wwPDB EM Validation Summary Report

Sep 29, 2026 – 09:57 PM JST

PDB ID	:	9K7V / pdb_00009k7v
EMDB ID	:	EMD-62153
Title	:	Structural insights into photosystem II supercomplex of a a siphonous green algae Bryopsis corticulans from intertidal zone
Authors	:	Liu, X.Y.; Wang, W.D.
Deposited on	:	2024-10-24
Resolution	:	3.07 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

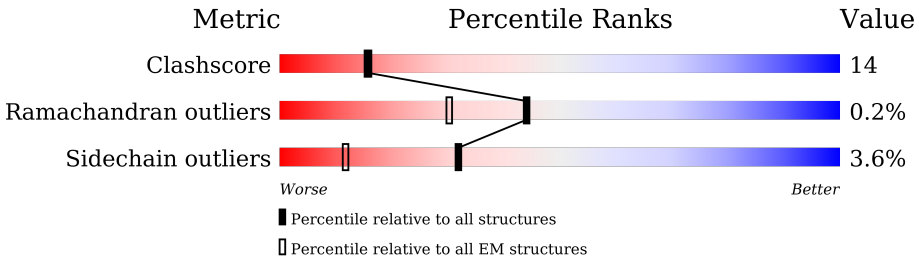
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

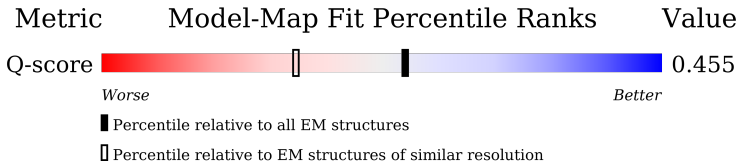
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.07 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	13977 (2.57 - 3.57)

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	Z	62	77% 21%
1	z	62	84% 15%
2	E	82	51% 27% 21%
2	e	82	67% 12% 21%

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Mol	Chain	Length	Quality of chain
3	H	75	64% 27% 9%
3	h	75	5% 63% 28% 9%
4	I	36	83% 11% 6%
4	i	36	83% 11% 6%
5	K	43	60% 23% 14%
5	k	43	72% 14% 14%
6	L	38	66% 26% 5%
6	l	38	63% 32%
7	M	33	9% 61% 30% 9%
7	m	33	9% 58% 30% 9%
8	R	267	16% 53% 29% 16%
8	r	267	17% 58% 24% 16%
9	F	42	55% 17% 26%
9	f	42	55% 17% 26%
10	1	212	58% 68% 30%
10	4	212	58% 73% 25%
11	2	256	10% 66% 20% 14%
11	5	256	9% 65% 21% 14%
12	3	254	54% 59% 23% 17%
12	6	254	58% 59% 26% 14%
12	7	254	56% 27% 14%
12	9	254	86% 53% 31% 14%
12	p	254	55% 27% 14%
12	u	254	86% 52% 32% 14%
13	S	308	51% 27% 19%

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Mol	Chain	Length	Quality of chain
13	s	308	52% 26% 19%
14	X	109	28% 69%
14	x	109	28% 69%
15	V	33	42% 48% 21% 6% 24%
15	v	33	39% 52% 21% 24%
16	T	31	65% 26% 10%
16	t	31	65% 26% 10%
17	8	280	51% 22% 26%
17	G	280	60% 57% 22% 20%
17	N	280	45% 49% 22% 26%
17	Y	280	58% 22% 20%
17	g	280	60% 56% 24% 20%
17	n	280	45% 49% 23% 26%
17	q	280	51% 22% 26%
17	y	280	59% 21% 20%
18	B	508	70% 22% 6%
18	b	508	72% 21% 6%
19	A	327	70% 28%
19	a	327	72% 27%
20	C	461	5% 75% 21%
20	c	461	5% 74% 21%
21	D	352	74% 21%
21	d	352	74% 22%
22	W	118	29% 7% 64%
22	w	118	30% 7% 64%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	NEX	1	303	-	-	X	-
28	NEX	3	318	-	-	X	-
28	NEX	4	303	-	-	X	-
28	NEX	6	303	-	-	X	-
28	NEX	7	304	-	-	X	-
28	NEX	G	304	-	-	X	-
28	NEX	S	617	-	-	X	-
28	NEX	p	304	-	-	X	-
28	NEX	s	401	-	-	X	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 95298 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	61	Total	C	N	O	S	0	0
			472	329	68	74	1		
1	z	61	Total	C	N	O	S	0	0
			472	329	68	74	1		

- Molecule 2 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	65	Total	C	N	O	0	0
			530	347	87	96		
2	e	65	Total	C	N	O	0	0
			530	347	87	96		

- Molecule 3 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	68	Total	C	N	O	S	0	0
			513	337	74	98	4		
3	h	68	Total	C	N	O	S	0	0
			513	337	74	98	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	34	Total	C	N	O	S	0	0
			275	189	40	45	1		
4	i	34	Total	C	N	O	S	0	0
			275	189	40	45	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	26	ASP	ASN	conflict	UNP A0A2P0QH95

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Chain	Residue	Modelled	Actual	Comment	Reference
i	26	ASP	ASN	conflict	UNP A0A2P0QH95

- Molecule 5 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	37	Total 299	C 208	N 43	O 48	0	0
5	k	37	Total 299	C 208	N 43	O 48	0	0

- Molecule 6 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	37	Total 304	C 204	N 48	O 52	0	0
6	l	37	Total 304	C 204	N 48	O 52	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	30	Total 231	C 159	N 33	O 39	0	0
7	m	30	Total 231	C 159	N 33	O 39	0	0

- Molecule 8 is a protein called PsbR.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	225	Total 1711	C 1092	N 284	O 326	S 9	0	0
8	r	225	Total 1707	C 1089	N 283	O 326	S 9	0	0

- Molecule 9 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	31	Total 246	C 167	N 40	O 38	S 1	0	0
9	f	31	Total 251	C 170	N 42	O 38	S 1	0	0

- Molecule 10 is a protein called Lhcb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	212	Total	C	N	O	S	0	0
			1609	1038	255	306	10		
10	4	212	Total	C	N	O	S	0	0
			1603	1035	252	306	10		

- Molecule 11 is a protein called Lhcb2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	221	Total	C	N	O	S	0	0
			1710	1108	278	316	8		
11	5	221	Total	C	N	O	S	0	0
			1711	1109	279	315	8		

- Molecule 12 is a protein called Lhcb3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3	211	Total	C	N	O	S	0	0
			1606	1033	260	304	9		
12	9	219	Total	C	N	O	S	0	0
			1680	1081	271	319	9		
12	6	219	Total	C	N	O	S	0	0
			1670	1073	271	317	9		
12	u	219	Total	C	N	O	S	0	0
			1683	1084	271	319	9		
12	p	219	Total	C	N	O	S	0	0
			1680	1081	271	319	9		
12	7	219	Total	C	N	O	S	0	0
			1677	1080	271	317	9		

- Molecule 13 is a protein called LhcbS.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	249	Total	C	N	O	S	0	0
			1867	1203	309	349	6		
13	s	249	Total	C	N	O	S	0	0
			1867	1203	309	349	6		

- Molecule 14 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	34	Total 226	C 146	N 36	O 44	0	0
14	x	34	Total 226	C 146	N 36	O 44	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	V	25	Total 179	C 118	N 30	O 31	0	0
15	v	25	Total 179	C 118	N 30	O 31	0	0

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	28	Total 236	C 165	N 34	O 36	S 1	0	0
16	t	28	Total 236	C 165	N 34	O 36	S 1	0	0

- Molecule 17 is a protein called LhcbG.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	223	Total 1690	C 1097	N 268	O 315	S 10	0	0
17	N	206	Total 1551	C 1002	N 247	O 292	S 10	0	0
17	Y	223	Total 1690	C 1097	N 268	O 315	S 10	0	0
17	8	206	Total 1554	C 1005	N 247	O 292	S 10	0	0
17	g	223	Total 1690	C 1097	N 268	O 315	S 10	0	0
17	n	206	Total 1545	C 998	N 247	O 290	S 10	0	0
17	y	223	Total 1690	C 1097	N 268	O 315	S 10	0	0
17	q	206	Total 1554	C 1005	N 247	O 292	S 10	0	0

- Molecule 18 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	478	Total	C	N	O	S	0	0
			3737	2447	625	652	13		
18	b	478	Total	C	N	O	S	0	0
			3737	2447	625	652	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	281	ALA	SER	conflict	UNP A0A0D6E1D0
B	353	GLU	GLN	conflict	UNP A0A0D6E1D0
B	355	HIS	TYR	conflict	UNP A0A0D6E1D0
b	281	ALA	SER	conflict	UNP A0A0D6E1D0
b	353	GLU	GLN	conflict	UNP A0A0D6E1D0
b	355	HIS	TYR	conflict	UNP A0A0D6E1D0

- Molecule 19 is a protein called PsbA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	327	Total	C	N	O	S	0	0
			2558	1669	422	453	14		
19	a	327	Total	C	N	O	S	0	0
			2558	1669	422	453	14		

- Molecule 20 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	C	448	Total	C	N	O	S	0	0
			3472	2281	581	599	11		
20	c	448	Total	C	N	O	S	0	0
			3472	2281	581	599	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	VAL	MET	conflict	UNP D0EVT6
c	1	VAL	MET	conflict	UNP D0EVT6

- Molecule 21 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	340	Total	C	N	O	S	0	0
			2719	1803	447	458	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	340	Total	C	N	O	S	0	0
			2719	1803	447	458	11		

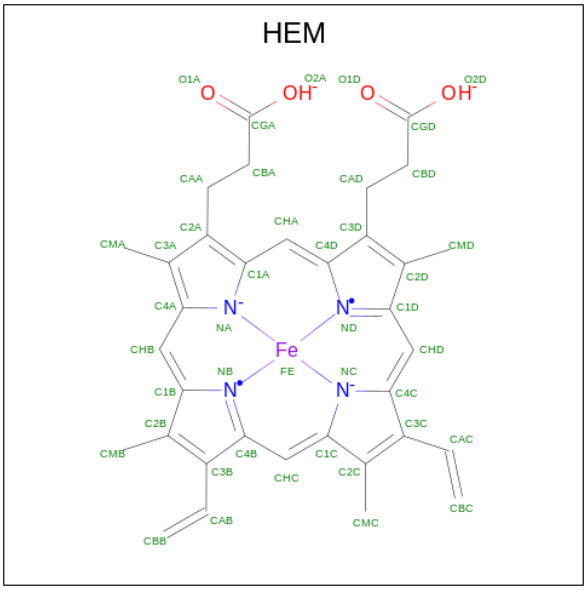
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	55	ILE	VAL	conflict	UNP A0A0B5GKA5
d	55	ILE	VAL	conflict	UNP A0A0B5GKA5

- Molecule 22 is a protein called PsbW.

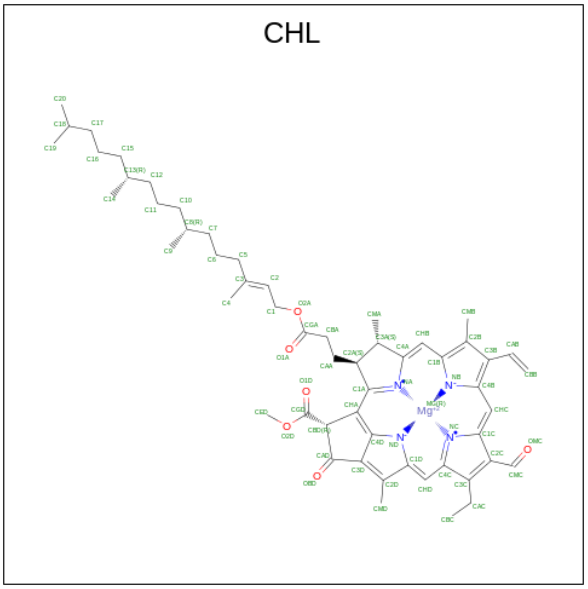
Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	43	Total	C	N	O	0	0
			304	191	49	64		
22	w	43	Total	C	N	O	0	0
			304	191	49	64		

- Molecule 23 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
23	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	R	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	3	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	3	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	S	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	G	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	G	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	N	1	Total	C	Mg	N	O	0
			54	43	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	N	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	N	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	Y	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	Y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	Y	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	6	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	g	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	u	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	u	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	u	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
24	n	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	y	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	p	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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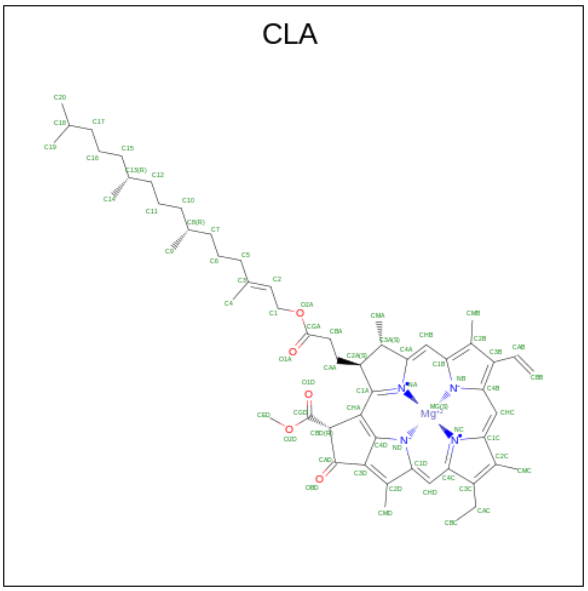
Mol	Chain	Residues	Atoms					AltConf
24	p	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	p	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	q	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	q	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
24	7	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
24	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 25 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
25	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
25	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	Y	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
25	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	u	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	u	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	u	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	u	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	y	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	q	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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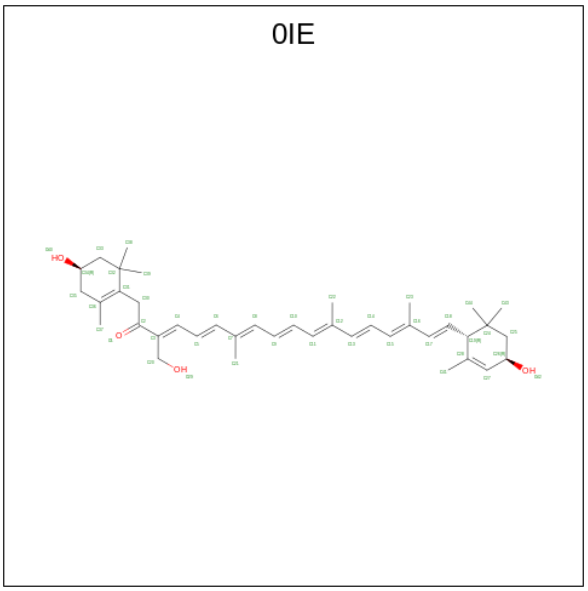
Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	s	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	s	1	Total 44	C 35	Mg 1	N 4	O 4	0
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	r	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	r	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	r	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	7	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	7	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	7	1	Total 52	C 42	Mg 1	N 4	O 5	0

- Molecule 26 is Siphonaxanthin (CCD ID: 0IE) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



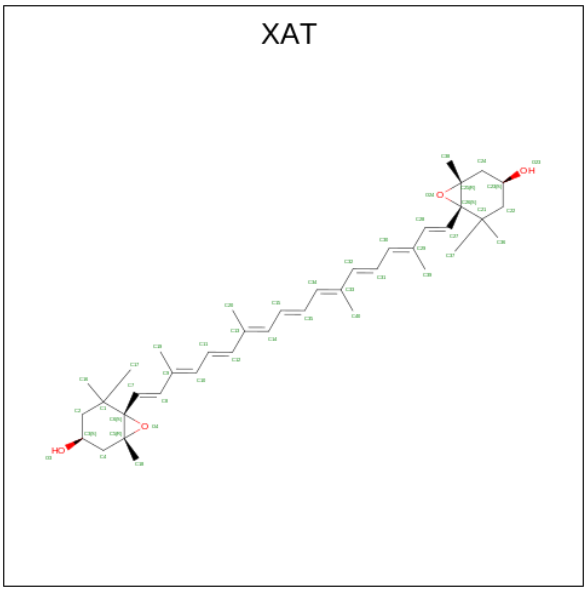
Mol	Chain	Residues	Atoms	AltConf
26	R	1	Total C O 44 40 4	0
26	1	1	Total C O 44 40 4	0
26	2	1	Total C O 44 40 4	0
26	2	1	Total C O 44 40 4	0
26	3	1	Total C O 43 39 4	0
26	3	1	Total C O 44 40 4	0
26	G	1	Total C O 44 40 4	0
26	G	1	Total C O 44 40 4	0
26	9	1	Total C O 44 40 4	0
26	9	1	Total C O 44 40 4	0
26	N	1	Total C O 44 40 4	0
26	Y	1	Total C O 44 40 4	0
26	Y	1	Total C O 44 40 4	0
26	8	1	Total C O 44 40 4	0

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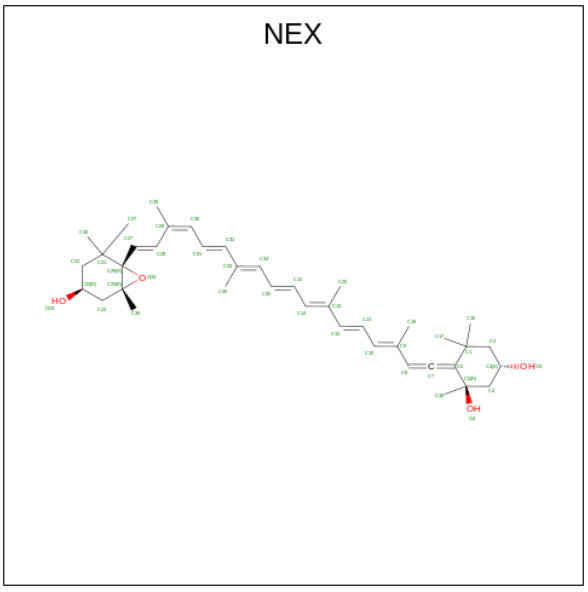
Mol	Chain	Residues	Atoms	AltConf
26	4	1	Total C O 44 40 4	0
26	5	1	Total C O 44 40 4	0
26	5	1	Total C O 44 40 4	0
26	6	1	Total C O 43 39 4	0
26	g	1	Total C O 44 40 4	0
26	g	1	Total C O 44 40 4	0
26	u	1	Total C O 44 40 4	0
26	u	1	Total C O 44 40 4	0
26	n	1	Total C O 44 40 4	0
26	y	1	Total C O 44 40 4	0
26	y	1	Total C O 44 40 4	0
26	p	1	Total C O 44 40 4	0
26	p	1	Total C O 44 40 4	0
26	q	1	Total C O 44 40 4	0
26	r	1	Total C O 44 40 4	0
26	7	1	Total C O 44 40 4	0
26	7	1	Total C O 44 40 4	0

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



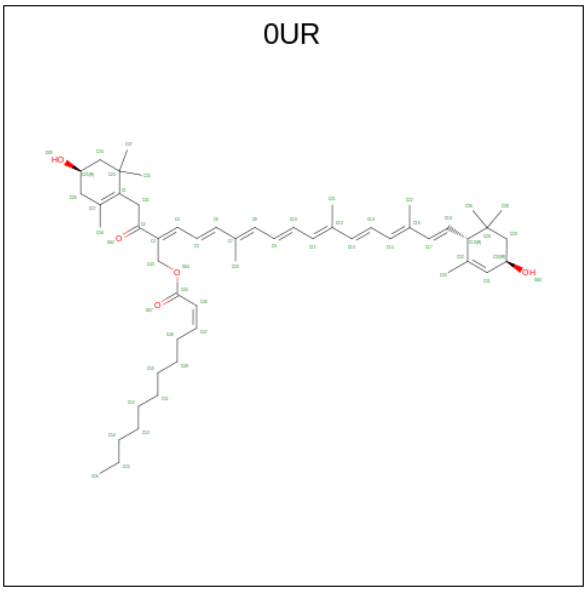
Mol	Chain	Residues	Atoms			AltConf
27	R	1	Total 44	C 40	O 4	0
27	r	1	Total 44	C 40	O 4	0

- Molecule 28 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	R	1	Total	C	O	0
			44	40	4	
28	1	1	Total	C	O	0
			44	40	4	
28	2	1	Total	C	O	0
			44	40	4	
28	3	1	Total	C	O	0
			44	40	4	
28	S	1	Total	C	O	0
			44	40	4	
28	G	1	Total	C	O	0
			44	40	4	
28	9	1	Total	C	O	0
			44	40	4	
28	N	1	Total	C	O	0
			44	40	4	
28	4	1	Total	C	O	0
			44	40	4	
28	5	1	Total	C	O	0
			44	40	4	
28	6	1	Total	C	O	0
			44	40	4	
28	g	1	Total	C	O	0
			44	40	4	
28	u	1	Total	C	O	0
			44	40	4	
28	n	1	Total	C	O	0
			44	40	4	
28	y	1	Total	C	O	0
			44	40	4	
28	p	1	Total	C	O	0
			44	40	4	
28	s	1	Total	C	O	0
			44	40	4	
28	r	1	Total	C	O	0
			44	40	4	
28	r	1	Total	C	O	0
			44	40	4	
28	7	1	Total	C	O	0
			44	40	4	

- Molecule 29 is Siphonein (CCD ID: 0UR) (formula: $C_{52}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



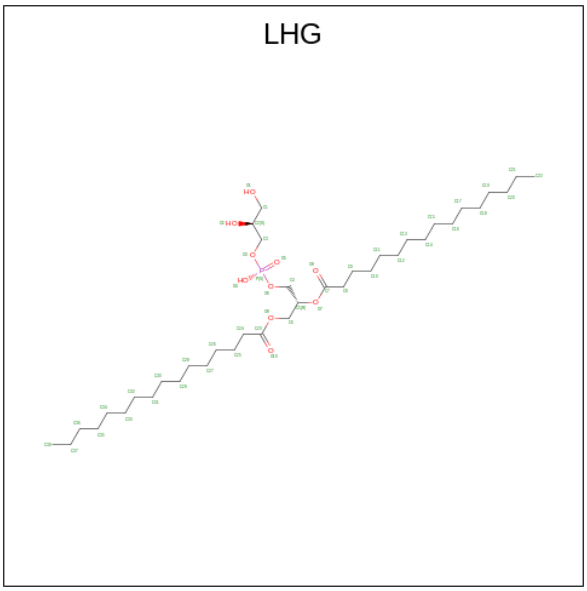
Mol	Chain	Residues	Atoms	AltConf
29	1	1	Total C O 52 47 5	0
29	2	1	Total C O 52 47 5	0
29	3	1	Total C O 52 47 5	0
29	G	1	Total C O 52 47 5	0
29	9	1	Total C O 52 47 5	0
29	N	1	Total C O 52 47 5	0
29	Y	1	Total C O 52 47 5	0
29	8	1	Total C O 52 47 5	0
29	4	1	Total C O 52 47 5	0
29	5	1	Total C O 52 47 5	0
29	6	1	Total C O 52 47 5	0
29	g	1	Total C O 52 47 5	0
29	u	1	Total C O 52 47 5	0
29	n	1	Total C O 52 47 5	0

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Mol	Chain	Residues	Atoms	AltConf
29	y	1	Total C O 52 47 5	0
29	p	1	Total C O 52 47 5	0
29	q	1	Total C O 52 47 5	0
29	7	1	Total C O 52 47 5	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



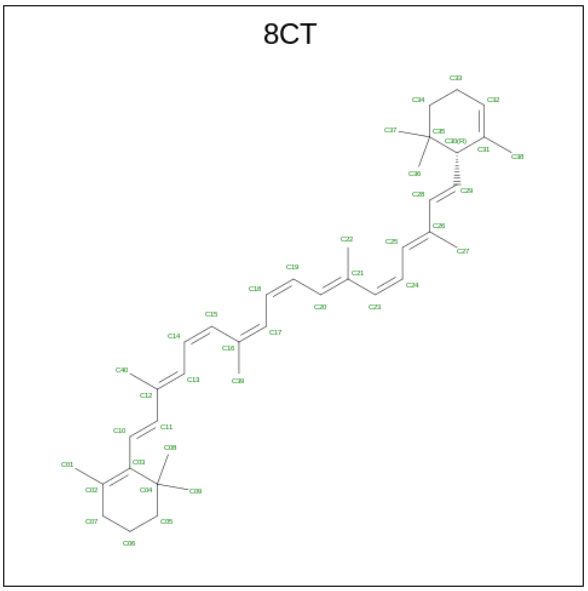
Mol	Chain	Residues	Atoms	AltConf
30	1	1	Total C O P 42 31 10 1	0
30	2	1	Total C O P 40 29 10 1	0
30	G	1	Total C O P 43 32 10 1	0
30	9	1	Total C O P 43 32 10 1	0
30	N	1	Total C O P 43 32 10 1	0
30	Y	1	Total C O P 43 32 10 1	0
30	A	1	Total C O P 45 34 10 1	0

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Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			44	33	10	1	
30	C	1	Total	C	O	P	0
			32	21	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			39	28	10	1	
30	4	1	Total	C	O	P	0
			42	31	10	1	
30	5	1	Total	C	O	P	0
			43	32	10	1	
30	g	1	Total	C	O	P	0
			43	32	10	1	
30	n	1	Total	C	O	P	0
			43	32	10	1	
30	y	1	Total	C	O	P	0
			43	32	10	1	
30	p	1	Total	C	O	P	0
			43	32	10	1	
30	a	1	Total	C	O	P	0
			45	34	10	1	
30	a	1	Total	C	O	P	0
			44	33	10	1	
30	c	1	Total	C	O	P	0
			32	21	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			39	28	10	1	
30	7	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 31 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



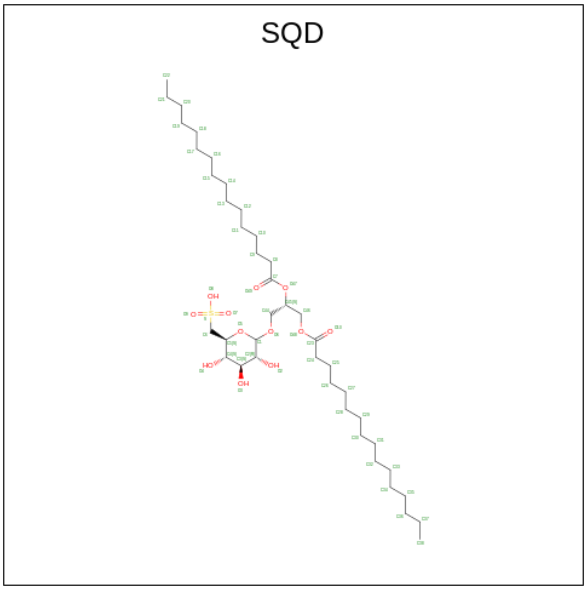
Mol	Chain	Residues	Atoms	AltConf
31	S	1	Total C 40 40	0
31	S	1	Total C 40 40	0
31	X	1	Total C 40 40	0
31	V	1	Total C 40 40	0
31	T	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	x	1	Total C 40 40	0
31	v	1	Total C 40 40	0
31	t	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
31	b	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	s	1	Total C 40 40	0
31	s	1	Total C 40 40	0

- Molecule 32 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).



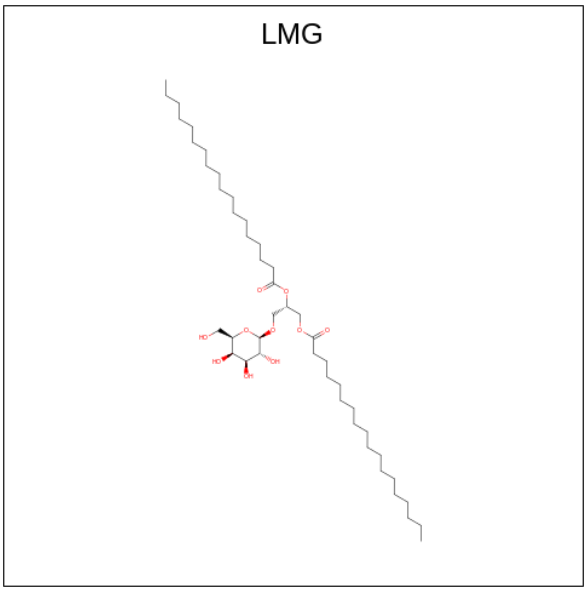
Mol	Chain	Residues	Atoms	AltConf
32	B	1	Total C O S 54 41 12 1	0
32	A	1	Total C O S 45 32 12 1	0

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Mol	Chain	Residues	Atoms				AltConf
32	D	1	Total	C	O	S	0
			44	31	12	1	
32	b	1	Total	C	O	S	0
			54	41	12	1	
32	a	1	Total	C	O	S	0
			45	32	12	1	
32	d	1	Total	C	O	S	0
			44	31	12	1	

- 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).



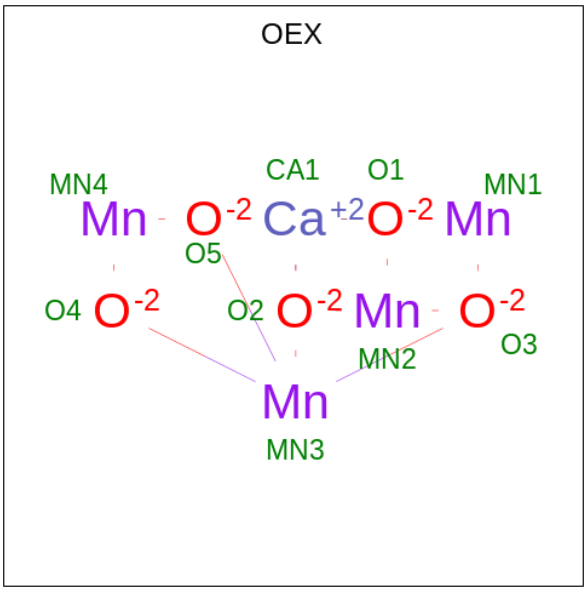
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			41	31	10	
33	C	1	Total	C	O	0
			42	32	10	
33	D	1	Total	C	O	0
			48	38	10	
33	D	1	Total	C	O	0
			46	36	10	
33	W	1	Total	C	O	0
			30	20	10	
33	i	1	Total	C	O	0
			48	38	10	
33	m	1	Total	C	O	0
			41	31	10	

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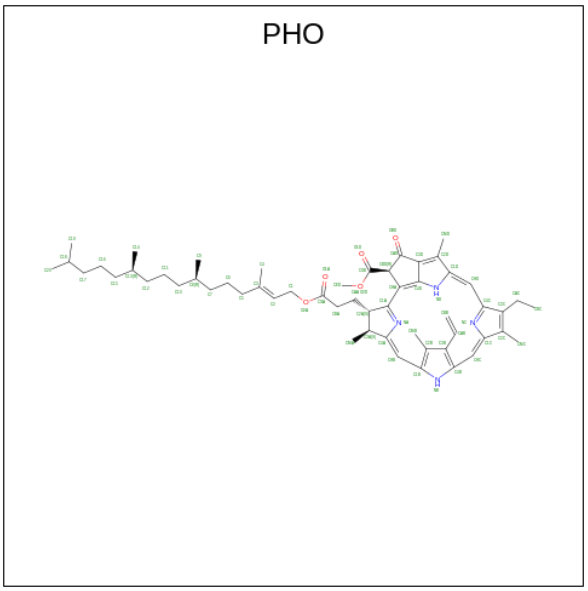
Mol	Chain	Residues	Atoms			AltConf
33	w	1	Total 36	C 26	O 10	0
33	d	1	Total 48	C 38	O 10	0
33	d	1	Total 46	C 36	O 10	0

- Molecule 34 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



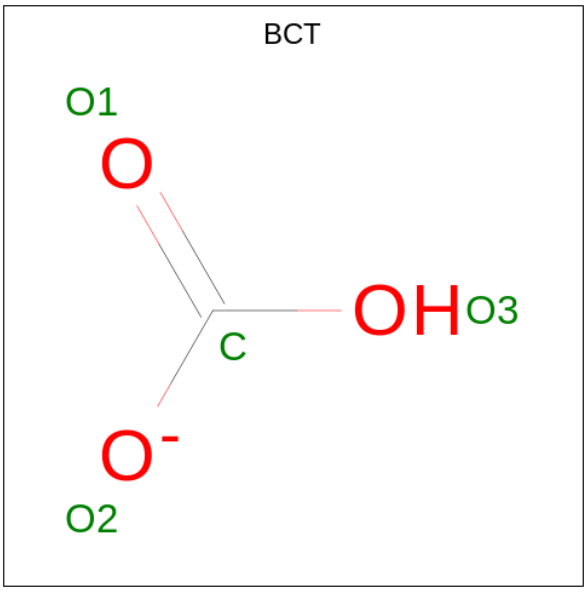
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total 10	Ca 1	Mn 4	O 5	0
34	a	1	Total 10	Ca 1	Mn 4	O 5	0

- Molecule 35 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



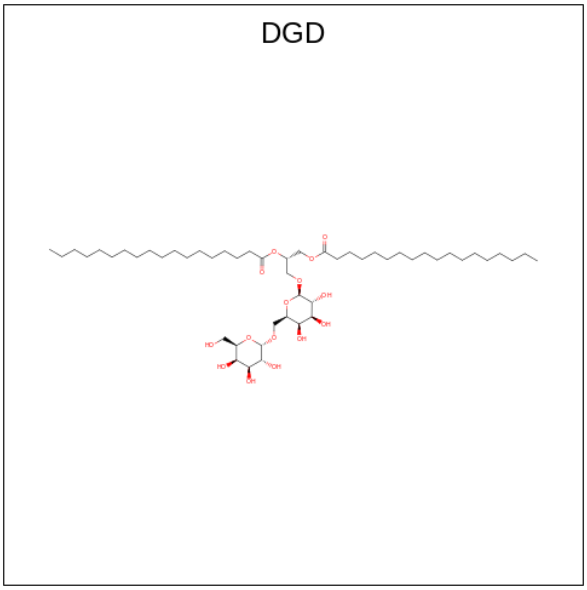
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	N	O	0
			64	55	4	5	
35	D	1	Total	C	N	O	0
			64	55	4	5	
35	a	1	Total	C	N	O	0
			64	55	4	5	
35	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

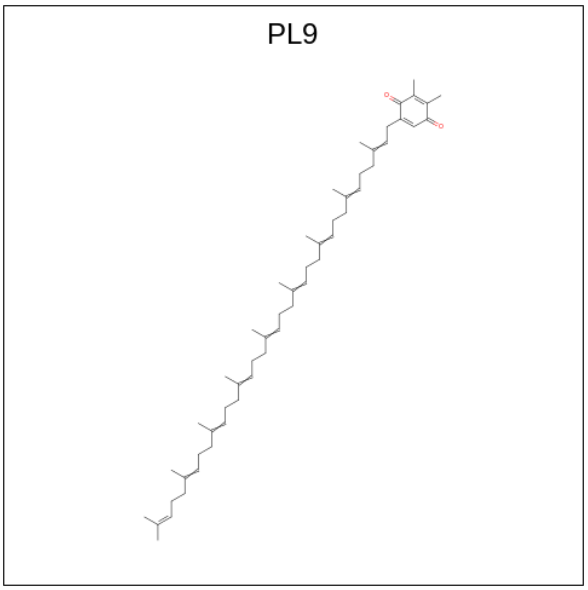


Mol	Chain	Residues	Atoms	AltConf
37	C	1	Total C O 50 35 15	0
37	C	1	Total C O 55 40 15	0
37	c	1	Total C O 50 35 15	0
37	c	1	Total C O 55 40 15	0

- Molecule 38 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
38	D	1	Total Fe 1 1	0
38	d	1	Total Fe 1 1	0

- Molecule 39 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



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

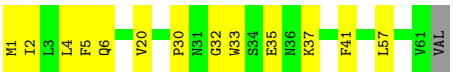
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II reaction center protein Z

Chain Z:





• Molecule 1: Photosystem II reaction center protein Z

Chain z:

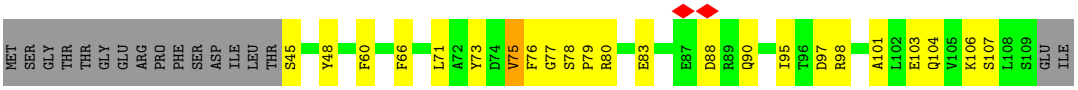




• Molecule 2: Cytochrome b559 subunit alpha

Chain E:





• Molecule 2: Cytochrome b559 subunit alpha

Chain e:

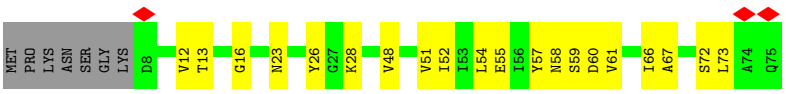




• Molecule 3: Photosystem II reaction center protein H

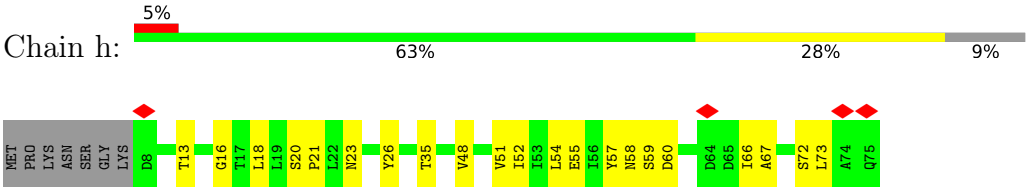
Chain H:





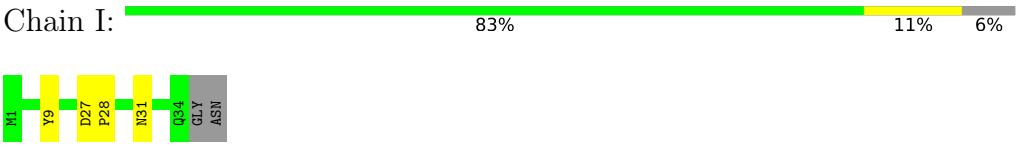
• Molecule 3: Photosystem II reaction center protein H

Chain h:



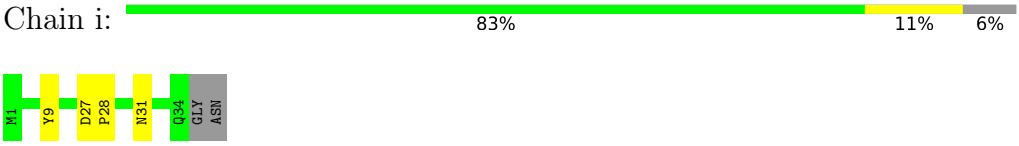
• Molecule 4: Photosystem II reaction center protein I

Chain I:



• Molecule 4: Photosystem II reaction center protein I

Chain i:



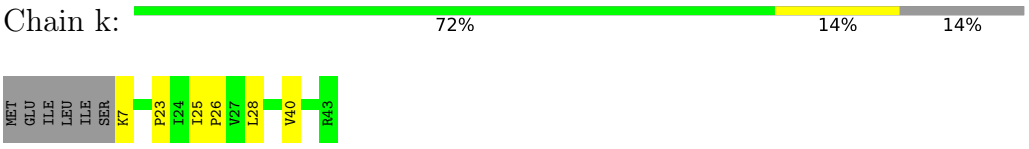
• Molecule 5: Photosystem II reaction center protein K

Chain K:



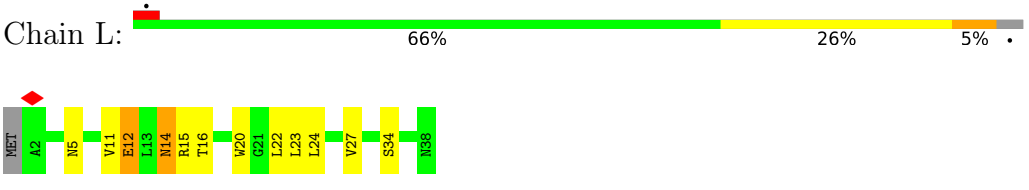
• Molecule 5: Photosystem II reaction center protein K

Chain k:



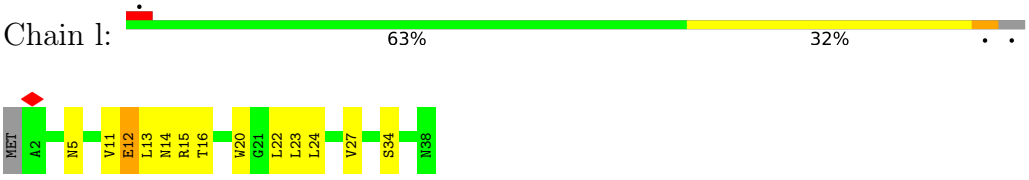
• Molecule 6: Photosystem II reaction center protein L

Chain L:

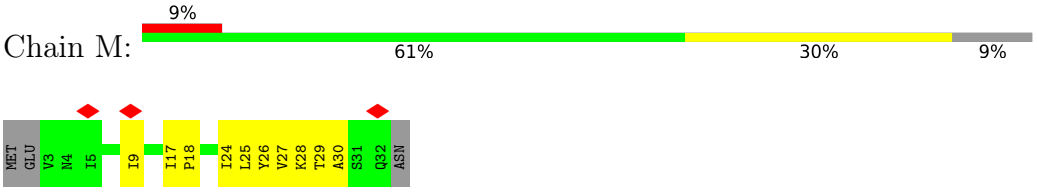


• Molecule 6: Photosystem II reaction center protein L

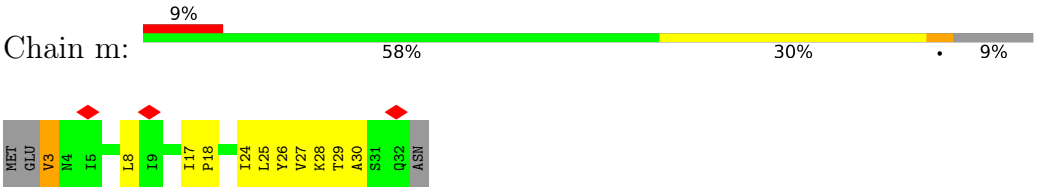
Chain l:



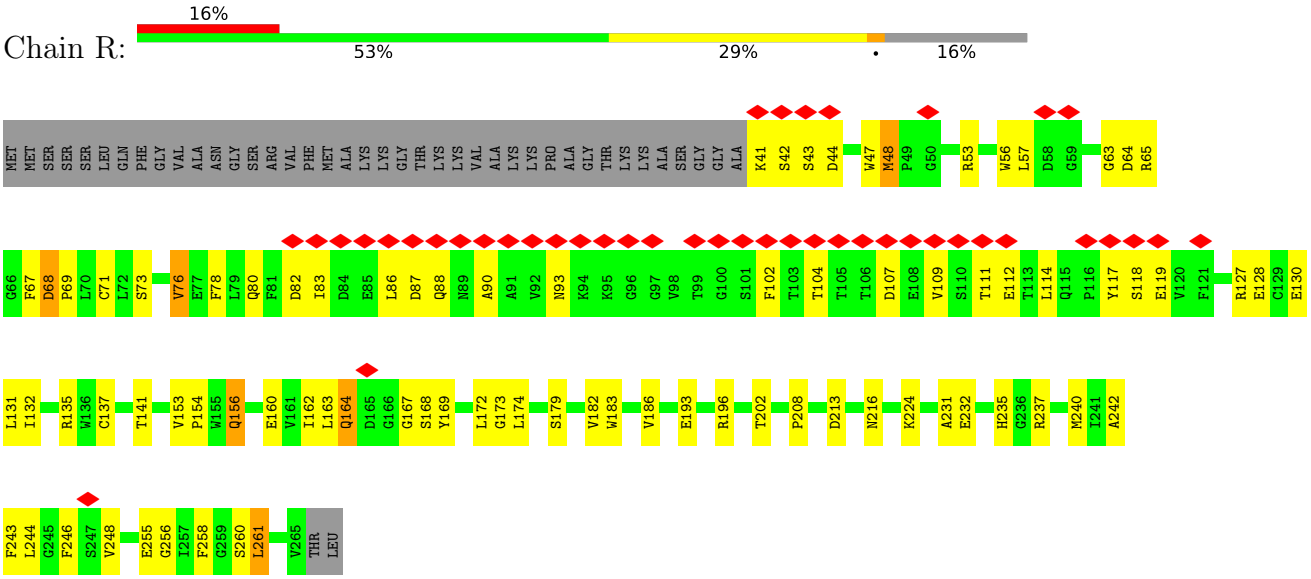
• Molecule 7: Photosystem II reaction center protein M



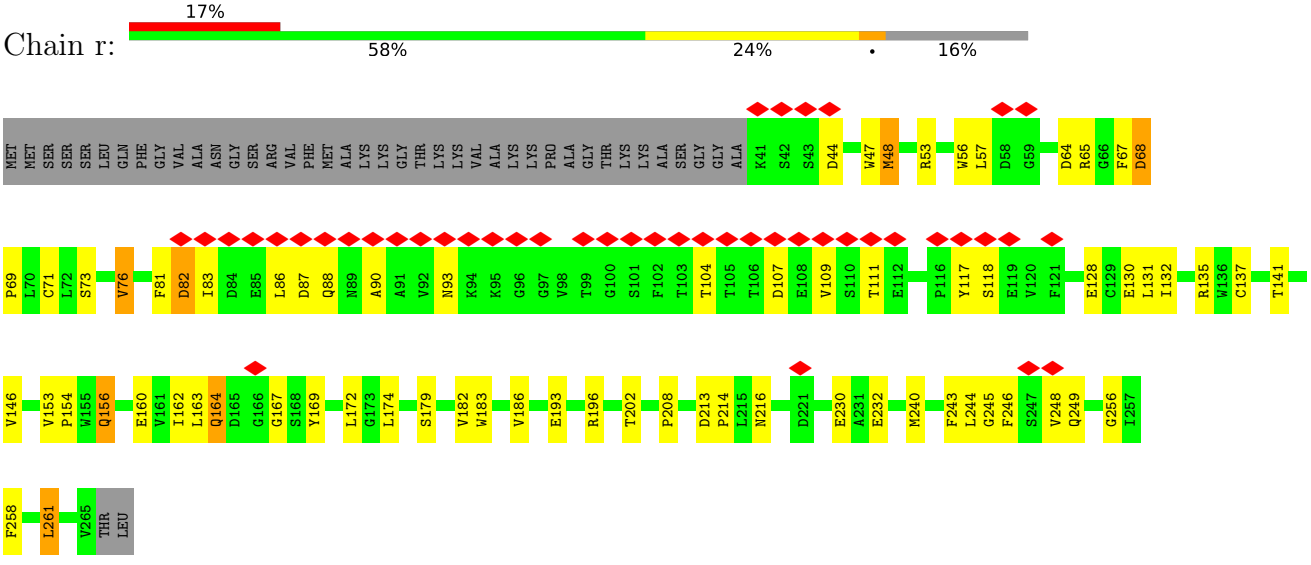
• Molecule 7: Photosystem II reaction center protein M



• Molecule 8: PsbR



• Molecule 8: PsbR



• Molecule 9: Cytochrome b559 subunit beta

Chain F:



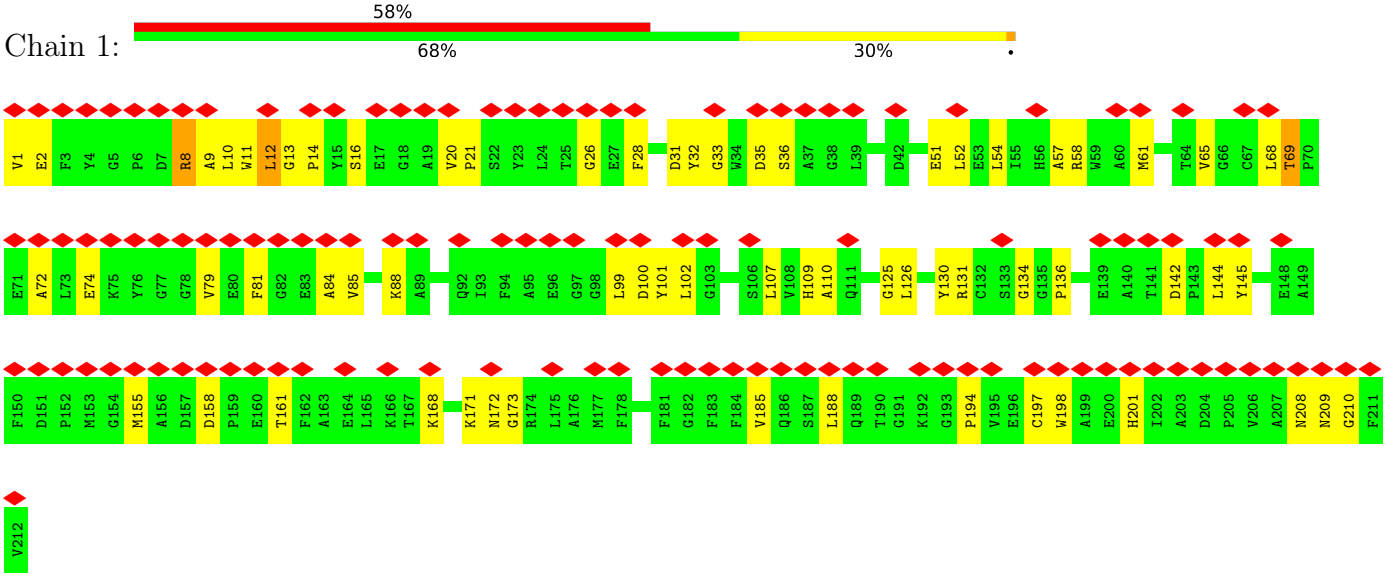
• Molecule 9: Cytochrome b559 subunit beta

Chain f:



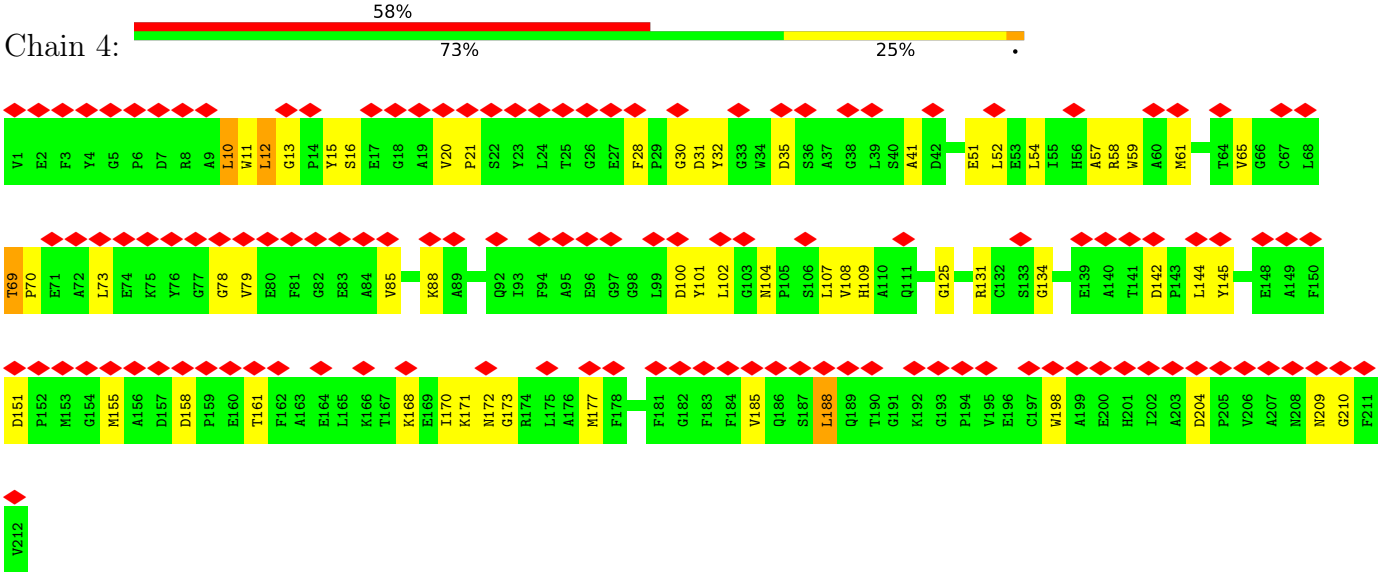
• Molecule 10: Lhcb1

Chain 1:



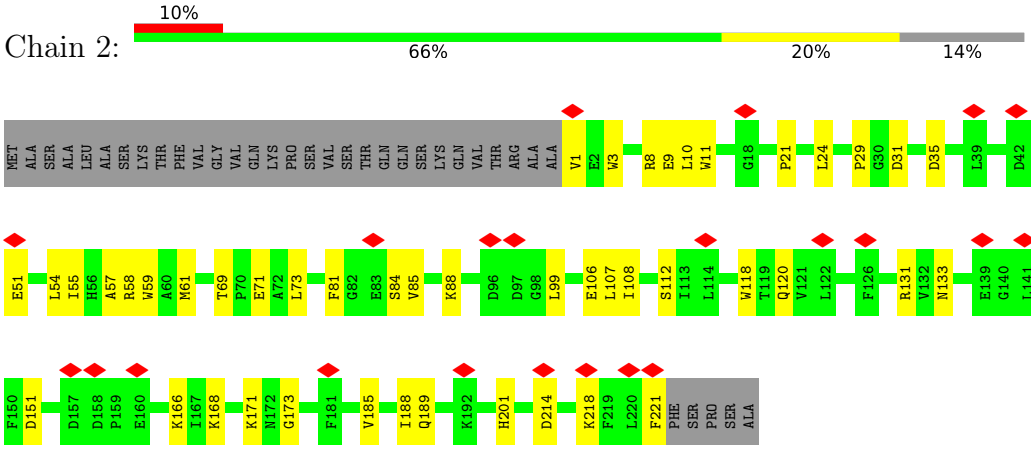
• Molecule 10: Lhcb1

Chain 4:



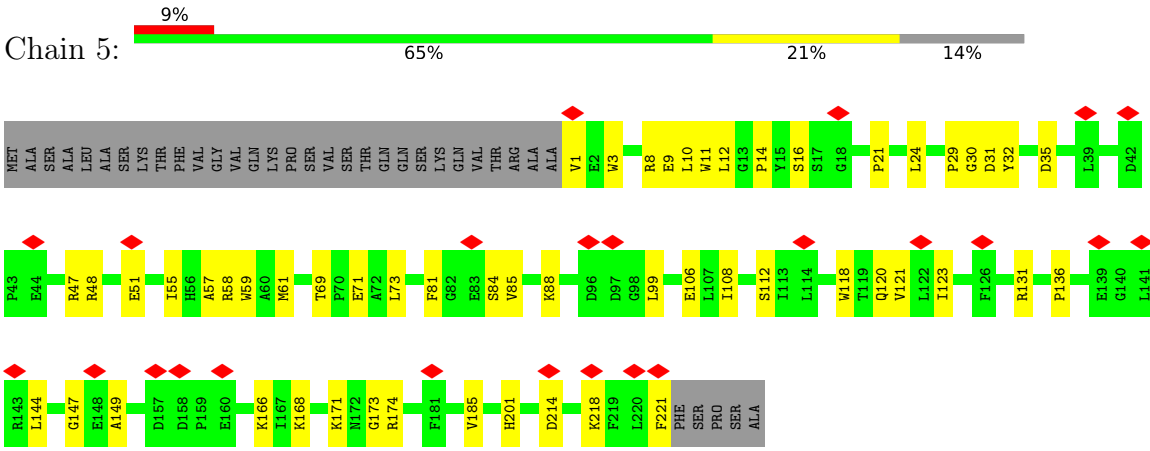
• Molecule 11: Lhcb2

Chain 2:



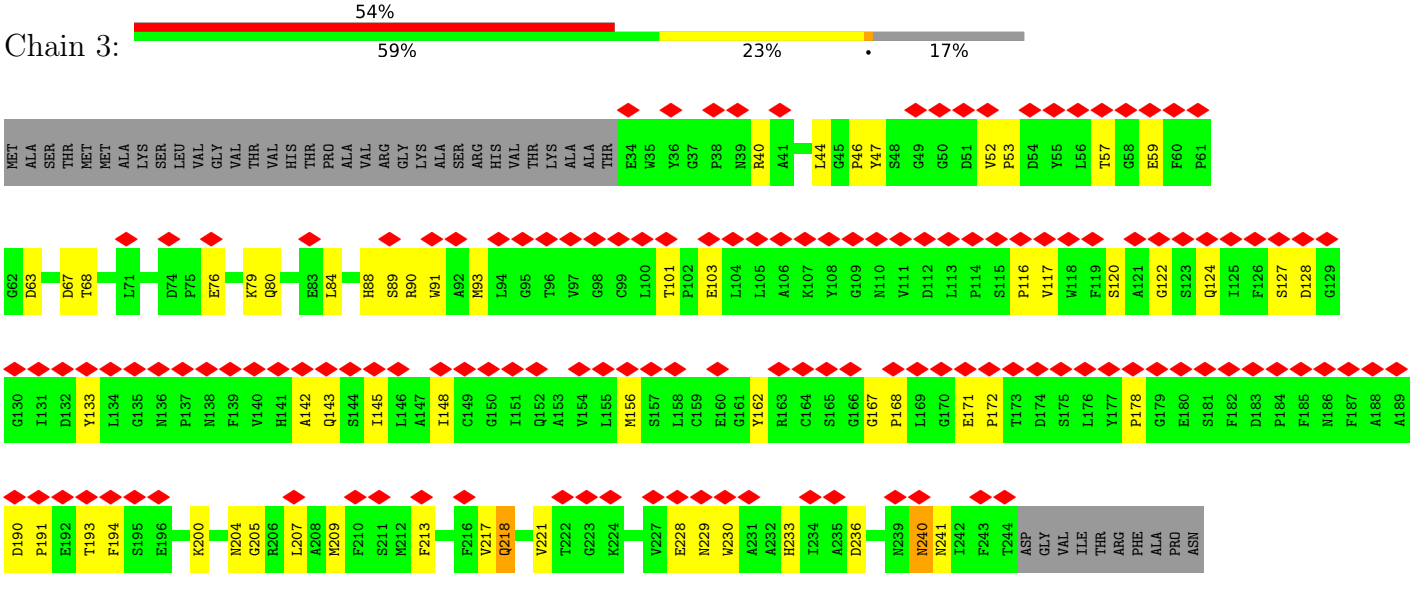
• Molecule 11: Lhcb2

Chain 5:



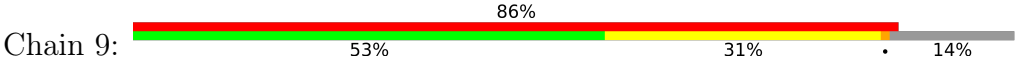
• Molecule 12: Lhcb3

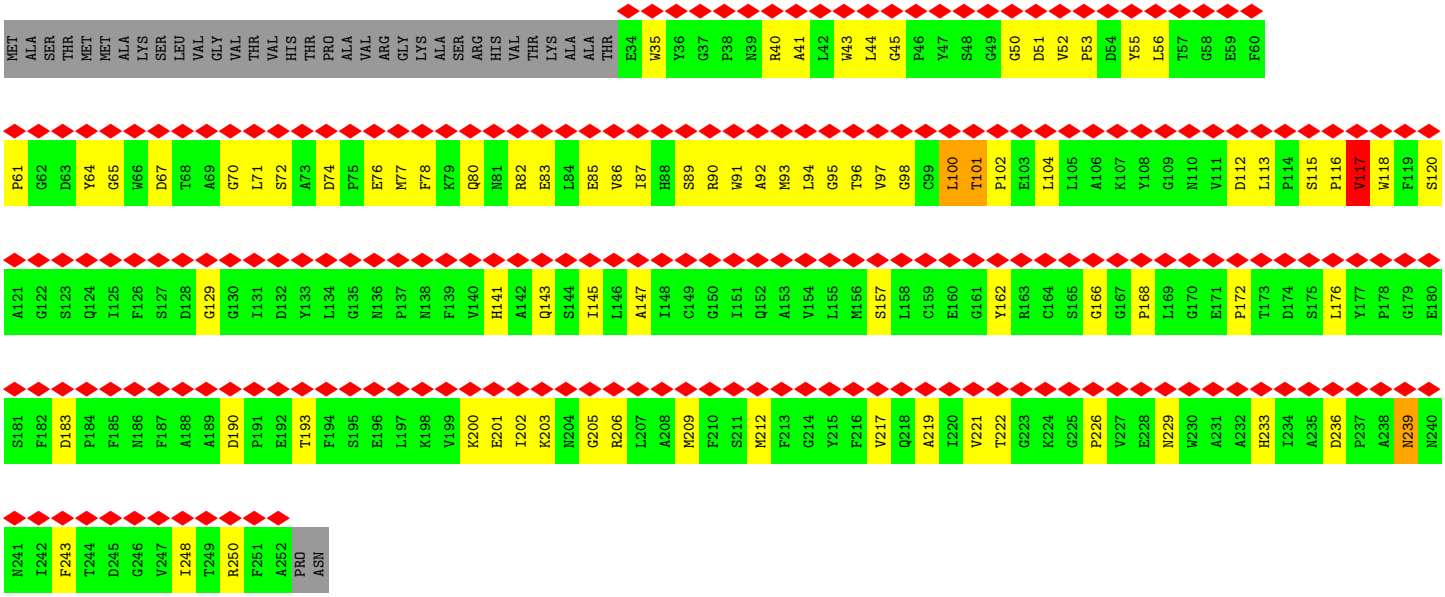
Chain 3:



• Molecule 12: Lhcb3

Chain 9:

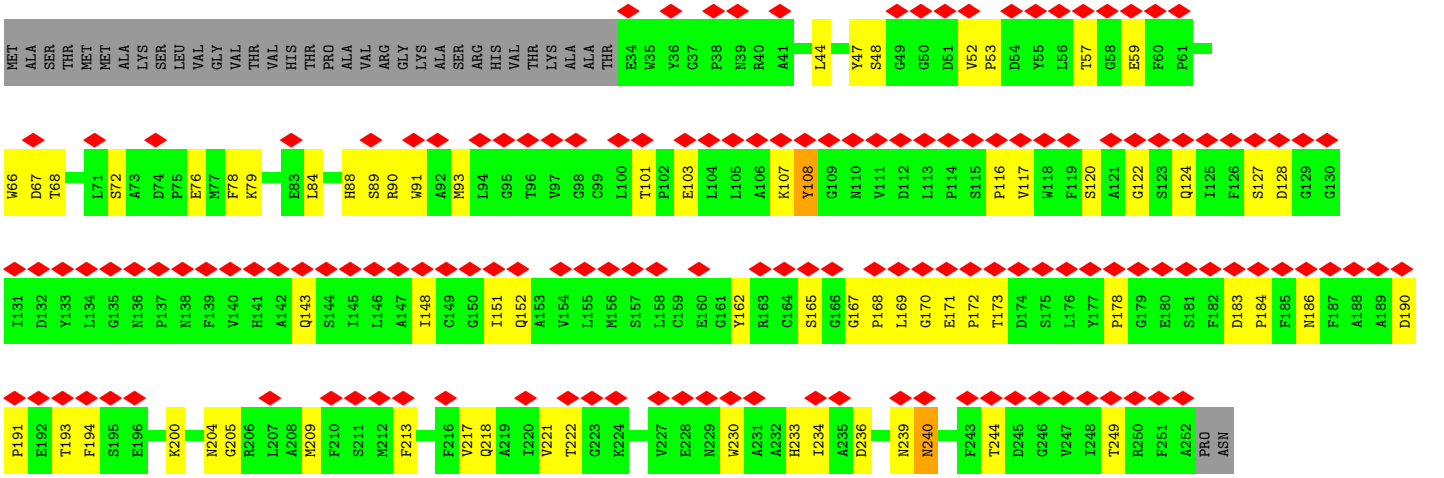




• Molecule 12: Lhcb3

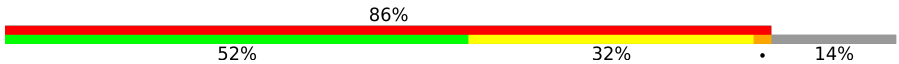
Chain 6:

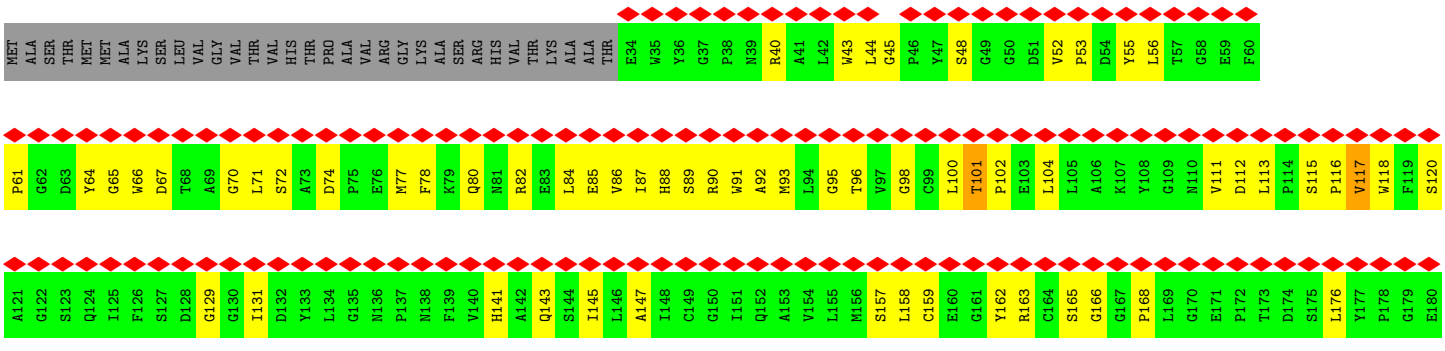


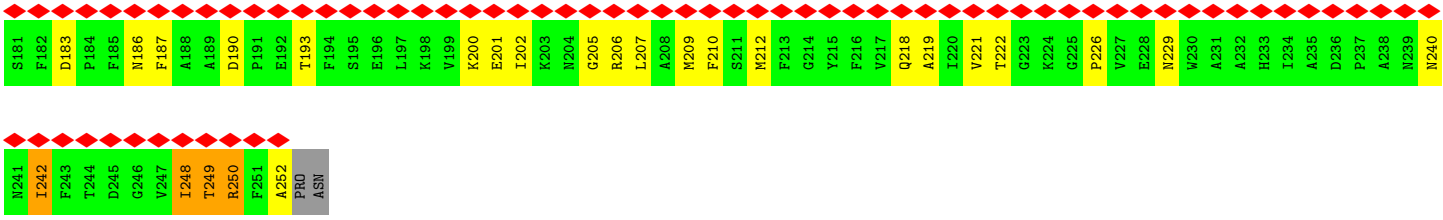


• Molecule 12: Lhcb3

Chain u:



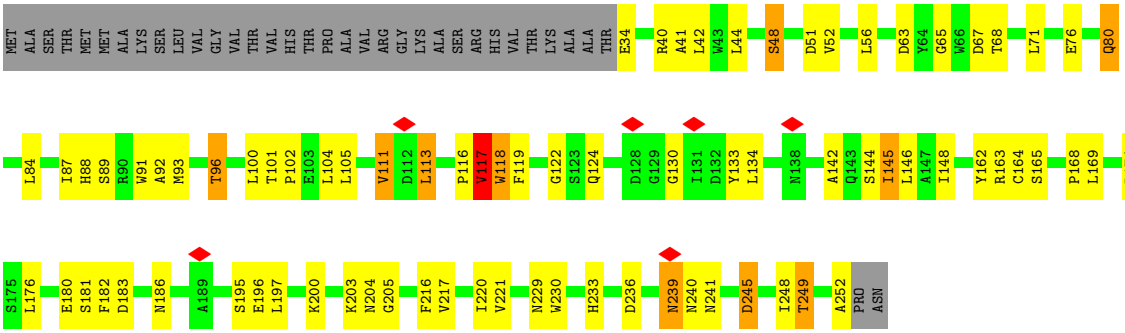




• Molecule 12: Lhcb3

Chain p:

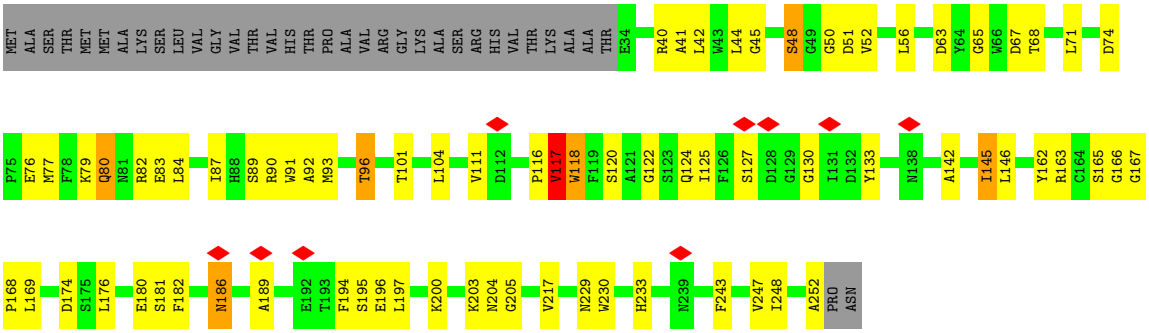




• Molecule 12: Lhcb3

Chain 7:

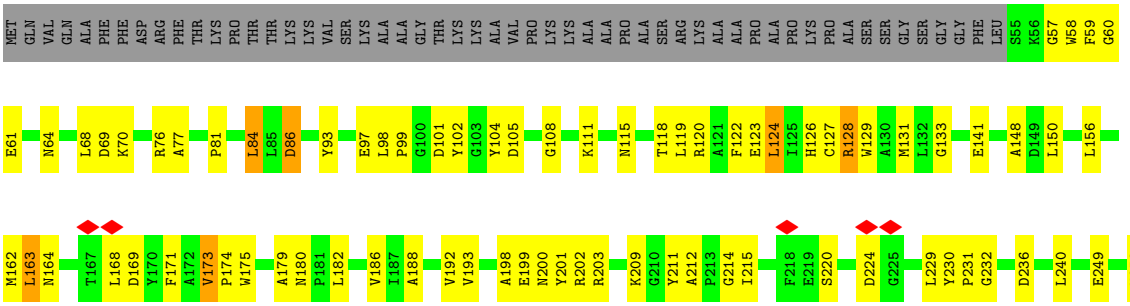


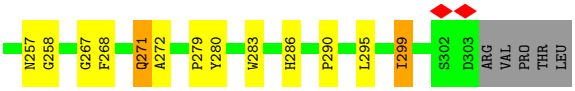


• Molecule 13: LhcbS

Chain S:

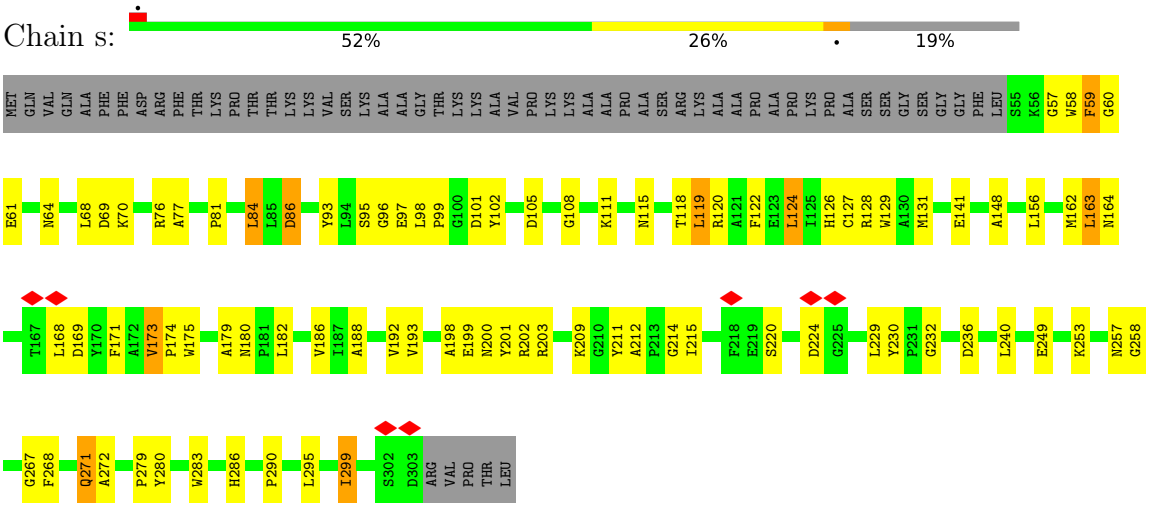






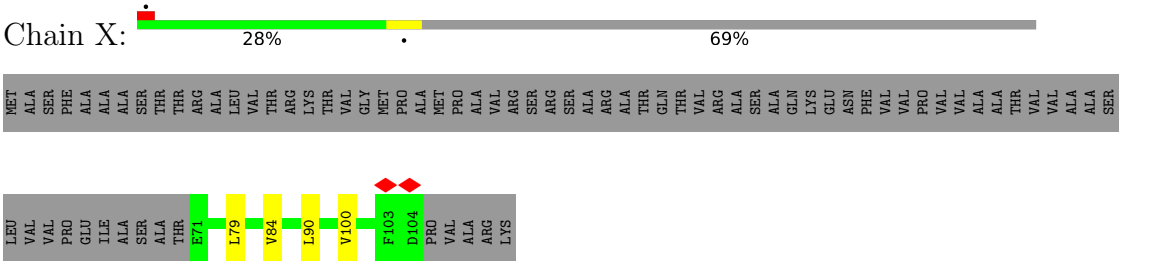
• Molecule 13: LhcbS

Chain s:



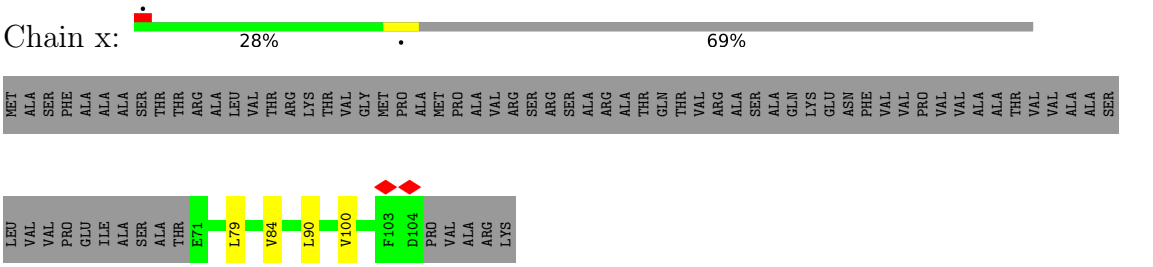
• Molecule 14: PsbX

Chain X:



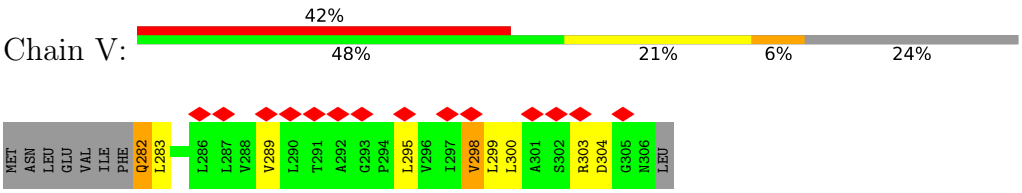
• Molecule 14: PsbX

Chain x:



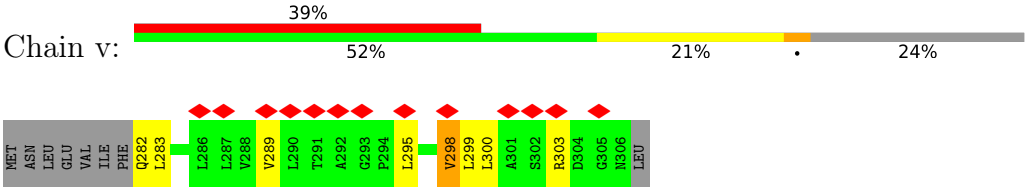
• Molecule 15: Photosystem II reaction center protein Psb30

Chain V:



• Molecule 15: Photosystem II reaction center protein Psb30

Chain v:



• Molecule 16: Photosystem II reaction center protein T

Chain T:



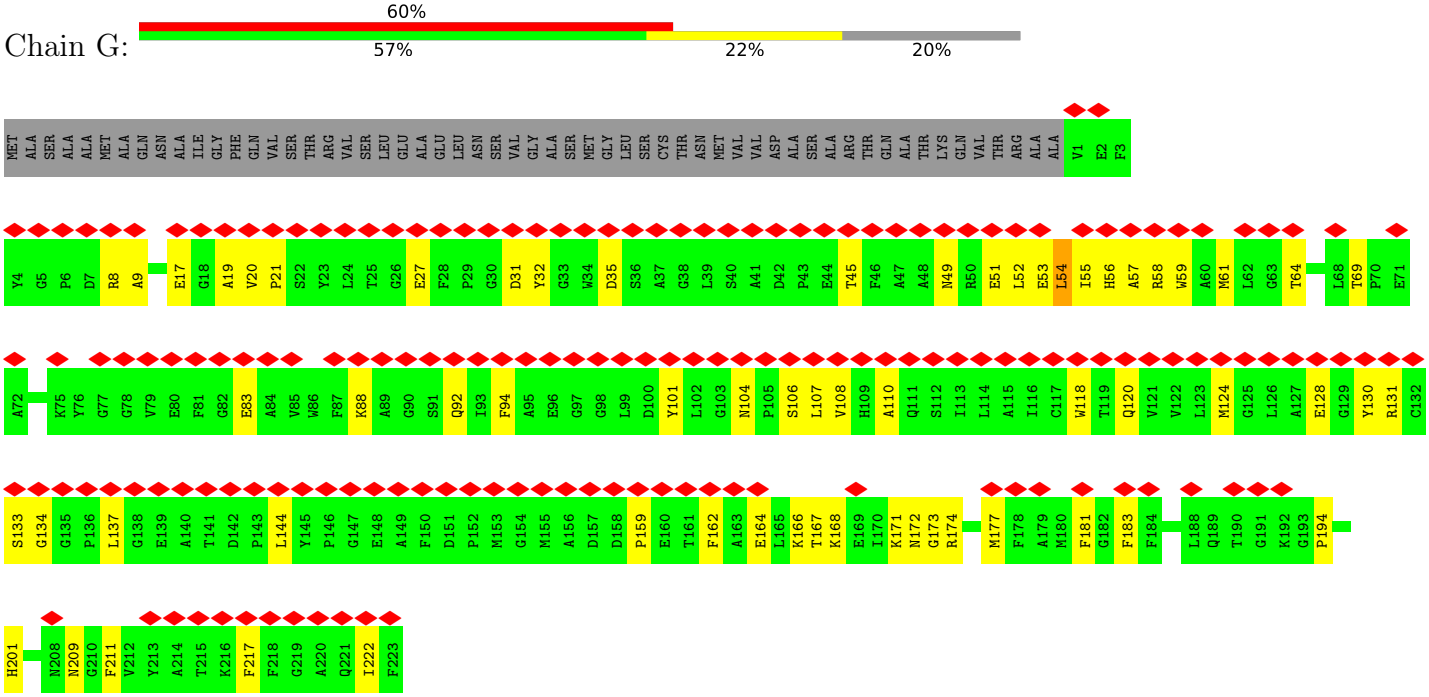
• Molecule 16: Photosystem II reaction center protein T

Chain t:



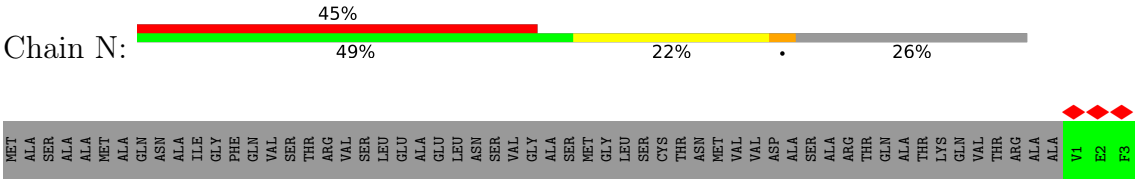
• Molecule 17: LhcbG

Chain G:



• Molecule 17: LhcbG

Chain N:

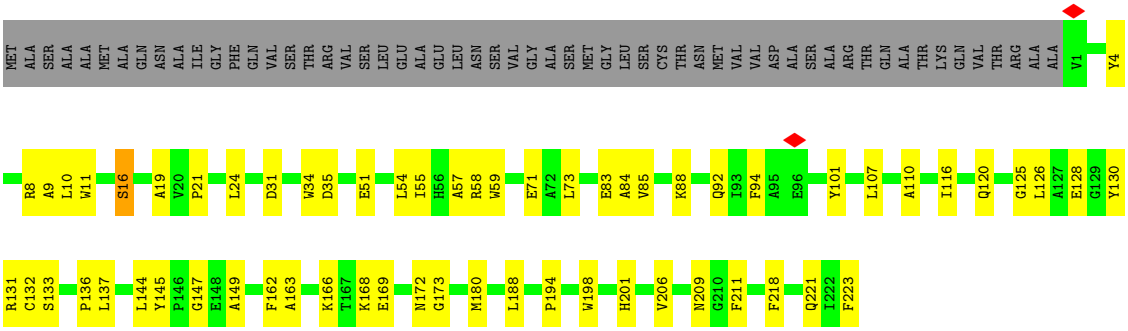




• Molecule 17: LhcbG

Chain Y:

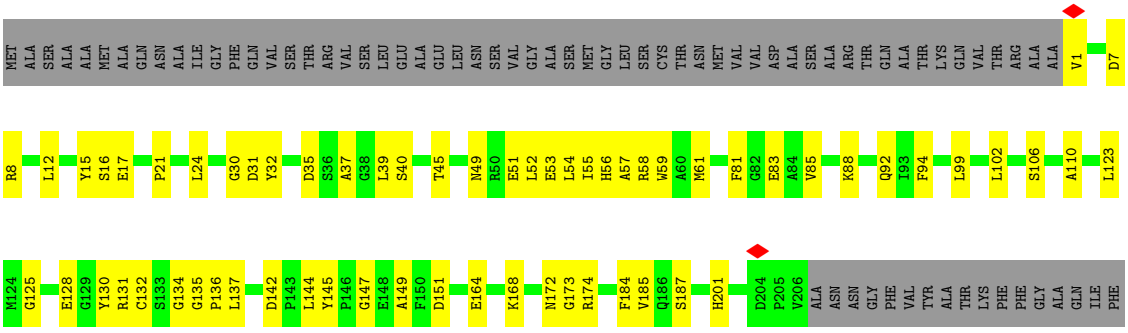




• Molecule 17: LhcbG

Chain 8:

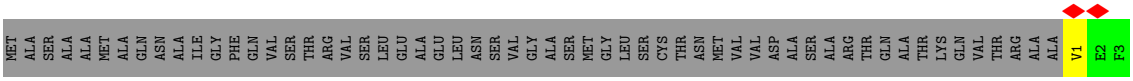




• Molecule 17: LhcbG

Chain g:



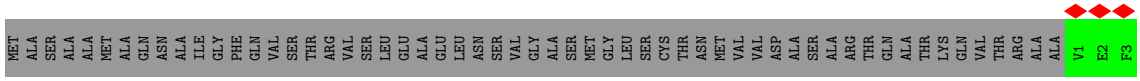


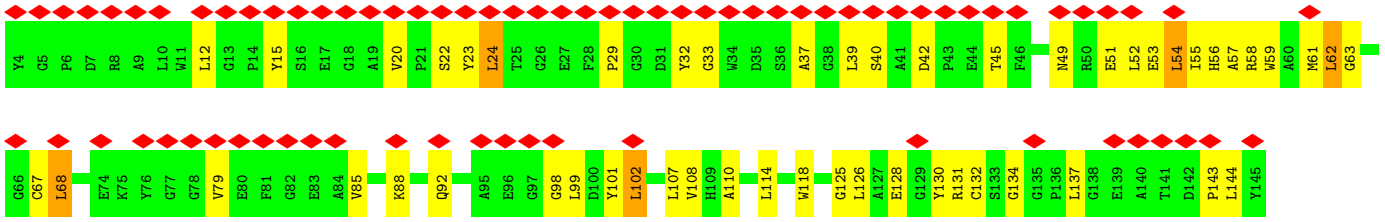


- Molecule 17: LhcbG

Chain n:



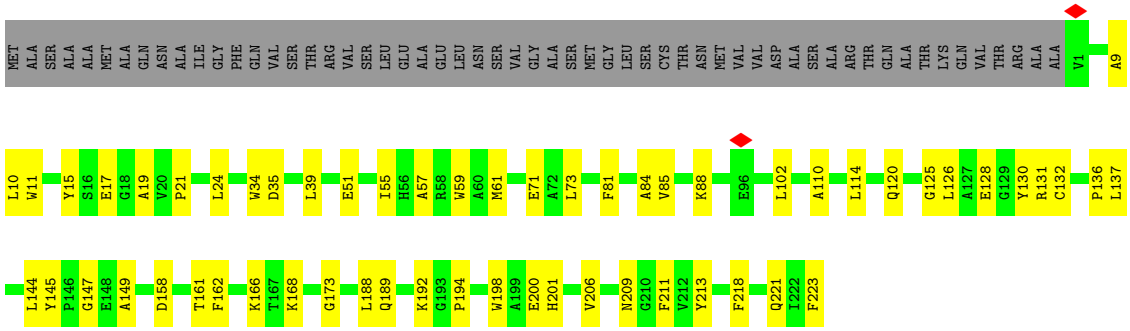




- Molecule 17: LhcbG

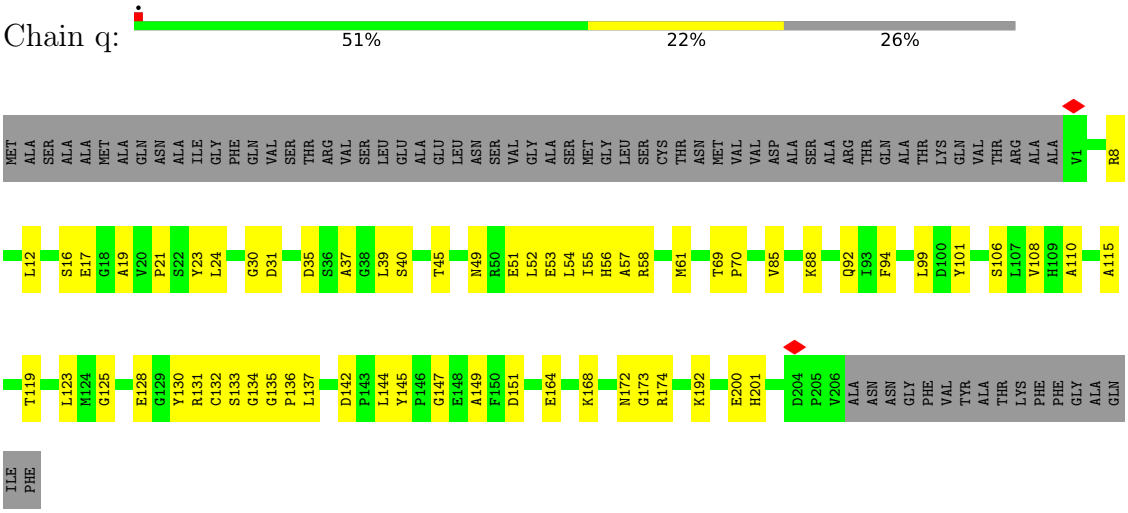
Chain y:





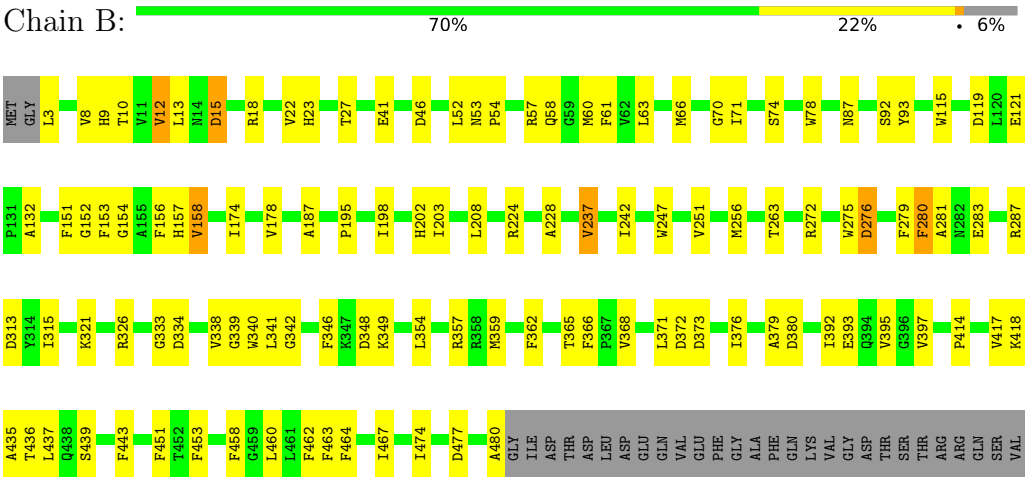
• Molecule 17: LhcbG

Chain q:



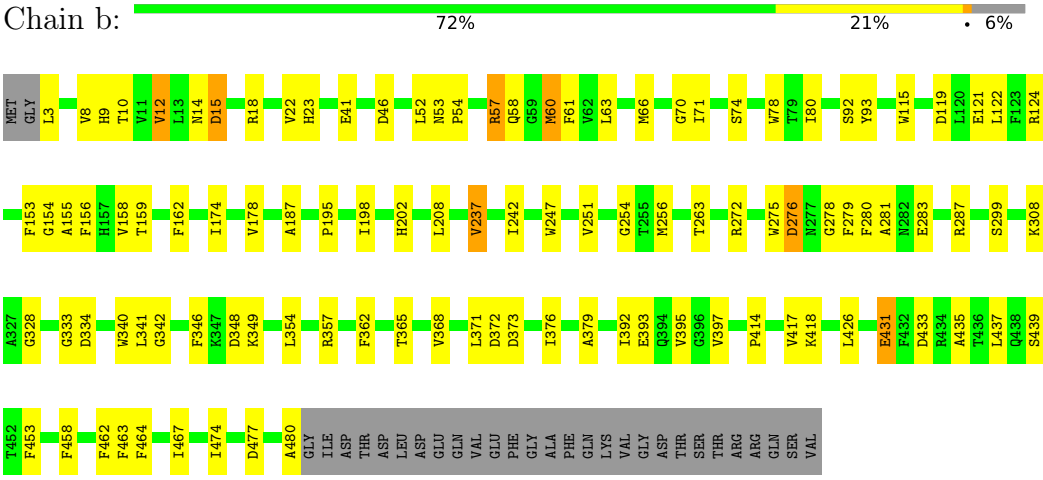
• Molecule 18: Photosystem II CP47 reaction center protein

Chain B:



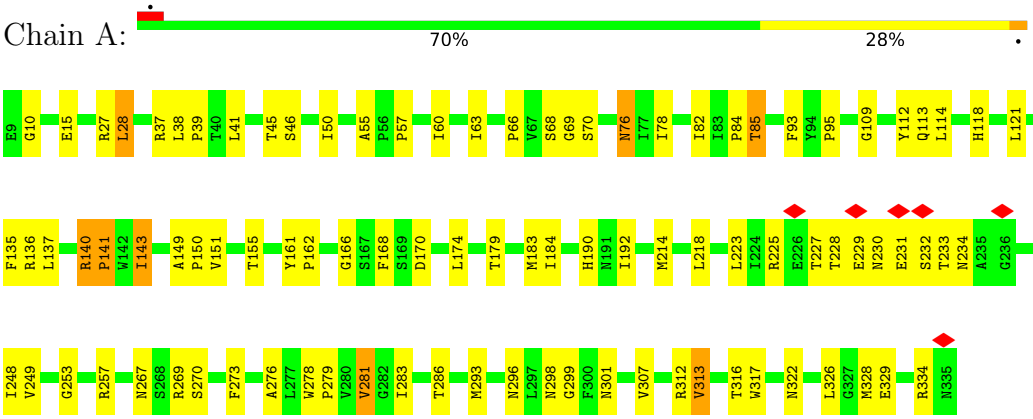
• Molecule 18: Photosystem II CP47 reaction center protein

Chain b:



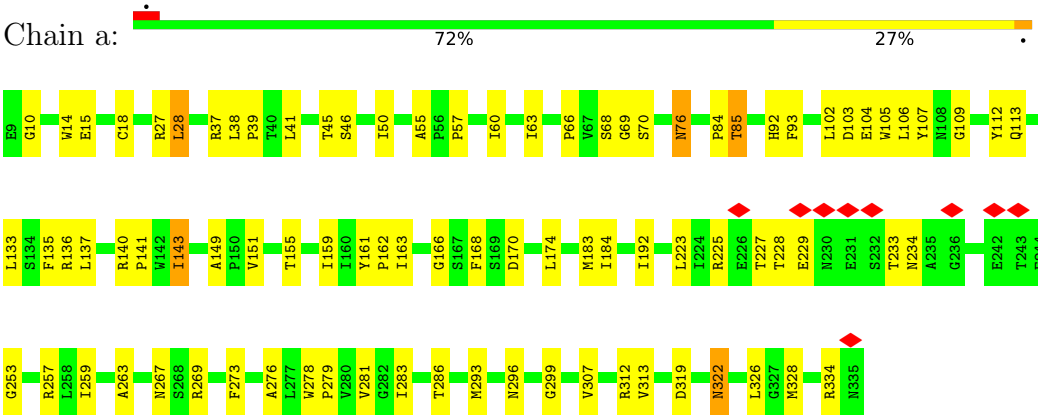
• Molecule 19: PsbA

Chain A:



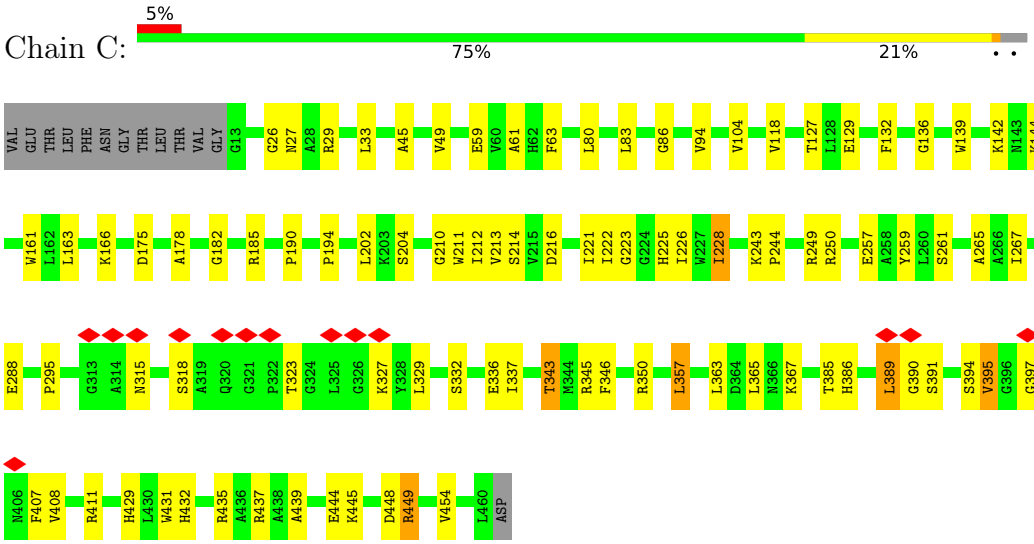
• Molecule 19: PsbA

Chain a:



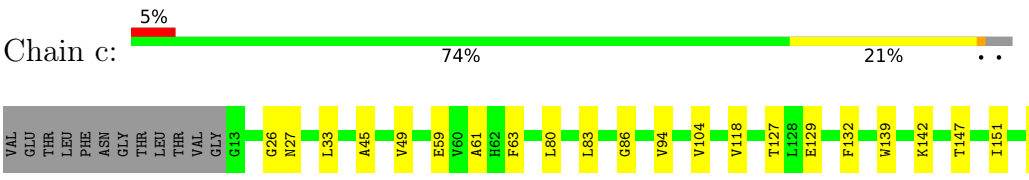
• Molecule 20: Photosystem II CP43 reaction center protein

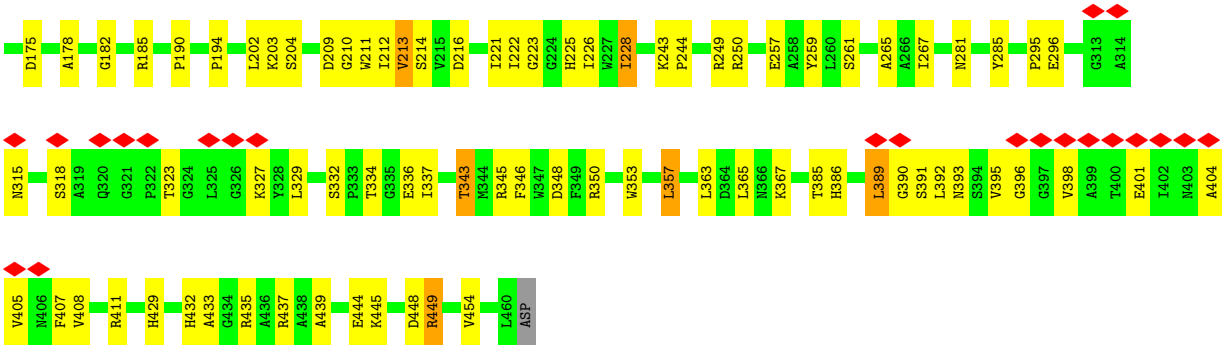
Chain C:



• Molecule 20: Photosystem II CP43 reaction center protein

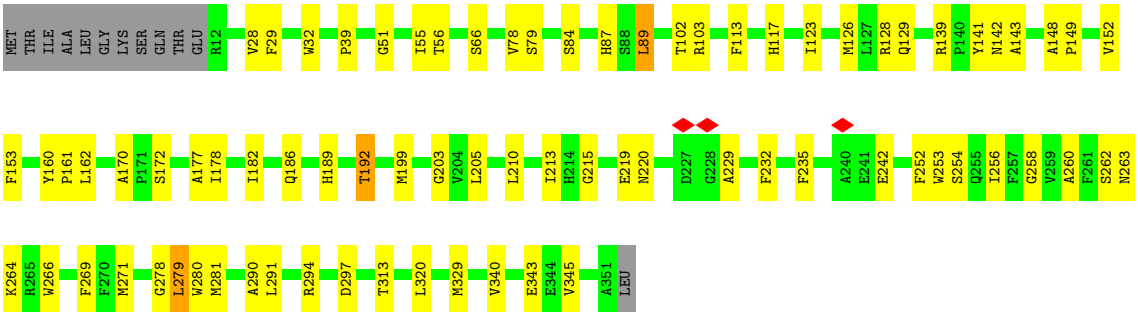
Chain c:





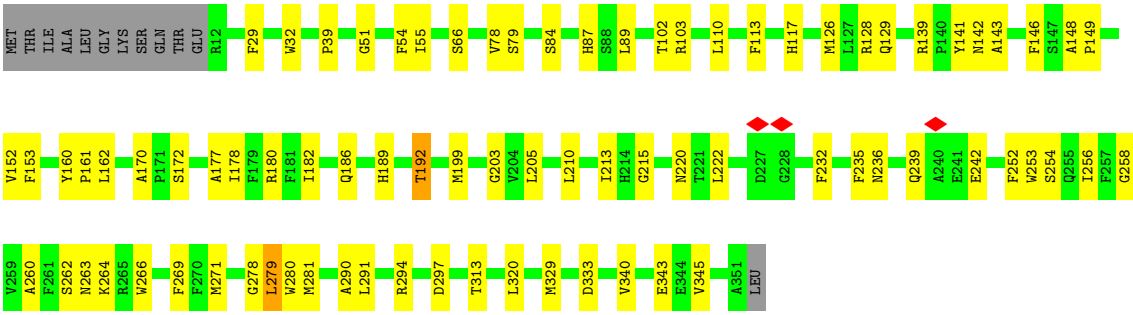
• Molecule 21: Photosystem II D2 protein





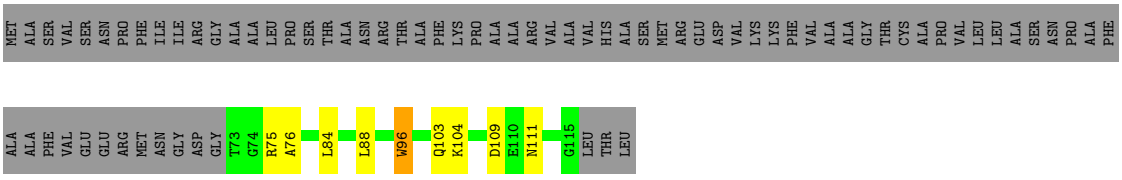
• Molecule 21: Photosystem II D2 protein





• Molecule 22: PsbW

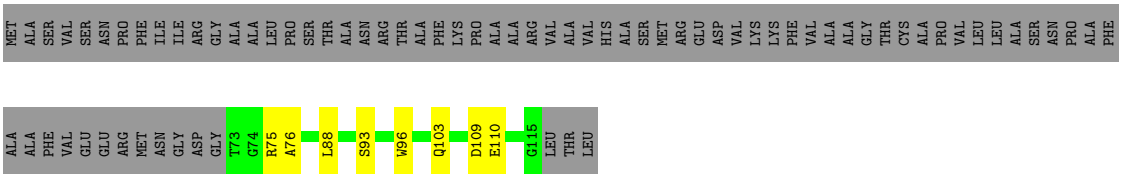




• Molecule 22: PsbW

Chain w:


30%
7%
64%


MET ALA SER VAL SER ASN PRO PHE ILE ILE ARG GLY ALA ALA LEU PRO SER THR ALA ASN ARG THR ALA PHE LYS PRO ALA ALA ARG VAL ALA VAL HIS ALA SER MET ARG GLU ASP VAL LYS LYS PHE VAL ALA ALA GLY THR CYS ALA PRO VAL LEU LEU ALA SER ASN PRO ALA PHE
ALA ALA PHE VAL GLU GLU ARG MET ASN GLY ASP GLY T73 G74 R75 A76 L88 S93 W96 Q103 D109 E110 G115 LEU THR LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 10	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	0.922	Depositor
Minimum map value	-0.284	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.204	Depositor
Map size (Å)	624.0, 624.0, 624.0	wwPDB
Map dimensions	600, 600, 600	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: BCT, FE2, DGD, 0UR, NEX, PHO, SQD, OEX, LMG, 8CT, 0IE, LHG, CHL, XAT, PL9, CLA, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	Z	0.18	0/486	0.28	0/664
1	z	0.17	0/486	0.28	0/664
2	E	0.42	0/546	0.54	1/745 (0.1%)
2	e	0.23	0/546	0.35	0/745
3	H	0.22	0/523	0.29	0/713
3	h	0.23	0/523	0.32	0/713
4	I	0.33	0/283	0.28	0/383
4	i	0.34	0/283	0.38	0/383
5	K	0.26	0/310	0.52	0/426
5	k	0.25	0/310	0.35	0/426
6	L	0.27	0/312	0.30	0/424
6	l	0.27	0/312	0.29	0/424
7	M	0.16	0/234	0.31	0/320
7	m	0.15	0/234	0.30	0/320
8	R	0.18	0/1749	0.41	2/2373 (0.1%)
8	r	0.18	0/1745	0.42	2/2369 (0.1%)
9	F	0.21	0/252	0.41	0/341
9	f	0.21	0/258	0.38	0/349
10	1	0.11	0/1658	0.30	0/2257
10	4	0.11	0/1652	0.30	0/2250
11	2	0.15	0/1763	0.33	0/2394
11	5	0.14	0/1764	0.29	0/2395
12	3	0.14	0/1657	0.36	0/2261
12	6	0.14	0/1722	0.40	1/2349 (0.0%)
12	7	0.19	0/1730	0.43	0/2359
12	9	0.12	0/1733	0.37	0/2363
12	p	0.19	0/1733	0.45	0/2363
12	u	0.13	0/1736	0.38	0/2367
13	S	0.25	0/1920	0.43	1/2621 (0.0%)
13	s	0.28	0/1920	0.45	1/2621 (0.0%)
14	X	0.14	0/227	0.22	0/308

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
14	x	0.14	0/227	0.22	0/308
15	V	0.13	0/179	0.38	0/245
15	v	0.13	0/179	0.36	0/245
16	T	0.30	0/244	0.36	0/329
16	t	0.31	0/244	0.35	0/329
17	8	0.19	0/1602	0.29	0/2182
17	G	0.11	0/1743	0.27	0/2371
17	N	0.14	0/1599	0.30	0/2178
17	Y	0.24	0/1743	0.31	0/2371
17	g	0.11	0/1743	0.26	0/2371
17	n	0.13	0/1592	0.29	0/2168
17	q	0.19	0/1602	0.29	0/2182
17	y	0.23	0/1743	0.29	0/2371
18	B	0.33	0/3866	0.37	1/5266 (0.0%)
18	b	0.27	0/3866	0.34	0/5266
19	A	0.33	0/2637	0.36	0/3595
19	a	0.41	0/2637	0.39	0/3595
20	C	0.30	0/3591	0.38	0/4895
20	c	0.30	0/3591	0.39	0/4895
21	D	0.33	0/2813	0.37	0/3832
21	d	0.35	0/2813	0.37	0/3832
22	W	0.24	0/308	0.51	0/417
22	w	0.23	0/308	0.51	0/417
All	All	0.25	0/71477	0.36	9/97350 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	77	GLY	N-CA-C	7.09	123.47	114.25
8	r	68	ASP	CA-C-N	-6.62	113.97	120.52
8	r	68	ASP	C-N-CA	-6.62	113.97	120.52
8	R	68	ASP	CA-C-N	-6.58	114.00	120.52
8	R	68	ASP	C-N-CA	-6.58	114.00	120.52

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	Z	472	0	496	9	0
1	z	472	0	496	6	0
2	E	530	0	517	20	0
2	e	530	0	517	9	0
3	H	513	0	517	18	0
3	h	513	0	517	17	0
4	I	275	0	282	4	0
4	i	275	0	282	4	0
5	K	299	0	311	7	0
5	k	299	0	311	4	0
6	L	304	0	313	16	0
6	l	304	0	313	14	0
7	M	231	0	261	9	0
7	m	231	0	261	11	0
8	R	1711	0	1670	83	0
8	r	1707	0	1659	70	0
9	F	246	0	256	4	0
9	f	251	0	261	4	0
10	1	1609	0	1517	52	0
10	4	1603	0	1506	50	0
11	2	1710	0	1616	46	0
11	5	1711	0	1620	48	0
12	3	1606	0	1501	44	0
12	6	1670	0	1564	50	0
12	7	1677	0	1573	66	0
12	9	1680	0	1575	71	0
12	p	1680	0	1575	65	0
12	u	1683	0	1584	74	0
13	S	1867	0	1797	79	0
13	s	1867	0	1797	75	0
14	X	226	0	242	4	0
14	x	226	0	242	2	0
15	V	179	0	205	7	0
15	v	179	0	205	5	0
16	T	236	0	239	5	0
16	t	236	0	239	5	0
17	8	1554	0	1467	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	G	1690	0	1593	57	0
17	N	1551	0	1458	64	0
17	Y	1690	0	1593	44	0
17	g	1690	0	1593	57	0
17	n	1545	0	1455	59	0
17	q	1554	0	1467	52	0
17	y	1690	0	1593	43	0
18	B	3737	0	3605	100	0
18	b	3737	0	3605	92	0
19	A	2558	0	2469	75	0
19	a	2558	0	2469	70	0
20	C	3472	0	3381	85	0
20	c	3472	0	3381	83	0
21	D	2719	0	2631	69	0
21	d	2719	0	2631	66	0
22	W	304	0	276	8	0
22	w	304	0	276	11	0
23	E	43	0	30	2	0
23	f	43	0	30	3	0
24	1	349	0	234	24	0
24	2	353	0	234	11	0
24	3	365	0	250	31	0
24	4	349	0	234	22	0
24	5	353	0	234	15	0
24	6	365	0	250	37	0
24	7	397	0	311	35	0
24	8	351	0	270	24	0
24	9	397	0	311	25	0
24	G	433	0	370	40	0
24	N	404	0	311	20	0
24	R	277	0	186	17	0
24	S	331	0	233	14	0
24	Y	486	0	411	26	0
24	g	433	0	370	28	0
24	n	404	0	311	21	0
24	p	397	0	311	37	0
24	q	404	0	311	23	0
24	r	277	0	186	19	0
24	s	331	0	233	14	0
24	u	397	0	311	21	0
24	y	433	0	370	26	0
25	1	268	0	204	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	2	305	0	258	10	0
25	3	256	0	186	6	0
25	4	268	0	204	23	0
25	5	305	0	258	11	0
25	6	256	0	186	7	0
25	7	321	0	280	27	0
25	8	310	0	267	12	0
25	9	324	0	284	16	0
25	A	280	0	271	12	0
25	B	980	0	1023	63	0
25	C	790	0	814	30	0
25	D	130	0	144	10	0
25	G	318	0	272	27	0
25	N	310	0	267	13	0
25	R	325	0	247	17	0
25	S	333	0	261	10	0
25	Y	321	0	278	8	0
25	a	280	0	271	13	0
25	b	980	0	1023	61	0
25	c	790	0	814	33	0
25	d	130	0	144	10	0
25	g	318	0	272	15	0
25	n	310	0	267	12	0
25	p	324	0	284	24	0
25	q	310	0	267	12	0
25	r	325	0	247	18	0
25	s	332	0	261	13	0
25	u	324	0	284	16	0
25	y	321	0	278	12	0
26	1	44	0	0	0	0
26	2	88	0	0	1	0
26	3	87	0	0	2	0
26	4	44	0	0	0	0
26	5	88	0	0	0	0
26	6	43	0	0	2	0
26	7	88	0	0	2	0
26	8	44	0	0	0	0
26	9	88	0	0	3	0
26	G	88	0	0	0	0
26	N	44	0	0	0	0
26	R	44	0	0	1	0
26	Y	88	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	g	88	0	0	0	0
26	n	44	0	0	0	0
26	p	88	0	0	2	0
26	q	44	0	0	0	0
26	r	44	0	0	1	0
26	u	88	0	0	1	0
26	y	88	0	0	2	0
27	R	44	0	56	16	0
27	r	44	0	56	8	0
28	1	44	0	56	22	0
28	2	44	0	56	9	0
28	3	44	0	56	22	0
28	4	44	0	56	21	0
28	5	44	0	56	10	0
28	6	44	0	56	21	0
28	7	44	0	56	32	0
28	9	44	0	56	6	0
28	G	44	0	56	32	0
28	N	44	0	56	7	0
28	R	44	0	56	6	0
28	S	44	0	56	24	0
28	g	44	0	56	15	0
28	n	44	0	56	7	0
28	p	44	0	56	27	0
28	r	88	0	112	15	0
28	s	44	0	56	21	0
28	u	44	0	56	9	0
28	y	44	0	56	4	0
29	1	52	0	0	0	0
29	2	52	0	0	1	0
29	3	52	0	0	0	0
29	4	52	0	0	1	0
29	5	52	0	0	0	0
29	6	52	0	0	1	0
29	7	52	0	0	0	0
29	8	52	0	0	1	0
29	9	52	0	0	1	0
29	G	52	0	0	1	0
29	N	52	0	0	0	0
29	Y	52	0	0	1	0
29	g	52	0	0	0	0
29	n	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	p	52	0	0	1	0
29	q	52	0	0	1	0
29	u	52	0	0	1	0
29	y	52	0	0	1	0
30	1	42	0	54	3	0
30	2	40	0	50	2	0
30	4	42	0	54	3	0
30	5	43	0	56	2	0
30	7	37	0	44	3	0
30	9	43	0	56	6	0
30	A	89	0	124	8	0
30	C	32	0	34	0	0
30	D	88	0	122	13	0
30	G	43	0	56	1	0
30	N	43	0	56	4	0
30	Y	43	0	56	0	0
30	a	89	0	124	7	0
30	c	32	0	34	0	0
30	d	88	0	122	11	0
30	g	43	0	56	2	0
30	n	43	0	56	4	0
30	p	43	0	56	3	0
30	y	43	0	56	2	0
31	A	40	0	0	0	0
31	B	40	0	0	0	0
31	C	120	0	0	1	0
31	D	40	0	0	0	0
31	S	80	0	0	0	0
31	T	40	0	0	0	0
31	V	40	0	0	1	0
31	X	40	0	0	0	0
31	a	40	0	0	0	0
31	b	40	0	0	0	0
31	c	120	0	0	1	0
31	d	40	0	0	0	0
31	s	80	0	0	0	0
31	t	40	0	0	0	0
31	v	40	0	0	1	0
31	x	40	0	0	0	0
32	A	45	0	54	2	0
32	B	54	0	78	4	0
32	D	44	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	a	45	0	54	4	0
32	b	54	0	78	5	0
32	d	44	0	52	1	0
33	B	41	0	52	5	0
33	C	42	0	54	6	0
33	D	94	0	128	8	0
33	W	30	0	30	2	0
33	d	94	0	128	8	0
33	i	48	0	66	3	0
33	m	41	0	52	6	0
33	w	36	0	42	6	0
34	A	10	0	0	0	0
34	a	10	0	0	0	0
35	A	64	0	74	4	0
35	D	64	0	74	6	0
35	a	64	0	74	4	0
35	d	64	0	74	6	0
36	A	4	0	1	0	0
36	a	4	0	1	0	0
37	C	105	0	126	7	0
37	c	105	0	126	8	0
38	D	1	0	0	0	0
38	d	1	0	0	0	0
39	D	55	0	80	2	0
39	d	55	0	80	2	0
All	All	95298	0	87326	2639	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 2639 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)
13:S:58:TRP:HZ2	28:S:617:NEX:H183	1.14	1.10
12:u:158:LEU:HD23	28:u:304:NEX:H203	1.35	1.07
13:S:58:TRP:CZ2	28:S:617:NEX:H183	1.89	1.06
28:p:304:NEX:H31	24:p:310:CHL:HBA1	1.38	1.04
13:S:58:TRP:HE1	28:S:617:NEX:H192	1.19	1.03

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	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
1	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
2	E	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
2	e	63/82 (77%)	63 (100%)	0	0	100	100
3	H	66/75 (88%)	63 (96%)	3 (4%)	0	100	100
3	h	66/75 (88%)	63 (96%)	3 (4%)	0	100	100
4	I	32/36 (89%)	32 (100%)	0	0	100	100
4	i	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
5	K	35/43 (81%)	33 (94%)	2 (6%)	0	100	100
5	k	35/43 (81%)	34 (97%)	1 (3%)	0	100	100
6	L	35/38 (92%)	35 (100%)	0	0	100	100
6	l	35/38 (92%)	35 (100%)	0	0	100	100
7	M	28/33 (85%)	27 (96%)	1 (4%)	0	100	100
7	m	28/33 (85%)	27 (96%)	1 (4%)	0	100	100
8	R	223/267 (84%)	199 (89%)	23 (10%)	1 (0%)	30	58
8	r	223/267 (84%)	203 (91%)	20 (9%)	0	100	100
9	F	29/42 (69%)	27 (93%)	2 (7%)	0	100	100
9	f	29/42 (69%)	28 (97%)	1 (3%)	0	100	100
10	1	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
10	4	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
11	2	219/256 (86%)	205 (94%)	14 (6%)	0	100	100
11	5	219/256 (86%)	204 (93%)	15 (7%)	0	100	100
12	3	209/254 (82%)	189 (90%)	20 (10%)	0	100	100
12	6	217/254 (85%)	196 (90%)	21 (10%)	0	100	100
12	7	217/254 (85%)	188 (87%)	27 (12%)	2 (1%)	14	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	9	217/254 (85%)	185 (85%)	31 (14%)	1 (0%)	24 54
12	p	217/254 (85%)	188 (87%)	26 (12%)	3 (1%)	9 31
12	u	217/254 (85%)	187 (86%)	30 (14%)	0	100 100
13	S	247/308 (80%)	211 (85%)	34 (14%)	2 (1%)	16 44
13	s	247/308 (80%)	209 (85%)	35 (14%)	3 (1%)	10 34
14	X	32/109 (29%)	32 (100%)	0	0	100 100
14	x	32/109 (29%)	32 (100%)	0	0	100 100
15	V	23/33 (70%)	18 (78%)	5 (22%)	0	100 100
15	v	23/33 (70%)	19 (83%)	4 (17%)	0	100 100
16	T	26/31 (84%)	24 (92%)	2 (8%)	0	100 100
16	t	26/31 (84%)	24 (92%)	2 (8%)	0	100 100
17	8	204/280 (73%)	195 (96%)	9 (4%)	0	100 100
17	G	221/280 (79%)	215 (97%)	6 (3%)	0	100 100
17	N	204/280 (73%)	196 (96%)	8 (4%)	0	100 100
17	Y	221/280 (79%)	212 (96%)	9 (4%)	0	100 100
17	g	221/280 (79%)	214 (97%)	7 (3%)	0	100 100
17	n	204/280 (73%)	192 (94%)	11 (5%)	1 (0%)	24 54
17	q	204/280 (73%)	196 (96%)	8 (4%)	0	100 100
17	y	221/280 (79%)	212 (96%)	9 (4%)	0	100 100
18	B	476/508 (94%)	455 (96%)	19 (4%)	2 (0%)	30 58
18	b	476/508 (94%)	457 (96%)	17 (4%)	2 (0%)	30 58
19	A	325/327 (99%)	307 (94%)	17 (5%)	1 (0%)	36 64
19	a	325/327 (99%)	304 (94%)	20 (6%)	1 (0%)	36 64
20	C	446/461 (97%)	409 (92%)	36 (8%)	1 (0%)	43 71
20	c	446/461 (97%)	407 (91%)	38 (8%)	1 (0%)	43 71
21	D	338/352 (96%)	313 (93%)	25 (7%)	0	100 100
21	d	338/352 (96%)	318 (94%)	20 (6%)	0	100 100
22	W	41/118 (35%)	30 (73%)	11 (27%)	0	100 100
22	w	41/118 (35%)	30 (73%)	11 (27%)	0	100 100
All	All	8900/10550 (84%)	8243 (93%)	636 (7%)	21 (0%)	44 71

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	B	279	PHE
18	B	299	SER
17	n	23	TYR
12	p	117	VAL
12	p	118	TRP

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	Z	51/52 (98%)	51 (100%)	0	100	100
1	z	51/52 (98%)	51 (100%)	0	100	100
2	E	58/73 (80%)	57 (98%)	1 (2%)	53	71
2	e	58/73 (80%)	57 (98%)	1 (2%)	53	71
3	H	56/62 (90%)	55 (98%)	1 (2%)	51	70
3	h	56/62 (90%)	55 (98%)	1 (2%)	51	70
4	I	31/32 (97%)	31 (100%)	0	100	100
4	i	31/32 (97%)	31 (100%)	0	100	100
5	K	33/39 (85%)	31 (94%)	2 (6%)	17	44
5	k	33/39 (85%)	32 (97%)	1 (3%)	36	62
6	L	34/35 (97%)	31 (91%)	3 (9%)	9	31
6	l	34/35 (97%)	32 (94%)	2 (6%)	18	45
7	M	27/30 (90%)	27 (100%)	0	100	100
7	m	27/30 (90%)	26 (96%)	1 (4%)	30	58
8	R	181/214 (85%)	173 (96%)	8 (4%)	25	54
8	r	180/214 (84%)	170 (94%)	10 (6%)	19	46
9	F	25/36 (69%)	22 (88%)	3 (12%)	5	19
9	f	26/36 (72%)	23 (88%)	3 (12%)	5	21
10	1	160/160 (100%)	153 (96%)	7 (4%)	25	54
10	4	159/160 (99%)	153 (96%)	6 (4%)	29	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	2	168/199 (84%)	168 (100%)	0	100	100
11	5	168/199 (84%)	168 (100%)	0	100	100
12	3	165/202 (82%)	158 (96%)	7 (4%)	26	55
12	6	172/202 (85%)	166 (96%)	6 (4%)	32	59
12	7	173/202 (86%)	164 (95%)	9 (5%)	21	49
12	9	174/202 (86%)	167 (96%)	7 (4%)	28	56
12	p	174/202 (86%)	161 (92%)	13 (8%)	12	37
12	u	175/202 (87%)	166 (95%)	9 (5%)	21	50
13	S	184/232 (79%)	172 (94%)	12 (6%)	15	42
13	s	184/232 (79%)	174 (95%)	10 (5%)	20	48
14	X	24/80 (30%)	23 (96%)	1 (4%)	26	55
14	x	24/80 (30%)	22 (92%)	2 (8%)	10	33
15	V	20/28 (71%)	18 (90%)	2 (10%)	7	26
15	v	20/28 (71%)	19 (95%)	1 (5%)	22	50
16	T	25/28 (89%)	23 (92%)	2 (8%)	11	35
16	t	25/28 (89%)	23 (92%)	2 (8%)	11	35
17	8	153/210 (73%)	152 (99%)	1 (1%)	76	80
17	G	165/210 (79%)	161 (98%)	4 (2%)	43	66
17	N	152/210 (72%)	143 (94%)	9 (6%)	18	45
17	Y	165/210 (79%)	162 (98%)	3 (2%)	51	70
17	g	165/210 (79%)	159 (96%)	6 (4%)	31	58
17	n	151/210 (72%)	144 (95%)	7 (5%)	24	53
17	q	153/210 (73%)	153 (100%)	0	100	100
17	y	165/210 (79%)	163 (99%)	2 (1%)	63	75
18	B	384/410 (94%)	371 (97%)	13 (3%)	32	60
18	b	384/410 (94%)	372 (97%)	12 (3%)	35	61
19	A	266/266 (100%)	251 (94%)	15 (6%)	19	46
19	a	266/266 (100%)	252 (95%)	14 (5%)	20	48
20	C	347/359 (97%)	338 (97%)	9 (3%)	40	65
20	c	347/359 (97%)	337 (97%)	10 (3%)	37	63
21	D	275/285 (96%)	266 (97%)	9 (3%)	33	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	d	275/285 (96%)	267 (97%)	8 (3%)	37 63
22	W	29/88 (33%)	27 (93%)	2 (7%)	14 40
22	w	29/88 (33%)	29 (100%)	0	100 100
All	All	7057/8308 (85%)	6800 (96%)	257 (4%)	32 58

5 of 257 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	s	119	LEU
8	r	48	MET
19	A	281	VAL
19	A	232	SER
8	r	156	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
20	C	451	ASN
11	5	215	GLN
12	7	81	ASN
19	a	315	ASN
21	D	197	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 528 ligands modelled in this entry, 2 are monoatomic - leaving 526 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CHL	G	313	-	70,74,74	1.98	18 (25%)	80,114,114	2.74	29 (36%)
25	CLA	1	307	-	45,49,73	1.52	9 (20%)	54,84,113	1.49	6 (11%)
25	CLA	G	314	-	59,63,73	1.35	8 (13%)	71,101,113	1.35	7 (9%)
25	CLA	y	316	17	49,53,73	1.48	10 (20%)	59,89,113	1.53	4 (6%)
24	CHL	2	310	-	46,50,74	2.30	19 (41%)	51,85,114	3.39	24 (47%)
25	CLA	7	316	12	49,53,73	1.47	10 (20%)	59,89,113	1.45	4 (6%)
26	0IE	G	303	-	42,45,45	1.40	6 (14%)	49,63,63	1.55	9 (18%)
24	CHL	4	310	-	47,51,74	2.24	18 (38%)	52,86,114	3.32	25 (48%)
29	0UR	u	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.79	13 (22%)
24	CHL	q	308	-	50,54,74	2.21	18 (36%)	56,90,114	3.33	28 (50%)
30	LHG	d	407	-	48,48,48	1.07	5 (10%)	51,54,54	0.96	2 (3%)
31	8CT	S	614	-	40,41,41	4.72	24 (60%)	50,56,56	2.96	18 (36%)
25	CLA	R	609	8	59,63,73	1.34	9 (15%)	71,101,113	1.36	6 (8%)
24	CHL	R	606	-	52,56,74	2.18	18 (34%)	58,92,114	3.23	25 (43%)
26	0IE	R	614	-	42,45,45	1.44	6 (14%)	49,63,63	1.54	10 (20%)
30	LHG	G	319	-	42,42,48	1.16	6 (14%)	45,48,54	0.99	2 (4%)
25	CLA	C	609	20	69,73,73	1.26	9 (13%)	83,113,113	1.36	8 (9%)
30	LHG	9	318	25	42,42,48	1.17	6 (14%)	45,48,54	0.98	2 (4%)
24	CHL	q	304	17	64,68,74	1.96	19 (29%)	72,106,114	2.92	30 (41%)
25	CLA	4	314	-	45,49,73	1.52	9 (20%)	54,84,113	1.51	5 (9%)
30	LHG	5	319	-	42,42,48	1.16	5 (11%)	45,48,54	1.04	4 (8%)
25	CLA	3	316	-	49,53,73	1.49	10 (20%)	59,89,113	1.46	7 (11%)
25	CLA	7	308	-	54,58,73	1.40	9 (16%)	65,95,113	1.40	5 (7%)
37	DGD	C	619	-	51,51,67	0.93	2 (3%)	65,65,81	1.24	5 (7%)
25	CLA	s	413	-	59,63,73	1.34	10 (16%)	70,100,113	1.39	6 (8%)
31	8CT	d	410	-	40,41,41	4.69	23 (57%)	50,56,56	2.50	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	2	305	11	48,52,74	2.21	17 (35%)	53,87,114	3.32	23 (43%)
25	CLA	Y	306	17	57,61,73	1.37	9 (15%)	68,98,113	1.40	6 (8%)
25	CLA	3	307	-	47,51,73	1.48	8 (17%)	56,86,113	1.46	4 (7%)
25	CLA	4	306	-	48,52,73	1.47	8 (16%)	56,87,113	1.46	6 (10%)
25	CLA	6	313	-	45,49,73	1.52	7 (15%)	54,84,113	1.52	8 (14%)
24	CHL	s	408	-	50,54,74	2.19	19 (38%)	56,90,114	3.32	24 (42%)
25	CLA	C	608	20	65,69,73	1.28	10 (15%)	78,108,113	1.38	8 (10%)
24	CHL	1	308	10	47,51,74	2.33	18 (38%)	52,86,114	3.37	24 (46%)
36	BCT	A	611	38	2,3,3	1.25	0	2,3,3	4.17	2 (100%)
24	CHL	G	309	-	47,51,74	2.36	18 (38%)	52,86,114	3.36	24 (46%)
25	CLA	g	317	17	59,63,73	1.35	9 (15%)	70,100,113	1.37	7 (10%)
25	CLA	u	314	-	59,63,73	1.35	7 (11%)	71,101,113	1.35	7 (9%)
25	CLA	r	305	-	45,49,73	1.52	10 (22%)	54,84,113	1.56	7 (12%)
25	CLA	y	314	17	59,63,73	1.34	10 (16%)	71,101,113	1.37	8 (11%)
30	LHG	A	612	-	43,43,48	1.15	5 (11%)	46,49,54	1.02	3 (6%)
24	CHL	2	318	11	46,50,74	2.37	18 (39%)	51,85,114	3.41	25 (49%)
30	LHG	C	617	-	31,31,48	1.31	5 (16%)	34,37,54	1.14	3 (8%)
25	CLA	9	316	12	59,63,73	1.36	9 (15%)	70,100,113	1.34	6 (8%)
24	CHL	g	306	-	68,72,74	1.91	19 (27%)	77,111,114	2.88	30 (38%)
24	CHL	u	318	-	46,50,74	2.43	19 (41%)	51,85,114	3.45	26 (50%)
24	CHL	Y	312	-	70,74,74	1.88	19 (27%)	80,114,114	2.77	27 (33%)
24	CHL	1	311	-	48,52,74	2.20	18 (37%)	53,87,114	3.29	24 (45%)
24	CHL	y	310	-	51,55,74	2.14	19 (37%)	57,91,114	3.31	28 (49%)
25	CLA	C	602	20	69,73,73	1.25	10 (14%)	83,113,113	1.32	6 (7%)
24	CHL	5	305	11	48,52,74	2.21	17 (35%)	53,87,114	3.33	24 (45%)
25	CLA	B	606	18	69,73,73	1.24	9 (13%)	83,113,113	1.36	8 (9%)
25	CLA	A	604	-	69,73,73	1.27	10 (14%)	83,113,113	1.31	7 (8%)
28	NEX	N	303	-	38,46,46	1.05	2 (5%)	50,70,70	2.82	17 (34%)
25	CLA	B	610	-	69,73,73	1.25	10 (14%)	83,113,113	1.33	7 (8%)
25	CLA	n	306	17	58,62,73	1.37	8 (13%)	69,99,113	1.38	6 (8%)
24	CHL	S	607	-	50,54,74	2.20	19 (38%)	56,90,114	3.30	24 (42%)
32	SQD	D	409	-	43,44,54	1.06	5 (11%)	52,55,65	1.57	9 (17%)
24	CHL	q	303	17	58,62,74	2.13	18 (31%)	65,99,114	3.05	27 (41%)
25	CLA	6	306	-	45,49,73	1.50	9 (20%)	54,84,113	1.51	6 (11%)
24	CHL	r	309	-	50,54,74	2.24	18 (36%)	56,90,114	3.21	27 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	s	410	-	59,63,73	1.33	10 (16%)	71,101,113	1.35	5 (7%)
25	CLA	R	613	-	51,55,73	1.46	8 (15%)	61,91,113	1.37	5 (8%)
31	8CT	s	415	-	40,41,41	4.72	24 (60%)	50,56,56	2.97	18 (36%)
25	CLA	B	608	-	59,63,73	1.35	10 (16%)	71,101,113	1.36	7 (9%)
31	8CT	V	401	-	40,41,41	4.66	23 (57%)	50,56,56	2.56	17 (34%)
25	CLA	R	612	-	49,53,73	1.49	8 (16%)	59,89,113	1.48	6 (10%)
24	CHL	u	309	12	47,51,74	2.34	18 (38%)	52,86,114	3.34	24 (46%)
28	NEX	p	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.91	19 (38%)
29	0UR	g	301	-	50,53,58	0.95	1 (2%)	58,72,77	1.73	16 (27%)
25	CLA	3	313	-	45,49,73	1.52	8 (17%)	54,84,113	1.52	8 (14%)
24	CHL	S	605	-	50,54,74	2.23	18 (36%)	56,90,114	3.24	23 (41%)
23	HEM	f	201	2,9	50,50,50	1.37	7 (14%)	66,82,82	1.09	3 (4%)
25	CLA	2	316	-	49,53,73	1.48	10 (20%)	59,89,113	1.47	4 (6%)
24	CHL	p	305	12	70,74,74	1.82	19 (27%)	80,114,114	2.88	31 (38%)
24	CHL	q	311	-	60,64,74	2.02	19 (31%)	68,102,114	3.00	28 (41%)
25	CLA	A	610	-	45,49,73	1.52	8 (17%)	54,84,113	1.53	7 (12%)
24	CHL	u	306	-	68,72,74	1.95	19 (27%)	77,111,114	2.81	27 (35%)
24	CHL	1	317	-	46,50,74	2.41	19 (41%)	51,85,114	3.40	25 (49%)
30	LHG	n	318	-	42,42,48	1.18	6 (14%)	45,48,54	0.97	2 (4%)
24	CHL	2	313	-	46,50,74	2.33	18 (39%)	51,85,114	3.34	25 (49%)
25	CLA	D	405	21	69,73,73	1.24	9 (13%)	83,113,113	1.34	6 (7%)
24	CHL	y	311	-	58,62,74	2.04	19 (32%)	65,99,114	3.18	31 (47%)
24	CHL	N	304	17	58,62,74	2.15	18 (31%)	65,99,114	3.04	27 (41%)
24	CHL	S	613	-	46,50,74	2.29	18 (39%)	51,85,114	3.43	27 (52%)
30	LHG	7	319	25	36,36,48	1.25	5 (13%)	39,42,54	1.08	2 (5%)
26	0IE	7	302	-	42,45,45	1.45	6 (14%)	49,63,63	1.60	12 (24%)
24	CHL	9	311	-	51,55,74	2.24	19 (37%)	57,91,114	3.22	25 (43%)
25	CLA	9	307	-	54,58,73	1.41	9 (16%)	65,95,113	1.43	5 (7%)
25	CLA	A	607	19	64,68,73	1.27	9 (14%)	77,107,113	1.41	8 (10%)
26	0IE	g	303	-	42,45,45	1.41	6 (14%)	49,63,63	1.54	9 (18%)
25	CLA	y	307	17	57,61,73	1.37	9 (15%)	68,98,113	1.41	7 (10%)
25	CLA	C	605	20	60,64,73	1.32	10 (16%)	72,102,113	1.40	7 (9%)
28	NEX	g	304	-	38,46,46	0.97	2 (5%)	50,70,70	4.90	19 (38%)
25	CLA	R	611	8	49,53,73	1.48	10 (20%)	59,89,113	1.45	5 (8%)
24	CHL	N	309	-	50,54,74	2.18	18 (36%)	56,90,114	3.34	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	S	601	13	50,54,74	2.18	19 (38%)	56,90,114	3.35	24 (42%)
24	CHL	n	308	17	47,51,74	2.30	18 (38%)	52,86,114	3.32	24 (46%)
31	8CT	v	401	-	40,41,41	4.67	23 (57%)	50,56,56	2.55	17 (34%)
25	CLA	3	306	-	45,49,73	1.52	9 (20%)	54,84,113	1.51	5 (9%)
25	CLA	b	604	18	66,70,73	1.27	9 (13%)	79,109,113	1.40	8 (10%)
25	CLA	C	611	20	69,73,73	1.25	11 (15%)	83,113,113	1.34	5 (6%)
26	0IE	5	302	-	42,45,45	1.40	6 (14%)	49,63,63	1.53	9 (18%)
24	CHL	7	312	-	51,55,74	2.09	18 (35%)	57,91,114	3.34	28 (49%)
25	CLA	n	307	-	54,58,73	1.40	8 (14%)	65,95,113	1.42	7 (10%)
24	CHL	4	308	10	47,51,74	2.33	18 (38%)	52,86,114	3.37	24 (46%)
25	CLA	9	313	-	59,63,73	1.35	7 (11%)	71,101,113	1.36	7 (9%)
25	CLA	C	607	-	69,73,73	1.23	11 (15%)	83,113,113	1.33	5 (6%)
24	CHL	n	312	-	60,64,74	2.06	18 (30%)	68,102,114	2.99	28 (41%)
25	CLA	r	311	-	49,53,73	1.47	8 (16%)	59,89,113	1.46	7 (11%)
26	0IE	1	302	-	42,45,45	1.44	6 (14%)	49,63,63	1.57	10 (20%)
25	CLA	B	602	18	69,73,73	1.24	10 (14%)	83,113,113	1.30	6 (7%)
33	LMG	w	201	-	36,36,55	1.05	2 (5%)	44,44,63	1.35	6 (13%)
24	CHL	9	317	-	46,50,74	2.43	19 (41%)	51,85,114	3.46	26 (50%)
26	0IE	6	302	-	41,44,45	1.45	6 (14%)	46,60,63	1.67	11 (23%)
37	DGD	c	618	-	51,51,67	0.93	2 (3%)	65,65,81	1.22	6 (9%)
25	CLA	7	315	30	67,71,73	1.25	10 (14%)	80,110,113	1.38	7 (8%)
25	CLA	N	314	-	67,71,73	1.26	8 (11%)	80,110,113	1.29	5 (6%)
25	CLA	C	604	-	69,73,73	1.24	9 (13%)	83,113,113	1.33	6 (7%)
24	CHL	y	312	-	55,59,74	2.07	18 (32%)	62,96,114	3.16	29 (46%)
30	LHG	y	319	25	42,42,48	1.15	5 (11%)	45,48,54	1.07	2 (4%)
30	LHG	D	407	-	48,48,48	1.08	5 (10%)	51,54,54	0.96	2 (3%)
25	CLA	g	314	-	59,63,73	1.35	9 (15%)	71,101,113	1.35	7 (9%)
25	CLA	b	614	18	60,64,73	1.33	10 (16%)	72,102,113	1.35	4 (5%)
24	CHL	N	310	-	57,61,74	2.17	18 (31%)	64,98,114	3.11	28 (43%)
25	CLA	5	307	11	47,51,73	1.48	9 (19%)	56,86,113	1.46	5 (8%)
24	CHL	2	306	-	51,55,74	2.17	19 (37%)	57,91,114	3.20	25 (43%)
24	CHL	p	311	-	50,54,74	2.26	19 (38%)	56,90,114	3.19	24 (42%)
25	CLA	c	608	20	65,69,73	1.28	9 (13%)	78,108,113	1.38	8 (10%)
24	CHL	9	308	12	47,51,74	2.36	18 (38%)	52,86,114	3.36	25 (48%)
25	CLA	u	315	-	67,71,73	1.28	7 (10%)	80,110,113	1.32	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	0UR	9	301	-	50,53,58	0.93	1 (2%)	58,72,77	1.76	13 (22%)
26	0IE	y	302	-	42,45,45	1.41	6 (14%)	49,63,63	1.54	10 (20%)
24	CHL	3	311	-	48,52,74	2.20	18 (37%)	53,87,114	3.36	25 (47%)
24	CHL	r	303	-	51,55,74	2.16	18 (35%)	57,91,114	3.25	26 (45%)
24	CHL	4	317	-	46,50,74	2.41	19 (41%)	51,85,114	3.41	25 (49%)
25	CLA	y	315	30	67,71,73	1.25	9 (13%)	80,110,113	1.28	5 (6%)
25	CLA	G	307	-	57,61,73	1.39	8 (14%)	68,98,113	1.34	5 (7%)
25	CLA	8	311	-	59,63,73	1.33	10 (16%)	71,101,113	1.38	7 (9%)
24	CHL	y	305	17	70,74,74	1.80	18 (25%)	80,114,114	2.87	29 (36%)
24	CHL	7	305	12	70,74,74	1.82	18 (25%)	80,114,114	2.88	31 (38%)
25	CLA	G	317	-	59,63,73	1.34	9 (15%)	70,100,113	1.37	7 (10%)
24	CHL	r	308	-	52,56,74	2.13	19 (36%)	58,92,114	3.31	27 (46%)
25	CLA	b	605	18	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
29	0UR	6	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.81	14 (24%)
25	CLA	r	312	8	49,53,73	1.48	10 (20%)	59,89,113	1.45	5 (8%)
26	0IE	3	302	-	41,44,45	1.44	6 (14%)	46,60,63	1.65	11 (23%)
25	CLA	C	612	20	58,62,73	1.34	10 (17%)	69,99,113	1.43	5 (7%)
24	CHL	g	311	-	58,62,74	2.14	18 (31%)	65,99,114	3.06	27 (41%)
28	NEX	s	401	25	38,46,46	1.06	2 (5%)	50,70,70	2.82	17 (34%)
24	CHL	N	311	-	54,58,74	2.14	19 (35%)	59,94,114	3.20	25 (42%)
25	CLA	1	316	10	46,50,73	1.51	7 (15%)	55,85,113	1.47	5 (9%)
28	NEX	u	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
26	0IE	G	302	-	42,45,45	1.42	6 (14%)	49,63,63	1.58	9 (18%)
25	CLA	5	315	-	67,71,73	1.26	9 (13%)	80,110,113	1.31	5 (6%)
24	CHL	Y	305	-	68,72,74	1.85	18 (26%)	77,111,114	2.92	29 (37%)
26	0IE	u	302	-	42,45,45	1.44	6 (14%)	49,63,63	1.53	11 (22%)
24	CHL	n	317	-	46,50,74	2.42	19 (41%)	51,85,114	3.45	26 (50%)
32	SQD	b	618	-	53,54,54	0.96	5 (9%)	62,65,65	1.55	11 (17%)
24	CHL	8	309	-	54,58,74	2.08	18 (33%)	59,94,114	3.19	26 (44%)
25	CLA	s	412	13	49,53,73	1.47	10 (20%)	59,89,113	1.48	6 (10%)
25	CLA	b	610	-	69,73,73	1.25	10 (14%)	83,113,113	1.33	7 (8%)
25	CLA	b	609	18	69,73,73	1.24	9 (13%)	83,113,113	1.32	8 (9%)
26	0IE	n	302	-	42,45,45	1.44	6 (14%)	49,63,63	1.58	11 (22%)
24	CHL	8	315	-	46,50,74	2.39	19 (41%)	51,85,114	3.42	25 (49%)
25	CLA	c	604	-	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	a	607	19	64,68,73	1.28	9 (14%)	77,107,113	1.42	9 (11%)
30	LHG	a	612	-	43,43,48	1.15	5 (11%)	46,49,54	1.02	3 (6%)
24	CHL	6	311	-	48,52,74	2.18	18 (37%)	53,87,114	3.36	25 (47%)
25	CLA	5	314	-	59,63,73	1.34	10 (16%)	71,101,113	1.35	6 (8%)
26	0IE	4	302	-	42,45,45	1.45	6 (14%)	49,63,63	1.58	10 (20%)
25	CLA	b	612	18	69,73,73	1.24	10 (14%)	83,113,113	1.35	9 (10%)
29	0UR	2	301	-	50,53,58	1.00	2 (4%)	58,72,77	1.84	15 (25%)
24	CHL	S	602	13	62,66,74	1.97	18 (29%)	70,104,114	2.98	28 (40%)
24	CHL	N	308	17	47,51,74	2.27	17 (36%)	52,86,114	3.30	24 (46%)
24	CHL	G	318	17	46,50,74	2.32	18 (39%)	51,85,114	3.42	25 (49%)
25	CLA	u	316	-	49,53,73	1.49	8 (16%)	59,89,113	1.44	4 (6%)
25	CLA	a	604	-	69,73,73	1.27	10 (14%)	83,113,113	1.30	7 (8%)
25	CLA	1	314	-	45,49,73	1.52	8 (17%)	54,84,113	1.51	5 (9%)
25	CLA	N	316	-	47,51,73	1.49	9 (19%)	56,86,113	1.41	4 (7%)
26	0IE	9	302	-	42,45,45	1.44	6 (14%)	49,63,63	1.58	10 (20%)
25	CLA	Y	315	17	49,53,73	1.47	10 (20%)	59,89,113	1.53	4 (6%)
29	0UR	3	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.71	12 (20%)
24	CHL	3	305	-	52,56,74	2.21	19 (36%)	58,92,114	3.15	25 (43%)
25	CLA	r	313	-	49,53,73	1.48	8 (16%)	59,89,113	1.51	7 (11%)
25	CLA	c	611	20	69,73,73	1.24	11 (15%)	83,113,113	1.32	5 (6%)
24	CHL	Y	311	-	55,59,74	2.08	18 (32%)	62,96,114	3.16	29 (46%)
28	NEX	R	616	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
25	CLA	S	610	-	49,53,73	1.47	10 (20%)	59,89,113	1.43	5 (8%)
25	CLA	1	313	-	59,63,73	1.35	8 (13%)	71,101,113	1.36	7 (9%)
24	CHL	9	312	-	47,51,74	2.33	17 (36%)	52,86,114	3.31	25 (48%)
25	CLA	5	308	-	54,58,73	1.39	8 (14%)	65,95,113	1.44	8 (12%)
25	CLA	c	612	20	58,62,73	1.34	10 (17%)	69,99,113	1.42	4 (5%)
31	8CT	A	608	-	40,41,41	4.63	23 (57%)	50,56,56	2.65	20 (40%)
24	CHL	1	305	10	50,54,74	2.23	19 (38%)	56,90,114	3.29	28 (50%)
25	CLA	C	606	20	57,61,73	1.37	10 (17%)	68,98,113	1.41	6 (8%)
24	CHL	G	306	17	68,72,74	1.92	19 (27%)	77,111,114	2.86	29 (37%)
25	CLA	q	314	17	49,53,73	1.48	8 (16%)	59,89,113	1.48	4 (6%)
25	CLA	G	316	17	49,53,73	1.49	10 (20%)	59,89,113	1.46	4 (6%)
24	CHL	6	309	-	55,59,74	2.19	18 (32%)	62,96,114	3.12	28 (45%)
24	CHL	s	402	13	50,54,74	2.19	19 (38%)	56,90,114	3.35	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	2	312	-	50,54,74	2.20	19 (38%)	56,90,114	3.27	25 (44%)
33	LMG	d	401	-	48,48,55	0.91	2 (4%)	56,56,63	1.19	5 (8%)
25	CLA	B	612	18	69,73,73	1.23	10 (14%)	83,113,113	1.36	8 (9%)
24	CHL	4	309	-	47,51,74	2.31	17 (36%)	52,86,114	3.29	25 (48%)
24	CHL	R	608	-	50,54,74	2.25	18 (36%)	56,90,114	3.21	27 (48%)
24	CHL	6	310	-	50,54,74	2.34	18 (36%)	56,90,114	3.20	24 (42%)
25	CLA	R	604	-	45,49,73	1.51	10 (22%)	54,84,113	1.55	8 (14%)
25	CLA	n	316	-	47,51,73	1.49	7 (14%)	56,86,113	1.41	4 (7%)
26	0IE	N	302	-	42,45,45	1.42	6 (14%)	49,63,63	1.58	11 (22%)
25	CLA	c	605	20	60,64,73	1.32	10 (16%)	72,102,113	1.39	6 (8%)
24	CHL	N	317	-	46,50,74	2.41	19 (41%)	51,85,114	3.45	26 (50%)
25	CLA	4	316	-	46,50,73	1.52	7 (15%)	55,85,113	1.46	5 (9%)
24	CHL	5	306	-	51,55,74	2.17	19 (37%)	57,91,114	3.20	25 (43%)
25	CLA	s	417	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	5 (8%)
27	XAT	r	316	-	39,47,47	0.92	0	54,74,74	2.72	19 (35%)
26	0IE	2	302	-	42,45,45	1.40	6 (14%)	49,63,63	1.52	9 (18%)
24	CHL	5	312	-	50,54,74	2.20	19 (38%)	56,90,114	3.27	24 (42%)
33	LMG	D	411	-	46,46,55	0.95	2 (4%)	54,54,63	1.13	4 (7%)
24	CHL	y	318	17	46,50,74	2.26	18 (39%)	51,85,114	3.43	27 (52%)
25	CLA	8	312	-	67,71,73	1.26	9 (13%)	80,110,113	1.29	6 (7%)
26	0IE	p	303	-	42,45,45	1.40	6 (14%)	49,63,63	1.57	9 (18%)
24	CHL	2	311	-	51,55,74	2.26	19 (37%)	57,91,114	3.14	25 (43%)
26	0IE	Y	302	-	42,45,45	1.41	6 (14%)	49,63,63	1.55	10 (20%)
24	CHL	g	312	-	55,59,74	2.17	19 (34%)	62,96,114	3.11	29 (46%)
24	CHL	q	307	17	47,51,74	2.24	18 (38%)	52,86,114	3.34	24 (46%)
26	0IE	q	302	-	42,45,45	1.40	6 (14%)	49,63,63	1.52	10 (20%)
25	CLA	B	615	18	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)
25	CLA	R	610	-	49,53,73	1.47	9 (18%)	59,89,113	1.45	6 (10%)
25	CLA	5	317	11	53,57,73	1.39	9 (16%)	62,93,113	1.45	6 (9%)
25	CLA	3	314	-	45,49,73	1.51	7 (15%)	54,84,113	1.47	7 (12%)
31	8CT	t	101	-	40,41,41	4.64	23 (57%)	50,56,56	3.04	18 (36%)
24	CHL	7	313	-	47,51,74	2.22	18 (38%)	52,86,114	3.30	23 (44%)
25	CLA	b	607	18	69,73,73	1.24	10 (14%)	83,113,113	1.34	8 (9%)
29	0UR	N	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.82	12 (20%)
31	8CT	C	613	-	40,41,41	4.60	23 (57%)	50,56,56	2.72	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	p	308	-	54,58,73	1.40	9 (16%)	65,95,113	1.39	5 (7%)
31	8CT	S	615	-	40,41,41	4.73	25 (62%)	50,56,56	7.31	22 (44%)
24	CHL	4	304	-	46,50,74	2.40	19 (41%)	51,85,114	3.38	26 (50%)
24	CHL	q	310	-	54,58,74	2.09	18 (33%)	59,94,114	3.18	26 (44%)
24	CHL	s	403	13	62,66,74	1.97	18 (29%)	70,104,114	2.97	28 (40%)
25	CLA	p	317	12	59,63,73	1.34	10 (16%)	70,100,113	1.39	6 (8%)
25	CLA	n	313	-	59,63,73	1.34	8 (13%)	71,101,113	1.36	7 (9%)
24	CHL	3	309	-	55,59,74	2.20	18 (32%)	62,96,114	3.12	28 (45%)
25	CLA	7	317	12	56,60,73	1.38	10 (17%)	67,97,113	1.42	6 (8%)
25	CLA	C	601	20	69,73,73	1.24	10 (14%)	83,113,113	1.37	8 (9%)
24	CHL	r	306	-	46,50,74	2.32	19 (41%)	51,85,114	3.36	25 (49%)
24	CHL	u	312	-	51,55,74	2.24	18 (35%)	57,91,114	3.22	24 (42%)
24	CHL	8	310	-	60,64,74	2.03	19 (31%)	68,102,114	3.00	27 (39%)
24	CHL	Y	319	-	57,61,74	2.09	18 (31%)	64,98,114	3.15	30 (46%)
25	CLA	c	616	20	50,54,73	1.43	10 (20%)	60,90,113	1.49	7 (11%)
36	BCT	a	611	38	2,3,3	1.25	0	2,3,3	4.16	2 (100%)
29	0UR	5	301	-	50,53,58	0.99	2 (4%)	58,72,77	1.84	15 (25%)
29	0UR	Y	301	-	50,53,58	0.99	1 (2%)	58,72,77	1.63	12 (20%)
26	0IE	5	303	-	42,45,45	1.43	6 (14%)	49,63,63	1.52	9 (18%)
25	CLA	4	315	10	49,53,73	1.49	8 (16%)	59,89,113	1.46	4 (6%)
25	CLA	c	607	-	69,73,73	1.25	11 (15%)	83,113,113	1.33	5 (6%)
25	CLA	p	314	-	59,63,73	1.34	10 (16%)	71,101,113	1.36	6 (8%)
25	CLA	a	610	-	45,49,73	1.52	8 (17%)	54,84,113	1.52	6 (11%)
25	CLA	A	603	19	69,73,73	1.26	11 (15%)	83,113,113	1.38	7 (8%)
26	0IE	7	303	-	42,45,45	1.40	6 (14%)	49,63,63	1.54	9 (18%)
24	CHL	6	304	12	52,56,74	2.23	18 (34%)	58,92,114	3.18	25 (43%)
24	CHL	9	309	-	50,54,74	2.32	19 (38%)	56,90,114	3.23	25 (44%)
25	CLA	b	616	18	51,55,73	1.43	9 (17%)	61,91,113	1.48	5 (8%)
24	CHL	8	303	17	58,62,74	2.14	18 (31%)	65,99,114	3.04	27 (41%)
24	CHL	g	305	17	70,74,74	1.92	18 (25%)	80,114,114	2.78	27 (33%)
25	CLA	p	307	12	60,64,73	1.33	9 (15%)	72,102,113	1.39	5 (6%)
33	LMG	C	618	-	42,42,55	0.99	2 (4%)	50,50,63	1.23	4 (8%)
25	CLA	S	611	13	49,53,73	1.47	10 (20%)	59,89,113	1.47	6 (10%)
26	0IE	9	303	-	42,45,45	1.45	6 (14%)	49,63,63	1.74	11 (22%)
31	8CT	c	615	-	40,41,41	4.62	23 (57%)	50,56,56	2.73	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	c	606	20	57,61,73	1.37	10 (17%)	68,98,113	1.41	6 (8%)
29	0UR	7	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.58	12 (20%)
37	DGD	c	619	-	56,56,67	0.95	3 (5%)	70,70,81	1.23	5 (7%)
25	CLA	q	313	-	67,71,73	1.25	8 (11%)	80,110,113	1.29	5 (6%)
23	HEM	E	201	2	50,50,50	1.35	6 (12%)	66,82,82	1.10	4 (6%)
24	CHL	6	308	-	47,51,74	2.33	18 (38%)	52,86,114	3.35	24 (46%)
25	CLA	B	603	18	69,73,73	1.25	11 (15%)	83,113,113	1.31	7 (8%)
25	CLA	6	315	12	49,53,73	1.49	10 (20%)	59,89,113	1.47	6 (10%)
25	CLA	9	306	-	60,64,73	1.35	8 (13%)	72,102,113	1.34	5 (6%)
34	OEX	A	602	19	0,14,14	-	-	-		
25	CLA	S	616	-	49,53,73	1.47	9 (18%)	59,89,113	1.43	5 (8%)
25	CLA	2	314	-	59,63,73	1.33	10 (16%)	71,101,113	1.34	7 (9%)
24	CHL	q	309	-	57,61,74	2.10	18 (31%)	64,98,114	3.13	29 (45%)
25	CLA	p	316	-	49,53,73	1.47	10 (20%)	59,89,113	1.46	4 (6%)
24	CHL	g	310	-	51,55,74	2.29	19 (37%)	57,91,114	3.20	25 (43%)
24	CHL	R	605	-	46,50,74	2.26	19 (41%)	51,85,114	3.46	27 (52%)
25	CLA	n	315	17	49,53,73	1.48	10 (20%)	59,89,113	1.45	4 (6%)
24	CHL	g	318	17	46,50,74	2.32	18 (39%)	51,85,114	3.42	26 (50%)
25	CLA	g	307	-	57,61,73	1.39	8 (14%)	68,98,113	1.34	5 (7%)
30	LHG	c	617	-	31,31,48	1.31	5 (16%)	34,37,54	1.14	3 (8%)
25	CLA	2	307	11	47,51,73	1.48	9 (19%)	56,86,113	1.45	5 (8%)
34	OEX	a	602	19	0,14,14	-	-	-		
24	CHL	p	309	12	47,51,74	2.35	18 (38%)	52,86,114	3.38	25 (48%)
24	CHL	N	305	-	64,68,74	1.98	19 (29%)	72,106,114	2.88	28 (38%)
25	CLA	A	605	-	53,57,73	1.40	9 (16%)	62,93,113	1.45	7 (11%)
25	CLA	n	314	-	67,71,73	1.27	8 (11%)	80,110,113	1.30	5 (6%)
29	0UR	1	301	-	50,53,58	0.99	2 (4%)	58,72,77	1.96	17 (29%)
35	PHO	d	403	-	58,69,69	1.95	9 (15%)	56,99,99	1.54	8 (14%)
25	CLA	p	315	30	67,71,73	1.25	10 (14%)	80,110,113	1.39	6 (7%)
25	CLA	B	607	18	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
35	PHO	A	606	-	58,69,69	1.95	11 (18%)	56,99,99	1.49	7 (12%)
25	CLA	b	615	18	69,73,73	1.24	9 (13%)	83,113,113	1.28	5 (6%)
25	CLA	y	308	-	54,58,73	1.39	10 (18%)	65,95,113	1.44	9 (13%)
30	LHG	A	601	-	44,44,48	1.13	5 (11%)	47,50,54	0.98	2 (4%)
25	CLA	Y	314	30	67,71,73	1.26	9 (13%)	80,110,113	1.27	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	G	308	-	54,58,73	1.40	7 (12%)	65,95,113	1.40	7 (10%)
24	CHL	n	309	-	50,54,74	2.18	19 (38%)	56,90,114	3.36	29 (51%)
25	CLA	2	317	-	53,57,73	1.40	9 (16%)	62,93,113	1.43	5 (8%)
25	CLA	B	614	18	60,64,73	1.32	9 (15%)	72,102,113	1.34	5 (6%)
26	0IE	2	303	-	42,45,45	1.42	6 (14%)	49,63,63	1.52	9 (18%)
31	8CT	c	614	-	40,41,41	4.56	23 (57%)	50,56,56	2.70	21 (42%)
24	CHL	7	309	12	47,51,74	2.36	18 (38%)	52,86,114	3.38	25 (48%)
31	8CT	c	613	-	40,41,41	4.60	23 (57%)	50,56,56	2.70	21 (42%)
25	CLA	g	316	17	49,53,73	1.47	10 (20%)	59,89,113	1.48	4 (6%)
25	CLA	3	315	12	49,53,73	1.49	10 (20%)	59,89,113	1.46	6 (10%)
31	8CT	C	614	-	40,41,41	4.56	23 (57%)	50,56,56	2.68	21 (42%)
25	CLA	d	404	21	69,73,73	1.24	10 (14%)	83,113,113	1.33	7 (8%)
28	NEX	r	317	-	38,46,46	0.96	2 (5%)	50,70,70	4.91	19 (38%)
24	CHL	6	317	12	46,50,74	2.37	18 (39%)	51,85,114	3.43	28 (54%)
24	CHL	G	311	-	58,62,74	2.13	18 (31%)	65,99,114	3.08	27 (41%)
25	CLA	S	604	-	47,51,73	1.47	8 (17%)	56,86,113	1.46	5 (8%)
25	CLA	B	616	18	51,55,73	1.43	9 (17%)	61,91,113	1.49	5 (8%)
31	8CT	T	101	-	40,41,41	4.64	23 (57%)	50,56,56	3.04	18 (36%)
24	CHL	1	309	-	47,51,74	2.31	18 (38%)	52,86,114	3.28	24 (46%)
25	CLA	7	314	-	59,63,73	1.34	10 (16%)	71,101,113	1.36	6 (8%)
30	LHG	D	408	-	38,38,48	1.21	5 (13%)	41,44,54	1.06	2 (4%)
24	CHL	7	306	-	68,72,74	1.84	18 (26%)	77,111,114	2.93	32 (41%)
25	CLA	q	306	28	54,58,73	1.40	10 (18%)	65,95,113	1.40	8 (12%)
25	CLA	2	308	-	54,58,73	1.40	8 (14%)	65,95,113	1.45	7 (10%)
25	CLA	D	404	21	69,73,73	1.24	11 (15%)	83,113,113	1.32	8 (9%)
25	CLA	N	315	17	49,53,73	1.48	10 (20%)	59,89,113	1.44	5 (8%)
28	NEX	2	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
28	NEX	r	301	-	38,46,46	1.06	2 (5%)	50,70,70	2.82	17 (34%)
31	8CT	a	608	-	40,41,41	4.63	23 (57%)	50,56,56	2.66	20 (40%)
33	LMG	W	201	-	30,30,55	1.14	2 (6%)	38,38,63	1.37	6 (15%)
24	CHL	8	307	17	47,51,74	2.24	18 (38%)	52,86,114	3.34	26 (50%)
25	CLA	7	307	12	60,64,73	1.33	8 (13%)	72,102,113	1.40	5 (6%)
31	8CT	C	615	-	40,41,41	4.62	23 (57%)	50,56,56	2.75	18 (36%)
24	CHL	s	409	-	51,55,74	2.20	18 (35%)	57,91,114	3.21	25 (43%)
25	CLA	y	317	17	59,63,73	1.33	10 (16%)	70,100,113	1.40	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	0UR	y	301	-	50,53,58	0.98	1 (2%)	58,72,77	1.63	14 (24%)
26	0IE	y	303	-	42,45,45	1.40	6 (14%)	49,63,63	1.50	9 (18%)
25	CLA	R	603	-	51,55,73	1.42	7 (13%)	61,91,113	1.44	5 (8%)
29	0UR	G	301	-	50,53,58	0.95	1 (2%)	58,72,77	1.75	15 (25%)
25	CLA	c	603	20	69,73,73	1.24	9 (13%)	83,113,113	1.34	8 (9%)
25	CLA	d	405	21	69,73,73	1.24	9 (13%)	83,113,113	1.34	5 (6%)
29	0UR	n	301	-	50,53,58	0.95	1 (2%)	58,72,77	1.81	12 (20%)
25	CLA	q	315	17	47,51,73	1.48	10 (21%)	56,86,113	1.44	4 (7%)
24	CHL	3	317	12	46,50,74	2.37	19 (41%)	51,85,114	3.44	27 (52%)
25	CLA	S	612	-	59,63,73	1.35	10 (16%)	70,100,113	1.37	6 (8%)
25	CLA	8	313	17	49,53,73	1.47	9 (18%)	59,89,113	1.47	4 (6%)
25	CLA	4	313	-	59,63,73	1.36	8 (13%)	71,101,113	1.35	8 (11%)
24	CHL	u	305	12	70,74,74	1.97	18 (25%)	80,114,114	2.81	27 (33%)
24	CHL	p	306	-	68,72,74	1.84	18 (26%)	77,111,114	2.94	32 (41%)
29	0UR	4	301	-	50,53,58	0.99	2 (4%)	58,72,77	1.96	17 (29%)
24	CHL	5	309	11	47,51,74	2.31	17 (36%)	52,86,114	3.35	24 (46%)
31	8CT	b	617	-	40,41,41	4.66	23 (57%)	50,56,56	2.84	18 (36%)
25	CLA	b	601	-	49,53,73	1.46	10 (20%)	59,89,113	1.47	6 (10%)
24	CHL	Y	317	17	46,50,74	2.27	18 (39%)	51,85,114	3.43	27 (52%)
24	CHL	g	313	-	70,74,74	1.98	18 (25%)	80,114,114	2.76	29 (36%)
27	XAT	R	615	-	39,47,47	0.91	0	54,74,74	2.74	20 (37%)
25	CLA	C	610	-	69,73,73	1.24	10 (14%)	83,113,113	1.32	8 (9%)
33	LMG	D	401	-	48,48,55	0.91	2 (4%)	56,56,63	1.17	5 (8%)
24	CHL	y	313	-	70,74,74	1.89	19 (27%)	80,114,114	2.75	26 (32%)
24	CHL	G	312	-	55,59,74	2.18	19 (34%)	62,96,114	3.10	27 (43%)
25	CLA	q	305	17	58,62,73	1.36	9 (15%)	69,99,113	1.39	5 (7%)
24	CHL	4	312	-	50,54,74	2.29	18 (36%)	56,90,114	3.18	25 (44%)
24	CHL	N	312	-	60,64,74	2.06	18 (30%)	68,102,114	2.99	28 (41%)
25	CLA	8	306	-	54,58,73	1.40	9 (16%)	65,95,113	1.40	7 (10%)
24	CHL	R	602	-	51,55,74	2.16	19 (37%)	57,91,114	3.25	26 (45%)
24	CHL	Y	309	-	51,55,74	2.13	18 (35%)	57,91,114	3.31	28 (49%)
24	CHL	u	310	-	50,54,74	2.34	19 (38%)	56,90,114	3.23	25 (44%)
26	0IE	g	302	-	42,45,45	1.42	6 (14%)	49,63,63	1.58	10 (20%)
24	CHL	u	311	-	50,54,74	2.31	19 (38%)	56,90,114	3.23	24 (42%)
24	CHL	S	608	-	51,55,74	2.19	19 (37%)	57,91,114	3.23	27 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	0IE	3	303	-	42,45,45	1.44	6 (14%)	49,63,63	1.70	9 (18%)
25	CLA	B	609	18	69,73,73	1.24	9 (13%)	83,113,113	1.32	8 (9%)
28	NEX	5	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
25	CLA	b	611	18	69,73,73	1.25	9 (13%)	83,113,113	1.39	7 (8%)
24	CHL	p	310	-	50,54,74	2.30	18 (36%)	56,90,114	3.23	26 (46%)
25	CLA	c	601	20	69,73,73	1.24	10 (14%)	83,113,113	1.40	9 (10%)
24	CHL	u	313	-	47,51,74	2.32	17 (36%)	52,86,114	3.32	25 (48%)
24	CHL	y	309	17	47,51,74	2.23	17 (36%)	52,86,114	3.38	25 (48%)
39	PL9	d	406	-	55,55,55	1.68	12 (21%)	68,69,69	1.57	12 (17%)
24	CHL	5	313	-	46,50,74	2.33	18 (39%)	51,85,114	3.35	24 (47%)
31	8CT	s	416	-	40,41,41	4.74	25 (62%)	50,56,56	7.31	22 (44%)
33	LMG	i	101	-	48,48,55	0.92	2 (4%)	56,56,63	1.20	4 (7%)
25	CLA	9	315	-	49,53,73	1.49	8 (16%)	59,89,113	1.45	4 (6%)
25	CLA	C	603	20	69,73,73	1.24	10 (14%)	83,113,113	1.34	8 (9%)
28	NEX	7	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
24	CHL	n	310	-	57,61,74	2.17	19 (33%)	64,98,114	3.11	28 (43%)
25	CLA	b	602	18	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
25	CLA	r	314	-	51,55,73	1.46	7 (13%)	61,91,113	1.37	5 (8%)
24	CHL	Y	304	17	70,74,74	1.81	18 (25%)	80,114,114	2.88	29 (36%)
25	CLA	5	316	-	49,53,73	1.47	10 (20%)	59,89,113	1.47	4 (6%)
24	CHL	1	310	-	47,51,74	2.24	18 (38%)	52,86,114	3.31	25 (48%)
25	CLA	s	405	-	47,51,73	1.47	8 (17%)	56,86,113	1.46	6 (10%)
30	LHG	g	319	-	42,42,48	1.16	5 (11%)	45,48,54	0.99	2 (4%)
29	0UR	q	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.79	14 (24%)
32	SQD	d	409	-	43,44,54	1.06	5 (11%)	52,55,65	1.57	8 (15%)
25	CLA	9	314	30	67,71,73	1.27	7 (10%)	80,110,113	1.33	5 (6%)
24	CHL	8	304	17	64,68,74	1.96	19 (29%)	72,106,114	2.91	29 (40%)
37	DGD	C	620	-	56,56,67	0.95	2 (3%)	70,70,81	1.21	6 (8%)
30	LHG	a	601	-	44,44,48	1.12	5 (11%)	47,50,54	0.98	3 (6%)
24	CHL	y	306	-	68,72,74	1.85	18 (26%)	77,111,114	2.91	29 (37%)
25	CLA	B	613	18	69,73,73	1.26	10 (14%)	83,113,113	1.27	7 (8%)
25	CLA	u	307	-	60,64,73	1.35	7 (11%)	72,102,113	1.34	4 (5%)
24	CHL	n	311	-	54,58,74	2.13	20 (37%)	59,94,114	3.19	25 (42%)
24	CHL	r	307	-	52,56,74	2.19	17 (32%)	58,92,114	3.20	25 (43%)
26	0IE	8	302	-	42,45,45	1.40	6 (14%)	49,63,63	1.52	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	g	308	-	54,58,73	1.40	8 (14%)	65,95,113	1.40	7 (10%)
24	CHL	Y	308	17	47,51,74	2.24	17 (36%)	52,86,114	3.38	24 (46%)
24	CHL	n	304	17	58,62,74	2.16	18 (31%)	65,99,114	3.04	27 (41%)
25	CLA	S	603	-	49,53,73	1.48	9 (18%)	59,89,113	1.46	6 (10%)
24	CHL	7	311	-	50,54,74	2.25	17 (34%)	56,90,114	3.22	26 (46%)
24	CHL	G	310	-	51,55,74	2.28	19 (37%)	57,91,114	3.19	25 (43%)
24	CHL	s	407	-	50,54,74	2.25	19 (38%)	56,90,114	3.21	25 (44%)
25	CLA	B	601	-	49,53,73	1.46	10 (20%)	59,89,113	1.47	6 (10%)
26	0IE	Y	303	-	42,45,45	1.39	6 (14%)	49,63,63	1.50	8 (16%)
24	CHL	6	312	-	47,51,74	2.31	17 (36%)	52,86,114	3.28	24 (46%)
30	LHG	N	318	-	42,42,48	1.17	6 (14%)	45,48,54	0.97	2 (4%)
28	NEX	9	319	-	38,46,46	0.95	2 (5%)	50,70,70	4.90	19 (38%)
24	CHL	5	310	-	46,50,74	2.29	19 (41%)	51,85,114	3.39	24 (47%)
31	8CT	B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.88	18 (36%)
25	CLA	C	616	20	50,54,73	1.44	10 (20%)	60,90,113	1.49	7 (11%)
24	CHL	R	607	-	52,56,74	2.13	19 (36%)	58,92,114	3.32	27 (46%)
24	CHL	2	309	11	47,51,74	2.29	18 (38%)	52,86,114	3.34	24 (46%)
24	CHL	G	305	17	70,74,74	1.91	18 (25%)	80,114,114	2.79	27 (33%)
24	CHL	q	316	-	46,50,74	2.39	19 (41%)	51,85,114	3.42	25 (49%)
26	0IE	p	302	-	42,45,45	1.45	6 (14%)	49,63,63	1.60	12 (24%)
24	CHL	1	304	-	46,50,74	2.40	18 (39%)	51,85,114	3.40	26 (50%)
25	CLA	2	315	-	67,71,73	1.26	8 (11%)	80,110,113	1.31	5 (6%)
25	CLA	c	609	20	69,73,73	1.27	9 (13%)	83,113,113	1.36	9 (10%)
24	CHL	s	414	-	46,50,74	2.29	18 (39%)	51,85,114	3.43	27 (52%)
24	CHL	1	312	10	50,54,74	2.29	18 (36%)	56,90,114	3.19	24 (42%)
25	CLA	B	611	18	69,73,73	1.25	9 (13%)	83,113,113	1.39	7 (8%)
24	CHL	4	305	-	50,54,74	2.23	19 (38%)	56,90,114	3.29	26 (46%)
28	NEX	1	303	-	38,46,46	0.97	2 (5%)	50,70,70	4.90	19 (38%)
30	LHG	Y	318	25	42,42,48	1.16	5 (11%)	45,48,54	1.10	3 (6%)
24	CHL	3	308	-	47,51,74	2.33	18 (38%)	52,86,114	3.34	24 (46%)
24	CHL	7	310	-	50,54,74	2.31	19 (38%)	56,90,114	3.24	26 (46%)
25	CLA	8	305	17	58,62,73	1.35	9 (15%)	69,99,113	1.38	5 (7%)
25	CLA	b	608	-	59,63,73	1.35	9 (15%)	71,101,113	1.37	7 (9%)
30	LHG	p	319	25	42,42,48	1.17	5 (11%)	45,48,54	1.02	3 (6%)
25	CLA	u	308	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	N	307	-	54,58,73	1.40	9 (16%)	65,95,113	1.41	7 (10%)
25	CLA	a	603	19	69,73,73	1.26	11 (15%)	83,113,113	1.38	7 (8%)
25	CLA	s	404	-	49,53,73	1.47	8 (16%)	59,89,113	1.45	6 (10%)
32	SQD	A	609	-	44,45,54	1.06	5 (11%)	53,56,65	1.55	10 (18%)
35	PHO	D	403	-	58,69,69	1.94	9 (15%)	56,99,99	1.53	7 (12%)
24	CHL	r	302	8	50,54,74	2.32	18 (36%)	56,90,114	3.24	25 (44%)
24	CHL	p	318	12	46,50,74	2.33	18 (39%)	51,85,114	3.39	27 (52%)
25	CLA	1	315	10	49,53,73	1.50	8 (16%)	59,89,113	1.46	4 (6%)
29	0UR	8	301	-	50,53,58	0.94	1 (2%)	58,72,77	1.78	14 (24%)
24	CHL	3	304	12	52,56,74	2.21	19 (36%)	58,92,114	3.17	24 (41%)
24	CHL	5	311	-	51,55,74	2.27	19 (37%)	57,91,114	3.13	25 (43%)
24	CHL	R	601	8	50,54,74	2.33	18 (36%)	56,90,114	3.26	25 (44%)
25	CLA	b	613	18	69,73,73	1.26	10 (14%)	83,113,113	1.28	7 (8%)
24	CHL	g	309	-	47,51,74	2.36	18 (38%)	52,86,114	3.36	24 (46%)
31	8CT	x	601	-	40,41,41	4.63	23 (57%)	50,56,56	2.59	19 (38%)
25	CLA	r	310	8	59,63,73	1.34	10 (16%)	71,101,113	1.36	5 (7%)
25	CLA	c	602	20	69,73,73	1.26	11 (15%)	83,113,113	1.33	6 (7%)
25	CLA	g	315	-	64,68,73	1.30	8 (12%)	77,107,113	1.29	5 (6%)
30	LHG	4	318	-	41,41,48	1.19	6 (14%)	44,47,54	0.97	3 (6%)
24	CHL	Y	310	-	58,62,74	2.03	19 (32%)	65,99,114	3.19	29 (44%)
28	NEX	y	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
33	LMG	B	619	-	41,41,55	0.97	2 (4%)	49,49,63	1.30	4 (8%)
24	CHL	s	406	-	50,54,74	2.24	18 (36%)	56,90,114	3.23	23 (41%)
25	CLA	B	605	18	69,73,73	1.25	10 (14%)	83,113,113	1.27	7 (8%)
28	NEX	3	318	-	38,46,46	1.06	2 (5%)	50,70,70	2.82	17 (34%)
28	NEX	G	304	-	38,46,46	0.96	2 (5%)	50,70,70	4.91	19 (38%)
24	CHL	5	318	11	46,50,74	2.38	18 (39%)	51,85,114	3.41	25 (49%)
24	CHL	n	305	-	64,68,74	1.98	19 (29%)	72,106,114	2.88	28 (38%)
26	0IE	u	303	-	42,45,45	1.45	6 (14%)	49,63,63	1.67	10 (20%)
29	0UR	p	301	-	50,53,58	0.93	1 (2%)	58,72,77	1.59	12 (20%)
25	CLA	Y	307	-	54,58,73	1.40	10 (18%)	65,95,113	1.45	9 (13%)
25	CLA	S	609	-	59,63,73	1.32	10 (16%)	71,101,113	1.34	5 (7%)
24	CHL	S	606	-	50,54,74	2.25	19 (38%)	56,90,114	3.22	25 (44%)
24	CHL	6	305	-	52,56,74	2.20	19 (36%)	58,92,114	3.16	26 (44%)
25	CLA	N	306	17	58,62,73	1.36	8 (13%)	69,99,113	1.38	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	NEX	S	617	-	38,46,46	0.95	2 (5%)	50,70,70	4.90	19 (38%)
25	CLA	a	605	-	53,57,73	1.39	9 (16%)	62,93,113	1.45	7 (11%)
24	CHL	9	304	12	70,74,74	1.93	18 (25%)	80,114,114	2.79	27 (33%)
24	CHL	4	311	-	48,52,74	2.21	18 (37%)	53,87,114	3.28	24 (45%)
25	CLA	s	411	-	48,52,73	1.51	11 (22%)	56,87,113	1.46	6 (10%)
26	0IE	r	315	-	42,45,45	1.44	6 (14%)	49,63,63	1.54	10 (20%)
35	PHO	a	606	-	58,69,69	1.95	10 (17%)	56,99,99	1.49	7 (12%)
25	CLA	b	606	18	69,73,73	1.23	10 (14%)	83,113,113	1.36	7 (8%)
25	CLA	b	603	18	69,73,73	1.25	11 (15%)	83,113,113	1.31	8 (9%)
25	CLA	c	610	-	69,73,73	1.24	11 (15%)	83,113,113	1.32	9 (10%)
32	SQD	B	618	-	53,54,54	0.95	5 (9%)	62,65,65	1.55	11 (17%)
25	CLA	4	307	28	45,49,73	1.52	9 (20%)	54,84,113	1.50	7 (12%)
25	CLA	u	317	12	59,63,73	1.37	9 (15%)	70,100,113	1.35	5 (7%)
24	CHL	3	310	-	50,54,74	2.33	18 (36%)	56,90,114	3.20	25 (44%)
24	CHL	p	312	-	51,55,74	2.11	18 (35%)	57,91,114	3.32	28 (49%)
24	CHL	7	318	12	46,50,74	2.34	18 (39%)	51,85,114	3.39	27 (52%)
39	PL9	D	406	-	55,55,55	1.67	12 (21%)	68,69,69	1.57	12 (17%)
28	NEX	6	303	-	38,46,46	1.06	2 (5%)	50,70,70	2.82	17 (34%)
30	LHG	1	318	-	41,41,48	1.19	6 (14%)	44,47,54	0.97	3 (6%)
33	LMG	m	101	-	41,41,55	0.98	2 (4%)	49,49,63	1.23	4 (8%)
24	CHL	9	305	-	68,72,74	1.94	19 (27%)	77,111,114	2.82	27 (35%)
30	LHG	d	408	-	38,38,48	0.98	2 (5%)	41,44,54	1.24	4 (9%)
24	CHL	9	310	-	50,54,74	2.32	19 (38%)	56,90,114	3.22	24 (42%)
25	CLA	B	604	18	66,70,73	1.28	9 (13%)	79,109,113	1.41	8 (10%)
25	CLA	6	316	-	49,53,73	1.48	9 (18%)	59,89,113	1.45	6 (10%)
31	8CT	X	601	-	40,41,41	4.63	23 (57%)	50,56,56	2.58	19 (38%)
25	CLA	r	304	-	51,55,73	1.42	8 (15%)	61,91,113	1.46	5 (8%)
24	CHL	3	312	-	47,51,74	2.32	17 (36%)	52,86,114	3.28	25 (48%)
25	CLA	6	307	-	47,51,73	1.48	8 (17%)	56,86,113	1.46	4 (7%)
25	CLA	Y	316	17	59,63,73	1.33	10 (16%)	70,100,113	1.41	6 (8%)
24	CHL	8	308	-	50,54,74	2.21	18 (36%)	56,90,114	3.31	27 (48%)
25	CLA	1	306	-	48,52,73	1.47	8 (16%)	56,87,113	1.45	6 (10%)
25	CLA	q	312	-	59,63,73	1.33	10 (16%)	71,101,113	1.39	7 (9%)
32	SQD	a	609	-	44,45,54	1.05	5 (11%)	53,56,65	1.67	10 (18%)
31	8CT	D	410	-	40,41,41	4.70	23 (57%)	50,56,56	2.47	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	p	313	-	47,51,74	2.22	18 (38%)	52,86,114	3.29	23 (44%)
28	NEX	n	303	-	38,46,46	1.06	2 (5%)	50,70,70	2.82	18 (36%)
25	CLA	G	315	-	64,68,73	1.30	8 (12%)	77,107,113	1.29	5 (6%)
25	CLA	Y	313	17	59,63,73	1.34	10 (16%)	71,101,113	1.37	8 (11%)
33	LMG	d	411	-	46,46,55	0.95	2 (4%)	54,54,63	1.14	5 (9%)
25	CLA	N	313	-	59,63,73	1.34	8 (13%)	71,101,113	1.37	8 (11%)
25	CLA	8	314	-	47,51,73	1.48	10 (21%)	56,86,113	1.46	5 (8%)
25	CLA	6	314	-	45,49,73	1.51	7 (15%)	54,84,113	1.50	6 (11%)
28	NEX	4	303	25	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
30	LHG	2	319	-	39,39,48	1.20	5 (12%)	42,45,54	1.06	3 (7%)

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
24	CHL	G	313	-	-	23/41/117/117	-
25	CLA	1	307	-	-	4/10/86/115	-
25	CLA	G	314	-	-	4/27/103/115	-
25	CLA	y	316	17	-	6/15/91/115	-
24	CHL	2	310	-	-	2/12/88/117	-
25	CLA	7	316	12	-	4/15/91/115	-
26	0IE	G	303	-	-	0/33/72/72	0/2/2/2
24	CHL	4	310	-	-	2/14/90/117	-
29	0UR	u	301	-	-	10/42/81/86	0/2/2/2
24	CHL	q	308	-	-	6/17/93/117	-
30	LHG	d	407	-	-	27/53/53/53	-
31	8CT	S	614	-	-	6/29/63/63	0/2/2/2
25	CLA	R	609	8	-	3/27/103/115	-
24	CHL	R	606	-	-	8/20/96/117	-
26	0IE	R	614	-	-	1/33/72/72	0/2/2/2
30	LHG	G	319	-	-	23/47/47/53	-
25	CLA	C	609	20	-	6/39/115/115	-
30	LHG	9	318	25	-	25/47/47/53	-
24	CHL	q	304	17	-	17/34/110/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	4	314	-	-	6/10/86/115	-
30	LHG	5	319	-	-	20/47/47/53	-
25	CLA	3	316	-	-	8/15/91/115	-
25	CLA	7	308	-	-	6/21/97/115	-
37	DGD	C	619	-	-	27/39/79/95	0/2/2/2
25	CLA	s	413	-	-	9/27/103/115	-
31	8CT	d	410	-	-	9/29/63/63	0/2/2/2
24	CHL	2	305	11	-	6/15/91/117	-
25	CLA	Y	306	17	-	5/25/101/115	-
25	CLA	3	307	-	-	6/13/89/115	-
25	CLA	4	306	-	-	6/13/90/115	-
25	CLA	6	313	-	-	2/10/86/115	-
24	CHL	s	408	-	-	6/17/93/117	-
25	CLA	C	608	20	-	10/35/111/115	-
24	CHL	1	308	10	-	2/14/90/117	-
24	CHL	G	309	-	-	2/14/90/117	-
25	CLA	g	317	17	-	6/27/103/115	-
25	CLA	u	314	-	-	3/27/103/115	-
25	CLA	r	305	-	-	3/10/86/115	-
25	CLA	y	314	17	-	5/27/103/115	-
30	LHG	A	612	-	-	15/48/48/53	-
24	CHL	2	318	11	-	6/12/88/117	-
30	LHG	C	617	-	-	17/36/36/53	-
25	CLA	9	316	12	-	11/27/103/115	-
24	CHL	g	306	-	-	26/39/115/117	-
24	CHL	u	318	-	-	6/12/88/117	-
24	CHL	Y	312	-	-	19/41/117/117	-
24	CHL	1	311	-	-	3/15/91/117	-
24	CHL	y	310	-	-	5/19/95/117	-
25	CLA	C	602	20	-	20/39/115/115	-
24	CHL	5	305	11	-	7/15/91/117	-
25	CLA	B	606	18	-	18/39/115/115	-
25	CLA	A	604	-	-	9/39/115/115	-
28	NEX	N	303	-	-	4/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	610	-	-	4/39/115/115	-
25	CLA	n	306	17	-	9/26/102/115	-
24	CHL	S	607	-	-	5/17/93/117	-
32	SQD	D	409	-	-	13/39/59/69	0/1/1/1
24	CHL	q	303	17	-	8/27/103/117	-
25	CLA	6	306	-	-	5/10/86/115	-
24	CHL	r	309	-	-	6/17/93/117	-
25	CLA	s	410	-	-	5/27/103/115	-
25	CLA	R	613	-	-	9/18/94/115	-
31	8CT	s	415	-	-	6/29/63/63	0/2/2/2
25	CLA	B	608	-	-	12/27/103/115	-
31	8CT	V	401	-	-	11/29/63/63	0/2/2/2
25	CLA	R	612	-	-	7/15/91/115	-
24	CHL	u	309	12	-	2/14/90/117	-
28	NEX	p	304	-	-	5/27/83/83	0/3/3/3
29	0UR	g	301	-	-	10/42/81/86	0/2/2/2
25	CLA	3	313	-	-	2/10/86/115	-
24	CHL	S	605	-	-	6/17/93/117	-
23	HEM	f	201	2,9	-	1/14/54/54	-
25	CLA	2	316	-	-	4/15/91/115	-
24	CHL	p	305	12	-	17/41/117/117	-
24	CHL	q	311	-	-	11/29/105/117	-
25	CLA	A	610	-	-	4/10/86/115	-
24	CHL	u	306	-	-	17/39/115/117	-
24	CHL	1	317	-	-	7/12/88/117	-
30	LHG	n	318	-	-	20/47/47/53	-
24	CHL	2	313	-	-	4/12/88/117	-
25	CLA	D	405	21	-	12/39/115/115	-
24	CHL	y	311	-	-	12/27/103/117	-
24	CHL	N	304	17	-	8/27/103/117	-
24	CHL	S	613	-	-	3/12/88/117	-
30	LHG	7	319	25	-	24/41/41/53	-
26	0IE	7	302	-	-	4/33/72/72	0/2/2/2
24	CHL	9	311	-	-	7/19/95/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	9	307	-	-	9/21/97/115	-
25	CLA	A	607	19	-	4/33/109/115	-
26	0IE	g	303	-	-	0/33/72/72	0/2/2/2
25	CLA	y	307	17	-	5/25/101/115	-
25	CLA	C	605	20	-	9/29/105/115	-
28	NEX	g	304	-	-	5/27/83/83	0/3/3/3
25	CLA	R	611	8	-	8/15/91/115	-
24	CHL	N	309	-	-	7/17/93/117	-
24	CHL	S	601	13	-	12/17/93/117	-
24	CHL	n	308	17	-	4/14/90/117	-
31	8CT	v	401	-	-	11/29/63/63	0/2/2/2
25	CLA	3	306	-	-	5/10/86/115	-
25	CLA	b	604	18	-	16/36/112/115	-
25	CLA	C	611	20	-	13/39/115/115	-
26	0IE	5	302	-	-	2/33/72/72	0/2/2/2
24	CHL	7	312	-	-	7/19/95/117	-
25	CLA	n	307	-	-	5/21/97/115	-
24	CHL	4	308	10	-	2/14/90/117	-
25	CLA	9	313	-	-	3/27/103/115	-
25	CLA	C	607	-	-	11/39/115/115	-
24	CHL	n	312	-	-	12/29/105/117	-
25	CLA	r	311	-	-	6/15/91/115	-
26	0IE	1	302	-	-	2/33/72/72	0/2/2/2
25	CLA	B	602	18	-	13/39/115/115	-
33	LMG	w	201	-	-	17/31/51/70	0/1/1/1
24	CHL	9	317	-	-	6/12/88/117	-
26	0IE	6	302	-	-	4/33/69/72	0/2/2/2
37	DGD	c	618	-	-	27/39/79/95	0/2/2/2
25	CLA	7	315	30	-	15/37/113/115	-
25	CLA	N	314	-	-	7/37/113/115	-
25	CLA	C	604	-	-	17/39/115/115	-
24	CHL	y	312	-	-	5/23/99/117	-
30	LHG	y	319	25	-	25/47/47/53	-
30	LHG	D	407	-	-	29/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	g	314	-	-	4/27/103/115	-
25	CLA	b	614	18	-	13/29/105/115	-
24	CHL	N	310	-	-	9/26/102/117	-
25	CLA	5	307	11	-	7/13/89/115	-
24	CHL	2	306	-	-	10/19/95/117	-
24	CHL	p	311	-	-	3/17/93/117	-
25	CLA	c	608	20	-	10/35/111/115	-
24	CHL	9	308	12	-	2/14/90/117	-
25	CLA	u	315	-	-	13/37/113/115	-
29	0UR	9	301	-	-	10/42/81/86	0/2/2/2
26	0IE	y	302	-	-	2/33/72/72	0/2/2/2
24	CHL	3	311	-	-	5/15/91/117	-
24	CHL	r	303	-	-	6/19/95/117	-
24	CHL	4	317	-	-	8/12/88/117	-
25	CLA	y	315	30	-	12/37/113/115	-
25	CLA	G	307	-	-	6/25/101/115	-
25	CLA	8	311	-	-	3/27/103/115	-
24	CHL	y	305	17	-	11/41/117/117	-
24	CHL	7	305	12	-	17/41/117/117	-
25	CLA	G	317	-	-	6/27/103/115	-
24	CHL	r	308	-	-	11/20/96/117	-
25	CLA	b	605	18	-	16/39/115/115	-
29	0UR	6	301	-	-	9/42/81/86	0/2/2/2
25	CLA	r	312	8	-	8/15/91/115	-
26	0IE	3	302	-	-	4/33/69/72	0/2/2/2
25	CLA	C	612	20	-	10/26/102/115	-
24	CHL	g	311	-	-	8/27/103/117	-
28	NEX	s	401	25	-	4/27/83/83	0/3/3/3
24	CHL	N	311	-	-	7/22/98/117	-
25	CLA	1	316	10	-	1/12/88/115	-
28	NEX	u	304	-	-	5/27/83/83	0/3/3/3
26	0IE	G	302	-	-	2/33/72/72	0/2/2/2
25	CLA	5	315	-	-	10/37/113/115	-
24	CHL	Y	305	-	-	22/39/115/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	0IE	u	302	-	-	4/33/72/72	0/2/2/2
24	CHL	n	317	-	-	4/12/88/117	-
32	SQD	b	618	-	-	15/49/69/69	0/1/1/1
24	CHL	8	309	-	-	5/22/98/117	-
25	CLA	s	412	13	-	6/15/91/115	-
25	CLA	b	610	-	-	5/39/115/115	-
25	CLA	b	609	18	-	19/39/115/115	-
26	0IE	n	302	-	-	2/33/72/72	0/2/2/2
24	CHL	8	315	-	-	0/12/88/117	-
25	CLA	c	604	-	-	18/39/115/115	-
25	CLA	a	607	19	-	4/33/109/115	-
30	LHG	a	612	-	-	15/48/48/53	-
24	CHL	6	311	-	-	4/15/91/117	-
25	CLA	5	314	-	-	5/27/103/115	-
26	0IE	4	302	-	-	2/33/72/72	0/2/2/2
25	CLA	b	612	18	-	11/39/115/115	-
29	0UR	2	301	-	-	14/42/81/86	0/2/2/2
24	CHL	S	602	13	-	16/32/108/117	-
24	CHL	N	308	17	-	4/14/90/117	-
24	CHL	G	318	17	-	8/12/88/117	-
25	CLA	u	316	-	-	6/15/91/115	-
25	CLA	a	604	-	-	10/39/115/115	-
25	CLA	1	314	-	-	6/10/86/115	-
25	CLA	N	316	-	-	2/13/89/115	-
26	0IE	9	302	-	-	4/33/72/72	0/2/2/2
25	CLA	Y	315	17	-	6/15/91/115	-
29	0UR	3	301	-	-	9/42/81/86	0/2/2/2
24	CHL	3	305	-	-	10/20/96/117	-
25	CLA	r	313	-	-	7/15/91/115	-
25	CLA	c	611	20	-	13/39/115/115	-
24	CHL	Y	311	-	-	5/23/99/117	-
28	NEX	R	616	-	-	5/27/83/83	0/3/3/3
25	CLA	S	610	-	-	2/15/91/115	-
25	CLA	1	313	-	-	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	9	312	-	-	4/14/90/117	-
25	CLA	5	308	-	-	4/21/97/115	-
25	CLA	c	612	20	-	10/26/102/115	-
31	8CT	A	608	-	-	8/29/63/63	0/2/2/2
24	CHL	1	305	10	-	8/17/93/117	-
25	CLA	C	606	20	-	9/25/101/115	-
24	CHL	G	306	17	-	26/39/115/117	-
25	CLA	q	314	17	-	4/15/91/115	-
25	CLA	G	316	17	-	6/15/91/115	-
24	CHL	6	309	-	-	7/23/99/117	-
24	CHL	s	402	13	-	12/17/93/117	-
24	CHL	2	312	-	-	7/17/93/117	-
33	LMG	d	401	-	-	12/43/63/70	0/1/1/1
25	CLA	B	612	18	-	12/39/115/115	-
24	CHL	4	309	-	-	4/14/90/117	-
24	CHL	R	608	-	-	6/17/93/117	-
24	CHL	6	310	-	-	7/17/93/117	-
25	CLA	R	604	-	-	5/10/86/115	-
25	CLA	n	316	-	-	3/13/89/115	-
26	0IE	N	302	-	-	2/33/72/72	0/2/2/2
25	CLA	c	605	20	-	9/29/105/115	-
24	CHL	N	317	-	-	4/12/88/117	-
25	CLA	4	316	-	-	0/12/88/115	-
24	CHL	5	306	-	-	9/19/95/117	-
25	CLA	s	417	-	-	8/15/91/115	-
27	XAT	r	316	-	-	0/31/93/93	0/4/4/4
26	0IE	2	302	-	-	2/33/72/72	0/2/2/2
24	CHL	5	312	-	-	7/17/93/117	-
33	LMG	D	411	-	-	26/41/61/70	0/1/1/1
24	CHL	y	318	17	-	6/12/88/117	-
25	CLA	8	312	-	-	10/37/113/115	-
26	0IE	p	303	-	-	2/33/72/72	0/2/2/2
24	CHL	2	311	-	-	7/19/95/117	-
26	0IE	Y	302	-	-	2/33/72/72	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	g	312	-	-	5/23/99/117	-
24	CHL	q	307	17	-	2/14/90/117	-
26	0IE	q	302	-	-	2/33/72/72	0/2/2/2
25	CLA	B	615	18	-	4/39/115/115	-
25	CLA	R	610	-	-	4/15/91/115	-
25	CLA	5	317	11	-	9/20/96/115	-
25	CLA	3	314	-	-	4/10/86/115	-
31	8CT	t	101	-	-	12/29/63/63	0/2/2/2
24	CHL	7	313	-	-	5/14/90/117	-
25	CLA	b	607	18	-	14/39/115/115	-
29	0UR	N	301	-	-	10/42/81/86	0/2/2/2
31	8CT	C	613	-	-	8/29/63/63	0/2/2/2
25	CLA	p	308	-	-	7/21/97/115	-
31	8CT	S	615	-	-	12/29/63/63	0/2/2/2
24	CHL	4	304	-	-	2/12/88/117	-
24	CHL	q	310	-	-	5/22/98/117	-
24	CHL	s	403	13	-	17/32/108/117	-
25	CLA	p	317	12	-	9/27/103/115	-
25	CLA	n	313	-	-	6/27/103/115	-
24	CHL	3	309	-	-	7/23/99/117	-
25	CLA	7	317	12	-	9/24/100/115	-
25	CLA	C	601	20	-	14/39/115/115	-
24	CHL	r	306	-	-	6/12/88/117	-
24	CHL	u	312	-	-	7/19/95/117	-
24	CHL	8	310	-	-	11/29/105/117	-
24	CHL	Y	319	-	-	8/26/102/117	-
25	CLA	c	616	20	-	4/17/93/115	-
29	0UR	5	301	-	-	14/42/81/86	0/2/2/2
29	0UR	Y	301	-	-	12/42/81/86	0/2/2/2
26	0IE	5	303	-	-	0/33/72/72	0/2/2/2
25	CLA	4	315	10	-	8/15/91/115	-
25	CLA	c	607	-	-	11/39/115/115	-
25	CLA	p	314	-	-	5/27/103/115	-
25	CLA	a	610	-	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	603	19	-	13/39/115/115	-
26	0IE	7	303	-	-	2/33/72/72	0/2/2/2
24	CHL	6	304	12	-	8/20/96/117	-
24	CHL	9	309	-	-	9/17/93/117	-
25	CLA	b	616	18	-	6/18/94/115	-
24	CHL	8	303	17	-	8/27/103/117	-
24	CHL	g	305	17	-	21/41/117/117	-
25	CLA	p	307	12	-	8/29/105/115	-
33	LMG	C	618	-	-	17/37/57/70	0/1/1/1
25	CLA	S	611	13	-	6/15/91/115	-
26	0IE	9	303	-	-	5/33/72/72	0/2/2/2
31	8CT	c	615	-	-	12/29/63/63	0/2/2/2
25	CLA	c	606	20	-	9/25/101/115	-
29	0UR	7	301	-	-	8/42/81/86	0/2/2/2
37	DGD	c	619	-	-	17/44/84/95	0/2/2/2
25	CLA	q	313	-	-	8/37/113/115	-
23	HEM	E	201	2	-	0/14/54/54	-
24	CHL	6	308	-	-	2/14/90/117	-
25	CLA	B	603	18	-	12/39/115/115	-
25	CLA	6	315	12	-	7/15/91/115	-
25	CLA	9	306	-	-	6/29/105/115	-
25	CLA	S	616	-	-	8/15/91/115	-
25	CLA	2	314	-	-	5/27/103/115	-
24	CHL	q	309	-	-	10/26/102/117	-
25	CLA	p	316	-	-	4/15/91/115	-
24	CHL	g	310	-	-	7/19/95/117	-
24	CHL	R	605	-	-	4/12/88/117	-
25	CLA	n	315	17	-	6/15/91/115	-
24	CHL	g	318	17	-	8/12/88/117	-
25	CLA	g	307	-	-	6/25/101/115	-
30	LHG	c	617	-	-	17/36/36/53	-
25	CLA	2	307	11	-	6/13/89/115	-
24	CHL	p	309	12	-	1/14/90/117	-
24	CHL	N	305	-	-	16/34/110/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	605	-	-	7/20/96/115	-
25	CLA	n	314	-	-	6/37/113/115	-
29	0UR	1	301	-	-	13/42/81/86	0/2/2/2
35	PHO	d	403	-	-	10/37/103/103	0/5/6/6
25	CLA	p	315	30	-	15/37/113/115	-
25	CLA	B	607	18	-	15/39/115/115	-
35	PHO	A	606	-	-	9/37/103/103	0/5/6/6
25	CLA	b	615	18	-	5/39/115/115	-
25	CLA	y	308	-	-	9/21/97/115	-
30	LHG	A	601	-	-	24/49/49/53	-
25	CLA	Y	314	30	-	13/37/113/115	-
25	CLA	G	308	-	-	10/21/97/115	-
24	CHL	n	309	-	-	7/17/93/117	-
25	CLA	2	317	-	-	9/20/96/115	-
25	CLA	B	614	18	-	13/29/105/115	-
26	0IE	2	303	-	-	0/33/72/72	0/2/2/2
31	8CT	c	614	-	-	14/29/63/63	0/2/2/2
24	CHL	7	309	12	-	0/14/90/117	-
31	8CT	c	613	-	-	8/29/63/63	0/2/2/2
25	CLA	g	316	17	-	5/15/91/115	-
25	CLA	3	315	12	-	6/15/91/115	-
31	8CT	C	614	-	-	14/29/63/63	0/2/2/2
25	CLA	d	404	21	-	11/39/115/115	-
28	NEX	r	317	-	-	5/27/83/83	0/3/3/3
24	CHL	6	317	12	-	0/12/88/117	-
24	CHL	G	311	-	-	10/27/103/117	-
25	CLA	S	604	-	-	4/13/89/115	-
25	CLA	B	616	18	-	6/18/94/115	-
31	8CT	T	101	-	-	12/29/63/63	0/2/2/2
24	CHL	1	309	-	-	3/14/90/117	-
25	CLA	7	314	-	-	7/27/103/115	-
30	LHG	D	408	-	-	21/43/43/53	-
24	CHL	7	306	-	-	27/39/115/117	-
25	CLA	q	306	28	-	5/21/97/115	-
25	CLA	2	308	-	-	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	D	404	21	-	9/39/115/115	-
25	CLA	N	315	17	-	7/15/91/115	-
28	NEX	2	304	-	-	5/27/83/83	0/3/3/3
28	NEX	r	301	-	-	4/27/83/83	0/3/3/3
31	8CT	a	608	-	-	8/29/63/63	0/2/2/2
33	LMG	W	201	-	-	11/25/45/70	0/1/1/1
24	CHL	8	307	17	-	2/14/90/117	-
25	CLA	7	307	12	-	7/29/105/115	-
31	8CT	C	615	-	-	13/29/63/63	0/2/2/2
24	CHL	s	409	-	-	7/19/95/117	-
25	CLA	y	317	17	-	11/27/103/115	-
29	0UR	y	301	-	-	12/42/81/86	0/2/2/2
26	0IE	y	303	-	-	0/33/72/72	0/2/2/2
25	CLA	R	603	-	-	6/18/94/115	-
29	0UR	G	301	-	-	10/42/81/86	0/2/2/2
25	CLA	c	603	20	-	13/39/115/115	-
25	CLA	d	405	21	-	12/39/115/115	-
29	0UR	n	301	-	-	9/42/81/86	0/2/2/2
25	CLA	q	315	17	-	5/13/89/115	-
24	CHL	3	317	12	-	2/12/88/117	-
25	CLA	S	612	-	-	9/27/103/115	-
25	CLA	8	313	17	-	4/15/91/115	-
25	CLA	4	313	-	-	6/27/103/115	-
24	CHL	u	305	12	-	15/41/117/117	-
24	CHL	p	306	-	-	26/39/115/117	-
29	0UR	4	301	-	-	13/42/81/86	0/2/2/2
24	CHL	5	309	11	-	3/14/90/117	-
31	8CT	b	617	-	-	14/29/63/63	0/2/2/2
25	CLA	b	601	-	-	11/15/91/115	-
24	CHL	Y	317	17	-	6/12/88/117	-
24	CHL	g	313	-	-	21/41/117/117	-
27	XAT	R	615	-	-	0/31/93/93	0/4/4/4
25	CLA	C	610	-	-	10/39/115/115	-
33	LMG	D	401	-	-	10/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	y	313	-	-	19/41/117/117	-
24	CHL	G	312	-	-	5/23/99/117	-
25	CLA	q	305	17	-	10/26/102/115	-
24	CHL	4	312	-	-	6/17/93/117	-
24	CHL	N	312	-	-	11/29/105/117	-
25	CLA	8	306	-	-	6/21/97/115	-
24	CHL	R	602	-	-	5/19/95/117	-
24	CHL	Y	309	-	-	5/19/95/117	-
24	CHL	u	310	-	-	9/17/93/117	-
26	0IE	g	302	-	-	2/33/72/72	0/2/2/2
24	CHL	u	311	-	-	4/17/93/117	-
24	CHL	S	608	-	-	7/19/95/117	-
26	0IE	3	303	-	-	1/33/72/72	0/2/2/2
25	CLA	B	609	18	-	16/39/115/115	-
28	NEX	5	304	-	-	5/27/83/83	0/3/3/3
25	CLA	b	611	18	-	6/39/115/115	-
24	CHL	p	310	-	-	7/17/93/117	-
25	CLA	c	601	20	-	14/39/115/115	-
24	CHL	u	313	-	-	5/14/90/117	-
24	CHL	y	309	17	-	5/14/90/117	-
39	PL9	d	406	-	-	11/53/73/73	0/1/1/1
24	CHL	5	313	-	-	3/12/88/117	-
31	8CT	s	416	-	-	12/29/63/63	0/2/2/2
33	LMG	i	101	-	-	14/43/63/70	0/1/1/1
25	CLA	9	315	-	-	6/15/91/115	-
25	CLA	C	603	20	-	14/39/115/115	-
28	NEX	7	304	-	-	5/27/83/83	0/3/3/3
24	CHL	n	310	-	-	9/26/102/117	-
25	CLA	b	602	18	-	13/39/115/115	-
25	CLA	r	314	-	-	9/18/94/115	-
24	CHL	Y	304	17	-	15/41/117/117	-
25	CLA	5	316	-	-	4/15/91/115	-
24	CHL	1	310	-	-	2/14/90/117	-
25	CLA	s	405	-	-	4/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	g	319	-	-	23/47/47/53	-
29	0UR	q	301	-	-	10/42/81/86	0/2/2/2
32	SQD	d	409	-	-	13/39/59/69	0/1/1/1
25	CLA	9	314	30	-	14/37/113/115	-
24	CHL	8	304	17	-	15/34/110/117	-
37	DGD	C	620	-	-	25/44/84/95	0/2/2/2
30	LHG	a	601	-	-	25/49/49/53	-
24	CHL	y	306	-	-	22/39/115/117	-
25	CLA	B	613	18	-	10/39/115/115	-
25	CLA	u	307	-	-	6/29/105/115	-
24	CHL	n	311	-	-	7/22/98/117	-
24	CHL	r	307	-	-	7/20/96/117	-
26	0IE	8	302	-	-	2/33/72/72	0/2/2/2
25	CLA	g	308	-	-	8/21/97/115	-
24	CHL	Y	308	17	-	5/14/90/117	-
24	CHL	n	304	17	-	8/27/103/117	-
25	CLA	S	603	-	-	5/15/91/115	-
24	CHL	7	311	-	-	2/17/93/117	-
24	CHL	G	310	-	-	9/19/95/117	-
24	CHL	s	407	-	-	6/17/93/117	-
25	CLA	B	601	-	-	11/15/91/115	-
26	0IE	Y	303	-	-	0/33/72/72	0/2/2/2
24	CHL	6	312	-	-	3/14/90/117	-
30	LHG	N	318	-	-	18/47/47/53	-
28	NEX	9	319	-	-	5/27/83/83	0/3/3/3
24	CHL	5	310	-	-	4/12/88/117	-
31	8CT	B	617	-	-	13/29/63/63	0/2/2/2
25	CLA	C	616	20	-	4/17/93/115	-
24	CHL	R	607	-	-	11/20/96/117	-
24	CHL	2	309	11	-	3/14/90/117	-
24	CHL	G	305	17	-	21/41/117/117	-
24	CHL	q	316	-	-	1/12/88/117	-
26	0IE	p	302	-	-	4/33/72/72	0/2/2/2
24	CHL	1	304	-	-	2/12/88/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	2	315	-	-	10/37/113/115	-
25	CLA	c	609	20	-	6/39/115/115	-
24	CHL	s	414	-	-	3/12/88/117	-
24	CHL	1	312	10	-	6/17/93/117	-
25	CLA	B	611	18	-	6/39/115/115	-
24	CHL	4	305	-	-	8/17/93/117	-
28	NEX	1	303	-	-	5/27/83/83	0/3/3/3
30	LHG	Y	318	25	-	23/47/47/53	-
24	CHL	3	308	-	-	3/14/90/117	-
24	CHL	7	310	-	-	7/17/93/117	-
25	CLA	8	305	17	-	11/26/102/115	-
25	CLA	b	608	-	-	10/27/103/115	-
30	LHG	p	319	25	-	26/47/47/53	-
25	CLA	u	308	-	-	7/21/97/115	-
25	CLA	N	307	-	-	6/21/97/115	-
25	CLA	a	603	19	-	13/39/115/115	-
25	CLA	s	404	-	-	5/15/91/115	-
32	SQD	A	609	-	-	16/40/60/69	0/1/1/1
35	PHO	D	403	-	-	11/37/103/103	0/5/6/6
24	CHL	r	302	8	-	5/17/93/117	-
24	CHL	p	318	12	-	5/12/88/117	-
25	CLA	1	315	10	-	8/15/91/115	-
29	0UR	8	301	-	-	10/42/81/86	0/2/2/2
24	CHL	3	304	12	-	8/20/96/117	-
24	CHL	5	311	-	-	7/19/95/117	-
24	CHL	R	601	8	-	5/17/93/117	-
25	CLA	b	613	18	-	10/39/115/115	-
24	CHL	g	309	-	-	2/14/90/117	-
31	8CT	x	601	-	-	10/29/63/63	0/2/2/2
25	CLA	r	310	8	-	4/27/103/115	-
25	CLA	c	602	20	-	17/39/115/115	-
25	CLA	g	315	-	-	6/33/109/115	-
30	LHG	4	318	-	-	21/46/46/53	-
24	CHL	Y	310	-	-	12/27/103/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	NEX	y	304	-	-	5/27/83/83	0/3/3/3
33	LMG	B	619	-	-	20/36/56/70	0/1/1/1
24	CHL	s	406	-	-	6/17/93/117	-
25	CLA	B	605	18	-	16/39/115/115	-
28	NEX	3	318	-	-	4/27/83/83	0/3/3/3
28	NEX	G	304	-	-	5/27/83/83	0/3/3/3
24	CHL	5	318	11	-	6/12/88/117	-
24	CHL	n	305	-	-	20/34/110/117	-
26	0IE	u	303	-	-	2/33/72/72	0/2/2/2
29	0UR	p	301	-	-	8/42/81/86	0/2/2/2
25	CLA	Y	307	-	-	9/21/97/115	-
25	CLA	S	609	-	-	5/27/103/115	-
24	CHL	S	606	-	-	6/17/93/117	-
24	CHL	6	305	-	-	12/20/96/117	-
25	CLA	N	306	17	-	10/26/102/115	-
28	NEX	S	617	-	-	5/27/83/83	0/3/3/3
25	CLA	a	605	-	-	8/20/96/115	-
24	CHL	9	304	12	-	15/41/117/117	-
24	CHL	4	311	-	-	3/15/91/117	-
25	CLA	s	411	-	-	4/13/90/115	-
26	0IE	r	315	-	-	1/33/72/72	0/2/2/2
35	PHO	a	606	-	-	7/37/103/103	0/5/6/6
25	CLA	b	606	18	-	18/39/115/115	-
25	CLA	b	603	18	-	12/39/115/115	-
25	CLA	c	610	-	-	9/39/115/115	-
32	SQD	B	618	-	-	16/49/69/69	0/1/1/1
25	CLA	4	307	28	-	4/10/86/115	-
25	CLA	u	317	12	-	8/27/103/115	-
24	CHL	3	310	-	-	7/17/93/117	-
24	CHL	p	312	-	-	7/19/95/117	-
24	CHL	7	318	12	-	5/12/88/117	-
39	PL9	D	406	-	-	13/53/73/73	0/1/1/1
28	NEX	6	303	-	-	4/27/83/83	0/3/3/3
30	LHG	1	318	-	-	23/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	m	101	-	-	19/36/56/70	0/1/1/1
24	CHL	9	305	-	-	17/39/115/117	-
30	LHG	d	408	-	-	25/43/43/53	-
24	CHL	9	310	-	-	4/17/93/117	-
25	CLA	B	604	18	-	16/36/112/115	-
25	CLA	6	316	-	-	11/15/91/115	-
31	8CT	X	601	-	-	10/29/63/63	0/2/2/2
25	CLA	r	304	-	-	6/18/94/115	-
24	CHL	3	312	-	-	5/14/90/117	-
25	CLA	6	307	-	-	8/13/89/115	-
25	CLA	Y	316	17	-	11/27/103/115	-
24	CHL	8	308	-	-	5/17/93/117	-
25	CLA	1	306	-	-	6/13/90/115	-
25	CLA	q	312	-	-	3/27/103/115	-
32	SQD	a	609	-	-	19/40/60/69	0/1/1/1
31	8CT	D	410	-	-	10/29/63/63	0/2/2/2
24	CHL	p	313	-	-	4/14/90/117	-
28	NEX	n	303	-	-	4/27/83/83	0/3/3/3
25	CLA	G	315	-	-	7/33/109/115	-
25	CLA	Y	313	17	-	5/27/103/115	-
33	LMG	d	411	-	-	21/41/61/70	0/1/1/1
25	CLA	N	313	-	-	5/27/103/115	-
25	CLA	8	314	-	-	5/13/89/115	-
25	CLA	6	314	-	-	4/10/86/115	-
28	NEX	4	303	25	-	5/27/83/83	0/3/3/3
30	LHG	2	319	-	-	20/44/44/53	-

The worst 5 of 6030 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	410	8CT	C02-C03	14.71	1.59	1.34
31	d	410	8CT	C02-C03	14.58	1.59	1.34
31	S	614	8CT	C02-C03	14.32	1.59	1.34
31	s	415	8CT	C02-C03	14.31	1.59	1.34
31	A	608	8CT	C02-C03	14.29	1.59	1.34

The worst 5 of 7347 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	416	8CT	C22-C21-C20	-31.40	78.94	122.92
31	S	615	8CT	C22-C21-C20	-31.38	78.96	122.92
31	S	615	8CT	C22-C21-C23	-25.32	78.18	118.08
31	s	416	8CT	C22-C21-C23	-25.31	78.20	118.08
31	S	615	8CT	C23-C21-C20	24.86	157.09	118.94

There are no chirality outliers.

5 of 4494 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	R	601	CHL	C3C-C2C-CMC-OMC
24	R	607	CHL	C3C-C2C-CMC-OMC
24	1	305	CHL	CHA-CBD-CGD-O1D
24	1	305	CHL	CHA-CBD-CGD-O2D
24	1	317	CHL	CHA-CBD-CGD-O1D

There are no ring outliers.

435 monomers are involved in 1342 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	313	CHL	10	0
25	1	307	CLA	9	0
25	G	314	CLA	2	0
25	y	316	CLA	3	0
25	7	316	CLA	3	0
24	4	310	CHL	3	0
29	u	301	0UR	1	0
24	q	308	CHL	3	0
30	d	407	LHG	7	0
25	R	609	CLA	1	0
24	R	606	CHL	2	0
26	R	614	0IE	1	0
30	G	319	LHG	1	0
25	C	609	CLA	2	0
30	9	318	LHG	6	0
24	q	304	CHL	4	0
25	4	314	CLA	1	0
30	5	319	LHG	2	0
25	3	316	CLA	2	0
25	7	308	CLA	15	0
37	C	619	DGD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	s	413	CLA	1	0
24	2	305	CHL	5	0
25	Y	306	CLA	2	0
25	3	307	CLA	2	0
24	s	408	CHL	1	0
24	G	309	CHL	2	0
25	g	317	CLA	1	0
25	u	314	CLA	2	0
25	r	305	CLA	9	0
25	y	314	CLA	2	0
30	A	612	LHG	2	0
25	9	316	CLA	4	0
24	g	306	CHL	3	0
24	u	318	CHL	1	0
24	Y	312	CHL	7	0
24	1	311	CHL	7	0
24	y	310	CHL	1	0
25	C	602	CLA	2	0
24	5	305	CHL	6	0
25	B	606	CLA	8	0
25	A	604	CLA	5	0
28	N	303	NEX	7	0
25	B	610	CLA	2	0
25	n	306	CLA	2	0
24	S	607	CHL	2	0
32	D	409	SQD	1	0
24	q	303	CHL	3	0
25	6	306	CLA	1	0
24	r	309	CHL	2	0
25	s	410	CLA	4	0
25	B	608	CLA	6	0
31	V	401	8CT	1	0
25	R	612	CLA	7	0
24	u	309	CHL	2	0
28	p	304	NEX	27	0
24	S	605	CHL	2	0
23	f	201	HEM	3	0
25	2	316	CLA	1	0
24	p	305	CHL	7	0
24	q	311	CHL	6	0
24	u	306	CHL	4	0
24	1	317	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	n	318	LHG	4	0
24	2	313	CHL	3	0
25	D	405	CLA	5	0
24	y	311	CHL	1	0
24	N	304	CHL	5	0
24	S	613	CHL	2	0
30	7	319	LHG	3	0
26	7	302	0IE	2	0
24	9	311	CHL	4	0
25	9	307	CLA	4	0
25	A	607	CLA	2	0
25	y	307	CLA	2	0
25	C	605	CLA	1	0
28	g	304	NEX	15	0
24	N	309	CHL	1	0
24	S	601	CHL	1	0
24	n	308	CHL	3	0
31	v	401	8CT	1	0
25	3	306	CLA	1	0
25	b	604	CLA	10	0
25	C	611	CLA	5	0
24	7	312	CHL	6	0
25	n	307	CLA	4	0
24	4	308	CHL	1	0
25	9	313	CLA	2	0
25	C	607	CLA	2	0
24	n	312	CHL	2	0
25	r	311	CLA	1	0
25	B	602	CLA	7	0
33	w	201	LMG	6	0
24	9	317	CHL	1	0
26	6	302	0IE	2	0
37	c	618	DGD	4	0
25	7	315	CLA	2	0
25	C	604	CLA	4	0
24	y	312	CHL	4	0
30	y	319	LHG	2	0
30	D	407	LHG	7	0
25	g	314	CLA	2	0
25	b	614	CLA	3	0
24	N	310	CHL	2	0
24	p	311	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	608	CLA	3	0
24	9	308	CHL	1	0
25	u	315	CLA	4	0
29	9	301	0UR	1	0
26	y	302	0IE	1	0
24	3	311	CHL	6	0
24	r	303	CHL	5	0
24	4	317	CHL	2	0
25	y	315	CLA	3	0
25	G	307	CLA	2	0
25	8	311	CLA	2	0
24	y	305	CHL	8	0
24	7	305	CHL	6	0
25	G	317	CLA	2	0
24	r	308	CHL	3	0
25	b	605	CLA	4	0
29	6	301	0UR	1	0
26	3	302	0IE	2	0
25	C	612	CLA	2	0
24	g	311	CHL	3	0
28	s	401	NEX	21	0
24	N	311	CHL	4	0
25	1	316	CLA	2	0
28	u	304	NEX	9	0
25	5	315	CLA	1	0
24	Y	305	CHL	2	0
26	u	302	0IE	1	0
32	b	618	SQD	5	0
24	8	309	CHL	5	0
25	s	412	CLA	3	0
25	b	610	CLA	3	0
25	b	609	CLA	4	0
25	c	604	CLA	3	0
25	a	607	CLA	2	0
30	a	612	LHG	2	0
24	6	311	CHL	9	0
25	5	314	CLA	2	0
25	b	612	CLA	8	0
29	2	301	0UR	1	0
24	S	602	CHL	5	0
24	N	308	CHL	3	0
24	G	318	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	u	316	CLA	4	0
25	a	604	CLA	6	0
25	1	314	CLA	1	0
25	N	316	CLA	4	0
26	9	302	0IE	2	0
25	Y	315	CLA	1	0
24	3	305	CHL	1	0
25	r	313	CLA	5	0
25	c	611	CLA	3	0
24	Y	311	CHL	4	0
28	R	616	NEX	6	0
25	1	313	CLA	2	0
24	9	312	CHL	3	0
25	5	308	CLA	5	0
25	c	612	CLA	4	0
24	1	305	CHL	2	0
24	G	306	CHL	6	0
25	q	314	CLA	1	0
25	G	316	CLA	3	0
24	6	309	CHL	20	0
24	s	402	CHL	3	0
24	2	312	CHL	2	0
33	d	401	LMG	3	0
25	B	612	CLA	8	0
24	4	309	CHL	7	0
24	R	608	CHL	2	0
24	6	310	CHL	2	0
25	R	604	CLA	7	0
25	n	316	CLA	4	0
25	c	605	CLA	2	0
25	4	316	CLA	2	0
25	s	417	CLA	4	0
27	r	316	XAT	8	0
24	5	312	CHL	3	0
33	D	411	LMG	5	0
24	y	318	CHL	2	0
25	8	312	CLA	1	0
26	Y	302	0IE	1	0
24	g	312	CHL	3	0
24	q	307	CHL	1	0
25	B	615	CLA	8	0
25	R	610	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	5	317	CLA	2	0
24	7	313	CHL	3	0
25	b	607	CLA	3	0
31	C	613	8CT	1	0
25	p	308	CLA	12	0
24	4	304	CHL	2	0
24	q	310	CHL	6	0
24	s	403	CHL	3	0
25	p	317	CLA	5	0
24	3	309	CHL	19	0
25	7	317	CLA	4	0
25	C	601	CLA	4	0
24	r	306	CHL	3	0
24	u	312	CHL	4	0
24	8	310	CHL	6	0
25	c	616	CLA	2	0
29	Y	301	0UR	1	0
25	4	315	CLA	2	0
25	c	607	CLA	3	0
25	p	314	CLA	2	0
25	A	603	CLA	5	0
24	6	304	CHL	3	0
24	9	309	CHL	3	0
25	b	616	CLA	3	0
24	8	303	CHL	3	0
24	g	305	CHL	4	0
25	p	307	CLA	2	0
33	C	618	LMG	6	0
25	S	611	CLA	1	0
26	9	303	0IE	1	0
37	c	619	DGD	4	0
25	q	313	CLA	1	0
23	E	201	HEM	2	0
24	6	308	CHL	1	0
25	B	603	CLA	3	0
25	6	315	CLA	1	0
25	9	306	CLA	1	0
25	S	616	CLA	4	0
25	2	314	CLA	1	0
25	p	316	CLA	2	0
24	g	310	CHL	6	0
24	R	605	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	n	315	CLA	2	0
24	g	318	CHL	2	0
25	g	307	CLA	2	0
24	p	309	CHL	3	0
24	N	305	CHL	2	0
25	A	605	CLA	1	0
35	d	403	PHO	6	0
25	p	315	CLA	2	0
25	B	607	CLA	4	0
35	A	606	PHO	4	0
25	b	615	CLA	7	0
25	y	308	CLA	1	0
30	A	601	LHG	6	0
25	Y	314	CLA	1	0
25	G	308	CLA	16	0
24	n	309	CHL	1	0
25	2	317	CLA	2	0
25	B	614	CLA	3	0
26	2	303	0IE	1	0
31	c	613	8CT	1	0
25	g	316	CLA	2	0
25	3	315	CLA	1	0
25	d	404	CLA	4	0
28	r	317	NEX	9	0
24	6	317	CHL	2	0
24	G	311	CHL	4	0
25	B	616	CLA	3	0
24	1	309	CHL	5	0
25	7	314	CLA	2	0
30	D	408	LHG	6	0
24	7	306	CHL	4	0
25	q	306	CLA	5	0
25	2	308	CLA	5	0
25	D	404	CLA	5	0
25	N	315	CLA	3	0
28	2	304	NEX	9	0
28	r	301	NEX	6	0
33	W	201	LMG	2	0
24	8	307	CHL	1	0
25	7	307	CLA	2	0
24	s	409	CHL	2	0
25	y	317	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	y	301	0UR	1	0
26	y	303	0IE	1	0
25	R	603	CLA	1	0
29	G	301	0UR	1	0
25	c	603	CLA	3	0
25	d	405	CLA	6	0
29	n	301	0UR	1	0
25	q	315	CLA	1	0
24	3	317	CHL	2	0
25	S	612	CLA	1	0
25	8	313	CLA	1	0
25	4	313	CLA	2	0
24	u	305	CHL	5	0
24	p	306	CHL	4	0
29	4	301	0UR	1	0
24	5	309	CHL	1	0
25	b	601	CLA	1	0
24	Y	317	CHL	2	0
24	g	313	CHL	6	0
27	R	615	XAT	16	0
25	C	610	CLA	4	0
33	D	401	LMG	3	0
24	y	313	CHL	6	0
24	G	312	CHL	12	0
25	q	305	CLA	2	0
24	4	312	CHL	3	0
24	N	312	CHL	4	0
25	8	306	CLA	4	0
24	R	602	CHL	4	0
24	Y	309	CHL	2	0
24	u	310	CHL	4	0
24	u	311	CHL	1	0
24	S	608	CHL	1	0
25	B	609	CLA	3	0
28	5	304	NEX	10	0
25	b	611	CLA	3	0
24	p	310	CHL	12	0
25	c	601	CLA	3	0
24	u	313	CHL	1	0
24	y	309	CHL	2	0
39	d	406	PL9	2	0
24	5	313	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	i	101	LMG	3	0
25	9	315	CLA	4	0
25	C	603	CLA	5	0
28	7	304	NEX	32	0
24	n	310	CHL	2	0
25	b	602	CLA	8	0
25	r	314	CLA	1	0
24	Y	304	CHL	5	0
25	5	316	CLA	2	0
24	1	310	CHL	3	0
30	g	319	LHG	2	0
29	q	301	0UR	1	0
32	d	409	SQD	1	0
25	9	314	CLA	3	0
24	8	304	CHL	6	0
37	C	620	DGD	2	0
30	a	601	LHG	5	0
24	y	306	CHL	2	0
25	B	613	CLA	5	0
25	u	307	CLA	2	0
24	n	311	CHL	4	0
24	r	307	CHL	4	0
25	g	308	CLA	6	0
24	Y	308	CHL	3	0
24	n	304	CHL	4	0
24	7	311	CHL	2	0
24	G	310	CHL	3	0
24	s	407	CHL	2	0
25	B	601	CLA	1	0
30	N	318	LHG	4	0
28	9	319	NEX	6	0
25	C	616	CLA	2	0
24	R	607	CHL	3	0
24	2	309	CHL	1	0
24	G	305	CHL	4	0
26	p	302	0IE	2	0
24	1	304	CHL	3	0
25	2	315	CLA	1	0
25	c	609	CLA	3	0
24	s	414	CHL	2	0
24	1	312	CHL	4	0
25	B	611	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	4	305	CHL	1	0
28	1	303	NEX	22	0
24	3	308	CHL	2	0
24	7	310	CHL	14	0
25	8	305	CLA	2	0
25	b	608	CLA	5	0
30	p	319	LHG	3	0
25	u	308	CLA	1	0
25	N	307	CLA	4	0
25	a	603	CLA	5	0
32	A	609	SQD	2	0
35	D	403	PHO	6	0
24	r	302	CHL	3	0
24	p	318	CHL	3	0
25	1	315	CLA	2	0
29	8	301	0UR	1	0
24	3	304	CHL	1	0
24	5	311	CHL	1	0
24	R	601	CHL	3	0
25	b	613	CLA	5	0
24	g	309	CHL	2	0
25	r	310	CLA	1	0
25	c	602	CLA	2	0
25	g	315	CLA	3	0
30	4	318	LHG	3	0
24	Y	310	CHL	1	0
28	y	304	NEX	4	0
33	B	619	LMG	5	0
24	s	406	CHL	2	0
25	B	605	CLA	6	0
28	3	318	NEX	22	0
28	G	304	NEX	32	0
24	n	305	CHL	5	0
29	p	301	0UR	1	0
25	S	609	CLA	4	0
24	S	606	CHL	2	0
24	6	305	CHL	1	0
25	N	306	CLA	1	0
28	S	617	NEX	24	0
25	a	605	CLA	1	0
24	9	304	CHL	6	0
24	4	311	CHL	5	0

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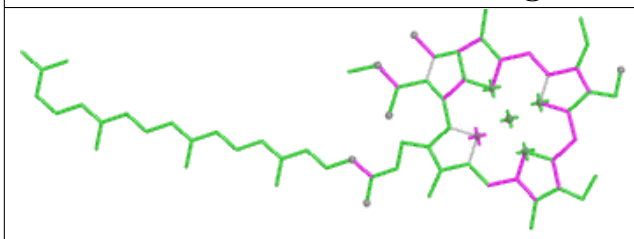
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	s	411	CLA	3	0
26	r	315	0IE	1	0
35	a	606	PHO	4	0
25	b	606	CLA	9	0
25	b	603	CLA	4	0
25	c	610	CLA	4	0
32	B	618	SQD	4	0
25	4	307	CLA	16	0
25	u	317	CLA	5	0
24	3	310	CHL	1	0
24	p	312	CHL	5	0
24	7	318	CHL	2	0
39	D	406	PL9	2	0
28	6	303	NEX	21	0
30	1	318	LHG	3	0
33	m	101	LMG	6	0
24	9	305	CHL	6	0
30	d	408	LHG	4	0
24	9	310	CHL	2	0
25	B	604	CLA	12	0
25	6	316	CLA	3	0
25	r	304	CLA	1	0
25	6	307	CLA	2	0
25	Y	316	CLA	2	0
24	8	308	CHL	3	0
25	q	312	CLA	2	0
32	a	609	SQD	4	0
24	p	313	CHL	3	0
28	n	303	NEX	7	0
25	G	315	CLA	3	0
25	Y	313	CLA	2	0
33	d	411	LMG	5	0
25	N	313	CLA	1	0
25	8	314	CLA	2	0
28	4	303	NEX	21	0
30	2	319	LHG	2	0

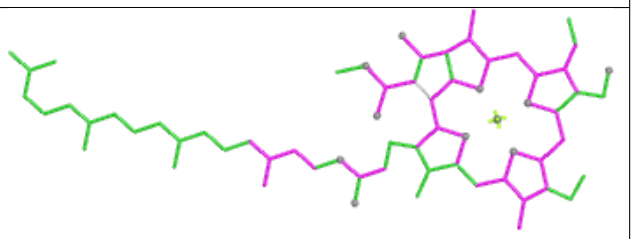
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

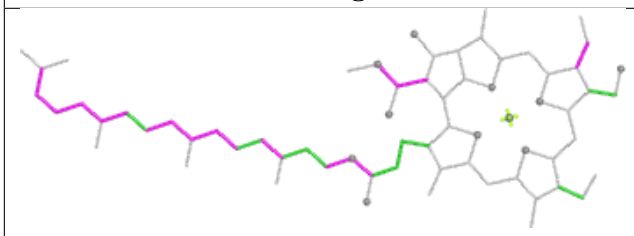
Ligand CHL G 313



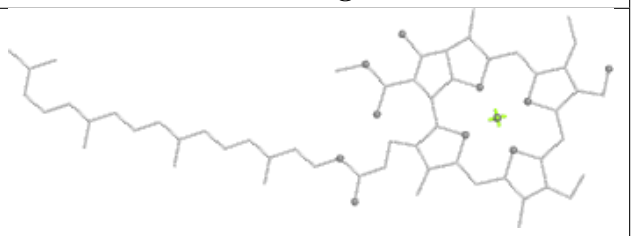
Bond lengths



Bond angles

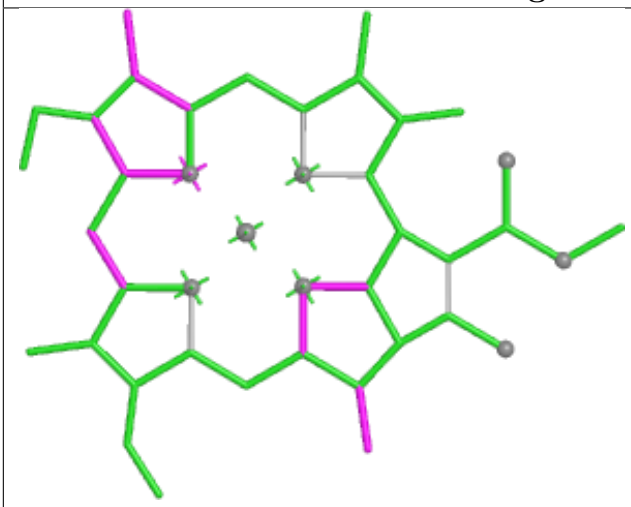


Torsions

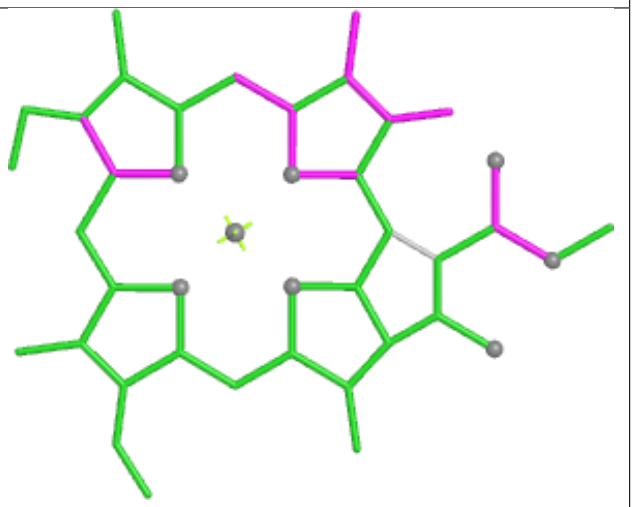


Rings

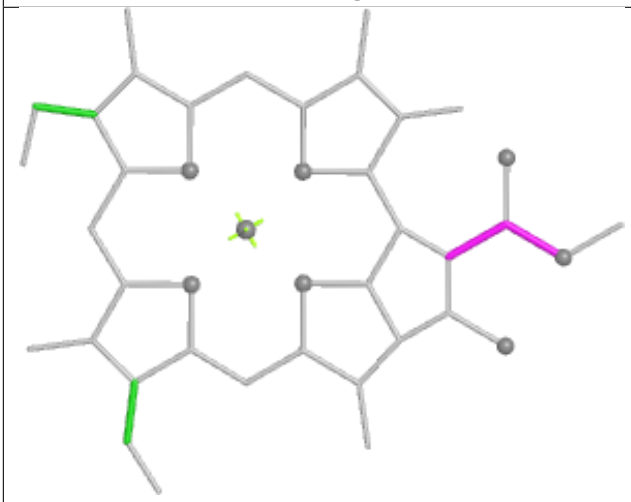
Ligand CLA 1 307



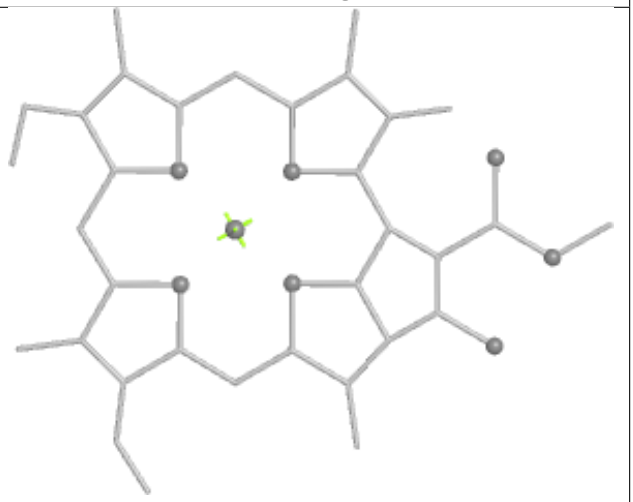
Bond lengths



Bond angles

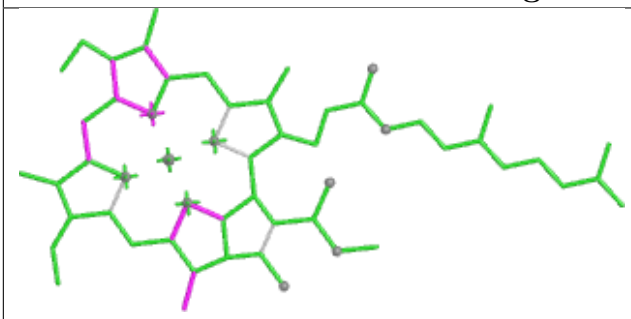


Torsions

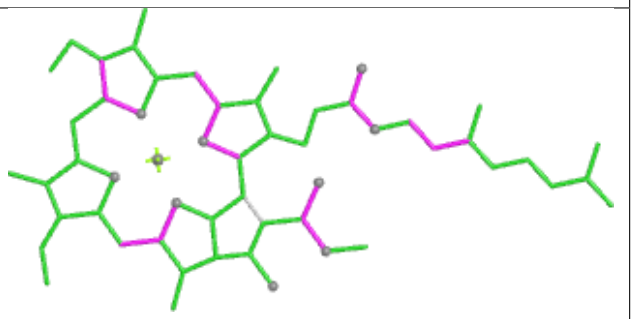


Rings

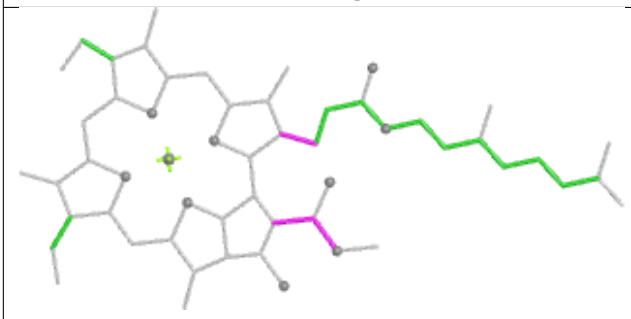
Ligand CLA G 314



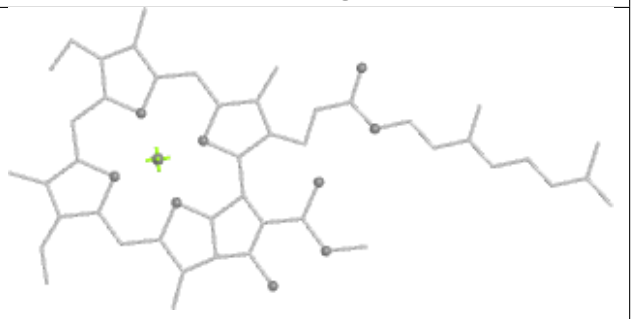
Bond lengths



Bond angles

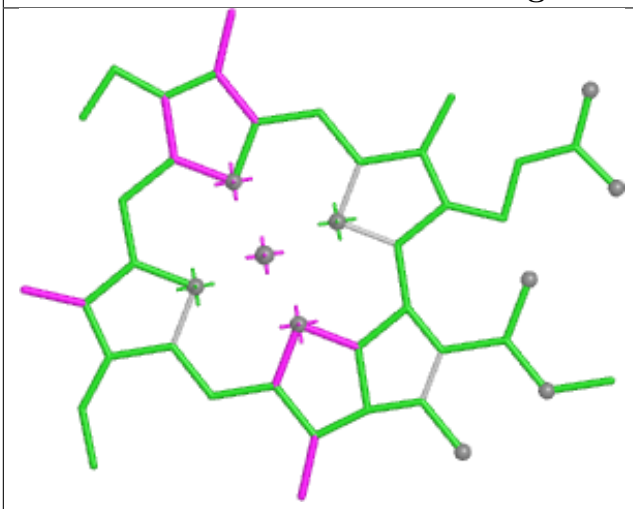


Torsions

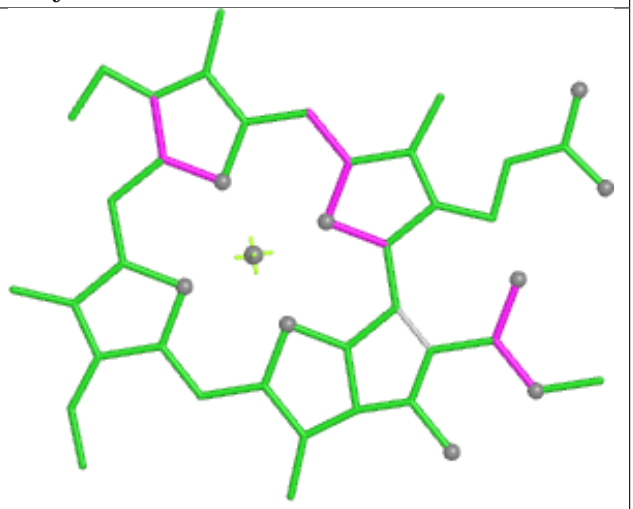


Rings

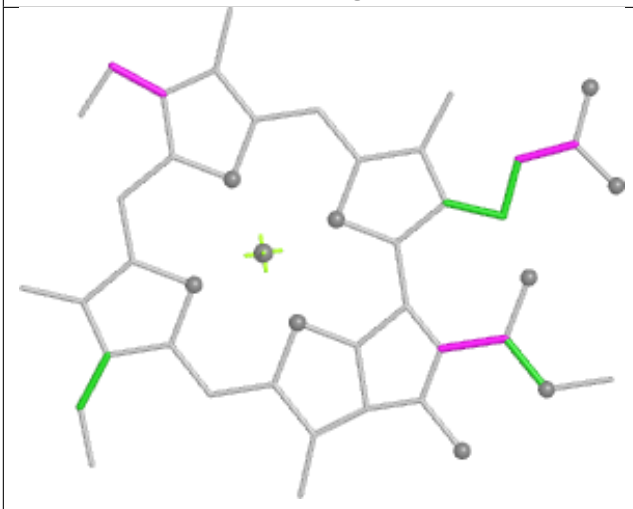
Ligand CLA y 316



Bond lengths



Bond angles

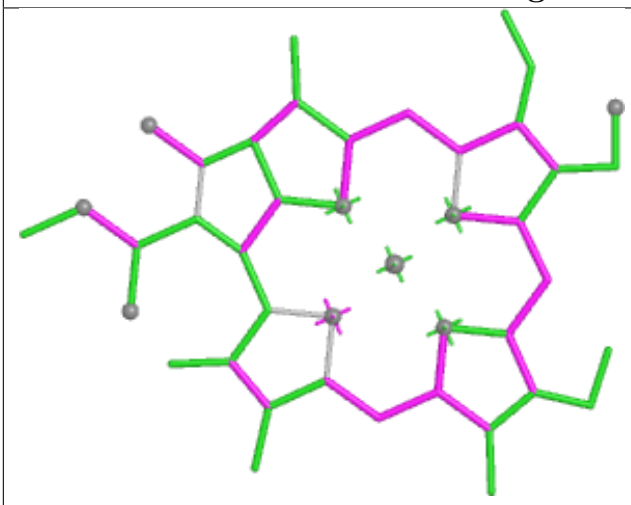


Torsions

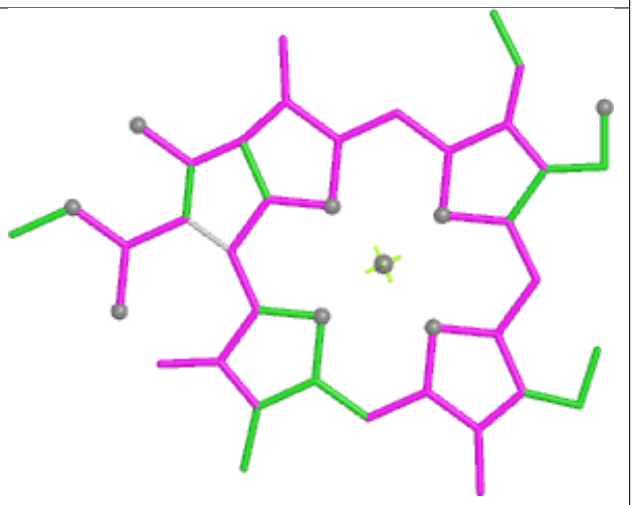


Rings

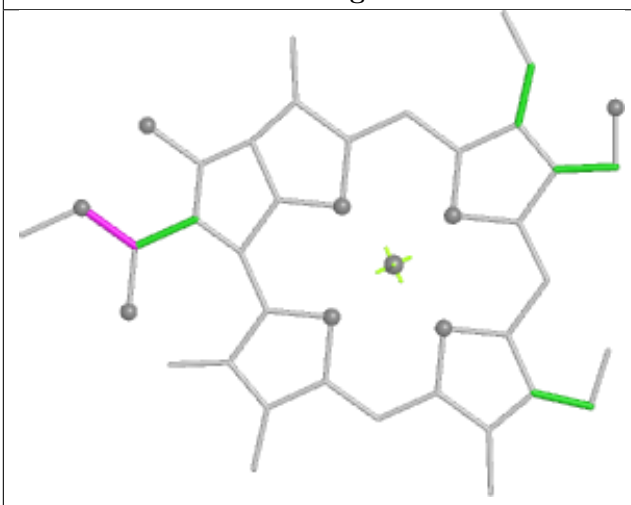
Ligand CHL 2 310



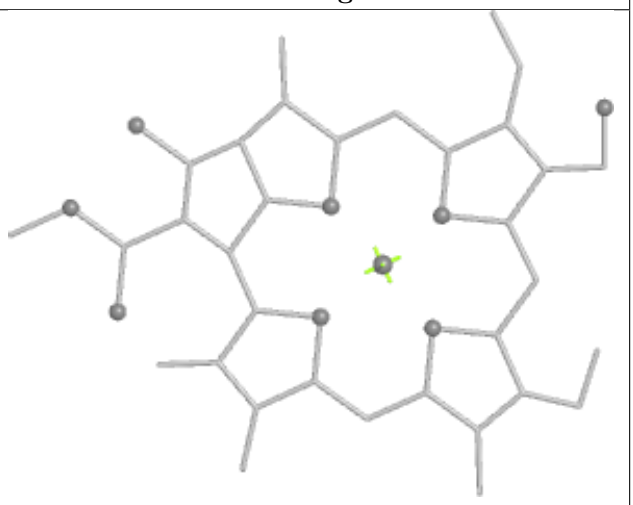
Bond lengths



Bond angles

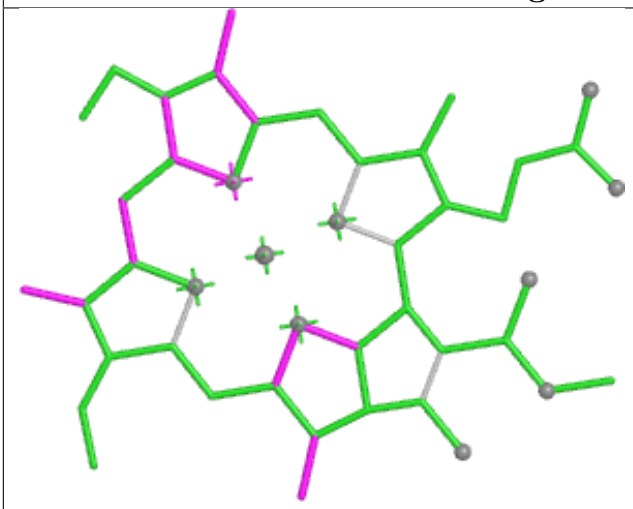


Torsions

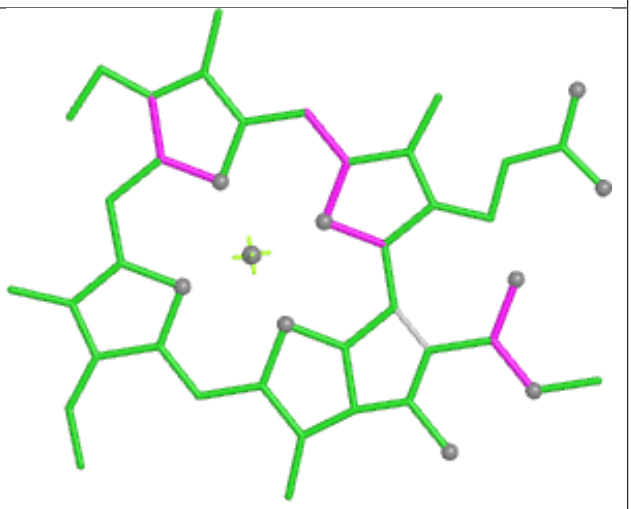


Rings

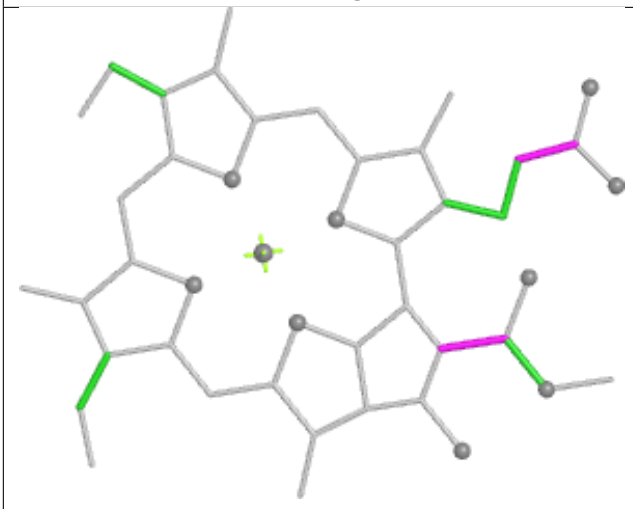
Ligand CLA 7 316



Bond lengths



Bond angles

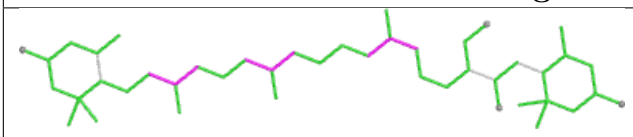


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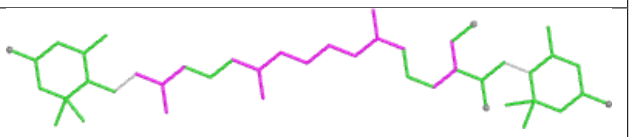


Rings

Ligand 0IE G 303



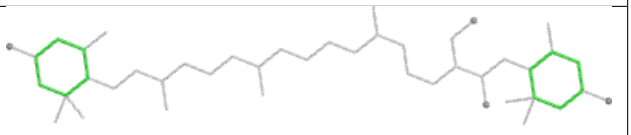
Bond lengths



Bond angles

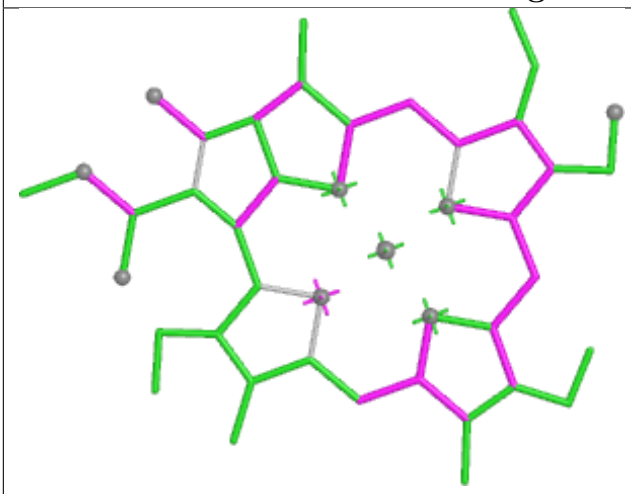


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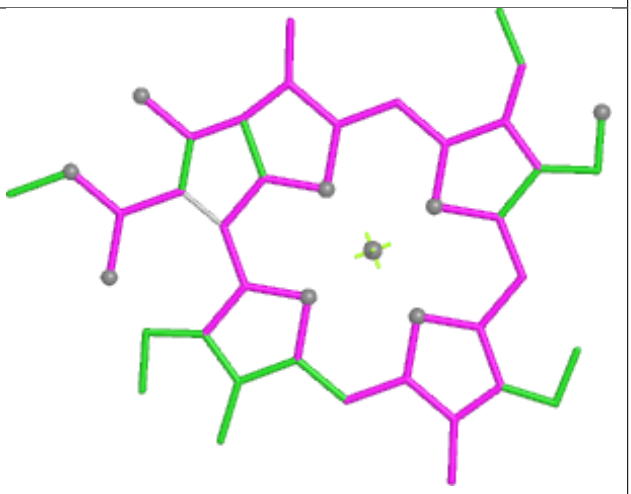


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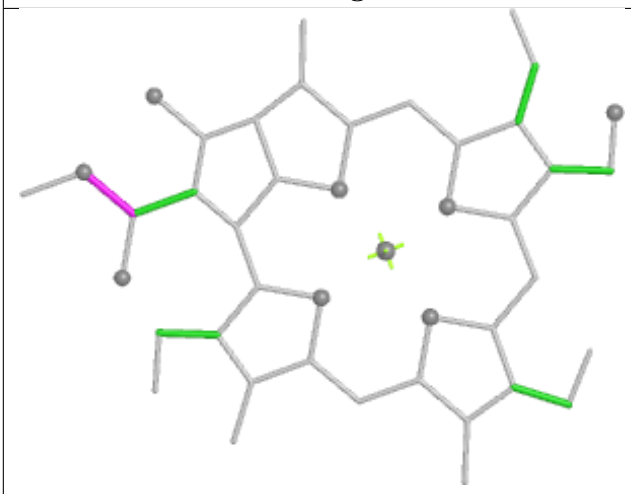
Ligand CHL 4 310



Bond lengths



Bond angles

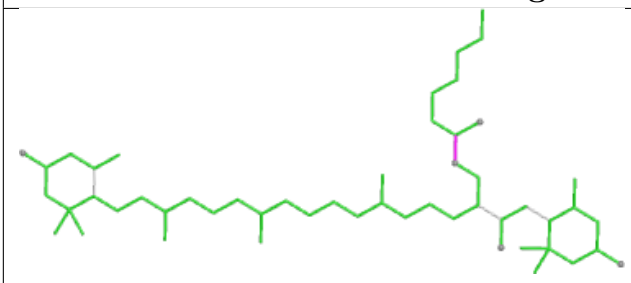


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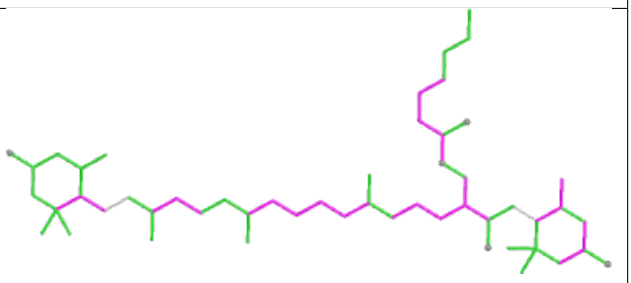


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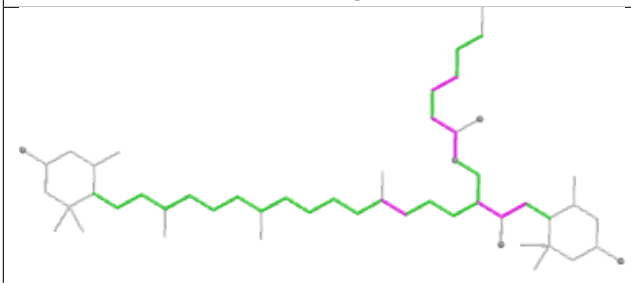
Ligand 0UR u 301



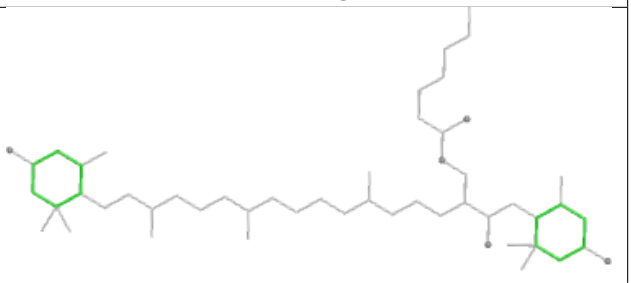
Bond lengths



Bond angles

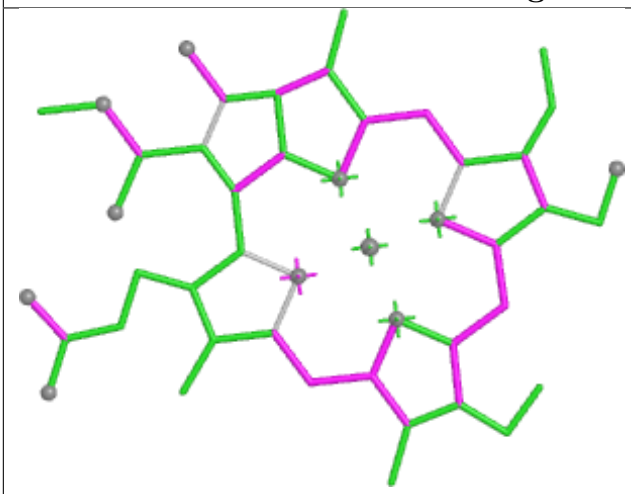


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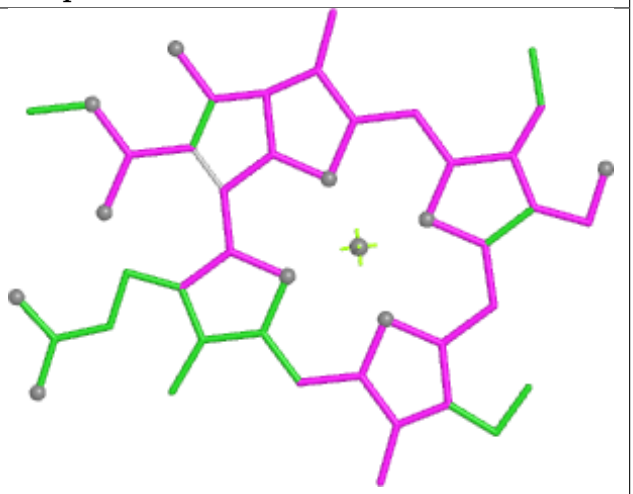


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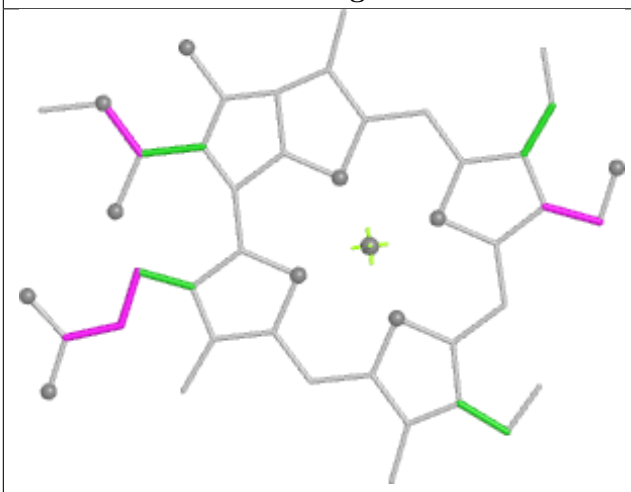
Ligand CHL q 308



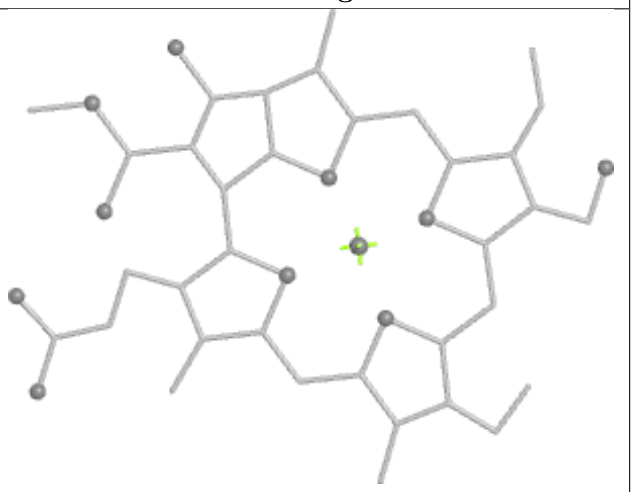
Bond lengths



Bond angles

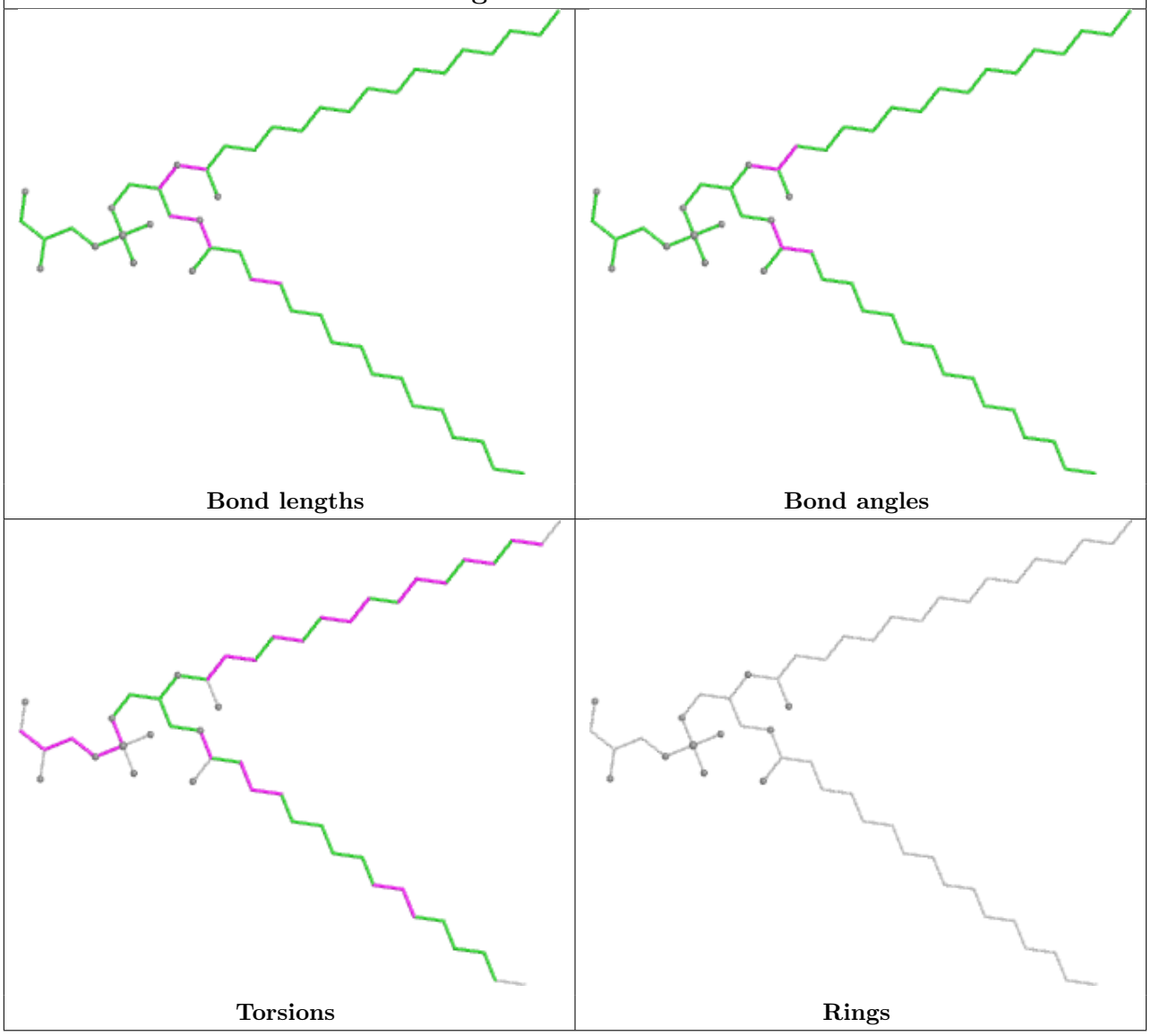


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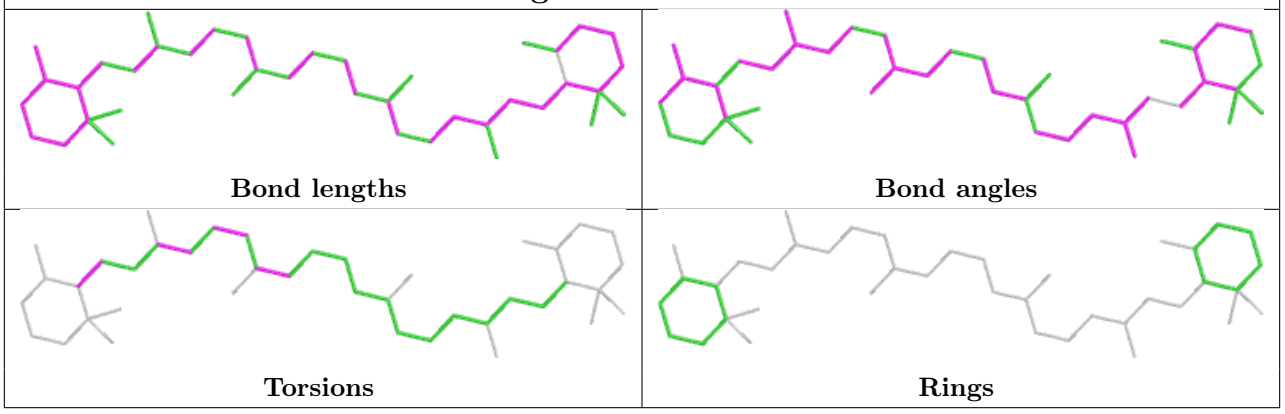


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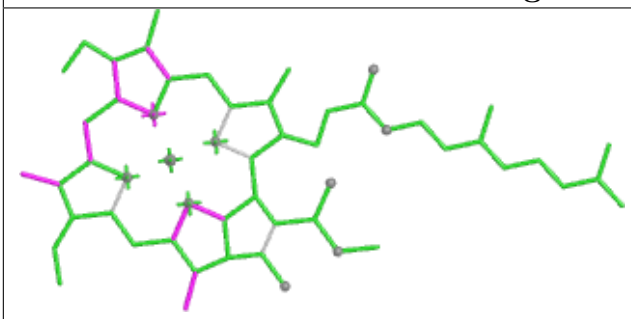
Ligand LHG d 407



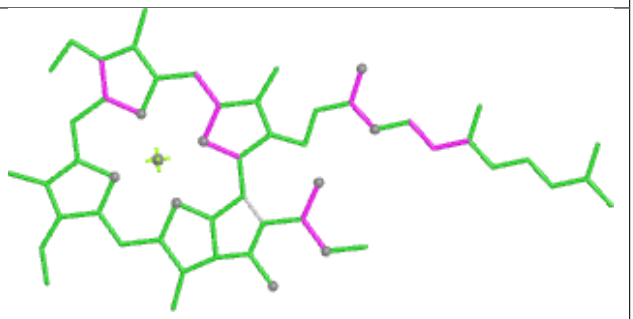
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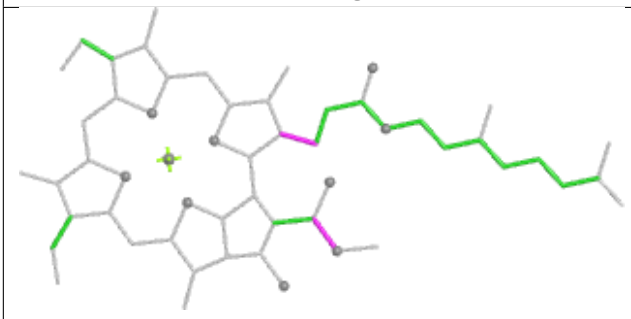
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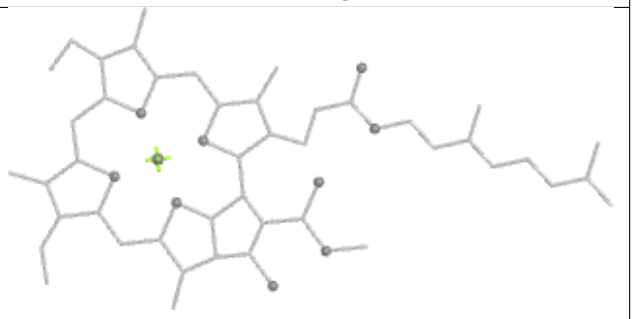
Bond lengths



Bond angles

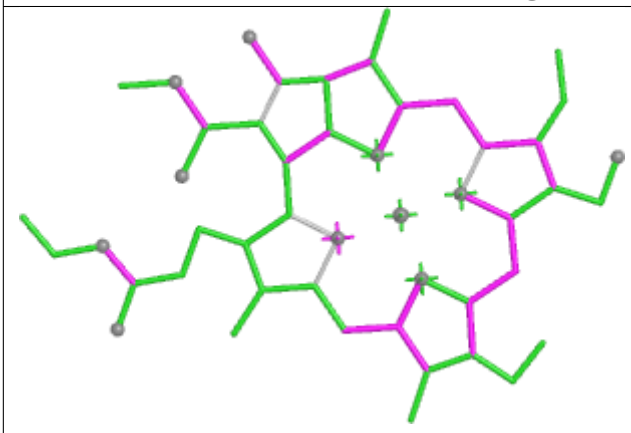


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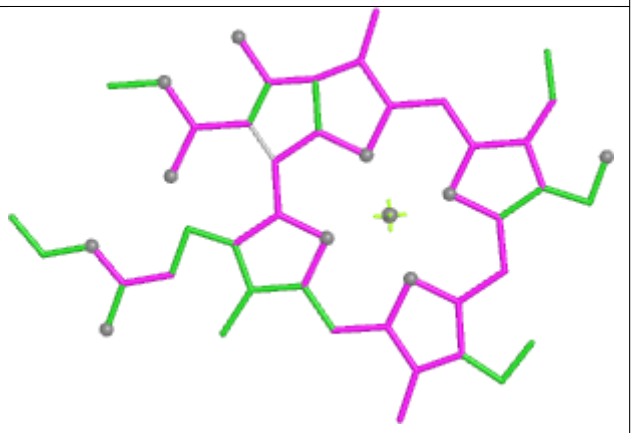


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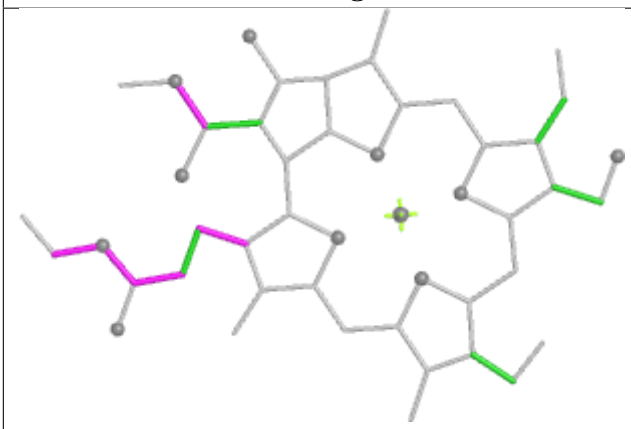
Ligand CHL R 606



Bond lengths



Bond angles

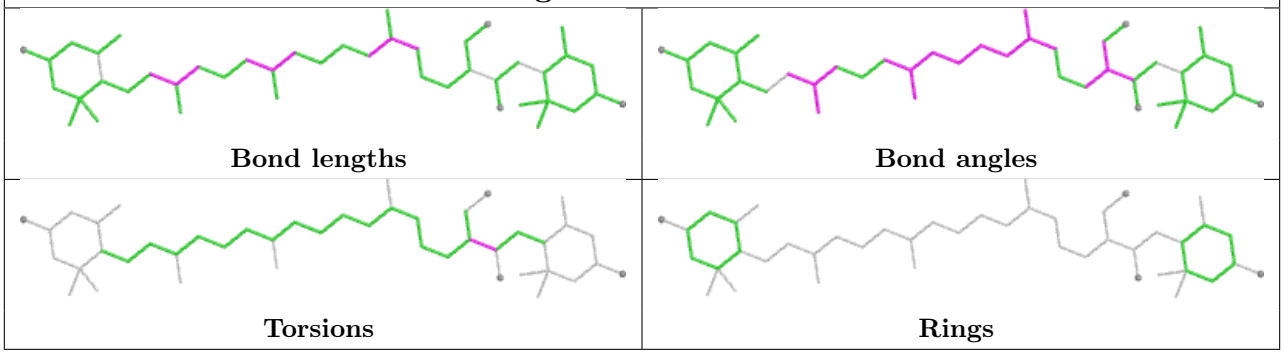


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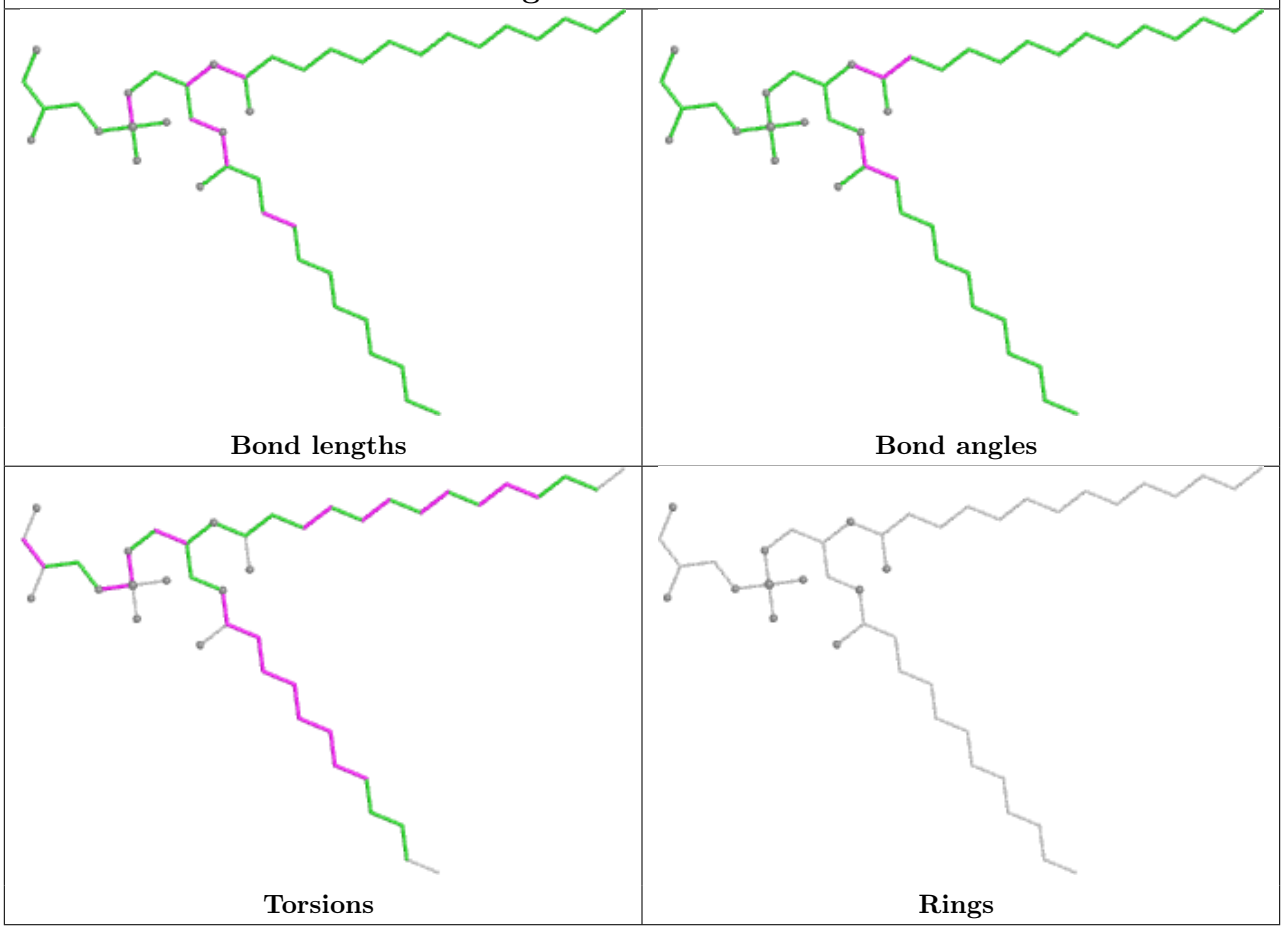


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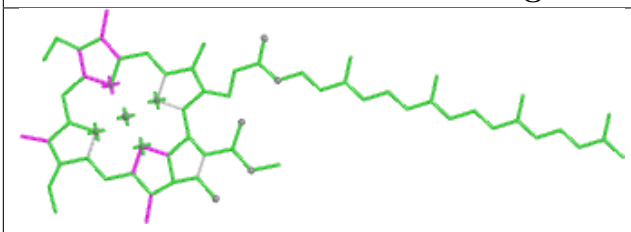
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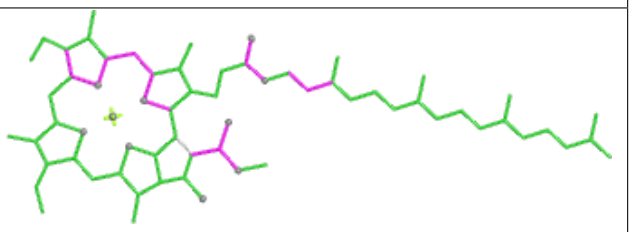
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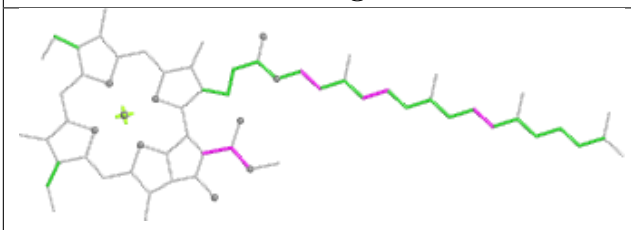
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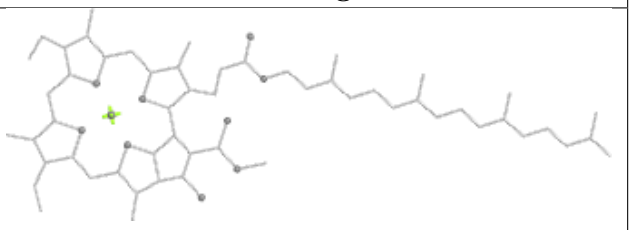
Bond lengths



Bond angles

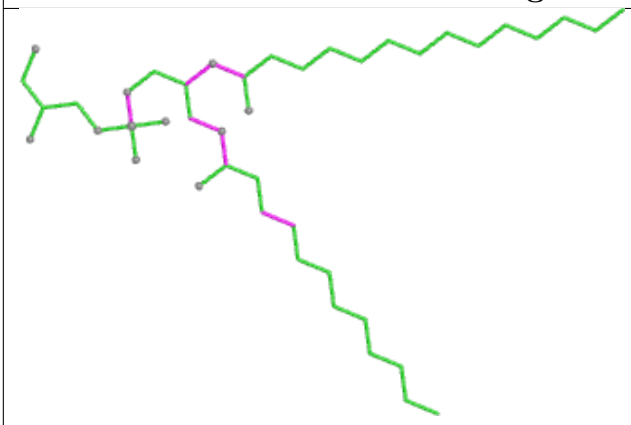


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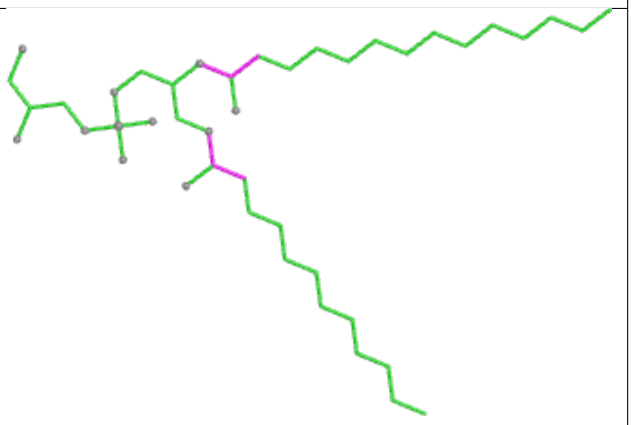


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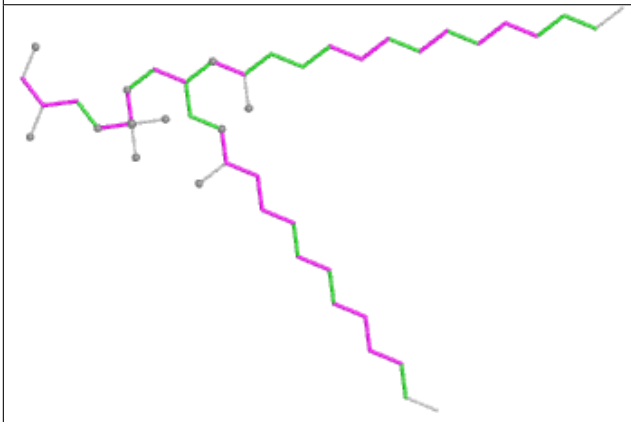
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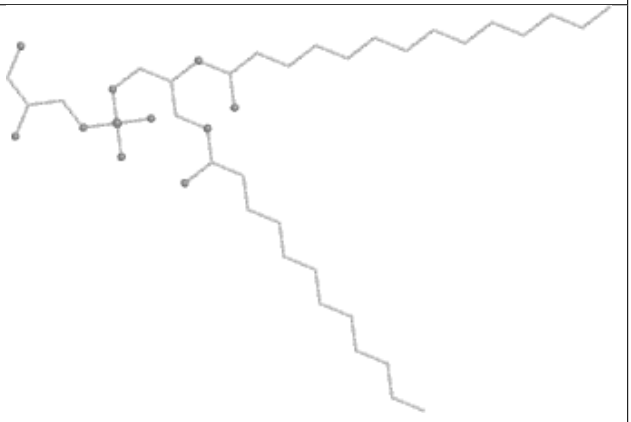
Bond lengths



Bond angles

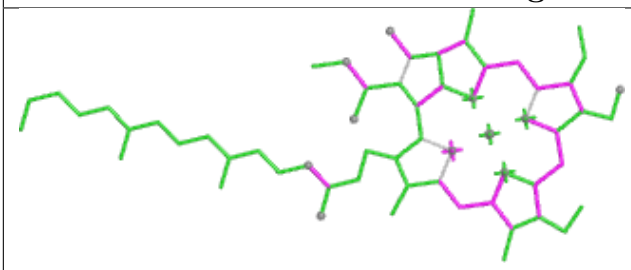


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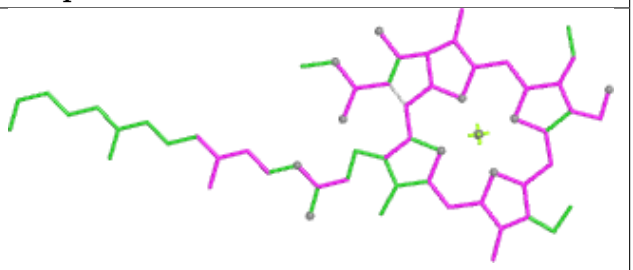


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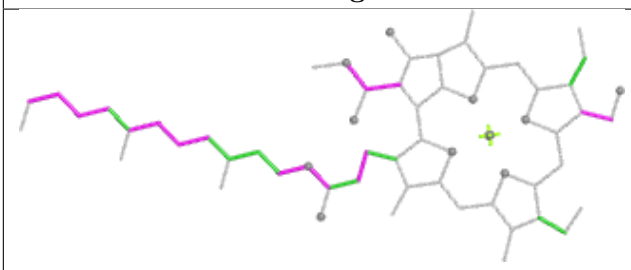
Ligand CHL q 304



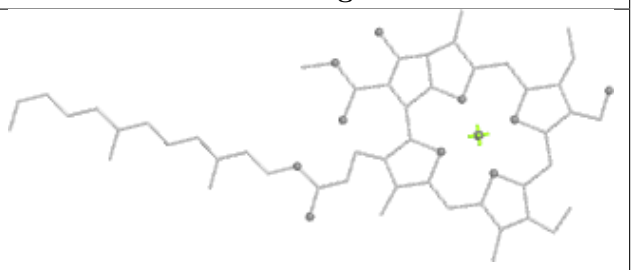
Bond lengths



Bond angles

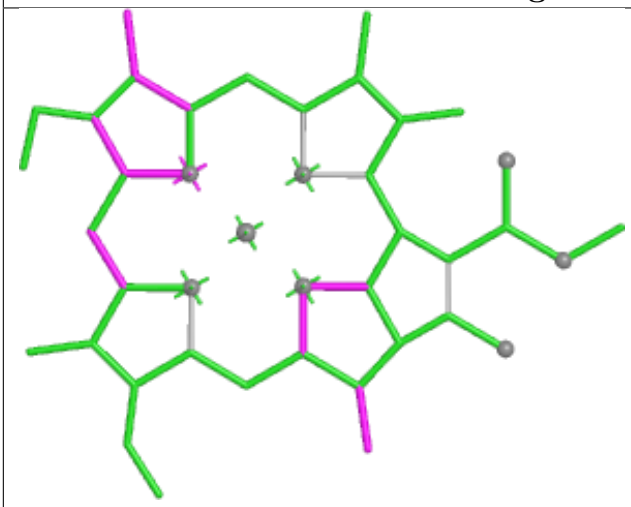


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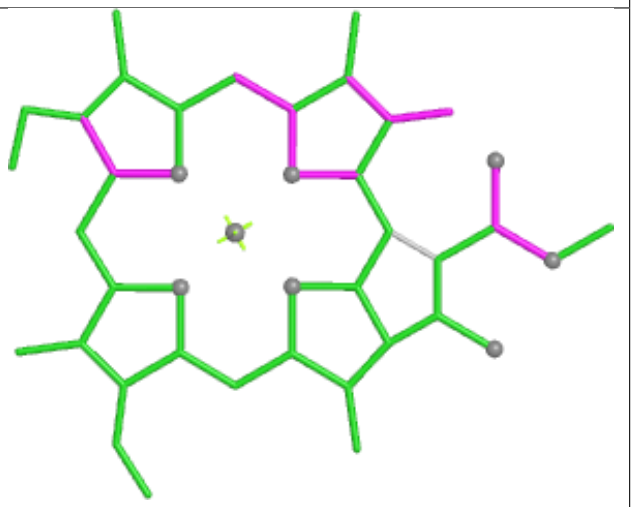


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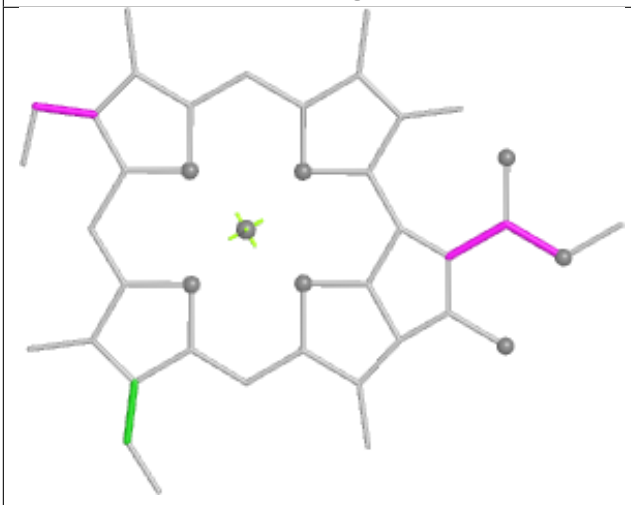
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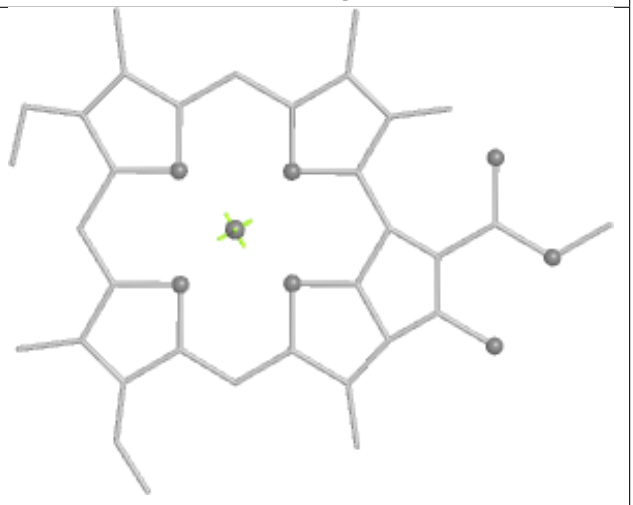
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Bond angles

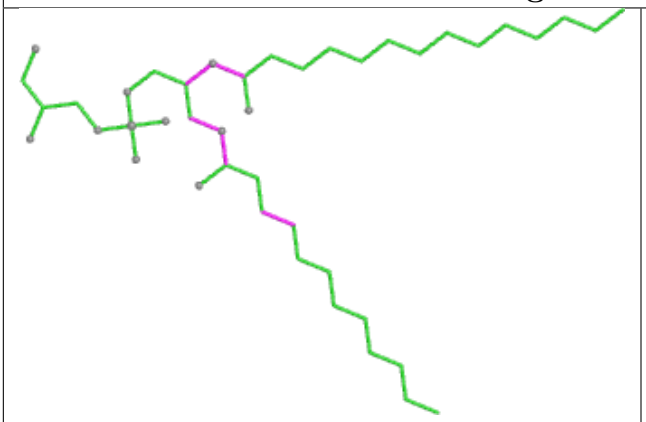


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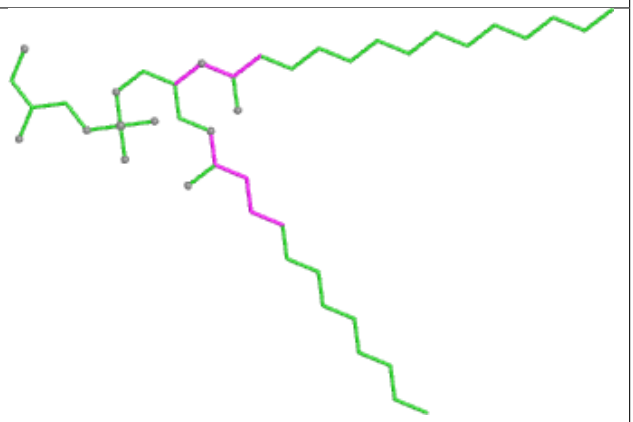


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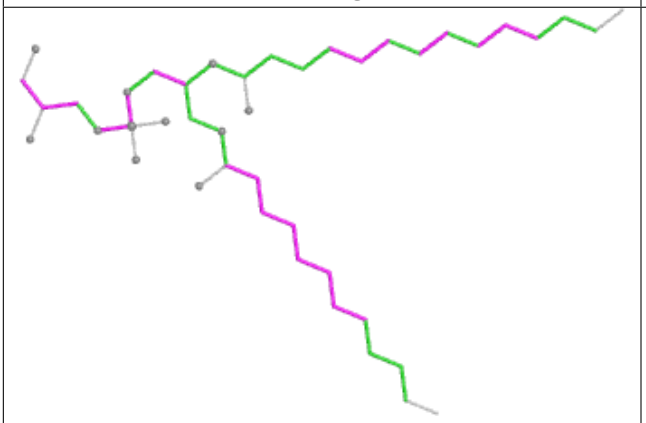
Ligand LHG 5 319



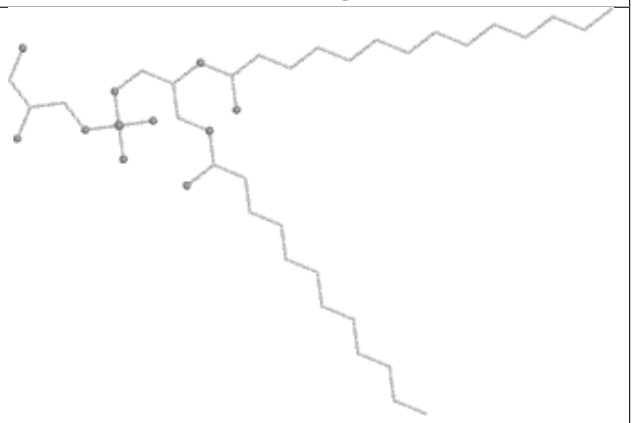
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Bond angles

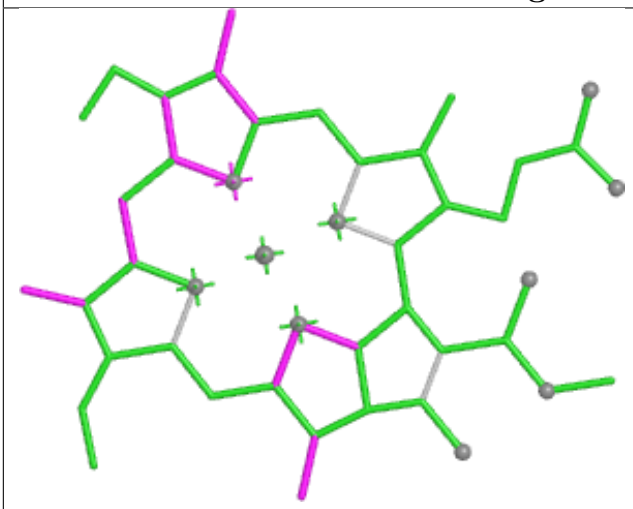


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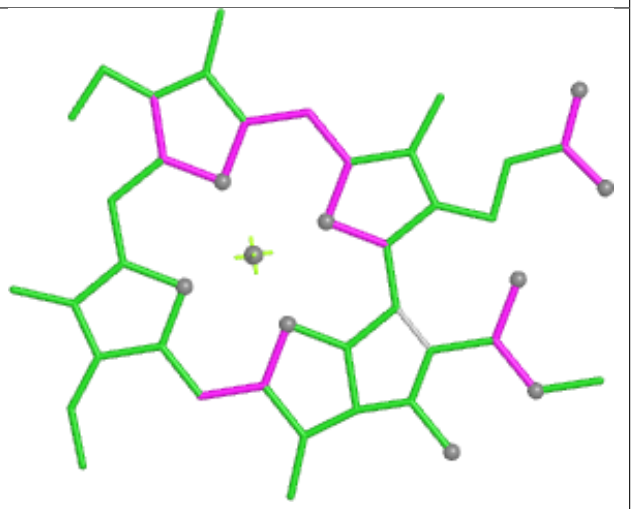


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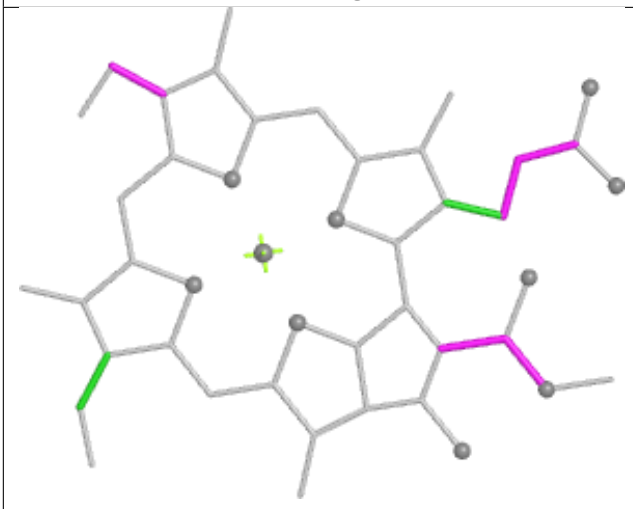
Ligand CLA 3 316



Bond lengths



Bond angles

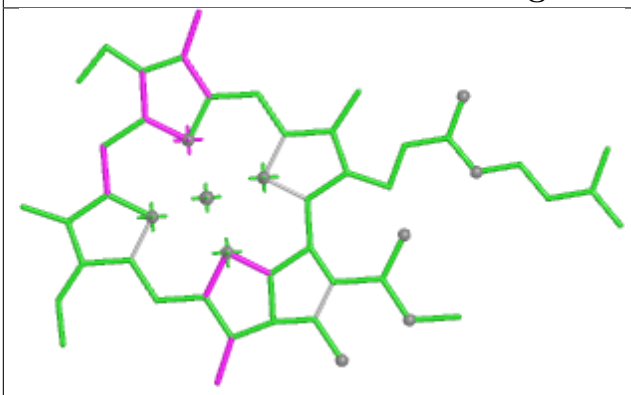


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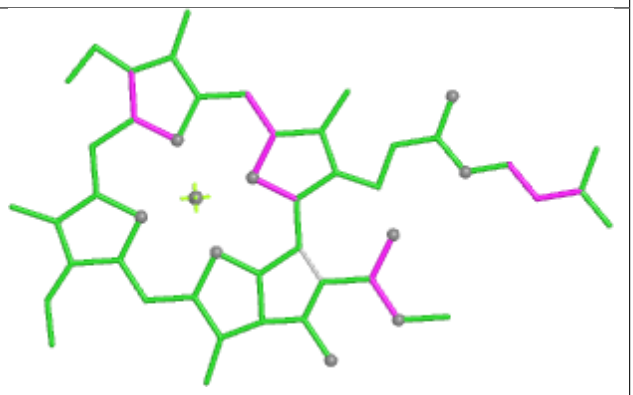


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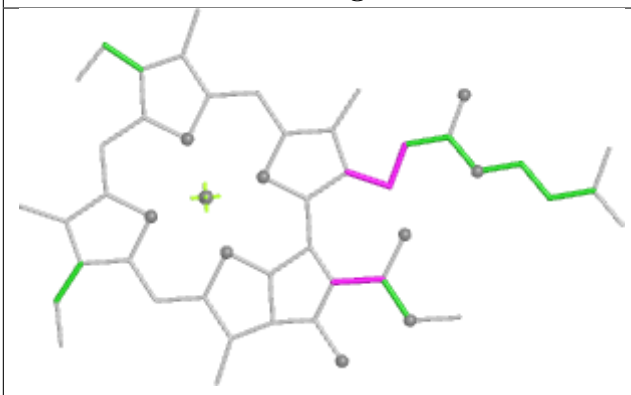
Ligand CLA 7 308



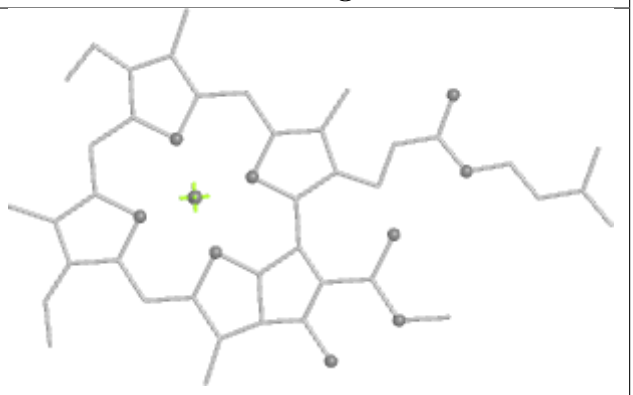
Bond lengths



Bond angles

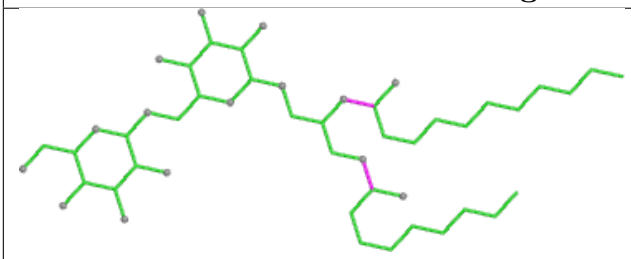


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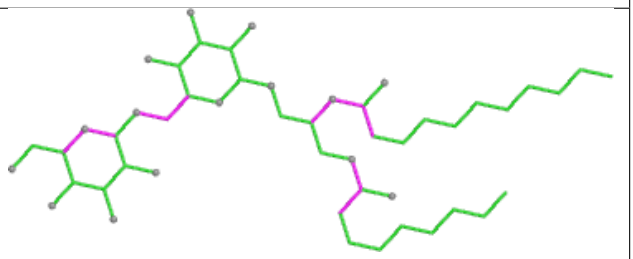


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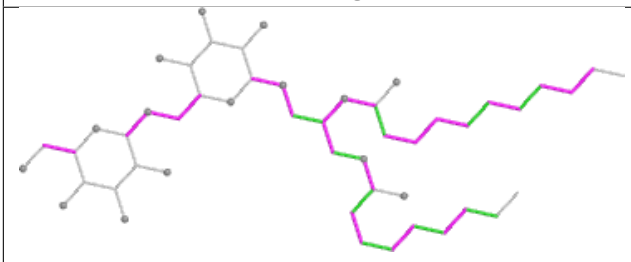
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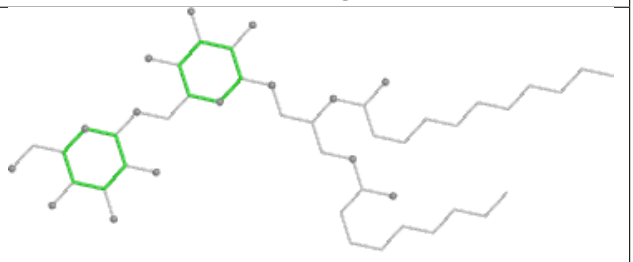
Bond lengths



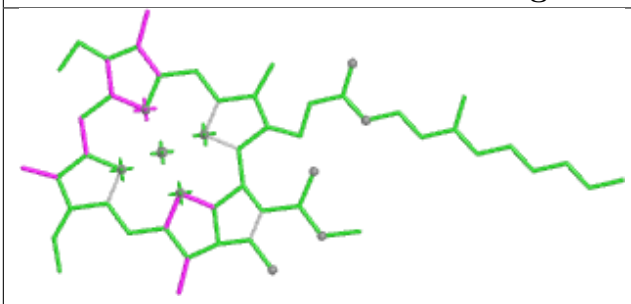
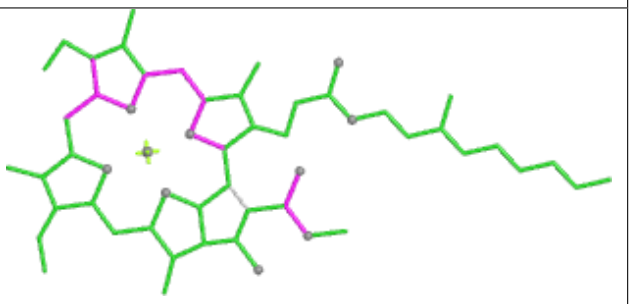
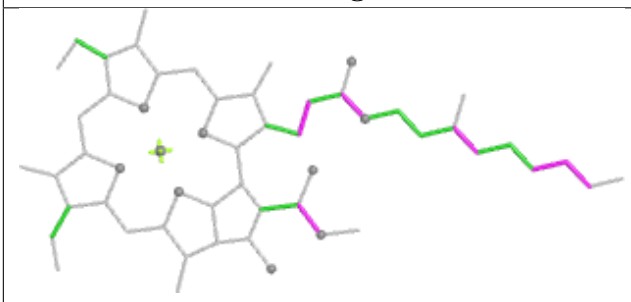
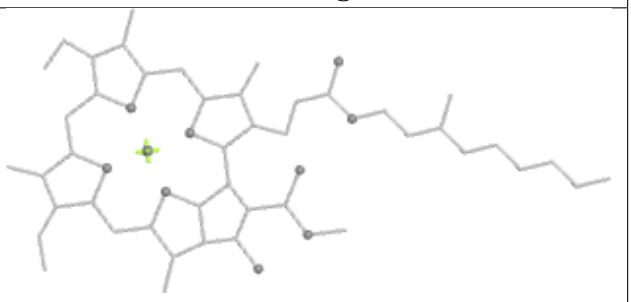
Bond angles

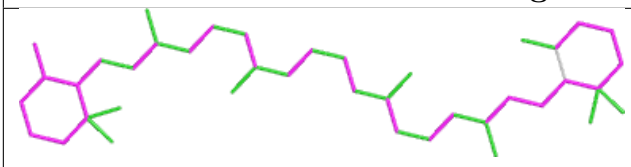
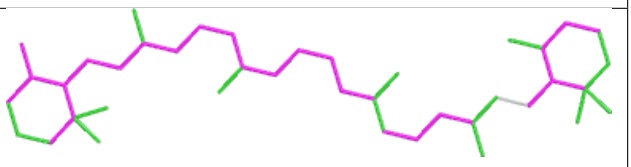
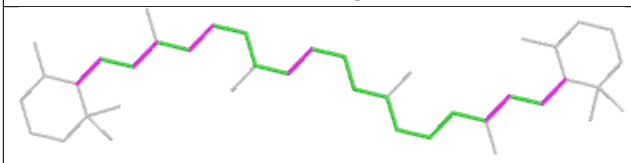
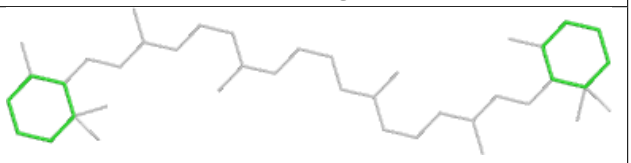


Torsions

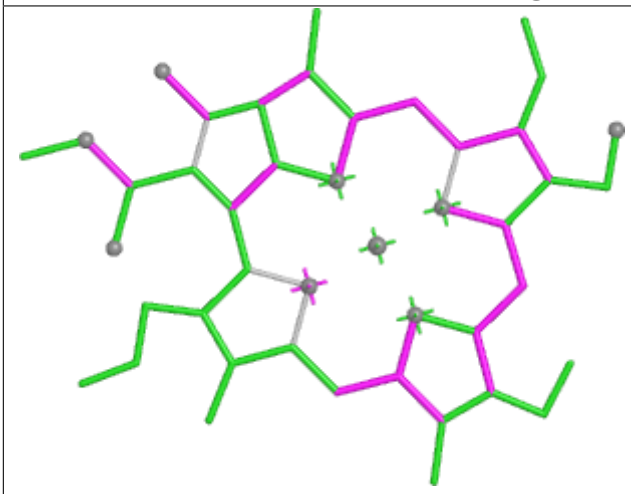


Rings

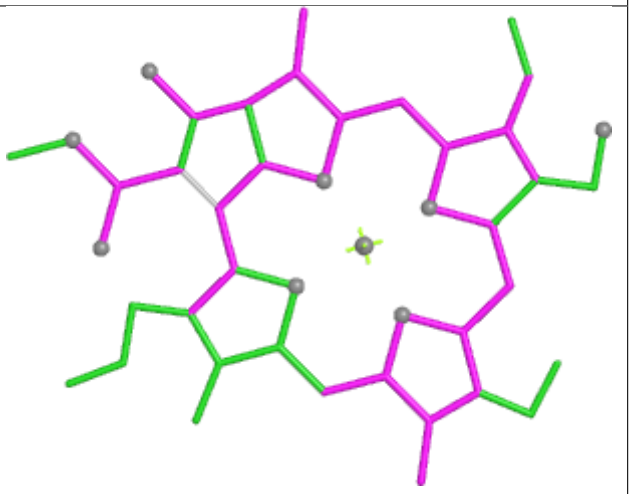
Ligand CLA s 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

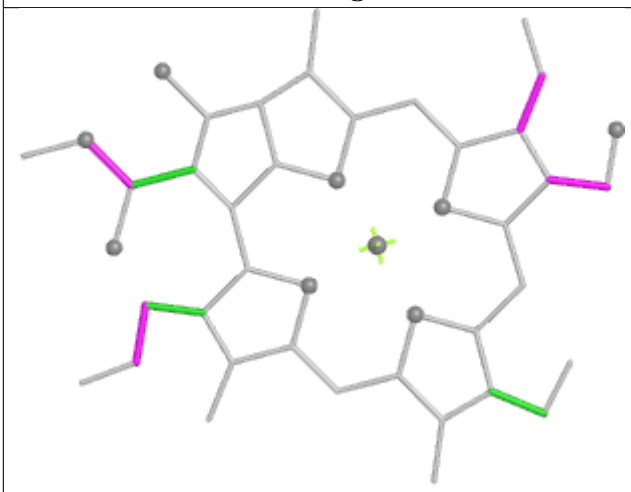
Ligand CHL 2 305



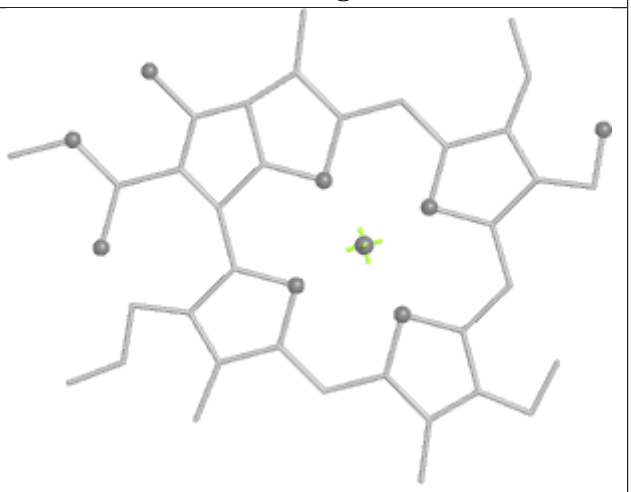
Bond lengths



Bond angles

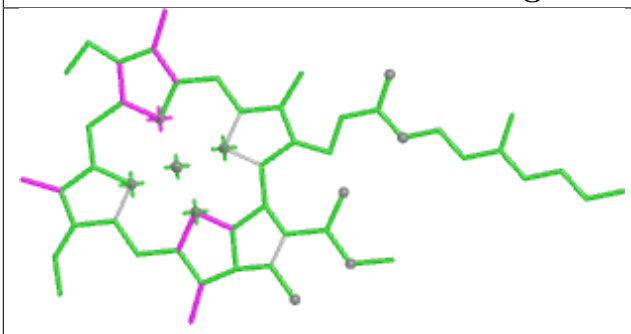


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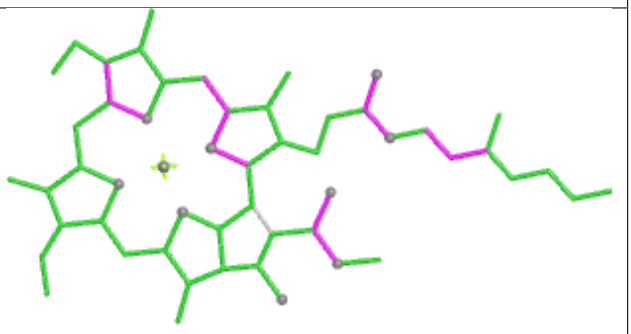


Rings

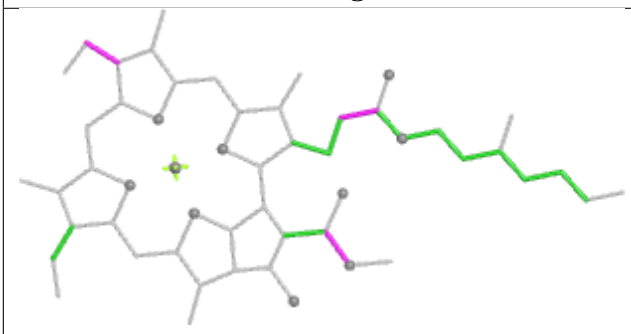
Ligand CLA Y 306



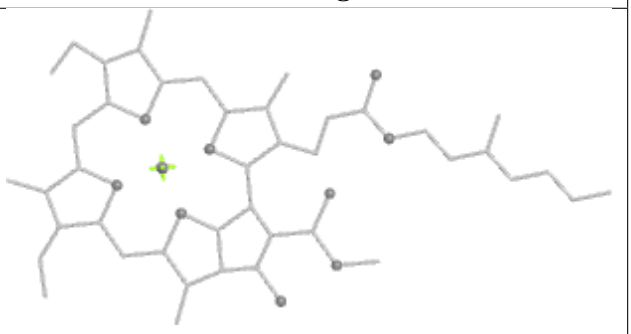
Bond lengths



Bond angles

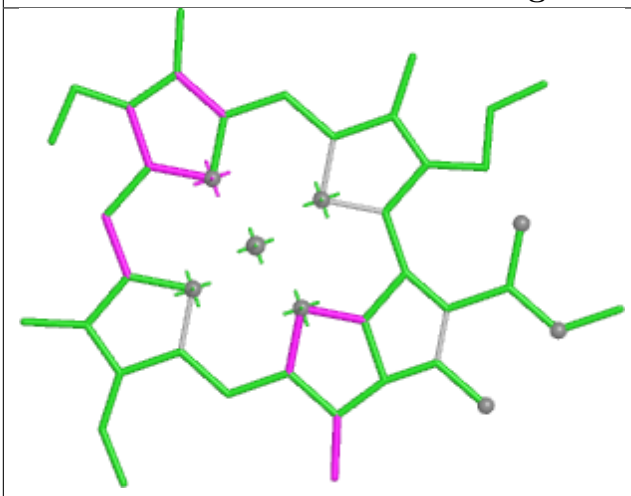


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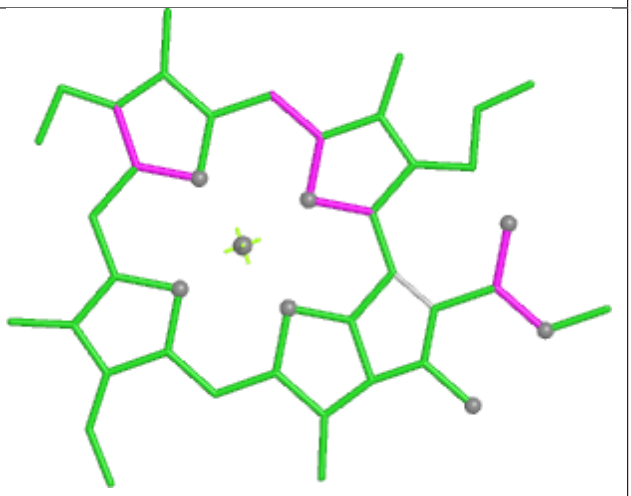


Rings

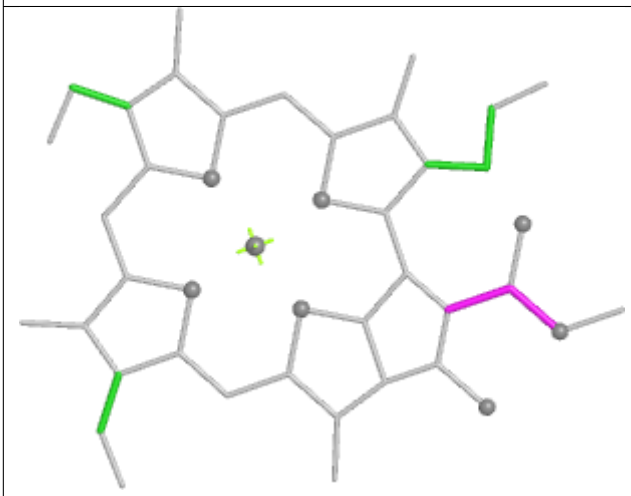
Ligand CLA 3 307



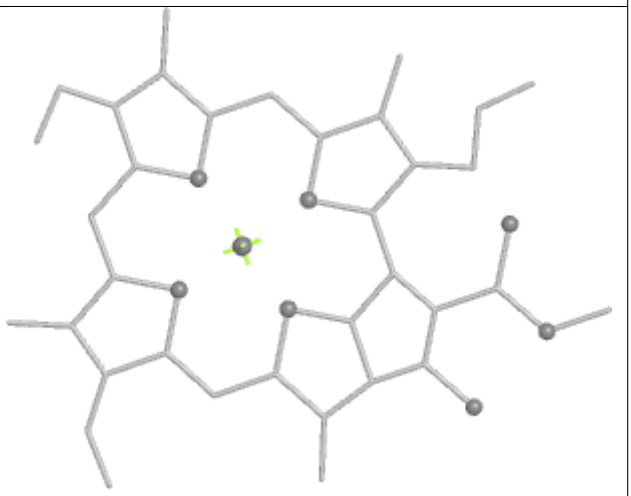
Bond lengths



Bond angles

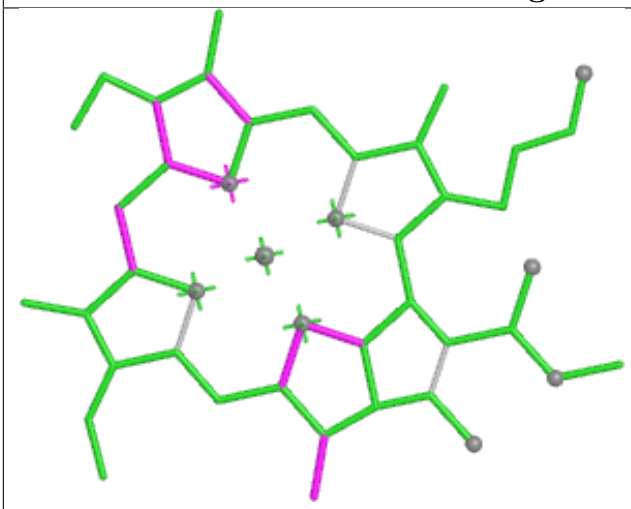


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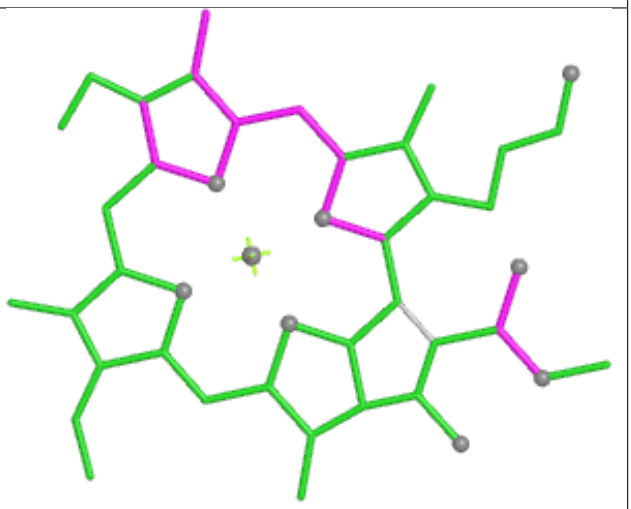


Rings

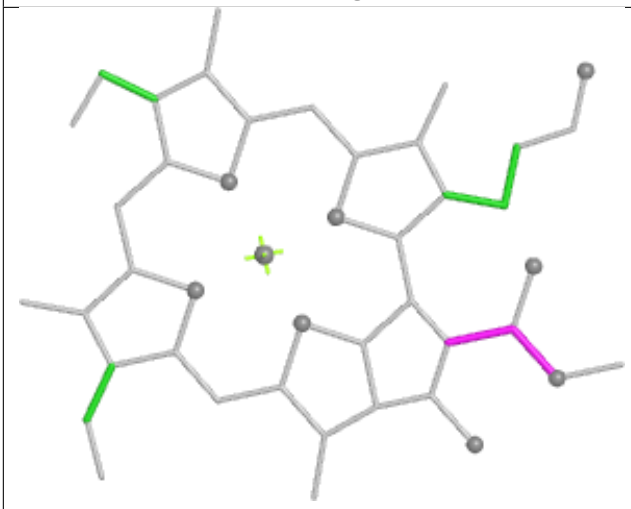
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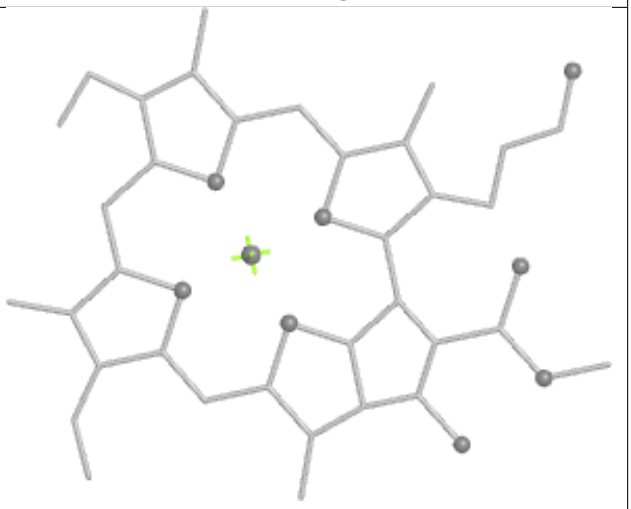
Bond lengths



Bond angles

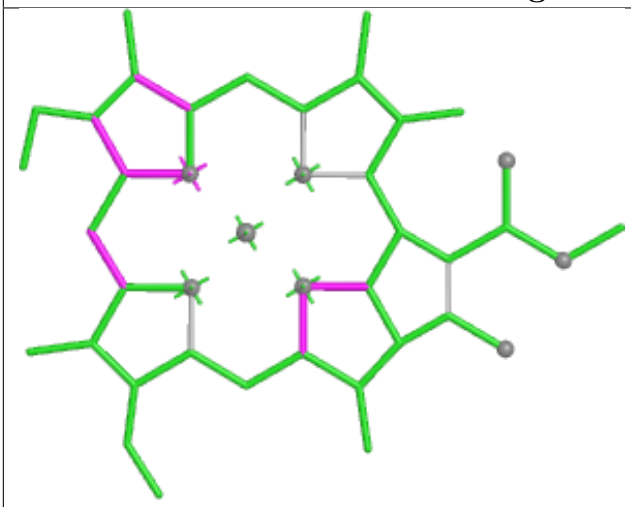


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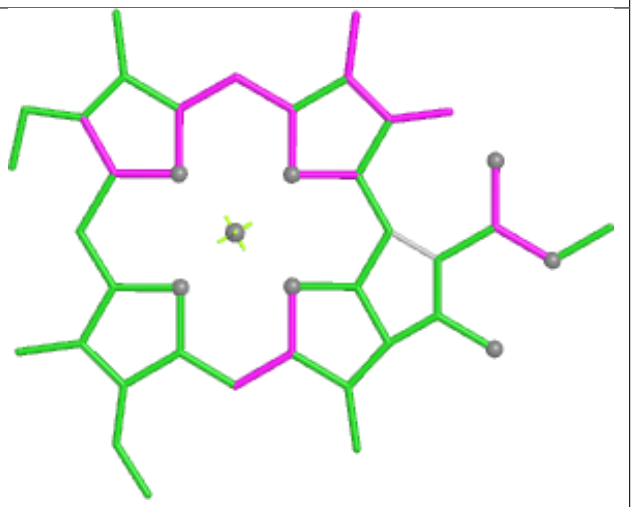


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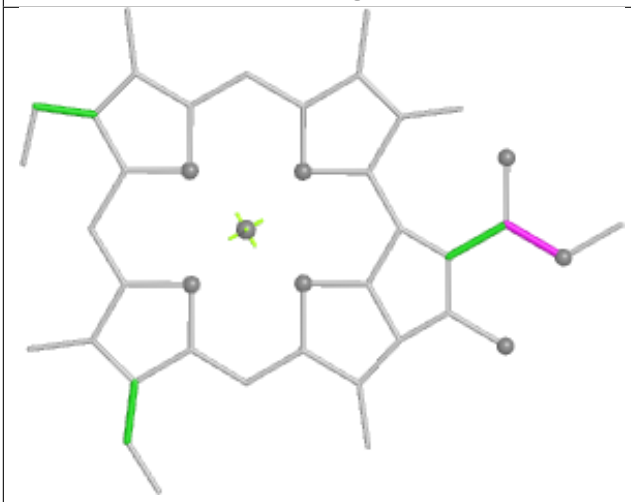
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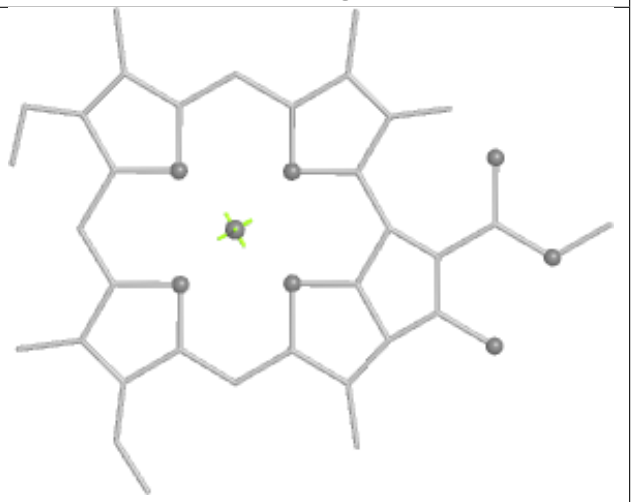
Bond lengths



Bond angles

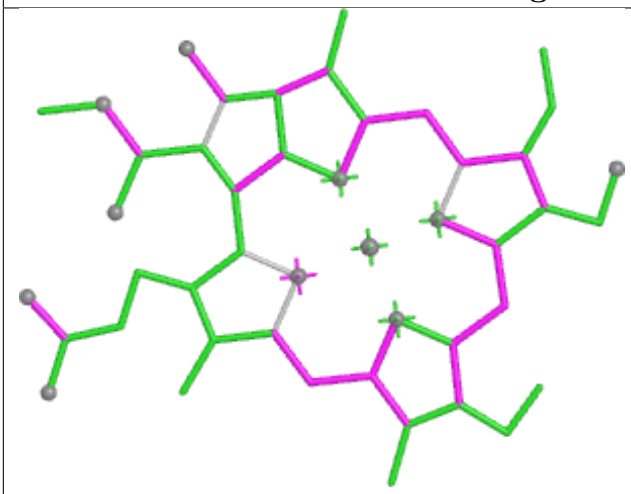


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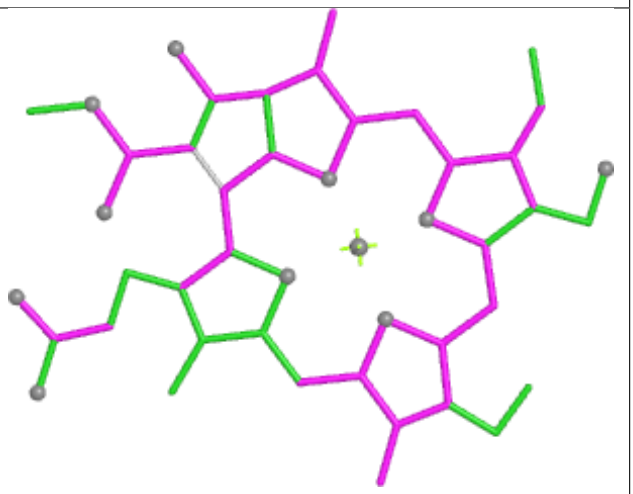


Rings

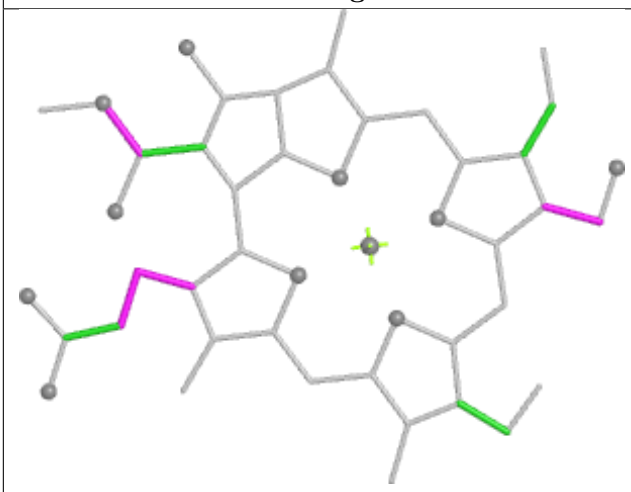
Ligand CHL s 408



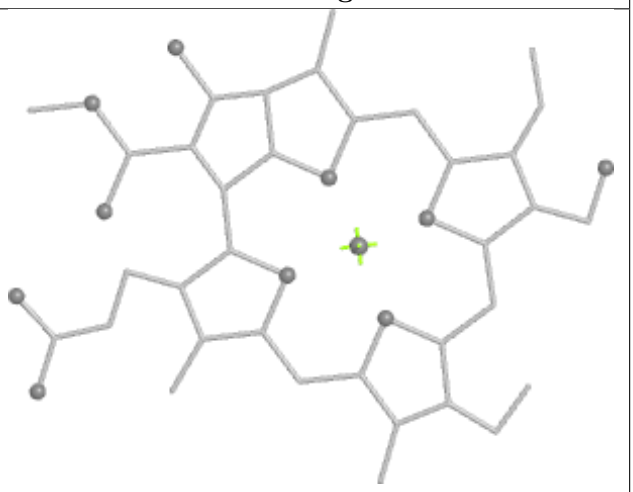
Bond lengths



Bond angles

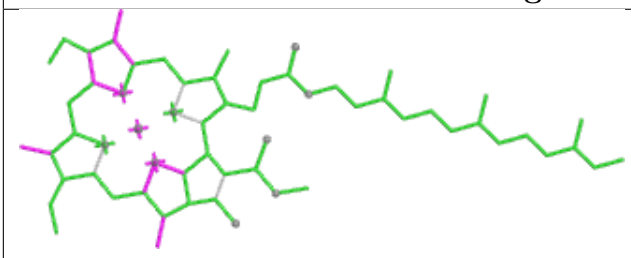


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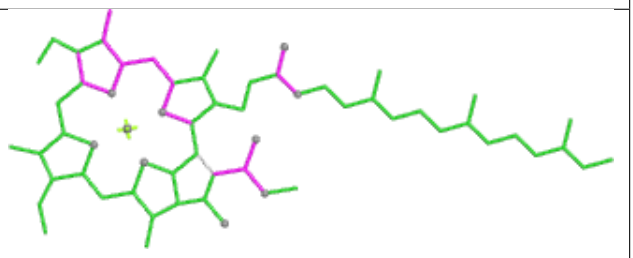


Rings

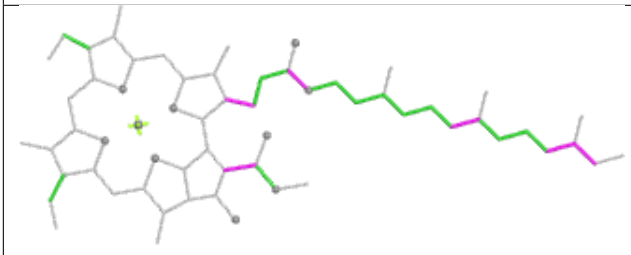
Ligand CLA C 608



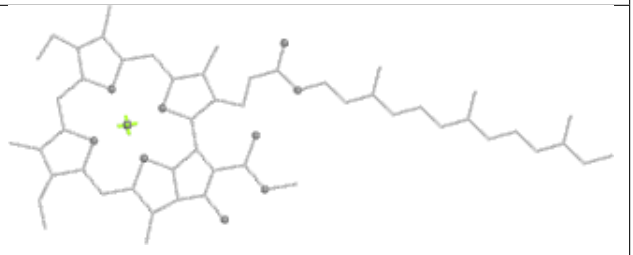
Bond lengths



Bond angles

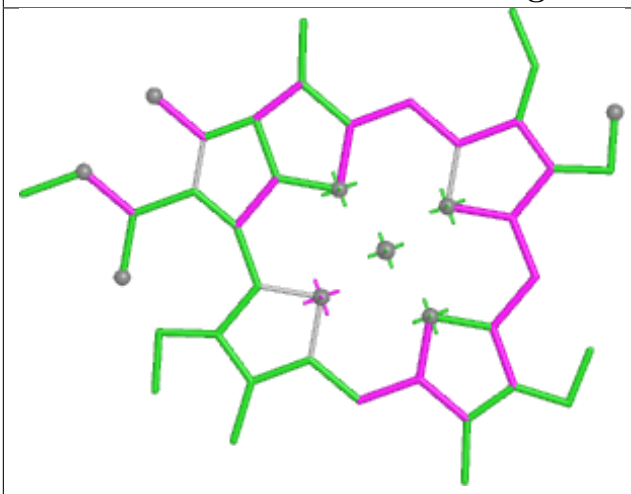


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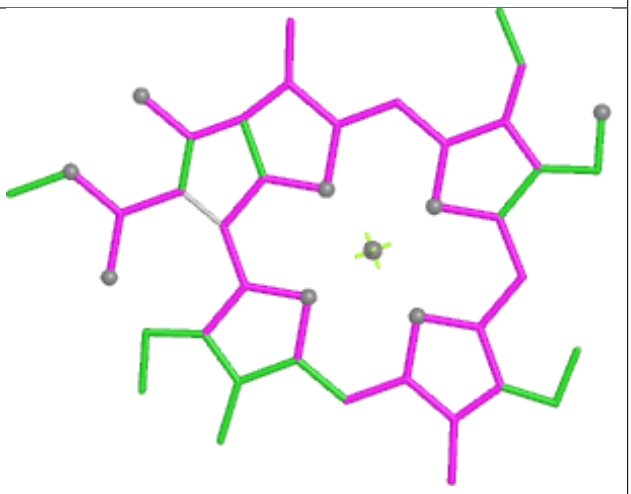


Rings

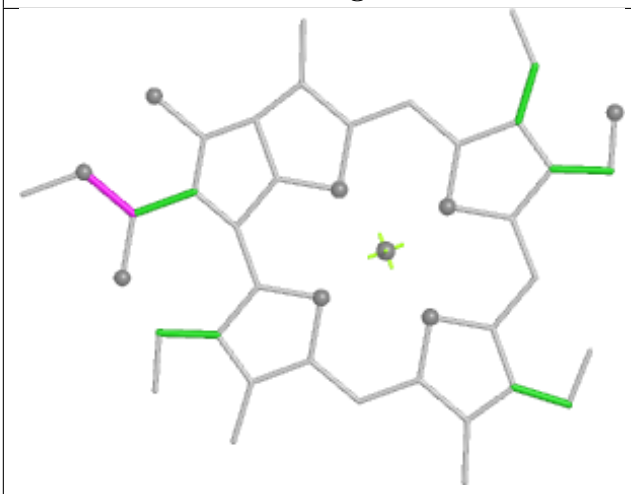
Ligand CHL 1 308



Bond lengths



Bond angles

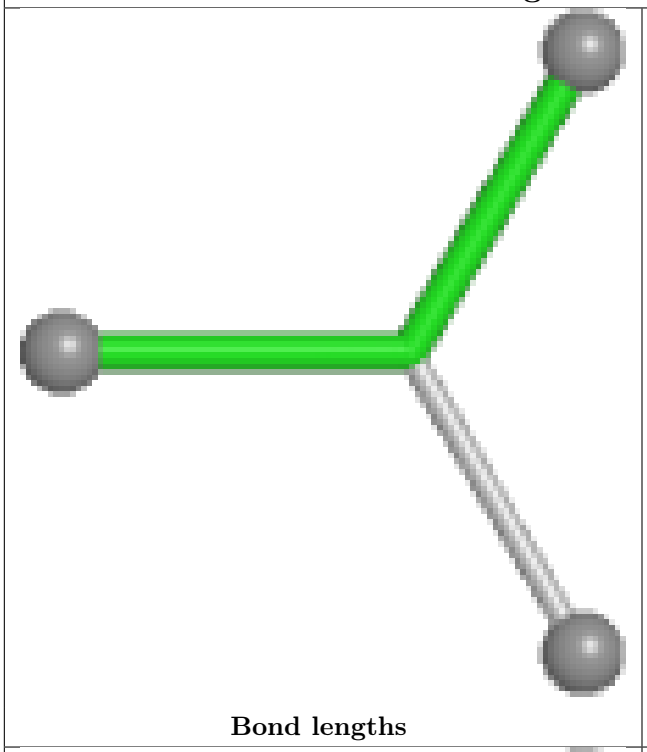


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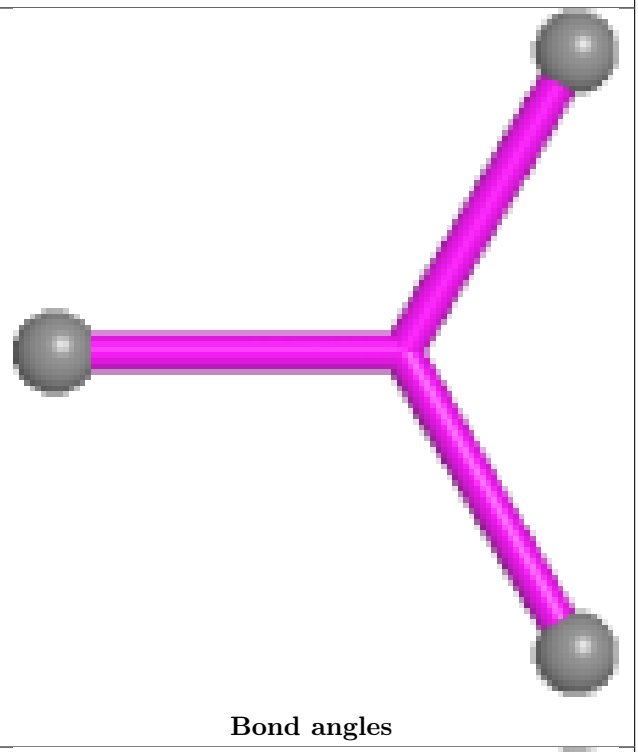


Rings

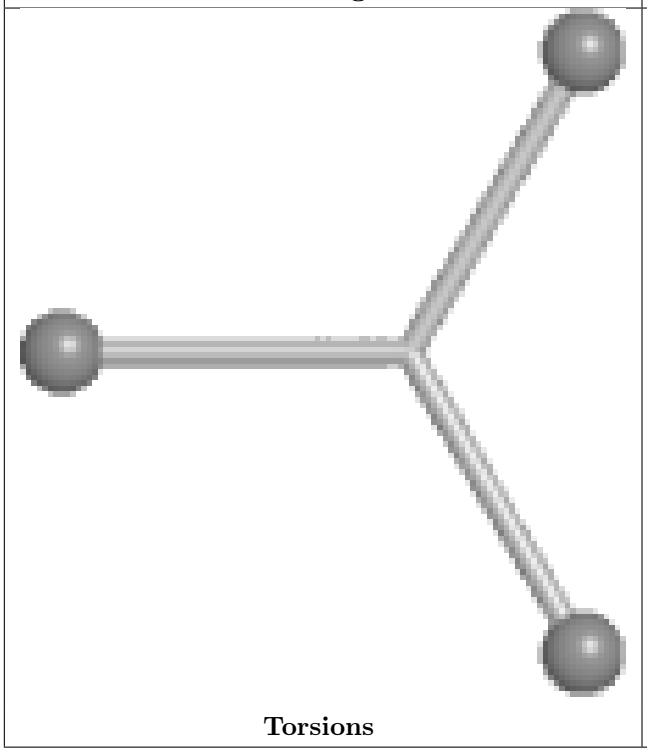
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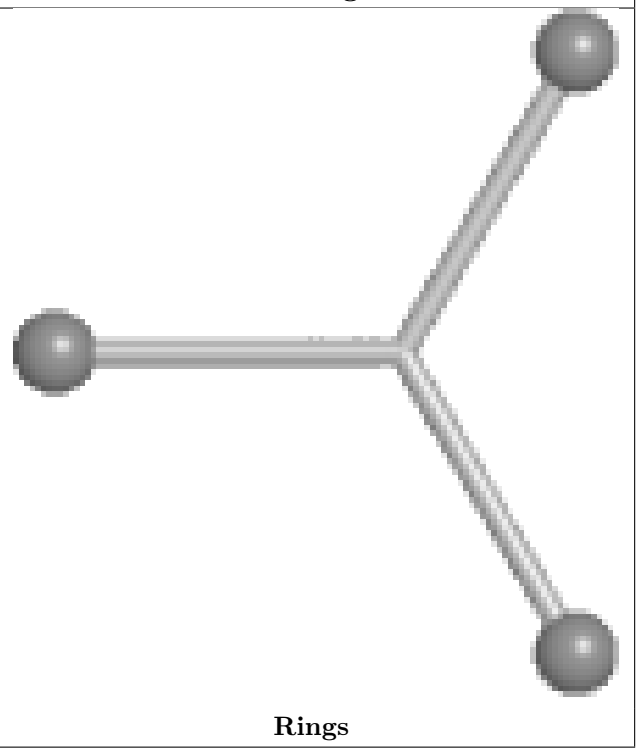
Bond lengths



Bond angles

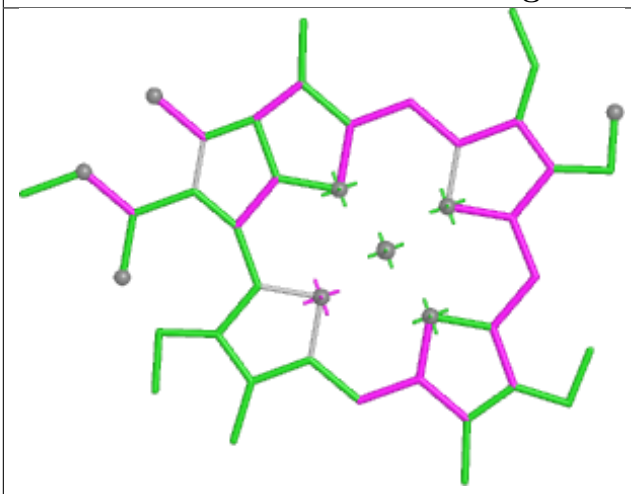


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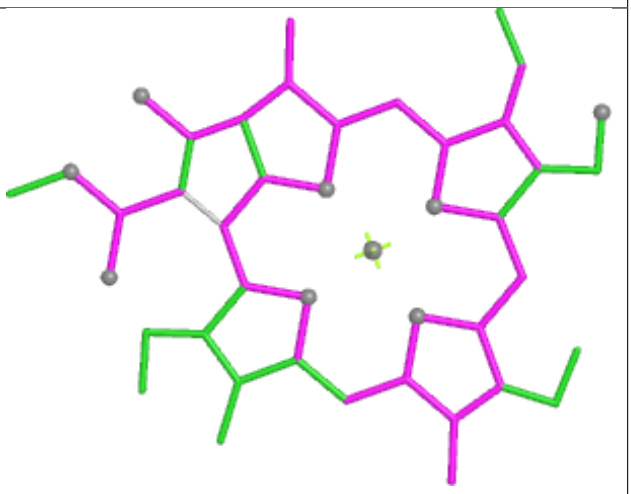


Rings

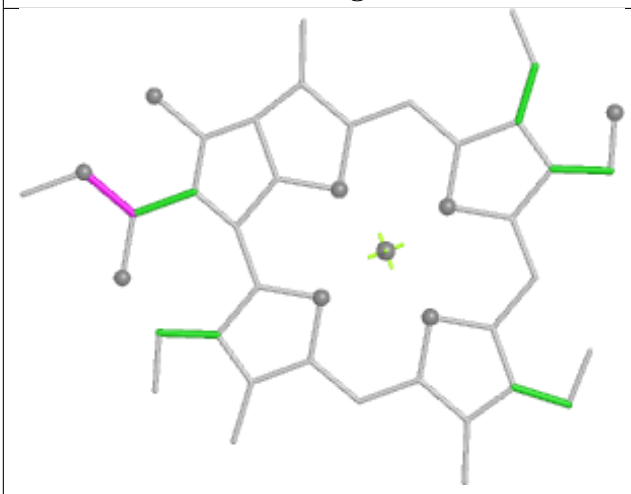
Ligand CHL G 309



Bond lengths



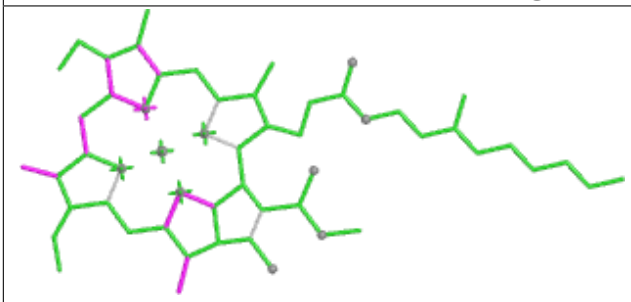
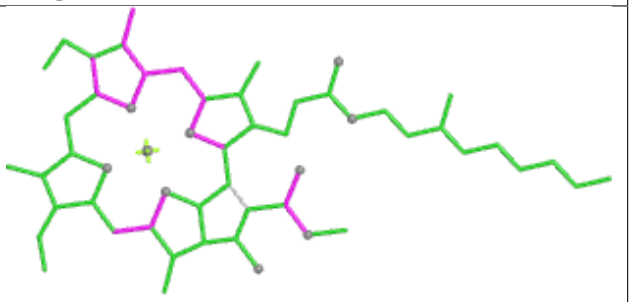
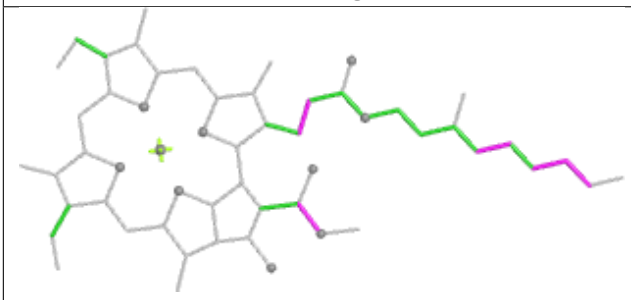
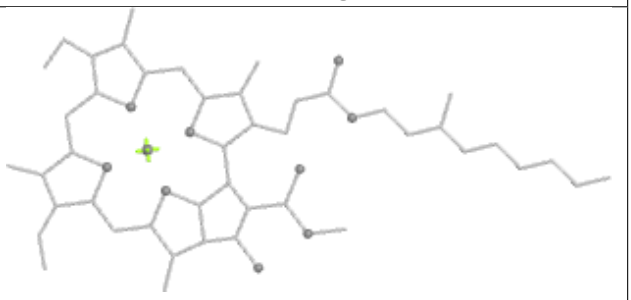
Bond angles

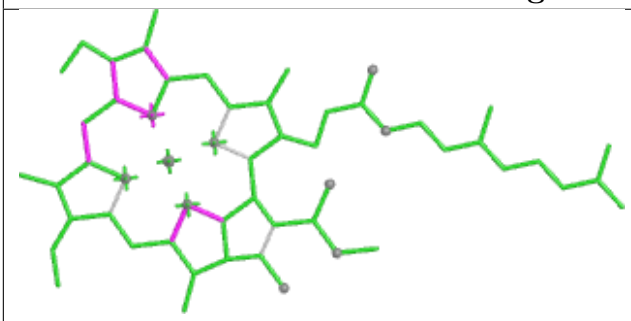
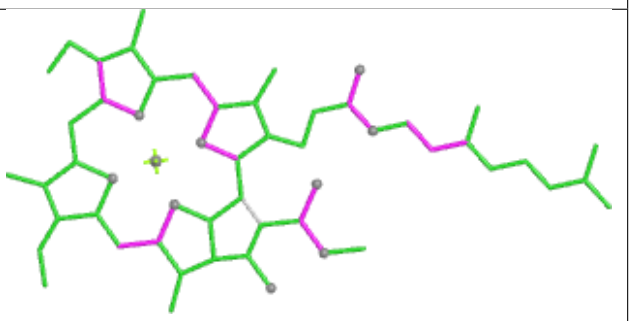
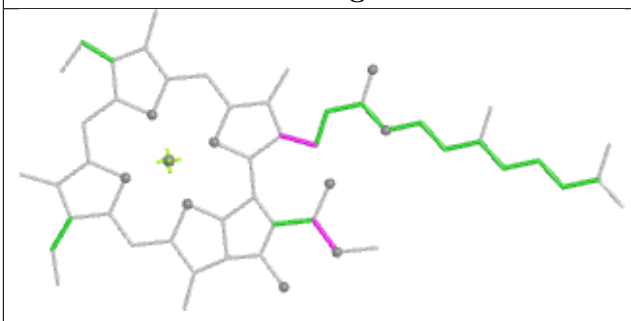
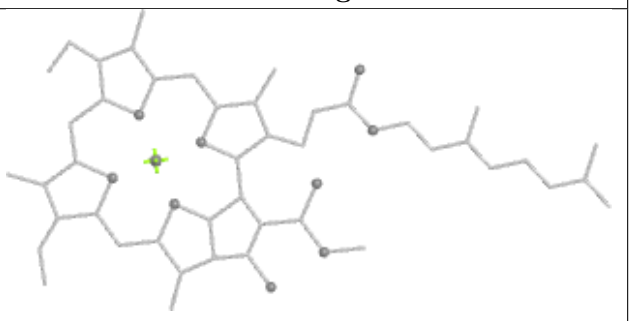


Torsions

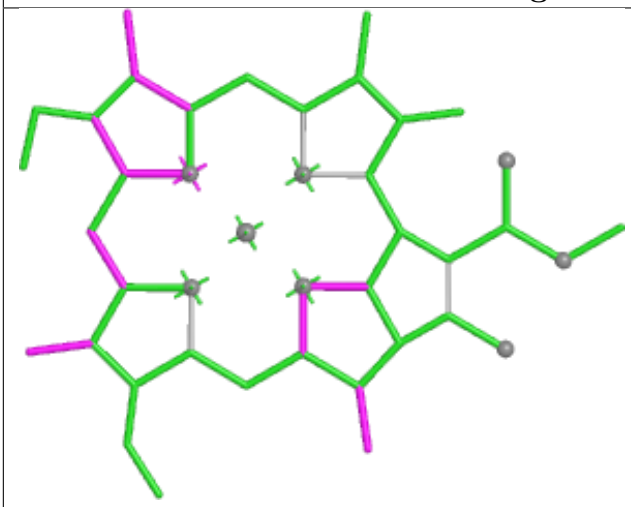


Rings

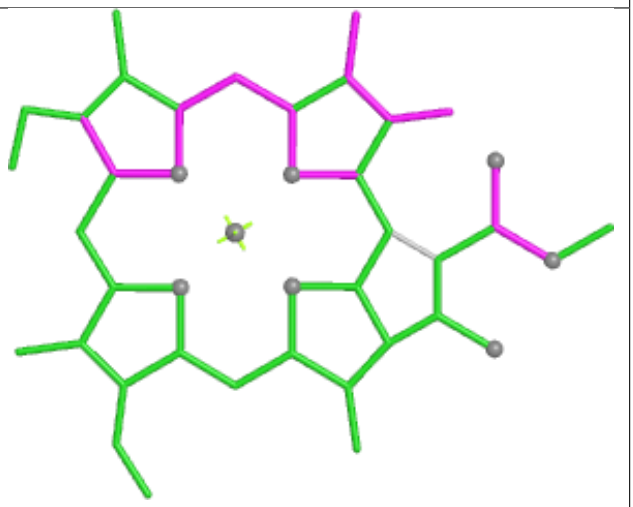
Ligand CLA g 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA u 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

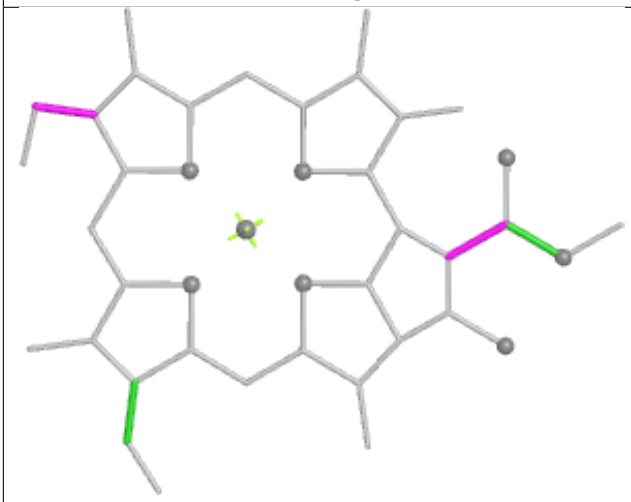
Ligand CLA r 305



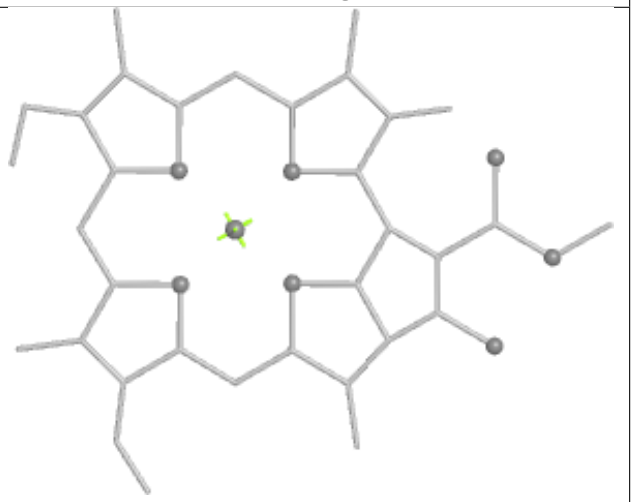
Bond lengths



Bond angles

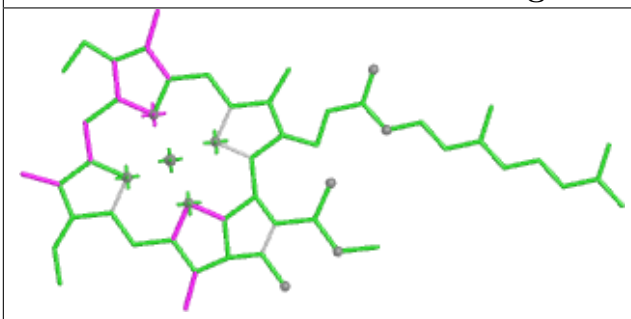


Torsions

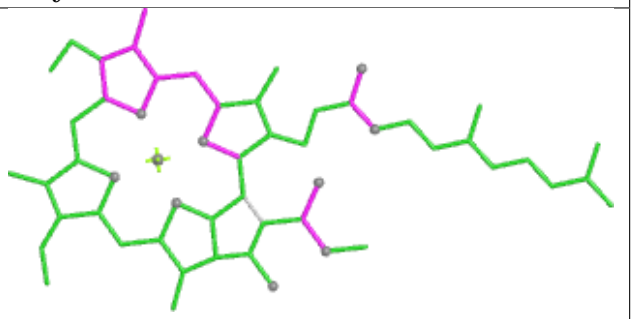


Rings

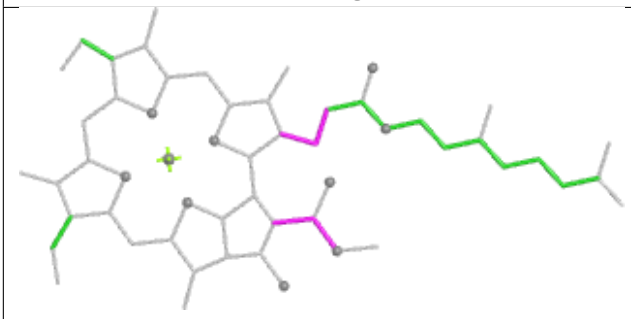
Ligand CLA y 314



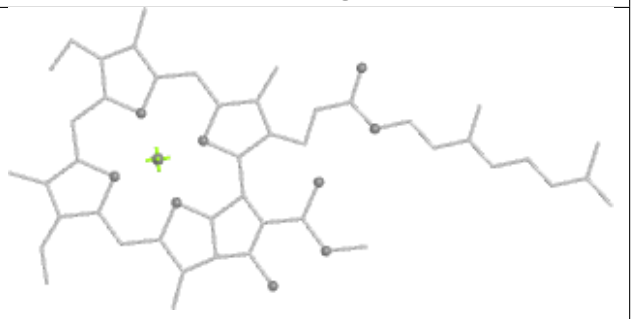
Bond lengths



Bond angles

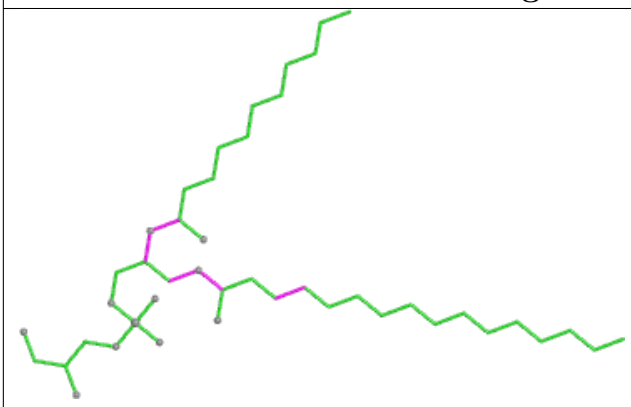


Torsions

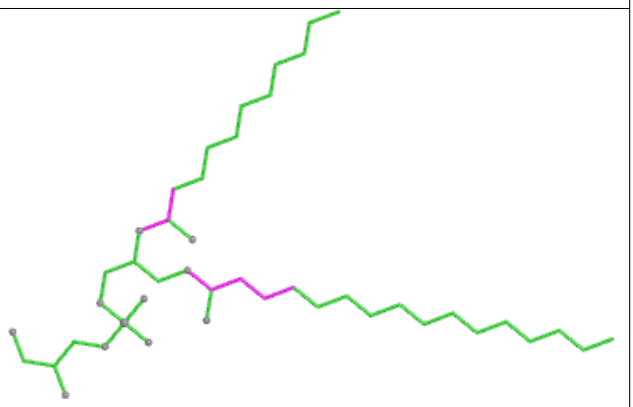


Rings

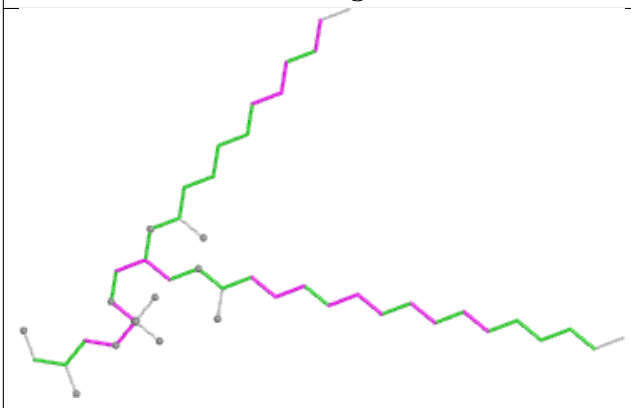
Ligand LHG A 612



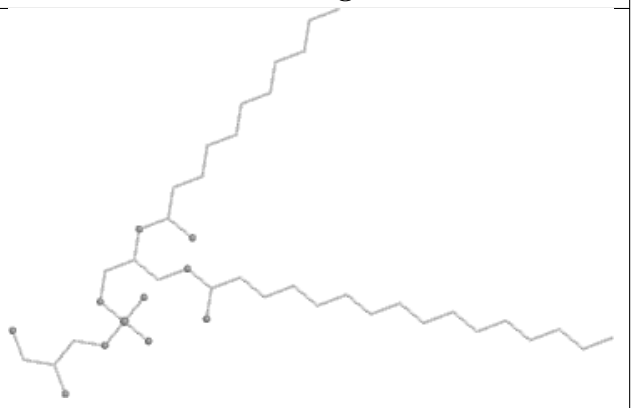
Bond lengths



Bond angles

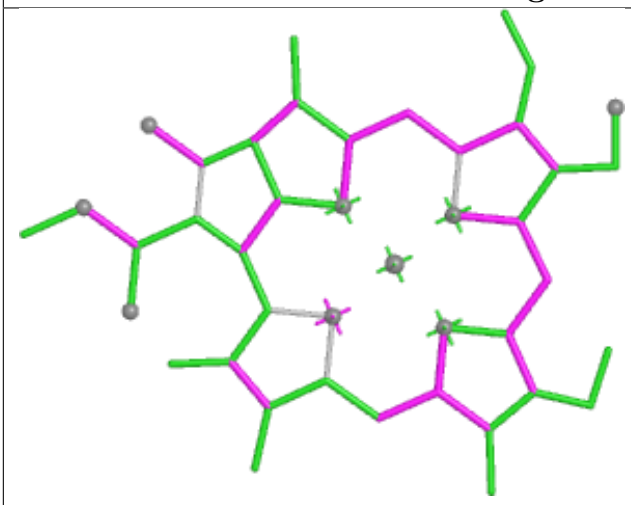


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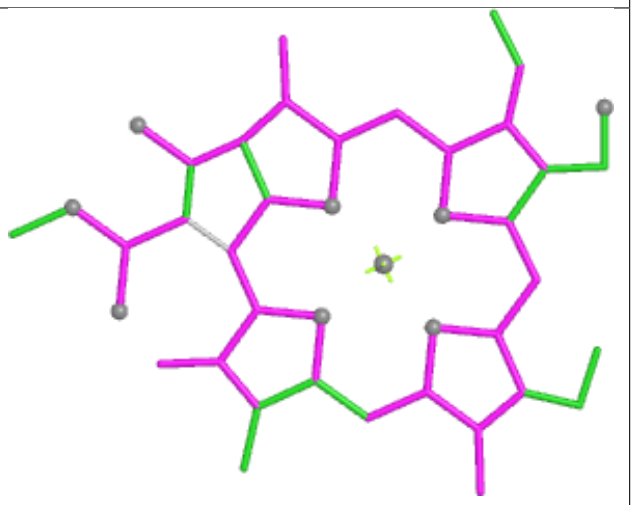


Rings

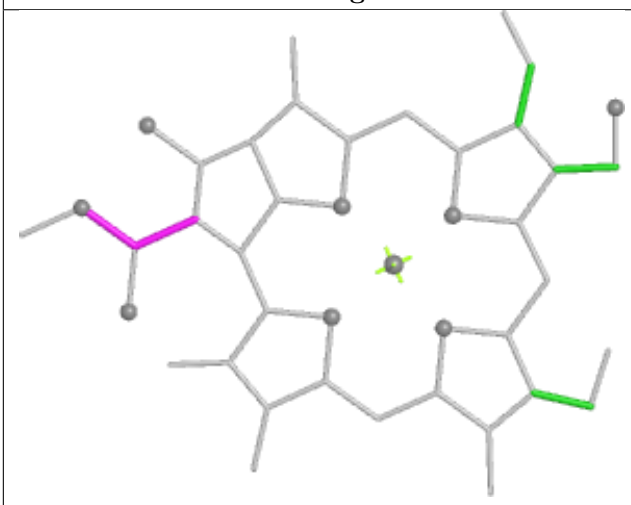
Ligand CHL 2 318



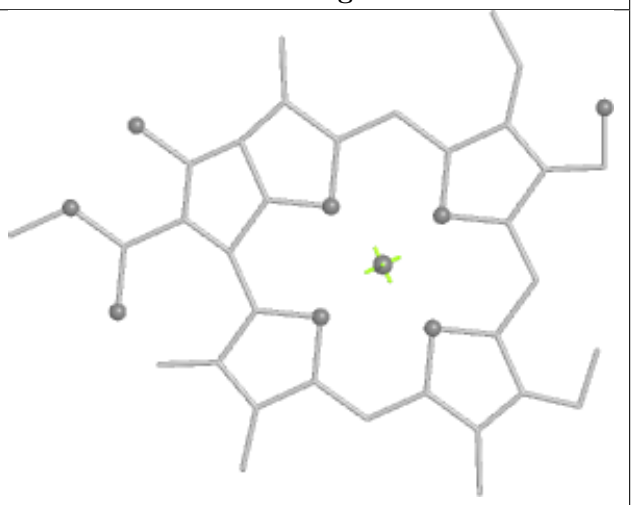
Bond lengths



Bond angles

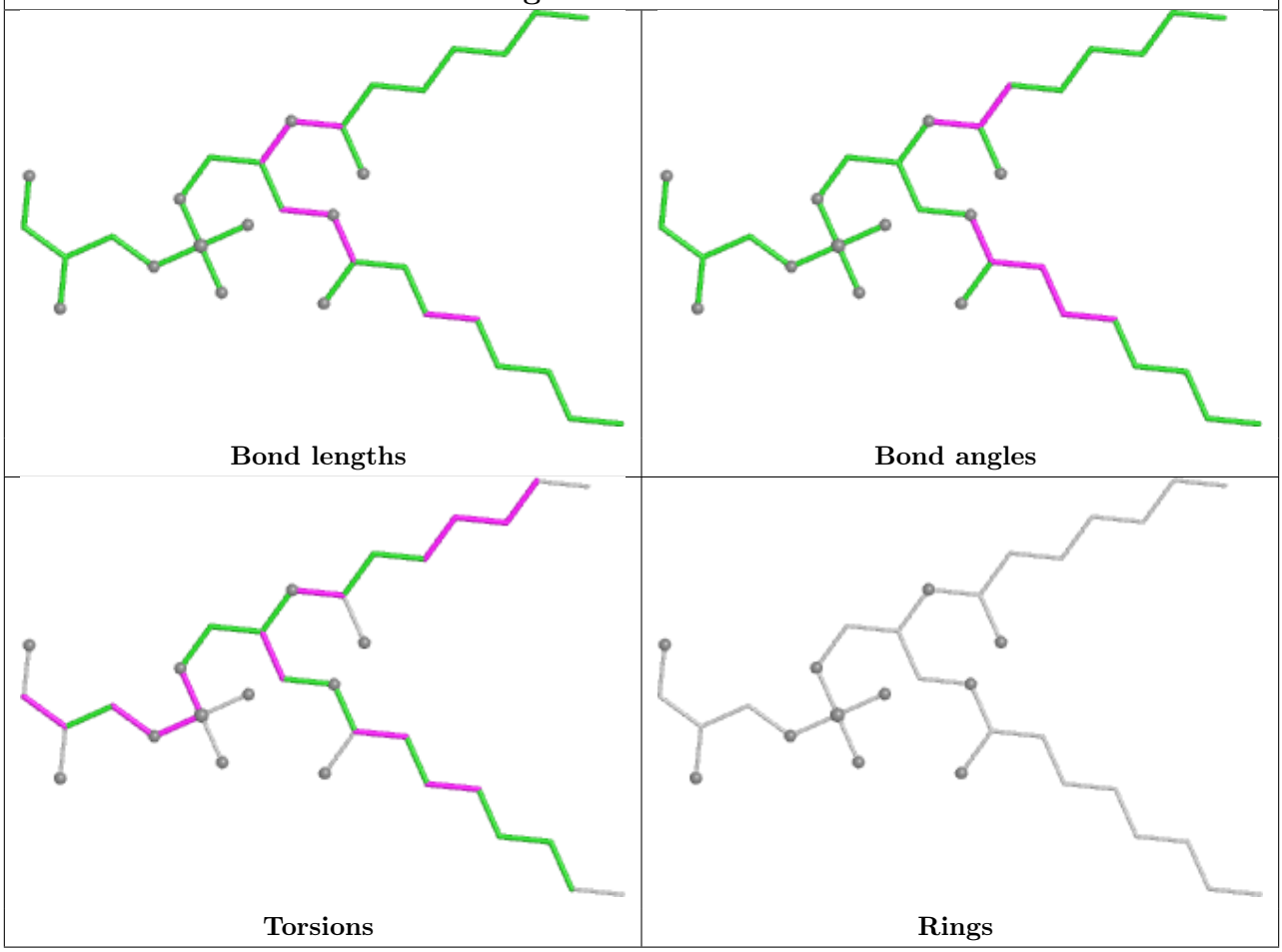


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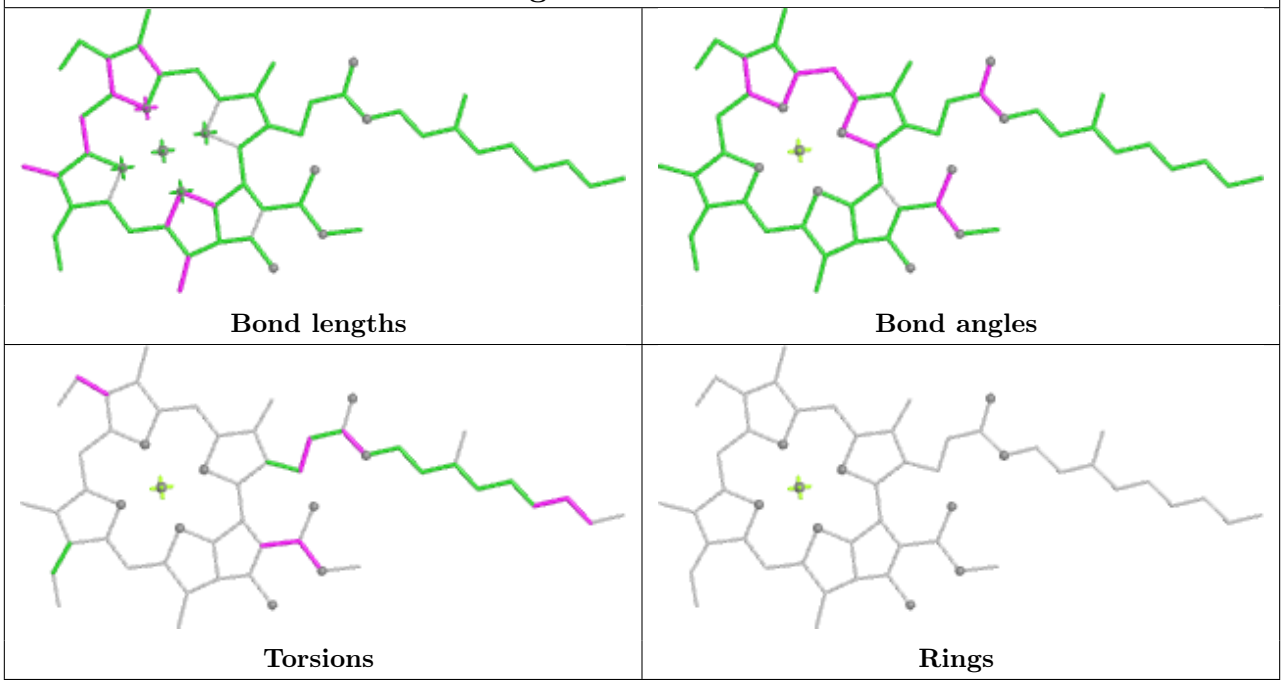


Rings

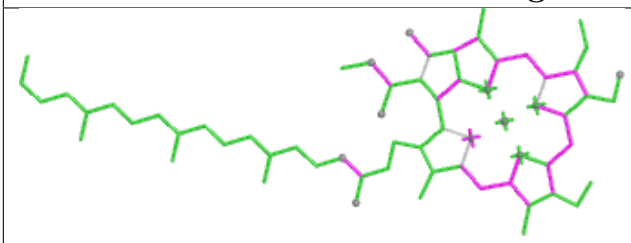
Ligand LHG C 617



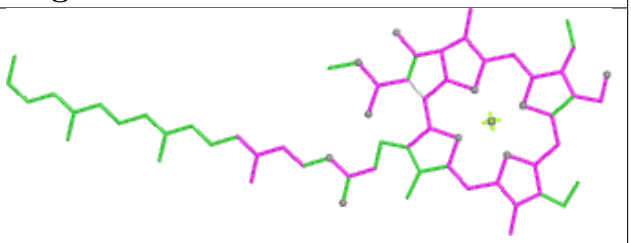
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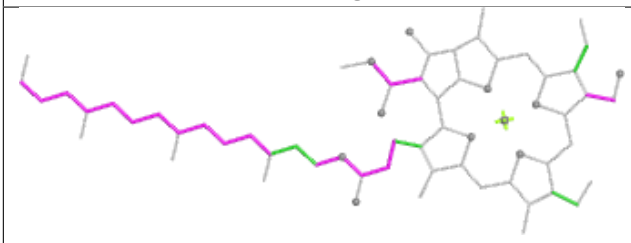
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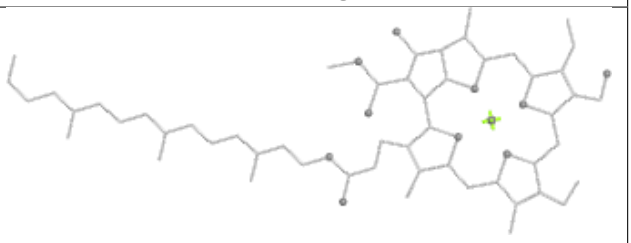
Bond lengths



Bond angles

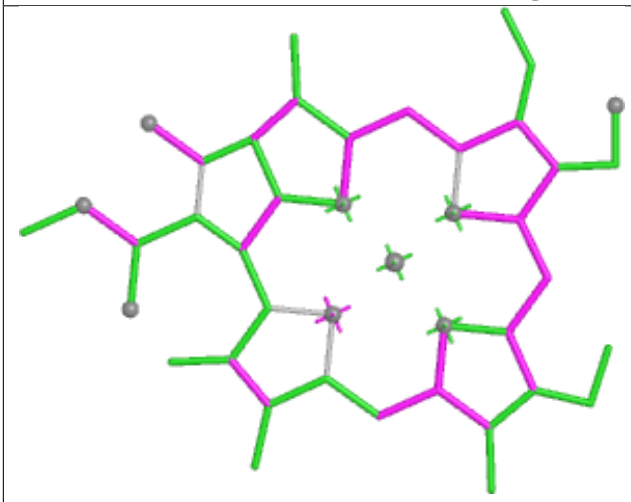


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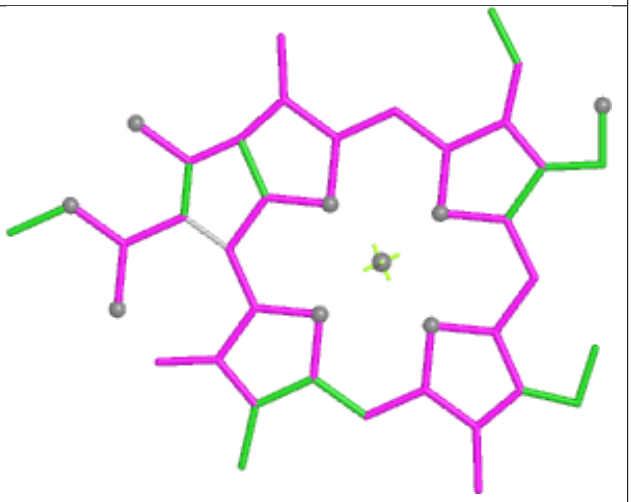


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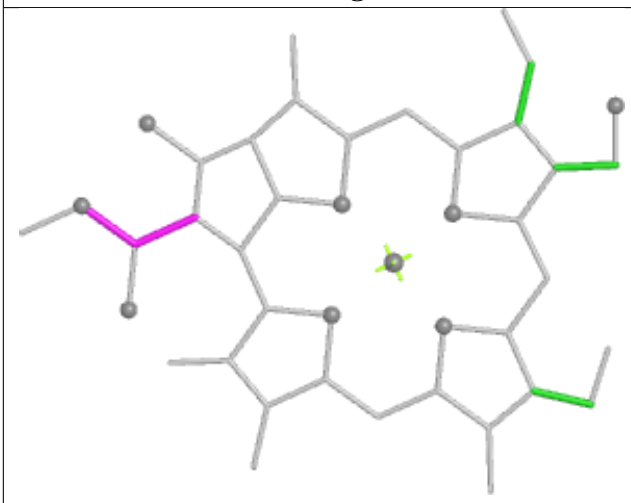
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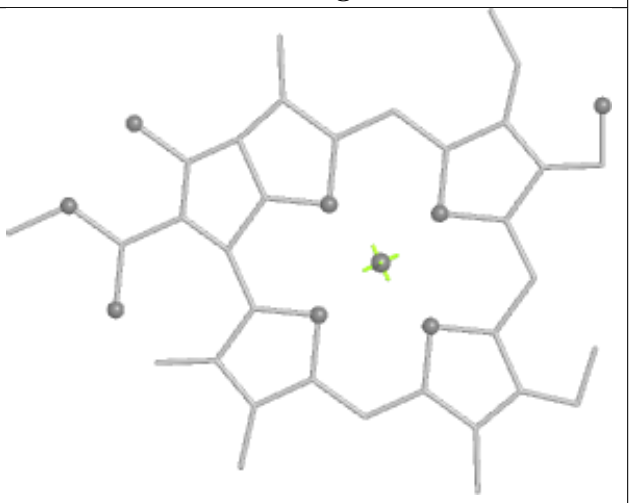
Bond lengths



Bond angles

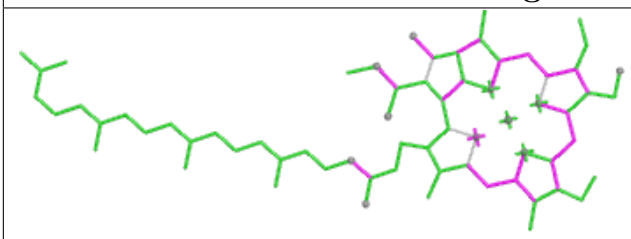


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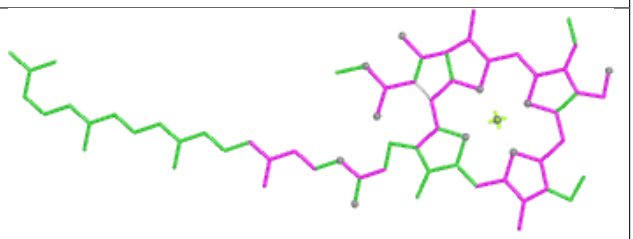


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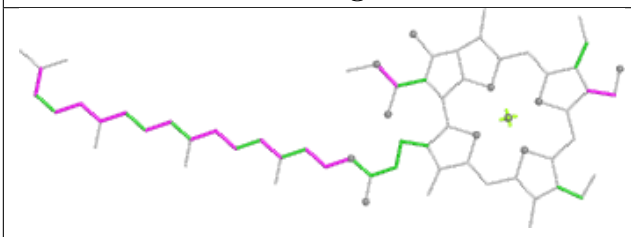
Ligand CHL Y 312



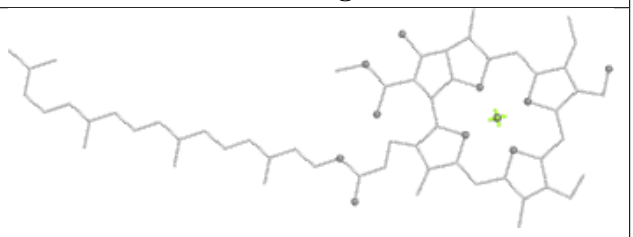
Bond lengths



Bond angles

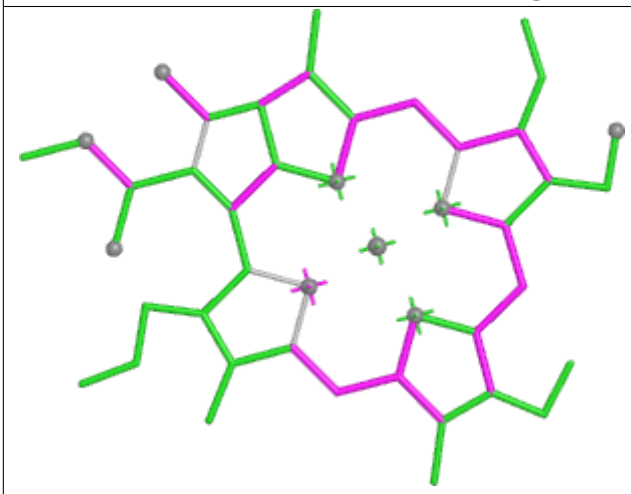


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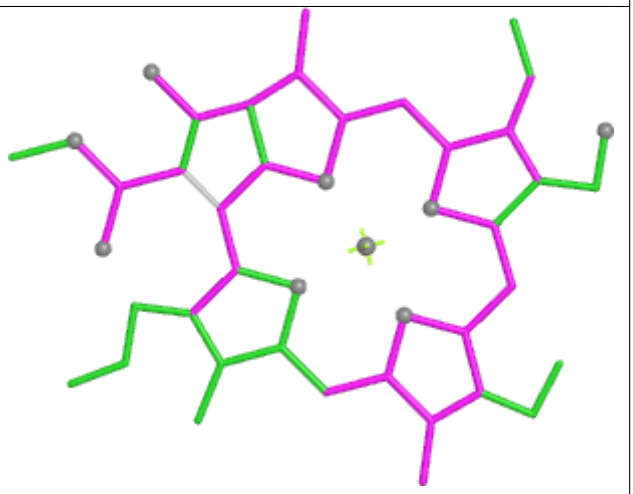


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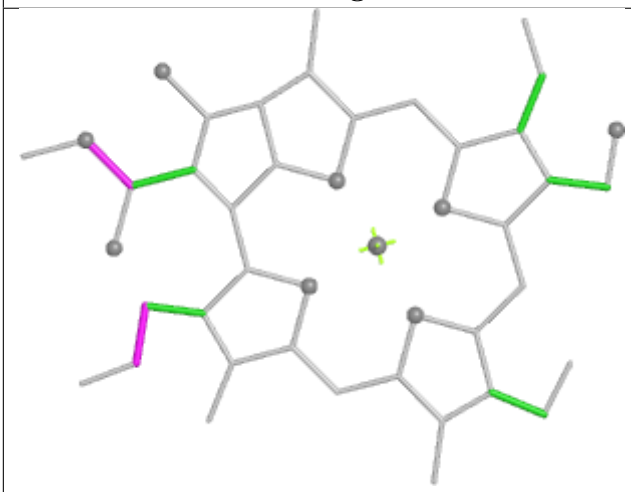
Ligand CHL 1 311



Bond lengths



Bond angles

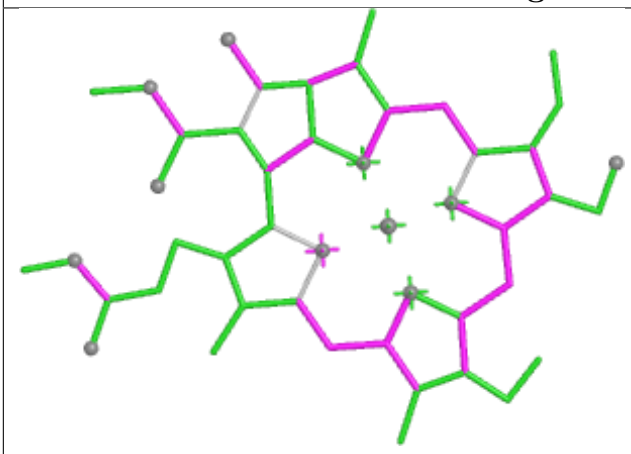


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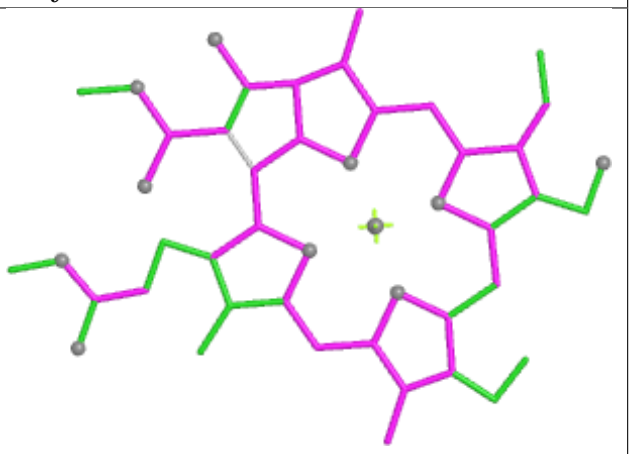


Rings

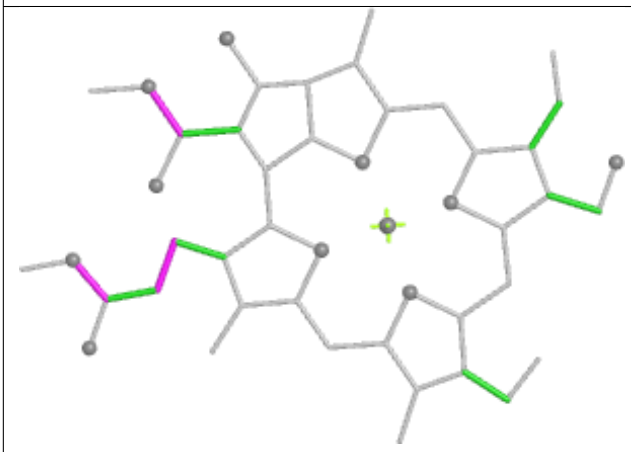
Ligand CHL y 310



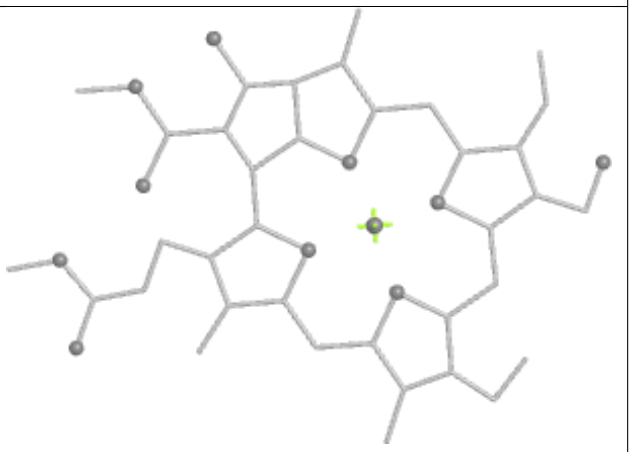
Bond lengths



Bond angles

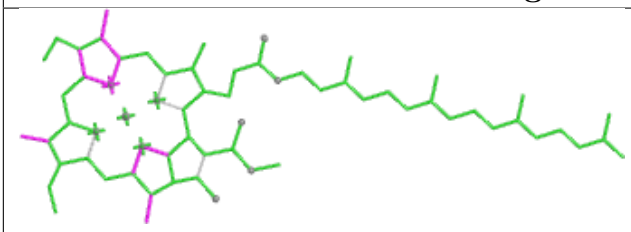


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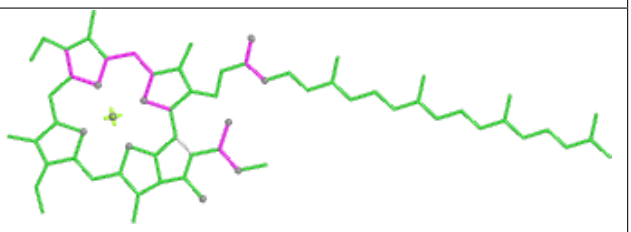


Rings

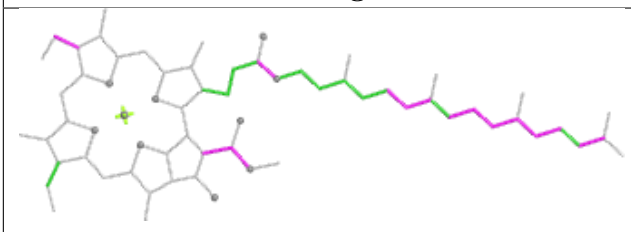
Ligand CLA C 602



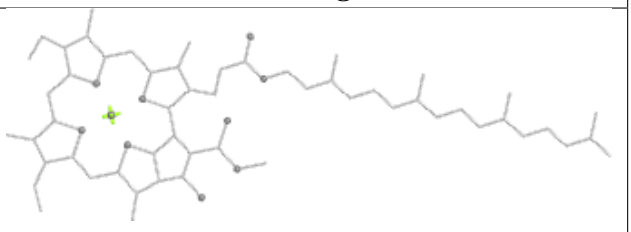
Bond lengths



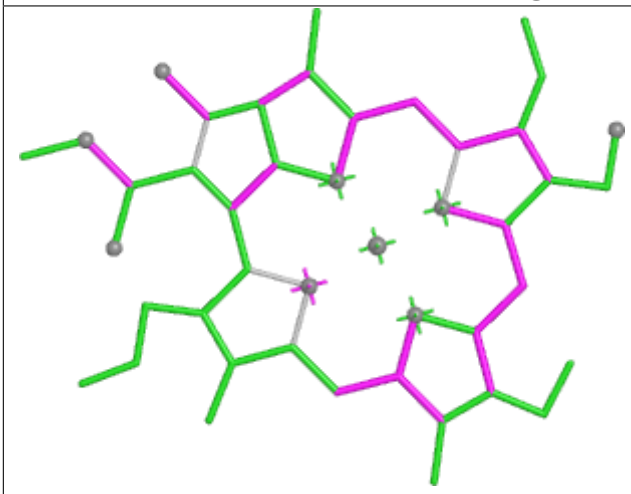
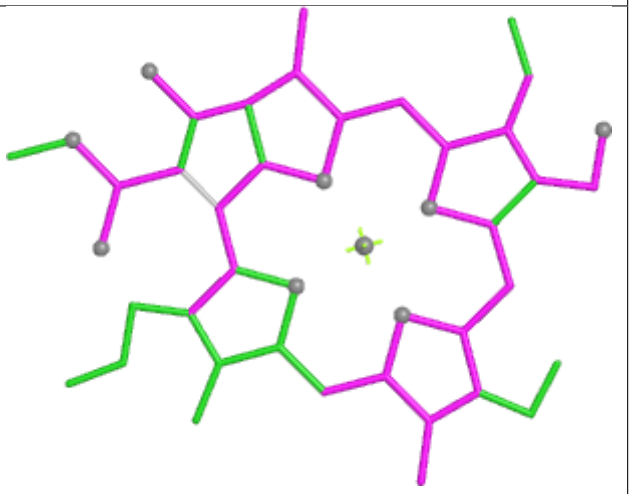
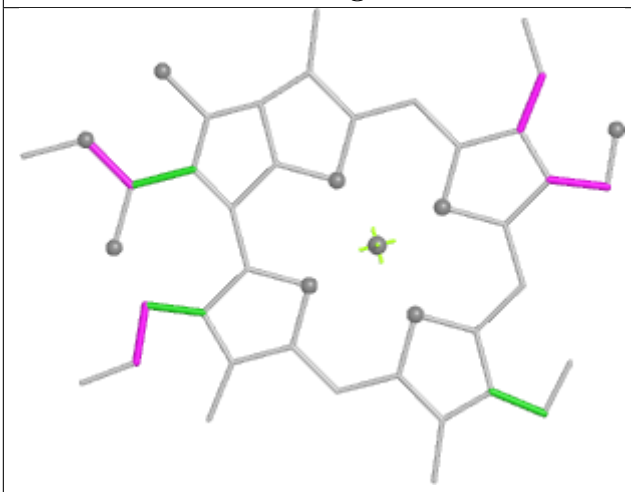
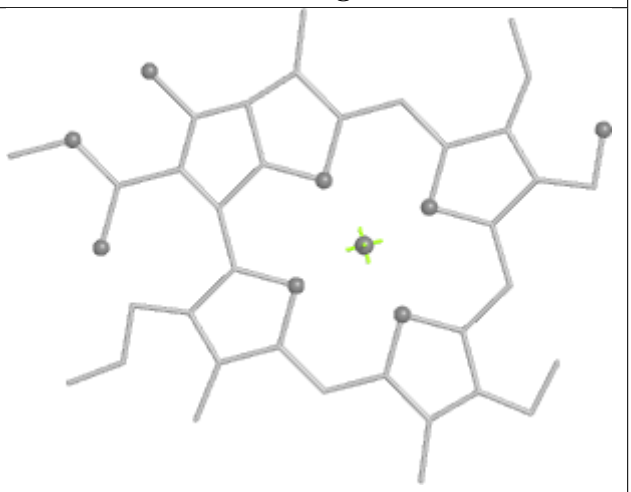
Bond angles

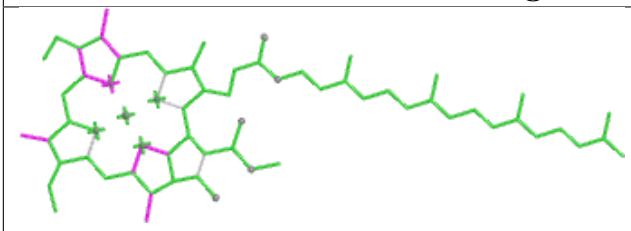
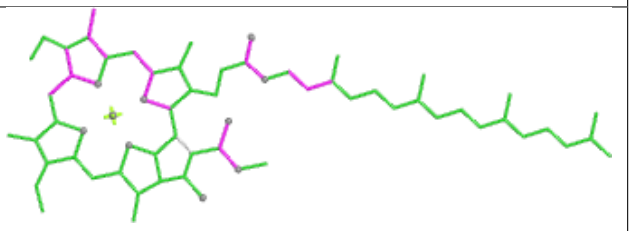
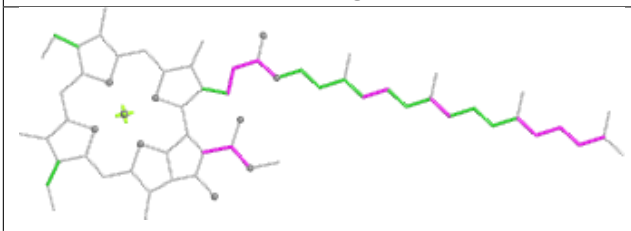
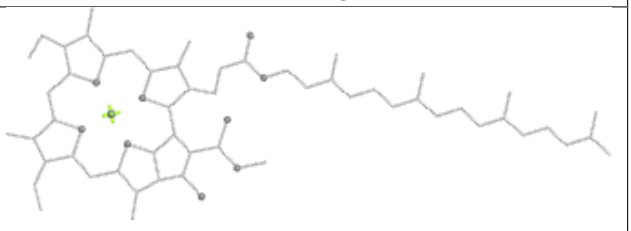


Torsions

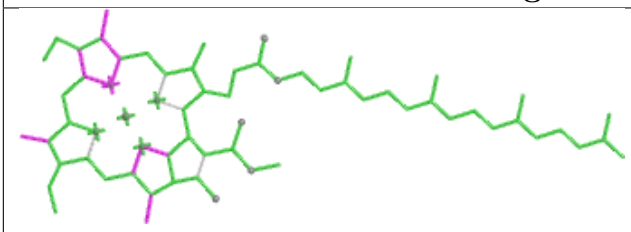


Rings

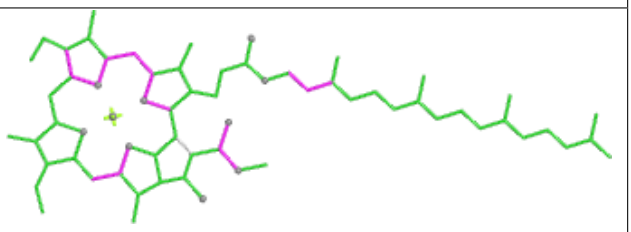
Ligand CHL 5 305	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 606	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

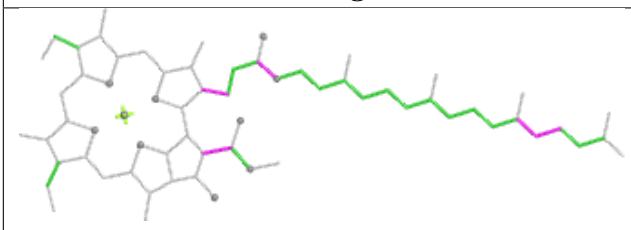
Ligand CLA A 604



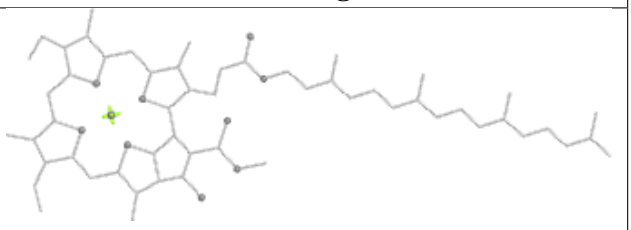
Bond lengths



Bond angles



Torsions



Rings

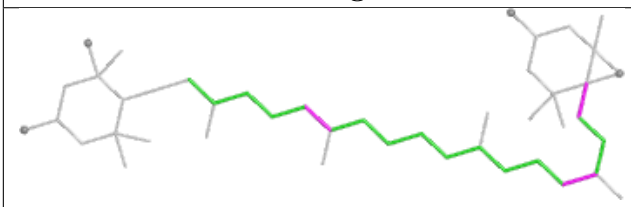
Ligand NEX N 303



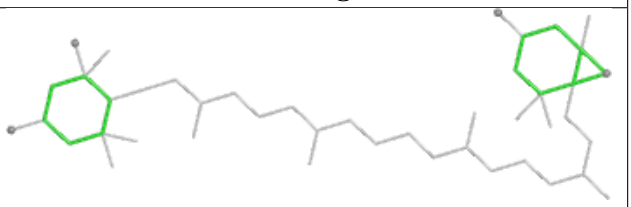
Bond lengths



Bond angles

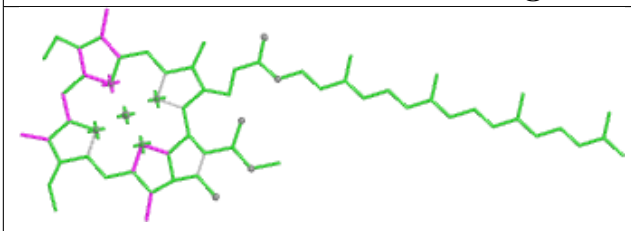


Torsions

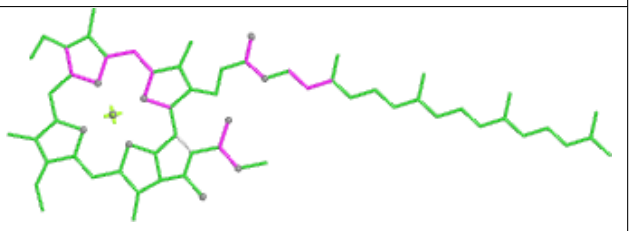


Rings

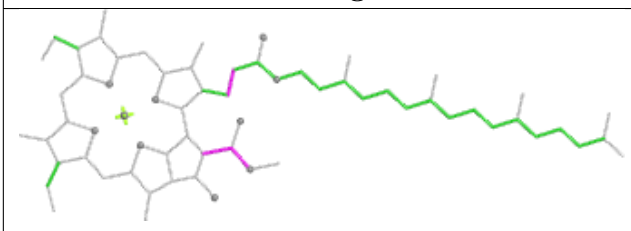
Ligand CLA B 610



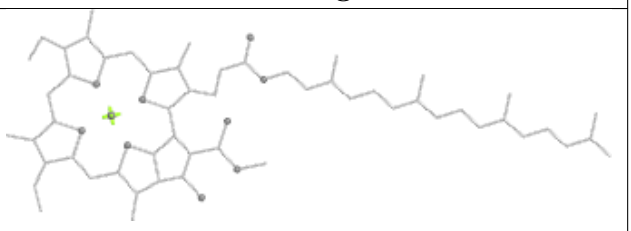
Bond lengths



Bond angles

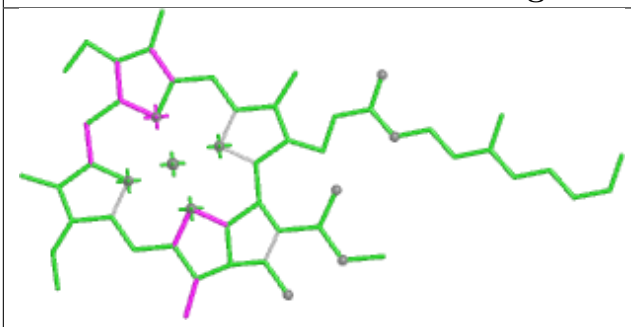


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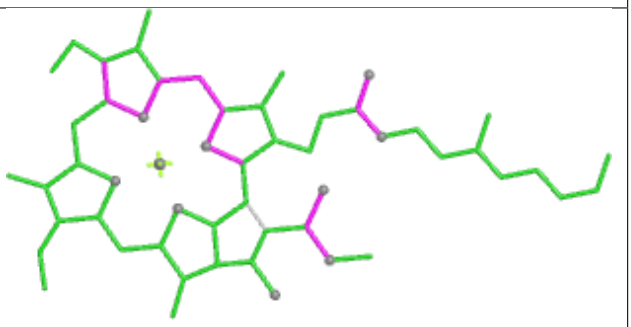


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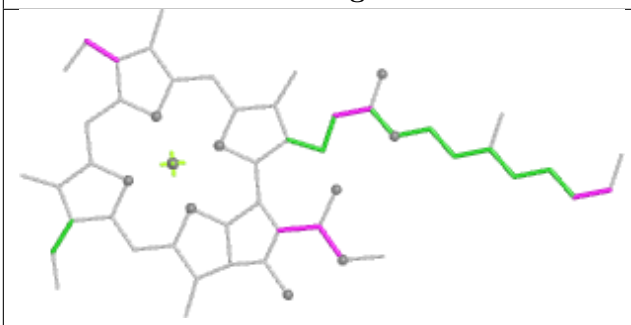
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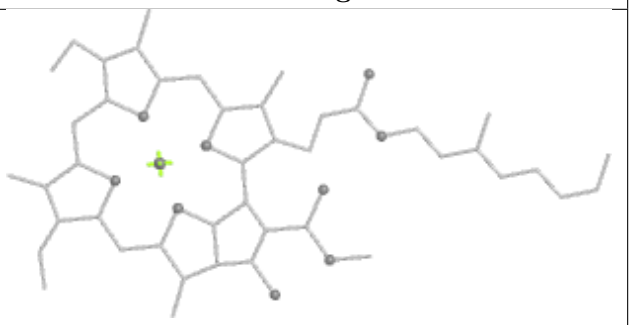
Bond lengths



Bond angles

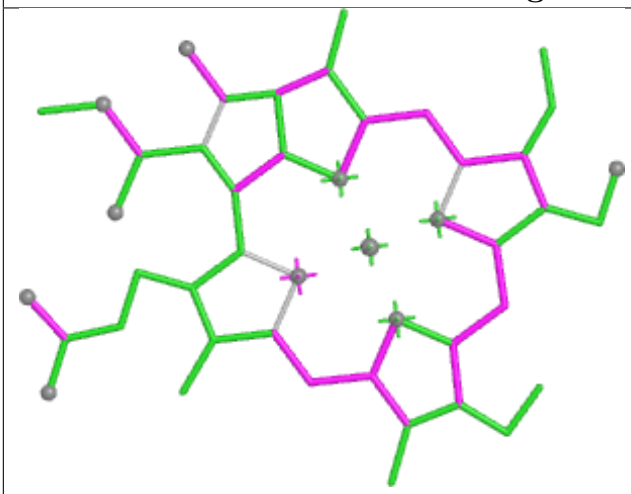


Torsions

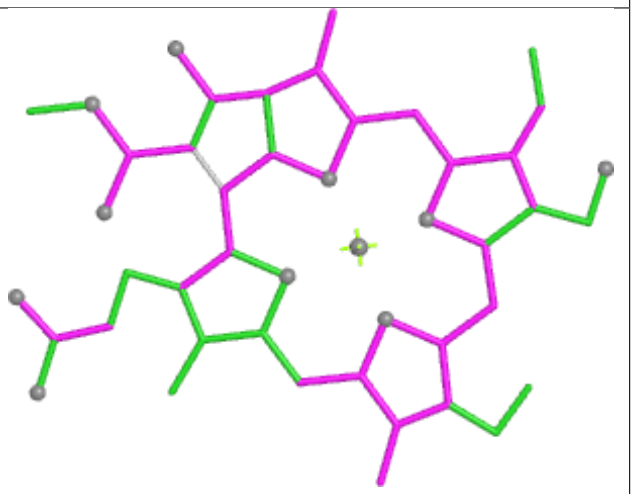


Rings

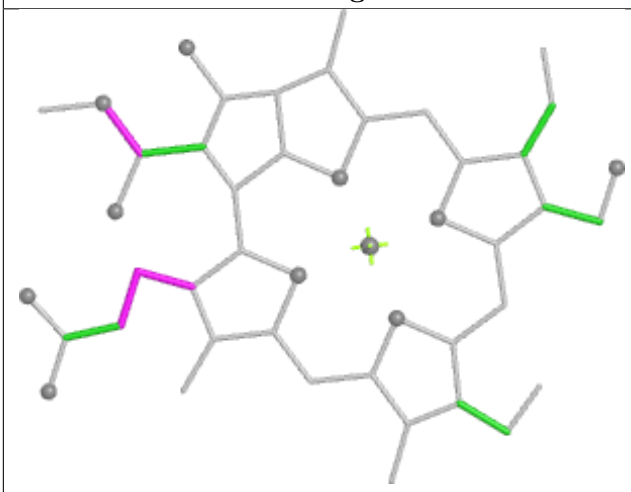
Ligand CHL S 607



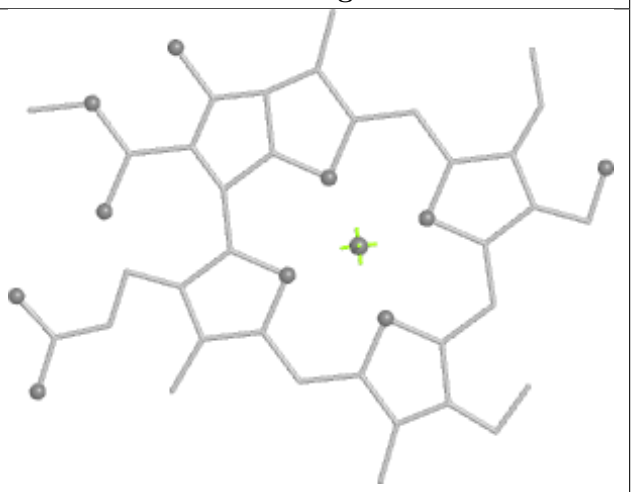
Bond lengths



Bond angles

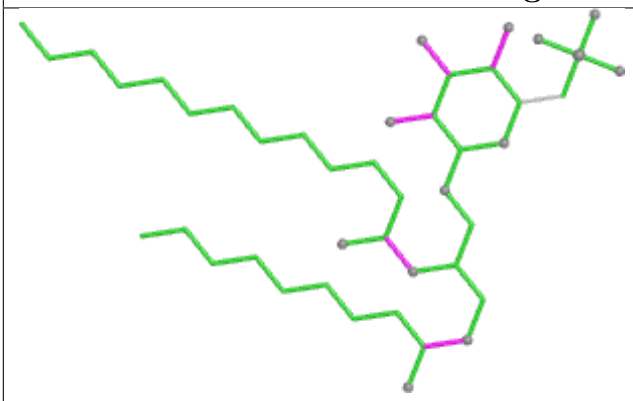


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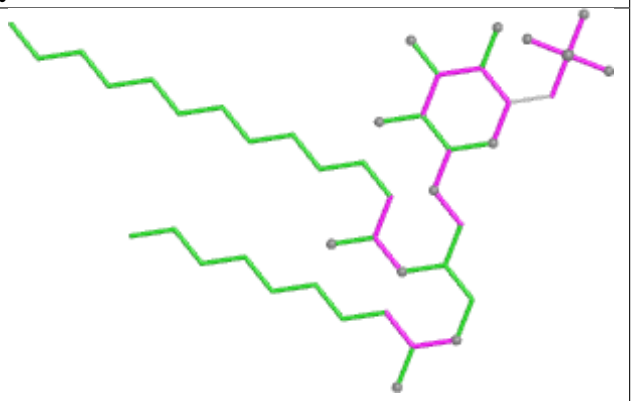


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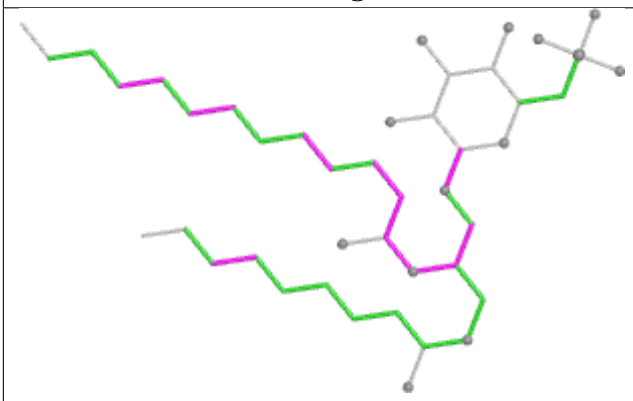
Ligand SQD D 409



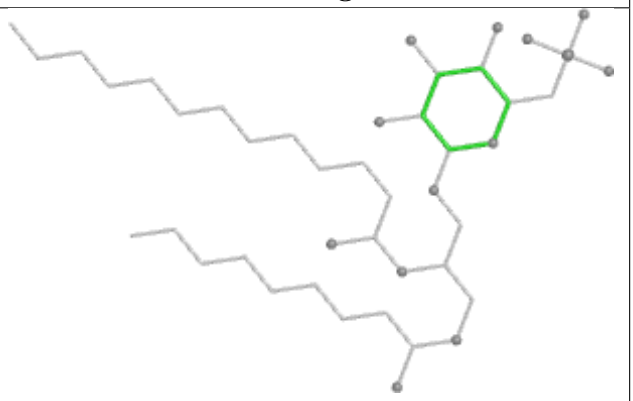
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Bond angles

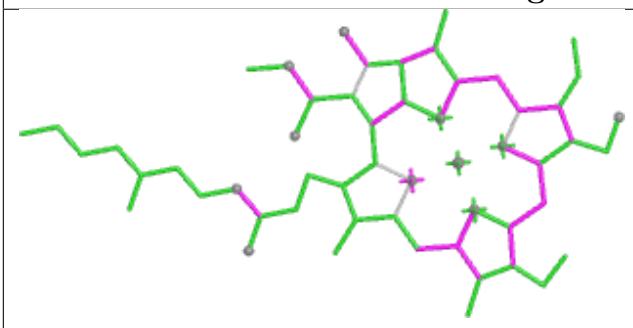


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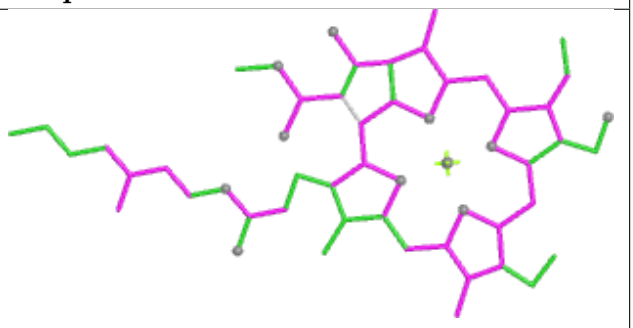


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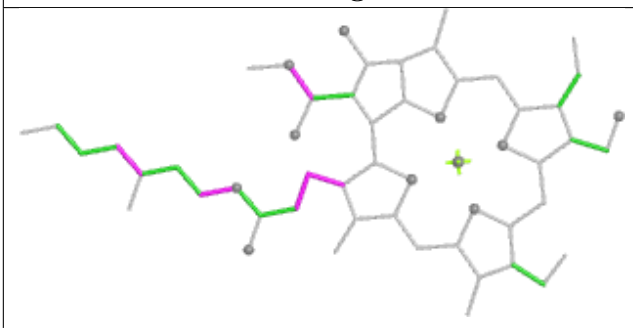
Ligand CHL q 303



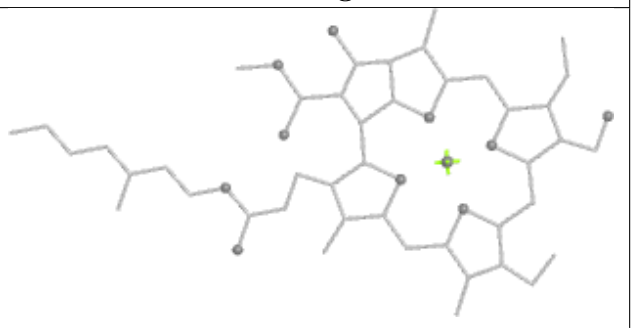
Bond lengths



Bond angles

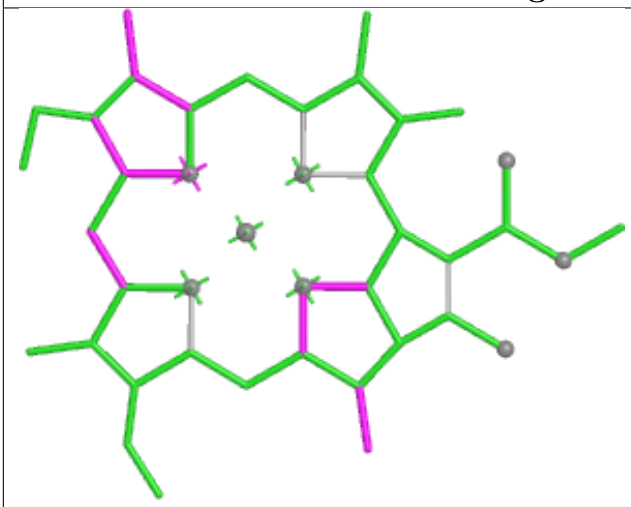


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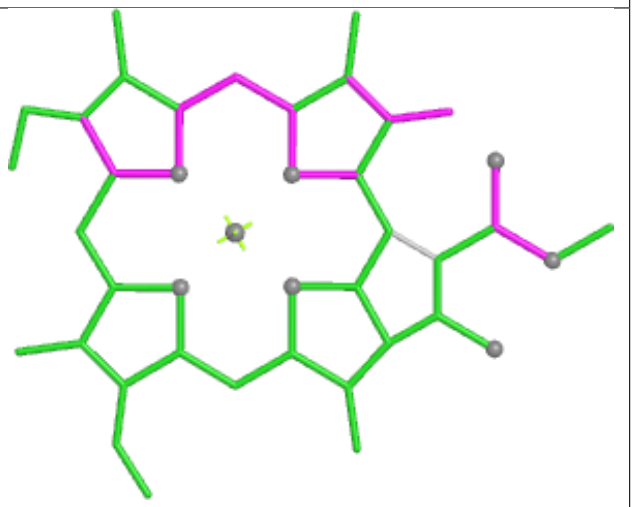


Rings

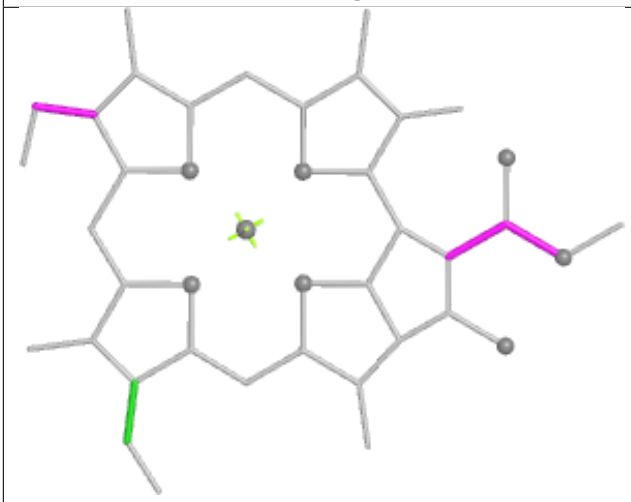
Ligand CLA 6 306



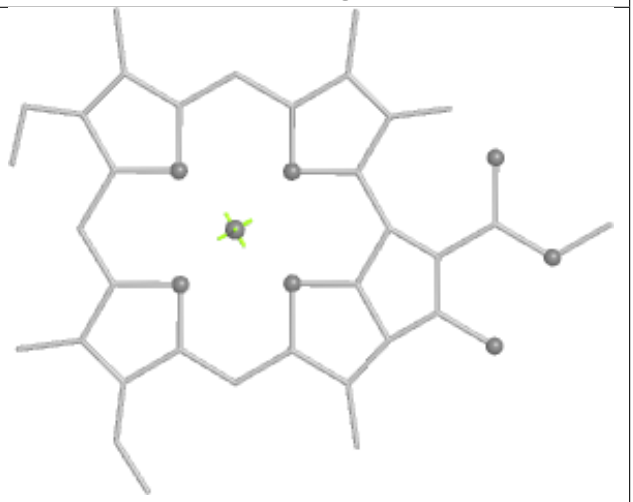
Bond lengths



Bond angles

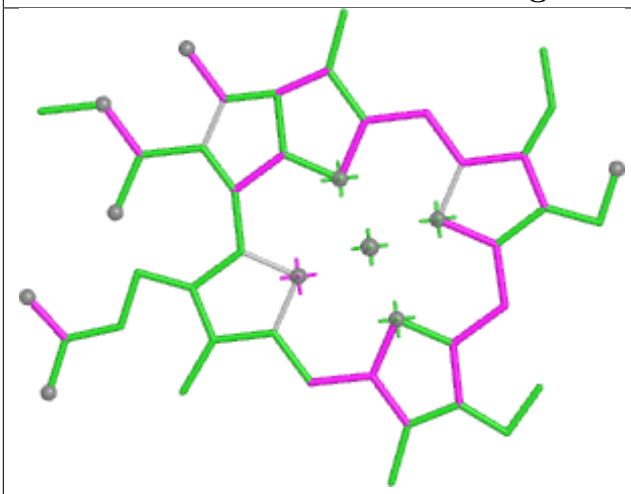


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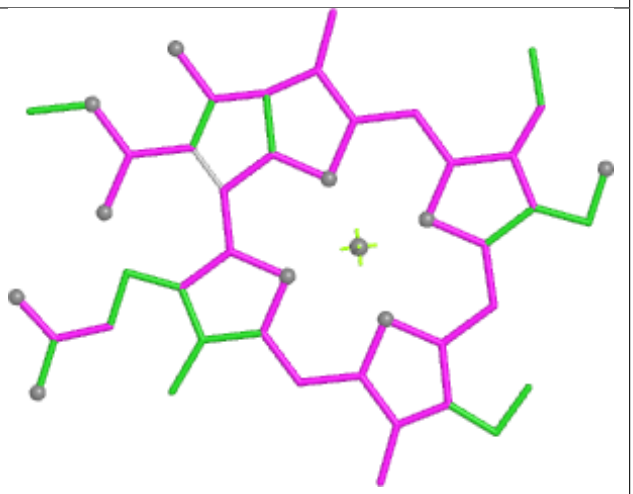


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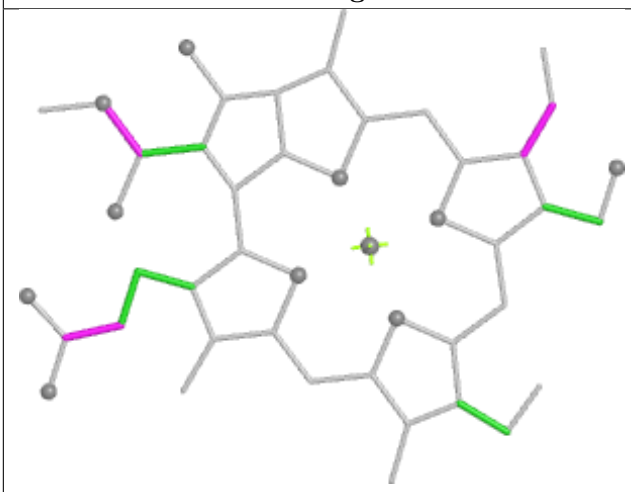
Ligand CHL r 309



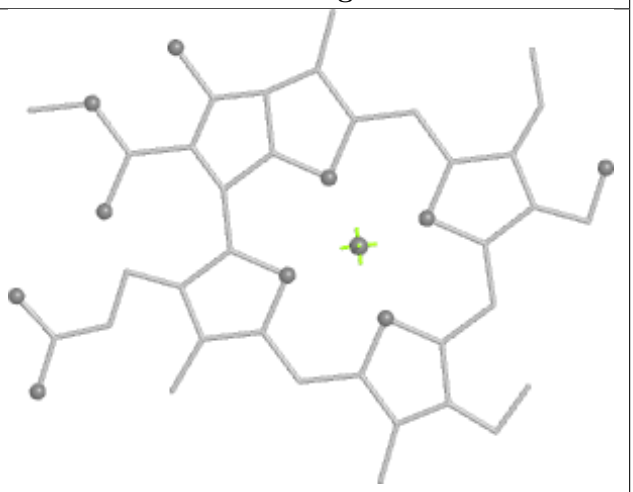
Bond lengths



Bond angles

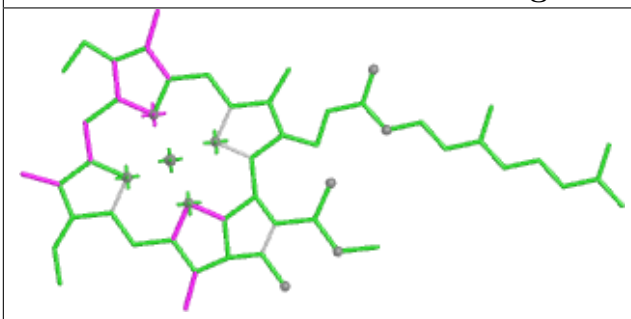


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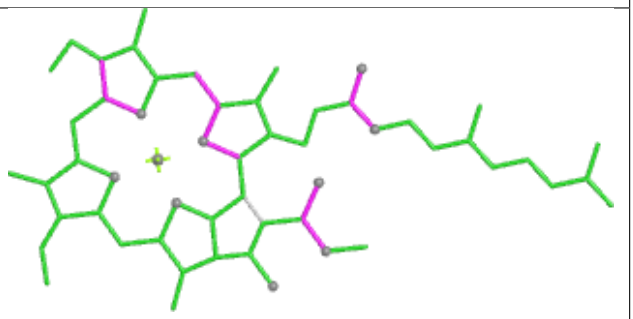


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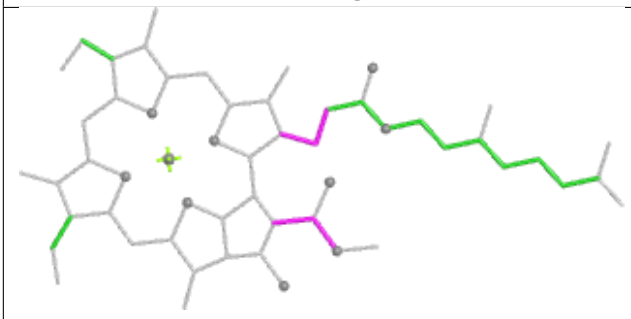
Ligand CLA s 410



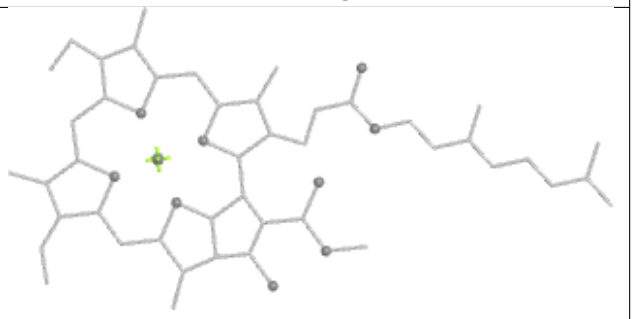
Bond lengths



Bond angles

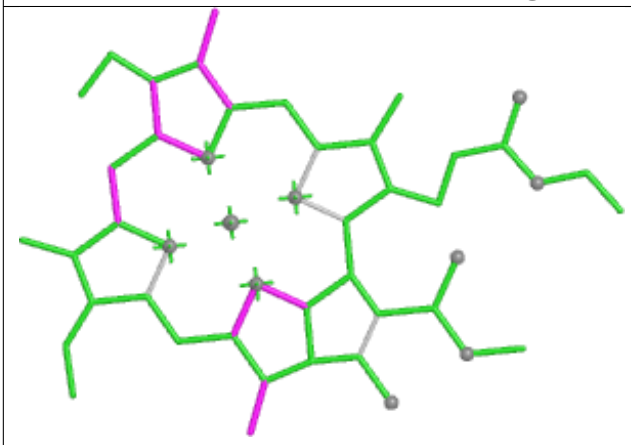


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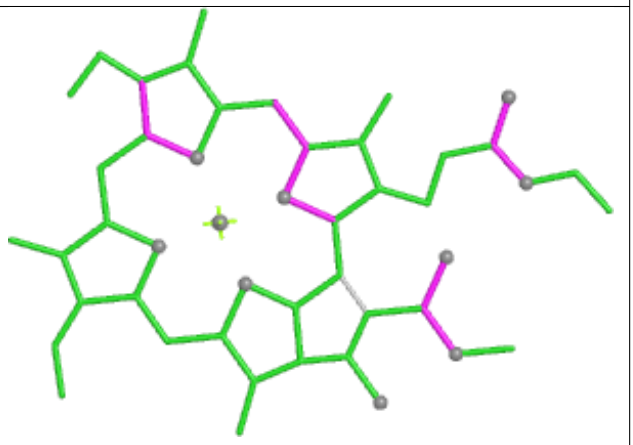


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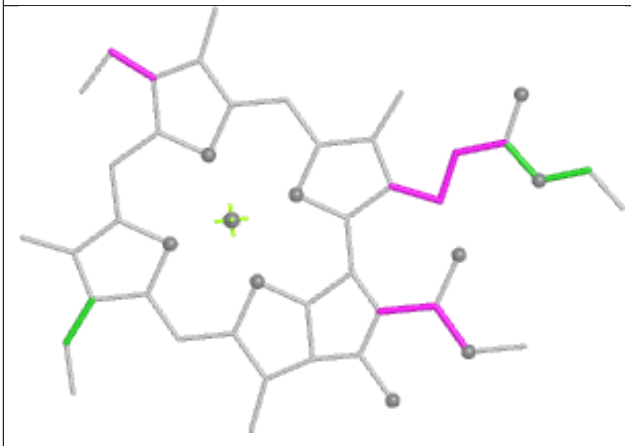
Ligand CLA R 613



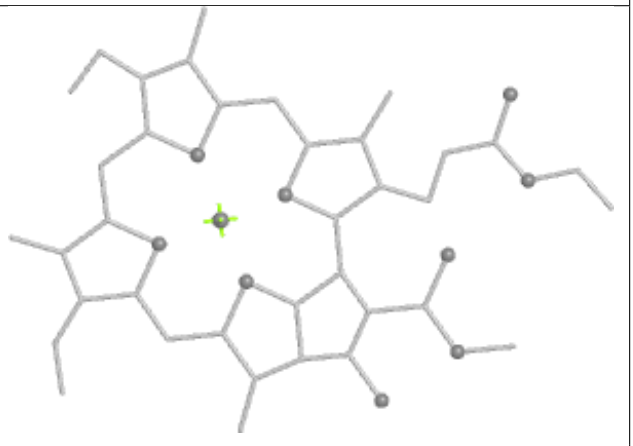
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Bond angles

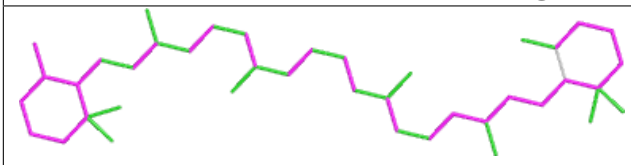


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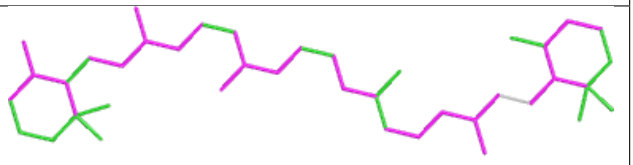


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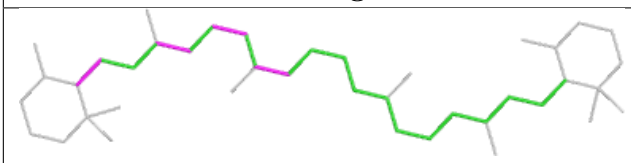
Ligand 8CT s 415



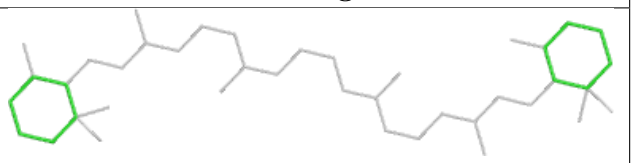
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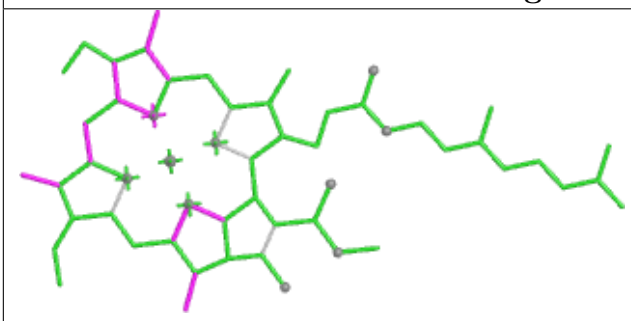


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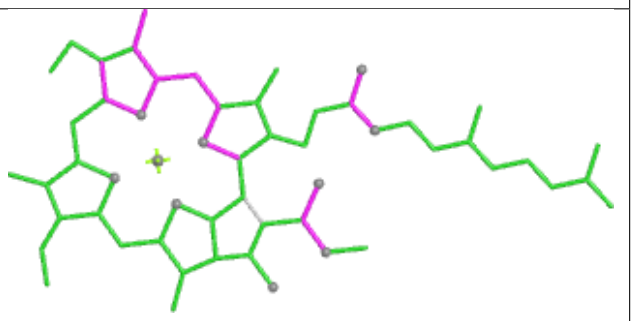


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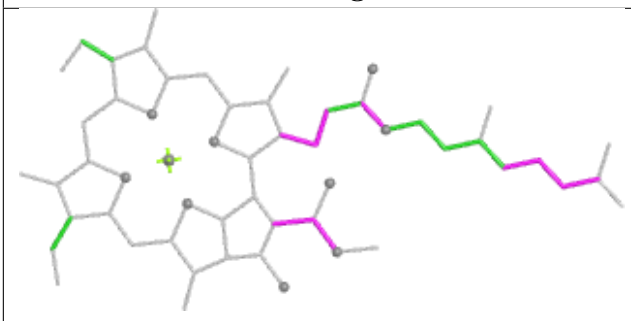
Ligand CLA B 608



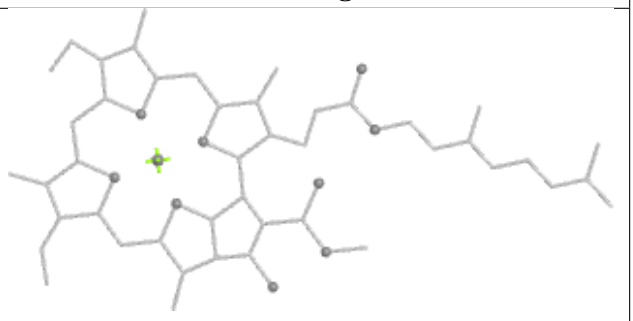
Bond lengths



Bond angles

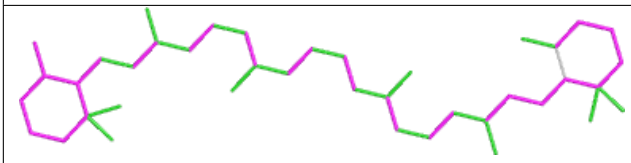


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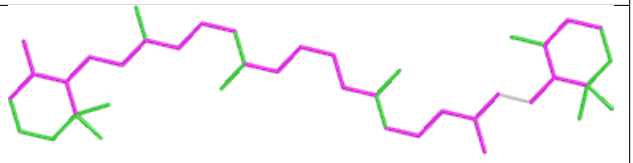


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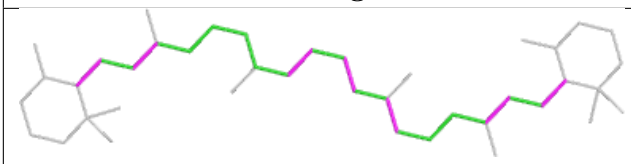
Ligand 8CT V 401



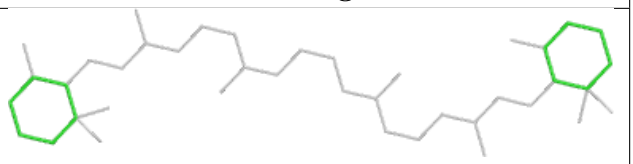
Bond lengths



Bond angles

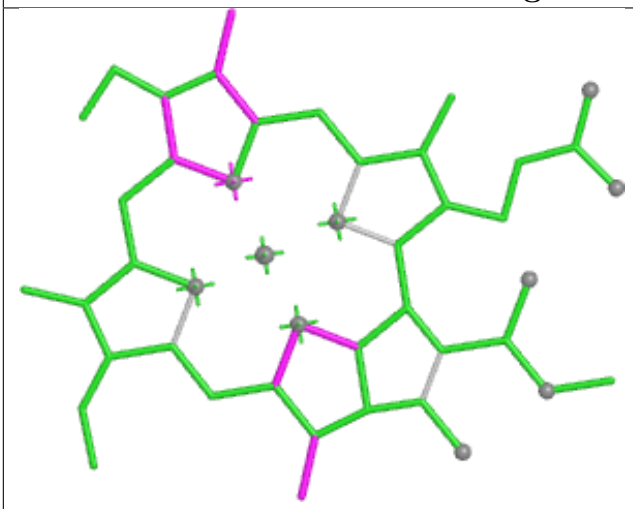


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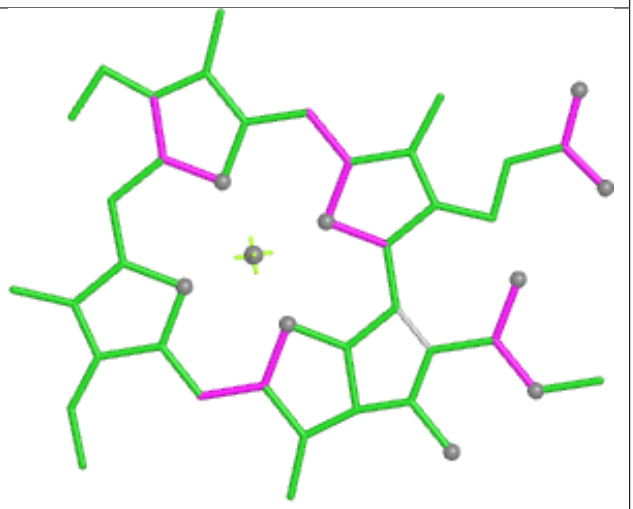


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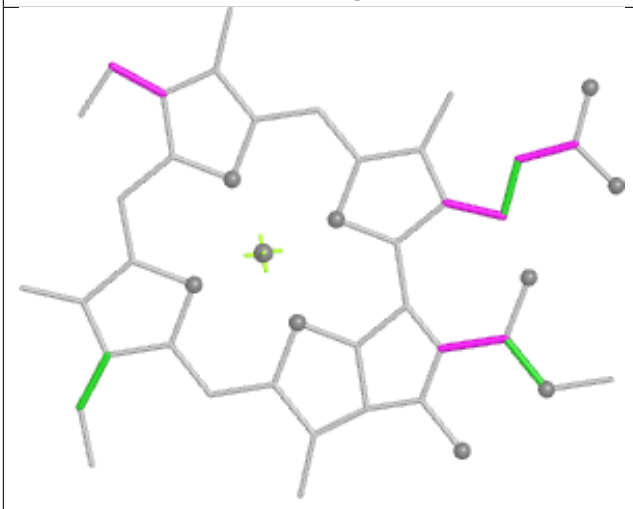
Ligand CLA R 612



Bond lengths



Bond angles

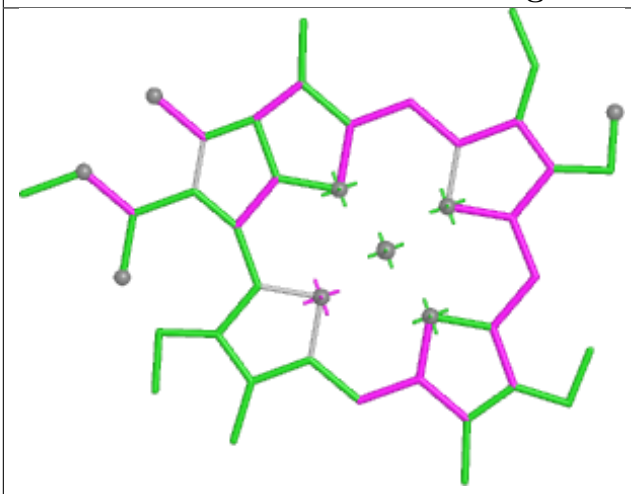


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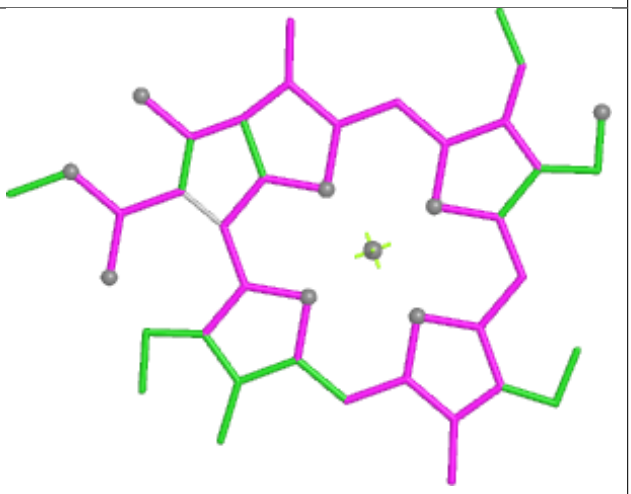


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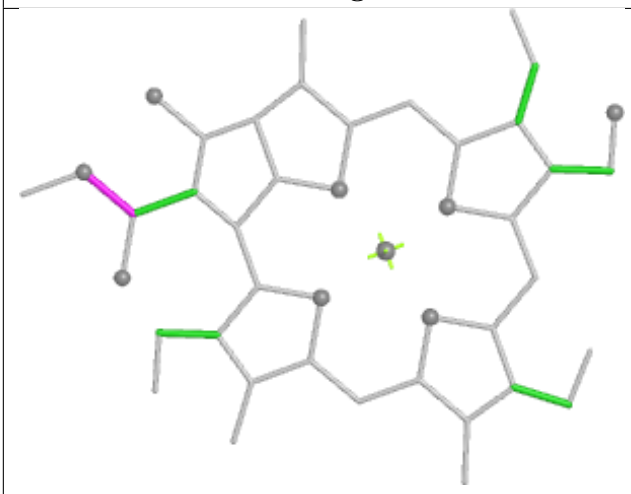
Ligand CHL u 309



Bond lengths



Bond angles



Torsions



Rings

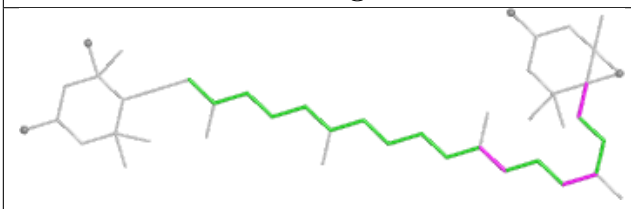
Ligand NEX p 304



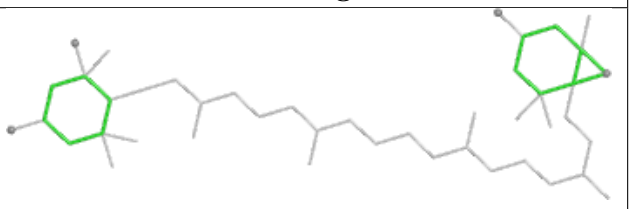
Bond lengths



Bond angles

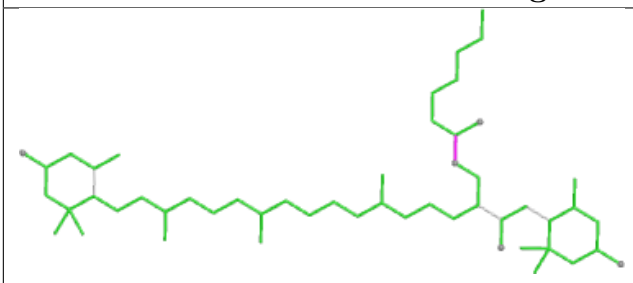


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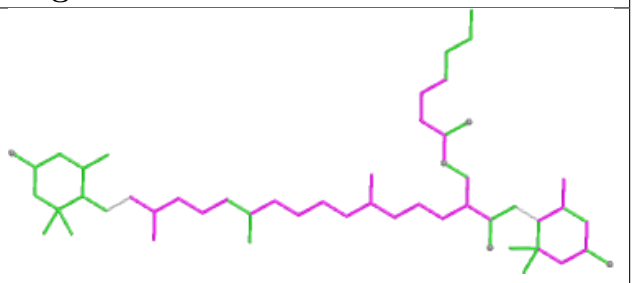


Rings

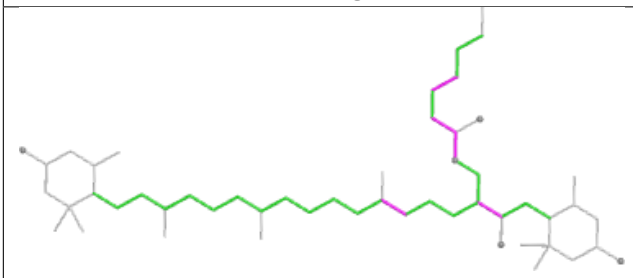
Ligand 0UR g 301



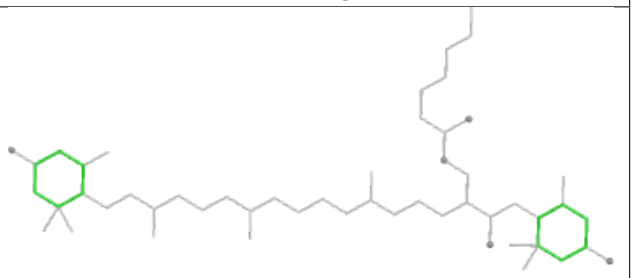
Bond lengths



Bond angles

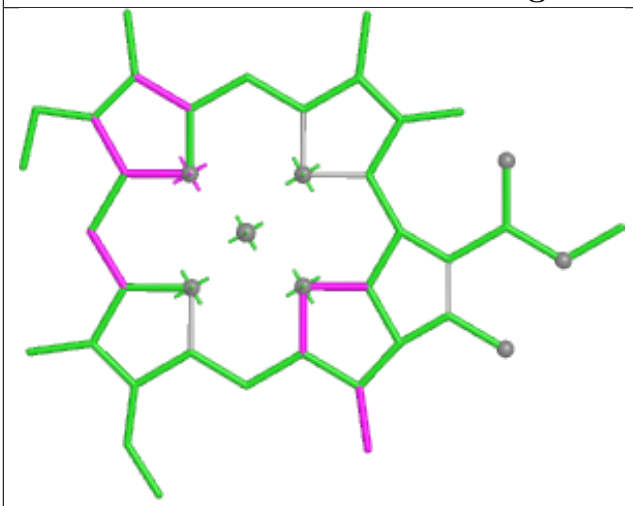


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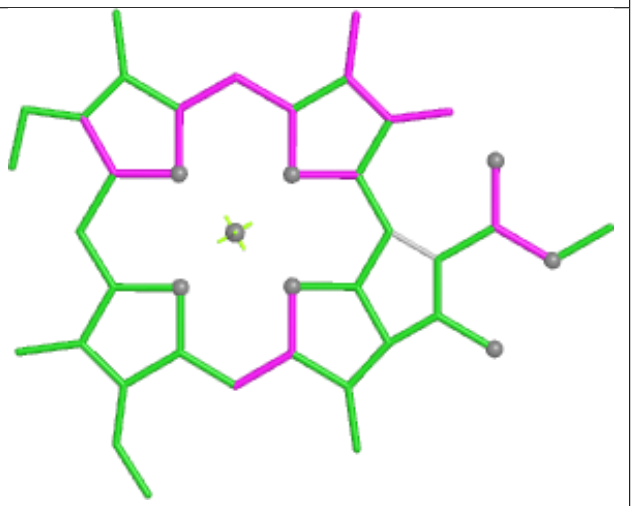


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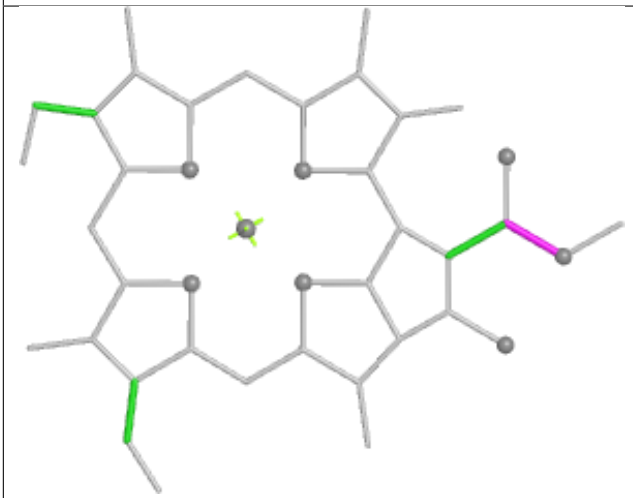
Ligand CLA 3 313



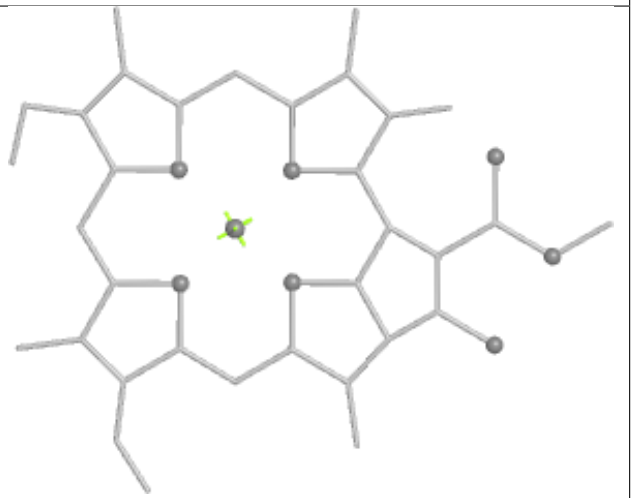
Bond lengths



Bond angles

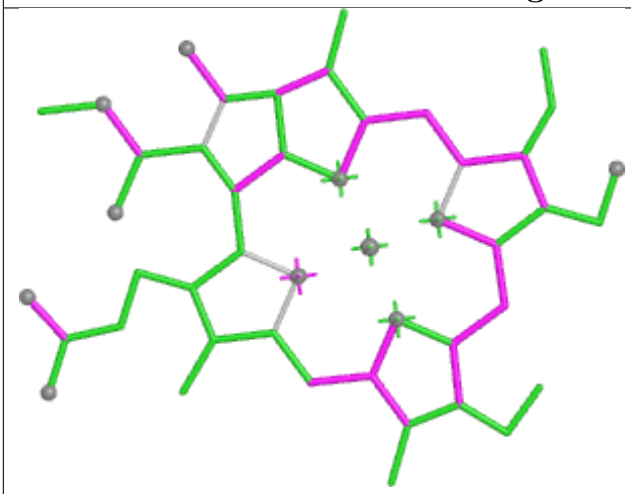


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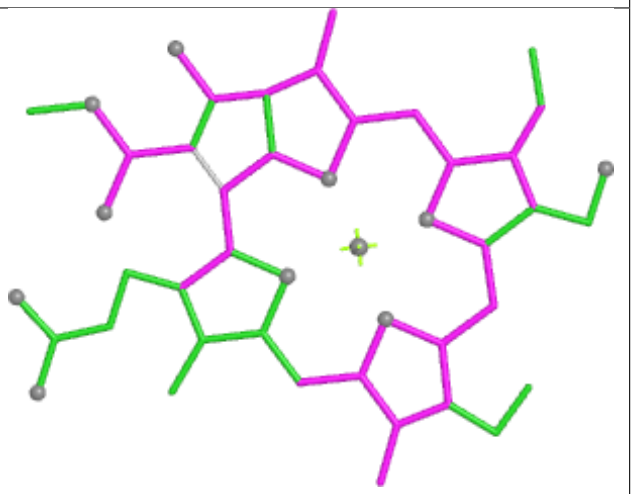


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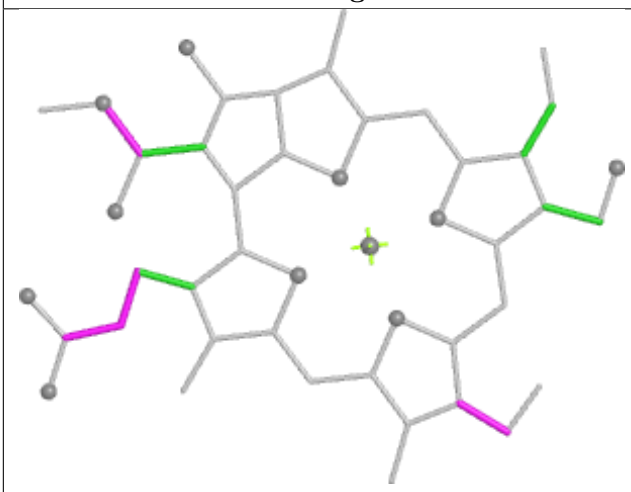
Ligand CHL S 605



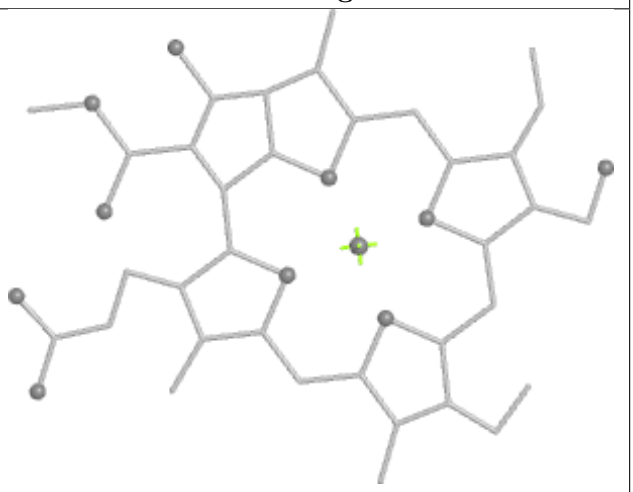
Bond lengths



Bond angles

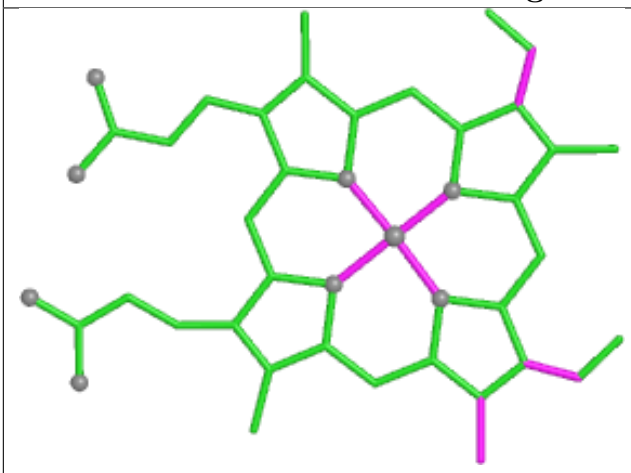


Torsions

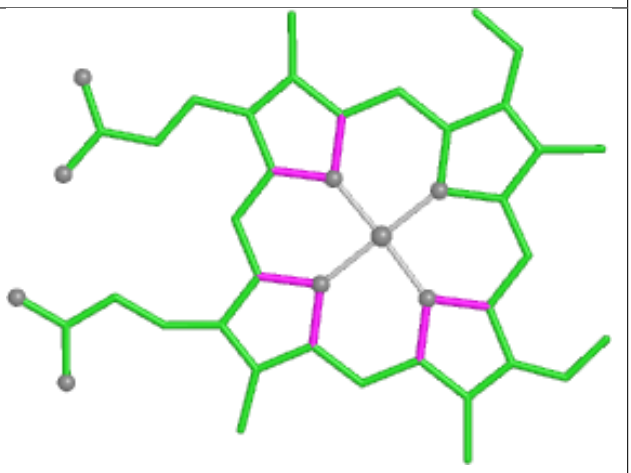


Rings

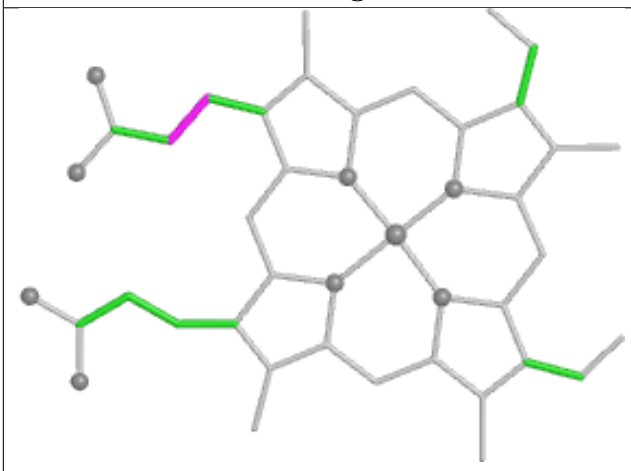
Ligand HEM f 201



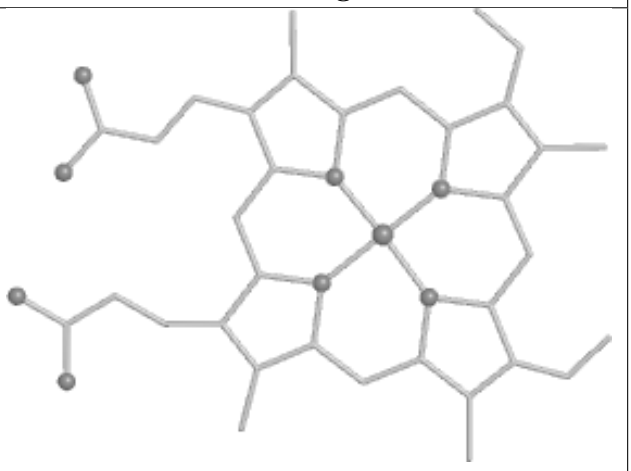
Bond lengths



Bond angles

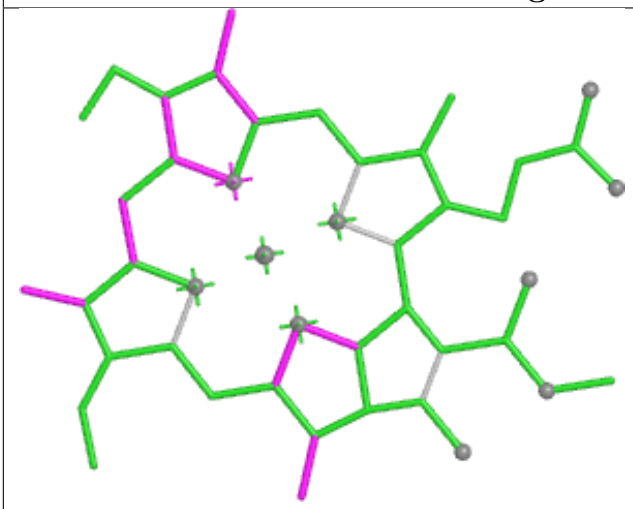


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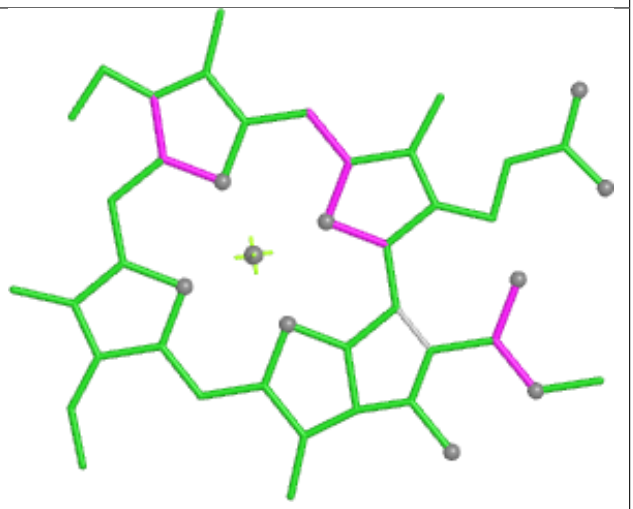


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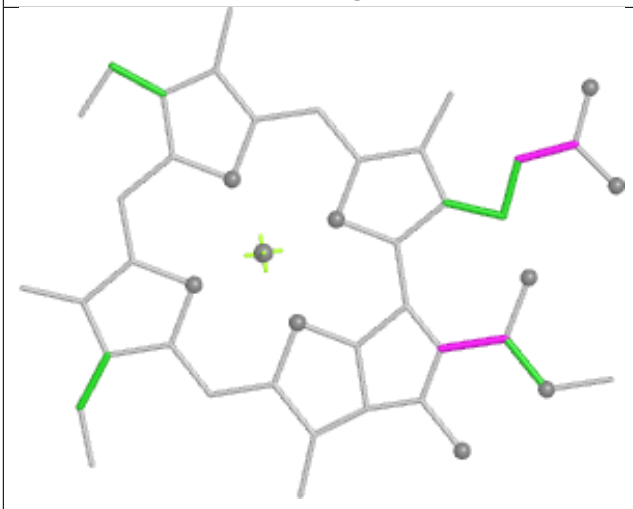
Ligand CLA 2 316



Bond lengths



Bond angles

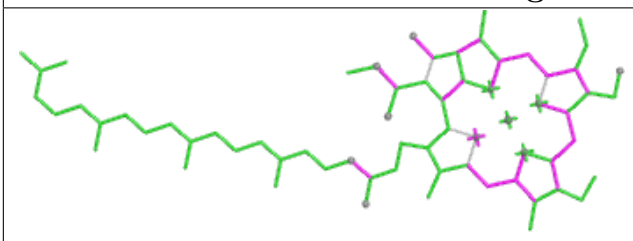


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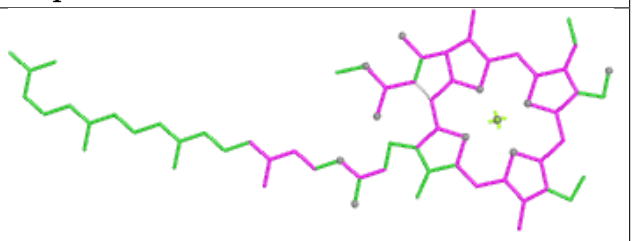


Rings

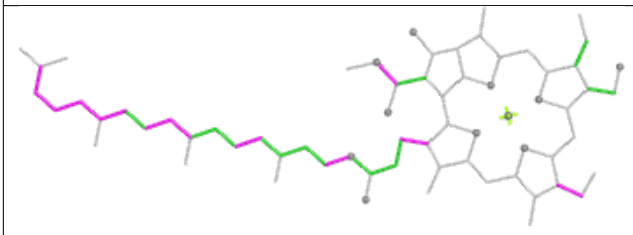
Ligand CHL p 305



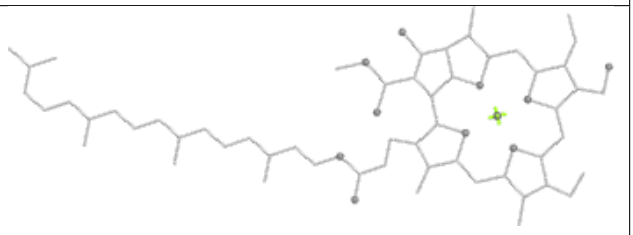
Bond lengths



Bond angles

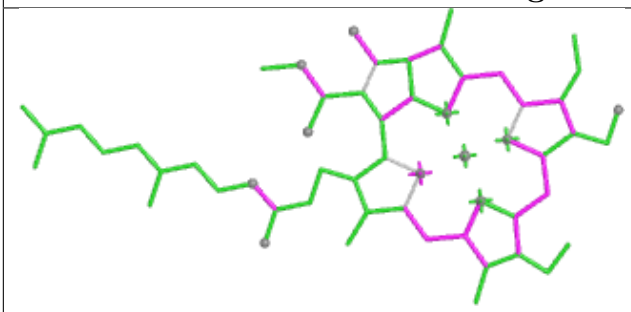


Torsions

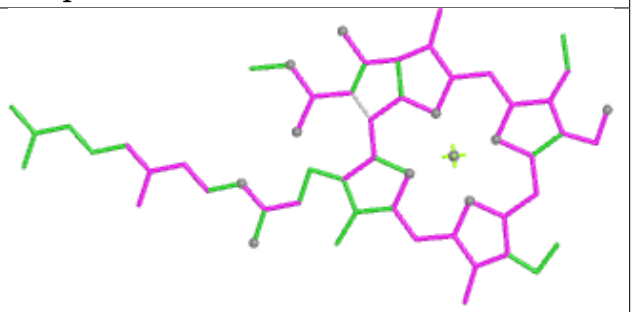


Rings

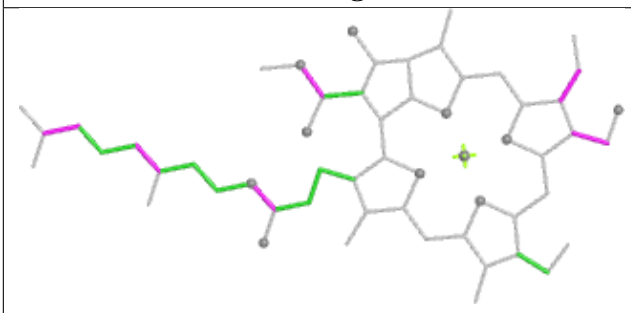
Ligand CHL q 311



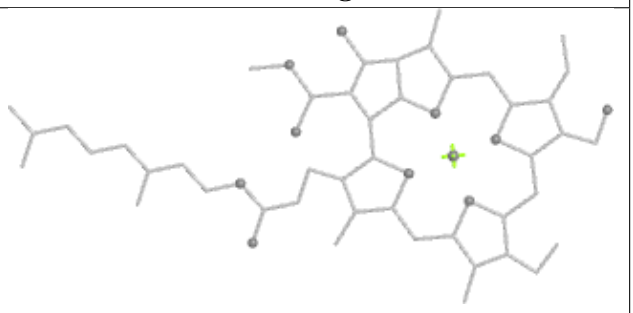
Bond lengths



Bond angles

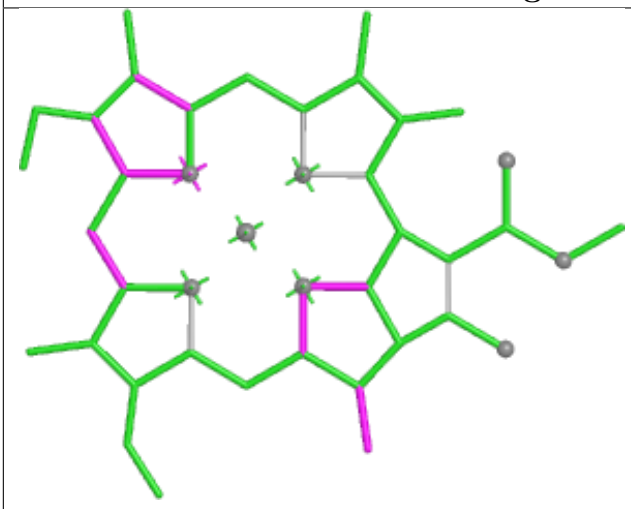


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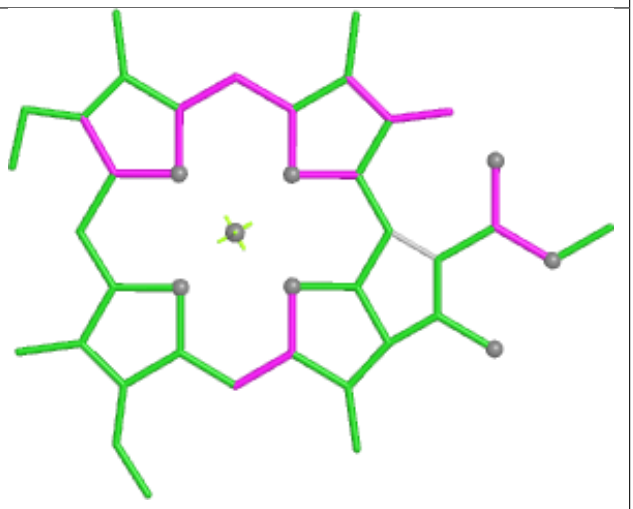


Rings

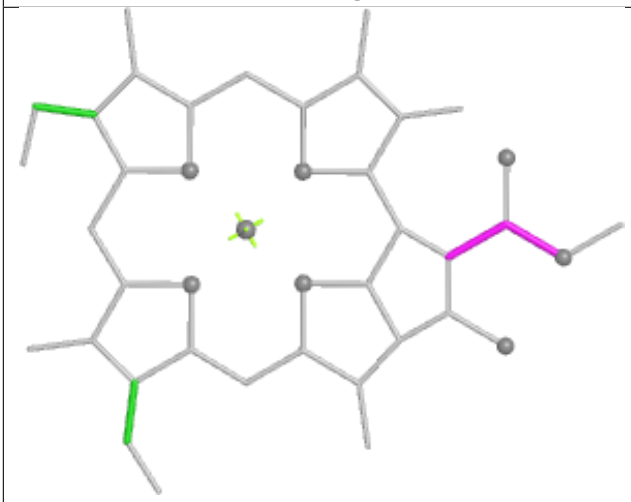
Ligand CLA A 610



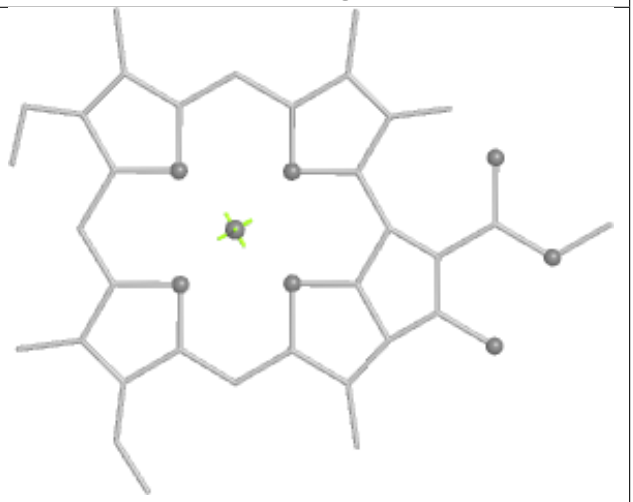
Bond lengths



Bond angles

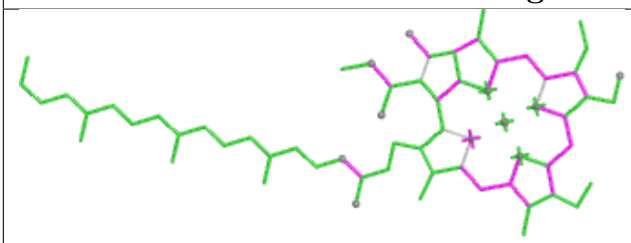


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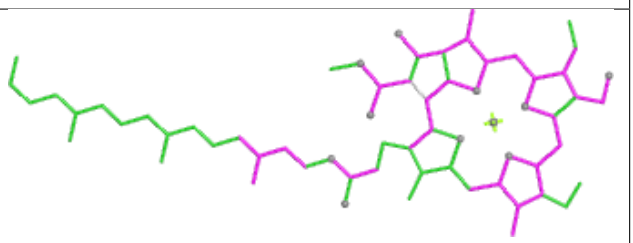


Rings

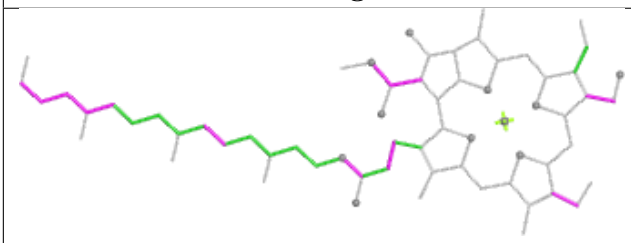
Ligand CHL u 306



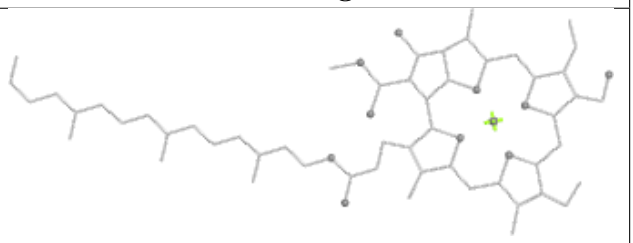
Bond lengths



Bond angles

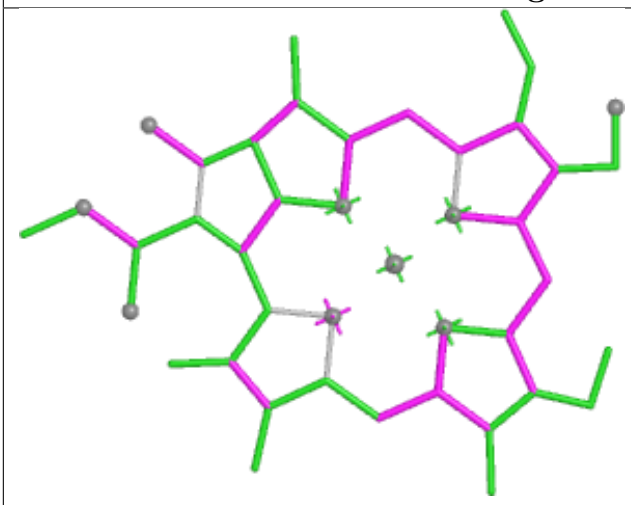


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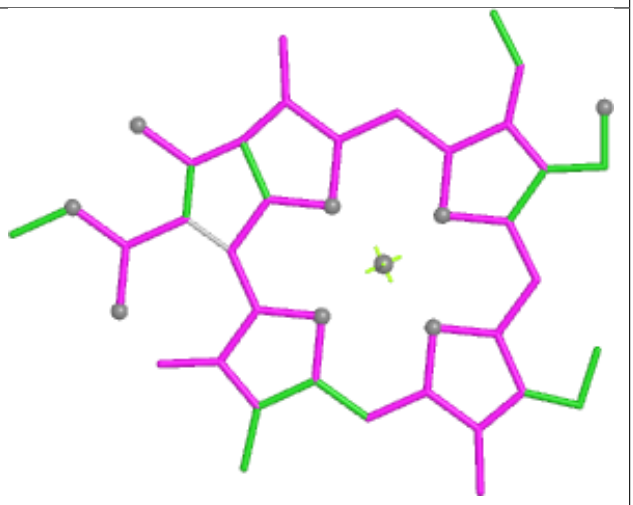


Rings

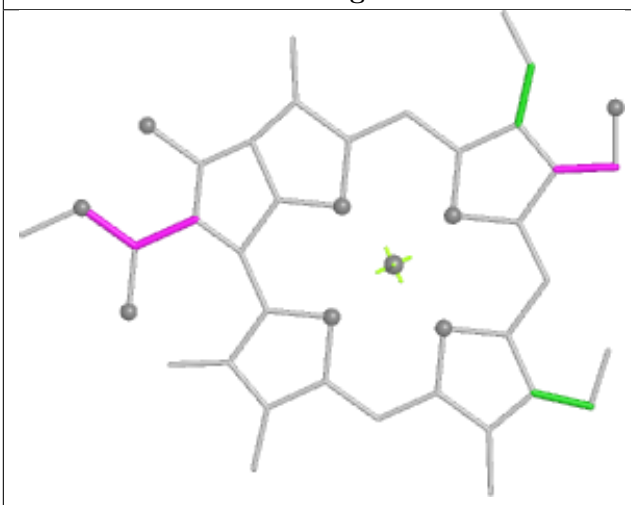
Ligand CHL 1 317



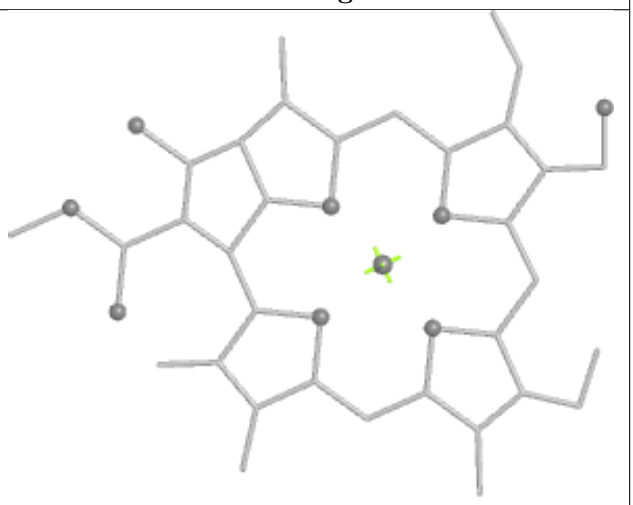
Bond lengths



Bond angles

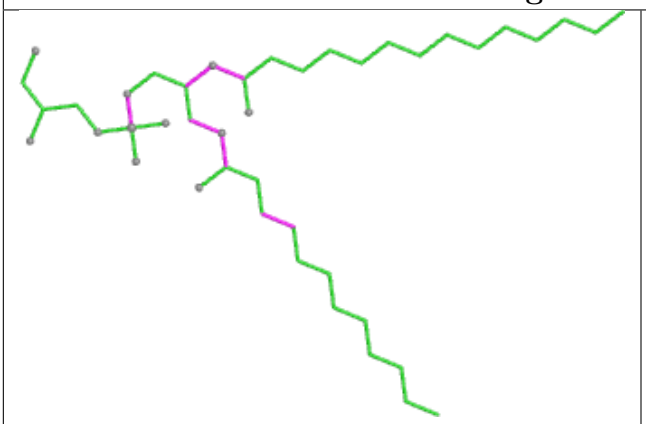


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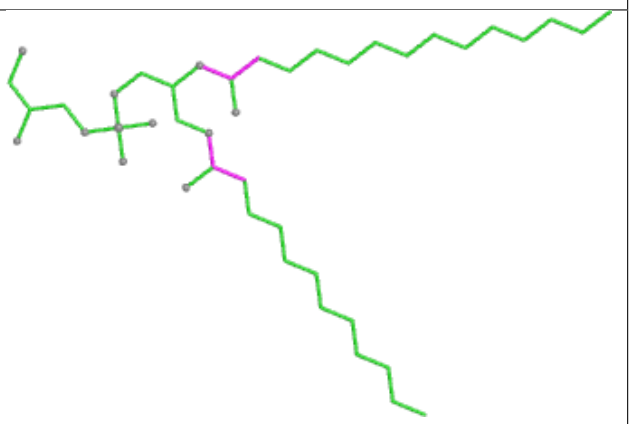


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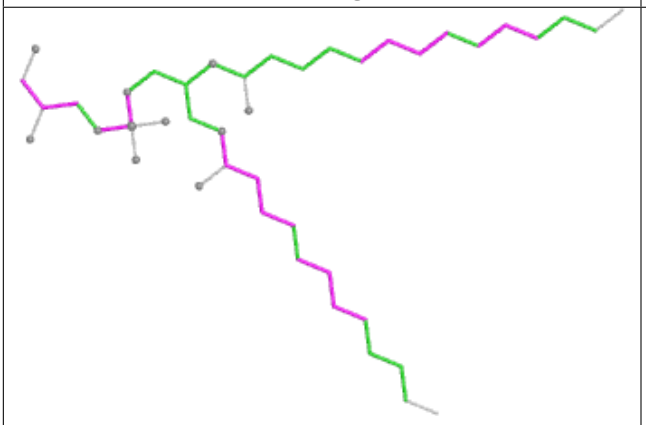
Ligand LHG n 318



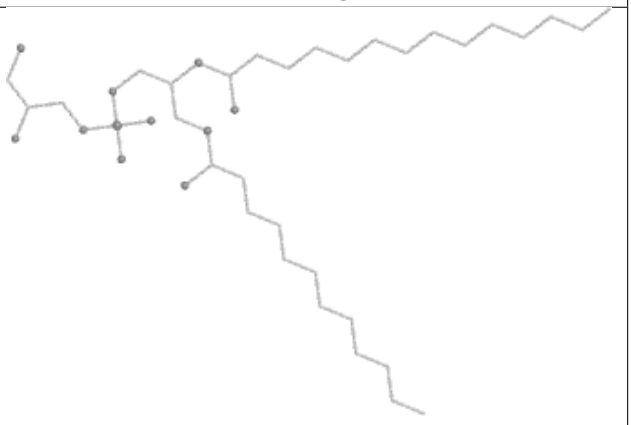
Bond lengths



Bond angles

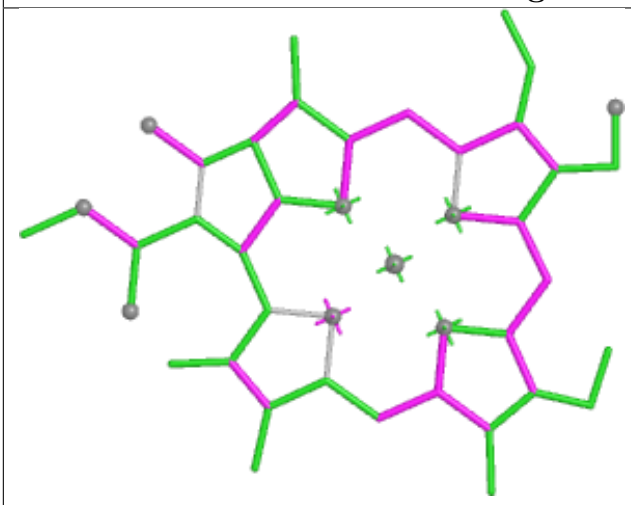


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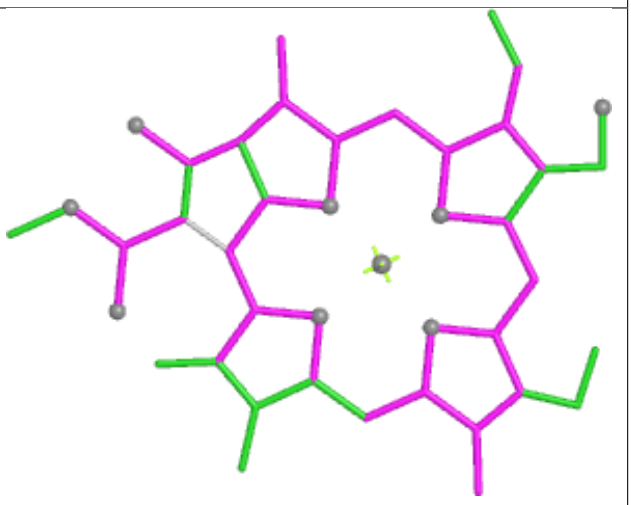


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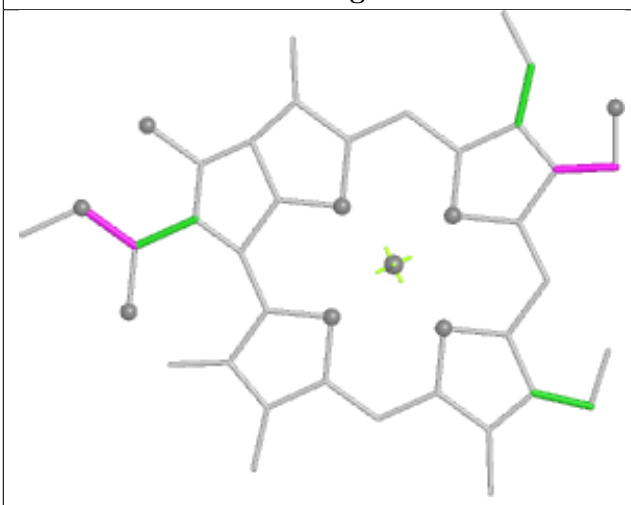
Ligand CHL 2 313



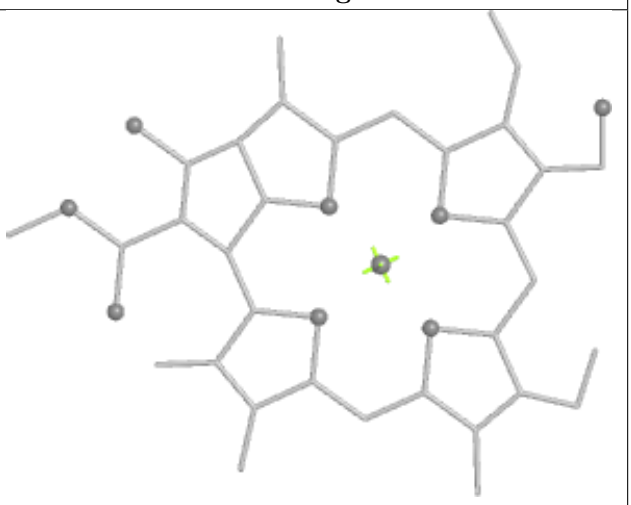
Bond lengths



Bond angles

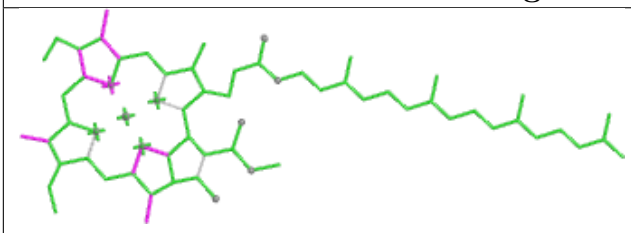


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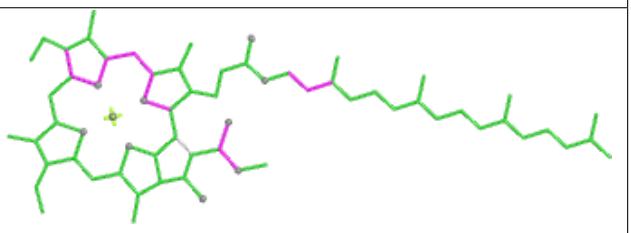


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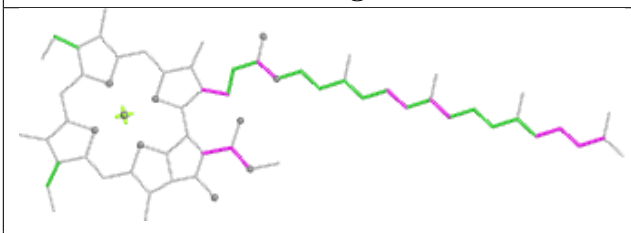
Ligand CLA D 405



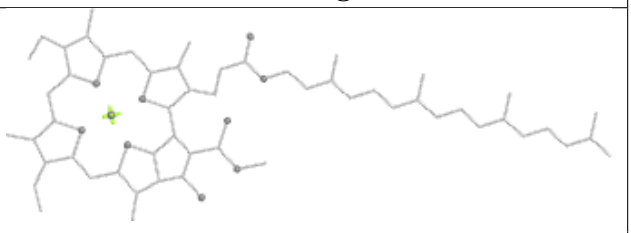
Bond lengths



Bond angles

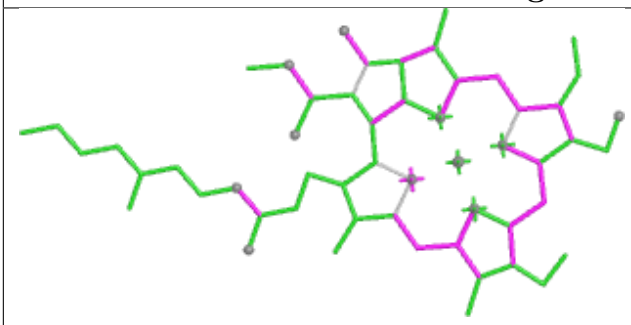


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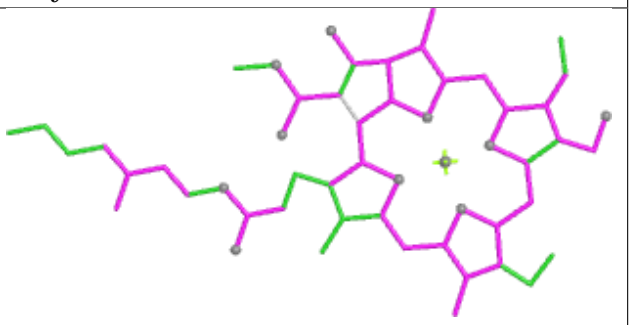


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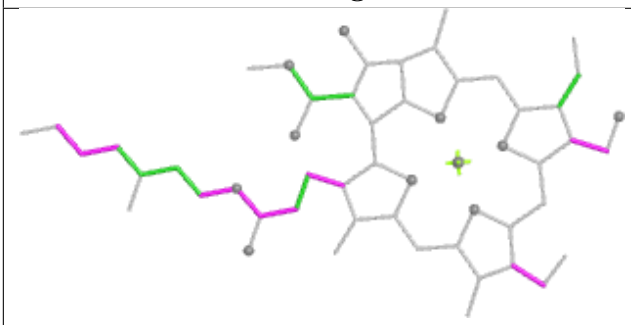
Ligand CHL y 311



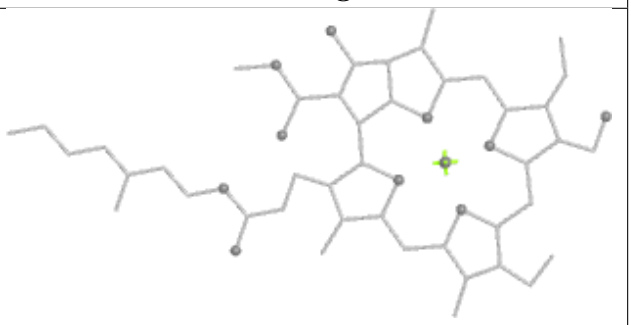
Bond lengths



Bond angles

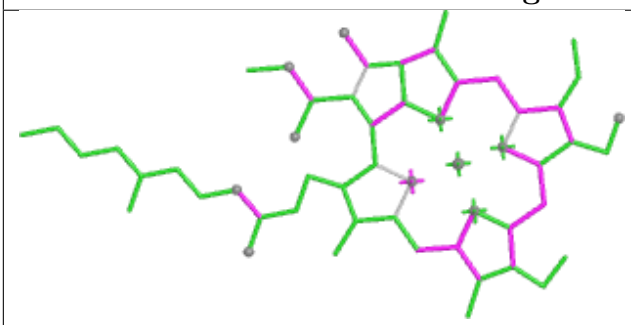


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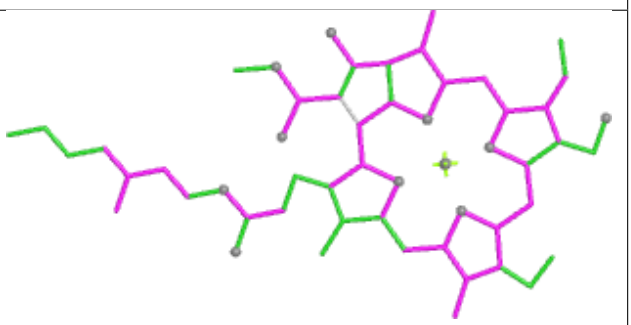


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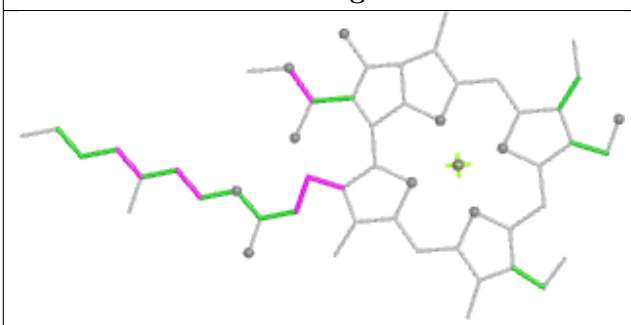
Ligand CHL N 304



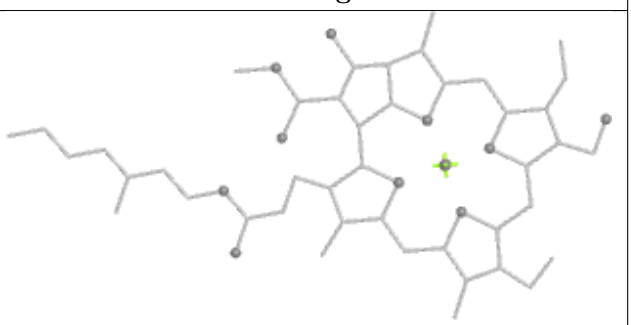
Bond lengths



Bond angles

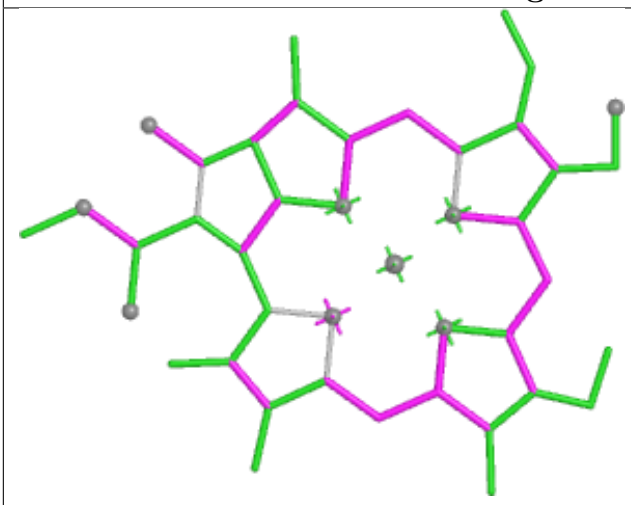


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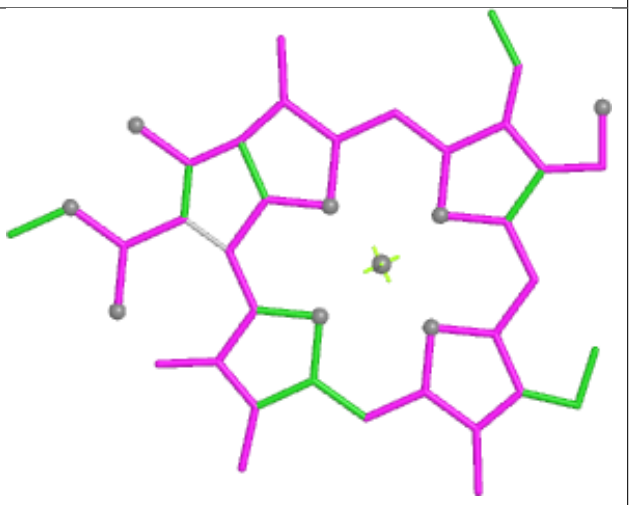


Rings

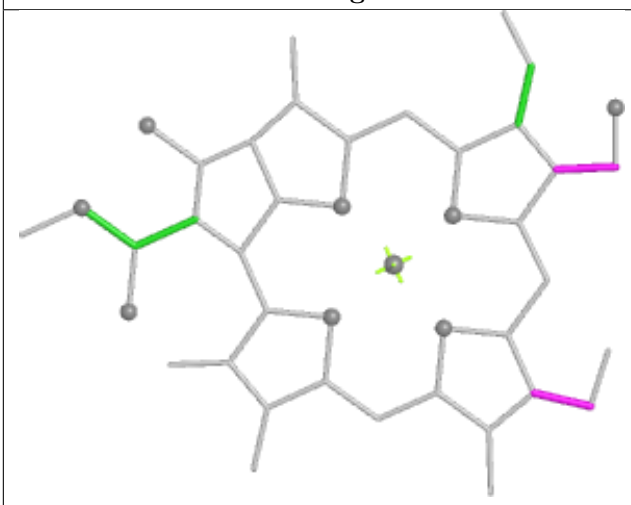
Ligand CHL S 613



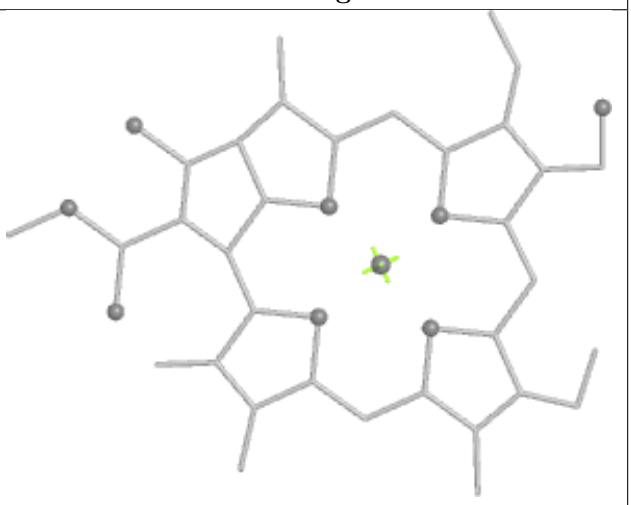
Bond lengths



Bond angles

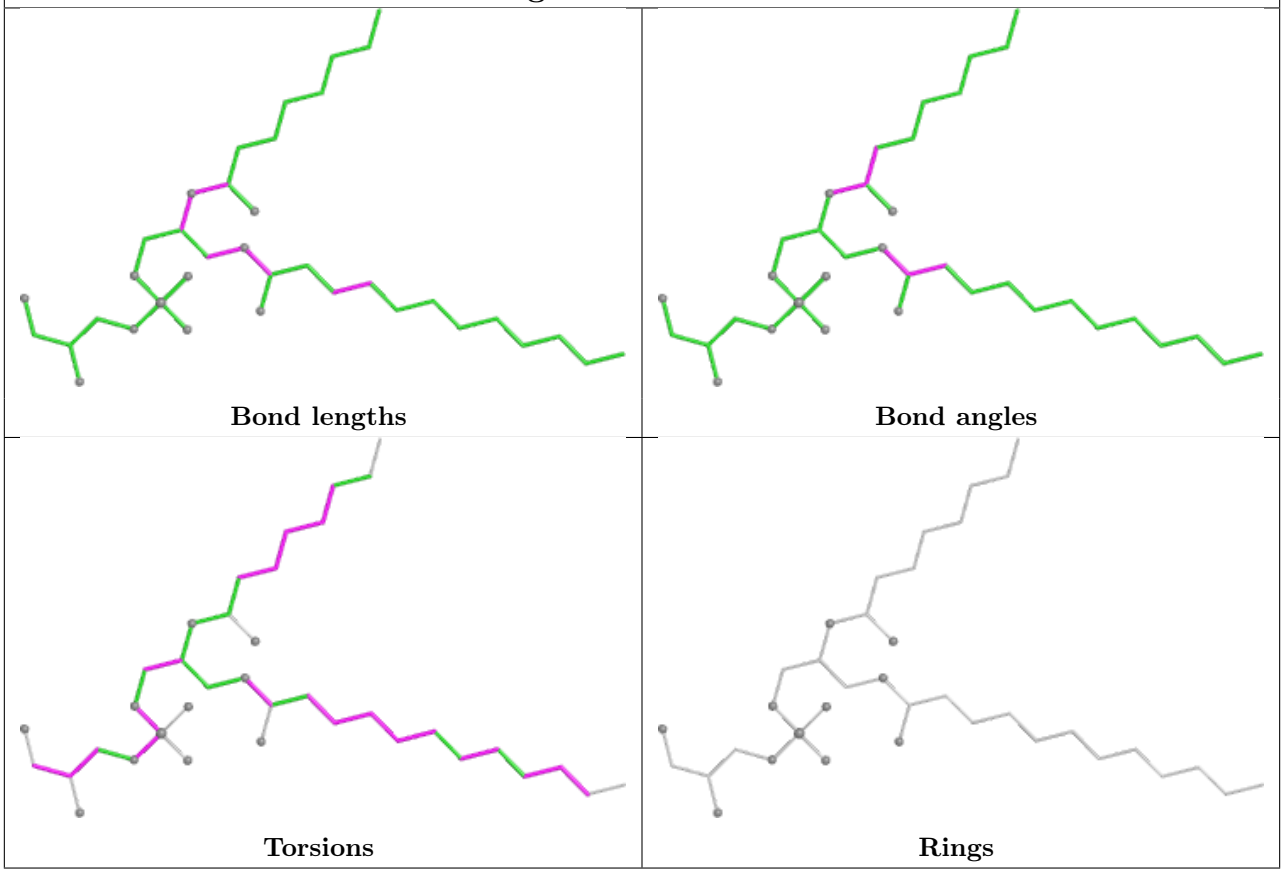


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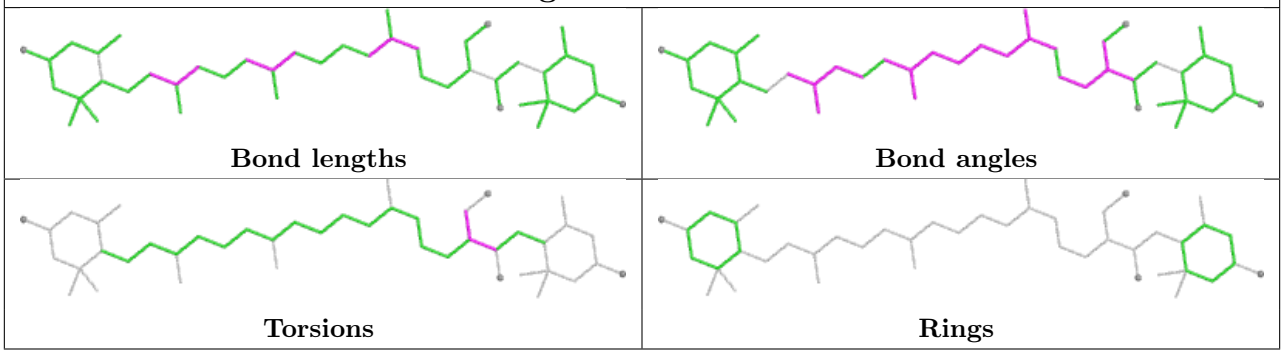


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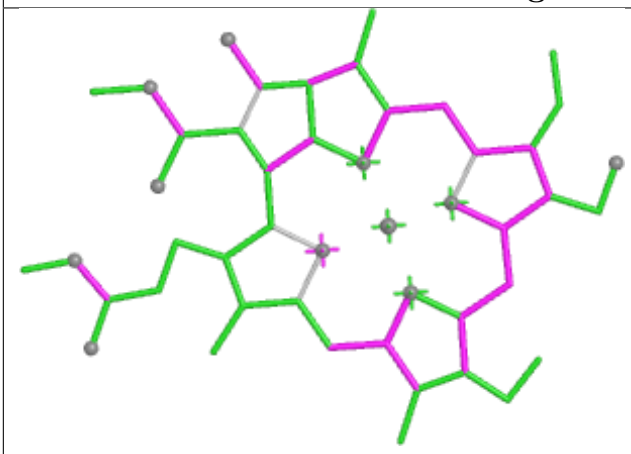
Ligand LHG 7 319



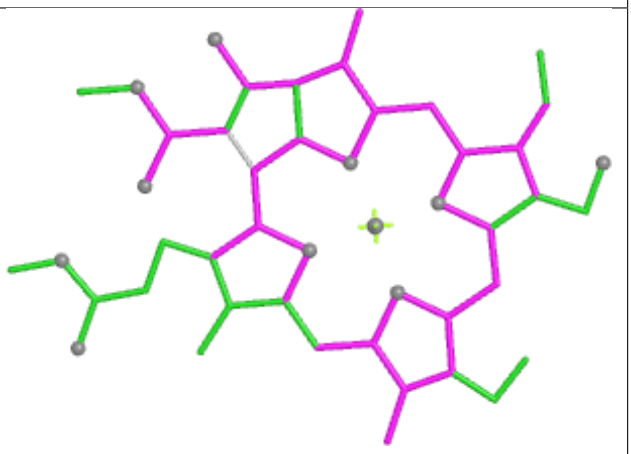
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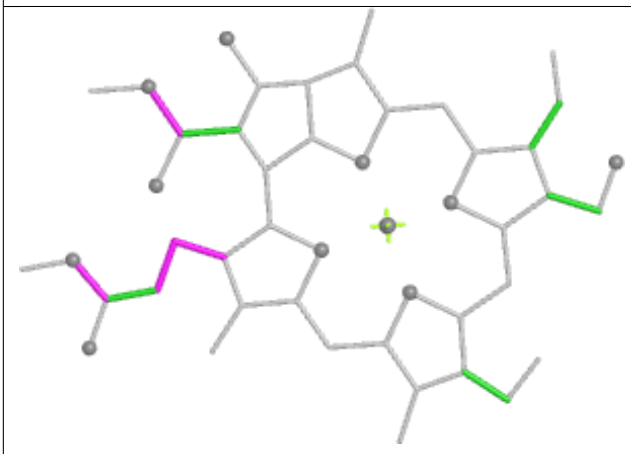
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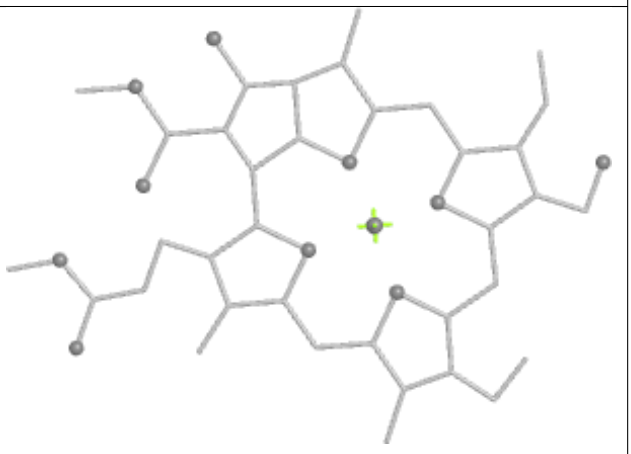
Bond lengths



Bond angles

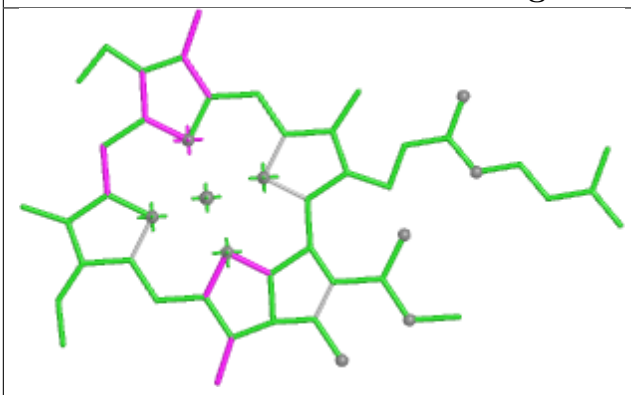


Torsions

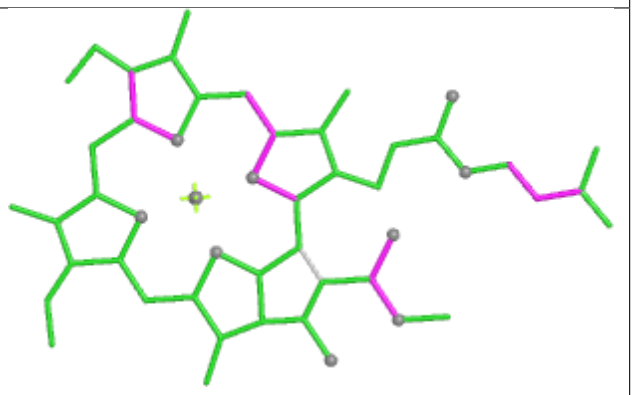


Rings

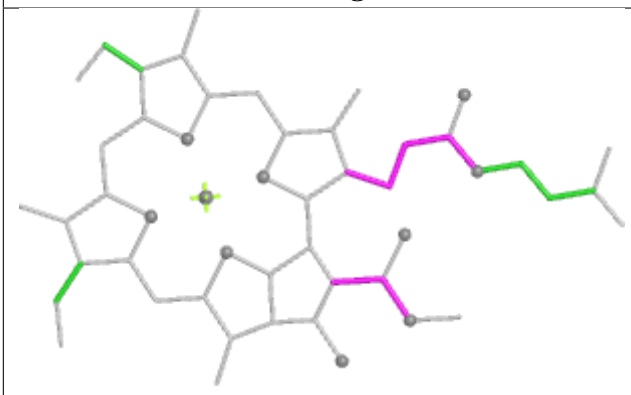
Ligand CLA 9 307



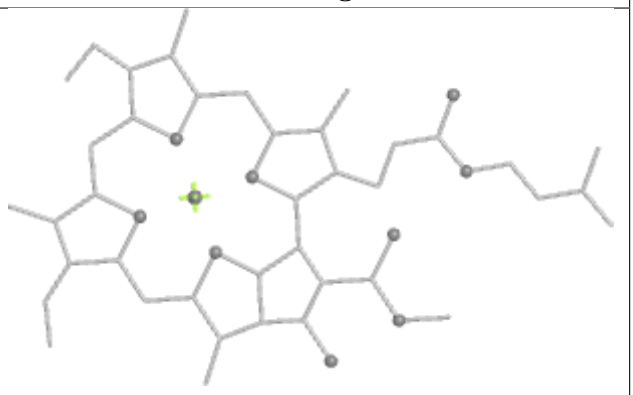
Bond lengths



Bond angles

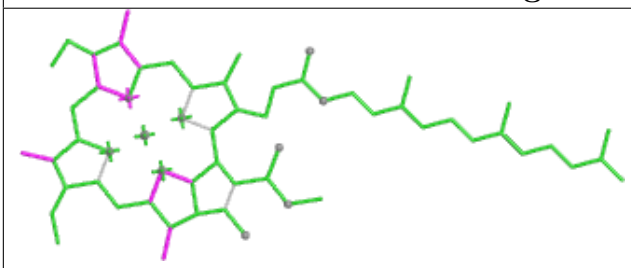


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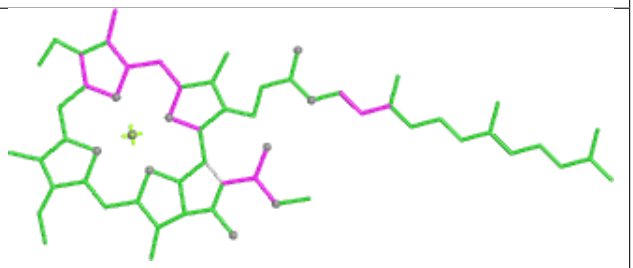


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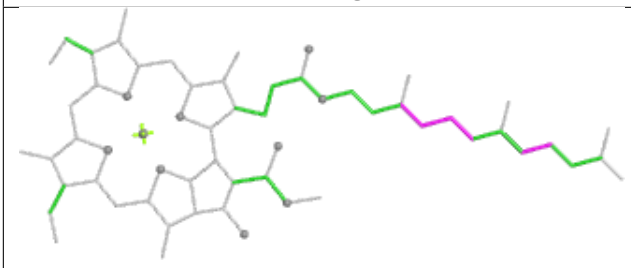
Ligand CLA A 607



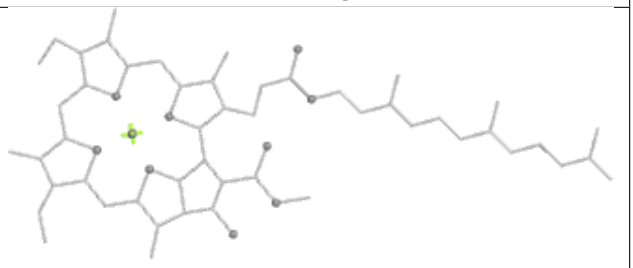
Bond lengths



Bond angles

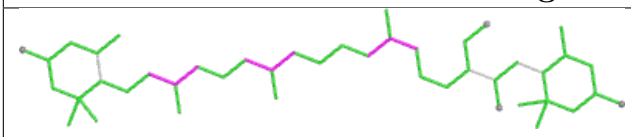


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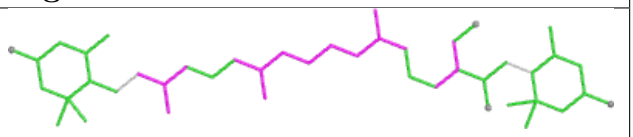


Rings

Ligand 0IE g 303



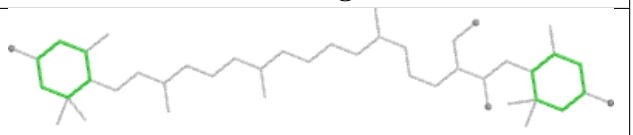
Bond lengths



Bond angles

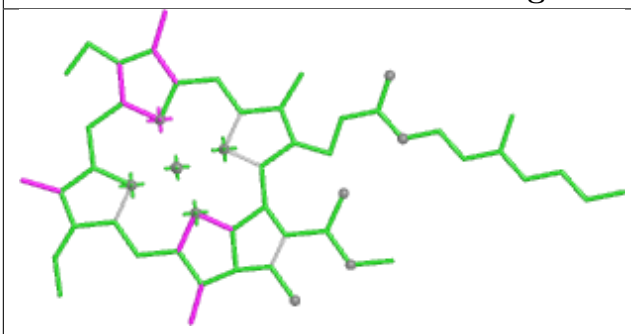


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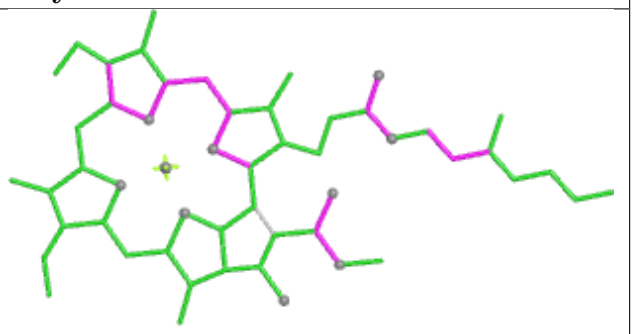


Rings

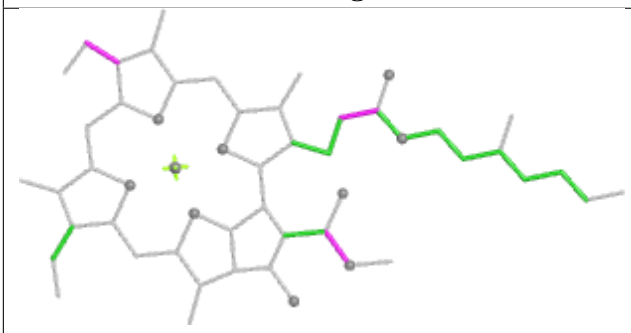
Ligand CLA y 307



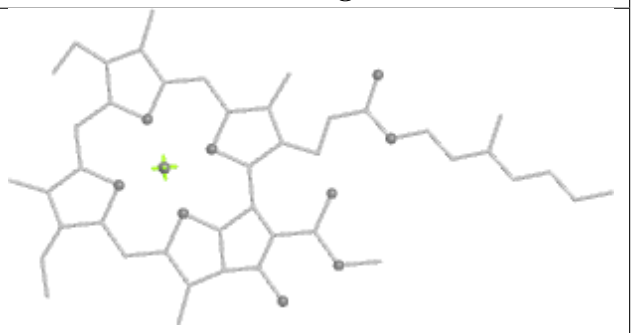
Bond lengths



Bond angles

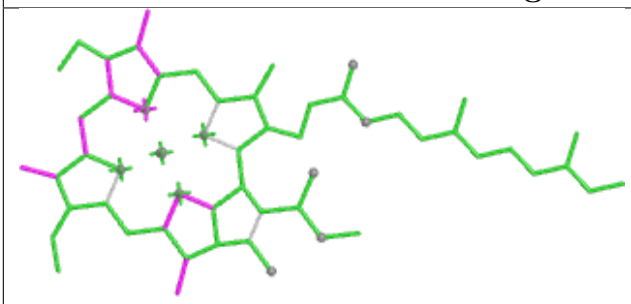


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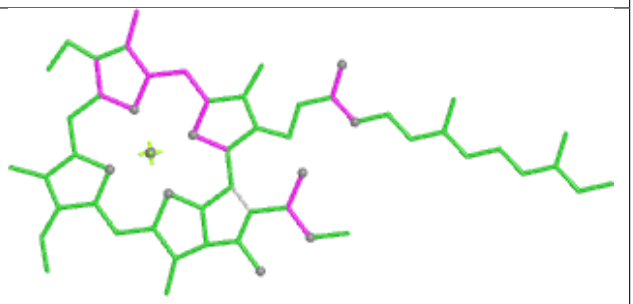


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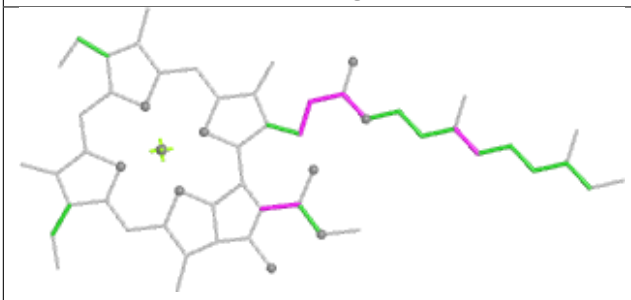
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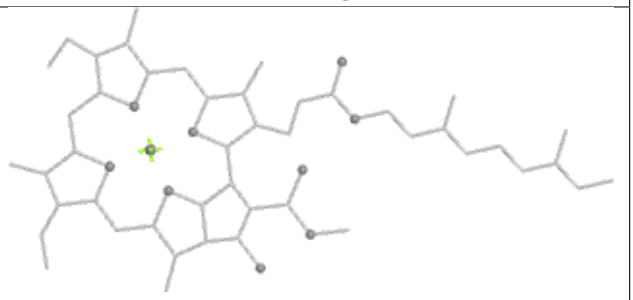
Bond lengths



Bond angles

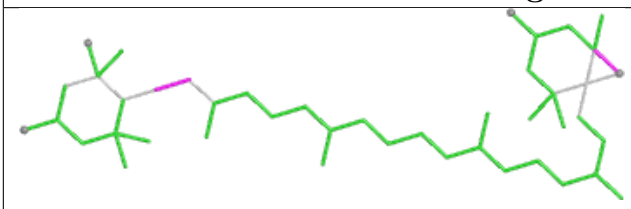


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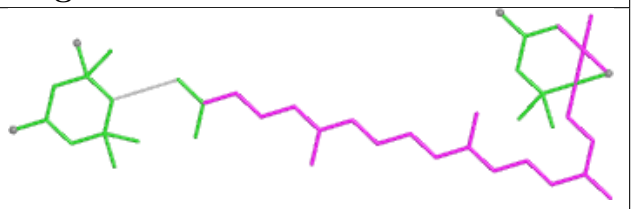


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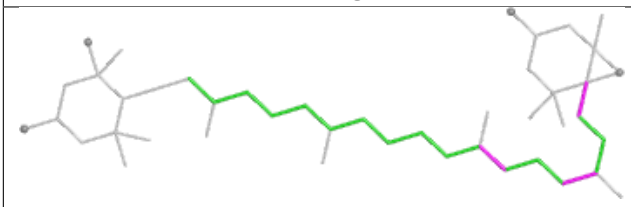
Ligand NEX g 304



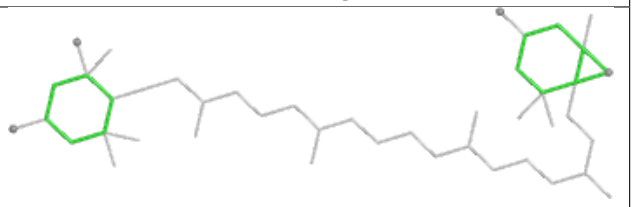
Bond lengths



Bond angles

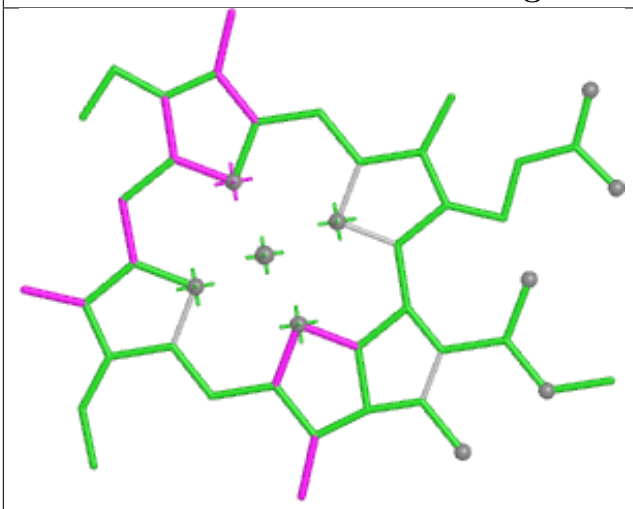


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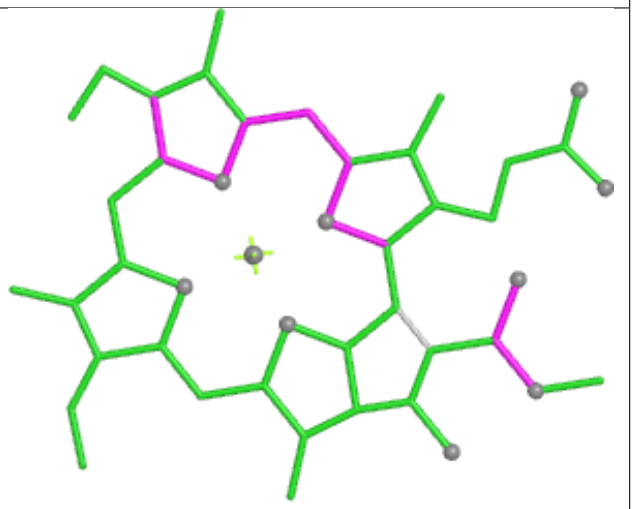


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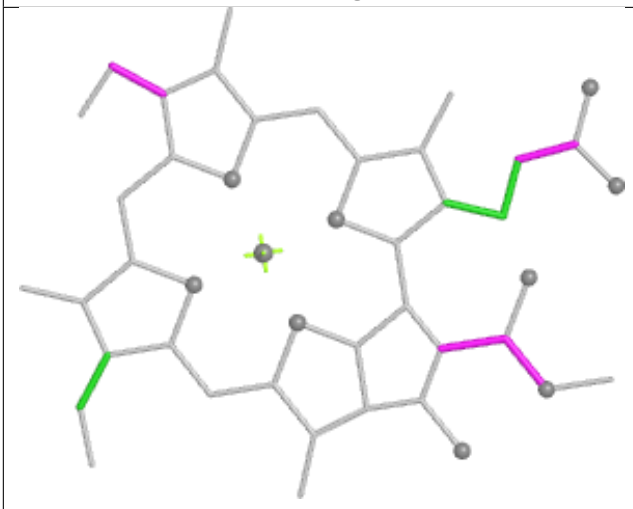
Ligand CLA R 611



Bond lengths



Bond angles

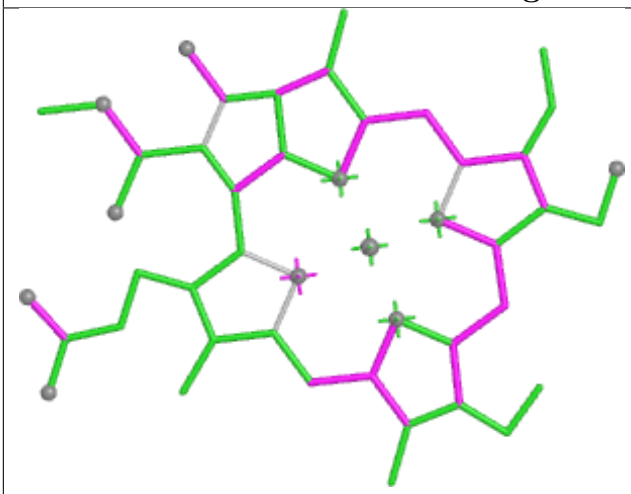


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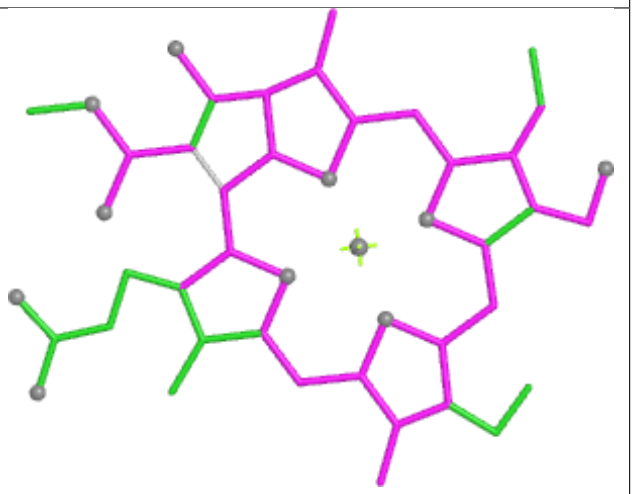


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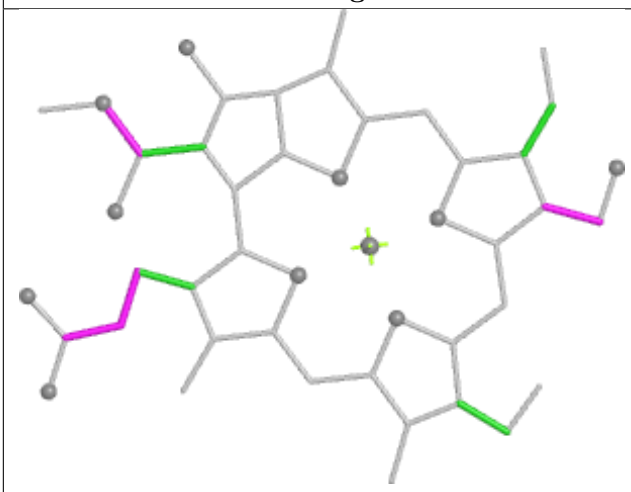
Ligand CHL N 309



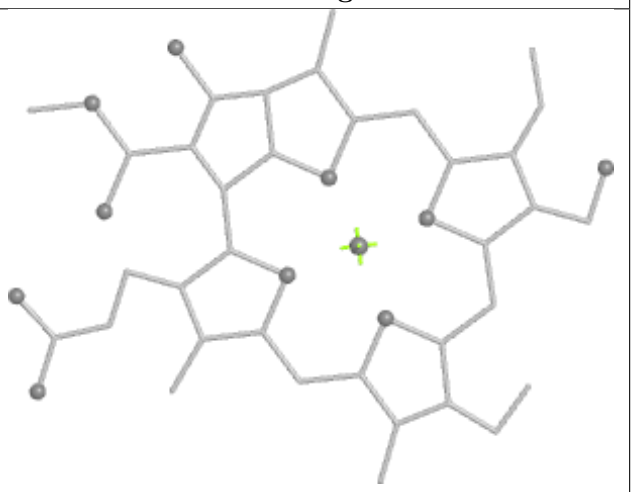
Bond lengths



Bond angles

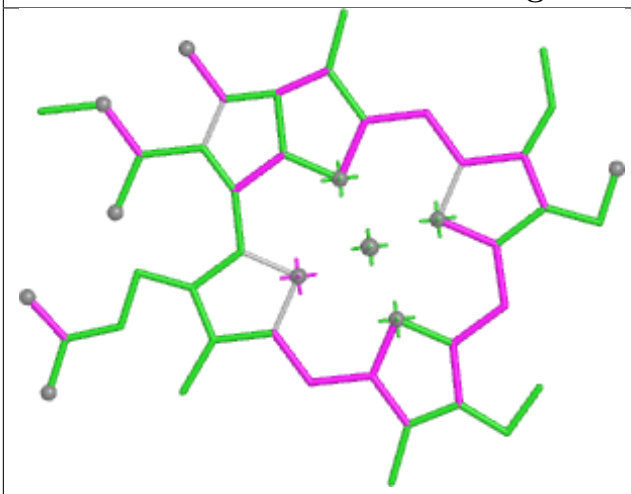


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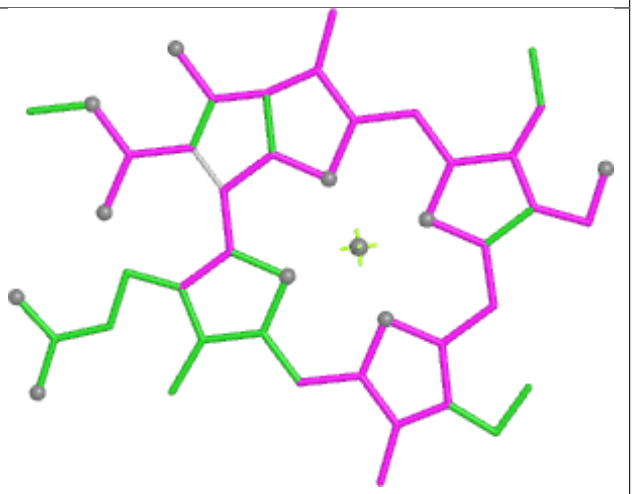


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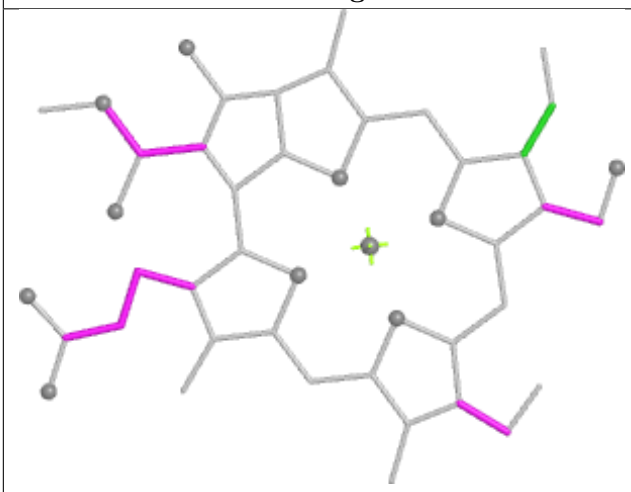
Ligand CHL S 601



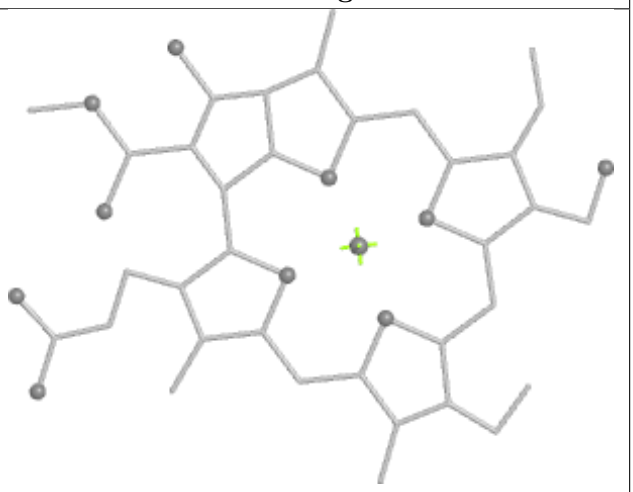
Bond lengths



Bond angles

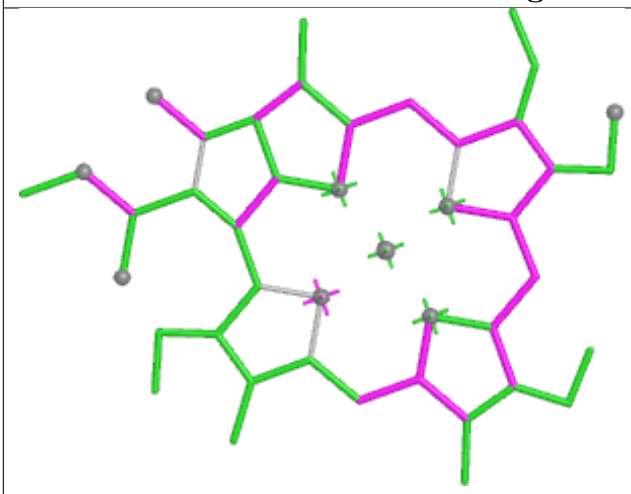


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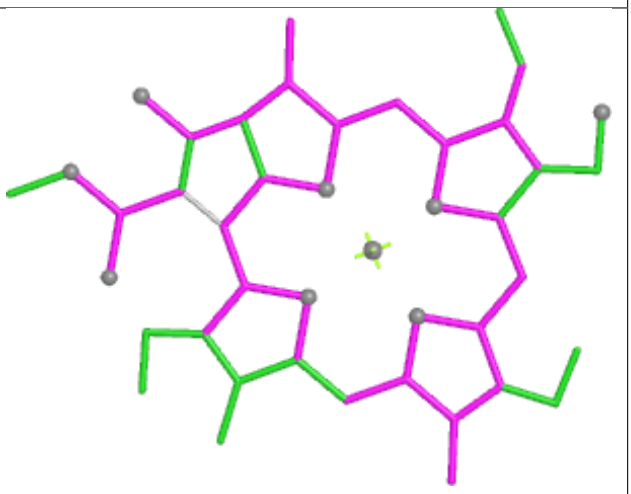


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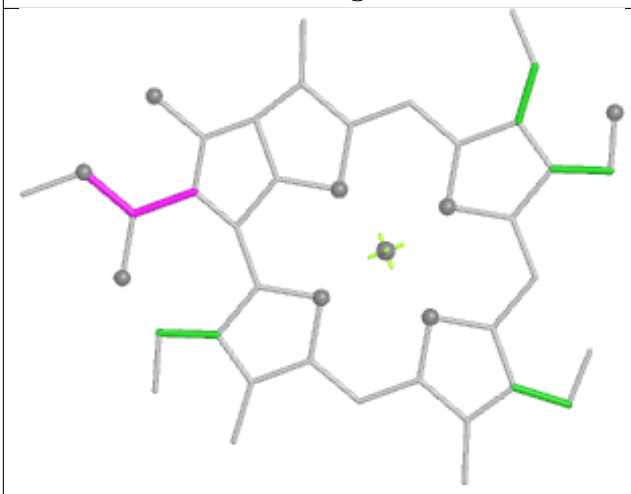
Ligand CHL n 308



Bond lengths



Bond angles

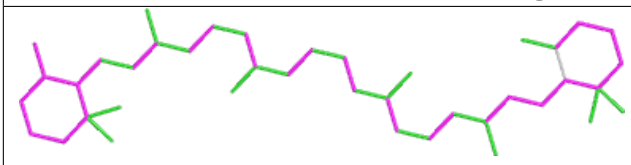


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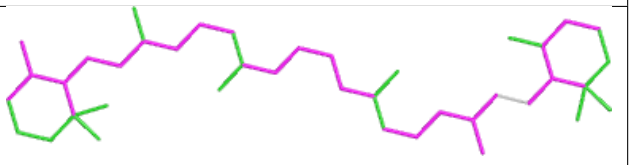


Rings

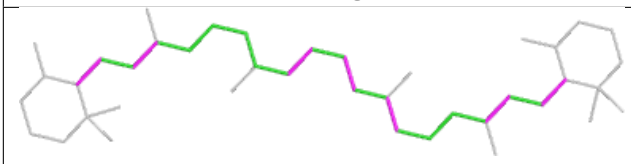
Ligand 8CT v 401



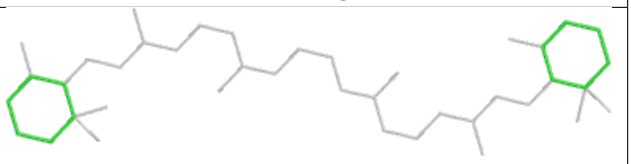
Bond lengths



Bond angles

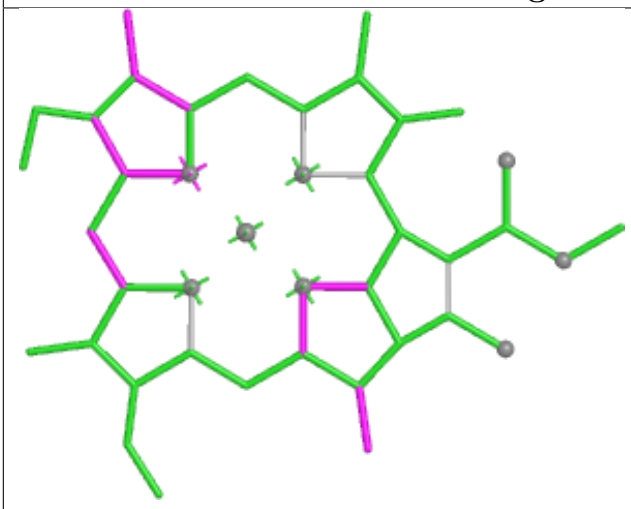


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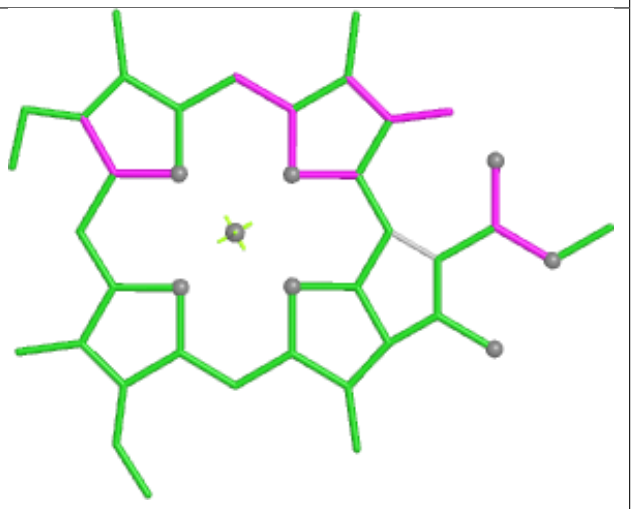


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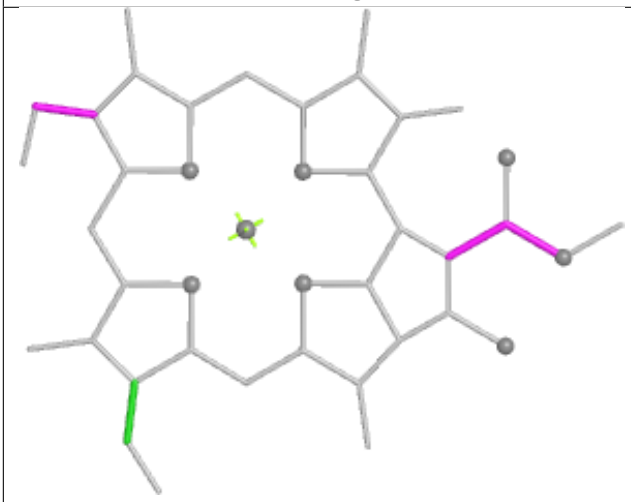
Ligand CLA 3 306



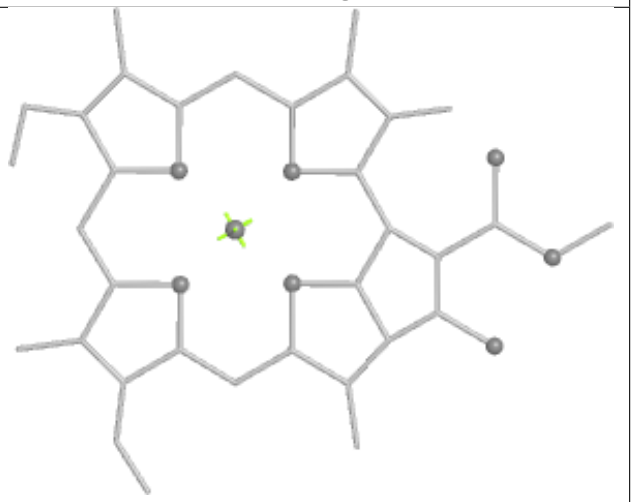
Bond lengths



Bond angles

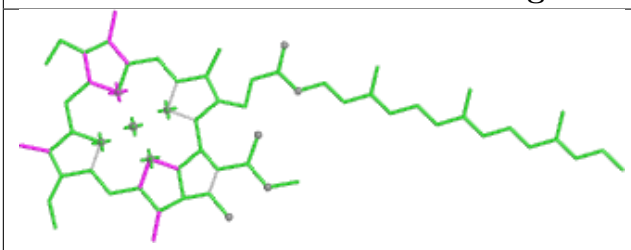


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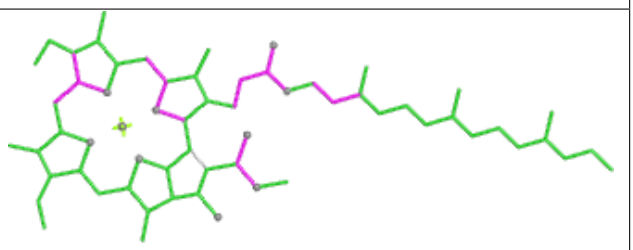


Rings

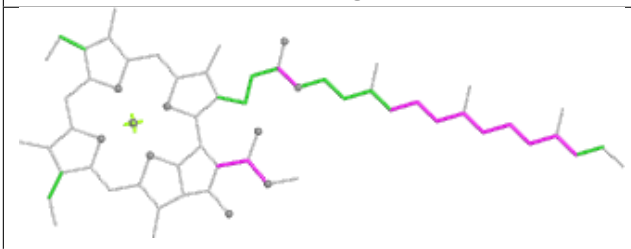
Ligand CLA b 604



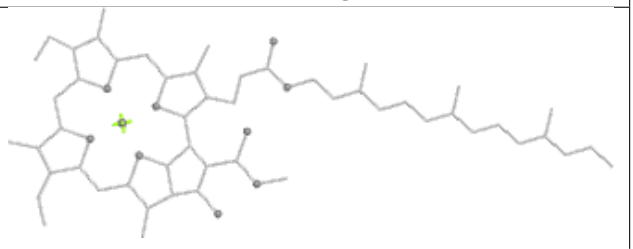
Bond lengths



Bond angles

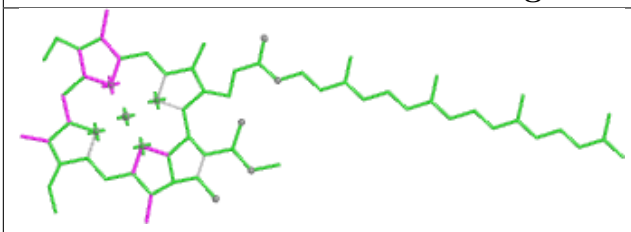


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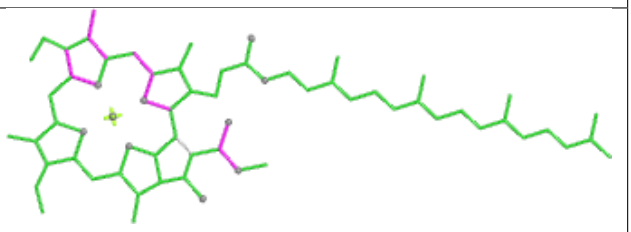


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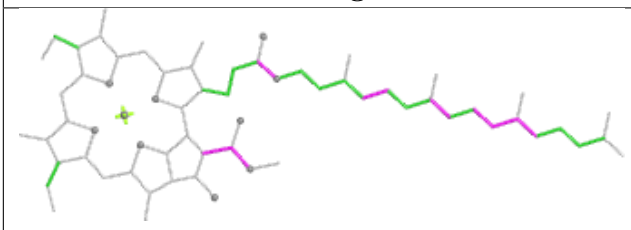
Ligand CLA C 611



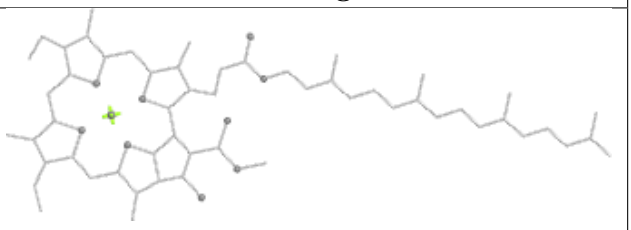
Bond lengths



Bond angles



Torsions

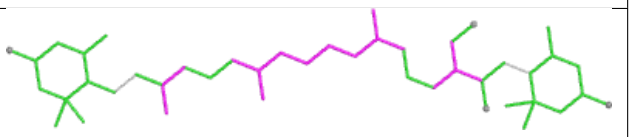


Rings

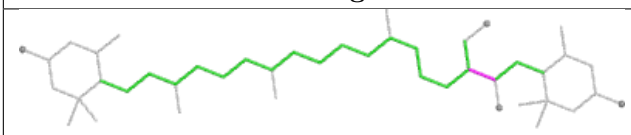
Ligand 0IE 5 302



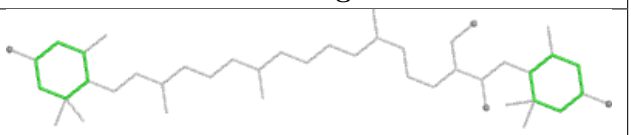
Bond lengths



Bond angles

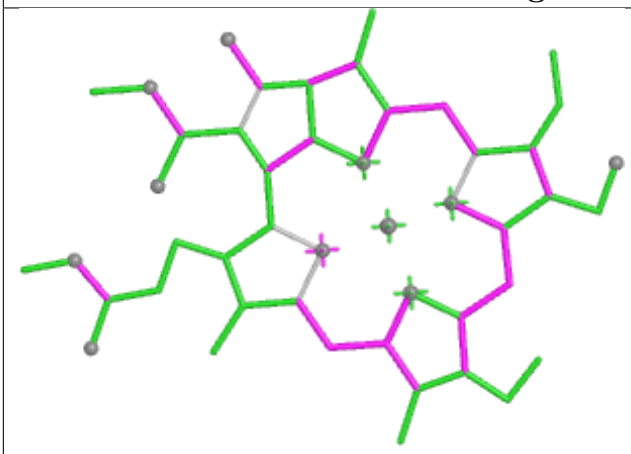


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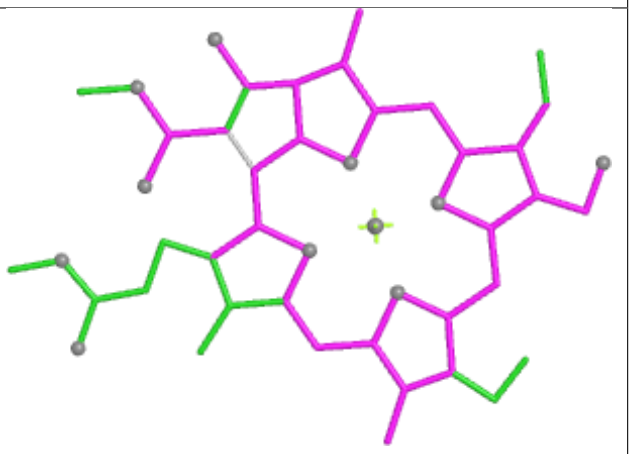


Rings

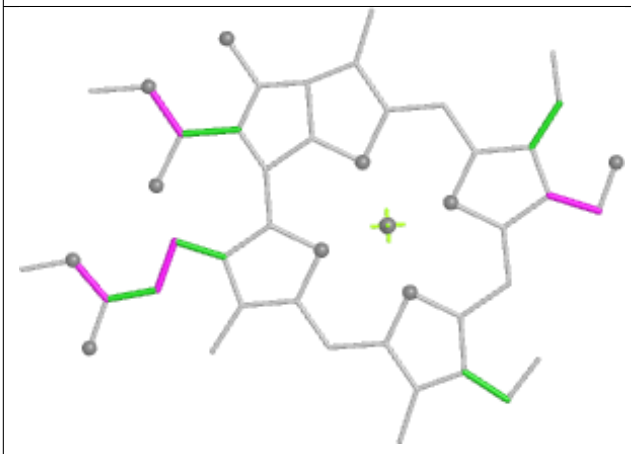
Ligand CHL 7 312



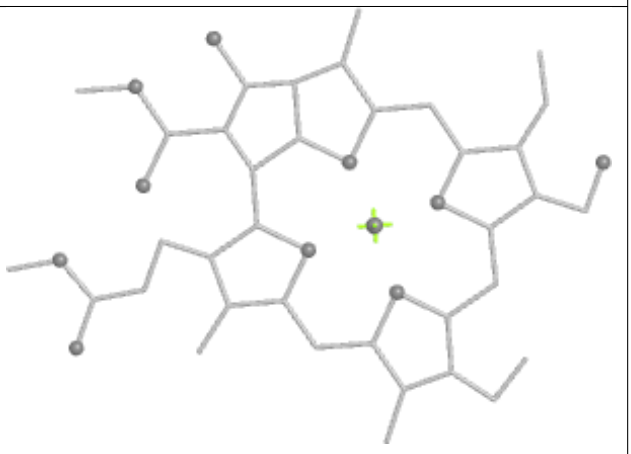
Bond lengths



Bond angles

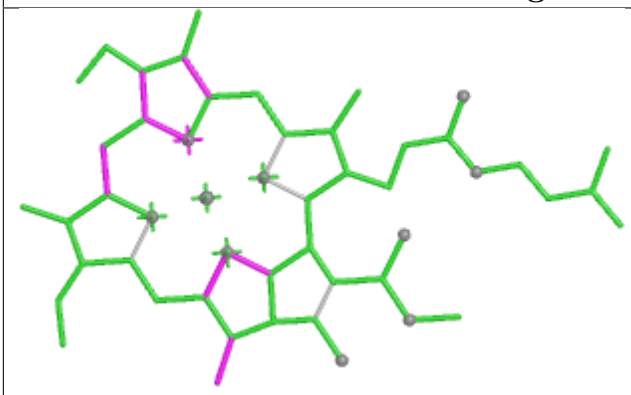


Torsions

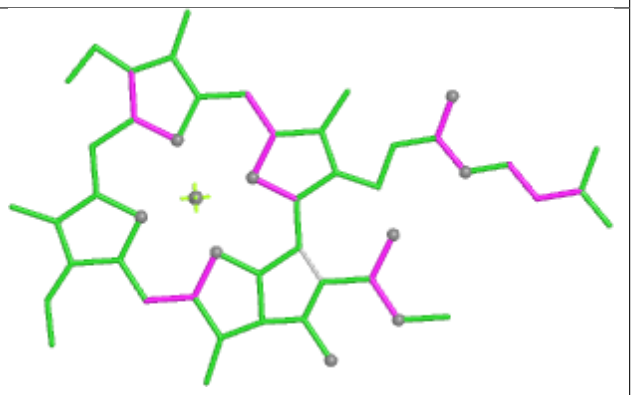


Rings

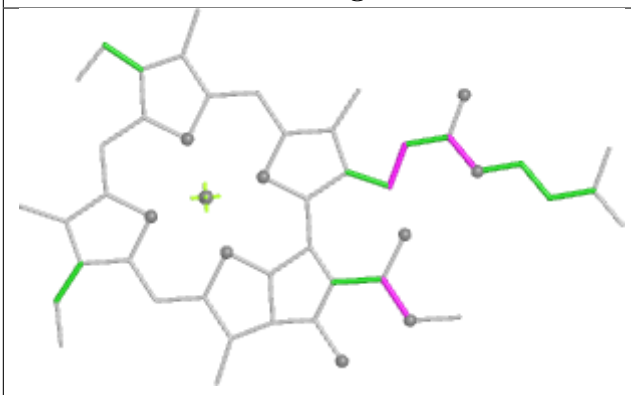
Ligand CLA n 307



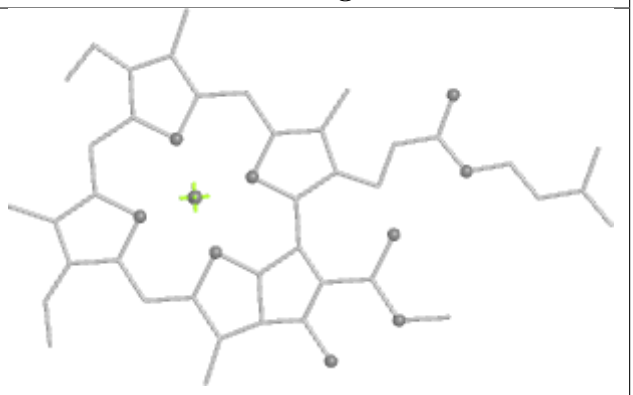
Bond lengths



Bond angles

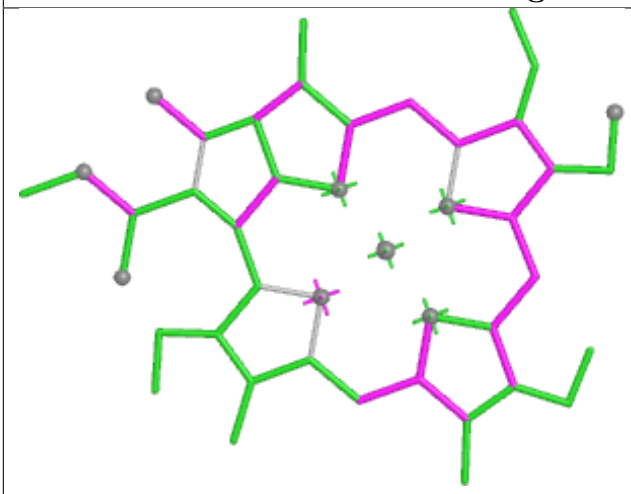


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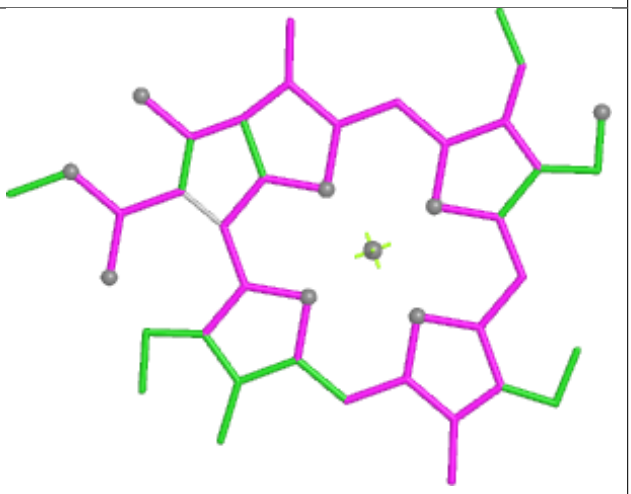


Rings

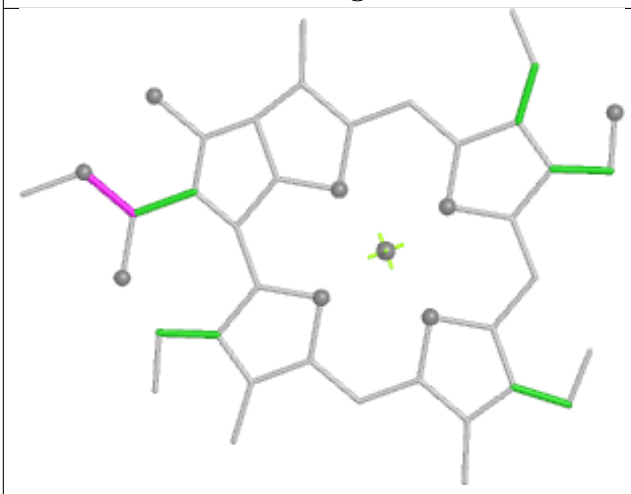
Ligand CHL 4 308



Bond lengths



Bond angles

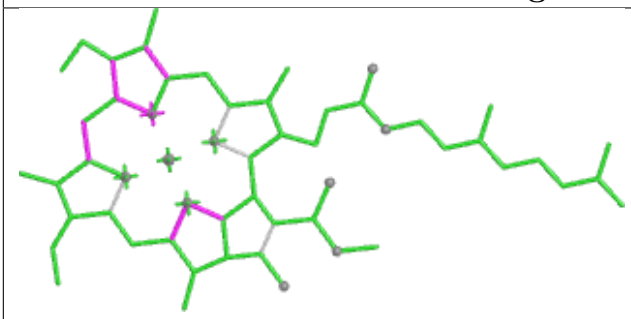


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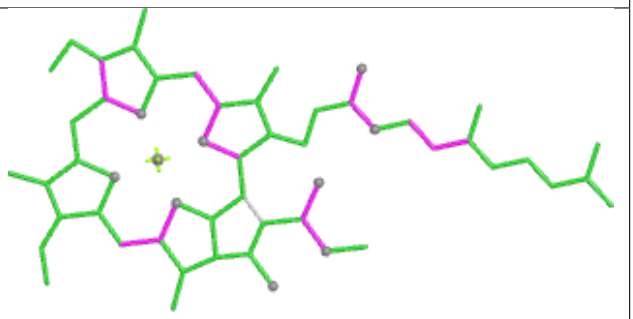


Rings

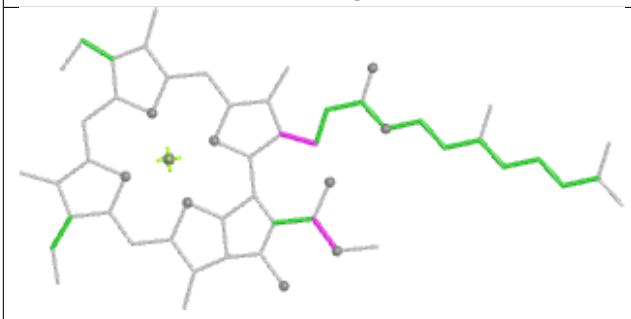
Ligand CLA 9 313



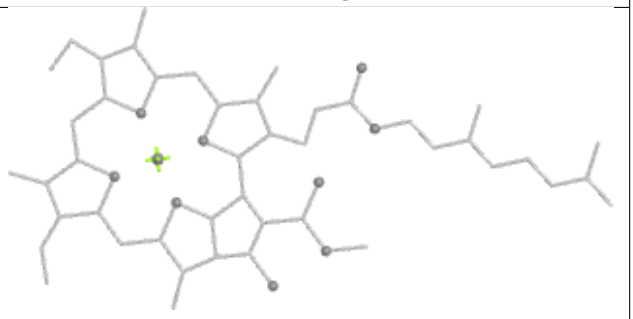
Bond lengths



Bond angles

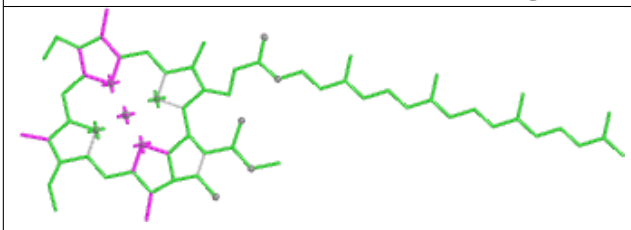


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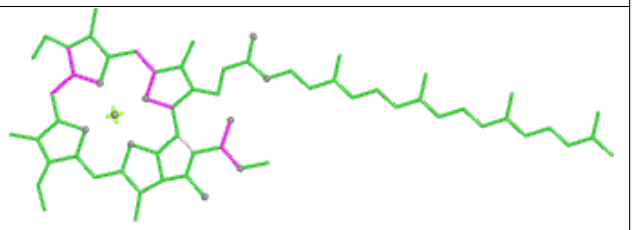


Rings

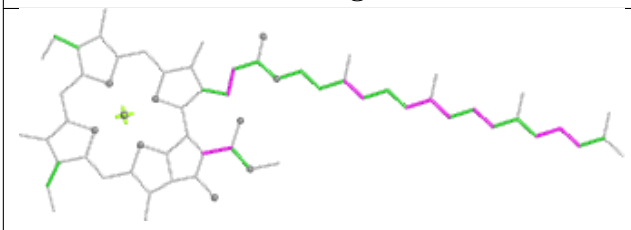
Ligand CLA C 607



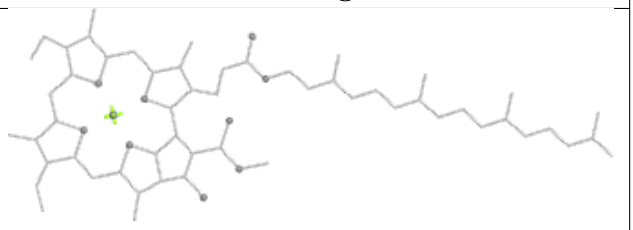
Bond lengths



Bond angles

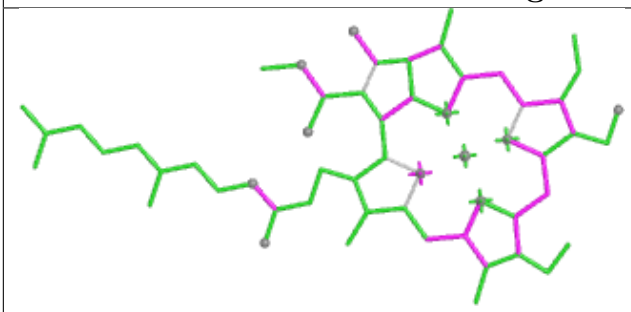


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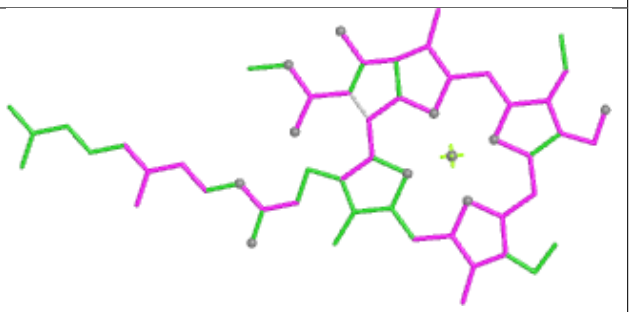


Rings

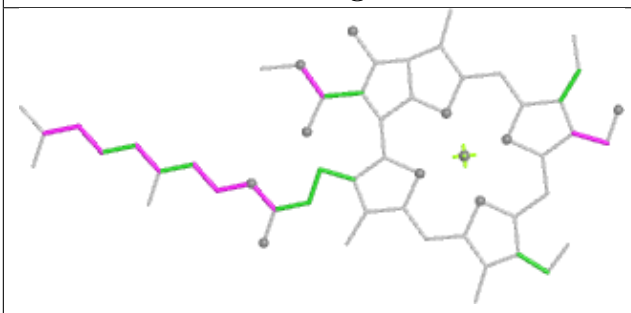
Ligand CHL n 312



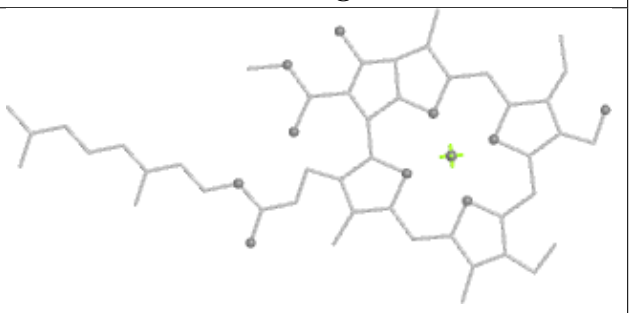
Bond lengths



Bond angles

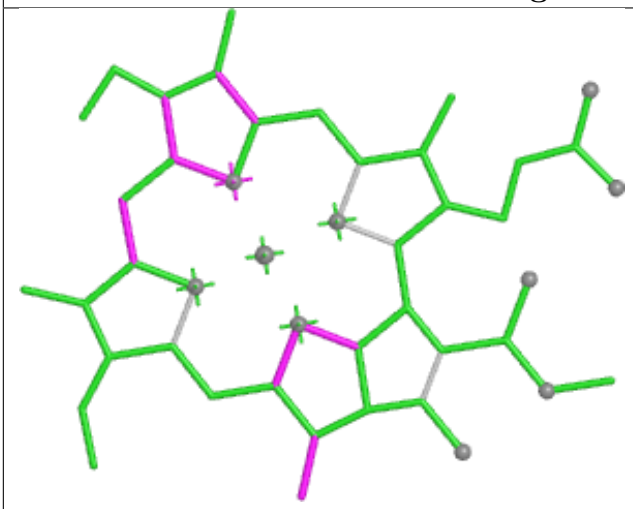


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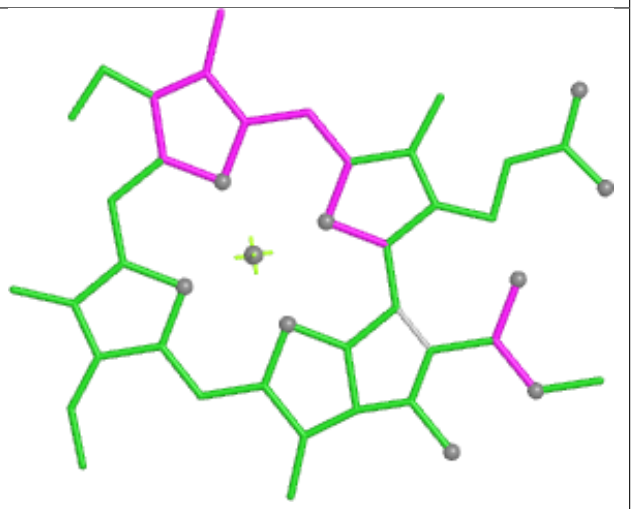


Rings

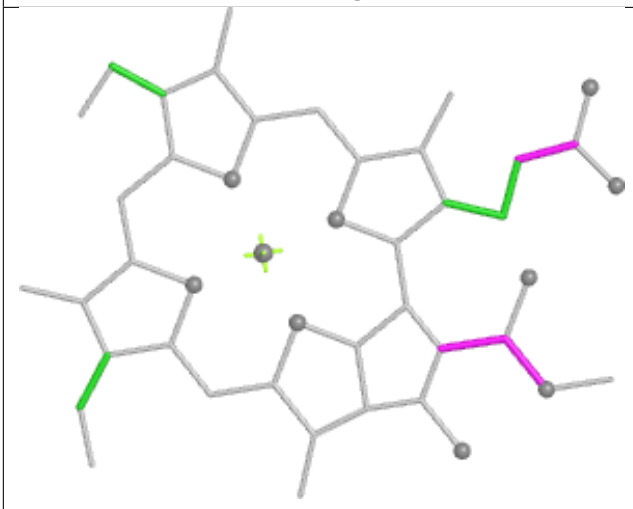
Ligand CLA r 311



Bond lengths



Bond angles

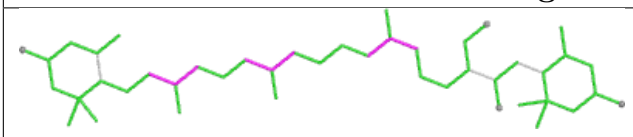


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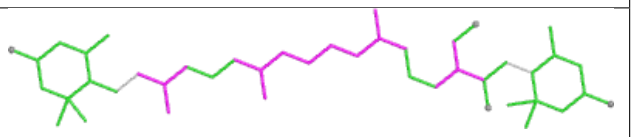


Rings

Ligand 0IE 1 302



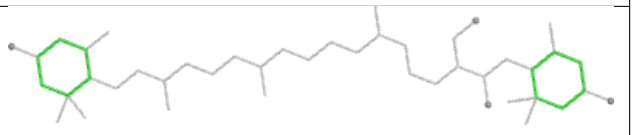
Bond lengths



Bond angles

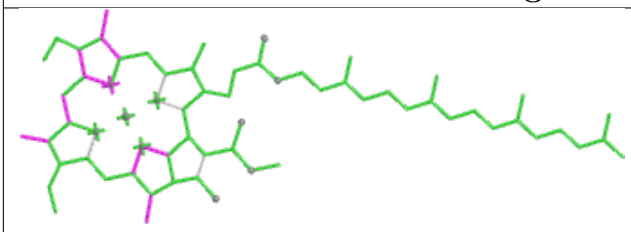


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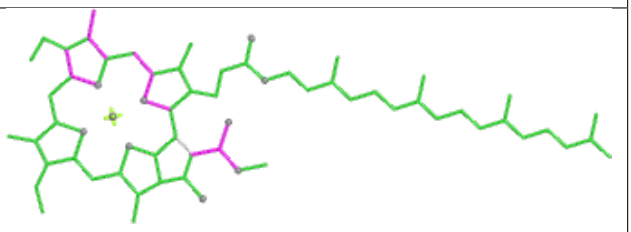


Rings

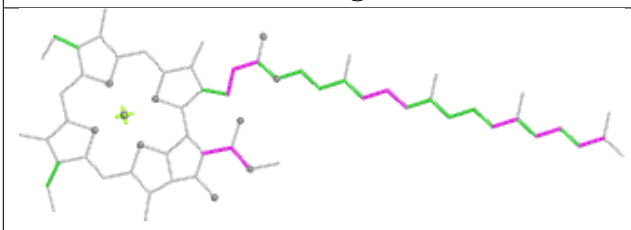
Ligand CLA B 602



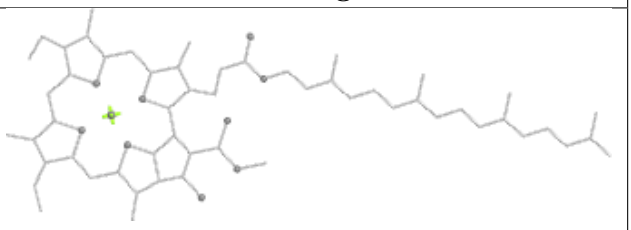
Bond lengths



Bond angles

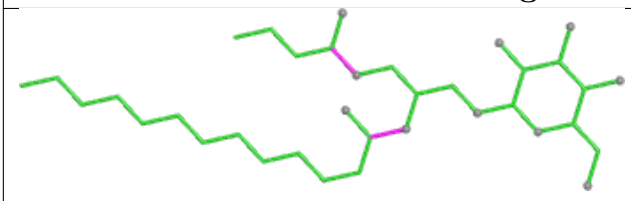


Torsions



Rings

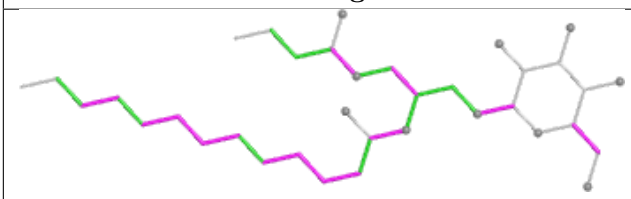
Ligand LMG w 201



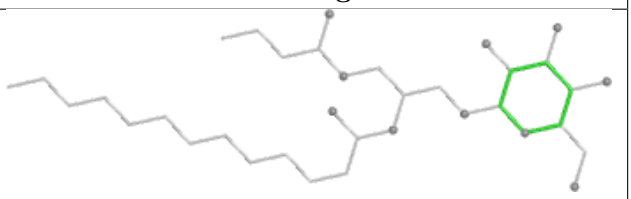
Bond lengths



Bond angles

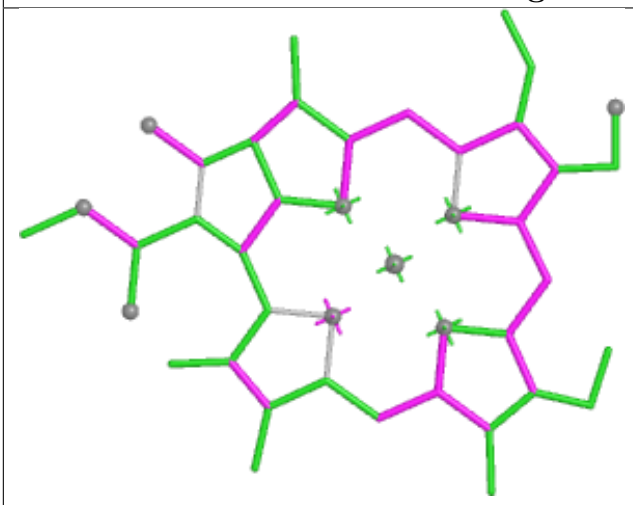


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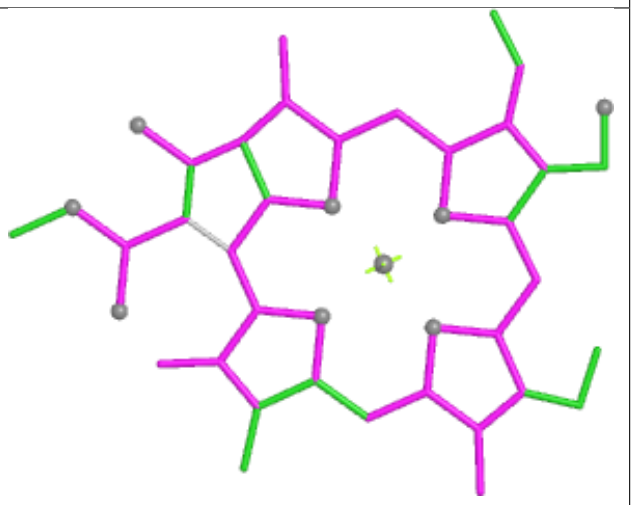


Rings

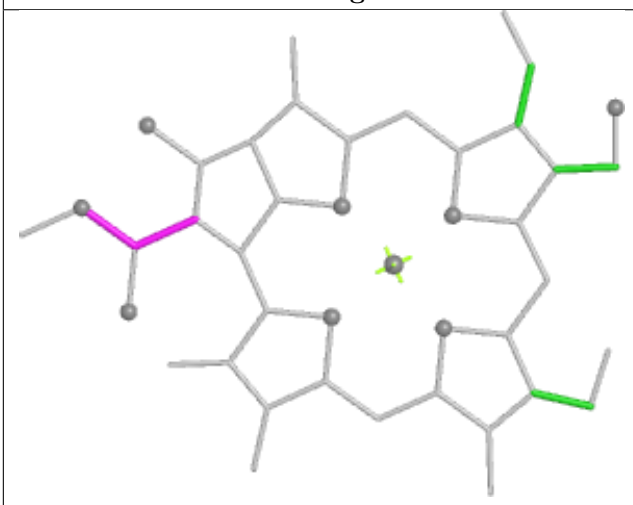
Ligand CHL 9 317



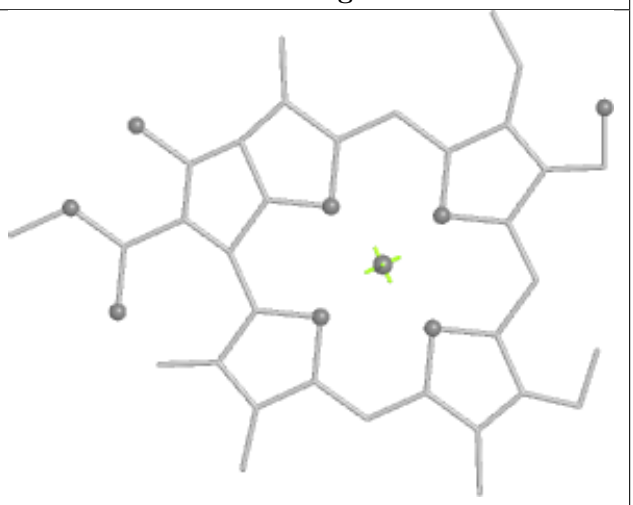
Bond lengths



Bond angles

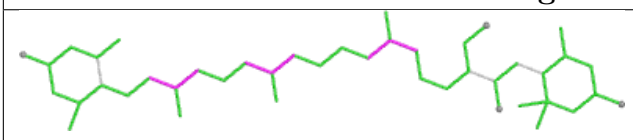


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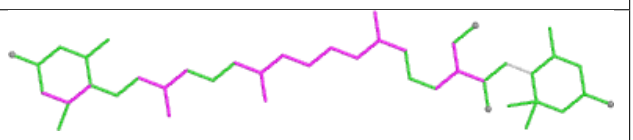


Rings

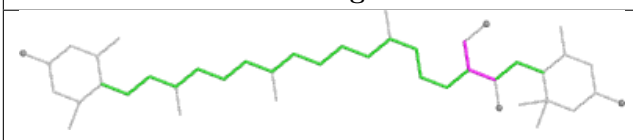
Ligand 0IE 6 302



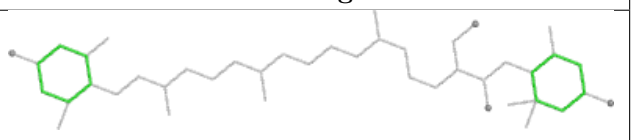
Bond lengths



Bond angles

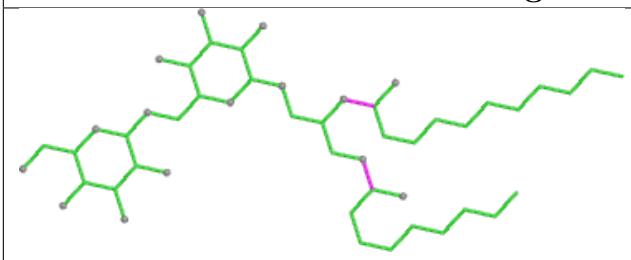


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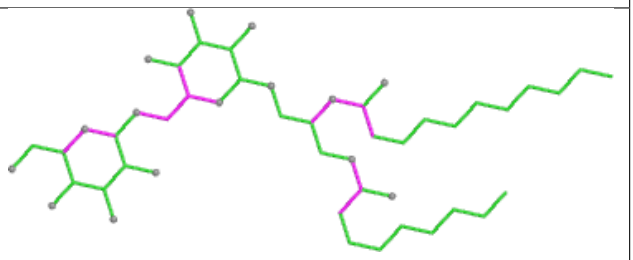


Rings

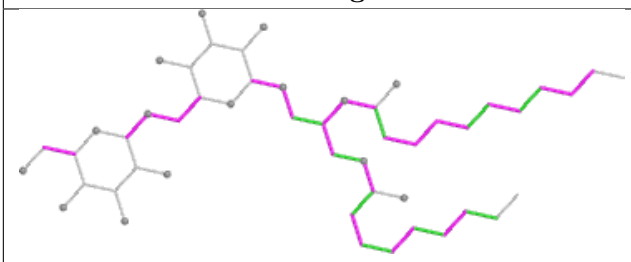
Ligand DGD c 618



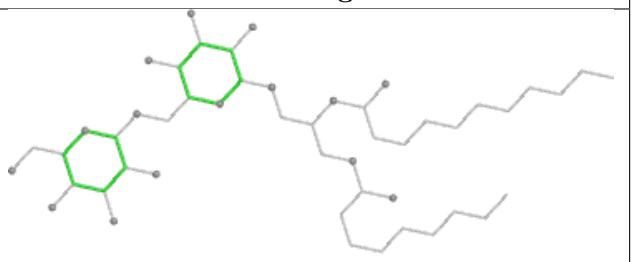
Bond lengths



Bond angles

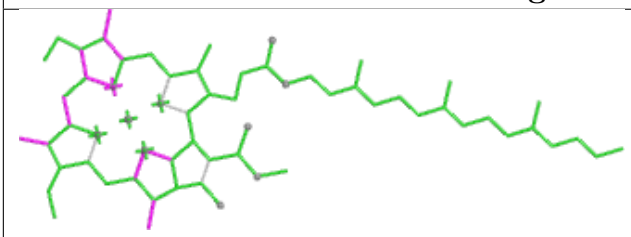


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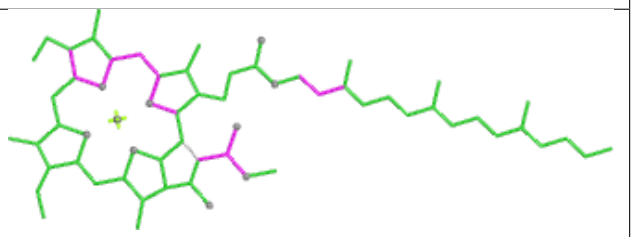


Rings

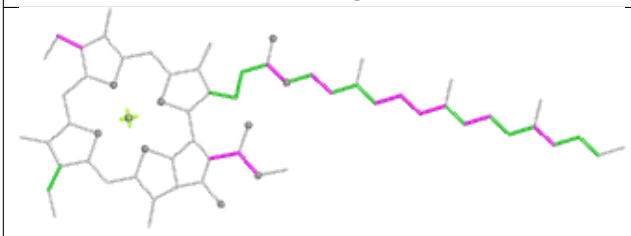
Ligand CLA 7 315



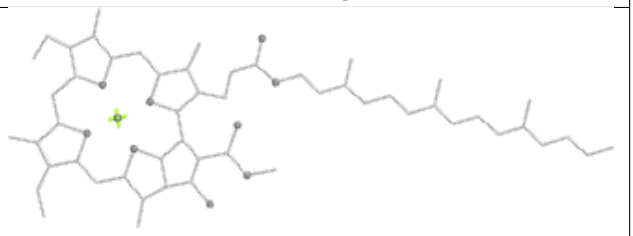
Bond lengths



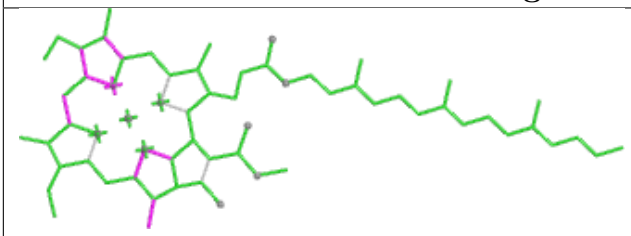
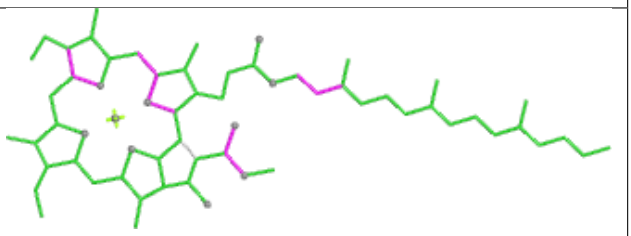
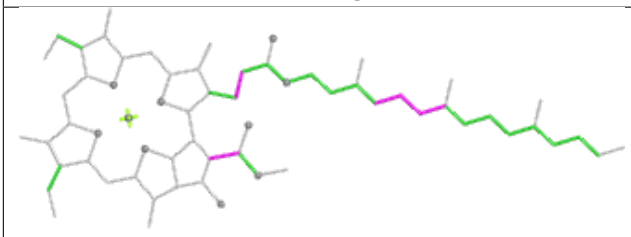
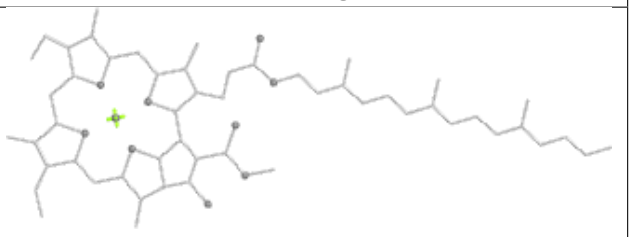
Bond angles

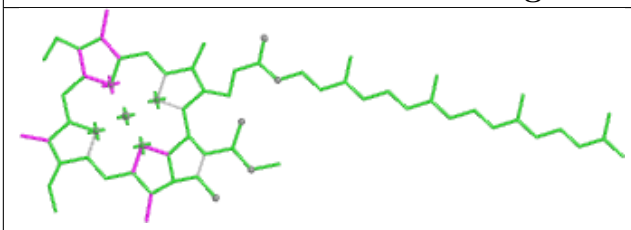
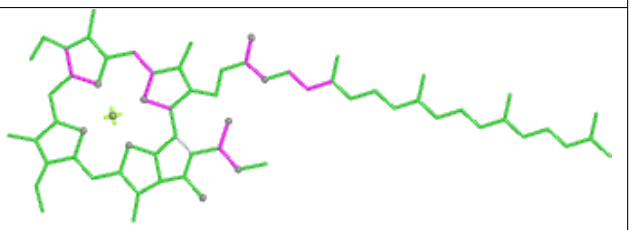
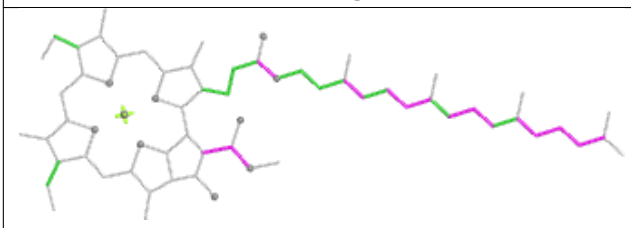
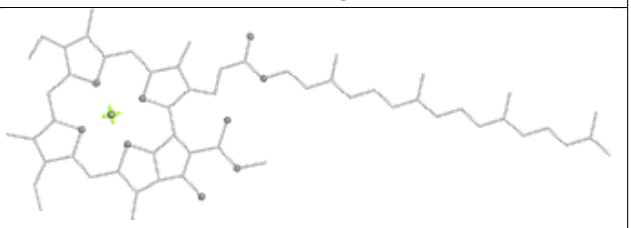


Torsions

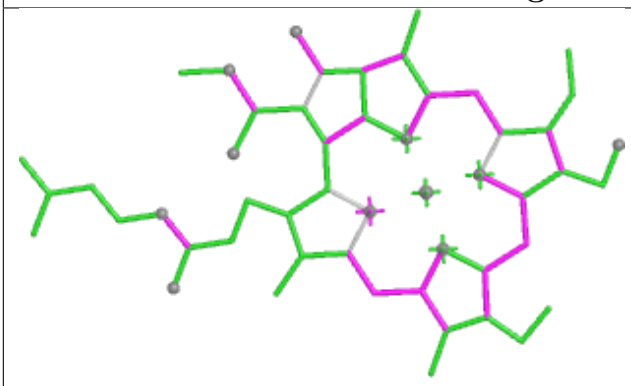


Rings

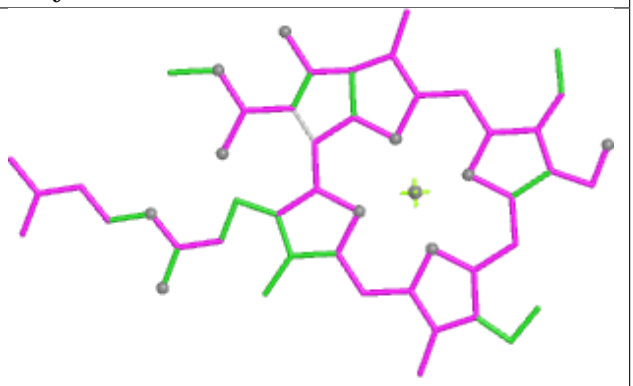
Ligand CLA N 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

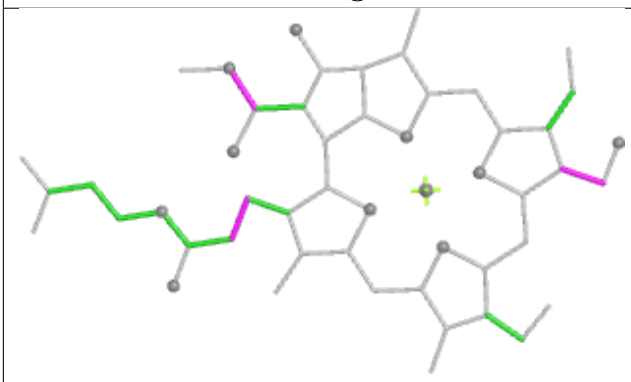
Ligand CHL y 312



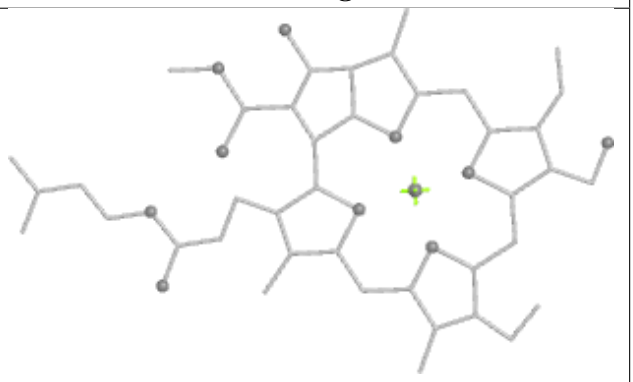
Bond lengths



Bond angles

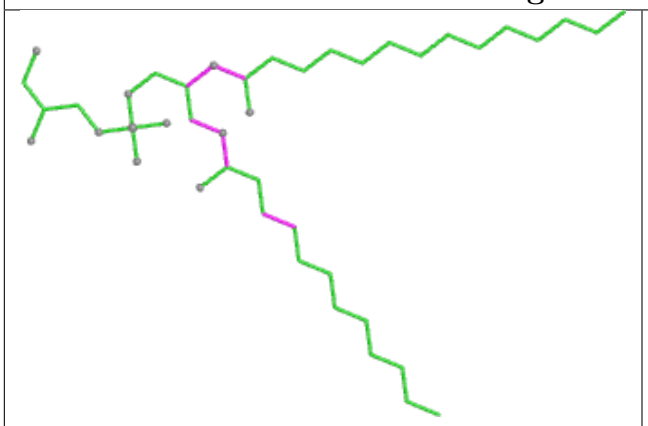


Torsions

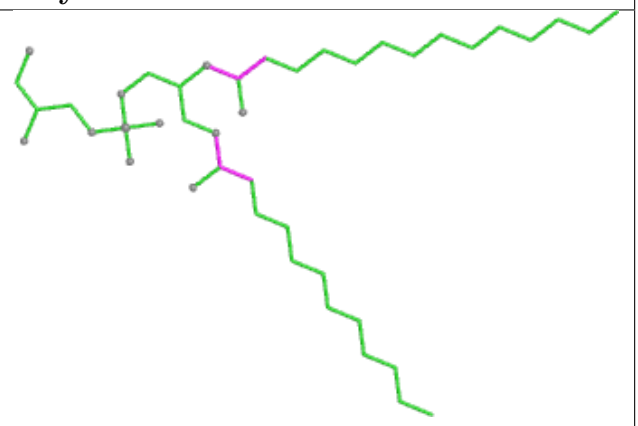


Rings

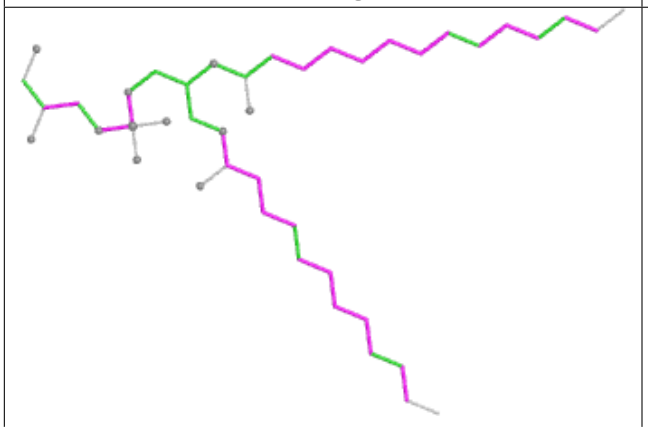
Ligand LHG y 319



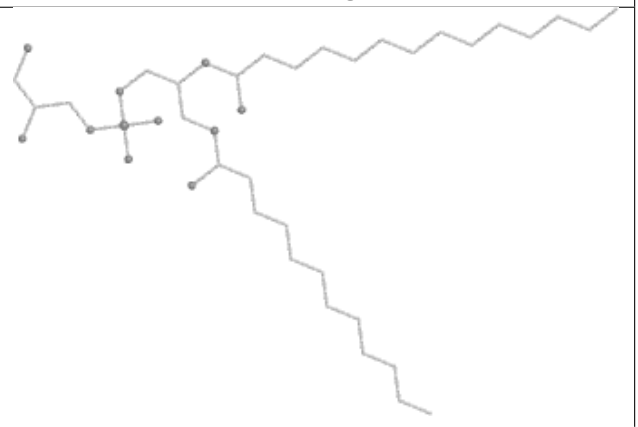
Bond lengths



Bond angles

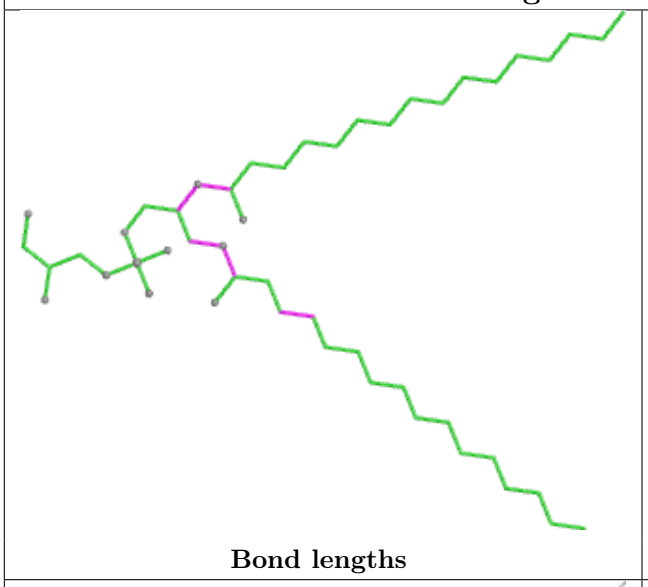


Torsions

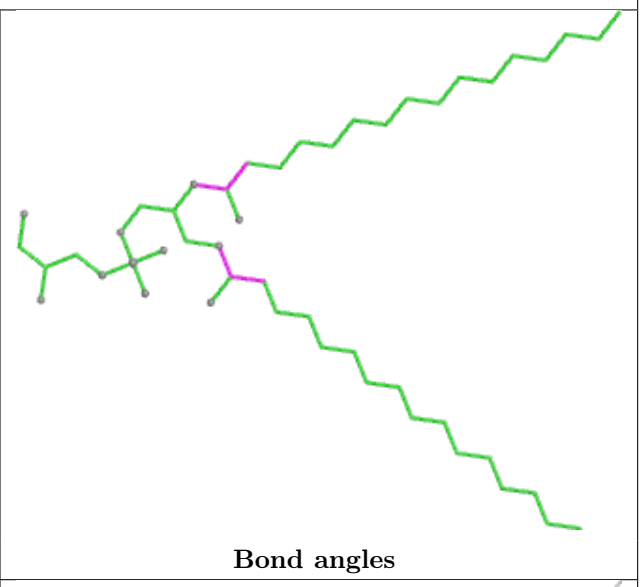


Rings

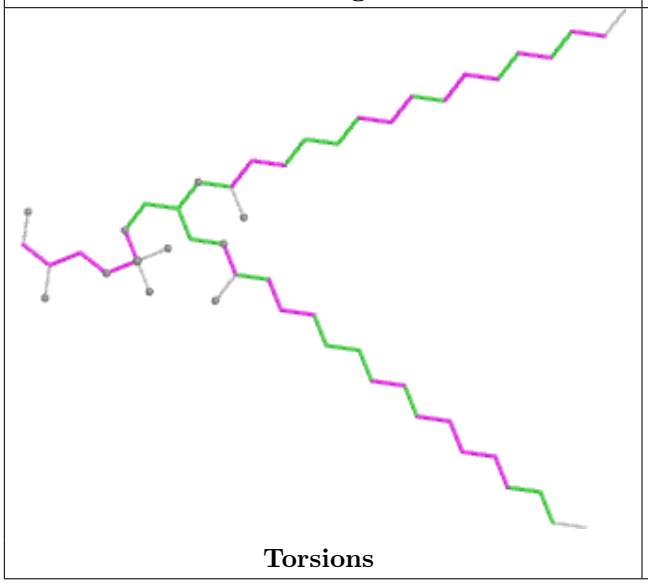
Ligand LHG D 407



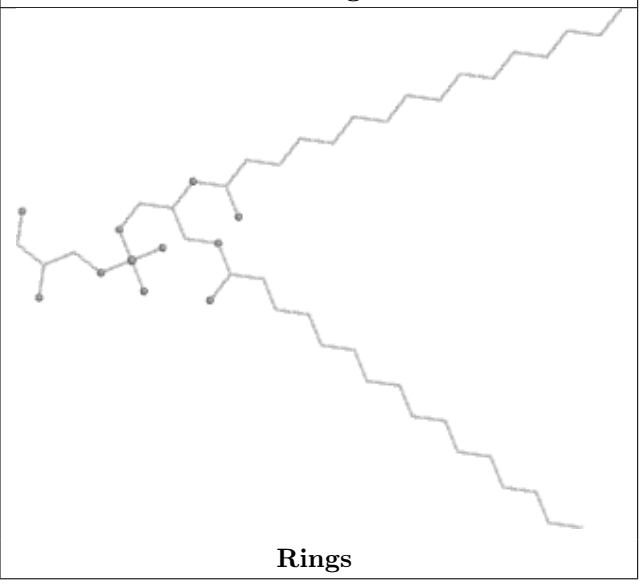
Bond lengths



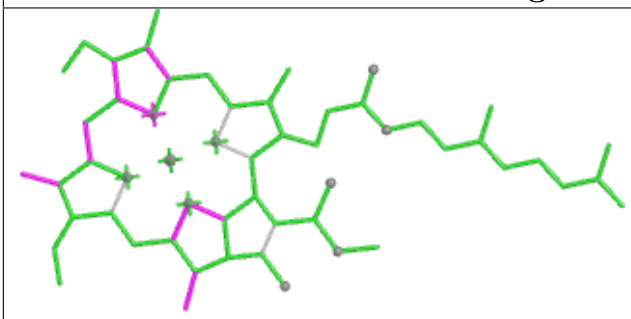
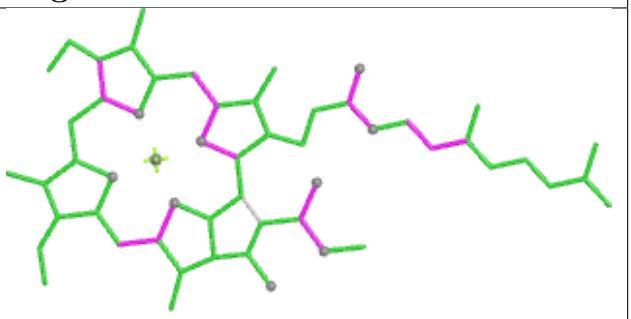
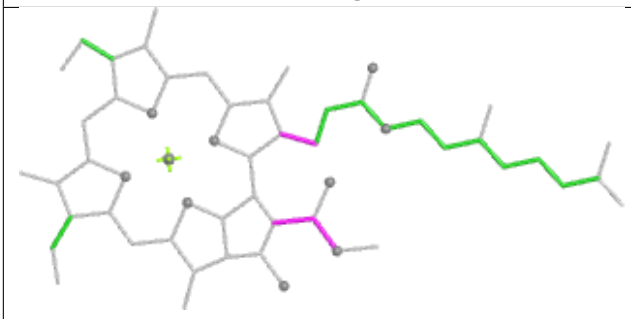
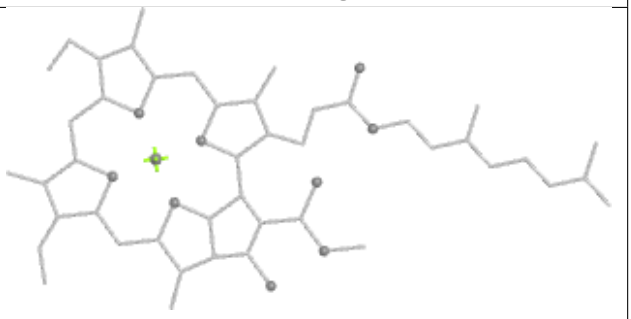
Bond angles

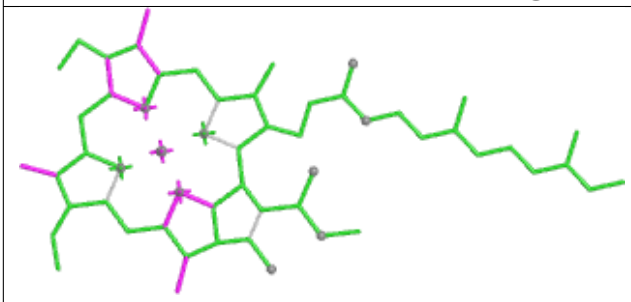
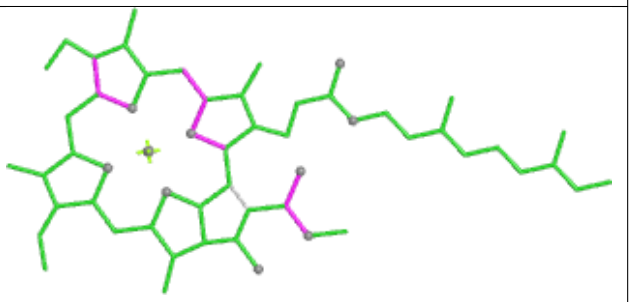
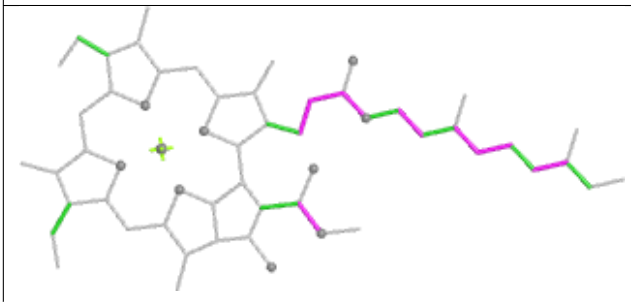
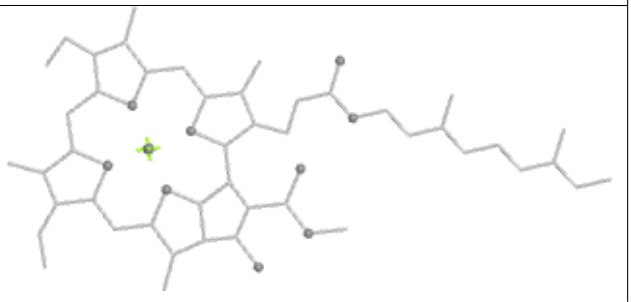


Torsions

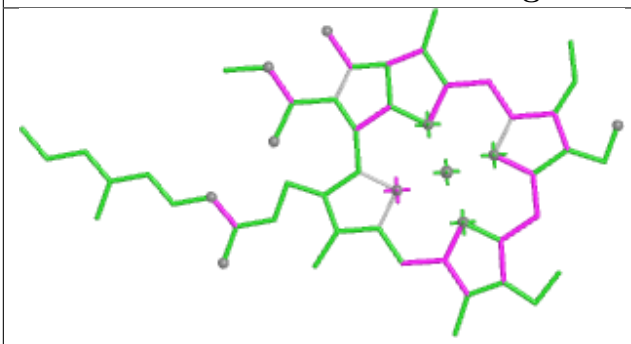


Rings

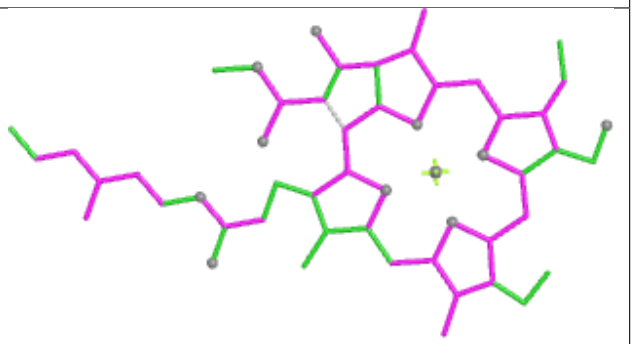
Ligand CLA g 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

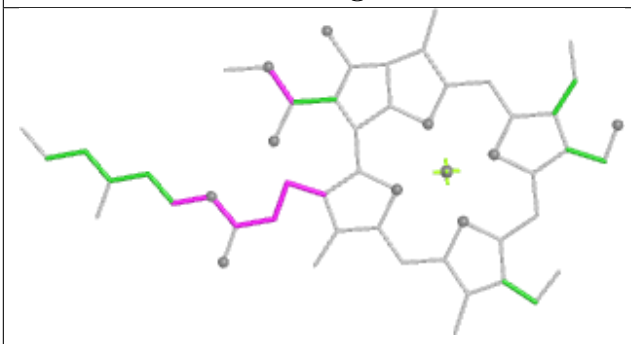
Ligand CHL N 310



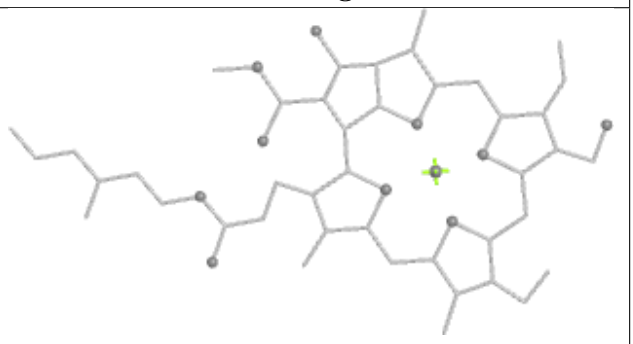
Bond lengths



Bond angles

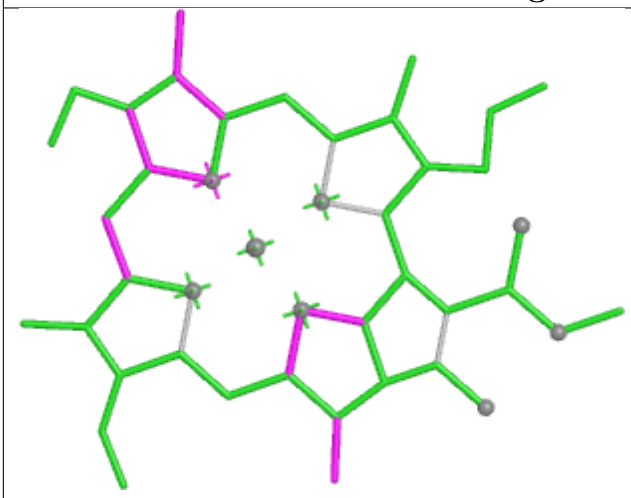


Torsions

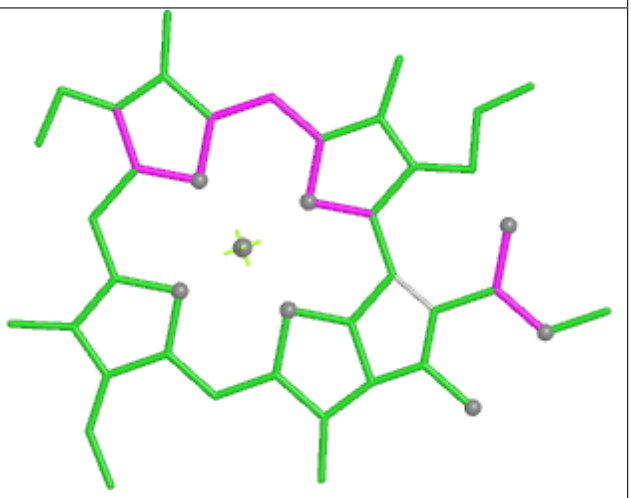


Rings

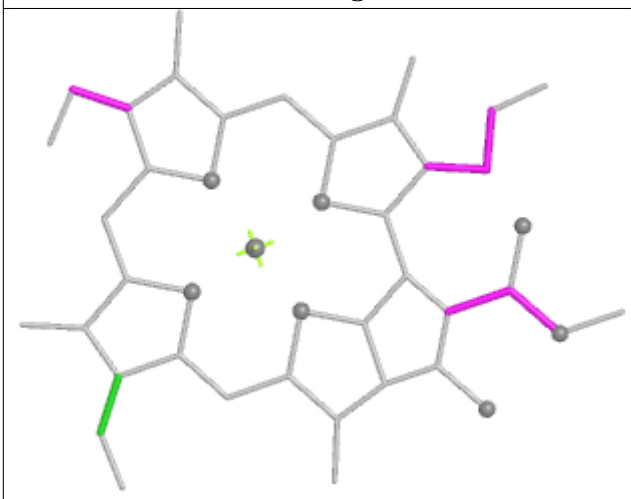
Ligand CLA 5 307



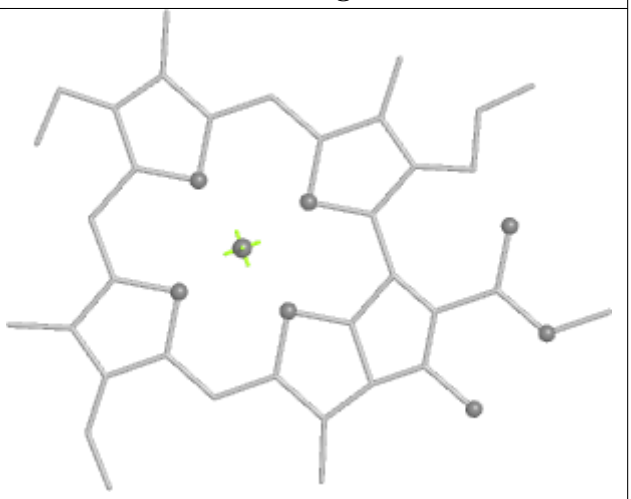
Bond lengths



Bond angles

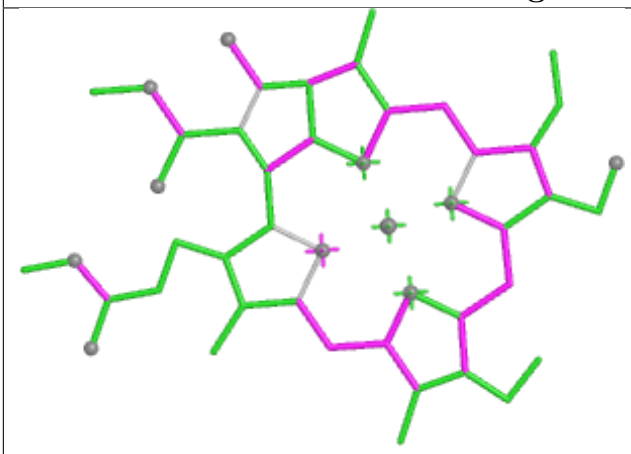


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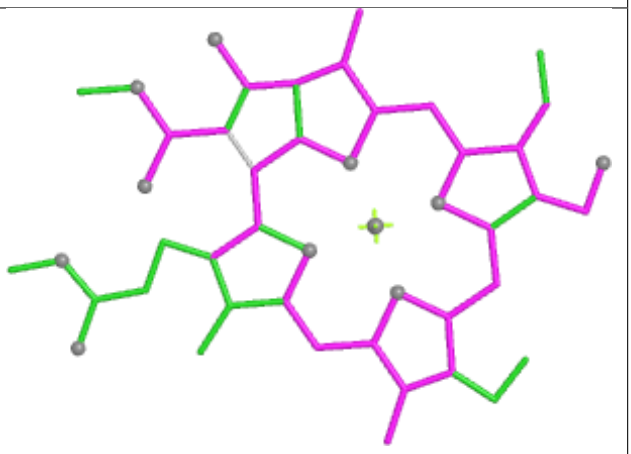


Rings

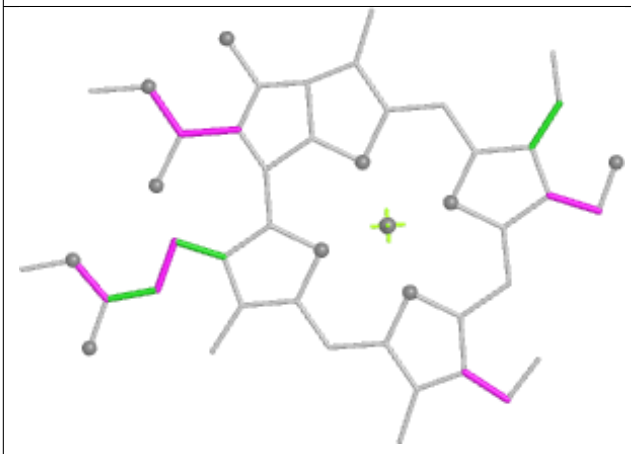
Ligand CHL 2 306



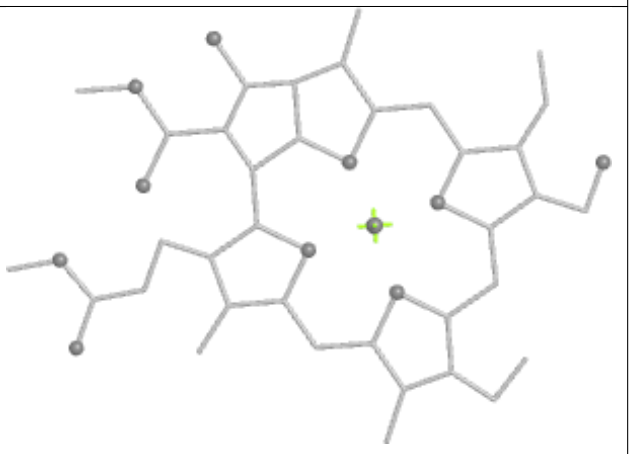
Bond lengths



Bond angles

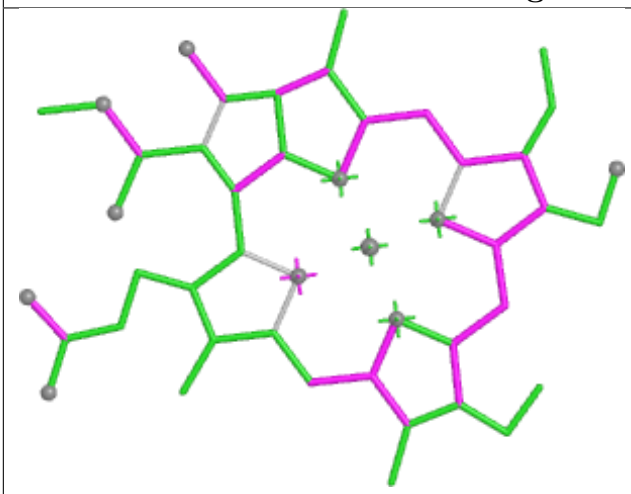


Torsions

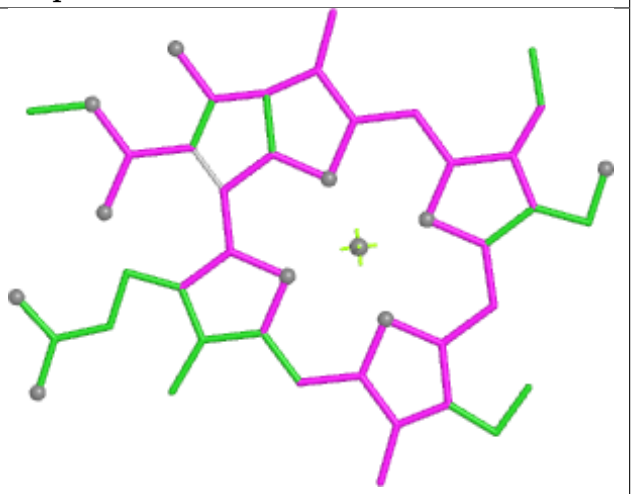


Rings

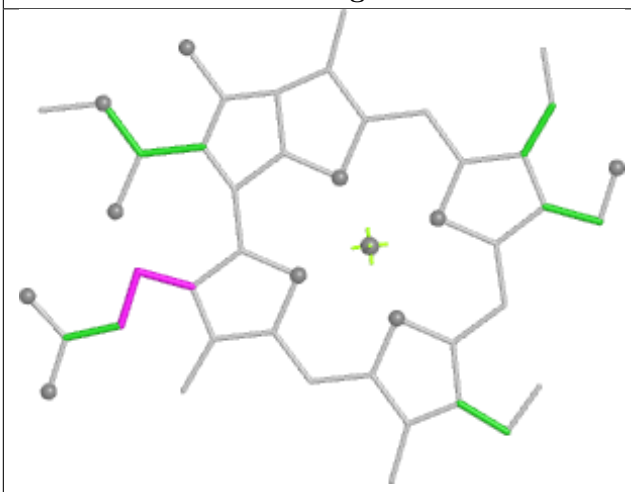
Ligand CHL p 311



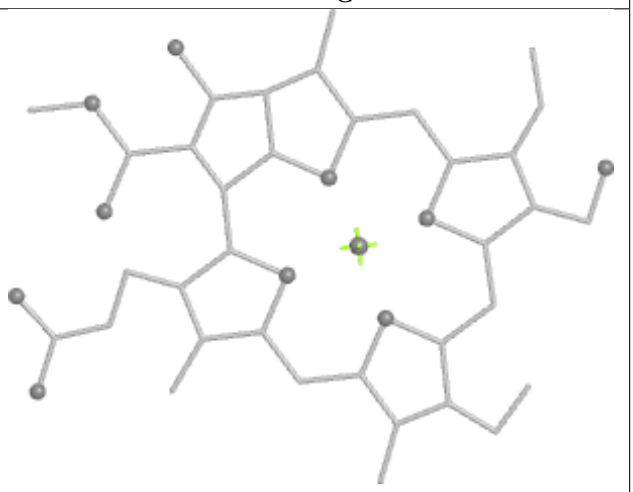
Bond lengths



Bond angles

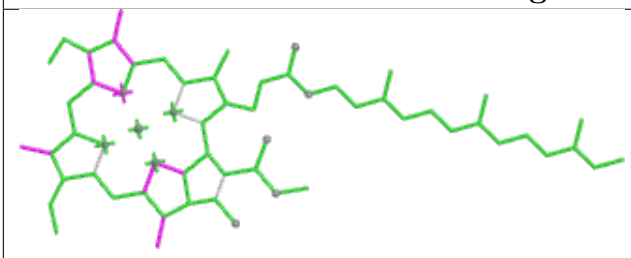


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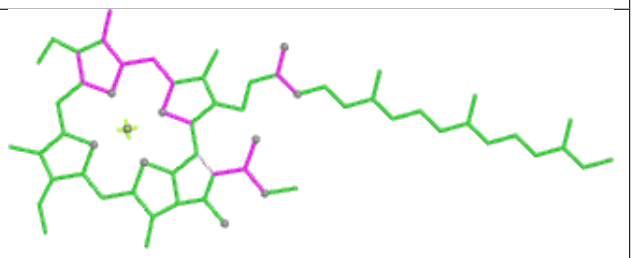


Rings

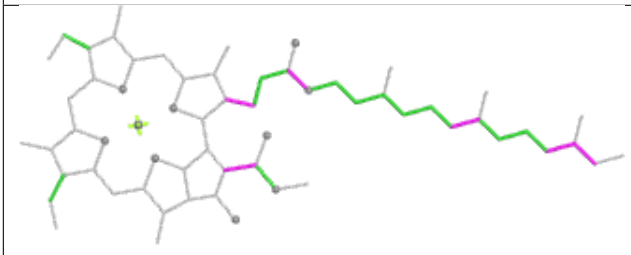
Ligand CLA c 608



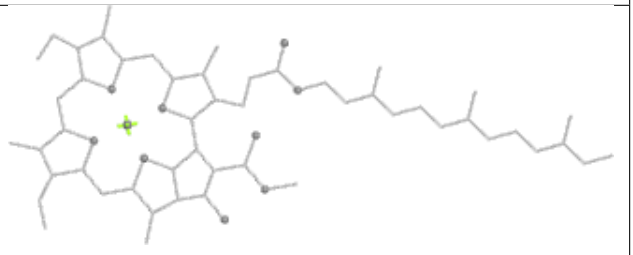
Bond lengths



Bond angles

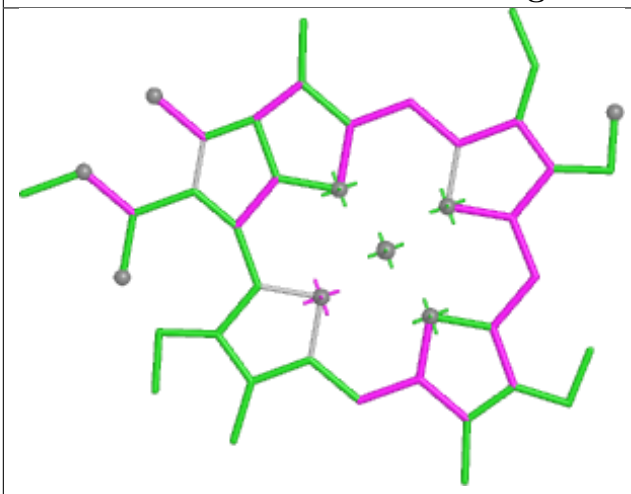


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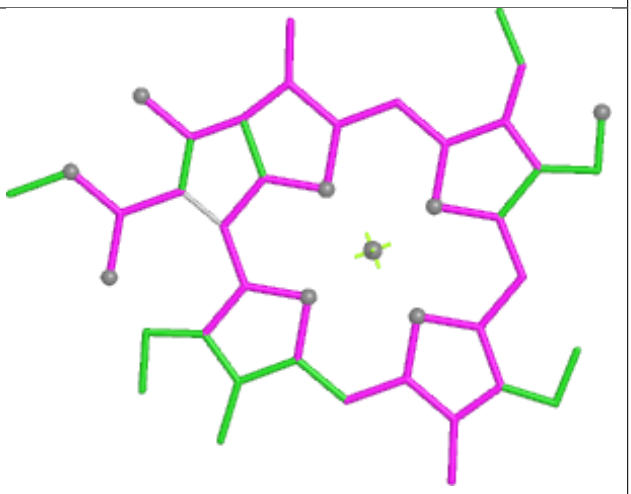


Rings

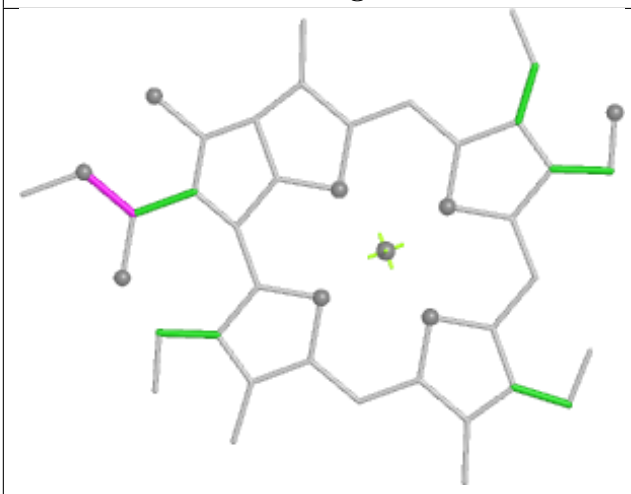
Ligand CHL 9 308



Bond lengths



Bond angles

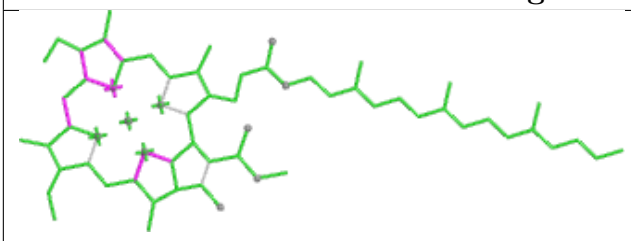


Torsions

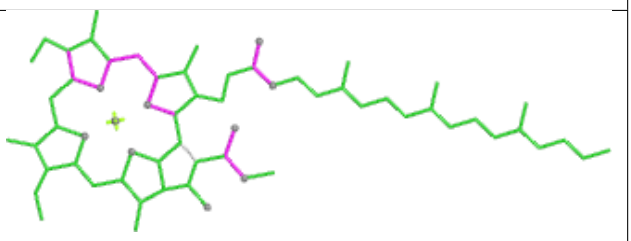


Rings

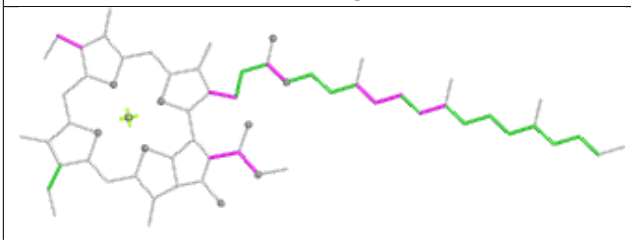
Ligand CLA u 315



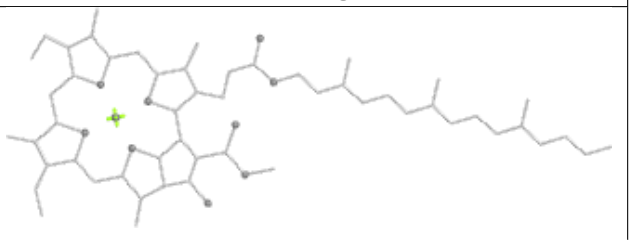
Bond lengths



Bond angles

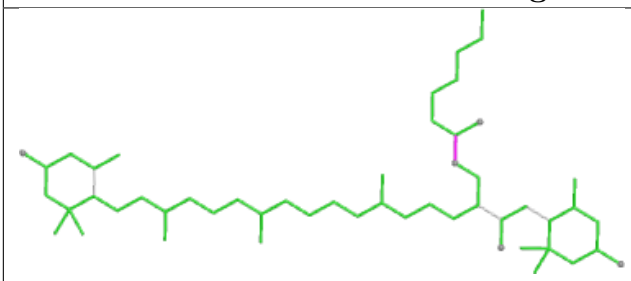


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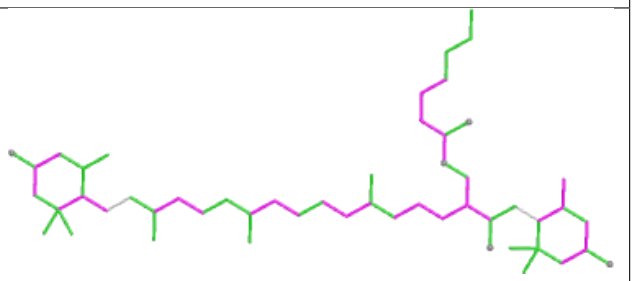


Rings

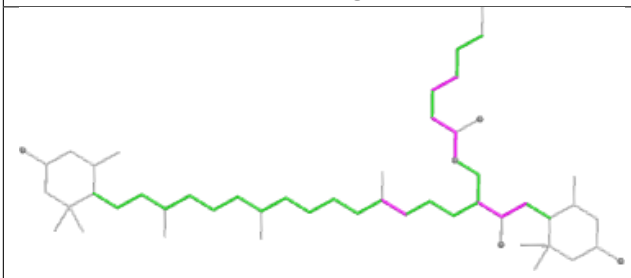
Ligand 0UR 9 301



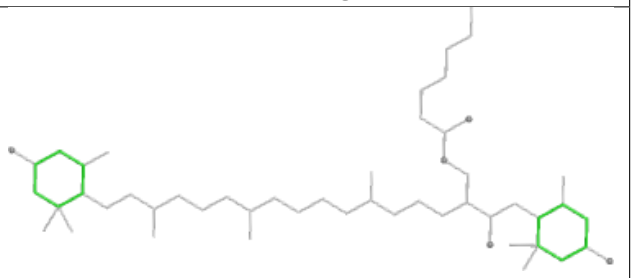
Bond lengths



Bond angles

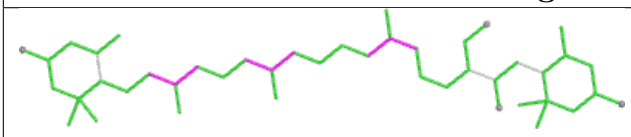


Torsions

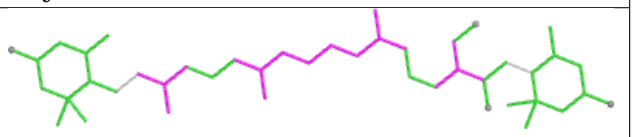


Rings

Ligand 0IE y 302



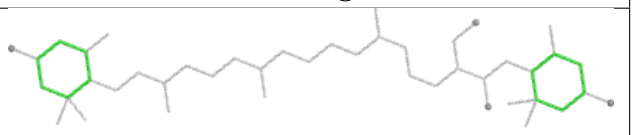
Bond lengths



Bond angles

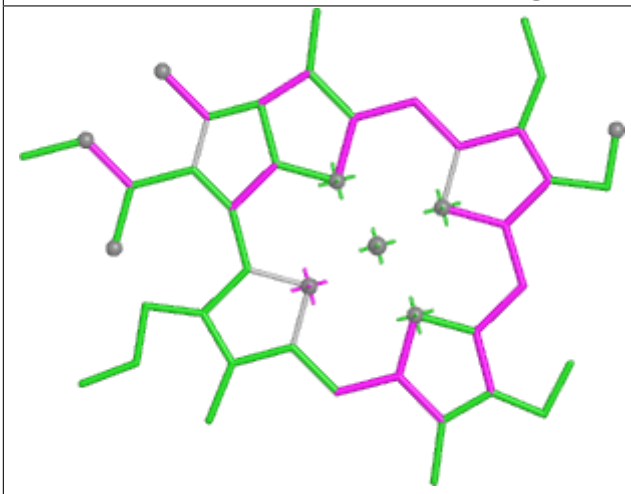


Torsions

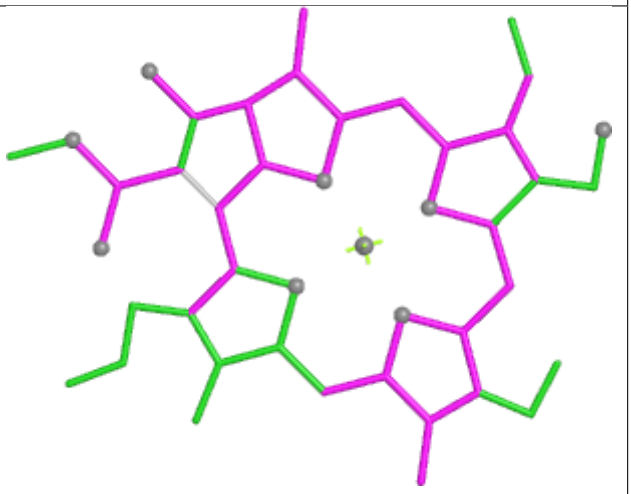


Rings

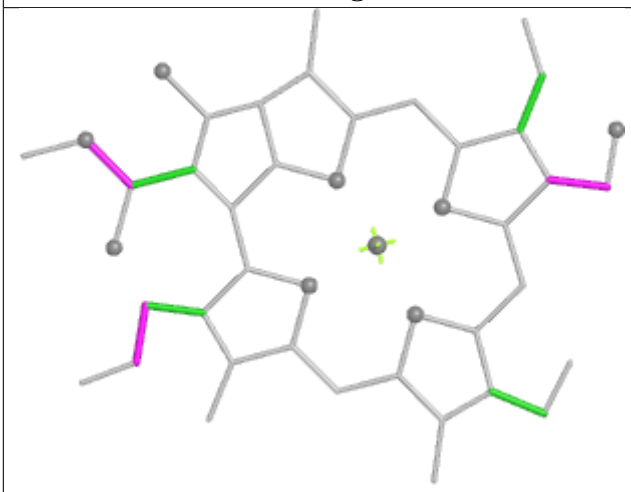
Ligand CHL 3 311



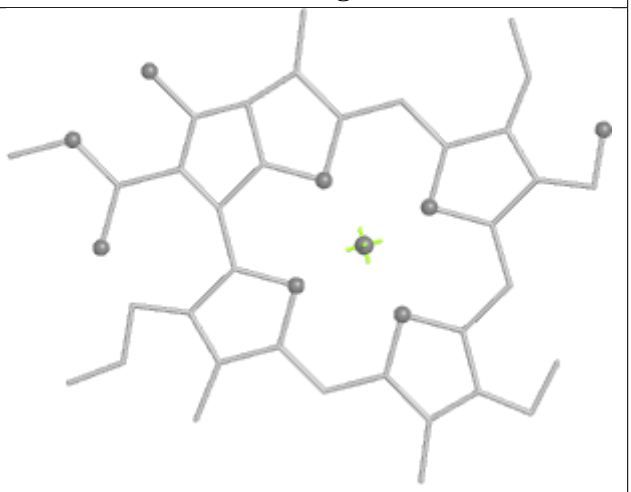
Bond lengths



Bond angles

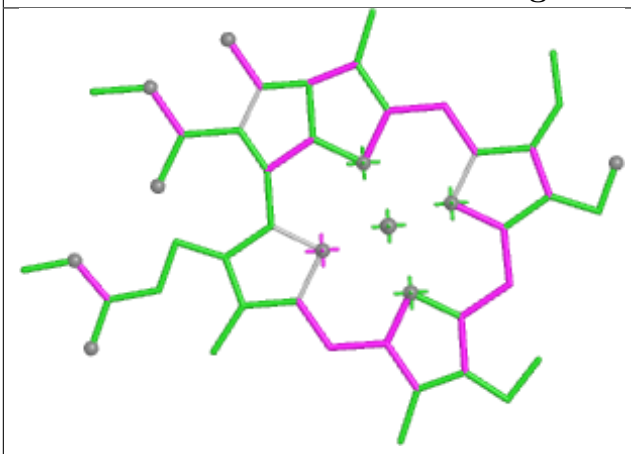


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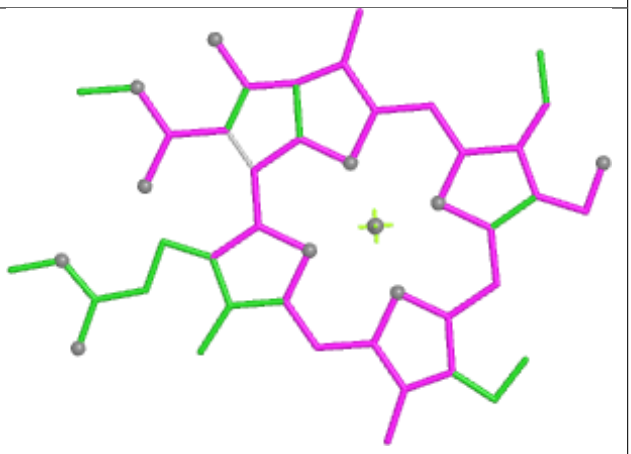


Rings

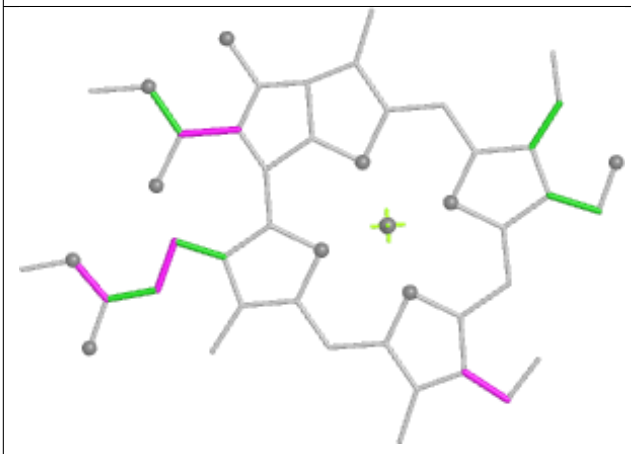
Ligand CHL r 303



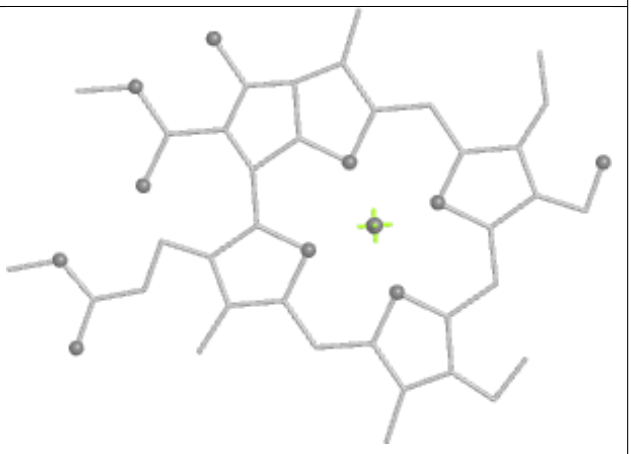
Bond lengths



Bond angles

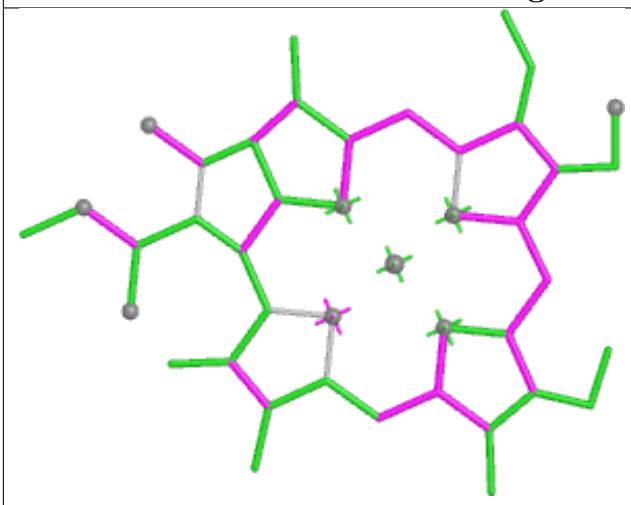


Torsions

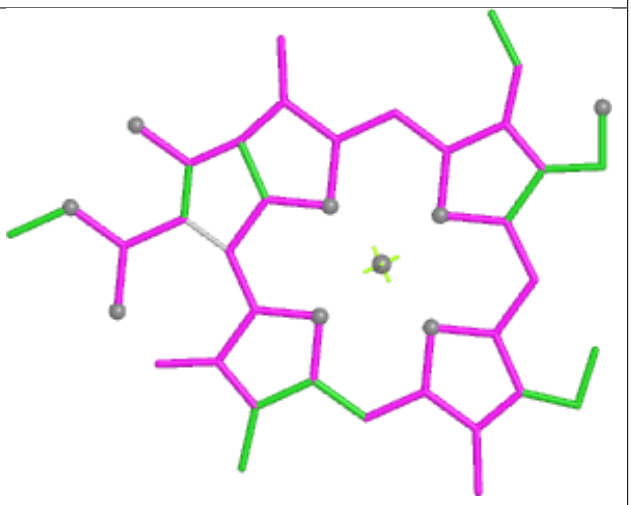


Rings

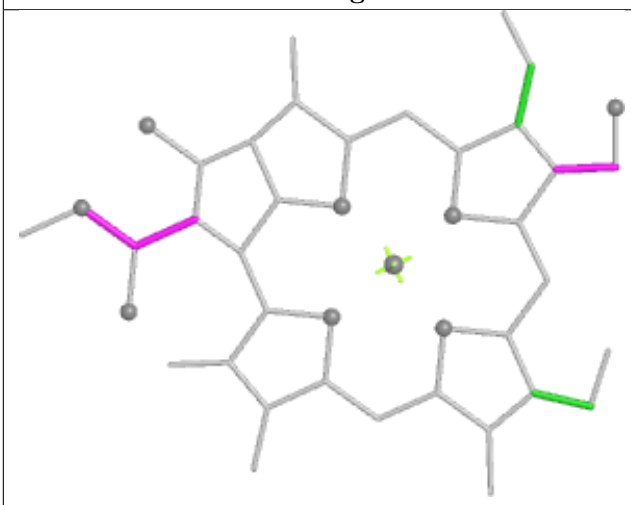
Ligand CHL 4 317



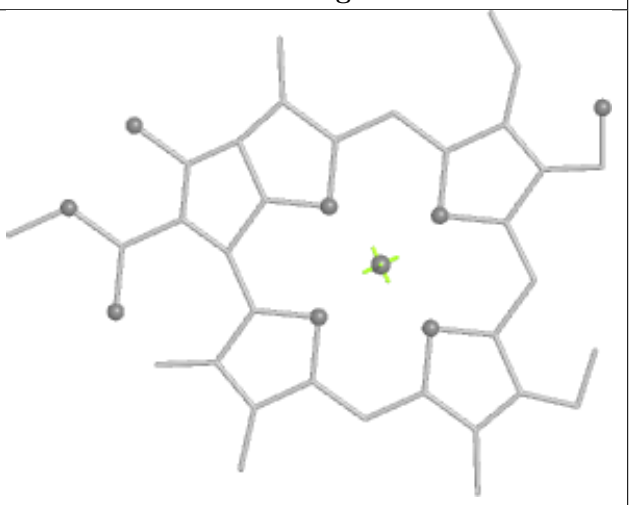
Bond lengths



Bond angles

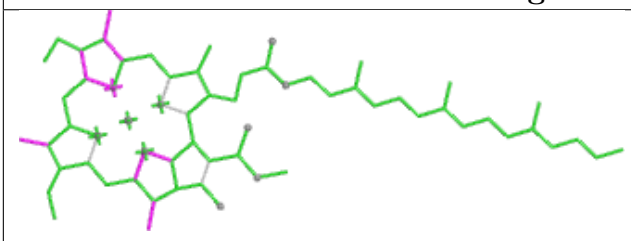


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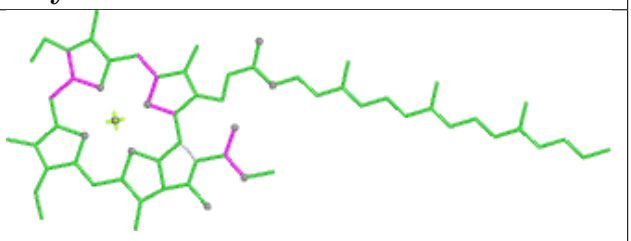


Rings

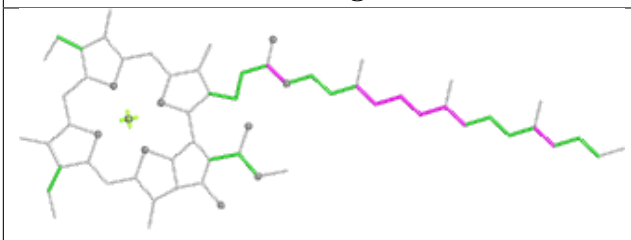
Ligand CLA y 315



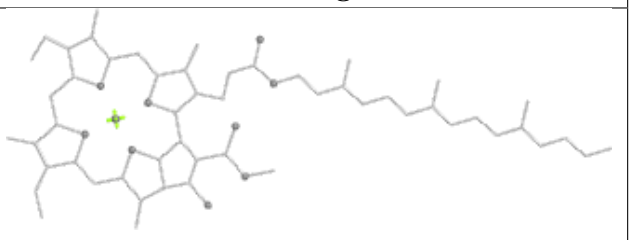
Bond lengths



Bond angles

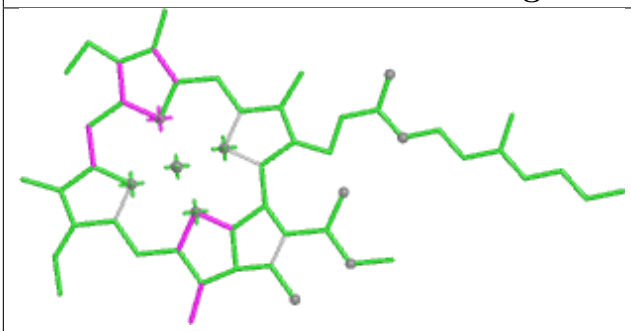


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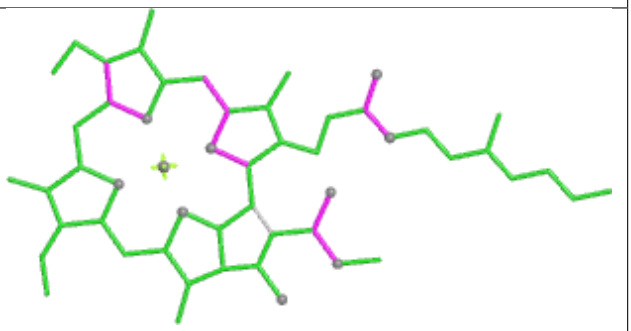


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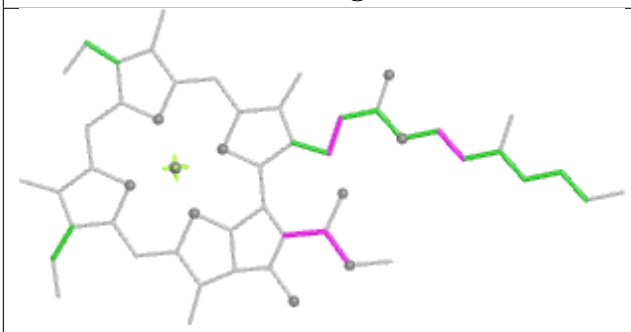
Ligand CLA G 307



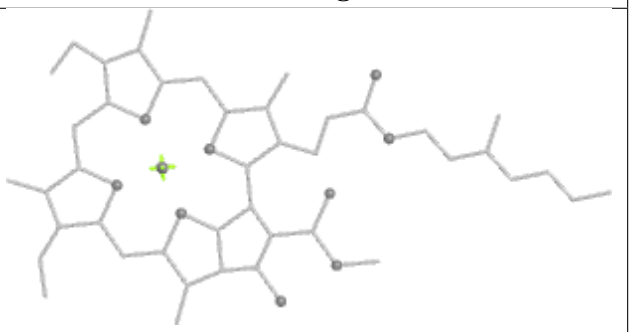
Bond lengths



Bond angles

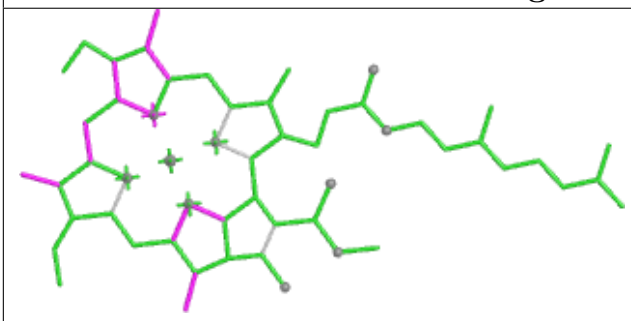


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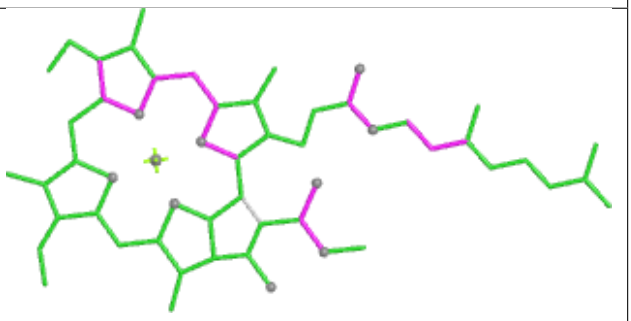


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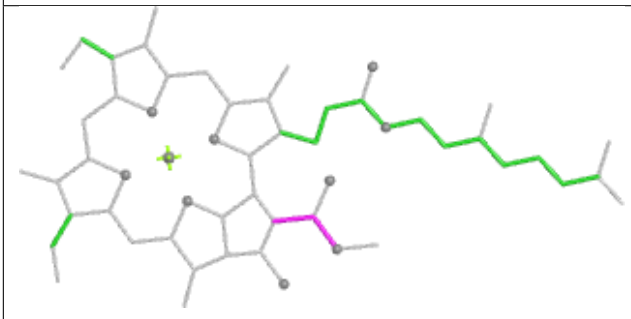
Ligand CLA 8 311



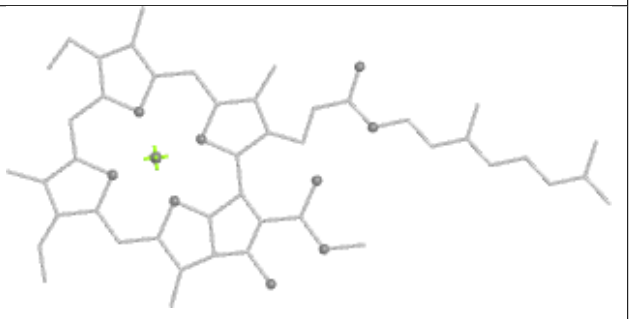
Bond lengths



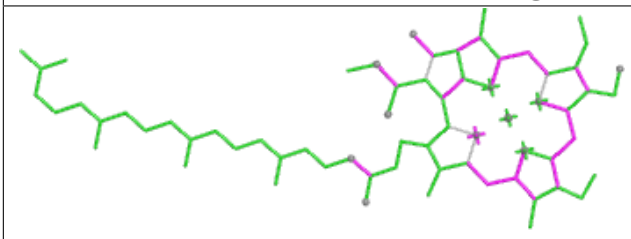
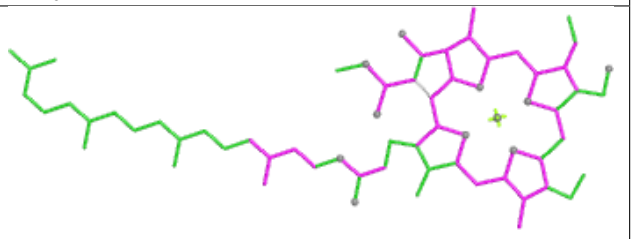
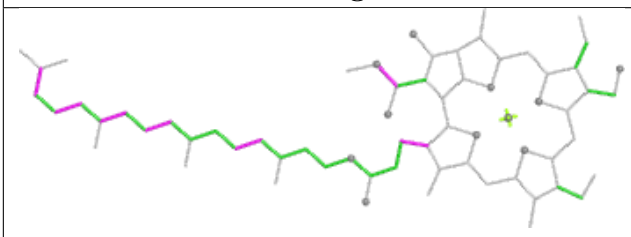
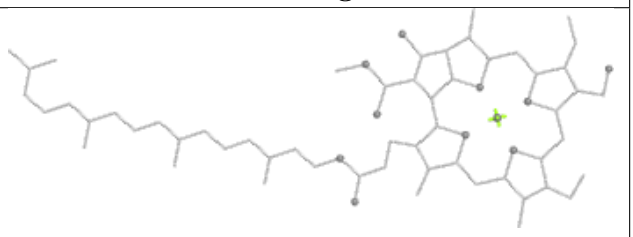
Bond angles

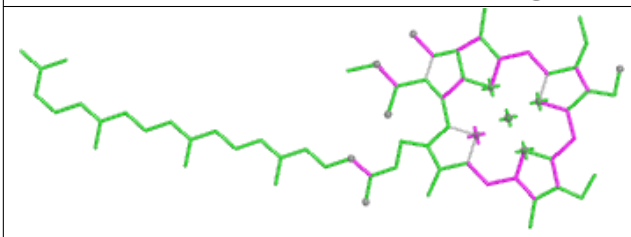
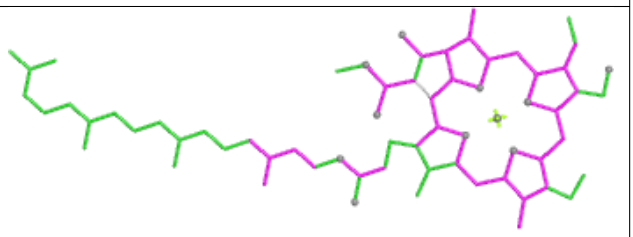
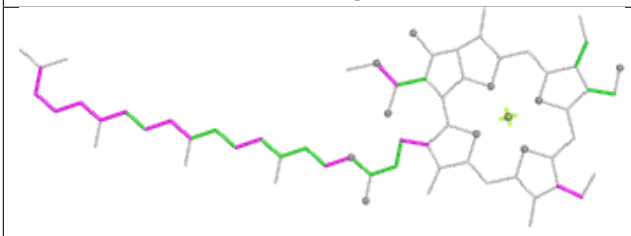
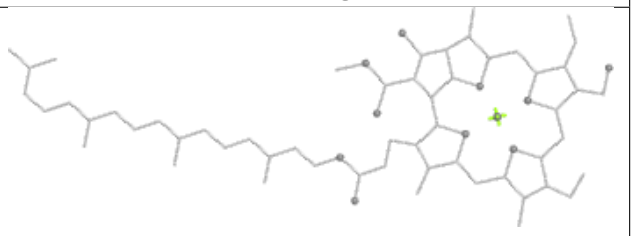


Torsions

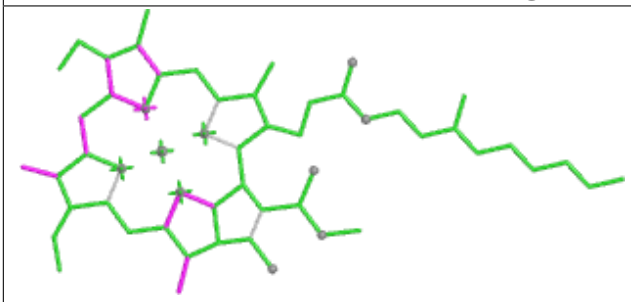


Rings

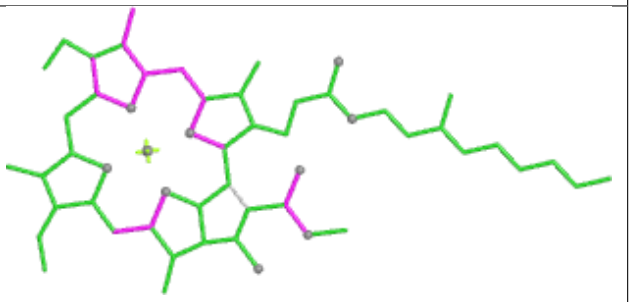
Ligand CHL y 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 7 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

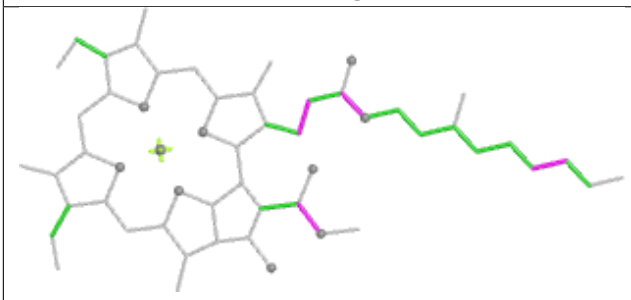
Ligand CLA G 317



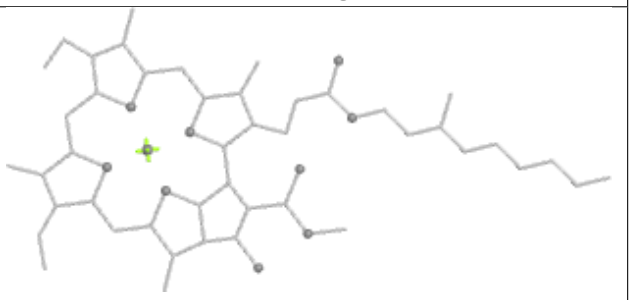
Bond lengths



Bond angles

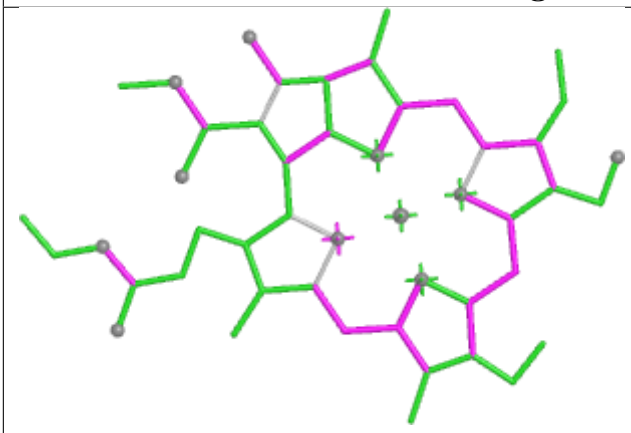


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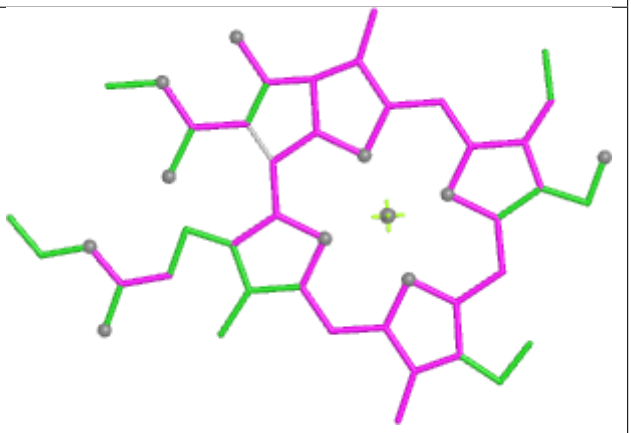


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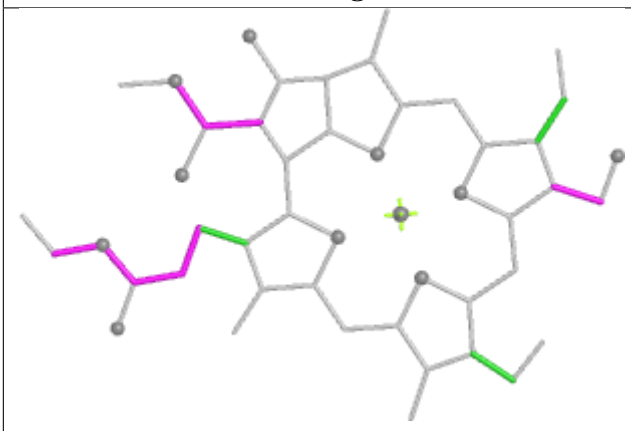
Ligand CHL r 308



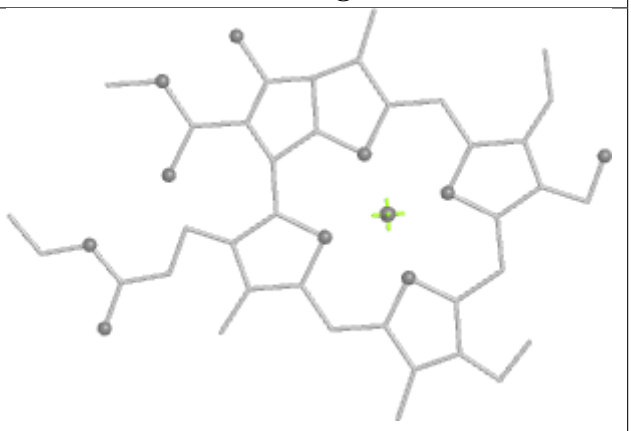
Bond lengths



Bond angles

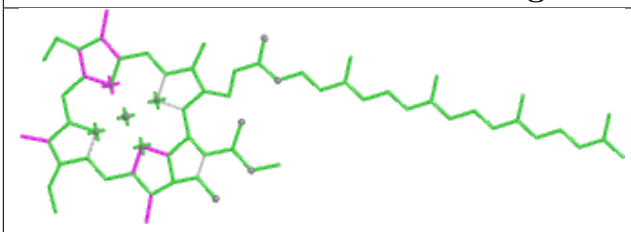


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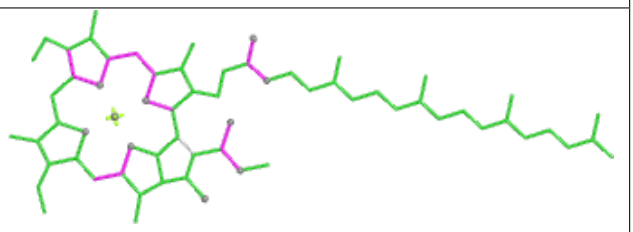


Rings

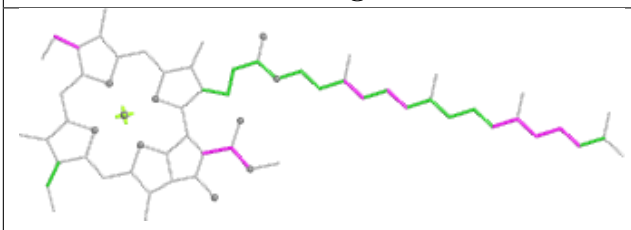
Ligand CLA b 605



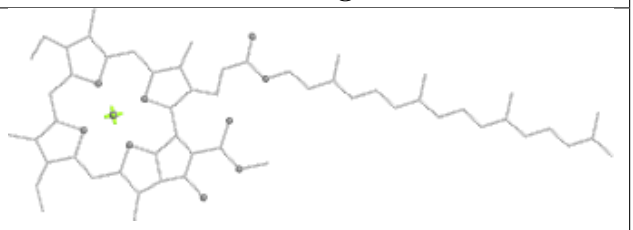
Bond lengths



Bond angles

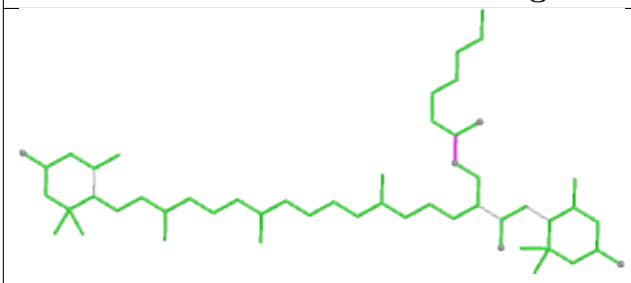


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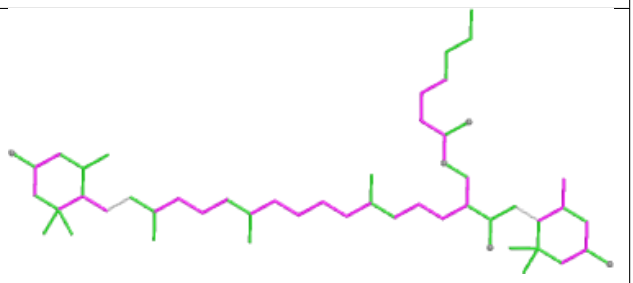


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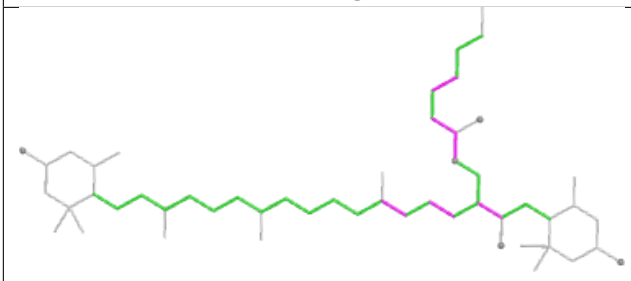
Ligand 0UR 6 301



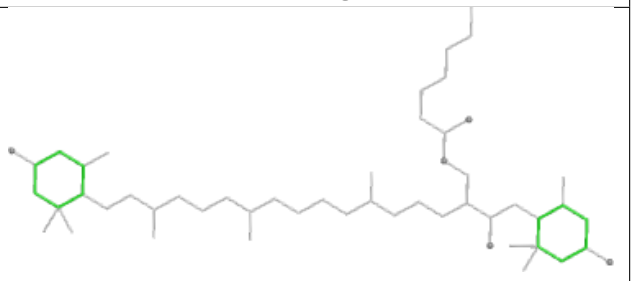
Bond lengths



Bond angles

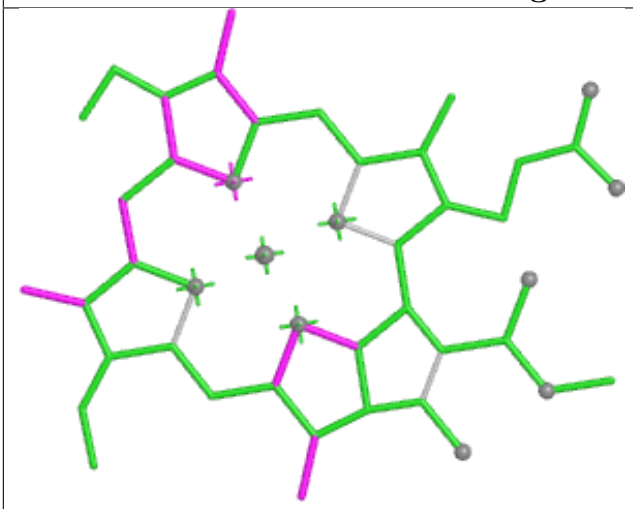


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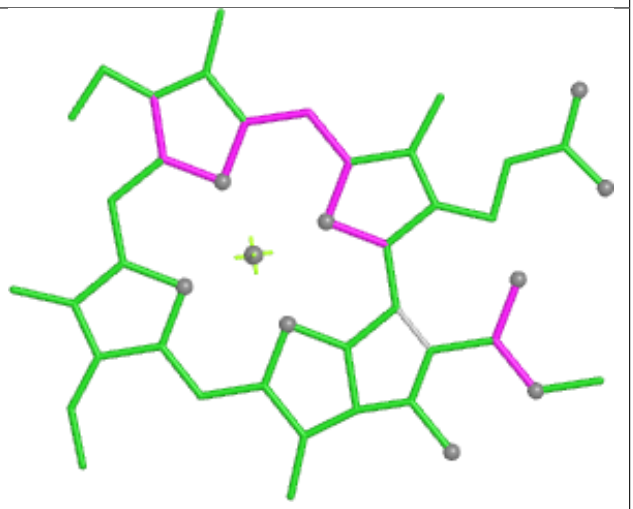


Rings

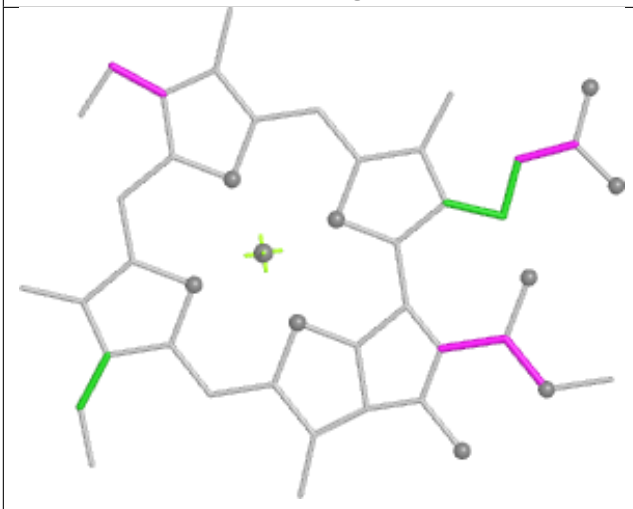
Ligand CLA r 312



Bond lengths



Bond angles

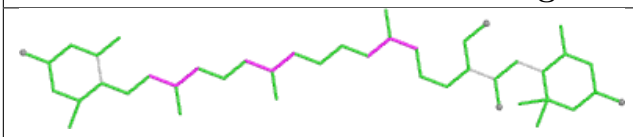


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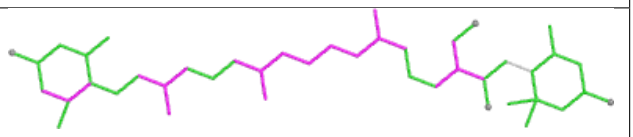


Rings

Ligand 0IE 3 302



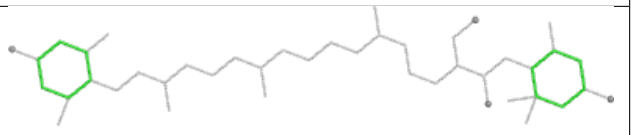
Bond lengths



Bond angles

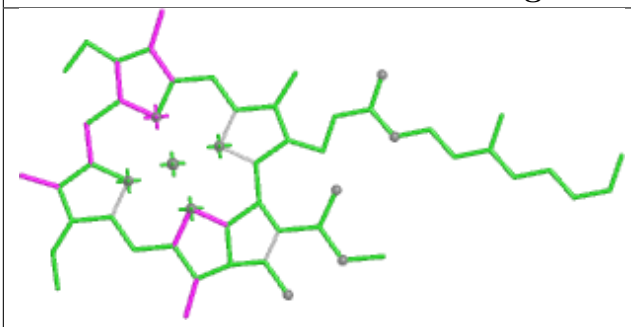


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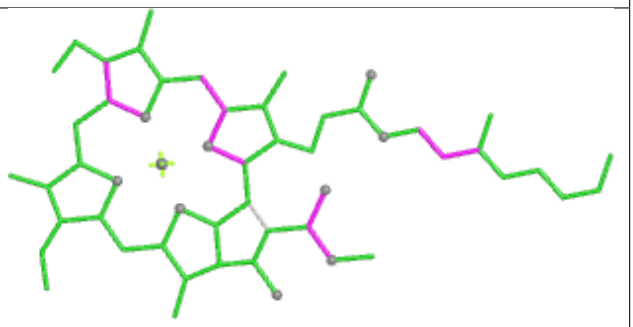


Rings

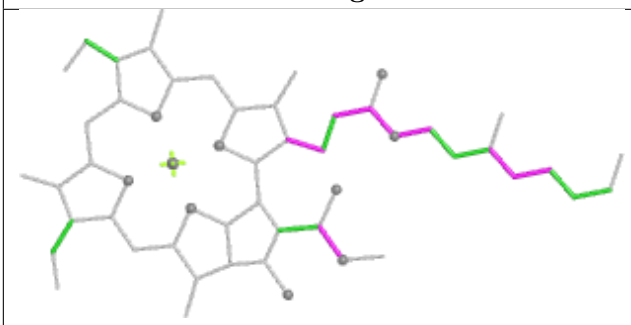
Ligand CLA C 612



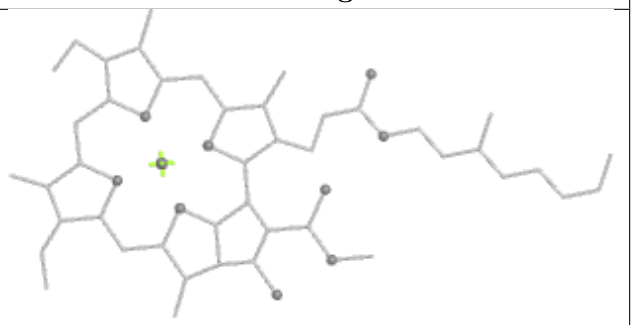
Bond lengths



Bond angles

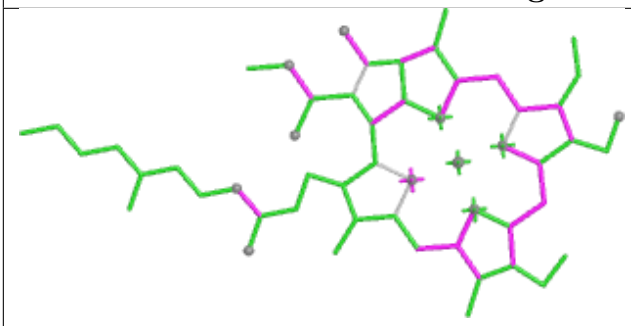


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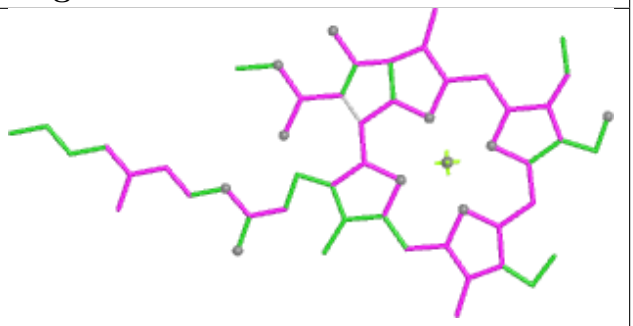


Rings

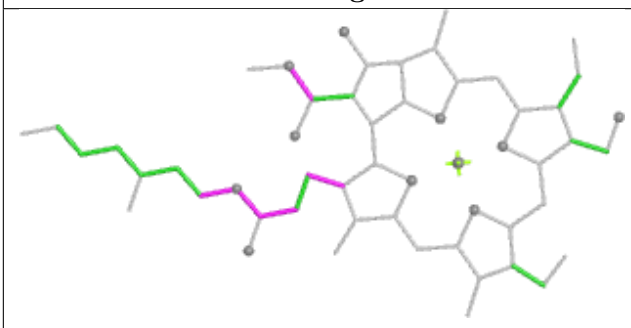
Ligand CHL g 311



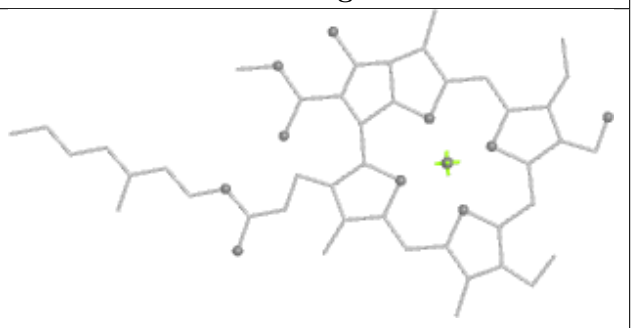
Bond lengths



Bond angles

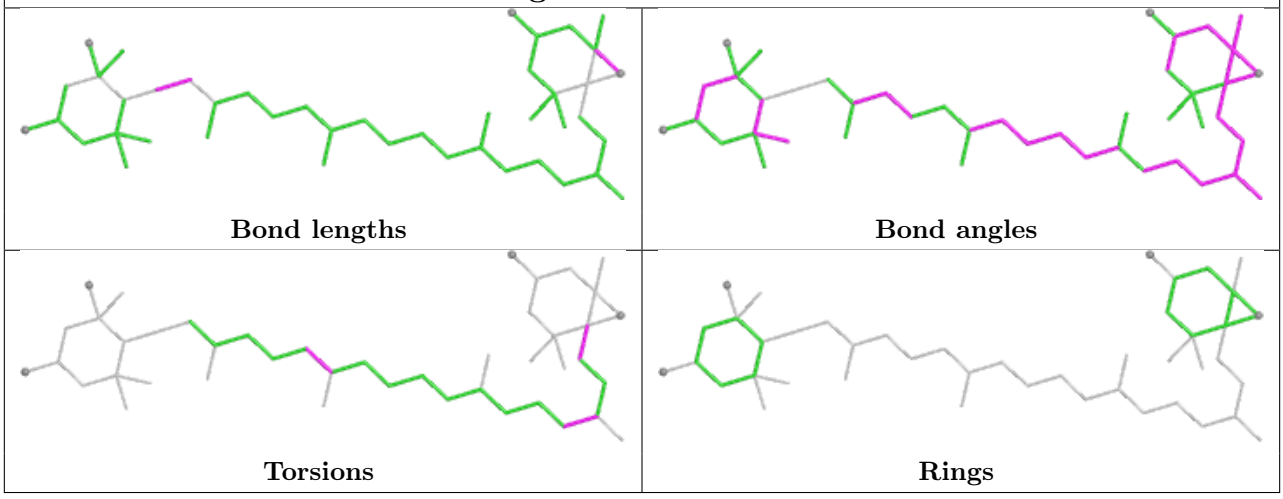


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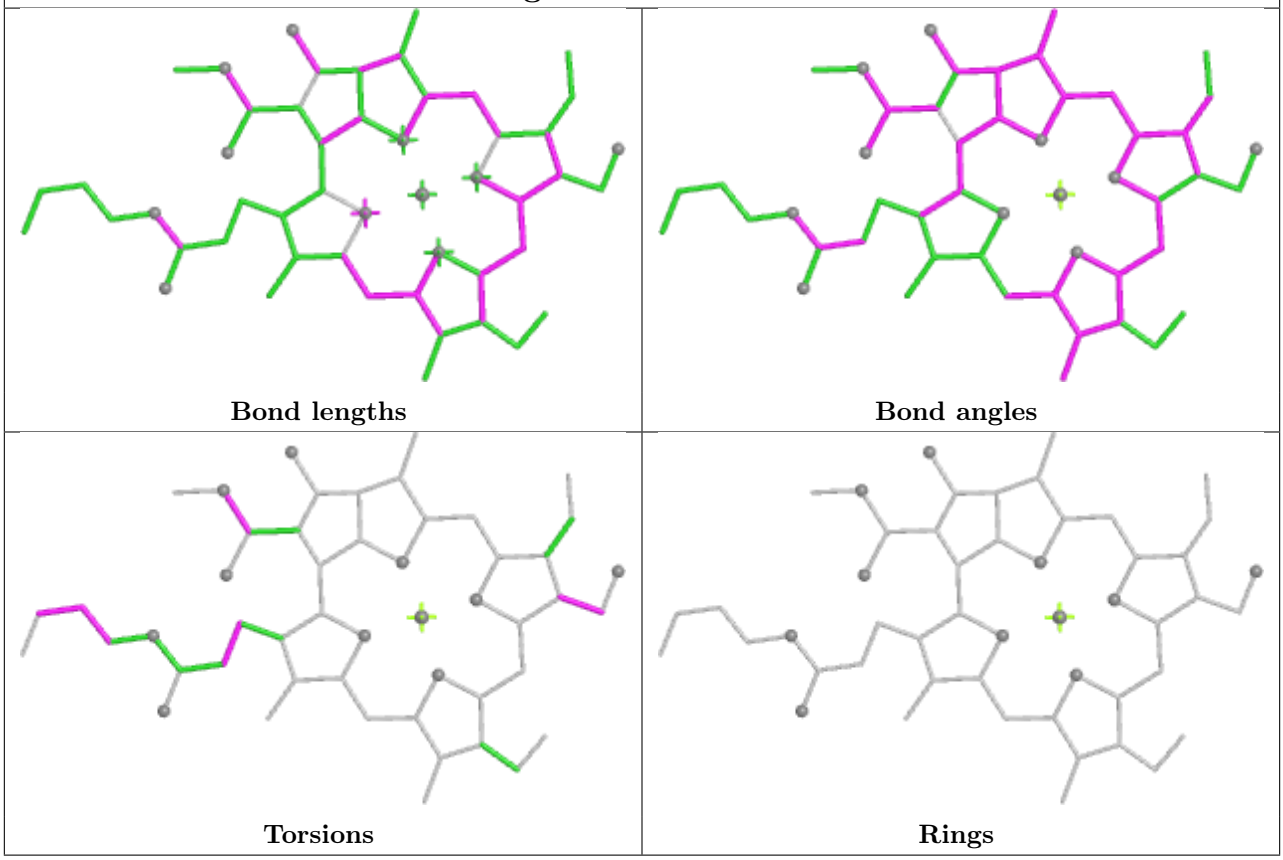


Rings

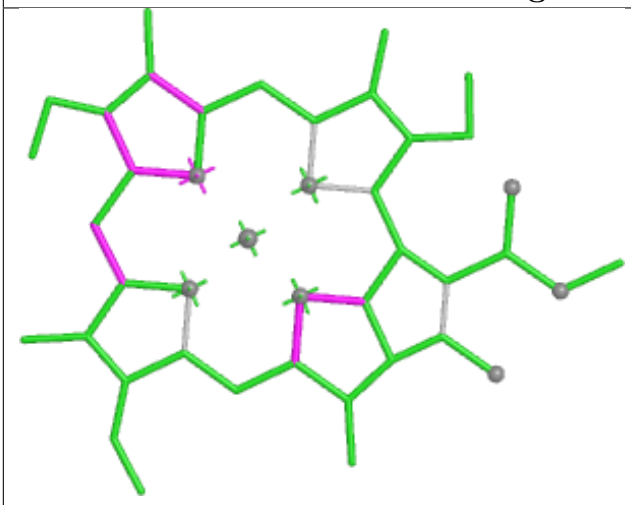
Ligand NEX s 401



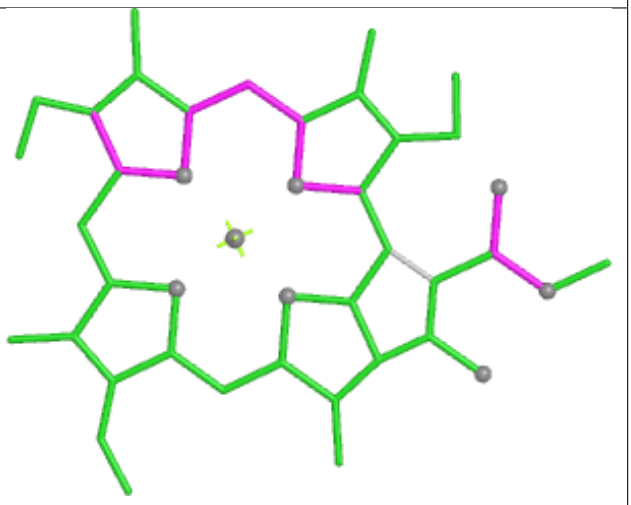
Ligand CHL N 311



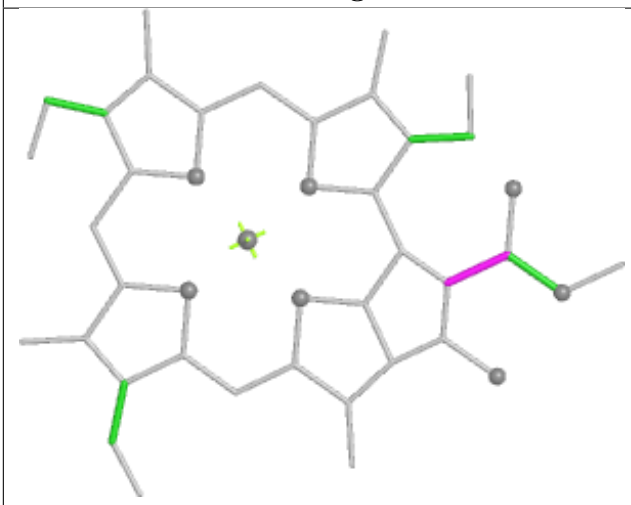
Ligand CLA 1 316



Bond lengths



Bond angles

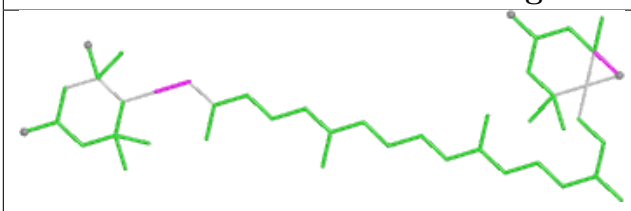


Torsions

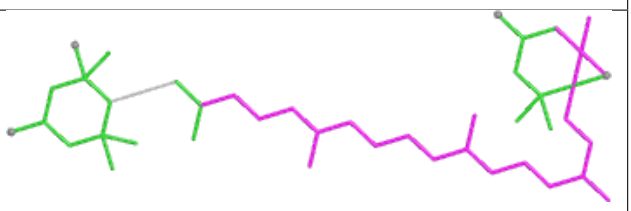


Rings

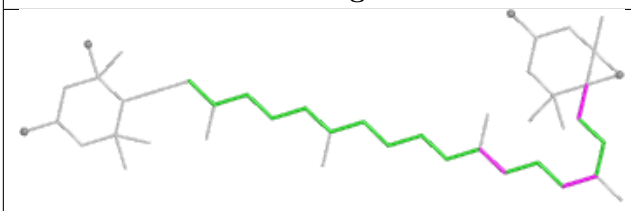
Ligand NEX u 304



Bond lengths



Bond angles

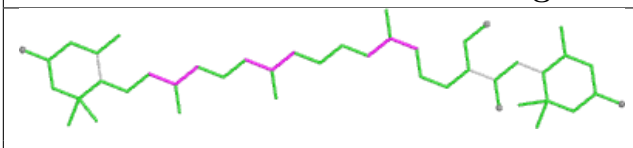


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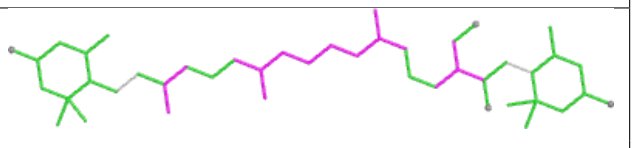


Rings

Ligand 0IE G 302



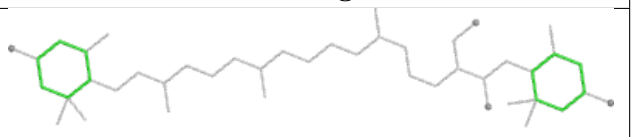
Bond lengths



Bond angles

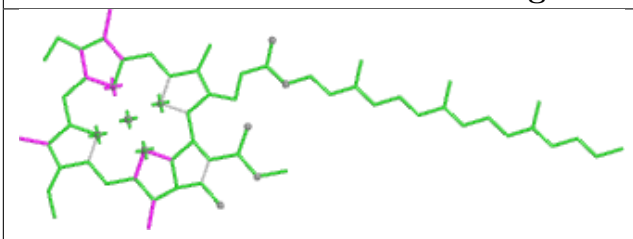


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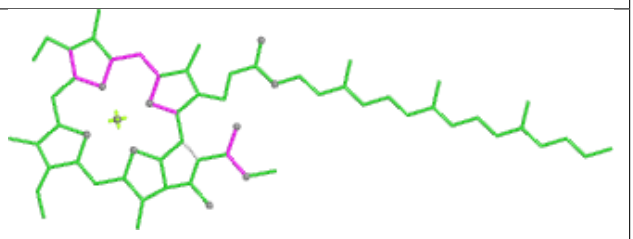


Rings

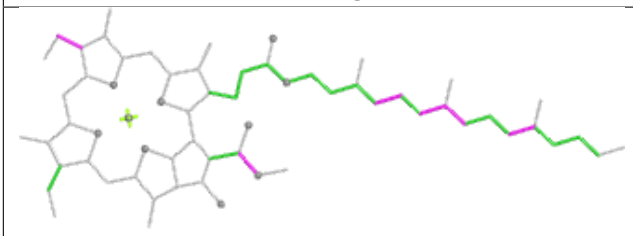
Ligand CLA 5 315



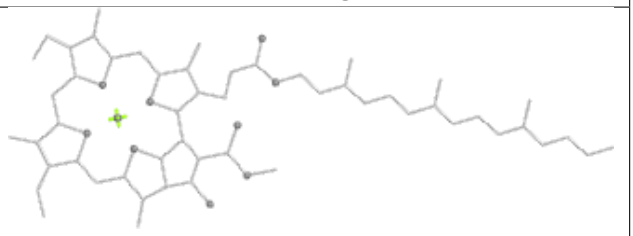
Bond lengths



Bond angles

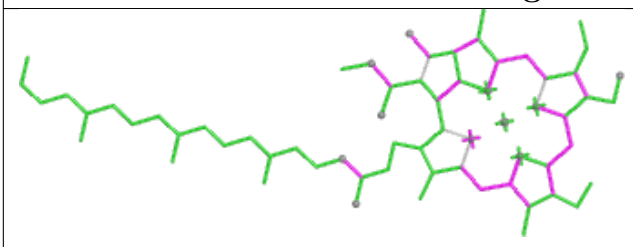


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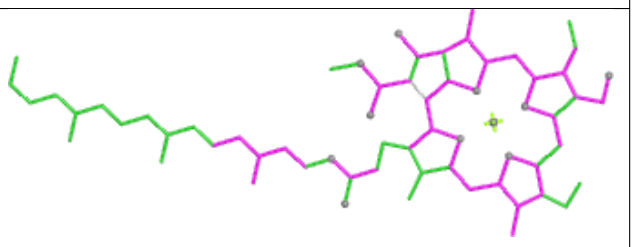


Rings

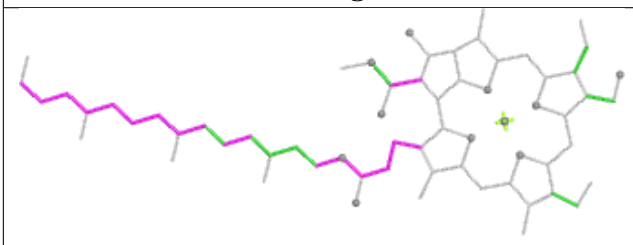
Ligand CHL Y 305



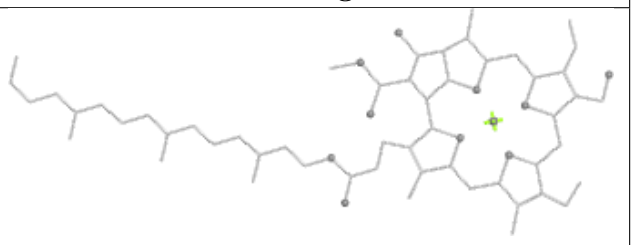
Bond lengths



Bond angles

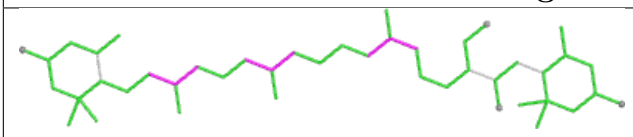


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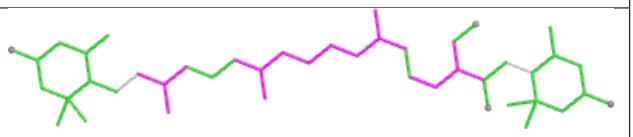


Rings

Ligand 0IE u 302



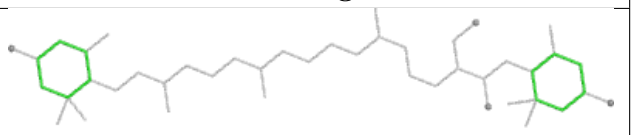
Bond lengths



Bond angles

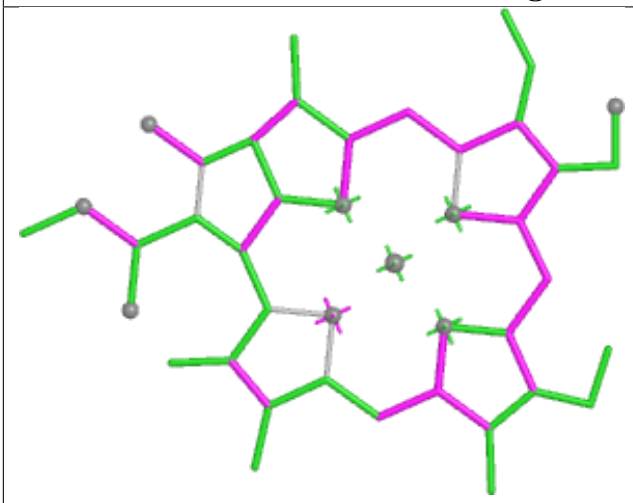


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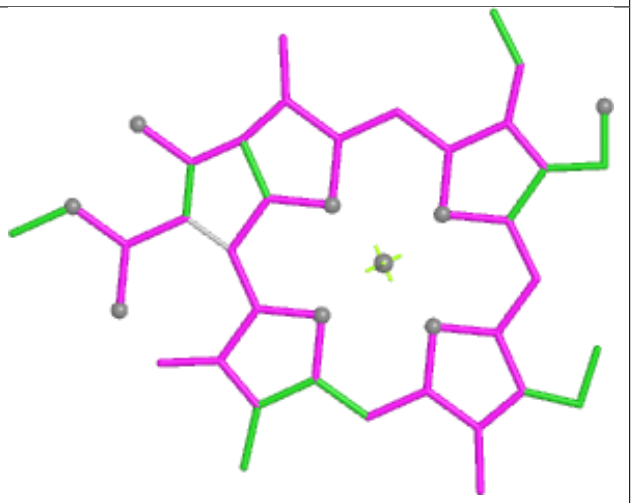


Rings

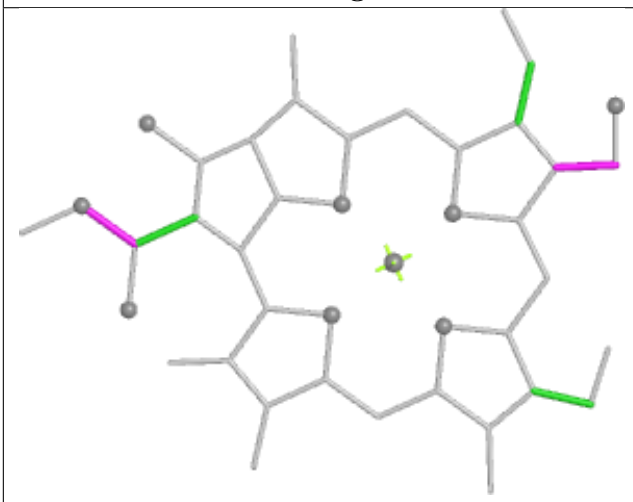
Ligand CHL n 317



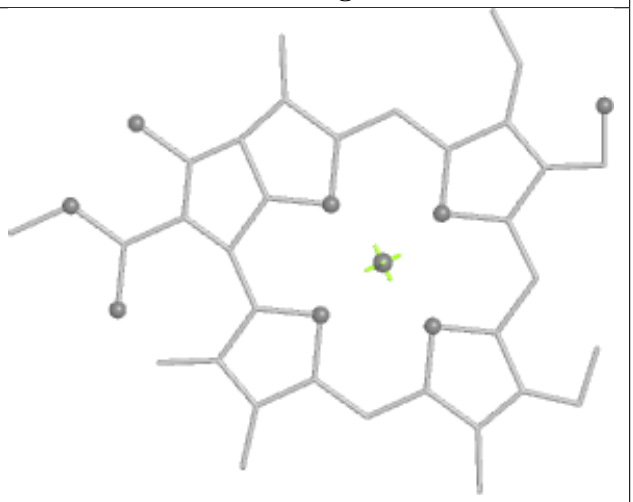
Bond lengths



Bond angles

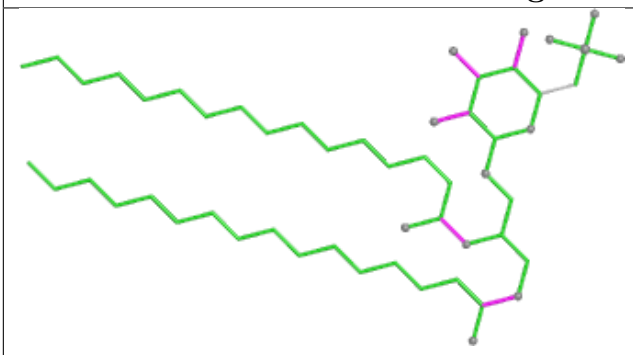


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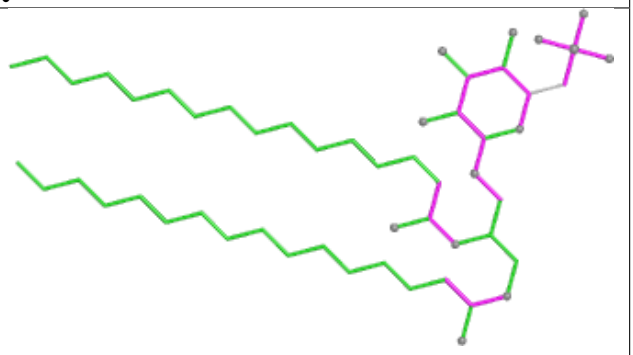


Rings

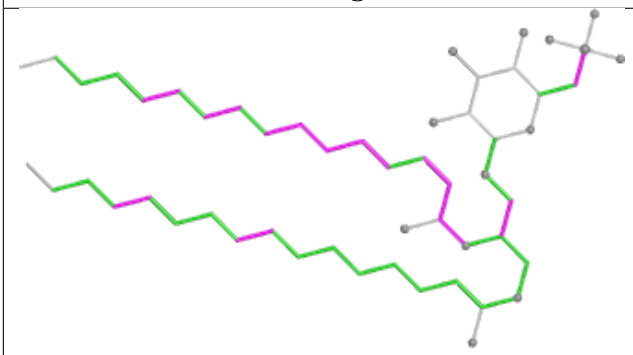
Ligand SQD b 618



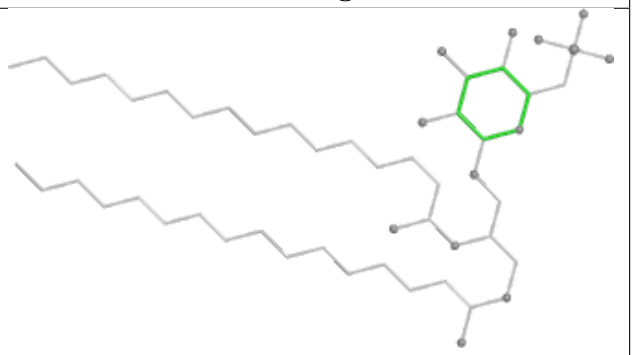
Bond lengths



Bond angles

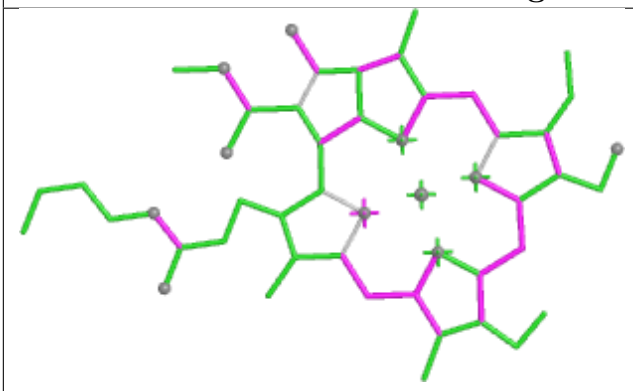


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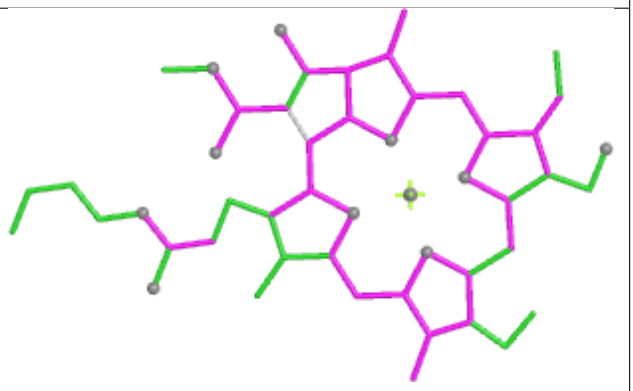


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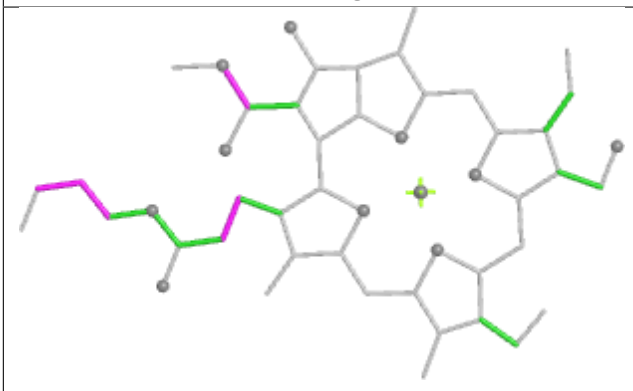
Ligand CHL 8 309



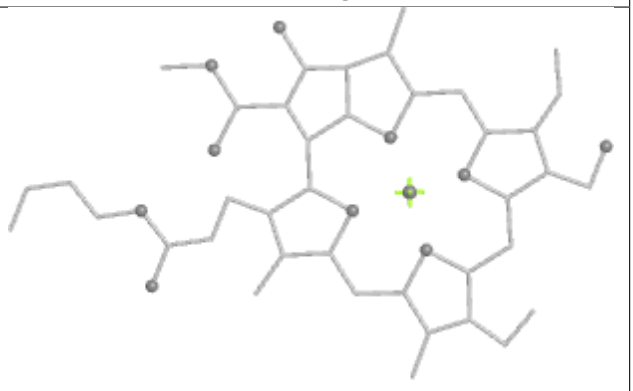
Bond lengths



Bond angles

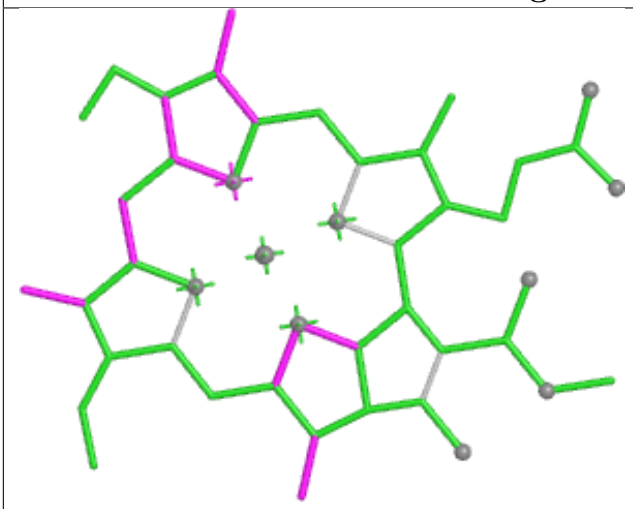


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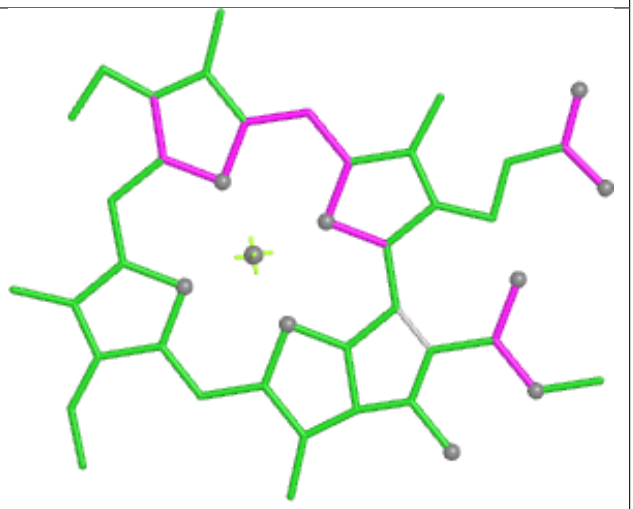


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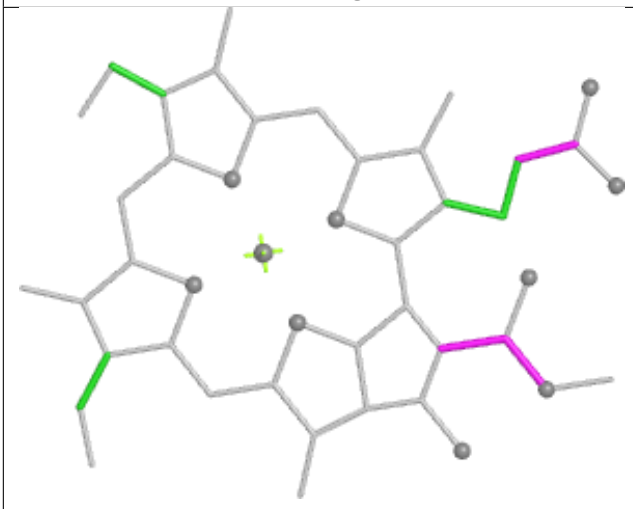
Ligand CLA s 412



Bond lengths



Bond angles

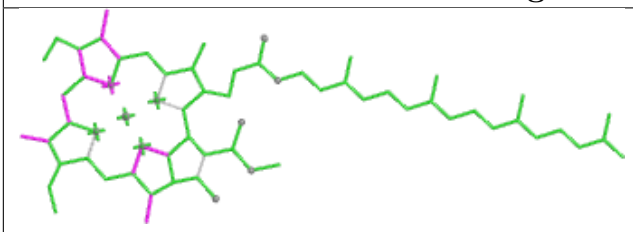


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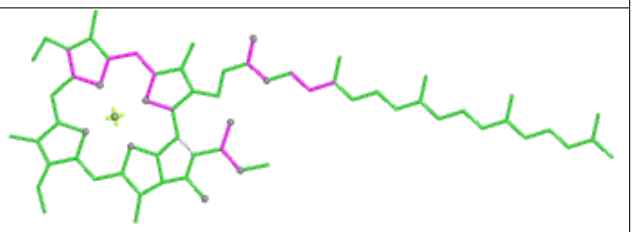


Rings

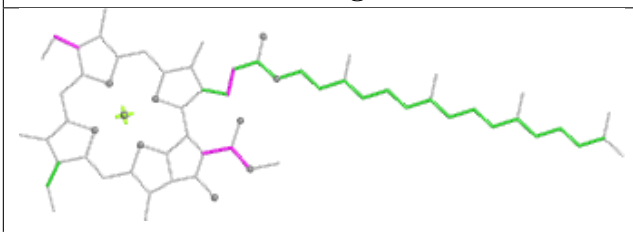
Ligand CLA b 610



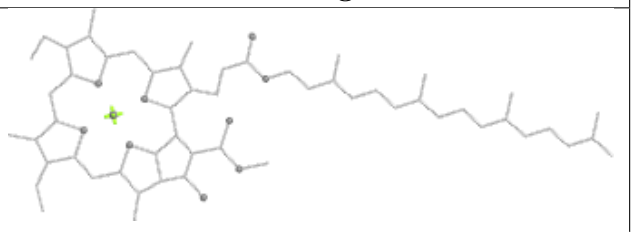
Bond lengths



Bond angles

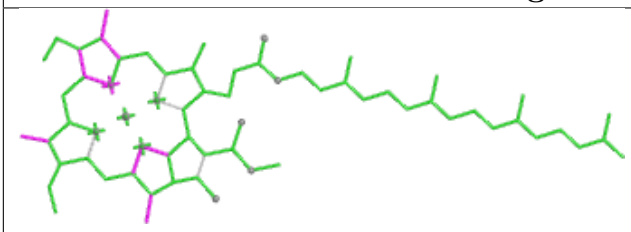


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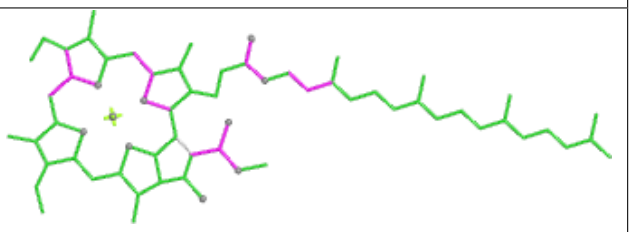


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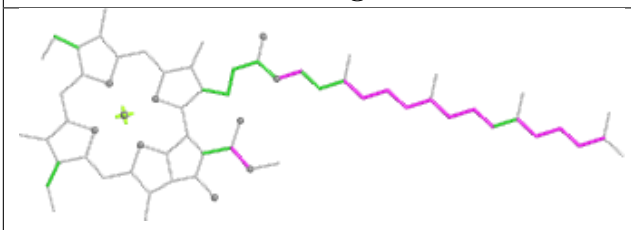
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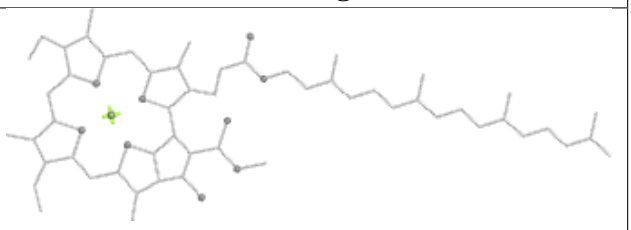
Bond lengths



Bond angles



Torsions

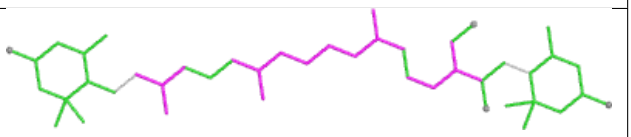


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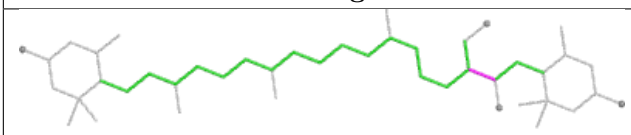
Ligand 0IE n 302



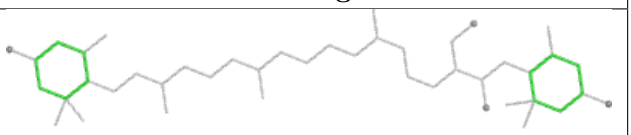
Bond lengths



Bond angles

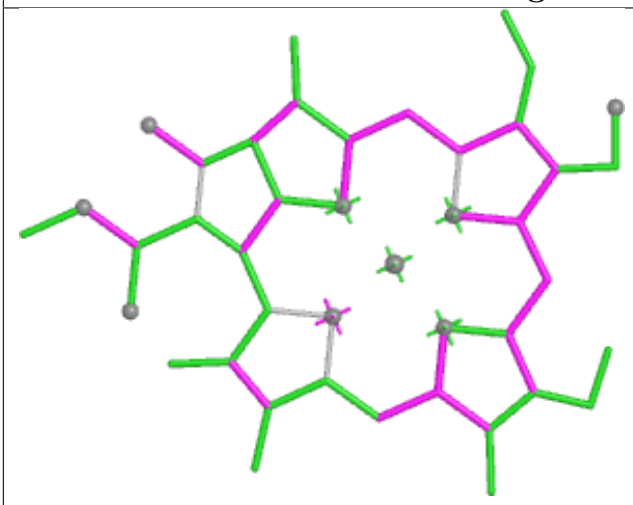


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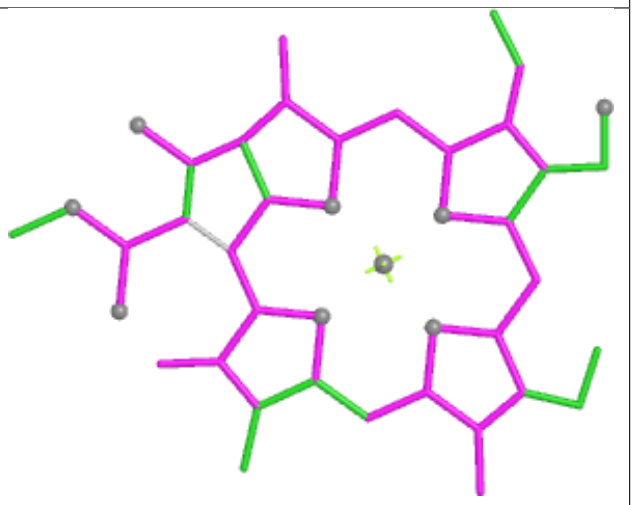


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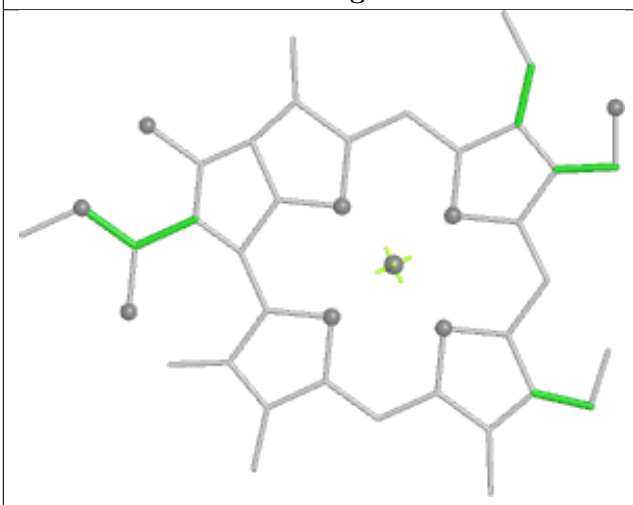
Ligand CHL 8 315



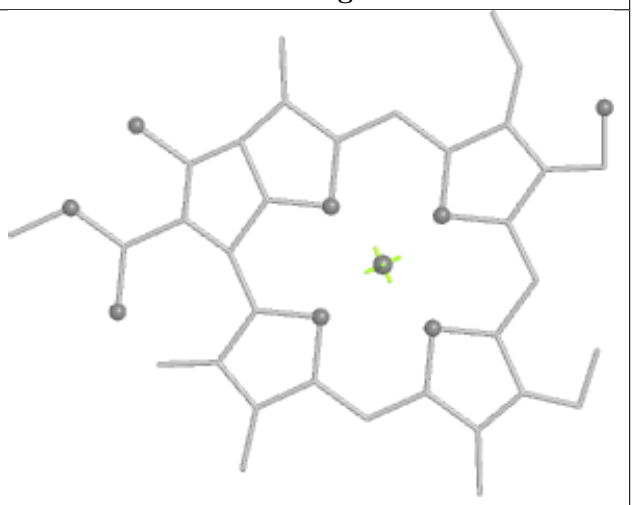
Bond lengths



Bond angles

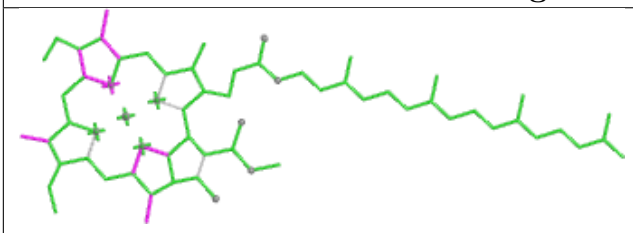


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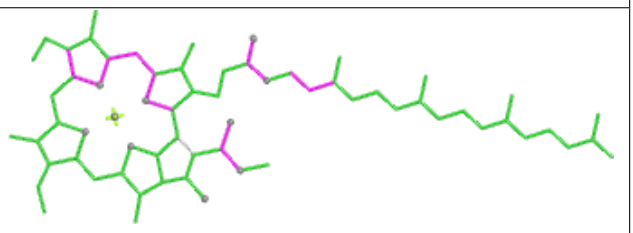


Rings

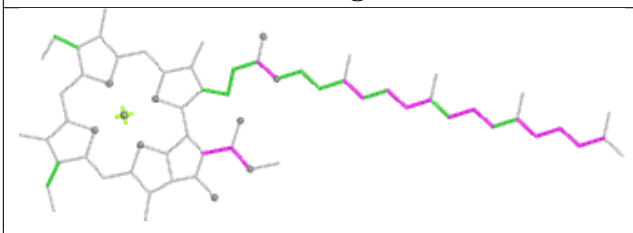
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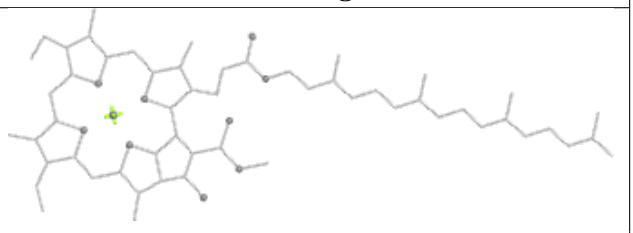
Bond lengths



Bond angles

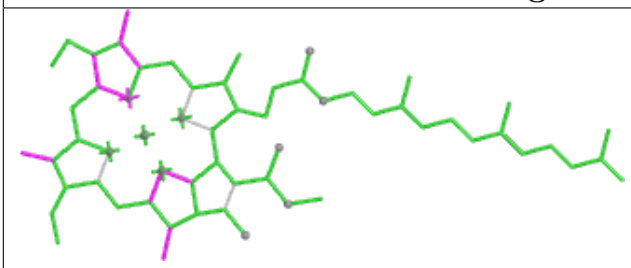


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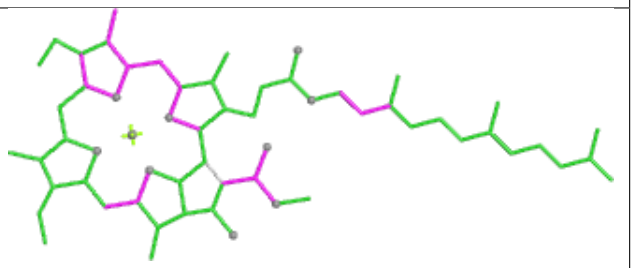


Rings

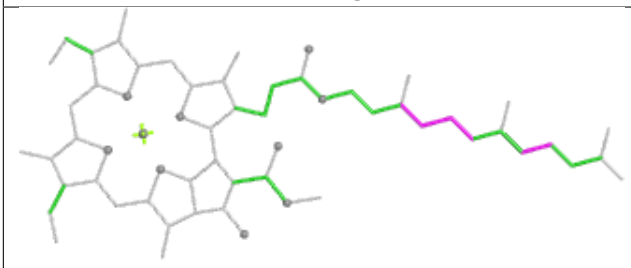
Ligand CLA a 607



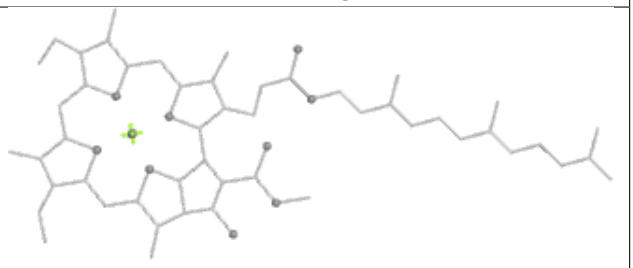
Bond lengths



Bond angles

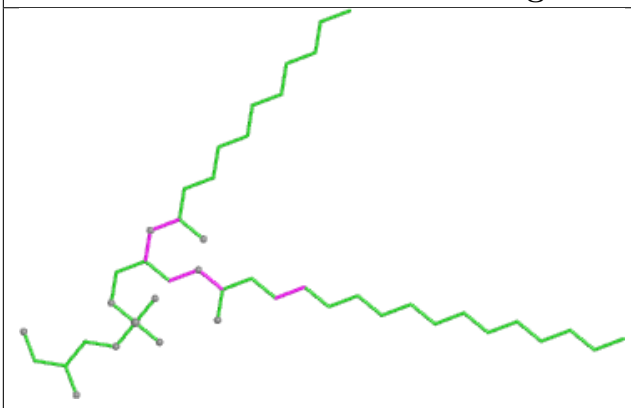


Torsions

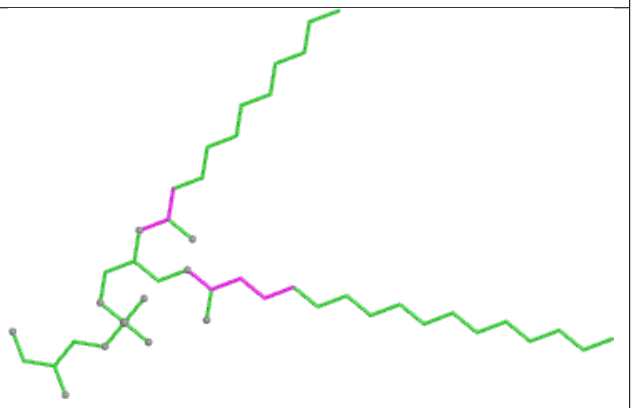


Rings

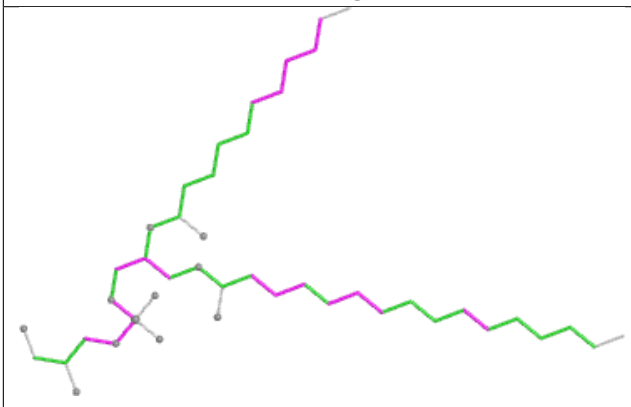
Ligand LHG a 612



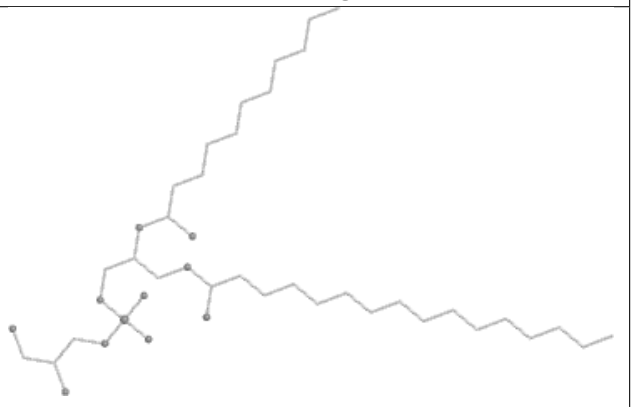
Bond lengths



Bond angles

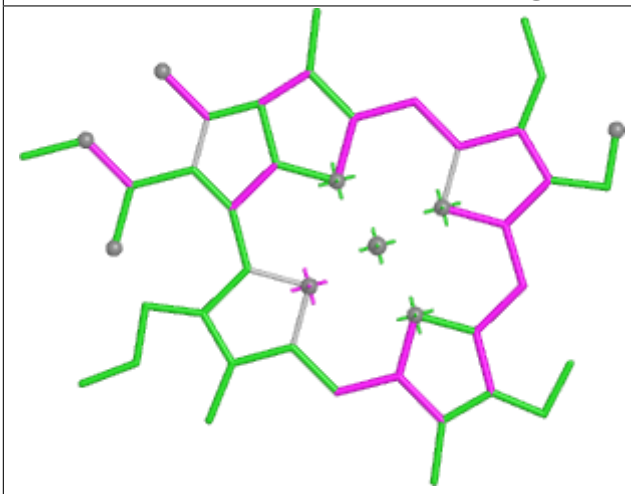


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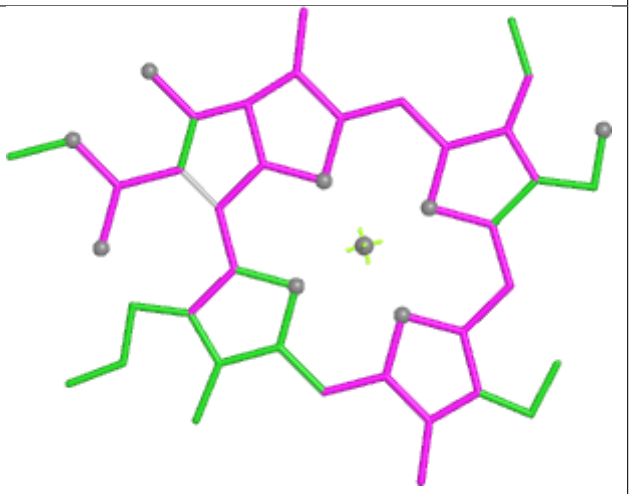


Rings

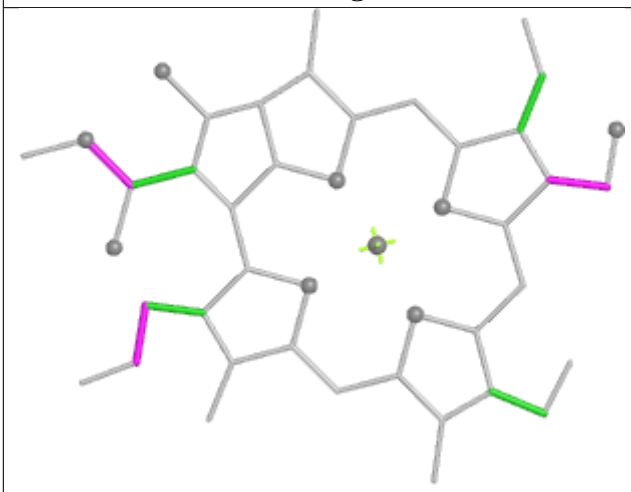
Ligand CHL 6 311



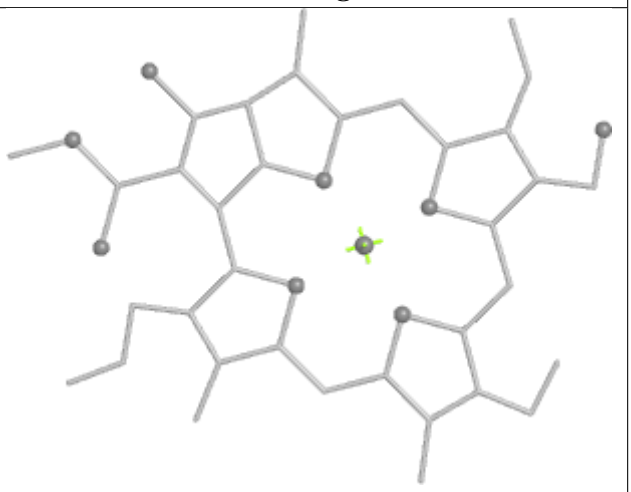
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Bond angles

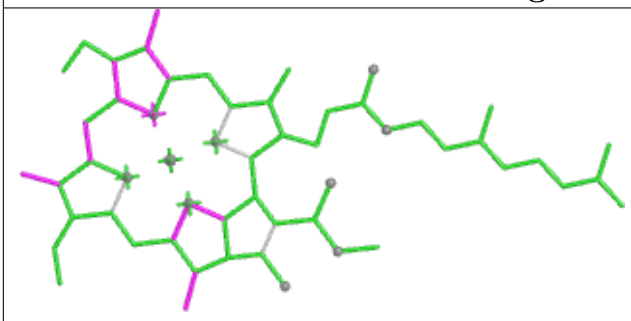


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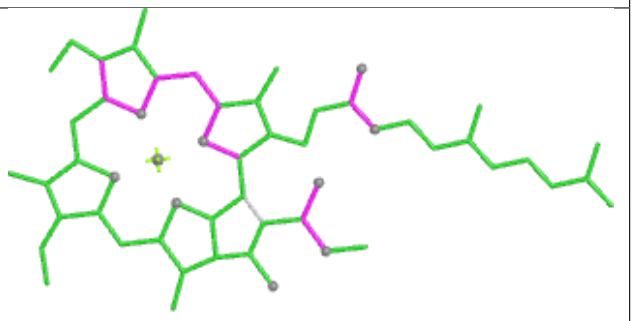


Rings

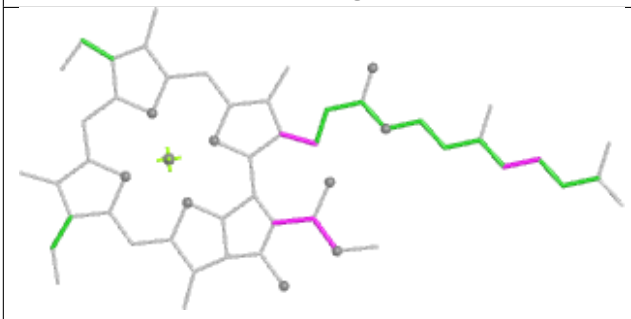
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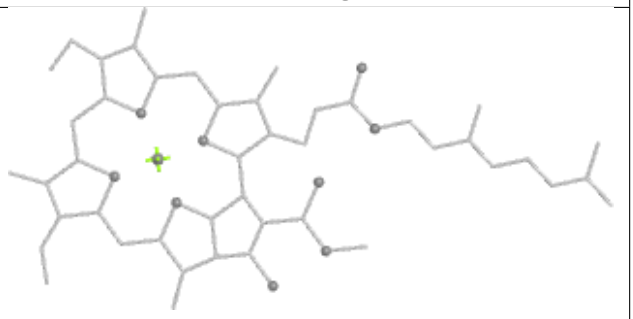
Bond lengths



Bond angles

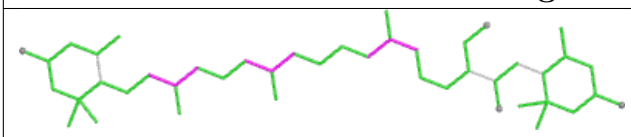


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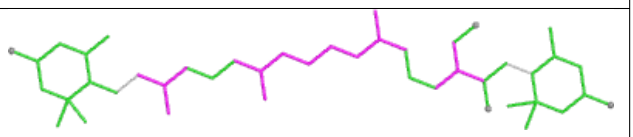


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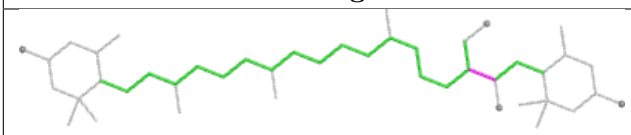
Ligand 0IE 4 302



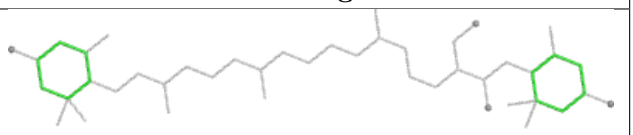
Bond lengths



Bond angles

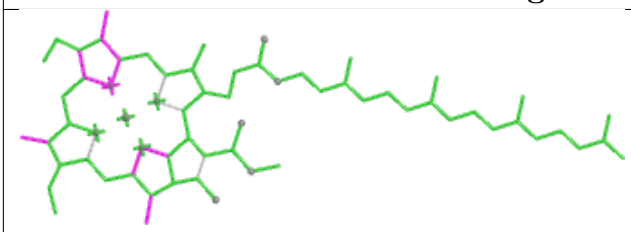


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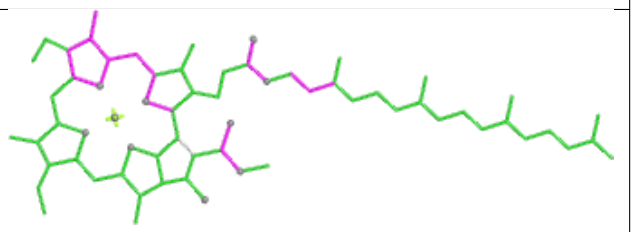


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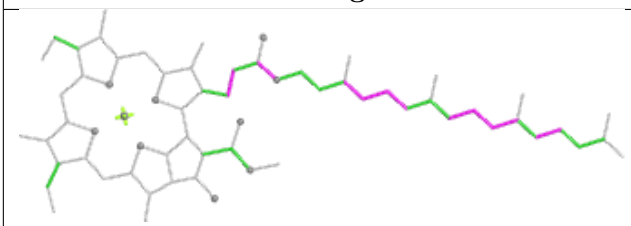
Ligand CLA b 612



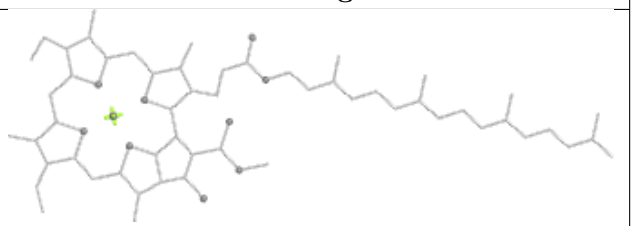
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Bond angles

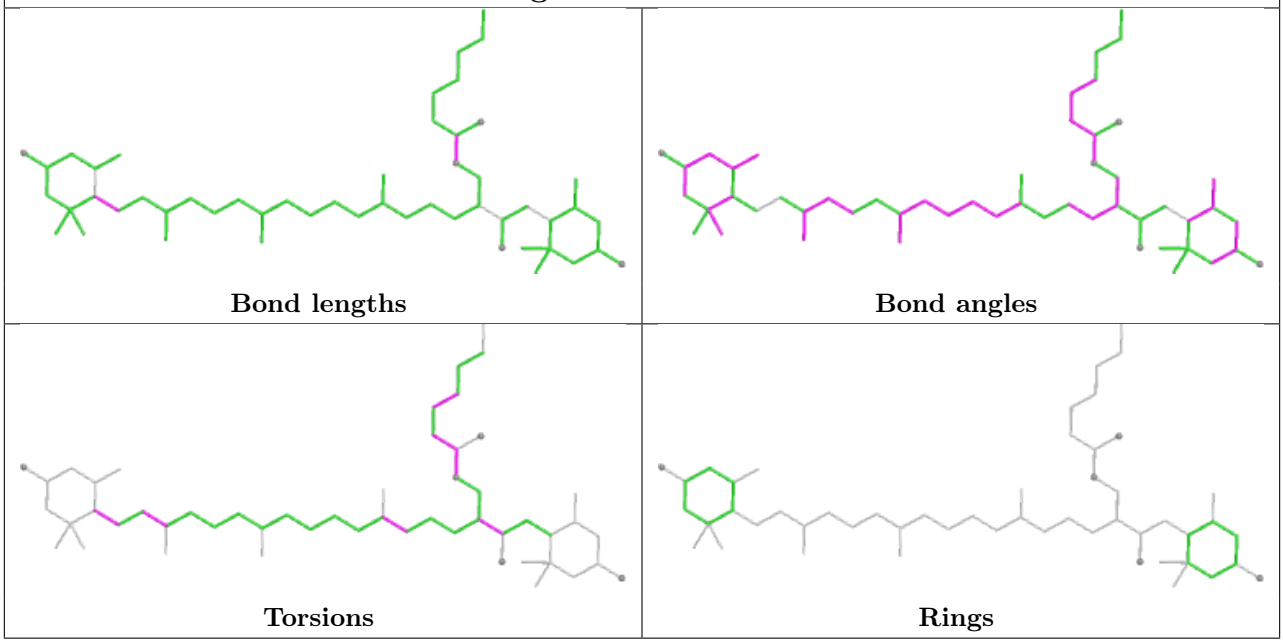


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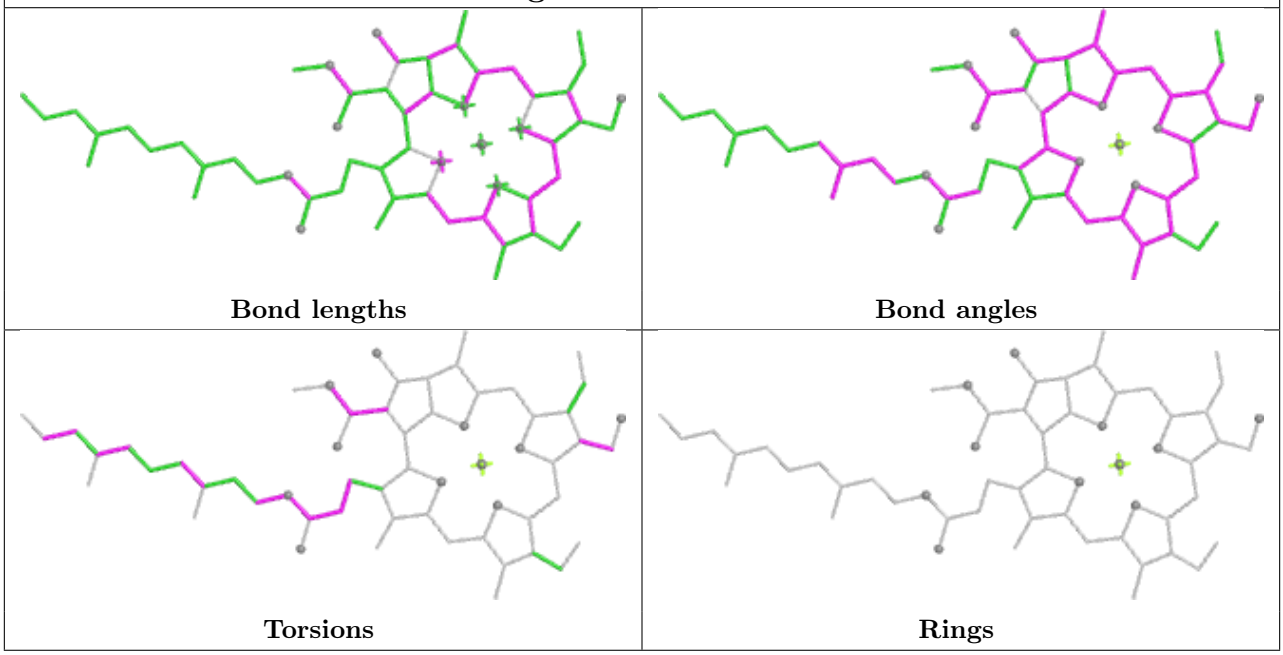


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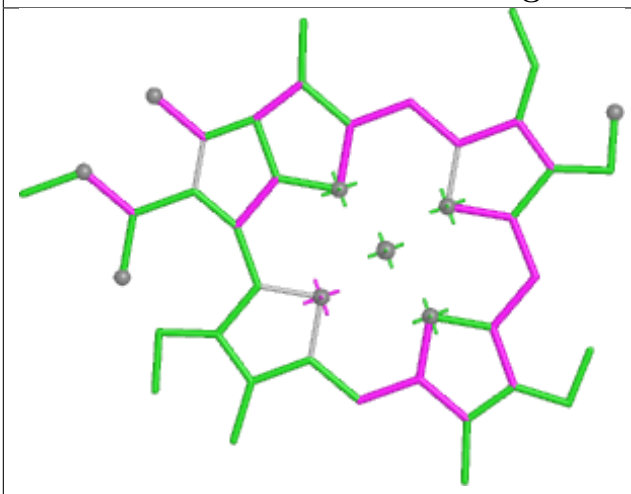
Ligand 0UR 2 301



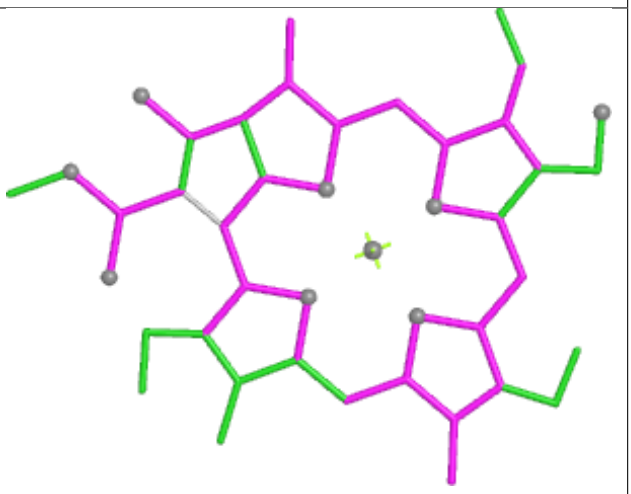
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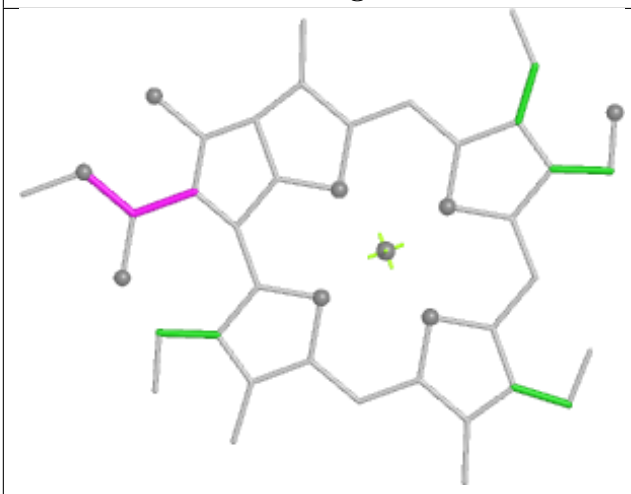
Ligand CHL N 308



Bond lengths



Bond angles

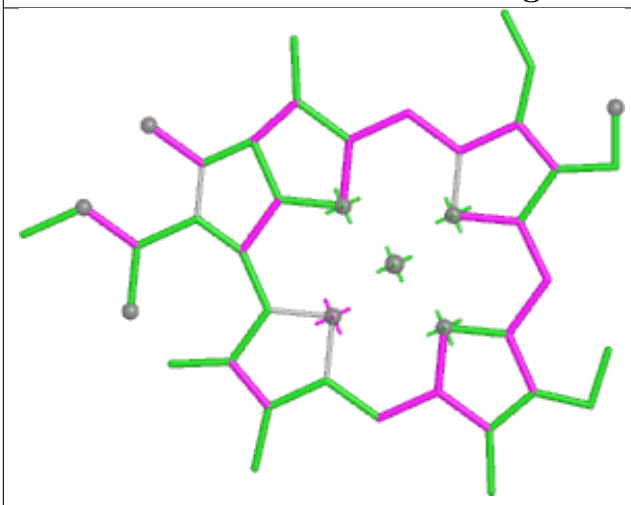


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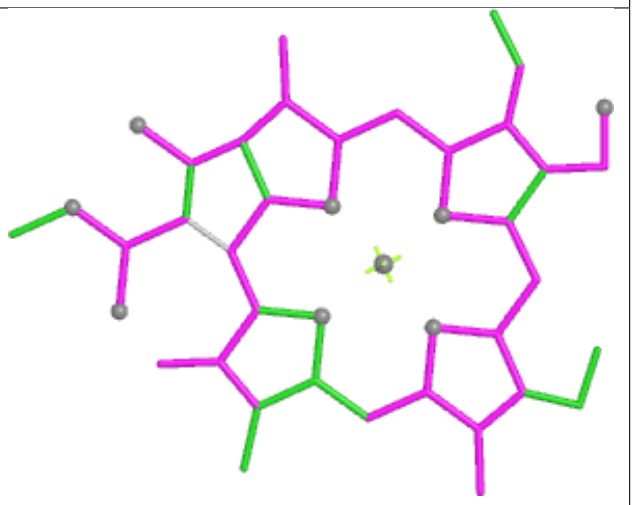


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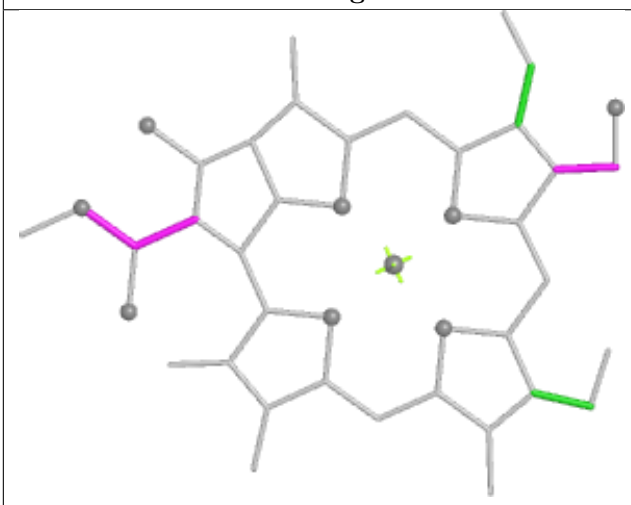
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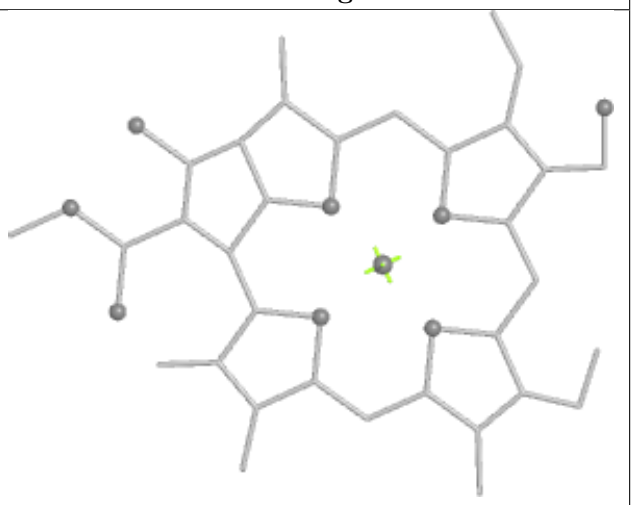
Bond lengths



Bond angles

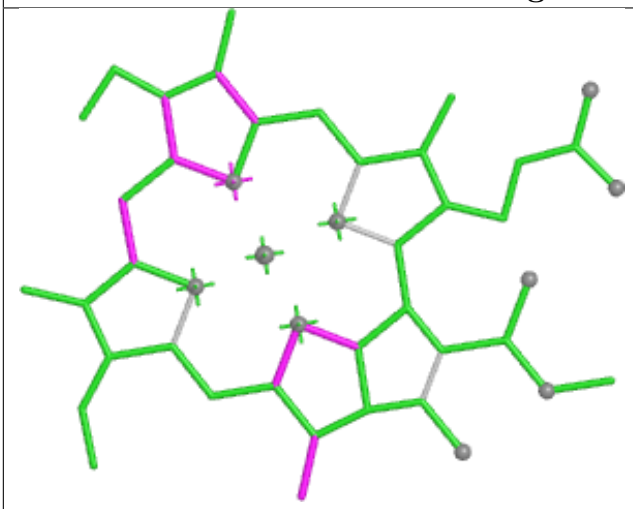


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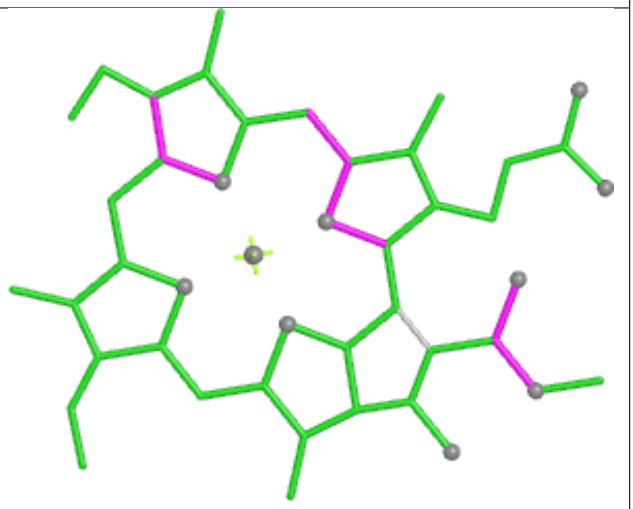


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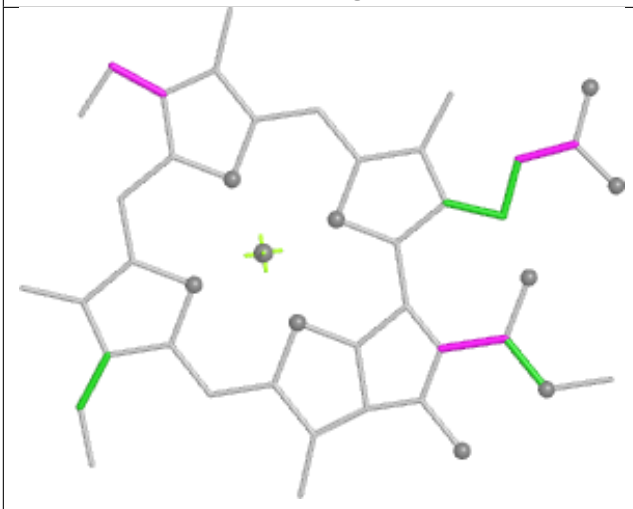
Ligand CLA u 316



Bond lengths



Bond angles

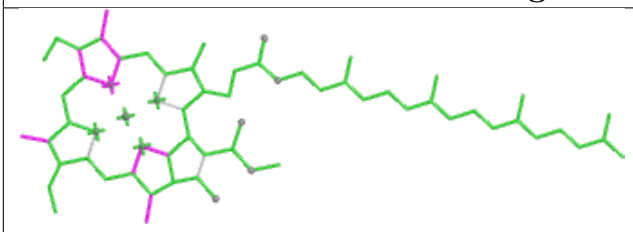


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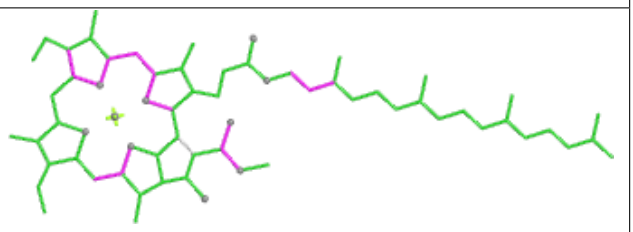


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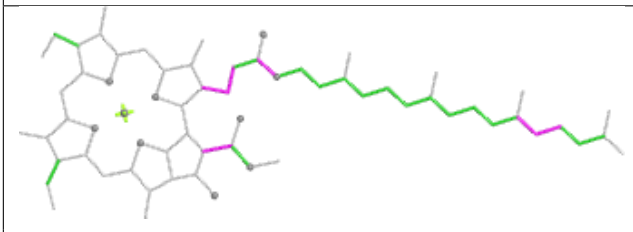
Ligand CLA a 604



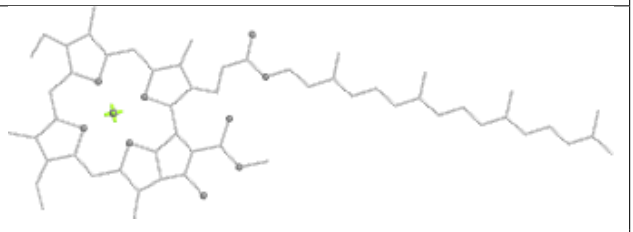
Bond lengths



Bond angles

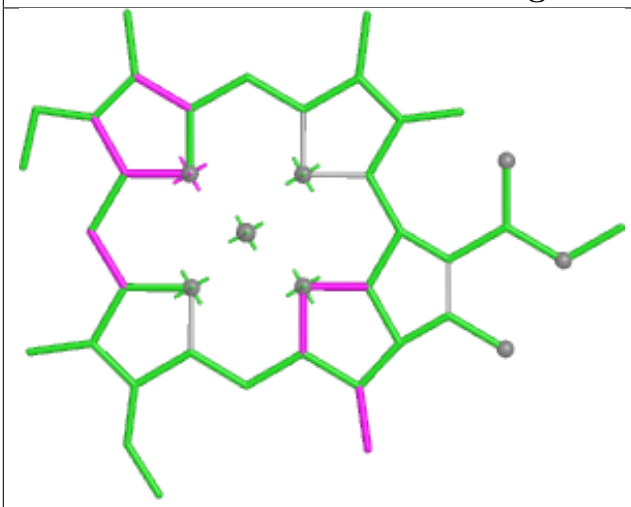


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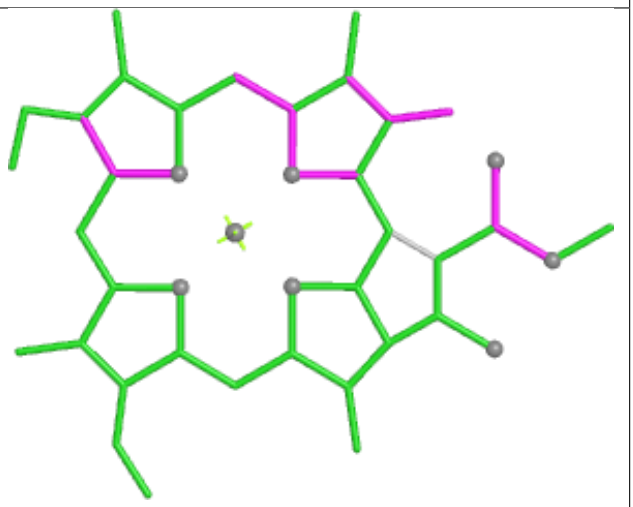


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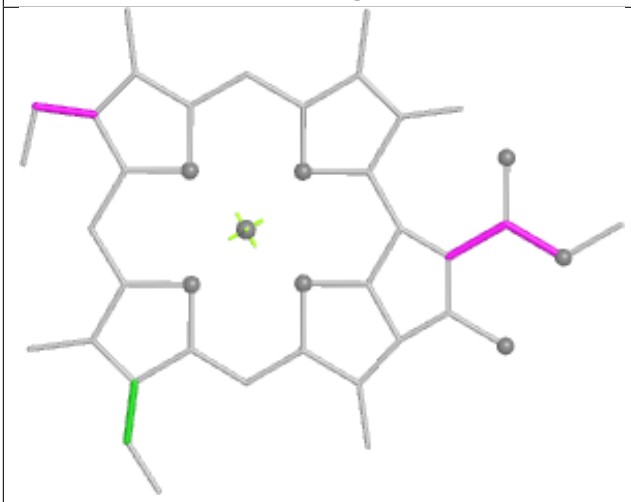
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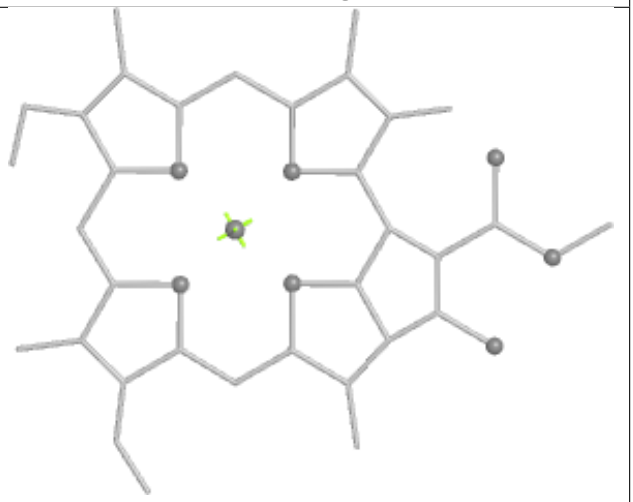
Bond lengths



Bond angles

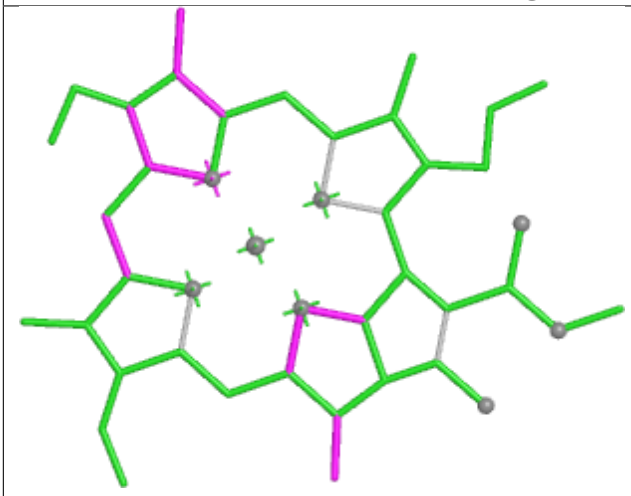


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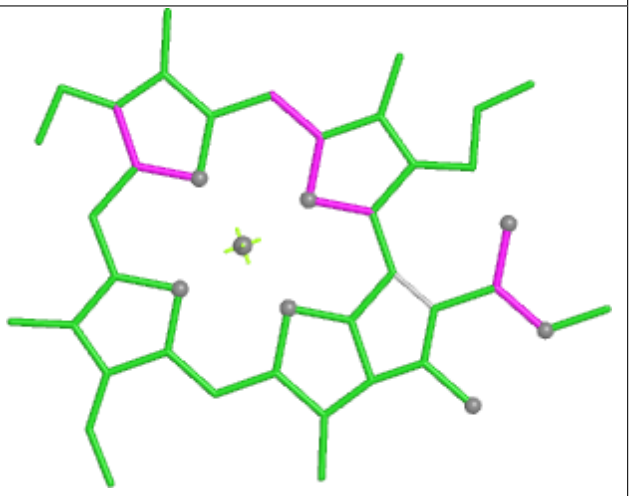


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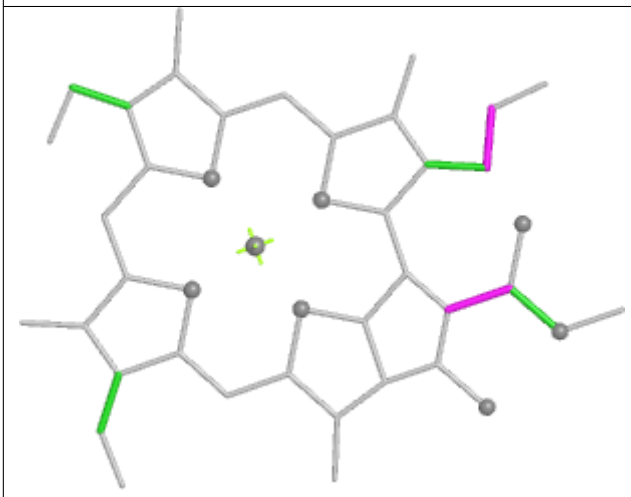
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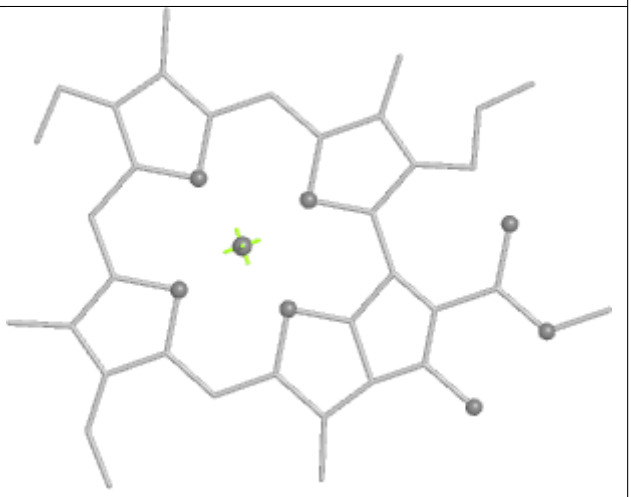
Bond lengths



Bond angles

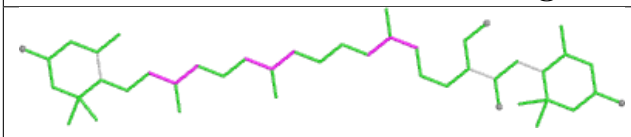


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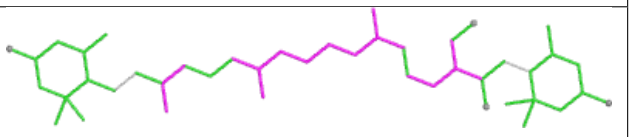


Rings

Ligand 0IE 9 302



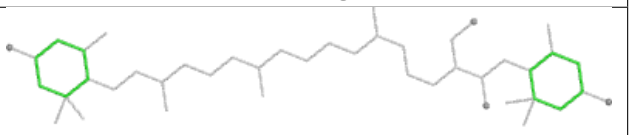
Bond lengths



Bond angles

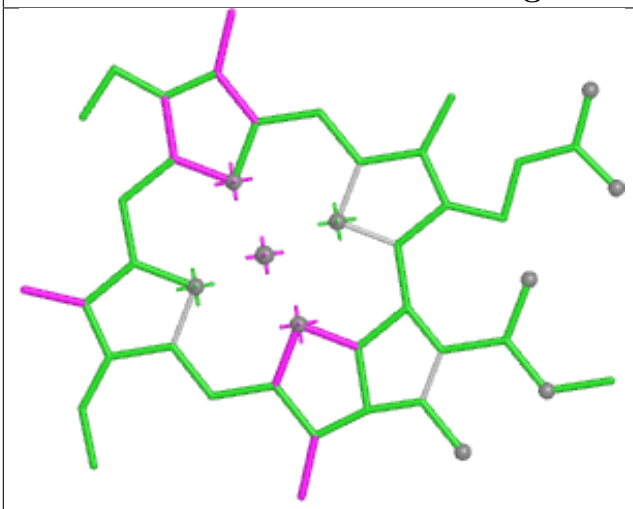


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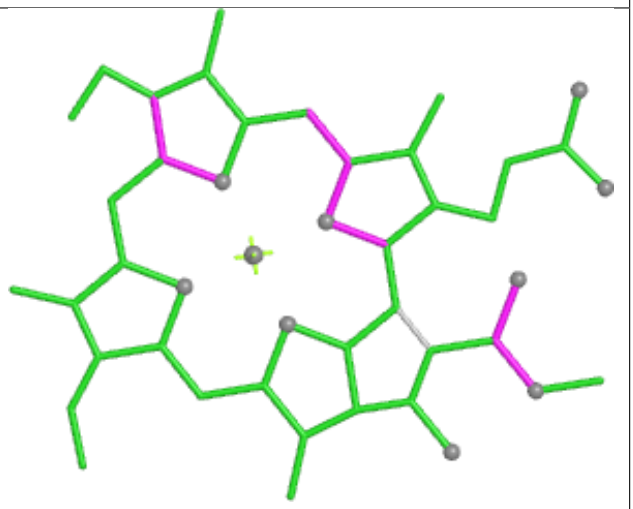


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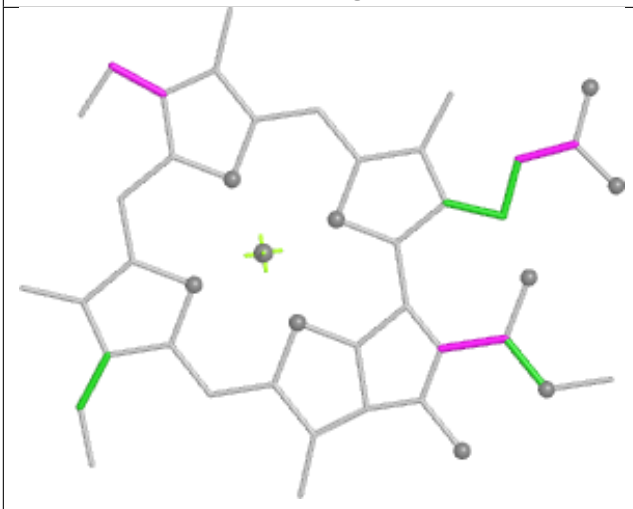
Ligand CLA Y 315



Bond lengths



Bond angles

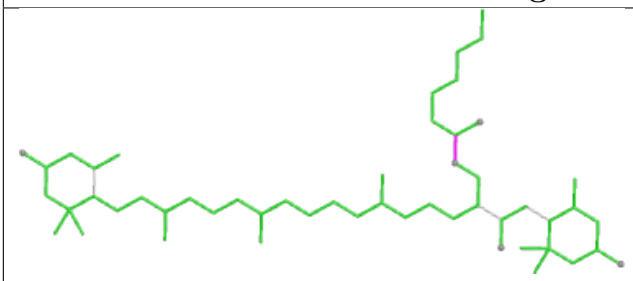


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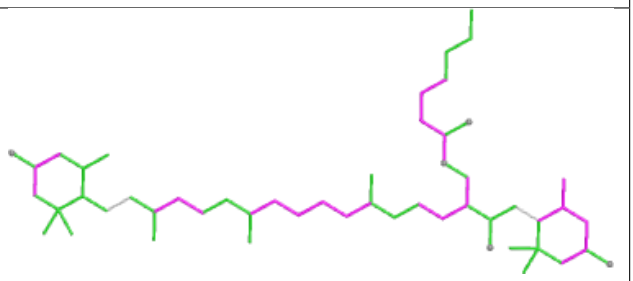


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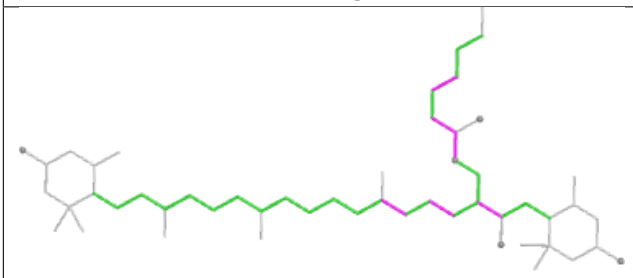
Ligand 0UR 3 301



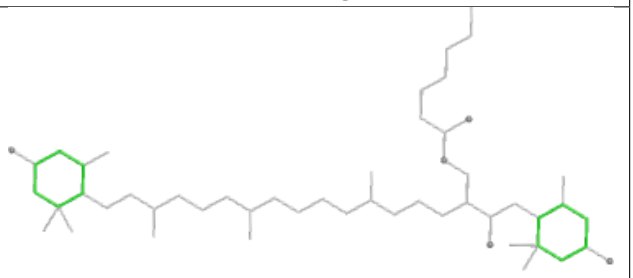
Bond lengths



Bond angles

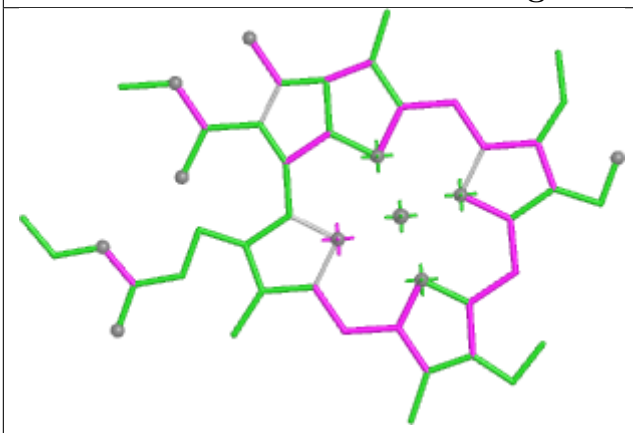


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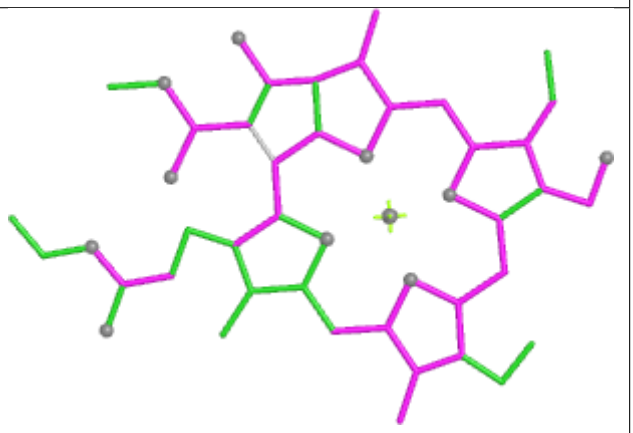


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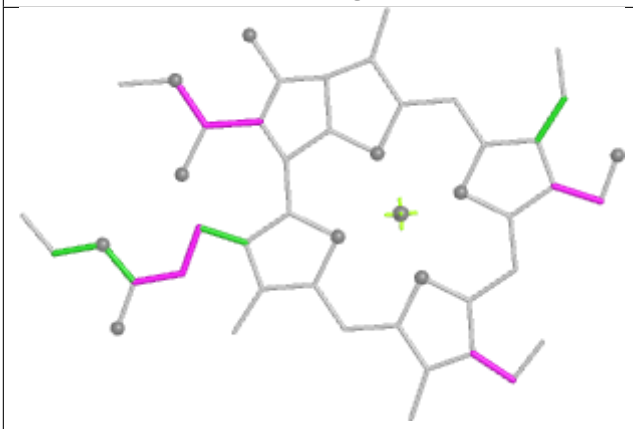
Ligand CHL 3 305



Bond lengths



Bond angles

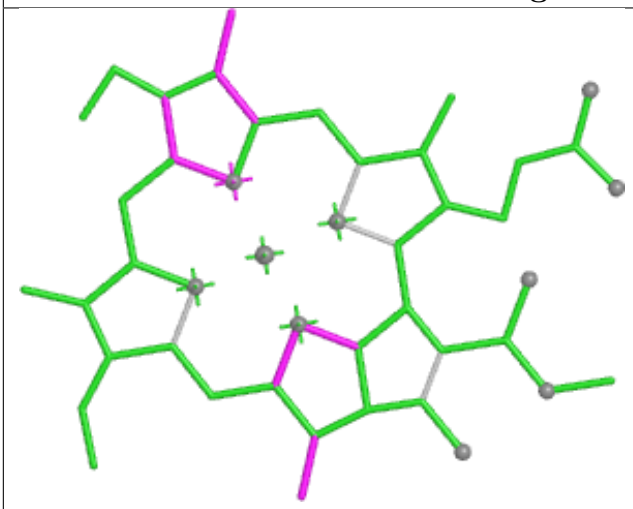


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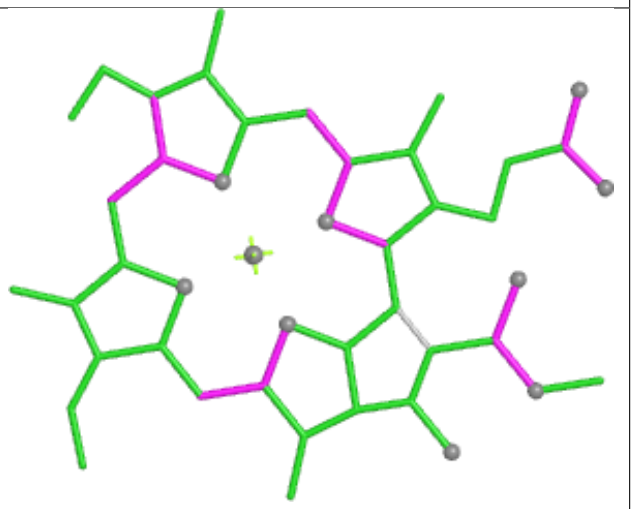


Rings

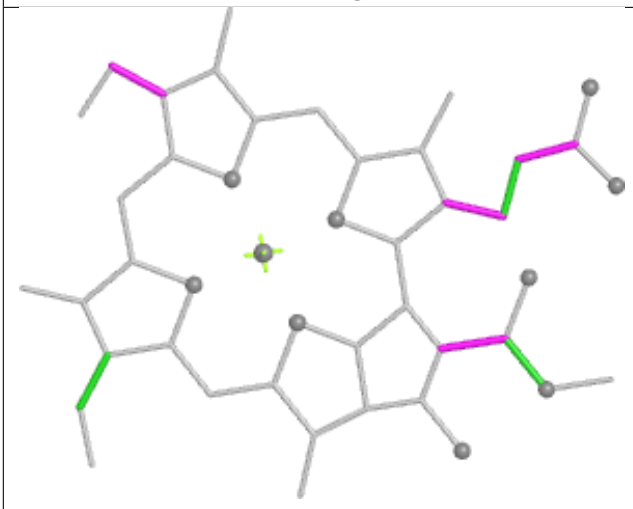
Ligand CLA r 313



Bond lengths



Bond angles

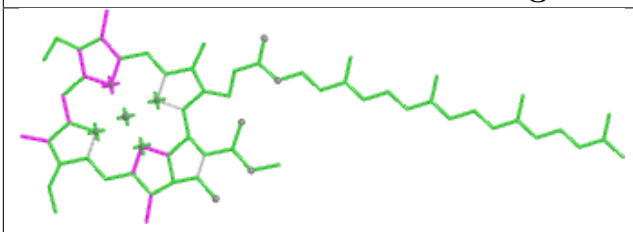


Torsions

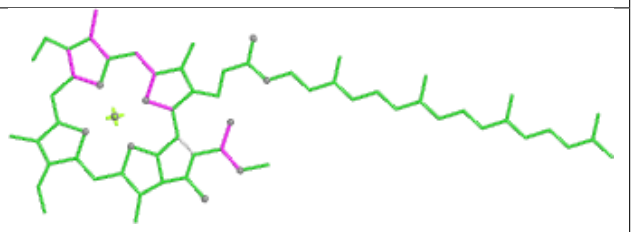


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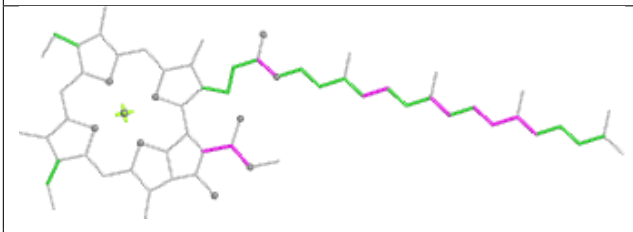
Ligand CLA c 611



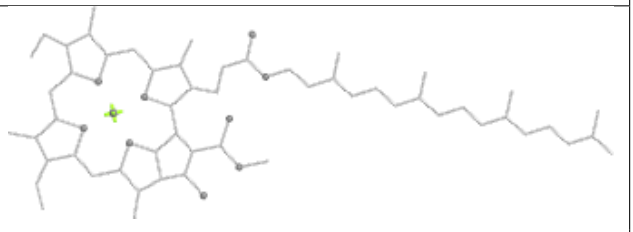
Bond lengths



Bond angles

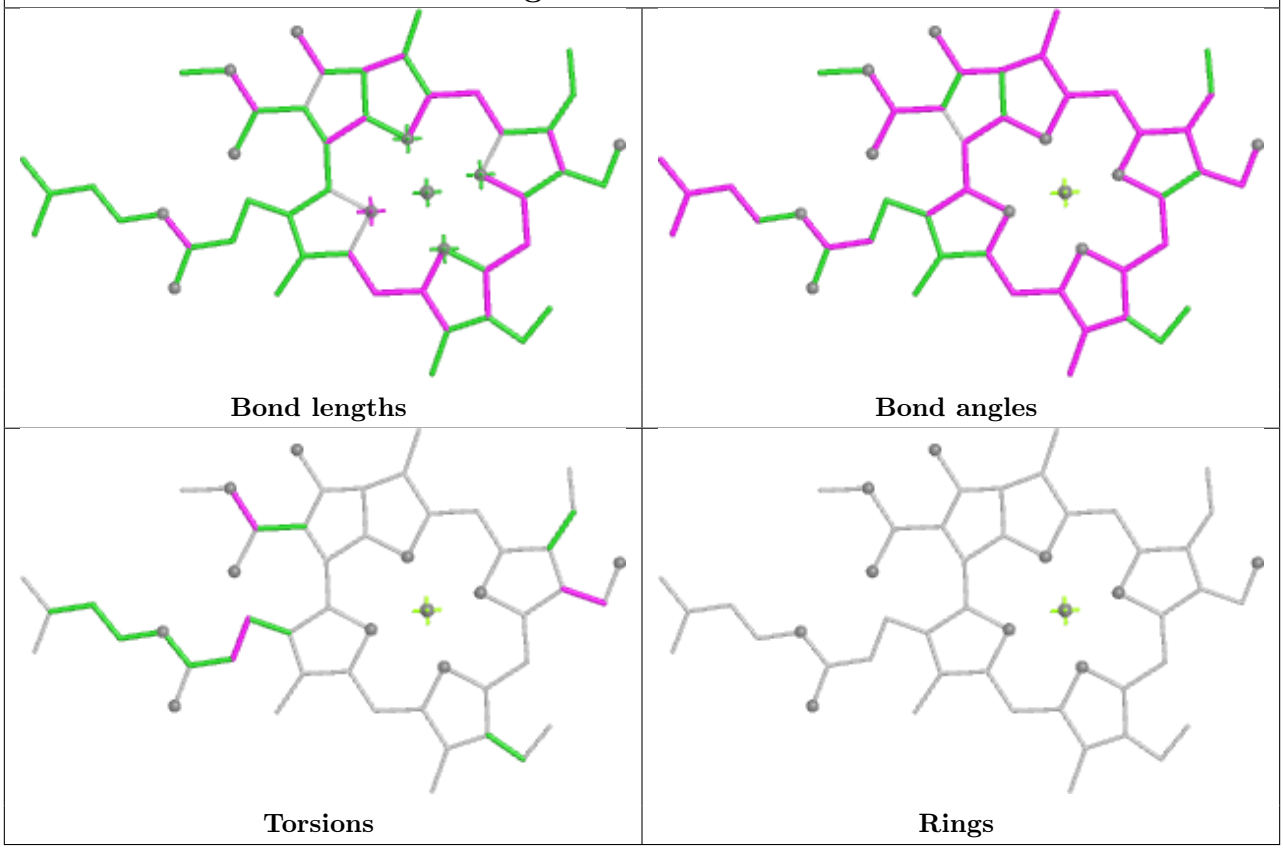


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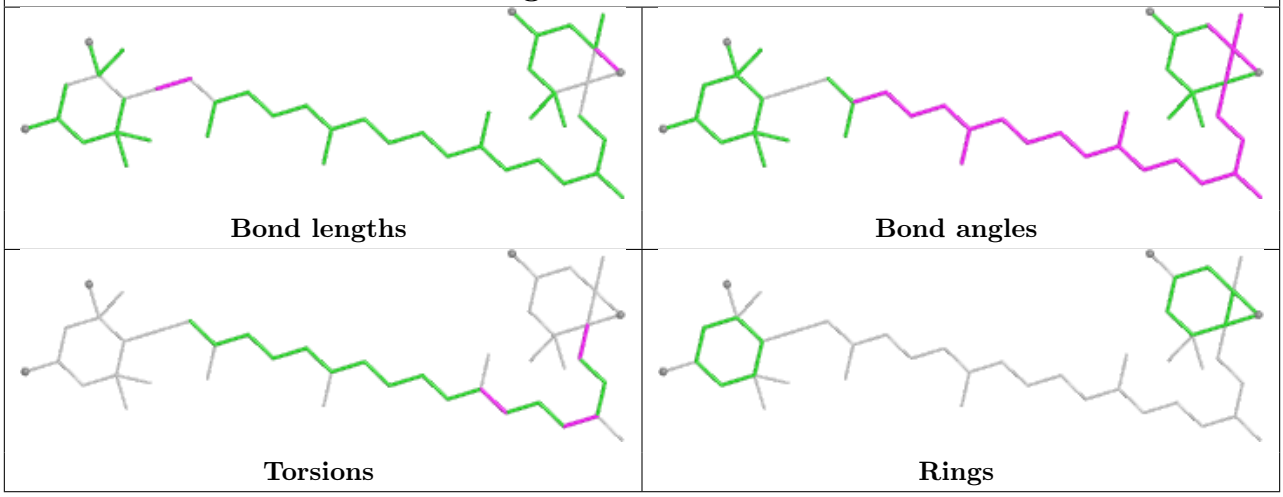


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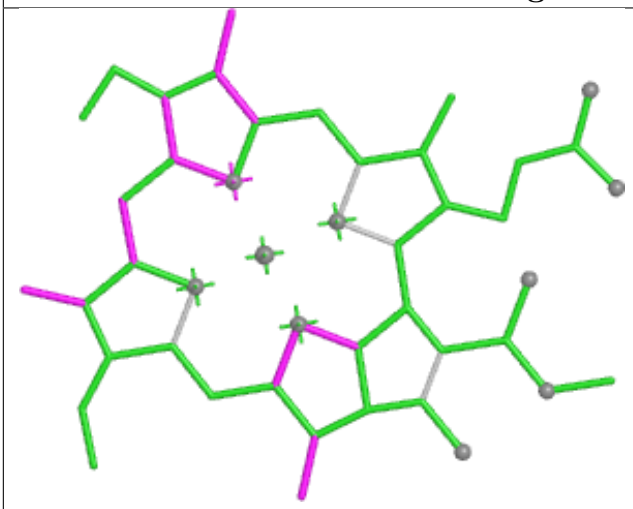
Ligand CHL Y 311



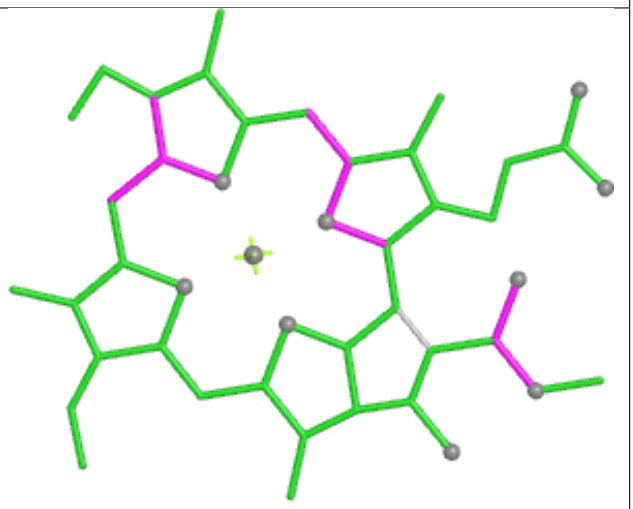
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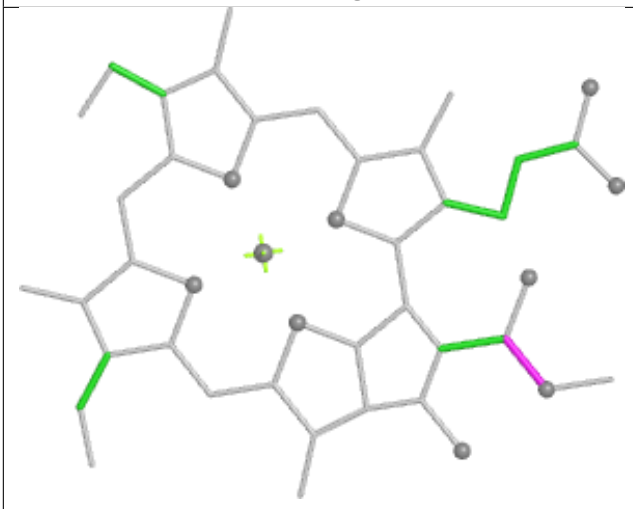
Ligand CLA S 610



Bond lengths



Bond angles

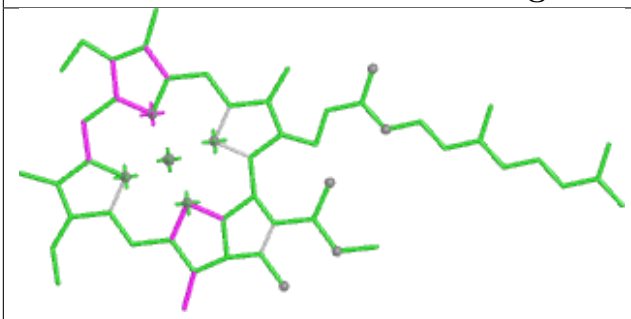


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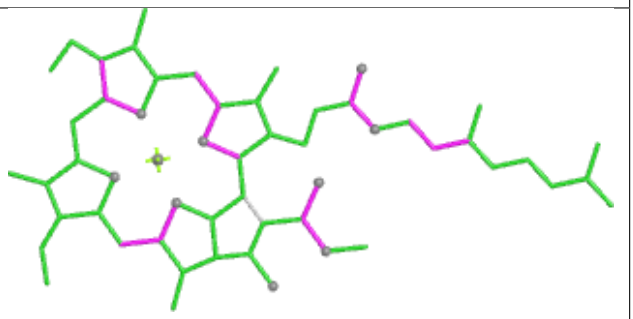


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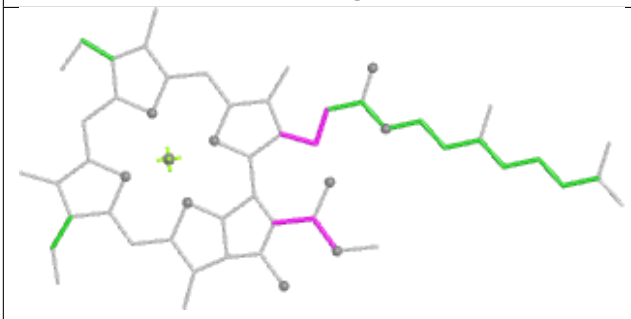
Ligand CLA 1 313



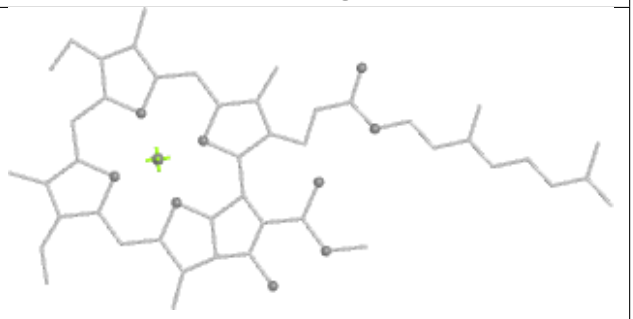
Bond lengths



Bond angles

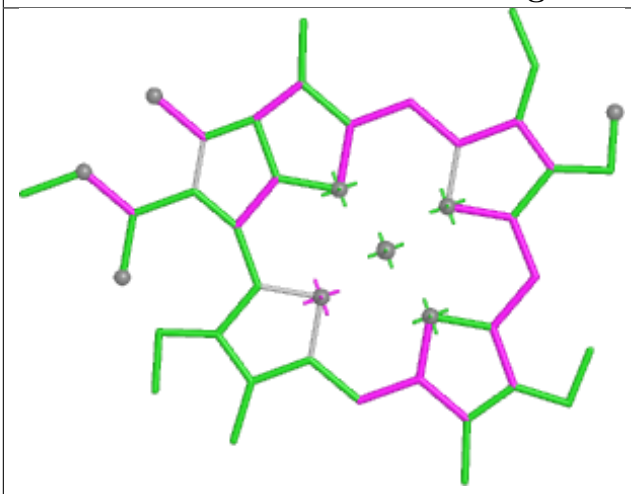


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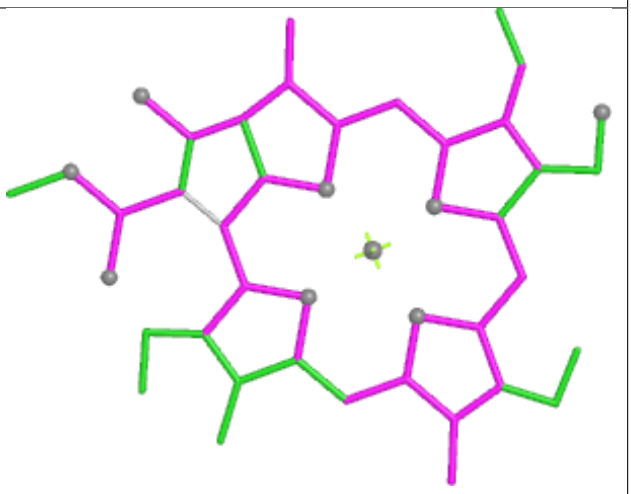


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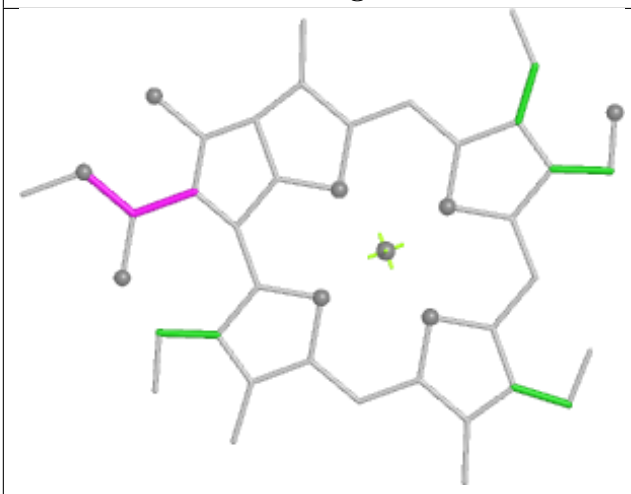
Ligand CHL 9 312



Bond lengths



Bond angles

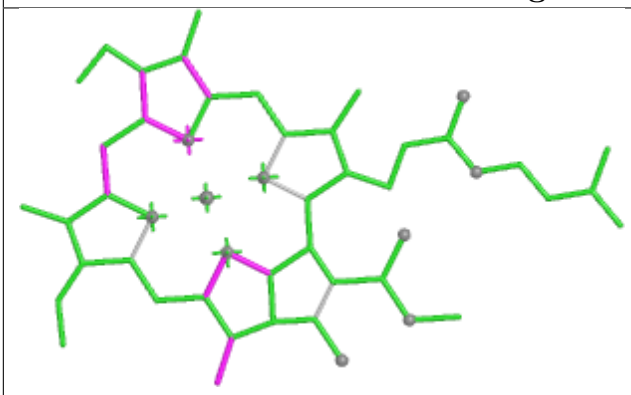


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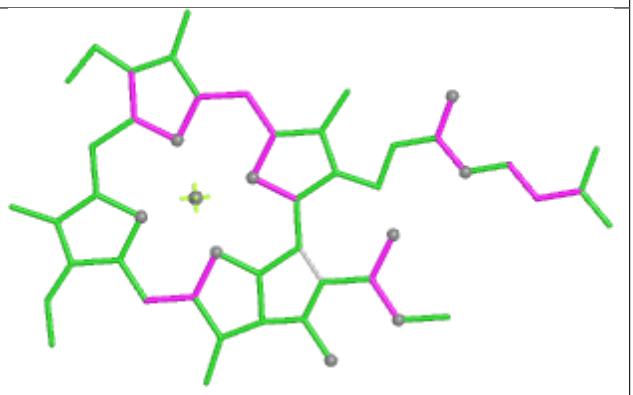


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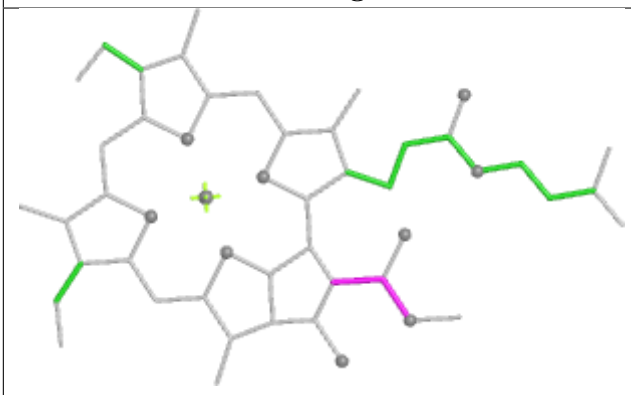
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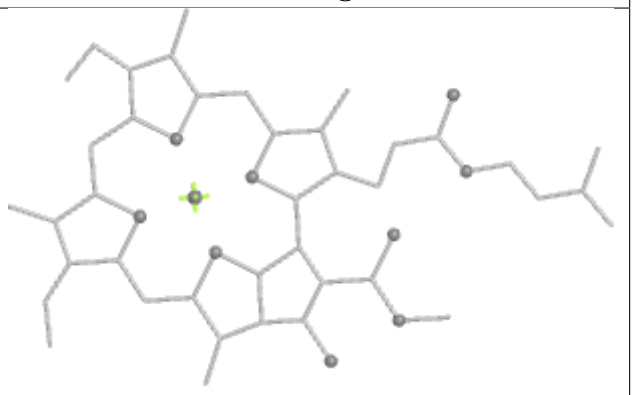
Bond lengths



Bond angles

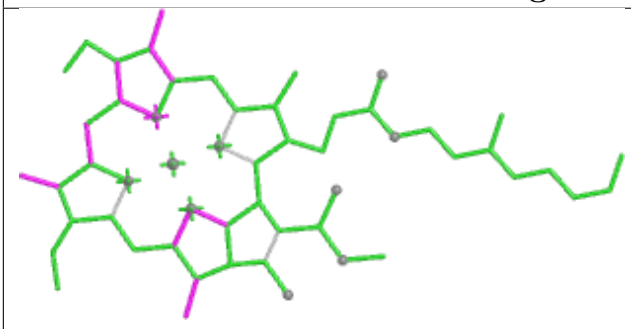


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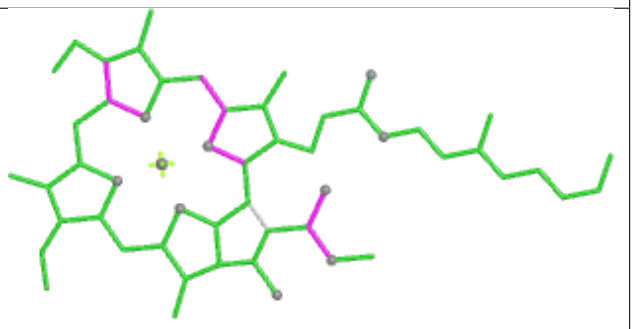


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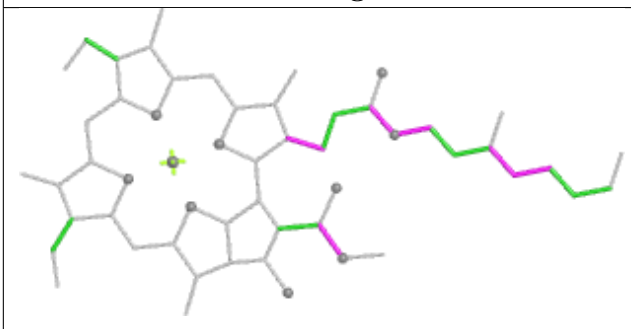
Ligand CLA c 612



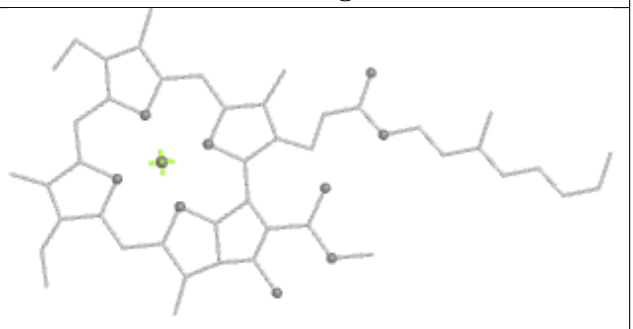
Bond lengths



Bond angles

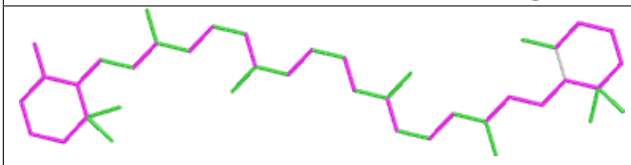


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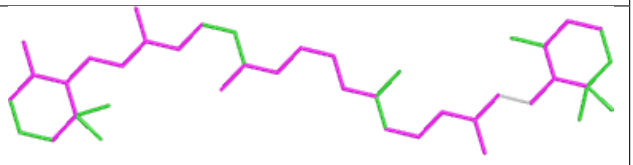


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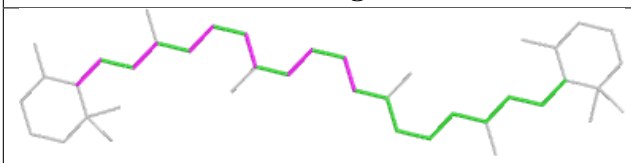
Ligand 8CT A 608



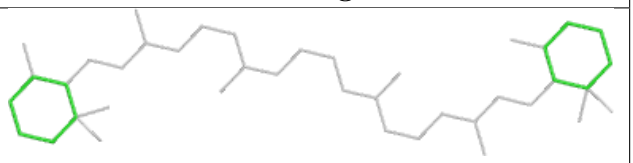
Bond lengths



Bond angles

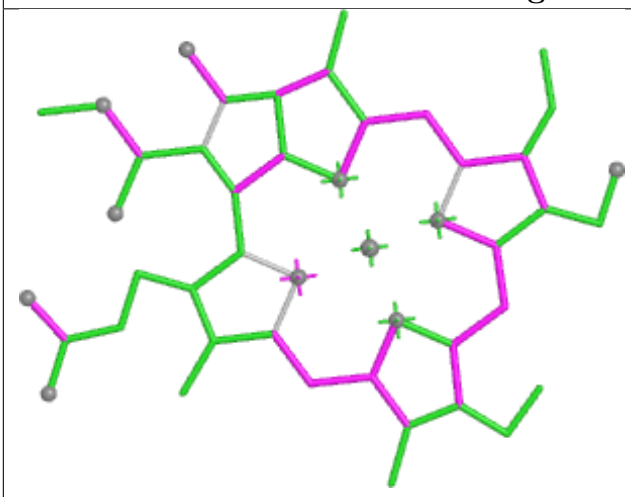


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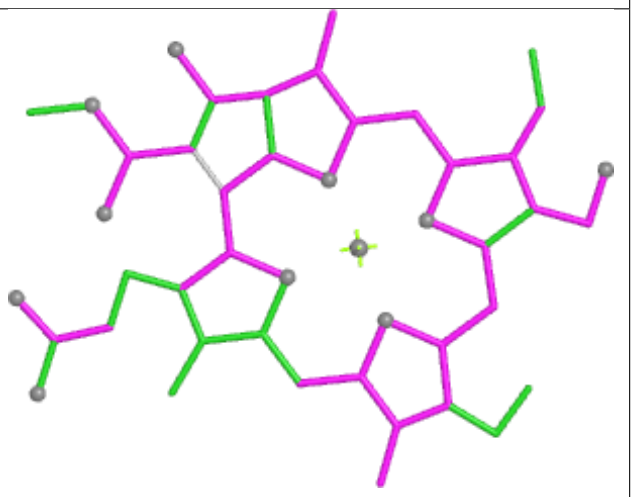


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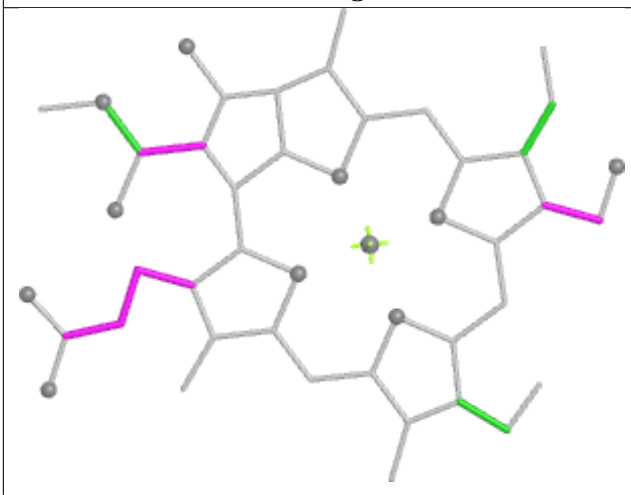
Ligand CHL 1 305



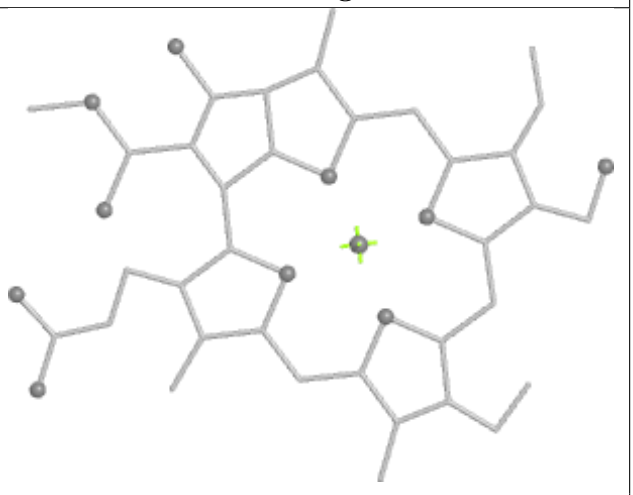
Bond lengths



Bond angles

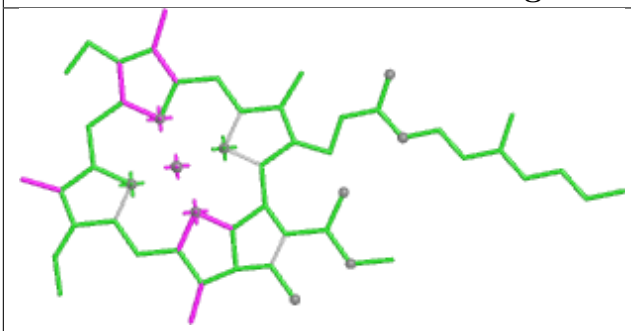


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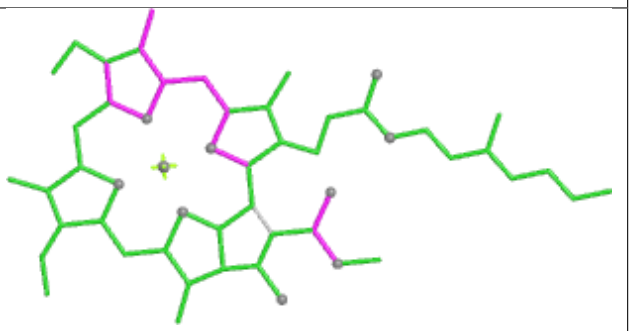


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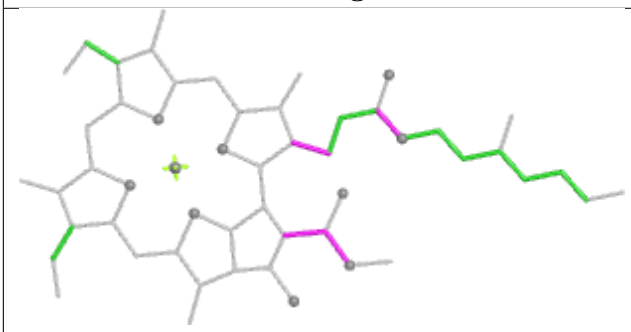
Ligand CLA C 606



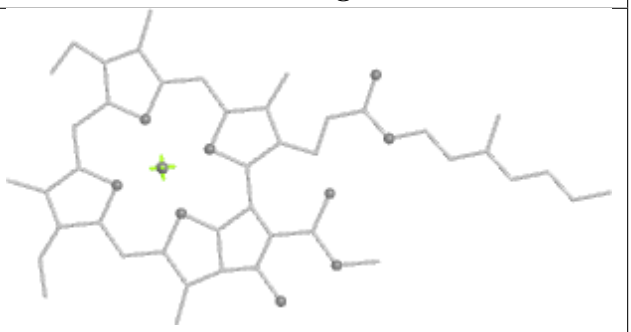
Bond lengths



Bond angles

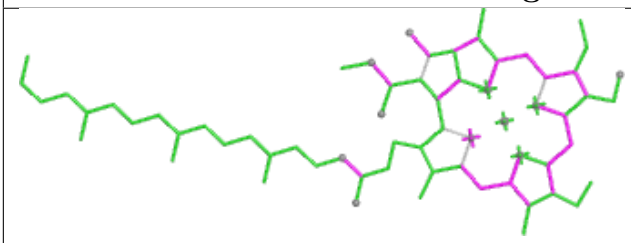


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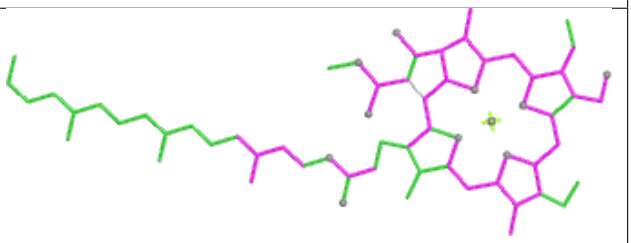


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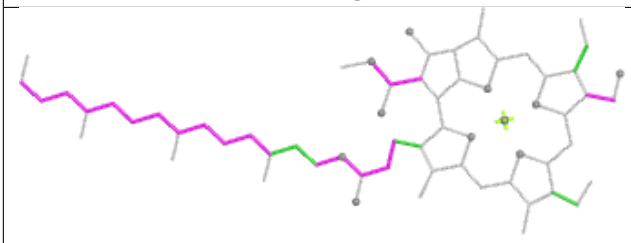
Ligand CHL G 306



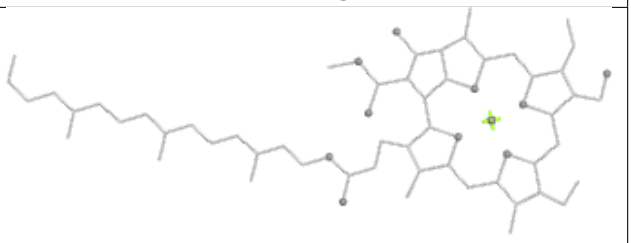
Bond lengths



Bond angles

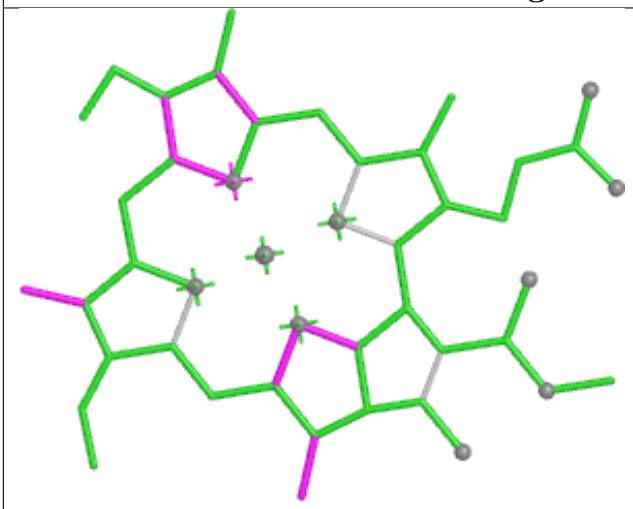


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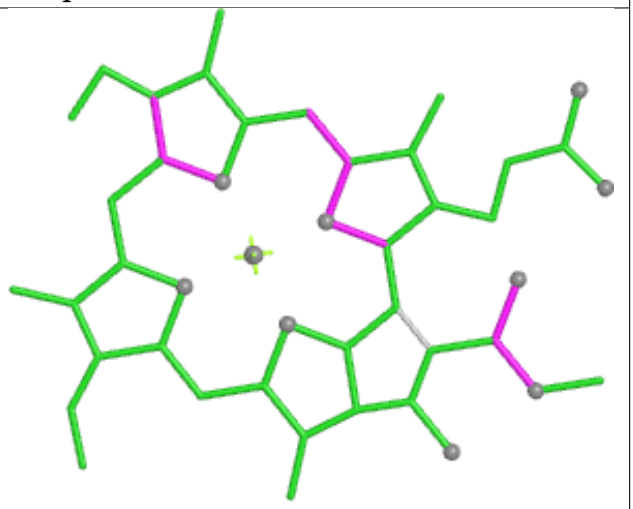


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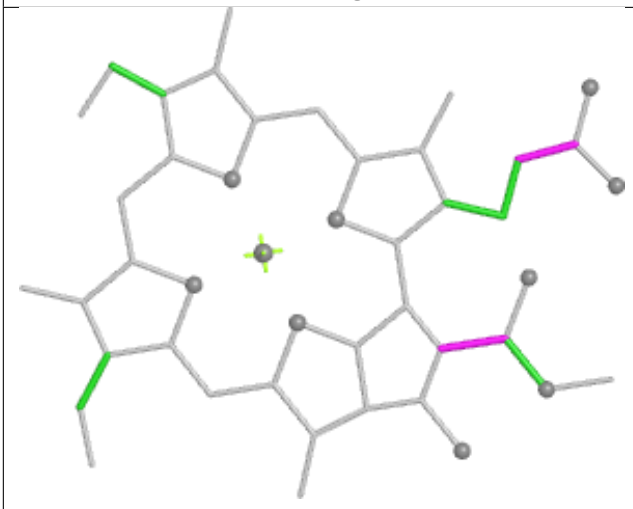
Ligand CLA q 314



Bond lengths



Bond angles

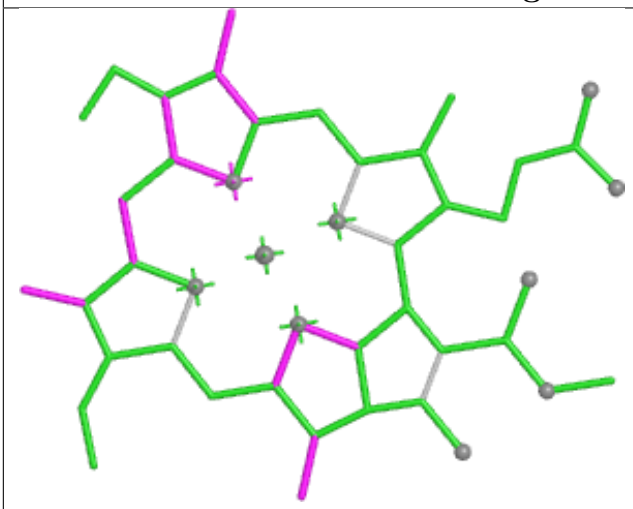


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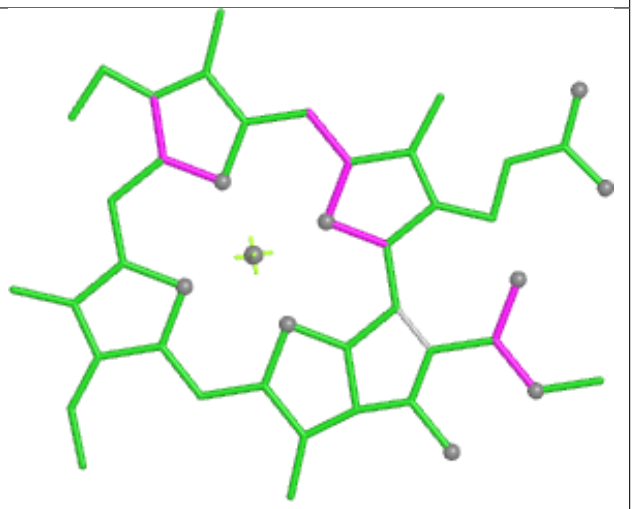


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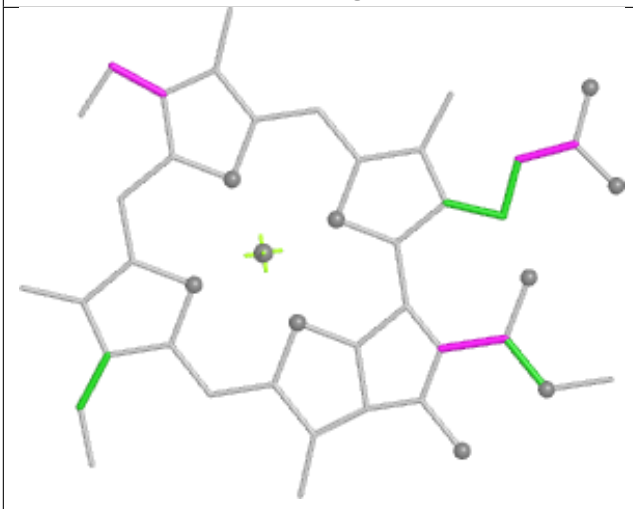
Ligand CLA G 316



Bond lengths



Bond angles

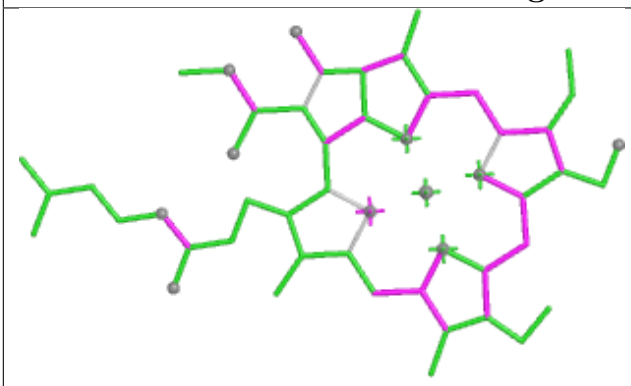


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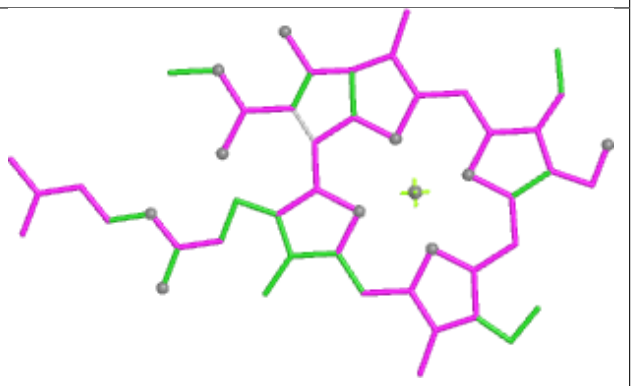


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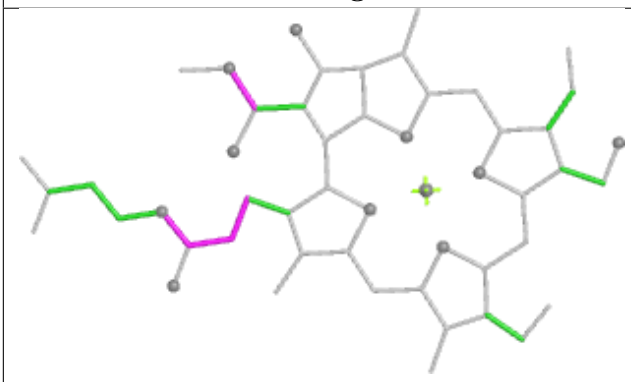
Ligand CHL 6 309



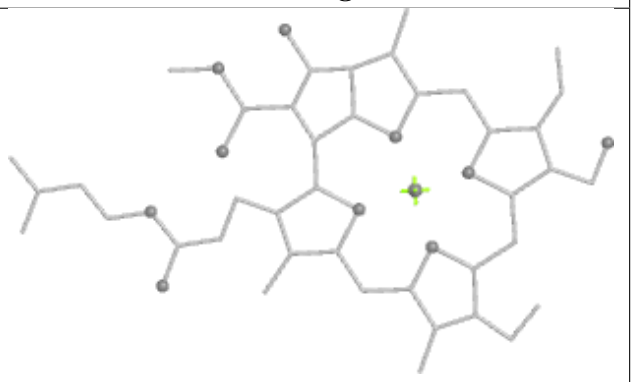
Bond lengths



Bond angles

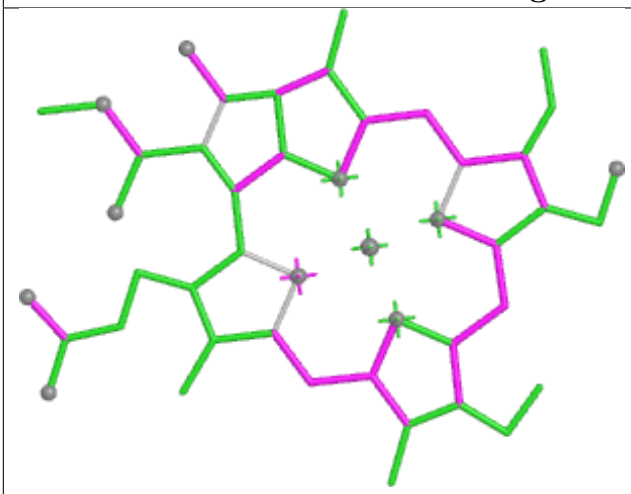


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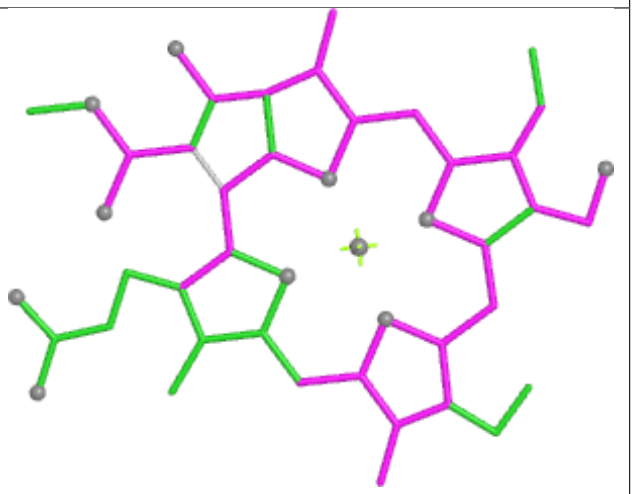


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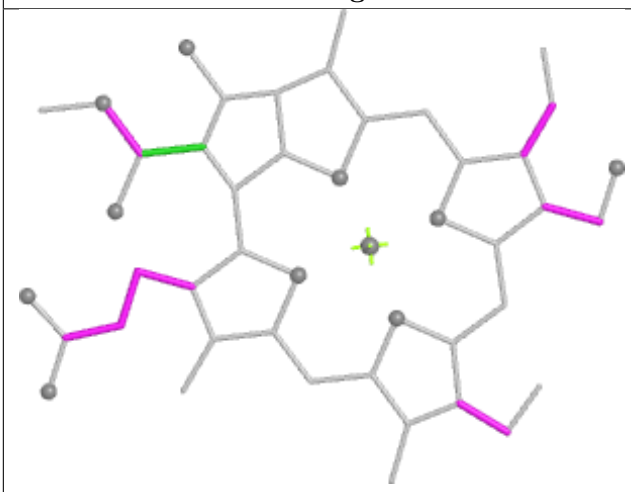
Ligand CHL s 402



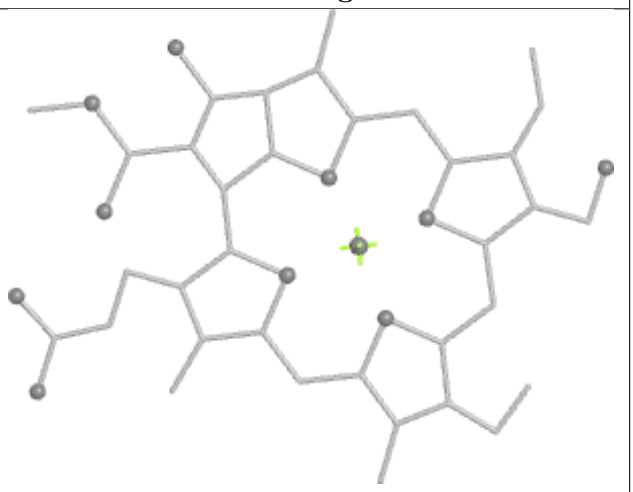
Bond lengths



Bond angles

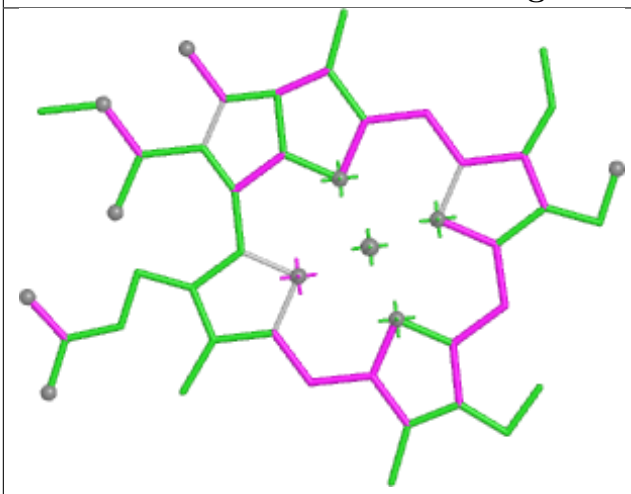


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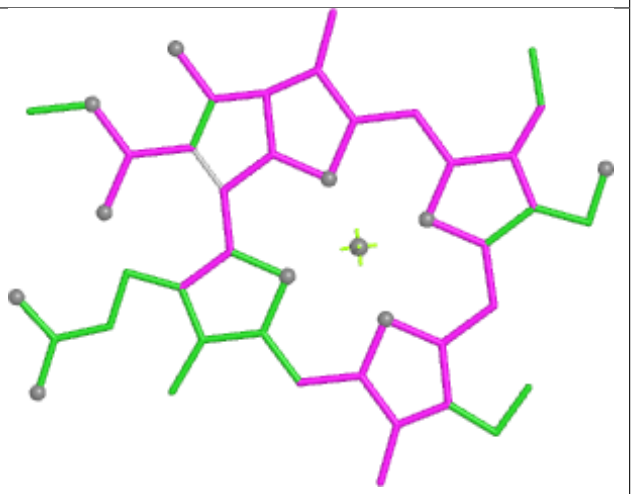


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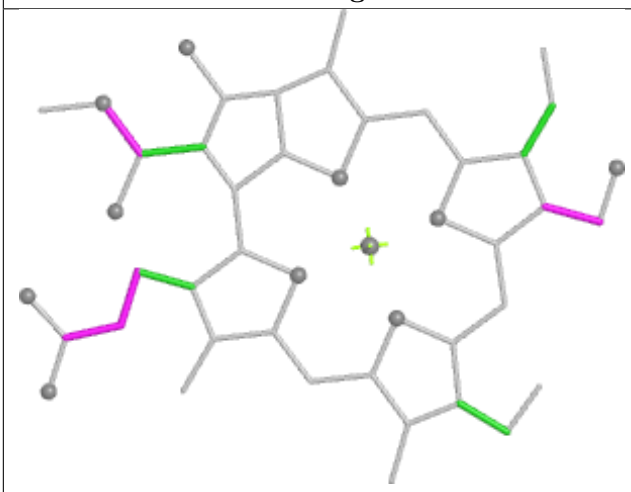
Ligand CHL 2 312



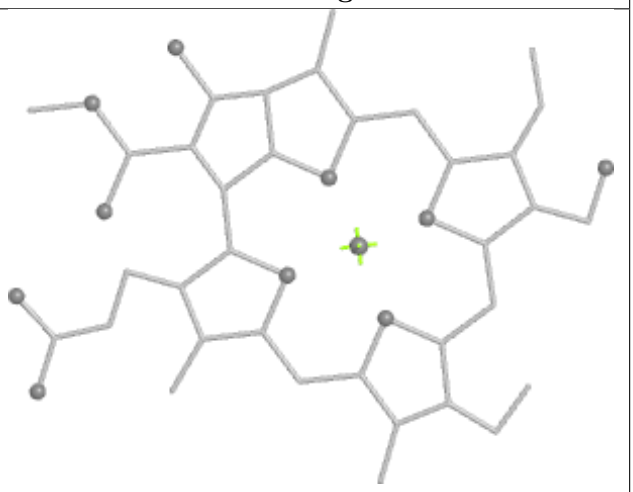
Bond lengths



Bond angles

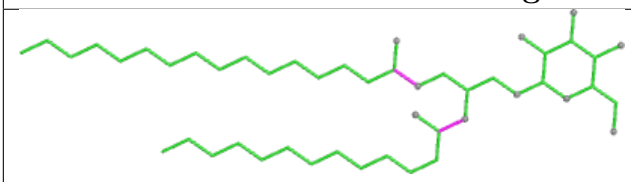


Torsions

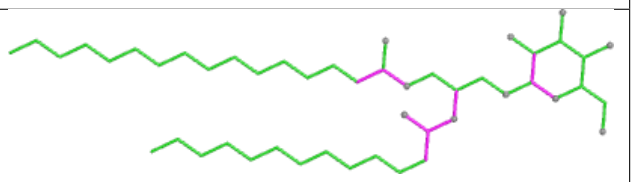


Rings

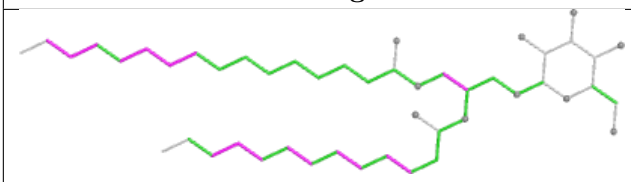
Ligand LMG d 401



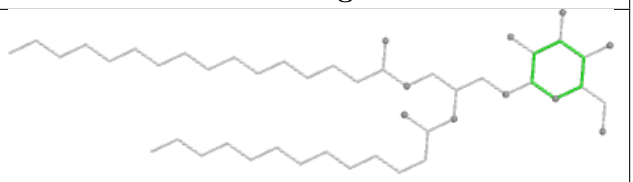
Bond lengths



Bond angles

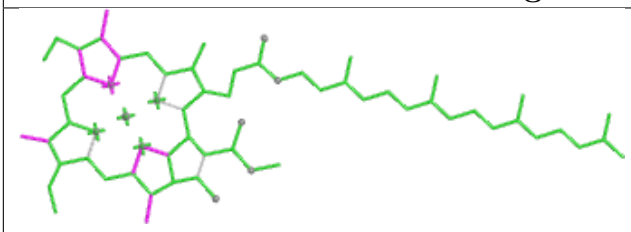


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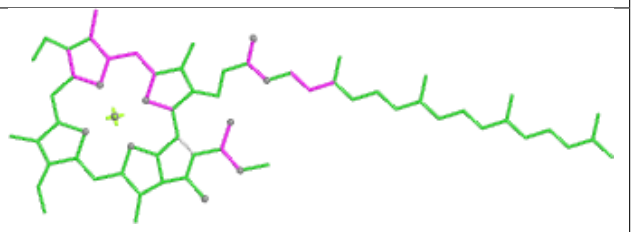


Rings

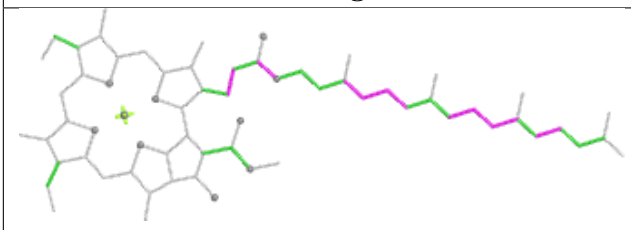
Ligand CLA B 612



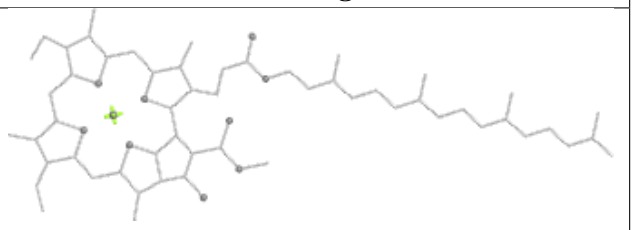
Bond lengths



Bond angles

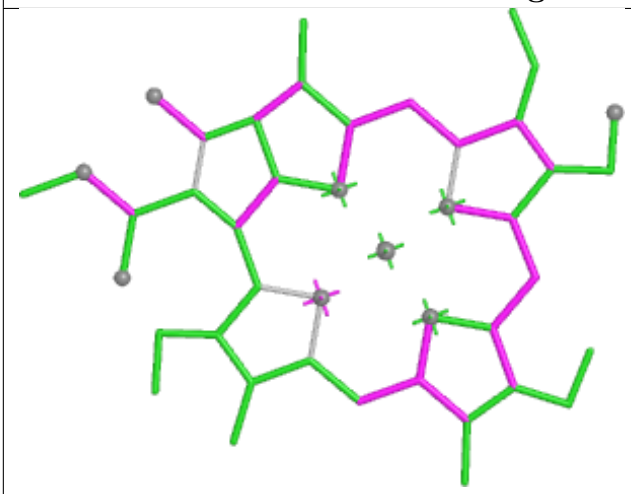


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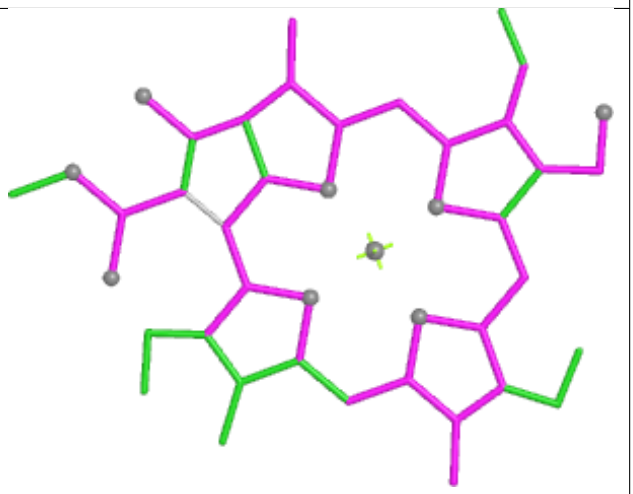


Rings

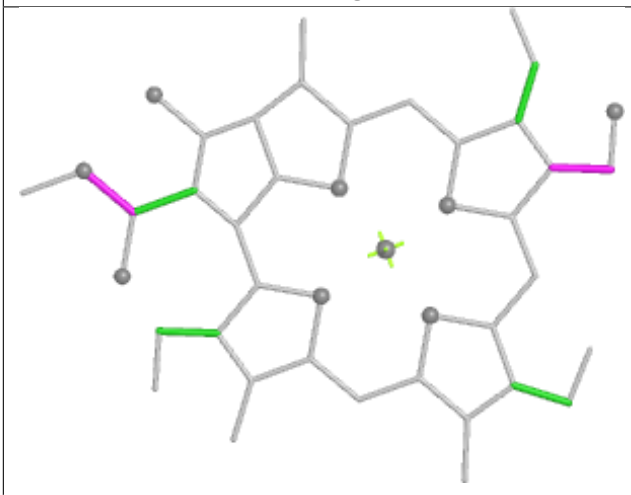
Ligand CHL 4 309



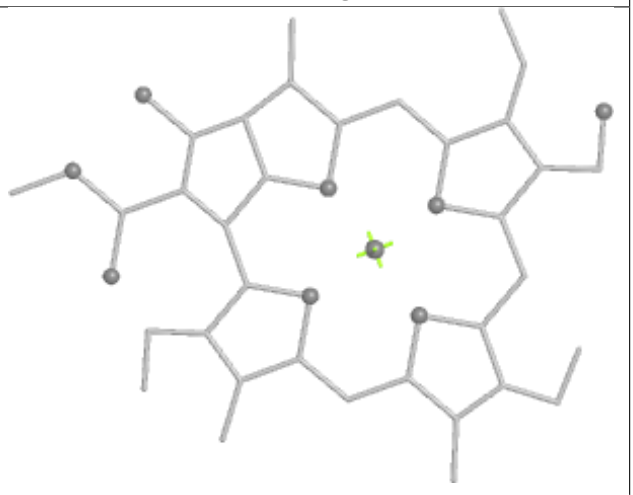
Bond lengths



Bond angles

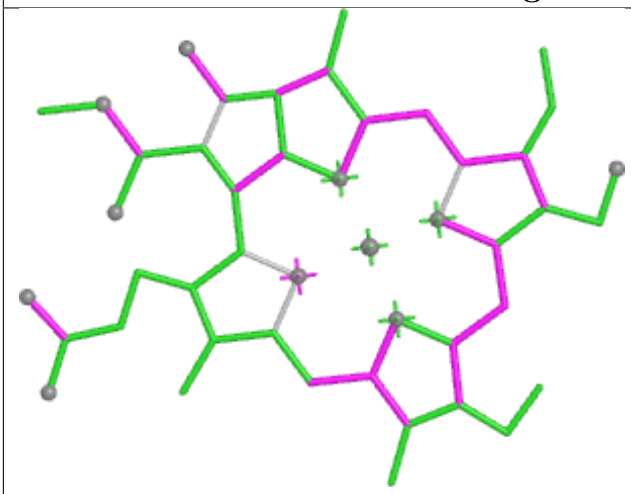


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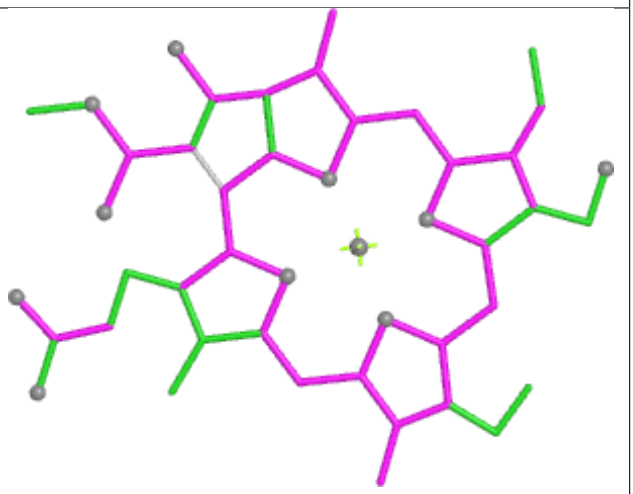


Rings

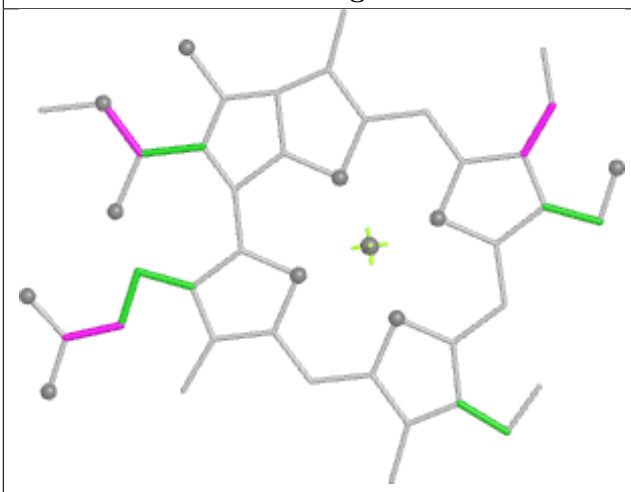
Ligand CHL R 608



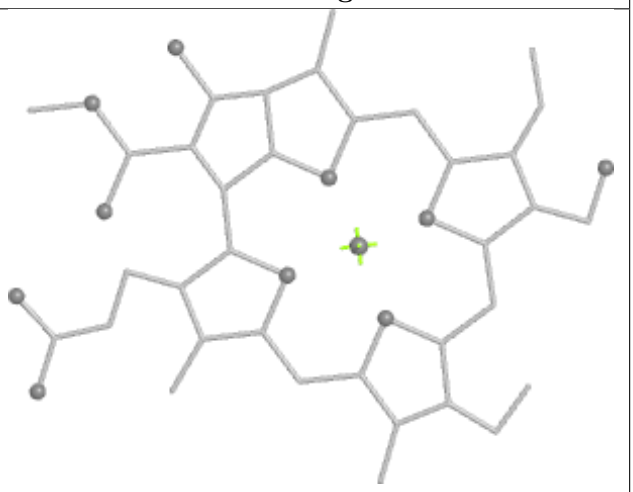
Bond lengths



Bond angles

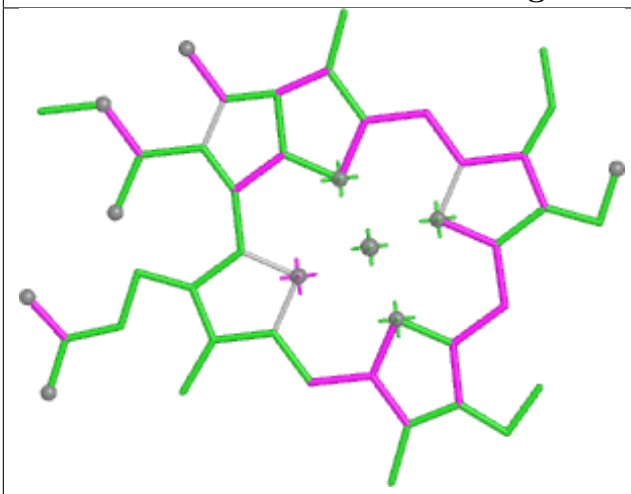


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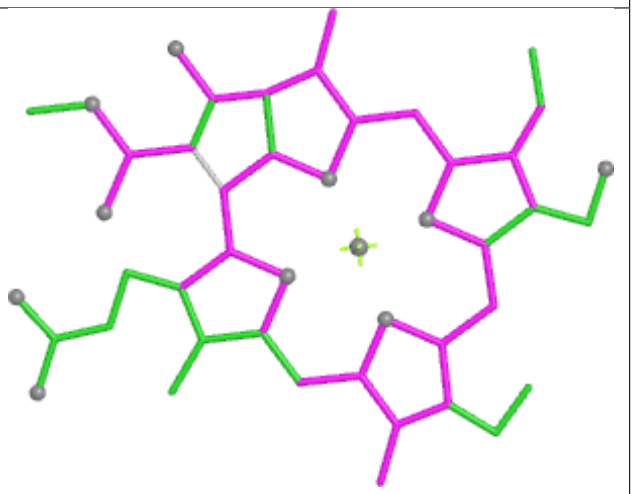


Rings

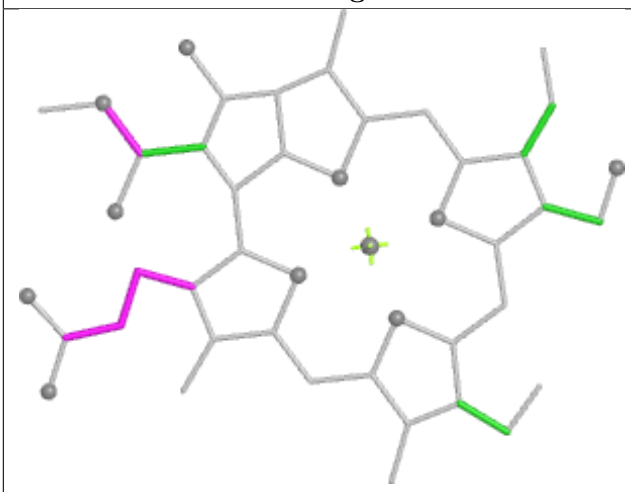
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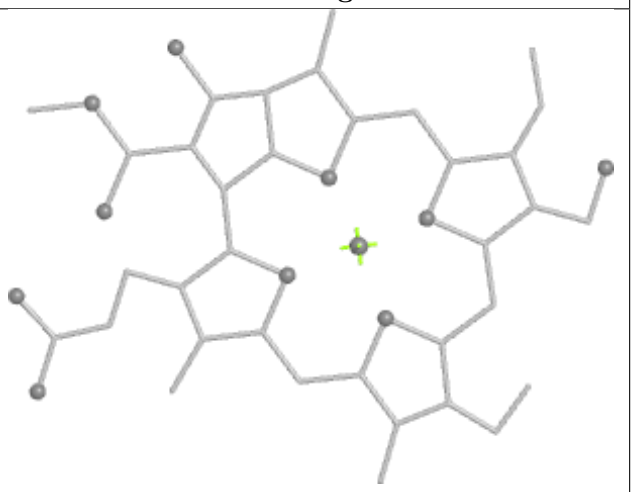
Bond lengths



Bond angles

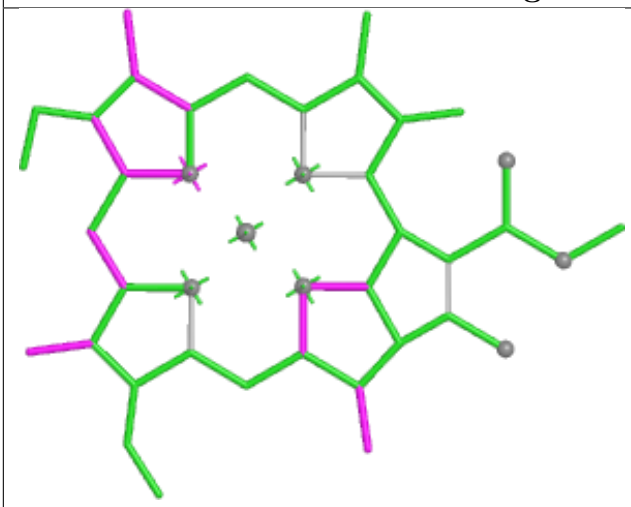


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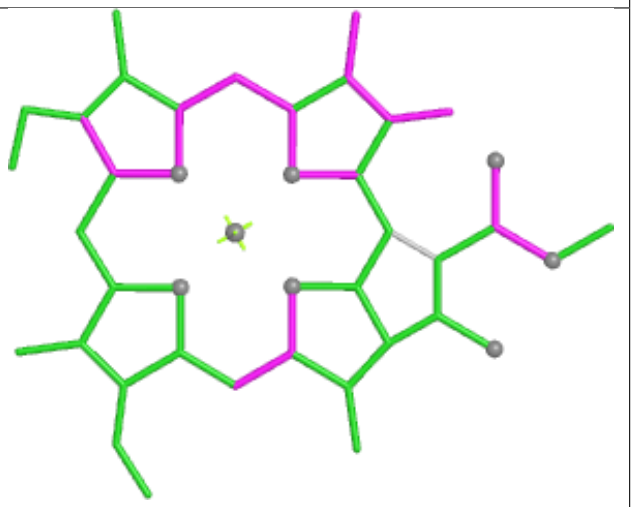


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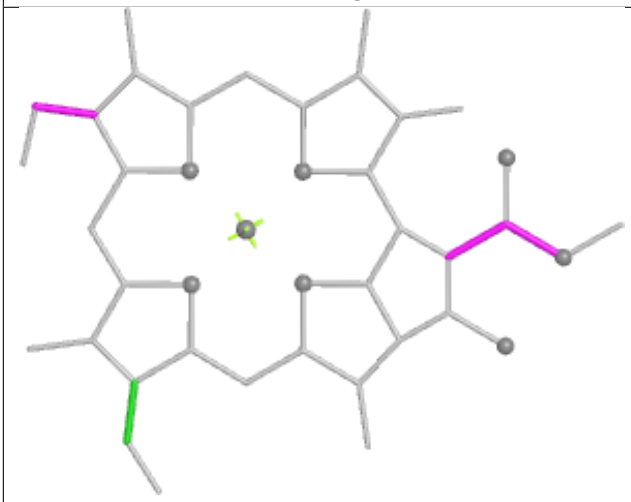
Ligand CLA R 604



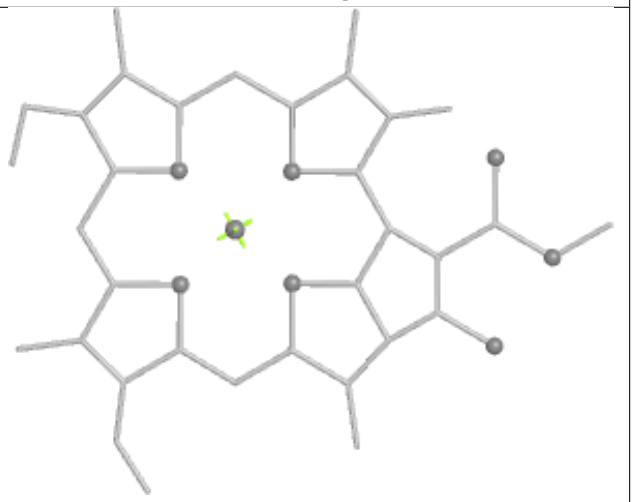
Bond lengths



Bond angles

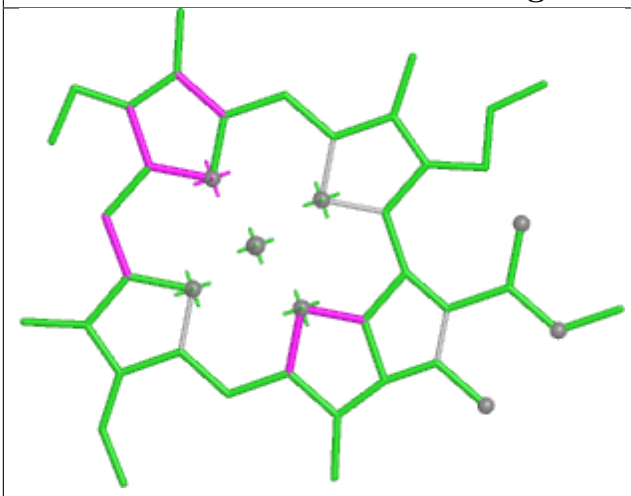


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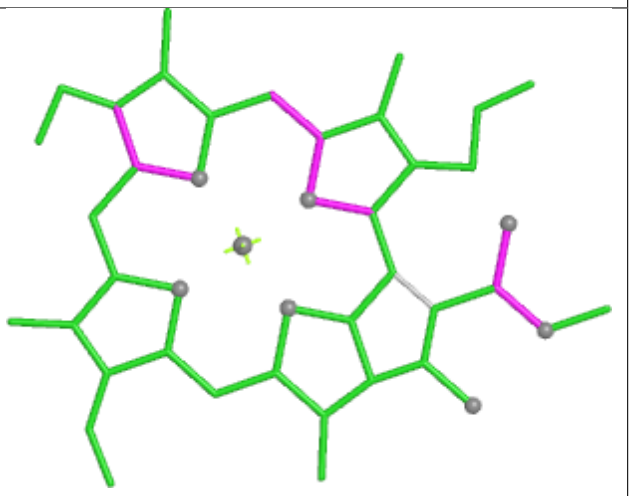


Rings

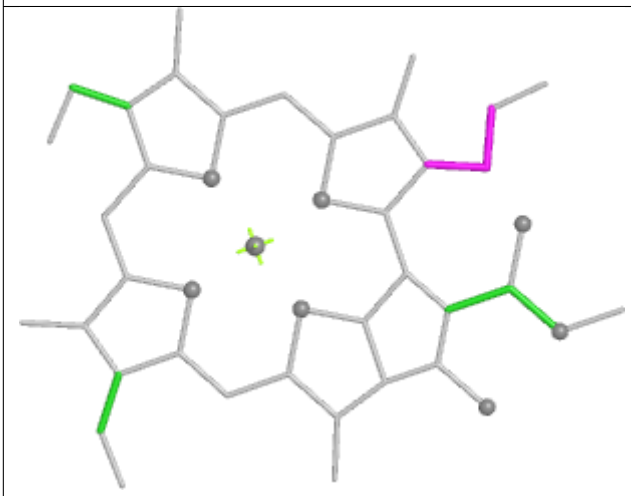
Ligand CLA n 316



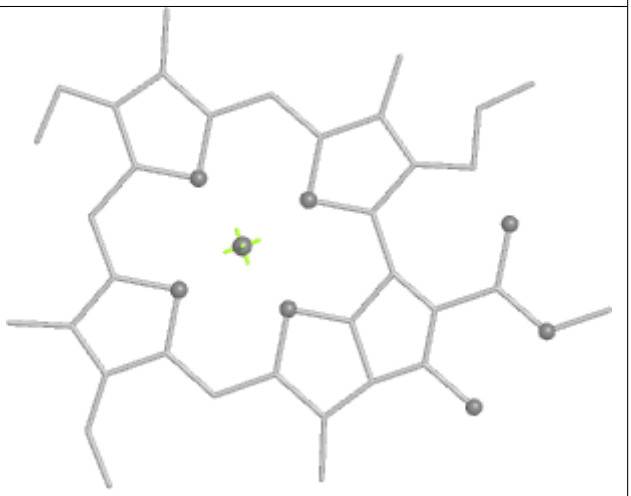
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Bond angles

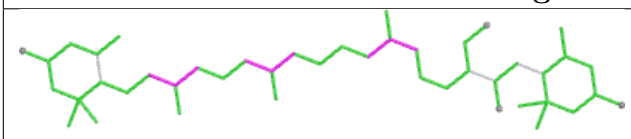


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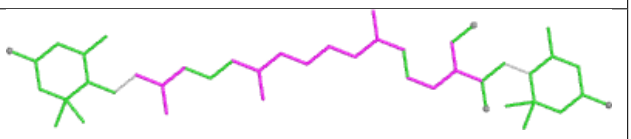


Rings

Ligand 0IE N 302



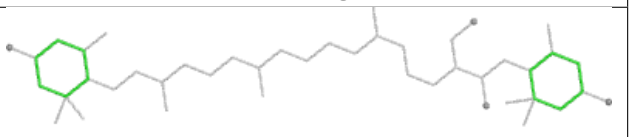
Bond lengths



Bond angles

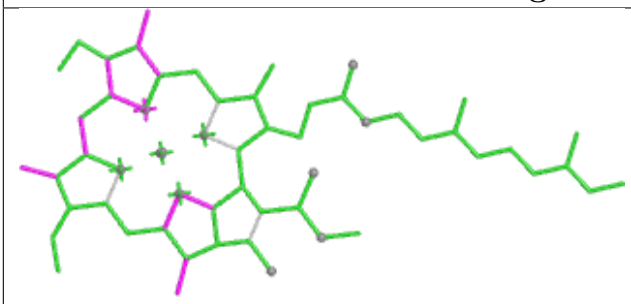


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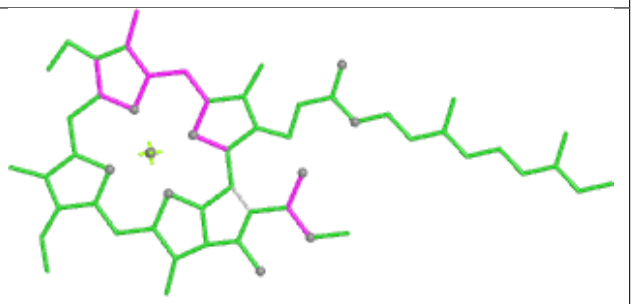


Rings

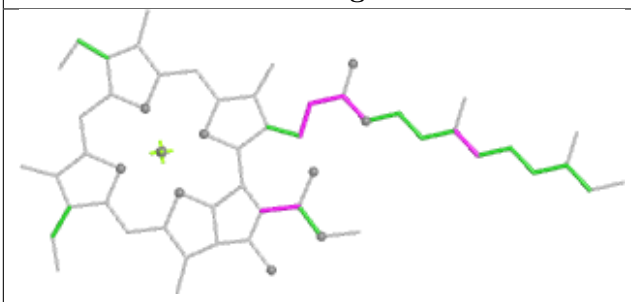
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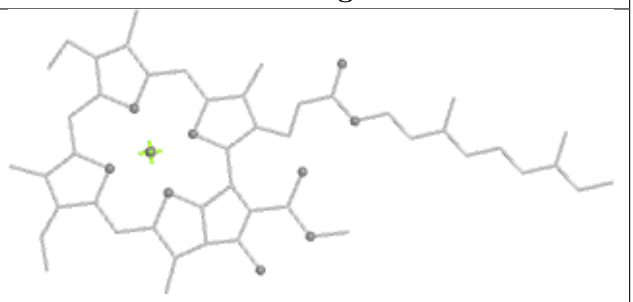
Bond lengths



Bond angles

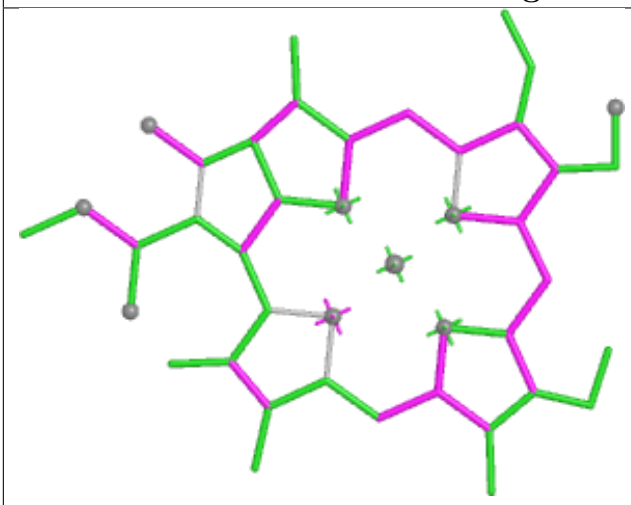


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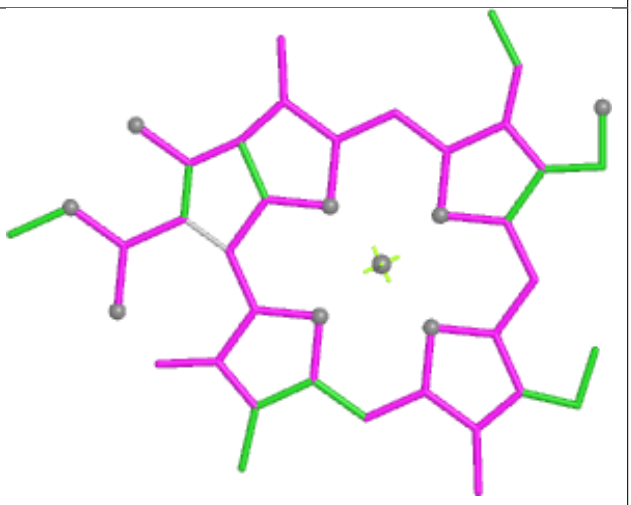


Rings

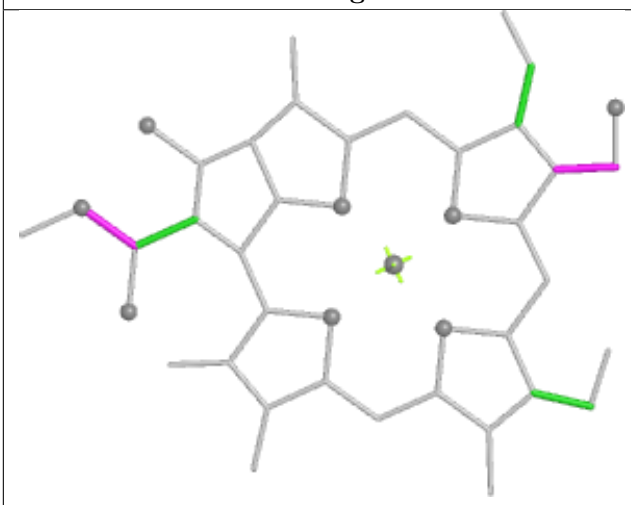
Ligand CHL N 317



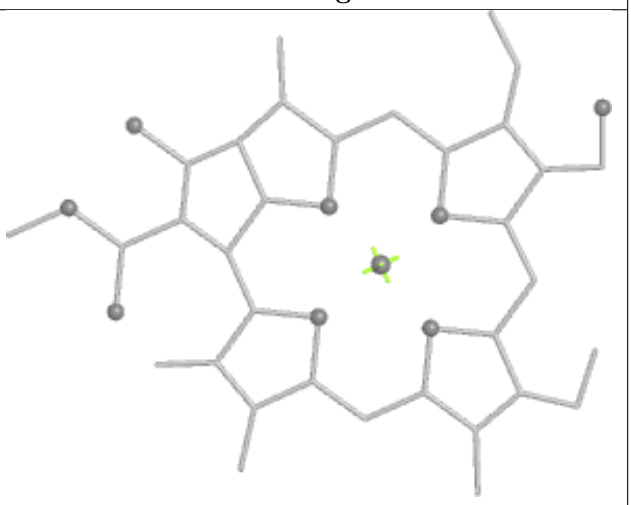
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Bond angles

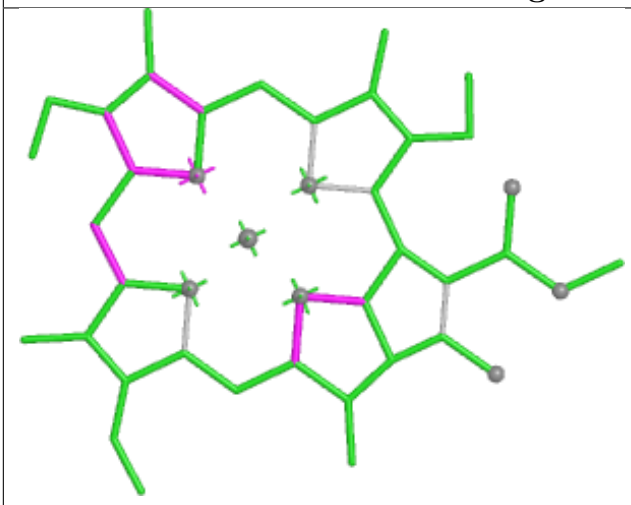


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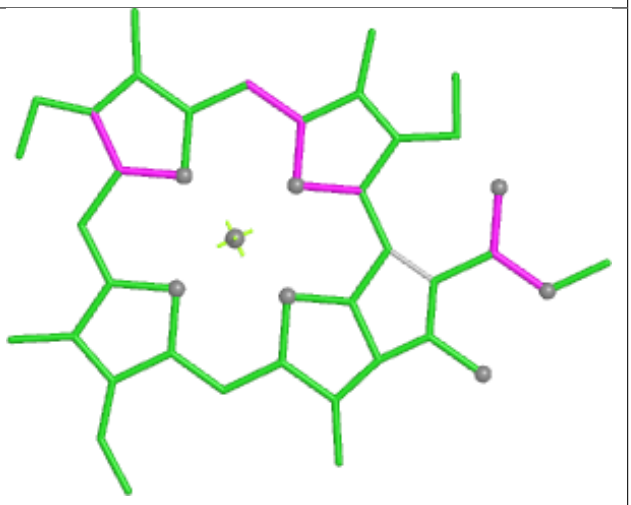


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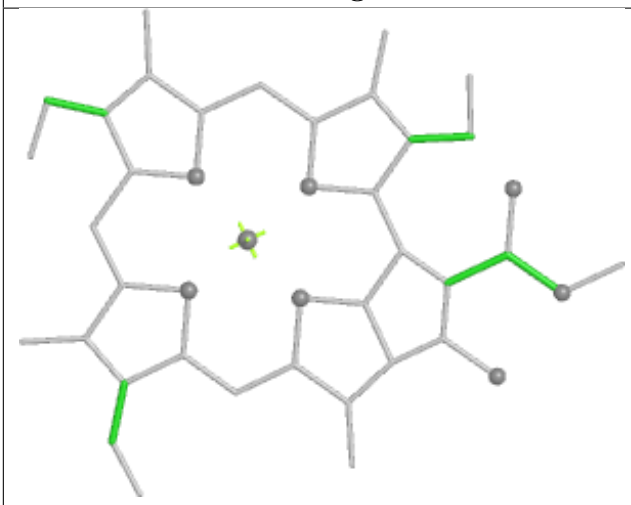
Ligand CLA 4 316



Bond lengths



Bond angles

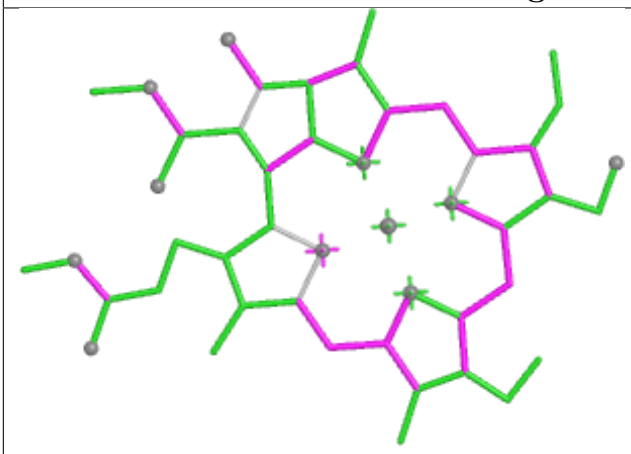


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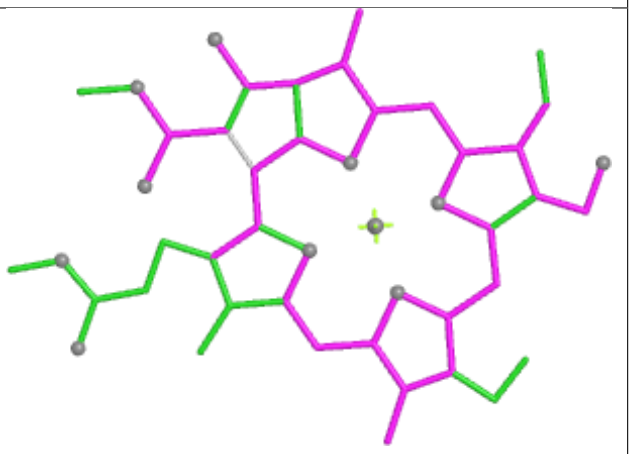


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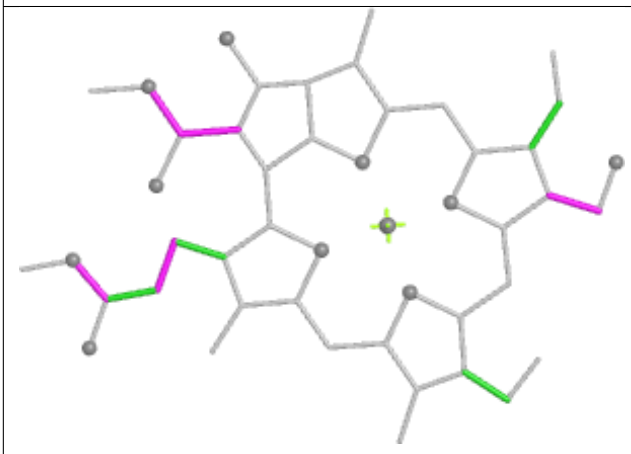
Ligand CHL 5 306



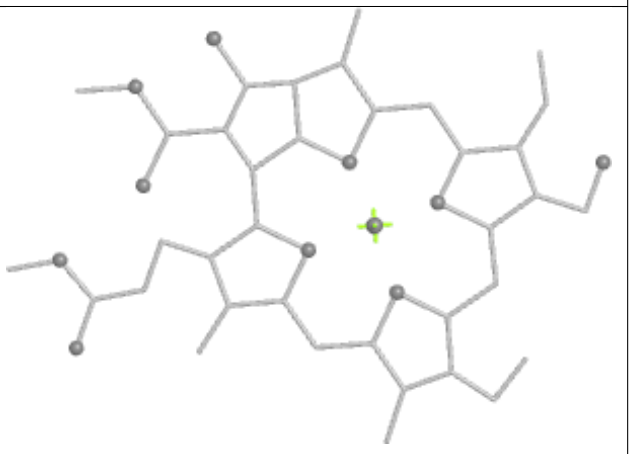
Bond lengths



Bond angles

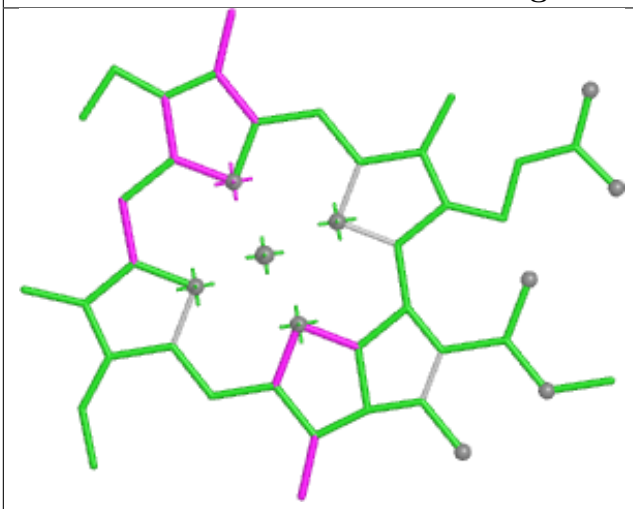


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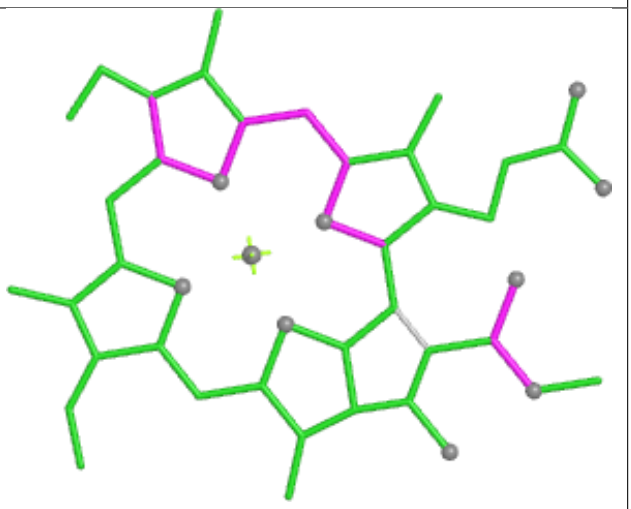


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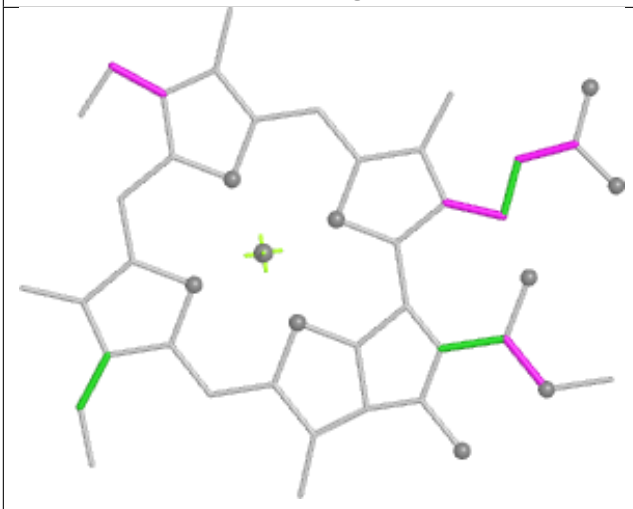
Ligand CLA s 417



Bond lengths



Bond angles

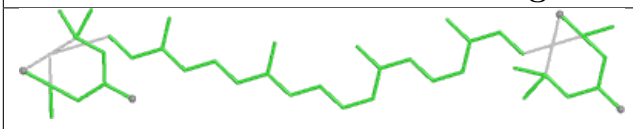


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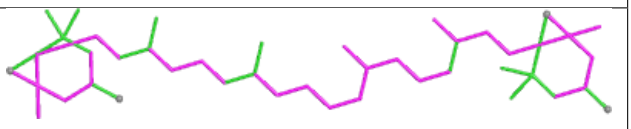


Rings

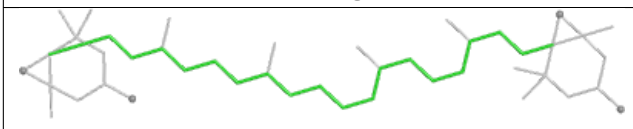
Ligand XAT r 316



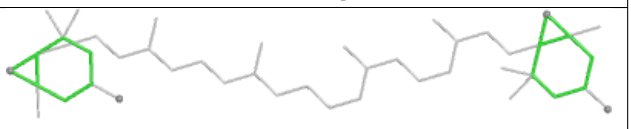
Bond lengths



Bond angles

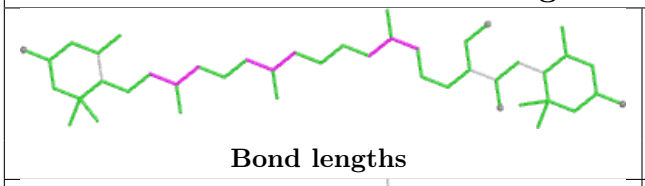


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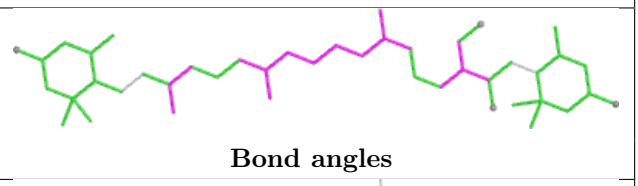


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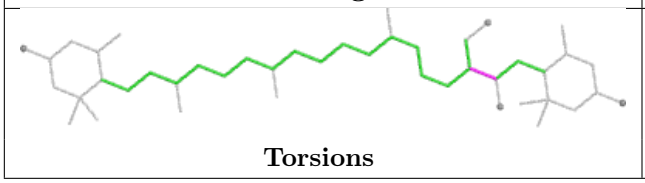
Ligand 0IE 2 302



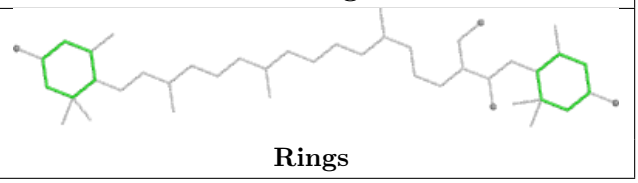
Bond lengths



Bond angles

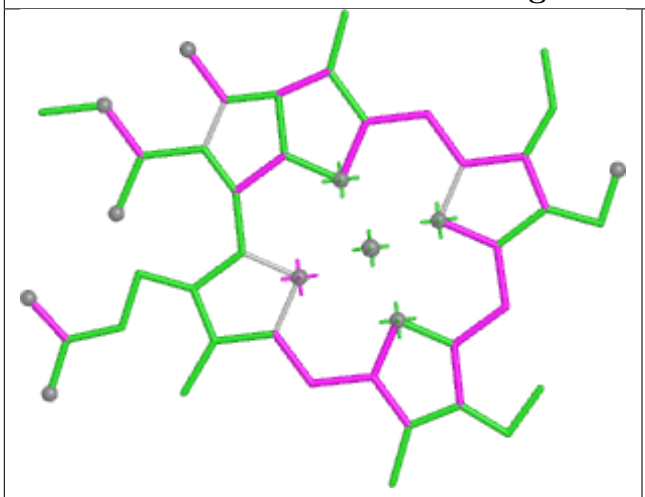


Torsions

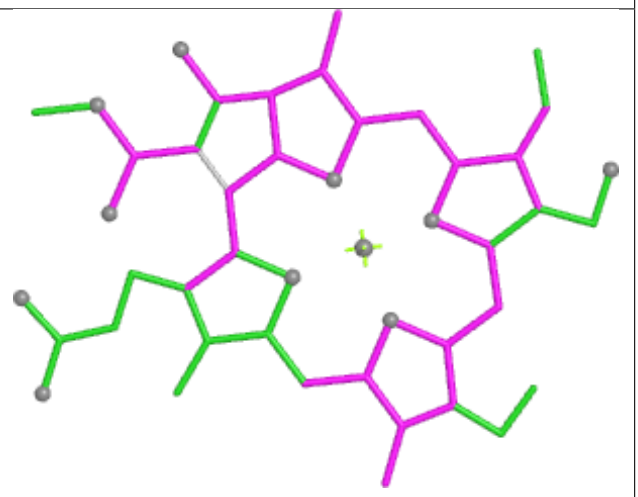


Rings

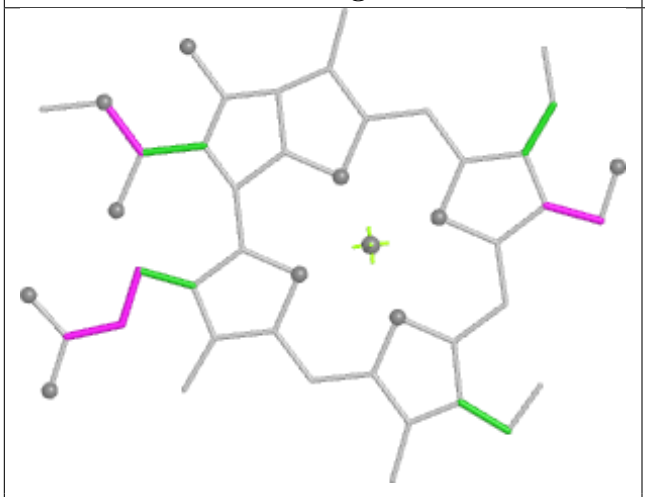
Ligand CHL 5 312



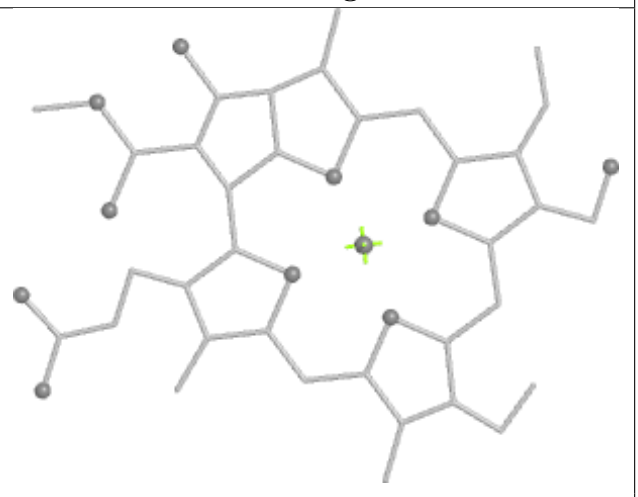
Bond lengths



Bond angles

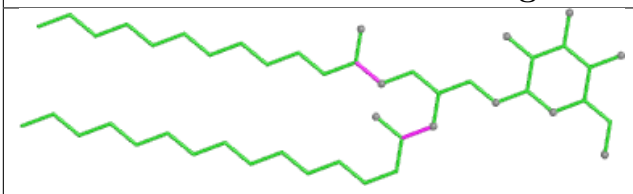


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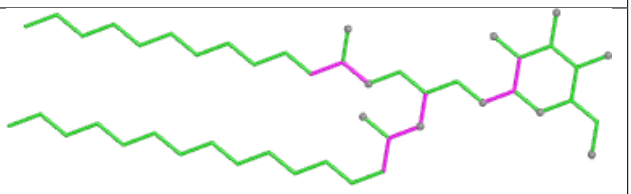


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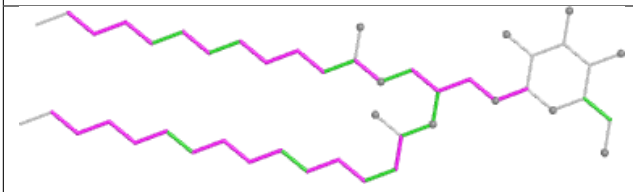
Ligand LMG D 411



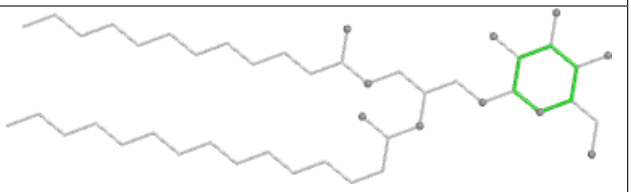
Bond lengths



Bond angles

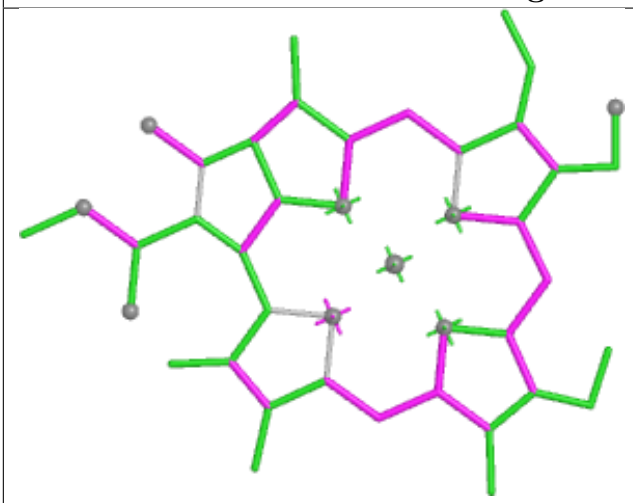


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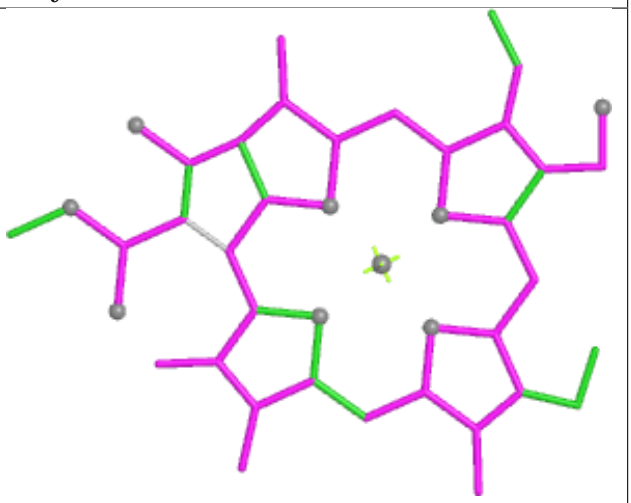


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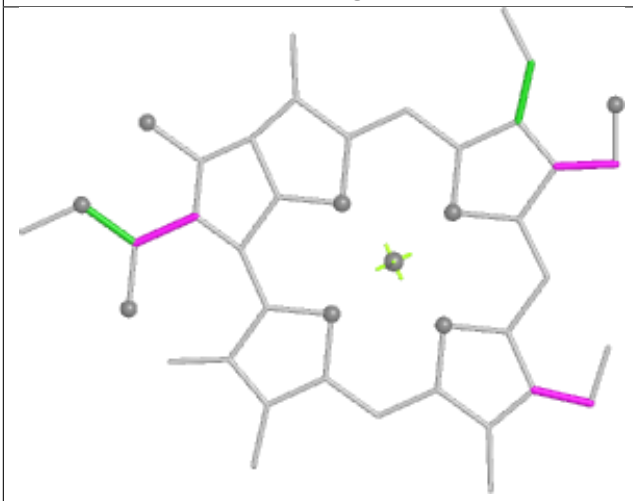
Ligand CHL y 318



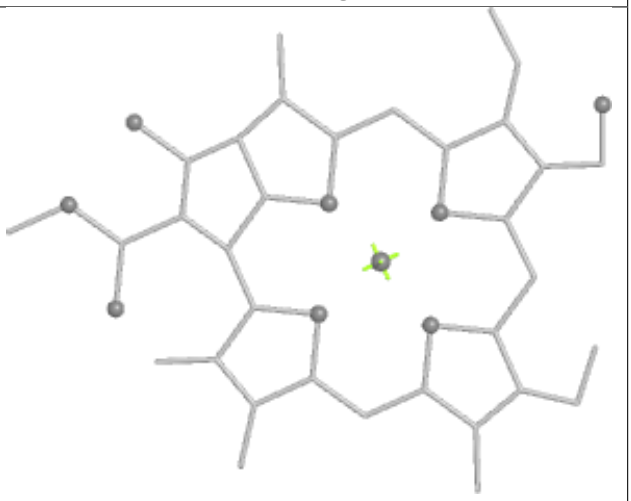
Bond lengths



Bond angles

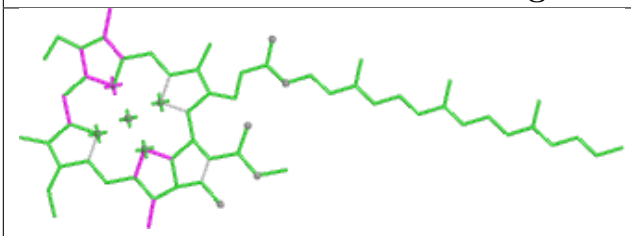


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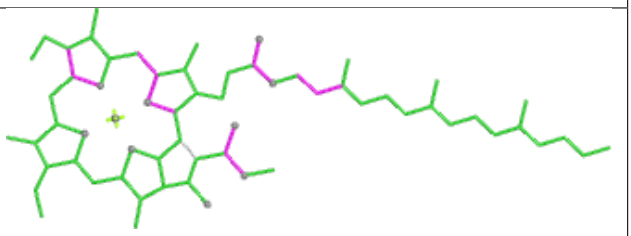


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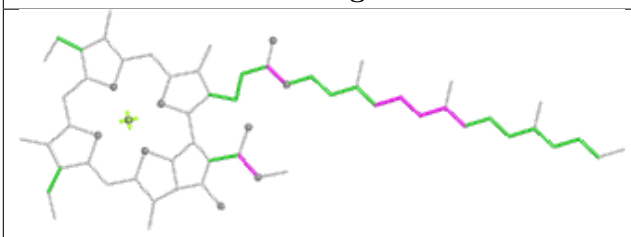
Ligand CLA 8 312



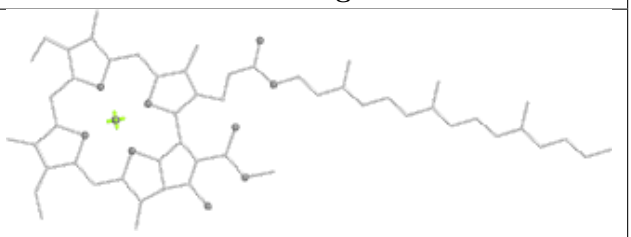
Bond lengths



Bond angles

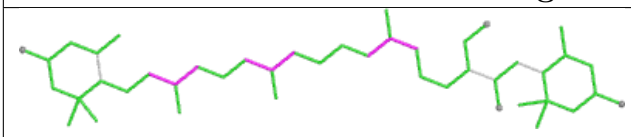


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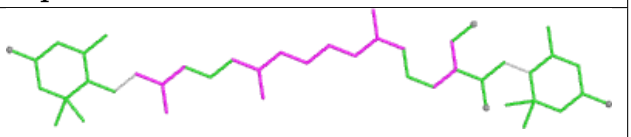


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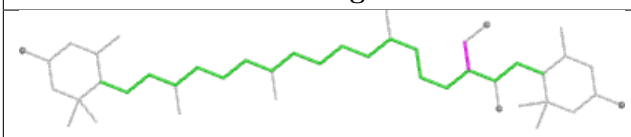
Ligand 0IE p 303



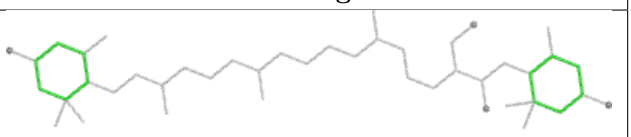
Bond lengths



Bond angles

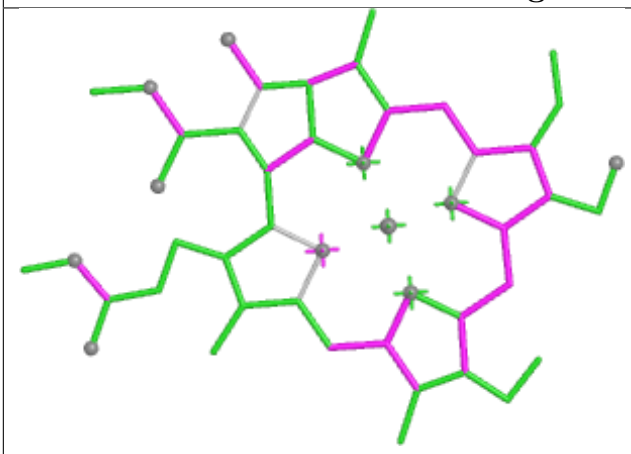


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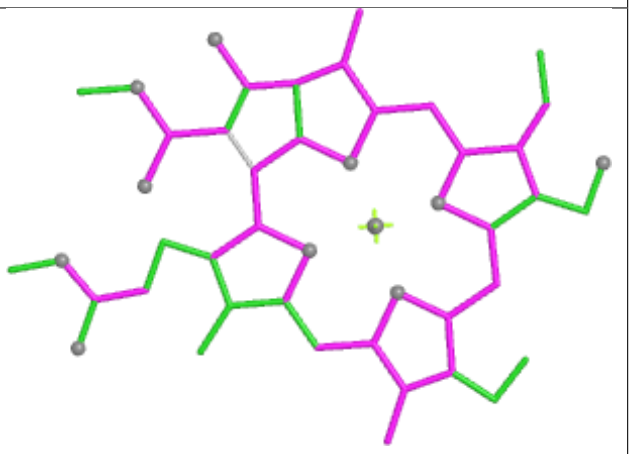


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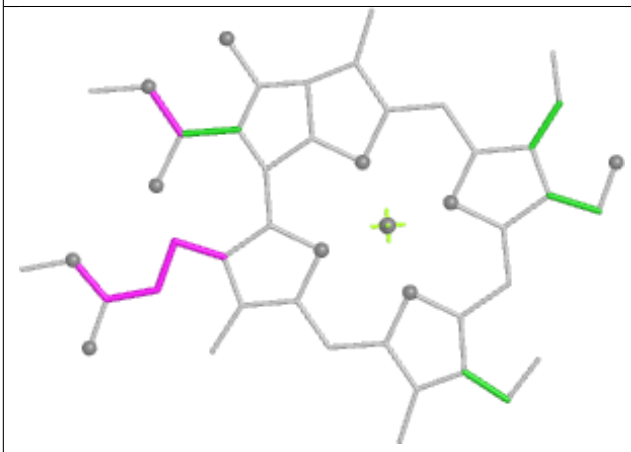
Ligand CHL 2 311



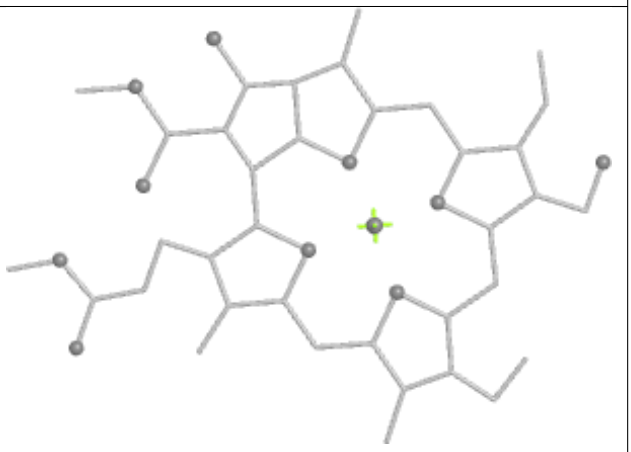
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Bond angles

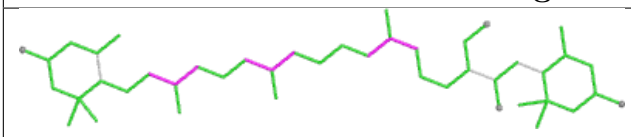


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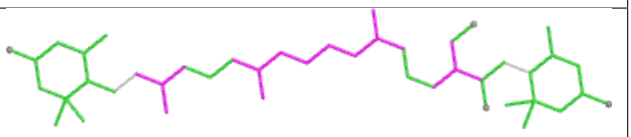


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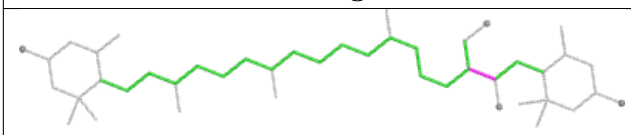
Ligand 0IE Y 302



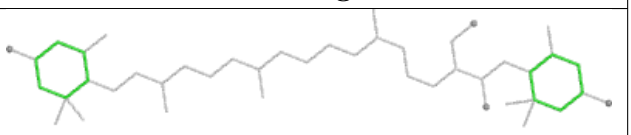
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Bond angles

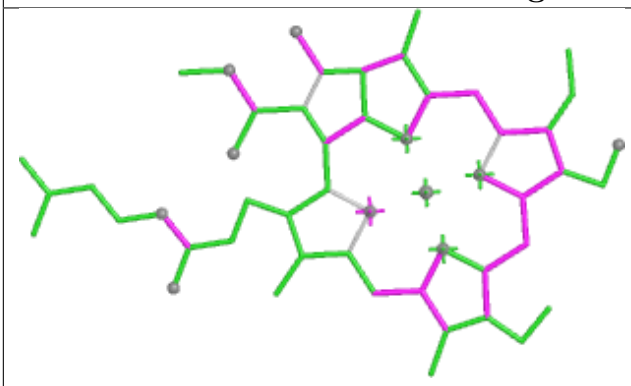


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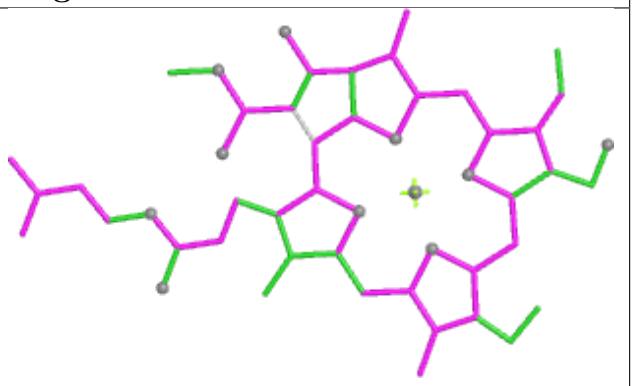


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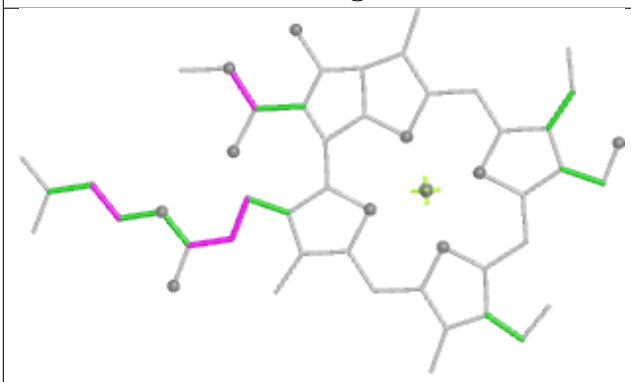
Ligand CHL g 312



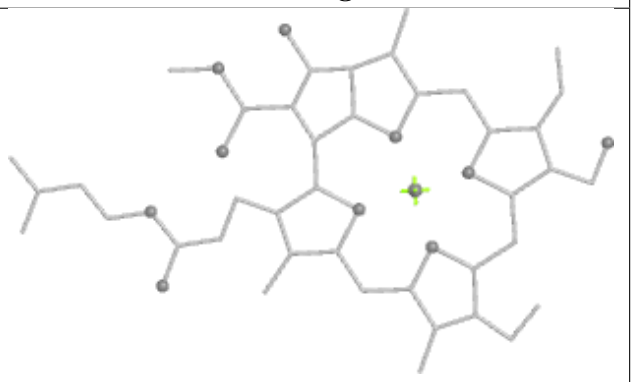
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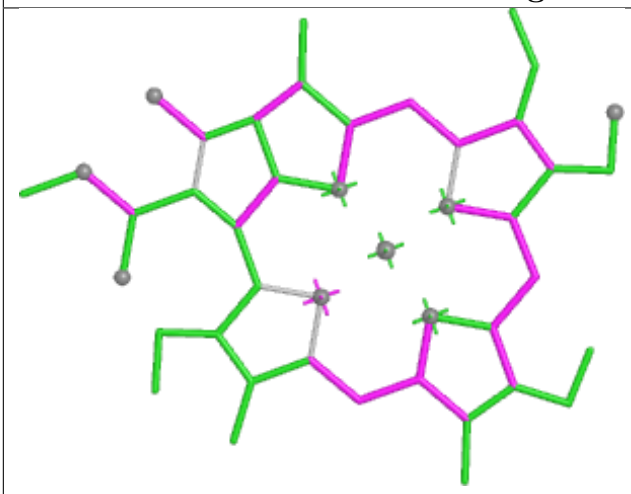


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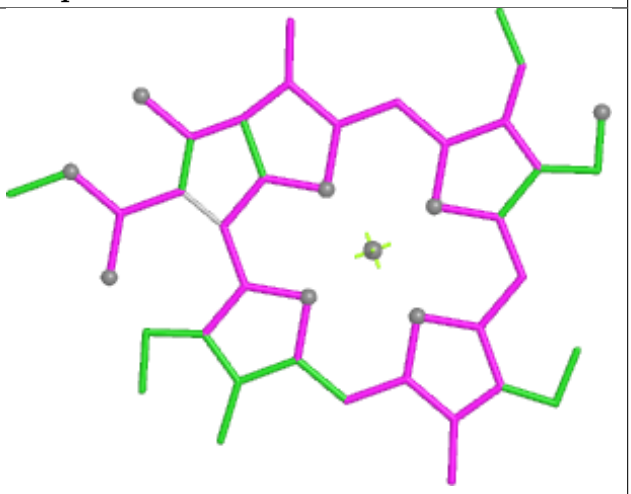


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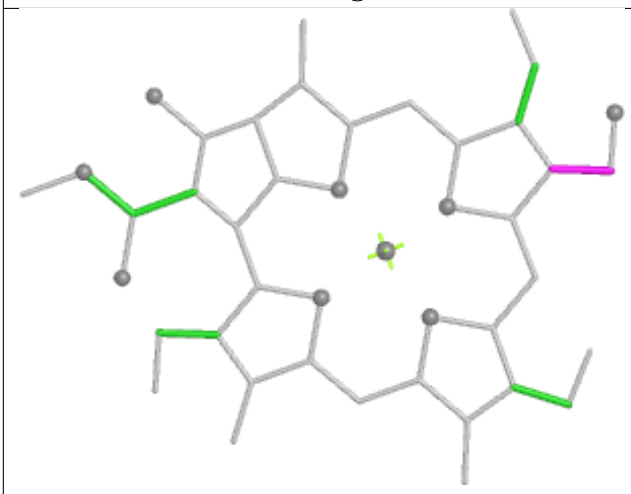
Ligand CHL q 307



Bond lengths



Bond angles



Torsions

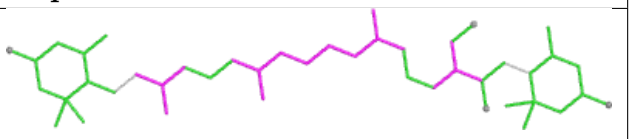


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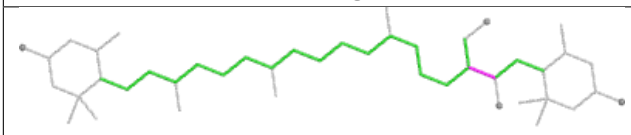
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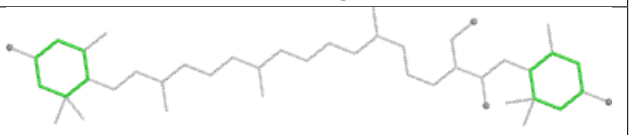
Bond lengths



Bond angles

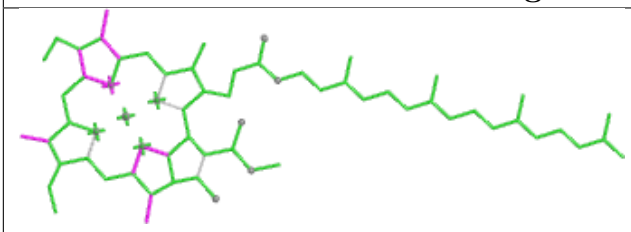


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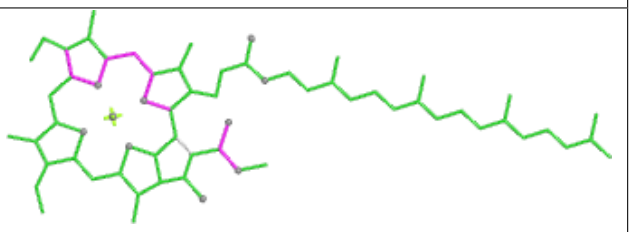


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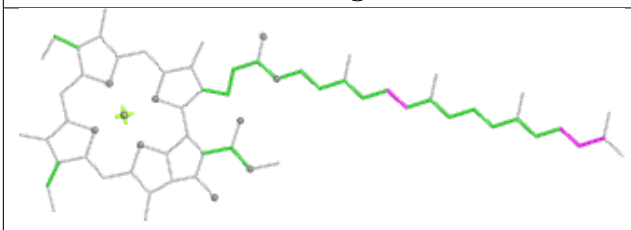
Ligand CLA B 615



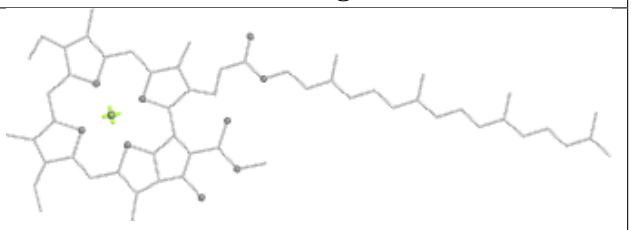
Bond lengths



Bond angles

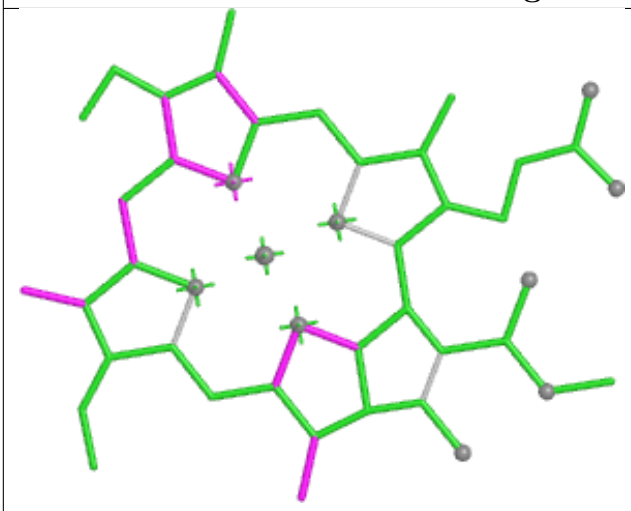


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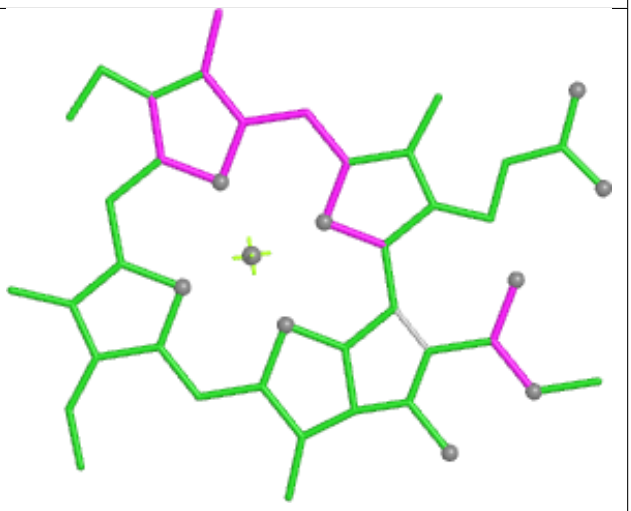


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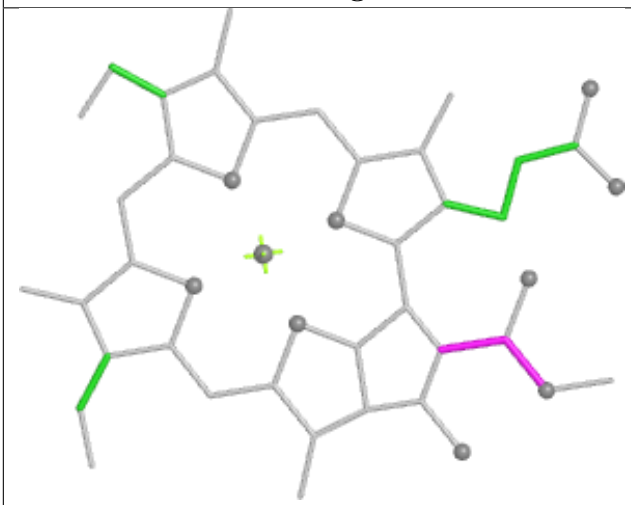
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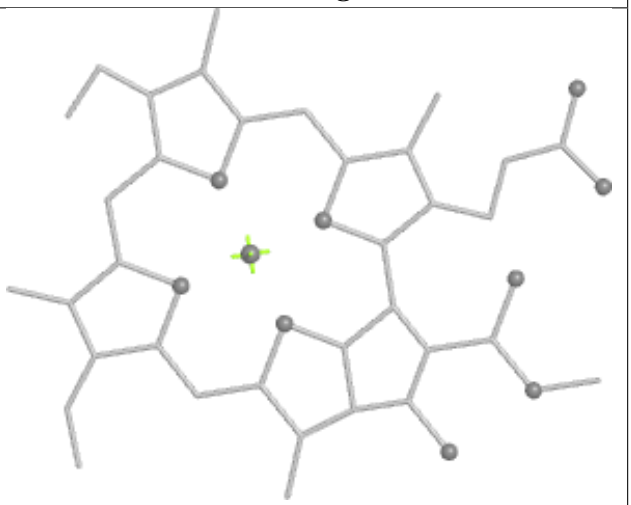
Bond lengths



Bond angles

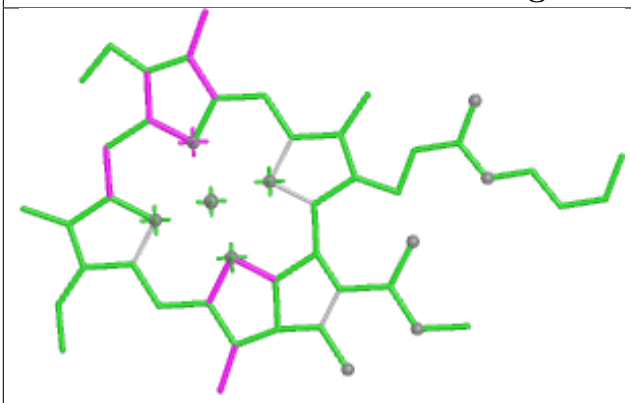


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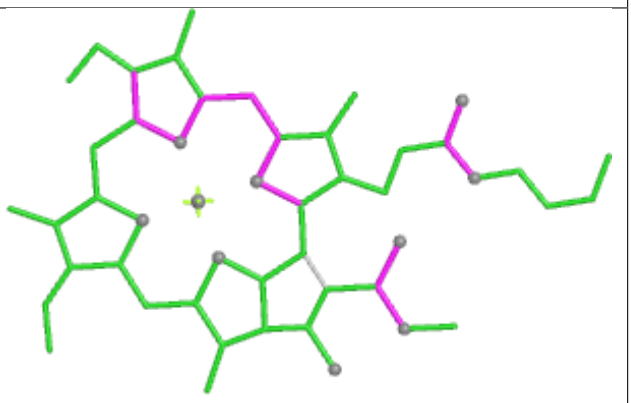


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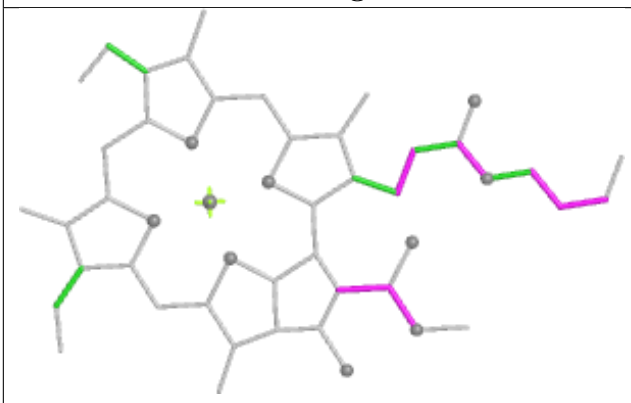
Ligand CLA 5 317



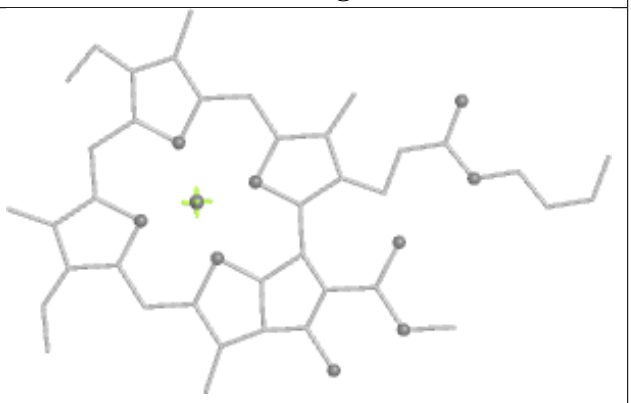
Bond lengths



Bond angles

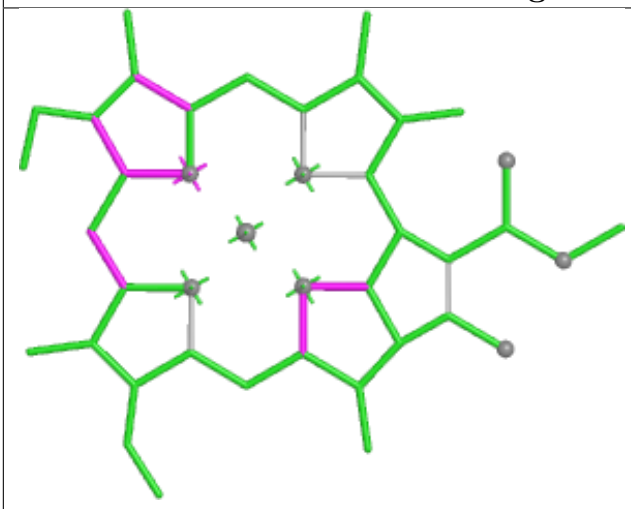


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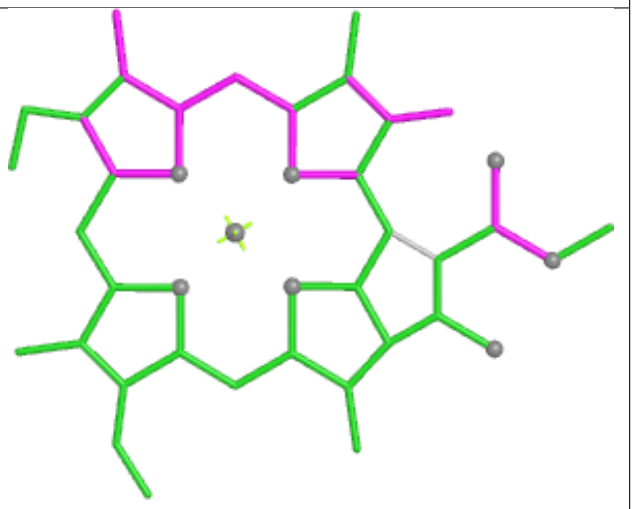


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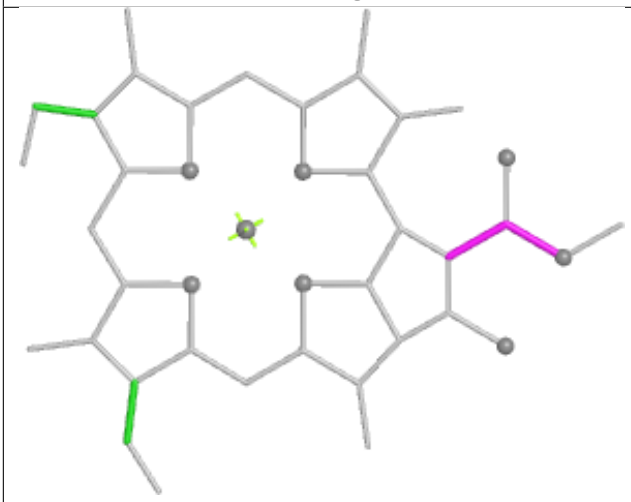
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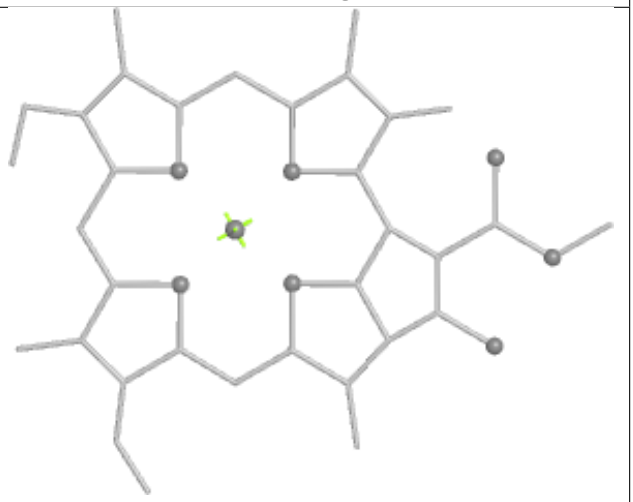
Bond lengths



Bond angles

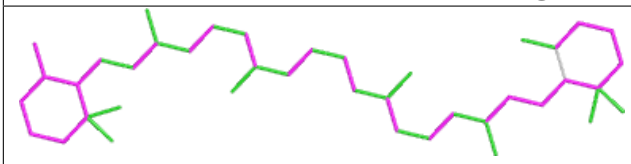


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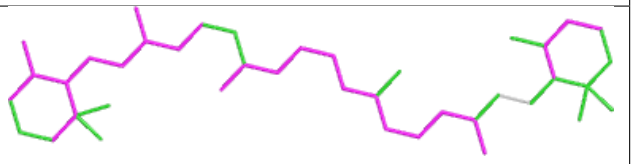


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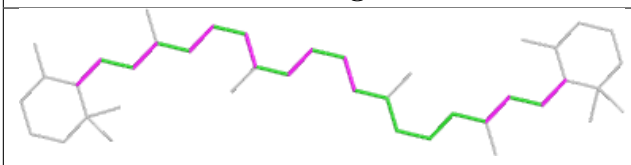
Ligand 8CT t 101



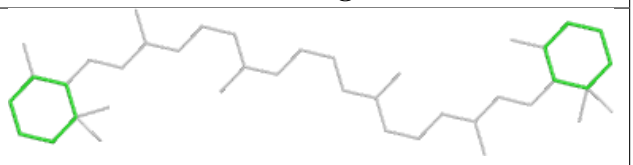
Bond lengths



Bond angles

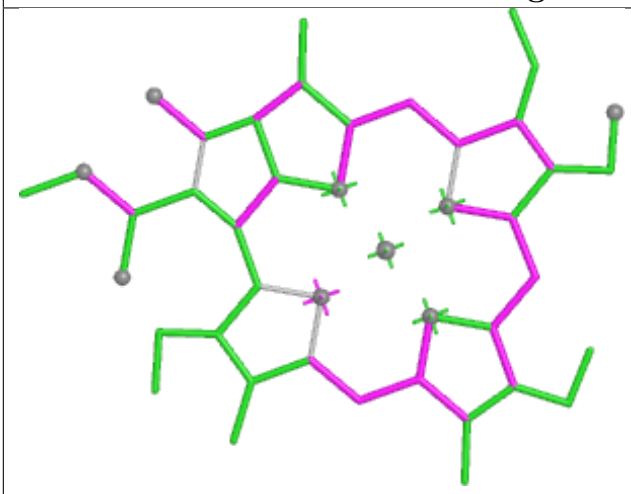


Torsions

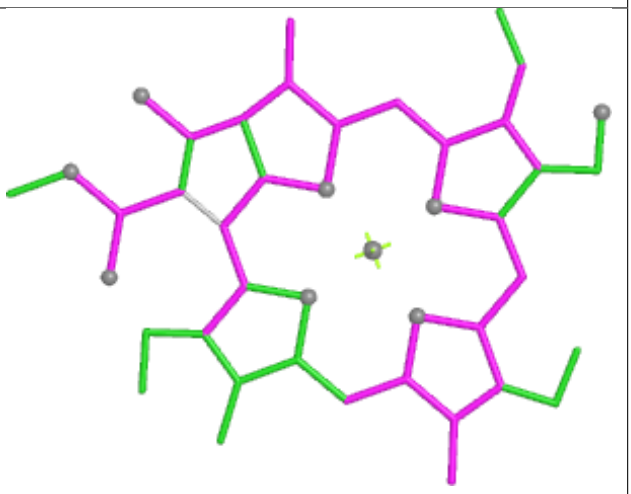


Rings

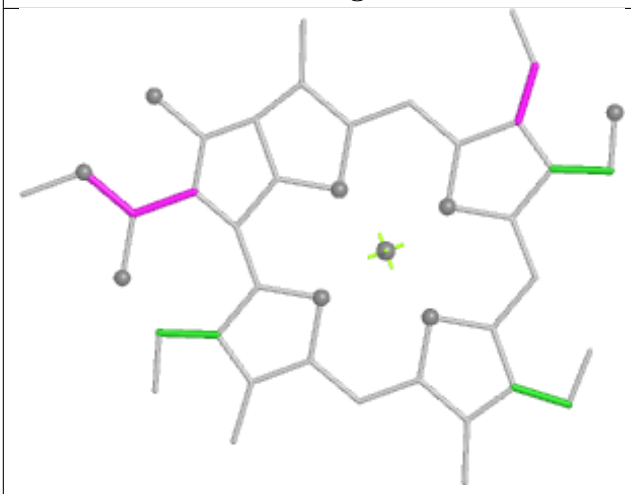
Ligand CHL 7 313



Bond lengths



Bond angles

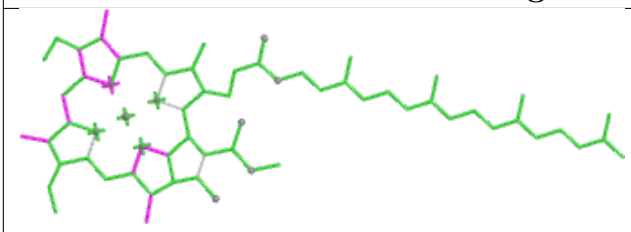


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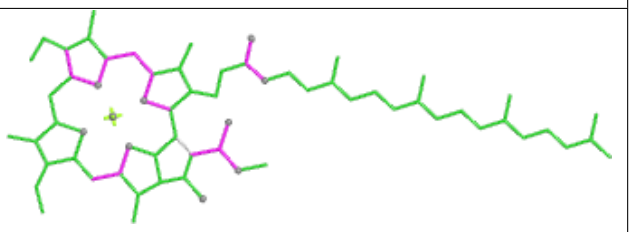


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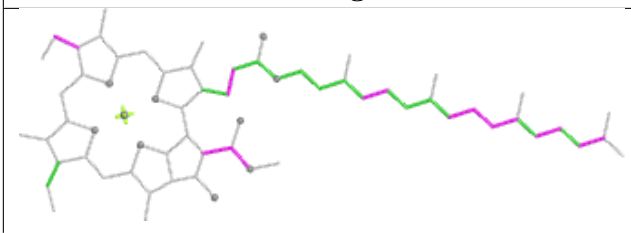
Ligand CLA b 607



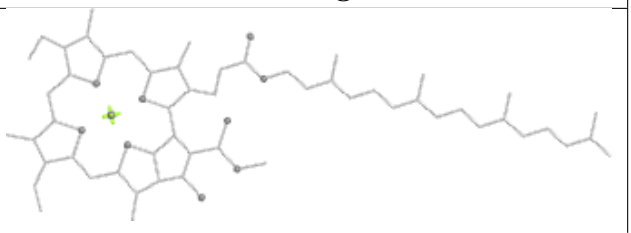
Bond lengths



Bond angles

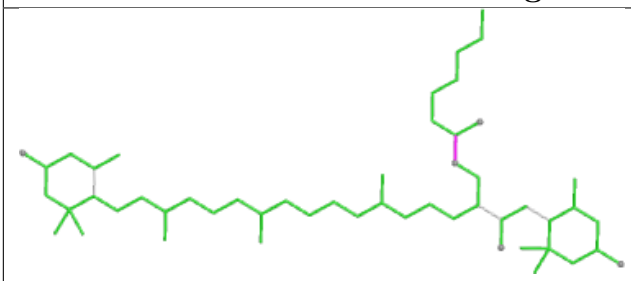


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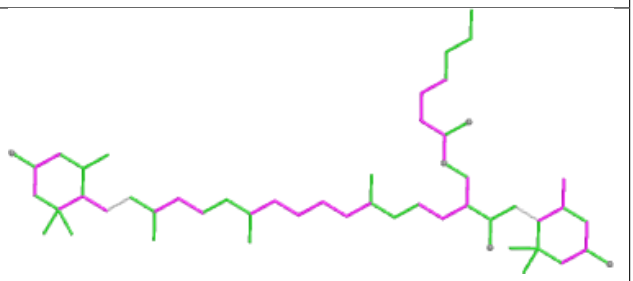


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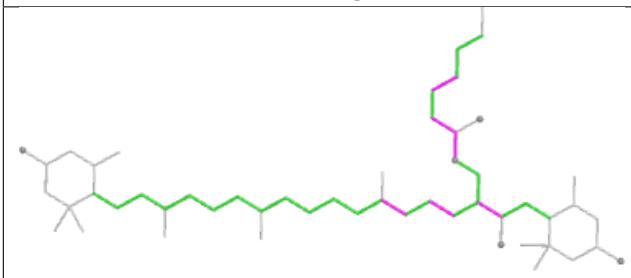
Ligand 0UR N 301



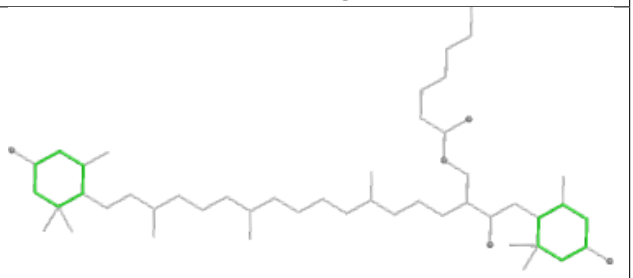
Bond lengths



Bond angles

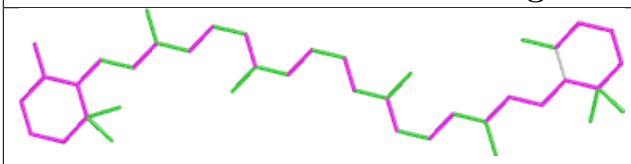


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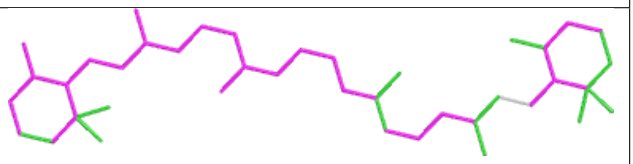


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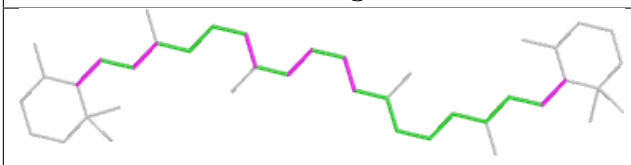
Ligand 8CT C 613



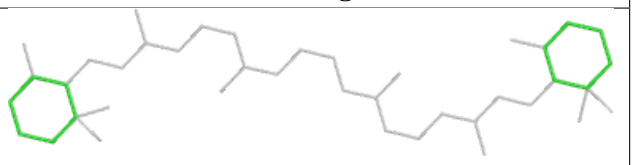
Bond lengths



Bond angles

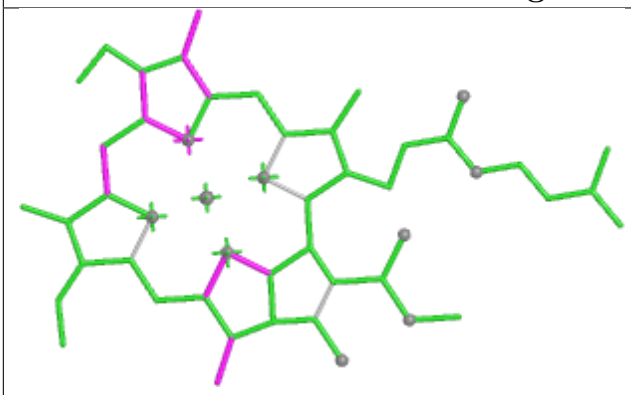


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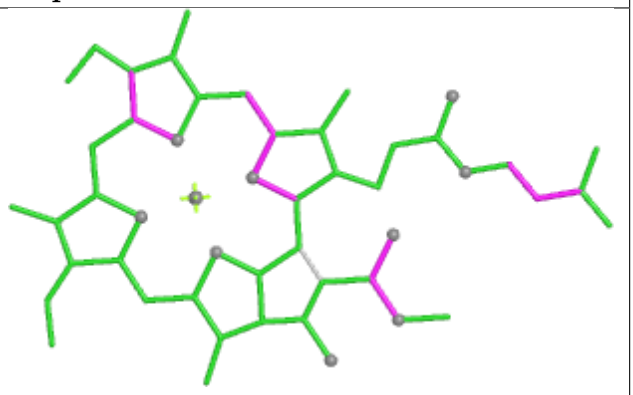


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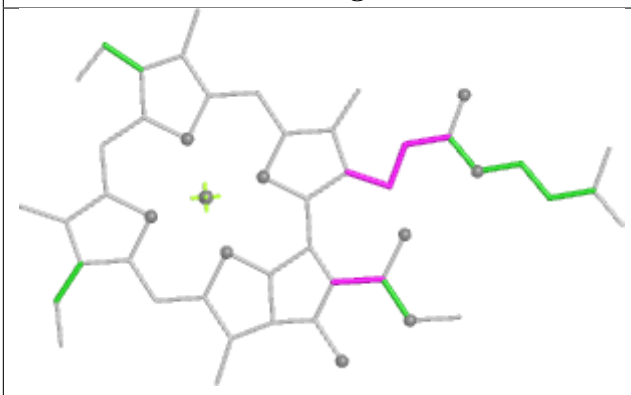
Ligand CLA p 308



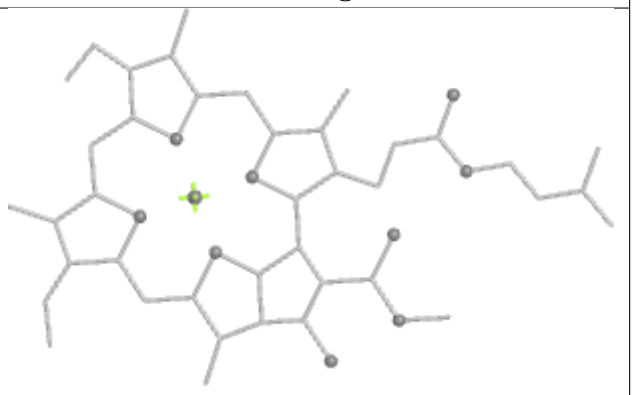
Bond lengths



Bond angles

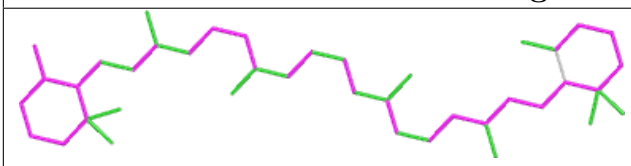


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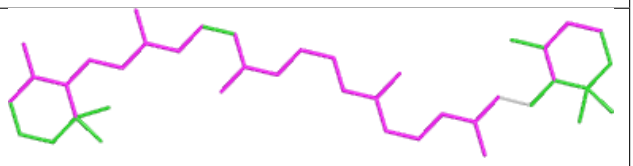


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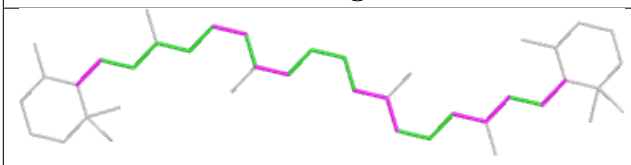
Ligand 8CT S 615



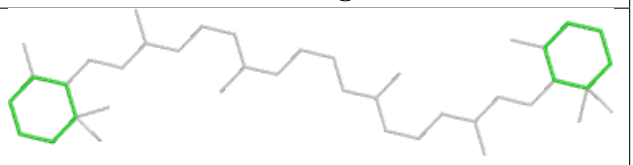
Bond lengths



Bond angles

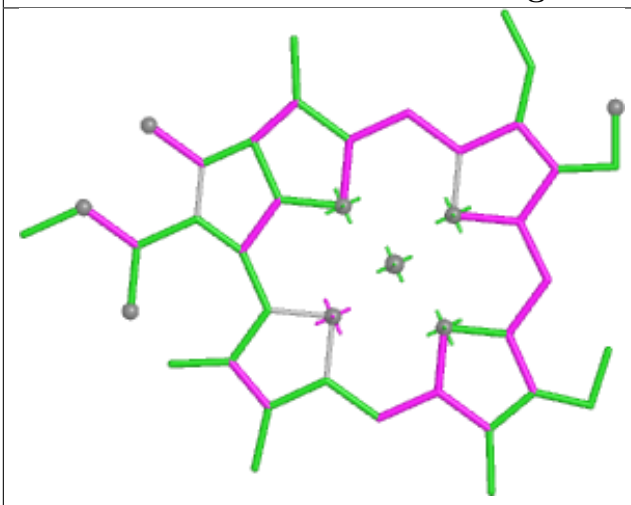


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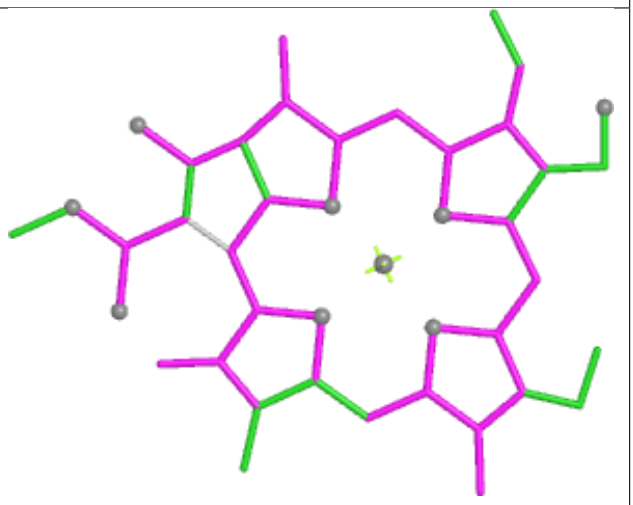


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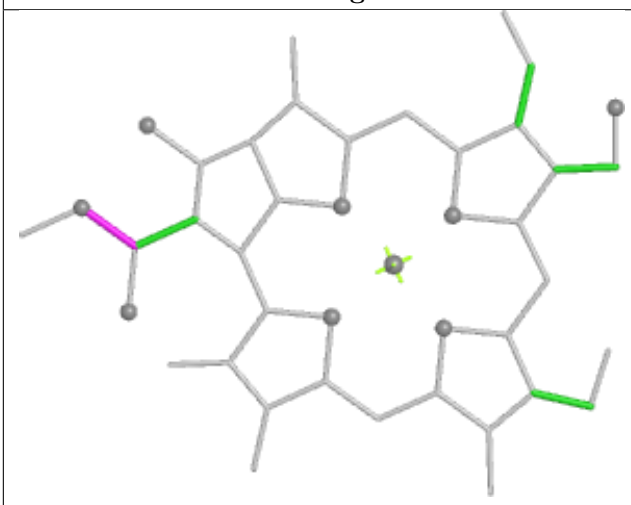
Ligand CHL 4 304



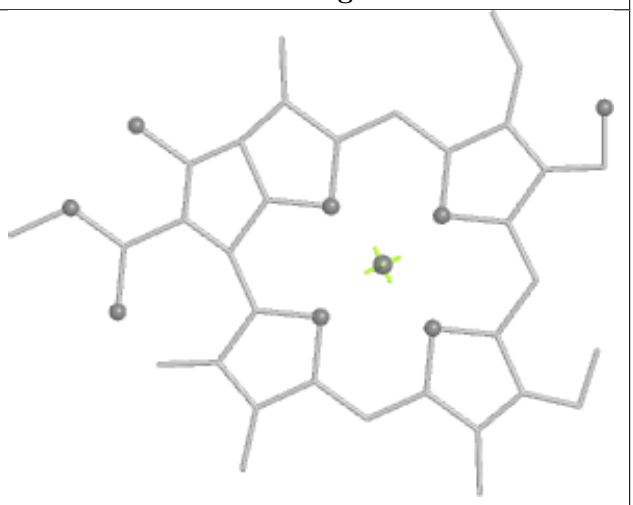
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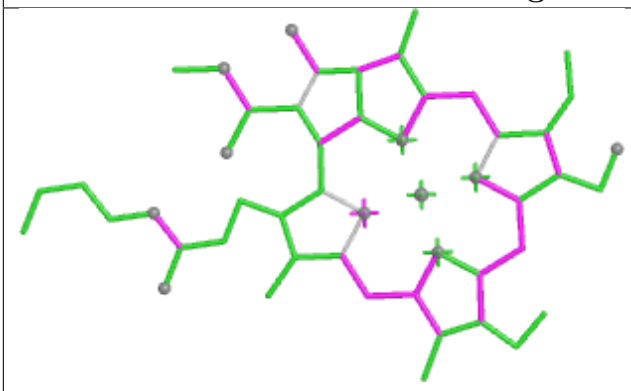


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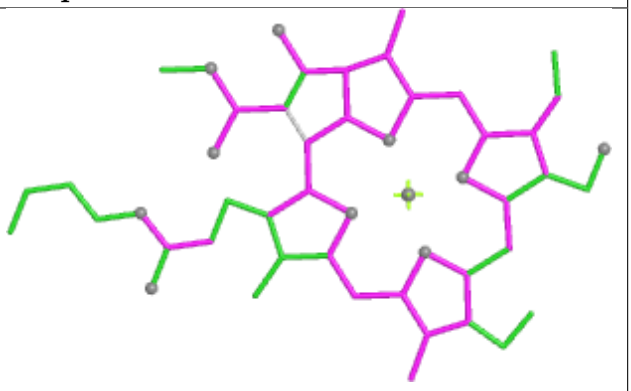


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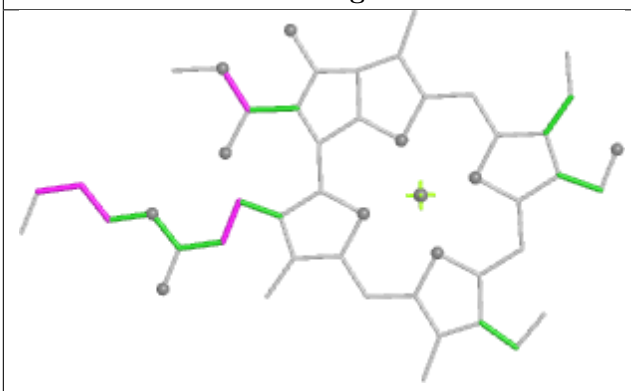
Ligand CHL q 310



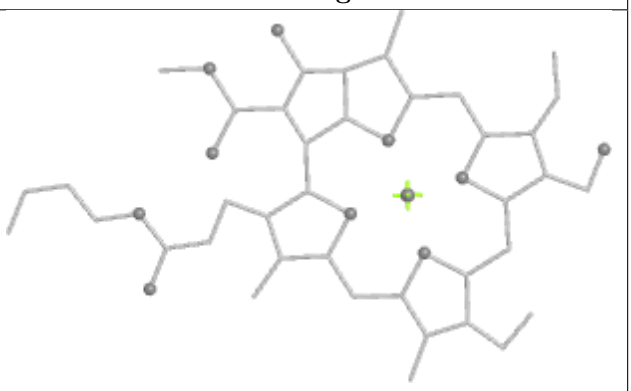
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Bond angles

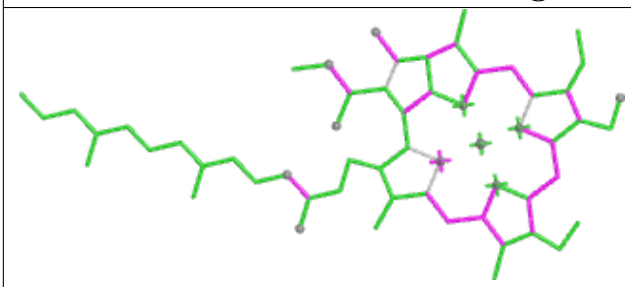


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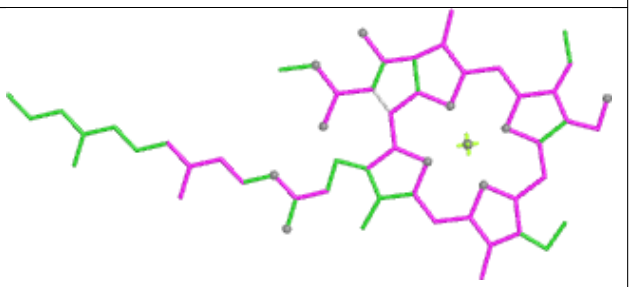


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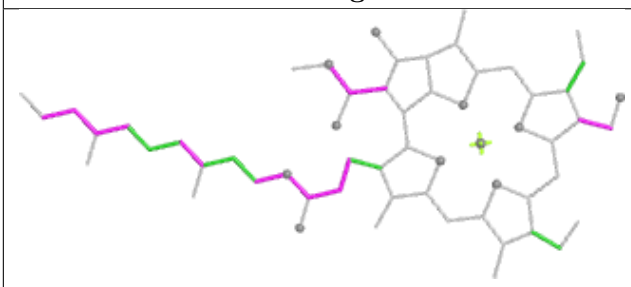
Ligand CHL s 403



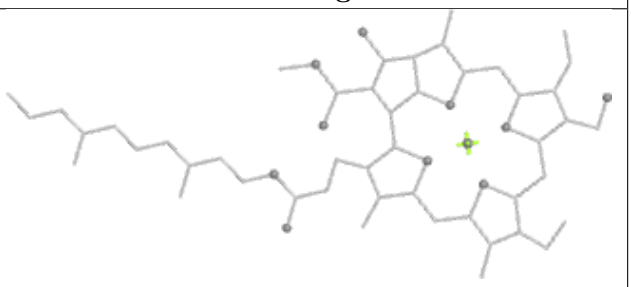
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Bond angles

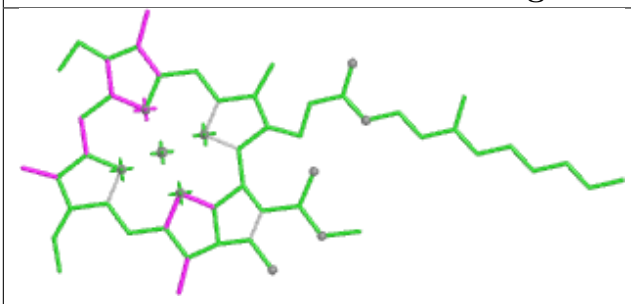


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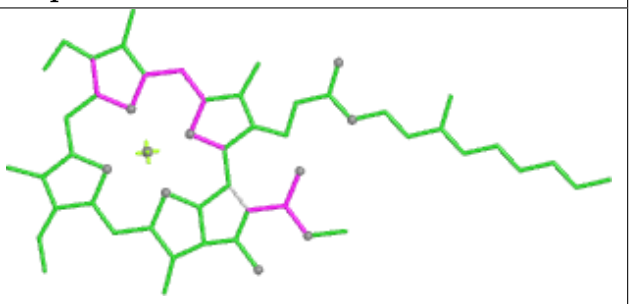


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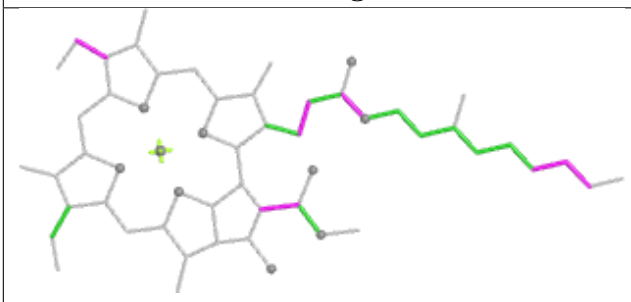
Ligand CLA p 317



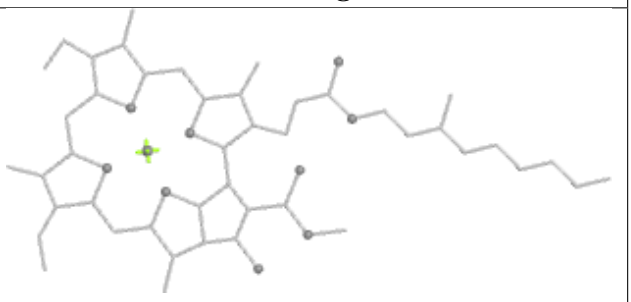
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Bond angles

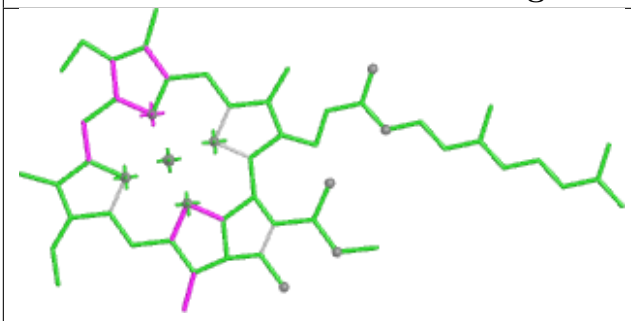


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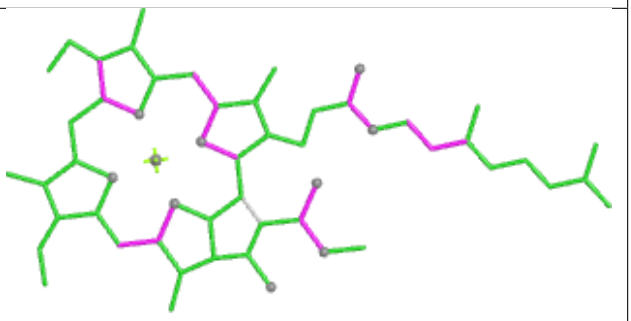


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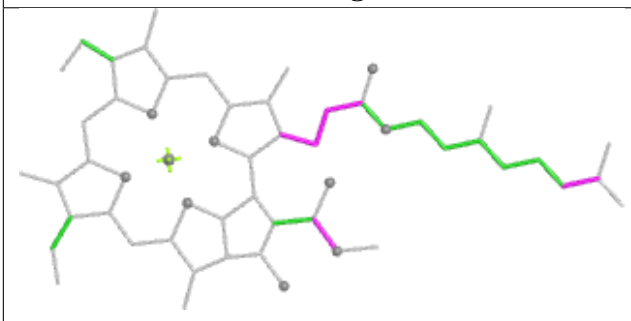
Ligand CLA n 313



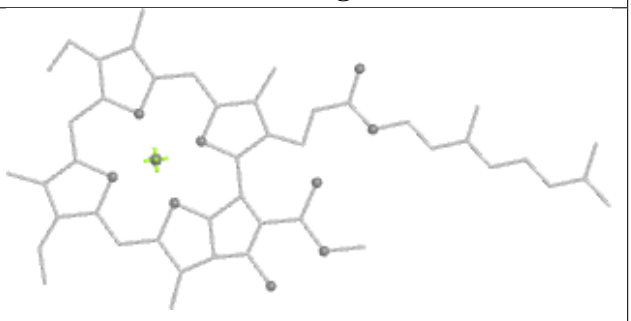
Bond lengths



Bond angles

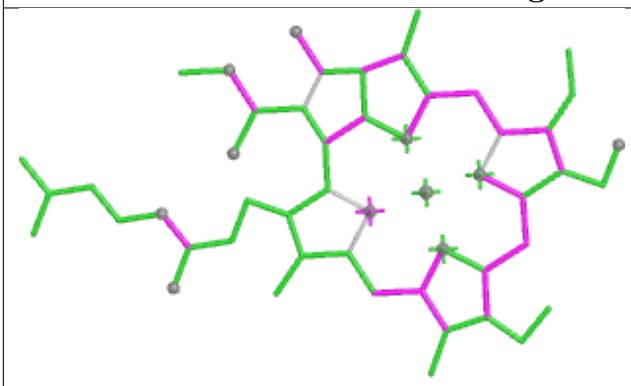


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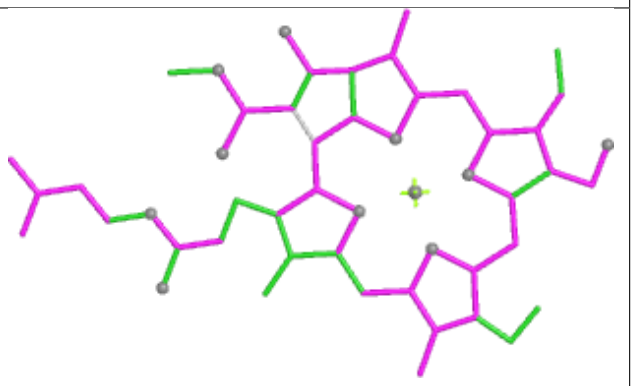


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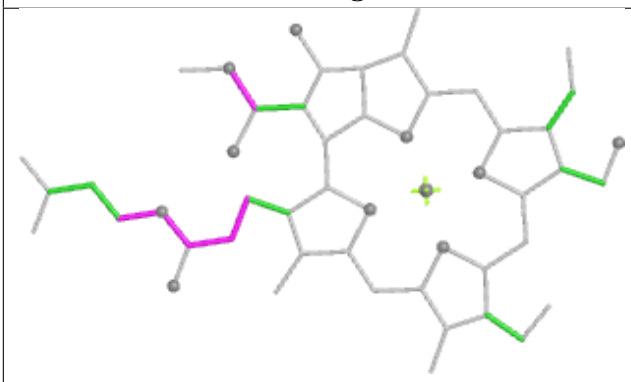
Ligand CHL 3 309



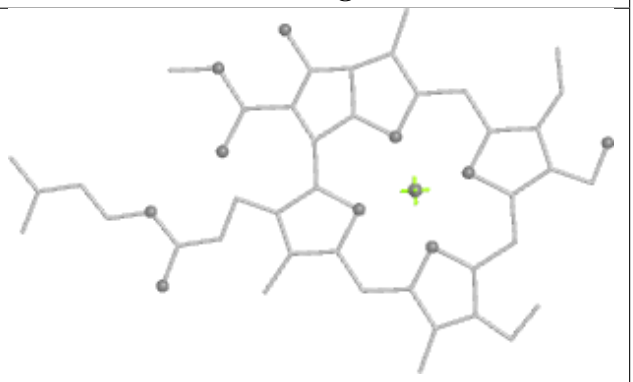
Bond lengths



Bond angles

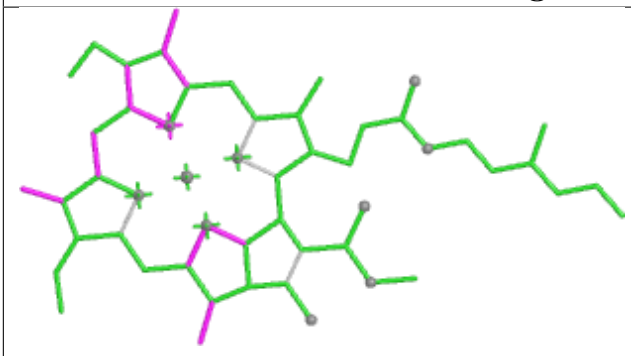


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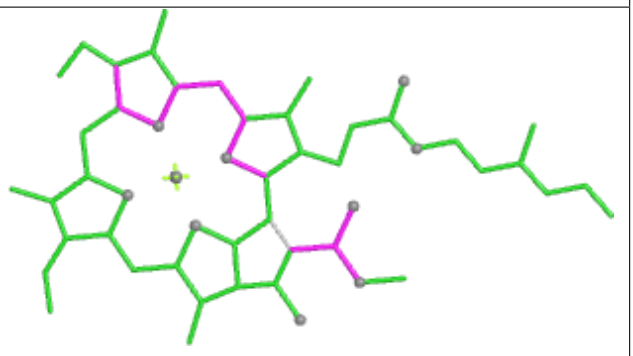


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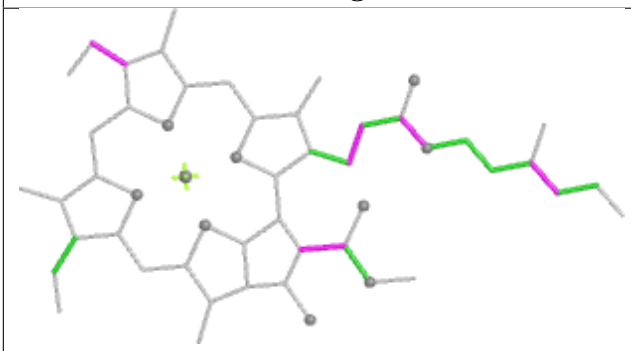
Ligand CLA 7 317



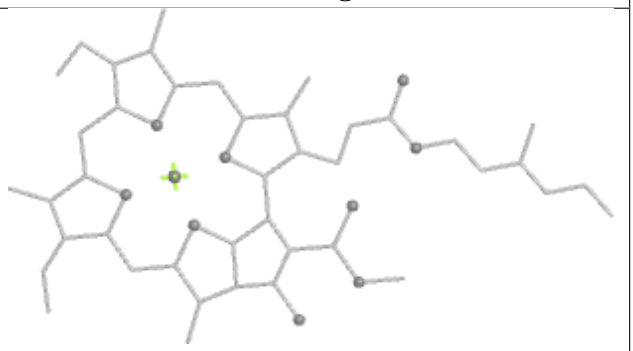
Bond lengths



Bond angles

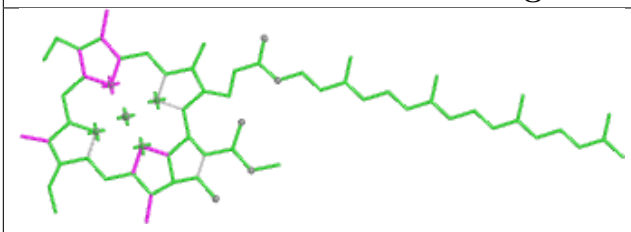


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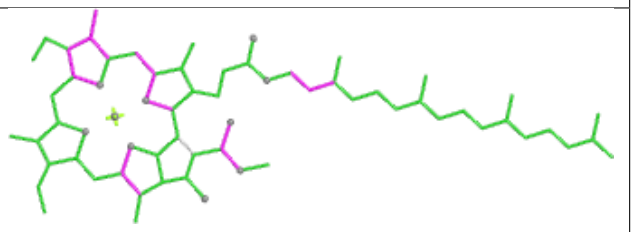


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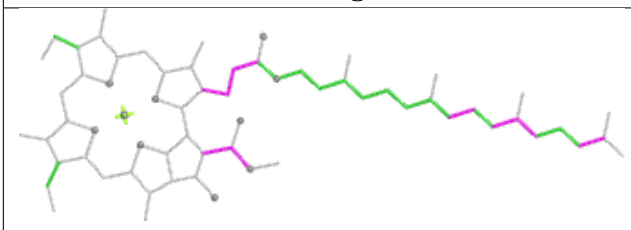
Ligand CLA C 601



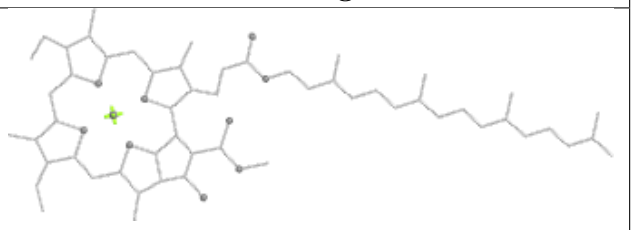
Bond lengths



Bond angles

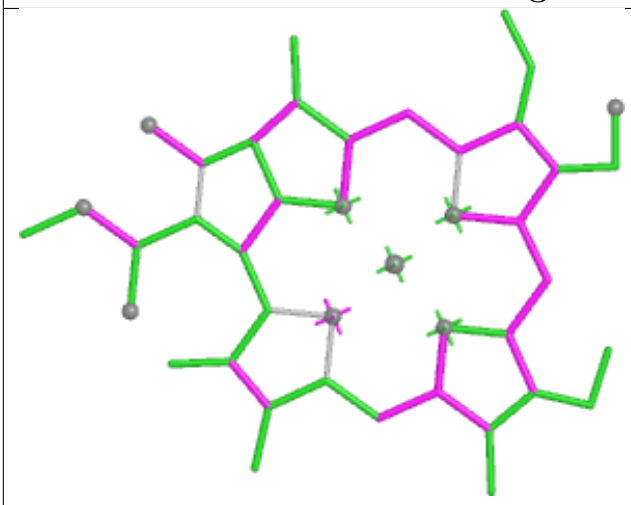


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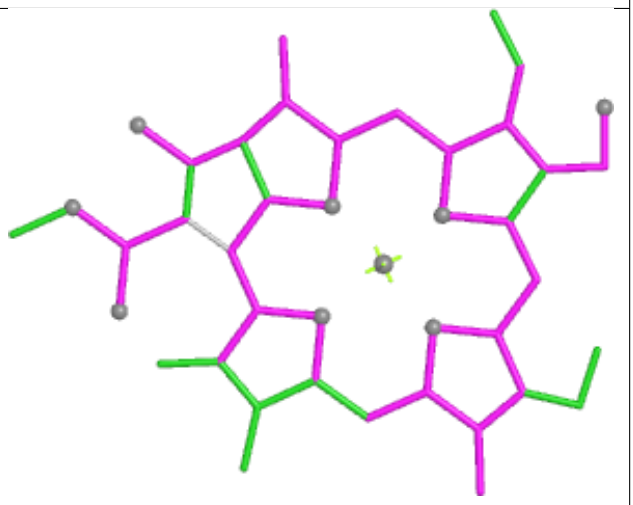


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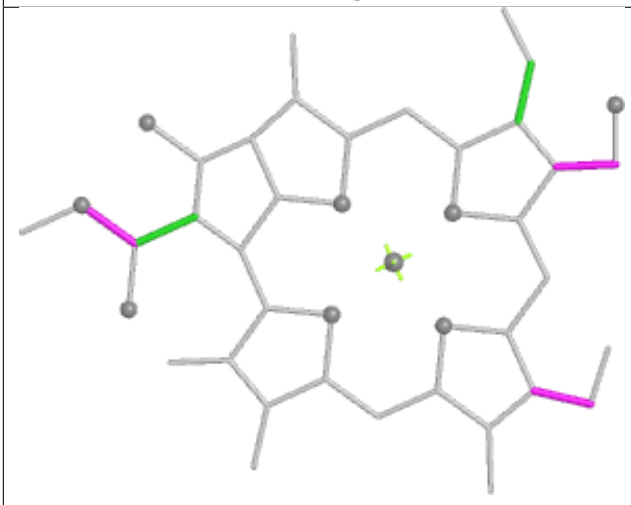
Ligand CHL r 306



Bond lengths



Bond angles

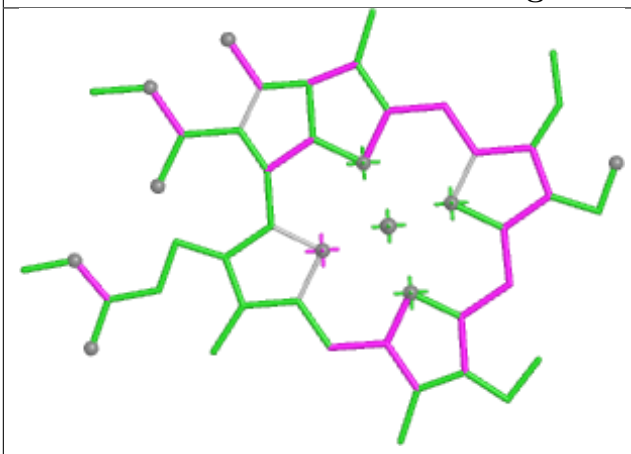


Torsions

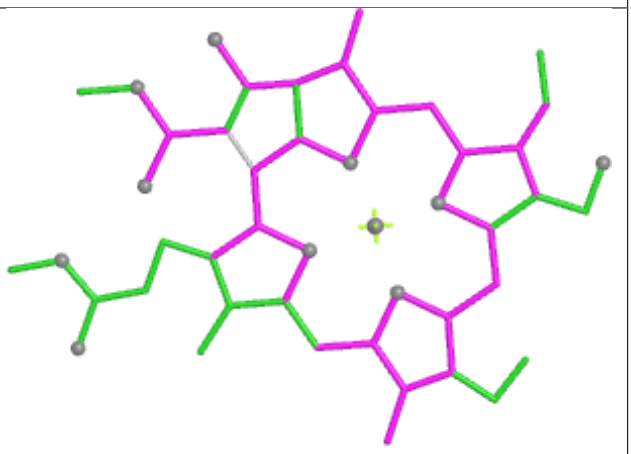


Rings

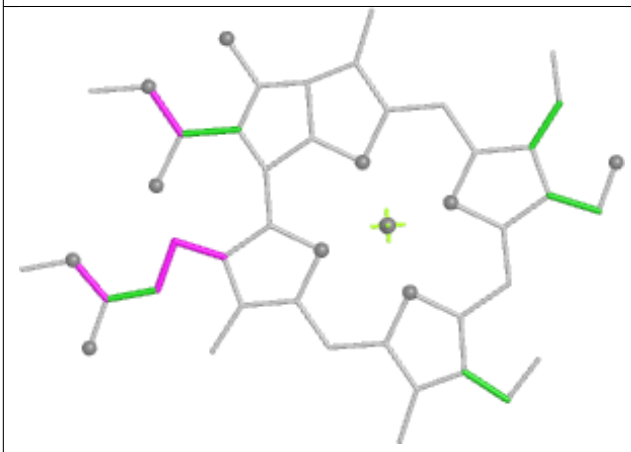
Ligand CHL u 312



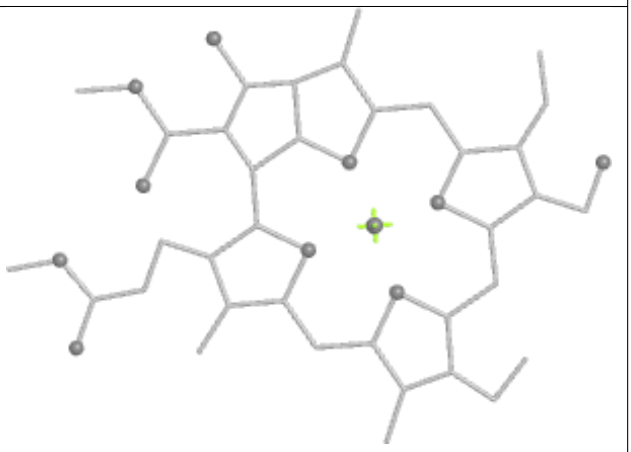
Bond lengths



Bond angles

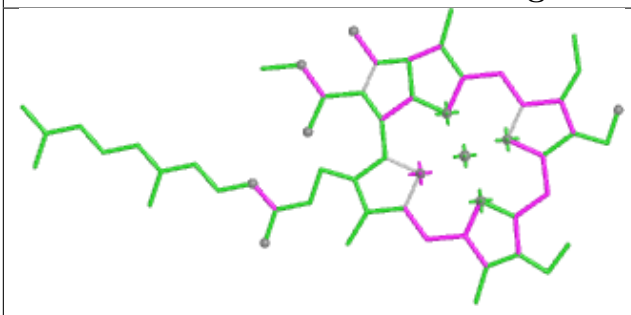


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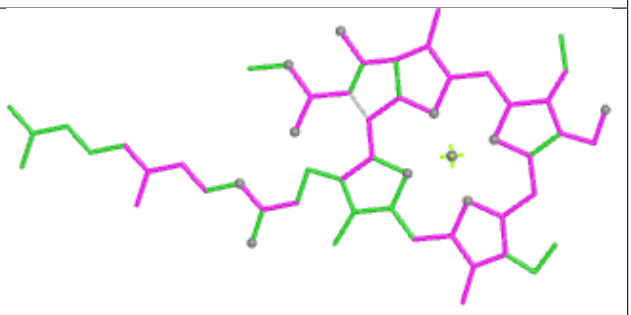


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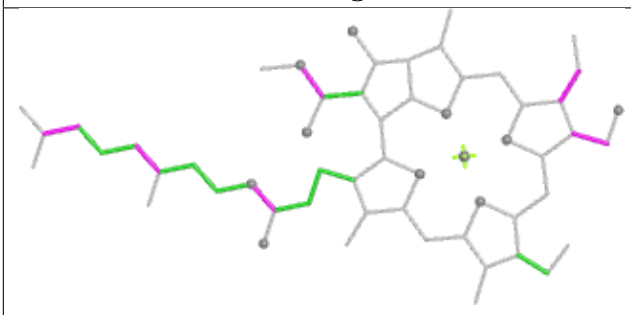
Ligand CHL 8 310



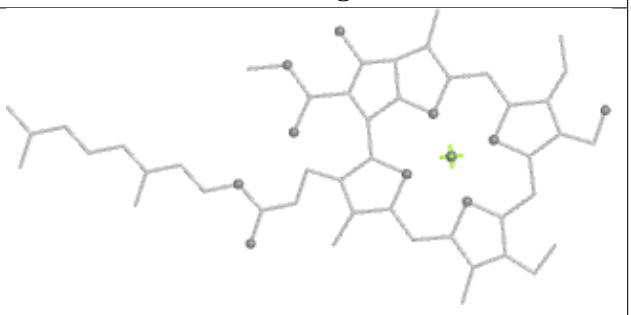
Bond lengths



Bond angles

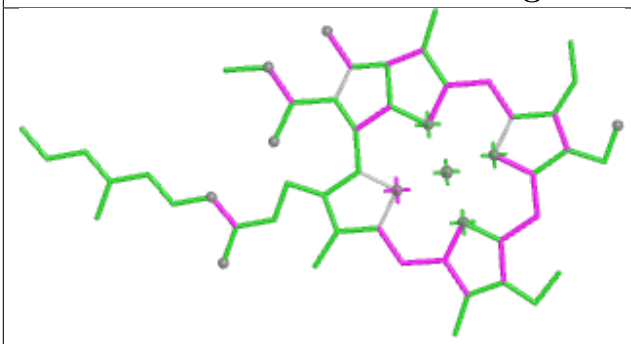


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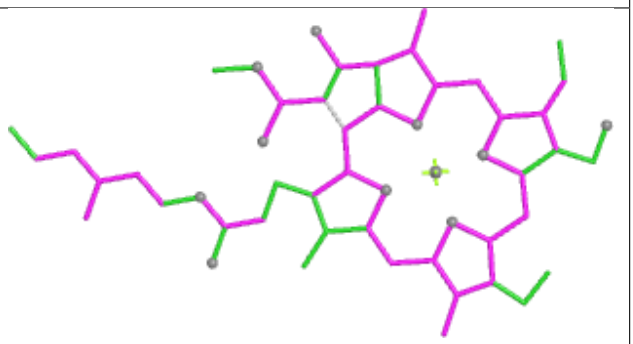


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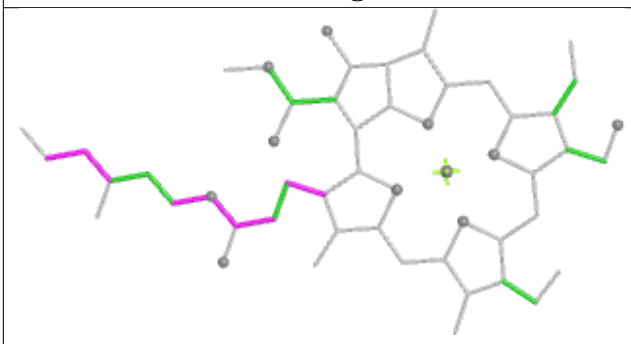
Ligand CHL Y 319



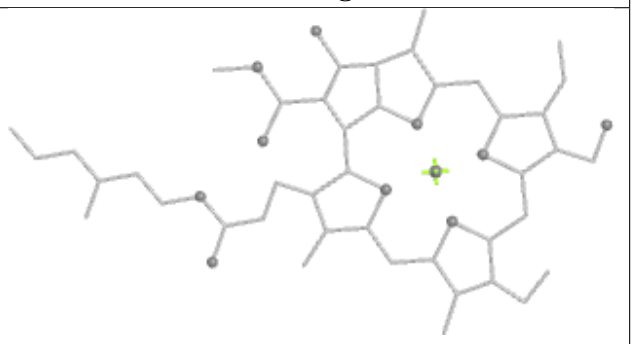
Bond lengths



Bond angles

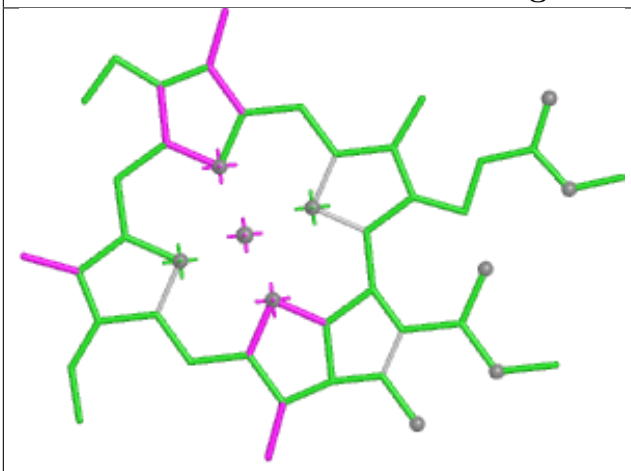


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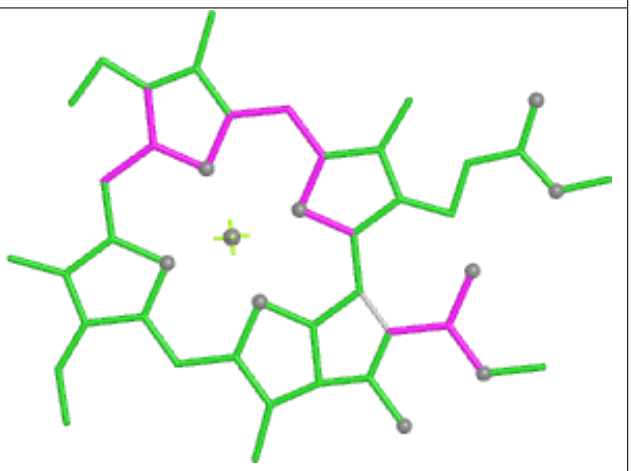


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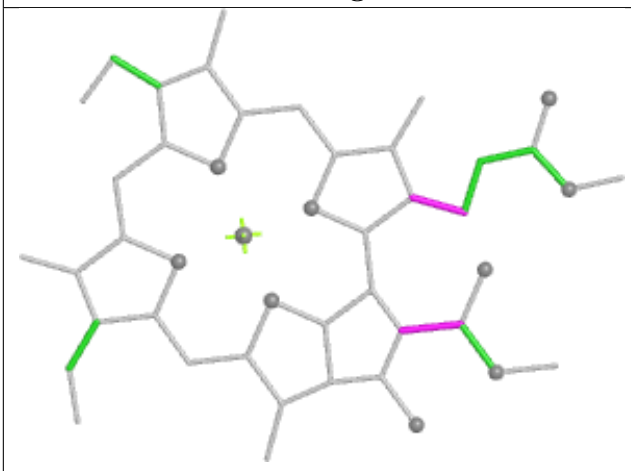
Ligand CLA c 616



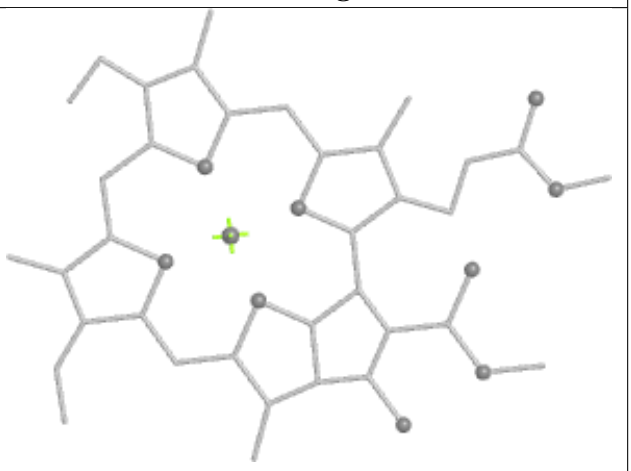
Bond lengths



Bond angles

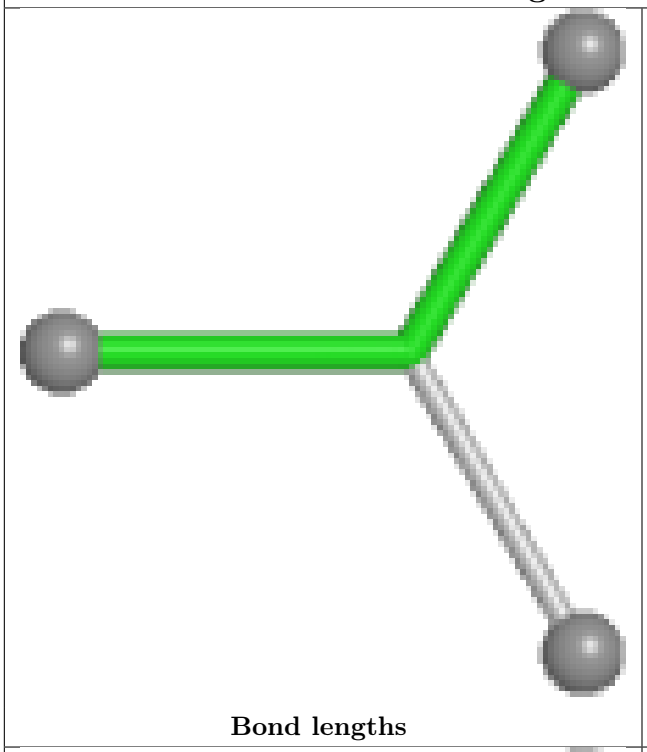


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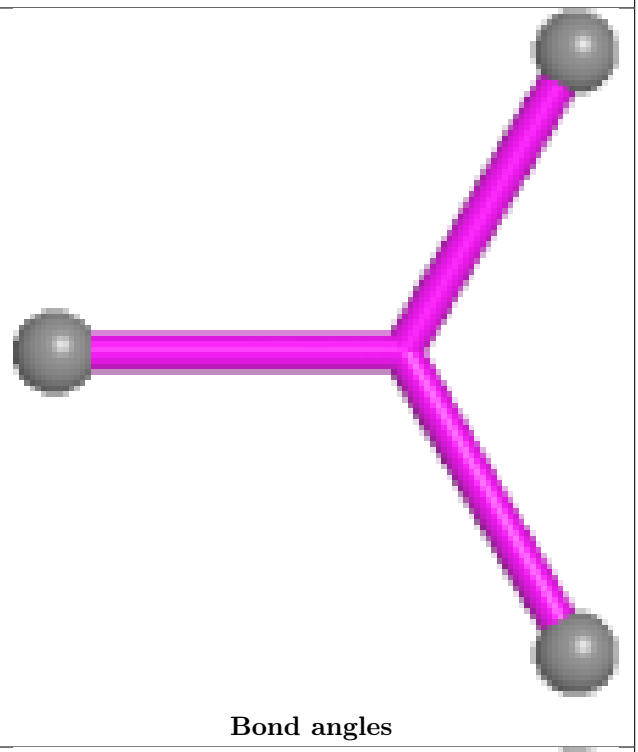


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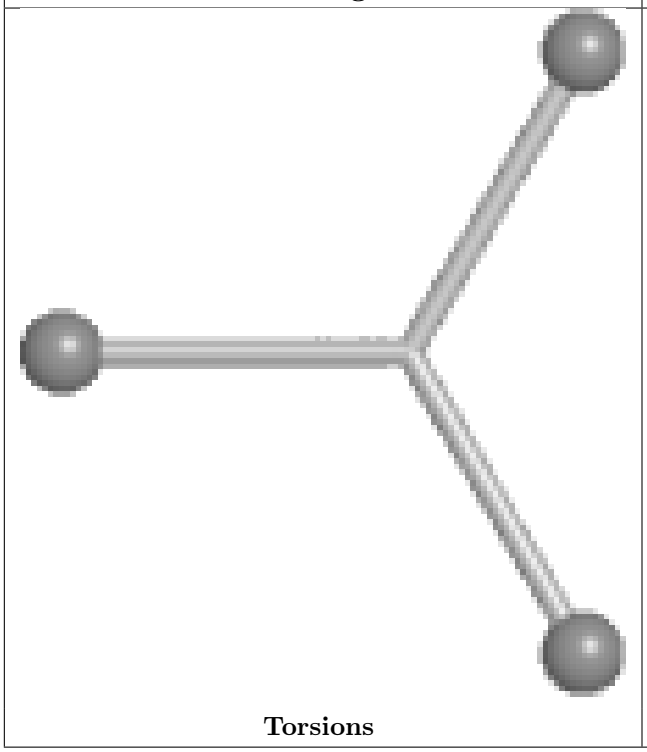
Ligand BCT a 611



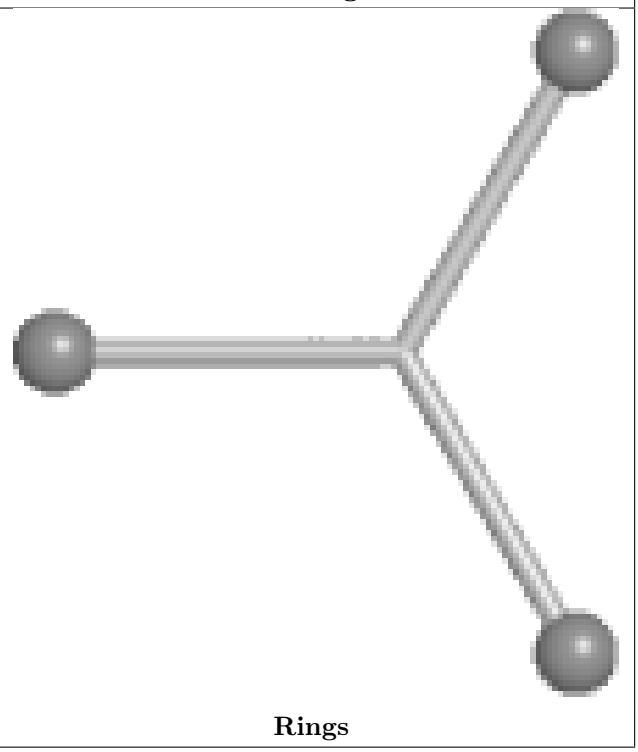
Bond lengths



Bond angles

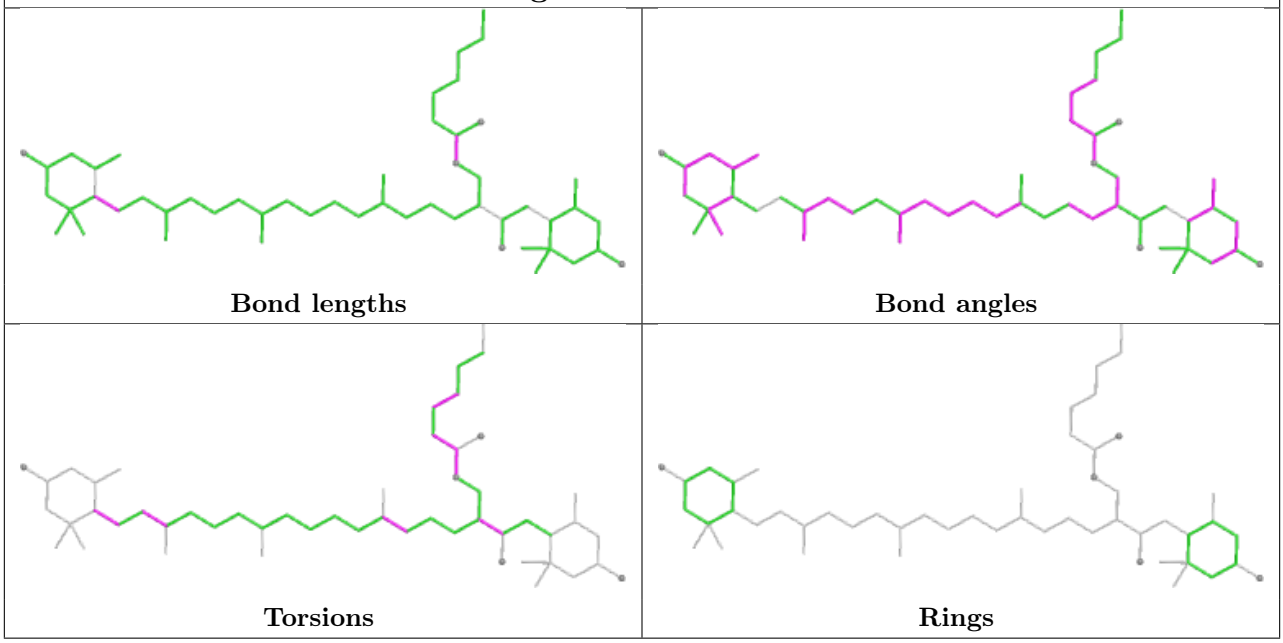


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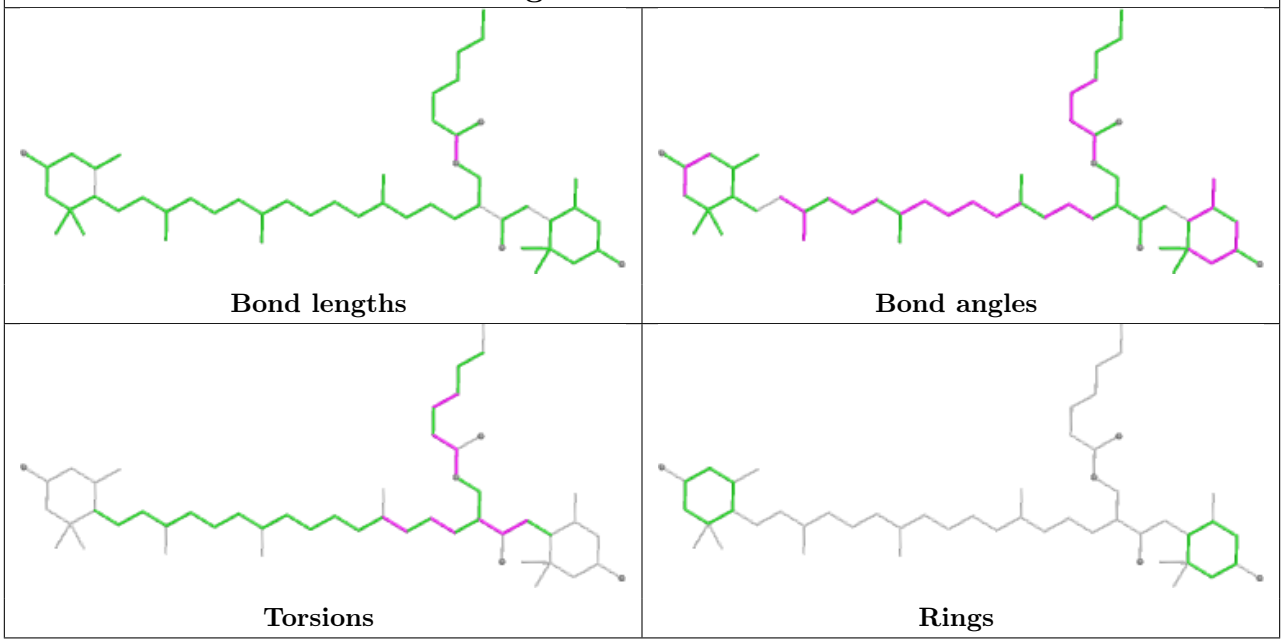


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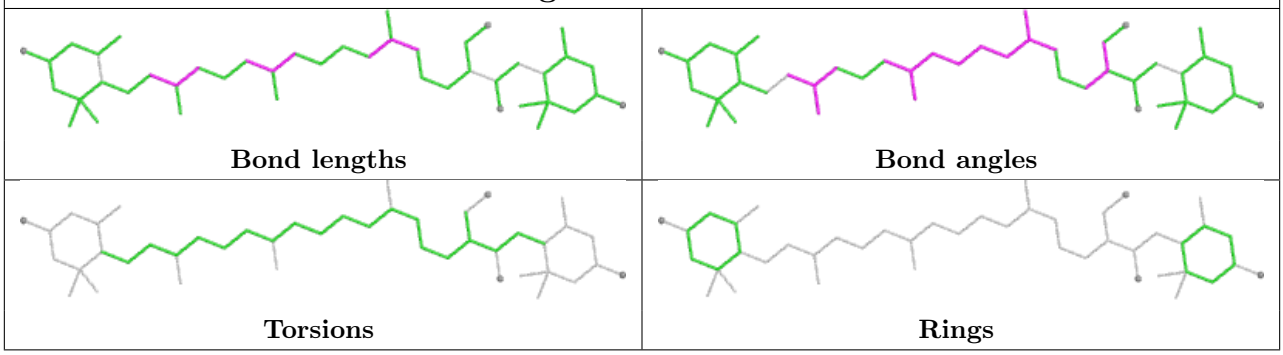
Ligand 0UR 5 301



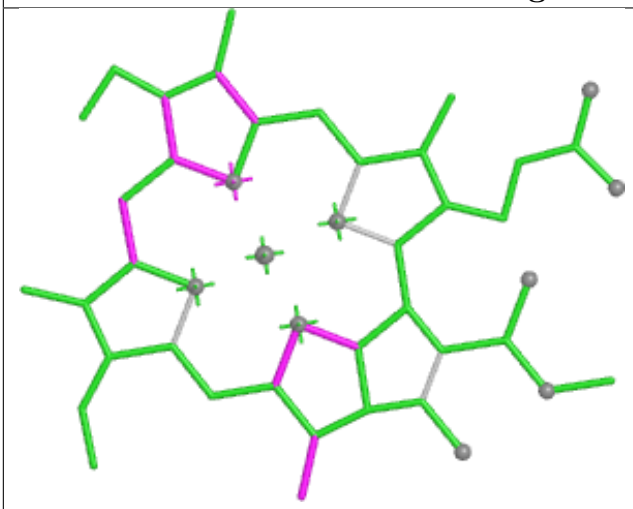
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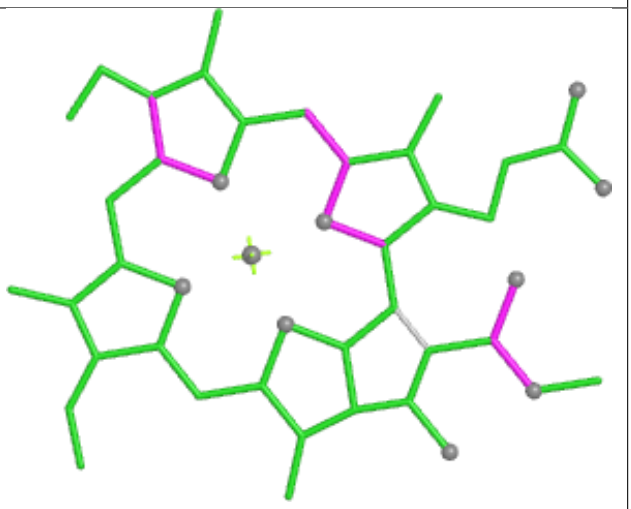
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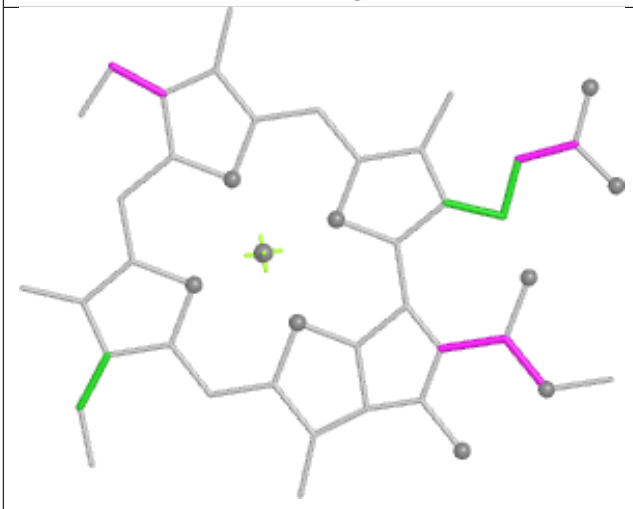
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Bond lengths



Bond angles

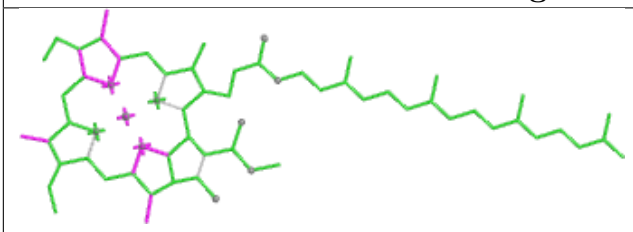


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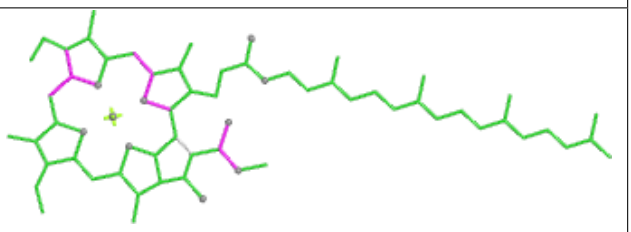


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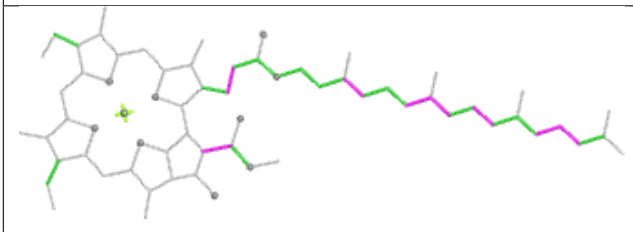
Ligand CLA c 607



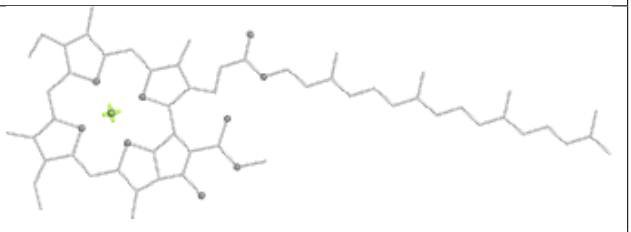
Bond lengths



Bond angles

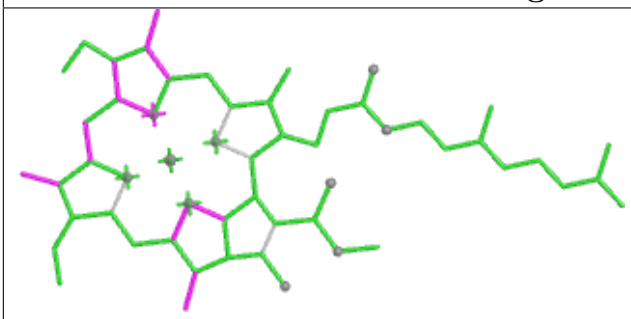


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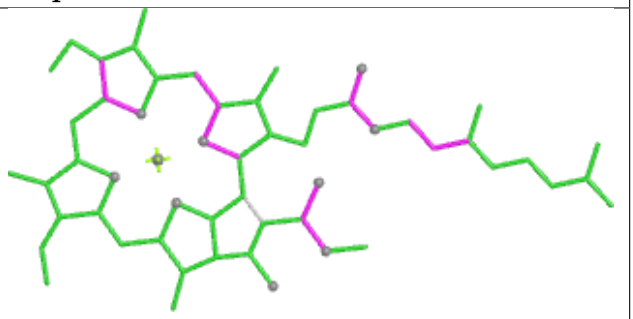


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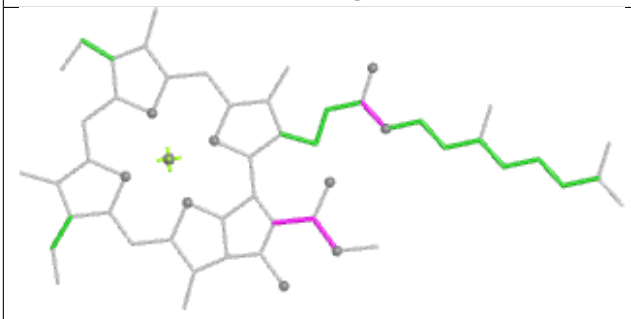
Ligand CLA p 314



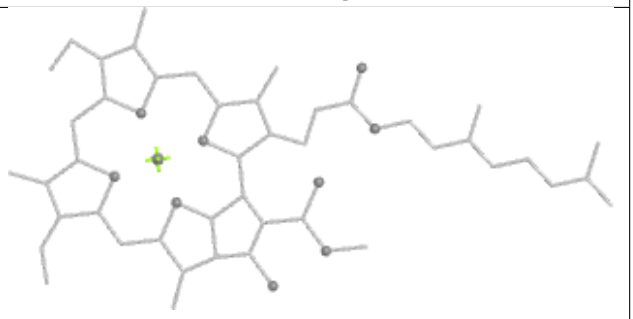
Bond lengths



Bond angles

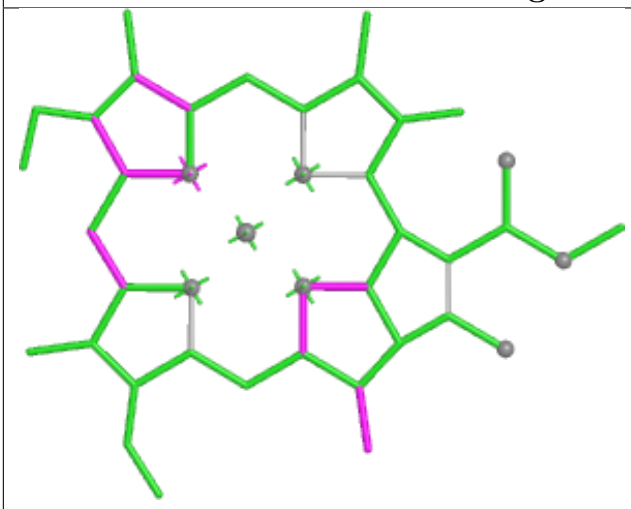


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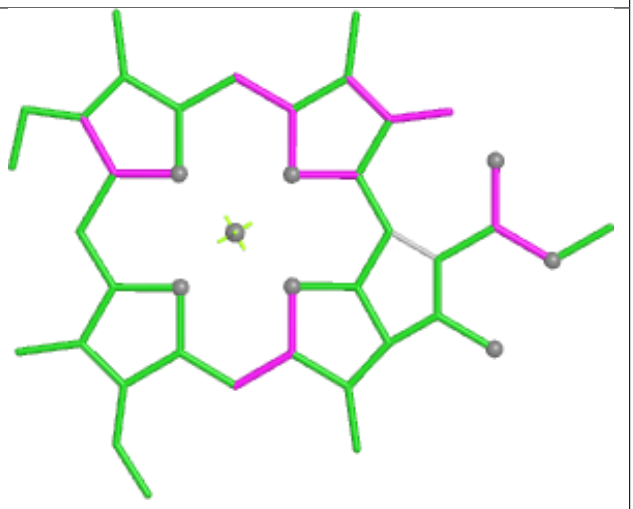


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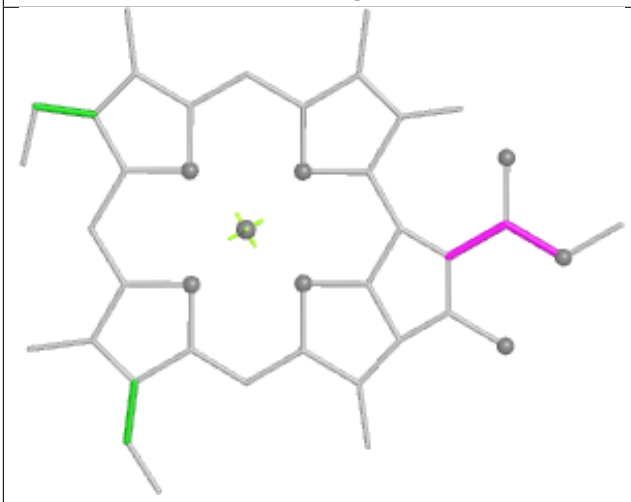
Ligand CLA a 610



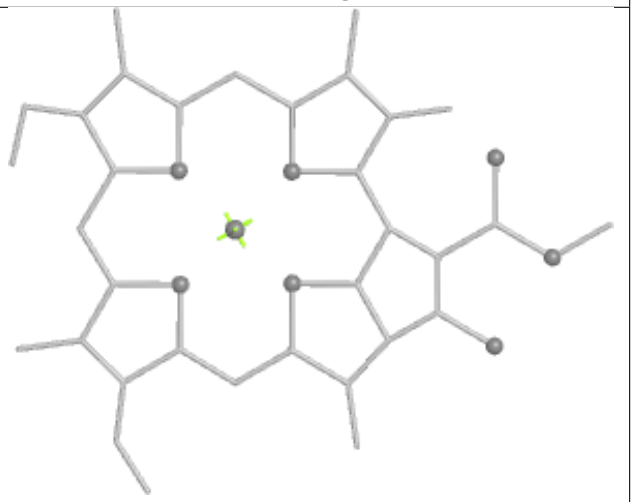
Bond lengths



Bond angles

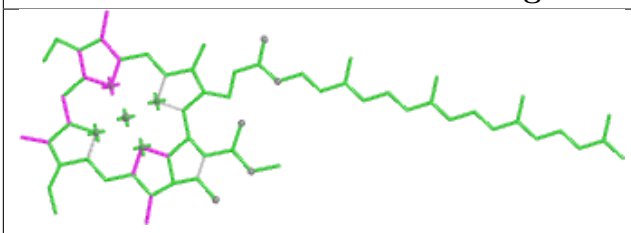


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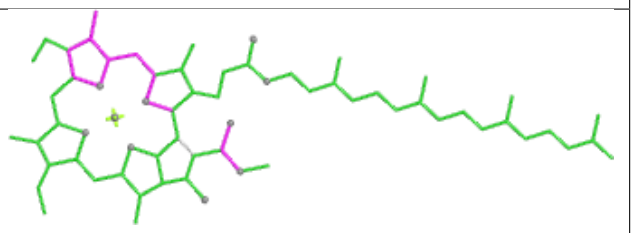


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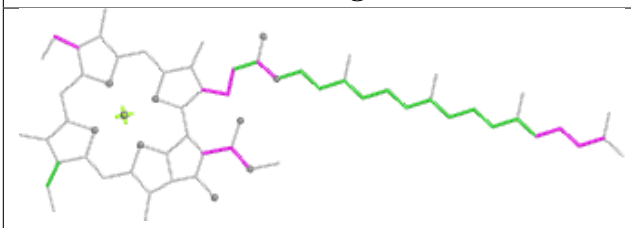
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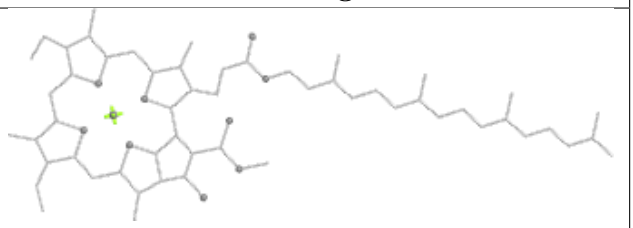
Bond lengths



Bond angles

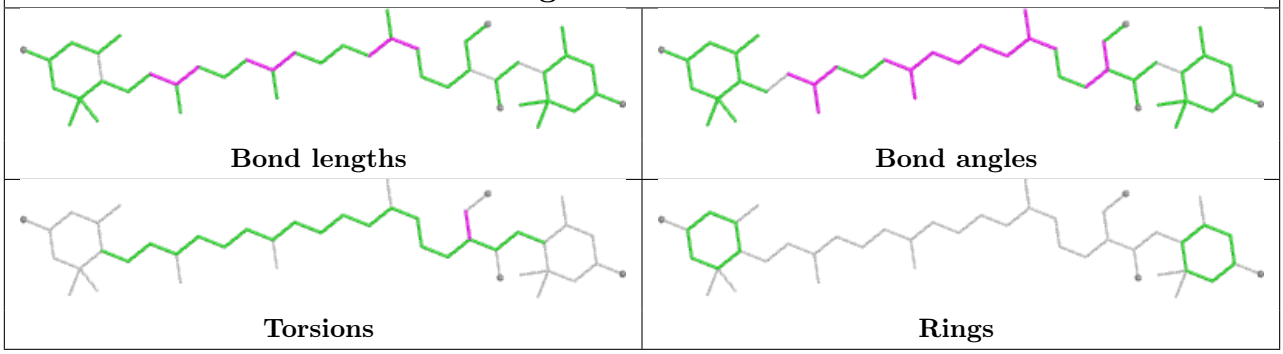


Torsions



Rings

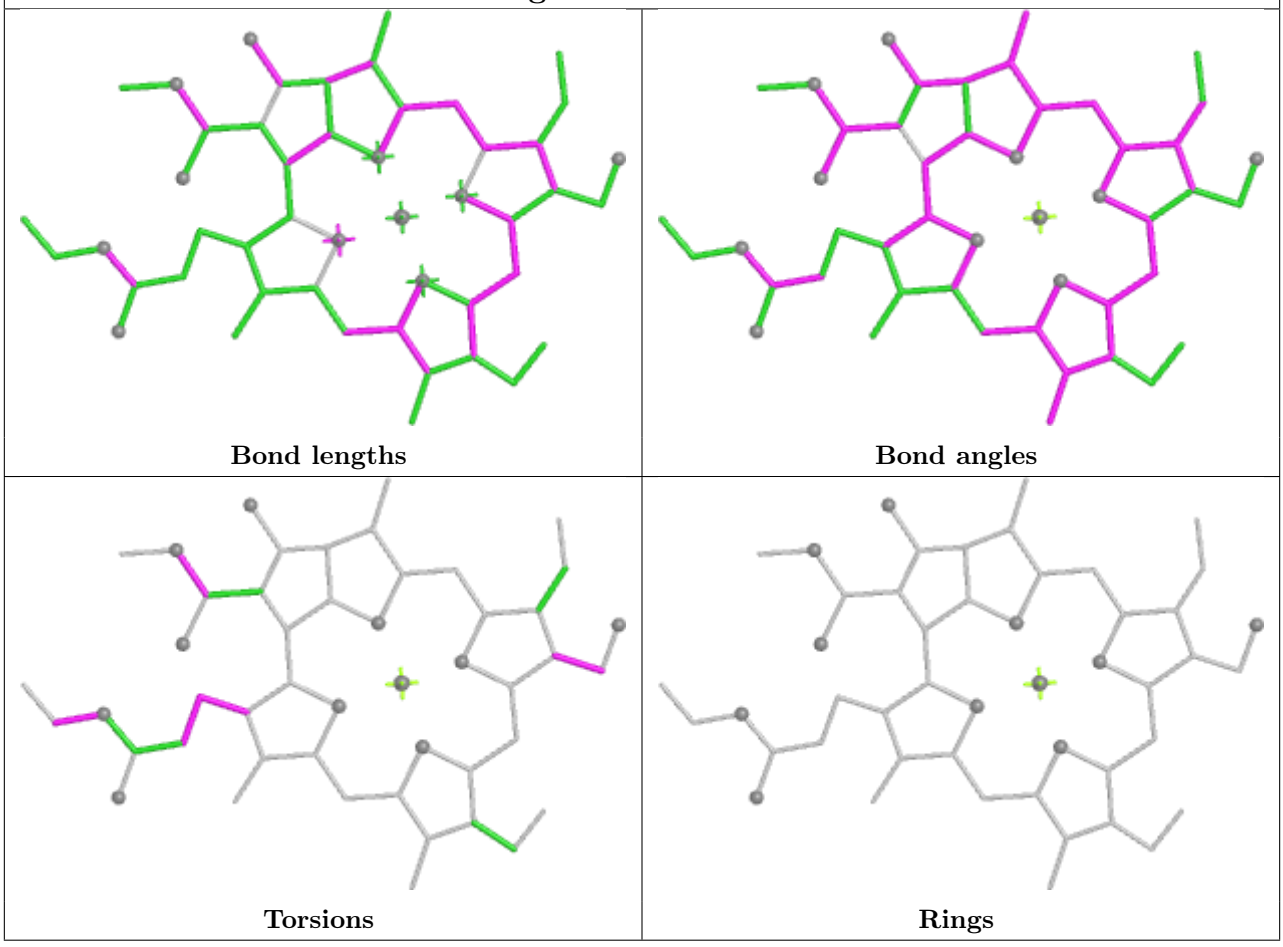
Ligand 0IE 7 303



Bond lengths | Bond angles

Torsions | Rings

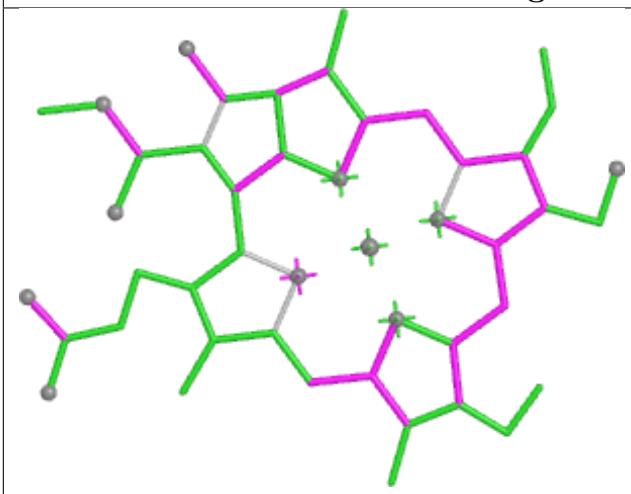
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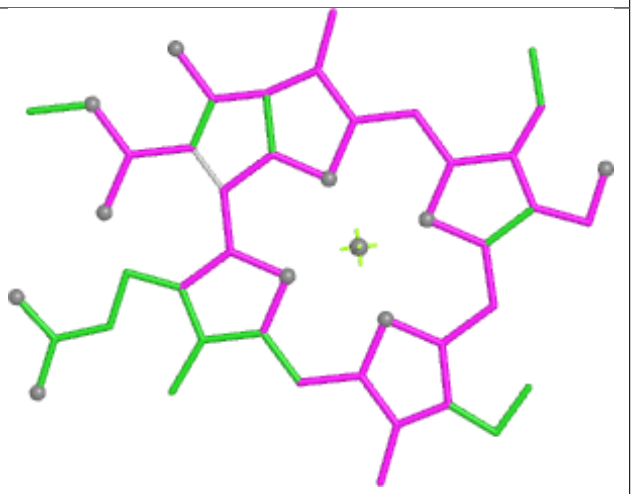
Bond lengths | Bond angles

Torsions | Rings

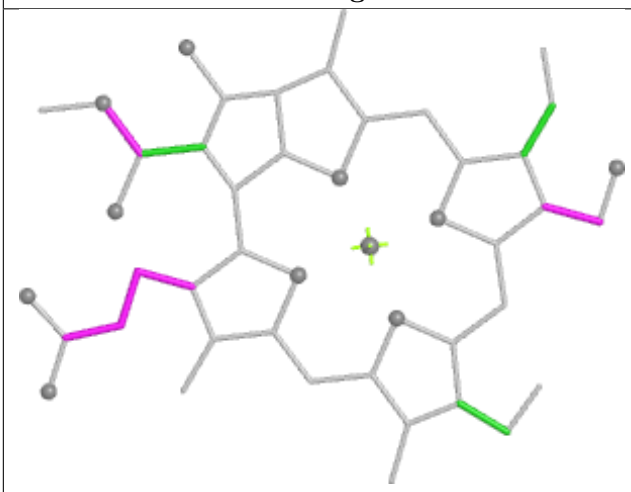
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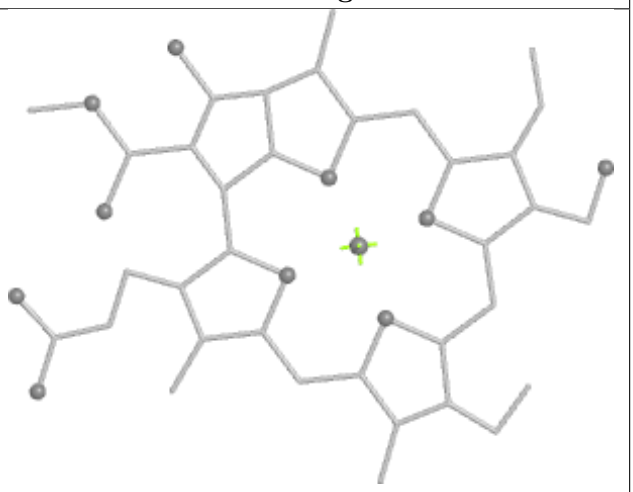
Bond lengths



Bond angles

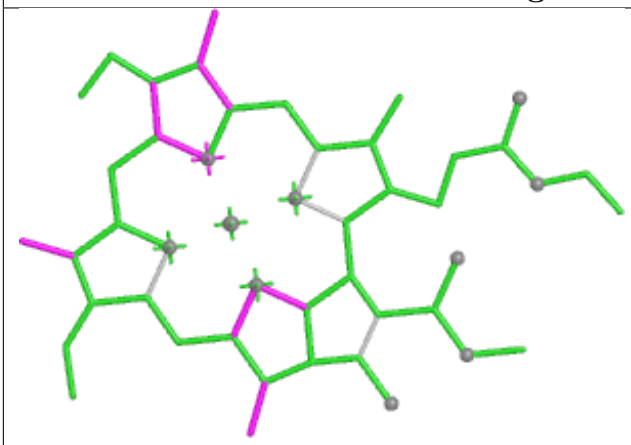


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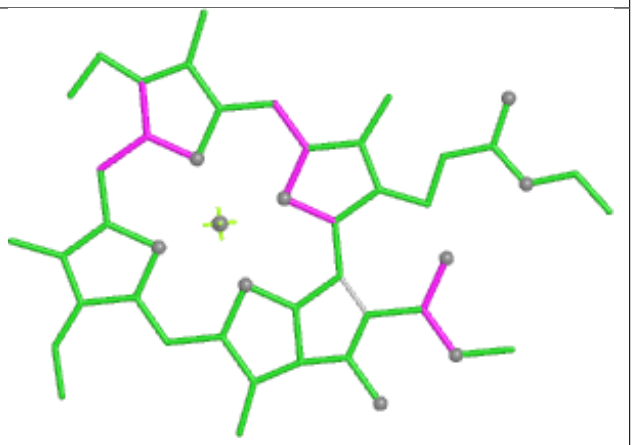


Rings

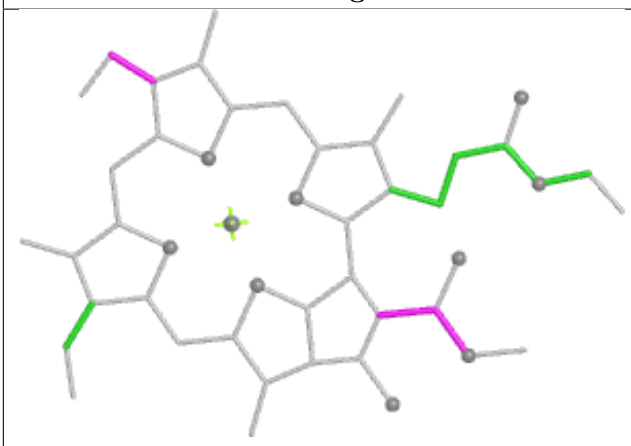
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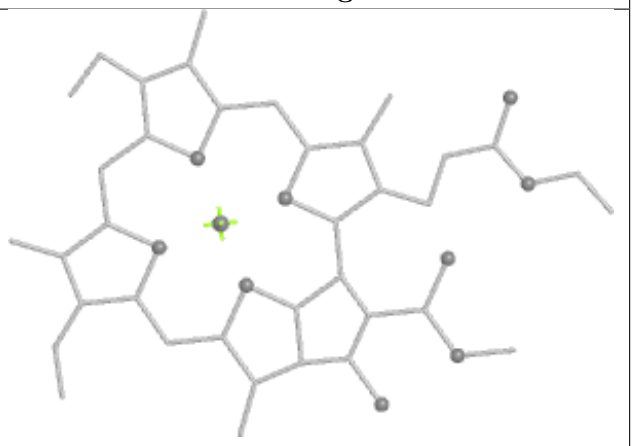
Bond lengths



Bond angles

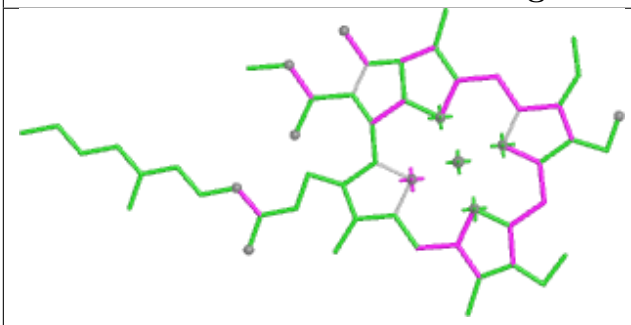


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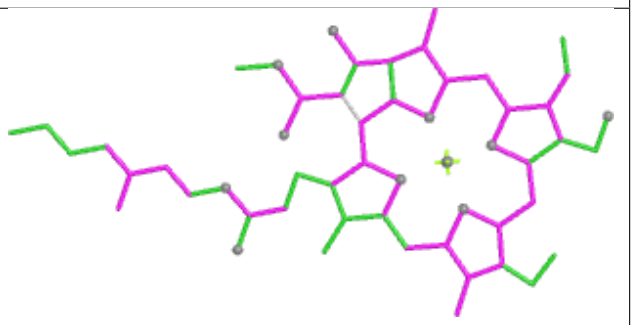


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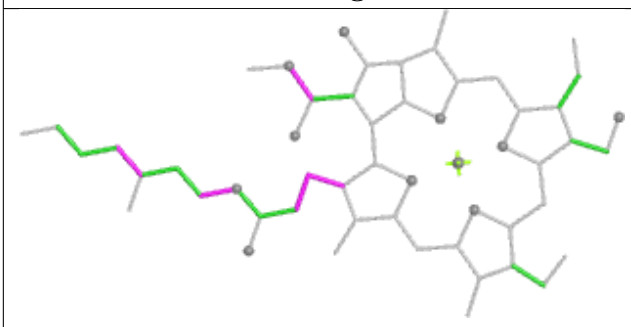
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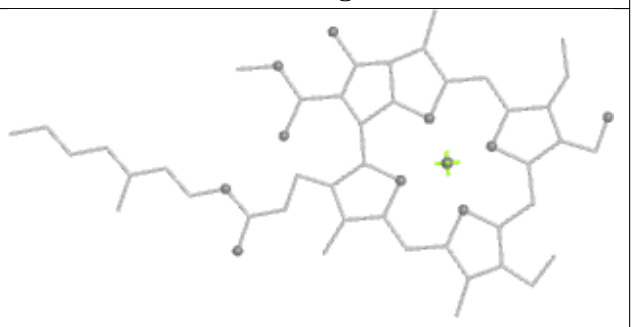
Bond lengths



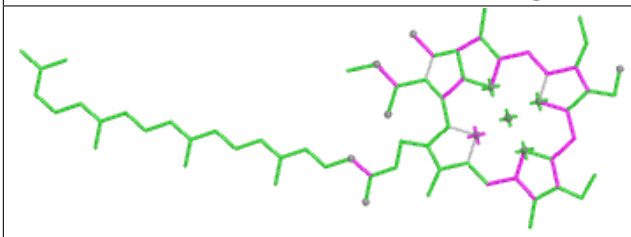
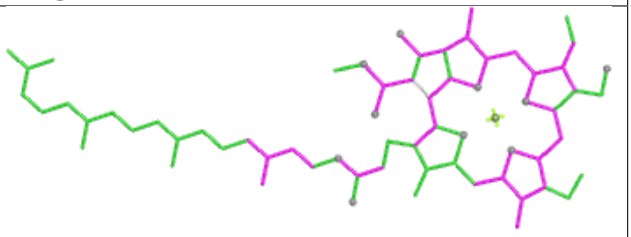
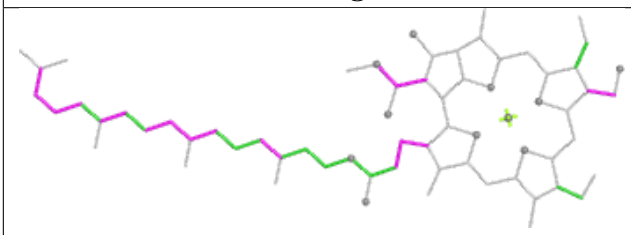
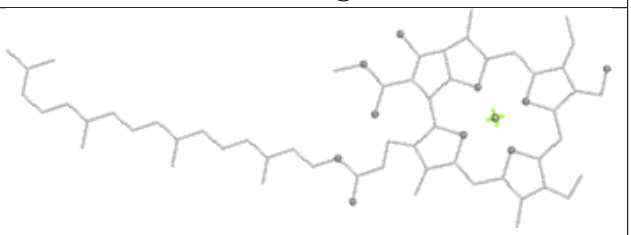
Bond angles

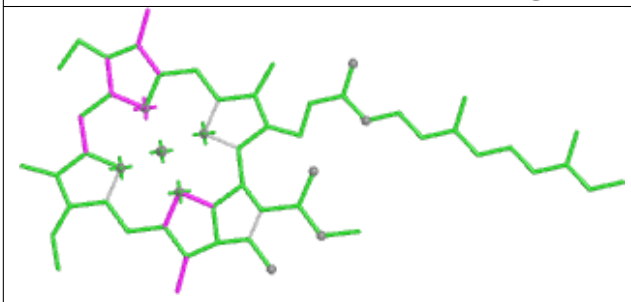
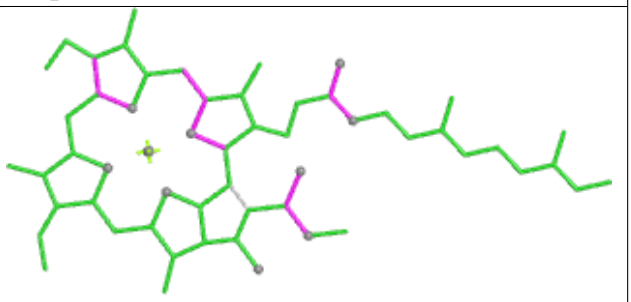
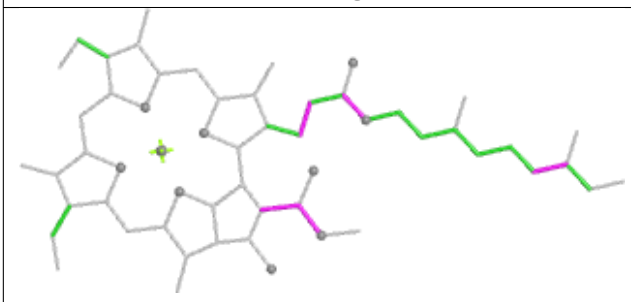
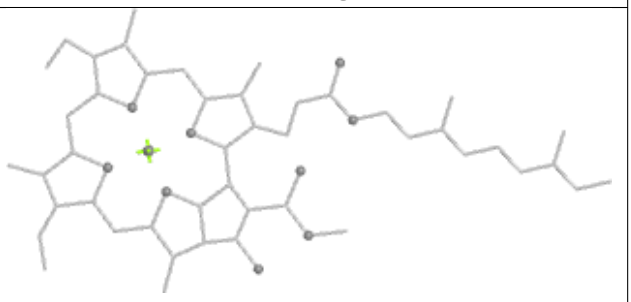


Torsions

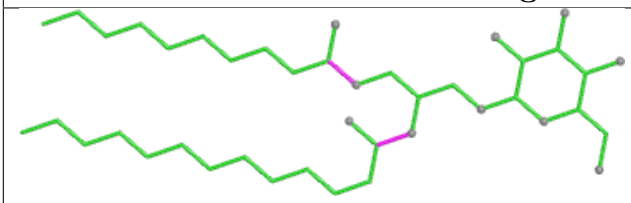


Rings

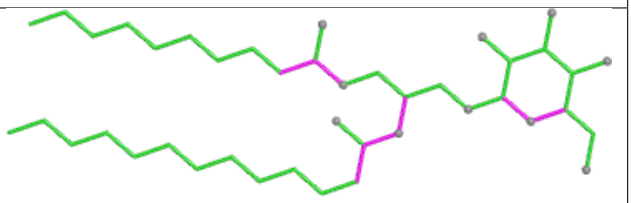
Ligand CHL g 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA p 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

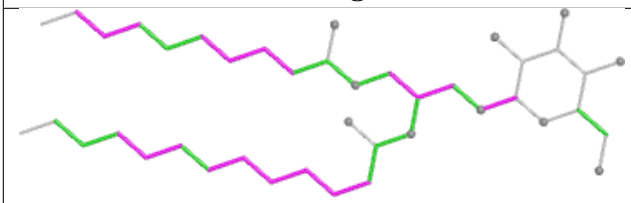
Ligand LMG C 618



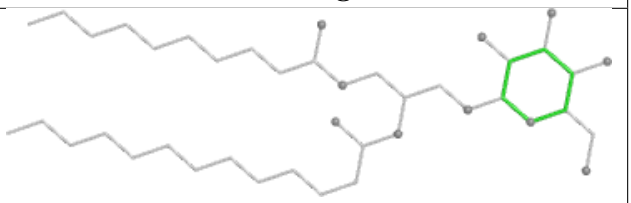
Bond lengths



Bond angles

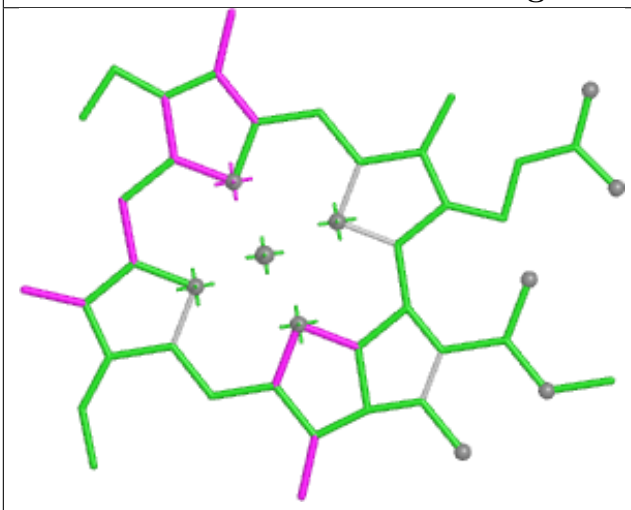


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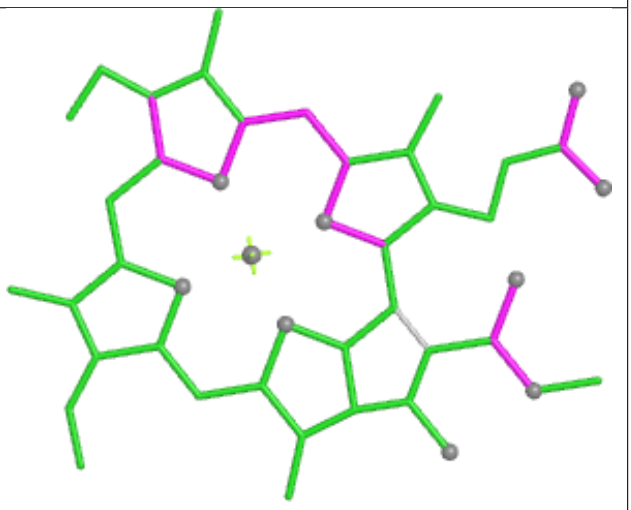


Rings

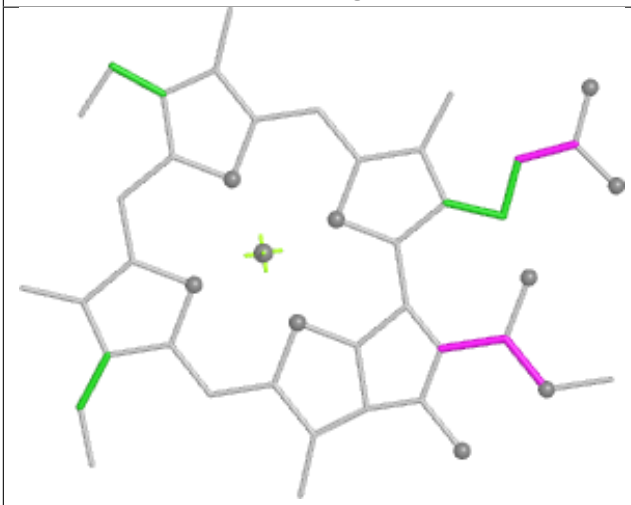
Ligand CLA S 611



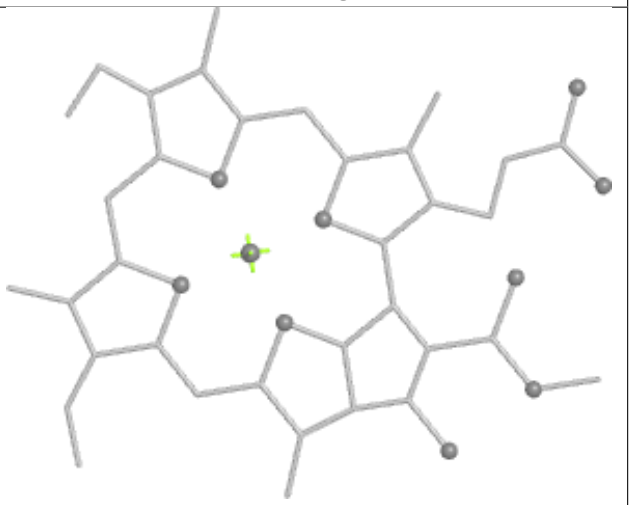
Bond lengths



Bond angles

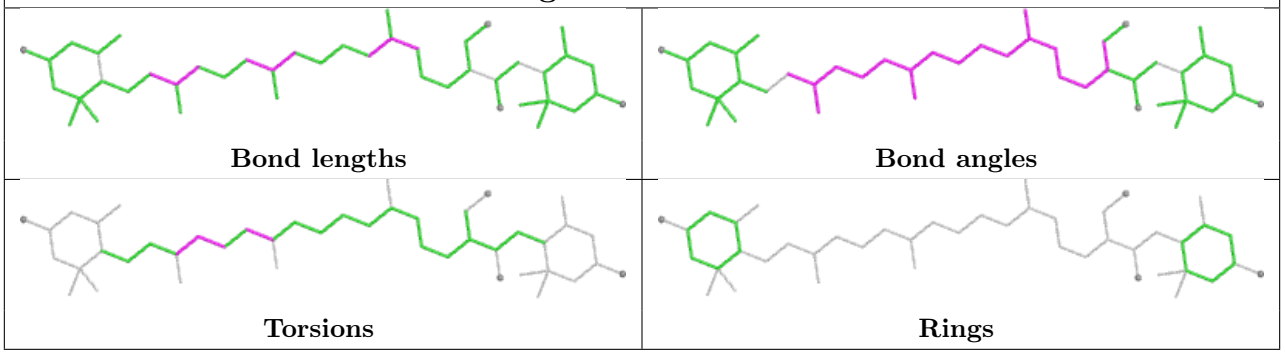


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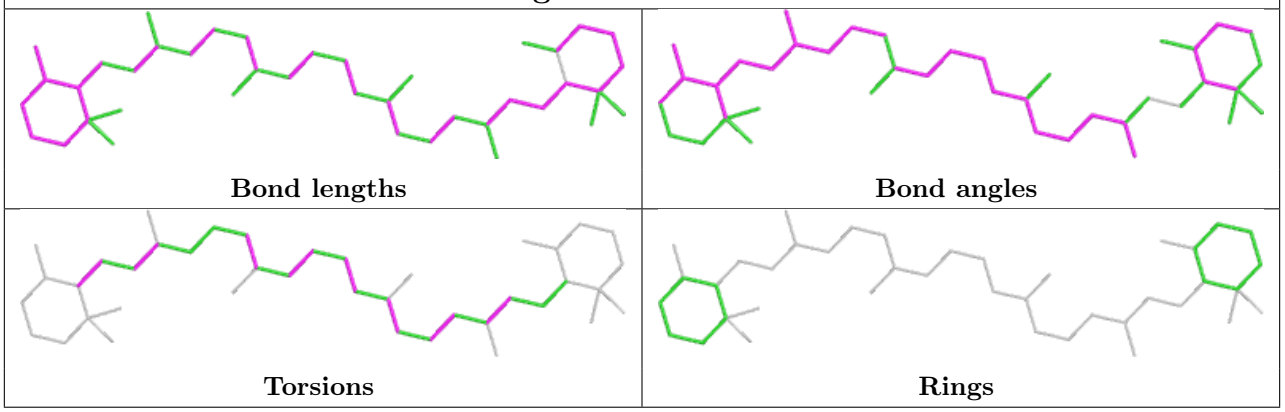


Rings

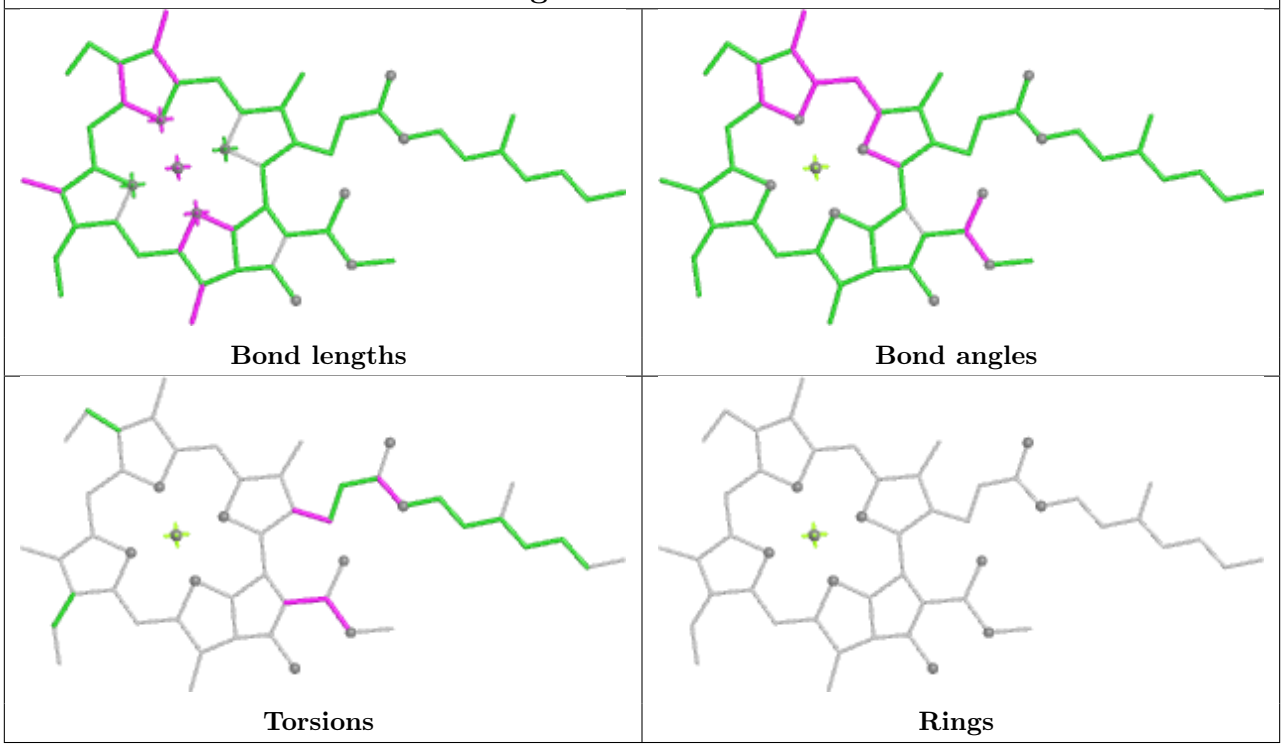
Ligand 0IE 9 303



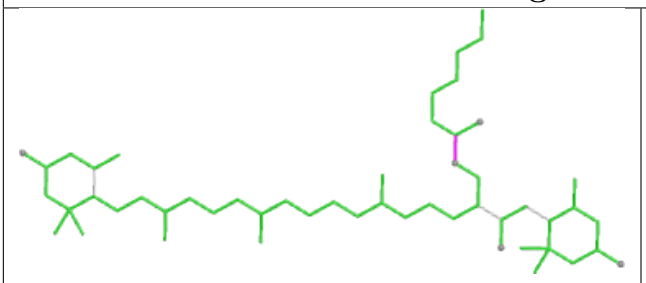
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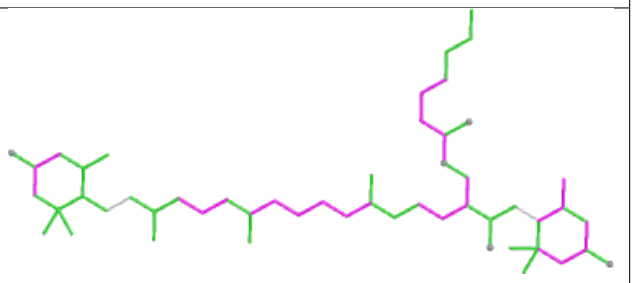
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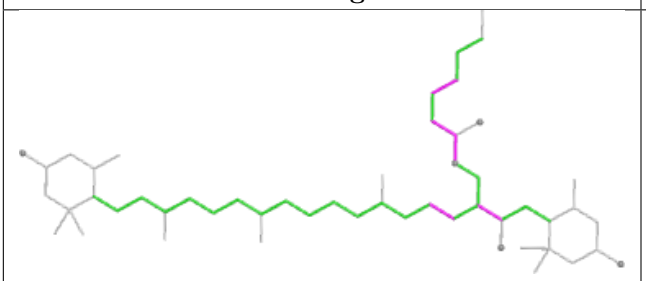
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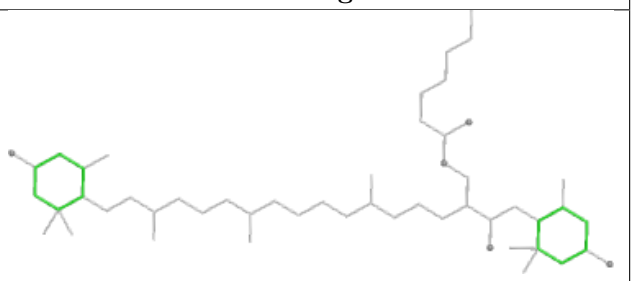
Bond lengths



Bond angles

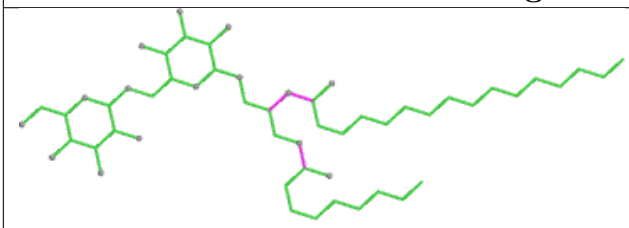


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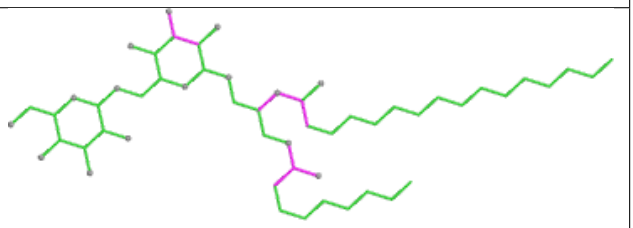


Rings

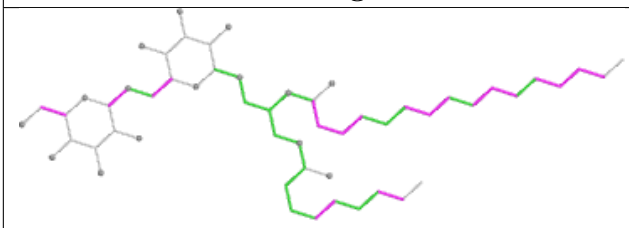
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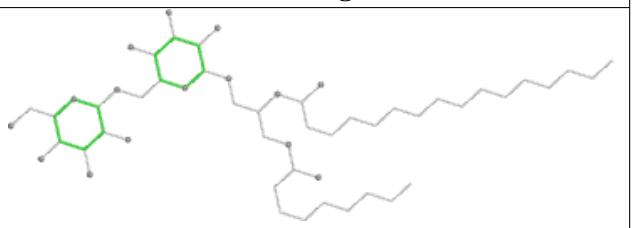
Bond lengths



Bond angles

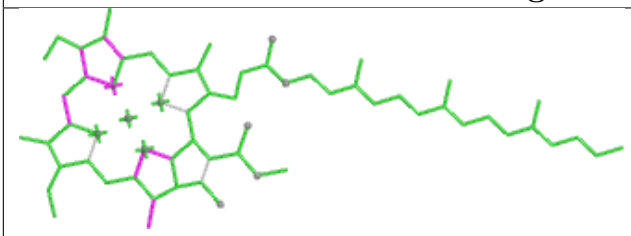


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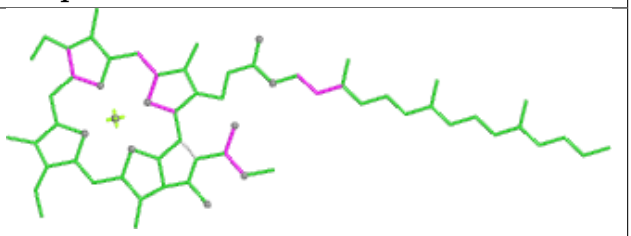


Rings

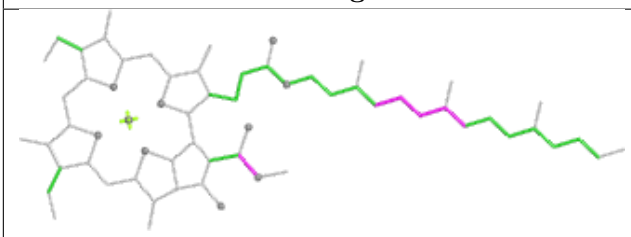
Ligand CLA q 313



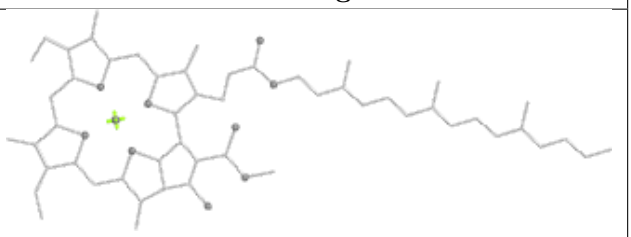
Bond lengths



Bond angles

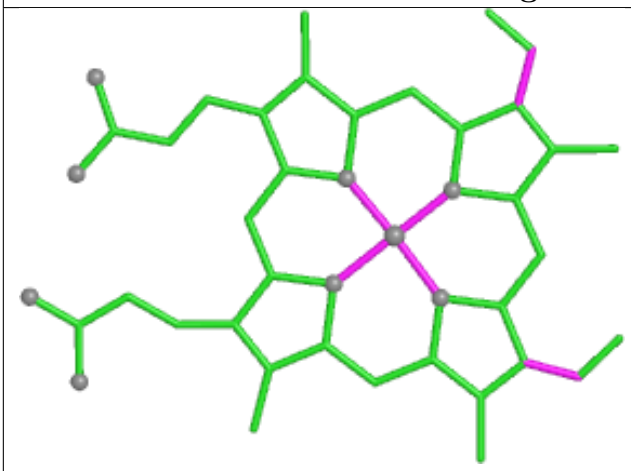


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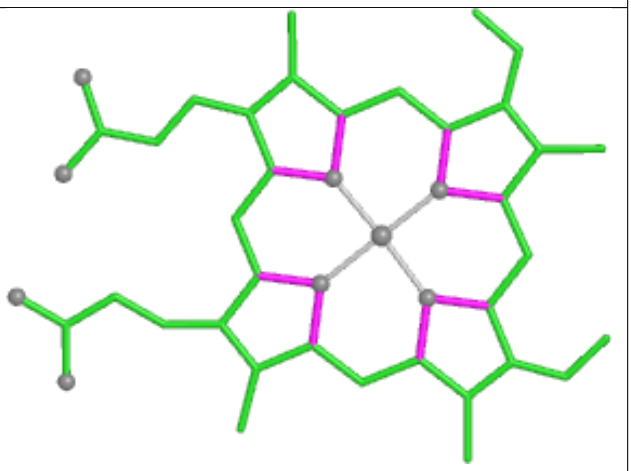


Rings

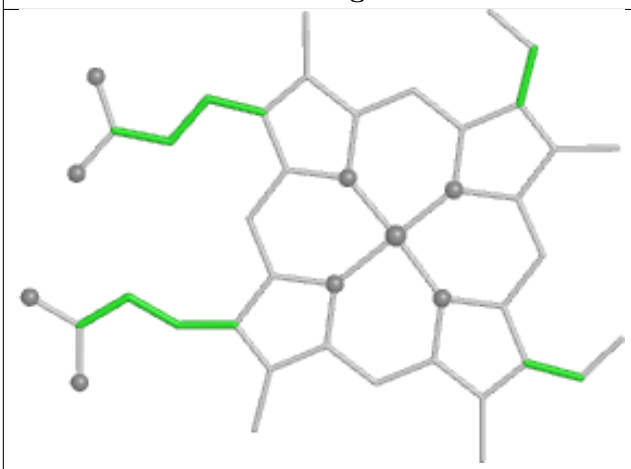
Ligand HEM E 201



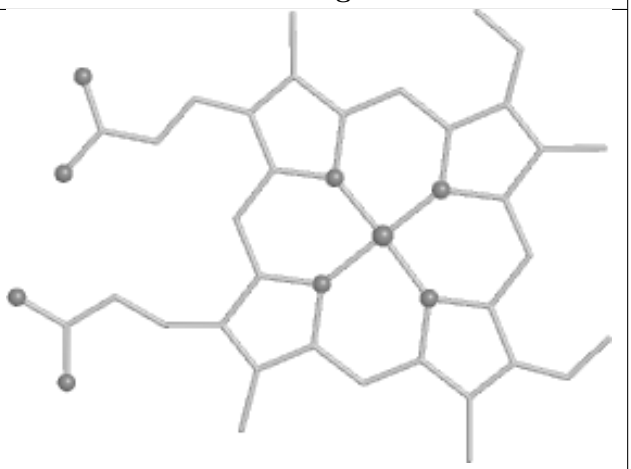
Bond lengths



Bond angles

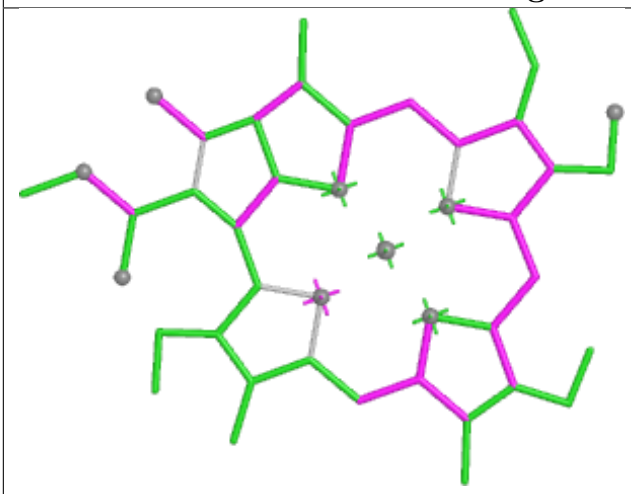


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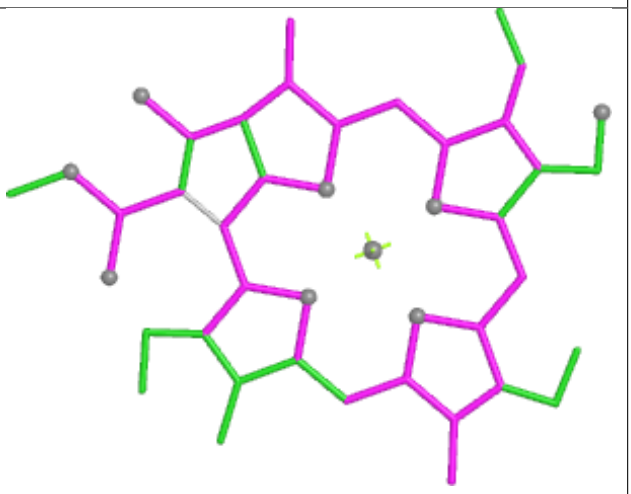


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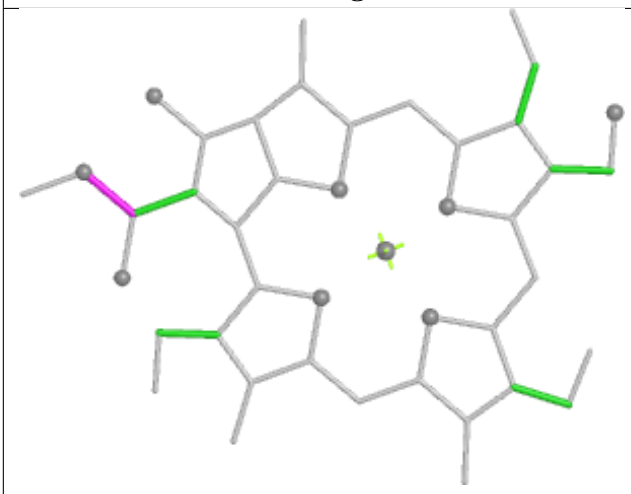
Ligand CHL 6 308



Bond lengths



Bond angles

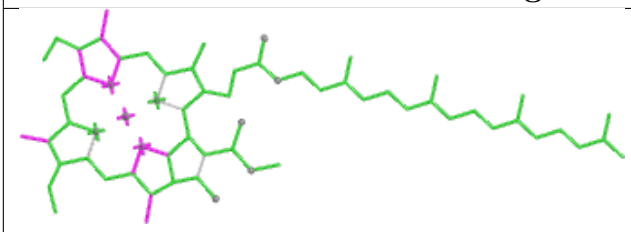


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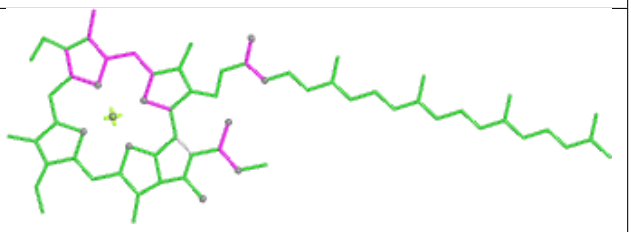


Rings

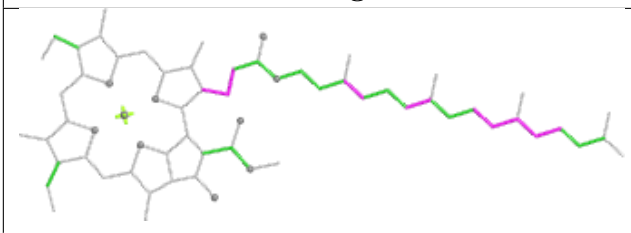
Ligand CLA B 603



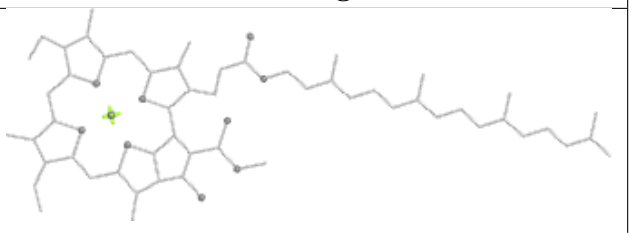
Bond lengths



Bond angles

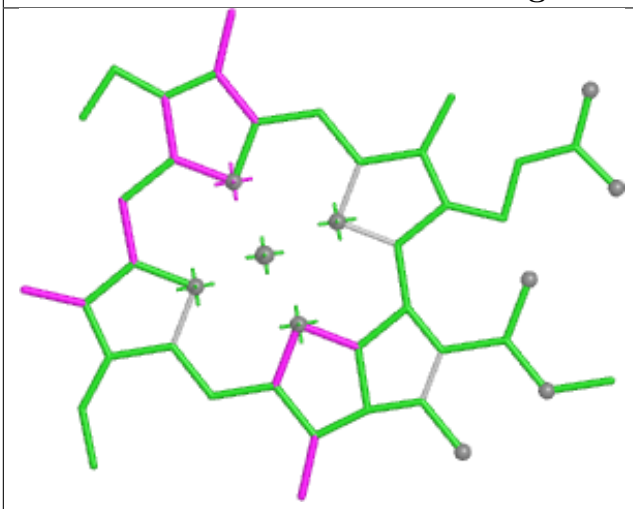


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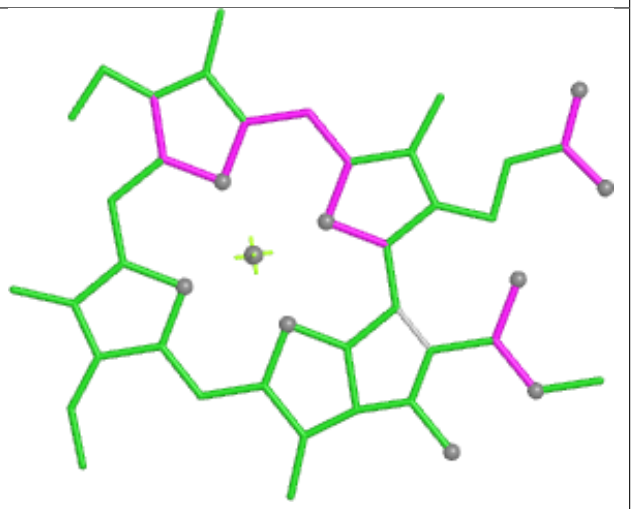


Rings

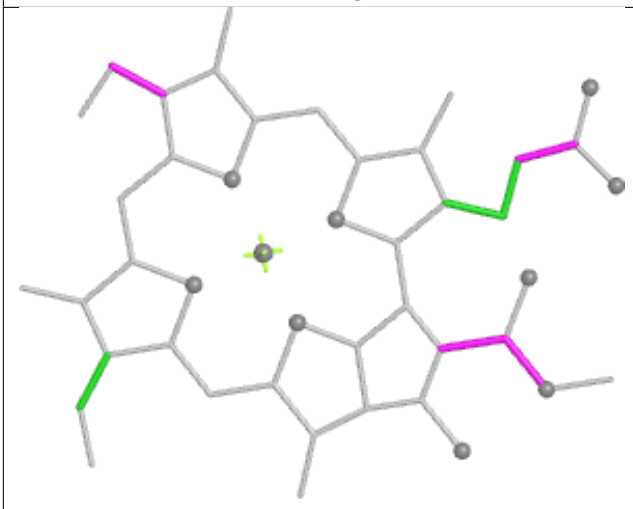
Ligand CLA 6 315



Bond lengths



Bond angles

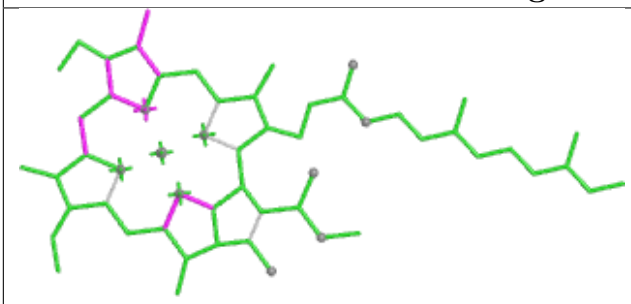


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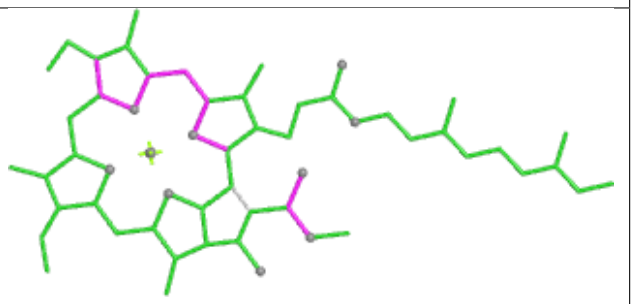


Rings

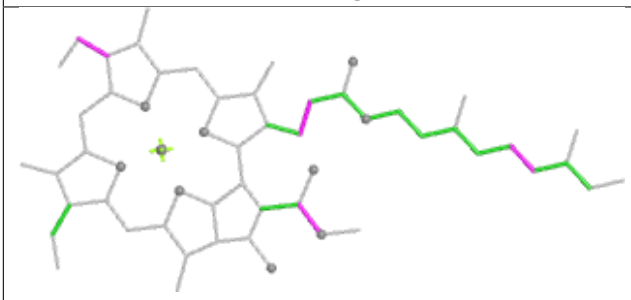
Ligand CLA 9 306



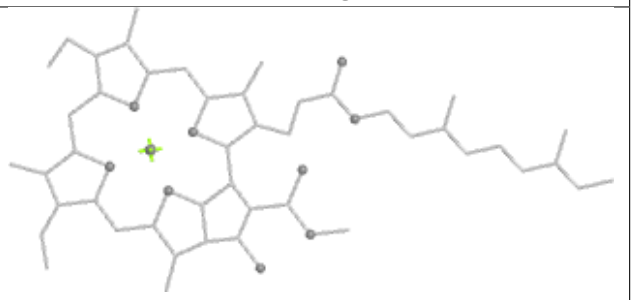
Bond lengths



Bond angles

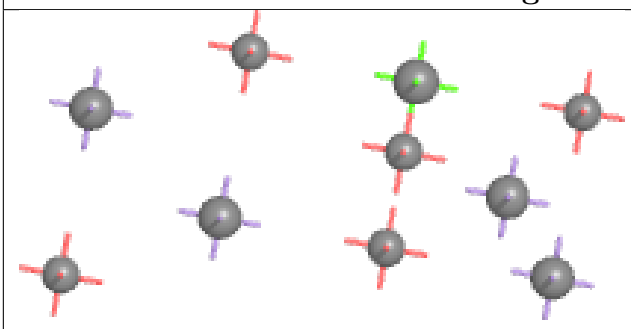


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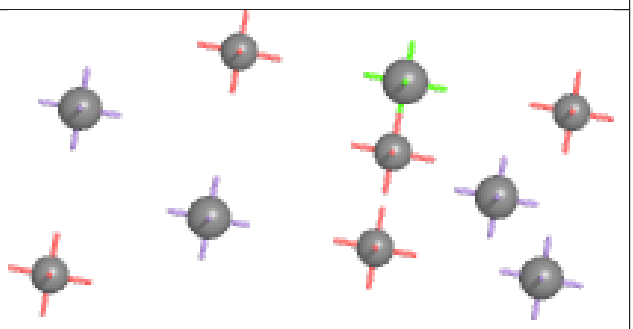


Rings

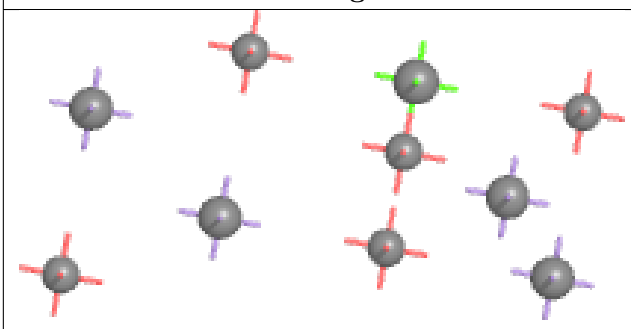
Ligand OEX A 602



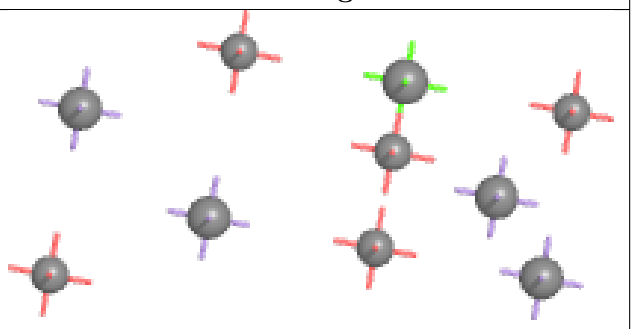
Bond lengths



Bond angles

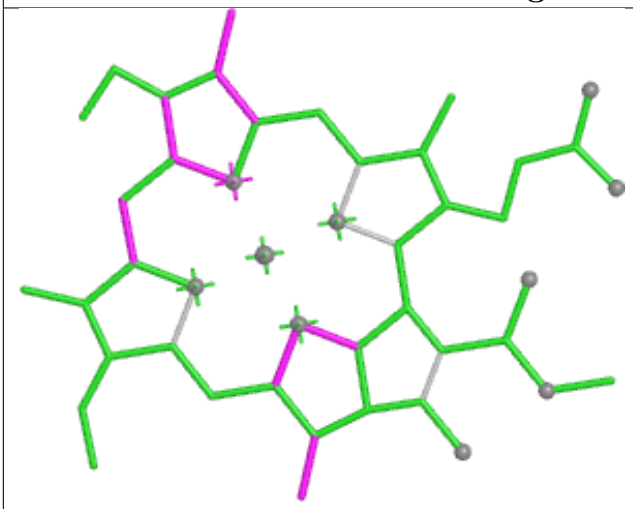


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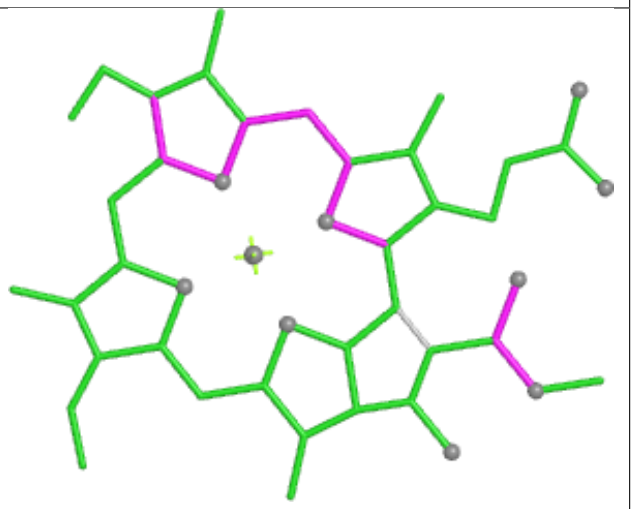


Rings

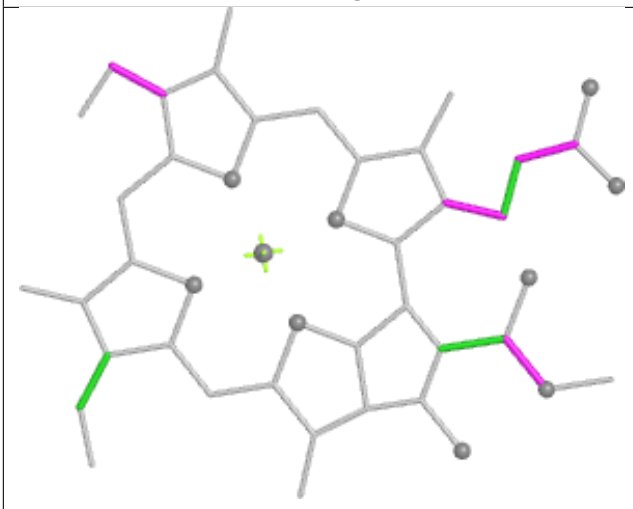
Ligand CLA S 616



Bond lengths



Bond angles

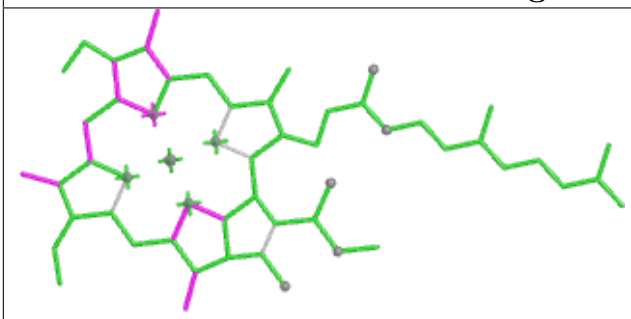


Torsions

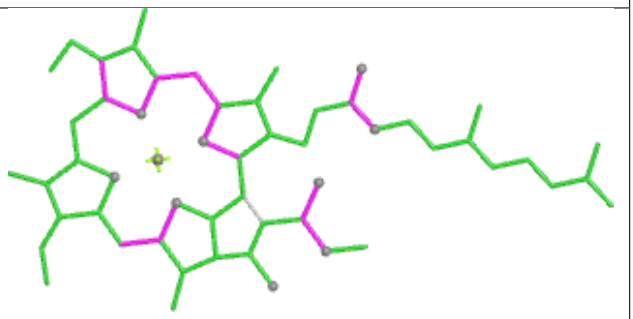


Rings

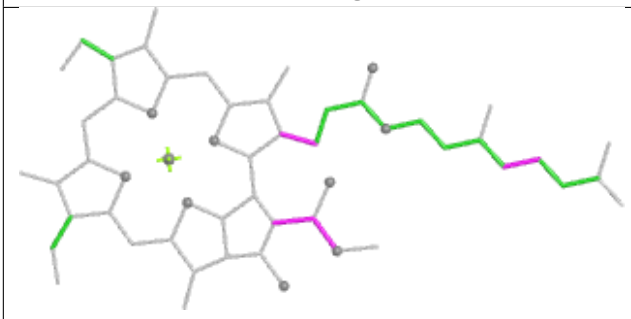
Ligand CLA 2 314



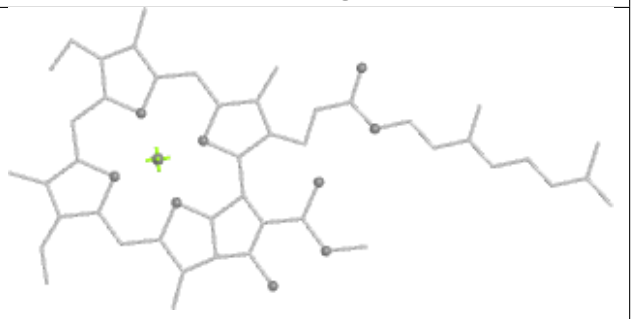
Bond lengths



Bond angles

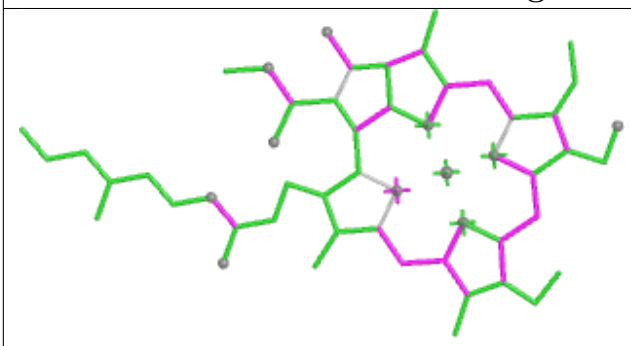


Torsions

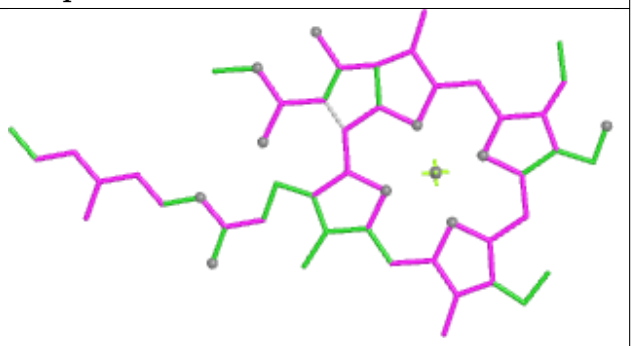


Rings

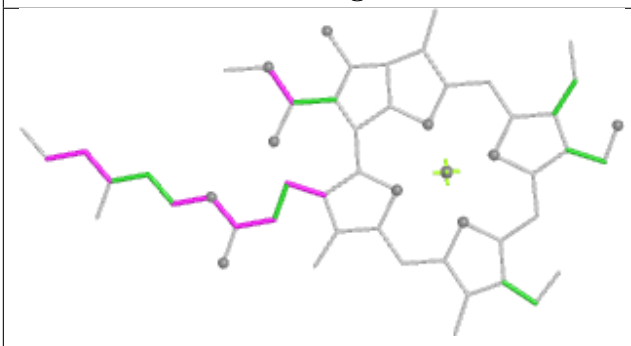
Ligand CHL q 309



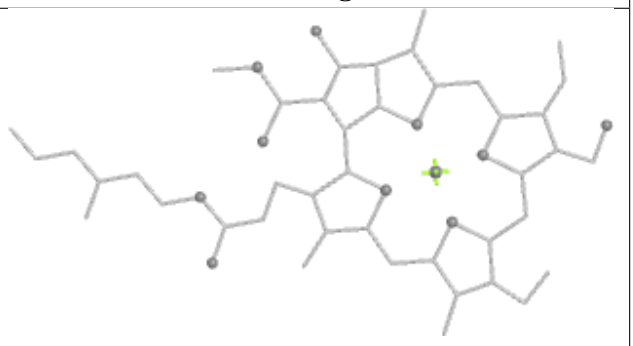
Bond lengths



Bond angles

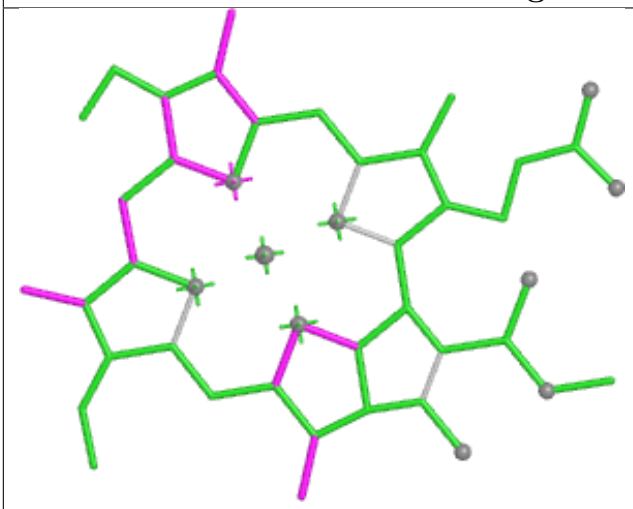


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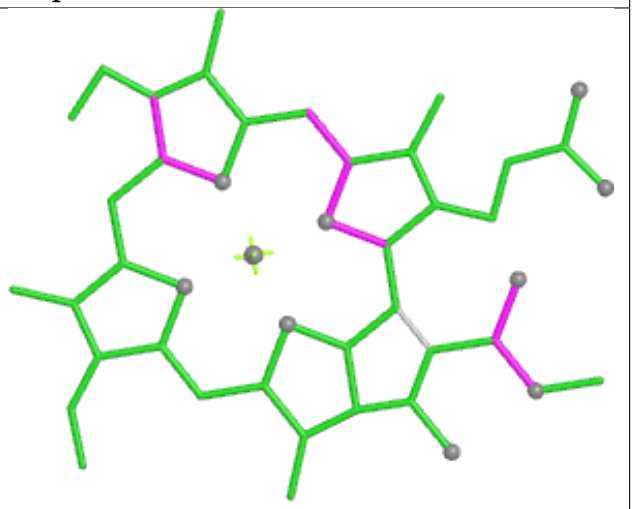


Rings

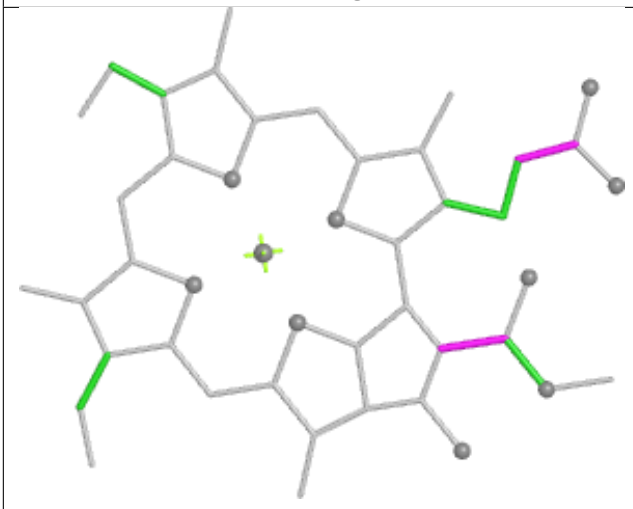
Ligand CLA p 316



Bond lengths



Bond angles

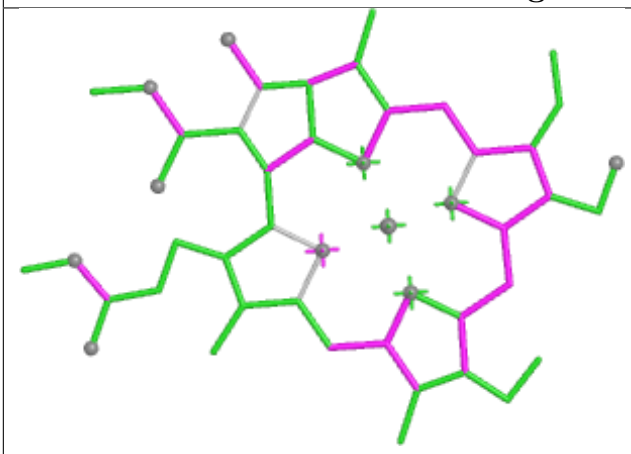


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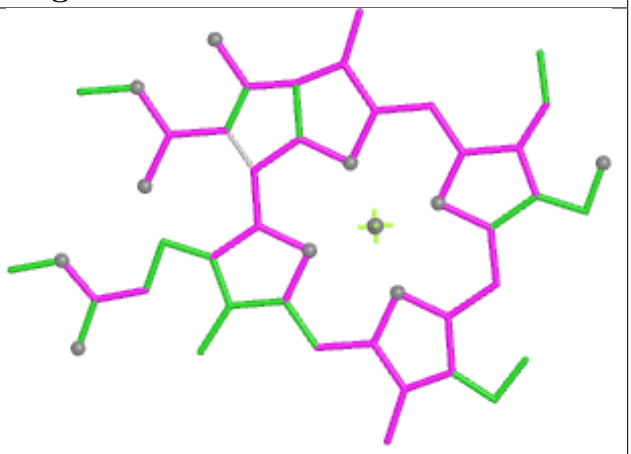


Rings

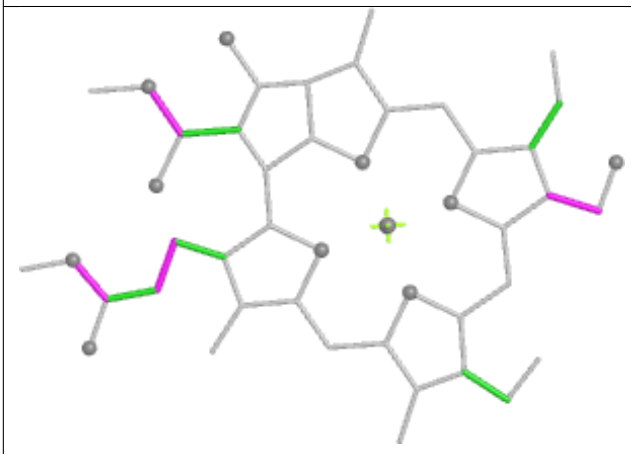
Ligand CHL g 310



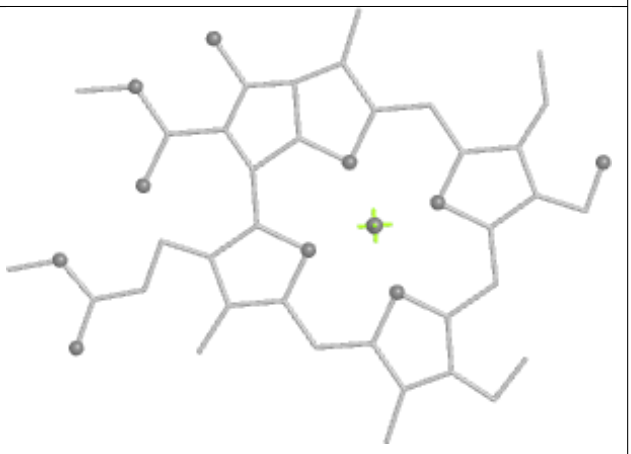
Bond lengths



Bond angles

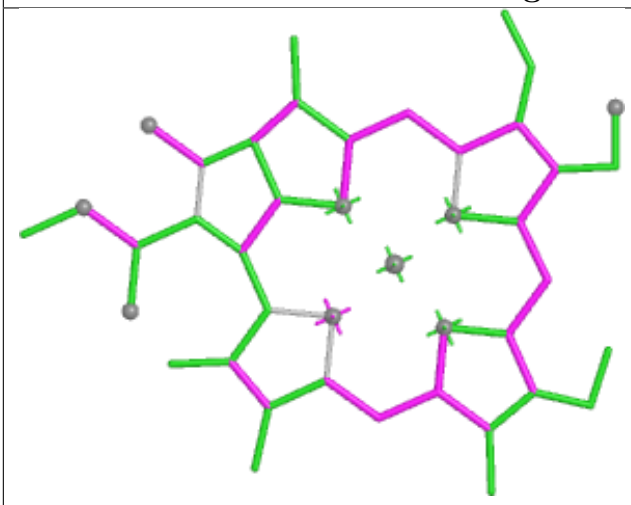


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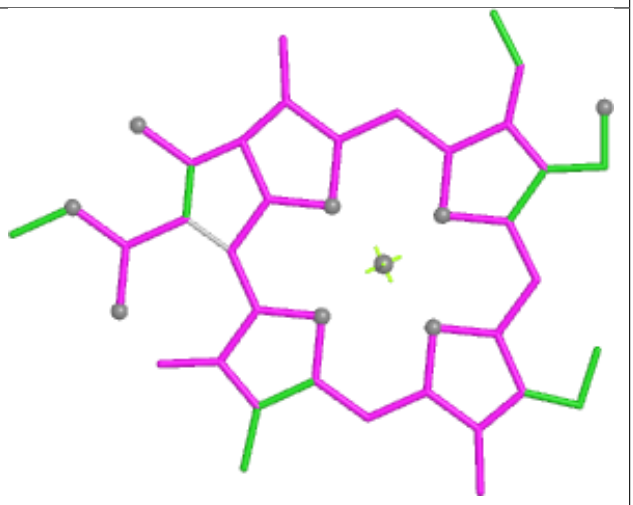


Rings

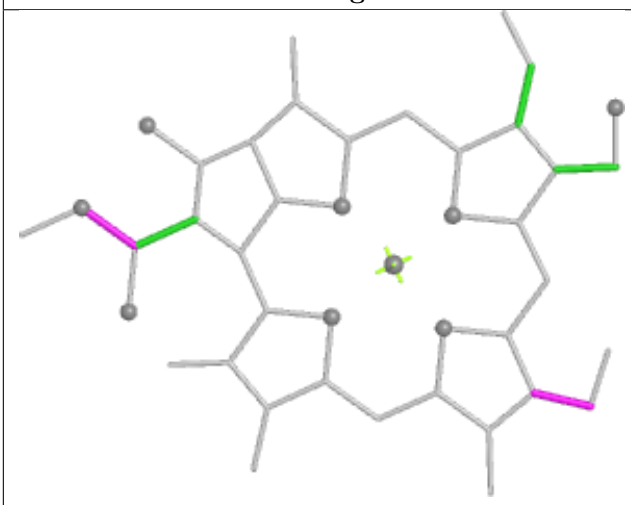
Ligand CHL R 605



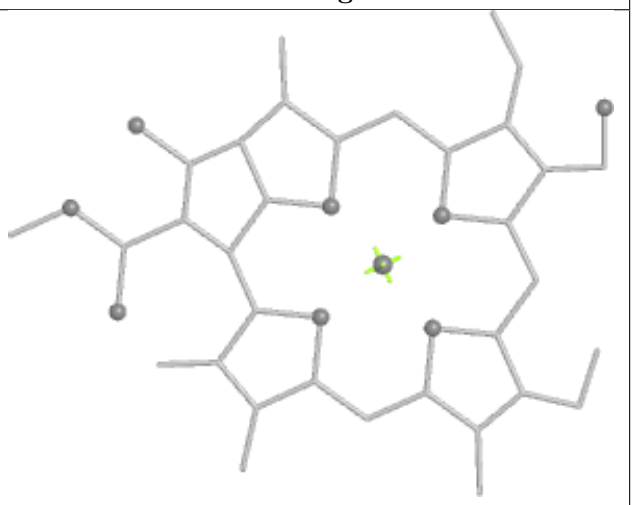
Bond lengths



Bond angles

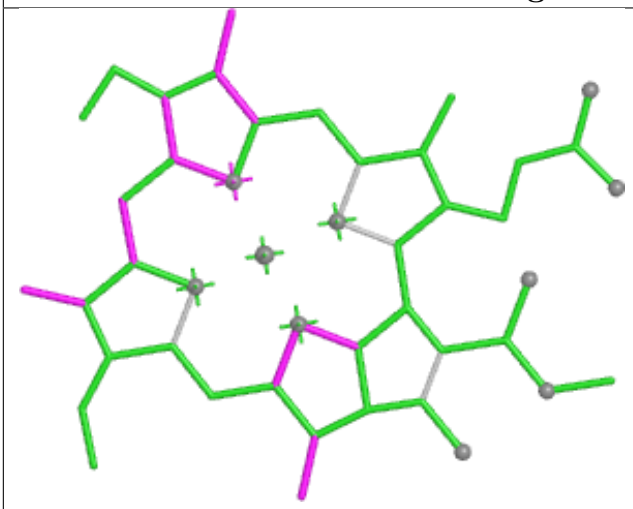


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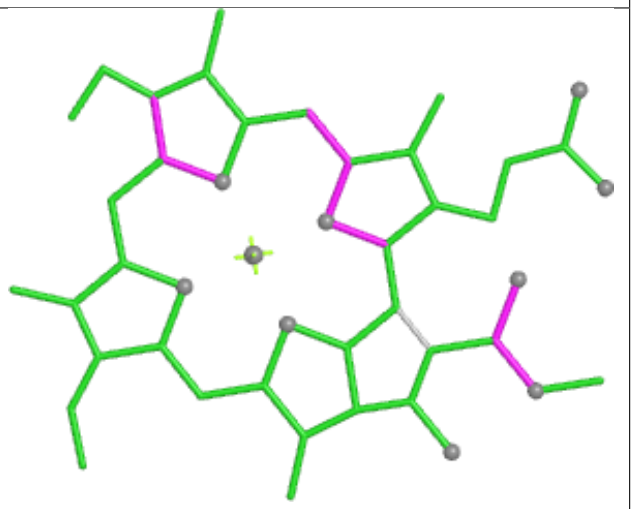


Rings

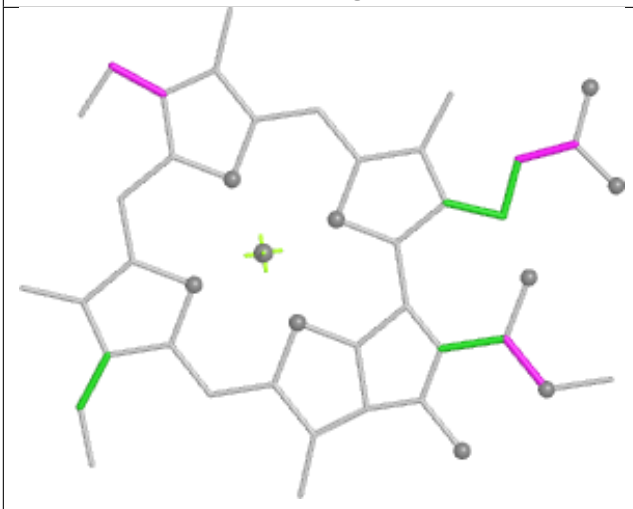
Ligand CLA n 315



Bond lengths



Bond angles

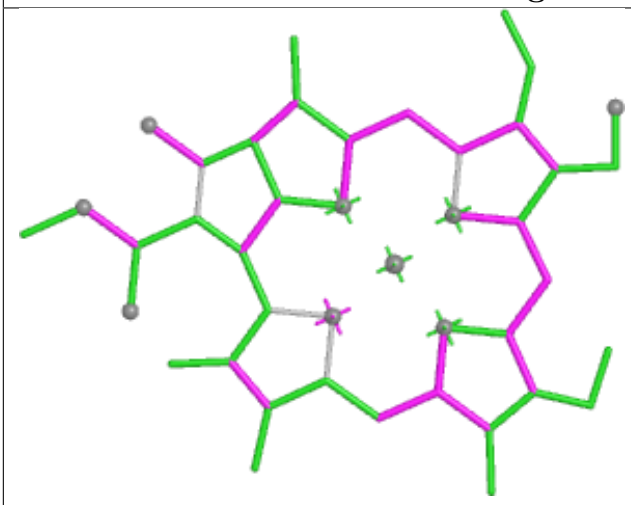


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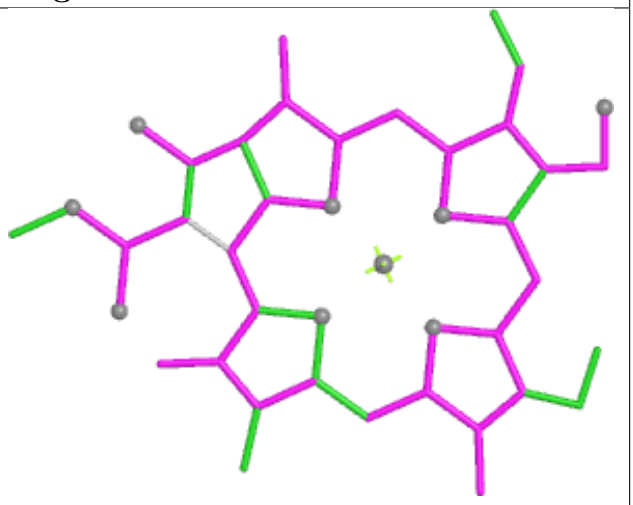


Rings

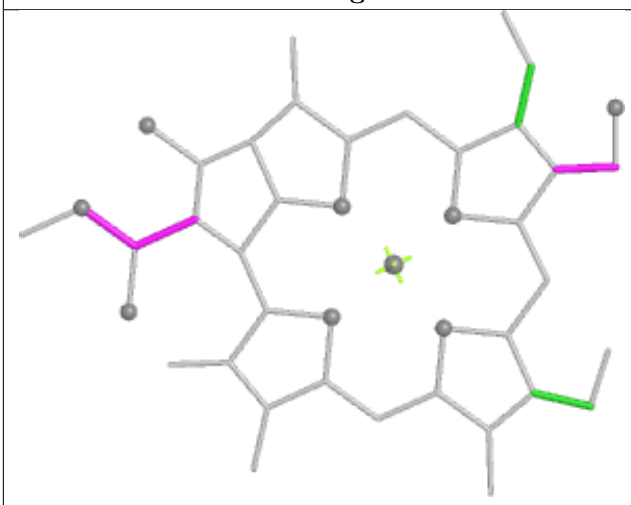
Ligand CHL g 318



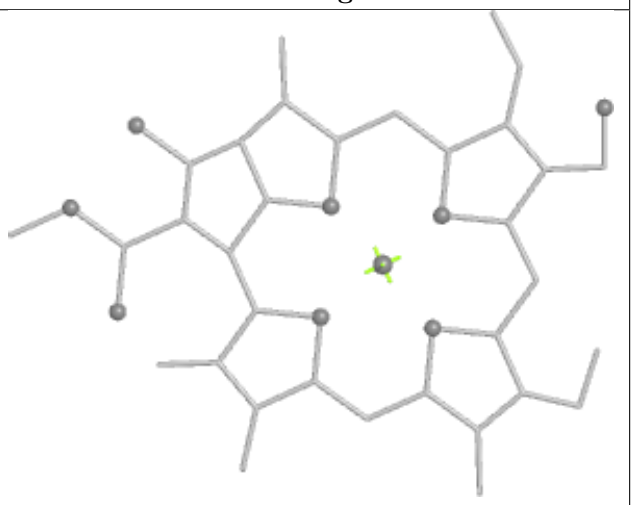
Bond lengths



Bond angles

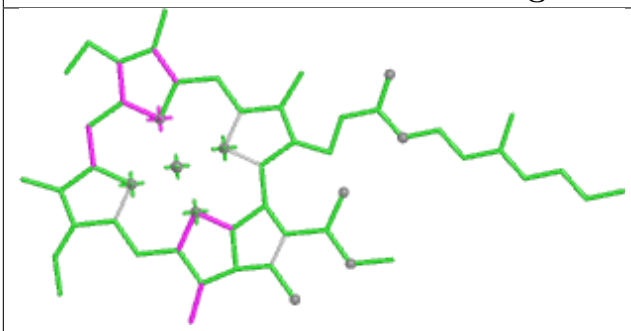


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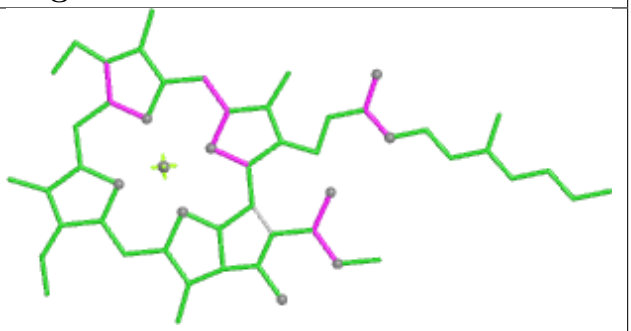


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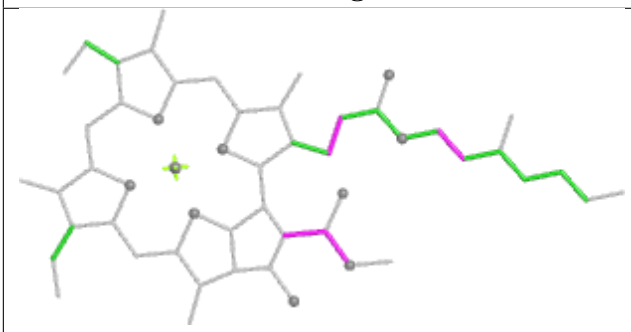
Ligand CLA g 307



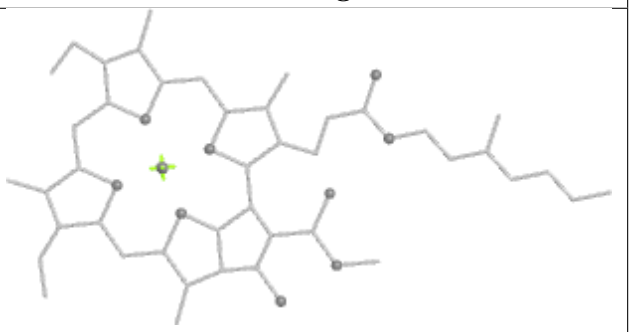
Bond lengths



Bond angles

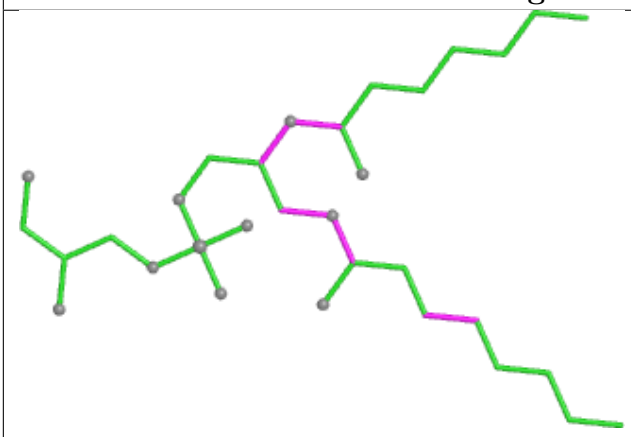


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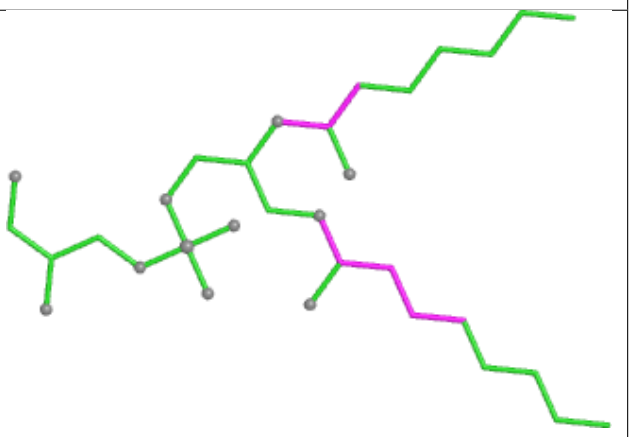


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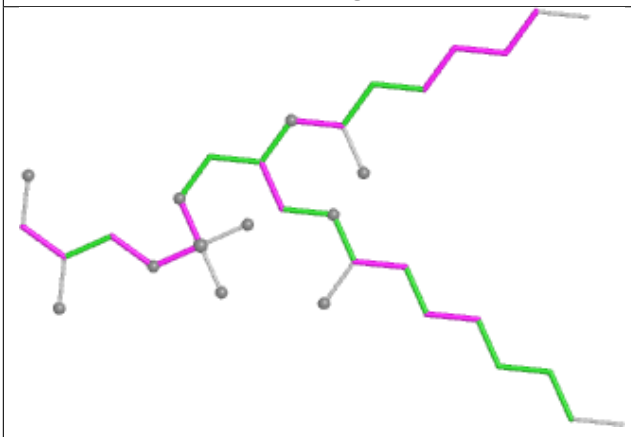
Ligand LHG c 617



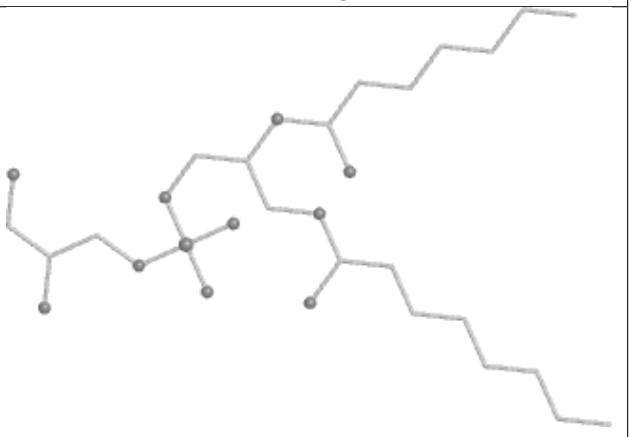
Bond lengths



Bond angles

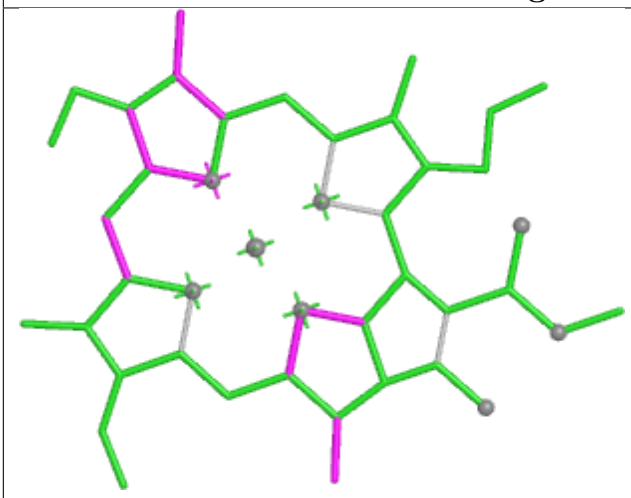


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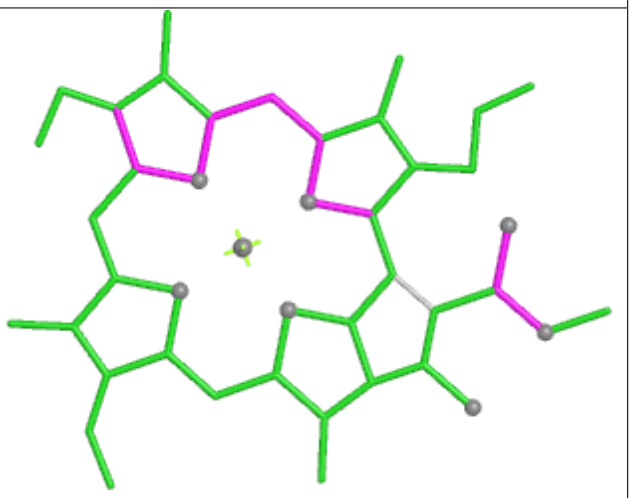


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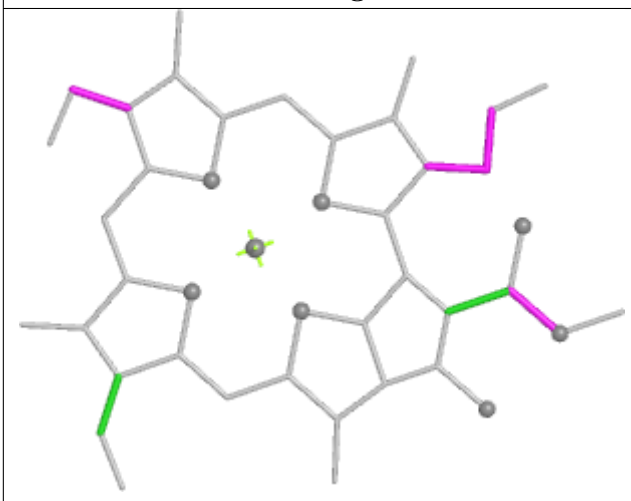
Ligand CLA 2 307



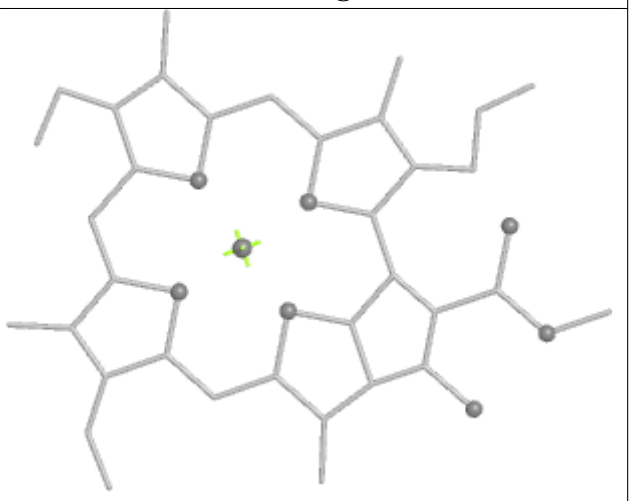
Bond lengths



Bond angles

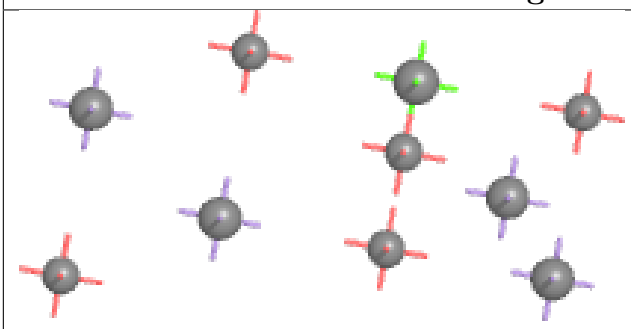


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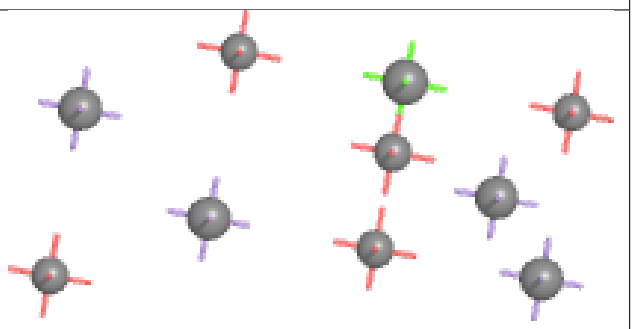


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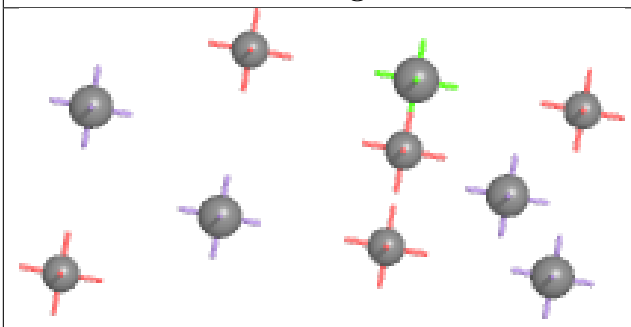
Ligand OEX a 602



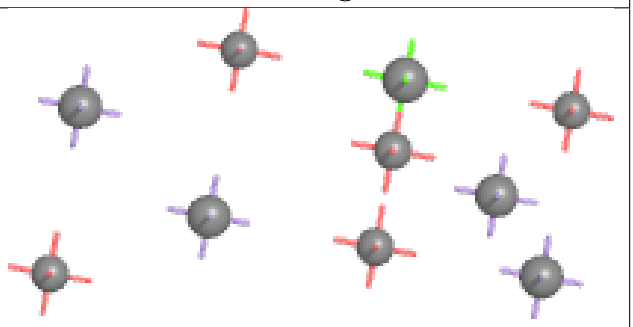
Bond lengths



Bond angles

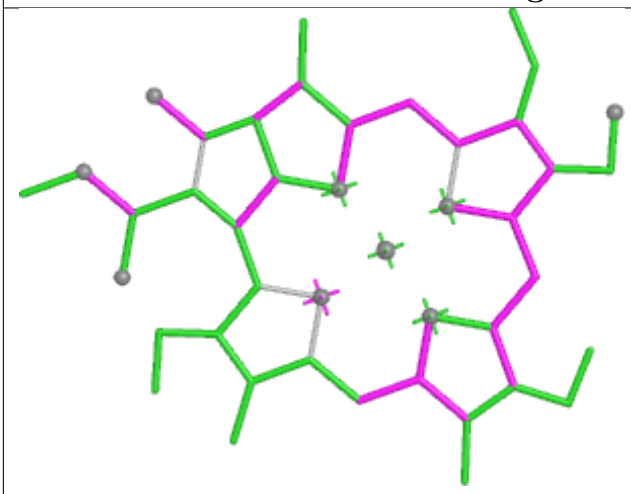


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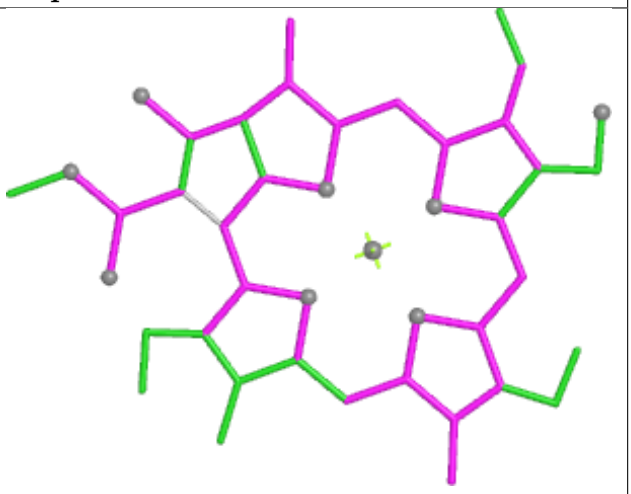


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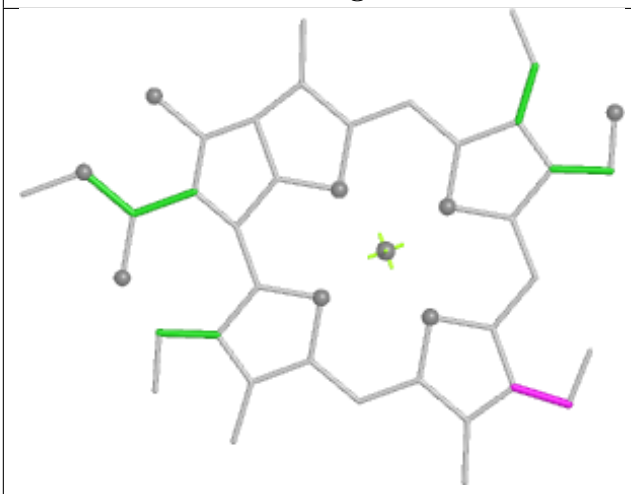
Ligand CHL p 309



Bond lengths



Bond angles

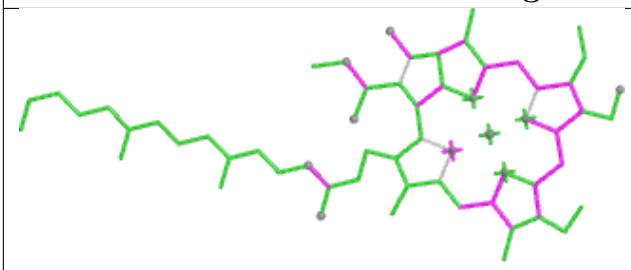


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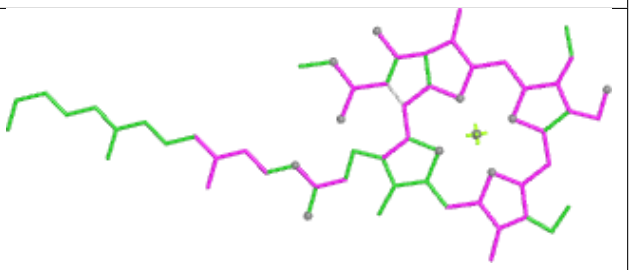


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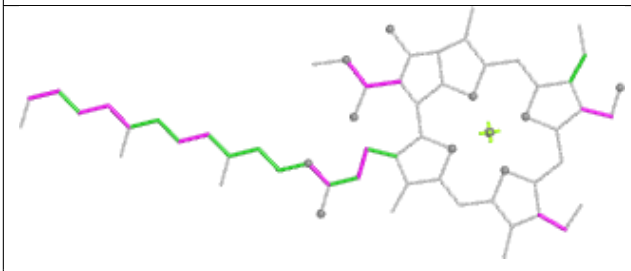
Ligand CHL N 305



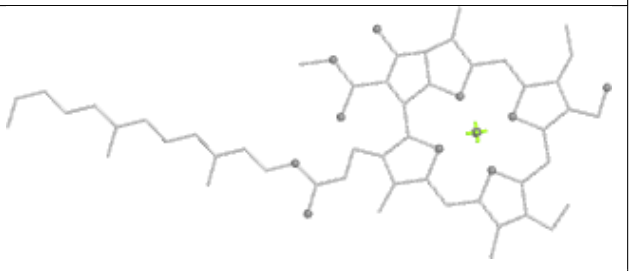
Bond lengths



Bond angles

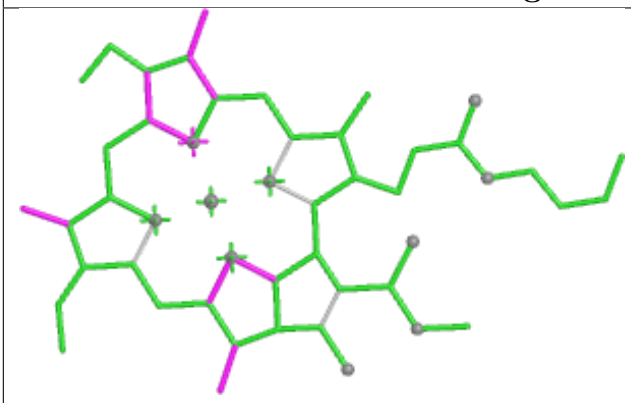


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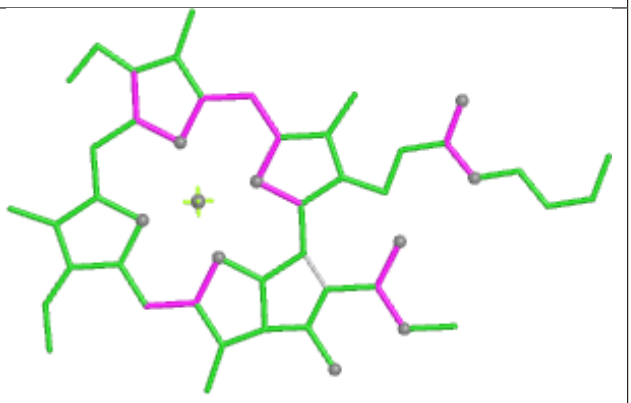


Rings

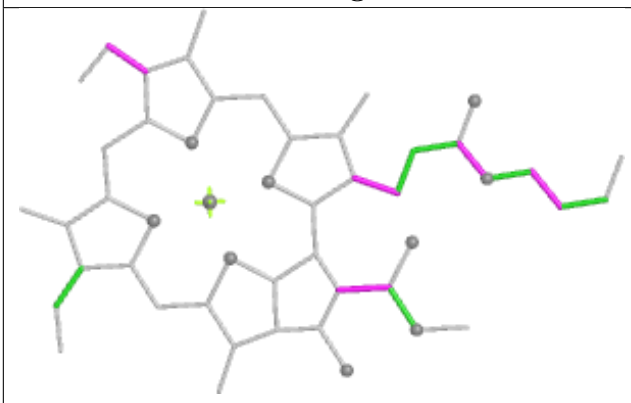
Ligand CLA A 605



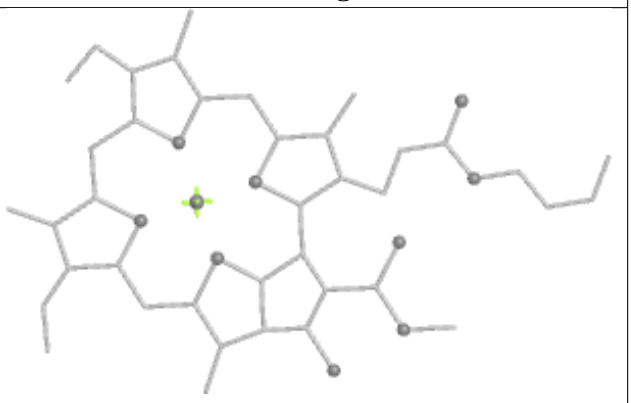
Bond lengths



Bond angles

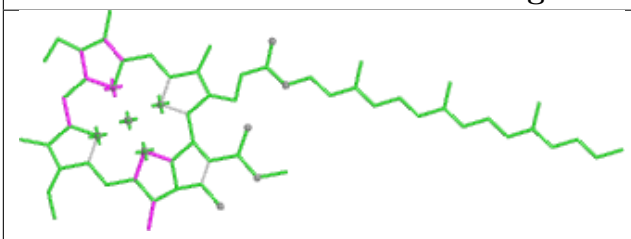


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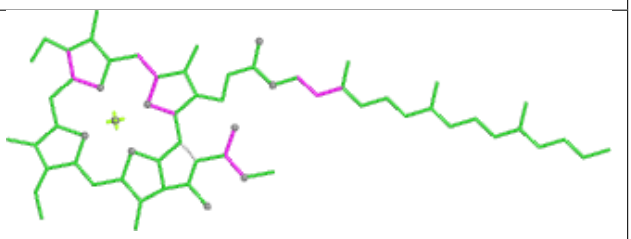


Rings

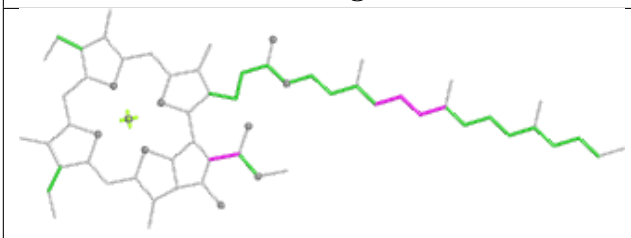
Ligand CLA n 314



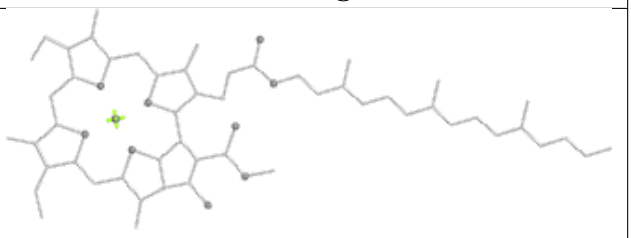
Bond lengths



Bond angles

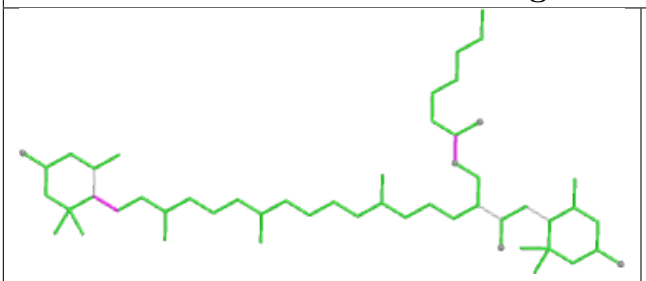


Torsions

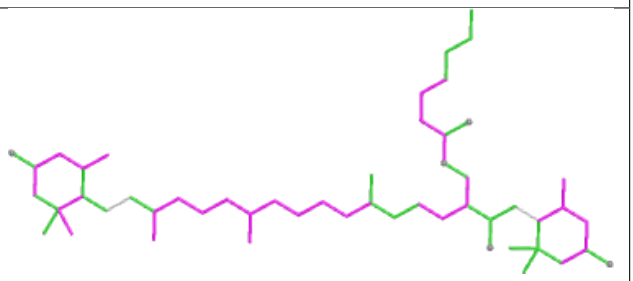


Rings

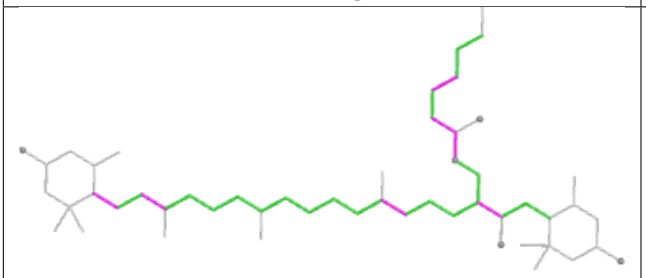
Ligand 0UR 1 301



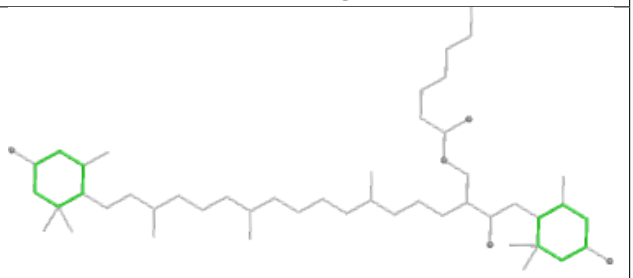
Bond lengths



Bond angles

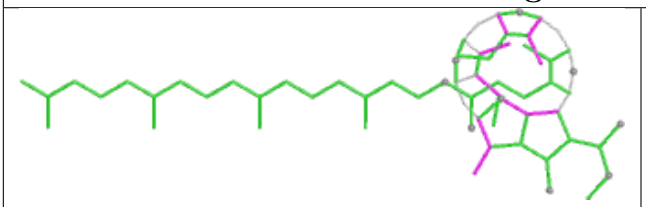


Torsions

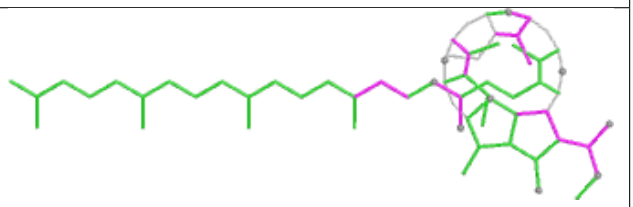


Rings

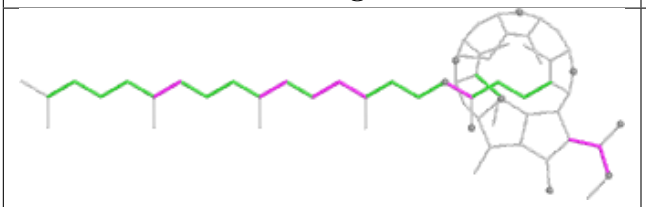
Ligand PHO d 403



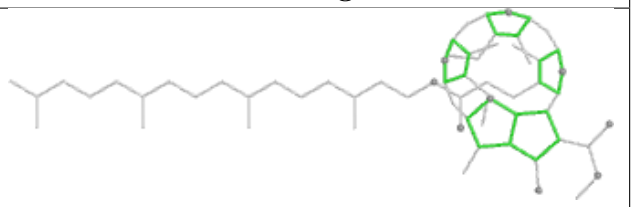
Bond lengths



Bond angles

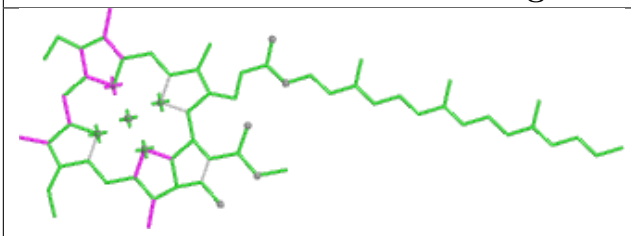


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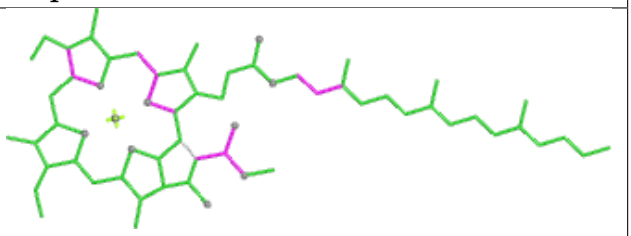


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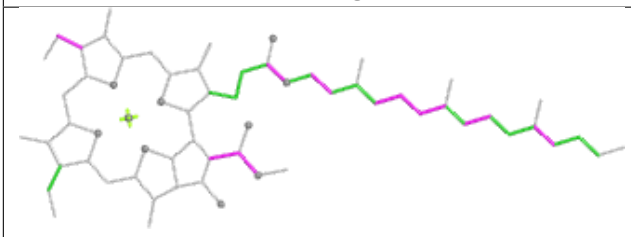
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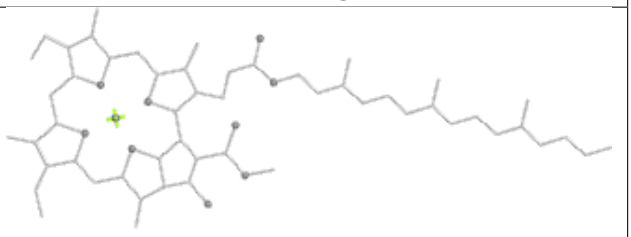
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Bond angles

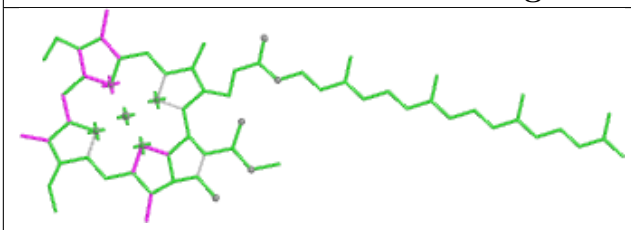


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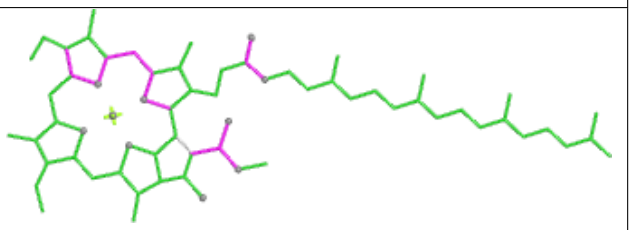


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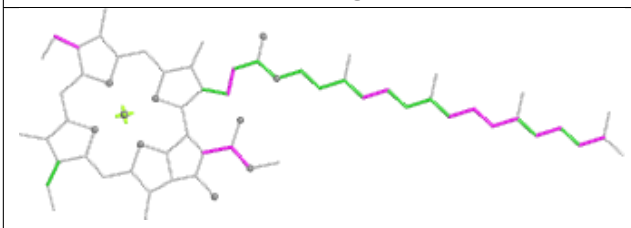
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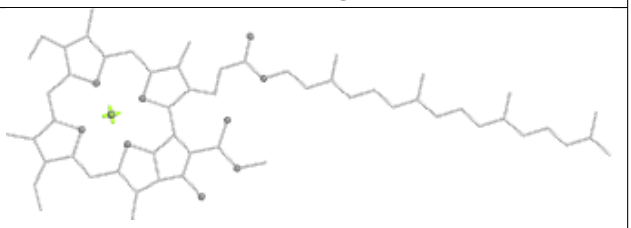
Bond lengths



Bond angles

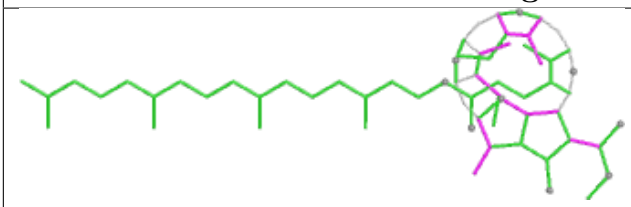


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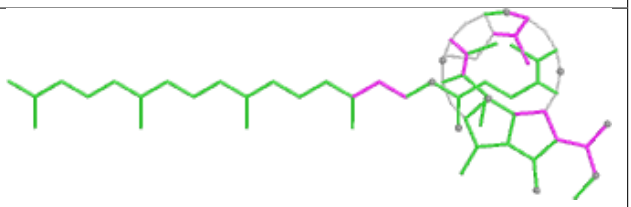


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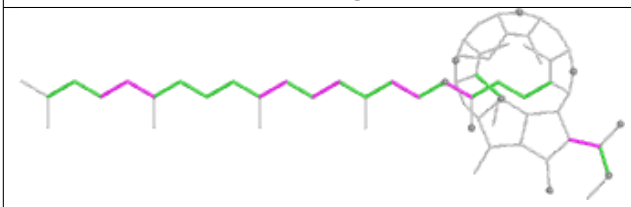
Ligand PHO A 606



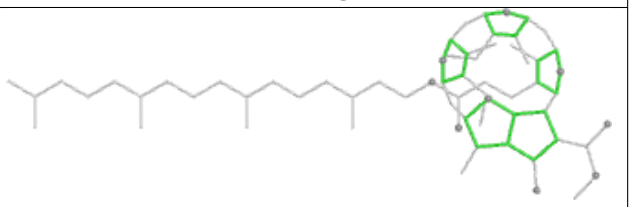
Bond lengths



Bond angles

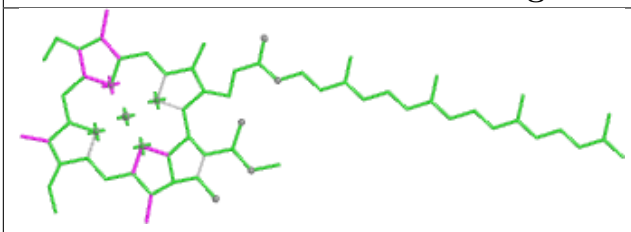


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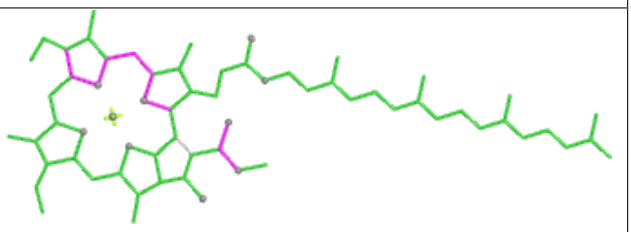


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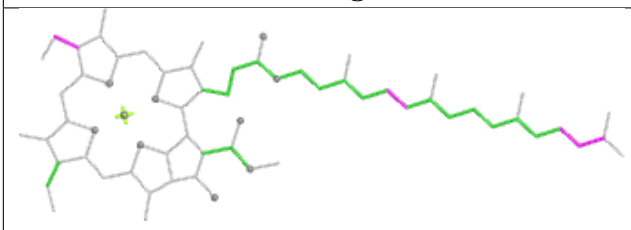
Ligand CLA b 615



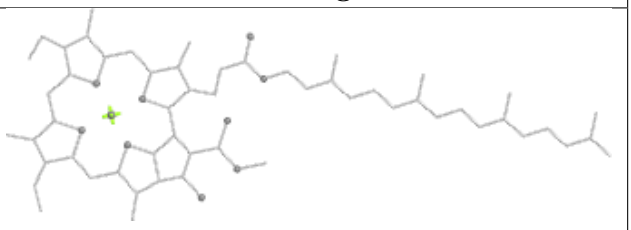
Bond lengths



Bond angles

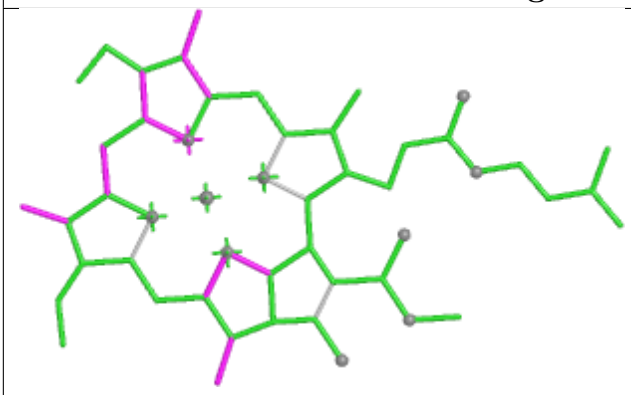


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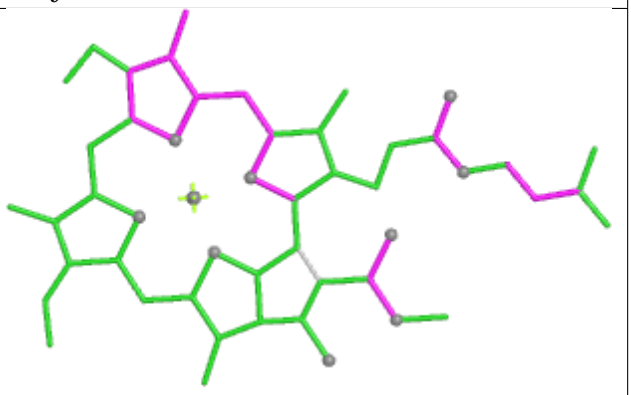


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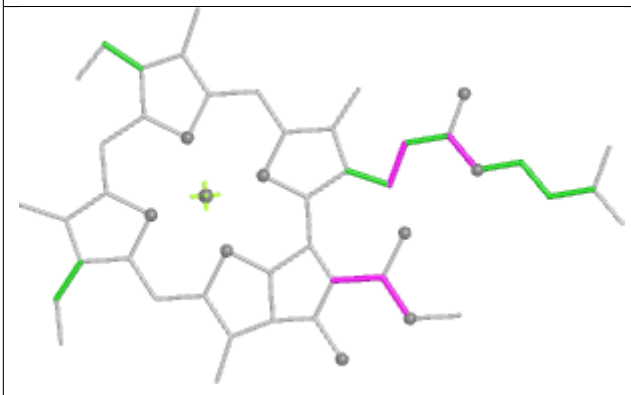
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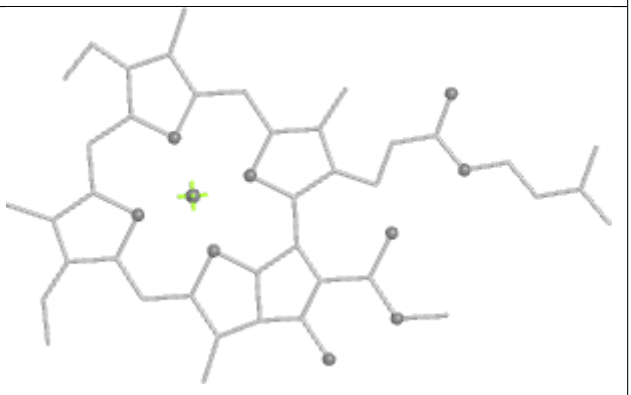
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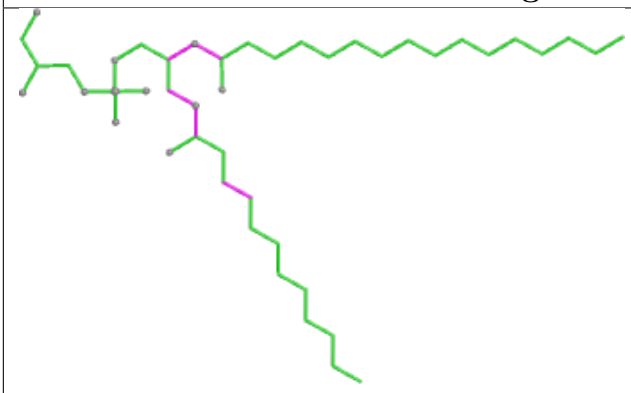


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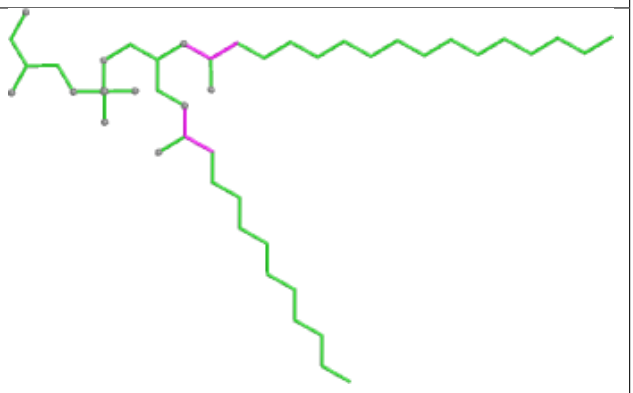


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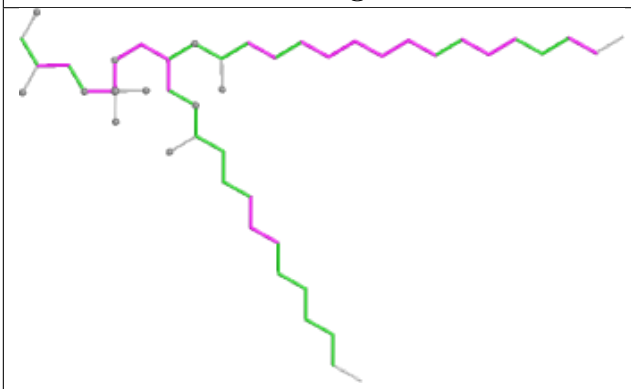
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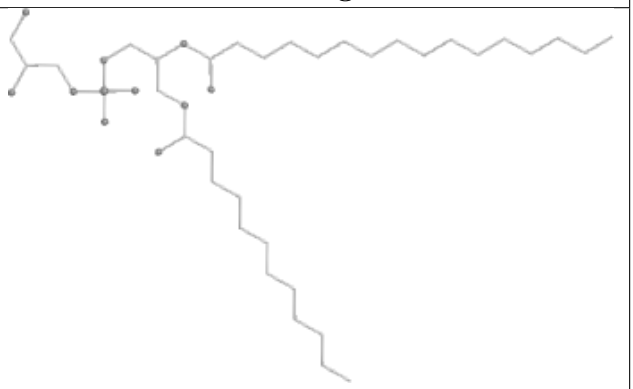
Bond lengths



Bond angles

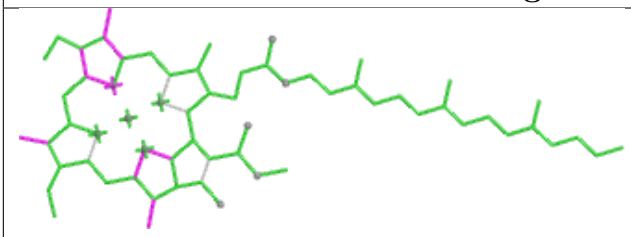


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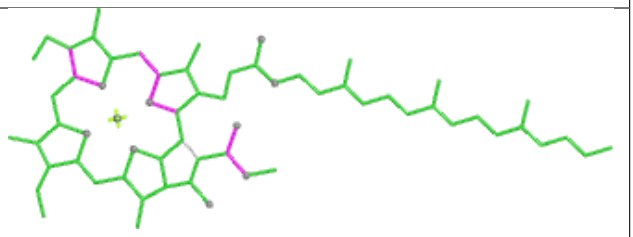


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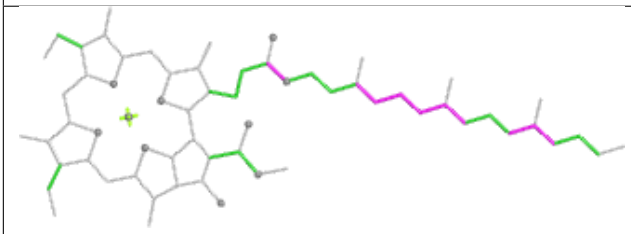
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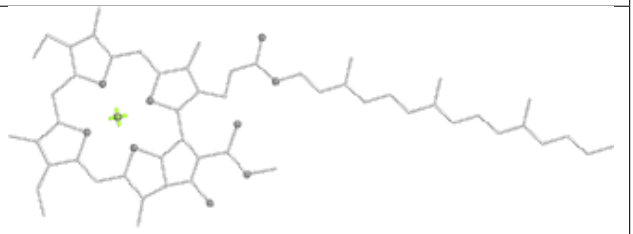
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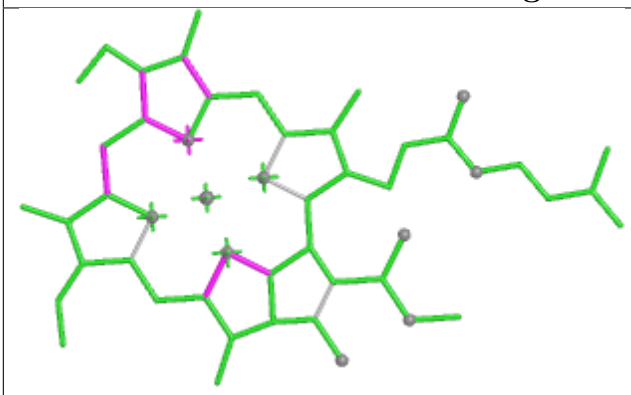


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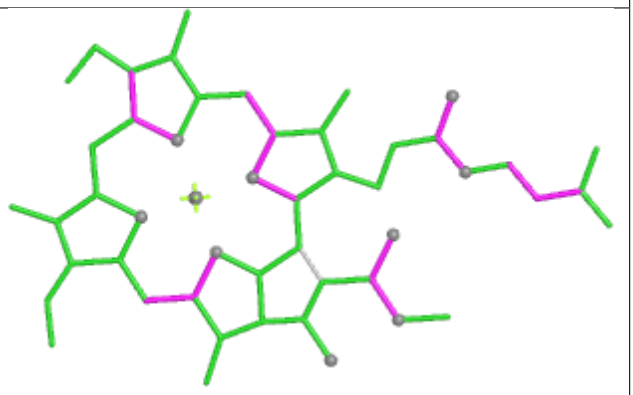


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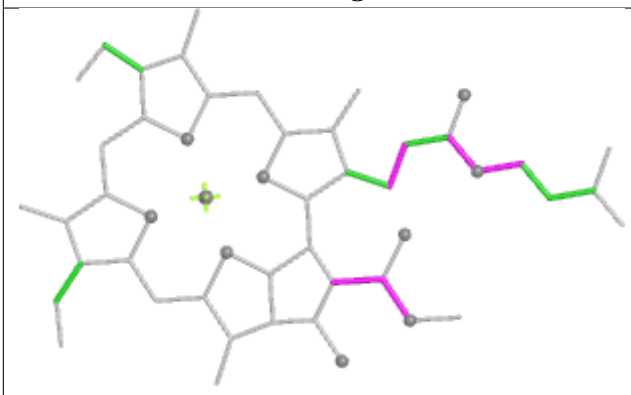
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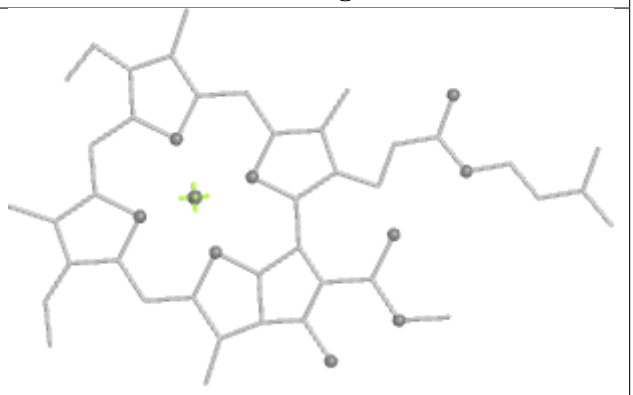
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Bond angles

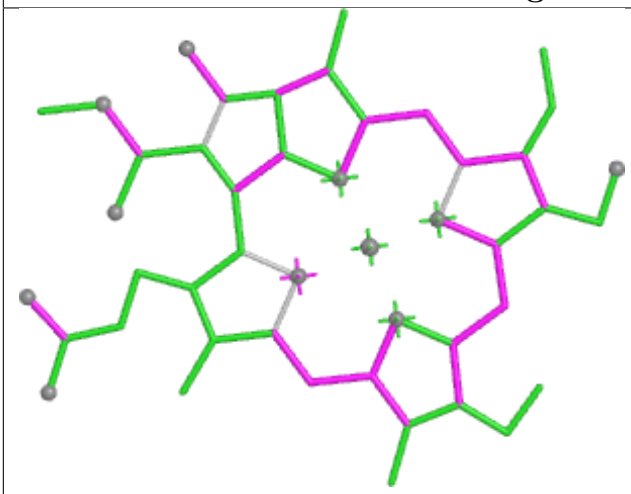


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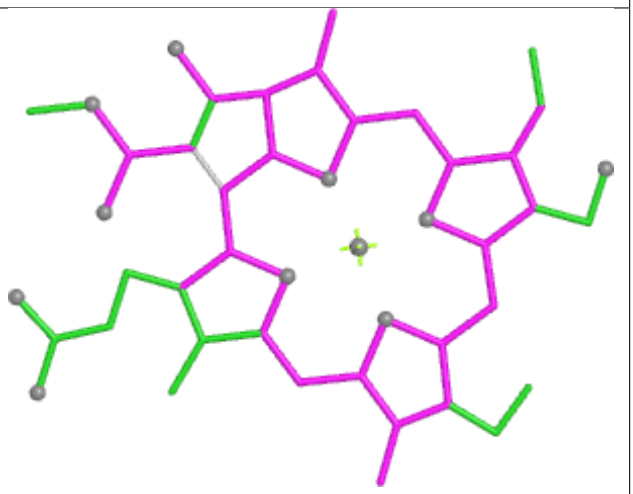


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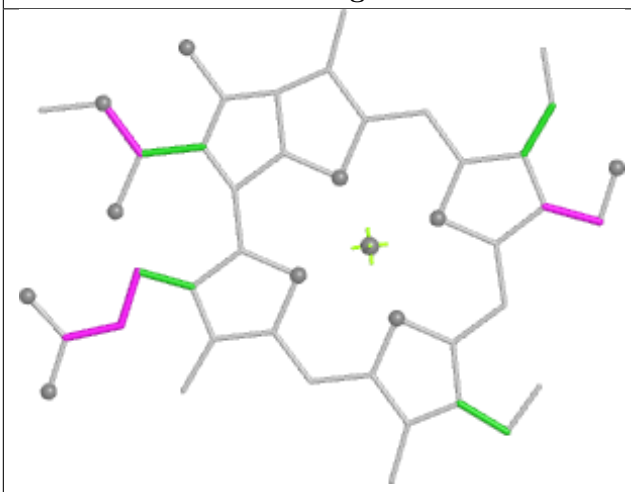
Ligand CHL n 309



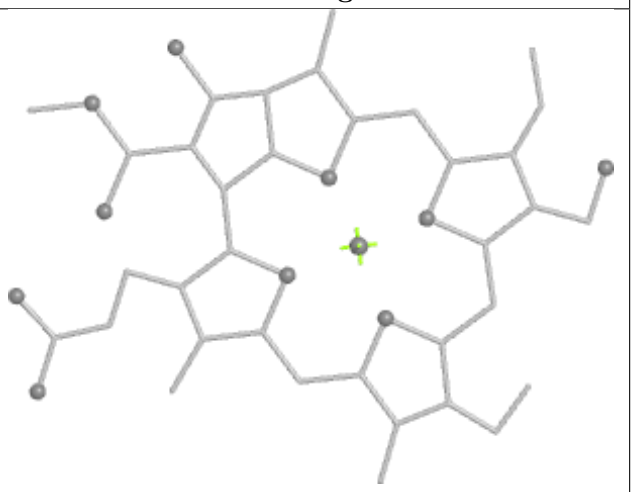
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Bond angles

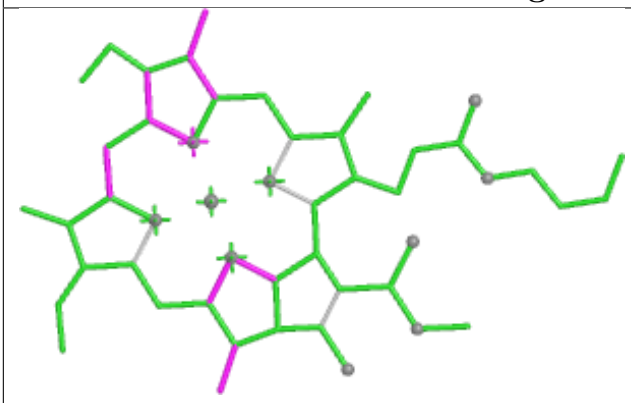


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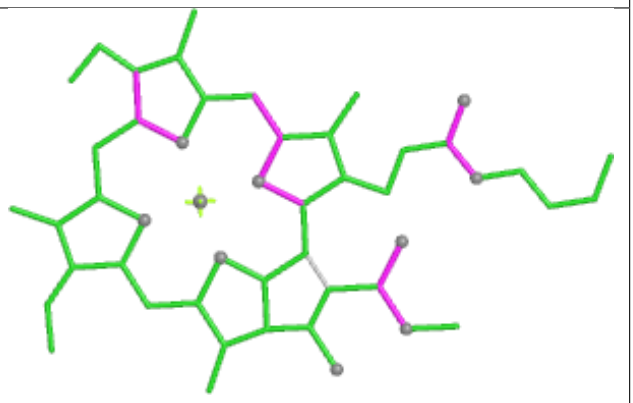


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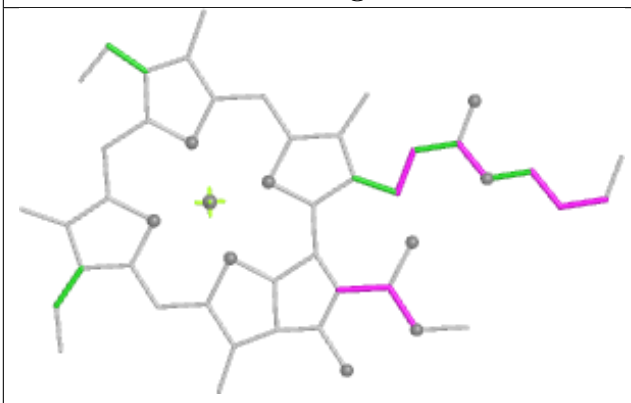
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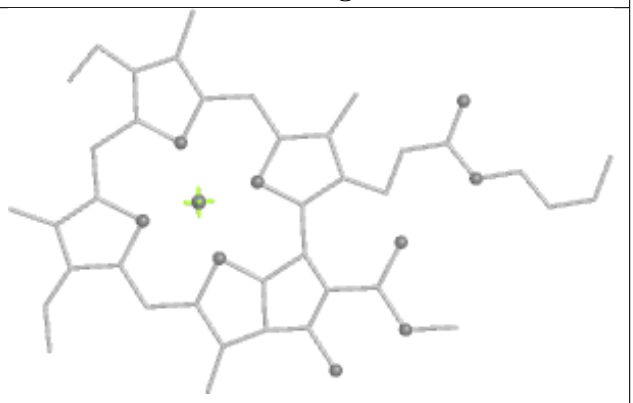
Bond lengths



Bond angles

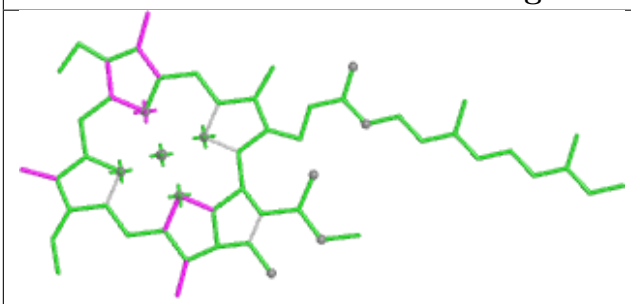


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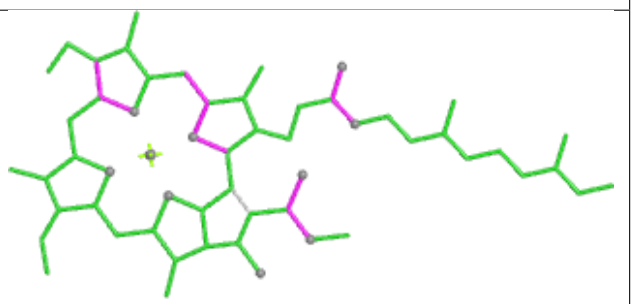


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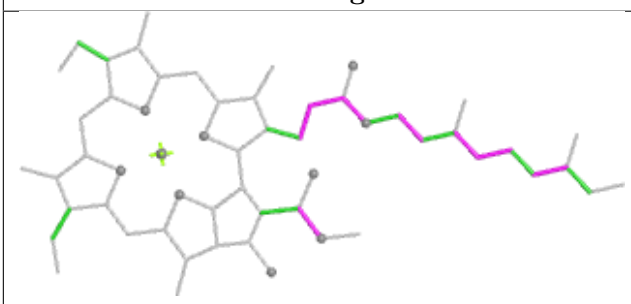
Ligand CLA B 614



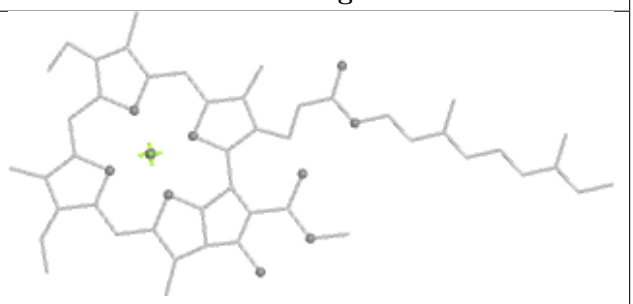
Bond lengths



Bond angles

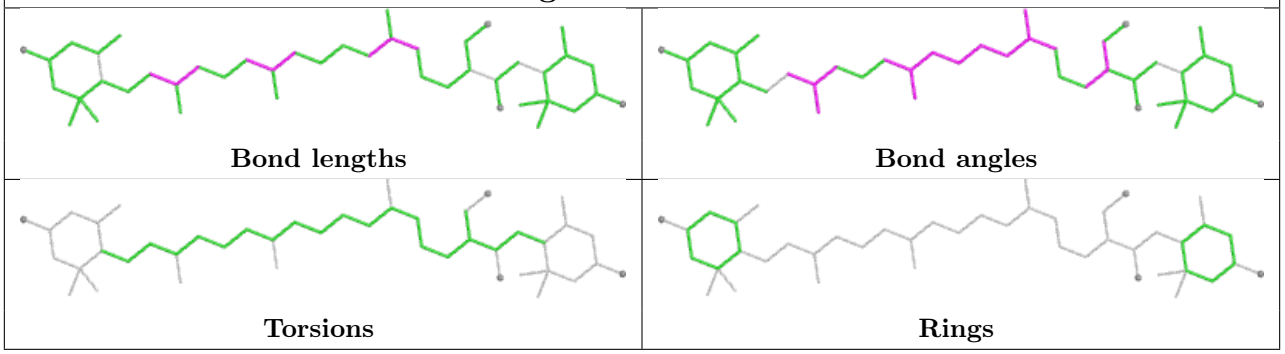


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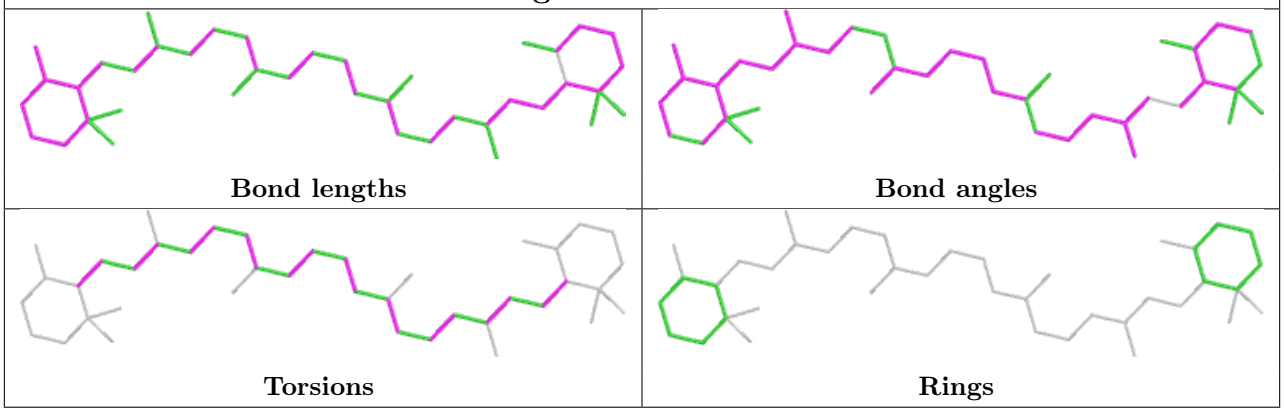


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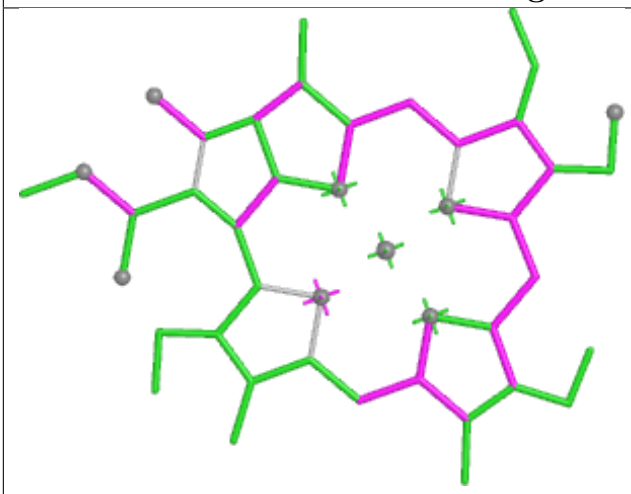
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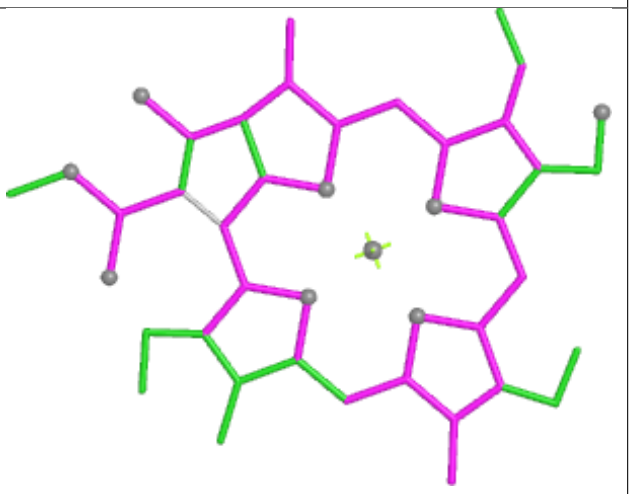
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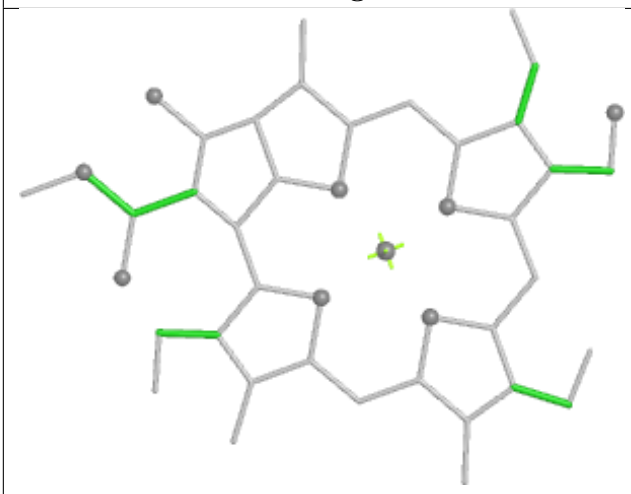
Ligand CHL 7 309



Bond lengths



Bond angles

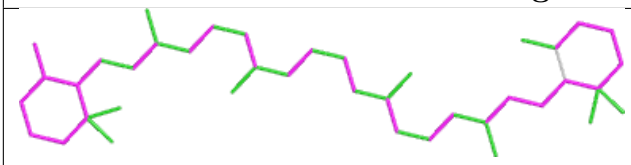


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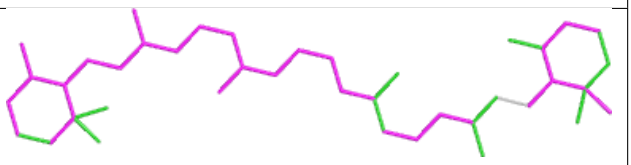


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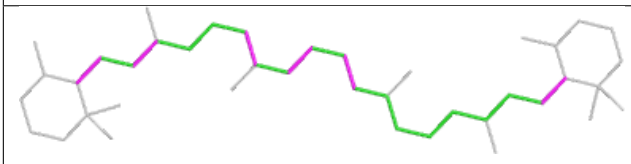
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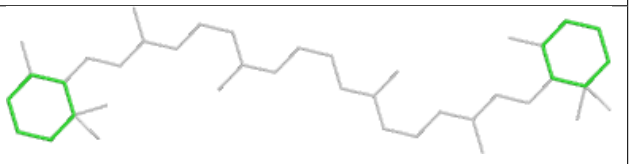
Bond lengths



Bond angles

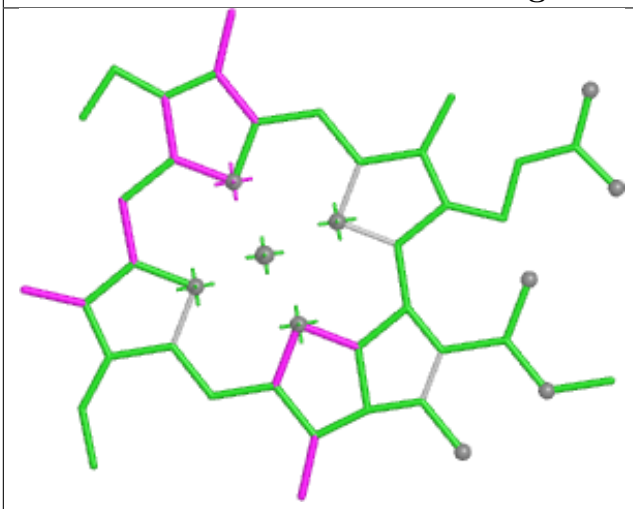


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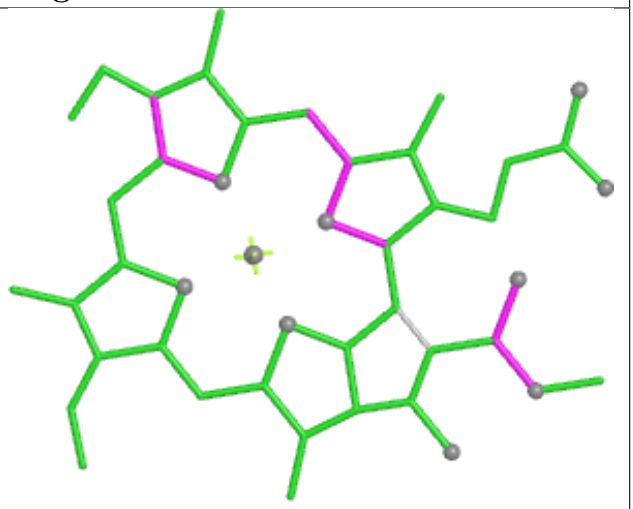


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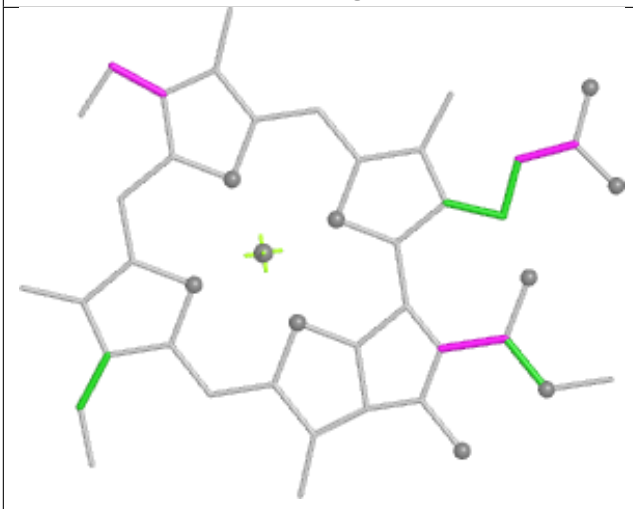
Ligand CLA g 316



Bond lengths



Bond angles

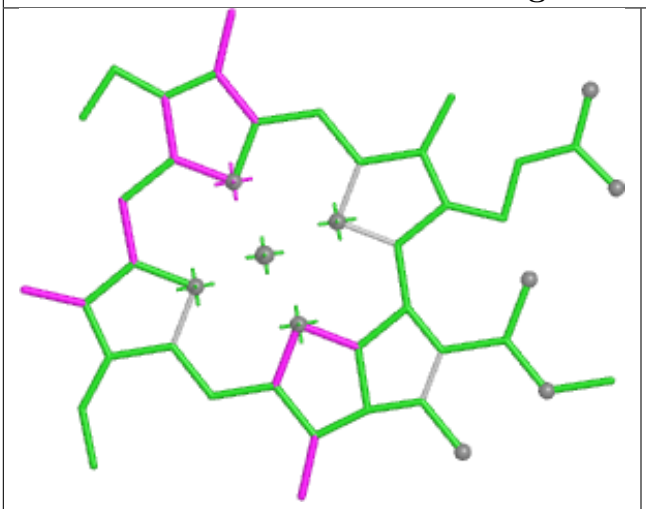


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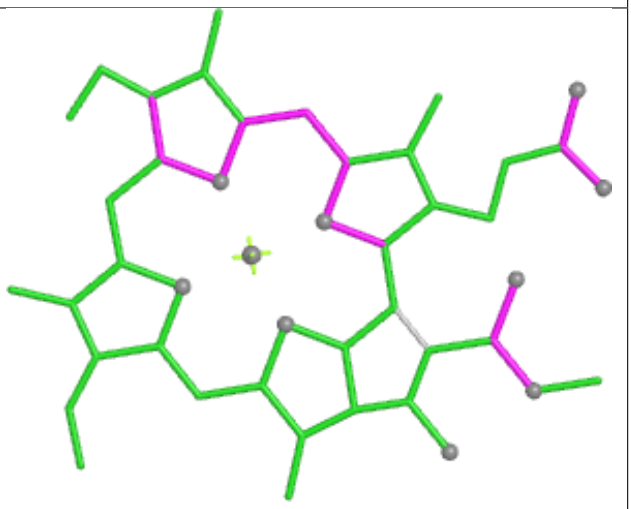


Rings

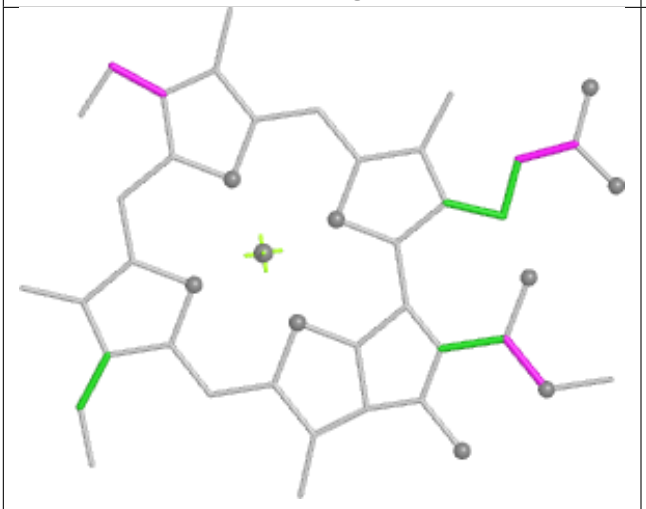
Ligand CLA 3 315



Bond lengths



Bond angles

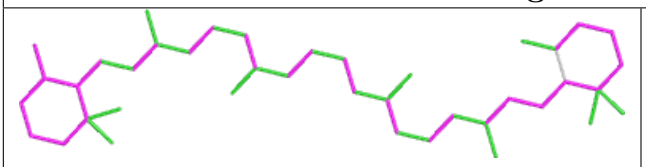


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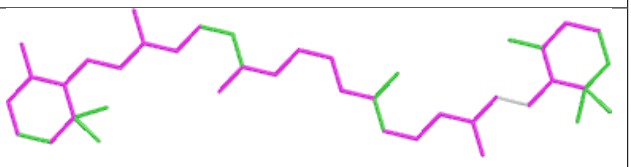


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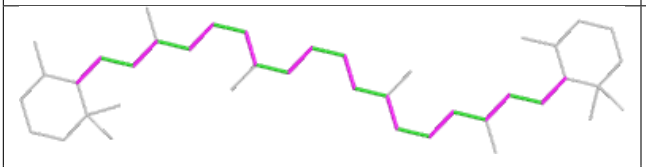
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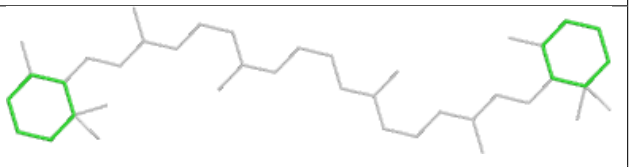
Bond lengths



Bond angles

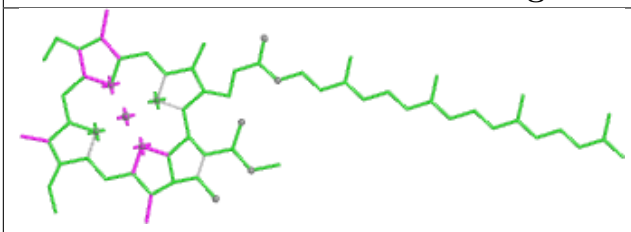


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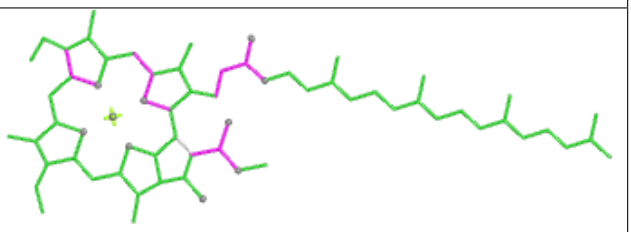


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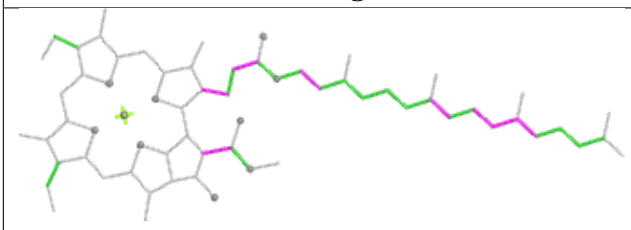
Ligand CLA d 404



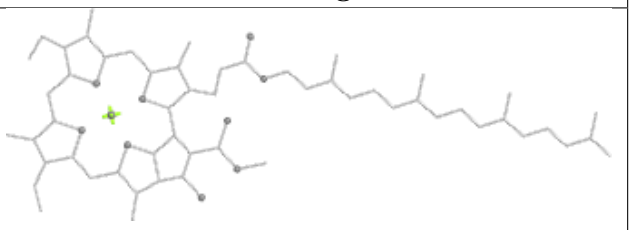
Bond lengths



Bond angles



Torsions



Rings

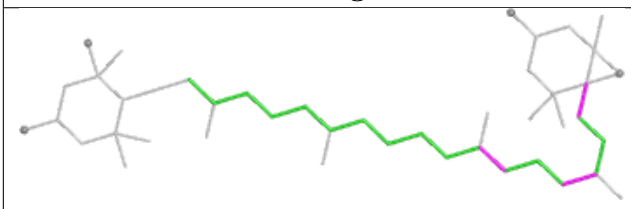
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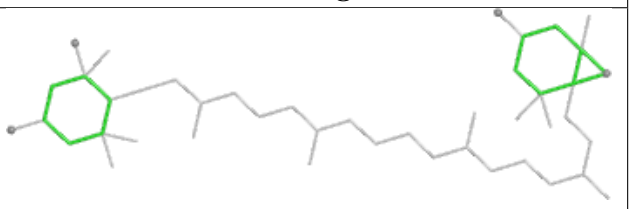
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Bond angles

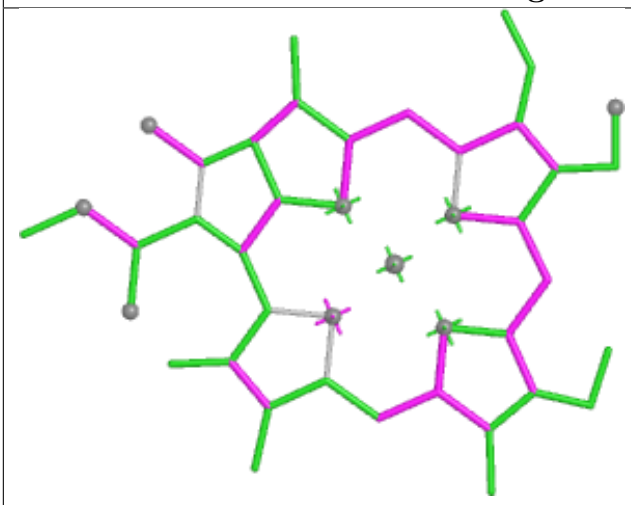


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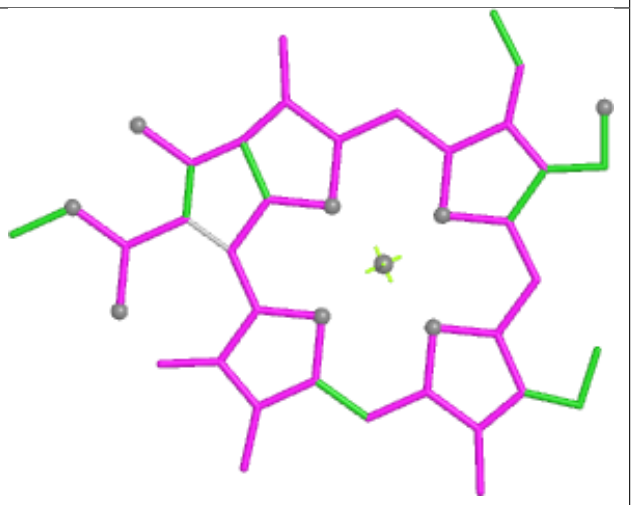


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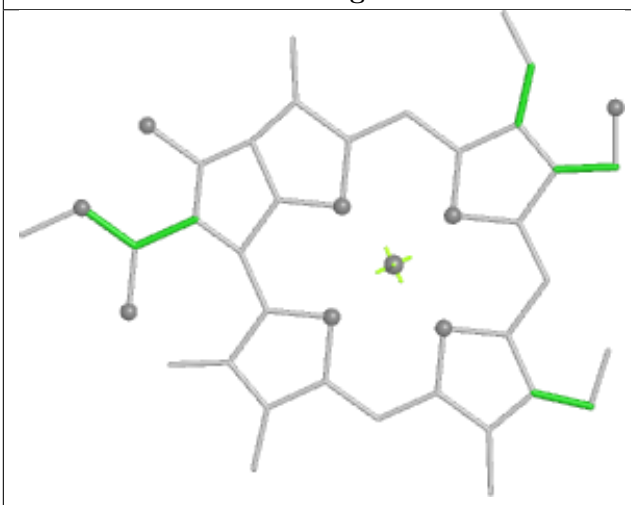
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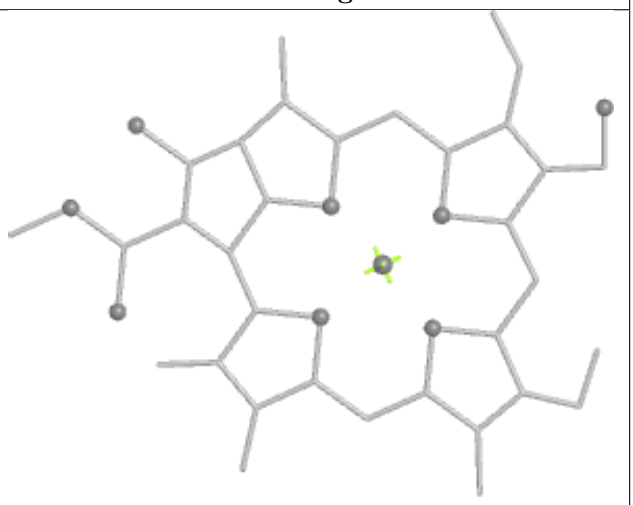
Bond lengths



Bond angles

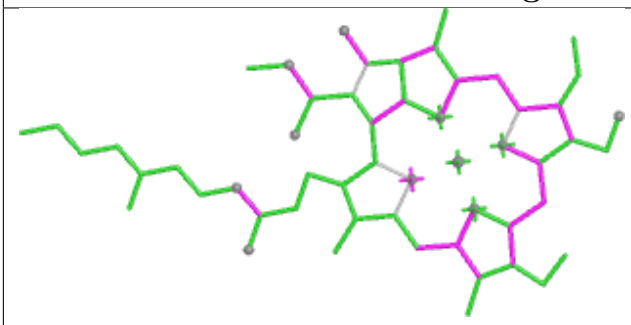


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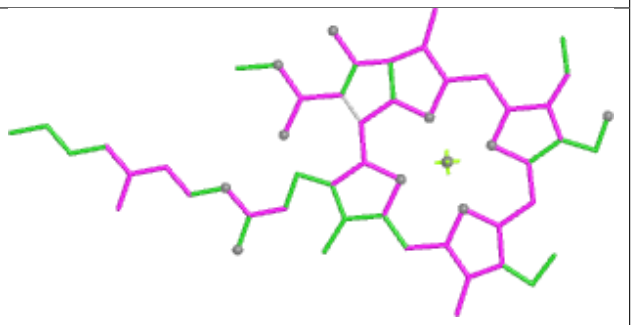


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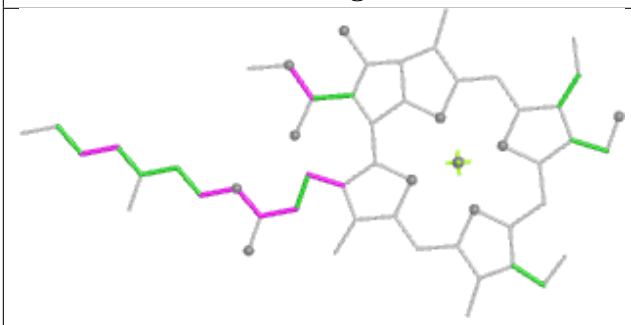
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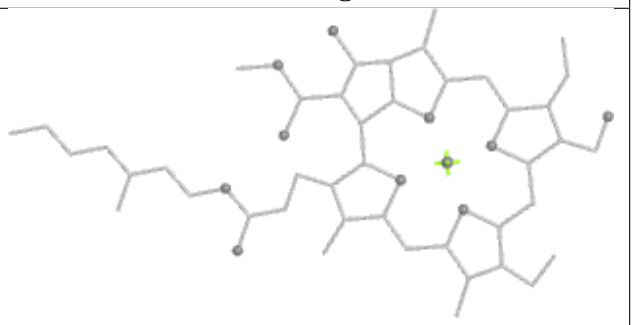
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Bond angles

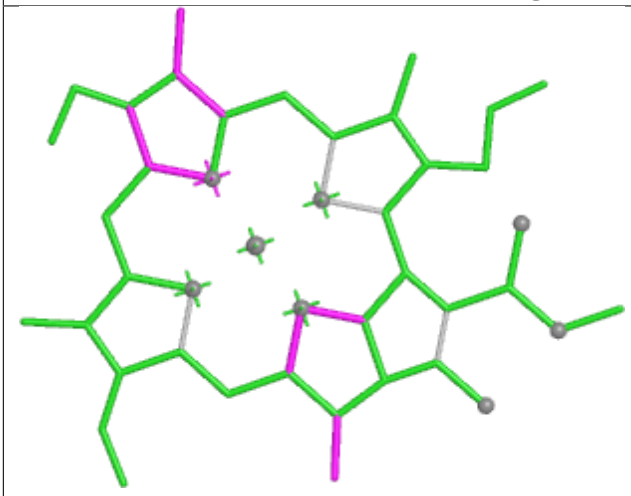


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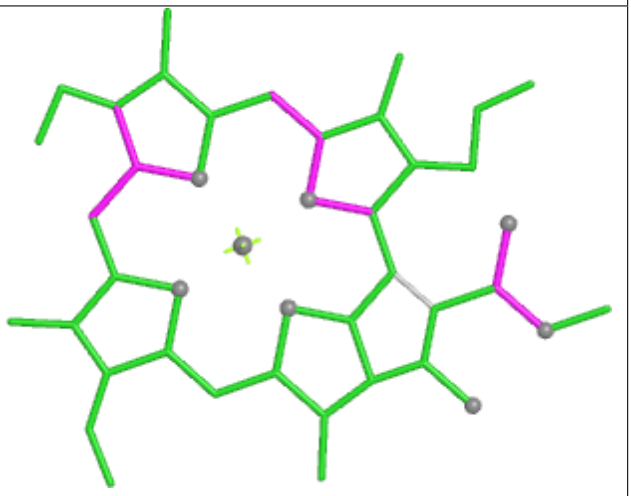


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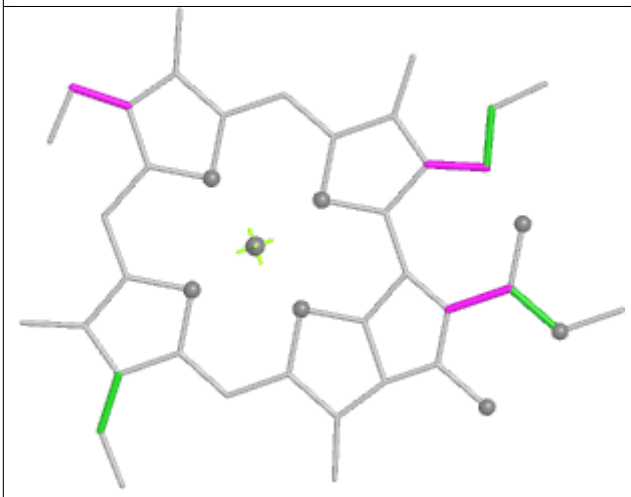
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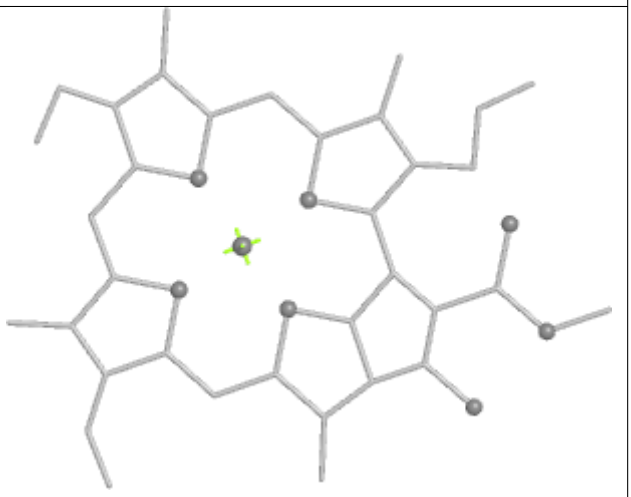
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Bond angles

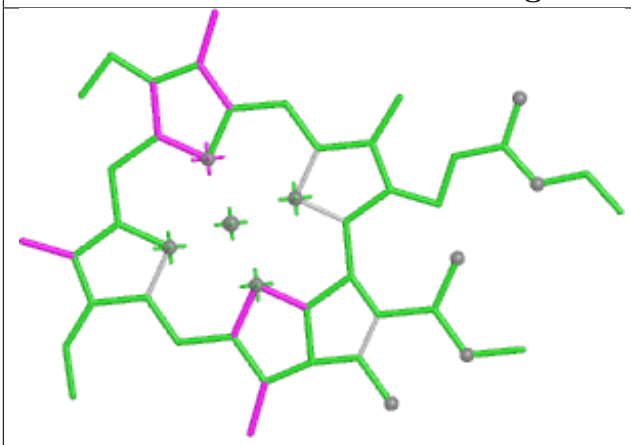


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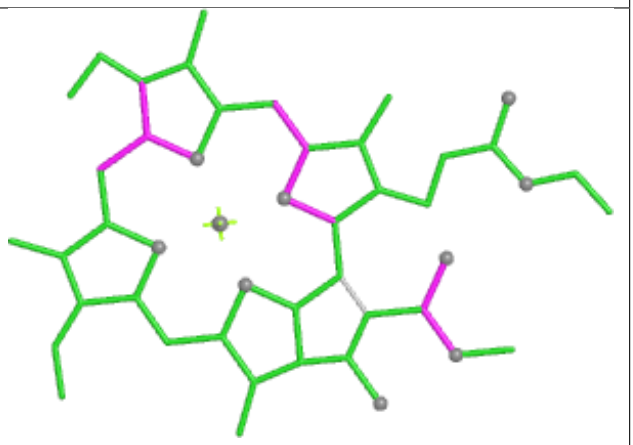


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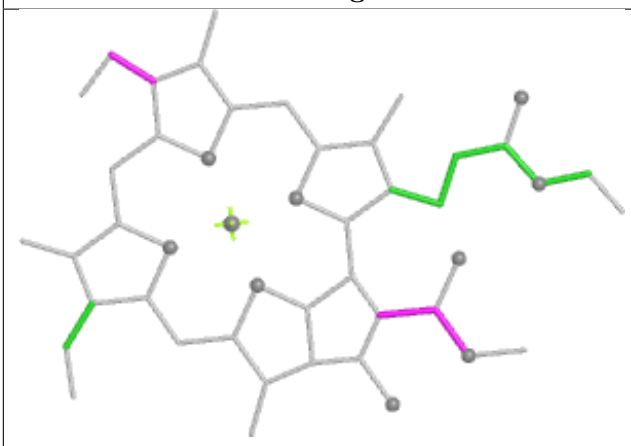
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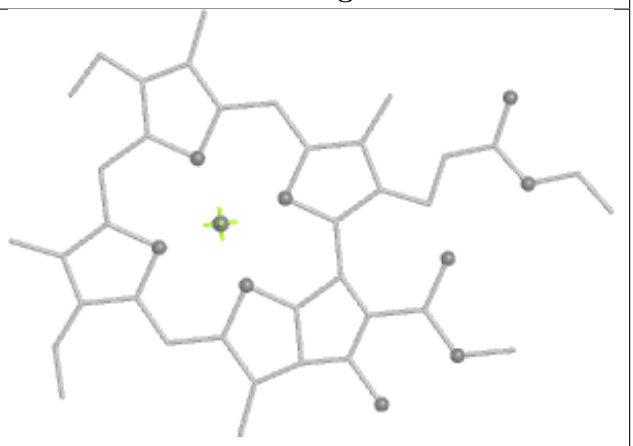
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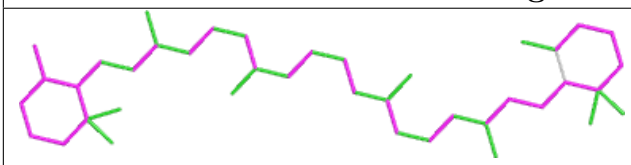


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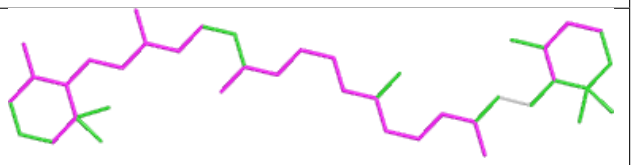


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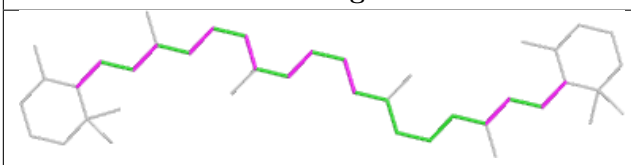
Ligand 8CT T 101



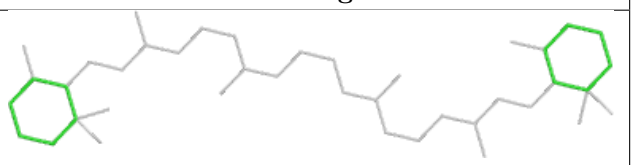
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Bond angles

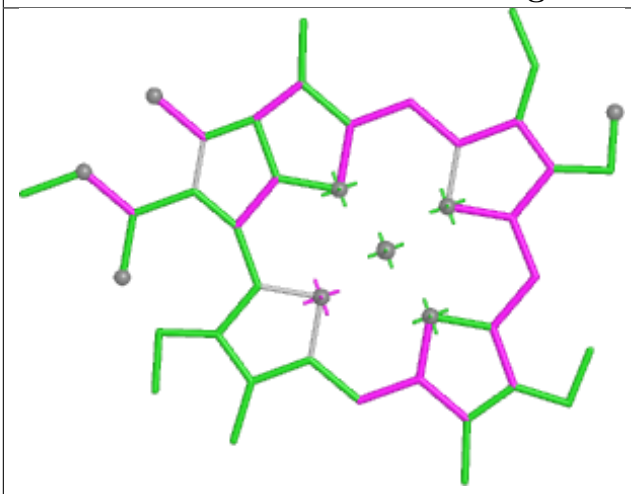


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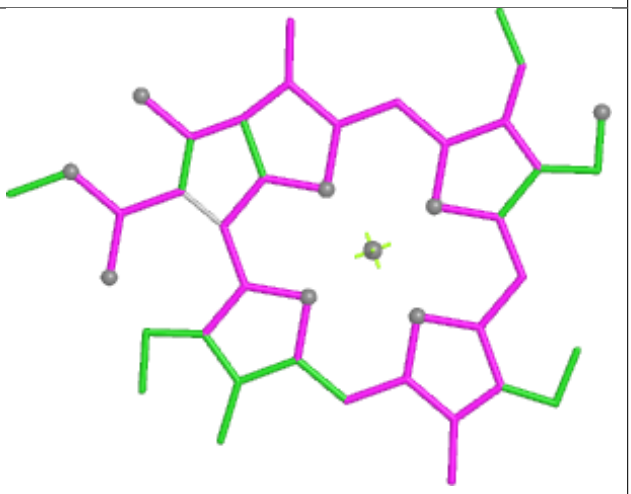


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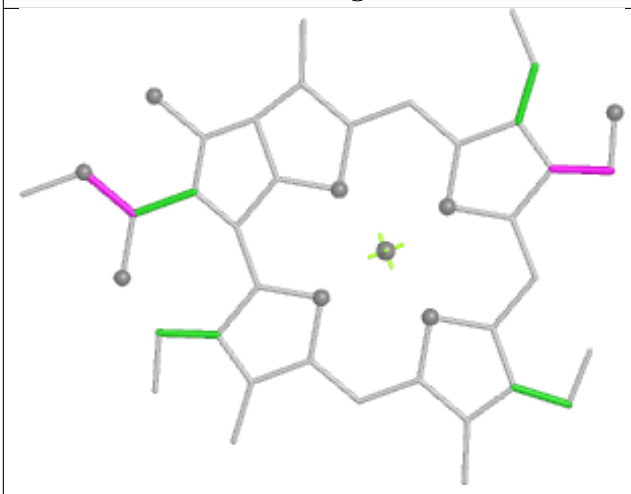
Ligand CHL 1 309



Bond lengths



Bond angles

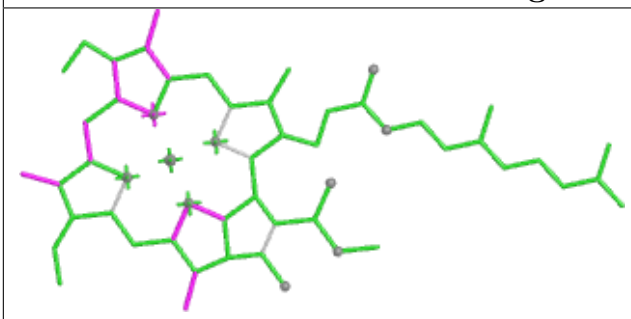


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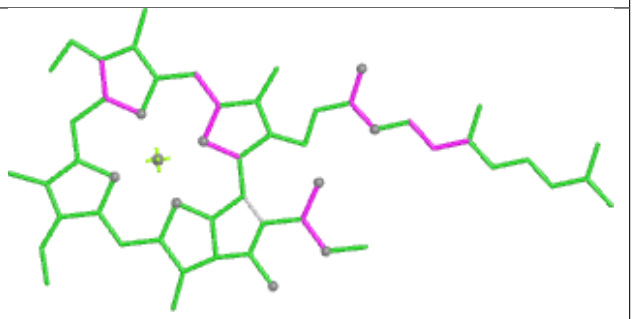


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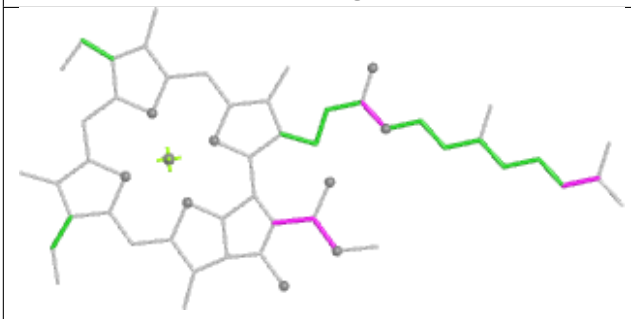
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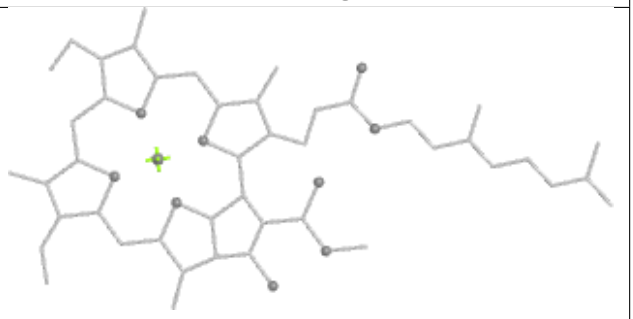
Bond lengths



Bond angles

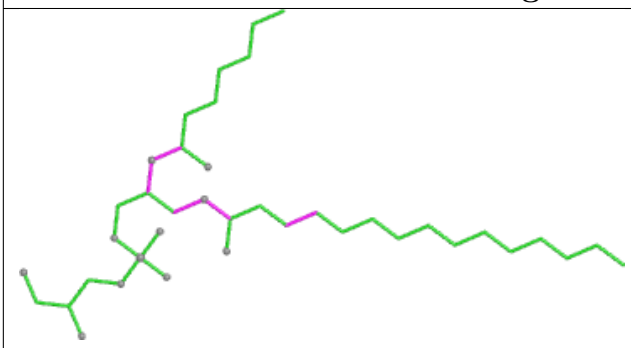


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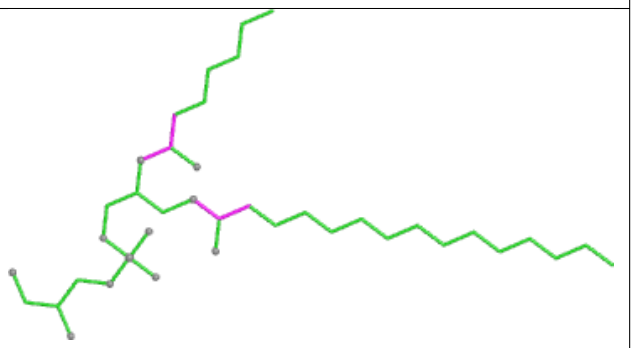


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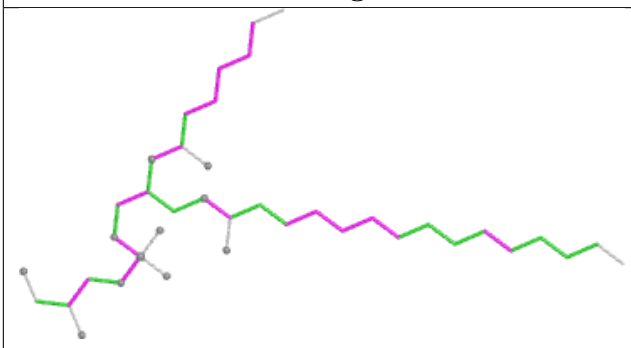
Ligand LHG D 408



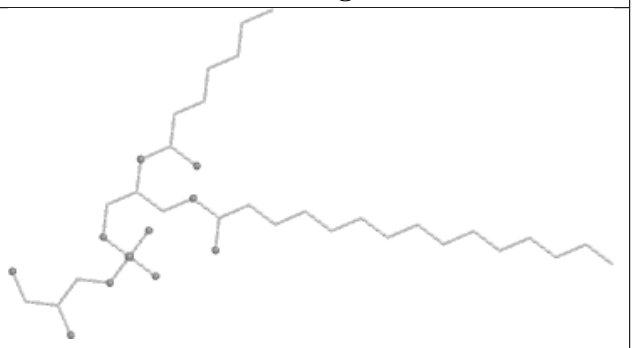
Bond lengths



Bond angles

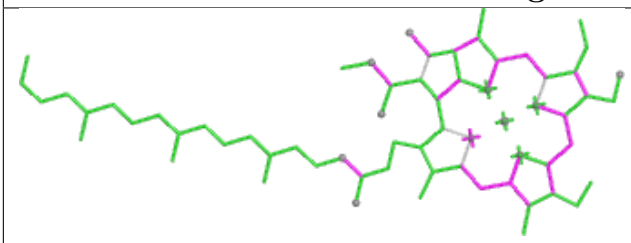


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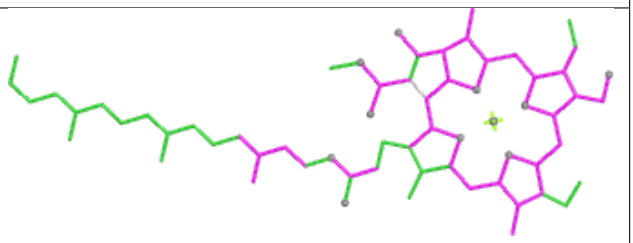


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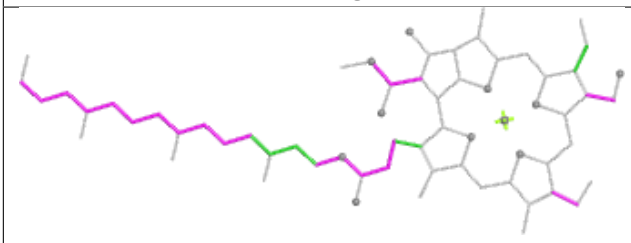
Ligand CHL 7 306



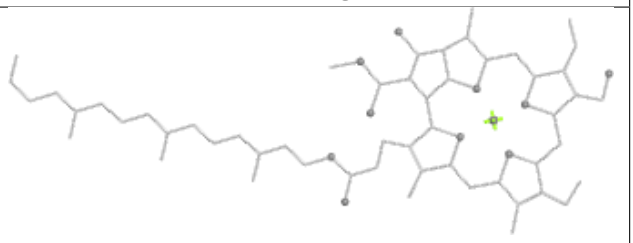
Bond lengths



Bond angles

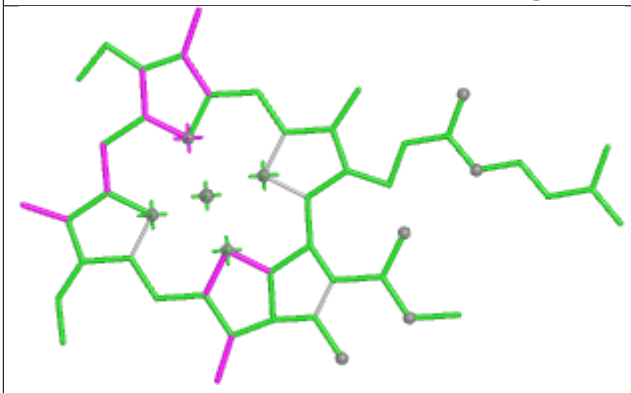


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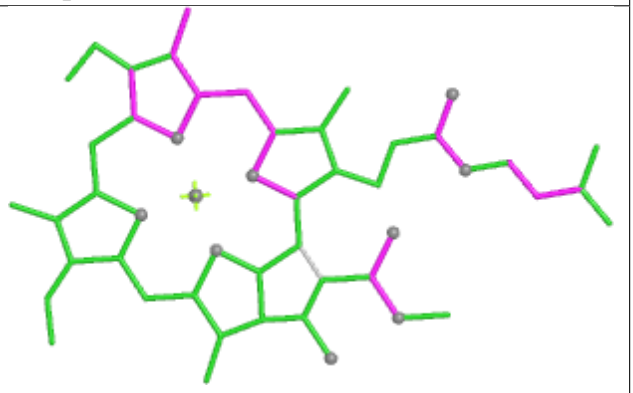


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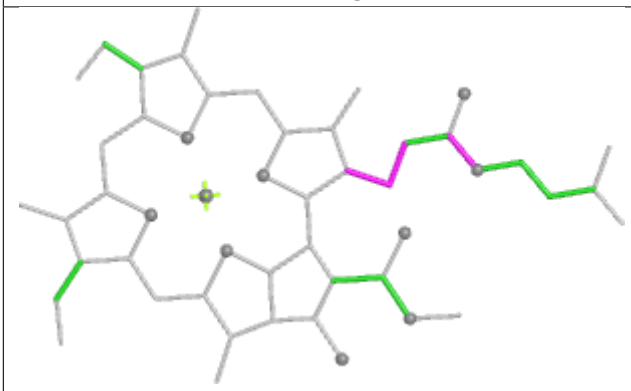
Ligand CLA q 306



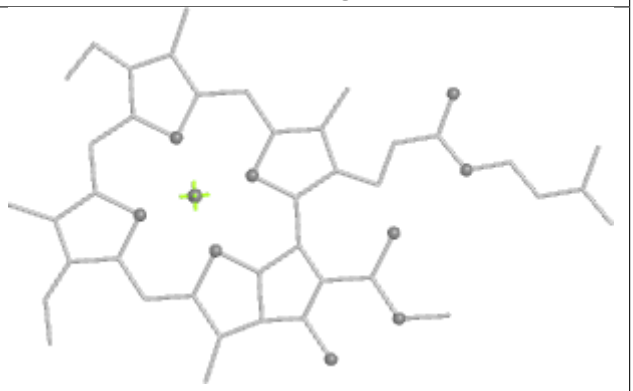
Bond lengths



Bond angles

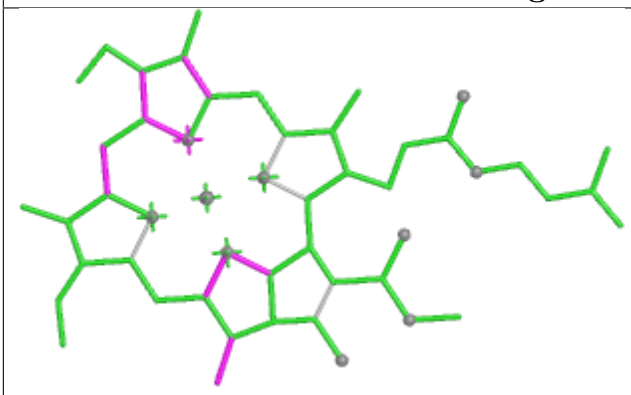


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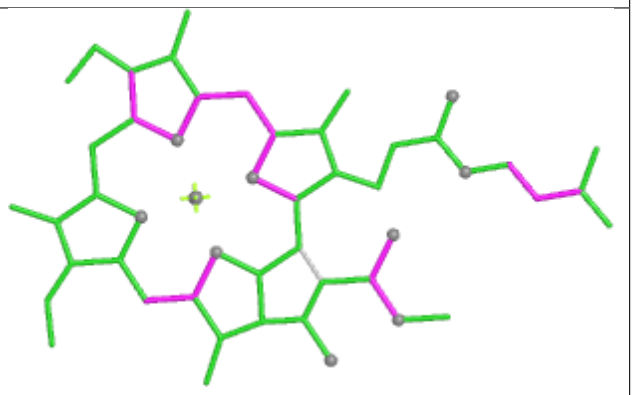


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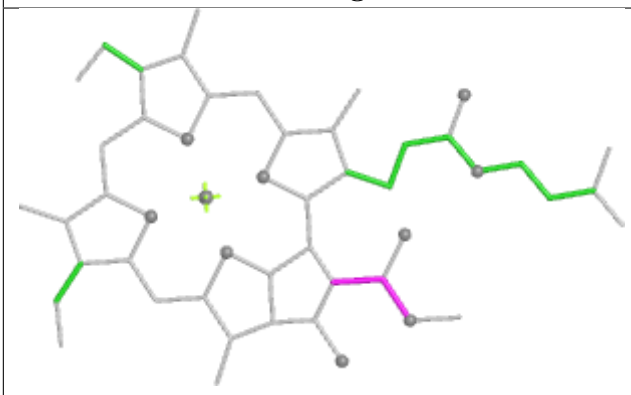
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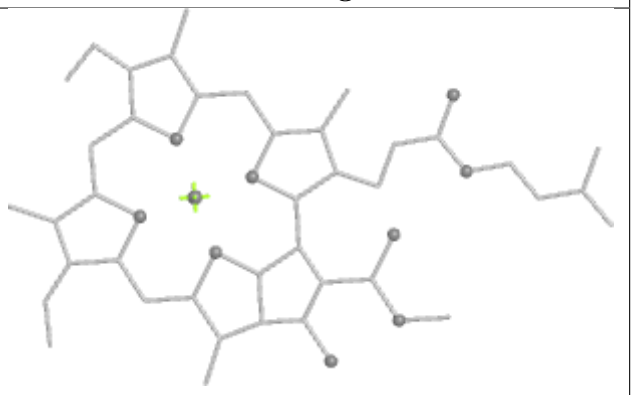
Bond lengths



Bond angles

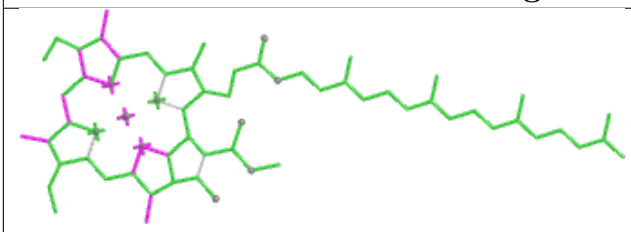


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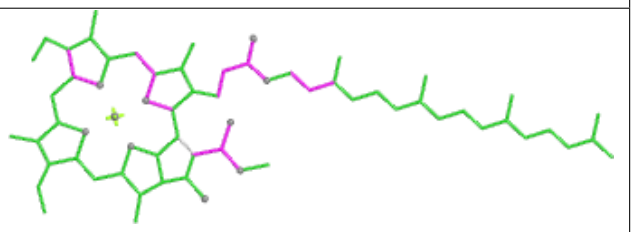


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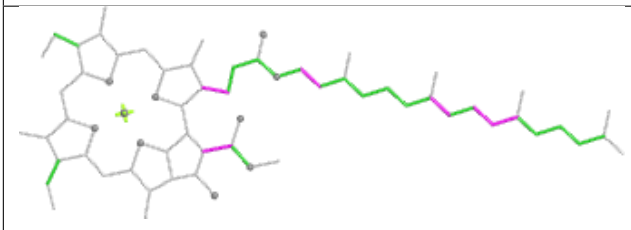
Ligand CLA D 404



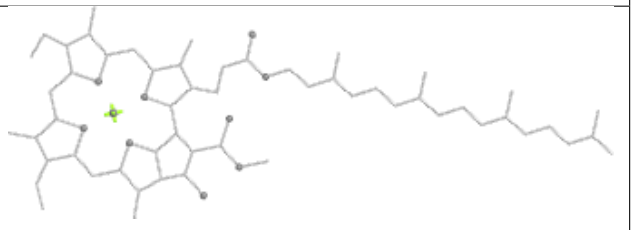
Bond lengths



Bond angles

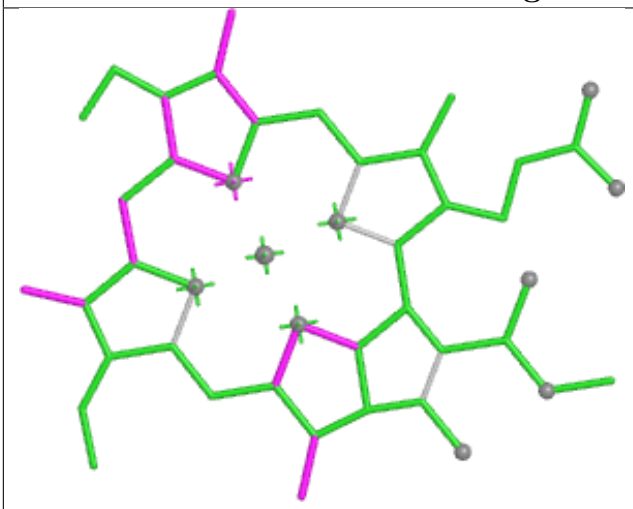


Torsions

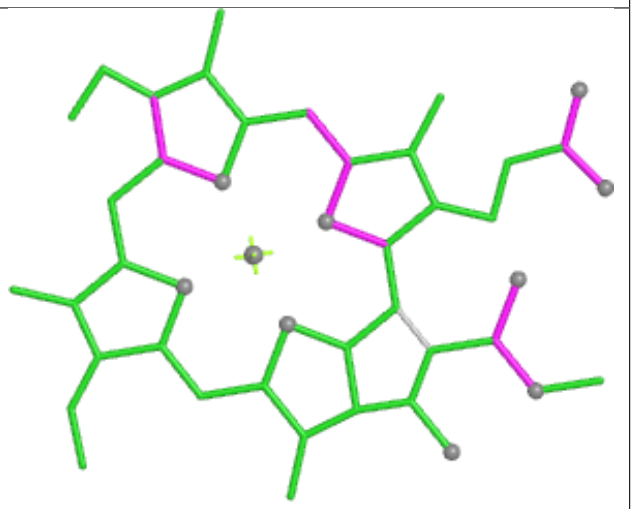


Rings

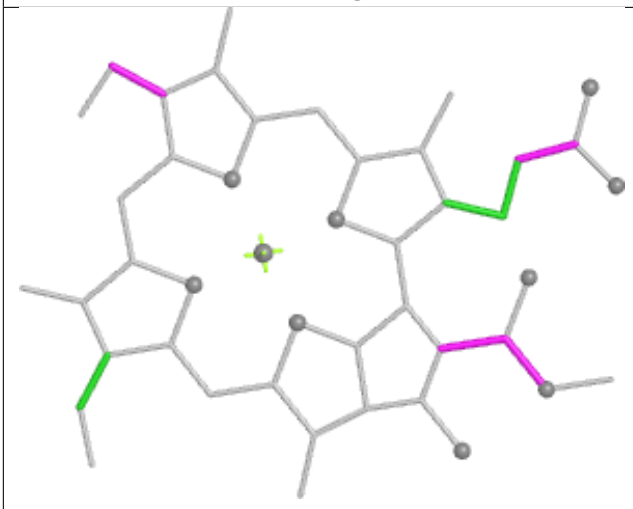
Ligand CLA N 315



Bond lengths



Bond angles

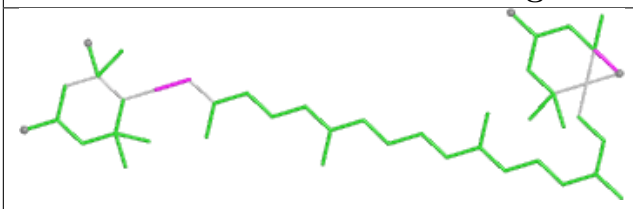


Torsions

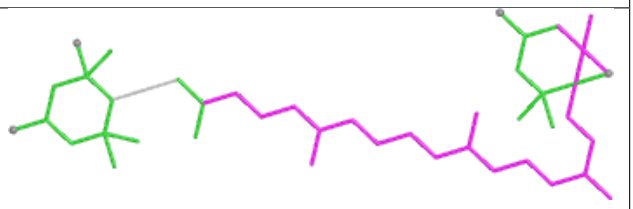


Rings

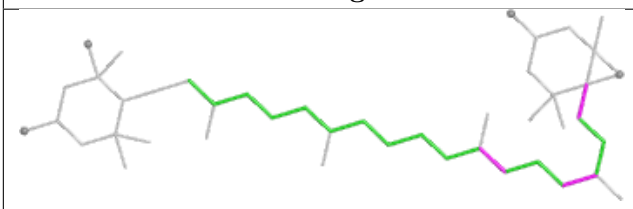
Ligand NEX 2 304



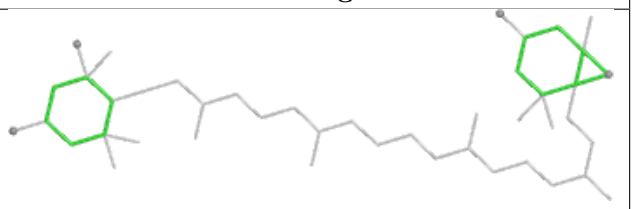
Bond lengths



Bond angles

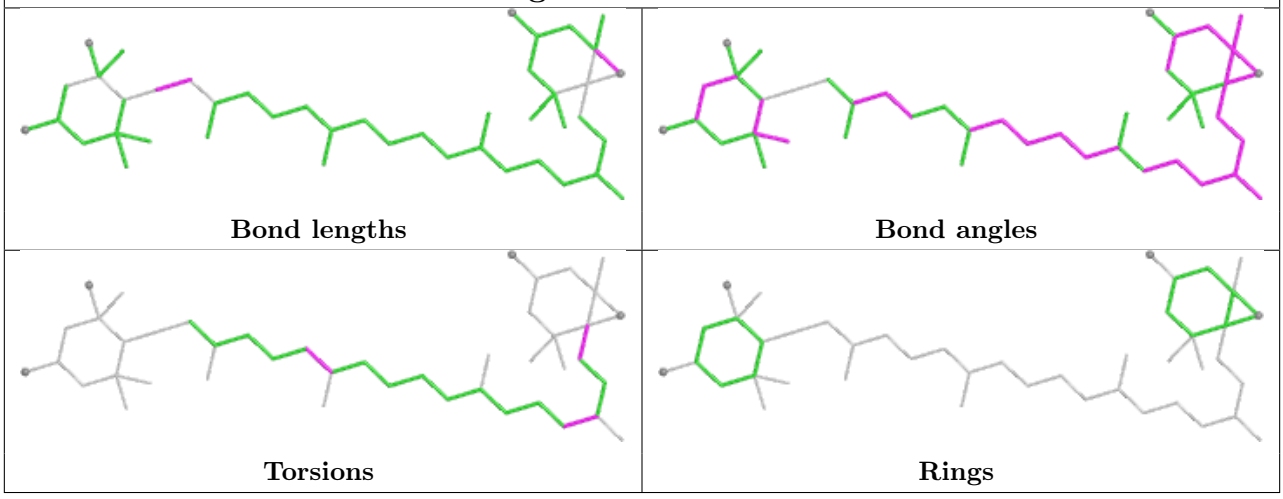


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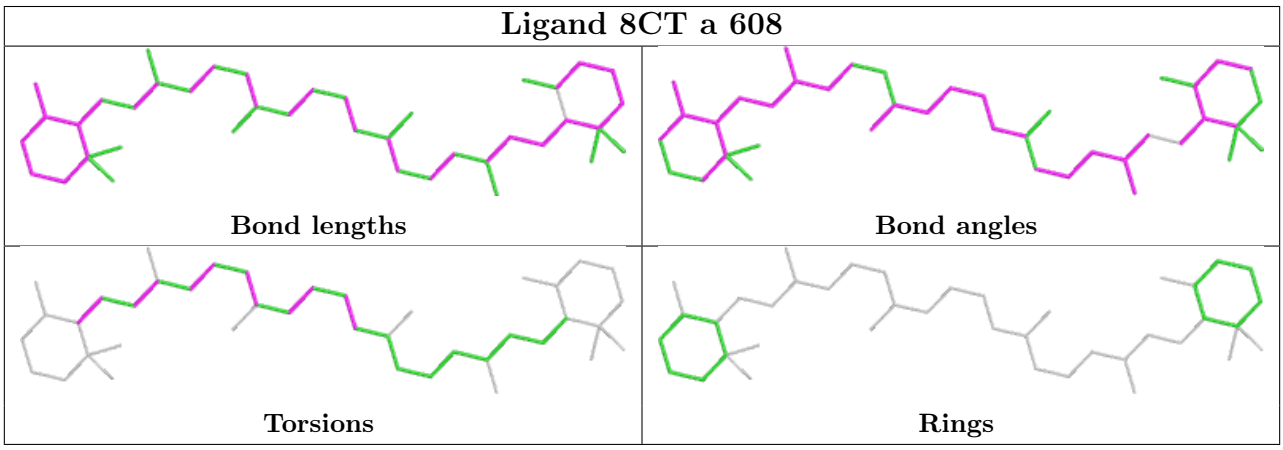


Rings

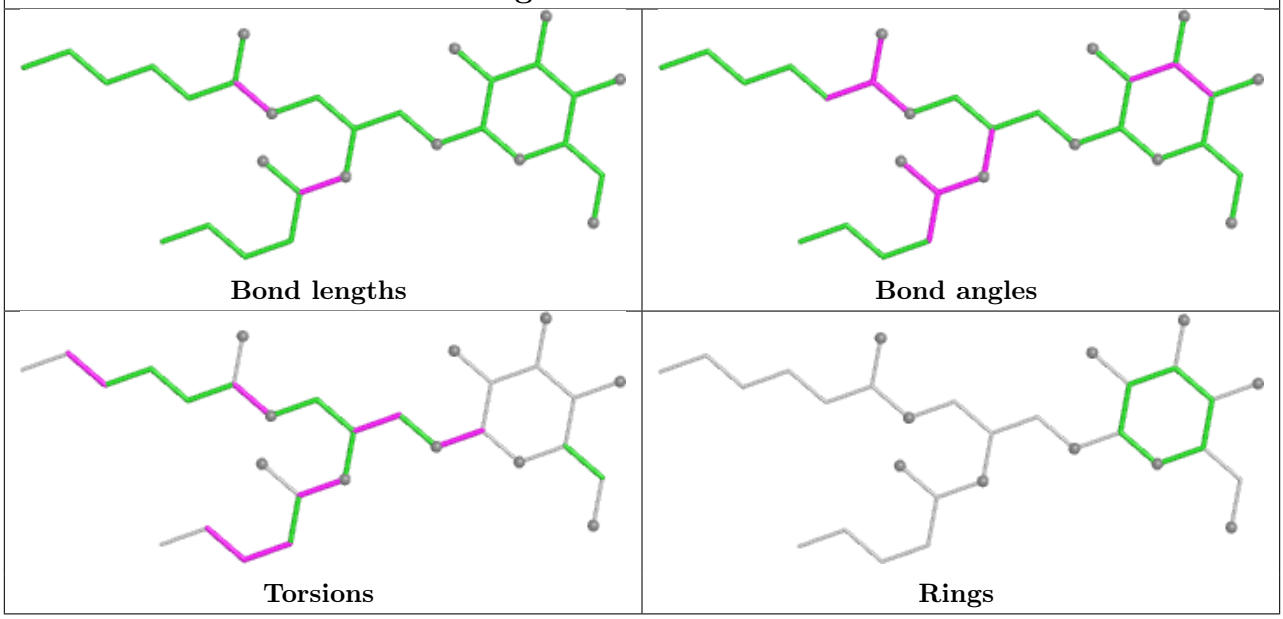
Ligand NEX r 301



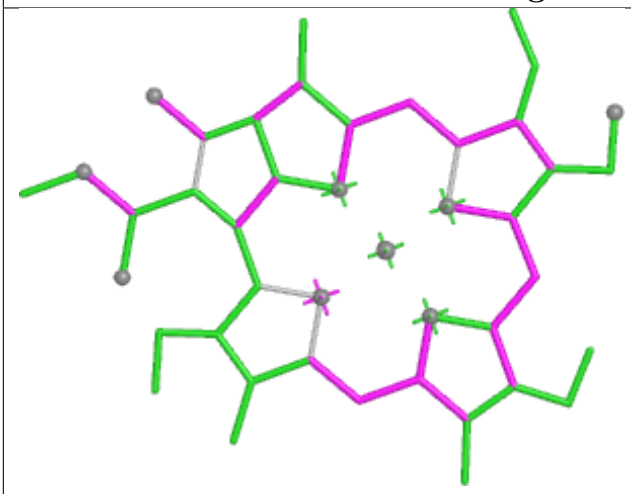
Ligand 8CT a 608



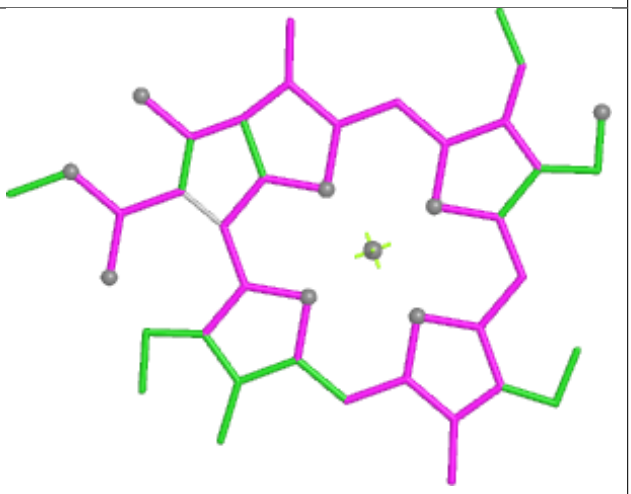
Ligand LMG W 201



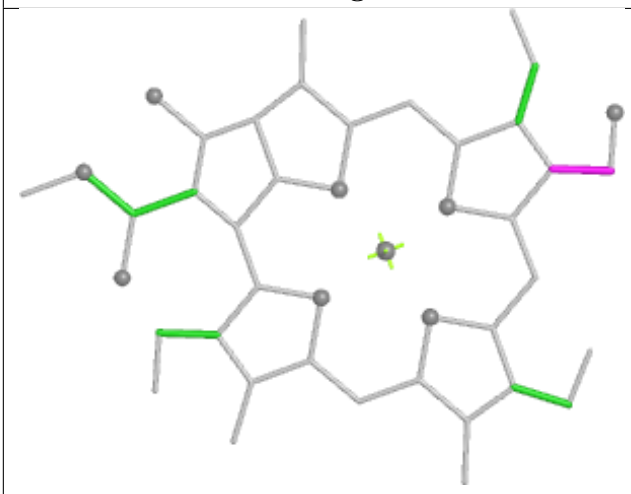
Ligand CHL 8 307



Bond lengths



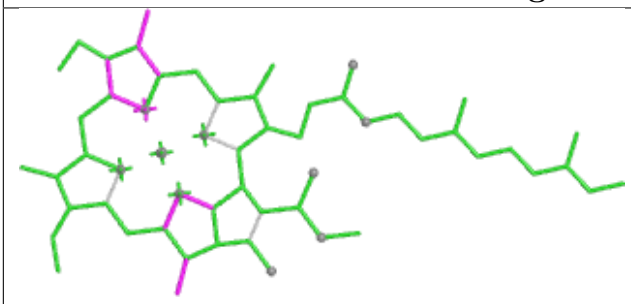
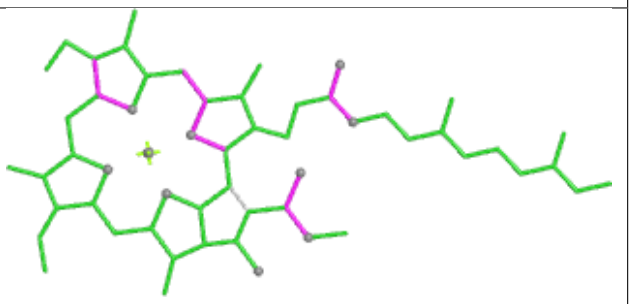
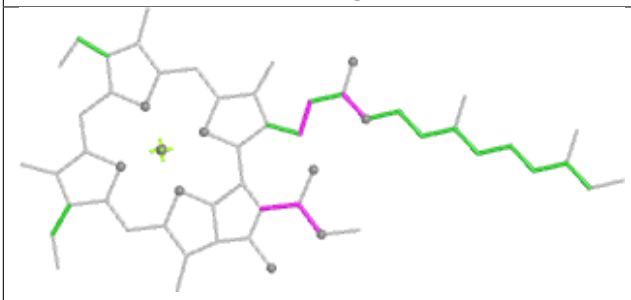
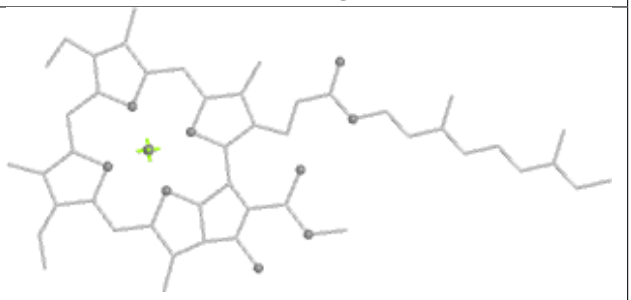
Bond angles

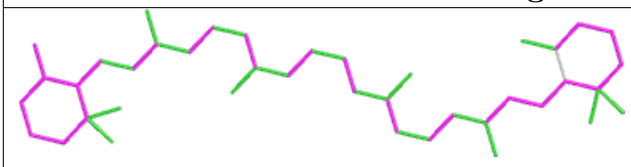
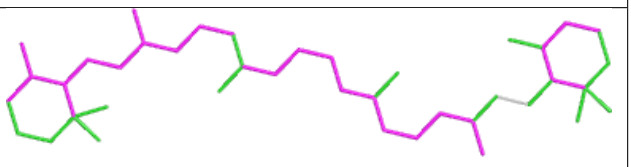
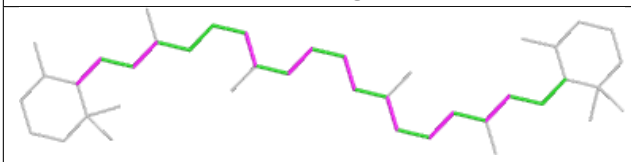
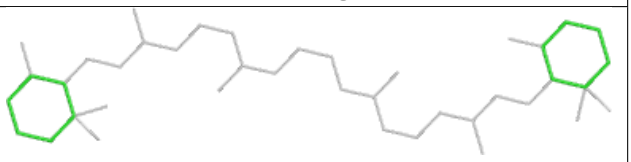


Torsions

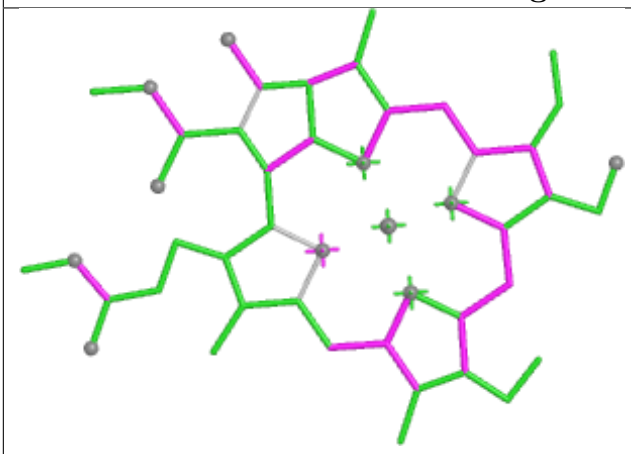


Rings

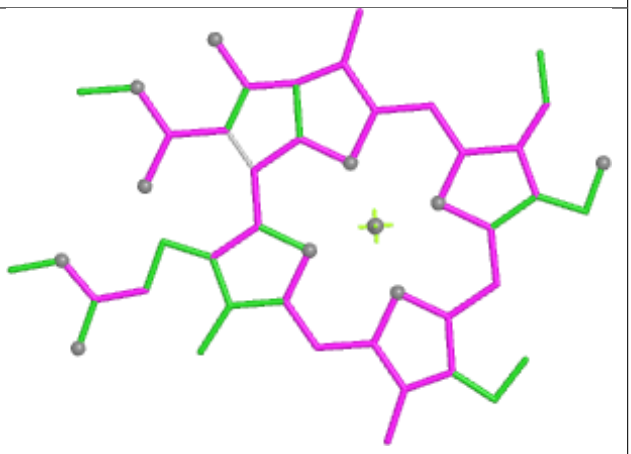
Ligand CLA 7 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT C 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

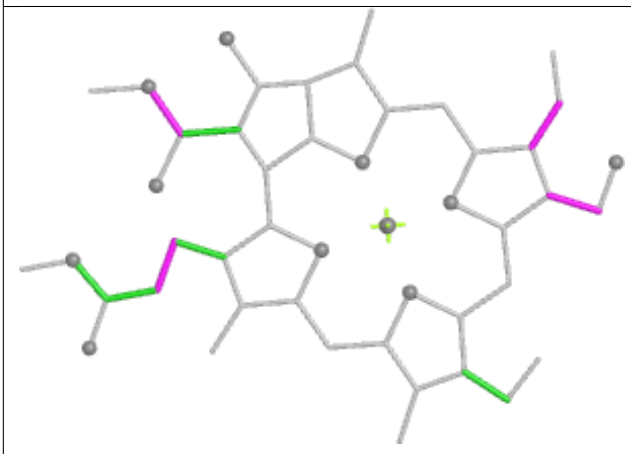
Ligand CHL s 409



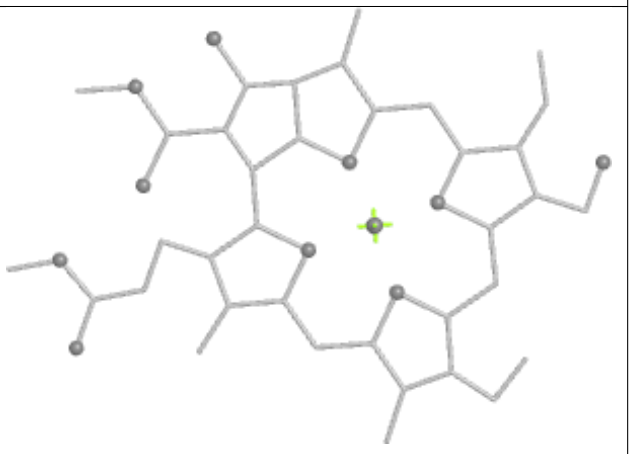
Bond lengths



Bond angles

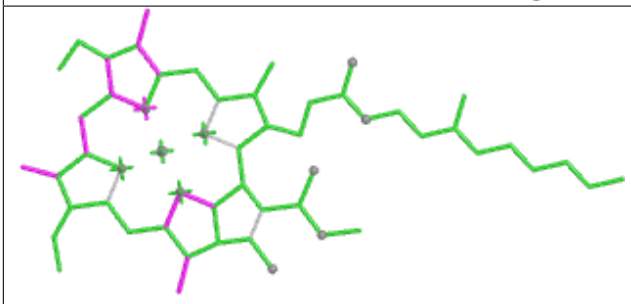


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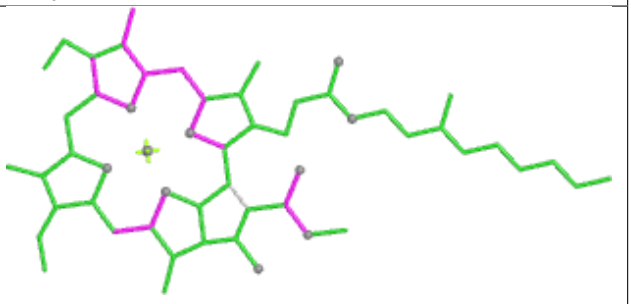


Rings

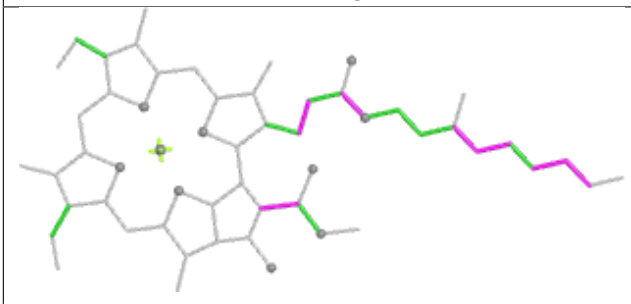
Ligand CLA y 317



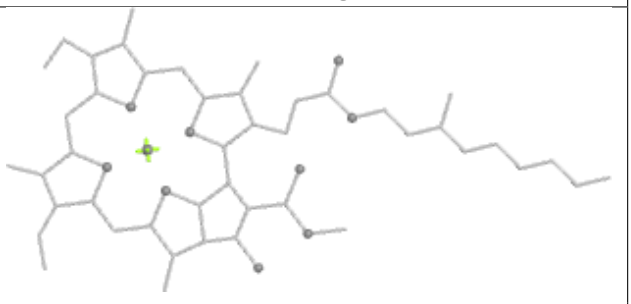
Bond lengths



Bond angles

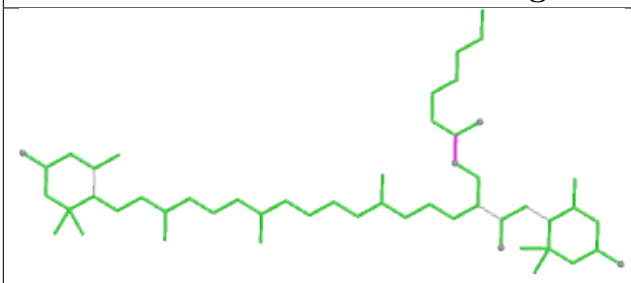


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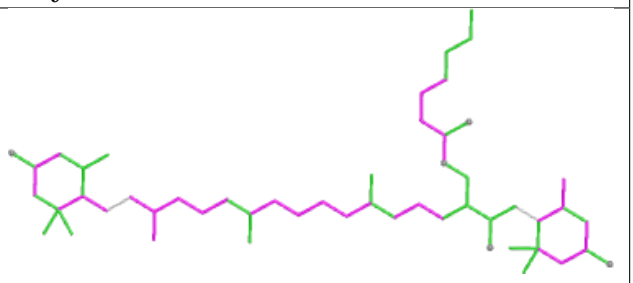


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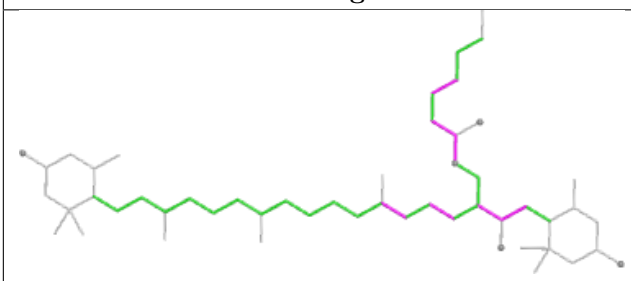
Ligand 0UR y 301



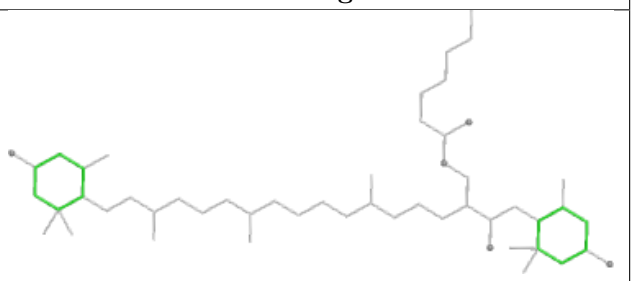
Bond lengths



Bond angles

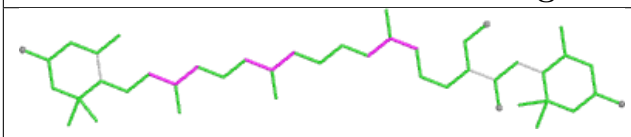


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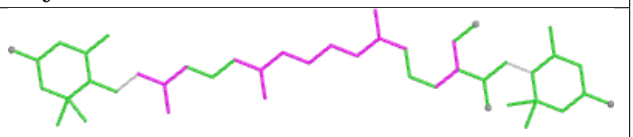


Rings

Ligand 0IE y 303



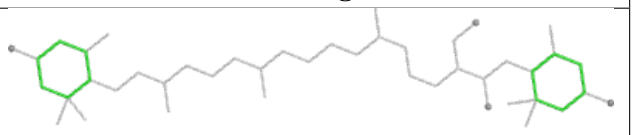
Bond lengths



Bond angles

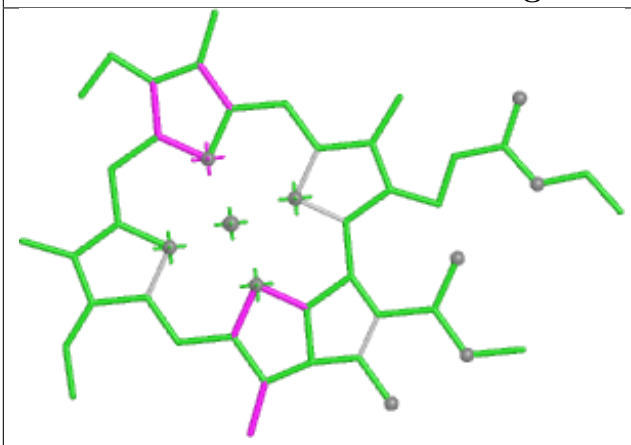


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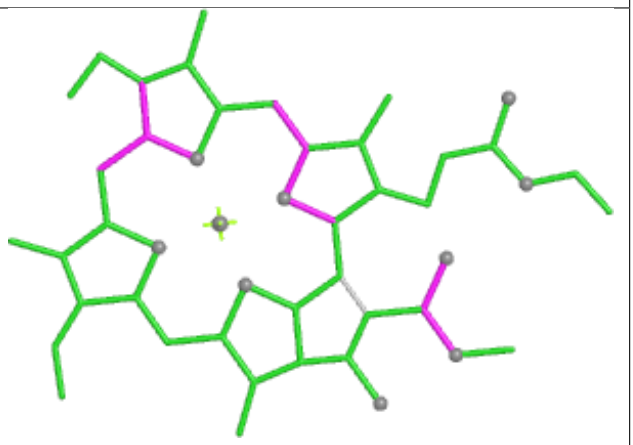


Rings

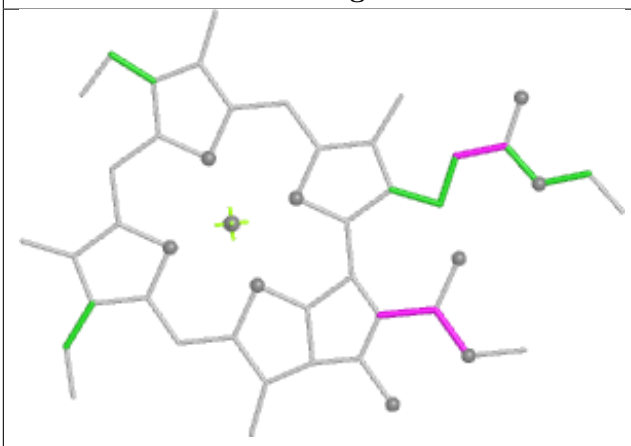
Ligand CLA R 603



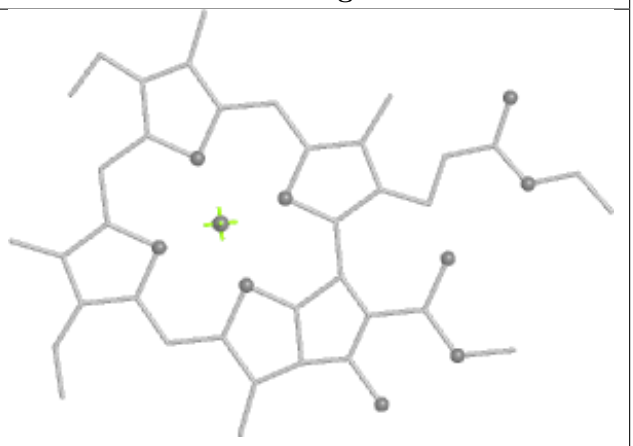
Bond lengths



Bond angles

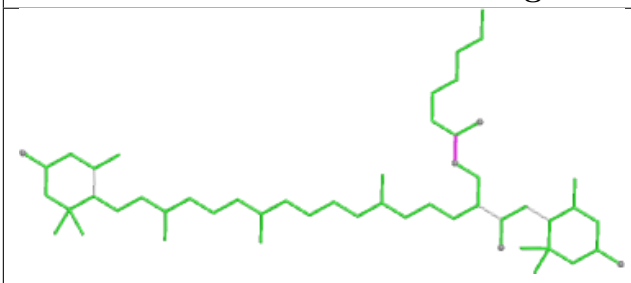


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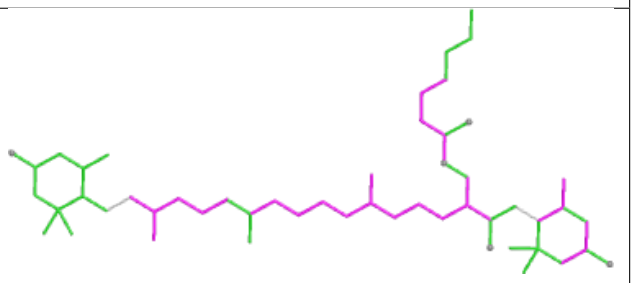


Rings

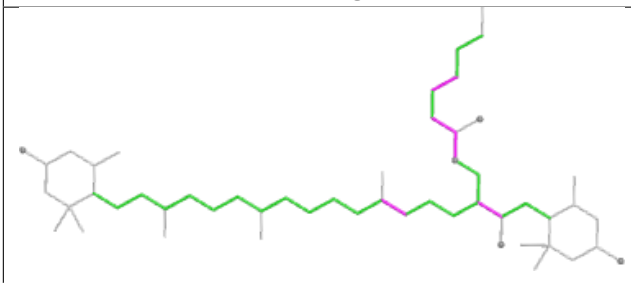
Ligand 0UR G 301



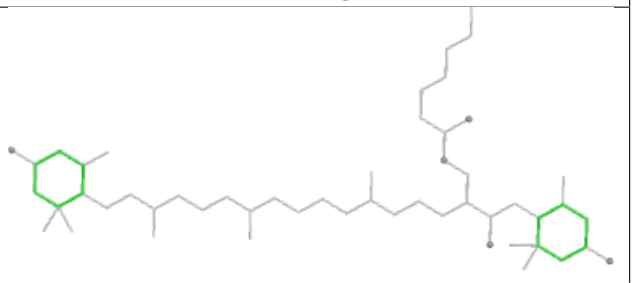
Bond lengths



Bond angles

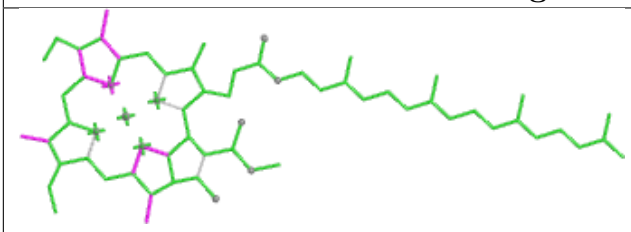


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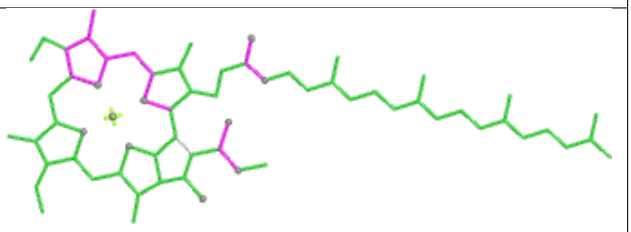


Rings

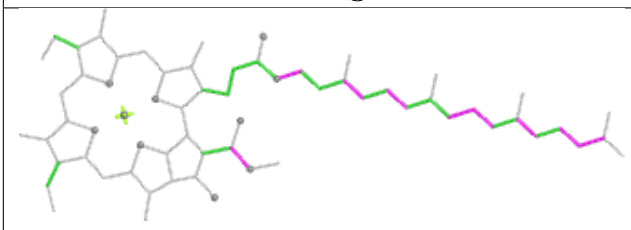
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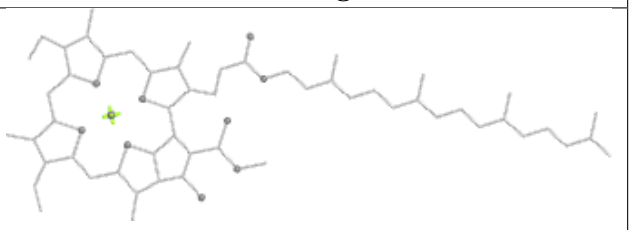
Bond lengths



Bond angles

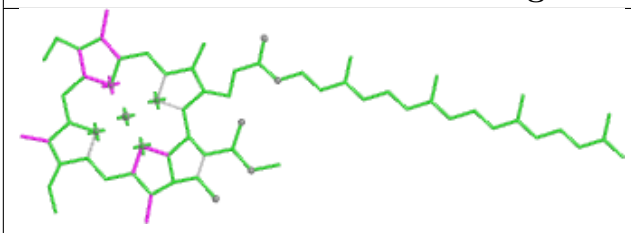


Torsions

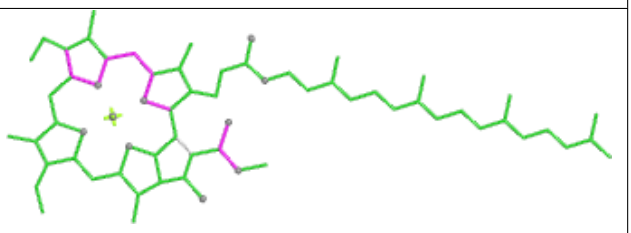


Rings

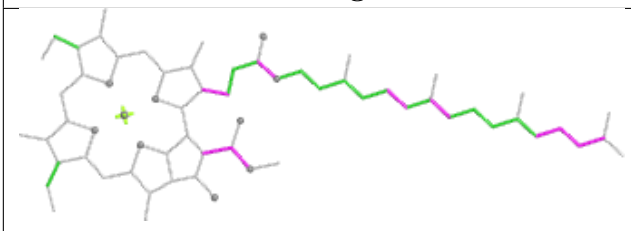
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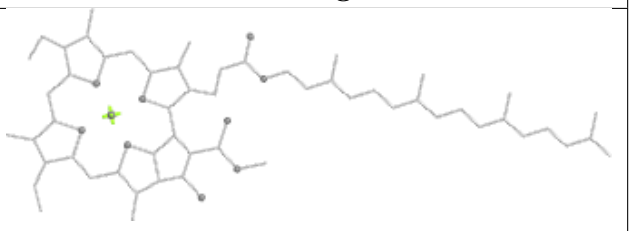
Bond lengths



Bond angles

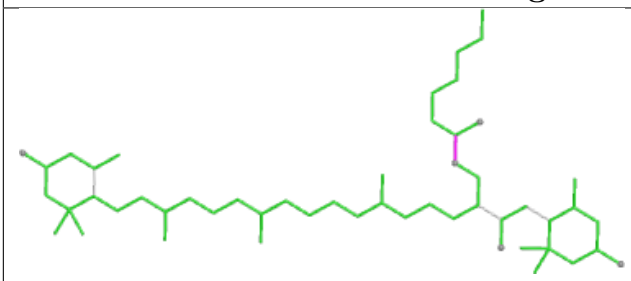


Torsions

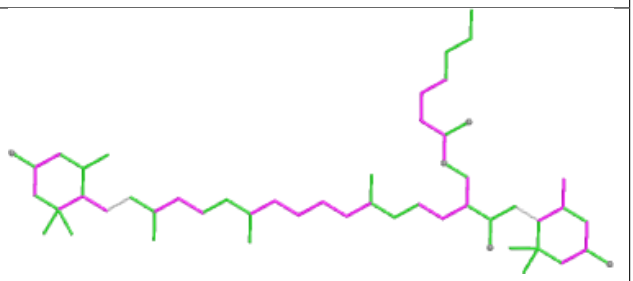


Rings

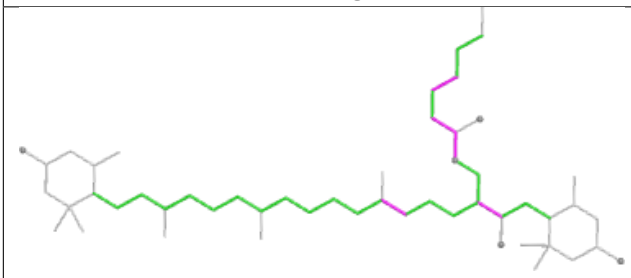
Ligand 0UR n 301



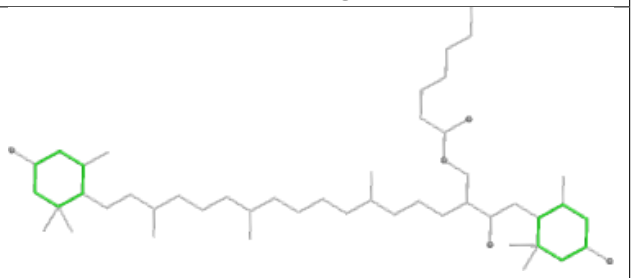
Bond lengths



Bond angles

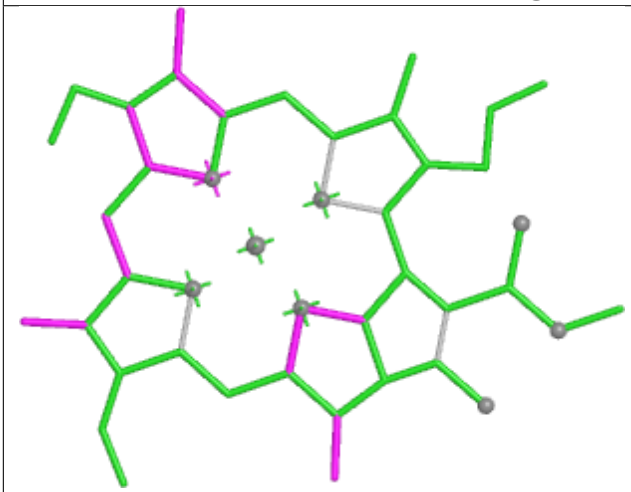


Torsions

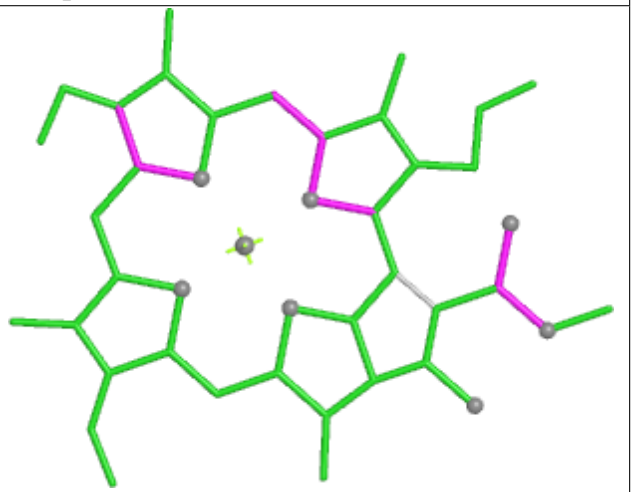


Rings

Ligand CLA q 315



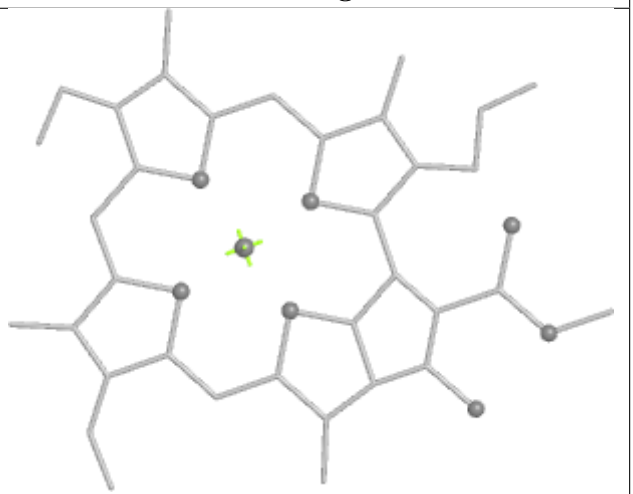
Bond lengths



Bond angles

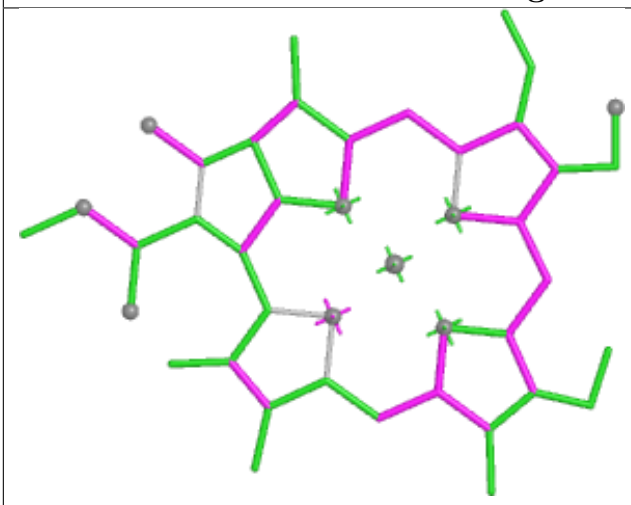


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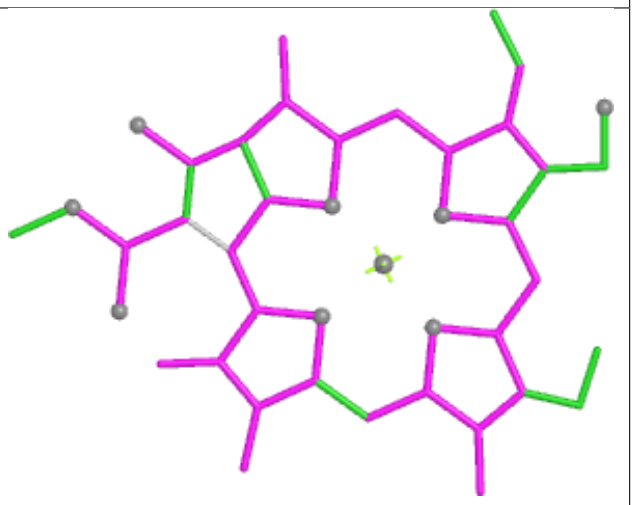


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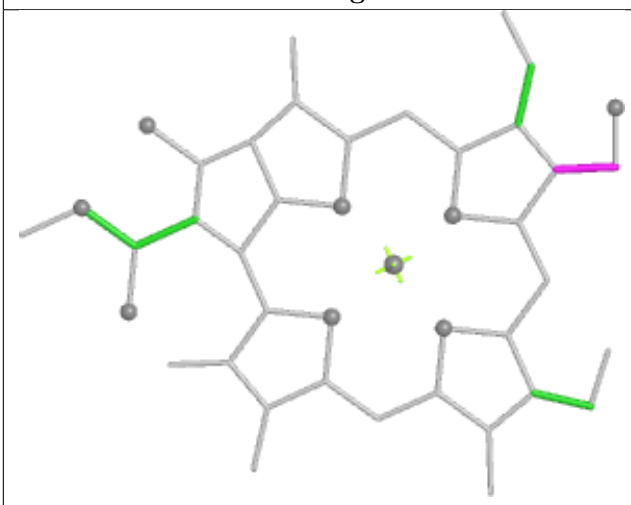
Ligand CHL 3 317



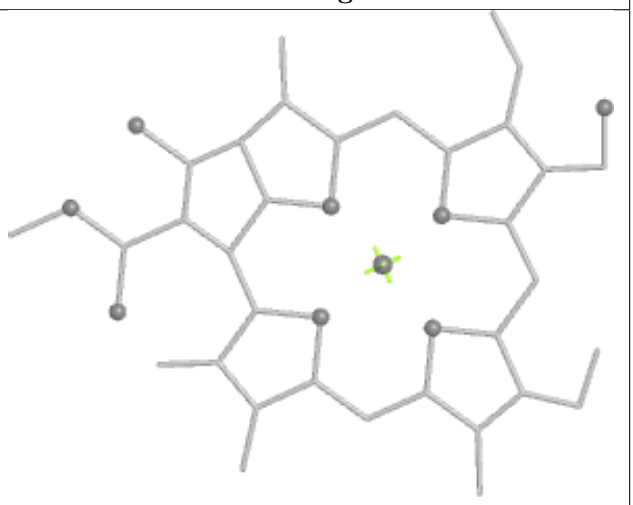
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Bond angles

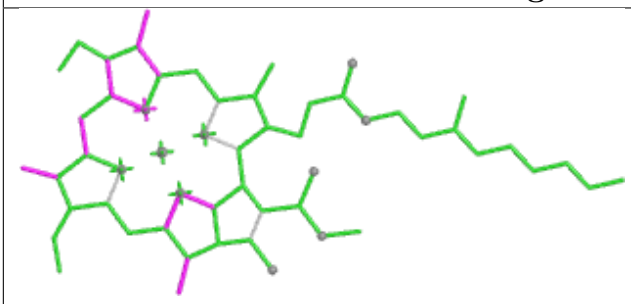


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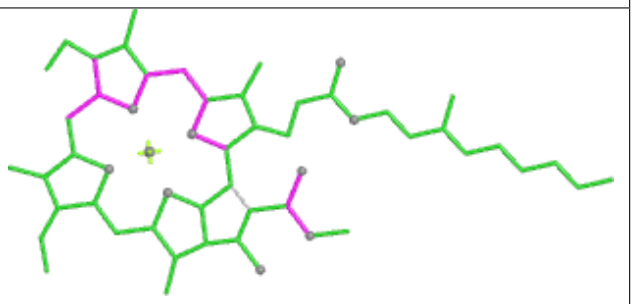


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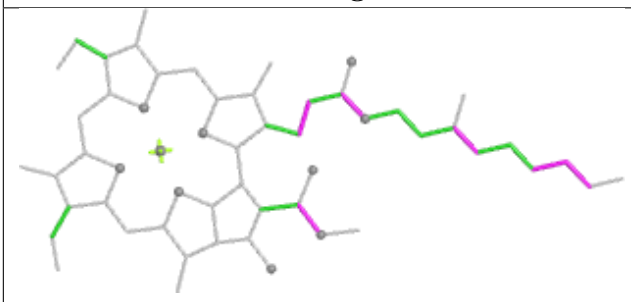
Ligand CLA S 612



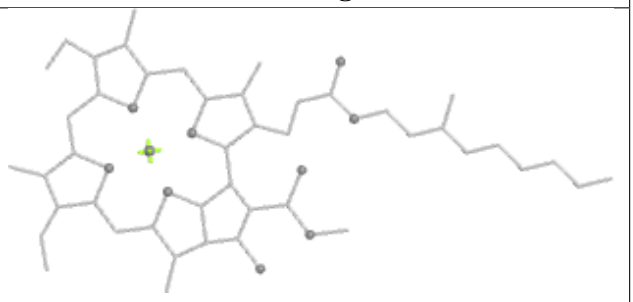
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Bond angles

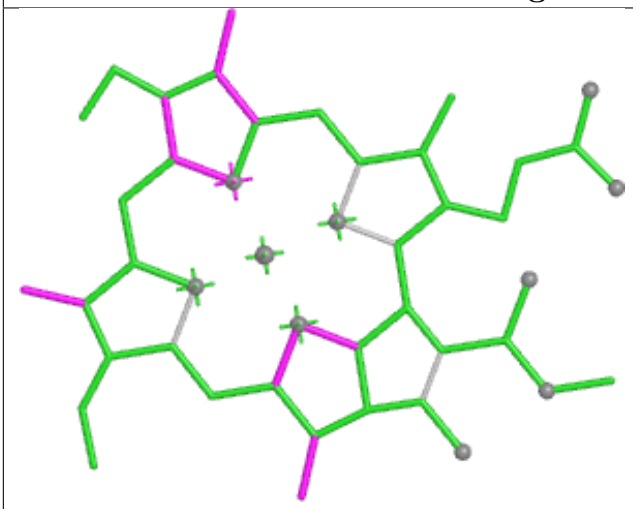


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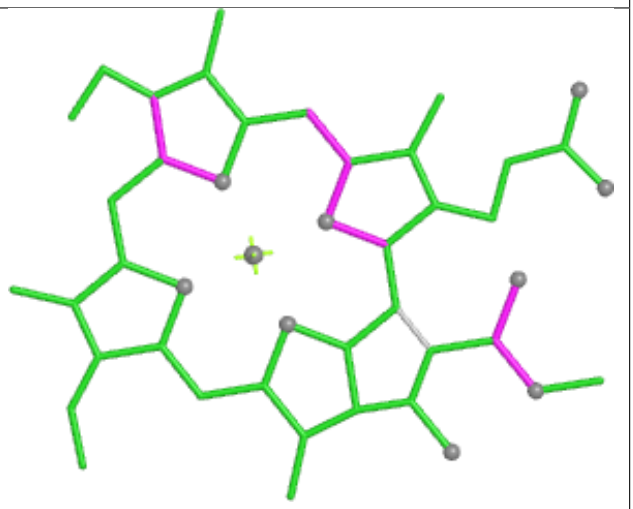


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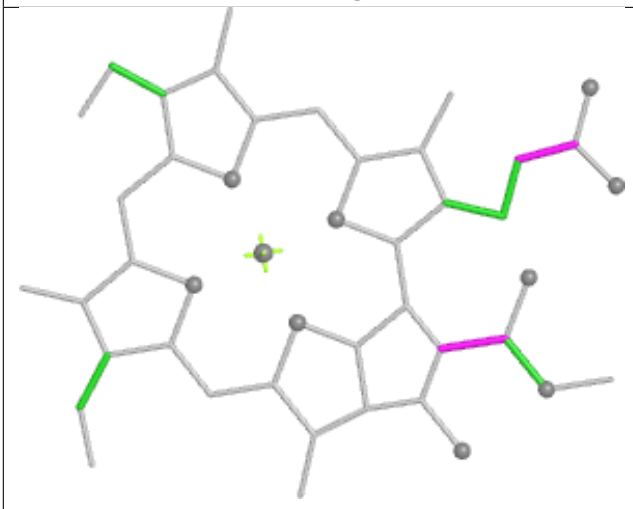
Ligand CLA 8 313



Bond lengths



Bond angles

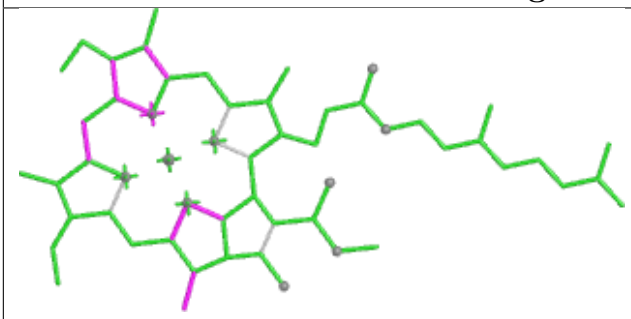


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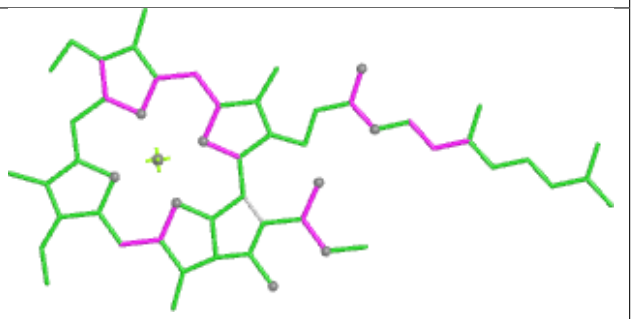


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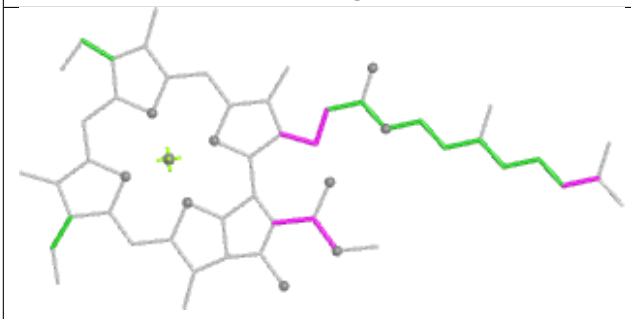
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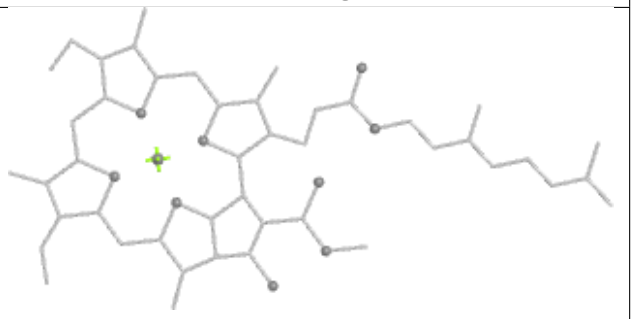
Bond lengths



Bond angles

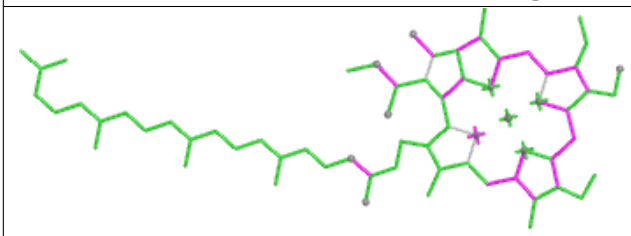


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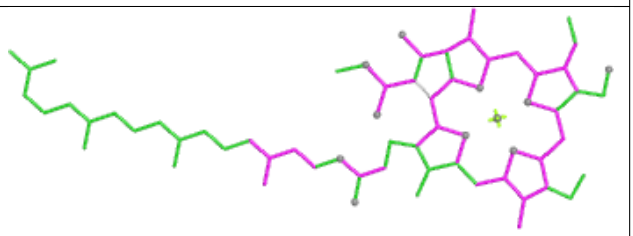


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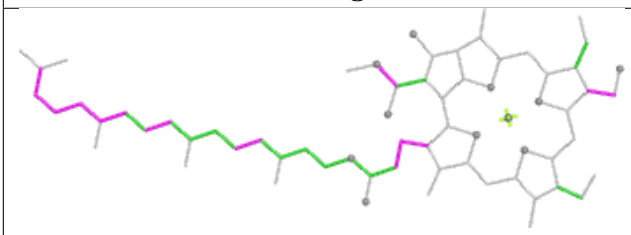
Ligand CHL u 305



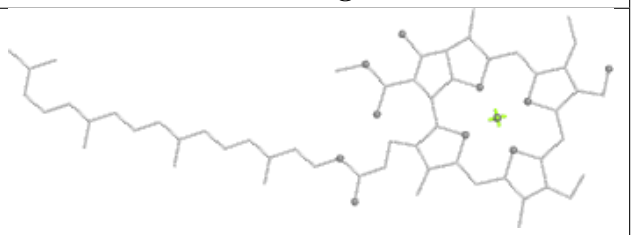
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Bond angles

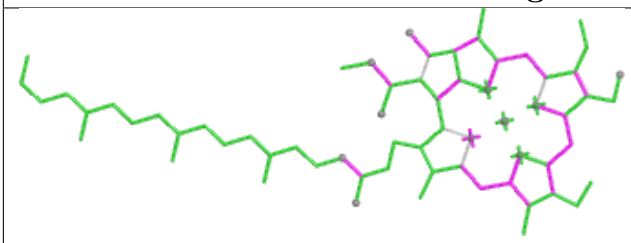


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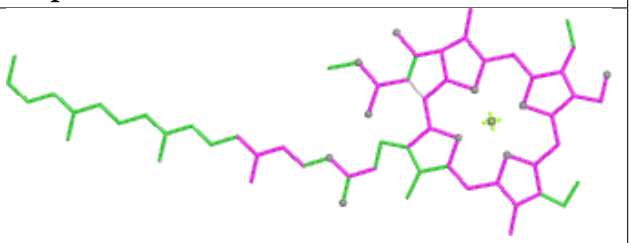


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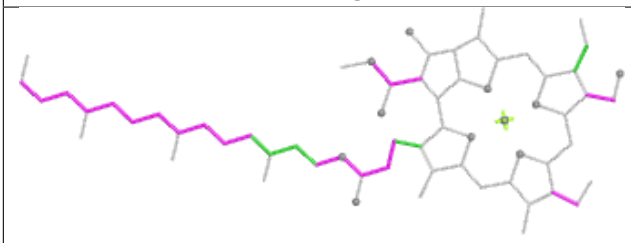
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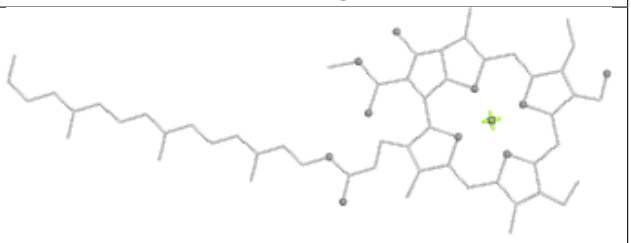
Bond lengths



Bond angles

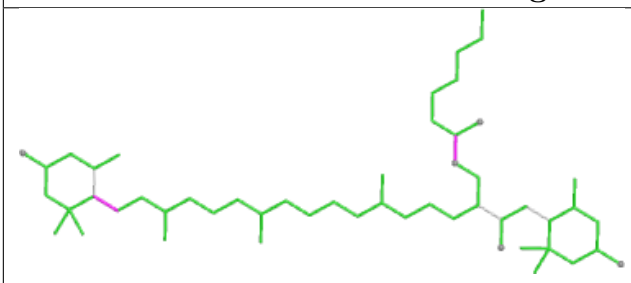


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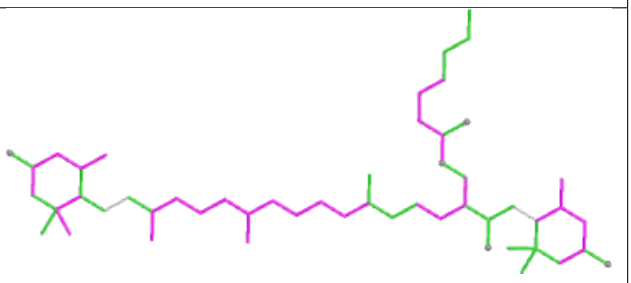


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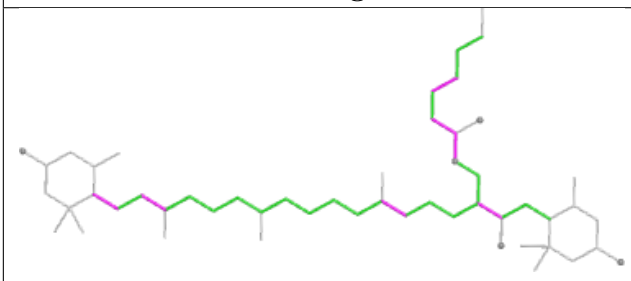
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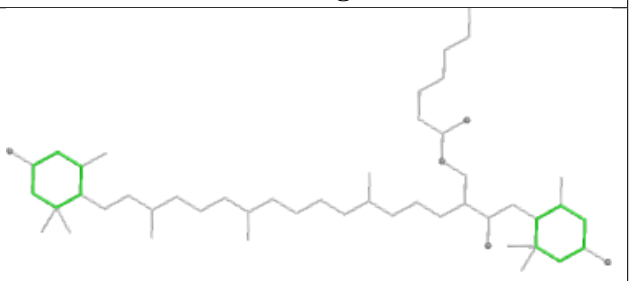
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Bond angles

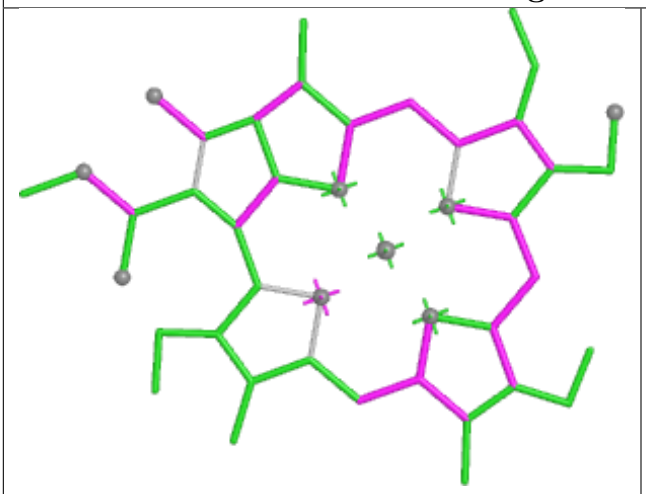


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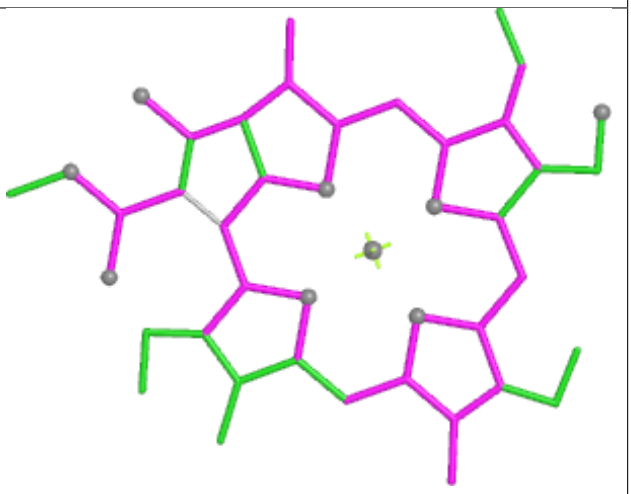


Rings

Ligand CHL 5 309



Bond lengths



Bond angles

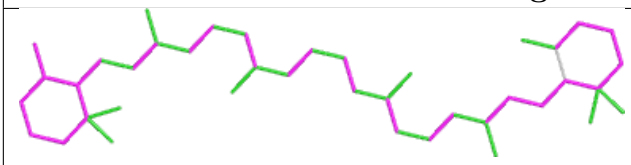


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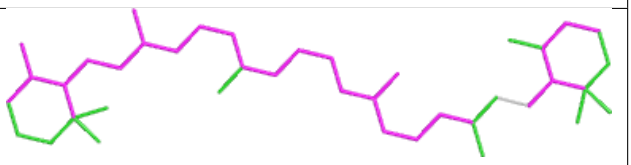


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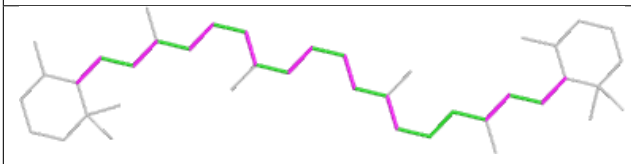
Ligand 8CT b 617



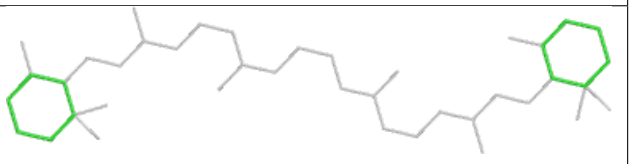
Bond lengths



Bond angles

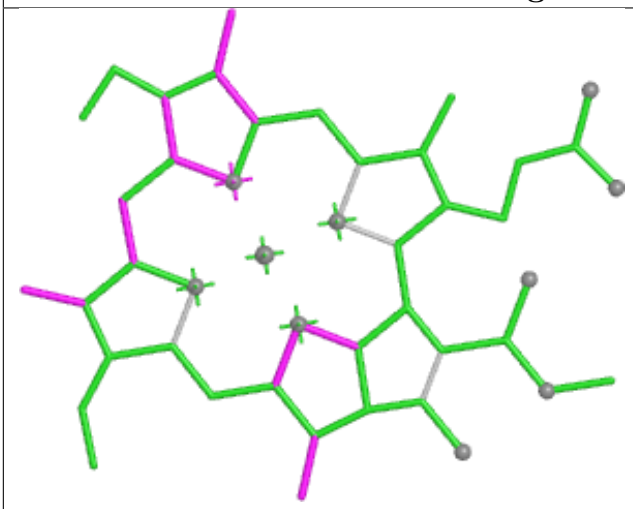


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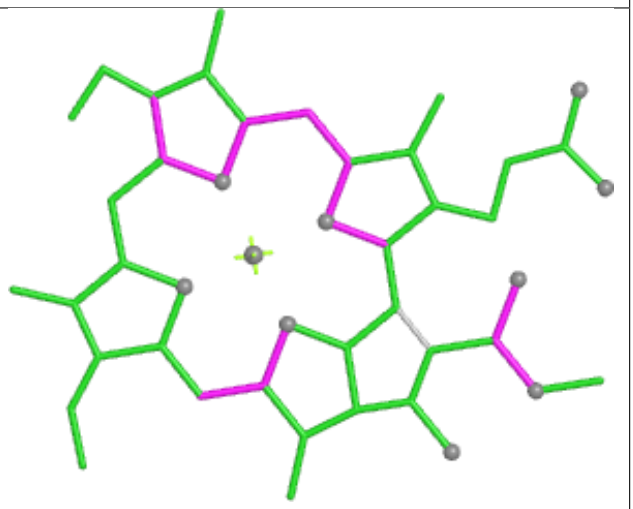


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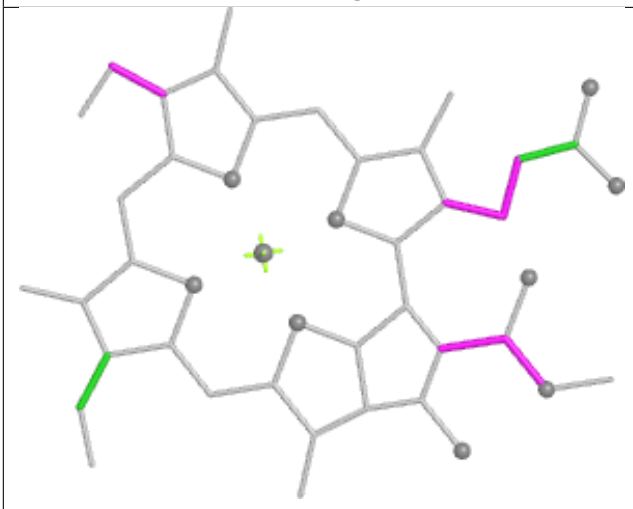
Ligand CLA b 601



Bond lengths



Bond angles

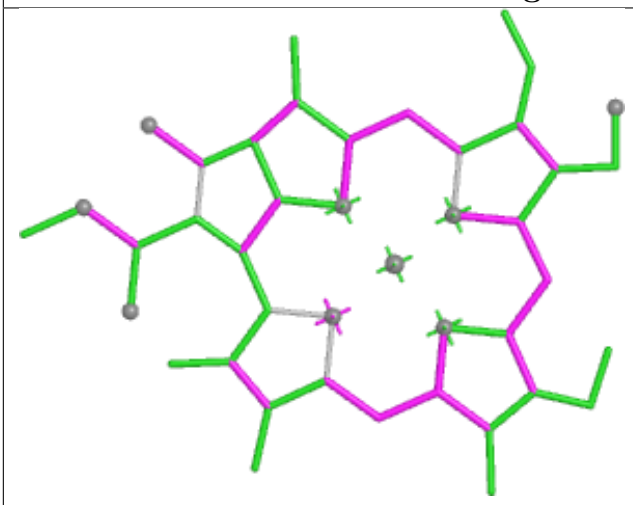


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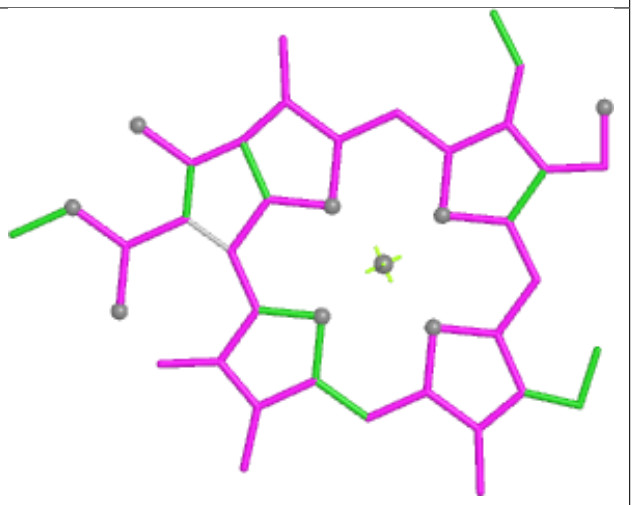


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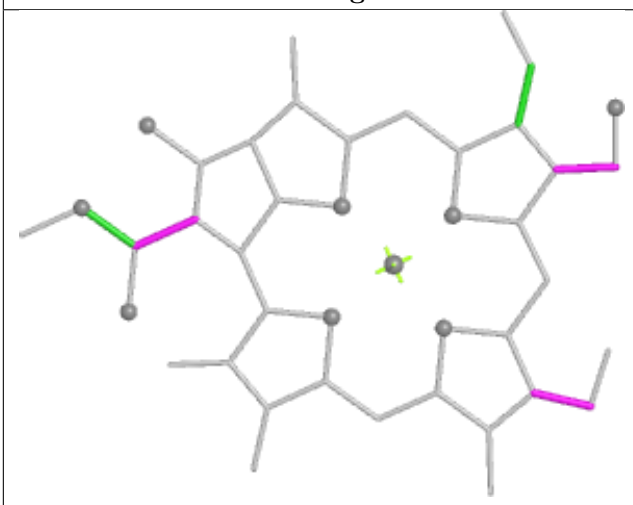
Ligand CHL Y 317



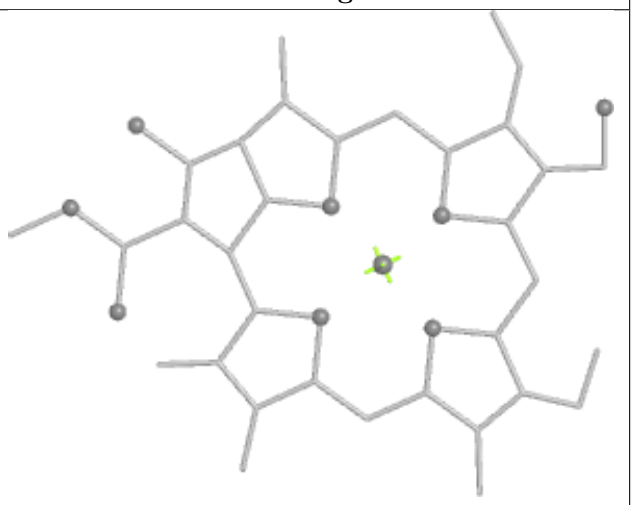
Bond lengths



Bond angles

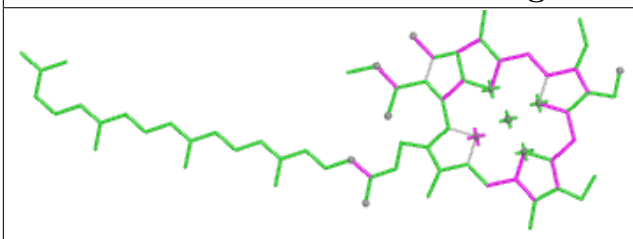


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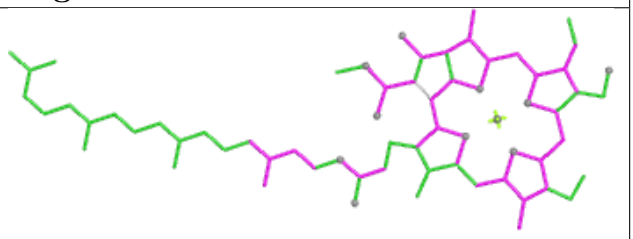


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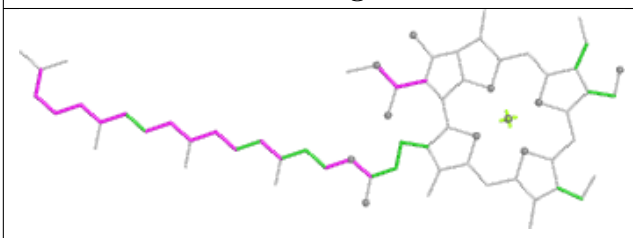
Ligand CHL g 313



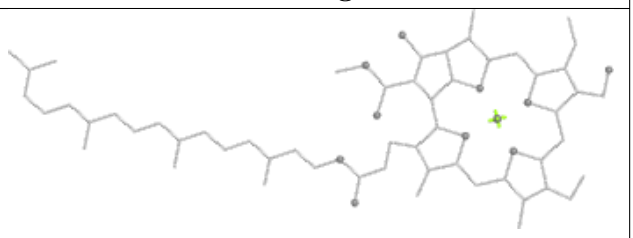
Bond lengths



Bond angles

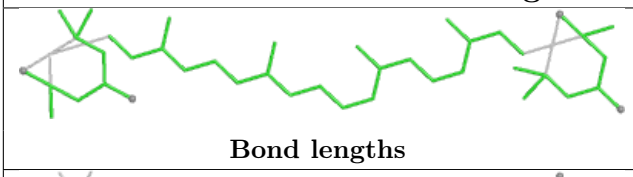


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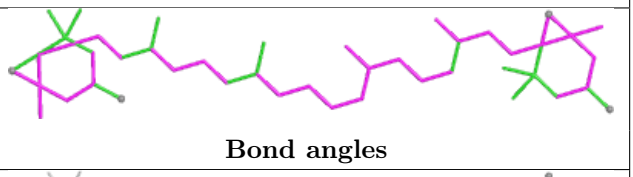


Rings

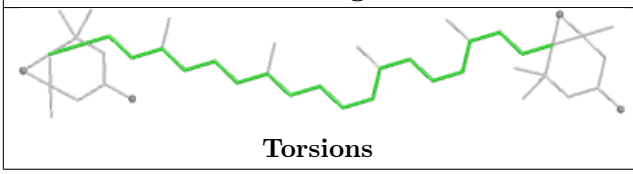
Ligand XAT R 615



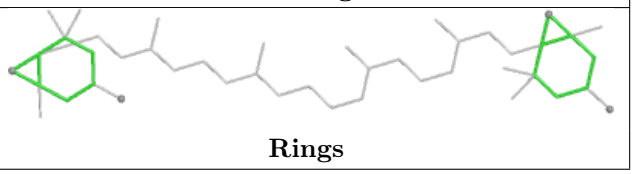
Bond lengths



Bond angles

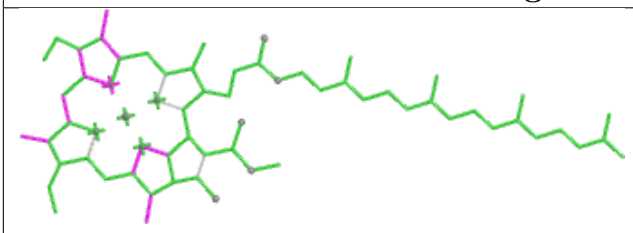


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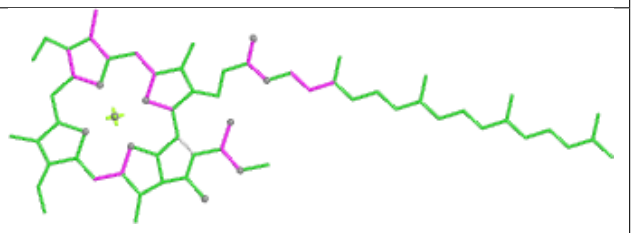


Rings

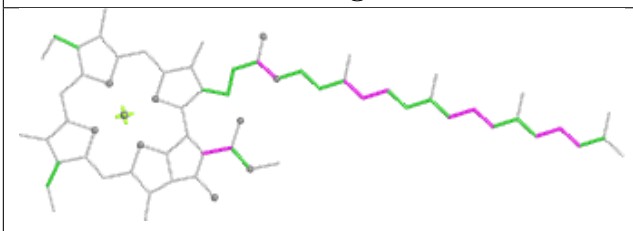
Ligand CLA C 610



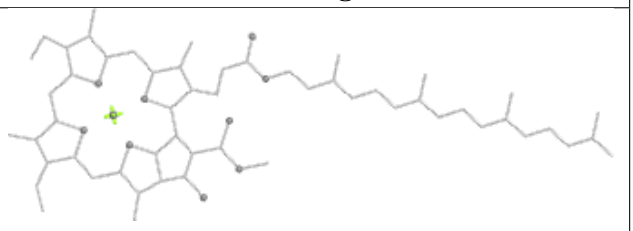
Bond lengths



Bond angles

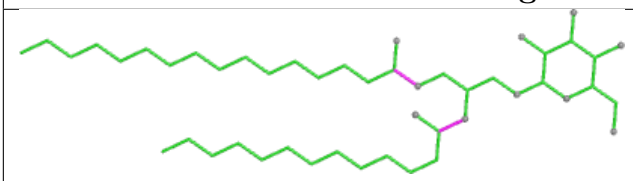


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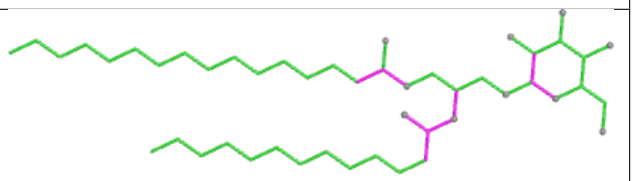


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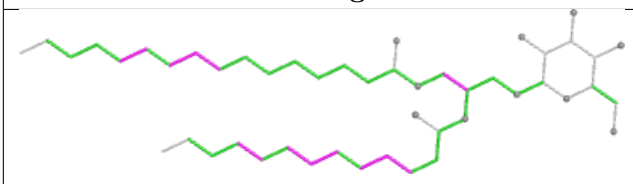
Ligand LMG D 401



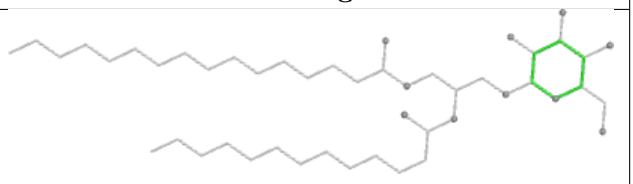
Bond lengths



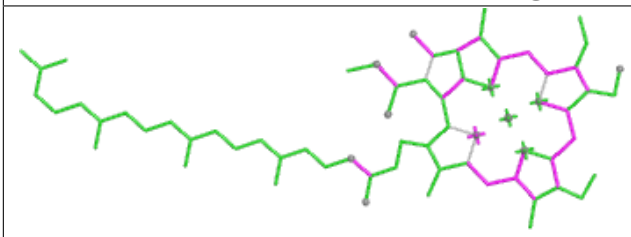
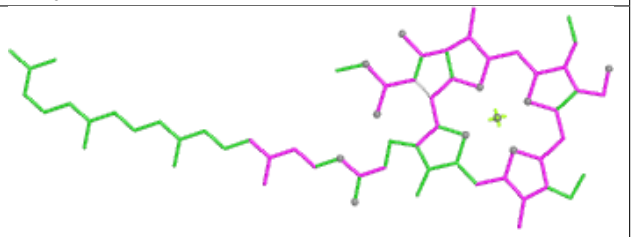
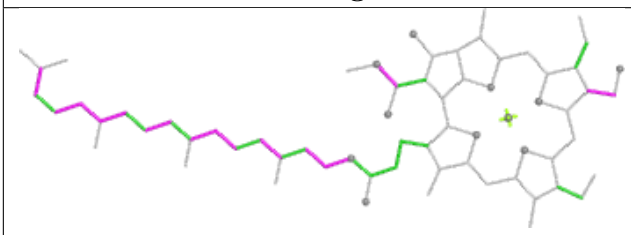
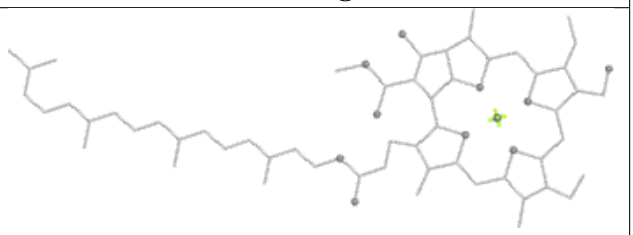
Bond angles

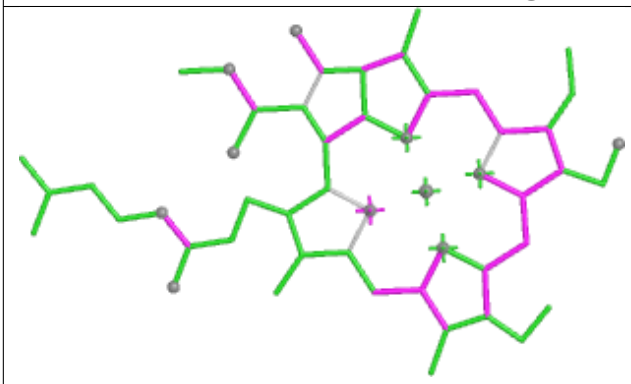
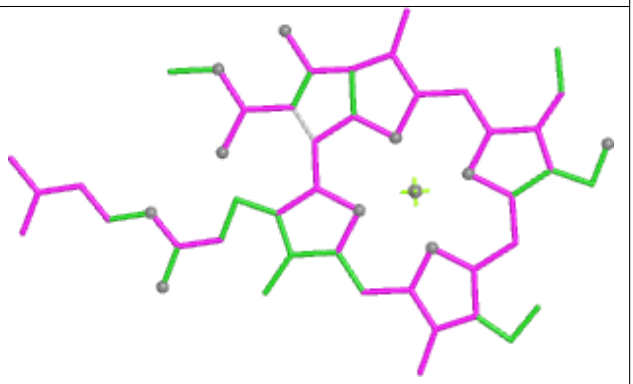
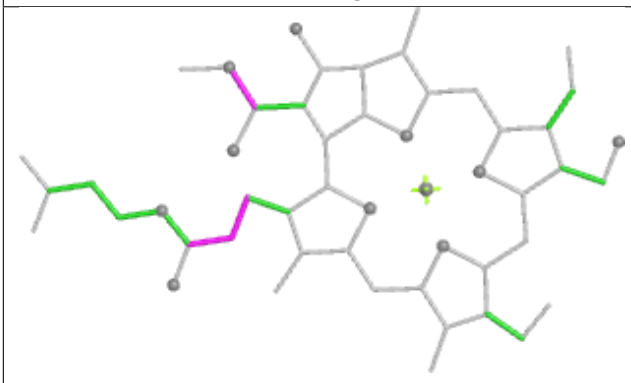
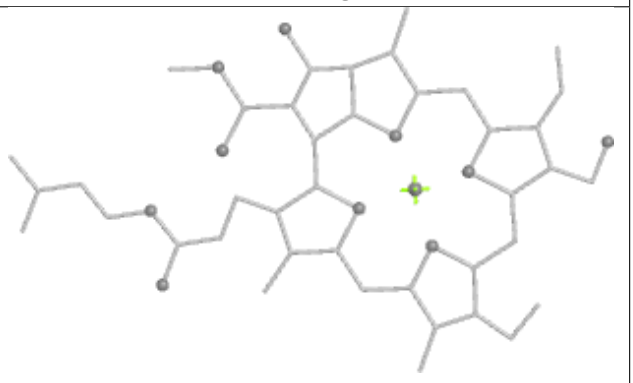


Torsions

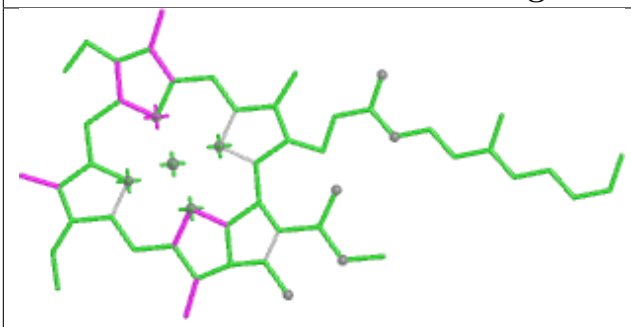


Rings

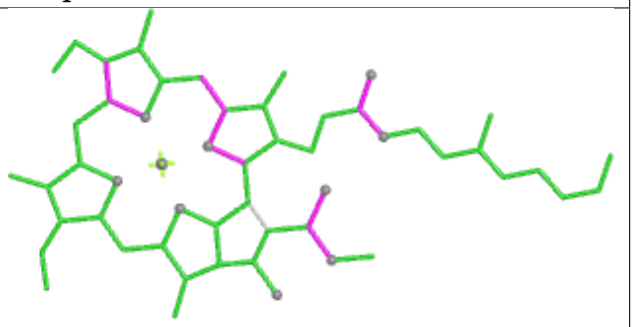
Ligand CHL y 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

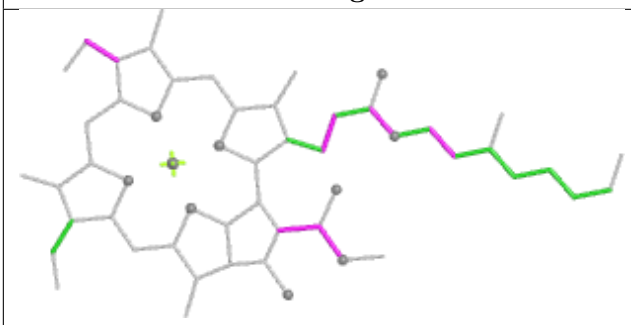
Ligand CLA q 305



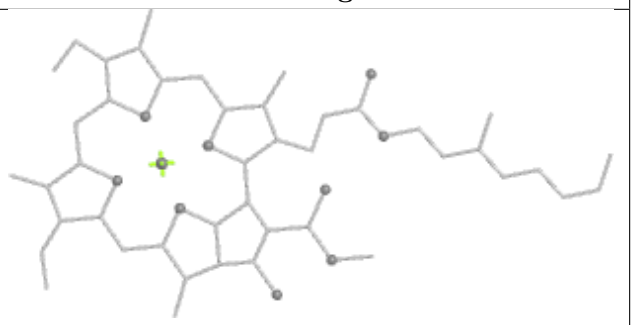
Bond lengths



Bond angles

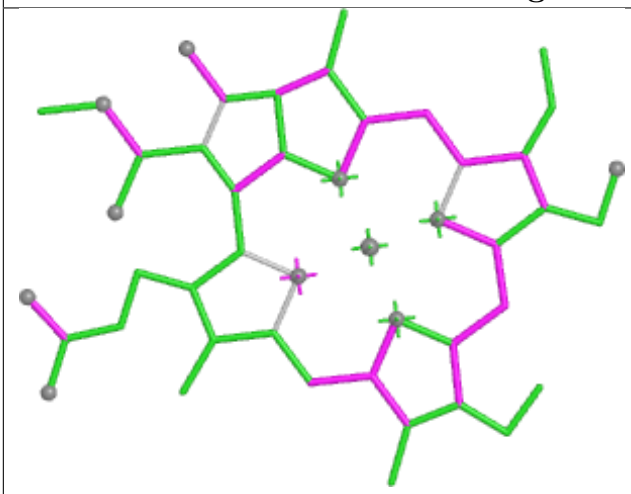


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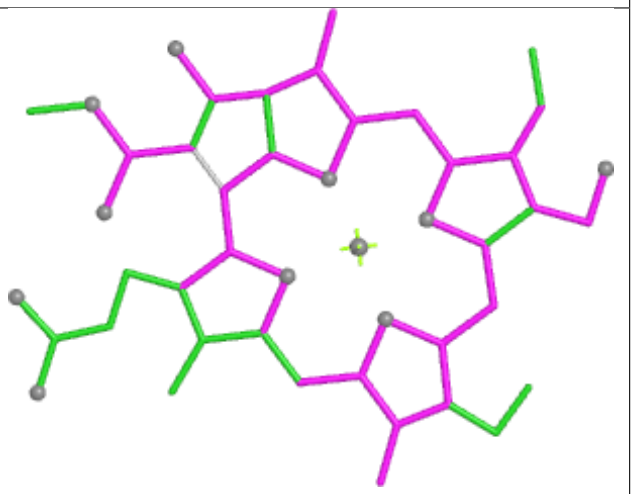


Rings

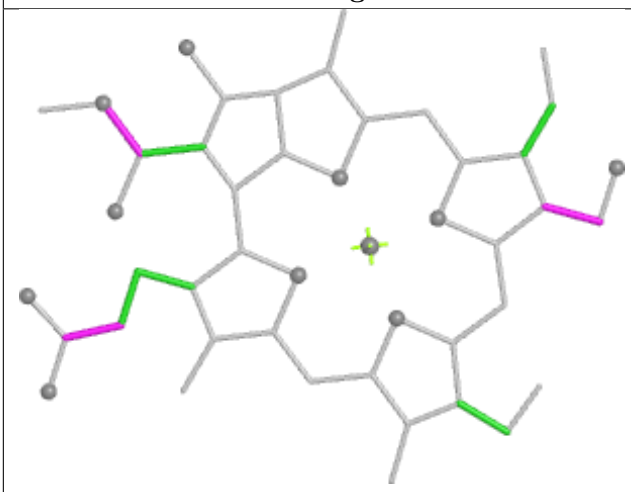
Ligand CHL 4 312



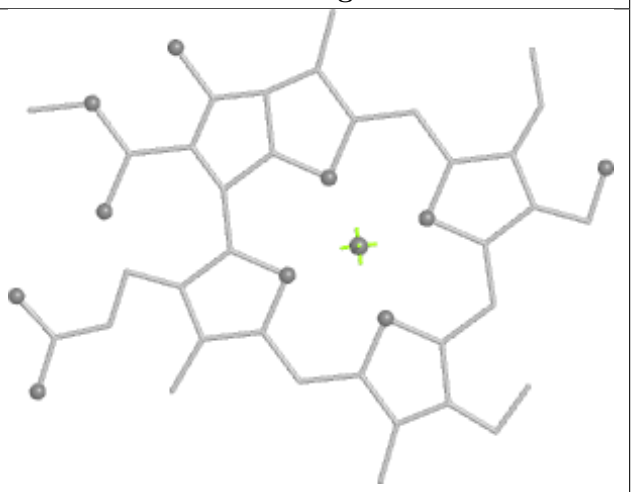
Bond lengths



Bond angles

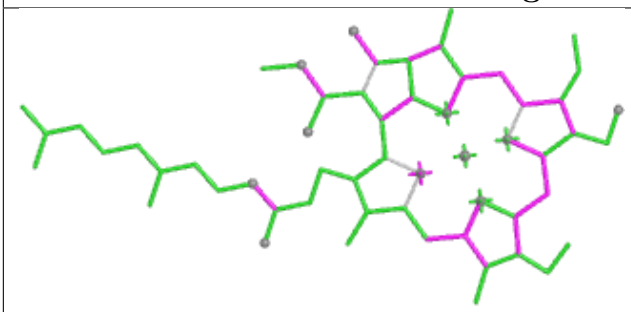


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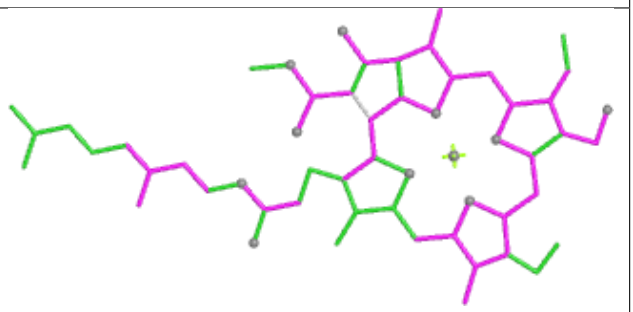


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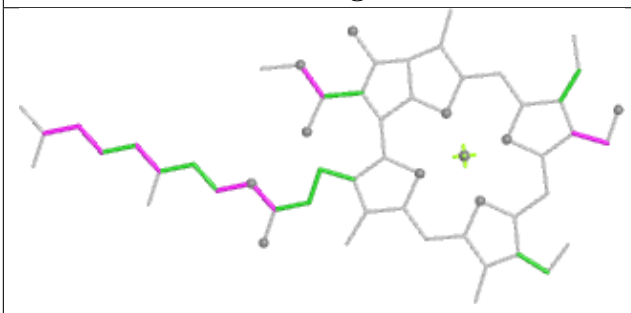
Ligand CHL N 312



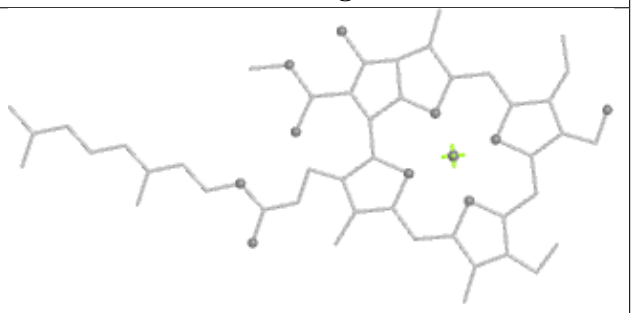
Bond lengths



Bond angles

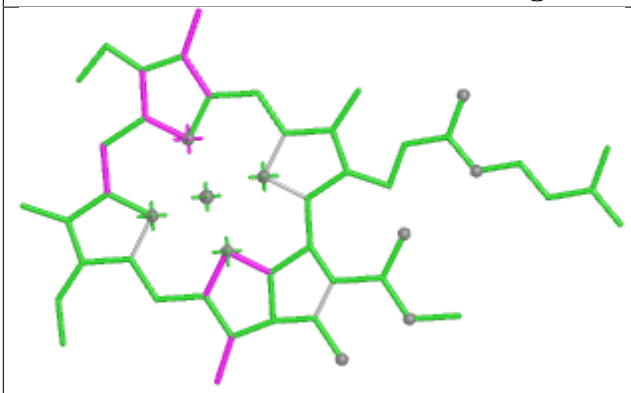


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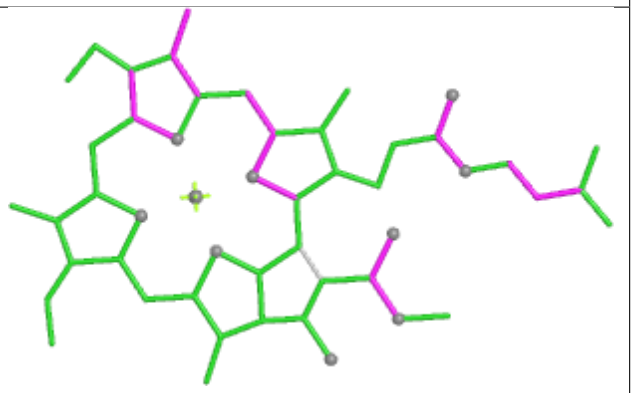


Rings

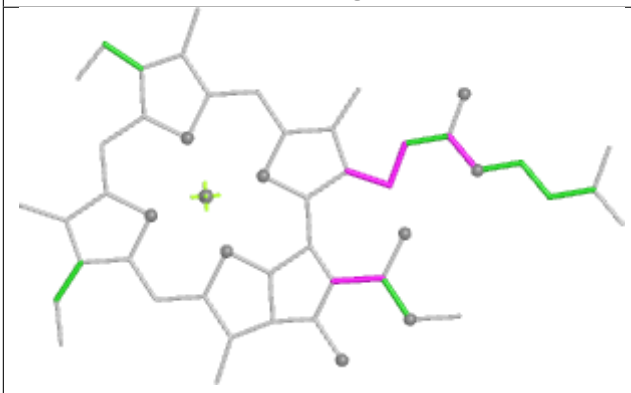
Ligand CLA 8 306



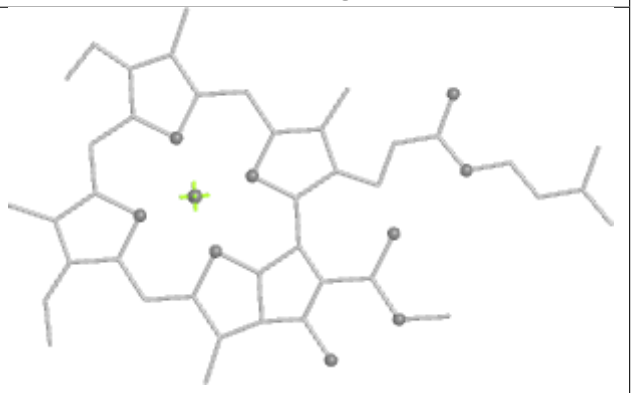
Bond lengths



Bond angles

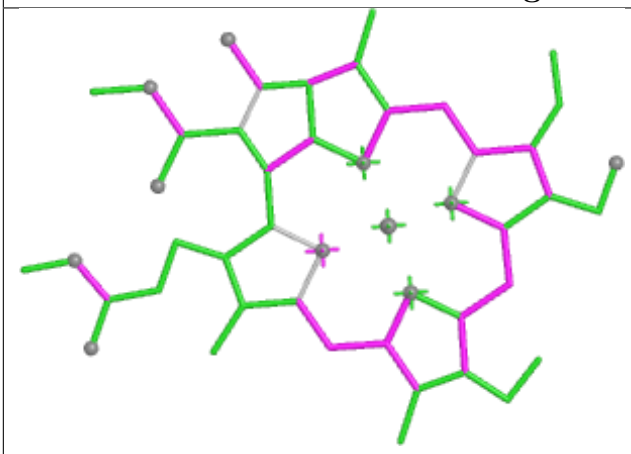


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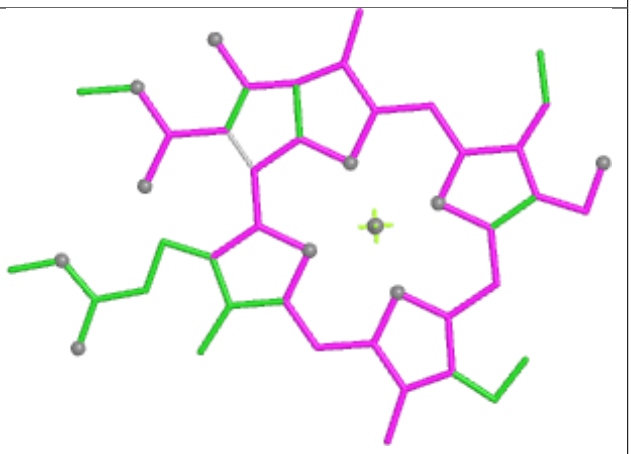


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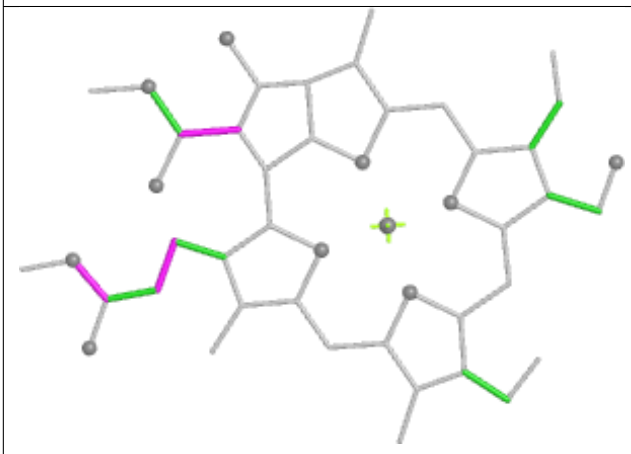
Ligand CHL R 602



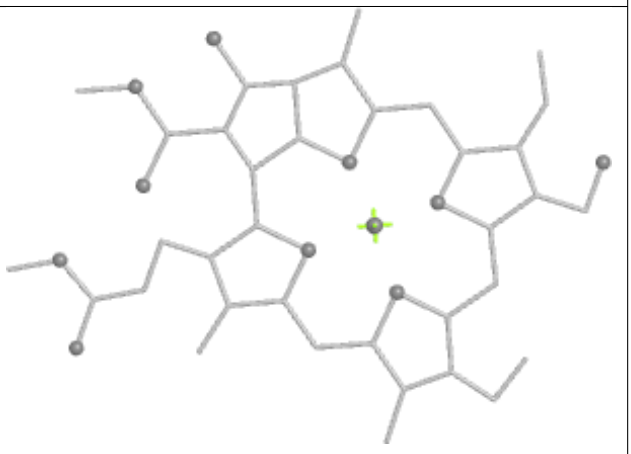
Bond lengths



Bond angles

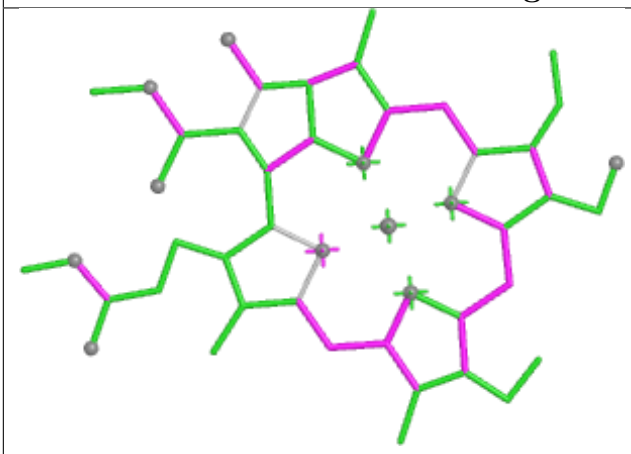


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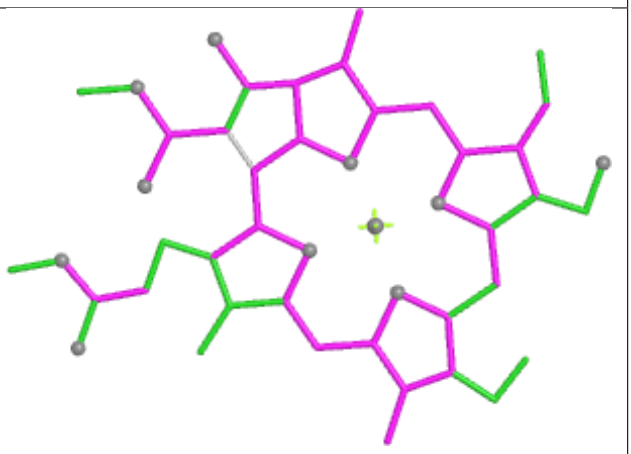


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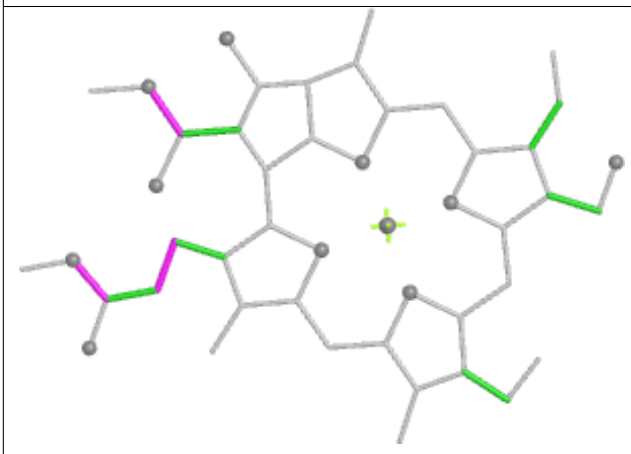
Ligand CHL Y 309



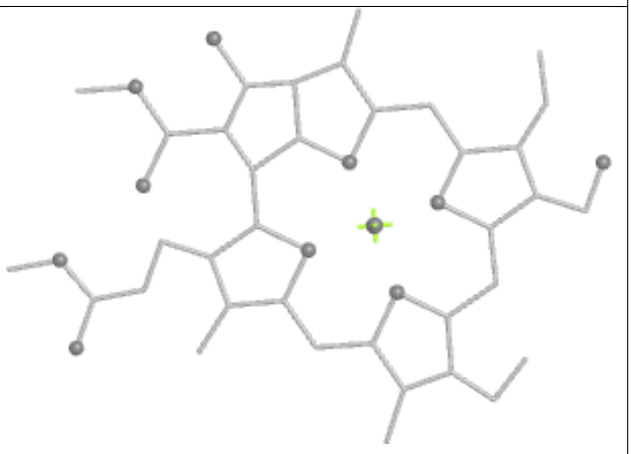
Bond lengths



Bond angles

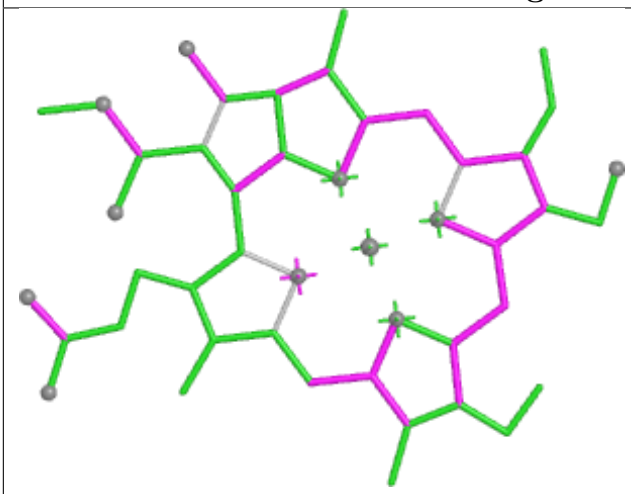


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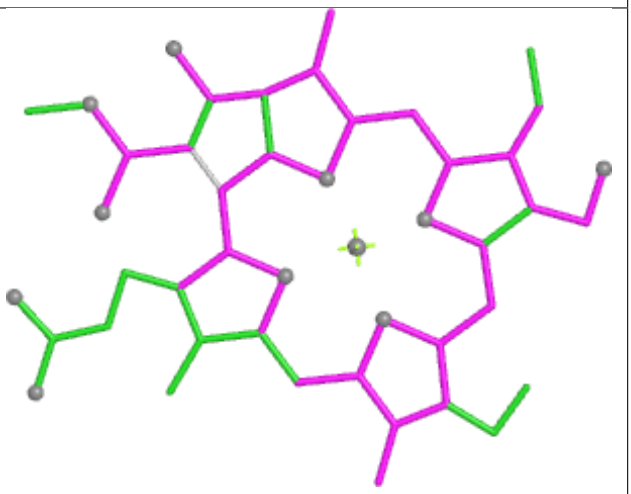


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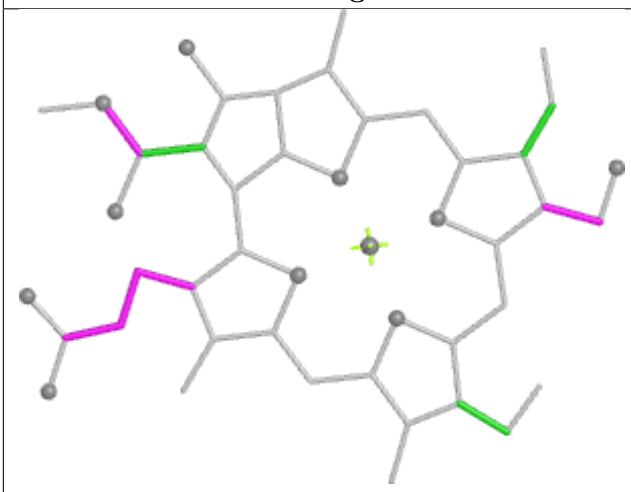
Ligand CHL u 310



Bond lengths



Bond angles



Torsions

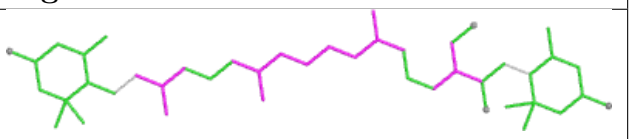


Rings

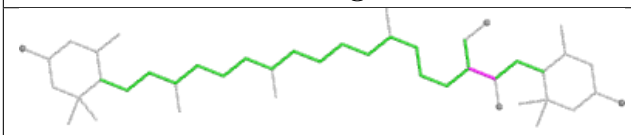
Ligand 0IE g 302



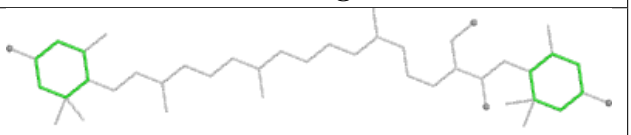
Bond lengths



Bond angles

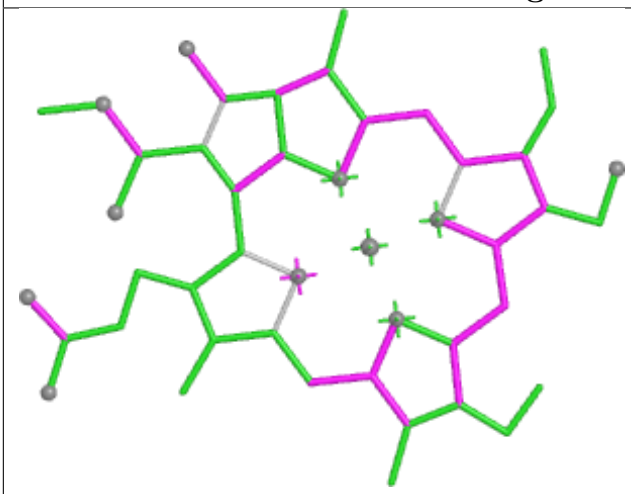


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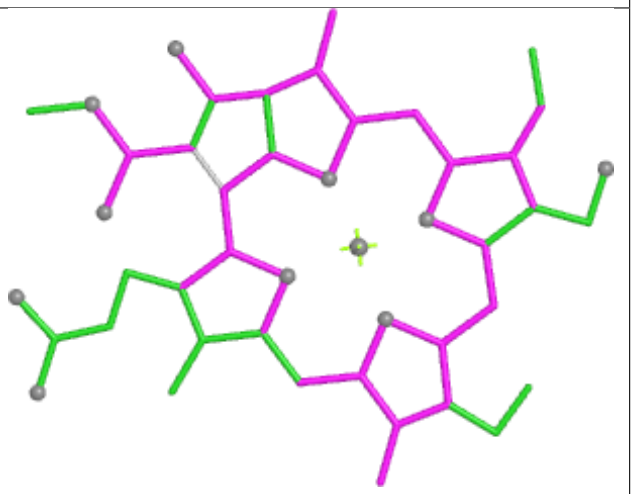


Rings

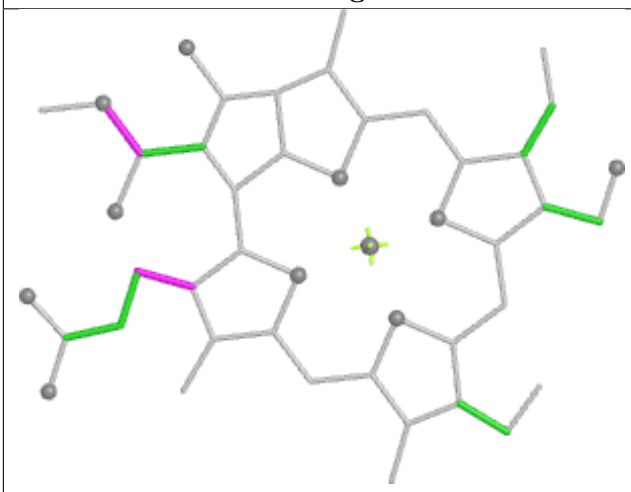
Ligand CHL u 311



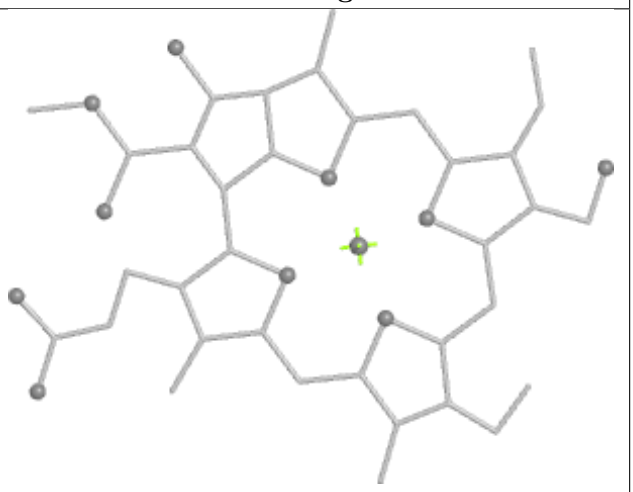
Bond lengths



Bond angles

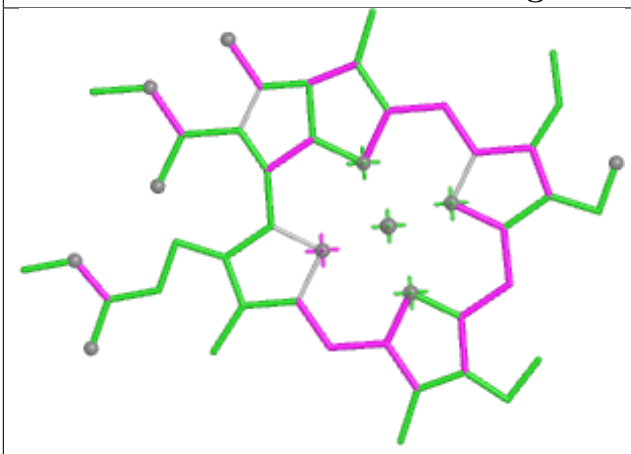


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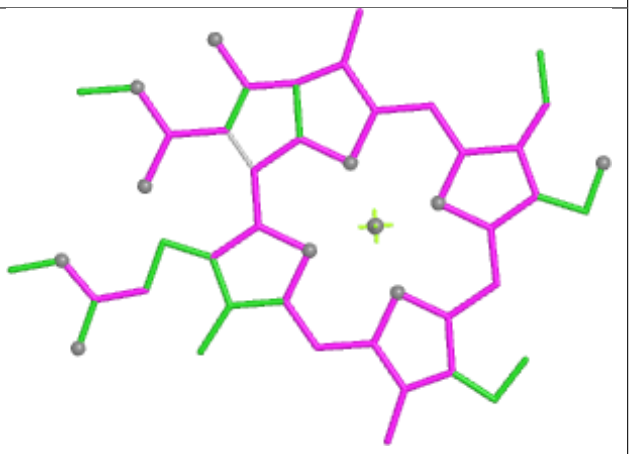


Rings

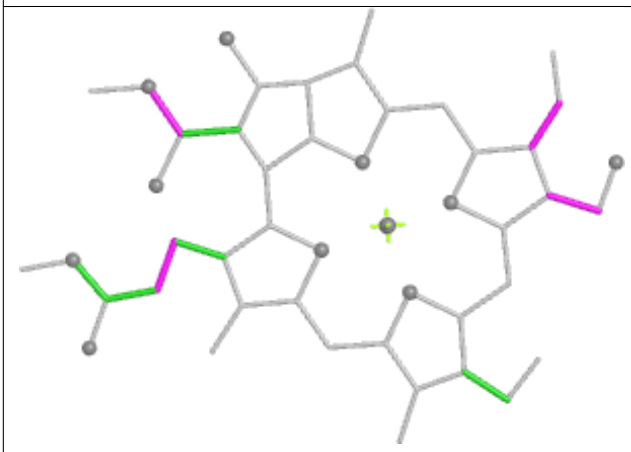
Ligand CHL S 608



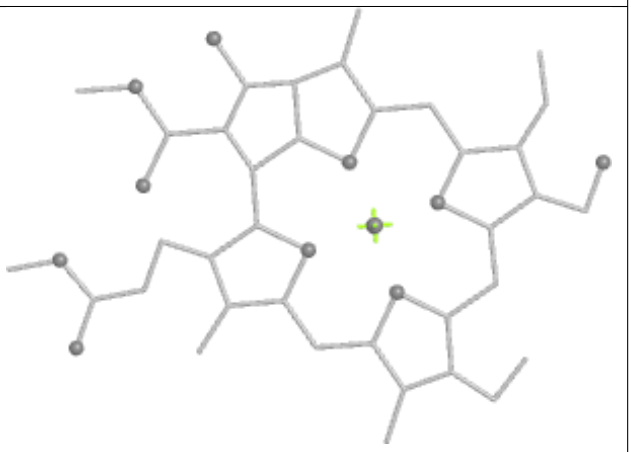
Bond lengths



Bond angles

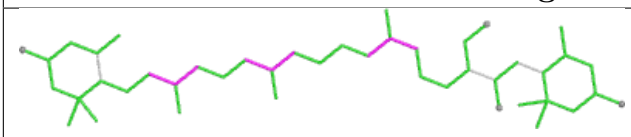


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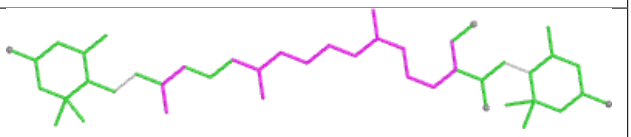


Rings

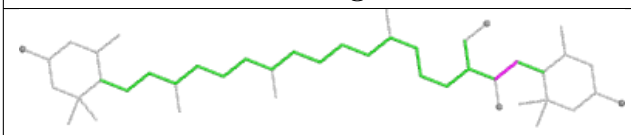
Ligand 0IE 3 303



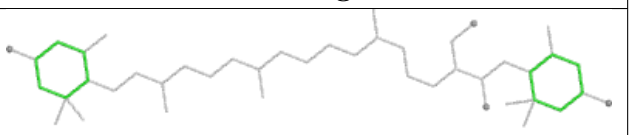
Bond lengths



Bond angles

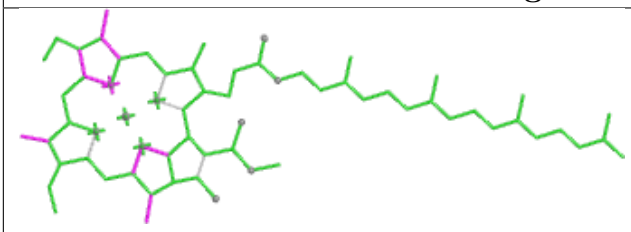


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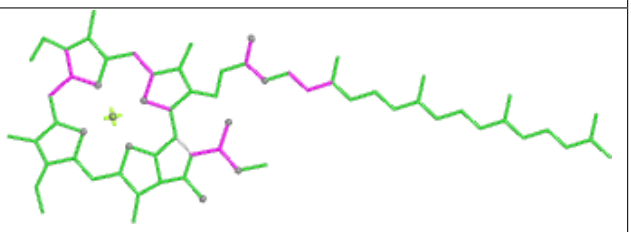


Rings

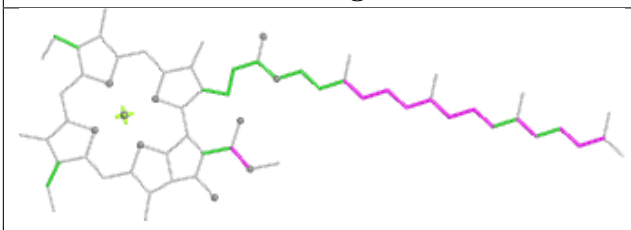
Ligand CLA B 609



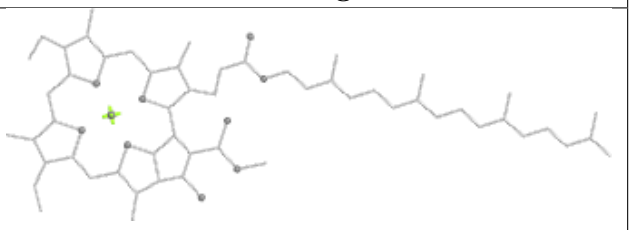
Bond lengths



Bond angles



Torsions



Rings

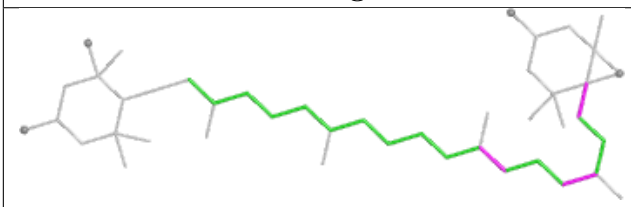
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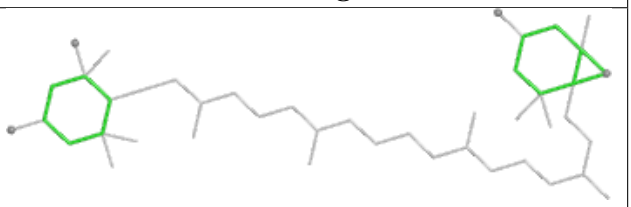
Bond lengths



Bond angles

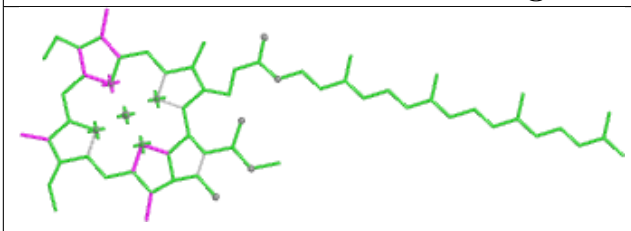


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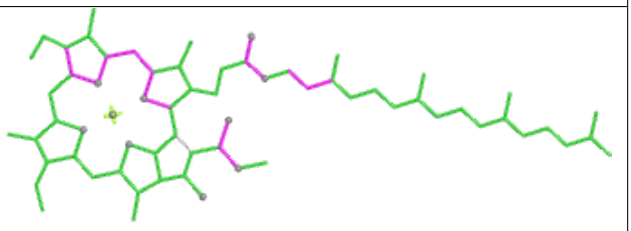


Rings

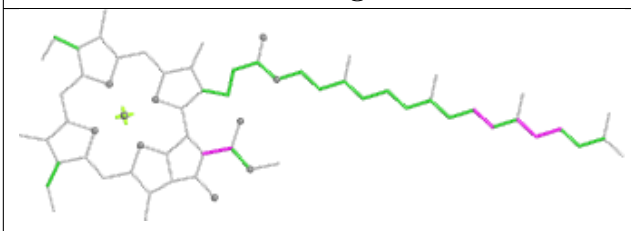
Ligand CLA b 611



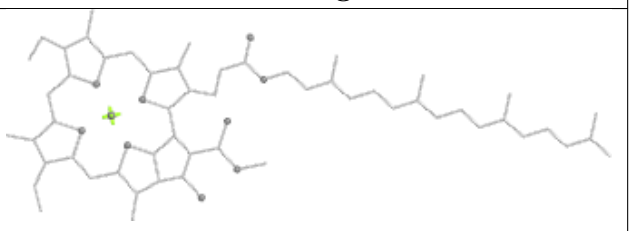
Bond lengths



Bond angles

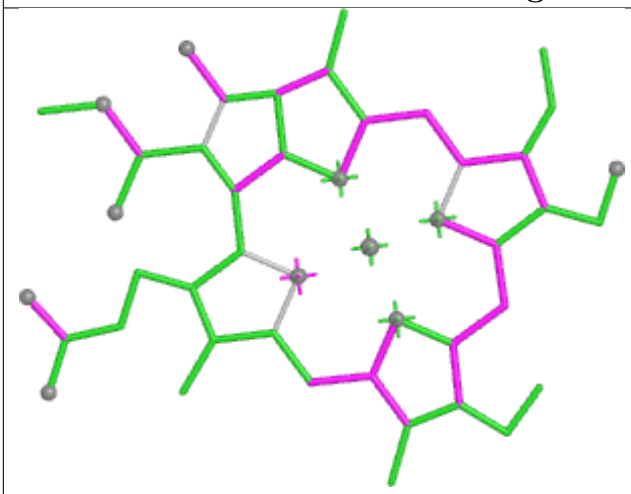


Torsions

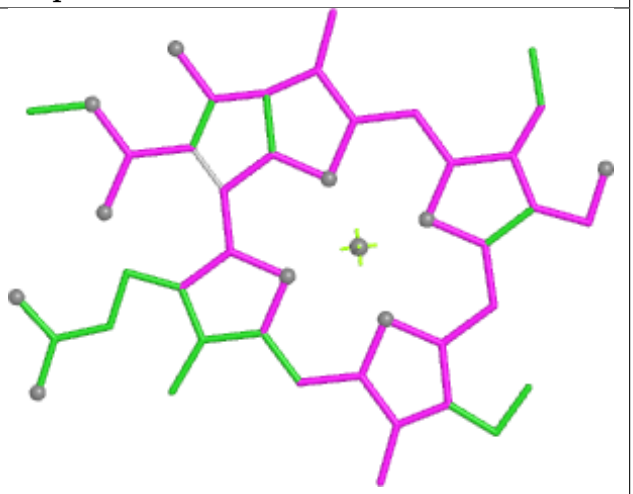


Rings

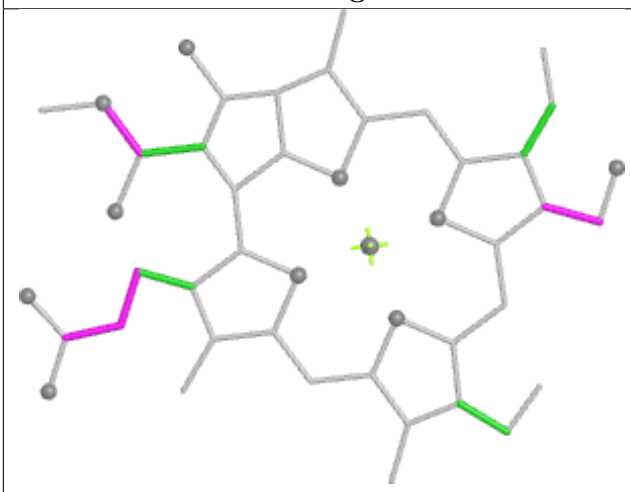
Ligand CHL p 310



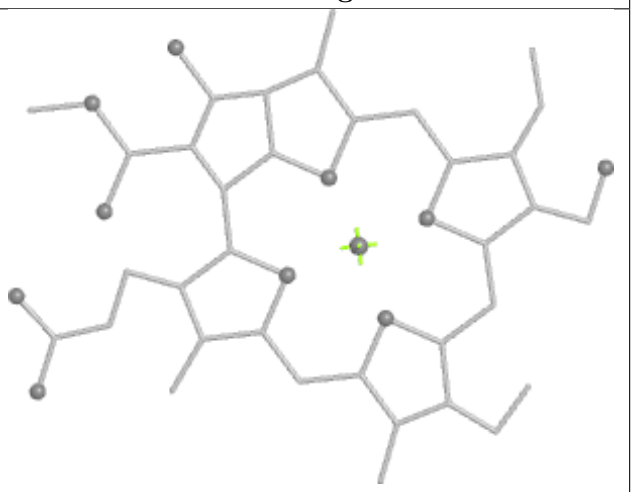
Bond lengths



Bond angles

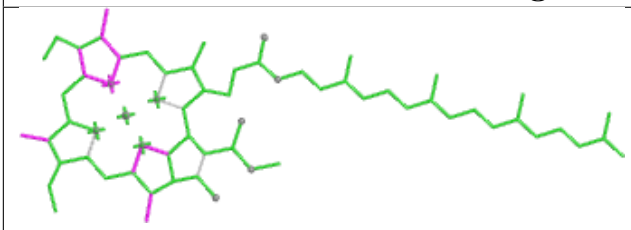


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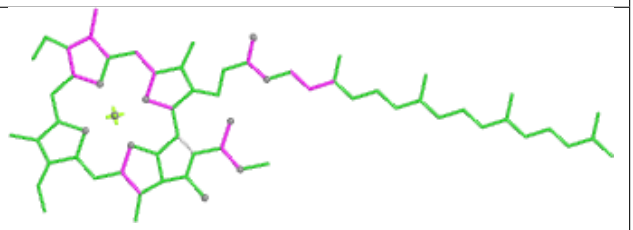


Rings

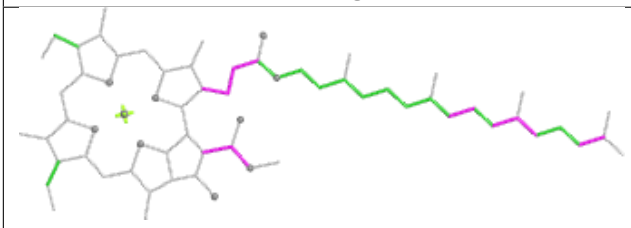
Ligand CLA c 601



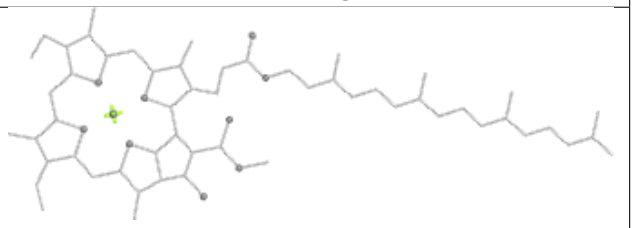
Bond lengths



Bond angles

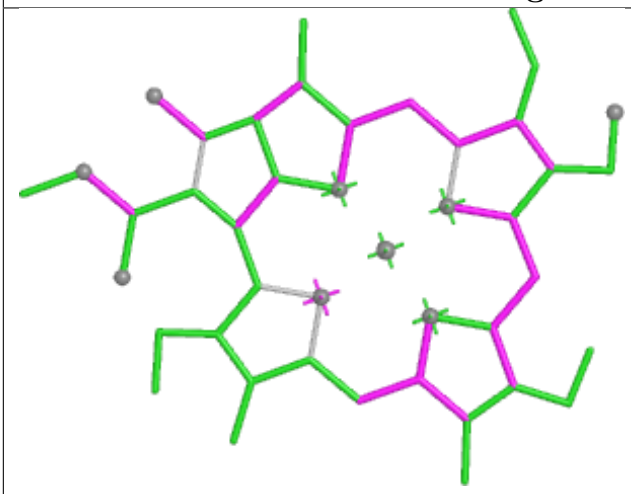


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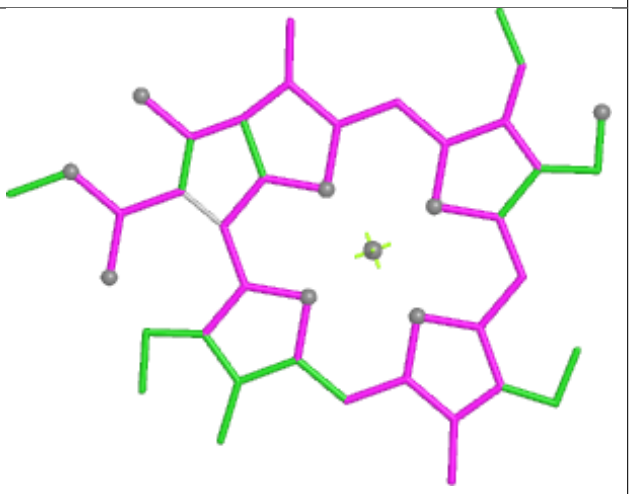


Rings

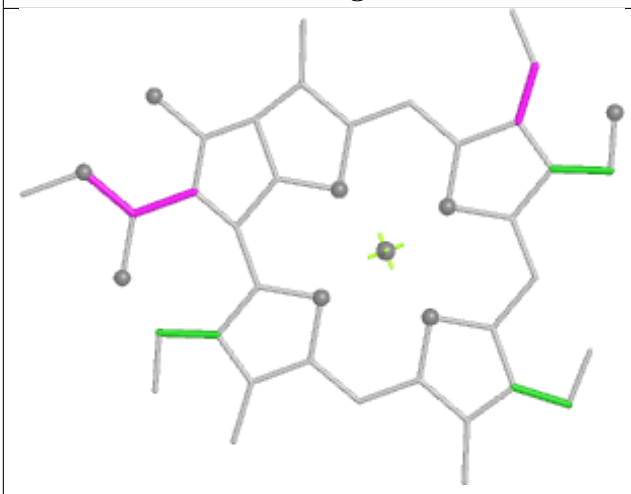
Ligand CHL u 313



Bond lengths



Bond angles

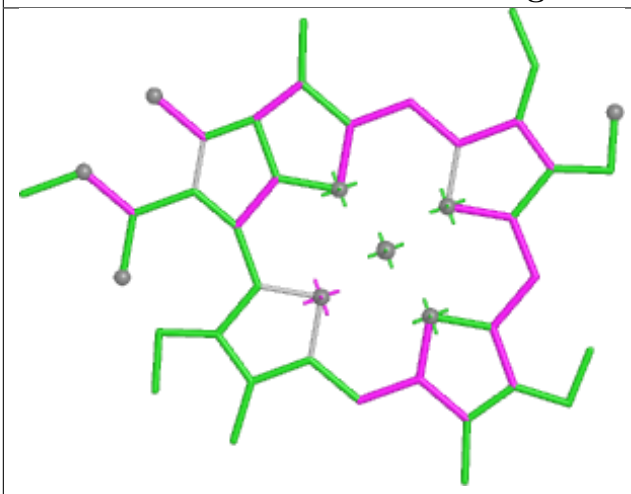


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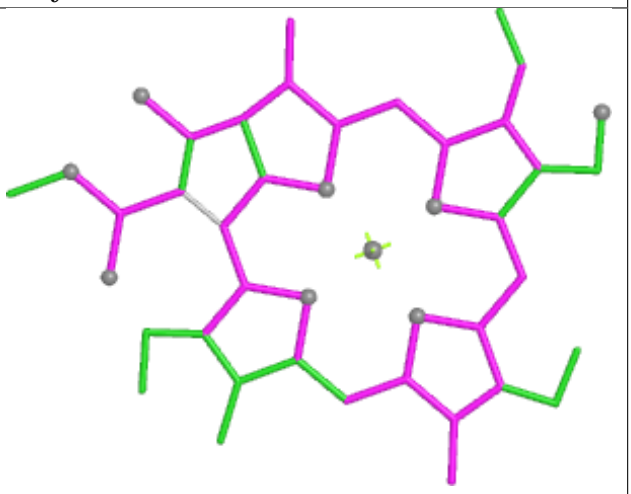


Rings

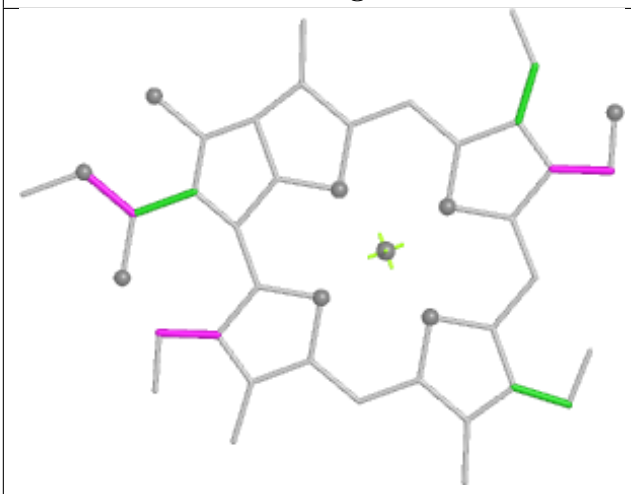
Ligand CHL y 309



Bond lengths



Bond angles



Torsions



Rings

Ligand PL9 d 406



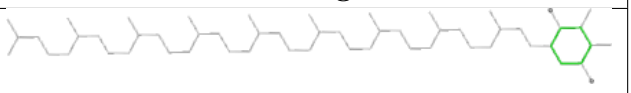
Bond lengths



Bond angles

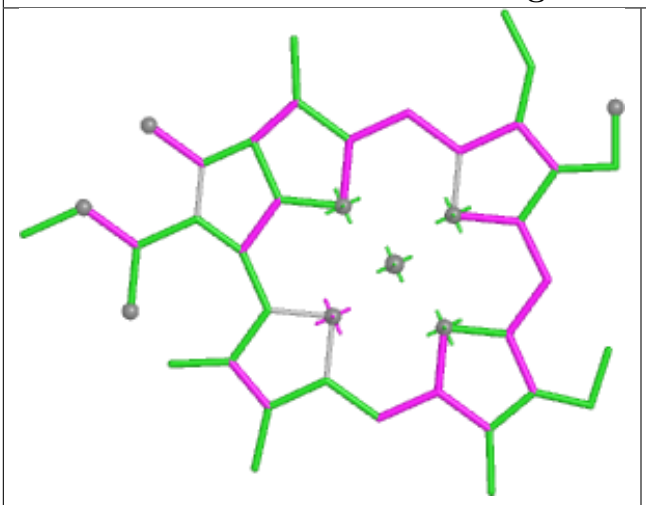


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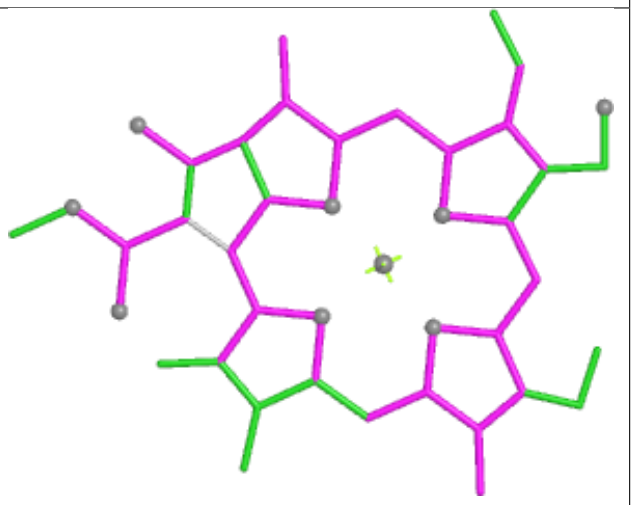


Rings

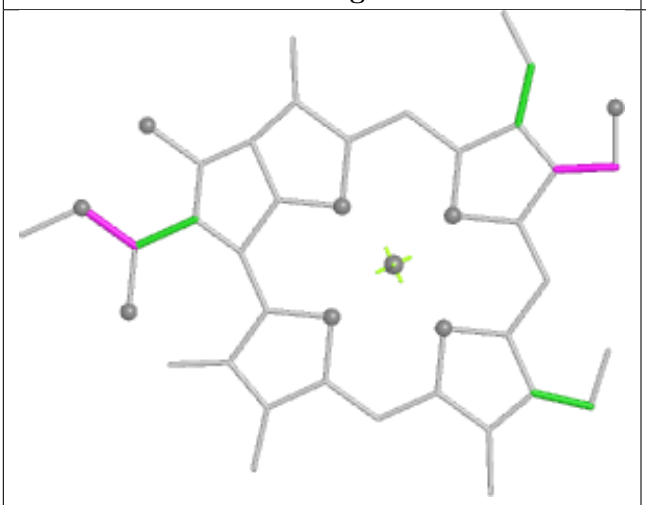
Ligand CHL 5 313



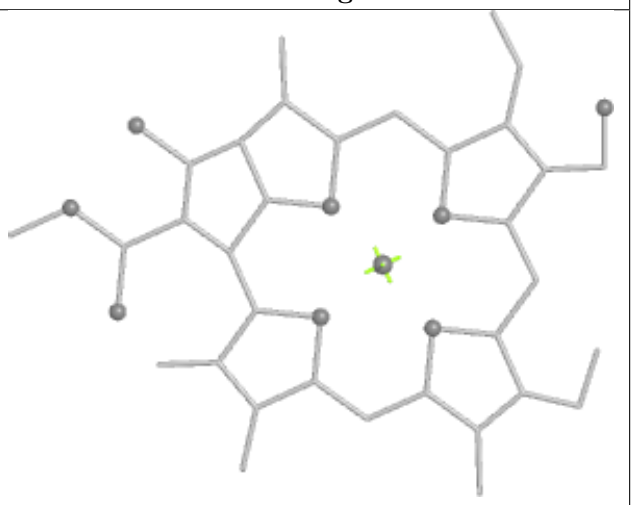
Bond lengths



Bond angles

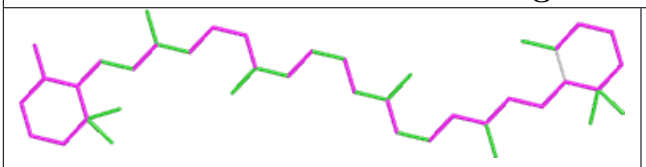


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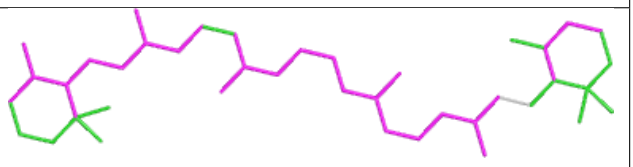


Rings

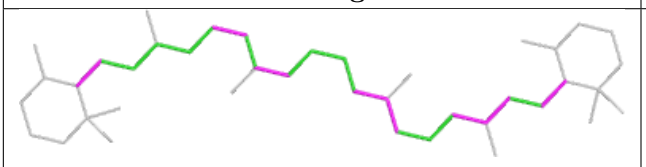
Ligand 8CT s 416



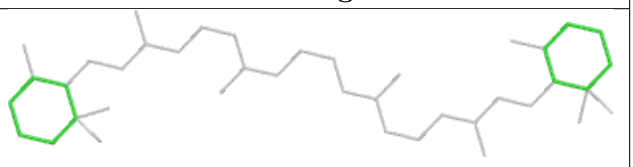
Bond lengths



Bond angles

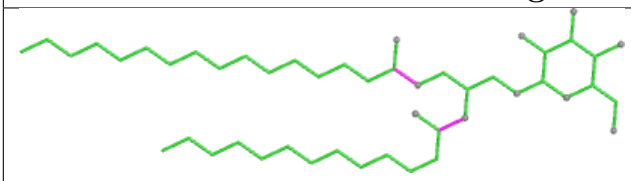


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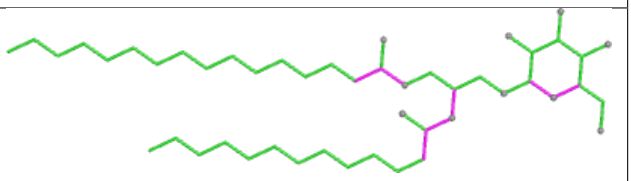


Rings

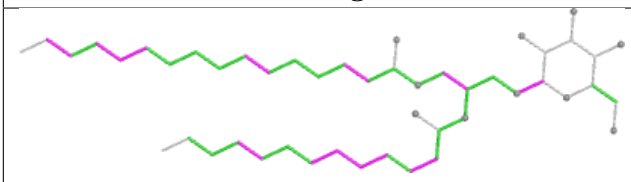
Ligand LMG i 101



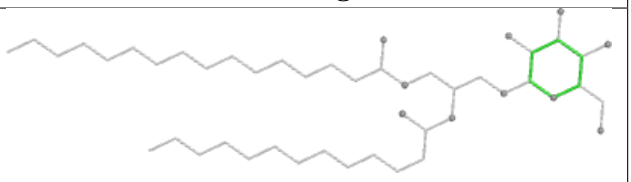
Bond lengths



Bond angles

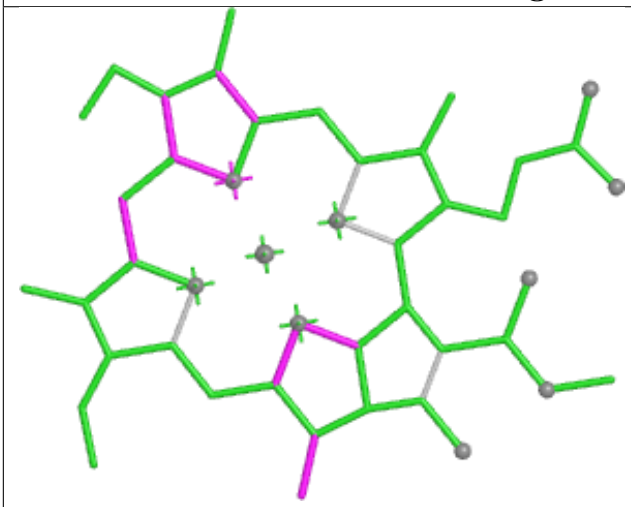


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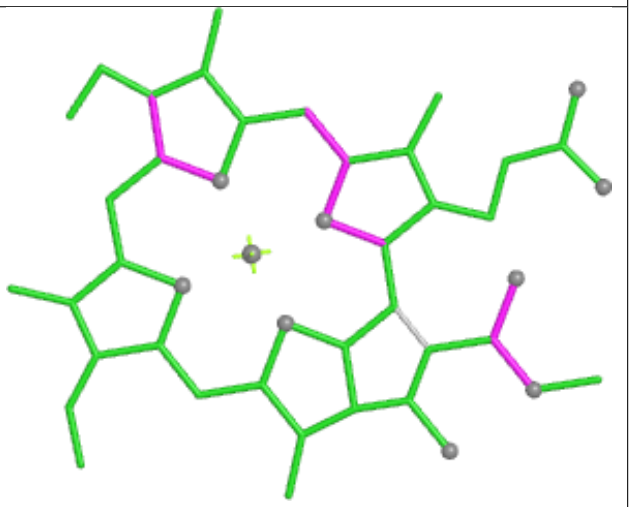


Rings

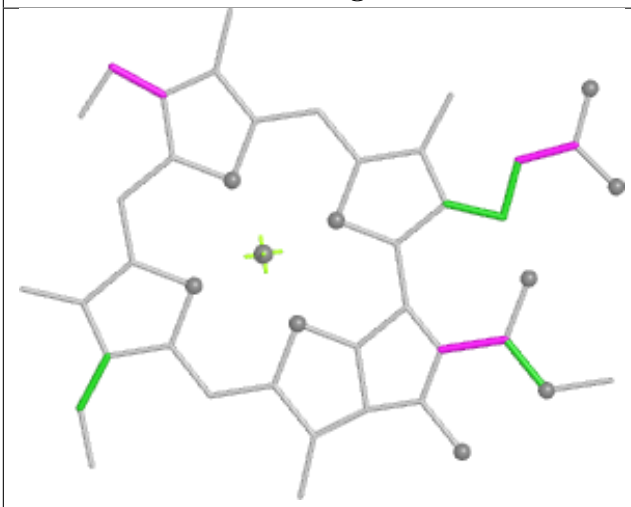
Ligand CLA 9 315



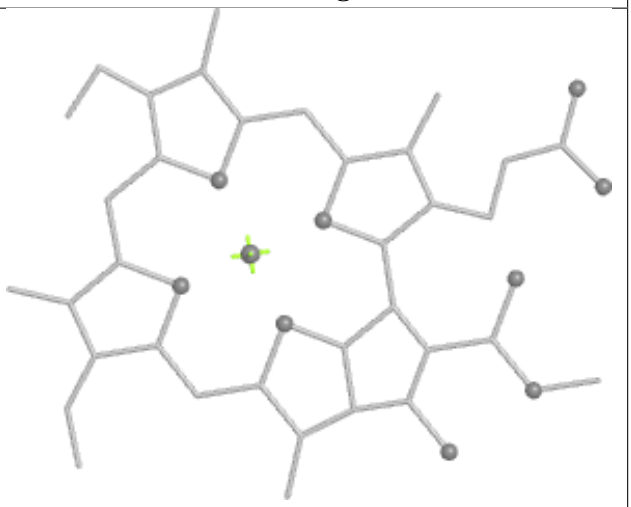
Bond lengths



Bond angles

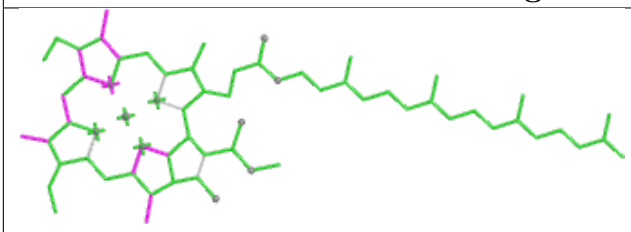


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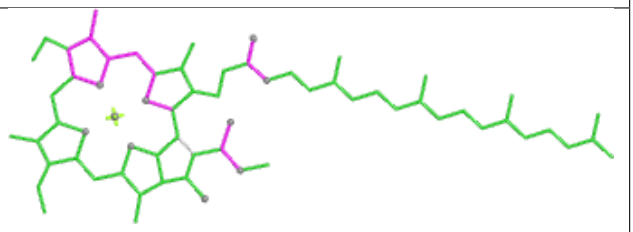


Rings

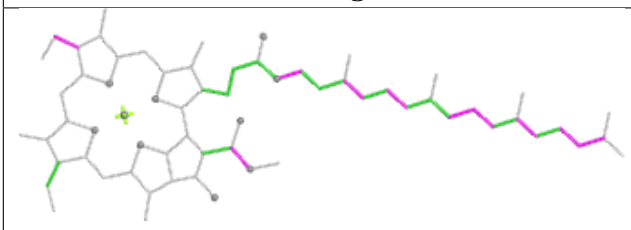
Ligand CLA C 603



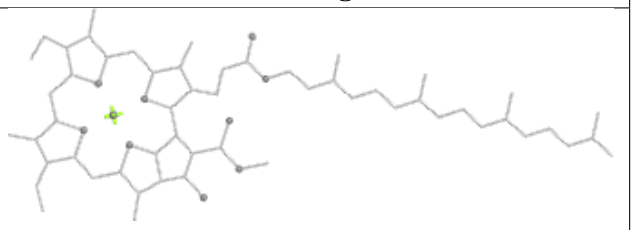
Bond lengths



Bond angles



Torsions



Rings

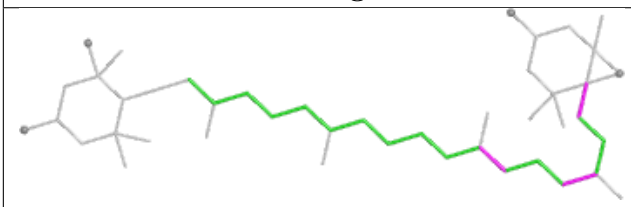
Ligand NEX 7 304



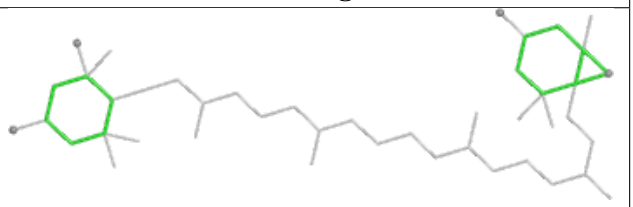
Bond lengths



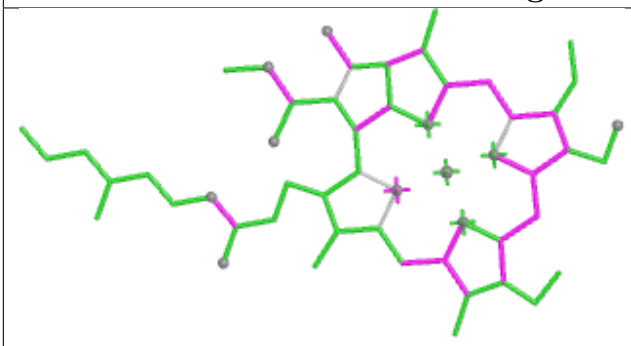
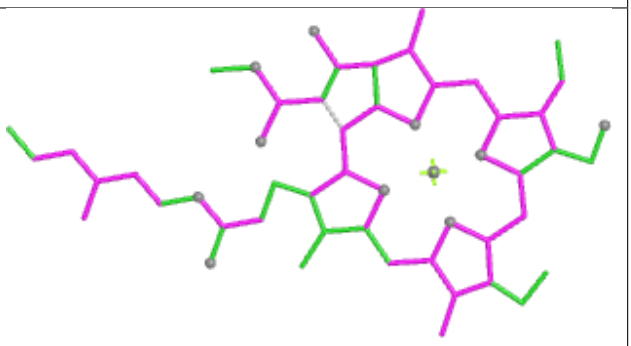
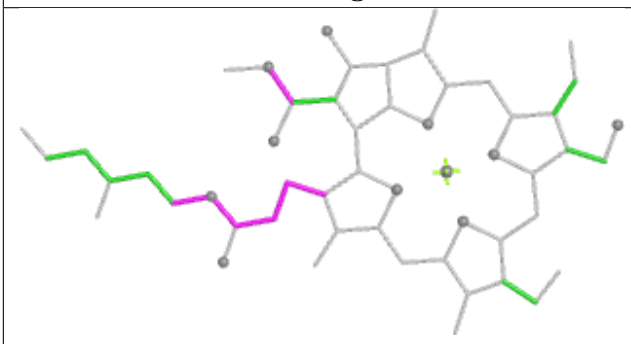
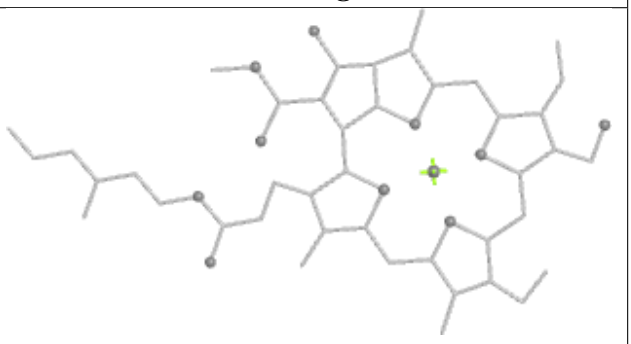
Bond angles

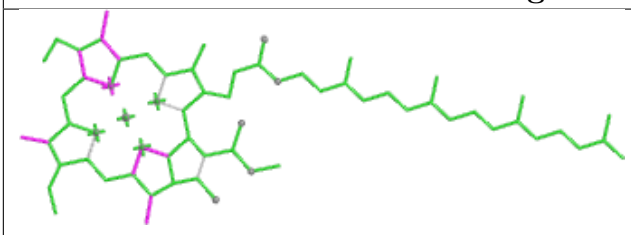
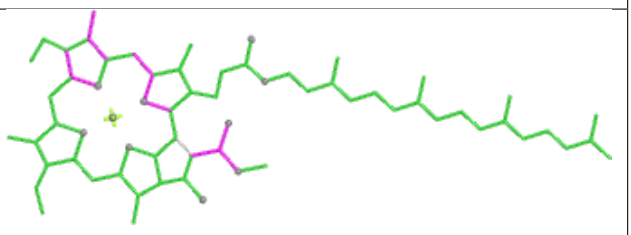
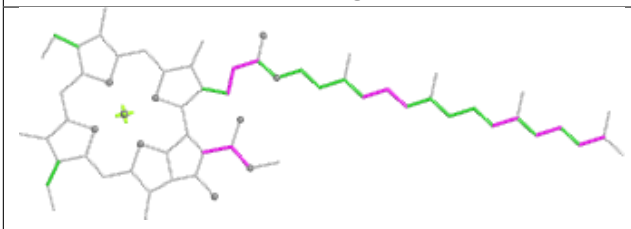
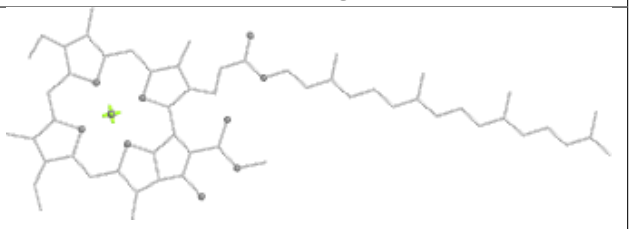


Torsions

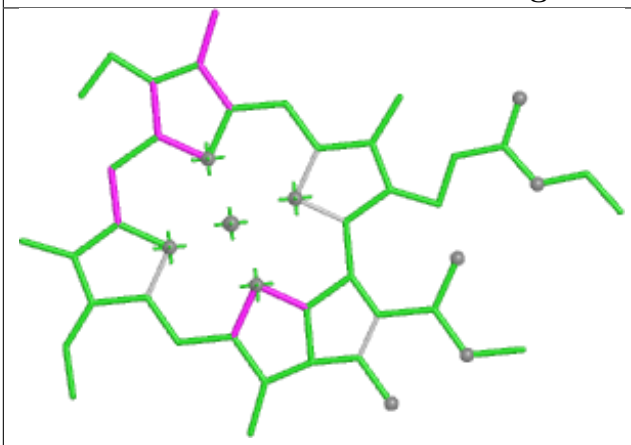


Rings

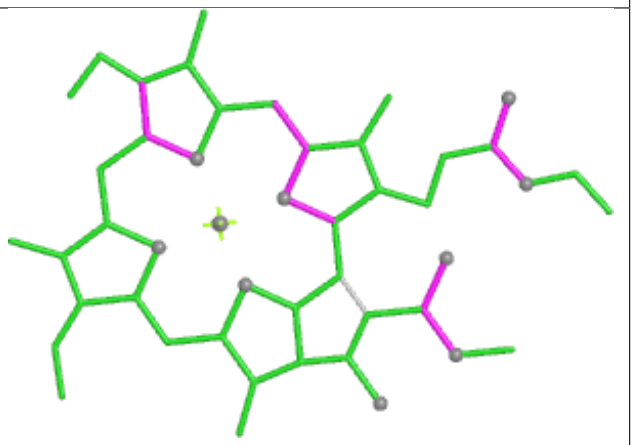
Ligand CHL n 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

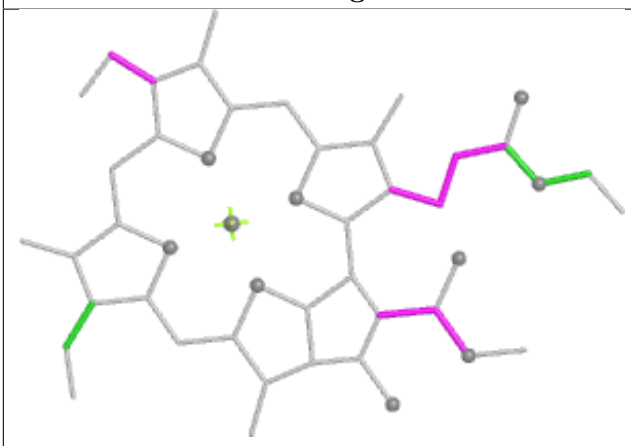
Ligand CLA r 314



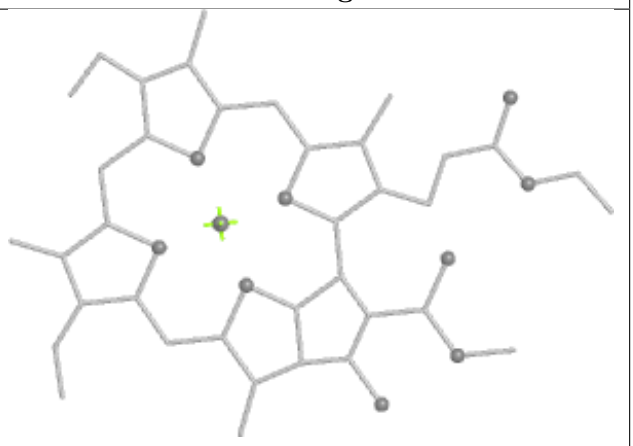
Bond lengths



Bond angles

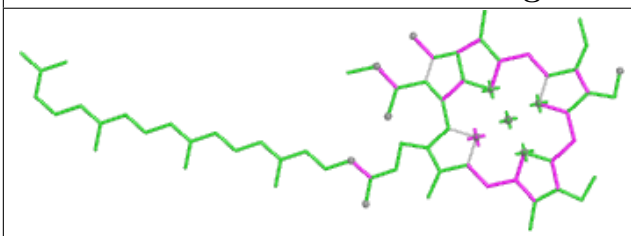


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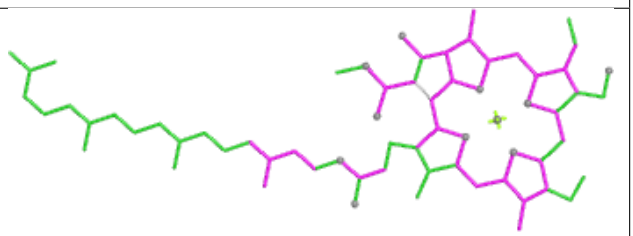


Rings

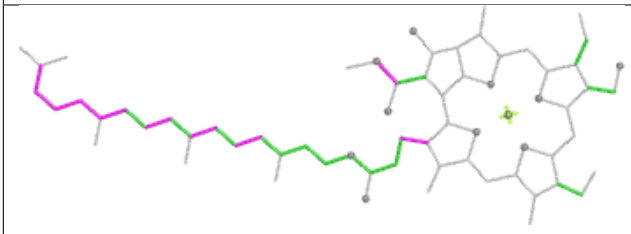
Ligand CHL Y 304



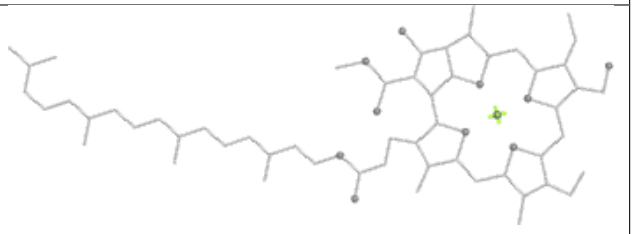
Bond lengths



Bond angles

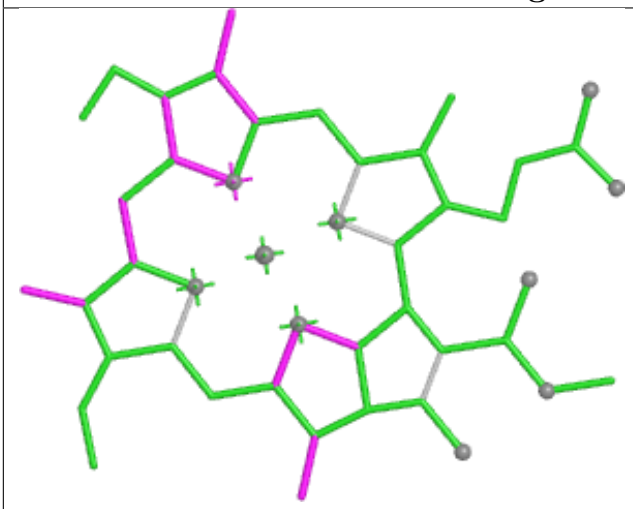


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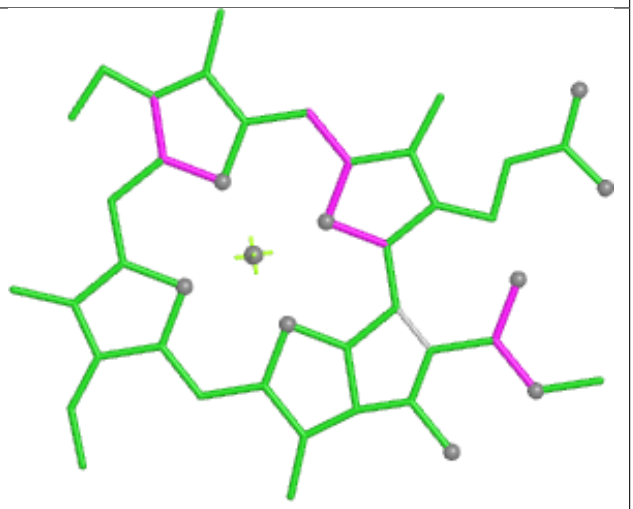


Rings

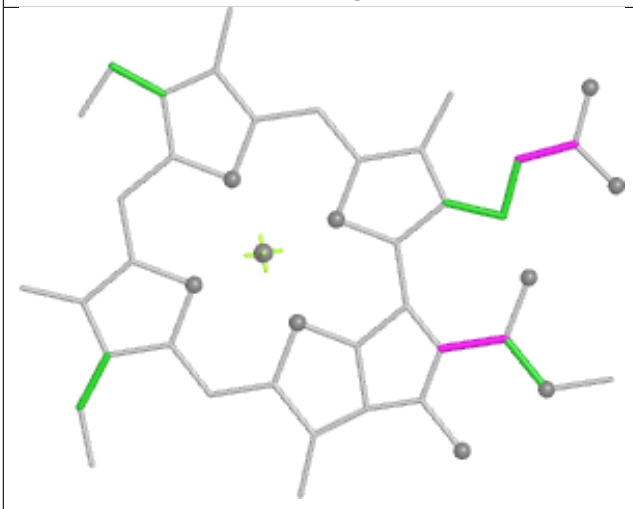
Ligand CLA 5 316



Bond lengths



Bond angles

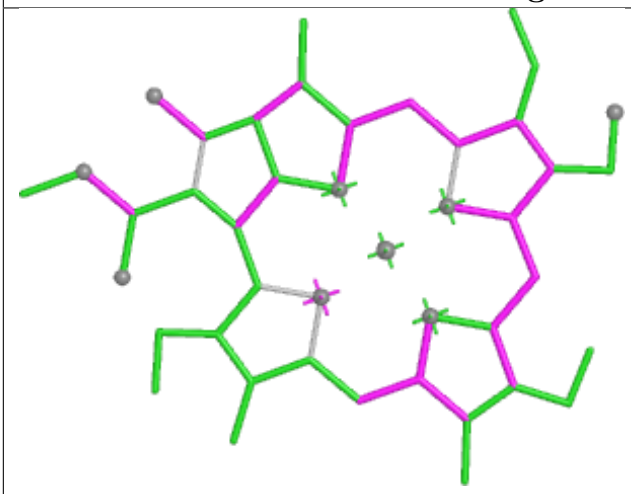


Torsions

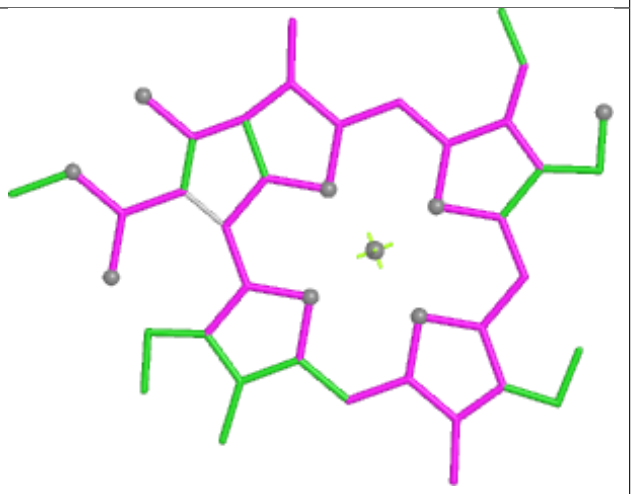


Rings

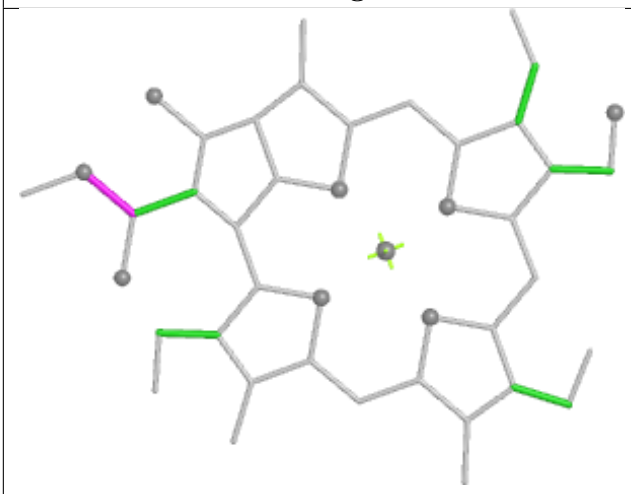
Ligand CHL 1 310



Bond lengths



Bond angles

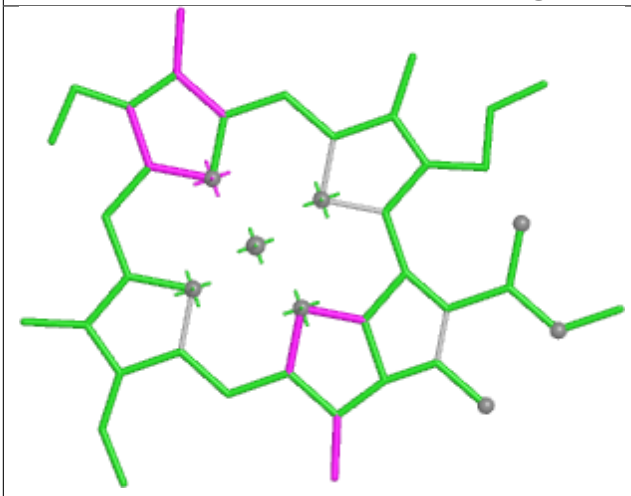


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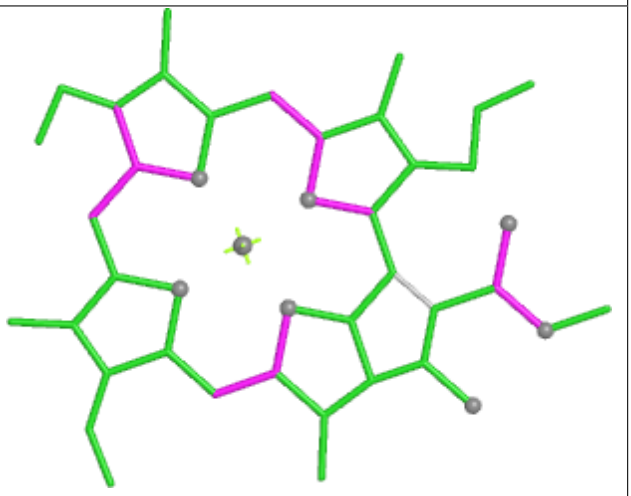


Rings

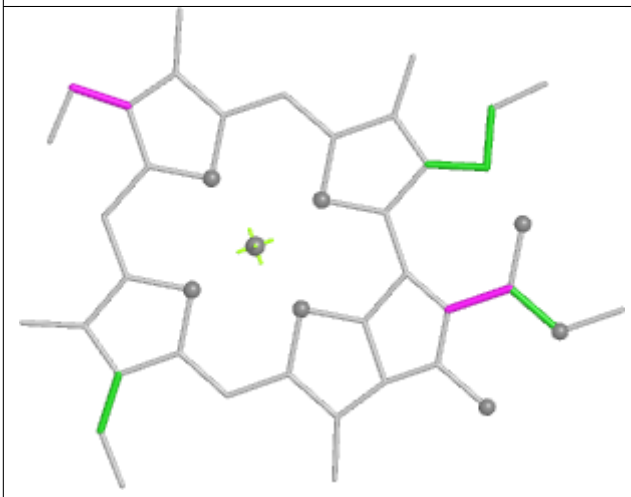
Ligand CLA s 405



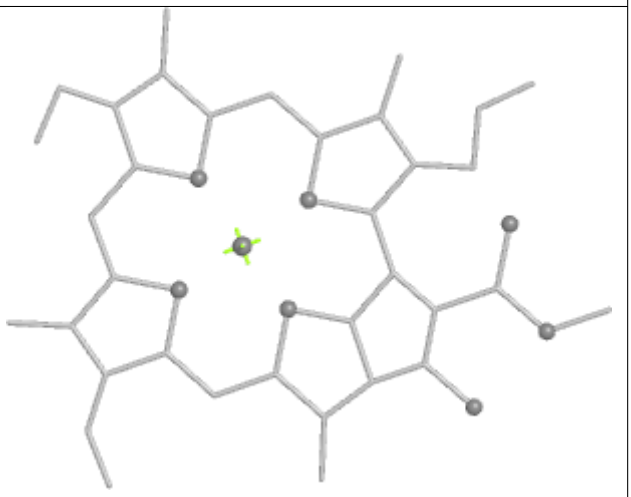
Bond lengths



Bond angles

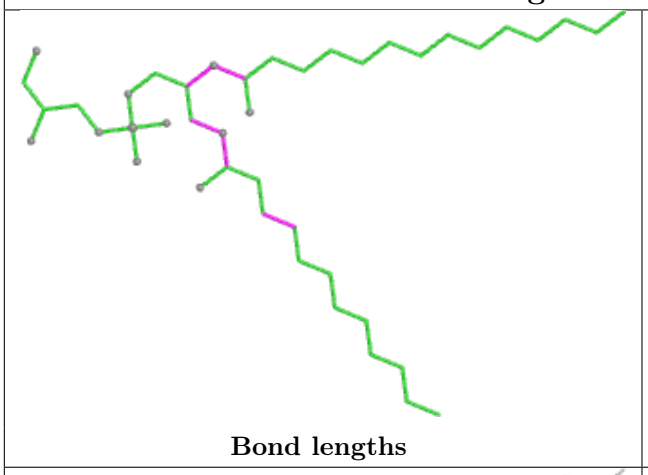


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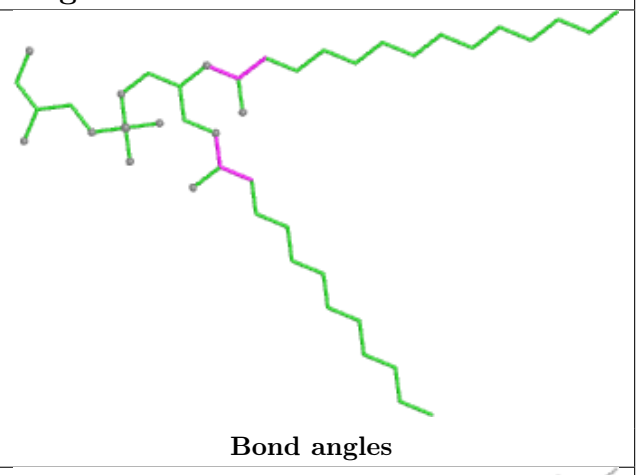


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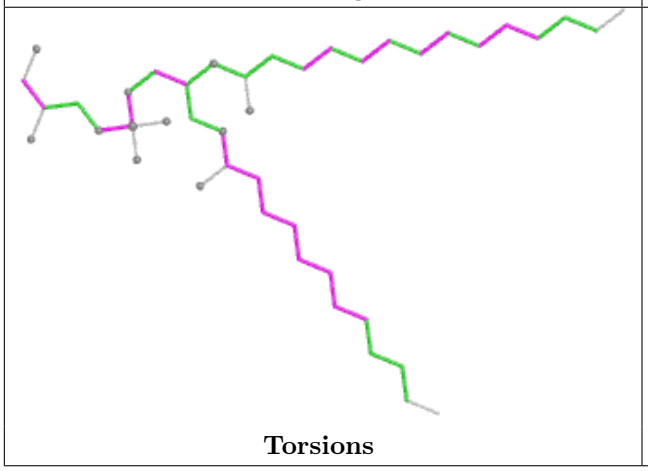
Ligand LHG g 319



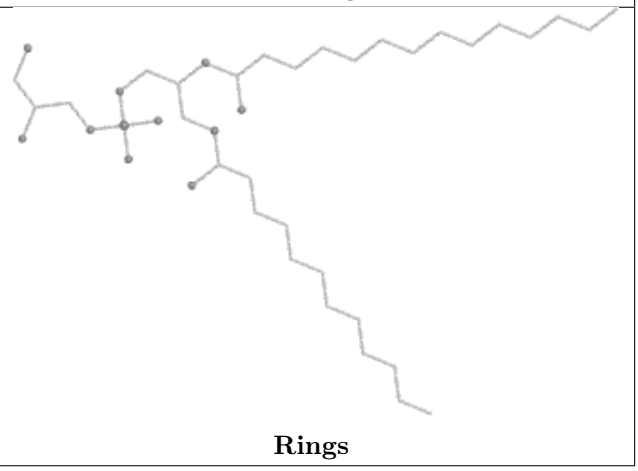
Bond lengths



Bond angles

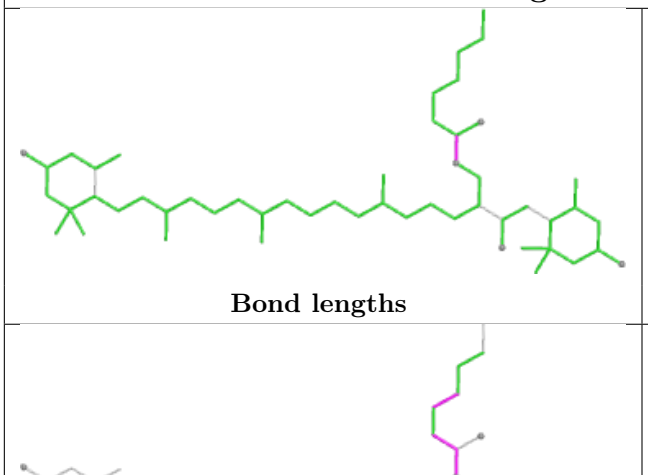


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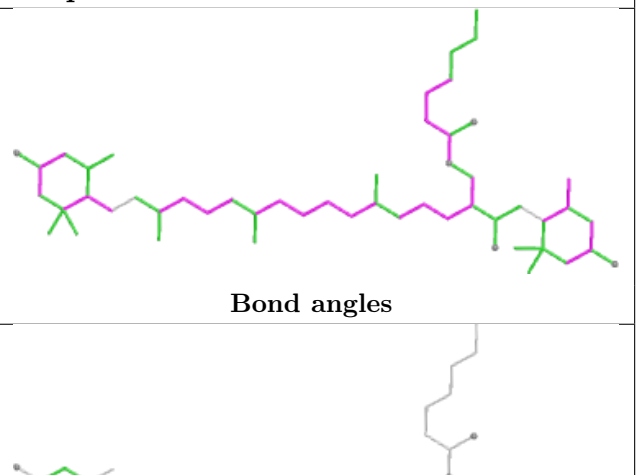


Rings

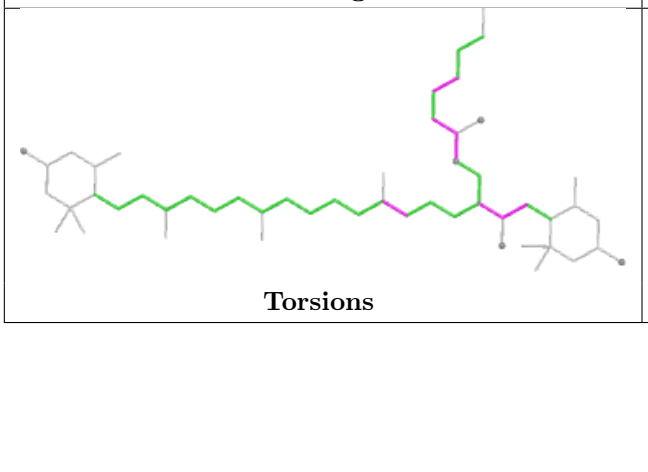
Ligand 0UR q 301



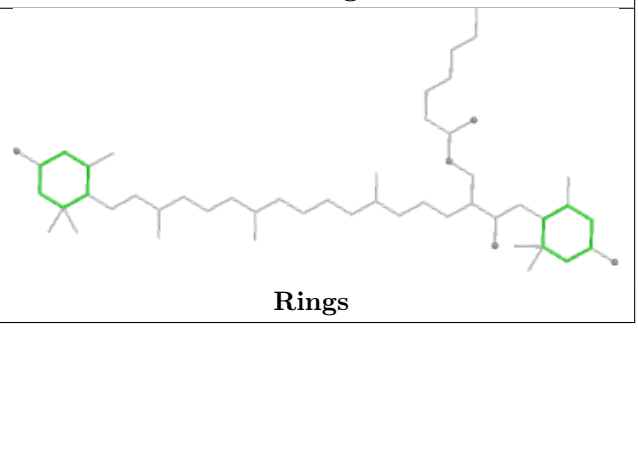
Bond lengths



Bond angles

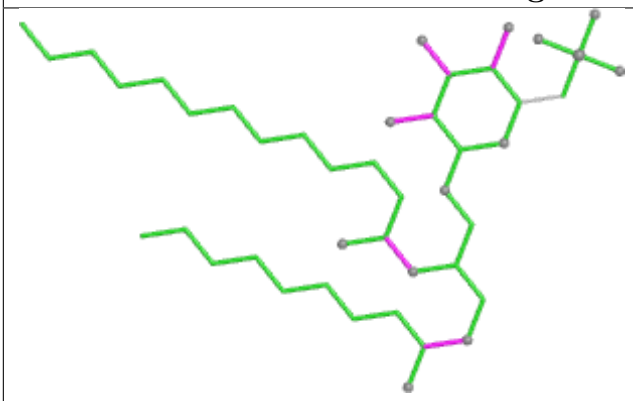


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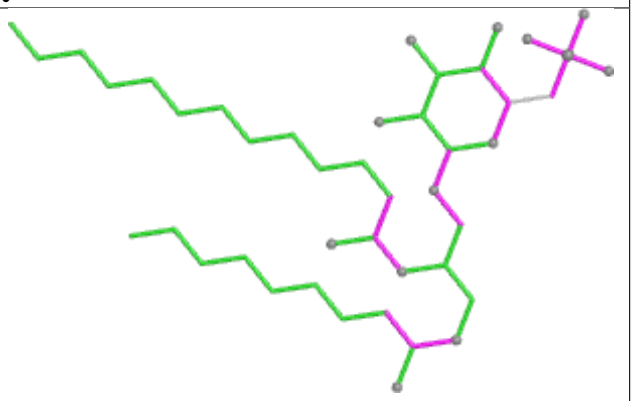


Rings

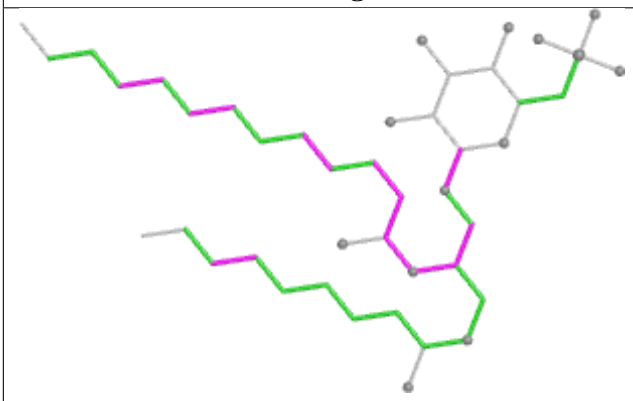
Ligand SQD d 409



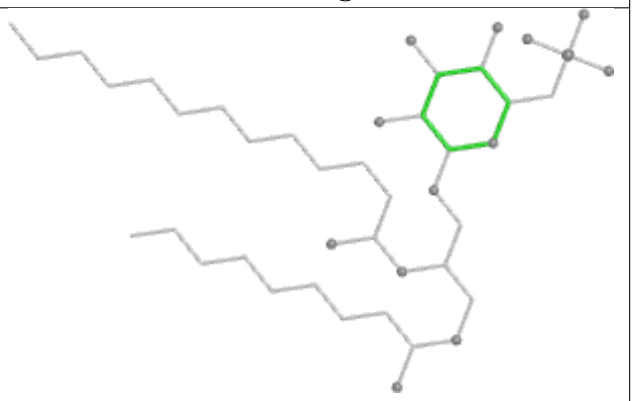
Bond lengths



Bond angles

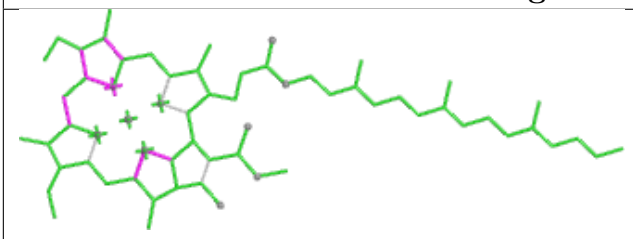


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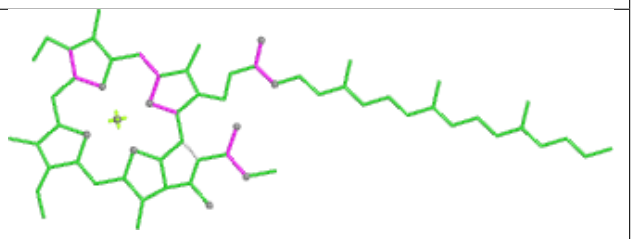


Rings

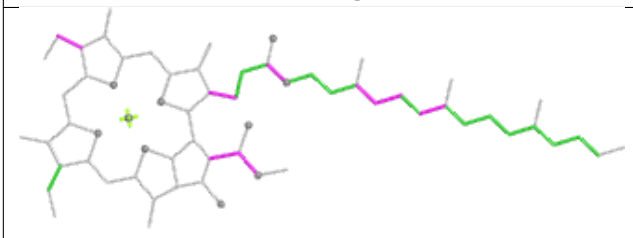
Ligand CLA 9 314



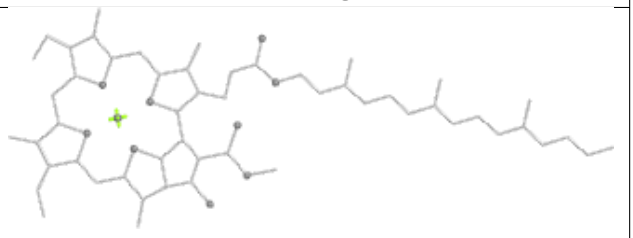
Bond lengths



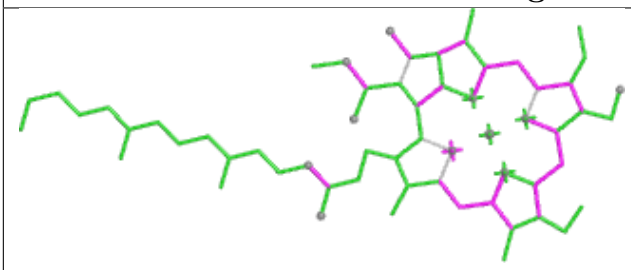
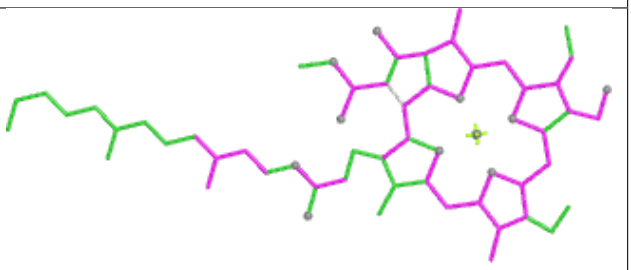
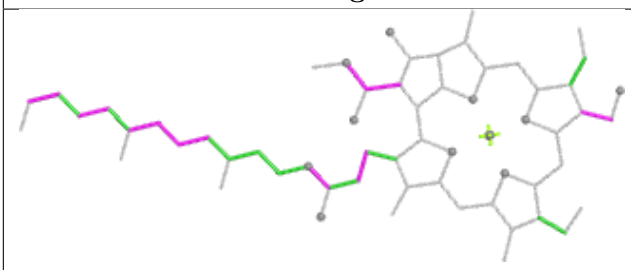
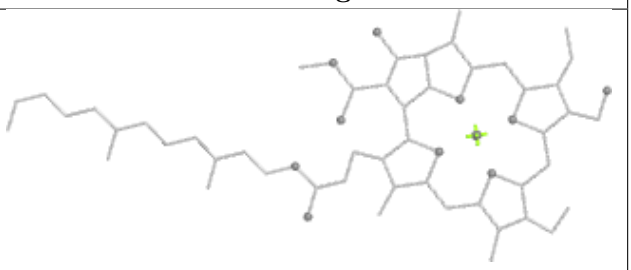
Bond angles

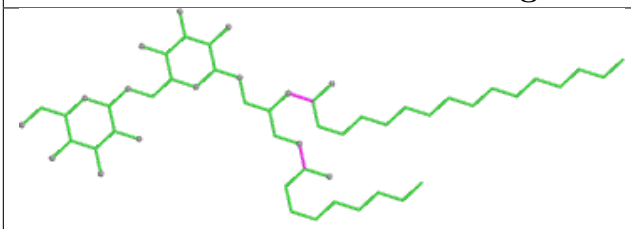
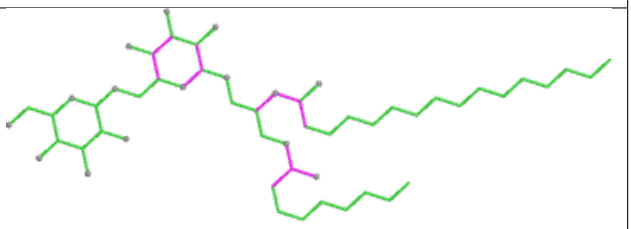
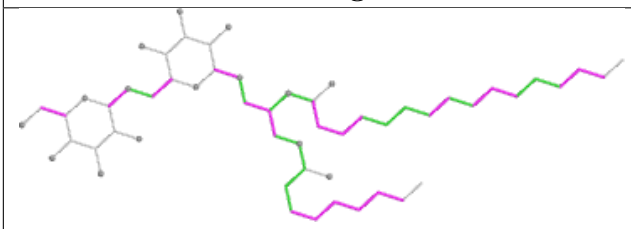
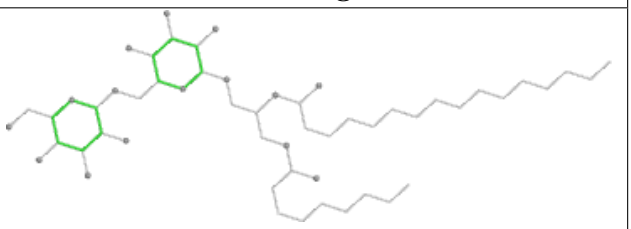


Torsions

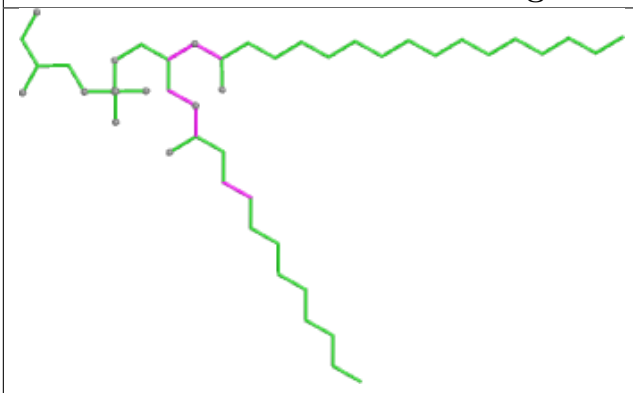


Rings

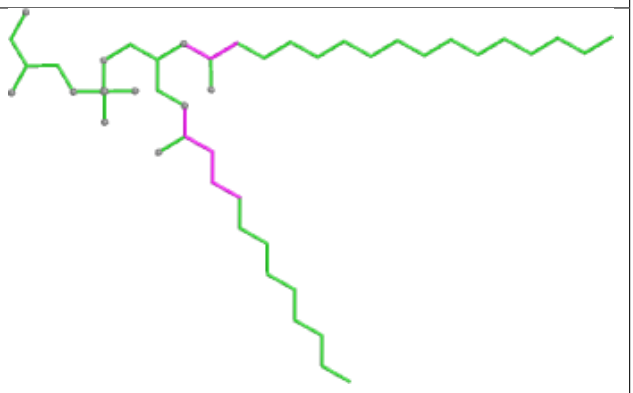
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD C 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

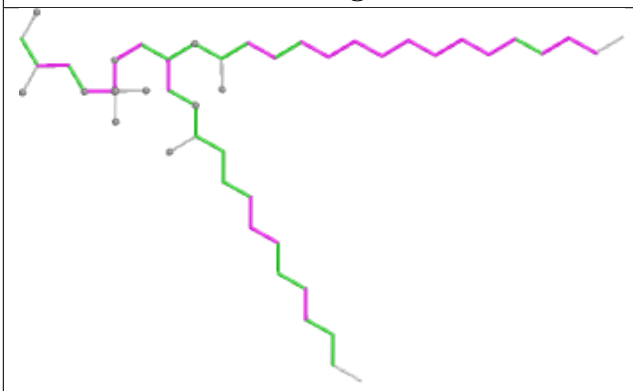
Ligand LHG a 601



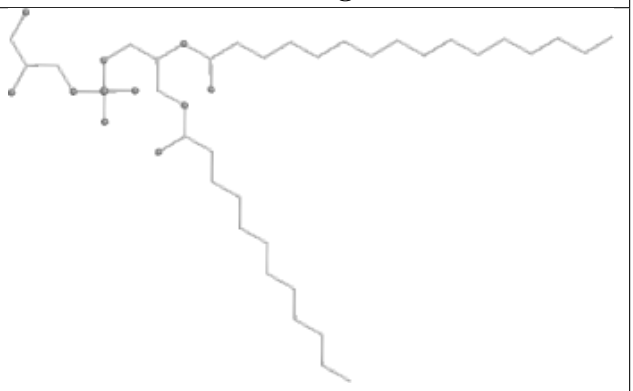
Bond lengths



Bond angles

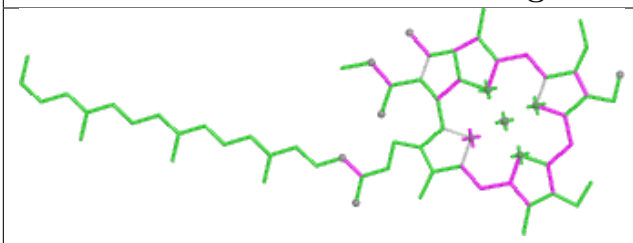


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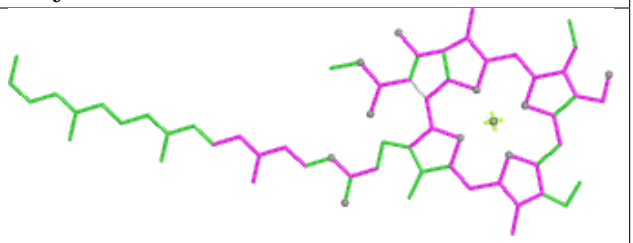


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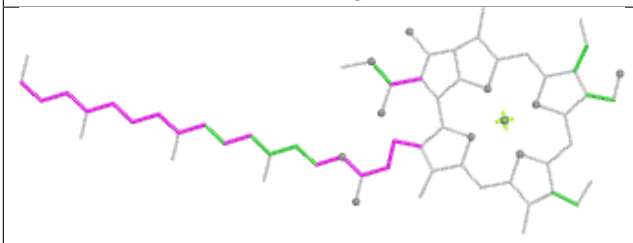
Ligand CHL y 306



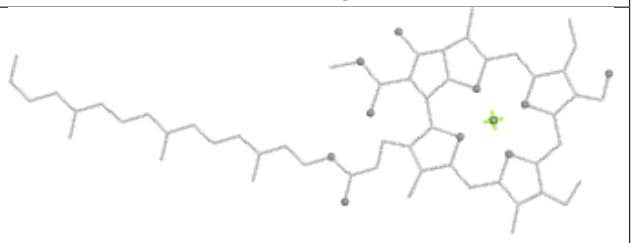
Bond lengths



Bond angles

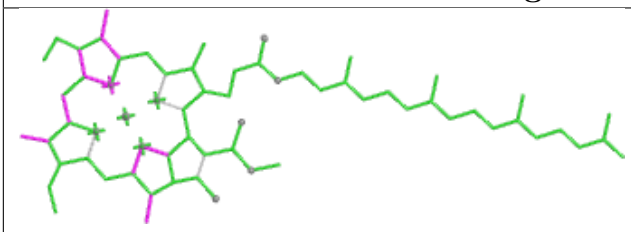


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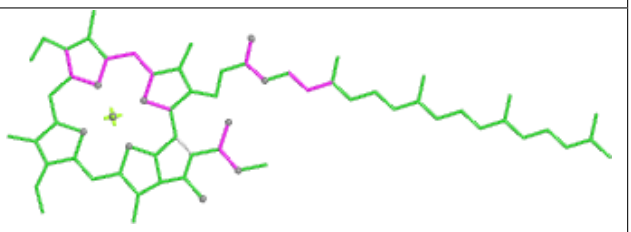


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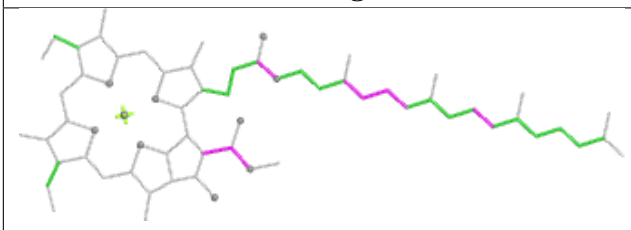
Ligand CLA B 613



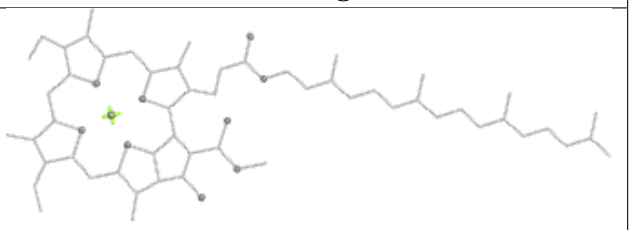
Bond lengths



Bond angles

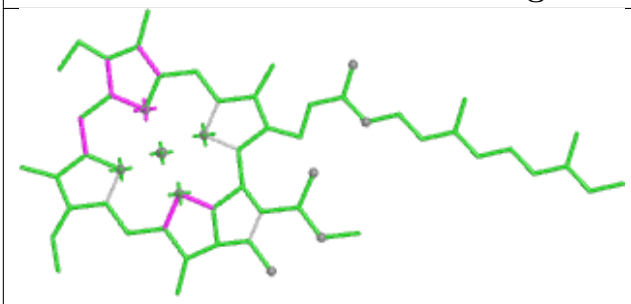


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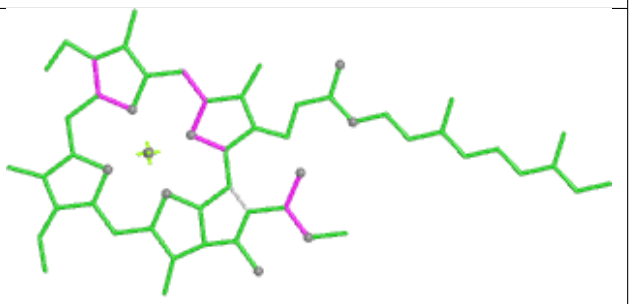


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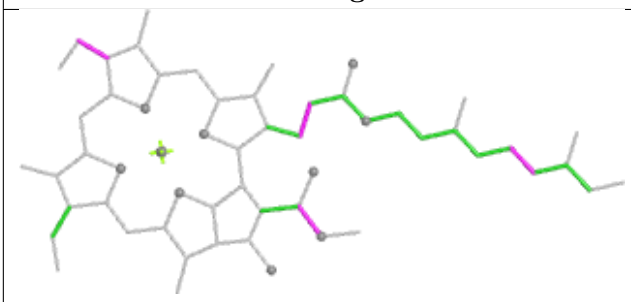
Ligand CLA u 307



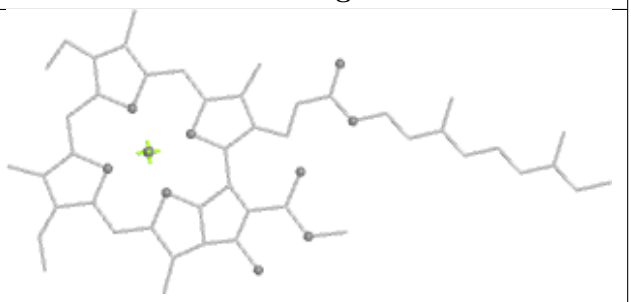
Bond lengths



Bond angles

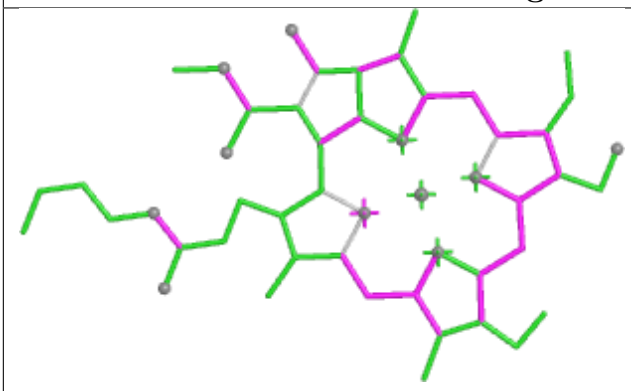


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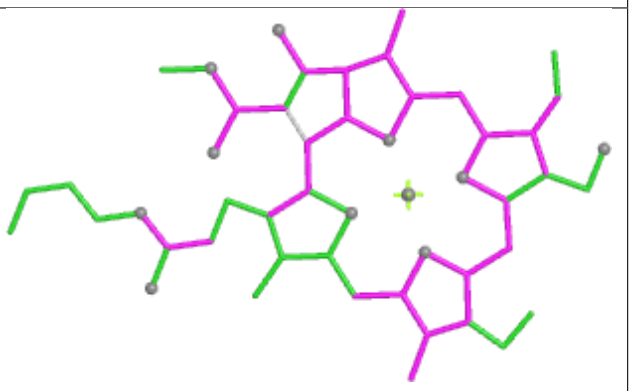


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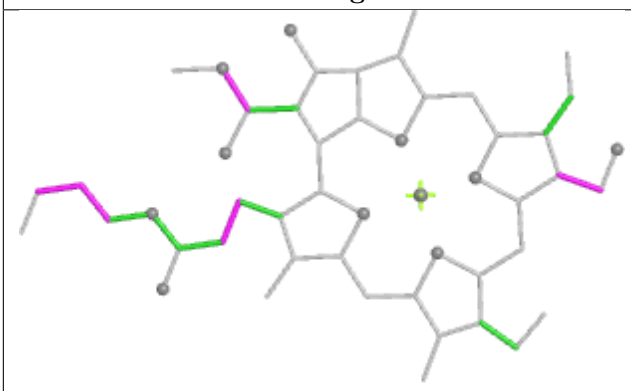
Ligand CHL n 311



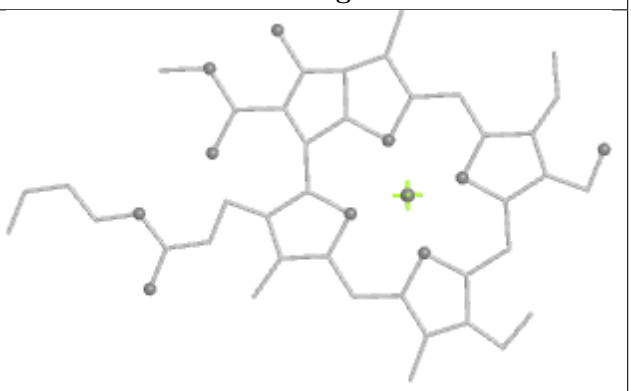
Bond lengths



Bond angles

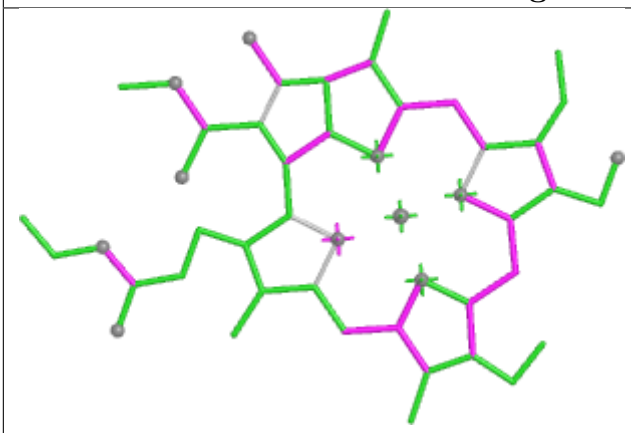


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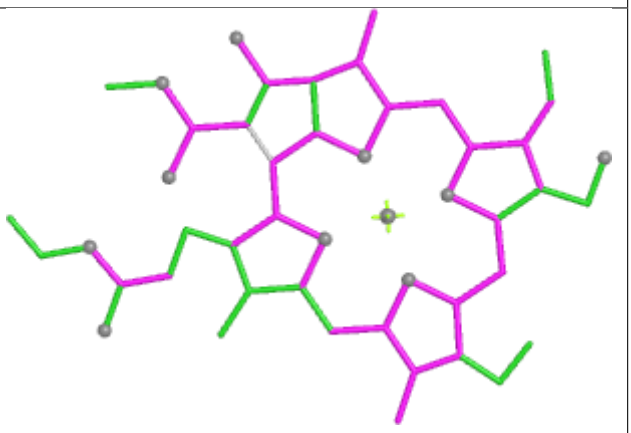


Rings

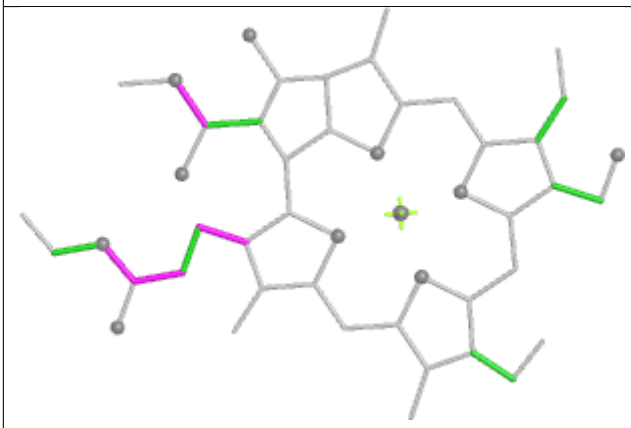
Ligand CHL r 307



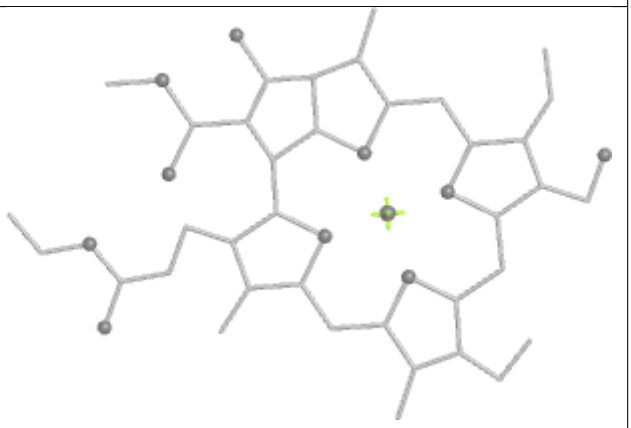
Bond lengths



Bond angles

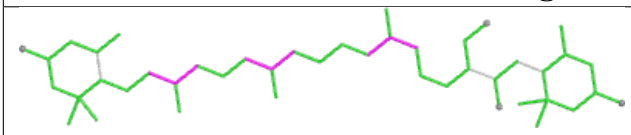


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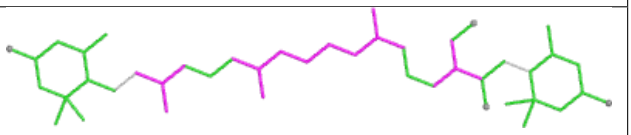


Rings

Ligand 0IE 8 302



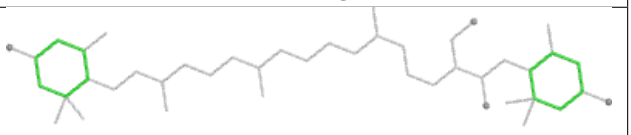
Bond lengths



Bond angles

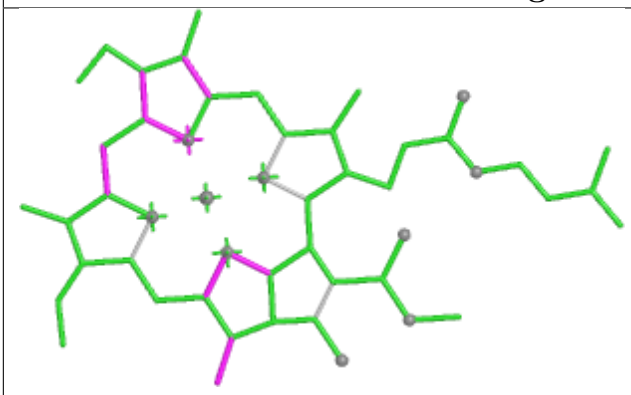


Torsions

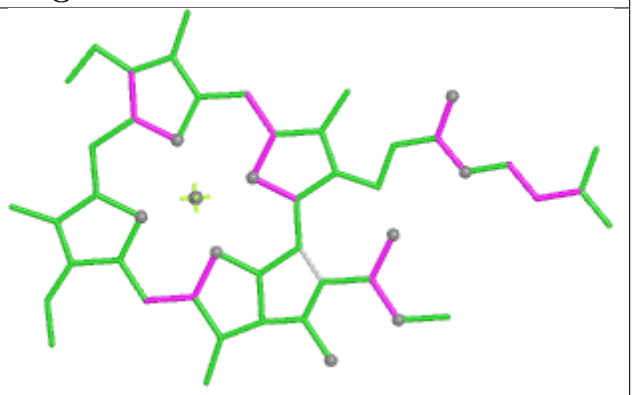


Rings

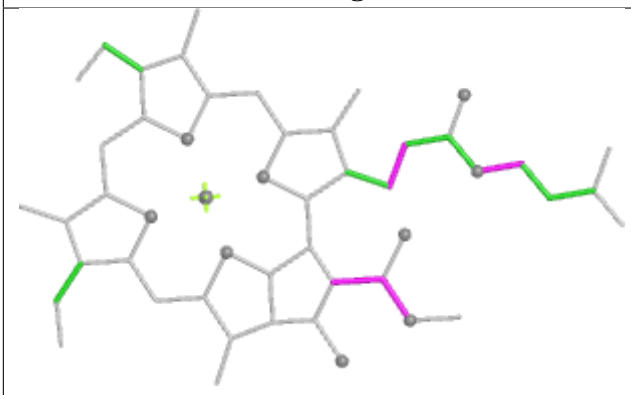
Ligand CLA g 308



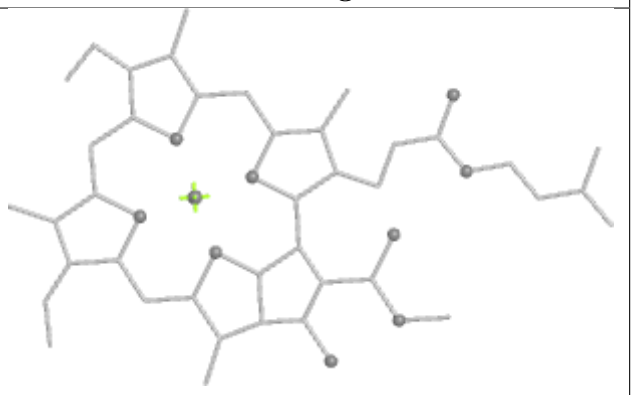
Bond lengths



Bond angles

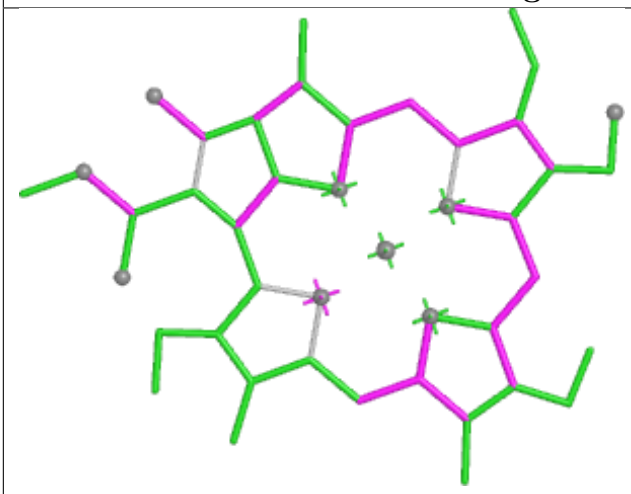


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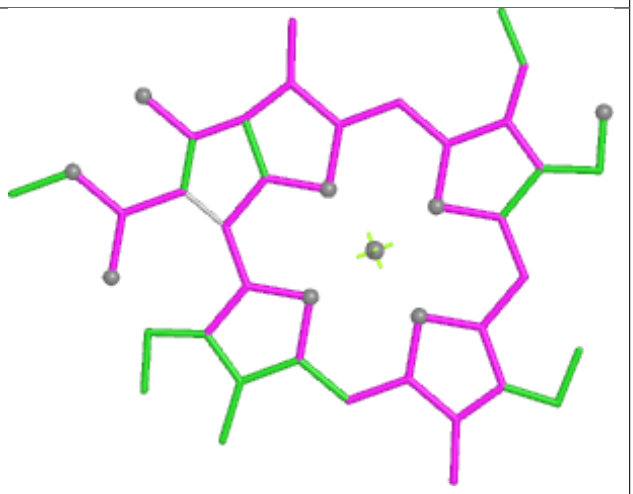


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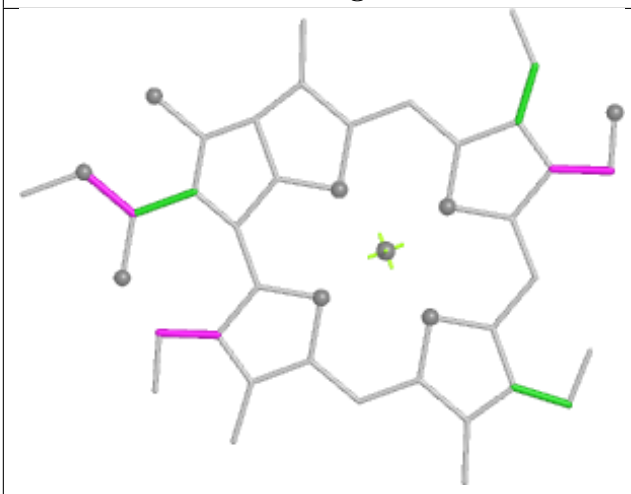
Ligand CHL Y 308



Bond lengths



Bond angles

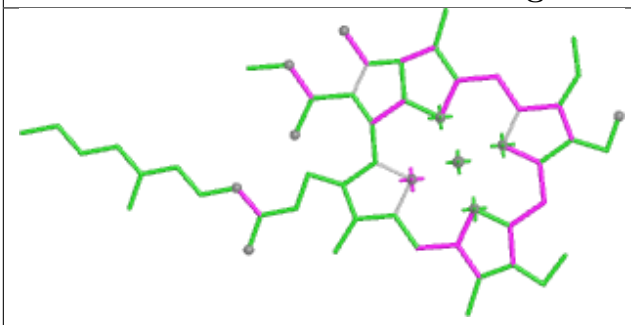


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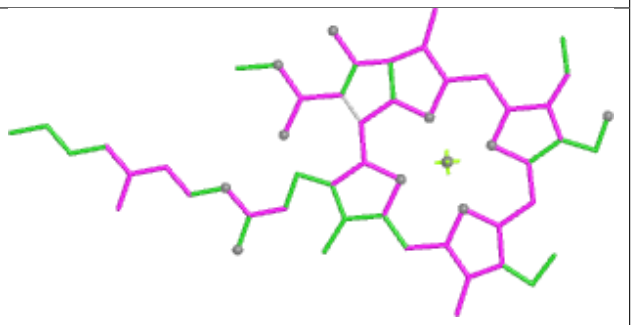


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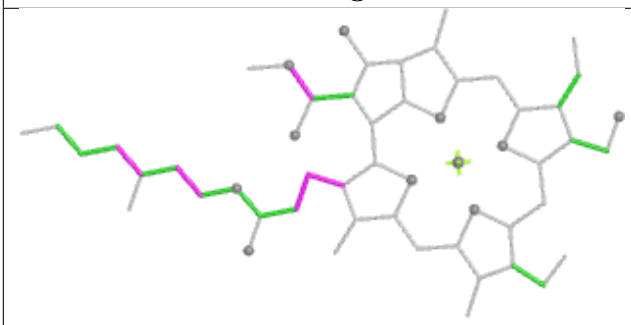
Ligand CHL n 304



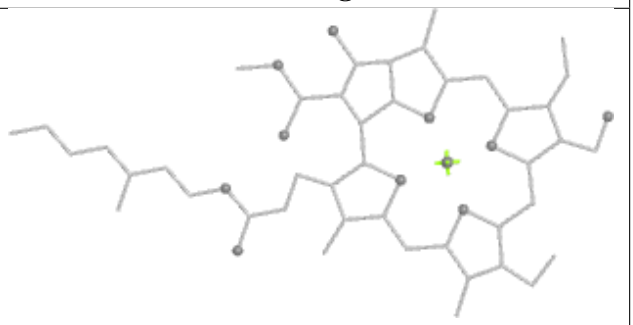
Bond lengths



Bond angles

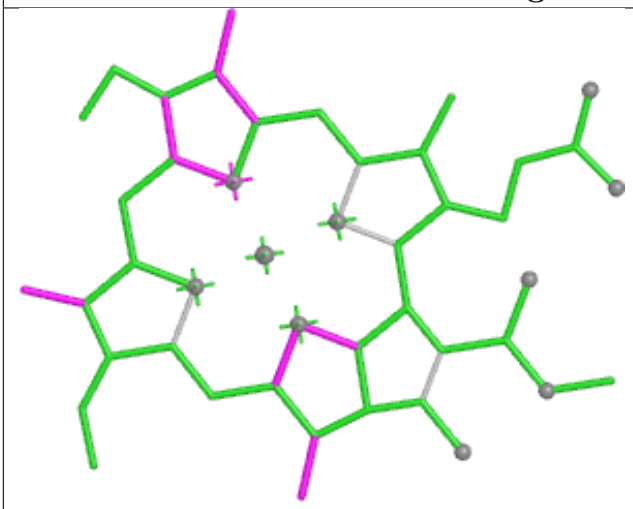


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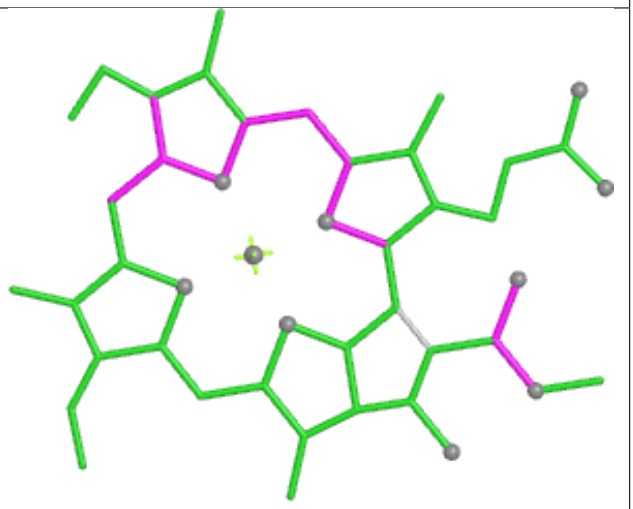


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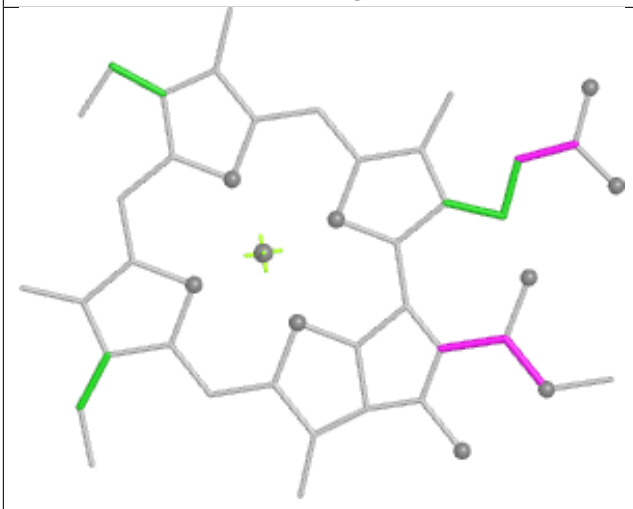
Ligand CLA S 603



Bond lengths



Bond angles

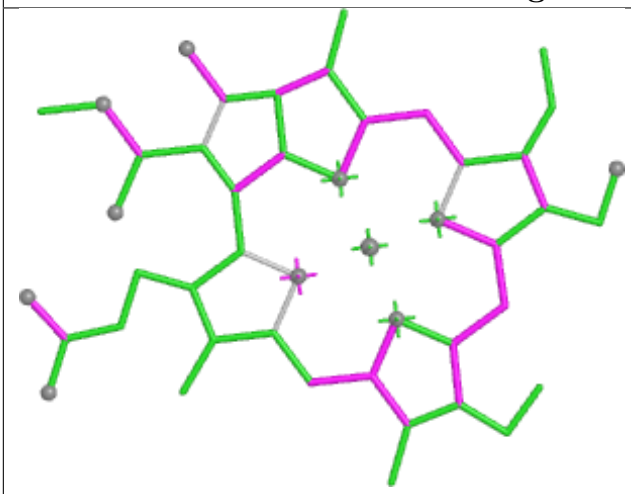


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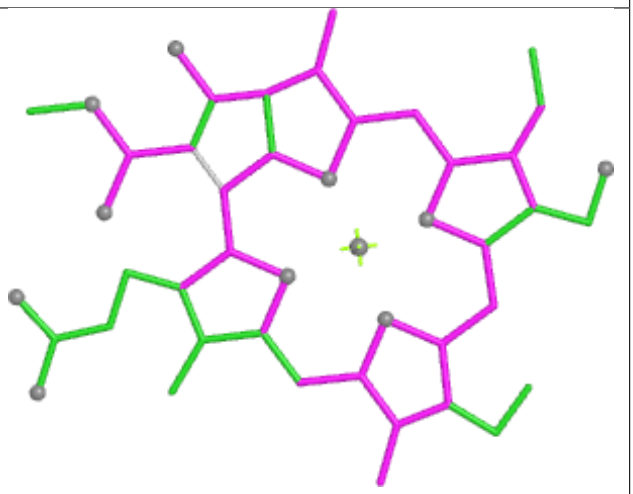


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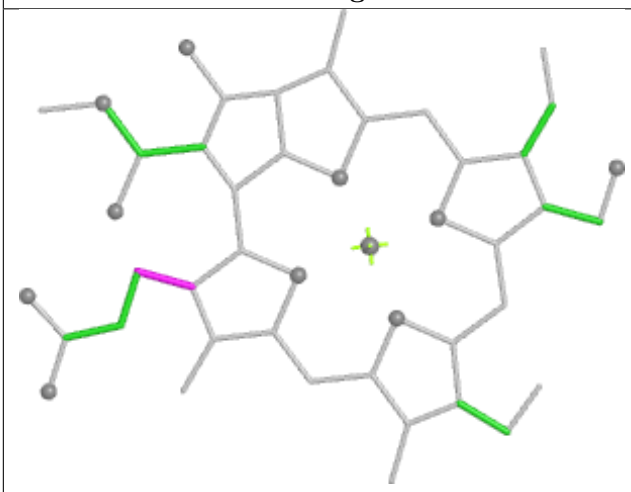
Ligand CHL 7 311



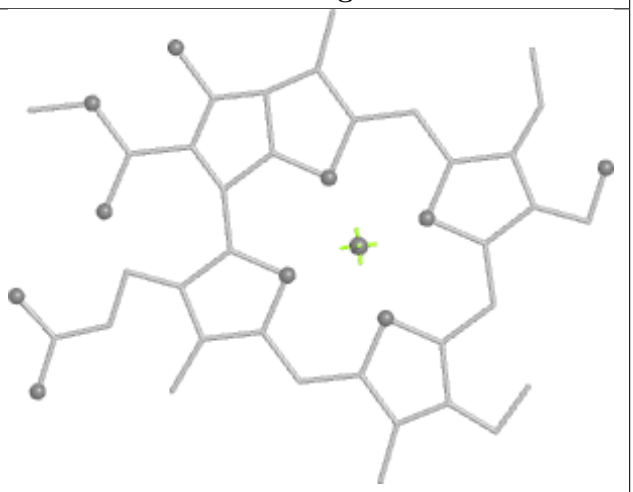
Bond lengths



Bond angles

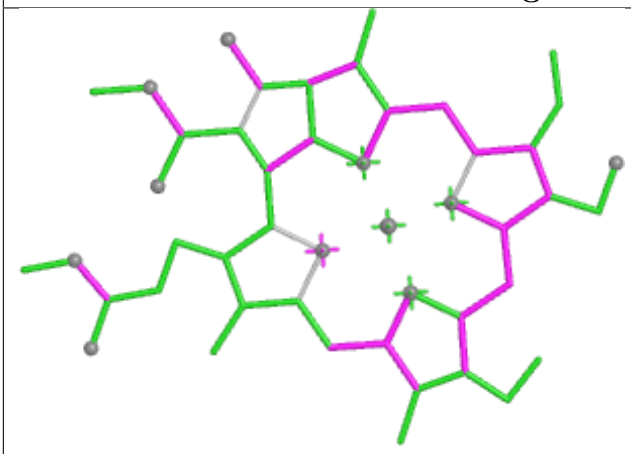


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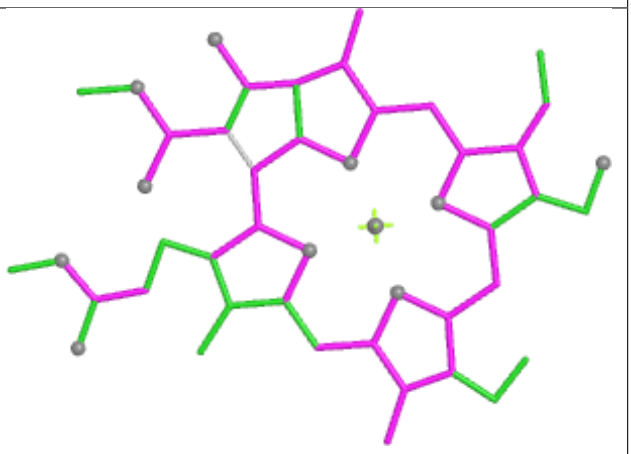


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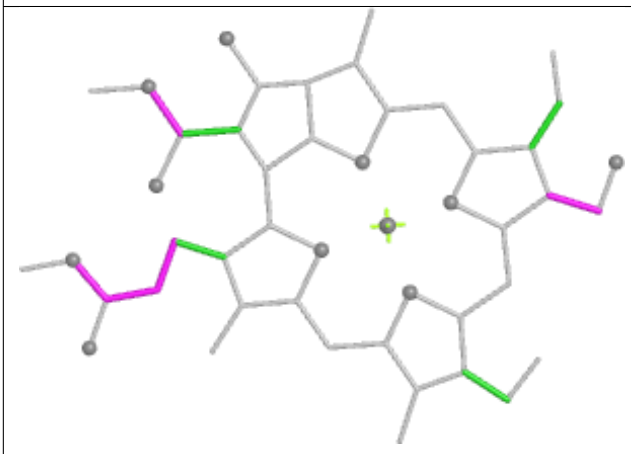
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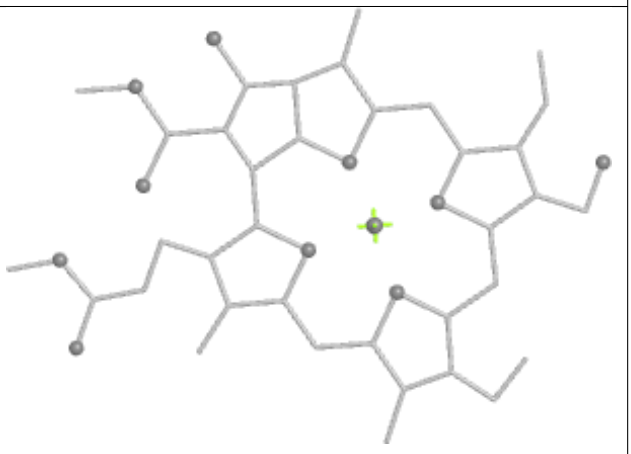
Bond lengths



Bond angles

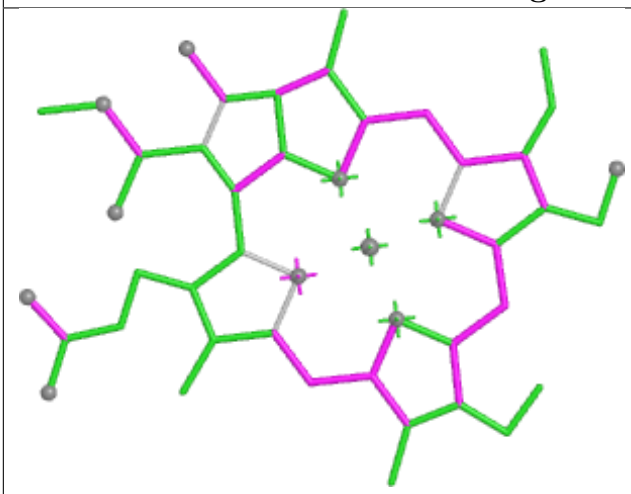


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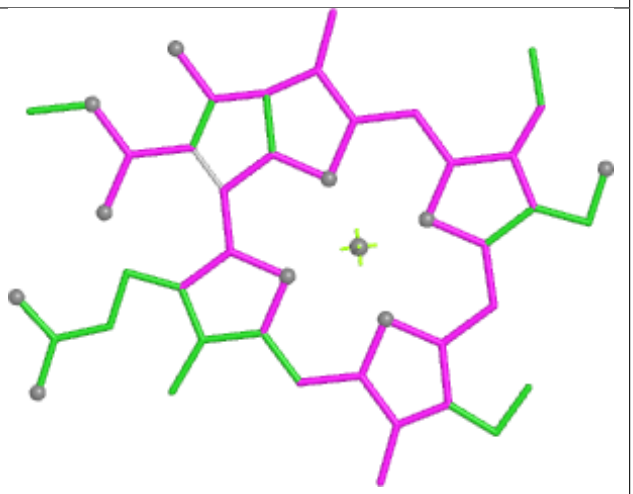


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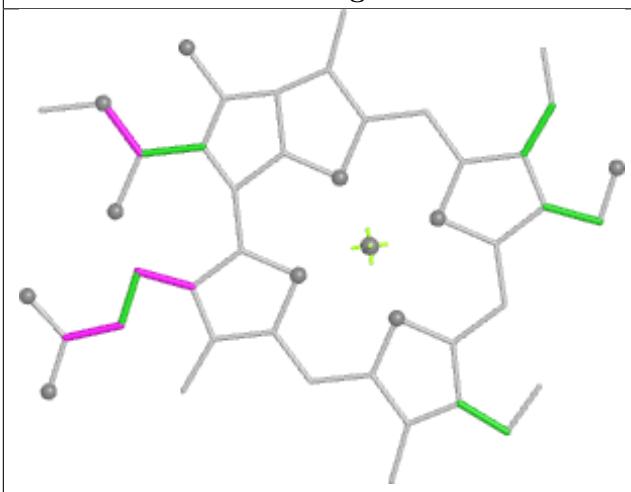
Ligand CHL s 407



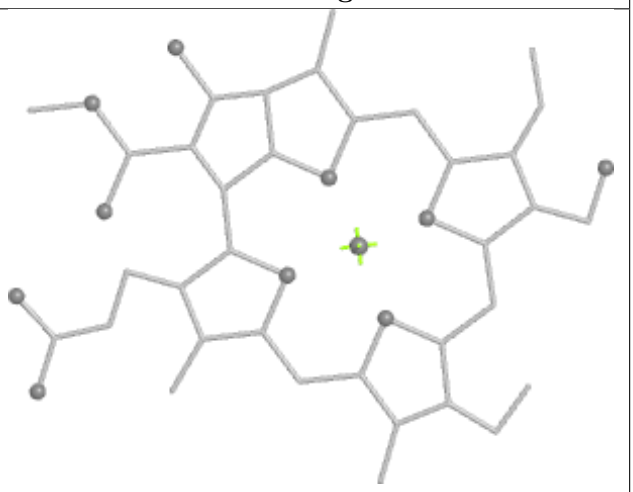
Bond lengths



Bond angles

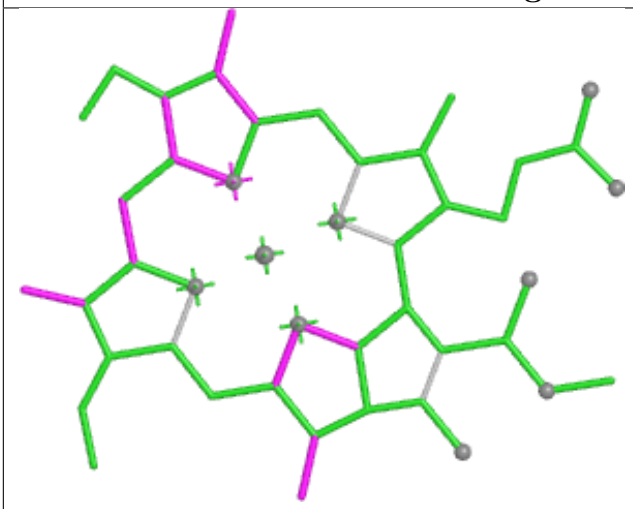


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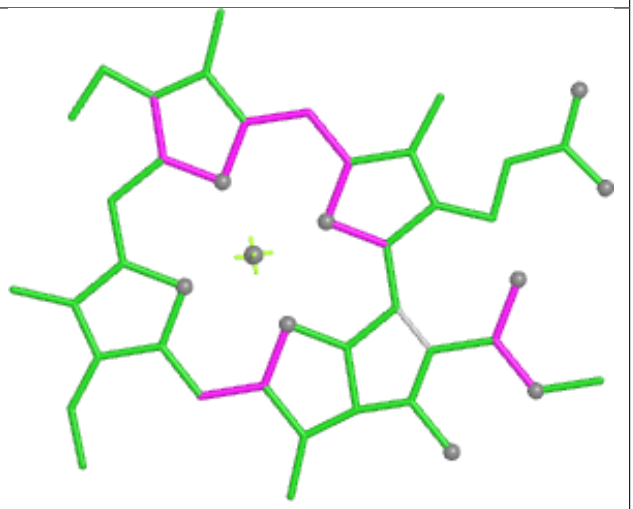


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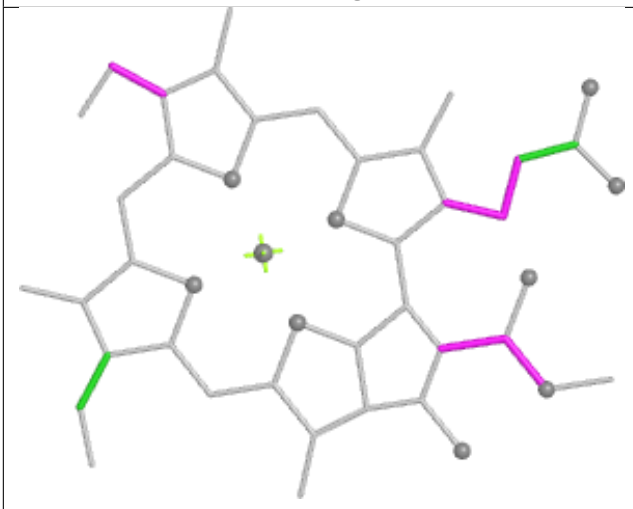
Ligand CLA B 601



Bond lengths



Bond angles

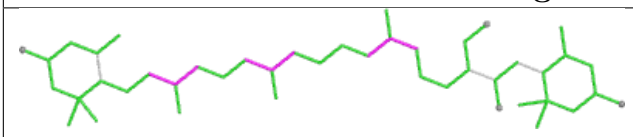


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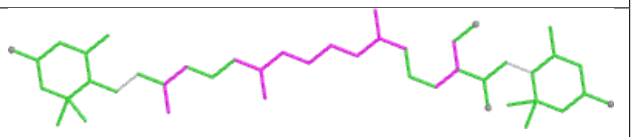


Rings

Ligand 0IE Y 303



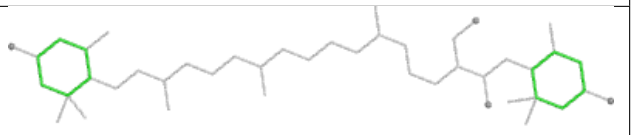
Bond lengths



Bond angles

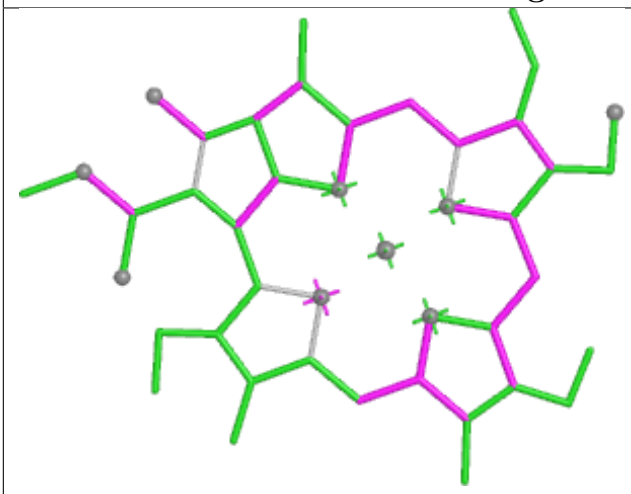


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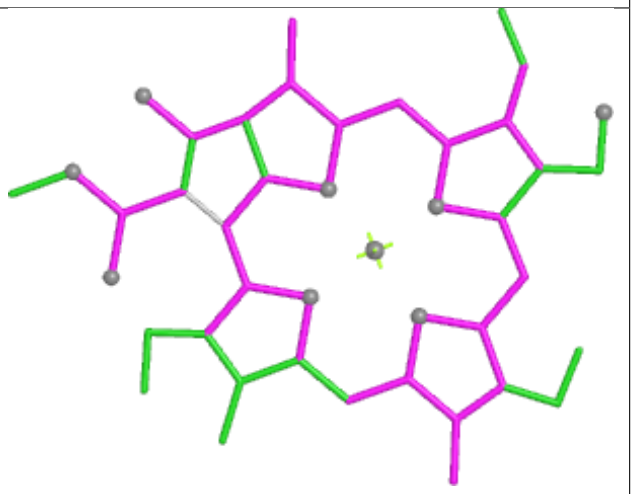


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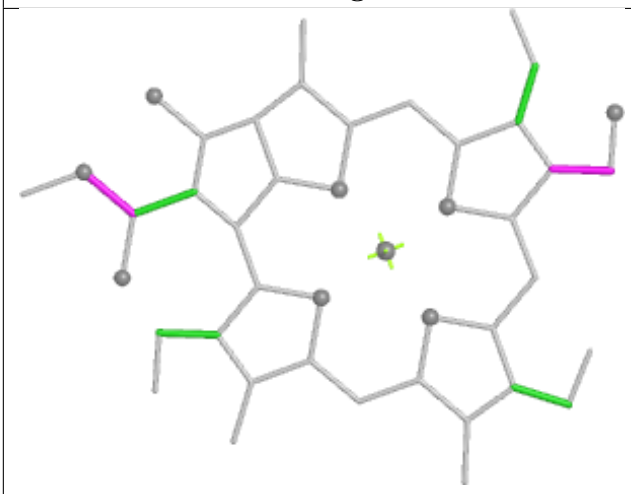
Ligand CHL 6 312



Bond lengths



Bond angles

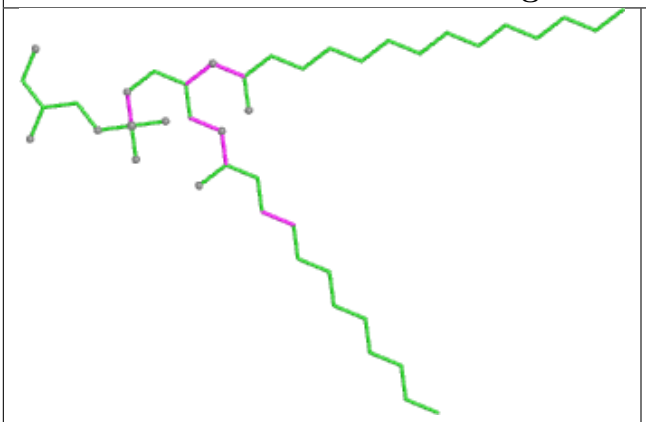


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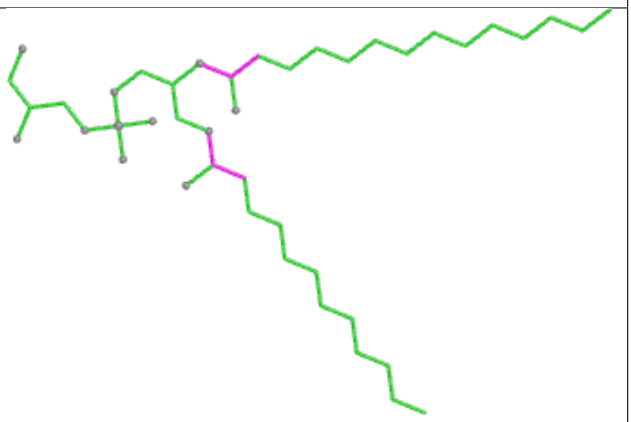


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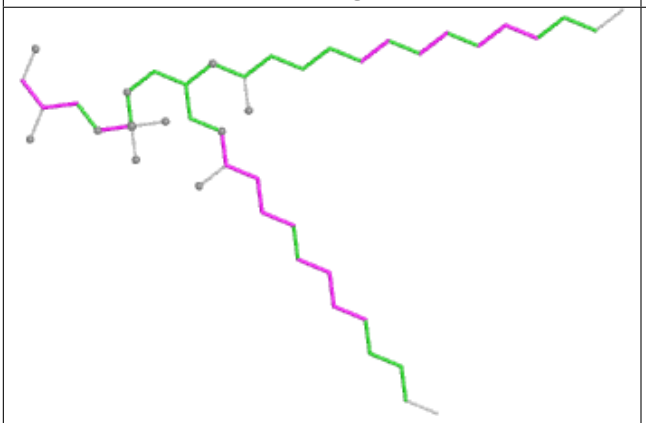
Ligand LHG N 318



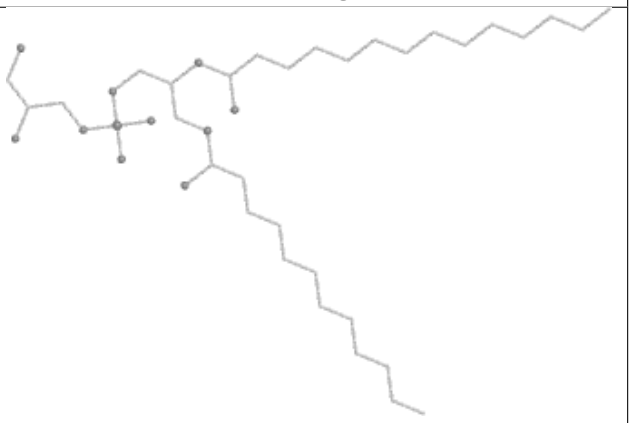
Bond lengths



Bond angles



Torsions



Rings

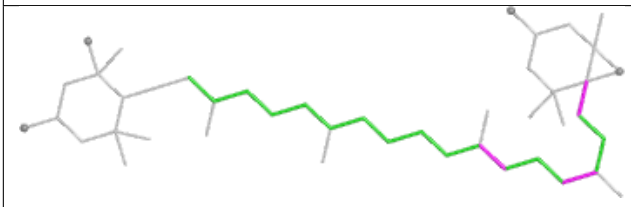
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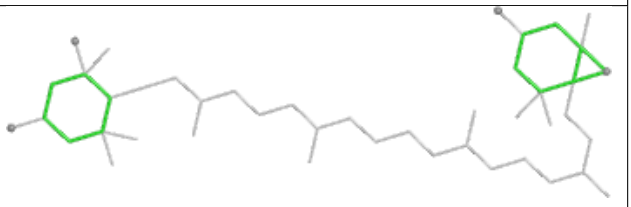
Bond lengths



Bond angles

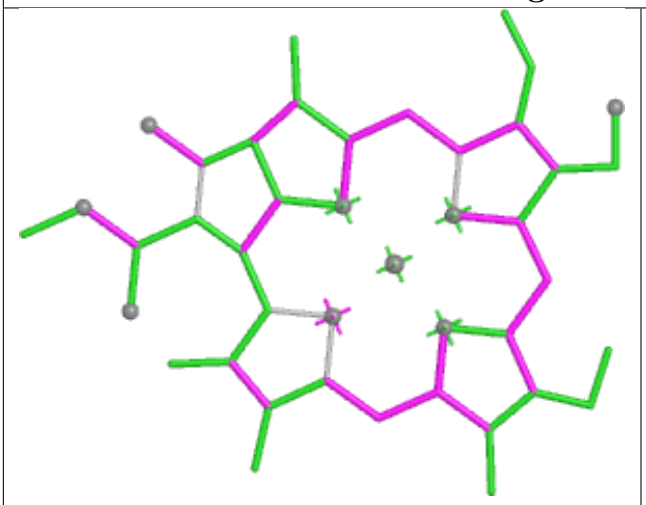


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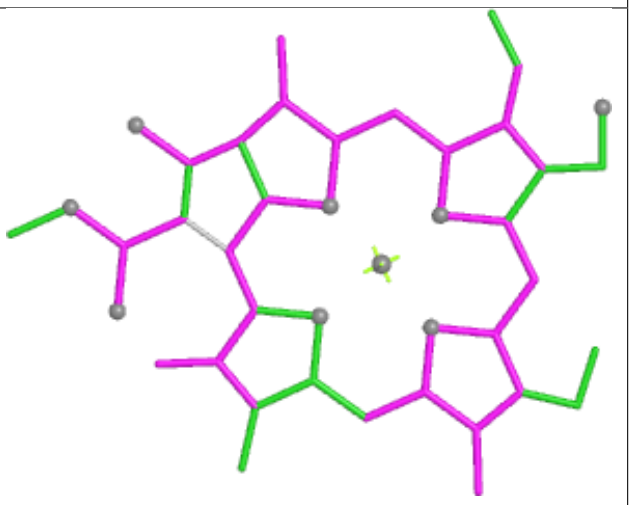


Rings

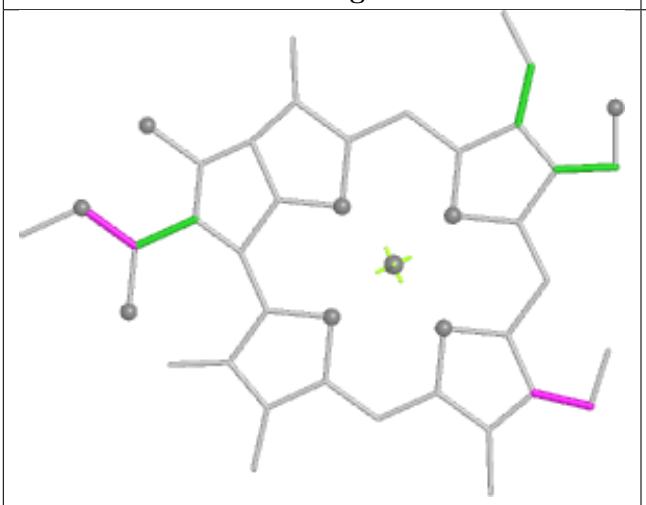
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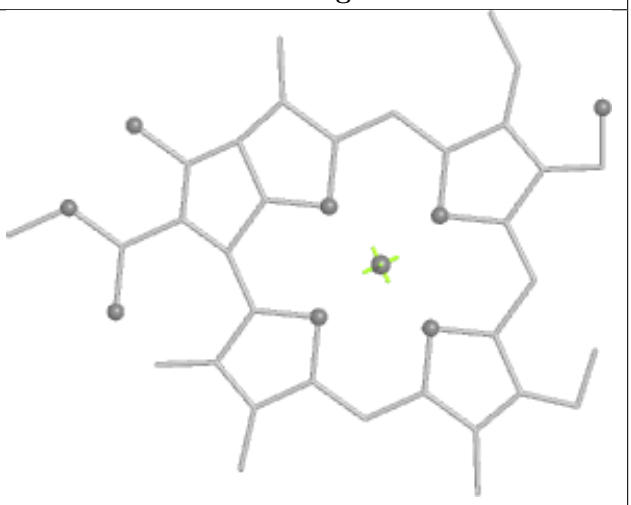
Bond lengths



Bond angles

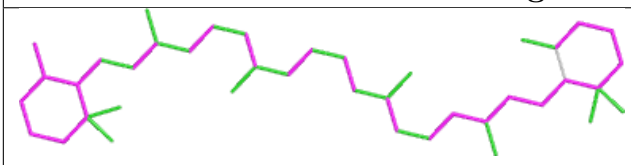


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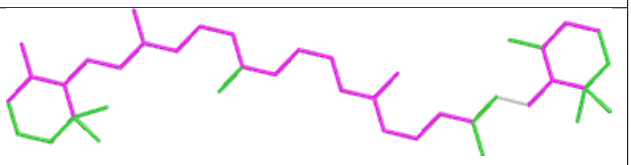


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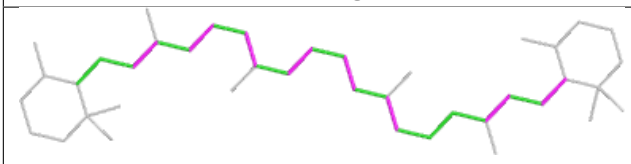
Ligand 8CT B 617



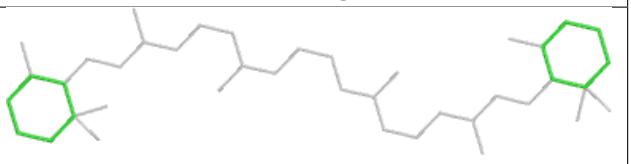
Bond lengths



Bond angles

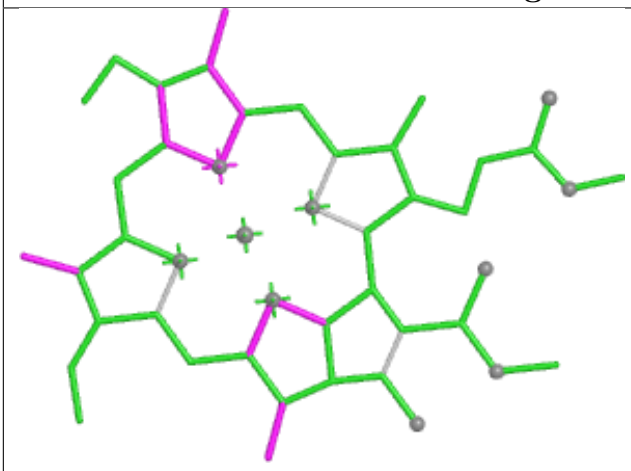


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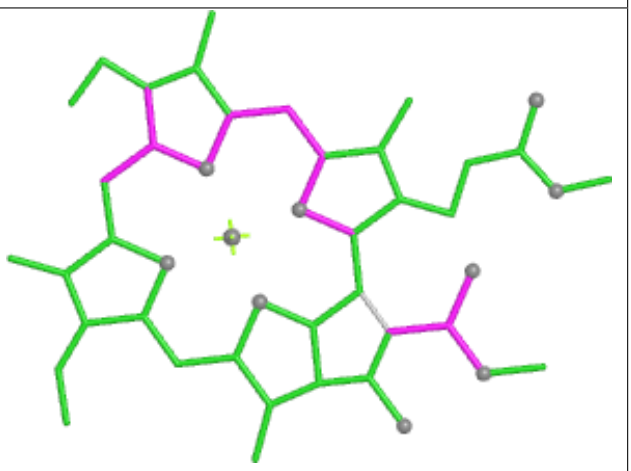


Rings

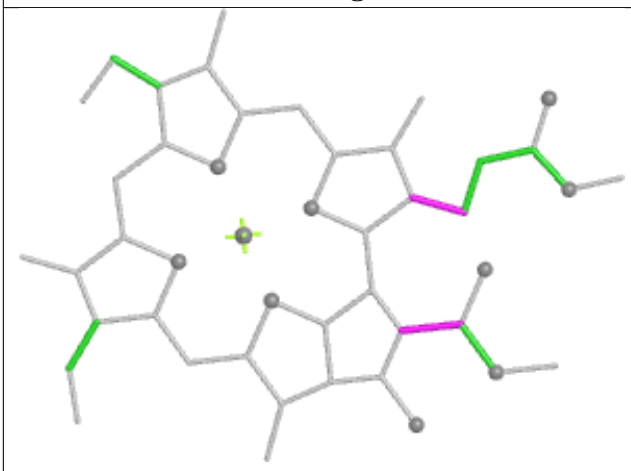
Ligand CLA C 616



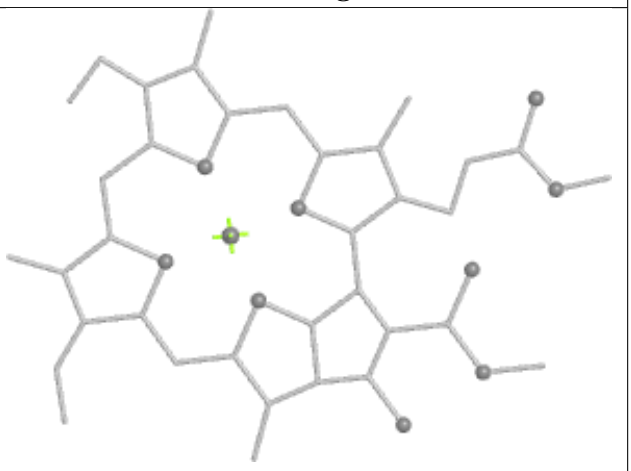
Bond lengths



Bond angles

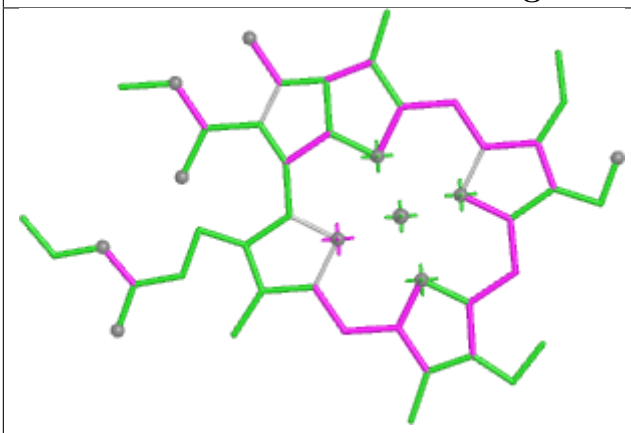


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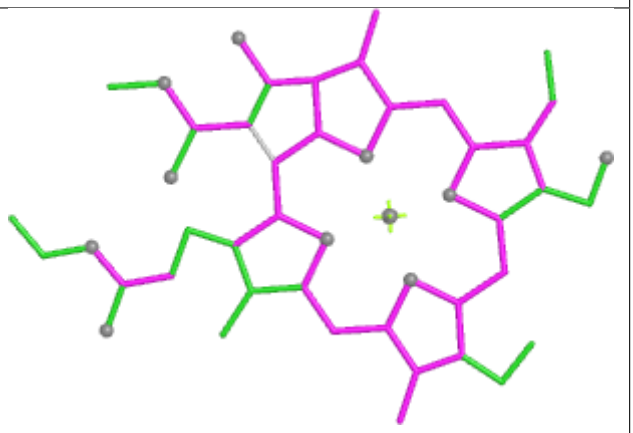


Rings

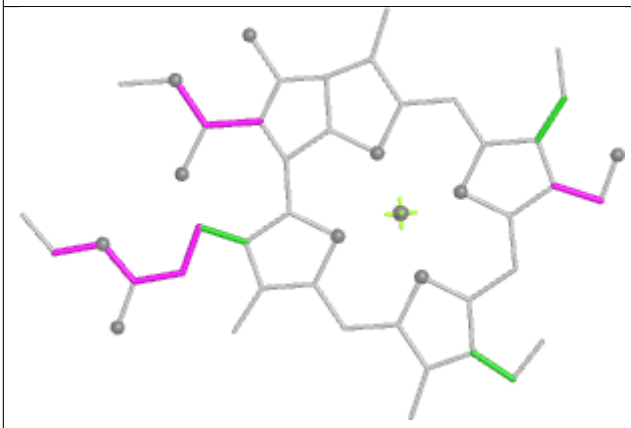
Ligand CHL R 607



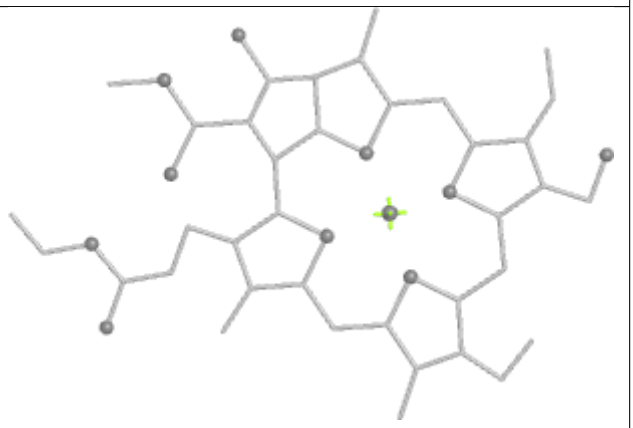
Bond lengths



Bond angles

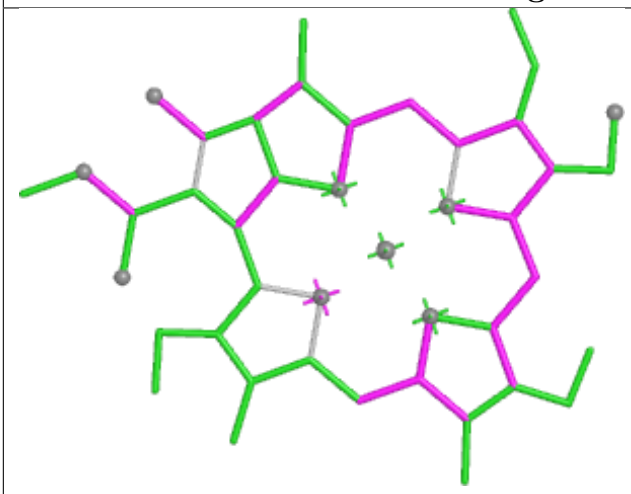


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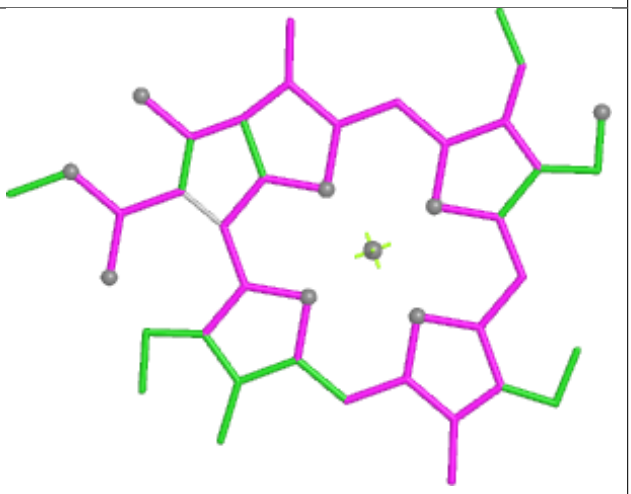


Rings

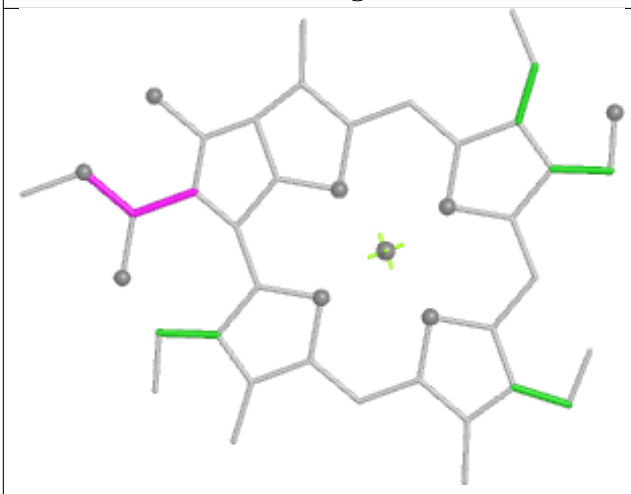
Ligand CHL 2 309



Bond lengths



Bond angles

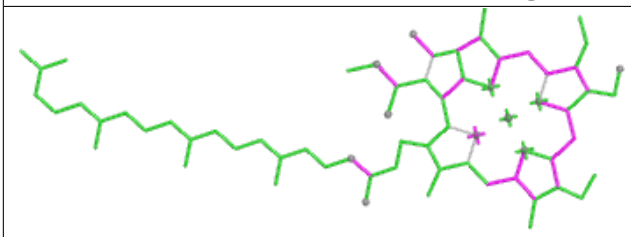


Torsions

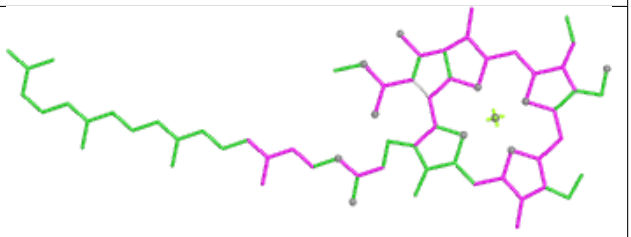


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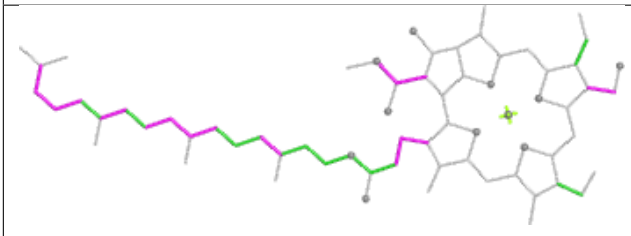
Ligand CHL G 305



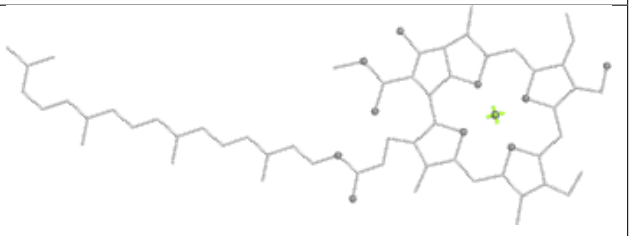
Bond lengths



Bond angles

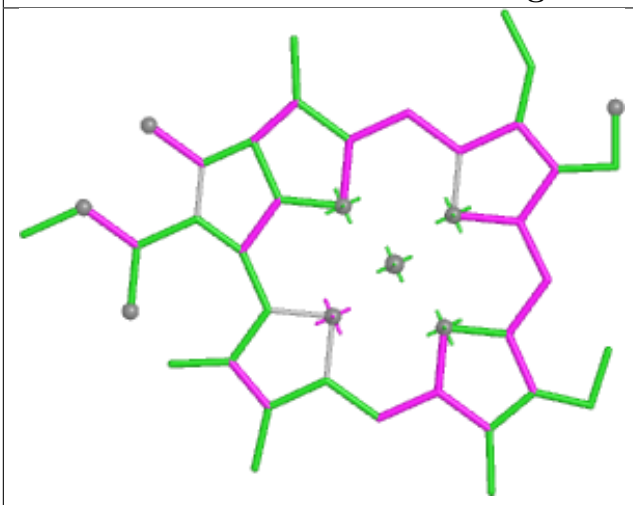


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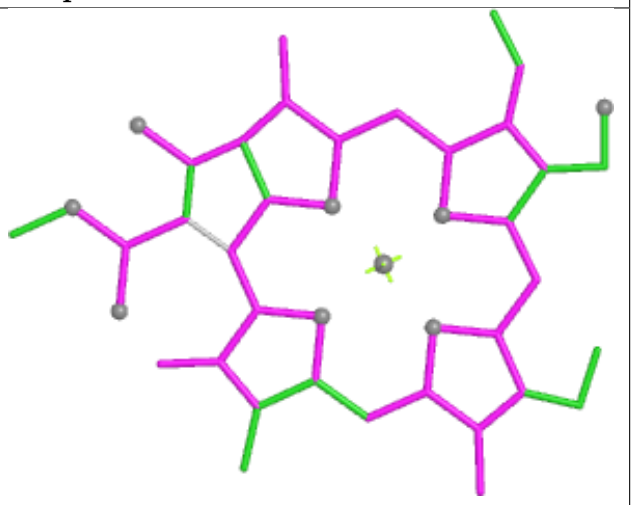


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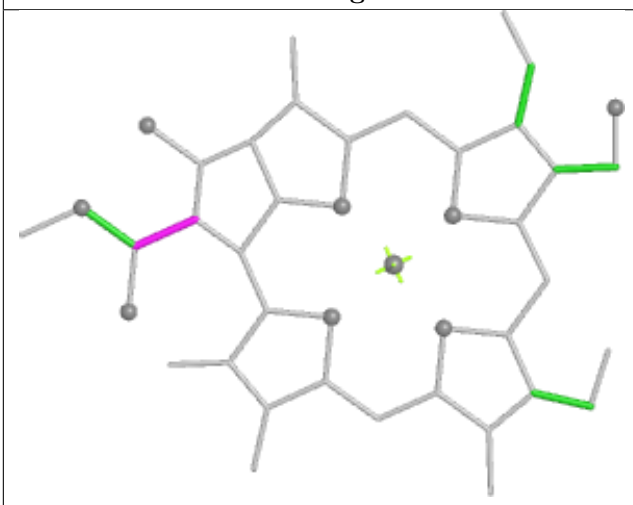
Ligand CHL q 316



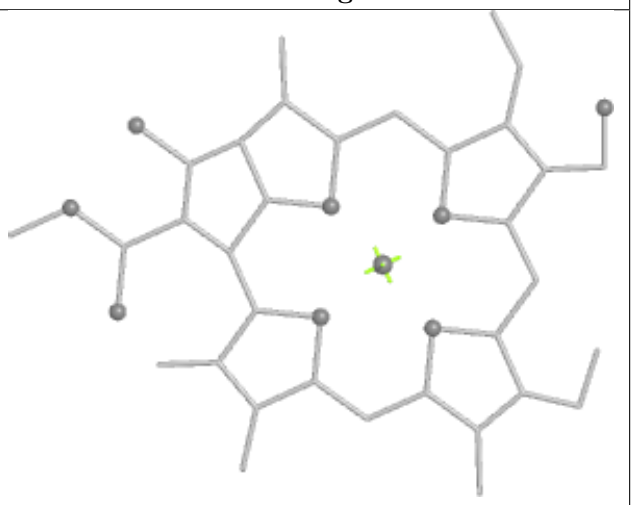
Bond lengths



Bond angles

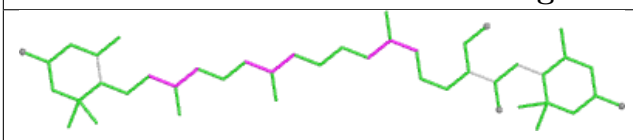


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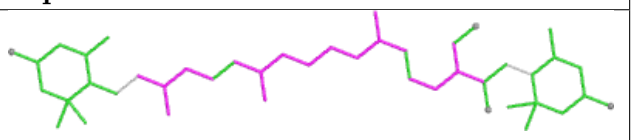


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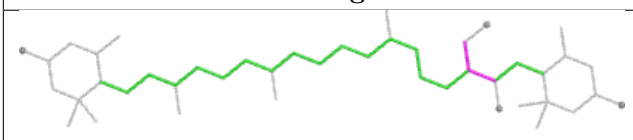
Ligand 0IE p 302



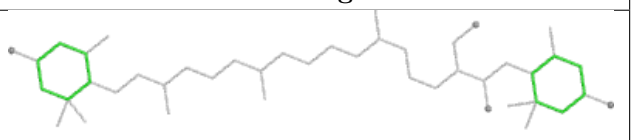
Bond lengths



Bond angles

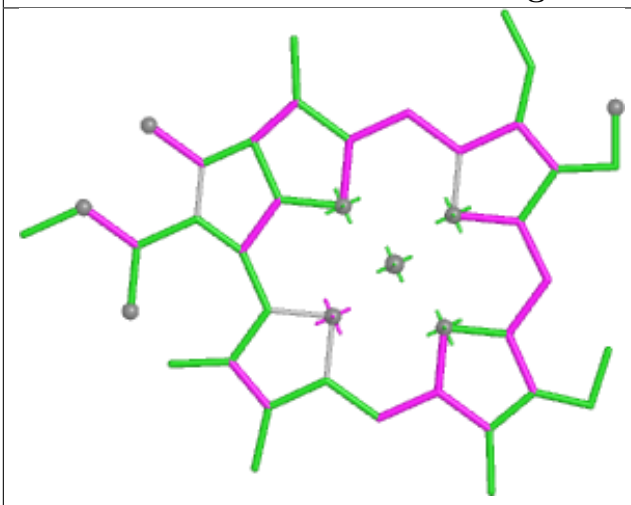


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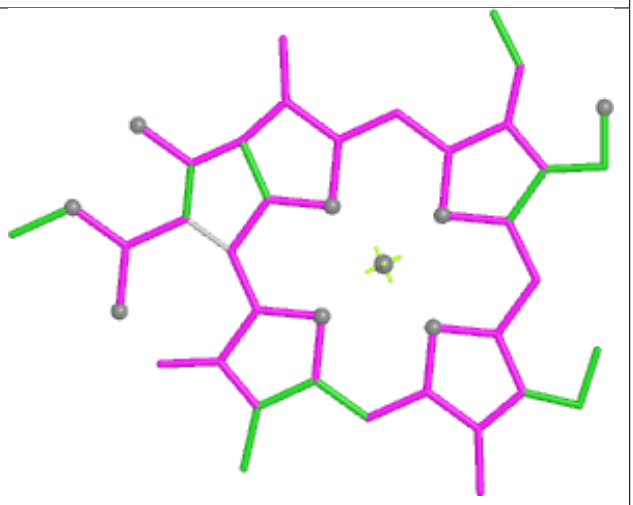


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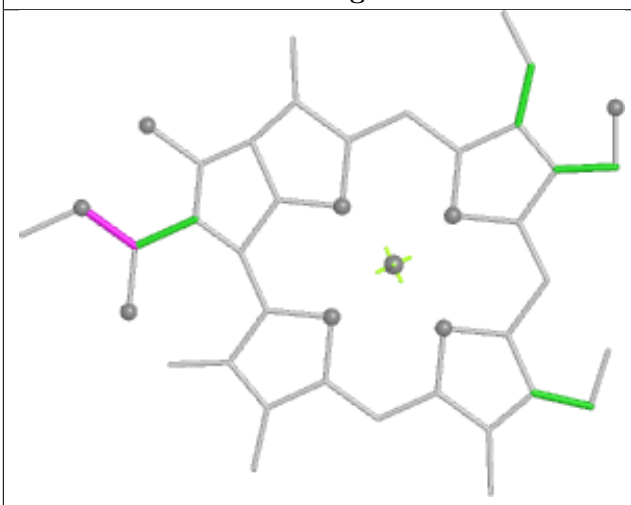
Ligand CHL 1 304



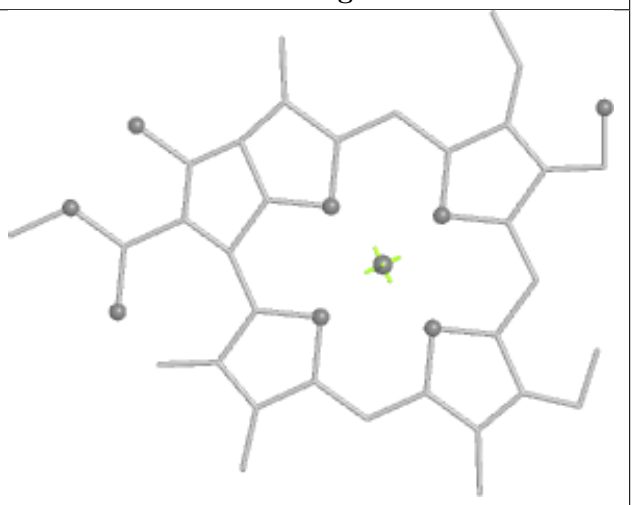
Bond lengths



Bond angles

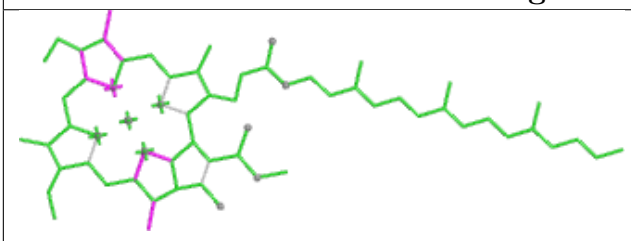


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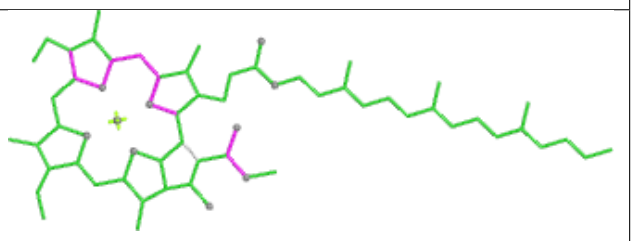


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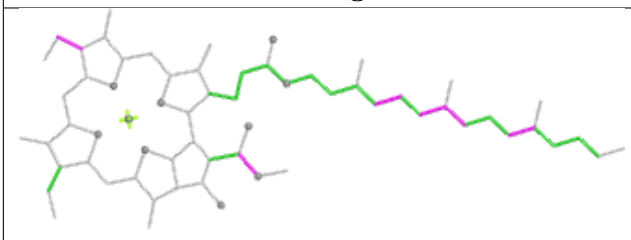
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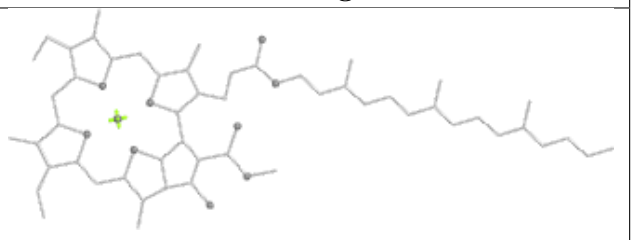
Bond lengths



Bond angles

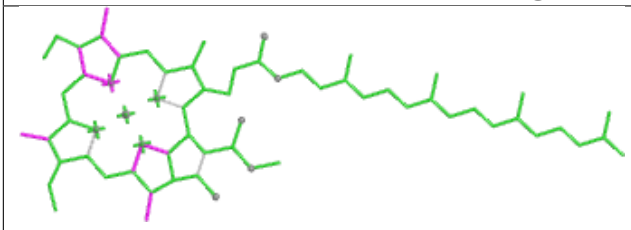


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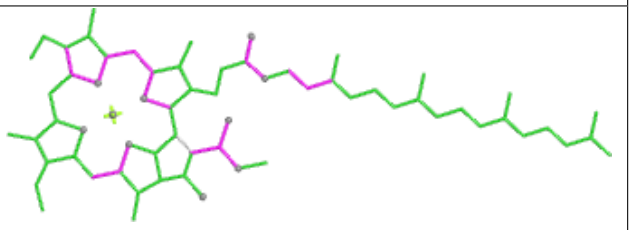


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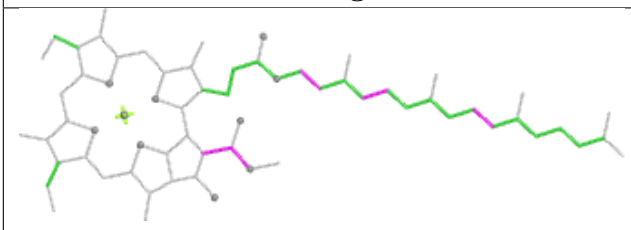
Ligand CLA c 609



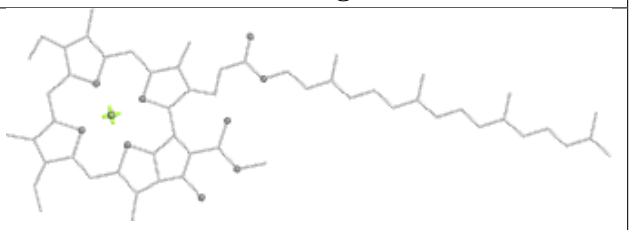
Bond lengths



Bond angles

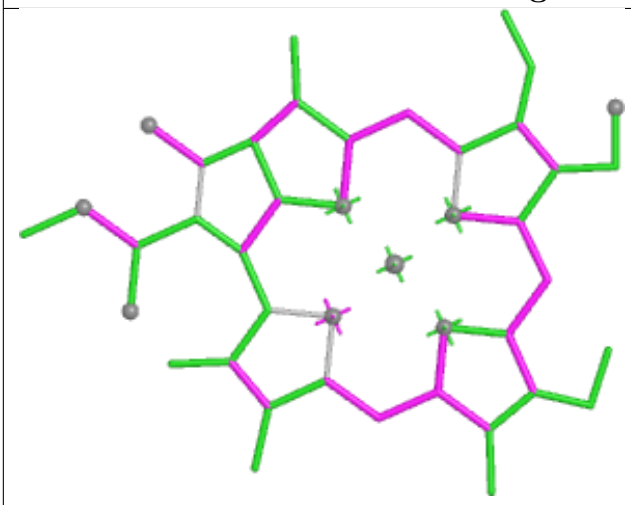


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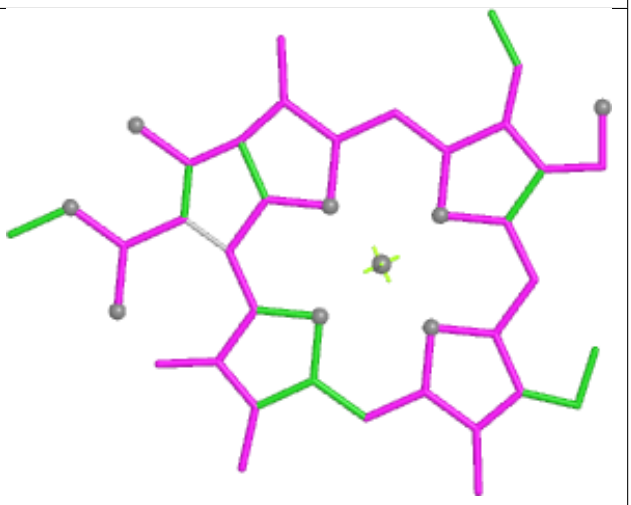


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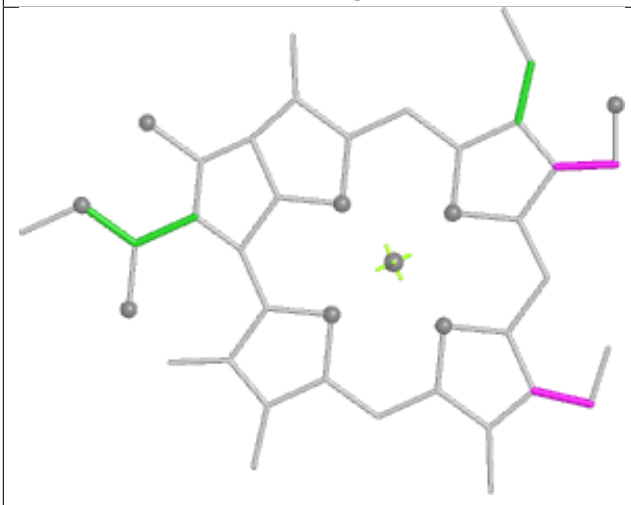
Ligand CHL s 414



Bond lengths



Bond angles

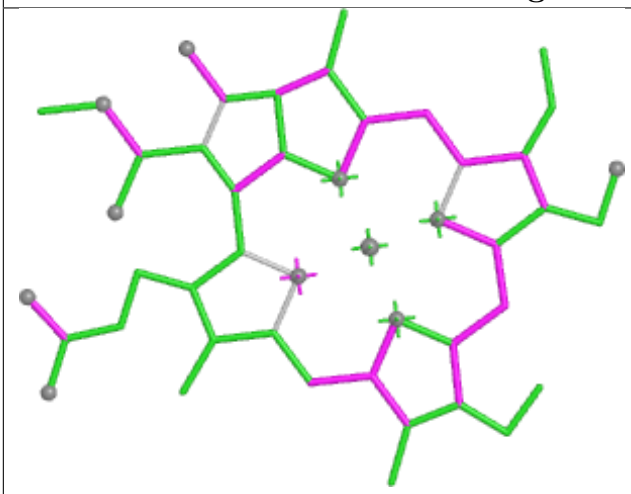


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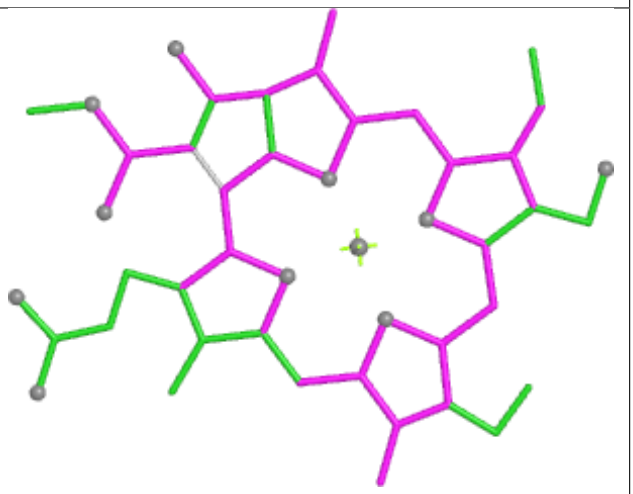


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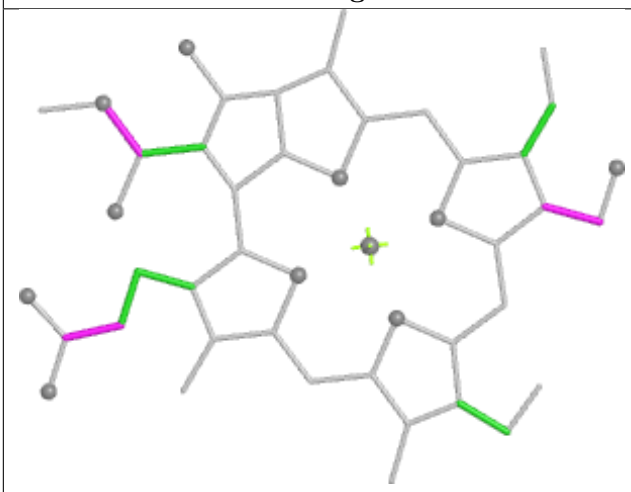
Ligand CHL 1 312



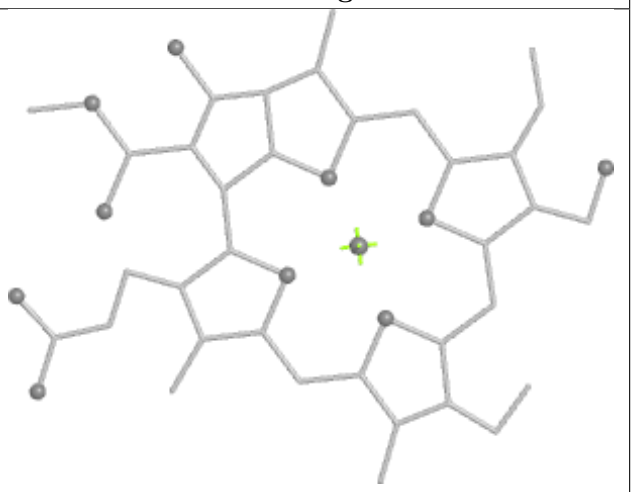
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Bond angles

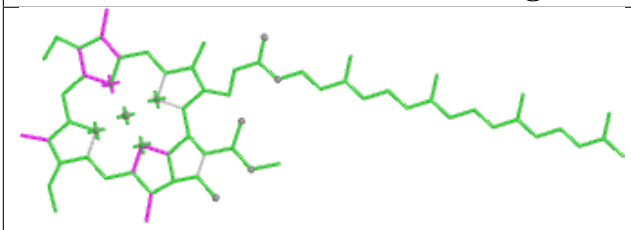


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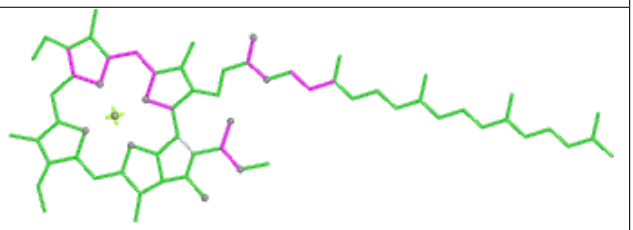


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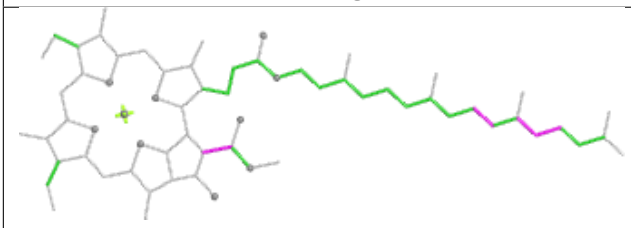
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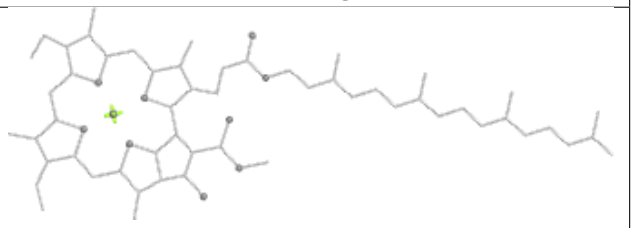
Bond lengths



Bond angles

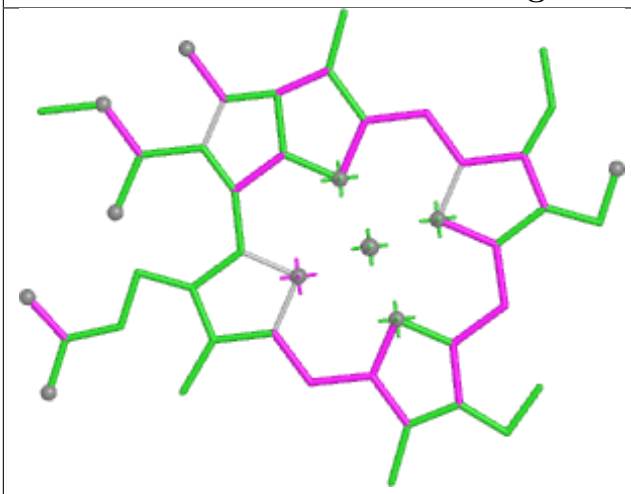


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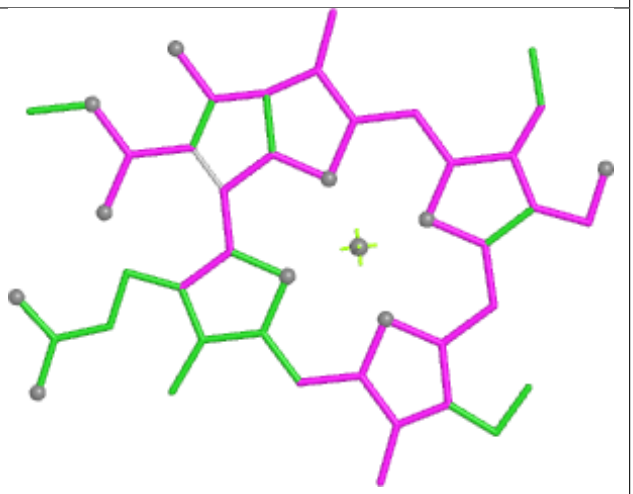


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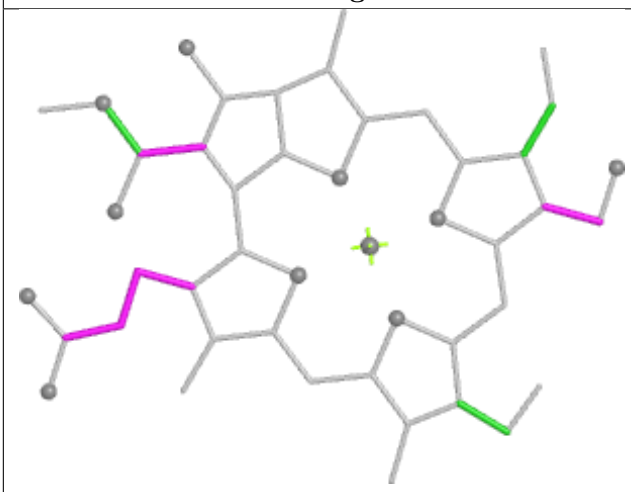
Ligand CHL 4 305



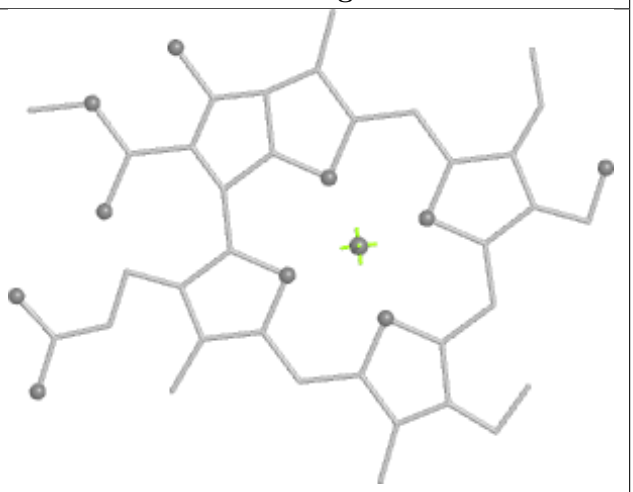
Bond lengths



Bond angles

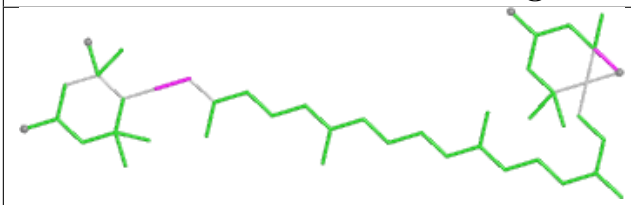


Torsions



Rings

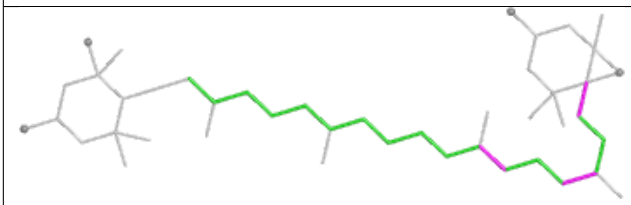
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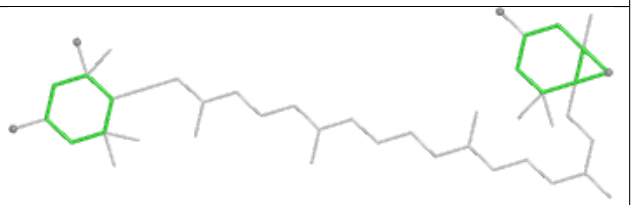
Bond lengths



Bond angles

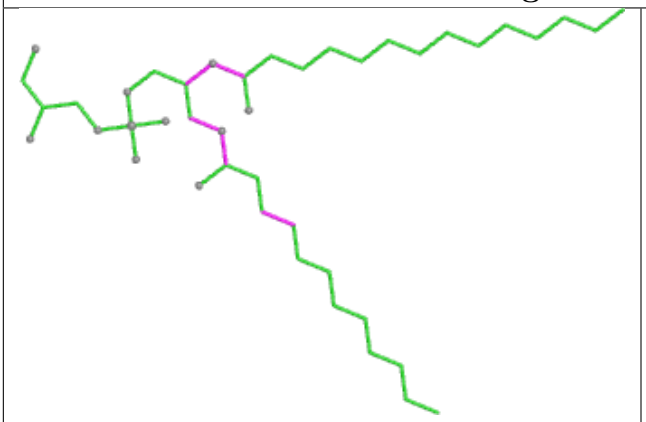


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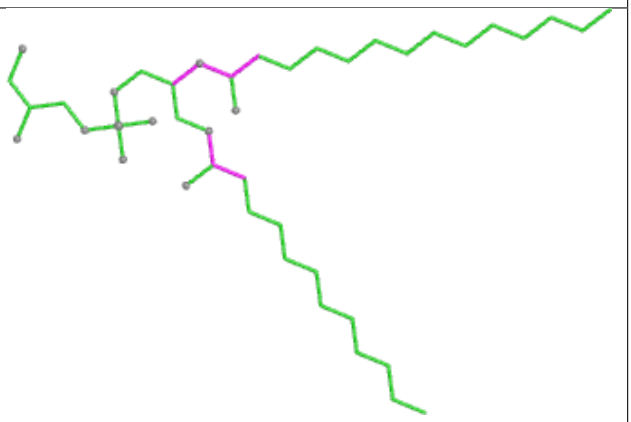


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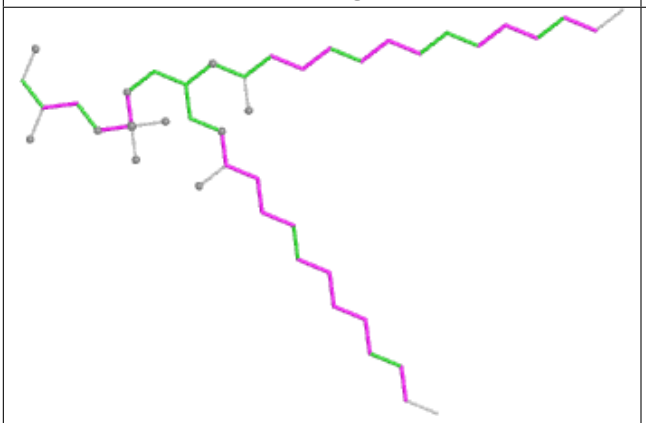
Ligand LHG Y 318



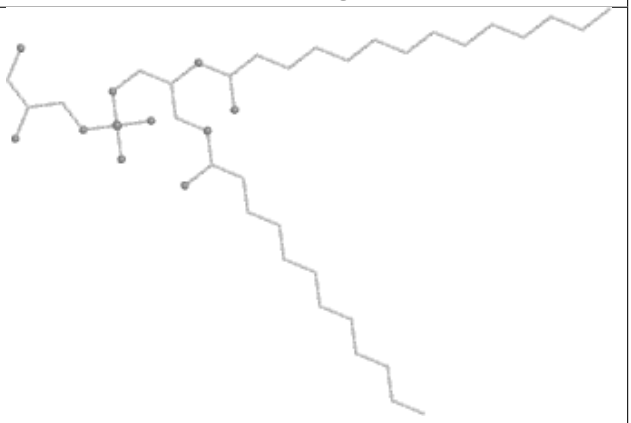
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Bond angles

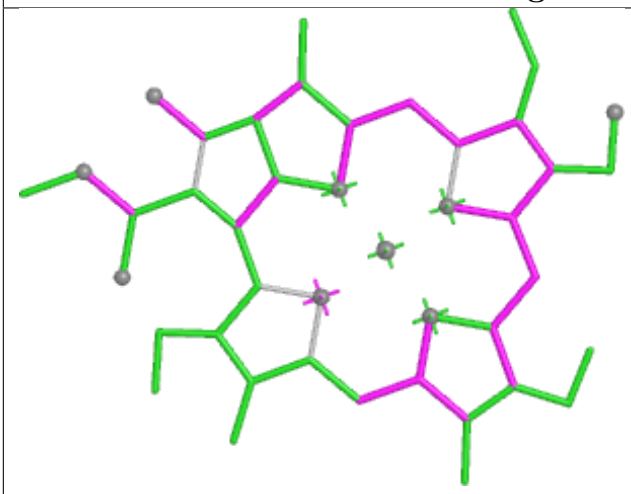


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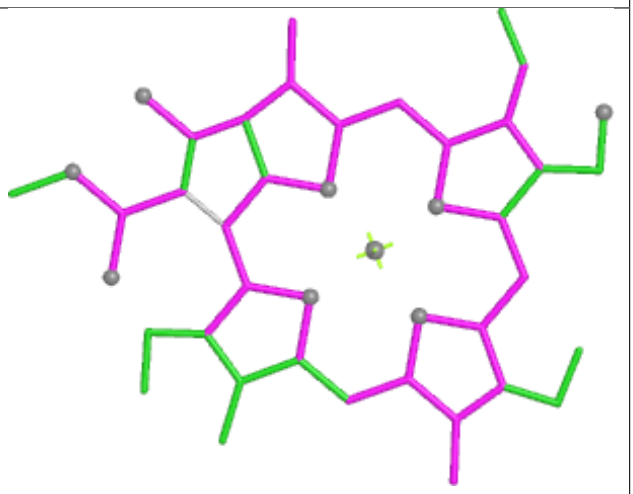


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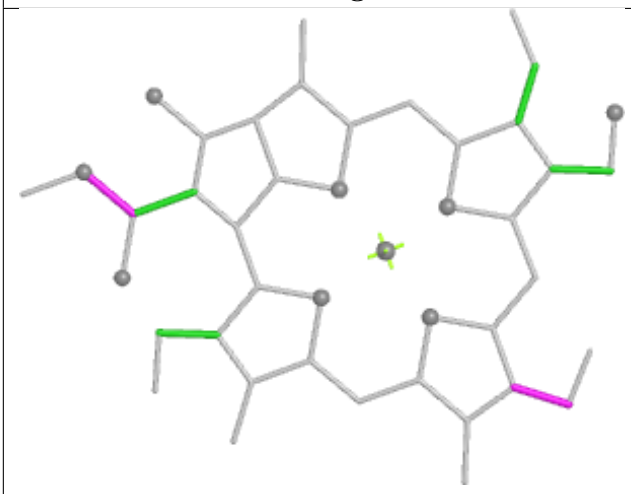
Ligand CHL 3 308



Bond lengths



Bond angles

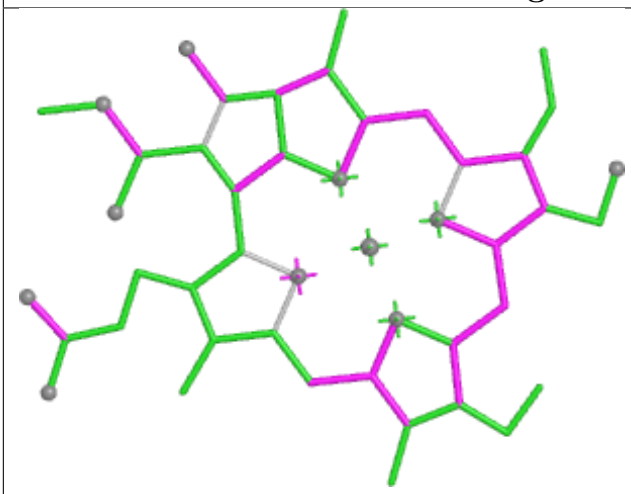


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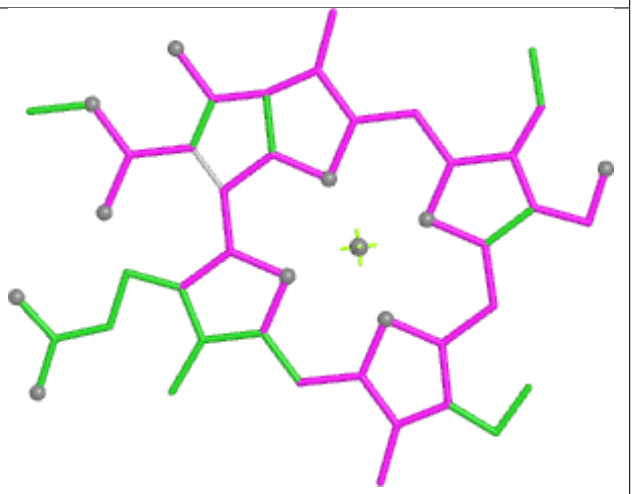


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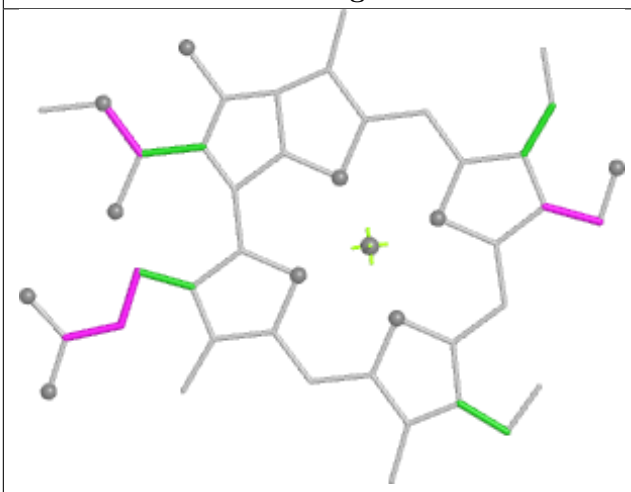
Ligand CHL 7 310



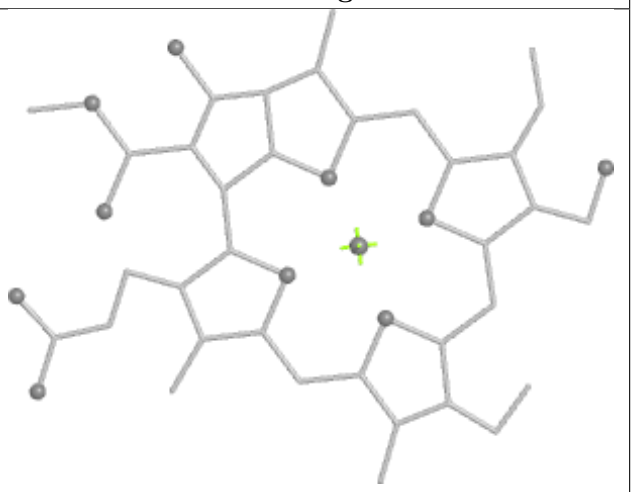
Bond lengths



Bond angles

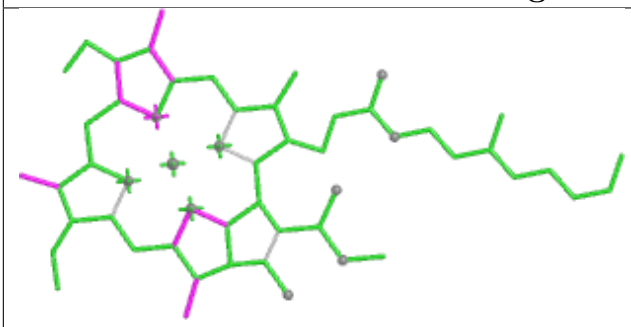


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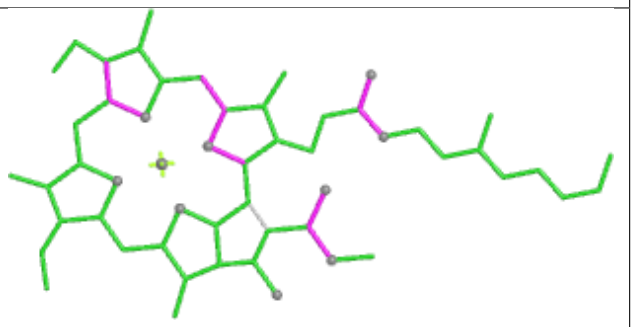


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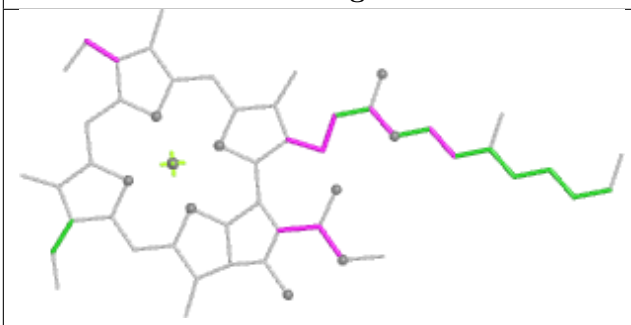
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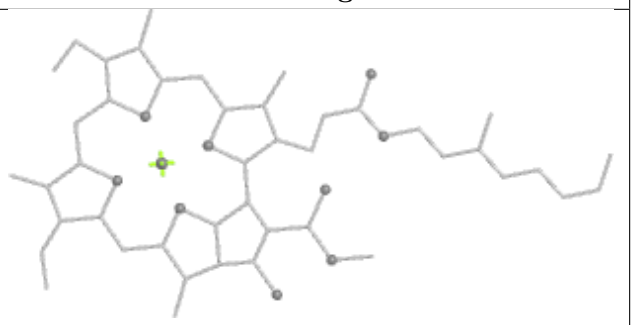
Bond lengths



Bond angles

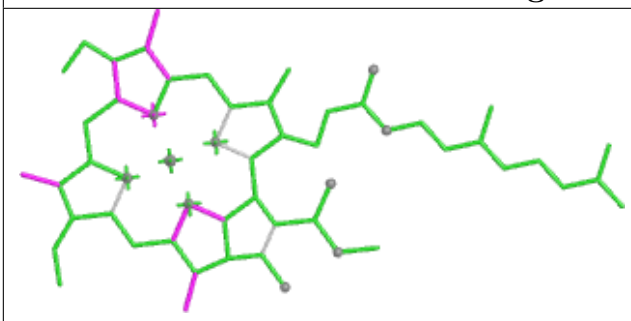


Torsions

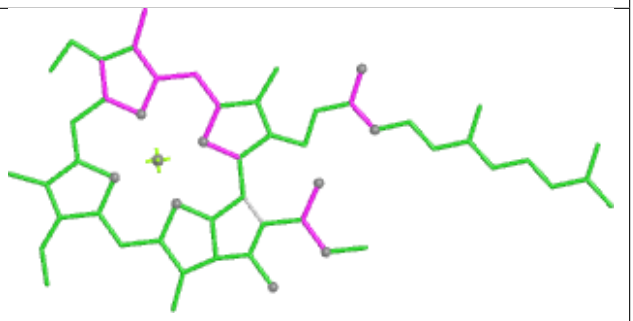


Rings

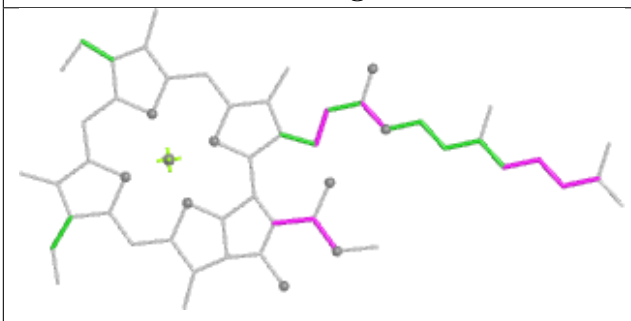
Ligand CLA b 608



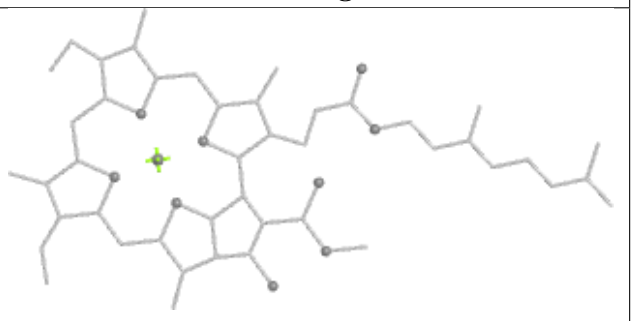
Bond lengths



Bond angles

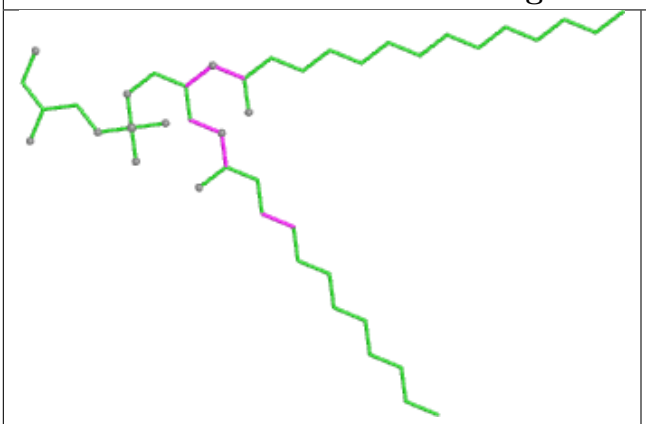


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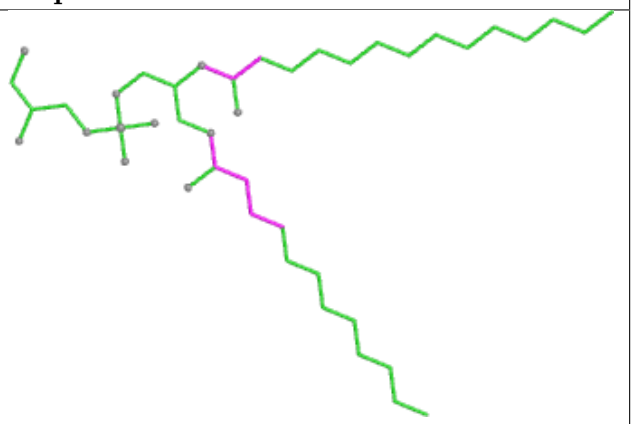


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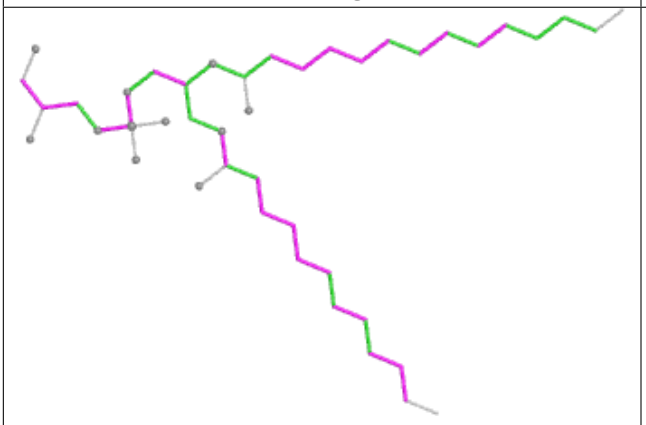
Ligand LHG p 319



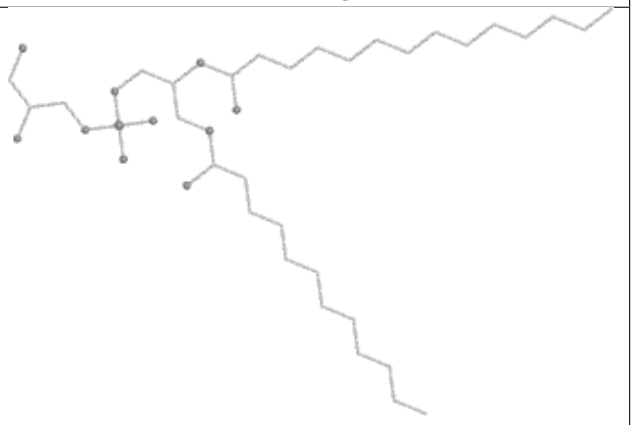
Bond lengths



Bond angles

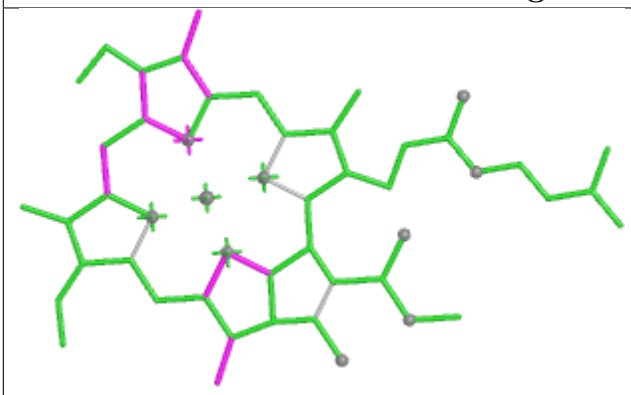


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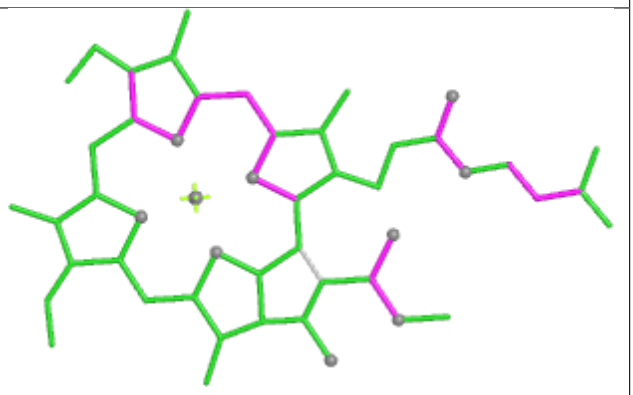


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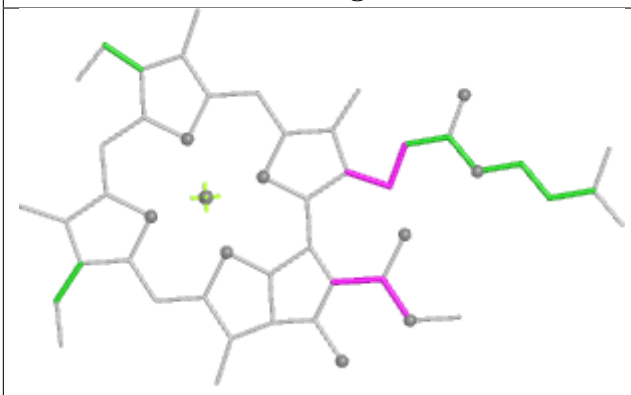
Ligand CLA u 308



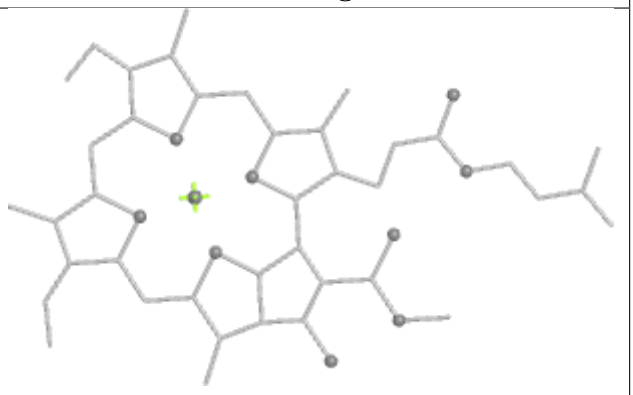
Bond lengths



Bond angles

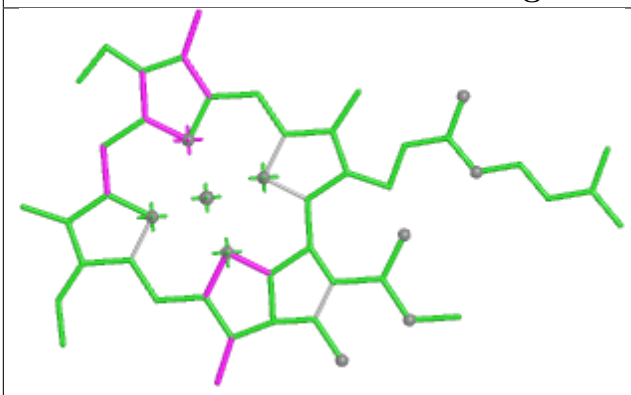


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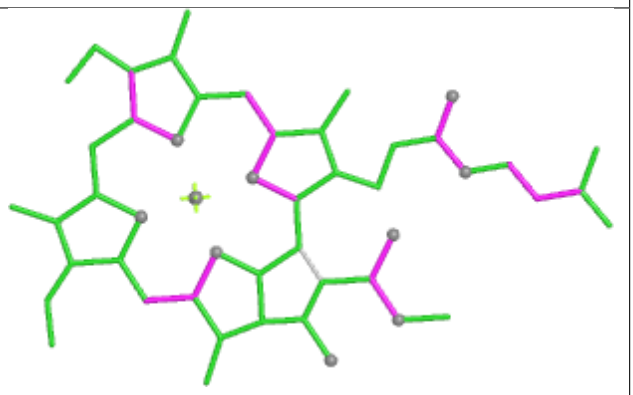


Rings

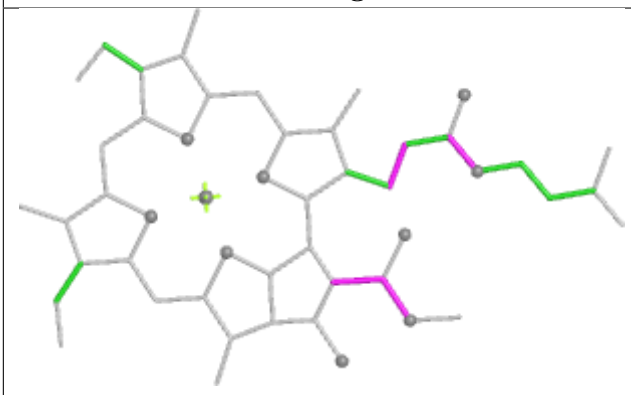
Ligand CLA N 307



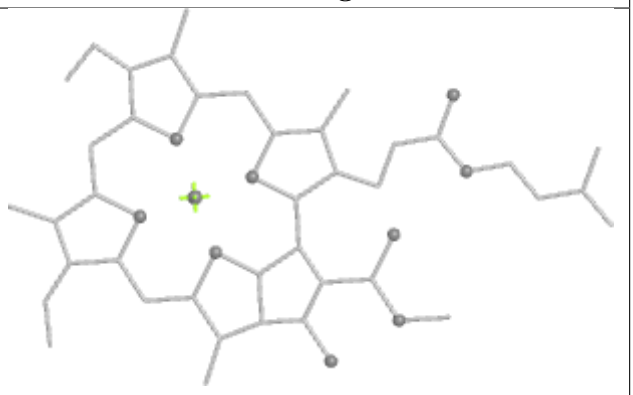
Bond lengths



Bond angles

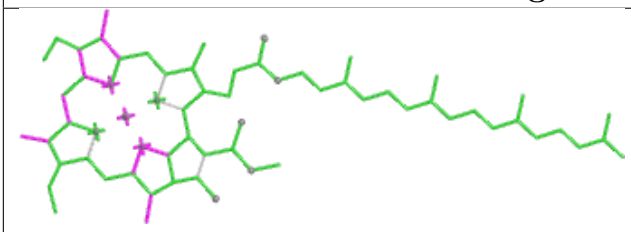


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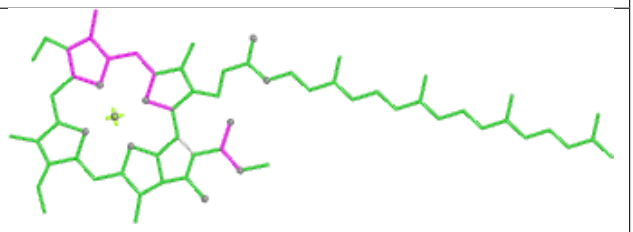


Rings

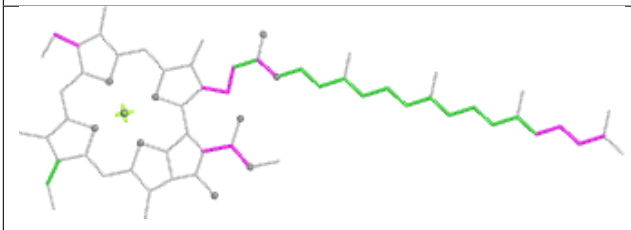
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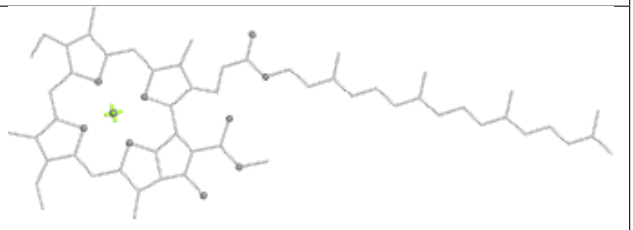
Bond lengths



Bond angles

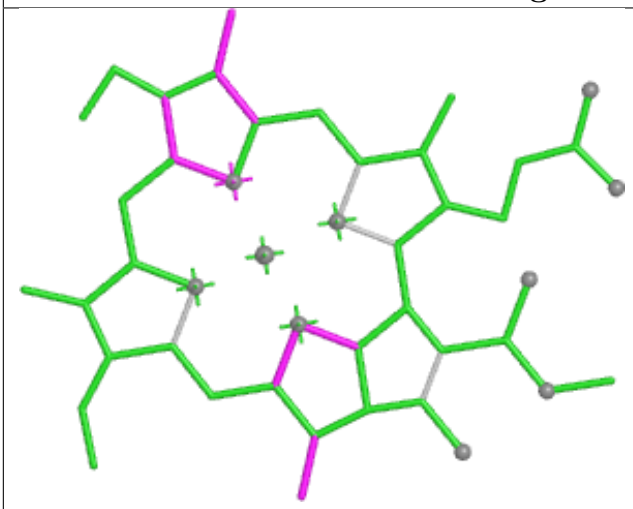


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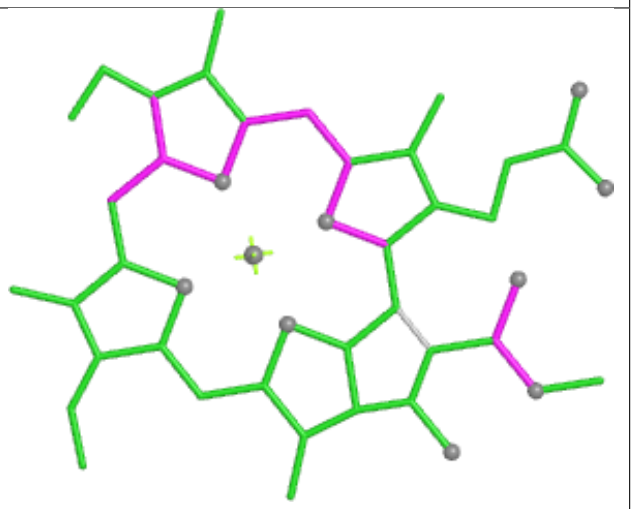


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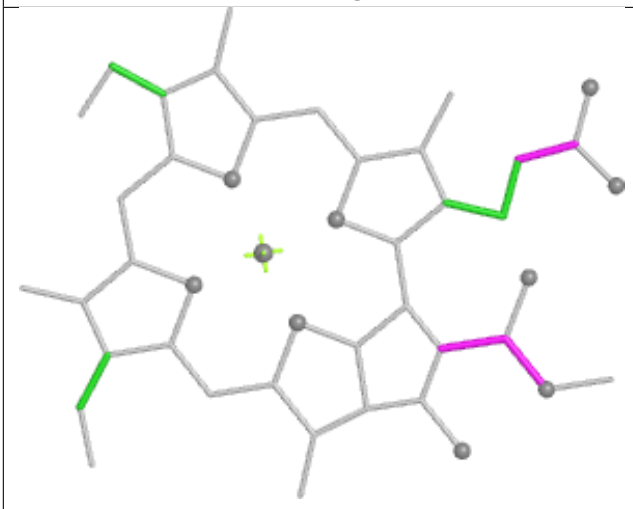
Ligand CLA s 404



Bond lengths



Bond angles

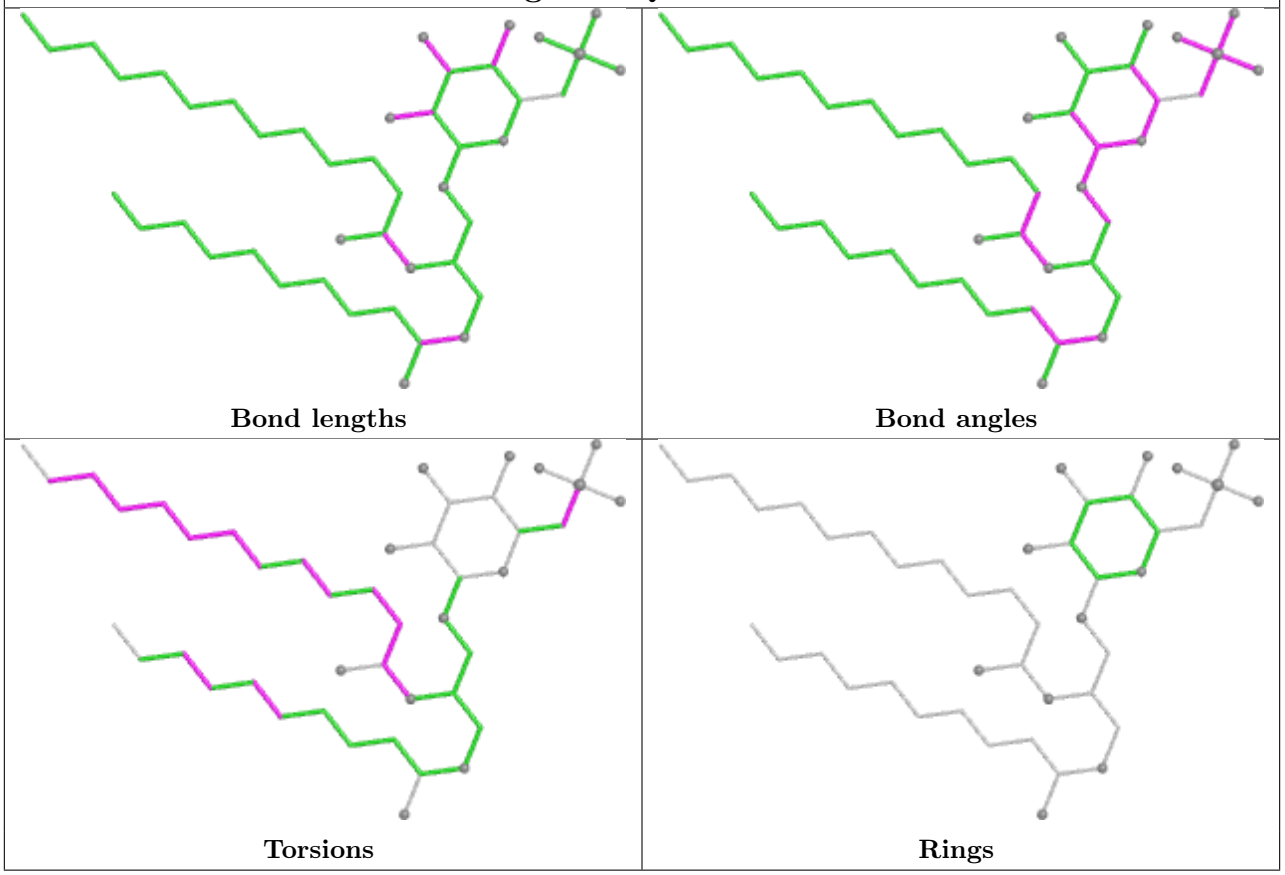


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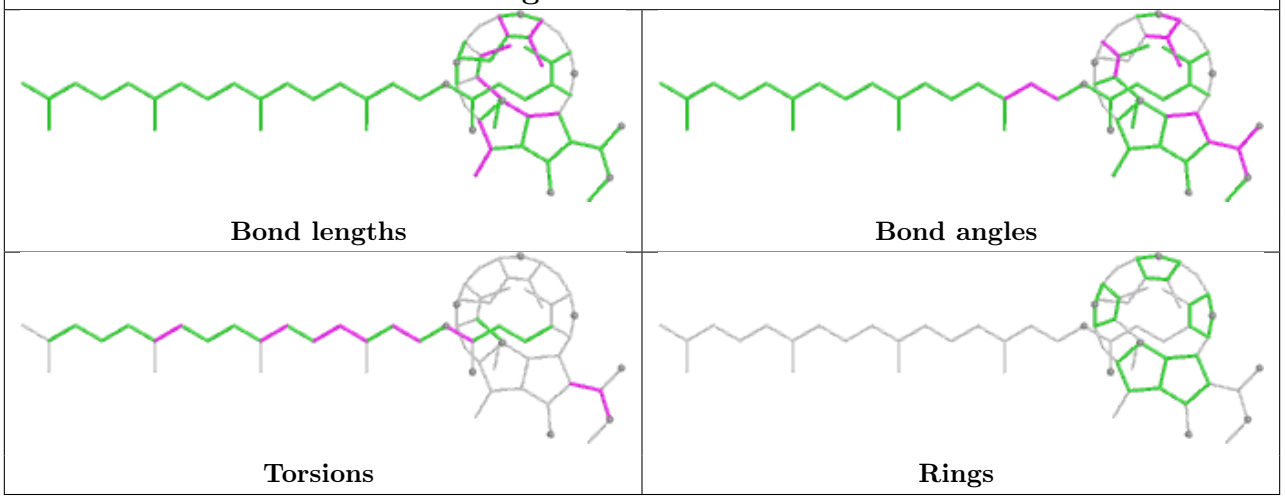


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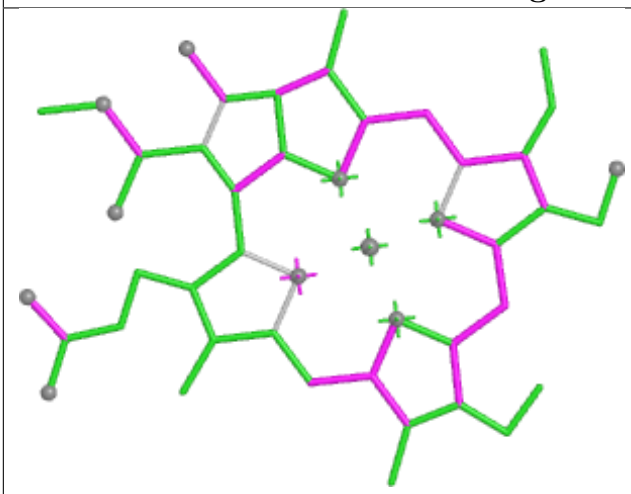
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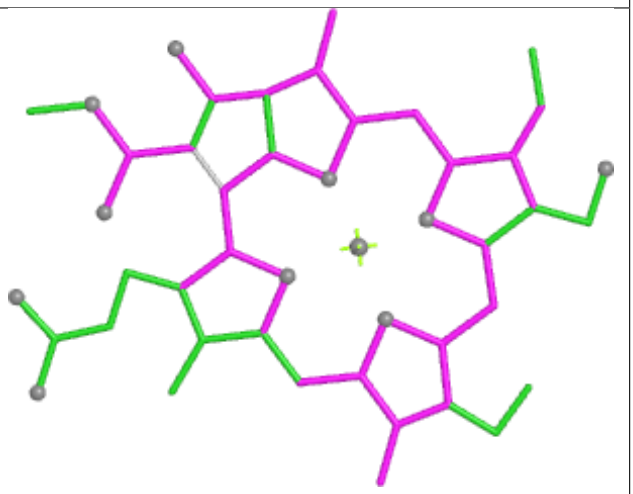
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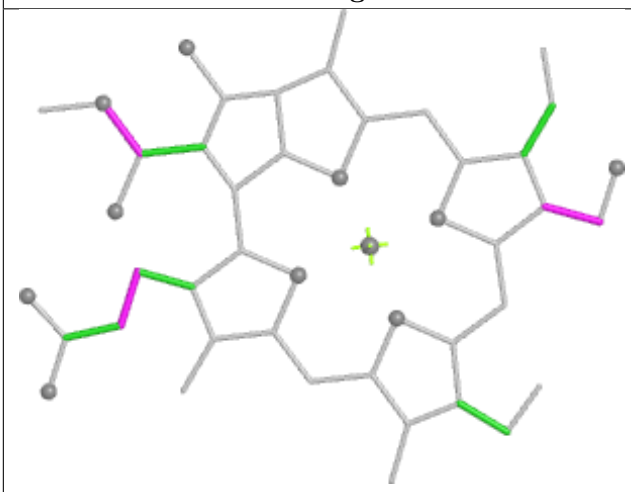
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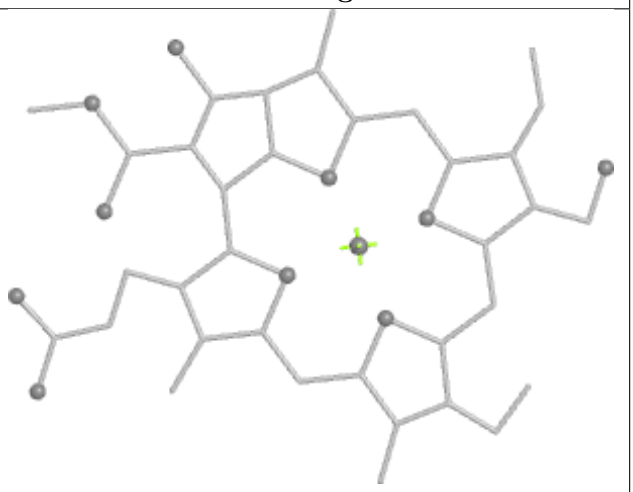
Bond lengths



Bond angles

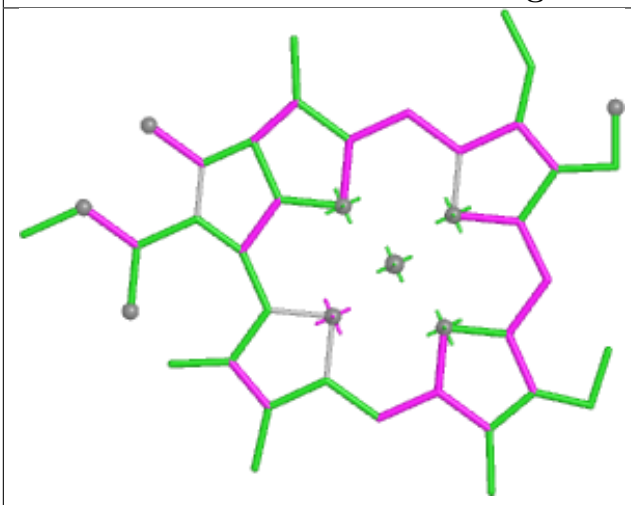


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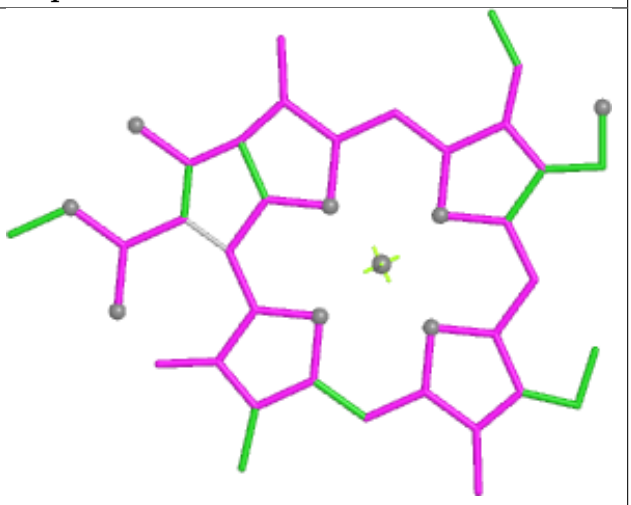


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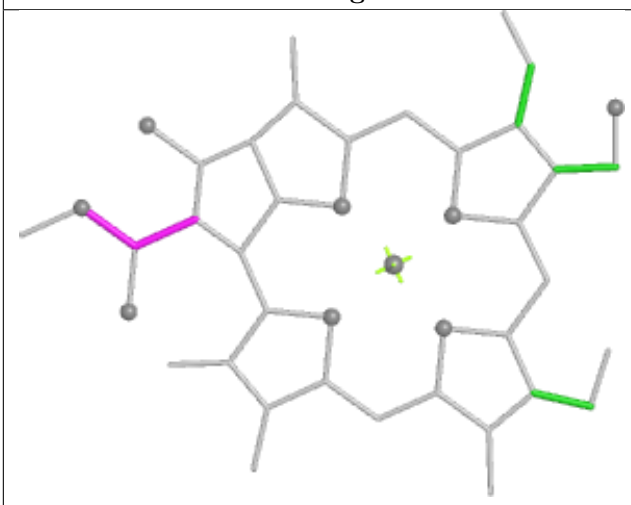
Ligand CHL p 318



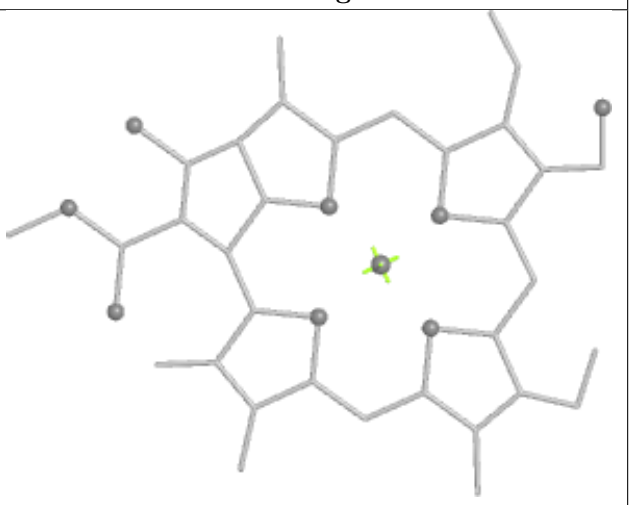
Bond lengths



Bond angles

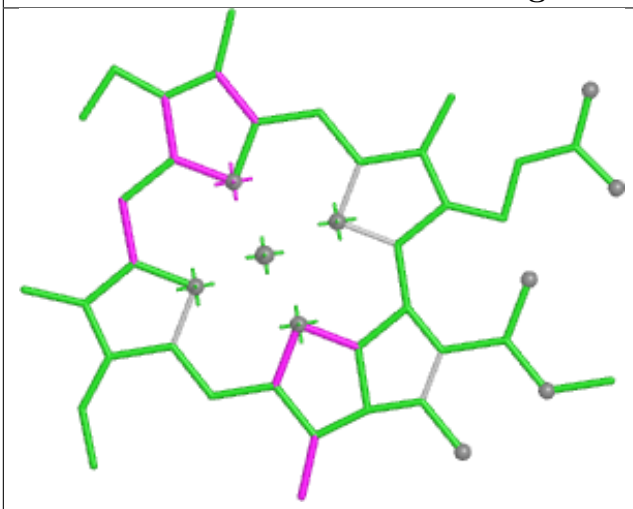


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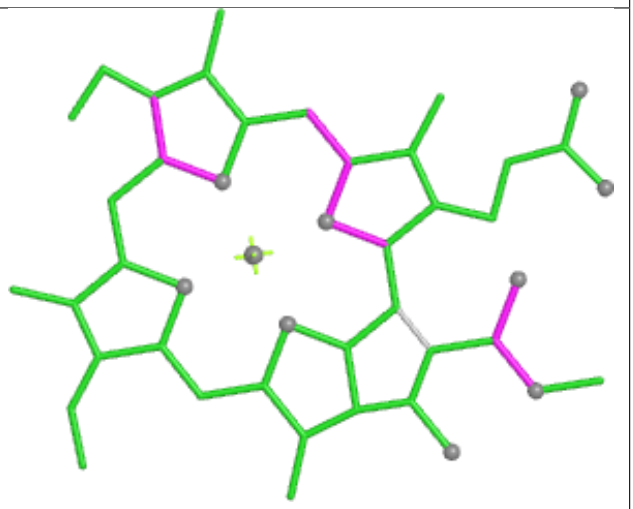


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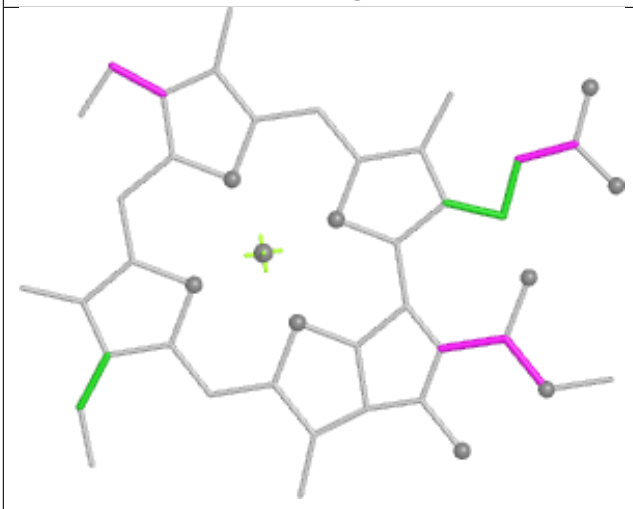
Ligand CLA 1 315



Bond lengths



Bond angles

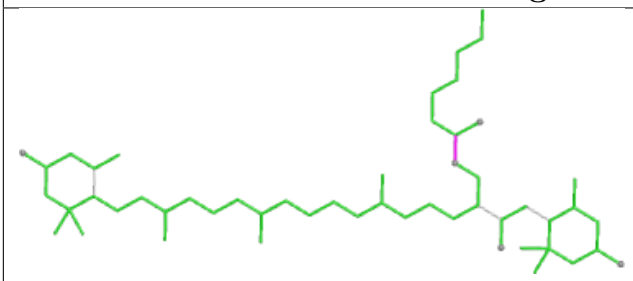


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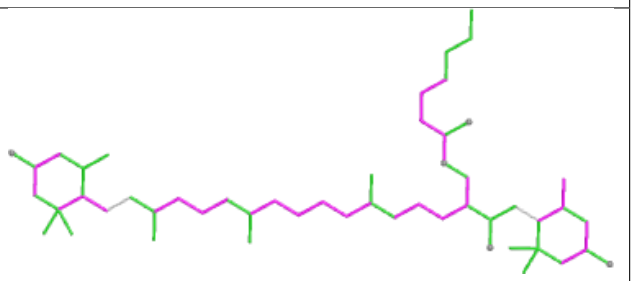


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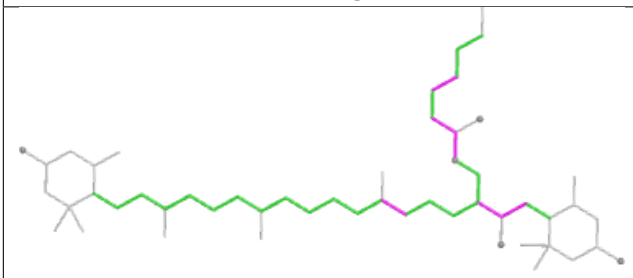
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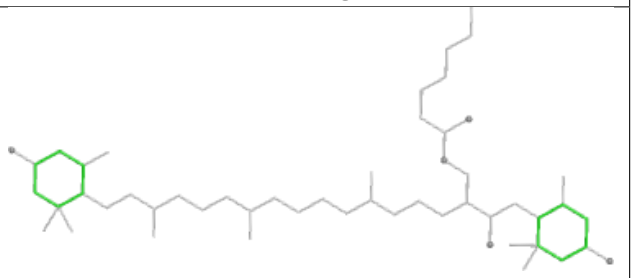
Bond lengths



Bond angles

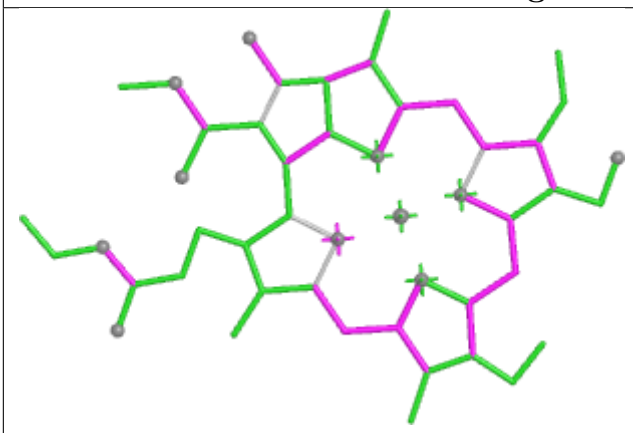


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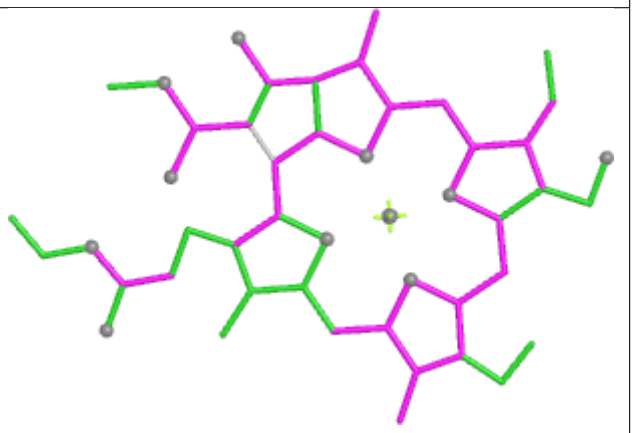


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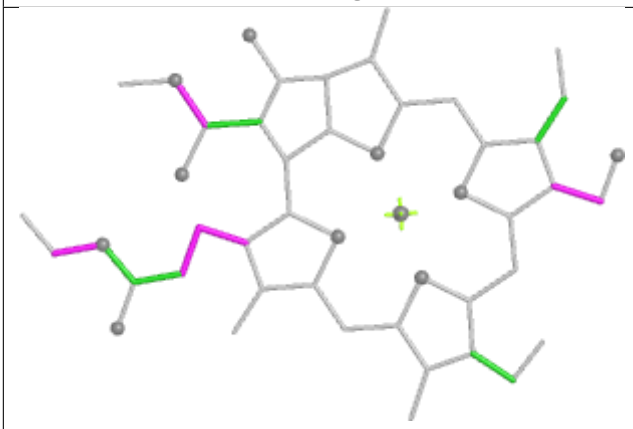
Ligand CHL 3 304



Bond lengths



Bond angles

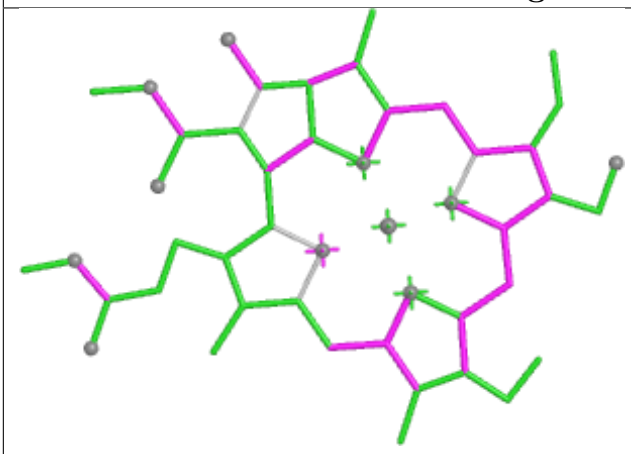


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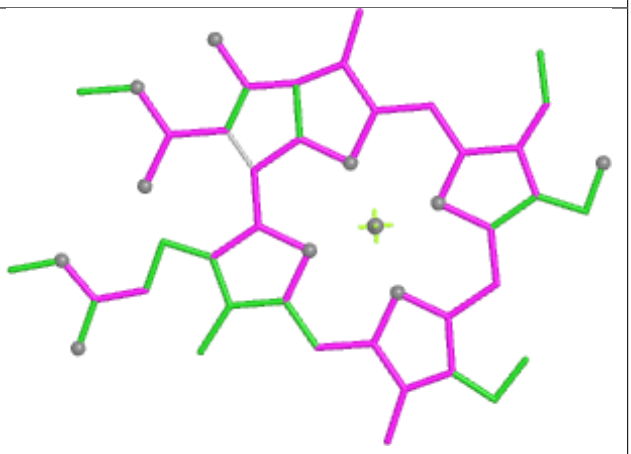


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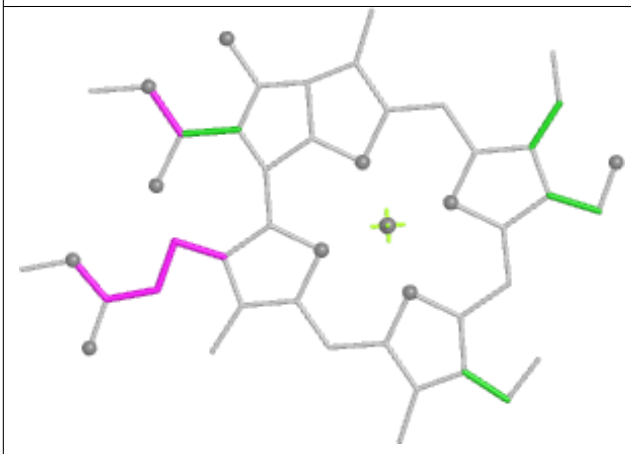
Ligand CHL 5 311



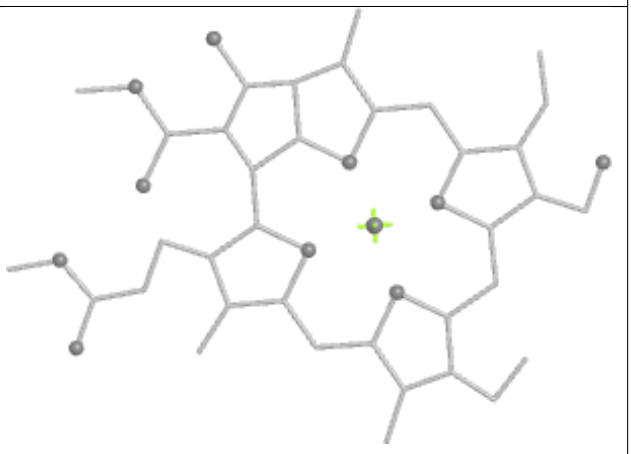
Bond lengths



Bond angles

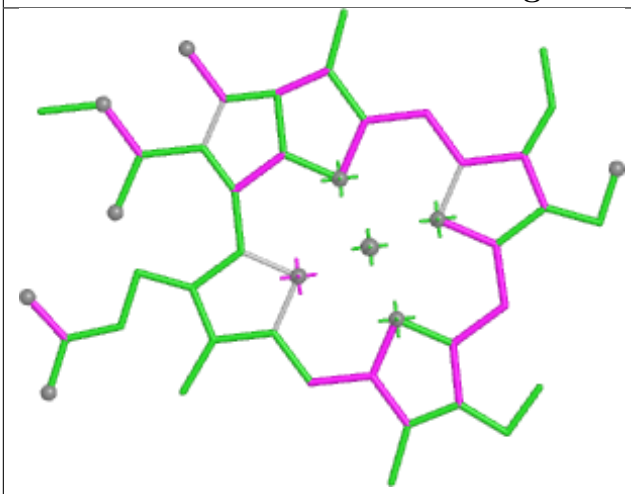


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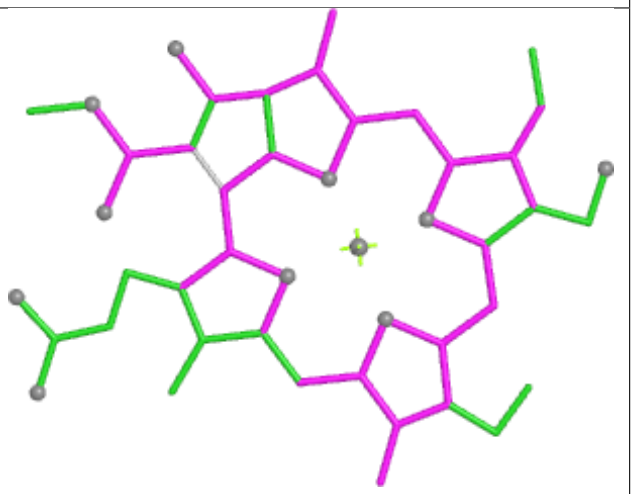


Rings

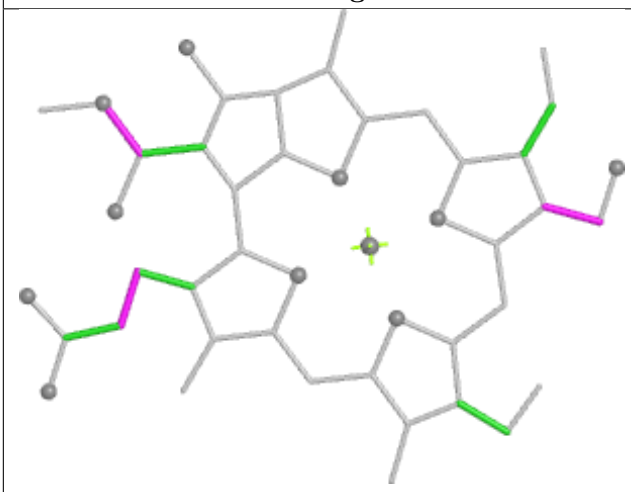
Ligand CHL R 601



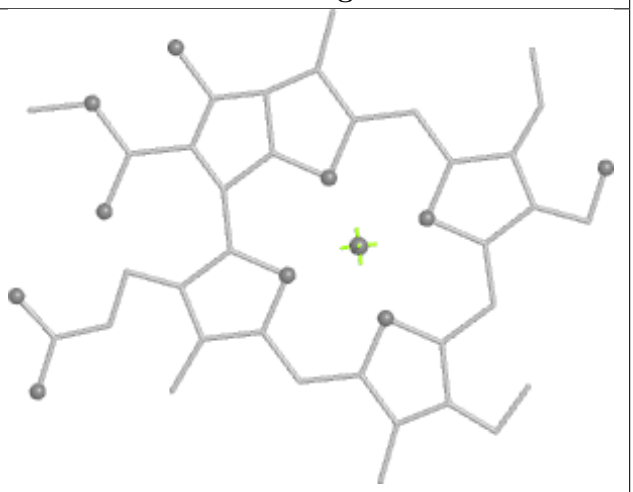
Bond lengths



Bond angles

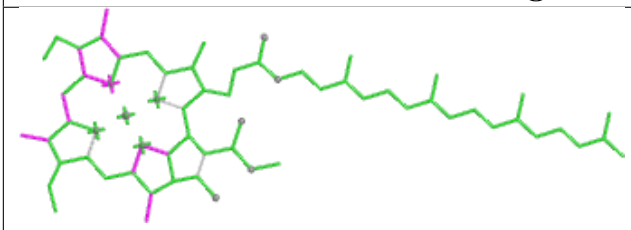


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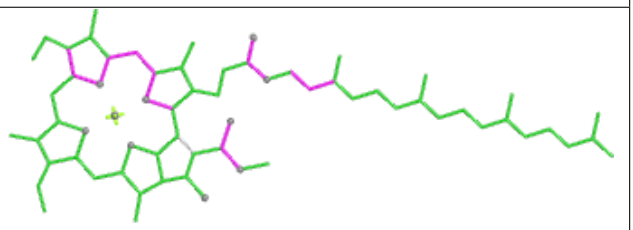


Rings

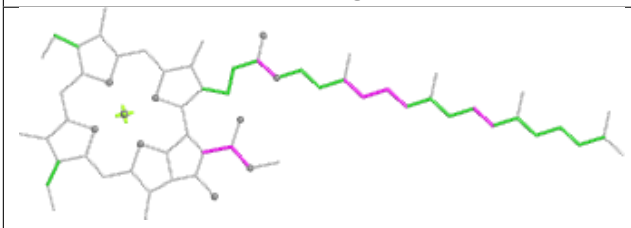
Ligand CLA b 613



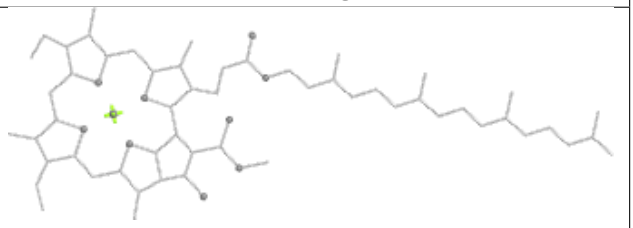
Bond lengths



Bond angles

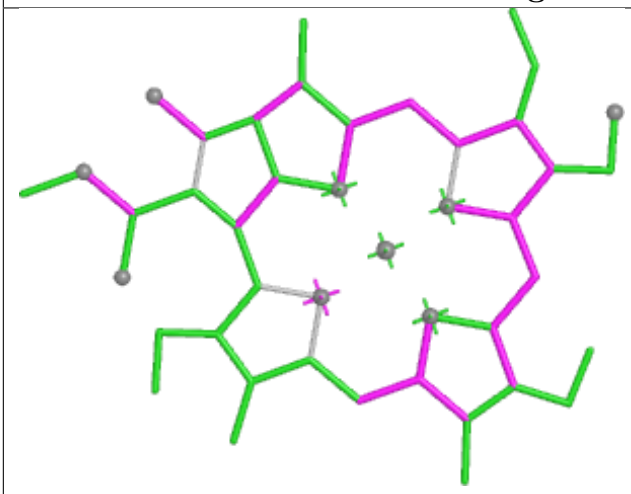


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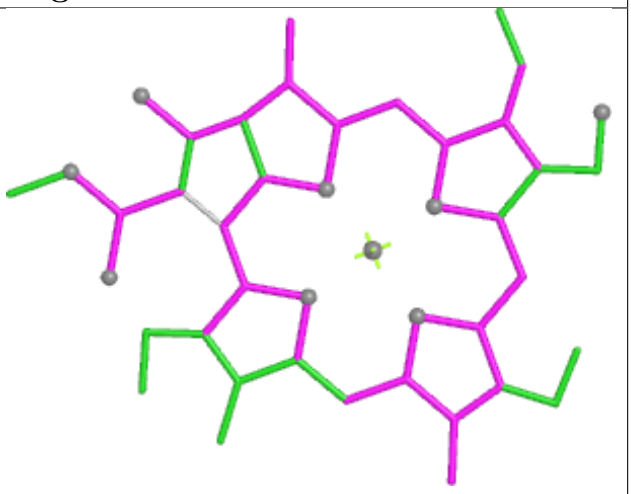


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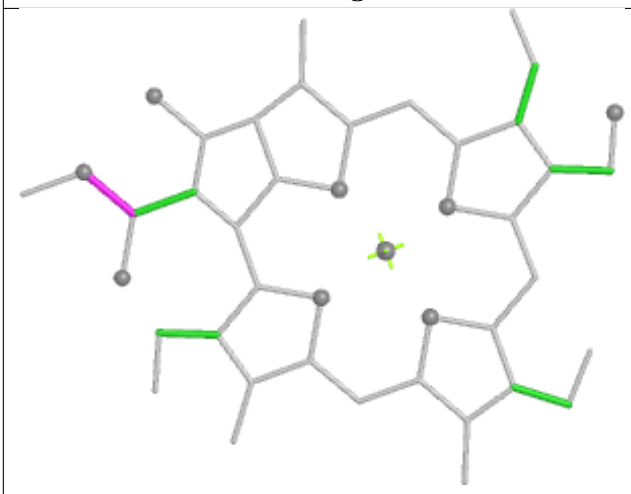
Ligand CHL g 309



Bond lengths



Bond angles

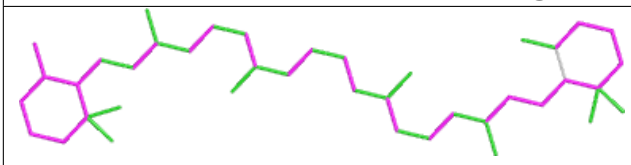


Torsions

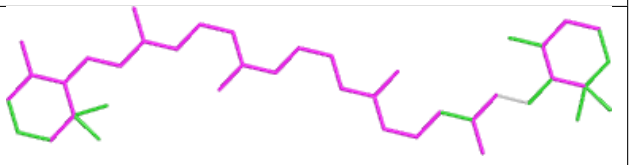


Rings

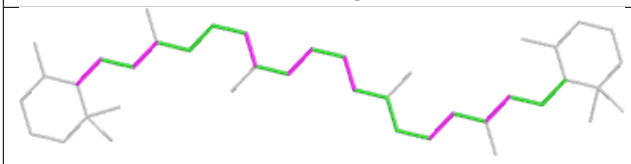
Ligand 8CT x 601



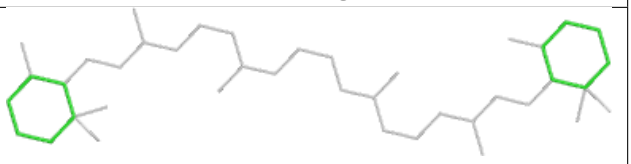
Bond lengths



Bond angles

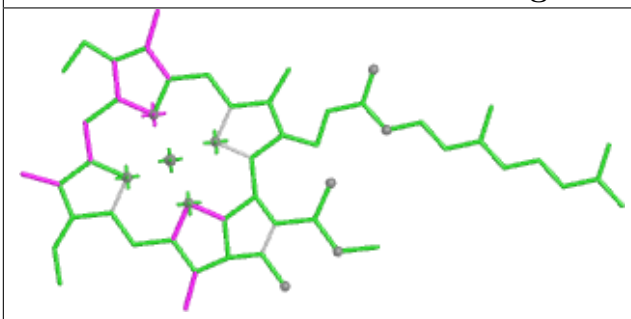


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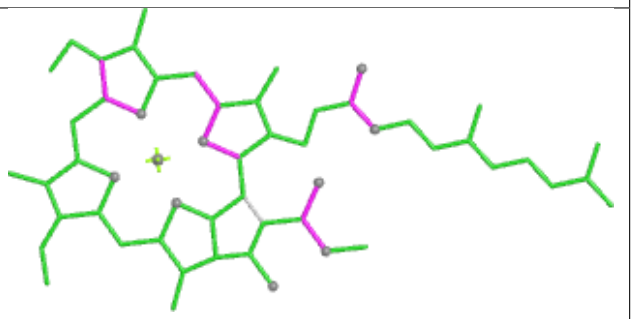


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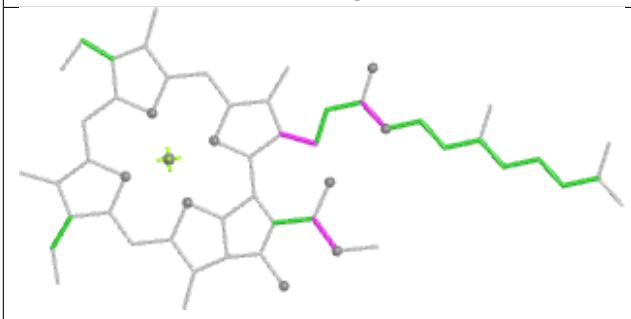
Ligand CLA r 310



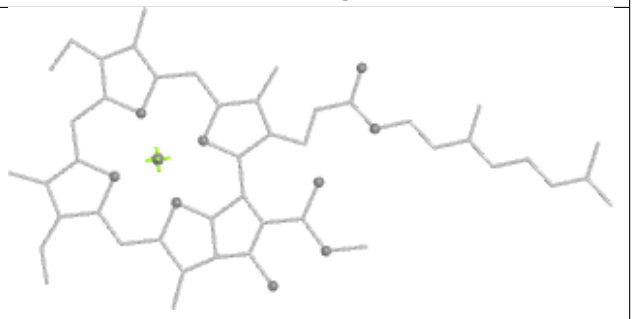
Bond lengths



Bond angles

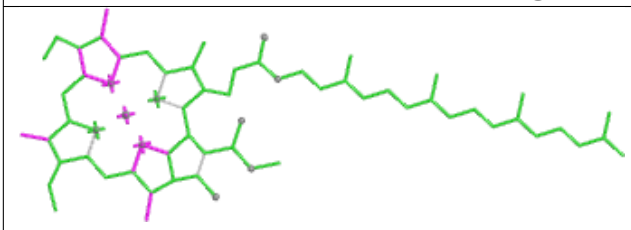


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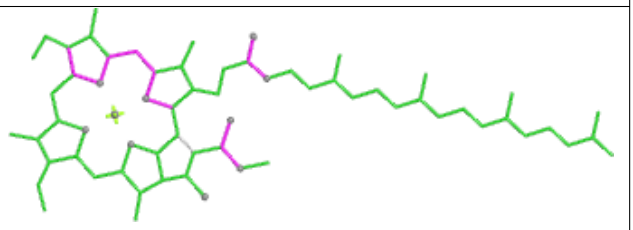


Rings

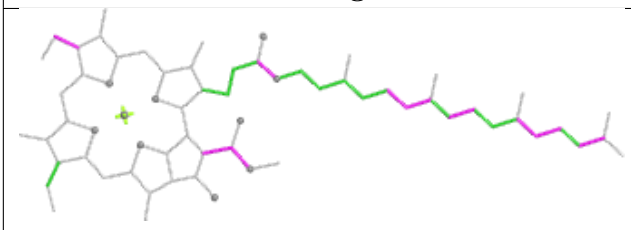
Ligand CLA c 602



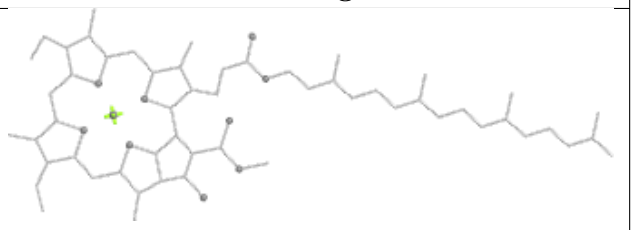
Bond lengths



Bond angles

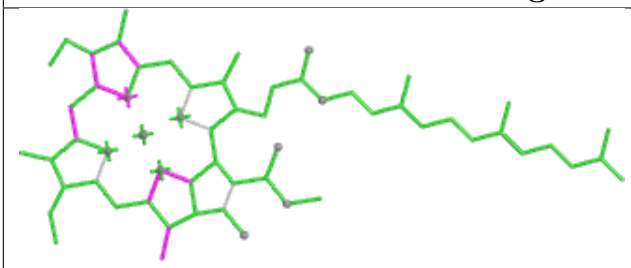


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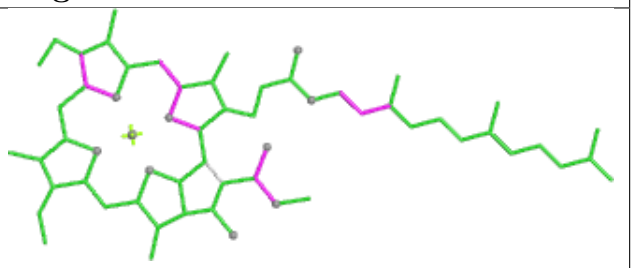


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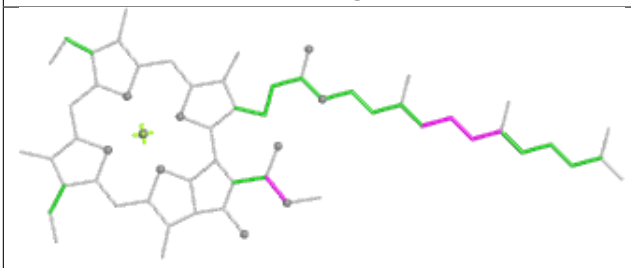
Ligand CLA g 315



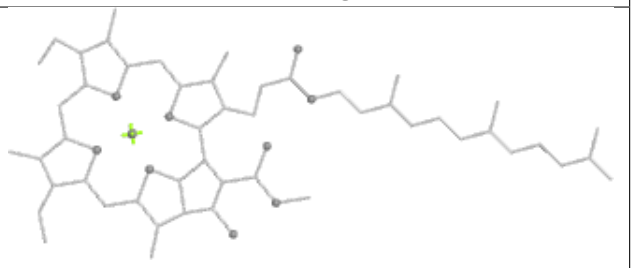
Bond lengths



Bond angles

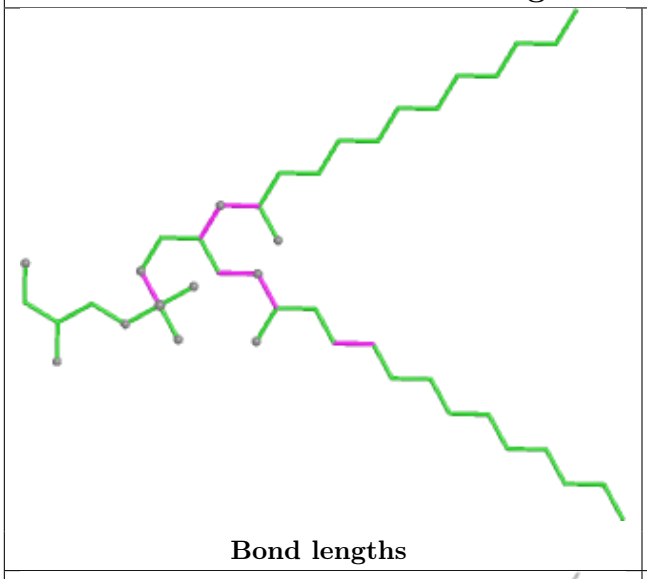


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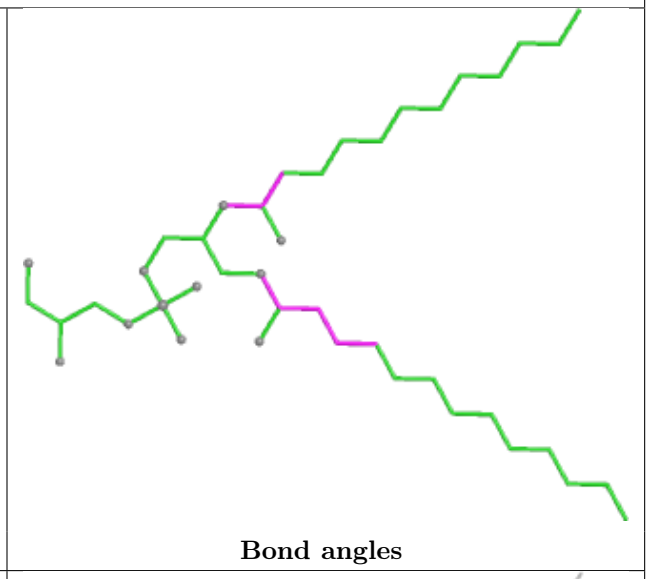


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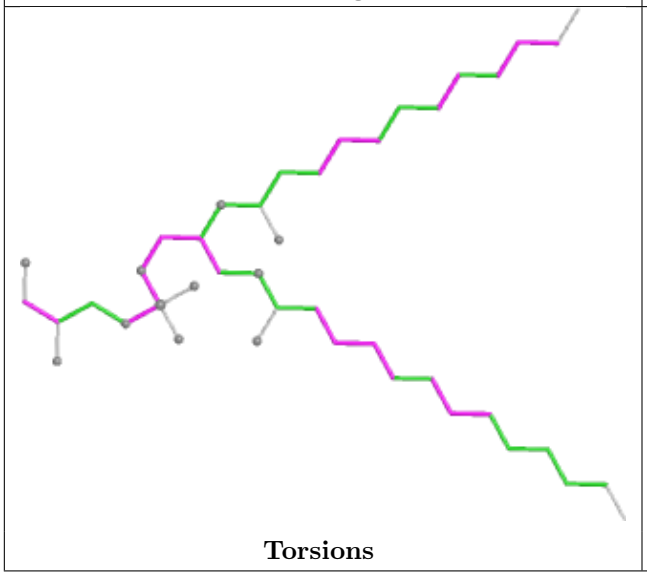
Ligand LHG 4 318



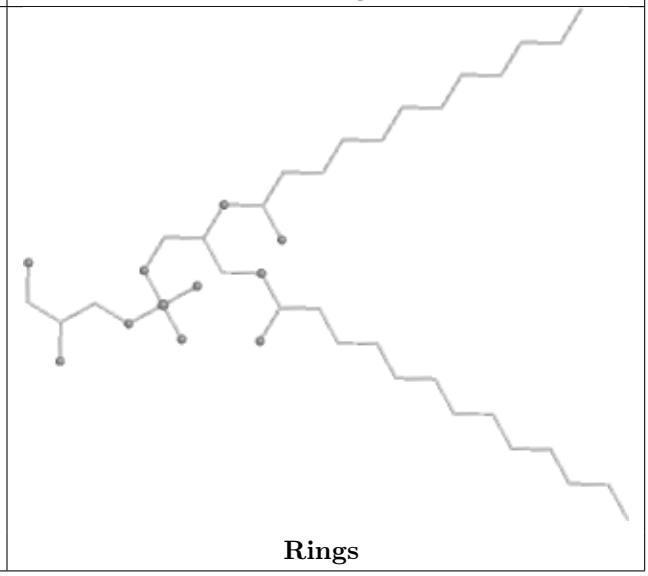
Bond lengths



Bond angles

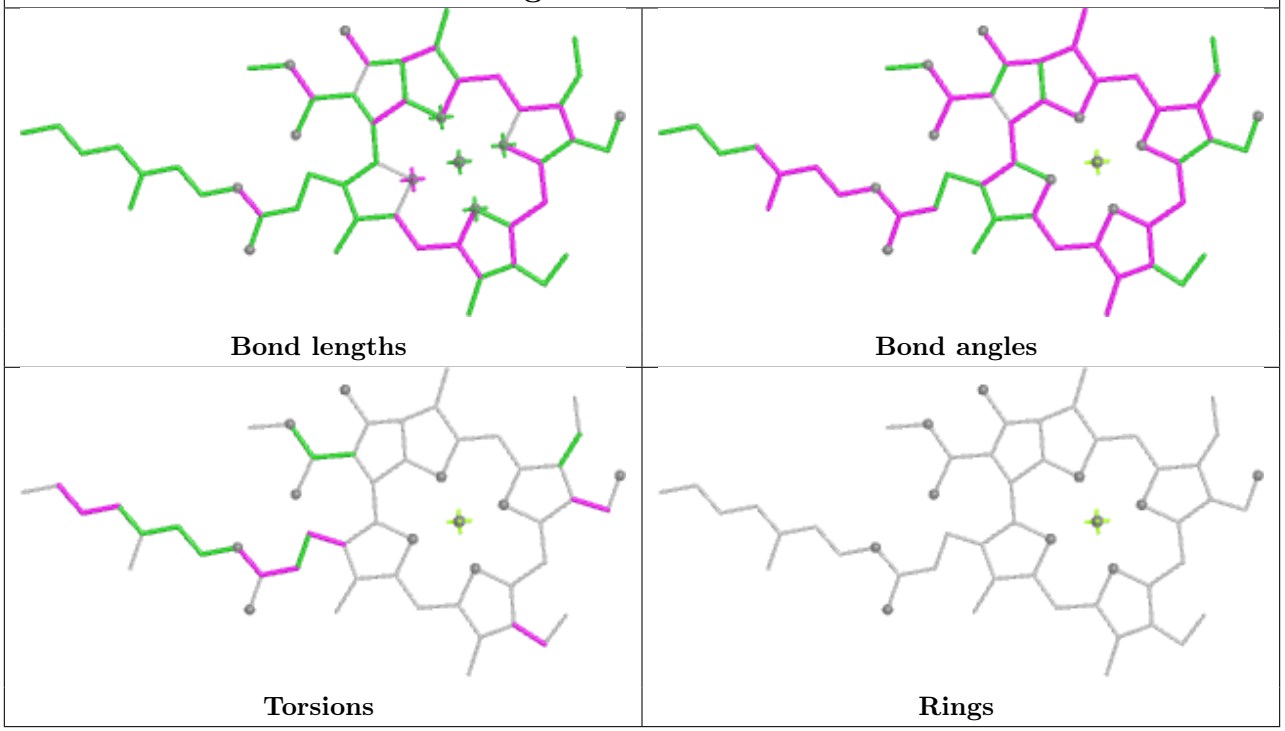


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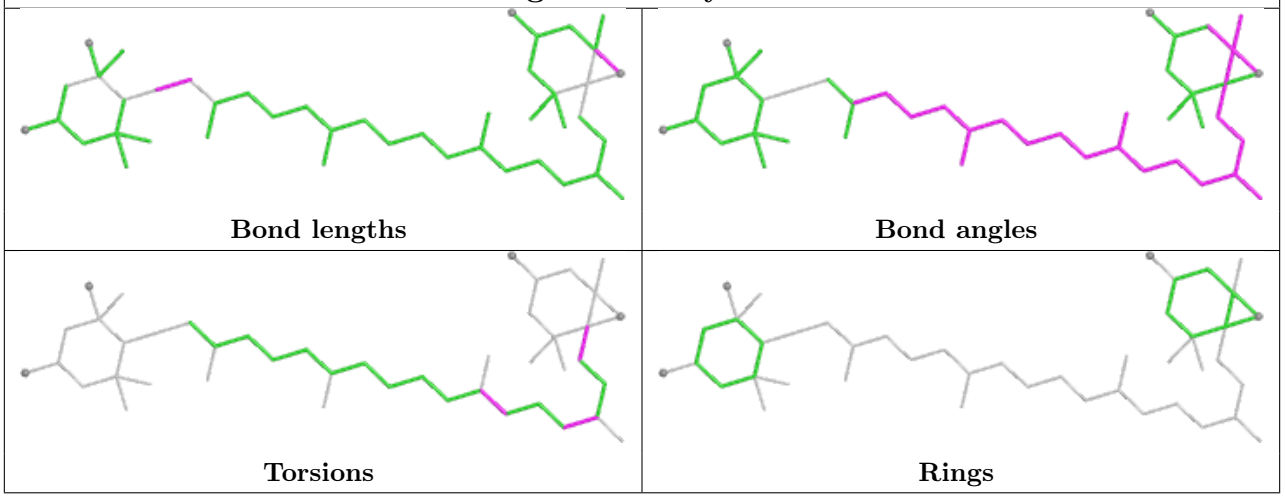


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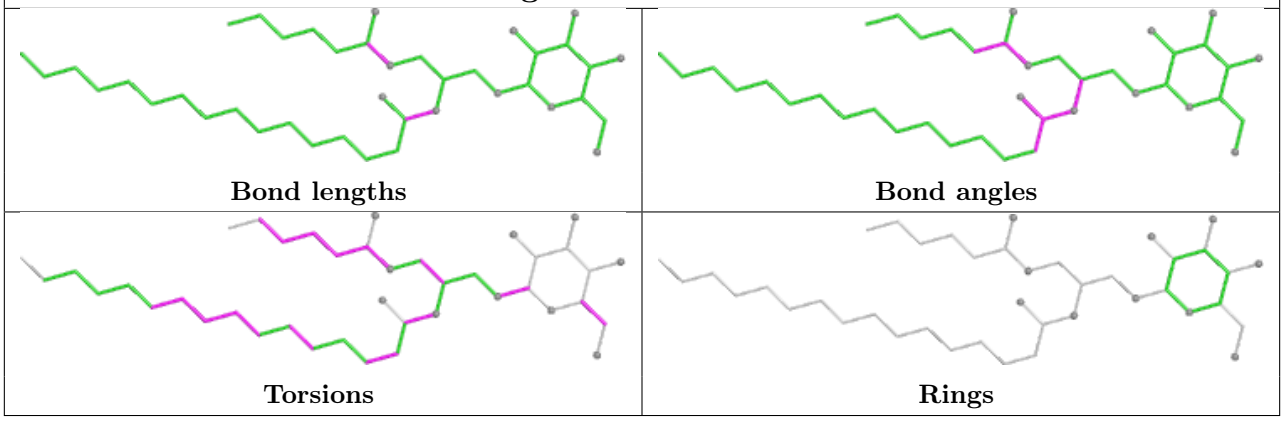
Ligand CHL Y 310



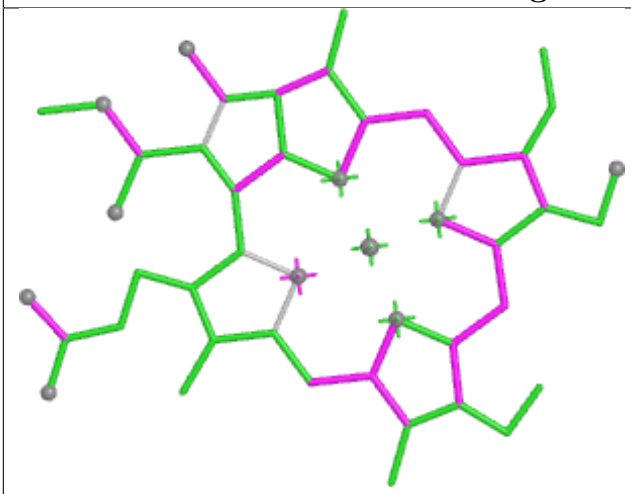
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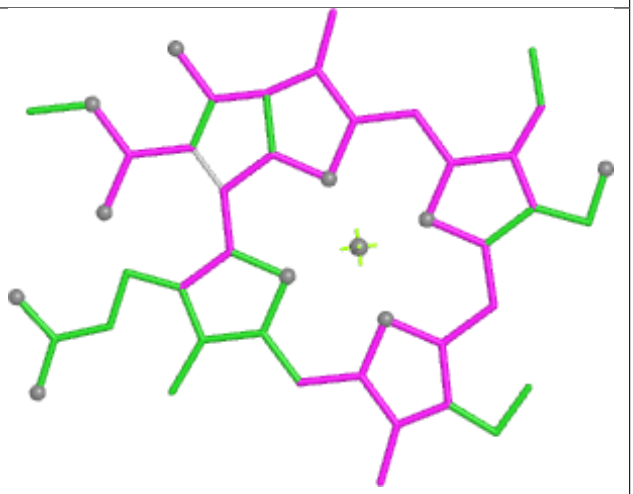
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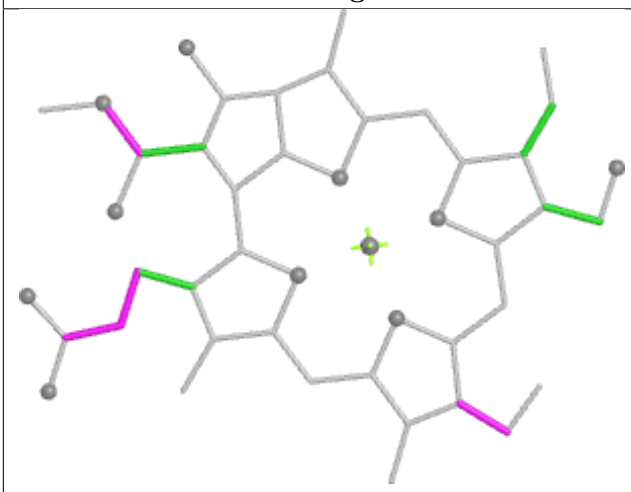
Ligand CHL s 406



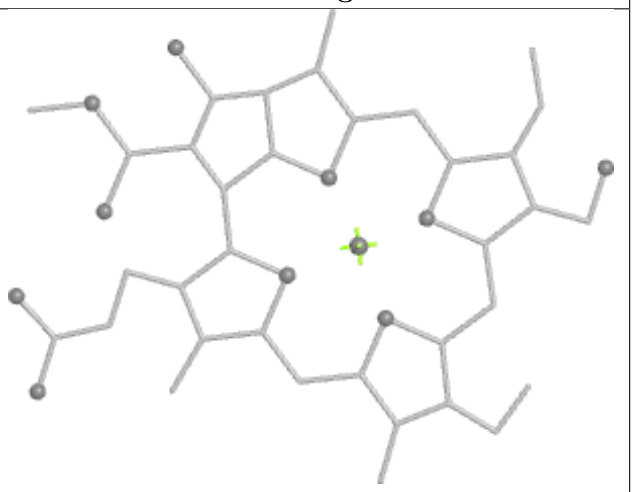
Bond lengths



Bond angles

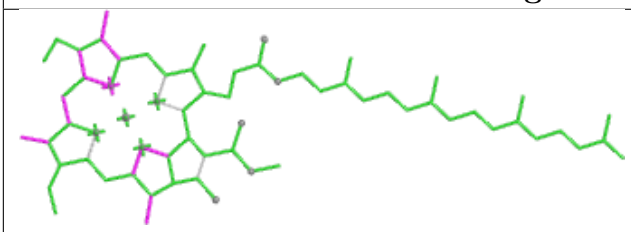


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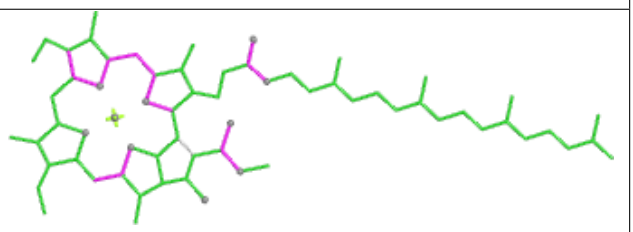


Rings

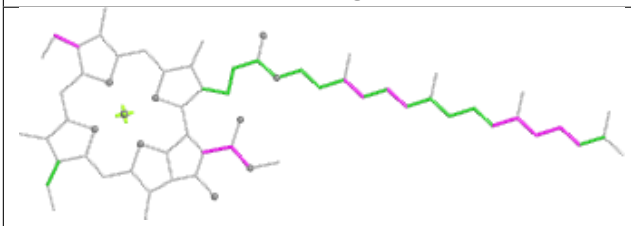
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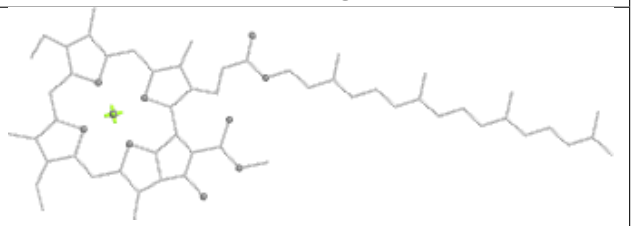
Bond lengths



Bond angles

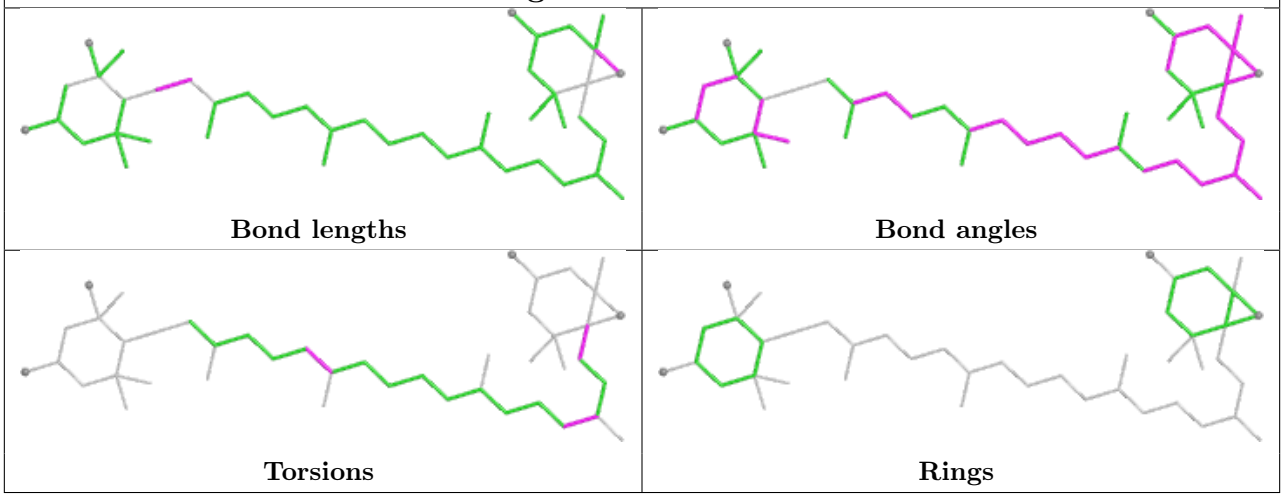


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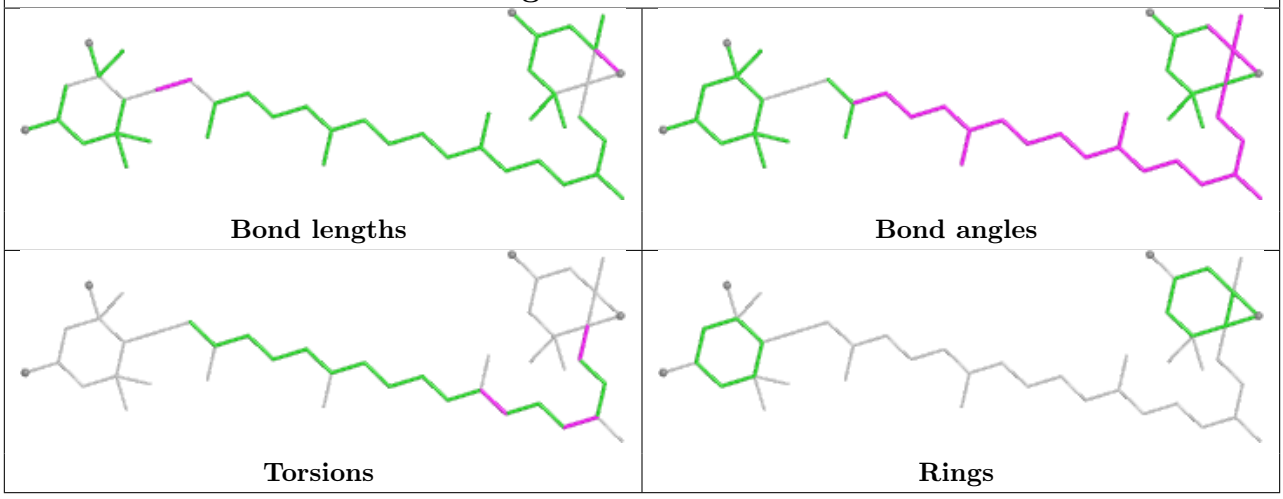


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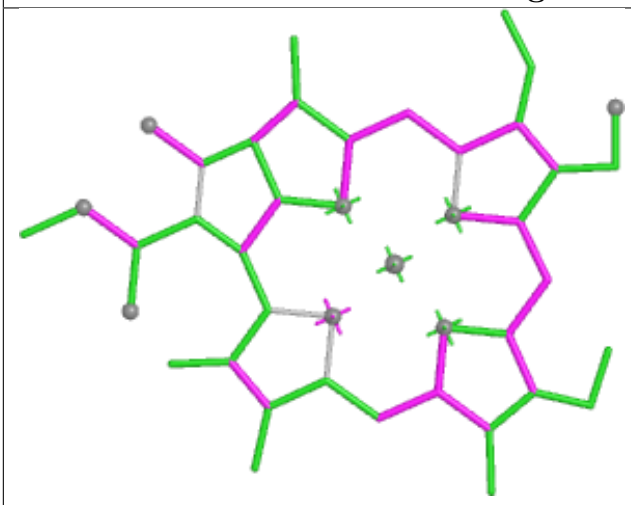
Ligand NEX 3 318



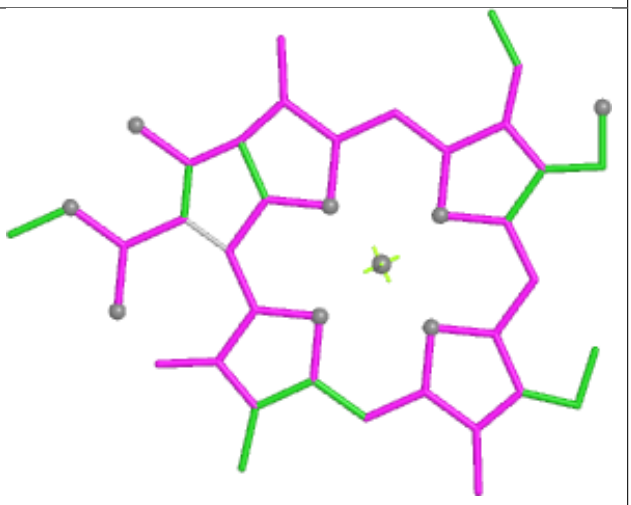
Ligand NEX G 304



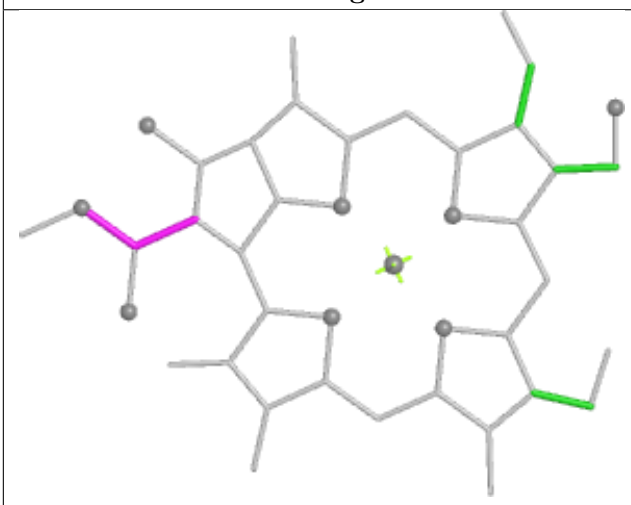
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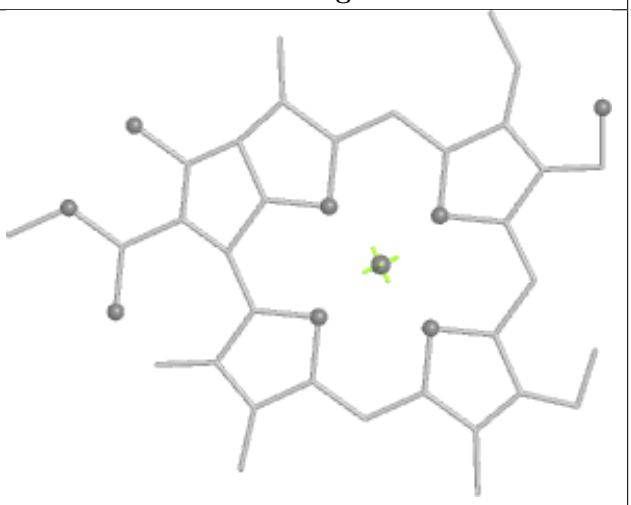
Bond lengths



Bond angles

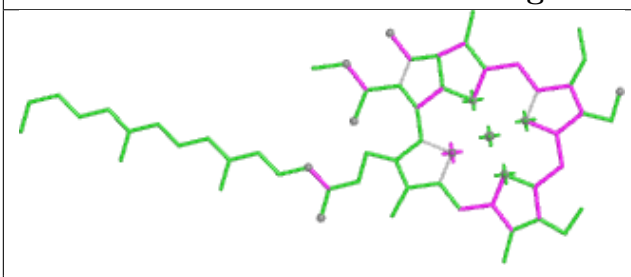


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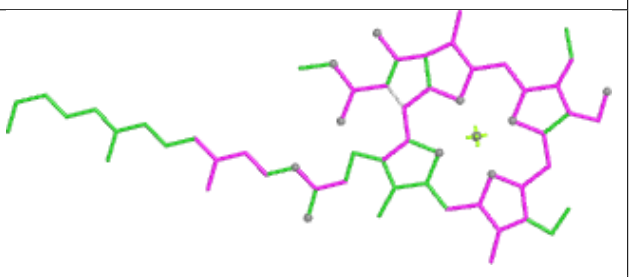


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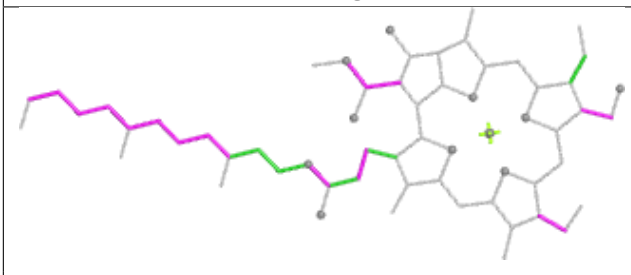
Ligand CHL n 305



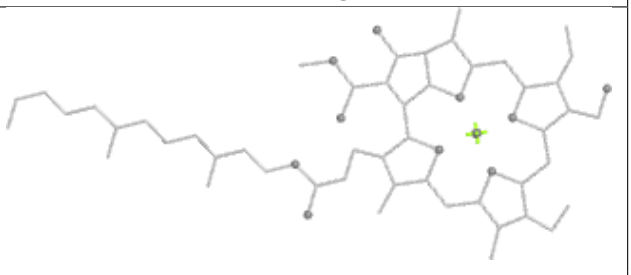
Bond lengths



Bond angles

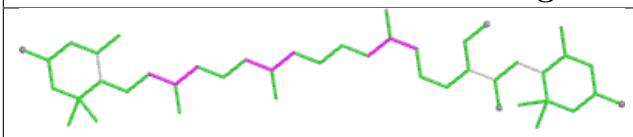


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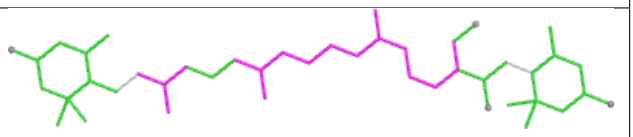


Rings

Ligand 0IE u 303



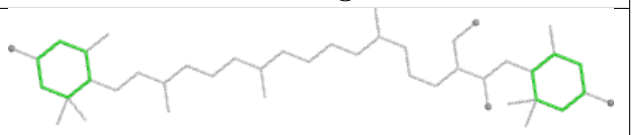
Bond lengths



Bond angles

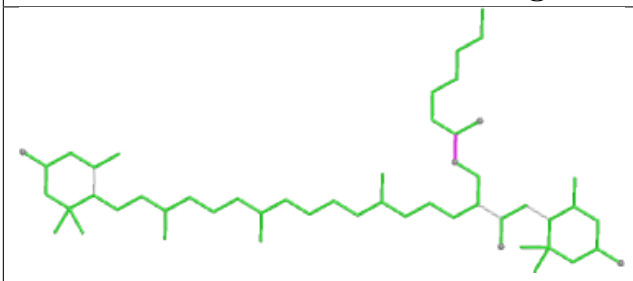


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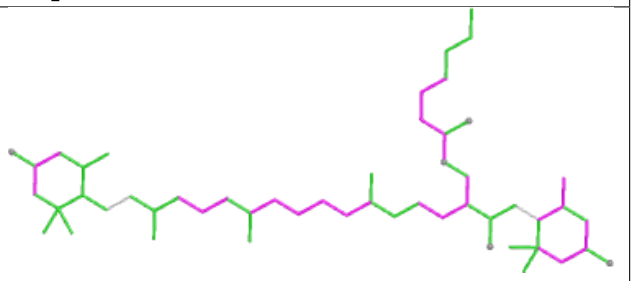


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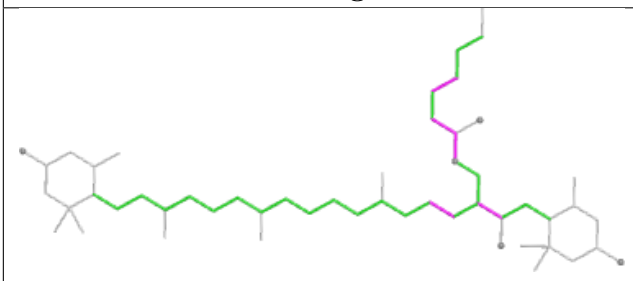
Ligand 0UR p 301



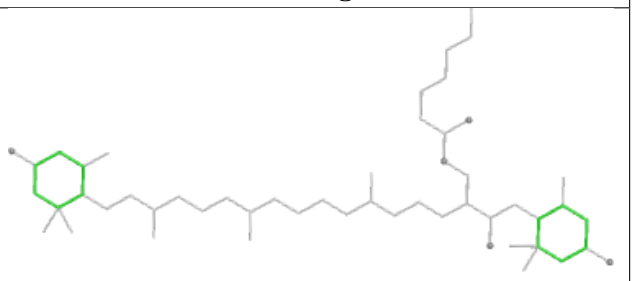
Bond lengths



Bond angles

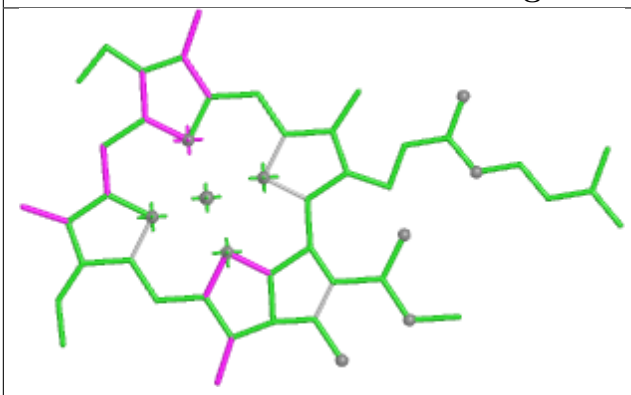


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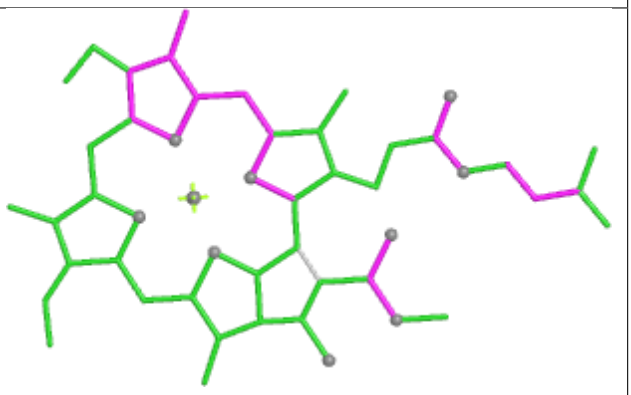


Rings

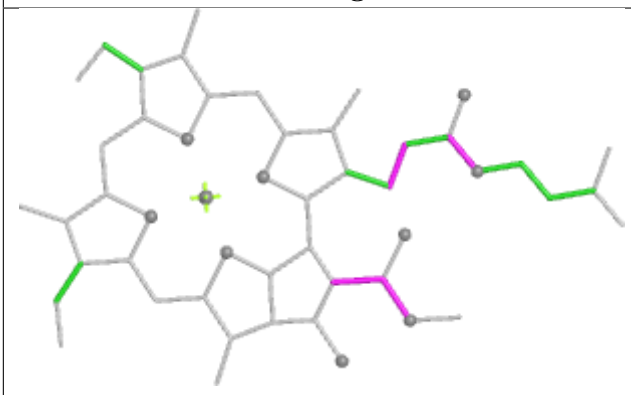
Ligand CLA Y 307



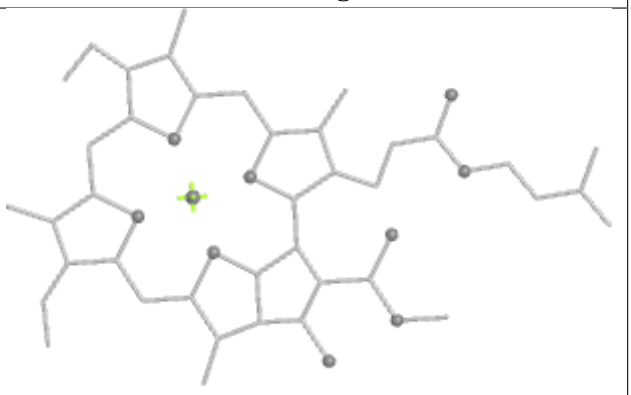
Bond lengths



Bond angles

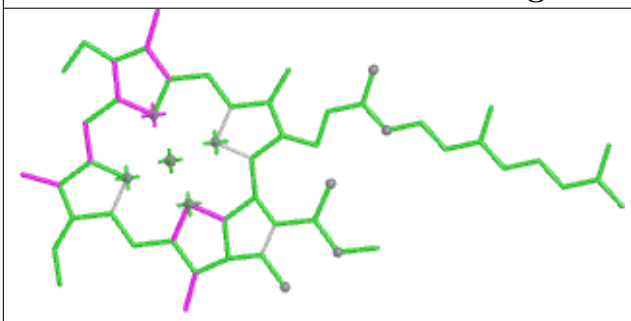


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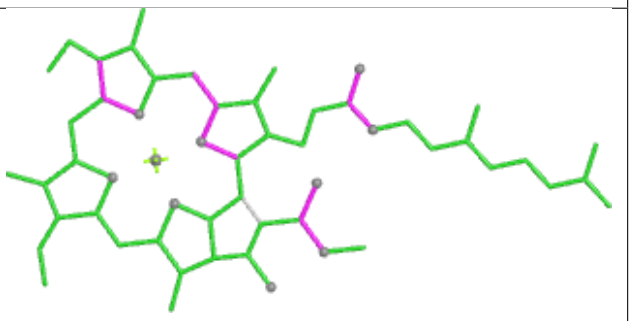


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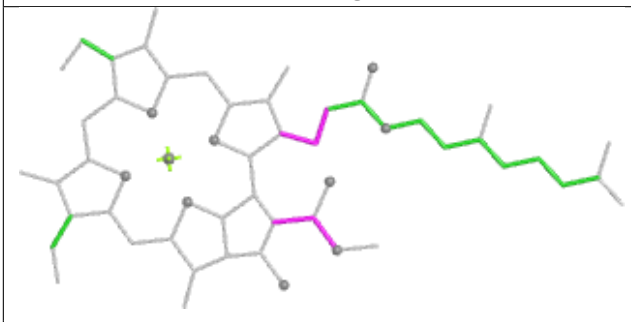
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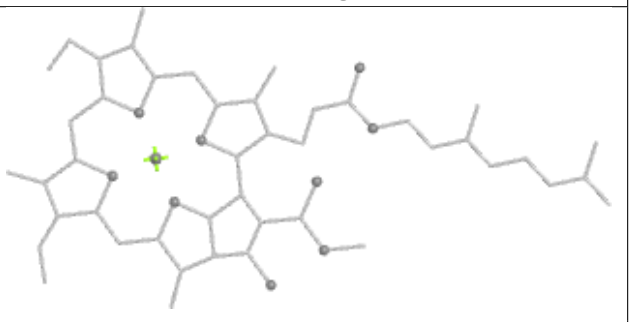
Bond lengths



Bond angles

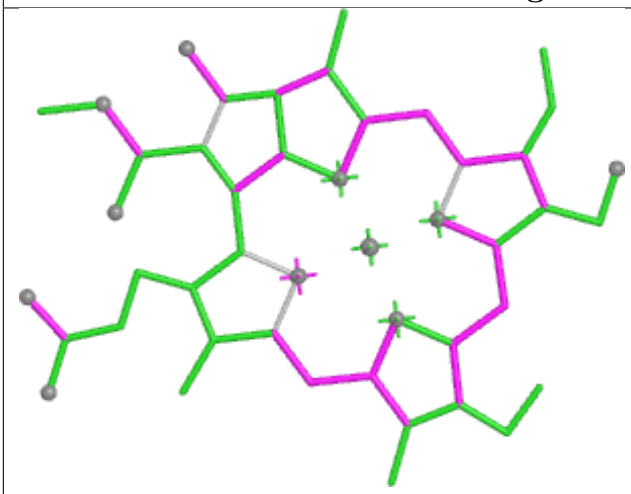


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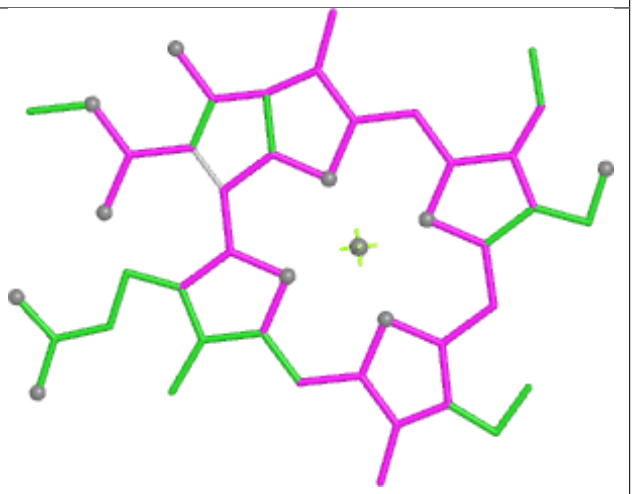


Rings

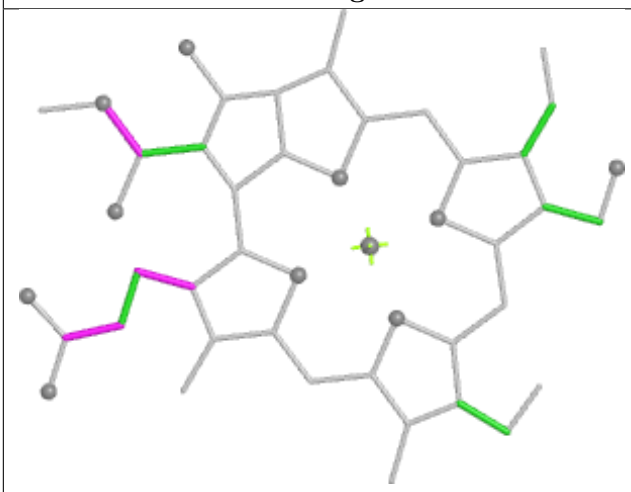
Ligand CHL S 606



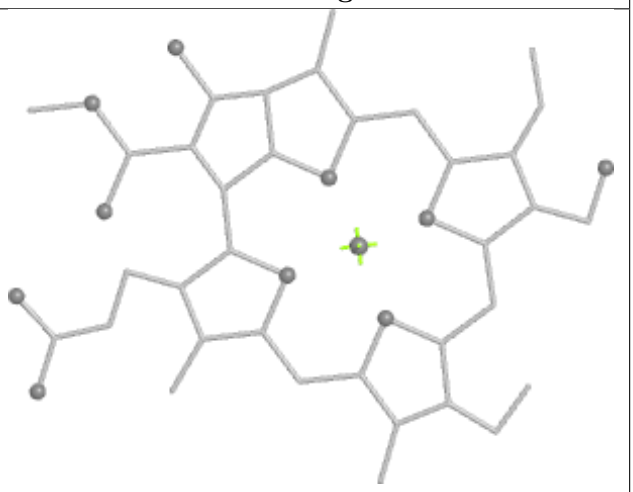
Bond lengths



Bond angles

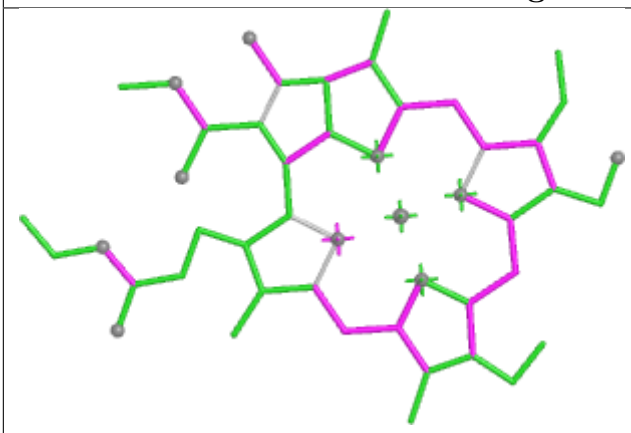


Torsions

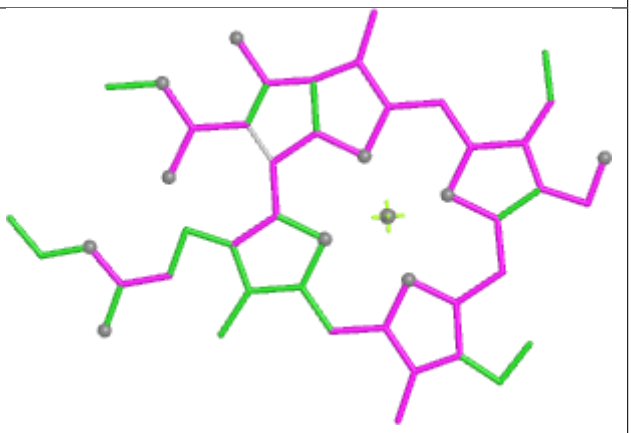


Rings

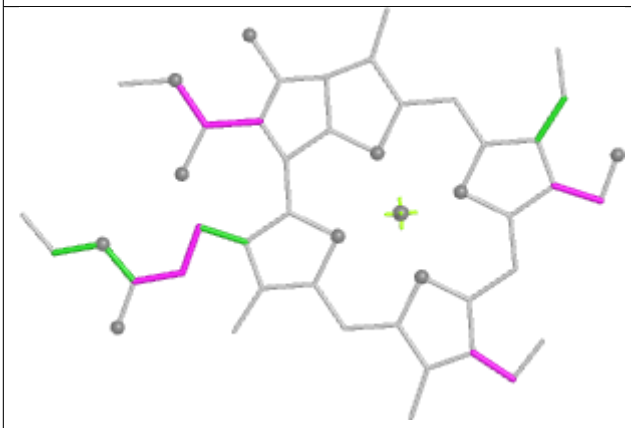
Ligand CHL 6 305



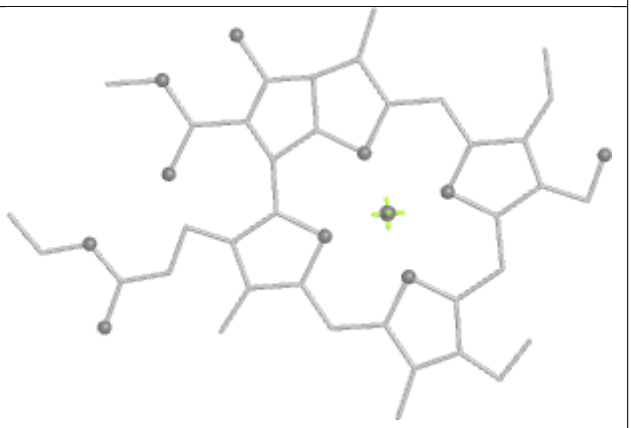
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Bond angles

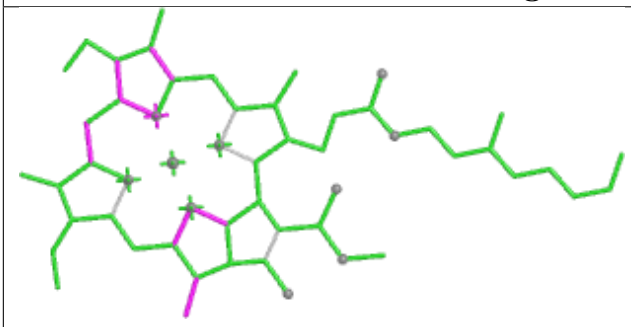


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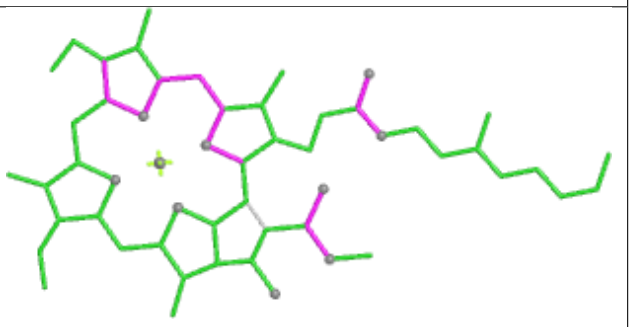


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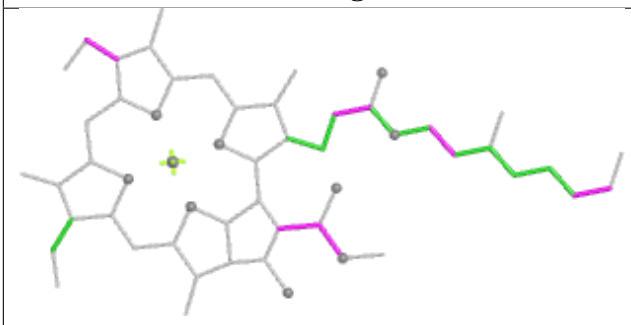
Ligand CLA N 306



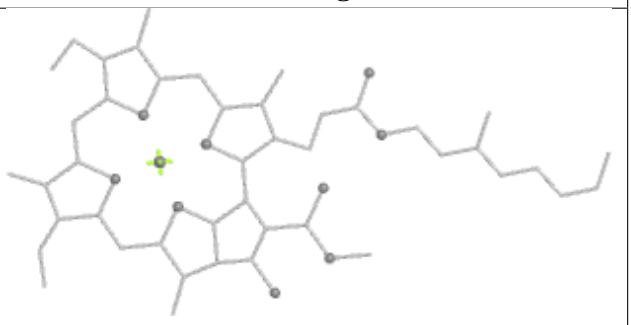
Bond lengths



Bond angles

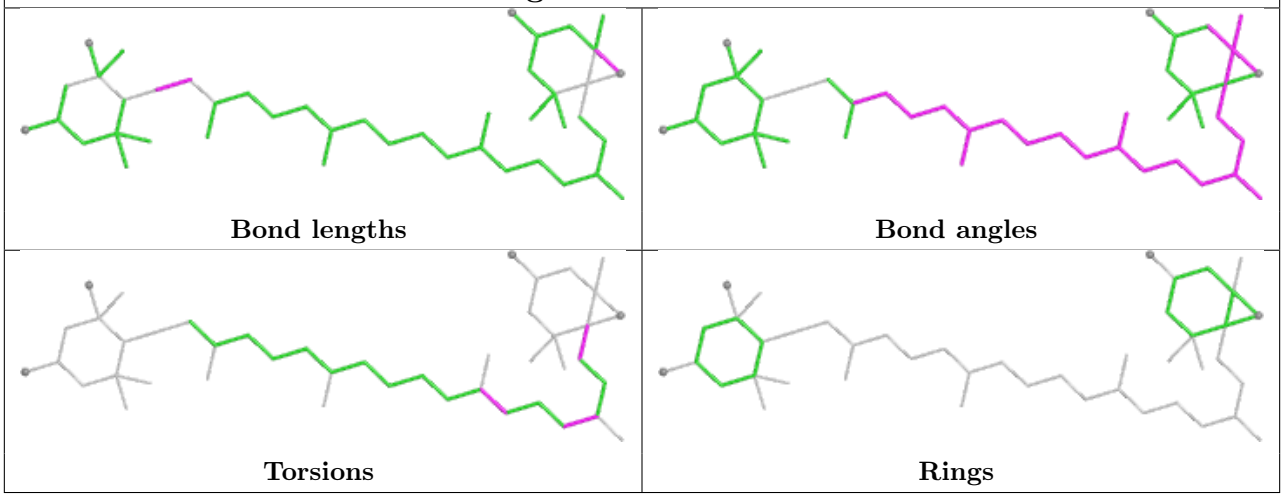


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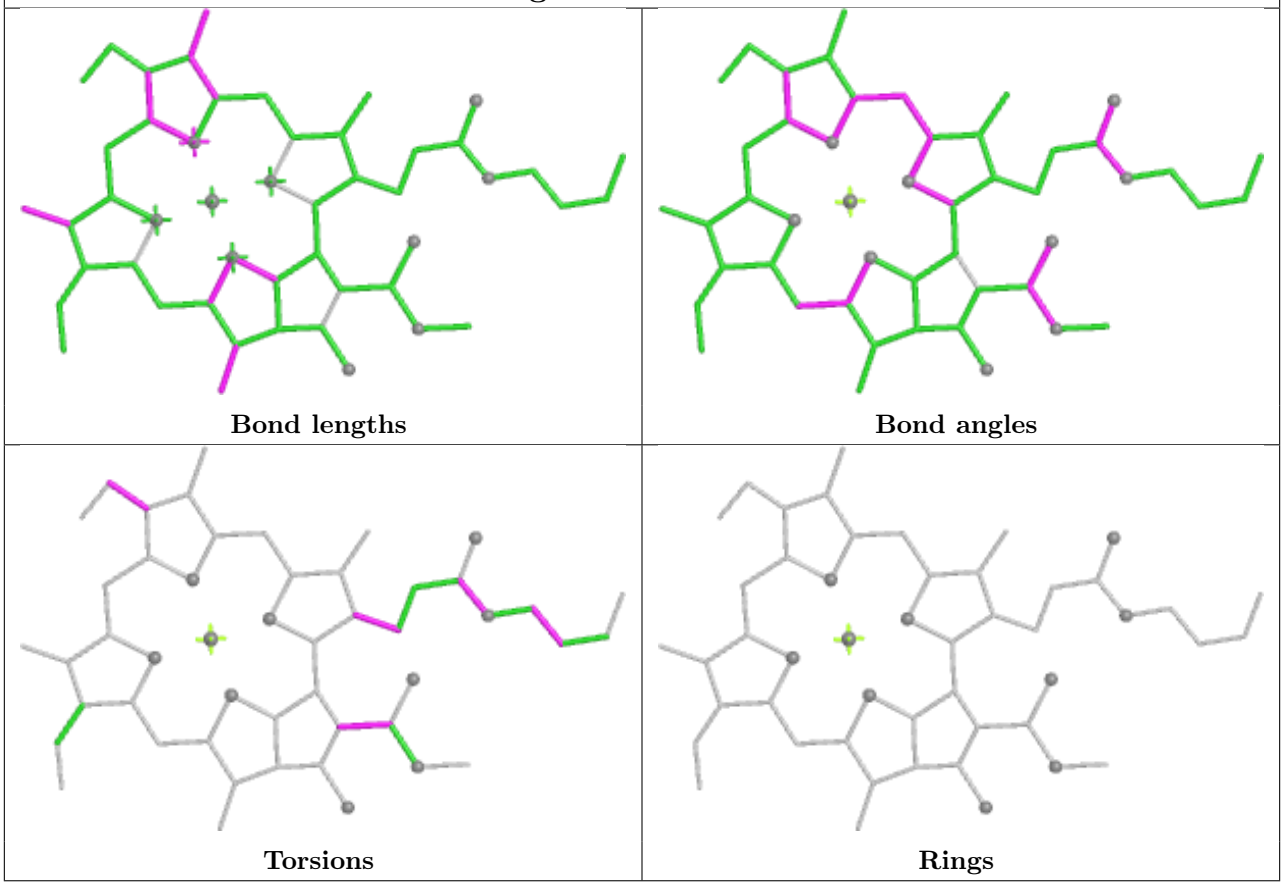


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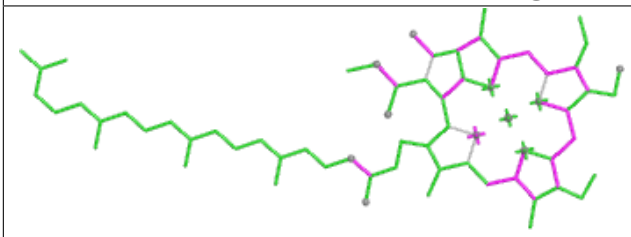
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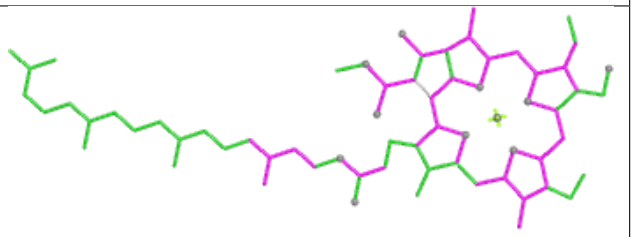
Ligand CLA a 605



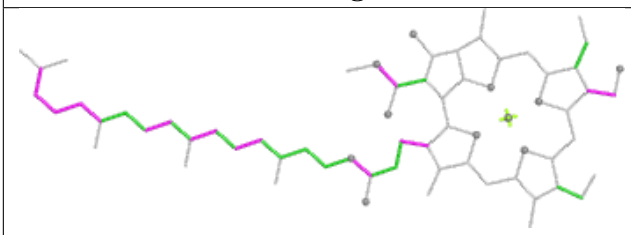
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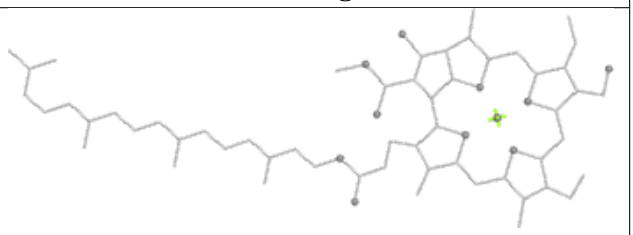
Bond lengths



Bond angles

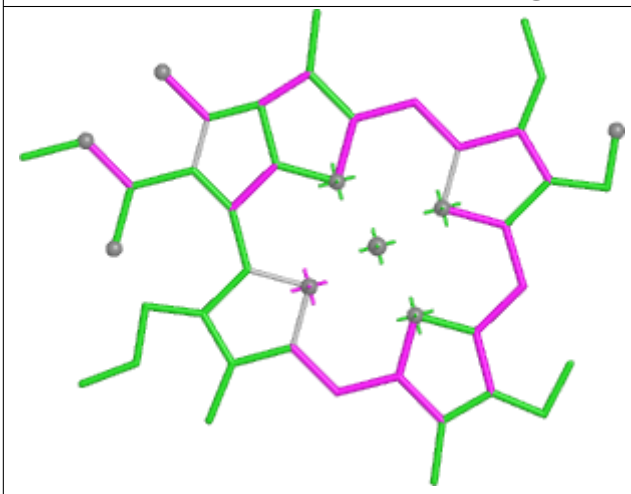


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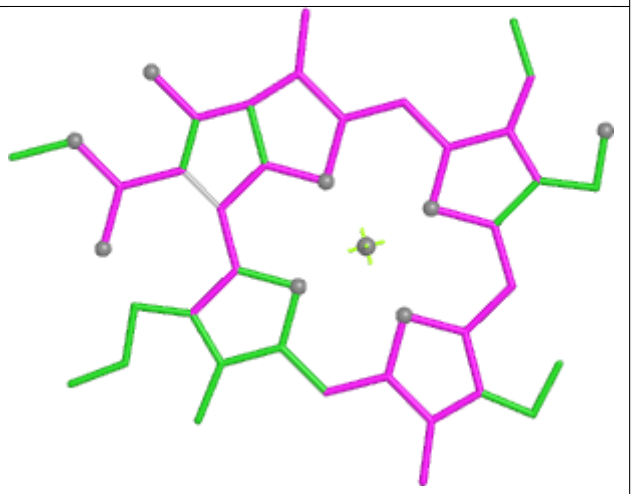


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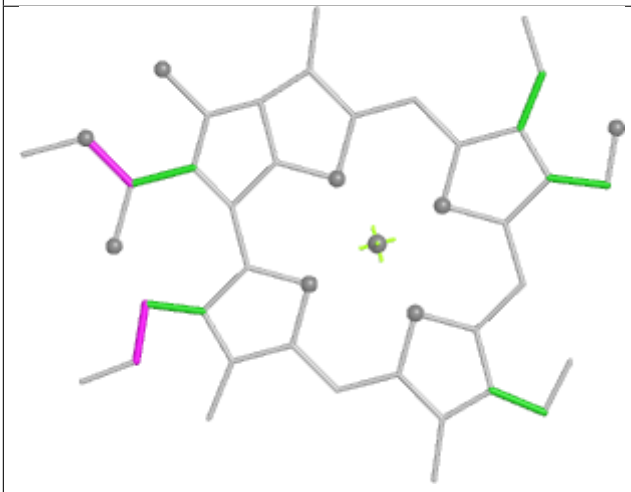
Ligand CHL 4 311



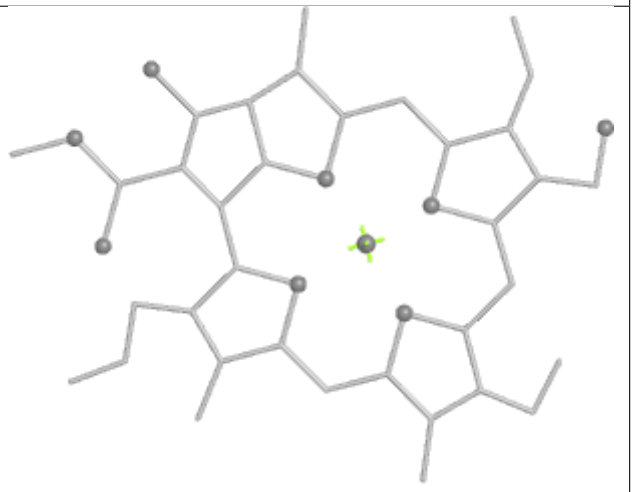
Bond lengths



Bond angles

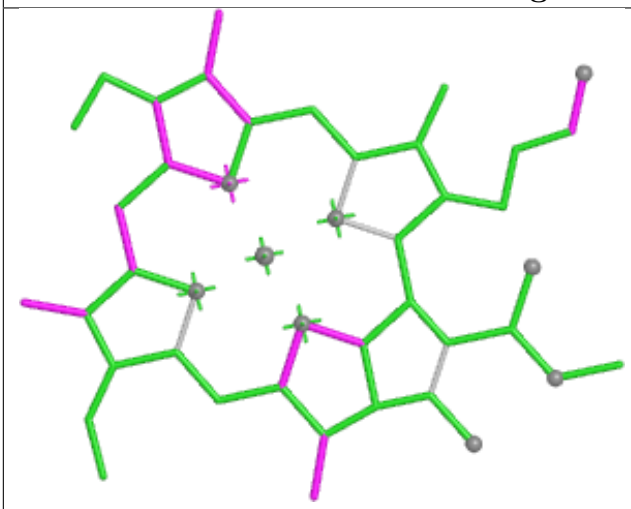


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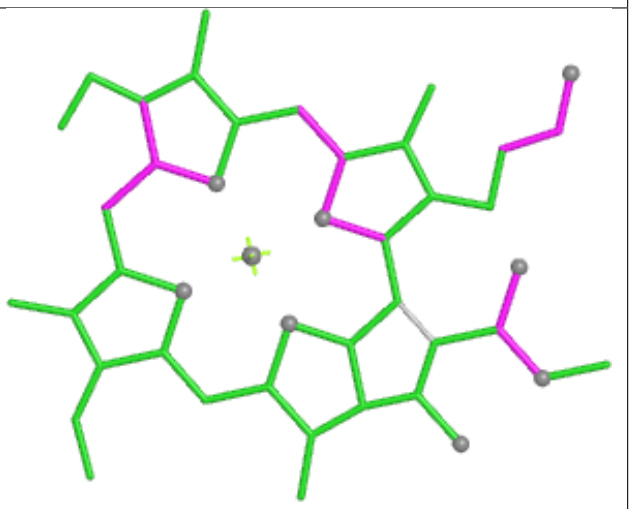


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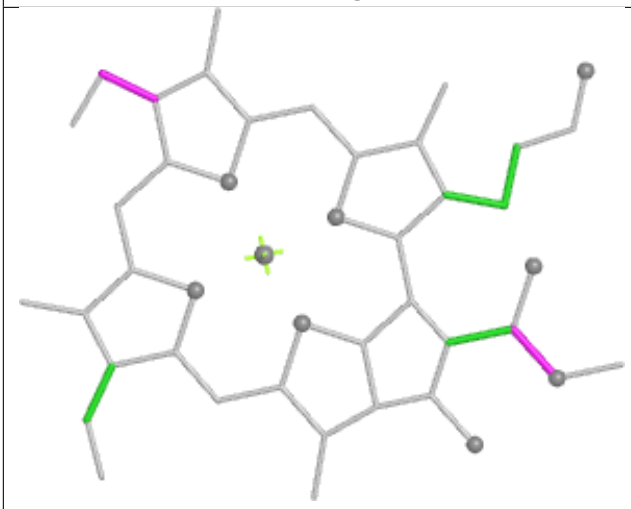
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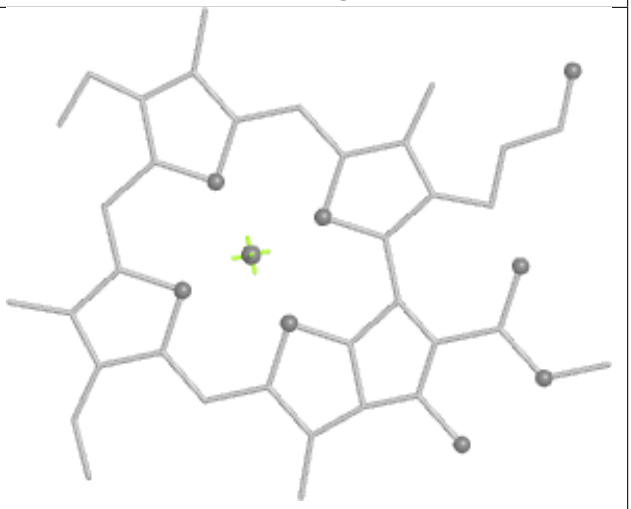
Bond lengths



Bond angles

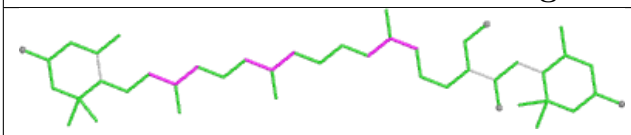


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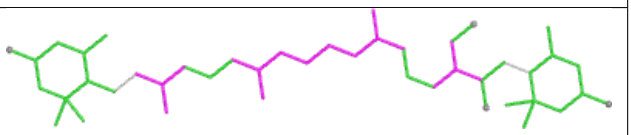


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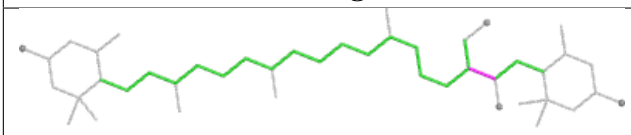
Ligand 0IE r 315



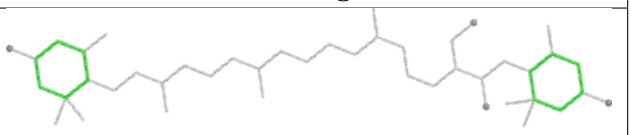
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Bond angles

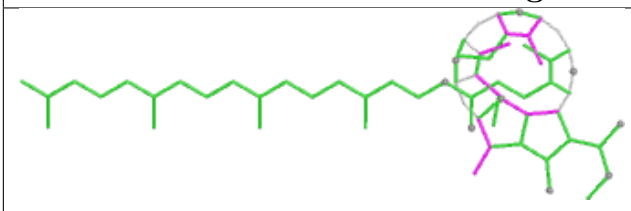


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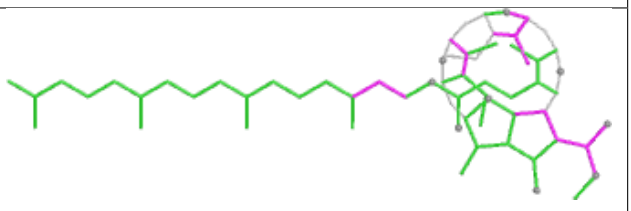


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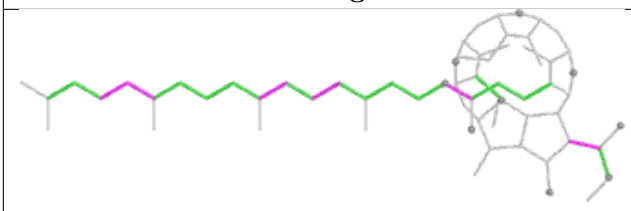
Ligand PHO a 606



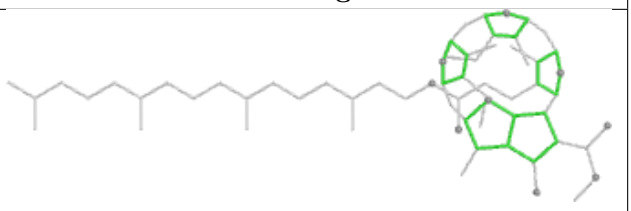
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Bond angles

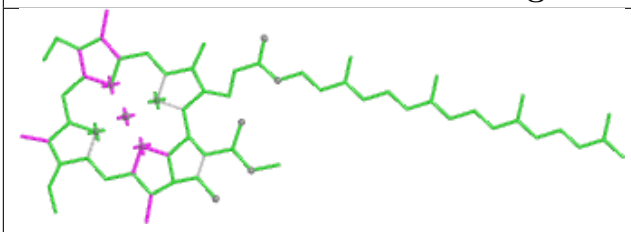


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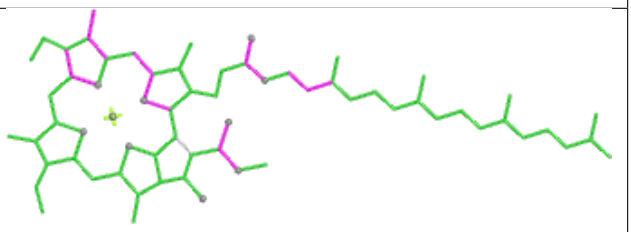


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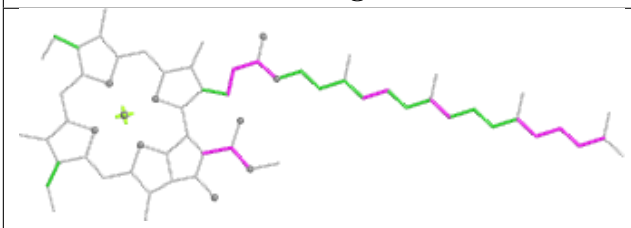
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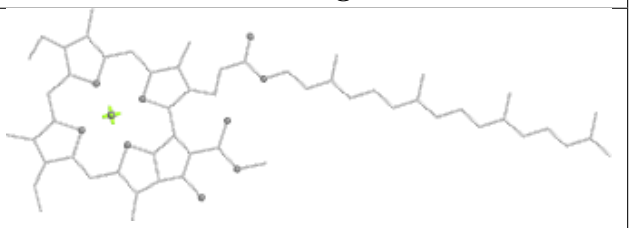
Bond lengths



Bond angles

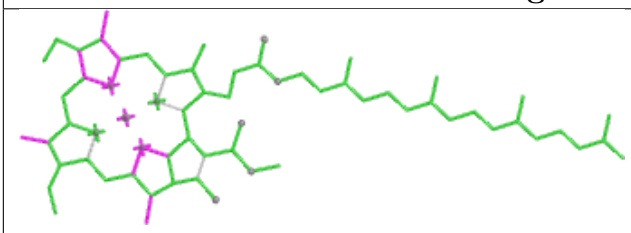


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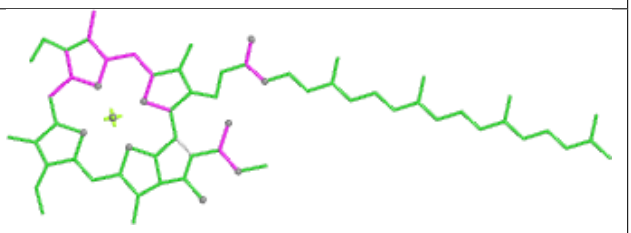


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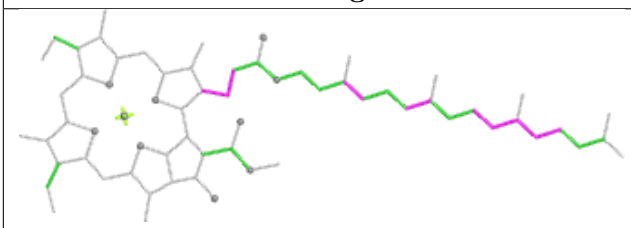
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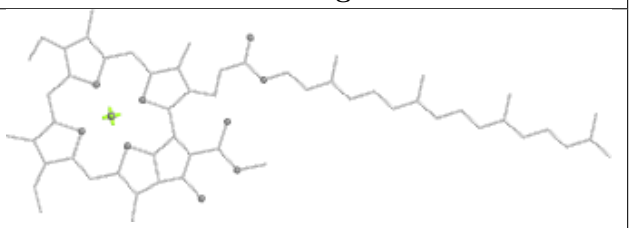
Bond lengths



Bond angles

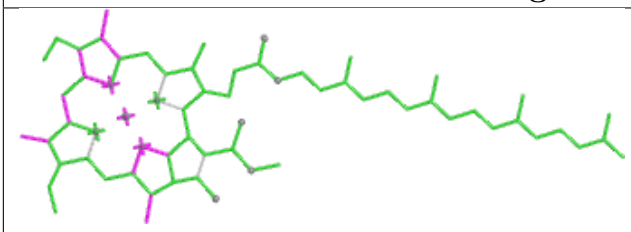


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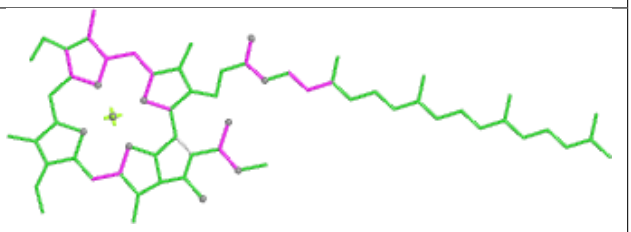


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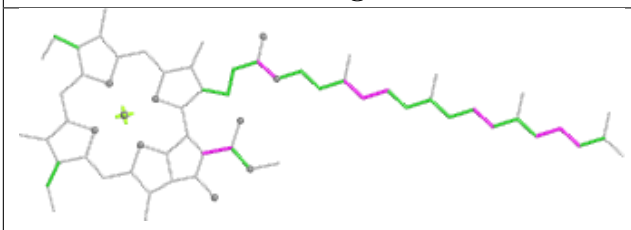
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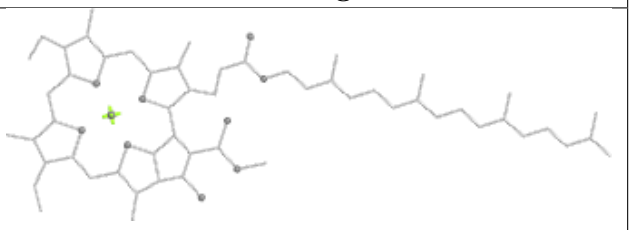
Bond lengths



Bond angles

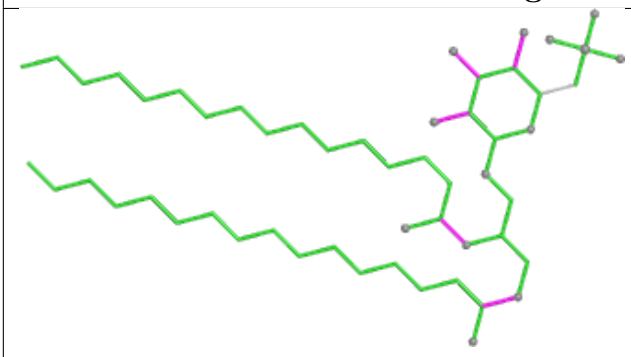


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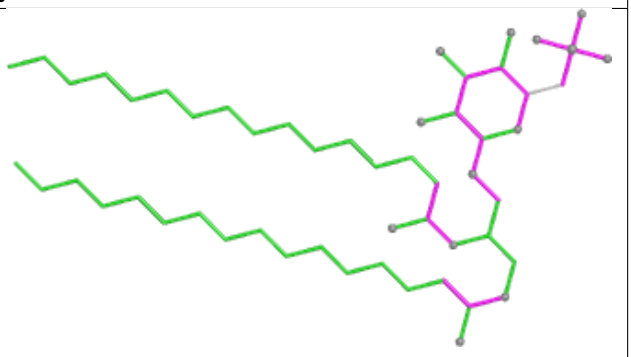


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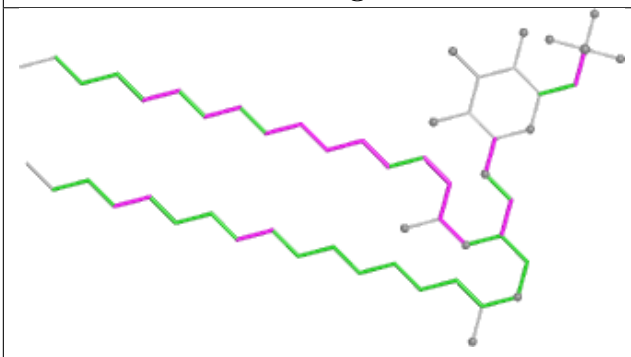
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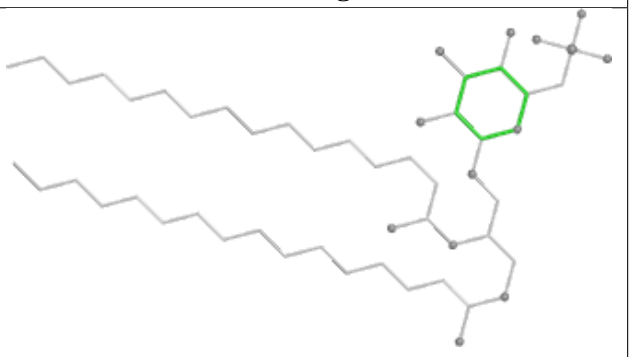
Bond lengths



Bond angles

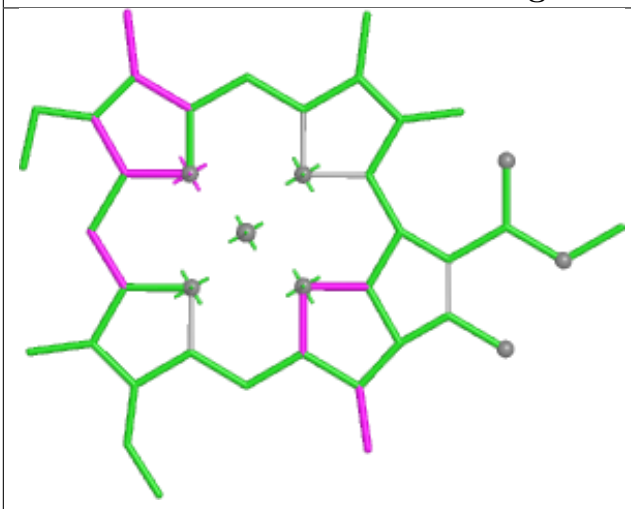


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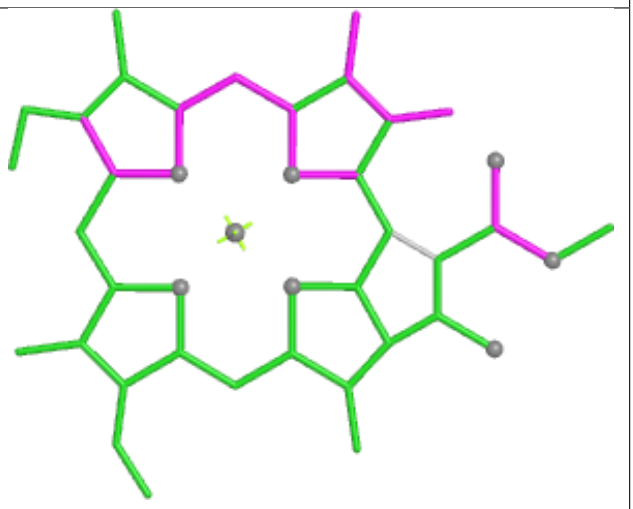


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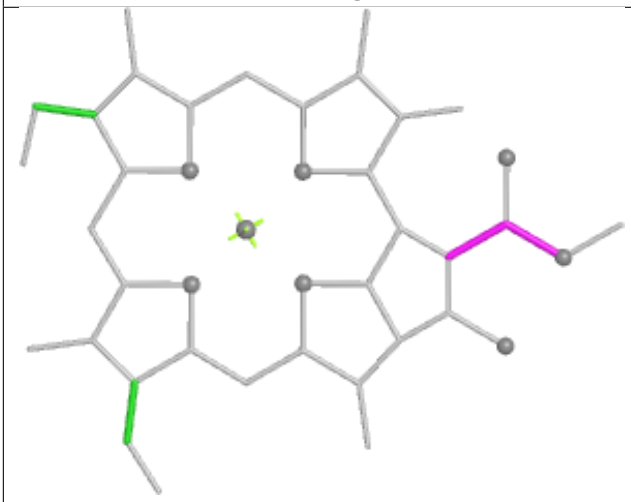
Ligand CLA 4 307



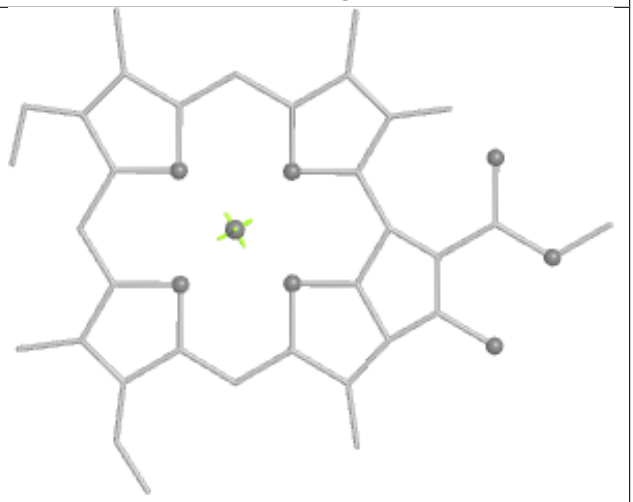
Bond lengths



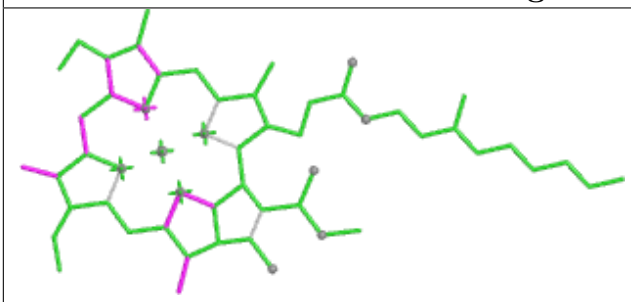
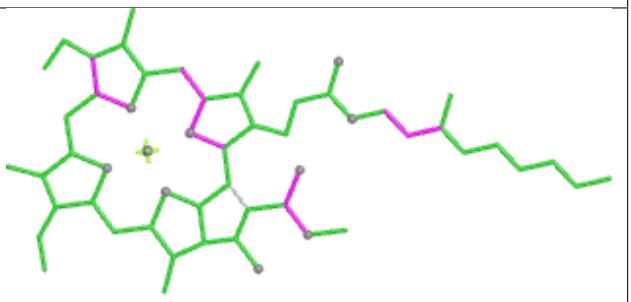
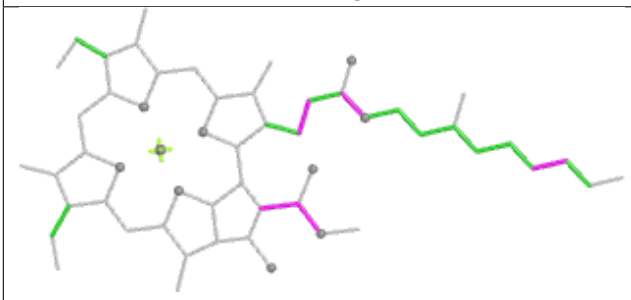
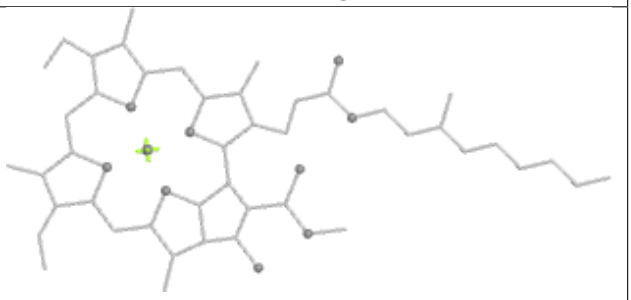
Bond angles



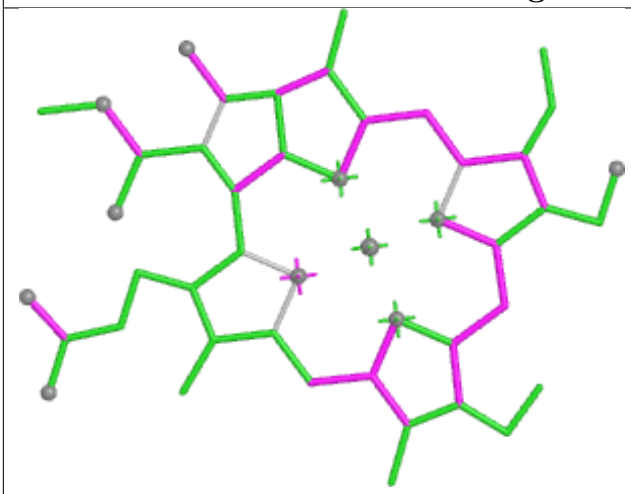
Torsions



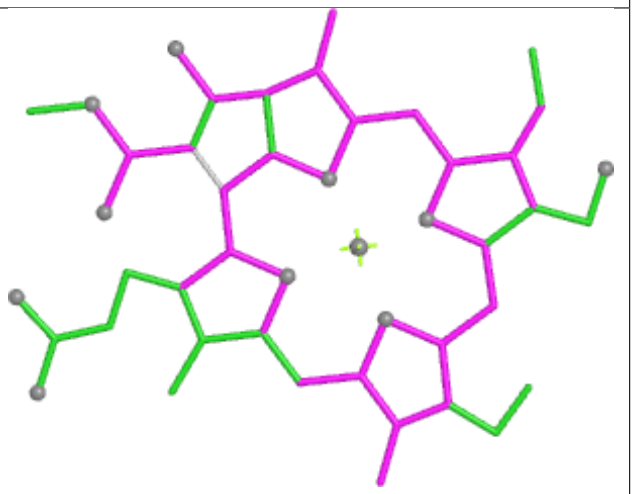
Rings

Ligand CLA u 317	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

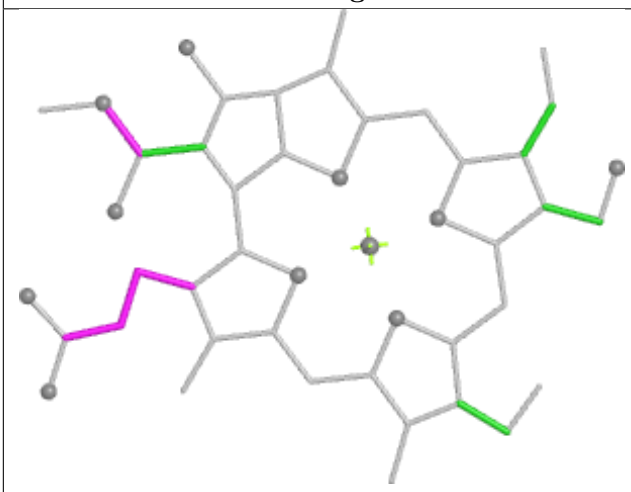
Ligand CHL 3 310



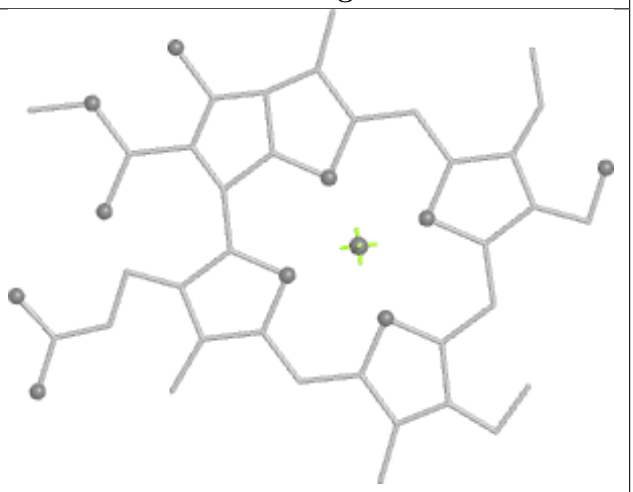
Bond lengths



Bond angles

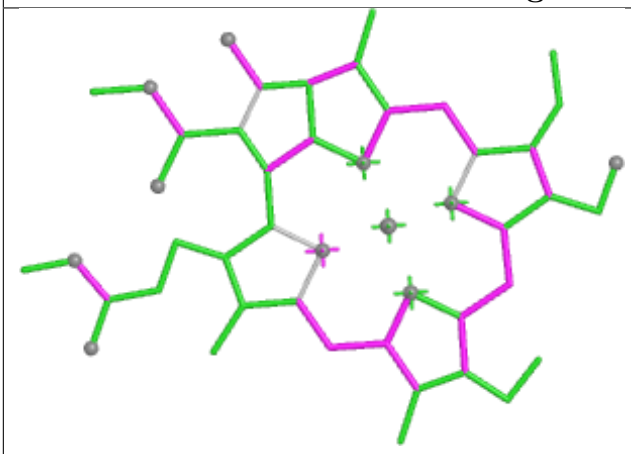


Torsions

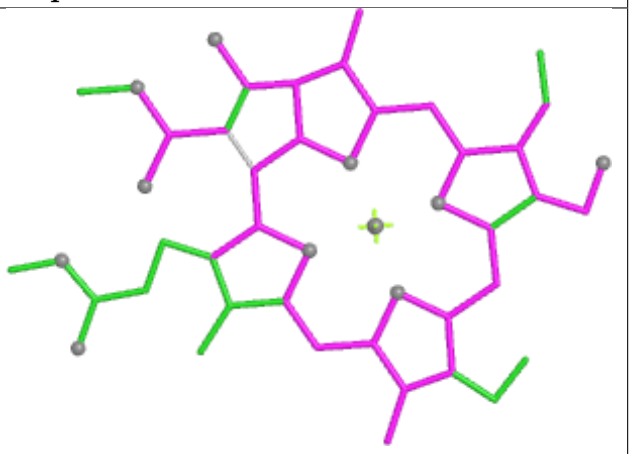


Rings

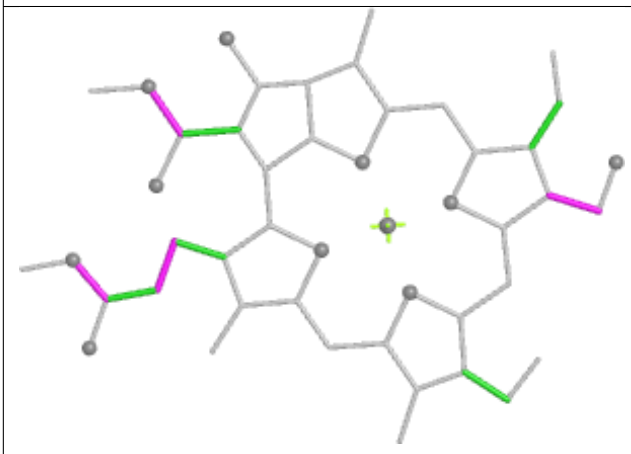
Ligand CHL p 312



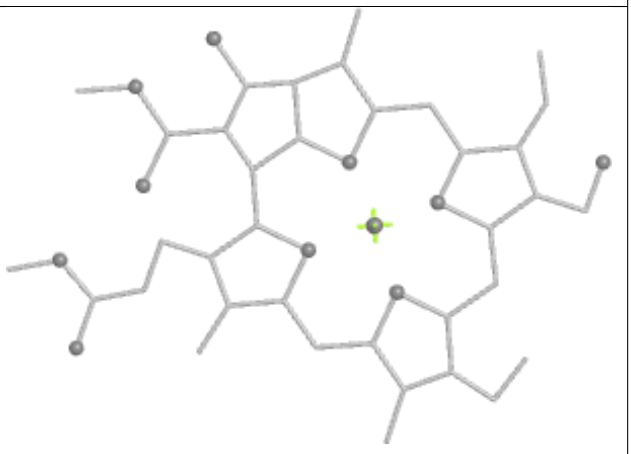
Bond lengths



Bond angles

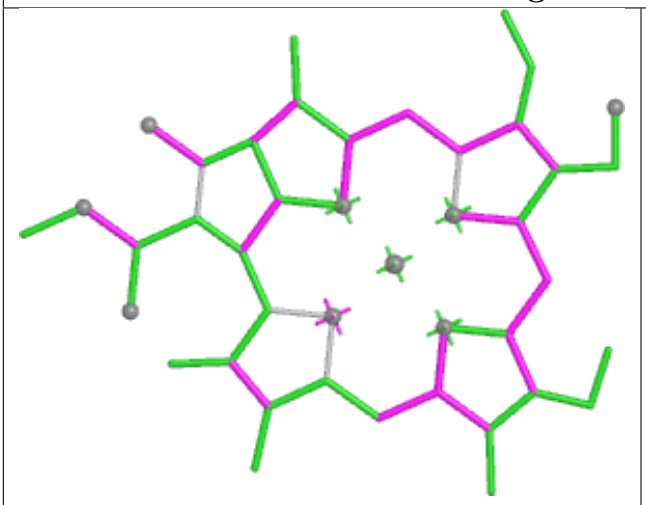


Torsions

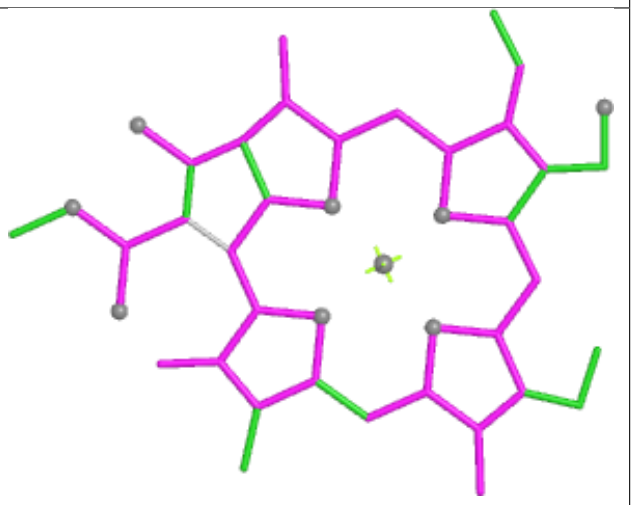


Rings

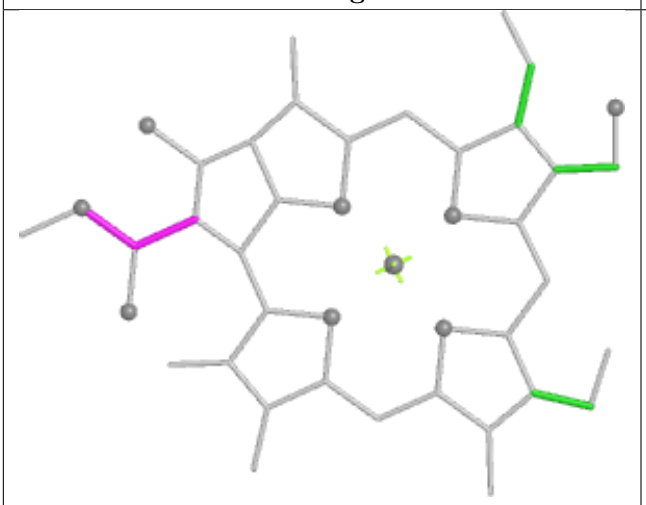
Ligand CHL 7 318



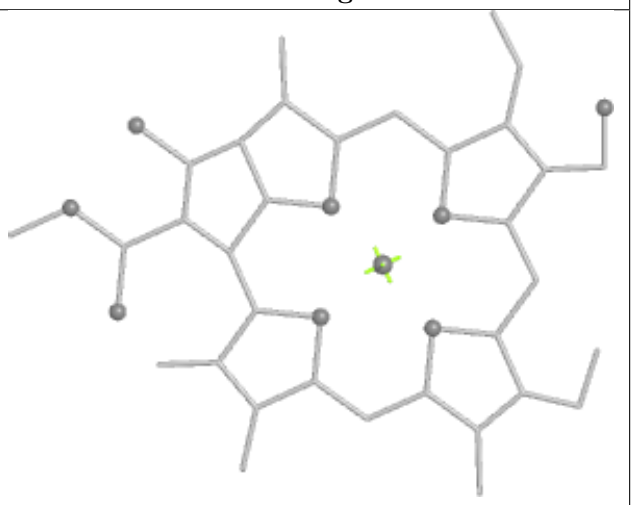
Bond lengths



Bond angles

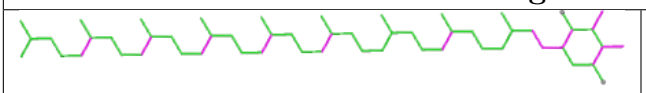


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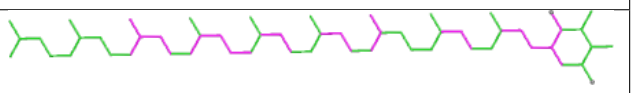


Rings

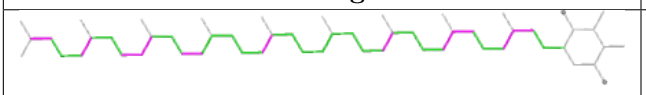
Ligand PL9 D 406



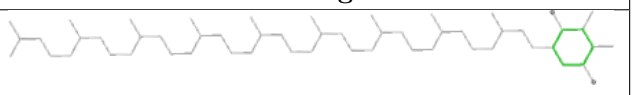
Bond lengths



Bond angles

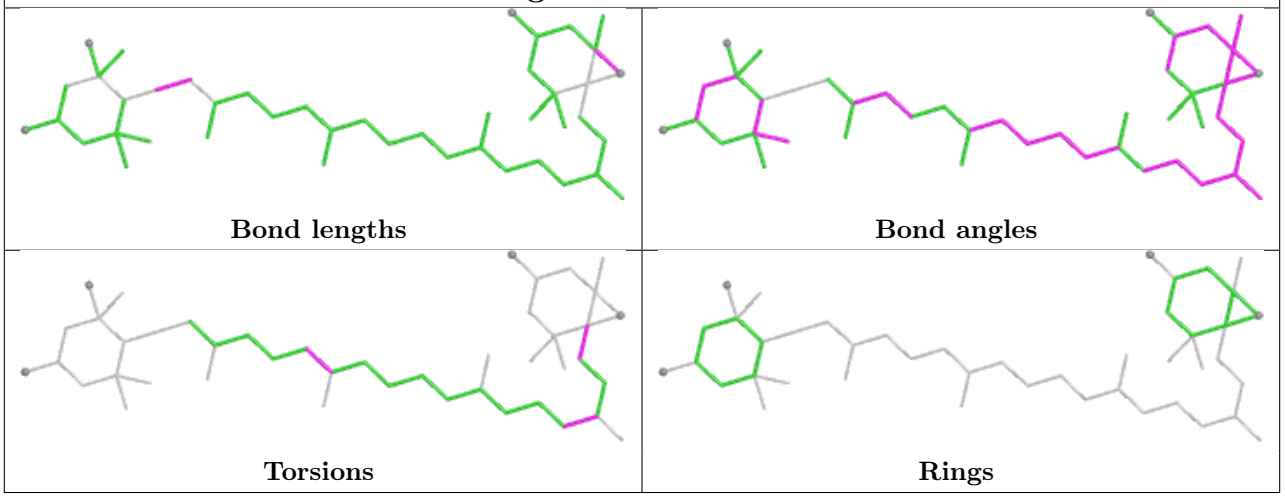


Torsions

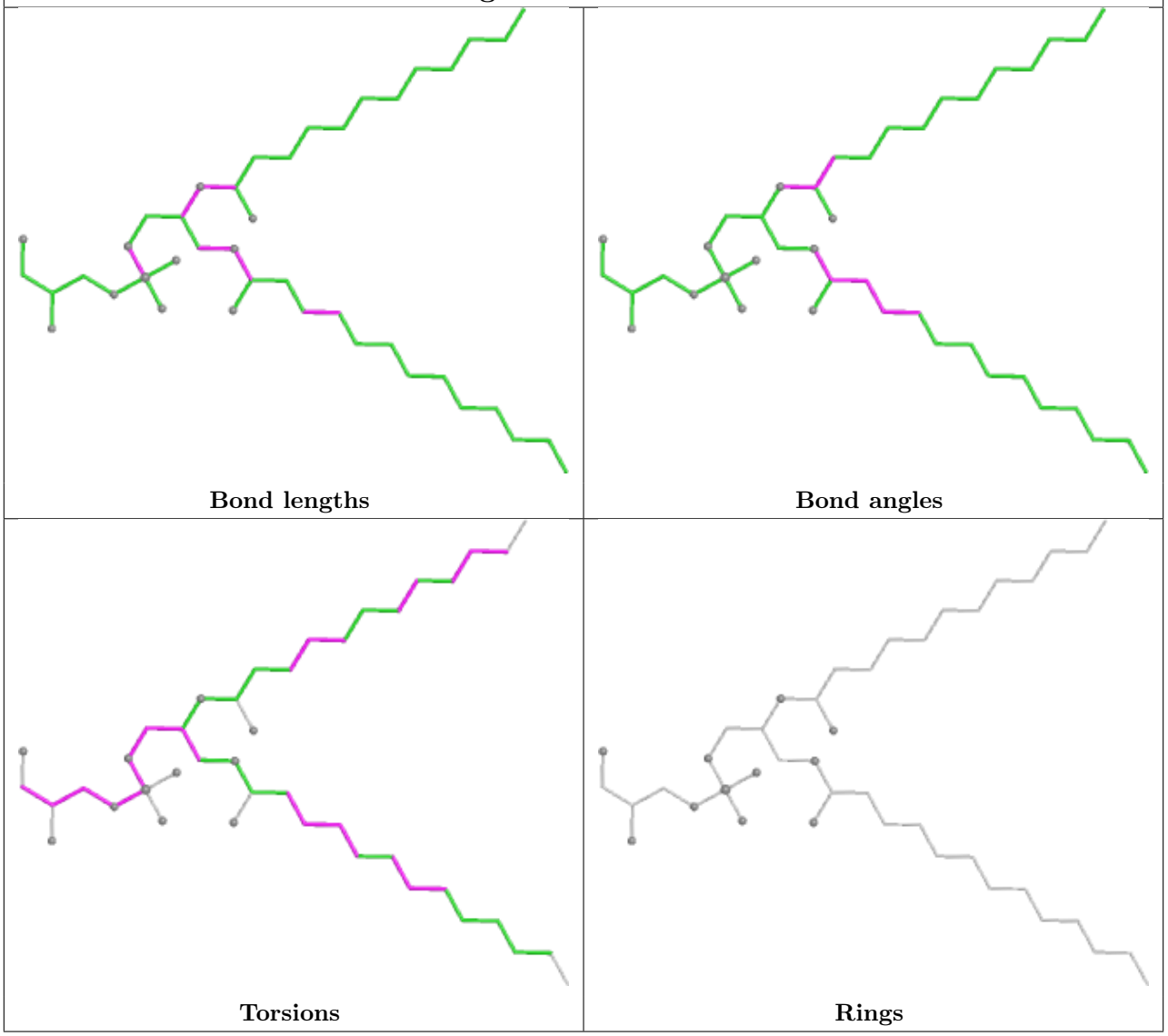


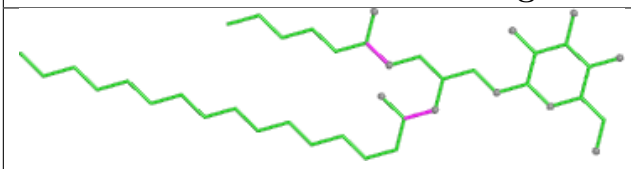
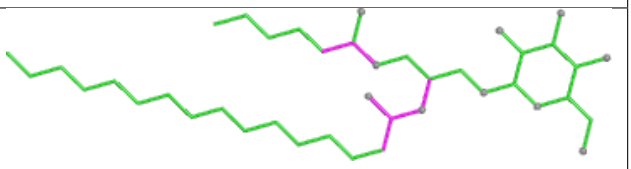
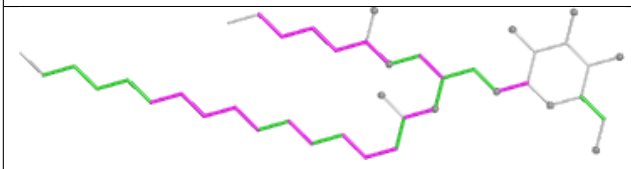
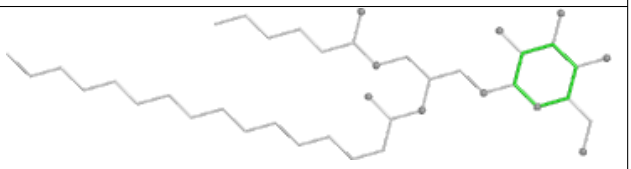
Rings

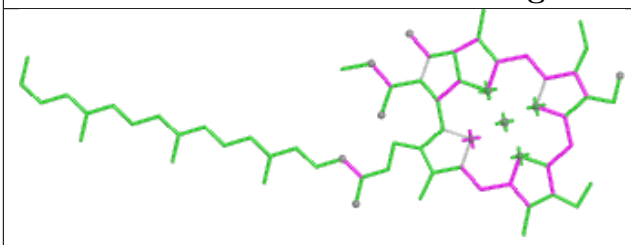
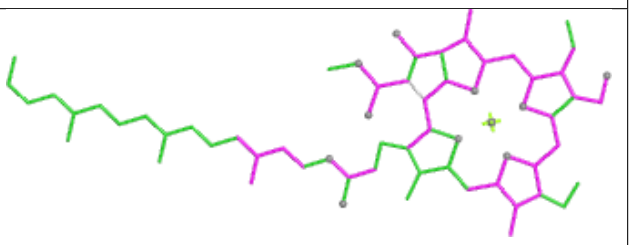
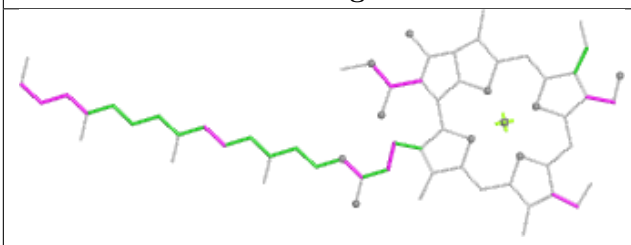
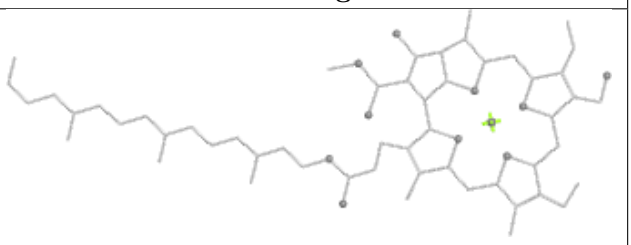
Ligand NEX 6 303



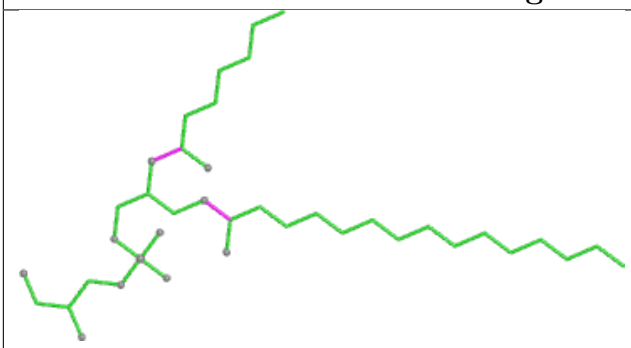
Ligand LHG 1 318



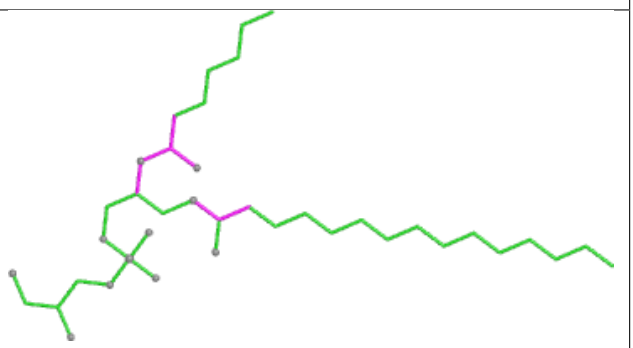
Ligand LMG m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 9 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

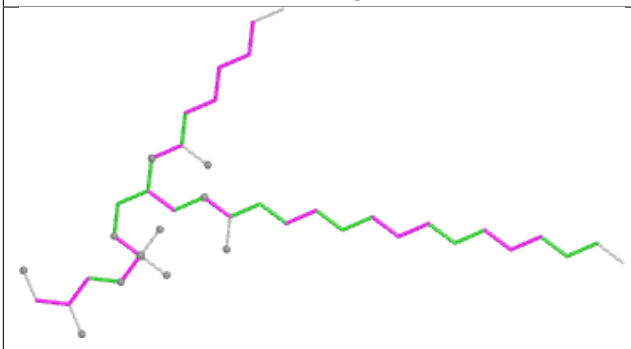
Ligand LHG d 408



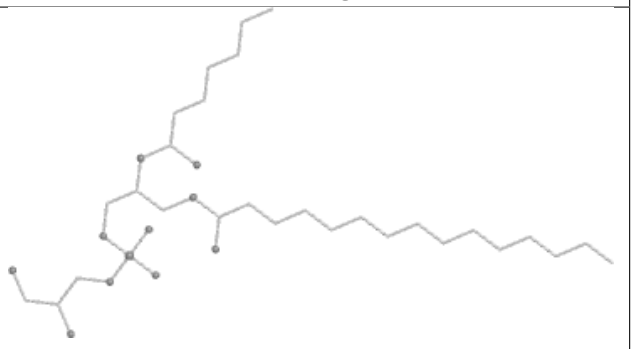
Bond lengths



Bond angles

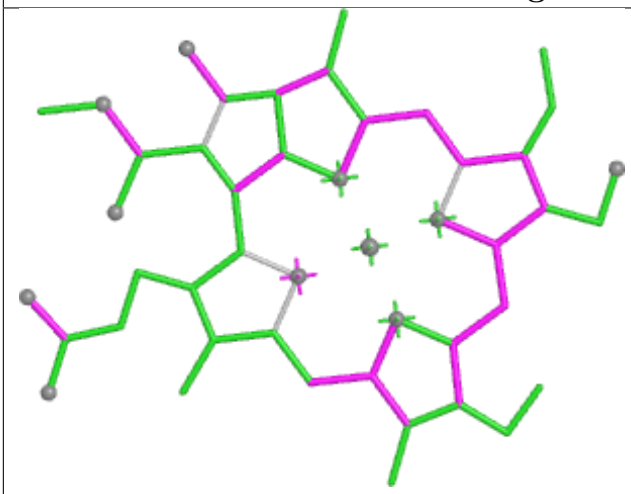


Torsions

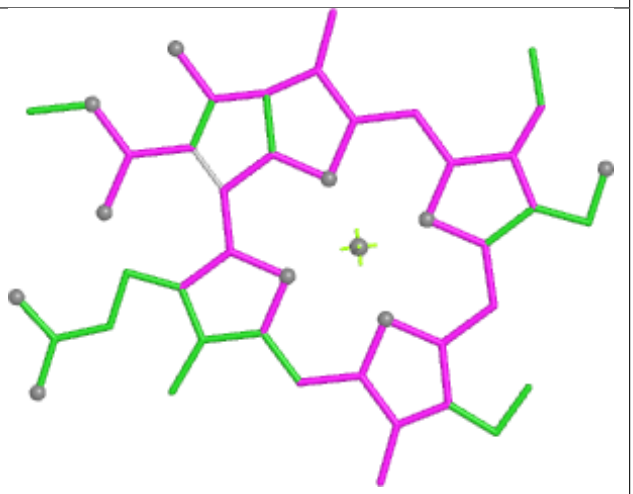


Rings

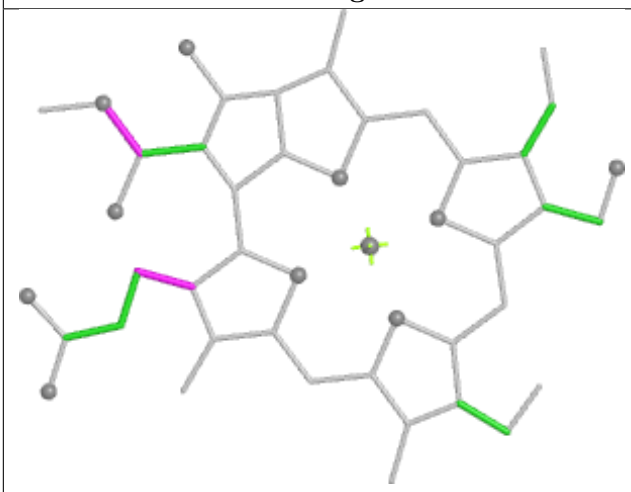
Ligand CHL 9 310



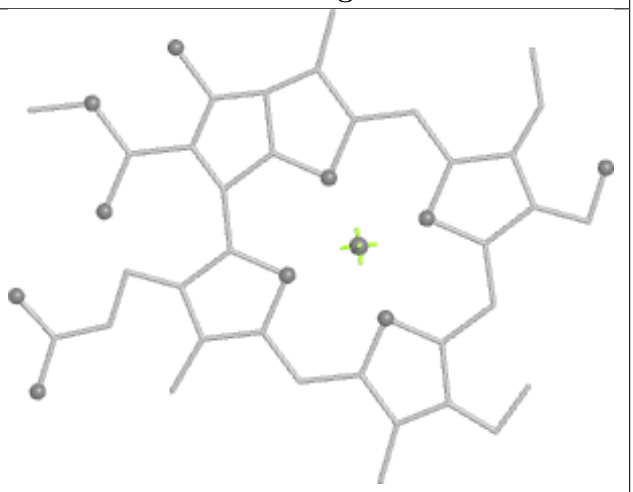
Bond lengths



Bond angles

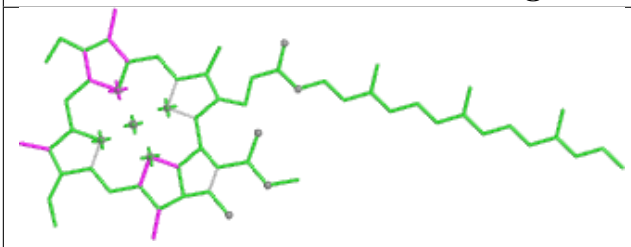


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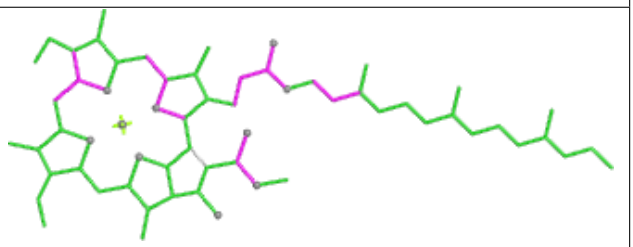


Rings

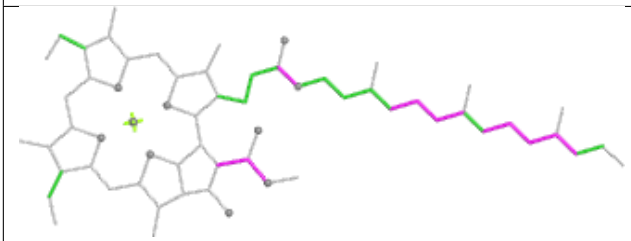
Ligand CLA B 604



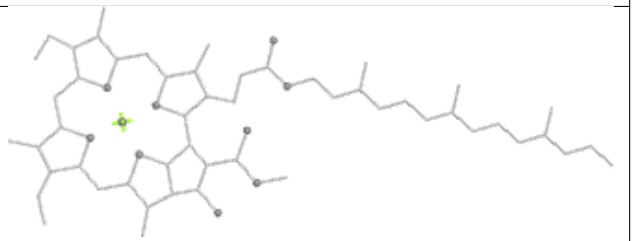
Bond lengths



Bond angles

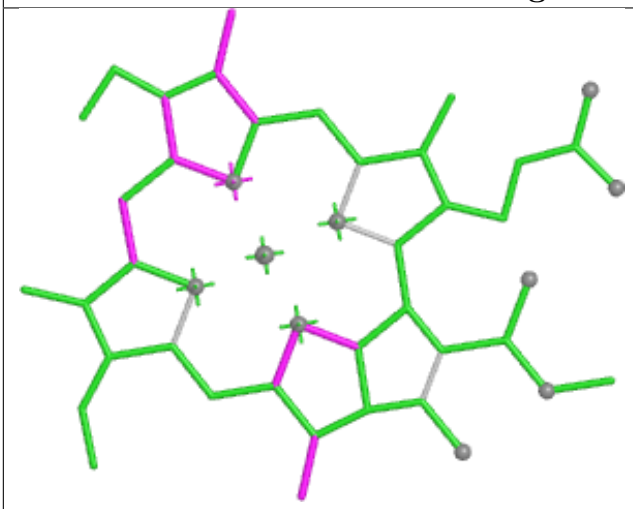


Torsions

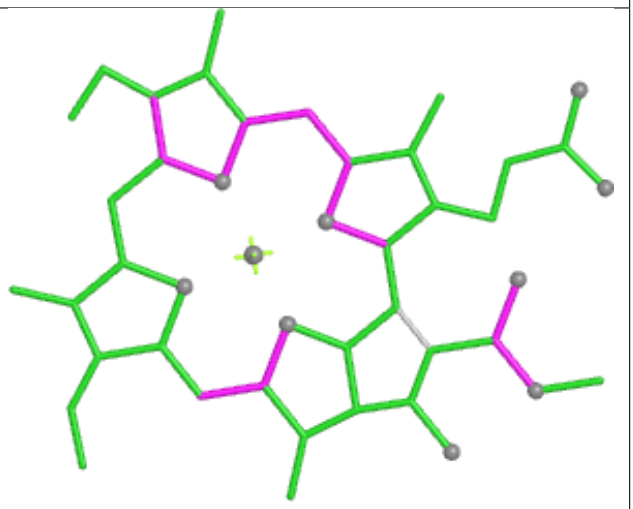


Rings

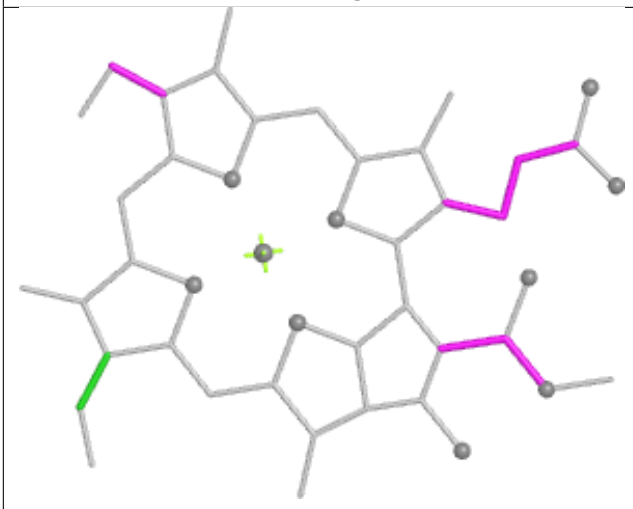
Ligand CLA 6 316



Bond lengths



Bond angles

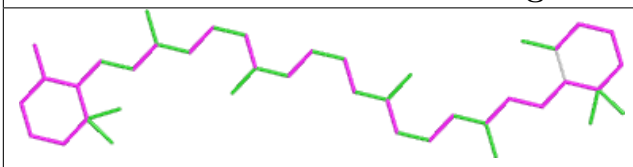


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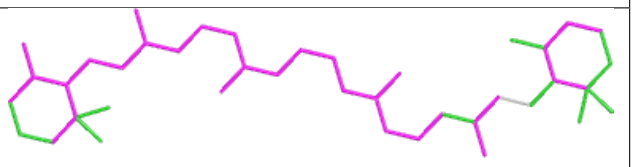


Rings

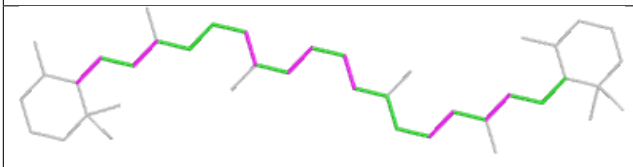
Ligand 8CT X 601



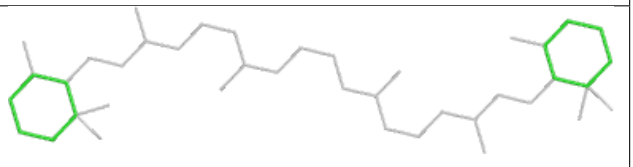
Bond lengths



Bond angles

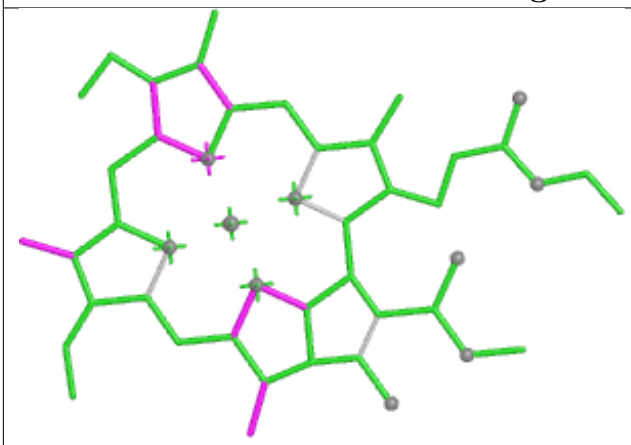


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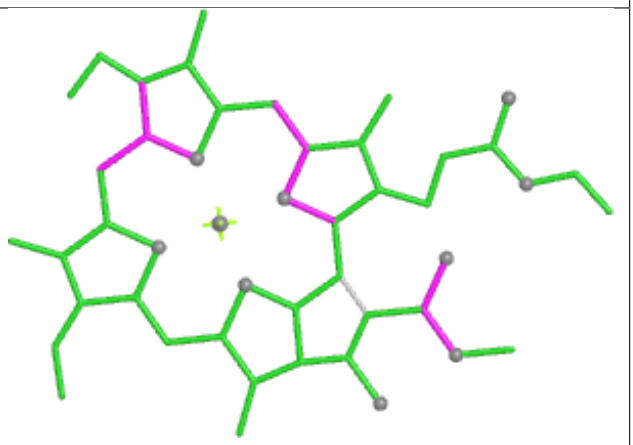


Rings

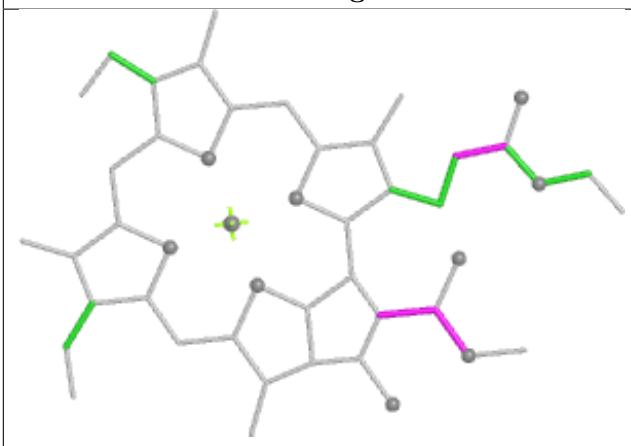
Ligand CLA r 304



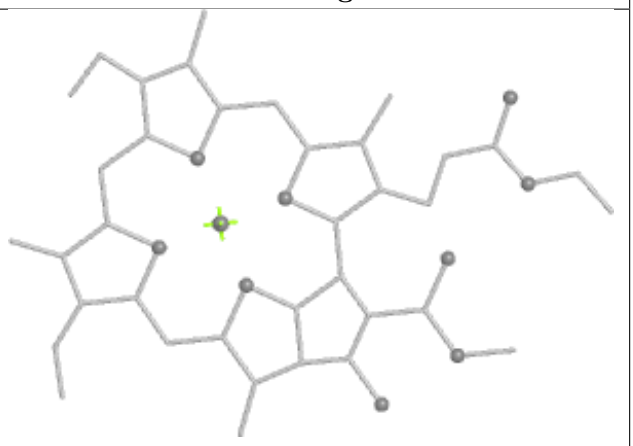
Bond lengths



Bond angles

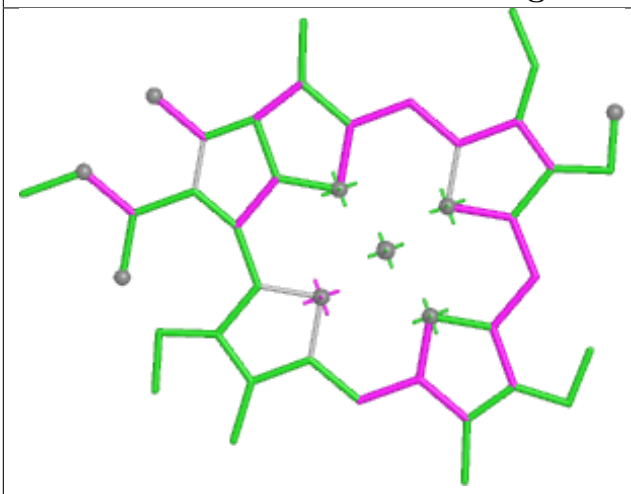


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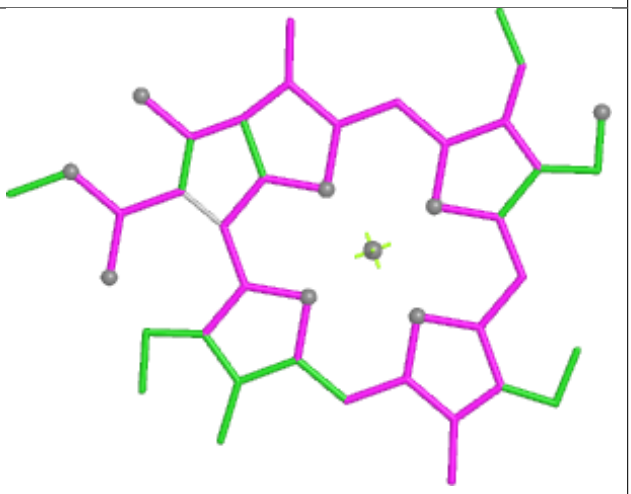


Rings

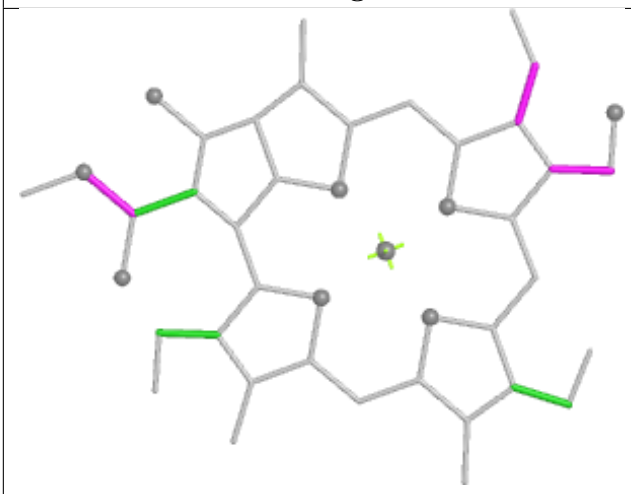
Ligand CHL 3 312



Bond lengths



Bond angles

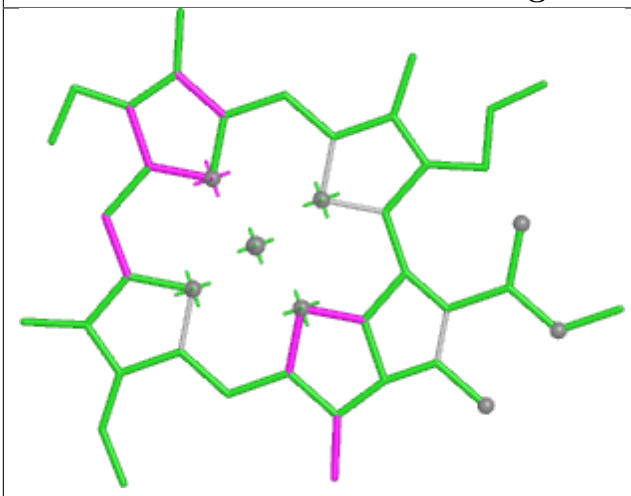


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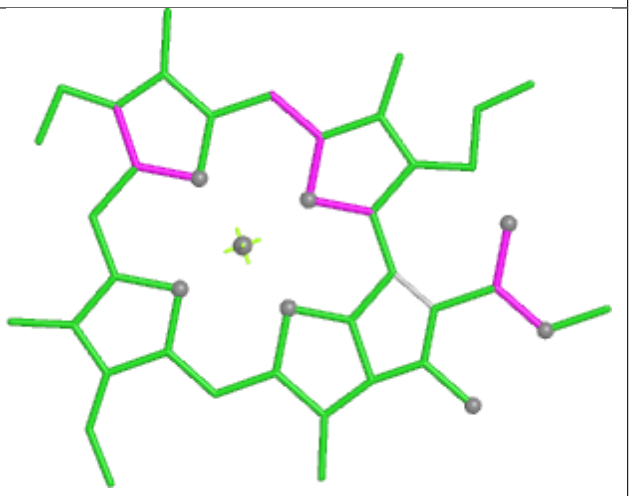


Rings

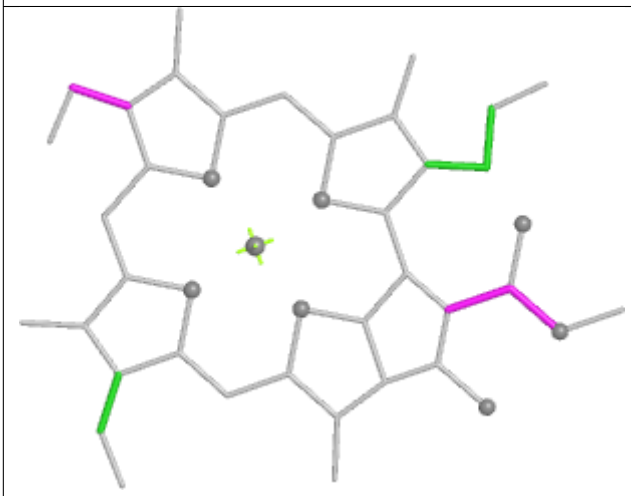
Ligand CLA 6 307



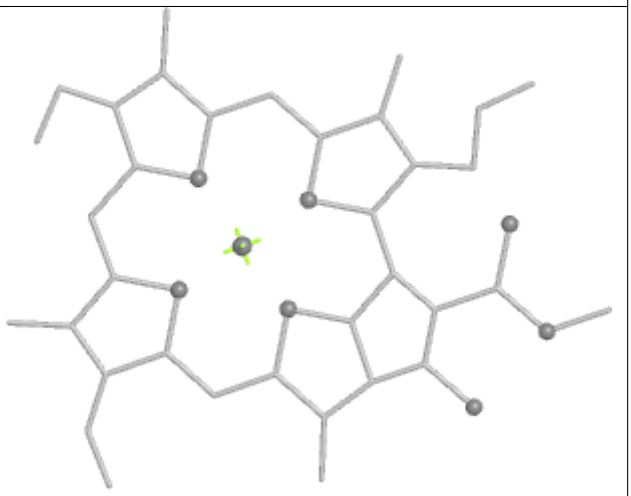
Bond lengths



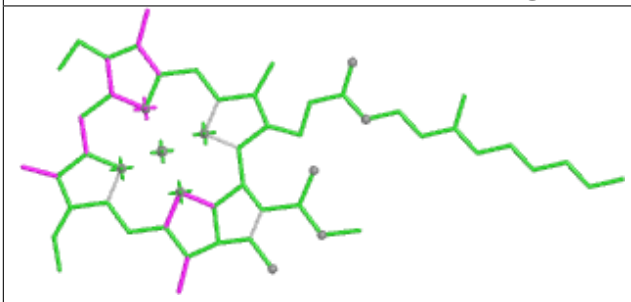
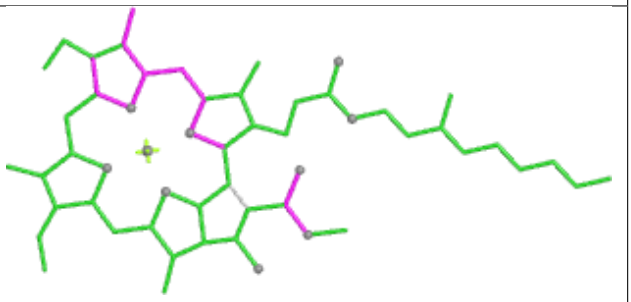
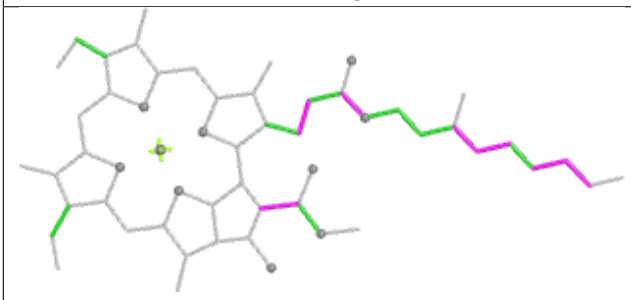
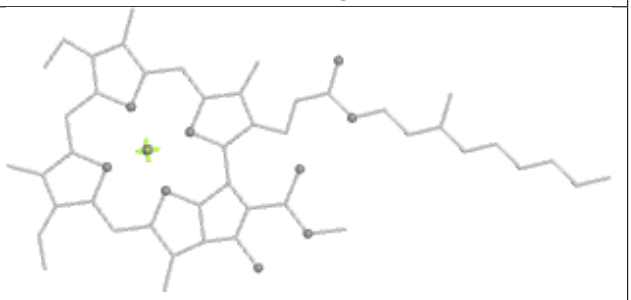
Bond angles



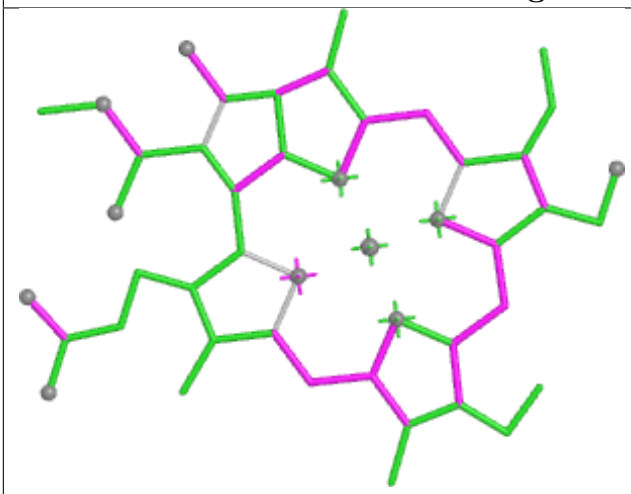
Torsions



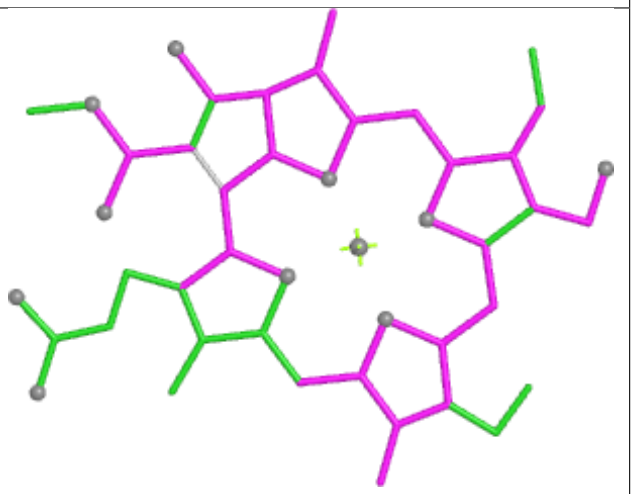
Rings

Ligand CLA Y 316	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

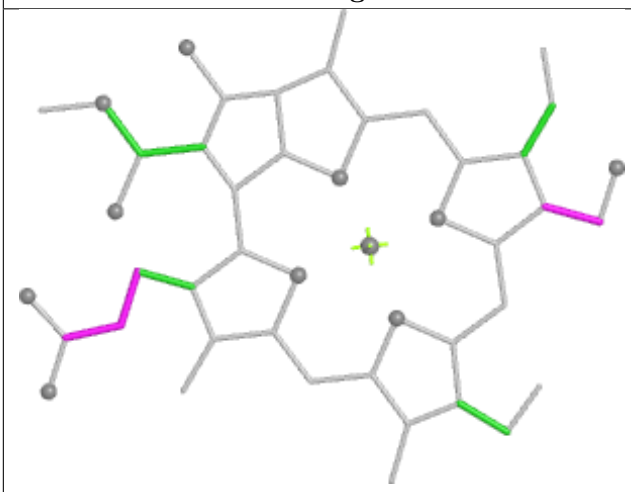
Ligand CHL 8 308



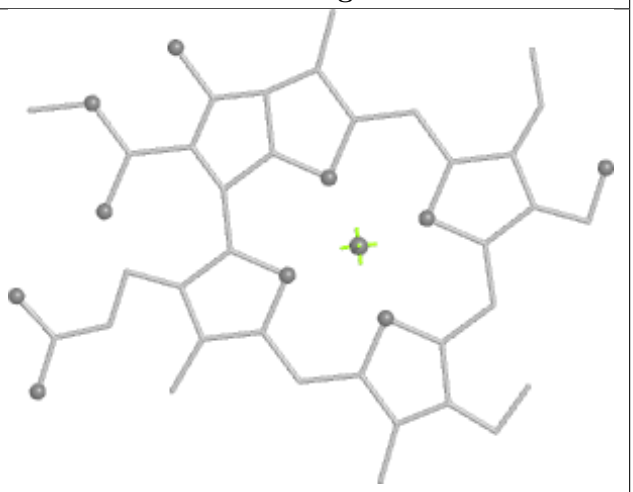
Bond lengths



Bond angles

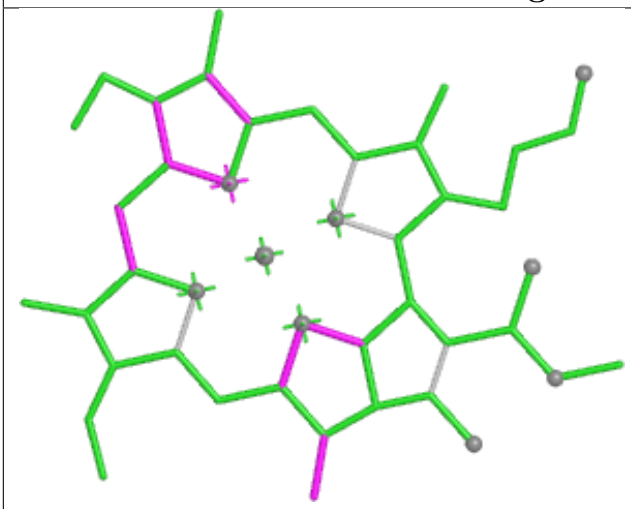


Torsions

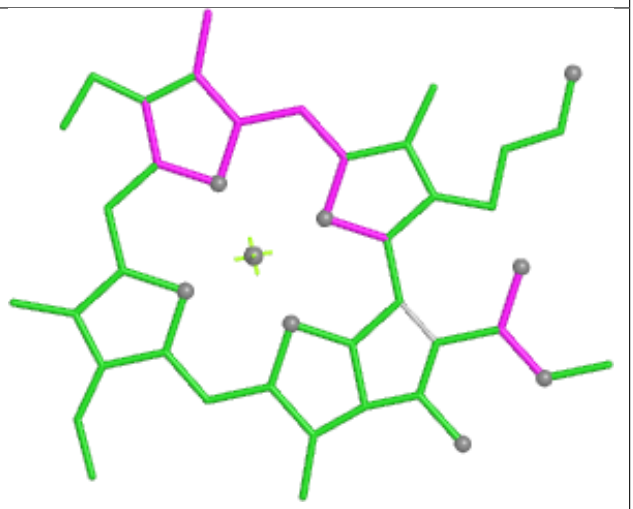


Rings

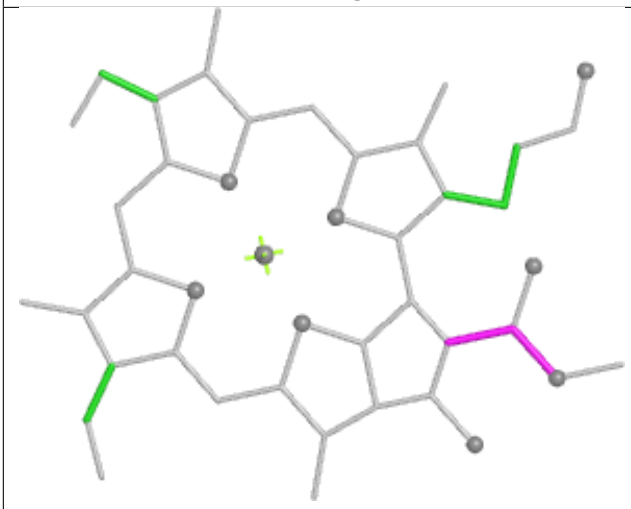
Ligand CLA 1 306



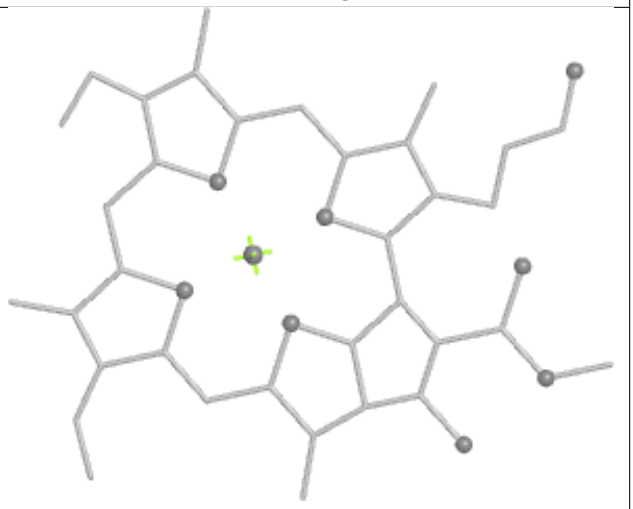
Bond lengths



Bond angles

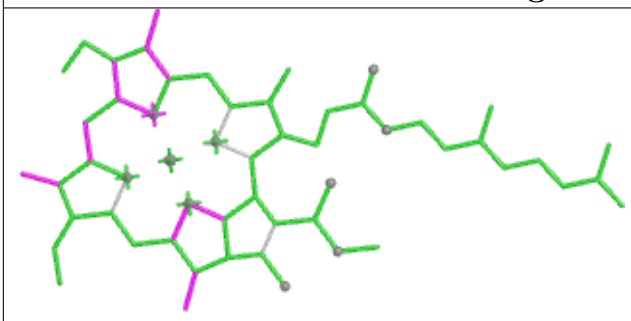


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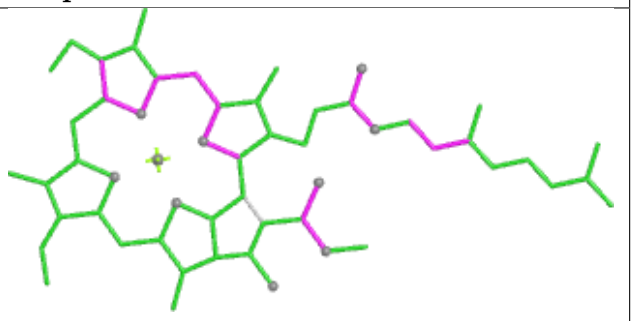


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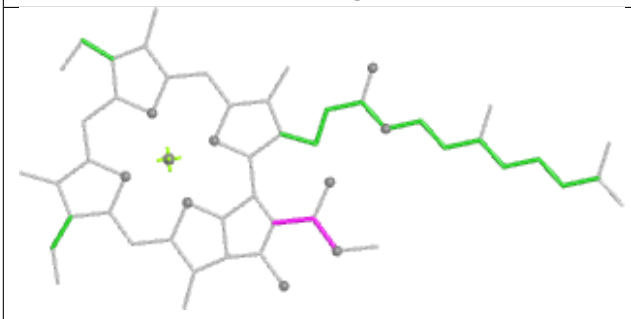
Ligand CLA q 312



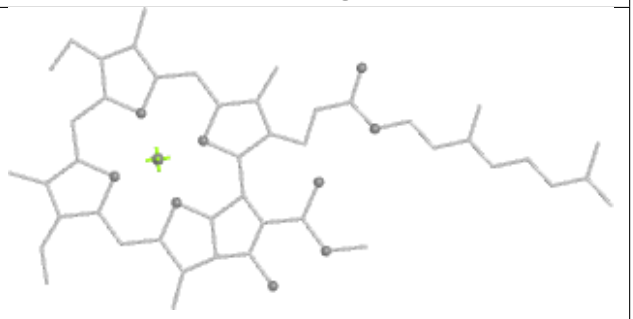
Bond lengths



Bond angles

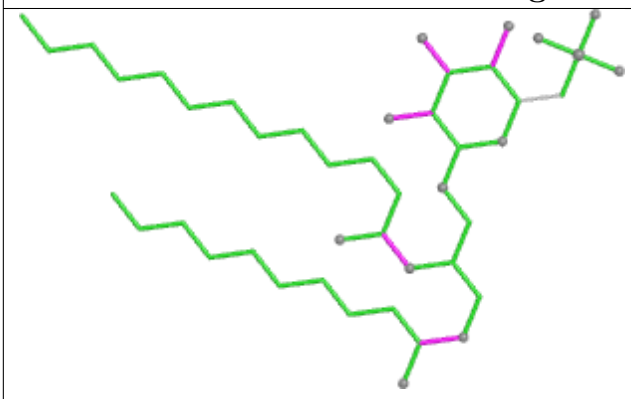


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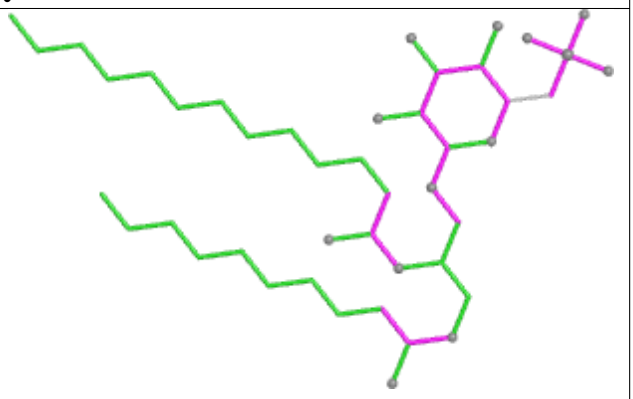


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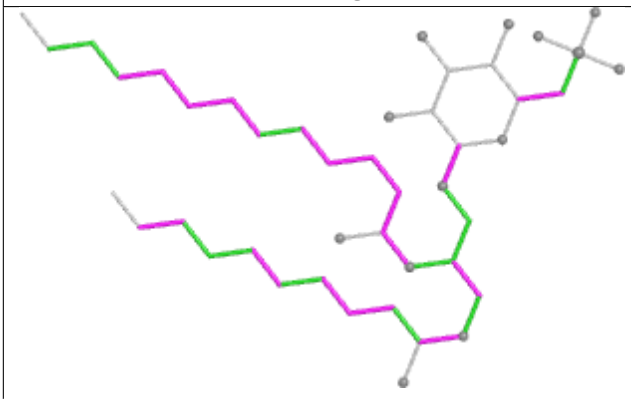
Ligand SQD a 609



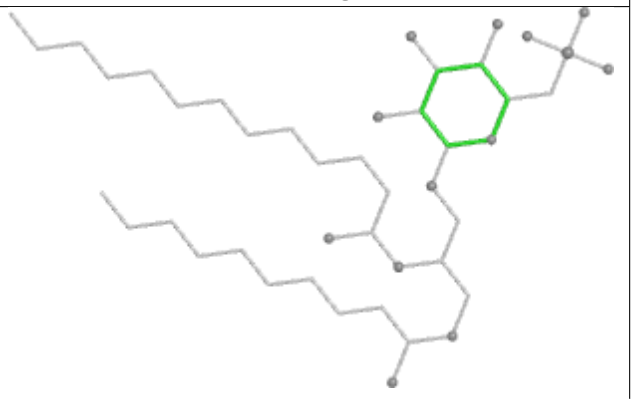
Bond lengths



Bond angles

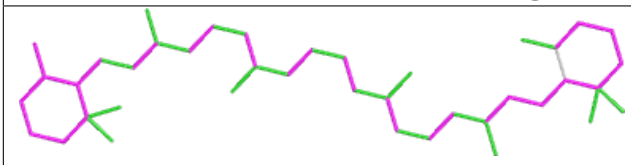


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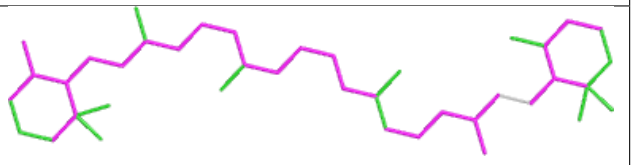


Rings

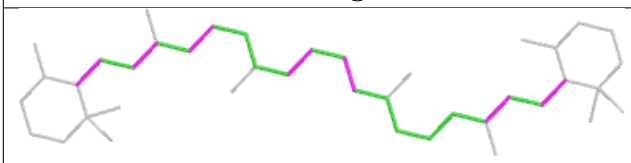
Ligand 8CT D 410



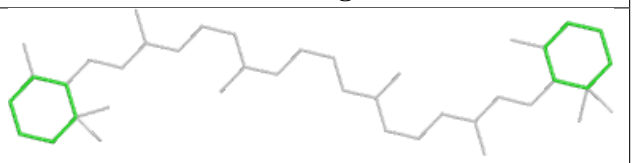
Bond lengths



Bond angles

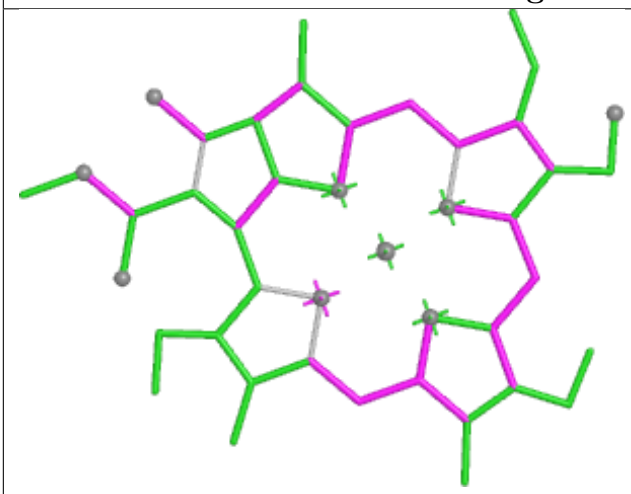


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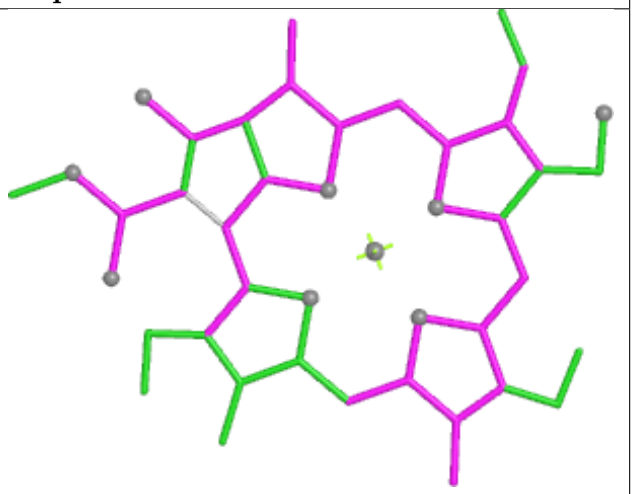


Rings

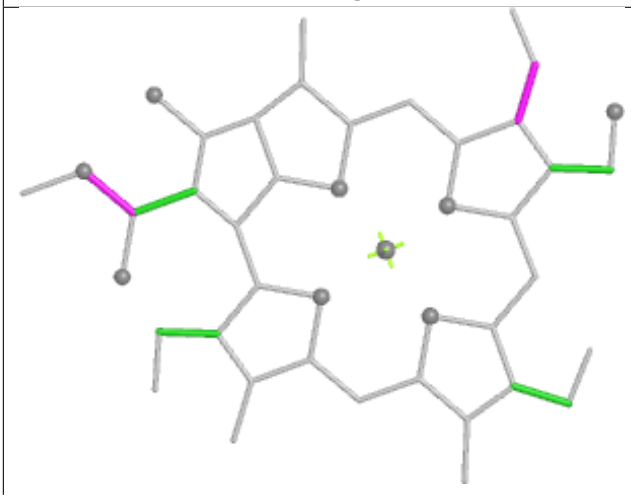
Ligand CHL p 313



Bond lengths



Bond angles

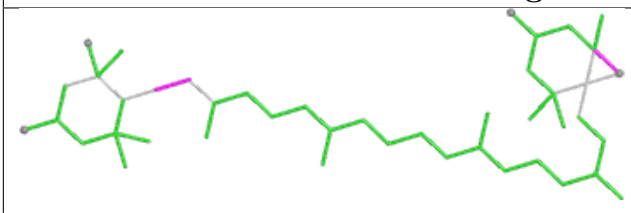


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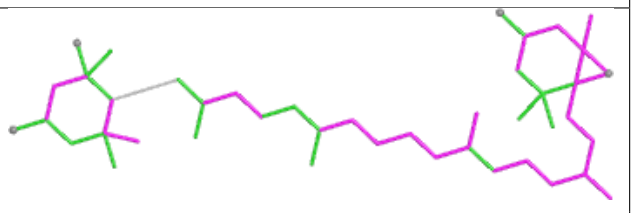


Rings

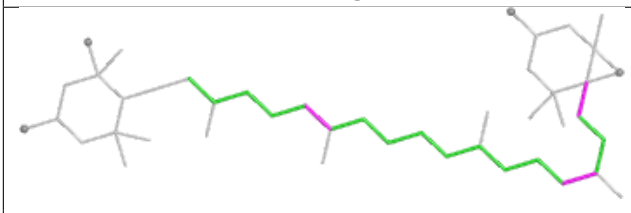
Ligand NEX n 303



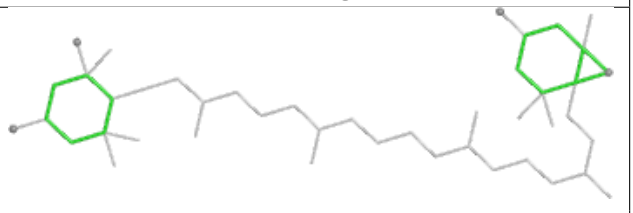
Bond lengths



Bond angles

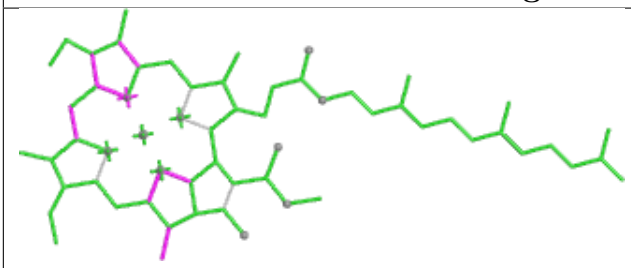


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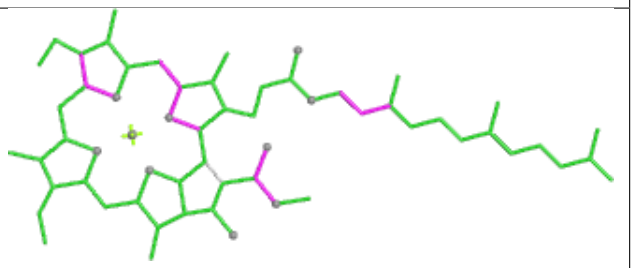


Rings

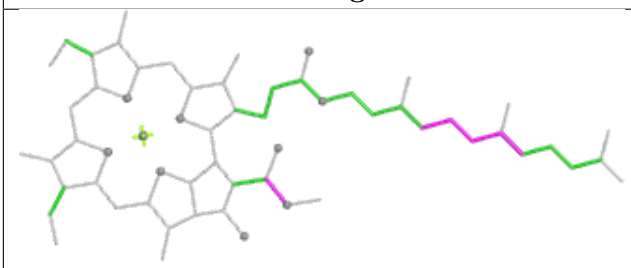
Ligand CLA G 315



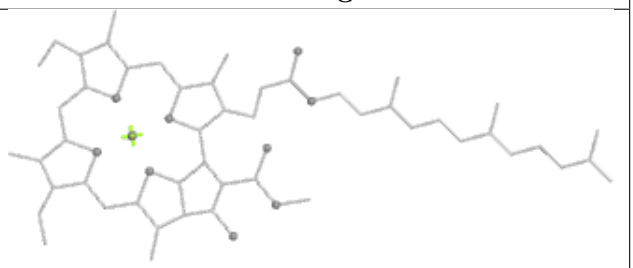
Bond lengths



Bond angles

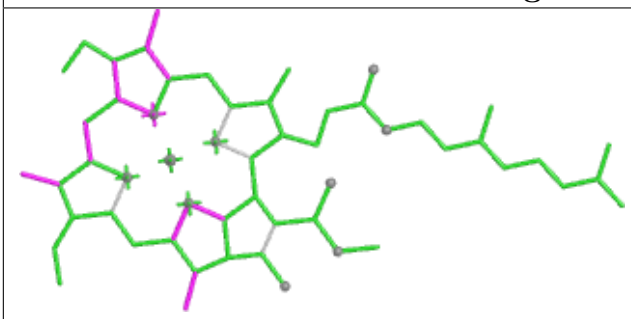


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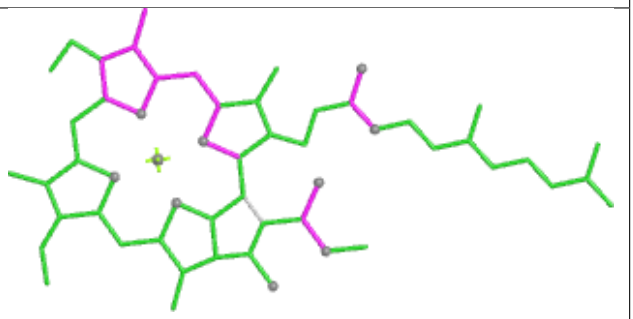


Rings

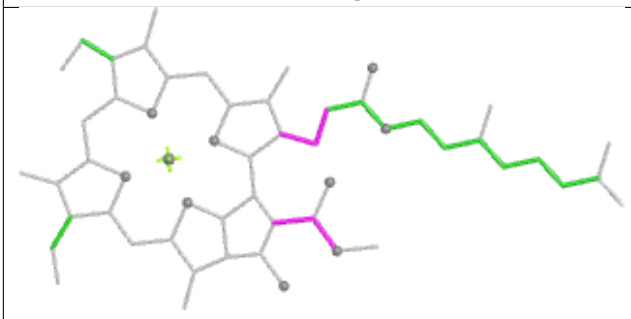
Ligand CLA Y 313



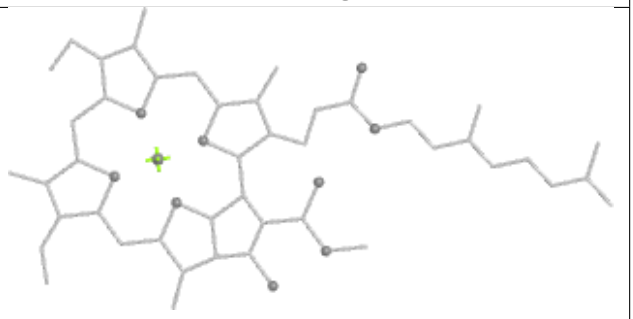
Bond lengths



Bond angles

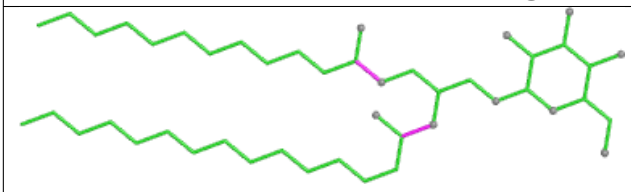


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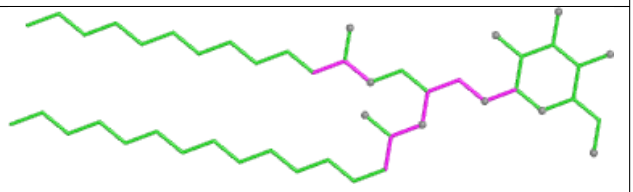


Rings

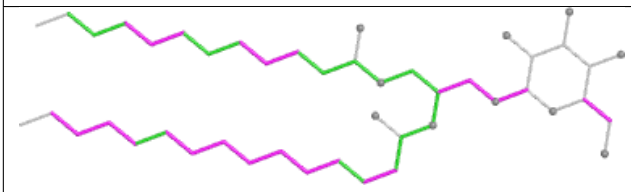
Ligand LMG d 411



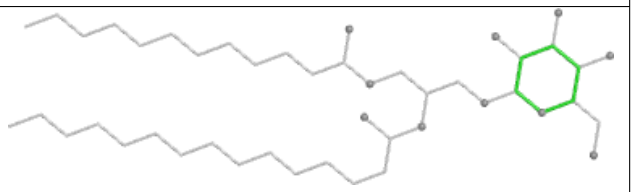
Bond lengths



Bond angles

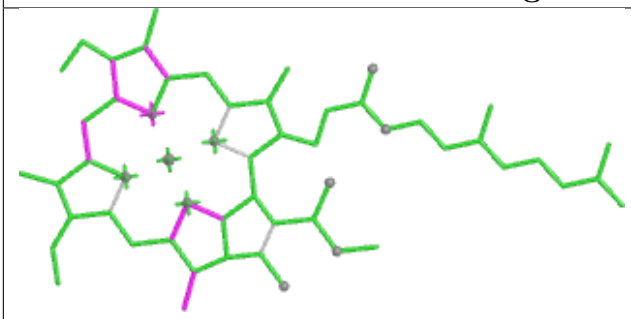


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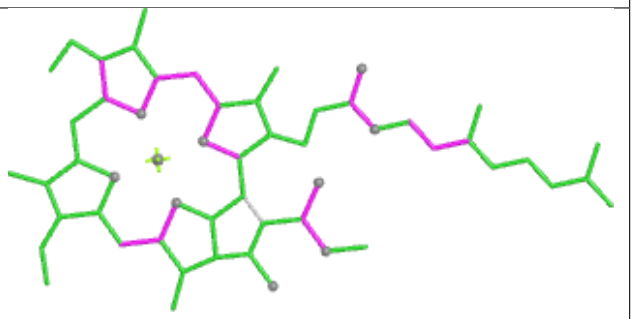


Rings

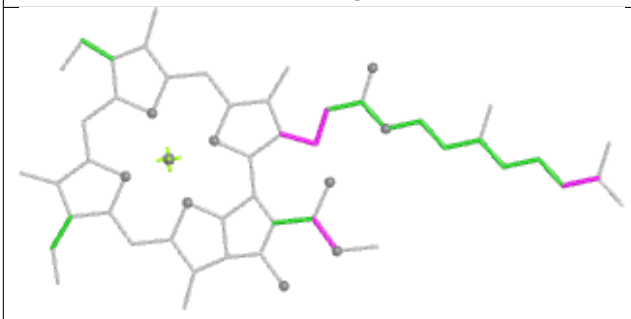
Ligand CLA N 313



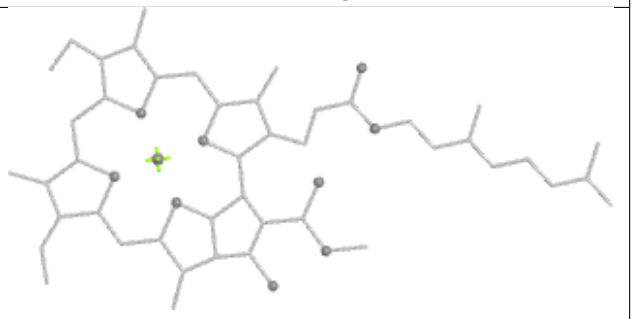
Bond lengths



Bond angles

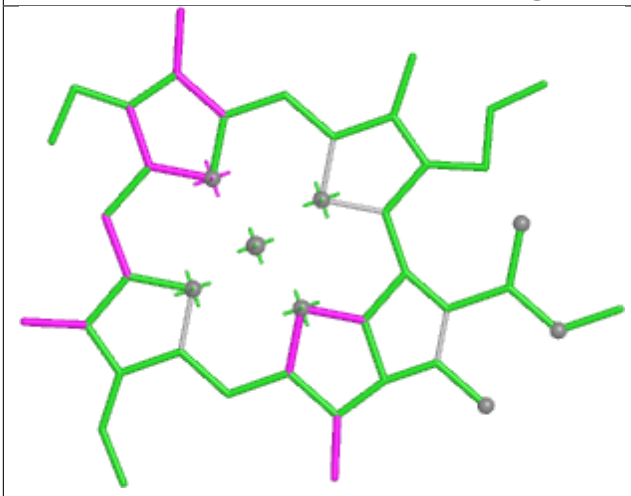


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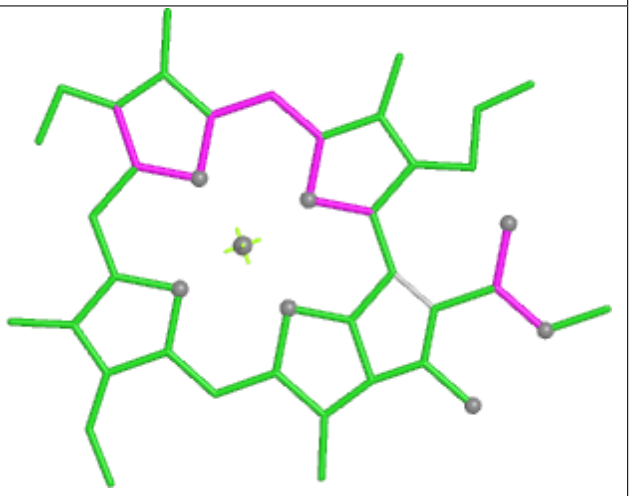


Rings

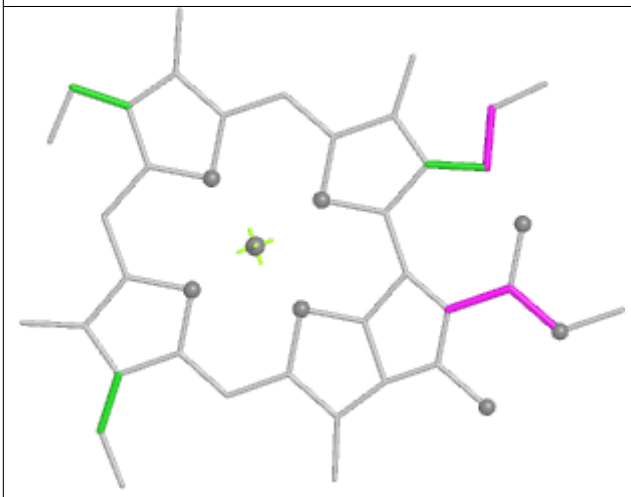
Ligand CLA 8 314



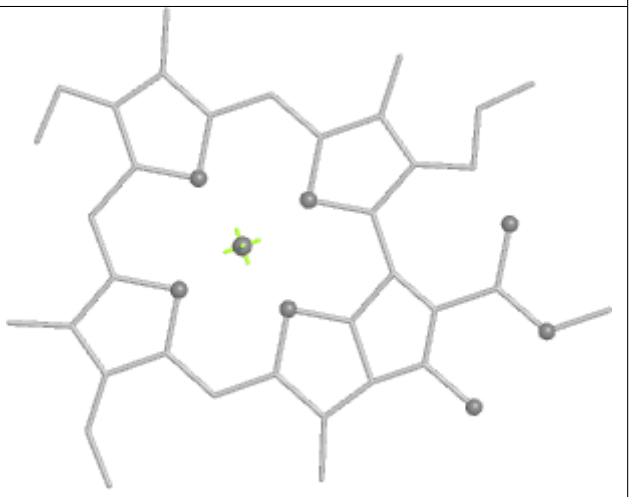
Bond lengths



Bond angles

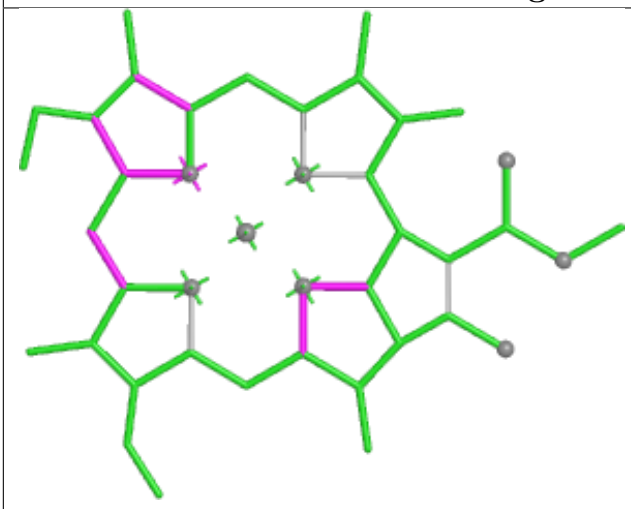


Torsions

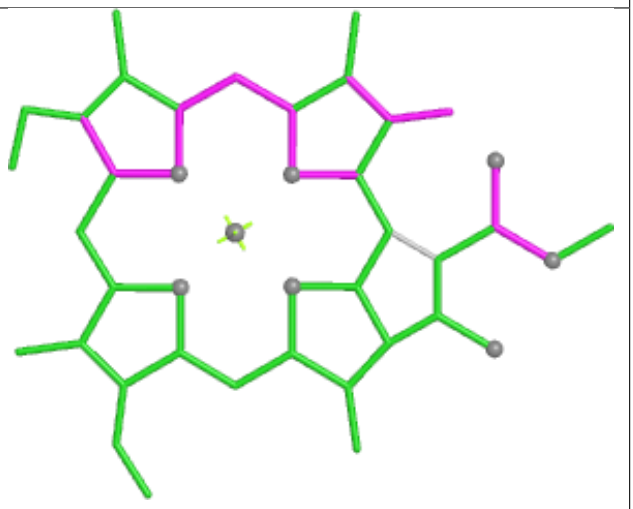


Rings

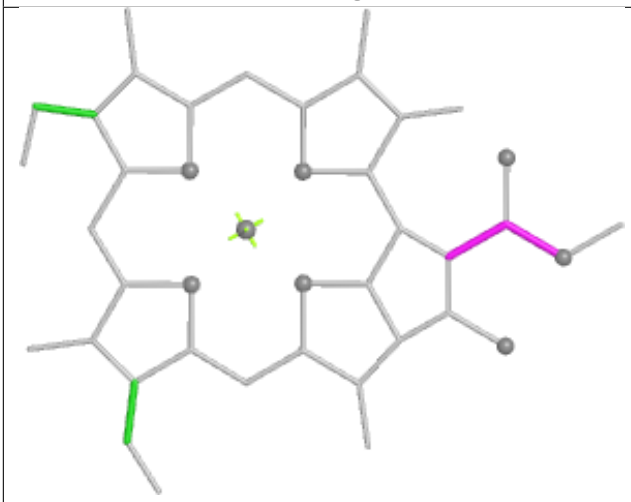
Ligand CLA 6 314



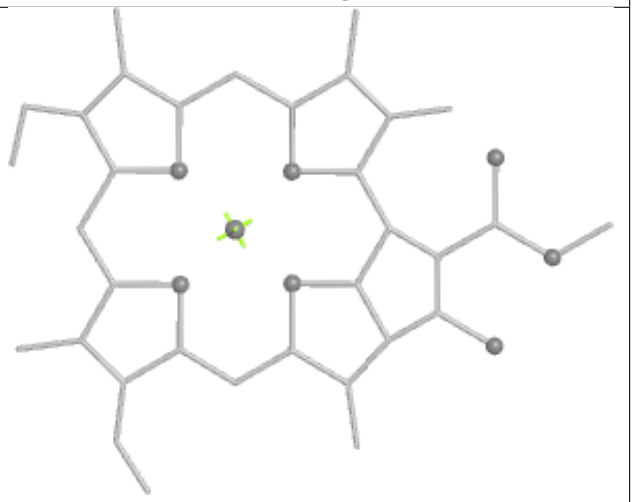
Bond lengths



Bond angles

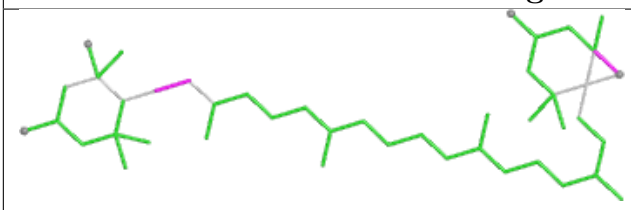


Torsions

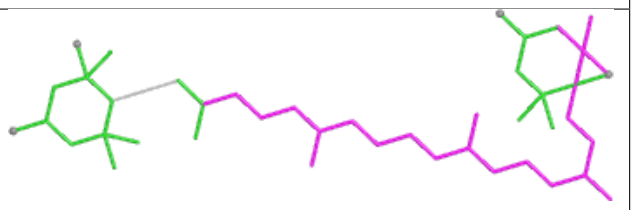


Rings

Ligand NEX 4 303



Bond lengths



Bond angles

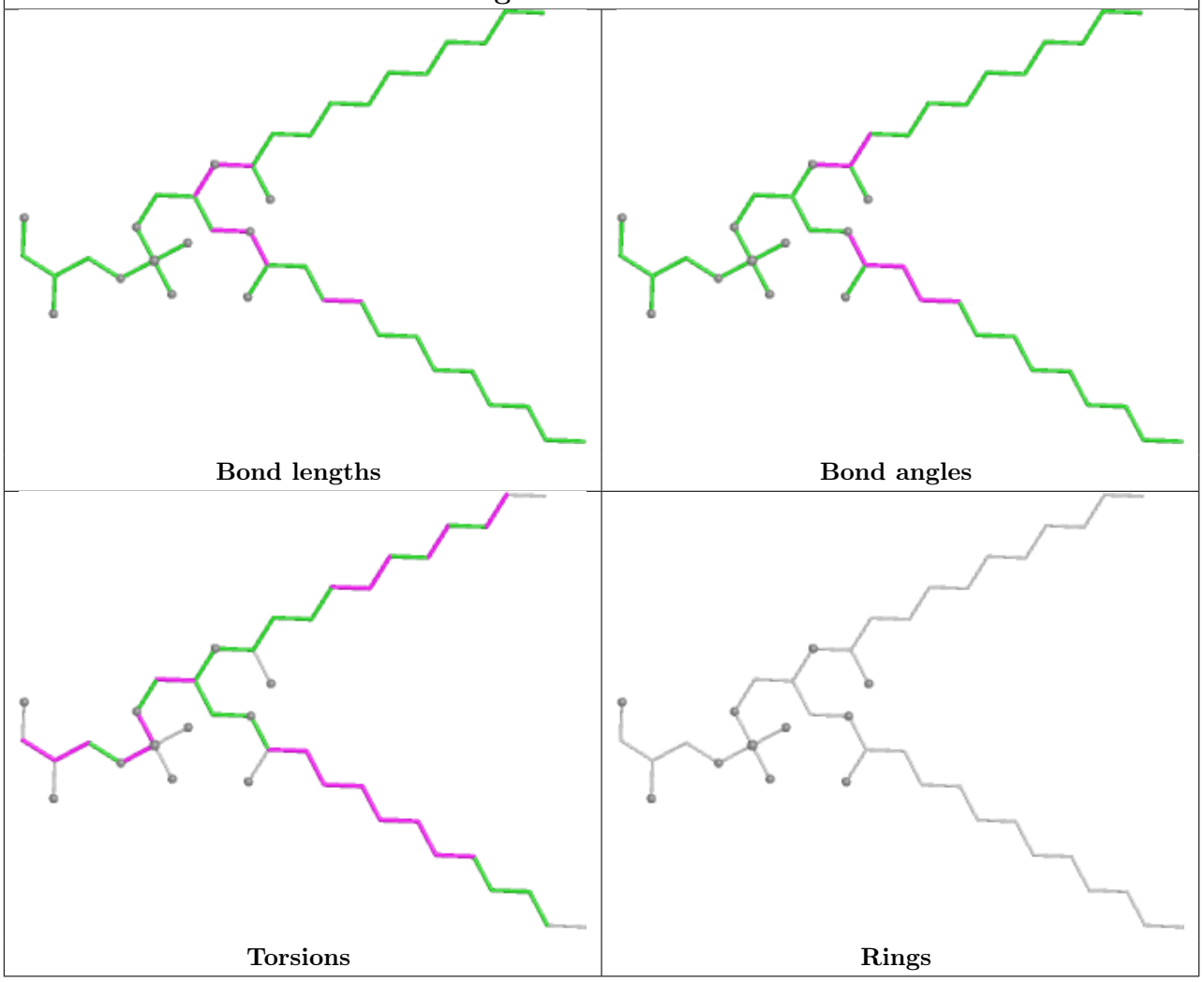


Torsions



Rings

Ligand LHG 2 319



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

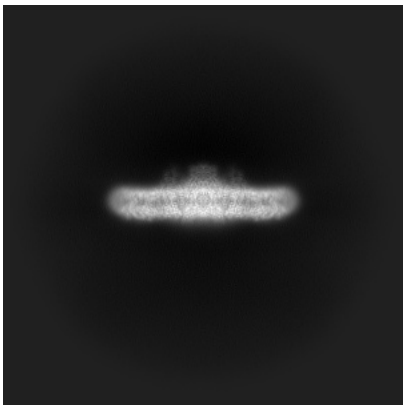
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62153. These allow visual inspection of the internal detail of the map and identification of artifacts.

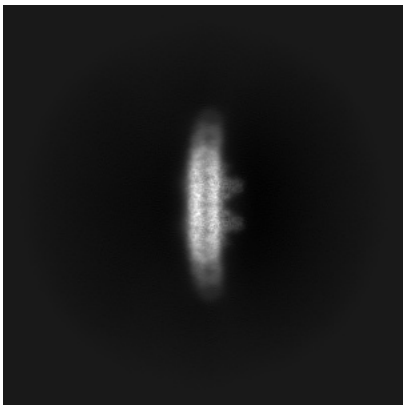
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

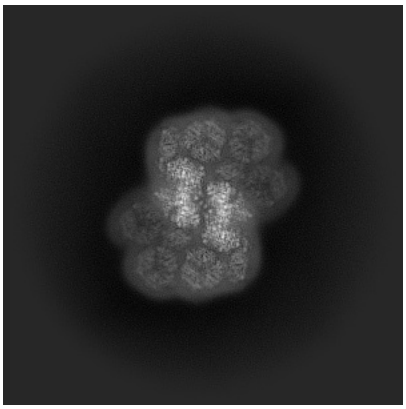
6.1.1 Primary map



X

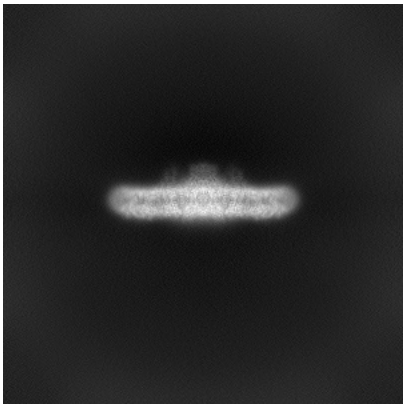


Y

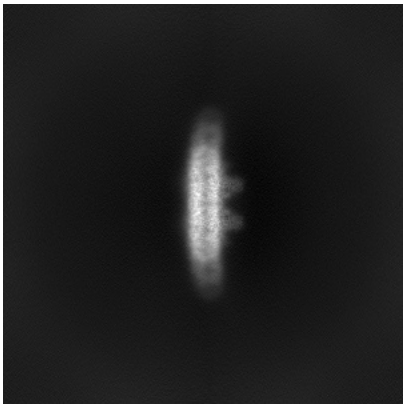


Z

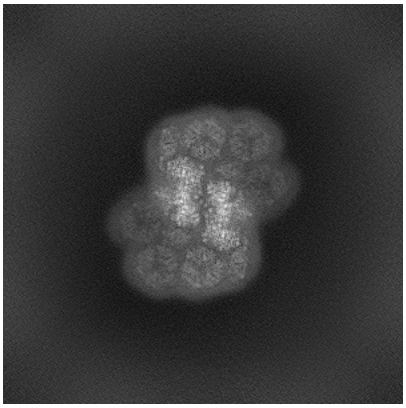
6.1.2 Raw map



X



Y

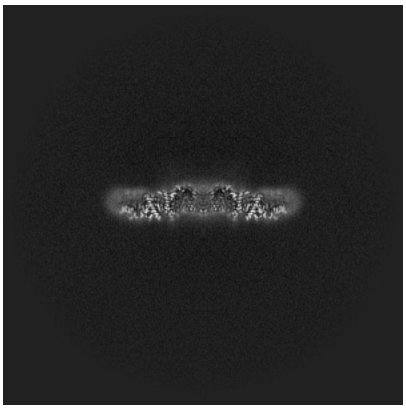


Z

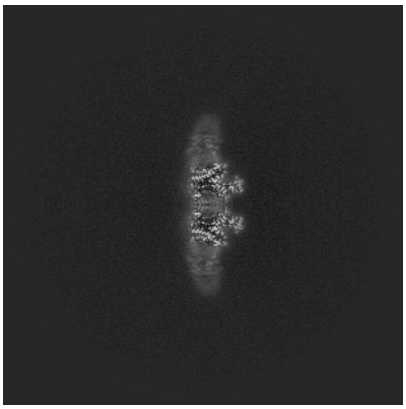
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

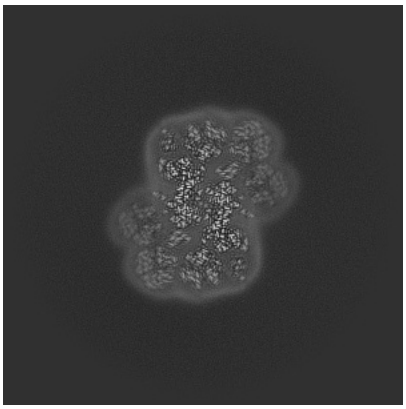
6.2.1 Primary map



X Index: 300

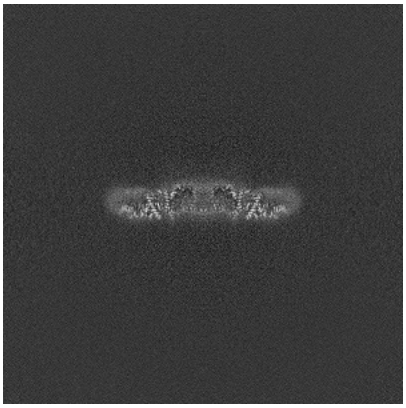


Y Index: 300

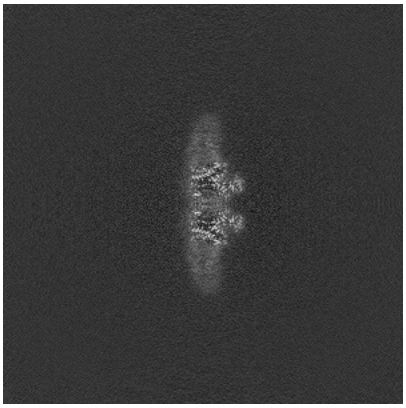


Z Index: 300

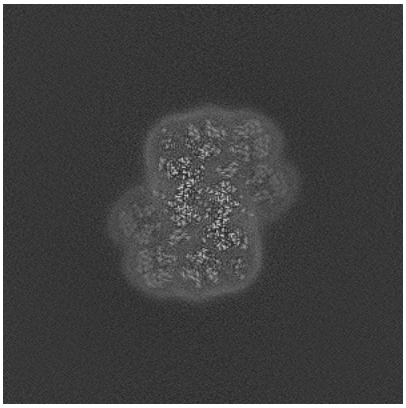
6.2.2 Raw map



X Index: 300



Y Index: 300

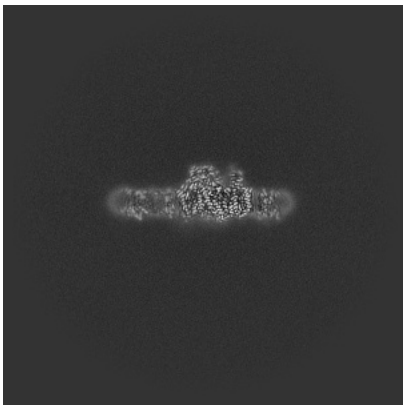


Z Index: 300

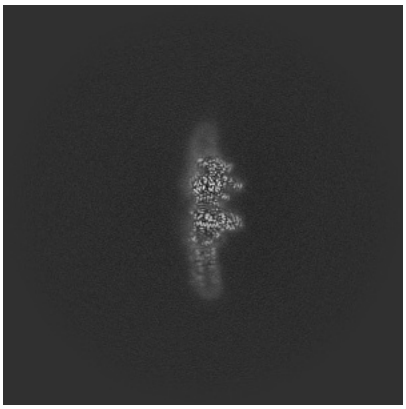
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

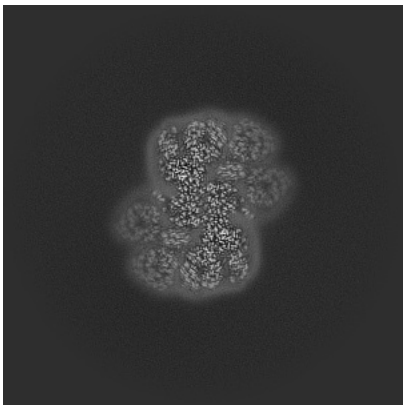
6.3.1 Primary map



X Index: 273

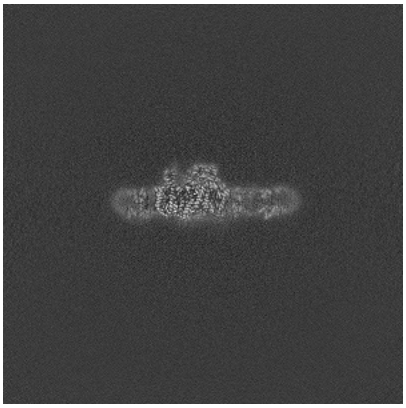


Y Index: 288

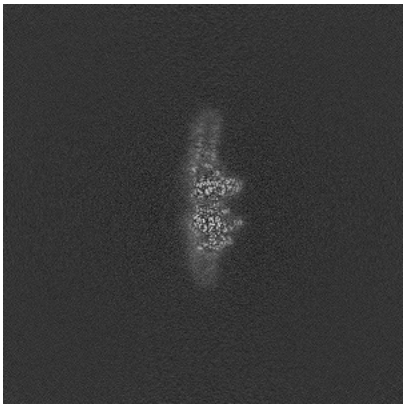


Z Index: 293

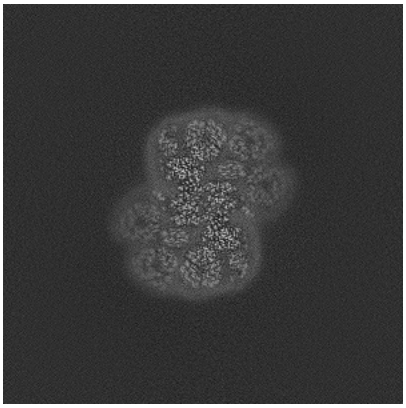
6.3.2 Raw map



X Index: 327



Y Index: 312

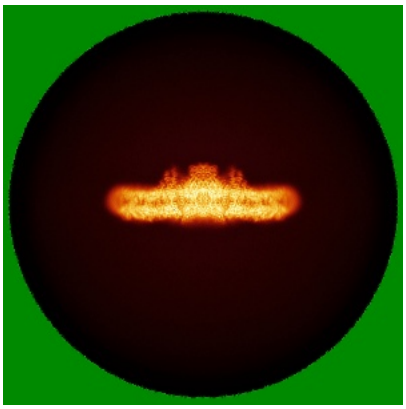


Z Index: 294

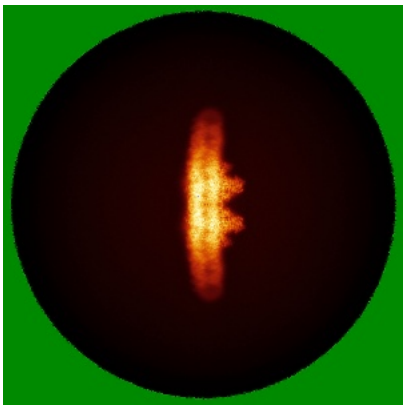
The images above show the largest variance slices of the map in three orthogonal directions.

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

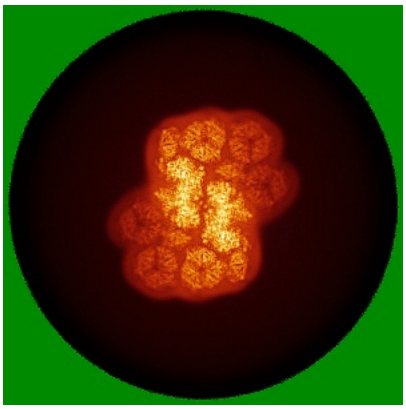
6.4.1 Primary map



X

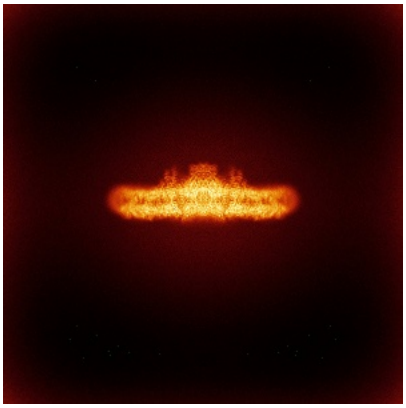


Y

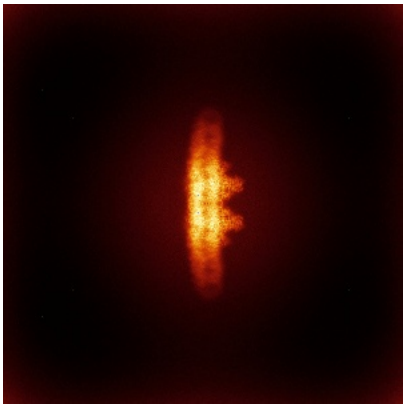


Z

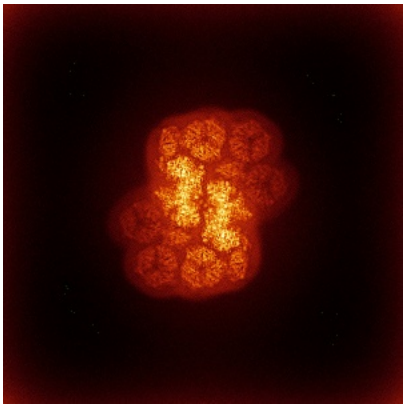
6.4.2 Raw map



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 0.204. 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.

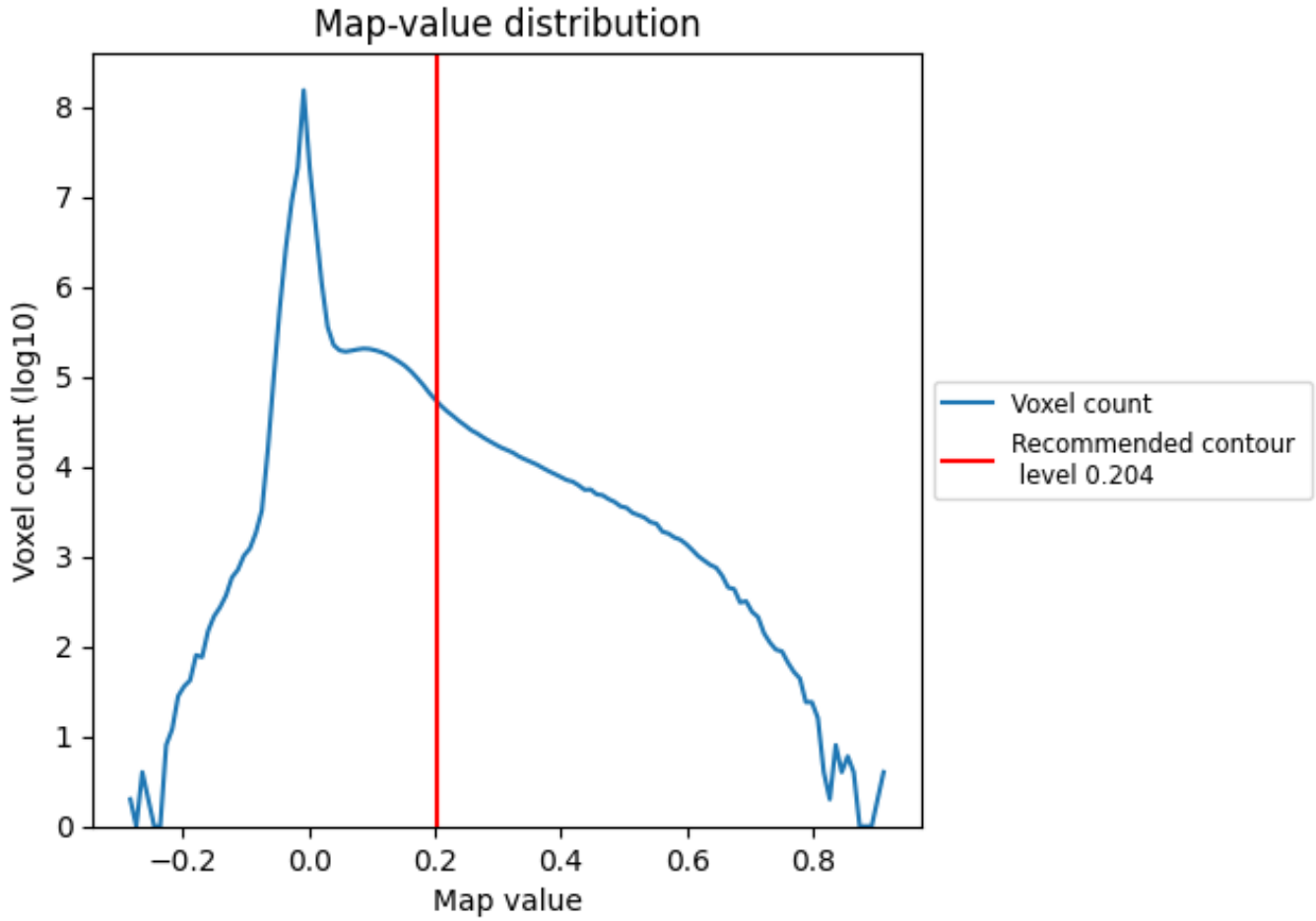
6.6 Mask visualisation (i)

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

7 Map analysis

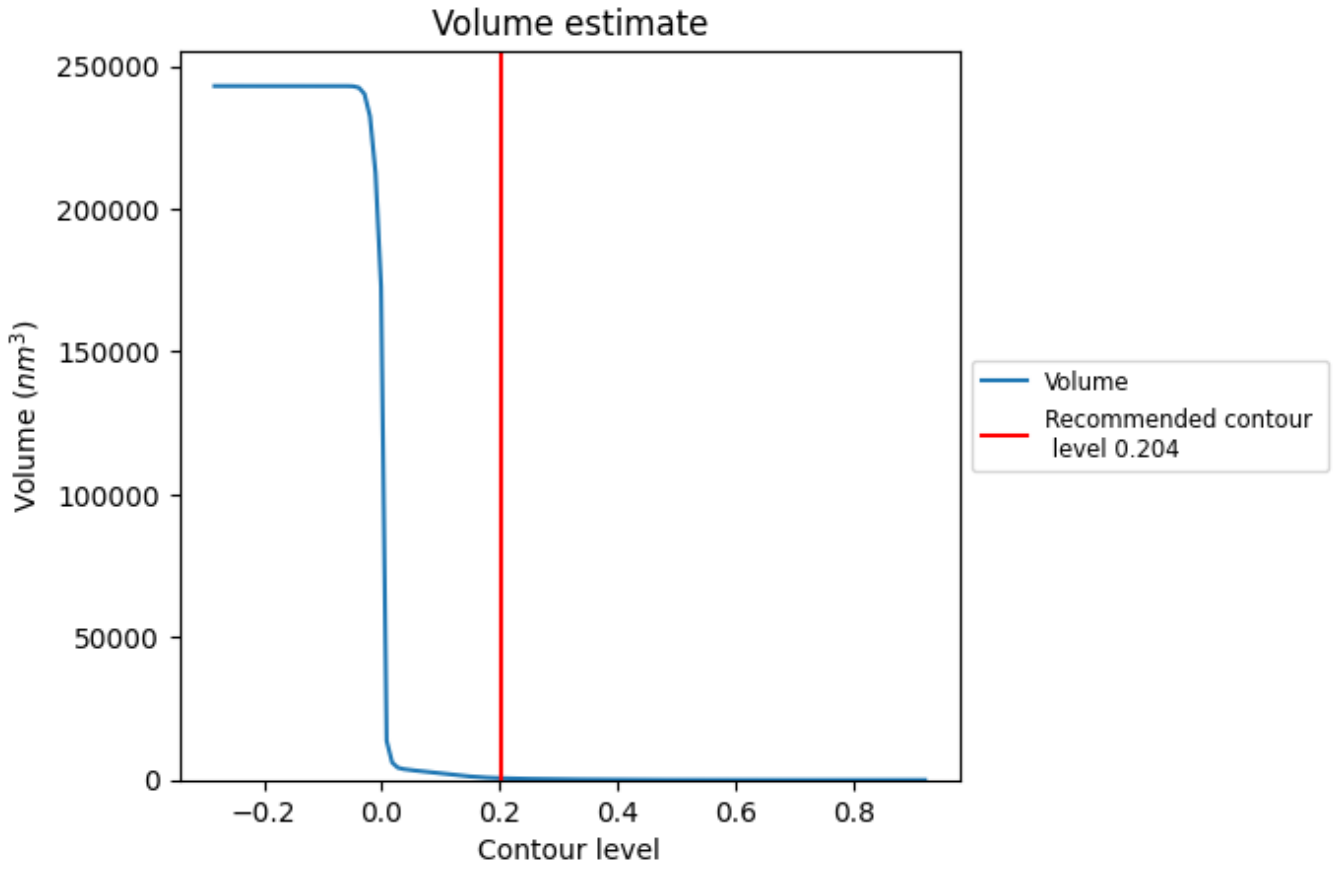
This section contains the results of statistical analysis of the map.

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.

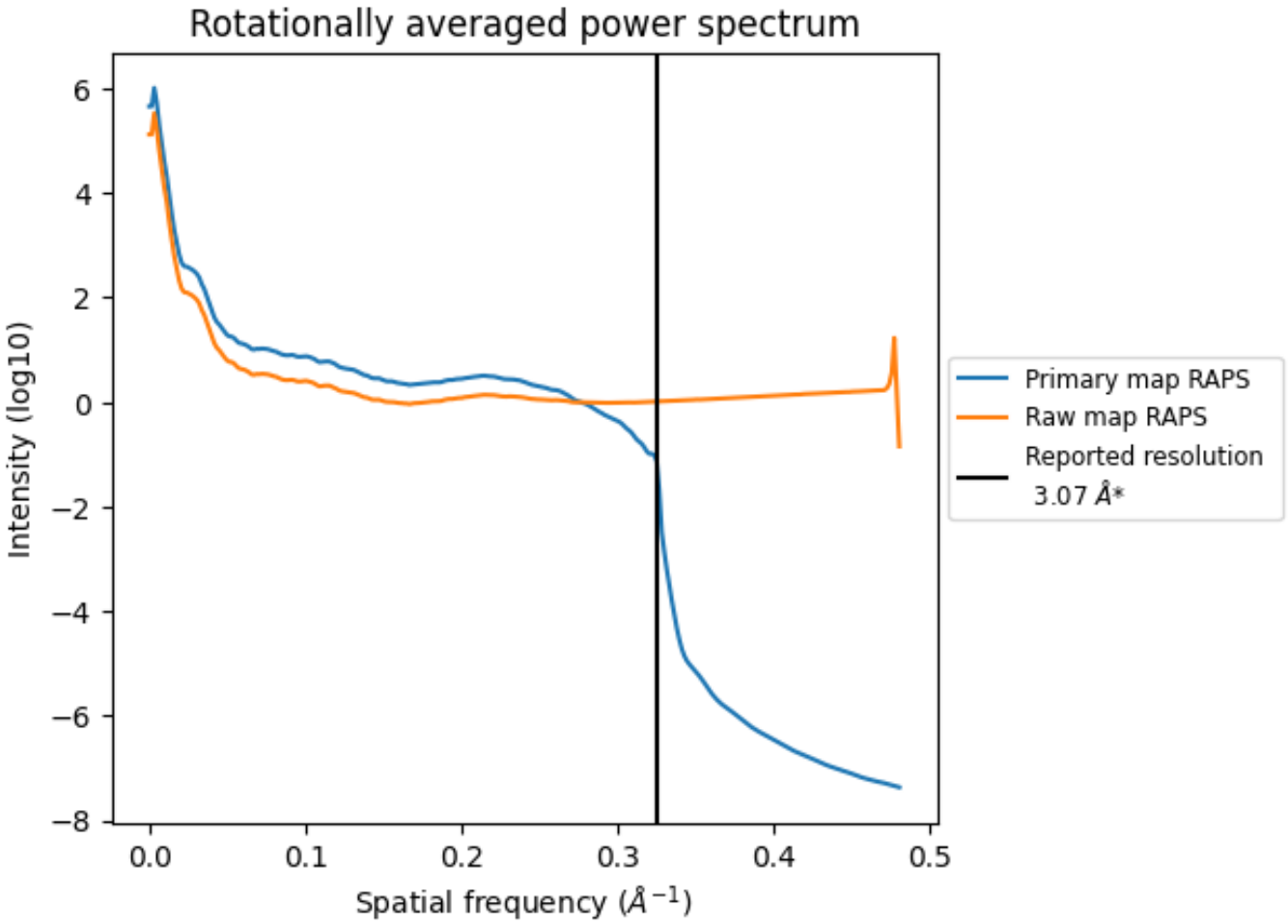
7.2 Volume estimate



The volume at the recommended contour level is 606 nm^3; this corresponds to an approximate mass of 548 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)

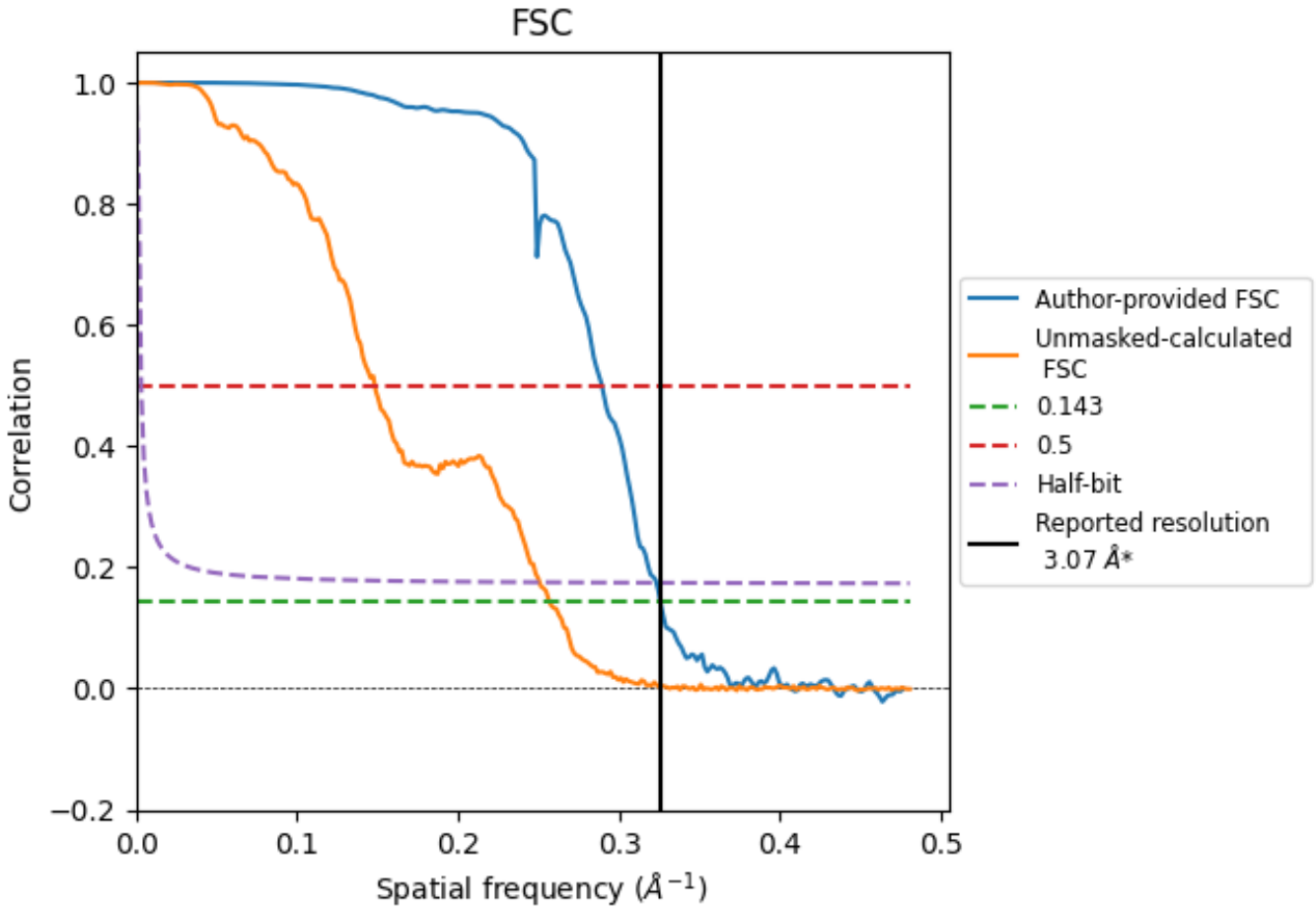


*Reported resolution corresponds to spatial frequency of 0.326 Å^{-1}

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 0.326 Å^{-1}

8.2 Resolution estimates (i)

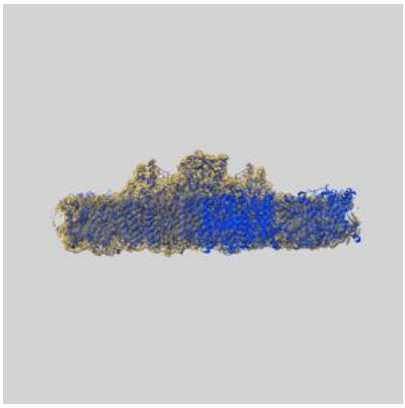
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.07	3.45	3.09
Unmasked-calculated*	3.89	6.74	3.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.07 by more than 10 %

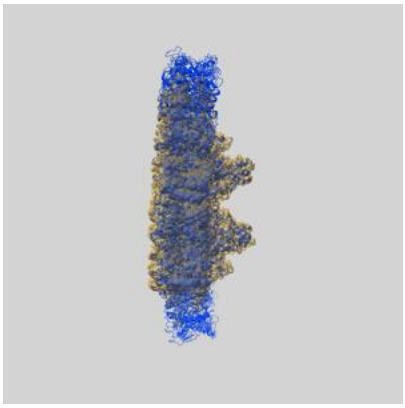
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62153 and PDB model 9K7V. Per-residue inclusion information can be found in section 3 on page 45.

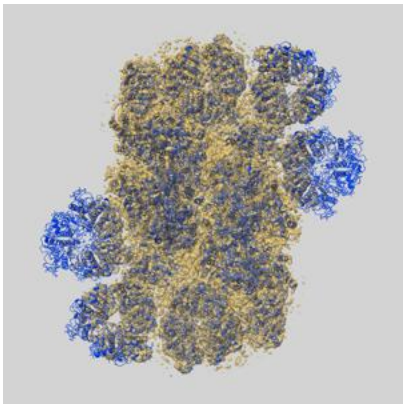
9.1 Map-model overlay



X



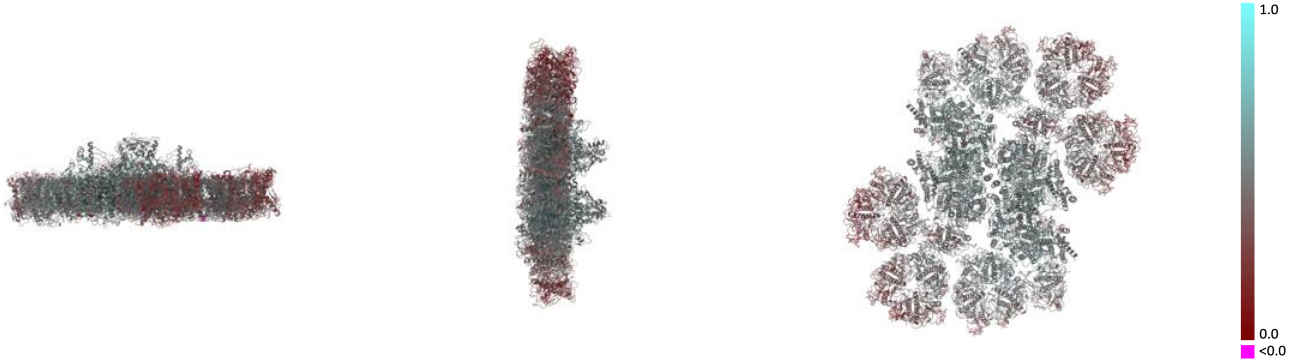
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.204 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.

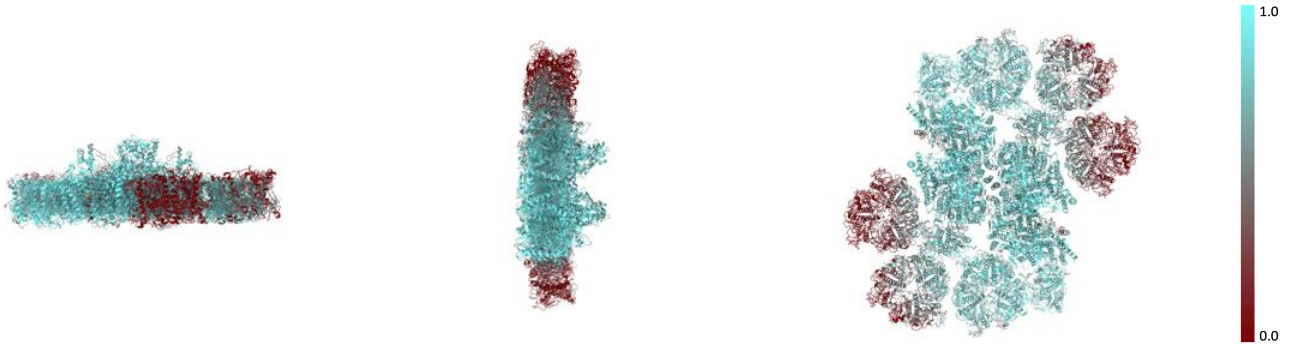
9.2 Q-score mapped to coordinate model



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.

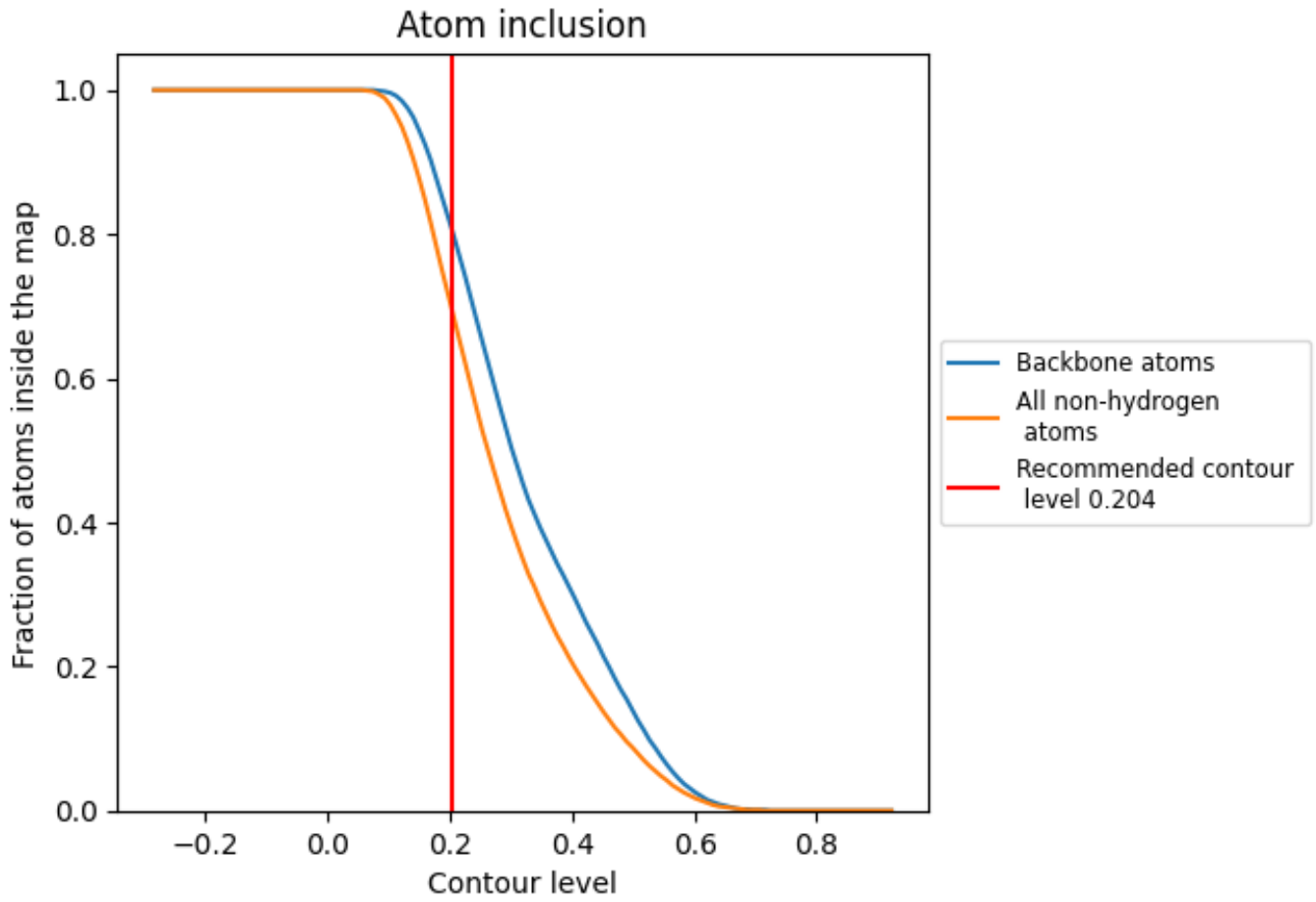
9.3 Atom inclusion mapped to coordinate model



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 (0.204).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 69% 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 (0.204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6920	0.4550
1	0.3620	0.3400
2	0.6680	0.4570
3	0.3050	0.3320
4	0.3660	0.3380
5	0.6660	0.4580
6	0.3020	0.3250
7	0.7880	0.4340
8	0.8580	0.4730
9	0.0130	0.2470
A	0.9160	0.5370
B	0.9140	0.5310
C	0.9100	0.5370
D	0.9260	0.5490
E	0.8090	0.4670
F	0.8670	0.4710
G	0.2460	0.3830
H	0.8510	0.5070
I	0.9600	0.5430
K	0.9220	0.5170
L	0.9060	0.5290
M	0.7130	0.4500
N	0.3140	0.3920
R	0.7010	0.4140
S	0.8320	0.4570
T	0.8600	0.5220
V	0.4290	0.3920
W	0.9000	0.5010
X	0.8040	0.4860
Y	0.9010	0.5210
Z	0.8080	0.4380
a	0.9160	0.5370
b	0.9140	0.5320
c	0.9080	0.5350
d	0.9240	0.5490



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Chain	Atom inclusion	Q-score
e	0.8140	0.4640
f	0.8530	0.4640
g	0.2490	0.3850
h	0.8430	0.5070
i	0.9500	0.5570
k	0.9290	0.5150
l	0.9100	0.5340
m	0.7310	0.4650
n	0.3180	0.3910
p	0.7870	0.4340
q	0.8550	0.4720
r	0.7020	0.4130
s	0.8340	0.4560
t	0.8640	0.5190
u	0.0150	0.2460
v	0.4470	0.3850
w	0.8840	0.4930
x	0.7970	0.4900
y	0.8990	0.5210
z	0.8080	0.4370