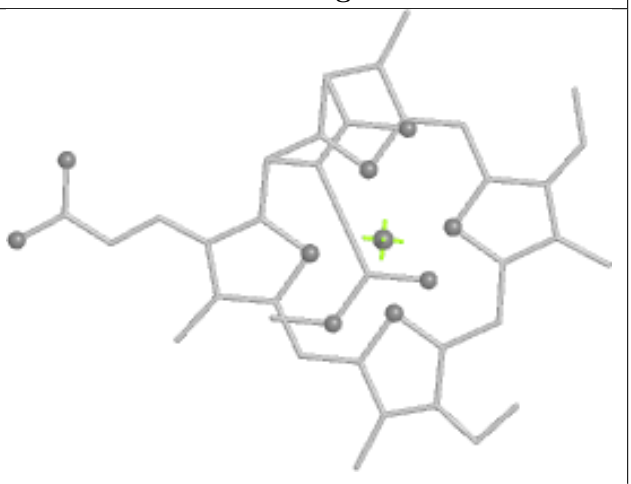
Bond lengths



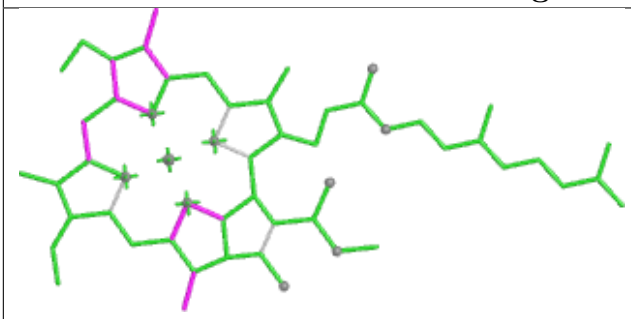
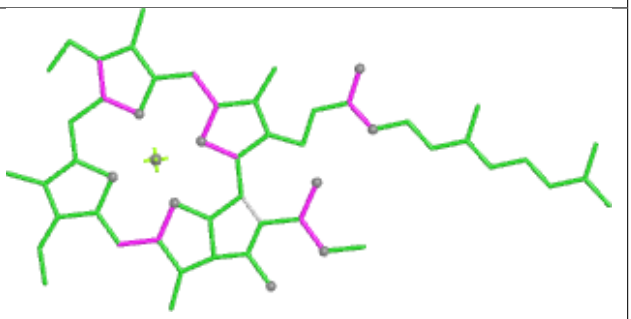
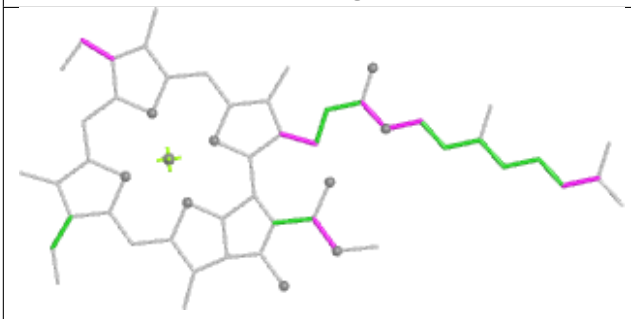
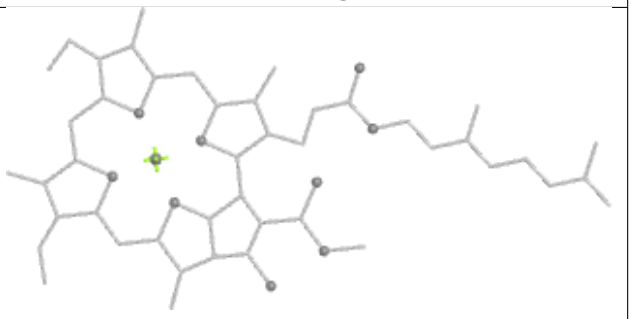
Bond angles

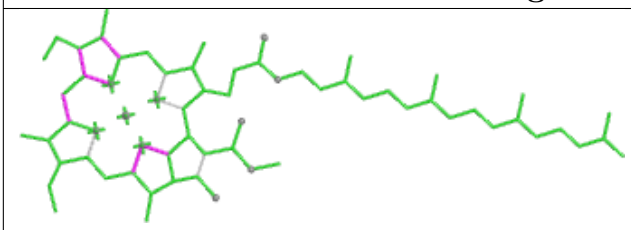
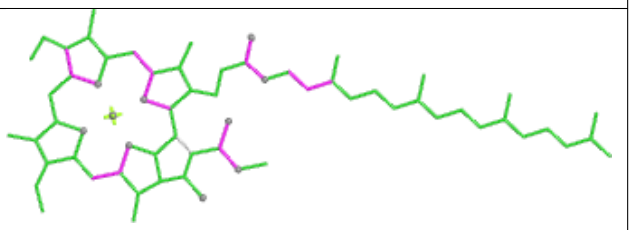
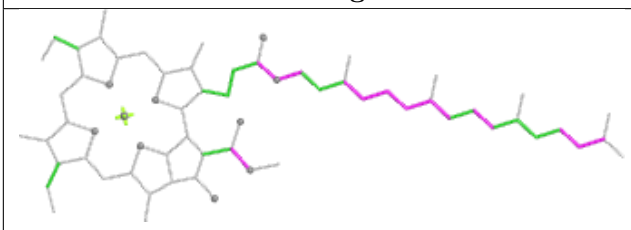
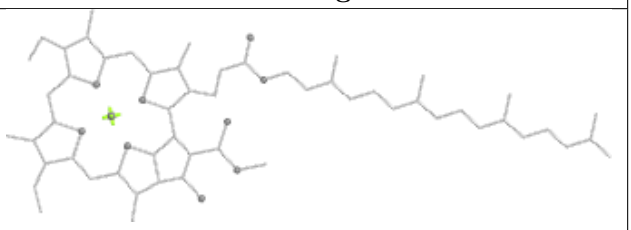


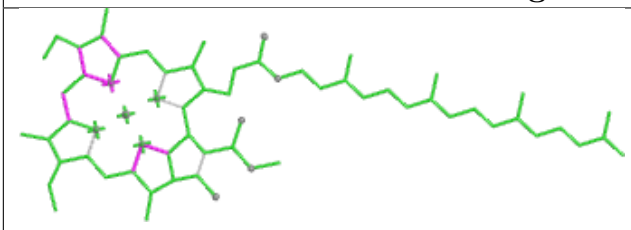
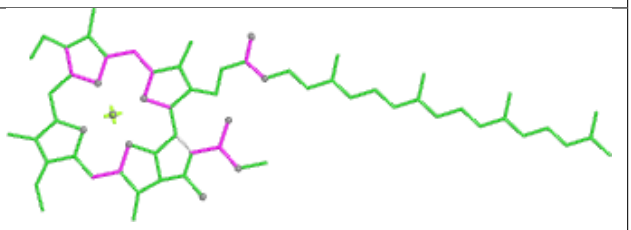
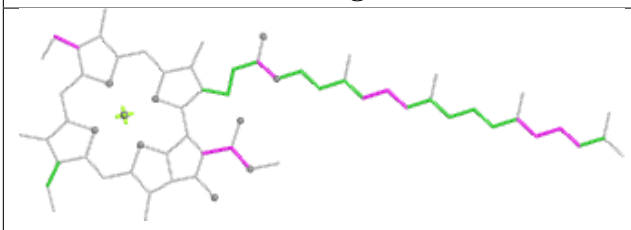
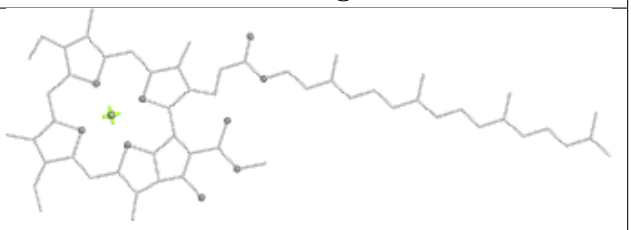
Torsions

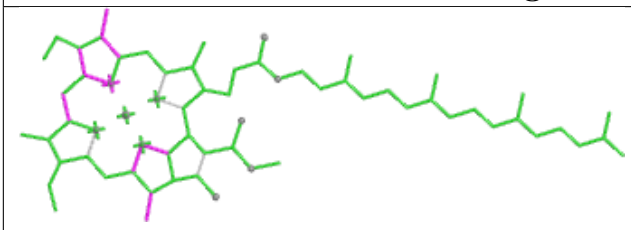
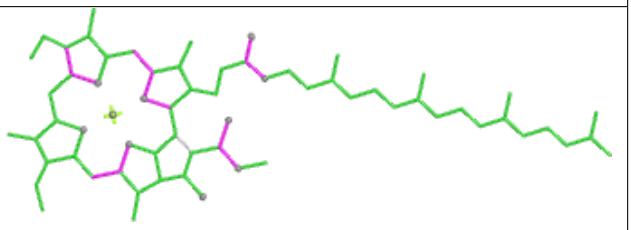
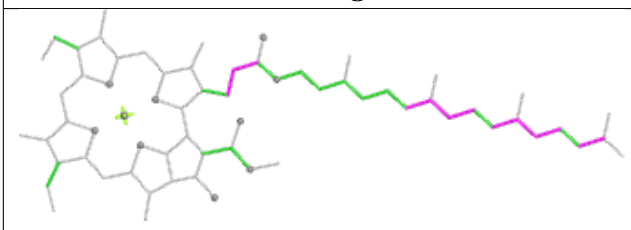
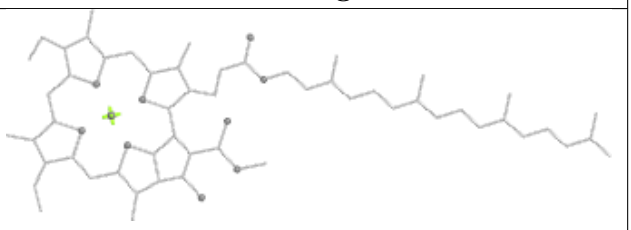


Rings

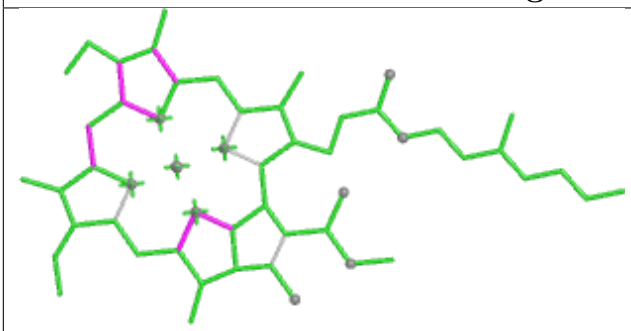
Ligand CLA f 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 707	
	
Bond lengths	Bond angles
	
Torsions	Rings

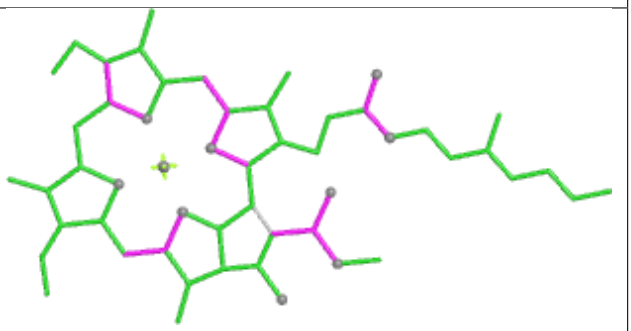
Ligand CLA a 726	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A 310	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

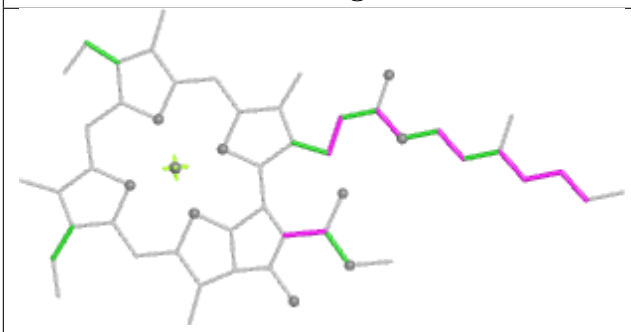
Ligand CLA L 309



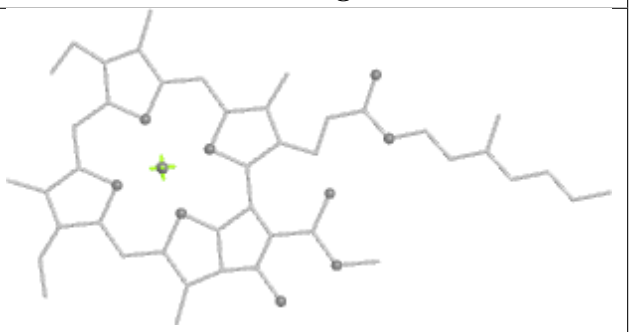
Bond lengths



Bond angles

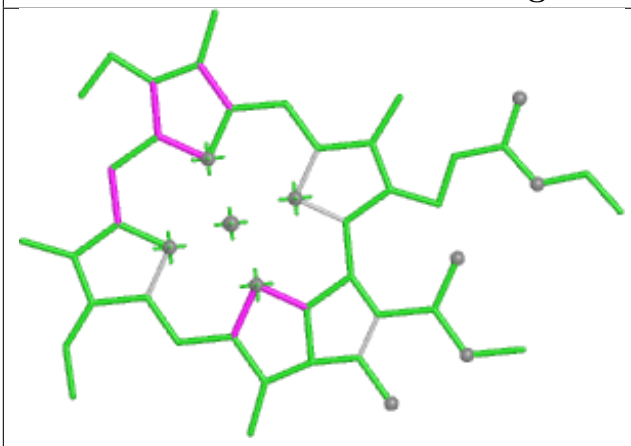


Torsions

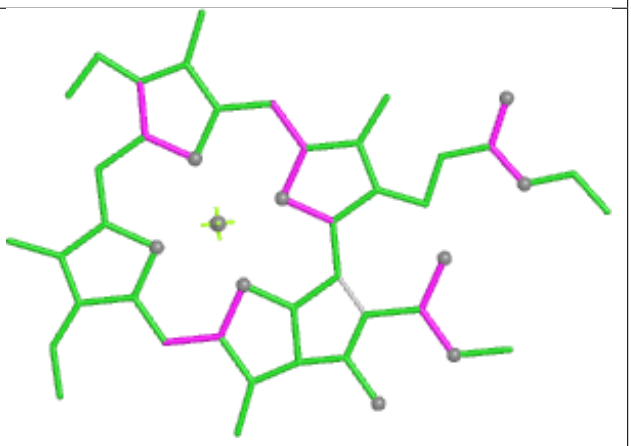


Rings

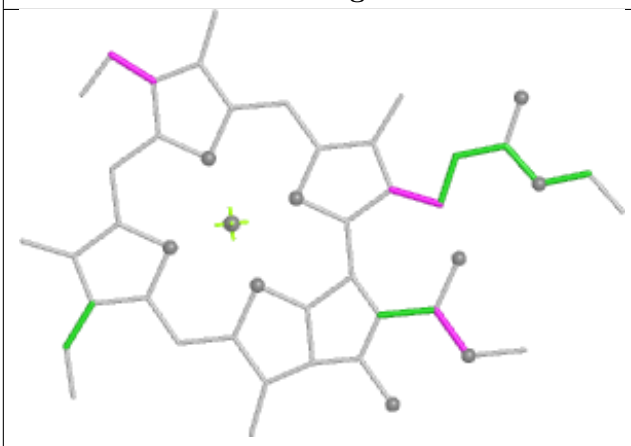
Ligand CLA a 716



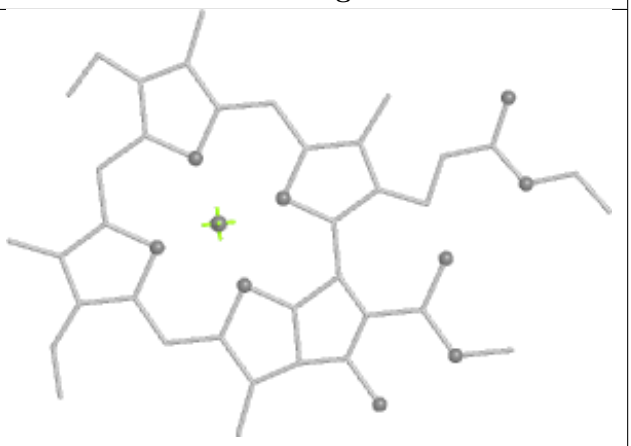
Bond lengths



Bond angles

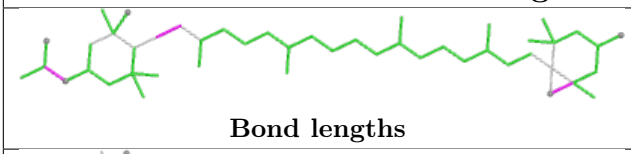


Torsions



Rings

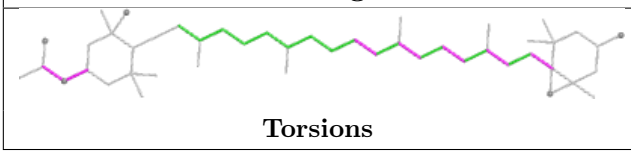
Ligand UIX J 305



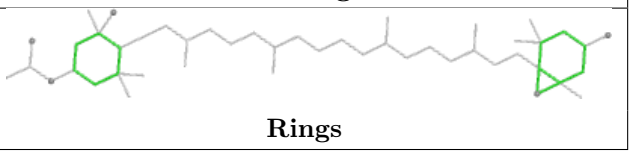
Bond lengths



Bond angles

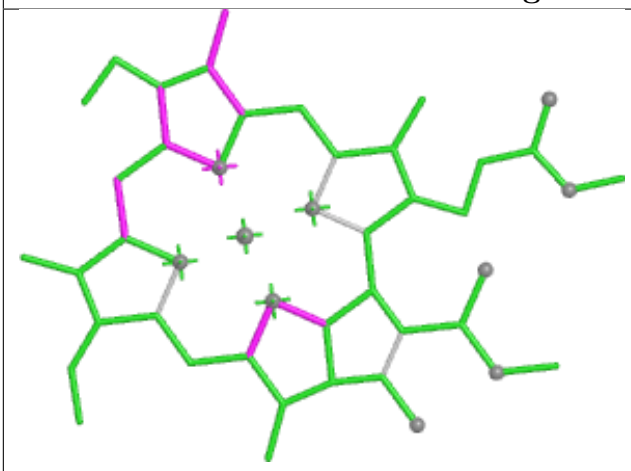


Torsions

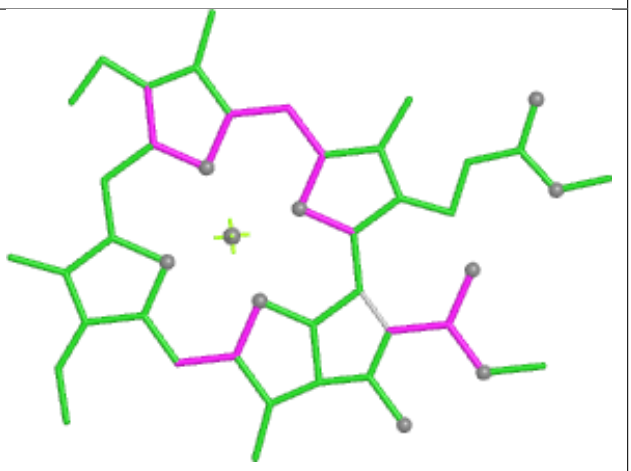


Rings

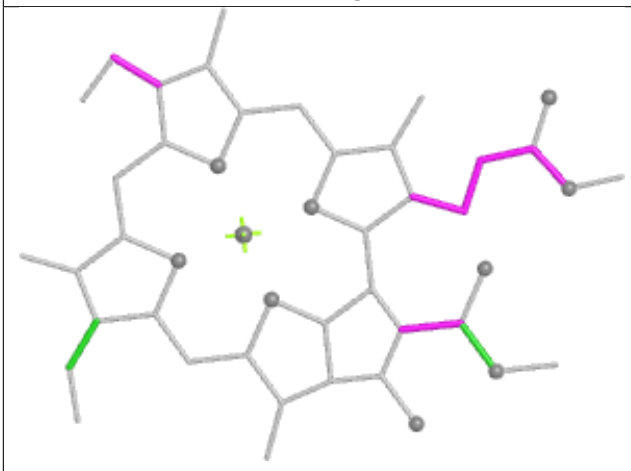
Ligand CLA G 518



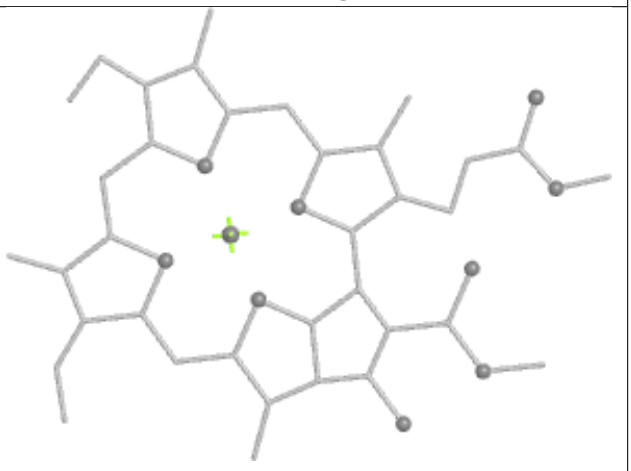
Bond lengths



Bond angles

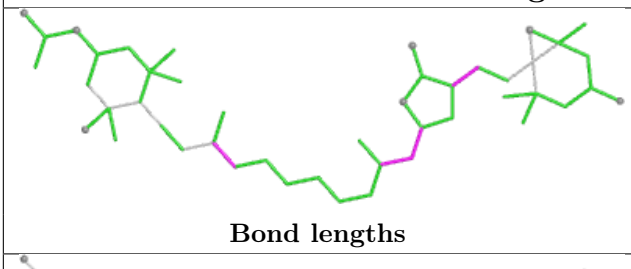


Torsions

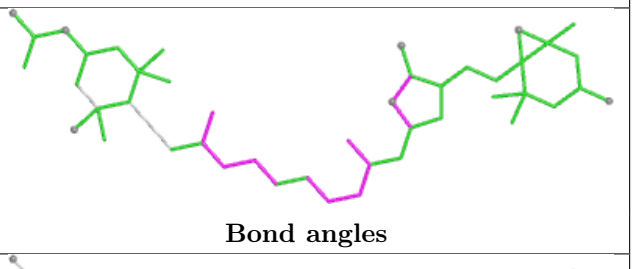


Rings

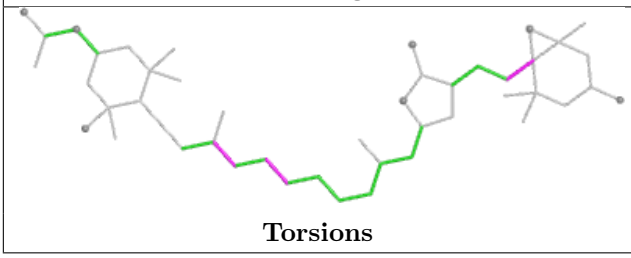
Ligand PID D 307



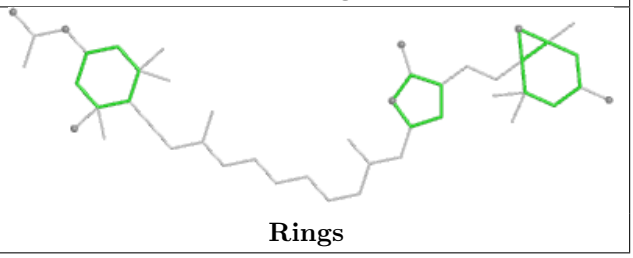
Bond lengths



Bond angles

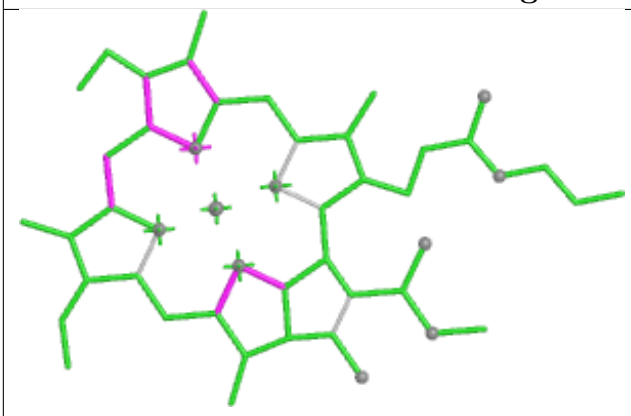


Torsions

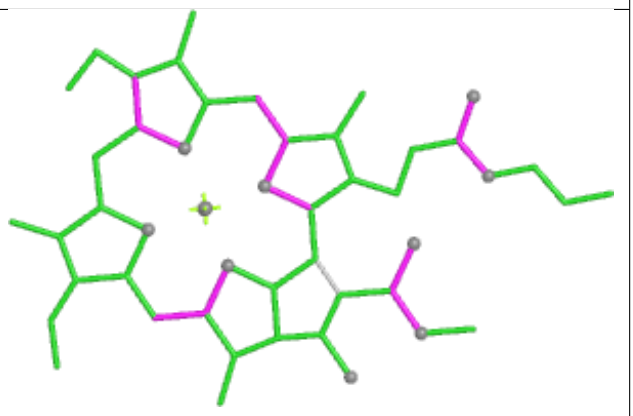


Rings

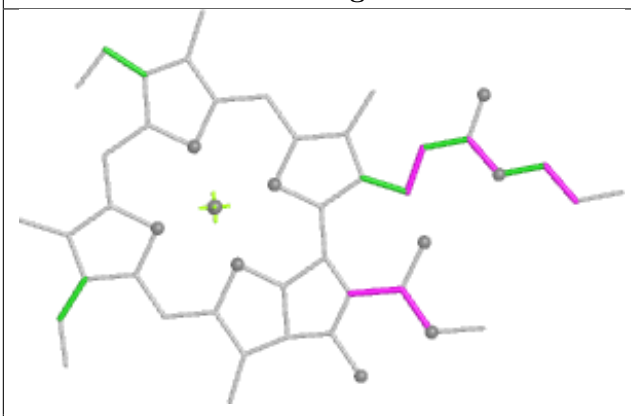
Ligand CLA M 310



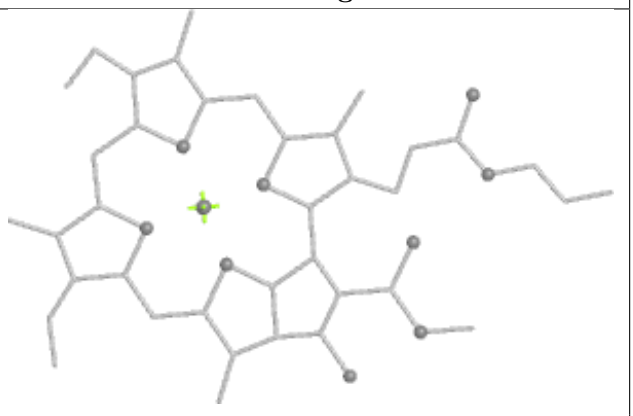
Bond lengths



Bond angles

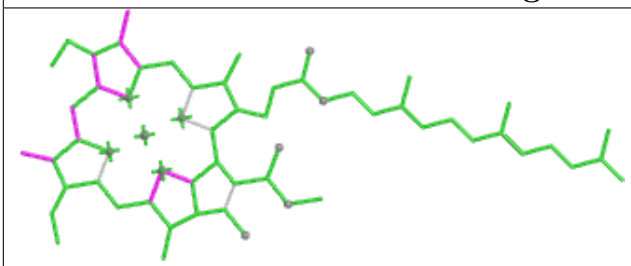


Torsions

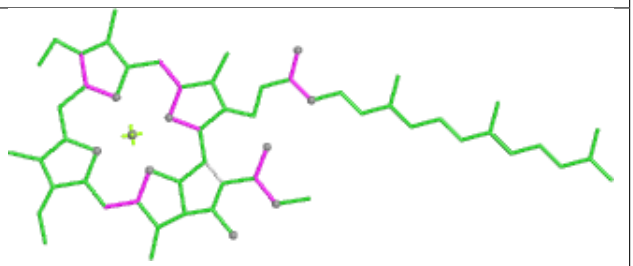


Rings

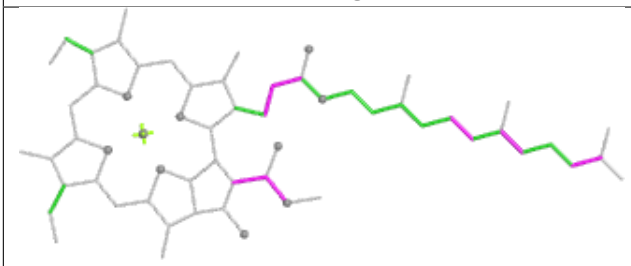
Ligand CLA G 512



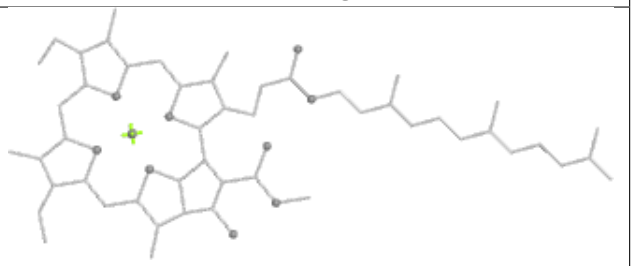
Bond lengths



Bond angles

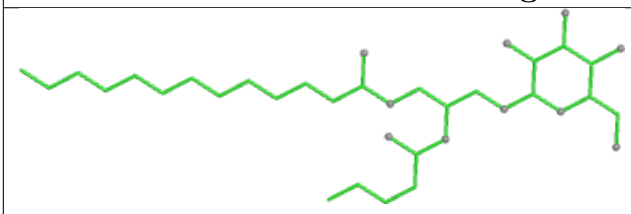


Torsions

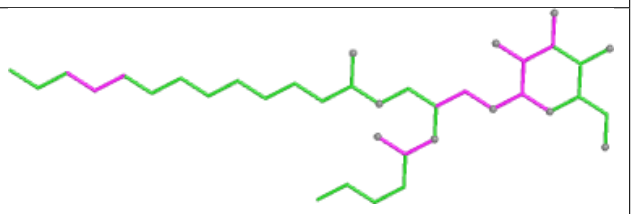


Rings

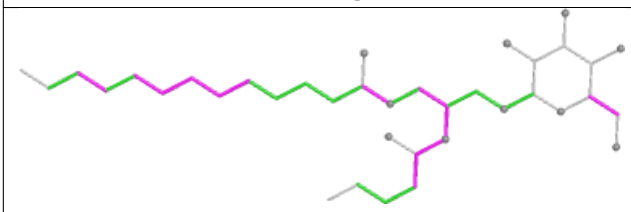
Ligand LMG B 318



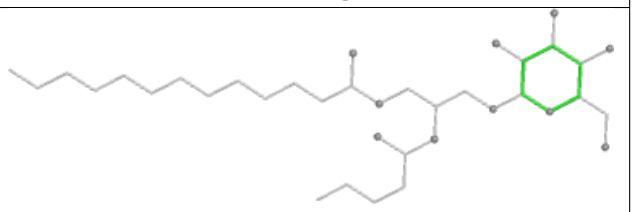
Bond lengths



Bond angles

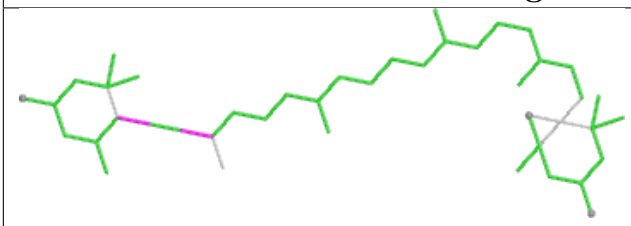


Torsions

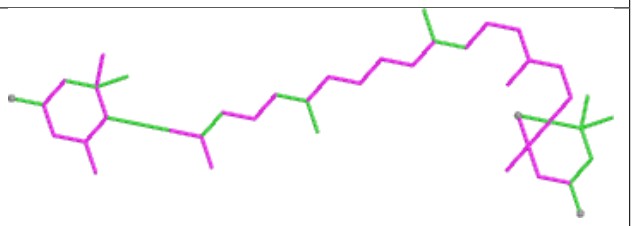


Rings

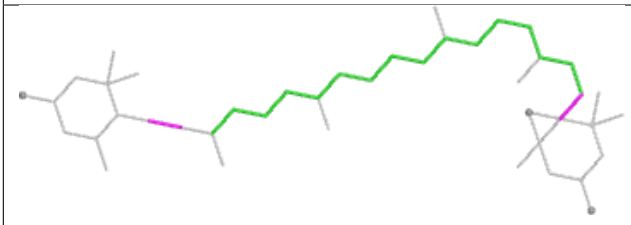
Ligand DD6 B 303



Bond lengths



Bond angles

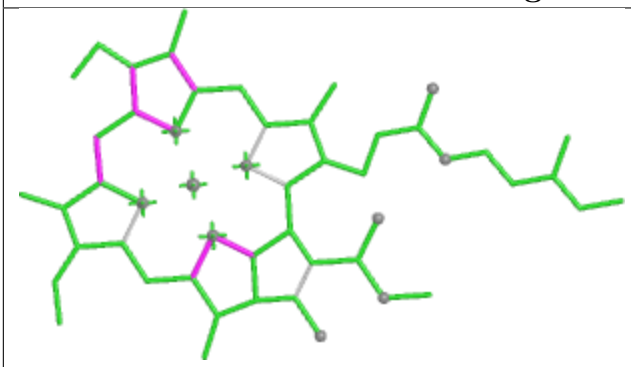


Torsions

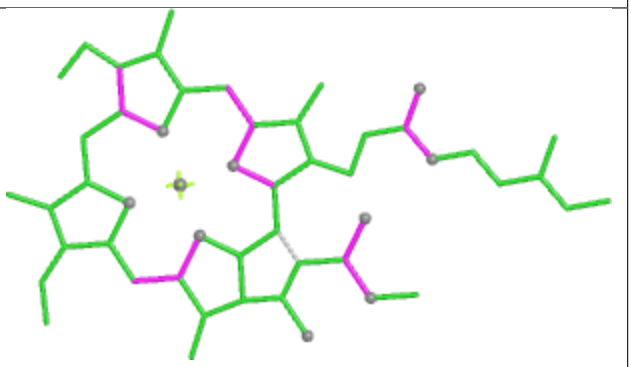


Rings

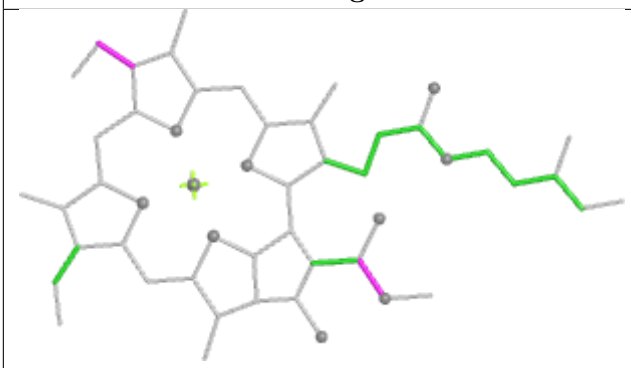
Ligand CLA B 312



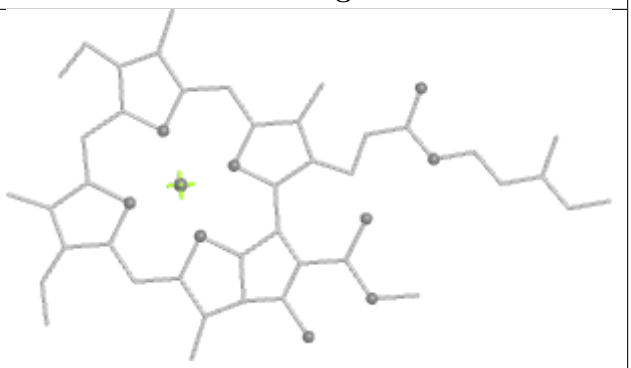
Bond lengths



Bond angles

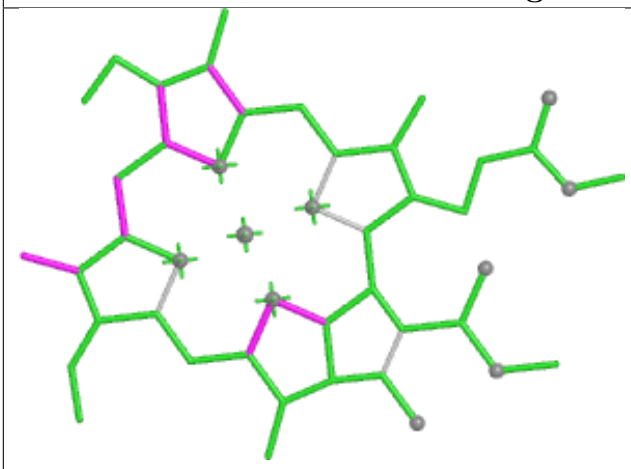


Torsions

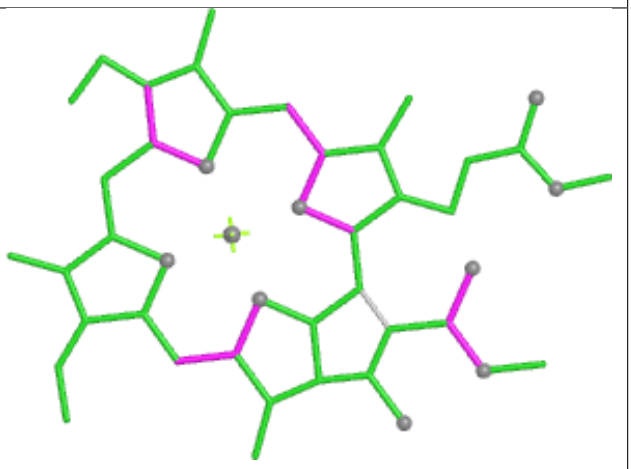


Rings

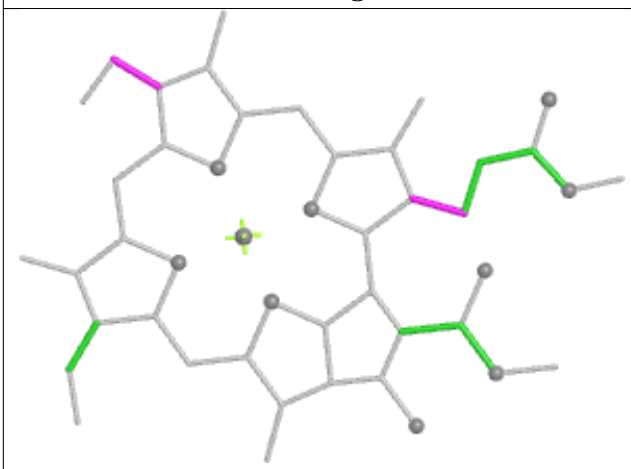
Ligand CLA F 308



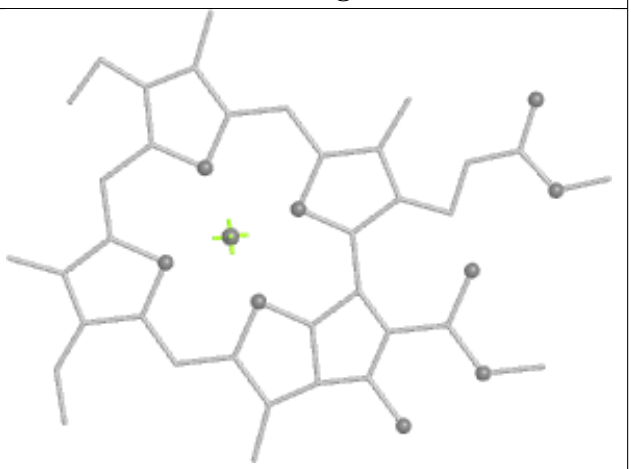
Bond lengths



Bond angles

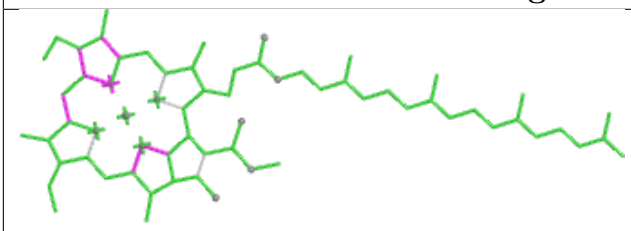


Torsions

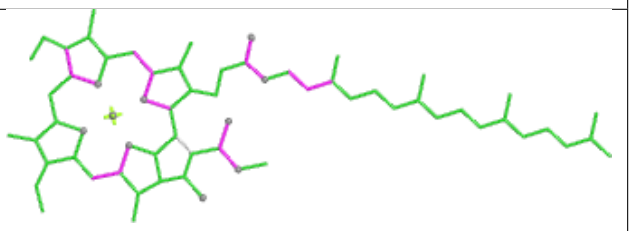


Rings

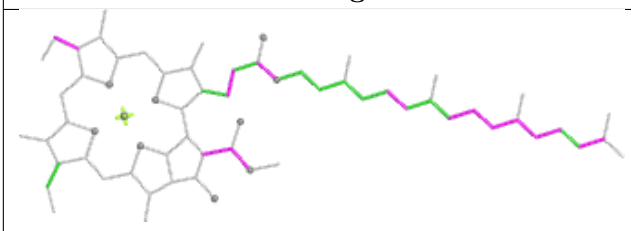
Ligand CLA a 721



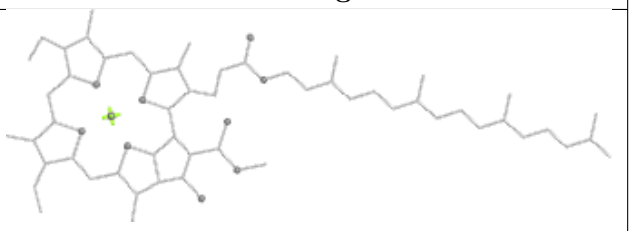
Bond lengths



Bond angles

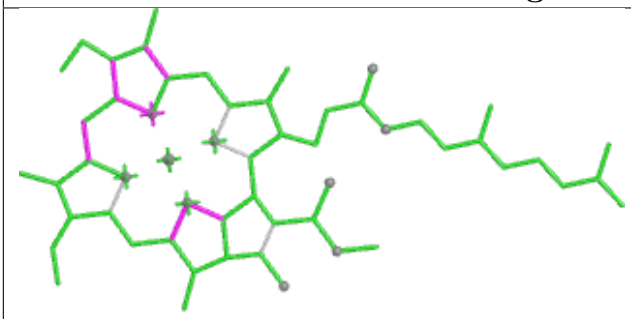


Torsions

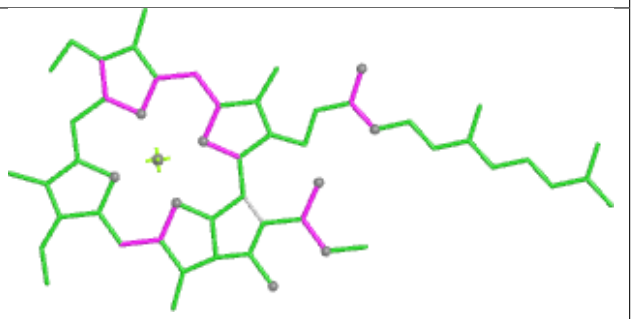


Rings

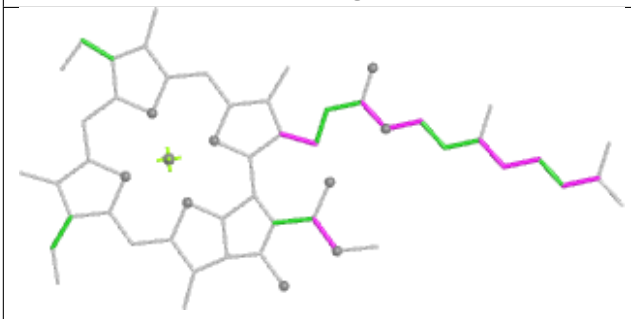
Ligand CLA L 313



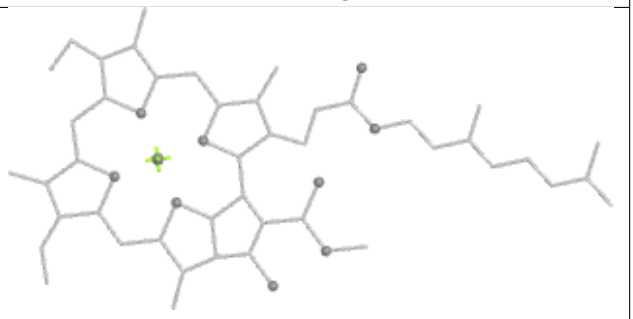
Bond lengths



Bond angles

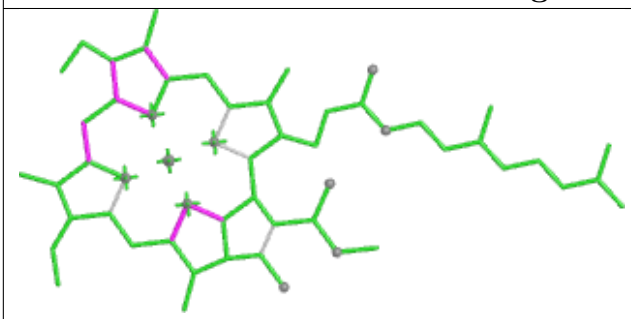


Torsions

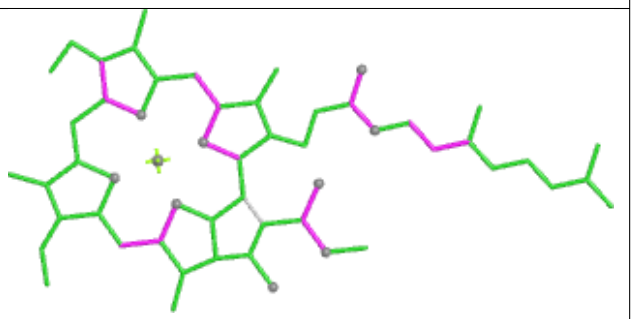


Rings

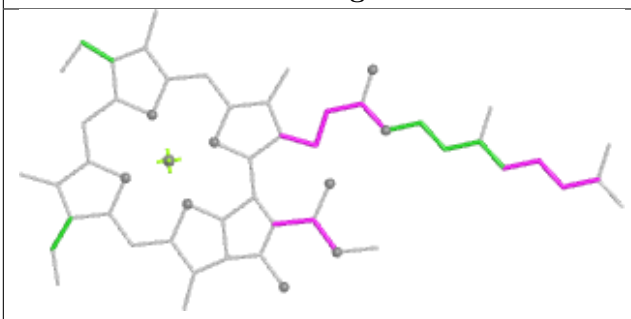
Ligand CLA I 316



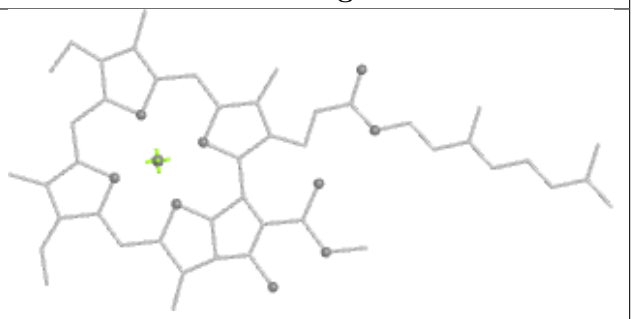
Bond lengths



Bond angles

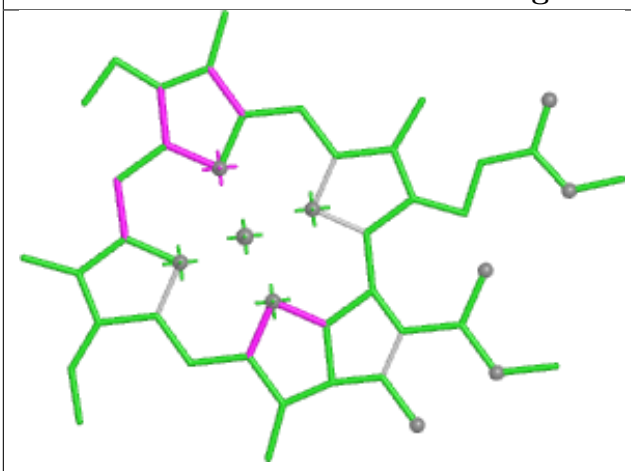


Torsions

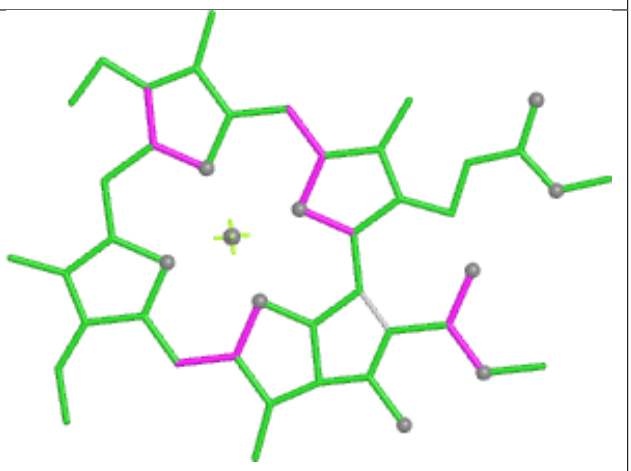


Rings

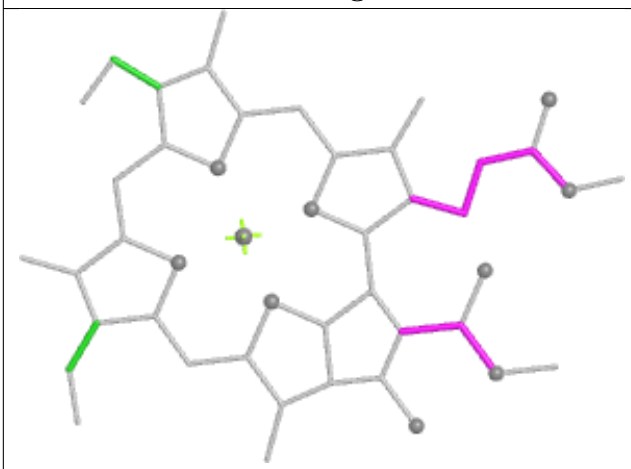
Ligand CLA f 303



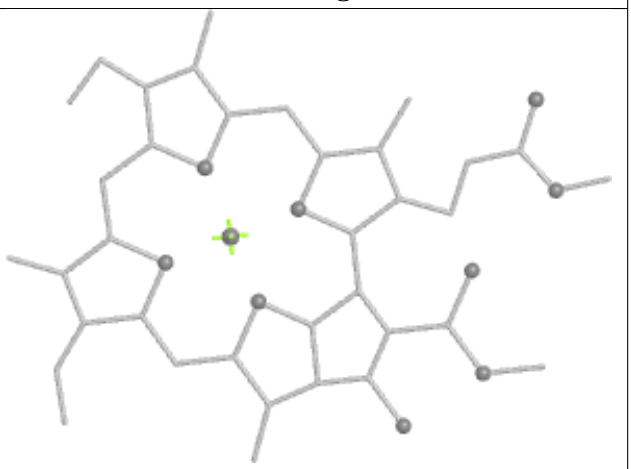
Bond lengths



Bond angles

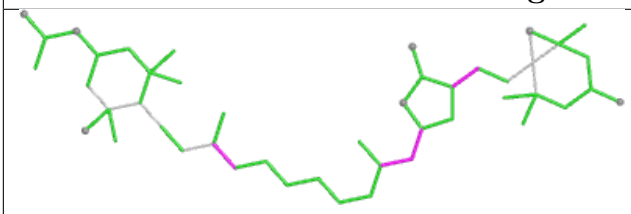


Torsions

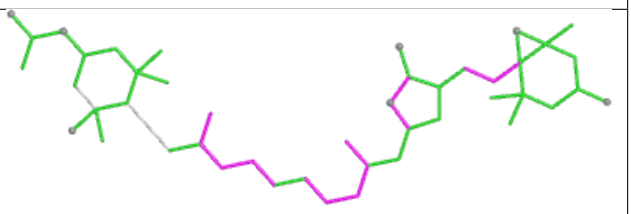


Rings

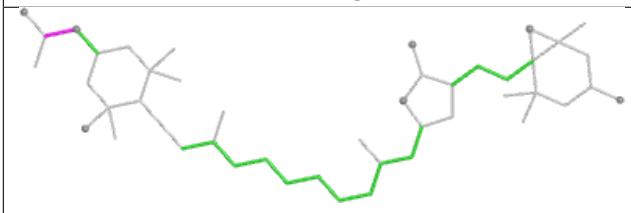
Ligand PID H 302



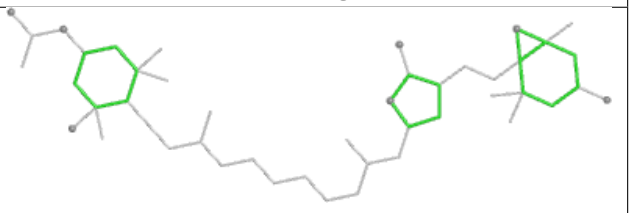
Bond lengths



Bond angles

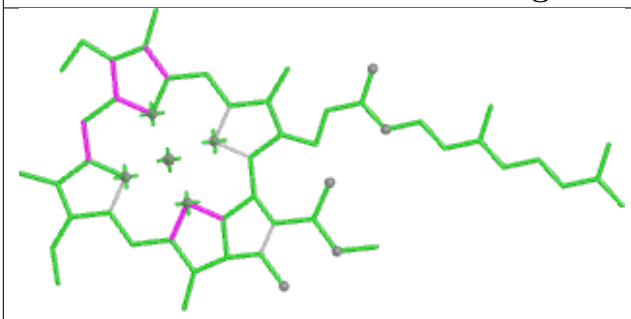


Torsions

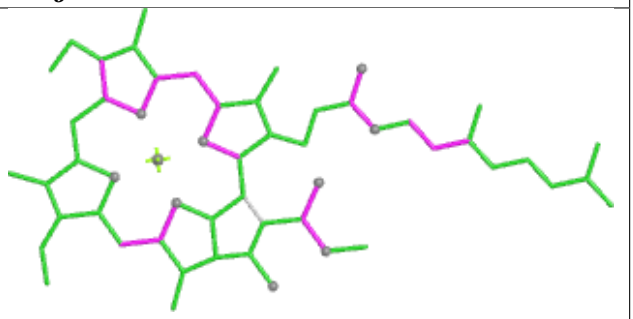


Rings

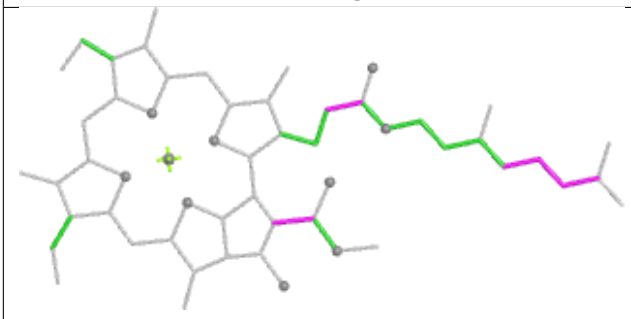
Ligand CLA j 104



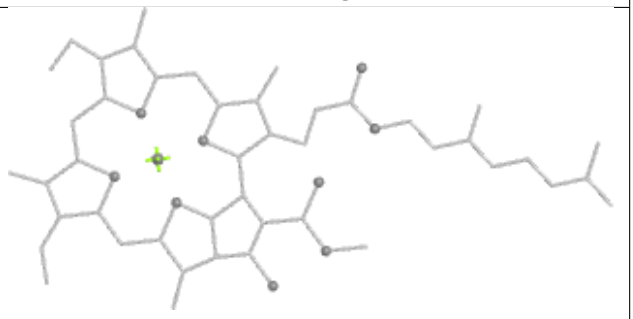
Bond lengths



Bond angles

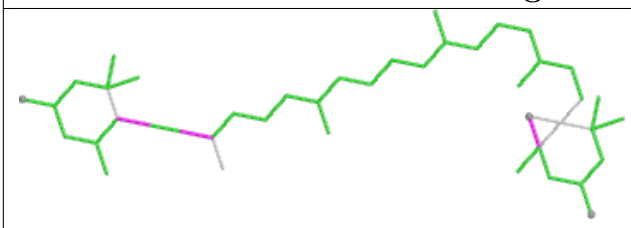


Torsions

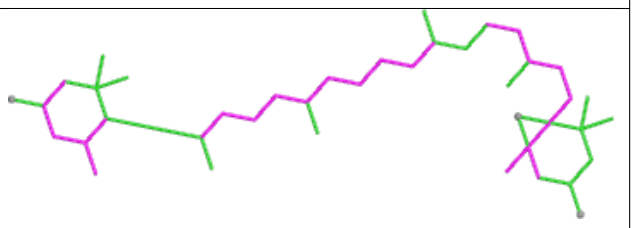


Rings

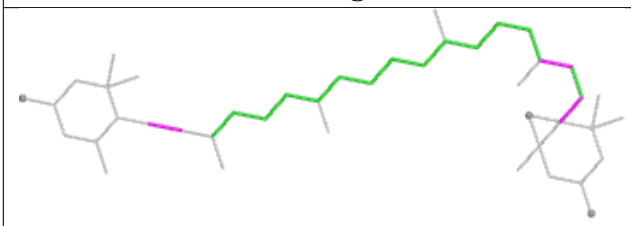
Ligand DD6 K 305



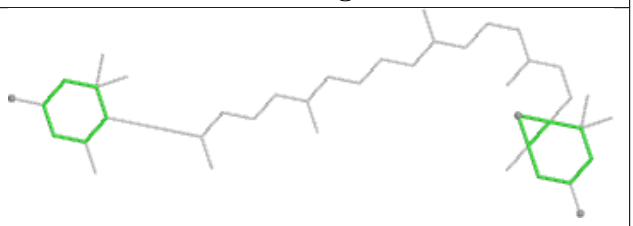
Bond lengths



Bond angles

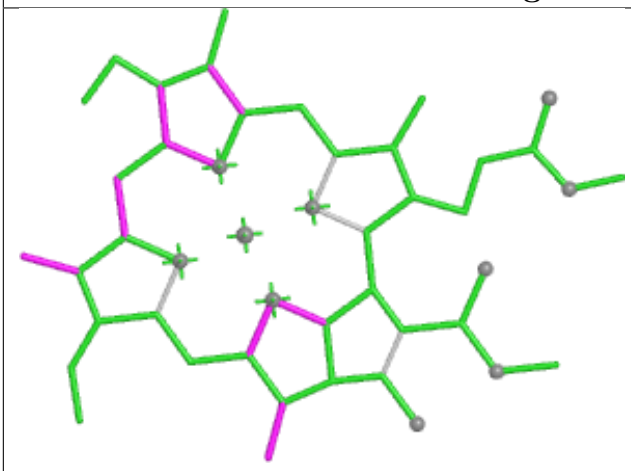


Torsions

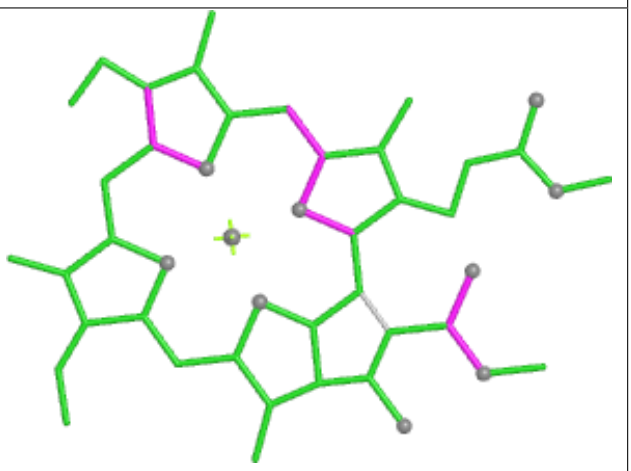


Rings

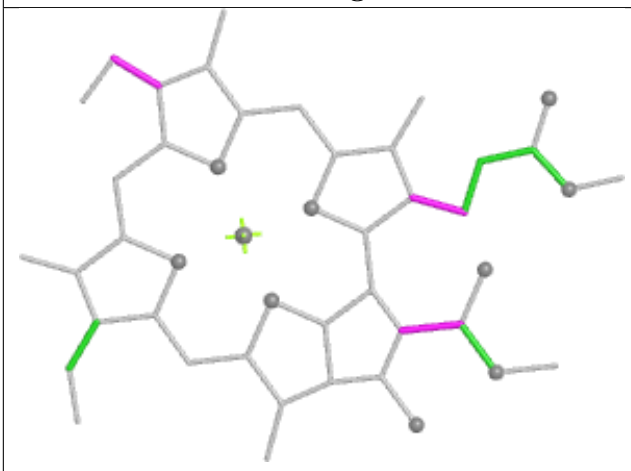
Ligand CLA N 309



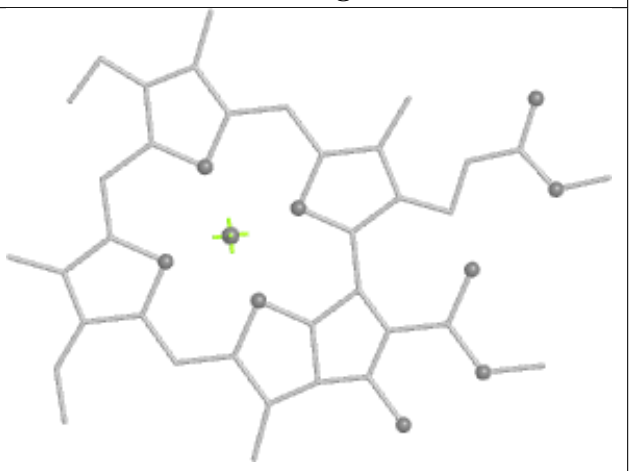
Bond lengths



Bond angles

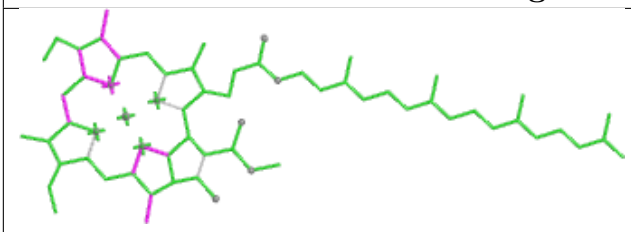


Torsions

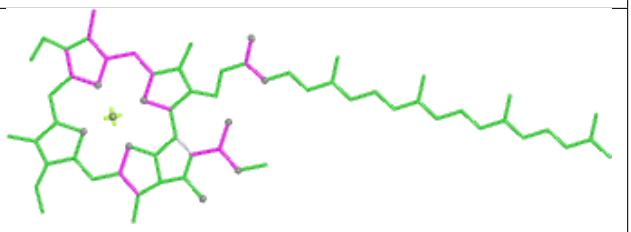


Rings

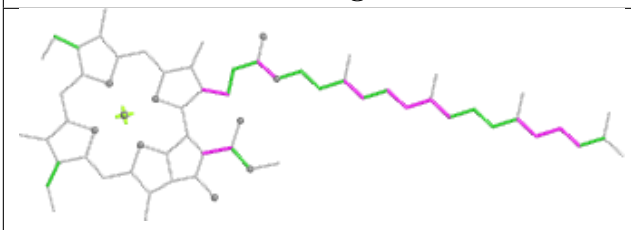
Ligand CLA a 724



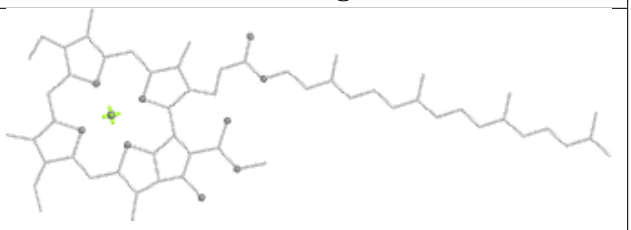
Bond lengths



Bond angles

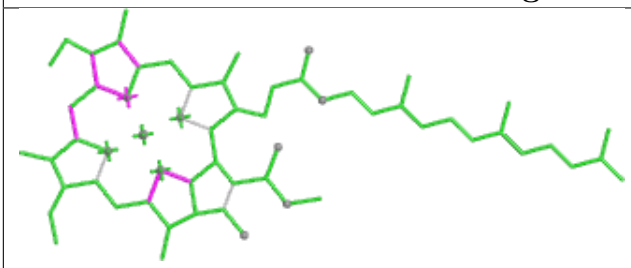


Torsions

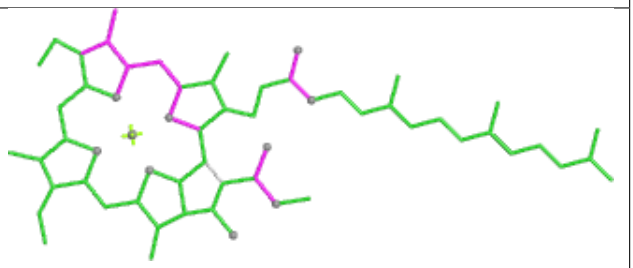


Rings

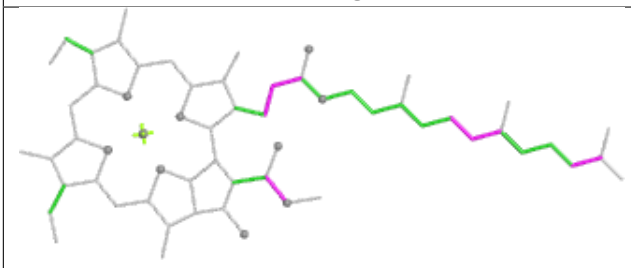
Ligand CLA m 202



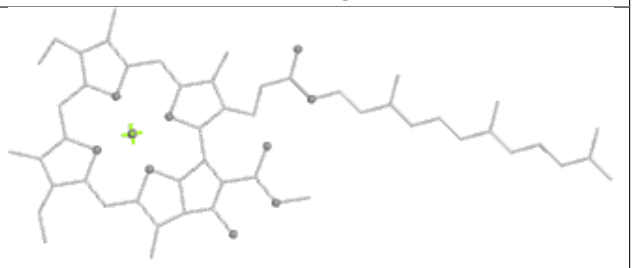
Bond lengths



Bond angles

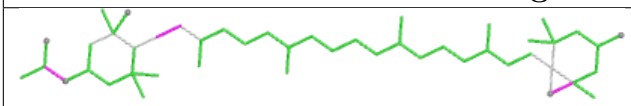


Torsions

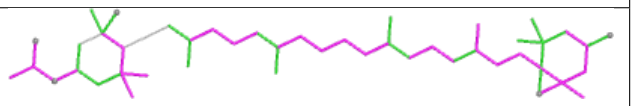


Rings

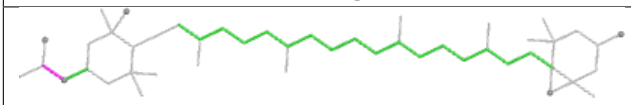
Ligand UIX h 201



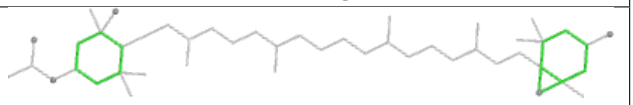
Bond lengths



Bond angles

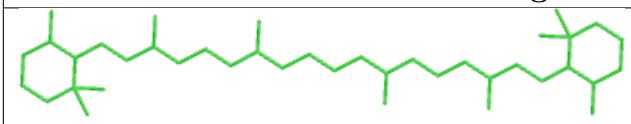


Torsions

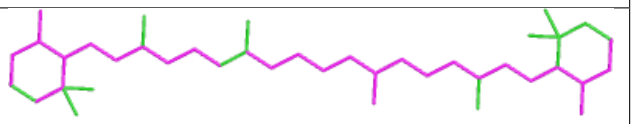


Rings

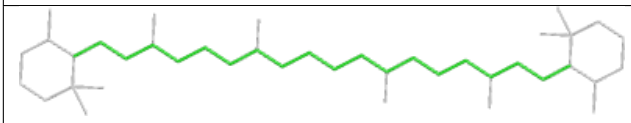
Ligand BCR l 307



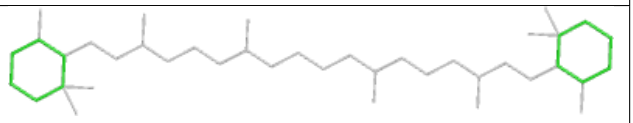
Bond lengths



Bond angles

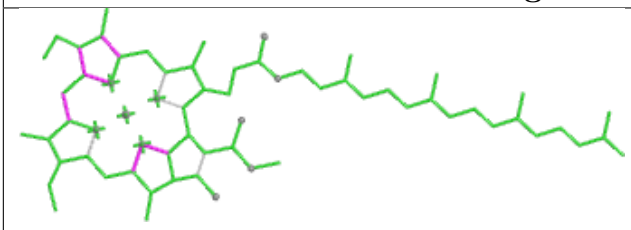


Torsions

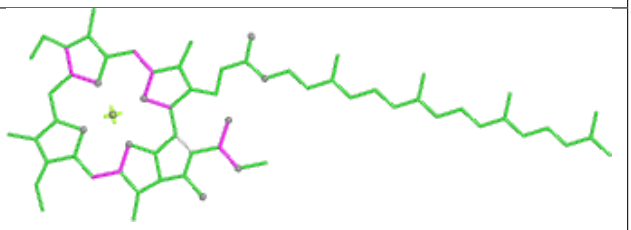


Rings

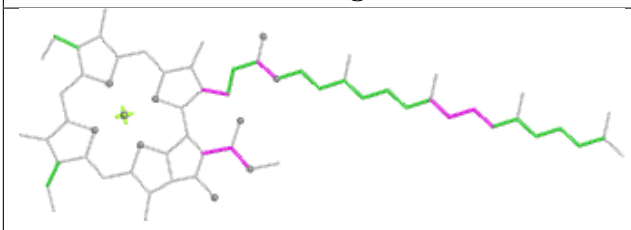
Ligand CLA B 313



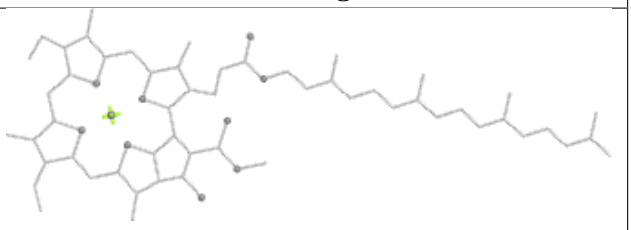
Bond lengths



Bond angles

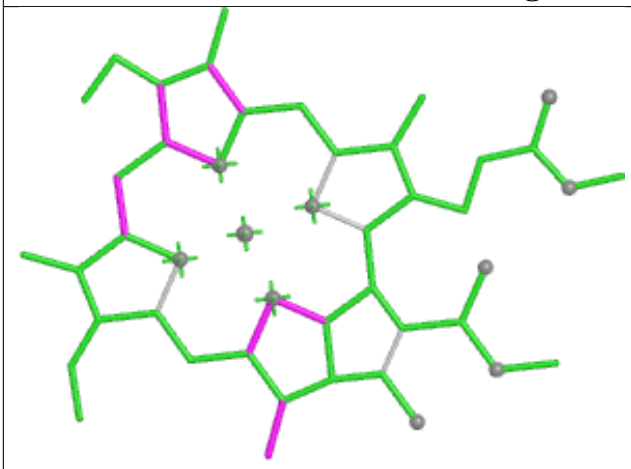


Torsions

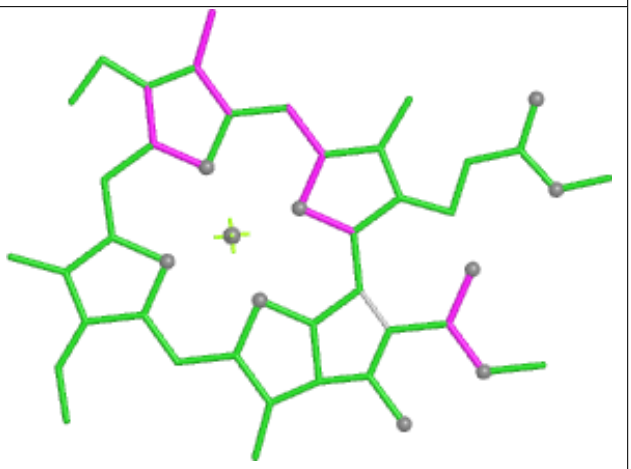


Rings

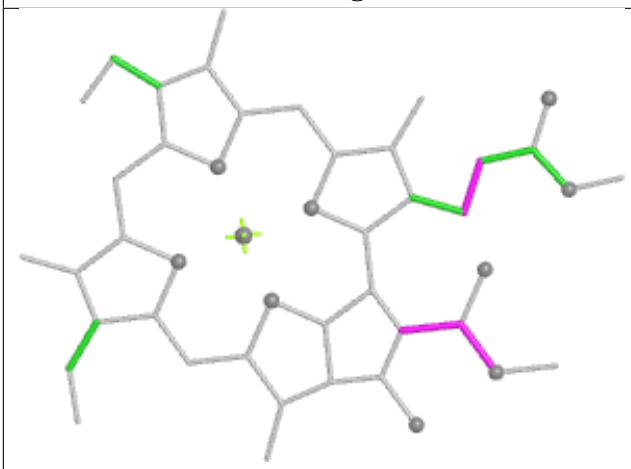
Ligand CLA O 313



Bond lengths



Bond angles

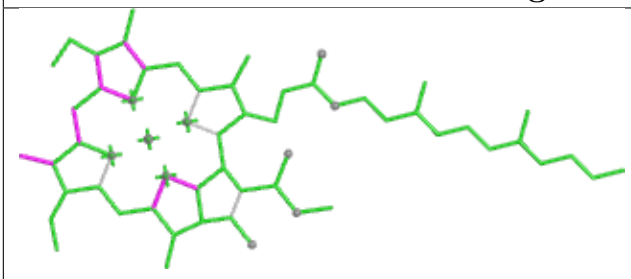


Torsions

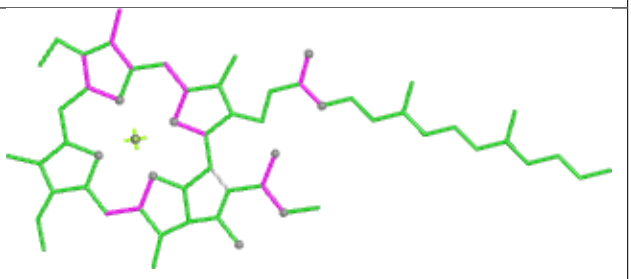


Rings

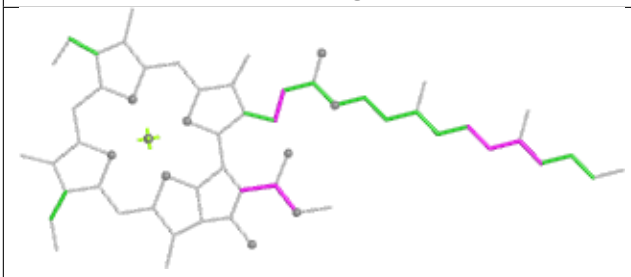
Ligand CLA a 722



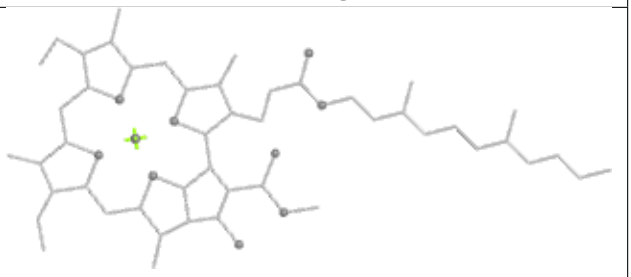
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

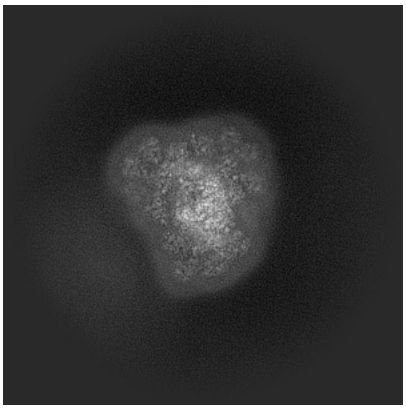
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36742. These allow visual inspection of the internal detail of the map and identification of artifacts.

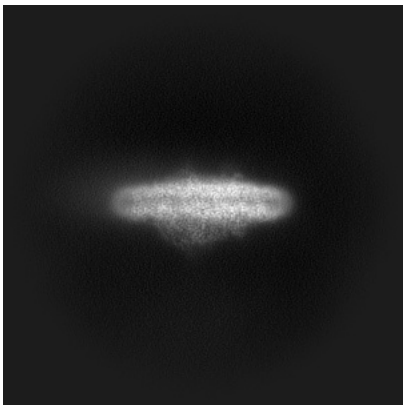
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

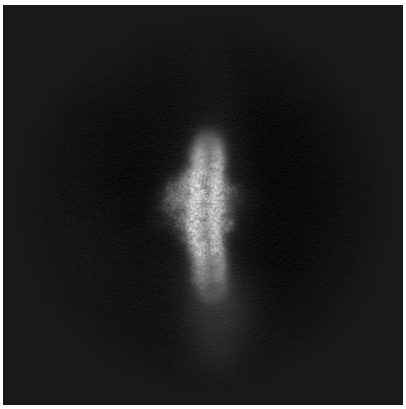
6.1.1 Primary map



X

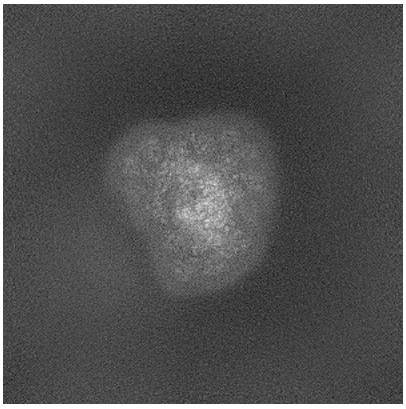


Y

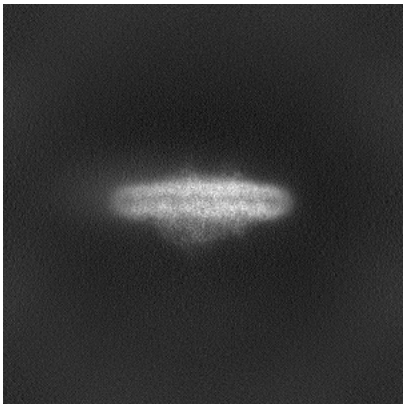


Z

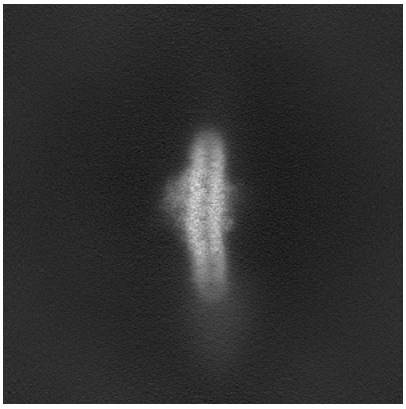
6.1.2 Raw map



X



Y

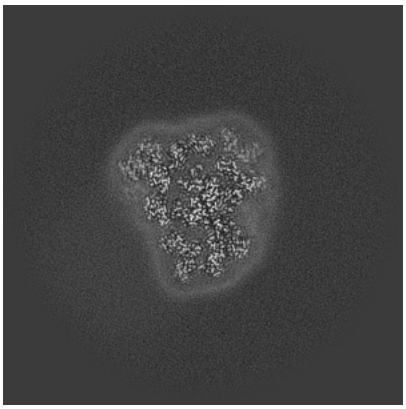


Z

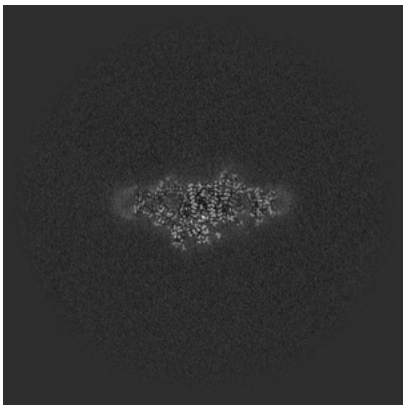
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

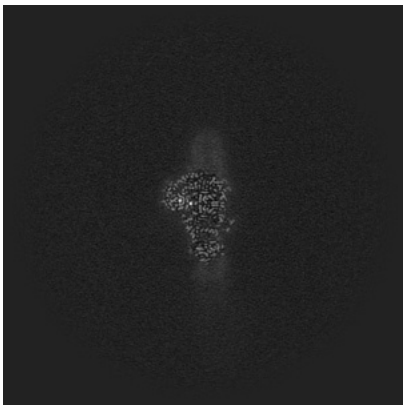
6.2.1 Primary map



X Index: 256

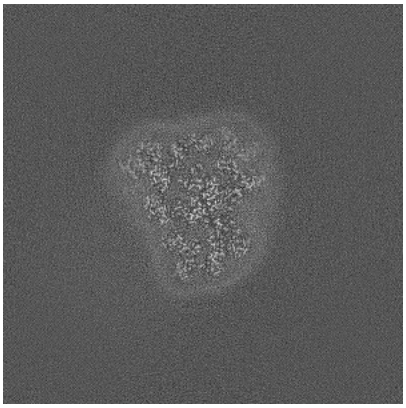


Y Index: 256

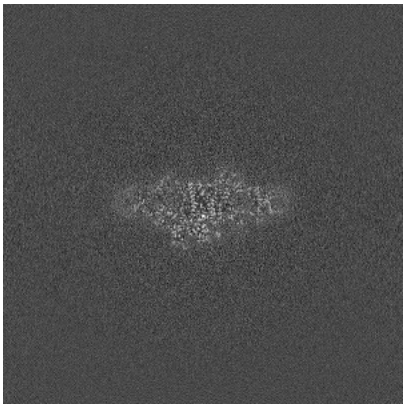


Z Index: 256

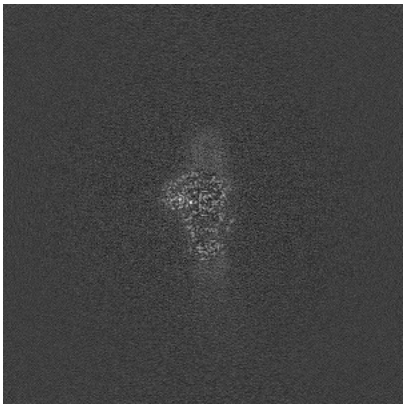
6.2.2 Raw map



X Index: 256



Y Index: 256

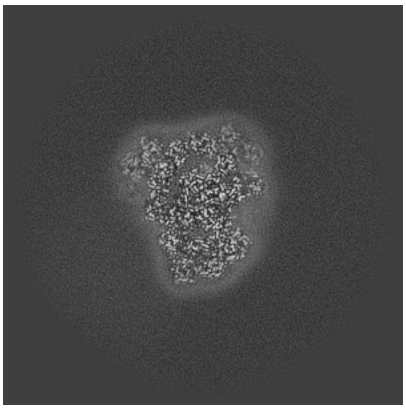


Z Index: 256

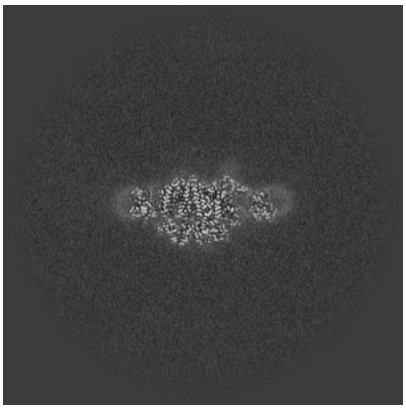
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

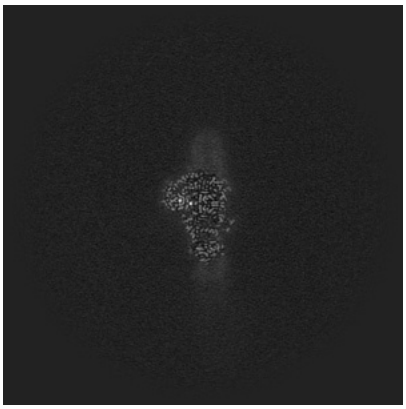
6.3.1 Primary map



X Index: 250

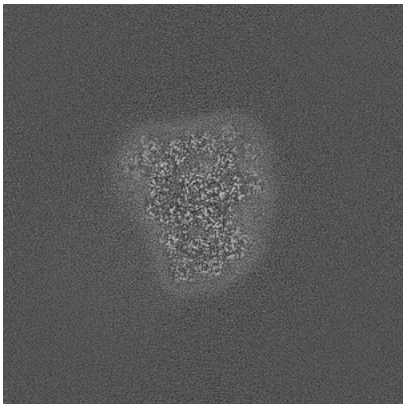


Y Index: 264

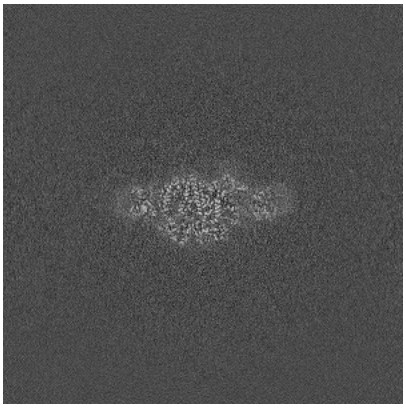


Z Index: 256

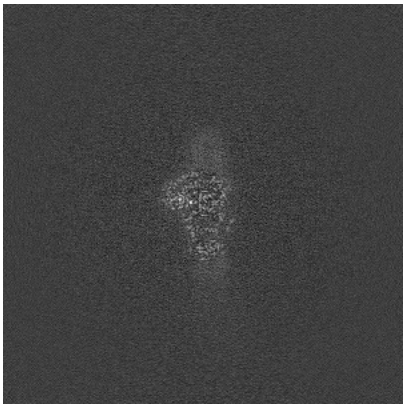
6.3.2 Raw map



X Index: 250



Y Index: 264

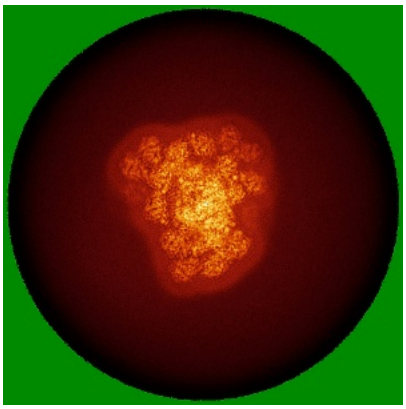


Z Index: 256

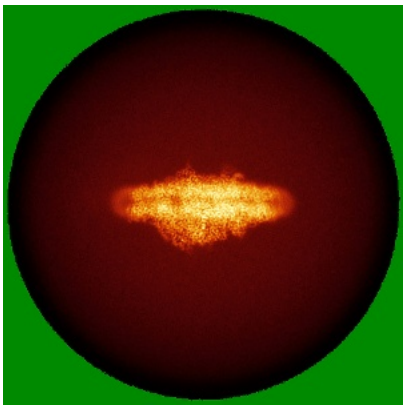
The images above show the largest variance slices of the map in three orthogonal directions.

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

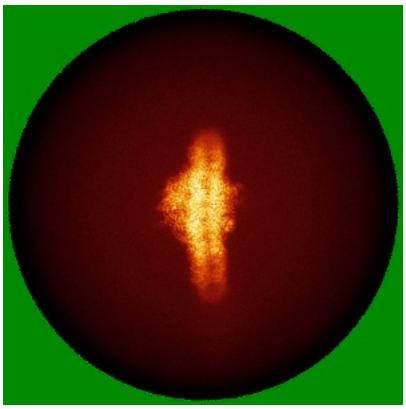
6.4.1 Primary map



X

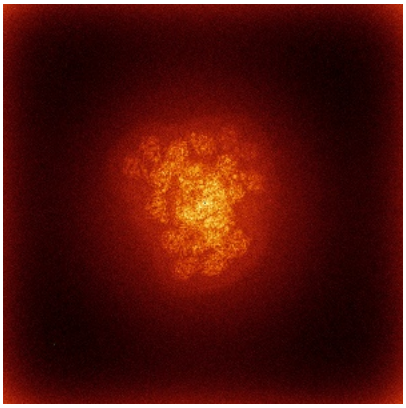


Y

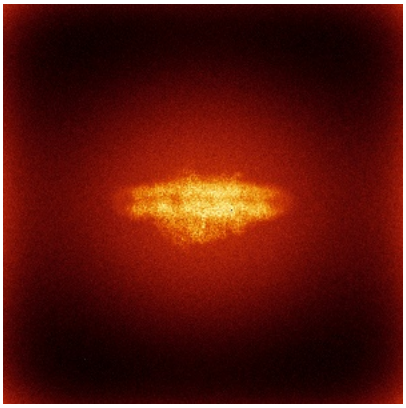


Z

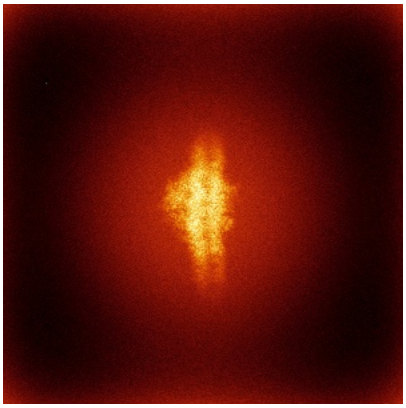
6.4.2 Raw map



X



Y

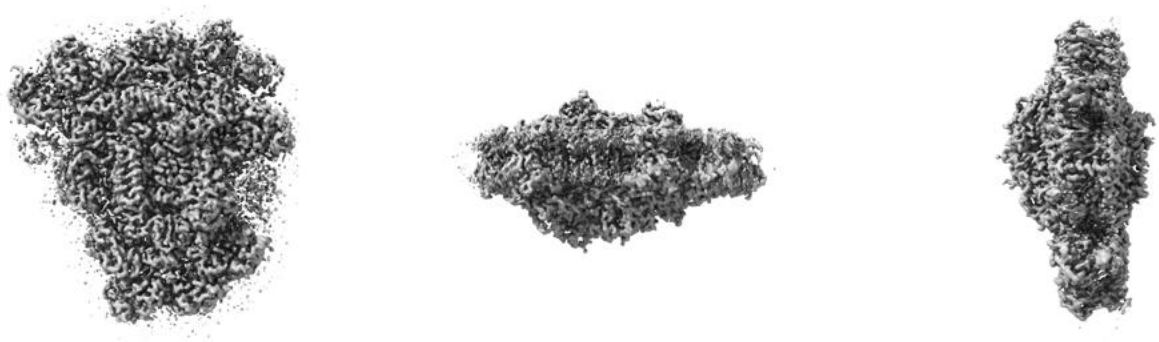


Z

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

6.5 Orthogonal surface views (i)

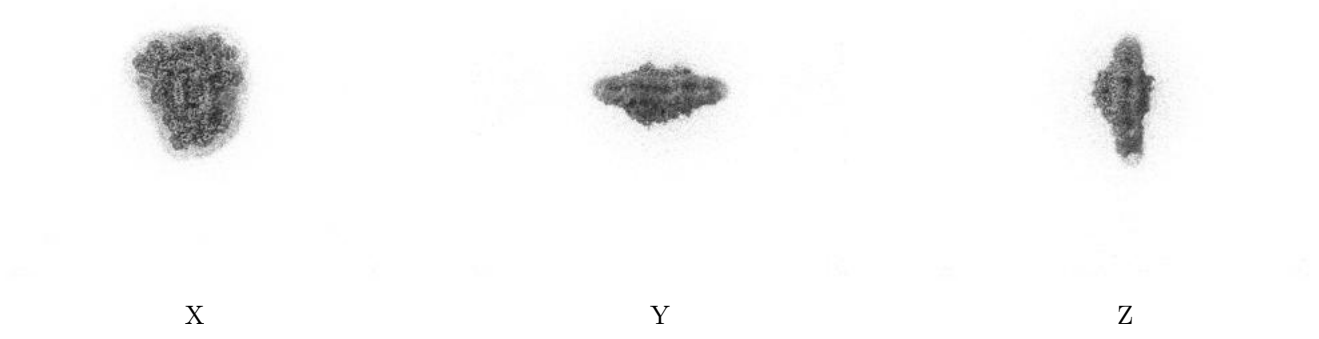
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.235. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

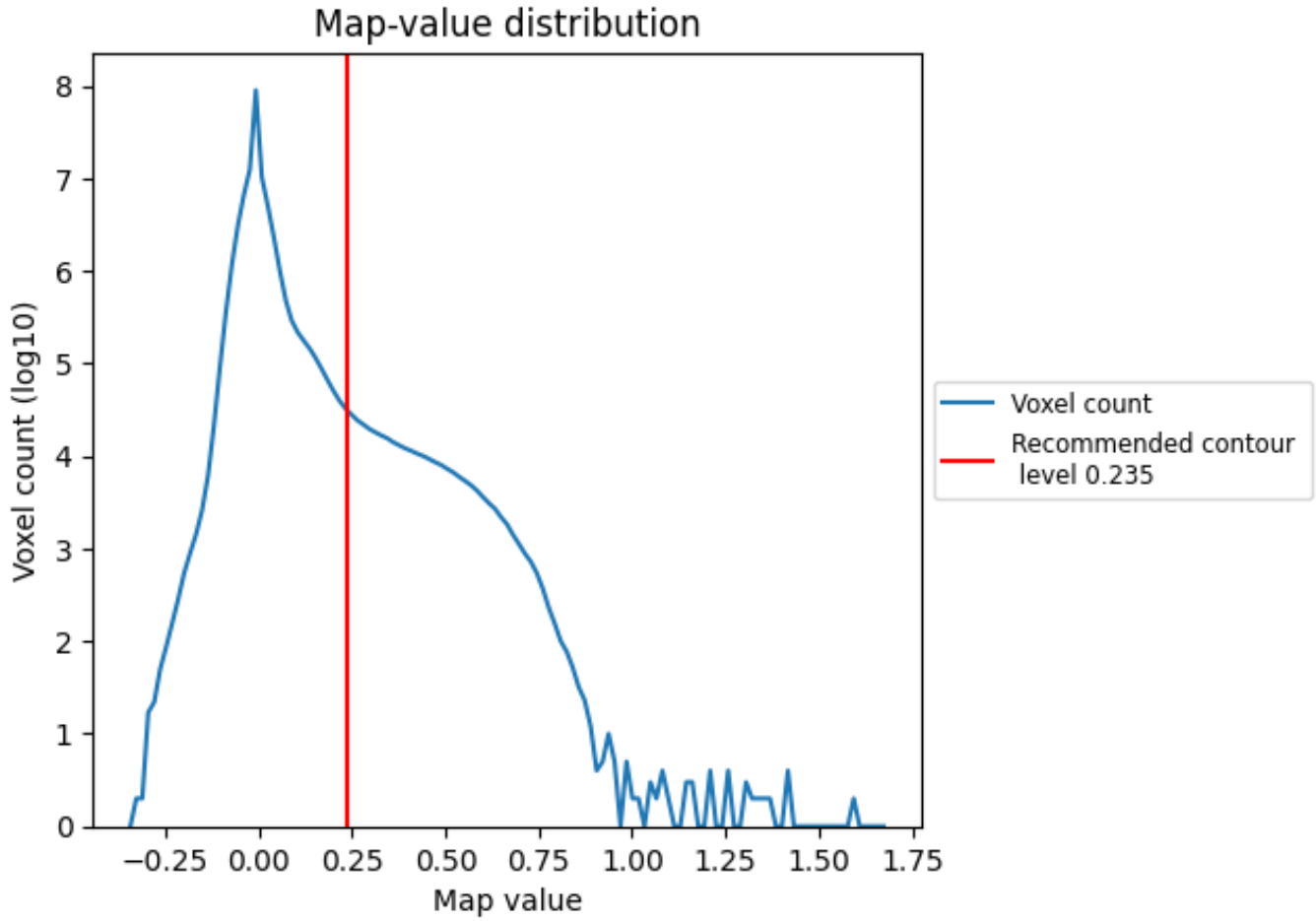
6.6 Mask visualisation (i)

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

7 Map analysis

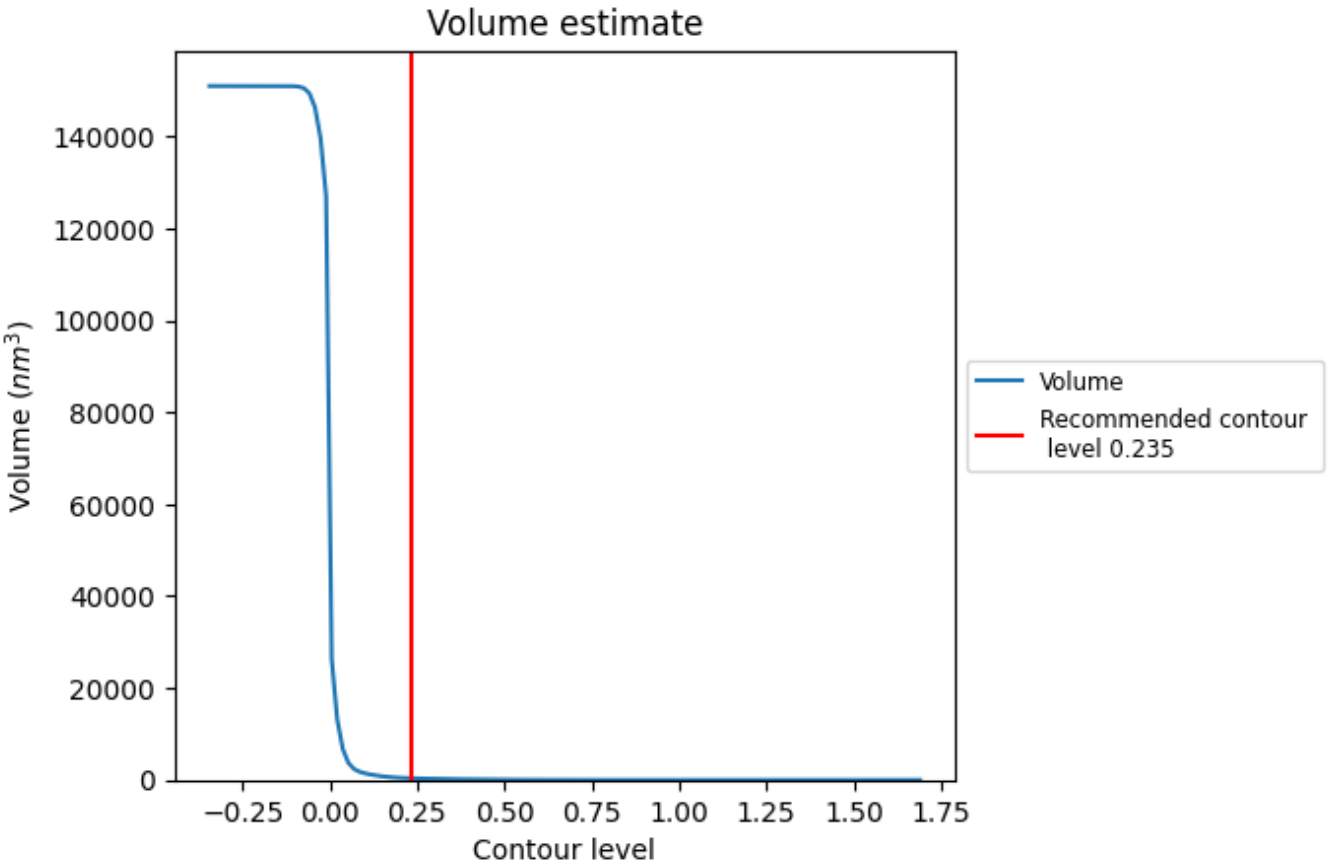
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

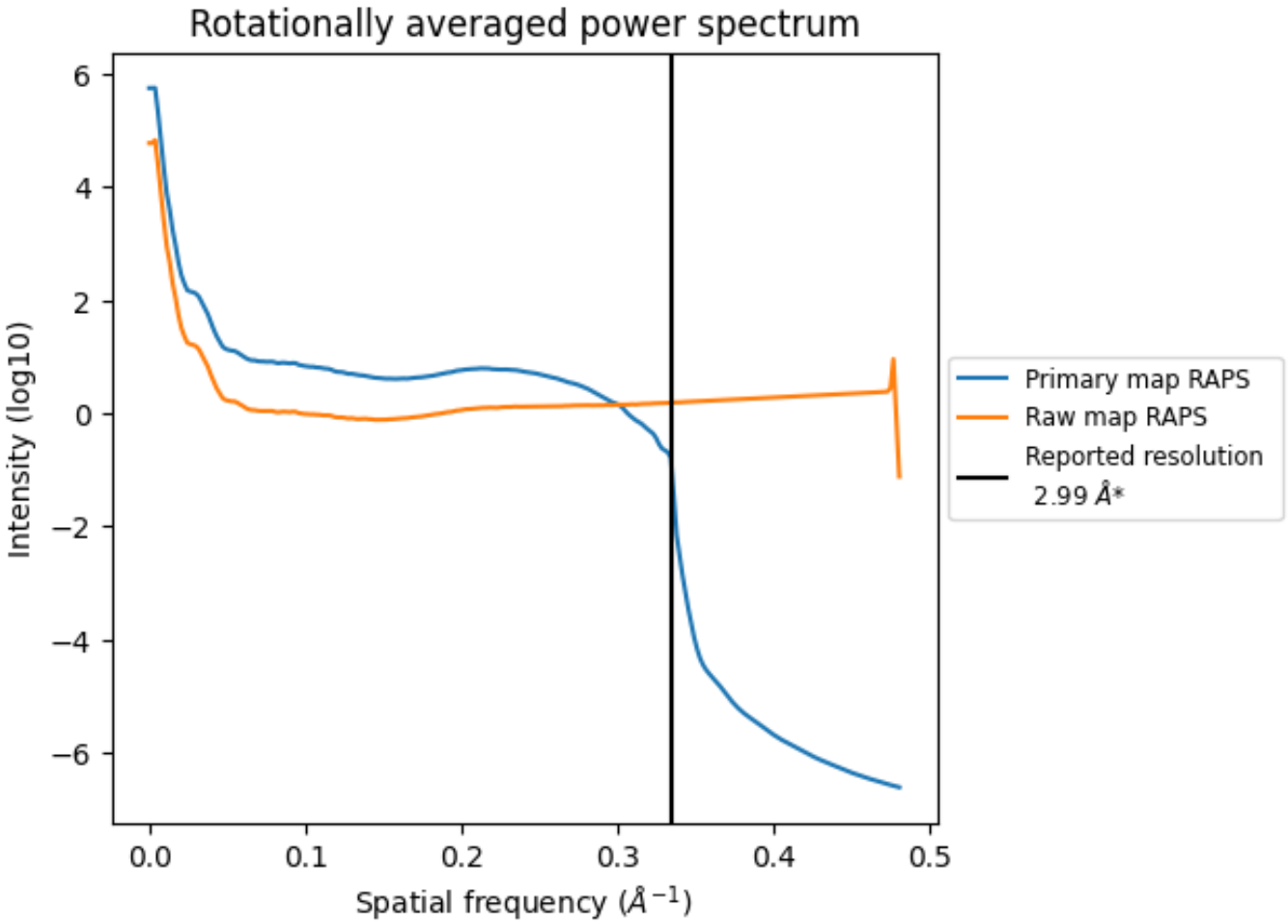
7.2 Volume estimate



The volume at the recommended contour level is 363 nm^3; this corresponds to an approximate mass of 328 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)

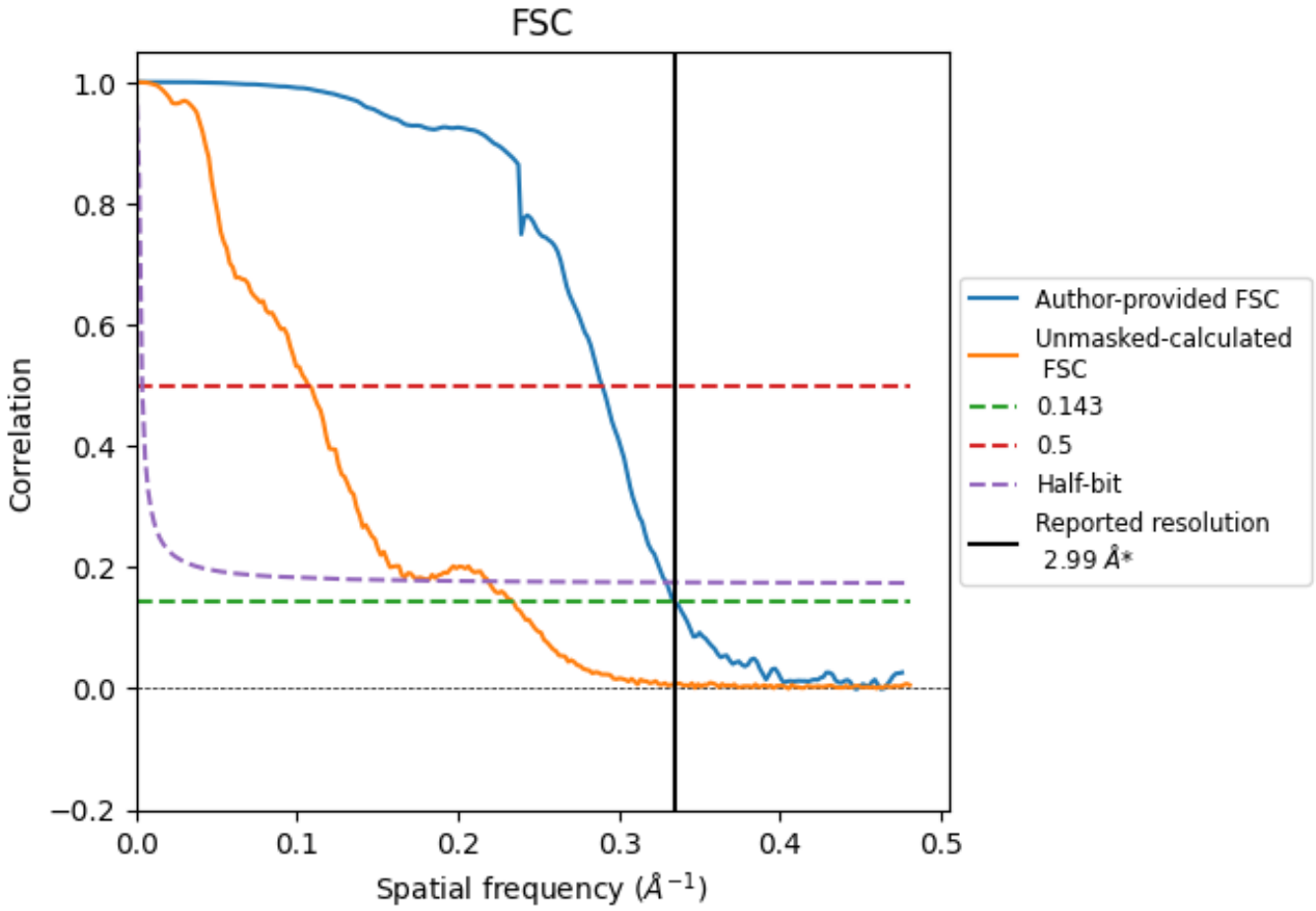


*Reported resolution corresponds to spatial frequency of 0.334 Å^{-1}

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 0.334 $Å^{-1}$

8.2 Resolution estimates (i)

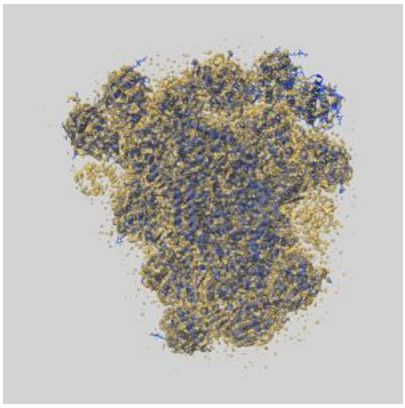
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.99	3.45	3.03
Unmasked-calculated*	4.27	9.35	4.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 2.99 by more than 10 %

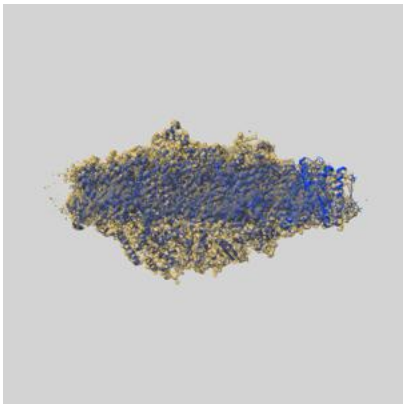
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36742 and PDB model 8JZE. Per-residue inclusion information can be found in section 3 on page 31.

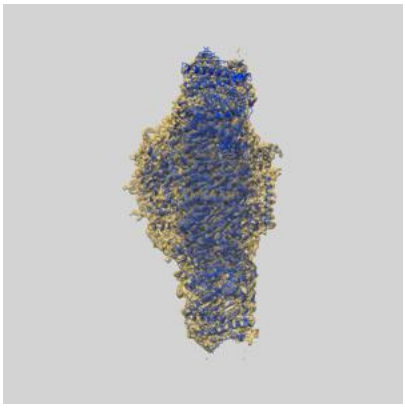
9.1 Map-model overlay



X



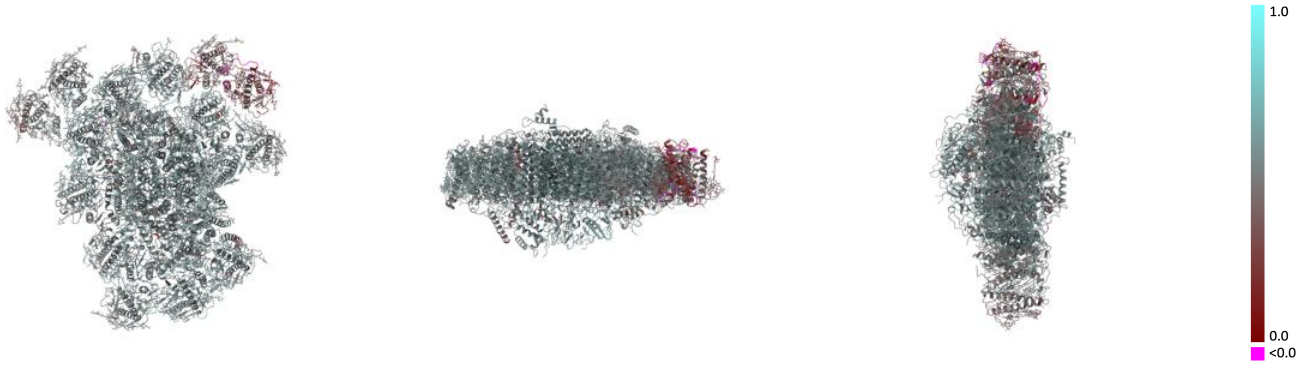
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.235 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.

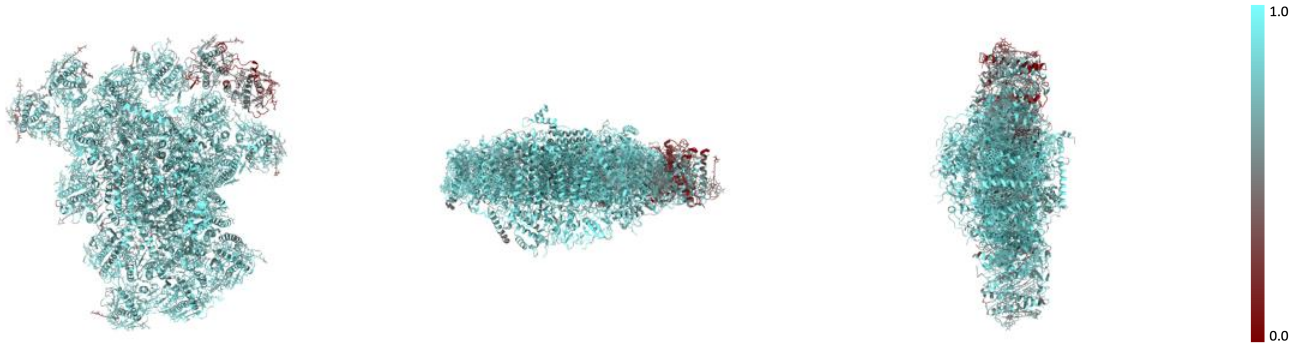
9.2 Q-score mapped to coordinate model



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.

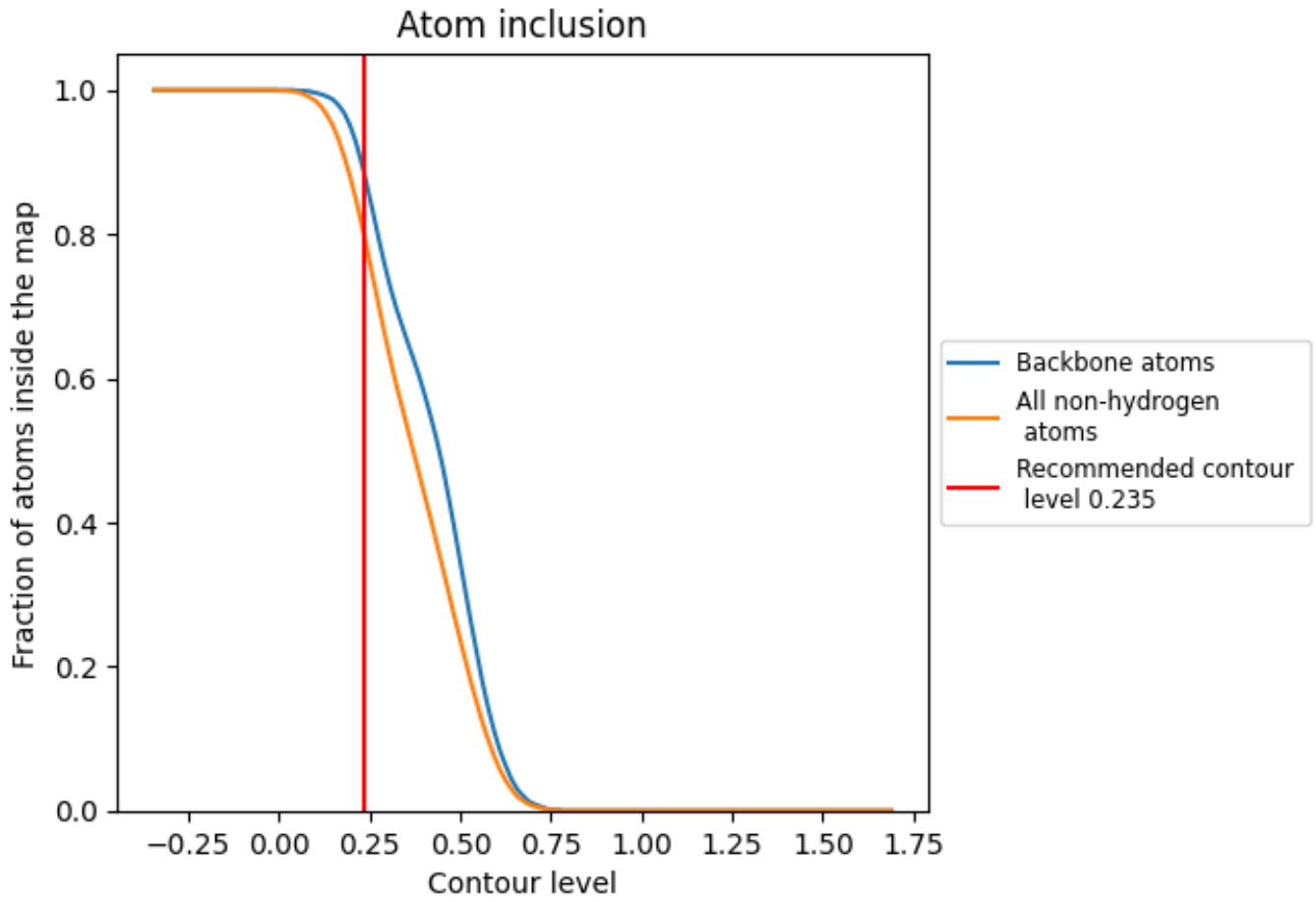
9.3 Atom inclusion mapped to coordinate model



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 (0.235).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 80% 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 (0.235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.5180
A	0.8360	0.5390
B	0.7940	0.5260
D	0.7490	0.5080
F	0.7320	0.4980
G	0.8000	0.5170
H	0.3060	0.2340
I	0.7850	0.5140
J	0.8410	0.5330
K	0.8600	0.5510
L	0.8440	0.5460
M	0.7800	0.5200
N	0.4940	0.3650
O	0.6780	0.4560
P	0.7250	0.4850
a	0.8560	0.5470
b	0.8710	0.5530
c	0.9280	0.5570
d	0.8550	0.5450
e	0.8990	0.5640
f	0.8330	0.5420
h	0.8660	0.5480
i	0.8360	0.5320
j	0.7800	0.5310
l	0.8610	0.5490
m	0.8270	0.5380
y	0.8670	0.5260
z	0.9150	0.5230

