wwPDB EM Validation Summary Report

Dec 18, 2022 – 05:38 pm GMT

PDB ID	:	6YP7
EMDB ID	:	EMD-10865
Title	:	PSII-LHCII C2S2 supercomplex from Pisum sativum grown in high light conditions
Authors	:	Grinzato, A.; Albanese, P.; Zanotti, G.; Pagliano, C.
Deposited on	:	2020-04-15
Resolution	:	3.80 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:

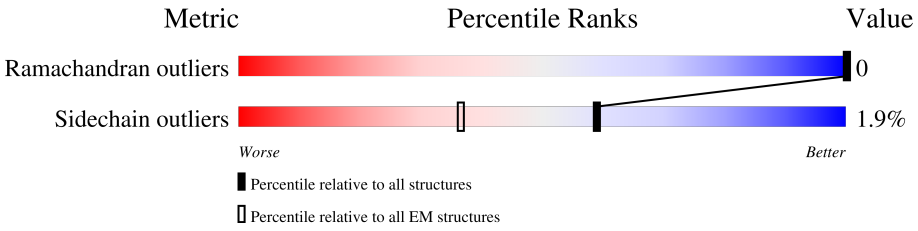
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.80 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	G	219	33% 98%
1	N	219	25% 98%
1	Y	219	13% 98%
1	g	219	34% 98%
1	n	219	22% 98%
1	y	219	11% 98%
2	A	334	5% 99%
2	a	334	99%
3	B	503	7% 99%

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Mol	Chain	Length	Quality of chain
3	b	503	7% 99%
4	C	450	6% 98%
4	c	450	5% 98%
5	D	341	8% 99%
5	d	341	8% 99%
6	E	75	17% 100%
6	e	75	8% 100%
7	F	30	10% 97%
7	f	30	10% 97%
8	H	60	18% 100%
8	h	60	20% 100%
9	I	34	6% 100%
9	i	34	6% 100%
10	J	35	74% 100%
10	j	35	69% 100%
11	K	37	16% 100%
11	k	37	16% 100%
12	L	37	14% 100%
12	l	37	16% 100%
13	M	33	36% 100%
13	m	33	39% 100%
14	O	248	23% 99%
14	o	248	27% 99%
15	T	32	25% 100%
15	t	32	25% 100%

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Mol	Chain	Length	Quality of chain
16	W	54	44% 94% 6%
16	w	54	31% 94% 6%
17	X	39	23% 100%
17	x	39	23% 100%
18	Z	62	21% 98%
18	z	62	18% 98%
19	R	222	34% 98%
19	r	222	32% 98%
20	S	218	24% 97%
20	s	218	24% 97%

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
21	CHL	G	601	X	-	-	-
21	CHL	G	605	X	-	-	-
21	CHL	G	606	X	-	-	-
21	CHL	G	607	X	-	-	-
21	CHL	G	608	X	-	-	-
21	CHL	G	609	X	-	-	-
21	CHL	N	601	X	-	-	-
21	CHL	N	605	X	-	-	-
21	CHL	N	606	X	-	-	-
21	CHL	N	607	X	-	-	-
21	CHL	N	608	X	-	-	-
21	CHL	R	305	X	-	-	-
21	CHL	R	306	X	-	-	-
21	CHL	R	307	X	-	-	-
21	CHL	S	301	X	-	-	-
21	CHL	S	302	X	-	-	-
21	CHL	S	306	X	-	-	-
21	CHL	S	307	X	-	-	-
21	CHL	Y	601	X	-	-	-
21	CHL	Y	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHL	Y	606	X	-	-	-
21	CHL	Y	607	X	-	-	-
21	CHL	Y	608	X	-	-	-
21	CHL	g	601	X	-	-	-
21	CHL	g	605	X	-	-	-
21	CHL	g	606	X	-	-	-
21	CHL	g	607	X	-	-	-
21	CHL	g	608	X	-	-	-
21	CHL	g	609	X	-	-	-
21	CHL	n	601	X	-	-	-
21	CHL	n	605	X	-	-	-
21	CHL	n	606	X	-	-	-
21	CHL	n	607	X	-	-	-
21	CHL	n	608	X	-	-	-
21	CHL	r	301	X	-	-	-
21	CHL	r	306	X	-	-	-
21	CHL	r	307	X	-	-	-
21	CHL	r	308	X	-	-	-
21	CHL	s	301	X	-	-	-
21	CHL	s	302	X	-	-	-
21	CHL	s	306	X	-	-	-
21	CHL	s	307	X	-	-	-
21	CHL	y	601	X	-	-	-
21	CHL	y	605	X	-	-	-
21	CHL	y	606	X	-	-	-
21	CHL	y	607	X	-	-	-
21	CHL	y	608	X	-	-	-
21	CHL	y	609	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	407	X	-	-	-
22	CLA	A	409	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	B	618	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	C	515	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	G	602	X	-	-	-
22	CLA	G	603	X	-	-	-
22	CLA	G	604	X	-	-	-
22	CLA	G	610	X	-	-	-
22	CLA	G	611	X	-	-	-
22	CLA	G	612	X	-	-	-
22	CLA	G	613	X	-	-	-
22	CLA	G	614	X	-	-	-
22	CLA	N	602	X	-	-	-
22	CLA	N	603	X	-	-	-
22	CLA	N	604	X	-	-	-
22	CLA	N	609	X	-	-	-
22	CLA	N	610	X	-	-	-
22	CLA	N	611	X	-	-	-
22	CLA	N	612	X	-	-	-
22	CLA	N	613	X	-	-	-
22	CLA	R	302	X	-	-	-
22	CLA	R	303	X	-	-	-
22	CLA	R	304	X	-	-	-
22	CLA	R	308	X	-	-	-
22	CLA	R	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	R	310	X	-	-	-
22	CLA	R	311	X	-	-	-
22	CLA	S	303	X	-	-	-
22	CLA	S	304	X	-	-	-
22	CLA	S	305	X	-	-	-
22	CLA	S	309	X	-	-	-
22	CLA	S	310	X	-	-	-
22	CLA	S	311	X	-	-	-
22	CLA	S	312	X	-	-	-
22	CLA	S	313	X	-	-	-
22	CLA	W	101	X	-	-	-
22	CLA	Y	602	X	-	-	-
22	CLA	Y	603	X	-	-	-
22	CLA	Y	604	X	-	-	-
22	CLA	Y	609	X	-	-	-
22	CLA	Y	610	X	-	-	-
22	CLA	Y	611	X	-	-	-
22	CLA	Y	612	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	g	602	X	-	-	-
22	CLA	g	603	X	-	-	-
22	CLA	g	604	X	-	-	-
22	CLA	g	610	X	-	-	-
22	CLA	g	611	X	-	-	-
22	CLA	g	612	X	-	-	-
22	CLA	g	613	X	-	-	-
22	CLA	g	614	X	-	-	-
22	CLA	n	602	X	-	-	-
22	CLA	n	603	X	-	-	-
22	CLA	n	604	X	-	-	-
22	CLA	n	609	X	-	-	-
22	CLA	n	610	X	-	-	-
22	CLA	n	611	X	-	-	-
22	CLA	n	612	X	-	-	-
22	CLA	n	613	X	-	-	-
22	CLA	r	303	X	-	-	-
22	CLA	r	304	X	-	-	-
22	CLA	r	305	X	-	-	-
22	CLA	r	309	X	-	-	-
22	CLA	r	310	X	-	-	-
22	CLA	r	311	X	-	-	-
22	CLA	r	312	X	-	-	-
22	CLA	s	303	X	-	-	-
22	CLA	s	304	X	-	-	-
22	CLA	s	305	X	-	-	-
22	CLA	s	309	X	-	-	-
22	CLA	s	310	X	-	-	-
22	CLA	s	311	X	-	-	-
22	CLA	s	312	X	-	-	-
22	CLA	s	313	X	-	-	-
22	CLA	w	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	x	101	X	-	-	-
22	CLA	y	602	X	-	-	-
22	CLA	y	603	X	-	-	-
22	CLA	y	604	X	-	-	-
22	CLA	y	610	X	-	-	-
22	CLA	y	611	X	-	-	-
22	CLA	y	612	X	-	-	-
22	CLA	y	613	X	-	-	-
24	XAT	G	617	X	-	-	-
24	XAT	N	616	X	-	-	-
24	XAT	R	313	X	-	-	-
24	XAT	Y	615	X	-	-	-
24	XAT	g	617	X	-	-	-
24	XAT	n	615	X	-	-	-
24	XAT	r	314	X	-	-	-
24	XAT	y	615	X	-	-	-
25	NEX	N	617	X	-	-	-
25	NEX	Y	616	X	-	-	-
25	NEX	g	618	X	-	-	-
25	NEX	n	616	X	-	-	-
25	NEX	r	315	X	-	-	-
25	NEX	y	616	X	-	-	-
25	NEX	y	618	X	-	-	-
33	SQD	D	402	X	-	-	-
33	SQD	d	402	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 71784 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	n	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	G	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	N	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	Y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		

- Molecule 2 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		
2	A	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		

- Molecule 3 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		
3	B	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		
4	C	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		
5	D	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	75	Total	C	N	O	0	0
			612	400	100	112		
6	E	75	Total	C	N	O	0	0
			612	400	100	112		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		
7	F	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	26	PHE	SER	conflict	UNP P62096
F	26	PHE	SER	conflict	UNP P62096

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	60	Total	C	N	O	S	0	0
			452	296	72	81	3		
8	H	60	Total	C	N	O	S	0	0
			452	296	72	81	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	34	Total	C	N	O	S	0	0
			278	191	43	43	1		
9	I	34	Total	C	N	O	S	0	0
			278	191	43	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	35	Total	C	N	O	0	0
			256	174	39	43		
10	J	35	Total	C	N	O	0	0
			256	174	39	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	37	Total	C	N	O	S	0	0
			306	215	44	46	1		
11	K	37	Total	C	N	O	S	0	0
			306	215	44	46	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	l	37	Total	C	N	O	0	0
			311	205	49	57		
12	L	37	Total	C	N	O	0	0
			311	205	49	57		

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	33	Total	C	N	O	S	0	0
			256	176	36	43	1		
13	M	33	Total	C	N	O	S	0	0
			256	176	36	43	1		

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		
14	O	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	t	32	Total	C	N	O	S	0	0
			261	182	37	41	1		
15	T	32	Total	C	N	O	S	0	0
			261	182	37	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	w	54	Total	C	N	O	S	0	0
			419	275	61	82	1		
16	W	54	Total	C	N	O	S	0	0
			419	275	61	82	1		

- Molecule 17 is a protein called Ultraviolet-B-repressible protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	x	39	Total	C	N	O	0	0
			276	180	46	50		
17	X	39	Total	C	N	O	0	0
			276	180	46	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		
18	Z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		

- Molecule 19 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	222	Total	C	N	O	S	0	0
			1732	1133	281	314	4		

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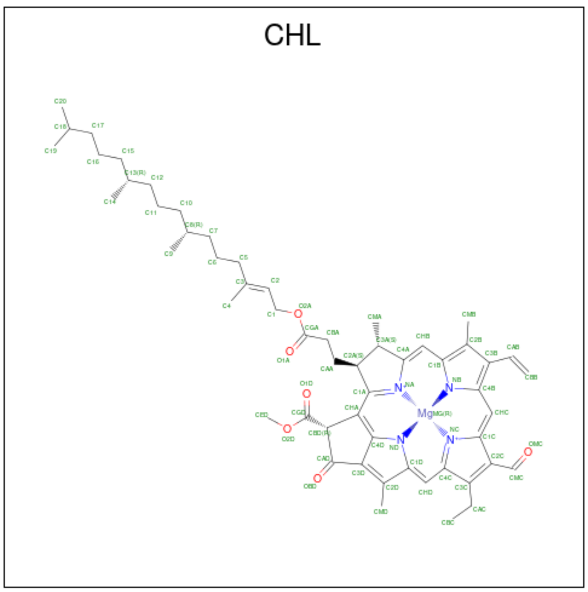
Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	222	Total 1732	C 1133	N 281	O 314	S 4	0	0

- Molecule 20 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	s	218	Total 1688	C 1105	N 271	O 308	S 4	0	0
20	S	218	Total 1688	C 1105	N 271	O 308	S 4	0	0

- Molecule 21 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
21	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
21	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
21	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
21	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
21	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
21	g	1	Total 355	C 289	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
21	n	1	Total 314	C 259	Mg 5	N 20	O 30	0
21	n	1	Total 314	C 259	Mg 5	N 20	O 30	0
21	n	1	Total 314	C 259	Mg 5	N 20	O 30	0
21	n	1	Total 314	C 259	Mg 5	N 20	O 30	0
21	n	1	Total 314	C 259	Mg 5	N 20	O 30	0
21	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
21	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
21	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
21	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
21	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
21	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
21	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
21	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
21	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
21	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
21	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
21	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
21	N	1	Total 314	C 259	Mg 5	N 20	O 30	0
21	N	1	Total 314	C 259	Mg 5	N 20	O 30	0
21	N	1	Total 314	C 259	Mg 5	N 20	O 30	0
21	N	1	Total 314	C 259	Mg 5	N 20	O 30	0

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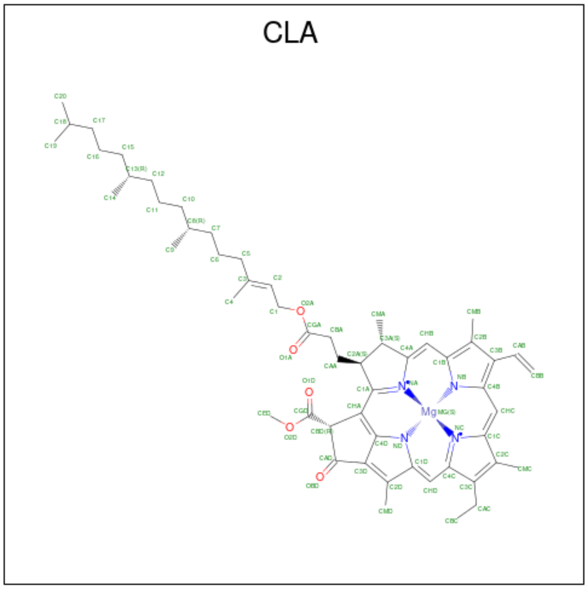
Mol	Chain	Residues	Atoms					AltConf
21	N	1	Total	C	Mg	N	O	0
			314	259	5	20	30	
21	Y	1	Total	C	Mg	N	O	0
			314	259	5	20	30	
21	Y	1	Total	C	Mg	N	O	0
			314	259	5	20	30	
21	Y	1	Total	C	Mg	N	O	0
			314	259	5	20	30	
21	Y	1	Total	C	Mg	N	O	0
			314	259	5	20	30	
21	Y	1	Total	C	Mg	N	O	0
			314	259	5	20	30	
21	r	1	Total	C	Mg	N	O	0
			231	187	4	16	24	
21	r	1	Total	C	Mg	N	O	0
			231	187	4	16	24	
21	r	1	Total	C	Mg	N	O	0
			231	187	4	16	24	
21	r	1	Total	C	Mg	N	O	0
			231	187	4	16	24	
21	s	1	Total	C	Mg	N	O	0
			186	142	4	16	24	
21	s	1	Total	C	Mg	N	O	0
			186	142	4	16	24	
21	s	1	Total	C	Mg	N	O	0
			186	142	4	16	24	
21	s	1	Total	C	Mg	N	O	0
			186	142	4	16	24	
21	S	1	Total	C	Mg	N	O	0
			186	142	4	16	24	
21	S	1	Total	C	Mg	N	O	0
			186	142	4	16	24	
21	S	1	Total	C	Mg	N	O	0
			186	142	4	16	24	
21	S	1	Total	C	Mg	N	O	0
			186	142	4	16	24	
21	R	1	Total	C	Mg	N	O	0
			183	150	3	12	18	
21	R	1	Total	C	Mg	N	O	0
			183	150	3	12	18	
21	R	1	Total	C	Mg	N	O	0
			183	150	3	12	18	

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	Y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	Y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	Y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	Y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	Y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	Y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	Y	1	Total 413	C 343	Mg 7	N 28	O 35	0
22	a	1	Total 240	C 200	Mg 4	N 16	O 20	0
22	a	1	Total 240	C 200	Mg 4	N 16	O 20	0
22	a	1	Total 240	C 200	Mg 4	N 16	O 20	0
22	a	1	Total 240	C 200	Mg 4	N 16	O 20	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	b	1	Total 975	C 825	Mg 15	N 60	O 75	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0

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Mol	Chain	Residues	Atoms					AltConf
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	d	1	Total 130	C 110	Mg 2	N 8	O 10	0
22	d	1	Total 130	C 110	Mg 2	N 8	O 10	0
22	w	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 240	C 200	Mg 4	N 16	O 20	0
22	A	1	Total 240	C 200	Mg 4	N 16	O 20	0
22	A	1	Total 240	C 200	Mg 4	N 16	O 20	0
22	A	1	Total 240	C 200	Mg 4	N 16	O 20	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0

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Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C Mg N O 1040 880 16 64 80	0
22	B	1	Total C Mg N O 1040 880 16 64 80	0
22	B	1	Total C Mg N O 1040 880 16 64 80	0
22	B	1	Total C Mg N O 1040 880 16 64 80	0
22	B	1	Total C Mg N O 1040 880 16 64 80	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	C	1	Total C Mg N O 845 715 13 52 65	0
22	D	1	Total C Mg N O 130 110 2 8 10	0
22	D	1	Total C Mg N O 130 110 2 8 10	0
22	W	1	Total C Mg N O 60 50 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
22	r	1	Total C Mg N O 400 330 7 28 35	0
22	r	1	Total C Mg N O 400 330 7 28 35	0
22	r	1	Total C Mg N O 400 330 7 28 35	0
22	r	1	Total C Mg N O 400 330 7 28 35	0
22	r	1	Total C Mg N O 400 330 7 28 35	0
22	r	1	Total C Mg N O 400 330 7 28 35	0
22	r	1	Total C Mg N O 400 330 7 28 35	0
22	s	1	Total C Mg N O 471 381 9 36 45	0
22	s	1	Total C Mg N O 471 381 9 36 45	0
22	s	1	Total C Mg N O 471 381 9 36 45	0
22	s	1	Total C Mg N O 471 381 9 36 45	0
22	s	1	Total C Mg N O 471 381 9 36 45	0
22	s	1	Total C Mg N O 471 381 9 36 45	0
22	s	1	Total C Mg N O 471 381 9 36 45	0
22	s	1	Total C Mg N O 471 381 9 36 45	0
22	s	1	Total C Mg N O 471 381 9 36 45	0
22	S	1	Total C Mg N O 471 381 9 36 45	0
22	S	1	Total C Mg N O 471 381 9 36 45	0
22	S	1	Total C Mg N O 471 381 9 36 45	0
22	S	1	Total C Mg N O 471 381 9 36 45	0
22	S	1	Total C Mg N O 471 381 9 36 45	0

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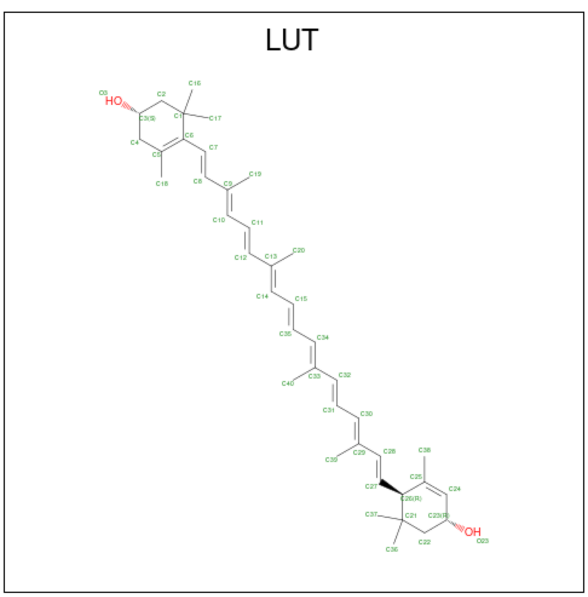
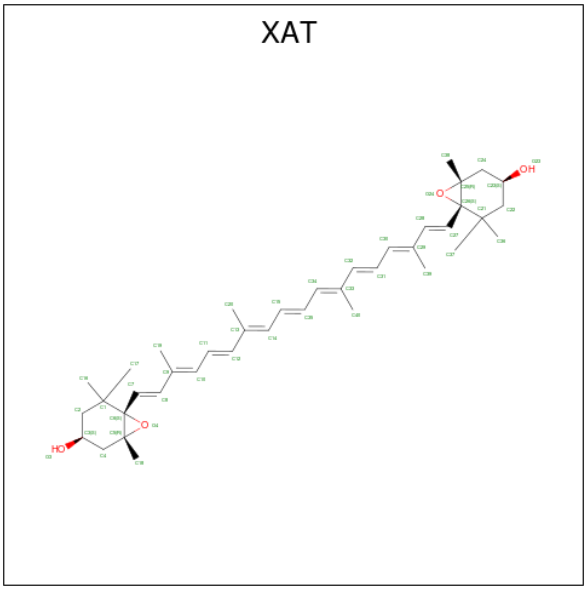
Mol	Chain	Residues	Atoms	AltConf
22	S	1	Total C Mg N O 471 381 9 36 45	0
22	S	1	Total C Mg N O 471 381 9 36 45	0
22	S	1	Total C Mg N O 471 381 9 36 45	0
22	S	1	Total C Mg N O 471 381 9 36 45	0
22	R	1	Total C Mg N O 400 330 7 28 35	0
22	R	1	Total C Mg N O 400 330 7 28 35	0
22	R	1	Total C Mg N O 400 330 7 28 35	0
22	R	1	Total C Mg N O 400 330 7 28 35	0
22	R	1	Total C Mg N O 400 330 7 28 35	0
22	R	1	Total C Mg N O 400 330 7 28 35	0
22	R	1	Total C Mg N O 400 330 7 28 35	0

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



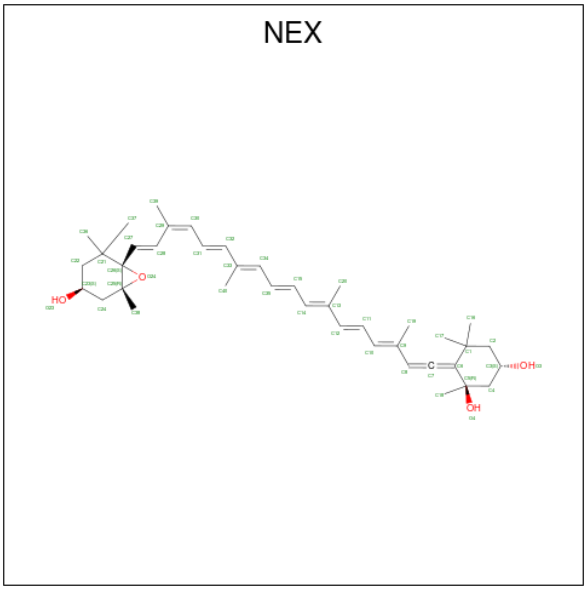
Mol	Chain	Residues	Atoms			AltConf
23	g	1	Total	C	O	0
			84	80	4	
23	g	1	Total	C	O	0
			84	80	4	
23	n	1	Total	C	O	0
			42	40	2	
23	y	1	Total	C	O	0
			42	40	2	
23	G	1	Total	C	O	0
			84	80	4	
23	G	1	Total	C	O	0
			84	80	4	
23	N	1	Total	C	O	0
			84	80	4	
23	N	1	Total	C	O	0
			84	80	4	
23	Y	1	Total	C	O	0
			84	80	4	
23	Y	1	Total	C	O	0
			84	80	4	
23	r	1	Total	C	O	0
			42	40	2	
23	R	1	Total	C	O	0
			42	40	2	

- Molecule 24 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 (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	AltConf
24	g	1	Total C O 44 40 4	0
24	n	1	Total C O 44 40 4	0
24	y	1	Total C O 44 40 4	0
24	G	1	Total C O 44 40 4	0
24	N	1	Total C O 44 40 4	0
24	Y	1	Total C O 44 40 4	0
24	r	1	Total C O 44 40 4	0
24	R	1	Total C O 44 40 4	0

- Molecule 25 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 (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	AltConf
25	g	1	Total C O 44 40 4	0
25	n	1	Total C O 44 40 4	0

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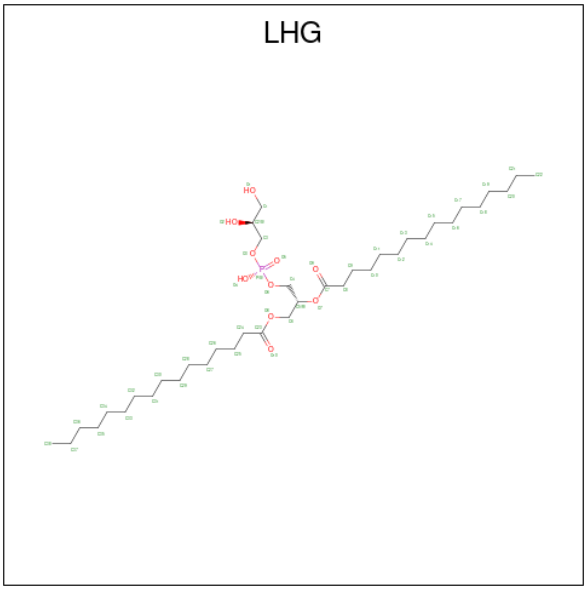
Mol	Chain	Residues	Atoms	AltConf
25	y	1	Total C O 88 80 8	0
25	y	1	Total C O 88 80 8	0
25	N	1	Total C O 44 40 4	0
25	Y	1	Total C O 44 40 4	0
25	r	1	Total C O 44 40 4	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
26	g	1	Total C O P 49 38 10 1	0
26	n	1	Total C O P 49 38 10 1	0
26	y	1	Total C O P 49 38 10 1	0
26	G	1	Total C O P 49 38 10 1	0
26	N	1	Total C O P 49 38 10 1	0
26	Y	1	Total C O P 49 38 10 1	0

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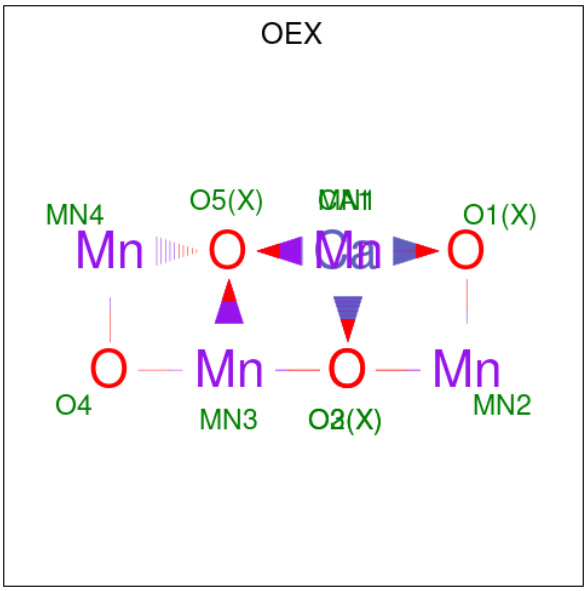
Mol	Chain	Residues	Atoms				AltConf
26	b	1	Total	C	O	P	0
			49	38	10	1	
26	c	1	Total	C	O	P	0
			147	114	30	3	
26	c	1	Total	C	O	P	0
			147	114	30	3	
26	c	1	Total	C	O	P	0
			147	114	30	3	
26	d	1	Total	C	O	P	0
			138	105	30	3	
26	d	1	Total	C	O	P	0
			138	105	30	3	
26	d	1	Total	C	O	P	0
			138	105	30	3	
26	l	1	Total	C	O	P	0
			49	38	10	1	
26	B	1	Total	C	O	P	0
			49	38	10	1	
26	C	1	Total	C	O	P	0
			147	114	30	3	
26	C	1	Total	C	O	P	0
			147	114	30	3	
26	C	1	Total	C	O	P	0
			147	114	30	3	
26	D	1	Total	C	O	P	0
			138	105	30	3	
26	D	1	Total	C	O	P	0
			138	105	30	3	
26	D	1	Total	C	O	P	0
			138	105	30	3	
26	L	1	Total	C	O	P	0
			49	38	10	1	
26	r	1	Total	C	O	P	0
			47	36	10	1	
26	s	1	Total	C	O	P	0
			49	38	10	1	
26	S	1	Total	C	O	P	0
			49	38	10	1	
26	R	1	Total	C	O	P	0
			47	36	10	1	

- Molecule 27 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

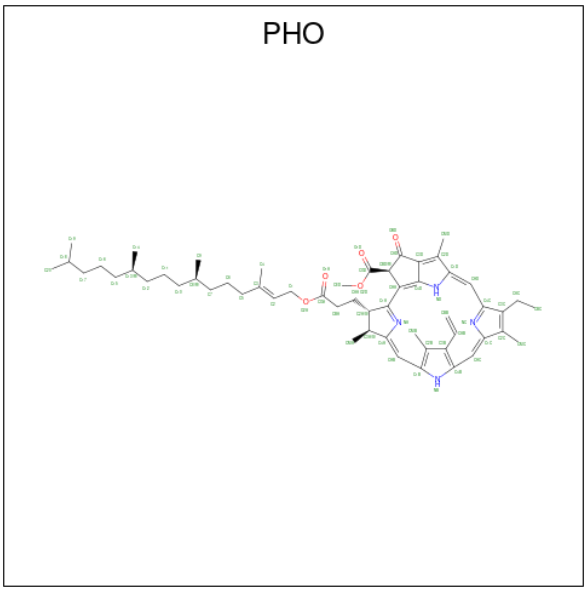
- Molecule 28 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 29 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

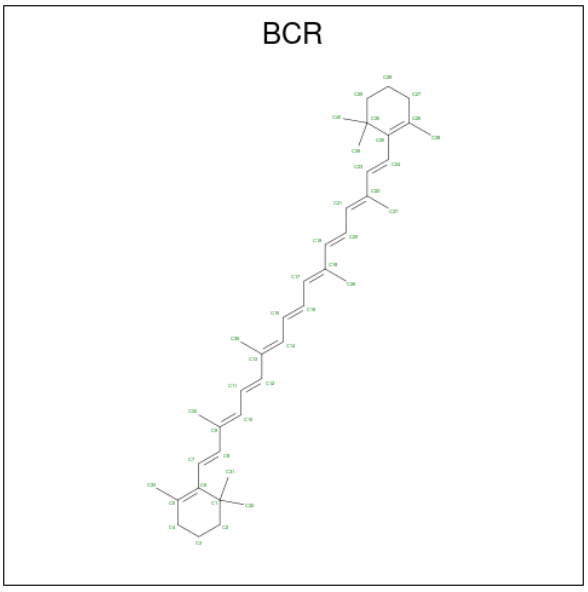
Mol	Chain	Residues	Atoms		AltConf
29	a	1	Total	Cl	0
			1	1	
29	c	1	Total	Cl	0
			1	1	
29	A	1	Total	Cl	0
			1	1	
29	C	1	Total	Cl	0
			1	1	

- Molecule 30 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



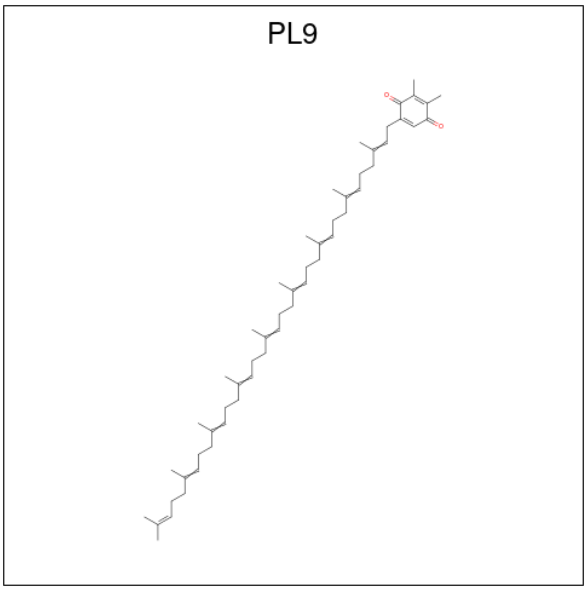
Mol	Chain	Residues	Atoms				AltConf
30	a	1	Total	C	N	O	0
			64	55	4	5	
30	d	1	Total	C	N	O	0
			64	55	4	5	
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



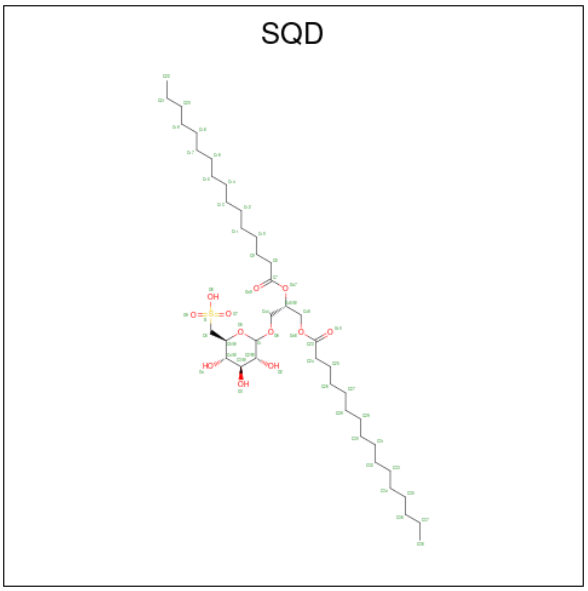
Mol	Chain	Residues	Atoms	AltConf
31	a	1	Total C 40 40	0
31	b	1	Total C 120 120	0
31	b	1	Total C 120 120	0
31	b	1	Total C 120 120	0
31	c	1	Total C 80 80	0
31	c	1	Total C 80 80	0
31	d	1	Total C 40 40	0
31	h	1	Total C 40 40	0
31	k	1	Total C 80 80	0
31	k	1	Total C 80 80	0
31	A	1	Total C 40 40	0
31	B	1	Total C 160 160	0
31	B	1	Total C 160 160	0
31	B	1	Total C 160 160	0
31	B	1	Total C 160 160	0
31	C	1	Total C 80 80	0
31	C	1	Total C 80 80	0
31	D	1	Total C 40 40	0
31	H	1	Total C 40 40	0
31	K	1	Total C 80 80	0
31	K	1	Total C 80 80	0
31	T	1	Total C 40 40	0

- Molecule 32 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 (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



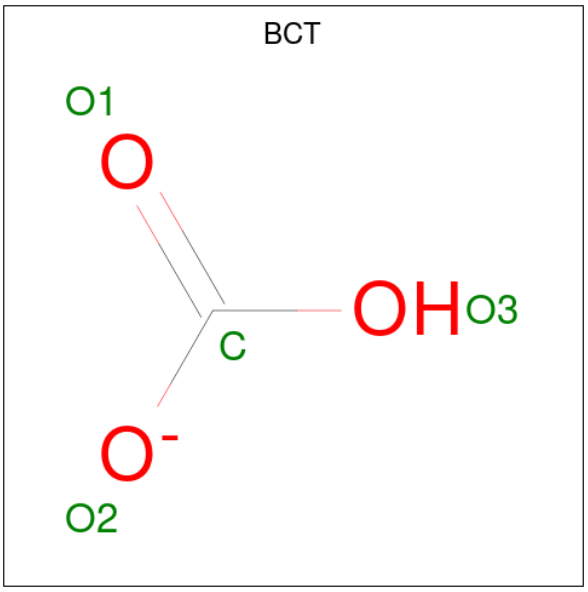
Mol	Chain	Residues	Atoms			AltConf
32	a	1	Total	C	O	0
			13	11	2	
32	d	1	Total	C	O	0
			55	53	2	
32	A	1	Total	C	O	0
			13	11	2	
32	D	1	Total	C	O	0
			55	53	2	

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



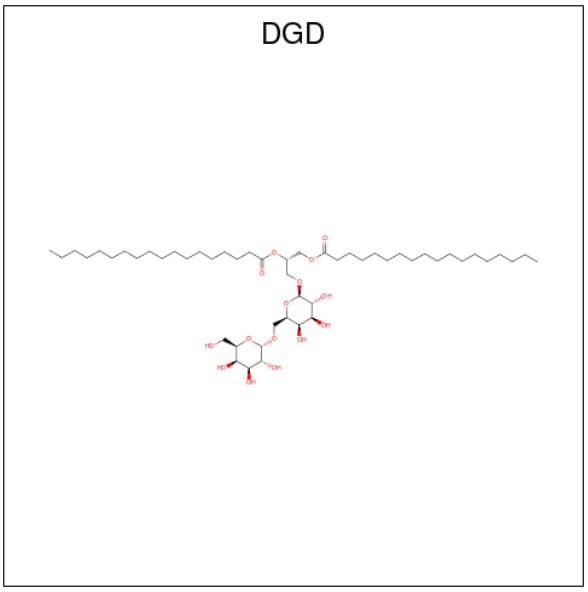
Mol	Chain	Residues	Atoms				AltConf
33	a	1	Total	C	O	S	0
			54	41	12	1	
33	d	1	Total	C	O	S	0
			50	37	12	1	
33	l	1	Total	C	O	S	0
			96	70	24	2	
33	l	1	Total	C	O	S	0
			96	70	24	2	
33	A	1	Total	C	O	S	0
			54	41	12	1	
33	D	1	Total	C	O	S	0
			50	37	12	1	
33	L	1	Total	C	O	S	0
			96	70	24	2	
33	L	1	Total	C	O	S	0
			96	70	24	2	

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
35	a	1	Total	C	O	0
			59	44	15	

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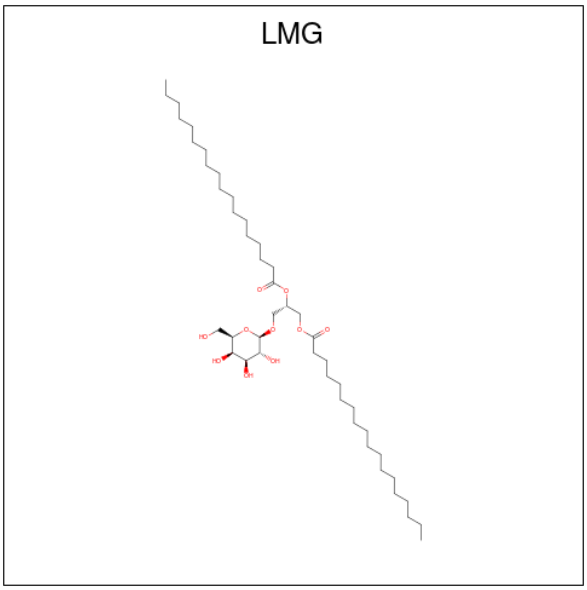
Mol	Chain	Residues	Atoms	AltConf
35	c	1	Total C O 177 132 45	0
35	c	1	Total C O 177 132 45	0
35	c	1	Total C O 177 132 45	0
35	h	1	Total C O 62 47 15	0
35	A	1	Total C O 59 44 15	0
35	C	1	Total C O 117 87 30	0
35	C	1	Total C O 117 87 30	0
35	H	1	Total C O 62 47 15	0
35	J	1	Total C O 60 45 15	0

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



Mol	Chain	Residues	Atoms	AltConf
36	b	1	Total C O 55 45 10	0
36	c	1	Total C O 51 41 10	0

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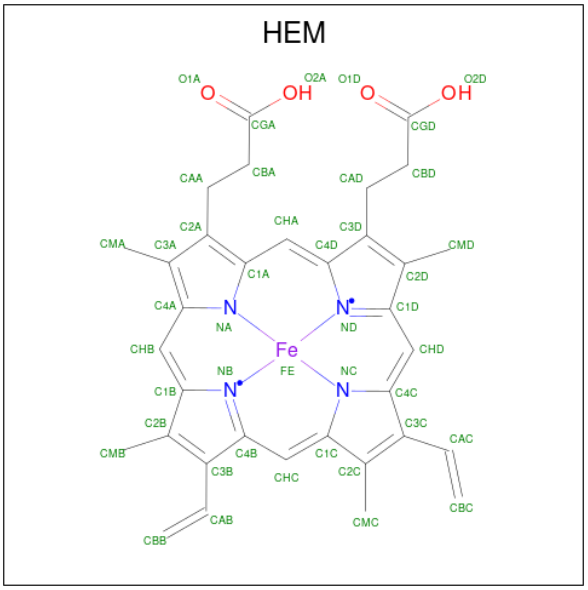
Mol	Chain	Residues	Atoms	AltConf
36	d	1	Total C O 46 36 10	0
36	k	1	Total C O 51 41 10	0
36	w	1	Total C O 48 38 10	0
36	B	1	Total C O 95 75 20	0
36	B	1	Total C O 95 75 20	0
36	C	1	Total C O 99 79 20	0
36	C	1	Total C O 99 79 20	0
36	D	1	Total C O 46 36 10	0
36	I	1	Total C O 40 30 10	0
36	K	1	Total C O 51 41 10	0
36	M	1	Total C O 51 41 10	0
36	T	1	Total C O 51 41 10	0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



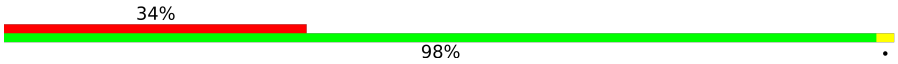
Mol	Chain	Residues	Atoms					AltConf
37	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
37	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

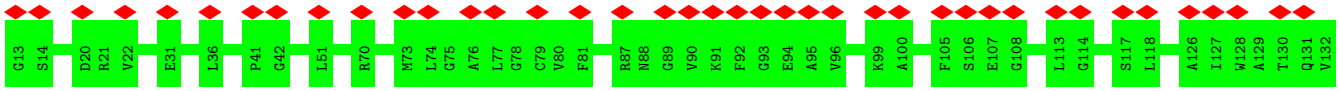
3 Residue-property plots (i)

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

• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

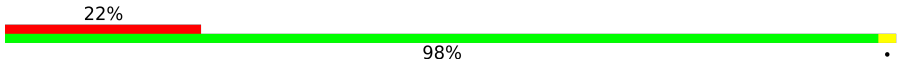
Chain g:

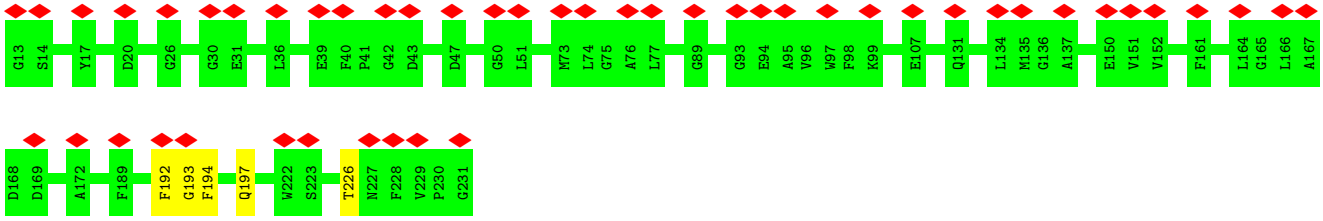




• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

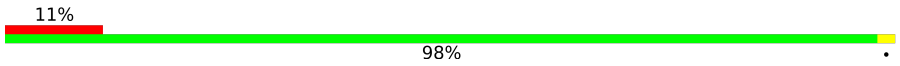
Chain n:

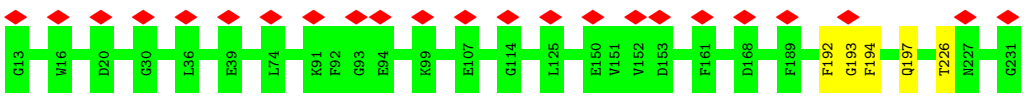




• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

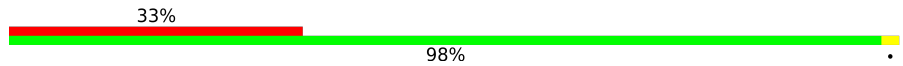
Chain y:

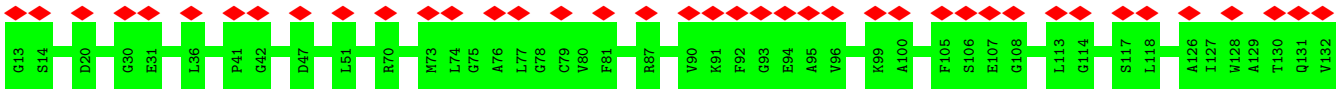


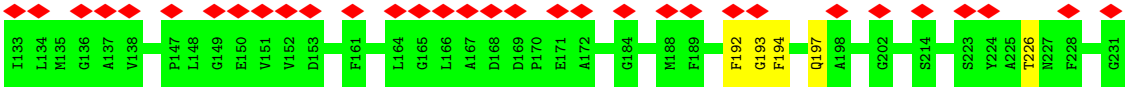


• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

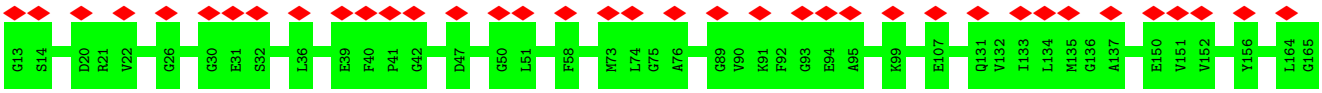
Chain G:

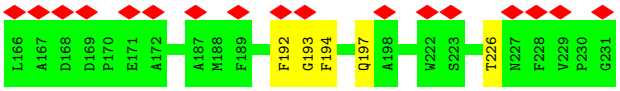




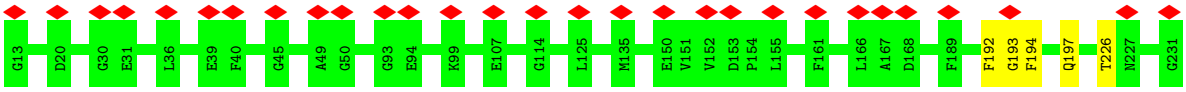


• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

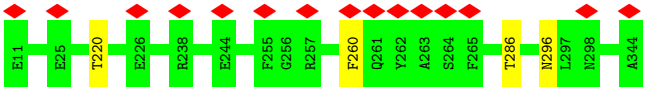




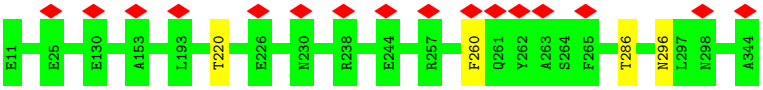
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



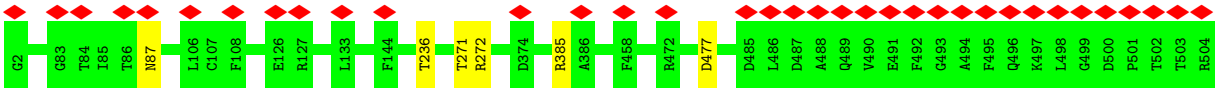
• Molecule 2: Photosystem II protein D1



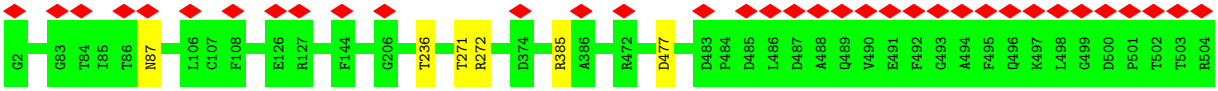
• Molecule 2: Photosystem II protein D1



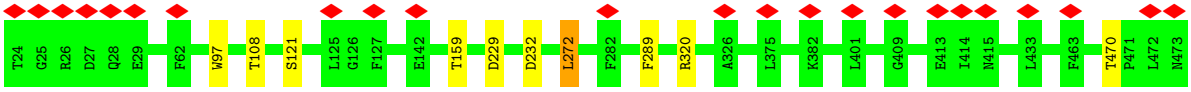
• Molecule 3: Photosystem II CP47 reaction center protein



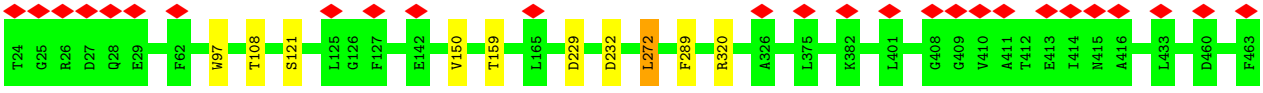
• Molecule 3: Photosystem II CP47 reaction center protein

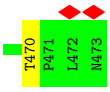


• Molecule 4: Photosystem II CP43 reaction center protein

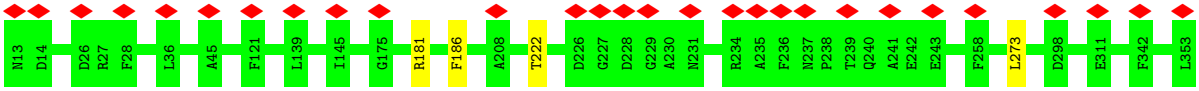


• Molecule 4: Photosystem II CP43 reaction center protein

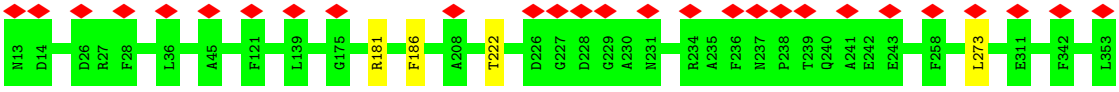




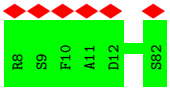
• Molecule 5: Photosystem II D2 protein



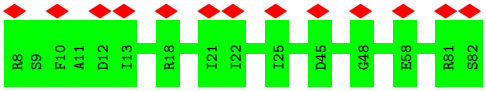
• Molecule 5: Photosystem II D2 protein



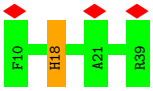
• Molecule 6: Cytochrome b559 subunit alpha



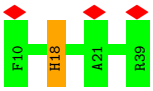
• Molecule 6: Cytochrome b559 subunit alpha



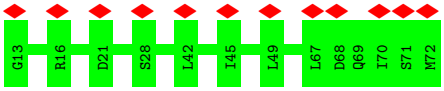
• Molecule 7: Cytochrome b559 subunit beta



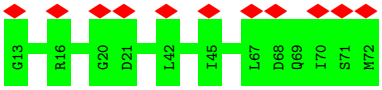
• Molecule 7: Cytochrome b559 subunit beta



• Molecule 8: Photosystem II reaction center protein H



• Molecule 8: Photosystem II reaction center protein H

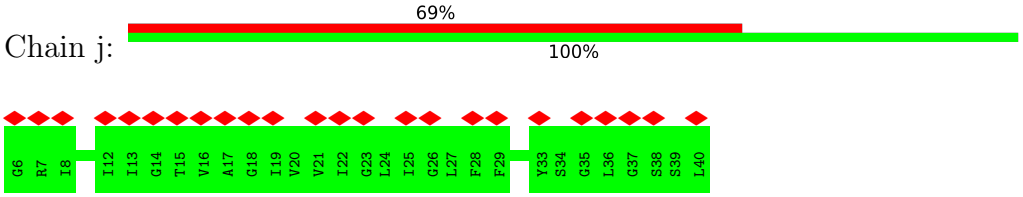


• Molecule 9: Photosystem II reaction center protein I

• Molecule 9: Photosystem II reaction center protein I

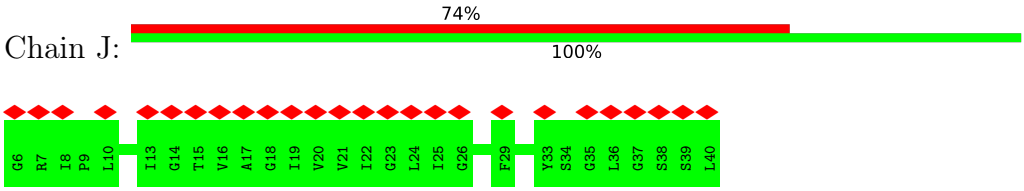
• Molecule 10: Photosystem II reaction center protein J

Chain j:



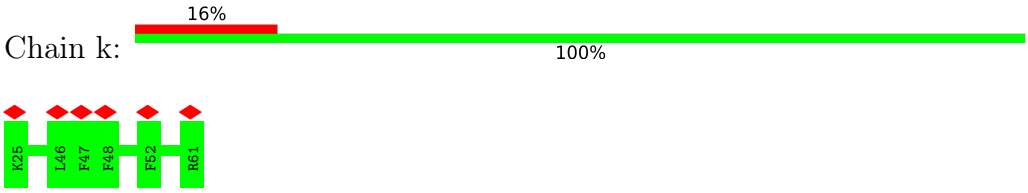
• Molecule 10: Photosystem II reaction center protein J

Chain J:



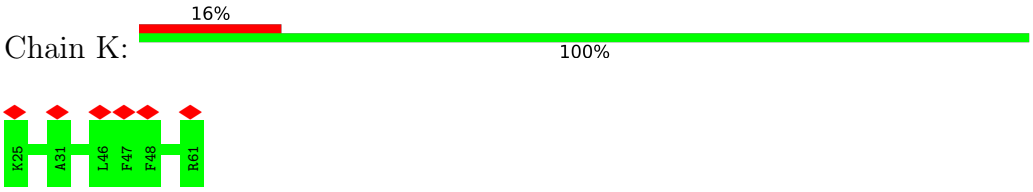
• Molecule 11: Photosystem II reaction center protein K

Chain k:



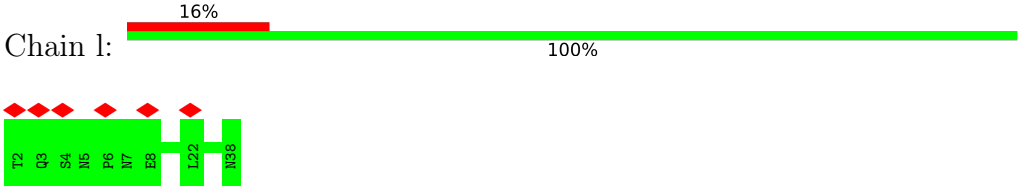
• Molecule 11: Photosystem II reaction center protein K

Chain K:



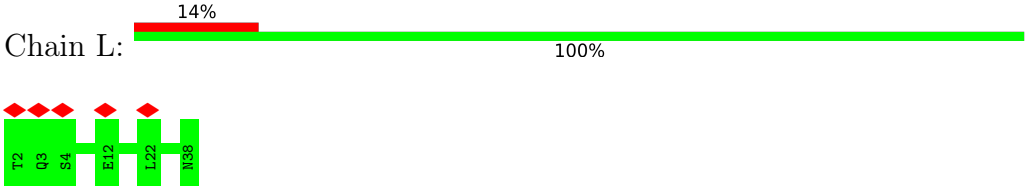
• Molecule 12: Photosystem II reaction center protein L

Chain l:



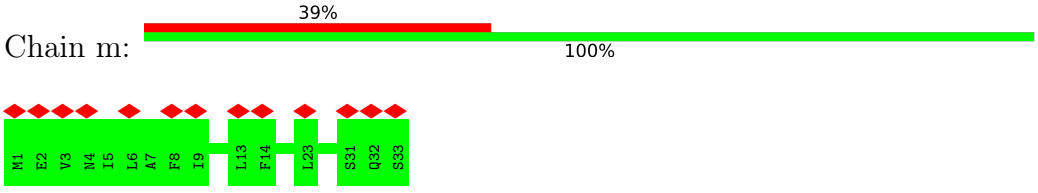
• Molecule 12: Photosystem II reaction center protein L

Chain L:



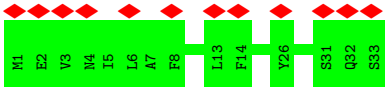
• Molecule 13: Photosystem II reaction center protein M

Chain m:



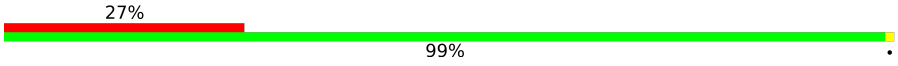
• Molecule 13: Photosystem II reaction center protein M

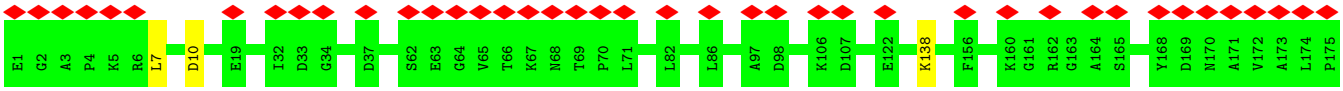
Chain M:

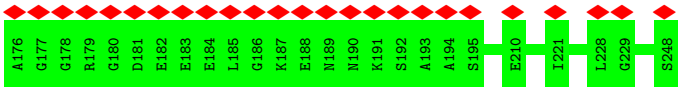


• Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o:

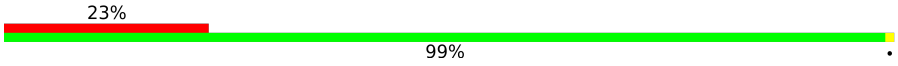


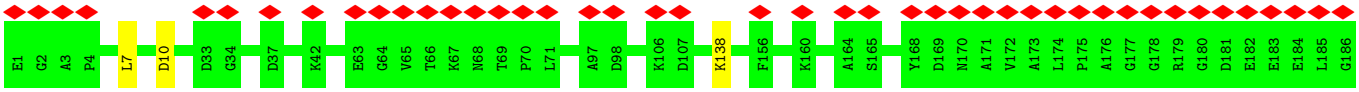


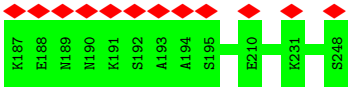


• Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O:

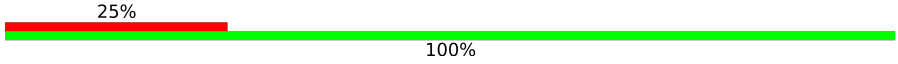


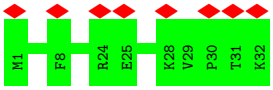




• Molecule 15: Photosystem II reaction center protein T

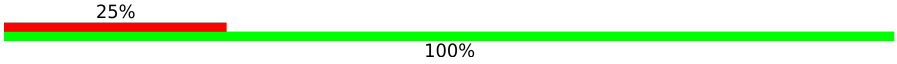
Chain t:

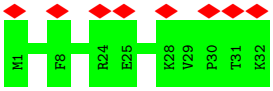




• Molecule 15: Photosystem II reaction center protein T

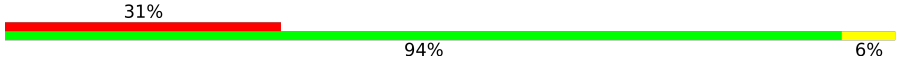
Chain T:

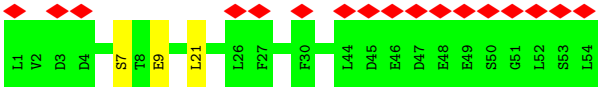




• Molecule 16: Photosystem II reaction center protein W

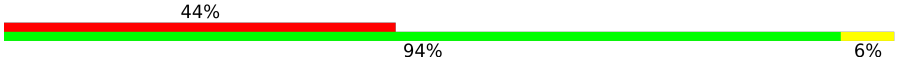
Chain w:

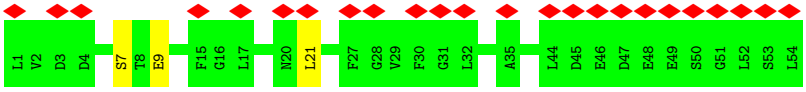




• Molecule 16: Photosystem II reaction center protein W

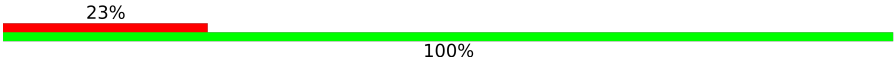
Chain W:

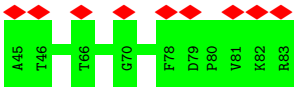




• Molecule 17: Ultraviolet-B-repressible protein

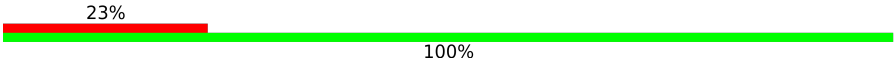
Chain x:

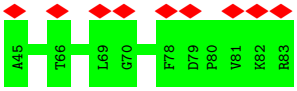




• Molecule 17: Ultraviolet-B-repressible protein

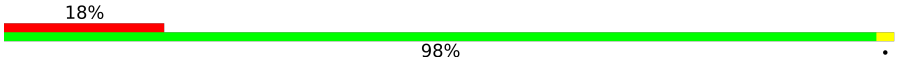
Chain X:

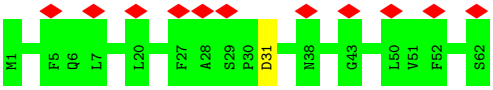




• Molecule 18: Photosystem II reaction center protein Z

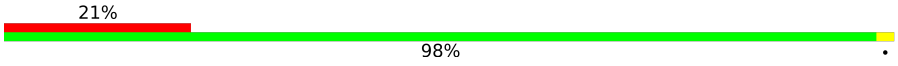
Chain z:

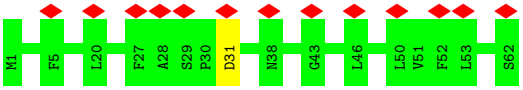




• Molecule 18: Photosystem II reaction center protein Z

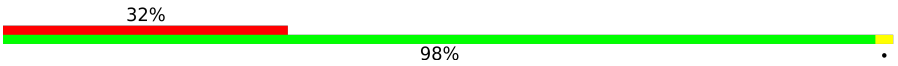
Chain Z:

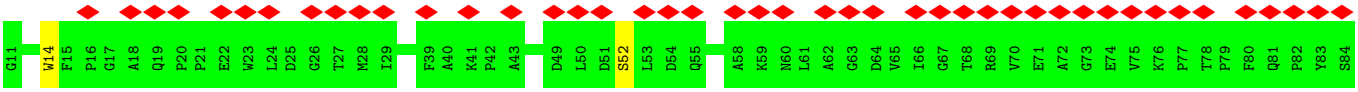


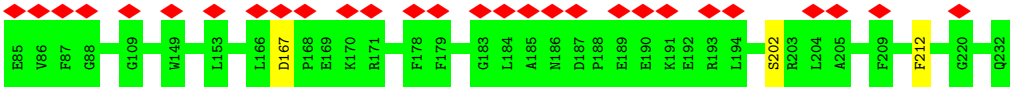


• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4.3

Chain r:

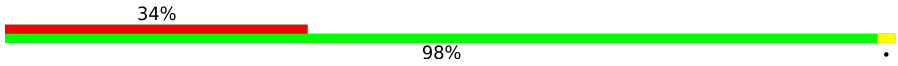


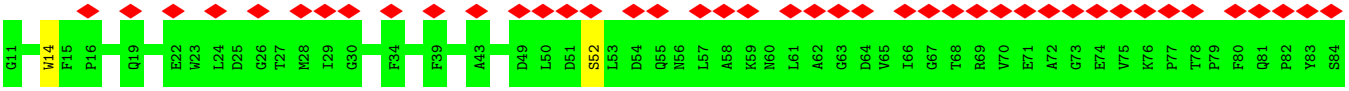


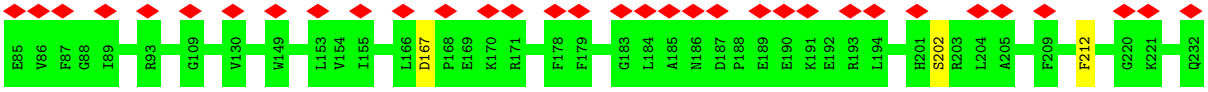


• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4.3

Chain R:

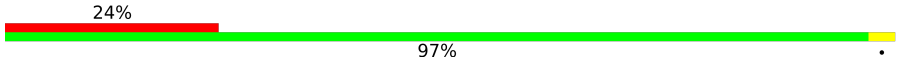


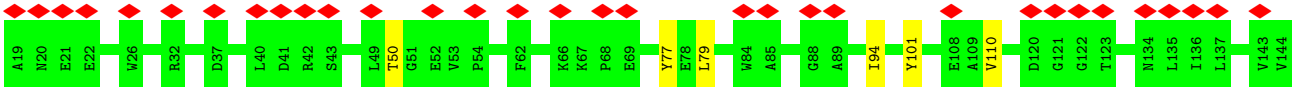


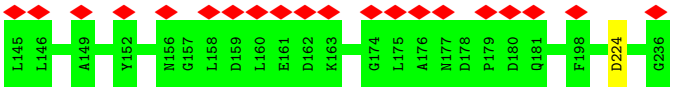


• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

Chain s:

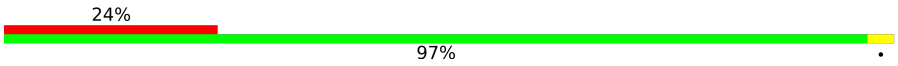


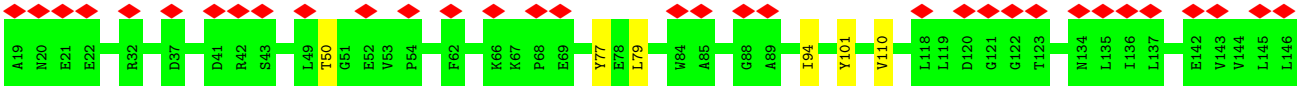


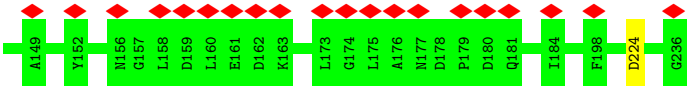


• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

Chain S:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	27942	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40, 40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k), GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.923	Depositor
Minimum map value	-0.630	Depositor
Average map value	0.055	Depositor
Map value standard deviation	0.166	Depositor
Recommended contour level	0.85	Depositor
Map size (Å)	374.0, 374.0, 374.0	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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, LMG, LUT, CL, HEM, CHL, BCR, FE2, SQD, CLA, XAT, OEX, DGD, LHG, PHO, PL9, NEX

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	G	0.30	0/1720	0.43	0/2342
1	N	0.30	0/1720	0.43	0/2342
1	Y	0.30	0/1720	0.43	0/2342
1	g	0.30	0/1720	0.43	0/2342
1	n	0.30	0/1720	0.43	0/2342
1	y	0.30	0/1720	0.43	0/2342
2	A	0.31	0/2697	0.43	0/3677
2	a	0.31	0/2697	0.43	0/3677
3	B	0.31	0/4081	0.41	0/5556
3	b	0.31	0/4081	0.41	0/5556
4	C	0.82	1/3614 (0.0%)	0.48	3/4922 (0.1%)
4	c	0.82	1/3614 (0.0%)	0.48	3/4922 (0.1%)
5	D	0.31	0/2804	0.42	0/3823
5	d	0.31	0/2804	0.42	0/3823
6	E	0.28	0/630	0.39	0/857
6	e	0.28	0/630	0.39	0/857
7	F	0.56	1/248 (0.4%)	0.47	0/335
7	f	0.56	1/248 (0.4%)	0.47	0/335
8	H	0.29	0/461	0.43	0/626
8	h	0.29	0/461	0.43	0/626
9	I	0.33	0/286	0.40	0/386
9	i	0.33	0/286	0.41	0/386
10	J	0.27	0/262	0.40	0/354
10	j	0.27	0/262	0.40	0/354
11	K	0.32	0/318	0.43	0/434
11	k	0.32	0/318	0.43	0/434
12	L	0.31	0/319	0.40	0/434
12	l	0.31	0/319	0.40	0/434
13	M	0.30	0/260	0.39	0/355
13	m	0.30	0/260	0.39	0/355
14	O	0.28	0/1906	0.45	0/2575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
14	o	0.28	0/1906	0.45	0/2575
15	T	0.35	0/269	0.39	0/365
15	t	0.35	0/269	0.39	0/365
16	W	0.36	0/429	0.43	0/581
16	w	0.36	0/429	0.42	0/581
17	X	0.28	0/279	0.40	0/380
17	x	0.28	0/279	0.39	0/380
18	Z	0.27	0/474	0.35	0/648
18	z	0.27	0/474	0.35	0/648
19	R	0.28	0/1780	0.40	0/2417
19	r	0.29	0/1780	0.40	0/2417
20	S	0.31	0/1737	0.42	0/2361
20	s	0.31	0/1737	0.42	0/2361
All	All	0.41	4/56028 (0.0%)	0.43	6/76224 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	2
1	N	0	2
1	Y	0	2
1	g	0	2
1	n	0	2
1	y	0	2
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	272	LEU	CG-CD1	45.67	3.20	1.51
4	C	272	LEU	CG-CD1	45.67	3.20	1.51
7	F	18	HIS	CB-CG	7.21	1.63	1.50
7	f	18	HIS	CB-CG	7.19	1.62	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	c	272	LEU	CB-CG-CD1	12.88	132.89	111.00
4	C	272	LEU	CB-CG-CD1	12.87	132.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	c	272	LEU	CA-CB-CG	7.25	131.97	115.30
4	C	272	LEU	CA-CB-CG	7.24	131.96	115.30
4	C	272	LEU	CB-CG-CD2	-6.80	99.44	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	g	193	GLY	Mainchain
1	g	197	GLN	Sidechain
1	n	193	GLY	Mainchain
1	n	197	GLN	Sidechain
1	y	193	GLY	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	G	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	N	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	Y	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	g	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	n	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	y	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
2	A	332/334 (99%)	320 (96%)	12 (4%)	0	100	100
2	a	332/334 (99%)	320 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	501/503 (100%)	485 (97%)	16 (3%)	0	100	100
3	b	501/503 (100%)	485 (97%)	16 (3%)	0	100	100
4	C	448/450 (100%)	428 (96%)	20 (4%)	0	100	100
4	c	448/450 (100%)	428 (96%)	20 (4%)	0	100	100
5	D	339/341 (99%)	326 (96%)	13 (4%)	0	100	100
5	d	339/341 (99%)	327 (96%)	12 (4%)	0	100	100
6	E	73/75 (97%)	73 (100%)	0	0	100	100
6	e	73/75 (97%)	73 (100%)	0	0	100	100
7	F	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
7	f	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
8	H	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
8	h	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
9	i	32/34 (94%)	32 (100%)	0	0	100	100
10	J	33/35 (94%)	33 (100%)	0	0	100	100
10	j	33/35 (94%)	33 (100%)	0	0	100	100
11	K	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
11	k	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
12	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
13	M	31/33 (94%)	31 (100%)	0	0	100	100
13	m	31/33 (94%)	31 (100%)	0	0	100	100
14	O	246/248 (99%)	230 (94%)	16 (6%)	0	100	100
14	o	246/248 (99%)	230 (94%)	16 (6%)	0	100	100
15	T	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
15	t	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
16	W	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
16	w	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
17	X	37/39 (95%)	37 (100%)	0	0	100	100
17	x	37/39 (95%)	37 (100%)	0	0	100	100
18	Z	60/62 (97%)	60 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	z	60/62 (97%)	60 (100%)	0	0	100	100
19	R	220/222 (99%)	207 (94%)	13 (6%)	0	100	100
19	r	220/222 (99%)	207 (94%)	13 (6%)	0	100	100
20	S	216/218 (99%)	198 (92%)	18 (8%)	0	100	100
20	s	216/218 (99%)	198 (92%)	18 (8%)	0	100	100
All	All	6914/7002 (99%)	6583 (95%)	331 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	G	171/171 (100%)	168 (98%)	3 (2%)	59	77
1	N	171/171 (100%)	168 (98%)	3 (2%)	59	77
1	Y	171/171 (100%)	168 (98%)	3 (2%)	59	77
1	g	171/171 (100%)	168 (98%)	3 (2%)	59	77
1	n	171/171 (100%)	168 (98%)	3 (2%)	59	77
1	y	171/171 (100%)	168 (98%)	3 (2%)	59	77
2	A	270/270 (100%)	266 (98%)	4 (2%)	65	81
2	a	270/270 (100%)	266 (98%)	4 (2%)	65	81
3	B	400/400 (100%)	394 (98%)	6 (2%)	65	81
3	b	400/400 (100%)	394 (98%)	6 (2%)	65	81
4	C	352/352 (100%)	341 (97%)	11 (3%)	40	65
4	c	352/352 (100%)	342 (97%)	10 (3%)	43	68
5	D	275/275 (100%)	271 (98%)	4 (2%)	65	81
5	d	275/275 (100%)	271 (98%)	4 (2%)	65	81
6	E	67/67 (100%)	67 (100%)	0	100	100
6	e	67/67 (100%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	F	25/25 (100%)	24 (96%)	1 (4%)	31 59
7	f	25/25 (100%)	24 (96%)	1 (4%)	31 59
8	H	49/49 (100%)	49 (100%)	0	100 100
8	h	49/49 (100%)	49 (100%)	0	100 100
9	I	31/31 (100%)	31 (100%)	0	100 100
9	i	31/31 (100%)	31 (100%)	0	100 100
10	J	26/26 (100%)	26 (100%)	0	100 100
10	j	26/26 (100%)	26 (100%)	0	100 100
11	K	32/32 (100%)	32 (100%)	0	100 100
11	k	32/32 (100%)	32 (100%)	0	100 100
12	L	35/35 (100%)	35 (100%)	0	100 100
12	l	35/35 (100%)	35 (100%)	0	100 100
13	M	29/29 (100%)	29 (100%)	0	100 100
13	m	29/29 (100%)	29 (100%)	0	100 100
14	O	204/204 (100%)	201 (98%)	3 (2%)	65 81
14	o	204/204 (100%)	201 (98%)	3 (2%)	65 81
15	T	29/29 (100%)	29 (100%)	0	100 100
15	t	29/29 (100%)	29 (100%)	0	100 100
16	W	44/44 (100%)	41 (93%)	3 (7%)	16 47
16	w	44/44 (100%)	41 (93%)	3 (7%)	16 47
17	X	32/32 (100%)	32 (100%)	0	100 100
17	x	32/32 (100%)	32 (100%)	0	100 100
18	Z	54/54 (100%)	53 (98%)	1 (2%)	57 76
18	z	54/54 (100%)	53 (98%)	1 (2%)	57 76
19	R	175/175 (100%)	170 (97%)	5 (3%)	42 67
19	r	175/175 (100%)	170 (97%)	5 (3%)	42 67
20	S	169/169 (100%)	162 (96%)	7 (4%)	30 59
20	s	169/169 (100%)	162 (96%)	7 (4%)	30 59
All	All	5622/5622 (100%)	5515 (98%)	107 (2%)	59 76

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	272	ARG
5	D	181	ARG
20	S	101	TYR
3	B	477	ASP
4	C	229	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
14	O	74	GLN
18	Z	58	ASN
20	S	81	HIS
1	Y	131	GLN
1	Y	122	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 325 ligands modelled in this entry, 6 are monoatomic - leaving 319 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	$\#\|Z\|>2$
31	BCR	h	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.31	6 (10%)
22	CLA	N	602	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
21	CHL	N	601	1	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
24	XAT	N	616	-	39,47,47	5.20	20 (51%)	54,74,74	13.62	31 (57%)
36	LMG	D	411	-	46,46,55	0.81	3 (6%)	54,54,63	1.39	7 (12%)
21	CHL	n	606	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	c	512	4	65,73,73	1.45	7 (10%)	76,113,113	1.42	8 (10%)
36	LMG	w	102	-	48,48,55	0.78	2 (4%)	56,56,63	1.41	8 (14%)
21	CHL	y	605	-	48,56,74	2.49	17 (35%)	51,92,114	2.83	17 (33%)
22	CLA	b	612	-	65,73,73	1.45	6 (9%)	76,113,113	1.35	6 (7%)
21	CHL	g	608	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
21	CHL	g	601	1	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	B	605	-	65,73,73	1.43	8 (12%)	76,113,113	1.40	8 (10%)
31	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
22	CLA	a	404	-	65,73,73	1.47	8 (12%)	76,113,113	1.40	8 (10%)
22	CLA	S	311	22,20	56,64,73	1.59	6 (10%)	65,102,113	1.42	7 (10%)
21	CHL	g	605	-	46,54,74	2.55	16 (34%)	49,90,114	2.88	16 (32%)
21	CHL	y	606	-	50,58,74	2.45	16 (32%)	52,94,114	2.82	17 (32%)
21	CHL	N	608	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	c	513	22	65,73,73	1.45	9 (13%)	76,113,113	1.32	6 (7%)
22	CLA	Y	603	-	65,73,73	1.46	7 (10%)	76,113,113	1.35	7 (9%)
21	CHL	g	606	-	50,58,74	2.45	17 (34%)	52,94,114	2.82	17 (32%)
22	CLA	y	610	-	60,68,73	1.54	7 (11%)	70,107,113	1.43	6 (8%)
26	LHG	G	618	-	48,48,48	0.64	1 (2%)	51,54,54	1.28	7 (13%)
22	CLA	R	309	19	65,73,73	1.48	6 (9%)	76,113,113	1.40	6 (7%)
21	CHL	y	608	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	s	305	20	50,58,73	1.66	6 (12%)	58,95,113	1.59	8 (13%)
22	CLA	R	310	23,19	49,57,73	1.75	7 (14%)	55,93,113	1.44	4 (7%)
26	LHG	c	521	-	48,48,48	0.61	1 (2%)	51,54,54	1.23	7 (13%)
26	LHG	C	522	-	48,48,48	0.60	1 (2%)	51,54,54	1.29	8 (15%)
22	CLA	s	311	22,20	56,64,73	1.58	6 (10%)	65,102,113	1.40	7 (10%)
22	CLA	s	309	22,20	55,63,73	1.58	5 (9%)	64,101,113	1.49	9 (14%)
24	XAT	r	314	-	39,47,47	5.21	19 (48%)	54,74,74	13.48	28 (51%)
21	CHL	y	607	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
23	LUT	R	312	22	42,43,43	5.91	19 (45%)	51,60,60	5.17	28 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	LMG	C	502	-	48,48,55	0.78	2 (4%)	56,56,63	1.42	8 (14%)
31	BCR	D	406	-	41,41,41	1.20	2 (4%)	56,56,56	1.24	7 (12%)
31	BCR	C	516	-	41,41,41	1.23	2 (4%)	56,56,56	1.26	6 (10%)
22	CLA	c	511	-	65,73,73	1.47	7 (10%)	76,113,113	1.36	8 (10%)
22	CLA	S	309	22,20	55,63,73	1.59	5 (9%)	64,101,113	1.49	9 (14%)
22	CLA	d	404	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
22	CLA	n	611	-	60,68,73	1.57	6 (10%)	70,107,113	1.39	7 (10%)
22	CLA	d	403	-	65,73,73	1.46	8 (12%)	76,113,113	1.36	7 (9%)
31	BCR	c	516	-	41,41,41	1.23	2 (4%)	56,56,56	1.28	7 (12%)
33	SQD	a	411	-	53,54,54	0.97	5 (9%)	62,65,65	1.60	12 (19%)
22	CLA	C	509	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	7 (9%)
31	BCR	C	517	-	41,41,41	1.21	2 (4%)	56,56,56	1.29	7 (12%)
22	CLA	C	511	-	65,73,73	3.57	12 (18%)	76,113,113	2.58	17 (22%)
22	CLA	g	612	-	60,68,73	1.56	6 (10%)	70,107,113	1.39	7 (10%)
22	CLA	a	405	-	65,73,73	1.44	10 (15%)	76,113,113	1.37	6 (7%)
21	CHL	N	606	-	66,74,74	2.14	16 (24%)	73,114,114	2.47	19 (26%)
26	LHG	s	314	22	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
22	CLA	A	409	-	60,68,73	1.50	7 (11%)	70,107,113	1.46	8 (11%)
22	CLA	y	603	-	65,73,73	1.45	7 (10%)	76,113,113	1.34	7 (9%)
22	CLA	N	604	25	50,58,73	1.64	8 (16%)	58,95,113	1.59	7 (12%)
22	CLA	C	505	-	65,73,73	1.42	6 (9%)	76,113,113	1.44	6 (7%)
25	NEX	n	616	22	38,46,46	5.17	15 (39%)	50,70,70	8.46	26 (52%)
22	CLA	A	406	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	6 (7%)
35	DGD	A	401	-	60,60,67	0.88	2 (3%)	74,74,81	1.44	12 (16%)
36	LMG	d	410	-	46,46,55	0.81	3 (6%)	54,54,63	1.38	7 (12%)
22	CLA	Y	609	-	60,68,73	1.54	6 (10%)	70,107,113	1.43	7 (10%)
26	LHG	y	617	-	48,48,48	0.64	1 (2%)	51,54,54	1.29	7 (13%)
36	LMG	b	620	-	55,55,55	0.85	3 (5%)	63,63,63	1.36	9 (14%)
22	CLA	S	313	22	55,63,73	1.59	6 (10%)	64,101,113	1.49	6 (9%)
36	LMG	B	601	-	40,40,55	0.84	0	48,48,63	1.30	5 (10%)
22	CLA	n	609	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	6 (7%)
21	CHL	n	607	-	66,74,74	2.14	16 (24%)	73,114,114	2.47	19 (26%)
23	LUT	y	614	-	42,43,43	5.89	19 (45%)	51,60,60	5.45	25 (49%)
25	NEX	g	618	22	38,46,46	5.10	15 (39%)	50,70,70	8.41	27 (54%)
26	LHG	B	622	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	SQD	D	402	-	49,50,54	1.01	5 (10%)	58,61,65	1.56	10 (17%)
22	CLA	y	611	-	60,68,73	1.53	7 (11%)	70,107,113	1.40	7 (10%)
22	CLA	B	612	-	65,73,73	1.44	7 (10%)	76,113,113	1.39	7 (9%)
26	LHG	C	520	22	48,48,48	0.81	4 (8%)	51,54,54	1.30	7 (13%)
21	CHL	G	606	-	50,58,74	2.45	16 (32%)	52,94,114	2.81	17 (32%)
22	CLA	b	614	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	6 (7%)
22	CLA	D	405	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
22	CLA	y	602	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
21	CHL	r	306	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	G	604	-	50,58,73	1.64	8 (16%)	58,95,113	1.57	7 (12%)
21	CHL	G	605	-	46,54,74	2.55	16 (34%)	49,90,114	2.87	16 (32%)
32	PL9	a	410	-	13,13,55	1.57	2 (15%)	17,17,69	1.66	4 (23%)
35	DGD	C	519	-	63,63,67	0.93	3 (4%)	77,77,81	1.47	10 (12%)
22	CLA	G	613	1	65,73,73	1.80	12 (18%)	76,113,113	1.88	15 (19%)
22	CLA	y	612	1	65,73,73	1.80	12 (18%)	76,113,113	1.88	15 (19%)
36	LMG	M	101	-	51,51,55	0.75	1 (1%)	59,59,63	1.35	7 (11%)
21	CHL	y	609	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
23	LUT	g	615	-	42,43,43	5.88	19 (45%)	51,60,60	5.45	25 (49%)
25	NEX	Y	616	22	38,46,46	5.13	15 (39%)	50,70,70	8.19	27 (54%)
22	CLA	N	613	-	48,56,73	1.71	5 (10%)	55,92,113	1.50	8 (14%)
30	PHO	d	401	-	51,69,69	1.03	4 (7%)	47,99,99	1.17	6 (12%)
21	CHL	N	605	-	50,58,74	2.44	16 (32%)	52,94,114	2.81	17 (32%)
22	CLA	W	101	-	60,68,73	1.56	6 (10%)	70,107,113	1.39	7 (10%)
22	CLA	b	601	-	65,73,73	1.45	8 (12%)	76,113,113	1.37	7 (9%)
31	BCR	k	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
21	CHL	S	307	20	46,54,74	2.55	16 (34%)	49,90,114	2.87	16 (32%)
31	BCR	d	405	-	41,41,41	1.21	2 (4%)	56,56,56	1.24	7 (12%)
24	XAT	g	617	-	39,47,47	5.24	20 (51%)	54,74,74	13.43	29 (53%)
21	CHL	Y	607	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
21	CHL	R	305	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	C	512	-	65,73,73	1.47	9 (13%)	76,113,113	1.37	8 (10%)
22	CLA	R	302	-	60,68,73	1.53	5 (8%)	70,107,113	1.42	8 (11%)
22	CLA	g	610	-	64,72,73	1.50	6 (9%)	74,111,113	1.42	6 (8%)
22	CLA	b	611	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	6 (7%)
22	CLA	s	313	22	55,63,73	1.58	6 (10%)	64,101,113	1.50	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	LHG	D	409	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	6 (11%)
22	CLA	b	610	-	65,73,73	1.47	8 (12%)	76,113,113	1.38	7 (9%)
35	DGD	c	518	-	63,63,67	0.93	3 (4%)	77,77,81	1.47	10 (12%)
36	LMG	T	101	-	51,51,55	0.74	1 (1%)	59,59,63	1.35	7 (11%)
22	CLA	c	506	-	65,73,73	1.46	8 (12%)	76,113,113	1.37	7 (9%)
32	PL9	A	411	-	13,13,55	1.59	2 (15%)	17,17,69	1.64	4 (23%)
22	CLA	x	101	-	65,73,73	1.49	7 (10%)	76,113,113	1.36	8 (10%)
22	CLA	B	606	-	65,73,73	1.44	6 (9%)	76,113,113	1.39	7 (9%)
22	CLA	c	502	-	65,73,73	1.45	9 (13%)	76,113,113	1.35	6 (7%)
22	CLA	g	604	25	50,58,73	1.64	8 (16%)	58,95,113	1.57	8 (13%)
22	CLA	c	514	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	7 (9%)
22	CLA	C	507	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	7 (9%)
22	CLA	g	602	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	7 (9%)
21	CHL	S	302	-	46,54,74	2.55	17 (36%)	49,90,114	2.88	16 (32%)
26	LHG	C	521	-	48,48,48	0.61	1 (2%)	51,54,54	1.23	7 (13%)
31	BCR	B	620	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	6 (10%)
37	HEM	f	101	7	41,50,50	4.46	10 (24%)	45,82,82	3.70	22 (48%)
35	DGD	a	413	-	60,60,67	0.88	2 (3%)	74,74,81	1.44	12 (16%)
22	CLA	n	603	-	65,73,73	1.46	7 (10%)	76,113,113	1.36	7 (9%)
22	CLA	r	310	19	65,73,73	1.47	6 (9%)	76,113,113	1.40	6 (7%)
22	CLA	a	408	-	60,68,73	1.50	7 (11%)	70,107,113	1.45	8 (11%)
22	CLA	B	608	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
22	CLA	c	508	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	7 (9%)
22	CLA	b	608	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	6 (7%)
22	CLA	s	312	20	49,57,73	1.71	7 (14%)	55,93,113	1.51	6 (10%)
22	CLA	b	615	-	65,73,73	1.45	6 (9%)	76,113,113	1.35	7 (9%)
22	CLA	G	603	-	65,73,73	1.45	6 (9%)	76,113,113	1.35	7 (9%)
22	CLA	r	303	-	60,68,73	1.53	5 (8%)	70,107,113	1.41	8 (11%)
22	CLA	s	308	20	45,53,73	1.82	6 (13%)	52,89,113	1.55	7 (13%)
26	LHG	R	301	19	46,46,48	0.64	1 (2%)	49,52,54	1.28	7 (14%)
22	CLA	B	609	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	7 (9%)
22	CLA	S	304	20	45,53,73	1.80	6 (13%)	52,89,113	1.55	7 (13%)
22	CLA	G	602	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
22	CLA	N	603	-	65,73,73	1.46	7 (10%)	76,113,113	1.35	7 (9%)
21	CHL	n	605	-	50,58,74	2.45	16 (32%)	52,94,114	2.81	17 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	BCR	b	616	-	41,41,41	1.22	2 (4%)	56,56,56	1.23	7 (12%)
22	CLA	a	406	-	50,58,73	1.67	8 (16%)	58,95,113	1.51	8 (13%)
21	CHL	n	608	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	B	604	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	7 (9%)
33	SQD	d	402	-	49,50,54	1.01	5 (10%)	58,61,65	1.56	10 (17%)
22	CLA	c	507	-	65,73,73	1.44	7 (10%)	76,113,113	1.41	7 (9%)
22	CLA	c	503	-	65,73,73	1.43	8 (12%)	76,113,113	1.39	8 (10%)
22	CLA	b	602	-	65,73,73	1.43	8 (12%)	76,113,113	1.40	8 (10%)
22	CLA	b	609	-	65,73,73	1.44	7 (10%)	76,113,113	1.39	7 (9%)
22	CLA	B	615	-	65,73,73	1.46	6 (9%)	76,113,113	1.36	6 (7%)
22	CLA	g	613	1	65,73,73	1.80	11 (16%)	76,113,113	1.89	15 (19%)
26	LHG	l	102	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	7 (13%)
21	CHL	R	306	-	56,64,74	2.31	17 (30%)	61,102,114	2.67	19 (31%)
26	LHG	d	408	-	48,48,48	0.63	1 (2%)	51,54,54	1.29	6 (11%)
22	CLA	g	614	-	48,56,73	1.71	6 (12%)	55,92,113	1.51	8 (14%)
21	CHL	G	609	-	61,69,74	2.21	16 (26%)	67,108,114	2.57	19 (28%)
33	SQD	l	101	-	41,42,54	1.08	5 (12%)	50,53,65	1.61	9 (18%)
22	CLA	A	407	-	50,58,73	1.67	8 (16%)	58,95,113	1.50	8 (13%)
22	CLA	D	404	-	65,73,73	1.46	8 (12%)	76,113,113	1.36	7 (9%)
22	CLA	b	613	-	65,73,73	1.45	7 (10%)	76,113,113	1.39	7 (9%)
22	CLA	y	613	-	48,56,73	1.71	5 (10%)	55,92,113	1.50	8 (14%)
26	LHG	N	618	-	48,48,48	0.63	1 (2%)	51,54,54	1.23	7 (13%)
21	CHL	r	307	-	56,64,74	2.32	17 (30%)	61,102,114	2.68	19 (31%)
21	CHL	y	601	1	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
31	BCR	B	602	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	6 (10%)
23	LUT	G	616	-	42,43,43	6.08	19 (45%)	51,60,60	4.93	22 (43%)
22	CLA	C	510	-	65,73,73	1.47	8 (12%)	76,113,113	1.37	8 (10%)
22	CLA	R	308	-	58,66,73	1.57	7 (12%)	67,104,113	1.42	7 (10%)
22	CLA	N	611	-	60,68,73	1.58	6 (10%)	70,107,113	1.40	7 (10%)
21	CHL	Y	601	1	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	c	505	-	65,73,73	1.45	7 (10%)	76,113,113	1.46	7 (9%)
22	CLA	B	617	-	65,73,73	1.46	7 (10%)	76,113,113	1.38	6 (7%)
21	CHL	s	301	-	48,56,74	2.50	16 (33%)	51,92,114	2.83	17 (33%)
22	CLA	c	504	-	65,73,73	1.43	7 (10%)	76,113,113	1.44	6 (7%)
32	PL9	d	406	-	55,55,55	1.33	4 (7%)	68,69,69	1.54	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	n	610	26	60,68,73	1.53	6 (10%)	70,107,113	1.40	7 (10%)
22	CLA	y	604	25	50,58,73	1.64	8 (16%)	58,95,113	1.57	7 (12%)
26	LHG	n	617	22	48,48,48	0.64	1 (2%)	51,54,54	1.29	7 (13%)
37	HEM	F	101	7	41,50,50	4.46	10 (24%)	45,82,82	3.69	22 (48%)
22	CLA	b	606	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	7 (9%)
31	BCR	c	515	-	41,41,41	1.23	2 (4%)	56,56,56	1.24	5 (8%)
22	CLA	Y	611	1	65,73,73	1.80	12 (18%)	76,113,113	1.89	15 (19%)
26	LHG	c	520	22	48,48,48	0.81	4 (8%)	51,54,54	1.30	7 (13%)
21	CHL	r	308	19	61,69,74	2.22	16 (26%)	67,108,114	2.57	19 (28%)
24	XAT	Y	615	-	39,47,47	5.30	20 (51%)	54,74,74	13.38	30 (55%)
23	LUT	Y	613	-	42,43,43	5.87	19 (45%)	51,60,60	5.44	25 (49%)
22	CLA	Y	610	26	60,68,73	1.53	7 (11%)	70,107,113	1.40	7 (10%)
21	CHL	G	608	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	C	514	22	65,73,73	1.44	8 (12%)	76,113,113	1.31	6 (7%)
26	LHG	D	410	-	42,42,48	0.67	1 (2%)	45,48,54	1.26	5 (11%)
22	CLA	S	312	20	49,57,73	1.70	7 (14%)	55,93,113	1.50	6 (10%)
22	CLA	r	311	23,19	49,57,73	1.74	7 (14%)	55,93,113	1.43	4 (7%)
22	CLA	b	605	-	65,73,73	1.44	6 (9%)	76,113,113	1.38	7 (9%)
26	LHG	Y	617	22	48,48,48	0.66	1 (2%)	51,54,54	1.26	7 (13%)
33	SQD	L	102	-	41,42,54	1.08	5 (12%)	50,53,65	1.61	9 (18%)
22	CLA	r	305	-	48,56,73	1.71	7 (14%)	55,92,113	1.52	8 (14%)
21	CHL	s	302	-	46,54,74	2.56	16 (34%)	49,90,114	2.87	16 (32%)
35	DGD	c	519	-	61,61,67	0.98	5 (8%)	75,75,81	1.53	10 (13%)
22	CLA	n	602	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
26	LHG	d	409	-	42,42,48	0.67	1 (2%)	45,48,54	1.26	5 (11%)
22	CLA	r	309	-	58,66,73	1.56	8 (13%)	67,104,113	1.42	7 (10%)
23	LUT	N	615	-	42,43,43	6.10	20 (47%)	51,60,60	4.66	27 (52%)
35	DGD	C	518	-	56,56,67	0.99	3 (5%)	70,70,81	1.56	13 (18%)
36	LMG	B	623	-	55,55,55	0.85	3 (5%)	63,63,63	1.36	9 (14%)
22	CLA	g	611	-	60,68,73	1.53	7 (11%)	70,107,113	1.40	8 (11%)
31	BCR	b	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	3 (5%)
22	CLA	B	607	-	65,73,73	1.45	9 (13%)	76,113,113	1.37	6 (7%)
21	CHL	s	306	20	46,54,74	2.55	16 (34%)	49,90,114	2.88	16 (32%)
35	DGD	c	517	-	56,56,67	1.00	4 (7%)	70,70,81	1.56	12 (17%)
25	NEX	r	315	-	38,46,46	5.12	16 (42%)	50,70,70	7.87	27 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	LUT	n	614	-	42,43,43	5.88	19 (45%)	51,60,60	5.44	25 (49%)
22	CLA	R	311	19	60,68,73	1.52	6 (10%)	70,107,113	1.40	6 (8%)
34	BCT	a	412	-	2,3,3	1.33	0	2,3,3	2.75	2 (100%)
22	CLA	R	303	-	60,68,73	1.53	6 (10%)	70,107,113	1.42	7 (10%)
30	PHO	a	407	-	51,69,69	1.06	5 (9%)	47,99,99	1.11	4 (8%)
31	BCR	k	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.25	8 (14%)
22	CLA	B	603	-	65,73,73	1.48	8 (12%)	76,113,113	1.35	8 (10%)
21	CHL	S	306	20	46,54,74	2.55	16 (34%)	49,90,114	2.87	16 (32%)
26	LHG	r	302	19	46,46,48	0.64	1 (2%)	49,52,54	1.28	7 (14%)
26	LHG	S	314	22	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
26	LHG	b	619	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
22	CLA	B	613	-	65,73,73	1.47	9 (13%)	76,113,113	1.38	7 (9%)
23	LUT	Y	614	-	42,43,43	6.05	20 (47%)	51,60,60	4.89	22 (43%)
22	CLA	Y	604	25	50,58,73	1.63	8 (16%)	58,95,113	1.58	8 (13%)
22	CLA	G	614	-	48,56,73	1.70	5 (10%)	55,92,113	1.51	8 (14%)
23	LUT	N	614	-	42,43,43	5.88	19 (45%)	51,60,60	5.44	25 (49%)
22	CLA	r	304	-	60,68,73	1.53	6 (10%)	70,107,113	1.42	7 (10%)
31	BCR	B	619	-	41,41,41	1.21	2 (4%)	56,56,56	1.23	7 (12%)
36	LMG	C	523	-	51,51,55	0.72	1 (1%)	59,59,63	1.38	7 (11%)
22	CLA	r	312	19	60,68,73	1.53	6 (10%)	70,107,113	1.42	6 (8%)
22	CLA	A	405	-	65,73,73	1.46	8 (12%)	76,113,113	1.41	7 (9%)
22	CLA	Y	602	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	9 (11%)
36	LMG	I	101	-	40,40,55	0.85	0	48,48,63	1.30	5 (10%)
31	BCR	A	410	-	41,41,41	1.22	2 (4%)	56,56,56	1.26	7 (12%)
25	NEX	y	618	-	38,46,46	5.13	16 (42%)	50,70,70	7.86	27 (54%)
22	CLA	B	618	-	65,73,73	1.46	6 (9%)	76,113,113	1.34	7 (9%)
22	CLA	C	503	-	65,73,73	1.46	9 (13%)	76,113,113	1.35	6 (7%)
22	CLA	s	304	20	45,53,73	1.80	6 (13%)	52,89,113	1.54	7 (13%)
31	BCR	B	621	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	3 (5%)
25	NEX	y	616	22	38,46,46	5.17	14 (36%)	50,70,70	8.58	27 (54%)
23	LUT	g	616	-	42,43,43	6.10	19 (45%)	51,60,60	4.92	22 (43%)
26	LHG	d	407	-	45,45,48	0.64	1 (2%)	48,51,54	1.23	4 (8%)
31	BCR	H	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.30	6 (10%)
22	CLA	C	504	-	65,73,73	1.44	7 (10%)	76,113,113	1.39	8 (10%)
22	CLA	b	607	-	65,73,73	1.44	7 (10%)	76,113,113	1.42	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	S	305	20	50,58,73	1.66	6 (12%)	58,95,113	1.60	8 (13%)
30	PHO	A	408	-	51,69,69	1.07	5 (9%)	47,99,99	1.12	4 (8%)
22	CLA	n	612	1	60,68,73	1.87	12 (20%)	70,107,113	1.95	14 (20%)
22	CLA	n	613	-	48,56,73	1.71	6 (12%)	55,92,113	1.51	8 (14%)
21	CHL	s	307	20	46,54,74	2.55	16 (34%)	49,90,114	2.88	16 (32%)
31	BCR	a	409	-	41,41,41	1.22	2 (4%)	56,56,56	1.26	7 (12%)
22	CLA	g	603	-	65,73,73	1.46	6 (9%)	76,113,113	1.35	7 (9%)
22	CLA	s	310	26	55,63,73	1.57	7 (12%)	64,101,113	1.47	7 (10%)
22	CLA	C	508	-	65,73,73	1.44	7 (10%)	76,113,113	1.40	6 (7%)
32	PL9	D	407	-	55,55,55	1.34	5 (9%)	68,69,69	1.54	13 (19%)
31	BCR	b	617	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	6 (10%)
31	BCR	T	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
22	CLA	G	612	-	60,68,73	1.58	6 (10%)	70,107,113	1.39	7 (10%)
24	XAT	n	615	-	39,47,47	5.22	20 (51%)	54,74,74	13.59	30 (55%)
26	LHG	c	522	-	48,48,48	0.60	1 (2%)	51,54,54	1.29	8 (15%)
22	CLA	B	616	-	65,73,73	1.44	7 (10%)	76,113,113	1.39	7 (9%)
22	CLA	S	310	26	55,63,73	1.58	7 (12%)	64,101,113	1.47	7 (10%)
22	CLA	Y	612	-	48,56,73	1.70	6 (12%)	55,92,113	1.51	8 (14%)
22	CLA	G	611	-	60,68,73	1.53	7 (11%)	70,107,113	1.41	7 (10%)
21	CHL	R	307	19	61,69,74	2.22	17 (27%)	67,108,114	2.57	19 (28%)
22	CLA	N	612	1	60,68,73	1.88	12 (20%)	70,107,113	1.95	15 (21%)
22	CLA	B	614	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	6 (7%)
24	XAT	G	617	-	39,47,47	5.24	20 (51%)	54,74,74	13.43	30 (55%)
22	CLA	G	610	-	64,72,73	1.50	6 (9%)	74,111,113	1.44	8 (10%)
22	CLA	n	604	25	50,58,73	1.64	8 (16%)	58,95,113	1.57	8 (13%)
22	CLA	R	304	-	48,56,73	1.70	7 (14%)	55,92,113	1.52	8 (14%)
21	CHL	Y	605	-	50,58,74	2.45	16 (32%)	52,94,114	2.81	17 (32%)
21	CHL	Y	608	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
35	DGD	H	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.48	14 (18%)
31	BCR	K	102	-	41,41,41	1.19	2 (4%)	56,56,56	1.26	8 (14%)
22	CLA	N	609	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	6 (7%)
33	SQD	L	101	12	53,54,54	0.97	5 (9%)	62,65,65	1.61	11 (17%)
22	CLA	c	509	-	65,73,73	1.47	9 (13%)	76,113,113	1.36	8 (10%)
35	DGD	h	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.48	14 (18%)
21	CHL	G	607	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CHL	r	301	19	48,56,74	2.49	16 (33%)	51,92,114	2.83	17 (33%)
27	OEX	a	401	2,4	0,15,15	-	-	-		
24	XAT	y	615	-	39,47,47	5.28	20 (51%)	54,74,74	13.37	29 (53%)
27	OEX	A	402	2,4	0,15,15	-	-	-		
33	SQD	A	412	-	53,54,54	0.97	5 (9%)	62,65,65	1.60	12 (19%)
22	CLA	S	308	20	45,53,73	1.82	6 (13%)	52,89,113	1.54	7 (13%)
36	LMG	c	523	-	51,51,55	0.72	1 (1%)	59,59,63	1.38	7 (11%)
22	CLA	w	101	16	60,68,73	1.57	6 (10%)	70,107,113	1.39	7 (10%)
22	CLA	b	603	-	65,73,73	1.44	7 (10%)	76,113,113	1.38	7 (9%)
33	SQD	l	103	12	53,54,54	0.97	5 (9%)	62,65,65	1.61	11 (17%)
21	CHL	g	609	-	61,69,74	2.22	16 (26%)	67,108,114	2.57	19 (28%)
36	LMG	K	103	-	51,51,55	0.72	0	59,59,63	1.34	6 (10%)
22	CLA	c	510	-	65,73,73	3.57	12 (18%)	76,113,113	2.58	18 (23%)
22	CLA	b	604	-	65,73,73	1.45	9 (13%)	76,113,113	1.36	6 (7%)
23	LUT	G	615	-	42,43,43	5.88	19 (45%)	51,60,60	5.45	25 (49%)
21	CHL	g	607	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
26	LHG	L	103	-	48,48,48	0.63	1 (2%)	51,54,54	1.29	7 (13%)
21	CHL	n	601	1	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	N	610	-	60,68,73	1.52	6 (10%)	70,107,113	1.40	8 (11%)
22	CLA	B	611	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	6 (7%)
24	XAT	R	313	-	39,47,47	5.20	17 (43%)	54,74,74	13.47	28 (51%)
22	CLA	C	513	4	65,73,73	1.46	7 (10%)	76,113,113	1.42	8 (10%)
26	LHG	g	619	-	48,48,48	0.61	1 (2%)	51,54,54	1.30	8 (15%)
21	CHL	N	607	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	s	303	20	61,69,73	1.54	7 (11%)	71,108,113	1.43	8 (11%)
21	CHL	Y	606	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
21	CHL	S	301	-	48,56,74	2.50	16 (33%)	51,92,114	2.84	17 (33%)
22	CLA	B	610	-	65,73,73	1.43	7 (10%)	76,113,113	1.42	8 (10%)
25	NEX	N	617	22	38,46,46	5.17	15 (39%)	50,70,70	8.67	26 (52%)
21	CHL	G	601	1	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	C	506	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	7 (9%)
35	DGD	J	101	-	61,61,67	0.98	5 (8%)	75,75,81	1.53	10 (13%)
23	LUT	r	313	22	42,43,43	5.90	19 (45%)	51,60,60	5.16	28 (54%)
22	CLA	C	515	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	7 (9%)
26	LHG	D	408	-	45,45,48	0.65	1 (2%)	48,51,54	1.23	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	PHO	D	401	-	51,69,69	1.02	4 (7%)	47,99,99	1.17	5 (10%)
22	CLA	S	303	20	61,69,73	1.54	6 (9%)	71,108,113	1.43	8 (11%)
34	BCT	D	403	-	2,3,3	1.33	0	2,3,3	2.74	2 (100%)
36	LMG	k	103	-	51,51,55	0.73	0	59,59,63	1.34	6 (10%)

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
31	BCR	h	101	-	-	7/29/63/63	0/2/2/2
22	CLA	N	602	-	1/1/15/20	13/37/115/115	-
21	CHL	N	601	1	4/4/20/26	24/39/137/137	-
24	XAT	N	616	-	2/2/12/26	17/31/93/93	0/4/4/4
36	LMG	D	411	-	-	12/41/61/70	0/1/1/1
21	CHL	n	606	-	4/4/20/26	18/39/137/137	-
22	CLA	c	512	4	1/1/15/20	14/37/115/115	-
36	LMG	w	102	-	-	16/43/63/70	0/1/1/1
21	CHL	y	605	-	3/3/16/26	11/18/116/137	-
22	CLA	b	612	-	1/1/15/20	8/37/115/115	-
21	CHL	g	608	-	4/4/20/26	23/39/137/137	-
21	CHL	g	601	1	4/4/20/26	24/39/137/137	-
22	CLA	B	605	-	1/1/15/20	13/37/115/115	-
31	BCR	K	101	-	-	16/29/63/63	0/2/2/2
22	CLA	a	404	-	1/1/15/20	4/37/115/115	-
22	CLA	S	311	22,20	1/1/13/20	13/27/105/115	-
21	CHL	g	605	-	3/3/16/26	9/15/113/137	-
21	CHL	y	606	-	3/3/16/26	13/20/118/137	-
21	CHL	N	608	-	4/4/20/26	15/39/137/137	-
22	CLA	c	513	22	1/1/15/20	21/37/115/115	-
22	CLA	Y	603	-	1/1/15/20	17/37/115/115	-
21	CHL	g	606	-	3/3/16/26	13/20/118/137	-
22	CLA	y	610	-	1/1/14/20	15/31/109/115	-
26	LHG	G	618	-	-	28/53/53/53	-
22	CLA	R	309	19	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	y	608	-	4/4/20/26	23/39/137/137	-
22	CLA	s	305	20	1/1/12/20	9/19/97/115	-
22	CLA	R	310	23,19	1/1/11/20	11/18/96/115	-
26	LHG	c	521	-	-	21/53/53/53	-
26	LHG	C	522	-	-	24/53/53/53	-
22	CLA	s	311	22,20	1/1/13/20	13/27/105/115	-
22	CLA	s	309	22,20	1/1/13/20	7/25/103/115	-
24	XAT	r	314	-	1/1/12/26	14/31/93/93	0/4/4/4
21	CHL	y	607	-	4/4/20/26	18/39/137/137	-
23	LUT	R	312	22	-	18/29/67/67	0/2/2/2
36	LMG	C	502	-	-	16/43/63/70	0/1/1/1
31	BCR	D	406	-	-	8/29/63/63	0/2/2/2
31	BCR	C	516	-	-	5/29/63/63	0/2/2/2
22	CLA	c	511	-	1/1/15/20	14/37/115/115	-
22	CLA	S	309	22,20	1/1/13/20	7/25/103/115	-
22	CLA	d	404	-	1/1/15/20	12/37/115/115	-
22	CLA	n	611	-	1/1/14/20	12/31/109/115	-
22	CLA	d	403	-	1/1/15/20	13/37/115/115	-
31	BCR	c	516	-	-	6/29/63/63	0/2/2/2
33	SQD	a	411	-	-	23/49/69/69	0/1/1/1
22	CLA	C	509	-	1/1/15/20	12/37/115/115	-
31	BCR	C	517	-	-	6/29/63/63	0/2/2/2
22	CLA	C	511	-	1/1/15/20	11/37/115/115	-
22	CLA	g	612	-	1/1/14/20	12/31/109/115	-
22	CLA	a	405	-	1/1/15/20	15/37/115/115	-
21	CHL	N	606	-	4/4/20/26	18/39/137/137	-
26	LHG	s	314	22	-	29/53/53/53	-
22	CLA	A	409	-	1/1/14/20	3/31/109/115	-
22	CLA	y	603	-	1/1/15/20	17/37/115/115	-
22	CLA	N	604	25	1/1/12/20	6/19/97/115	-
22	CLA	C	505	-	1/1/15/20	14/37/115/115	-
25	NEX	n	616	22	2/2/12/25	16/27/83/83	0/3/3/3
22	CLA	A	406	-	1/1/15/20	15/37/115/115	-
35	DGD	A	401	-	-	21/48/88/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMG	d	410	-	-	11/41/61/70	0/1/1/1
22	CLA	Y	609	-	1/1/14/20	15/31/109/115	-
26	LHG	y	617	-	-	22/53/53/53	-
36	LMG	b	620	-	-	22/50/70/70	0/1/1/1
22	CLA	S	313	22	1/1/13/20	12/25/103/115	-
36	LMG	B	601	-	-	18/35/55/70	0/1/1/1
22	CLA	n	609	-	1/1/15/20	18/37/115/115	-
21	CHL	n	607	-	4/4/20/26	23/39/137/137	-
25	NEX	g	618	22	2/2/12/25	15/27/83/83	0/3/3/3
23	LUT	y	614	-	-	17/29/67/67	0/2/2/2
26	LHG	B	622	-	-	28/53/53/53	-
33	SQD	D	402	-	1/1/9/9	18/45/65/69	0/1/1/1
22	CLA	y	611	-	1/1/14/20	8/31/109/115	-
22	CLA	B	612	-	1/1/15/20	11/37/115/115	-
26	LHG	C	520	22	-	31/53/53/53	-
21	CHL	G	606	-	3/3/16/26	13/20/118/137	-
22	CLA	b	614	-	1/1/15/20	20/37/115/115	-
22	CLA	D	405	-	1/1/15/20	12/37/115/115	-
22	CLA	y	602	-	1/1/15/20	13/37/115/115	-
21	CHL	r	306	-	4/4/20/26	20/39/137/137	-
22	CLA	G	604	-	1/1/12/20	6/19/97/115	-
21	CHL	G	605	-	3/3/16/26	9/15/113/137	-
32	PL9	a	410	-	-	3/5/18/73	0/1/1/1
35	DGD	C	519	-	-	26/51/91/95	0/2/2/2
22	CLA	G	613	1	1/1/15/20	20/37/115/115	-
22	CLA	y	612	1	1/1/15/20	20/37/115/115	-
36	LMG	M	101	-	-	23/46/66/70	0/1/1/1
21	CHL	y	609	-	4/4/20/26	14/39/137/137	-
23	LUT	g	615	-	-	17/29/67/67	0/2/2/2
25	NEX	Y	616	22	2/2/12/25	14/27/83/83	0/3/3/3
22	CLA	N	613	-	1/1/11/20	9/17/95/115	-
30	PHO	d	401	-	-	15/37/103/103	0/5/6/6
21	CHL	N	605	-	3/3/16/26	13/20/118/137	-
22	CLA	W	101	-	1/1/14/20	12/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	601	-	1/1/15/20	18/37/115/115	-
31	BCR	k	101	-	-	16/29/63/63	0/2/2/2
21	CHL	S	307	20	3/3/16/26	12/15/113/137	-
31	BCR	d	405	-	-	8/29/63/63	0/2/2/2
24	XAT	g	617	-	2/2/12/26	17/31/93/93	0/4/4/4
21	CHL	Y	607	-	4/4/20/26	23/39/137/137	-
21	CHL	R	305	-	4/4/20/26	20/39/137/137	-
22	CLA	C	512	-	1/1/15/20	14/37/115/115	-
22	CLA	R	302	-	1/1/14/20	8/31/109/115	-
22	CLA	g	610	-	1/1/14/20	16/36/114/115	-
22	CLA	b	611	-	1/1/15/20	17/37/115/115	-
22	CLA	s	313	22	1/1/13/20	12/25/103/115	-
26	LHG	D	409	-	-	21/53/53/53	-
22	CLA	b	610	-	1/1/15/20	13/37/115/115	-
35	DGD	c	518	-	-	26/51/91/95	0/2/2/2
36	LMG	T	101	-	-	23/46/66/70	0/1/1/1
22	CLA	c	506	-	1/1/15/20	14/37/115/115	-
32	PL9	A	411	-	-	3/5/18/73	0/1/1/1
22	CLA	x	101	-	1/1/15/20	16/37/115/115	-
22	CLA	B	606	-	1/1/15/20	12/37/115/115	-
22	CLA	c	502	-	1/1/15/20	18/37/115/115	-
22	CLA	g	604	25	1/1/12/20	6/19/97/115	-
22	CLA	c	514	-	1/1/15/20	16/37/115/115	-
22	CLA	C	507	-	1/1/15/20	14/37/115/115	-
22	CLA	g	602	-	1/1/15/20	13/37/115/115	-
21	CHL	S	302	-	3/3/16/26	9/15/113/137	-
26	LHG	C	521	-	-	21/53/53/53	-
31	BCR	B	620	-	-	7/29/63/63	0/2/2/2
37	HEM	f	101	7	-	4/12/54/54	-
35	DGD	a	413	-	-	21/48/88/95	0/2/2/2
22	CLA	n	603	-	1/1/15/20	17/37/115/115	-
22	CLA	r	310	19	1/1/15/20	18/37/115/115	-
22	CLA	a	408	-	1/1/14/20	3/31/109/115	-
22	CLA	B	608	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	508	-	1/1/15/20	12/37/115/115	-
22	CLA	b	608	-	1/1/15/20	7/37/115/115	-
22	CLA	s	312	20	1/1/11/20	7/18/96/115	-
22	CLA	b	615	-	1/1/15/20	12/37/115/115	-
22	CLA	G	603	-	1/1/15/20	17/37/115/115	-
22	CLA	r	303	-	1/1/14/20	8/31/109/115	-
22	CLA	s	308	20	-	8/13/91/115	-
26	LHG	R	301	19	-	27/51/51/53	-
22	CLA	B	609	-	1/1/15/20	6/37/115/115	-
22	CLA	S	304	20	1/1/11/20	7/13/91/115	-
22	CLA	G	602	-	1/1/15/20	13/37/115/115	-
22	CLA	N	603	-	1/1/15/20	17/37/115/115	-
21	CHL	n	605	-	3/3/16/26	13/20/118/137	-
31	BCR	b	616	-	-	7/29/63/63	0/2/2/2
22	CLA	a	406	-	1/1/12/20	8/19/97/115	-
21	CHL	n	608	-	4/4/20/26	15/39/137/137	-
22	CLA	B	604	-	1/1/15/20	18/37/115/115	-
33	SQD	d	402	-	1/1/9/9	18/45/65/69	0/1/1/1
22	CLA	c	507	-	1/1/15/20	10/37/115/115	-
22	CLA	c	503	-	1/1/15/20	17/37/115/115	-
22	CLA	b	602	-	1/1/15/20	13/37/115/115	-
22	CLA	b	609	-	1/1/15/20	11/37/115/115	-
22	CLA	B	615	-	1/1/15/20	8/37/115/115	-
22	CLA	g	613	1	1/1/15/20	18/37/115/115	-
26	LHG	l	102	-	-	19/53/53/53	-
21	CHL	R	306	-	4/4/18/26	16/27/125/137	-
26	LHG	d	408	-	-	21/53/53/53	-
22	CLA	g	614	-	1/1/11/20	9/17/95/115	-
21	CHL	G	609	-	4/4/19/26	10/33/131/137	-
33	SQD	l	101	-	-	13/37/57/69	0/1/1/1
22	CLA	A	407	-	1/1/12/20	8/19/97/115	-
22	CLA	D	404	-	1/1/15/20	13/37/115/115	-
22	CLA	b	613	-	1/1/15/20	14/37/115/115	-
22	CLA	y	613	-	1/1/11/20	9/17/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	N	618	-	-	29/53/53/53	-
21	CHL	r	307	-	4/4/18/26	16/27/125/137	-
21	CHL	y	601	1	4/4/20/26	24/39/137/137	-
31	BCR	B	602	-	-	20/29/63/63	0/2/2/2
23	LUT	G	616	-	-	16/29/67/67	0/2/2/2
22	CLA	C	510	-	1/1/15/20	13/37/115/115	-
22	CLA	R	308	-	1/1/13/20	9/29/107/115	-
22	CLA	N	611	-	1/1/14/20	12/31/109/115	-
21	CHL	Y	601	1	4/4/20/26	24/39/137/137	-
22	CLA	c	505	-	1/1/15/20	8/37/115/115	-
22	CLA	B	617	-	1/1/15/20	20/37/115/115	-
21	CHL	s	301	-	3/3/16/26	10/18/116/137	-
22	CLA	c	504	-	1/1/15/20	14/37/115/115	-
32	PL9	d	406	-	-	17/53/73/73	0/1/1/1
22	CLA	n	610	26	1/1/14/20	8/31/109/115	-
22	CLA	y	604	25	1/1/12/20	6/19/97/115	-
26	LHG	n	617	22	-	25/53/53/53	-
37	HEM	F	101	7	-	4/12/54/54	-
22	CLA	b	606	-	1/1/15/20	6/37/115/115	-
31	BCR	c	515	-	-	5/29/63/63	0/2/2/2
22	CLA	Y	611	1	1/1/15/20	18/37/115/115	-
26	LHG	c	520	22	-	31/53/53/53	-
21	CHL	r	308	19	4/4/19/26	17/33/131/137	-
24	XAT	Y	615	-	2/2/12/26	18/31/93/93	0/4/4/4
23	LUT	Y	613	-	-	17/29/67/67	0/2/2/2
22	CLA	Y	610	26	1/1/14/20	8/31/109/115	-
21	CHL	G	608	-	4/4/20/26	23/39/137/137	-
22	CLA	C	514	22	1/1/15/20	21/37/115/115	-
26	LHG	D	410	-	-	19/47/47/53	-
22	CLA	S	312	20	1/1/11/20	7/18/96/115	-
22	CLA	r	311	23,19	1/1/11/20	11/18/96/115	-
22	CLA	b	605	-	1/1/15/20	10/37/115/115	-
26	LHG	Y	617	22	-	29/53/53/53	-
33	SQD	L	102	-	-	13/37/57/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	r	305	-	1/1/11/20	7/17/95/115	-
21	CHL	s	302	-	3/3/16/26	9/15/113/137	-
35	DGD	c	519	-	-	16/49/89/95	0/2/2/2
22	CLA	n	602	-	1/1/15/20	13/37/115/115	-
26	LHG	d	409	-	-	19/47/47/53	-
22	CLA	r	309	-	1/1/13/20	9/29/107/115	-
23	LUT	N	615	-	-	15/29/67/67	0/2/2/2
35	DGD	C	518	-	-	18/44/84/95	0/2/2/2
36	LMG	B	623	-	-	22/50/70/70	0/1/1/1
22	CLA	g	611	-	1/1/14/20	8/31/109/115	-
31	BCR	b	618	-	-	5/29/63/63	0/2/2/2
22	CLA	B	607	-	1/1/15/20	15/37/115/115	-
21	CHL	s	306	20	3/3/16/26	10/15/113/137	-
35	DGD	c	517	-	-	18/44/84/95	0/2/2/2
25	NEX	r	315	-	2/2/12/25	14/27/83/83	0/3/3/3
23	LUT	n	614	-	-	17/29/67/67	0/2/2/2
22	CLA	R	311	19	1/1/14/20	12/31/109/115	-
22	CLA	R	303	-	1/1/14/20	9/31/109/115	-
30	PHO	a	407	-	-	13/37/103/103	0/5/6/6
31	BCR	k	102	-	-	5/29/63/63	0/2/2/2
22	CLA	B	603	-	1/1/15/20	16/37/115/115	-
21	CHL	S	306	20	3/3/16/26	10/15/113/137	-
26	LHG	r	302	19	-	27/51/51/53	-
26	LHG	S	314	22	-	29/53/53/53	-
26	LHG	b	619	-	-	28/53/53/53	-
22	CLA	B	613	-	1/1/15/20	13/37/115/115	-
23	LUT	Y	614	-	-	14/29/67/67	0/2/2/2
22	CLA	Y	604	25	1/1/12/20	6/19/97/115	-
22	CLA	G	614	-	1/1/11/20	9/17/95/115	-
23	LUT	N	614	-	-	17/29/67/67	0/2/2/2
22	CLA	r	304	-	1/1/14/20	9/31/109/115	-
31	BCR	B	619	-	-	7/29/63/63	0/2/2/2
36	LMG	C	523	-	-	20/46/66/70	0/1/1/1
22	CLA	r	312	19	1/1/14/20	12/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	405	-	1/1/15/20	4/37/115/115	-
22	CLA	Y	602	-	1/1/15/20	13/37/115/115	-
36	LMG	I	101	-	-	18/35/55/70	0/1/1/1
31	BCR	A	410	-	-	5/29/63/63	0/2/2/2
25	NEX	y	618	-	2/2/12/25	14/27/83/83	0/3/3/3
22	CLA	B	618	-	1/1/15/20	12/37/115/115	-
22	CLA	C	503	-	1/1/15/20	18/37/115/115	-
22	CLA	s	304	20	1/1/11/20	7/13/91/115	-
31	BCR	B	621	-	-	5/29/63/63	0/2/2/2
25	NEX	y	616	22	2/2/12/25	15/27/83/83	0/3/3/3
23	LUT	g	616	-	-	15/29/67/67	0/2/2/2
26	LHG	d	407	-	-	25/50/50/53	-
31	BCR	H	101	-	-	7/29/63/63	0/2/2/2
22	CLA	C	504	-	1/1/15/20	17/37/115/115	-
22	CLA	b	607	-	1/1/15/20	13/37/115/115	-
22	CLA	S	305	20	1/1/12/20	9/19/97/115	-
30	PHO	A	408	-	-	13/37/103/103	0/5/6/6
22	CLA	n	612	1	1/1/14/20	16/31/109/115	-
22	CLA	n	613	-	1/1/11/20	9/17/95/115	-
21	CHL	s	307	20	3/3/16/26	12/15/113/137	-
31	BCR	a	409	-	-	5/29/63/63	0/2/2/2
22	CLA	g	603	-	1/1/15/20	17/37/115/115	-
22	CLA	s	310	26	1/1/13/20	16/25/103/115	-
22	CLA	C	508	-	1/1/15/20	10/37/115/115	-
32	PL9	D	407	-	-	17/53/73/73	0/1/1/1
31	BCR	b	617	-	-	7/29/63/63	0/2/2/2
31	BCR	T	102	-	-	21/29/63/63	0/2/2/2
22	CLA	G	612	-	1/1/14/20	12/31/109/115	-
24	XAT	n	615	-	2/2/12/26	16/31/93/93	0/4/4/4
26	LHG	c	522	-	-	23/53/53/53	-
22	CLA	B	616	-	1/1/15/20	14/37/115/115	-
22	CLA	S	310	26	1/1/13/20	16/25/103/115	-
22	CLA	Y	612	-	1/1/11/20	9/17/95/115	-
22	CLA	G	611	-	1/1/14/20	8/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	R	307	19	4/4/19/26	17/33/131/137	-
22	CLA	N	612	1	1/1/14/20	16/31/109/115	-
22	CLA	B	614	-	1/1/15/20	17/37/115/115	-
24	XAT	G	617	-	3/3/12/26	17/31/93/93	0/4/4/4
22	CLA	G	610	-	1/1/14/20	19/36/114/115	-
22	CLA	n	604	25	1/1/12/20	6/19/97/115	-
22	CLA	R	304	-	1/1/11/20	7/17/95/115	-
21	CHL	Y	605	-	3/3/16/26	13/20/118/137	-
21	CHL	Y	608	-	4/4/20/26	12/39/137/137	-
35	DGD	H	102	-	-	19/51/91/95	0/2/2/2
31	BCR	K	102	-	-	6/29/63/63	0/2/2/2
22	CLA	N	609	-	1/1/15/20	16/37/115/115	-
33	SQD	L	101	12	-	18/49/69/69	0/1/1/1
22	CLA	c	509	-	1/1/15/20	13/37/115/115	-
35	DGD	h	102	-	-	19/51/91/95	0/2/2/2
21	CHL	G	607	-	4/4/20/26	18/39/137/137	-
21	CHL	r	301	19	3/3/16/26	8/18/116/137	-
24	XAT	y	615	-	2/2/12/26	18/31/93/93	0/4/4/4
33	SQD	A	412	-	-	23/49/69/69	0/1/1/1
22	CLA	S	308	20	-	8/13/91/115	-
36	LMG	c	523	-	-	20/46/66/70	0/1/1/1
22	CLA	w	101	16	1/1/14/20	12/31/109/115	-
22	CLA	b	603	-	1/1/15/20	12/37/115/115	-
33	SQD	l	103	12	-	18/49/69/69	0/1/1/1
21	CHL	g	609	-	4/4/19/26	10/33/131/137	-
36	LMG	K	103	-	-	26/46/66/70	0/1/1/1
22	CLA	c	510	-	1/1/15/20	11/37/115/115	-
22	CLA	b	604	-	1/1/15/20	15/37/115/115	-
23	LUT	G	615	-	-	17/29/67/67	0/2/2/2
21	CHL	g	607	-	4/4/20/26	18/39/137/137	-
26	LHG	L	103	-	-	19/53/53/53	-
21	CHL	n	601	1	4/4/20/26	24/39/137/137	-
22	CLA	N	610	-	1/1/14/20	8/31/109/115	-
22	CLA	B	611	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	XAT	R	313	-	1/1/12/26	14/31/93/93	0/4/4/4
22	CLA	C	513	4	1/1/15/20	14/37/115/115	-
26	LHG	g	619	-	-	22/53/53/53	-
21	CHL	N	607	-	4/4/20/26	23/39/137/137	-
22	CLA	s	303	20	1/1/14/20	12/33/111/115	-
21	CHL	Y	606	-	4/4/20/26	18/39/137/137	-
21	CHL	S	301	-	3/3/16/26	10/18/116/137	-
22	CLA	B	610	-	1/1/15/20	13/37/115/115	-
25	NEX	N	617	22	2/2/12/25	15/27/83/83	0/3/3/3
21	CHL	G	601	1	4/4/20/26	24/39/137/137	-
22	CLA	C	506	-	1/1/15/20	8/37/115/115	-
35	DGD	J	101	-	-	16/49/89/95	0/2/2/2
23	LUT	r	313	22	-	18/29/67/67	0/2/2/2
22	CLA	C	515	-	1/1/15/20	16/37/115/115	-
26	LHG	D	408	-	-	25/50/50/53	-
30	PHO	D	401	-	-	15/37/103/103	0/5/6/6
22	CLA	S	303	20	1/1/14/20	12/33/111/115	-
36	LMG	k	103	-	-	26/46/66/70	0/1/1/1

The worst 5 of 2557 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	f	101	HEM	FE-NB	25.25	3.21	1.96
37	F	101	HEM	FE-NB	25.23	3.21	1.96
23	N	615	LUT	C24-C25	17.30	1.54	1.33
23	N	614	LUT	C24-C25	17.28	1.54	1.33
23	n	614	LUT	C24-C25	17.28	1.54	1.33

The worst 5 of 3429 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	617	XAT	O24-C25-C24	-78.18	54.66	113.38
24	N	616	XAT	O24-C25-C24	-78.01	54.78	113.38
24	R	313	XAT	O24-C25-C24	-77.64	55.06	113.38
24	r	314	XAT	O24-C25-C24	-77.61	55.08	113.38
24	g	617	XAT	O24-C25-C24	-77.46	55.19	113.38

5 of 353 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	g	601	CHL	NC
21	g	601	CHL	C8
21	g	601	CHL	ND
21	g	601	CHL	NA
21	g	605	CHL	NC

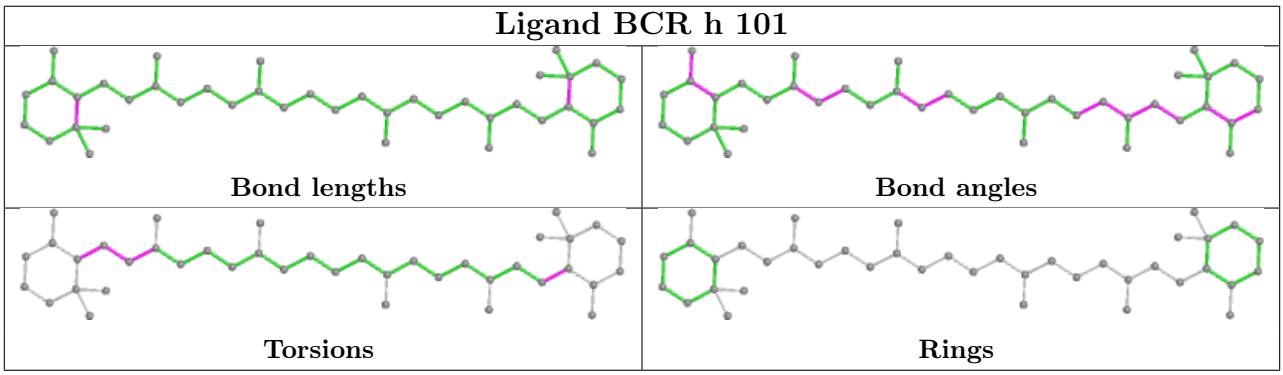
5 of 4559 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	g	601	CHL	C1A-C2A-CAA-CBA
21	g	601	CHL	C1C-C2C-CMC-OMC
21	g	601	CHL	C3C-C2C-CMC-OMC
21	g	605	CHL	C1C-C2C-CMC-OMC
21	g	605	CHL	C3C-C2C-CMC-OMC

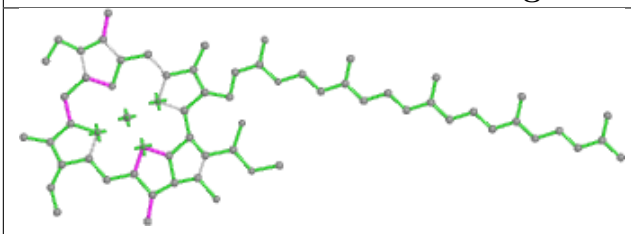
There are no ring outliers.

No monomer is involved in short contacts.

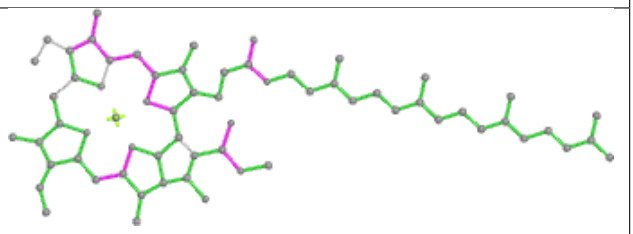
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



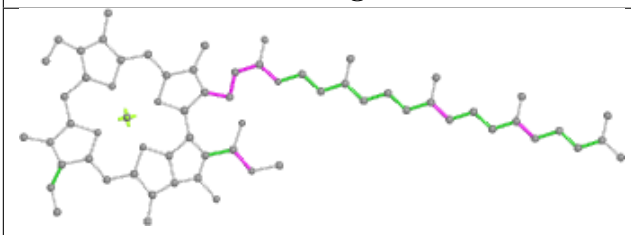
Ligand CLA N 602



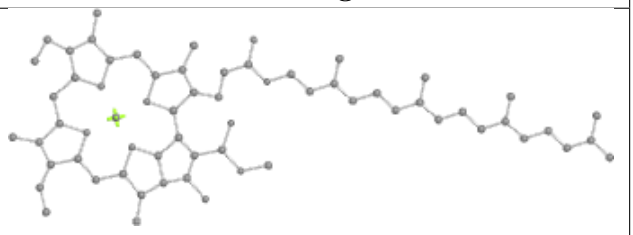
Bond lengths



Bond angles

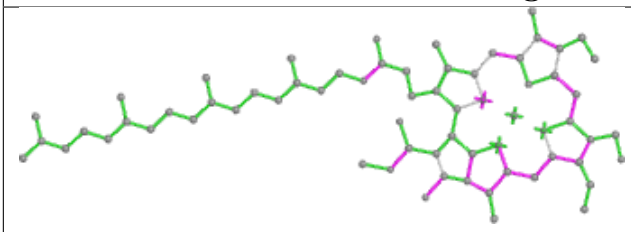


Torsions

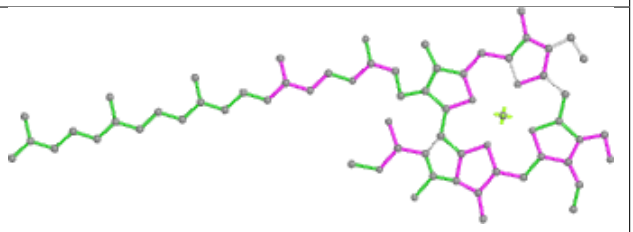


Rings

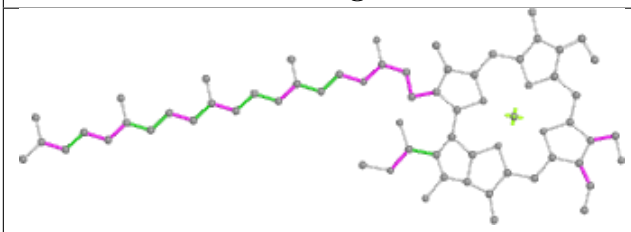
Ligand CHL N 601



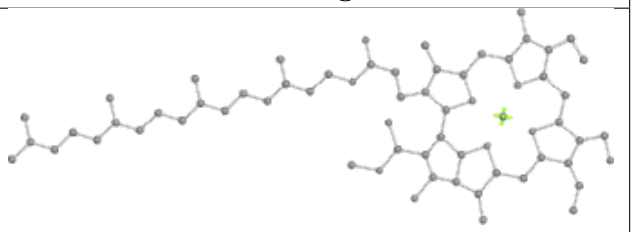
Bond lengths



Bond angles

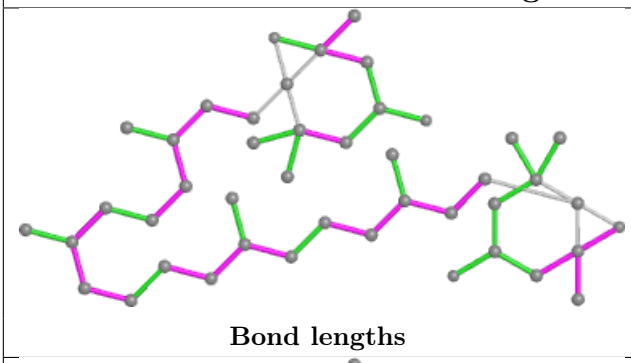


Torsions

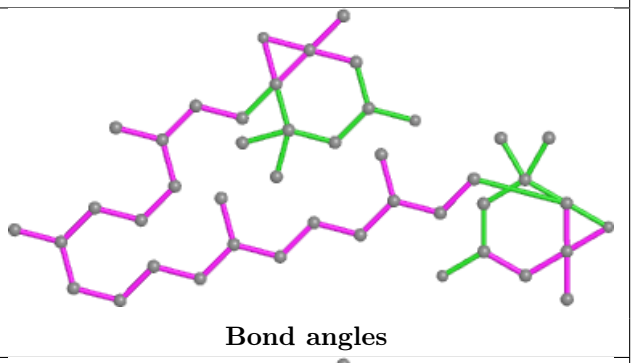


Rings

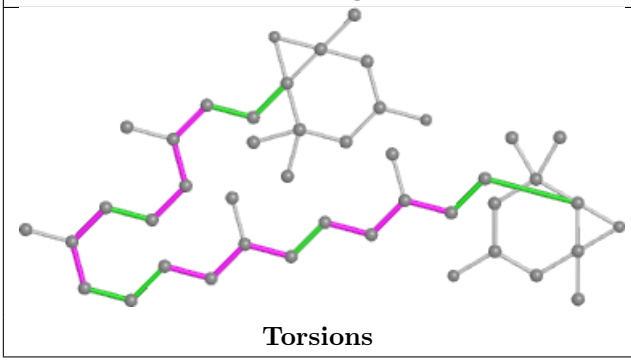
Ligand XAT N 616



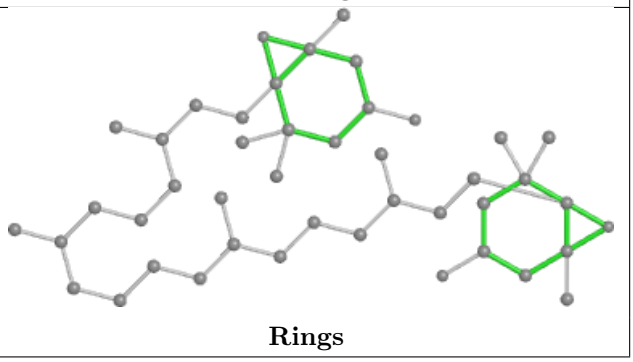
Bond lengths



Bond angles

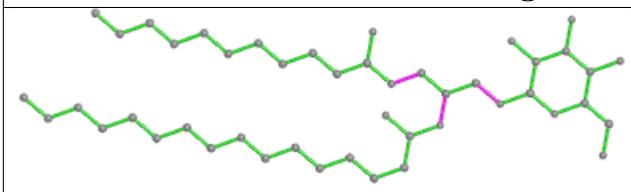


Torsions

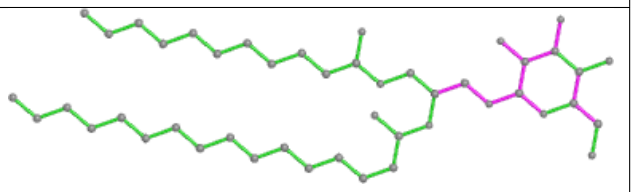


Rings

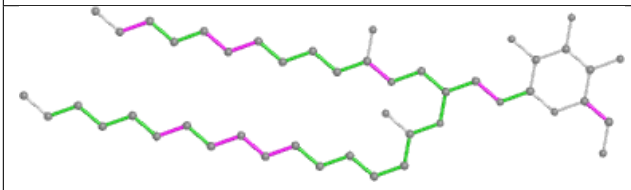
Ligand LMG D 411



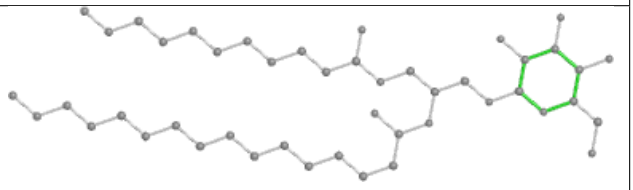
Bond lengths



Bond angles

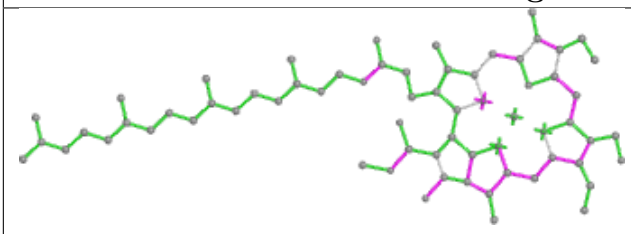


Torsions

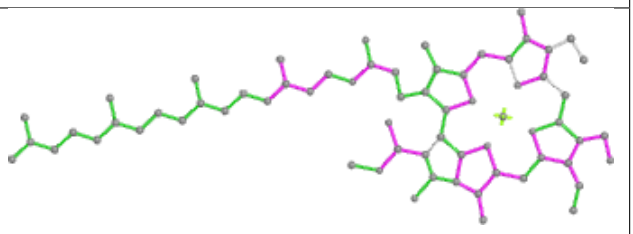


Rings

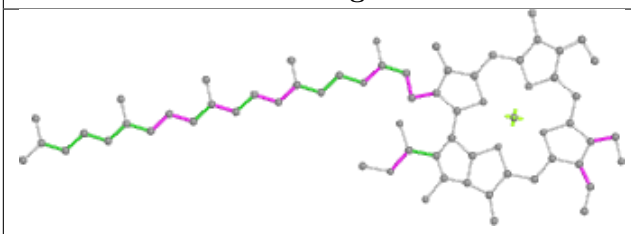
Ligand CHL n 606



Bond lengths



Bond angles



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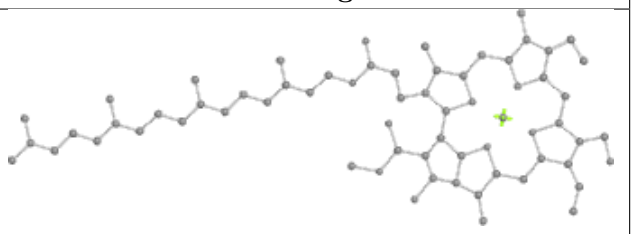
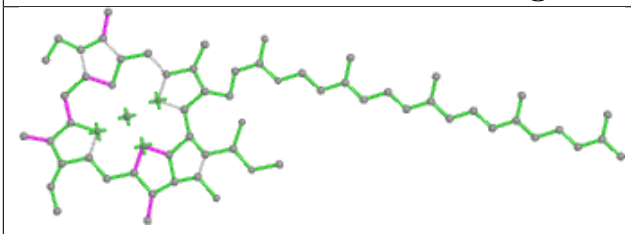


Rings

Ligand CLA c 512



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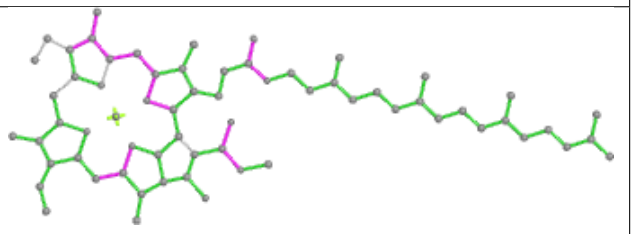
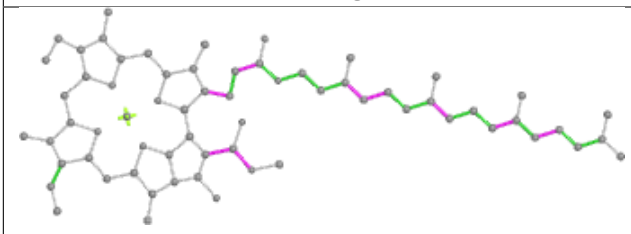


Bond angles



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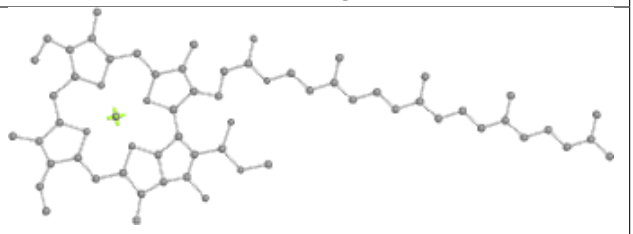
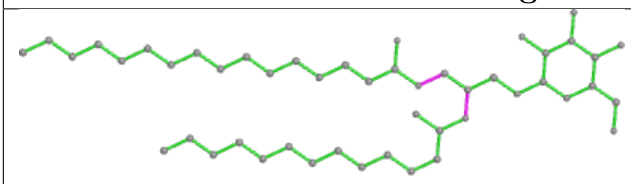


Rings

Ligand LMG w 102



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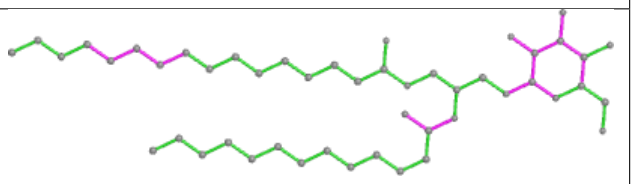
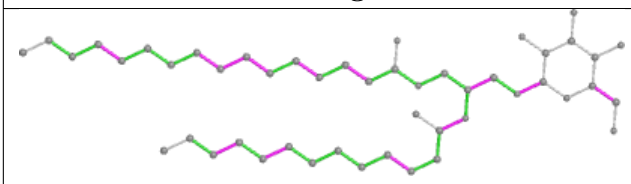
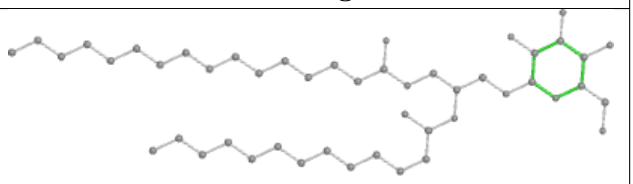


Bond angles

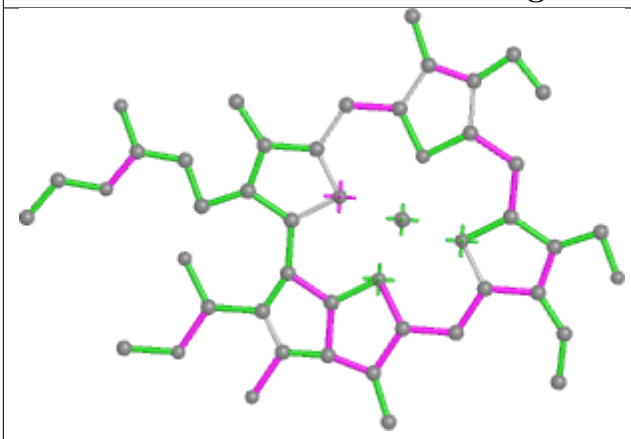


Torsions



Rings

Ligand CHL y 605



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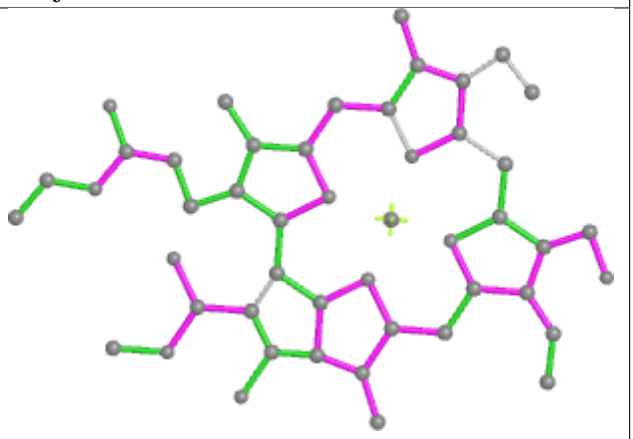
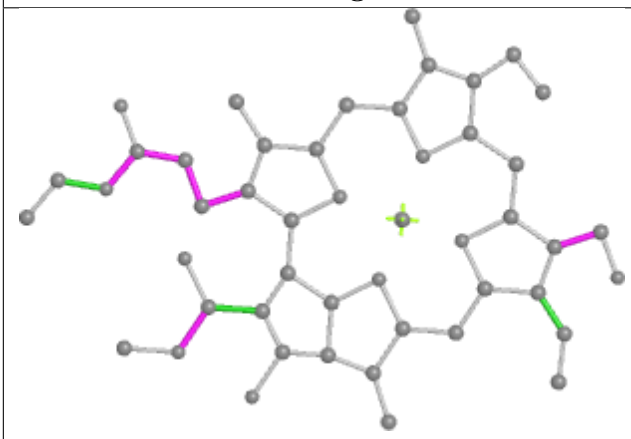


Bond angles



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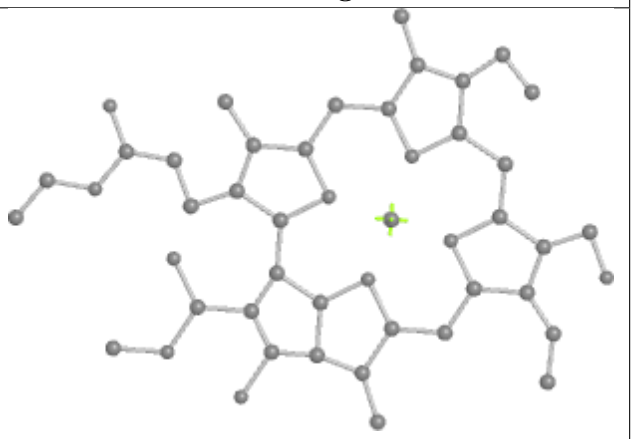
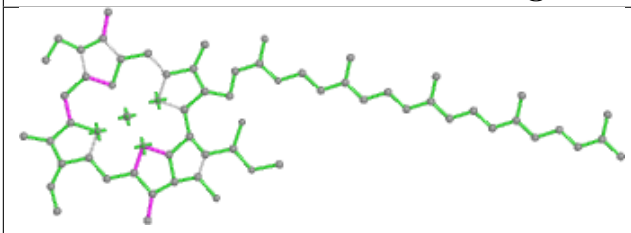
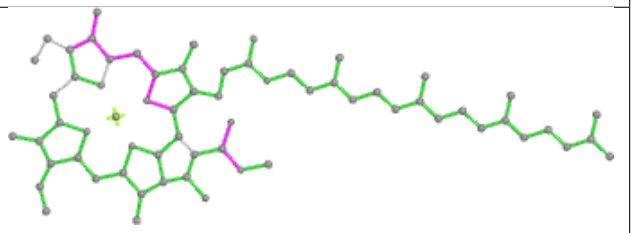


Rings

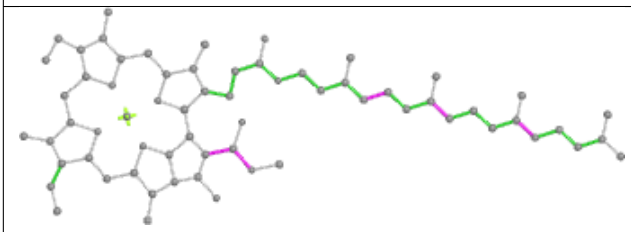
Ligand CLA b 612



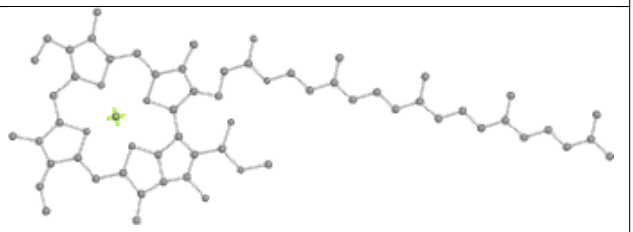
Bond lengths



Bond angles

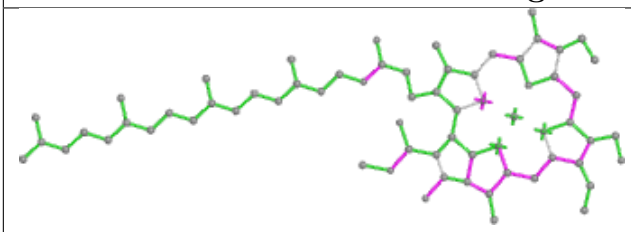


Torsions



Rings

Ligand CHL g 608



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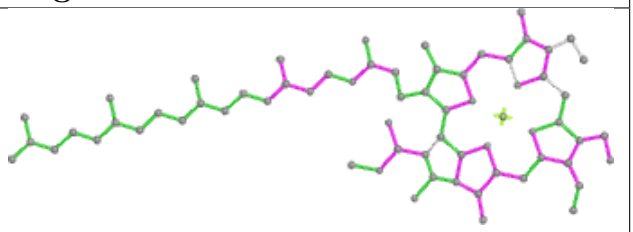
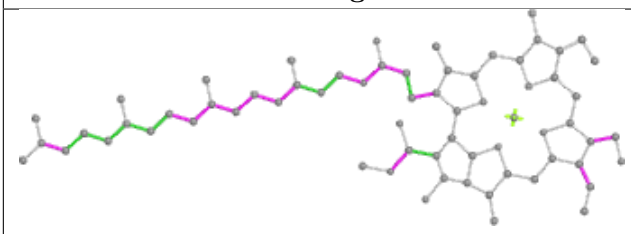
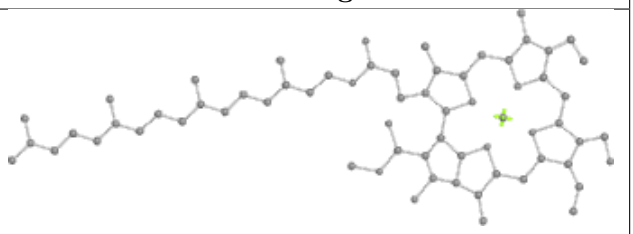


Bond angles

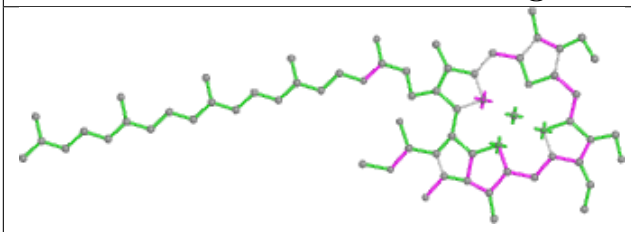


Torsions



Rings

Ligand CHL g 601



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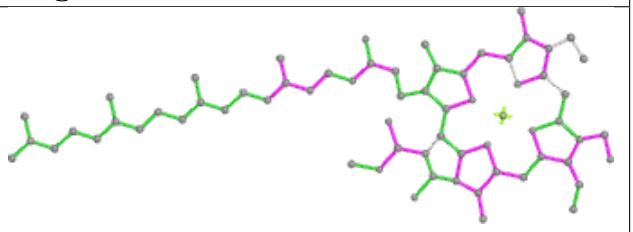
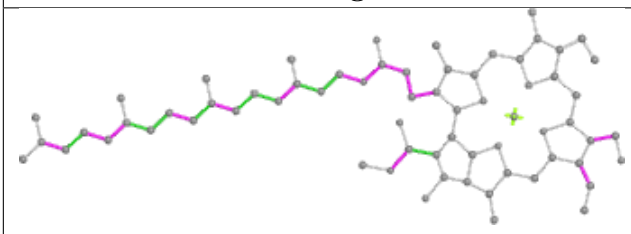


Bond angles



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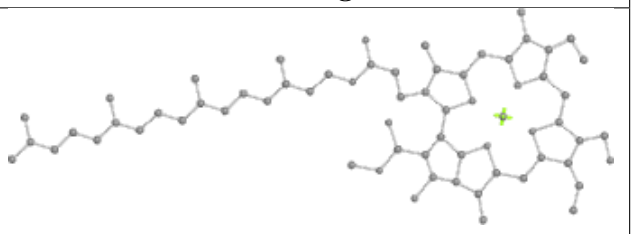
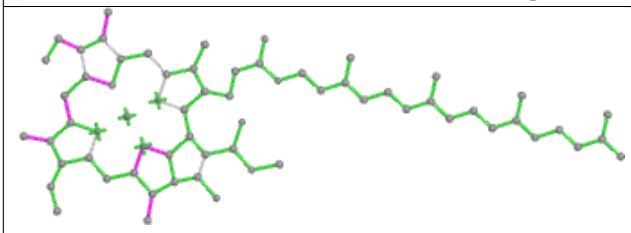
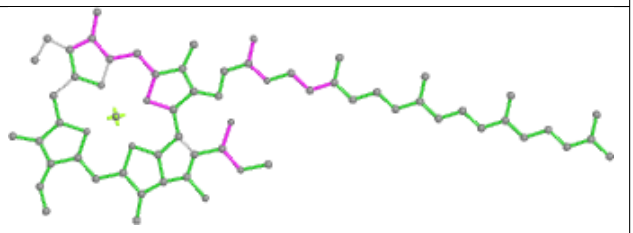


Rings

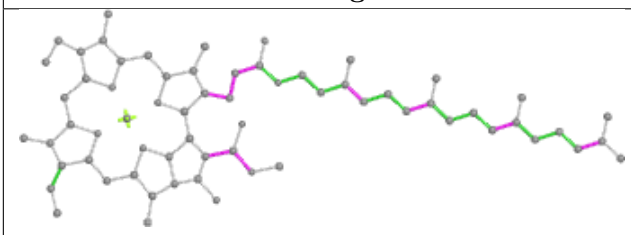
Ligand CLA B 605



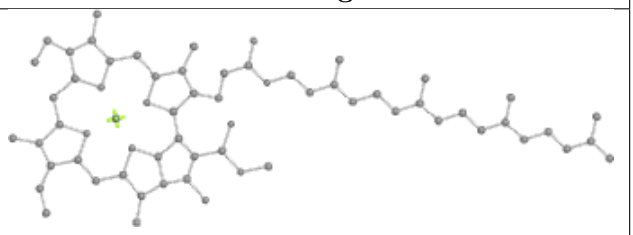
Bond lengths



Bond angles

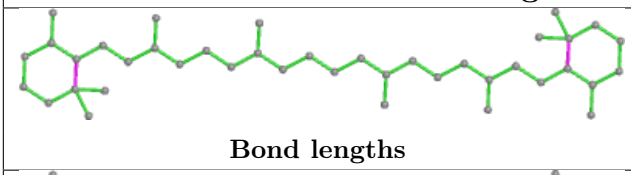


Torsions

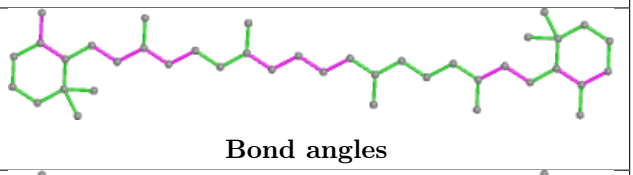


Rings

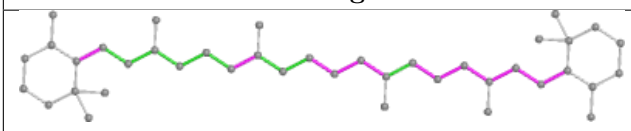
Ligand BCR K 101



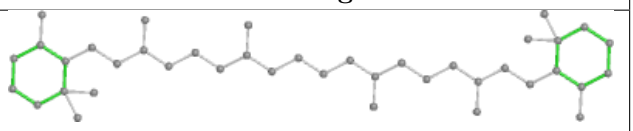
Bond lengths



Bond angles

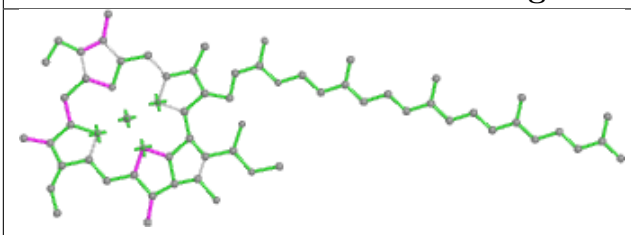


Torsions

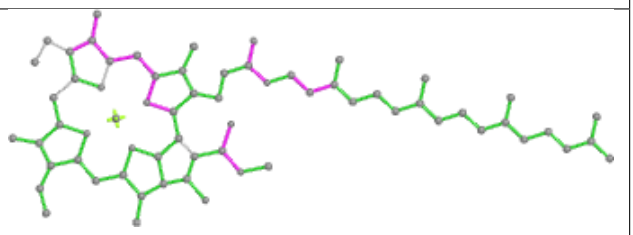


Rings

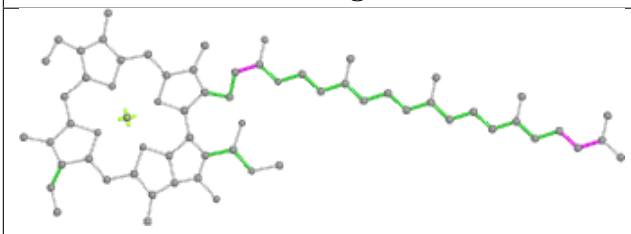
Ligand CLA a 404



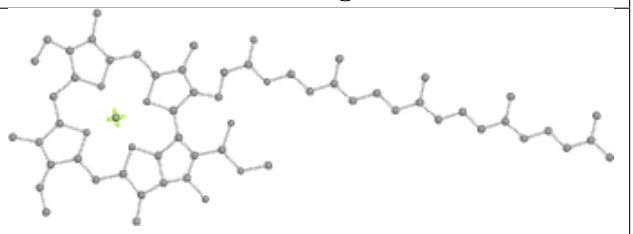
Bond lengths



Bond angles

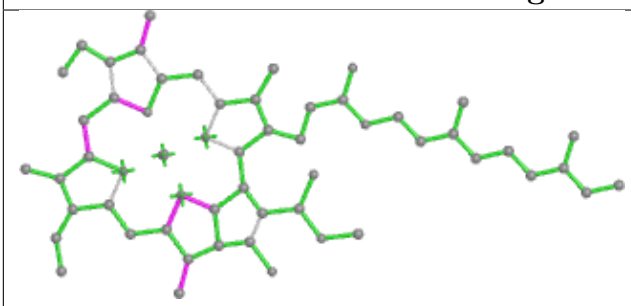


Torsions



Rings

Ligand CLA S 311



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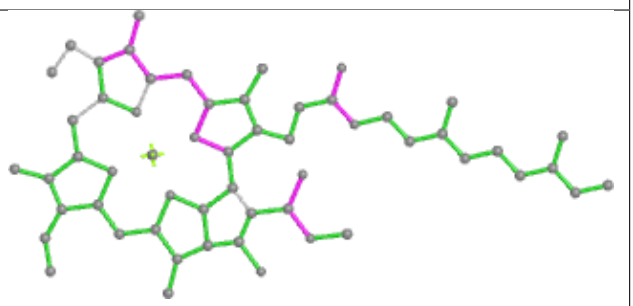
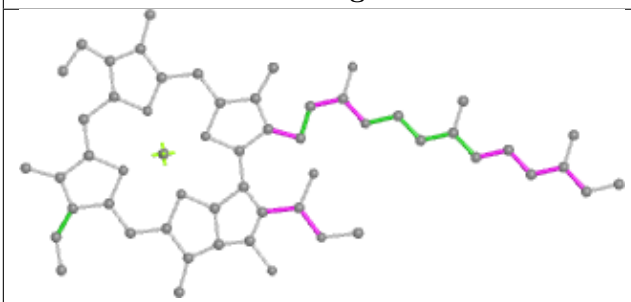
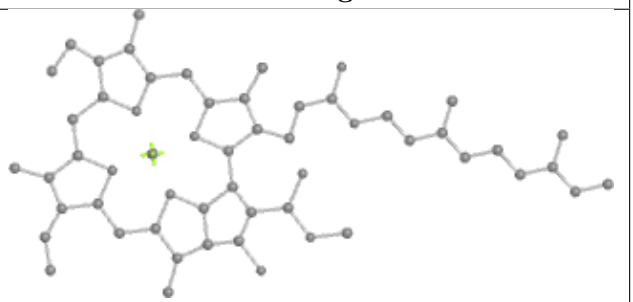


Bond angles

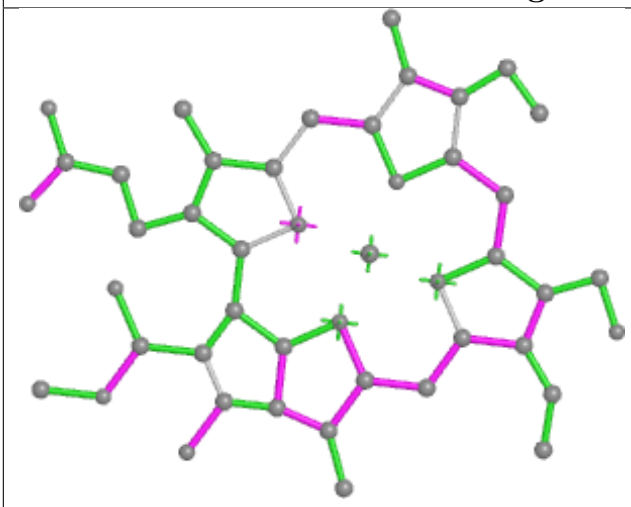


Torsions



Rings

Ligand CHL g 605



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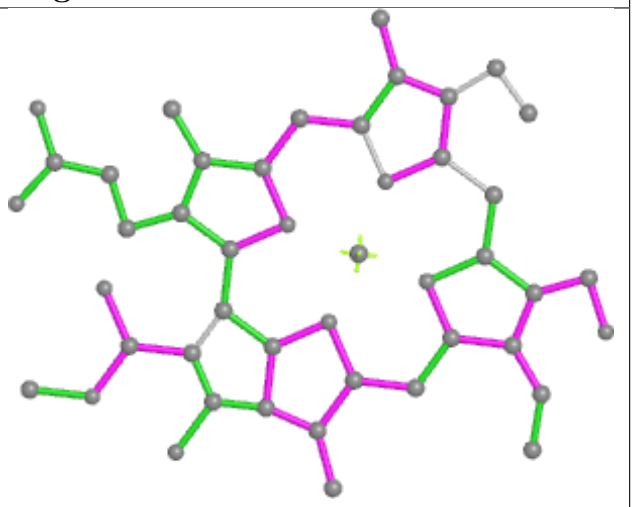
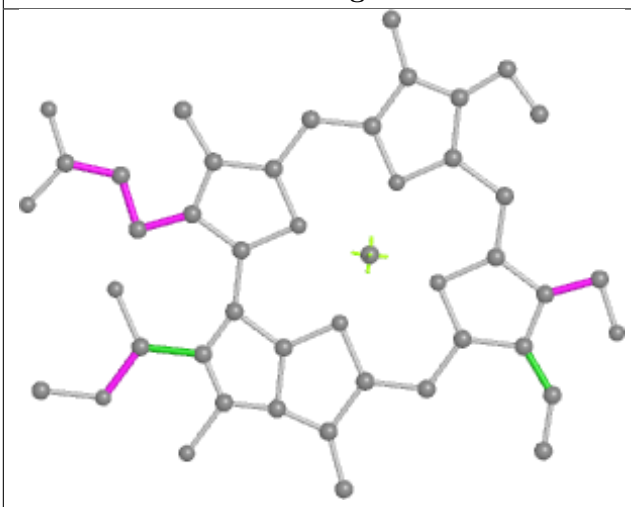
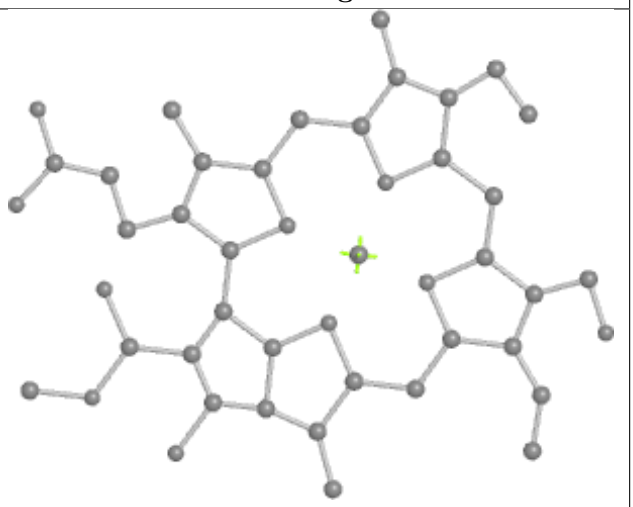


Bond angles

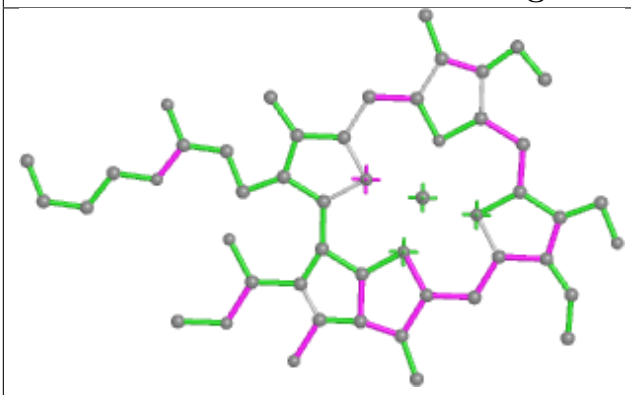


Torsions

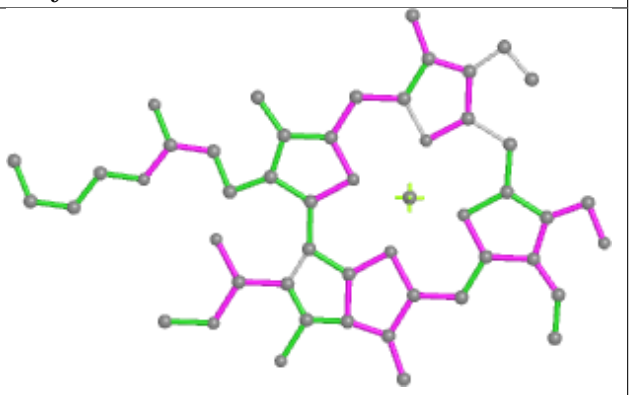


Rings

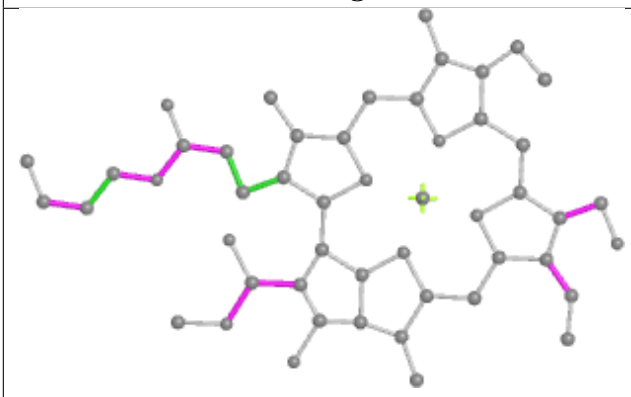
Ligand CHL y 606



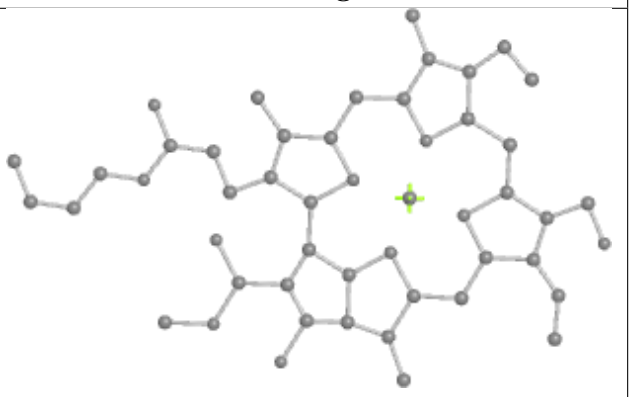
Bond lengths



Bond angles

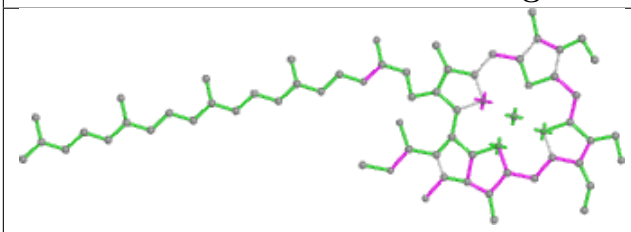


Torsions

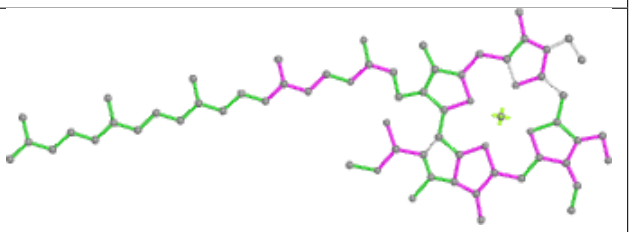


Rings

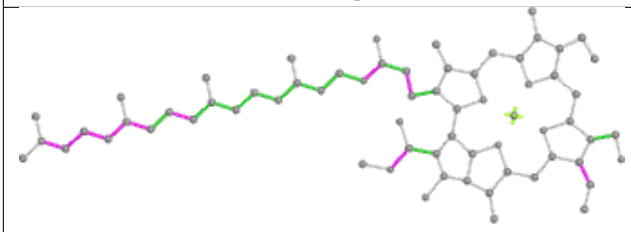
Ligand CHL N 608



Bond lengths



Bond angles



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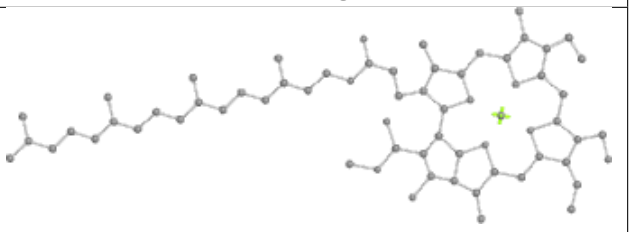
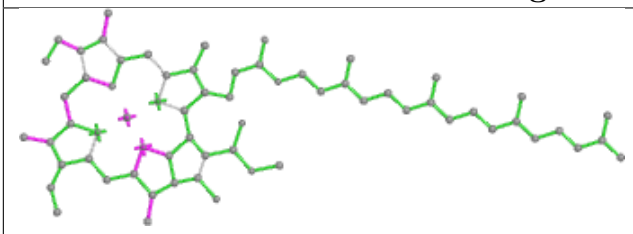
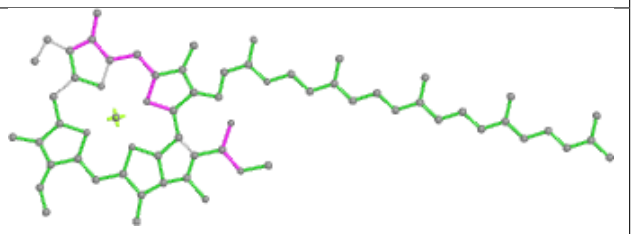


Rings

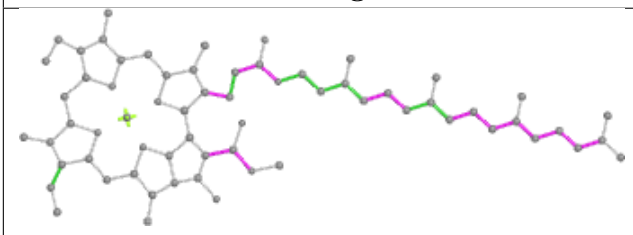
Ligand CLA c 513



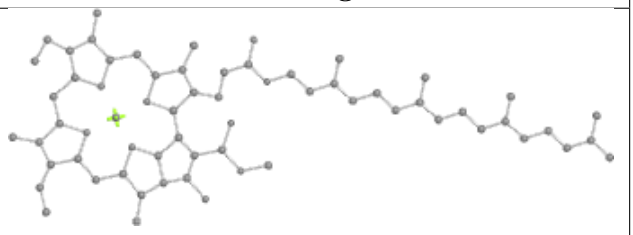
Bond lengths



Bond angles

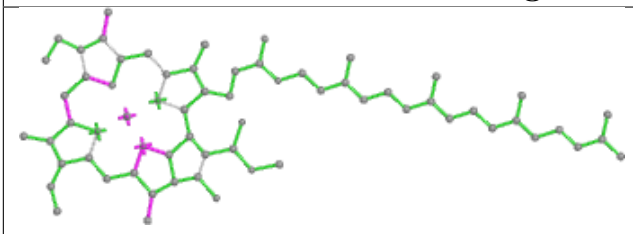


Torsions



Rings

Ligand CLA Y 603



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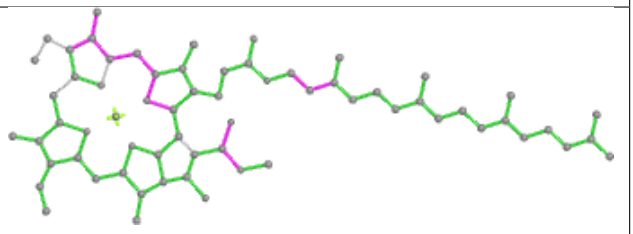
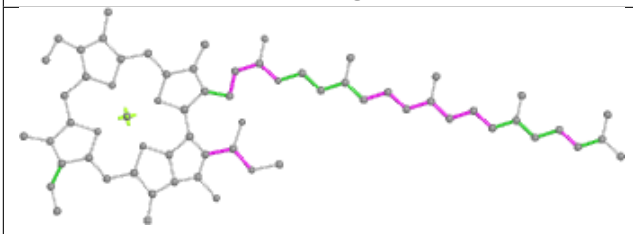


Bond angles



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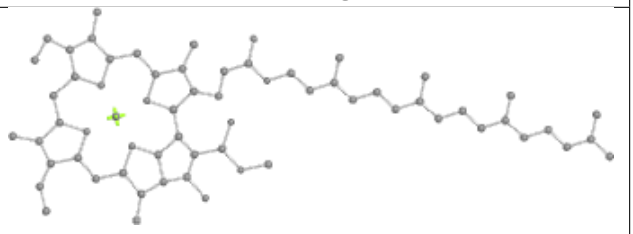
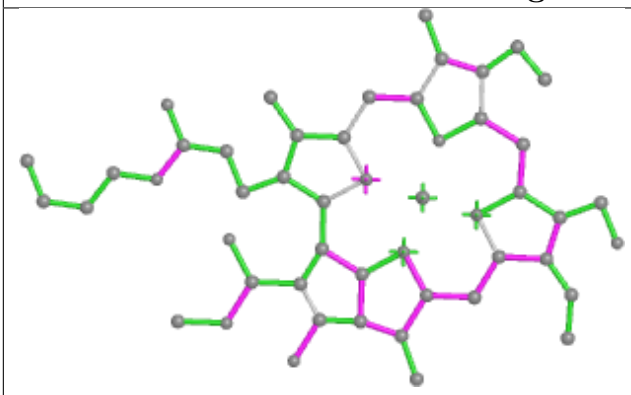


Rings

Ligand CHL g 606



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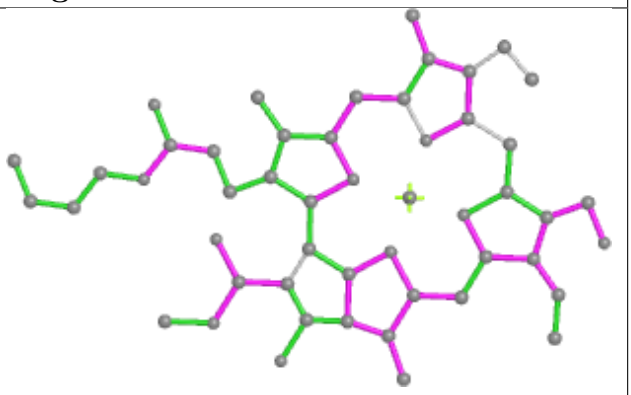
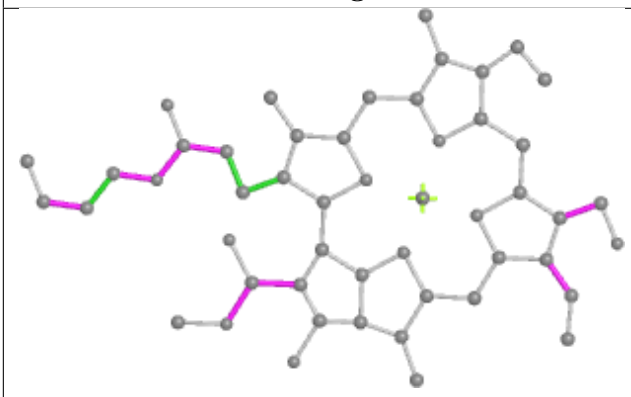


Bond angles



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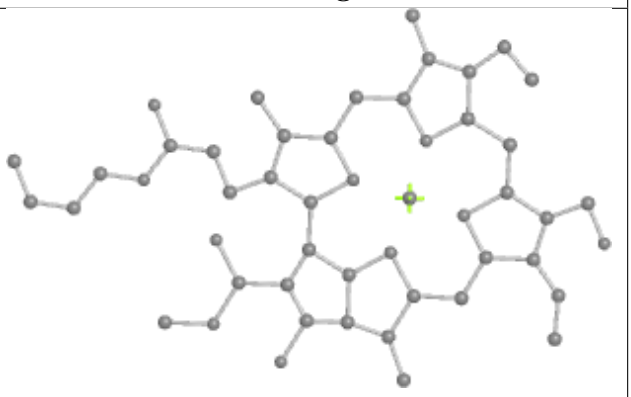
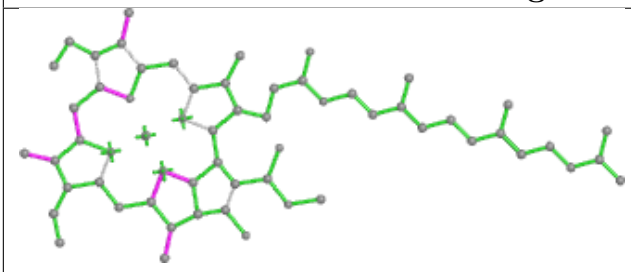
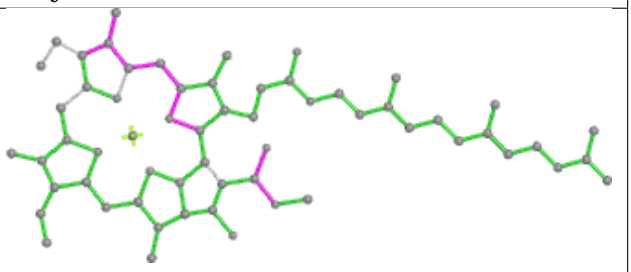


Rings

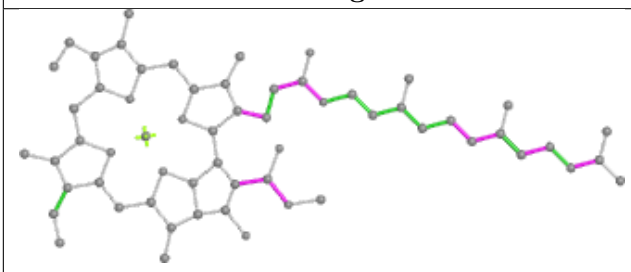
Ligand CLA y 610



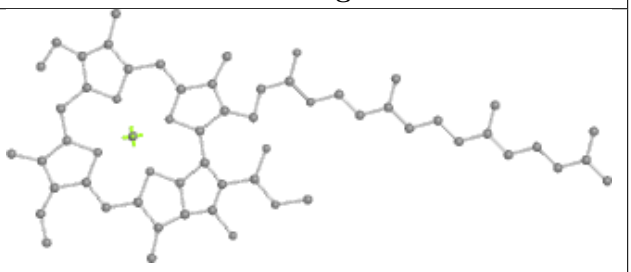
Bond lengths



Bond angles

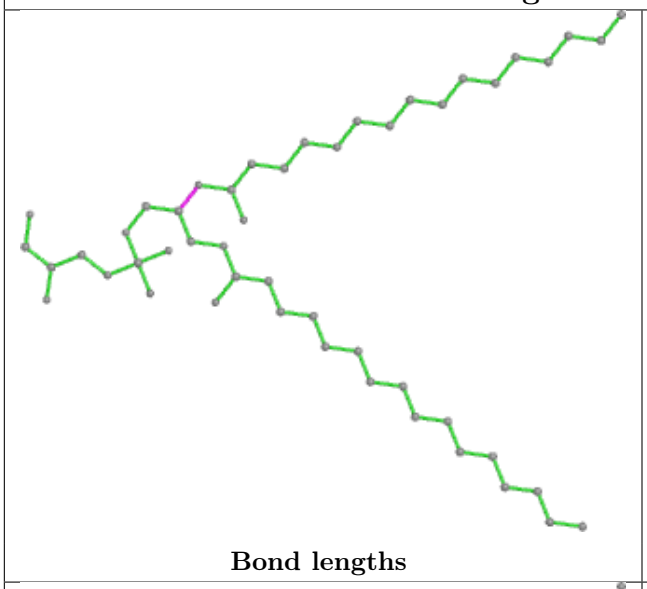


Torsions



Rings

Ligand LHG G 618



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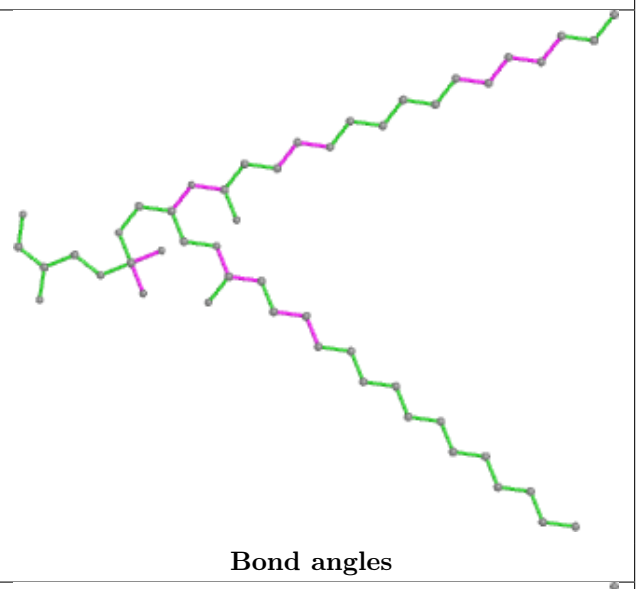
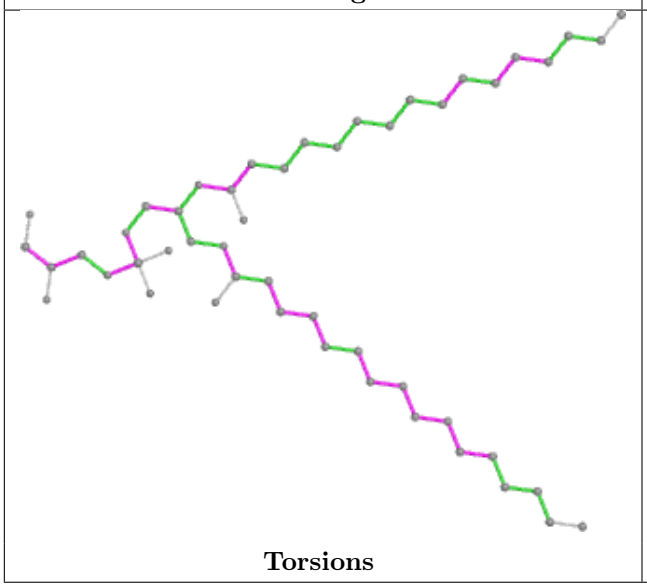
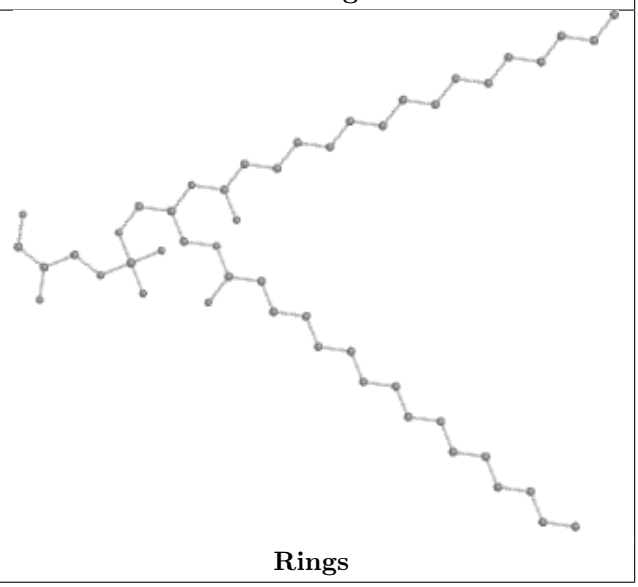


Bond angles

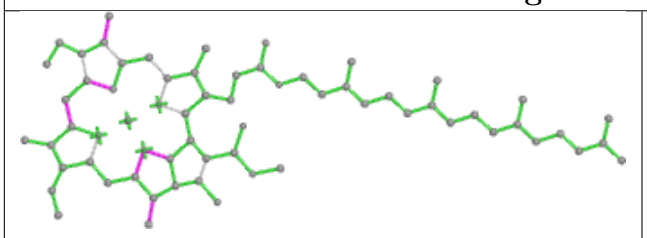


Torsions

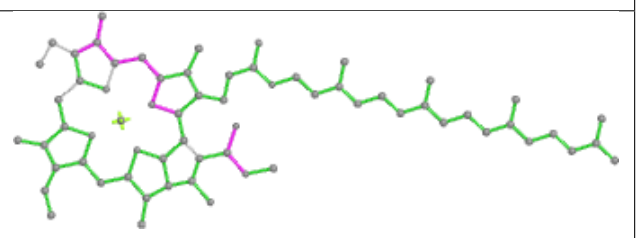


Rings

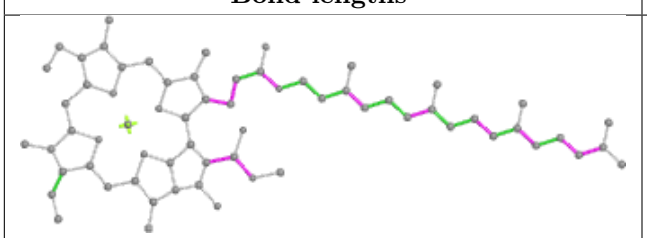
Ligand CLA R 309



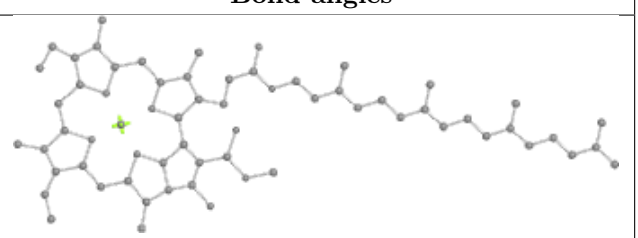
Bond lengths



Bond angles

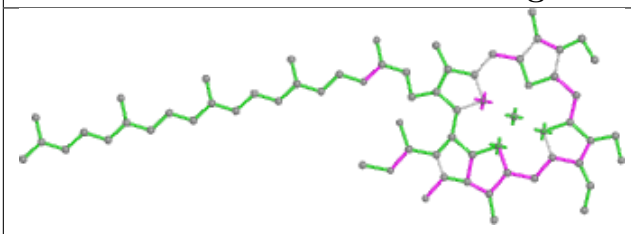


Torsions



Rings

Ligand CHL y 608



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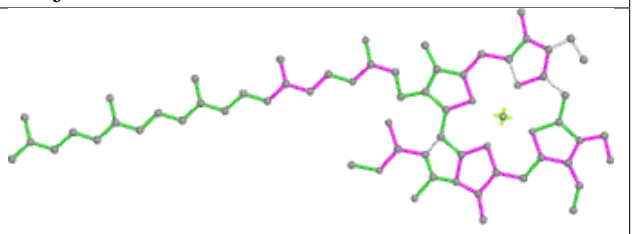
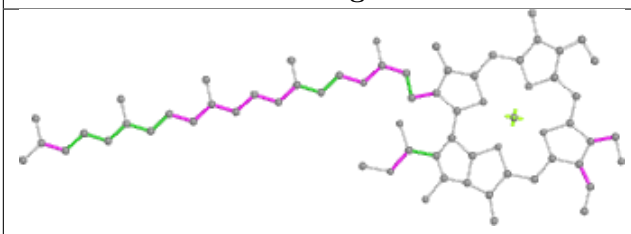
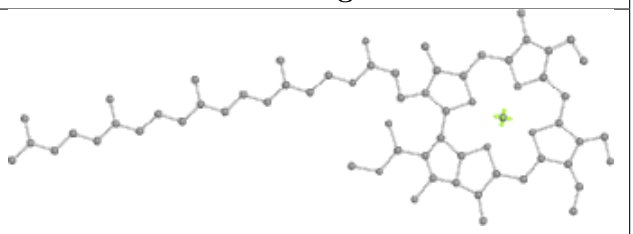


Bond angles

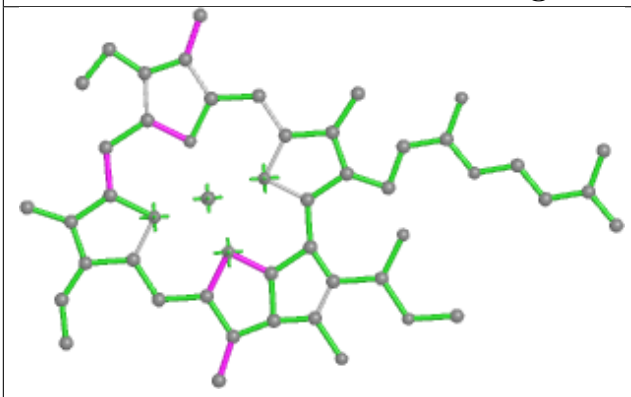


Torsions

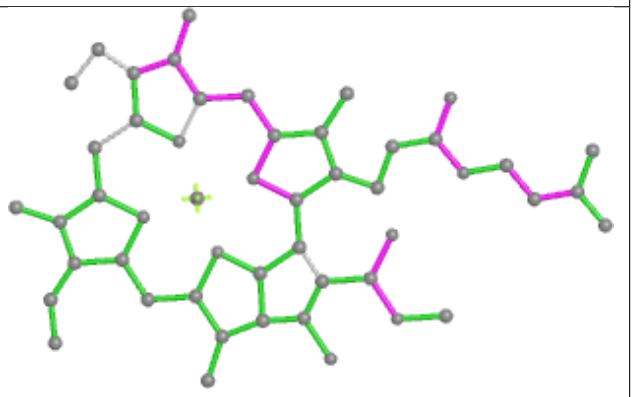


Rings

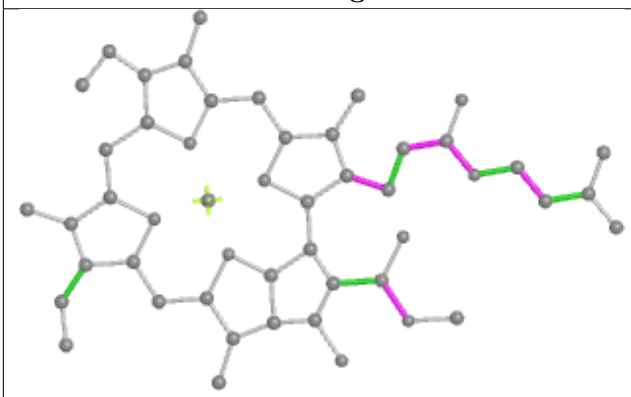
Ligand CLA s 305



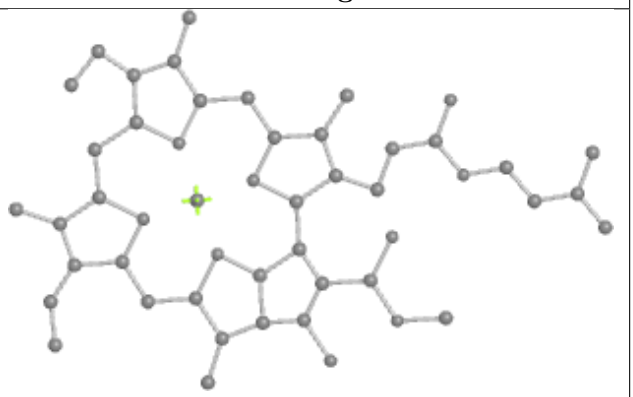
Bond lengths



Bond angles

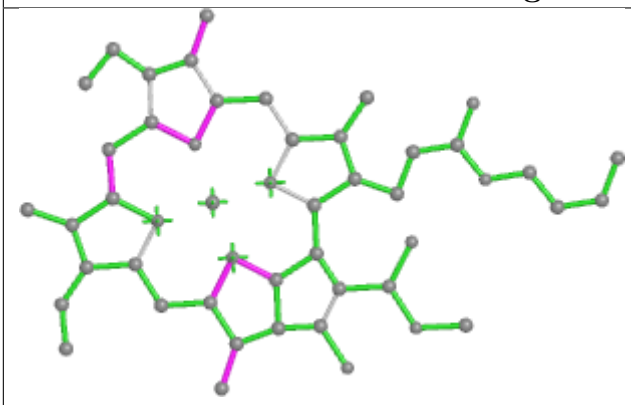


Torsions

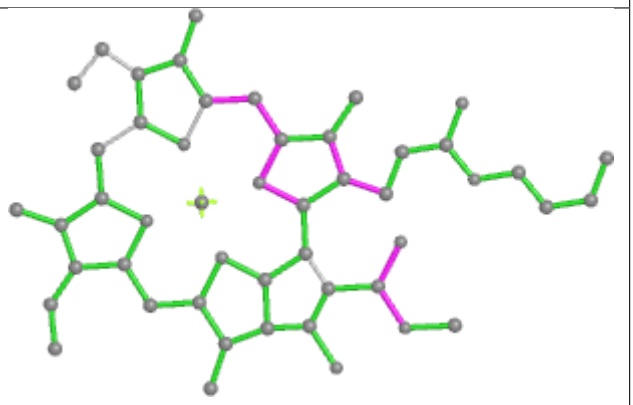


Rings

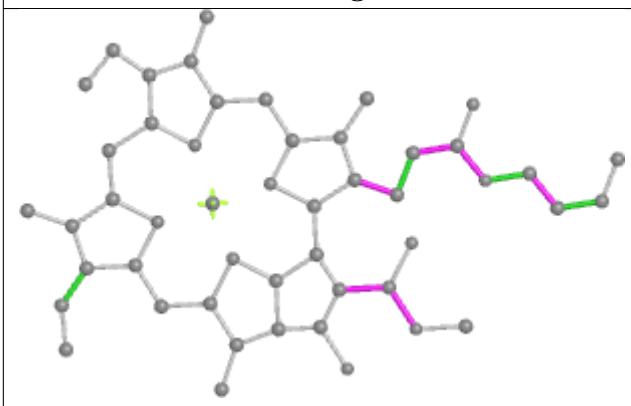
Ligand CLA R 310



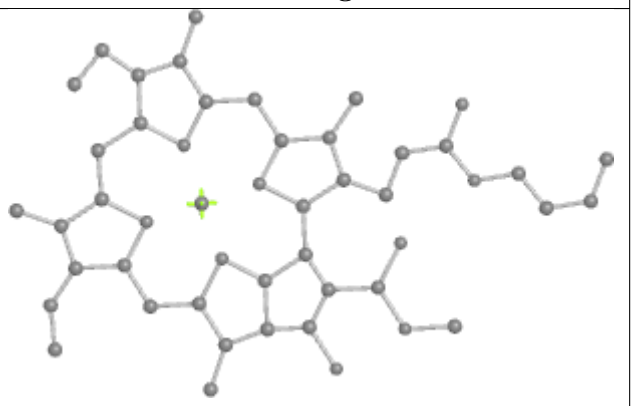
Bond lengths



Bond angles

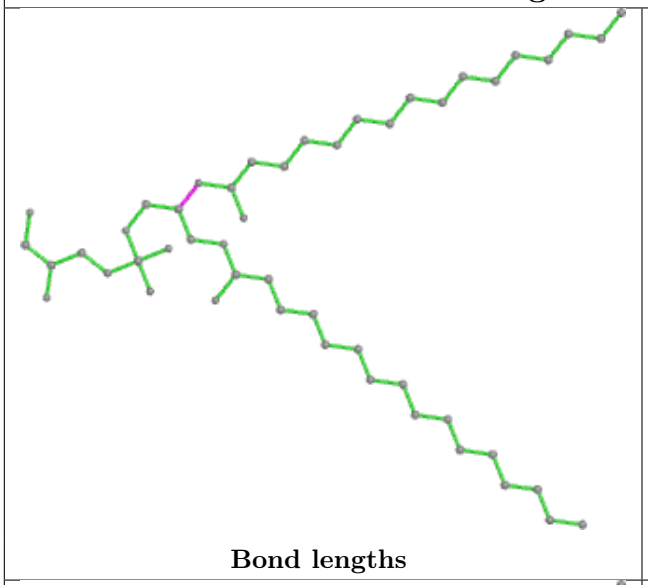


Torsions



Rings

Ligand LHG c 521



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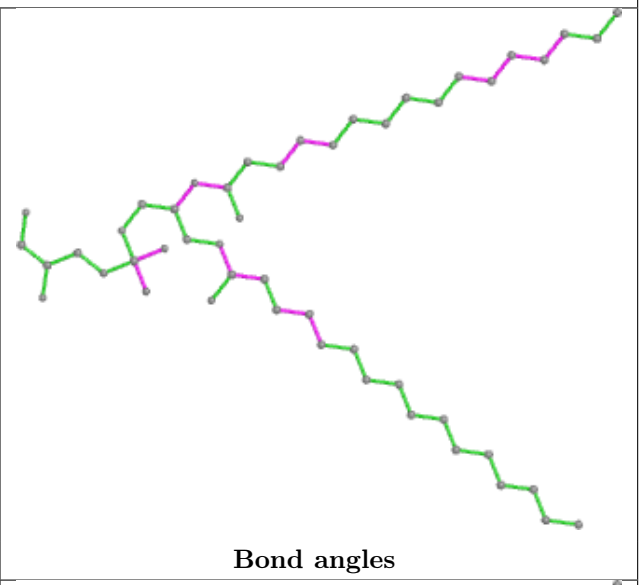
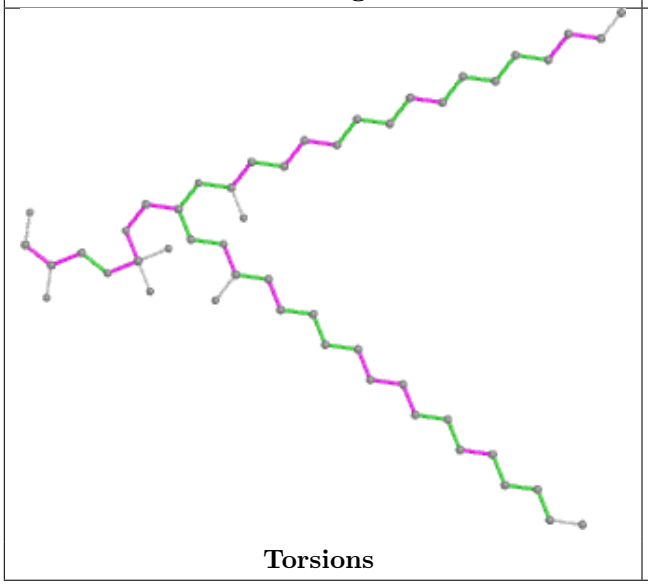
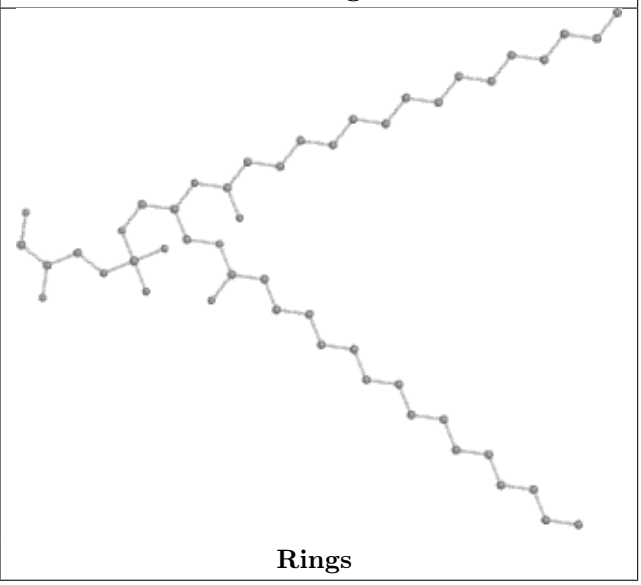


Bond angles

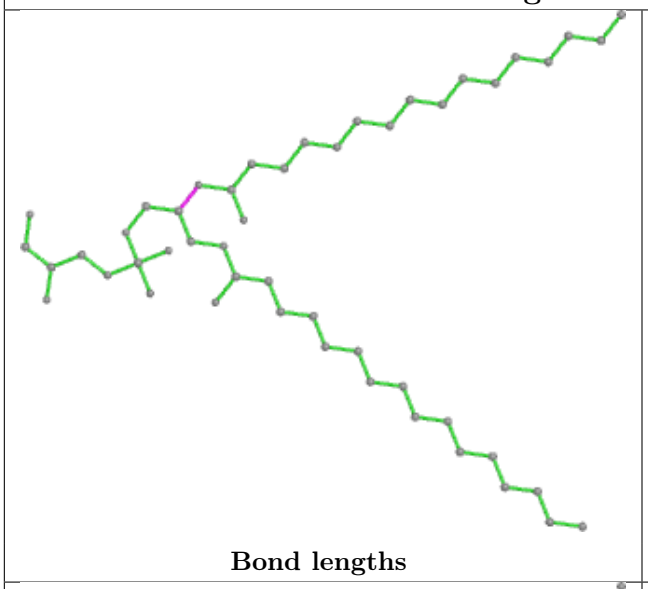


Torsions

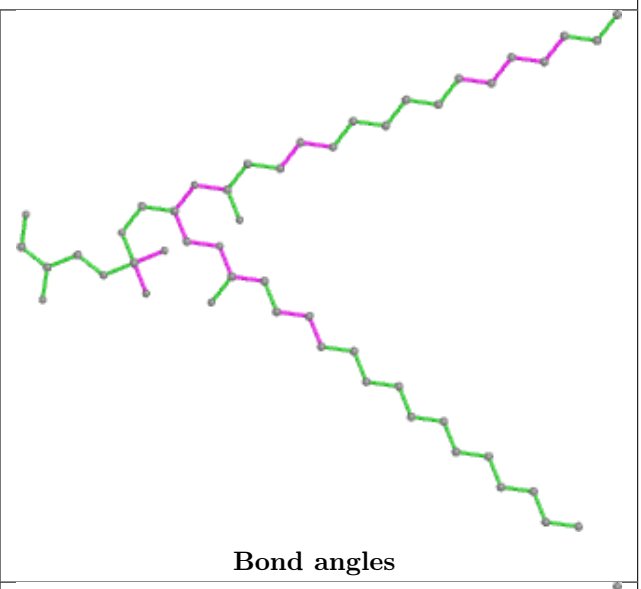


Rings

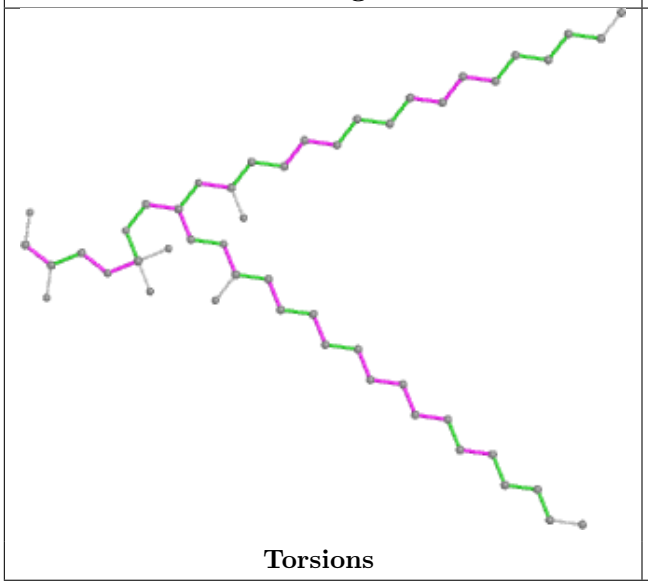
Ligand LHG C 522



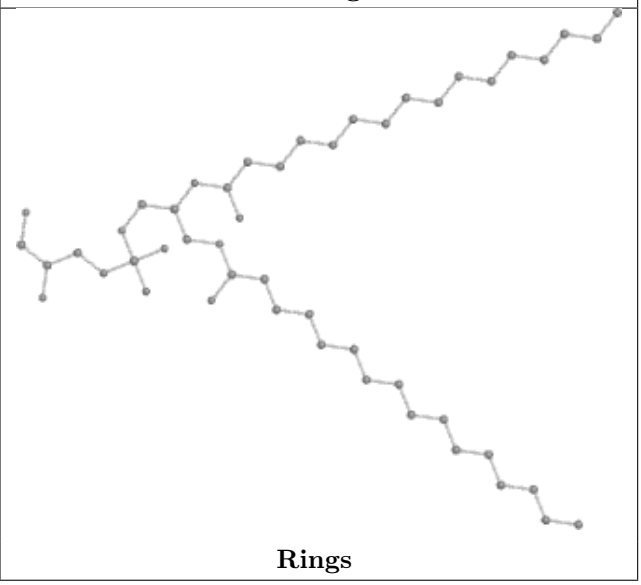
Bond lengths



Bond angles

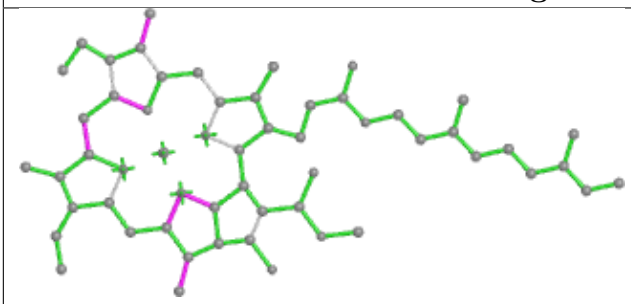


Torsions

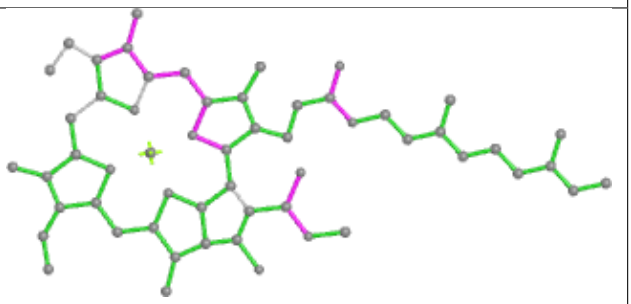


Rings

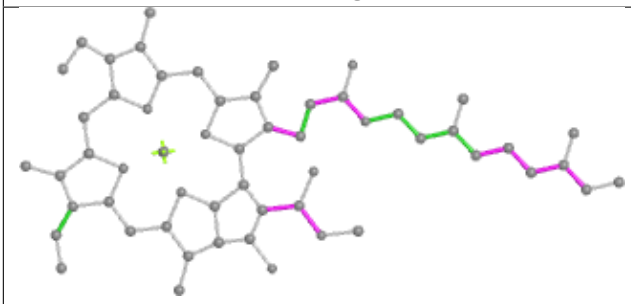
Ligand CLA s 311



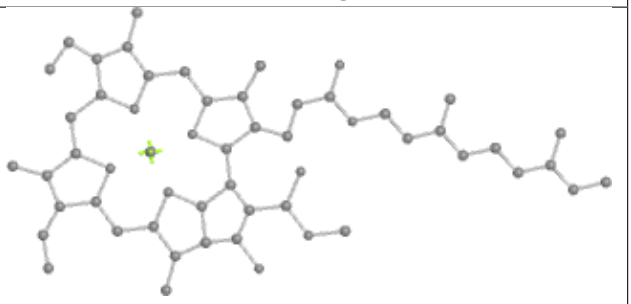
Bond lengths



Bond angles

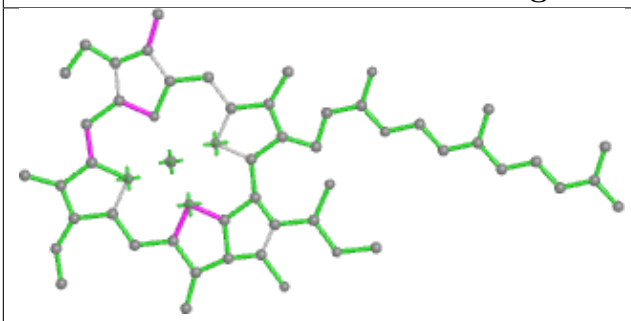


Torsions

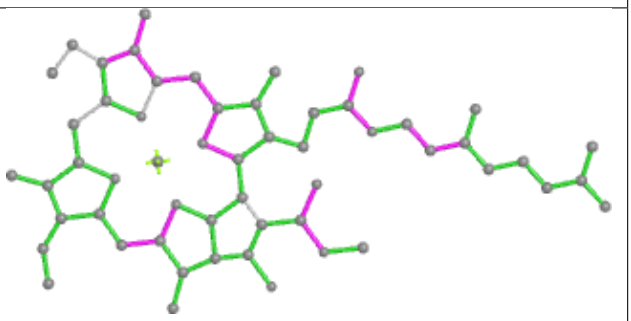


Rings

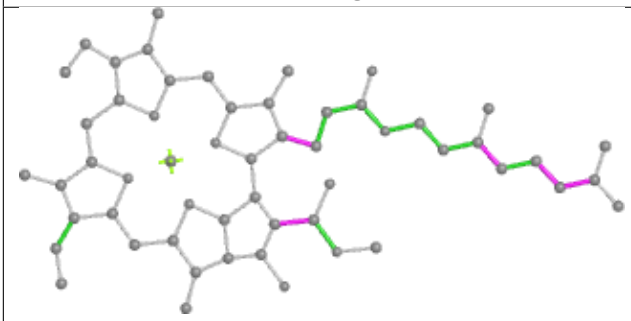
Ligand CLA s 309



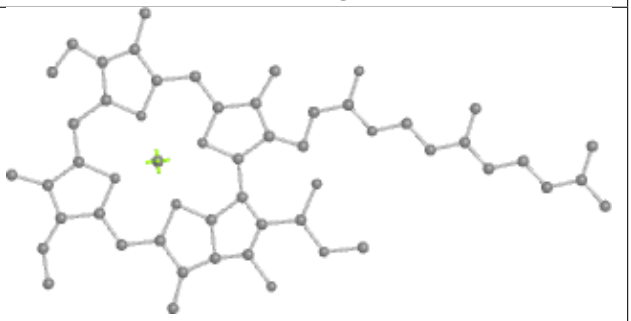
Bond lengths



Bond angles

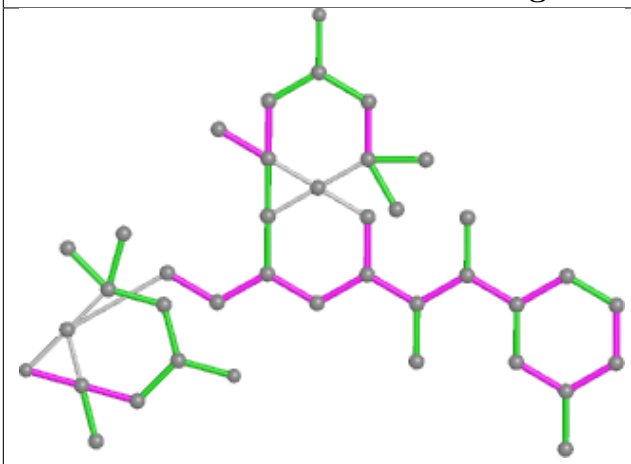


Torsions

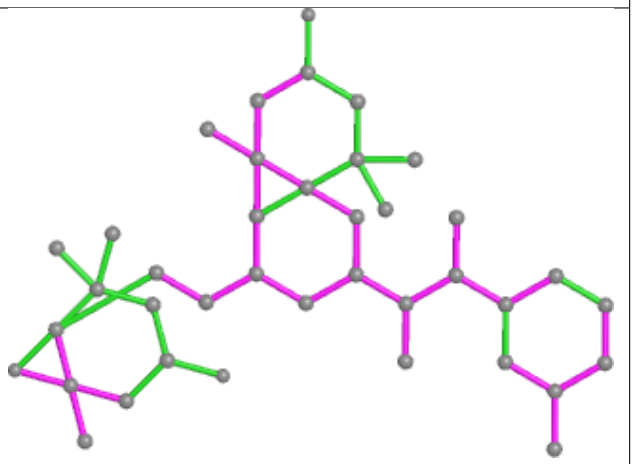


Rings

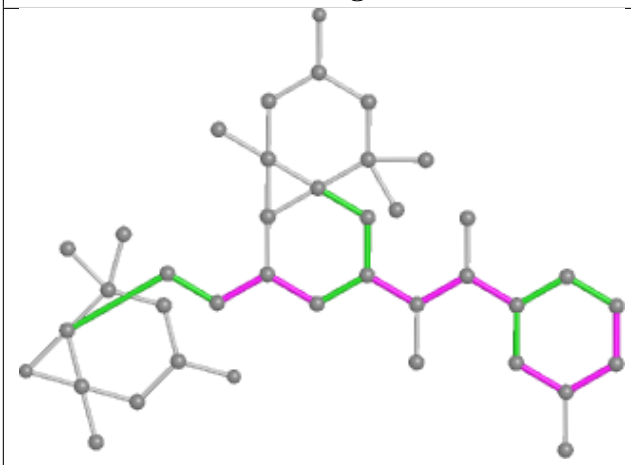
Ligand XAT r 314



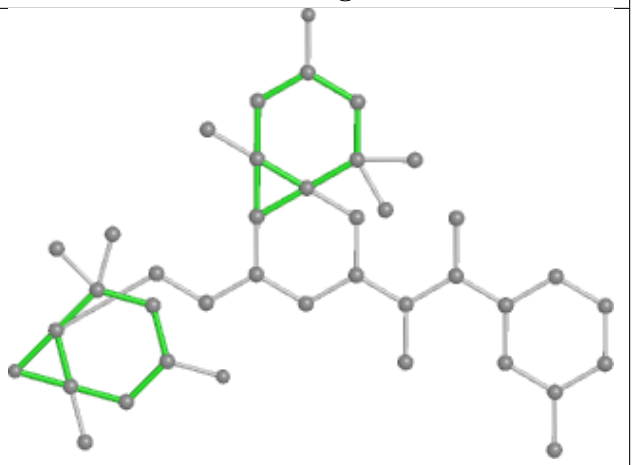
Bond lengths



Bond angles

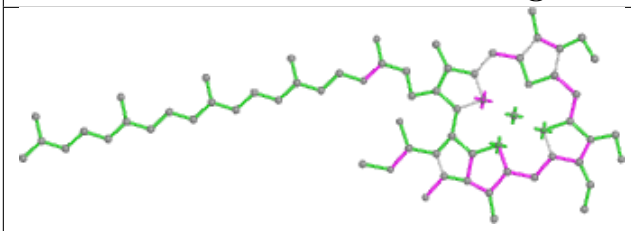


Torsions

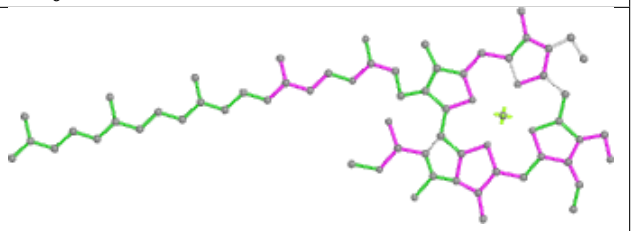


Rings

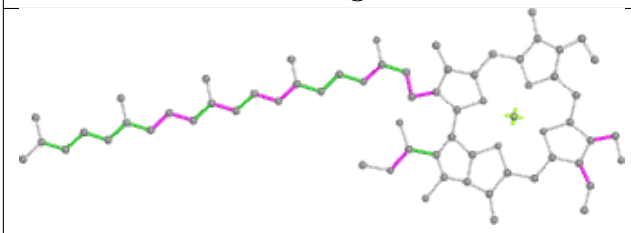
Ligand CHL y 607



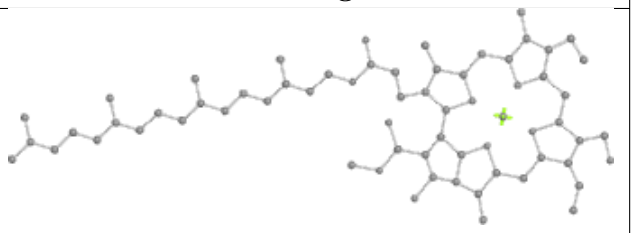
Bond lengths



Bond angles



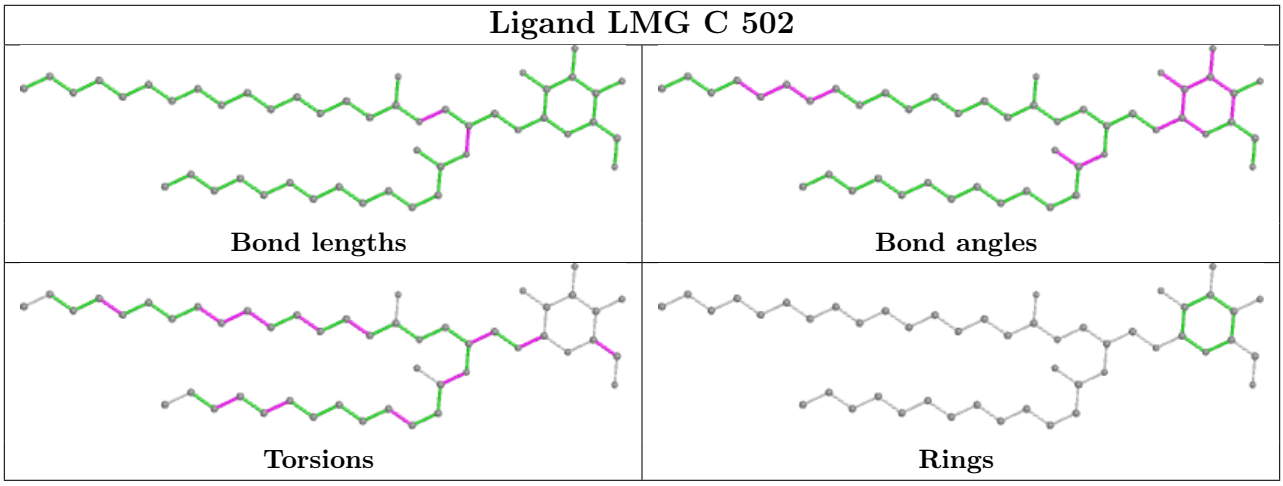
Torsions



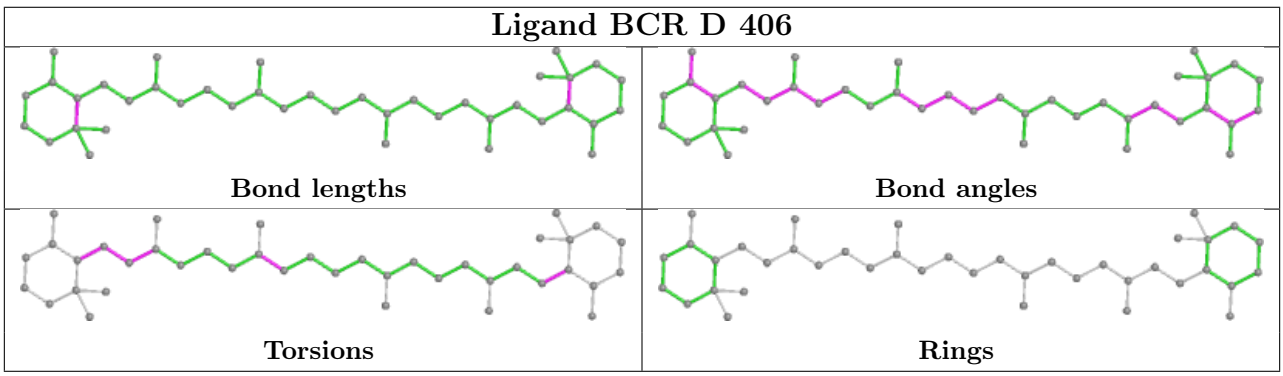
Rings

Ligand LUT R 312

Ligand LMG C 502



Ligand BCR D 406



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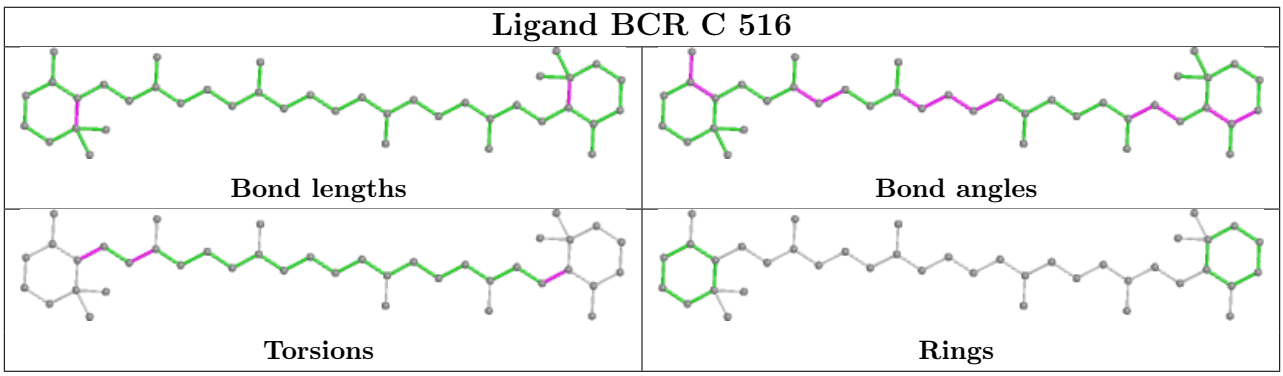
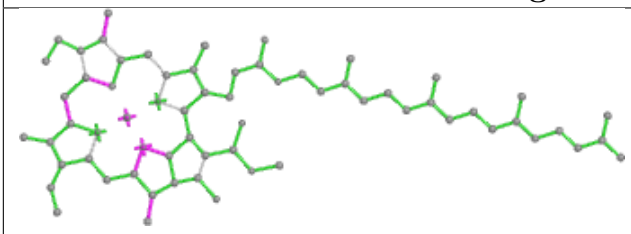
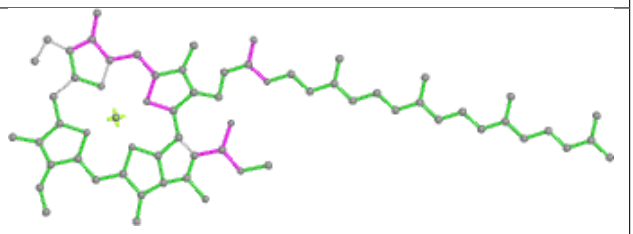


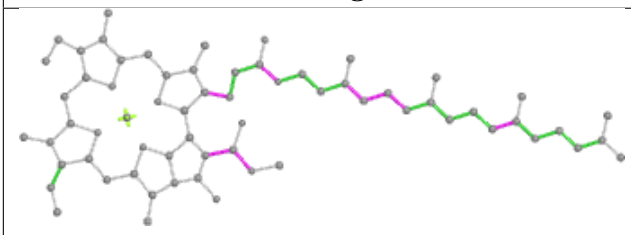
Ligand CLA c 511



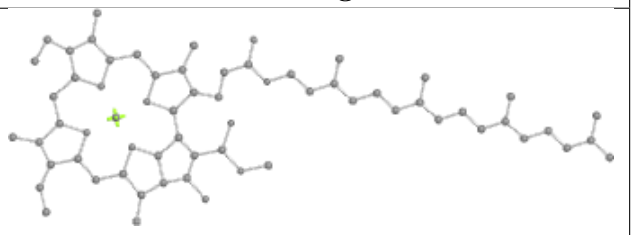
Bond lengths



Bond angles

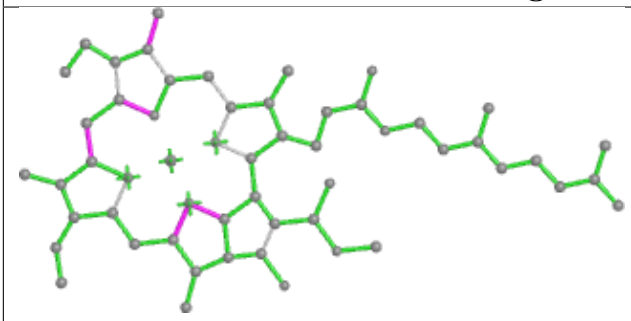


Torsions

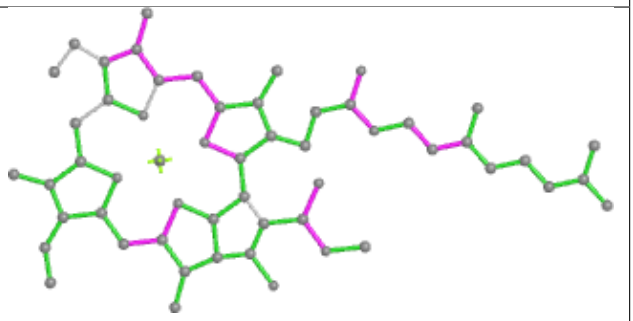


Rings

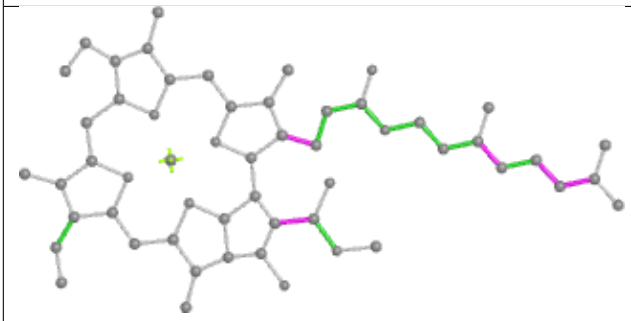
Ligand CLA S 309



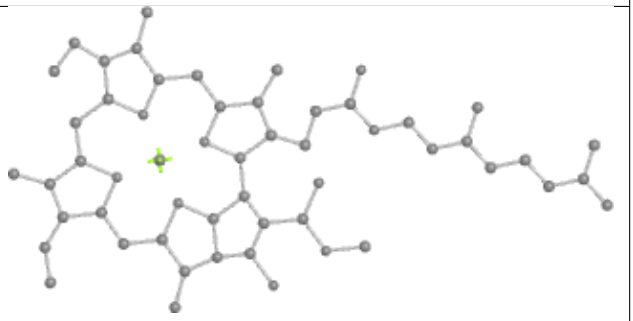
Bond lengths



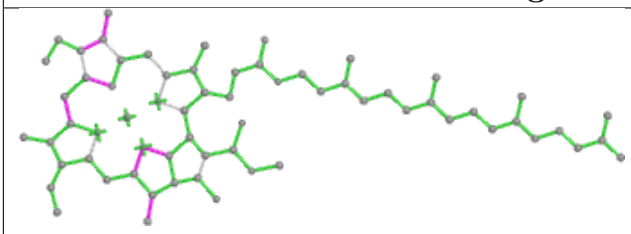
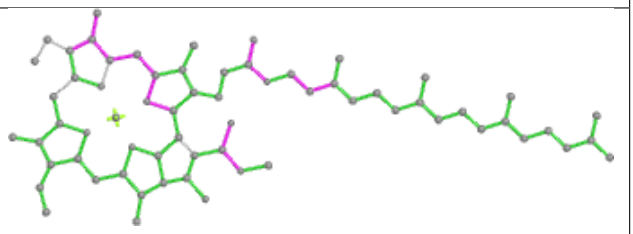
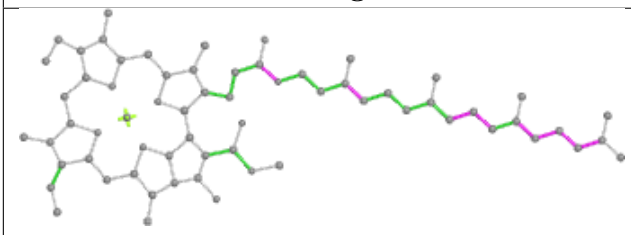
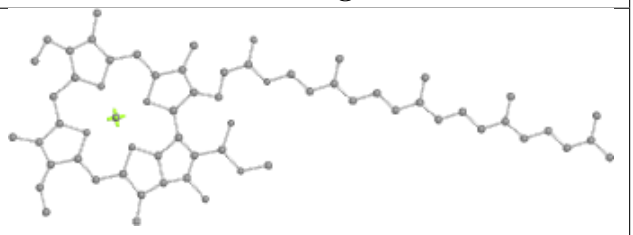
Bond angles

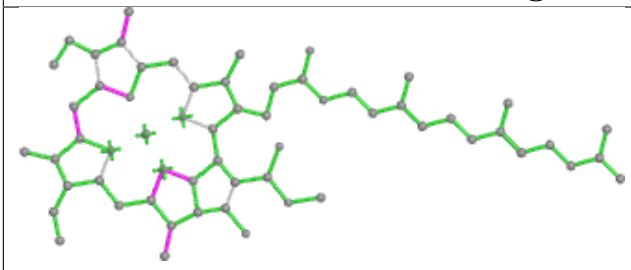
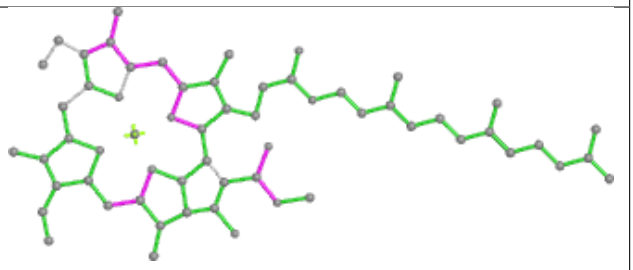
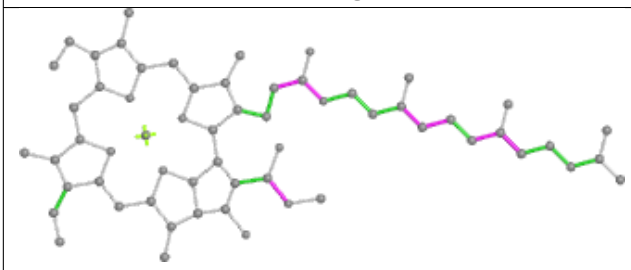
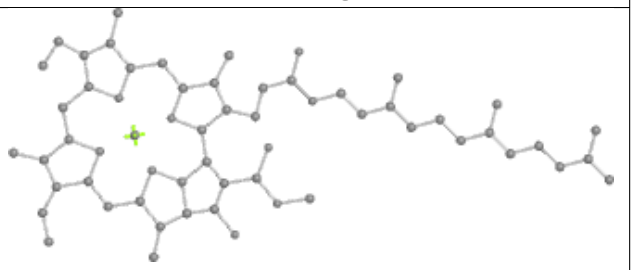


Torsions

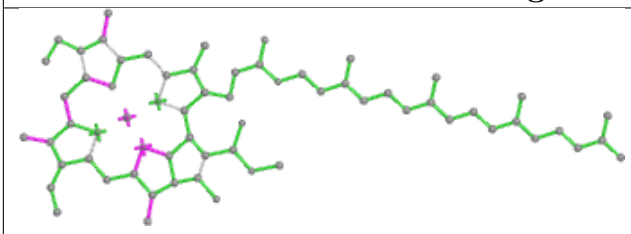


Rings

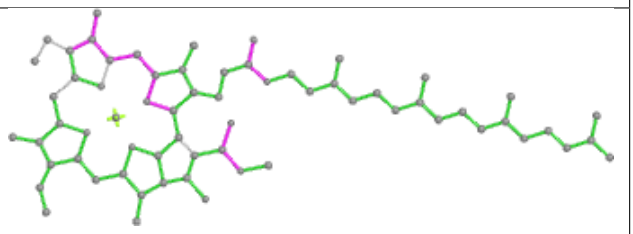
Ligand CLA d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

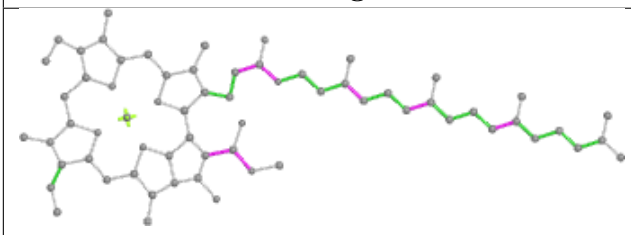
Ligand CLA d 403



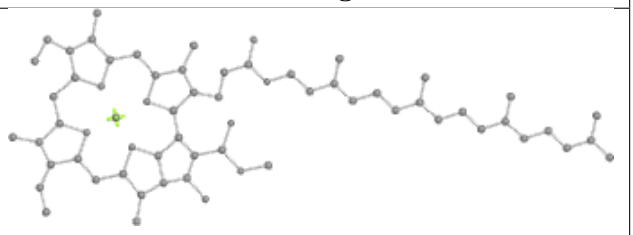
Bond lengths



Bond angles

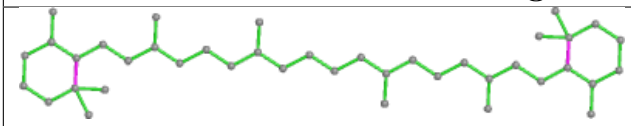


Torsions

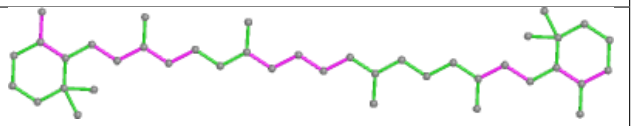


Rings

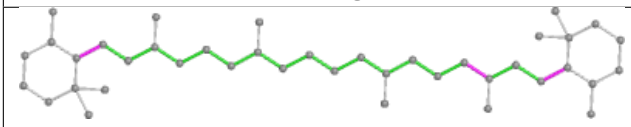
Ligand BCR c 516



Bond lengths



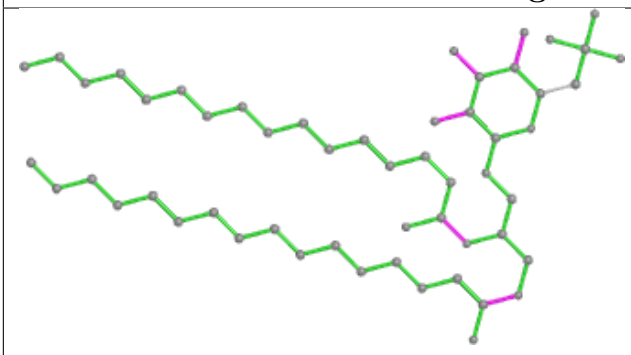
Bond angles



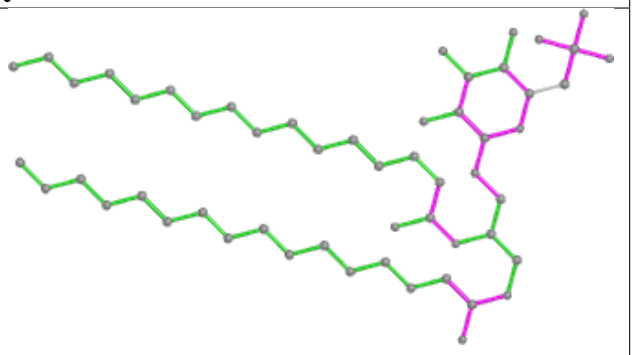
Torsions

Rings

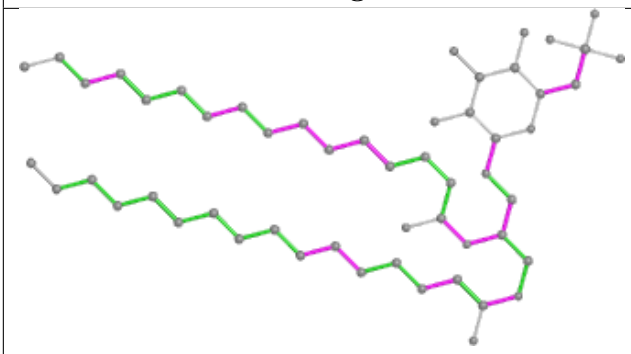
Ligand SQD a 411



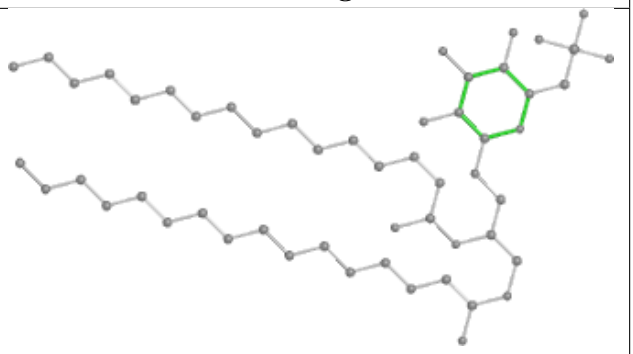
Bond lengths



Bond angles

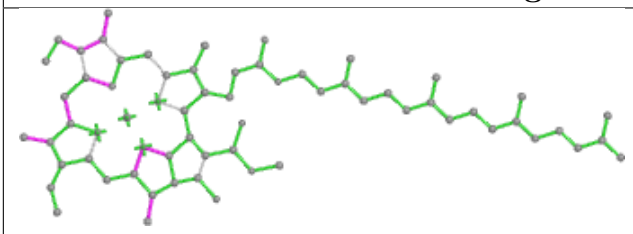


Torsions

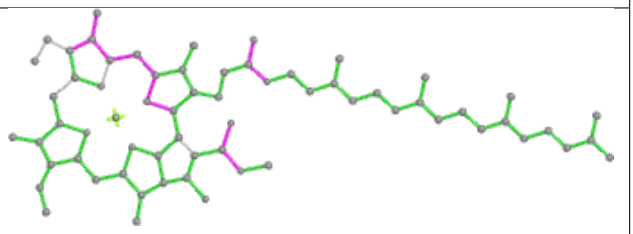


Rings

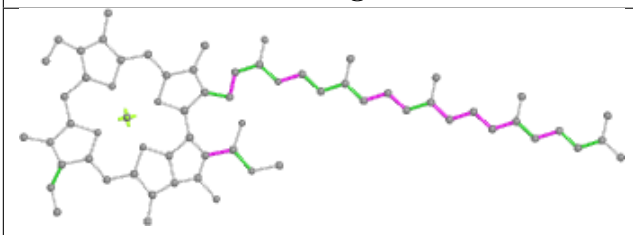
Ligand CLA C 509



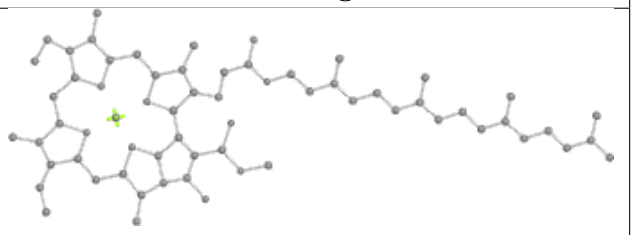
Bond lengths



Bond angles

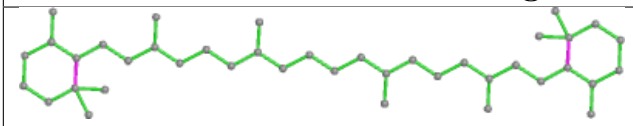


Torsions

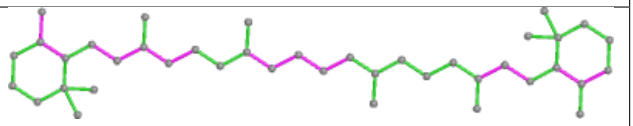


Rings

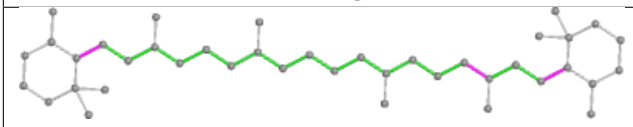
Ligand BCR C 517



Bond lengths



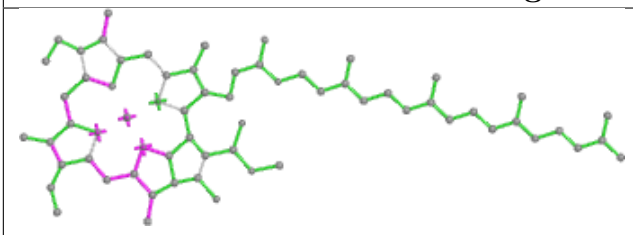
Bond angles



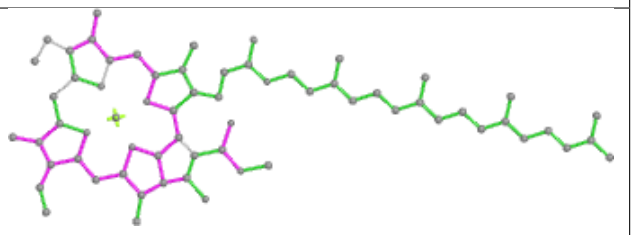
Torsions

Rings

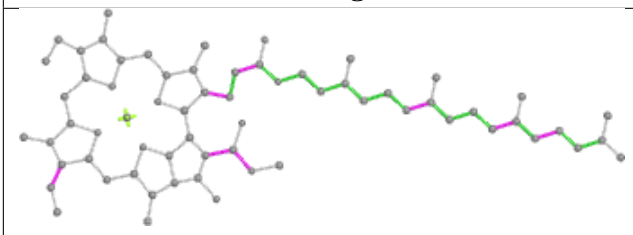
Ligand CLA C 511



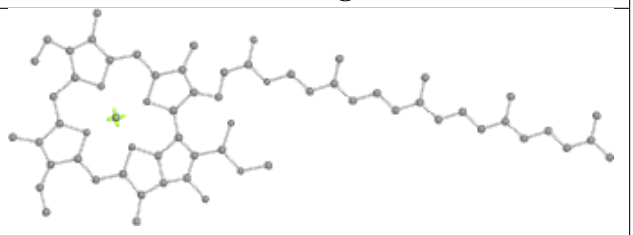
Bond lengths



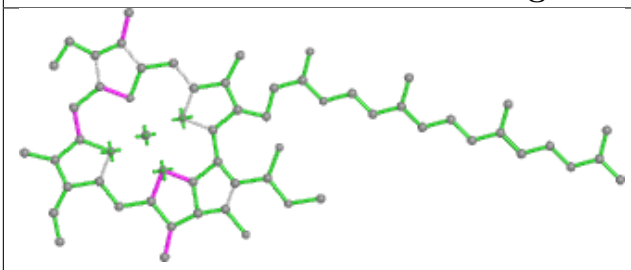
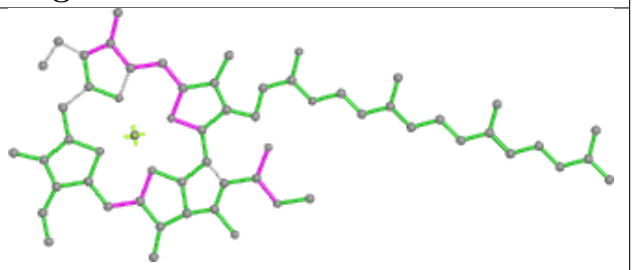
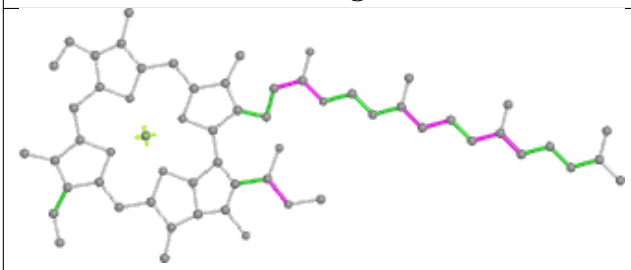
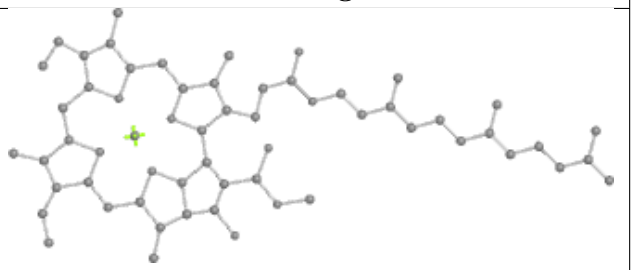
Bond angles

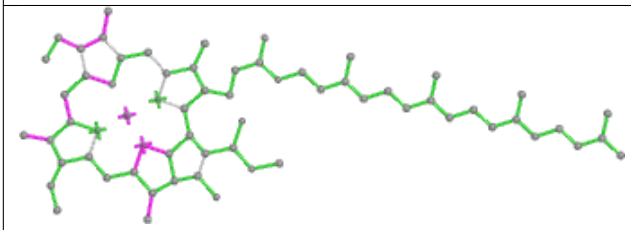
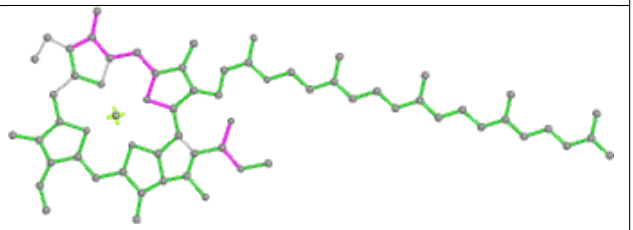
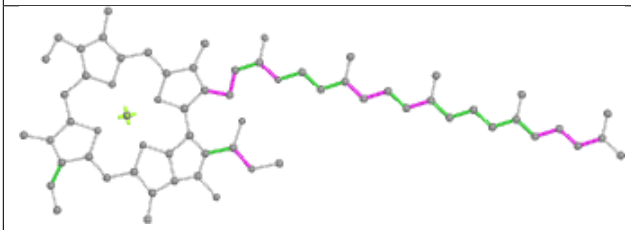
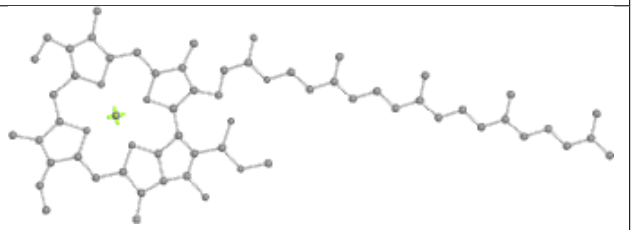


Torsions

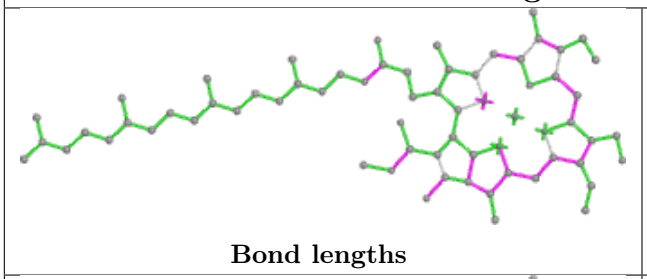


Rings

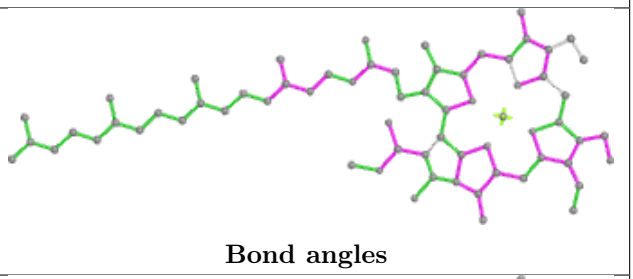
Ligand CLA g 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

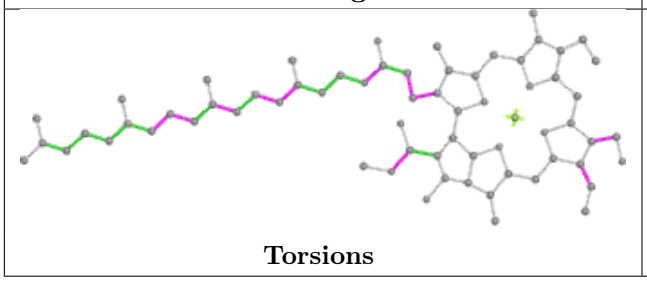
Ligand CHL N 606



Bond lengths



Bond angles



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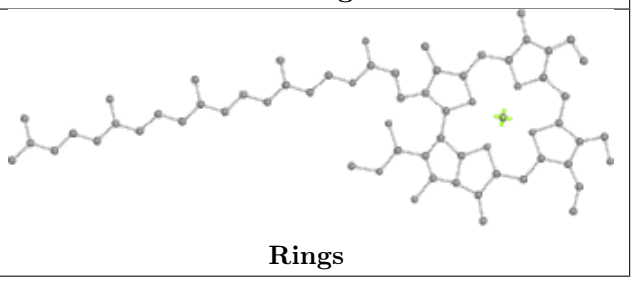
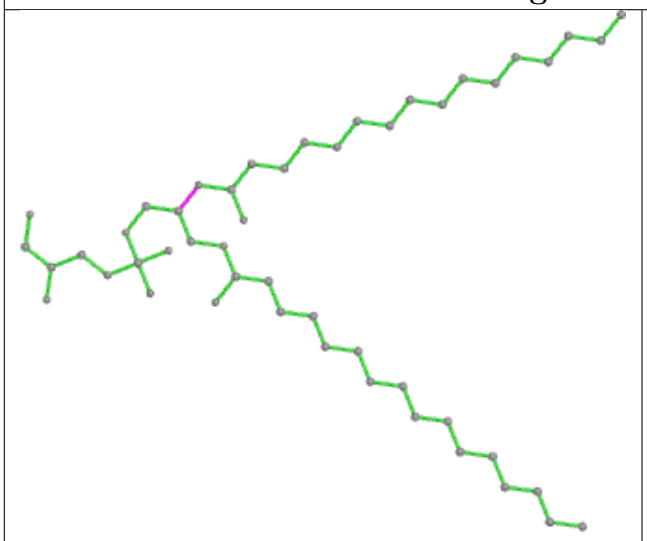


Rings

Ligand LHG s 314



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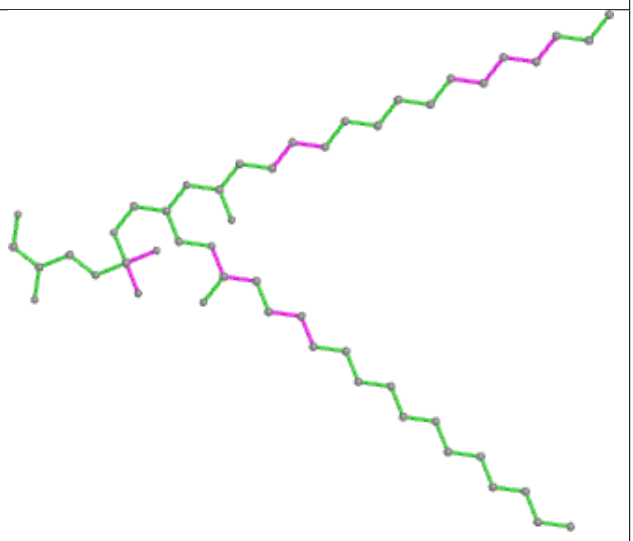
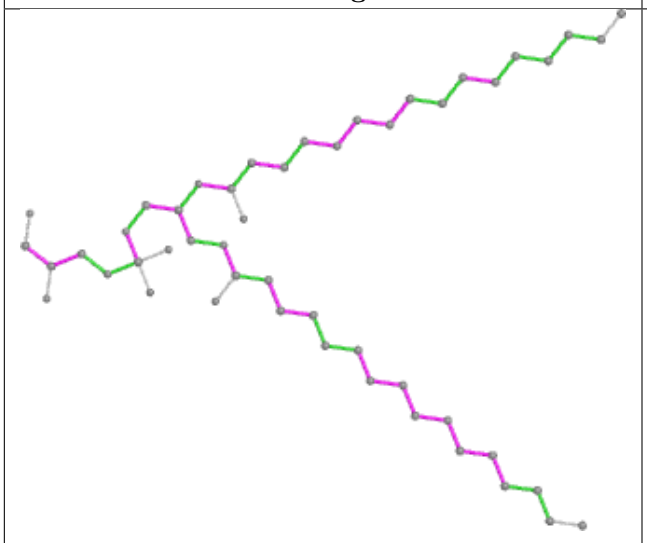


Bond angles



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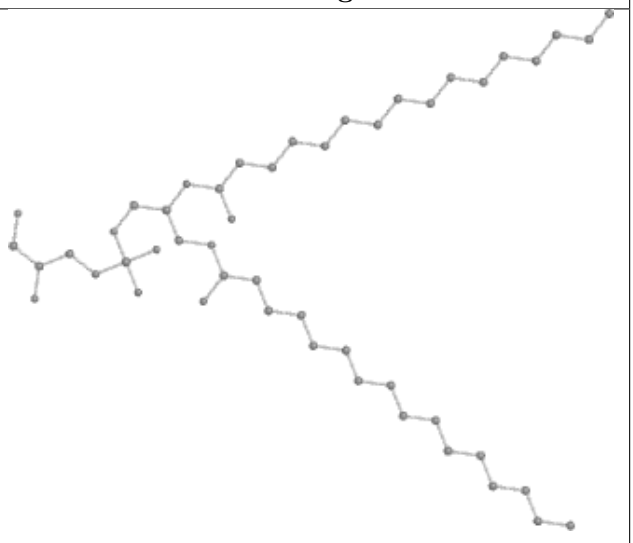
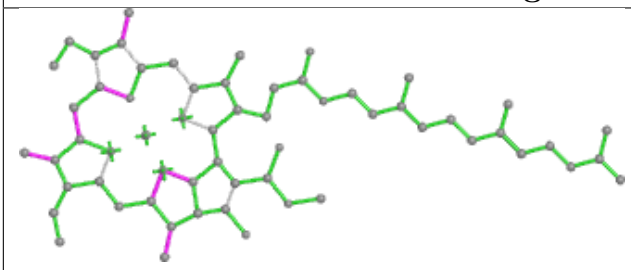
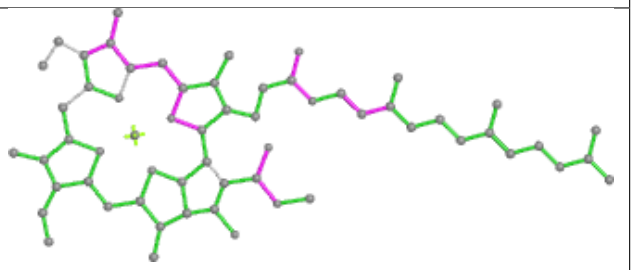
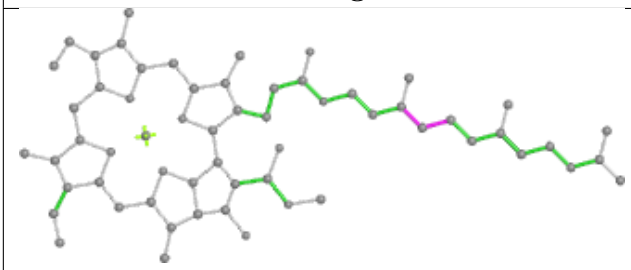
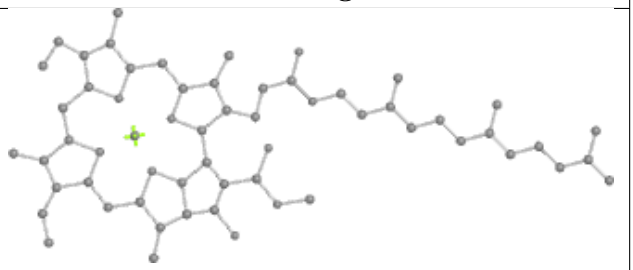
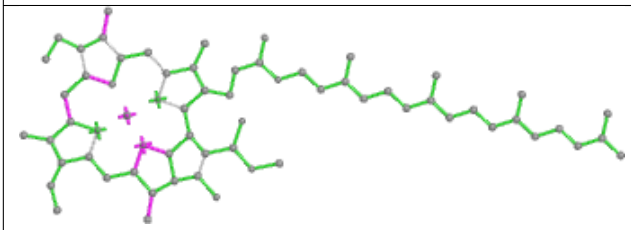
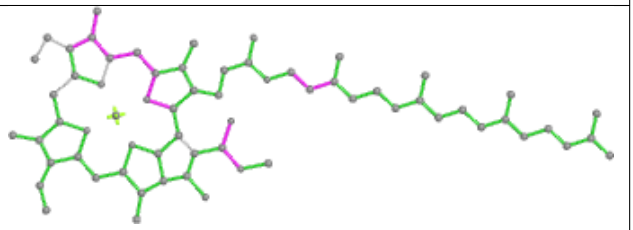
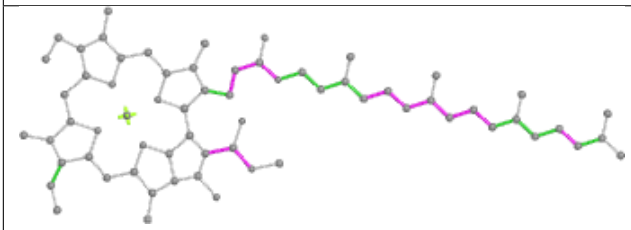
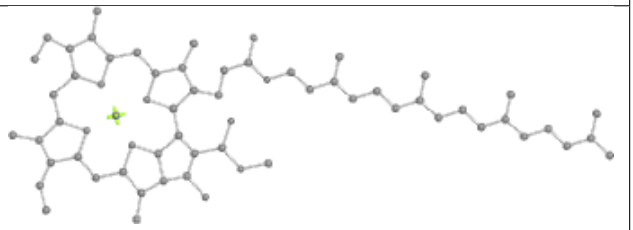
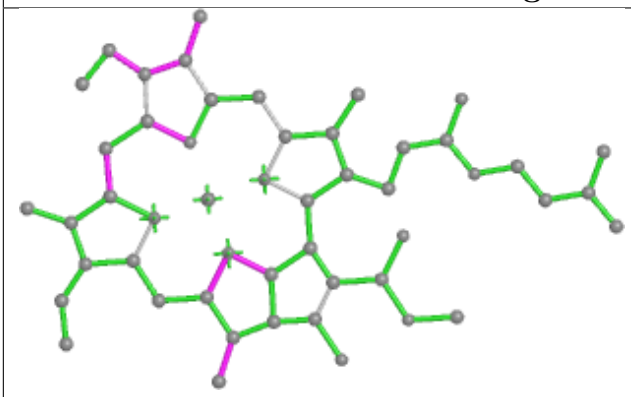
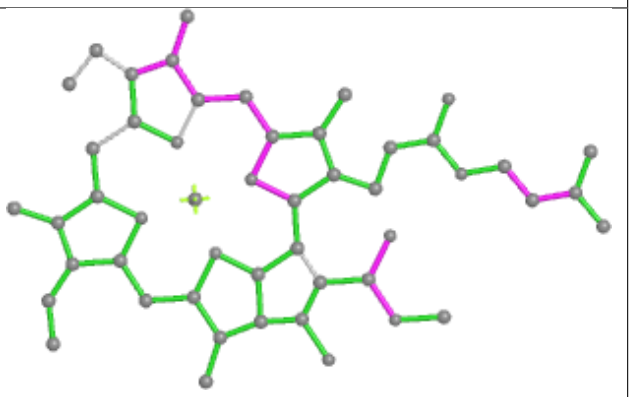
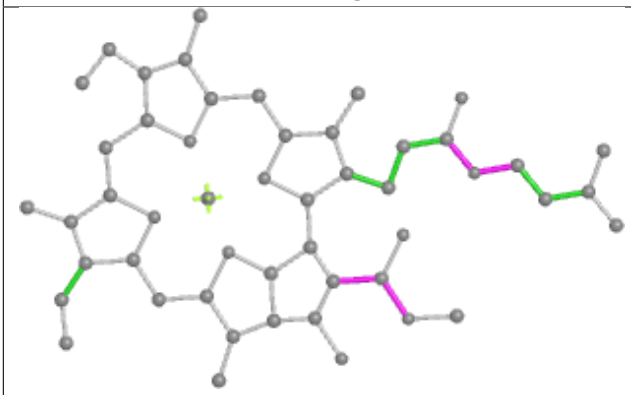
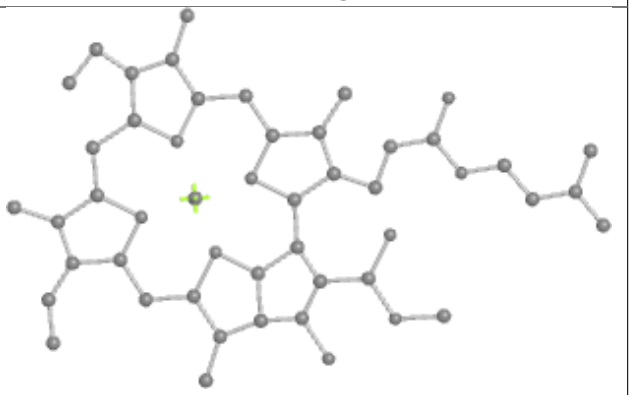
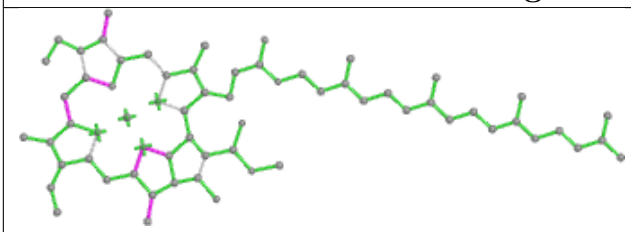
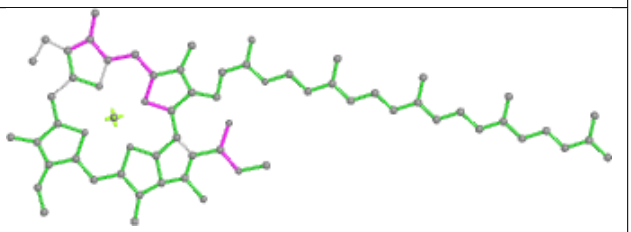
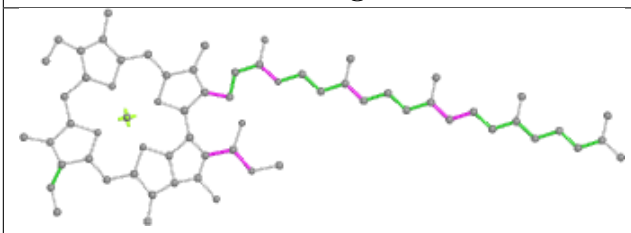
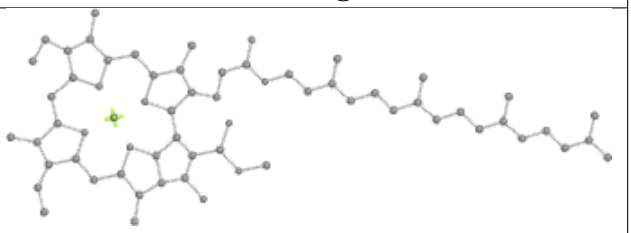


Rings

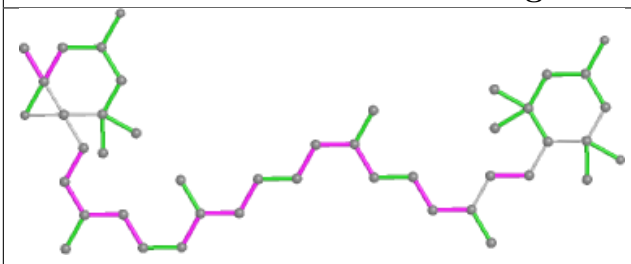
Ligand CLA A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA y 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

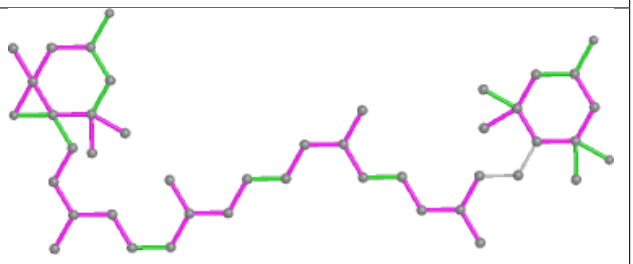
Ligand CLA N 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

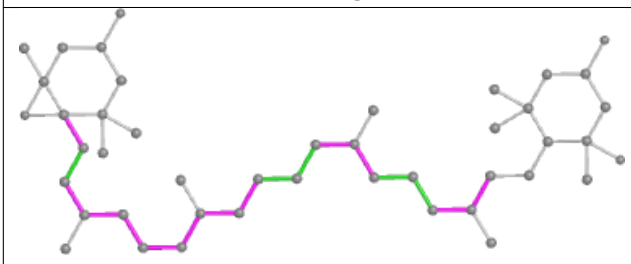
Ligand NEX n 616



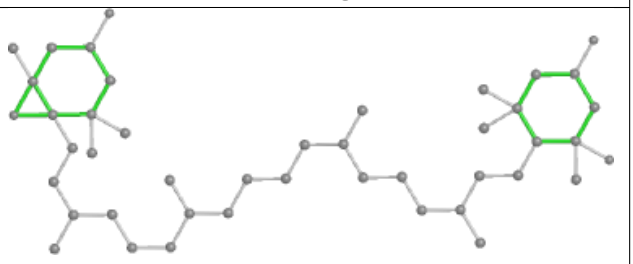
Bond lengths



Bond angles

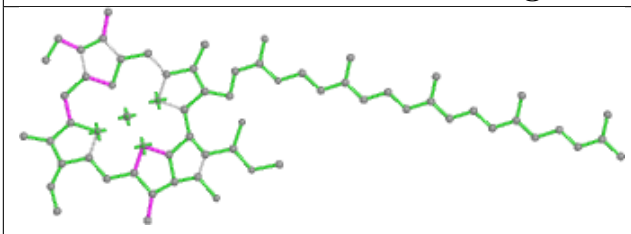


Torsions



Rings

Ligand CLA A 406



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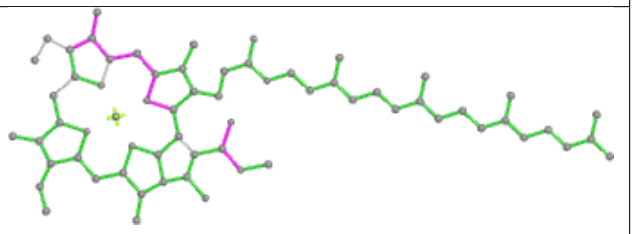
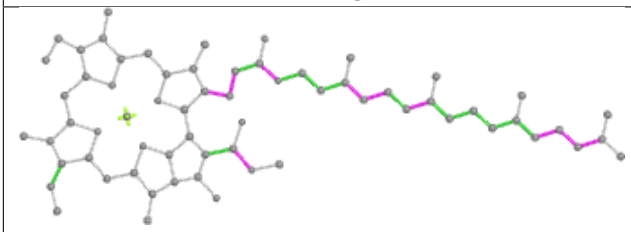


Bond angles



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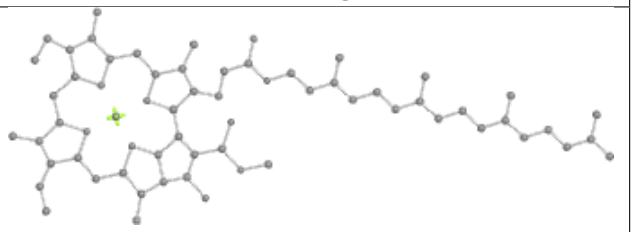
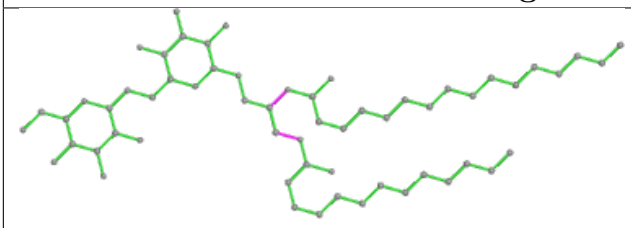
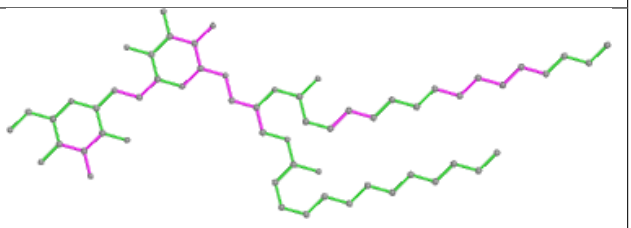


Rings

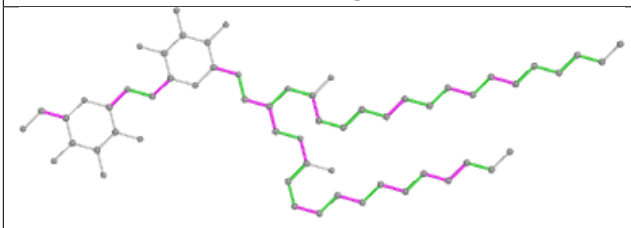
Ligand DGD A 401



Bond lengths



Bond angles



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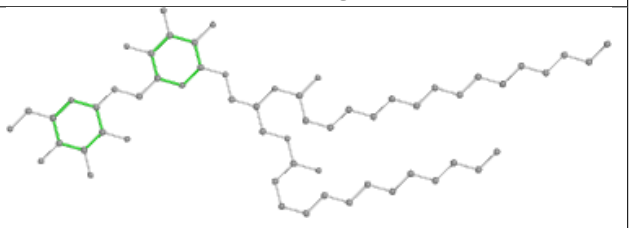
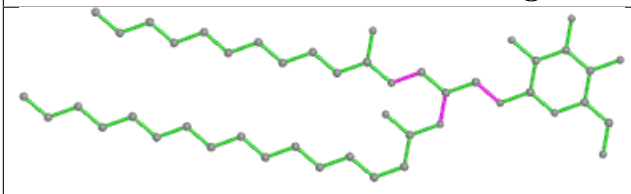


Rings

Ligand LMG d 410



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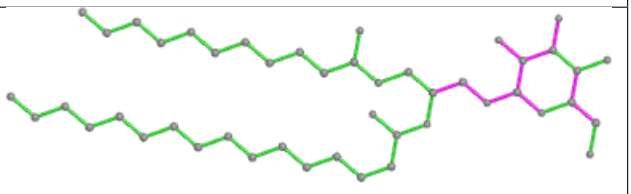
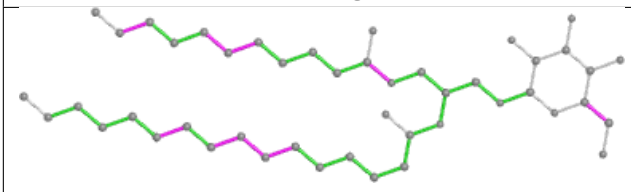
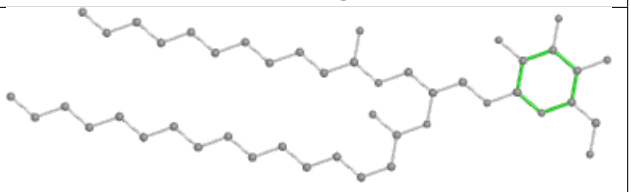


Bond angles

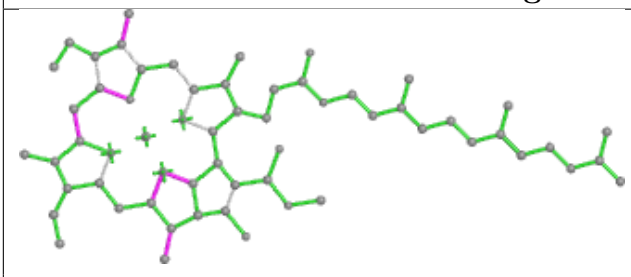


Torsions



Rings

Ligand CLA Y 609



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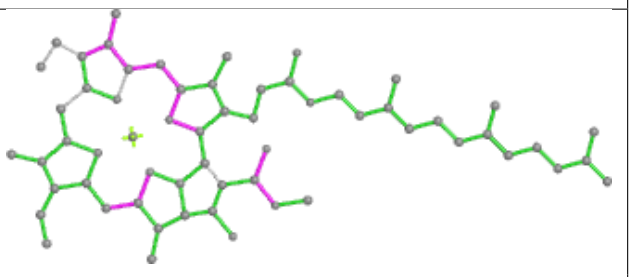
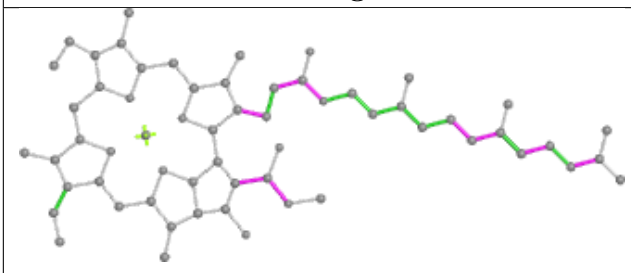
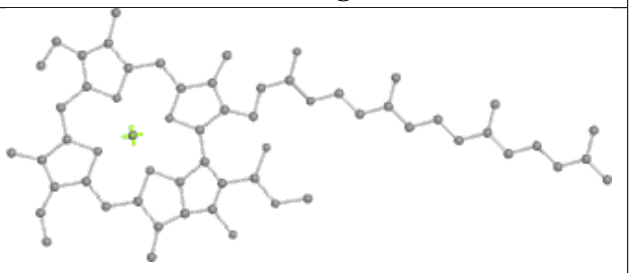


Bond angles

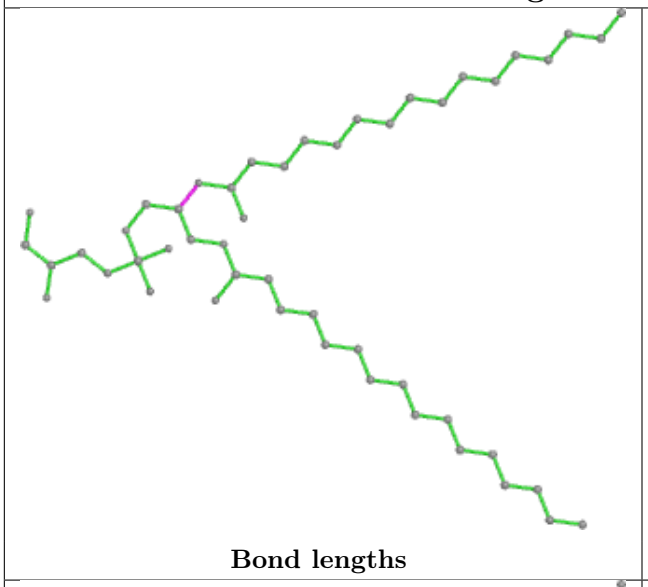


Torsions



Rings

Ligand LHG y 617



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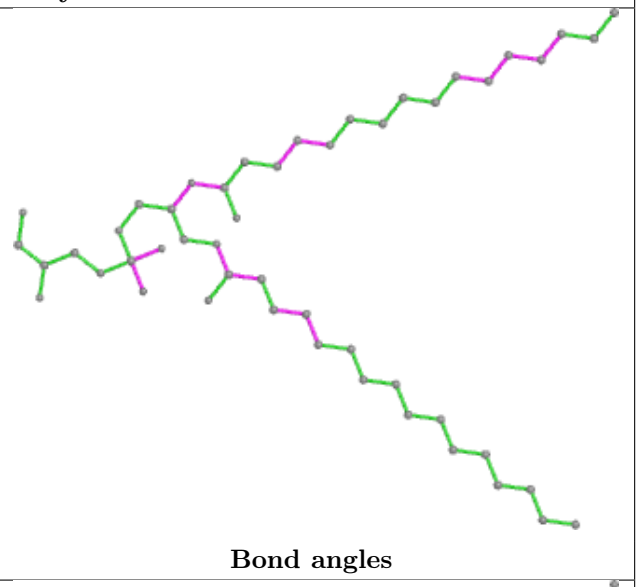
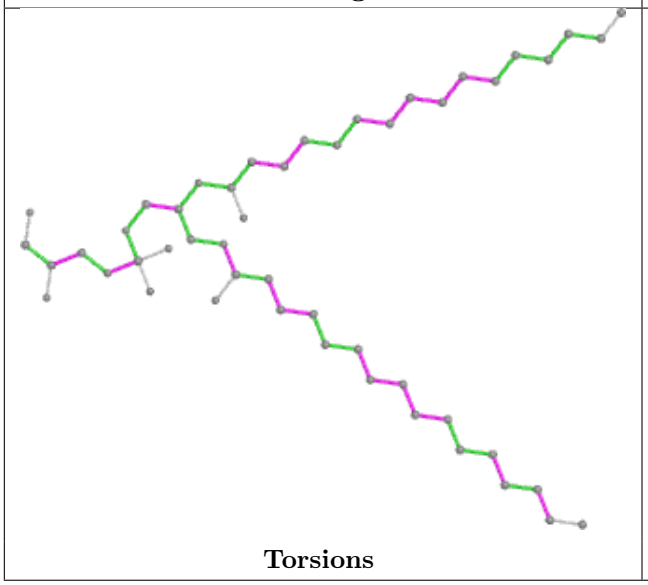
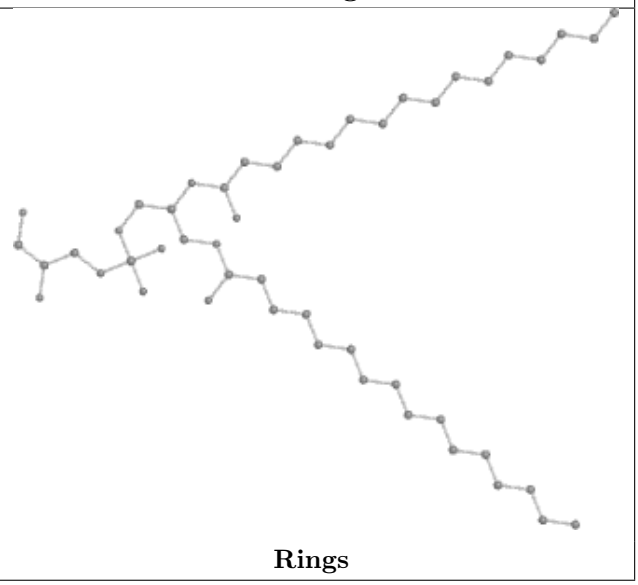


Bond angles

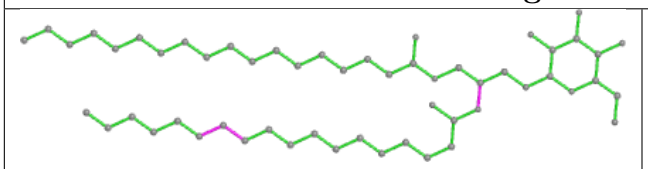


Torsions

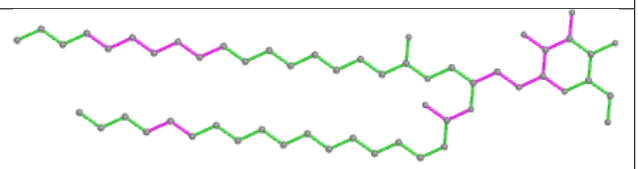


Rings

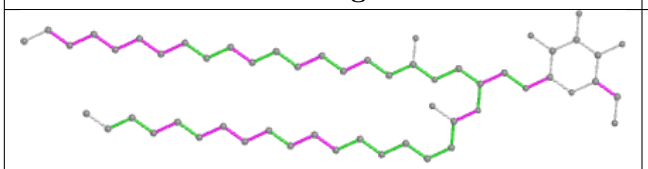
Ligand LMG b 620



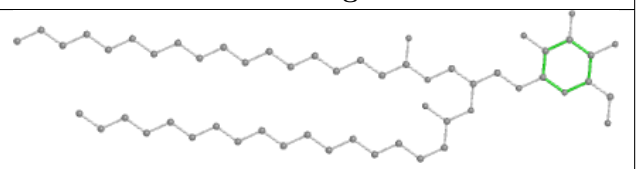
Bond lengths



Bond angles

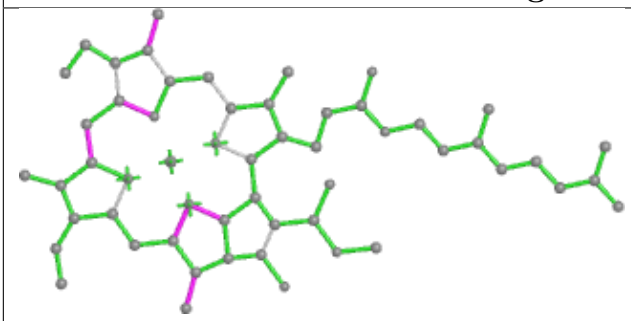


Torsions

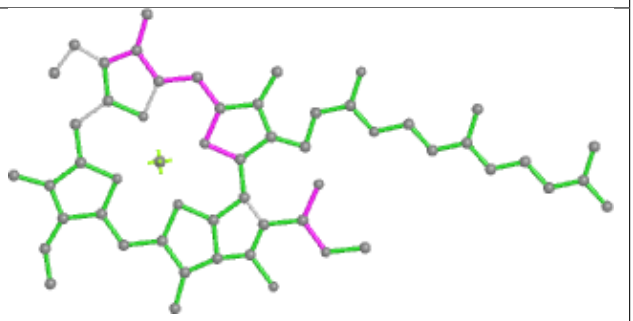


Rings

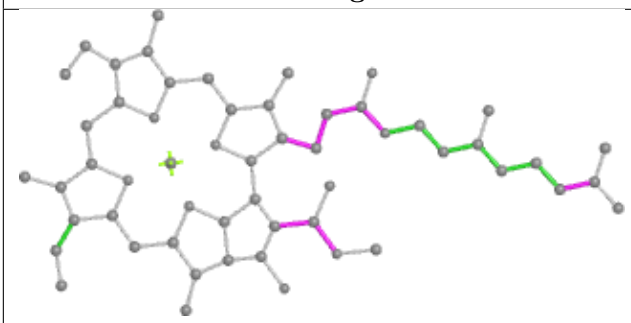
Ligand CLA S 313



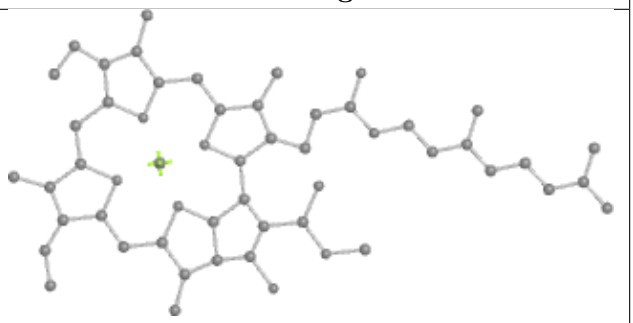
Bond lengths



Bond angles

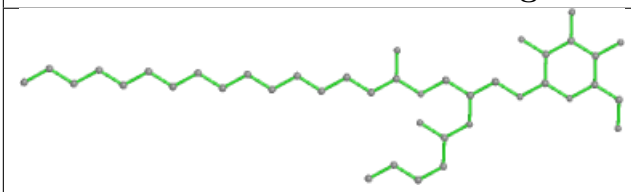


Torsions

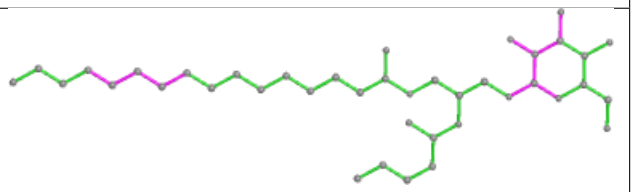


Rings

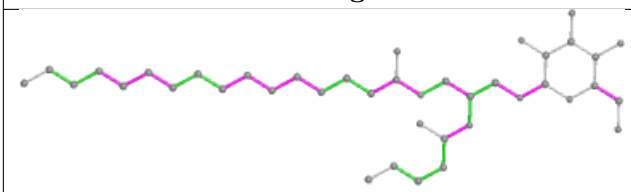
Ligand LMG B 601



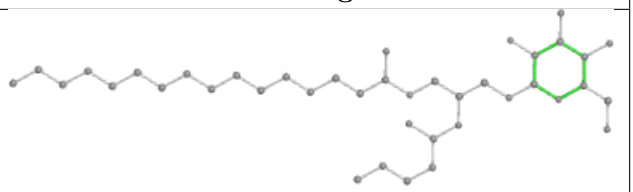
Bond lengths



Bond angles

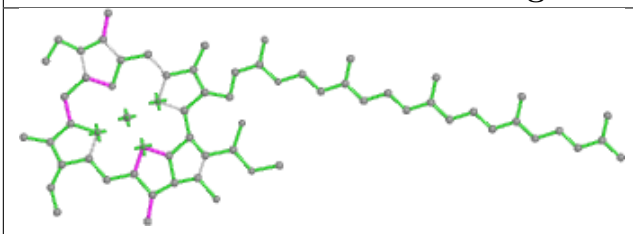


Torsions



Rings

Ligand CLA n 609



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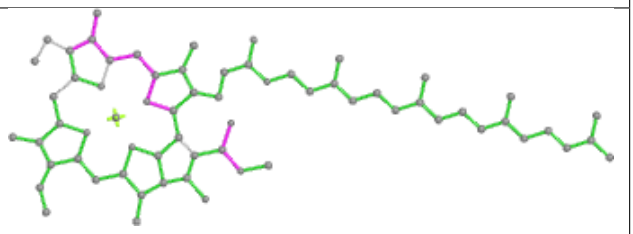
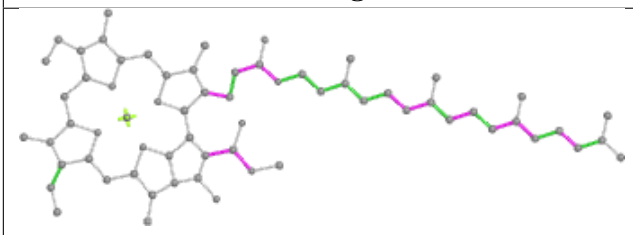


Bond angles



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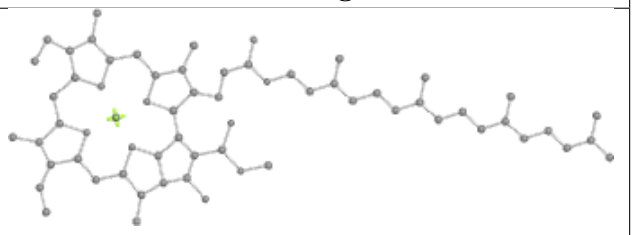
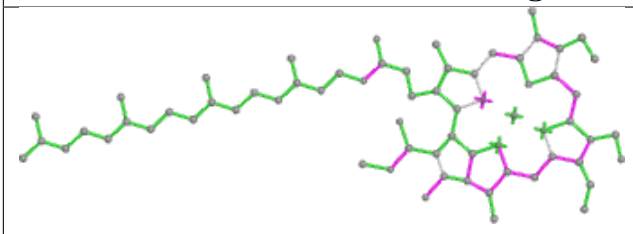


Rings

Ligand CHL n 607



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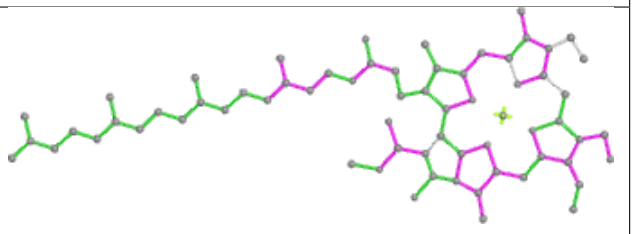
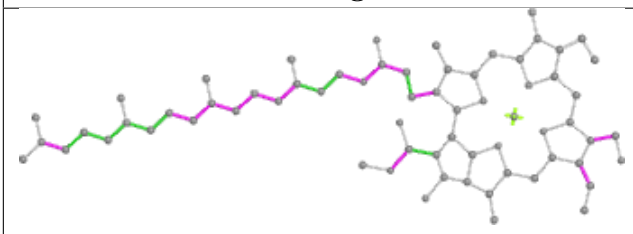
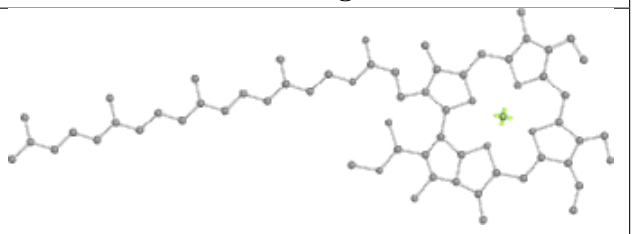


Bond angles

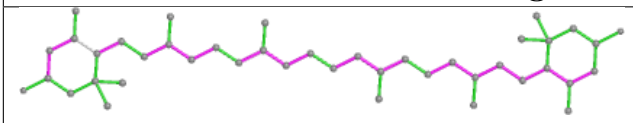


Torsions



Rings

Ligand LUT y 614



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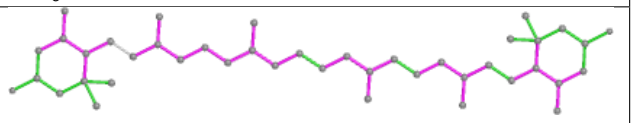
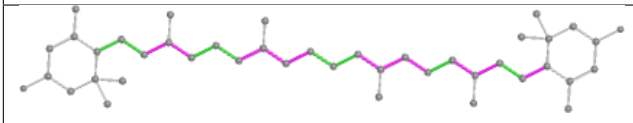


Bond angles



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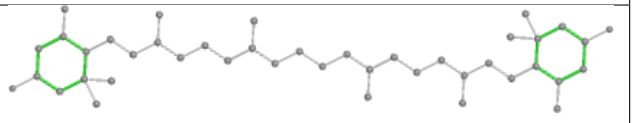
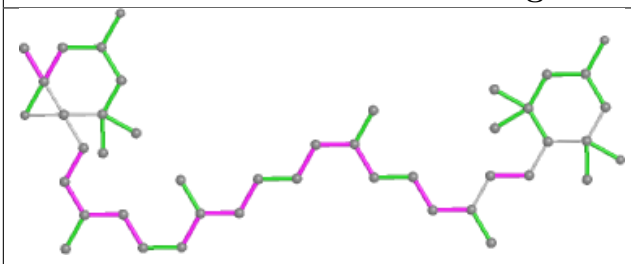


Rings

Ligand NEX g 618



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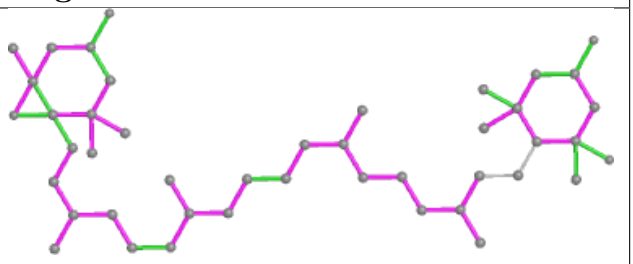
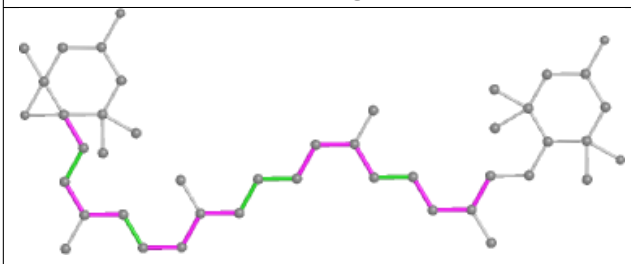


Bond angles



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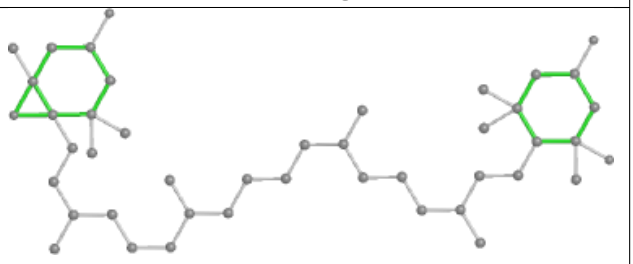
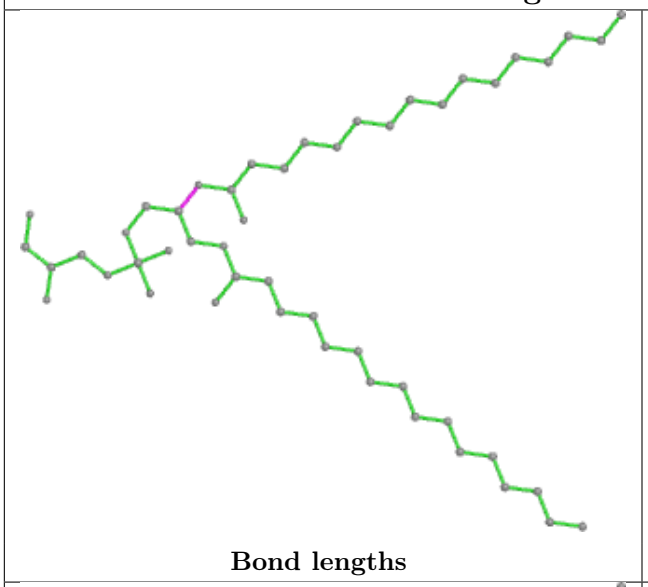
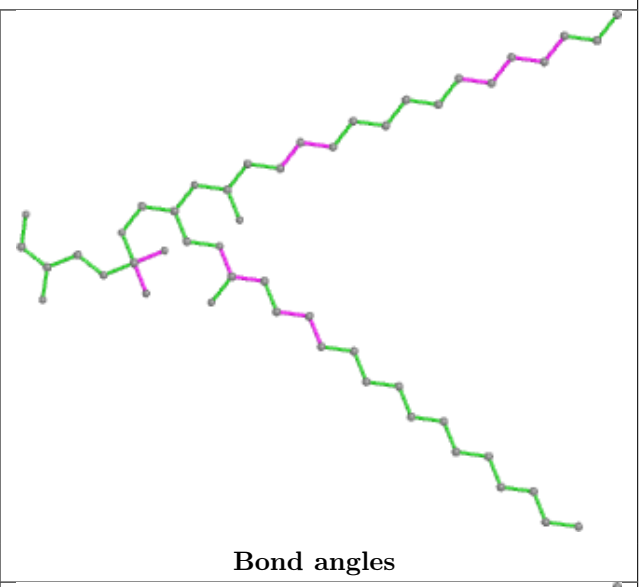


Rings

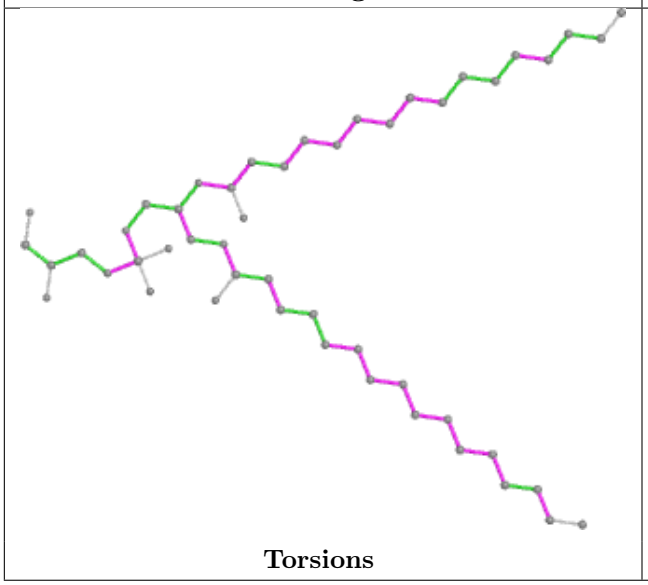
Ligand LHG B 622



Bond lengths



Bond angles



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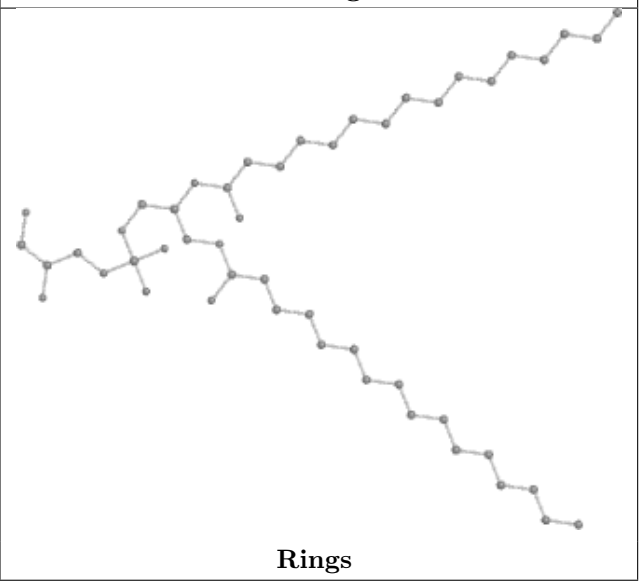
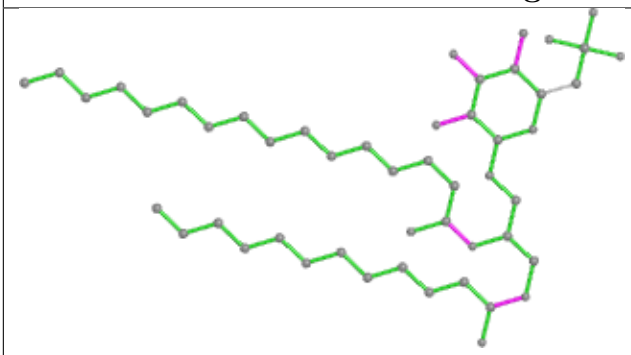
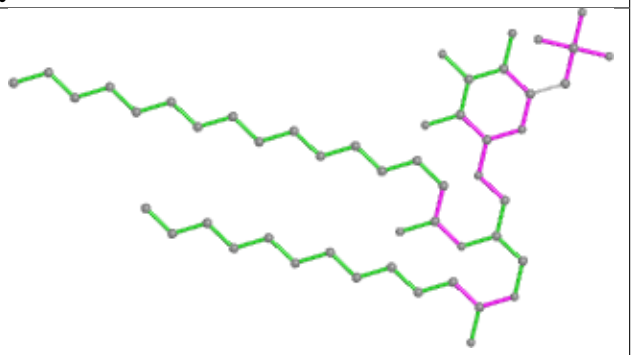


Rings

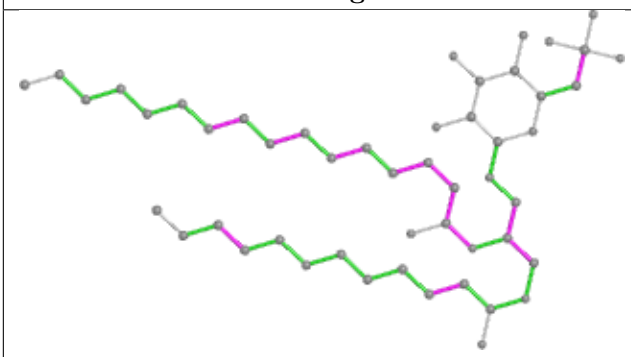
Ligand SQD D 402



Bond lengths



Bond angles



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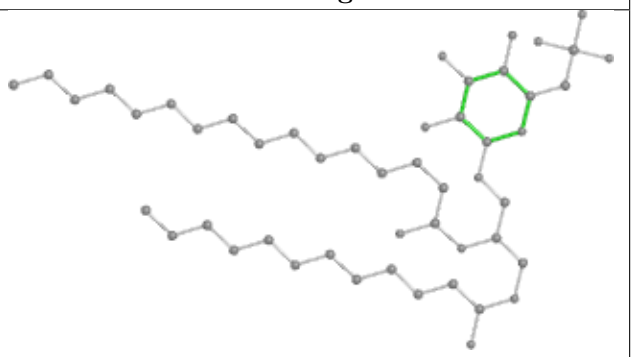
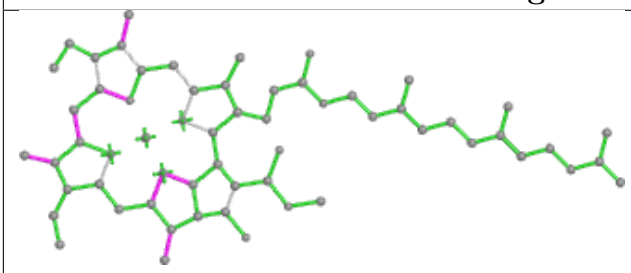


Rings

Ligand CLA y 611



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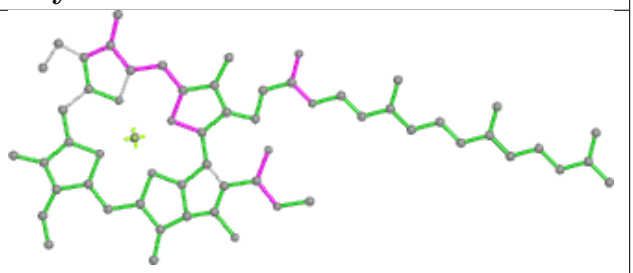
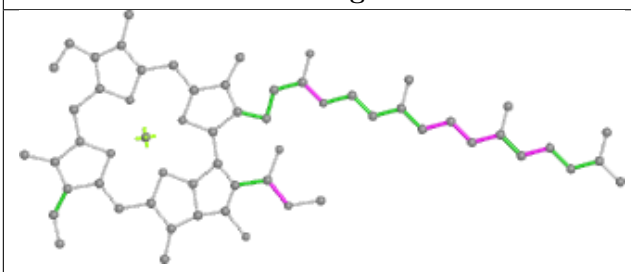


Bond angles



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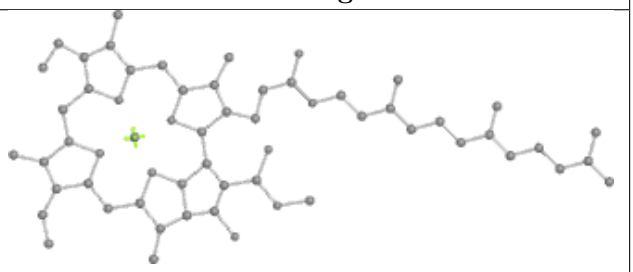
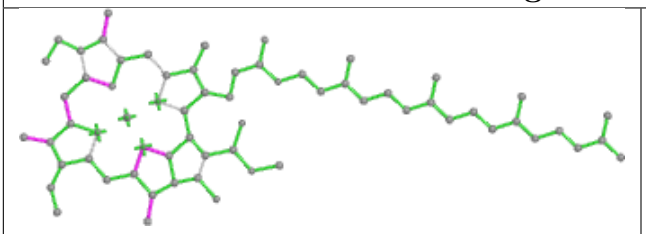


Rings

Ligand CLA B 612



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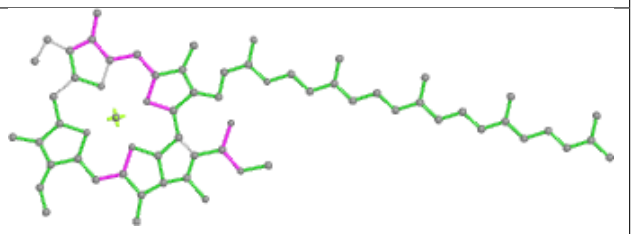
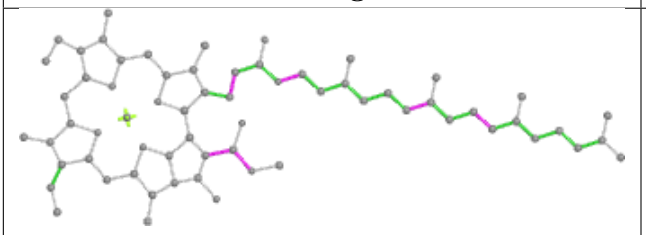


Bond angles



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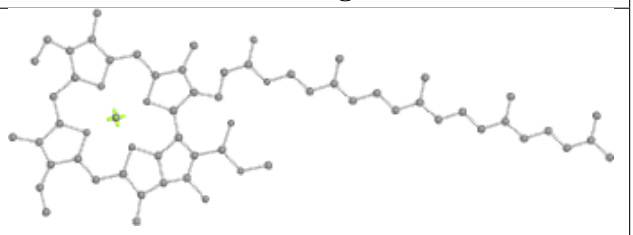
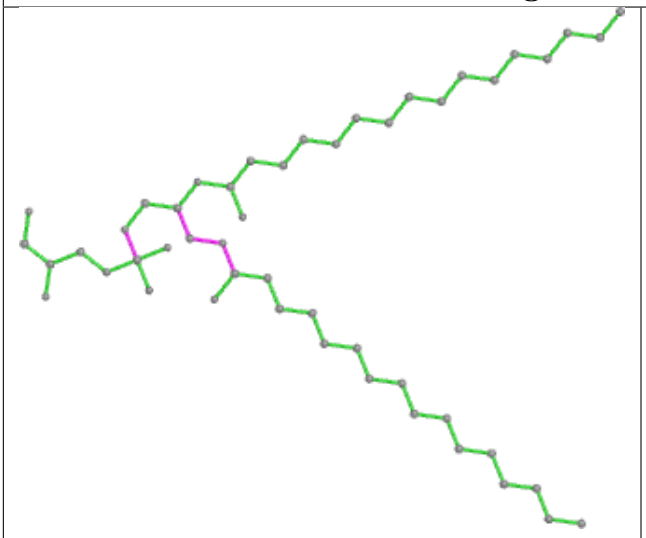


Rings

Ligand LHG C 520



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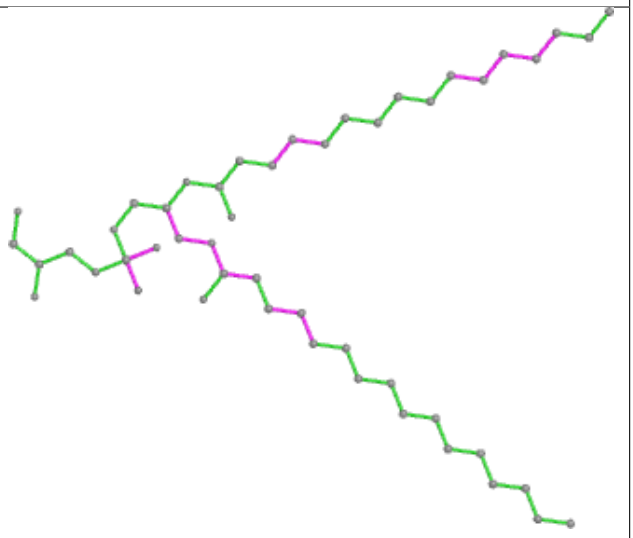
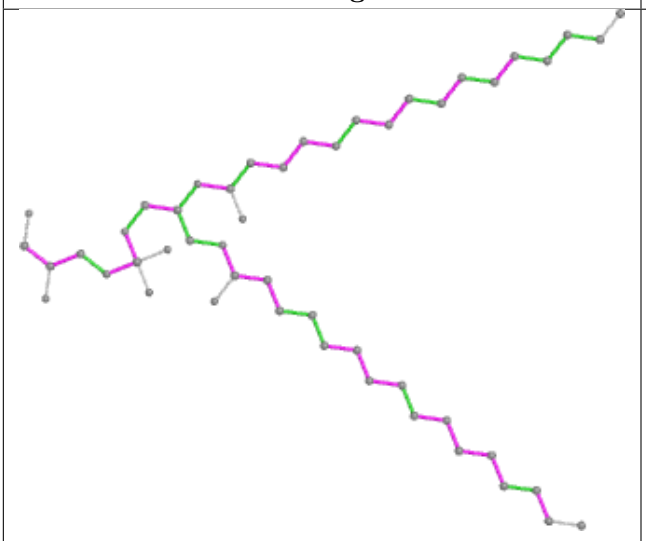
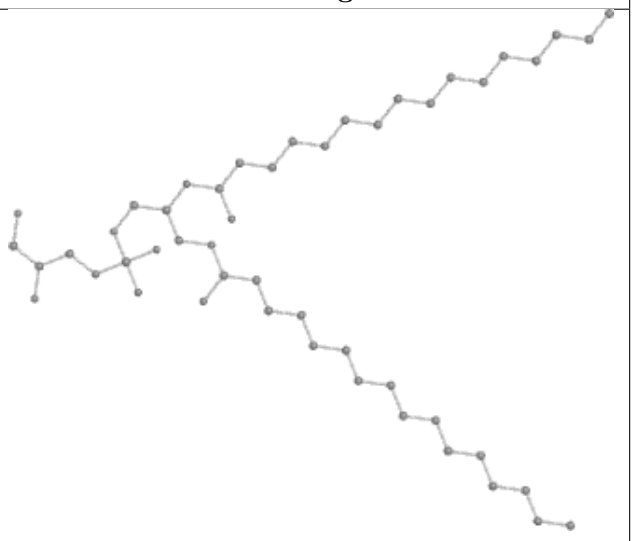


Bond angles

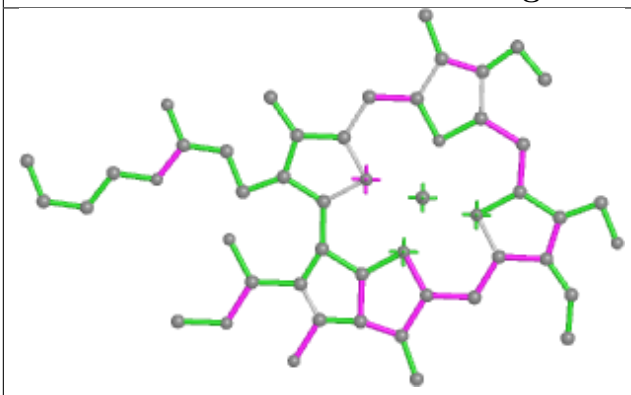


Torsions



Rings

Ligand CHL G 606



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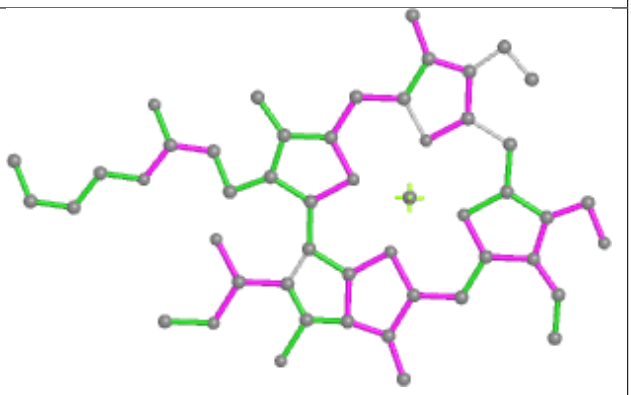
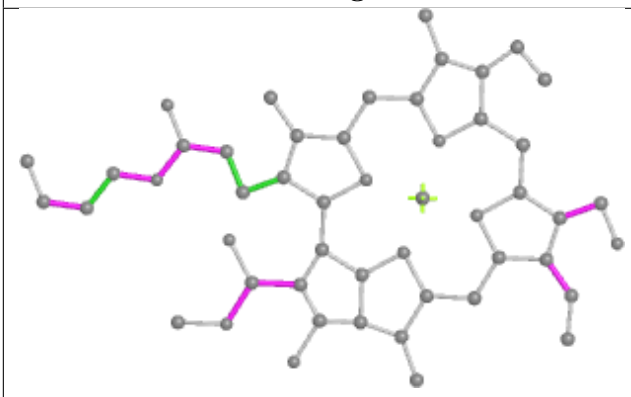


Bond angles



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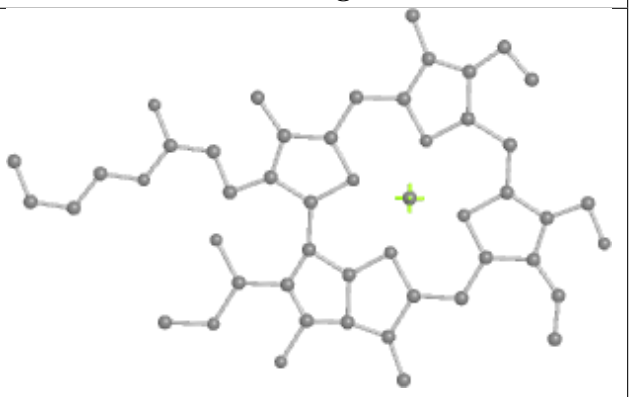
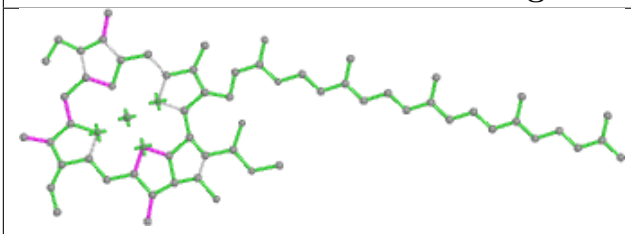


Rings

Ligand CLA b 614



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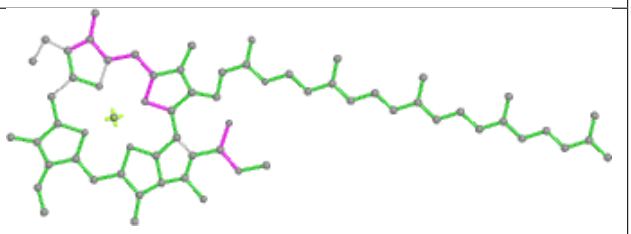
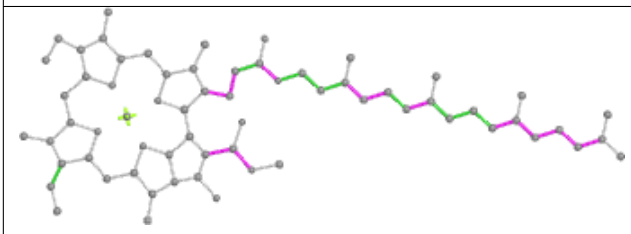
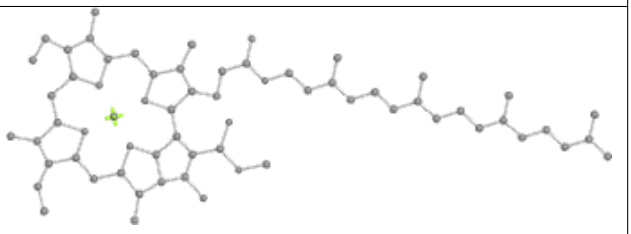


Bond angles

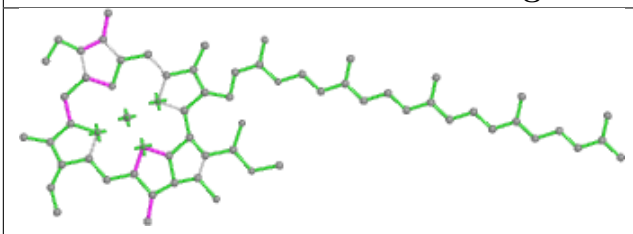


Torsions

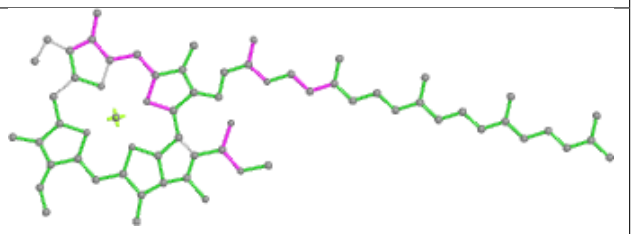


Rings

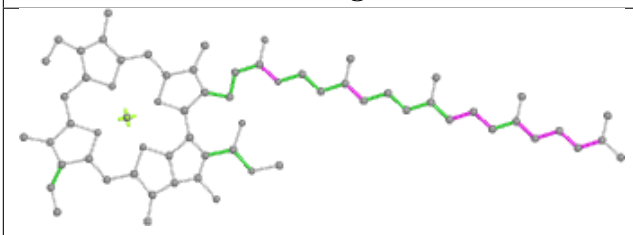
Ligand CLA D 405



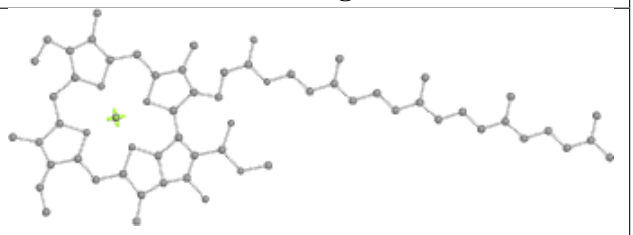
Bond lengths



Bond angles

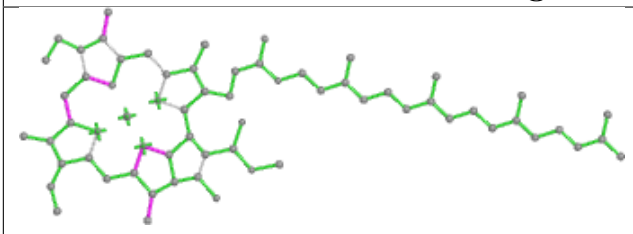


Torsions



Rings

Ligand CLA y 602



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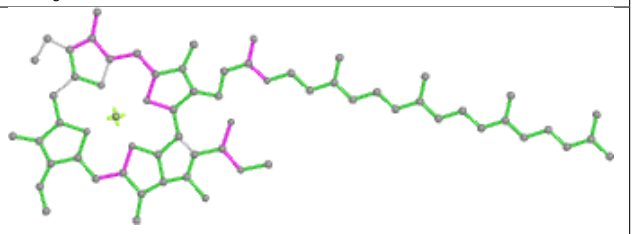
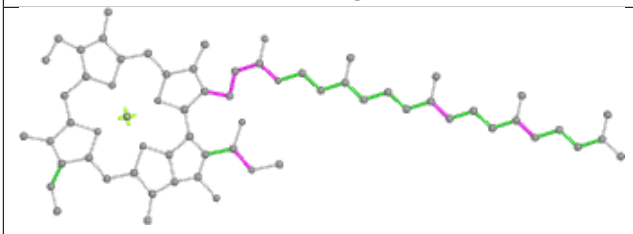
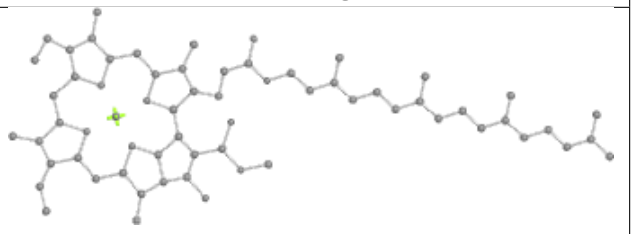


Bond angles

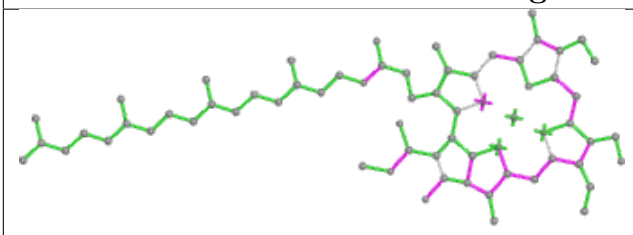


Torsions

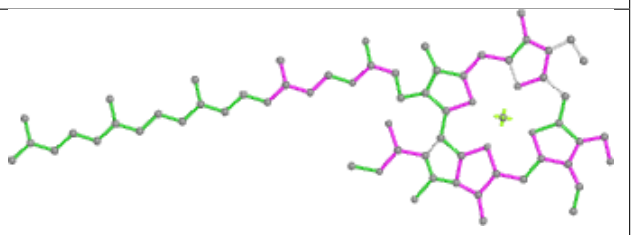


Rings

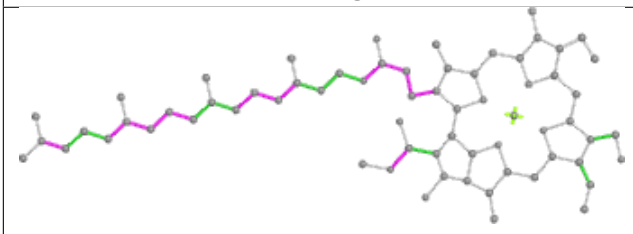
Ligand CHL r 306



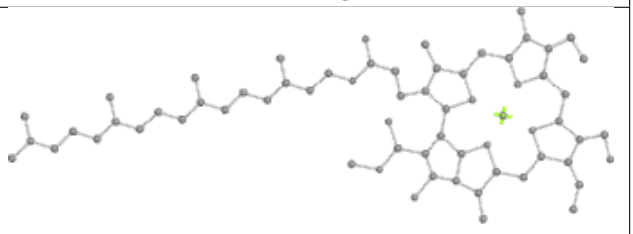
Bond lengths



Bond angles

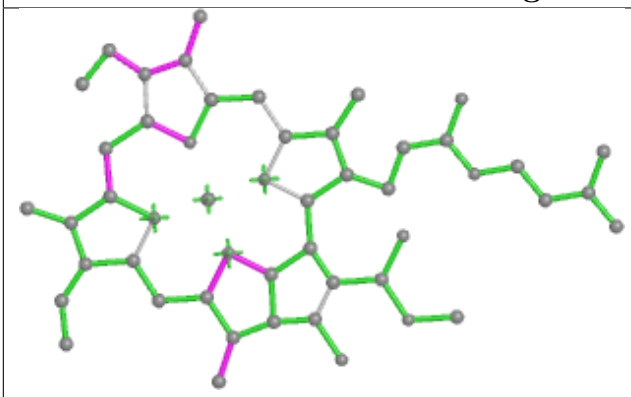


Torsions

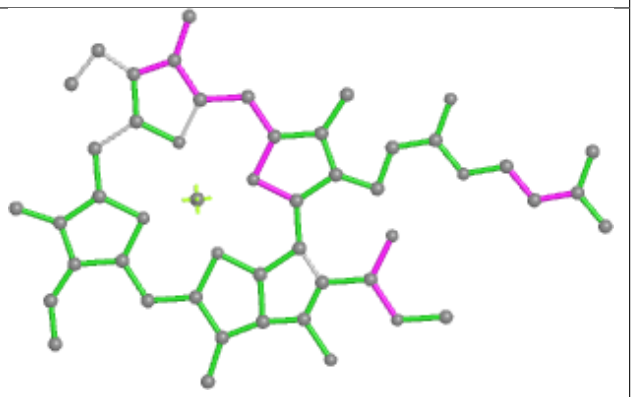


Rings

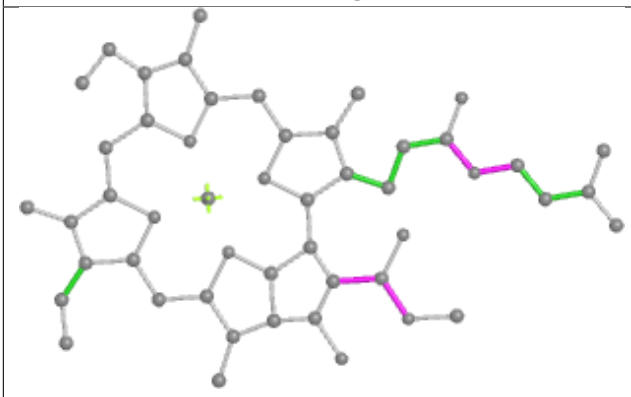
Ligand CLA G 604



Bond lengths



Bond angles



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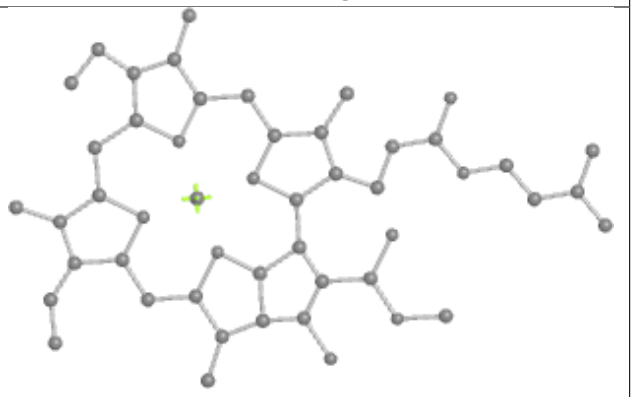
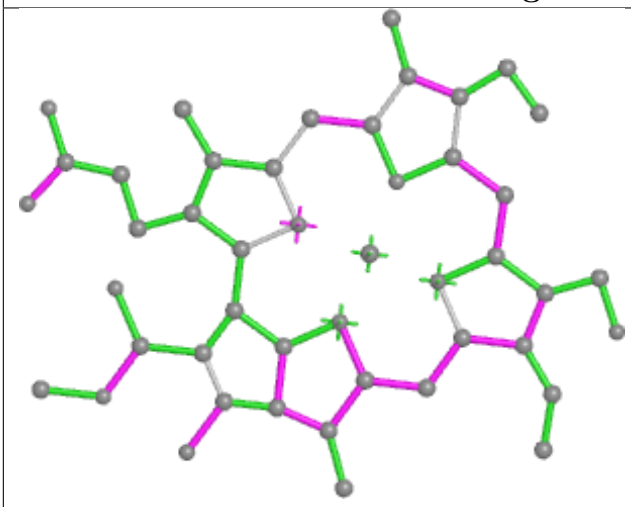


Rings

Ligand CHL G 605



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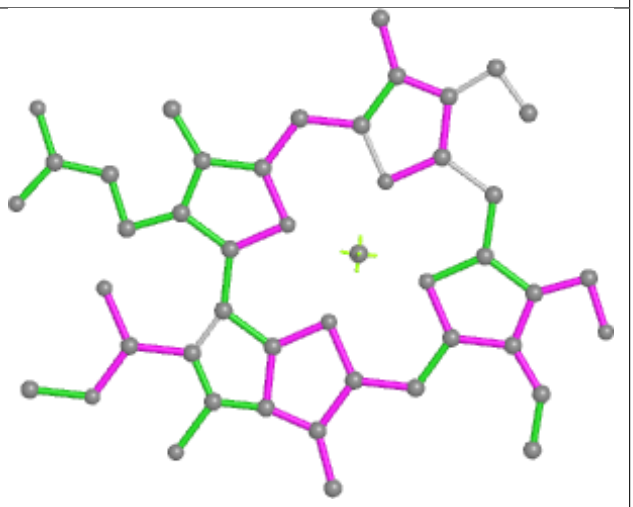
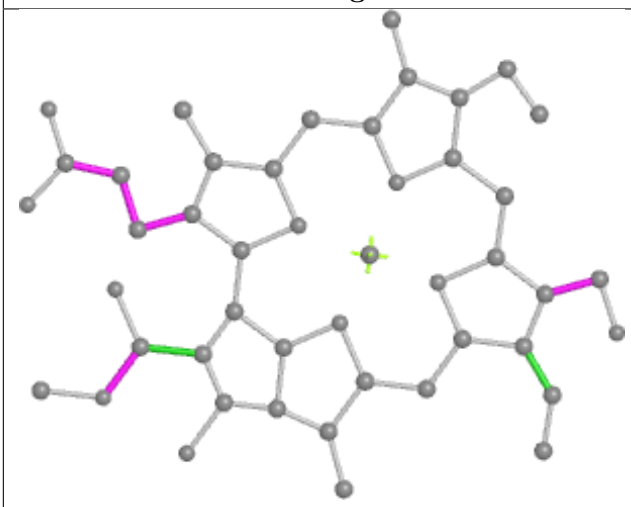


Bond angles



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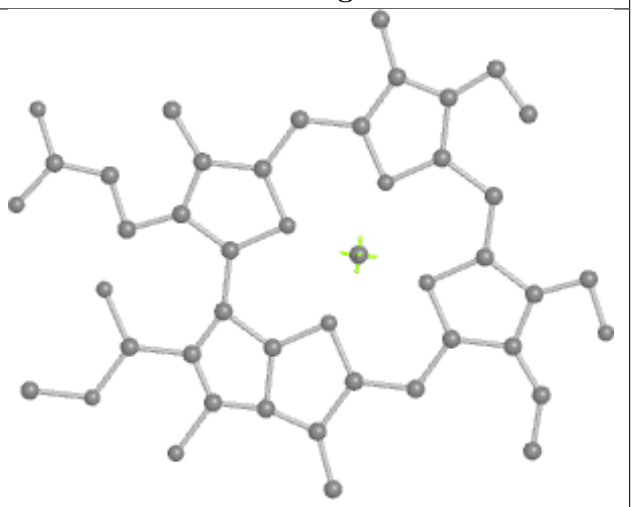
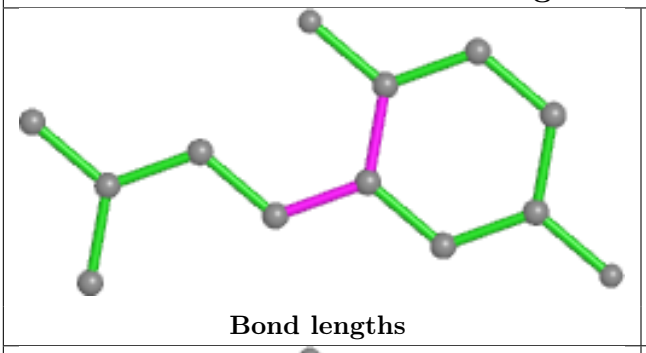


Rings

Ligand PL9 a 410



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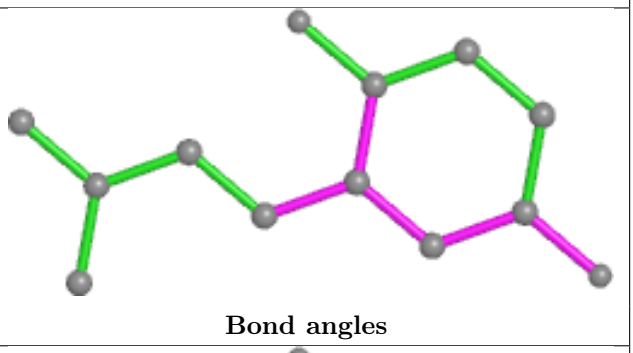
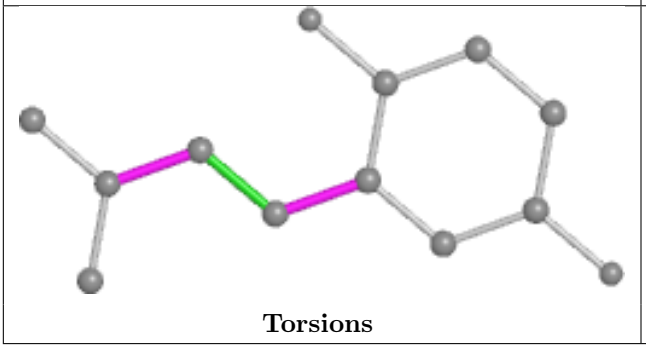


Bond angles



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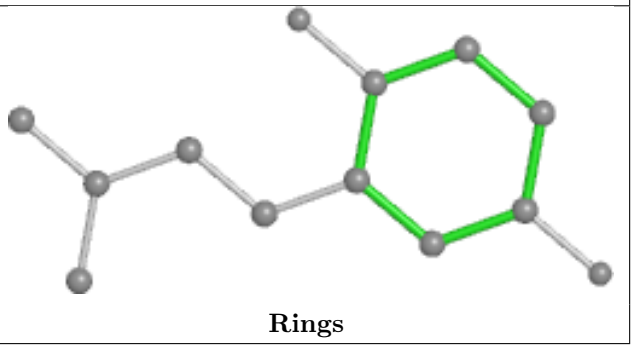
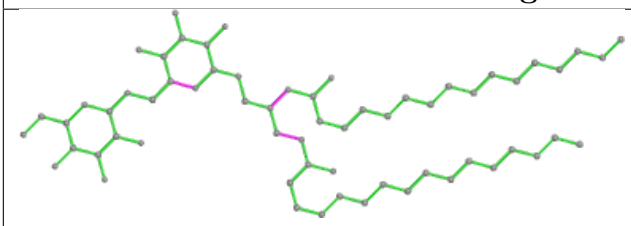


Rings

Ligand DGD C 519



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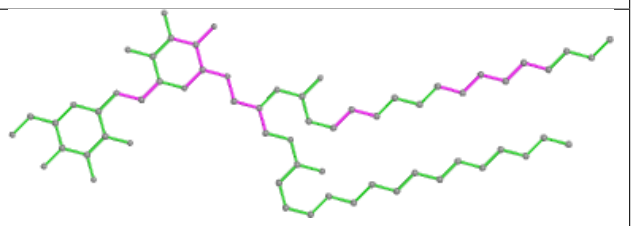
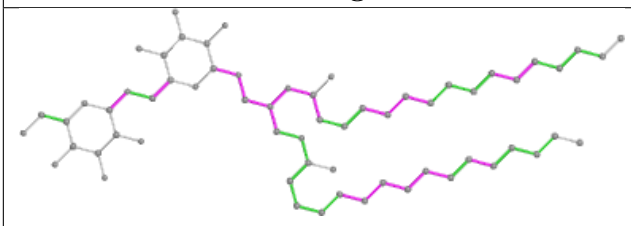
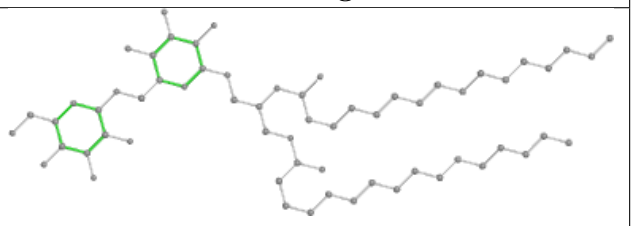


Bond angles

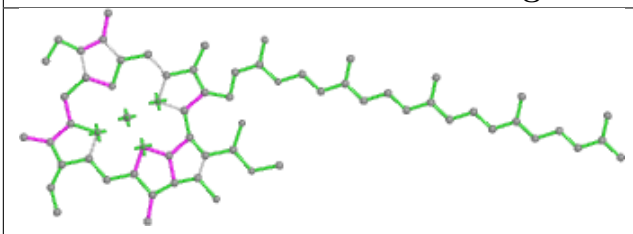


Torsions



Rings

Ligand CLA G 613



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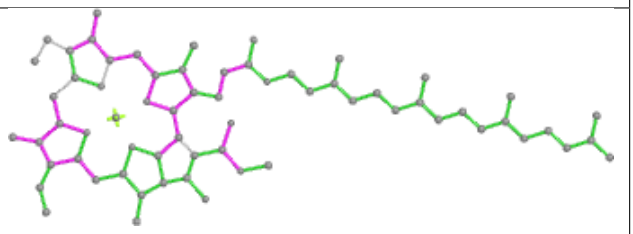
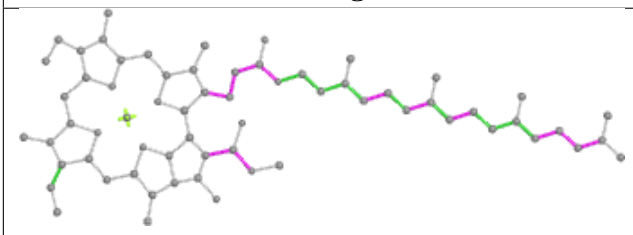


Bond angles



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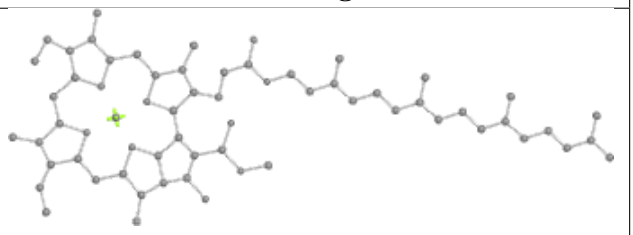
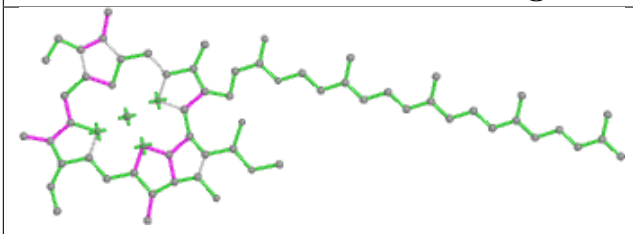
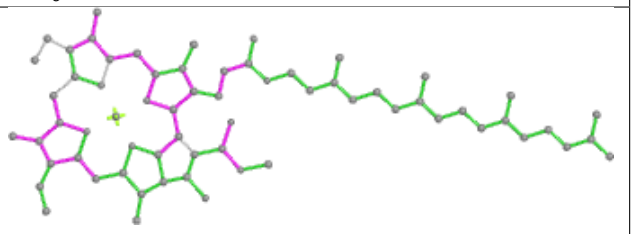


Rings

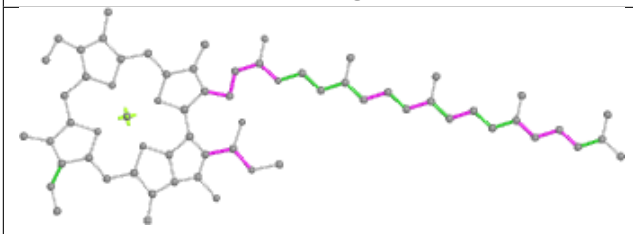
Ligand CLA y 612



Bond lengths



Bond angles



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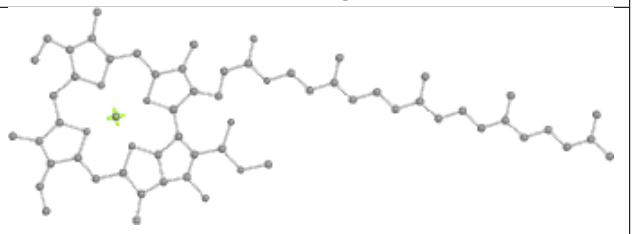
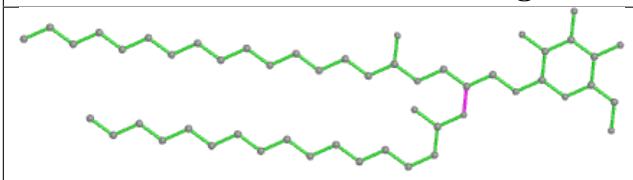


Rings

Ligand LMG M 101



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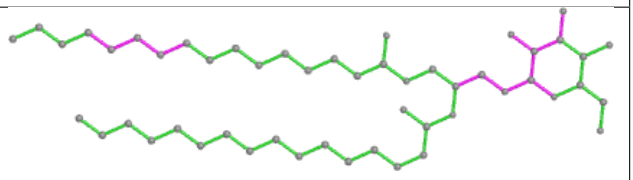
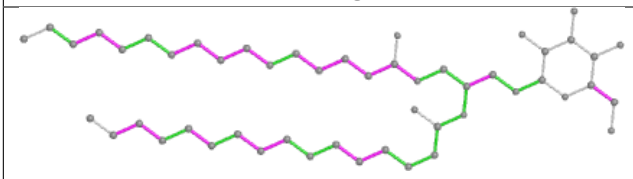


Bond angles



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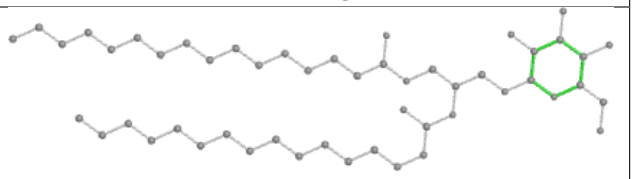
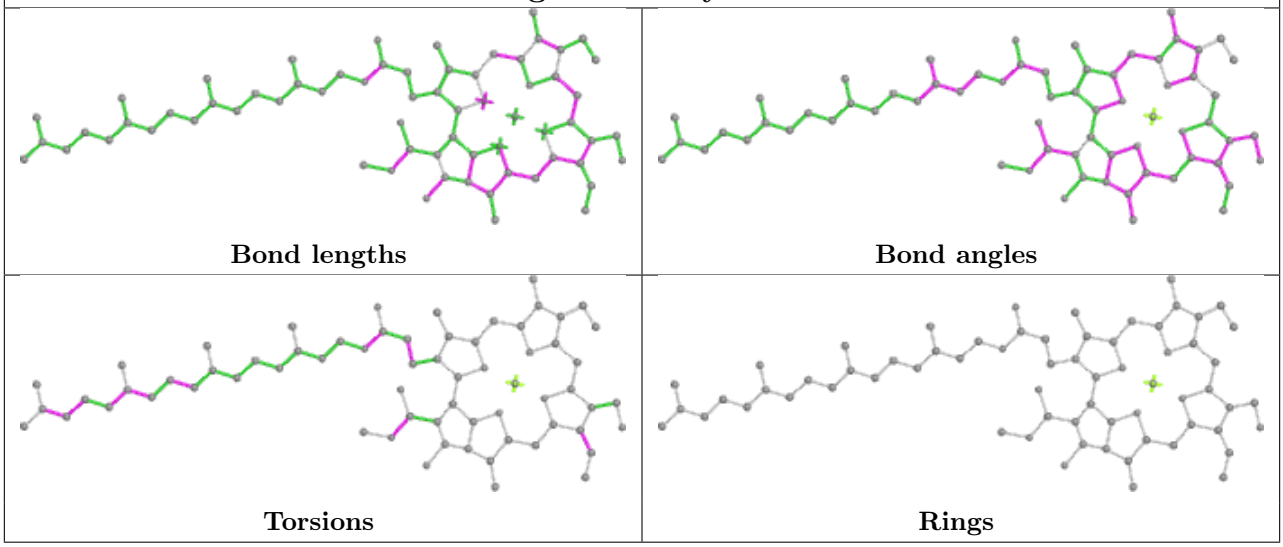


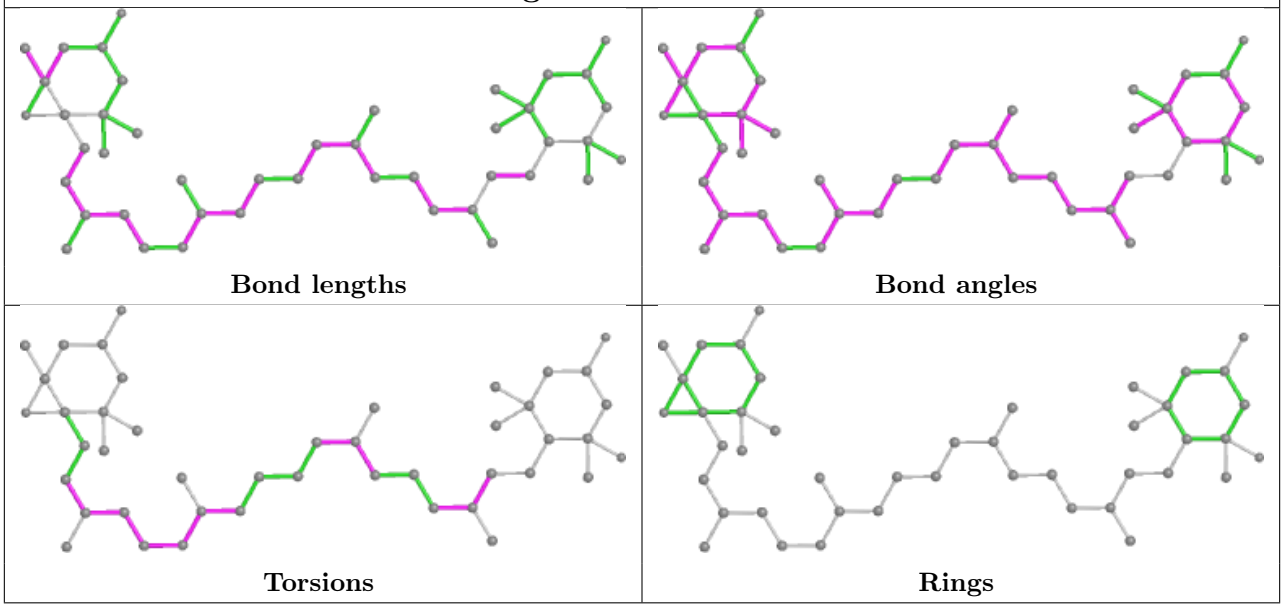
Rings

Ligand CHL y 609

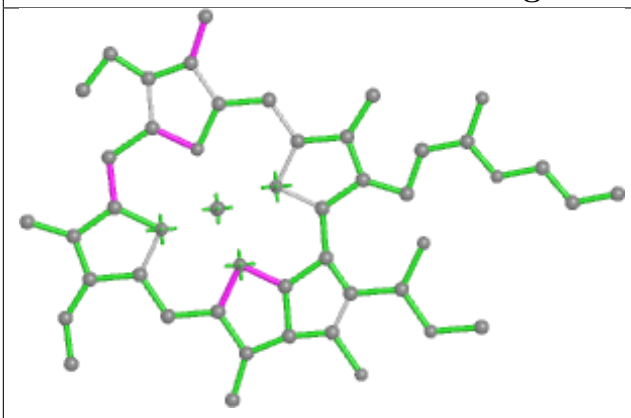


Ligand LUT g 615

Ligand NEX Y 616



Ligand CLA N 613



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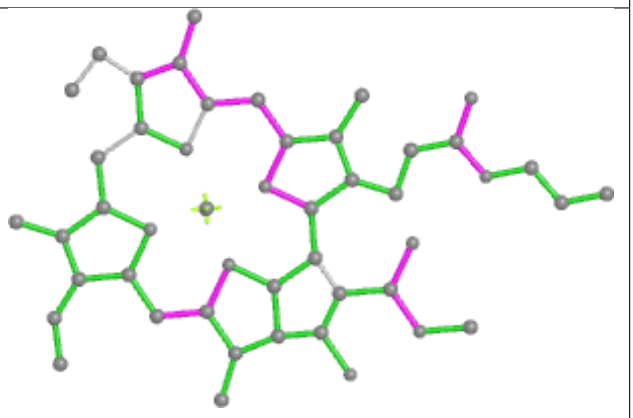
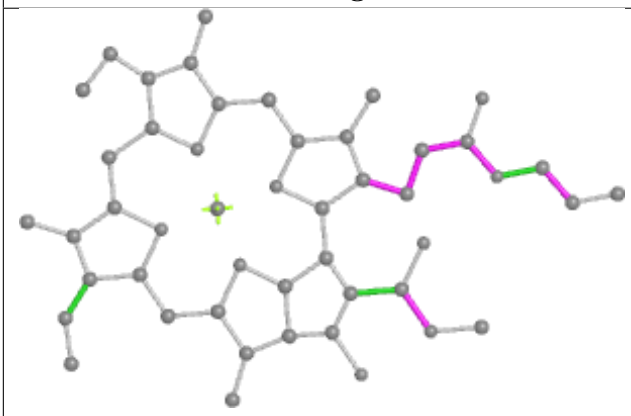
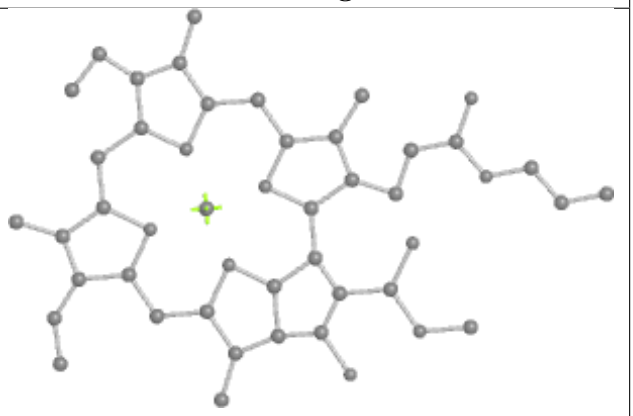


Bond angles

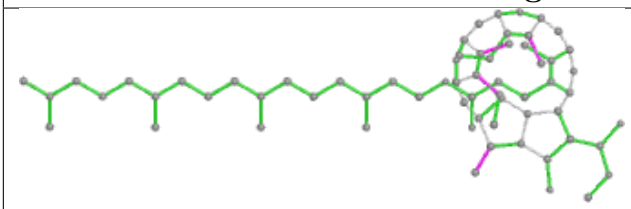


Torsions

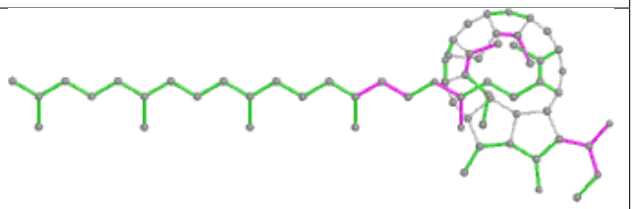


Rings

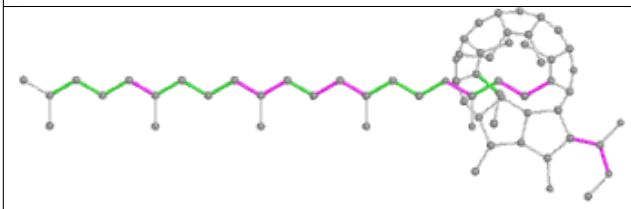
Ligand PHO d 401



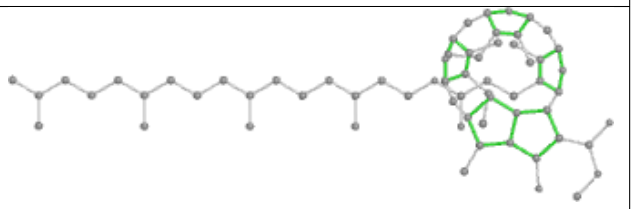
Bond lengths



Bond angles

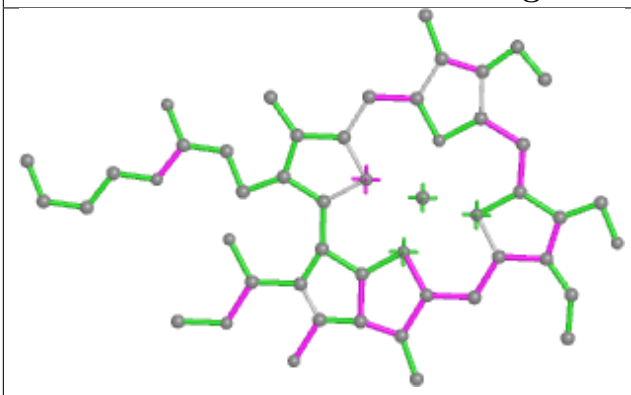


Torsions



Rings

Ligand CHL N 605



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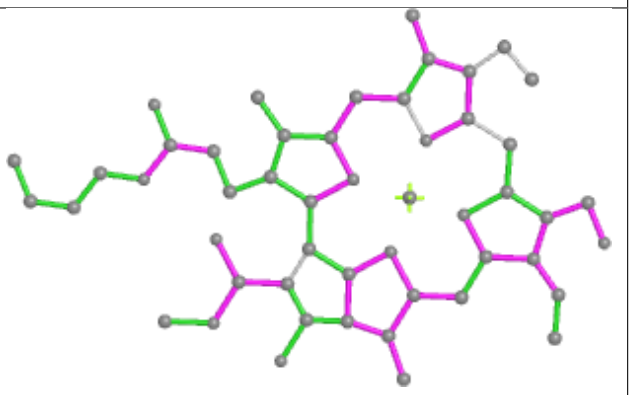
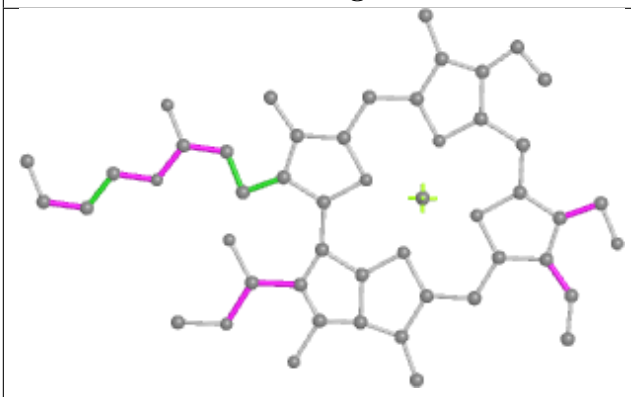
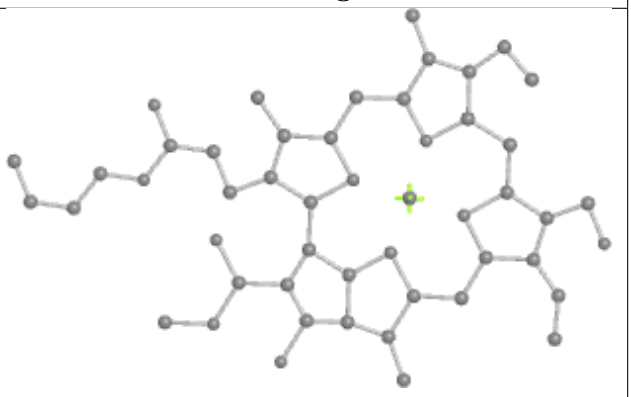


Bond angles

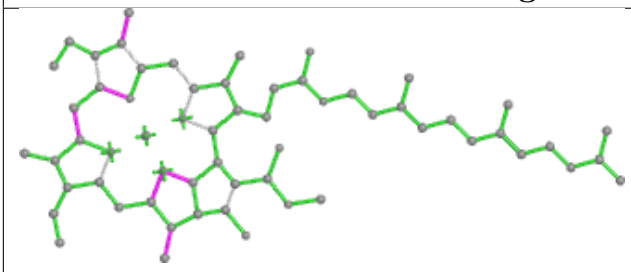


Torsions



Rings

Ligand CLA W 101



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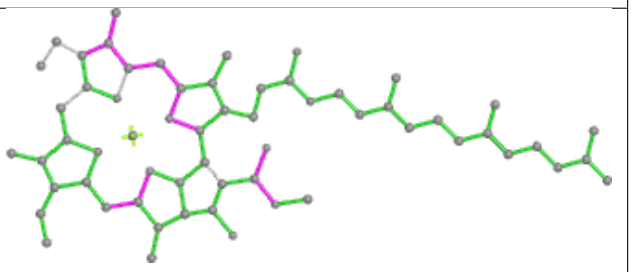
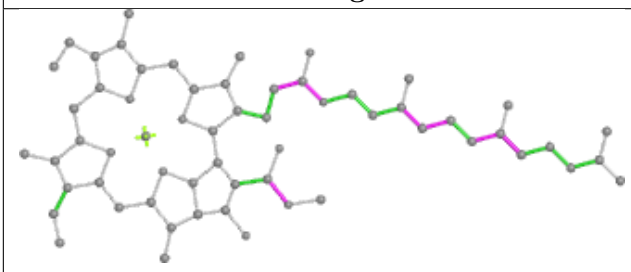
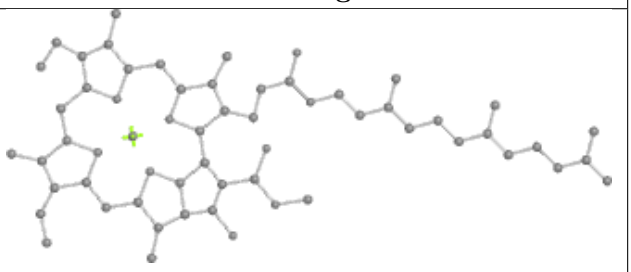


Bond angles

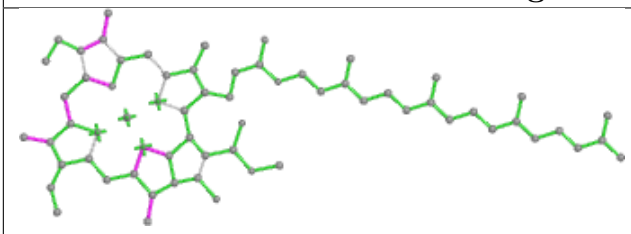


Torsions

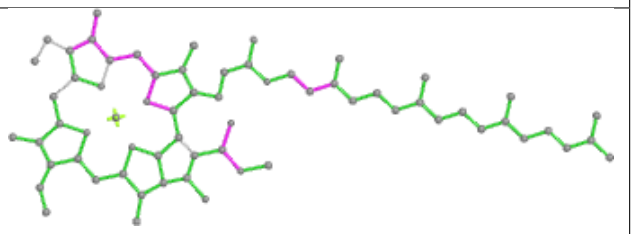


Rings

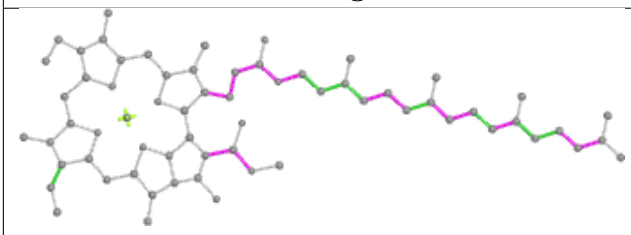
Ligand CLA b 601



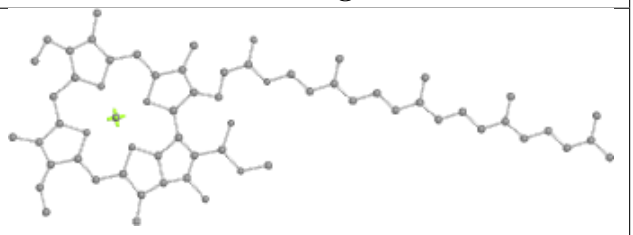
Bond lengths



Bond angles

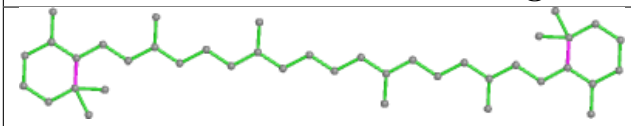


Torsions

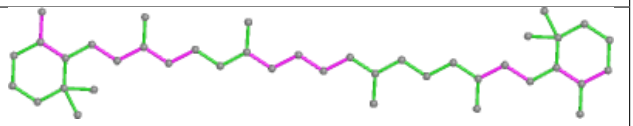


Rings

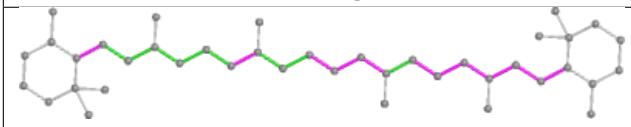
Ligand BCR k 101



Bond lengths



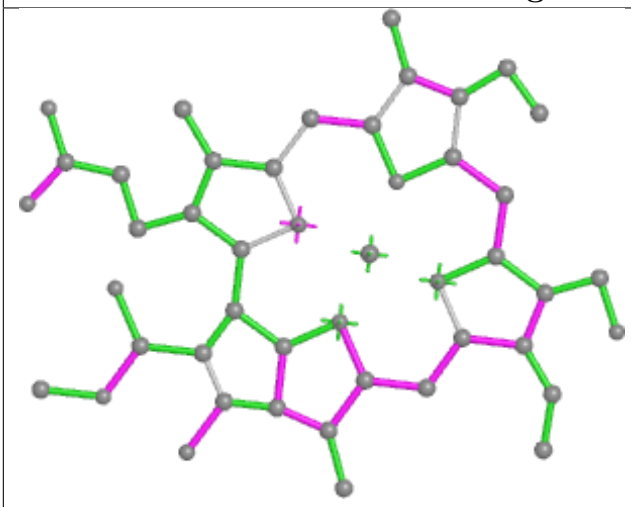
Bond angles



Torsions

Rings

Ligand CHL S 307



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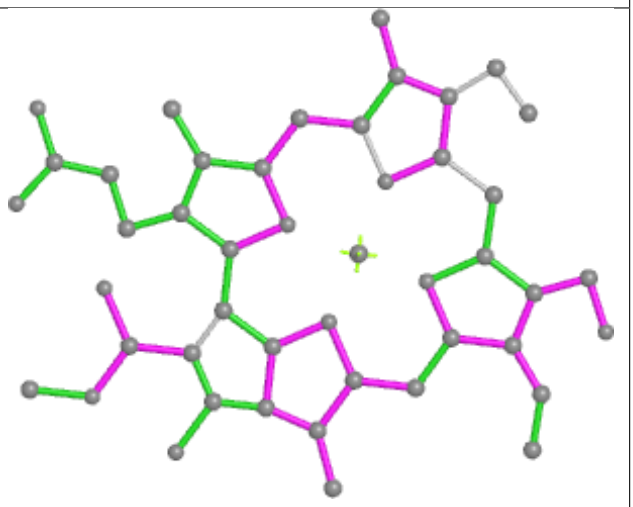
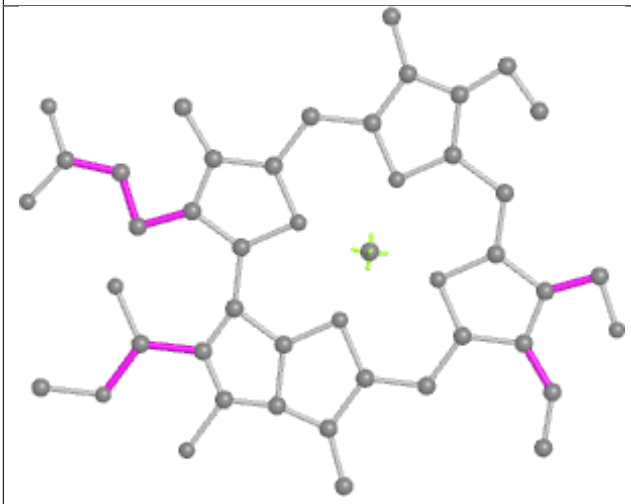
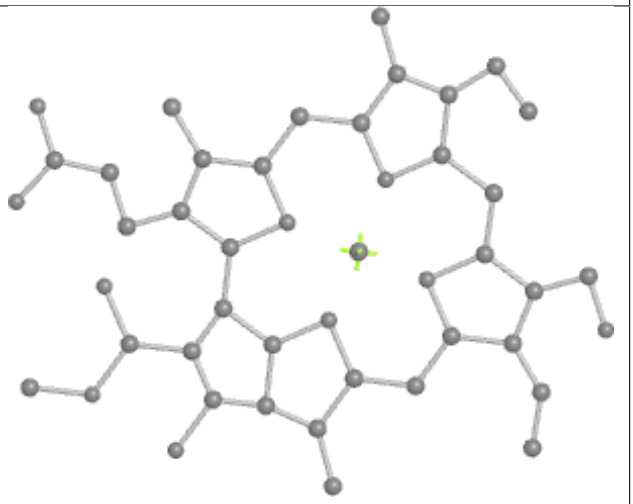


Bond angles

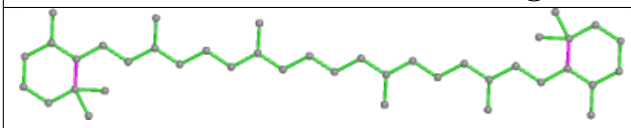


Torsions

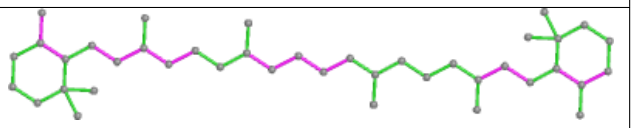


Rings

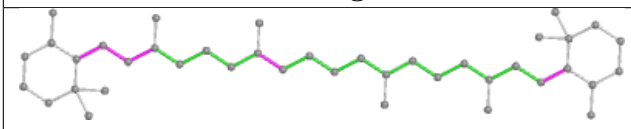
Ligand BCR d 405



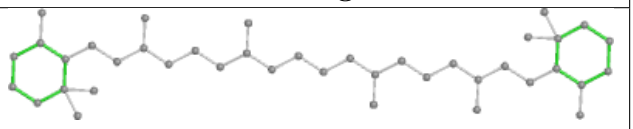
Bond lengths



Bond angles

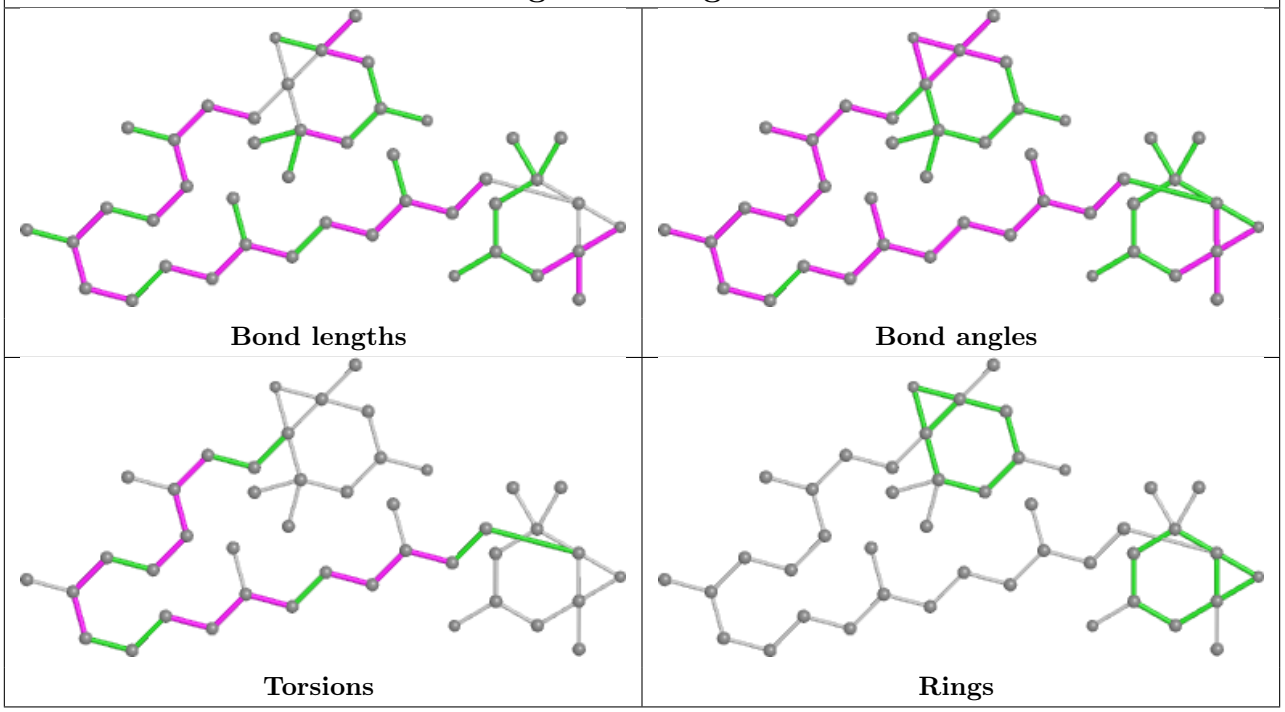


Torsions

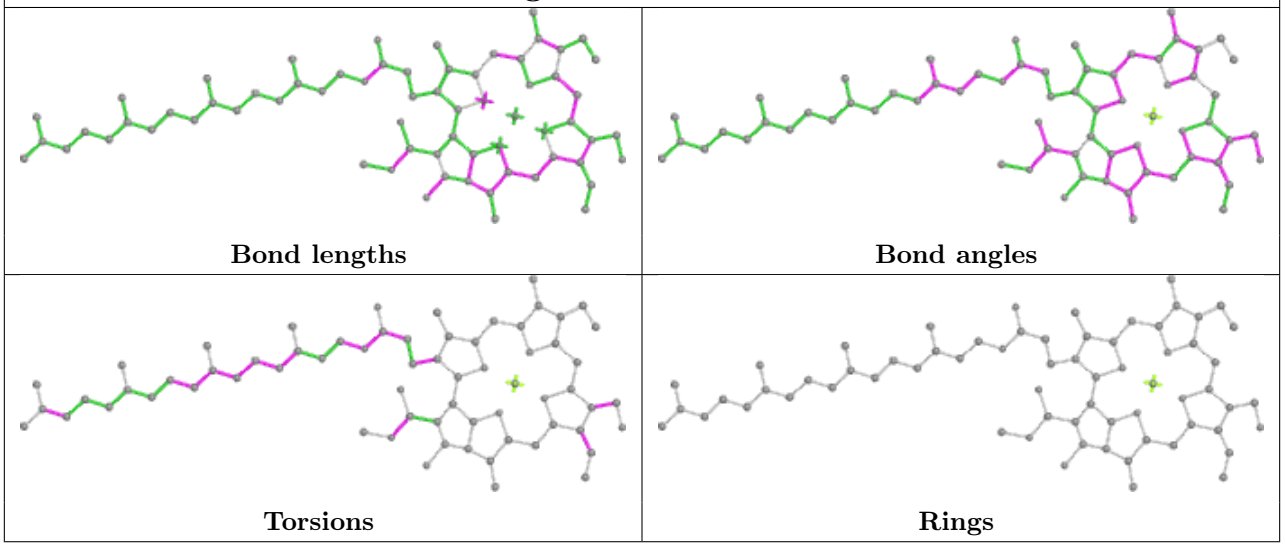


Rings

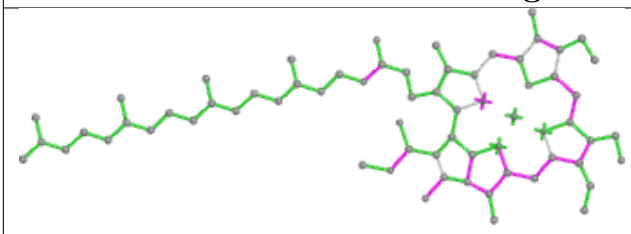
Ligand XAT g 617



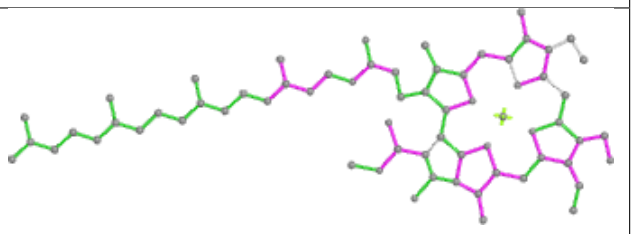
Ligand CHL Y 607



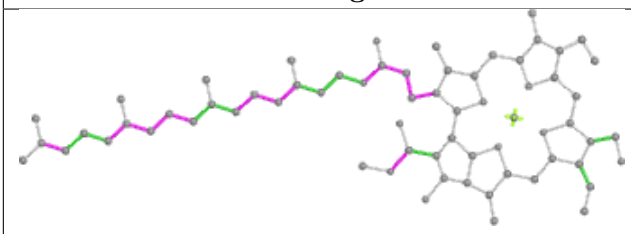
Ligand CHL R 305



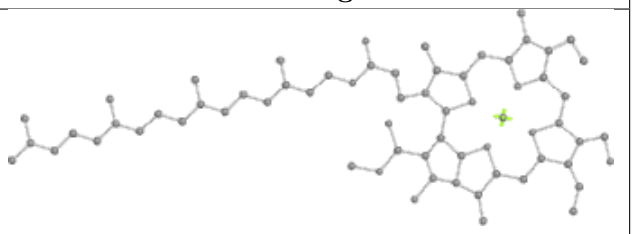
Bond lengths



Bond angles

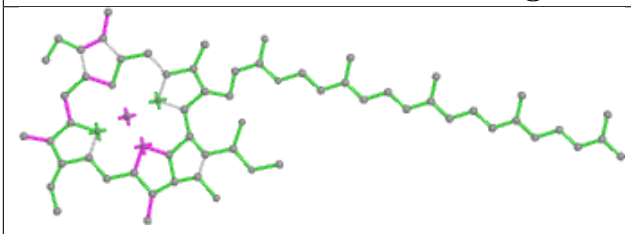


Torsions



Rings

Ligand CLA C 512



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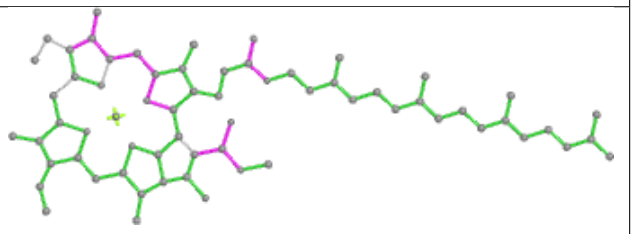
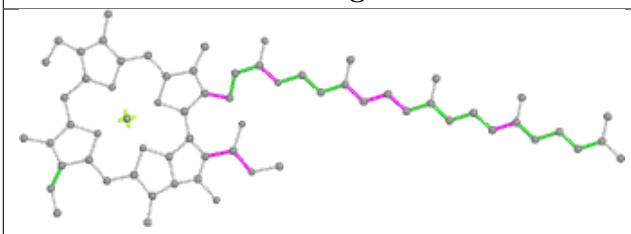


Bond angles



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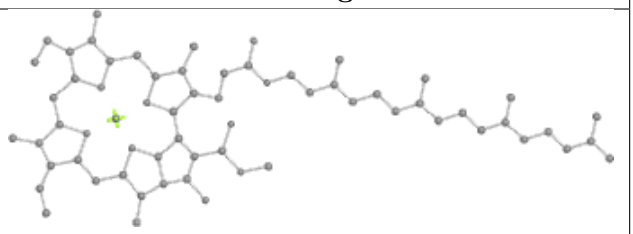
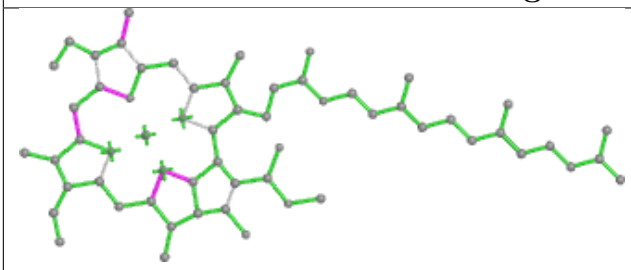
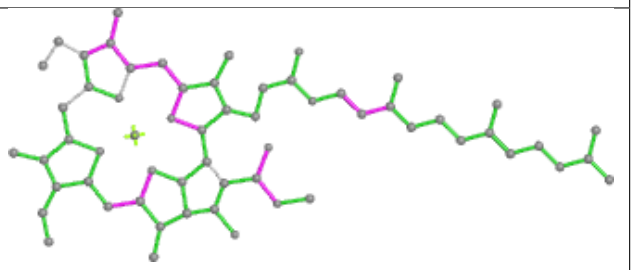


Rings

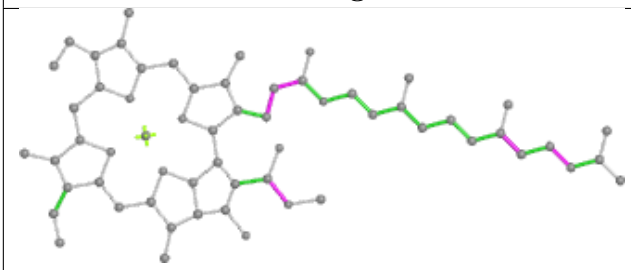
Ligand CLA R 302



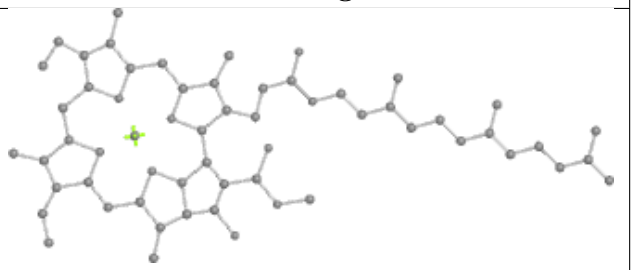
Bond lengths



Bond angles

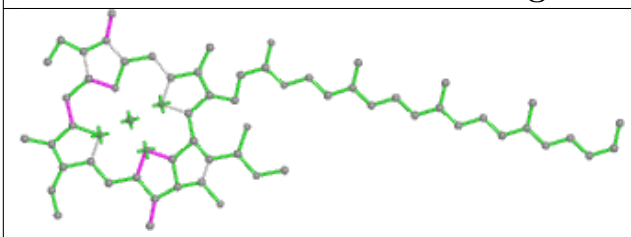


Torsions



Rings

Ligand CLA g 610



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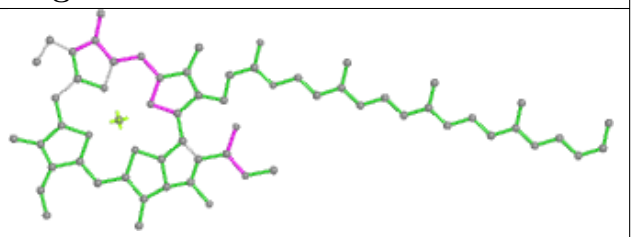
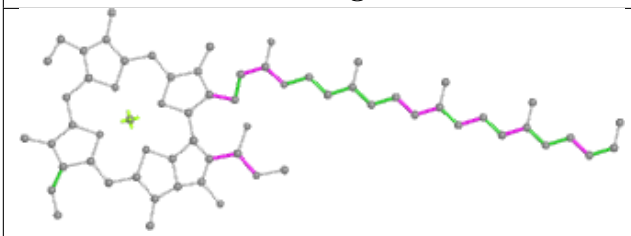


Bond angles



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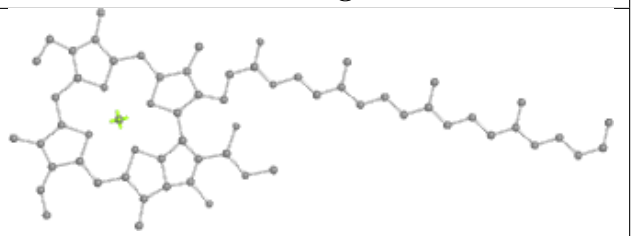
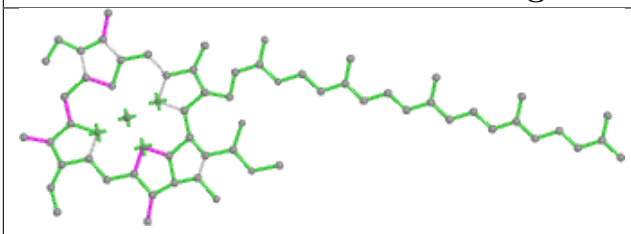
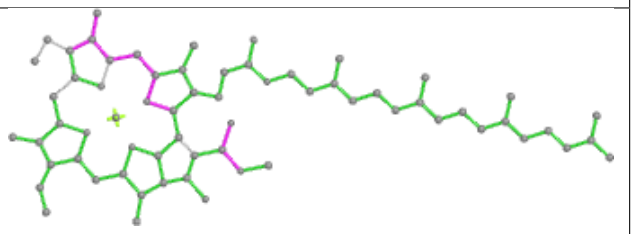


Rings

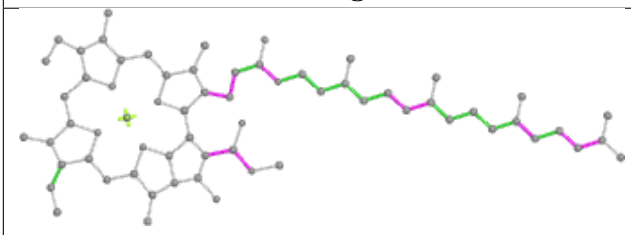
Ligand CLA b 611



Bond lengths



Bond angles



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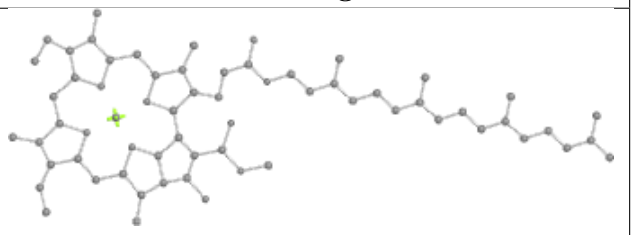
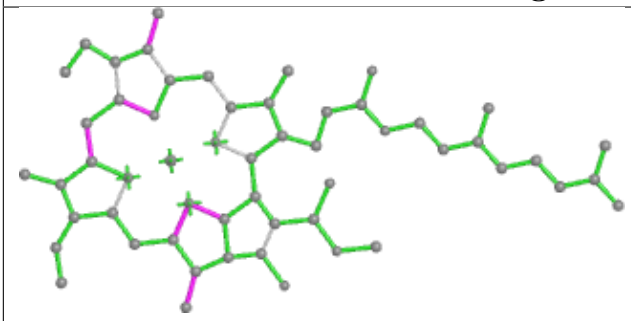
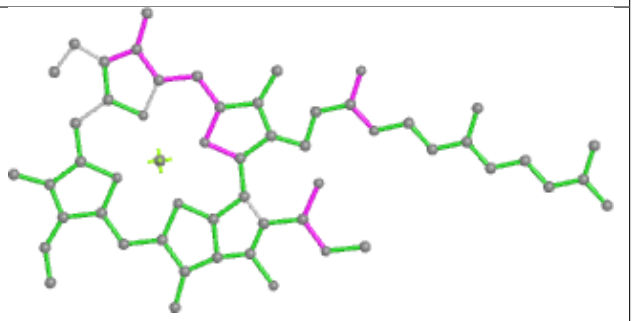


Rings

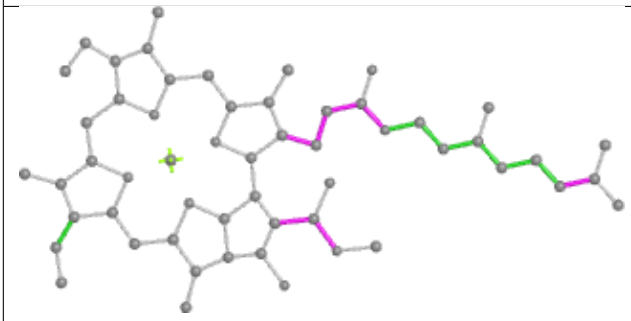
Ligand CLA s 313



Bond lengths



Bond angles



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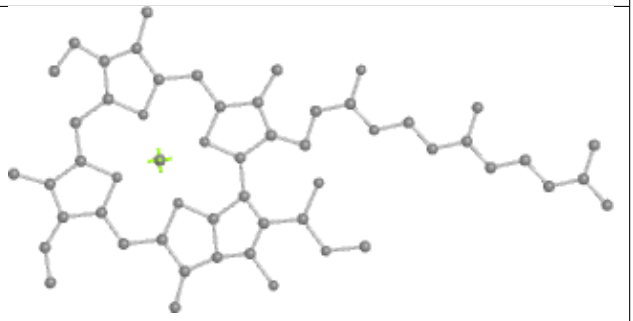
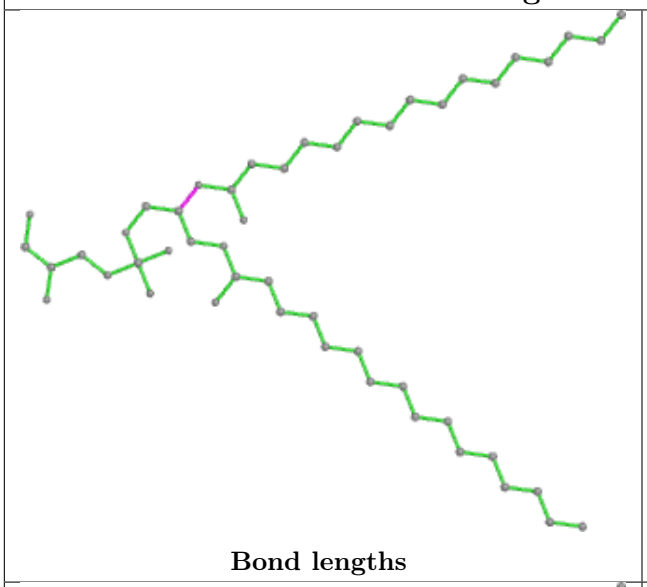
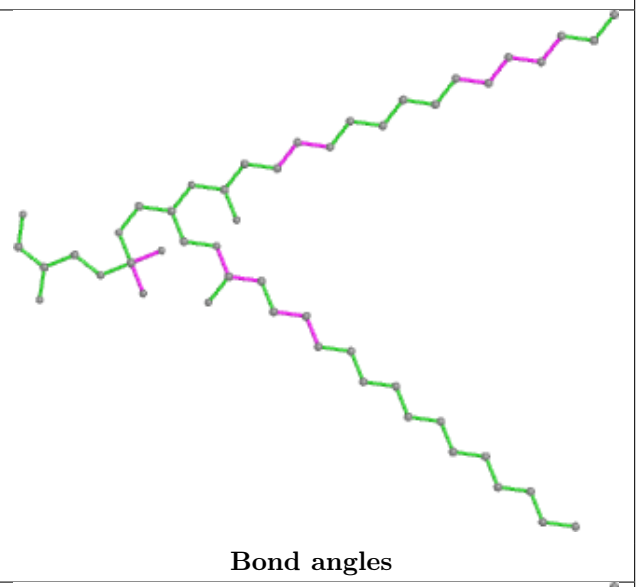


Rings

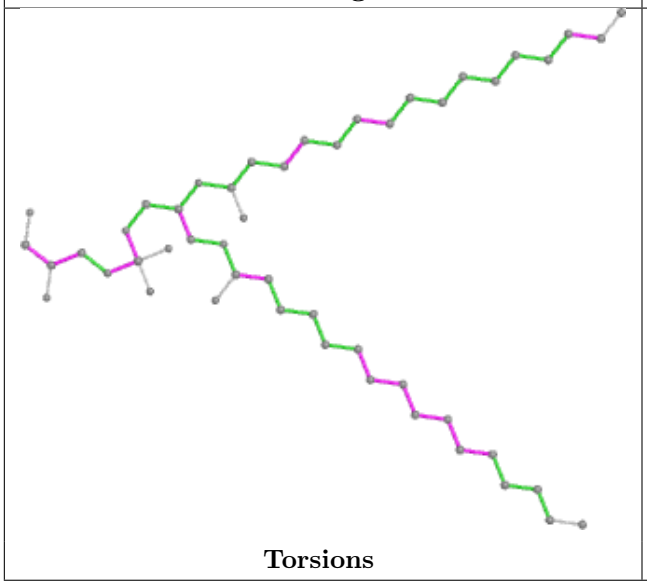
Ligand LHG D 409



Bond lengths



Bond angles



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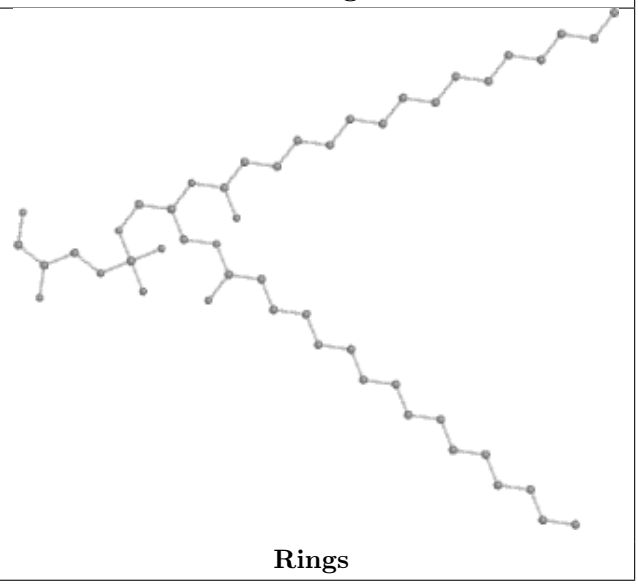
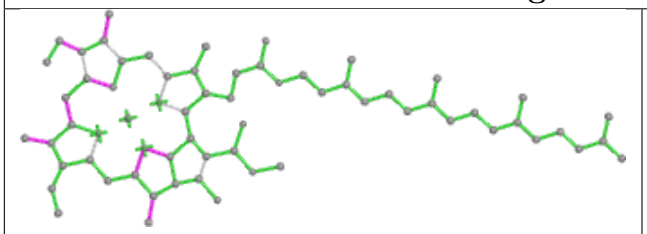


Rings

Ligand CLA b 610



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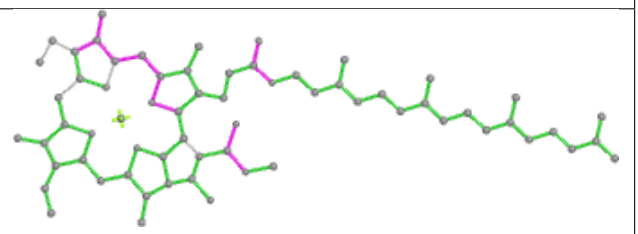
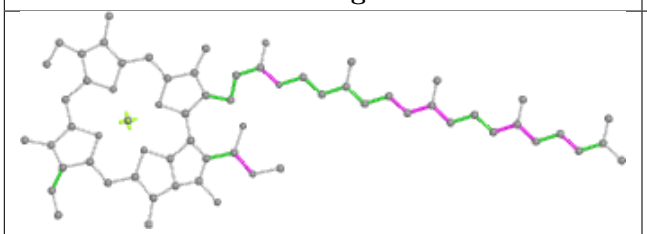
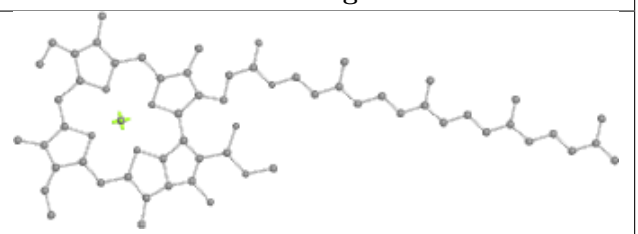


Bond angles

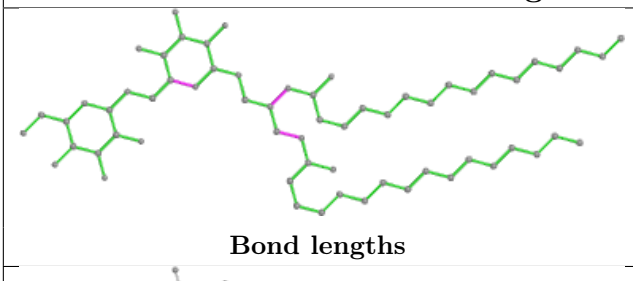


Torsions

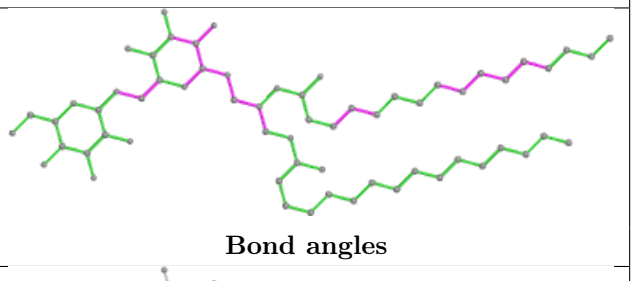


Rings

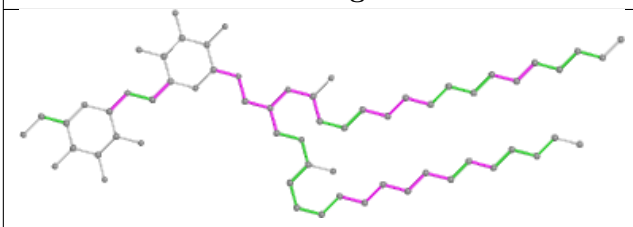
Ligand DGD c 518



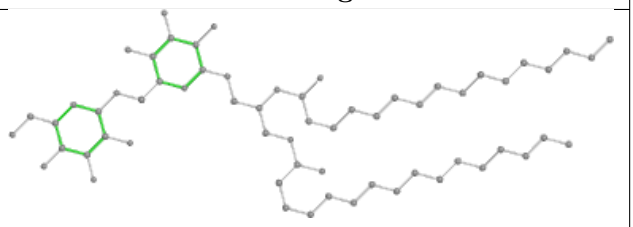
Bond lengths



Bond angles

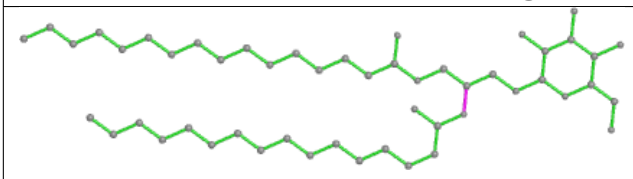


Torsions

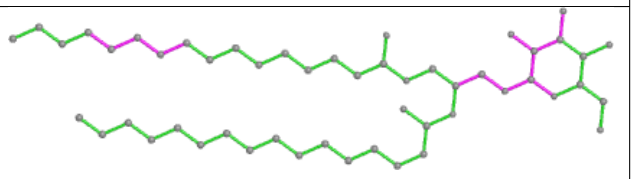


Rings

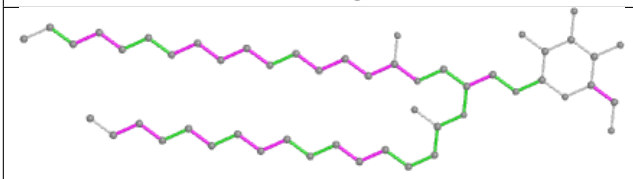
Ligand LMG T 101



Bond lengths



Bond angles



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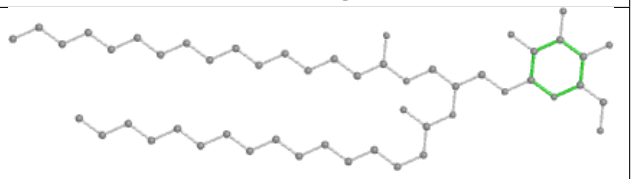
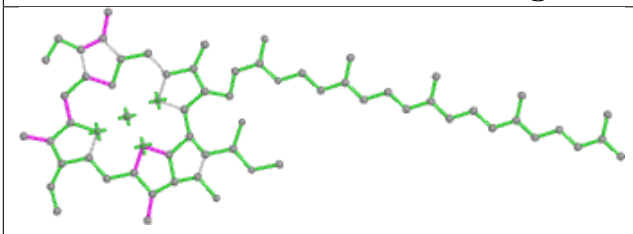


Rings

Ligand CLA c 506



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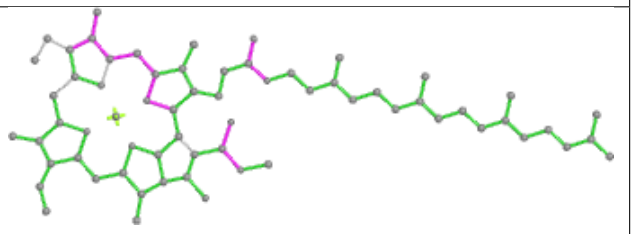
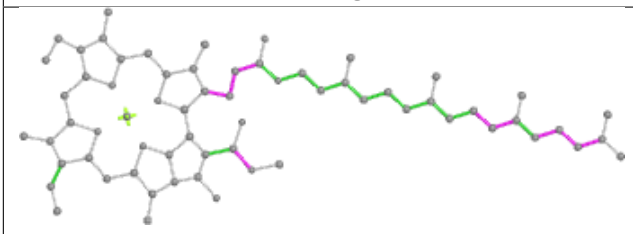


Bond angles



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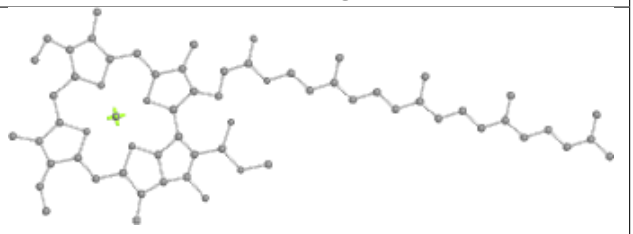
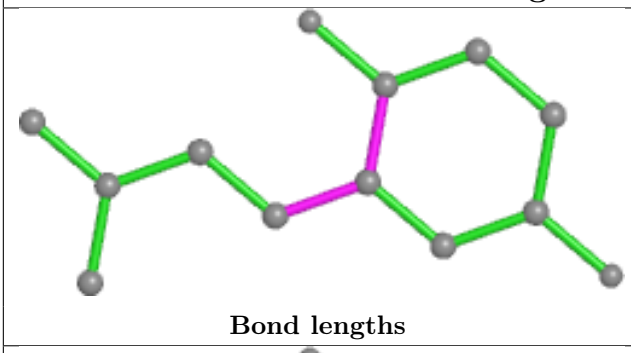


Rings

Ligand PL9 A 411



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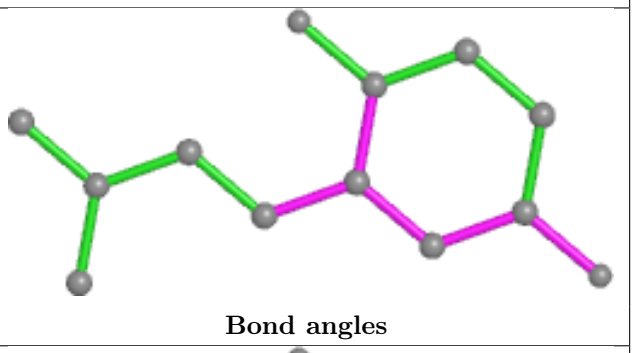
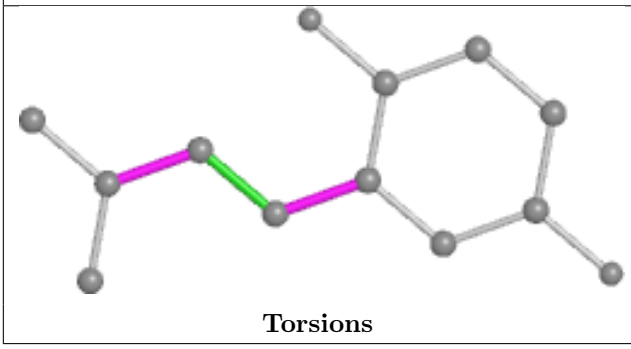
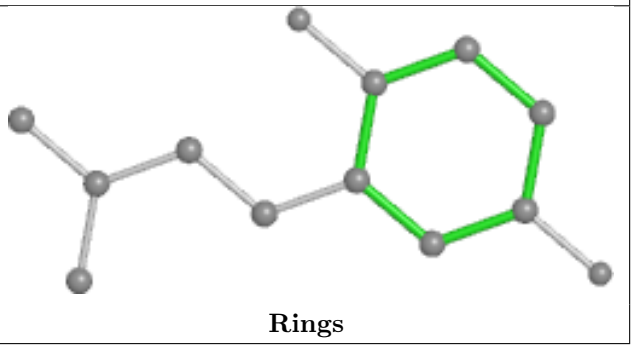


Bond angles

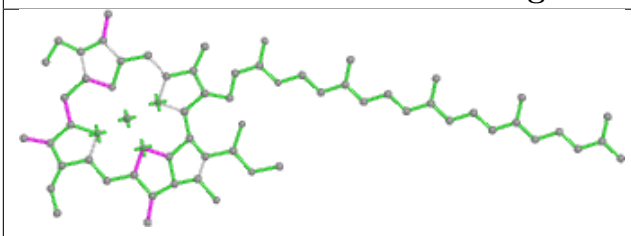


Torsions

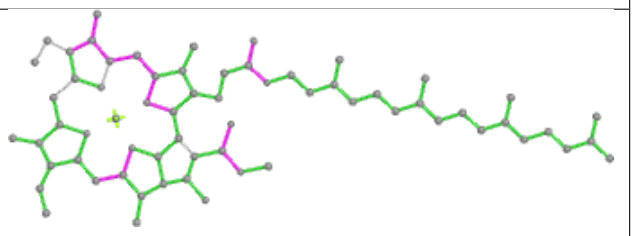


Rings

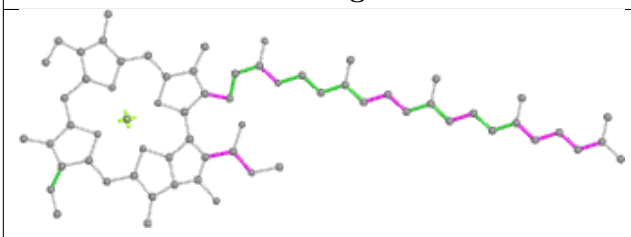
Ligand CLA x 101



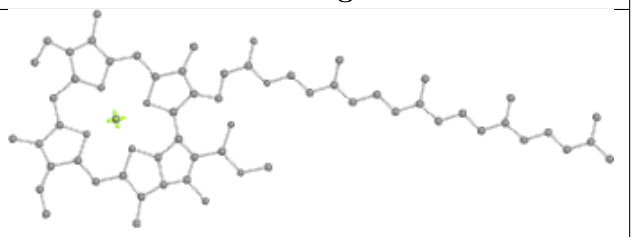
Bond lengths



Bond angles

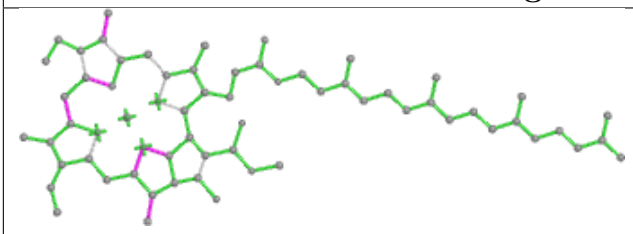


Torsions

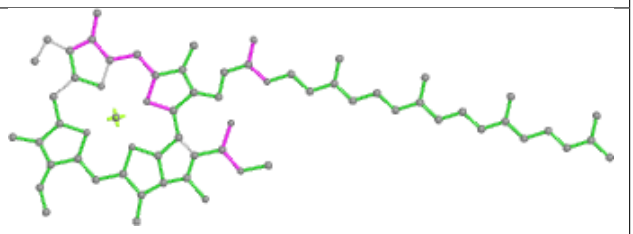


Rings

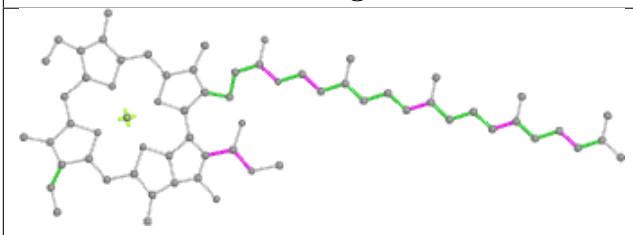
Ligand CLA B 606



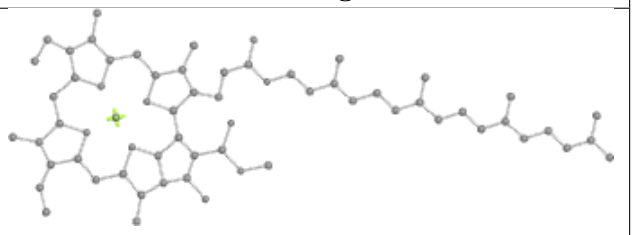
Bond lengths



Bond angles

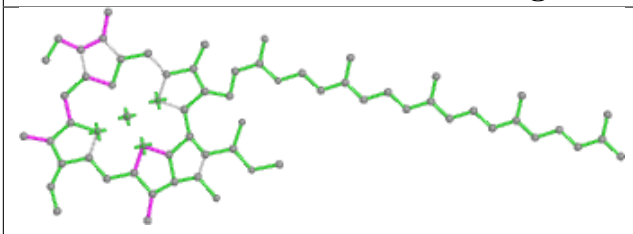


Torsions

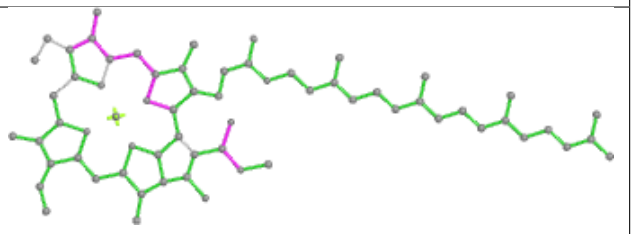


Rings

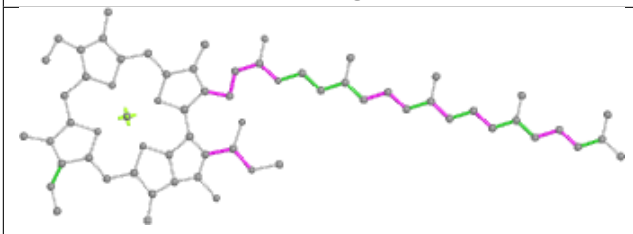
Ligand CLA c 502



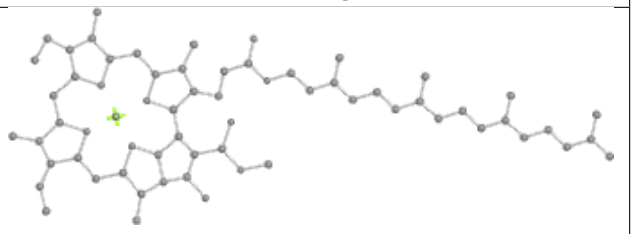
Bond lengths



Bond angles

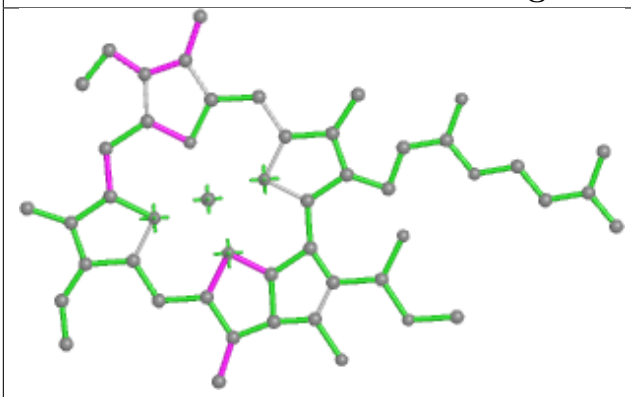


Torsions

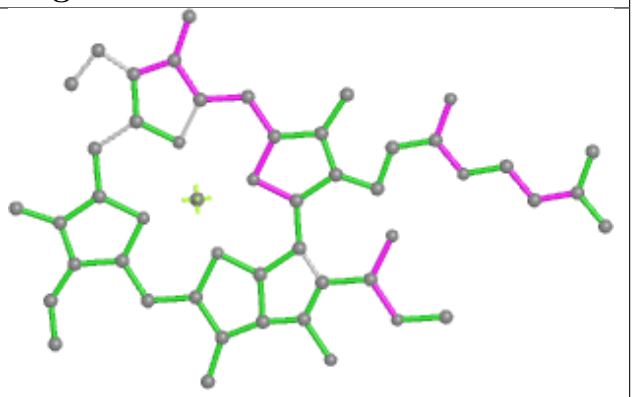


Rings

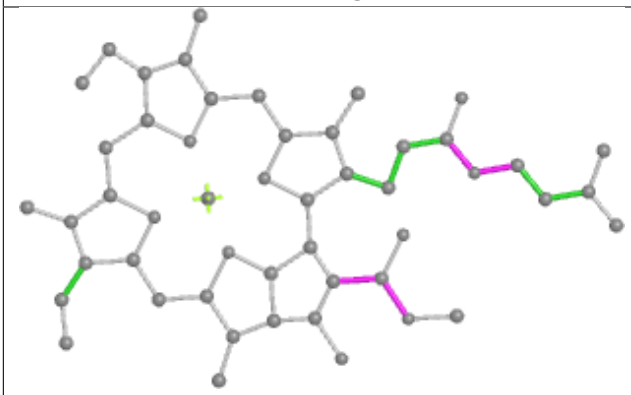
Ligand CLA g 604



Bond lengths



Bond angles



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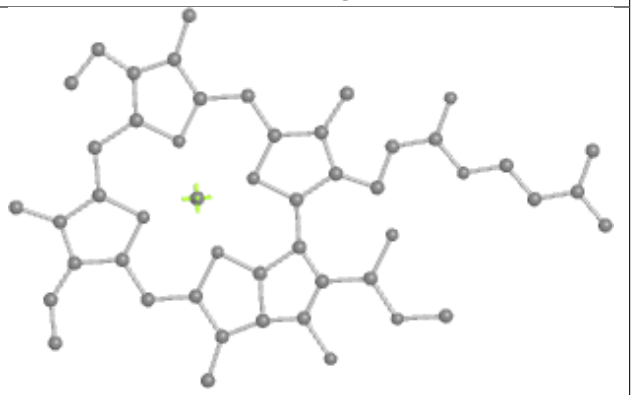
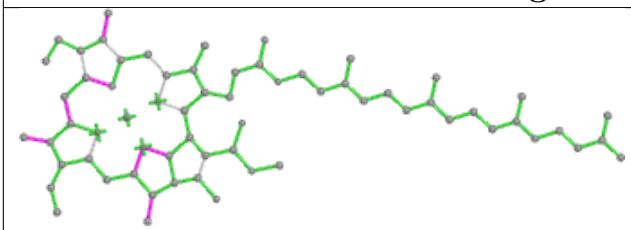


Rings

Ligand CLA c 514



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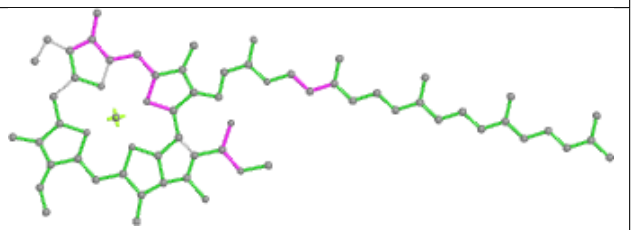
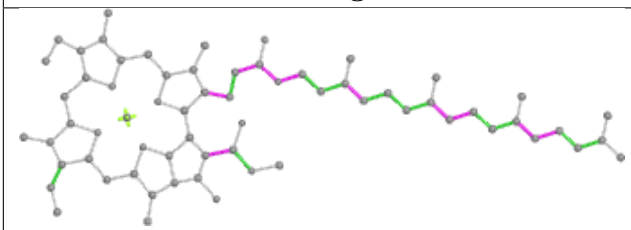


Bond angles



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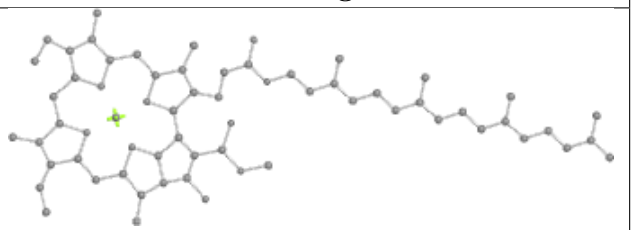
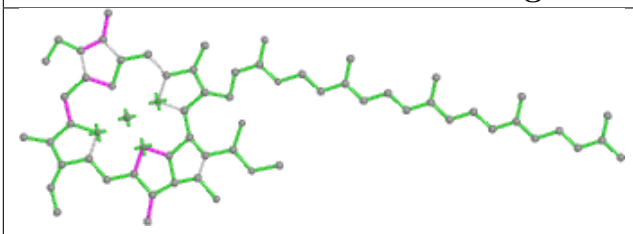


Rings

Ligand CLA C 507



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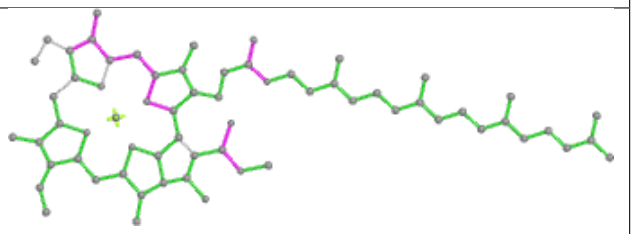
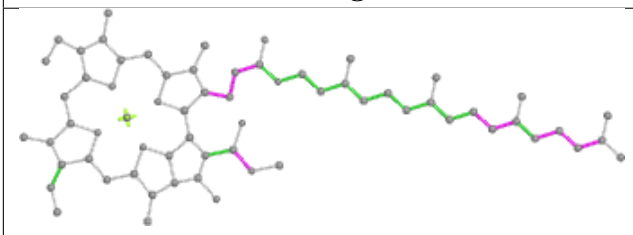


Bond angles



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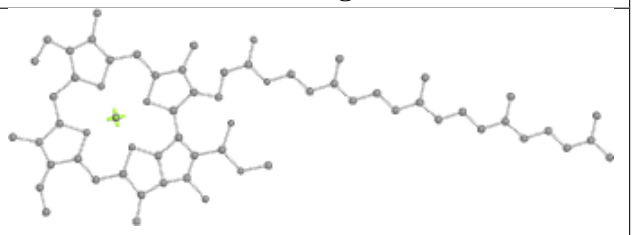
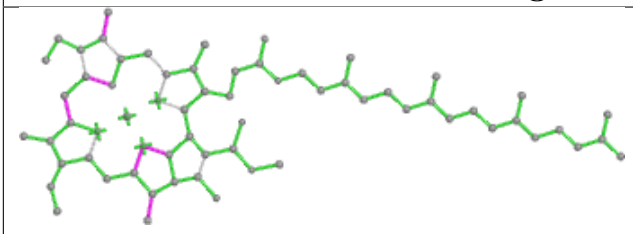
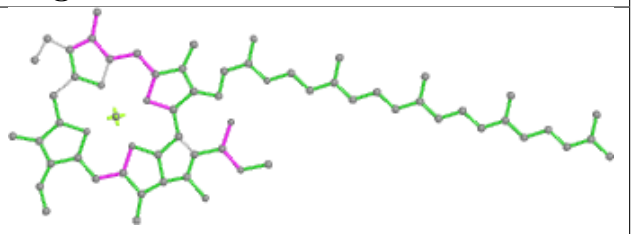


Rings

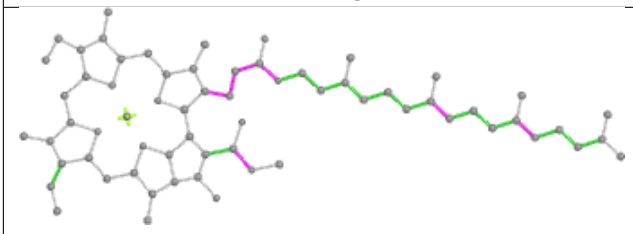
Ligand CLA g 602



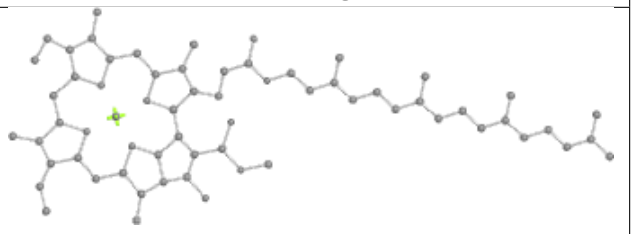
Bond lengths



Bond angles

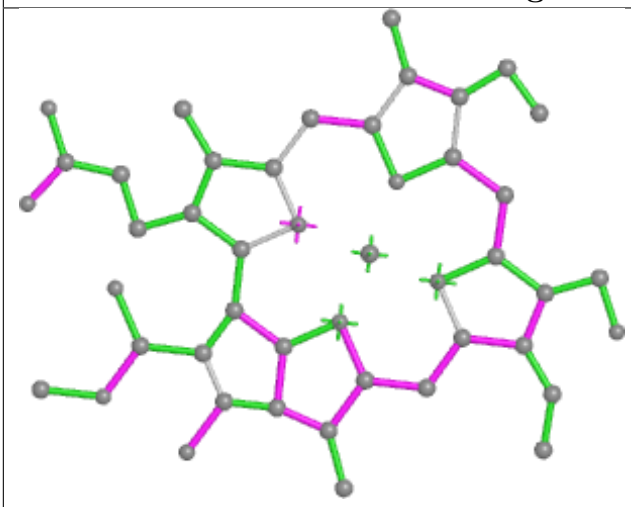


Torsions



Rings

Ligand CHL S 302



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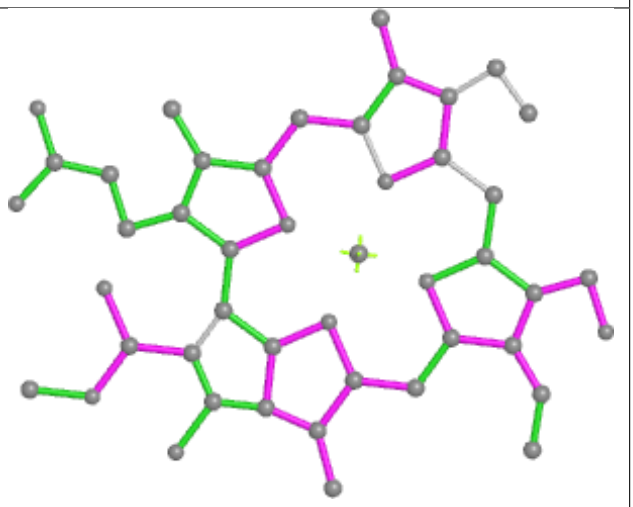
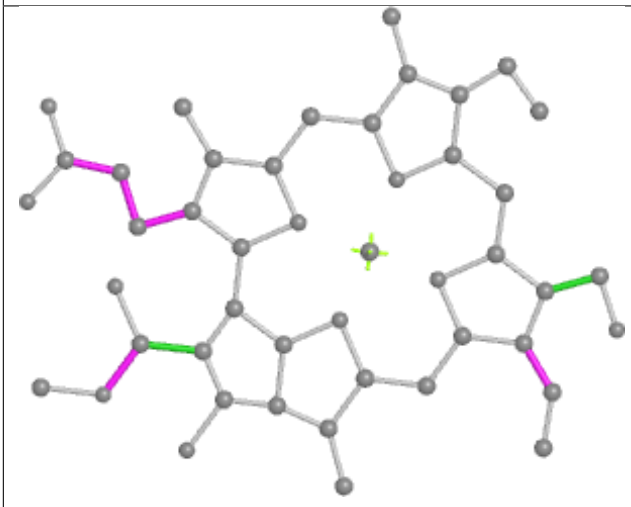


Bond angles



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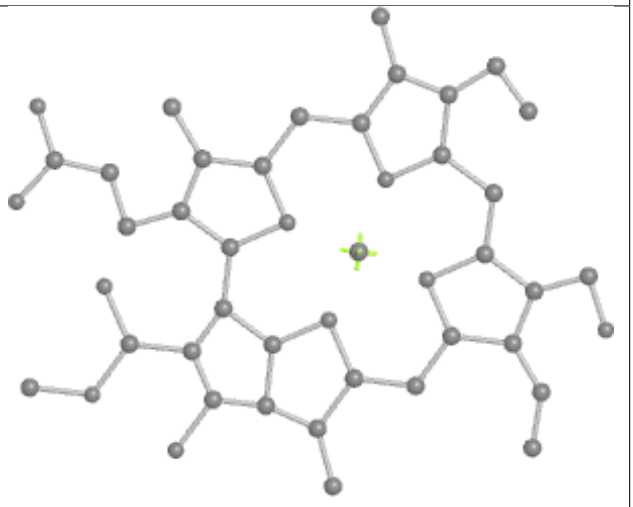
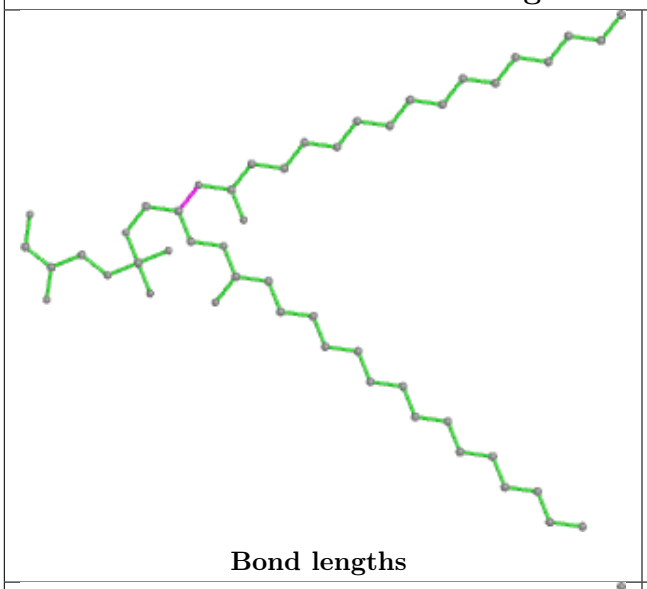


Rings

Ligand LHG C 521



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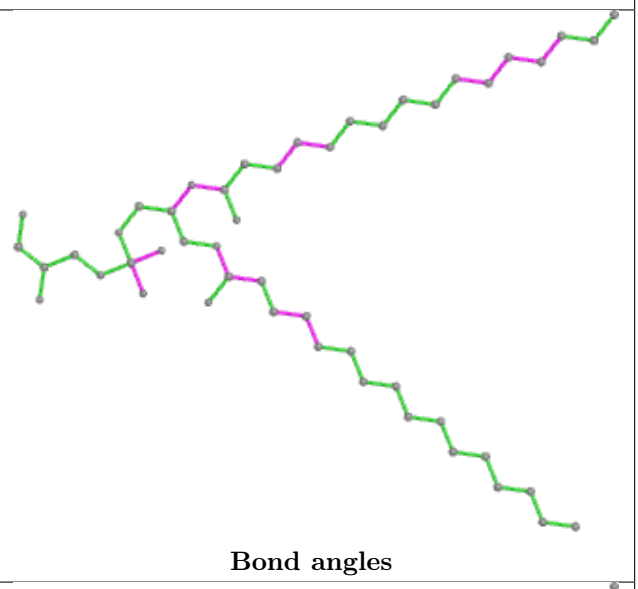
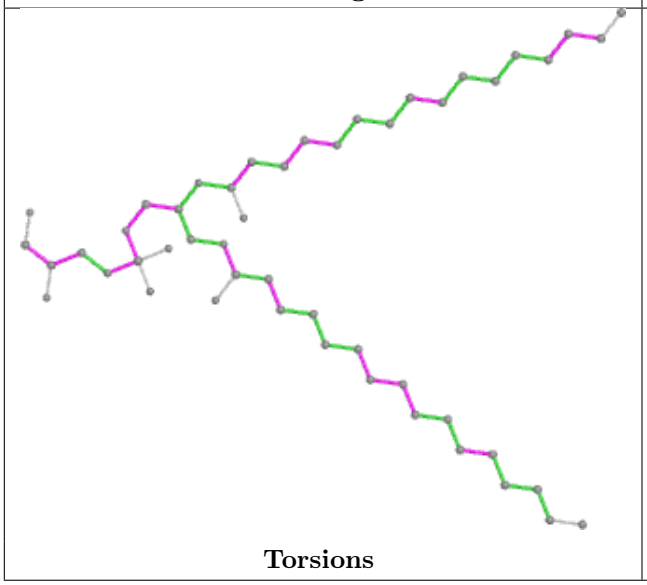


Bond angles



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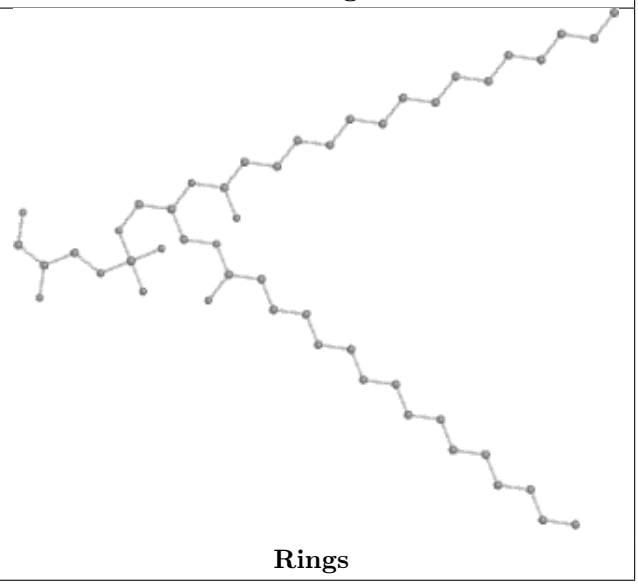
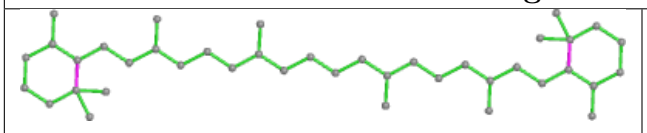
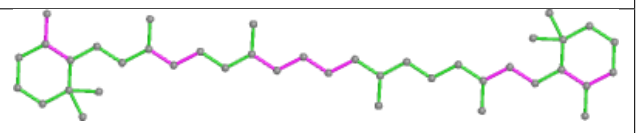


Rings

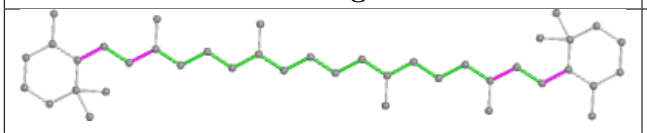
Ligand BCR B 620



Bond lengths



Bond angles



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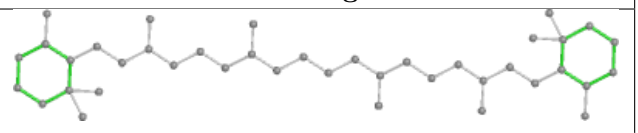
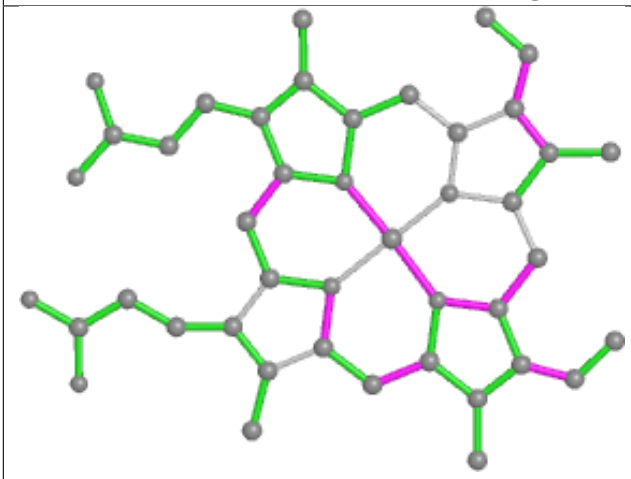


Rings

Ligand HEM f 101



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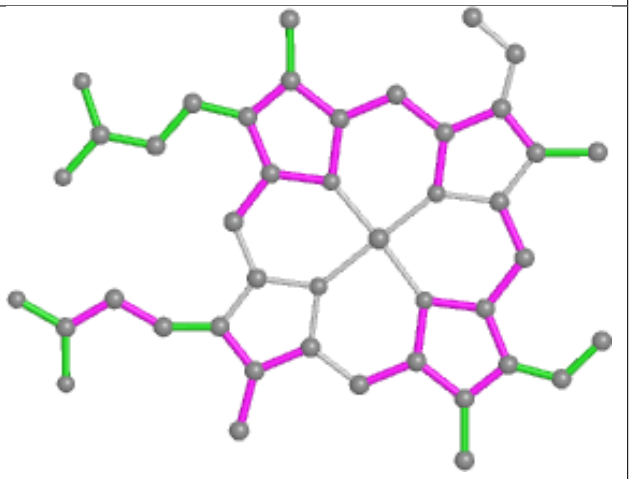
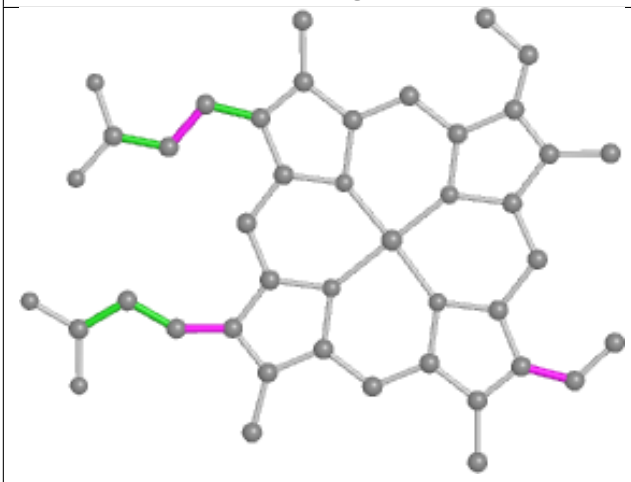


Bond angles



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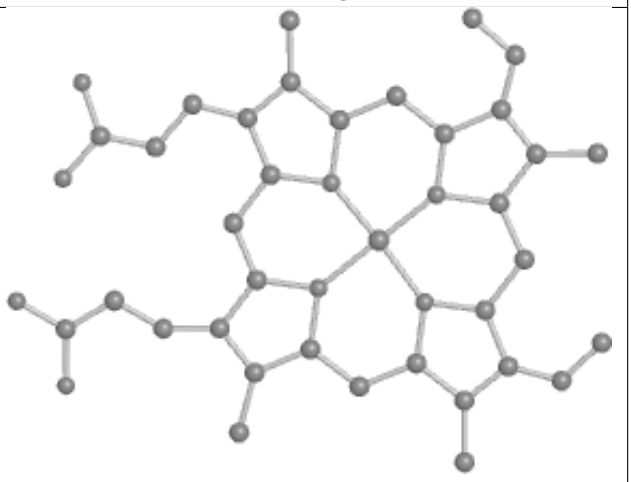
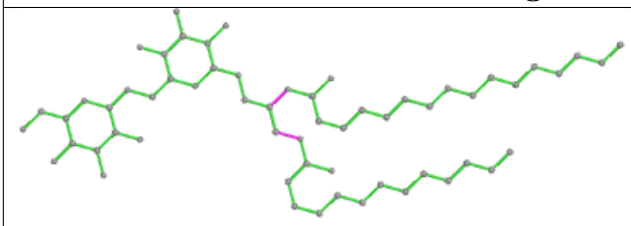
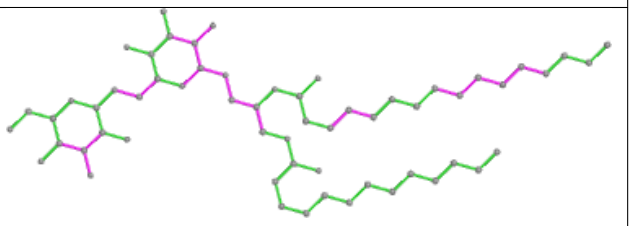


Rings

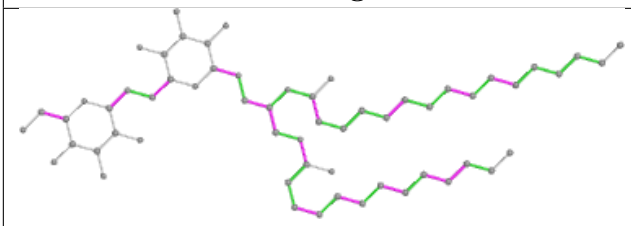
Ligand DGD a 413



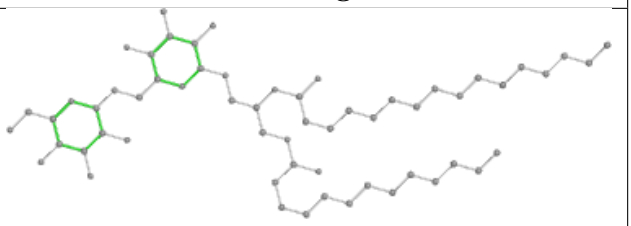
Bond lengths



Bond angles

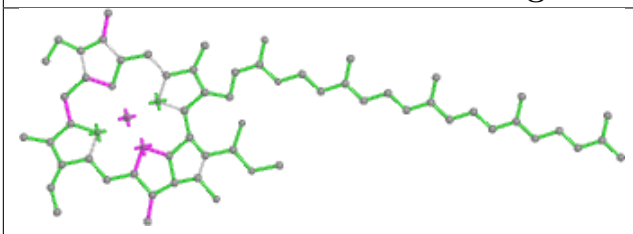


Torsions

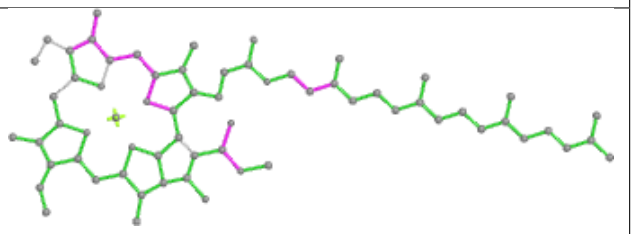


Rings

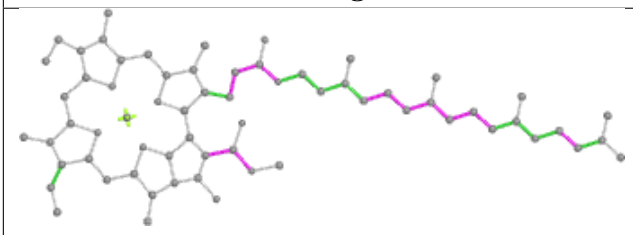
Ligand CLA n 603



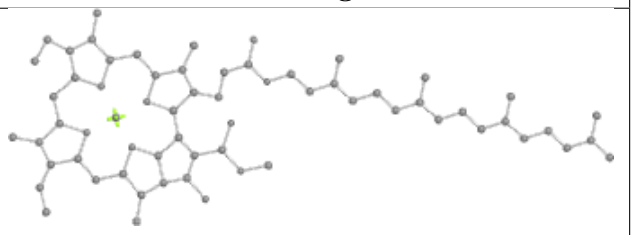
Bond lengths



Bond angles

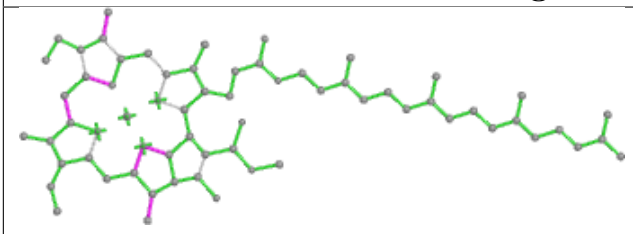


Torsions



Rings

Ligand CLA r 310



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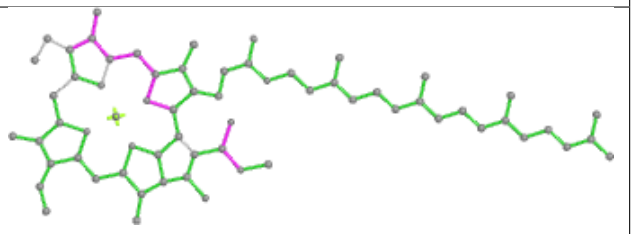
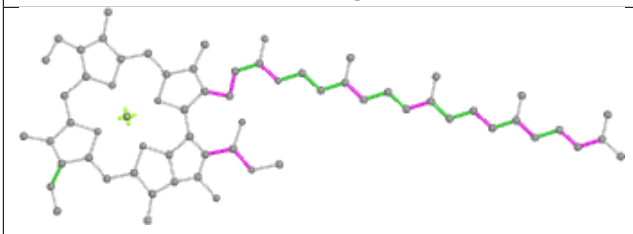


Bond angles



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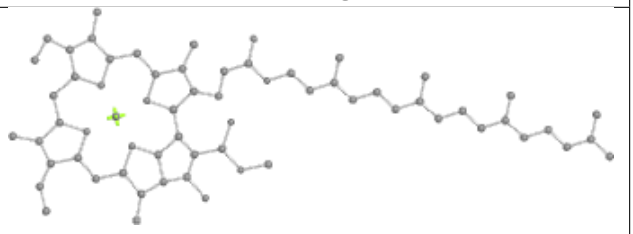
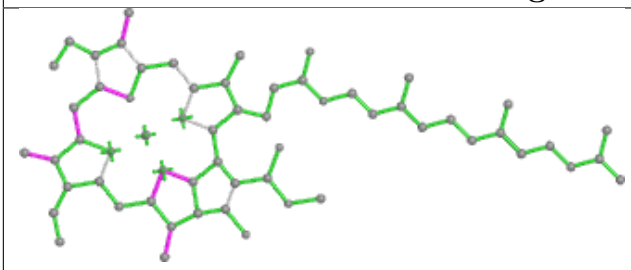
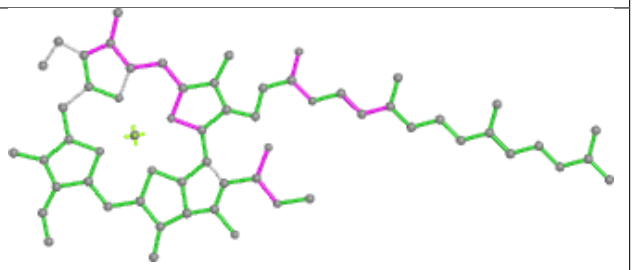
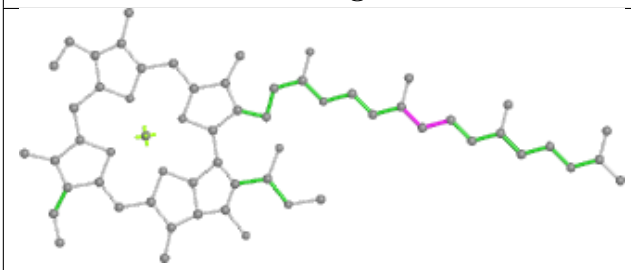
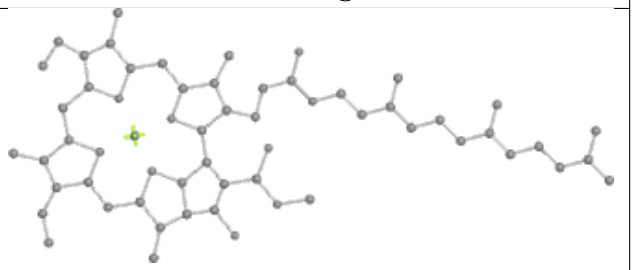
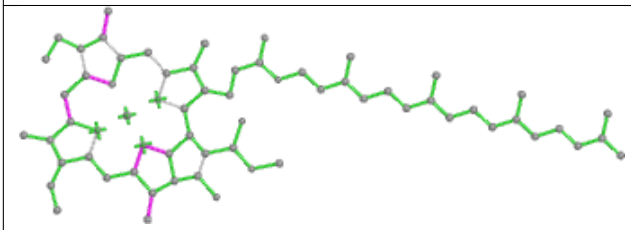
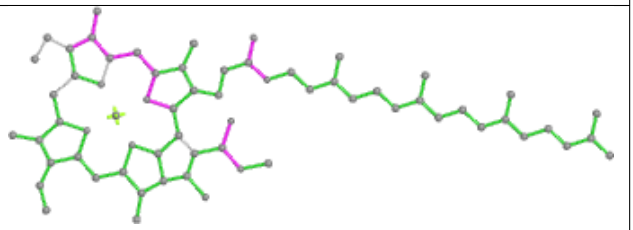
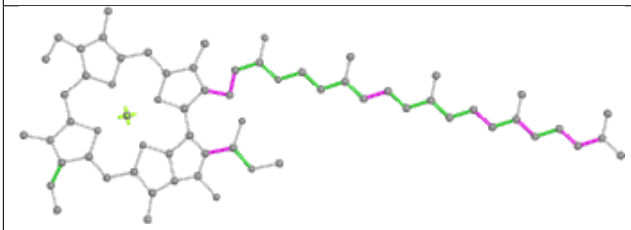
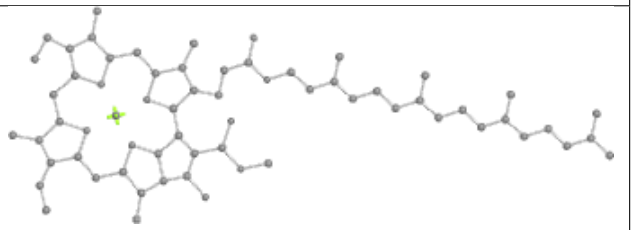
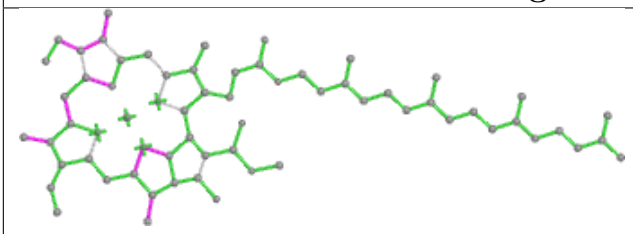


Rings

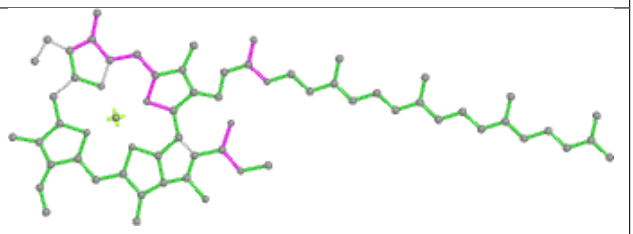
Ligand CLA a 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

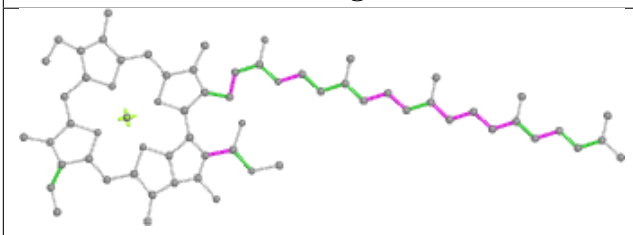
Ligand CLA c 508



Bond lengths



Bond angles



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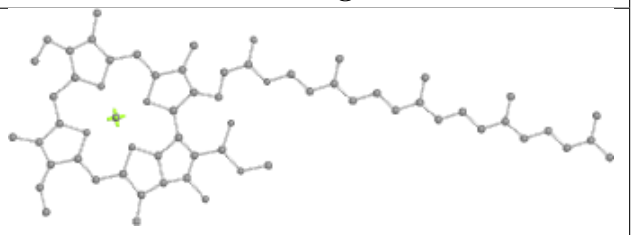
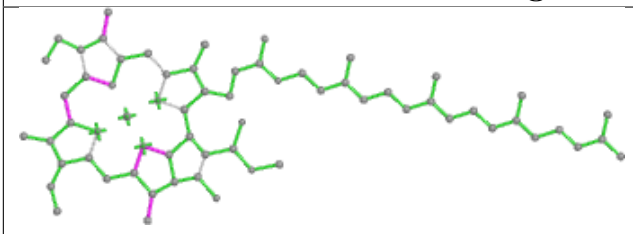
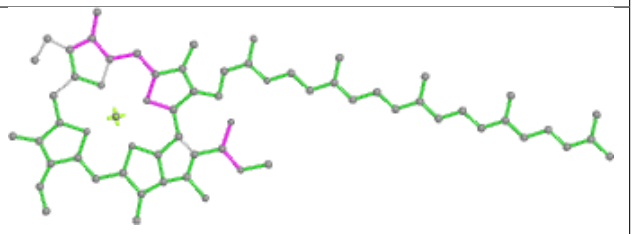


Rings

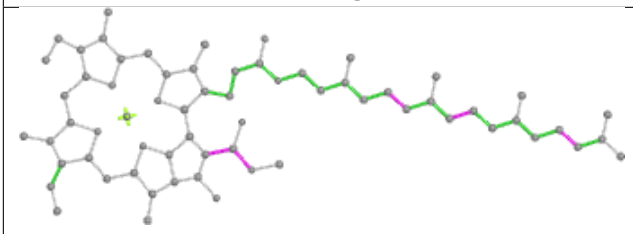
Ligand CLA b 608



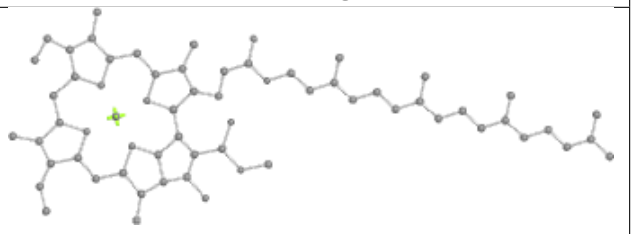
Bond lengths



Bond angles

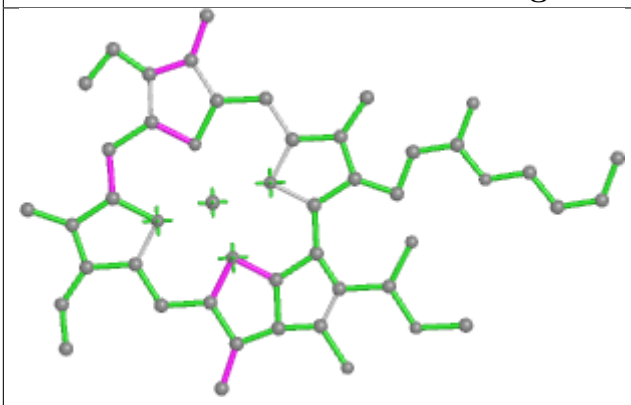


Torsions

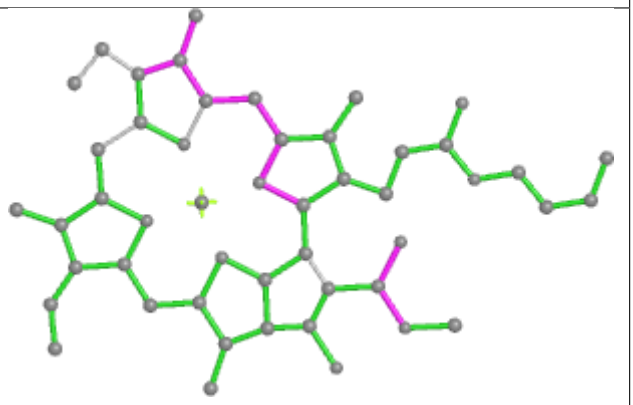


Rings

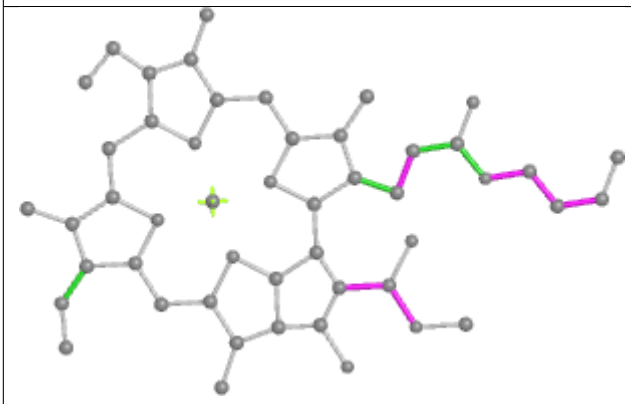
Ligand CLA s 312



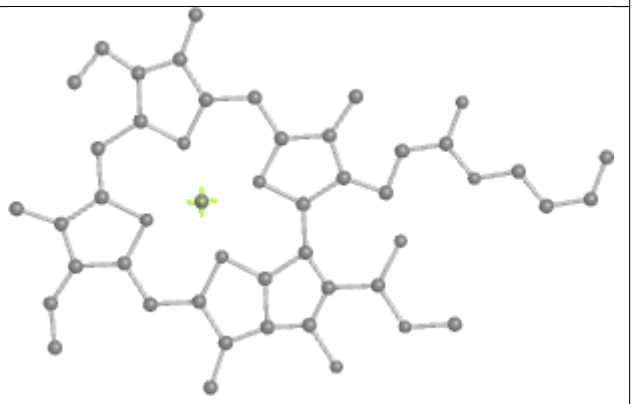
Bond lengths



Bond angles

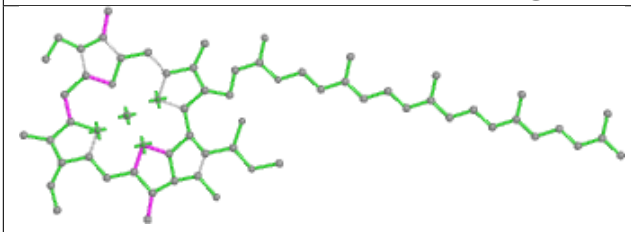


Torsions

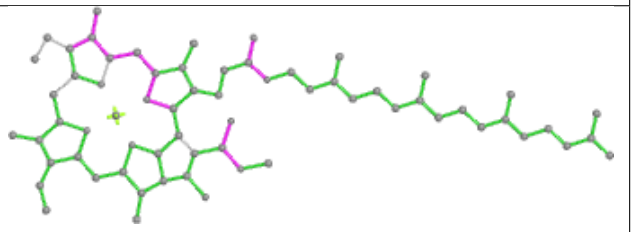


Rings

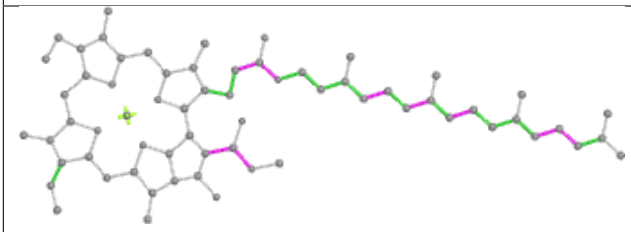
Ligand CLA b 615



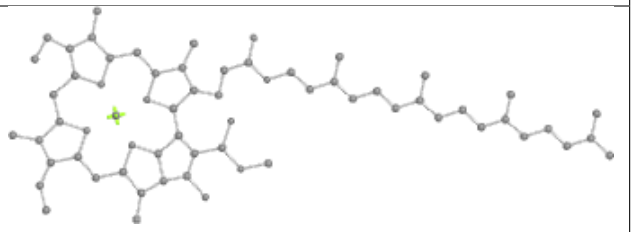
Bond lengths



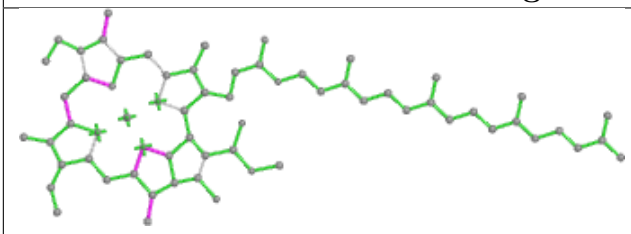
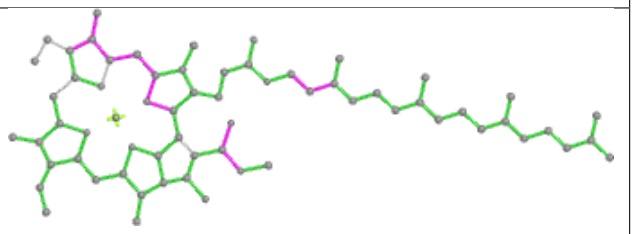
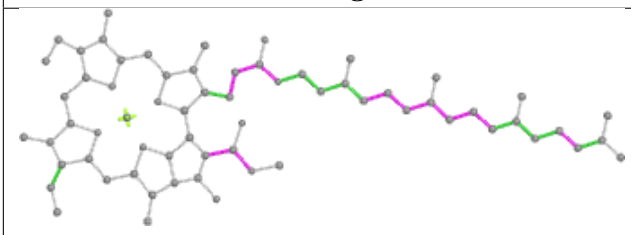
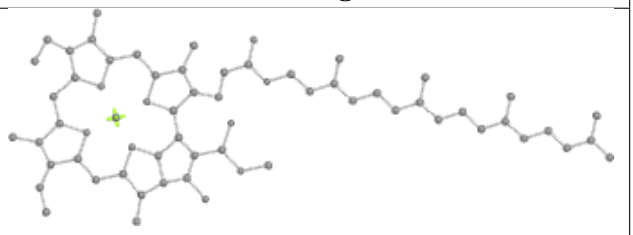
Bond angles

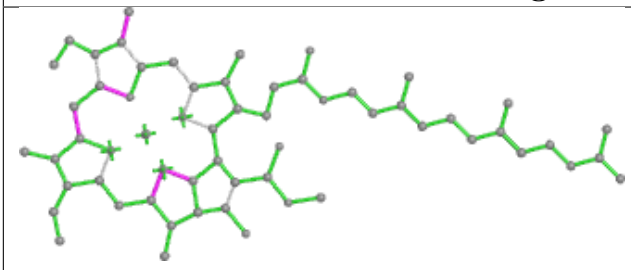
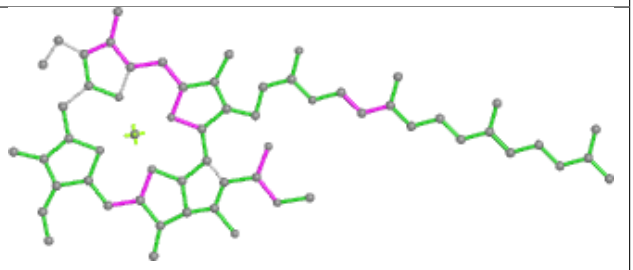
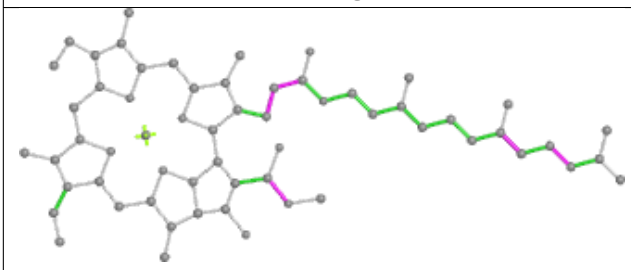
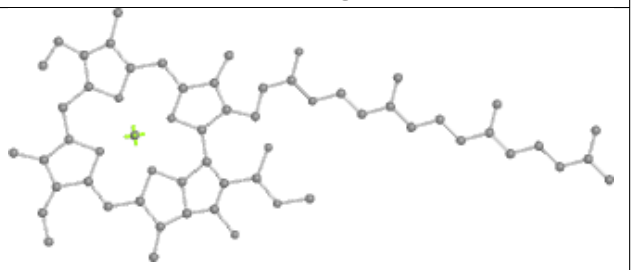


Torsions

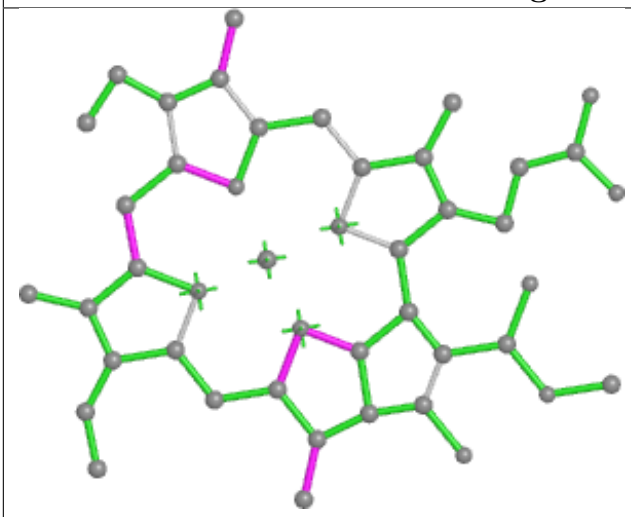


Rings

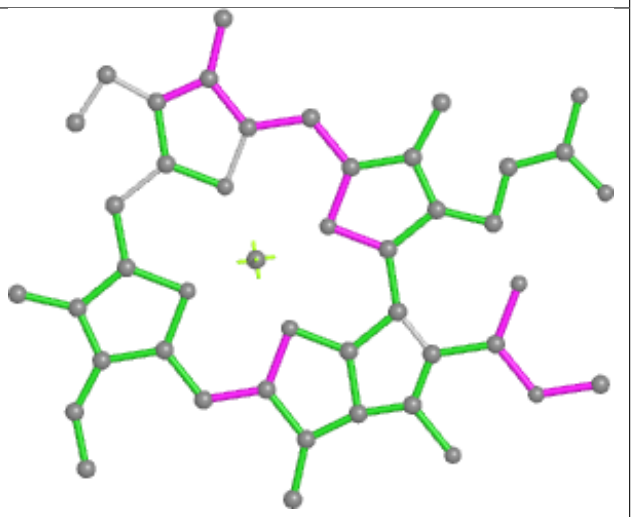
Ligand CLA G 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

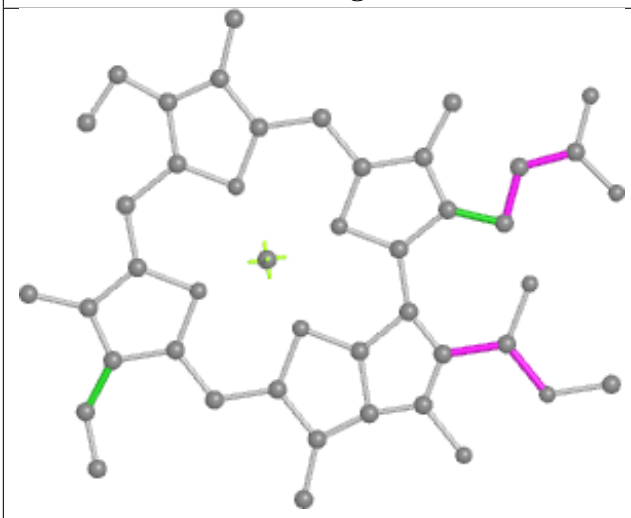
Ligand CLA s 308



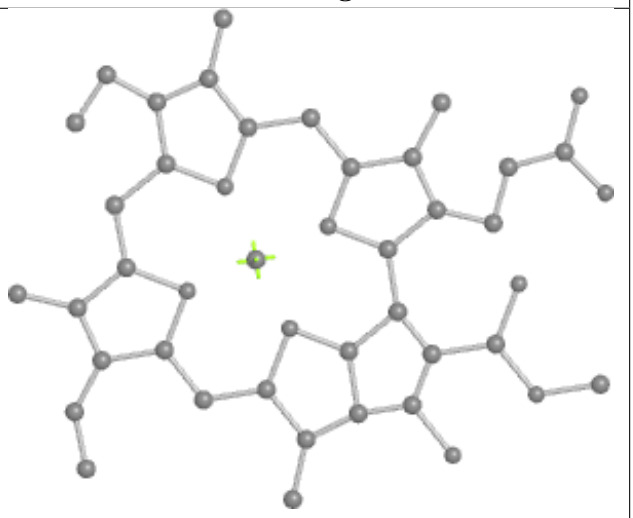
Bond lengths



Bond angles

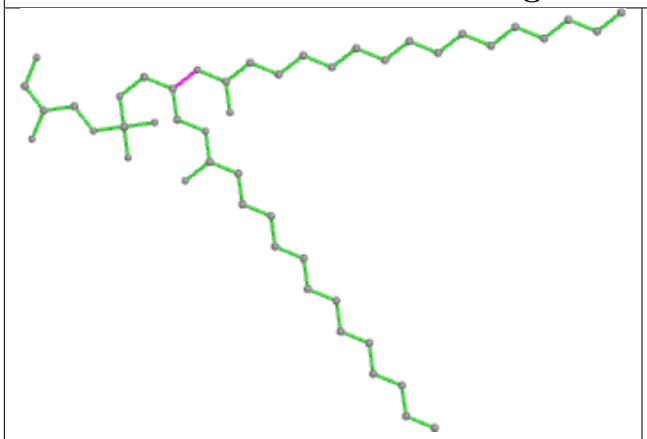


Torsions

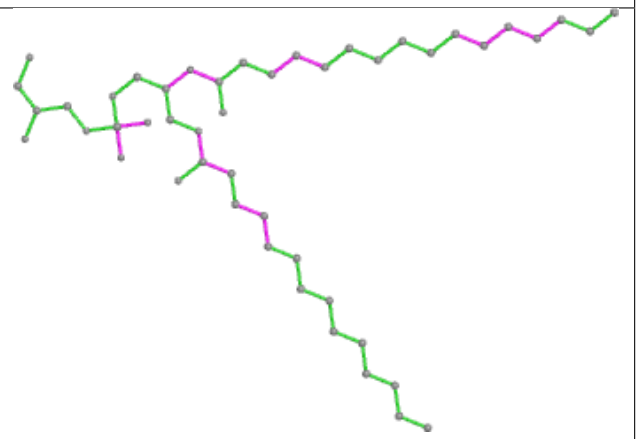


Rings

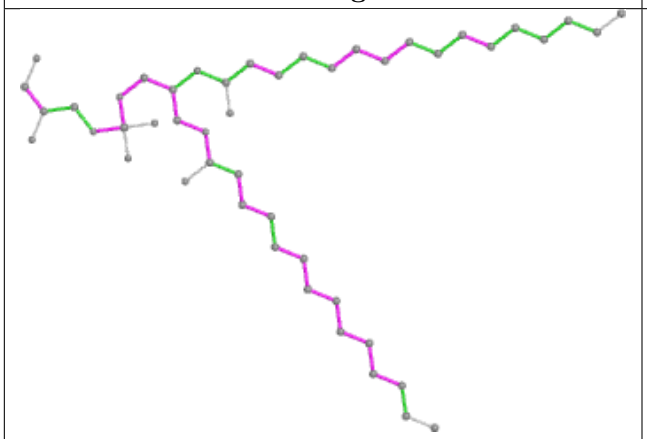
Ligand LHG R 301



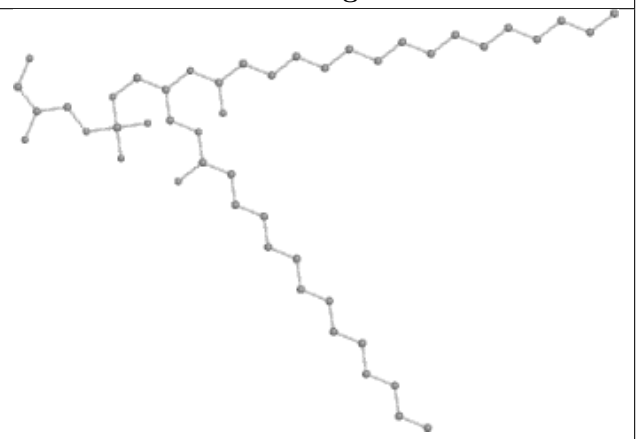
Bond lengths



Bond angles

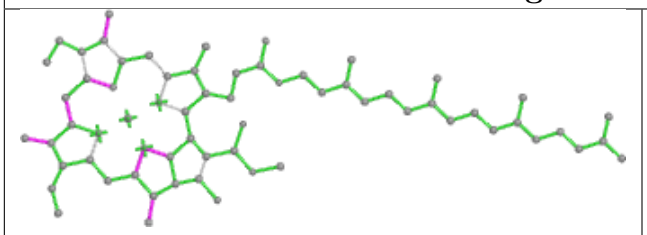


Torsions

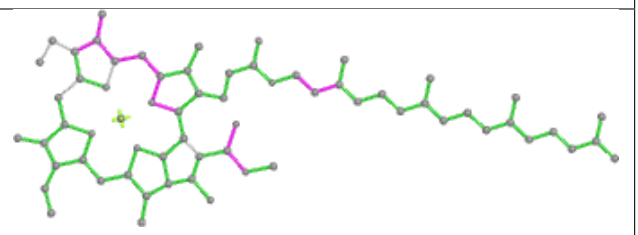


Rings

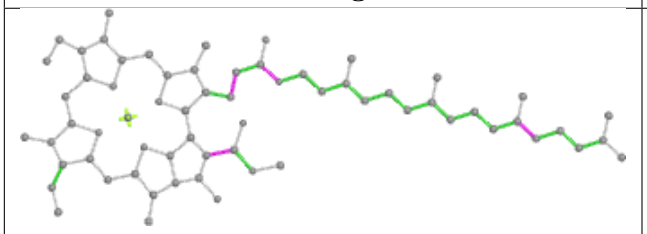
Ligand CLA B 609



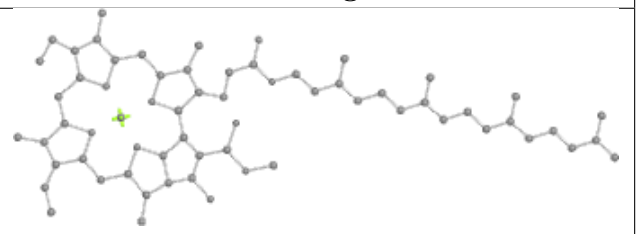
Bond lengths



Bond angles

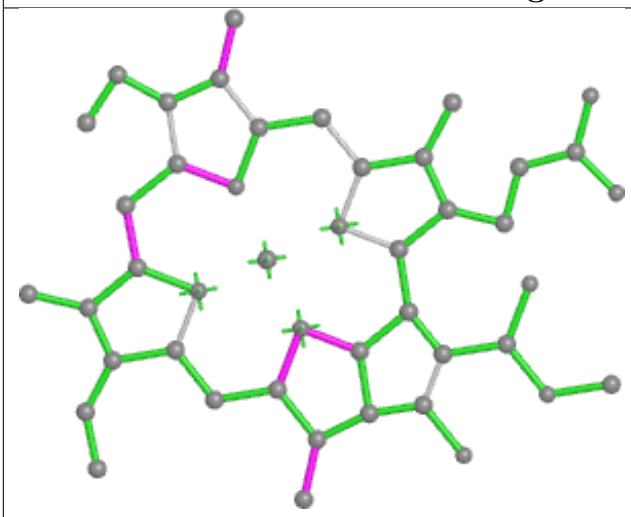


Torsions

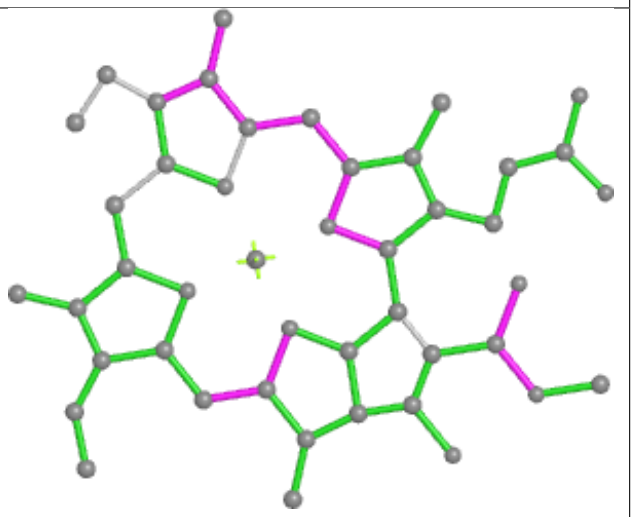


Rings

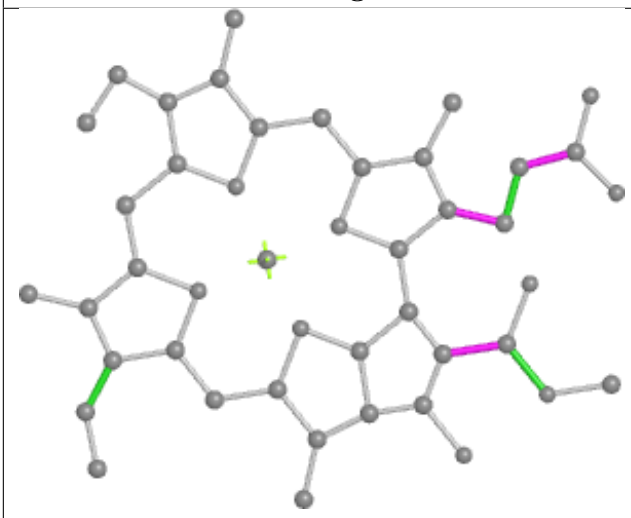
Ligand CLA S 304



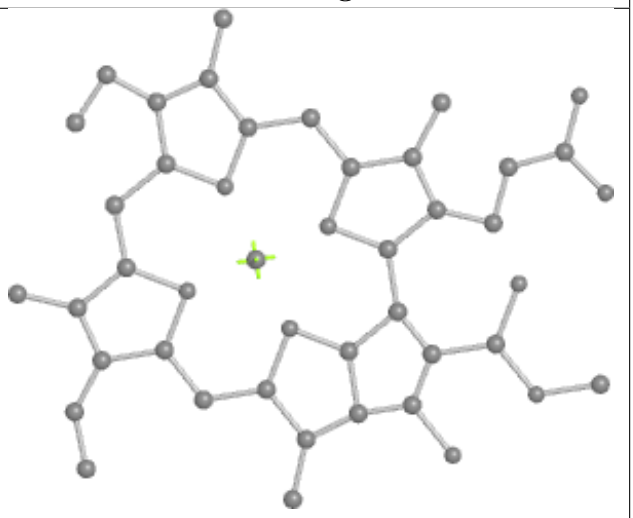
Bond lengths



Bond angles

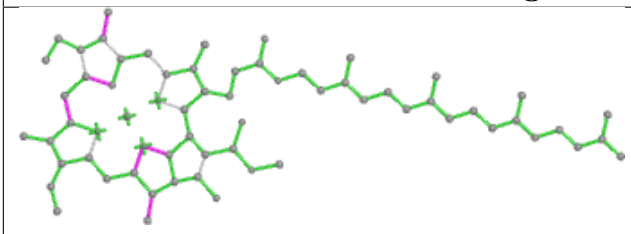


Torsions

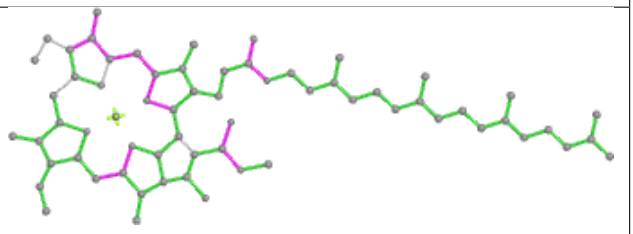


Rings

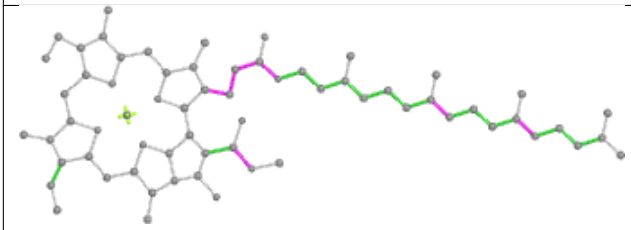
Ligand CLA G 602



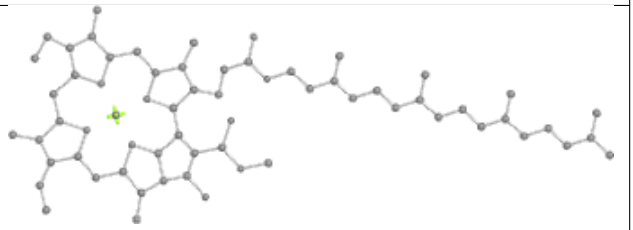
Bond lengths



Bond angles

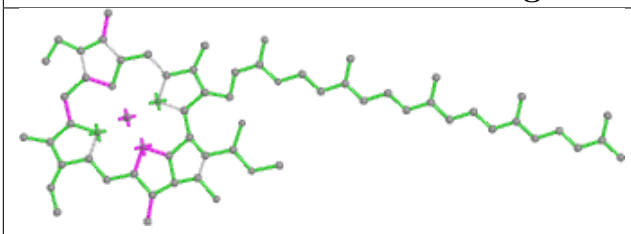


Torsions

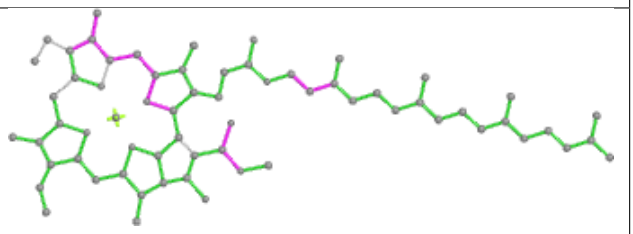


Rings

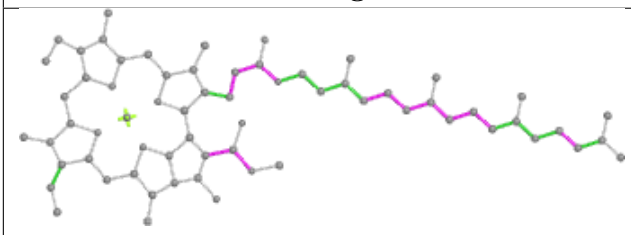
Ligand CLA N 603



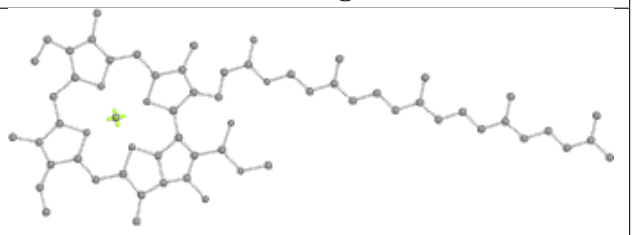
Bond lengths



Bond angles

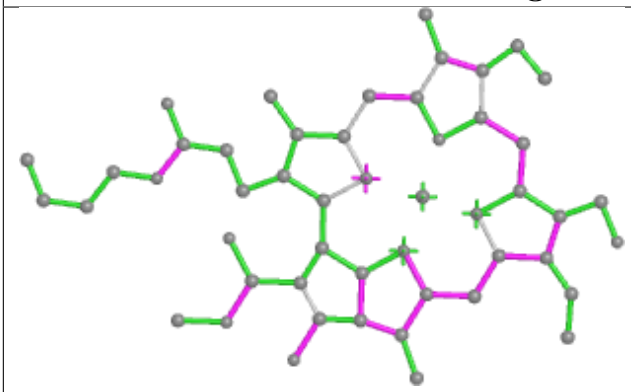


Torsions

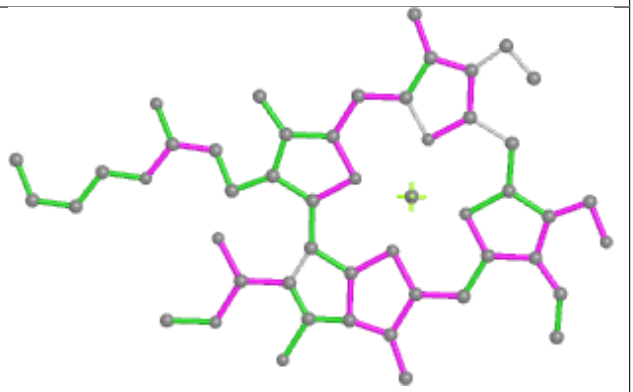


Rings

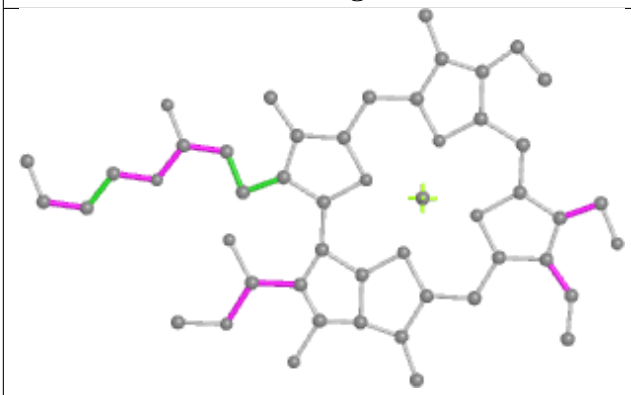
Ligand CHL n 605



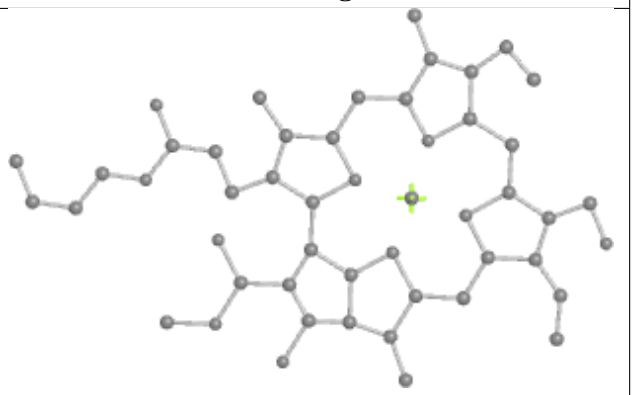
Bond lengths



Bond angles

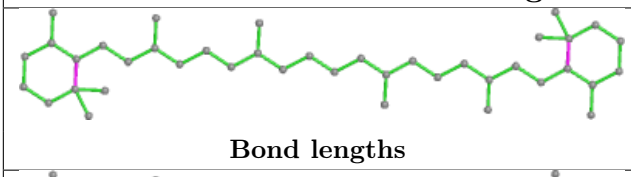


Torsions

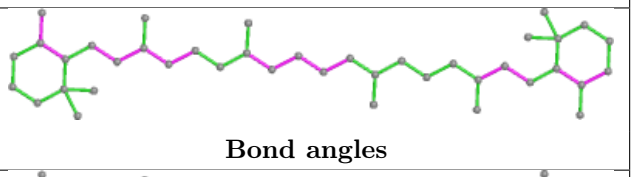


Rings

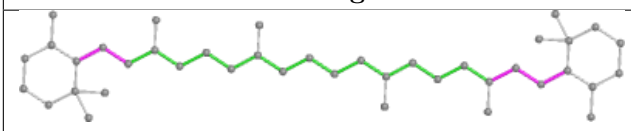
Ligand BCR b 616



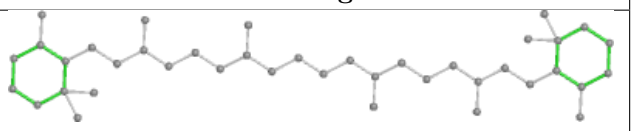
Bond lengths



Bond angles

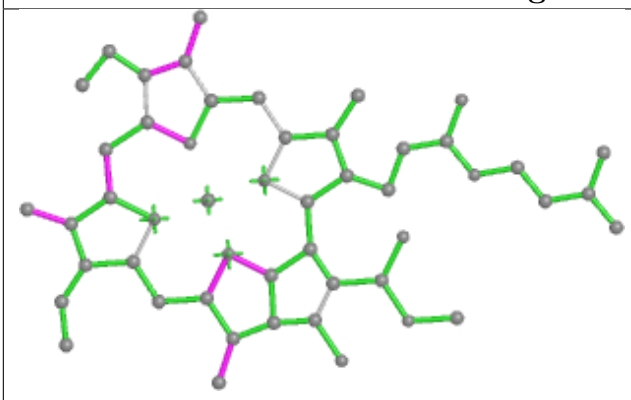


Torsions

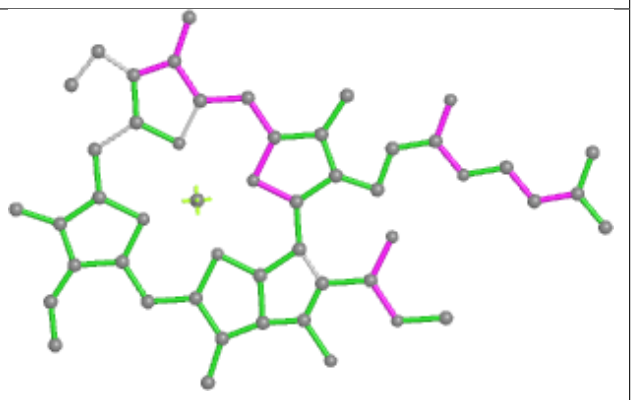


Rings

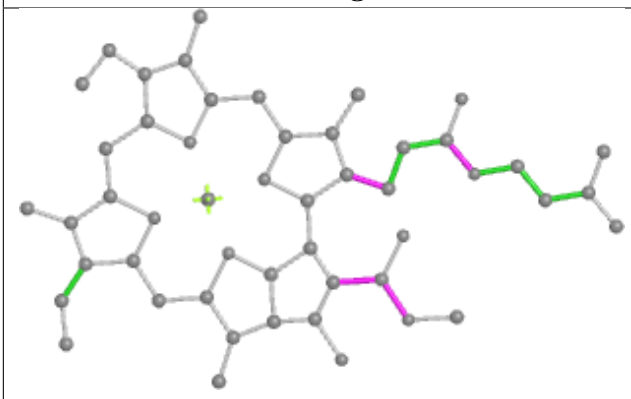
Ligand CLA a 406



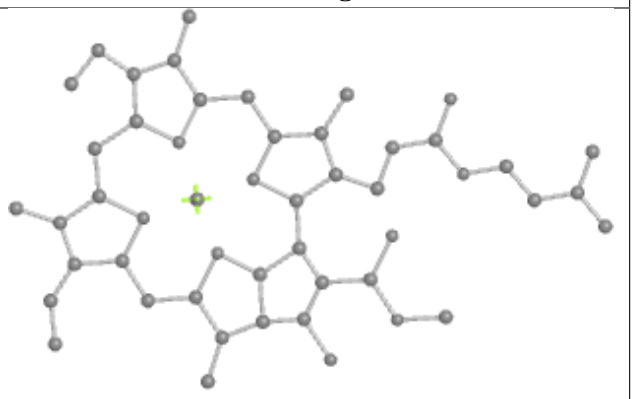
Bond lengths



Bond angles

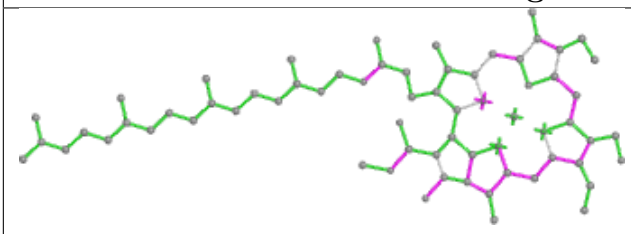


Torsions

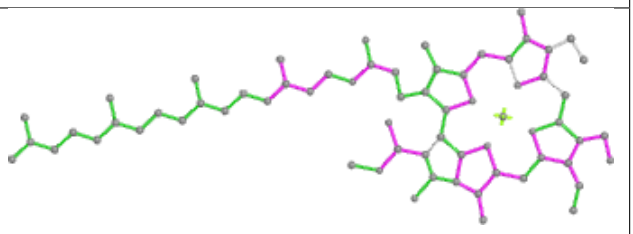


Rings

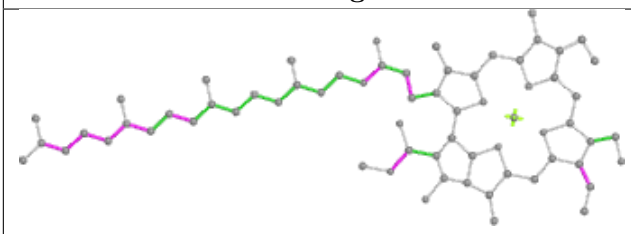
Ligand CHL n 608



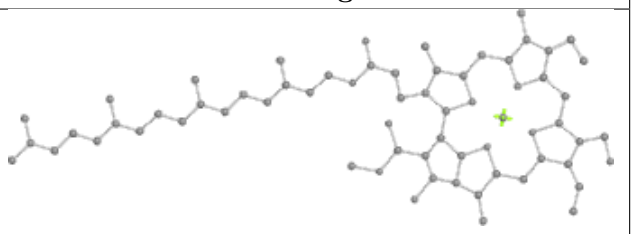
Bond lengths



Bond angles

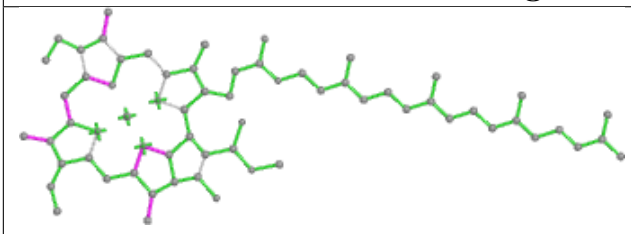


Torsions

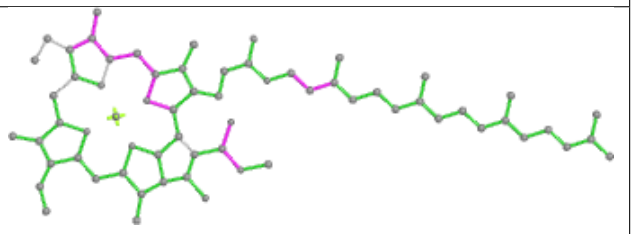


Rings

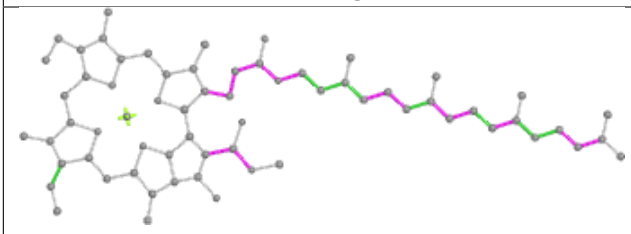
Ligand CLA B 604



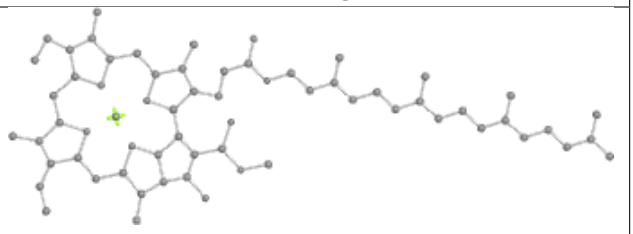
Bond lengths



Bond angles

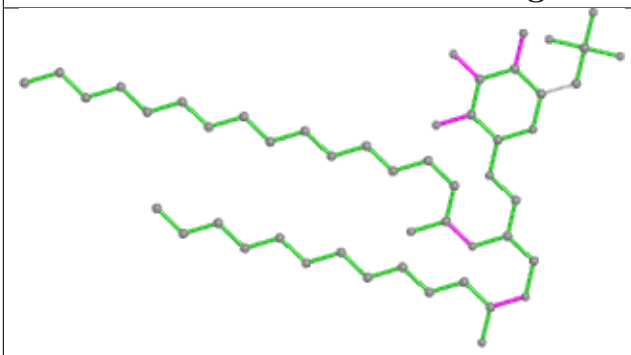


Torsions

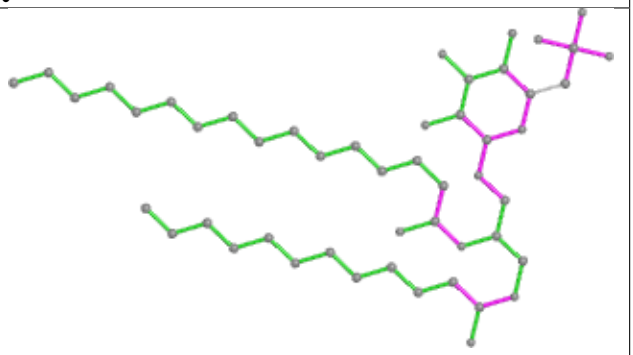


Rings

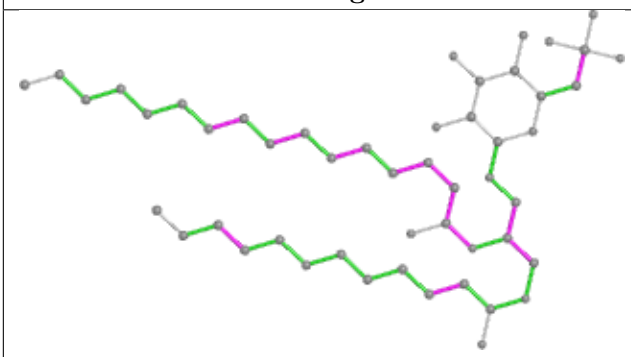
Ligand SQD d 402



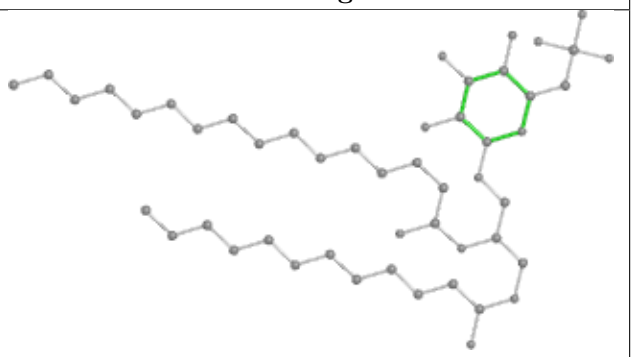
Bond lengths



Bond angles

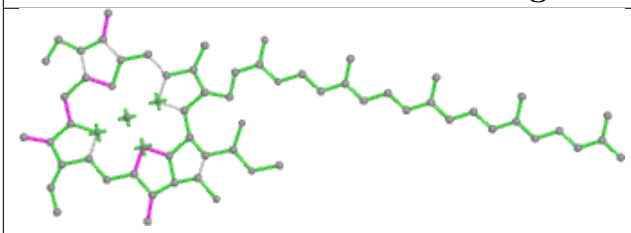


Torsions

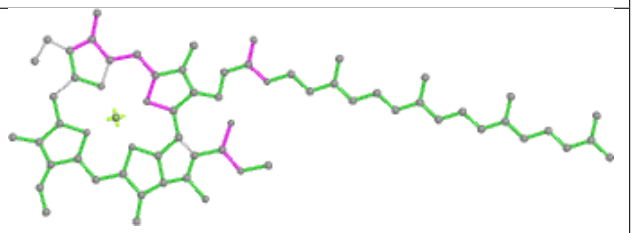


Rings

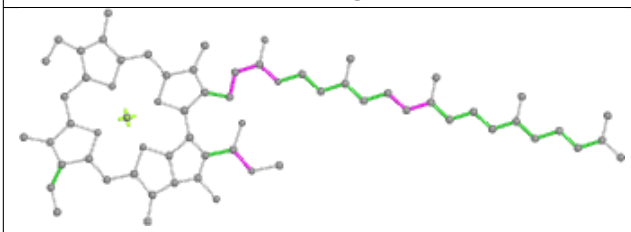
Ligand CLA c 507



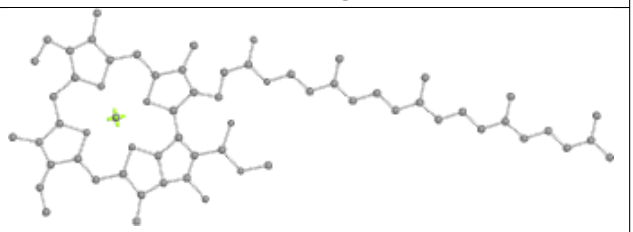
Bond lengths



Bond angles

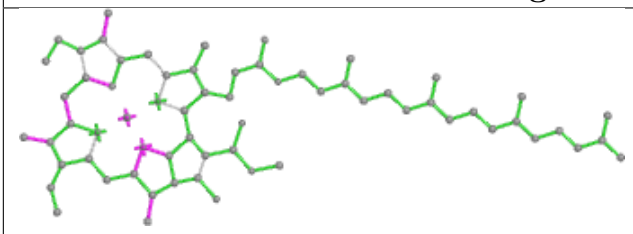


Torsions

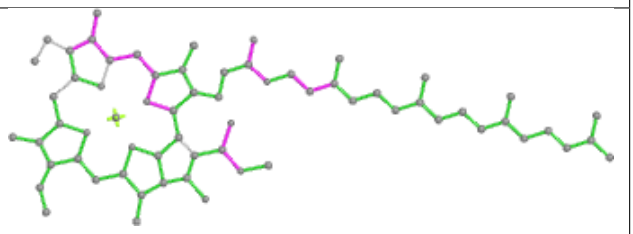


Rings

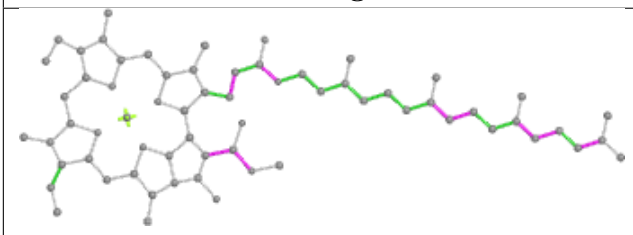
Ligand CLA c 503



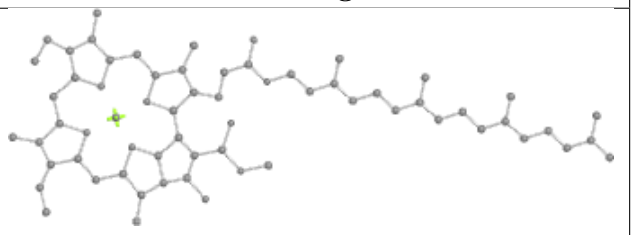
Bond lengths



Bond angles

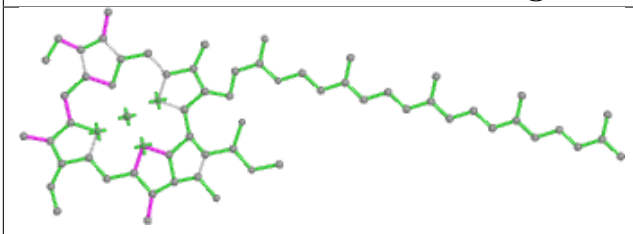


Torsions

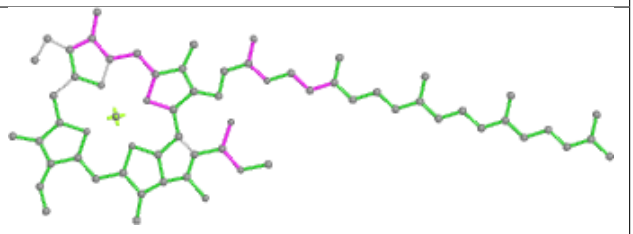


Rings

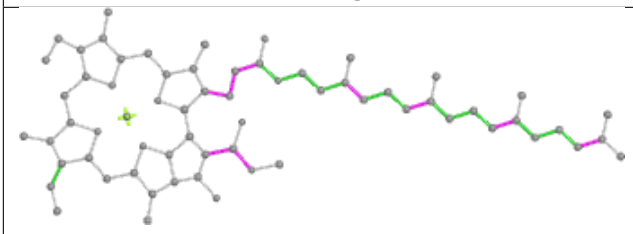
Ligand CLA b 602



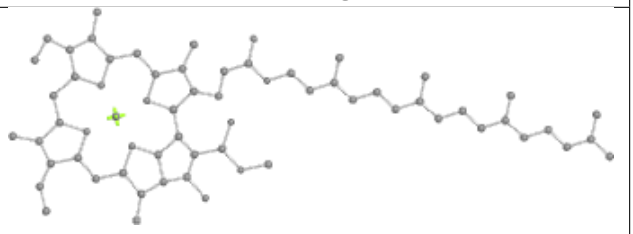
Bond lengths



Bond angles

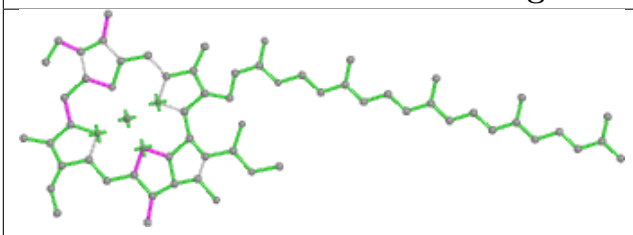


Torsions

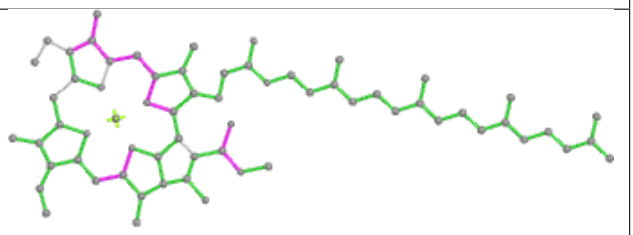


Rings

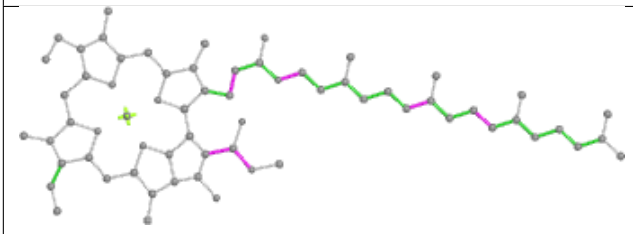
Ligand CLA b 609



Bond lengths



Bond angles



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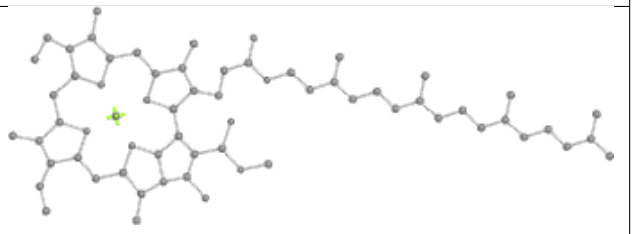
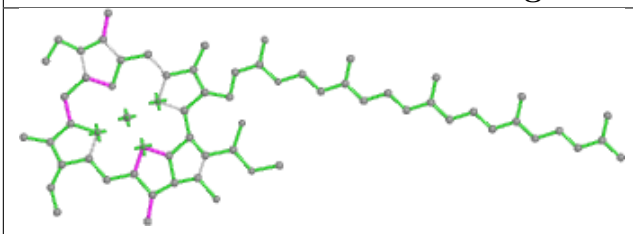
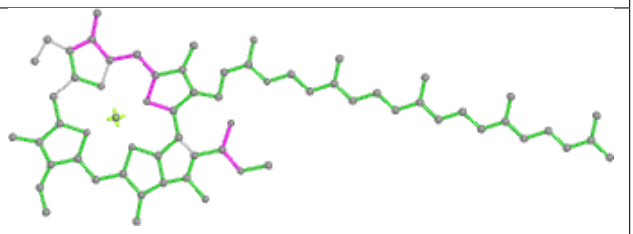


Rings

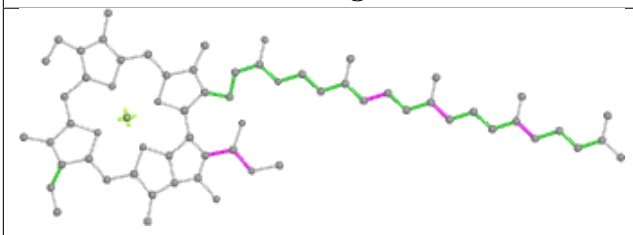
Ligand CLA B 615



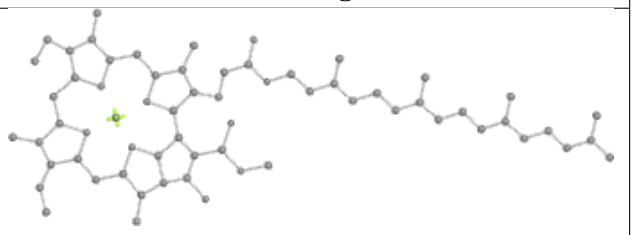
Bond lengths



Bond angles

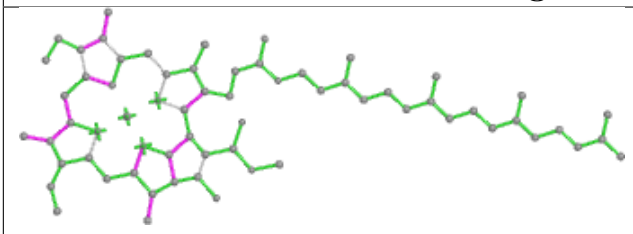


Torsions

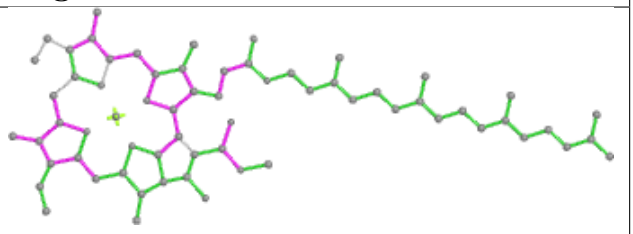


Rings

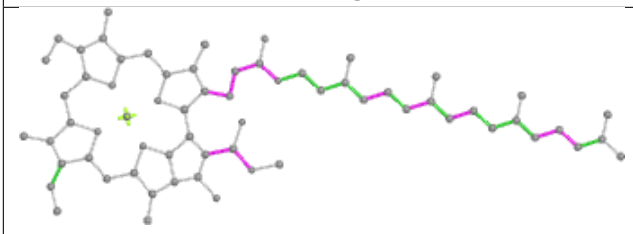
Ligand CLA g 613



Bond lengths



Bond angles



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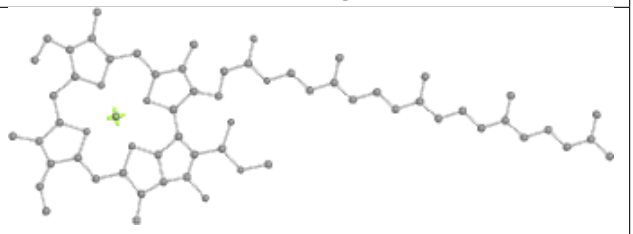
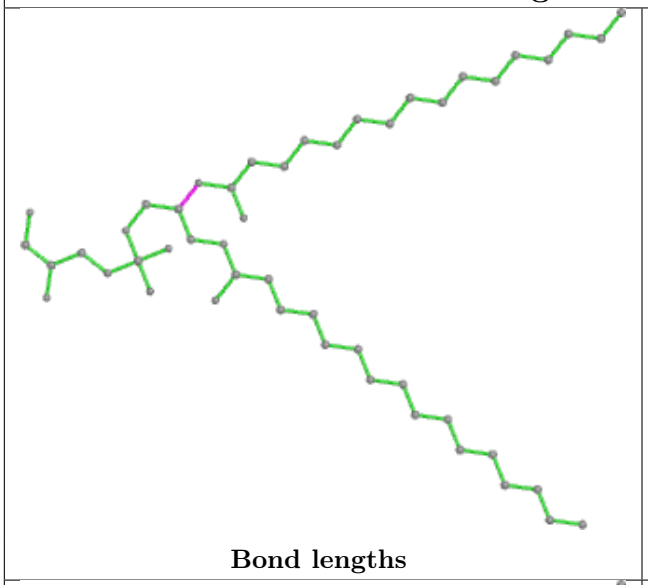


Rings

Ligand LHG l 102



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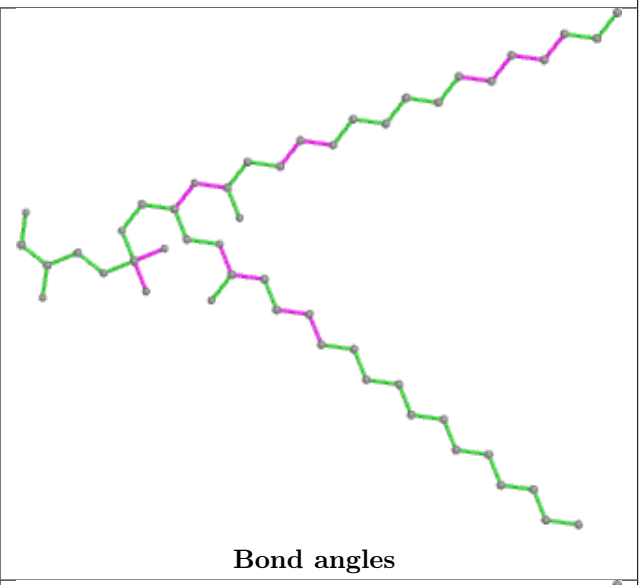
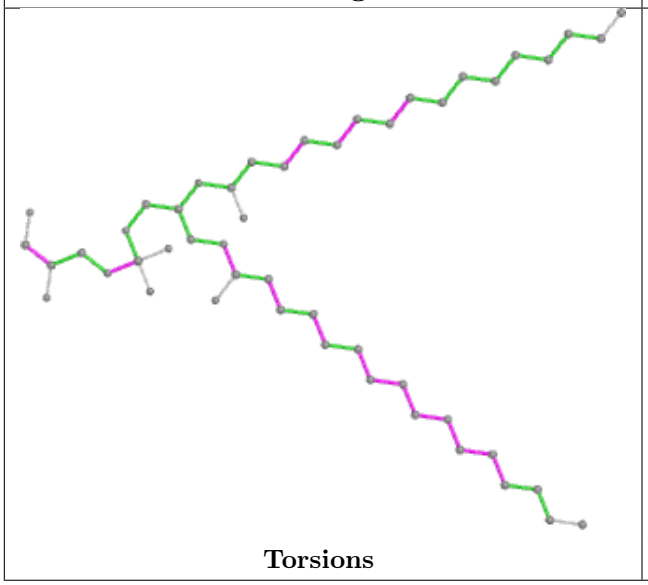


Bond angles



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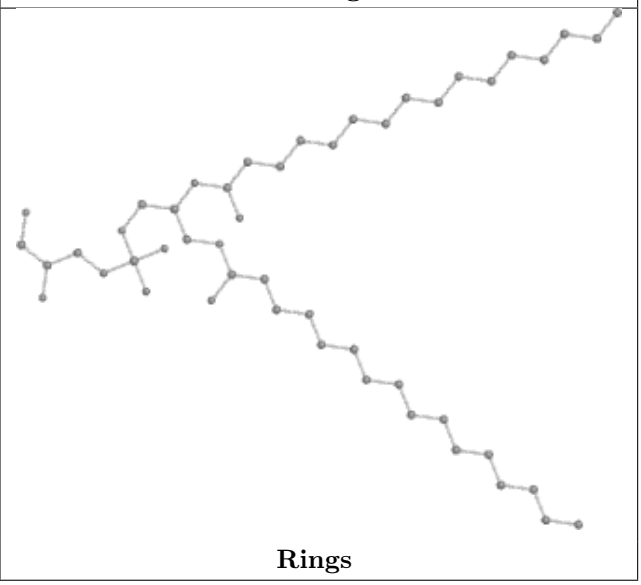
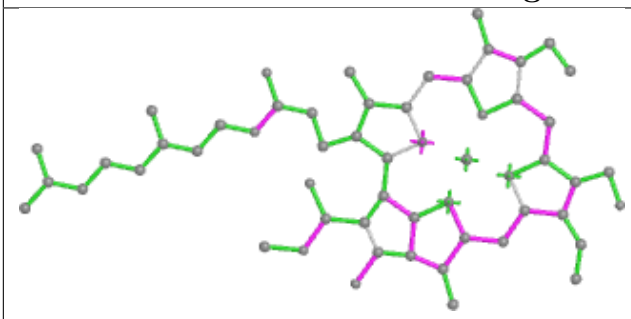
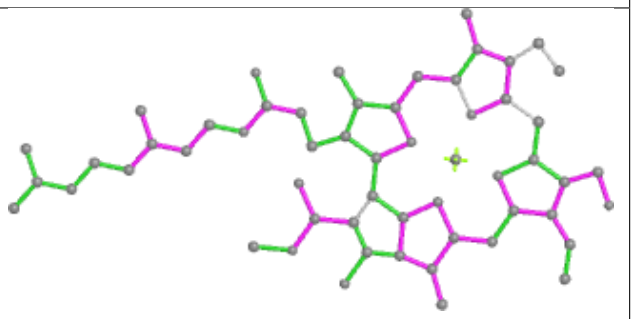


Rings

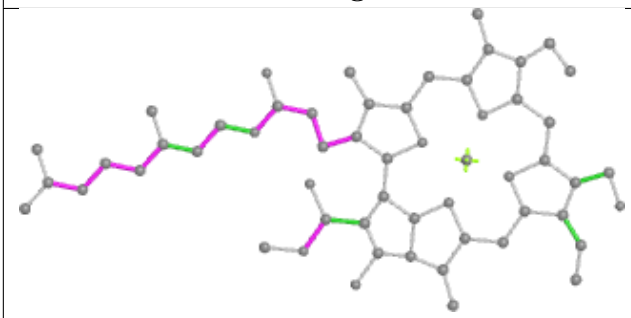
Ligand CHL R 306



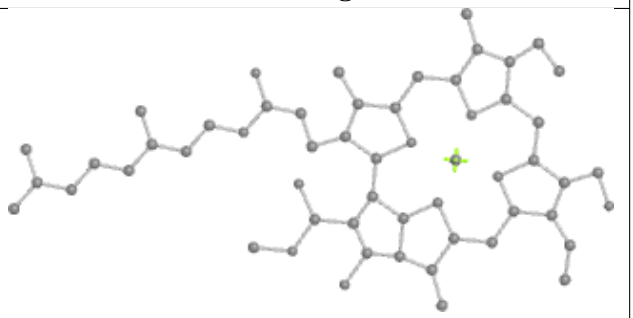
Bond lengths



Bond angles

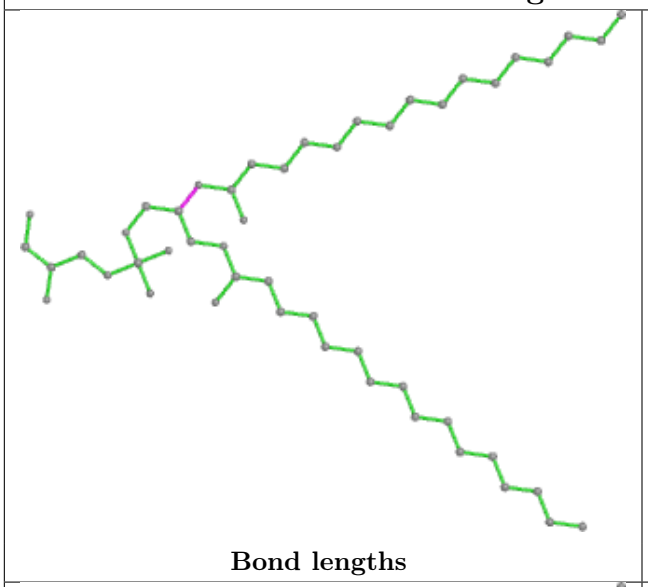


Torsions

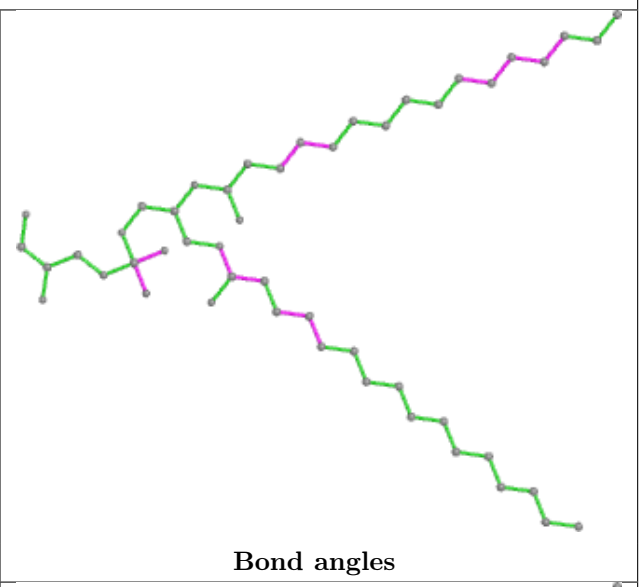


Rings

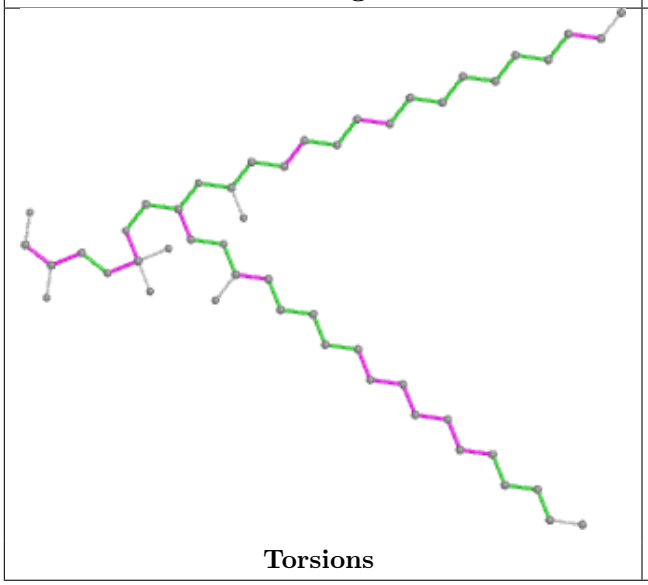
Ligand LHG d 408



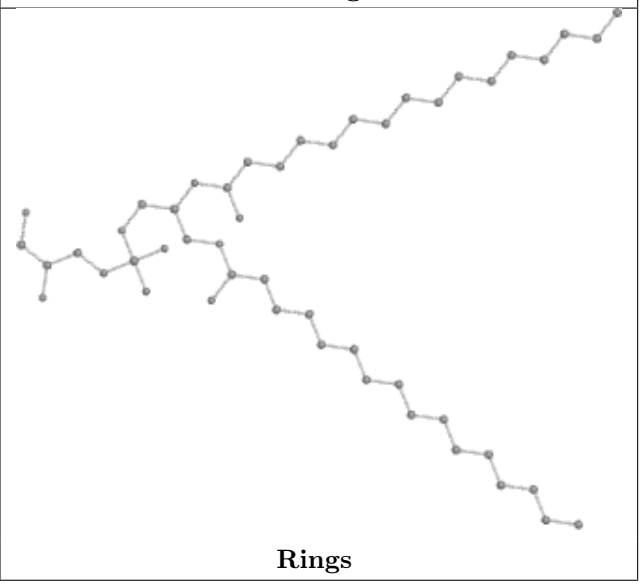
Bond lengths



Bond angles

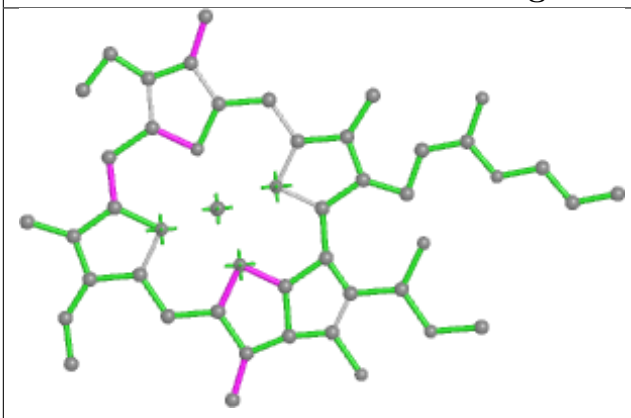


Torsions



Rings

Ligand CLA g 614



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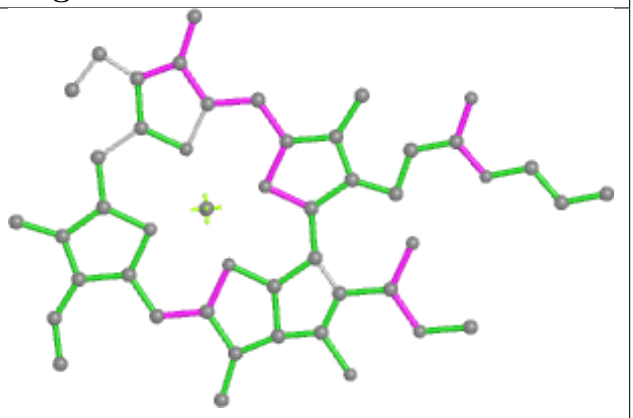
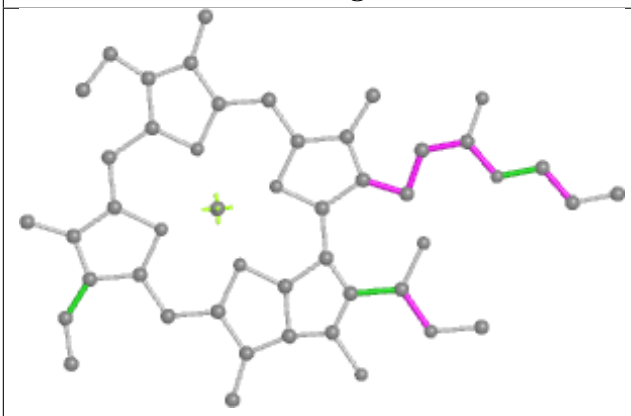


Bond angles



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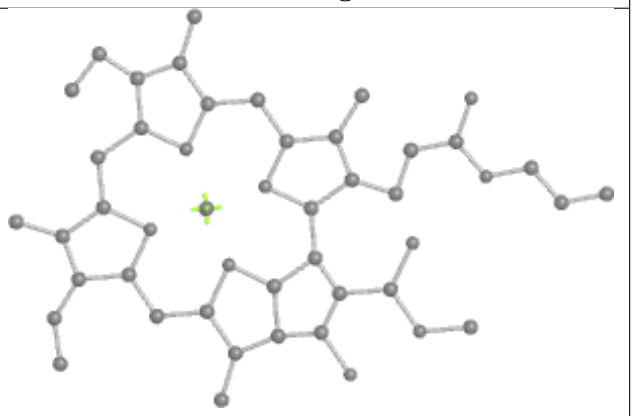
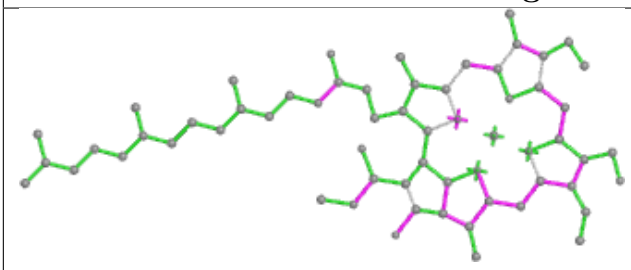


Rings

Ligand CHL G 609



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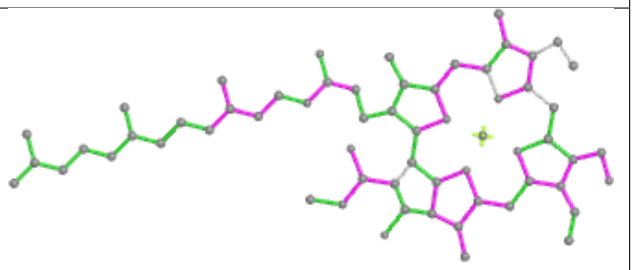
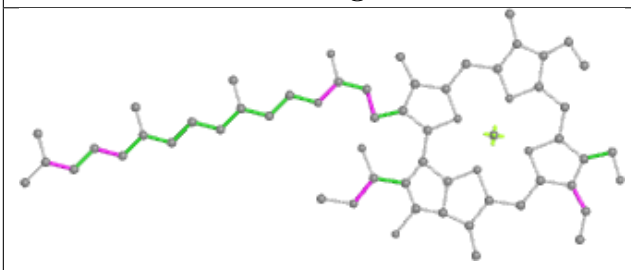
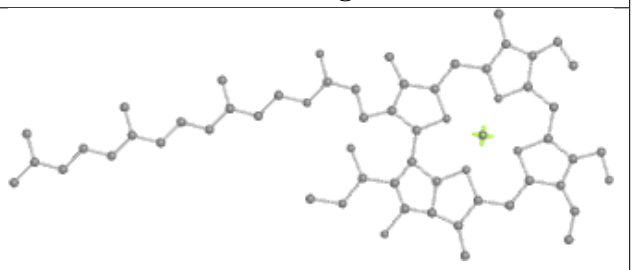


Bond angles

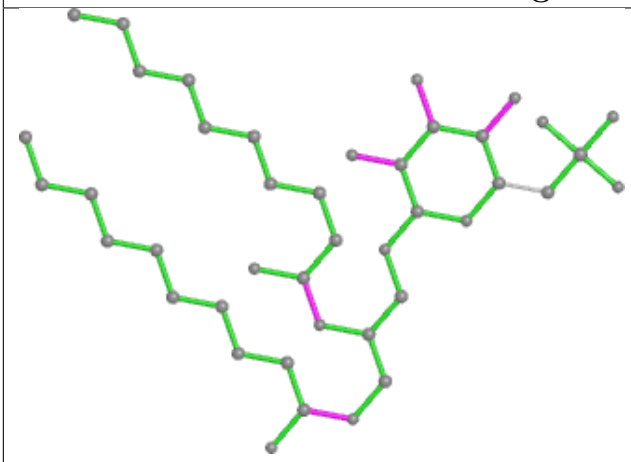


Torsions

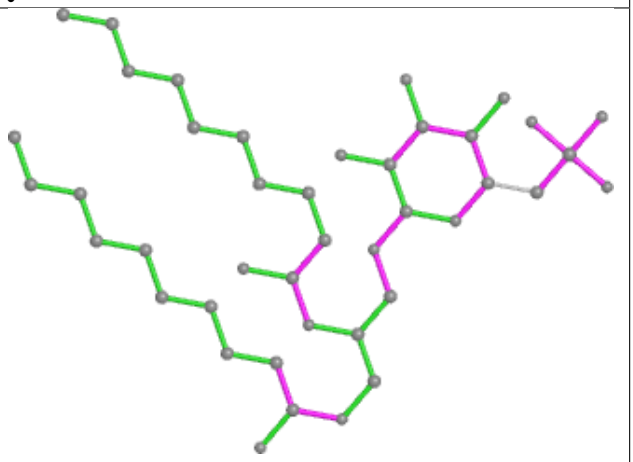


Rings

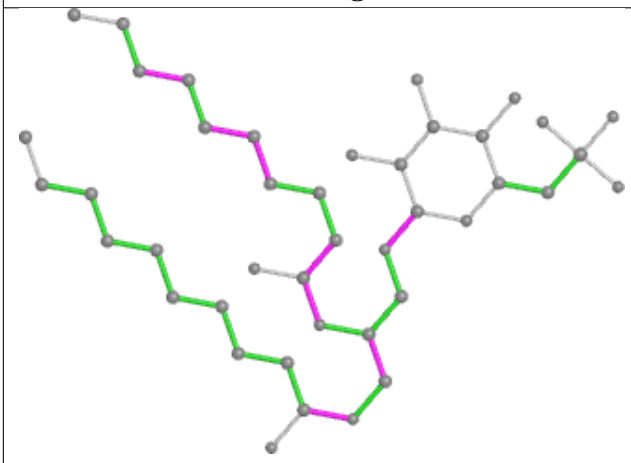
Ligand SQD l 101



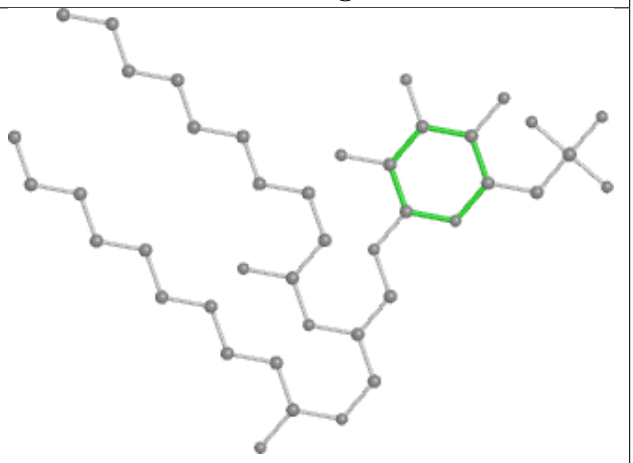
Bond lengths



Bond angles

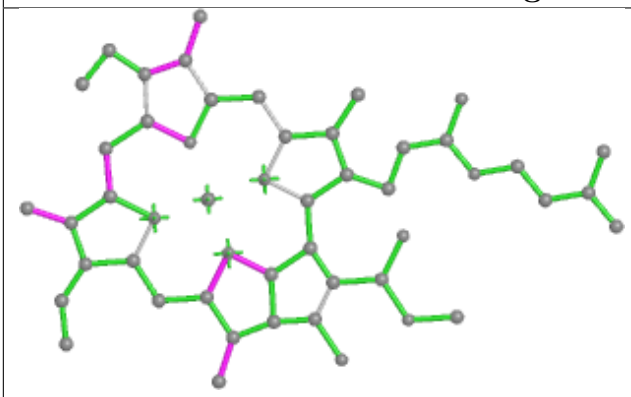


Torsions

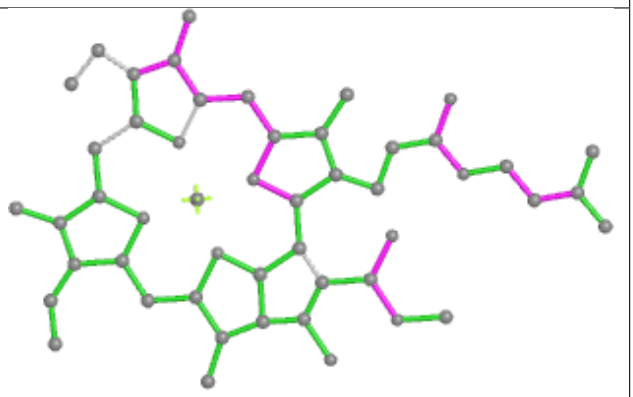


Rings

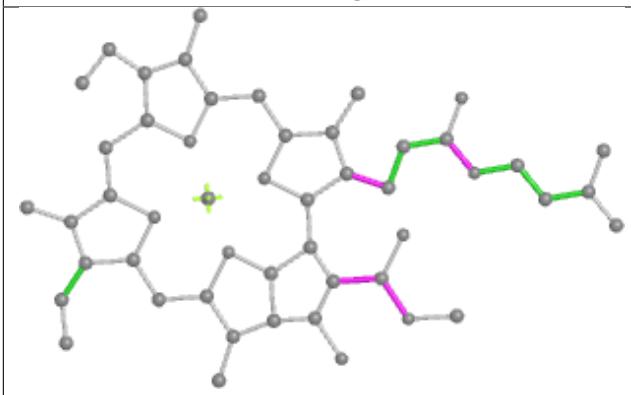
Ligand CLA A 407



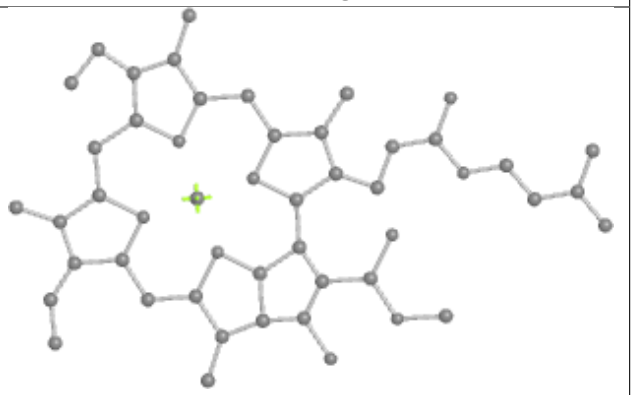
Bond lengths



Bond angles

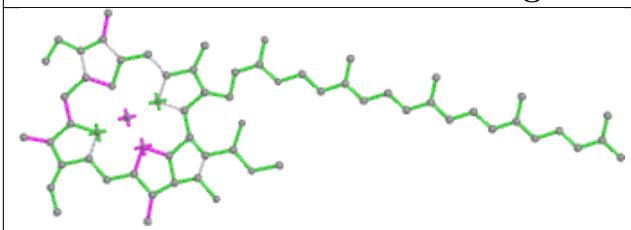


Torsions

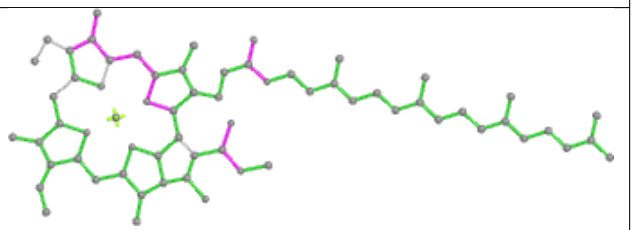


Rings

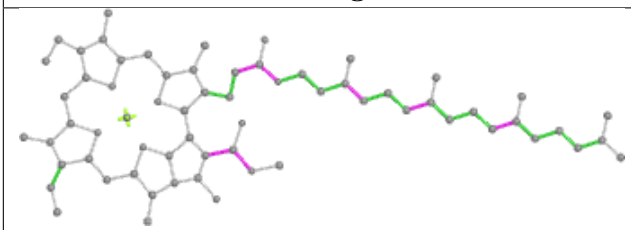
Ligand CLA D 404



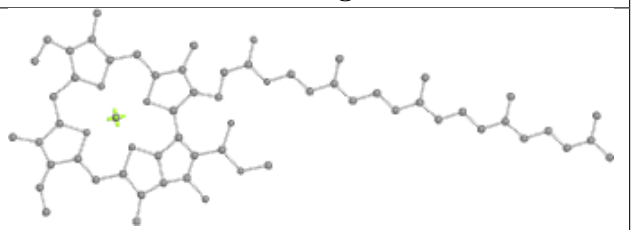
Bond lengths



Bond angles

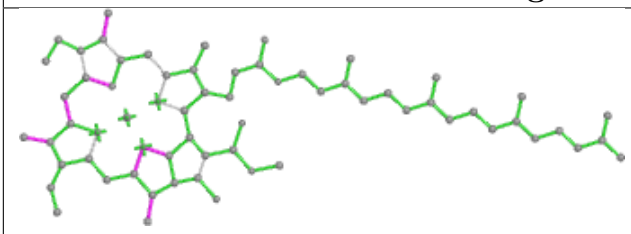


Torsions

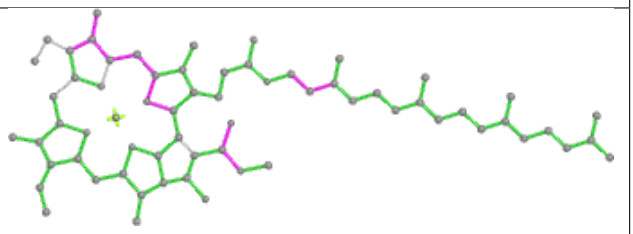


Rings

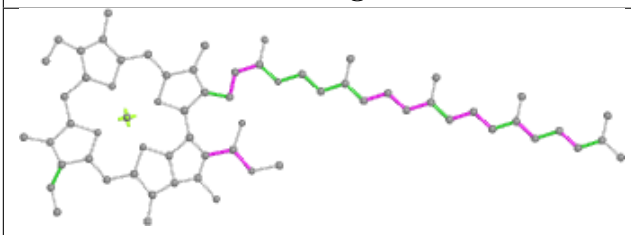
Ligand CLA b 613



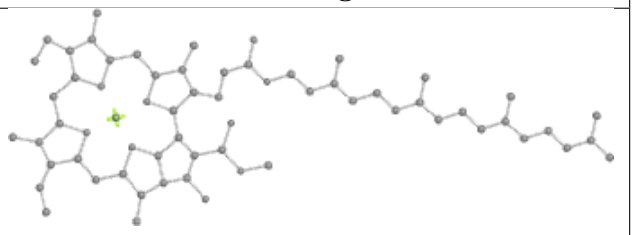
Bond lengths



Bond angles

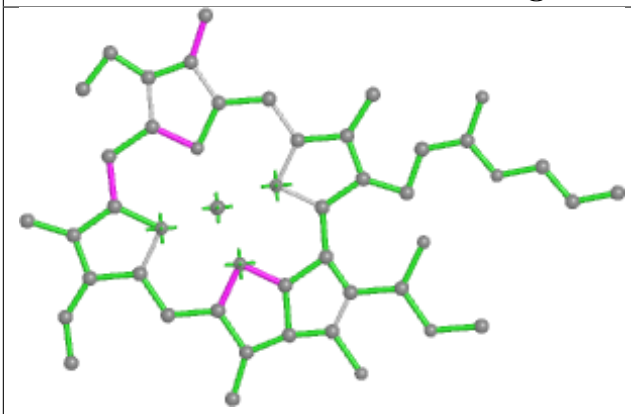


Torsions

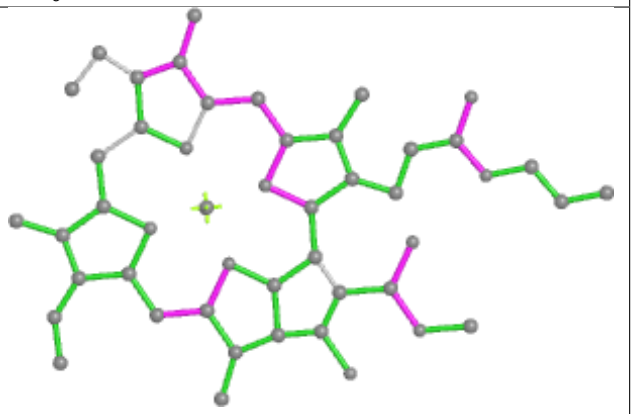


Rings

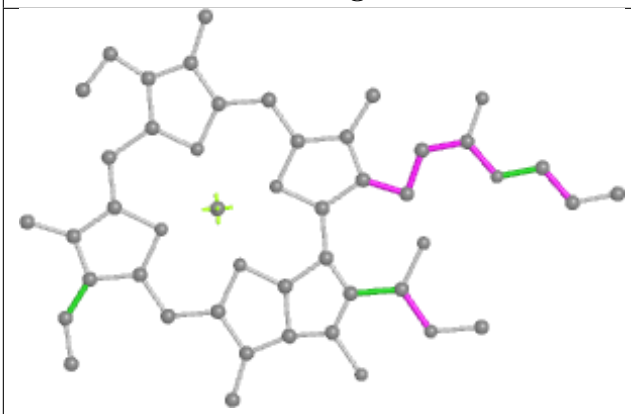
Ligand CLA y 613



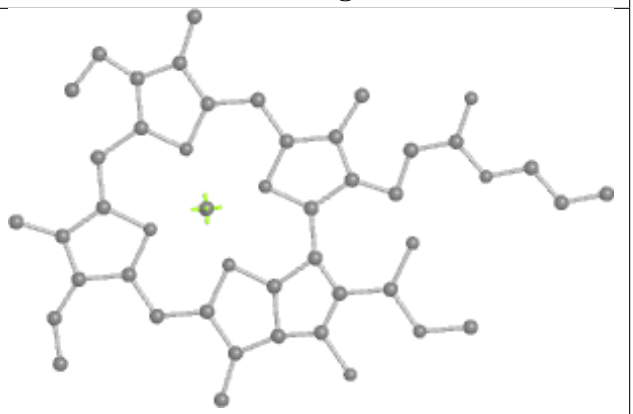
Bond lengths



Bond angles

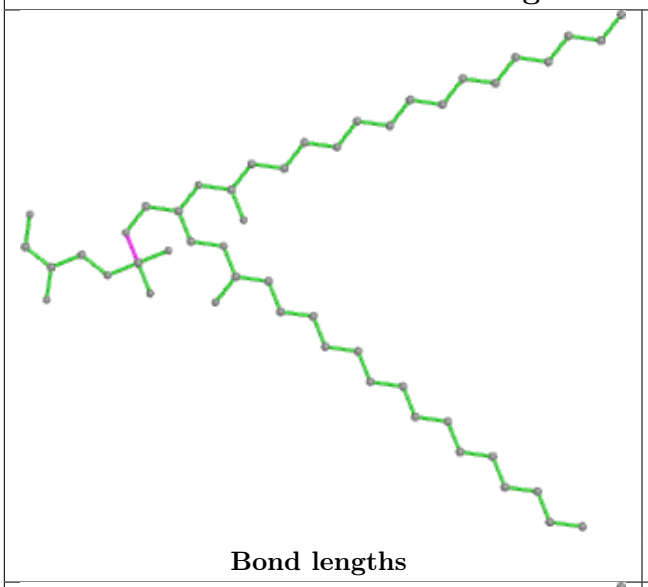


Torsions



Rings

Ligand LHG N 618



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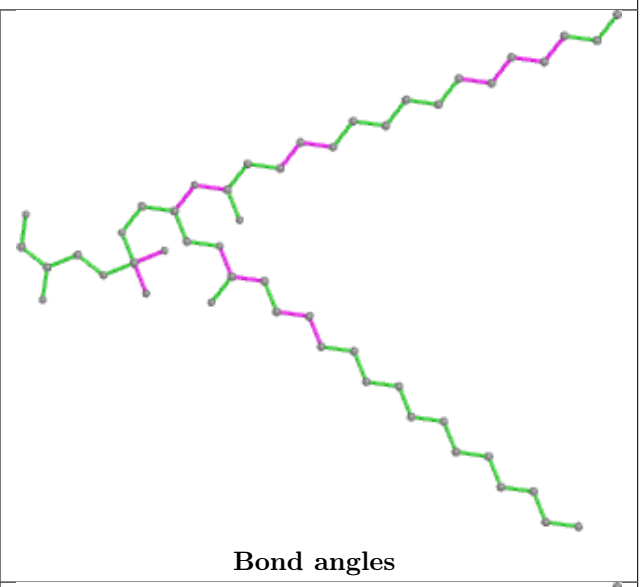
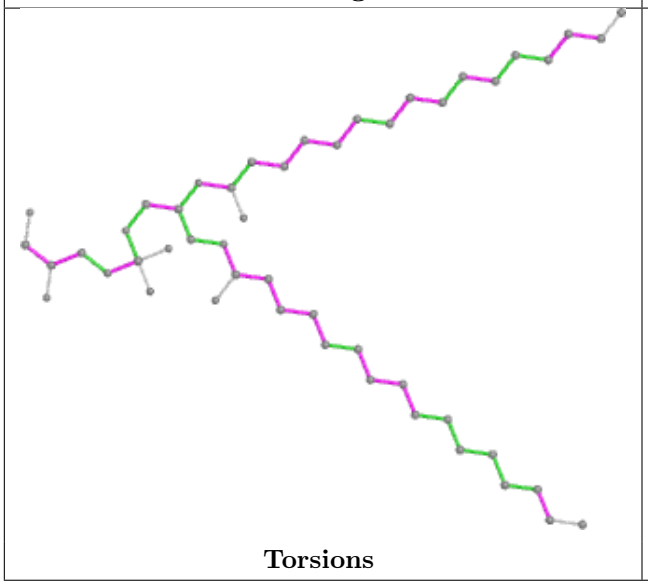
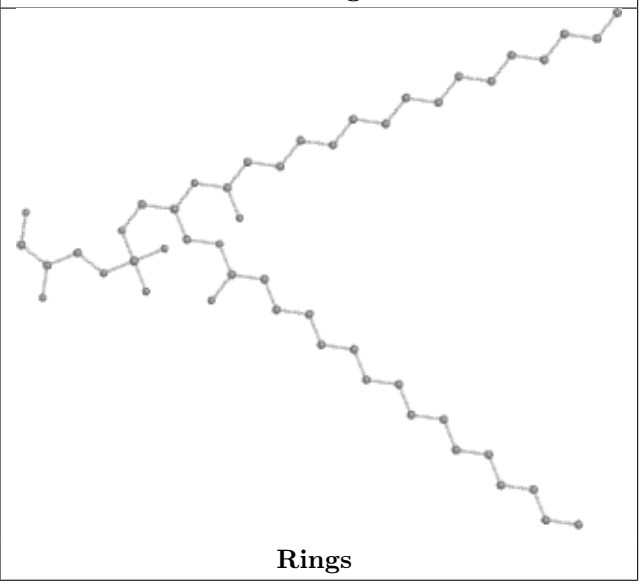


Bond angles

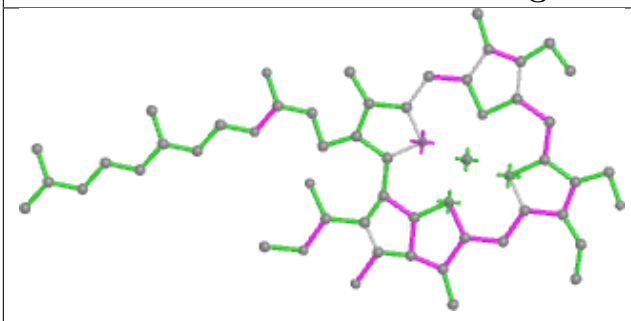


Torsions



Rings

Ligand CHL r 307



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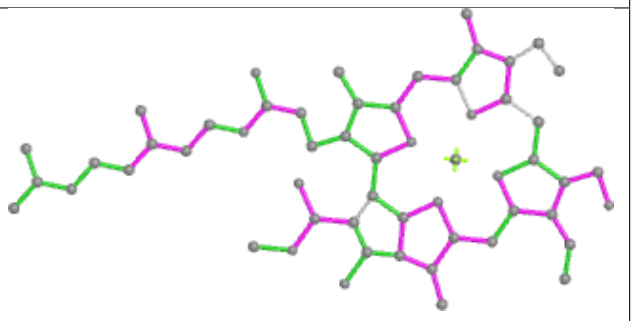
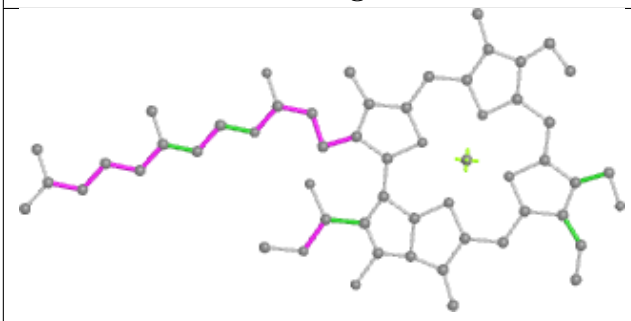
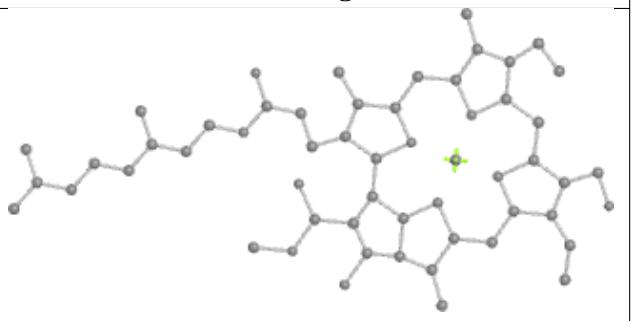


Bond angles

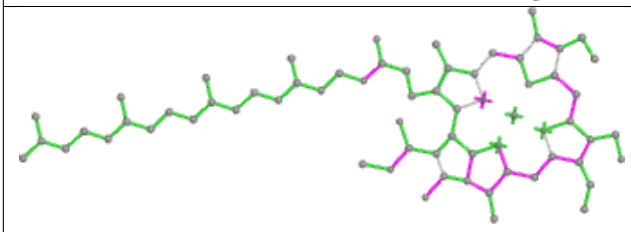


Torsions



Rings

Ligand CHL y 601



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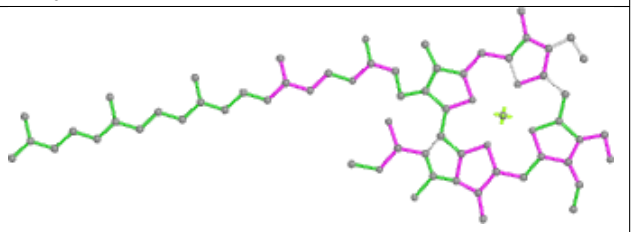
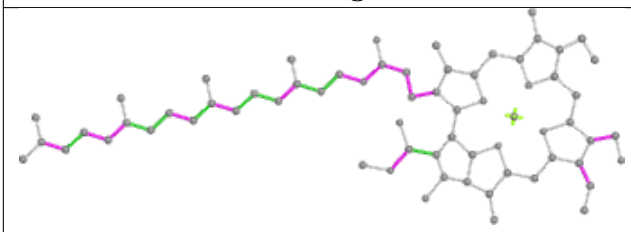


Bond angles



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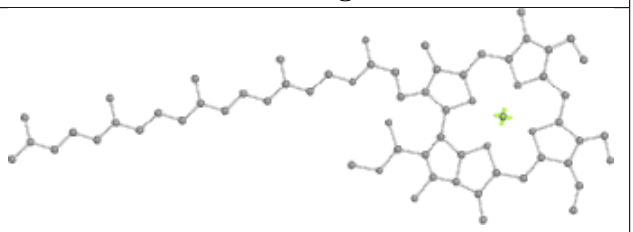
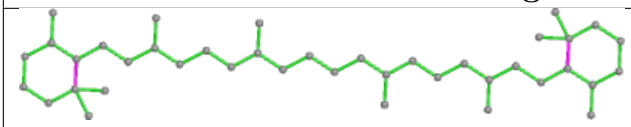
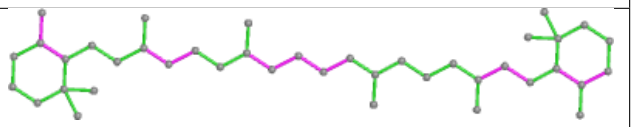


Rings

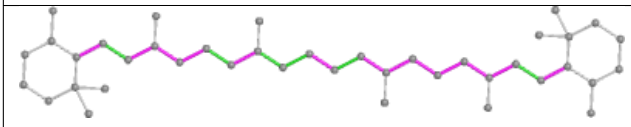
Ligand BCR B 602



Bond lengths



Bond angles



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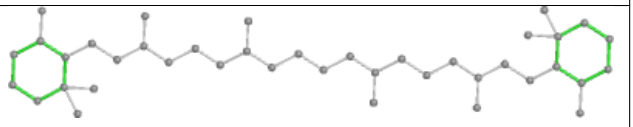
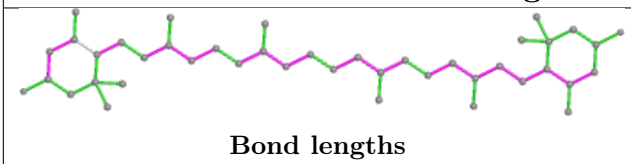
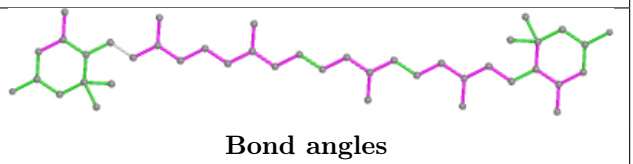


Rings

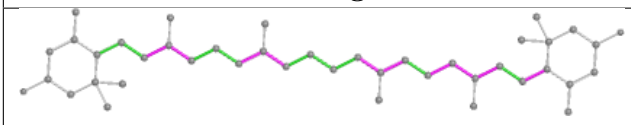
Ligand LUT G 616



Bond lengths



Bond angles



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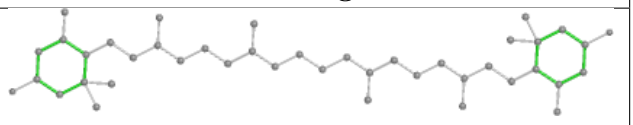
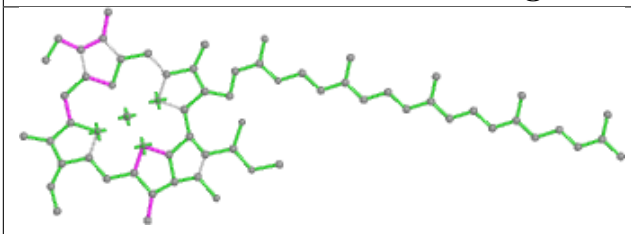
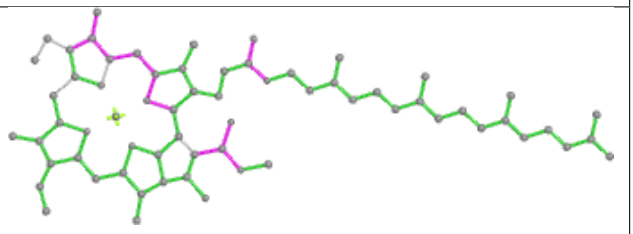


Rings

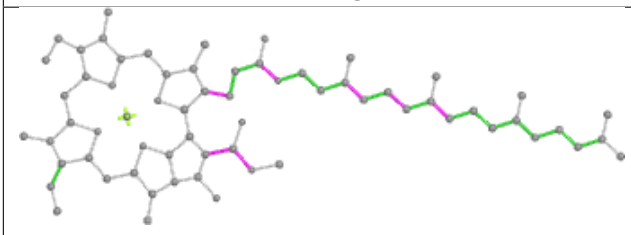
Ligand CLA C 510



Bond lengths



Bond angles



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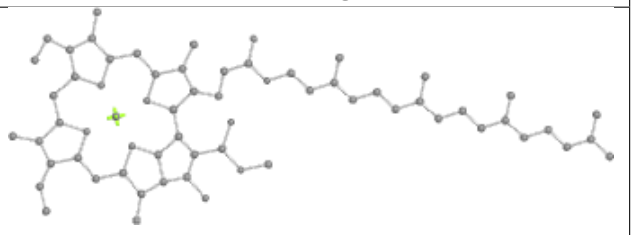
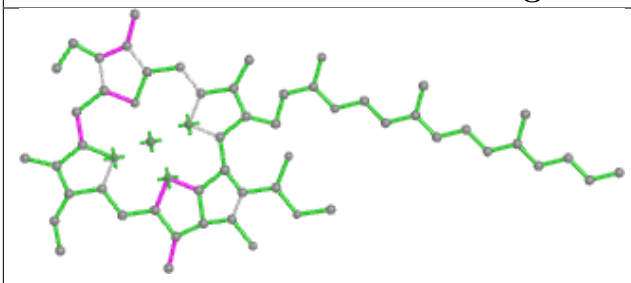
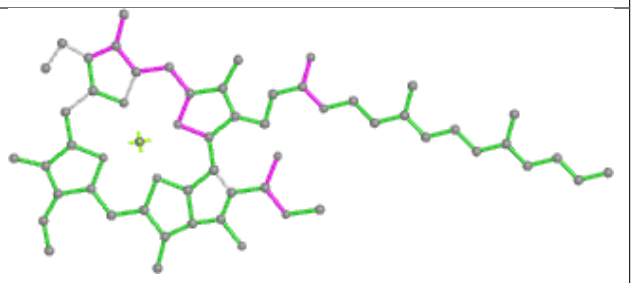


Rings

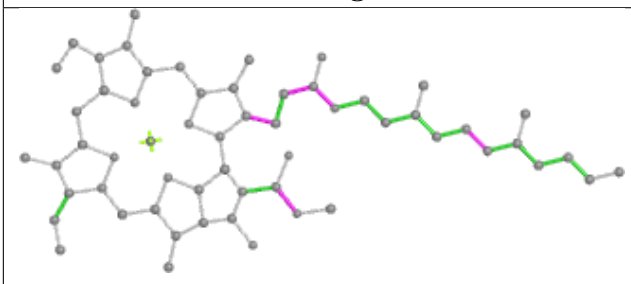
Ligand CLA R 308



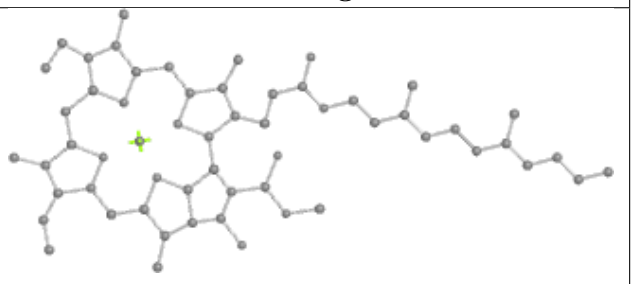
Bond lengths



Bond angles

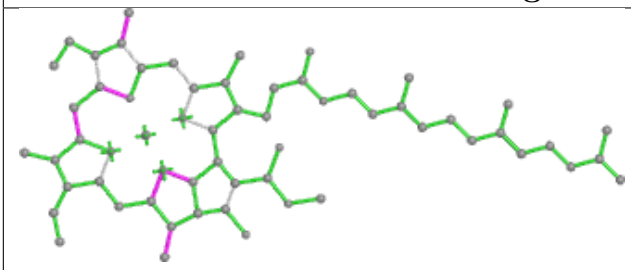


Torsions

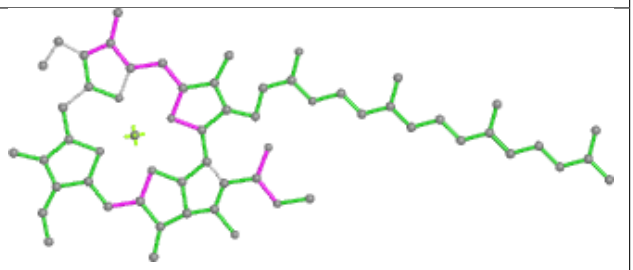


Rings

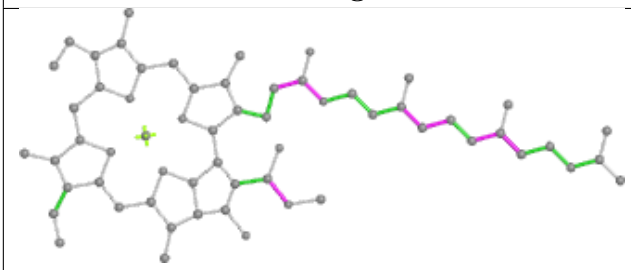
Ligand CLA N 611



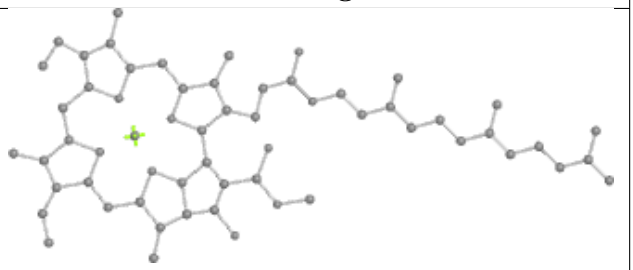
Bond lengths



Bond angles

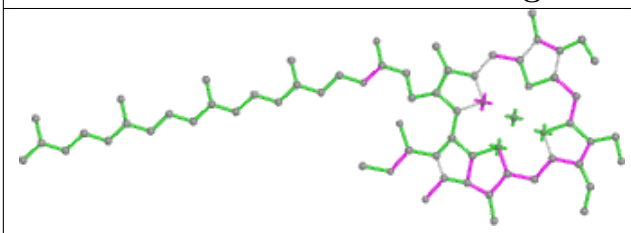


Torsions



Rings

Ligand CHL Y 601



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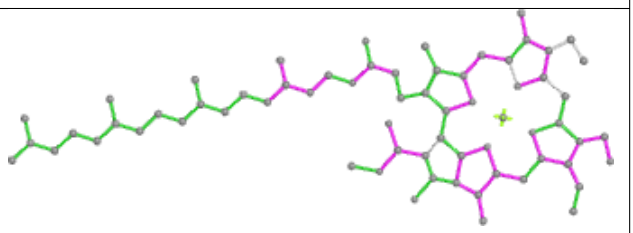
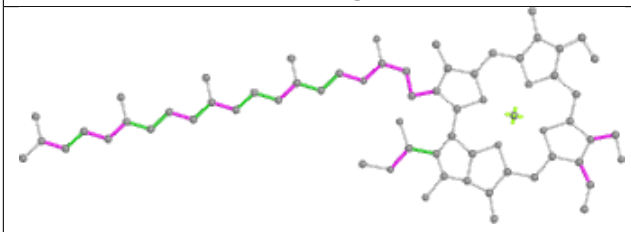
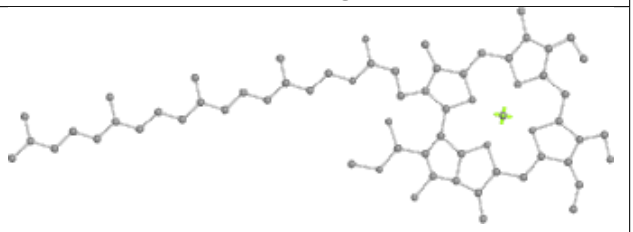


Bond angles

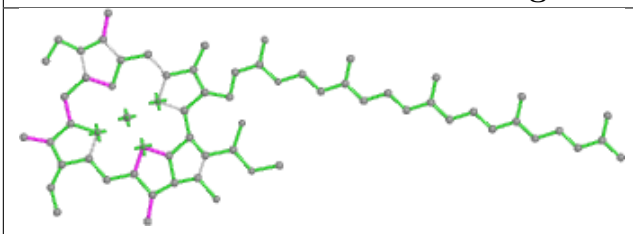


Torsions



Rings

Ligand CLA c 505



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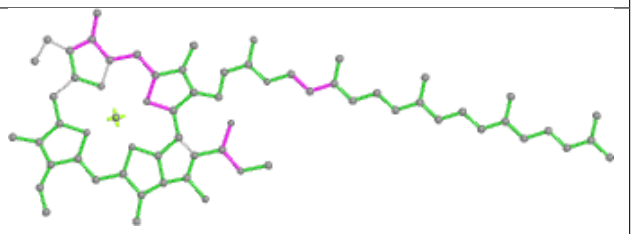
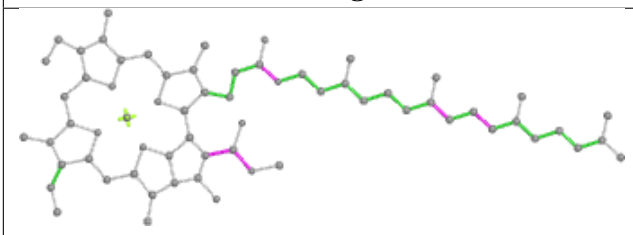


Bond angles



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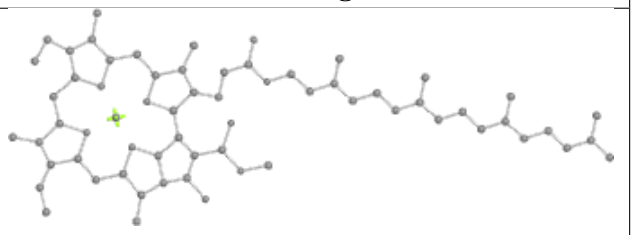
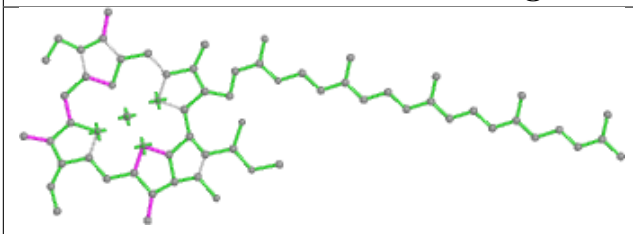


Rings

Ligand CLA B 617



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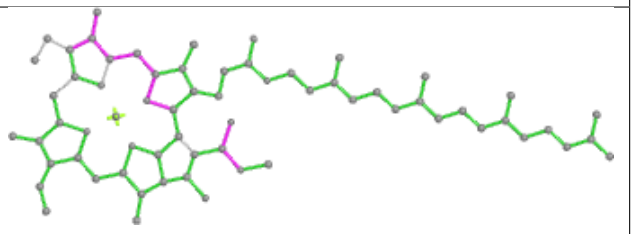
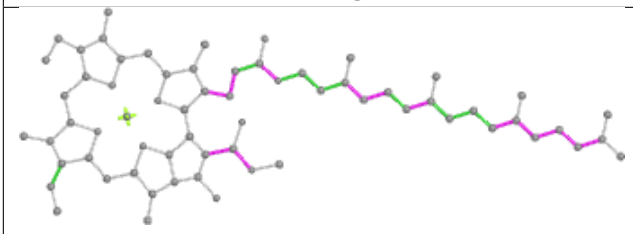
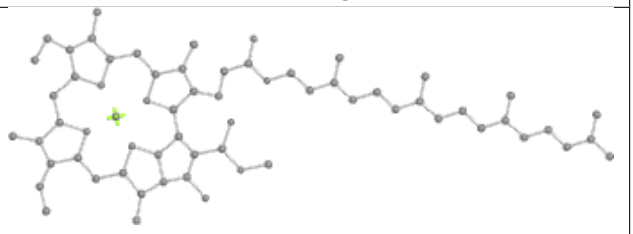


Bond angles

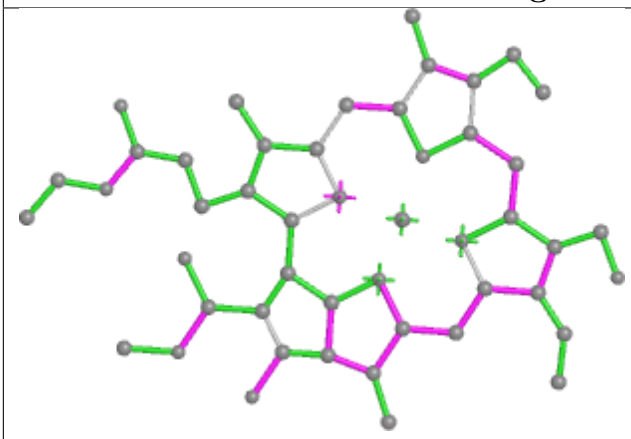


Torsions

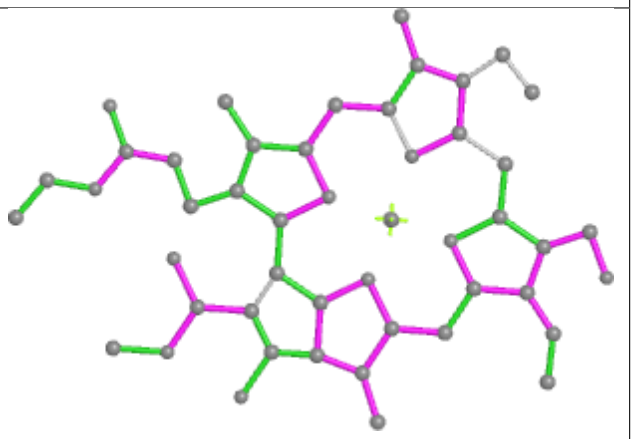


Rings

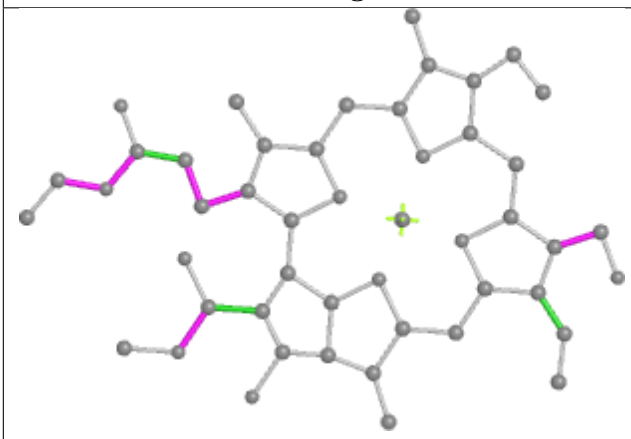
Ligand CHL s 301



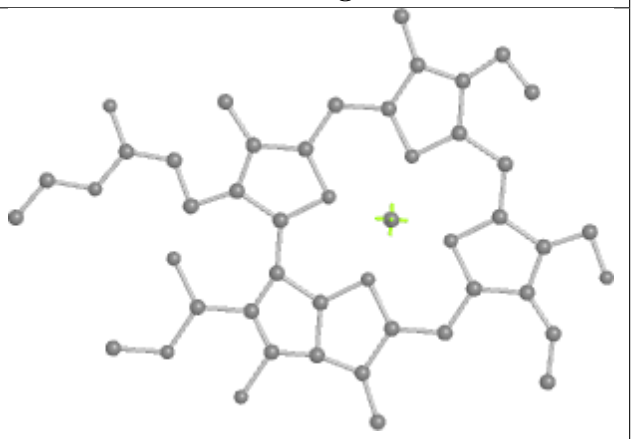
Bond lengths



Bond angles

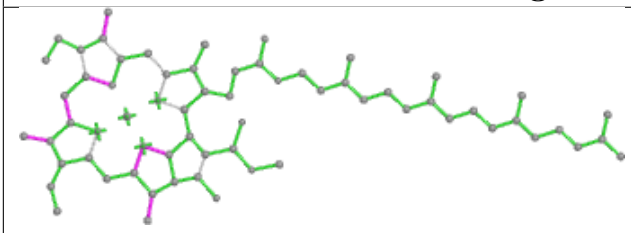


Torsions



Rings

Ligand CLA c 504



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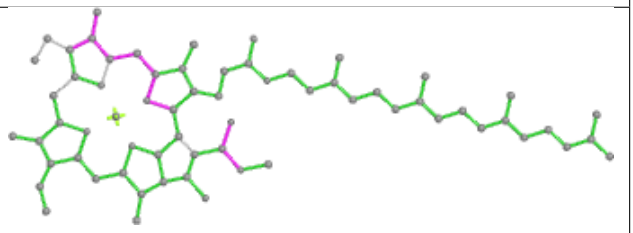
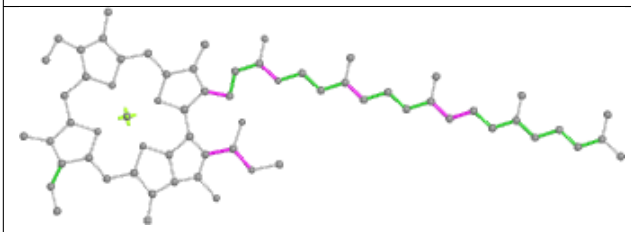
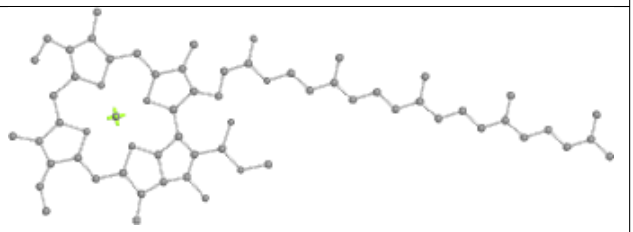


Bond angles

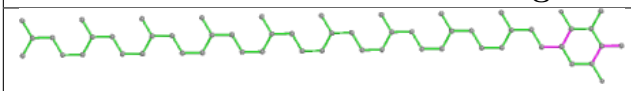


Torsions

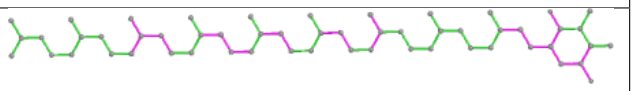


Rings

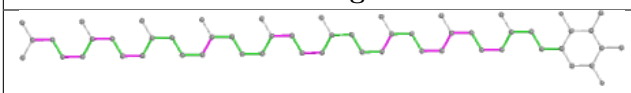
Ligand PL9 d 406



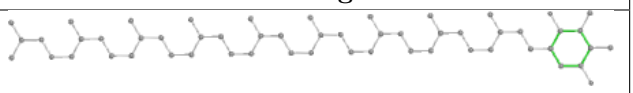
Bond lengths



Bond angles

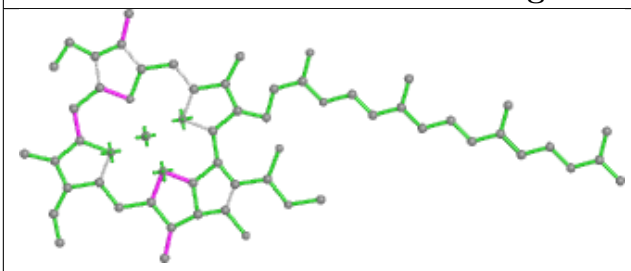


Torsions

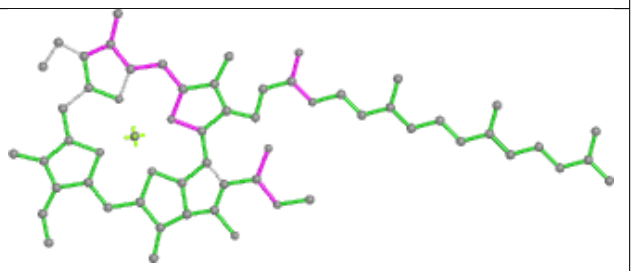


Rings

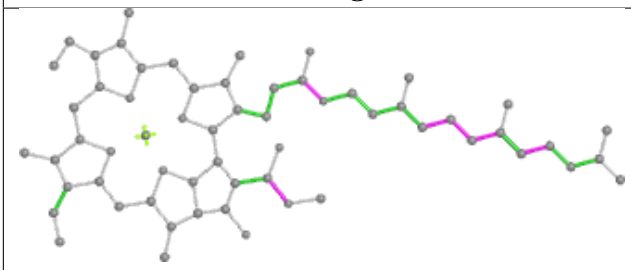
Ligand CLA n 610



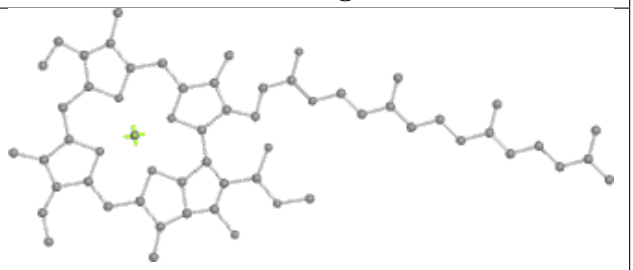
Bond lengths



Bond angles

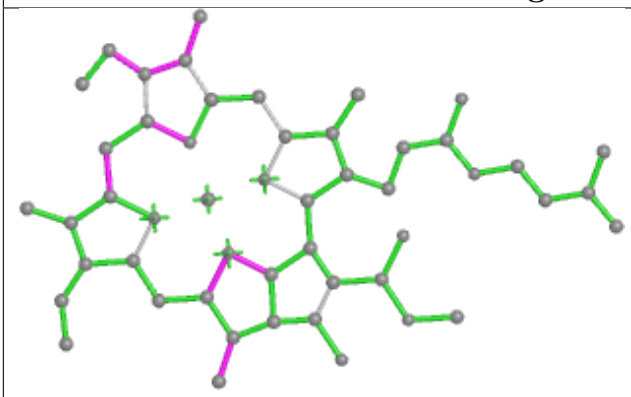


Torsions

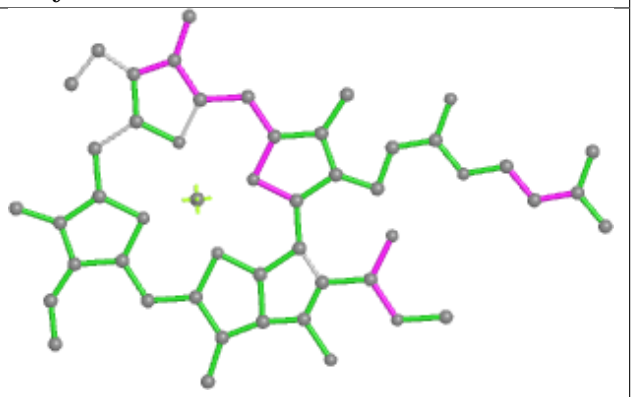


Rings

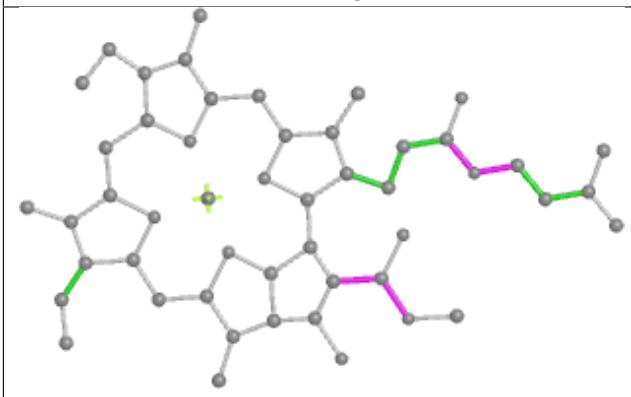
Ligand CLA y 604



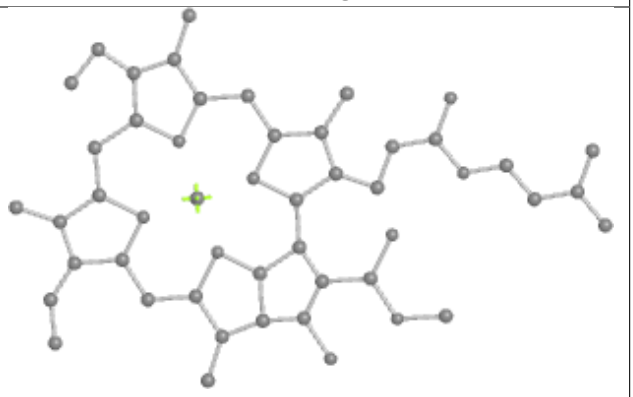
Bond lengths



Bond angles

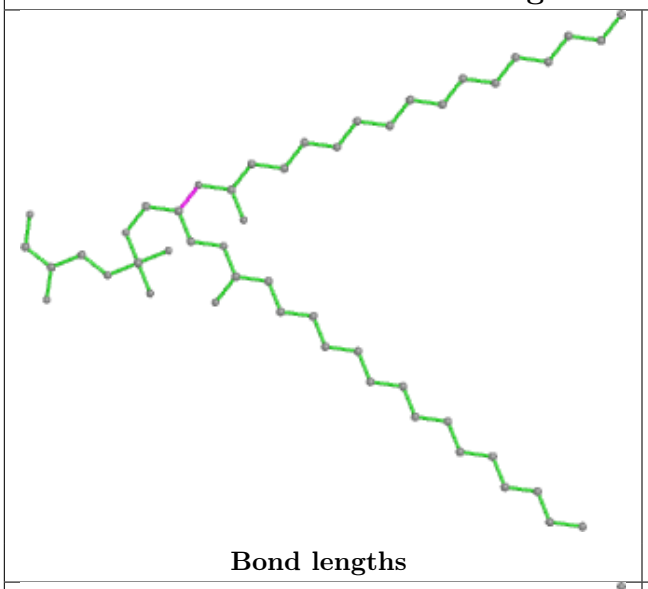


Torsions

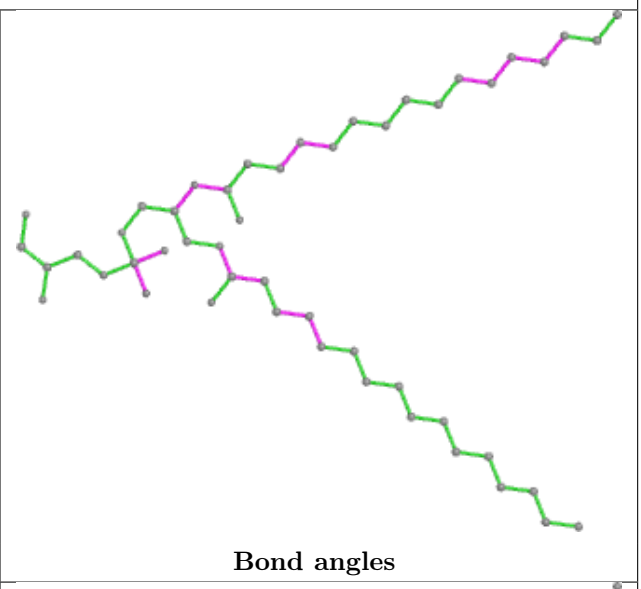


Rings

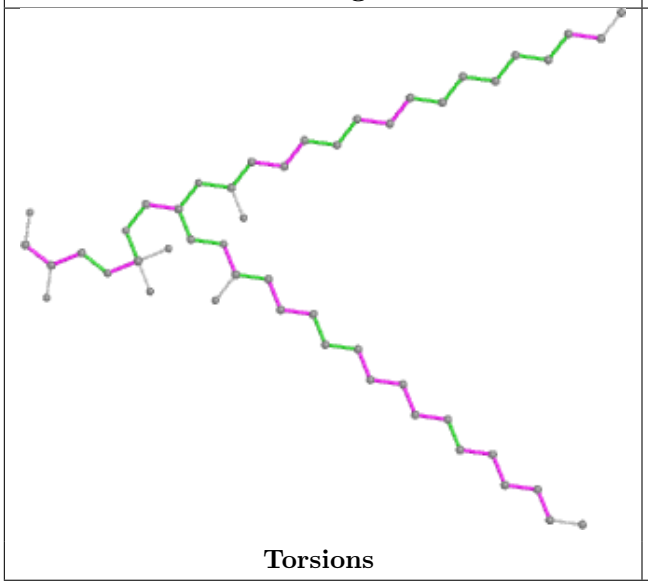
Ligand LHG n 617



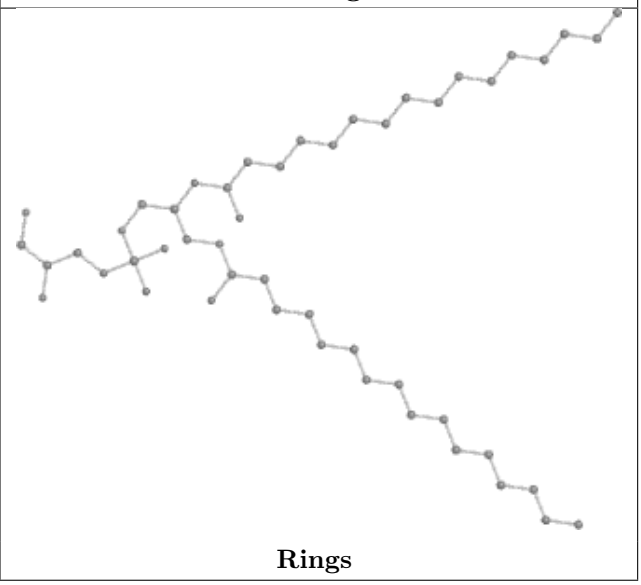
Bond lengths



Bond angles

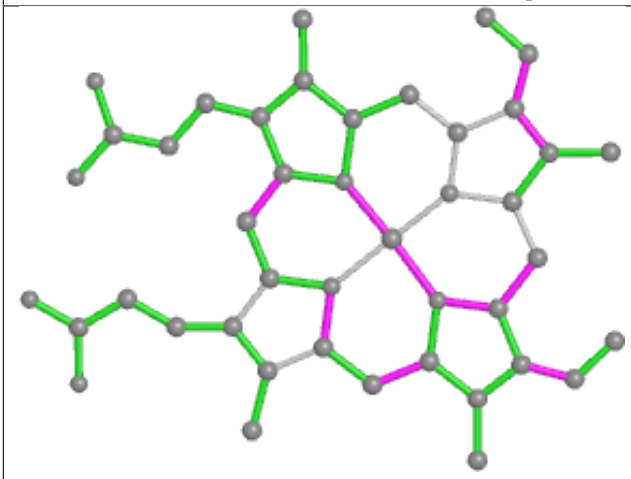


Torsions

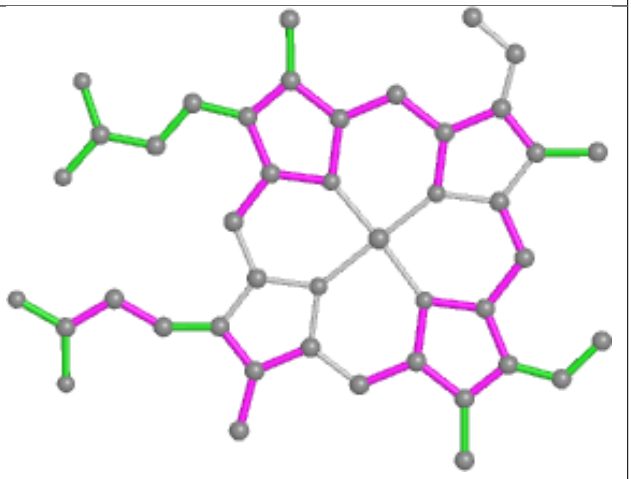


Rings

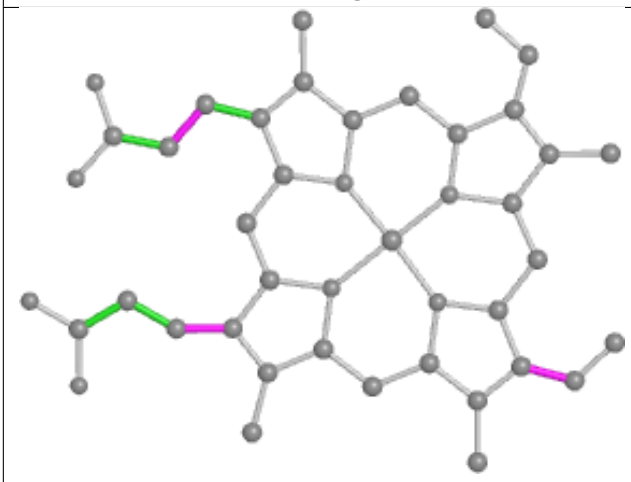
Ligand HEM F 101



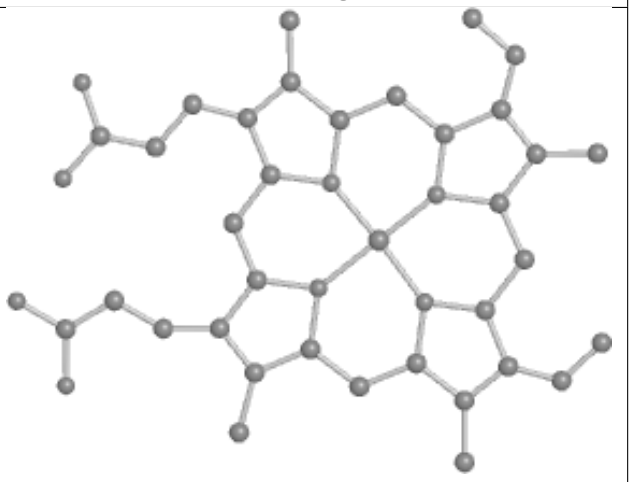
Bond lengths



Bond angles

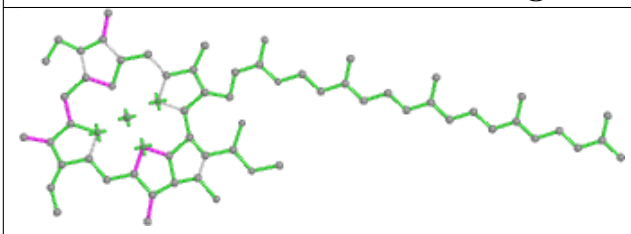


Torsions

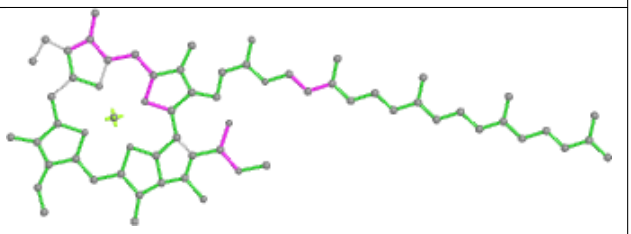


Rings

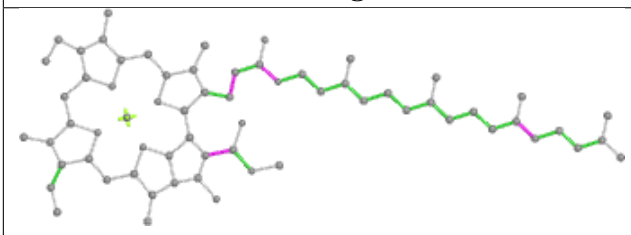
Ligand CLA b 606



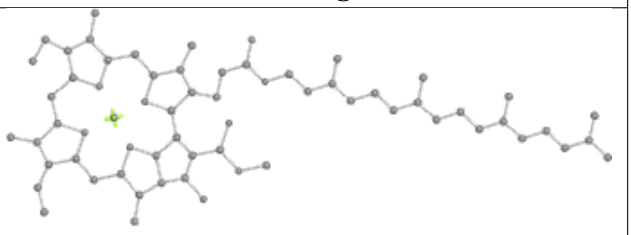
Bond lengths



Bond angles

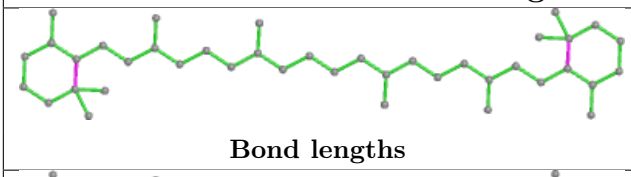


Torsions

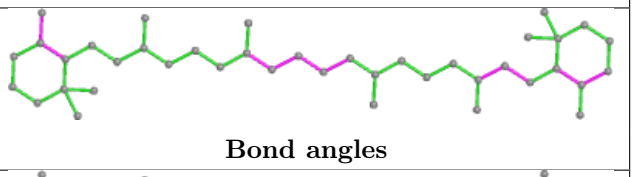


Rings

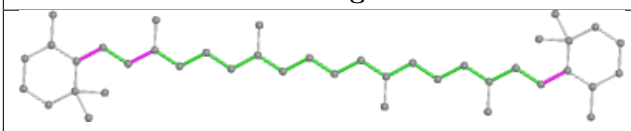
Ligand BCR c 515



Bond lengths



Bond angles



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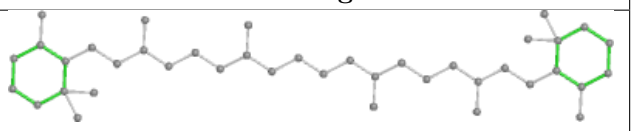
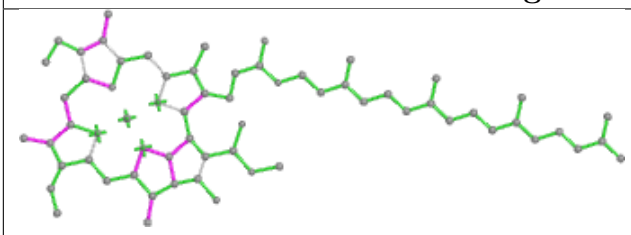
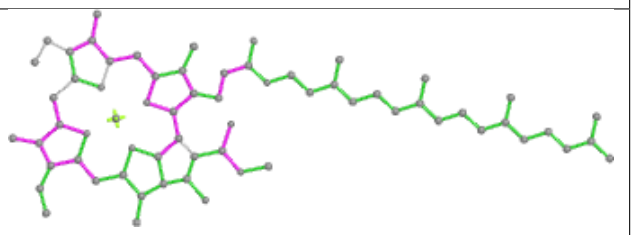


Rings

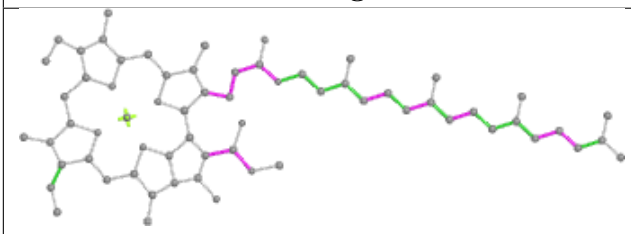
Ligand CLA Y 611



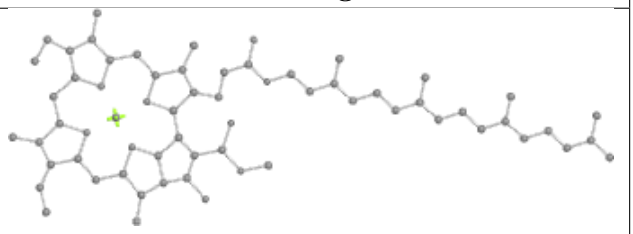
Bond lengths



Bond angles

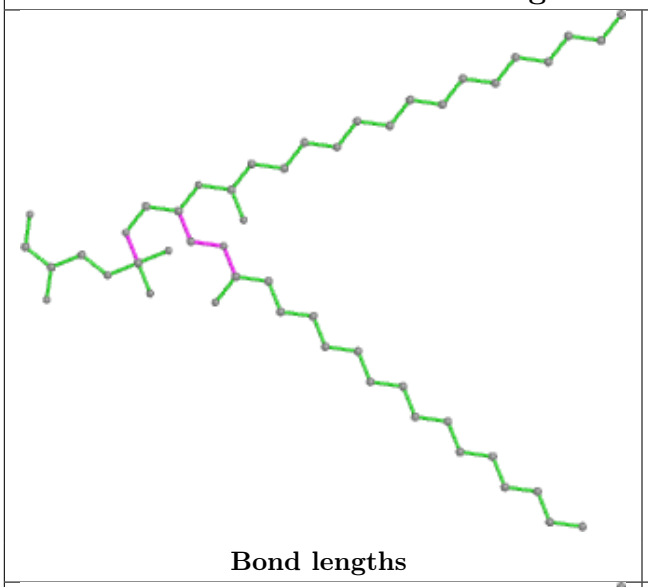


Torsions

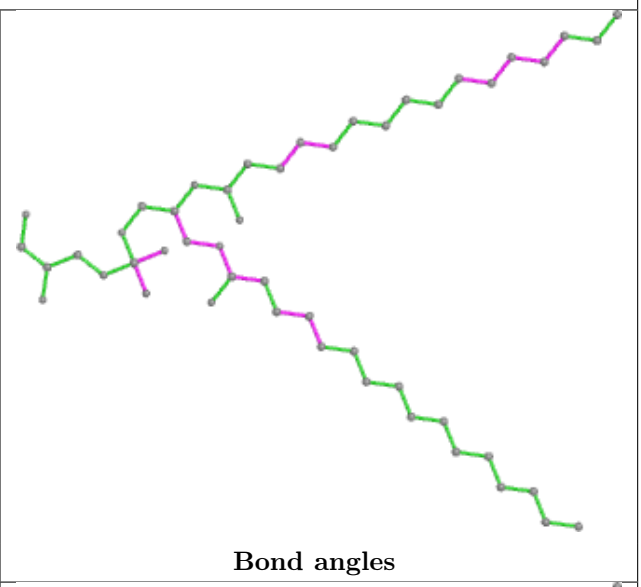


Rings

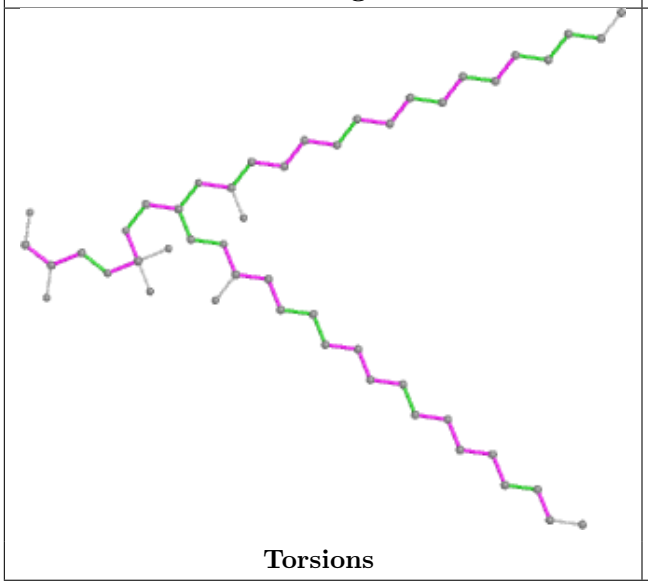
Ligand LHG c 520



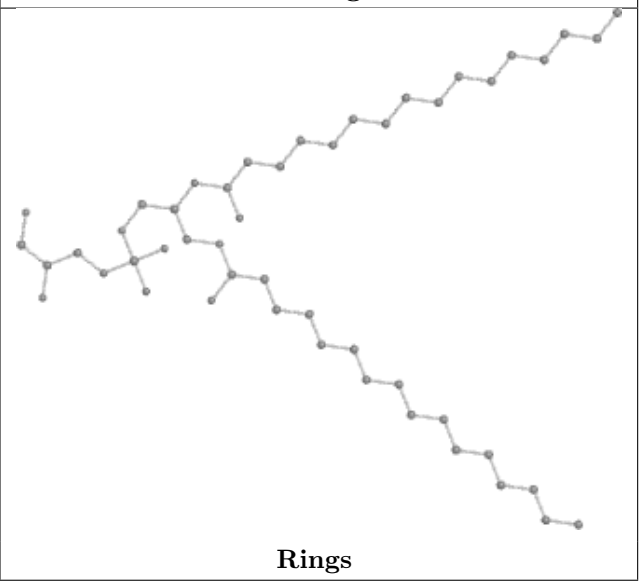
Bond lengths



Bond angles

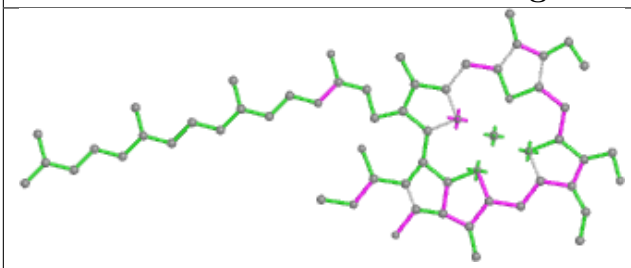


Torsions

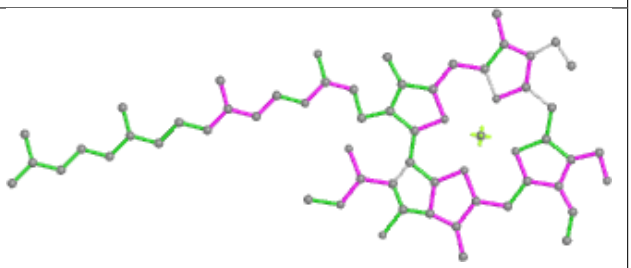


Rings

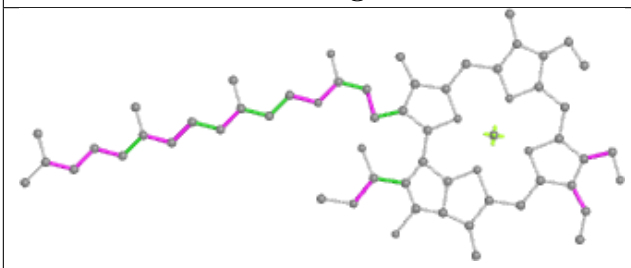
Ligand CHL r 308



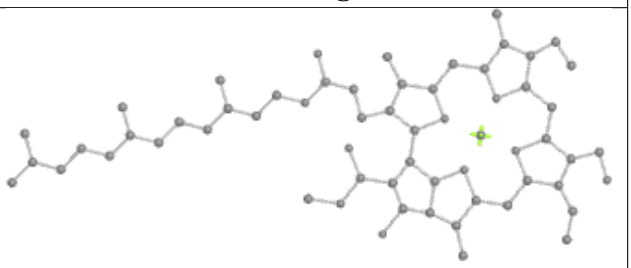
Bond lengths



Bond angles

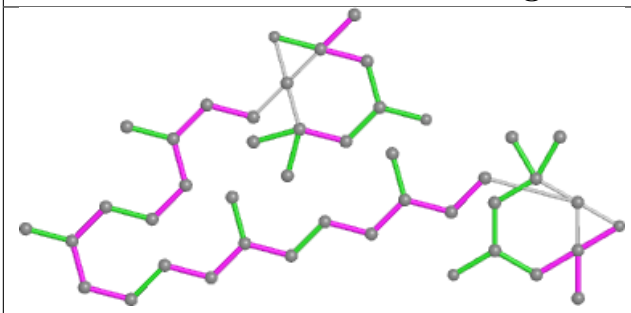


Torsions

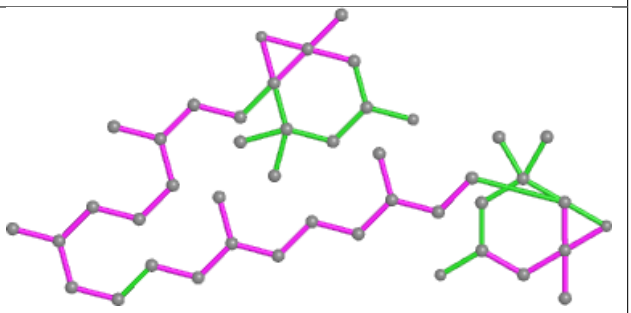


Rings

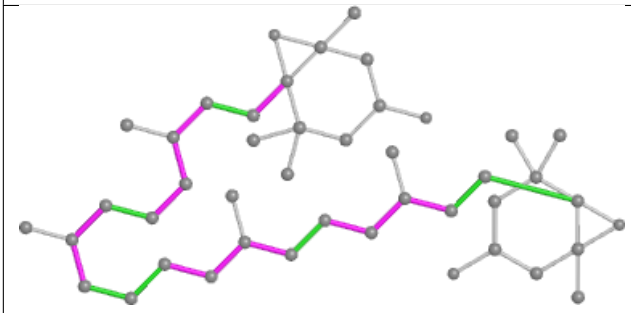
Ligand XAT Y 615



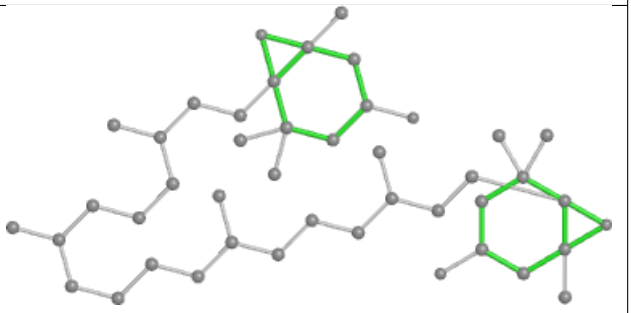
Bond lengths



Bond angles

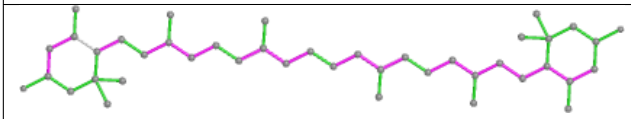


Torsions



Rings

Ligand LUT Y 613



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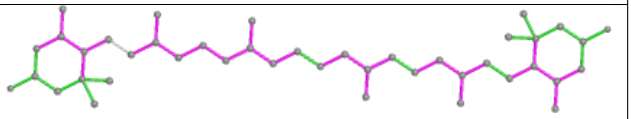
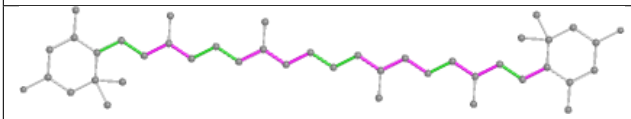


Bond angles



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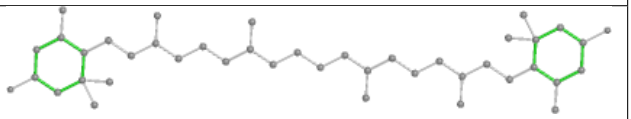
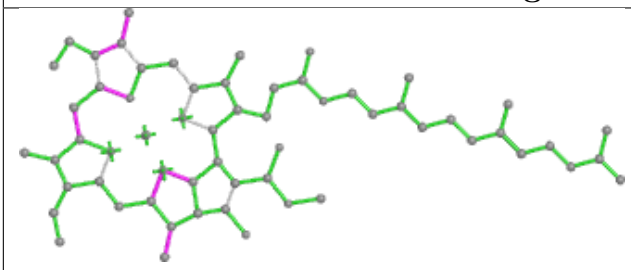


Rings

Ligand CLA Y 610



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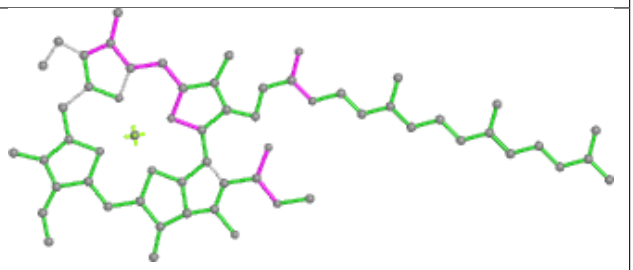
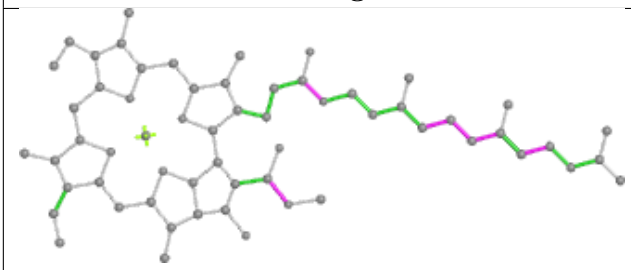
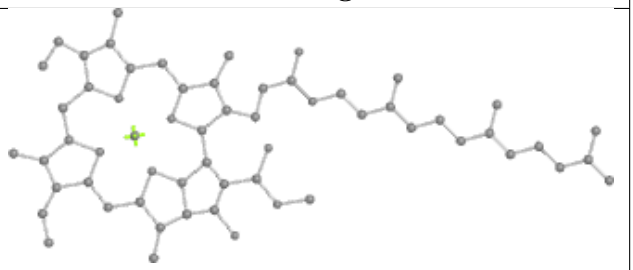


Bond angles

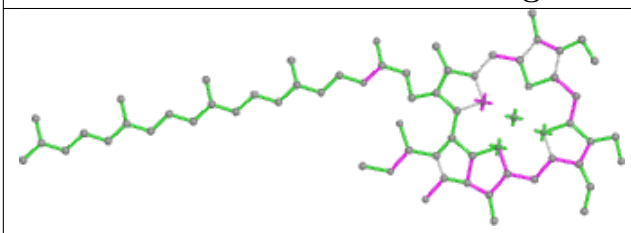


Torsions



Rings

Ligand CHL G 608



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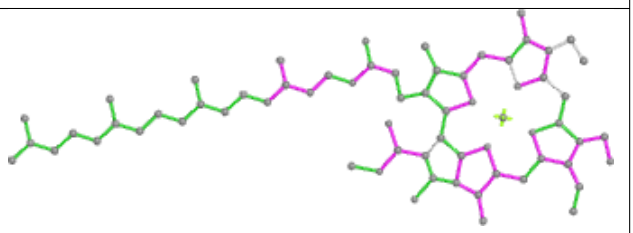
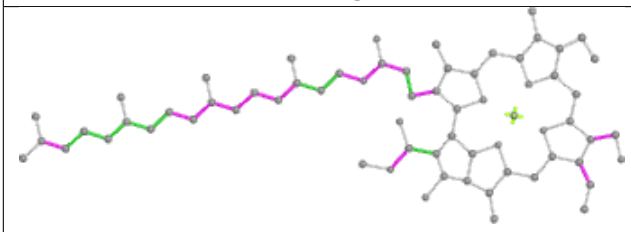
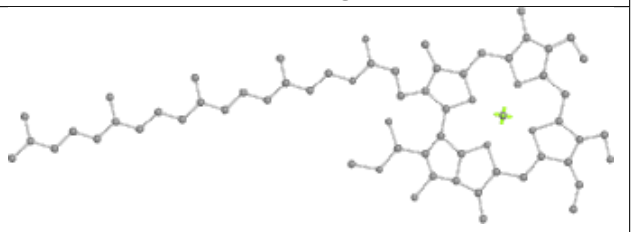


Bond angles

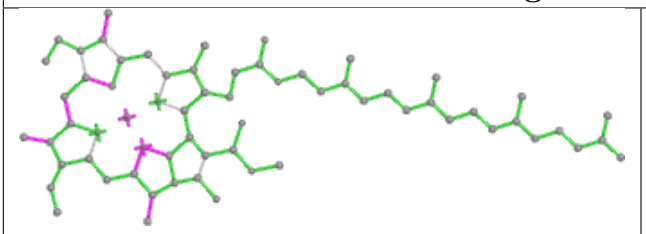


Torsions

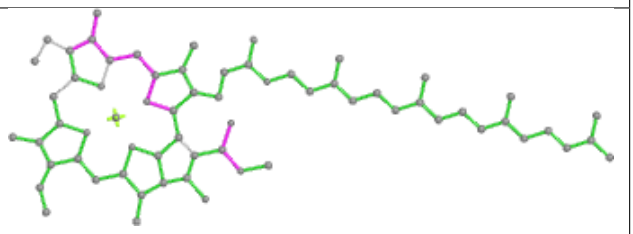


Rings

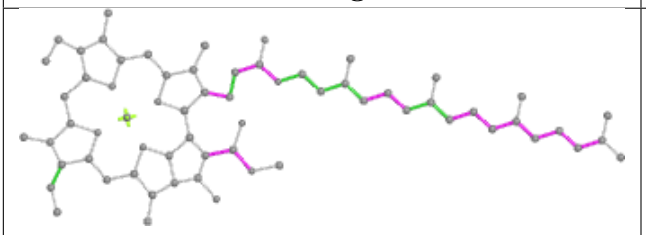
Ligand CLA C 514



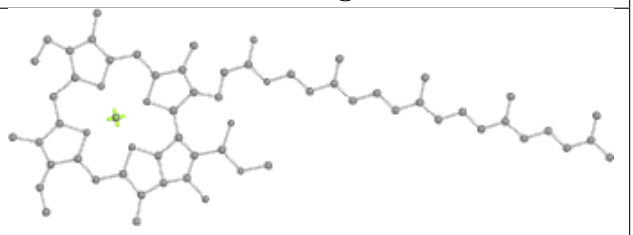
Bond lengths



Bond angles

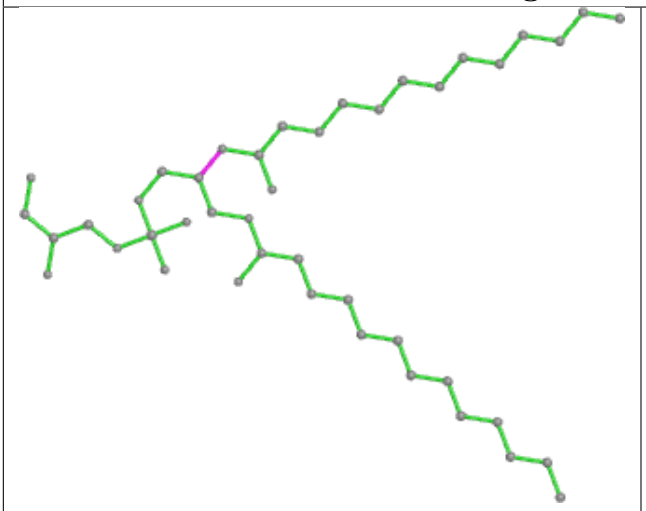


Torsions

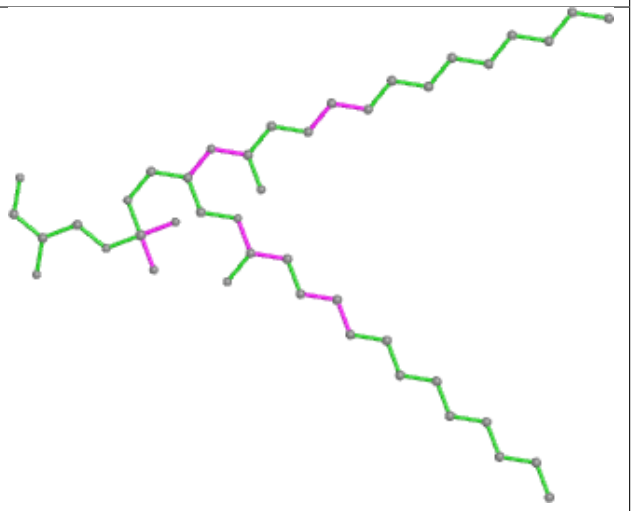


Rings

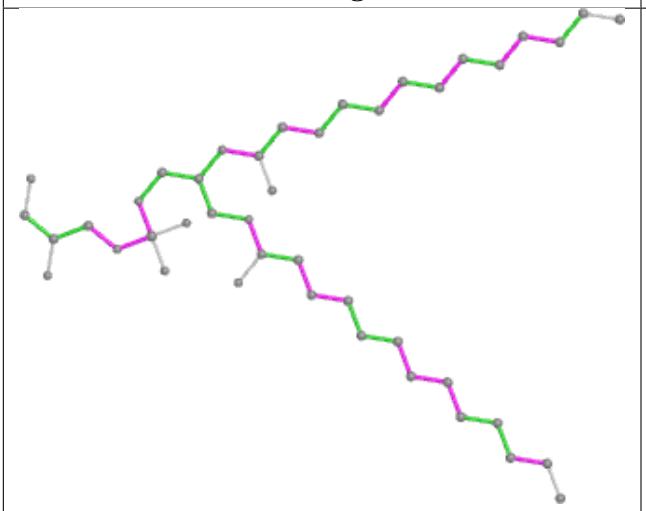
Ligand LHG D 410



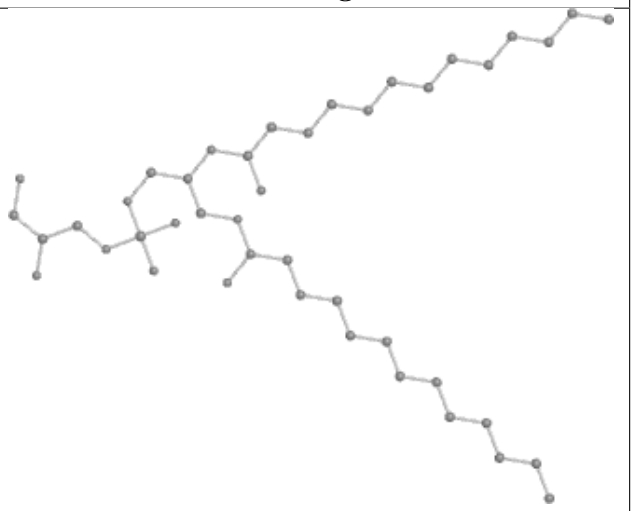
Bond lengths



Bond angles

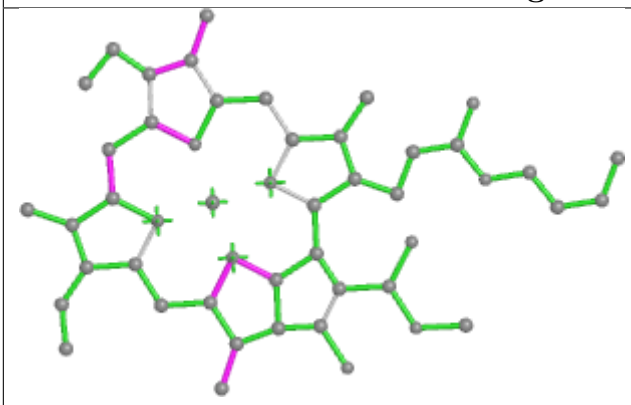


Torsions

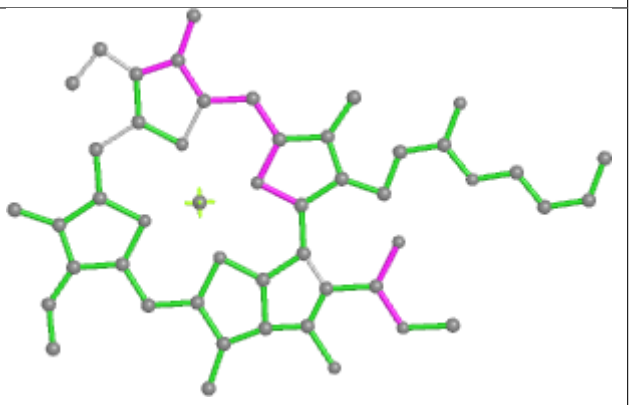


Rings

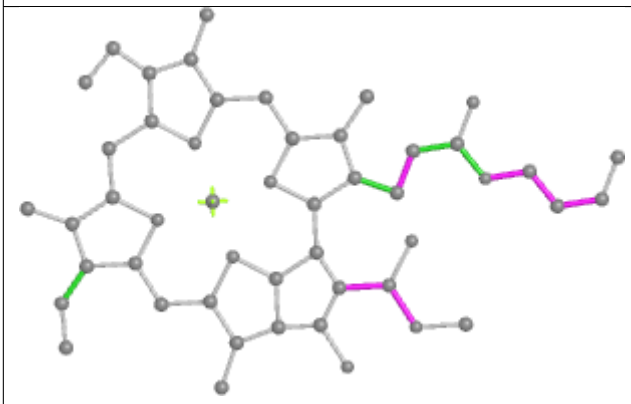
Ligand CLA S 312



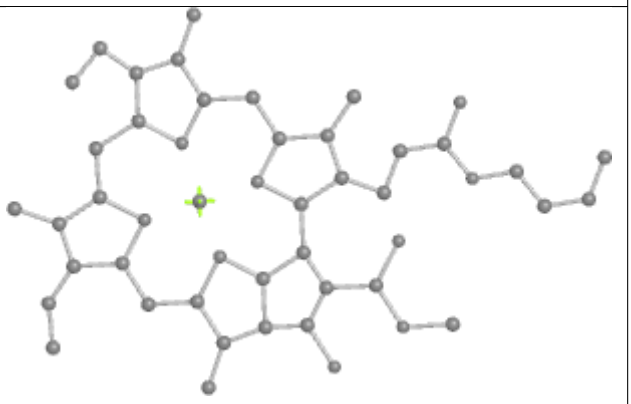
Bond lengths



Bond angles

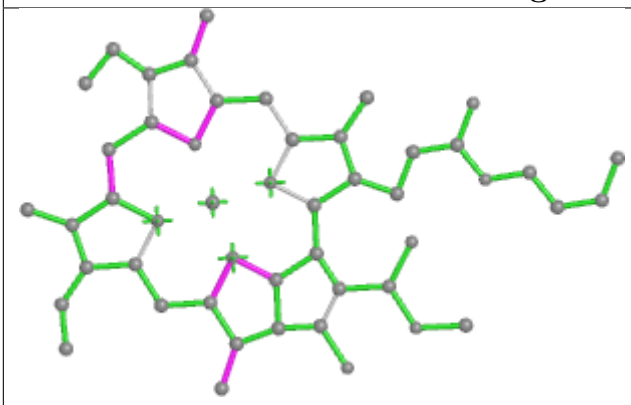


Torsions

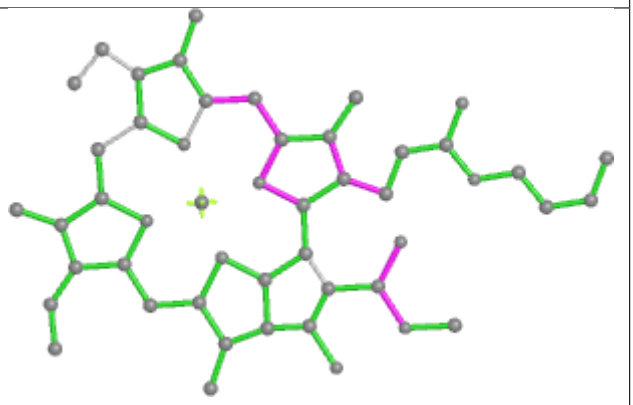


Rings

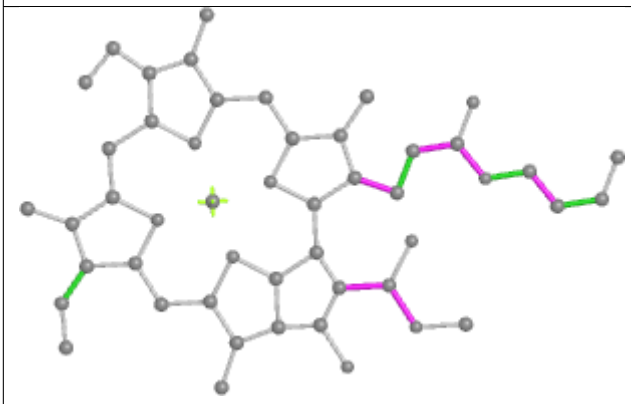
Ligand CLA r 311



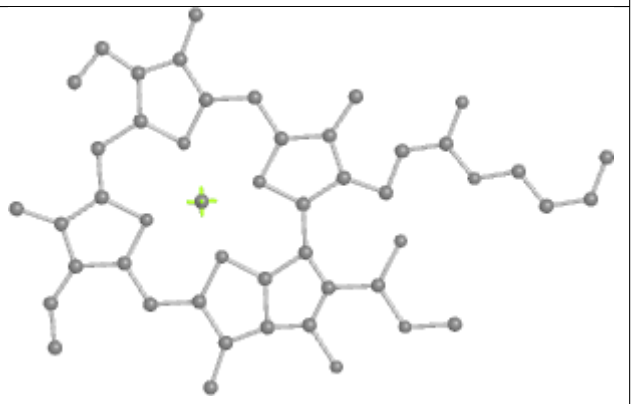
Bond lengths



Bond angles

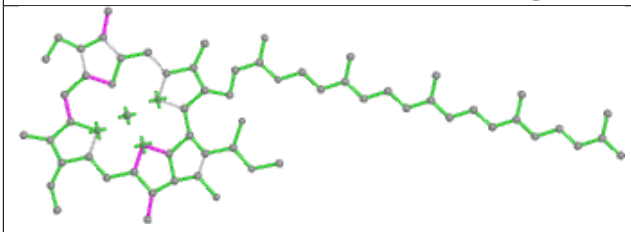


Torsions

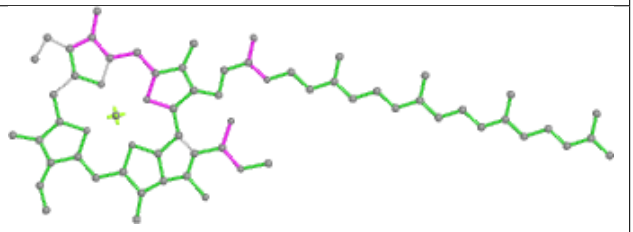


Rings

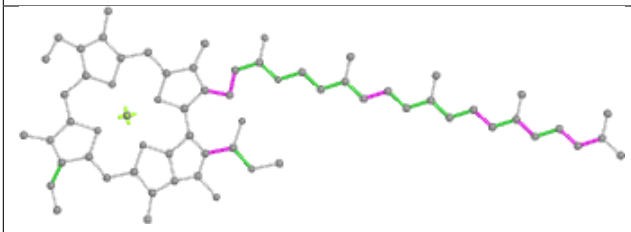
Ligand CLA b 605



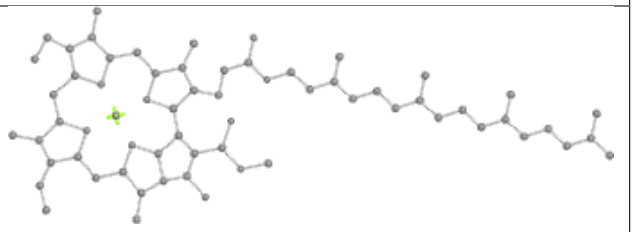
Bond lengths



Bond angles

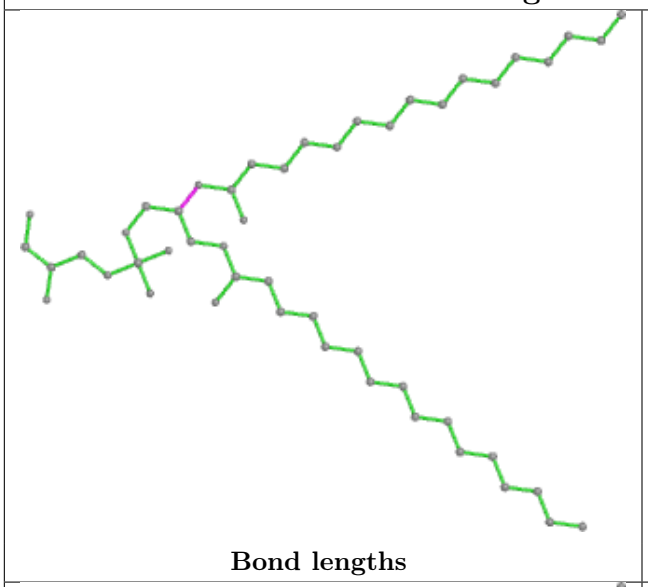


Torsions

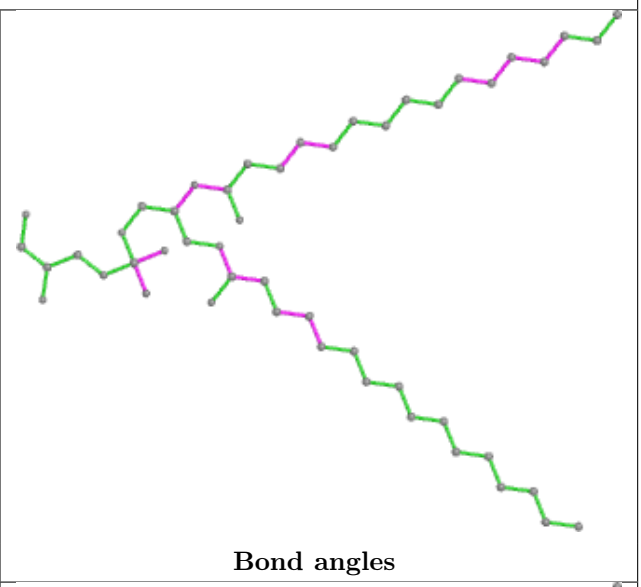


Rings

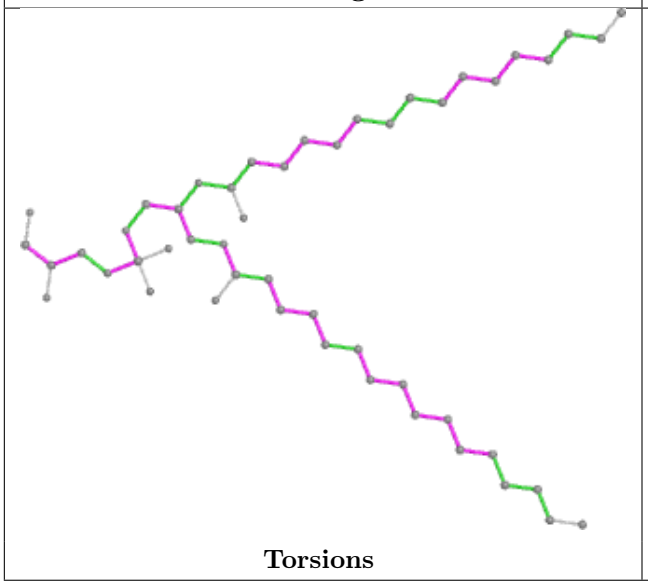
Ligand LHG Y 617



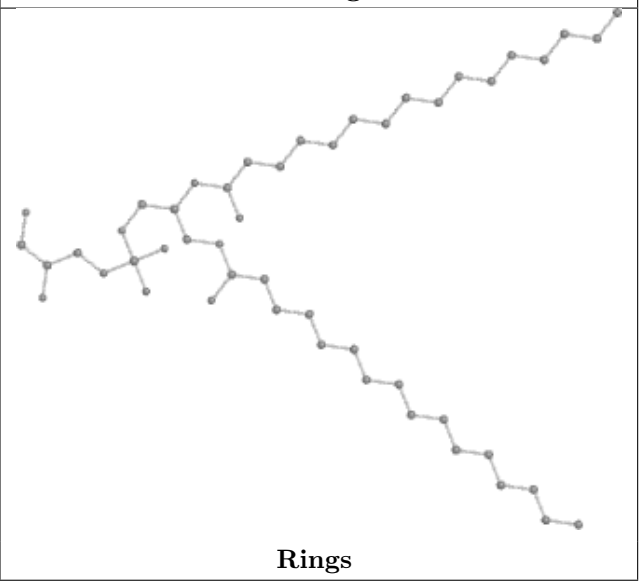
Bond lengths



Bond angles

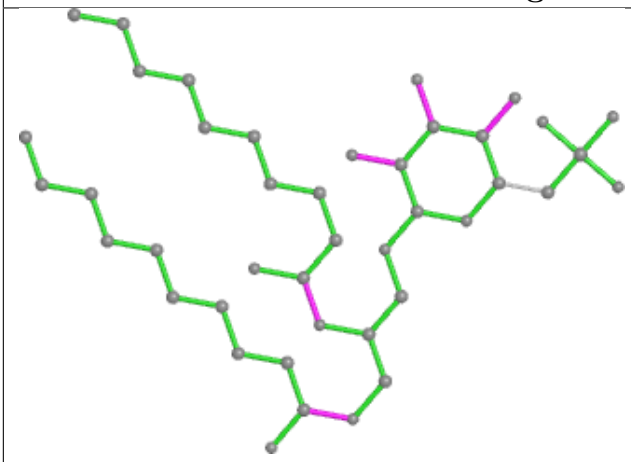


Torsions

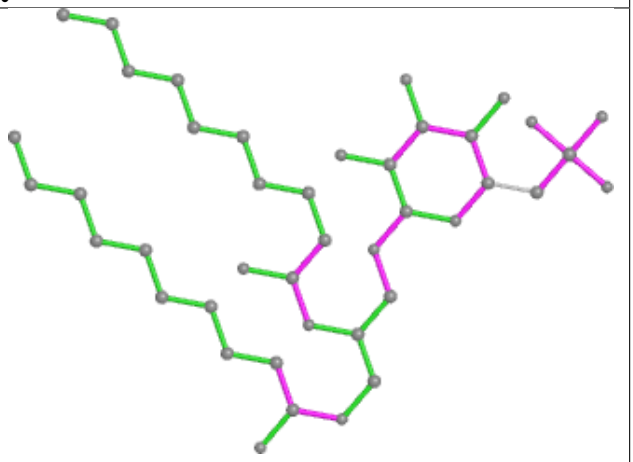


Rings

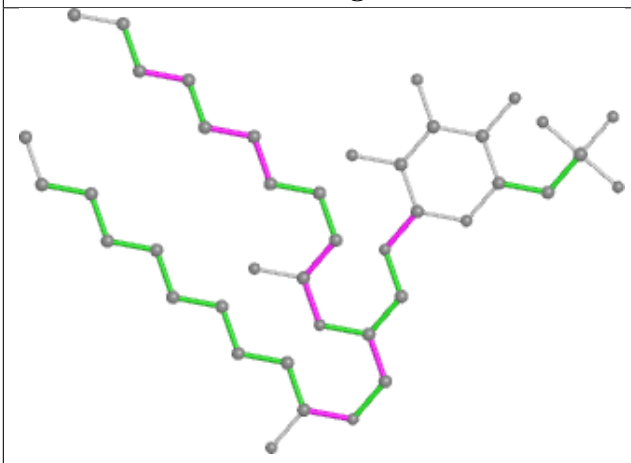
Ligand SQD L 102



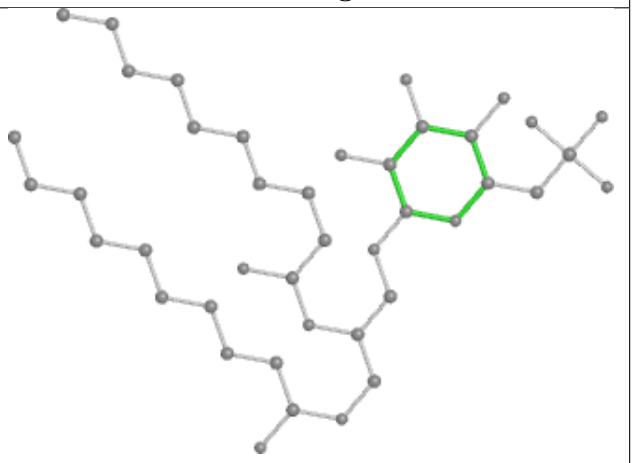
Bond lengths



Bond angles

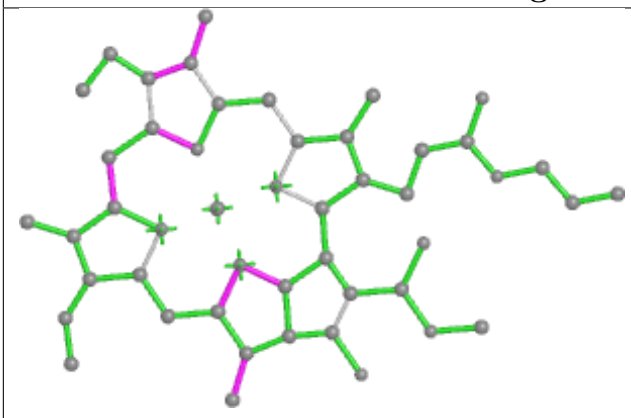


Torsions

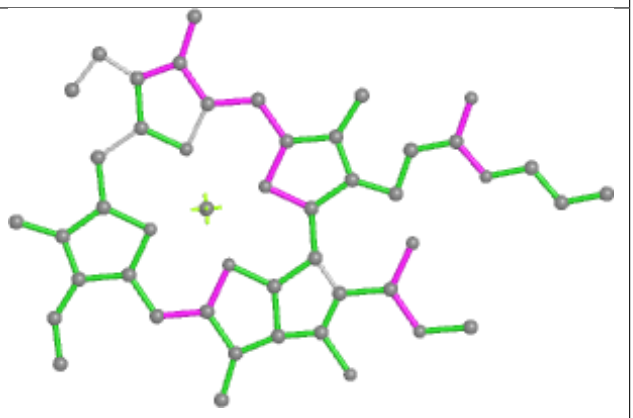


Rings

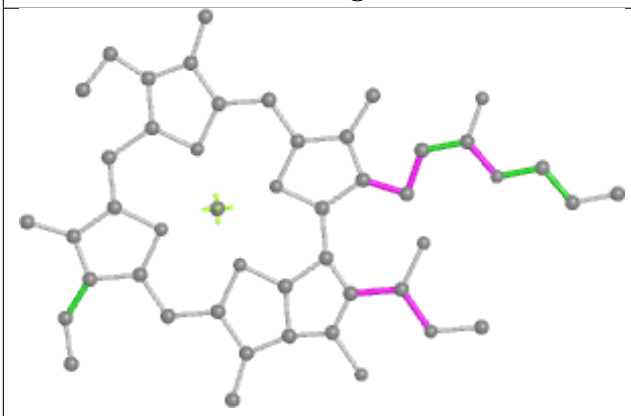
Ligand CLA r 305



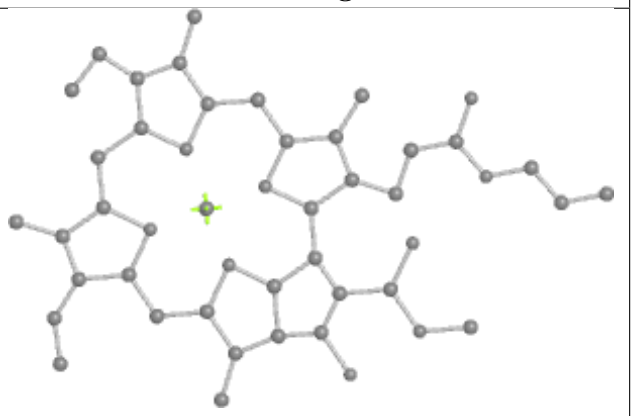
Bond lengths



Bond angles

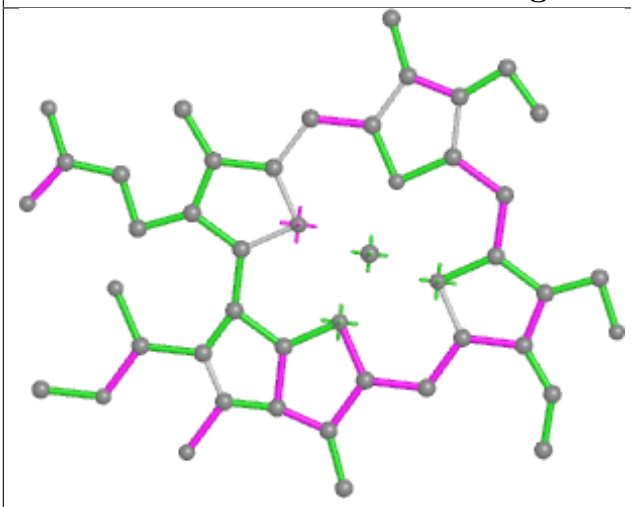


Torsions

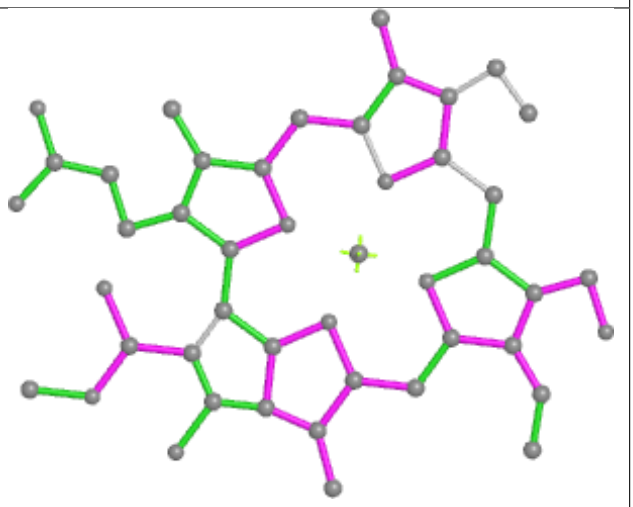


Rings

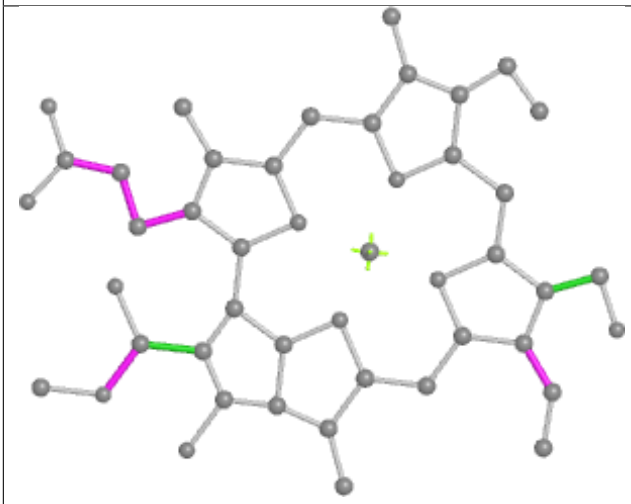
Ligand CHL s 302



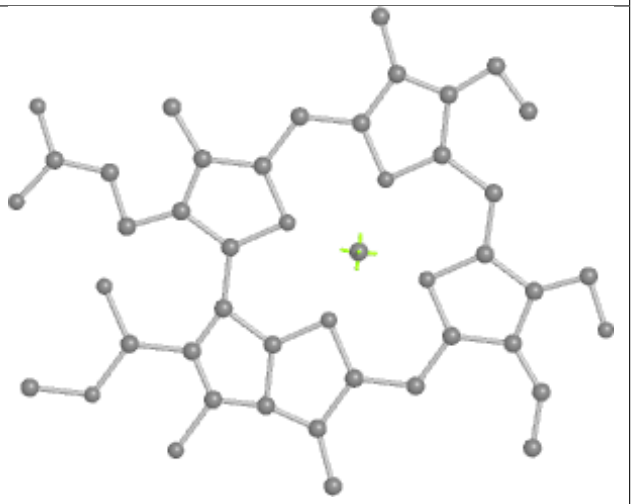
Bond lengths



Bond angles

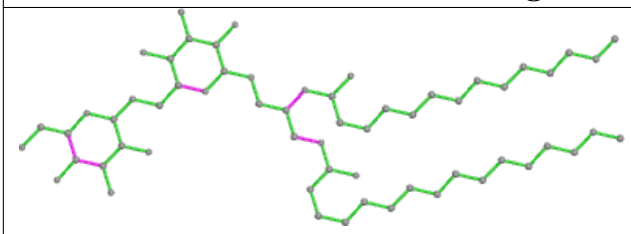


Torsions

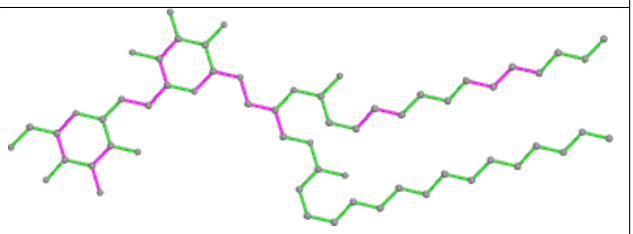


Rings

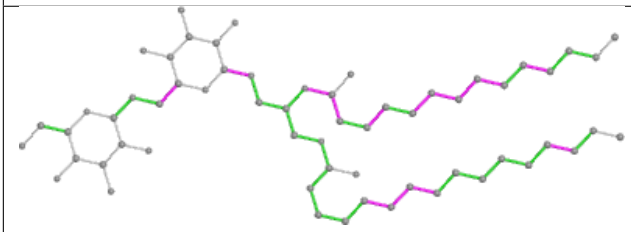
Ligand DGD c 519



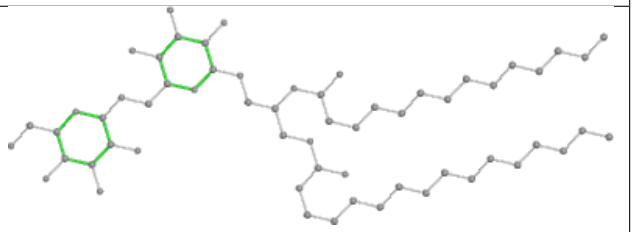
Bond lengths



Bond angles

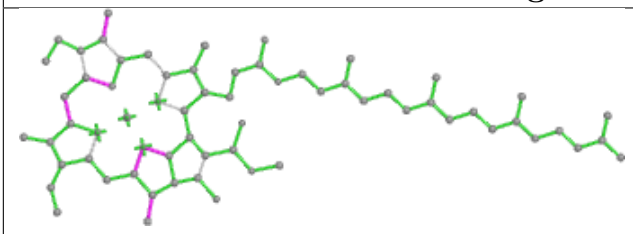


Torsions

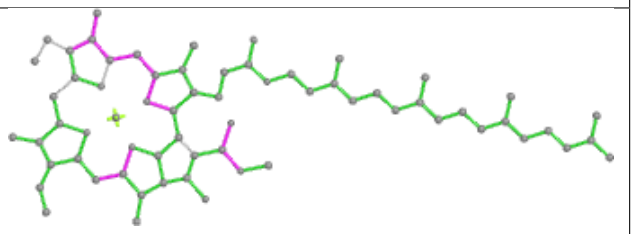


Rings

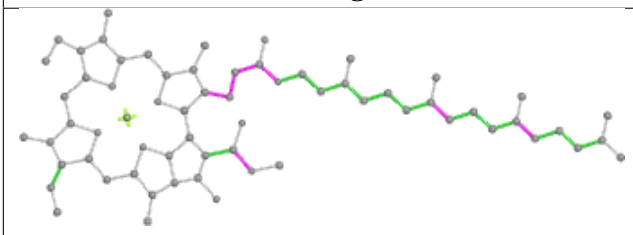
Ligand CLA n 602



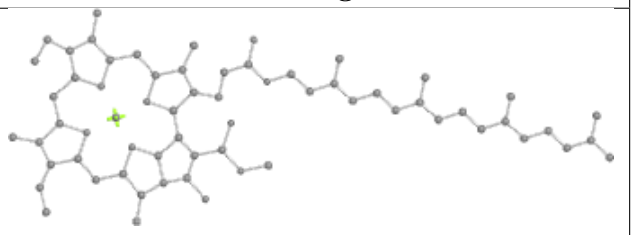
Bond lengths



Bond angles

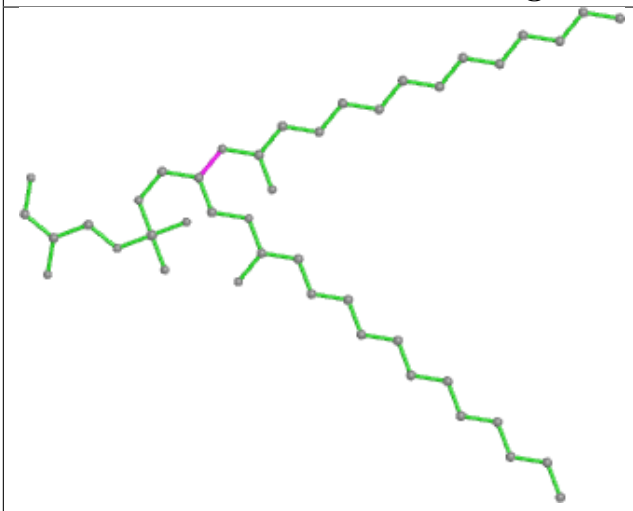


Torsions

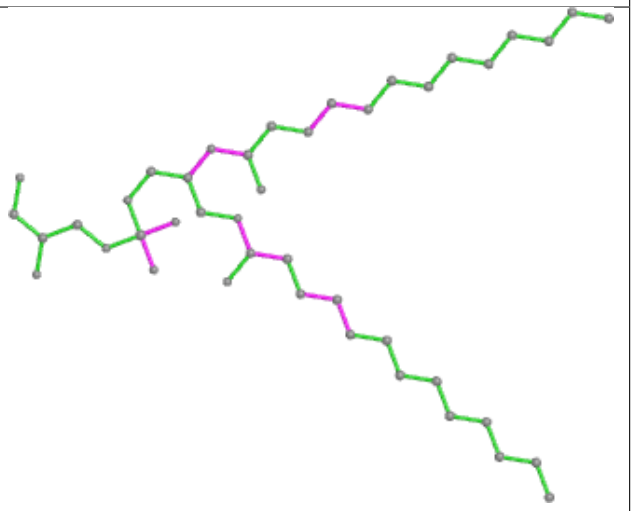


Rings

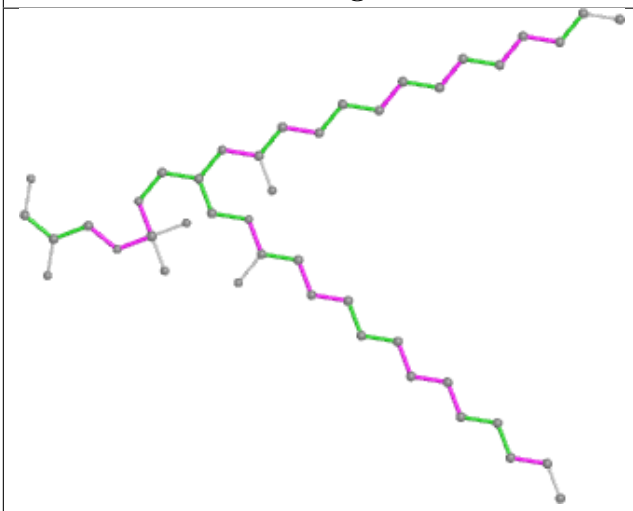
Ligand LHG d 409



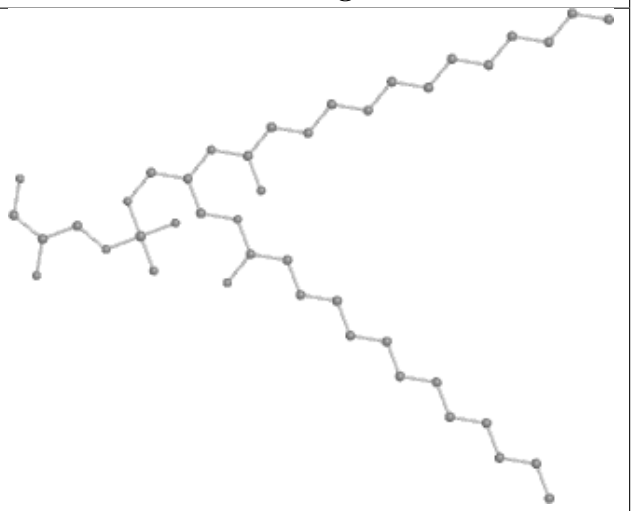
Bond lengths



Bond angles

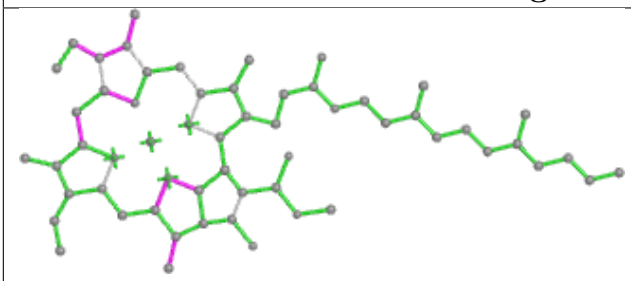


Torsions

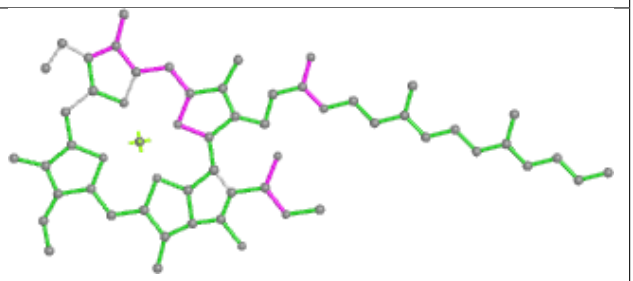


Rings

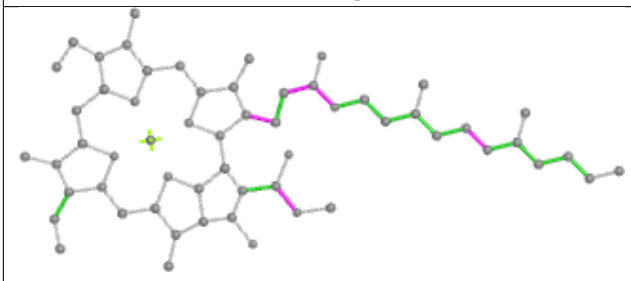
Ligand CLA r 309



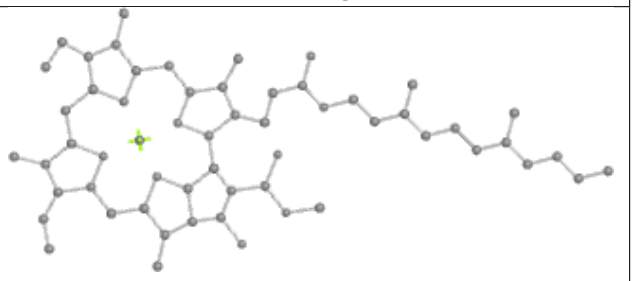
Bond lengths



Bond angles

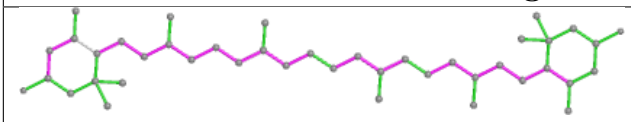


Torsions

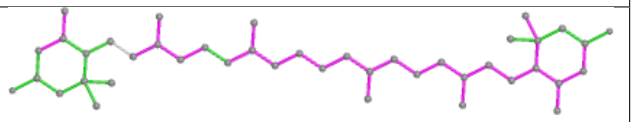


Rings

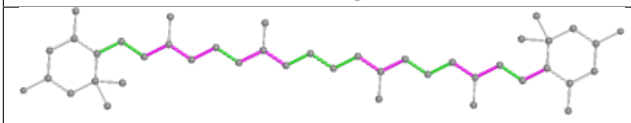
Ligand LUT N 615



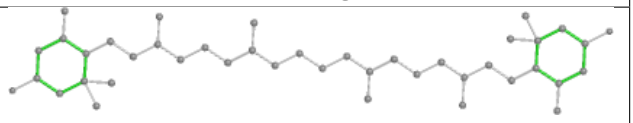
Bond lengths



Bond angles

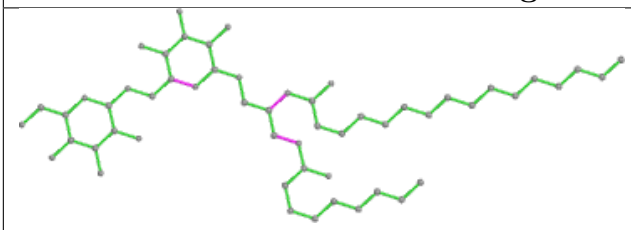


Torsions

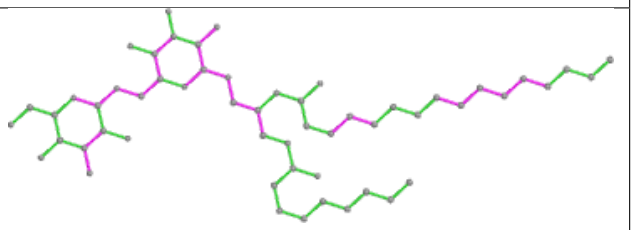


Rings

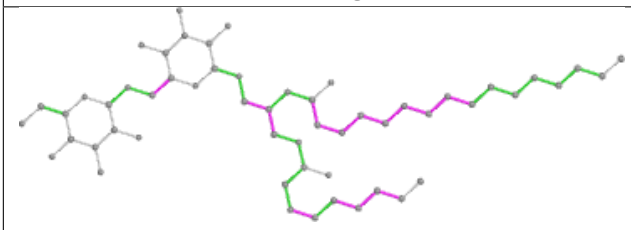
Ligand DGD C 518



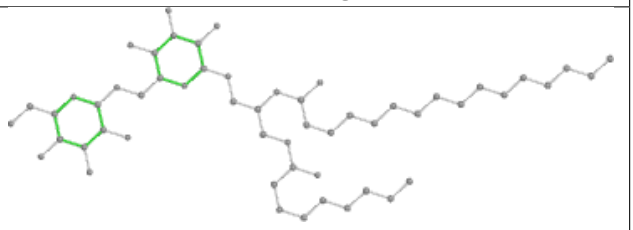
Bond lengths



Bond angles

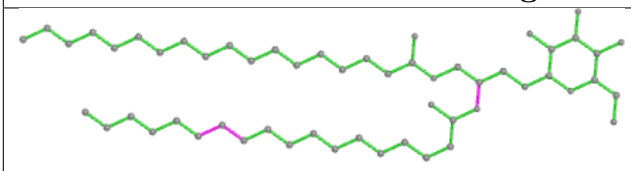


Torsions

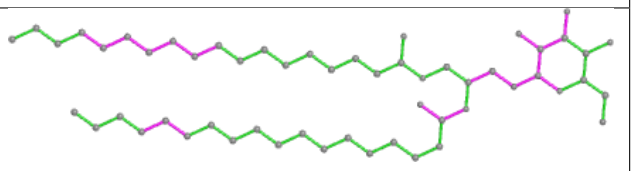


Rings

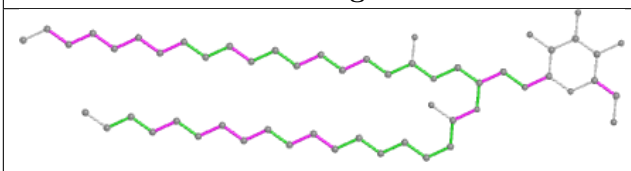
Ligand LMG B 623



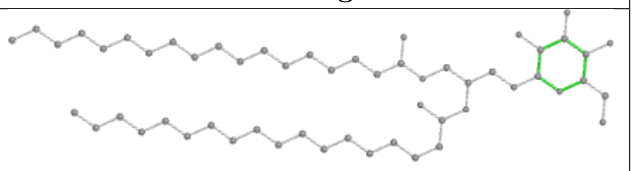
Bond lengths



Bond angles

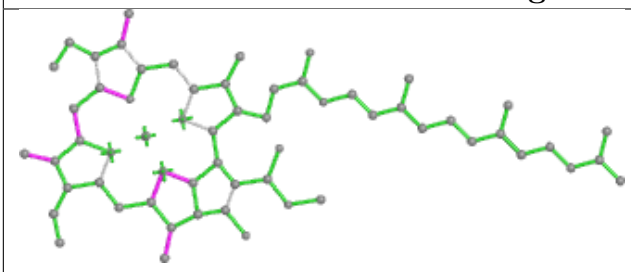


Torsions

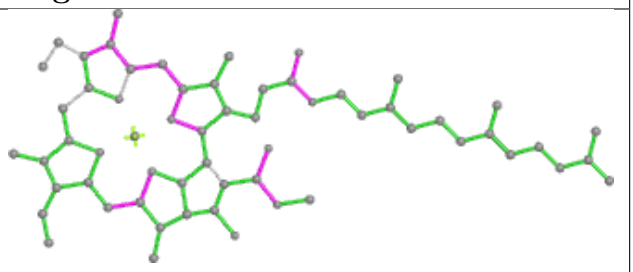


Rings

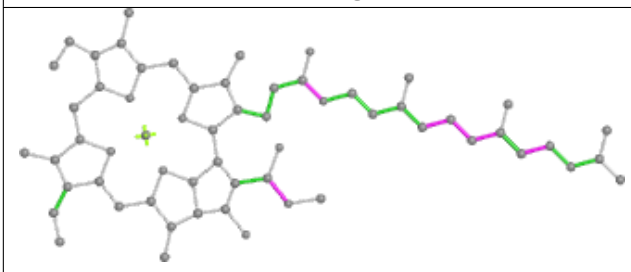
Ligand CLA g 611



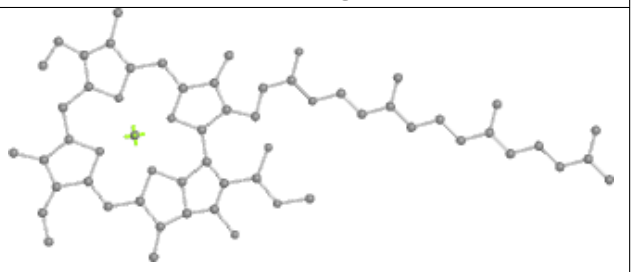
Bond lengths



Bond angles

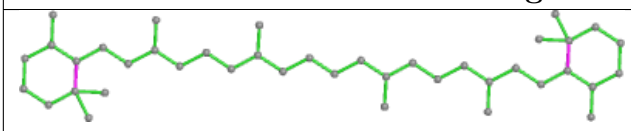


Torsions

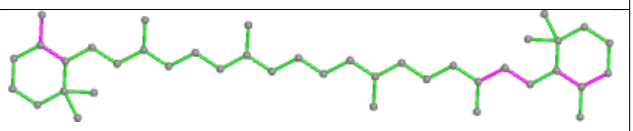


Rings

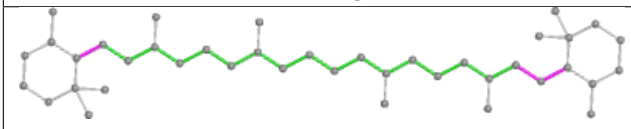
Ligand BCR b 618



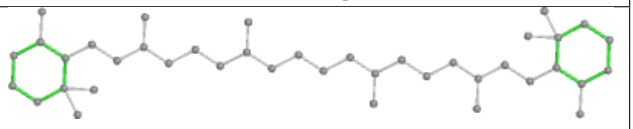
Bond lengths



Bond angles

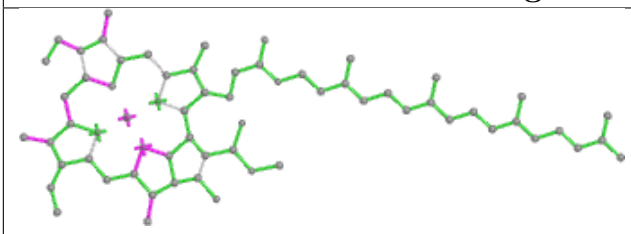


Torsions

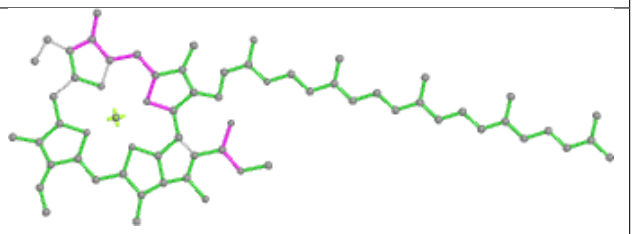


Rings

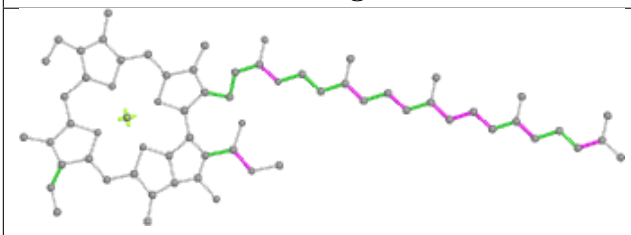
Ligand CLA B 607



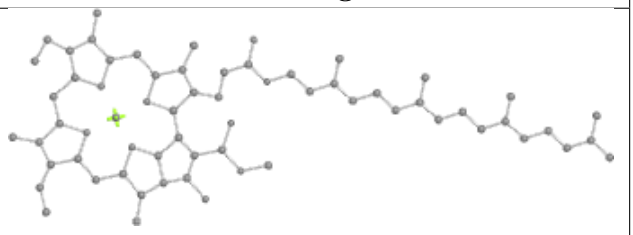
Bond lengths



Bond angles

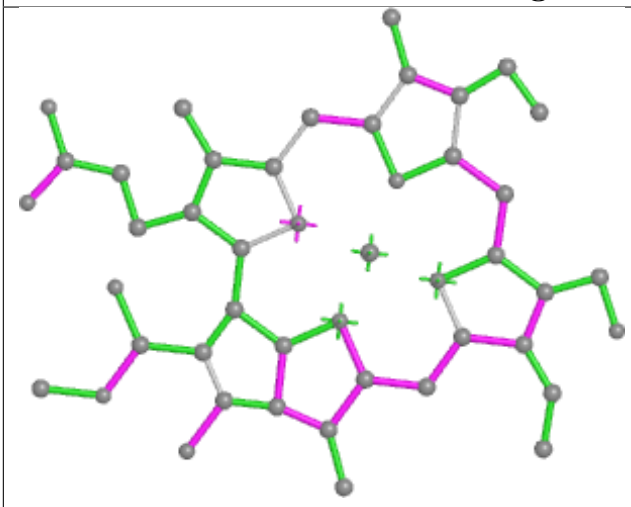


Torsions

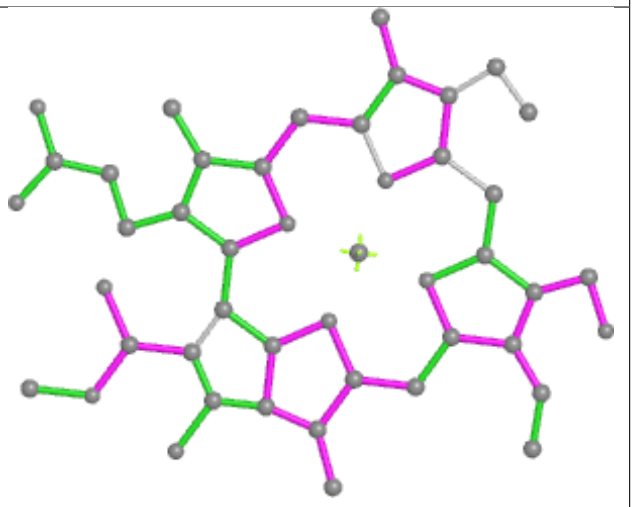


Rings

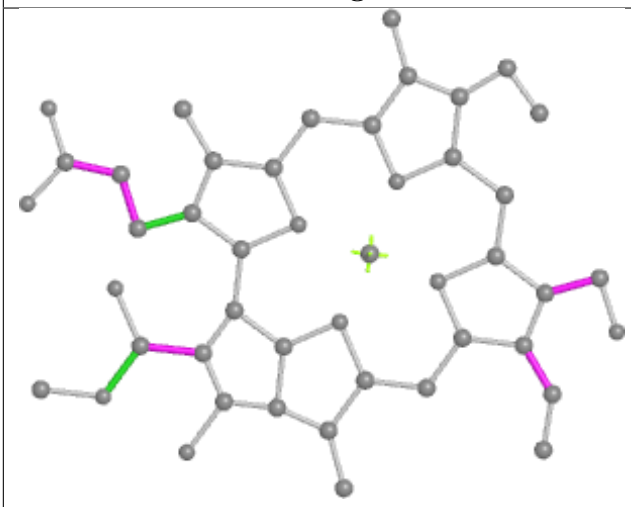
Ligand CHL s 306



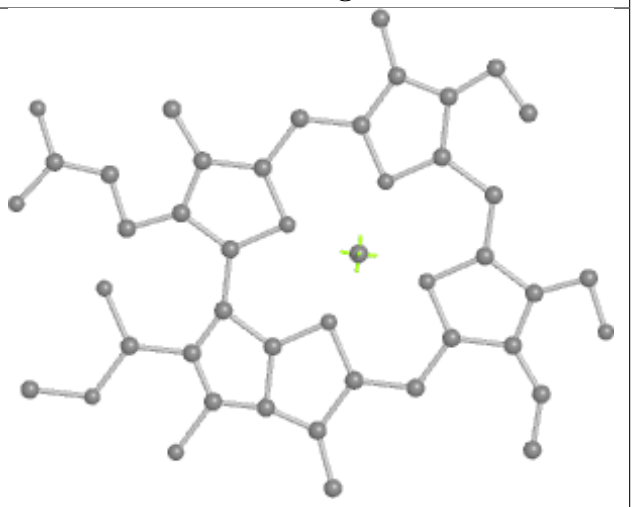
Bond lengths



Bond angles

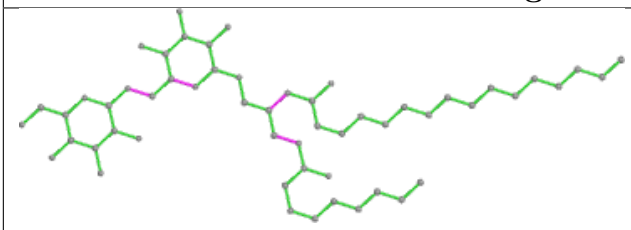


Torsions



Rings

Ligand DGD c 517



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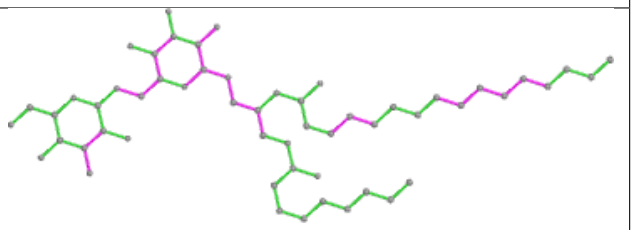
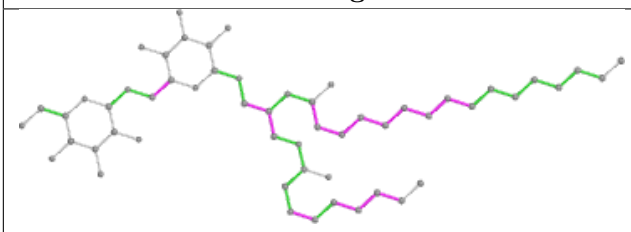
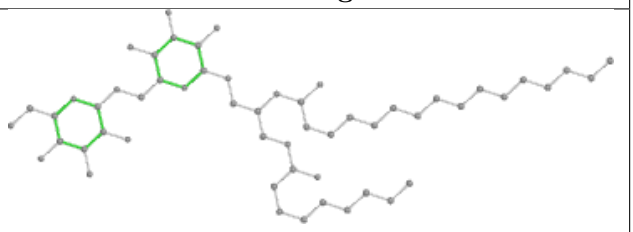


Bond angles

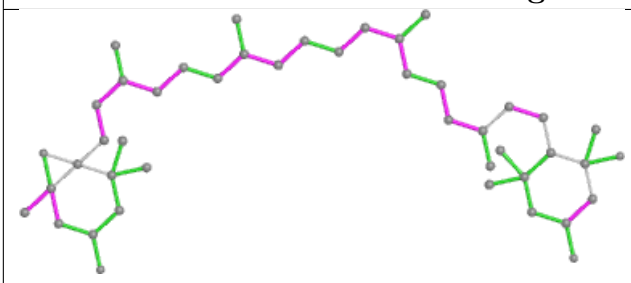


Torsions

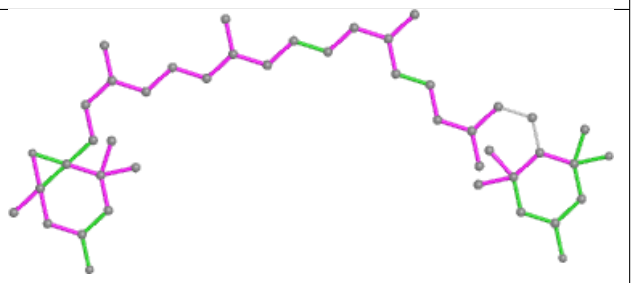


Rings

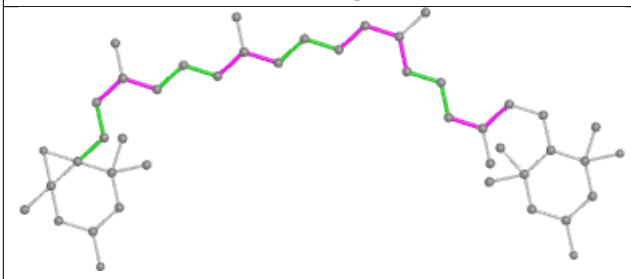
Ligand NEX r 315



Bond lengths



Bond angles



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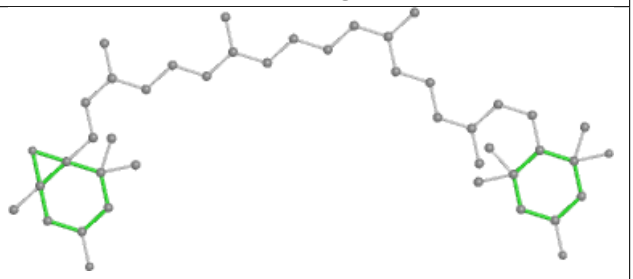
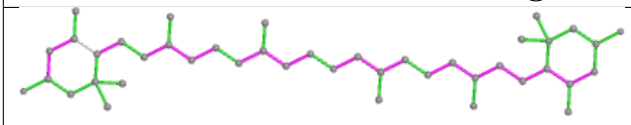
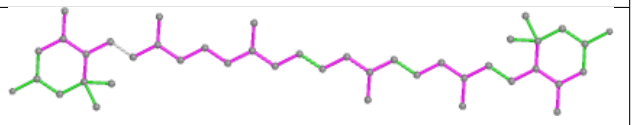


Rings

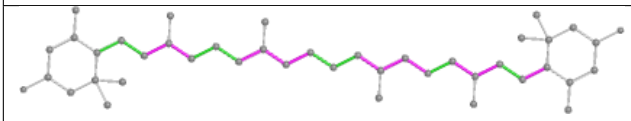
Ligand LUT n 614



Bond lengths



Bond angles



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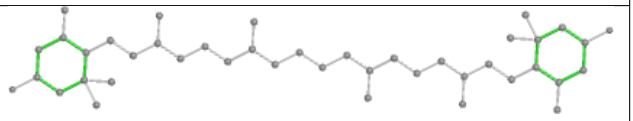
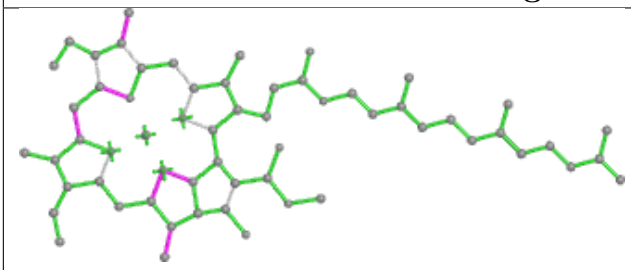
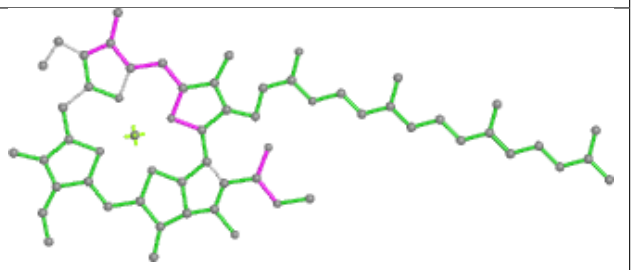


Rings

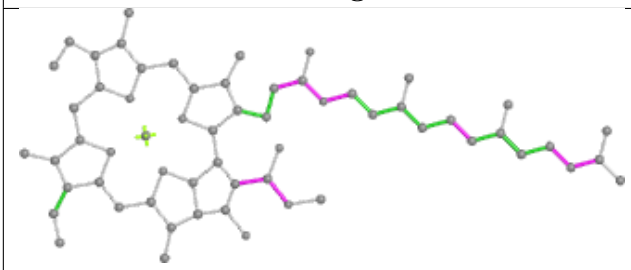
Ligand CLA R 311



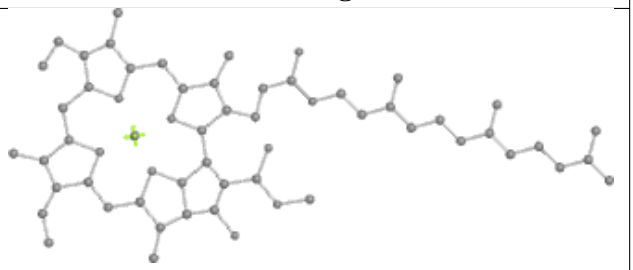
Bond lengths



Bond angles

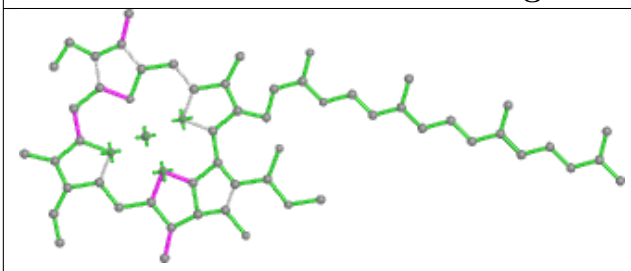


Torsions

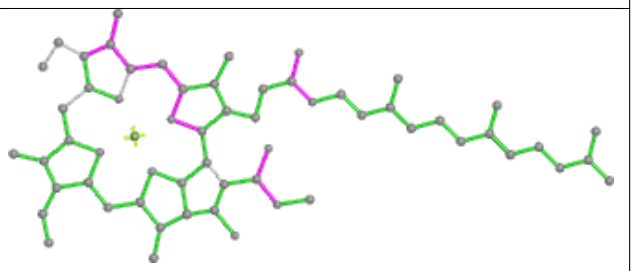


Rings

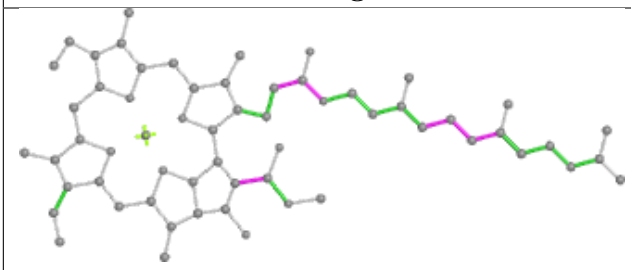
Ligand CLA R 303



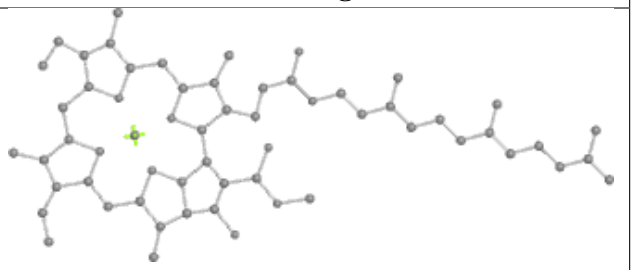
Bond lengths



Bond angles

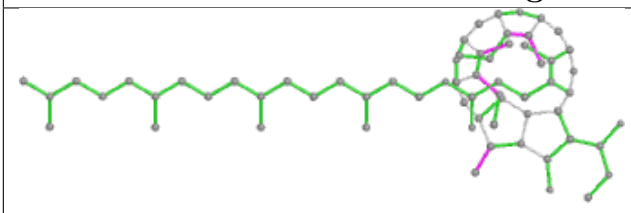


Torsions



Rings

Ligand PHO a 407



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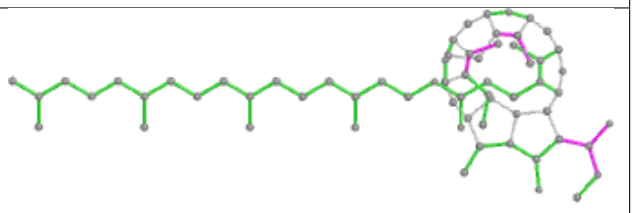
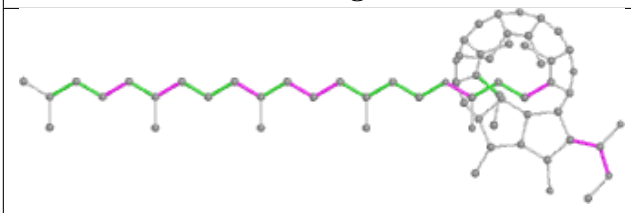
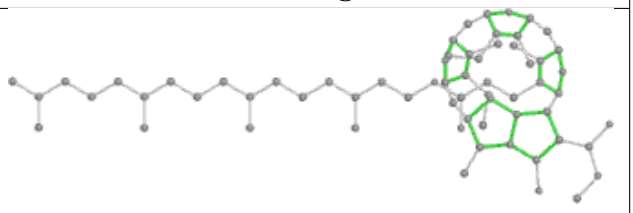


Bond angles



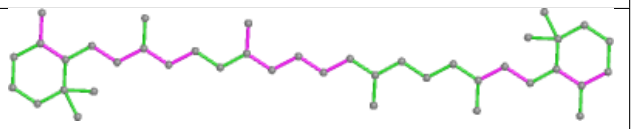
Torsions



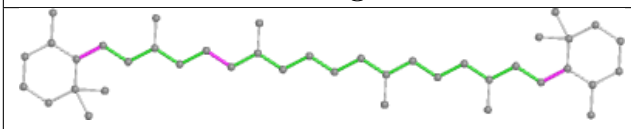
Rings

Ligand BCR k 102

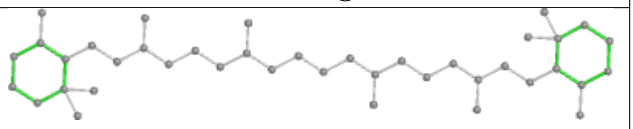
Bond lengths



Bond angles

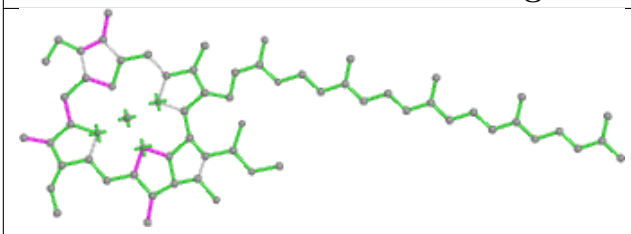


Torsions

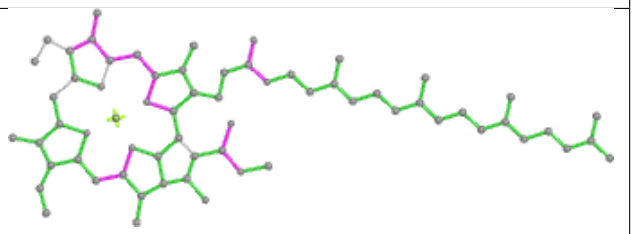


Rings

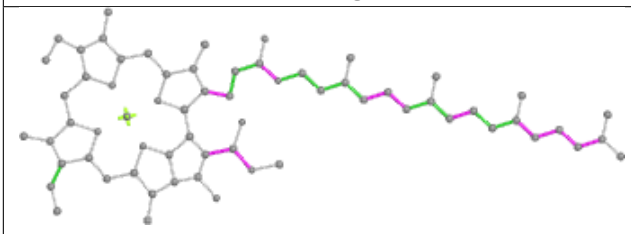
Ligand CLA B 603



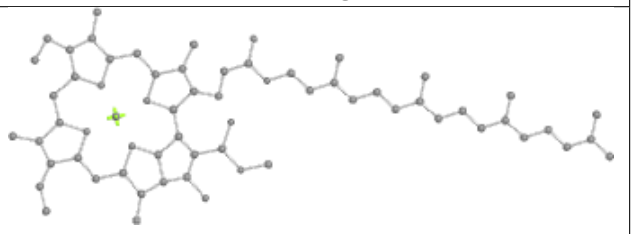
Bond lengths



Bond angles

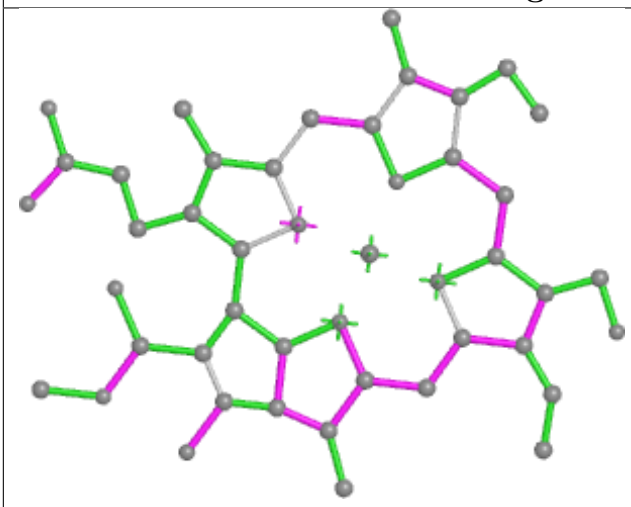


Torsions



Rings

Ligand CHL S 306



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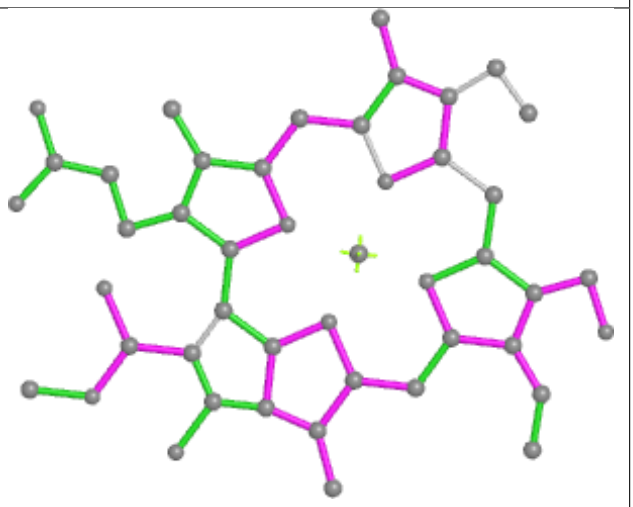
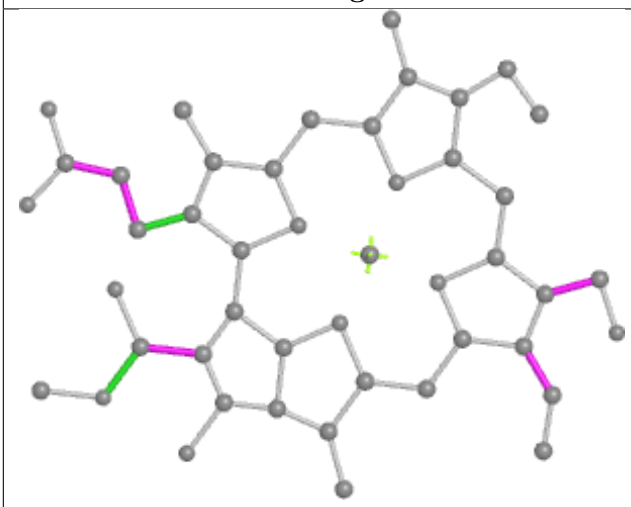
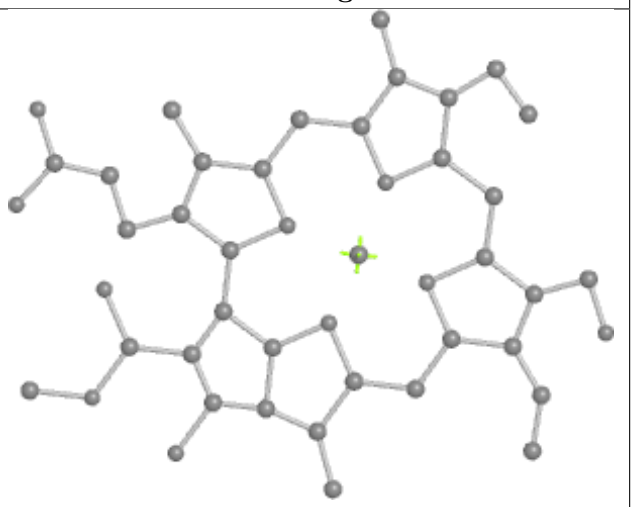


Bond angles

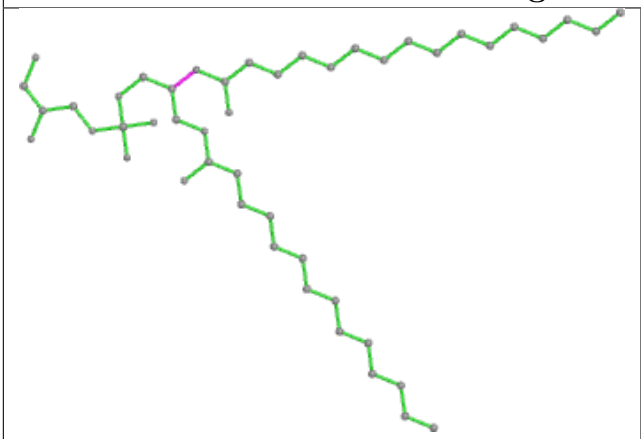


Torsions



Rings

Ligand LHG r 302



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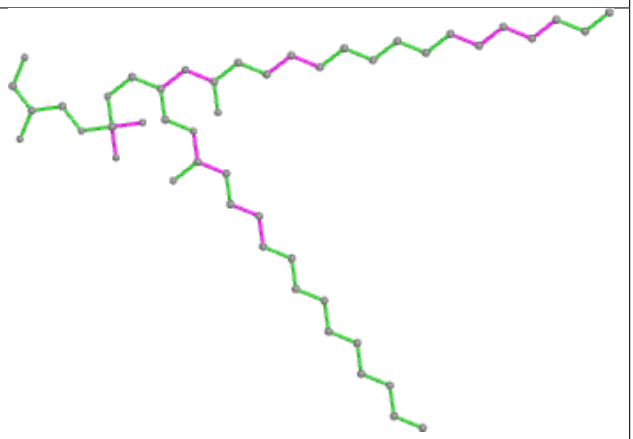
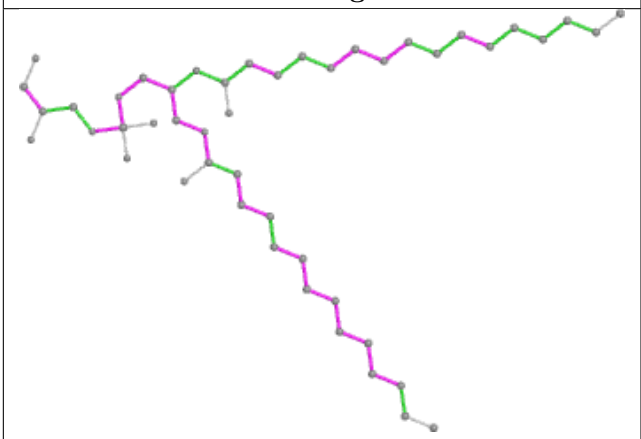
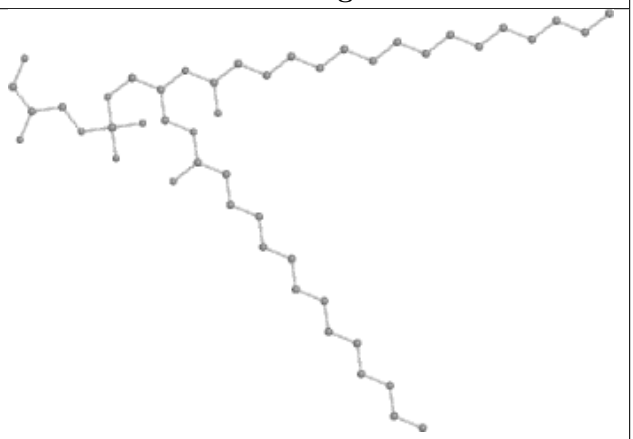


Bond angles

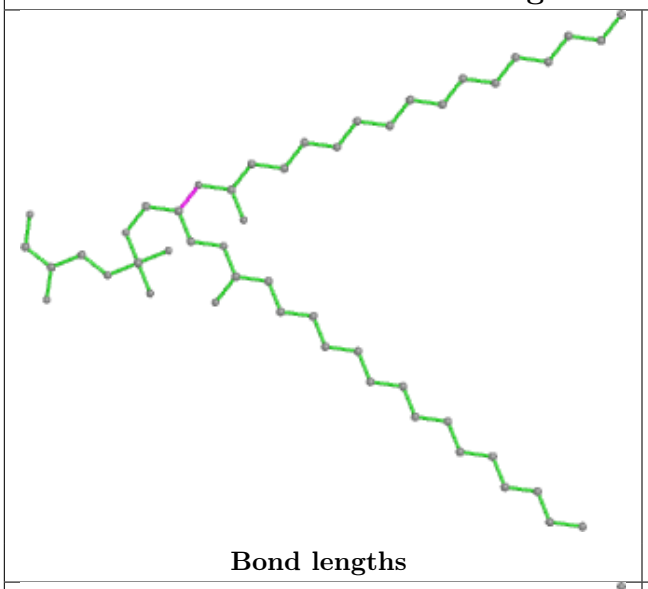


Torsions

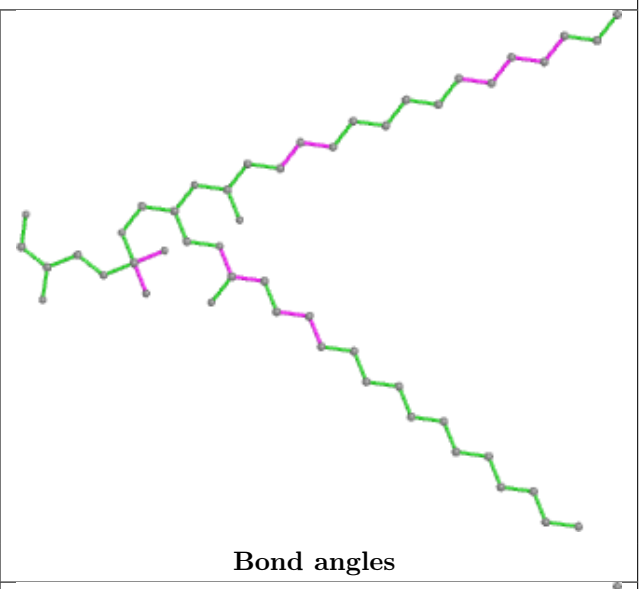


Rings

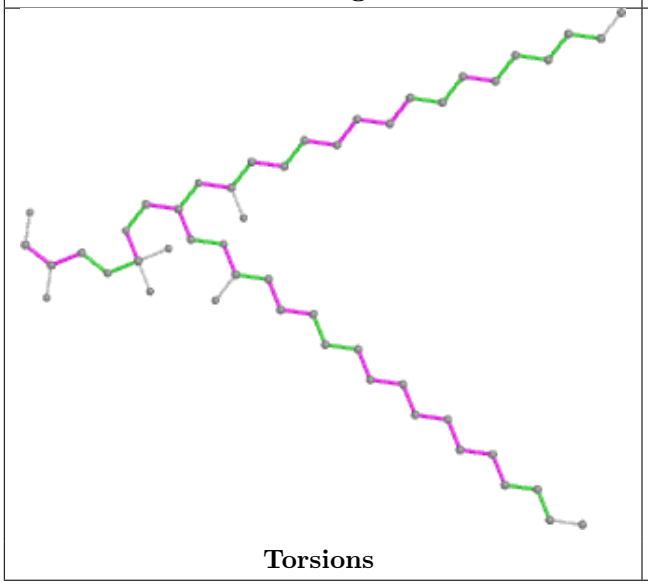
Ligand LHG S 314



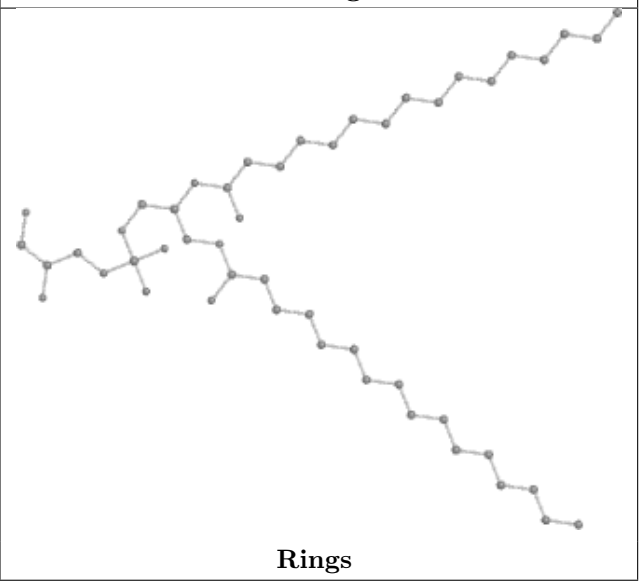
Bond lengths



Bond angles

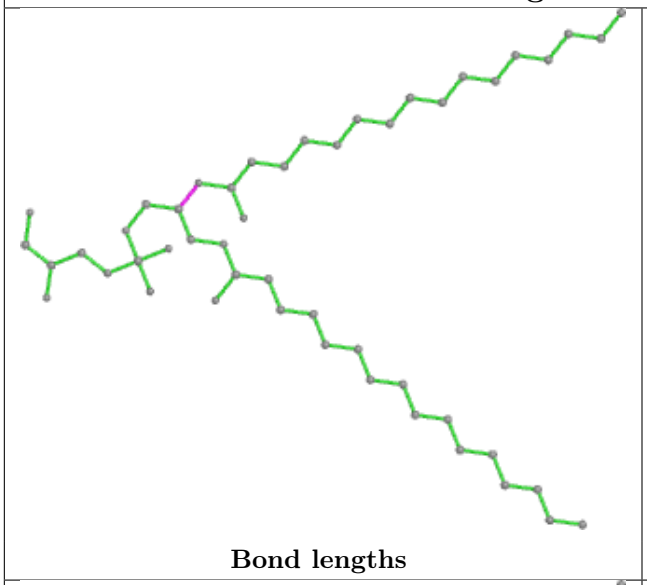


Torsions

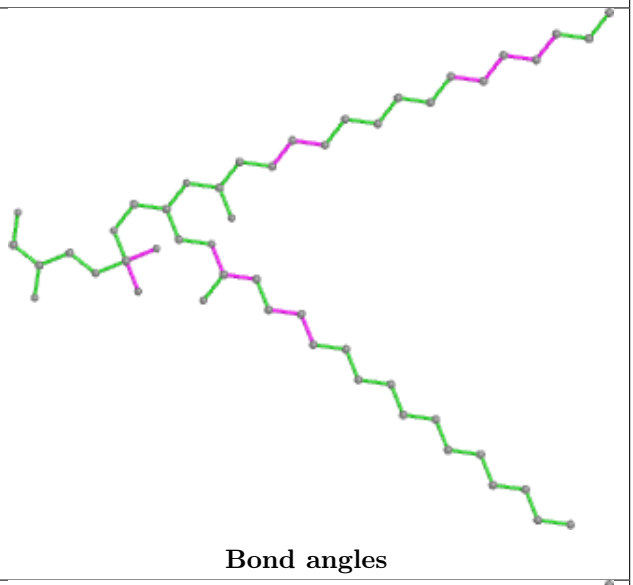


Rings

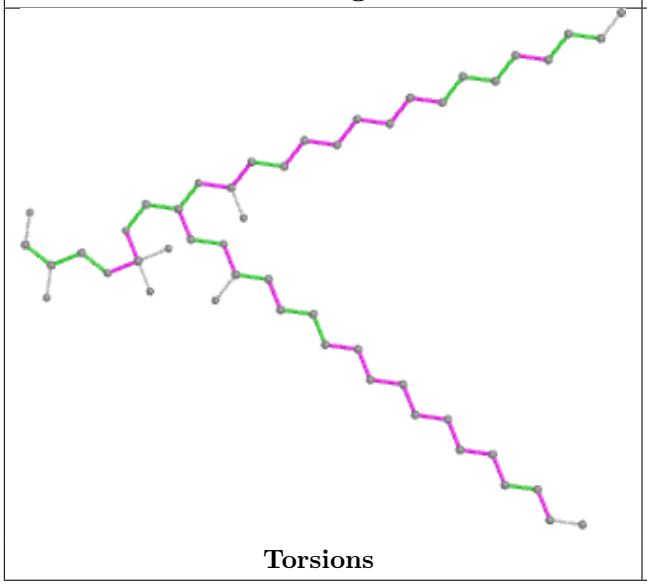
Ligand LHG b 619



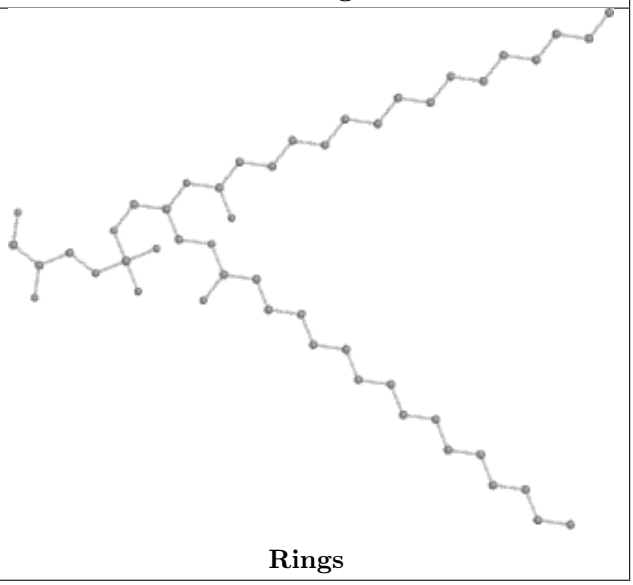
Bond lengths



Bond angles

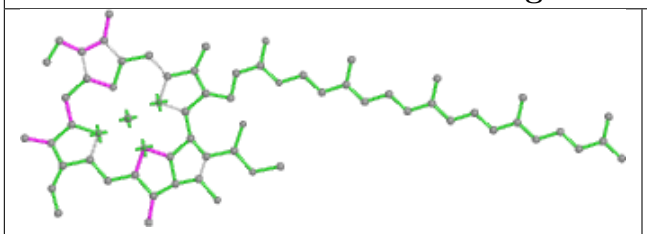


Torsions

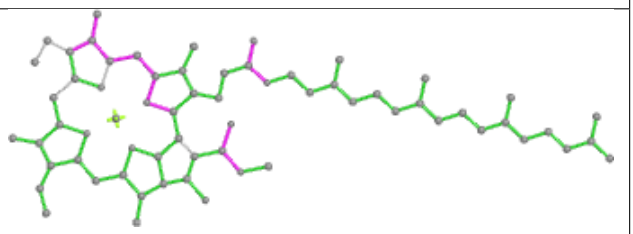


Rings

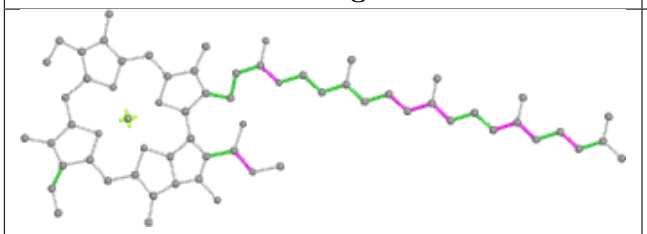
Ligand CLA B 613



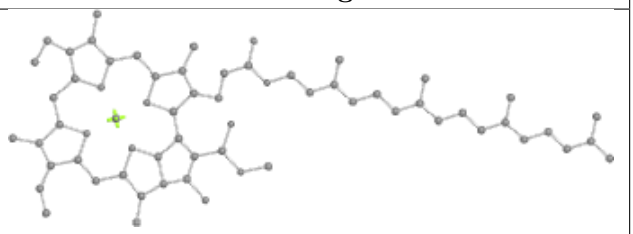
Bond lengths



Bond angles

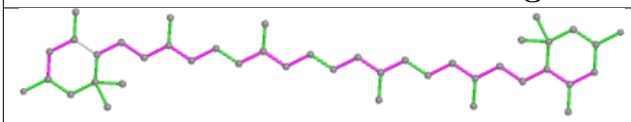


Torsions

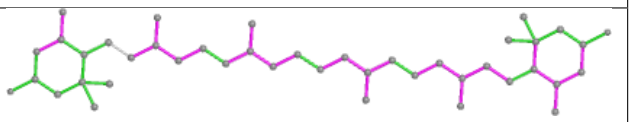


Rings

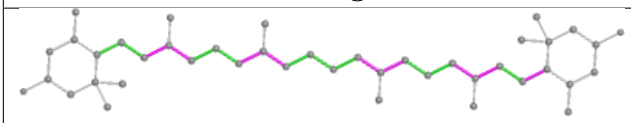
Ligand LUT Y 614



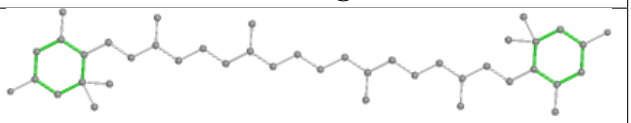
Bond lengths



Bond angles

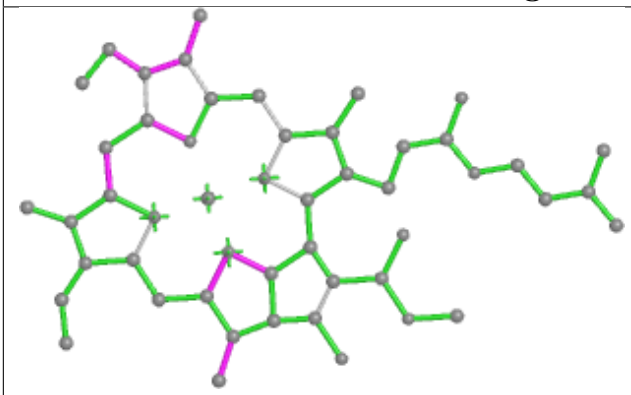


Torsions

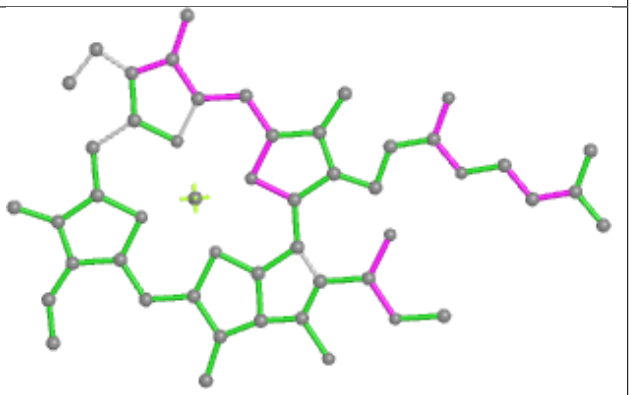


Rings

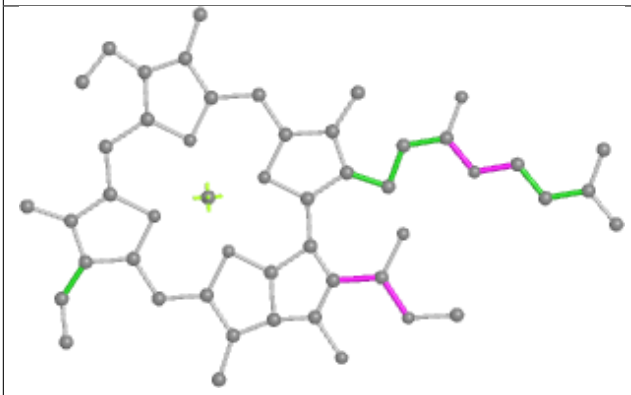
Ligand CLA Y 604



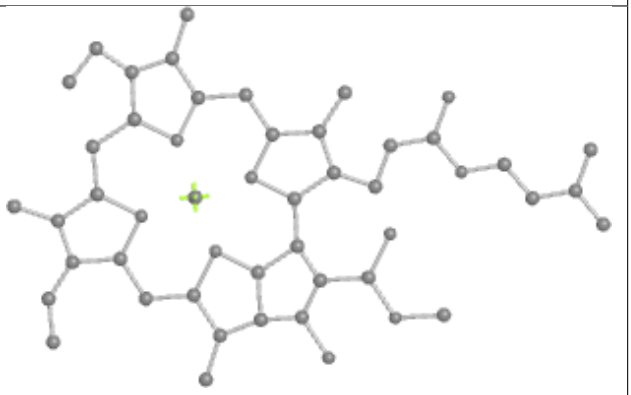
Bond lengths



Bond angles

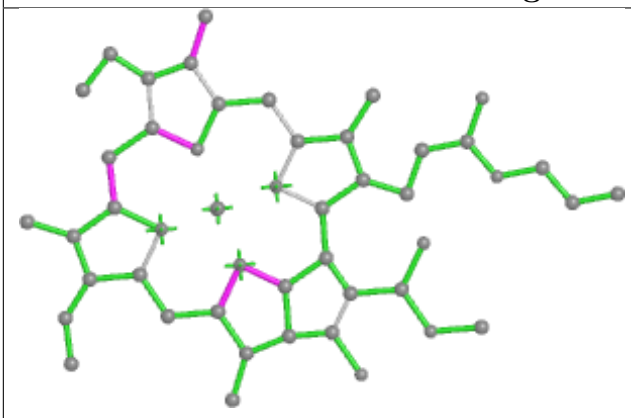


Torsions

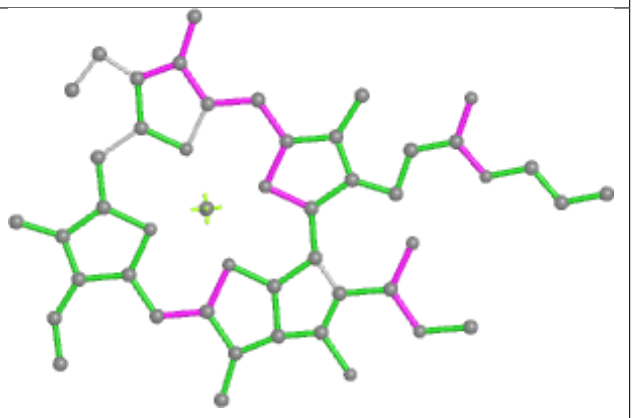


Rings

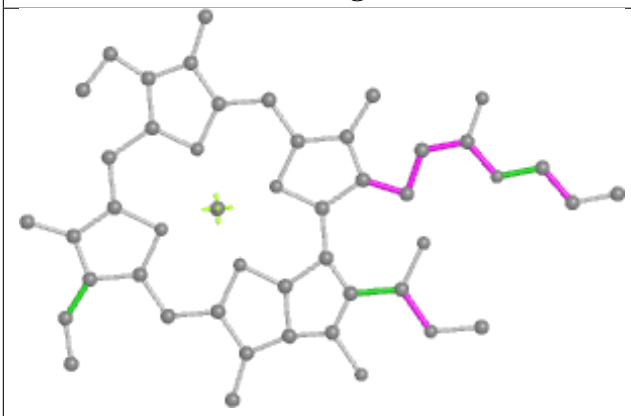
Ligand CLA G 614



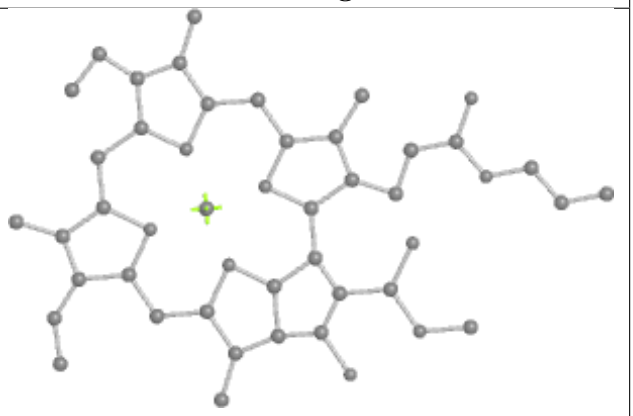
Bond lengths



Bond angles

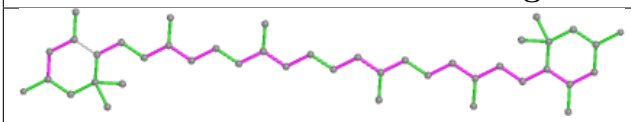


Torsions

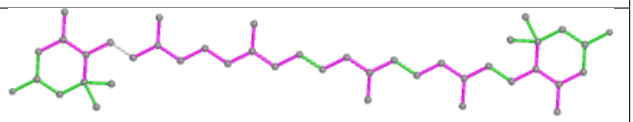


Rings

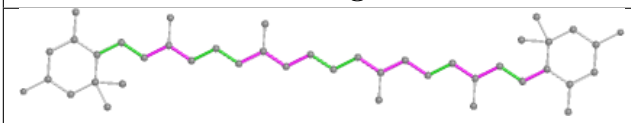
Ligand LUT N 614



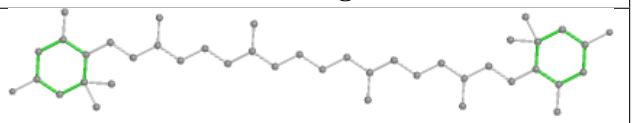
Bond lengths



Bond angles

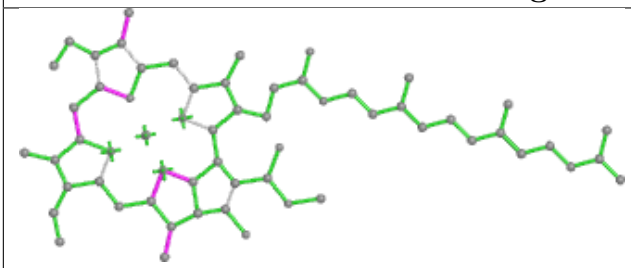


Torsions

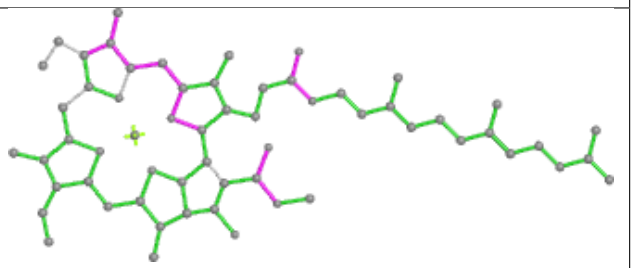


Rings

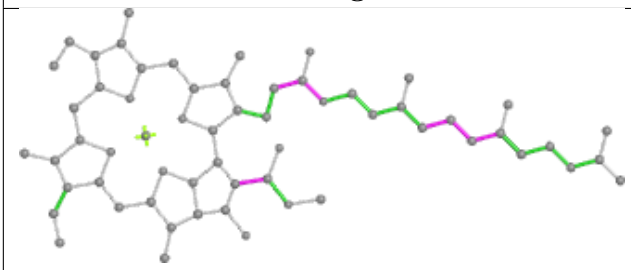
Ligand CLA r 304



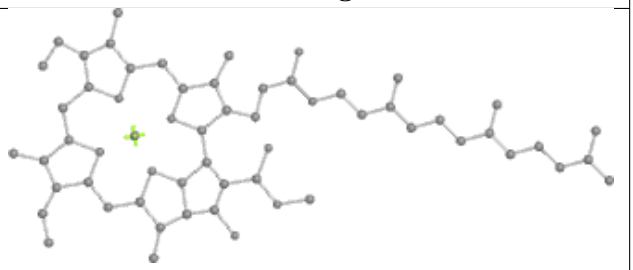
Bond lengths



Bond angles

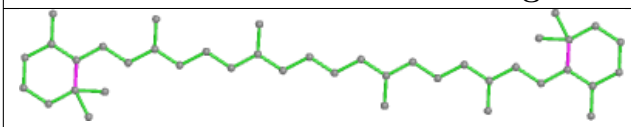


Torsions

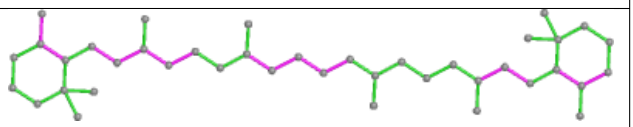


Rings

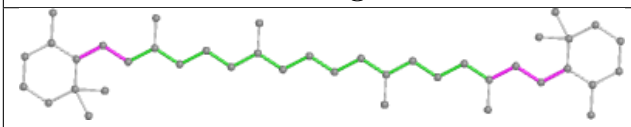
Ligand BCR B 619



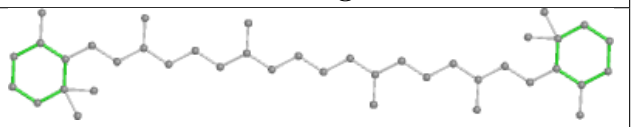
Bond lengths



Bond angles

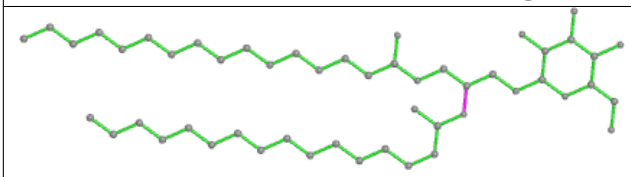


Torsions

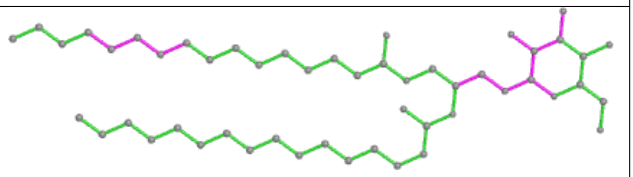


Rings

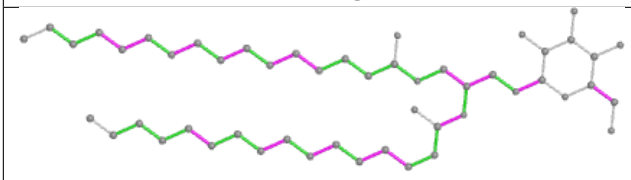
Ligand LMG C 523



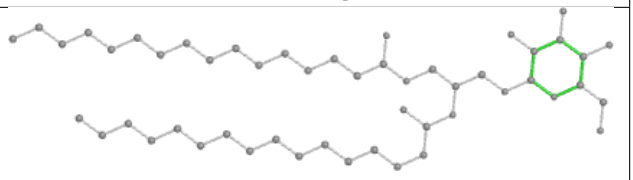
Bond lengths



Bond angles

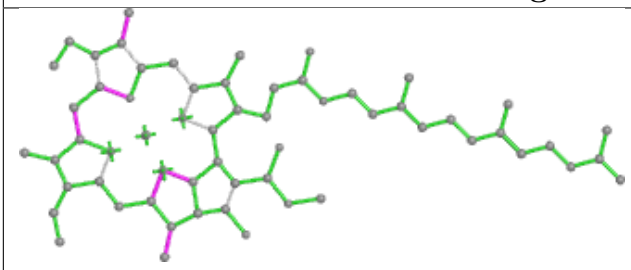


Torsions

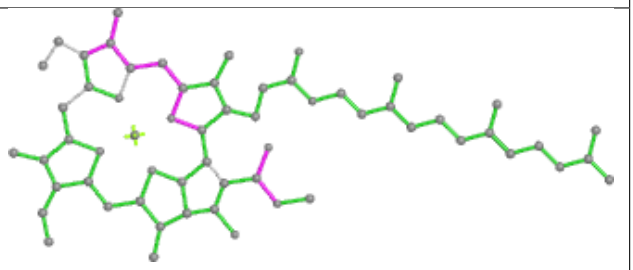


Rings

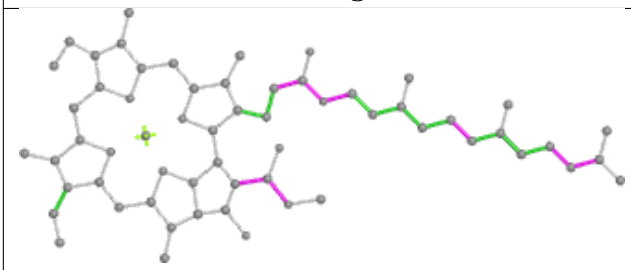
Ligand CLA r 312



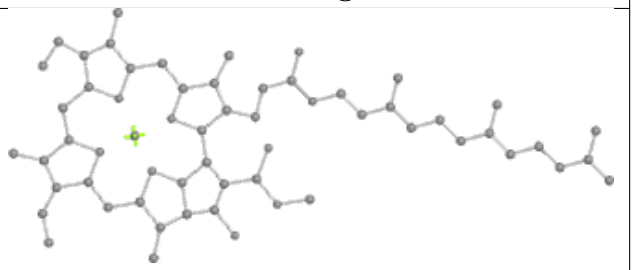
Bond lengths



Bond angles

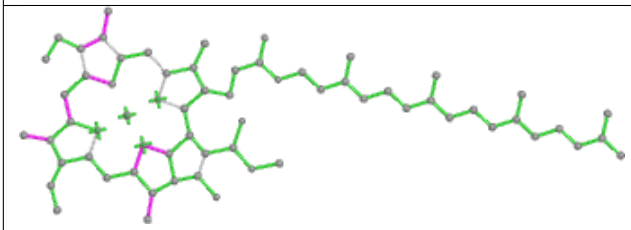


Torsions

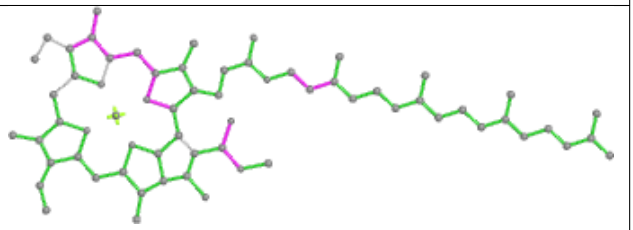


Rings

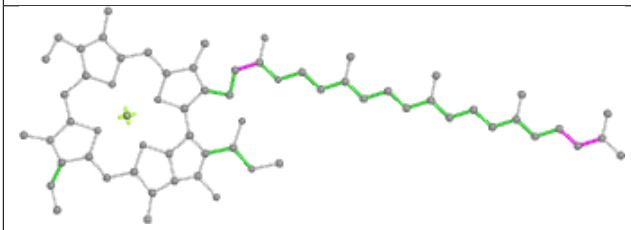
Ligand CLA A 405



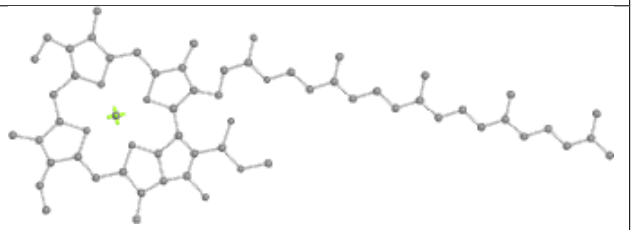
Bond lengths



Bond angles

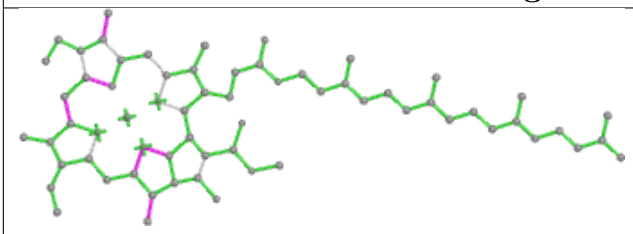


Torsions

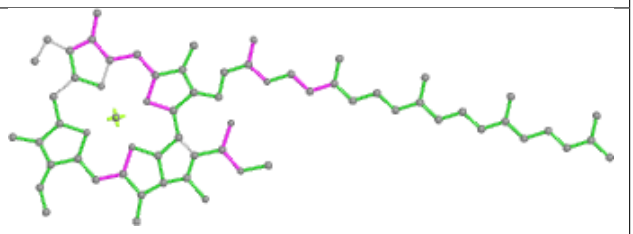


Rings

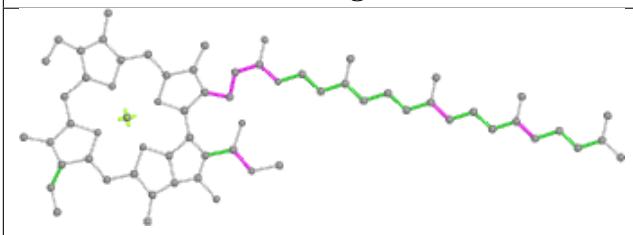
Ligand CLA Y 602



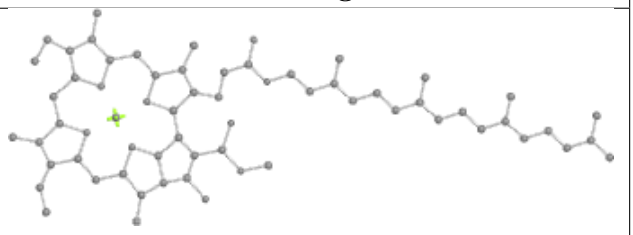
Bond lengths



Bond angles

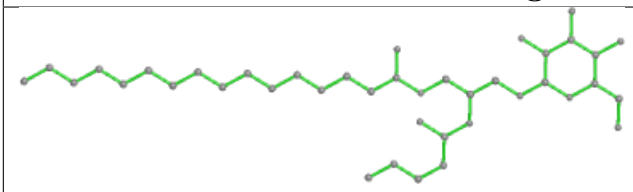


Torsions

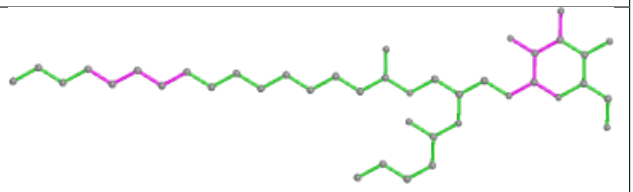


Rings

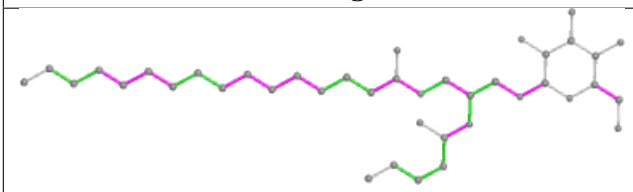
Ligand LMG I 101



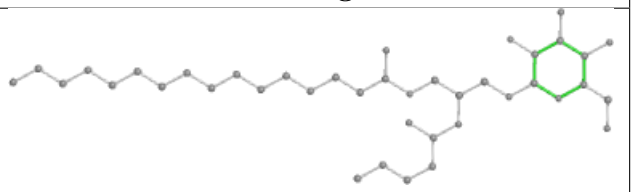
Bond lengths



Bond angles

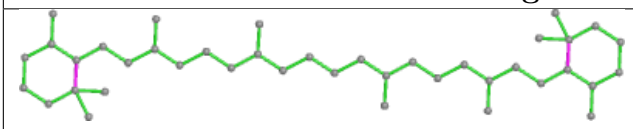


Torsions

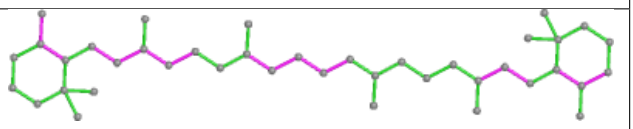


Rings

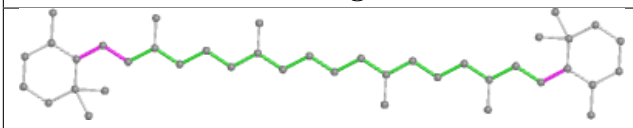
Ligand BCR A 410



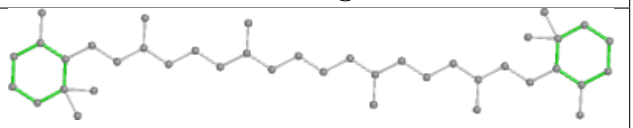
Bond lengths



Bond angles

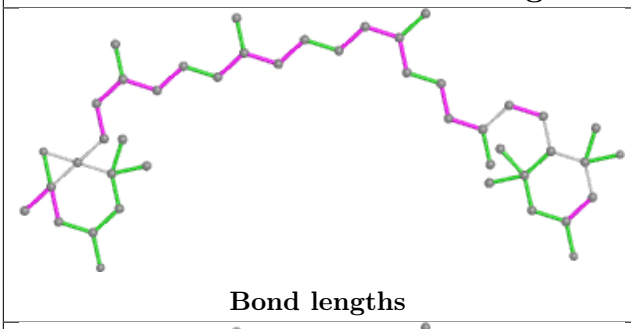


Torsions

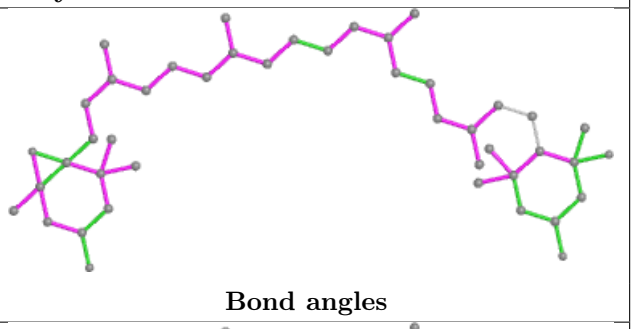


Rings

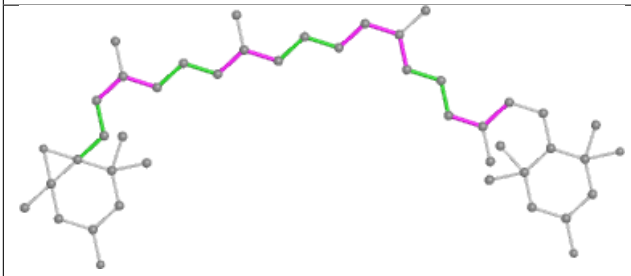
Ligand NEX y 618



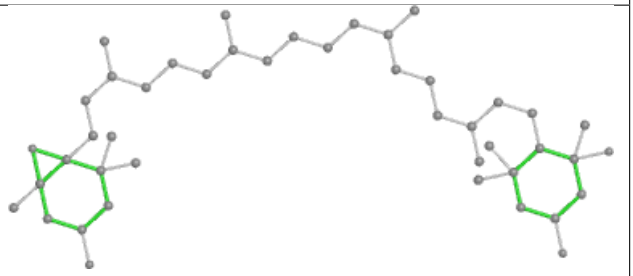
Bond lengths



Bond angles

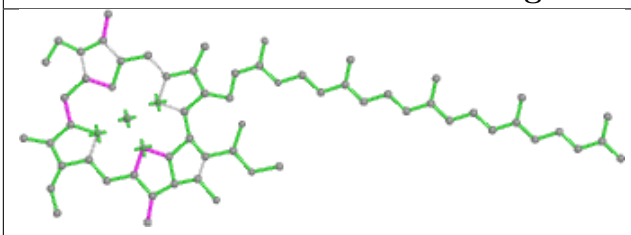


Torsions

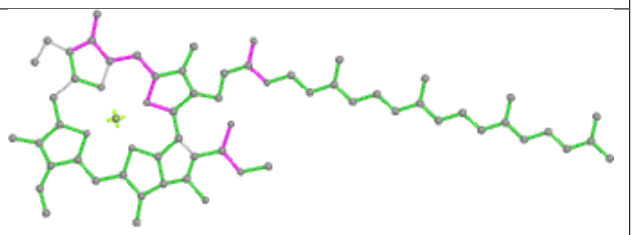


Rings

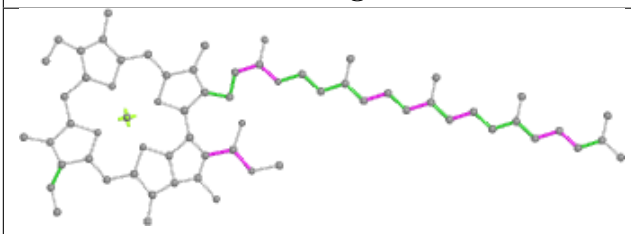
Ligand CLA B 618



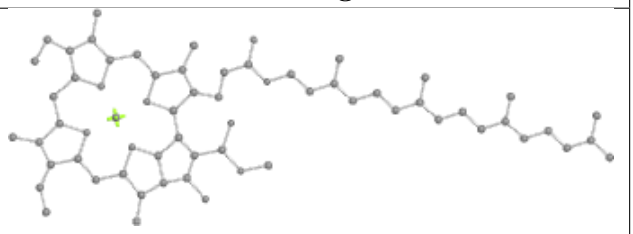
Bond lengths



Bond angles

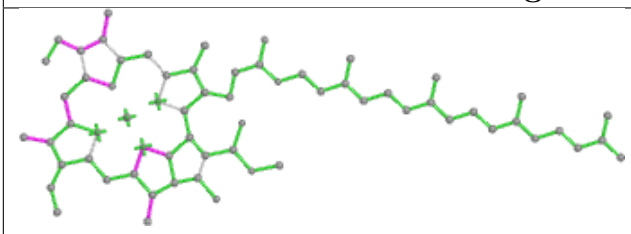


Torsions

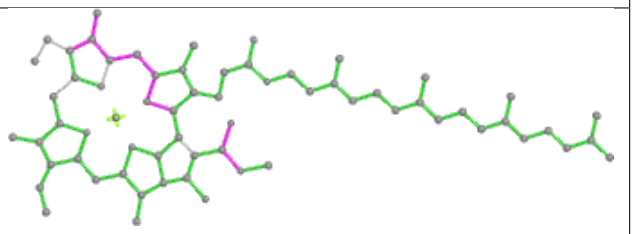


Rings

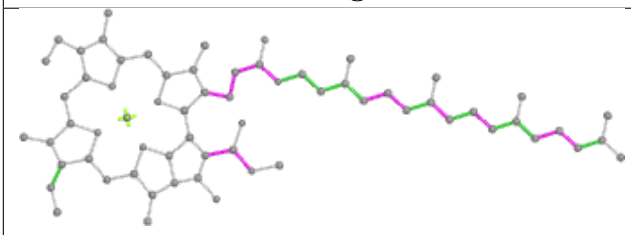
Ligand CLA C 503



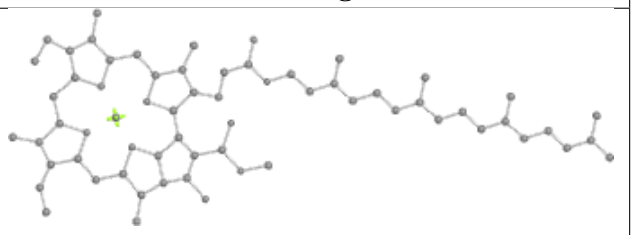
Bond lengths



Bond angles

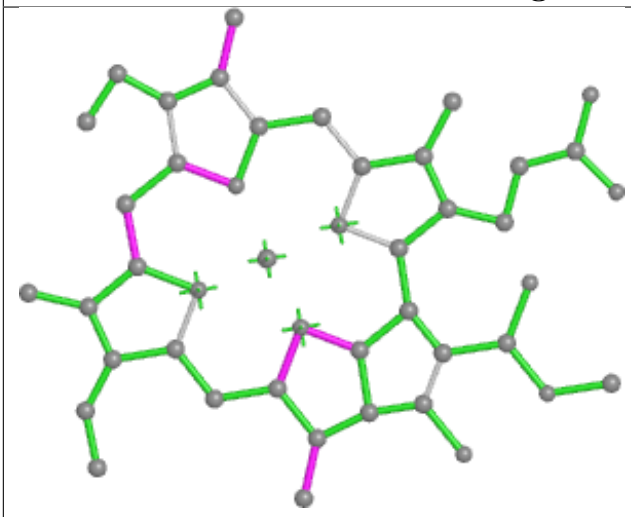


Torsions

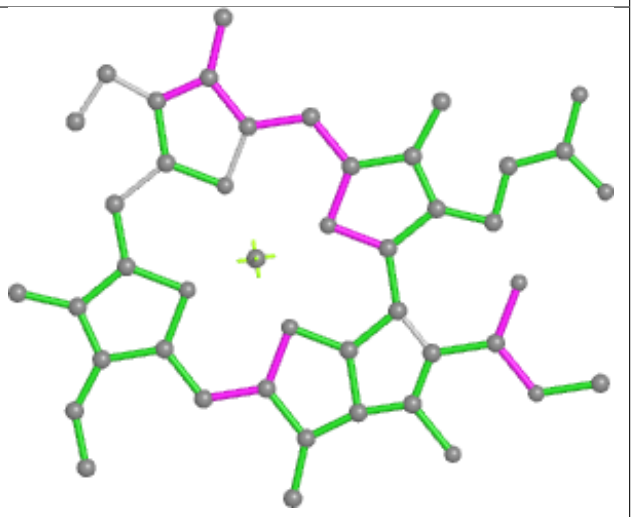


Rings

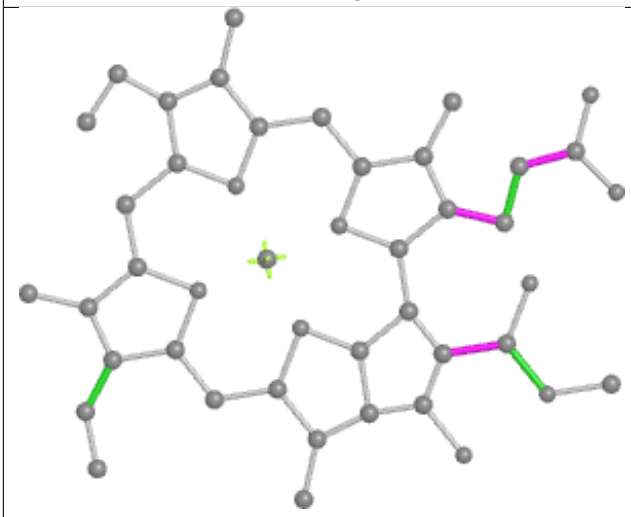
Ligand CLA s 304



Bond lengths



Bond angles



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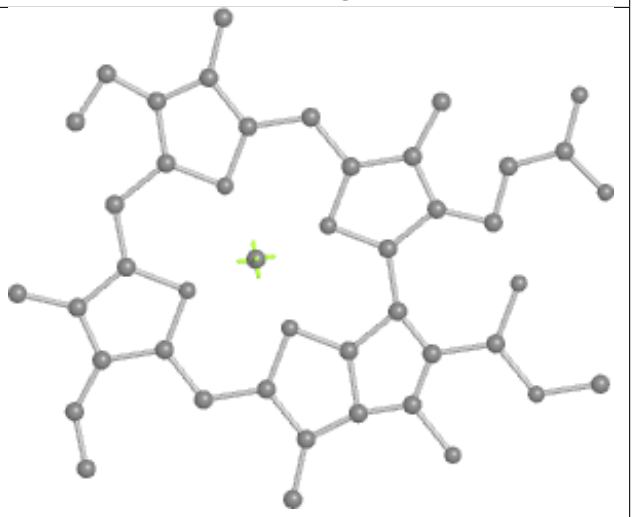
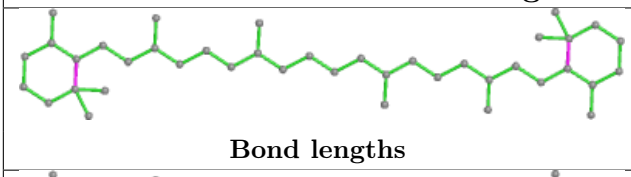


Rings

Ligand BCR B 621



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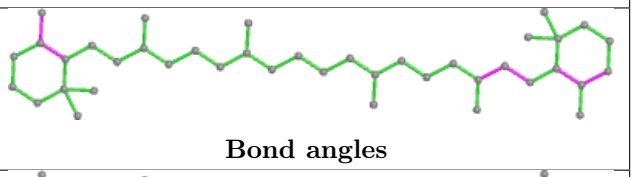
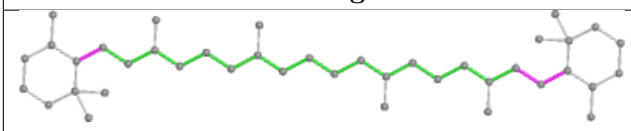
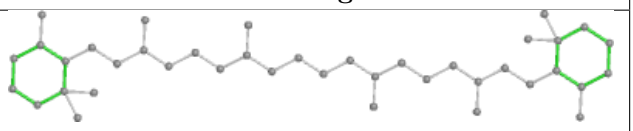


Bond angles

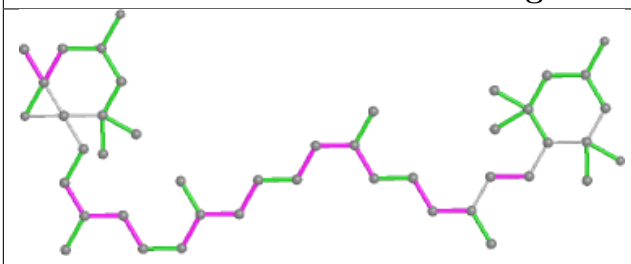


Torsions

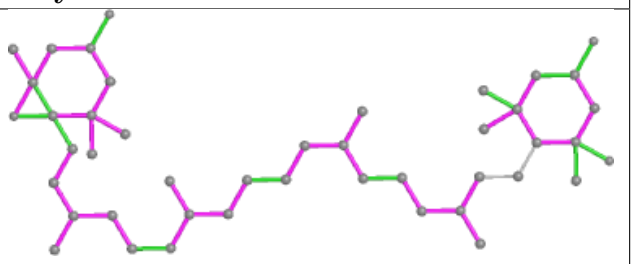


Rings

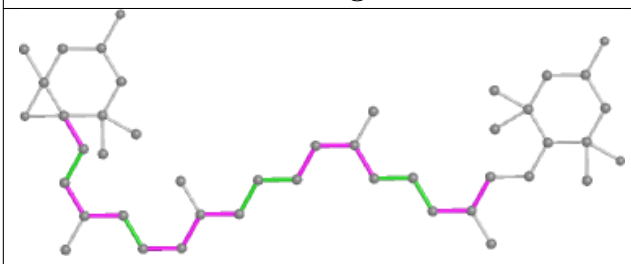
Ligand NEX y 616



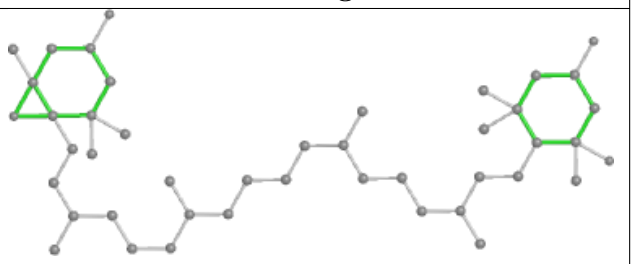
Bond lengths



Bond angles

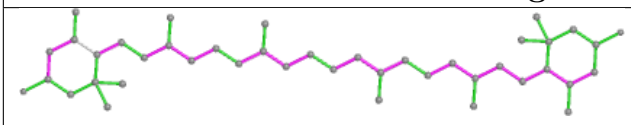


Torsions



Rings

Ligand LUT g 616



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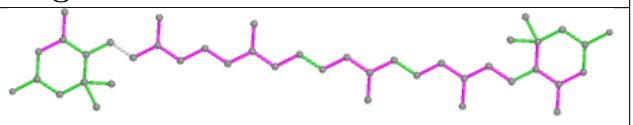
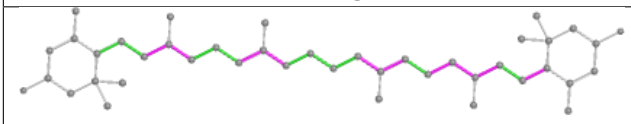


Bond angles



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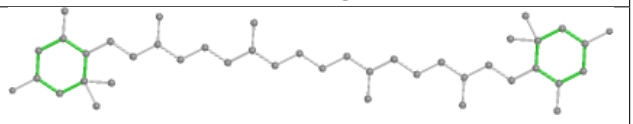
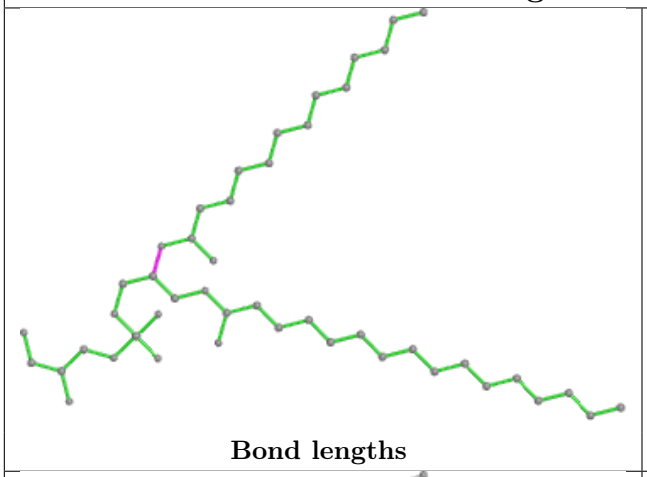
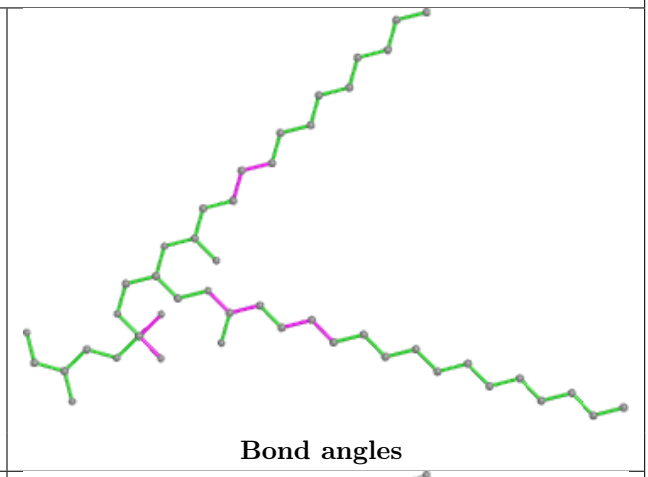


Rings

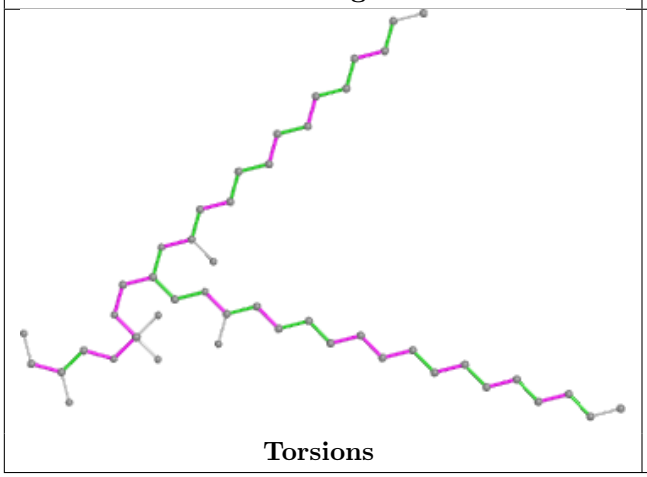
Ligand LHG d 407



Bond lengths



Bond angles



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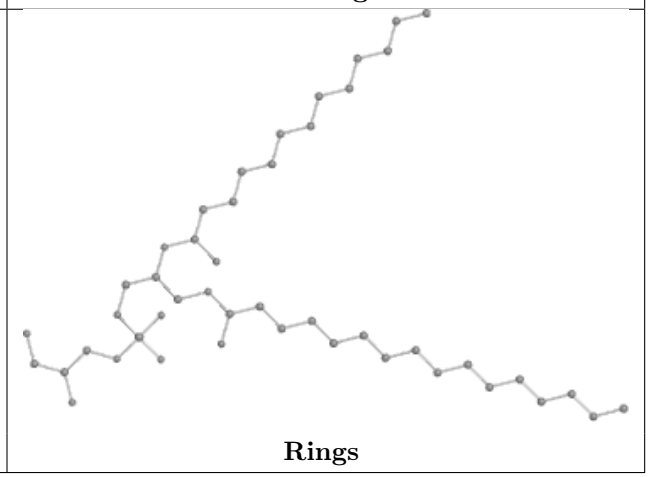
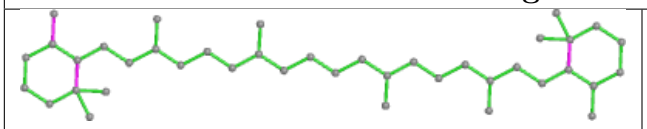
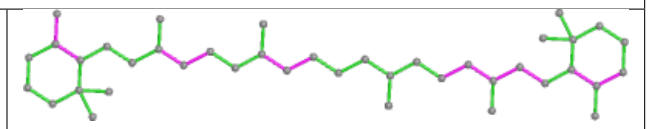


Rings

Ligand BCR H 101

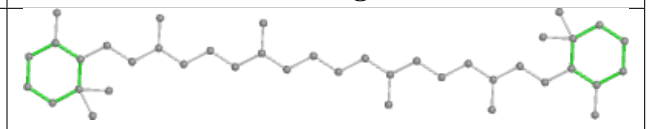


Bond lengths



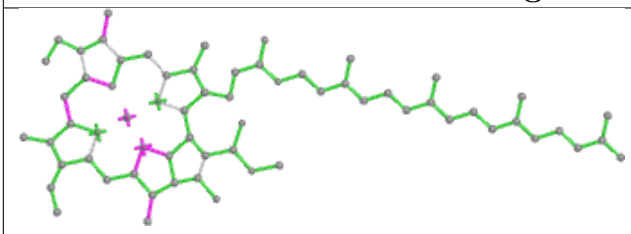
Bond angles

Torsions

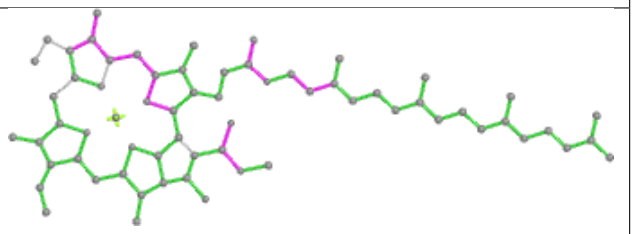


Rings

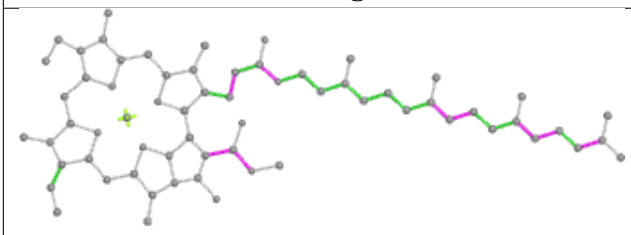
Ligand CLA C 504



Bond lengths



Bond angles



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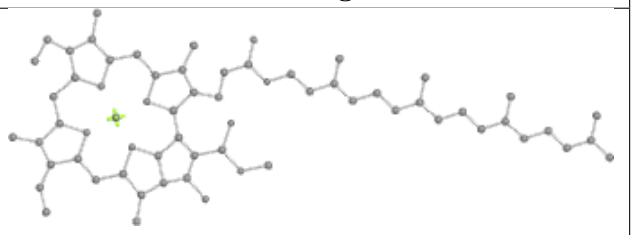
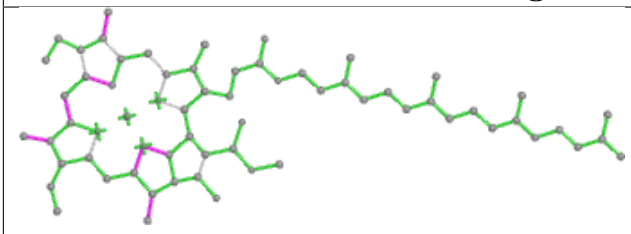
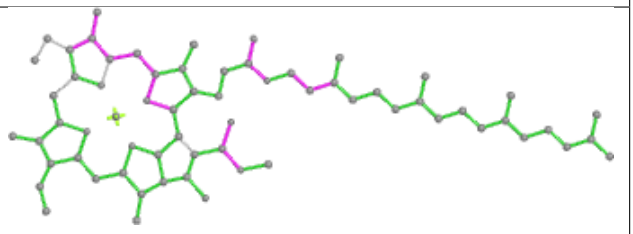


Rings

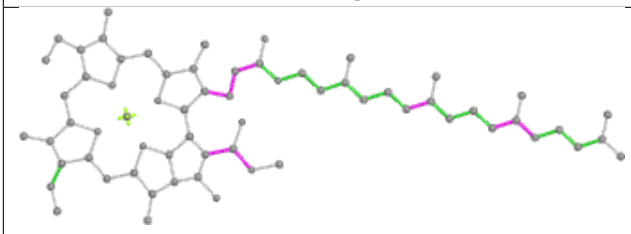
Ligand CLA b 607



Bond lengths



Bond angles



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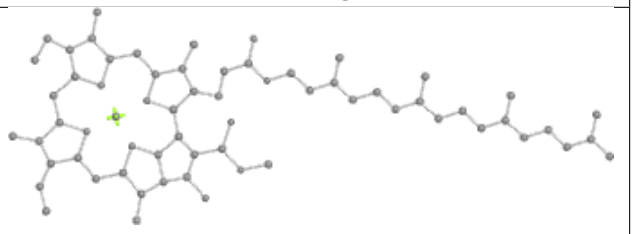
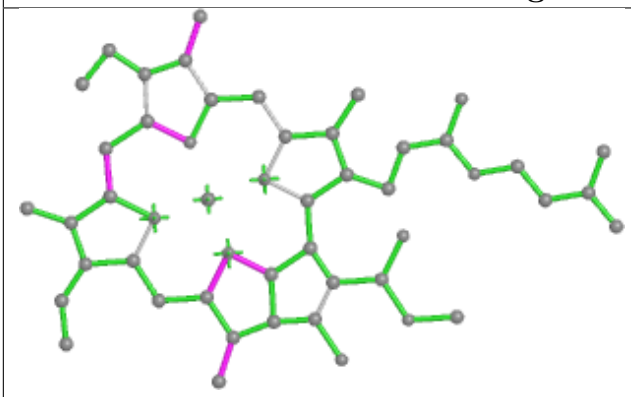
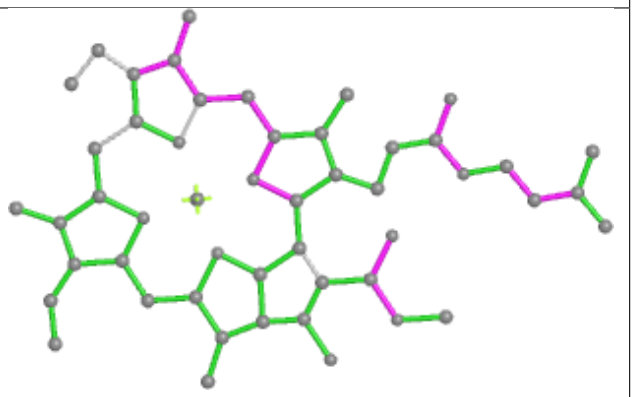


Rings

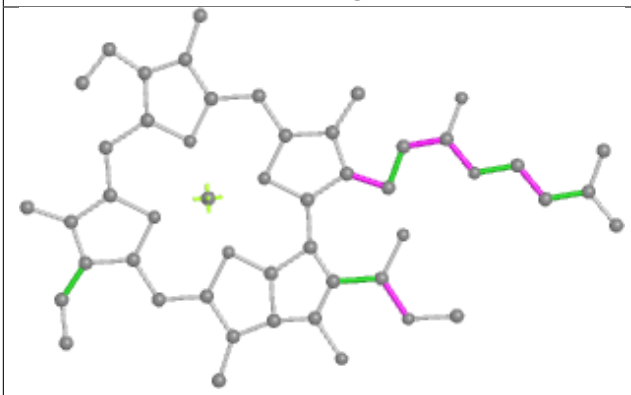
Ligand CLA S 305



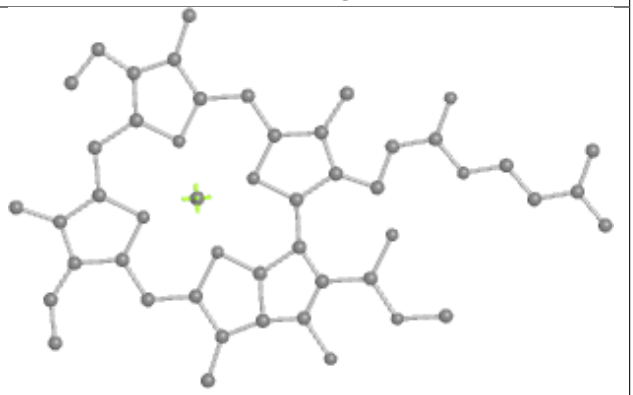
Bond lengths



Bond angles

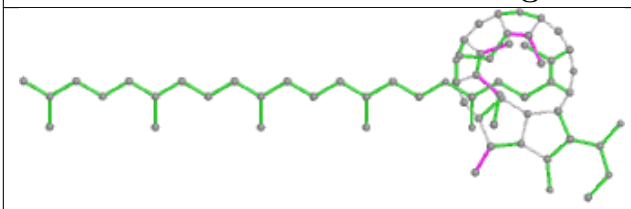


Torsions



Rings

Ligand PHO A 408



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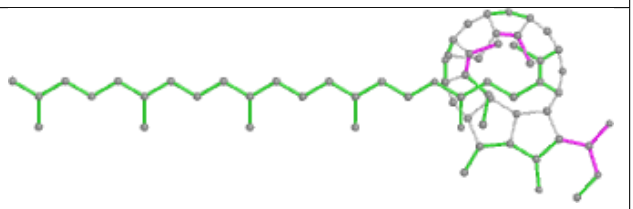
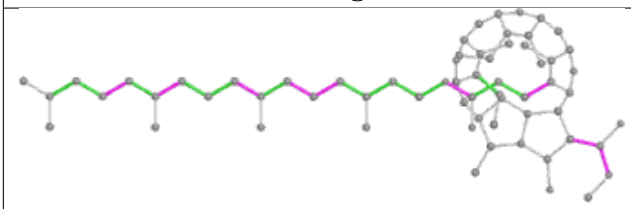


Bond angles



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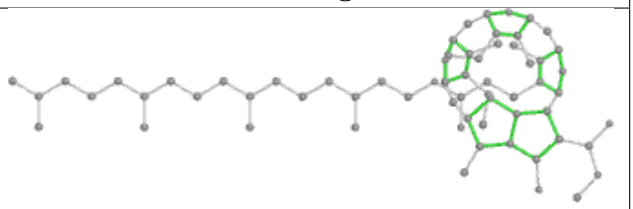
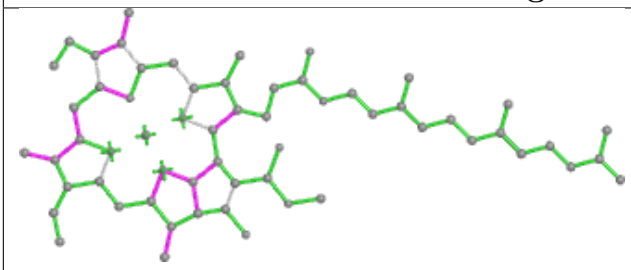


Rings

Ligand CLA n 612



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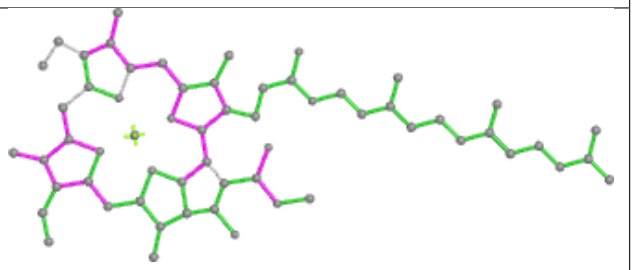
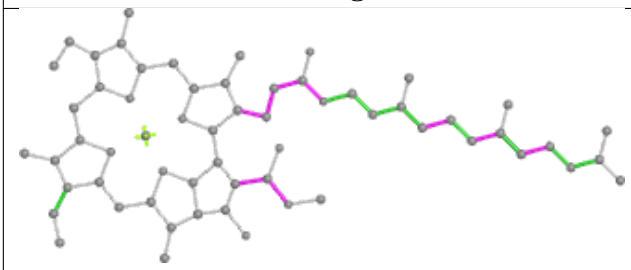
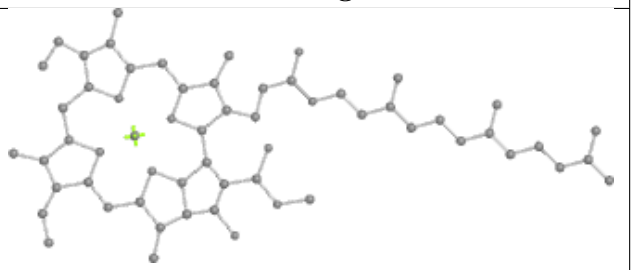


Bond angles

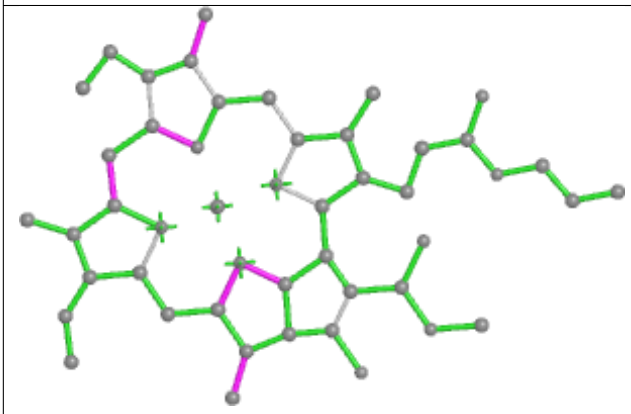


Torsions



Rings

Ligand CLA n 613



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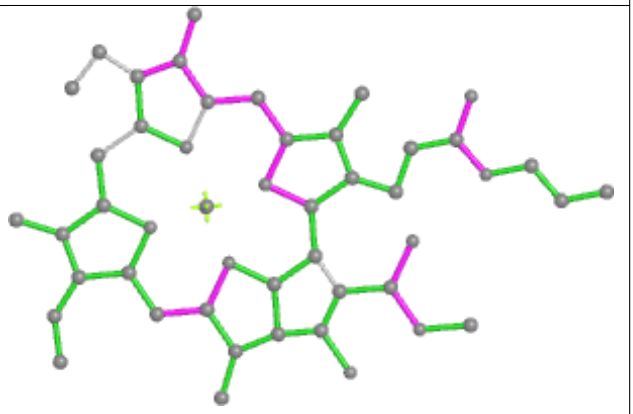
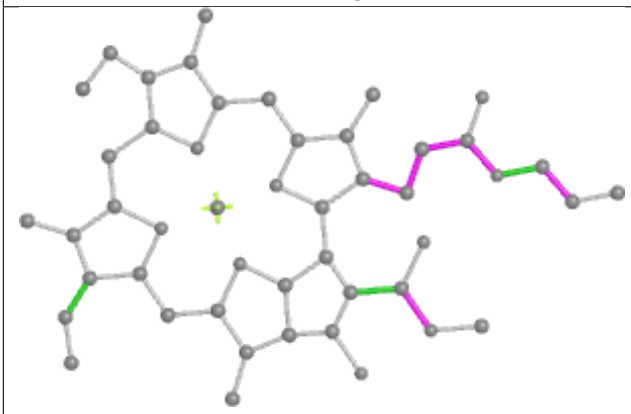
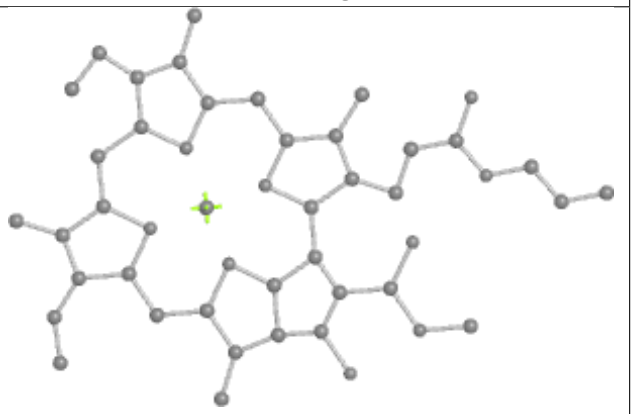


Bond angles

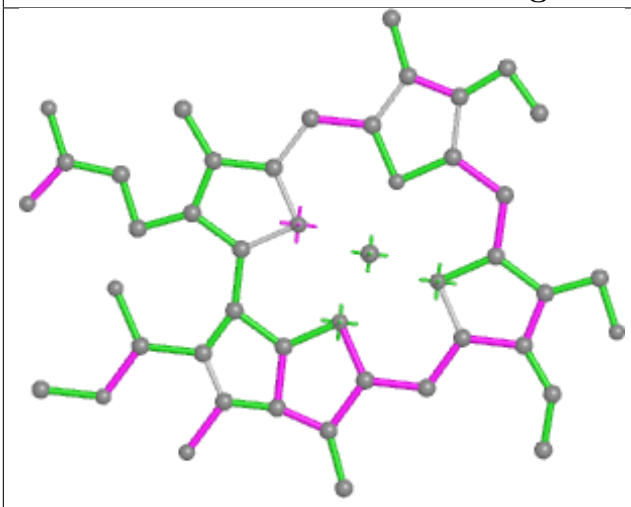


Torsions



Rings

Ligand CHL s 307



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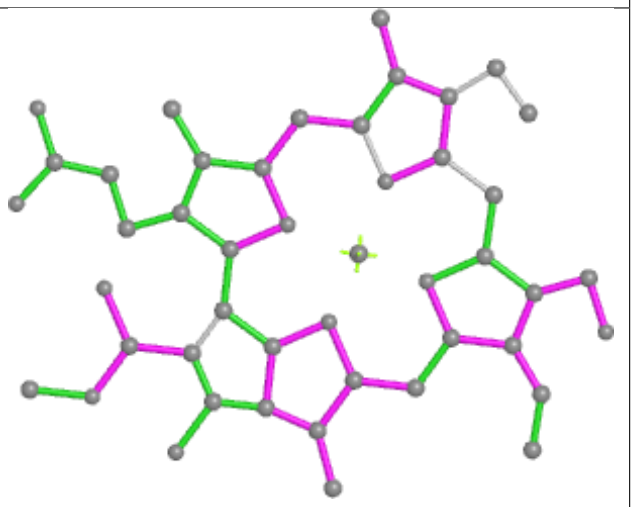
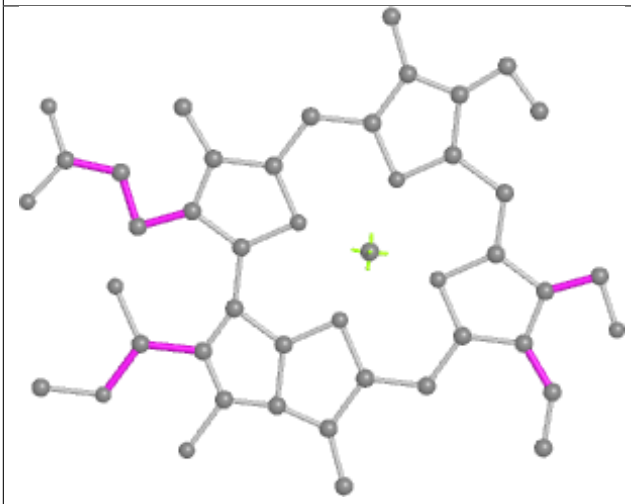
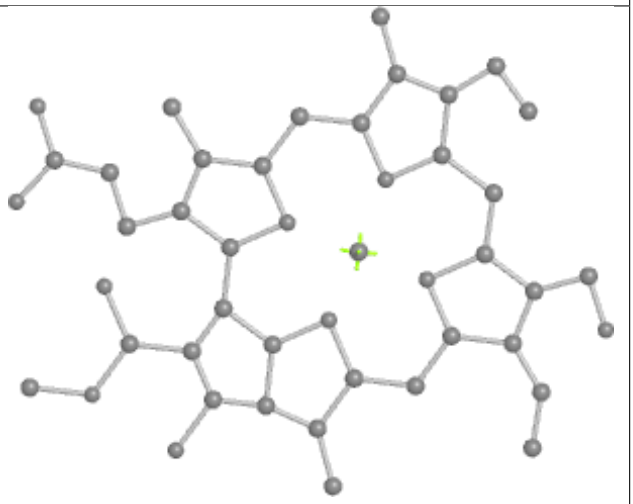


Bond angles

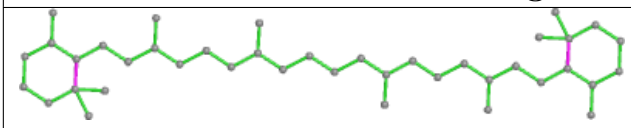


Torsions

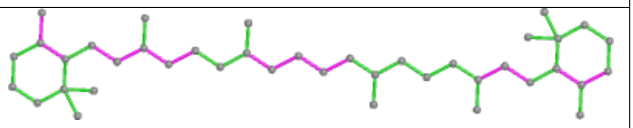


Rings

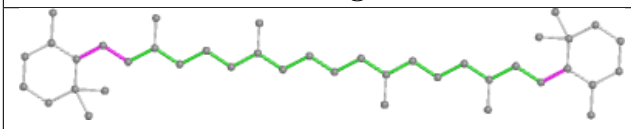
Ligand BCR a 409



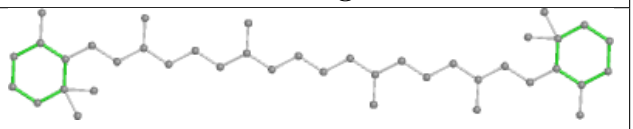
Bond lengths



Bond angles

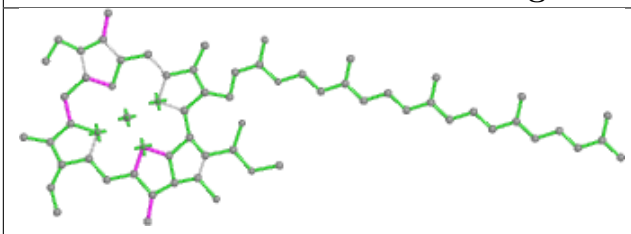


Torsions

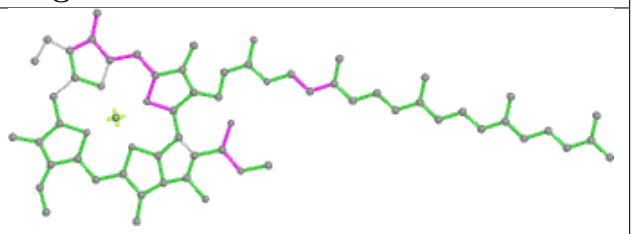


Rings

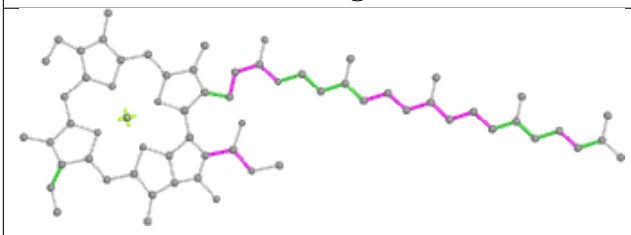
Ligand CLA g 603



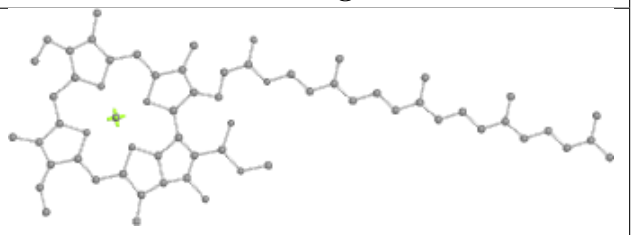
Bond lengths



Bond angles

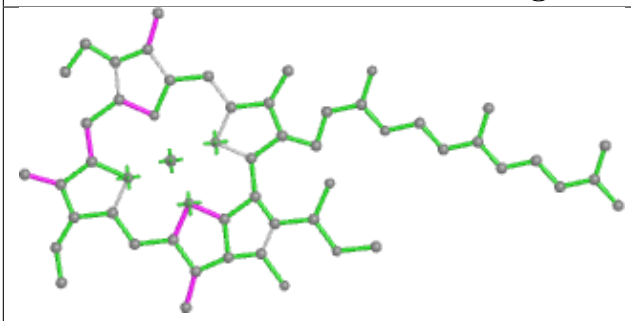


Torsions

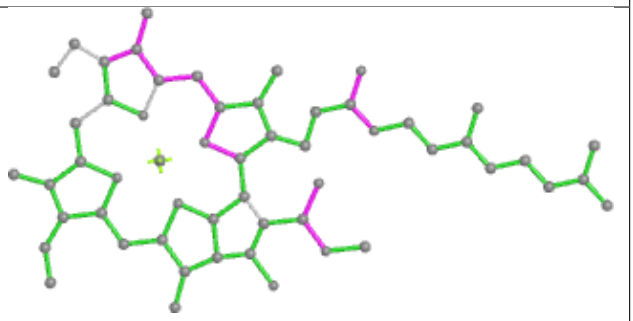


Rings

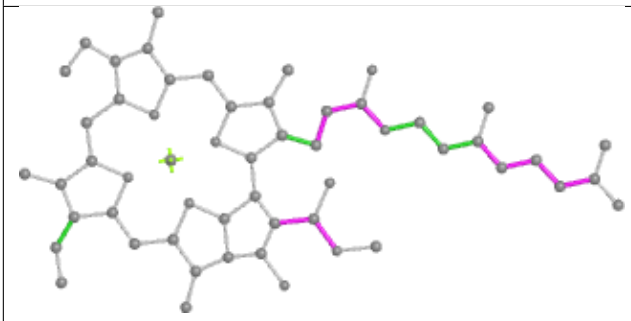
Ligand CLA s 310



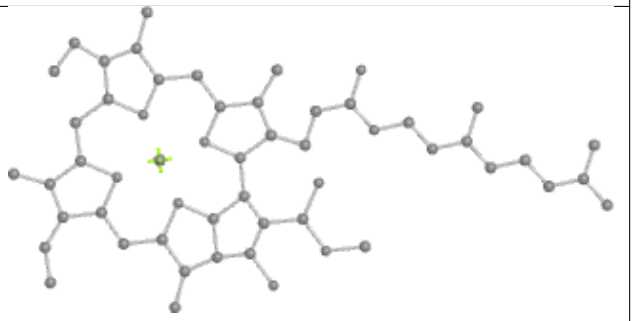
Bond lengths



Bond angles

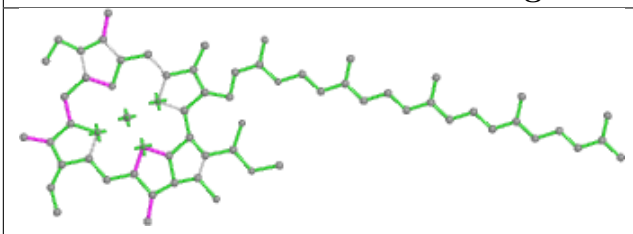


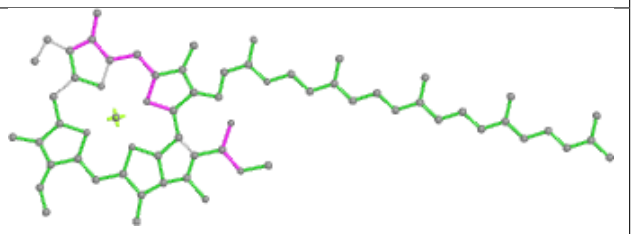
Torsions

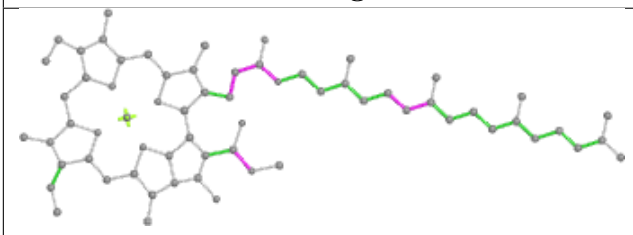


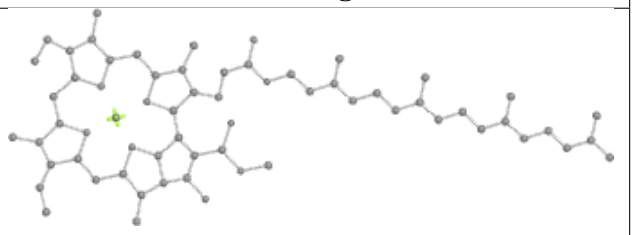
Rings

Ligand CLA C 508

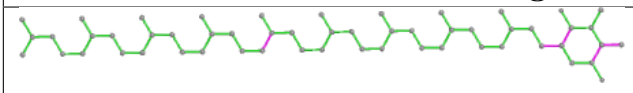

Bond lengths

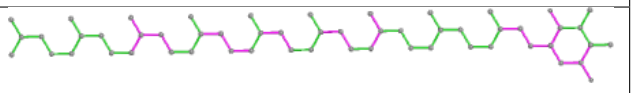

Bond angles

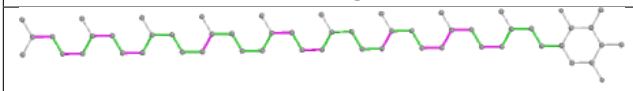

Torsions

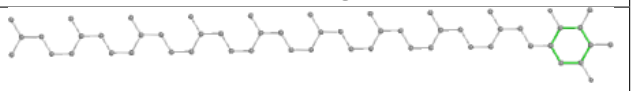

Rings

Ligand PL9 D 407

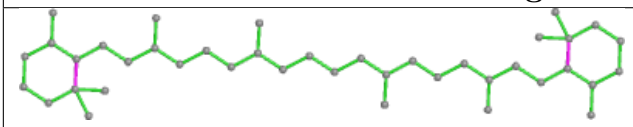

Bond lengths

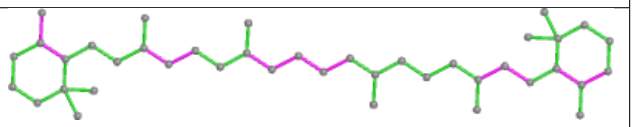

Bond angles

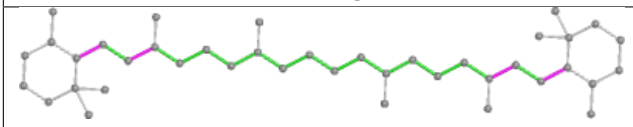

Torsions

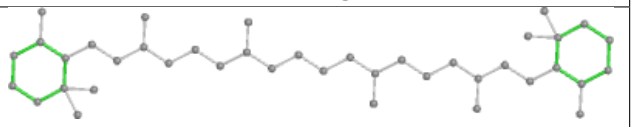

Rings

Ligand BCR b 617

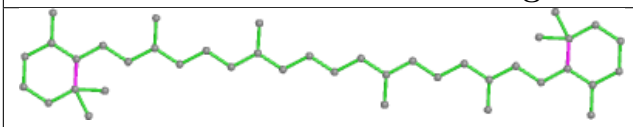

Bond lengths

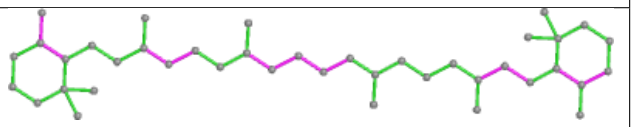

Bond angles

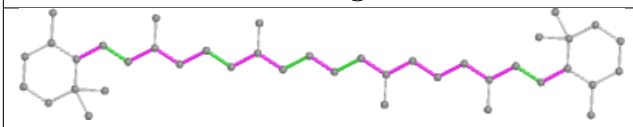

Torsions

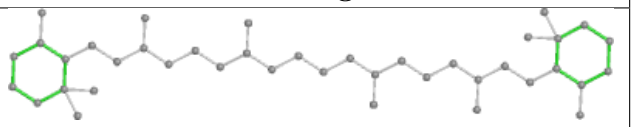

Rings

Ligand BCR T 102

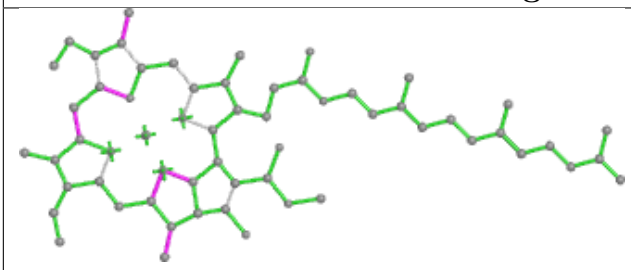

Bond lengths


Bond angles

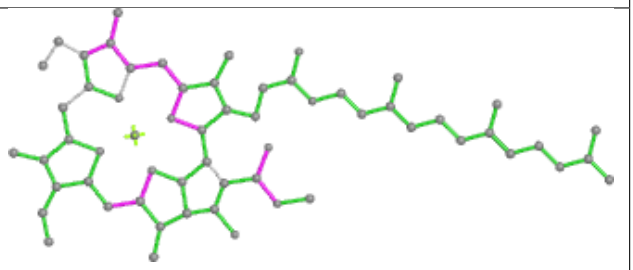

Torsions


Rings

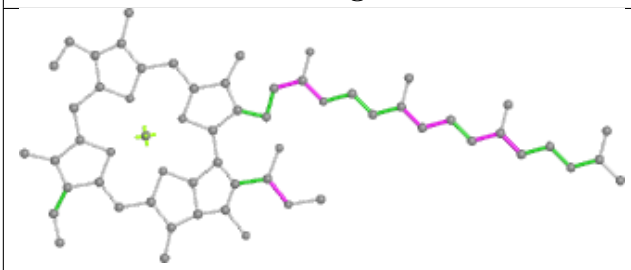
Ligand CLA G 612



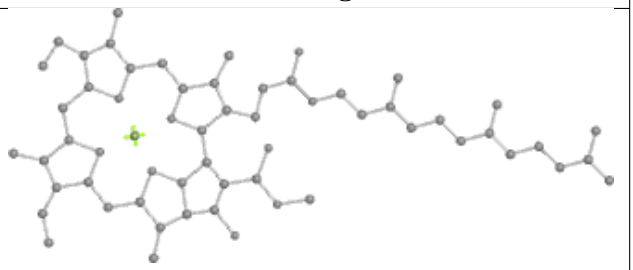
Bond lengths



Bond angles

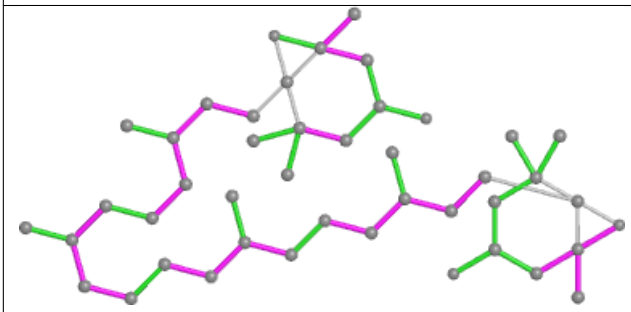


Torsions

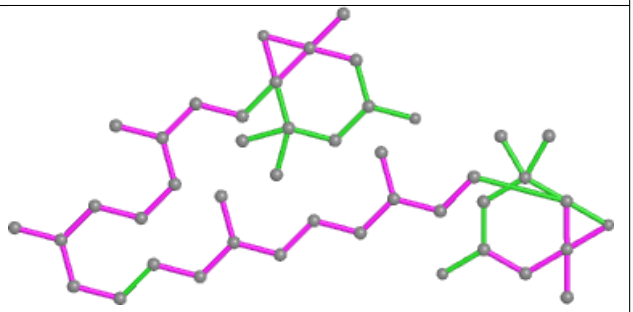


Rings

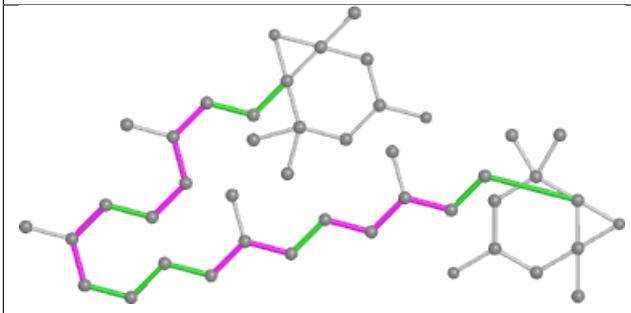
Ligand XAT n 615



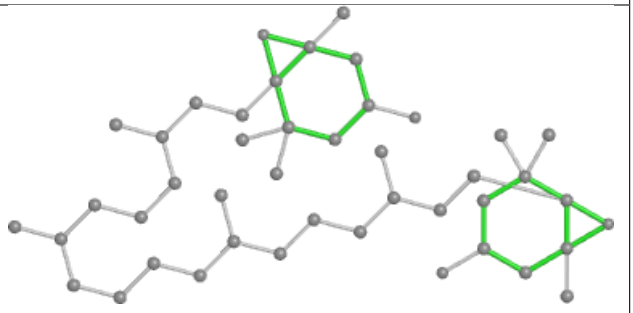
Bond lengths



Bond angles

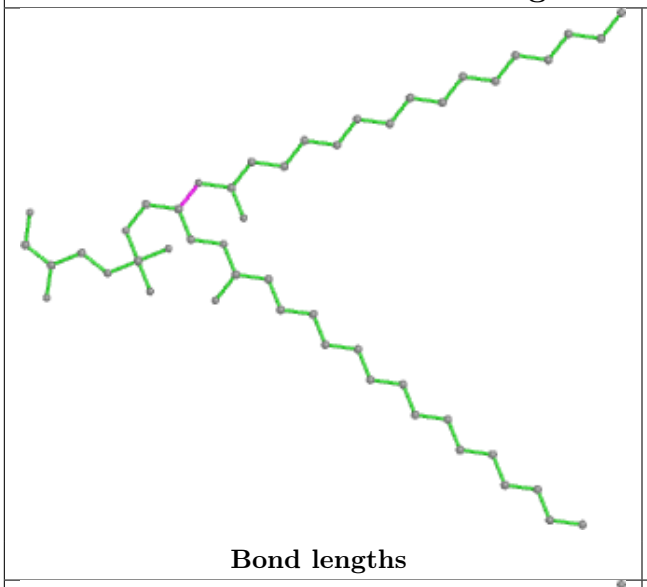


Torsions

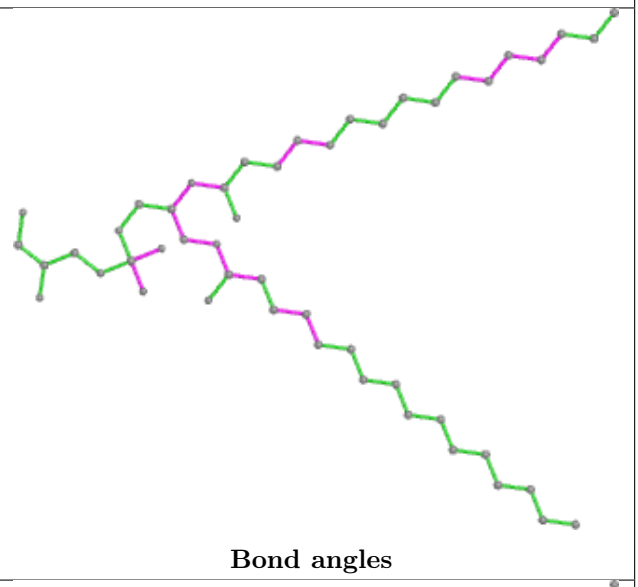


Rings

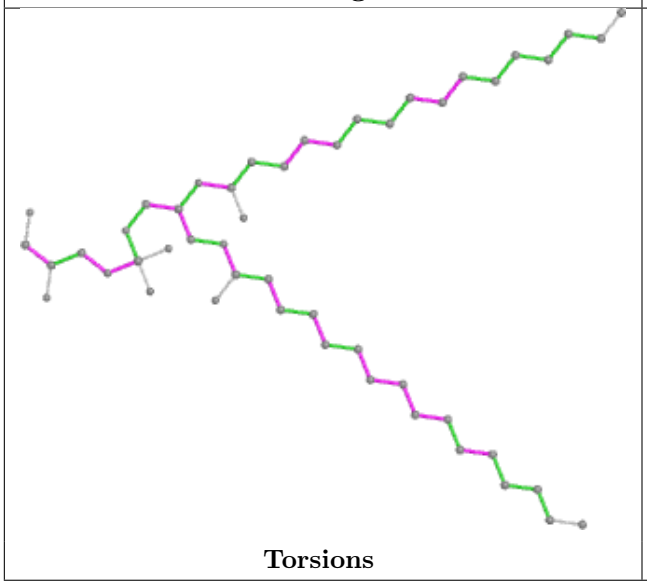
Ligand LHG c 522



Bond lengths



Bond angles



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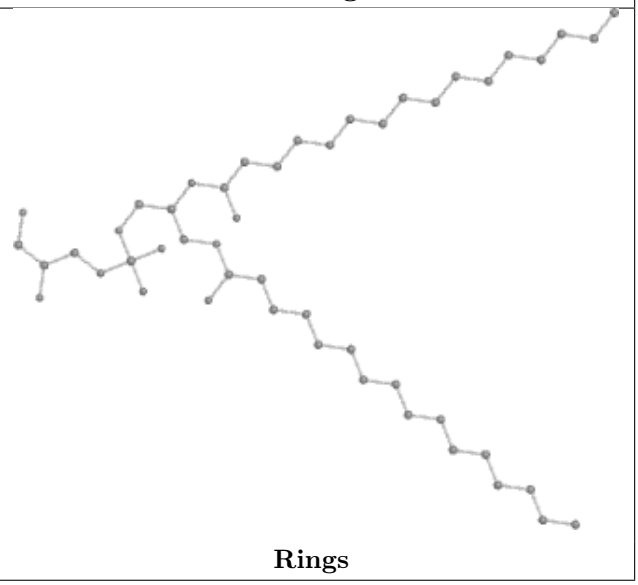
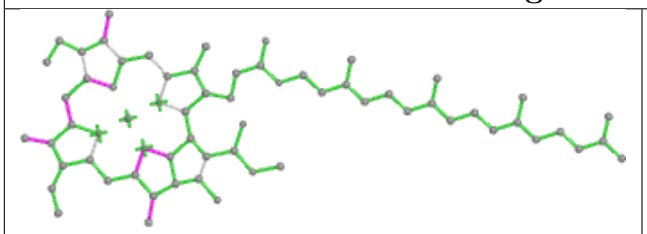


Rings

Ligand CLA B 616



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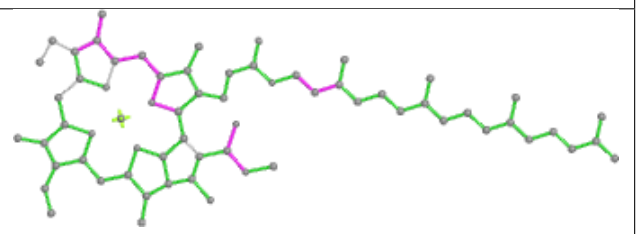
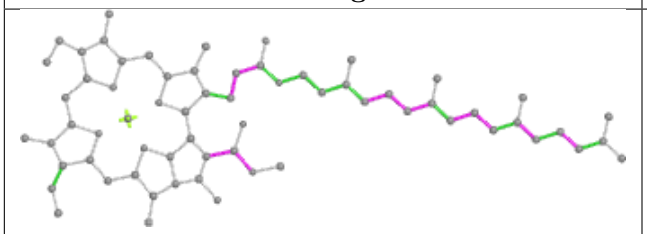
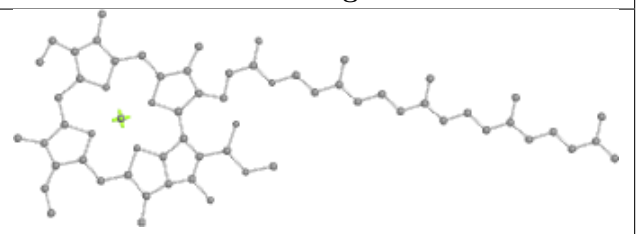


Bond angles

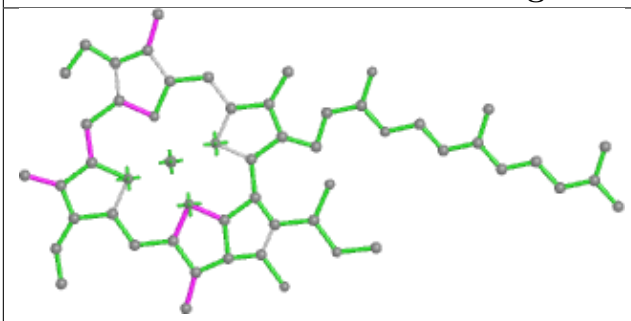


Torsions

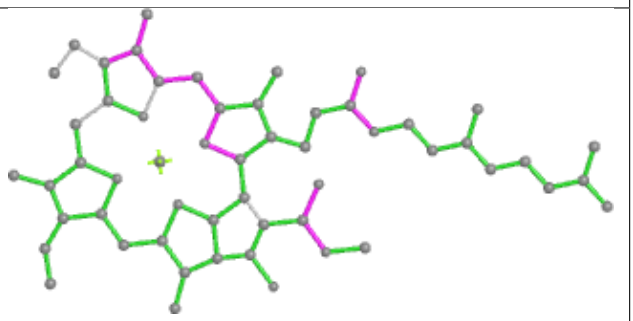


Rings

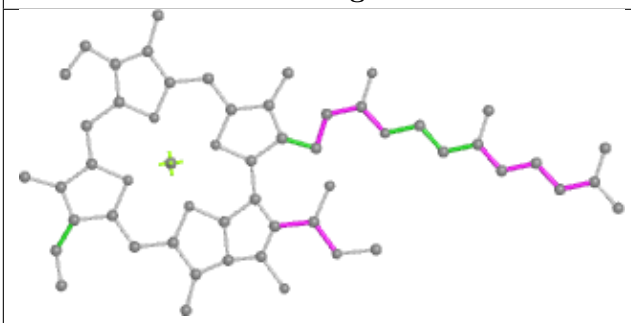
Ligand CLA S 310



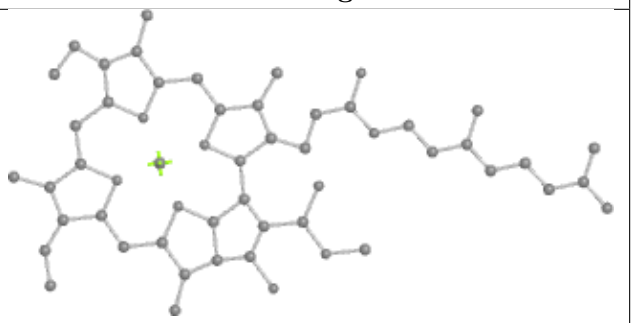
Bond lengths



Bond angles

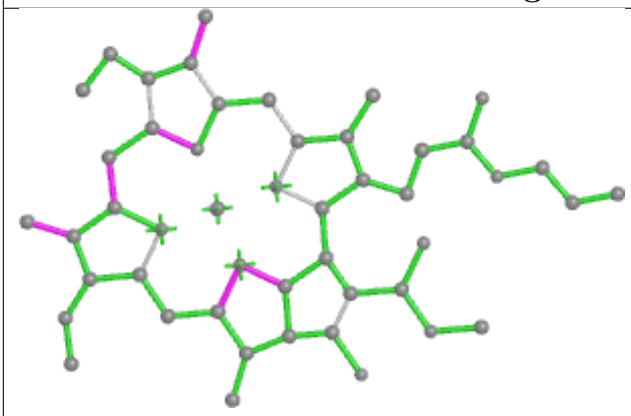


Torsions

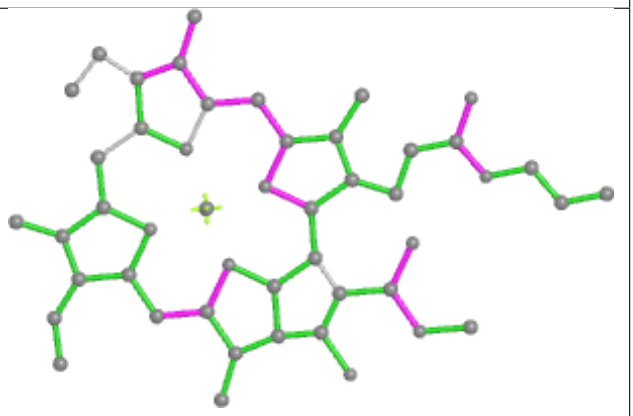


Rings

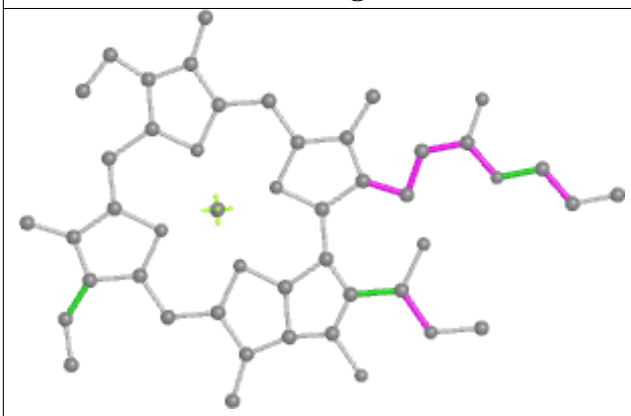
Ligand CLA Y 612



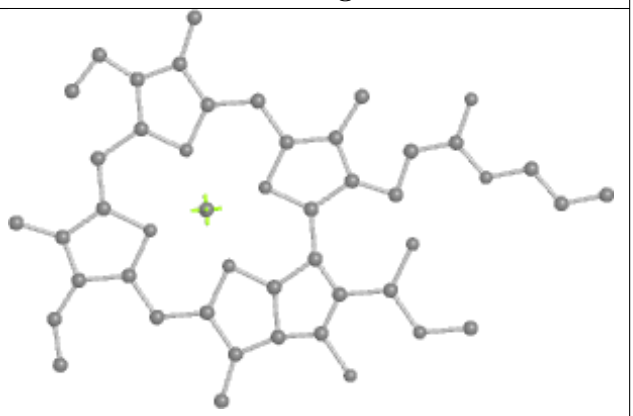
Bond lengths



Bond angles

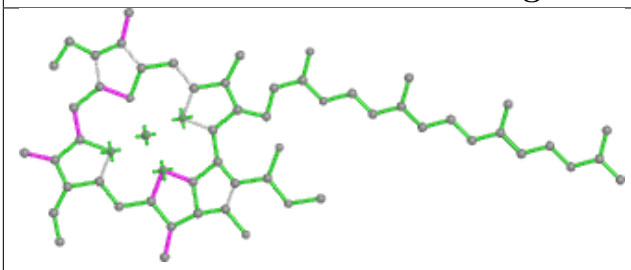


Torsions

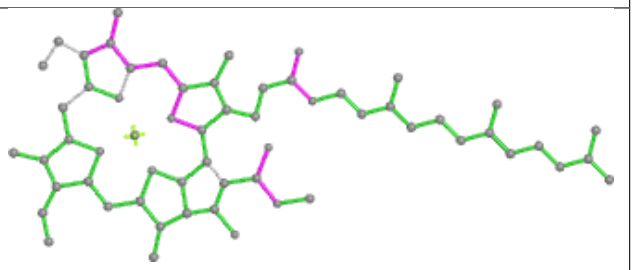


Rings

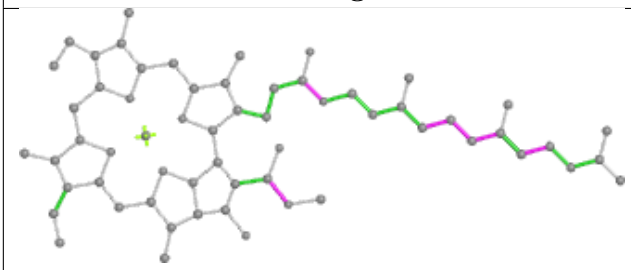
Ligand CLA G 611



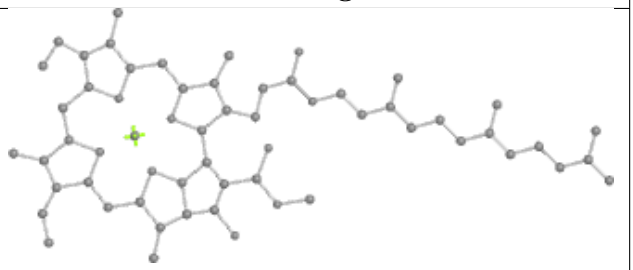
Bond lengths



Bond angles

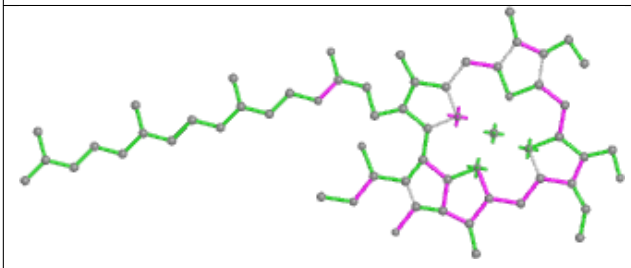


Torsions

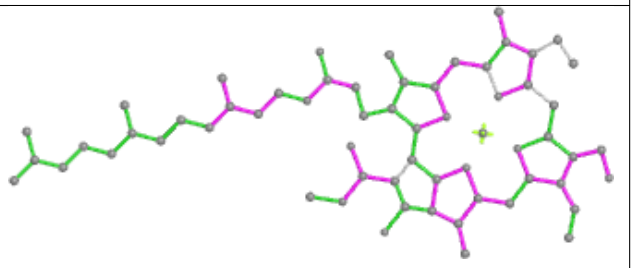


Rings

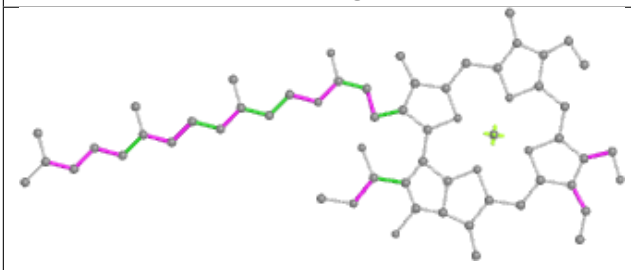
Ligand CHL R 307



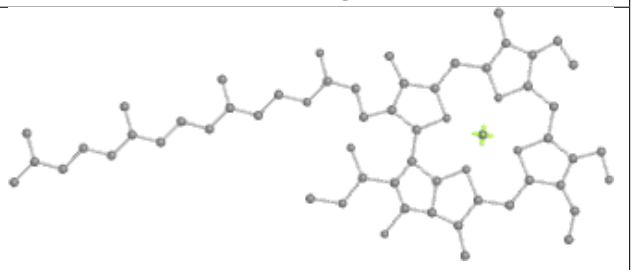
Bond lengths



Bond angles

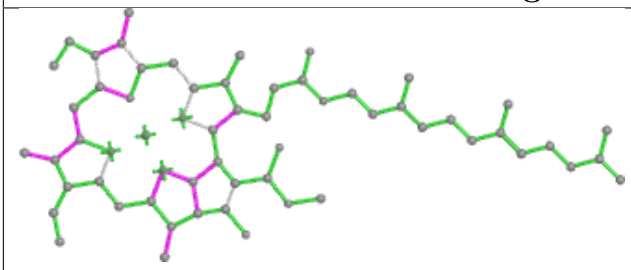


Torsions

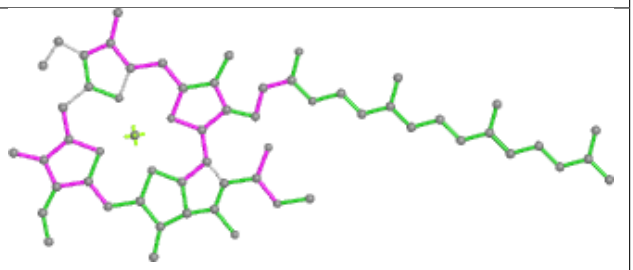


Rings

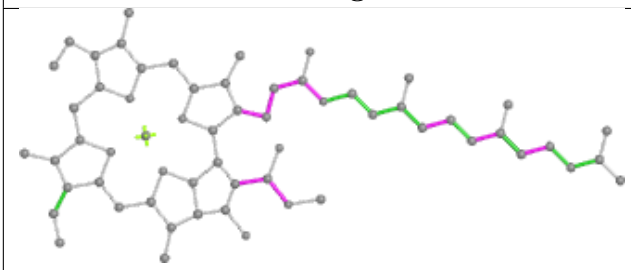
Ligand CLA N 612



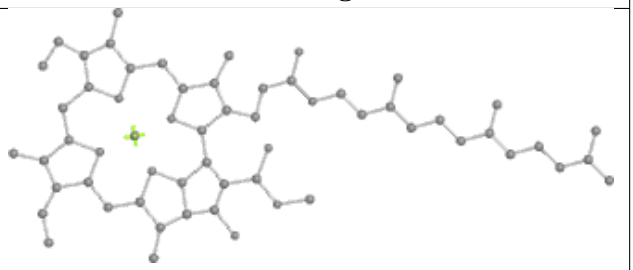
Bond lengths



Bond angles

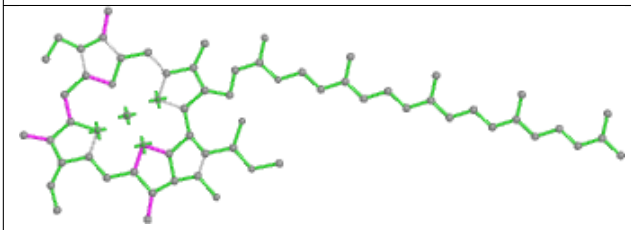


Torsions

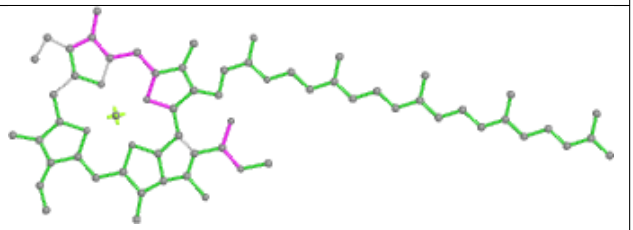


Rings

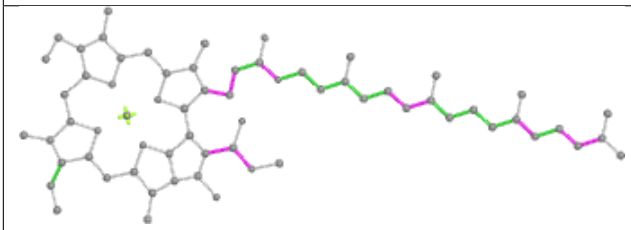
Ligand CLA B 614



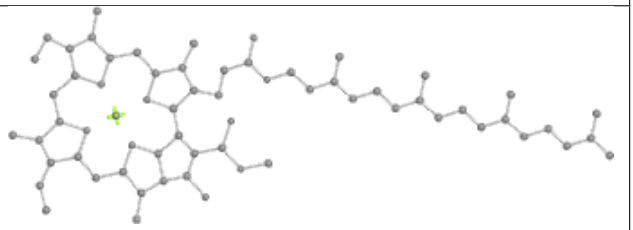
Bond lengths



Bond angles

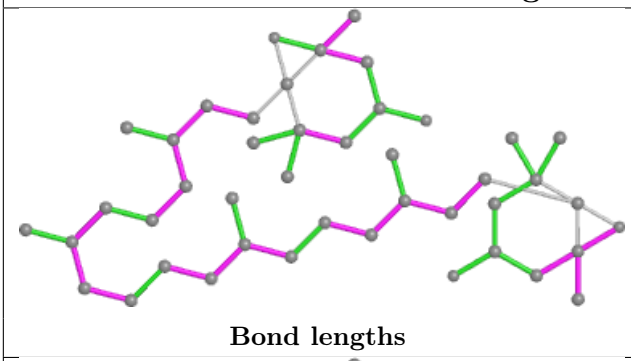


Torsions

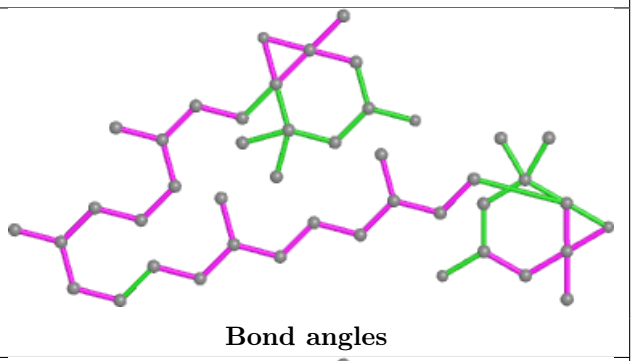


Rings

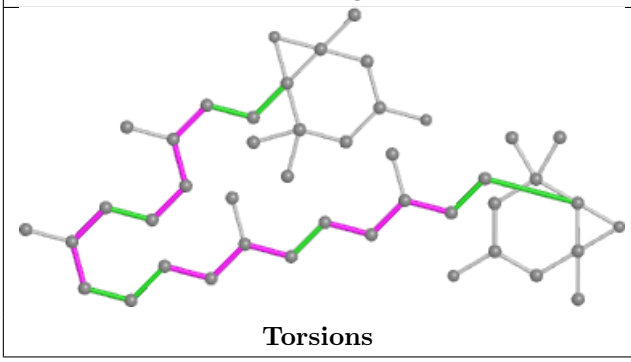
Ligand XAT G 617



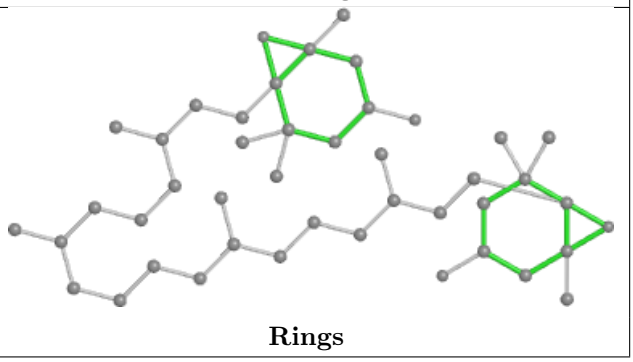
Bond lengths



Bond angles

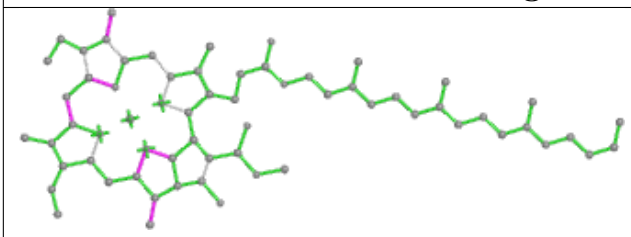


Torsions

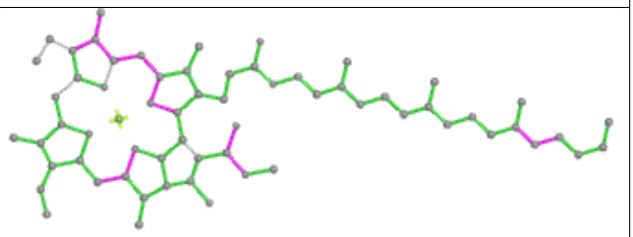


Rings

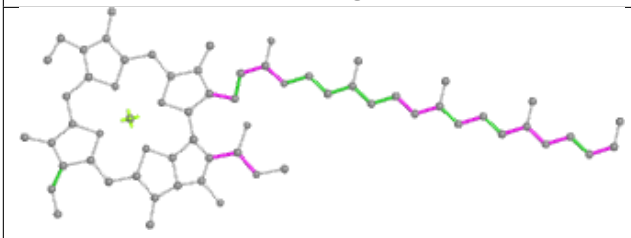
Ligand CLA G 610



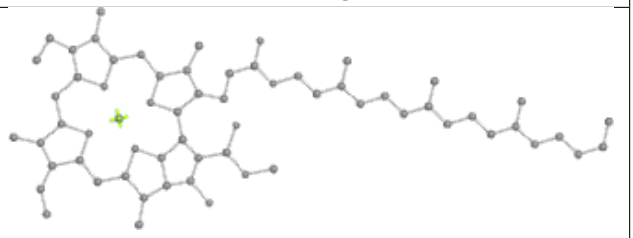
Bond lengths



Bond angles

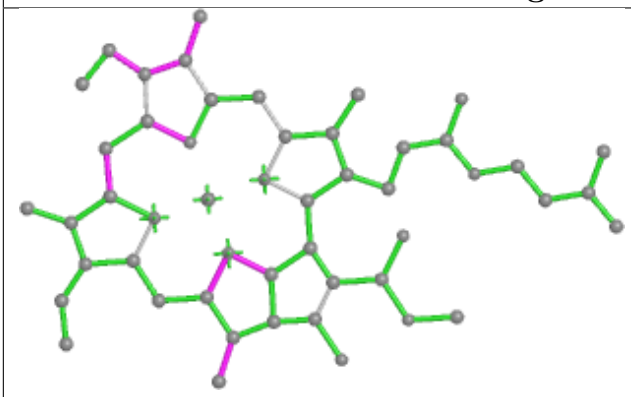


Torsions

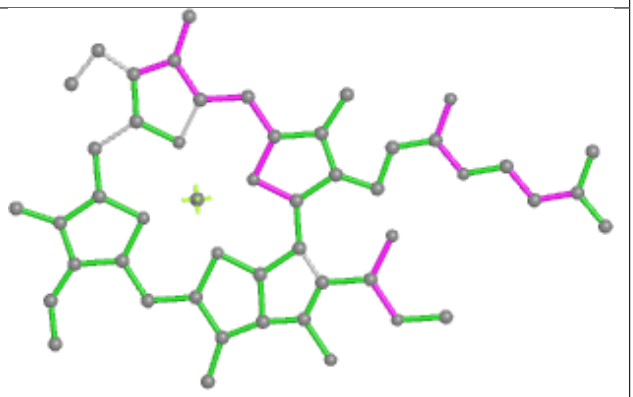


Rings

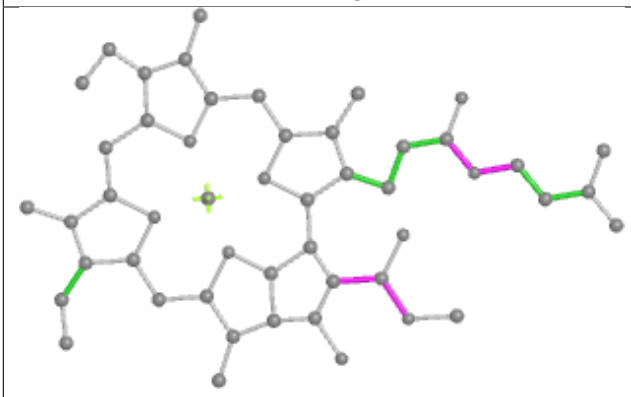
Ligand CLA n 604



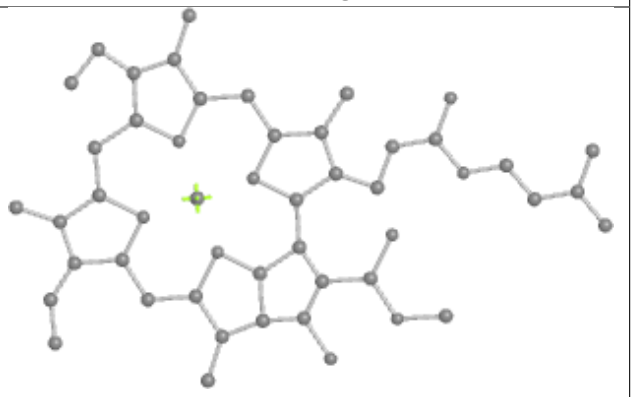
Bond lengths



Bond angles

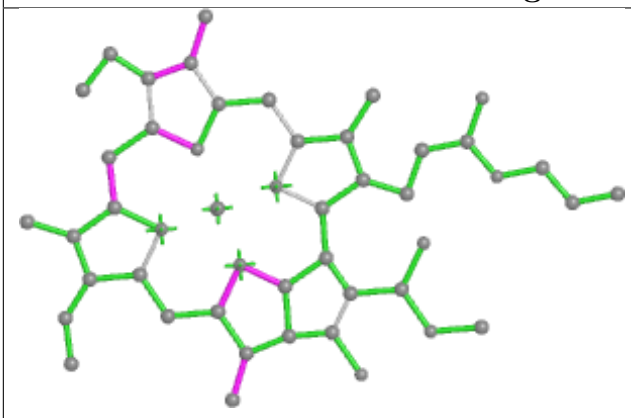


Torsions



Rings

Ligand CLA R 304



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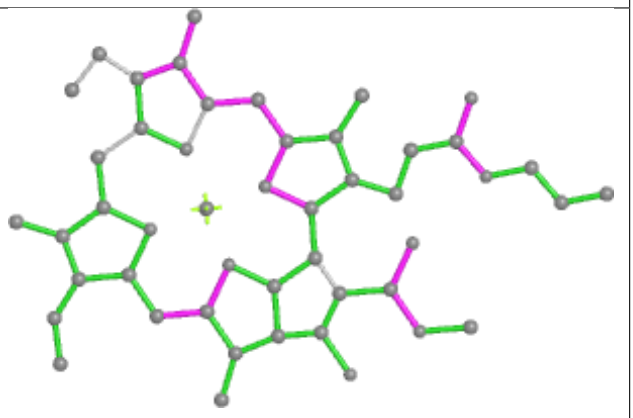
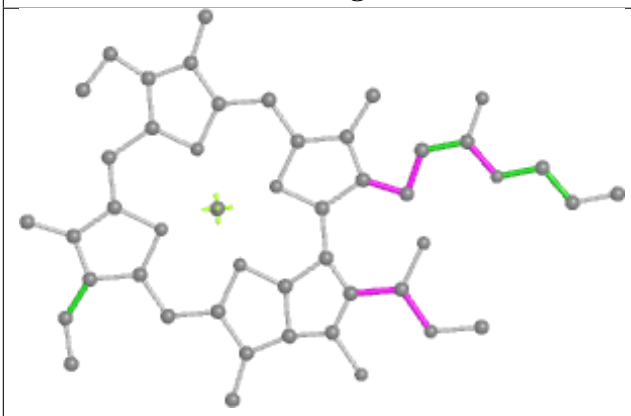
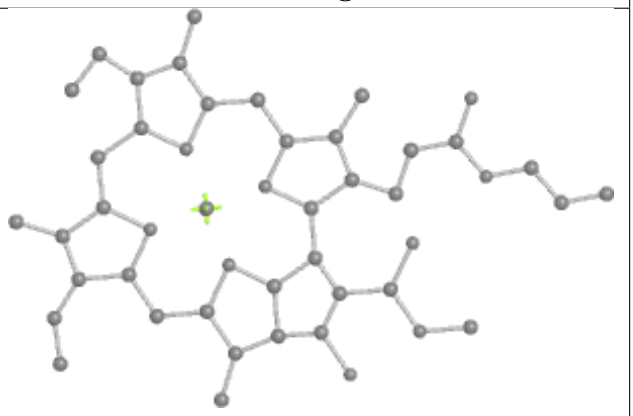


Bond angles

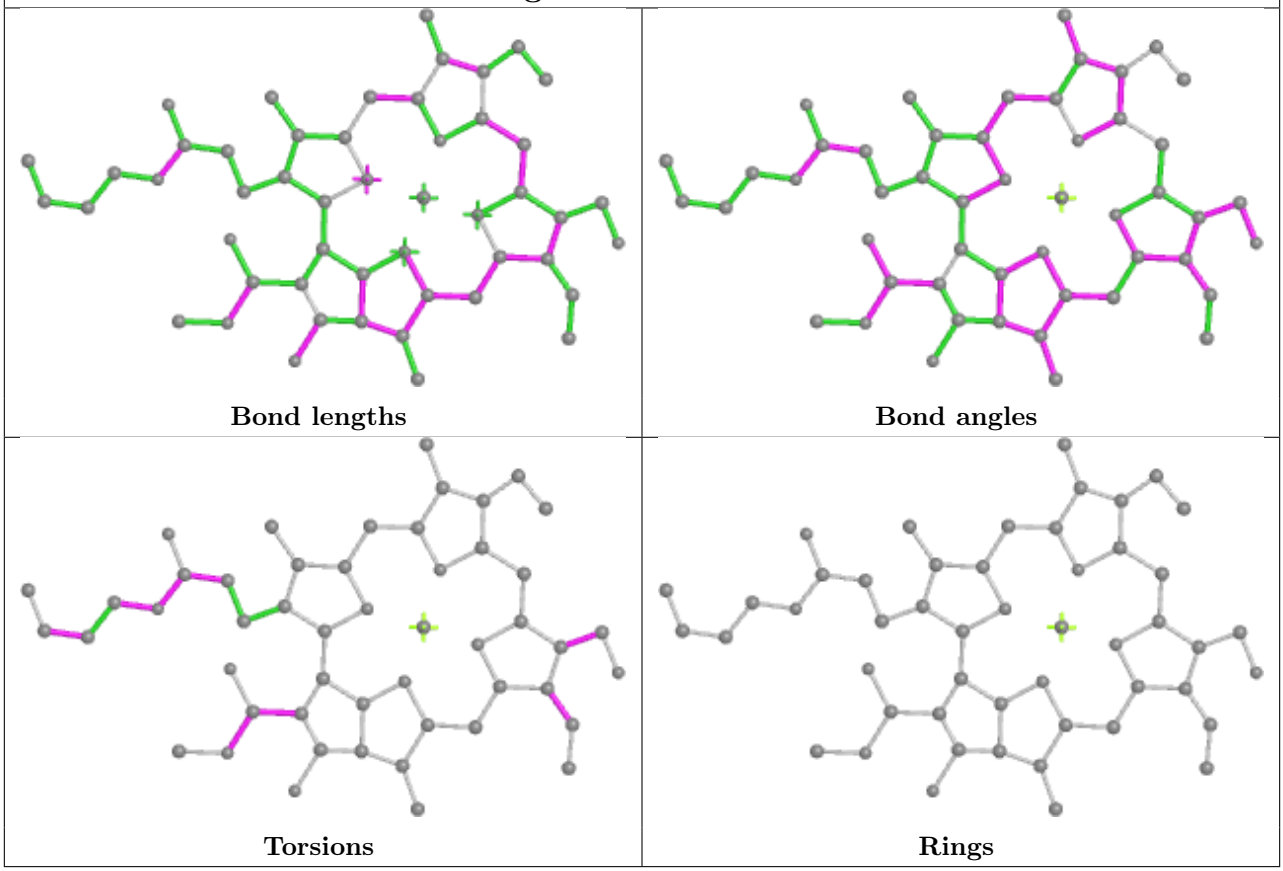


Torsions

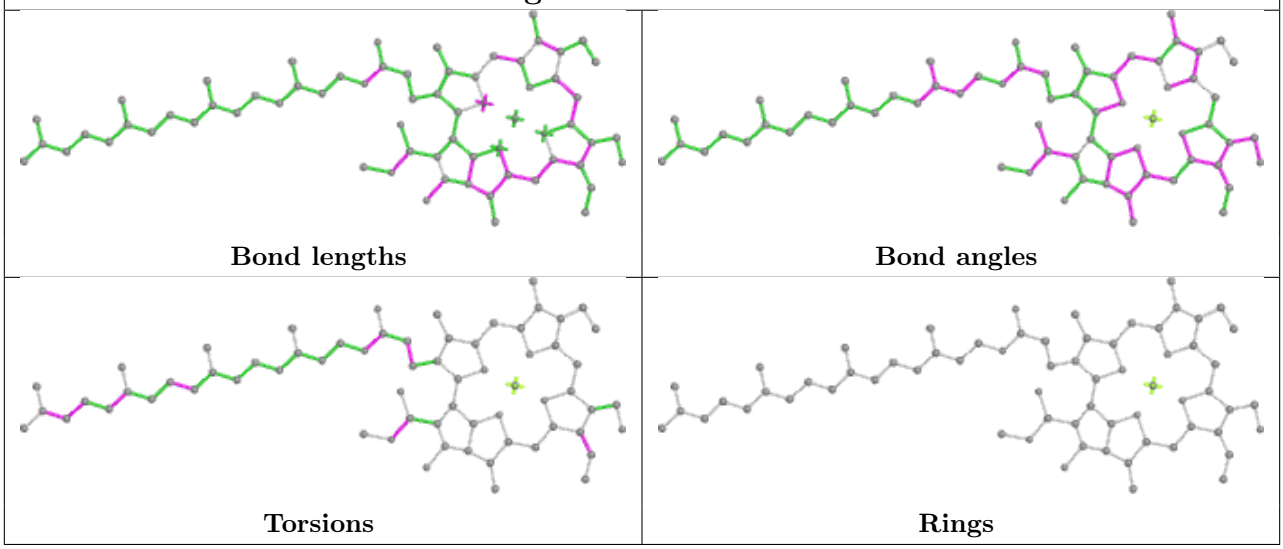


Rings

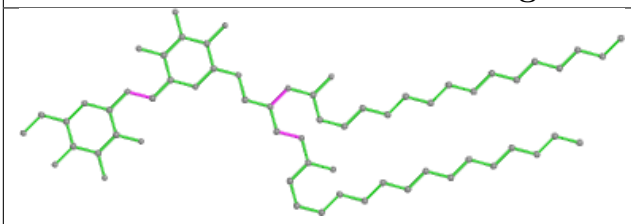
Ligand CHL Y 605



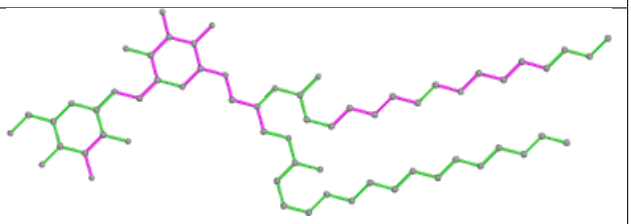
Ligand CHL Y 608



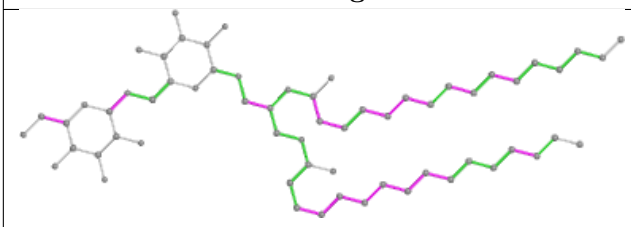
Ligand DGD H 102



Bond lengths



Bond angles



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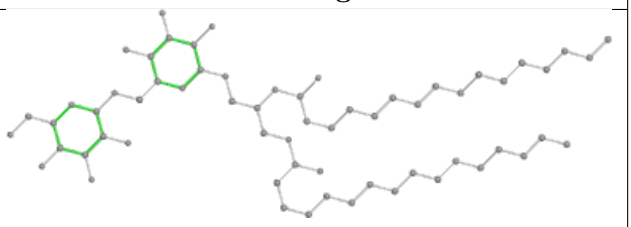
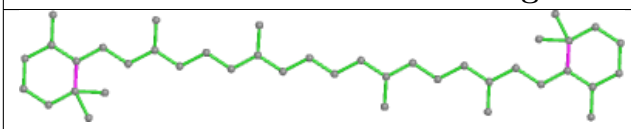
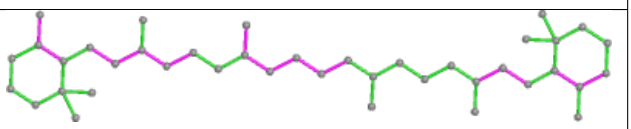


Rings

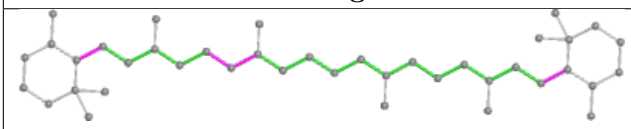
Ligand BCR K 102



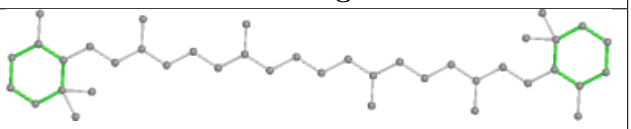
Bond lengths



Bond angles

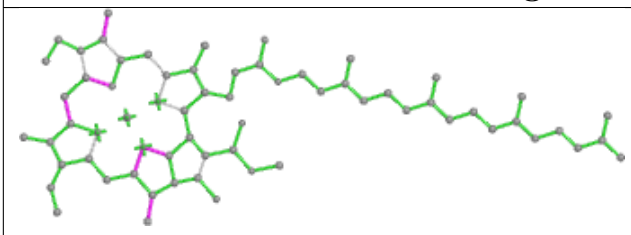


Torsions

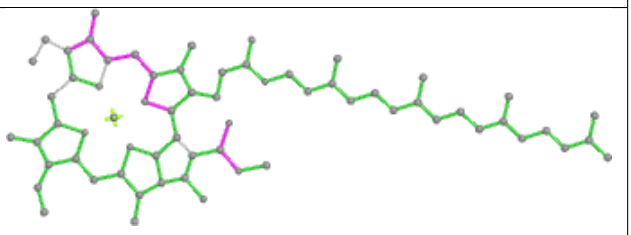


Rings

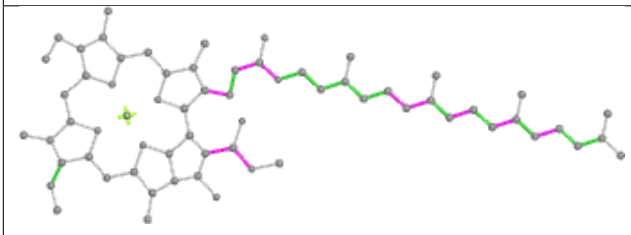
Ligand CLA N 609



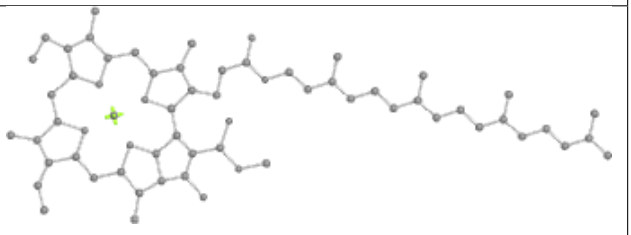
Bond lengths



Bond angles

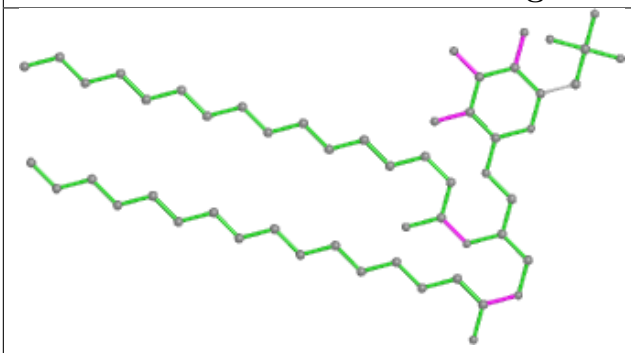


Torsions

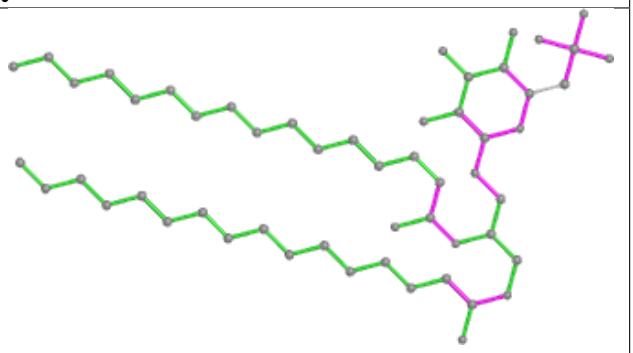


Rings

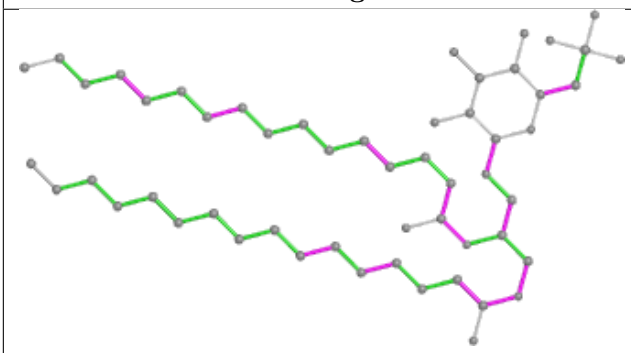
Ligand SQD L 101



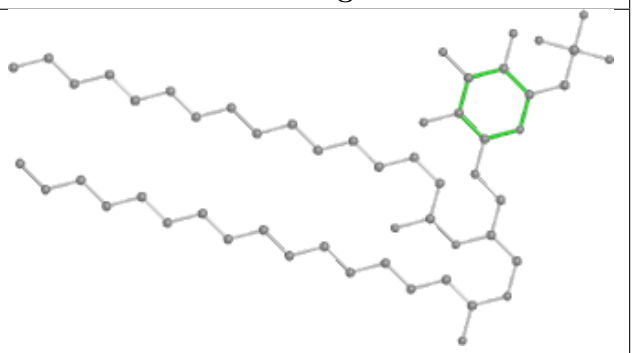
Bond lengths



Bond angles

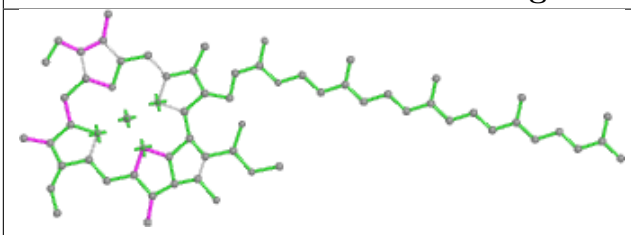


Torsions

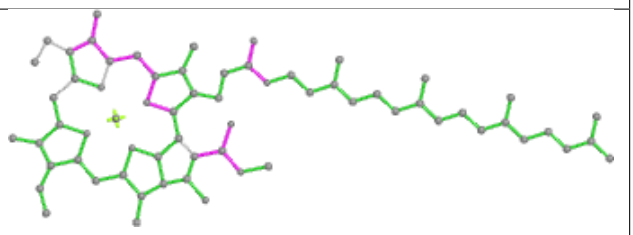


Rings

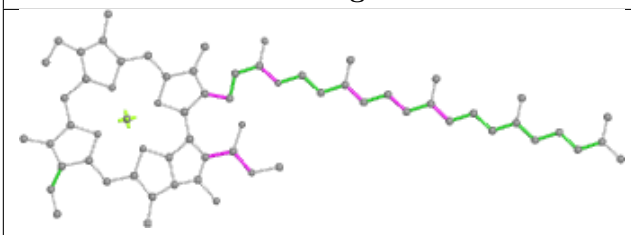
Ligand CLA c 509



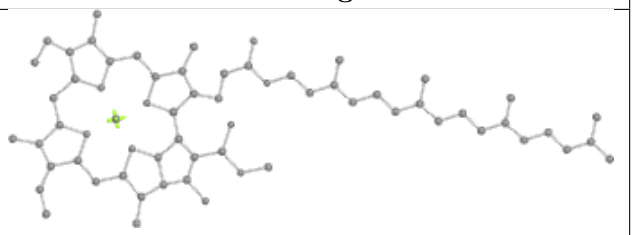
Bond lengths



Bond angles

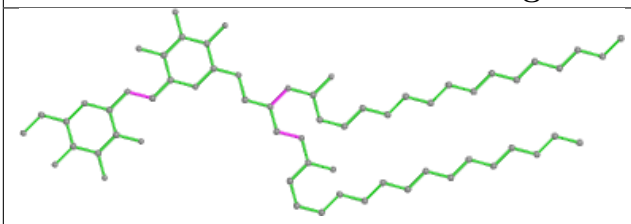


Torsions

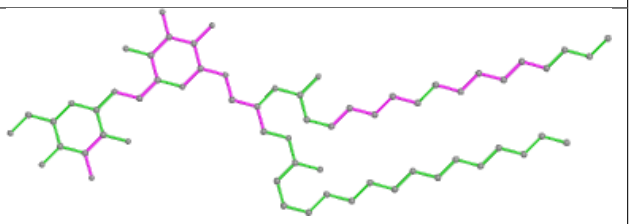


Rings

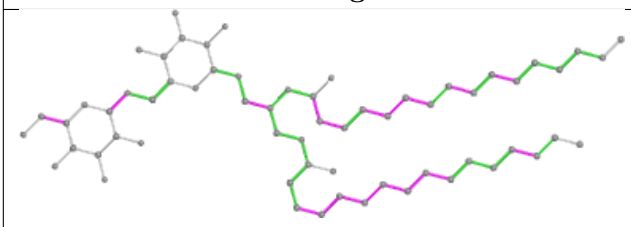
Ligand DGD h 102



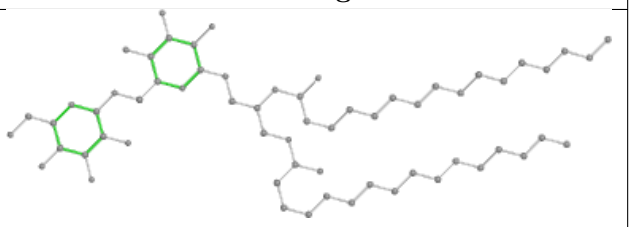
Bond lengths



Bond angles

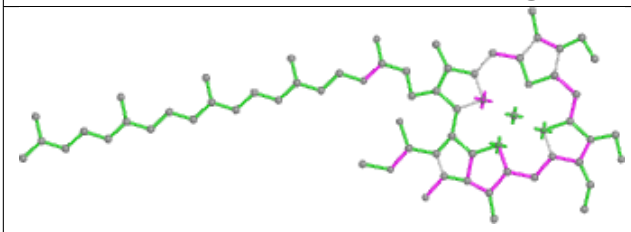


Torsions

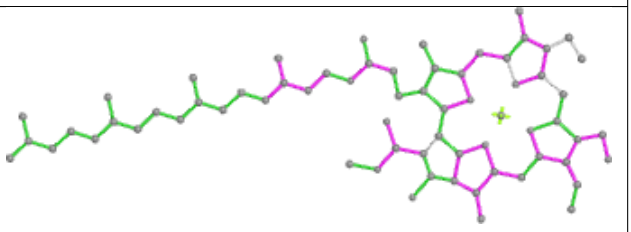


Rings

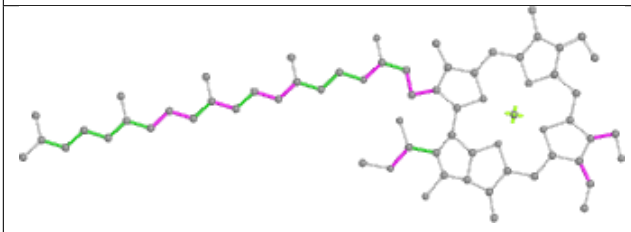
Ligand CHL G 607



Bond lengths



Bond angles



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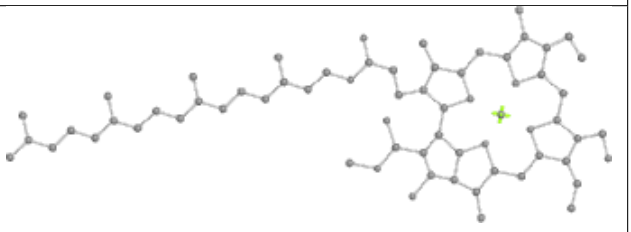
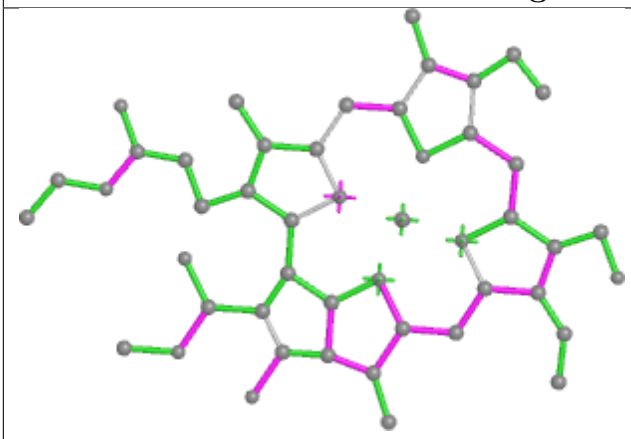


Rings

Ligand CHL r 301



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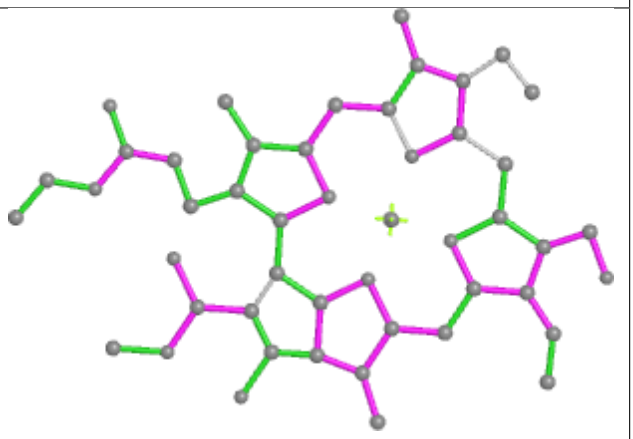
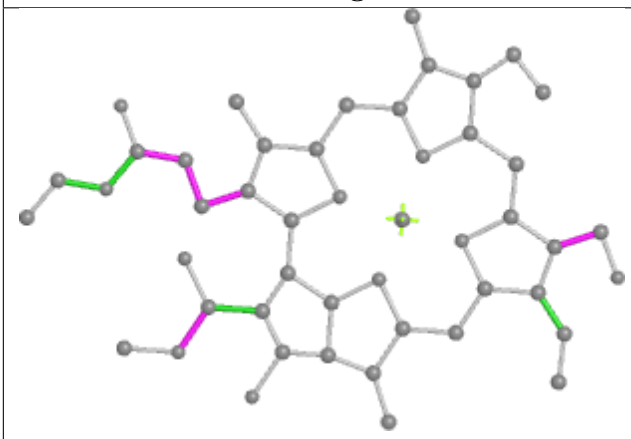


Bond angles



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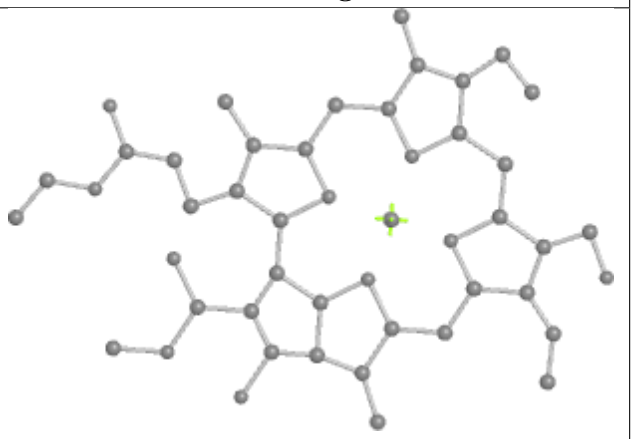
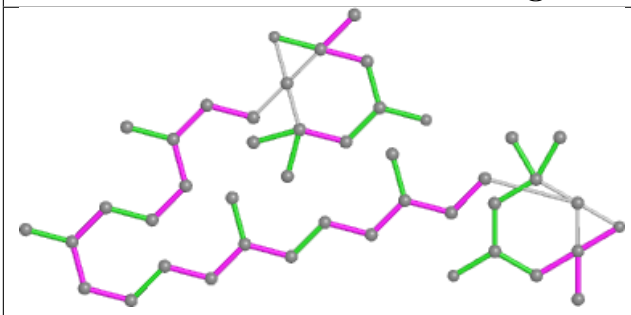
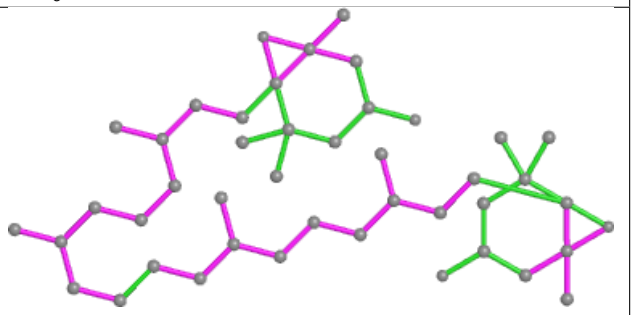


Rings

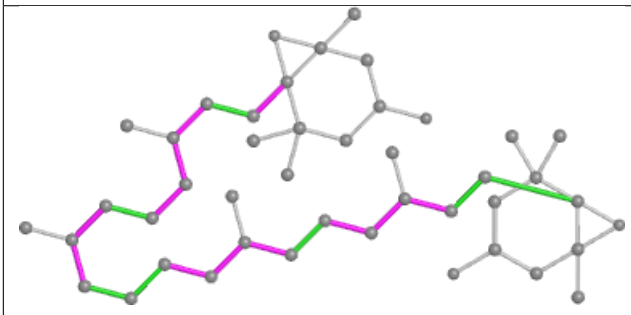
Ligand XAT y 615



Bond lengths



Bond angles



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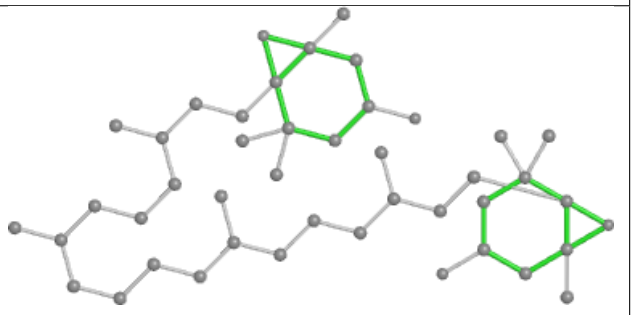
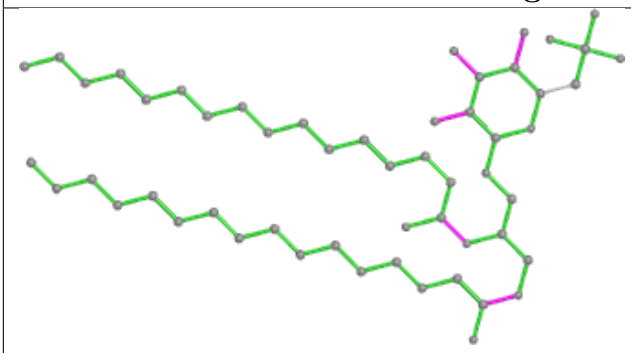
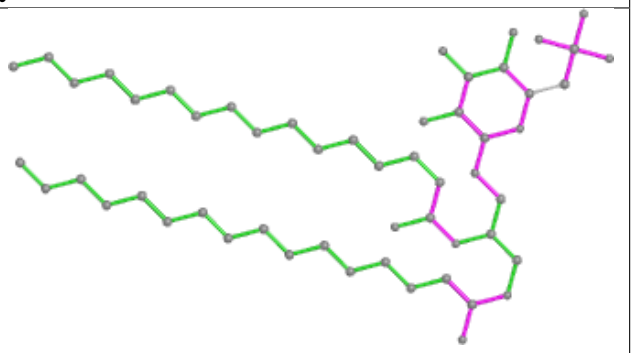


Rings

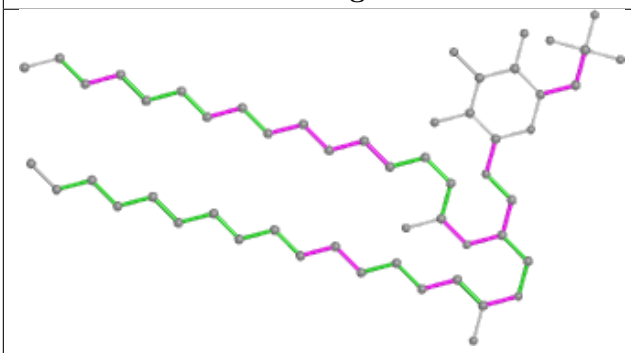
Ligand SQD A 412



Bond lengths



Bond angles



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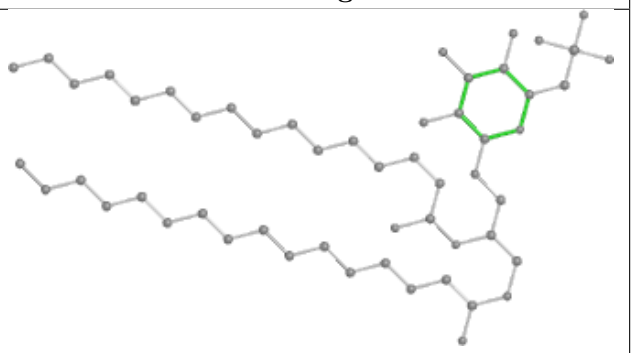
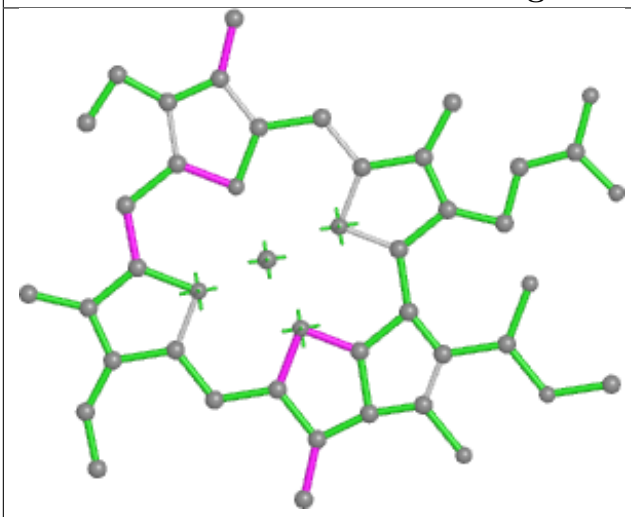
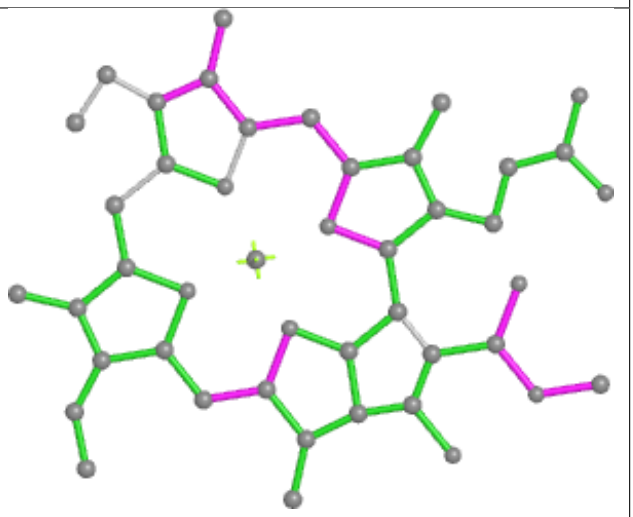


Rings

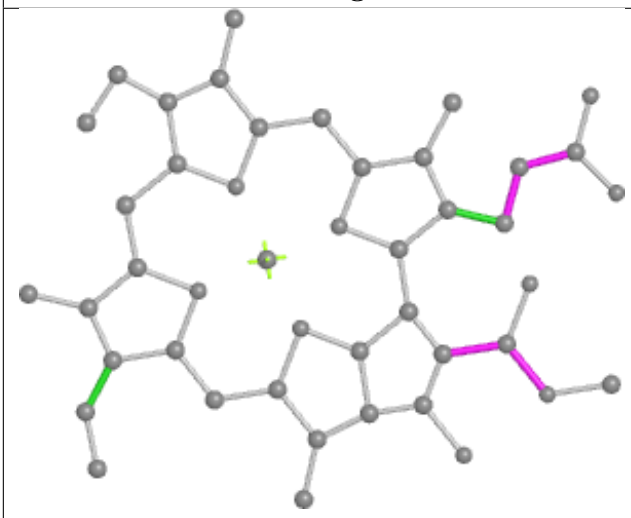
Ligand CLA S 308



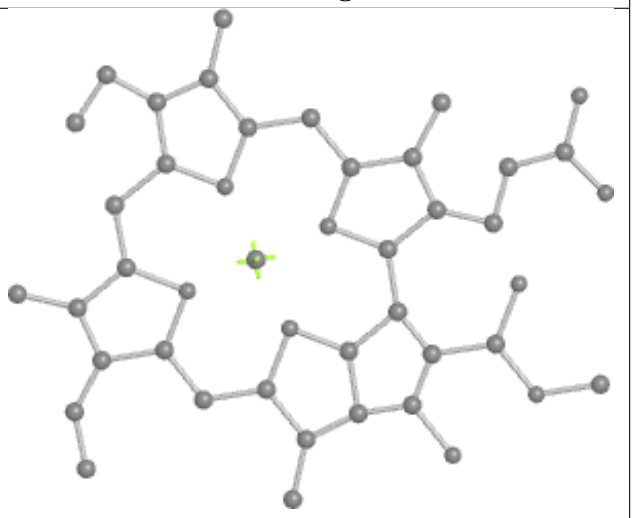
Bond lengths



Bond angles

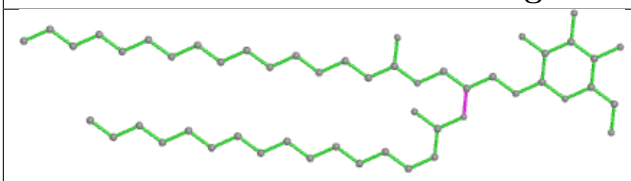


Torsions

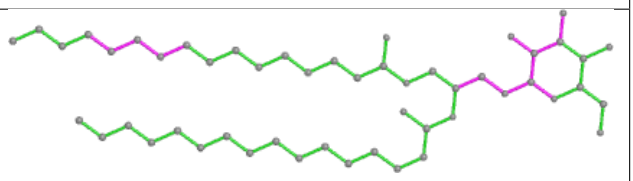


Rings

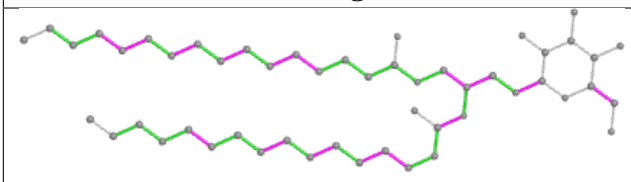
Ligand LMG c 523



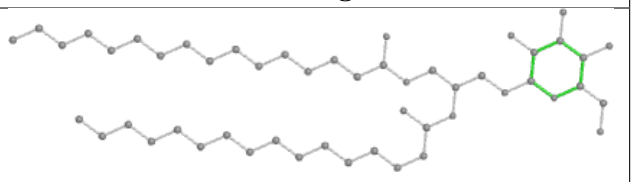
Bond lengths



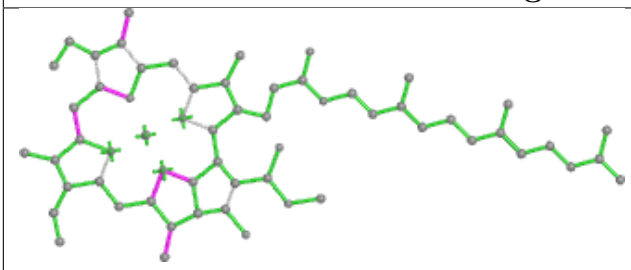
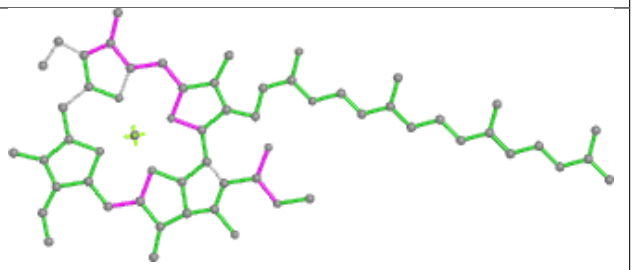
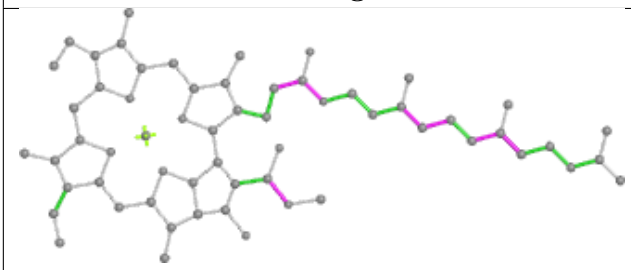
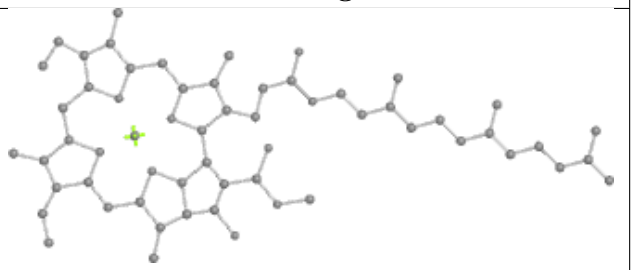
Bond angles

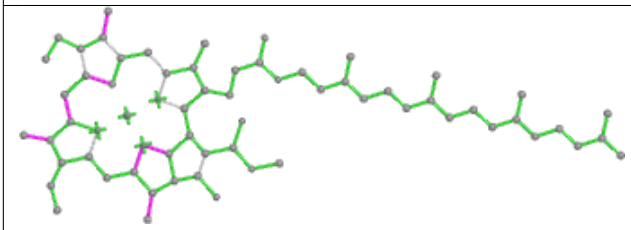
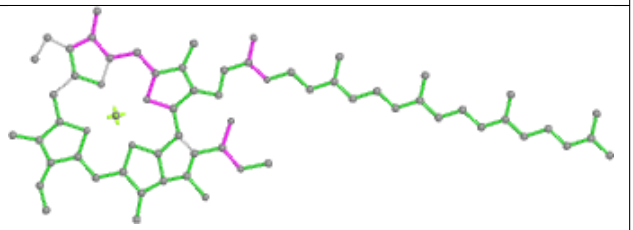
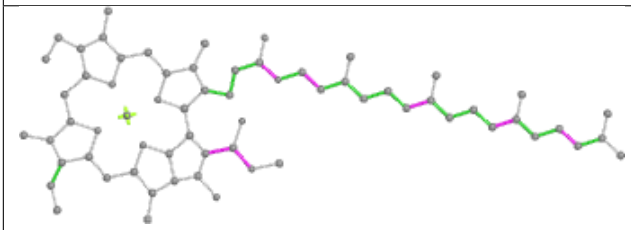
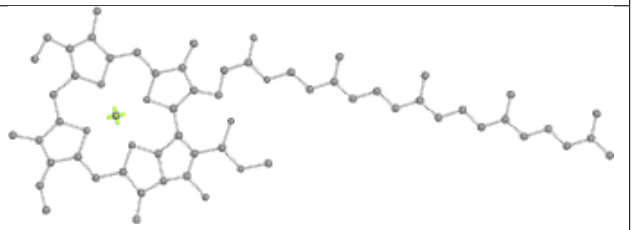


Torsions

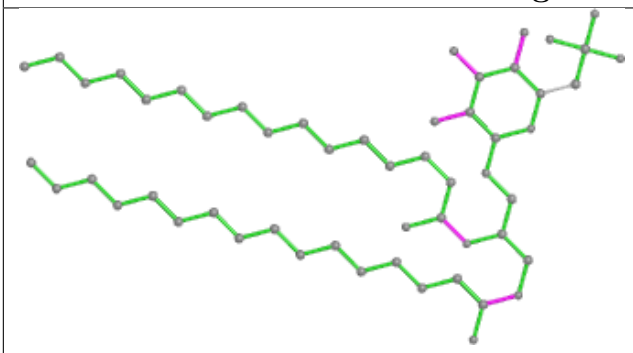


Rings

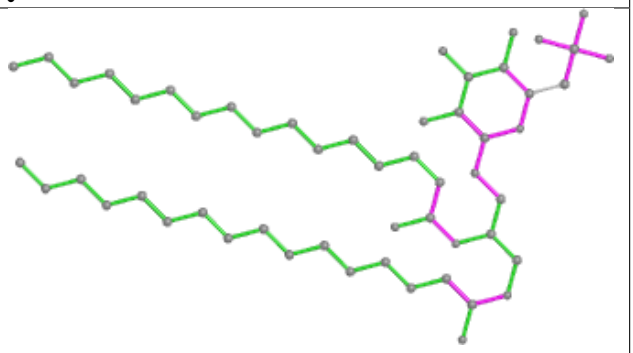
Ligand CLA w 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

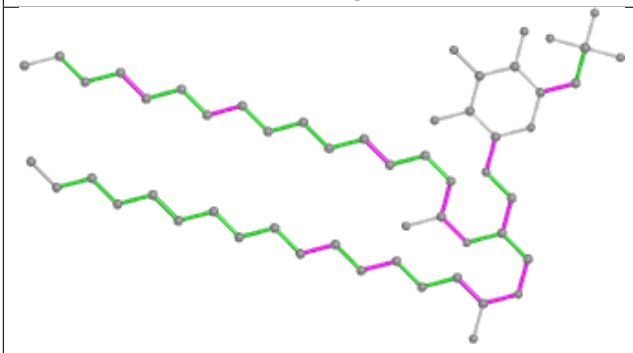
Ligand SQD l 103



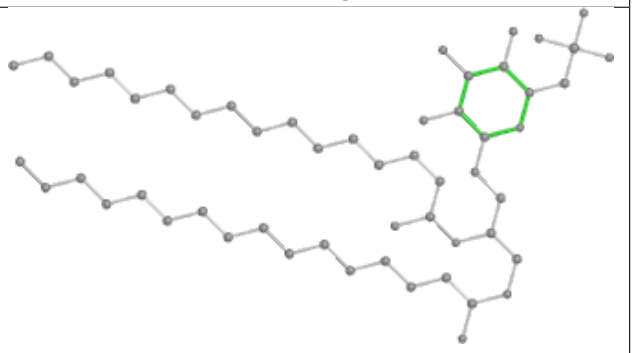
Bond lengths



Bond angles

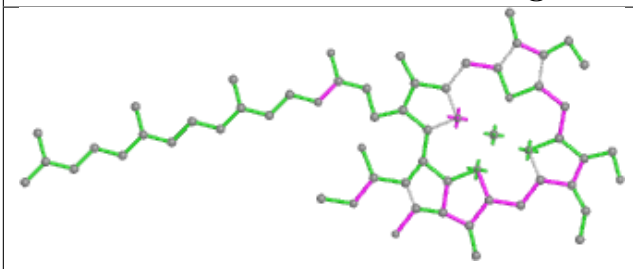


Torsions

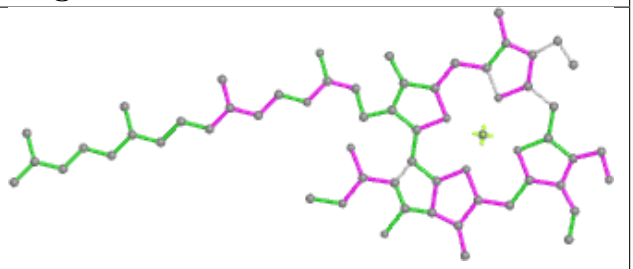


Rings

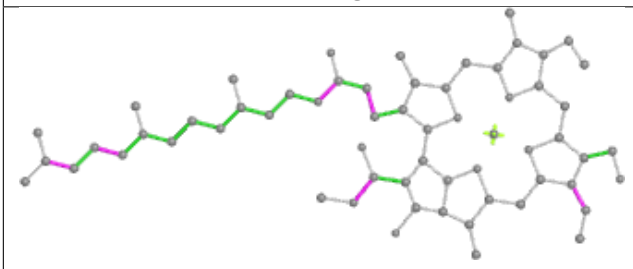
Ligand CHL g 609



Bond lengths



Bond angles



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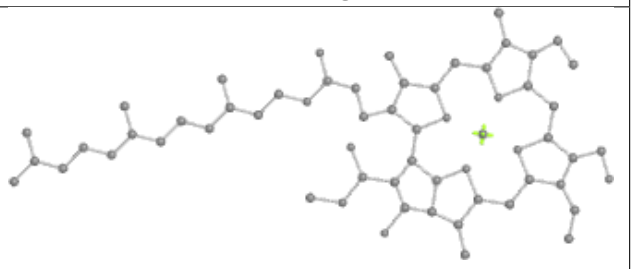
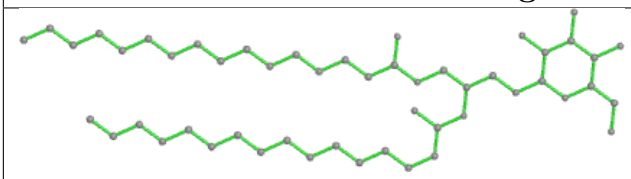
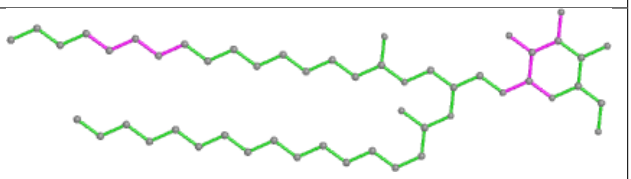


Rings

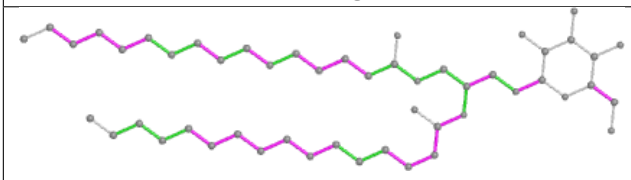
Ligand LMG K 103



Bond lengths



Bond angles



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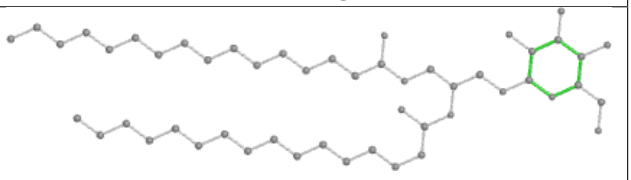
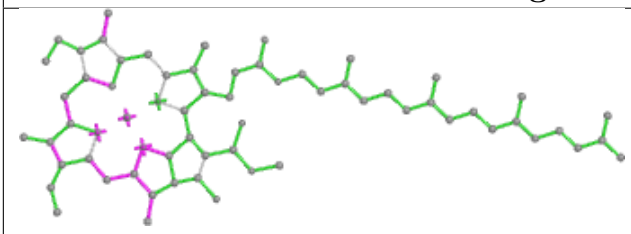


Rings

Ligand CLA c 510



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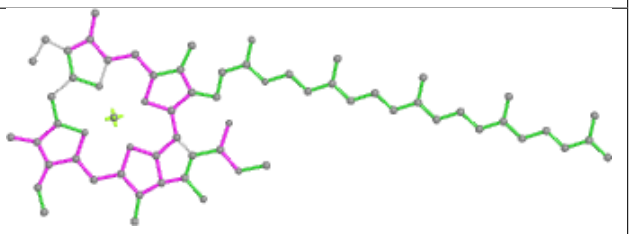
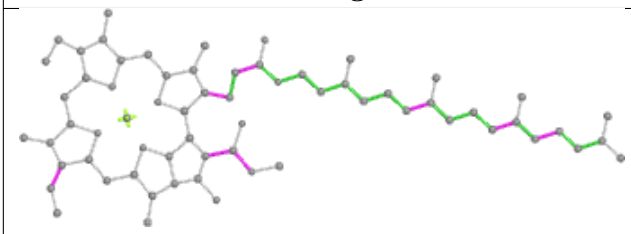


Bond angles



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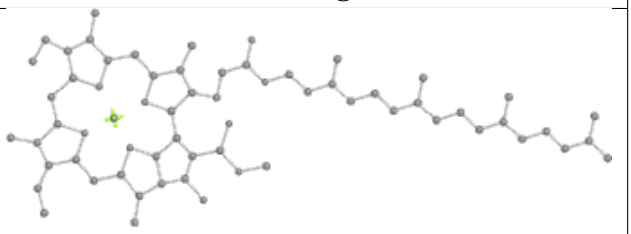
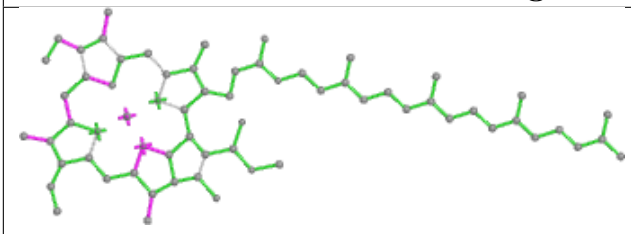


Rings

Ligand CLA b 604



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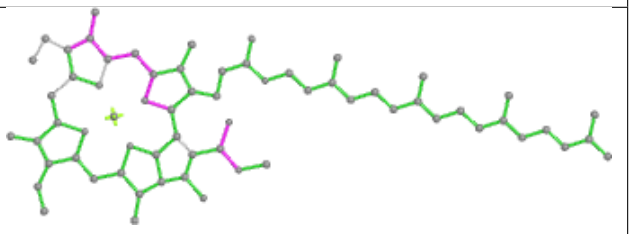
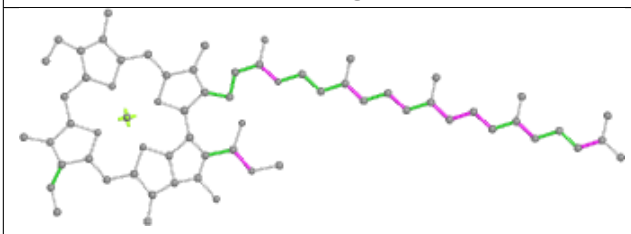


Bond angles



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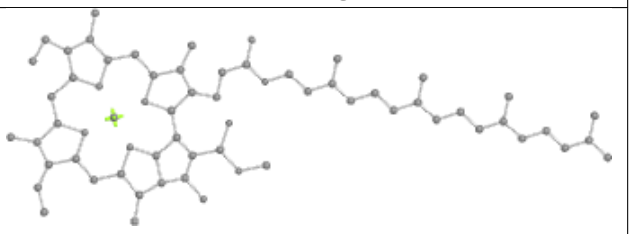
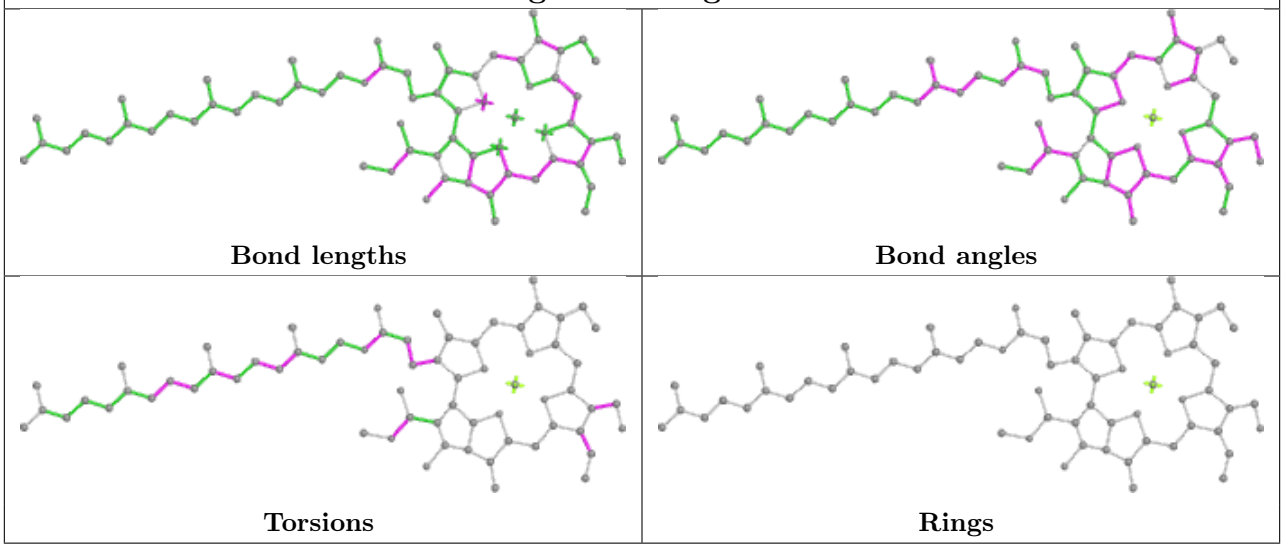


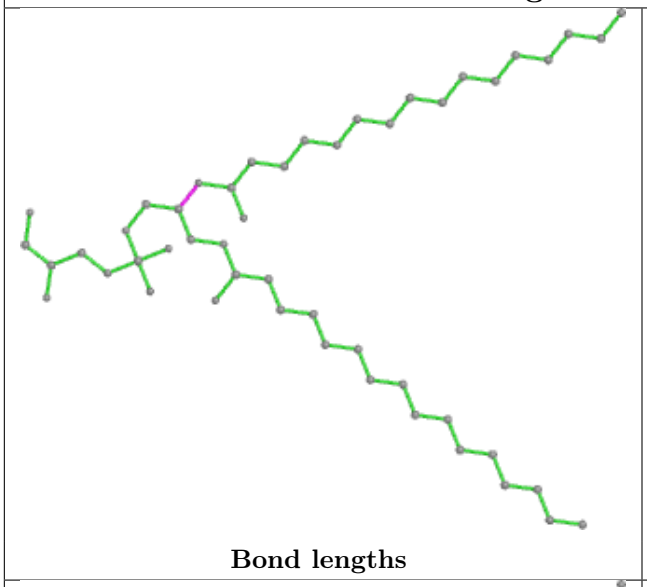
Rings

Ligand LUT G 615

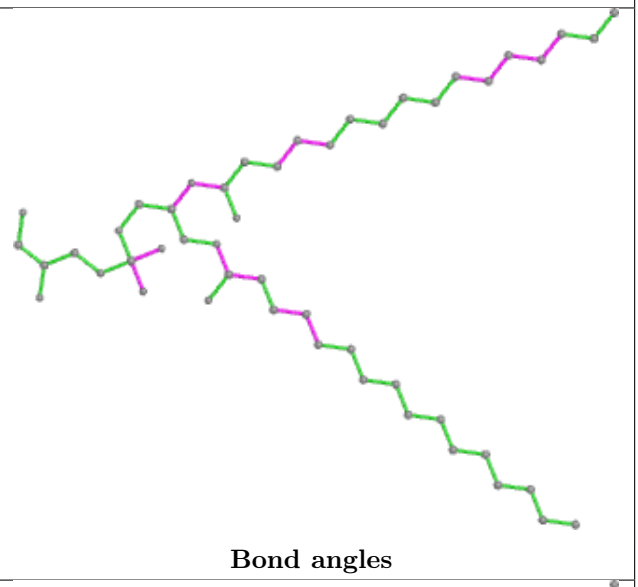
Ligand CHL g 607



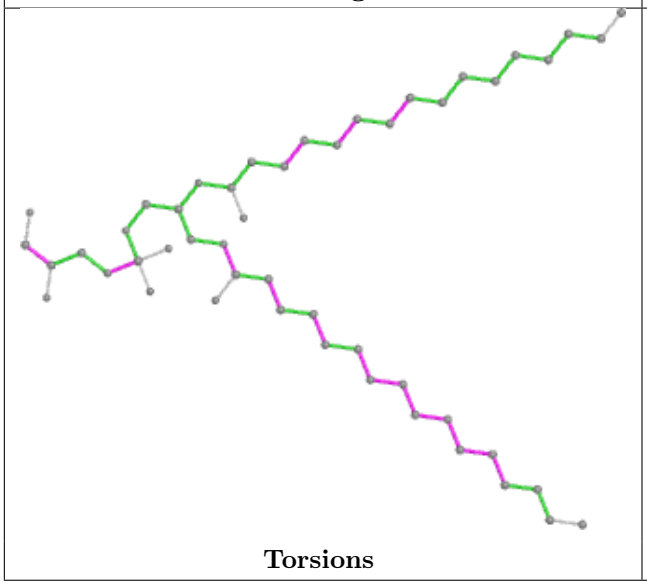
Ligand LHG L 103



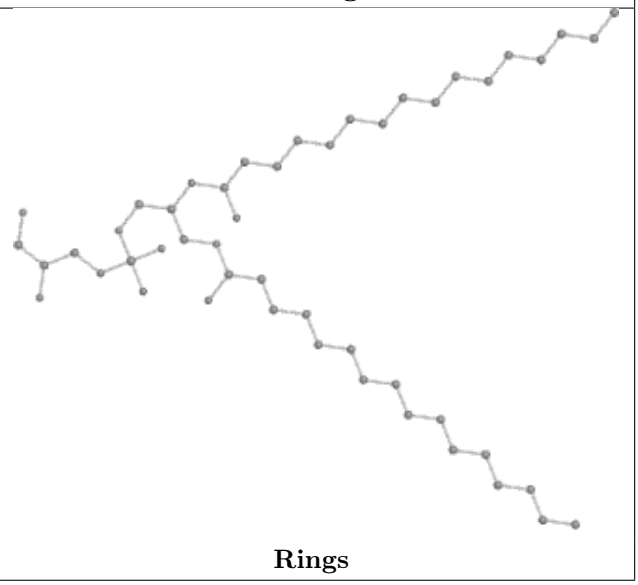
Bond lengths



Bond angles

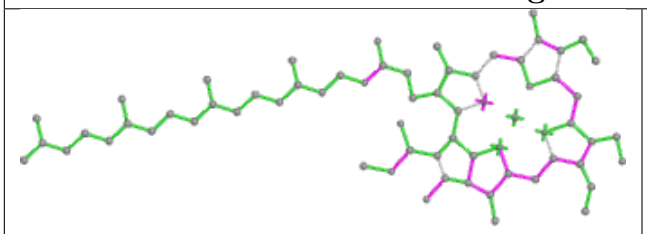


Torsions

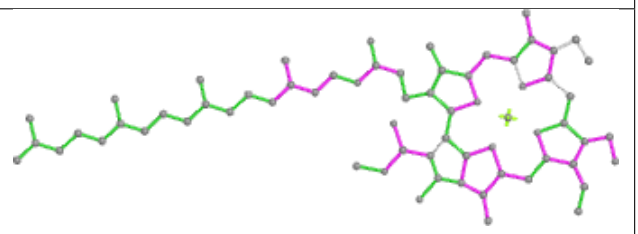


Rings

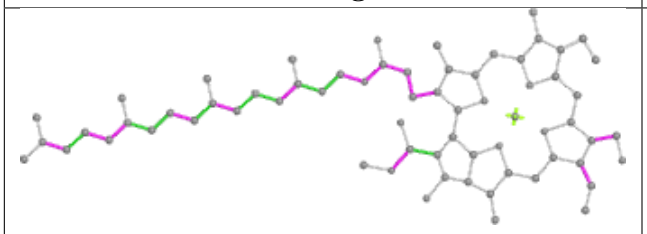
Ligand CHL n 601



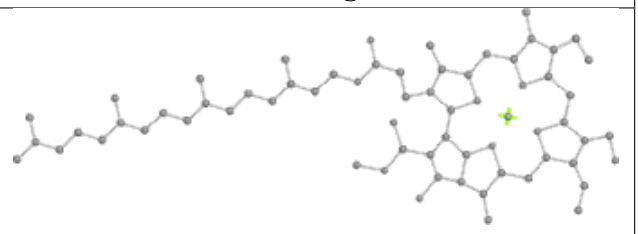
Bond lengths



Bond angles

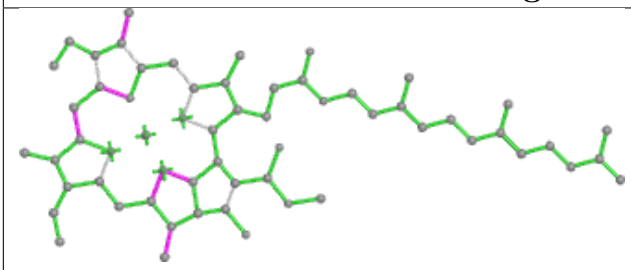


Torsions

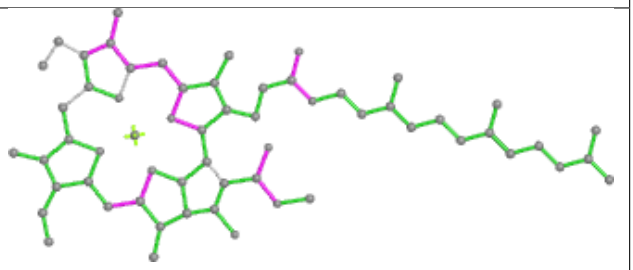


Rings

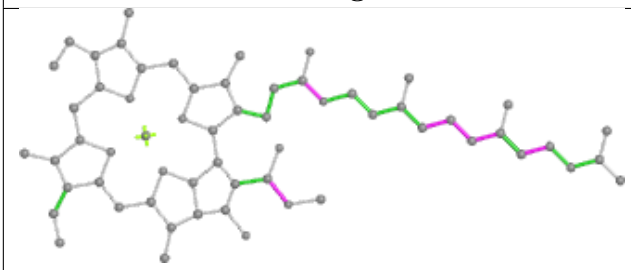
Ligand CLA N 610



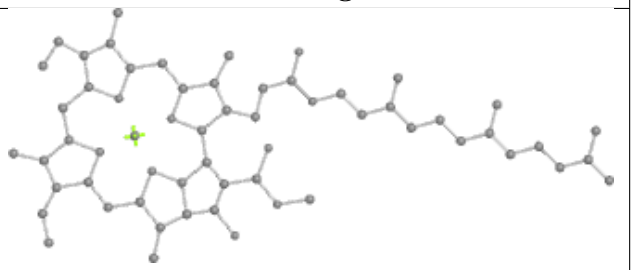
Bond lengths



Bond angles

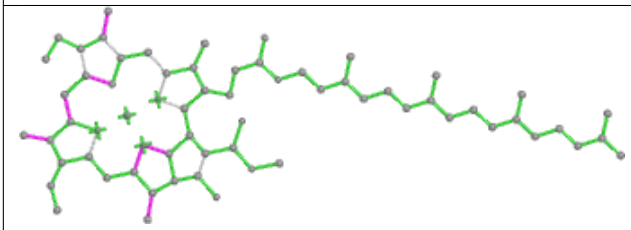


Torsions



Rings

Ligand CLA B 611



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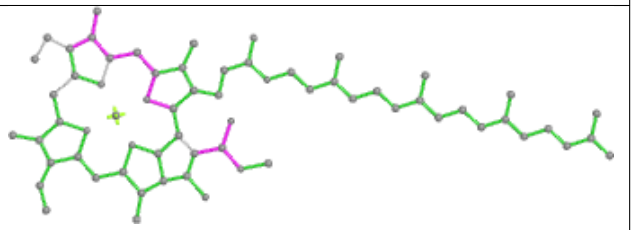
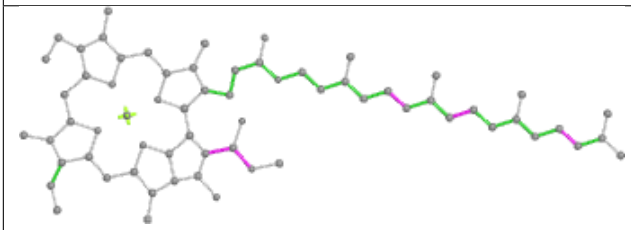
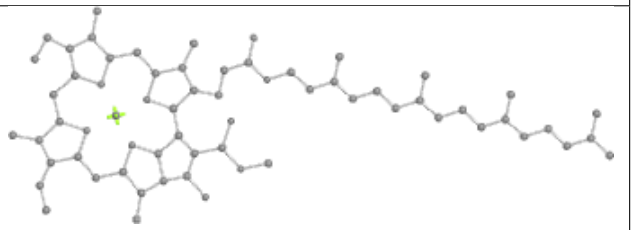


Bond angles

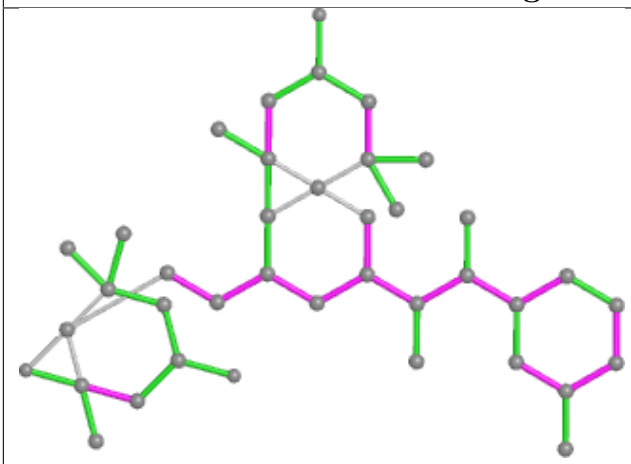


Torsions

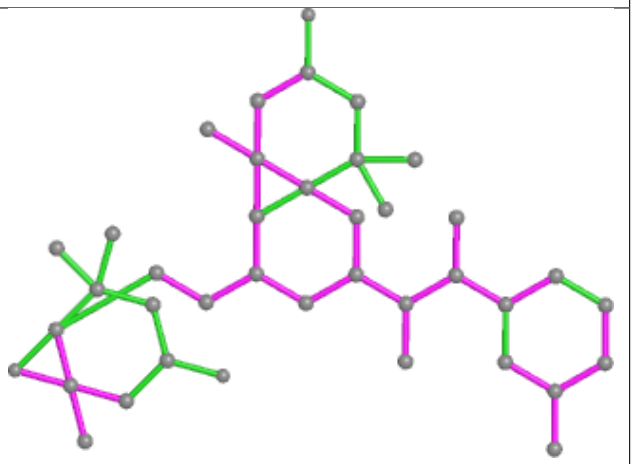


Rings

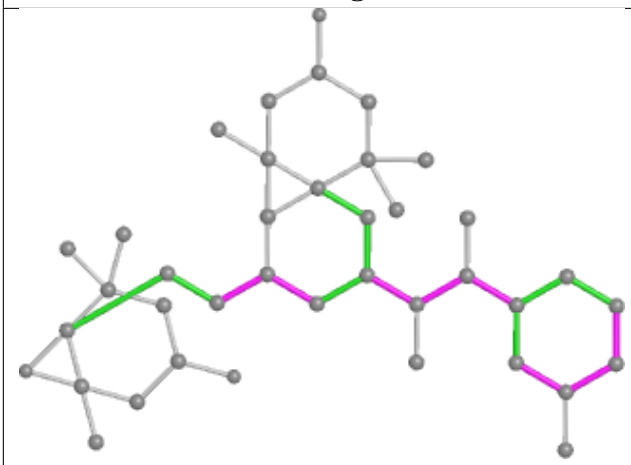
Ligand XAT R 313



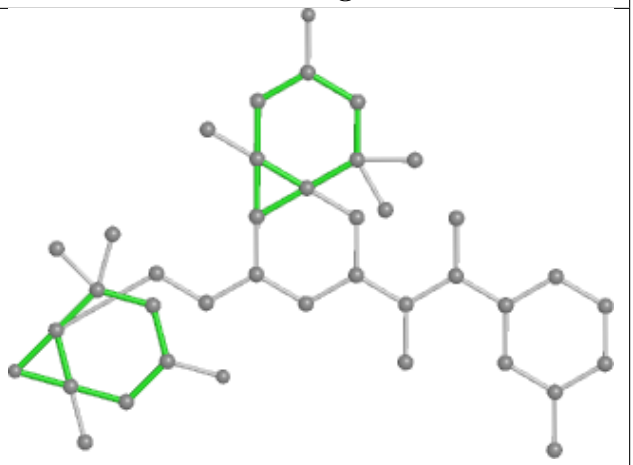
Bond lengths



Bond angles

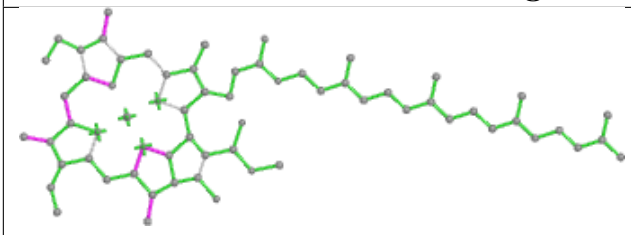


Torsions

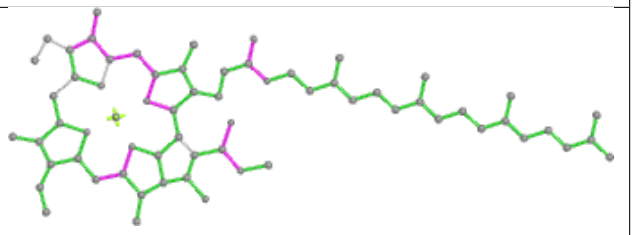


Rings

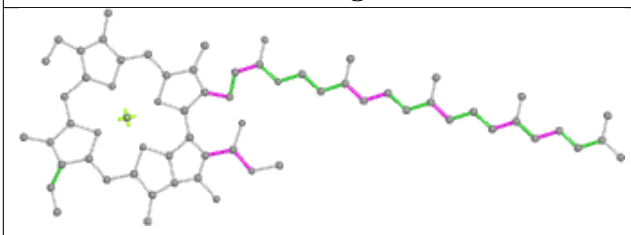
Ligand CLA C 513



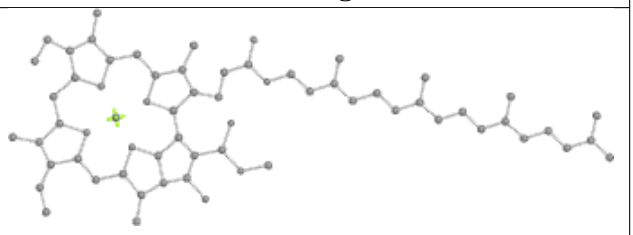
Bond lengths



Bond angles

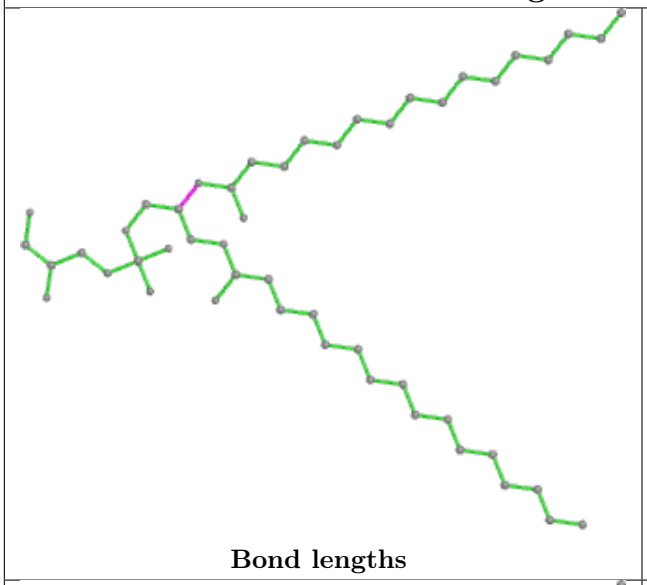


Torsions

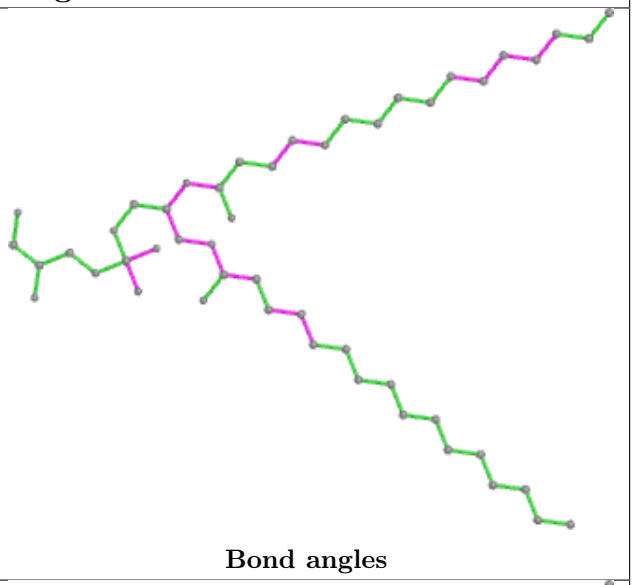


Rings

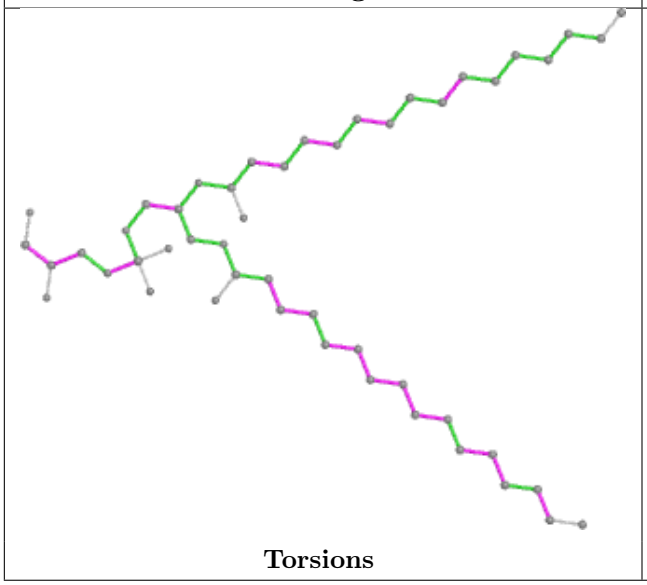
Ligand LHG g 619



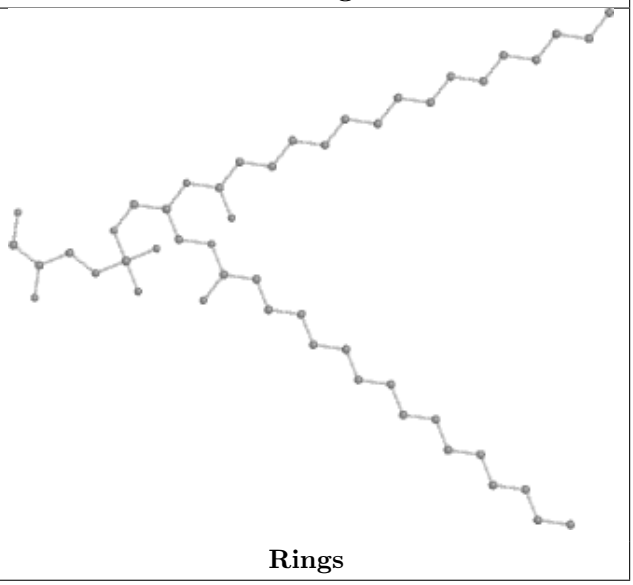
Bond lengths



Bond angles

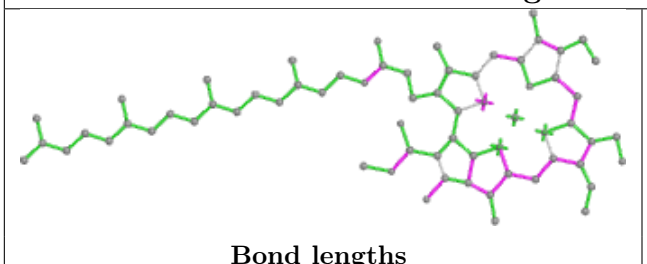


Torsions

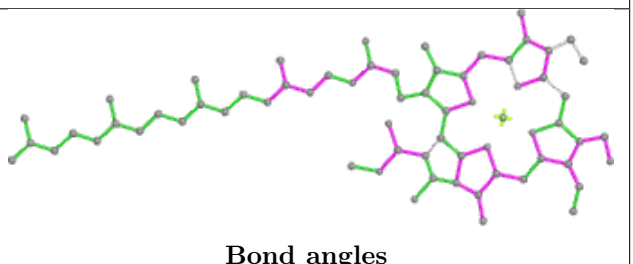


Rings

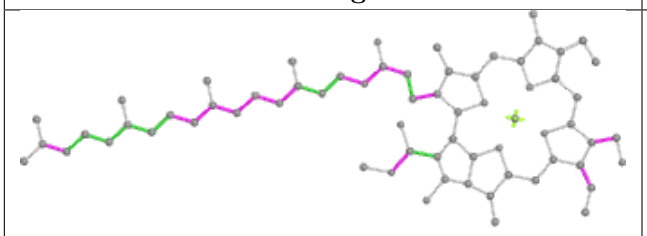
Ligand CHL N 607



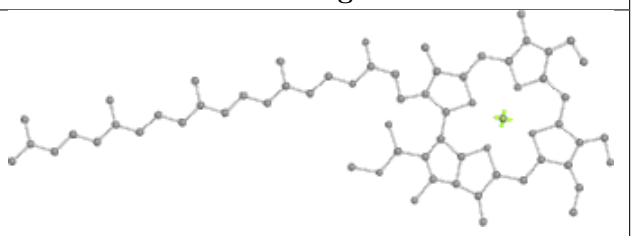
Bond lengths



Bond angles

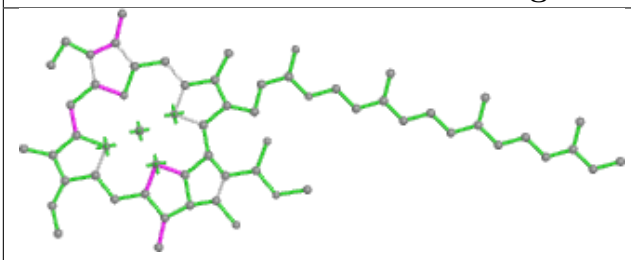


Torsions

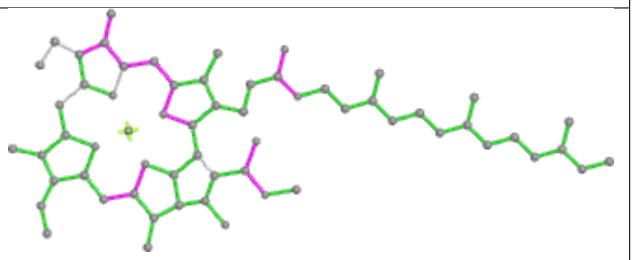


Rings

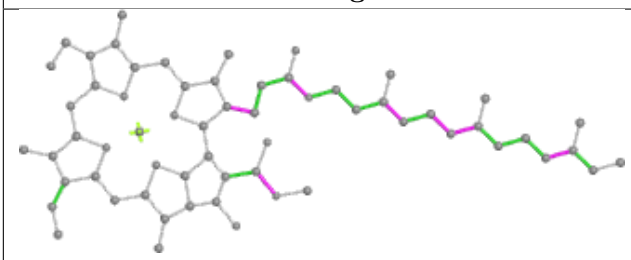
Ligand CLA s 303



Bond lengths



Bond angles



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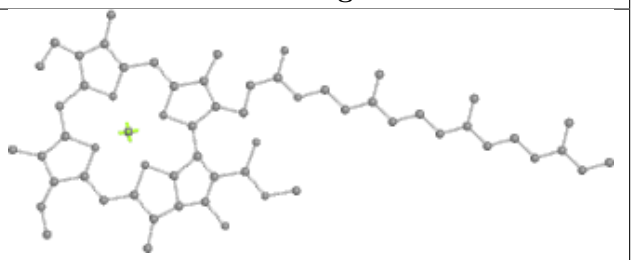
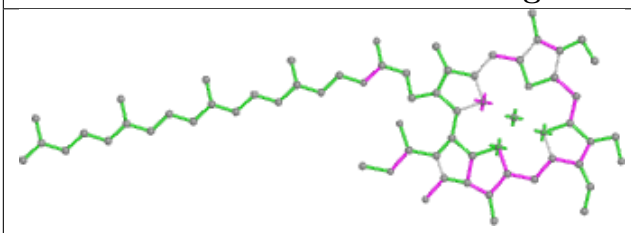
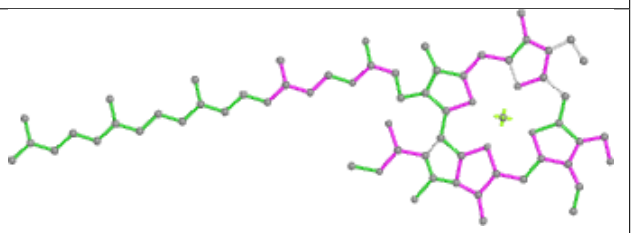


Rings

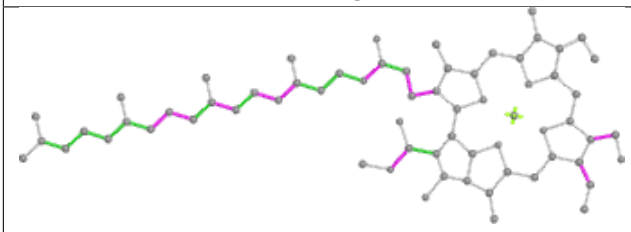
Ligand CHL Y 606



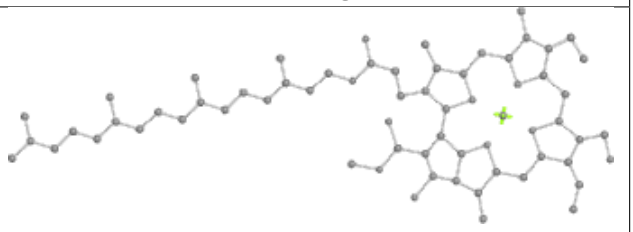
Bond lengths



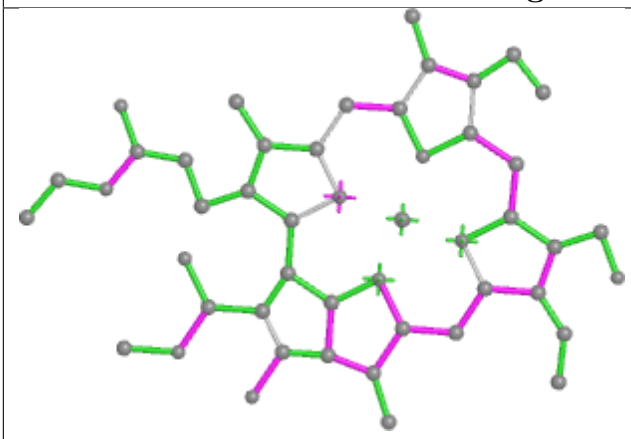
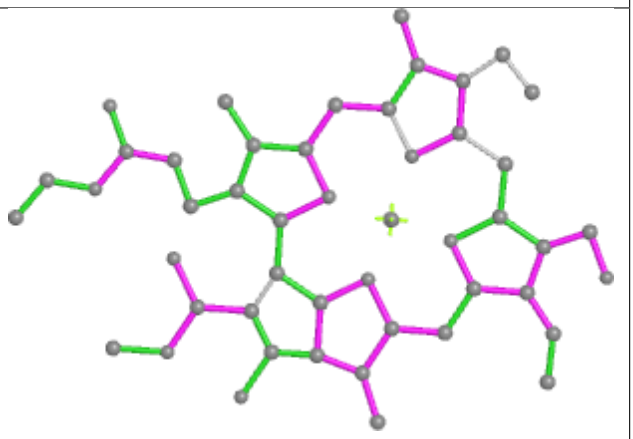
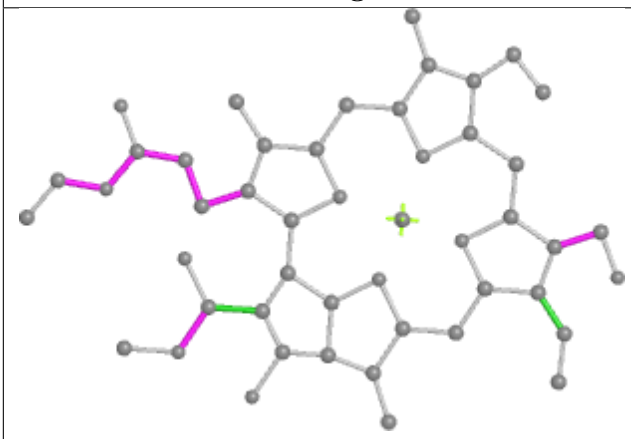
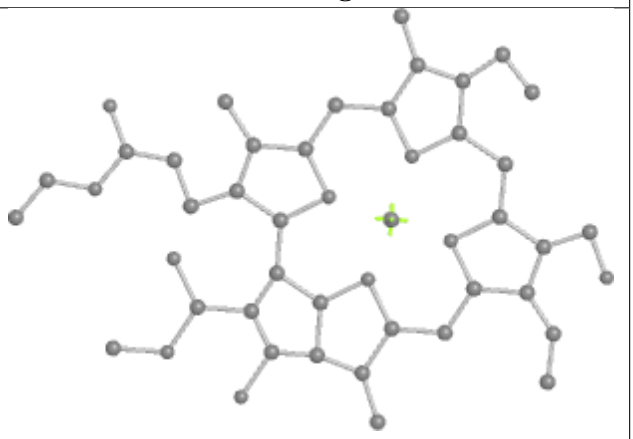
Bond angles

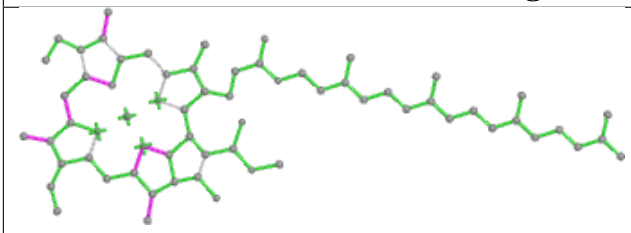
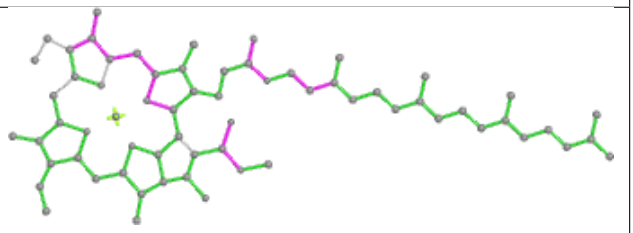
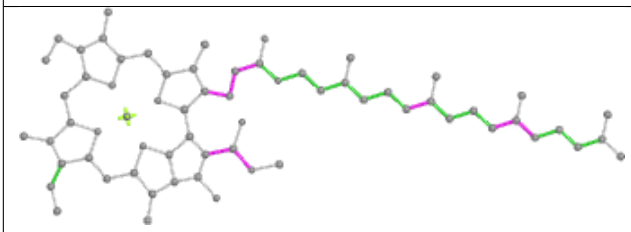
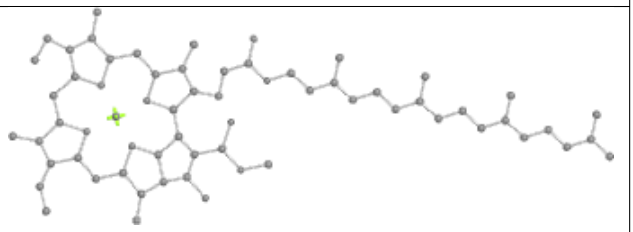


Torsions

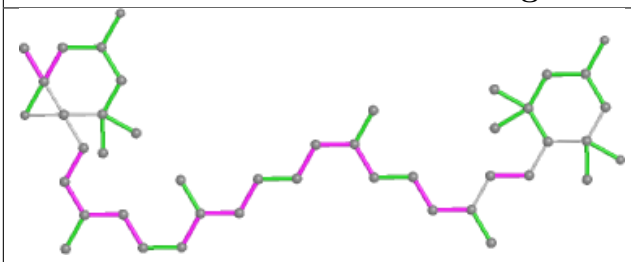


Rings

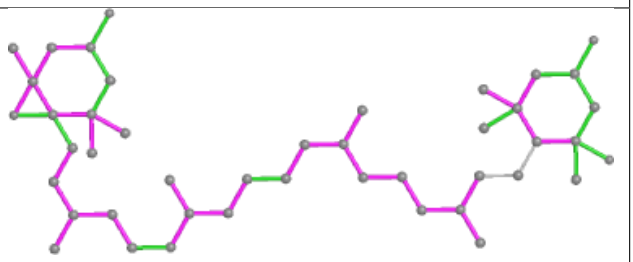
Ligand CHL S 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

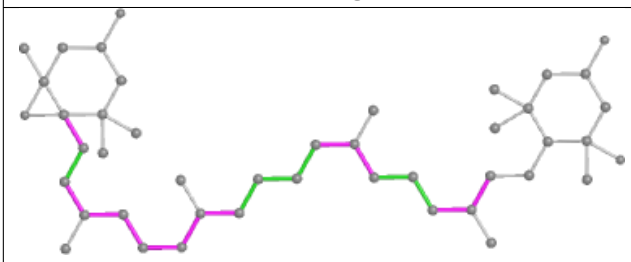
Ligand NEX N 617



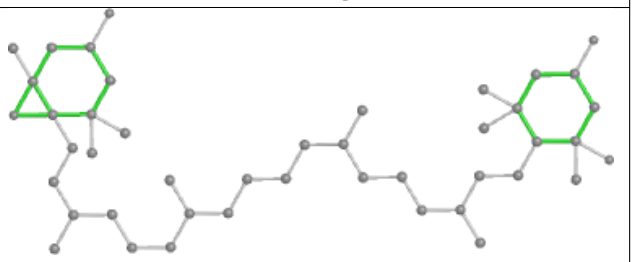
Bond lengths



Bond angles

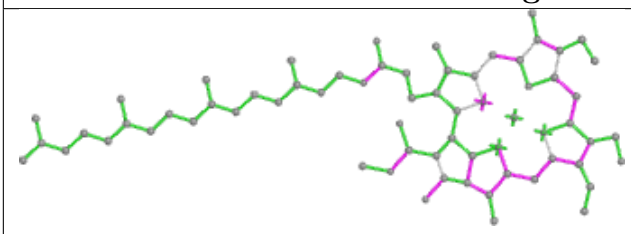


Torsions

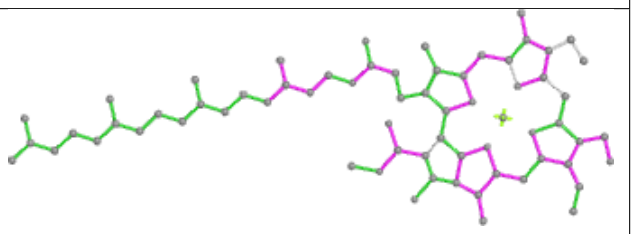


Rings

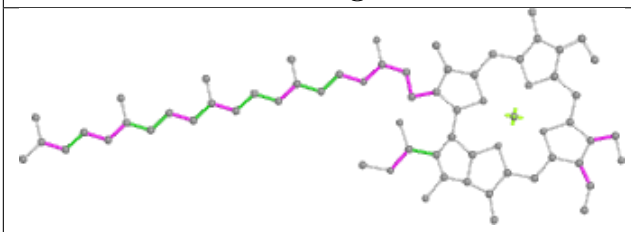
Ligand CHL G 601



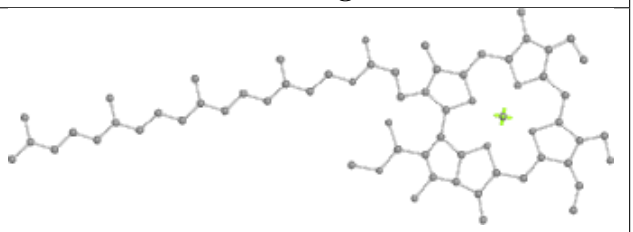
Bond lengths



Bond angles

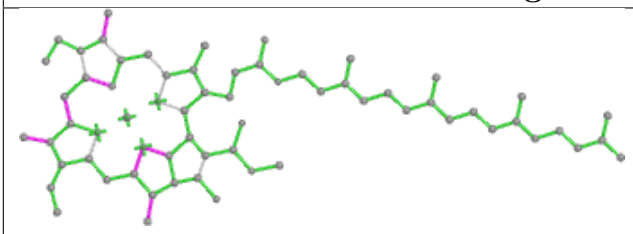


Torsions

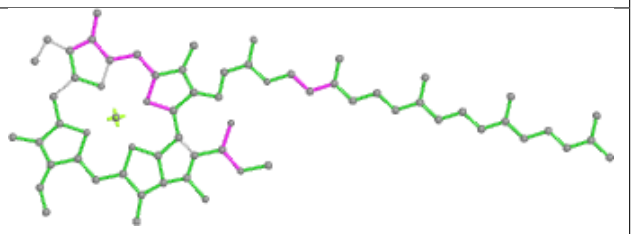


Rings

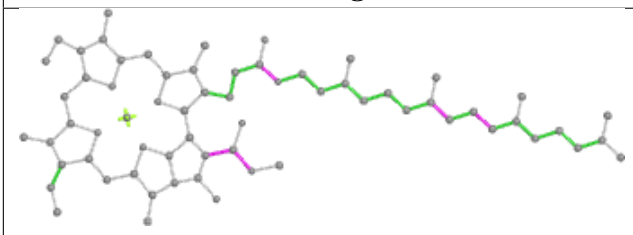
Ligand CLA C 506



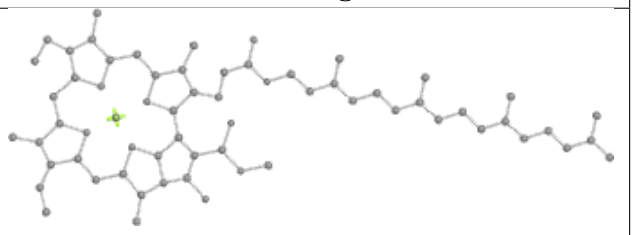
Bond lengths



Bond angles

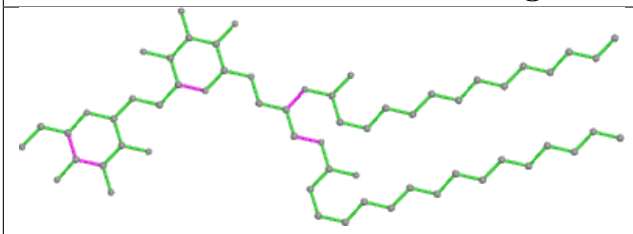


Torsions

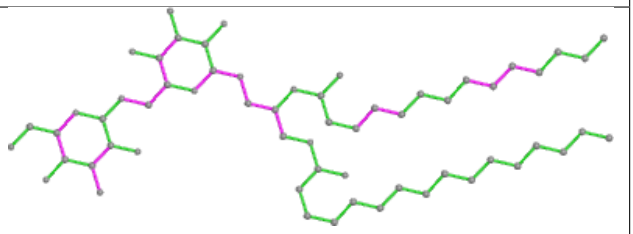


Rings

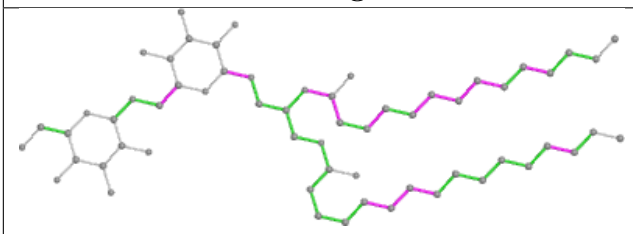
Ligand DGD J 101



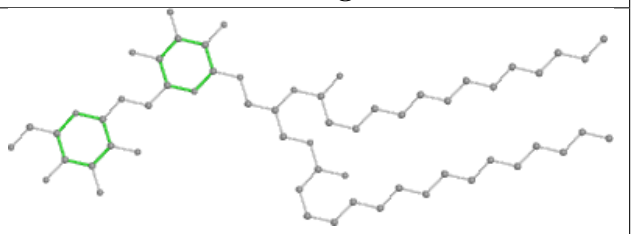
Bond lengths



Bond angles

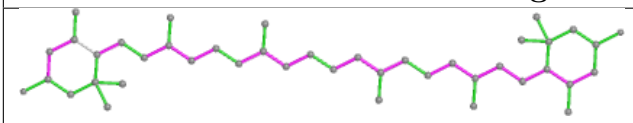


Torsions

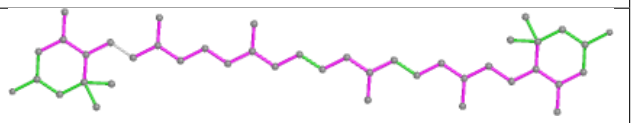


Rings

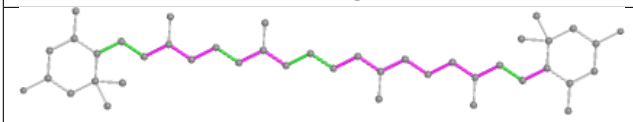
Ligand LUT r 313



Bond lengths



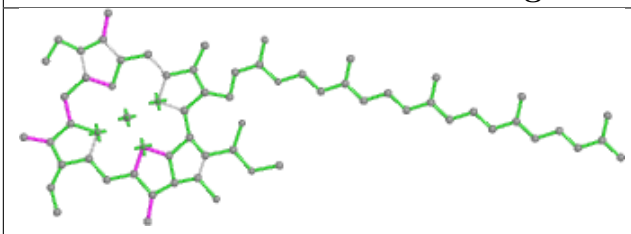
Bond angles



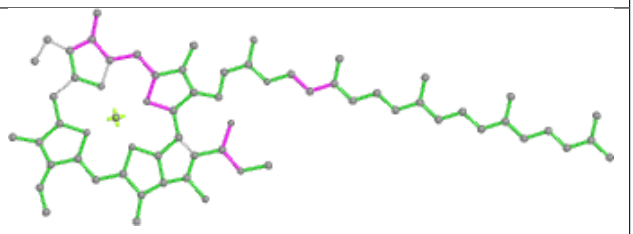
Torsions

Rings

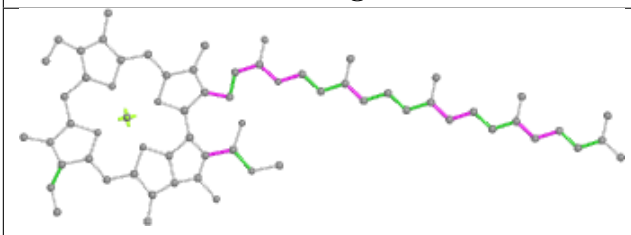
Ligand CLA C 515



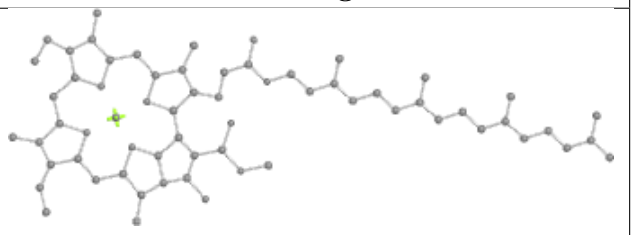
Bond lengths



Bond angles

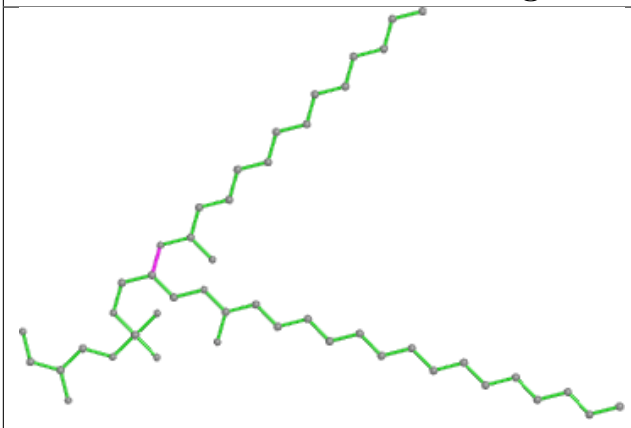


Torsions

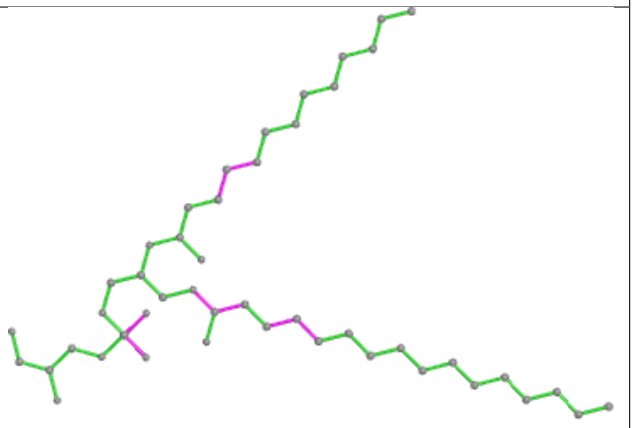


Rings

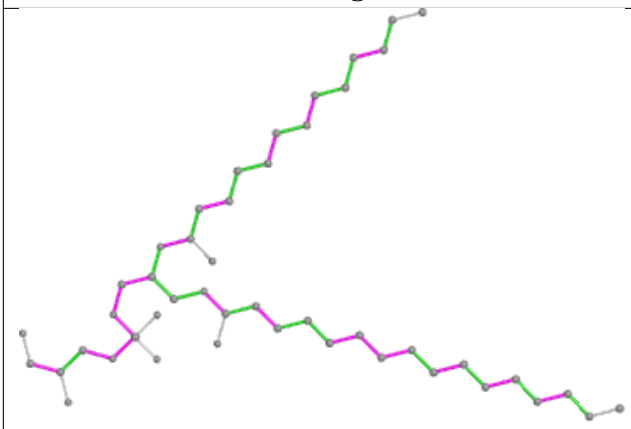
Ligand LHG D 408



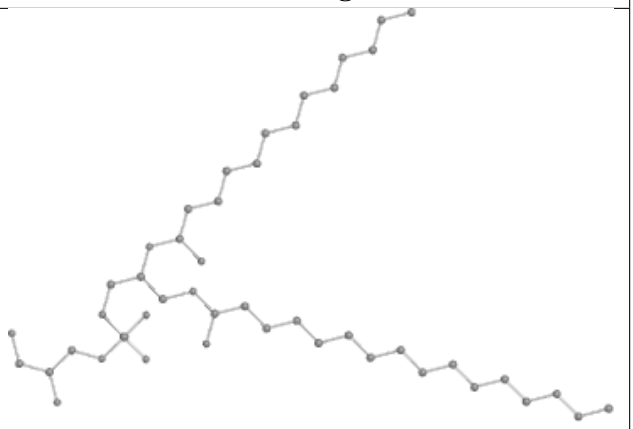
Bond lengths



Bond angles

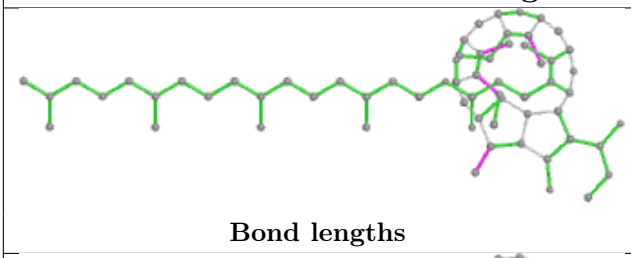


Torsions

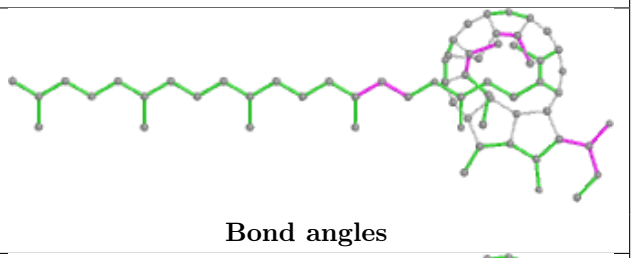


Rings

Ligand PHO D 401

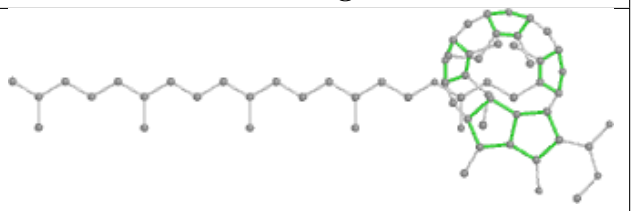


Bond lengths



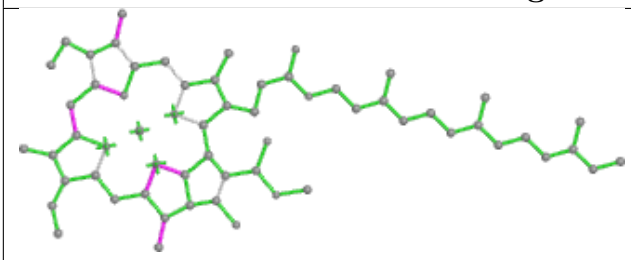
Bond angles

Torsions

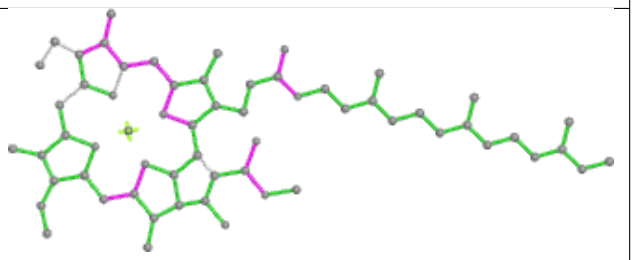


Rings

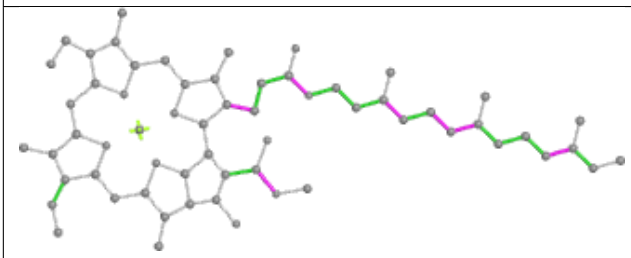
Ligand CLA S 303



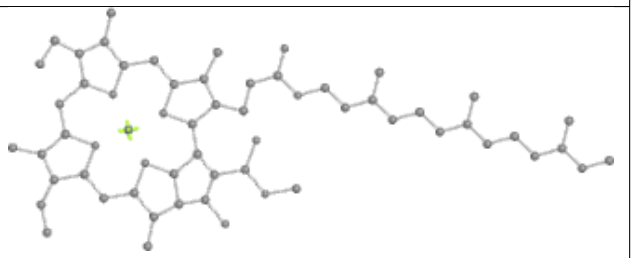
Bond lengths



Bond angles

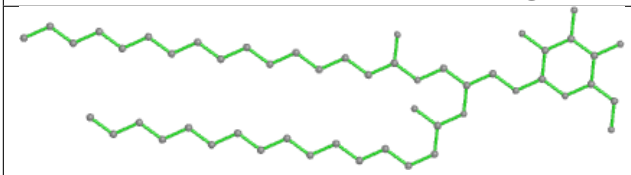


Torsions

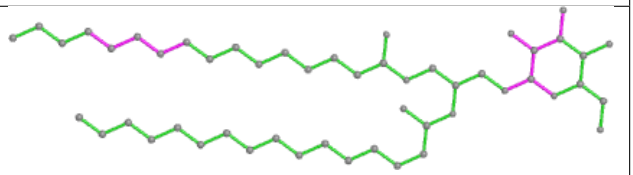


Rings

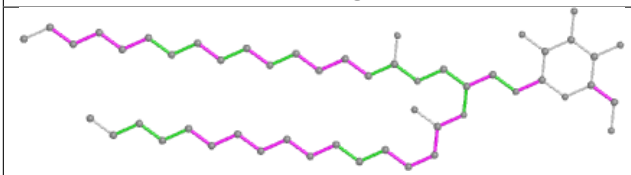
Ligand LMG k 103



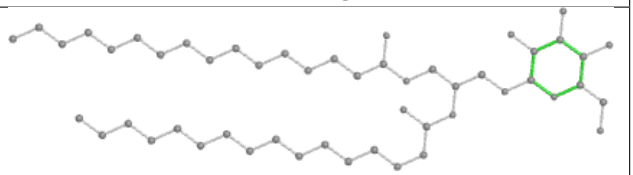
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

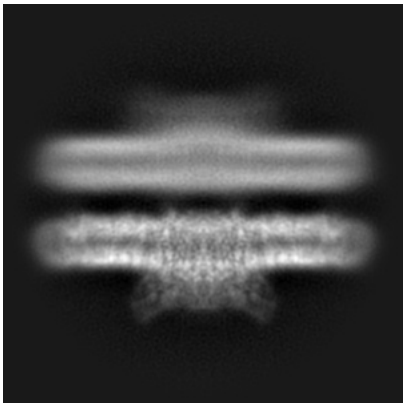
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10865. These allow visual inspection of the internal detail of the map and identification of artifacts.

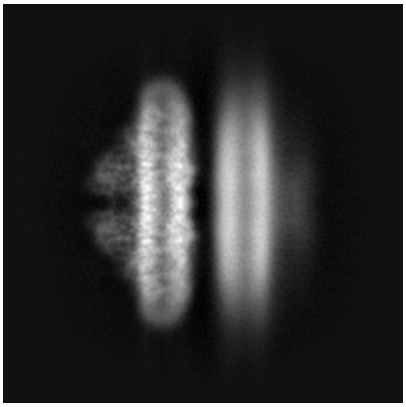
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

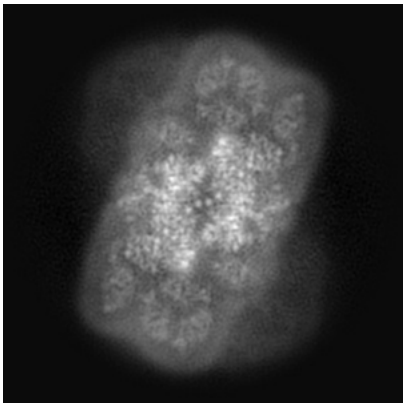
6.1.1 Primary map



X



Y

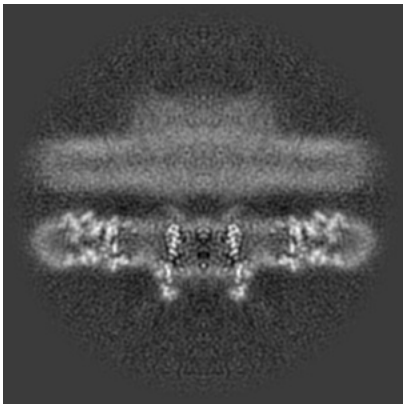


Z

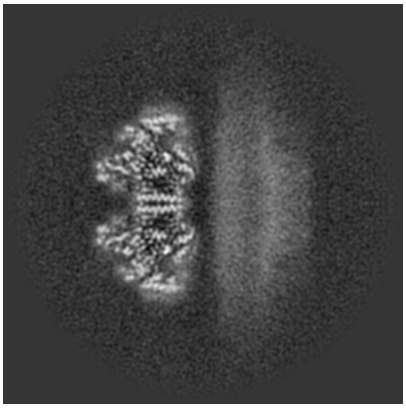
The images above show the map projected in three orthogonal directions.

6.2 Central slices

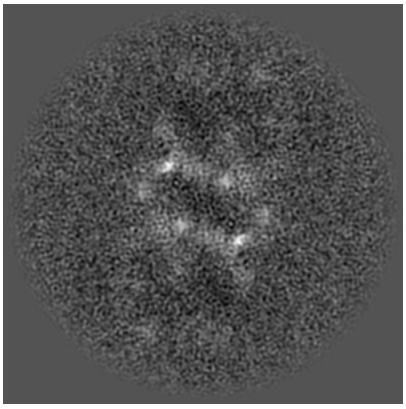
6.2.1 Primary map



X Index: 170



Y Index: 170

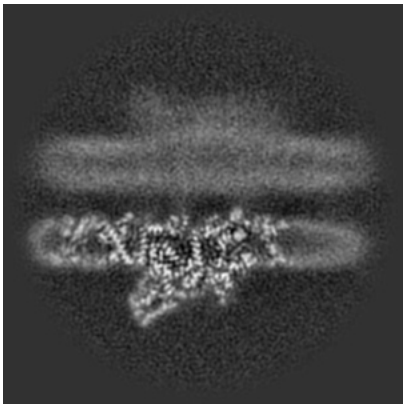


Z Index: 170

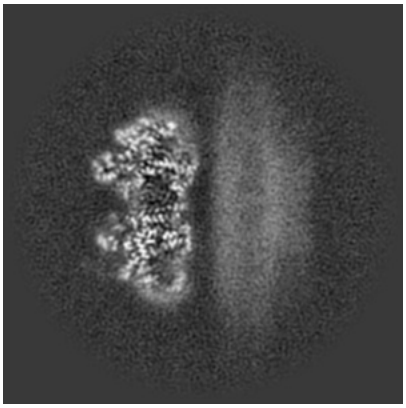
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

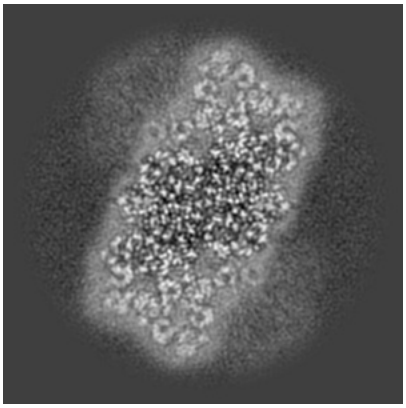
6.3.1 Primary map



X Index: 156



Y Index: 166

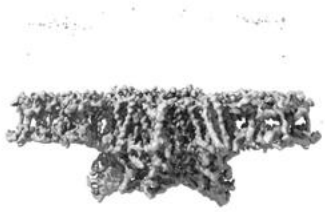


Z Index: 121

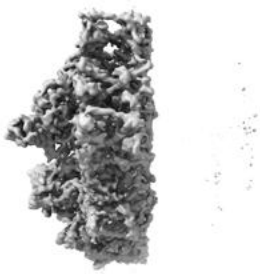
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

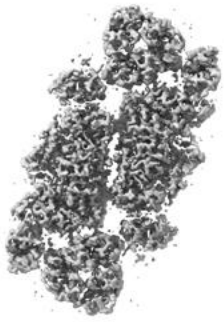
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

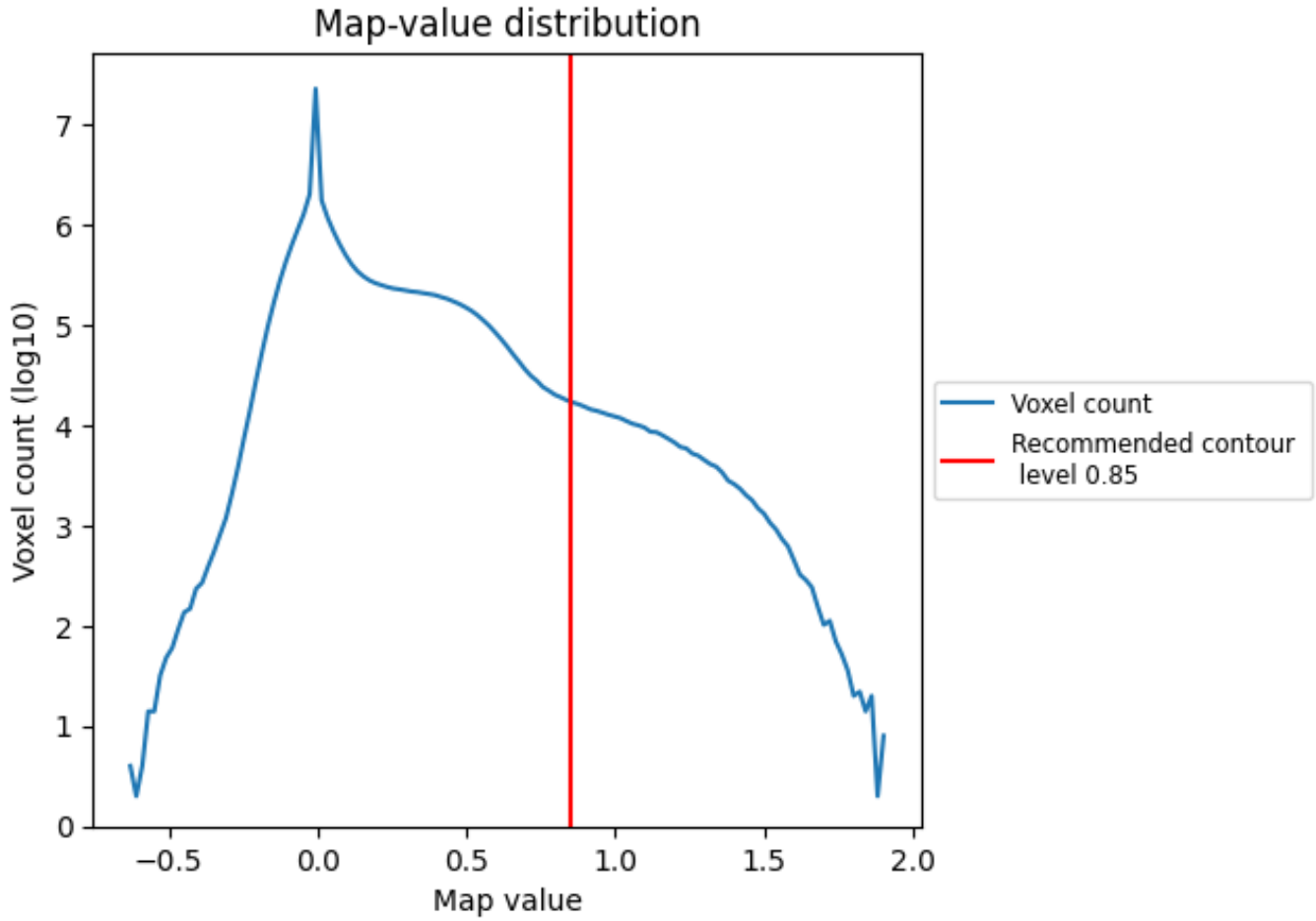
6.5 Mask visualisation (i)

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

7 Map analysis

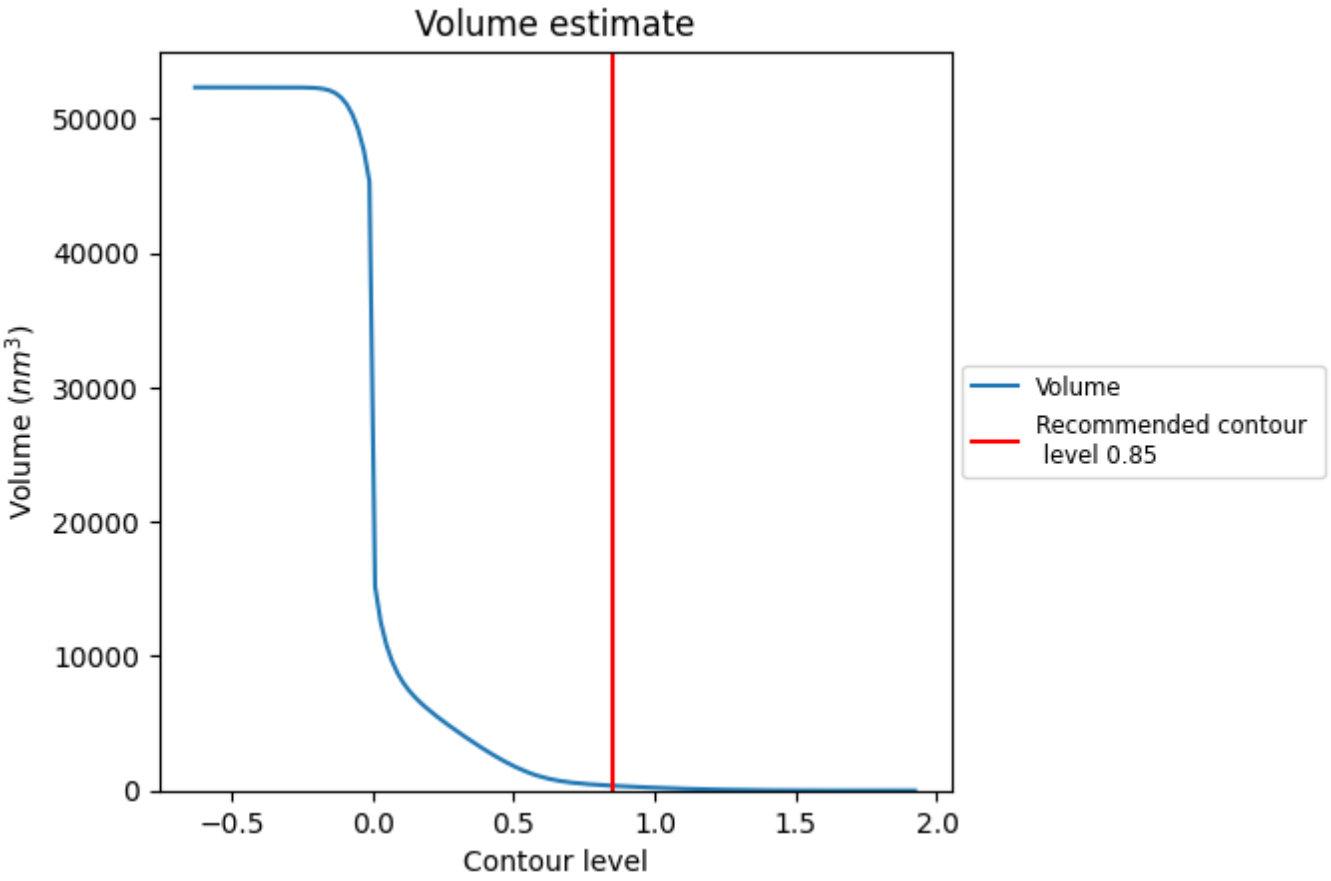
This section contains the results of statistical analysis of the map.

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.

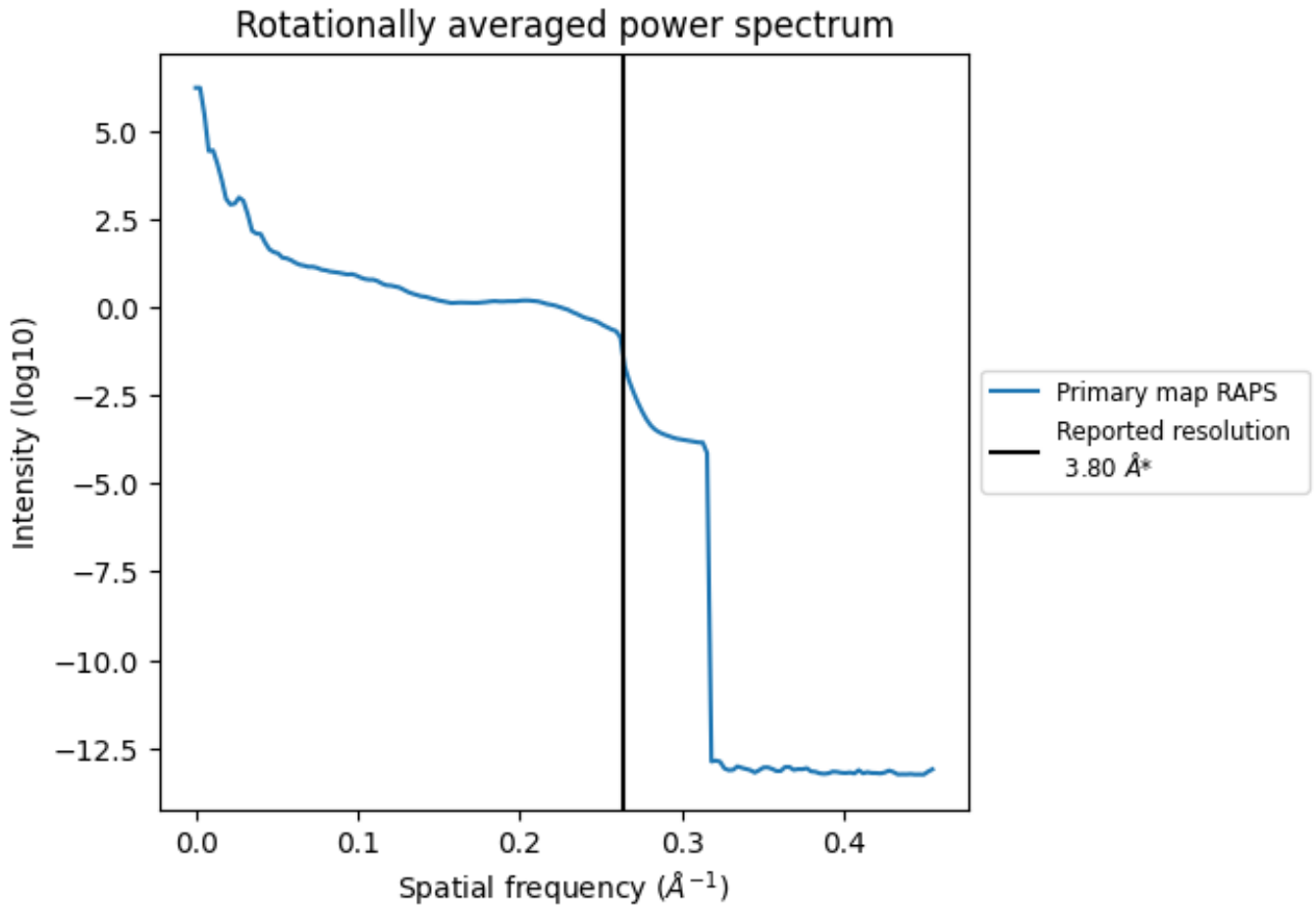
7.2 Volume estimate (i)



The volume at the recommended contour level is 360 nm^3; this corresponds to an approximate mass of 325 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 0.263 Å^{-1}

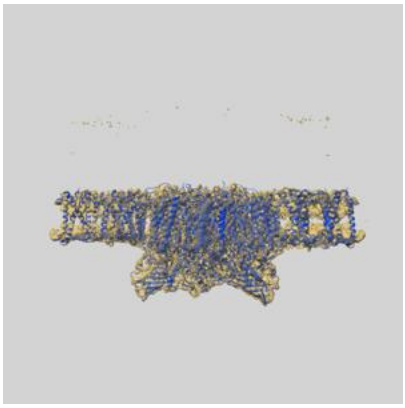
8 Fourier-Shell correlation

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

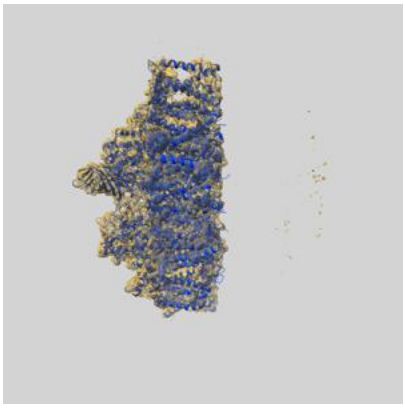
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10865 and PDB model 6YP7. Per-residue inclusion information can be found in section 3 on page 38.

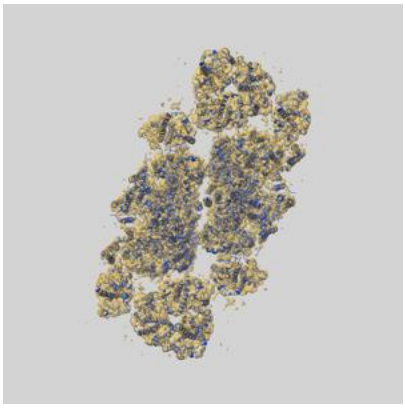
9.1 Map-model overlay



X



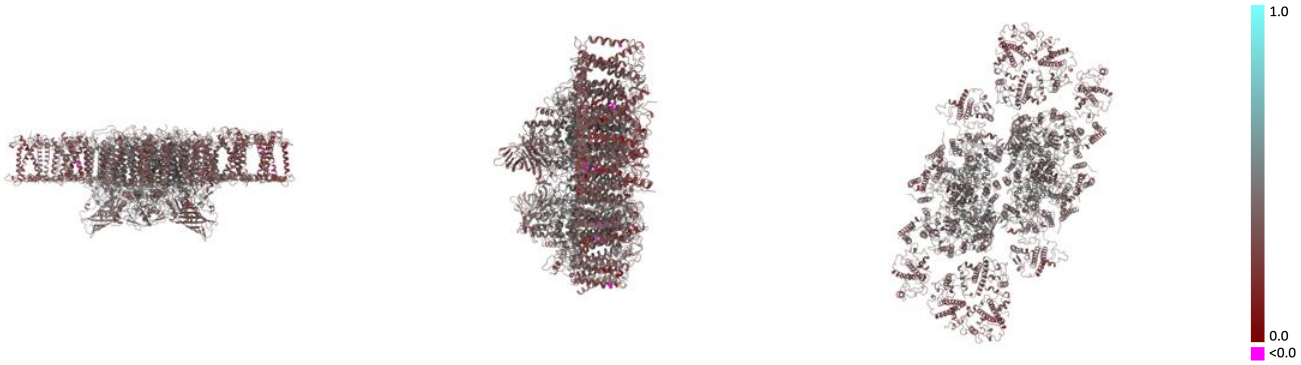
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.85 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.

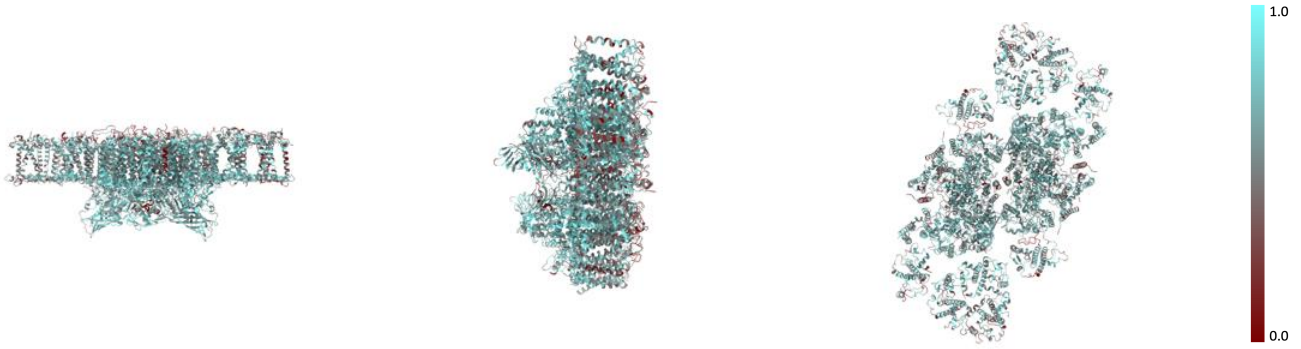
9.2 Q-score mapped to coordinate model



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.

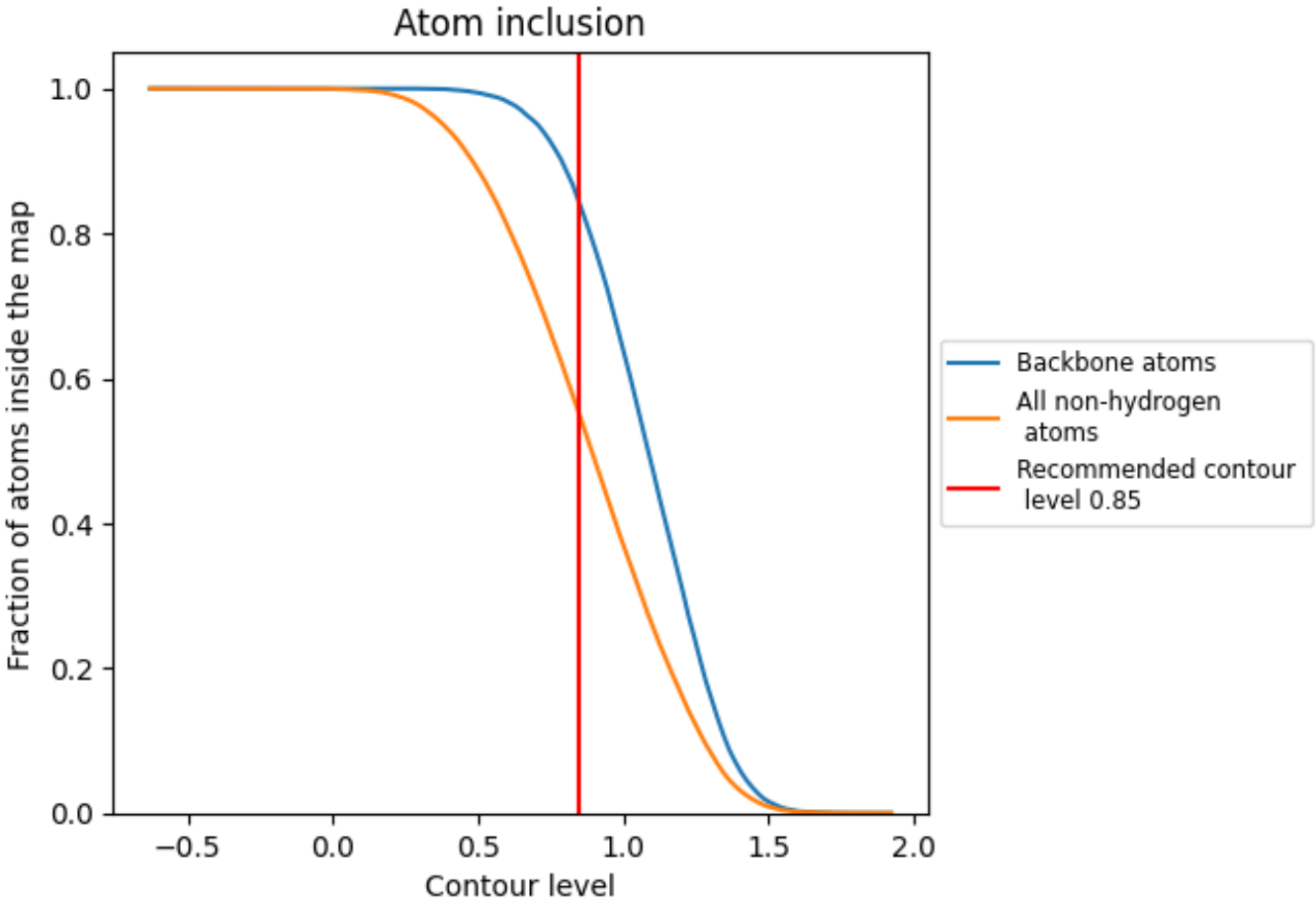
9.3 Atom inclusion mapped to coordinate model



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 (0.85).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 55% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5489	0.3820
A	0.6073	0.4440
B	0.6106	0.4330
C	0.6011	0.4200
D	0.5869	0.4380
E	0.6387	0.3060
F	0.5964	0.3180
G	0.4516	0.2780
H	0.5192	0.3920
I	0.5272	0.4460
J	0.2669	0.3740
K	0.4342	0.4020
L	0.4013	0.4420
M	0.3529	0.3940
N	0.4788	0.2880
O	0.5686	0.4020
R	0.4706	0.3470
S	0.5432	0.3340
T	0.3668	0.4390
W	0.4435	0.3460
X	0.5219	0.3380
Y	0.5448	0.3440
Z	0.5281	0.3270
a	0.6190	0.4440
b	0.6220	0.4350
c	0.6053	0.4220
d	0.5892	0.4410
e	0.6739	0.3500
f	0.5964	0.3260
g	0.4415	0.2710
h	0.5356	0.4140
i	0.6044	0.4440
j	0.2789	0.3520
k	0.4296	0.4000
l	0.3947	0.4490

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Chain	Atom inclusion	Q-score
m	0.4157	0.3850
n	0.4894	0.2920
o	0.5422	0.3560
r	0.4676	0.3520
s	0.5427	0.3330
t	0.4961	0.4360
w	0.4700	0.4050
x	0.5254	0.3640
y	0.5440	0.3470
z	0.5411	0.3310