wwPDB EM Validation Summary Report (i)

Dec 12, 2022 – 11:10 PM EST

PDB ID	:	3JCU
EMDB ID	:	EMD-6617
Title	:	Cryo-EM structure of spinach PSII-LHCII supercomplex at 3.2 Angstrom resolution
Authors	:	Wei, X.P.; Zhang, X.Z.; Su, X.D.; Cao, P.; Liu, X.Y.; Li, M.; Chang, W.R.; Liu, Z.F.
Deposited on	:	2016-03-10
Resolution	:	3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

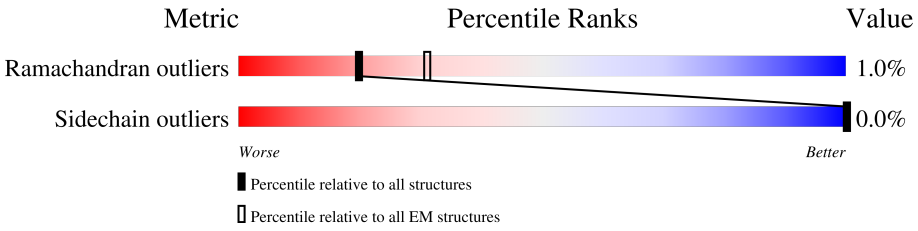
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.20 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	A	344	9% 97% .
1	a	344	9% 97% .
2	B	508	8% 95% . .
2	b	508	8% 95% . .
3	C	473	10% 95% 5%
3	c	473	10% 95% 5%
4	D	353	9% 96% .
4	d	353	10% 96% .
5	E	83	28% 95% 5%

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Mol	Chain	Length	Quality of chain
5	e	83	28% 95% 5%
6	F	39	13% 82% 18%
6	f	39	13% 82% 18%
7	G	267	21% 81% 18%
7	N	267	16% 81% 18%
7	Y	267	5% 81% 18%
7	g	267	21% 81% 18%
7	n	267	16% 81% 18%
7	y	267	6% 81% 18%
8	H	73	5% 81% 19%
8	h	73	81% 19%
9	I	36	14% 97%
9	i	36	14% 97%
10	J	40	80% 85% 15%
10	j	40	80% 85% 15%
11	K	59	12% 63% 37%
11	k	59	12% 63% 37%
12	L	38	8% 97%
12	l	38	8% 97%
13	M	34	32% 97%
13	m	34	32% 97%
14	O	332	34% 72% 27%
14	o	332	35% 72% 27%
15	P	267	64% 64% 36%
15	p	267	64% 64% 36%

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Mol	Chain	Length	Quality of chain
16	Q	232	64% 62% 36%
16	q	232	64% 62% 36%
17	R	243	37% 92% 5%
17	r	243	37% 92% 5%
18	S	295	30% 69% 27%
18	s	295	29% 69% 27%
19	T	33	15% 91% 9%
19	t	33	15% 91% 9%
20	U	99	24% 75%
20	u	99	24% 75%
21	W	137	13% 39% 61%
21	w	137	13% 39% 61%
22	X	117	6% 30% 70%
22	x	117	6% 30% 70%
23	Z	62	40% 98%
23	z	62	40% 98%

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
27	CLA	A	405	X	-	-	-
27	CLA	A	406	X	-	-	-
27	CLA	A	407	X	-	-	-
27	CLA	A	410	X	-	-	-
27	CLA	B	602	X	-	-	-
27	CLA	B	603	X	-	-	-
27	CLA	B	604	X	-	-	-
27	CLA	B	605	X	-	-	-
27	CLA	B	606	X	-	-	-
27	CLA	B	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	608	X	-	-	-
27	CLA	B	609	X	-	-	-
27	CLA	B	610	X	-	-	-
27	CLA	B	611	X	-	-	-
27	CLA	B	612	X	-	-	-
27	CLA	B	613	X	-	-	-
27	CLA	B	614	X	-	-	-
27	CLA	B	615	X	-	-	-
27	CLA	B	616	X	-	-	-
27	CLA	B	617	X	-	-	-
27	CLA	C	501	X	-	-	-
27	CLA	C	502	X	-	-	-
27	CLA	C	503	X	-	-	-
27	CLA	C	504	X	-	-	-
27	CLA	C	505	X	-	-	-
27	CLA	C	506	X	-	-	-
27	CLA	C	507	X	-	-	-
27	CLA	C	508	X	-	-	-
27	CLA	C	509	X	-	-	-
27	CLA	C	510	X	-	-	-
27	CLA	C	511	X	-	-	-
27	CLA	C	512	X	-	-	-
27	CLA	C	513	X	-	-	-
27	CLA	D	402	X	-	-	-
27	CLA	D	403	X	-	-	-
27	CLA	G	602	X	-	-	-
27	CLA	G	603	X	-	-	-
27	CLA	G	604	X	-	-	-
27	CLA	G	610	X	-	-	-
27	CLA	G	611	X	-	-	-
27	CLA	G	612	X	-	-	-
27	CLA	G	613	X	-	-	-
27	CLA	G	614	X	-	-	-
27	CLA	N	602	X	-	-	-
27	CLA	N	603	X	-	-	-
27	CLA	N	604	X	-	-	-
27	CLA	N	610	X	-	-	-
27	CLA	N	611	X	-	-	-
27	CLA	N	612	X	-	-	-
27	CLA	N	613	X	-	-	-
27	CLA	N	614	X	-	-	-
27	CLA	R	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	R	602	X	-	-	-
27	CLA	R	603	X	-	-	-
27	CLA	R	604	X	-	-	-
27	CLA	R	609	X	-	-	-
27	CLA	R	610	X	-	-	-
27	CLA	R	611	X	-	-	-
27	CLA	R	612	X	-	-	-
27	CLA	R	613	X	-	-	-
27	CLA	R	616	X	-	-	-
27	CLA	S	602	X	-	-	-
27	CLA	S	604	X	-	-	-
27	CLA	S	609	X	-	-	-
27	CLA	S	610	X	-	-	-
27	CLA	S	611	X	-	-	-
27	CLA	S	612	X	-	-	-
27	CLA	S	613	X	-	-	-
27	CLA	S	614	X	-	-	-
27	CLA	Y	602	X	-	-	-
27	CLA	Y	603	X	-	-	-
27	CLA	Y	604	X	-	-	-
27	CLA	Y	610	X	-	-	-
27	CLA	Y	611	X	-	-	-
27	CLA	Y	612	X	-	-	-
27	CLA	Y	613	X	-	-	-
27	CLA	Y	614	X	-	-	-
27	CLA	a	405	X	-	-	-
27	CLA	a	406	X	-	-	-
27	CLA	a	407	X	-	-	-
27	CLA	a	410	X	-	-	-
27	CLA	b	602	X	-	-	-
27	CLA	b	603	X	-	-	-
27	CLA	b	604	X	-	-	-
27	CLA	b	605	X	-	-	-
27	CLA	b	606	X	-	-	-
27	CLA	b	607	X	-	-	-
27	CLA	b	608	X	-	-	-
27	CLA	b	609	X	-	-	-
27	CLA	b	610	X	-	-	-
27	CLA	b	611	X	-	-	-
27	CLA	b	612	X	-	-	-
27	CLA	b	613	X	-	-	-
27	CLA	b	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	615	X	-	-	-
27	CLA	b	616	X	-	-	-
27	CLA	b	617	X	-	-	-
27	CLA	c	501	X	-	-	-
27	CLA	c	502	X	-	-	-
27	CLA	c	503	X	-	-	-
27	CLA	c	504	X	-	-	-
27	CLA	c	505	X	-	-	-
27	CLA	c	506	X	-	-	-
27	CLA	c	507	X	-	-	-
27	CLA	c	508	X	-	-	-
27	CLA	c	509	X	-	-	-
27	CLA	c	510	X	-	-	-
27	CLA	c	511	X	-	-	-
27	CLA	c	512	X	-	-	-
27	CLA	c	513	X	-	-	-
27	CLA	d	402	X	-	-	-
27	CLA	d	403	X	-	-	-
27	CLA	g	602	X	-	-	-
27	CLA	g	603	X	-	-	-
27	CLA	g	604	X	-	-	-
27	CLA	g	610	X	-	-	-
27	CLA	g	611	X	-	-	-
27	CLA	g	612	X	-	-	-
27	CLA	g	613	X	-	-	-
27	CLA	g	614	X	-	-	-
27	CLA	n	602	X	-	-	-
27	CLA	n	603	X	-	-	-
27	CLA	n	604	X	-	-	-
27	CLA	n	610	X	-	-	-
27	CLA	n	611	X	-	-	-
27	CLA	n	612	X	-	-	-
27	CLA	n	613	X	-	-	-
27	CLA	n	614	X	-	-	-
27	CLA	r	601	X	-	-	-
27	CLA	r	602	X	-	-	-
27	CLA	r	603	X	-	-	-
27	CLA	r	604	X	-	-	-
27	CLA	r	609	X	-	-	-
27	CLA	r	610	X	-	-	-
27	CLA	r	611	X	-	-	-
27	CLA	r	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	r	613	X	-	-	-
27	CLA	r	616	X	-	-	-
27	CLA	s	602	X	-	-	-
27	CLA	s	604	X	-	-	-
27	CLA	s	609	X	-	-	-
27	CLA	s	610	X	-	-	-
27	CLA	s	611	X	-	-	-
27	CLA	s	612	X	-	-	-
27	CLA	s	613	X	-	-	-
27	CLA	s	614	X	-	-	-
27	CLA	y	602	X	-	-	-
27	CLA	y	603	X	-	-	-
27	CLA	y	604	X	-	-	-
27	CLA	y	610	X	-	-	-
27	CLA	y	611	X	-	-	-
27	CLA	y	612	X	-	-	-
27	CLA	y	613	X	-	-	-
27	CLA	y	614	X	-	-	-
37	CHL	G	601	X	-	-	-
37	CHL	G	605	X	-	-	-
37	CHL	G	606	X	-	-	-
37	CHL	G	607	X	-	-	-
37	CHL	G	608	X	-	-	-
37	CHL	G	609	X	-	-	-
37	CHL	N	601	X	-	-	-
37	CHL	N	605	X	-	-	-
37	CHL	N	606	X	-	-	-
37	CHL	N	607	X	-	-	-
37	CHL	N	608	X	-	-	-
37	CHL	N	609	X	-	-	-
37	CHL	R	606	X	-	-	-
37	CHL	R	607	X	-	-	-
37	CHL	R	608	X	-	-	-
37	CHL	S	601	X	-	-	-
37	CHL	S	606	X	-	-	-
37	CHL	S	607	X	-	-	-
37	CHL	S	608	X	-	-	-
37	CHL	Y	601	X	-	-	-
37	CHL	Y	605	X	-	-	-
37	CHL	Y	606	X	-	-	-
37	CHL	Y	607	X	-	-	-
37	CHL	Y	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CHL	Y	609	X	-	-	-
37	CHL	g	601	X	-	-	-
37	CHL	g	605	X	-	-	-
37	CHL	g	606	X	-	-	-
37	CHL	g	607	X	-	-	-
37	CHL	g	608	X	-	-	-
37	CHL	g	609	X	-	-	-
37	CHL	n	601	X	-	-	-
37	CHL	n	605	X	-	-	-
37	CHL	n	606	X	-	-	-
37	CHL	n	607	X	-	-	-
37	CHL	n	608	X	-	-	-
37	CHL	n	609	X	-	-	-
37	CHL	r	606	X	-	-	-
37	CHL	r	607	X	-	-	-
37	CHL	r	608	X	-	-	-
37	CHL	s	601	X	-	-	-
37	CHL	s	606	X	-	-	-
37	CHL	s	607	X	-	-	-
37	CHL	s	608	X	-	-	-
37	CHL	y	601	X	-	-	-
37	CHL	y	605	X	-	-	-
37	CHL	y	606	X	-	-	-
37	CHL	y	607	X	-	-	-
37	CHL	y	608	X	-	-	-
37	CHL	y	609	X	-	-	-

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 75994 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2614	1707	430	464	13		
1	a	334	Total	C	N	O	S	0	0
			2614	1707	430	464	13		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	487	Total	C	N	O	S	0	0
			3820	2501	640	667	12		
2	b	487	Total	C	N	O	S	0	0
			3820	2501	640	667	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3475	2284	581	599	11		
3	c	449	Total	C	N	O	S	0	0
			3475	2284	581	599	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	340	Total	C	N	O	S	0	0
			2703	1786	443	462	12		
4	d	340	Total	C	N	O	S	0	0
			2703	1786	443	462	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	79	Total 636	C 412	N 104	O 120	0	0
5	e	79	Total 636	C 412	N 104	O 120	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	32	Total 257	C 174	N 43	O 39	S 1	0	0
6	f	32	Total 257	C 174	N 43	O 39	S 1	0	0

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total 1661	C 1079	N 270	O 305	S 7	0	0
7	N	218	Total 1661	C 1079	N 270	O 305	S 7	0	0
7	Y	218	Total 1661	C 1079	N 270	O 305	S 7	0	0
7	g	218	Total 1661	C 1079	N 270	O 305	S 7	0	0
7	n	218	Total 1661	C 1079	N 270	O 305	S 7	0	0
7	y	218	Total 1661	C 1079	N 270	O 305	S 7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	59	Total 434	C 288	N 65	O 78	S 3	0	0
8	h	59	Total 434	C 288	N 65	O 78	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total 286	C 195	N 44	O 46	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	35	Total 286	C 195	N 44	O 46	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	34	Total 247	C 168	N 38	O 41	0	0
10	j	34	Total 247	C 168	N 38	O 41	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total 307	C 217	N 43	O 46	S 1	0	0
11	k	37	Total 307	C 217	N 43	O 46	S 1	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	33	Total 258	C 176	N 37	O 45	0	0
13	m	33	Total 258	C 176	N 37	O 45	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	243	Total 1844	C 1164	N 301	O 376	S 3	0	0
14	o	243	Total 1844	C 1164	N 301	O 376	S 3	0	0

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	172	Total	C	N	O	S	0	0
			1324	841	215	266	2		
15	p	172	Total	C	N	O	S	0	0
			1324	841	215	266	2		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	148	Total	C	N	O	0	0
			1162	736	202	224		
16	q	148	Total	C	N	O	0	0
			1162	736	202	224		

- Molecule 17 is a protein called Chlorophyll A-B Binding protein 29 kD (CP29).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	232	Total	C	N	O	S	0	0
			1806	1170	293	339	4		
17	r	232	Total	C	N	O	S	0	0
			1806	1170	293	339	4		

- Molecule 18 is a protein called Chlorophyll A-B Binding protein 26 kD (CP26).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	214	Total	C	N	O	S	0	0
			1653	1080	269	299	5		
18	s	214	Total	C	N	O	S	0	0
			1653	1080	269	299	5		

- Molecule 19 is a protein called Photosystem II Reaction Center protein Tc.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	30	Total	C	N	O	S	0	0
			245	171	34	39	1		
19	t	30	Total	C	N	O	S	0	0
			245	171	34	39	1		

- Molecule 20 is a protein called Photosystem II Reaction Center Tn protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	25	Total	C	N	O	S	0	0
			193	123	35	32	3		
20	u	25	Total	C	N	O	S	0	0
			193	123	35	32	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	54	Total	C	N	O	S	0	0
			419	276	61	81	1		
21	w	54	Total	C	N	O	S	0	0
			419	276	61	81	1		

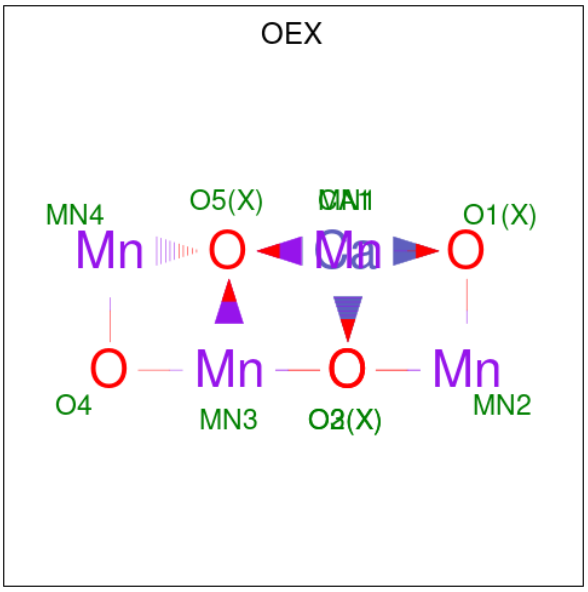
- Molecule 22 is a protein called Photosystem II Reaction Center X protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	35	Total	C	N	O	0	0
			246	163	38	45		
22	x	35	Total	C	N	O	0	0
			246	163	38	45		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Z	61	Total	C	N	O	0	0
			454	306	68	80		
23	z	61	Total	C	N	O	0	0
			454	306	68	80		

- Molecule 24 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

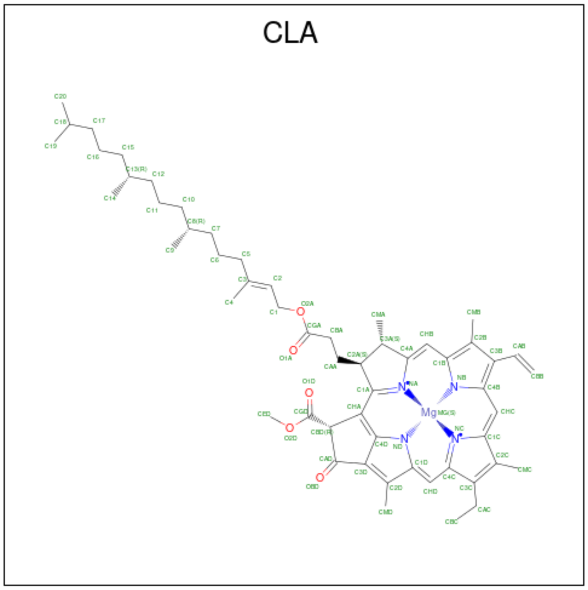
- Molecule 25 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 26 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Cl	0
			2	2	
26	a	2	Total	Cl	0
			2	2	

- Molecule 27 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total 239	C 199	Mg 4	N 16	O 20	0
27	A	1	Total 239	C 199	Mg 4	N 16	O 20	0
27	A	1	Total 239	C 199	Mg 4	N 16	O 20	0
27	A	1	Total 239	C 199	Mg 4	N 16	O 20	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	C	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	D	1	Total 130	C 110	Mg 2	N 8	O 10	0
27	D	1	Total 130	C 110	Mg 2	N 8	O 10	0

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Mol	Chain	Residues	Atoms					AltConf
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0

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Mol	Chain	Residues	Atoms					AltConf
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	S	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	S	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	S	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	S	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	S	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	S	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	S	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	S	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	S	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	Y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	Y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	Y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	Y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	Y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	Y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	Y	1	Total 472	C 392	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
27	Y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
27	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
27	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
27	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0

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Mol	Chain	Residues	Atoms					AltConf
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	c	1	Total 829	C 699	Mg 13	N 52	O 65	0
27	d	1	Total 130	C 110	Mg 2	N 8	O 10	0
27	d	1	Total 130	C 110	Mg 2	N 8	O 10	0
27	g	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	g	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	g	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	g	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	g	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	g	1	Total 424	C 344	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
27	g	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	g	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0

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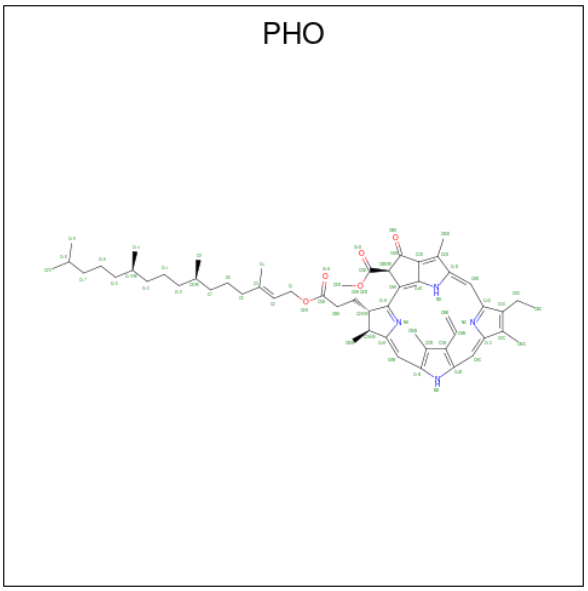
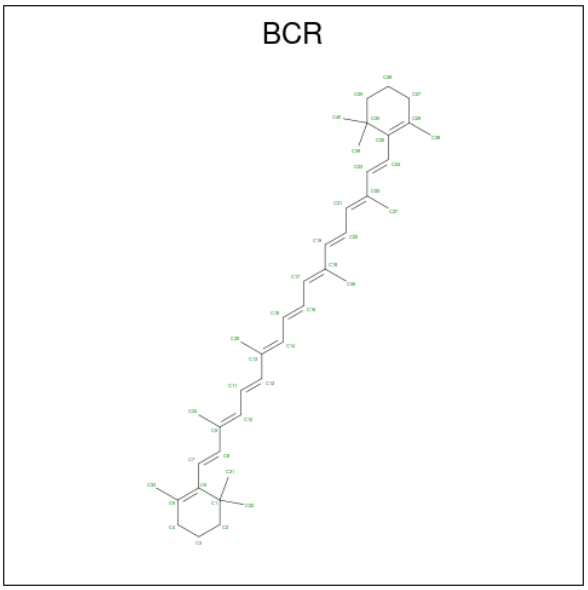
Mol	Chain	Residues	Atoms					AltConf
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0

- Molecule 28 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



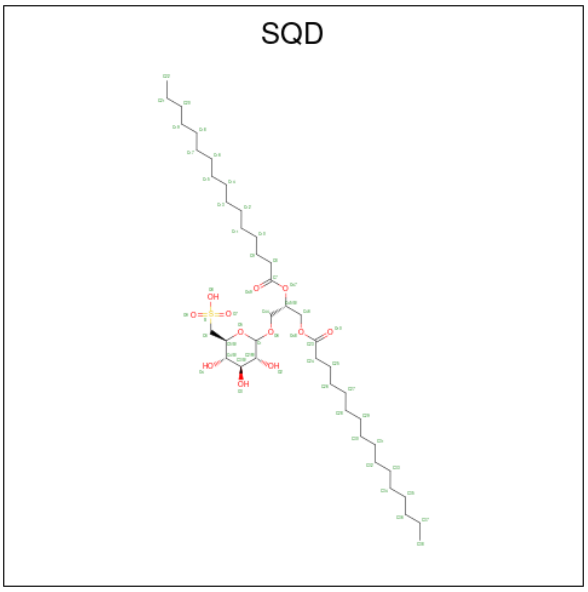
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total 128	C 110	N 8	O 10	0
28	A	1	Total 128	C 110	N 8	O 10	0
28	a	1	Total 128	C 110	N 8	O 10	0
28	a	1	Total 128	C 110	N 8	O 10	0

- Molecule 29 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



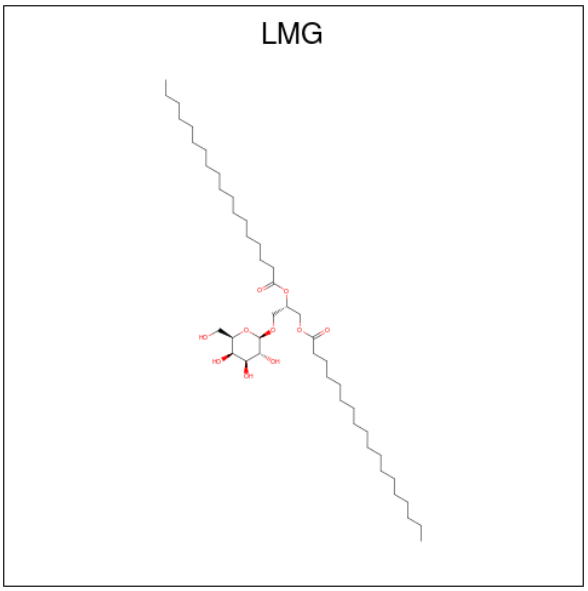
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	B	1	Total C 120 120	0
29	B	1	Total C 120 120	0
29	B	1	Total C 120 120	0
29	C	1	Total C 160 160	0
29	C	1	Total C 160 160	0
29	C	1	Total C 160 160	0
29	C	1	Total C 160 160	0
29	D	1	Total C 40 40	0
29	H	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	b	1	Total C 120 120	0
29	b	1	Total C 120 120	0
29	b	1	Total C 120 120	0
29	c	1	Total C 160 160	0
29	c	1	Total C 160 160	0
29	c	1	Total C 160 160	0
29	c	1	Total C 160 160	0
29	d	1	Total C 40 40	0
29	h	1	Total C 40 40	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



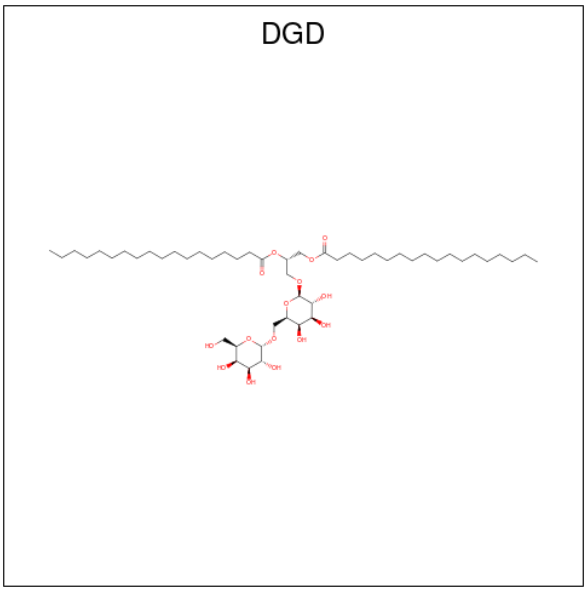
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			108	82	24	2	
30	A	1	Total	C	O	S	0
			108	82	24	2	
30	B	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			108	82	24	2	
30	a	1	Total	C	O	S	0
			108	82	24	2	
30	b	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



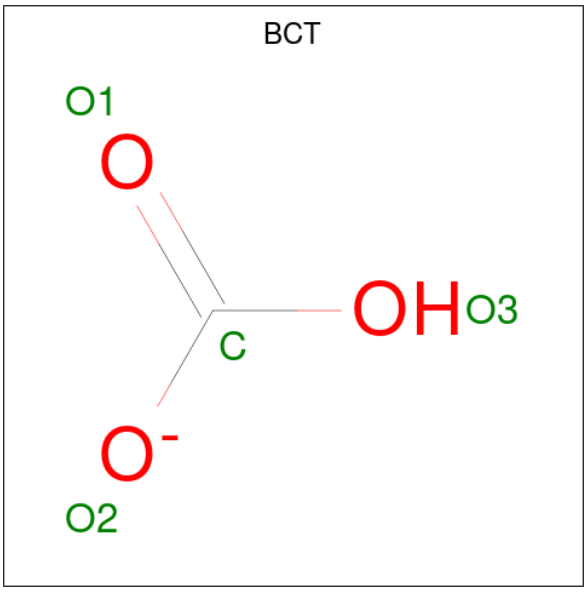
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C O 48 38 10	0
31	B	1	Total C O 51 41 10	0
31	C	1	Total C O 51 41 10	0
31	D	1	Total C O 46 36 10	0
31	Z	1	Total C O 51 41 10	0
31	a	1	Total C O 48 38 10	0
31	b	1	Total C O 51 41 10	0
31	c	1	Total C O 51 41 10	0
31	d	1	Total C O 46 36 10	0
31	z	1	Total C O 51 41 10	0

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



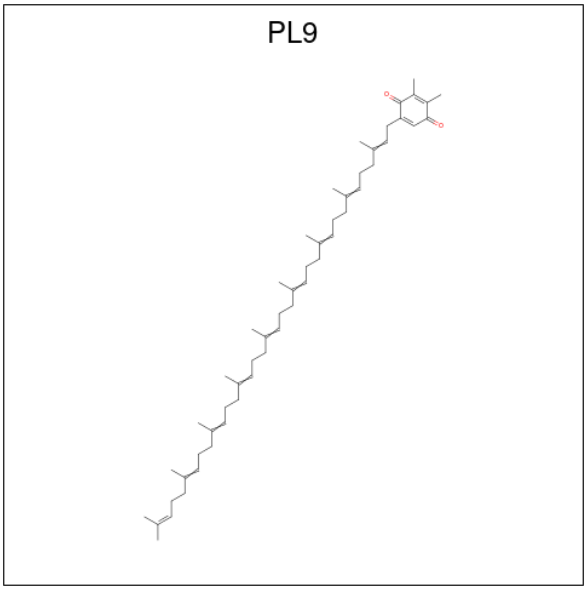
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total 179	C 134	O 45	0
32	C	1	Total 179	C 134	O 45	0
32	C	1	Total 179	C 134	O 45	0
32	H	1	Total 62	C 47	O 15	0
32	c	1	Total 179	C 134	O 45	0
32	c	1	Total 179	C 134	O 45	0
32	c	1	Total 179	C 134	O 45	0
32	h	1	Total 62	C 47	O 15	0

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



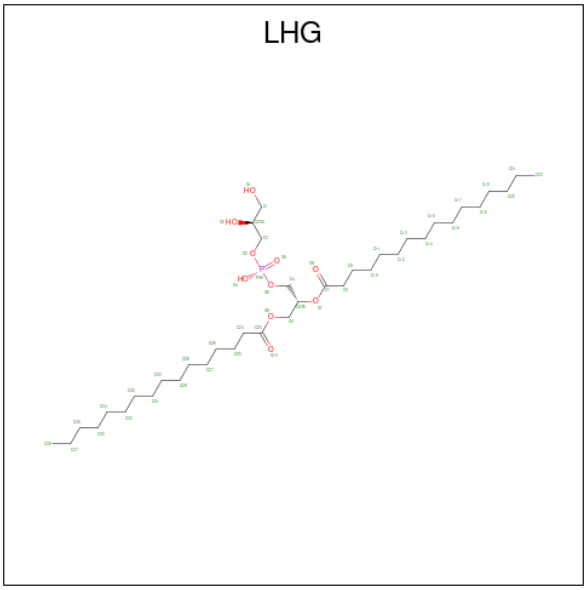
Mol	Chain	Residues	Atoms			AltConf
33	D	1	Total	C	O	0
			4	1	3	
33	d	1	Total	C	O	0
			4	1	3	

- Molecule 34 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
34	D	1	Total 55	C 53	O 2	0
34	d	1	Total 55	C 53	O 2	0

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



Mol	Chain	Residues	Atoms				AltConf
35	D	1	Total 129	C 96	O 30	P 3	0
35	D	1	Total 129	C 96	O 30	P 3	0
35	D	1	Total 129	C 96	O 30	P 3	0
35	G	1	Total 49	C 38	O 10	P 1	0
35	L	1	Total 49	C 38	O 10	P 1	0
35	N	1	Total 49	C 38	O 10	P 1	0
35	R	1	Total 49	C 38	O 10	P 1	0
35	S	1	Total 49	C 38	O 10	P 1	0
35	Y	1	Total 49	C 38	O 10	P 1	0

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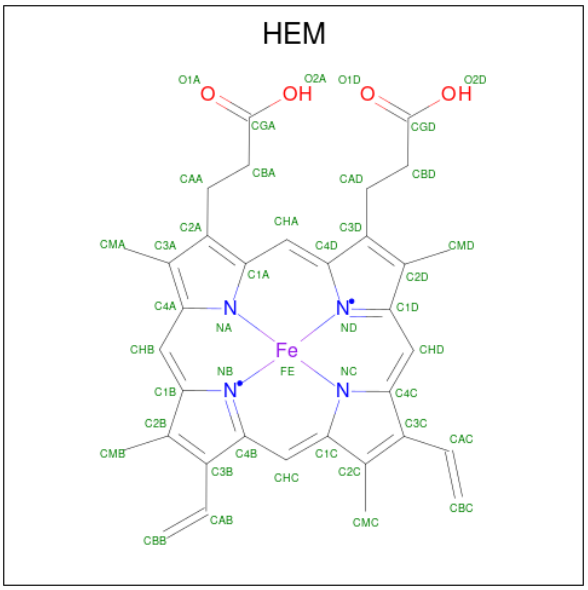
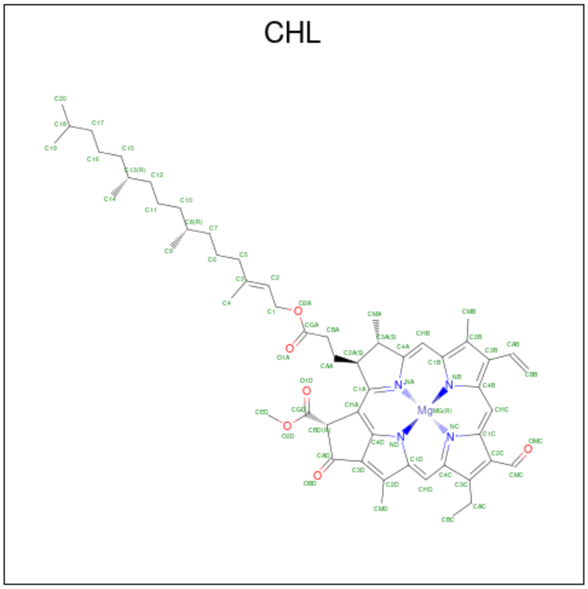
Mol	Chain	Residues	Atoms				AltConf
35	d	1	Total	C	O	P	0
			129	96	30	3	
35	d	1	Total	C	O	P	0
			129	96	30	3	
35	d	1	Total	C	O	P	0
			129	96	30	3	
35	g	1	Total	C	O	P	0
			49	38	10	1	
35	l	1	Total	C	O	P	0
			49	38	10	1	
35	n	1	Total	C	O	P	0
			49	38	10	1	
35	r	1	Total	C	O	P	0
			49	38	10	1	
35	s	1	Total	C	O	P	0
			49	38	10	1	
35	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 37 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
37	G	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	G	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	G	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	G	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	G	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	G	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	N	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	N	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	N	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	N	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	N	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	N	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	R	1	Total 150	C 117	Mg 3	N 12	O 18	0

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Mol	Chain	Residues	Atoms					AltConf
37	R	1	Total 150	C 117	Mg 3	N 12	O 18	0
37	R	1	Total 150	C 117	Mg 3	N 12	O 18	0
37	S	1	Total 201	C 157	Mg 4	N 16	O 24	0
37	S	1	Total 201	C 157	Mg 4	N 16	O 24	0
37	S	1	Total 201	C 157	Mg 4	N 16	O 24	0
37	S	1	Total 201	C 157	Mg 4	N 16	O 24	0
37	Y	1	Total 330	C 264	Mg 6	N 24	O 36	0
37	Y	1	Total 330	C 264	Mg 6	N 24	O 36	0
37	Y	1	Total 330	C 264	Mg 6	N 24	O 36	0
37	Y	1	Total 330	C 264	Mg 6	N 24	O 36	0
37	Y	1	Total 330	C 264	Mg 6	N 24	O 36	0
37	Y	1	Total 330	C 264	Mg 6	N 24	O 36	0
37	g	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	g	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	g	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	g	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	g	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	g	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	n	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	n	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	n	1	Total 314	C 248	Mg 6	N 24	O 36	0

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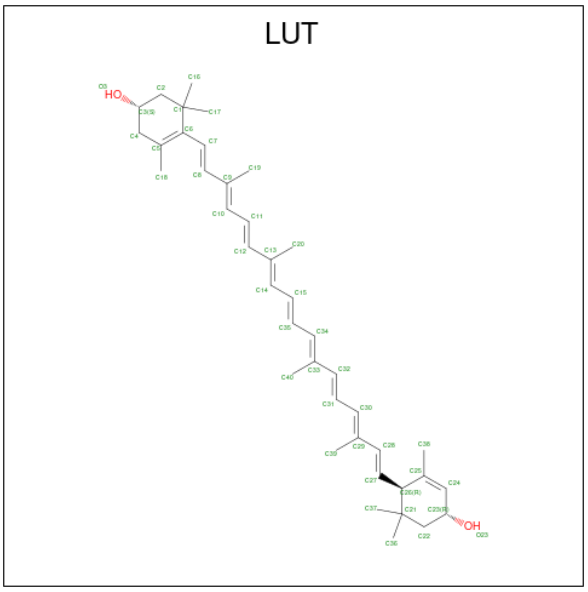
Mol	Chain	Residues	Atoms					AltConf
37	n	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	n	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	n	1	Total 314	C 248	Mg 6	N 24	O 36	0
37	r	1	Total 150	C 117	Mg 3	N 12	O 18	0
37	r	1	Total 150	C 117	Mg 3	N 12	O 18	0
37	r	1	Total 150	C 117	Mg 3	N 12	O 18	0
37	s	1	Total 201	C 157	Mg 4	N 16	O 24	0
37	s	1	Total 201	C 157	Mg 4	N 16	O 24	0
37	s	1	Total 201	C 157	Mg 4	N 16	O 24	0
37	s	1	Total 201	C 157	Mg 4	N 16	O 24	0
37	y	1	Total 330	C 264	Mg 6	N 24	O 36	0
37	y	1	Total 330	C 264	Mg 6	N 24	O 36	0
37	y	1	Total 330	C 264	Mg 6	N 24	O 36	0
37	y	1	Total 330	C 264	Mg 6	N 24	O 36	0
37	y	1	Total 330	C 264	Mg 6	N 24	O 36	0
37	y	1	Total 330	C 264	Mg 6	N 24	O 36	0

- Molecule 38 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
38	G	1	Total C O 84 80 4	0
38	G	1	Total C O 84 80 4	0
38	N	1	Total C O 84 80 4	0
38	N	1	Total C O 84 80 4	0
38	R	1	Total C O 42 40 2	0
38	S	1	Total C O 84 80 4	0
38	S	1	Total C O 84 80 4	0
38	Y	1	Total C O 84 80 4	0
38	Y	1	Total C O 84 80 4	0
38	g	1	Total C O 84 80 4	0
38	g	1	Total C O 84 80 4	0
38	n	1	Total C O 84 80 4	0
38	n	1	Total C O 84 80 4	0
38	r	1	Total C O 42 40 2	0

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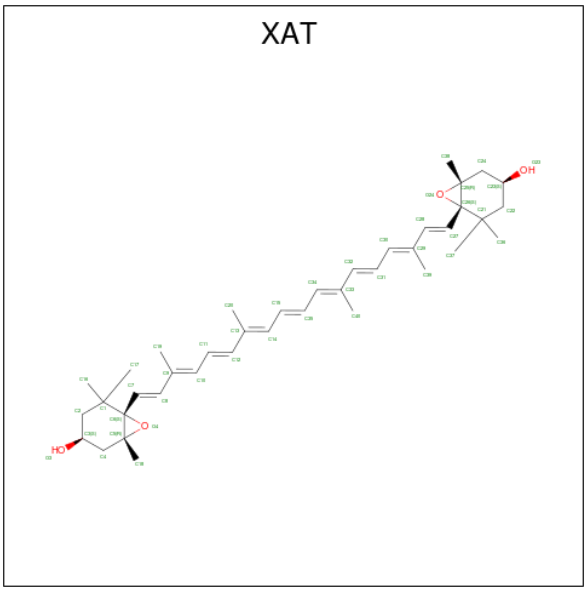
Mol	Chain	Residues	Atoms	AltConf
38	s	1	Total C O 84 80 4	0
38	s	1	Total C O 84 80 4	0
38	y	1	Total C O 84 80 4	0
38	y	1	Total C O 84 80 4	0

- Molecule 39 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
39	G	1	Total C O 44 40 4	0
39	N	1	Total C O 44 40 4	0
39	R	1	Total C O 44 40 4	0
39	Y	1	Total C O 44 40 4	0
39	g	1	Total C O 44 40 4	0
39	n	1	Total C O 44 40 4	0
39	r	1	Total C O 44 40 4	0

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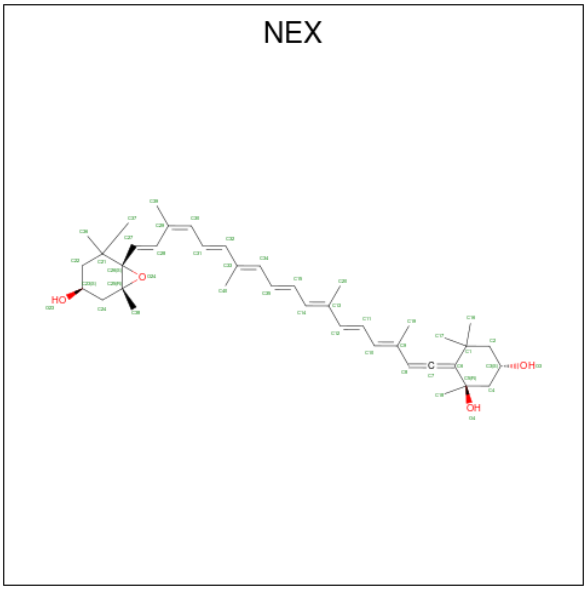
Mol	Chain	Residues	Atoms	AltConf
39	y	1	Total C O 44 40 4	0

- Molecule 40 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
40	G	1	Total C O 44 40 4	0
40	N	1	Total C O 44 40 4	0
40	R	1	Total C O 44 40 4	0
40	S	1	Total C O 44 40 4	0
40	Y	1	Total C O 44 40 4	0
40	g	1	Total C O 44 40 4	0
40	n	1	Total C O 44 40 4	0
40	r	1	Total C O 44 40 4	0
40	s	1	Total C O 44 40 4	0

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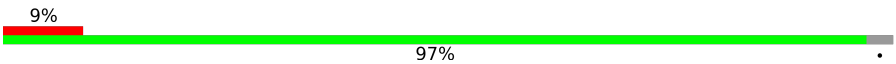
Mol	Chain	Residues	Atoms			AltConf
40	y	1	Total	C	O	0
			44	40	4	

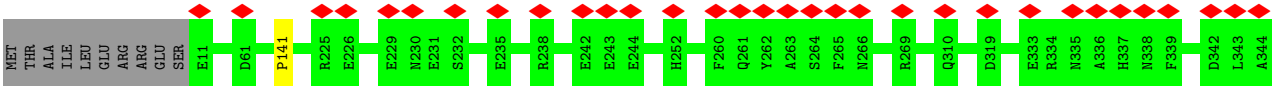
3 Residue-property plots (i)

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: Photosystem II protein D1

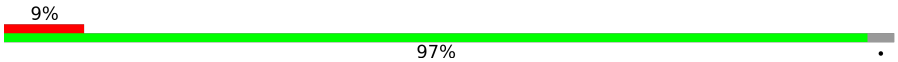
Chain A:

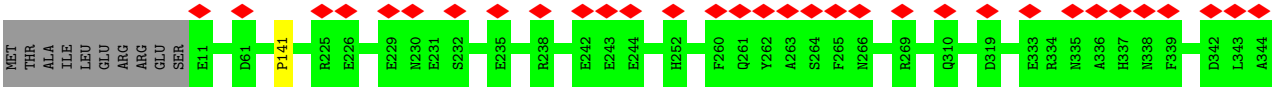




• Molecule 1: Photosystem II protein D1

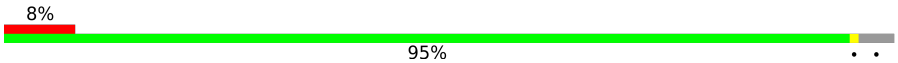
Chain a:

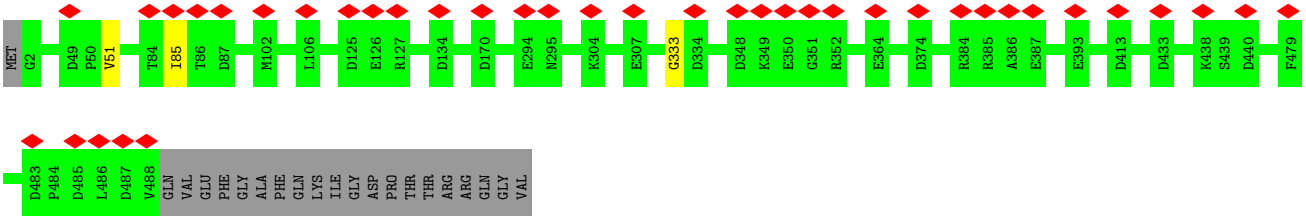




• Molecule 2: Photosystem II CP47 reaction center protein

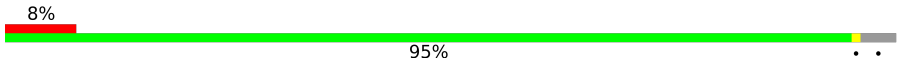
Chain B:

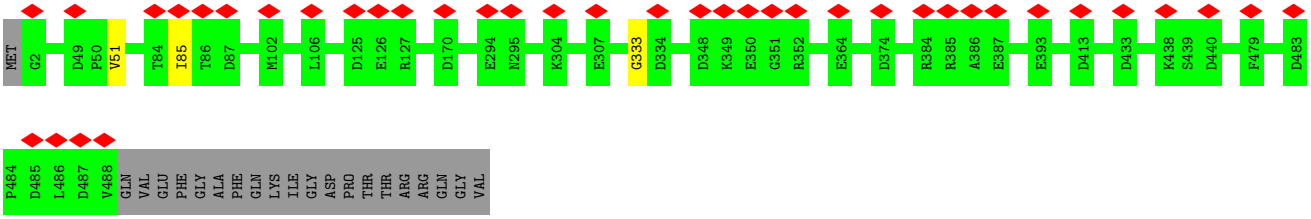




• Molecule 2: Photosystem II CP47 reaction center protein

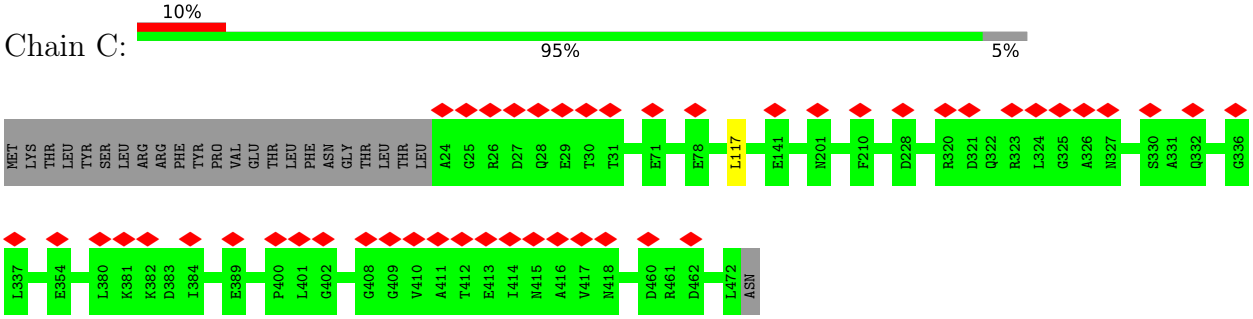
Chain b:





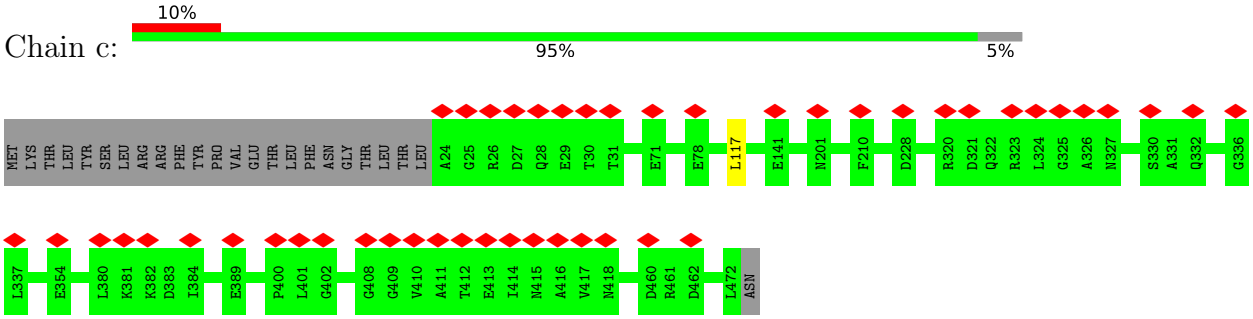
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



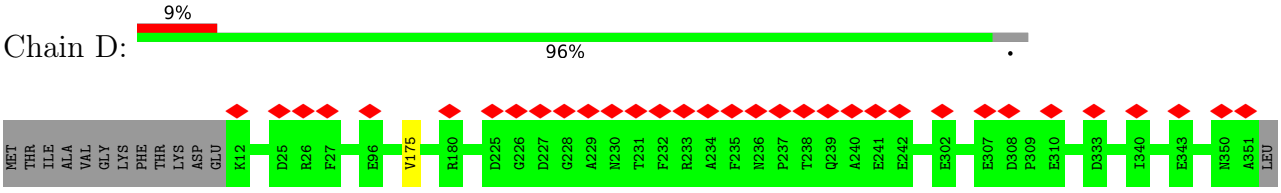
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



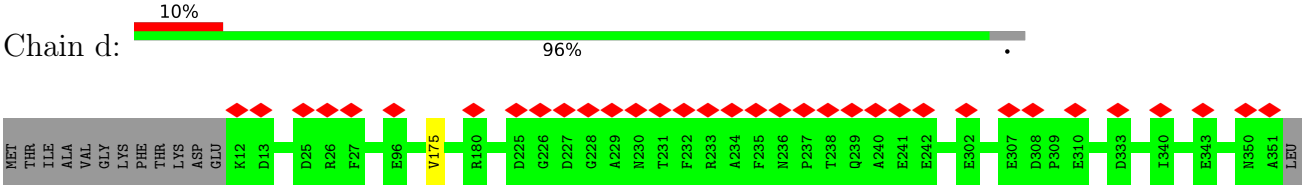
• Molecule 4: Photosystem II D2 protein

Chain D:



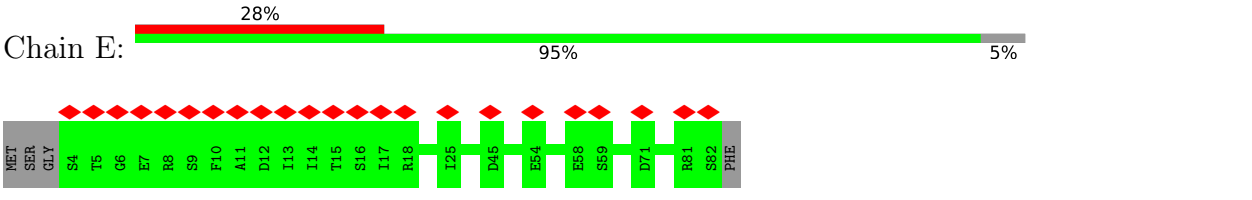
• Molecule 4: Photosystem II D2 protein

Chain d:



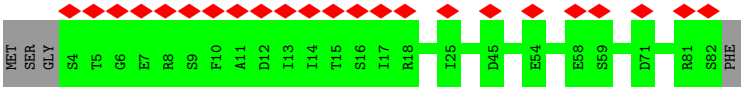
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

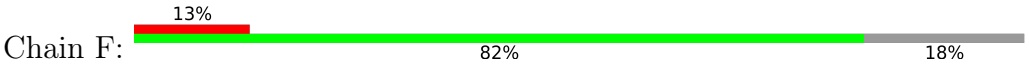


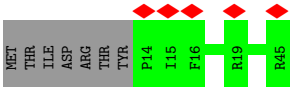
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

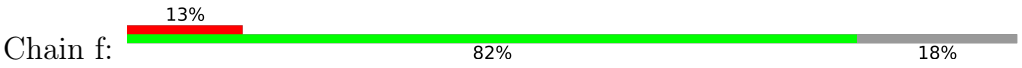


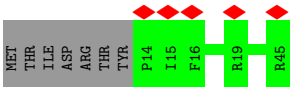
• Molecule 6: Cytochrome b559 subunit beta



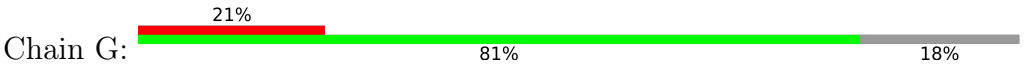


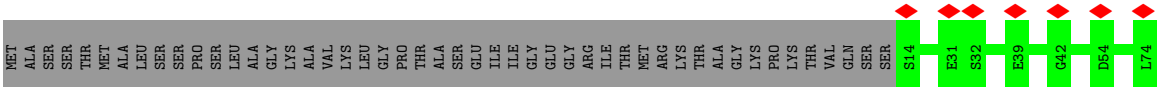
• Molecule 6: Cytochrome b559 subunit beta

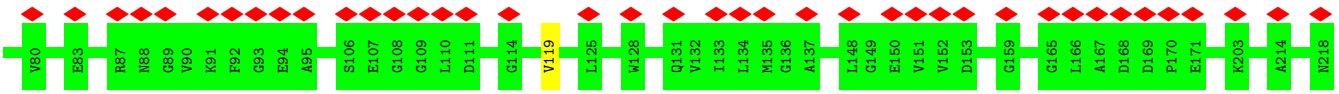


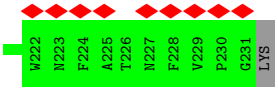


• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

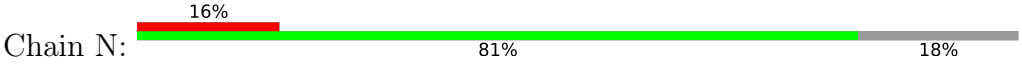


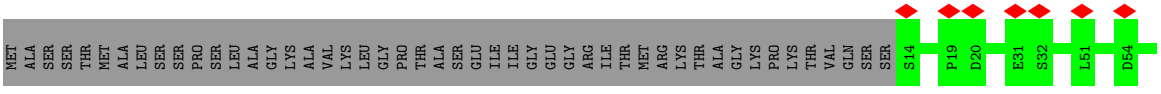


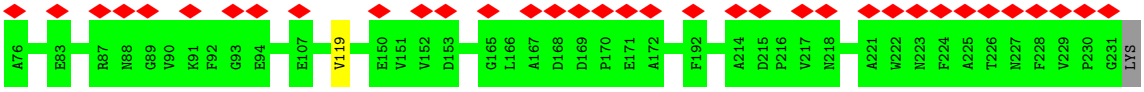




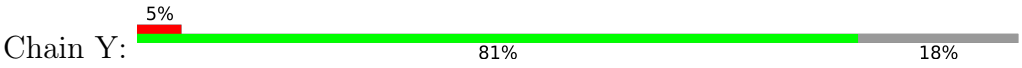
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

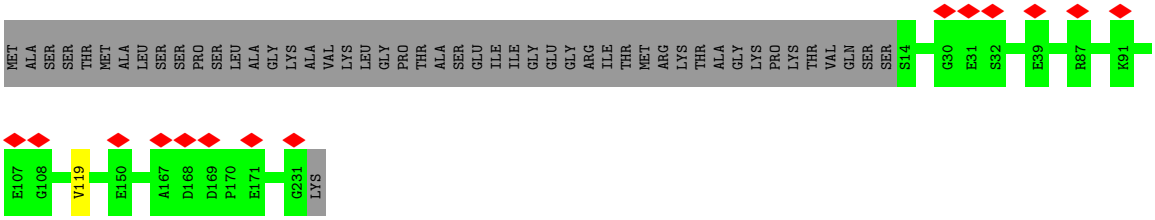




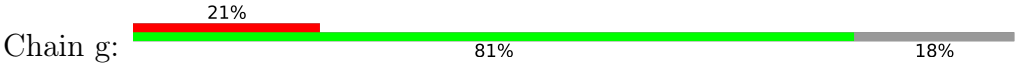


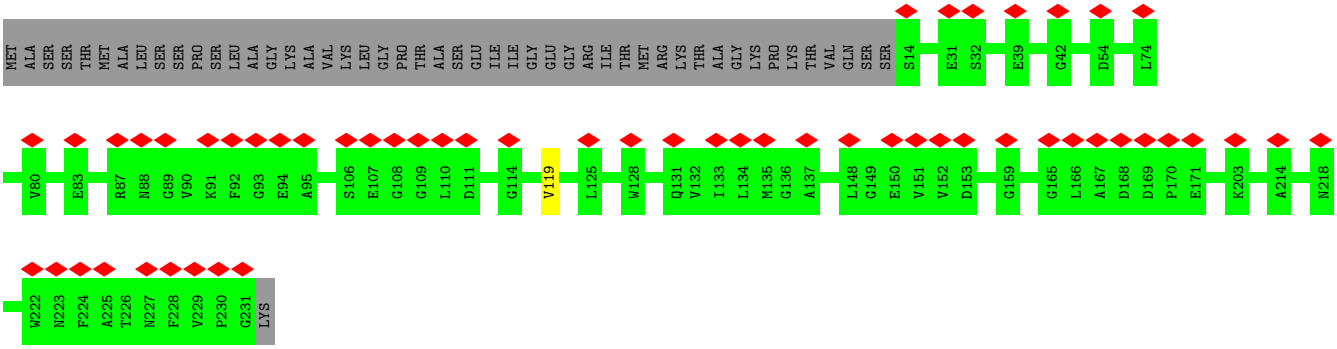
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic



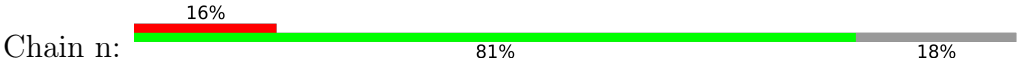


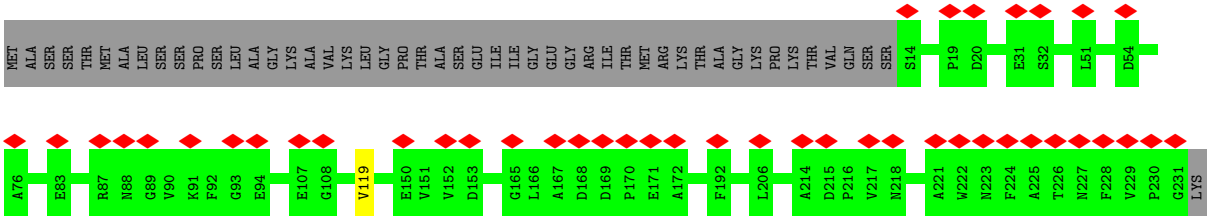
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic



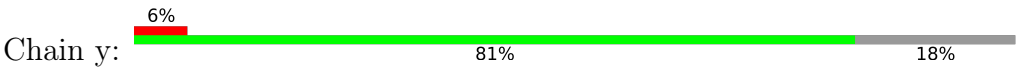


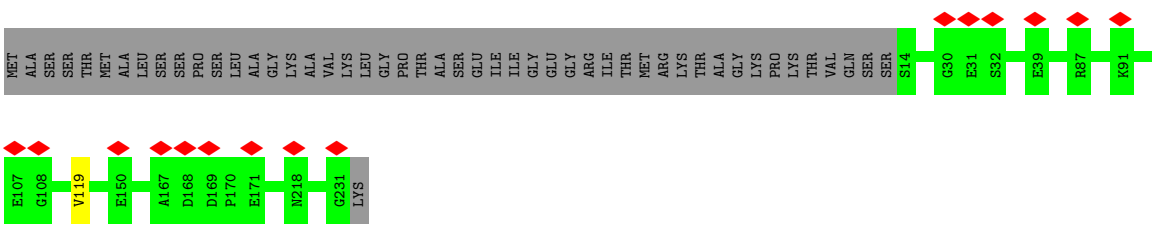
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic



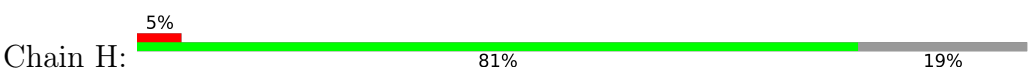


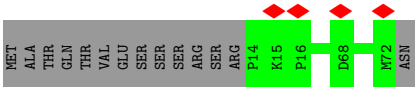
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic





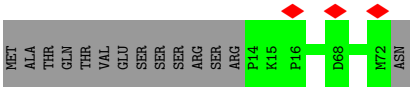
• Molecule 8: Photosystem II reaction center protein H





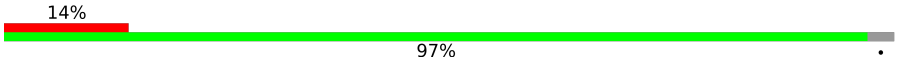
• Molecule 8: Photosystem II reaction center protein H

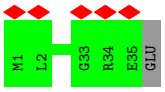
Chain h:



• Molecule 9: Protein Photosystem II reaction center protein I

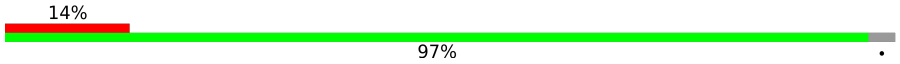
Chain I:

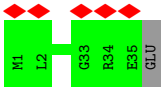




• Molecule 9: Protein Photosystem II reaction center protein I

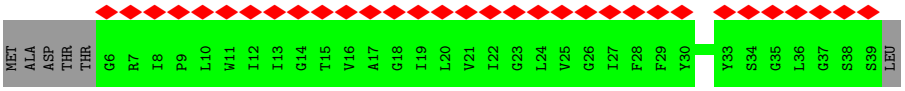
Chain i:





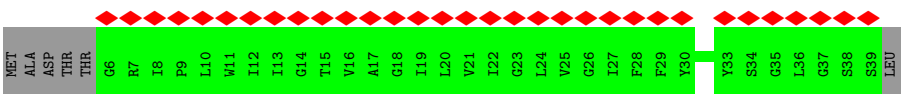
• Molecule 10: Photosystem II reaction center protein J

Chain J:



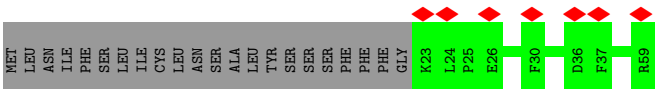
• Molecule 10: Photosystem II reaction center protein J

Chain j:



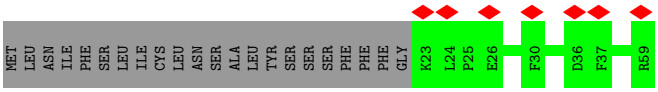
• Molecule 11: Photosystem II reaction center protein K

Chain K:



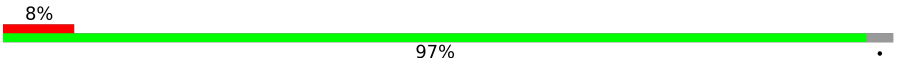
• Molecule 11: Photosystem II reaction center protein K

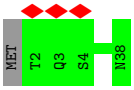
Chain k:



• Molecule 12: Protein Photosystem II reaction center protein L

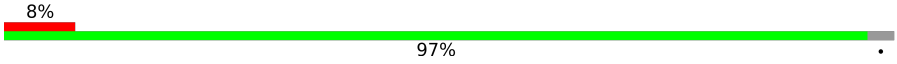
Chain L:

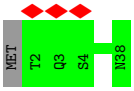




• Molecule 12: Protein Photosystem II reaction center protein L

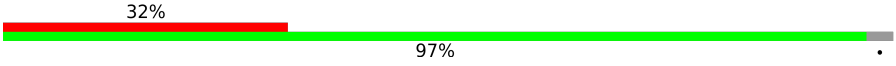
Chain l:

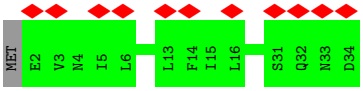




• Molecule 13: Photosystem II reaction center protein M

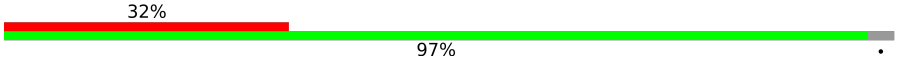
Chain M:

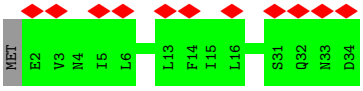




• Molecule 13: Photosystem II reaction center protein M

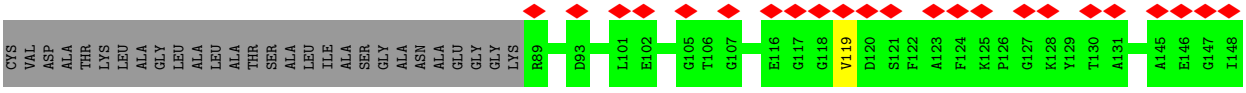
Chain m:

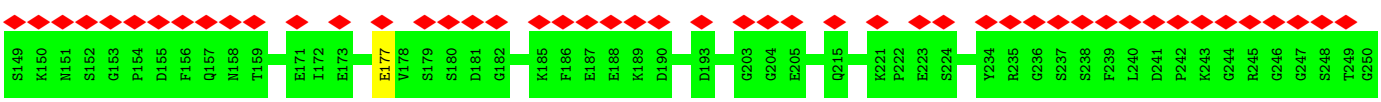


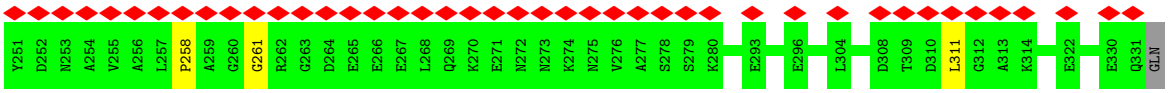


• Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O:

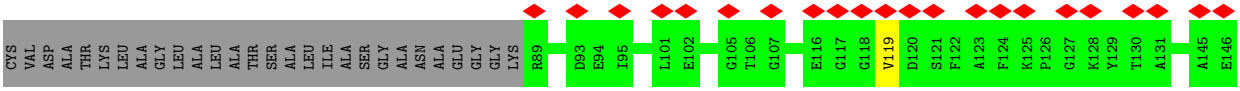


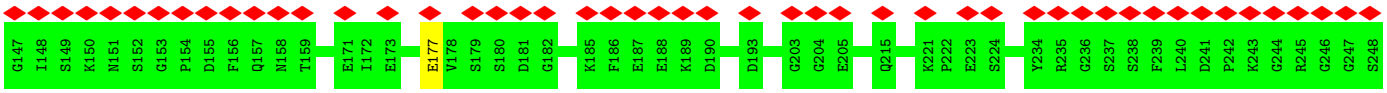




• Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

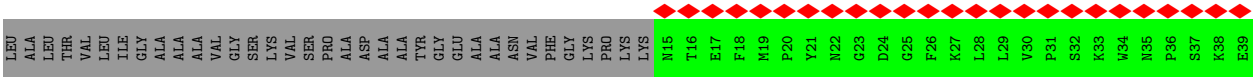
Chain o:

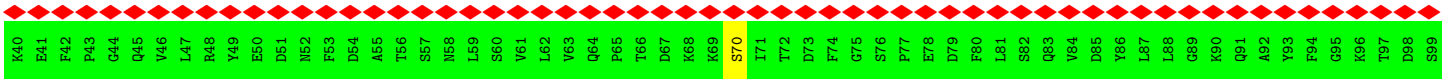


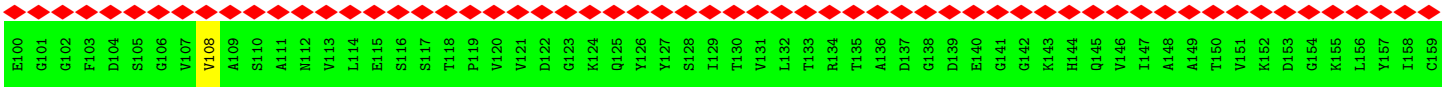


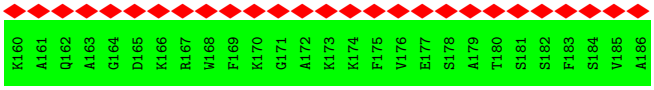
• Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain P:



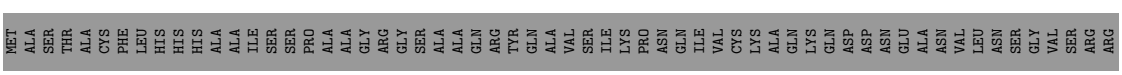


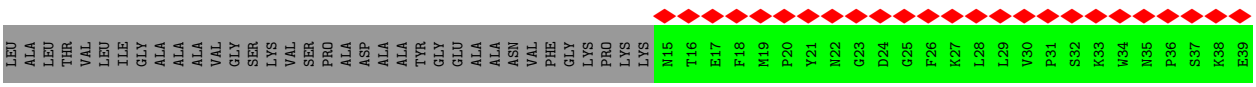




• Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain p:





K40 E41 F42 P43 G44 Q45 V46 L47 R48 Y49 E50 D51 N52 F53 D54 A55 T56 S57 N58 L59 S60 V61 L62 V63 Q64 P65 T66 D67 K68 K69 S70 I71 T72 D73 F74 G75 S76 P77 E78 D79 F80 L81 S82 Q83 Y84 D85 Y86 L87 L88 G89 K90 Q91 A92 Y93 F94 G95 K96 T97 D98 S99

E100 G101 G102 F103 D104 S105 G106 V107 V108 A109 S110 A111 N112 V113 L114 E115 S116 S117 T118 P119 V120 V121 D122 G123 K124 Q125 Y126 Y127 S128 I129 T130 V131 L132 T133 R134 T135 A136 D137 G138 D139 E140 G141 G142 K143 H144 Q145 V146 I147 A148 A149 T150 V151 K152 D153 G154 K155 L156 Y157 I158 C159

K160 A161 Q162 A163 G164 D165 K166 R167 W168 F169 K170 G171 A172 K173 K174 F175 V176 E177 S178 A179 T180 S181 S182 F183 S184 V185 A186

• Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic

Chain Q:

MET ALA GLN ALA MET ALA SER MET ALA GLY LEU ARG GLY ALA SER GLN ALA VAL LEU GLU GLY SER LEU GLN ILE SER GLY SER ASN ARG LEU SER GLY PRO THR THR SER ARG VAL ALA VAL PRO LYS MET GLY LEU ASN ILE ARG ALA GLN GLN VAL SER ALA GLU ALA GLU THR SER

ARG ARG ALA MET LEU GLY PHE VAL ALA ALA GLY LEU ALA SER GLY SER PHE VAL LYS ALA VAL LEU ALA E1 A2 R3 P4 I5 V6 V7 G8 P9 P10 P11 P12 L13 S14 G15 G16 L17 P18 G19 T20 E21 N22 S23 D24 Q25 A26 R27 D28 G29 T30 L31 P32 Y33 T34 K35 D36 R37

F38 Y39 L40 Q41 P42 L43 P44 P45 T46 E47 A48 A49 Q50 R51 A52 K53 V54 S55 A56 S57 E58 I59 L60 N61 V62 K63 Q64 F65 I66 D67 R68 K69 A70 W71 F72 S73 L74 Q75 N76 D77 L78 R79 L80 R81 A82 S83 Y84 L85 R86 Y87 D88 L89 K90 T91 V92 I93 S94 A95 K96 P97

K98 D99 E100 K101 K102 S103 L104 Q105 E106 L107 T108 S109 K110 L111 F112 S113 S114 I115 D116 N117 L118 D119 H120 A121 A122 K123 I124 K125 S126 P127 T128 E129 A130 E131 K132 Y133 Y134 G135 Q136 T137 V138 S139 N140 I141 N142 E143 V144 L145 A146 K147 L148 GLY

• Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic

Chain q:

MET ALA GLN ALA MET ALA SER MET ALA GLY LEU ARG GLY ALA SER GLN ALA VAL LEU GLU GLY SER LEU GLN ILE SER GLY SER ASN ARG LEU SER GLY PRO THR THR SER ARG VAL ALA VAL PRO LYS MET GLY LEU ASN ILE ARG ALA GLN GLN VAL SER ALA GLU ALA GLU THR SER

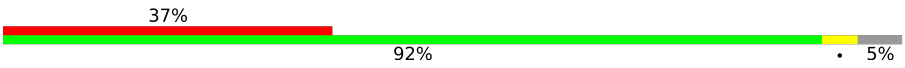
ARG ARG ALA MET LEU GLY PHE VAL ALA ALA GLY LEU ALA SER GLY SER PHE VAL LYS ALA VAL LEU ALA E1 A2 R3 P4 I5 V6 V7 G8 P9 P10 P11 P12 L13 S14 G15 G16 L17 P18 G19 T20 E21 N22 S23 D24 Q25 A26 R27 D28 G29 T30 L31 P32 Y33 T34 K35 D36 R37

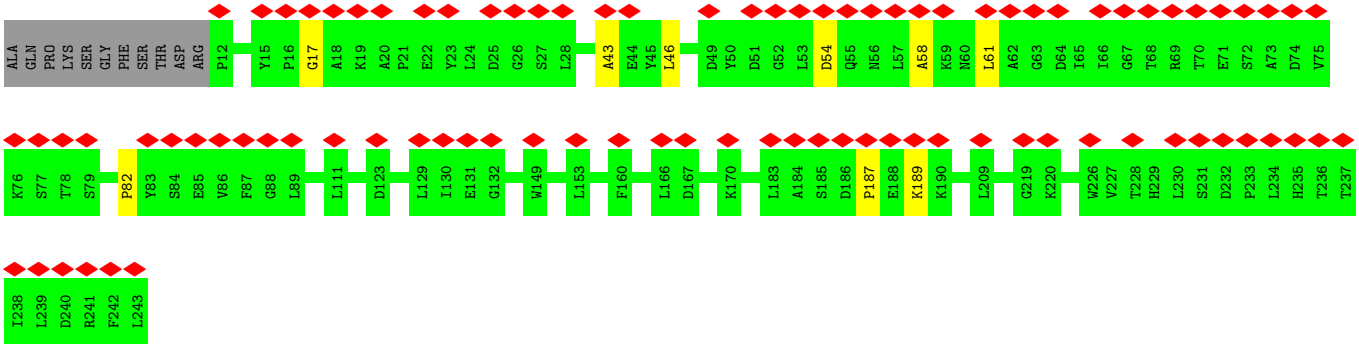
F38 Y39 L40 Q41 P42 L43 P44 P45 T46 E47 A48 A49 Q50 R51 A52 K53 V54 S55 A56 S57 E58 I59 L60 N61 V62 K63 Q64 F65 I66 D67 R68 K69 A70 W71 F72 S73 L74 Q75 N76 D77 L78 R79 L80 R81 A82 S83 Y84 L85 R86 Y87 D88 L89 K90 T91 V92 I93 S94 A95 K96 P97

K98 D99 E100 K101 K102 S103 L104 Q105 E106 L107 T108 S109 K110 L111 F112 S113 S114 I115 D116 N117 L118 D119 H120 A121 A122 K123 I124 K125 S126 P127 T128 E129 A130 E131 K132 Y133 Y134 G135 Q136 T137 V138 S139 N140 I141 N142 E143 V144 L145 A146 K147 L148 GLY

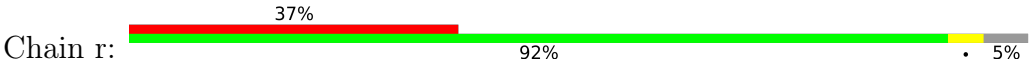
• Molecule 17: Chlorophyll A-B Binding protein 29 kD (CP29)

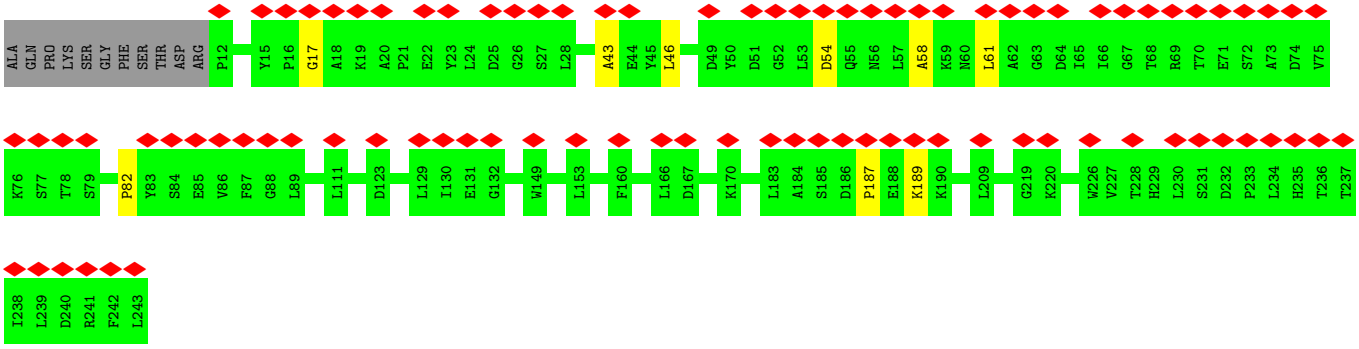
Chain R:



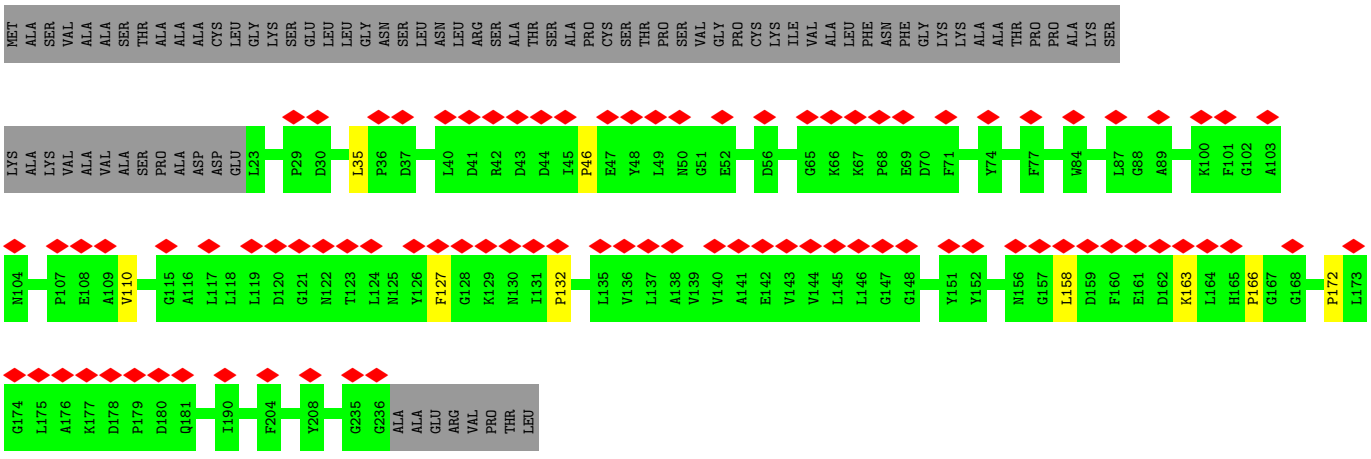


• Molecule 17: Chlorophyll A-B Binding protein 29 kD (CP29)

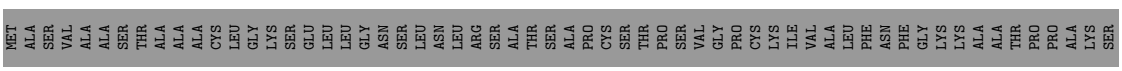




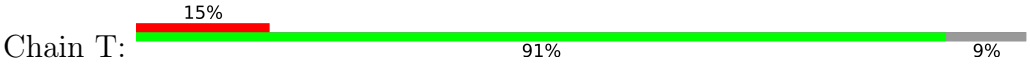
• Molecule 18: Chlorophyll A-B Binding protein 26 kD (CP26)

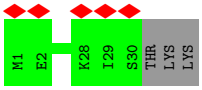


• Molecule 18: Chlorophyll A-B Binding protein 26 kD (CP26)

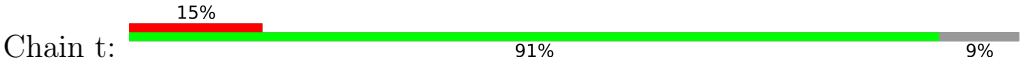


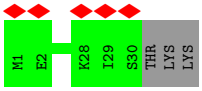
• Molecule 19: Photosystem II Reaction Center protein Tc



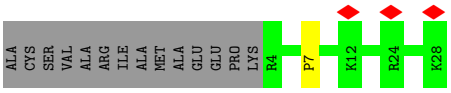


• Molecule 19: Photosystem II Reaction Center protein Tc

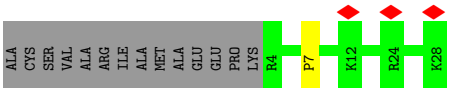




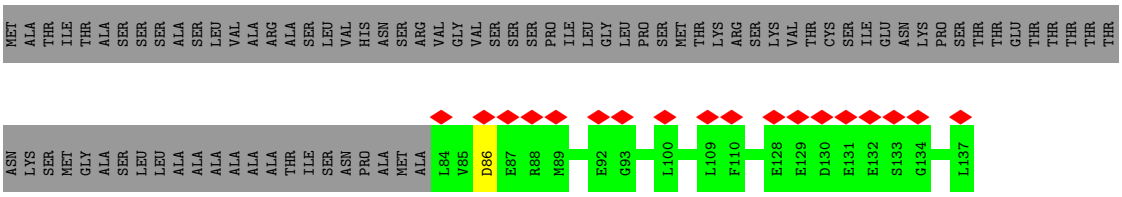
• Molecule 20: Photosystem II Reaction Center Tn protein



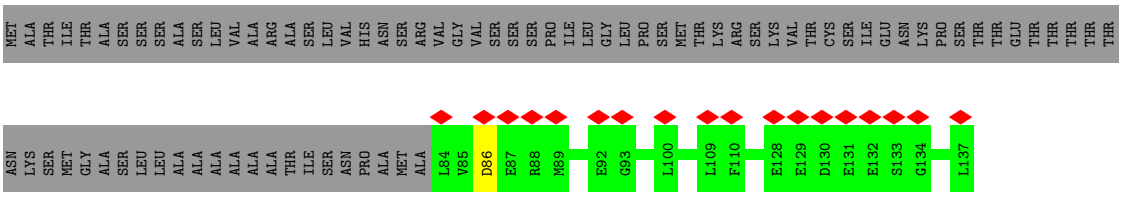
• Molecule 20: Photosystem II Reaction Center Tn protein



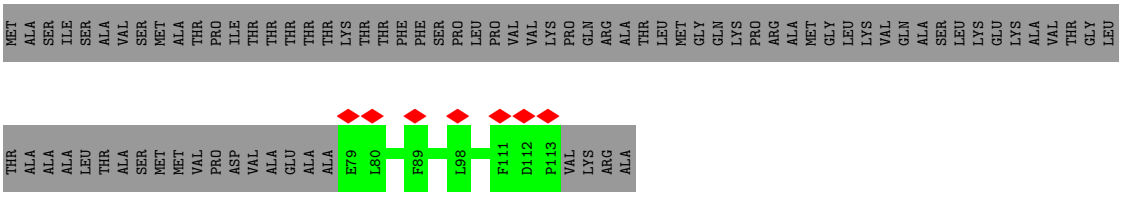
• Molecule 21: Photosystem II reaction center W protein, chloroplastic



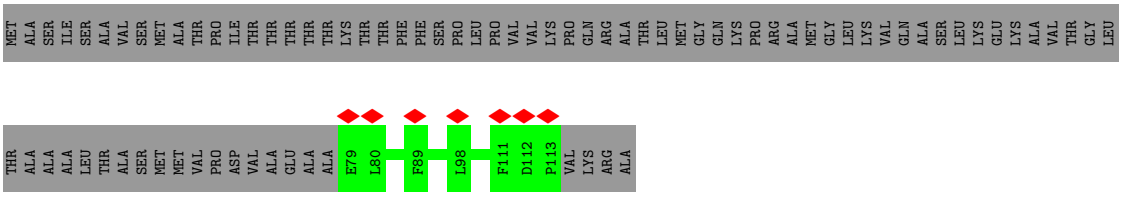
• Molecule 21: Photosystem II reaction center W protein, chloroplastic



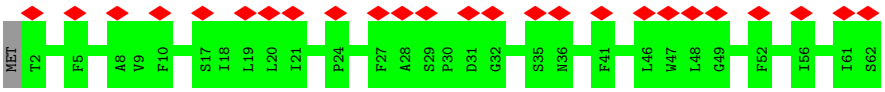
• Molecule 22: Photosystem II Reaction Center X protein



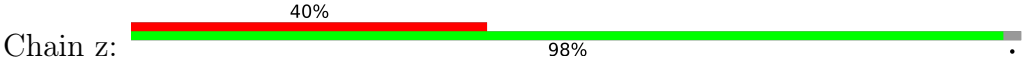
• Molecule 22: Photosystem II Reaction Center X protein

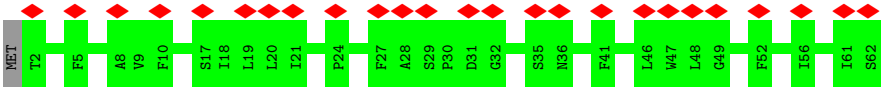


• Molecule 23: Photosystem II reaction center protein Z



• Molecule 23: Photosystem II reaction center protein Z





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	109042	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	59000	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.393	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	337.5, 337.5, 216.0	wwPDB
Map dimensions	250, 250, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.60	0/2695	0.59	0/3674
1	a	0.60	0/2695	0.59	0/3674
2	B	0.59	0/3951	0.55	0/5379
2	b	0.59	0/3951	0.55	0/5379
3	C	0.56	0/3589	0.55	0/4891
3	c	0.56	0/3589	0.55	0/4891
4	D	0.62	0/2796	0.56	0/3811
4	d	0.62	0/2796	0.56	0/3811
5	E	0.42	0/654	0.48	0/889
5	e	0.42	0/654	0.48	0/889
6	F	0.42	0/265	0.48	0/358
6	f	0.43	0/265	0.48	0/358
7	G	0.42	0/1713	0.49	0/2333
7	N	0.42	0/1713	0.49	0/2333
7	Y	0.51	0/1713	0.51	0/2333
7	g	0.42	0/1713	0.49	0/2333
7	n	0.41	0/1713	0.49	0/2333
7	y	0.51	0/1713	0.51	0/2333
8	H	0.49	0/444	0.53	0/605
8	h	0.49	0/444	0.53	0/605
9	I	0.62	0/294	0.57	0/397
9	i	0.62	0/294	0.58	0/397
10	J	0.28	0/253	0.45	0/343
10	j	0.29	0/253	0.45	0/343
11	K	0.49	0/320	0.49	0/436
11	k	0.49	0/320	0.49	0/436
12	L	0.60	0/319	0.49	0/434
12	l	0.60	0/319	0.49	0/434
13	M	0.52	0/262	0.55	0/359
13	m	0.52	0/262	0.55	0/359
14	O	0.39	0/1880	0.51	0/2541

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
14	o	0.39	0/1880	0.51	0/2541
15	P	0.28	0/1353	0.49	0/1828
15	p	0.28	0/1353	0.49	0/1828
16	Q	0.28	0/1186	0.57	2/1609 (0.1%)
16	q	0.28	0/1186	0.57	2/1609 (0.1%)
17	R	0.41	0/1853	0.55	0/2522
17	r	0.41	0/1853	0.55	0/2522
18	S	0.39	0/1700	0.62	0/2310
18	s	0.39	0/1700	0.62	0/2310
19	T	0.56	0/252	0.55	0/341
19	t	0.56	0/252	0.55	0/341
20	U	0.44	0/197	0.55	0/264
20	u	0.44	0/197	0.55	0/264
21	W	0.49	0/429	0.60	0/582
21	w	0.49	0/429	0.60	0/582
22	X	0.42	0/250	0.50	0/342
22	x	0.43	0/250	0.50	0/342
23	Z	0.38	0/464	0.53	0/636
23	z	0.38	0/464	0.53	0/636
All	All	0.50	0/61090	0.54	4/83100 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	a	0	1
18	S	0	1
18	s	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	q	42	PRO	CA-C-N	5.67	129.68	117.20
16	Q	42	PRO	CA-C-N	5.67	129.67	117.20
16	Q	42	PRO	C-N-CA	5.03	134.26	121.70
16	q	42	PRO	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	PRO	Peptide
18	S	35	LEU	Peptide
1	a	141	PRO	Peptide
18	s	35	LEU	Peptide

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	A	332/344 (96%)	321 (97%)	11 (3%)	0	100	100
1	a	332/344 (96%)	321 (97%)	11 (3%)	0	100	100
2	B	485/508 (96%)	469 (97%)	13 (3%)	3 (1%)	25	64
2	b	485/508 (96%)	469 (97%)	13 (3%)	3 (1%)	25	64
3	C	447/473 (94%)	424 (95%)	23 (5%)	0	100	100
3	c	447/473 (94%)	424 (95%)	23 (5%)	0	100	100
4	D	338/353 (96%)	317 (94%)	20 (6%)	1 (0%)	41	74
4	d	338/353 (96%)	317 (94%)	20 (6%)	1 (0%)	41	74
5	E	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
5	e	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
6	F	30/39 (77%)	30 (100%)	0	0	100	100
6	f	30/39 (77%)	30 (100%)	0	0	100	100
7	G	216/267 (81%)	208 (96%)	7 (3%)	1 (0%)	29	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	N	216/267 (81%)	210 (97%)	5 (2%)	1 (0%)	29	67
7	Y	216/267 (81%)	205 (95%)	10 (5%)	1 (0%)	29	67
7	g	216/267 (81%)	208 (96%)	7 (3%)	1 (0%)	29	67
7	n	216/267 (81%)	210 (97%)	5 (2%)	1 (0%)	29	67
7	y	216/267 (81%)	205 (95%)	10 (5%)	1 (0%)	29	67
8	H	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
8	h	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
9	I	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
9	i	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
10	J	32/40 (80%)	32 (100%)	0	0	100	100
10	j	32/40 (80%)	32 (100%)	0	0	100	100
11	K	35/59 (59%)	35 (100%)	0	0	100	100
11	k	35/59 (59%)	35 (100%)	0	0	100	100
12	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
12	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
13	M	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
13	m	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
14	O	241/332 (73%)	210 (87%)	26 (11%)	5 (2%)	7	37
14	o	241/332 (73%)	210 (87%)	26 (11%)	5 (2%)	7	37
15	P	170/267 (64%)	148 (87%)	20 (12%)	2 (1%)	13	49
15	p	170/267 (64%)	148 (87%)	20 (12%)	2 (1%)	13	49
16	Q	146/232 (63%)	134 (92%)	8 (6%)	4 (3%)	5	30
16	q	146/232 (63%)	134 (92%)	8 (6%)	4 (3%)	5	30
17	R	230/243 (95%)	211 (92%)	10 (4%)	9 (4%)	3	22
17	r	230/243 (95%)	211 (92%)	10 (4%)	9 (4%)	3	22
18	S	212/295 (72%)	187 (88%)	17 (8%)	8 (4%)	3	22
18	s	212/295 (72%)	187 (88%)	17 (8%)	8 (4%)	3	22
19	T	28/33 (85%)	28 (100%)	0	0	100	100
19	t	28/33 (85%)	28 (100%)	0	0	100	100
20	U	23/99 (23%)	21 (91%)	1 (4%)	1 (4%)	2	20
20	u	23/99 (23%)	21 (91%)	1 (4%)	1 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	W	52/137 (38%)	46 (88%)	5 (10%)	1 (2%)	8 39
21	w	52/137 (38%)	46 (88%)	5 (10%)	1 (2%)	8 39
22	X	33/117 (28%)	33 (100%)	0	0	100 100
22	x	33/117 (28%)	33 (100%)	0	0	100 100
23	Z	59/62 (95%)	56 (95%)	3 (5%)	0	100 100
23	z	59/62 (95%)	56 (95%)	3 (5%)	0	100 100
All	All	7548/9396 (80%)	7100 (94%)	374 (5%)	74 (1%)	20 54

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	85	ILE
14	O	258	PRO
14	O	311	LEU
15	P	108	VAL
18	S	110	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/279 (97%)	270 (100%)	0	100 100
1	a	270/279 (97%)	270 (100%)	0	100 100
2	B	389/406 (96%)	389 (100%)	0	100 100
2	b	389/406 (96%)	389 (100%)	0	100 100
3	C	351/374 (94%)	350 (100%)	1 (0%)	92 96
3	c	351/374 (94%)	350 (100%)	1 (0%)	92 96
4	D	272/283 (96%)	272 (100%)	0	100 100
4	d	272/283 (96%)	272 (100%)	0	100 100
5	E	70/73 (96%)	70 (100%)	0	100 100
5	e	70/73 (96%)	70 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	27/34 (79%)	27 (100%)	0	100	100
6	f	27/34 (79%)	27 (100%)	0	100	100
7	G	168/206 (82%)	168 (100%)	0	100	100
7	N	168/206 (82%)	168 (100%)	0	100	100
7	Y	168/206 (82%)	168 (100%)	0	100	100
7	g	168/206 (82%)	168 (100%)	0	100	100
7	n	168/206 (82%)	168 (100%)	0	100	100
7	y	168/206 (82%)	168 (100%)	0	100	100
8	H	48/61 (79%)	48 (100%)	0	100	100
8	h	48/61 (79%)	48 (100%)	0	100	100
9	I	32/33 (97%)	32 (100%)	0	100	100
9	i	32/33 (97%)	32 (100%)	0	100	100
10	J	25/30 (83%)	25 (100%)	0	100	100
10	j	25/30 (83%)	25 (100%)	0	100	100
11	K	32/52 (62%)	32 (100%)	0	100	100
11	k	32/52 (62%)	32 (100%)	0	100	100
12	L	35/36 (97%)	35 (100%)	0	100	100
12	l	35/36 (97%)	35 (100%)	0	100	100
13	M	29/30 (97%)	29 (100%)	0	100	100
13	m	29/30 (97%)	29 (100%)	0	100	100
14	O	202/269 (75%)	202 (100%)	0	100	100
14	o	202/269 (75%)	202 (100%)	0	100	100
15	P	144/212 (68%)	144 (100%)	0	100	100
15	p	144/212 (68%)	144 (100%)	0	100	100
16	Q	129/187 (69%)	129 (100%)	0	100	100
16	q	129/187 (69%)	129 (100%)	0	100	100
17	R	189/198 (96%)	189 (100%)	0	100	100
17	r	189/198 (96%)	189 (100%)	0	100	100
18	S	167/226 (74%)	167 (100%)	0	100	100
18	s	167/226 (74%)	167 (100%)	0	100	100
19	T	27/30 (90%)	27 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	t	27/30 (90%)	27 (100%)	0	100	100
20	U	21/80 (26%)	21 (100%)	0	100	100
20	u	21/80 (26%)	21 (100%)	0	100	100
21	W	44/110 (40%)	44 (100%)	0	100	100
21	w	44/110 (40%)	44 (100%)	0	100	100
22	X	26/90 (29%)	26 (100%)	0	100	100
22	x	26/90 (29%)	26 (100%)	0	100	100
23	Z	52/53 (98%)	52 (100%)	0	100	100
23	z	52/53 (98%)	52 (100%)	0	100	100
All	All	6170/7528 (82%)	6168 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	117	LEU
3	c	117	LEU

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

Mol	Chain	Res	Type
13	m	32	GLN
7	y	103	GLN
7	n	208	ASN
17	r	55	GLN
14	O	331	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 322 ligands modelled in this entry, 6 are monoatomic - leaving 316 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	$\#\|Z\| > 2$
27	CLA	C	513	-	49,57,73	1.63	10 (20%)	55,93,113	1.69	7 (12%)
37	CHL	r	608	-	50,58,74	2.16	16 (32%)	52,94,114	2.89	18 (34%)
27	CLA	A	407	-	49,57,73	1.63	9 (18%)	55,93,113	1.63	8 (14%)
37	CHL	y	605	7	48,56,74	2.14	13 (27%)	51,92,114	2.84	19 (37%)
37	CHL	Y	601	7	66,74,74	1.87	14 (21%)	73,114,114	2.43	23 (31%)
37	CHL	Y	605	7	48,56,74	2.15	13 (27%)	51,92,114	2.84	19 (37%)
37	CHL	s	601	18	52,60,74	2.12	15 (28%)	56,97,114	2.75	24 (42%)
27	CLA	N	610	7	65,73,73	1.44	9 (13%)	76,113,113	1.45	9 (11%)
37	CHL	r	606	-	50,58,74	2.09	14 (28%)	52,94,114	2.85	20 (38%)
37	CHL	y	609	7	66,74,74	1.84	13 (19%)	73,114,114	2.45	24 (32%)
37	CHL	G	606	-	50,58,74	2.19	14 (28%)	52,94,114	2.81	20 (38%)
27	CLA	c	503	-	65,73,73	1.45	11 (16%)	76,113,113	1.39	8 (10%)
27	CLA	y	613	7	65,73,73	1.44	10 (15%)	76,113,113	1.41	8 (10%)
37	CHL	S	601	18	52,60,74	2.11	14 (26%)	56,97,114	2.76	24 (42%)
27	CLA	C	511	3	65,73,73	1.46	10 (15%)	76,113,113	1.54	7 (9%)
37	CHL	G	608	-	50,58,74	2.16	14 (28%)	52,94,114	2.73	19 (36%)
33	BCT	d	401	-	2,3,3	0.69	0	2,3,3	1.05	0
27	CLA	N	613	7	49,57,73	1.64	9 (18%)	55,93,113	1.59	6 (10%)
27	CLA	s	609	18	49,57,73	1.70	6 (12%)	55,93,113	1.54	7 (12%)
35	LHG	Y	2630	27	48,48,48	0.74	1 (2%)	51,54,54	1.31	6 (11%)
29	BCR	B	619	-	41,41,41	0.92	3 (7%)	56,56,56	2.08	17 (30%)
27	CLA	Y	610	7	65,73,73	1.45	9 (13%)	76,113,113	1.47	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	G	604	-	49,57,73	1.65	10 (20%)	55,93,113	1.52	6 (10%)
27	CLA	c	510	-	65,73,73	1.42	9 (13%)	76,113,113	1.46	7 (9%)
27	CLA	r	612	-	49,57,73	1.67	7 (14%)	55,93,113	1.50	7 (12%)
27	CLA	B	604	-	65,73,73	1.46	10 (15%)	76,113,113	1.37	6 (7%)
35	LHG	L	101	-	48,48,48	0.72	1 (2%)	51,54,54	1.32	7 (13%)
37	CHL	Y	609	7	66,74,74	1.85	13 (19%)	73,114,114	2.46	24 (32%)
31	LMG	a	413	-	48,48,55	0.81	1 (2%)	56,56,63	1.56	13 (23%)
37	CHL	s	607	-	50,58,74	2.27	16 (32%)	52,94,114	2.74	22 (42%)
27	CLA	R	604	-	49,57,73	1.65	8 (16%)	55,93,113	1.65	7 (12%)
27	CLA	R	601	17	49,57,73	1.66	7 (14%)	55,93,113	1.63	9 (16%)
31	LMG	d	411	-	46,46,55	0.84	4 (8%)	54,54,63	1.41	7 (12%)
31	LMG	D	411	-	46,46,55	0.84	4 (8%)	54,54,63	1.41	6 (11%)
27	CLA	N	602	7	65,73,73	1.46	8 (12%)	76,113,113	1.39	6 (7%)
27	CLA	y	611	35	65,73,73	1.44	9 (13%)	76,113,113	1.39	7 (9%)
29	BCR	C	516	-	41,41,41	0.79	0	56,56,56	2.30	18 (32%)
35	LHG	R	2630	27	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
30	SQD	A	418	-	53,54,54	0.98	5 (9%)	62,65,65	1.49	10 (16%)
37	CHL	n	601	7	50,58,74	2.23	15 (30%)	52,94,114	2.77	21 (40%)
37	CHL	g	608	-	50,58,74	2.17	15 (30%)	52,94,114	2.73	19 (36%)
27	CLA	n	603	-	49,57,73	1.67	9 (18%)	55,93,113	1.60	6 (10%)
27	CLA	G	611	35	49,57,73	1.67	9 (18%)	55,93,113	1.60	9 (16%)
37	CHL	N	601	7	50,58,74	2.23	15 (30%)	52,94,114	2.78	21 (40%)
27	CLA	a	406	-	65,73,73	1.42	10 (15%)	76,113,113	1.52	8 (10%)
38	LUT	G	1621	-	42,43,43	0.92	1 (2%)	51,60,60	1.86	17 (33%)
38	LUT	N	1621	-	42,43,43	0.91	2 (4%)	51,60,60	1.76	15 (29%)
27	CLA	c	511	3	65,73,73	1.45	10 (15%)	76,113,113	1.53	7 (9%)
27	CLA	G	614	-	49,57,73	1.68	6 (12%)	55,93,113	1.57	7 (12%)
27	CLA	S	614	-	49,57,73	1.65	10 (20%)	55,93,113	1.54	7 (12%)
29	BCR	d	404	-	41,41,41	0.81	0	56,56,56	2.20	14 (25%)
27	CLA	S	612	18	49,57,73	1.64	9 (18%)	55,93,113	1.53	7 (12%)
28	PHO	a	408	-	51,69,69	1.14	6 (11%)	47,99,99	1.26	5 (10%)
27	CLA	Y	611	35	65,73,73	1.44	9 (13%)	76,113,113	1.39	7 (9%)
35	LHG	S	2630	27	48,48,48	0.64	1 (2%)	51,54,54	1.28	6 (11%)
32	DGD	h	102	-	63,63,67	0.99	4 (6%)	77,77,81	1.48	8 (10%)
27	CLA	N	604	-	49,57,73	1.64	9 (18%)	55,93,113	1.63	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	BCR	B	618	-	41,41,41	0.91	3 (7%)	56,56,56	2.19	18 (32%)
35	LHG	d	409	-	48,48,48	0.76	1 (2%)	51,54,54	1.36	9 (17%)
27	CLA	C	512	-	65,73,73	1.41	10 (15%)	76,113,113	1.43	7 (9%)
27	CLA	B	607	-	65,73,73	1.46	10 (15%)	76,113,113	1.46	11 (14%)
27	CLA	s	612	18	49,57,73	1.65	9 (18%)	55,93,113	1.53	7 (12%)
27	CLA	G	602	7	65,73,73	1.44	9 (13%)	76,113,113	1.43	6 (7%)
27	CLA	n	612	7	49,57,73	1.66	7 (14%)	55,93,113	1.59	8 (14%)
29	BCR	C	517	-	41,41,41	0.96	4 (9%)	56,56,56	2.33	16 (28%)
31	LMG	b	622	-	51,51,55	0.80	2 (3%)	59,59,63	1.45	8 (13%)
27	CLA	n	614	-	49,57,73	1.64	6 (12%)	55,93,113	1.61	7 (12%)
27	CLA	C	508	-	65,73,73	1.47	11 (16%)	76,113,113	1.57	8 (10%)
37	CHL	n	605	7	48,56,74	2.25	15 (31%)	51,92,114	2.82	21 (41%)
38	LUT	s	1620	-	42,43,43	0.86	1 (2%)	51,60,60	1.89	15 (29%)
37	CHL	G	605	7	48,56,74	2.28	16 (33%)	51,92,114	2.75	19 (37%)
37	CHL	S	607	-	50,58,74	2.26	16 (32%)	52,94,114	2.74	22 (42%)
27	CLA	Y	602	7	65,73,73	1.44	10 (15%)	76,113,113	1.48	8 (10%)
37	CHL	R	607	-	50,58,74	2.16	15 (30%)	52,94,114	2.80	21 (40%)
29	BCR	B	620	-	41,41,41	0.96	2 (4%)	56,56,56	2.12	17 (30%)
27	CLA	s	602	18	49,57,73	1.68	7 (14%)	55,93,113	1.59	8 (14%)
27	CLA	r	604	-	49,57,73	1.63	8 (16%)	55,93,113	1.64	7 (12%)
27	CLA	R	616	17	49,57,73	1.67	7 (14%)	55,93,113	1.60	9 (16%)
27	CLA	d	403	-	65,73,73	1.40	9 (13%)	76,113,113	1.47	8 (10%)
27	CLA	B	605	-	65,73,73	1.45	12 (18%)	76,113,113	1.60	9 (11%)
38	LUT	S	1620	-	42,43,43	0.87	1 (2%)	51,60,60	1.89	15 (29%)
37	CHL	N	607	-	66,74,74	1.86	13 (19%)	73,114,114	2.43	23 (31%)
37	CHL	n	609	7	50,58,74	2.16	14 (28%)	52,94,114	2.81	22 (42%)
31	LMG	z	101	-	51,51,55	0.72	0	59,59,63	1.35	6 (10%)
27	CLA	C	506	-	65,73,73	1.46	10 (15%)	76,113,113	1.47	8 (10%)
27	CLA	g	604	-	49,57,73	1.65	10 (20%)	55,93,113	1.52	6 (10%)
27	CLA	S	609	18	49,57,73	1.71	6 (12%)	55,93,113	1.54	7 (12%)
27	CLA	b	603	-	65,73,73	1.44	10 (15%)	76,113,113	1.38	7 (9%)
27	CLA	B	609	-	65,73,73	1.41	9 (13%)	76,113,113	1.44	9 (11%)
40	NEX	N	1623	-	38,46,46	1.03	2 (5%)	50,70,70	2.51	15 (30%)
27	CLA	s	603	-	49,57,73	1.64	7 (14%)	55,93,113	1.56	6 (10%)
27	CLA	c	513	-	49,57,73	1.64	10 (20%)	55,93,113	1.70	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	D	403	-	65,73,73	1.41	8 (12%)	76,113,113	1.47	8 (10%)
27	CLA	C	502	-	65,73,73	1.42	10 (15%)	76,113,113	1.45	7 (9%)
29	BCR	c	517	-	41,41,41	0.96	3 (7%)	56,56,56	2.33	16 (28%)
27	CLA	c	505	-	65,73,73	1.45	9 (13%)	76,113,113	1.55	8 (10%)
40	NEX	R	623	-	38,46,46	1.09	2 (5%)	50,70,70	2.41	21 (42%)
27	CLA	b	606	-	65,73,73	1.50	10 (15%)	76,113,113	1.37	9 (11%)
27	CLA	c	508	-	65,73,73	1.48	11 (16%)	76,113,113	1.58	8 (10%)
27	CLA	Y	603	-	49,57,73	1.68	9 (18%)	55,93,113	1.53	6 (10%)
28	PHO	a	409	-	51,69,69	1.14	7 (13%)	47,99,99	1.38	6 (12%)
27	CLA	Y	613	7	65,73,73	1.45	10 (15%)	76,113,113	1.40	7 (9%)
34	PL9	D	405	-	55,55,55	1.88	12 (21%)	68,69,69	1.57	15 (22%)
35	LHG	s	2630	27	48,48,48	0.64	1 (2%)	51,54,54	1.28	6 (11%)
27	CLA	s	611	35	49,57,73	1.65	10 (20%)	55,93,113	1.58	8 (14%)
32	DGD	c	518	-	56,56,67	1.14	9 (16%)	70,70,81	1.71	16 (22%)
39	XAT	R	622	-	39,47,47	0.98	1 (2%)	54,74,74	2.85	22 (40%)
27	CLA	N	612	7	49,57,73	1.66	9 (18%)	55,93,113	1.60	8 (14%)
27	CLA	R	609	17	49,57,73	1.64	7 (14%)	55,93,113	1.57	7 (12%)
37	CHL	G	601	7	66,74,74	1.86	14 (21%)	73,114,114	2.44	24 (32%)
37	CHL	N	605	7	48,56,74	2.24	15 (31%)	51,92,114	2.82	21 (41%)
35	LHG	N	2630	27	48,48,48	0.61	1 (2%)	51,54,54	1.28	6 (11%)
38	LUT	y	1620	-	42,43,43	0.93	2 (4%)	51,60,60	1.83	18 (35%)
27	CLA	A	410	-	60,68,73	1.46	11 (18%)	70,107,113	1.57	8 (11%)
27	CLA	b	611	-	65,73,73	1.44	10 (15%)	76,113,113	1.45	8 (10%)
27	CLA	c	512	-	65,73,73	1.41	10 (15%)	76,113,113	1.43	7 (9%)
27	CLA	G	610	7	65,73,73	1.45	7 (10%)	76,113,113	1.45	8 (10%)
27	CLA	y	612	7	65,73,73	1.43	10 (15%)	76,113,113	1.37	8 (10%)
29	BCR	D	404	-	41,41,41	0.80	0	56,56,56	2.20	14 (25%)
32	DGD	C	518	-	56,56,67	1.14	8 (14%)	70,70,81	1.71	16 (22%)
28	PHO	A	408	-	51,69,69	1.14	6 (11%)	47,99,99	1.26	5 (10%)
24	OEX	A	401	3,1	0,15,15	-	-	-		
27	CLA	g	603	-	49,57,73	1.67	8 (16%)	55,93,113	1.59	7 (12%)
27	CLA	R	610	17	65,73,73	1.45	7 (10%)	76,113,113	1.44	7 (9%)
38	LUT	G	1620	-	42,43,43	0.87	1 (2%)	51,60,60	1.78	15 (29%)
27	CLA	C	504	-	65,73,73	1.44	10 (15%)	76,113,113	1.44	6 (7%)
27	CLA	B	610	-	65,73,73	1.45	10 (15%)	76,113,113	1.42	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	R	603	-	49,57,73	1.66	9 (18%)	55,93,113	1.53	7 (12%)
27	CLA	r	613	17	49,57,73	1.64	8 (16%)	55,93,113	1.63	7 (12%)
37	CHL	R	606	-	50,58,74	2.09	14 (28%)	52,94,114	2.85	20 (38%)
27	CLA	N	611	35	49,57,73	1.65	7 (14%)	55,93,113	1.63	8 (14%)
27	CLA	c	509	-	65,73,73	1.45	10 (15%)	76,113,113	1.56	12 (15%)
35	LHG	n	2630	27	48,48,48	0.61	1 (2%)	51,54,54	1.28	6 (11%)
27	CLA	b	617	-	65,73,73	1.47	9 (13%)	76,113,113	1.43	7 (9%)
27	CLA	B	615	-	65,73,73	1.42	10 (15%)	76,113,113	1.38	7 (9%)
27	CLA	n	604	-	49,57,73	1.63	9 (18%)	55,93,113	1.63	6 (10%)
27	CLA	g	613	7	49,57,73	1.68	10 (20%)	55,93,113	1.57	7 (12%)
37	CHL	y	606	-	50,58,74	2.11	14 (28%)	52,94,114	2.82	20 (38%)
27	CLA	R	613	17	49,57,73	1.64	8 (16%)	55,93,113	1.61	7 (12%)
27	CLA	G	612	7	49,57,73	1.70	10 (20%)	55,93,113	1.55	7 (12%)
30	SQD	b	621	-	53,54,54	0.95	5 (9%)	62,65,65	1.56	10 (16%)
27	CLA	g	610	7	65,73,73	1.45	7 (10%)	76,113,113	1.45	9 (11%)
39	XAT	n	1622	-	39,47,47	1.00	1 (2%)	54,74,74	3.05	23 (42%)
32	DGD	H	102	-	63,63,67	0.99	4 (6%)	77,77,81	1.48	8 (10%)
27	CLA	Y	604	-	49,57,73	1.67	10 (20%)	55,93,113	1.64	7 (12%)
32	DGD	c	519	-	63,63,67	0.98	4 (6%)	77,77,81	1.51	13 (16%)
37	CHL	G	609	7	50,58,74	2.20	15 (30%)	52,94,114	2.80	19 (36%)
37	CHL	g	607	-	50,58,74	2.12	14 (28%)	52,94,114	2.78	19 (36%)
27	CLA	B	611	-	65,73,73	1.43	10 (15%)	76,113,113	1.45	8 (10%)
27	CLA	D	402	-	65,73,73	1.46	10 (15%)	76,113,113	1.49	8 (10%)
27	CLA	c	507	-	65,73,73	1.49	10 (15%)	76,113,113	1.35	8 (10%)
27	CLA	c	501	-	65,73,73	1.46	10 (15%)	76,113,113	1.40	8 (10%)
27	CLA	B	617	-	65,73,73	1.47	9 (13%)	76,113,113	1.43	7 (9%)
29	BCR	C	514	-	41,41,41	0.91	1 (2%)	56,56,56	2.02	18 (32%)
27	CLA	R	611	35	49,57,73	1.66	6 (12%)	55,93,113	1.53	7 (12%)
27	CLA	C	507	-	65,73,73	1.49	10 (15%)	76,113,113	1.36	8 (10%)
29	BCR	a	411	-	41,41,41	0.91	2 (4%)	56,56,56	2.09	17 (30%)
27	CLA	Y	614	-	49,57,73	1.60	8 (16%)	55,93,113	1.56	7 (12%)
37	CHL	R	608	-	50,58,74	2.16	16 (32%)	52,94,114	2.88	19 (36%)
27	CLA	S	604	-	49,57,73	1.62	8 (16%)	55,93,113	1.69	7 (12%)
27	CLA	b	616	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	6 (7%)
27	CLA	r	611	35	49,57,73	1.66	6 (12%)	55,93,113	1.53	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	CHL	S	608	-	49,57,74	2.34	15 (30%)	52,93,114	2.65	21 (40%)
38	LUT	g	1620	-	42,43,43	0.85	1 (2%)	51,60,60	1.79	15 (29%)
27	CLA	N	603	-	49,57,73	1.68	9 (18%)	55,93,113	1.59	6 (10%)
27	CLA	c	504	-	65,73,73	1.44	10 (15%)	76,113,113	1.43	6 (7%)
40	NEX	n	1623	-	38,46,46	1.02	1 (2%)	50,70,70	2.50	16 (32%)
38	LUT	N	1620	-	42,43,43	0.85	1 (2%)	51,60,60	1.83	16 (31%)
29	BCR	b	619	-	41,41,41	0.92	3 (7%)	56,56,56	2.09	17 (30%)
37	CHL	s	608	-	49,57,74	2.34	15 (30%)	52,93,114	2.65	20 (38%)
37	CHL	g	601	7	66,74,74	1.86	13 (19%)	73,114,114	2.44	22 (30%)
27	CLA	d	402	-	65,73,73	1.46	10 (15%)	76,113,113	1.49	8 (10%)
27	CLA	r	601	17	49,57,73	1.66	6 (12%)	55,93,113	1.62	9 (16%)
30	SQD	a	412	-	53,54,54	0.97	5 (9%)	62,65,65	1.45	9 (14%)
37	CHL	Y	606	-	50,58,74	2.11	14 (28%)	52,94,114	2.82	20 (38%)
37	CHL	n	607	-	66,74,74	1.86	14 (21%)	73,114,114	2.44	22 (30%)
27	CLA	s	614	-	49,57,73	1.65	10 (20%)	55,93,113	1.53	7 (12%)
39	XAT	r	622	-	39,47,47	0.99	1 (2%)	54,74,74	2.84	21 (38%)
27	CLA	r	616	17	49,57,73	1.67	7 (14%)	55,93,113	1.59	9 (16%)
29	BCR	c	515	-	41,41,41	0.90	1 (2%)	56,56,56	2.15	18 (32%)
37	CHL	s	606	-	50,58,74	2.22	16 (32%)	52,94,114	2.74	20 (38%)
27	CLA	c	506	-	65,73,73	1.46	10 (15%)	76,113,113	1.48	8 (10%)
27	CLA	b	609	-	65,73,73	1.41	10 (15%)	76,113,113	1.44	9 (11%)
40	NEX	Y	1623	-	38,46,46	1.10	2 (5%)	50,70,70	2.50	16 (32%)
27	CLA	b	605	-	65,73,73	1.45	12 (18%)	76,113,113	1.60	10 (13%)
39	XAT	N	1622	-	39,47,47	1.00	1 (2%)	54,74,74	3.06	23 (42%)
29	BCR	C	515	-	41,41,41	0.90	1 (2%)	56,56,56	2.15	18 (32%)
27	CLA	S	602	18	49,57,73	1.68	7 (14%)	55,93,113	1.60	7 (12%)
27	CLA	R	602	17	65,73,73	1.44	8 (12%)	76,113,113	1.40	7 (9%)
27	CLA	B	602	-	65,73,73	1.45	10 (15%)	76,113,113	1.39	8 (10%)
37	CHL	n	608	-	50,58,74	2.09	14 (28%)	52,94,114	2.87	20 (38%)
27	CLA	G	613	7	49,57,73	1.68	10 (20%)	55,93,113	1.57	7 (12%)
38	LUT	g	1621	-	42,43,43	0.91	1 (2%)	51,60,60	1.87	17 (33%)
40	NEX	S	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.42	14 (28%)
38	LUT	r	620	-	42,43,43	0.82	1 (2%)	51,60,60	1.66	15 (29%)
37	CHL	y	607	-	50,58,74	2.09	15 (30%)	52,94,114	2.77	21 (40%)
27	CLA	r	609	17	49,57,73	1.65	7 (14%)	55,93,113	1.57	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	B	608	-	65,73,73	1.43	10 (15%)	76,113,113	1.46	8 (10%)
35	LHG	D	409	-	48,48,48	0.76	1 (2%)	51,54,54	1.36	8 (15%)
27	CLA	Y	612	7	65,73,73	1.43	10 (15%)	76,113,113	1.38	8 (10%)
39	XAT	g	1622	-	39,47,47	0.96	2 (5%)	54,74,74	2.99	19 (35%)
27	CLA	a	410	-	60,68,73	1.47	11 (18%)	70,107,113	1.57	8 (11%)
27	CLA	B	614	-	65,73,73	1.46	10 (15%)	76,113,113	1.37	8 (10%)
27	CLA	g	602	7	65,73,73	1.44	9 (13%)	76,113,113	1.43	6 (7%)
29	BCR	A	411	-	41,41,41	0.92	2 (4%)	56,56,56	2.09	17 (30%)
27	CLA	B	612	-	65,73,73	1.47	10 (15%)	76,113,113	1.52	9 (11%)
39	XAT	Y	1622	-	39,47,47	0.90	0	54,74,74	3.05	20 (37%)
35	LHG	d	410	-	36,36,48	0.70	0	39,42,54	1.27	4 (10%)
35	LHG	D	410	-	36,36,48	0.70	0	39,42,54	1.27	4 (10%)
38	LUT	y	1621	-	42,43,43	1.01	3 (7%)	51,60,60	1.94	18 (35%)
27	CLA	b	610	-	65,73,73	1.45	10 (15%)	76,113,113	1.42	8 (10%)
27	CLA	a	407	-	49,57,73	1.64	10 (20%)	55,93,113	1.63	8 (14%)
31	LMG	C	521	-	51,51,55	0.74	0	59,59,63	1.39	8 (13%)
40	NEX	r	623	-	38,46,46	1.09	1 (2%)	50,70,70	2.41	21 (42%)
29	BCR	h	101	-	41,41,41	0.87	1 (2%)	56,56,56	2.00	19 (33%)
27	CLA	b	613	-	65,73,73	1.43	9 (13%)	76,113,113	1.55	8 (10%)
37	CHL	g	609	7	50,58,74	2.20	15 (30%)	52,94,114	2.80	19 (36%)
27	CLA	b	615	-	65,73,73	1.43	10 (15%)	76,113,113	1.38	7 (9%)
27	CLA	b	614	-	65,73,73	1.46	10 (15%)	76,113,113	1.36	9 (11%)
27	CLA	n	613	7	49,57,73	1.64	9 (18%)	55,93,113	1.59	6 (10%)
31	LMG	c	521	-	51,51,55	0.74	0	59,59,63	1.39	7 (11%)
40	NEX	y	1623	-	38,46,46	1.09	2 (5%)	50,70,70	2.50	16 (32%)
37	CHL	n	606	-	50,58,74	2.11	14 (28%)	52,94,114	2.92	20 (38%)
36	HEM	F	101	5,6	41,50,50	1.92	5 (12%)	45,82,82	1.43	5 (11%)
33	BCT	D	401	-	2,3,3	0.69	0	2,3,3	1.05	0
27	CLA	n	610	7	65,73,73	1.45	10 (15%)	76,113,113	1.44	9 (11%)
37	CHL	g	605	7	48,56,74	2.28	16 (33%)	51,92,114	2.74	19 (37%)
27	CLA	r	603	-	49,57,73	1.67	9 (18%)	55,93,113	1.55	7 (12%)
31	LMG	A	413	-	48,48,55	0.81	1 (2%)	56,56,63	1.56	13 (23%)
37	CHL	N	609	7	50,58,74	2.15	13 (26%)	52,94,114	2.81	22 (42%)
37	CHL	Y	607	-	50,58,74	2.09	15 (30%)	52,94,114	2.77	20 (38%)
37	CHL	y	608	-	50,58,74	2.11	13 (26%)	52,94,114	2.77	18 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	HEM	f	101	5,6	41,50,50	1.91	5 (12%)	45,82,82	1.42	5 (11%)
35	LHG	G	2630	27	48,48,48	0.61	1 (2%)	51,54,54	1.28	7 (13%)
27	CLA	b	604	-	65,73,73	1.45	10 (15%)	76,113,113	1.37	6 (7%)
27	CLA	a	405	-	65,73,73	1.46	9 (13%)	76,113,113	1.51	8 (10%)
27	CLA	S	603	-	49,57,73	1.64	7 (14%)	55,93,113	1.56	6 (10%)
35	LHG	d	408	-	42,42,48	0.77	1 (2%)	45,48,54	1.28	5 (11%)
30	SQD	A	412	-	53,54,54	0.98	5 (9%)	62,65,65	1.44	10 (16%)
27	CLA	B	616	-	65,73,73	1.44	9 (13%)	76,113,113	1.38	6 (7%)
32	DGD	c	520	-	63,63,67	0.97	4 (6%)	77,77,81	1.51	11 (14%)
27	CLA	N	614	-	49,57,73	1.63	7 (14%)	55,93,113	1.62	7 (12%)
40	NEX	s	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.43	14 (28%)
27	CLA	n	611	35	49,57,73	1.64	8 (16%)	55,93,113	1.63	8 (14%)
38	LUT	s	1621	-	42,43,43	0.87	1 (2%)	51,60,60	1.76	17 (33%)
27	CLA	r	610	17	65,73,73	1.46	7 (10%)	76,113,113	1.44	7 (9%)
27	CLA	B	606	-	65,73,73	1.51	10 (15%)	76,113,113	1.36	9 (11%)
27	CLA	S	613	18	49,57,73	1.63	9 (18%)	55,93,113	1.58	6 (10%)
38	LUT	Y	1620	-	42,43,43	0.93	2 (4%)	51,60,60	1.83	18 (35%)
27	CLA	y	614	-	49,57,73	1.61	8 (16%)	55,93,113	1.58	7 (12%)
27	CLA	b	607	-	65,73,73	1.46	10 (15%)	76,113,113	1.46	11 (14%)
37	CHL	Y	608	-	50,58,74	2.11	13 (26%)	52,94,114	2.77	19 (36%)
27	CLA	S	610	18	49,57,73	1.63	7 (14%)	55,93,113	1.63	7 (12%)
35	LHG	D	408	-	42,42,48	0.77	1 (2%)	45,48,54	1.28	5 (11%)
37	CHL	S	606	-	50,58,74	2.22	16 (32%)	52,94,114	2.74	19 (36%)
37	CHL	g	606	-	50,58,74	2.18	15 (30%)	52,94,114	2.81	20 (38%)
40	NEX	g	1623	-	38,46,46	1.01	2 (5%)	50,70,70	2.59	16 (32%)
27	CLA	R	612	-	49,57,73	1.65	6 (12%)	55,93,113	1.50	7 (12%)
29	BCR	c	516	-	41,41,41	0.78	0	56,56,56	2.30	18 (32%)
27	CLA	b	602	-	65,73,73	1.45	10 (15%)	76,113,113	1.39	8 (10%)
38	LUT	n	1621	-	42,43,43	0.90	2 (4%)	51,60,60	1.77	15 (29%)
27	CLA	B	603	-	65,73,73	1.44	10 (15%)	76,113,113	1.38	7 (9%)
27	CLA	y	610	7	65,73,73	1.45	9 (13%)	76,113,113	1.46	8 (10%)
34	PL9	d	405	-	55,55,55	1.88	12 (21%)	68,69,69	1.57	15 (22%)
27	CLA	y	603	-	49,57,73	1.68	9 (18%)	55,93,113	1.54	6 (10%)
27	CLA	C	505	-	65,73,73	1.45	9 (13%)	76,113,113	1.55	8 (10%)
29	BCR	H	101	-	41,41,41	0.86	1 (2%)	56,56,56	2.01	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	BCR	b	618	-	41,41,41	0.92	3 (7%)	56,56,56	2.20	18 (32%)
35	LHG	r	2630	27	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
27	CLA	c	502	-	65,73,73	1.41	10 (15%)	76,113,113	1.45	7 (9%)
27	CLA	b	608	-	65,73,73	1.43	10 (15%)	76,113,113	1.46	9 (11%)
27	CLA	g	612	7	49,57,73	1.69	10 (20%)	55,93,113	1.56	7 (12%)
27	CLA	S	611	35	49,57,73	1.66	10 (20%)	55,93,113	1.57	7 (12%)
30	SQD	B	621	-	53,54,54	0.95	5 (9%)	62,65,65	1.56	10 (16%)
35	LHG	g	2630	27	48,48,48	0.61	1 (2%)	51,54,54	1.29	7 (13%)
27	CLA	g	611	35	49,57,73	1.68	9 (18%)	55,93,113	1.61	9 (16%)
27	CLA	n	602	7	65,73,73	1.48	8 (12%)	76,113,113	1.38	6 (7%)
27	CLA	b	612	-	65,73,73	1.48	10 (15%)	76,113,113	1.52	9 (11%)
28	PHO	A	409	-	51,69,69	1.14	7 (13%)	47,99,99	1.37	6 (12%)
27	CLA	r	602	17	65,73,73	1.43	8 (12%)	76,113,113	1.40	7 (9%)
38	LUT	R	620	-	42,43,43	0.82	1 (2%)	51,60,60	1.65	15 (29%)
38	LUT	Y	1621	-	42,43,43	1.01	3 (7%)	51,60,60	1.93	18 (35%)
35	LHG	y	2630	27	48,48,48	0.74	1 (2%)	51,54,54	1.31	6 (11%)
37	CHL	G	607	-	50,58,74	2.12	14 (28%)	52,94,114	2.78	19 (36%)
24	OEX	a	401	3,1	0,15,15	-	-	-		
27	CLA	C	509	-	65,73,73	1.45	10 (15%)	76,113,113	1.56	12 (15%)
37	CHL	y	601	7	66,74,74	1.87	14 (21%)	73,114,114	2.42	23 (31%)
32	DGD	C	519	-	63,63,67	0.99	4 (6%)	77,77,81	1.51	14 (18%)
40	NEX	G	1623	-	38,46,46	1.01	2 (5%)	50,70,70	2.60	16 (32%)
27	CLA	C	510	-	65,73,73	1.41	9 (13%)	76,113,113	1.46	7 (9%)
39	XAT	y	1622	-	39,47,47	0.90	0	54,74,74	3.05	21 (38%)
37	CHL	N	608	-	50,58,74	2.09	14 (28%)	52,94,114	2.87	20 (38%)
27	CLA	y	602	7	65,73,73	1.44	10 (15%)	76,113,113	1.48	7 (9%)
27	CLA	y	604	-	49,57,73	1.65	10 (20%)	55,93,113	1.64	7 (12%)
32	DGD	C	520	-	63,63,67	0.97	4 (6%)	77,77,81	1.51	11 (14%)
29	BCR	c	514	-	41,41,41	0.90	1 (2%)	56,56,56	2.03	18 (32%)
38	LUT	S	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.76	17 (33%)
30	SQD	a	418	-	53,54,54	0.98	5 (9%)	62,65,65	1.48	10 (16%)
27	CLA	s	610	18	49,57,73	1.63	7 (14%)	55,93,113	1.63	7 (12%)
27	CLA	A	405	-	65,73,73	1.46	10 (15%)	76,113,113	1.50	8 (10%)
27	CLA	C	503	-	65,73,73	1.45	11 (16%)	76,113,113	1.38	8 (10%)
27	CLA	C	501	-	65,73,73	1.46	10 (15%)	76,113,113	1.40	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	XAT	G	1622	-	39,47,47	0.97	2 (5%)	54,74,74	2.99	18 (33%)
27	CLA	B	613	-	65,73,73	1.43	9 (13%)	76,113,113	1.55	8 (10%)
37	CHL	N	606	-	50,58,74	2.11	14 (28%)	52,94,114	2.92	20 (38%)
29	BCR	b	620	-	41,41,41	0.96	3 (7%)	56,56,56	2.12	17 (30%)
37	CHL	r	607	-	50,58,74	2.16	15 (30%)	52,94,114	2.80	21 (40%)
31	LMG	Z	101	-	51,51,55	0.72	0	59,59,63	1.35	6 (10%)
27	CLA	G	603	-	49,57,73	1.67	8 (16%)	55,93,113	1.59	7 (12%)
27	CLA	s	613	18	49,57,73	1.64	9 (18%)	55,93,113	1.58	6 (10%)
38	LUT	n	1620	-	42,43,43	0.83	1 (2%)	51,60,60	1.84	16 (31%)
27	CLA	g	614	-	49,57,73	1.67	6 (12%)	55,93,113	1.57	7 (12%)
35	LHG	l	101	-	48,48,48	0.72	1 (2%)	51,54,54	1.32	7 (13%)
31	LMG	B	622	-	51,51,55	0.80	2 (3%)	59,59,63	1.45	8 (13%)
27	CLA	A	406	-	65,73,73	1.41	9 (13%)	76,113,113	1.53	8 (10%)
27	CLA	s	604	-	49,57,73	1.62	9 (18%)	55,93,113	1.68	7 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	C	513	-	1/1/11/20	6/18/96/115	-
37	CHL	r	608	-	3/3/16/26	12/20/118/137	-
27	CLA	A	407	-	1/1/11/20	6/18/96/115	-
37	CHL	y	605	7	3/3/16/26	8/18/116/137	-
37	CHL	Y	601	7	4/4/20/26	17/39/137/137	-
37	CHL	Y	605	7	3/3/16/26	8/18/116/137	-
37	CHL	s	601	18	3/3/17/26	9/23/121/137	-
27	CLA	N	610	7	1/1/15/20	10/37/115/115	-
37	CHL	r	606	-	3/3/16/26	10/20/118/137	-
37	CHL	y	609	7	4/4/20/26	19/39/137/137	-
37	CHL	G	606	-	3/3/16/26	3/20/118/137	-
27	CLA	c	503	-	1/1/15/20	12/37/115/115	-
27	CLA	y	613	7	1/1/15/20	14/37/115/115	-
37	CHL	S	601	18	3/3/17/26	9/23/121/137	-
27	CLA	C	511	3	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CHL	G	608	-	3/3/16/26	10/20/118/137	-
27	CLA	N	613	7	1/1/11/20	7/18/96/115	-
27	CLA	s	609	18	1/1/11/20	8/18/96/115	-
35	LHG	Y	2630	27	-	20/53/53/53	-
29	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	CLA	Y	610	7	1/1/15/20	15/37/115/115	-
27	CLA	G	604	-	1/1/11/20	9/18/96/115	-
27	CLA	c	510	-	1/1/15/20	18/37/115/115	-
27	CLA	r	612	-	1/1/11/20	4/18/96/115	-
27	CLA	B	604	-	1/1/15/20	13/37/115/115	-
35	LHG	L	101	-	-	27/53/53/53	-
37	CHL	Y	609	7	4/4/20/26	19/39/137/137	-
37	CHL	s	607	-	3/3/16/26	9/20/118/137	-
31	LMG	a	413	-	-	15/43/63/70	0/1/1/1
27	CLA	R	604	-	1/1/11/20	9/18/96/115	-
27	CLA	R	601	17	1/1/11/20	13/18/96/115	-
31	LMG	d	411	-	-	13/41/61/70	0/1/1/1
31	LMG	D	411	-	-	13/41/61/70	0/1/1/1
27	CLA	N	602	7	1/1/15/20	10/37/115/115	-
27	CLA	y	611	35	1/1/15/20	9/37/115/115	-
29	BCR	C	516	-	-	7/29/63/63	0/2/2/2
35	LHG	R	2630	27	-	13/53/53/53	-
30	SQD	A	418	-	-	20/49/69/69	0/1/1/1
37	CHL	n	601	7	3/3/16/26	6/20/118/137	-
37	CHL	g	608	-	3/3/16/26	10/20/118/137	-
27	CLA	n	603	-	1/1/11/20	11/18/96/115	-
27	CLA	G	611	35	1/1/11/20	6/18/96/115	-
37	CHL	N	601	7	3/3/16/26	6/20/118/137	-
27	CLA	a	406	-	1/1/15/20	12/37/115/115	-
38	LUT	G	1621	-	-	1/29/67/67	0/2/2/2
38	LUT	N	1621	-	-	3/29/67/67	0/2/2/2
27	CLA	c	511	3	1/1/15/20	9/37/115/115	-
27	CLA	G	614	-	1/1/11/20	7/18/96/115	-
27	CLA	S	614	-	1/1/11/20	7/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	d	404	-	-	9/29/63/63	0/2/2/2
27	CLA	S	612	18	1/1/11/20	5/18/96/115	-
28	PHO	a	408	-	-	10/37/103/103	0/5/6/6
27	CLA	Y	611	35	1/1/15/20	9/37/115/115	-
35	LHG	S	2630	27	-	23/53/53/53	-
32	DGD	h	102	-	-	19/51/91/95	0/2/2/2
27	CLA	N	604	-	1/1/11/20	4/18/96/115	-
29	BCR	B	618	-	-	4/29/63/63	0/2/2/2
35	LHG	d	409	-	-	15/53/53/53	-
27	CLA	C	512	-	1/1/15/20	17/37/115/115	-
27	CLA	B	607	-	1/1/15/20	5/37/115/115	-
27	CLA	s	612	18	1/1/11/20	5/18/96/115	-
27	CLA	G	602	7	1/1/15/20	15/37/115/115	-
27	CLA	n	612	7	1/1/11/20	9/18/96/115	-
29	BCR	C	517	-	-	1/29/63/63	0/2/2/2
31	LMG	b	622	-	-	23/46/66/70	0/1/1/1
27	CLA	n	614	-	1/1/11/20	10/18/96/115	-
27	CLA	C	508	-	1/1/15/20	11/37/115/115	-
37	CHL	n	605	7	3/3/16/26	9/18/116/137	-
38	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
37	CHL	G	605	7	3/3/16/26	5/18/116/137	-
37	CHL	S	607	-	3/3/16/26	9/20/118/137	-
27	CLA	Y	602	7	1/1/15/20	12/37/115/115	-
37	CHL	R	607	-	3/3/16/26	9/20/118/137	-
29	BCR	B	620	-	-	6/29/63/63	0/2/2/2
27	CLA	s	602	18	1/1/11/20	7/18/96/115	-
27	CLA	r	604	-	1/1/11/20	9/18/96/115	-
27	CLA	R	616	17	1/1/11/20	9/18/96/115	-
27	CLA	d	403	-	1/1/15/20	12/37/115/115	-
27	CLA	B	605	-	1/1/15/20	17/37/115/115	-
38	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
37	CHL	N	607	-	4/4/20/26	16/39/137/137	-
37	CHL	n	609	7	3/3/16/26	7/20/118/137	-
31	LMG	z	101	-	-	22/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	C	506	-	1/1/15/20	18/37/115/115	-
27	CLA	g	604	-	1/1/11/20	9/18/96/115	-
27	CLA	S	609	18	1/1/11/20	8/18/96/115	-
27	CLA	b	603	-	1/1/15/20	16/37/115/115	-
27	CLA	B	609	-	1/1/15/20	16/37/115/115	-
40	NEX	N	1623	-	-	5/27/83/83	0/3/3/3
27	CLA	s	603	-	-	11/18/96/115	-
27	CLA	c	513	-	1/1/11/20	6/18/96/115	-
27	CLA	D	403	-	1/1/15/20	12/37/115/115	-
27	CLA	C	502	-	1/1/15/20	14/37/115/115	-
29	BCR	c	517	-	-	1/29/63/63	0/2/2/2
27	CLA	c	505	-	1/1/15/20	10/37/115/115	-
40	NEX	R	623	-	-	3/27/83/83	0/3/3/3
27	CLA	b	606	-	1/1/15/20	14/37/115/115	-
27	CLA	c	508	-	1/1/15/20	11/37/115/115	-
27	CLA	Y	603	-	1/1/11/20	4/18/96/115	-
28	PHO	a	409	-	-	17/37/103/103	0/5/6/6
27	CLA	Y	613	7	1/1/15/20	14/37/115/115	-
34	PL9	D	405	-	-	14/53/73/73	0/1/1/1
35	LHG	s	2630	27	-	23/53/53/53	-
27	CLA	s	611	35	1/1/11/20	7/18/96/115	-
32	DGD	c	518	-	-	17/44/84/95	0/2/2/2
39	XAT	R	622	-	-	2/31/93/93	0/4/4/4
27	CLA	N	612	7	1/1/11/20	9/18/96/115	-
27	CLA	R	609	17	1/1/11/20	8/18/96/115	-
37	CHL	G	601	7	4/4/20/26	20/39/137/137	-
37	CHL	N	605	7	3/3/16/26	9/18/116/137	-
35	LHG	N	2630	27	-	24/53/53/53	-
38	LUT	y	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	A	410	-	1/1/14/20	11/31/109/115	-
27	CLA	b	611	-	1/1/15/20	10/37/115/115	-
27	CLA	c	512	-	1/1/15/20	17/37/115/115	-
27	CLA	G	610	7	1/1/15/20	15/37/115/115	-
27	CLA	y	612	7	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	D	404	-	-	9/29/63/63	0/2/2/2
32	DGD	C	518	-	-	17/44/84/95	0/2/2/2
28	PHO	A	408	-	-	10/37/103/103	0/5/6/6
27	CLA	g	603	-	1/1/11/20	6/18/96/115	-
27	CLA	R	610	17	1/1/15/20	15/37/115/115	-
38	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	C	504	-	1/1/15/20	14/37/115/115	-
27	CLA	B	610	-	1/1/15/20	13/37/115/115	-
27	CLA	R	603	-	1/1/11/20	6/18/96/115	-
27	CLA	r	613	17	1/1/11/20	7/18/96/115	-
37	CHL	R	606	-	3/3/16/26	10/20/118/137	-
27	CLA	N	611	35	1/1/11/20	6/18/96/115	-
27	CLA	c	509	-	1/1/15/20	9/37/115/115	-
35	LHG	n	2630	27	-	24/53/53/53	-
27	CLA	b	617	-	1/1/15/20	15/37/115/115	-
27	CLA	B	615	-	1/1/15/20	14/37/115/115	-
27	CLA	n	604	-	1/1/11/20	4/18/96/115	-
27	CLA	g	613	7	1/1/11/20	6/18/96/115	-
37	CHL	y	606	-	3/3/16/26	6/20/118/137	-
27	CLA	R	613	17	1/1/11/20	7/18/96/115	-
27	CLA	G	612	7	1/1/11/20	6/18/96/115	-
30	SQD	b	621	-	-	24/49/69/69	0/1/1/1
27	CLA	g	610	7	1/1/15/20	15/37/115/115	-
39	XAT	n	1622	-	-	1/31/93/93	0/4/4/4
32	DGD	H	102	-	-	19/51/91/95	0/2/2/2
27	CLA	Y	604	-	1/1/11/20	6/18/96/115	-
32	DGD	c	519	-	-	23/51/91/95	0/2/2/2
37	CHL	G	609	7	3/3/16/26	11/20/118/137	-
37	CHL	g	607	-	3/3/16/26	9/20/118/137	-
27	CLA	B	611	-	1/1/15/20	10/37/115/115	-
27	CLA	D	402	-	1/1/15/20	10/37/115/115	-
27	CLA	c	507	-	1/1/15/20	15/37/115/115	-
27	CLA	c	501	-	1/1/15/20	12/37/115/115	-
27	CLA	B	617	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	C	514	-	-	4/29/63/63	0/2/2/2
27	CLA	R	611	35	1/1/11/20	9/18/96/115	-
27	CLA	C	507	-	1/1/15/20	15/37/115/115	-
29	BCR	a	411	-	-	0/29/63/63	0/2/2/2
27	CLA	Y	614	-	1/1/11/20	8/18/96/115	-
37	CHL	R	608	-	3/3/16/26	12/20/118/137	-
27	CLA	S	604	-	1/1/11/20	11/18/96/115	-
27	CLA	b	616	-	1/1/15/20	11/37/115/115	-
27	CLA	r	611	35	1/1/11/20	9/18/96/115	-
37	CHL	S	608	-	3/3/16/26	5/19/117/137	-
38	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	N	603	-	1/1/11/20	11/18/96/115	-
27	CLA	c	504	-	1/1/15/20	14/37/115/115	-
40	NEX	n	1623	-	-	5/27/83/83	0/3/3/3
38	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
29	BCR	b	619	-	-	0/29/63/63	0/2/2/2
37	CHL	s	608	-	3/3/16/26	5/19/117/137	-
37	CHL	g	601	7	4/4/20/26	20/39/137/137	-
27	CLA	d	402	-	1/1/15/20	10/37/115/115	-
27	CLA	r	601	17	1/1/11/20	13/18/96/115	-
30	SQD	a	412	-	-	28/49/69/69	0/1/1/1
37	CHL	Y	606	-	3/3/16/26	6/20/118/137	-
37	CHL	n	607	-	4/4/20/26	16/39/137/137	-
27	CLA	s	614	-	1/1/11/20	7/18/96/115	-
39	XAT	r	622	-	-	2/31/93/93	0/4/4/4
27	CLA	r	616	17	1/1/11/20	9/18/96/115	-
37	CHL	s	606	-	3/3/16/26	10/20/118/137	-
29	BCR	c	515	-	-	0/29/63/63	0/2/2/2
27	CLA	c	506	-	1/1/15/20	18/37/115/115	-
27	CLA	b	609	-	1/1/15/20	16/37/115/115	-
40	NEX	Y	1623	-	-	3/27/83/83	0/3/3/3
27	CLA	b	605	-	1/1/15/20	17/37/115/115	-
39	XAT	N	1622	-	-	1/31/93/93	0/4/4/4
29	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	CLA	S	602	18	1/1/11/20	7/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	R	602	17	1/1/15/20	15/37/115/115	-
27	CLA	B	602	-	1/1/15/20	19/37/115/115	-
37	CHL	n	608	-	3/3/16/26	7/20/118/137	-
27	CLA	G	613	7	1/1/11/20	6/18/96/115	-
38	LUT	g	1621	-	-	1/29/67/67	0/2/2/2
40	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
38	LUT	r	620	-	-	2/29/67/67	0/2/2/2
37	CHL	y	607	-	3/3/16/26	8/20/118/137	-
27	CLA	r	609	17	1/1/11/20	8/18/96/115	-
27	CLA	B	608	-	1/1/15/20	8/37/115/115	-
35	LHG	D	409	-	-	15/53/53/53	-
27	CLA	Y	612	7	1/1/15/20	10/37/115/115	-
39	XAT	g	1622	-	-	3/31/93/93	0/4/4/4
27	CLA	a	410	-	1/1/14/20	11/31/109/115	-
27	CLA	B	614	-	1/1/15/20	9/37/115/115	-
27	CLA	g	602	7	1/1/15/20	15/37/115/115	-
29	BCR	A	411	-	-	0/29/63/63	0/2/2/2
27	CLA	B	612	-	1/1/15/20	15/37/115/115	-
39	XAT	Y	1622	-	-	3/31/93/93	0/4/4/4
35	LHG	d	410	-	-	21/41/41/53	-
35	LHG	D	410	-	-	21/41/41/53	-
38	LUT	y	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	b	610	-	1/1/15/20	13/37/115/115	-
27	CLA	a	407	-	1/1/11/20	6/18/96/115	-
31	LMG	C	521	-	-	20/46/66/70	0/1/1/1
40	NEX	r	623	-	-	3/27/83/83	0/3/3/3
29	BCR	h	101	-	-	4/29/63/63	0/2/2/2
27	CLA	b	613	-	1/1/15/20	17/37/115/115	-
37	CHL	g	609	7	3/3/16/26	11/20/118/137	-
27	CLA	b	615	-	1/1/15/20	14/37/115/115	-
27	CLA	b	614	-	1/1/15/20	9/37/115/115	-
27	CLA	n	613	7	1/1/11/20	7/18/96/115	-
31	LMG	c	521	-	-	20/46/66/70	0/1/1/1
40	NEX	y	1623	-	-	3/27/83/83	0/3/3/3
37	CHL	n	606	-	3/3/16/26	4/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HEM	F	101	5,6	-	0/12/54/54	-
27	CLA	n	610	7	1/1/15/20	10/37/115/115	-
37	CHL	g	605	7	3/3/16/26	5/18/116/137	-
27	CLA	r	603	-	1/1/11/20	6/18/96/115	-
31	LMG	A	413	-	-	15/43/63/70	0/1/1/1
37	CHL	N	609	7	3/3/16/26	7/20/118/137	-
37	CHL	Y	607	-	3/3/16/26	8/20/118/137	-
37	CHL	y	608	-	3/3/16/26	9/20/118/137	-
36	HEM	f	101	5,6	-	0/12/54/54	-
35	LHG	G	2630	27	-	30/53/53/53	-
27	CLA	b	604	-	1/1/15/20	13/37/115/115	-
27	CLA	a	405	-	1/1/15/20	14/37/115/115	-
27	CLA	S	603	-	-	11/18/96/115	-
35	LHG	d	408	-	-	20/47/47/53	-
30	SQD	A	412	-	-	28/49/69/69	0/1/1/1
27	CLA	B	616	-	1/1/15/20	11/37/115/115	-
32	DGD	c	520	-	-	14/51/91/95	0/2/2/2
27	CLA	N	614	-	1/1/11/20	11/18/96/115	-
40	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
27	CLA	n	611	35	1/1/11/20	6/18/96/115	-
38	LUT	s	1621	-	-	3/29/67/67	0/2/2/2
27	CLA	r	610	17	1/1/15/20	15/37/115/115	-
27	CLA	B	606	-	1/1/15/20	14/37/115/115	-
27	CLA	S	613	18	1/1/11/20	6/18/96/115	-
38	LUT	Y	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	y	614	-	1/1/11/20	8/18/96/115	-
27	CLA	b	607	-	1/1/15/20	4/37/115/115	-
37	CHL	Y	608	-	3/3/16/26	9/20/118/137	-
27	CLA	S	610	18	1/1/11/20	5/18/96/115	-
35	LHG	D	408	-	-	20/47/47/53	-
37	CHL	S	606	-	3/3/16/26	10/20/118/137	-
37	CHL	g	606	-	3/3/16/26	3/20/118/137	-
40	NEX	g	1623	-	-	5/27/83/83	0/3/3/3
27	CLA	R	612	-	1/1/11/20	4/18/96/115	-
29	BCR	c	516	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	602	-	1/1/15/20	19/37/115/115	-
38	LUT	n	1621	-	-	3/29/67/67	0/2/2/2
27	CLA	B	603	-	1/1/15/20	15/37/115/115	-
27	CLA	y	610	7	1/1/15/20	15/37/115/115	-
34	PL9	d	405	-	-	14/53/73/73	0/1/1/1
27	CLA	y	603	-	1/1/11/20	4/18/96/115	-
27	CLA	C	505	-	1/1/15/20	10/37/115/115	-
29	BCR	H	101	-	-	4/29/63/63	0/2/2/2
29	BCR	b	618	-	-	4/29/63/63	0/2/2/2
35	LHG	r	2630	27	-	13/53/53/53	-
27	CLA	c	502	-	1/1/15/20	14/37/115/115	-
27	CLA	b	608	-	1/1/15/20	8/37/115/115	-
27	CLA	g	612	7	1/1/11/20	6/18/96/115	-
27	CLA	S	611	35	1/1/11/20	7/18/96/115	-
30	SQD	B	621	-	-	24/49/69/69	0/1/1/1
35	LHG	g	2630	27	-	30/53/53/53	-
27	CLA	g	611	35	1/1/11/20	6/18/96/115	-
27	CLA	n	602	7	1/1/15/20	10/37/115/115	-
27	CLA	b	612	-	1/1/15/20	15/37/115/115	-
28	PHO	A	409	-	-	17/37/103/103	0/5/6/6
27	CLA	r	602	17	1/1/15/20	15/37/115/115	-
38	LUT	R	620	-	-	2/29/67/67	0/2/2/2
38	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
35	LHG	y	2630	27	-	20/53/53/53	-
37	CHL	G	607	-	3/3/16/26	9/20/118/137	-
27	CLA	C	509	-	1/1/15/20	10/37/115/115	-
37	CHL	y	601	7	4/4/20/26	17/39/137/137	-
32	DGD	C	519	-	-	23/51/91/95	0/2/2/2
40	NEX	G	1623	-	-	5/27/83/83	0/3/3/3
27	CLA	C	510	-	1/1/15/20	18/37/115/115	-
39	XAT	y	1622	-	-	3/31/93/93	0/4/4/4
37	CHL	N	608	-	3/3/16/26	7/20/118/137	-
27	CLA	y	602	7	1/1/15/20	12/37/115/115	-
27	CLA	y	604	-	1/1/11/20	6/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	DGD	C	520	-	-	14/51/91/95	0/2/2/2
29	BCR	c	514	-	-	4/29/63/63	0/2/2/2
38	LUT	S	1621	-	-	3/29/67/67	0/2/2/2
30	SQD	a	418	-	-	20/49/69/69	0/1/1/1
27	CLA	s	610	18	1/1/11/20	5/18/96/115	-
27	CLA	A	405	-	1/1/15/20	14/37/115/115	-
27	CLA	C	503	-	1/1/15/20	12/37/115/115	-
27	CLA	C	501	-	1/1/15/20	12/37/115/115	-
39	XAT	G	1622	-	-	3/31/93/93	0/4/4/4
27	CLA	B	613	-	1/1/15/20	17/37/115/115	-
37	CHL	N	606	-	3/3/16/26	4/20/118/137	-
29	BCR	b	620	-	-	6/29/63/63	0/2/2/2
37	CHL	r	607	-	3/3/16/26	9/20/118/137	-
31	LMG	Z	101	-	-	22/46/66/70	0/1/1/1
27	CLA	G	603	-	1/1/11/20	6/18/96/115	-
27	CLA	s	613	18	1/1/11/20	6/18/96/115	-
38	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	g	614	-	1/1/11/20	7/18/96/115	-
35	LHG	l	101	-	-	27/53/53/53	-
31	LMG	B	622	-	-	23/46/66/70	0/1/1/1
27	CLA	A	406	-	1/1/15/20	12/37/115/115	-
27	CLA	s	604	-	1/1/11/20	11/18/96/115	-

The worst 5 of 2376 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	101	HEM	C3D-C2D	7.74	1.53	1.36
36	f	101	HEM	C3D-C2D	7.73	1.53	1.36
27	S	609	CLA	C4B-NB	7.39	1.41	1.35
27	s	609	CLA	C4B-NB	7.33	1.41	1.35
27	R	601	CLA	C4B-NB	7.11	1.41	1.35

The worst 5 of 3583 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	Y	1622	XAT	O4-C5-C4	11.88	122.31	113.38
39	y	1622	XAT	O4-C5-C4	11.85	122.28	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	G	1622	XAT	O4-C5-C4	10.80	121.50	113.38
39	g	1622	XAT	O4-C5-C4	10.77	121.47	113.38
40	G	1623	NEX	O24-C25-C24	9.46	120.49	113.38

5 of 312 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	405	CLA	ND
27	A	406	CLA	ND
27	A	407	CLA	ND
27	A	410	CLA	ND
27	B	602	CLA	ND

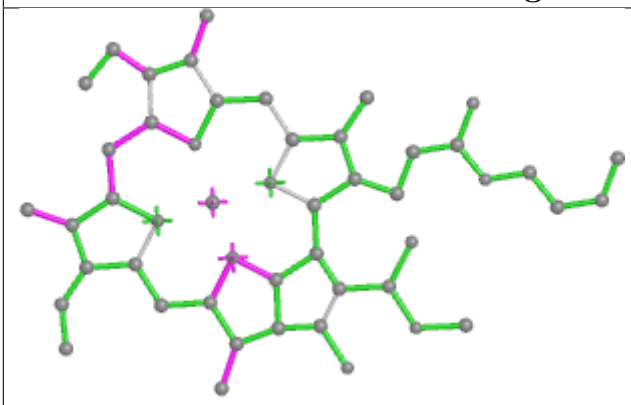
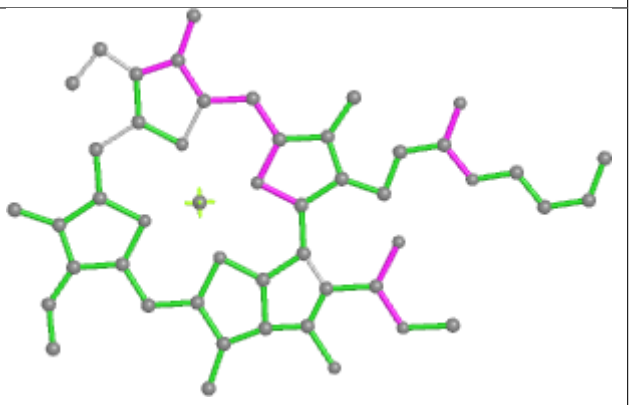
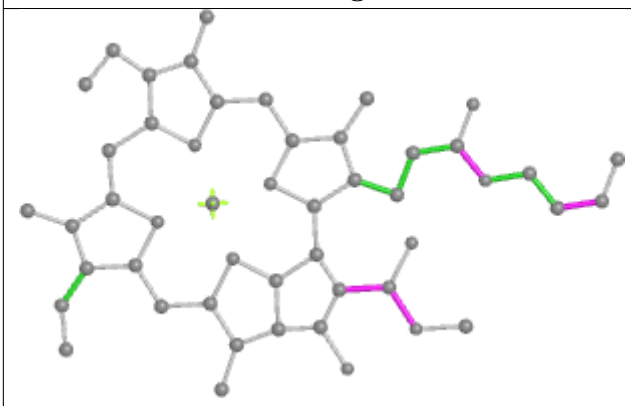
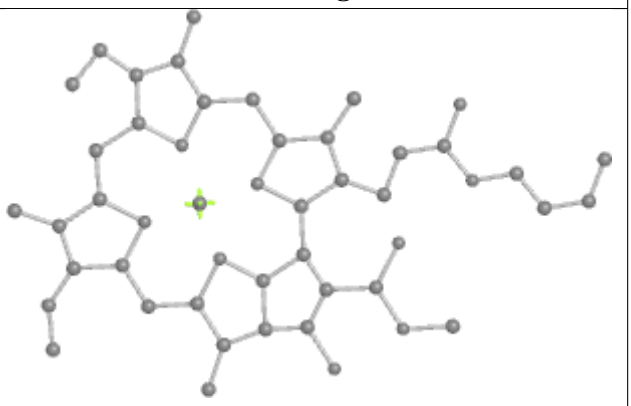
5 of 3220 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	405	CLA	CBD-CGD-O2D-CED
27	A	406	CLA	CHA-CBD-CGD-O1D
27	A	406	CLA	CHA-CBD-CGD-O2D
27	A	407	CLA	CBD-CGD-O2D-CED
27	B	602	CLA	C1A-C2A-CAA-CBA

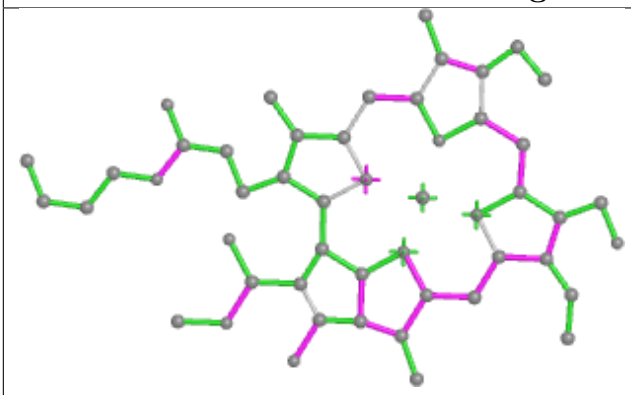
There are no ring outliers.

No monomer is involved in short contacts.

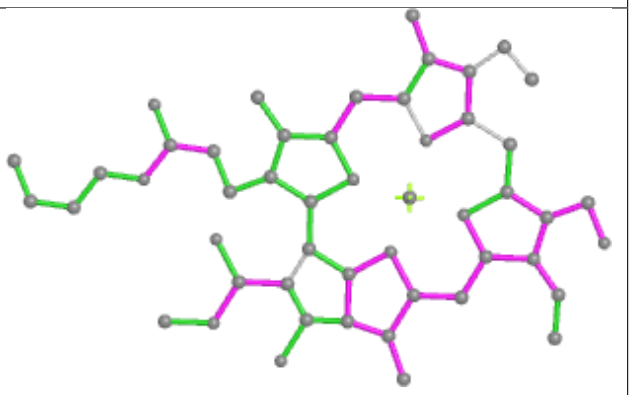
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 C 513	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

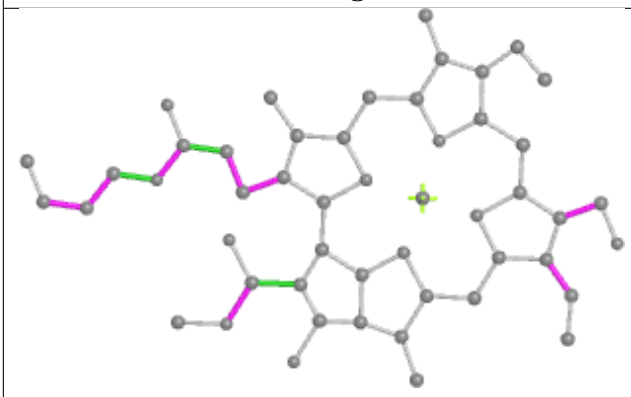
Ligand CHL r 608



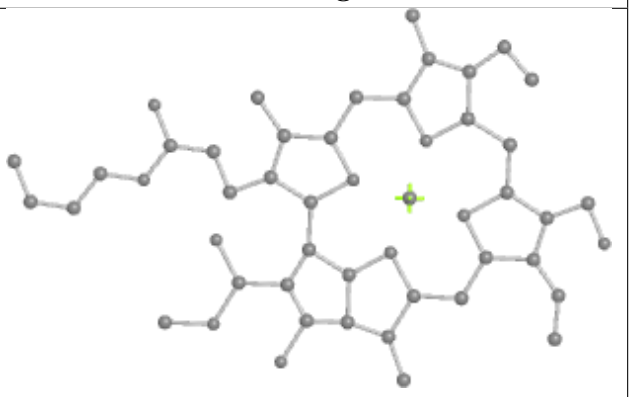
Bond lengths



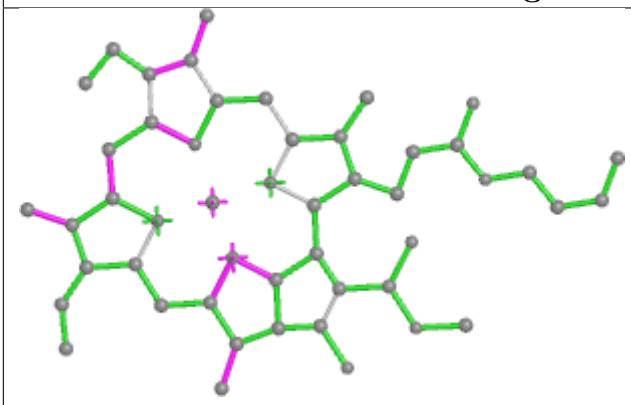
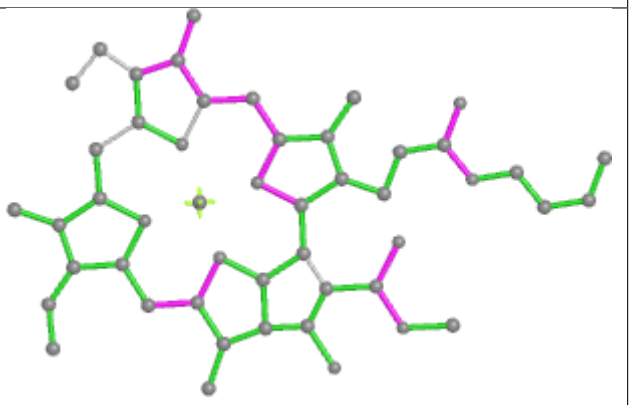
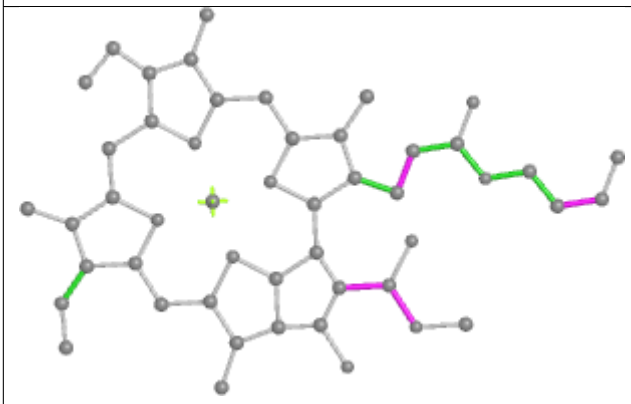
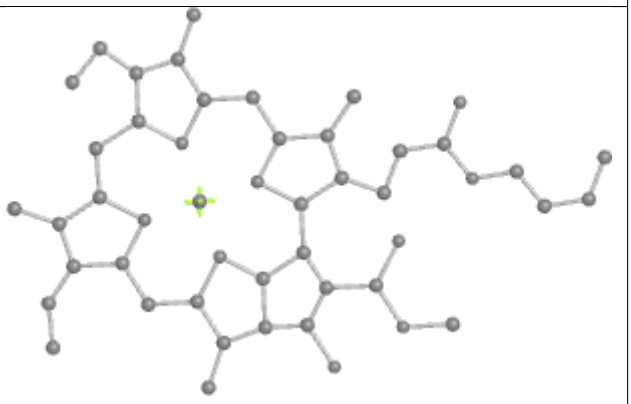
Bond angles



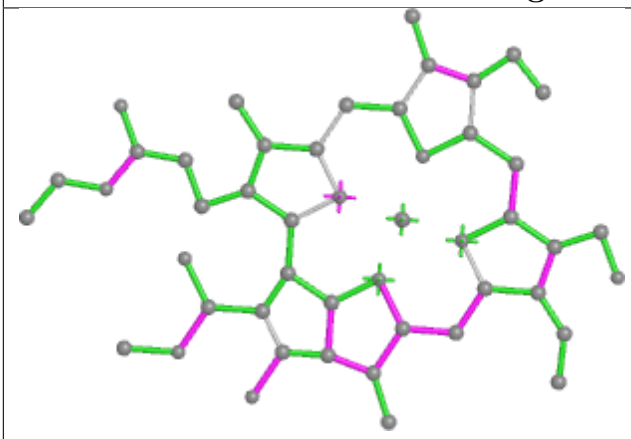
Torsions



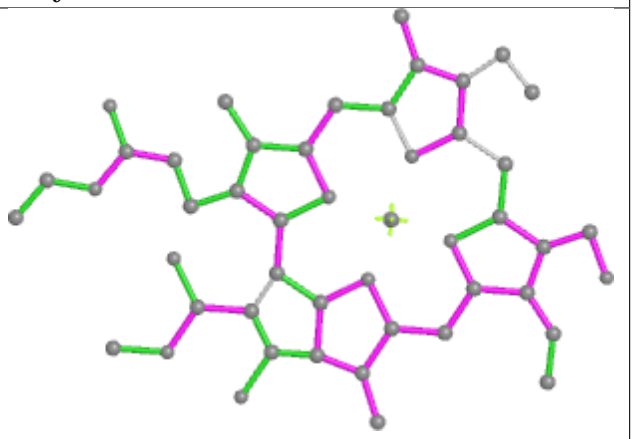
Rings

Ligand CLA A 407	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

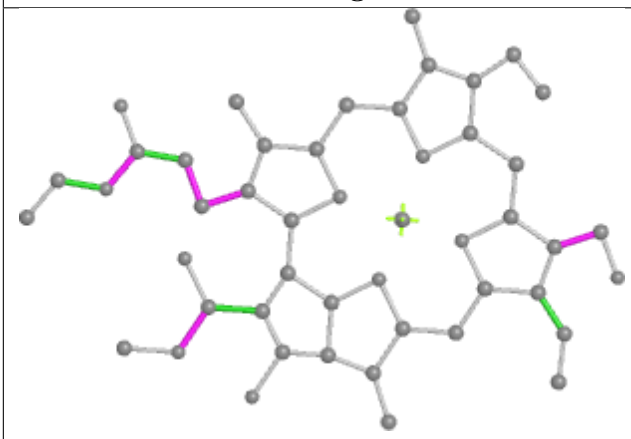
Ligand CHL y 605



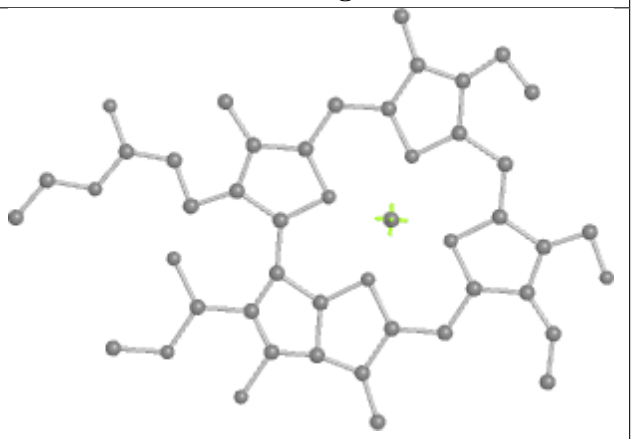
Bond lengths



Bond angles

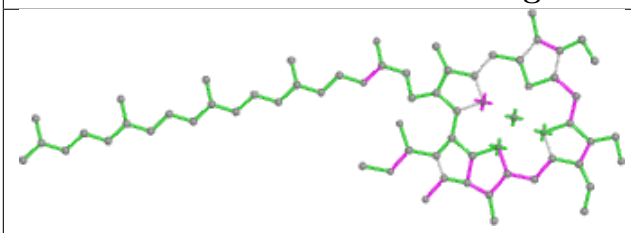


Torsions

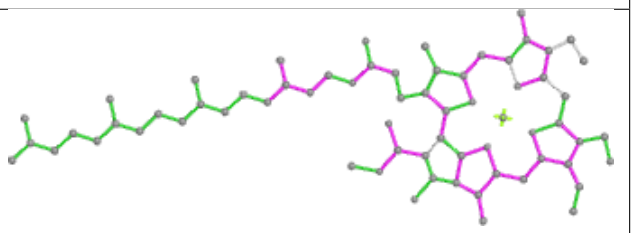


Rings

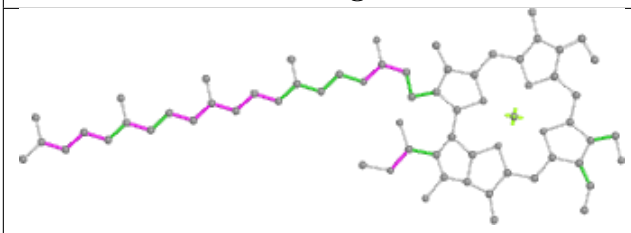
Ligand CHL Y 601



Bond lengths



Bond angles



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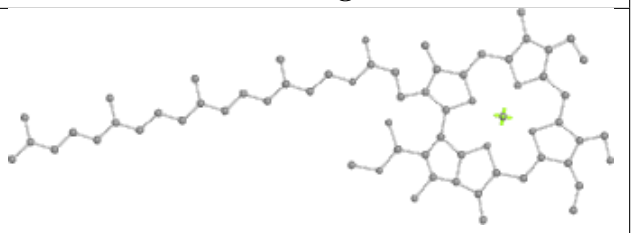
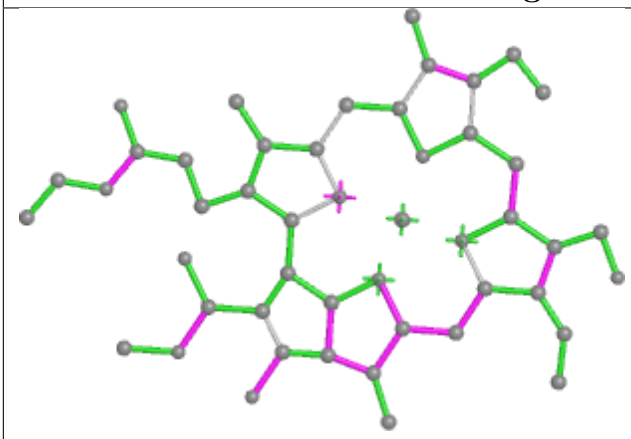
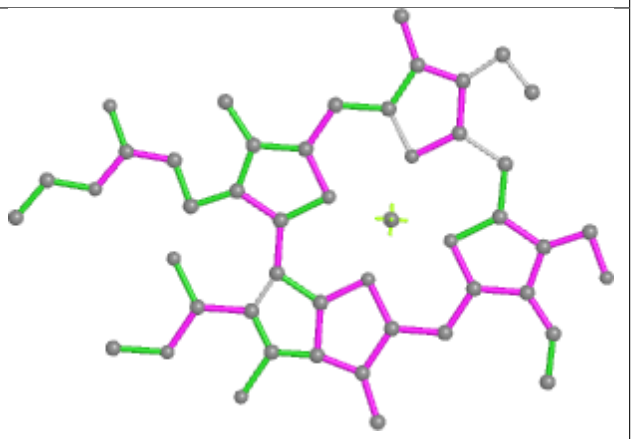


Rings

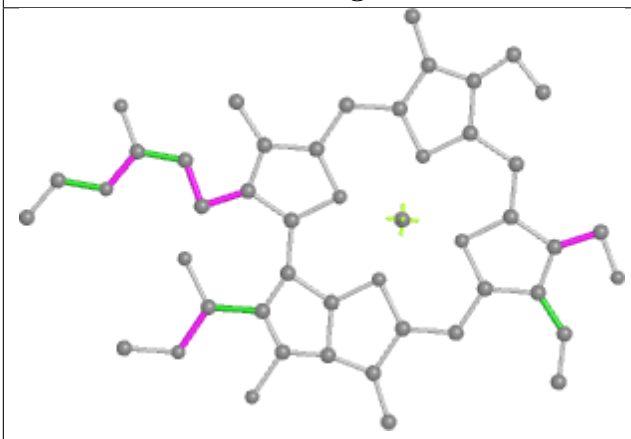
Ligand CHL Y 605



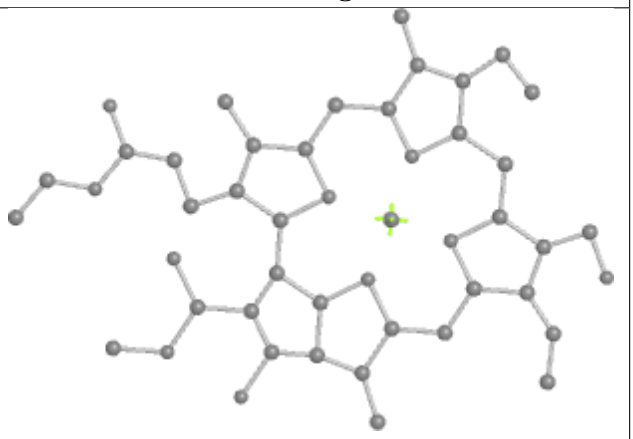
Bond lengths



Bond angles

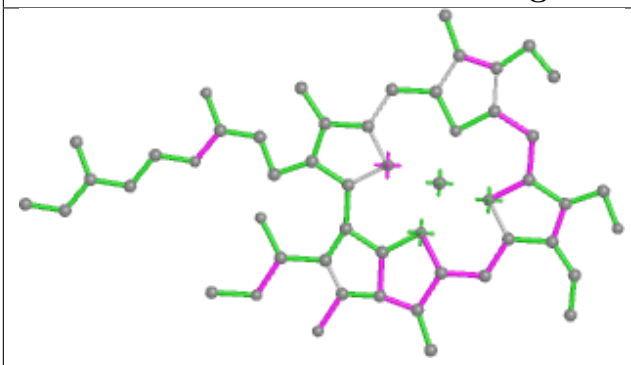


Torsions

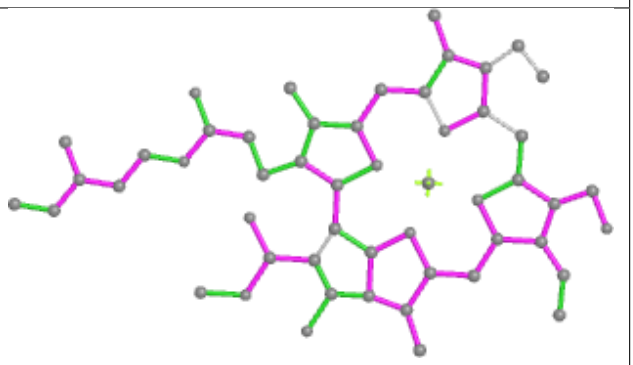


Rings

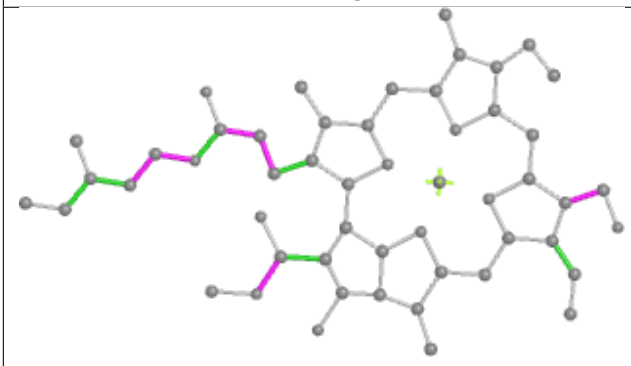
Ligand CHL s 601



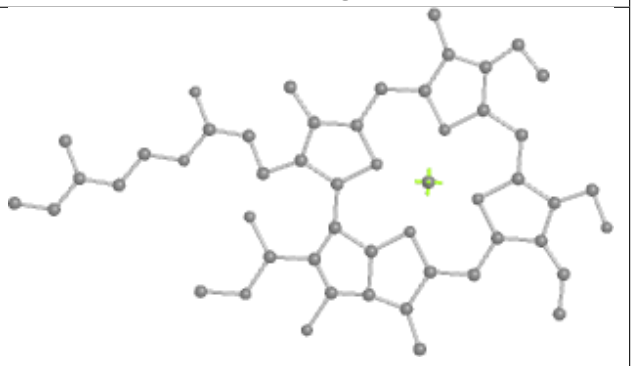
Bond lengths



Bond angles

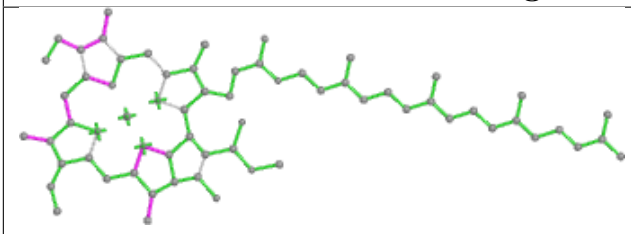


Torsions



Rings

Ligand CLA N 610



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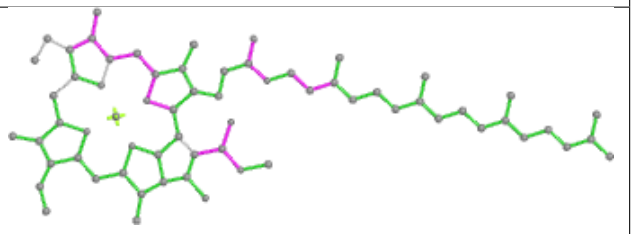

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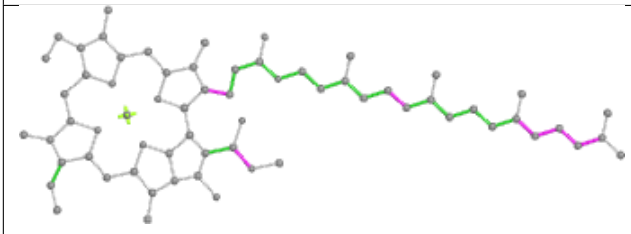

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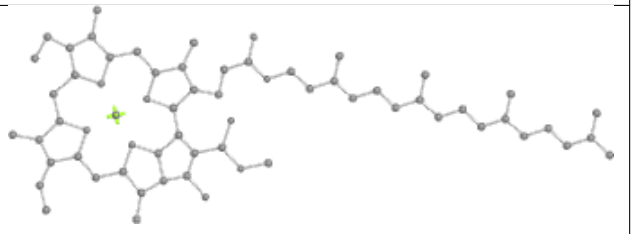
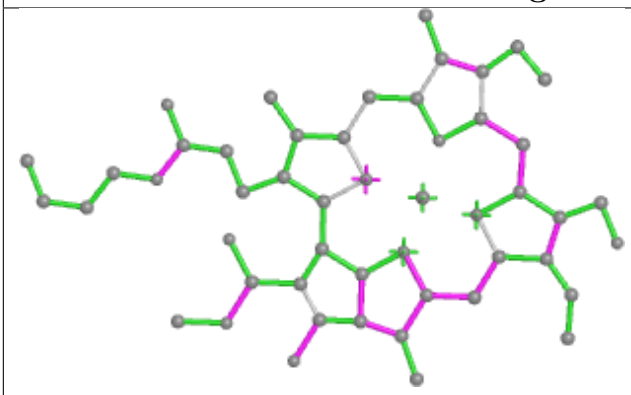


Rings

Ligand CHL r 606



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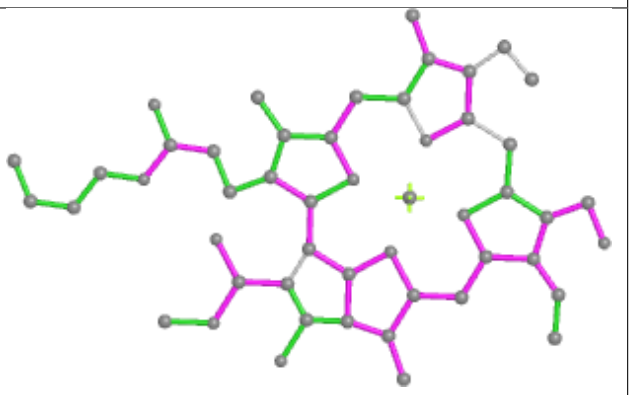

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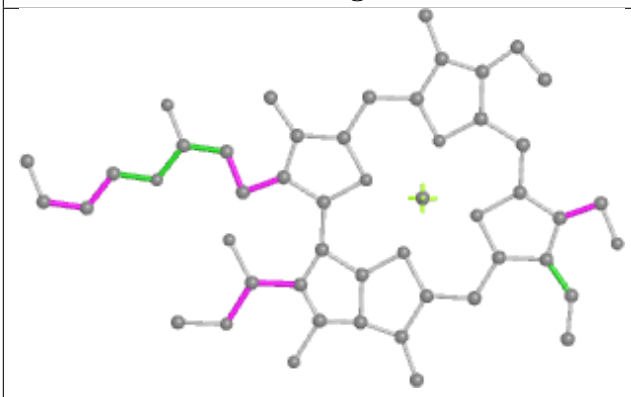

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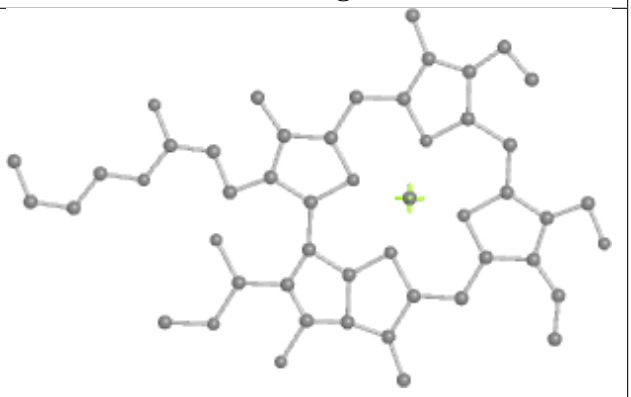
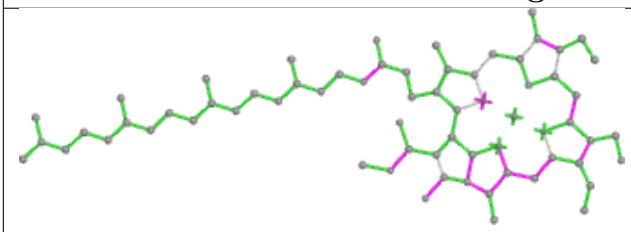


Rings

Ligand CHL y 609



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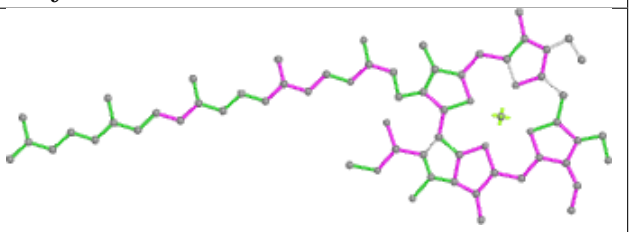
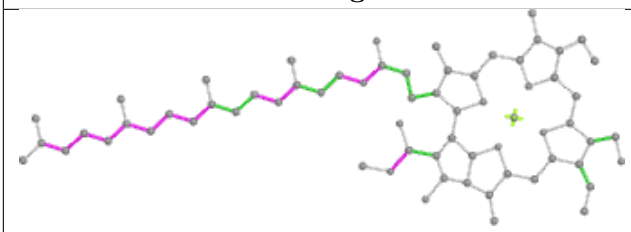


Bond angles



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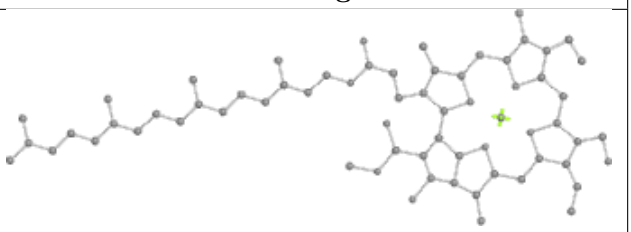
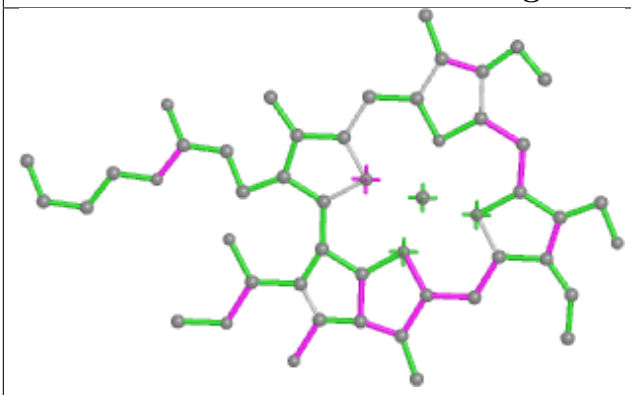


Rings

Ligand CHL G 606



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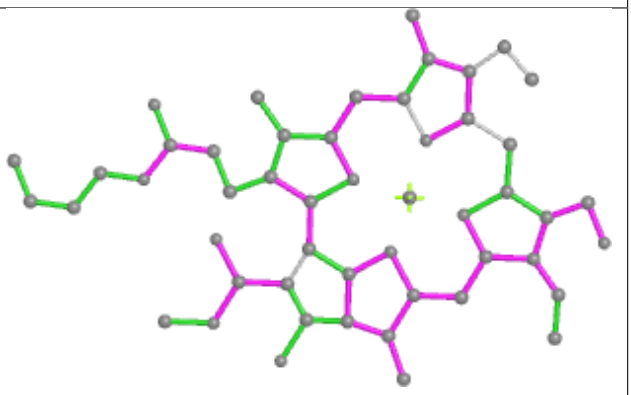
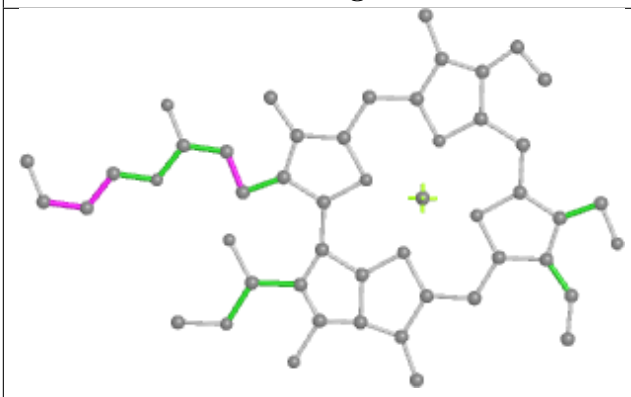


Bond angles



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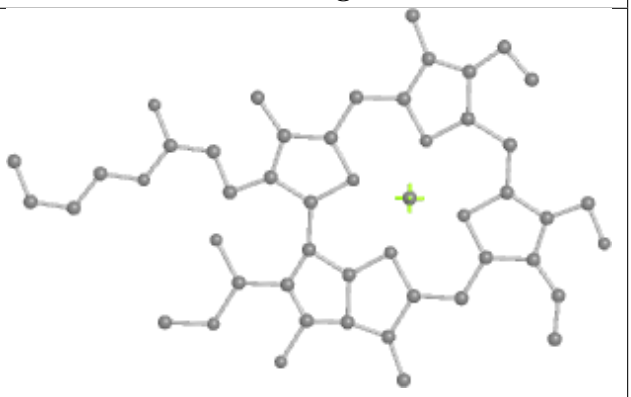
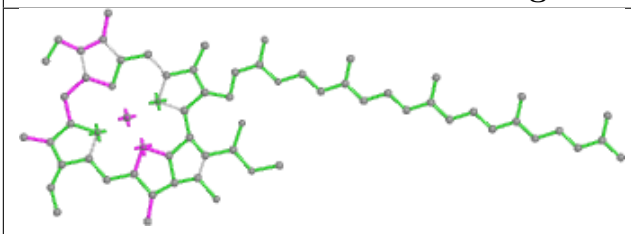


Rings

Ligand CLA c 503



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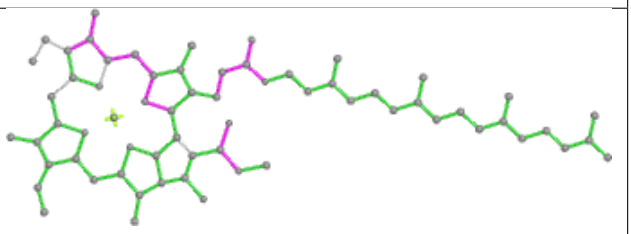
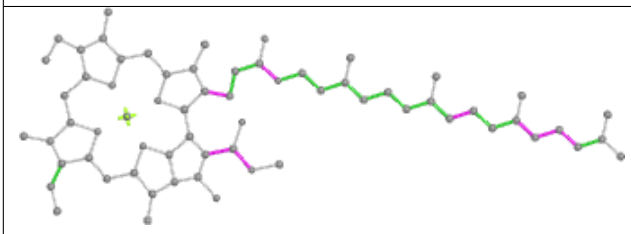


Bond angles



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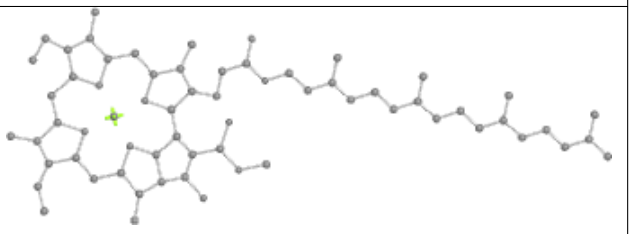
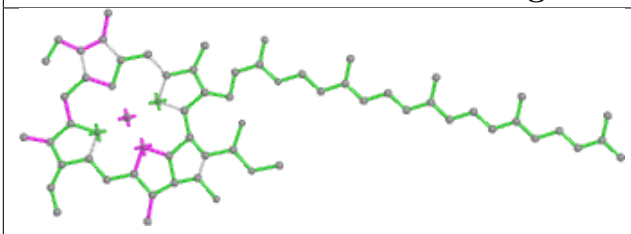


Rings

Ligand CLA y 613



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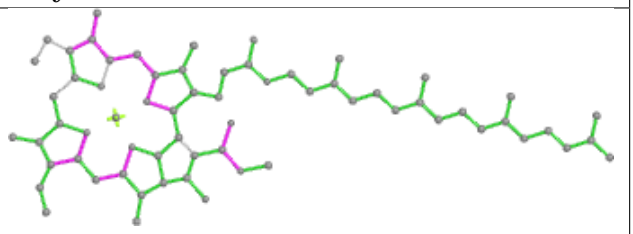

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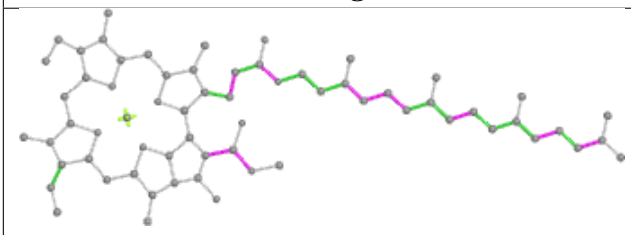

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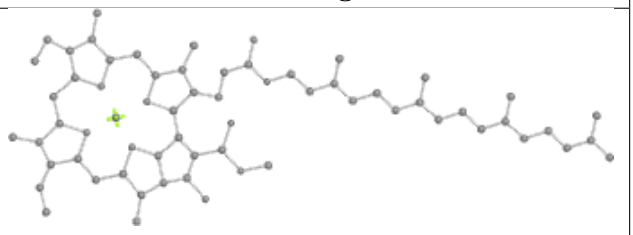
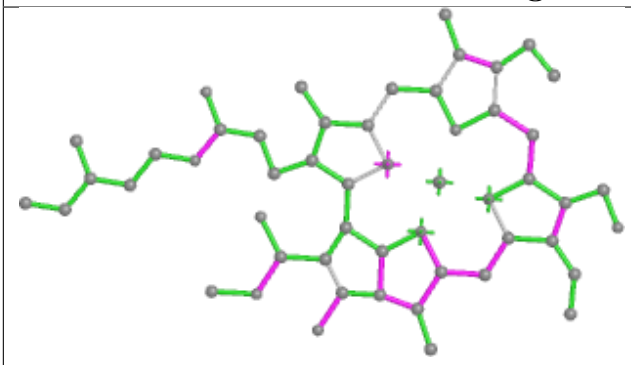


Rings

Ligand CHL S 601



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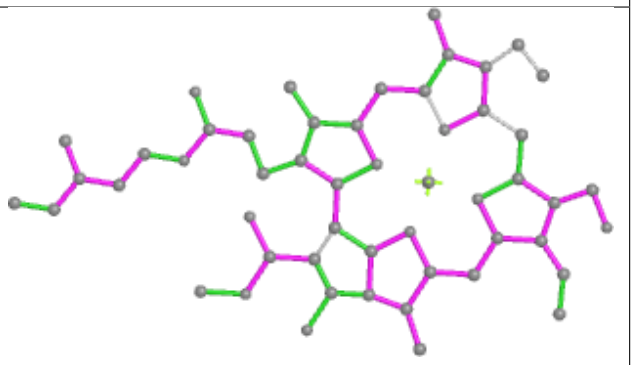
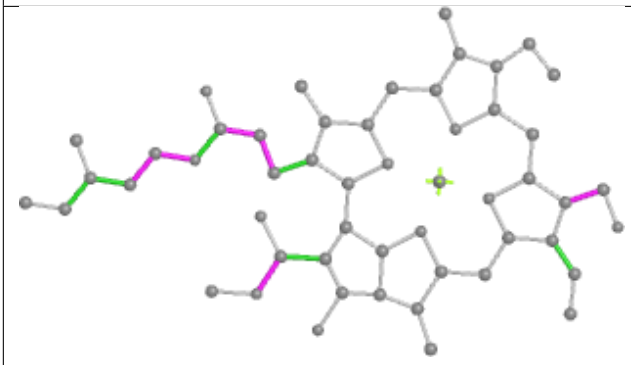


Bond angles



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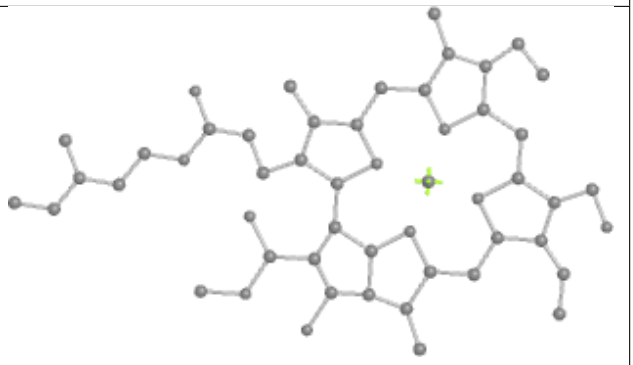
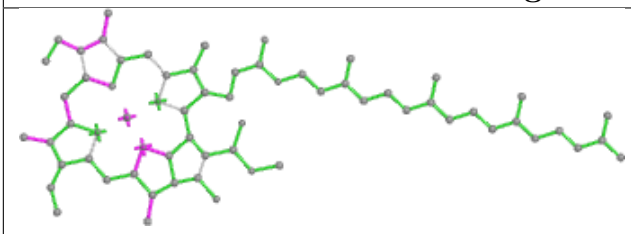


Rings

Ligand CLA C 511



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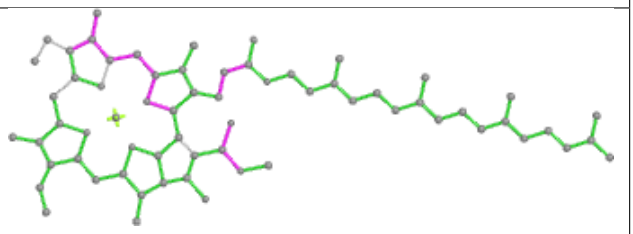
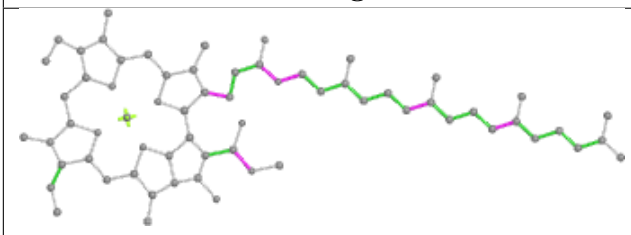


Bond angles



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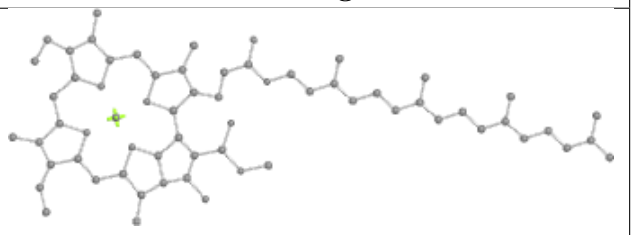
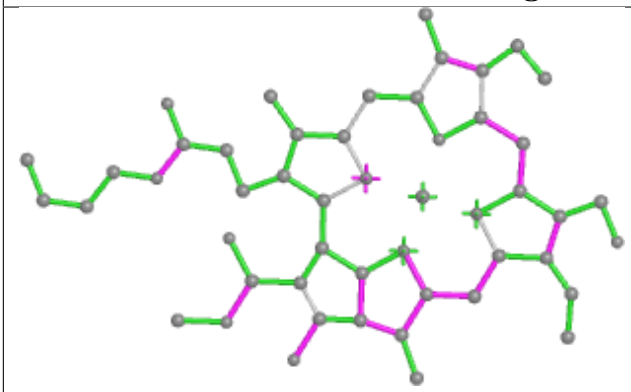


Rings

Ligand CHL G 608



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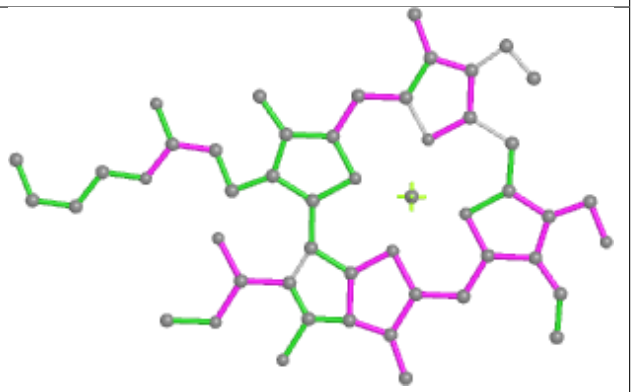
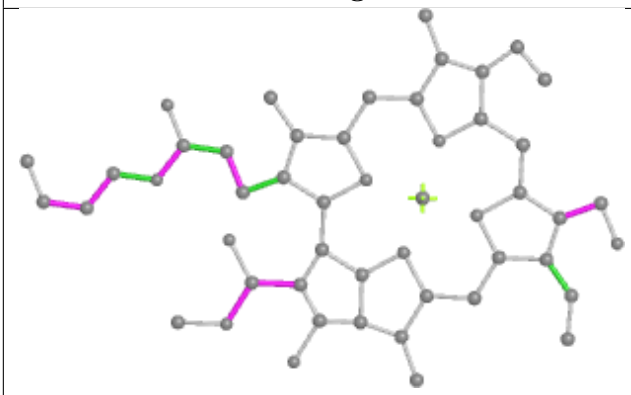


Bond angles



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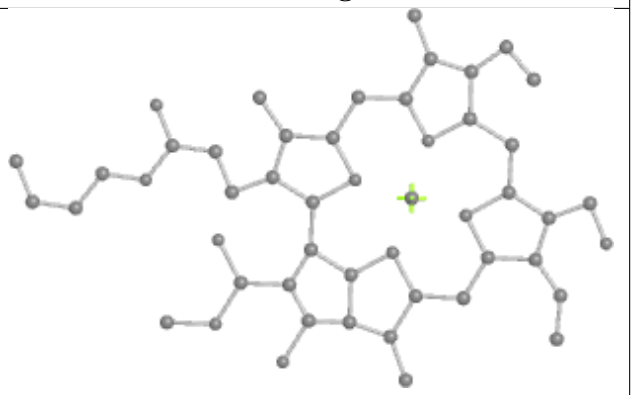
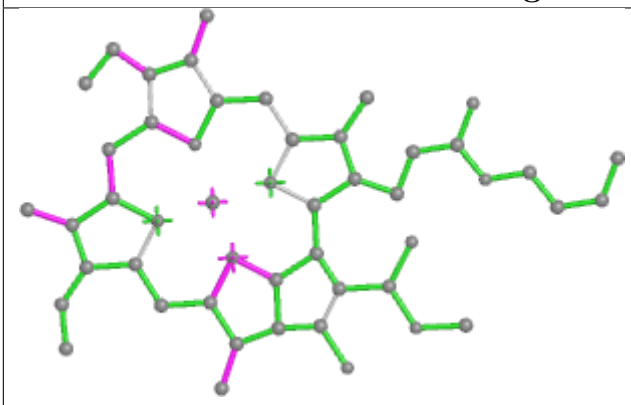


Rings

Ligand CLA N 613



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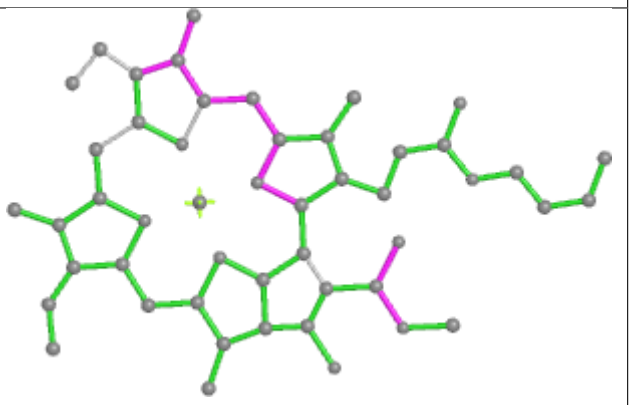
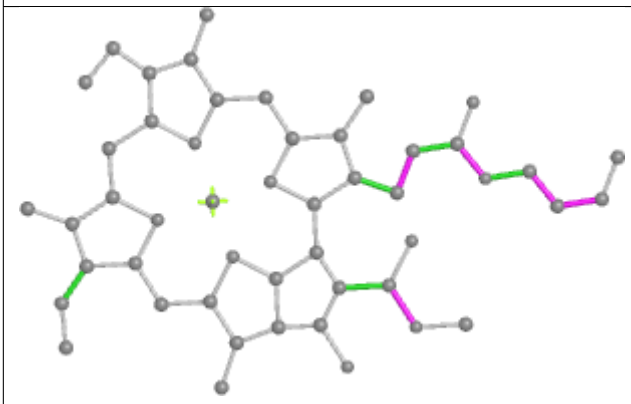


Bond angles



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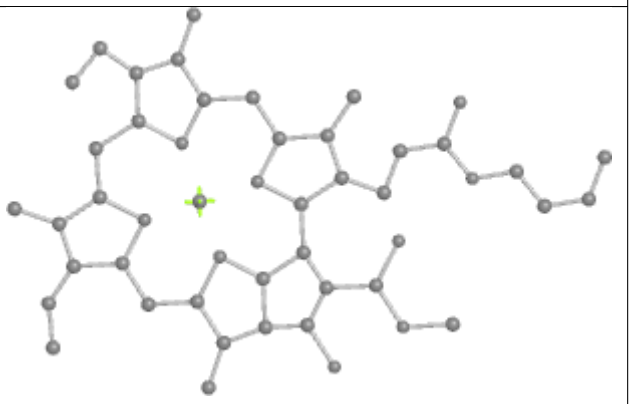
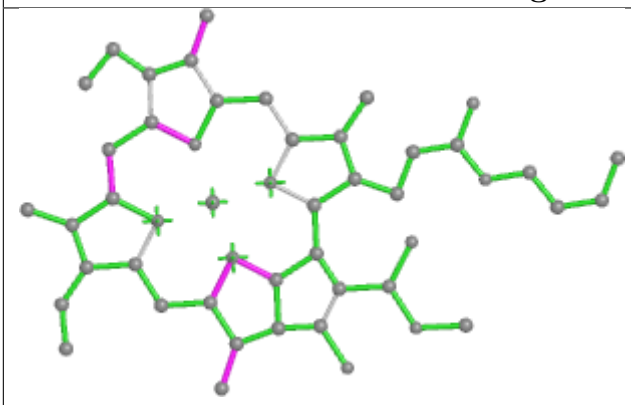
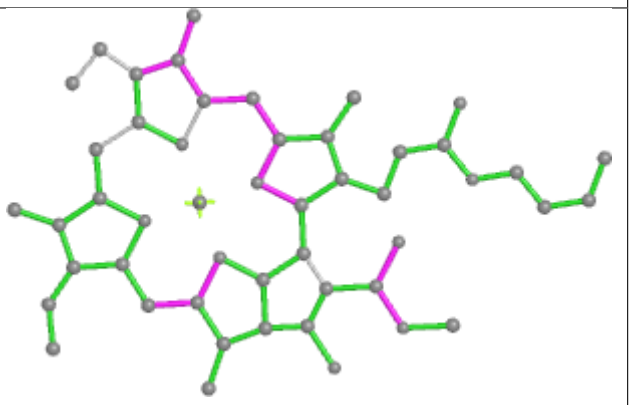
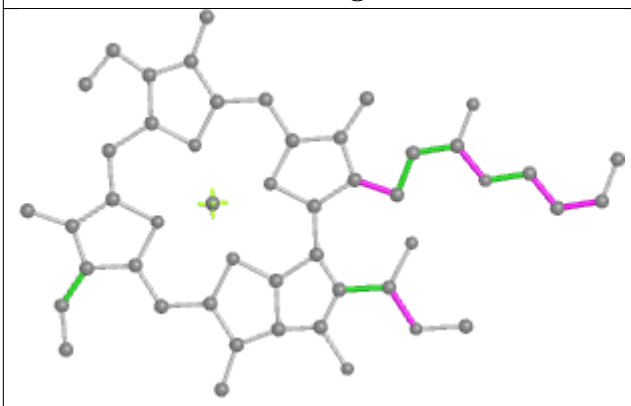
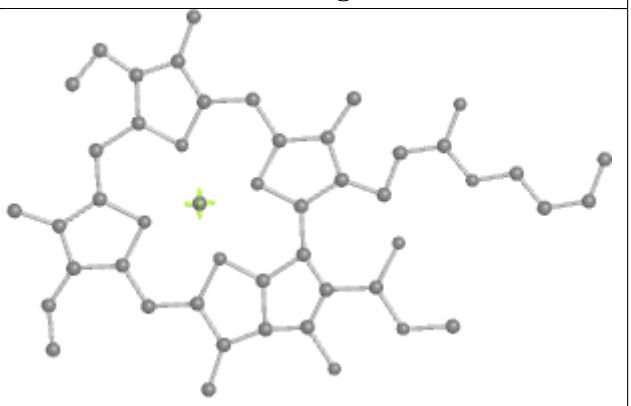
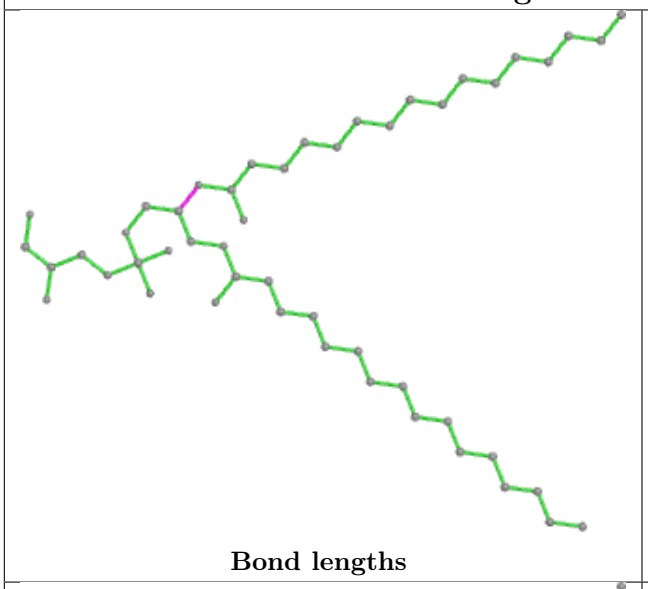


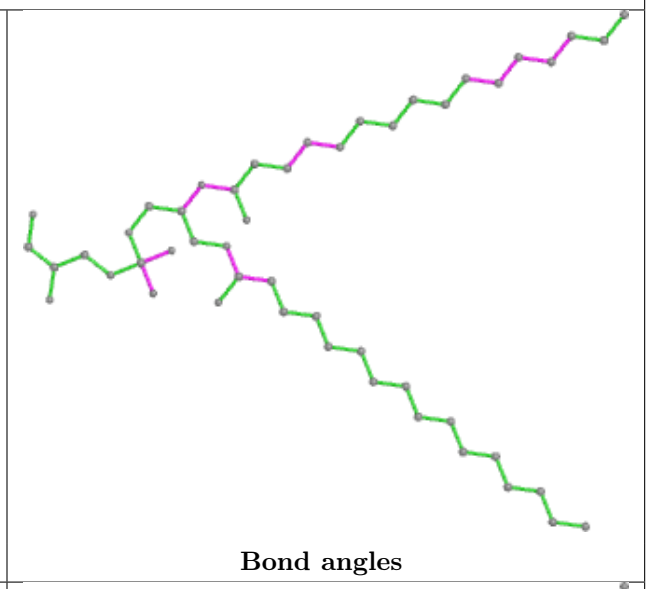
Rings

Ligand CLA s 609	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

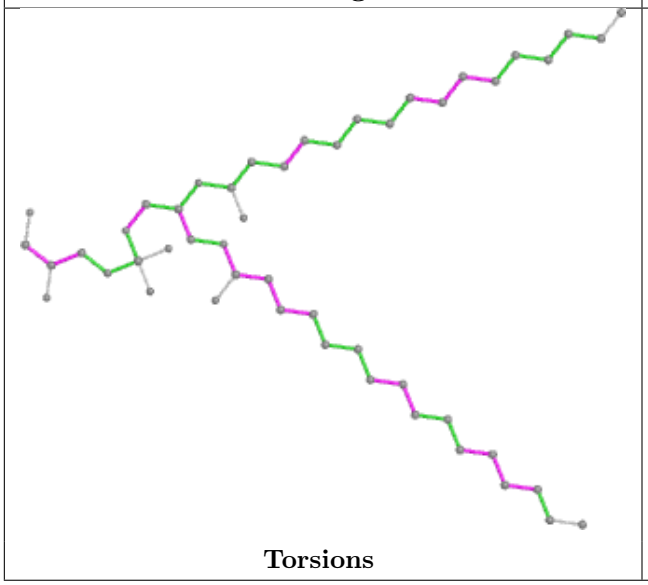
Ligand LHG Y 2630



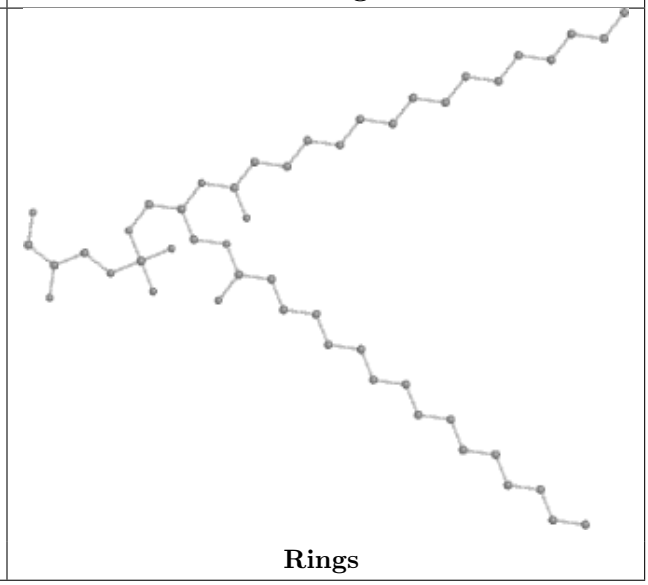
Bond lengths



Bond angles

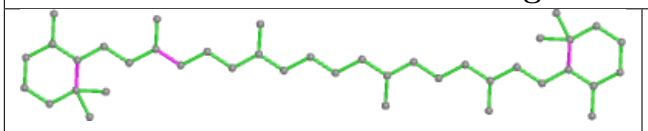


Torsions

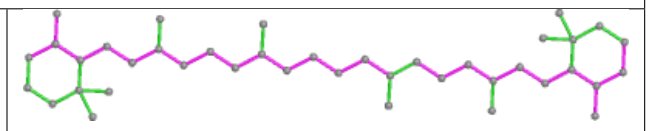


Rings

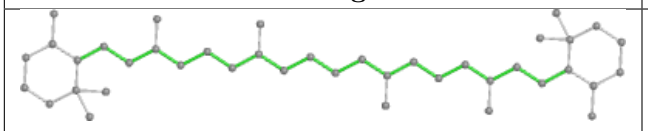
Ligand BCR B 619



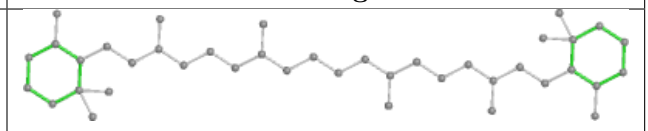
Bond lengths



Bond angles

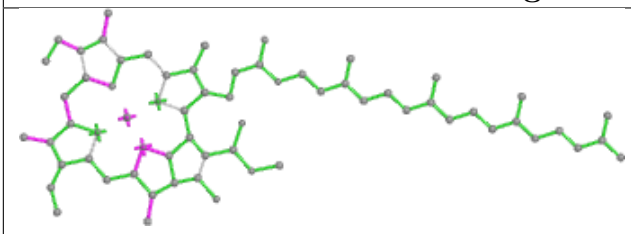


Torsions



Rings

Ligand CLA Y 610



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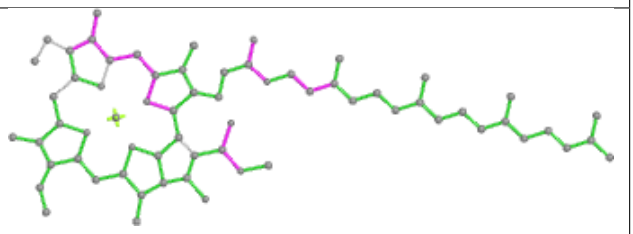
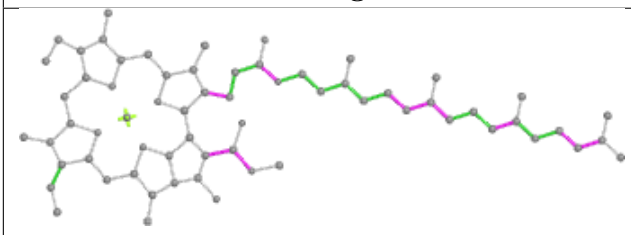
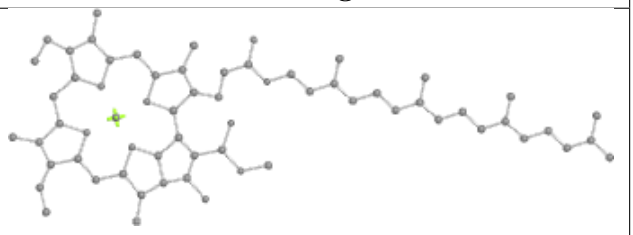


Bond angles

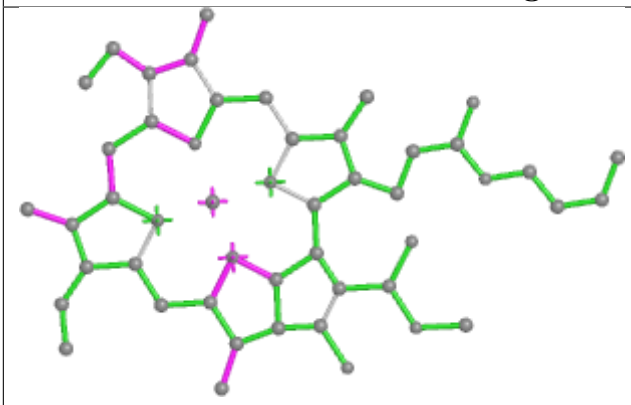


Torsions

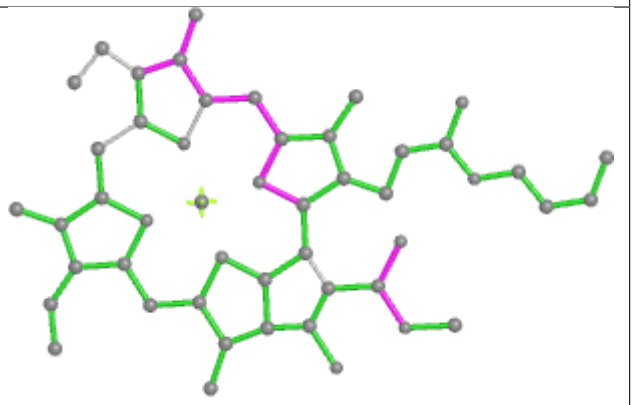


Rings

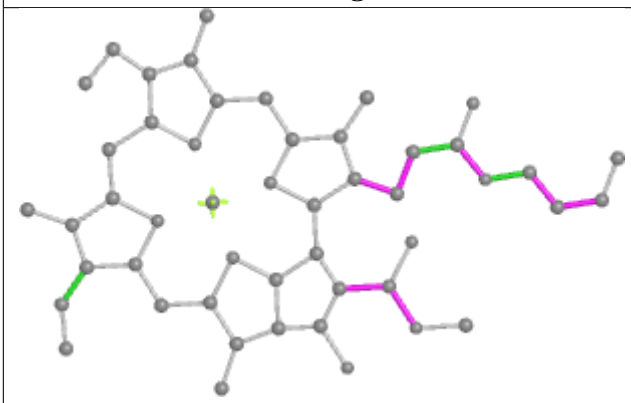
Ligand CLA G 604



Bond lengths



Bond angles



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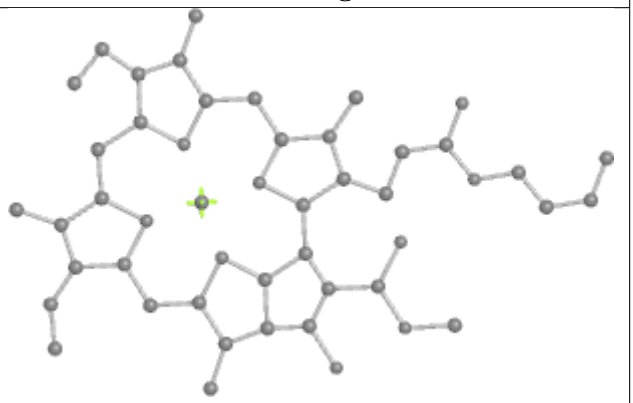
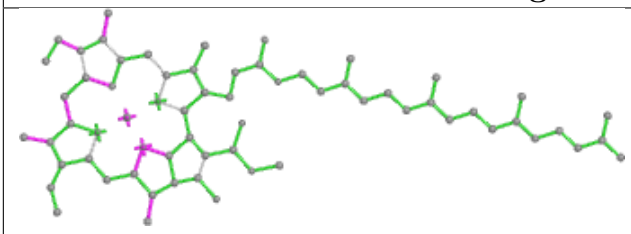
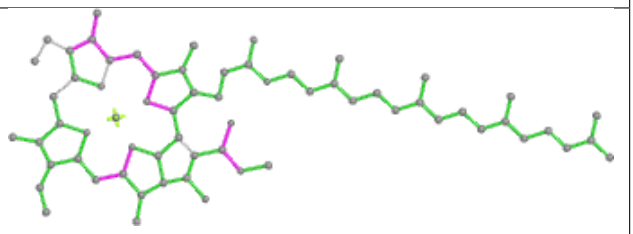


Rings

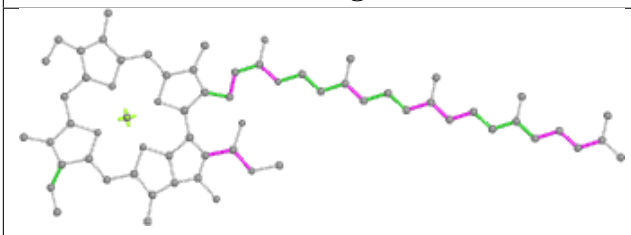
Ligand CLA c 510



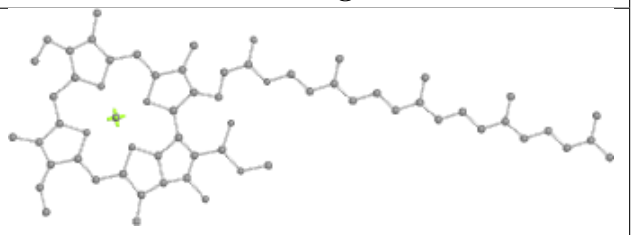
Bond lengths



Bond angles

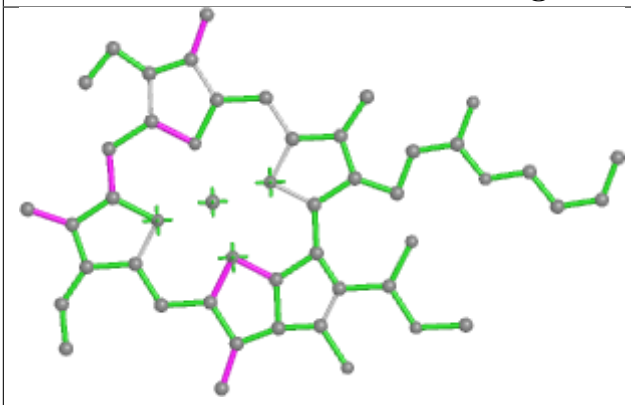


Torsions



Rings

Ligand CLA r 612



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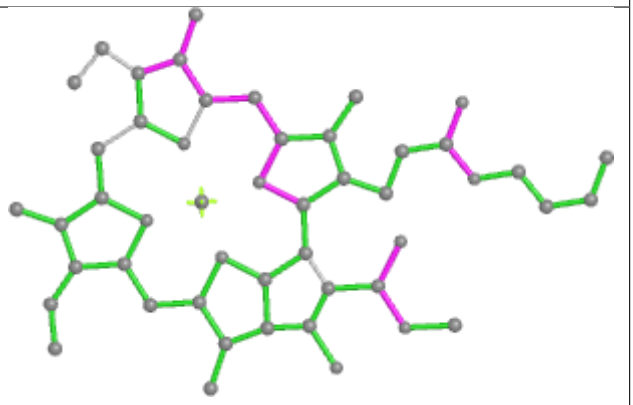
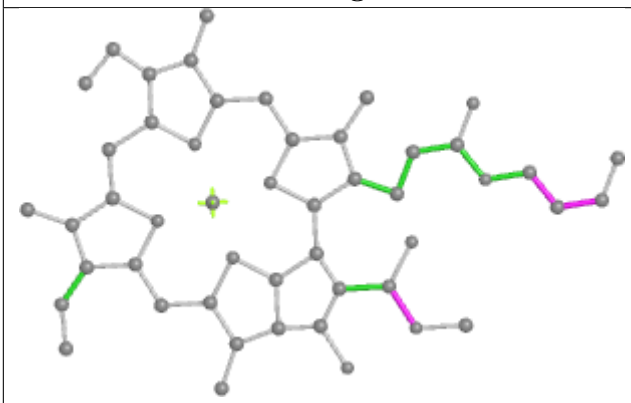


Bond angles



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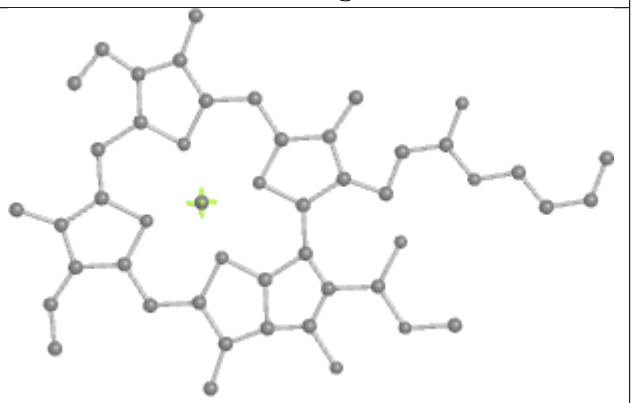
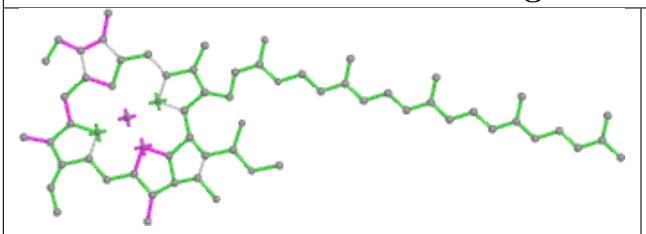


Rings

Ligand CLA B 604



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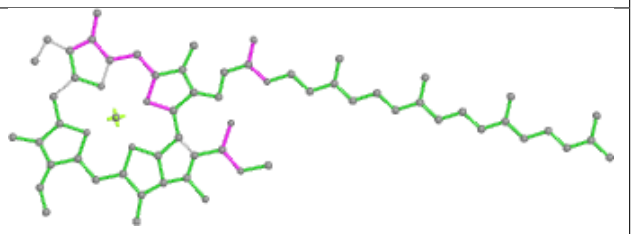
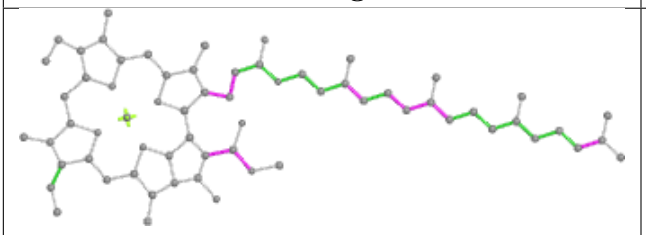
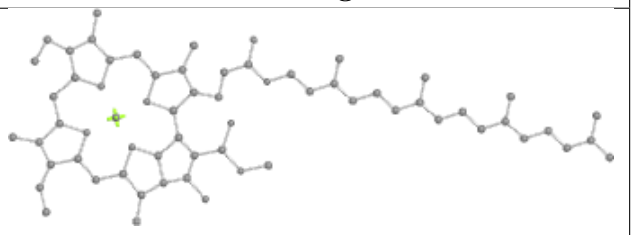


Bond angles

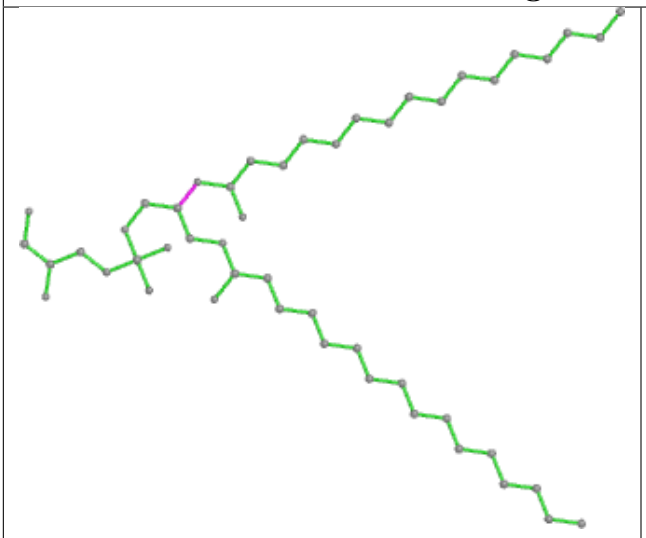


Torsions



Rings

Ligand LHG L 101



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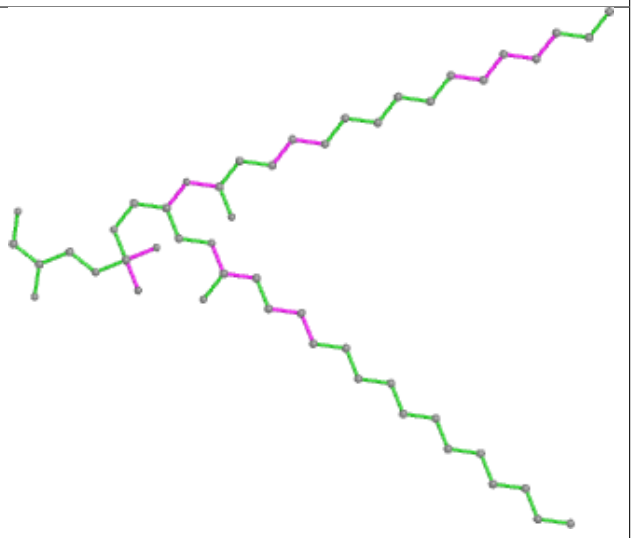
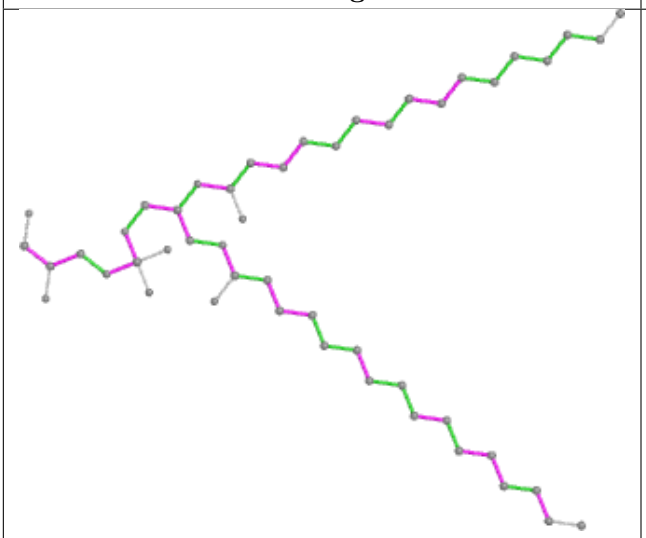


Bond angles



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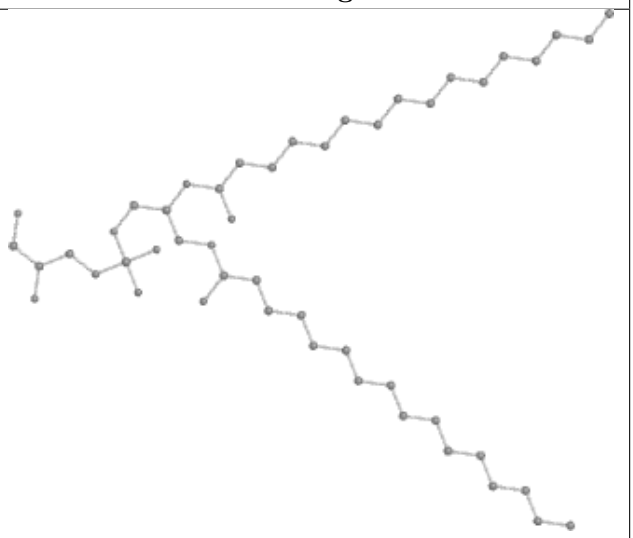
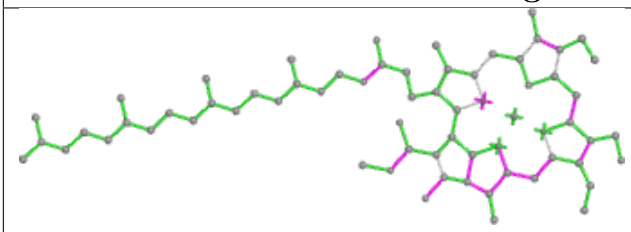


Rings

Ligand CHL Y 609



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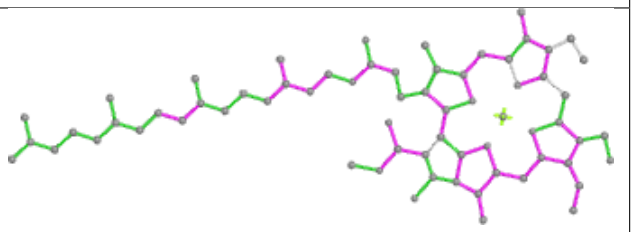
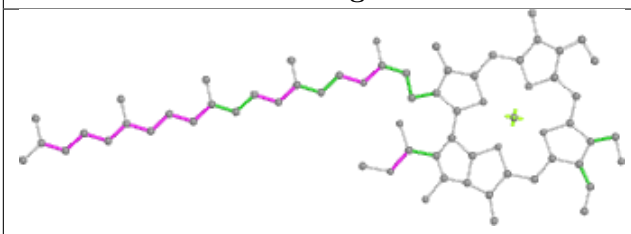


Bond angles



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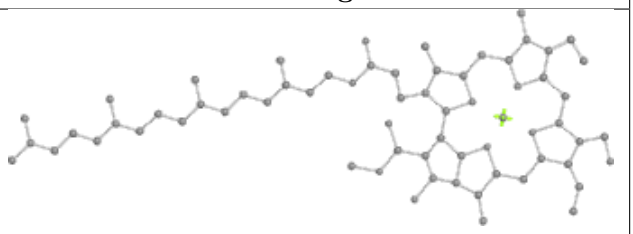
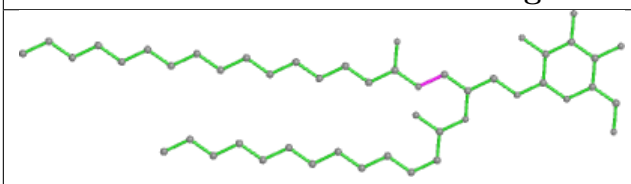


Rings

Ligand LMG a 413



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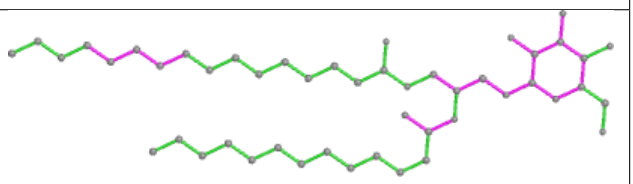
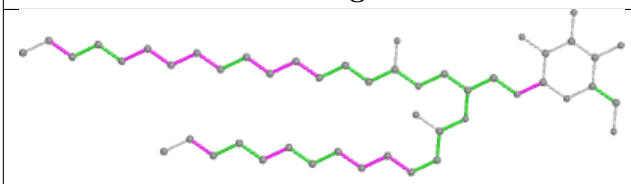


Bond angles



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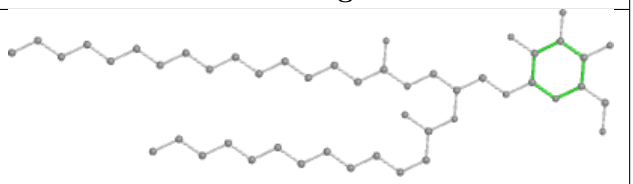
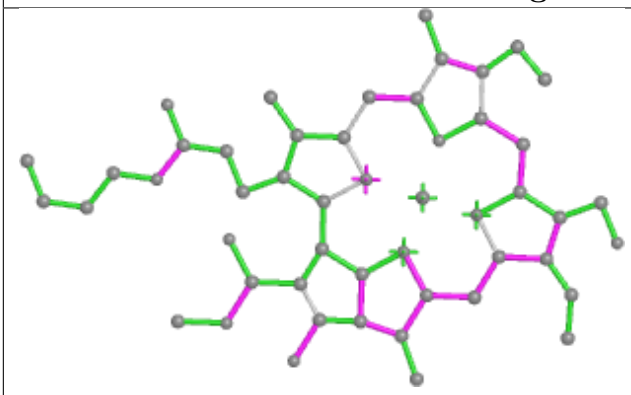


Rings

Ligand CHL s 607



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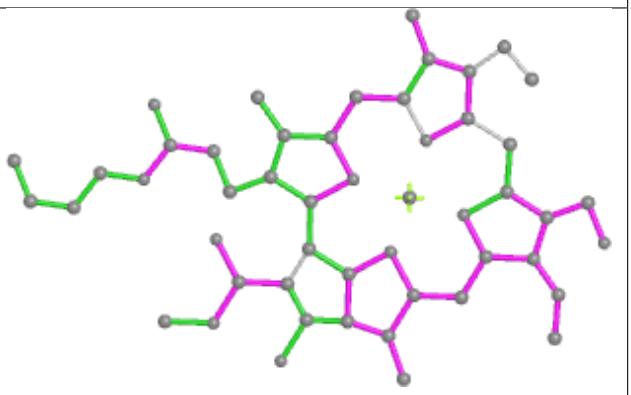
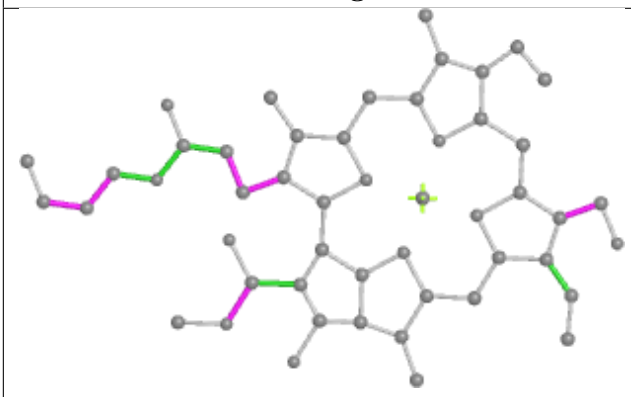
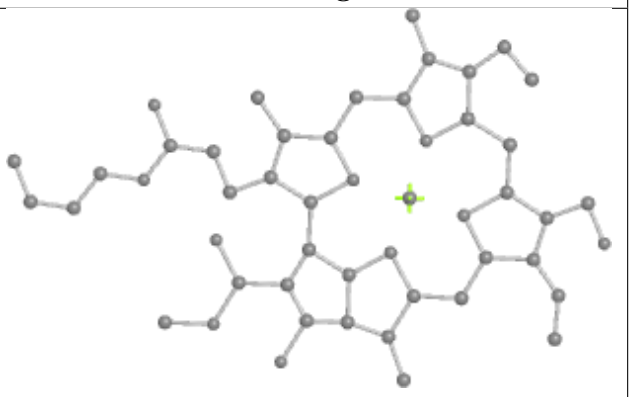


Bond angles

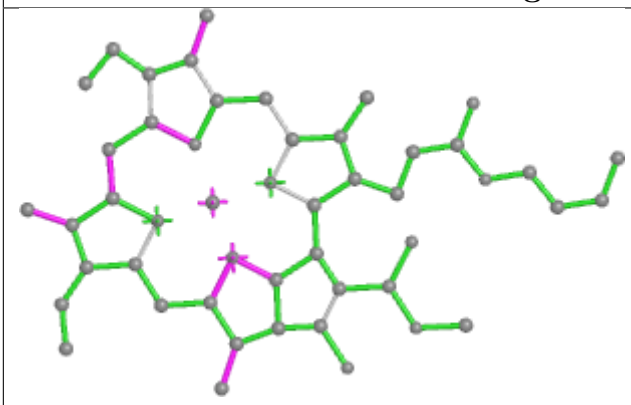


Torsions

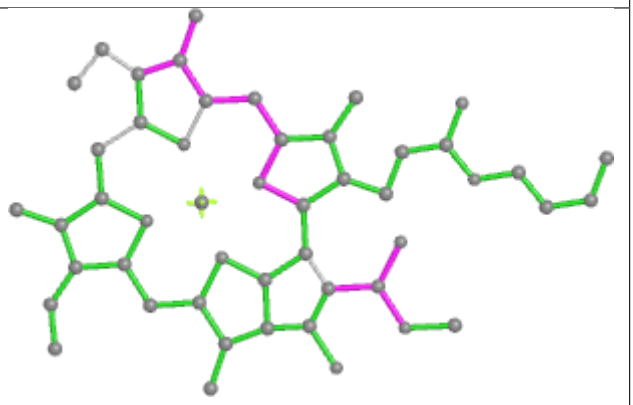


Rings

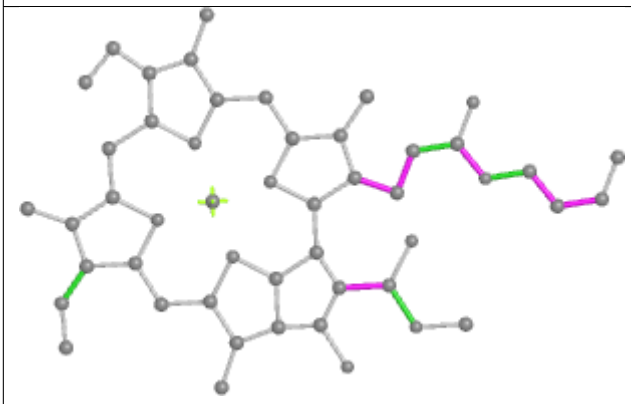
Ligand CLA R 604



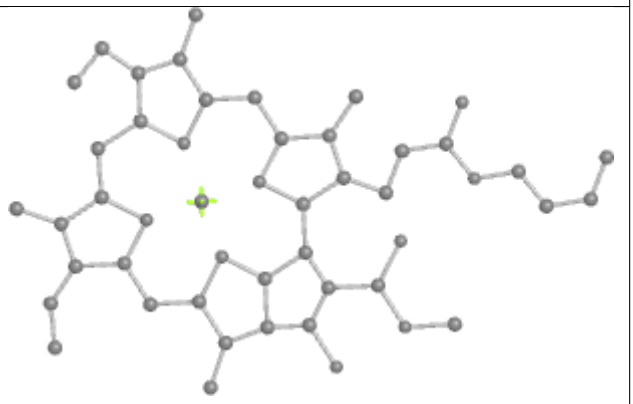
Bond lengths



Bond angles

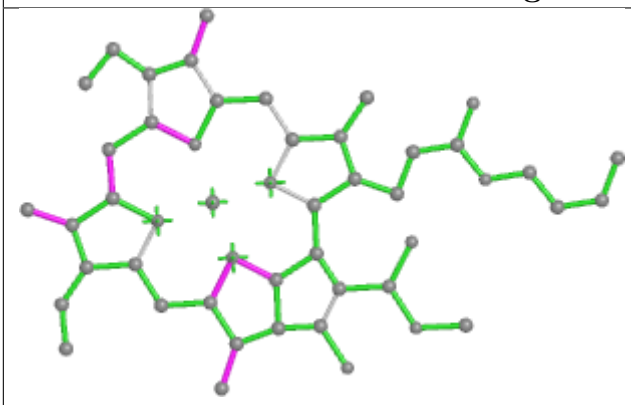


Torsions



Rings

Ligand CLA R 601



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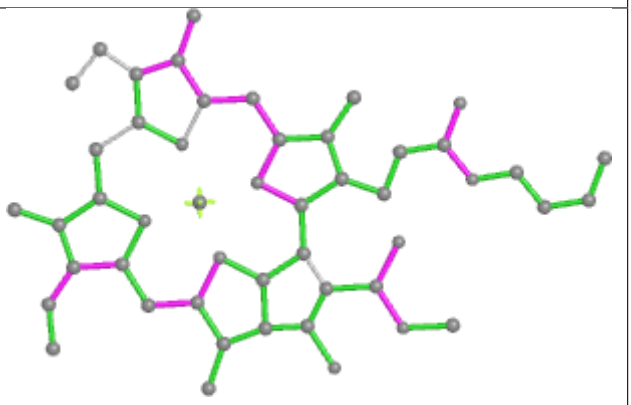
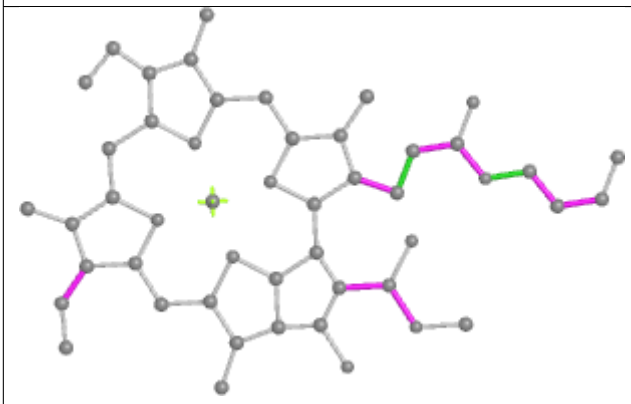


Bond angles



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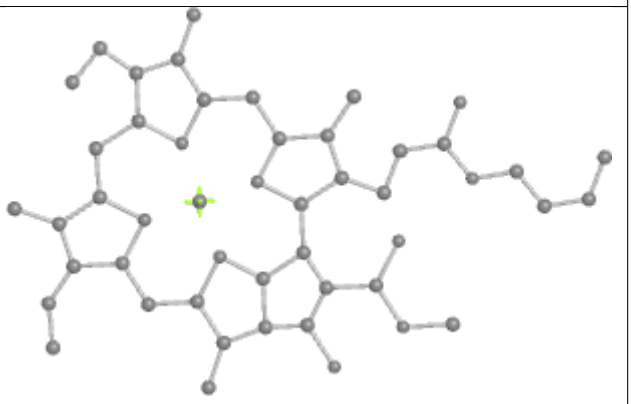
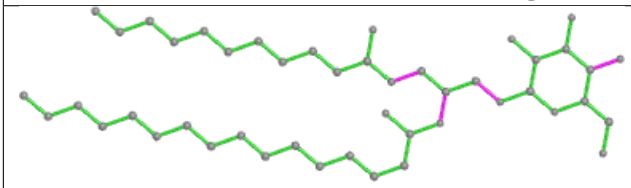


Rings

Ligand LMG d 411



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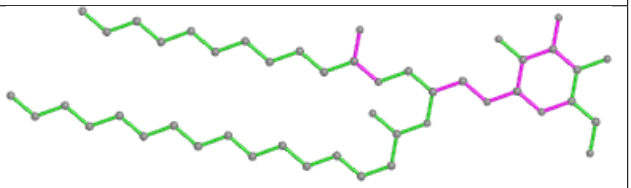
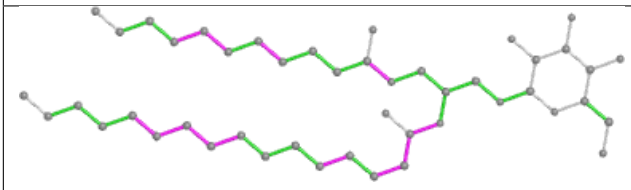


Bond angles



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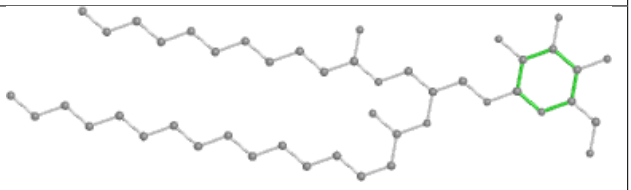
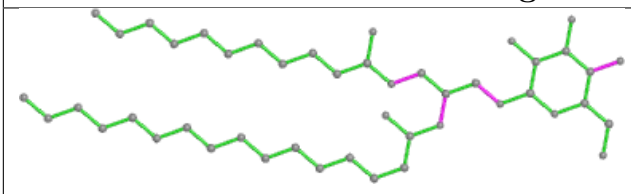
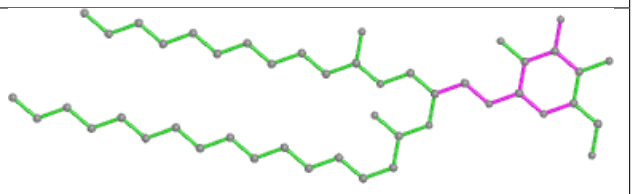


Rings

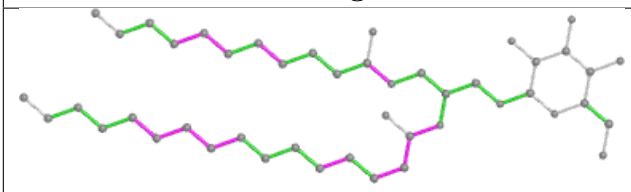
Ligand LMG D 411



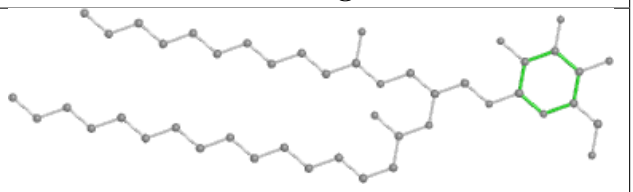
Bond lengths



Bond angles

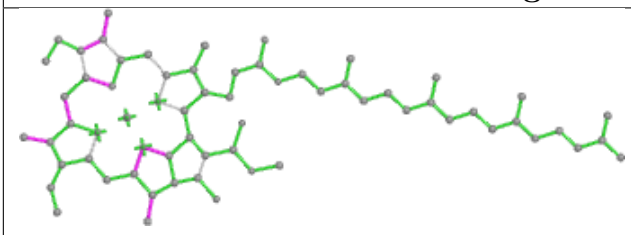


Torsions

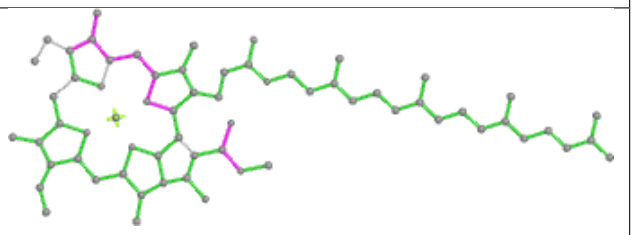


Rings

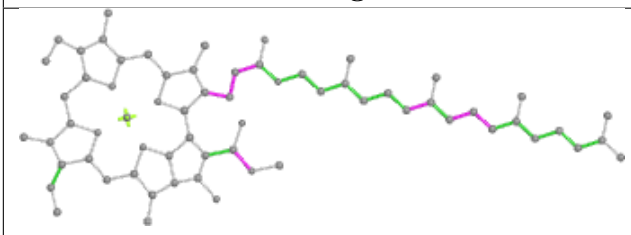
Ligand CLA N 602



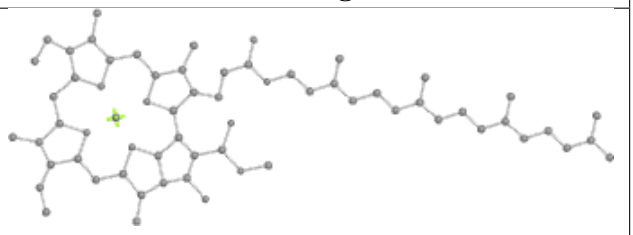
Bond lengths



Bond angles

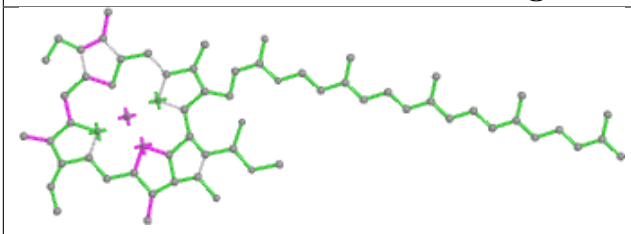


Torsions

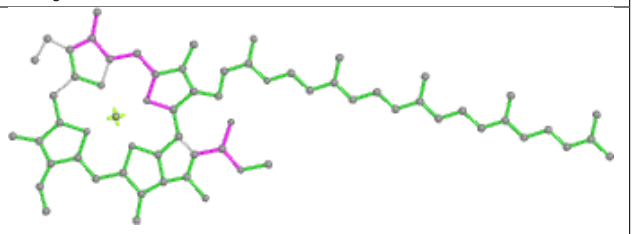


Rings

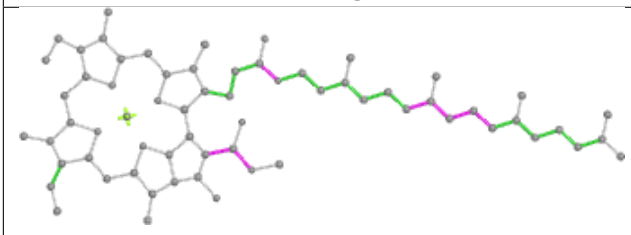
Ligand CLA y 611



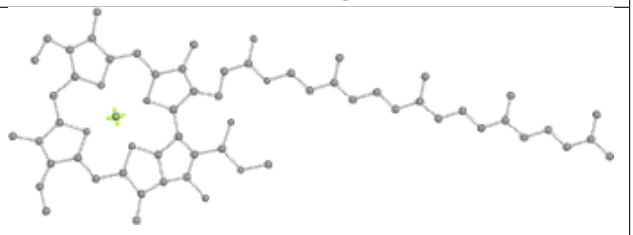
Bond lengths



Bond angles

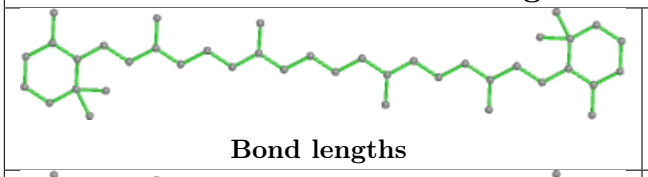


Torsions

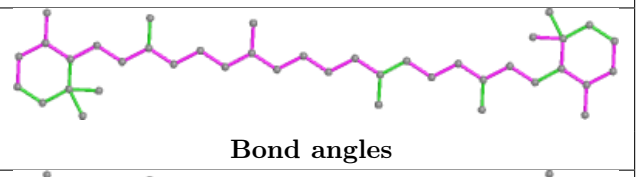


Rings

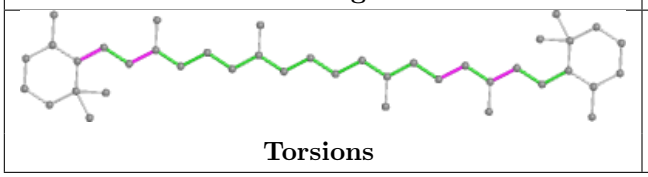
Ligand BCR C 516



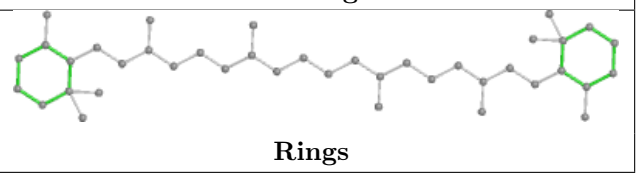
Bond lengths



Bond angles

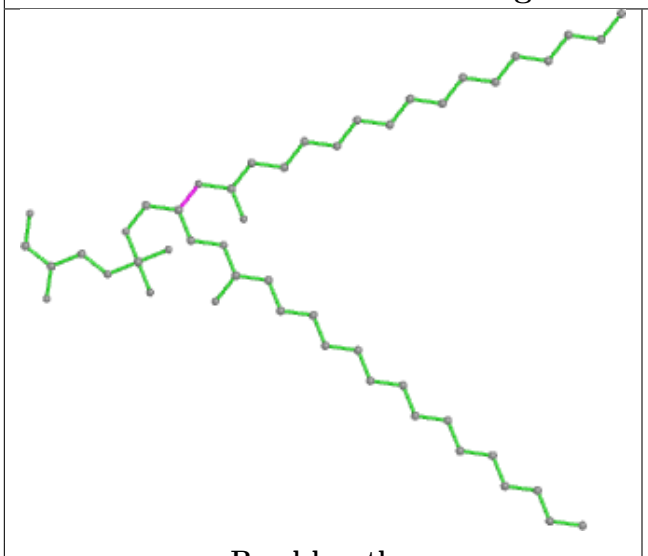


Torsions

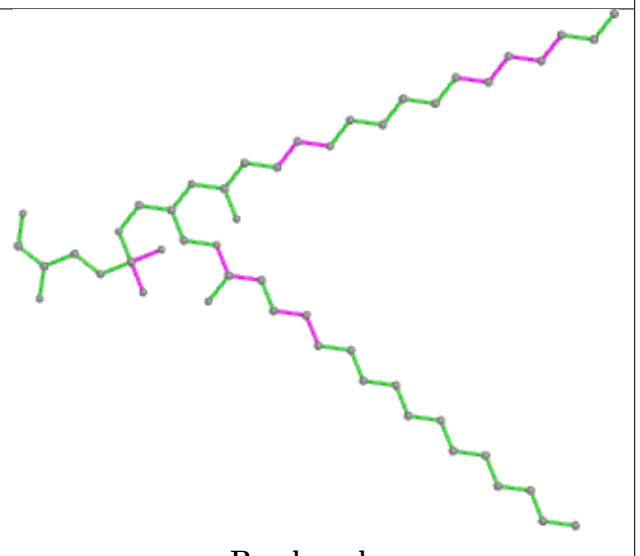


Rings

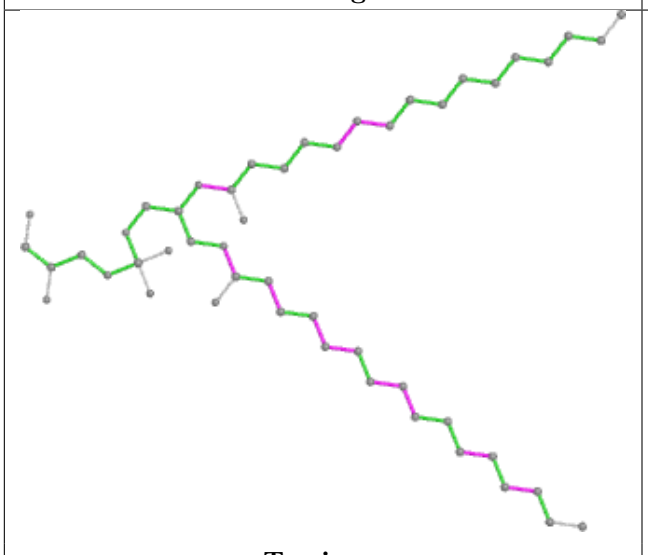
Ligand LHG R 2630



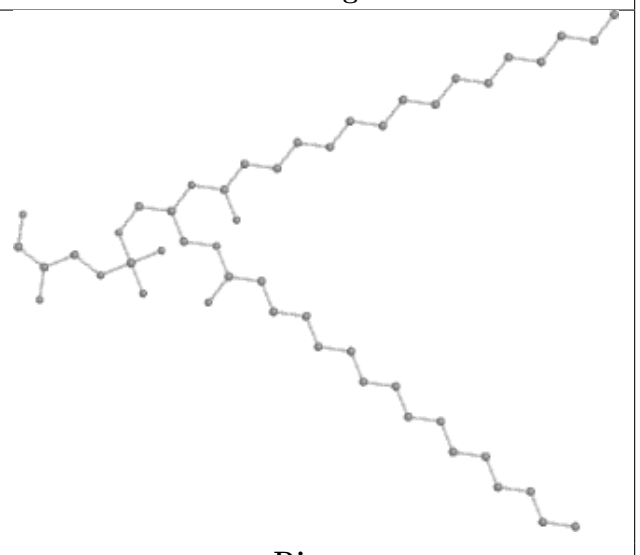
Bond lengths



Bond angles

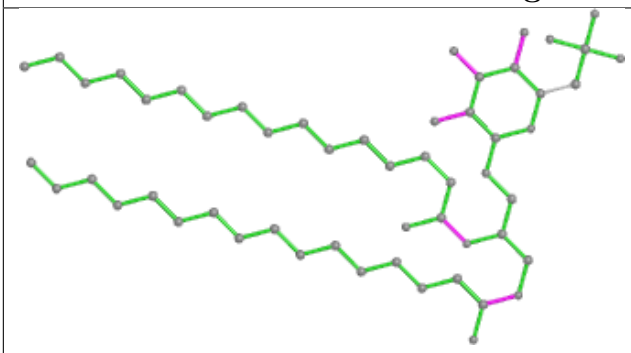


Torsions

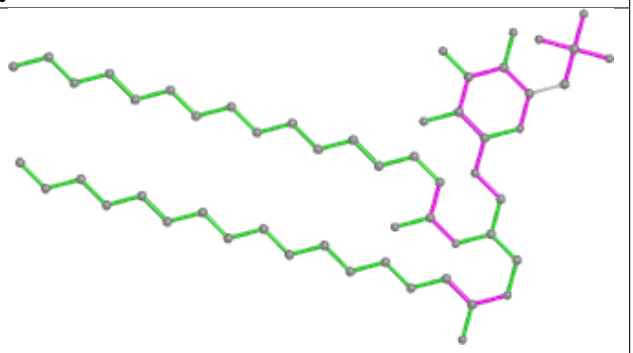


Rings

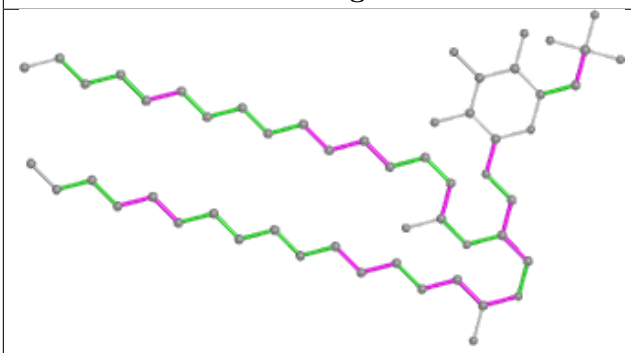
Ligand SQD A 418



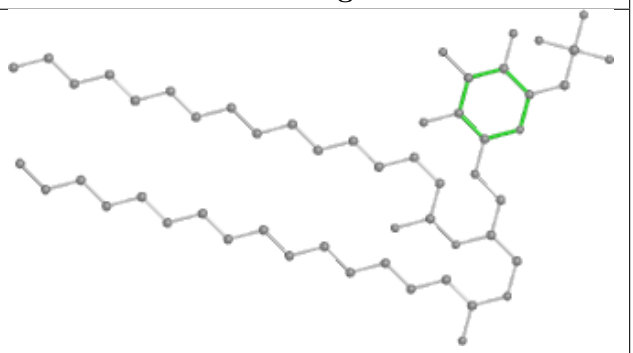
Bond lengths



Bond angles

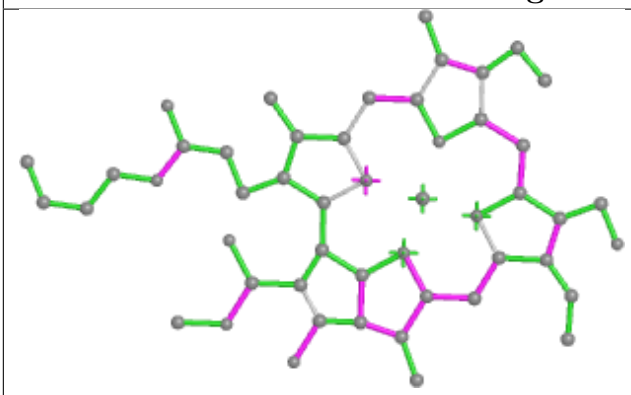


Torsions

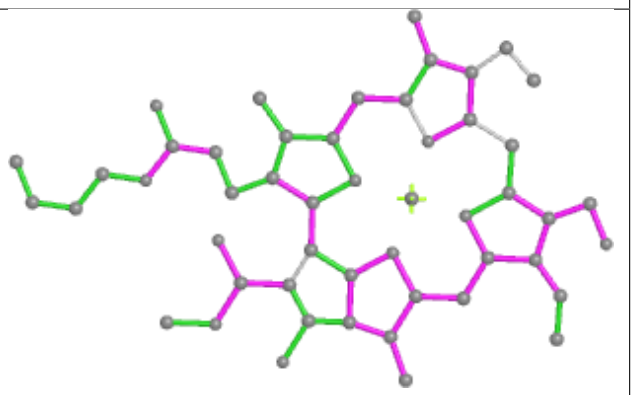


Rings

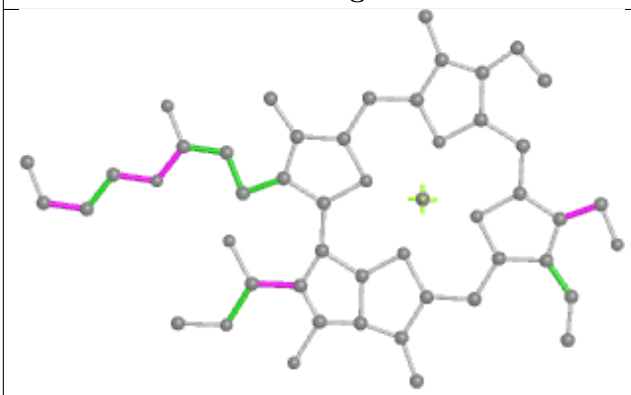
Ligand CHL n 601



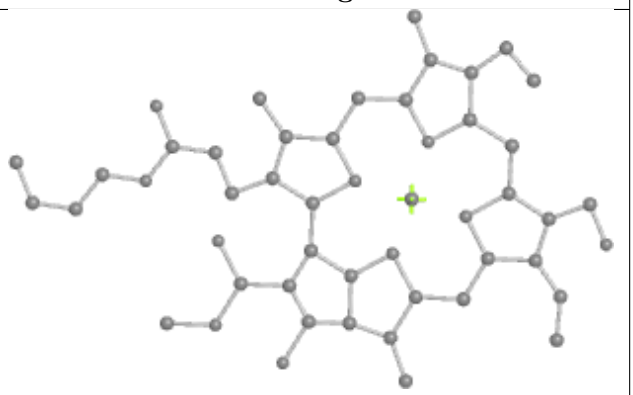
Bond lengths



Bond angles

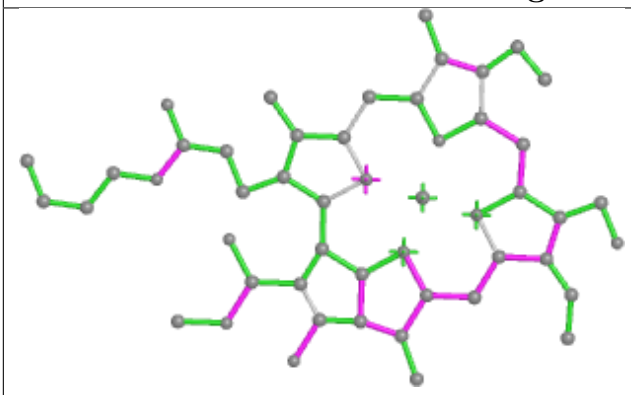


Torsions

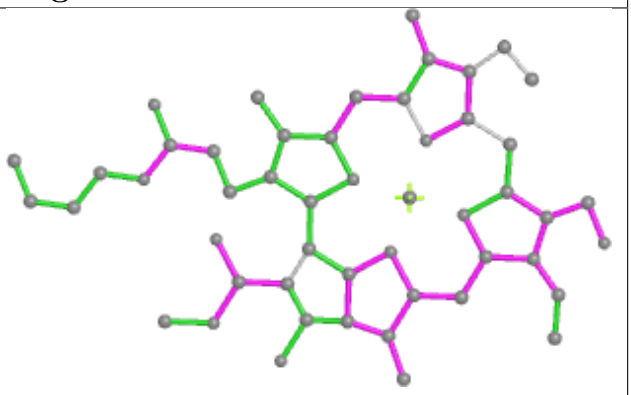


Rings

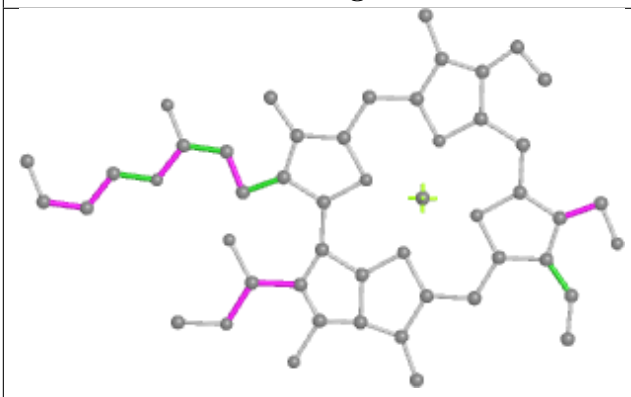
Ligand CHL g 608



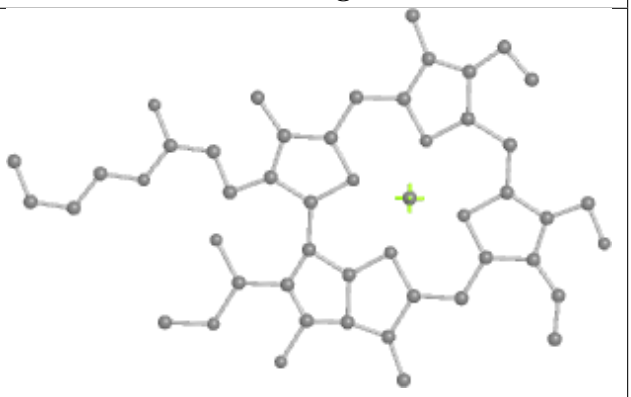
Bond lengths



Bond angles

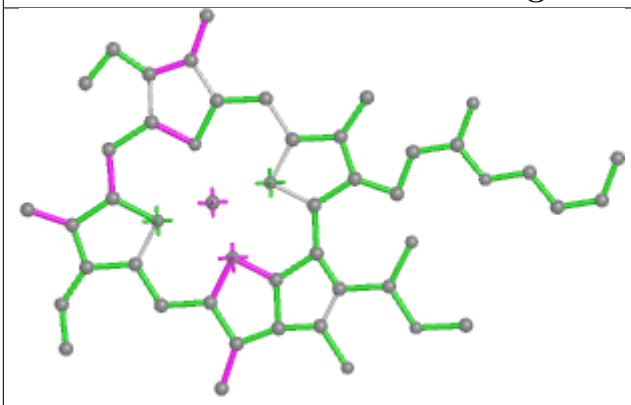


Torsions

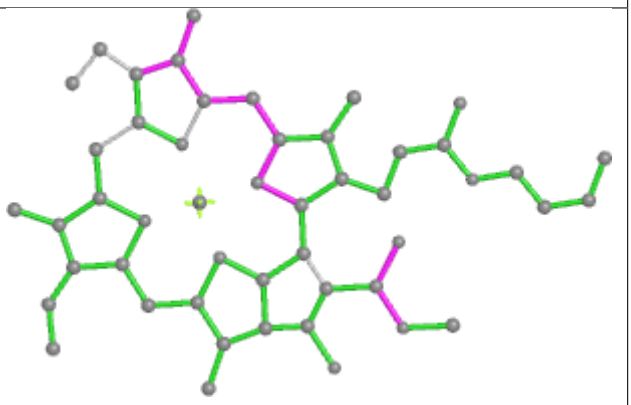


Rings

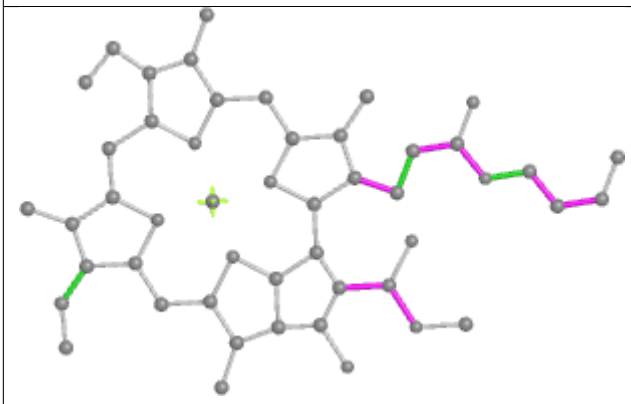
Ligand CLA n 603



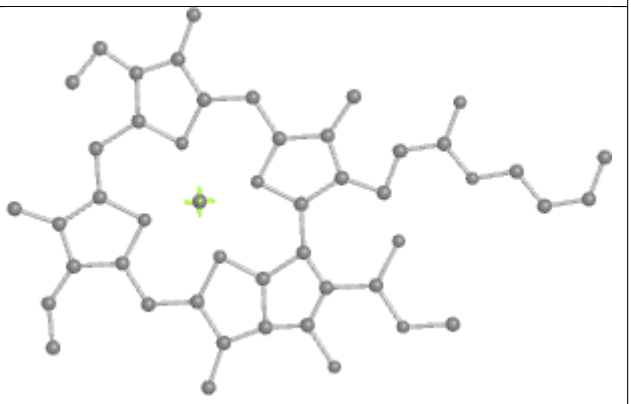
Bond lengths



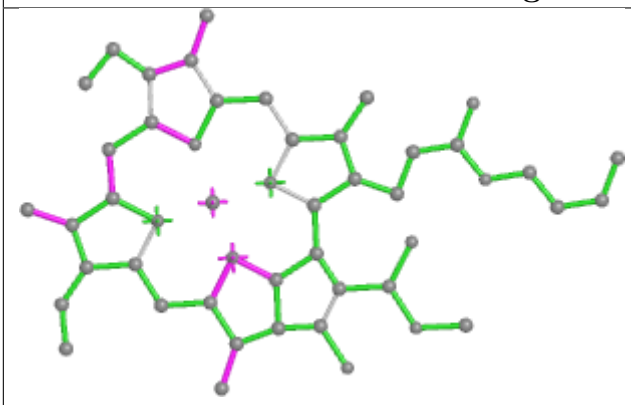
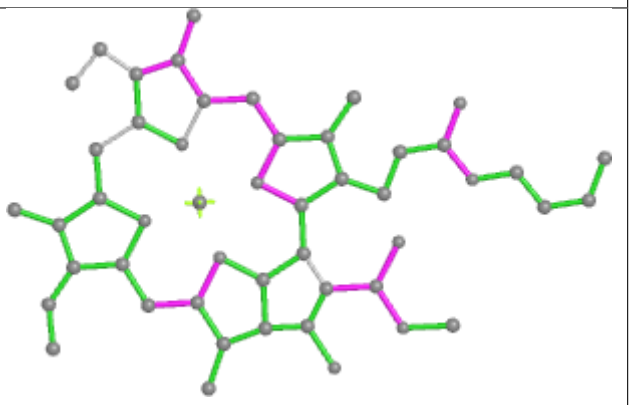
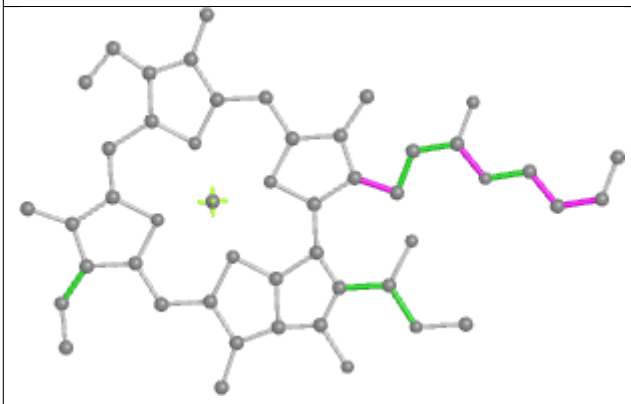
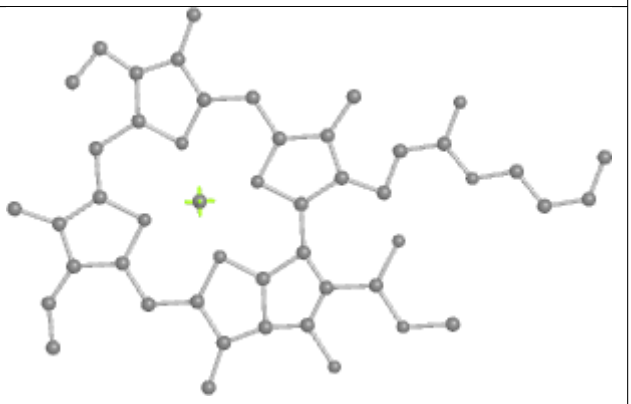
Bond angles



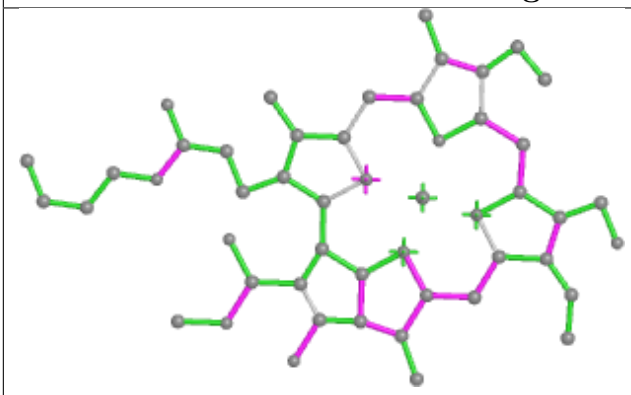
Torsions



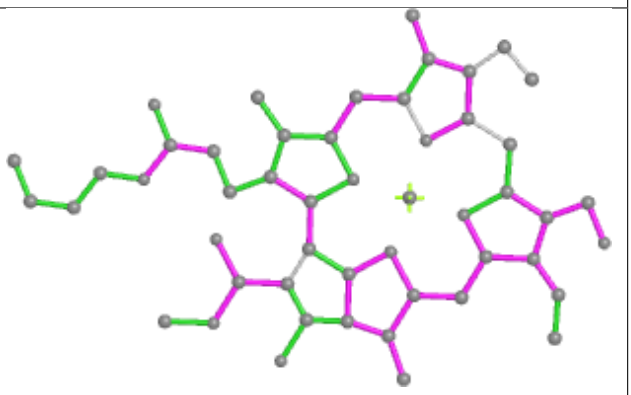
Rings

Ligand CLA G 611	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

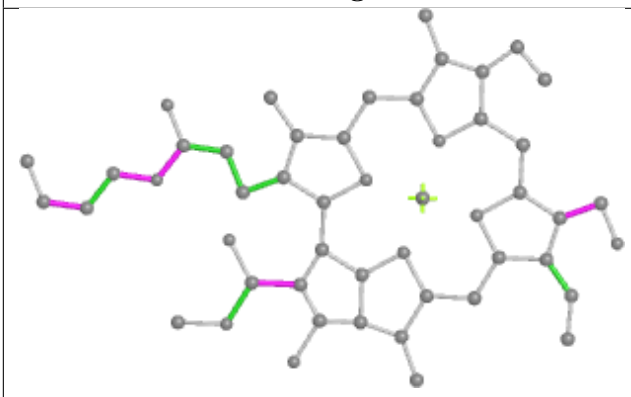
Ligand CHL N 601



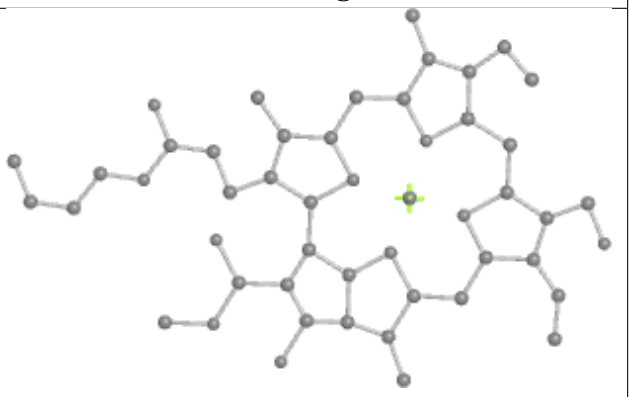
Bond lengths



Bond angles

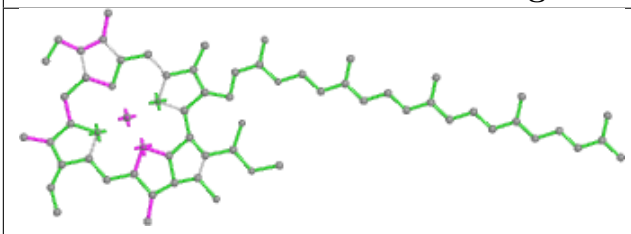


Torsions

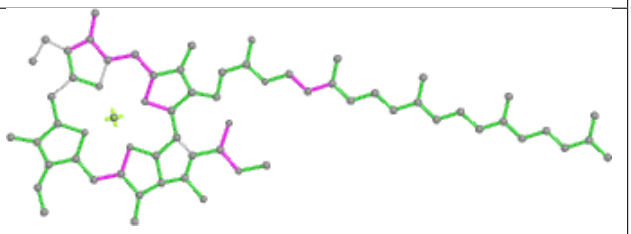


Rings

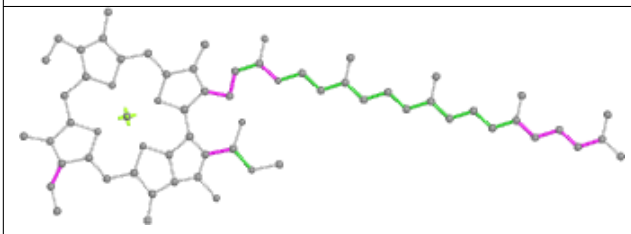
Ligand CLA a 406



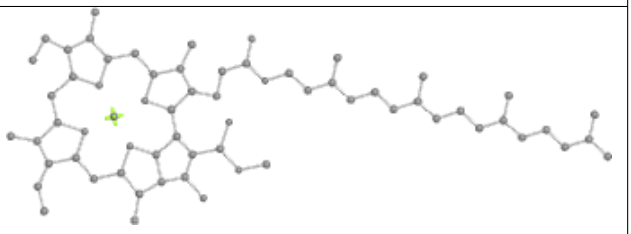
Bond lengths



Bond angles

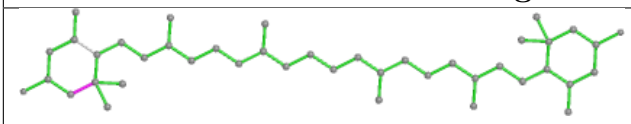


Torsions

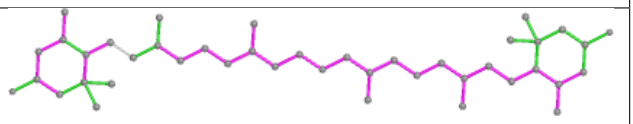


Rings

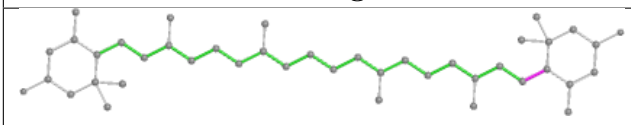
Ligand LUT G 1621



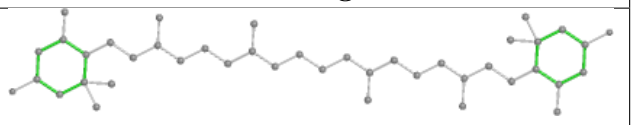
Bond lengths



Bond angles

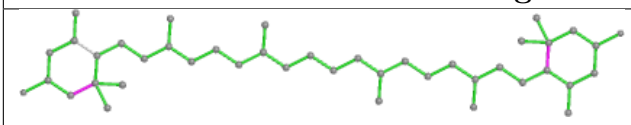


Torsions

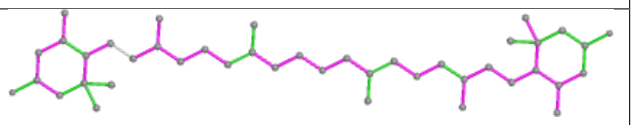


Rings

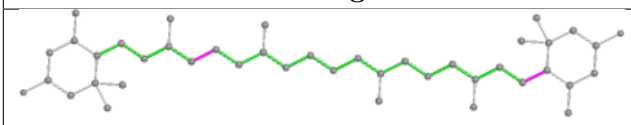
Ligand LUT N 1621



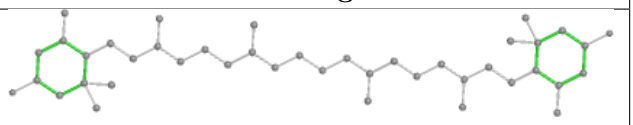
Bond lengths



Bond angles

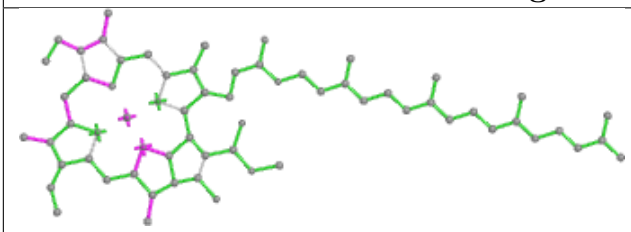


Torsions

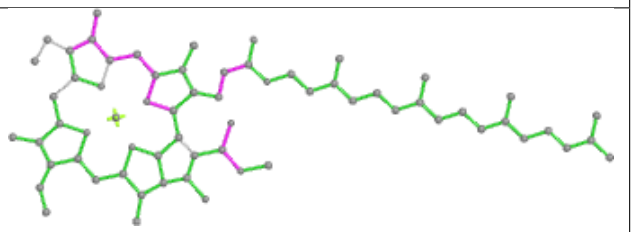


Rings

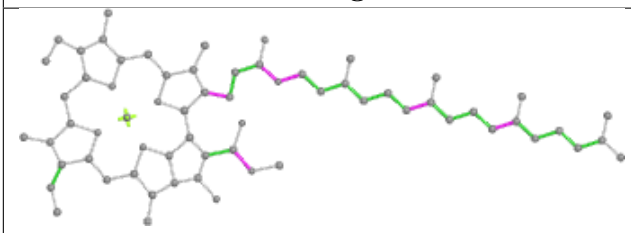
Ligand CLA c 511



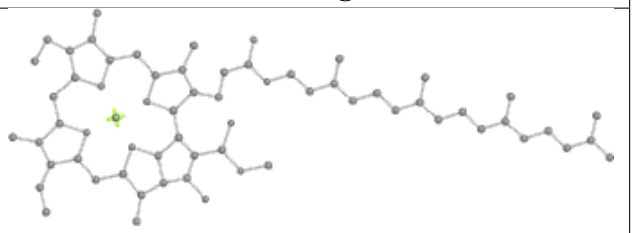
Bond lengths



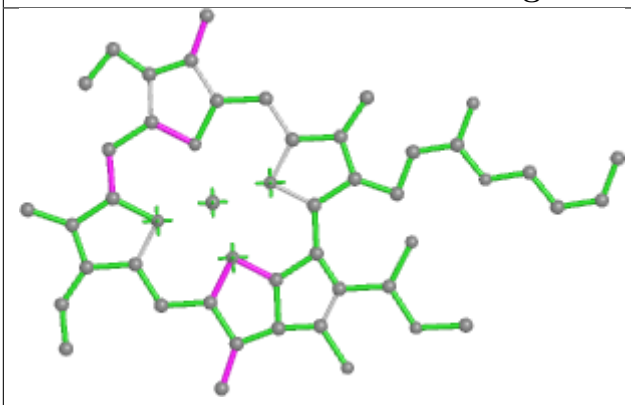
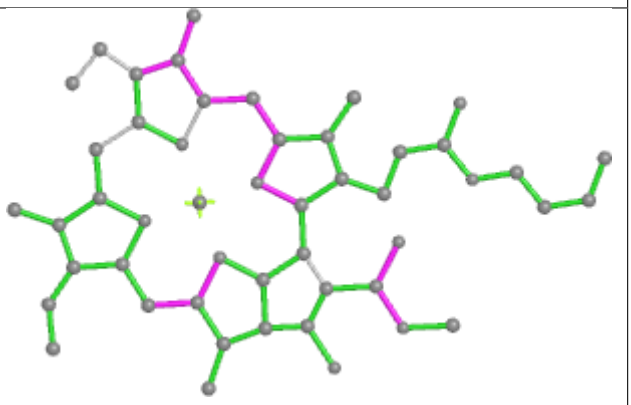
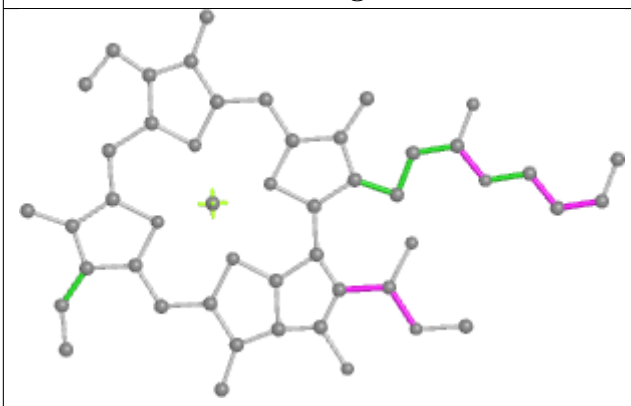
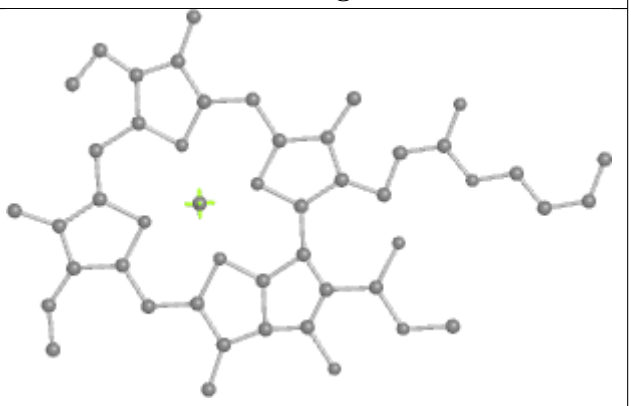
Bond angles



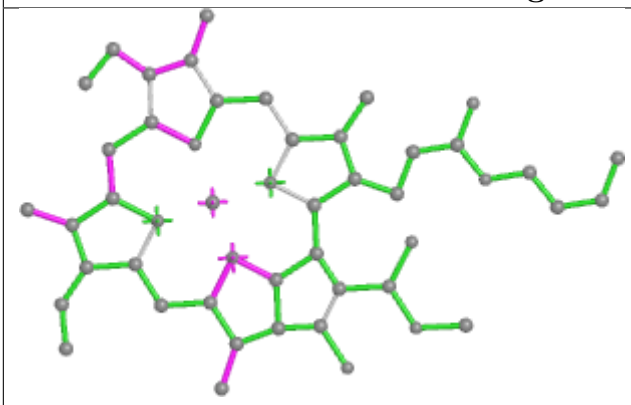
Torsions



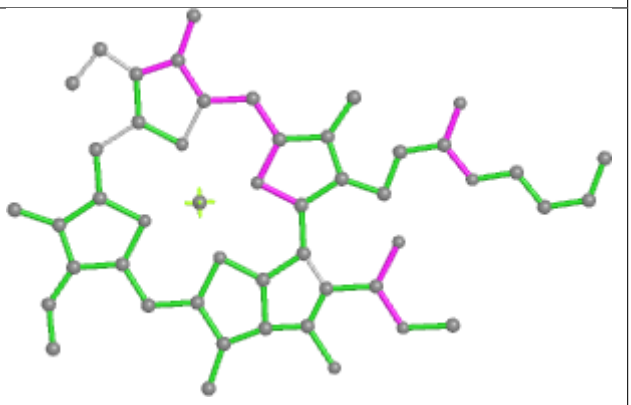
Rings

Ligand CLA G 614	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

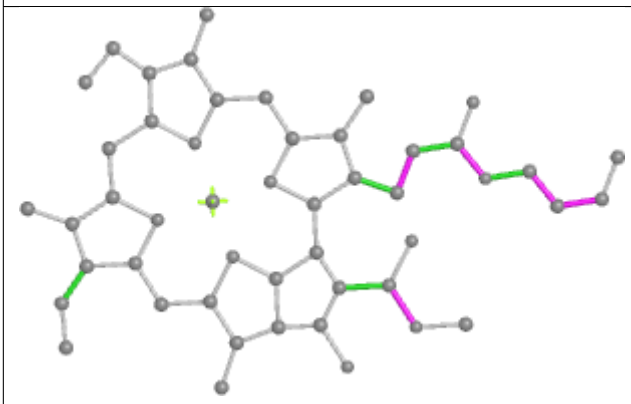
Ligand CLA S 614



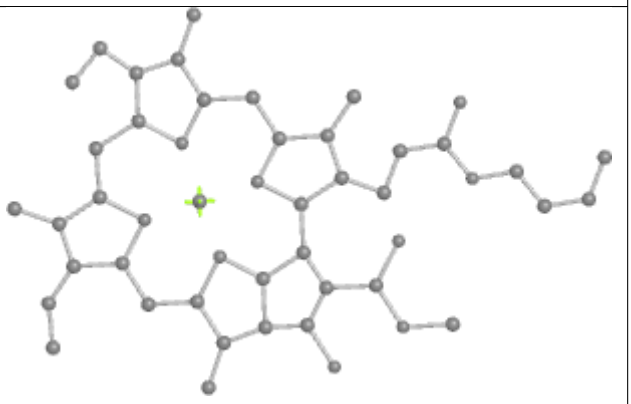
Bond lengths



Bond angles

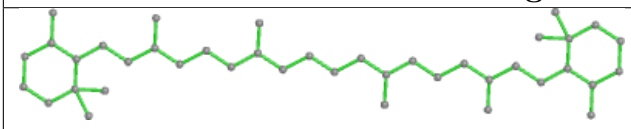


Torsions

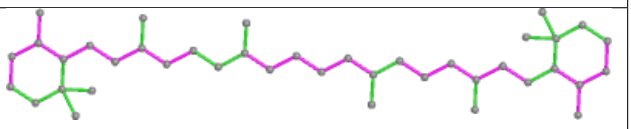


Rings

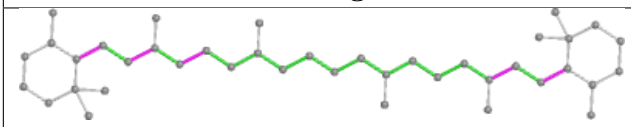
Ligand BCR d 404



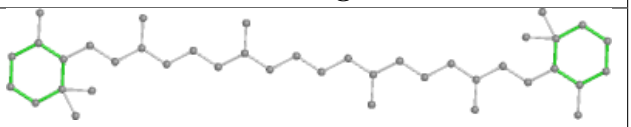
Bond lengths



Bond angles

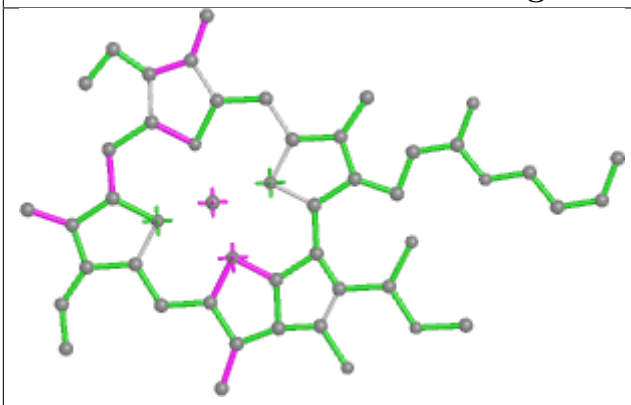


Torsions



Rings

Ligand CLA S 612



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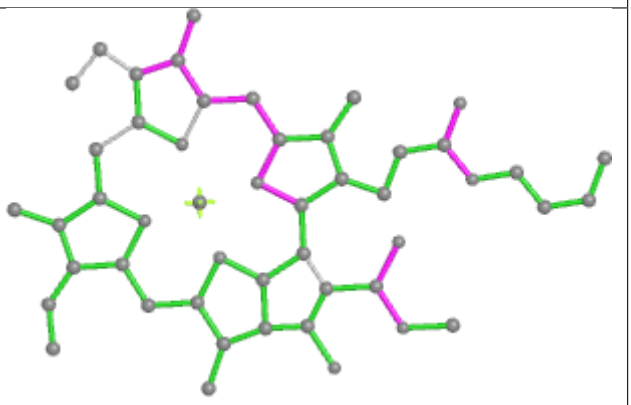

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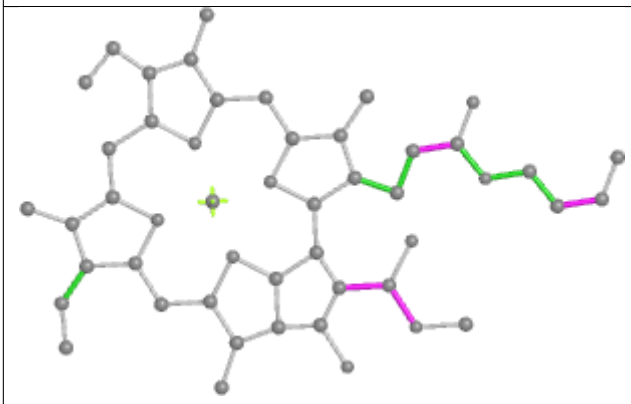

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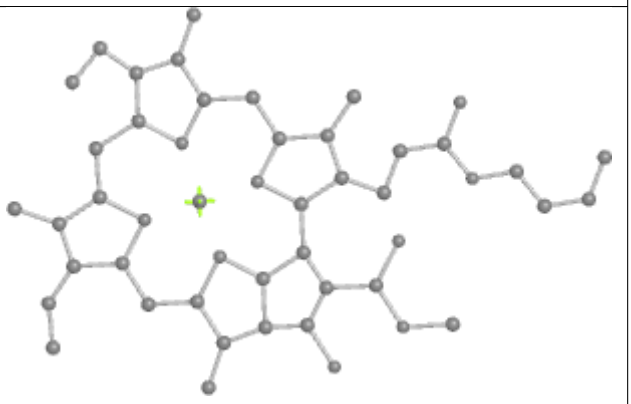
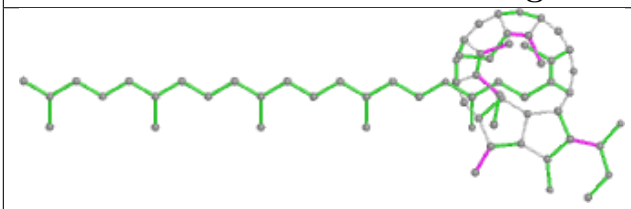


Rings

Ligand PHO a 408



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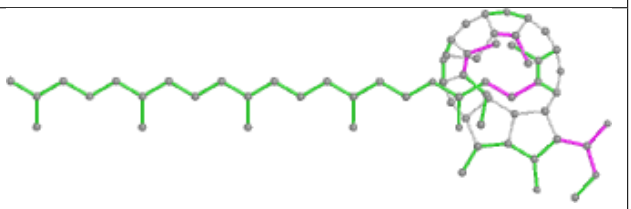
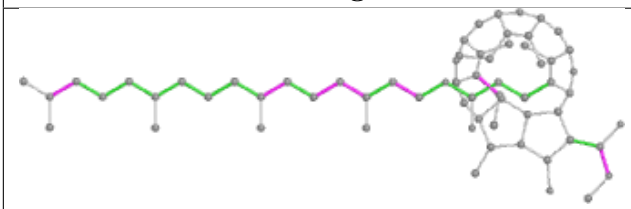


Bond angles



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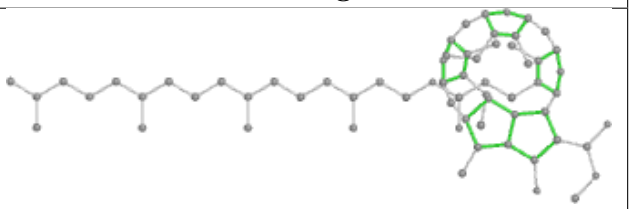
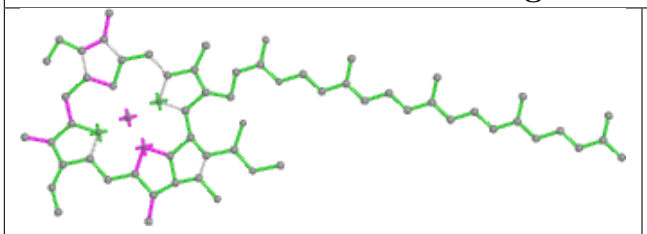


Rings

Ligand CLA Y 611



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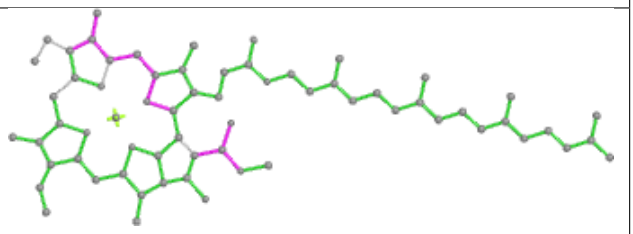
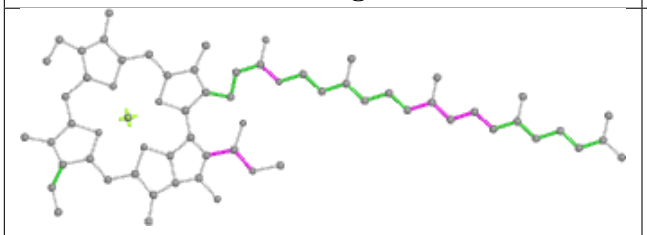


Bond angles



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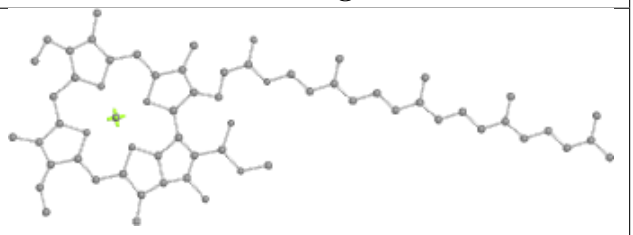
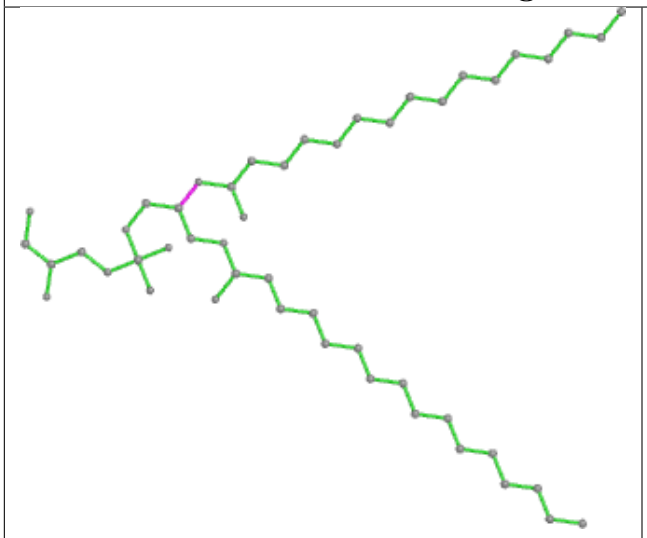


Rings

Ligand LHG S 2630



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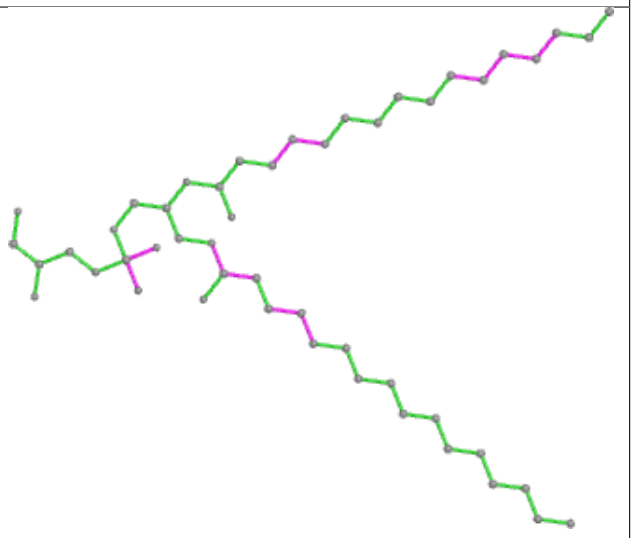
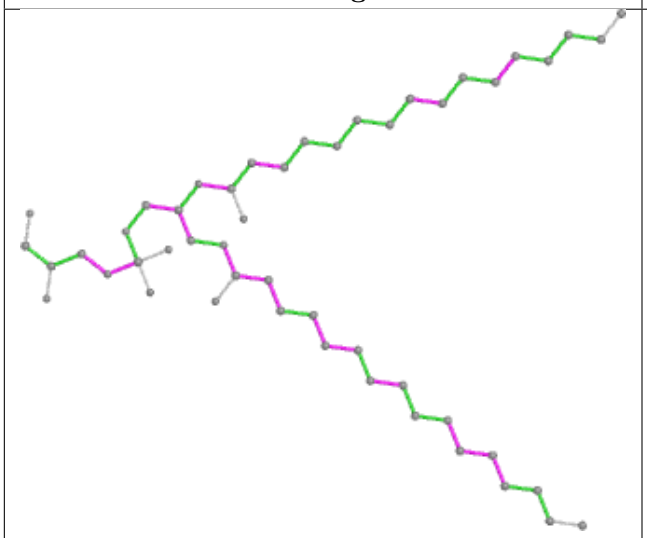


Bond angles



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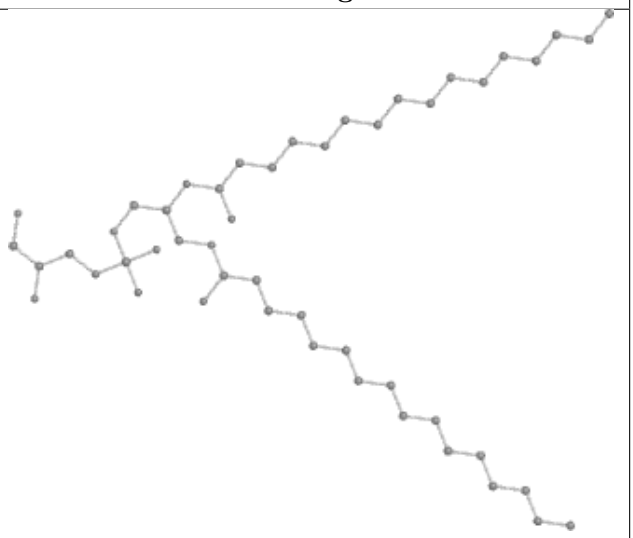
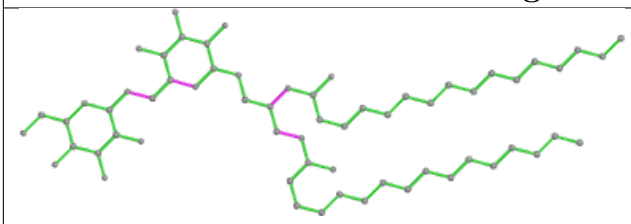


Rings

Ligand DGD h 102



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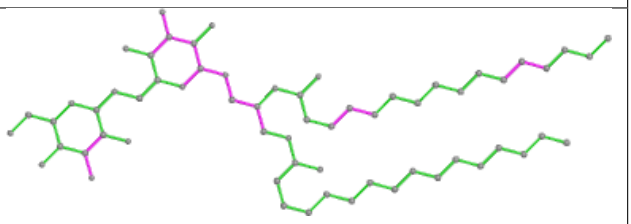
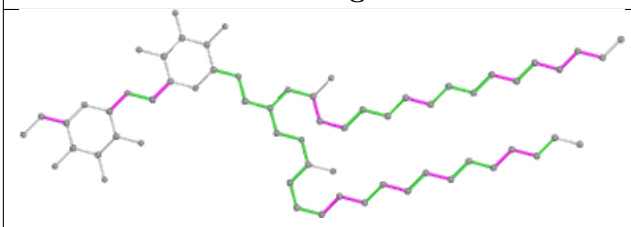


Bond angles



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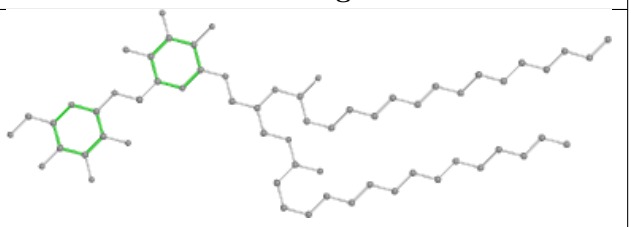
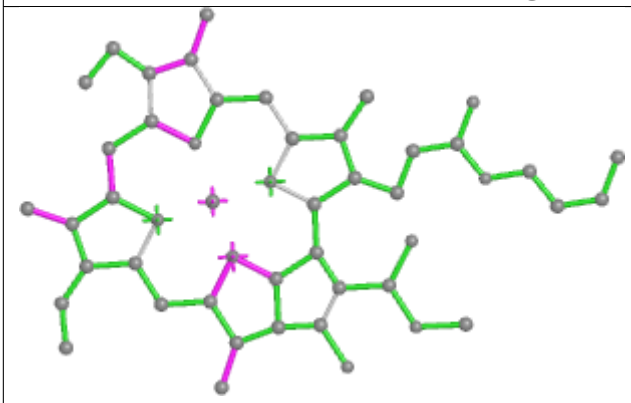


Rings

Ligand CLA N 604



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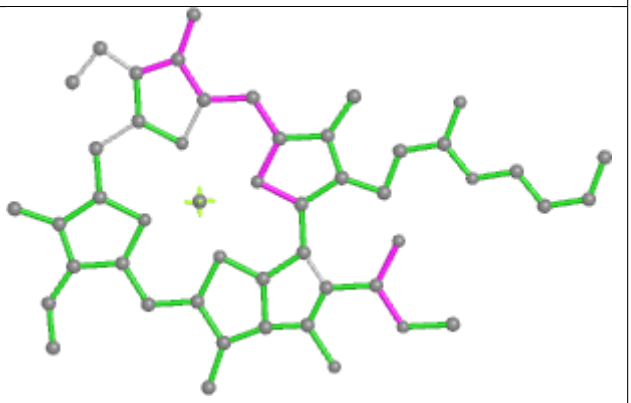
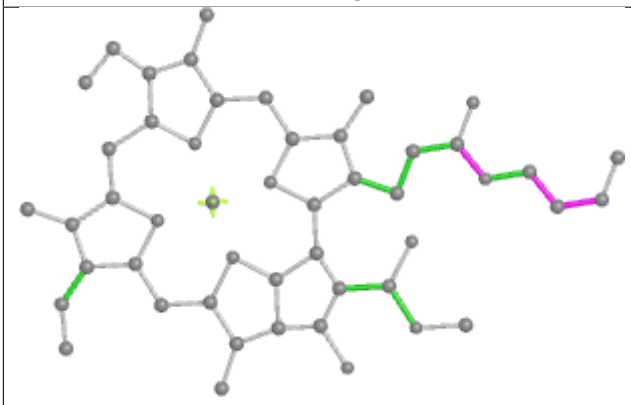


Bond angles



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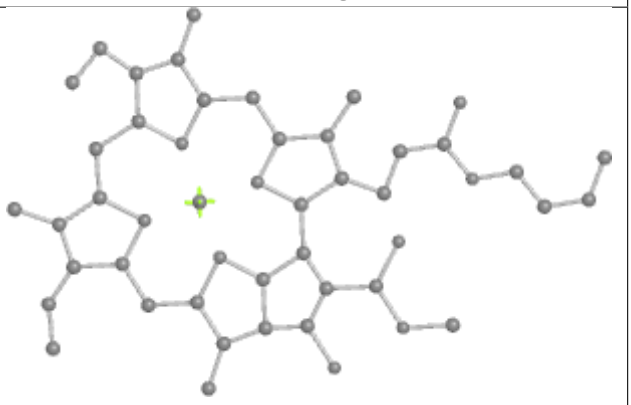
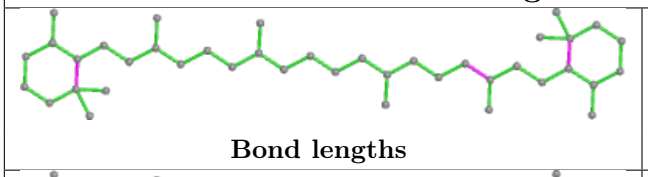


Rings

Ligand BCR B 618



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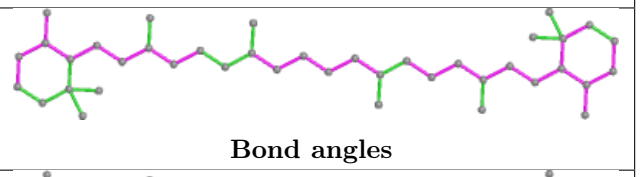
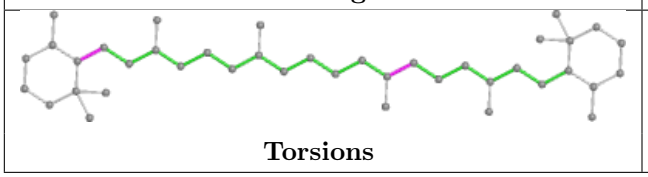


Bond angles



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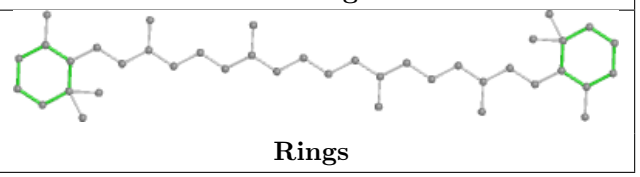
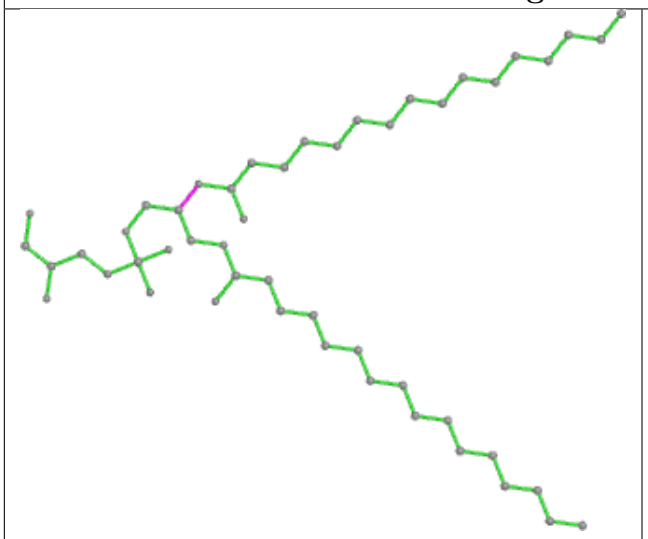


Rings

Ligand LHG d 409



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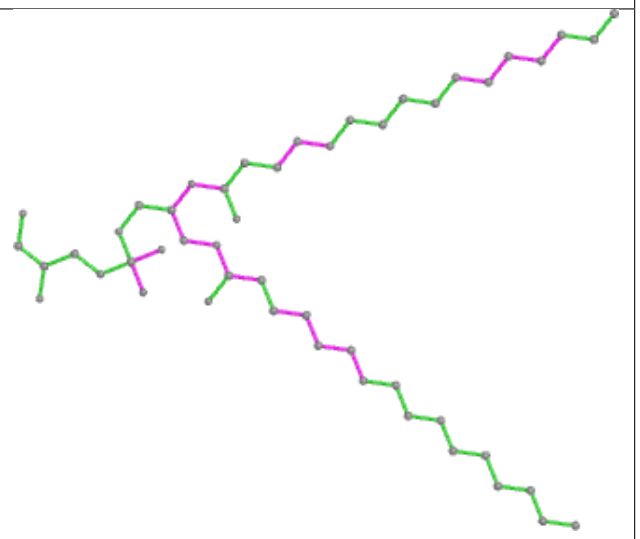
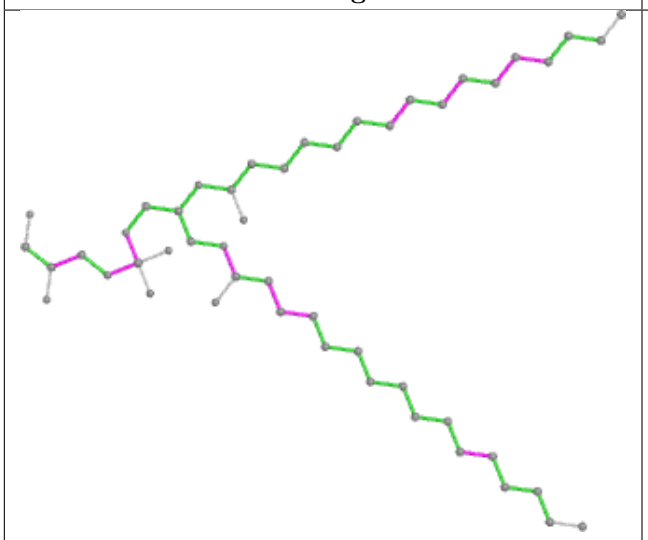
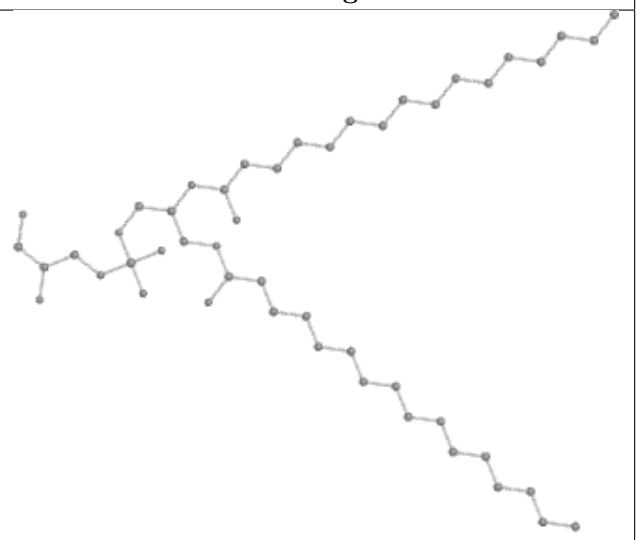


Bond angles

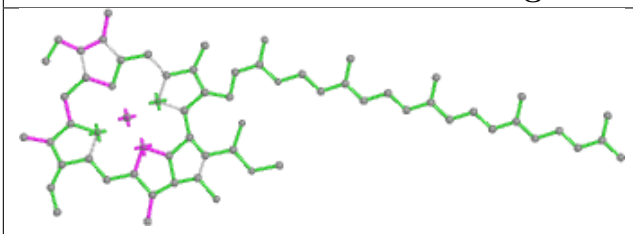


Torsions



Rings

Ligand CLA C 512



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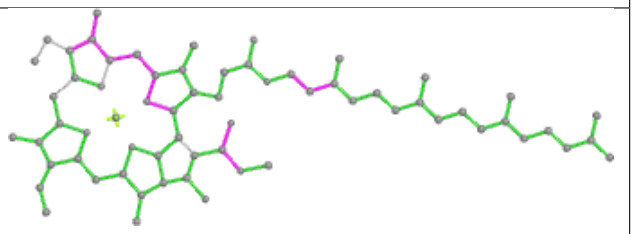
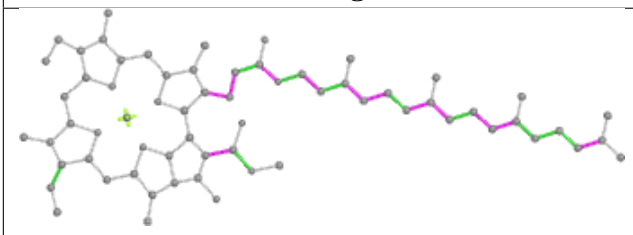
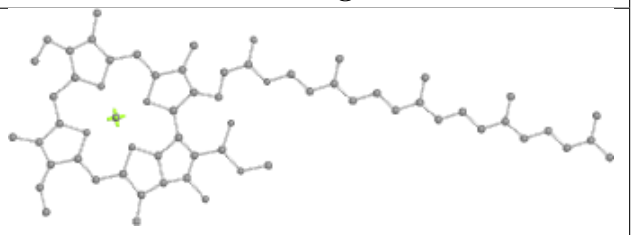


Bond angles

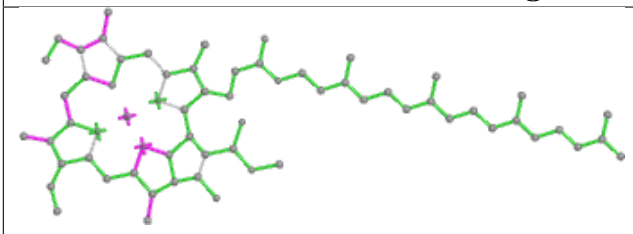


Torsions



Rings

Ligand CLA B 607



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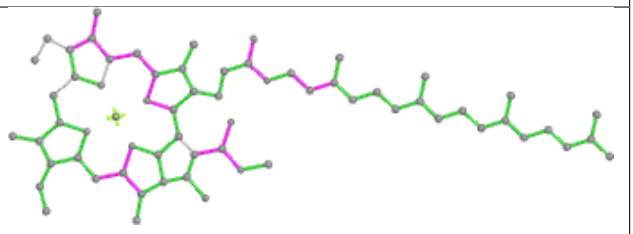
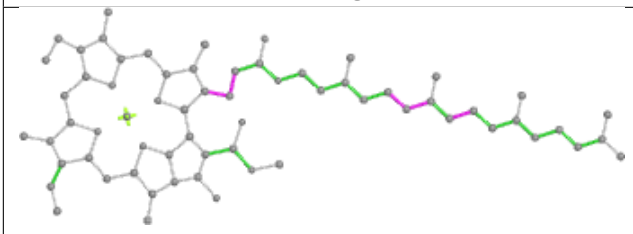


Bond angles



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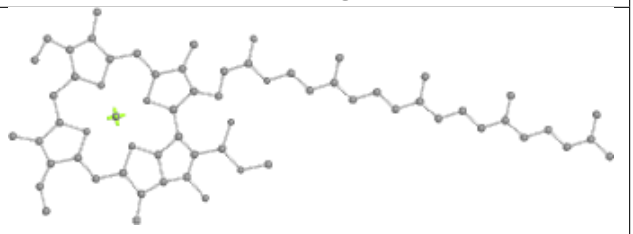
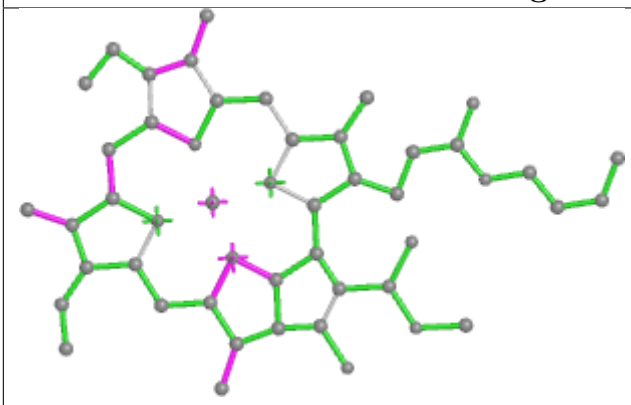


Rings

Ligand CLA s 612



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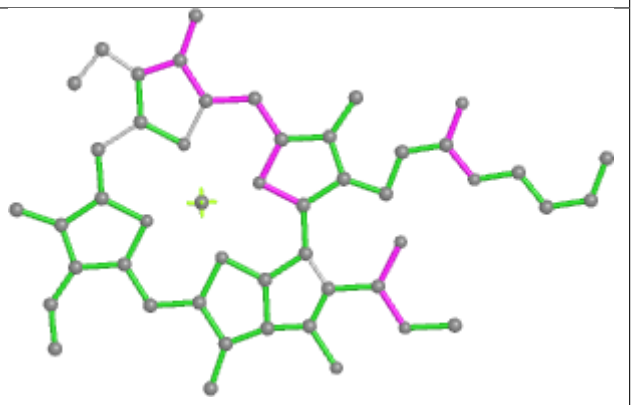
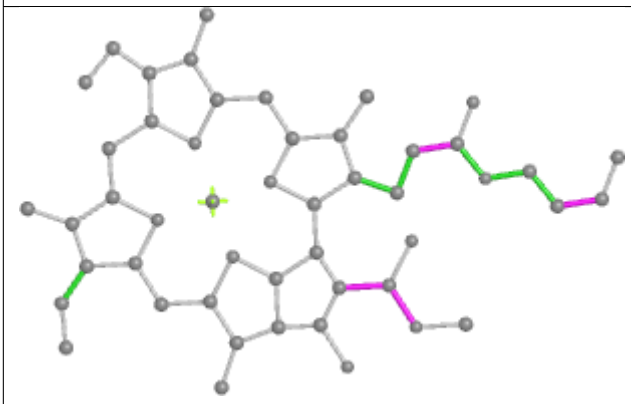
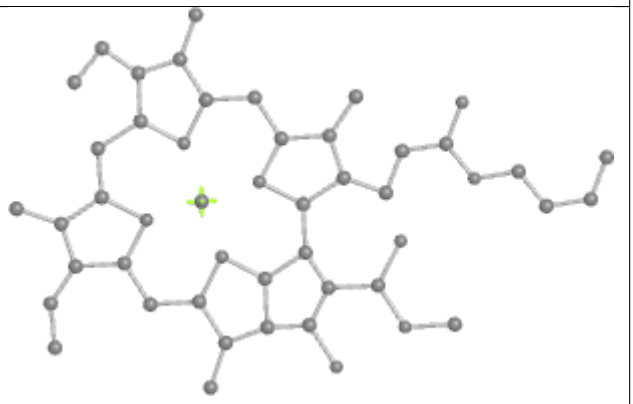


Bond angles

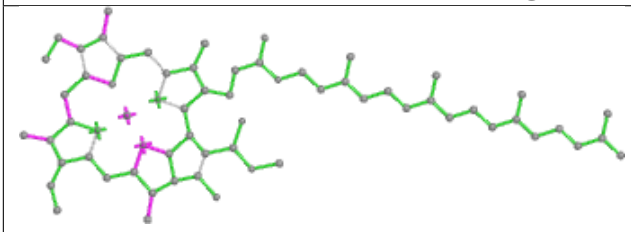


Torsions

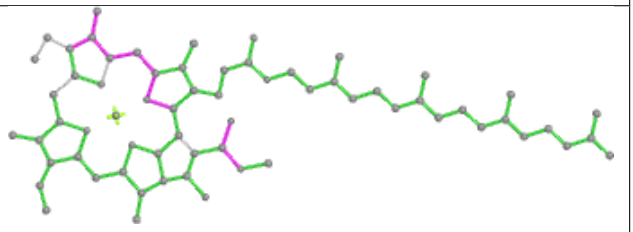


Rings

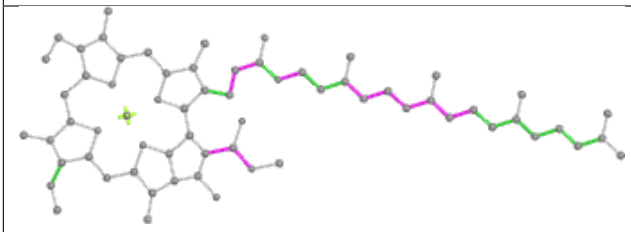
Ligand CLA G 602



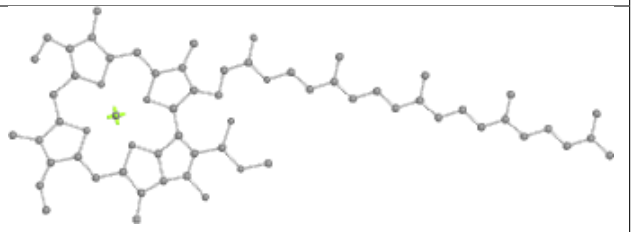
Bond lengths



Bond angles

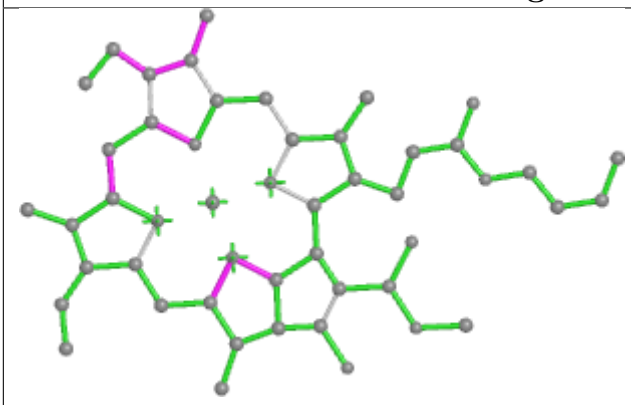


Torsions

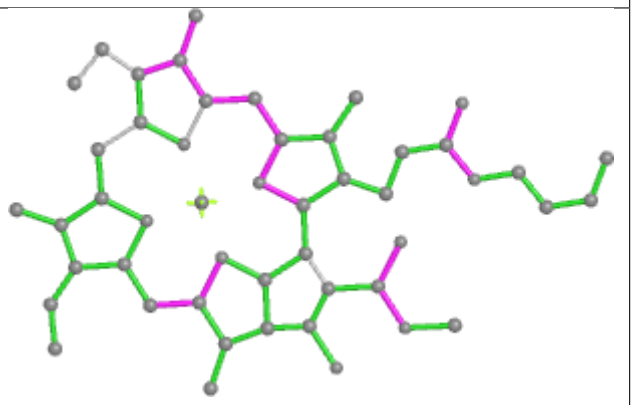


Rings

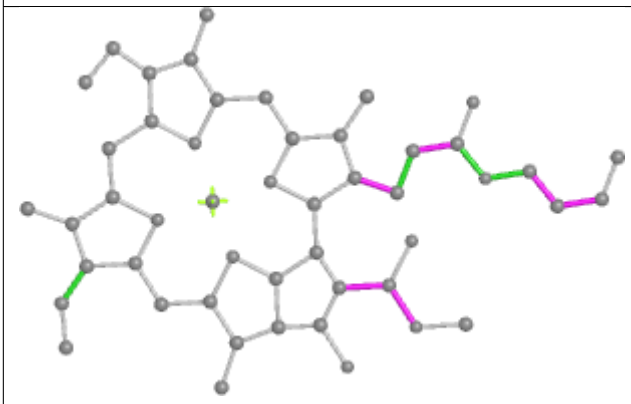
Ligand CLA n 612



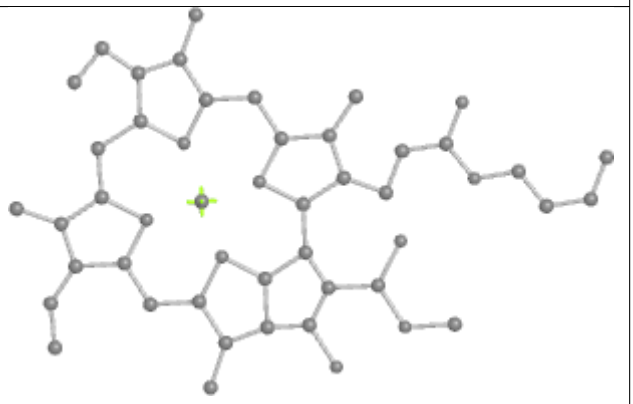
Bond lengths



Bond angles

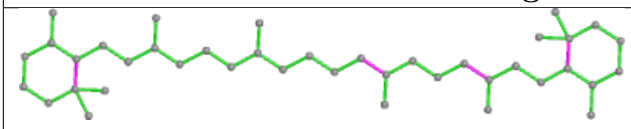


Torsions

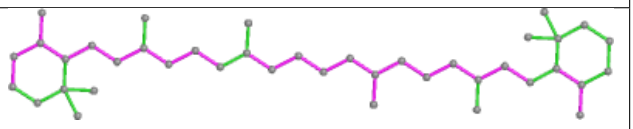


Rings

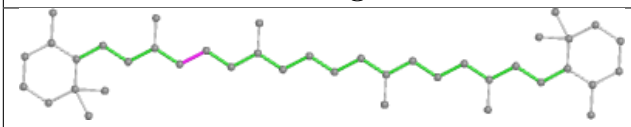
Ligand BCR C 517



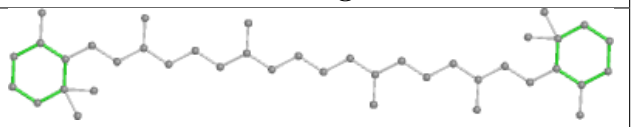
Bond lengths



Bond angles

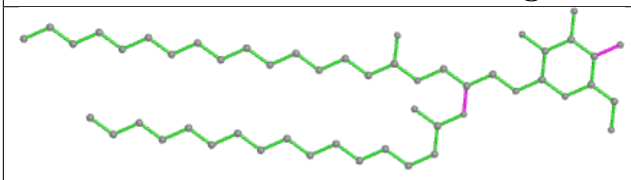


Torsions

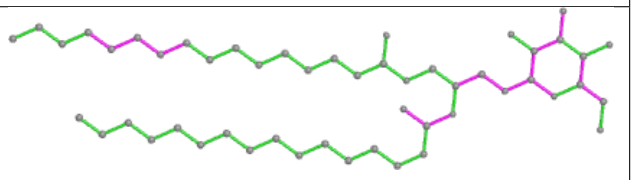


Rings

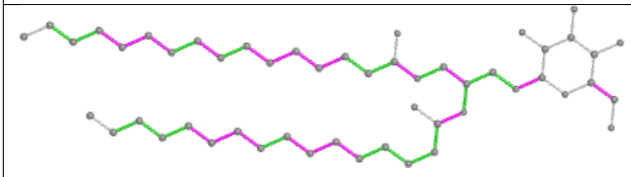
Ligand LMG b 622



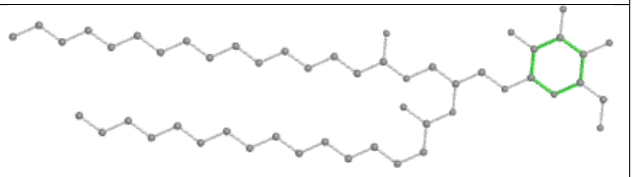
Bond lengths



Bond angles

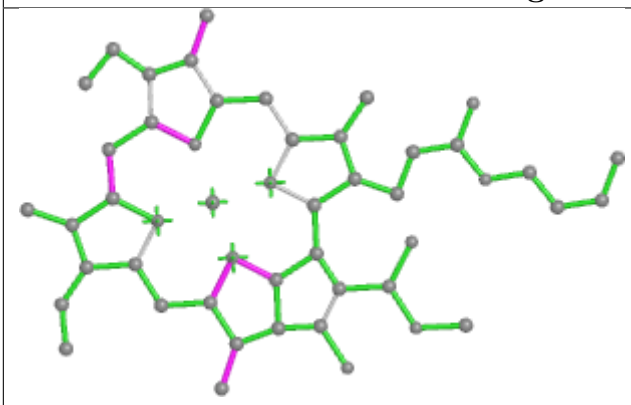


Torsions



Rings

Ligand CLA n 614



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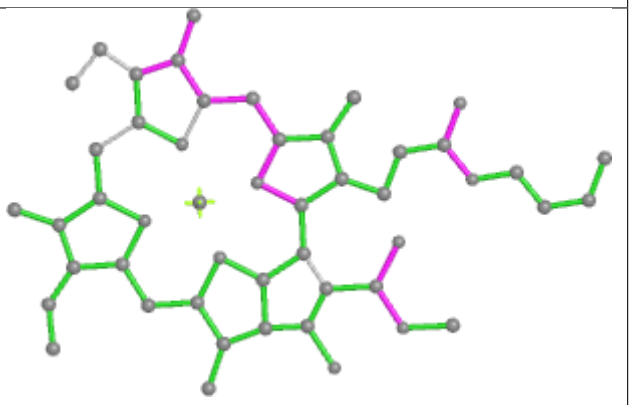
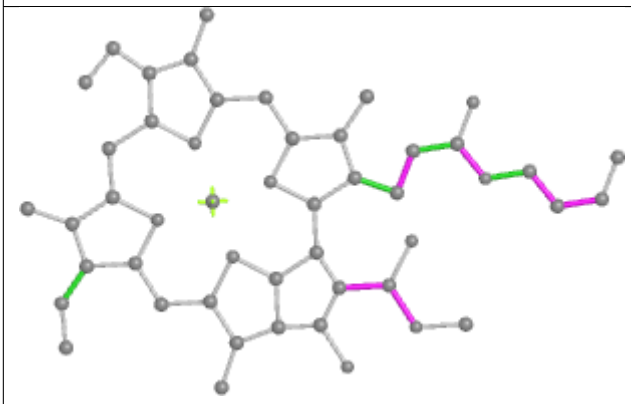
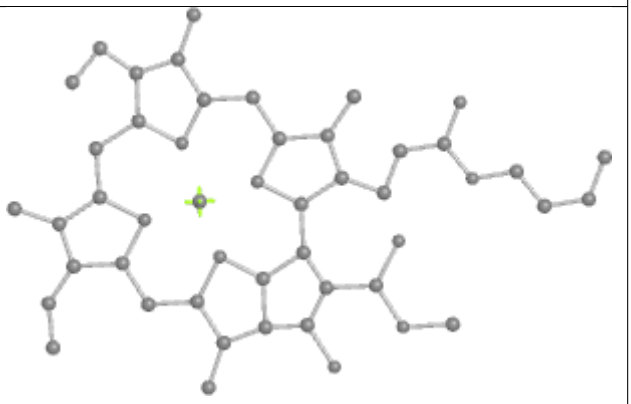


Bond angles

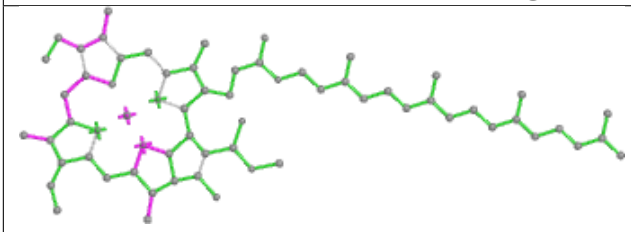


Torsions



Rings

Ligand CLA C 508



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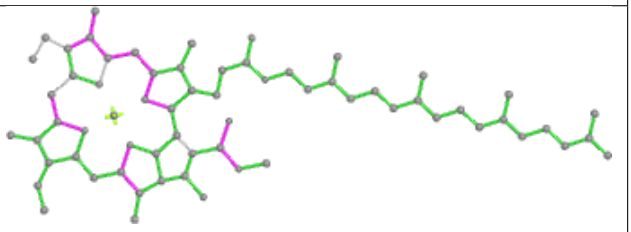
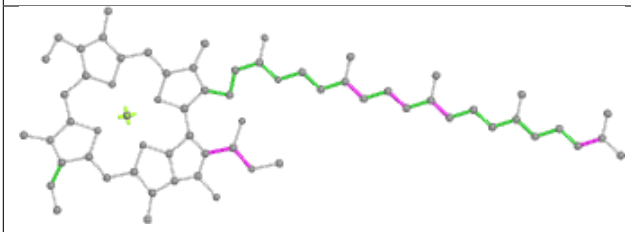
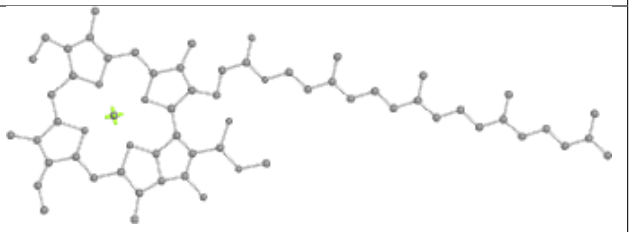


Bond angles

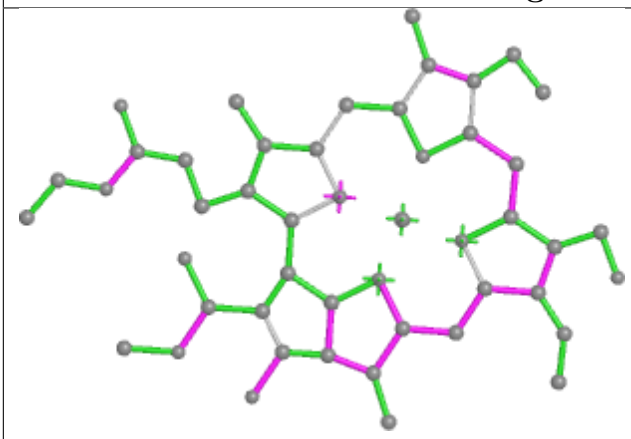


Torsions

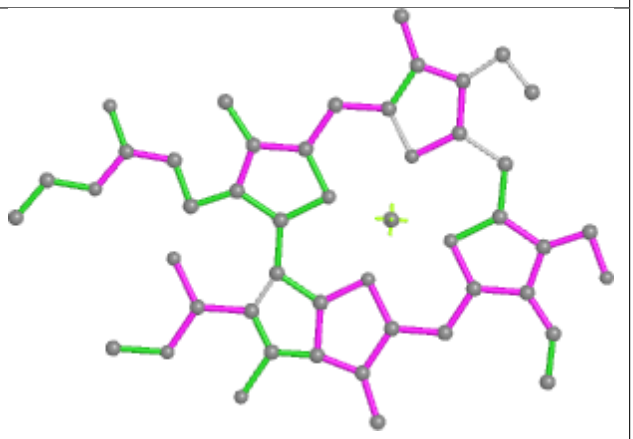


Rings

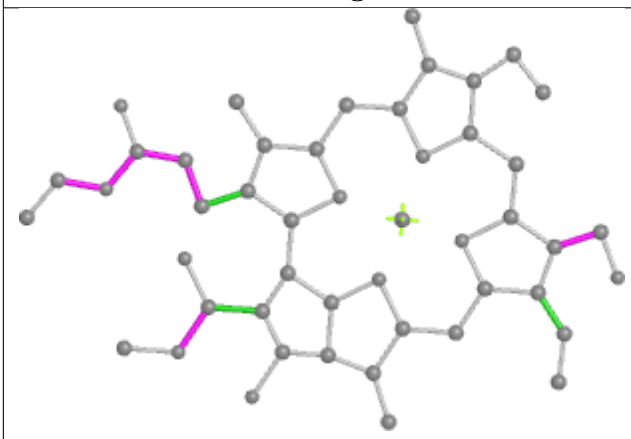
Ligand CHL n 605



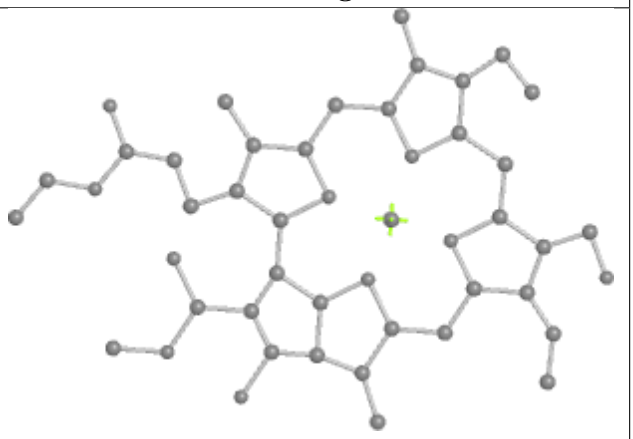
Bond lengths



Bond angles

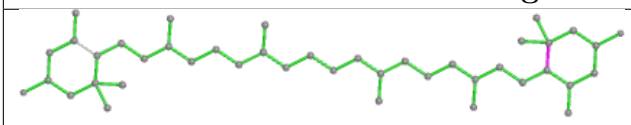


Torsions



Rings

Ligand LUT s 1620



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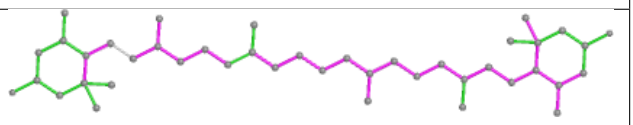
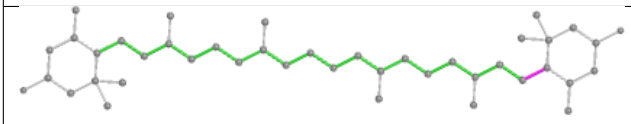


Bond angles



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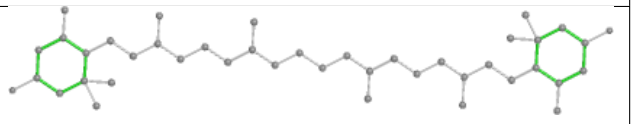
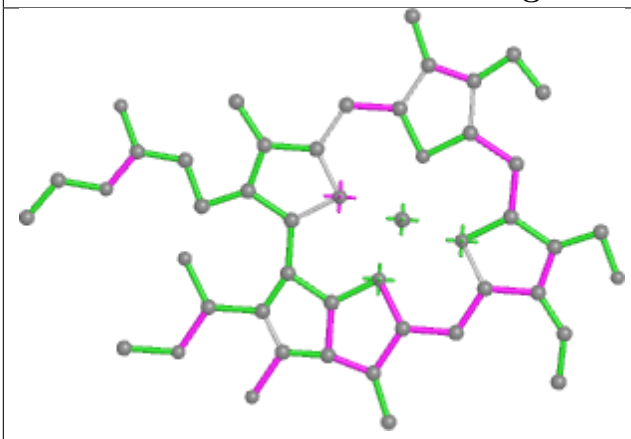


Rings

Ligand CHL G 605



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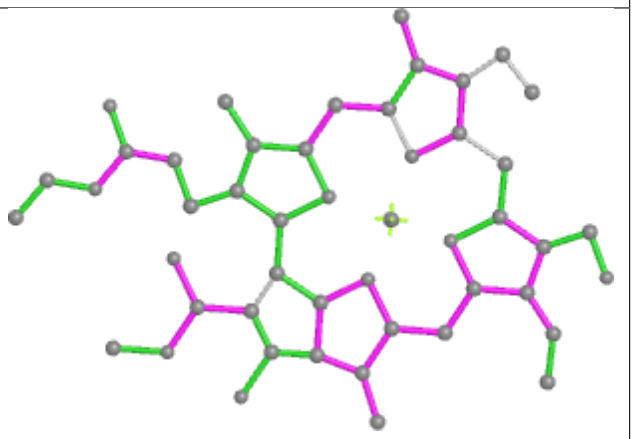
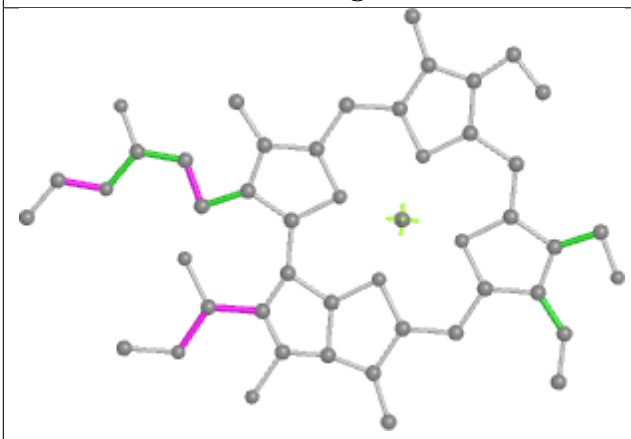


Bond angles



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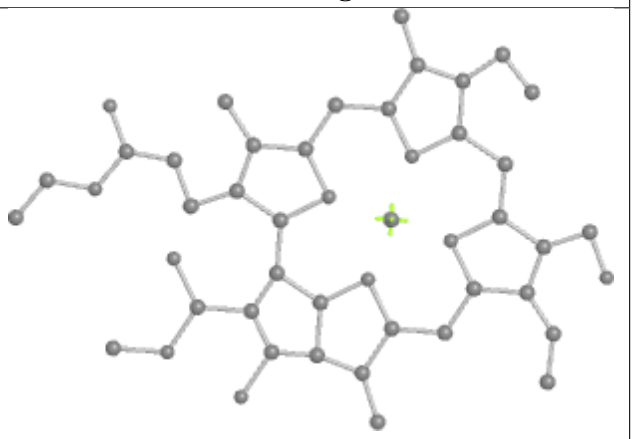
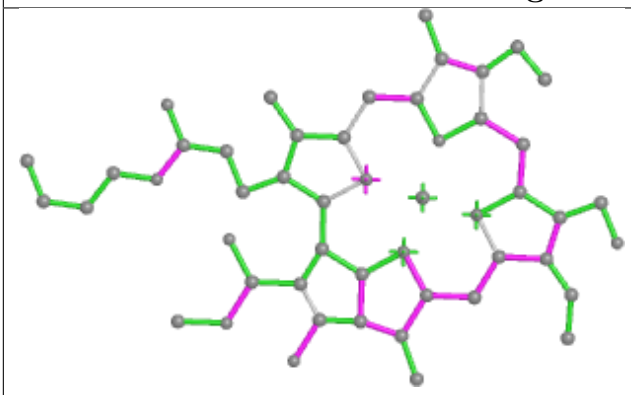


Rings

Ligand CHL S 607



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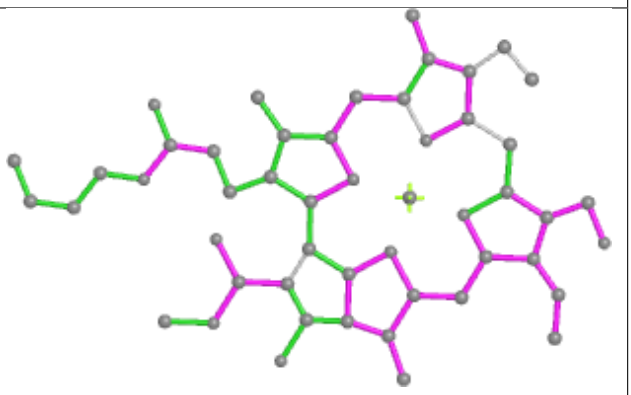
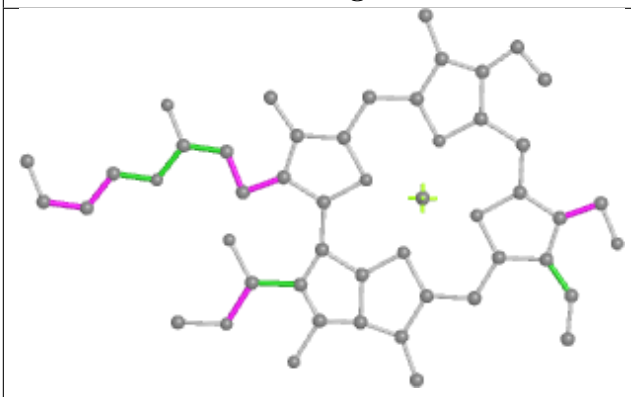
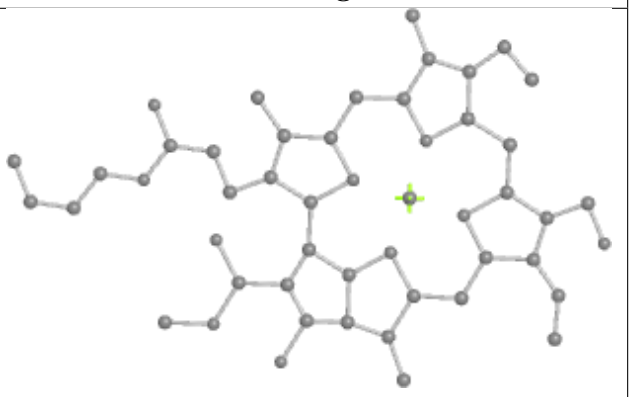


Bond angles

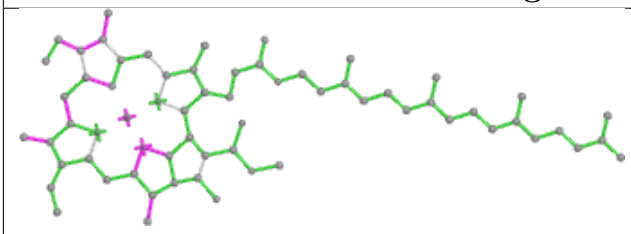


Torsions

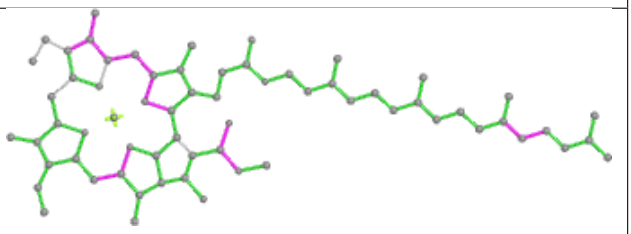


Rings

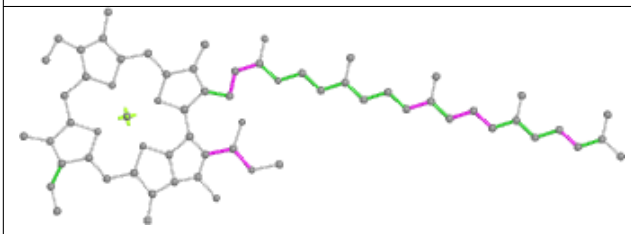
Ligand CLA Y 602



Bond lengths



Bond angles



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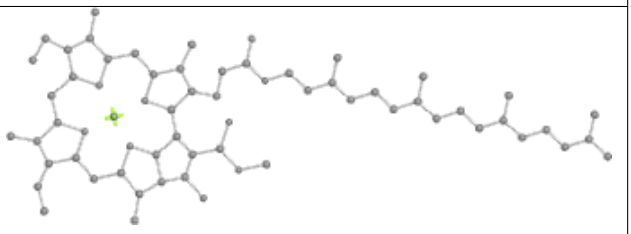
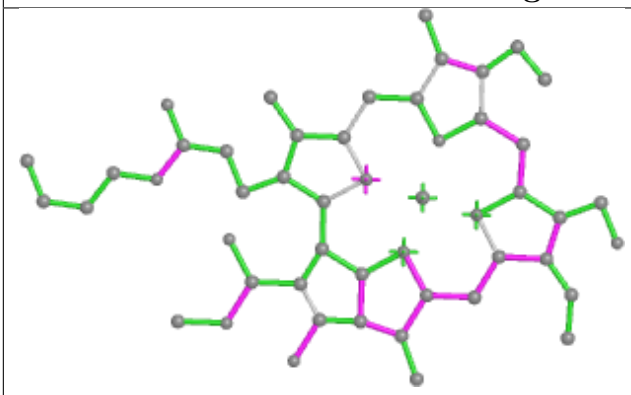
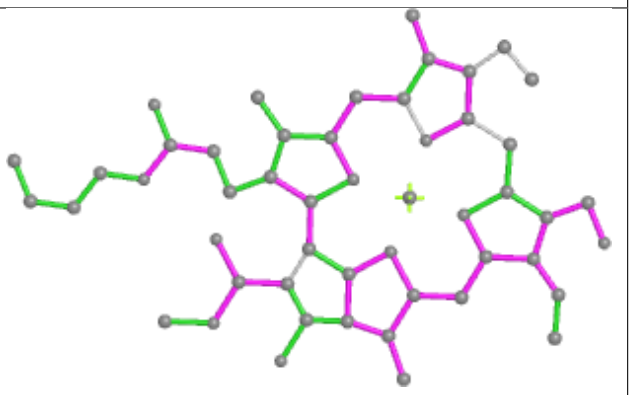


Rings

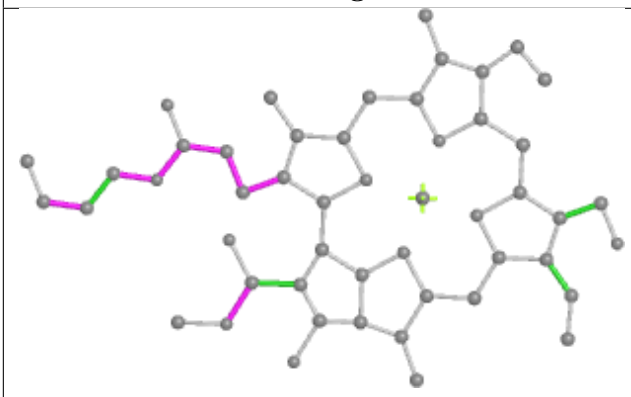
Ligand CHL R 607



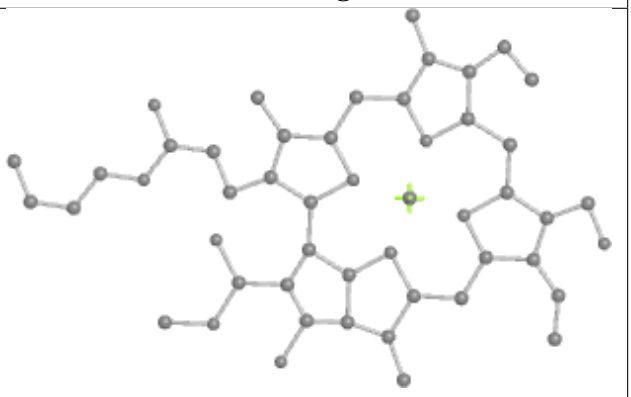
Bond lengths



Bond angles

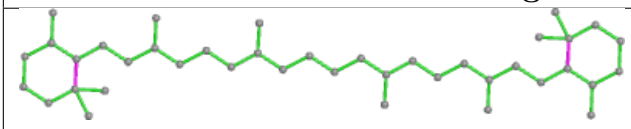


Torsions

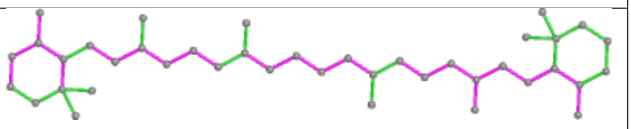


Rings

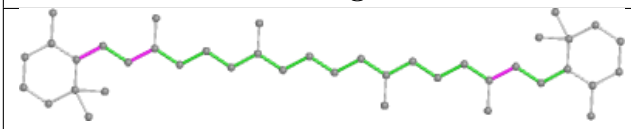
Ligand BCR B 620



Bond lengths



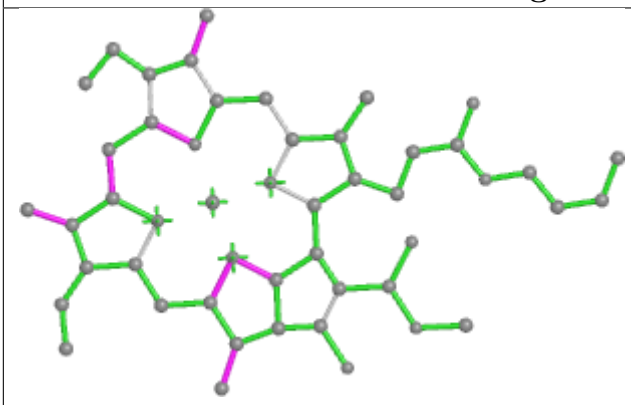
Bond angles



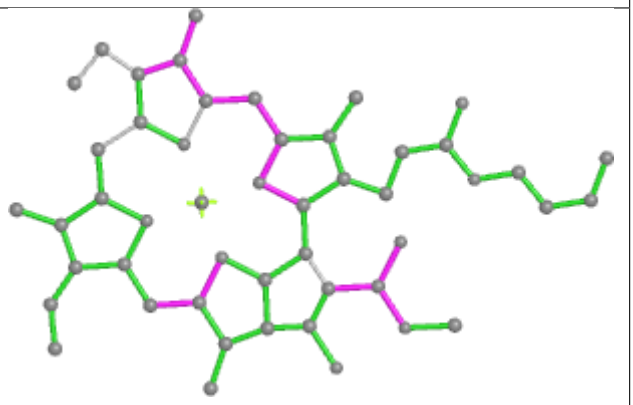
Torsions

Rings

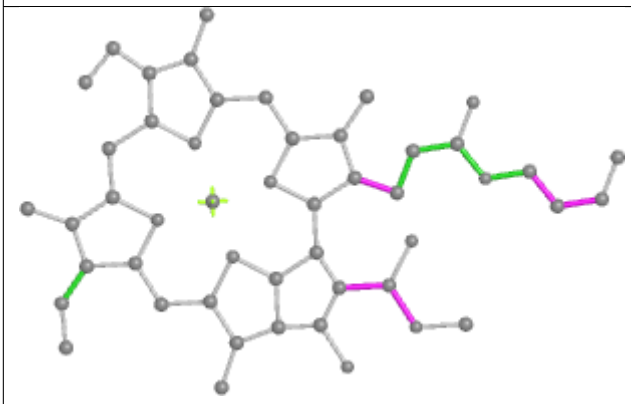
Ligand CLA s 602



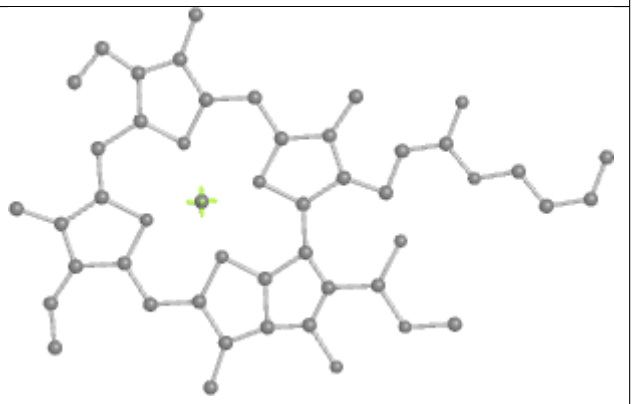
Bond lengths



Bond angles

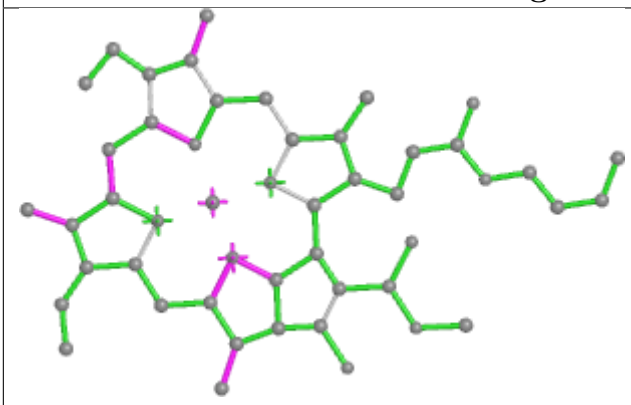


Torsions

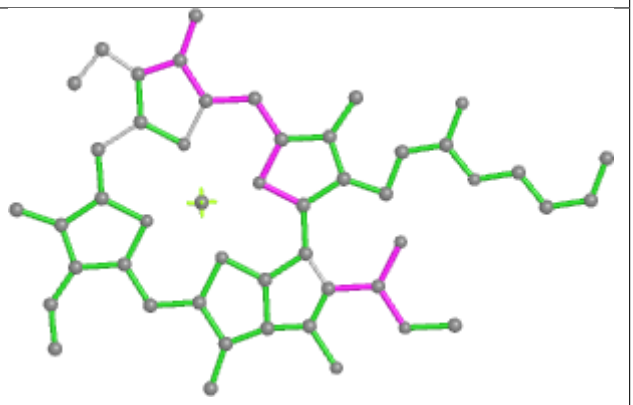


Rings

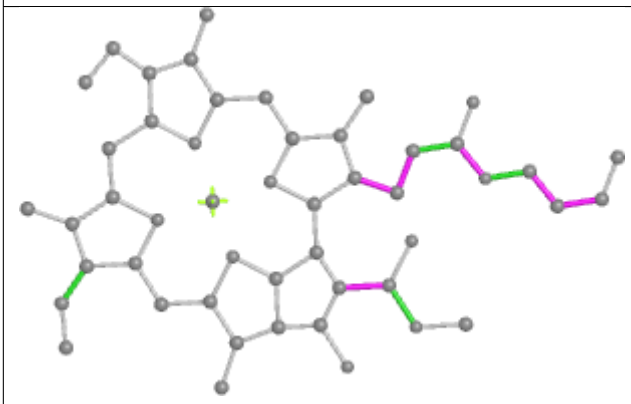
Ligand CLA r 604



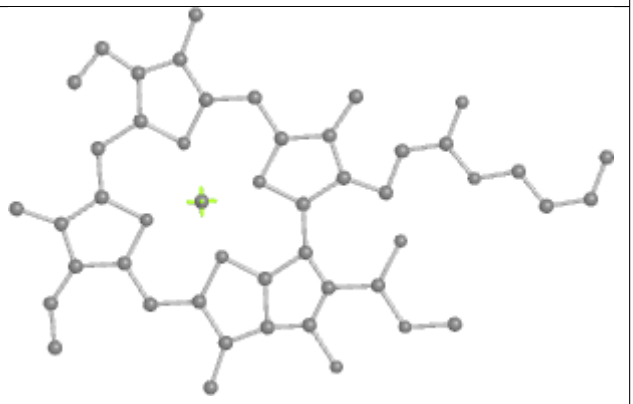
Bond lengths



Bond angles

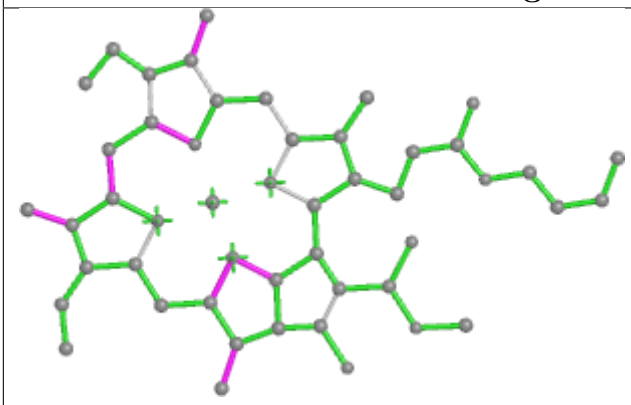


Torsions

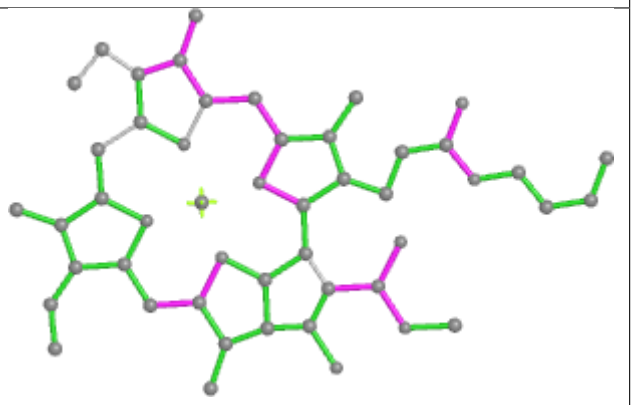


Rings

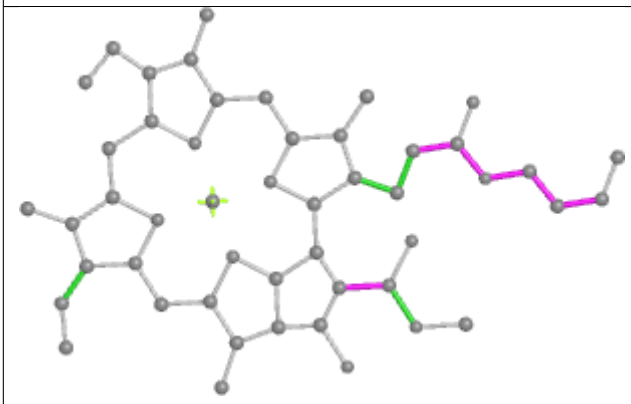
Ligand CLA R 616



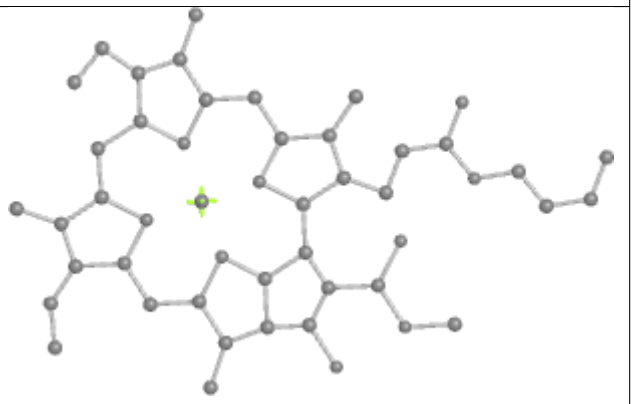
Bond lengths



Bond angles

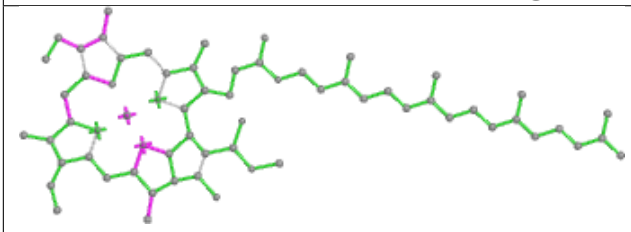


Torsions

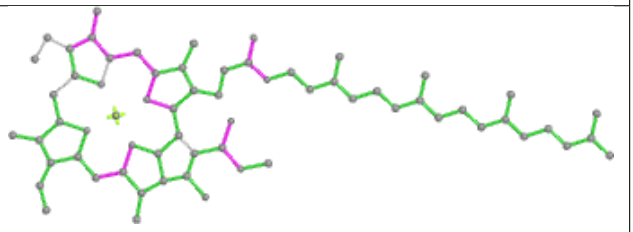


Rings

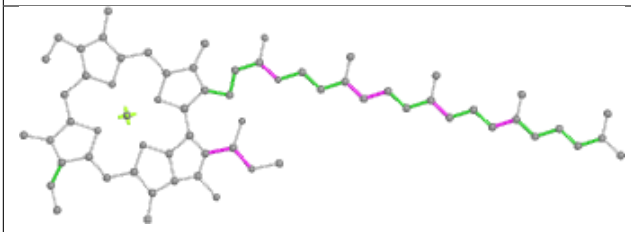
Ligand CLA d 403



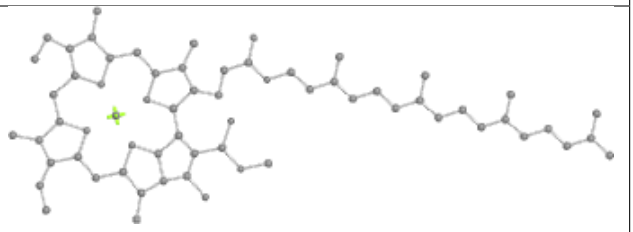
Bond lengths



Bond angles

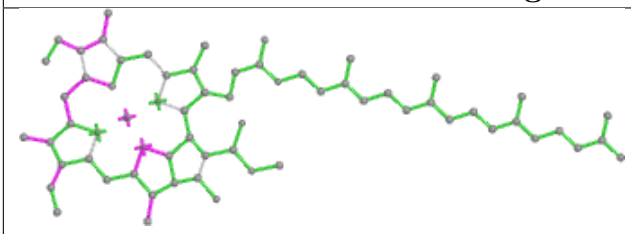


Torsions

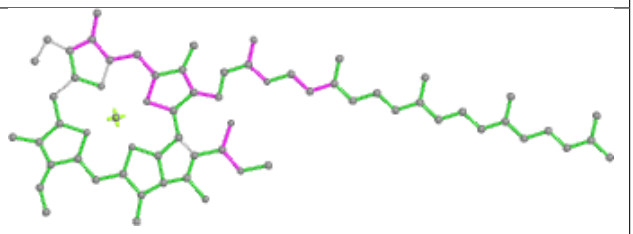


Rings

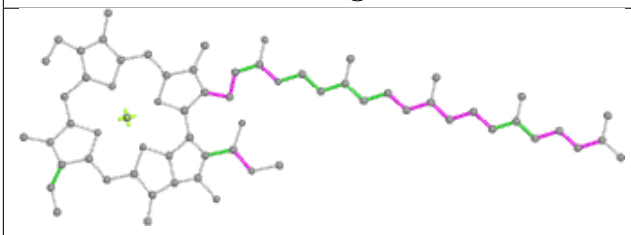
Ligand CLA B 605



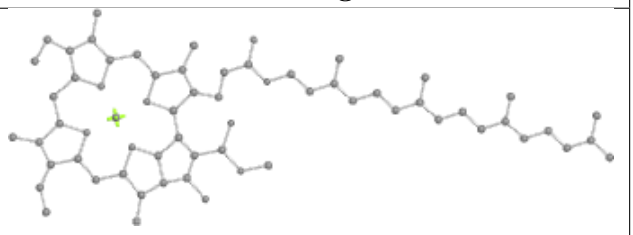
Bond lengths



Bond angles

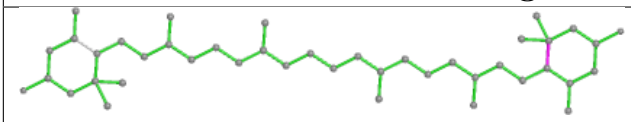


Torsions

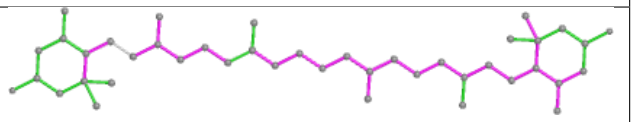


Rings

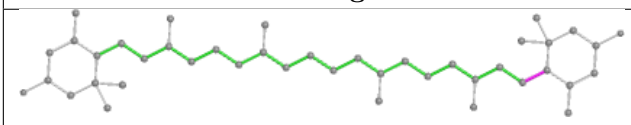
Ligand LUT S 1620



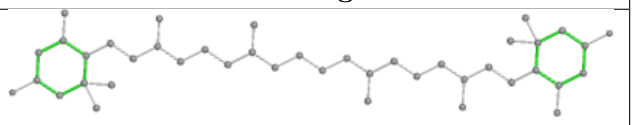
Bond lengths



Bond angles

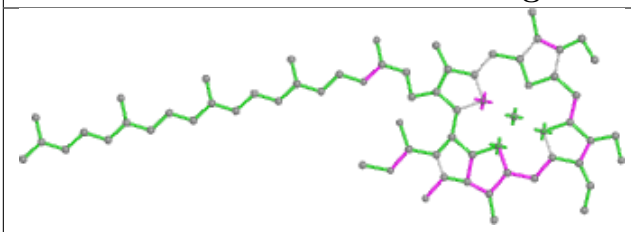


Torsions

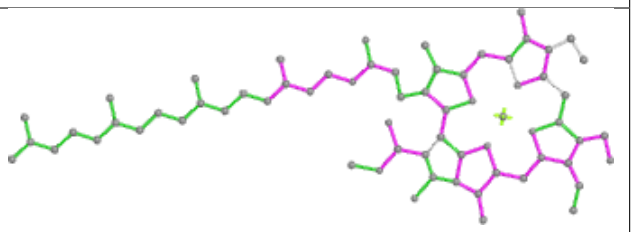


Rings

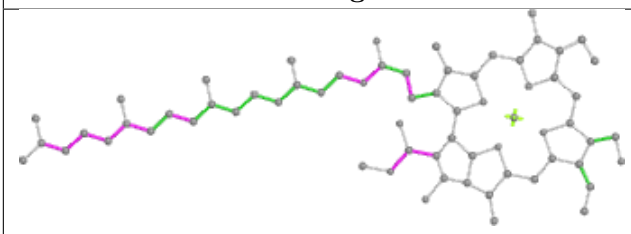
Ligand CHL N 607



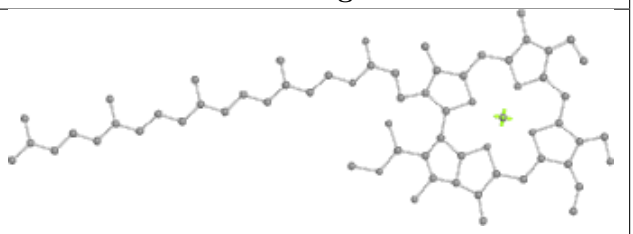
Bond lengths



Bond angles

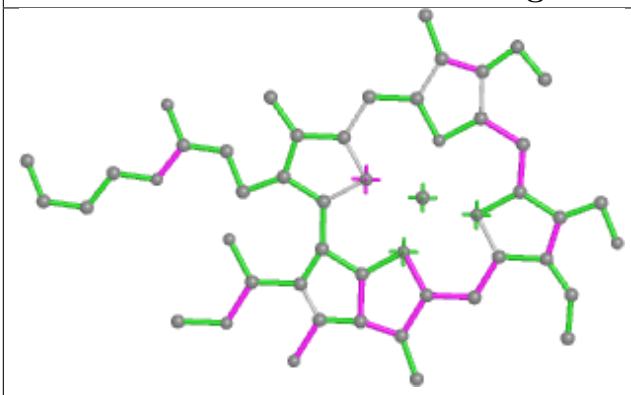


Torsions



Rings

Ligand CHL n 609



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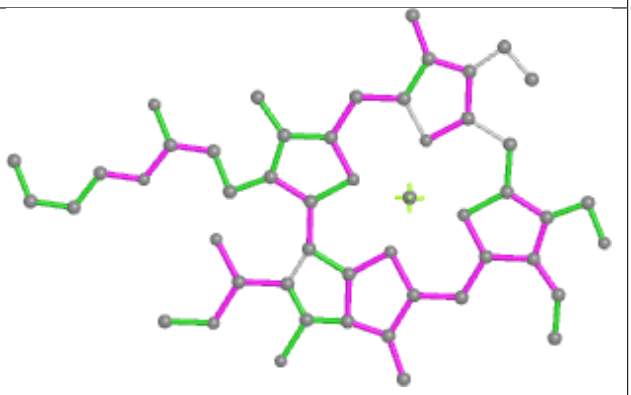
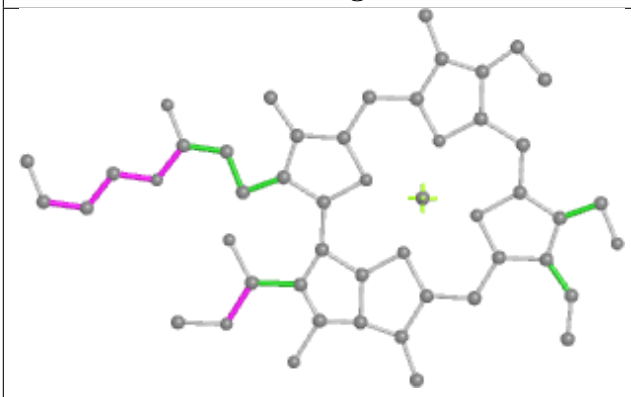
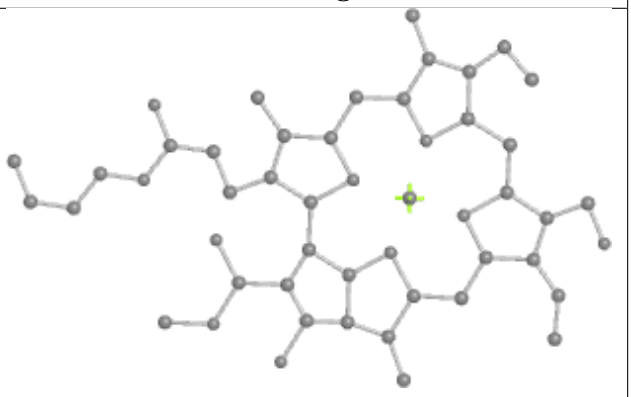


Bond angles

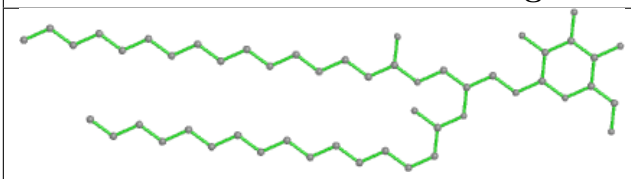


Torsions

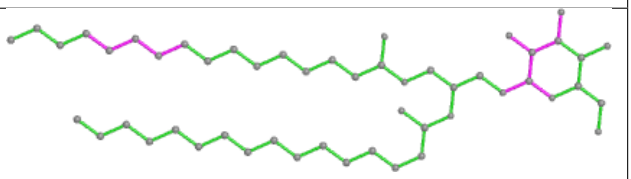


Rings

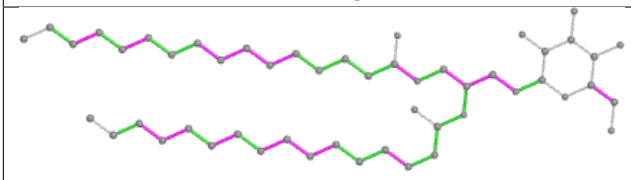
Ligand LMG z 101



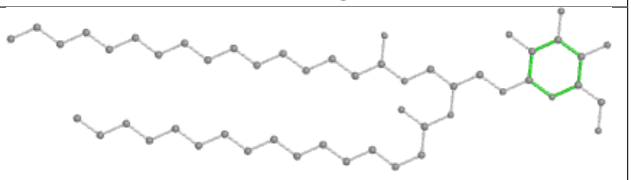
Bond lengths



Bond angles

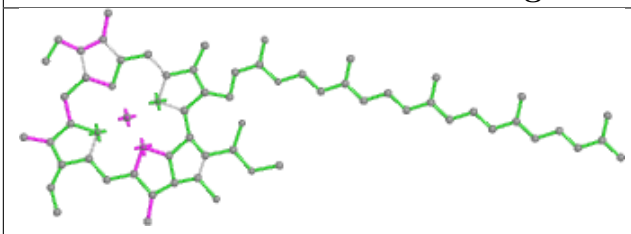


Torsions

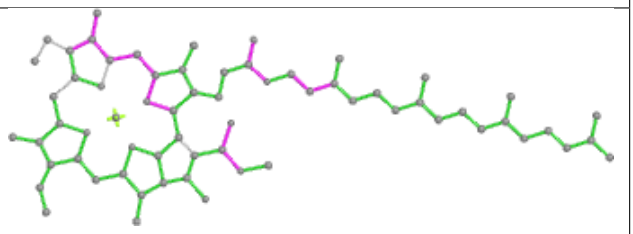


Rings

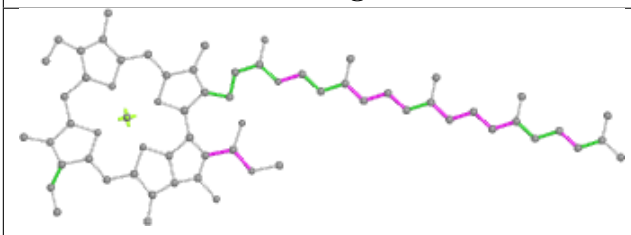
Ligand CLA C 506



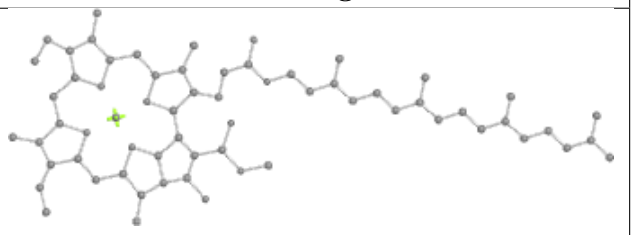
Bond lengths



Bond angles

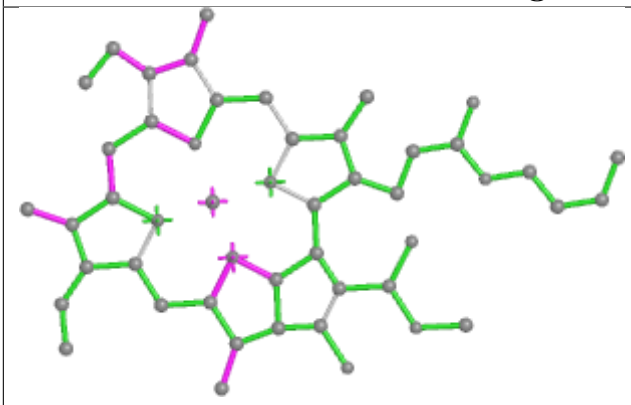


Torsions

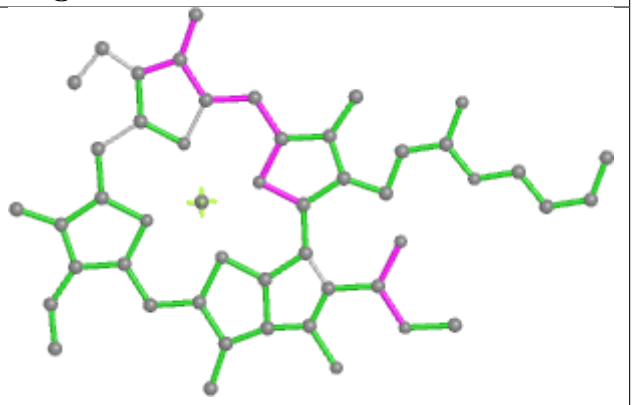


Rings

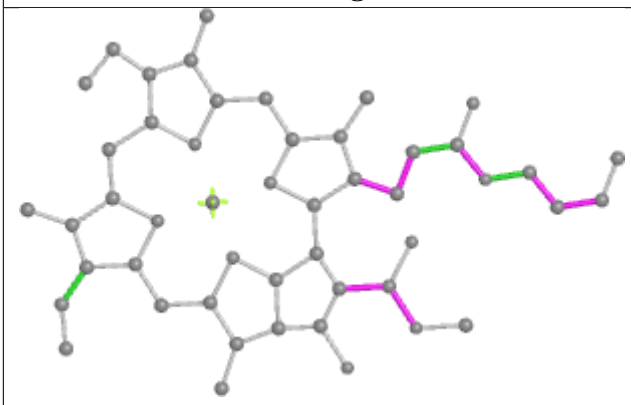
Ligand CLA g 604



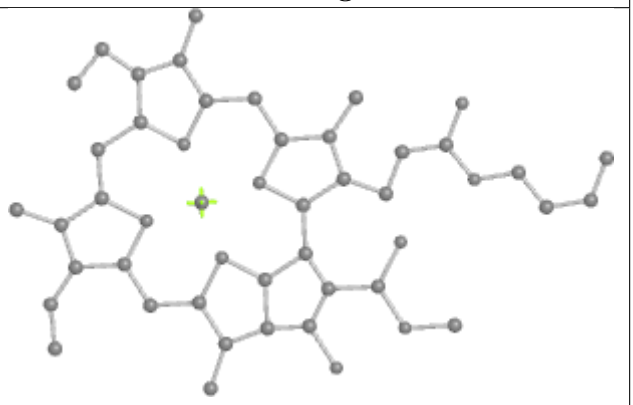
Bond lengths



Bond angles

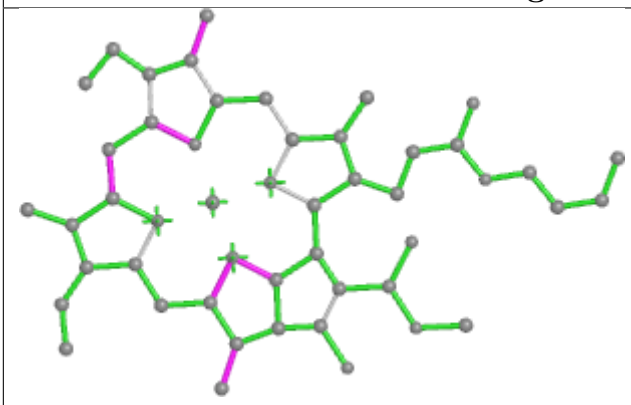


Torsions

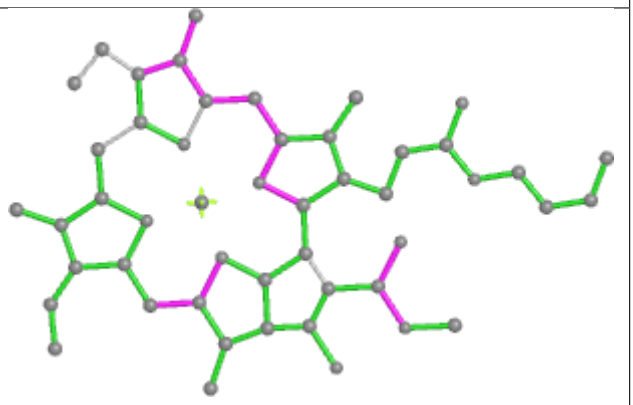


Rings

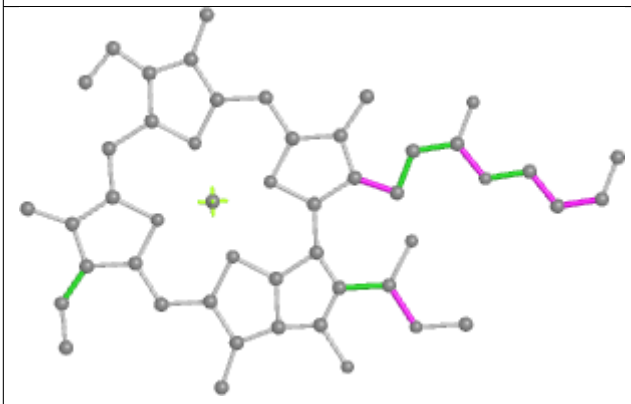
Ligand CLA S 609



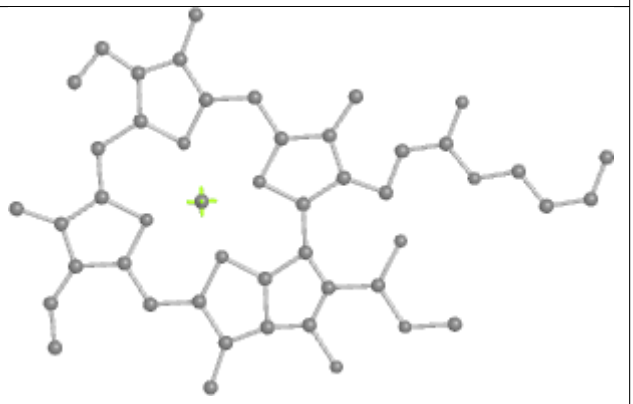
Bond lengths



Bond angles

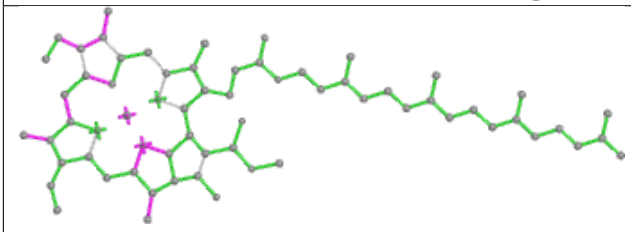


Torsions



Rings

Ligand CLA b 603



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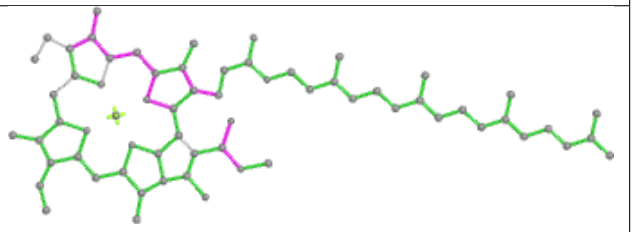
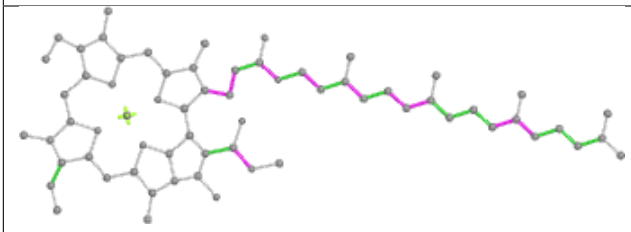
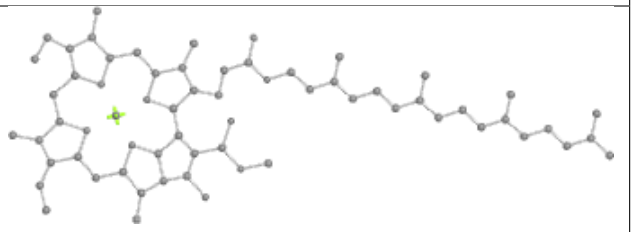


Bond angles

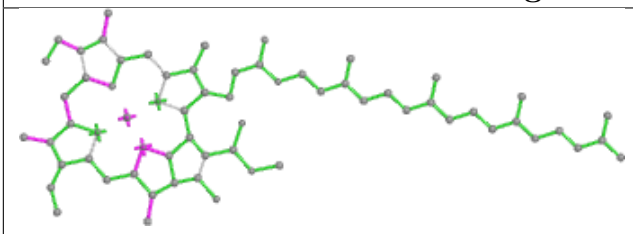


Torsions



Rings

Ligand CLA B 609



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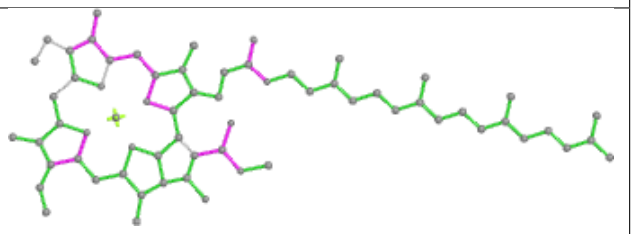
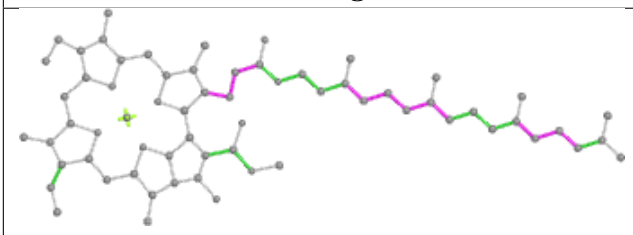
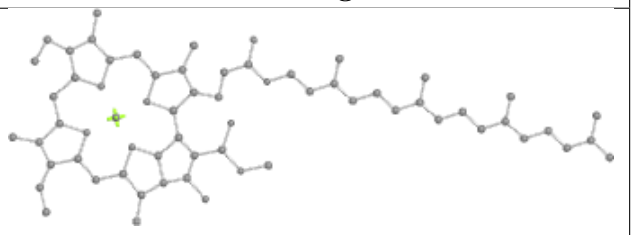


Bond angles

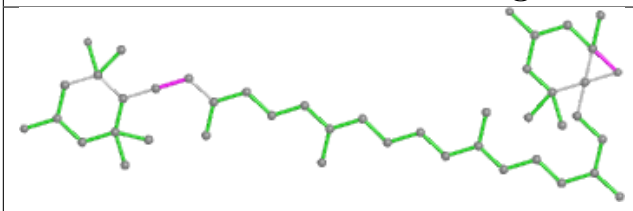


Torsions

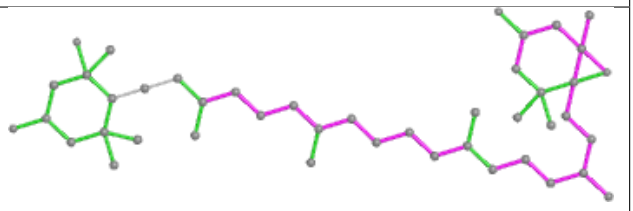


Rings

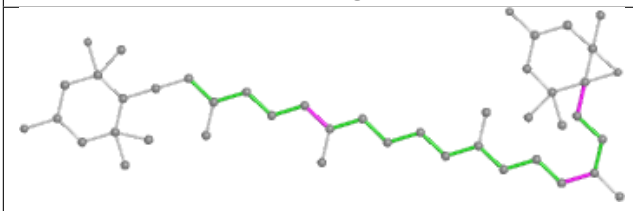
Ligand NEX N 1623



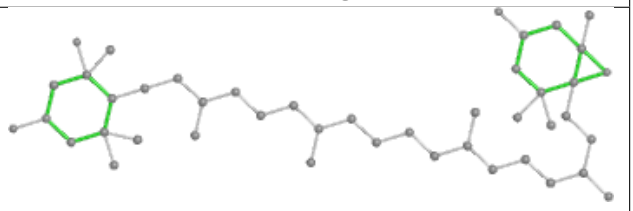
Bond lengths



Bond angles

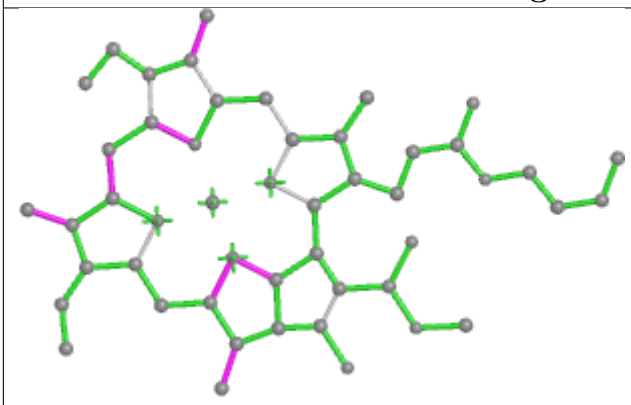


Torsions

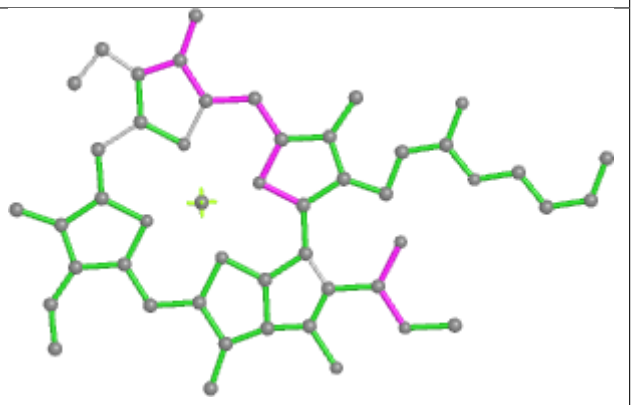


Rings

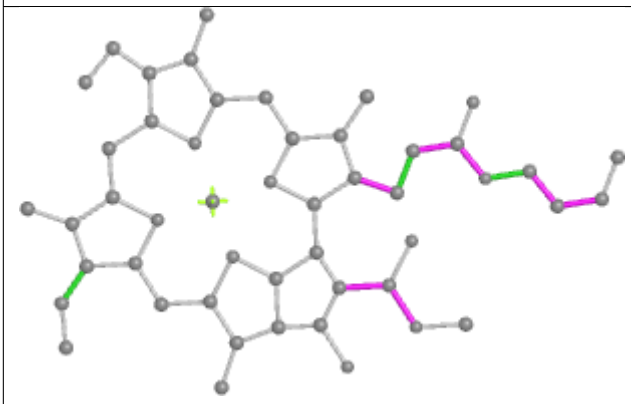
Ligand CLA s 603



Bond lengths



Bond angles



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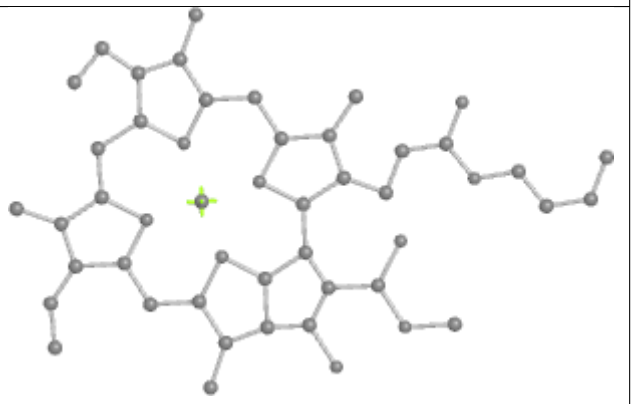
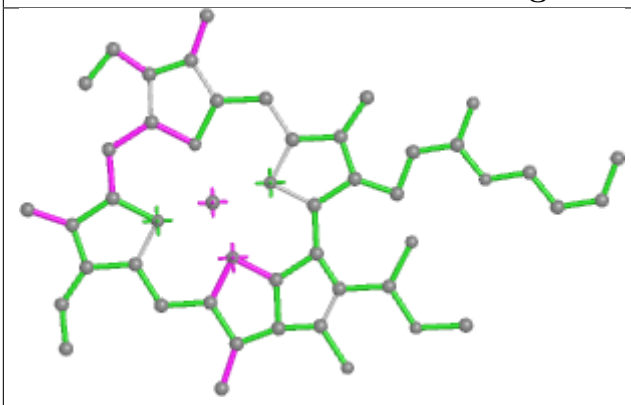
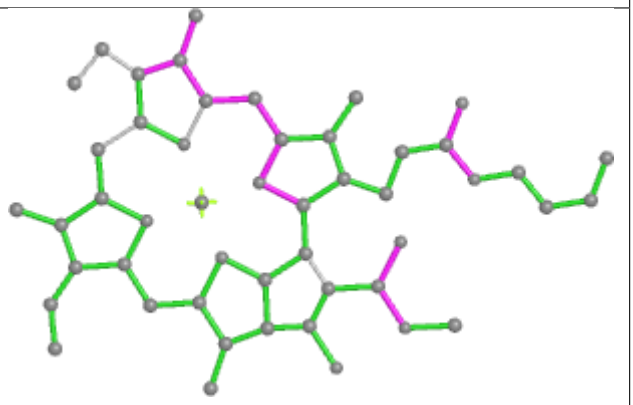


Rings

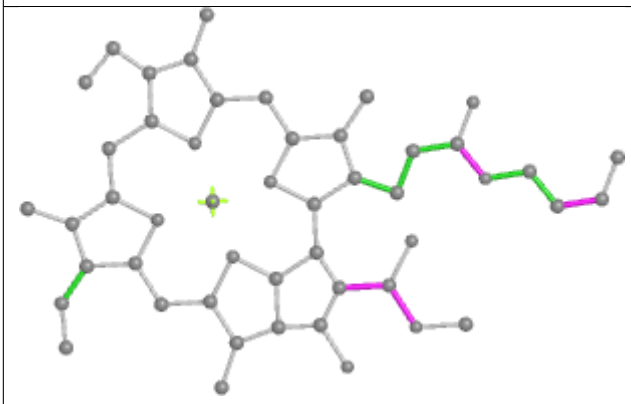
Ligand CLA c 513



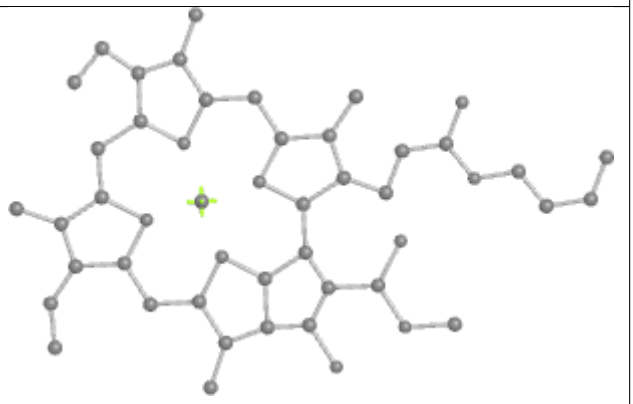
Bond lengths



Bond angles

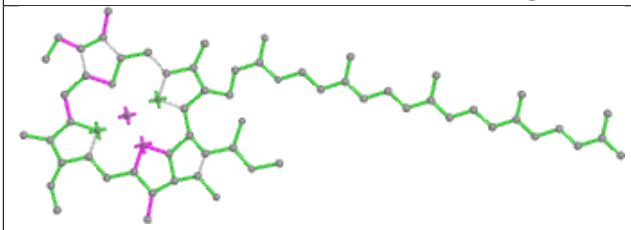


Torsions

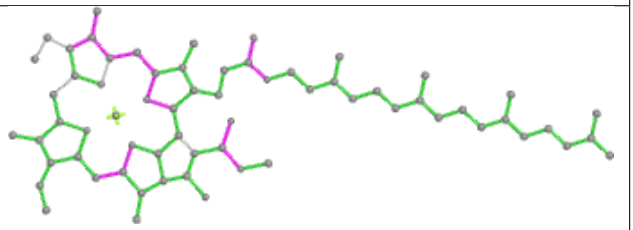


Rings

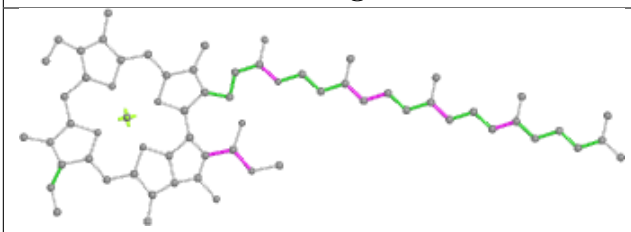
Ligand CLA D 403



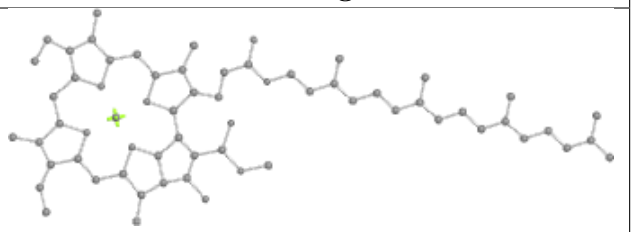
Bond lengths



Bond angles

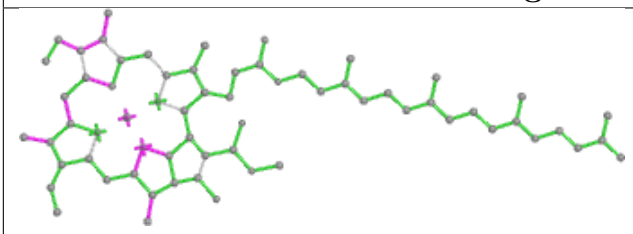


Torsions

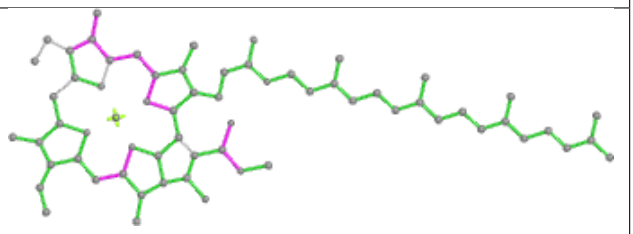


Rings

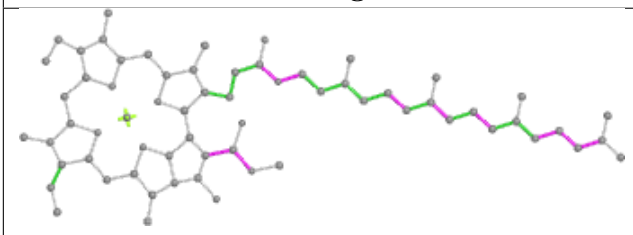
Ligand CLA C 502



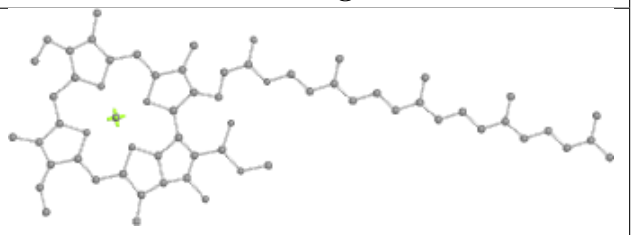
Bond lengths



Bond angles

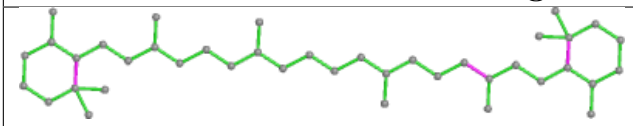


Torsions

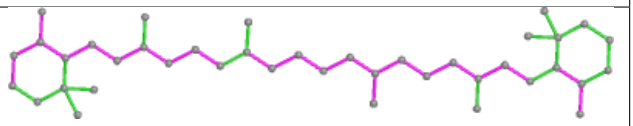


Rings

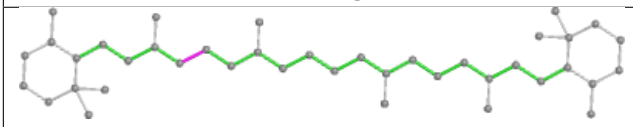
Ligand BCR c 517



Bond lengths



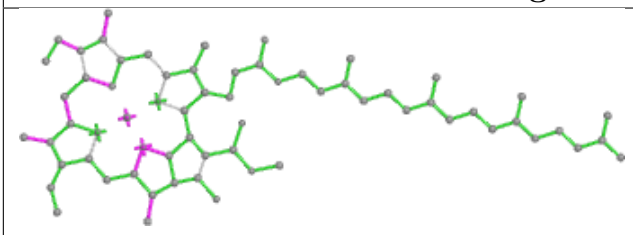
Bond angles



Torsions

Rings

Ligand CLA c 505



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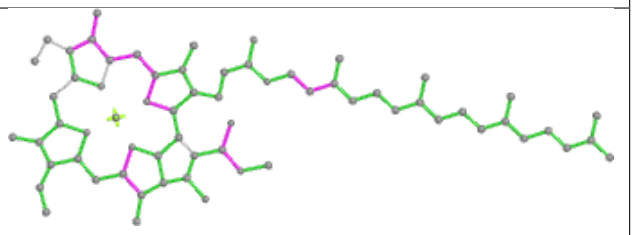
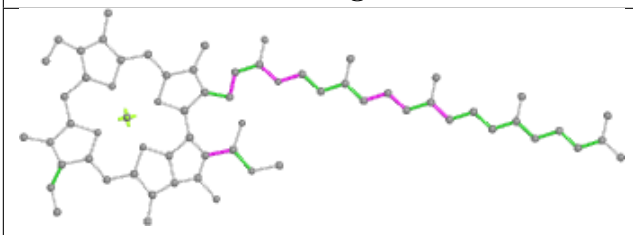
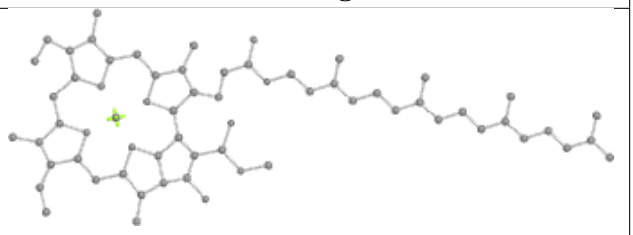


Bond angles

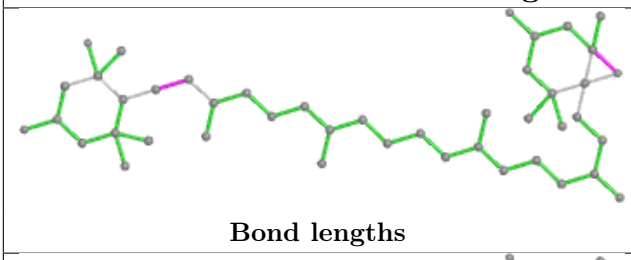


Torsions

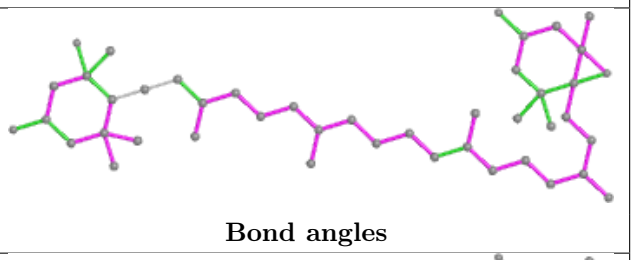


Rings

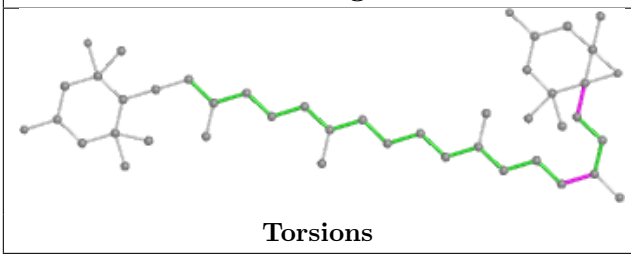
Ligand NEX R 623



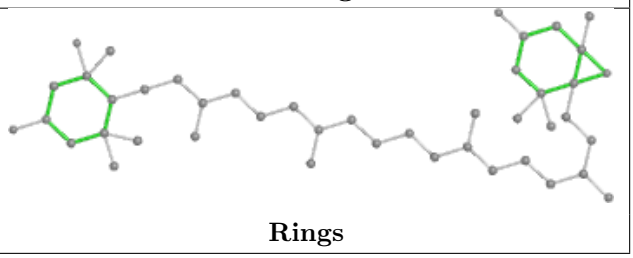
Bond lengths



Bond angles

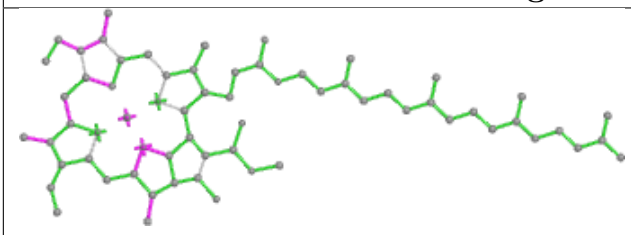


Torsions

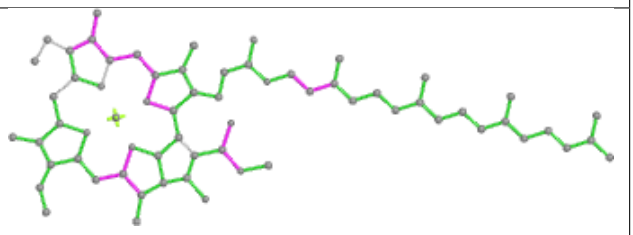


Rings

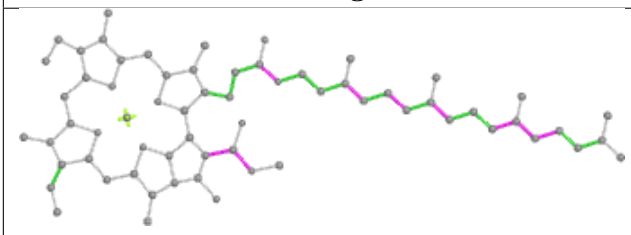
Ligand CLA b 606



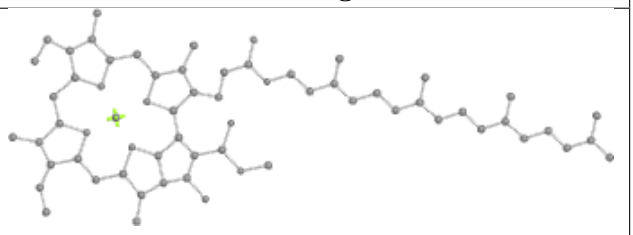
Bond lengths



Bond angles

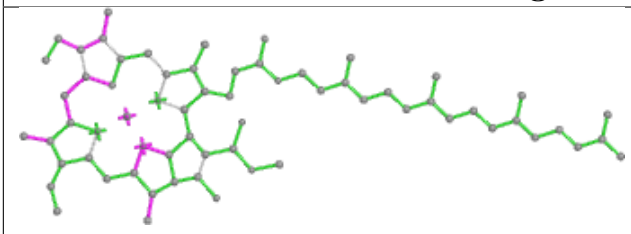


Torsions

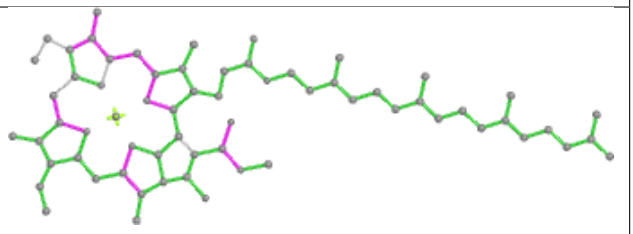


Rings

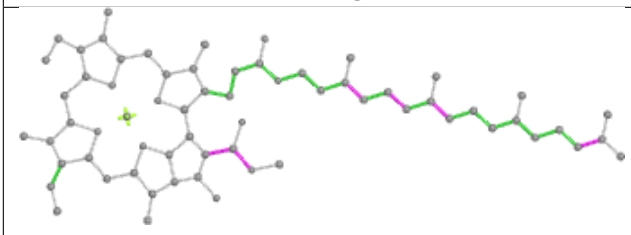
Ligand CLA c 508



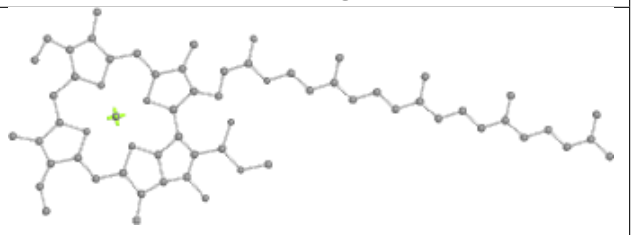
Bond lengths



Bond angles

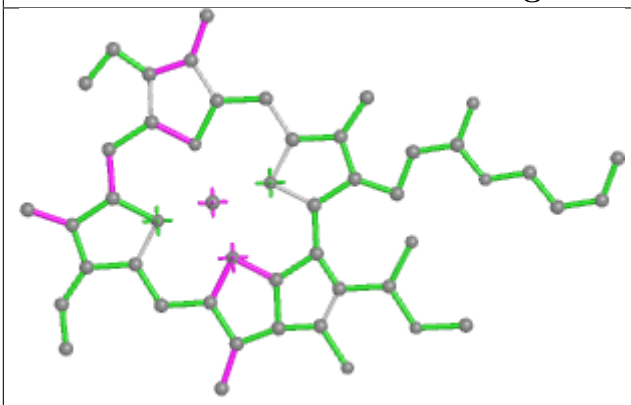


Torsions



Rings

Ligand CLA Y 603



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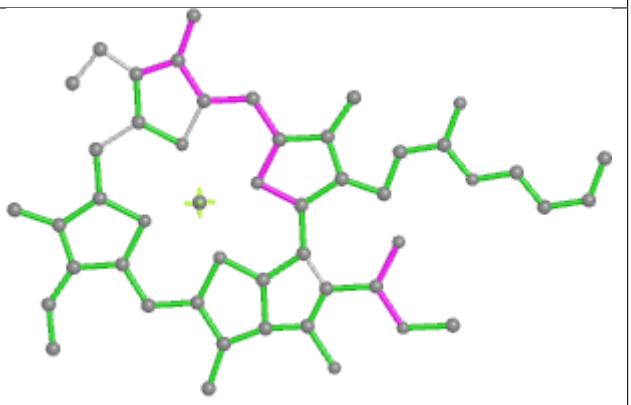
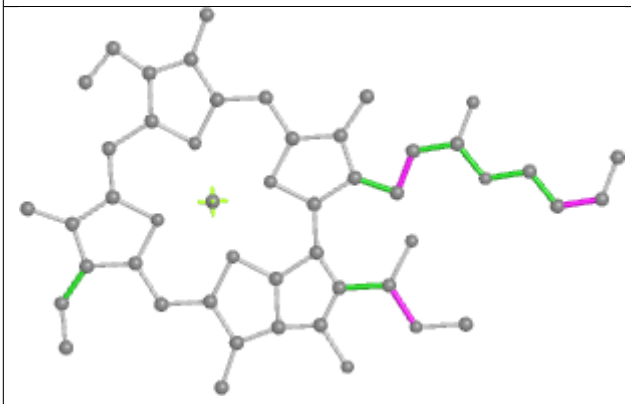
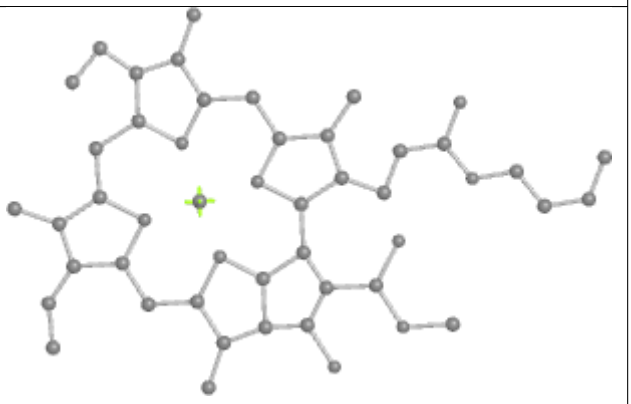


Bond angles

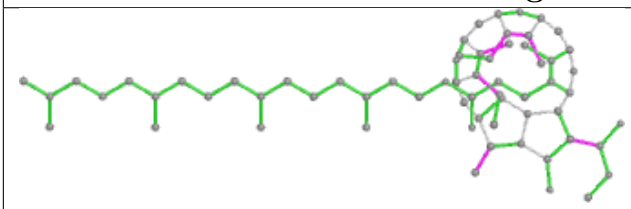


Torsions

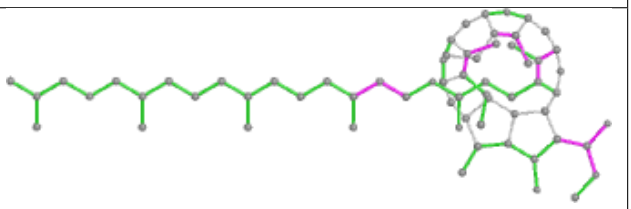


Rings

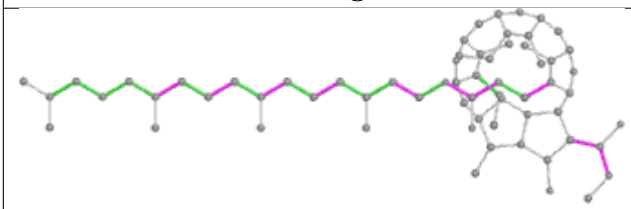
Ligand PHO a 409



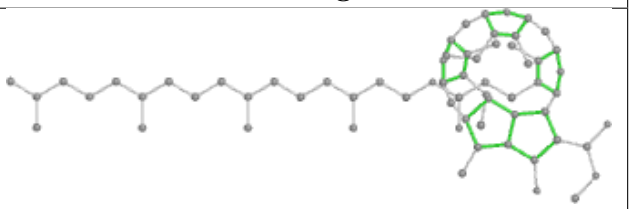
Bond lengths



Bond angles

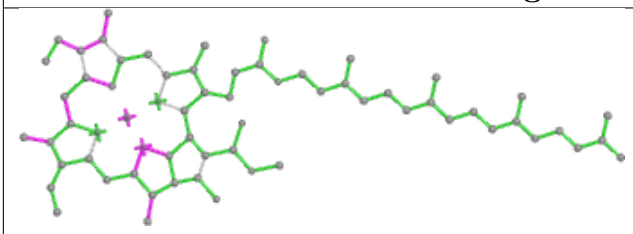


Torsions

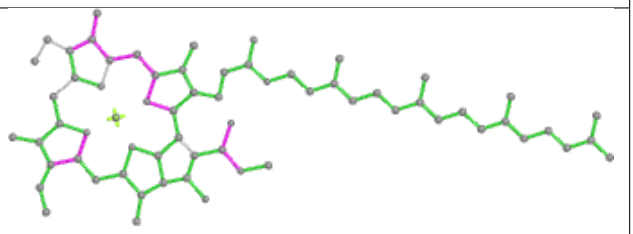


Rings

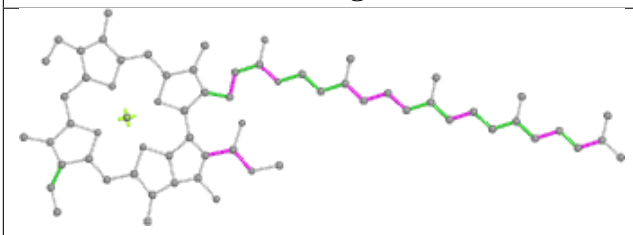
Ligand CLA Y 613



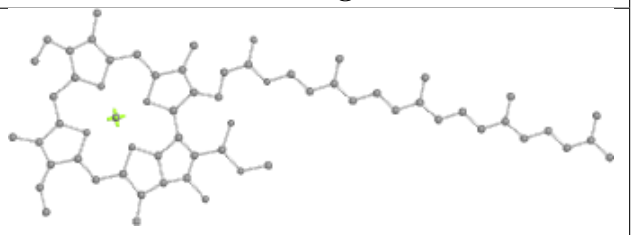
Bond lengths



Bond angles

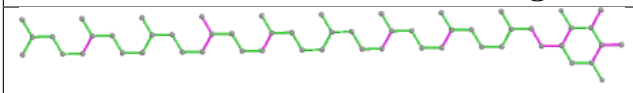


Torsions

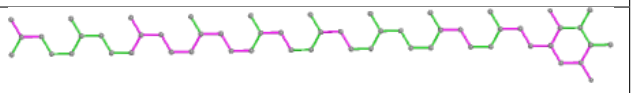


Rings

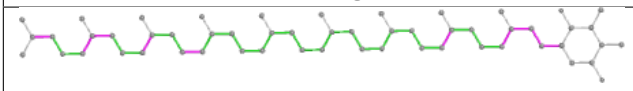
Ligand PL9 D 405



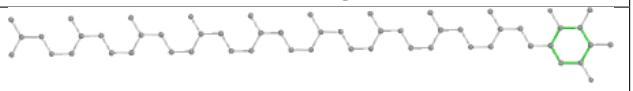
Bond lengths



Bond angles

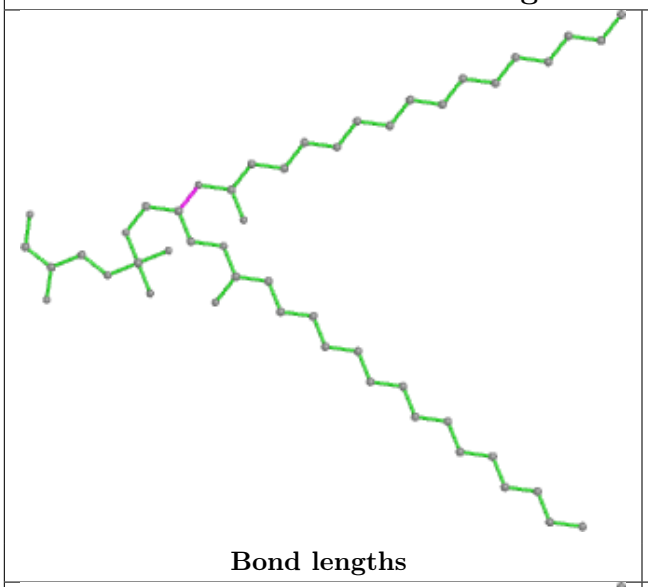


Torsions



Rings

Ligand LHG s 2630



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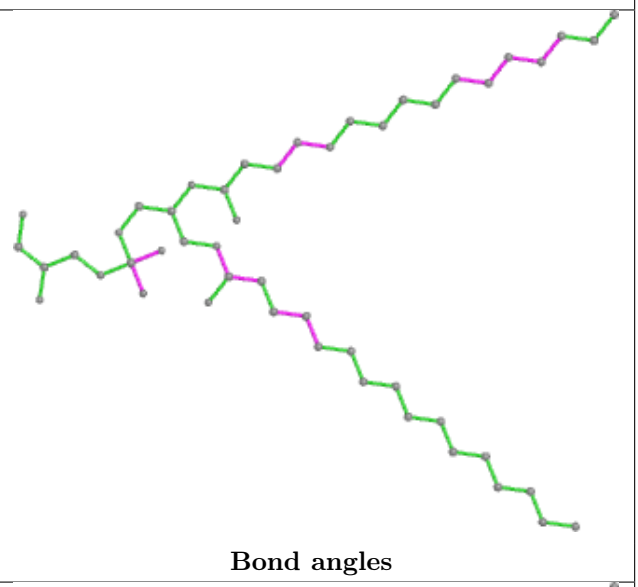
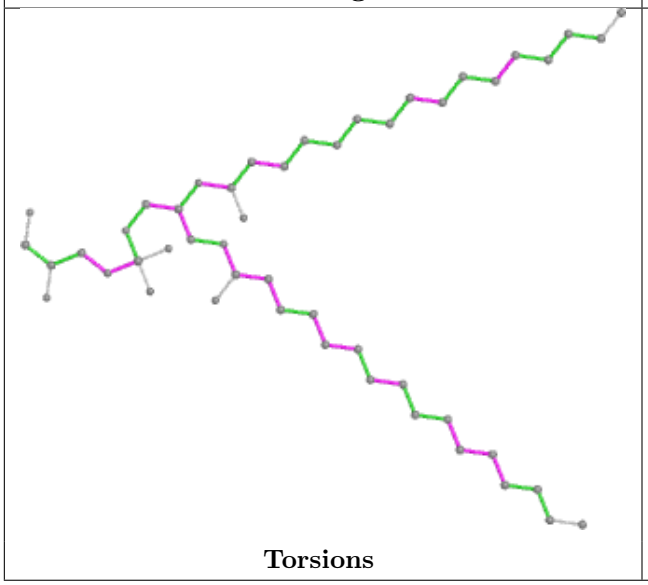
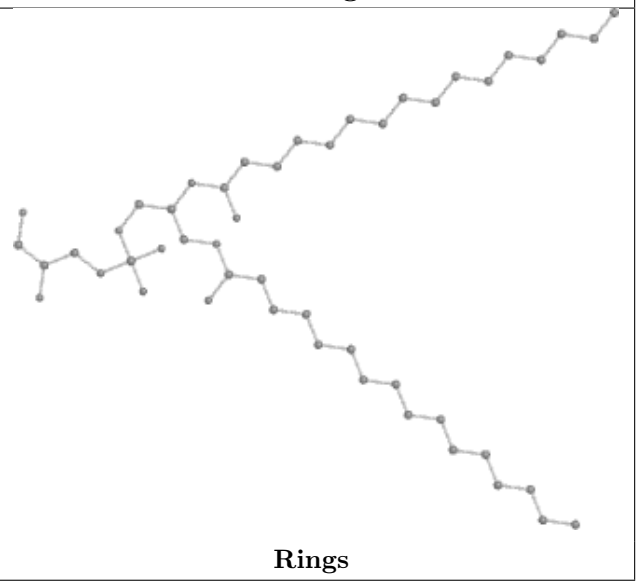


Bond angles

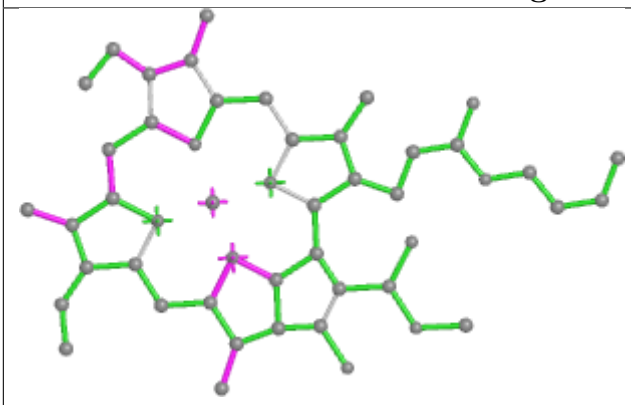


Torsions



Rings

Ligand CLA s 611



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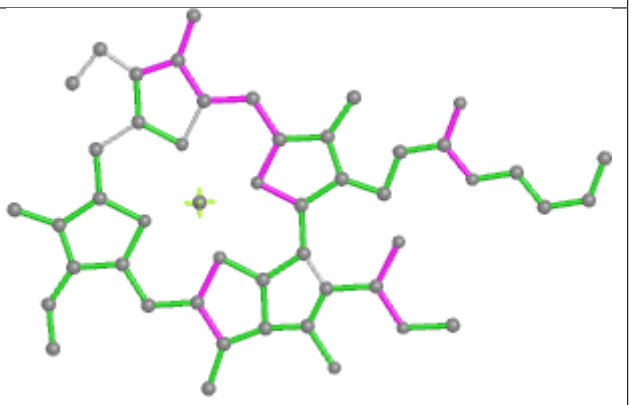
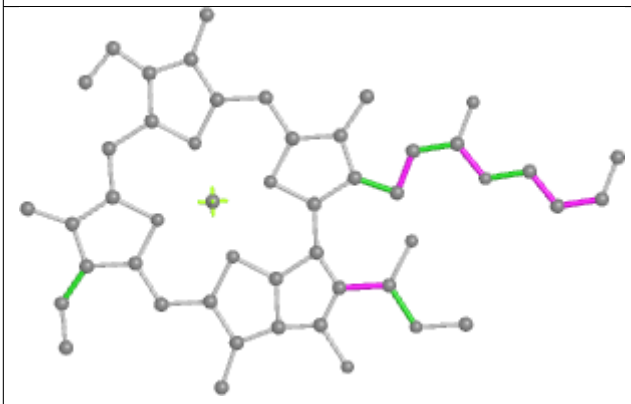
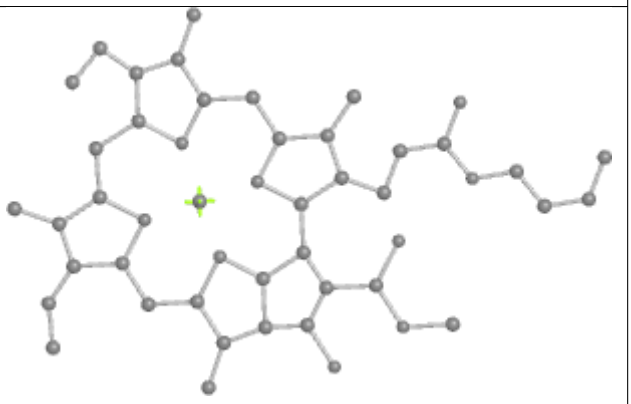


Bond angles

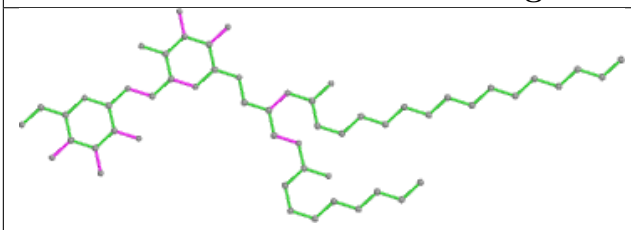


Torsions

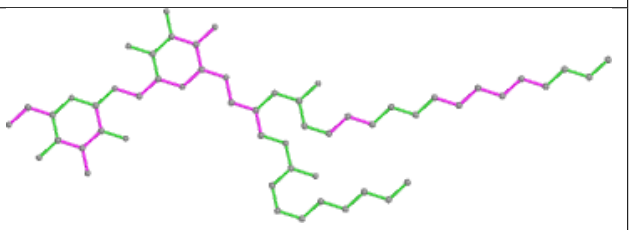


Rings

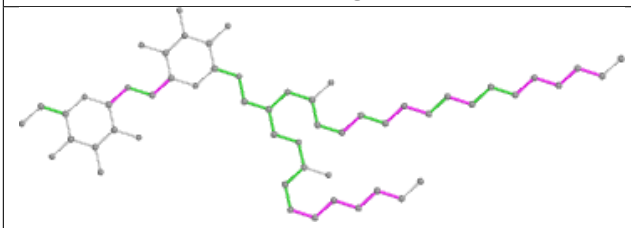
Ligand DGD c 518



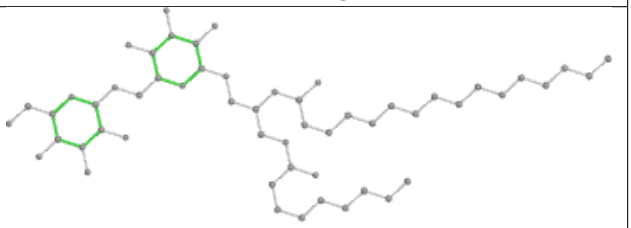
Bond lengths



Bond angles

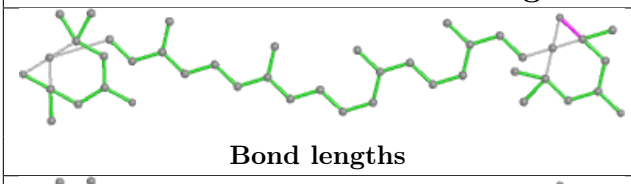


Torsions

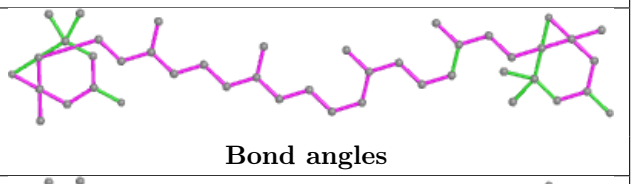


Rings

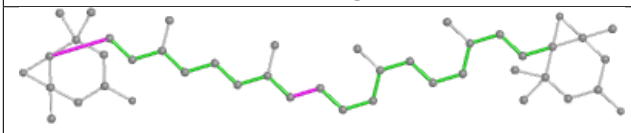
Ligand XAT R 622



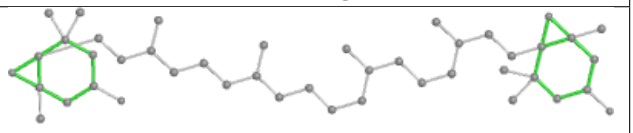
Bond lengths



Bond angles

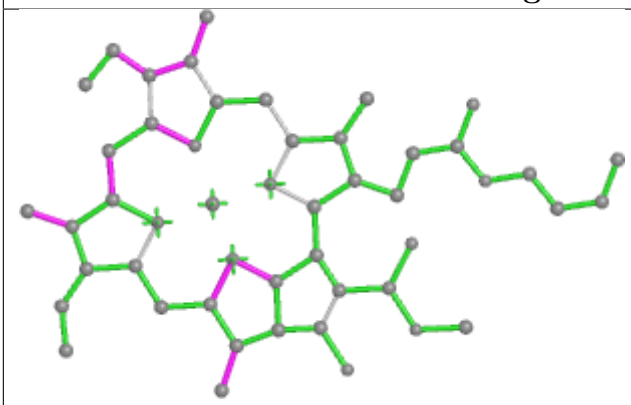


Torsions

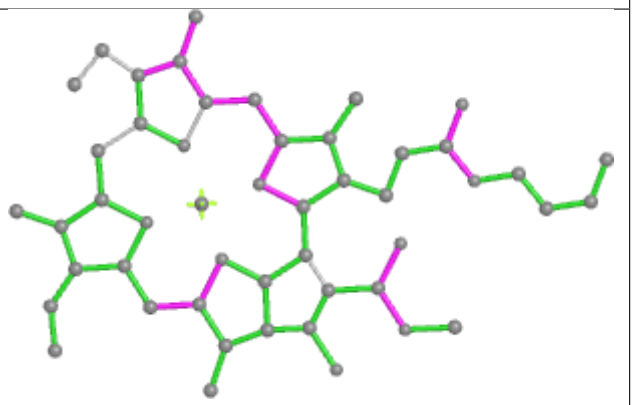


Rings

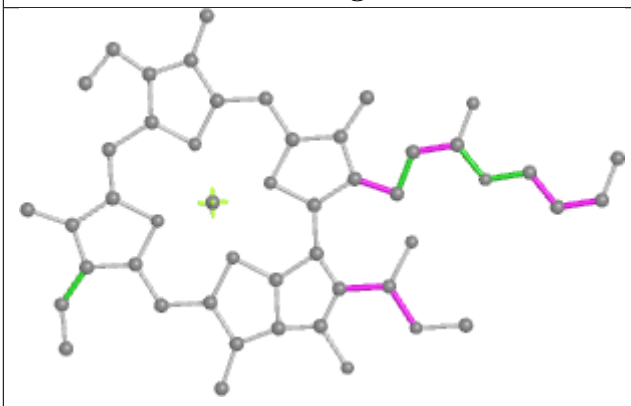
Ligand CLA N 612



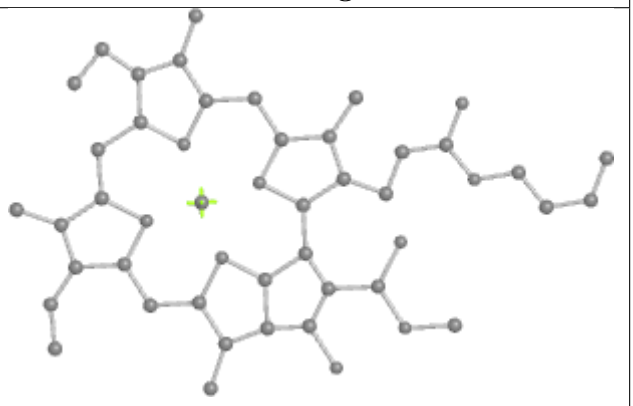
Bond lengths



Bond angles

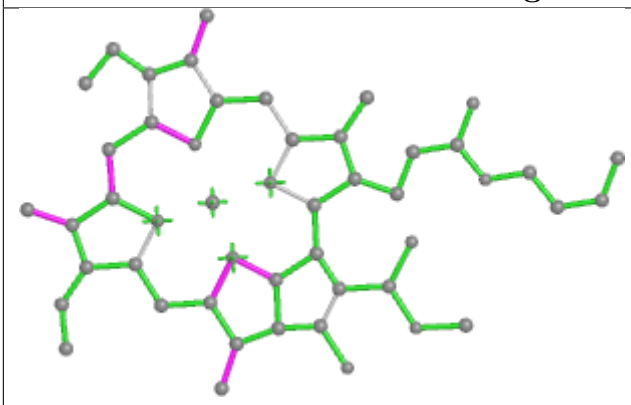


Torsions

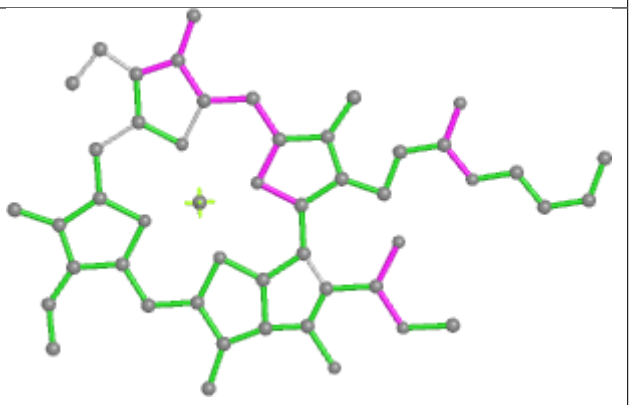


Rings

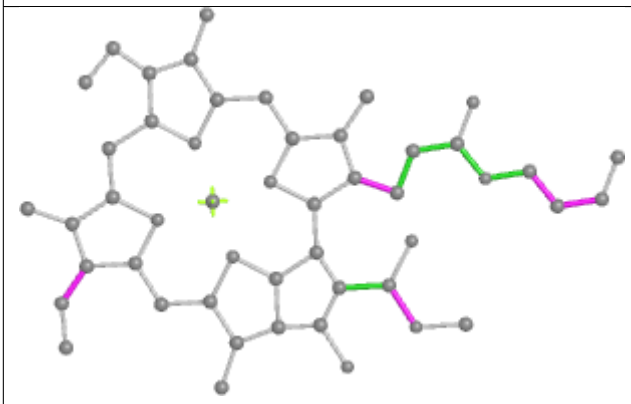
Ligand CLA R 609



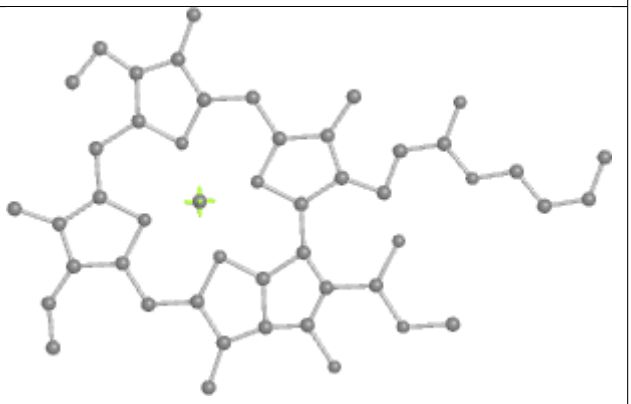
Bond lengths



Bond angles

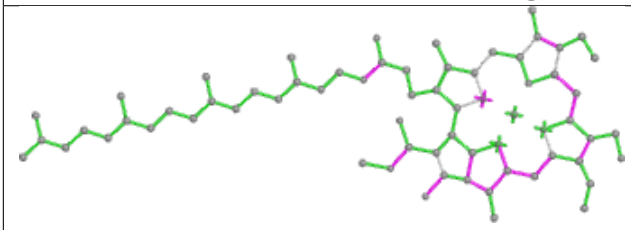


Torsions

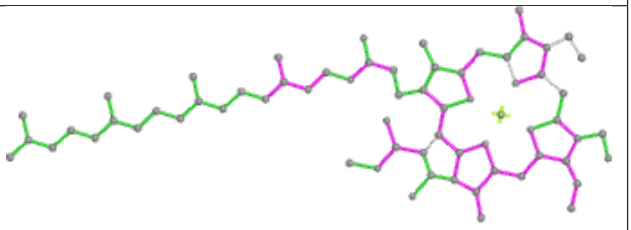


Rings

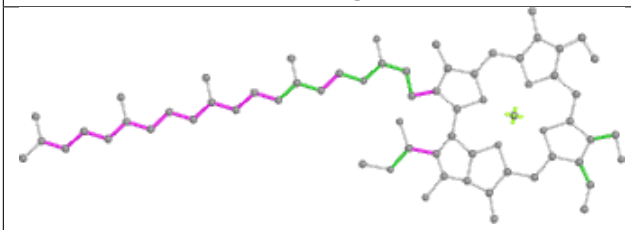
Ligand CHL G 601



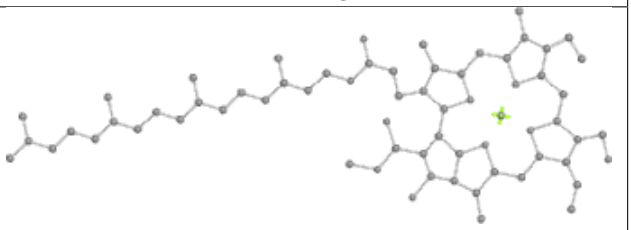
Bond lengths



Bond angles

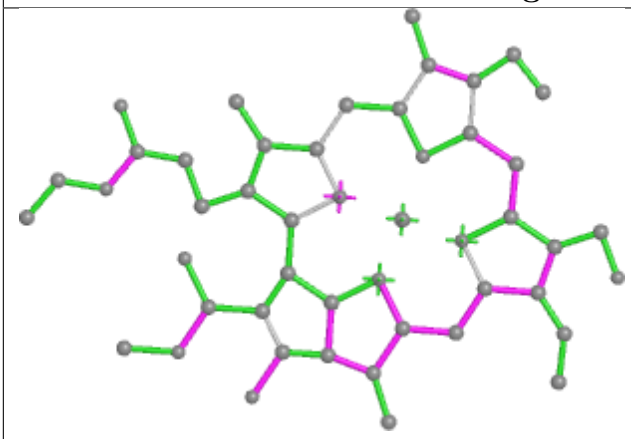


Torsions

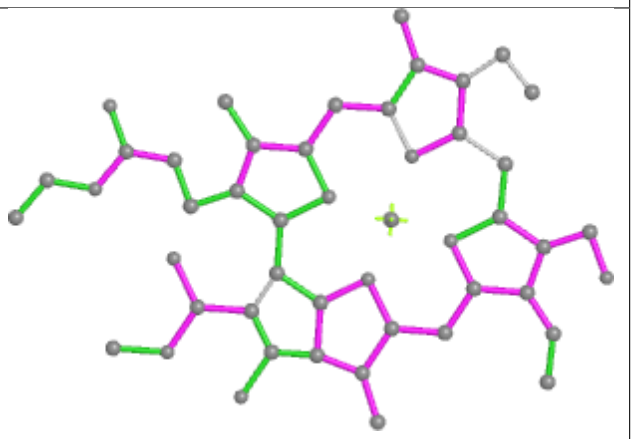


Rings

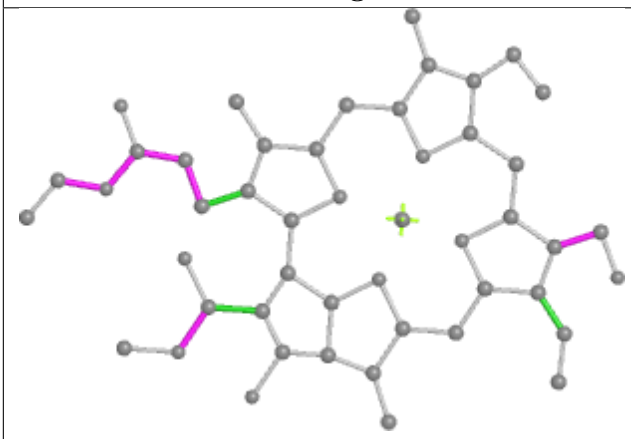
Ligand CHL N 605



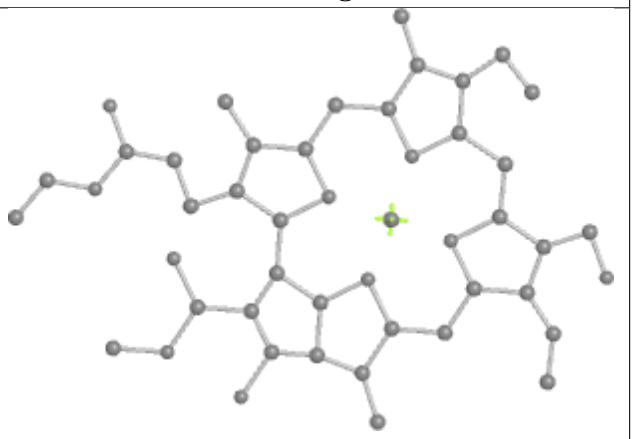
Bond lengths



Bond angles

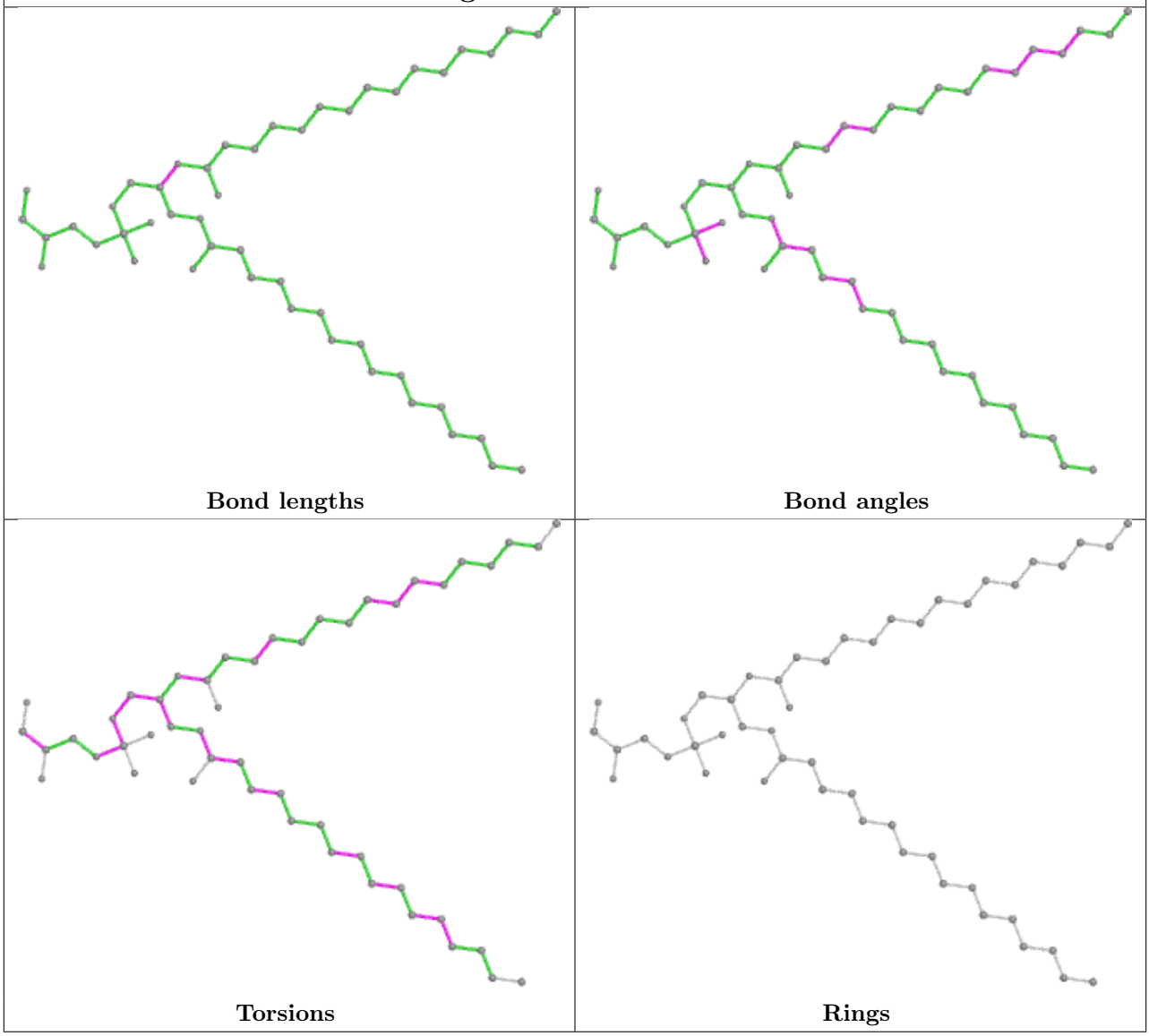


Torsions

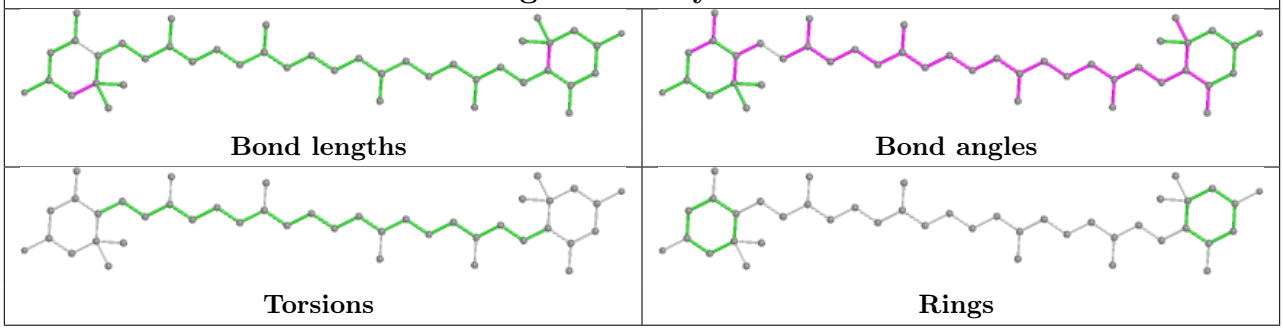


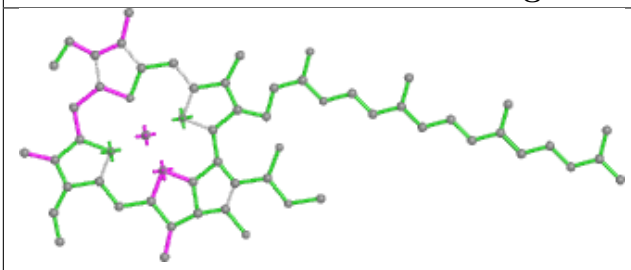
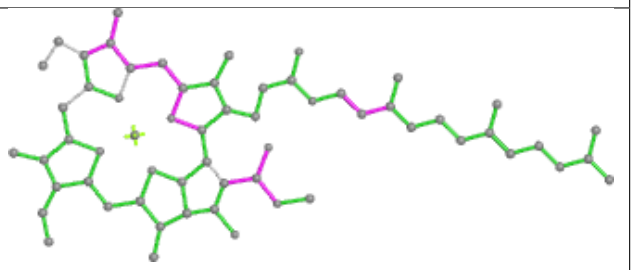
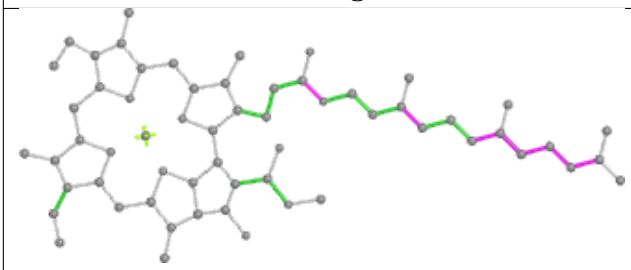
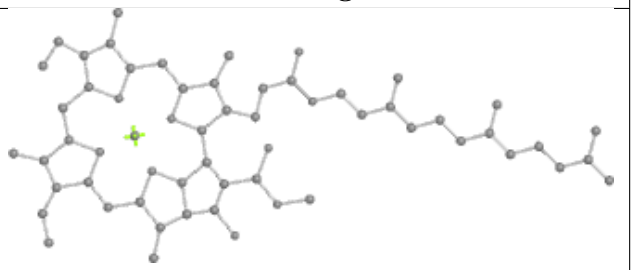
Rings

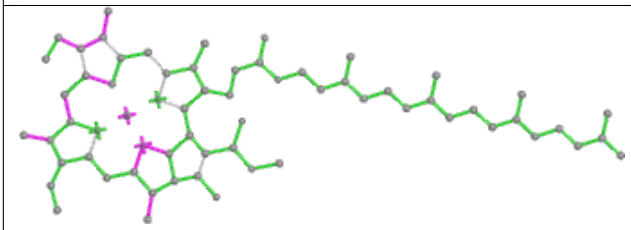
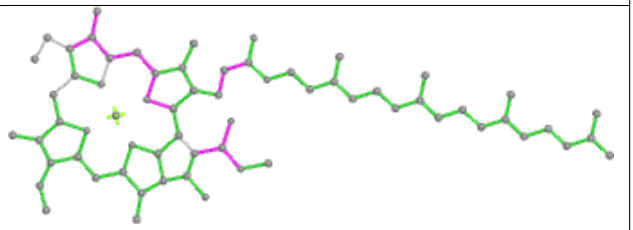
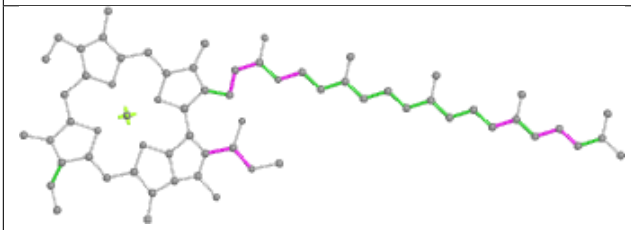
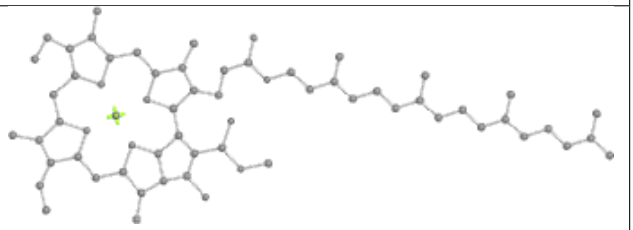
Ligand LHG N 2630



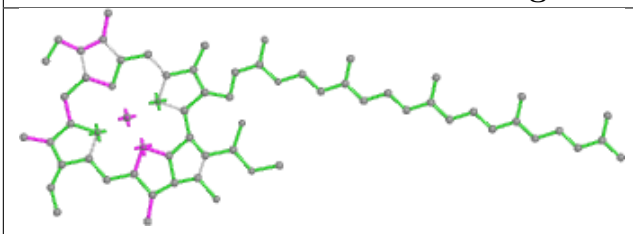
Ligand LUT y 1620



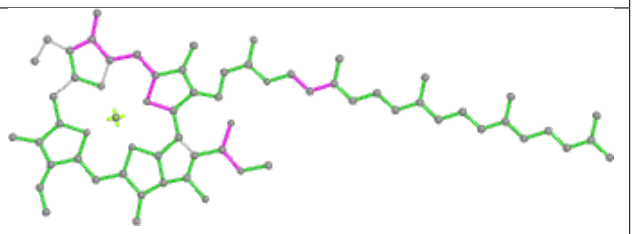
Ligand CLA A 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

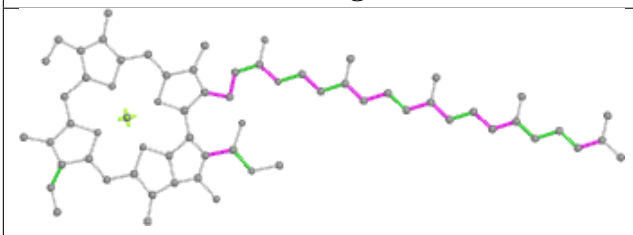
Ligand CLA c 512



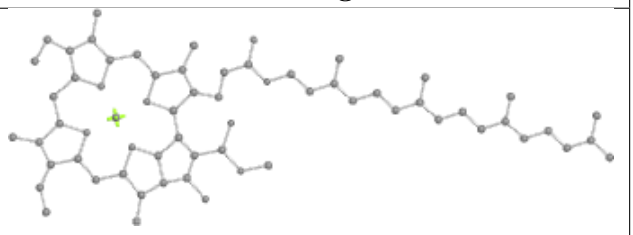
Bond lengths



Bond angles

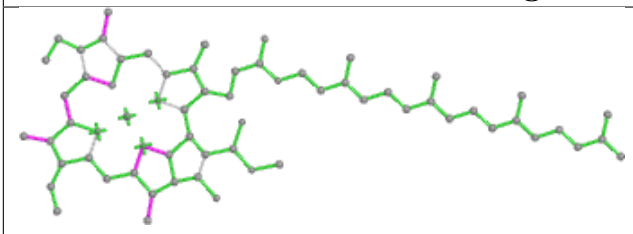


Torsions



Rings

Ligand CLA G 610



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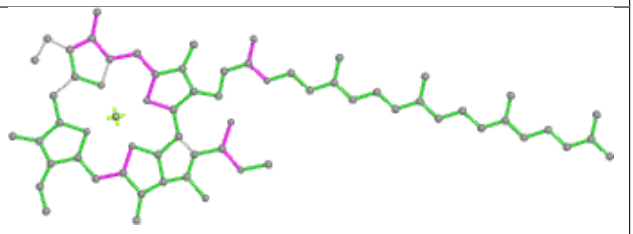
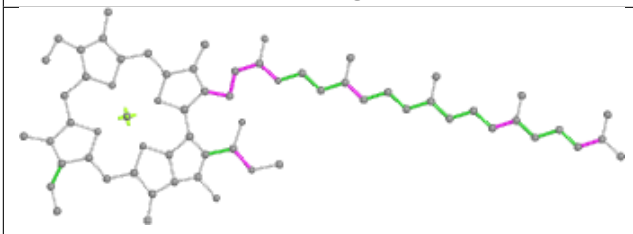


Bond angles



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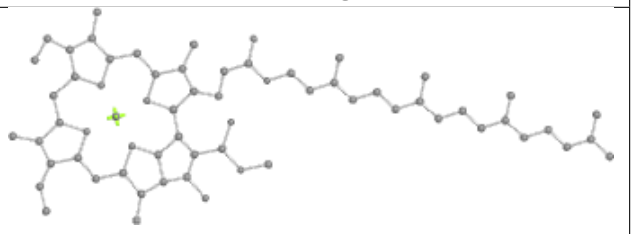
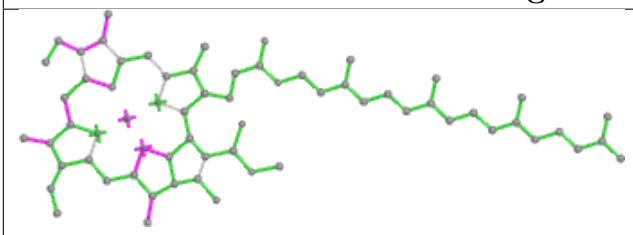
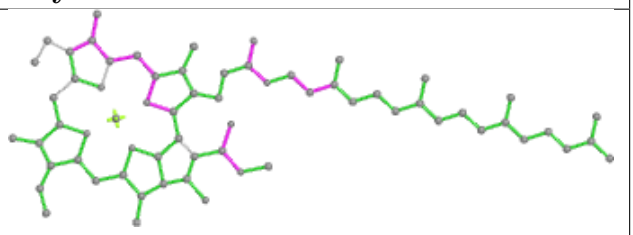


Rings

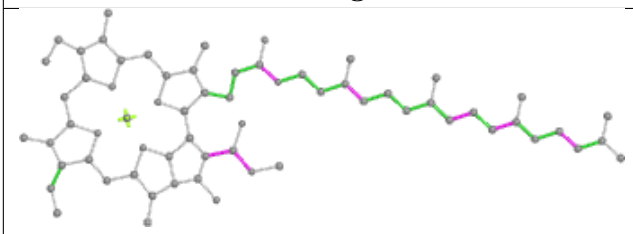
Ligand CLA y 612



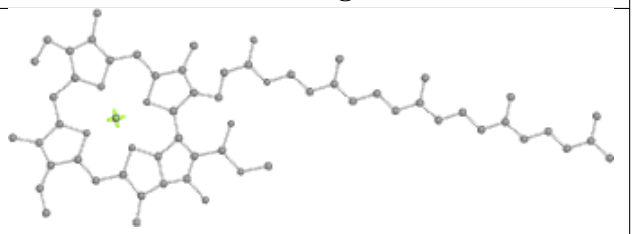
Bond lengths



Bond angles

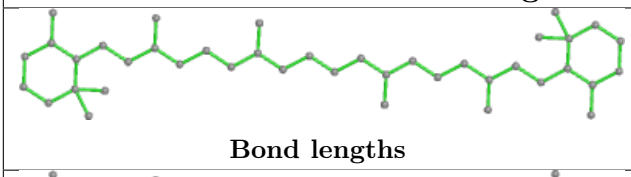


Torsions

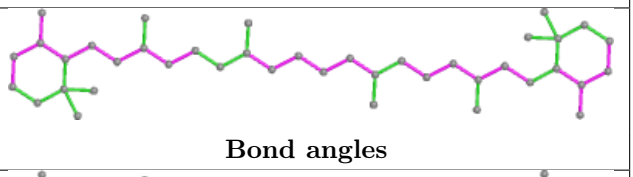


Rings

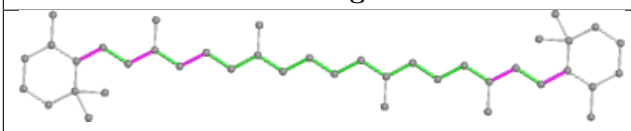
Ligand BCR D 404



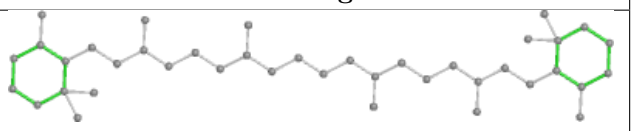
Bond lengths



Bond angles

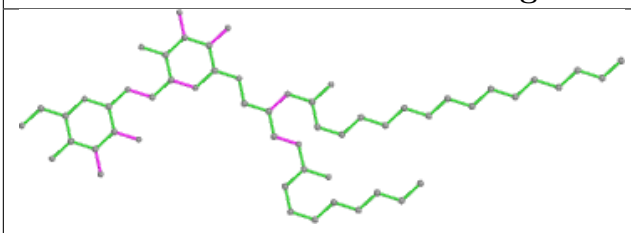


Torsions



Rings

Ligand DGD C 518



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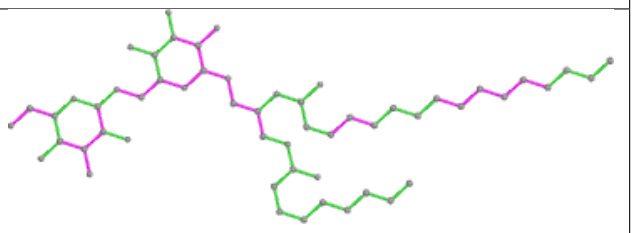
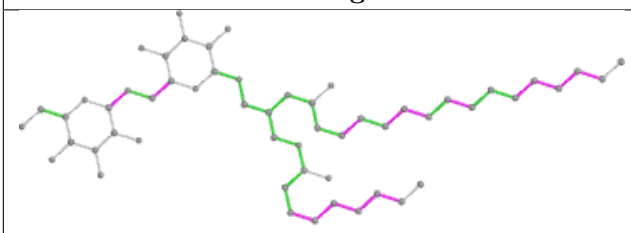
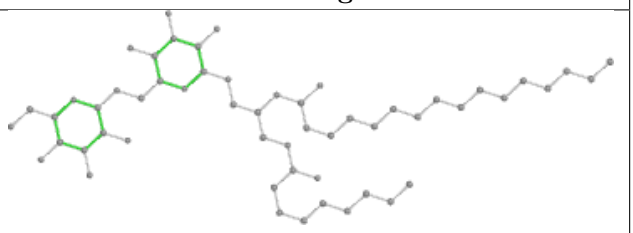


Bond angles

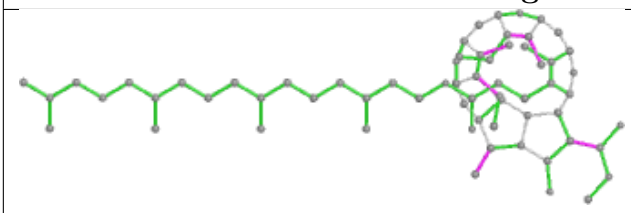


Torsions

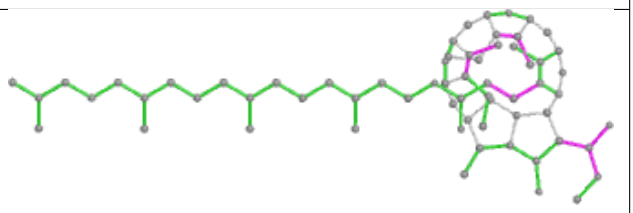


Rings

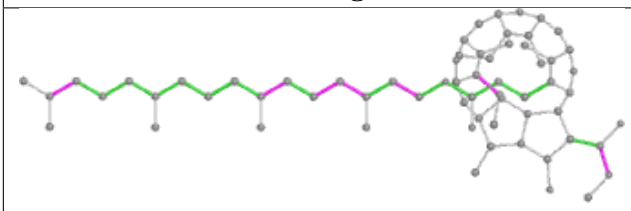
Ligand PHO A 408



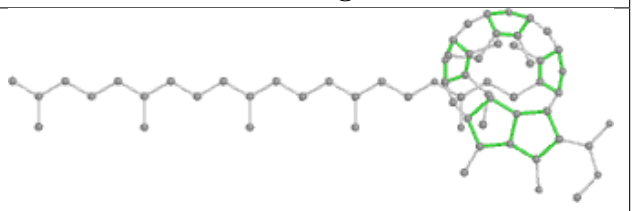
Bond lengths



Bond angles

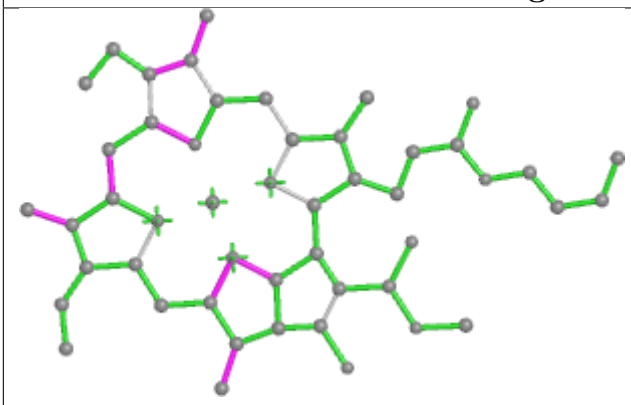


Torsions

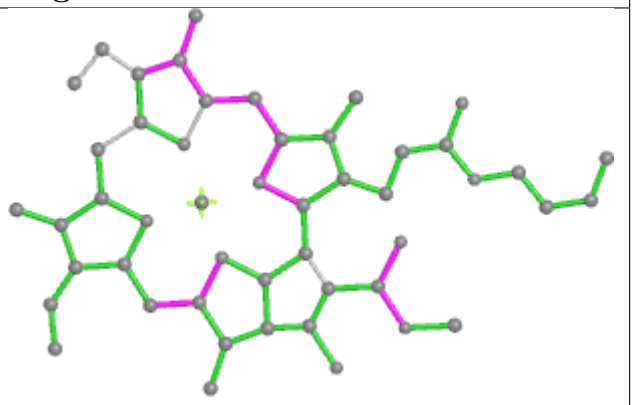


Rings

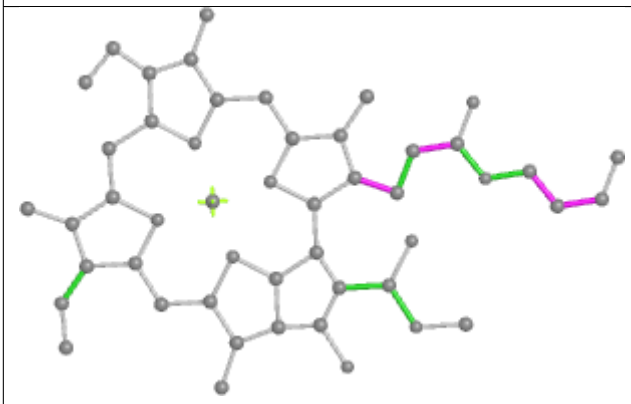
Ligand CLA g 603



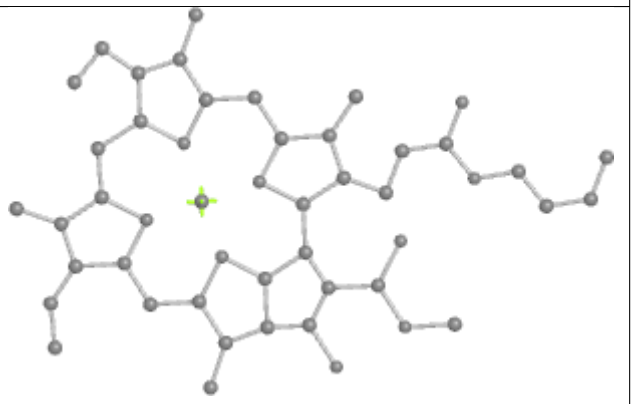
Bond lengths



Bond angles

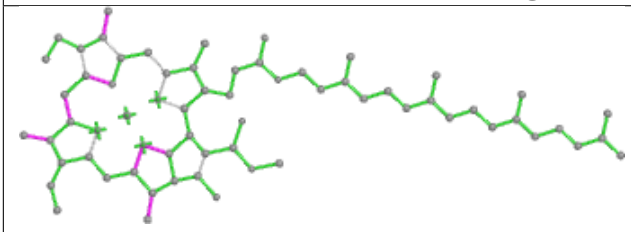


Torsions

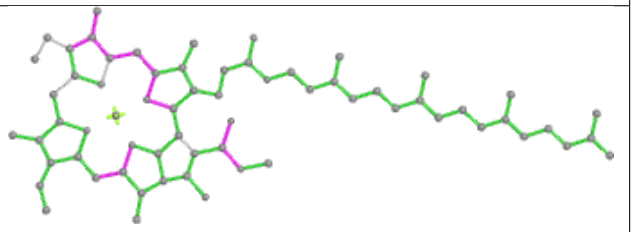


Rings

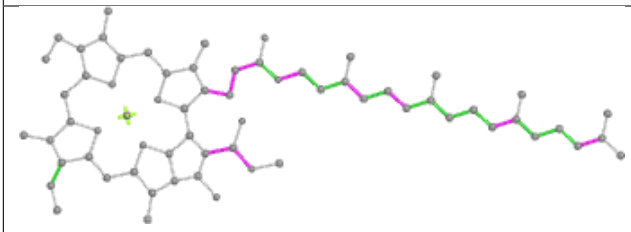
Ligand CLA R 610



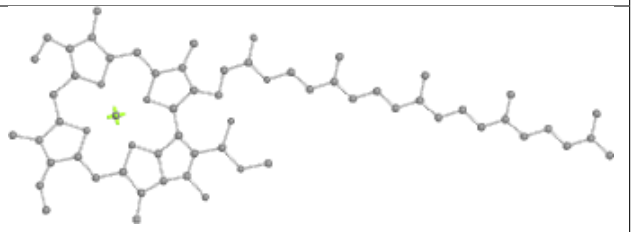
Bond lengths



Bond angles

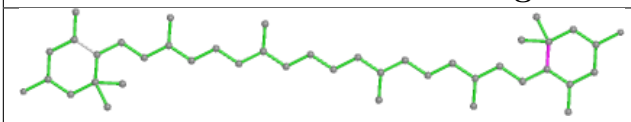


Torsions

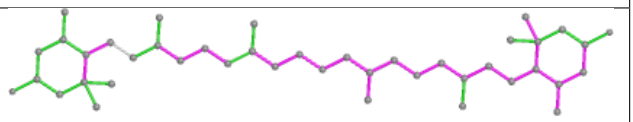


Rings

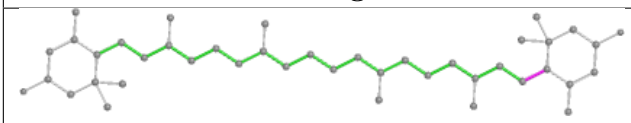
Ligand LUT G 1620



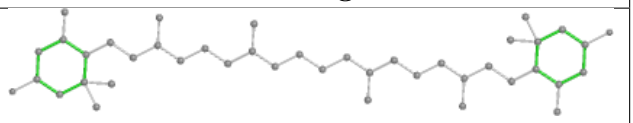
Bond lengths



Bond angles

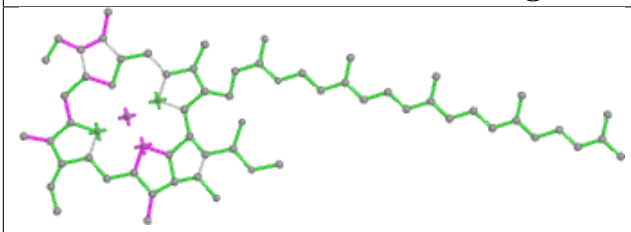


Torsions

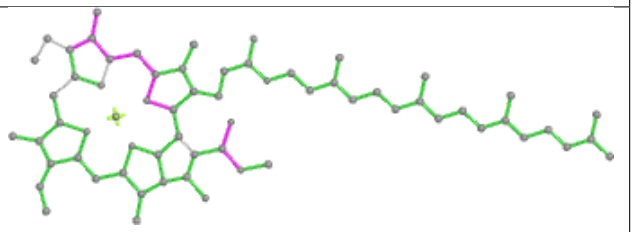


Rings

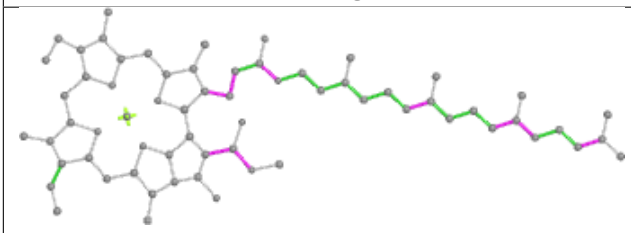
Ligand CLA C 504



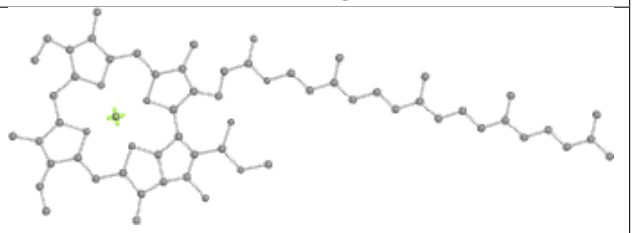
Bond lengths



Bond angles

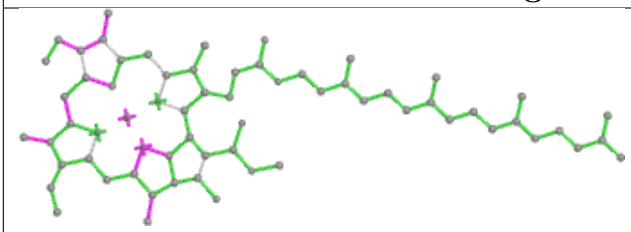


Torsions

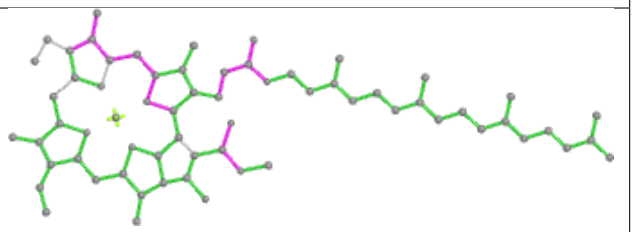


Rings

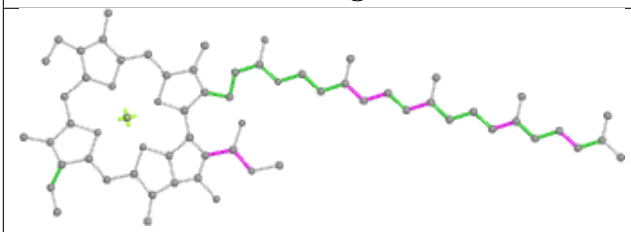
Ligand CLA B 610



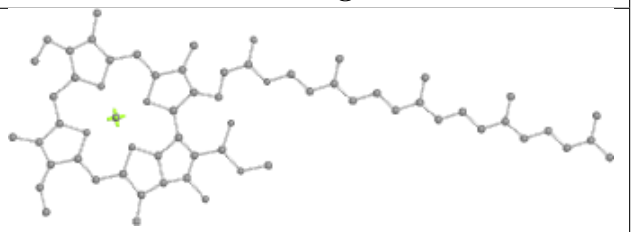
Bond lengths



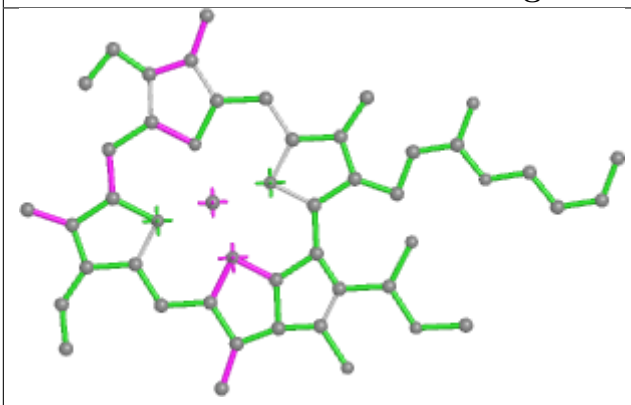
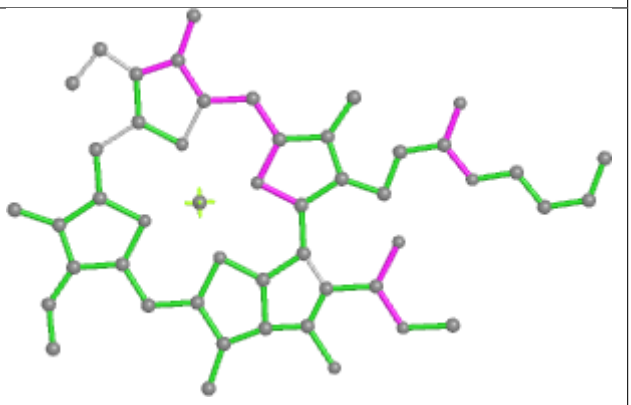
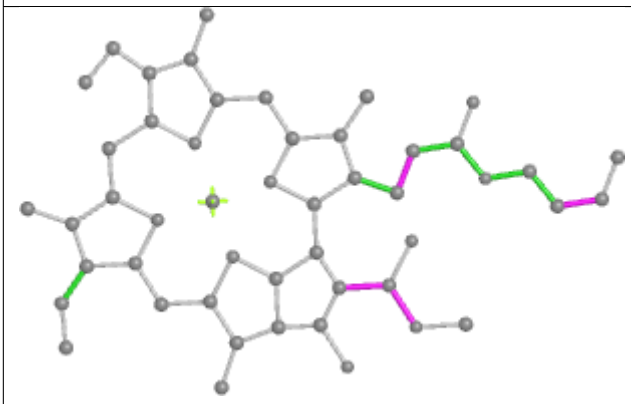
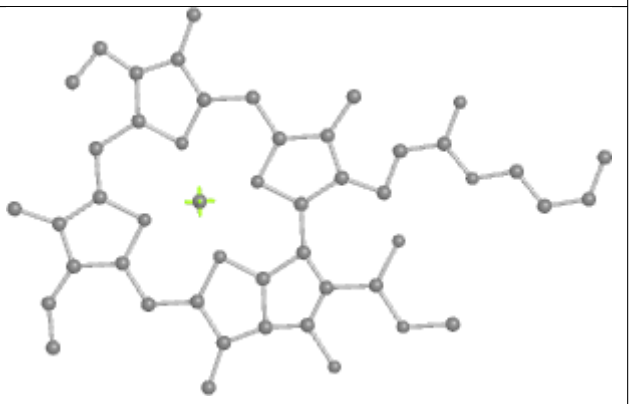
Bond angles



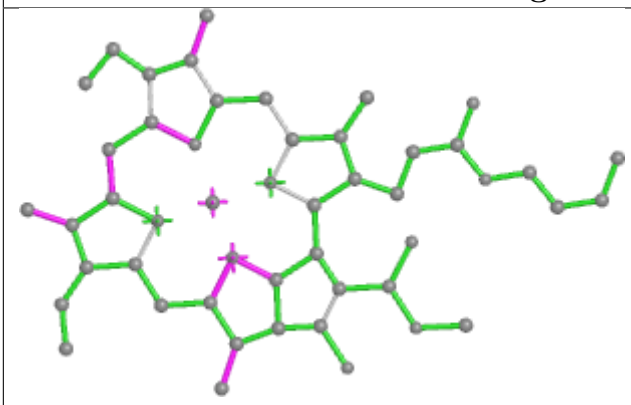
Torsions



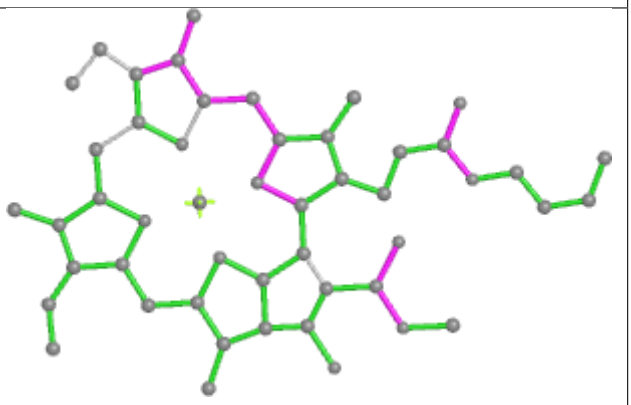
Rings

Ligand CLA R 603	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

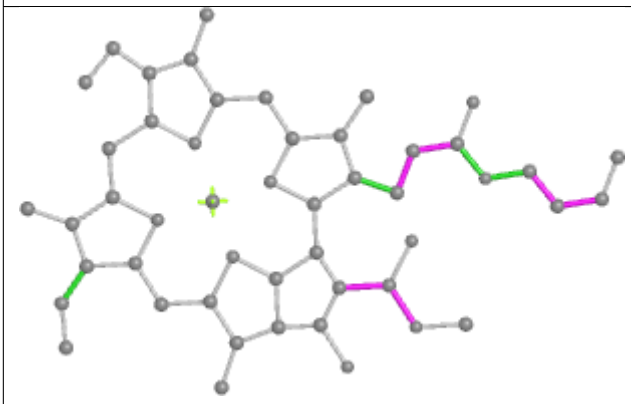
Ligand CLA r 613



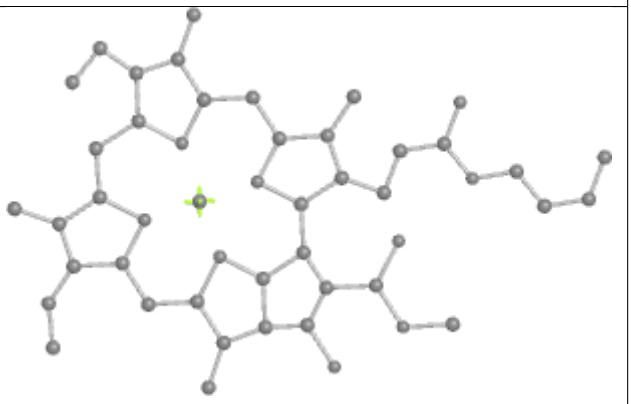
Bond lengths



Bond angles

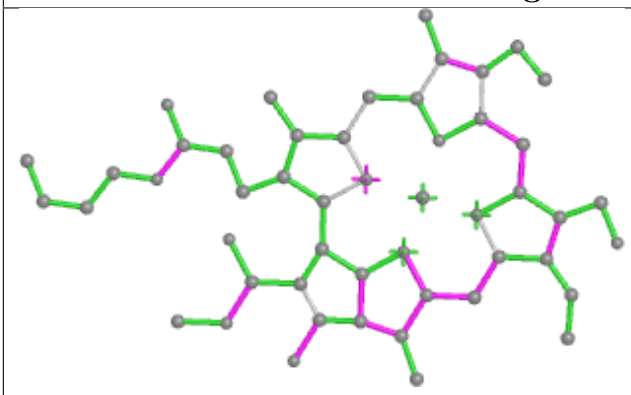


Torsions

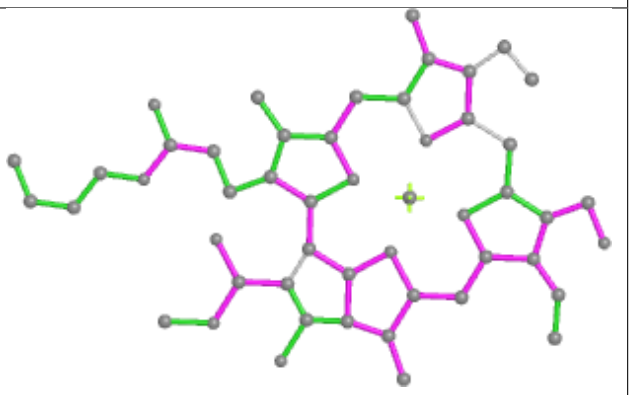


Rings

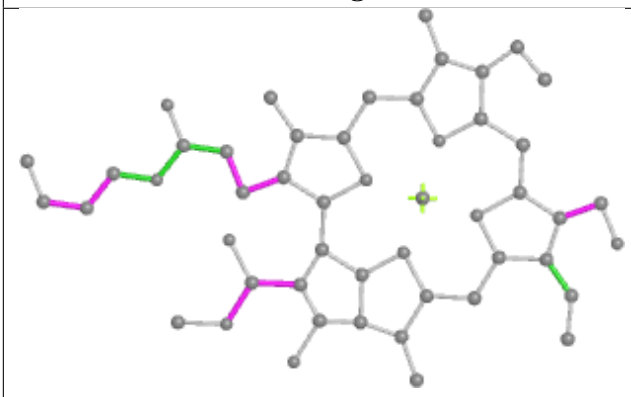
Ligand CHL R 606



Bond lengths



Bond angles



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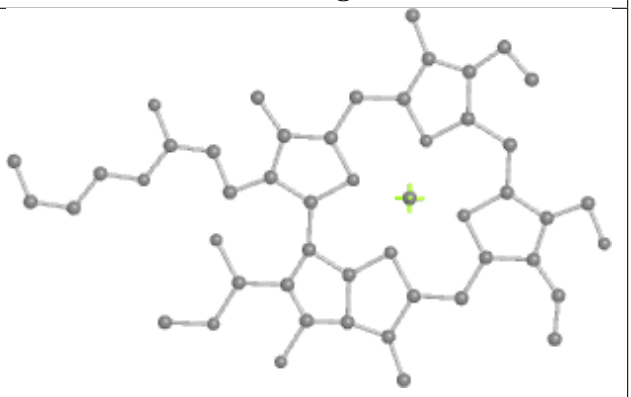
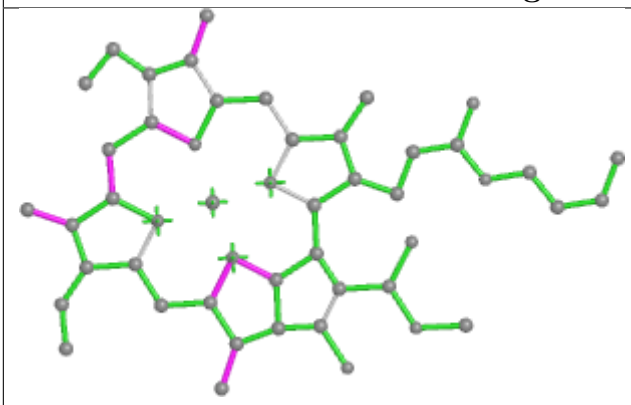
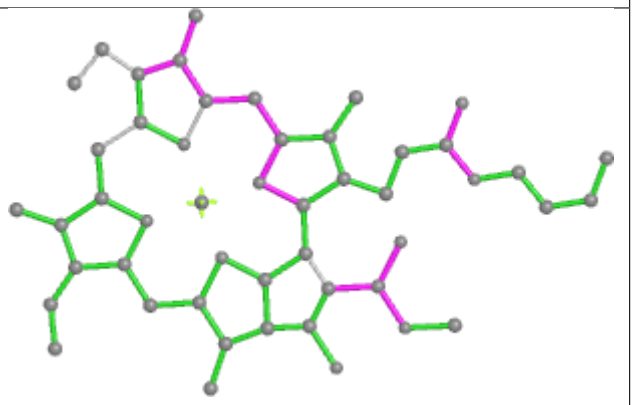


Rings

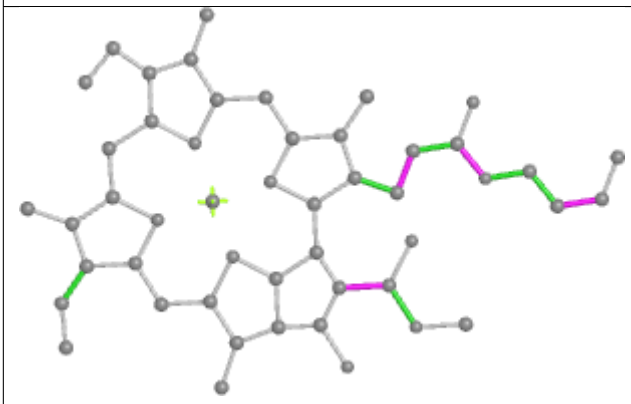
Ligand CLA N 611



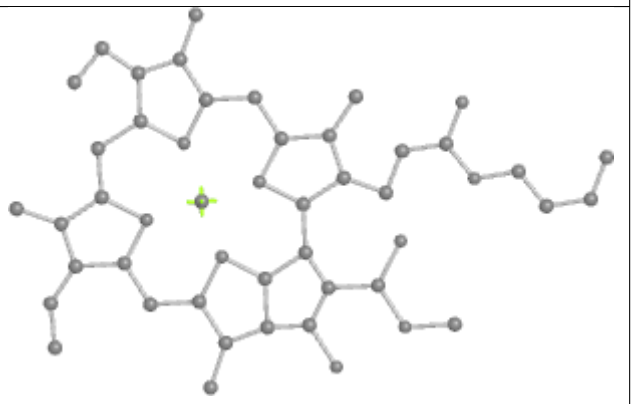
Bond lengths



Bond angles

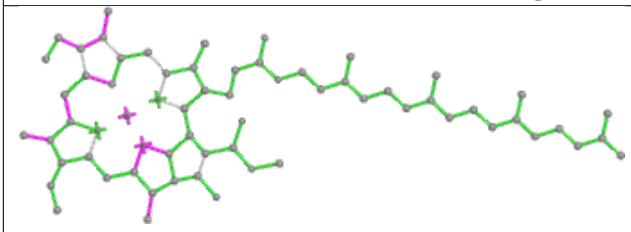


Torsions

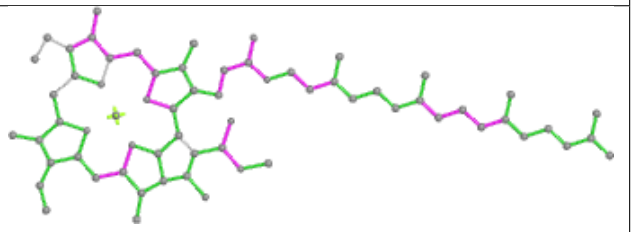


Rings

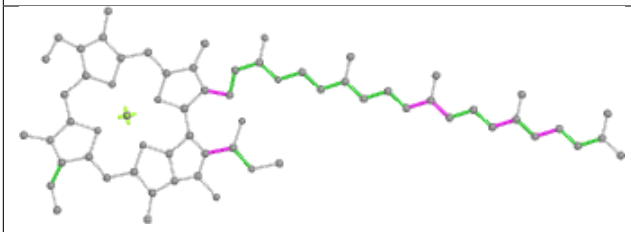
Ligand CLA c 509



Bond lengths



Bond angles



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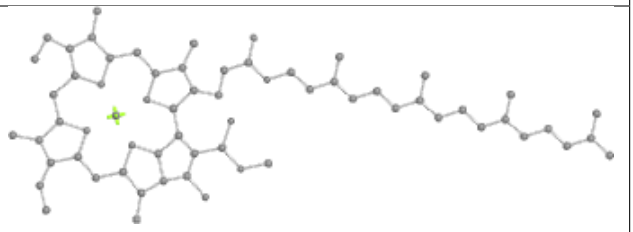
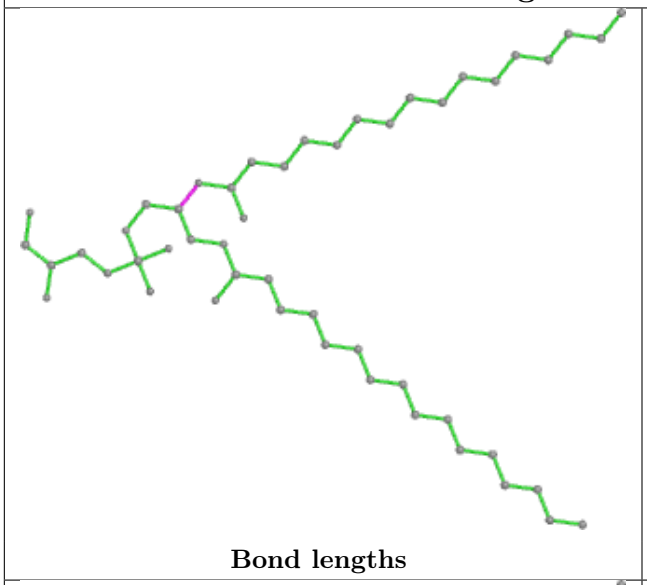


Rings

Ligand LHG n 2630



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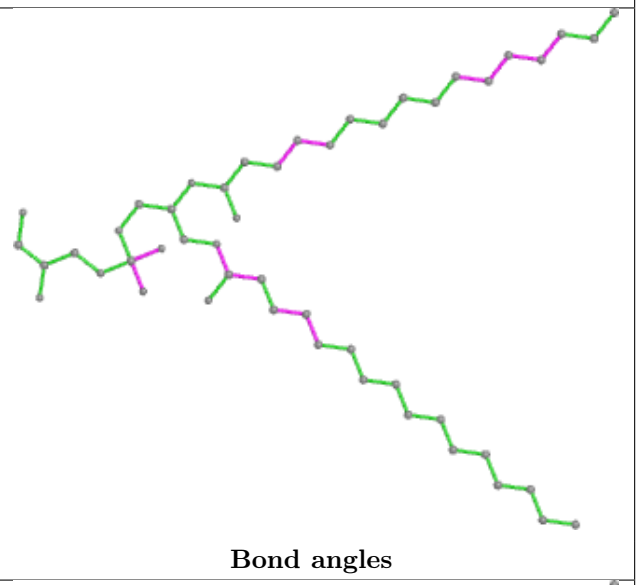
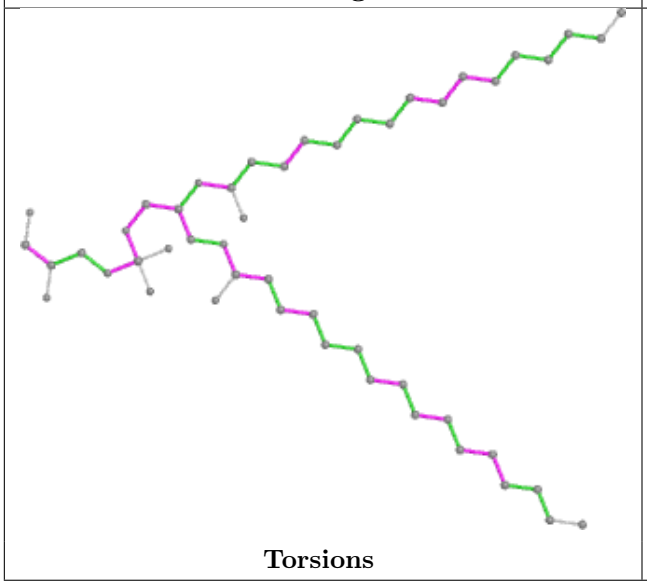


Bond angles



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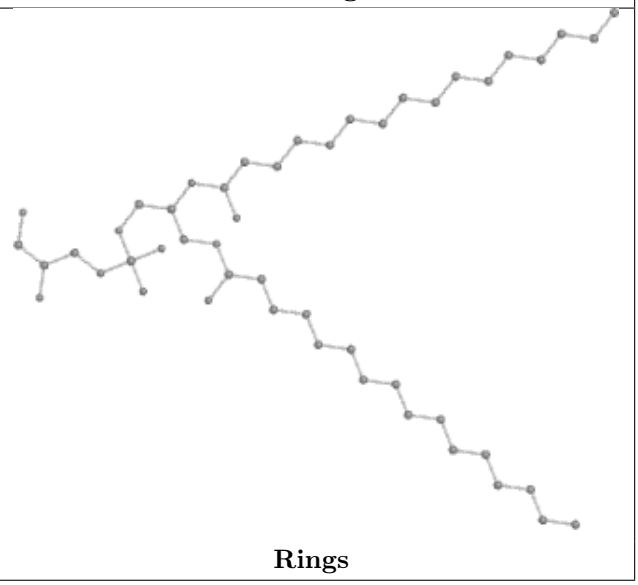
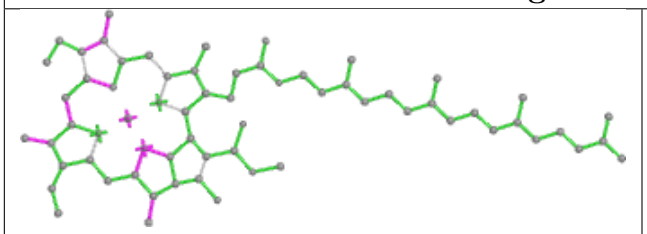


Rings

Ligand CLA b 617



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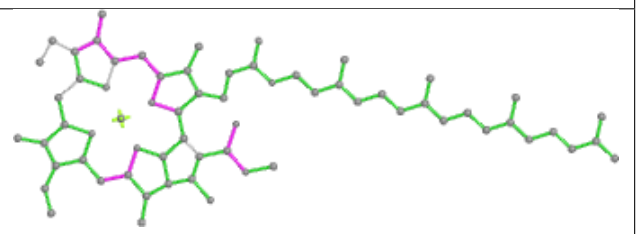
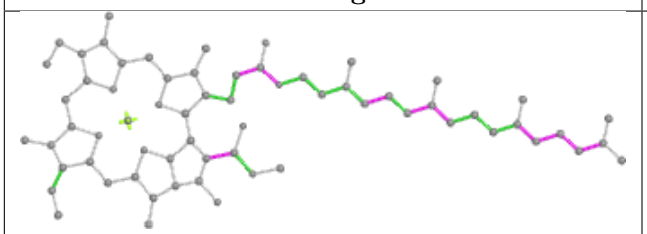


Bond angles



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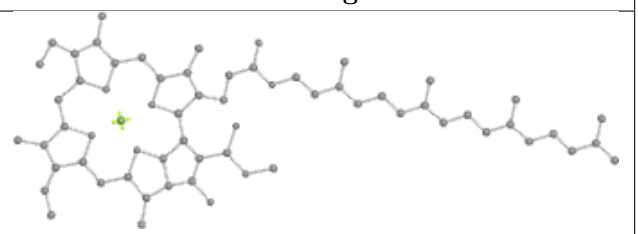
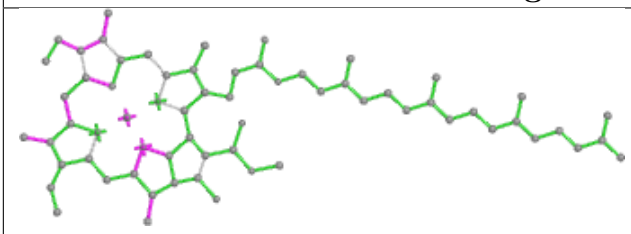
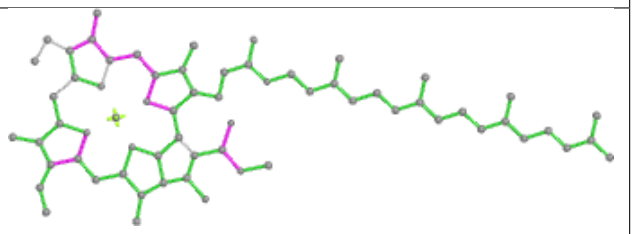


Rings

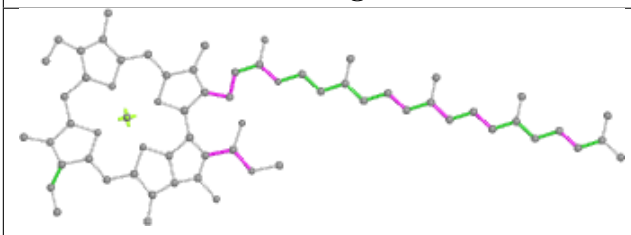
Ligand CLA B 615



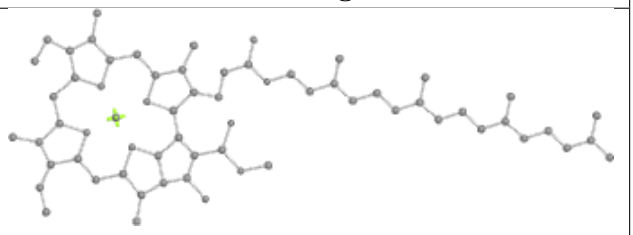
Bond lengths



Bond angles

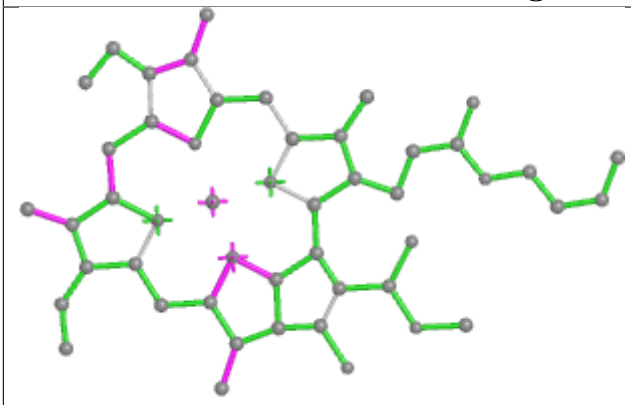


Torsions

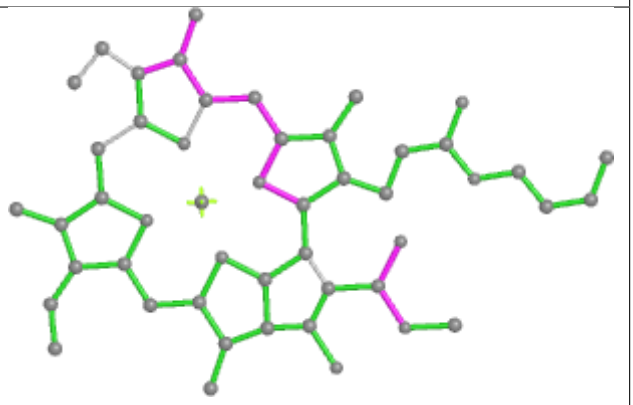


Rings

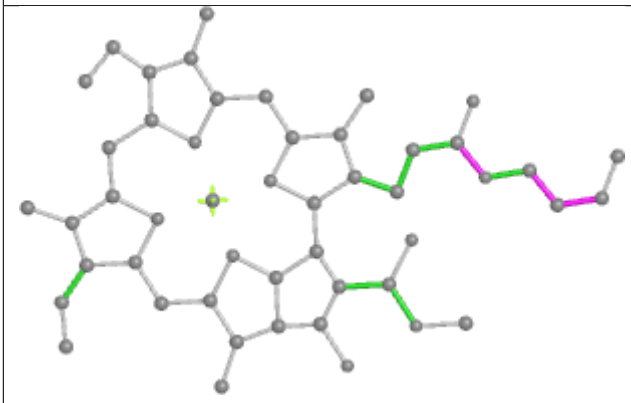
Ligand CLA n 604



Bond lengths



Bond angles



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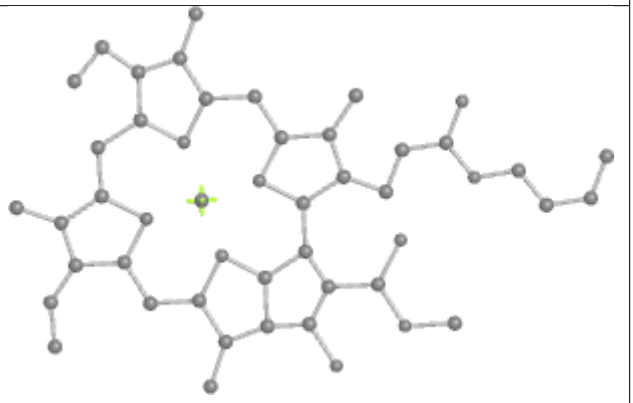
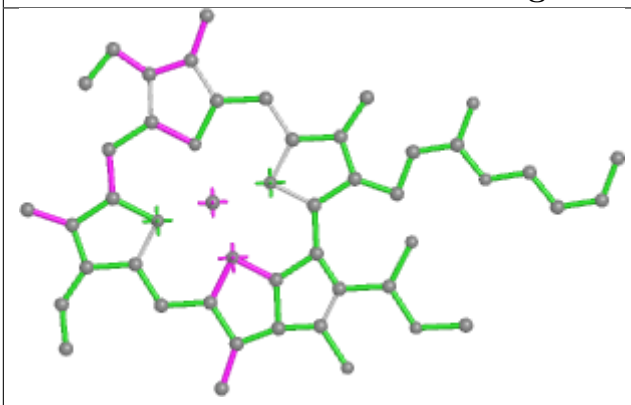


Rings

Ligand CLA g 613



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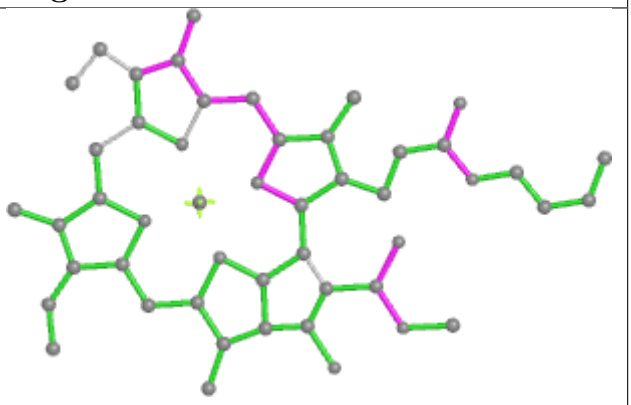

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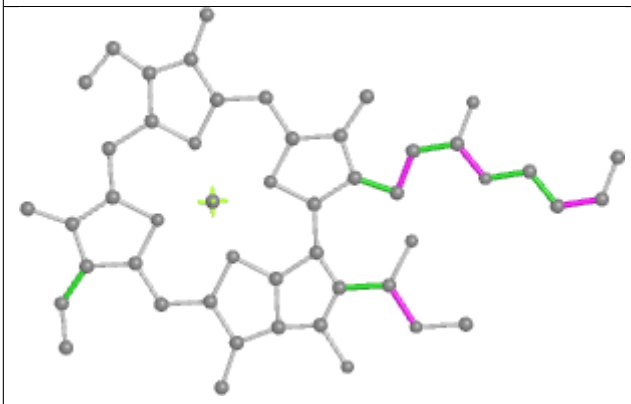
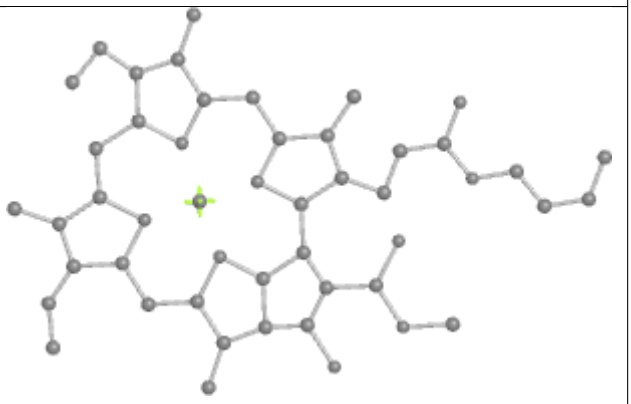
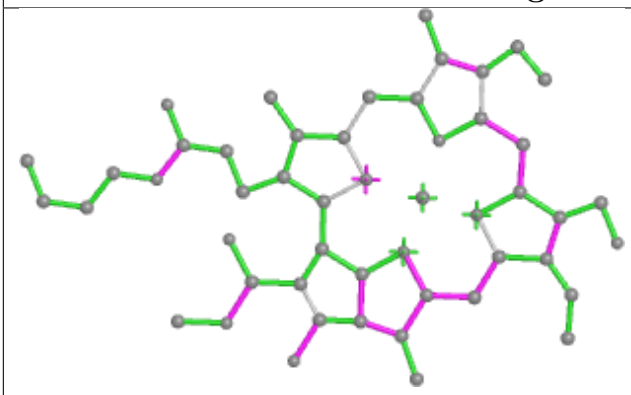


Torsions

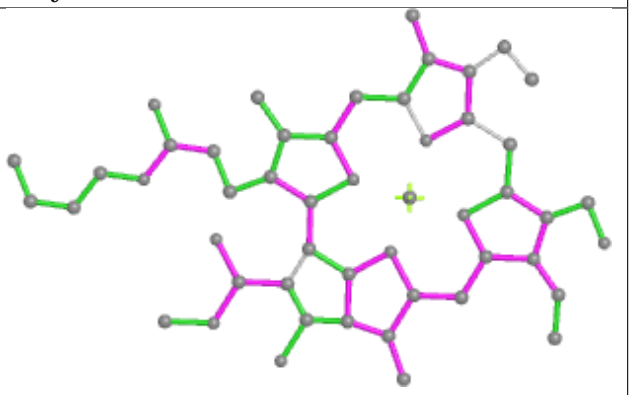


Rings

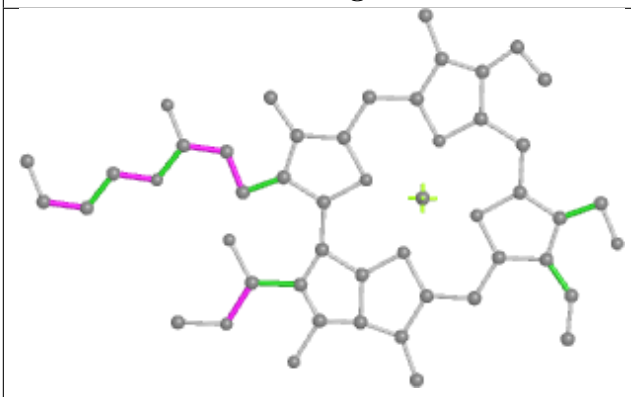
Ligand CHL y 606



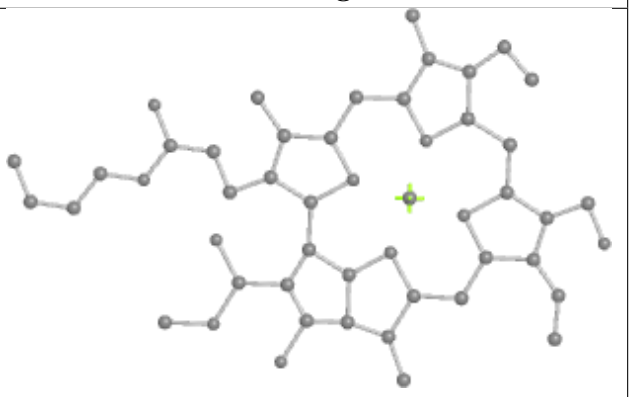
Bond lengths



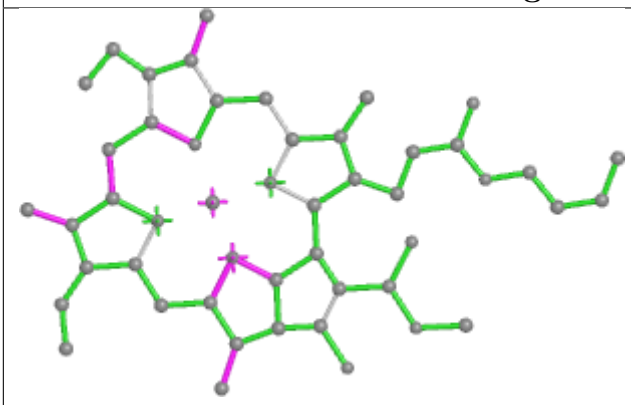
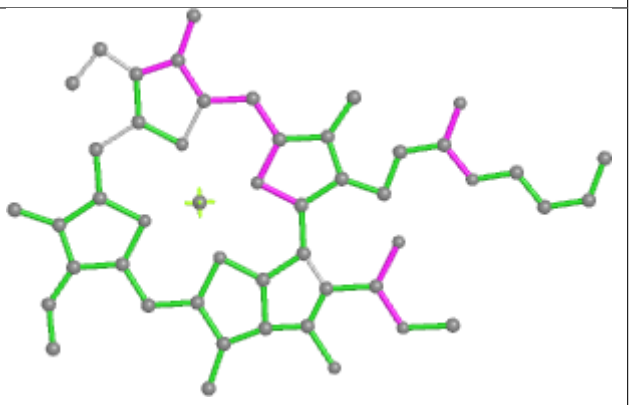
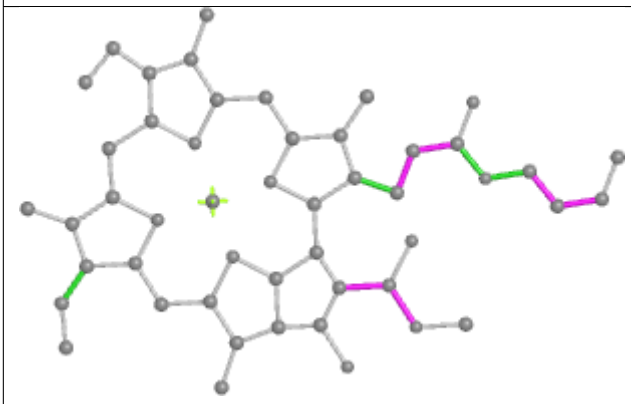
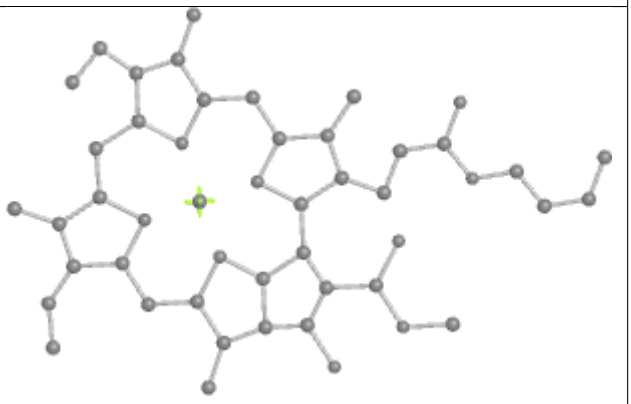
Bond angles



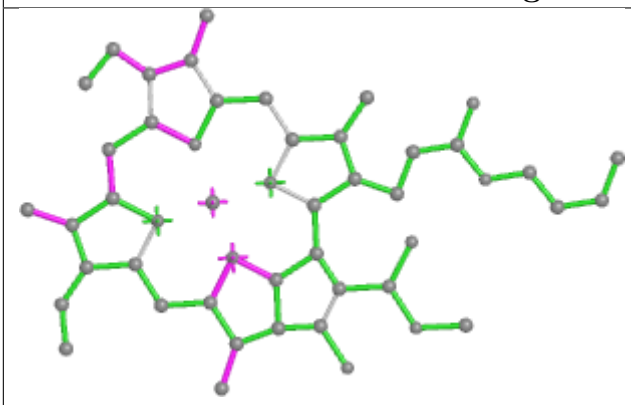
Torsions



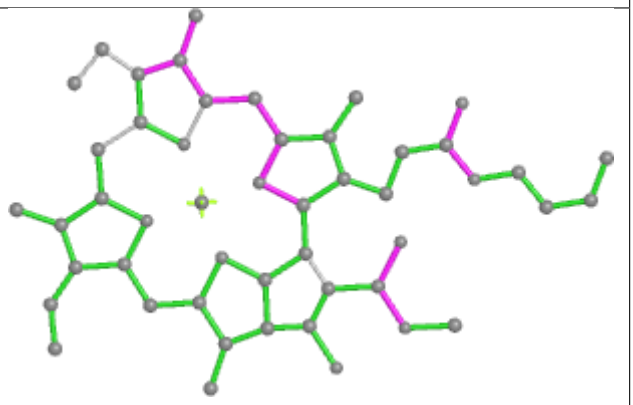
Rings

Ligand CLA R 613	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

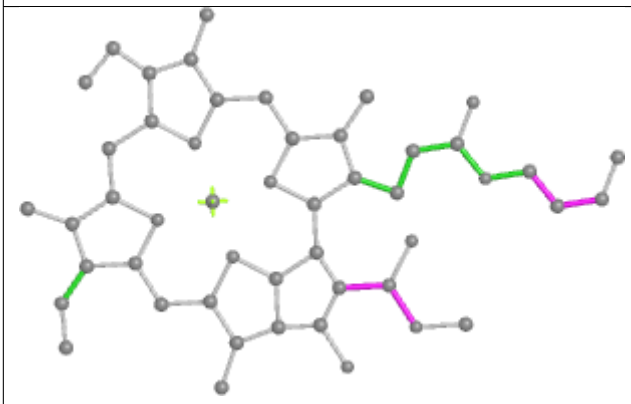
Ligand CLA G 612



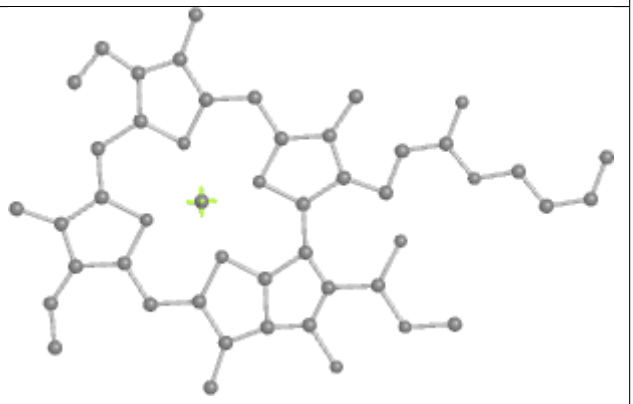
Bond lengths



Bond angles

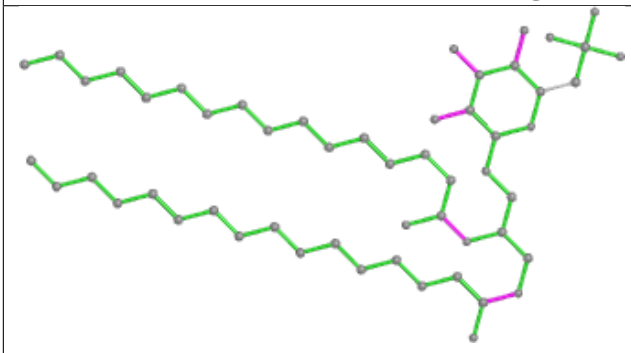


Torsions

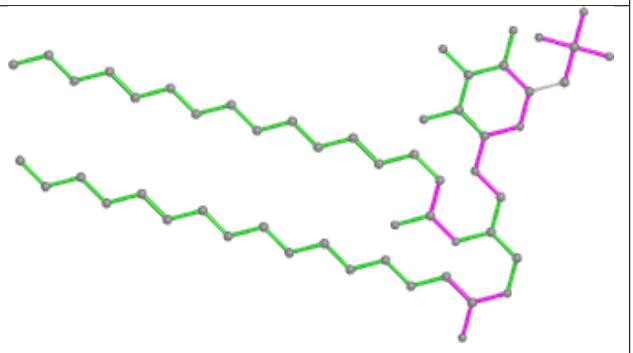


Rings

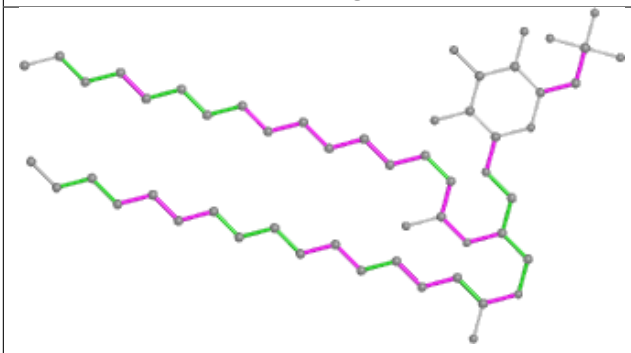
Ligand SQD b 621



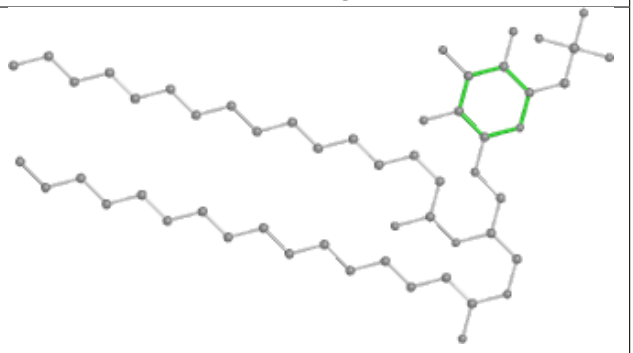
Bond lengths



Bond angles

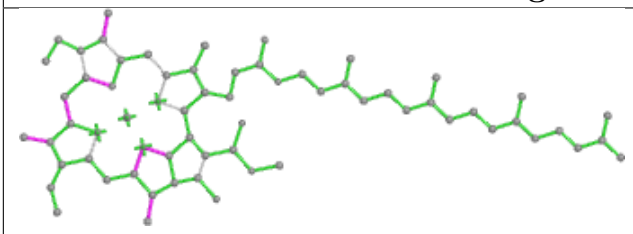


Torsions

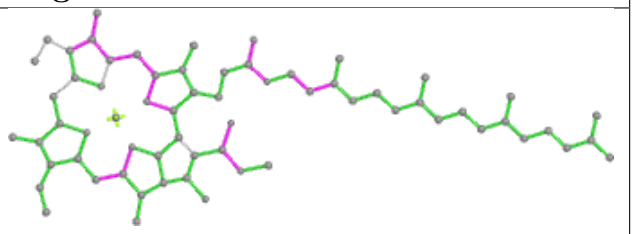


Rings

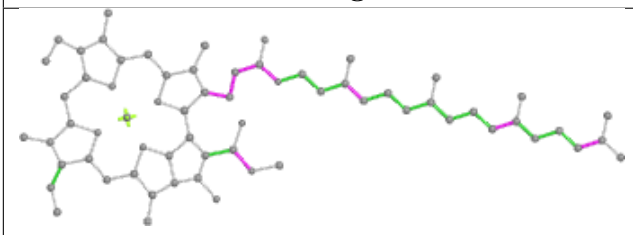
Ligand CLA g 610



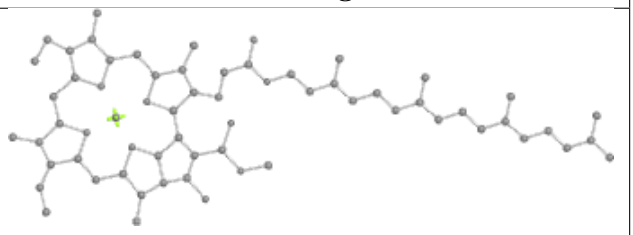
Bond lengths



Bond angles

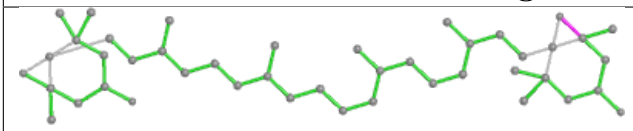


Torsions

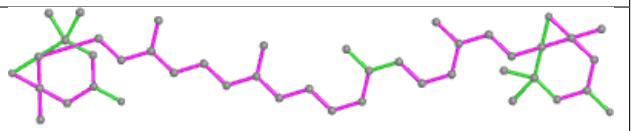


Rings

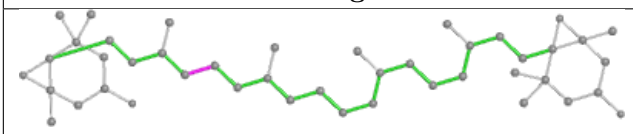
Ligand XAT n 1622



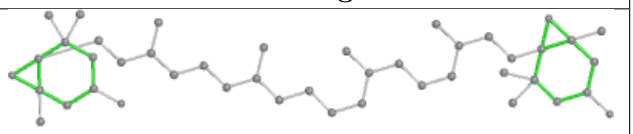
Bond lengths



Bond angles

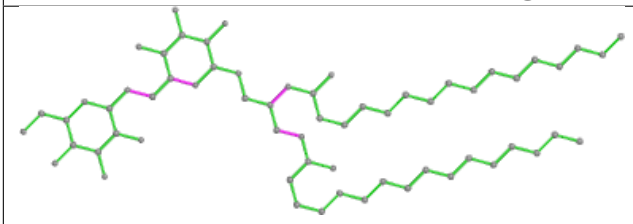


Torsions



Rings

Ligand DGD H 102



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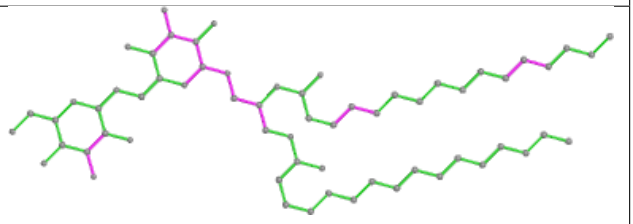
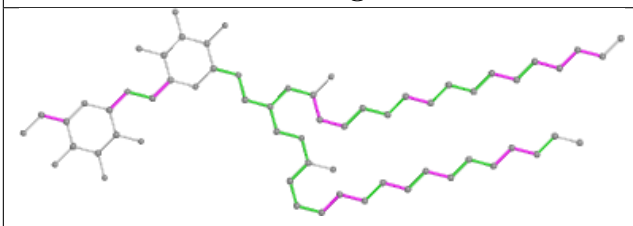
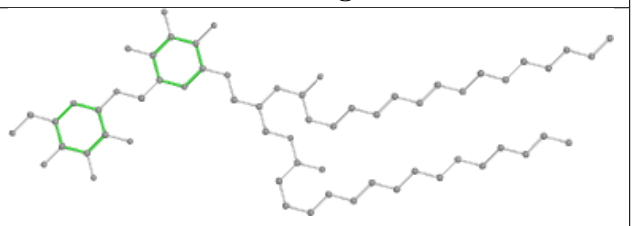


Bond angles

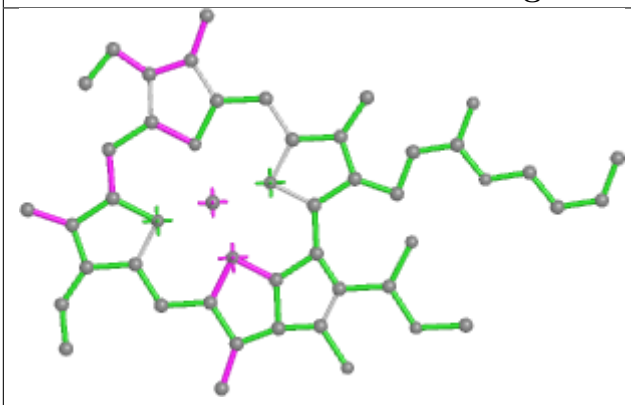


Torsions



Rings

Ligand CLA Y 604



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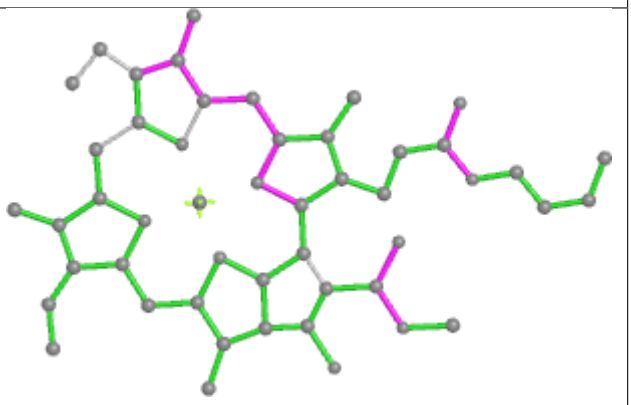
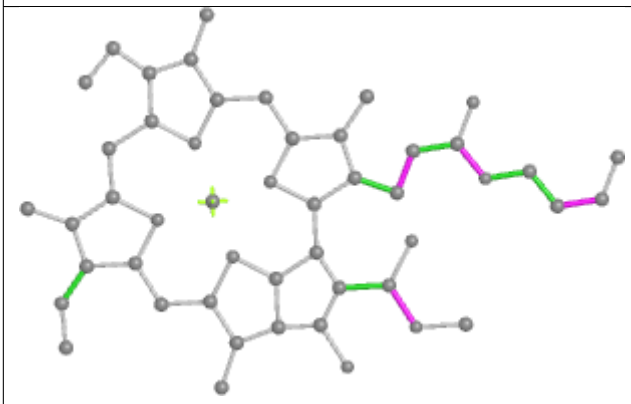
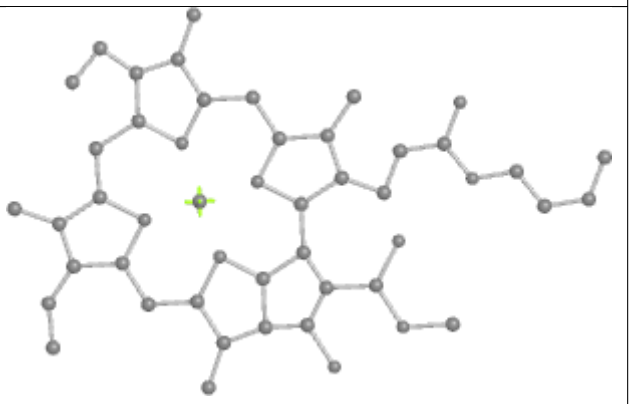


Bond angles

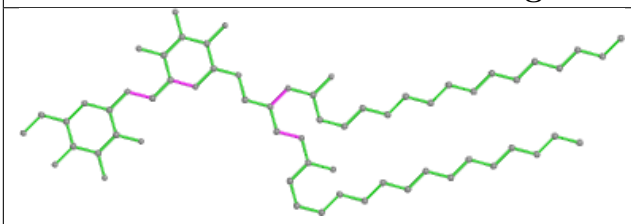


Torsions

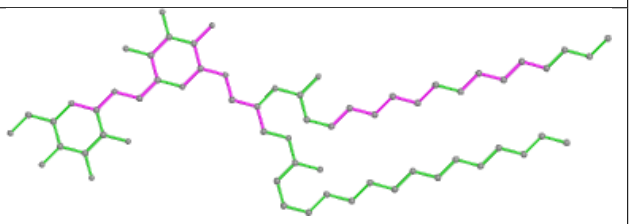


Rings

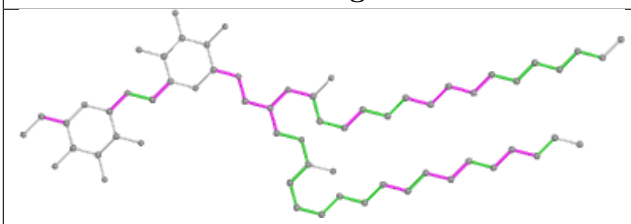
Ligand DGD c 519



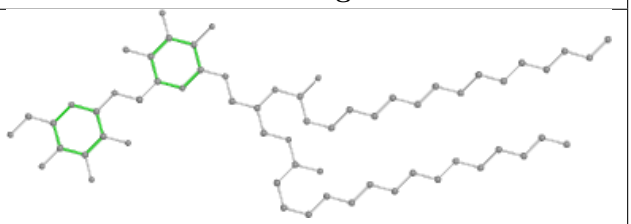
Bond lengths



Bond angles

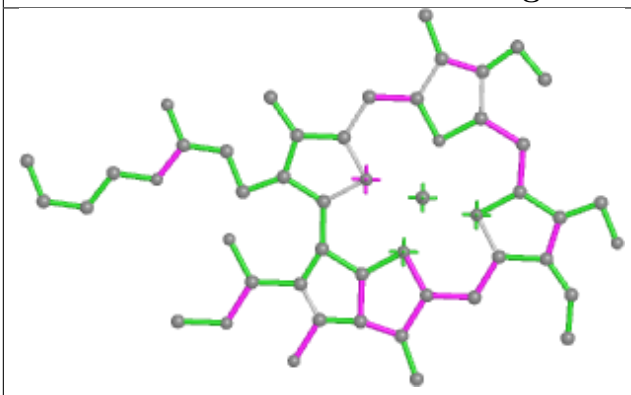


Torsions



Rings

Ligand CHL G 609



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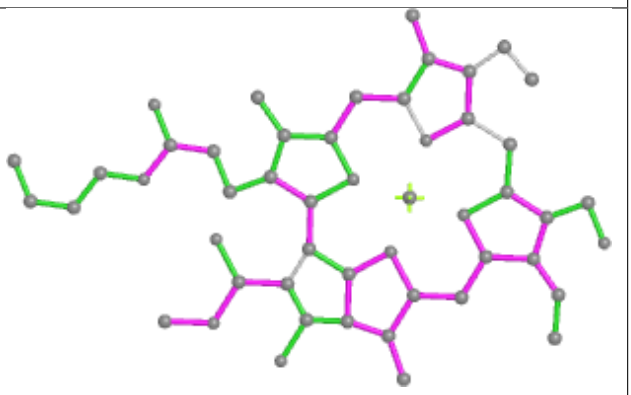
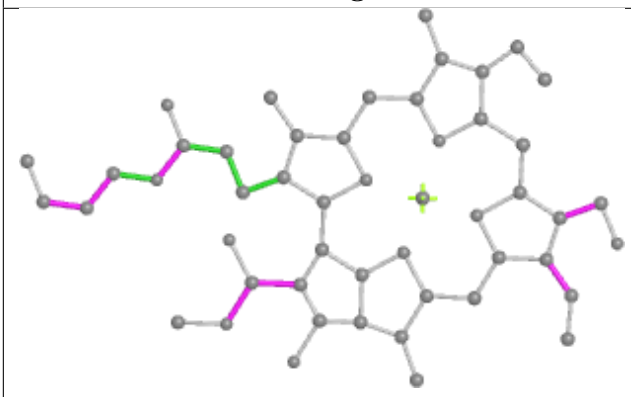
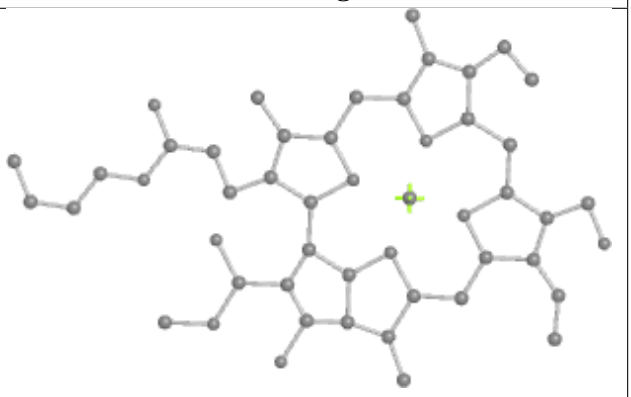


Bond angles

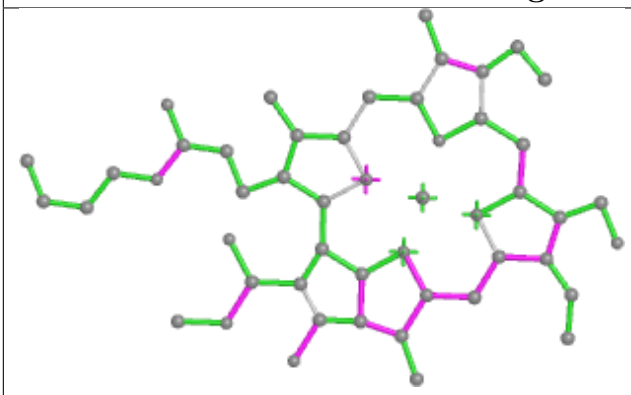


Torsions

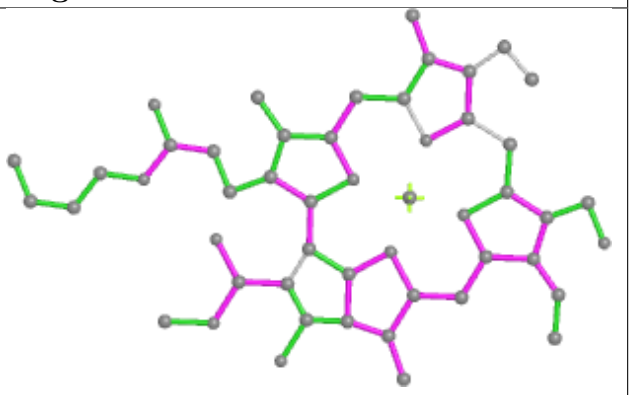


Rings

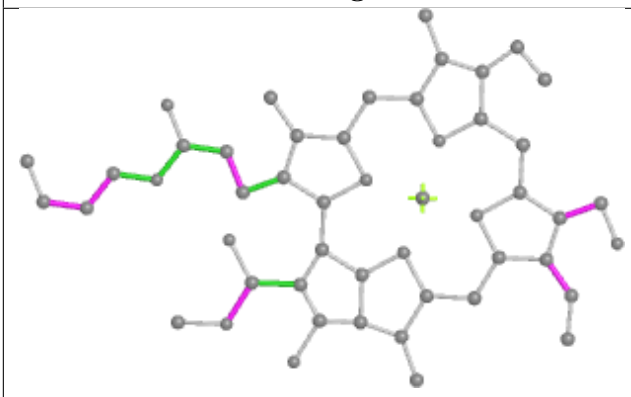
Ligand CHL g 607



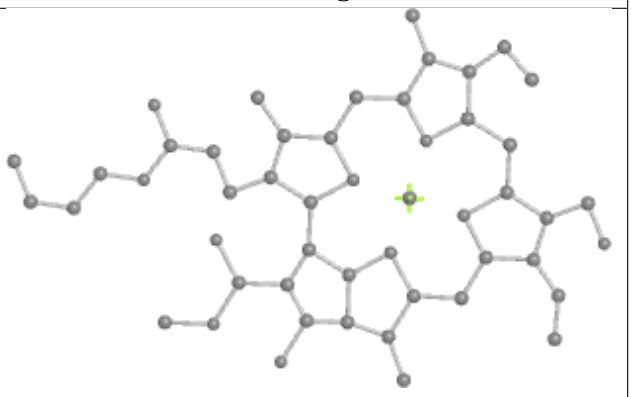
Bond lengths



Bond angles

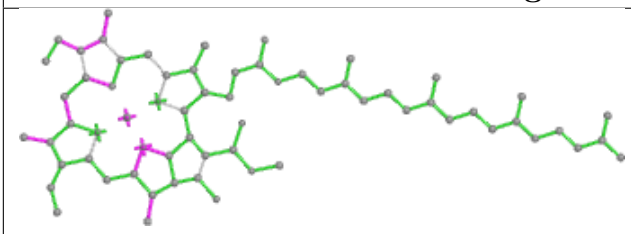


Torsions



Rings

Ligand CLA B 611



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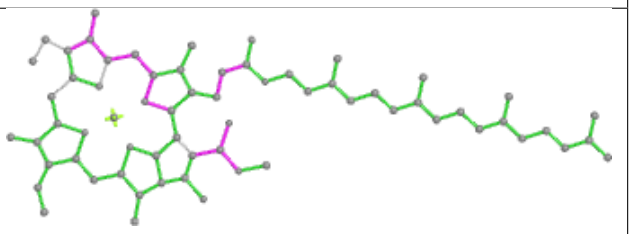
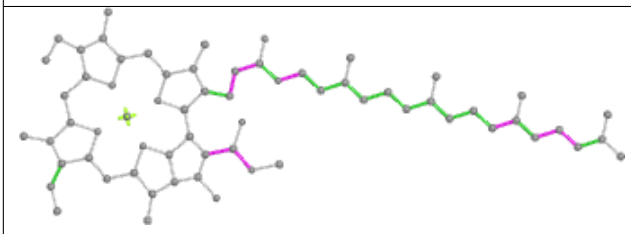
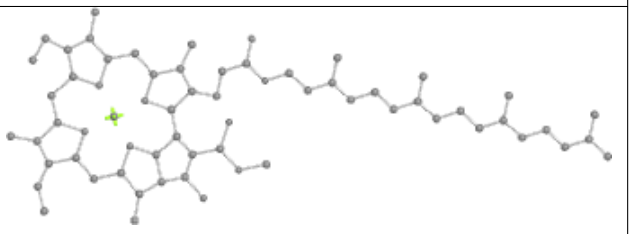


Bond angles

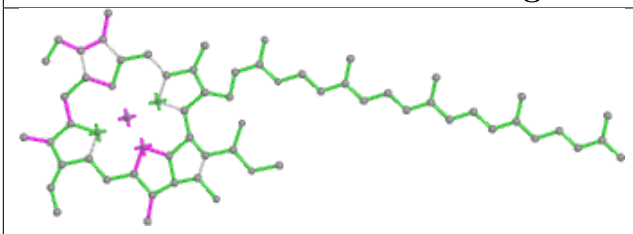


Torsions



Rings

Ligand CLA D 402



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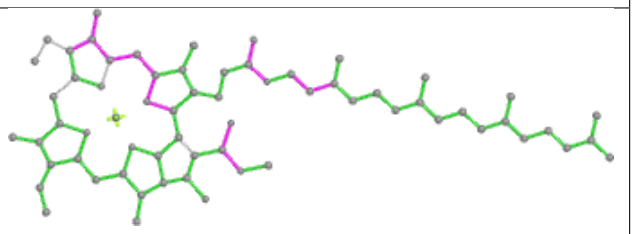
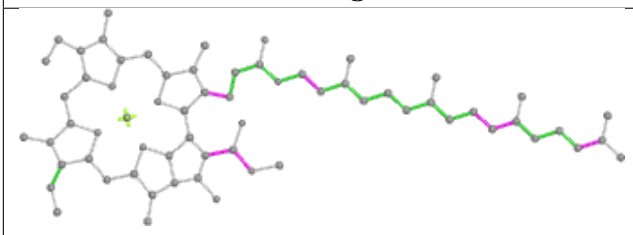
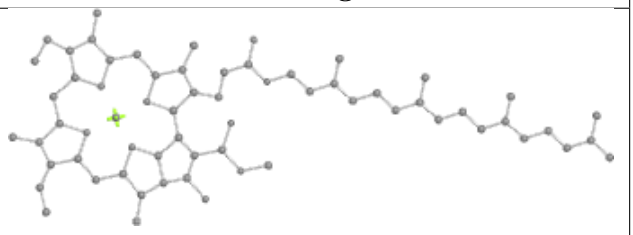


Bond angles

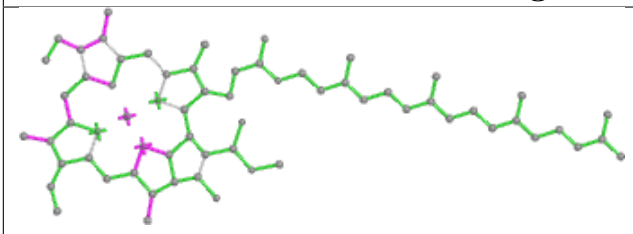


Torsions

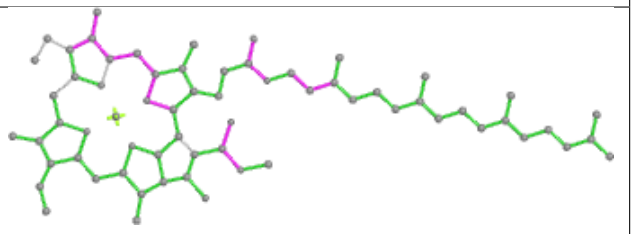


Rings

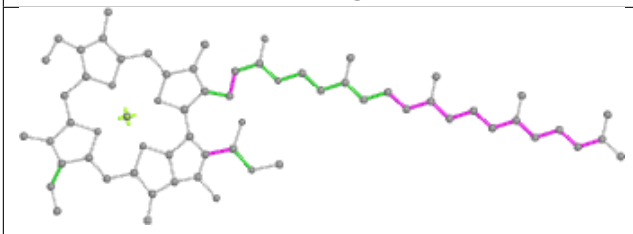
Ligand CLA c 507



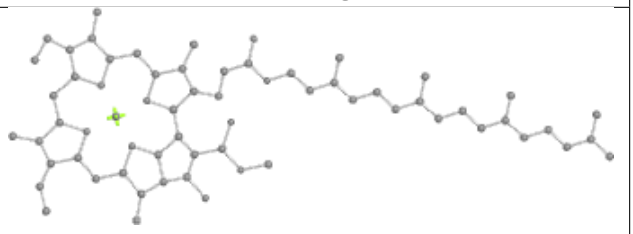
Bond lengths



Bond angles

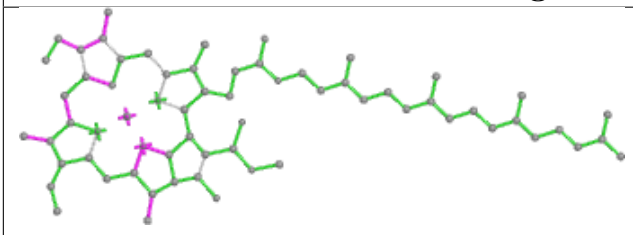


Torsions

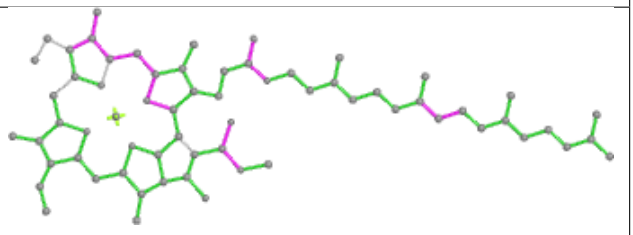


Rings

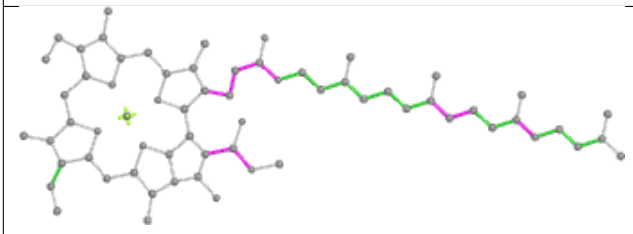
Ligand CLA c 501



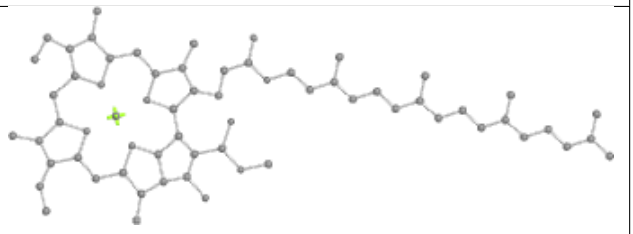
Bond lengths



Bond angles

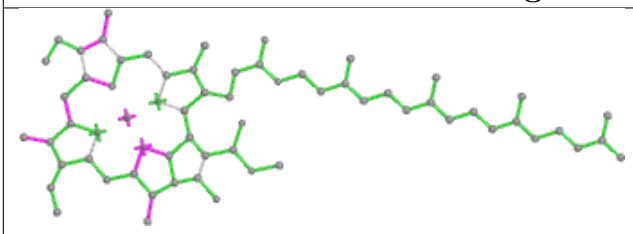


Torsions

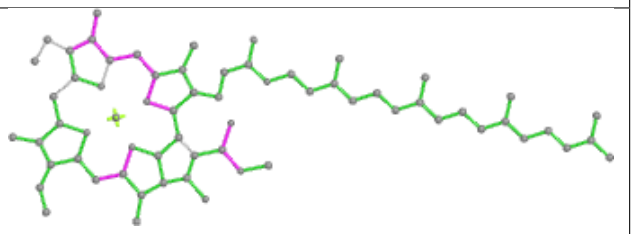


Rings

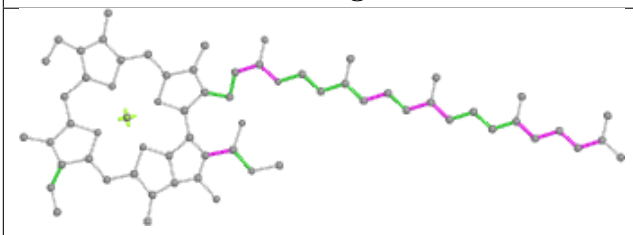
Ligand CLA B 617



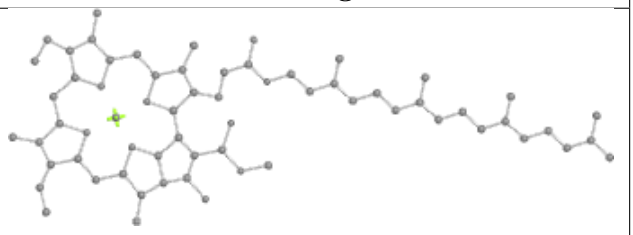
Bond lengths



Bond angles

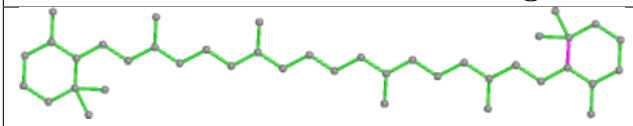


Torsions

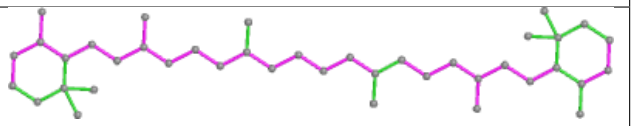


Rings

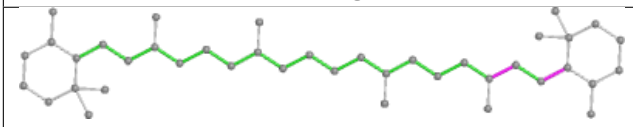
Ligand BCR C 514



Bond lengths



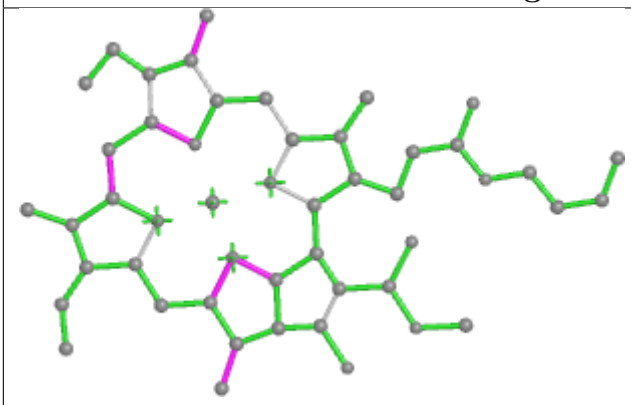
Bond angles



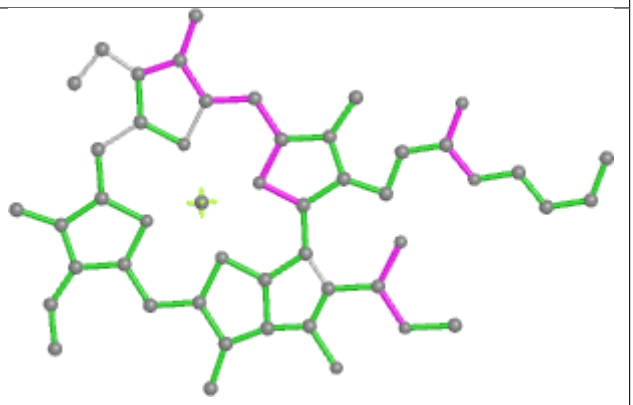
Torsions

Rings

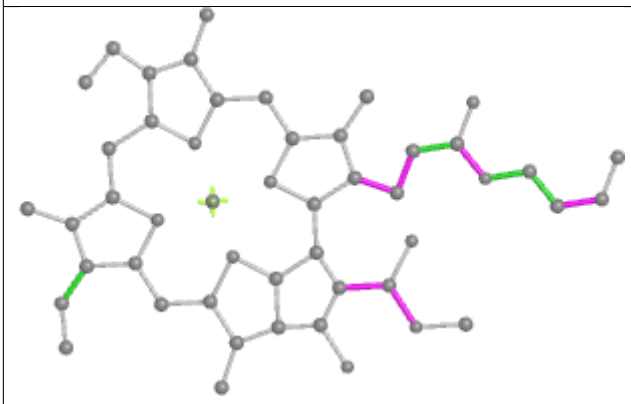
Ligand CLA R 611



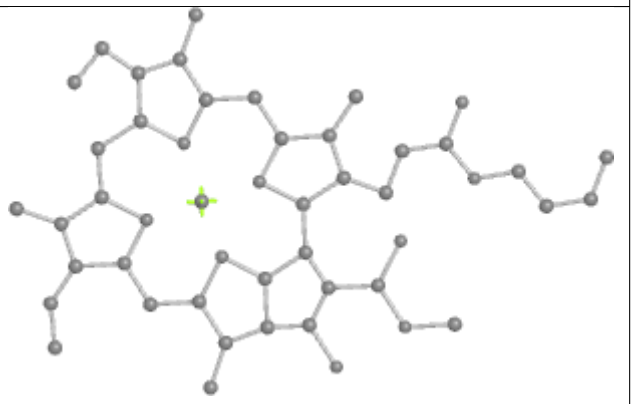
Bond lengths



Bond angles

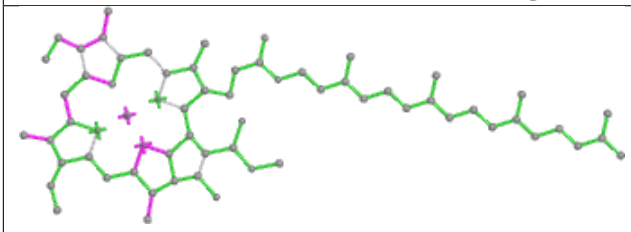


Torsions

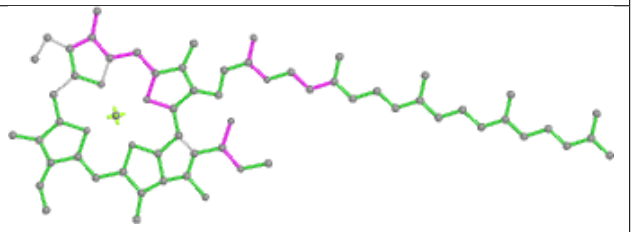


Rings

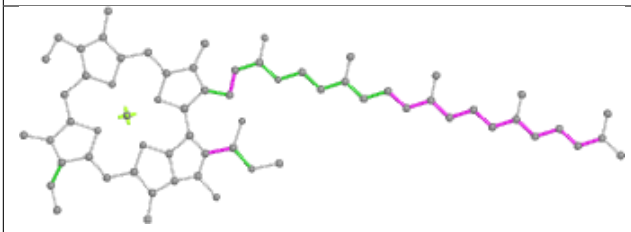
Ligand CLA C 507



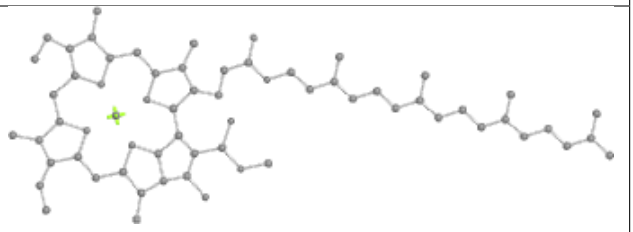
Bond lengths



Bond angles

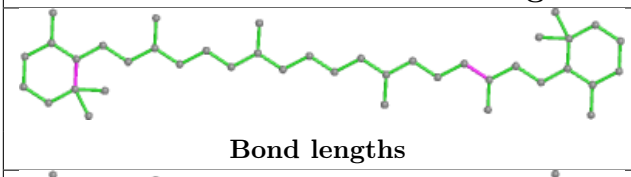


Torsions

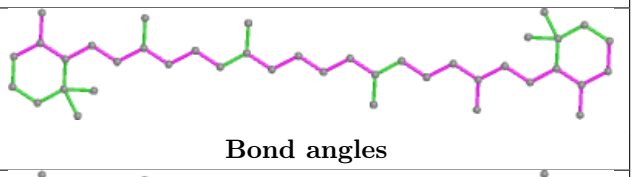


Rings

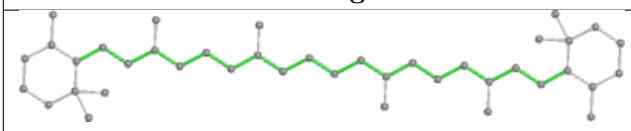
Ligand BCR a 411



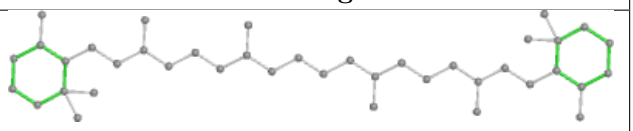
Bond lengths



Bond angles

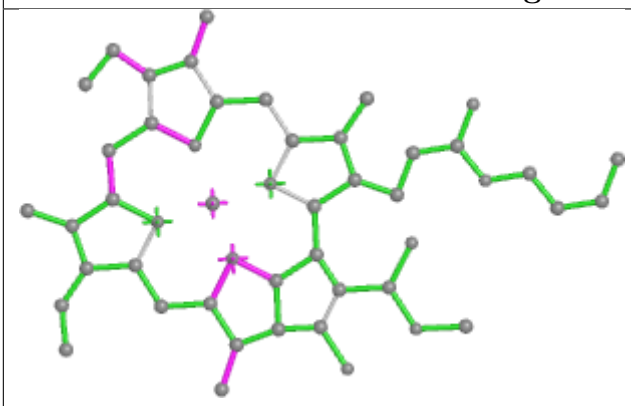


Torsions

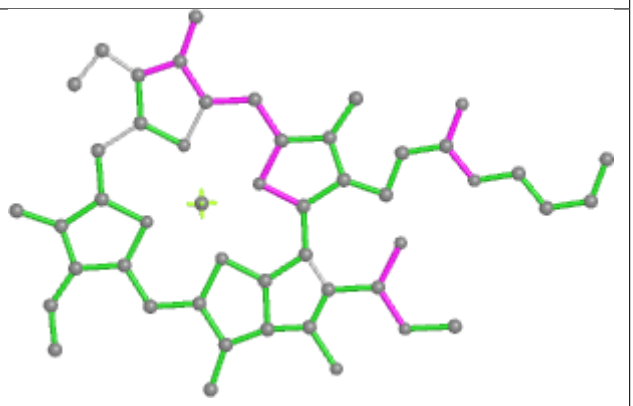


Rings

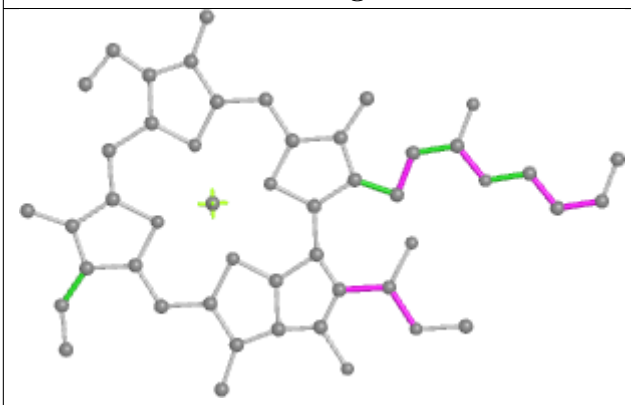
Ligand CLA Y 614



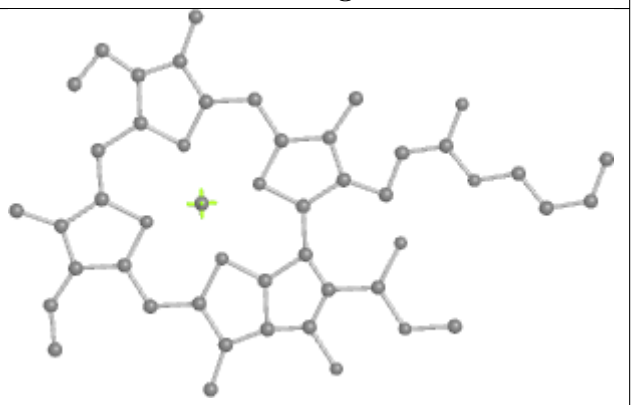
Bond lengths



Bond angles

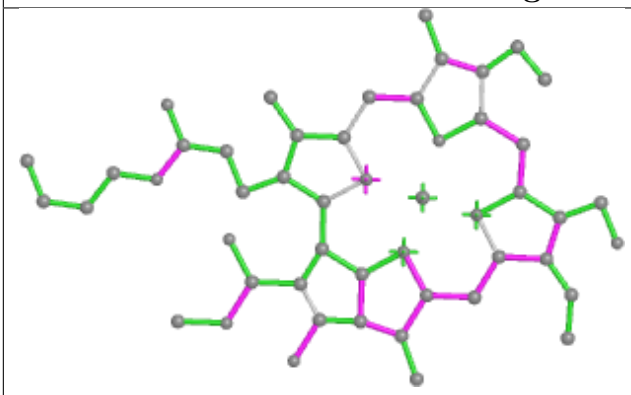


Torsions

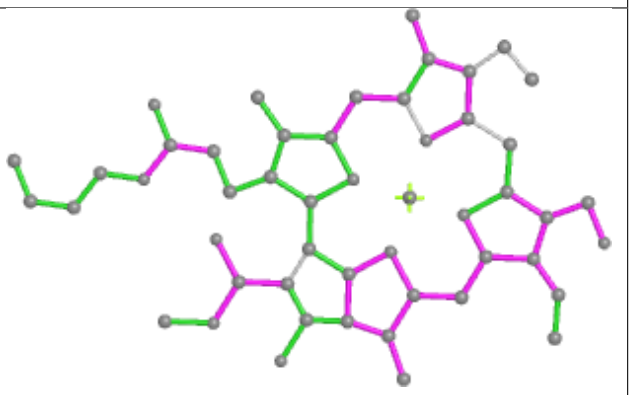


Rings

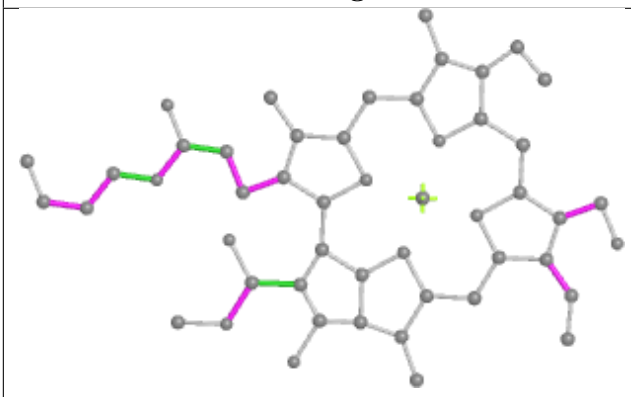
Ligand CHL R 608



Bond lengths



Bond angles



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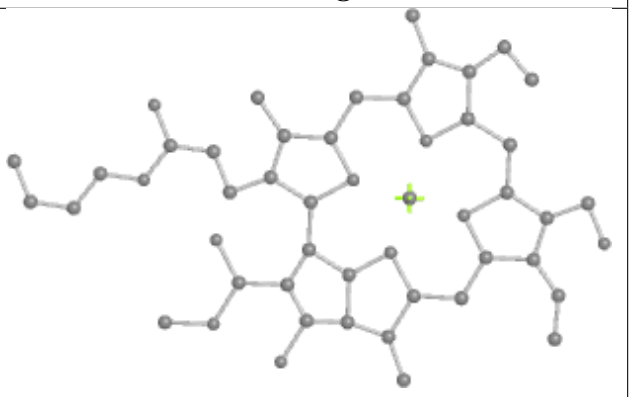
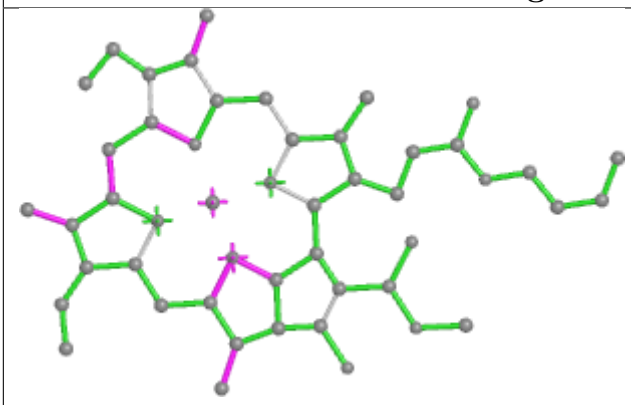


Rings

Ligand CLA S 604



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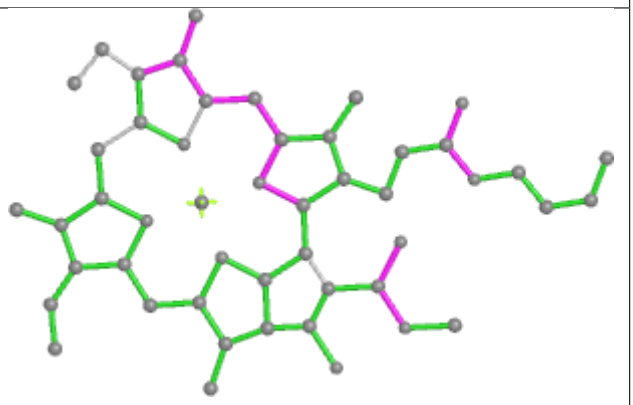
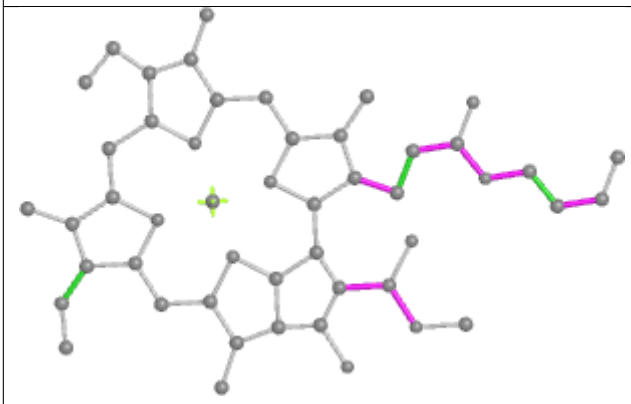


Bond angles



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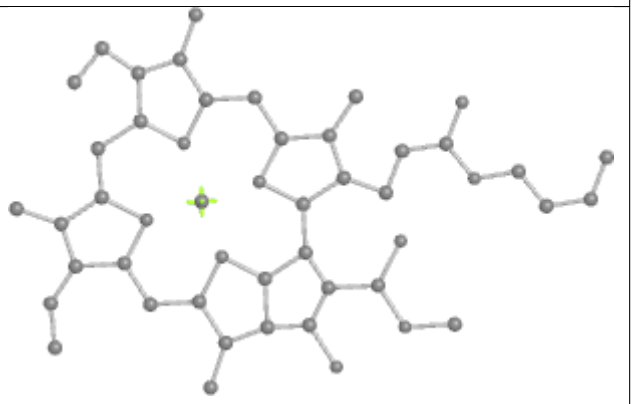
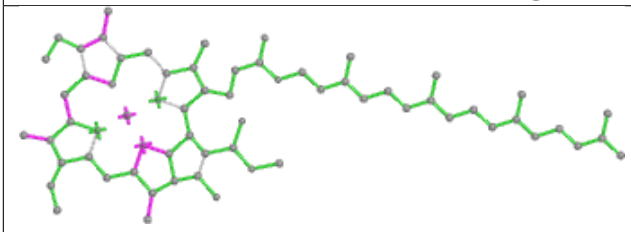
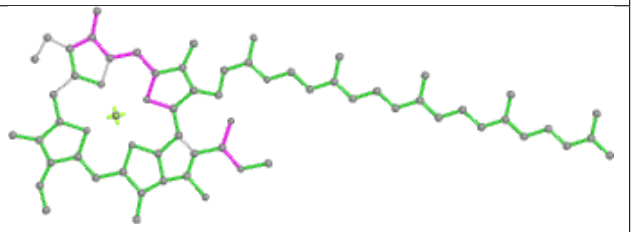


Rings

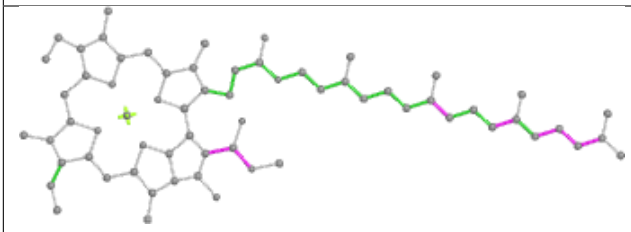
Ligand CLA b 616



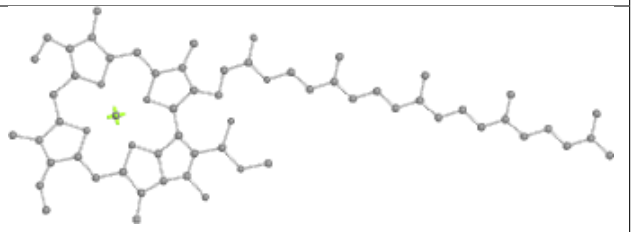
Bond lengths



Bond angles

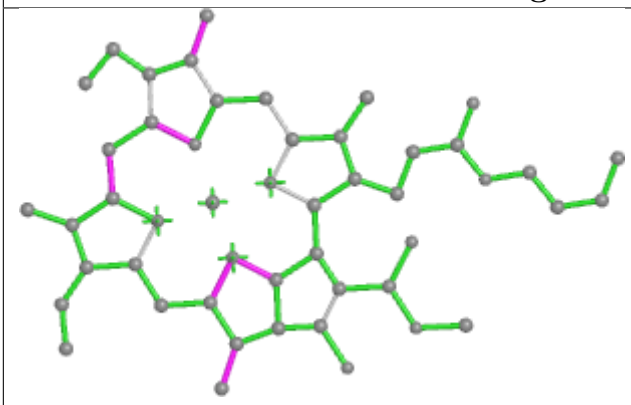


Torsions



Rings

Ligand CLA r 611



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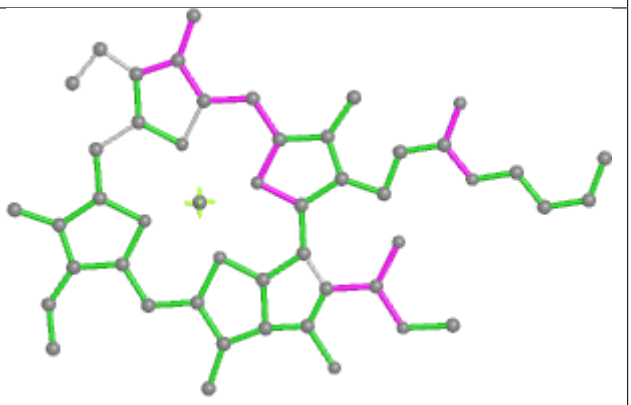
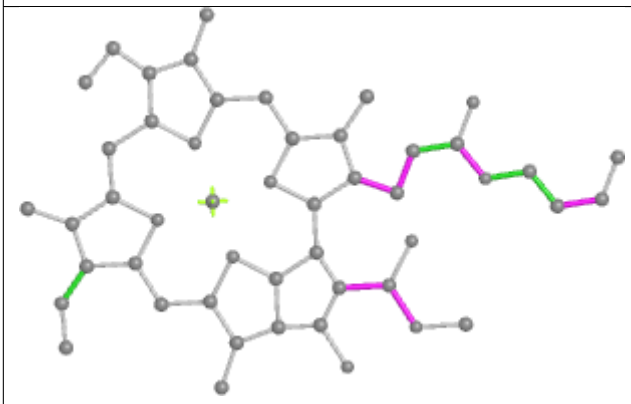
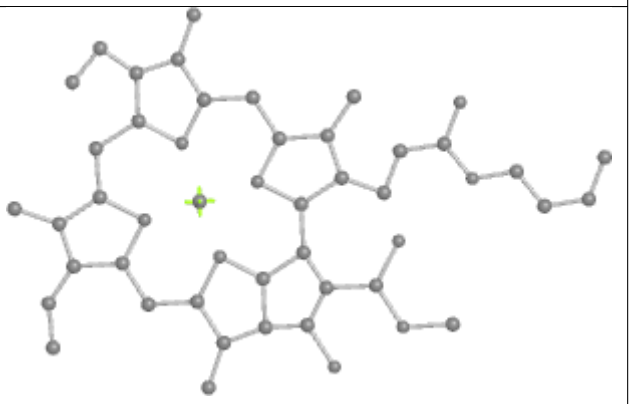


Bond angles

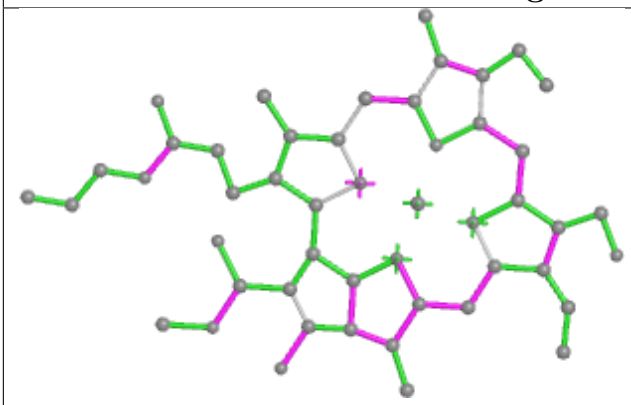


Torsions

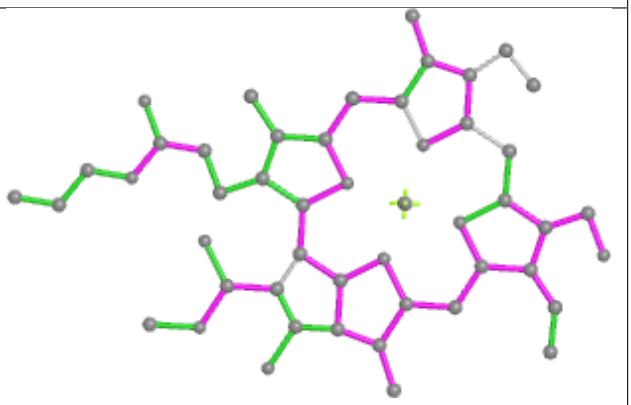


Rings

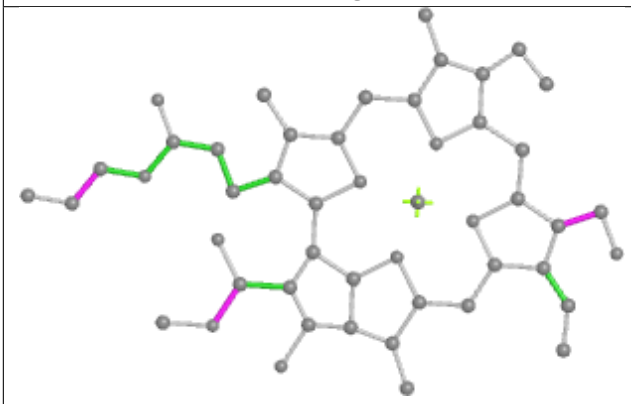
Ligand CHL S 608



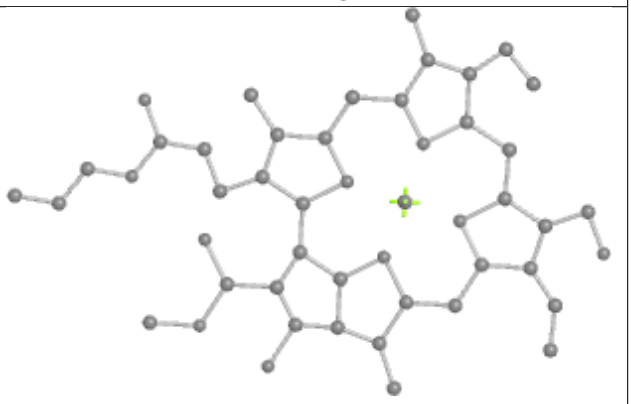
Bond lengths



Bond angles

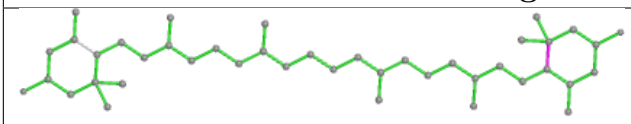


Torsions

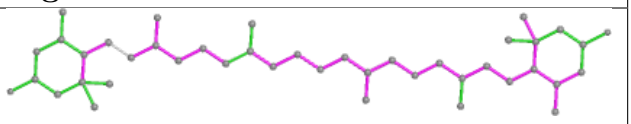


Rings

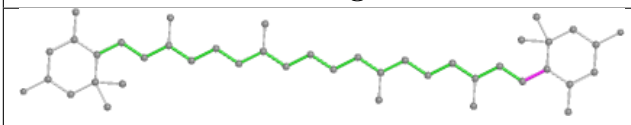
Ligand LUT g 1620



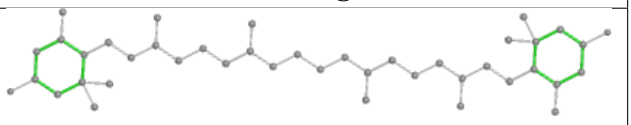
Bond lengths



Bond angles

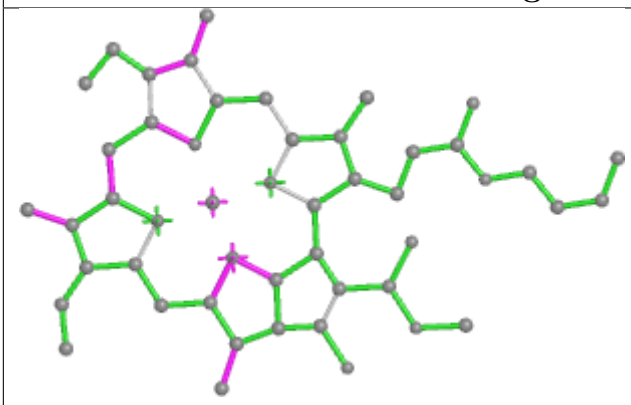


Torsions



Rings

Ligand CLA N 603



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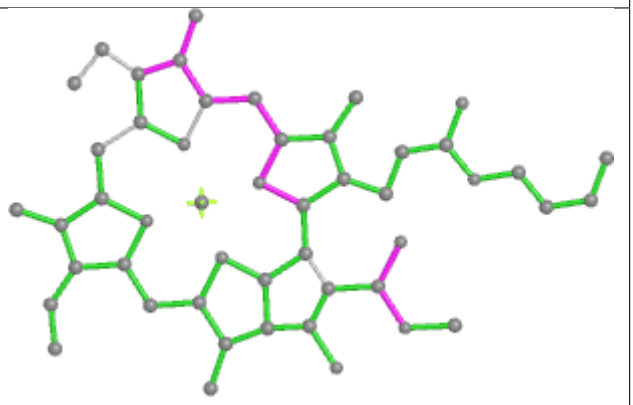
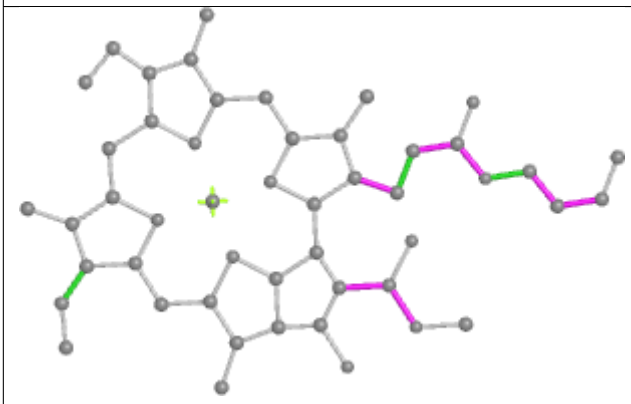
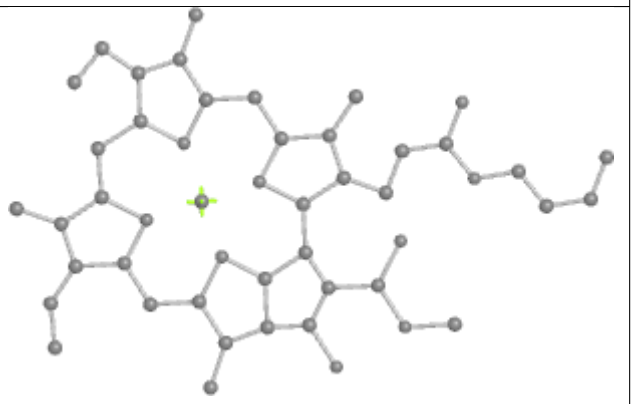


Bond angles

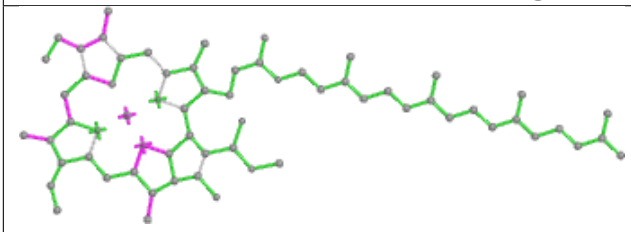


Torsions



Rings

Ligand CLA c 504



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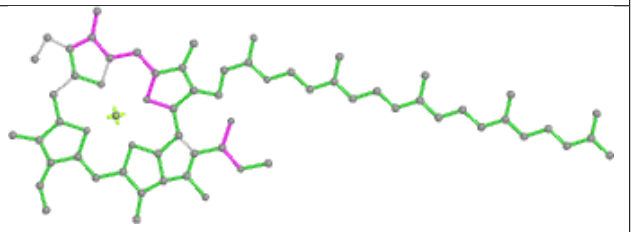
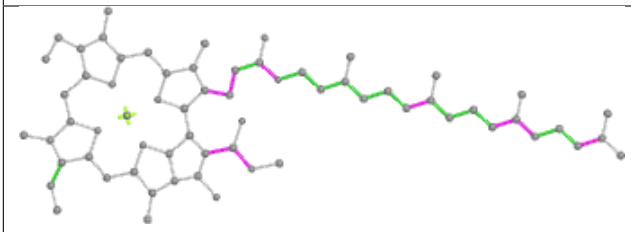
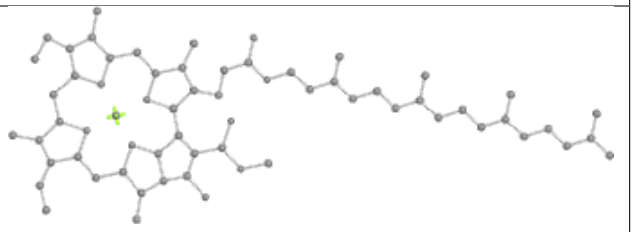


Bond angles

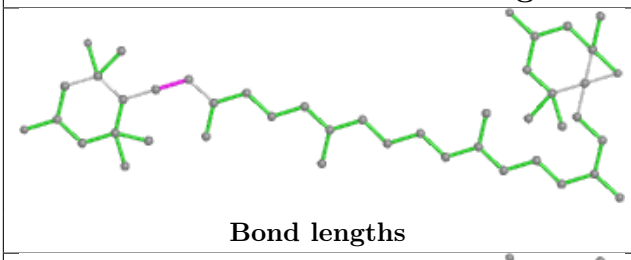


Torsions

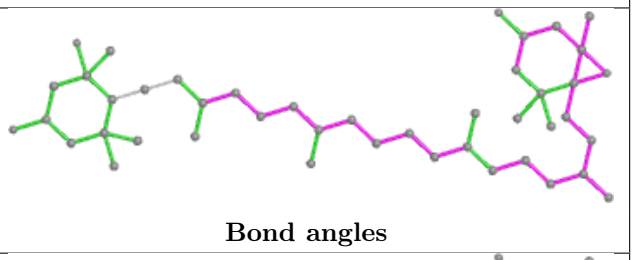


Rings

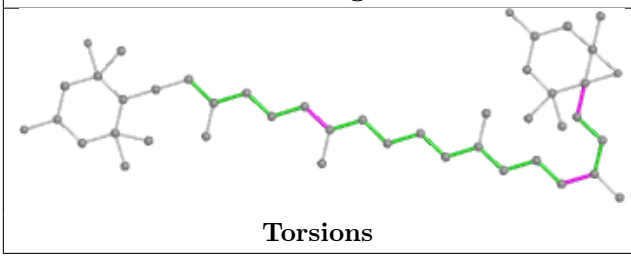
Ligand NEX n 1623



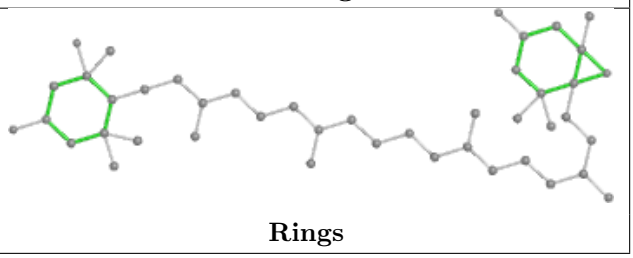
Bond lengths



Bond angles

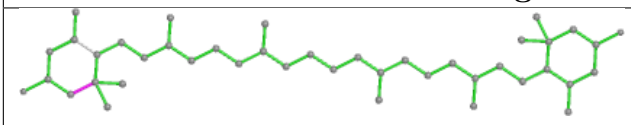


Torsions

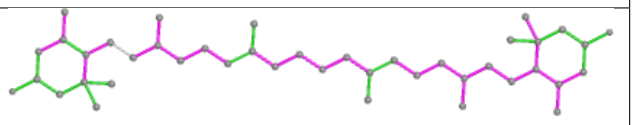


Rings

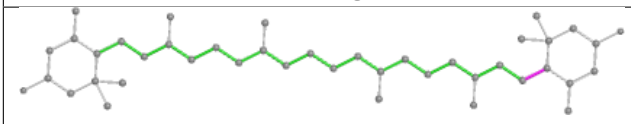
Ligand LUT N 1620



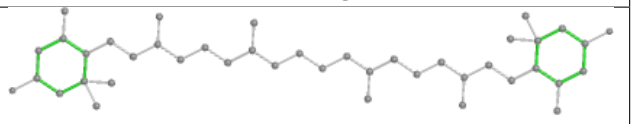
Bond lengths



Bond angles

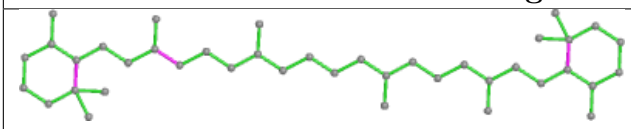


Torsions

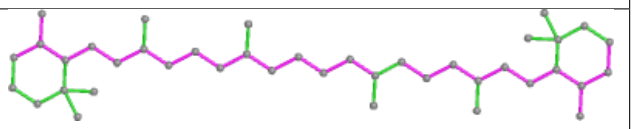


Rings

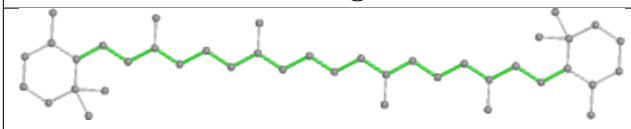
Ligand BCR b 619



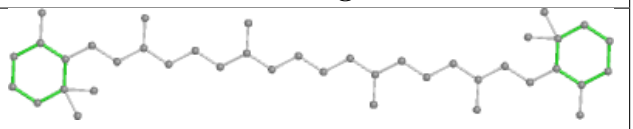
Bond lengths



Bond angles

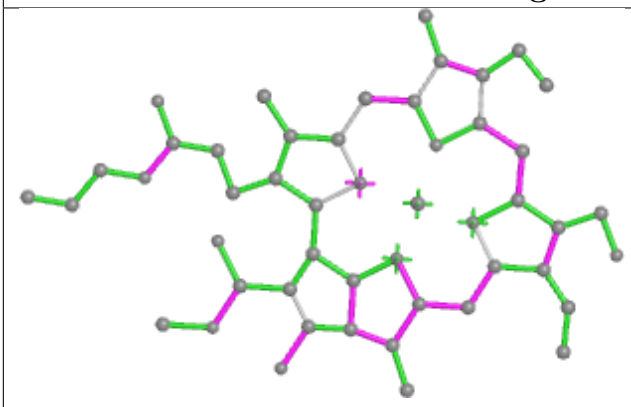


Torsions

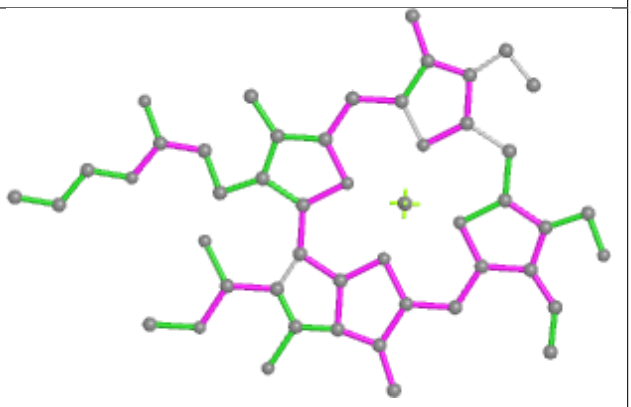


Rings

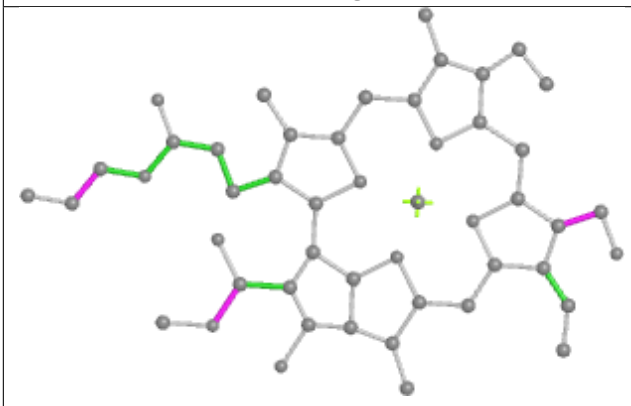
Ligand CHL s 608



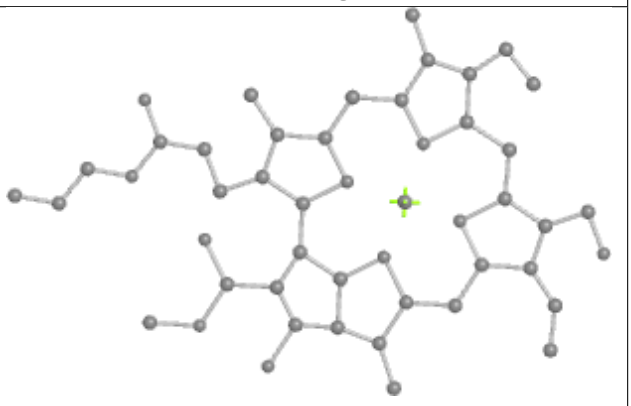
Bond lengths



Bond angles

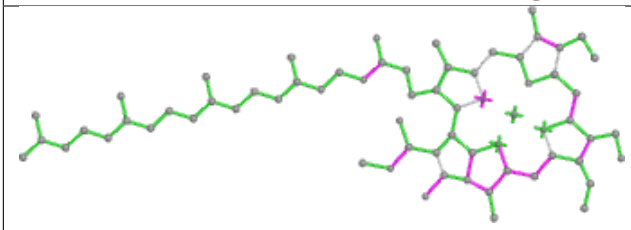


Torsions

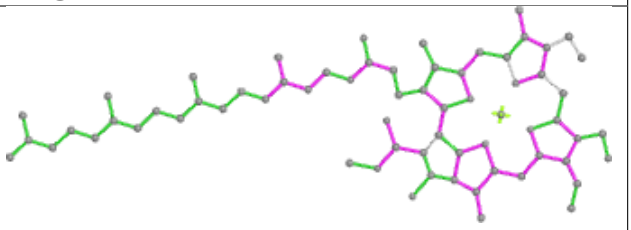


Rings

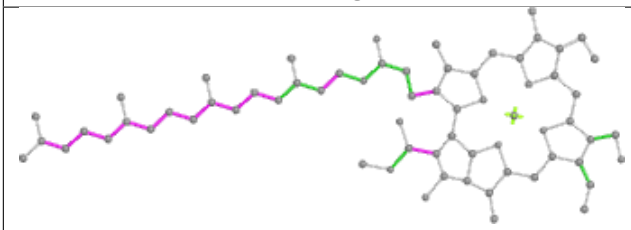
Ligand CHL g 601



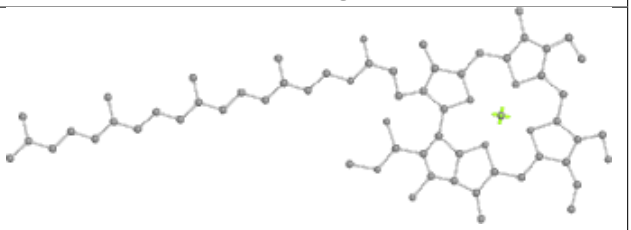
Bond lengths



Bond angles

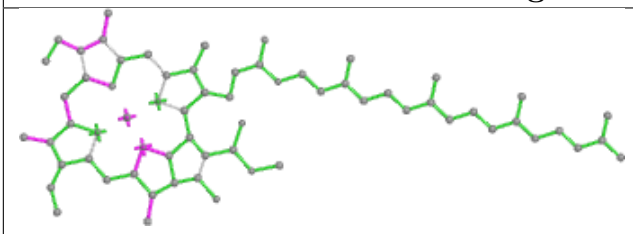


Torsions



Rings

Ligand CLA d 402



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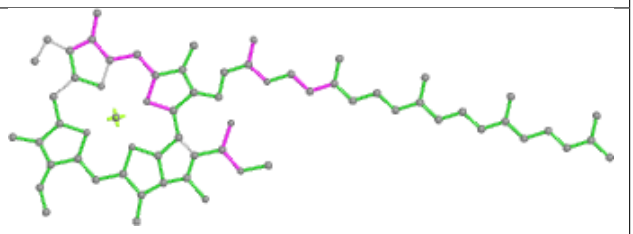
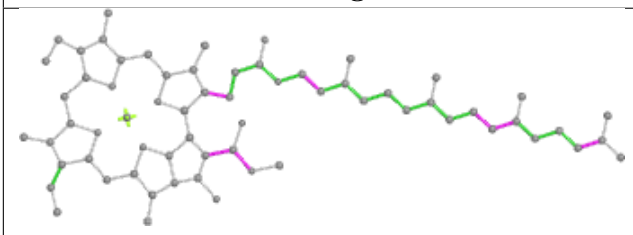
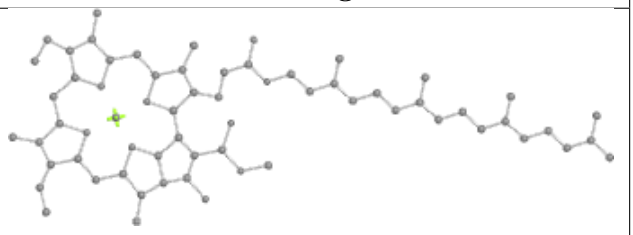


Bond angles

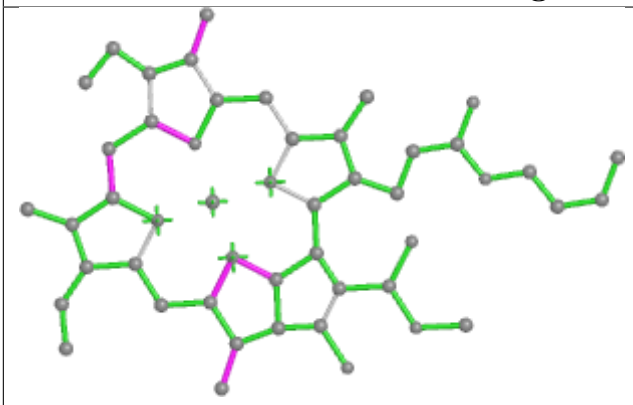


Torsions



Rings

Ligand CLA r 601



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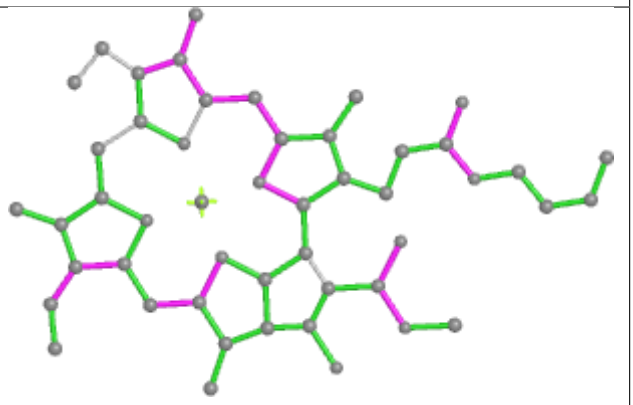
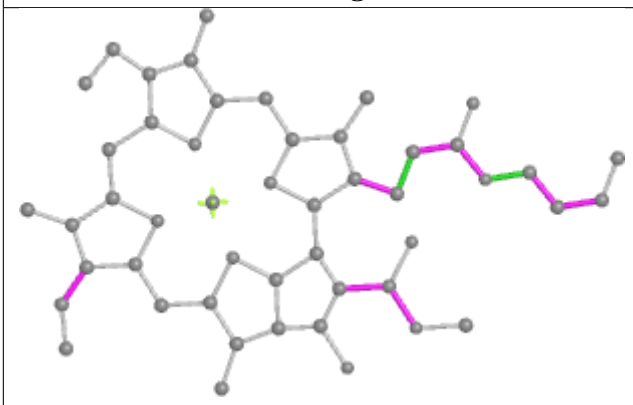
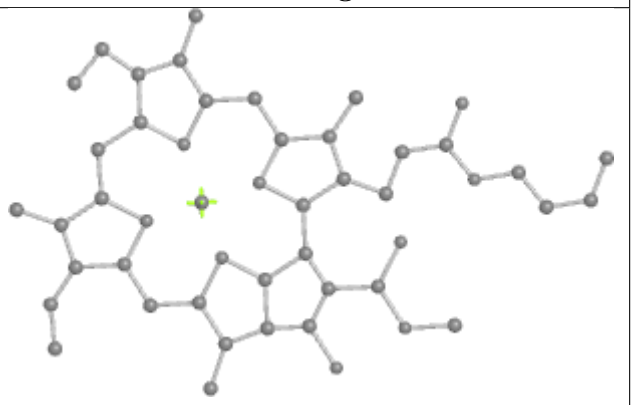


Bond angles

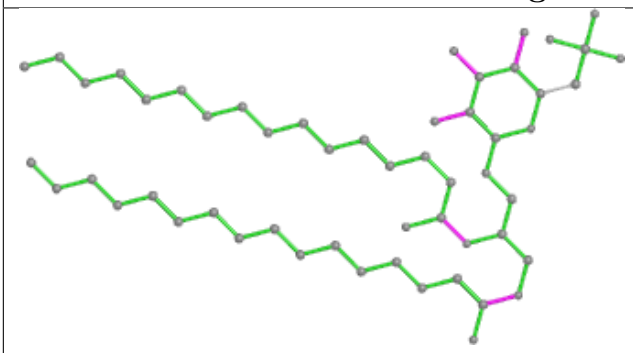


Torsions



Rings

Ligand SQD a 412



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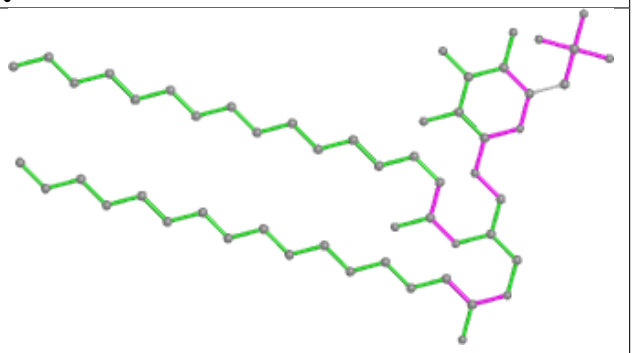
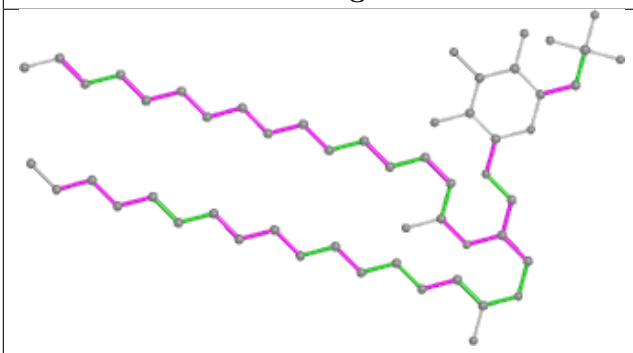
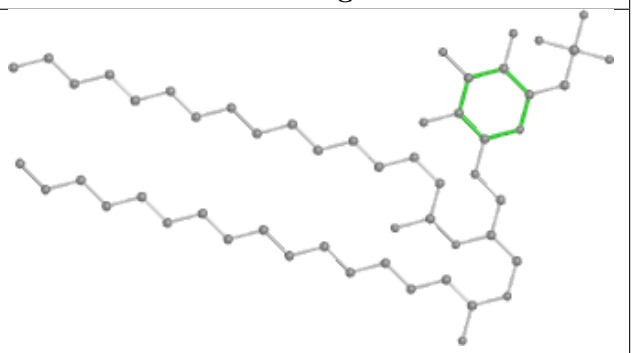


Bond angles

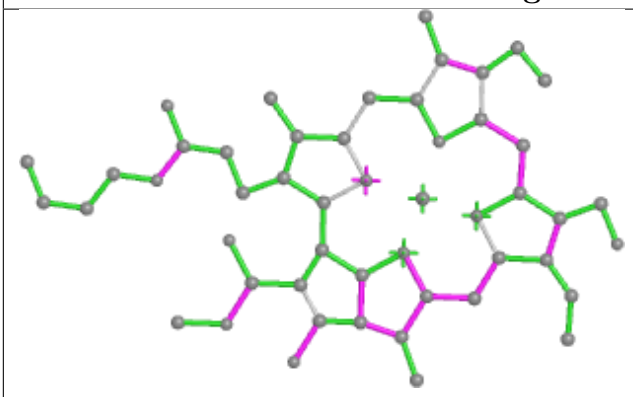


Torsions



Rings

Ligand CHL Y 606



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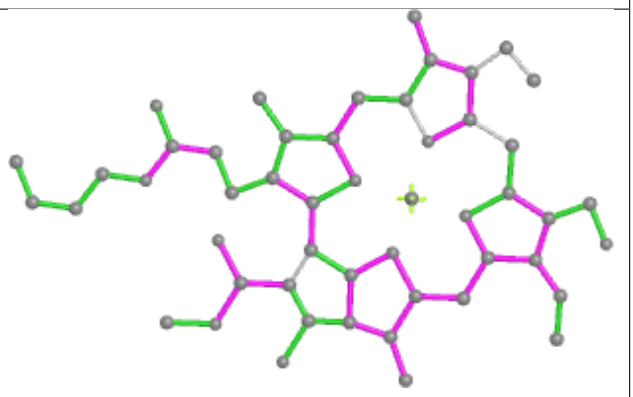
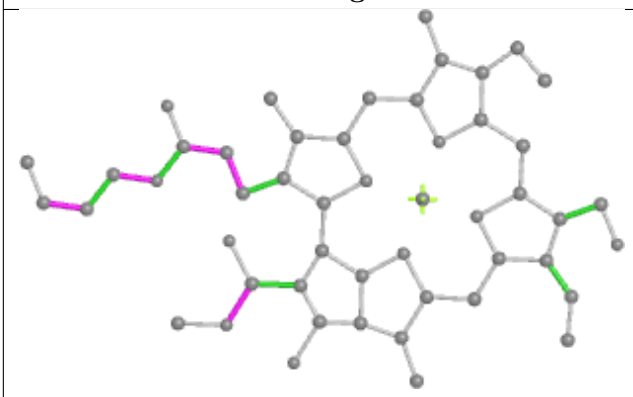
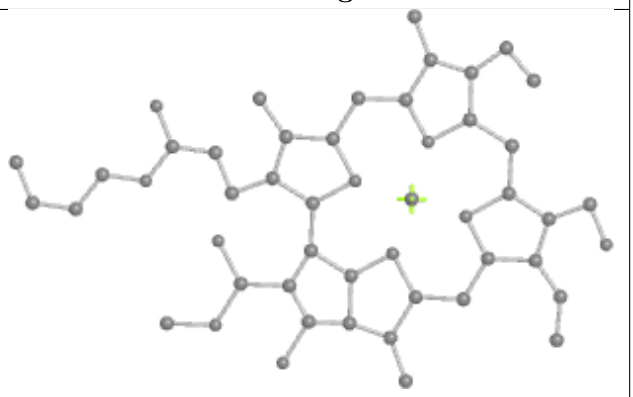


Bond angles

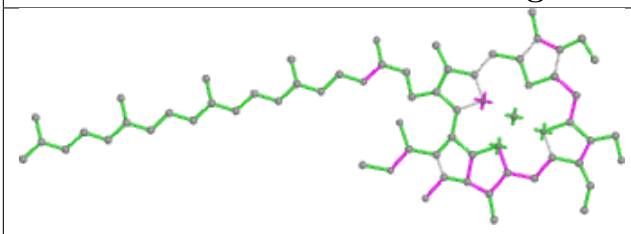


Torsions



Rings

Ligand CHL n 607



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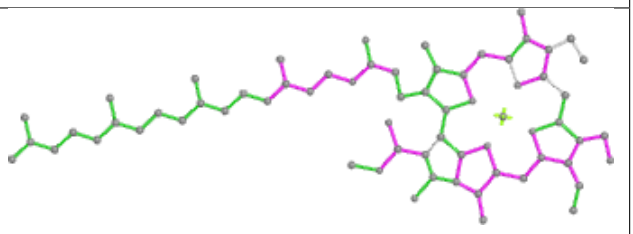
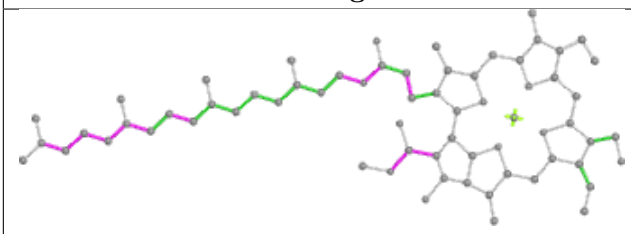
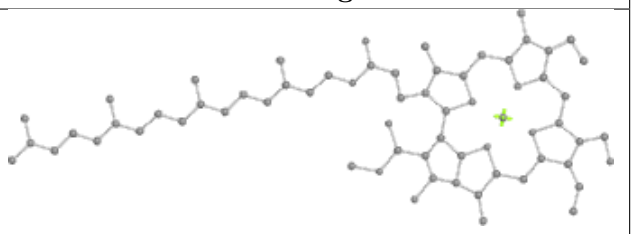


Bond angles

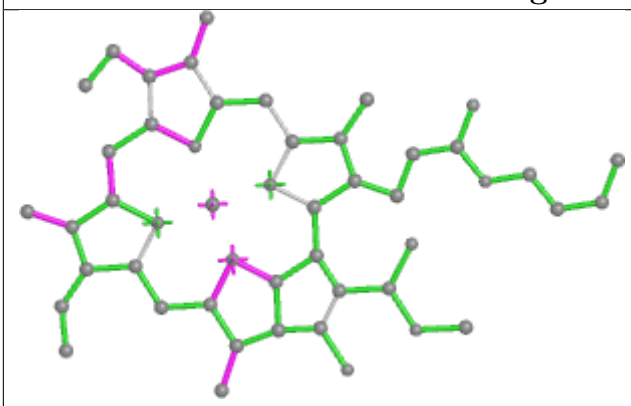


Torsions

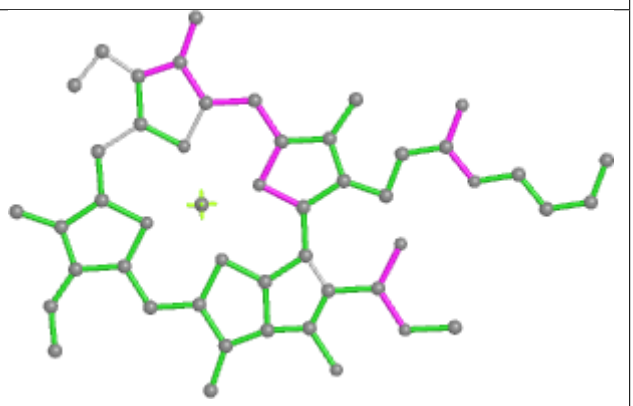


Rings

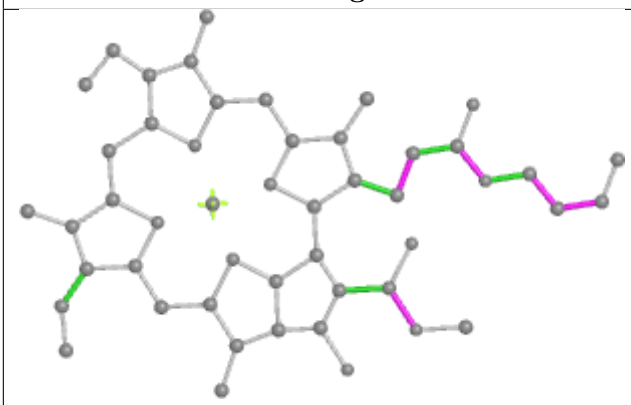
Ligand CLA s 614



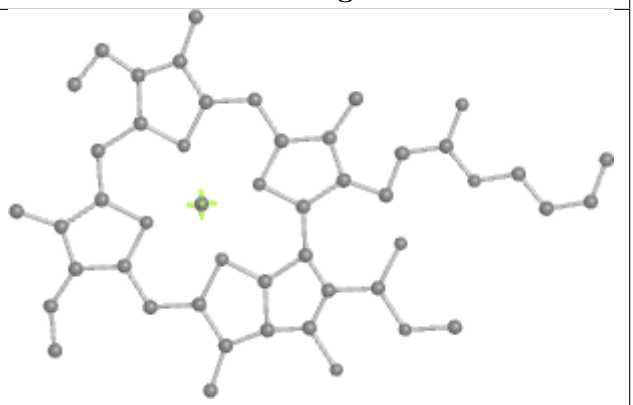
Bond lengths



Bond angles

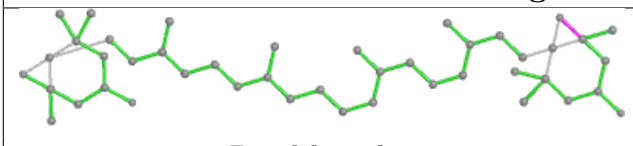


Torsions

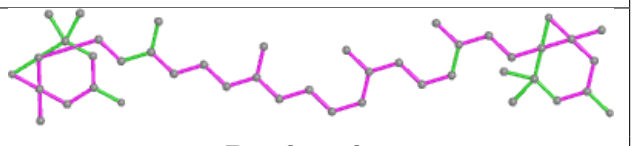


Rings

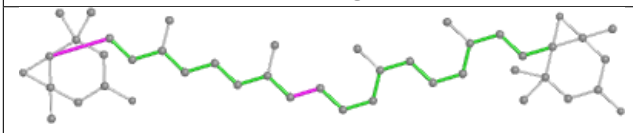
Ligand XAT r 622



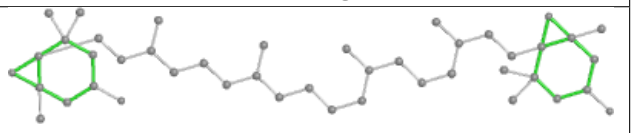
Bond lengths



Bond angles

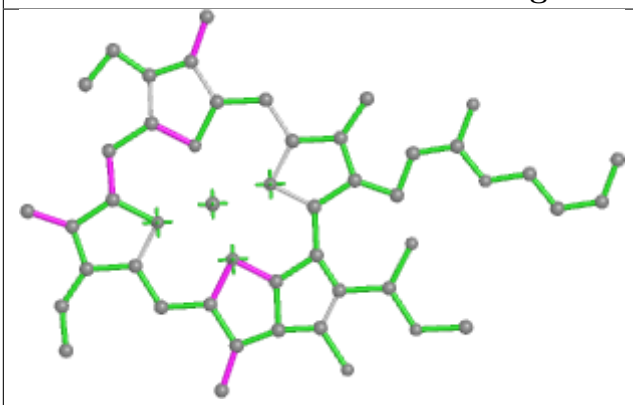


Torsions



Rings

Ligand CLA r 616



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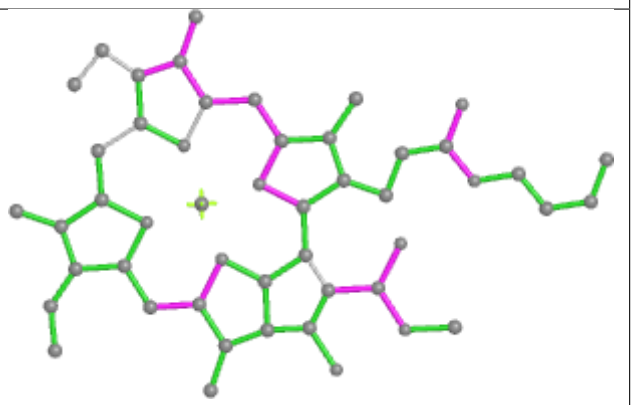
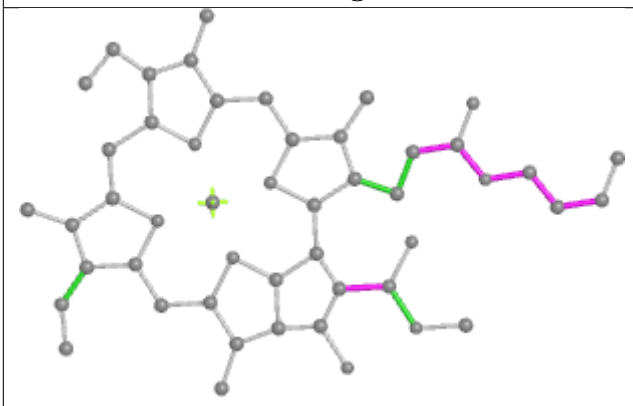
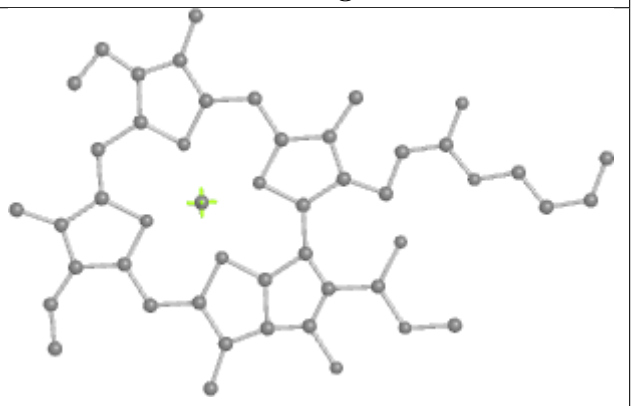


Bond angles

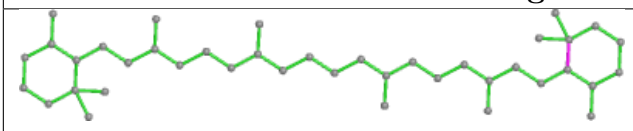


Torsions

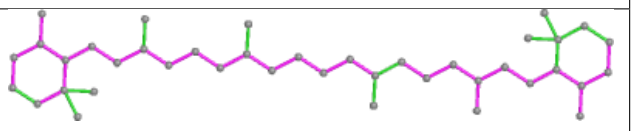


Rings

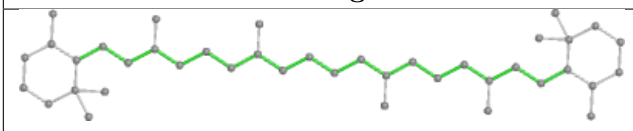
Ligand BCR c 515



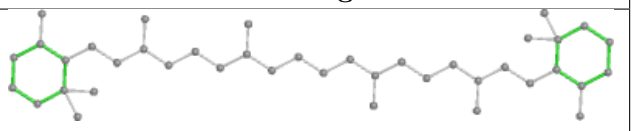
Bond lengths



Bond angles

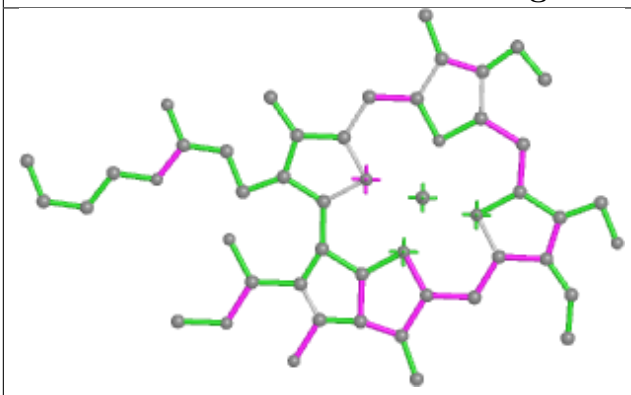


Torsions



Rings

Ligand CHL s 606



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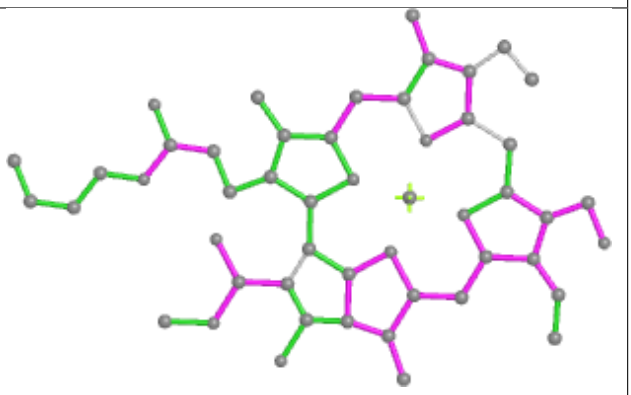
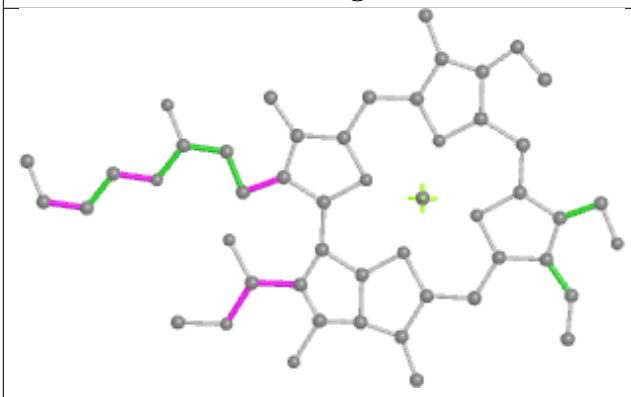
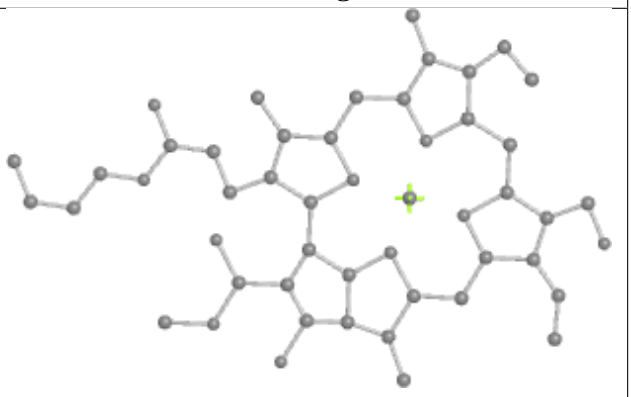


Bond angles

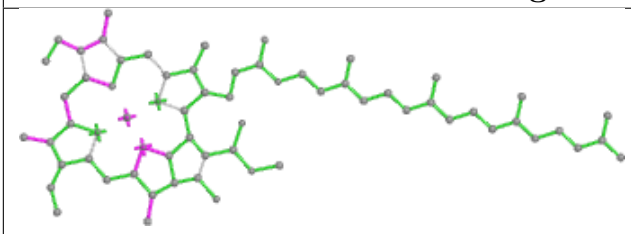


Torsions

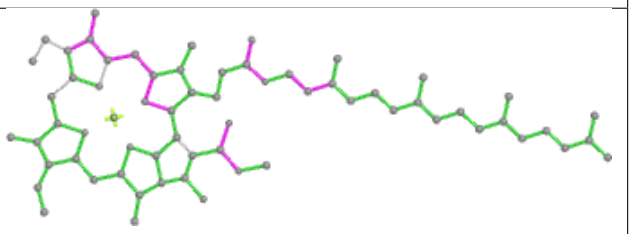


Rings

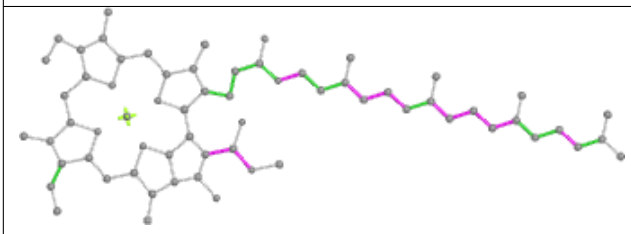
Ligand CLA c 506



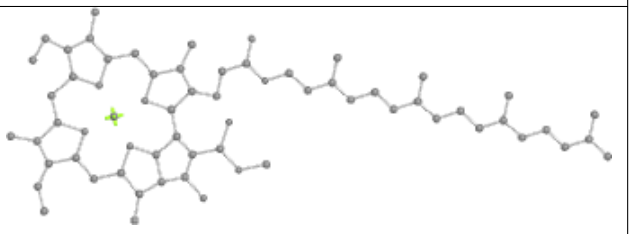
Bond lengths



Bond angles

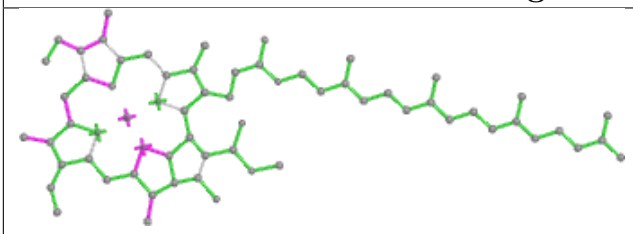


Torsions

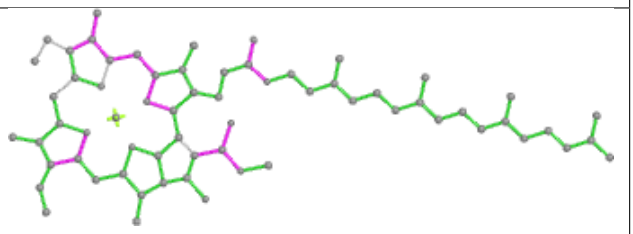


Rings

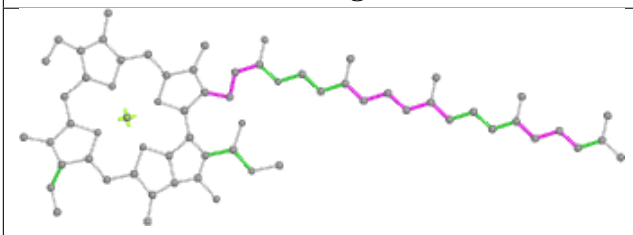
Ligand CLA b 609



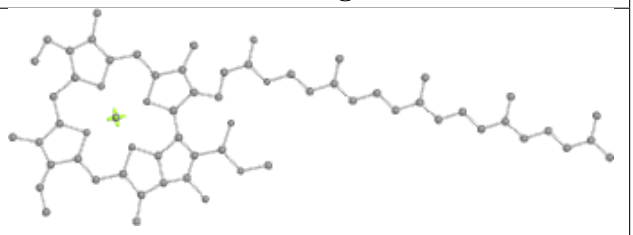
Bond lengths



Bond angles

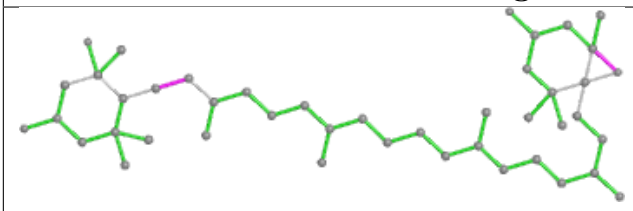


Torsions

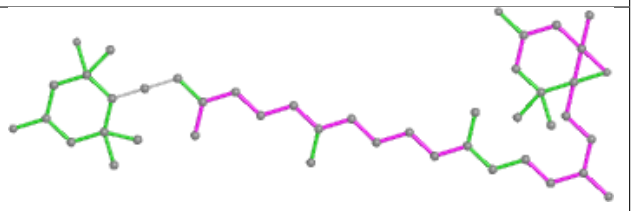


Rings

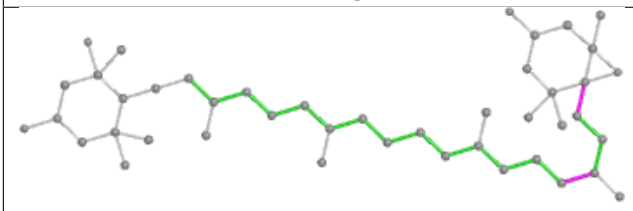
Ligand NEX Y 1623



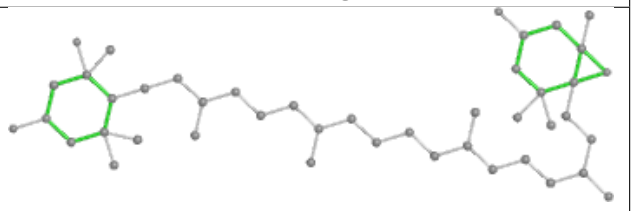
Bond lengths



Bond angles

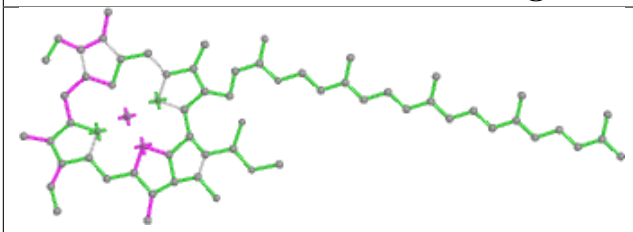


Torsions



Rings

Ligand CLA b 605



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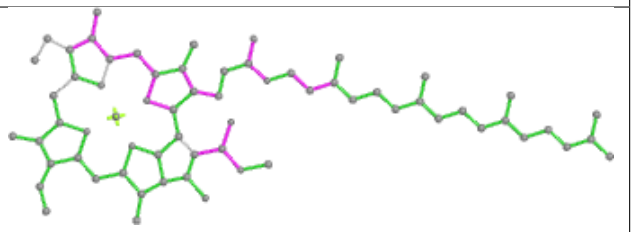
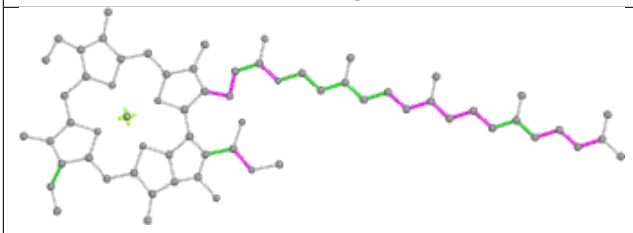


Bond angles



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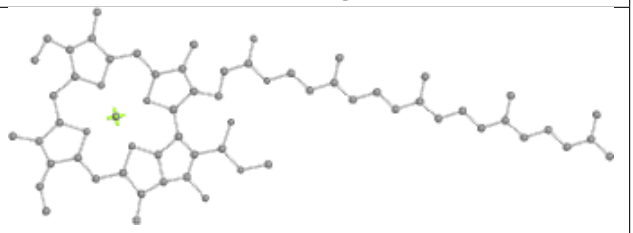
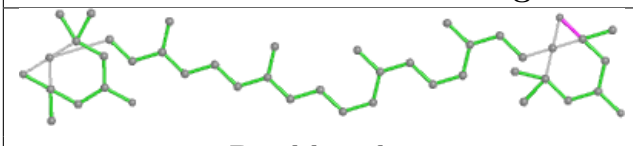
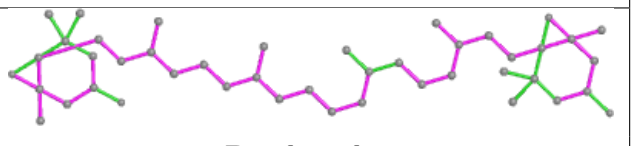


Rings

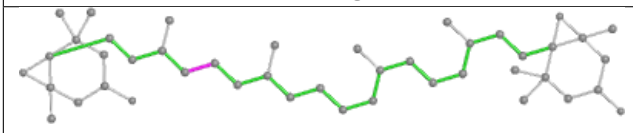
Ligand XAT N 1622



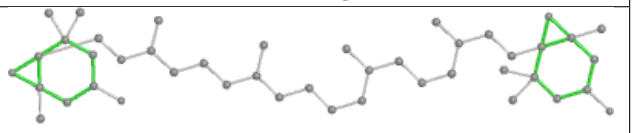
Bond lengths



Bond angles

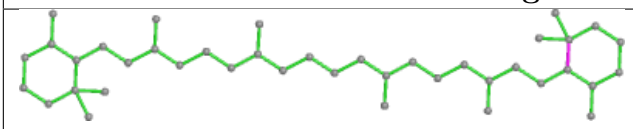


Torsions

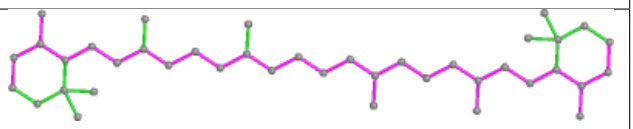


Rings

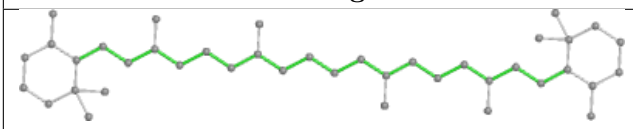
Ligand BCR C 515



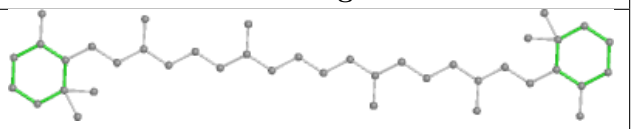
Bond lengths



Bond angles

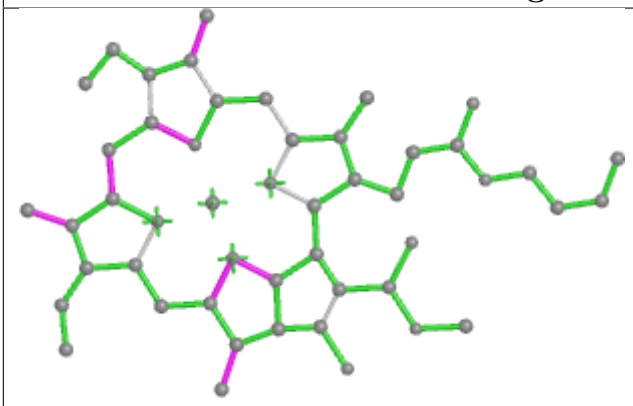


Torsions

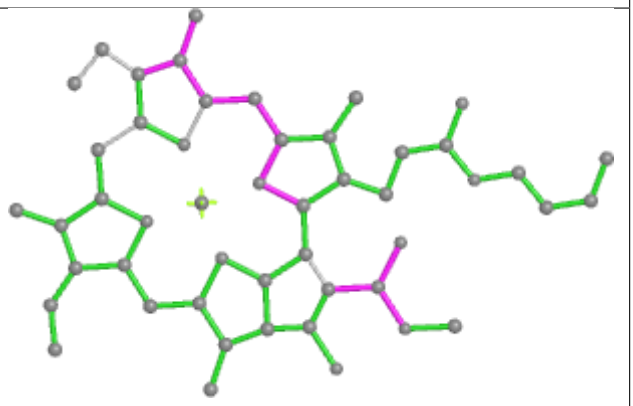


Rings

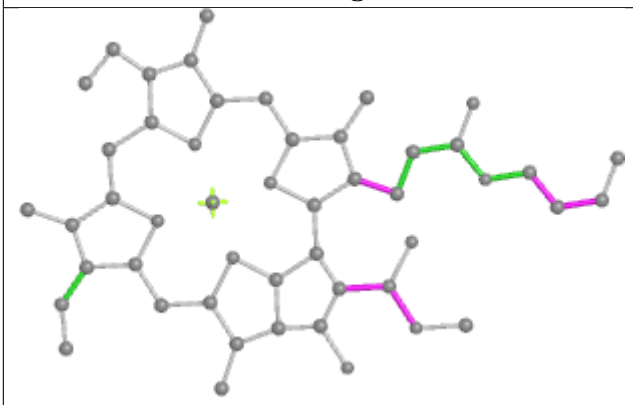
Ligand CLA S 602



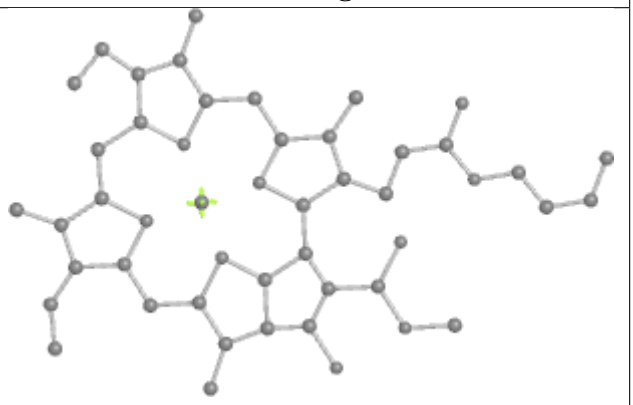
Bond lengths



Bond angles

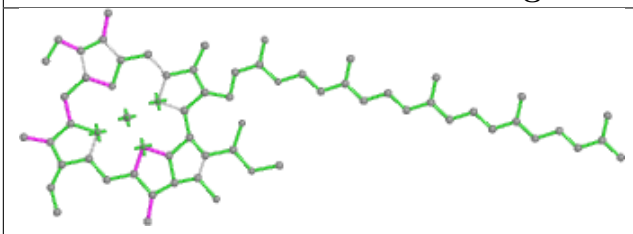


Torsions



Rings

Ligand CLA R 602



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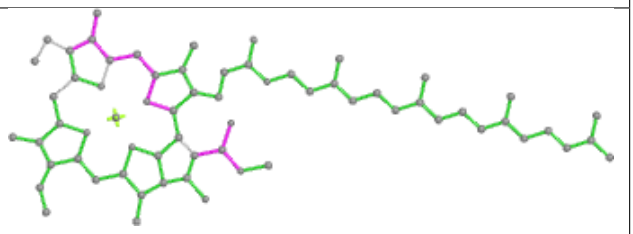
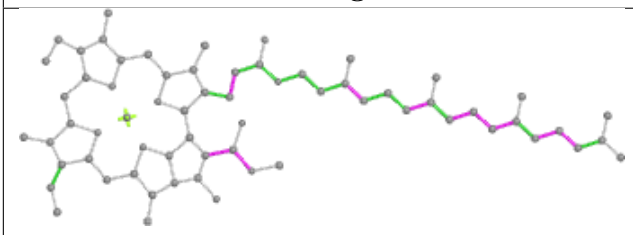


Bond angles



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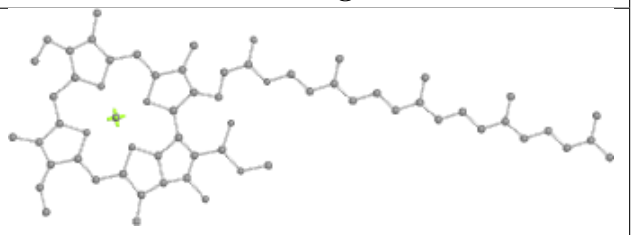
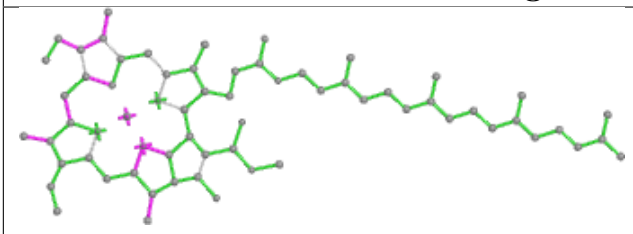


Rings

Ligand CLA B 602



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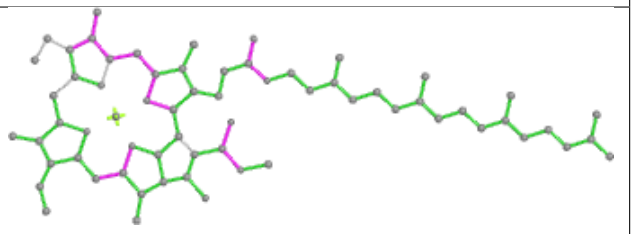
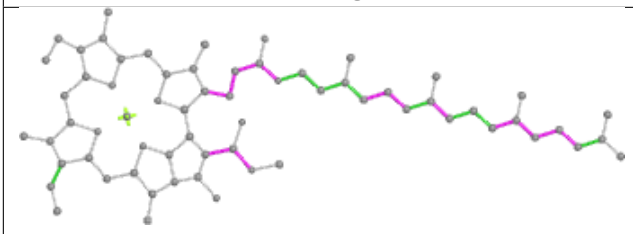


Bond angles



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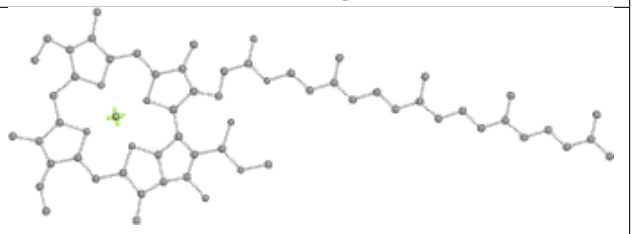
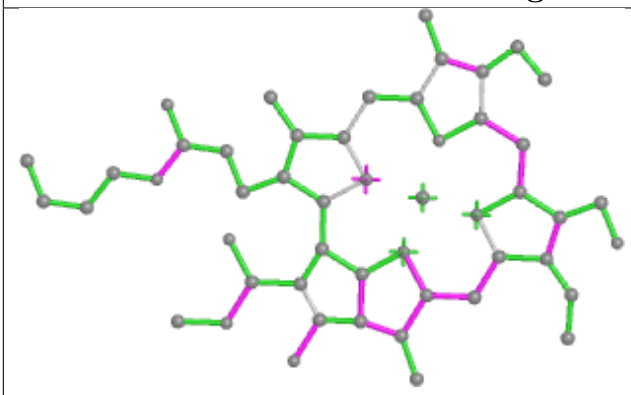


Rings

Ligand CHL n 608



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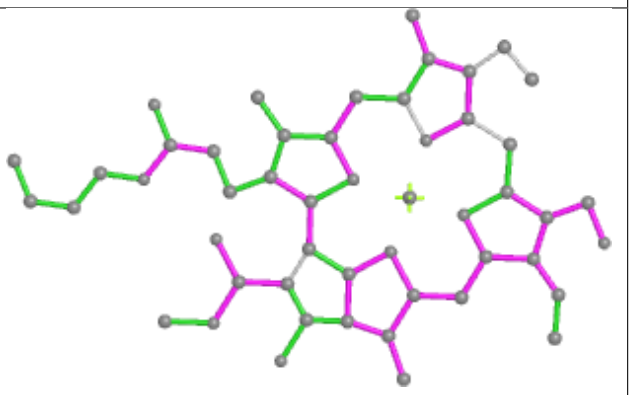
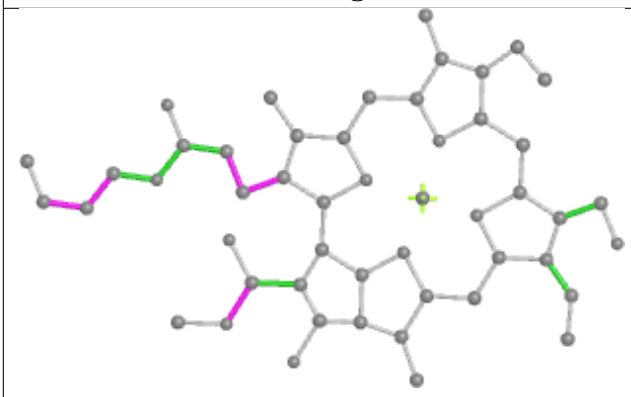
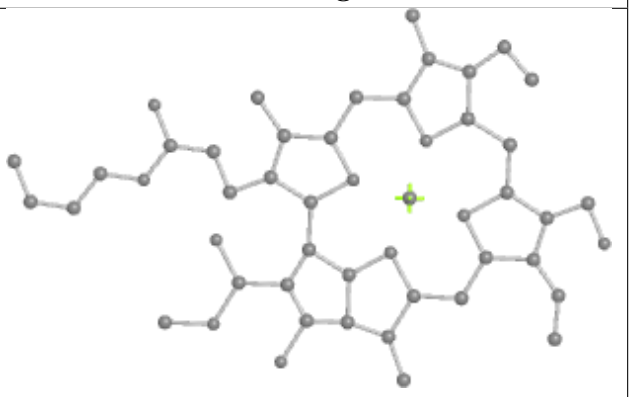


Bond angles

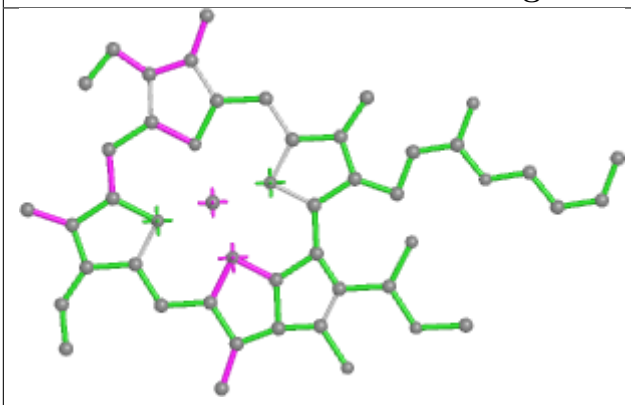


Torsions



Rings

Ligand CLA G 613



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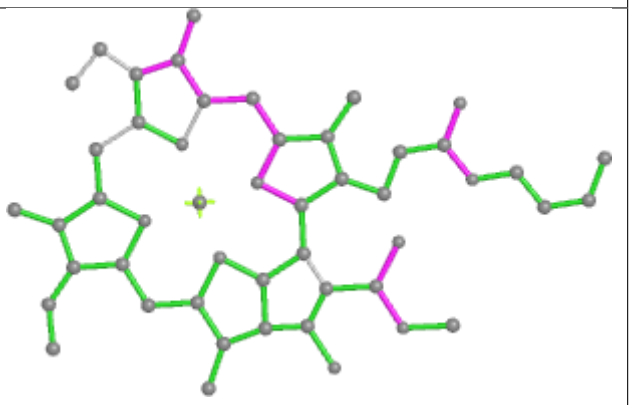
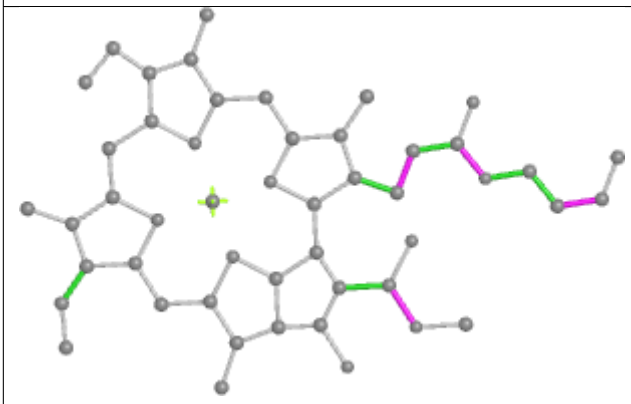
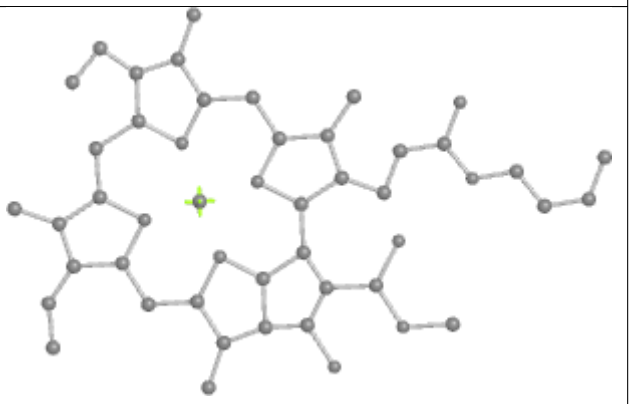


Bond angles

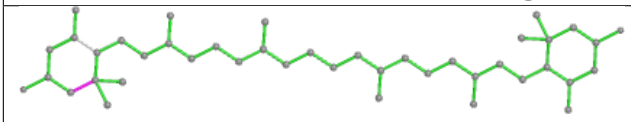


Torsions

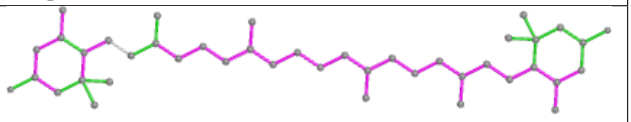


Rings

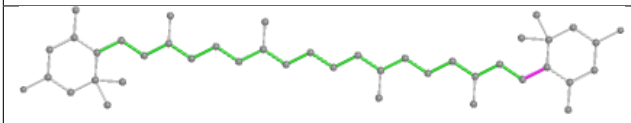
Ligand LUT g 1621



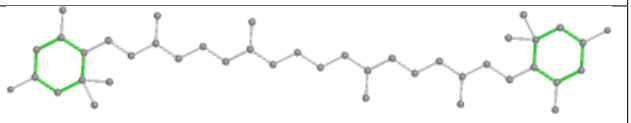
Bond lengths



Bond angles

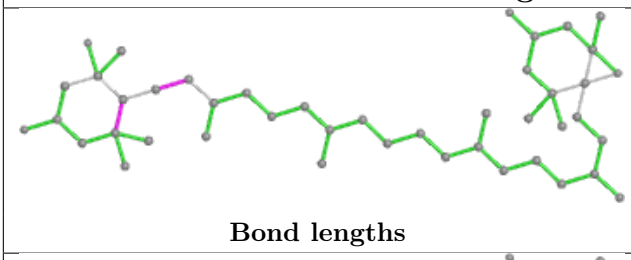


Torsions



Rings

Ligand NEX S 1623



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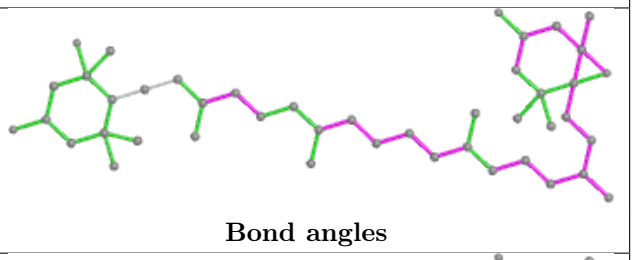
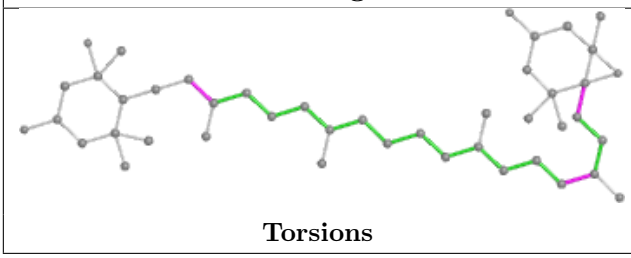
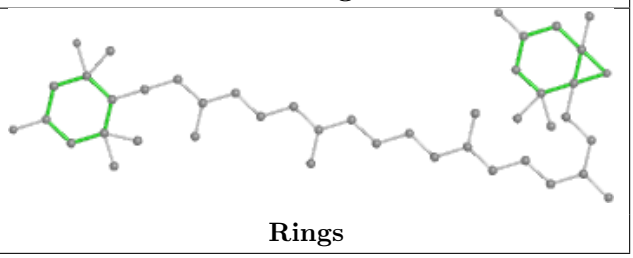


Bond angles

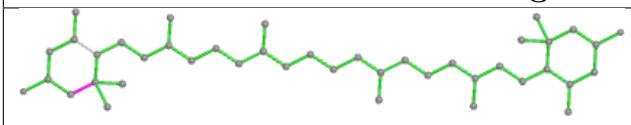


Torsions

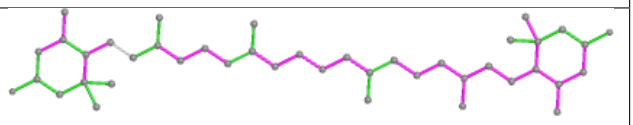


Rings

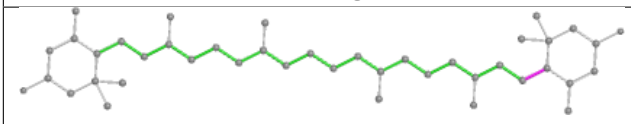
Ligand LUT r 620



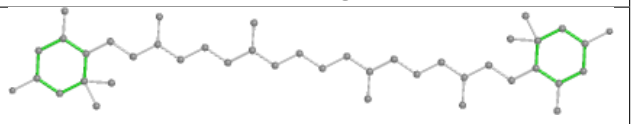
Bond lengths



Bond angles

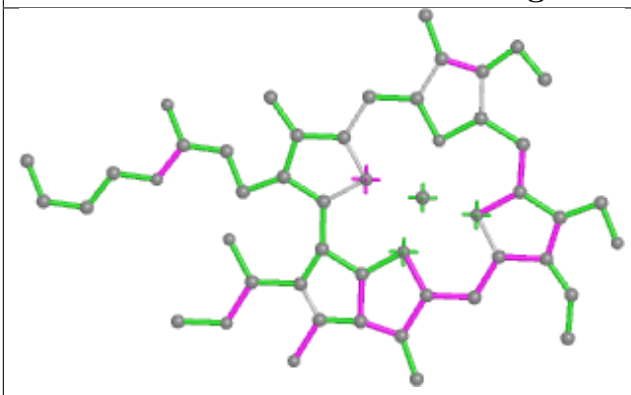


Torsions

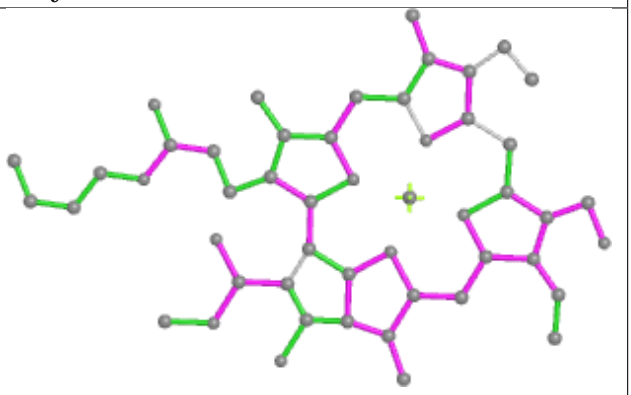


Rings

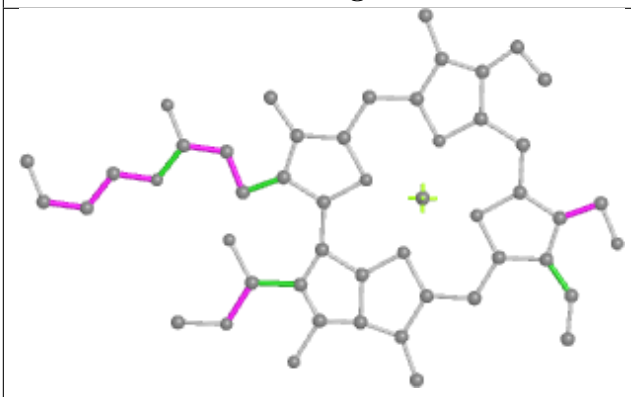
Ligand CHL y 607



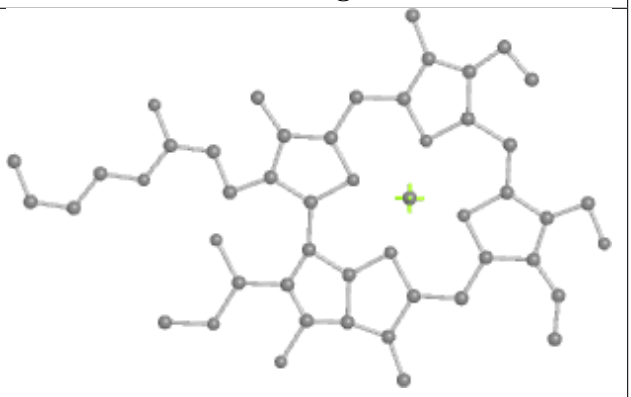
Bond lengths



Bond angles

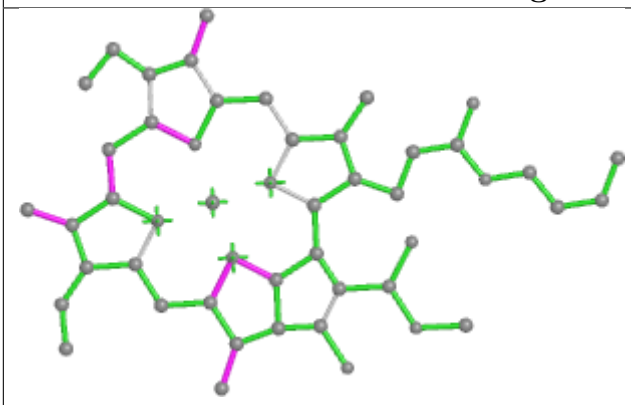


Torsions

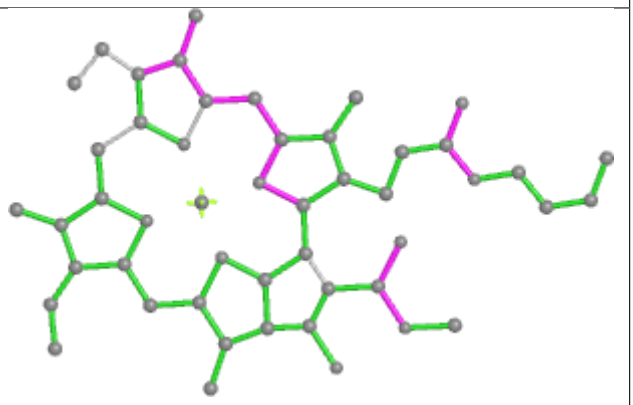


Rings

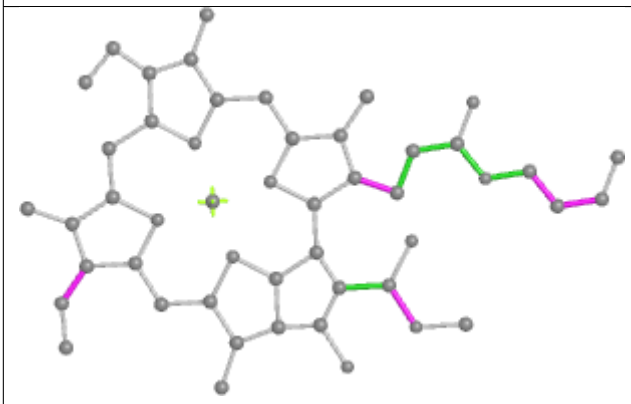
Ligand CLA r 609



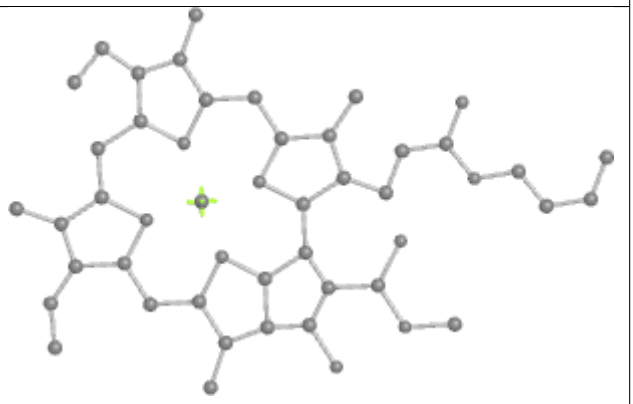
Bond lengths



Bond angles

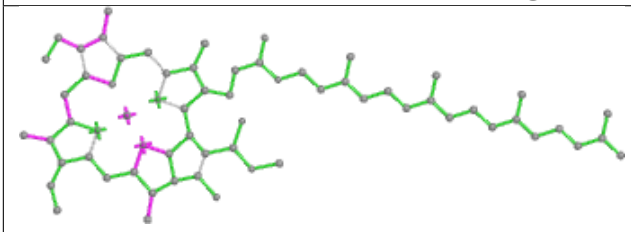


Torsions

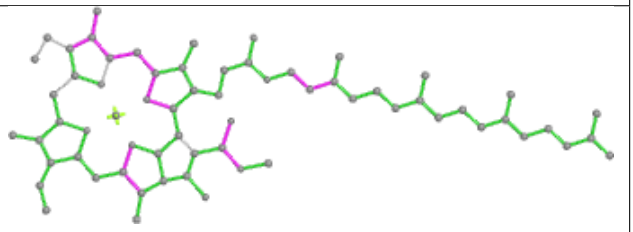


Rings

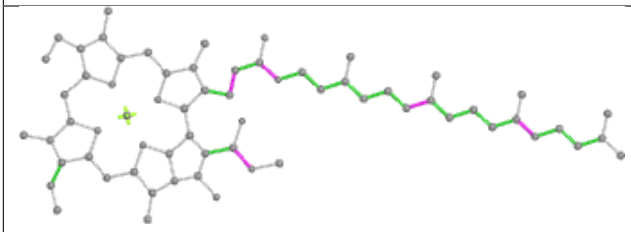
Ligand CLA B 608



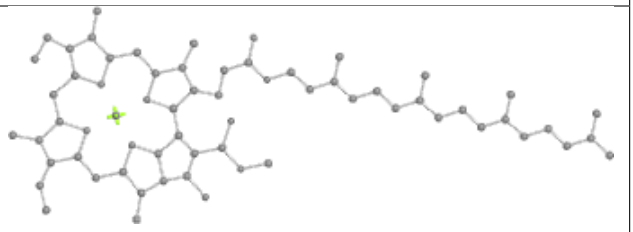
Bond lengths



Bond angles

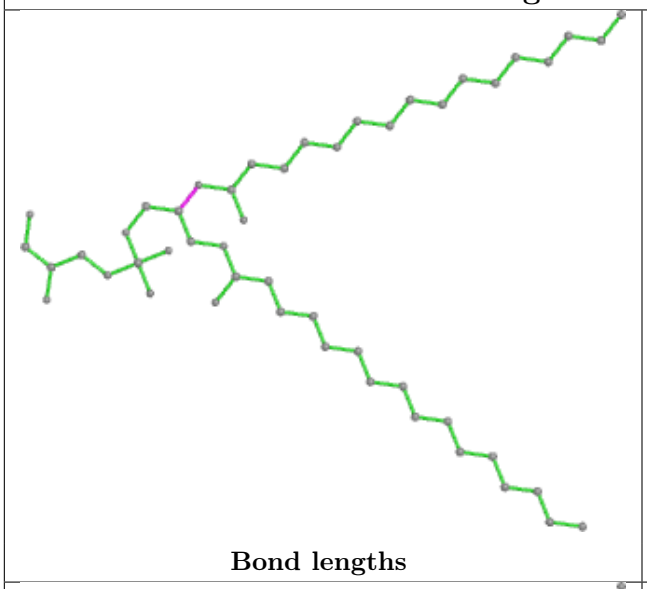


Torsions

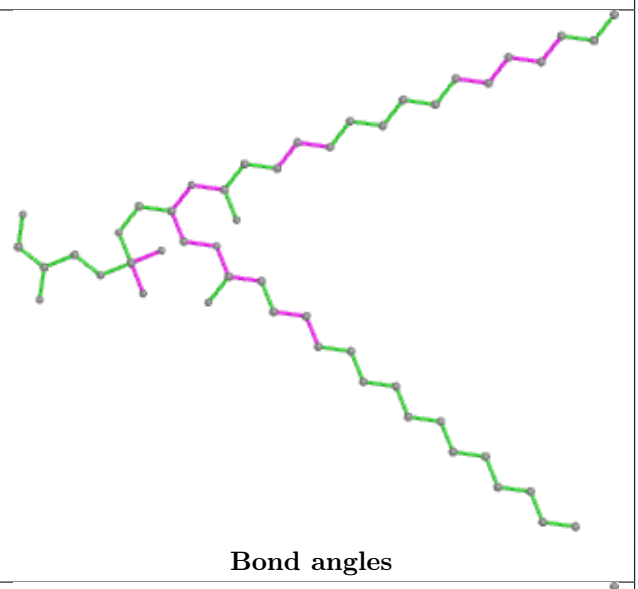


Rings

Ligand LHG D 409



Bond lengths



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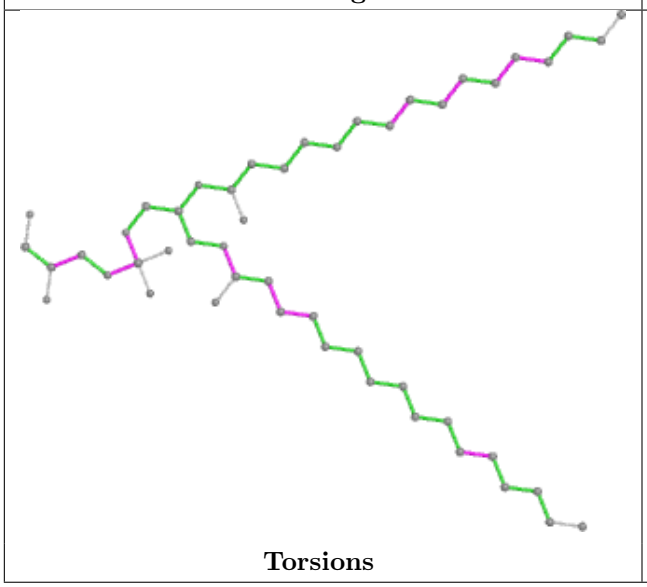
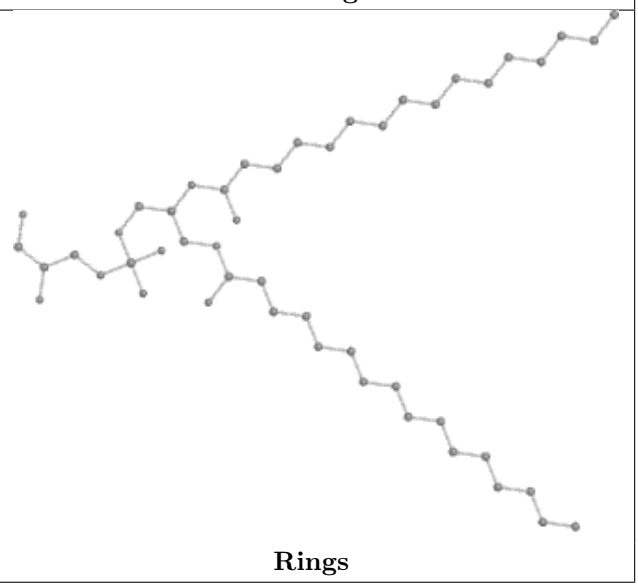
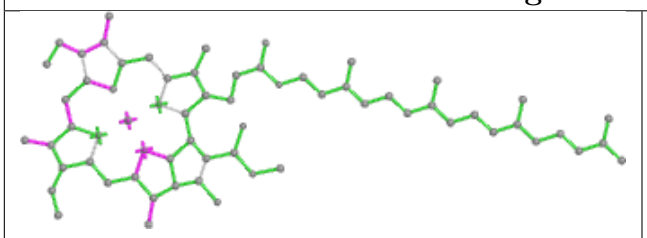


Torsions



Rings

Ligand CLA Y 612



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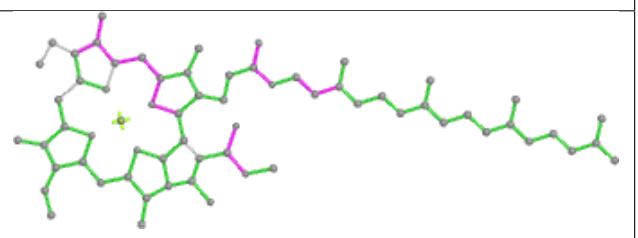
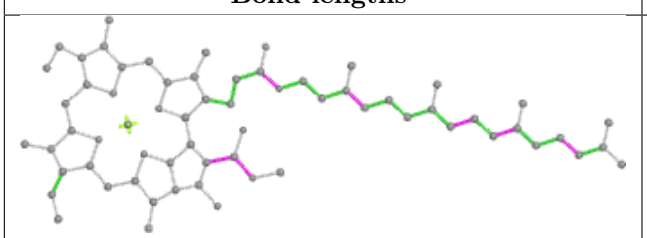
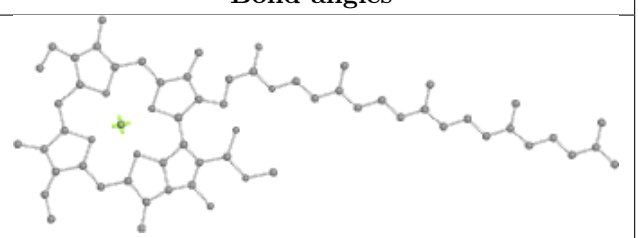


Bond angles

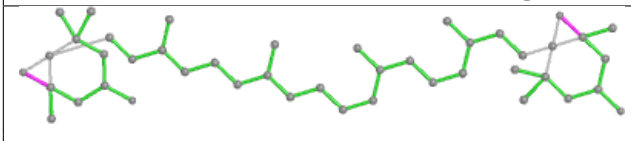


Torsions



Rings

Ligand XAT g 1622



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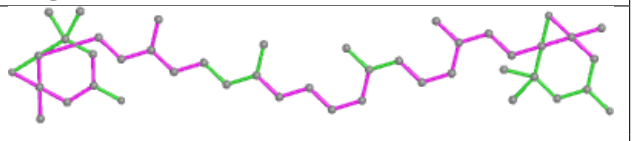
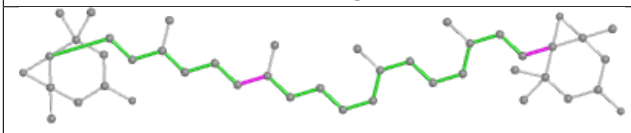
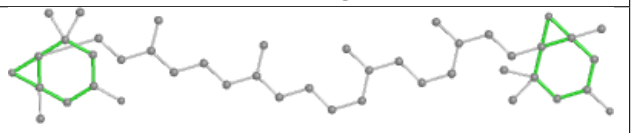


Bond angles

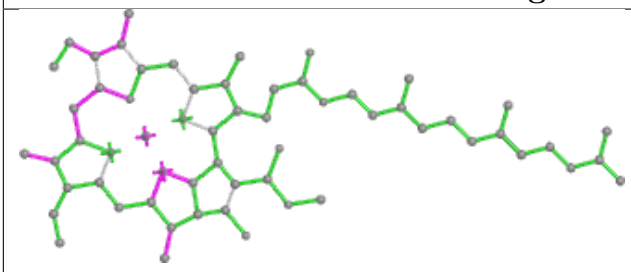


Torsions



Rings

Ligand CLA a 410



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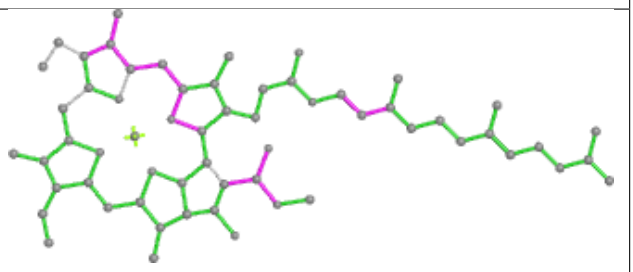
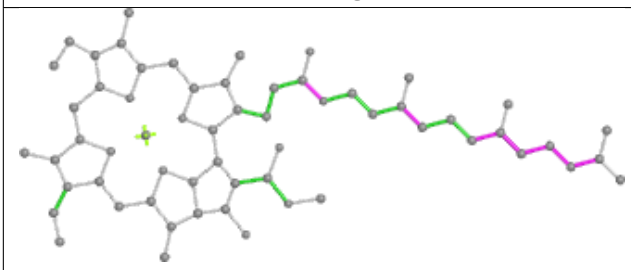
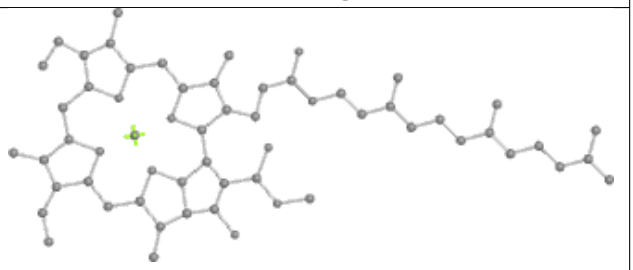


Bond angles

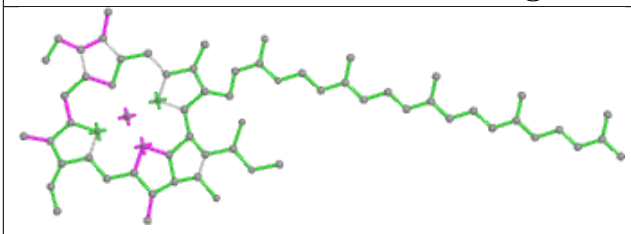


Torsions



Rings

Ligand CLA B 614



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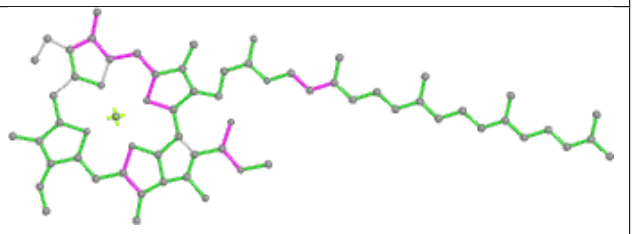
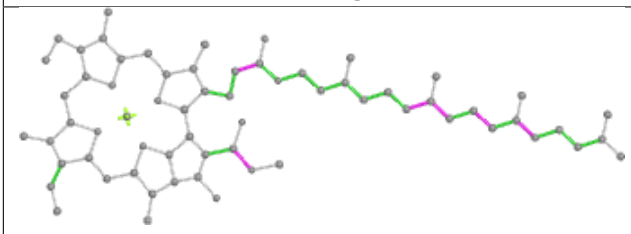


Bond angles



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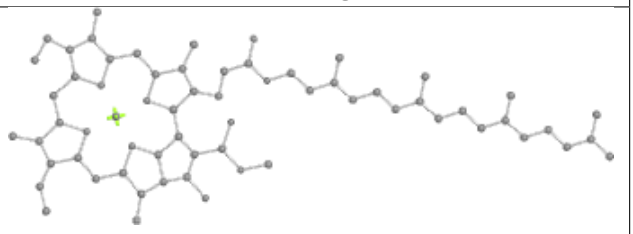
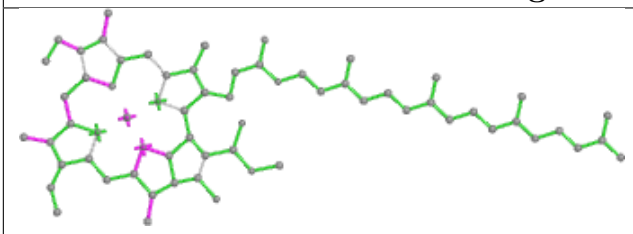


Rings

Ligand CLA g 602



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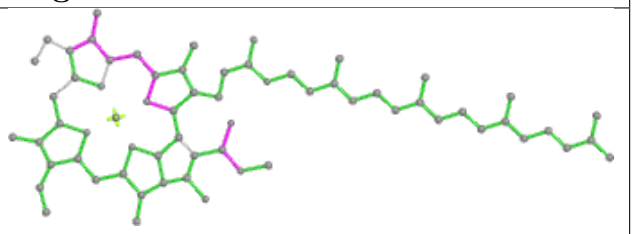
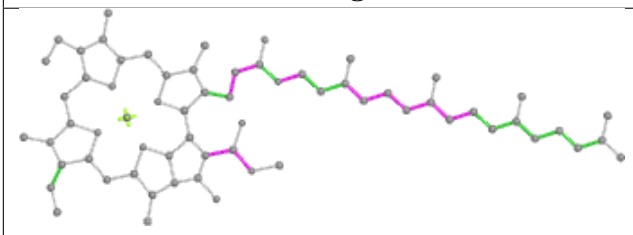


Bond angles



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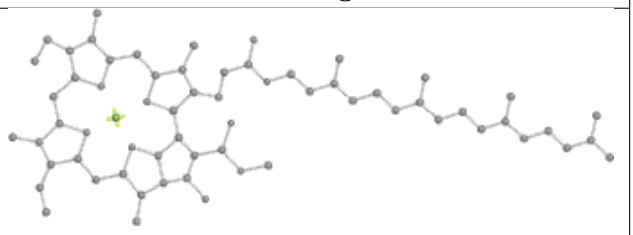
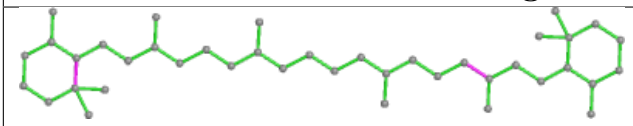


Rings

Ligand BCR A 411



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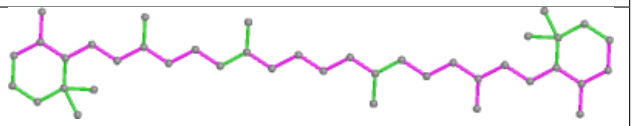

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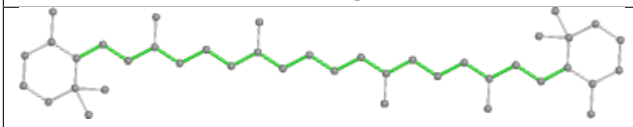
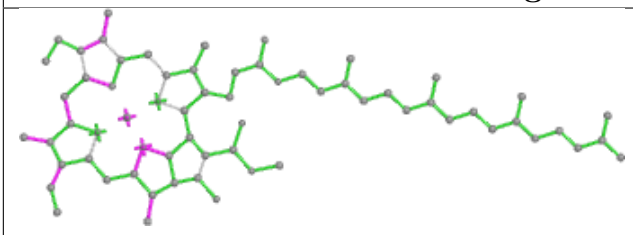


Torsions

Rings

Ligand CLA B 612



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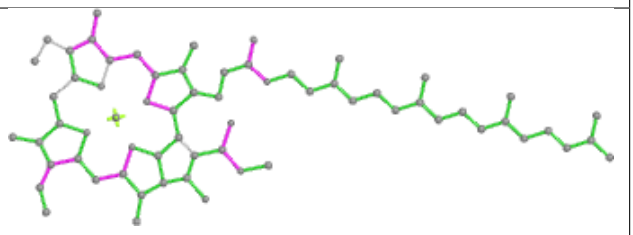
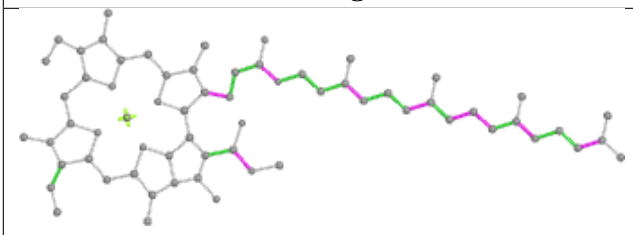
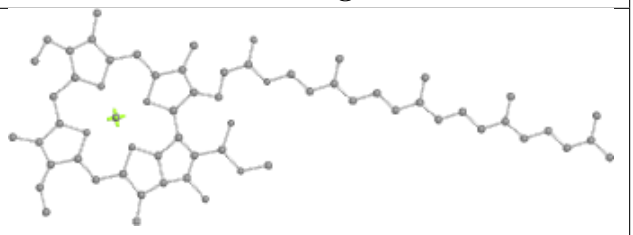


Bond angles

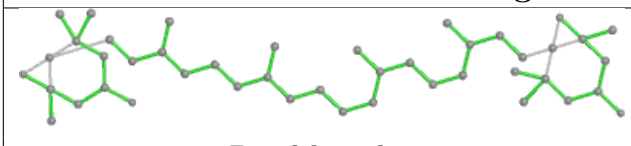


Torsions



Rings

Ligand XAT Y 1622



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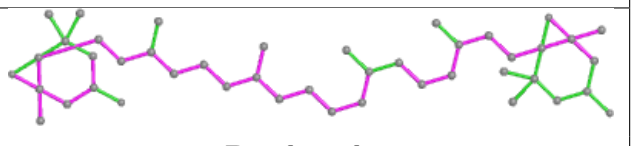
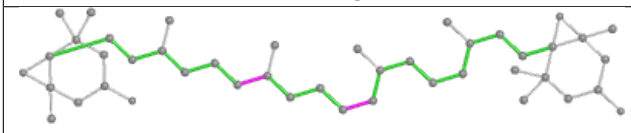
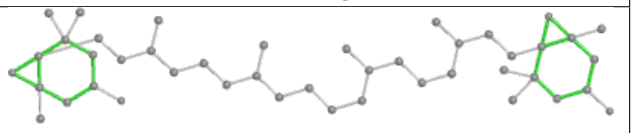


Bond angles

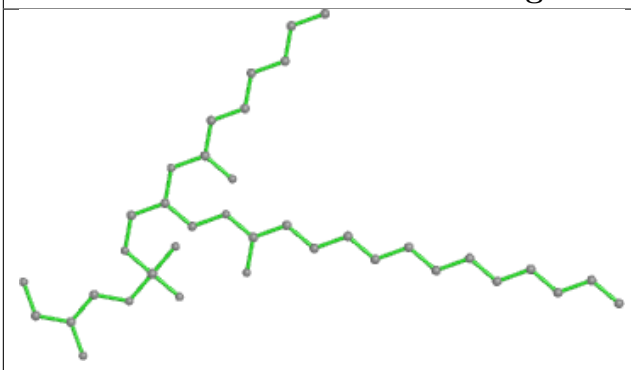


Torsions



Rings

Ligand LHG d 410



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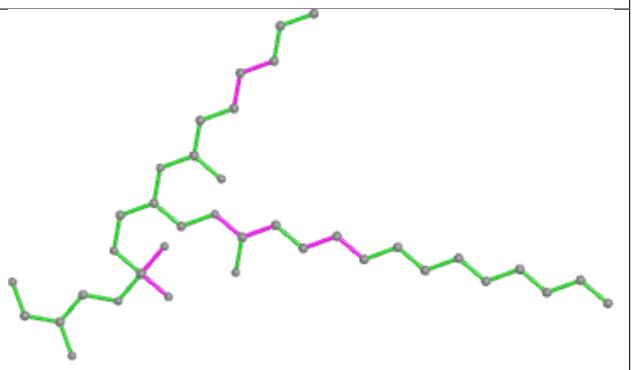
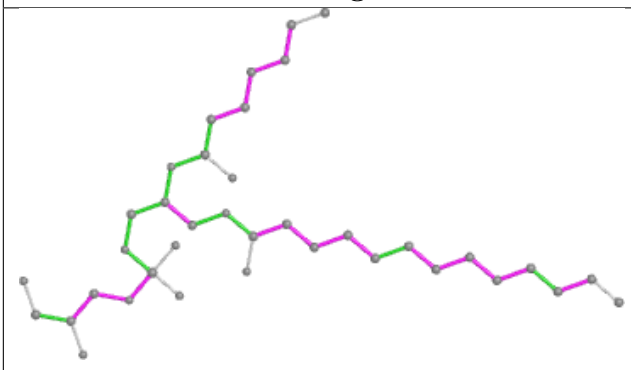
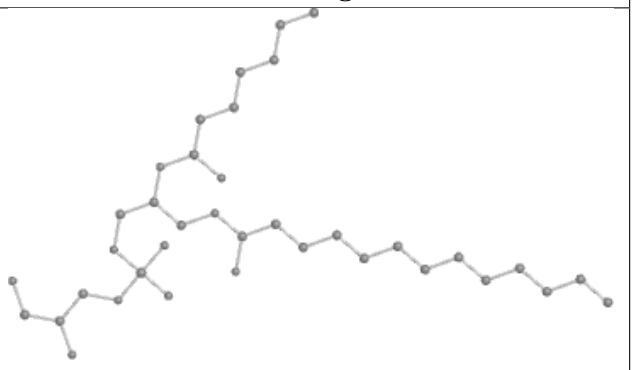


Bond angles

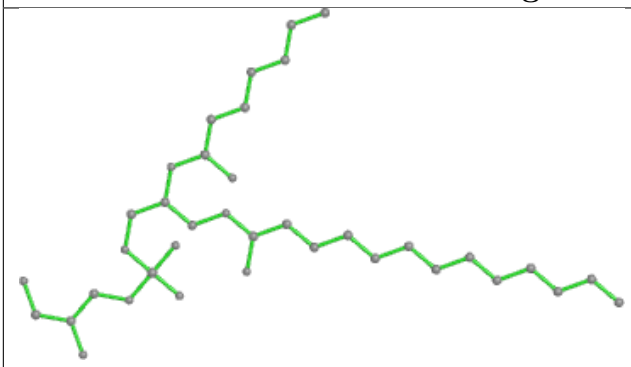


Torsions



Rings

Ligand LHG D 410



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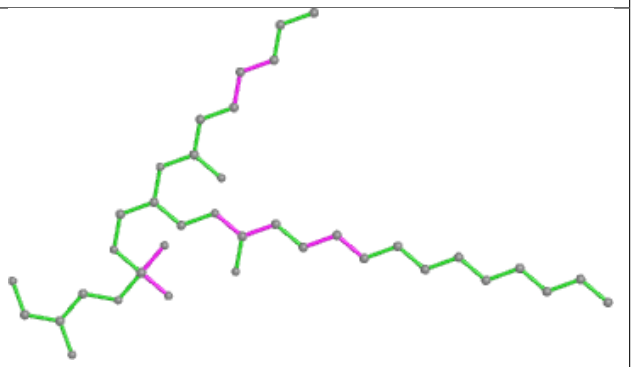
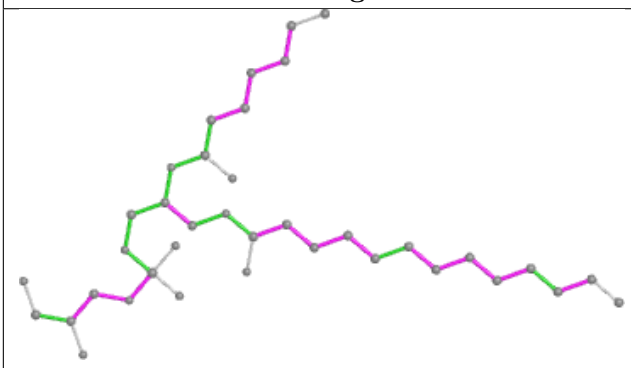


Bond angles



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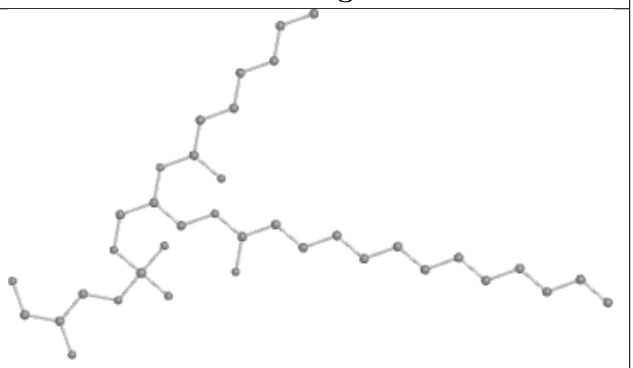
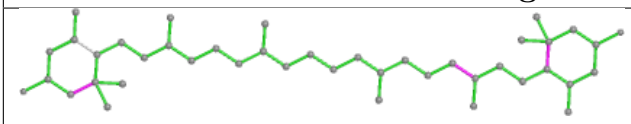


Rings

Ligand LUT y 1621



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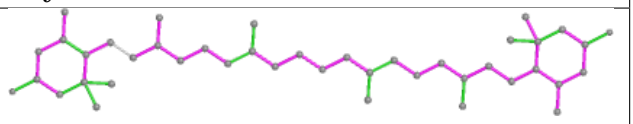
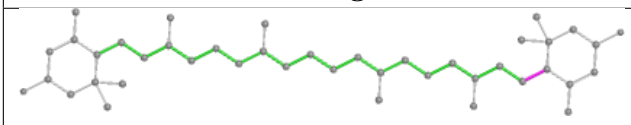


Bond angles



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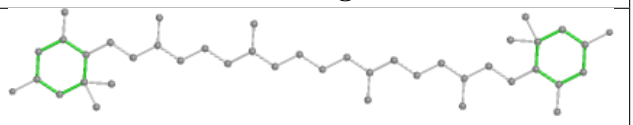
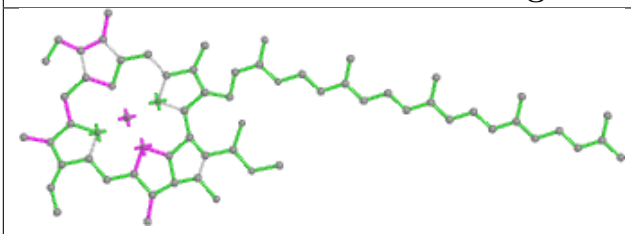
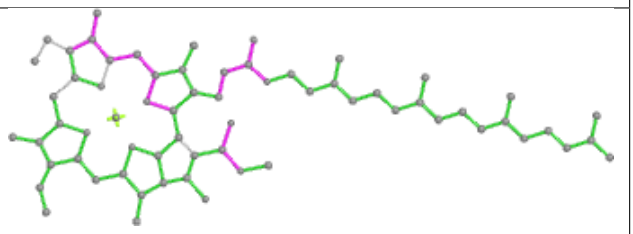


Rings

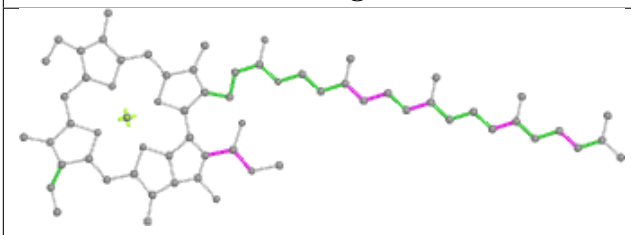
Ligand CLA b 610



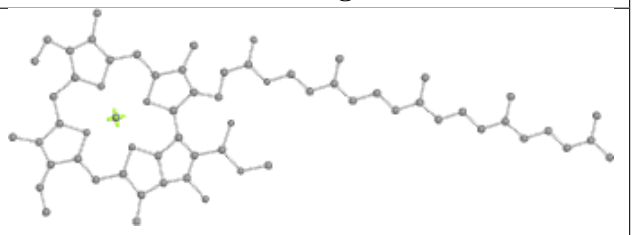
Bond lengths



Bond angles

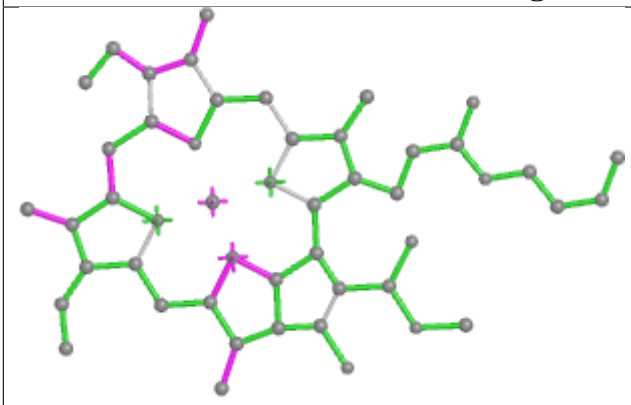


Torsions

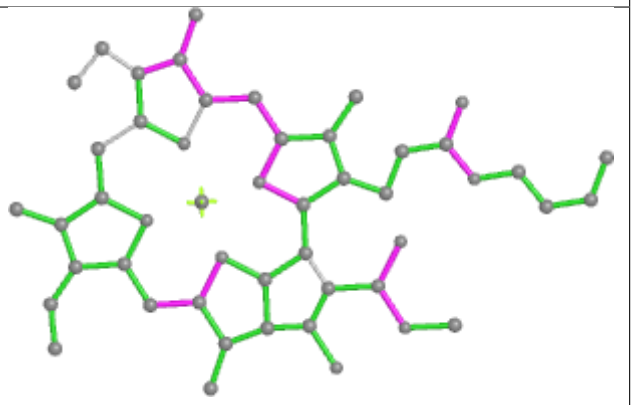


Rings

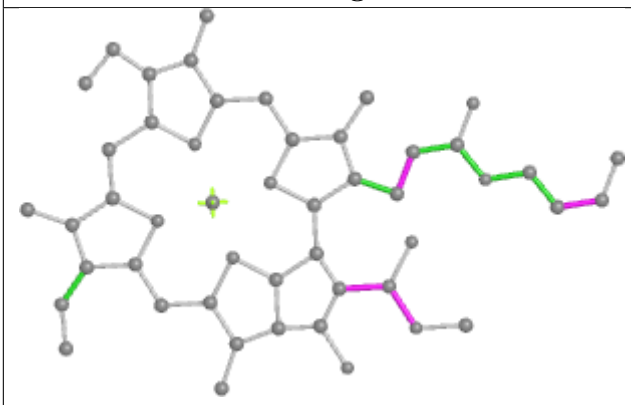
Ligand CLA a 407



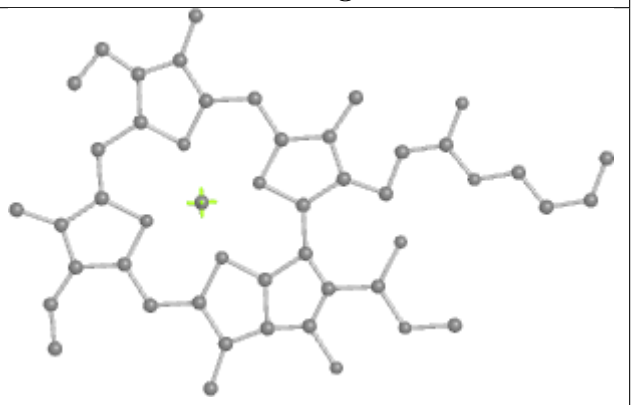
Bond lengths



Bond angles

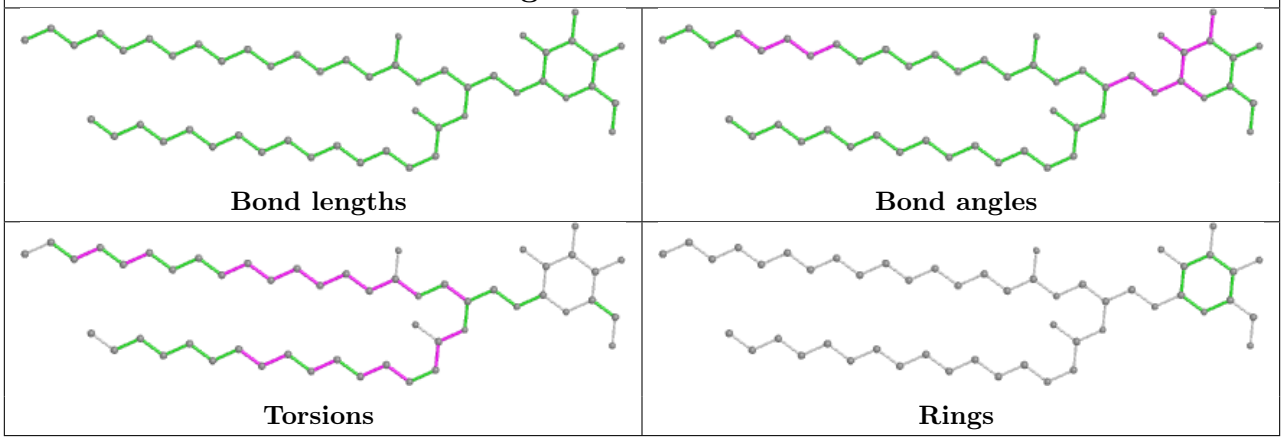


Torsions

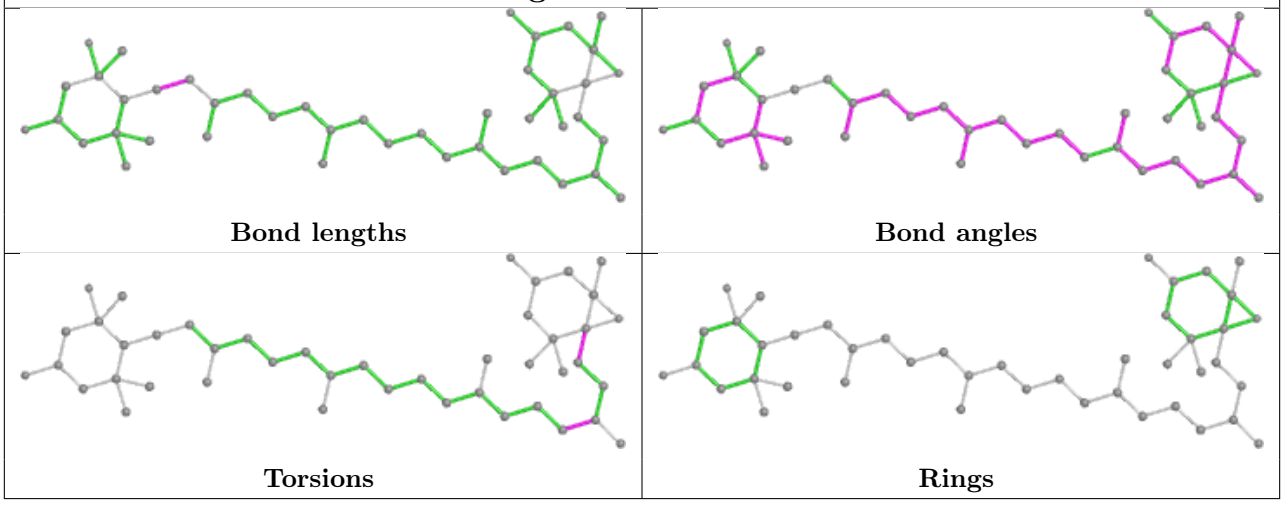


Rings

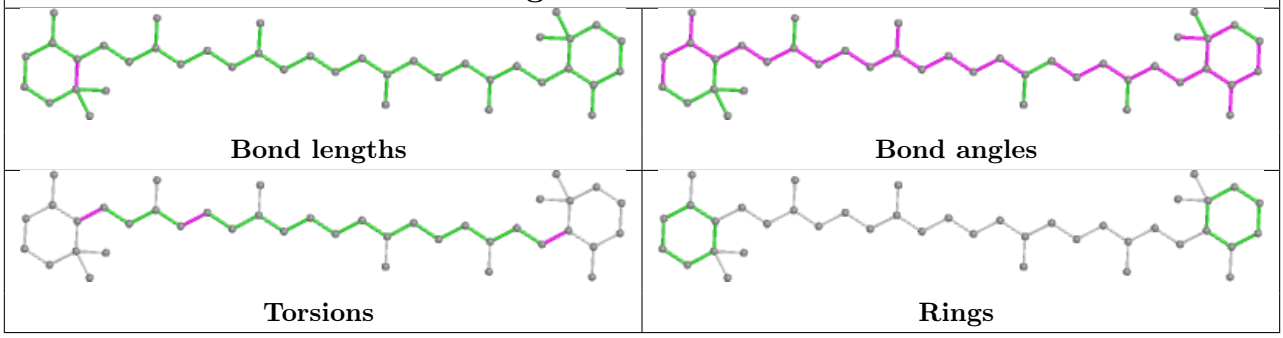
Ligand LMG C 521



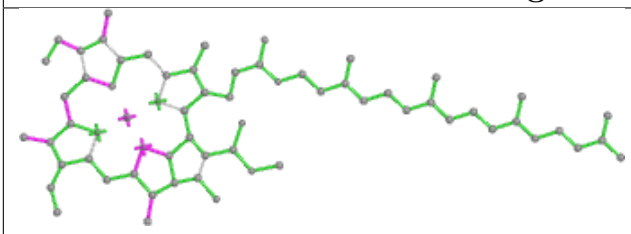
Ligand NEX r 623



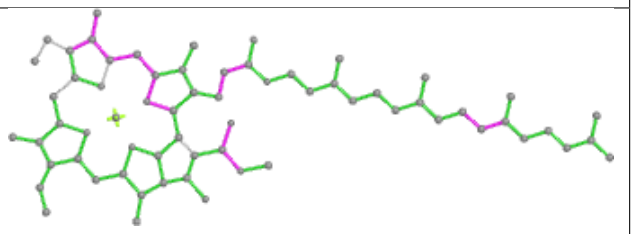
Ligand BCR h 101



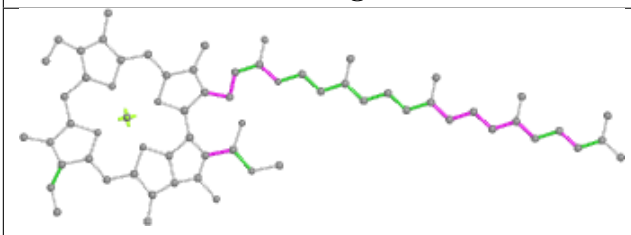
Ligand CLA b 613



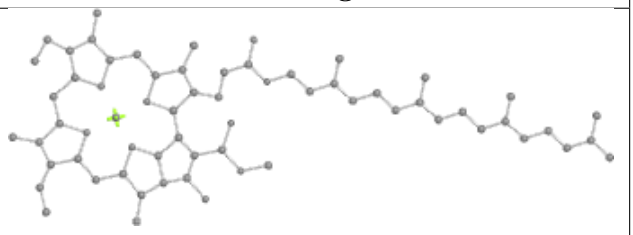
Bond lengths



Bond angles

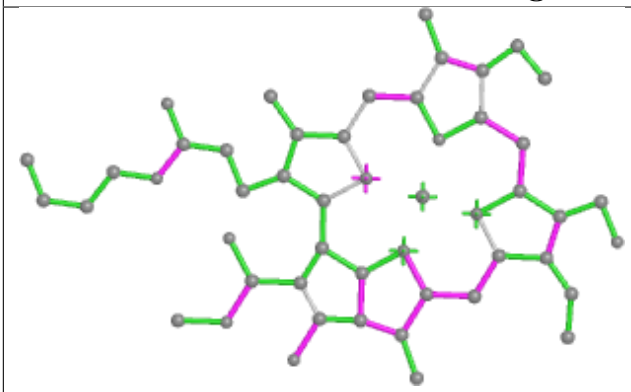


Torsions



Rings

Ligand CHL g 609



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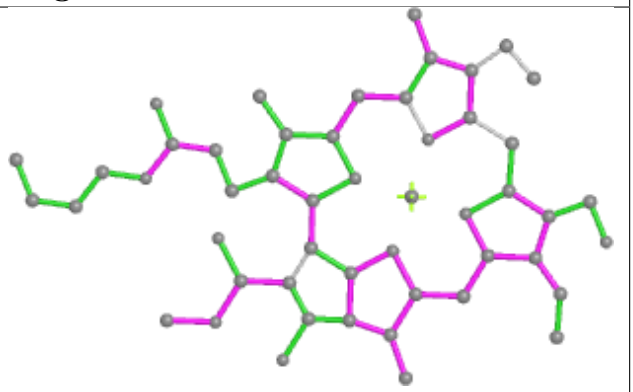
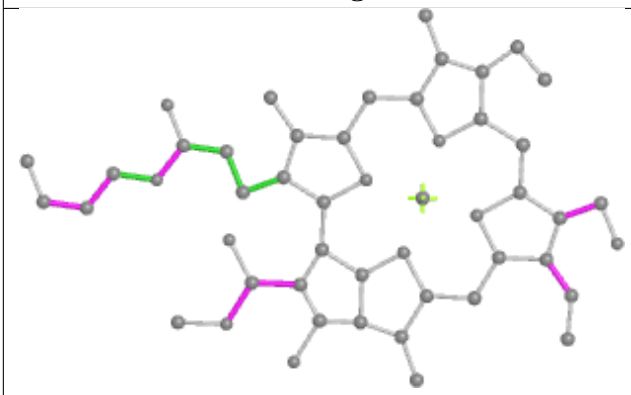
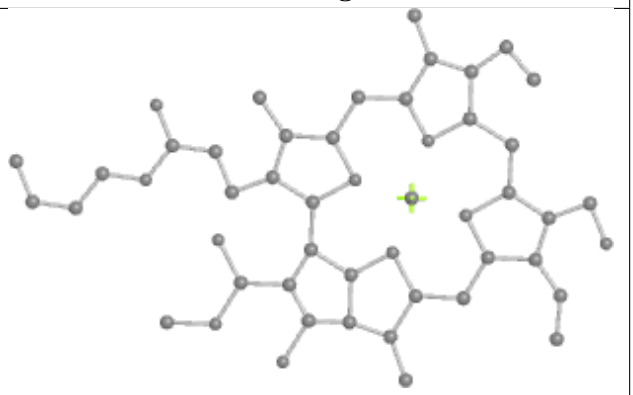


Bond angles

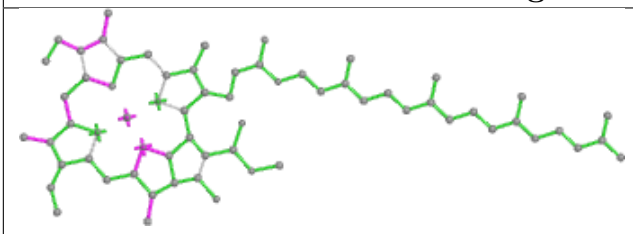


Torsions

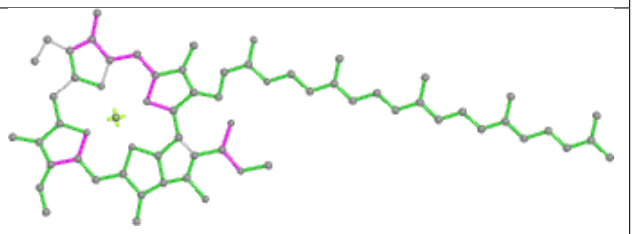


Rings

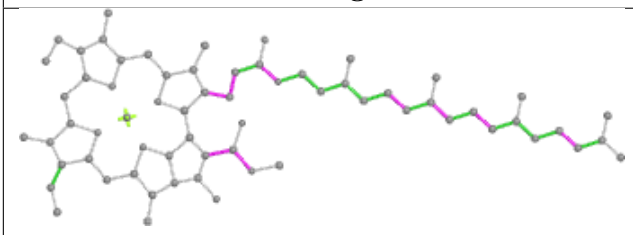
Ligand CLA b 615



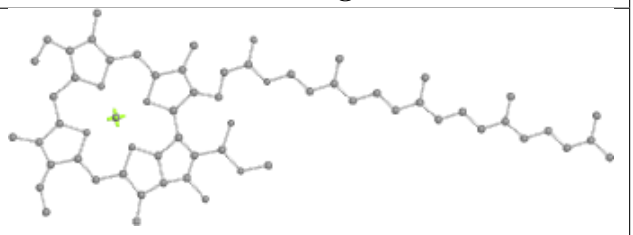
Bond lengths



Bond angles

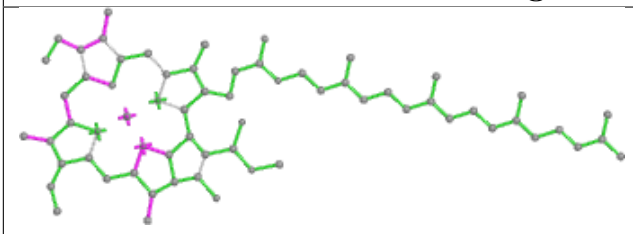


Torsions



Rings

Ligand CLA b 614



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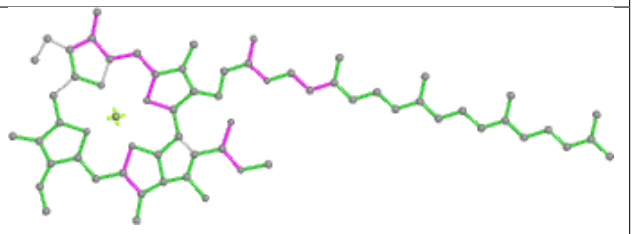
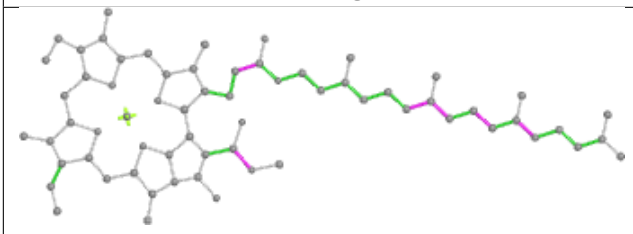
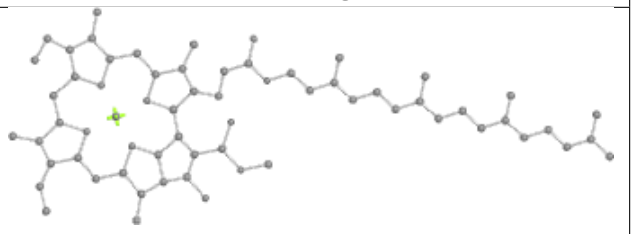


Bond angles

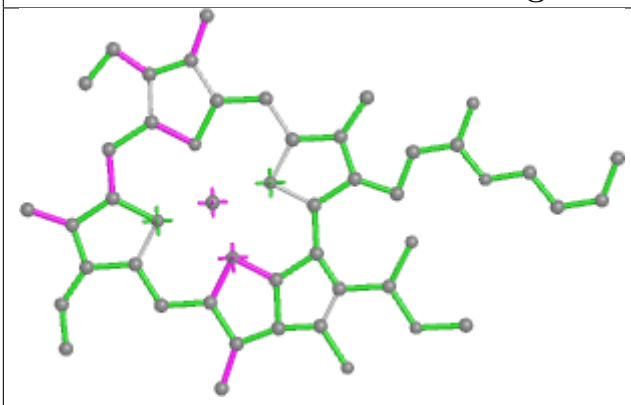


Torsions



Rings

Ligand CLA n 613



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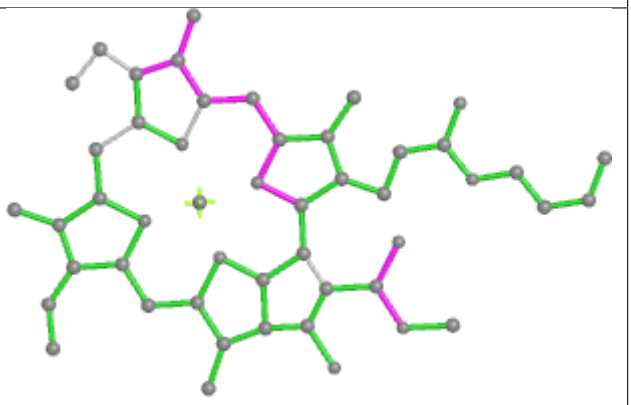
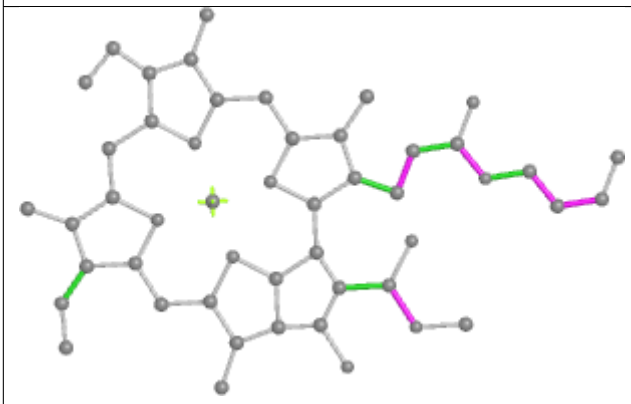
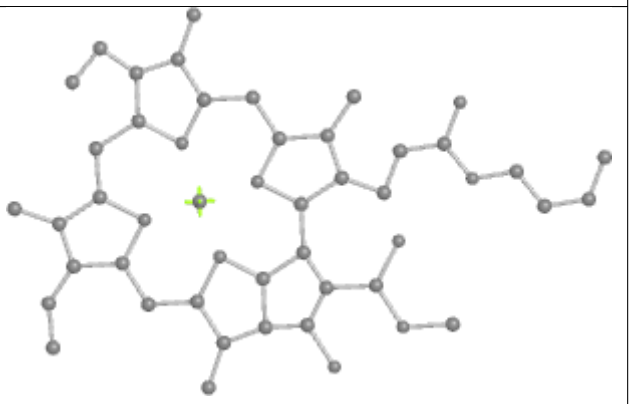


Bond angles

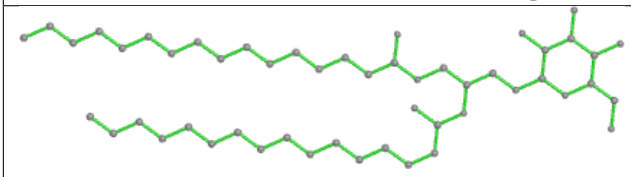


Torsions

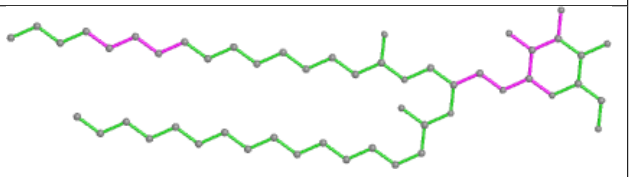


Rings

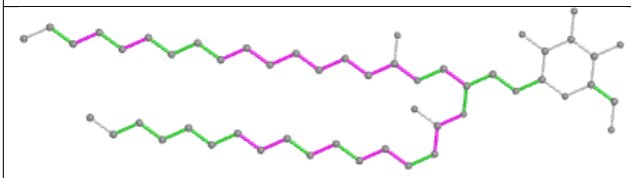
Ligand LMG c 521



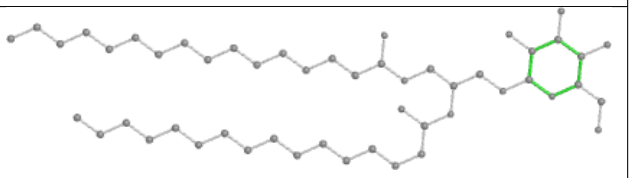
Bond lengths



Bond angles

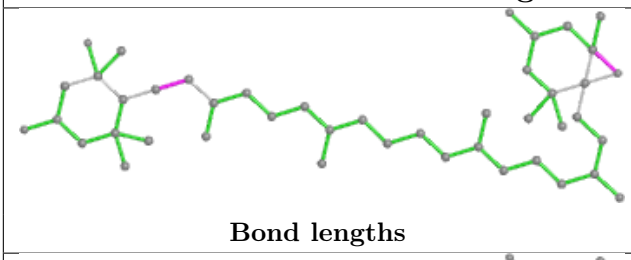


Torsions



Rings

Ligand NEX y 1623



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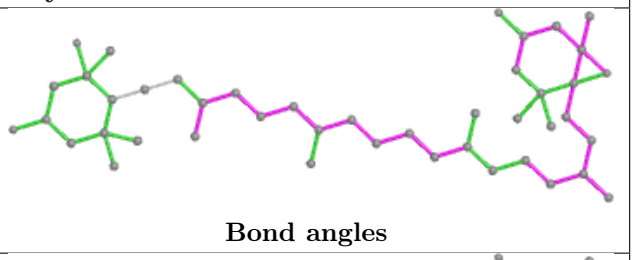
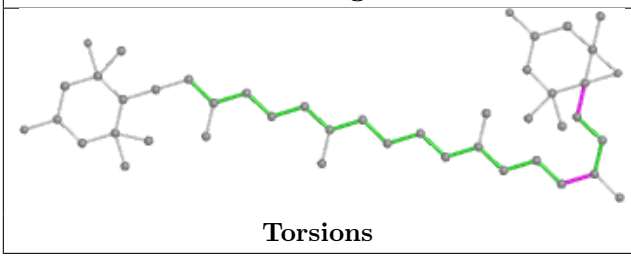
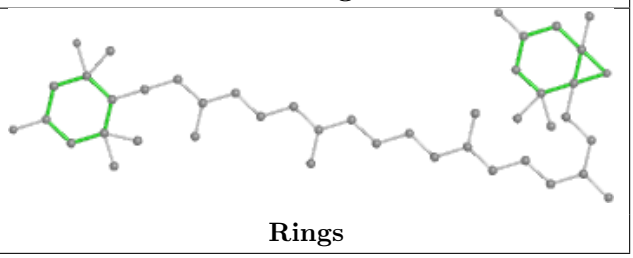


Bond angles

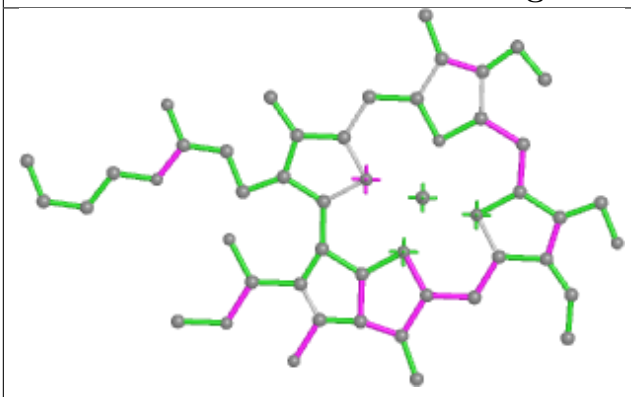


Torsions

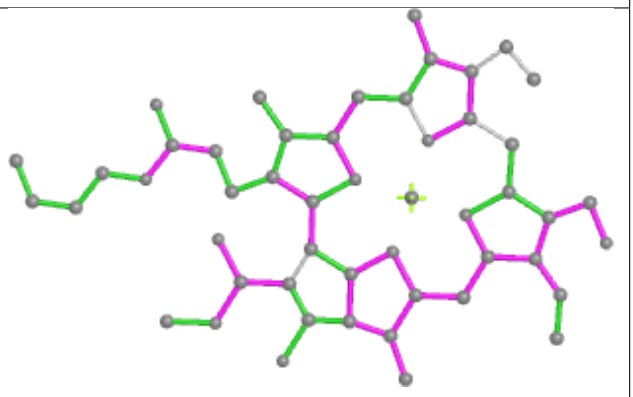


Rings

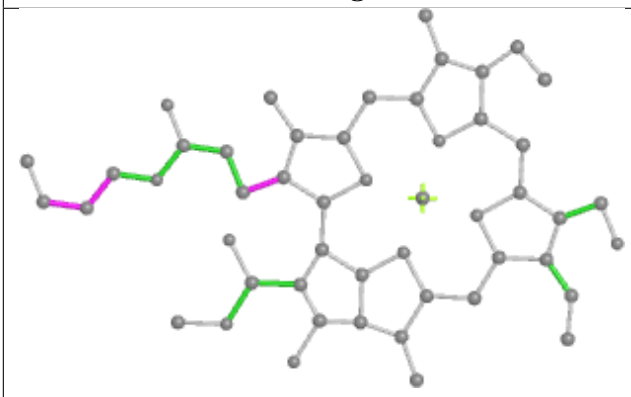
Ligand CHL n 606



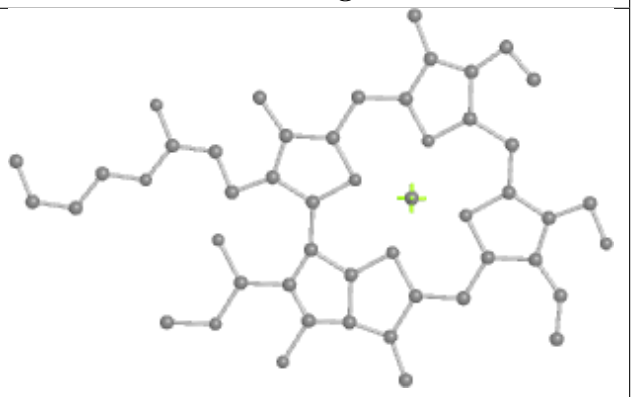
Bond lengths



Bond angles

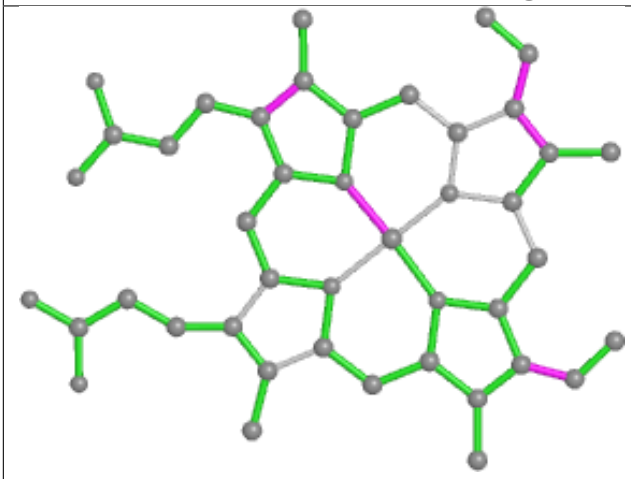


Torsions

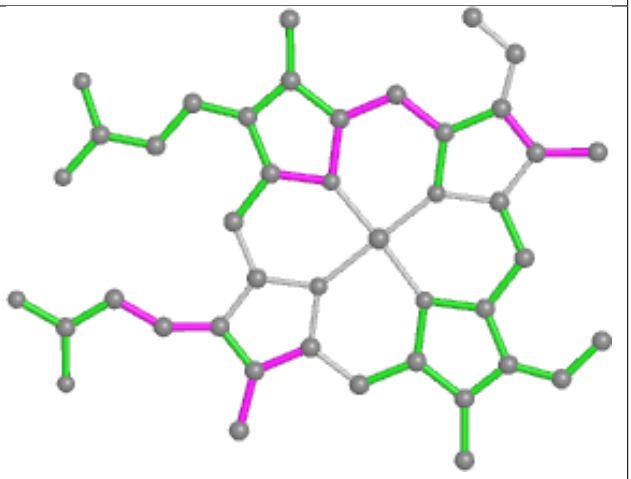


Rings

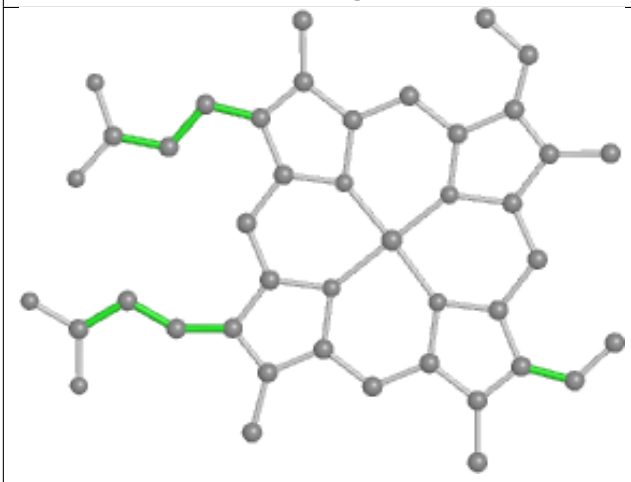
Ligand HEM F 101



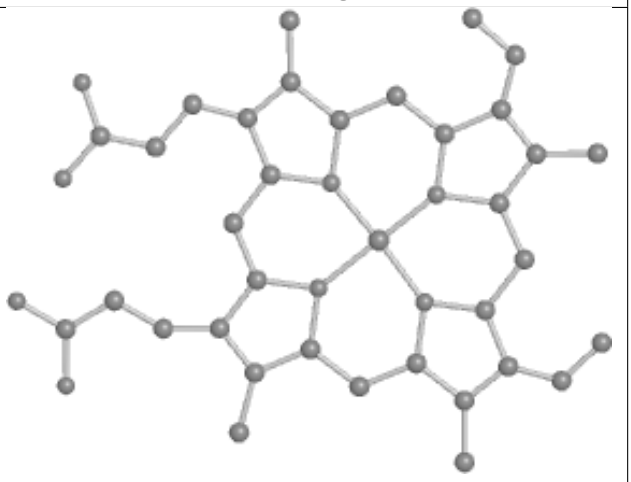
Bond lengths



Bond angles

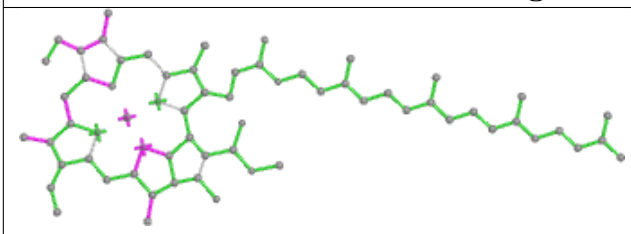


Torsions

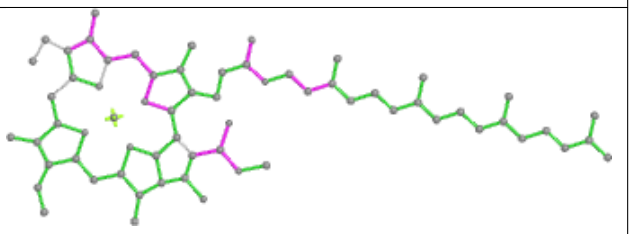


Rings

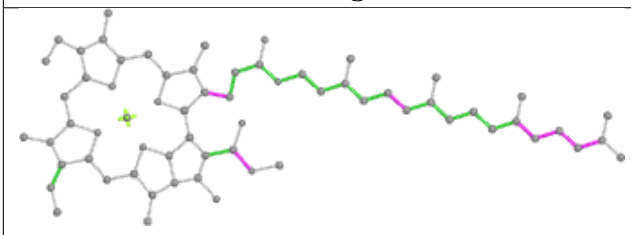
Ligand CLA n 610



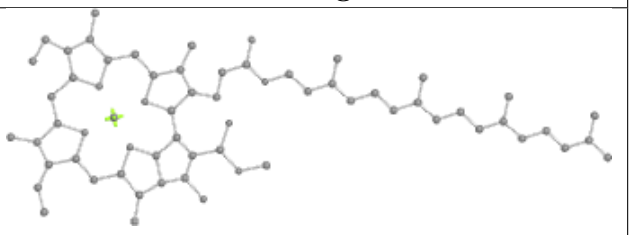
Bond lengths



Bond angles

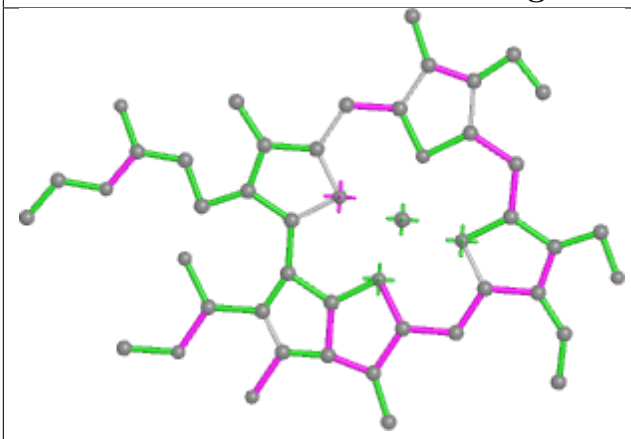


Torsions



Rings

Ligand CHL g 605



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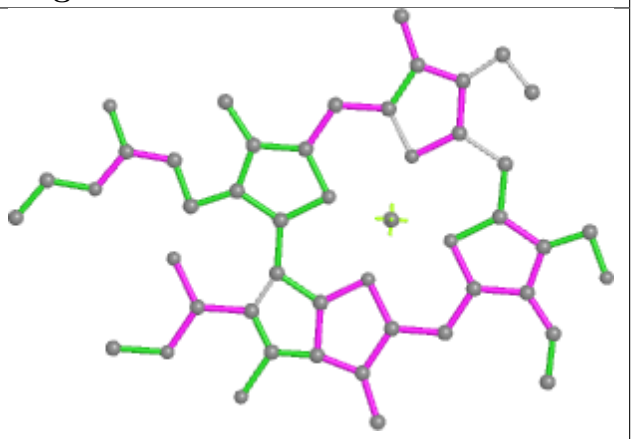
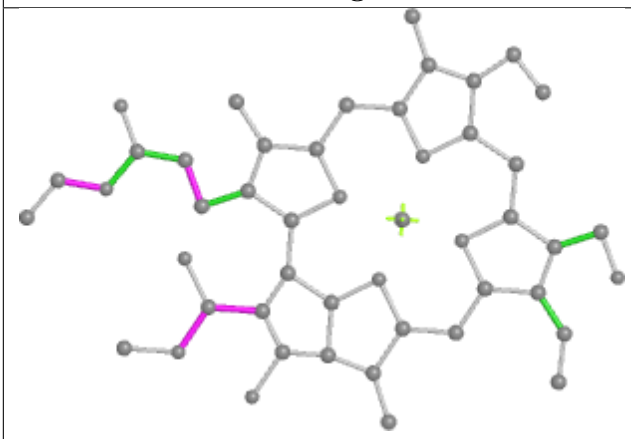
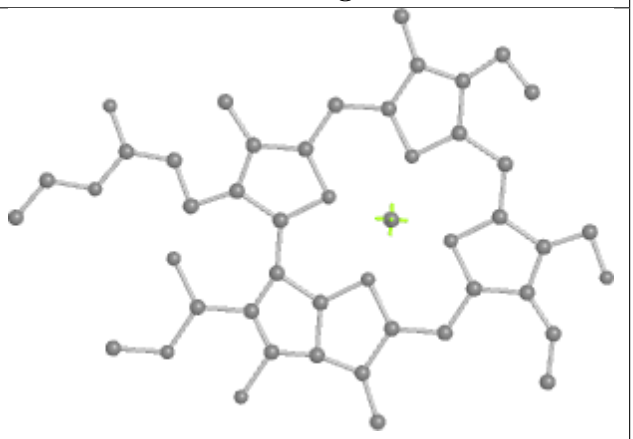


Bond angles

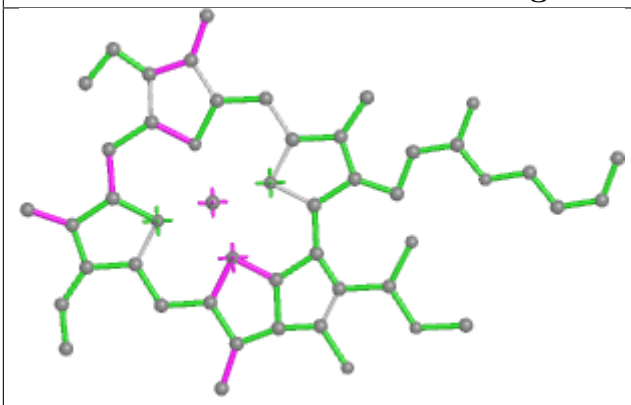


Torsions

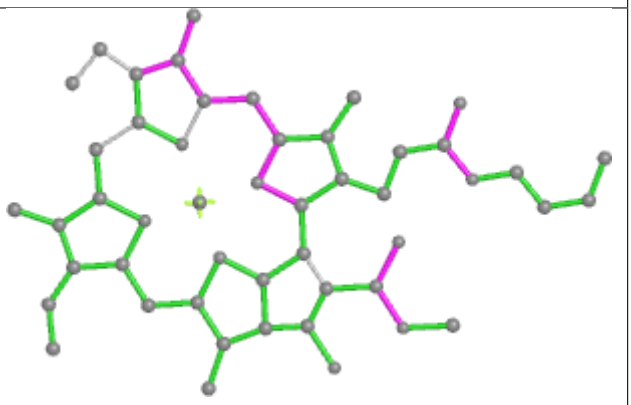


Rings

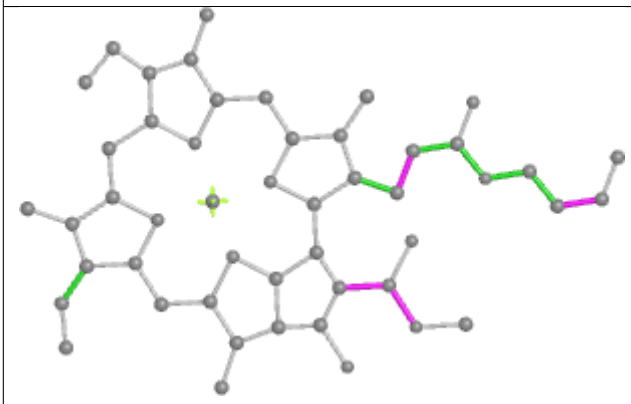
Ligand CLA r 603



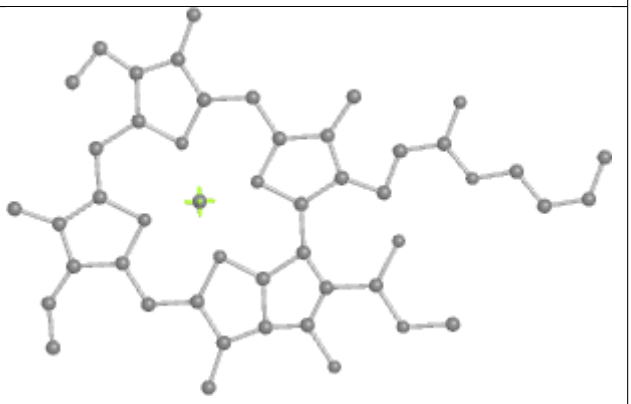
Bond lengths



Bond angles

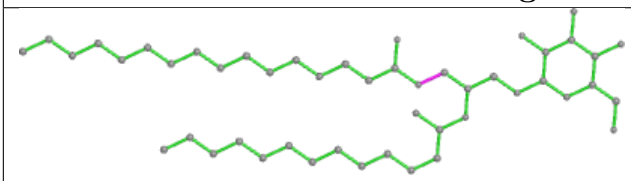


Torsions

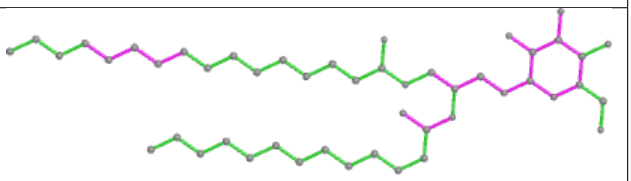


Rings

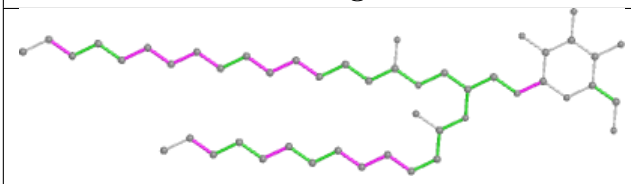
Ligand LMG A 413



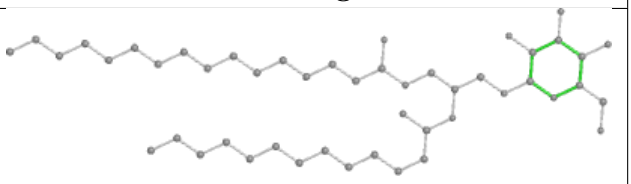
Bond lengths



Bond angles

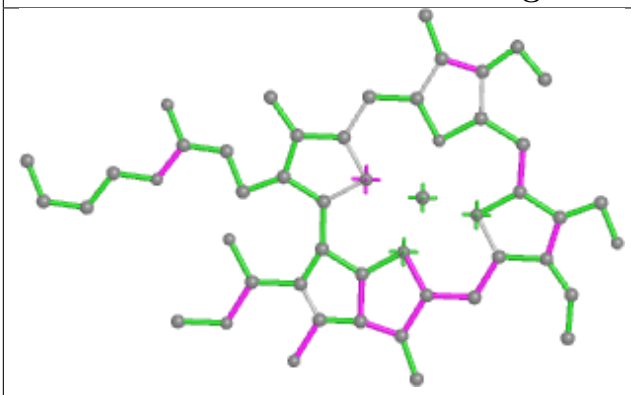


Torsions

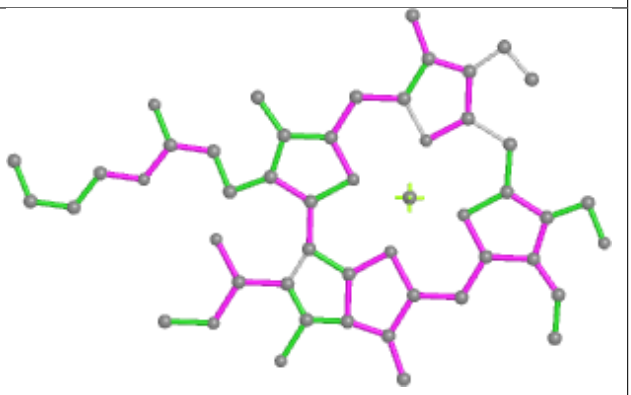


Rings

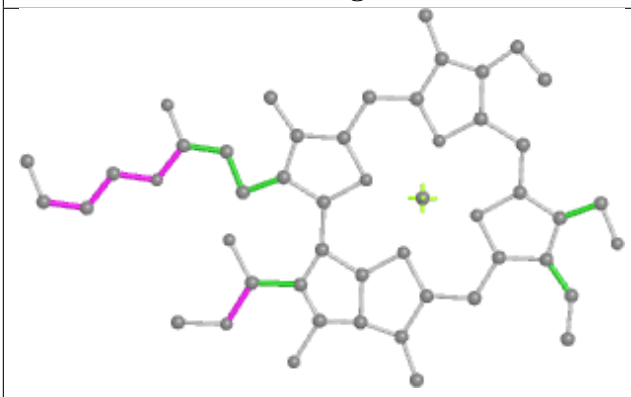
Ligand CHL N 609



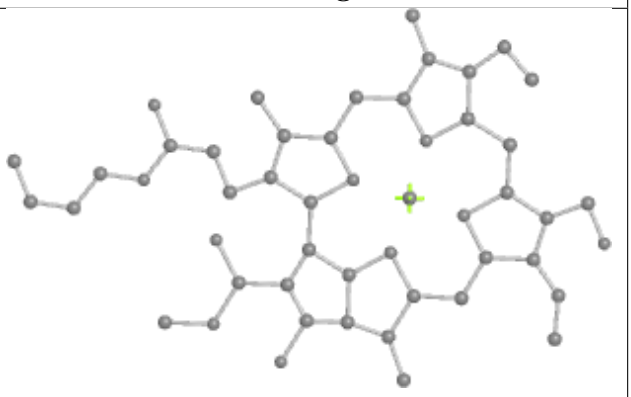
Bond lengths



Bond angles

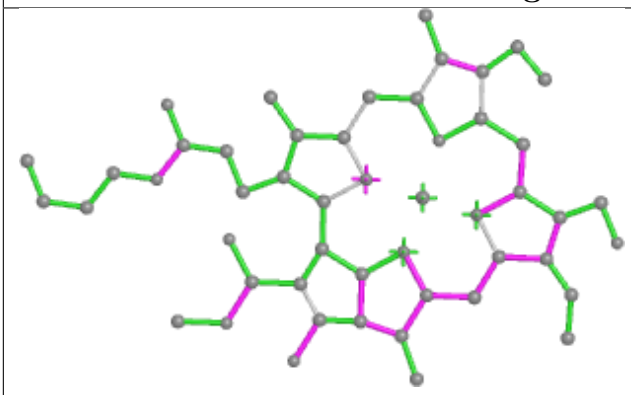


Torsions

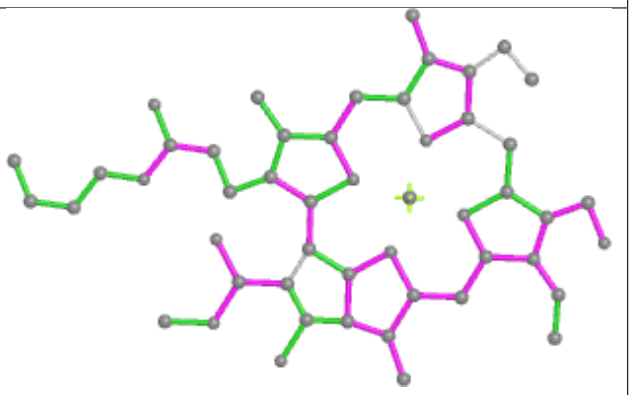


Rings

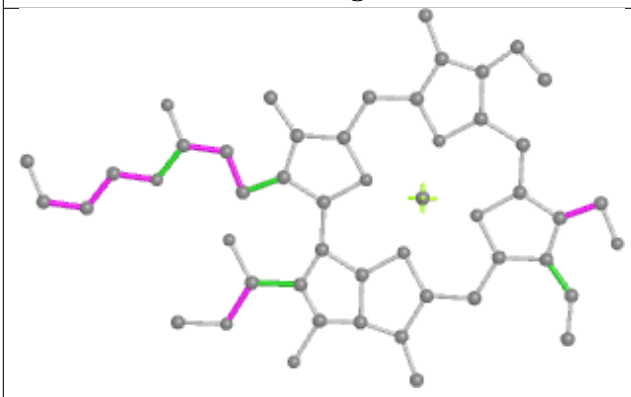
Ligand CHL Y 607



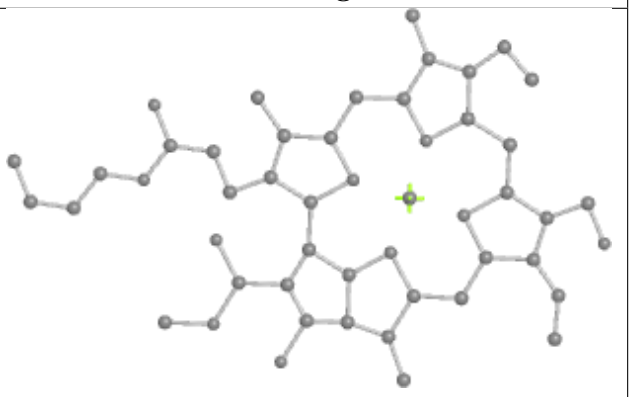
Bond lengths



Bond angles

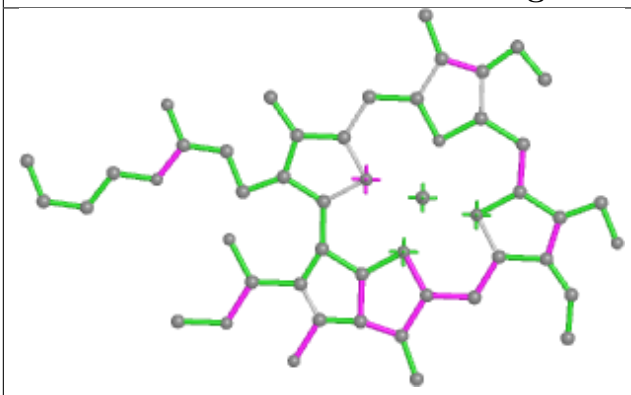


Torsions



Rings

Ligand CHL y 608



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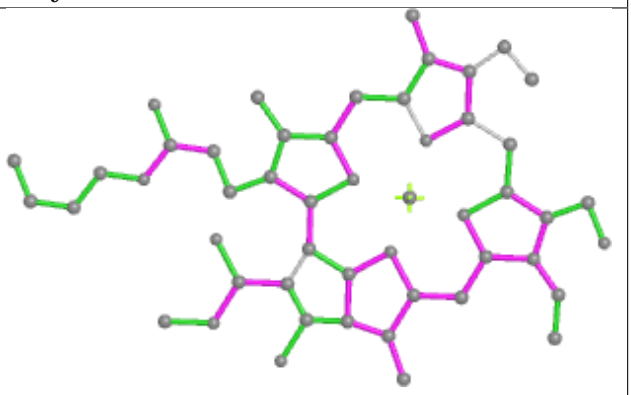
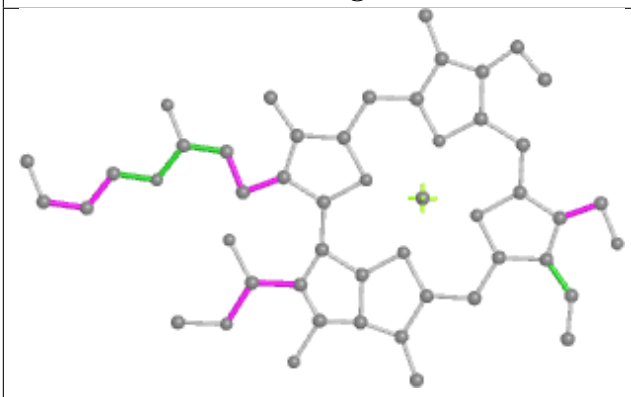
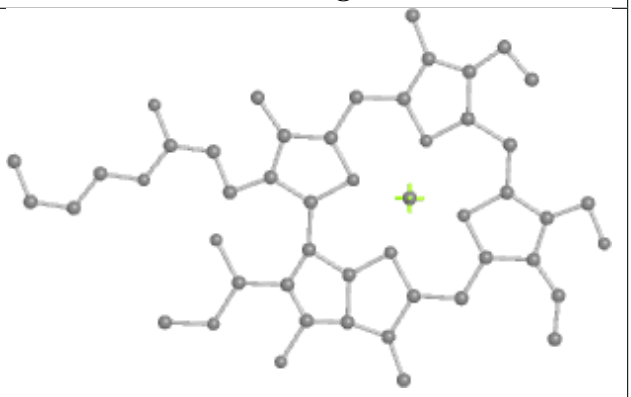


Bond angles

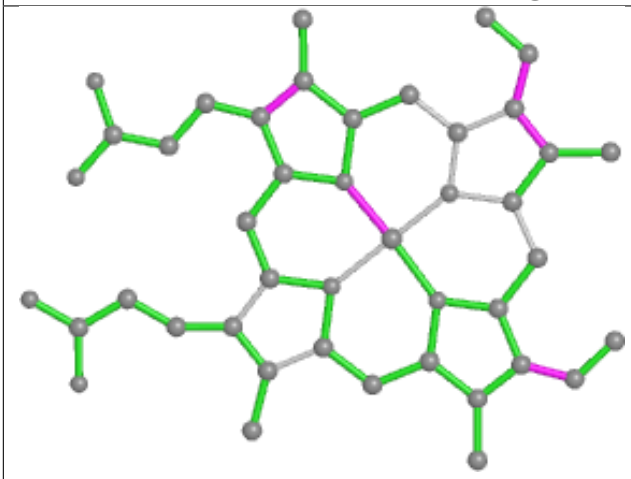


Torsions

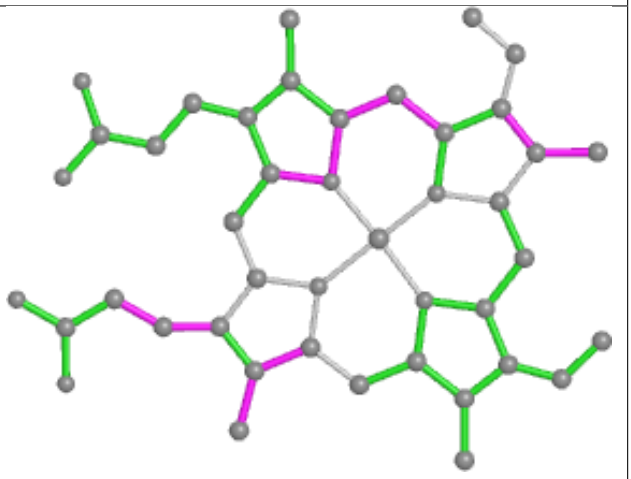


Rings

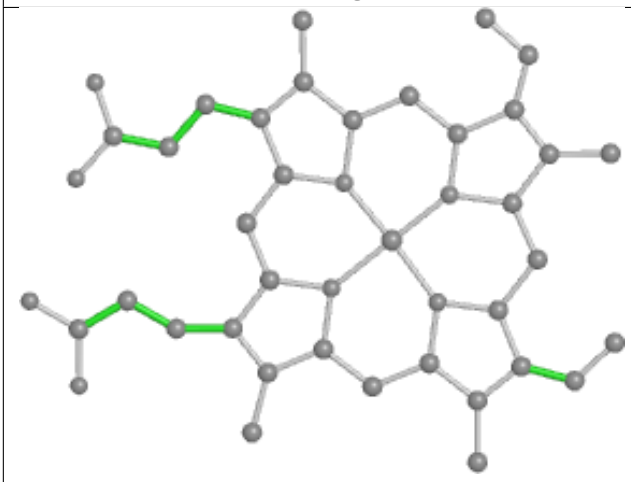
Ligand HEM f 101



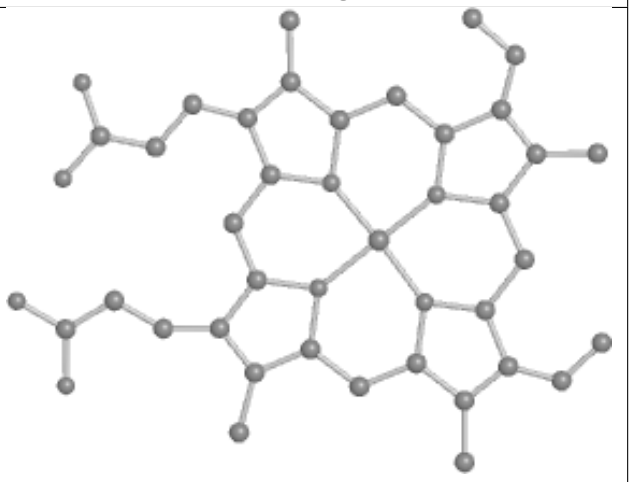
Bond lengths



Bond angles

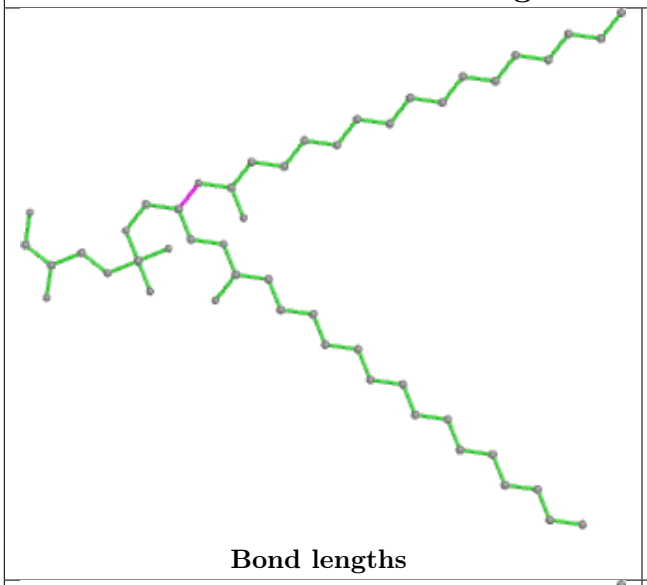


Torsions

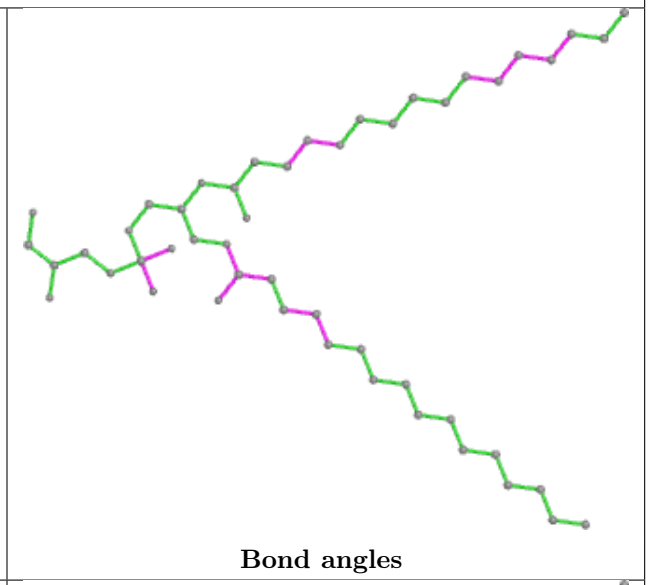


Rings

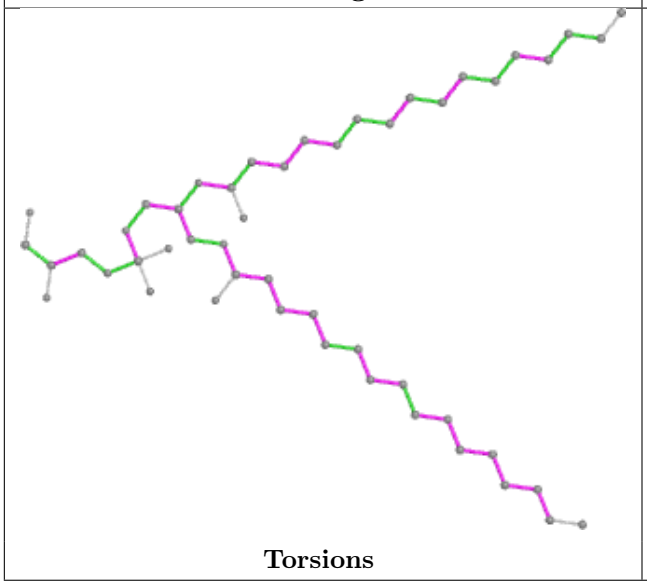
Ligand LHG G 2630



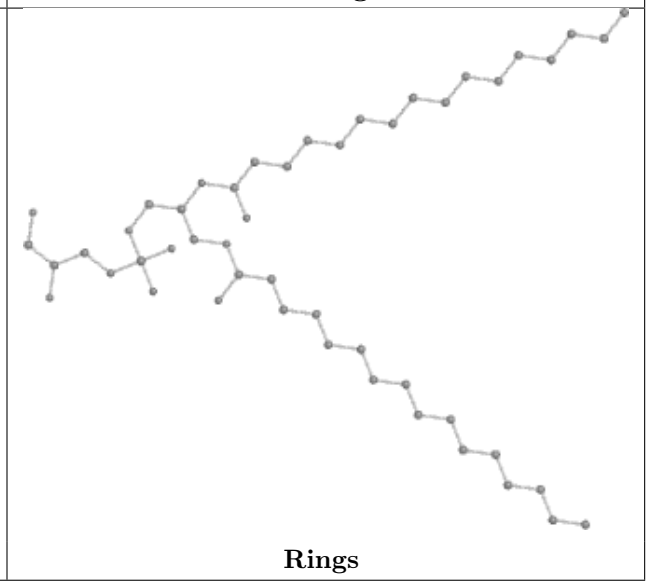
Bond lengths



Bond angles

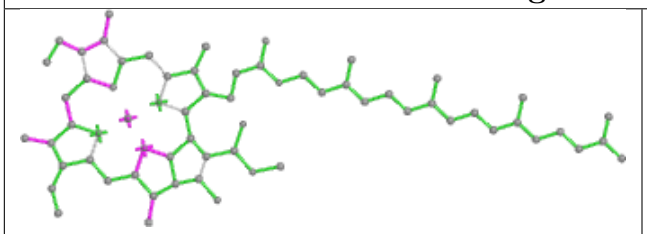


Torsions

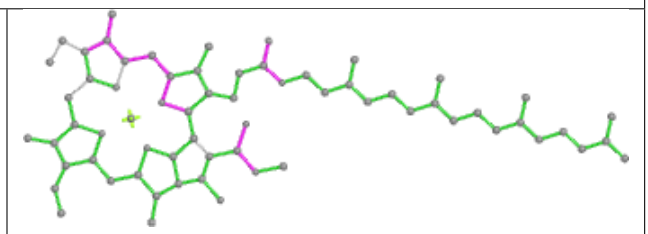


Rings

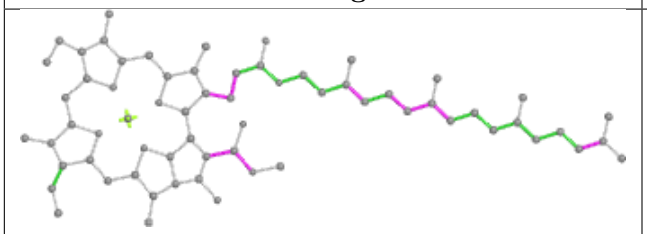
Ligand CLA b 604



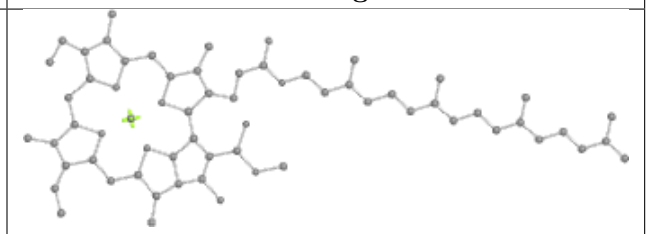
Bond lengths



Bond angles

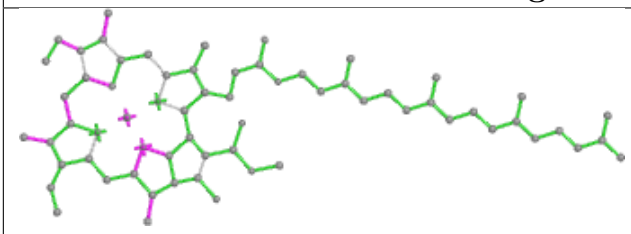


Torsions

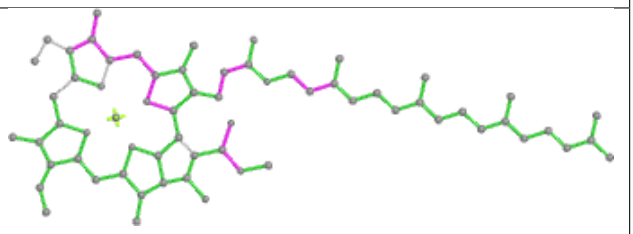


Rings

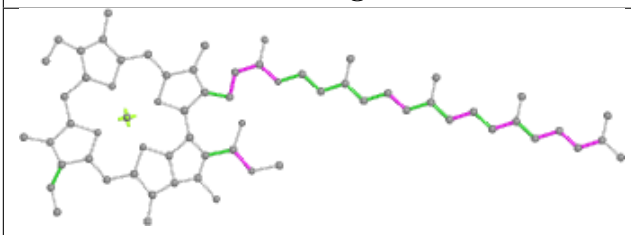
Ligand CLA a 405



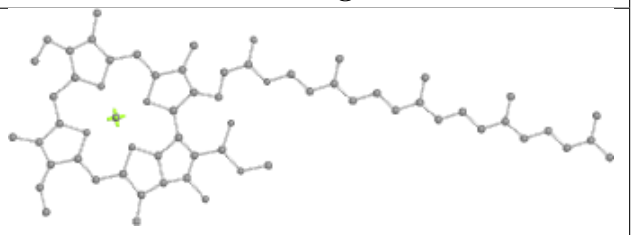
Bond lengths



Bond angles

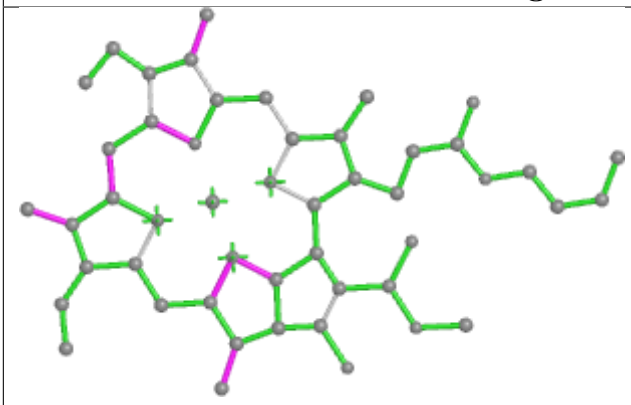


Torsions

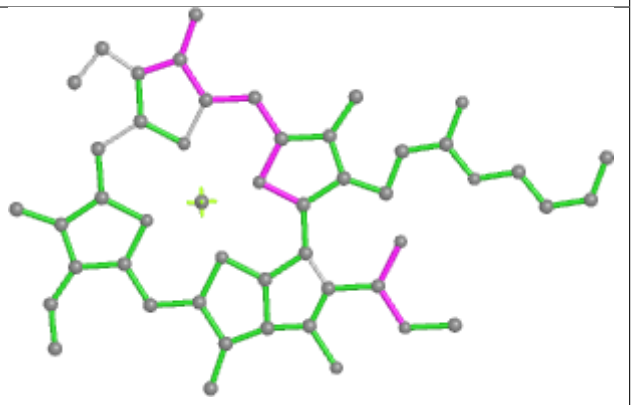


Rings

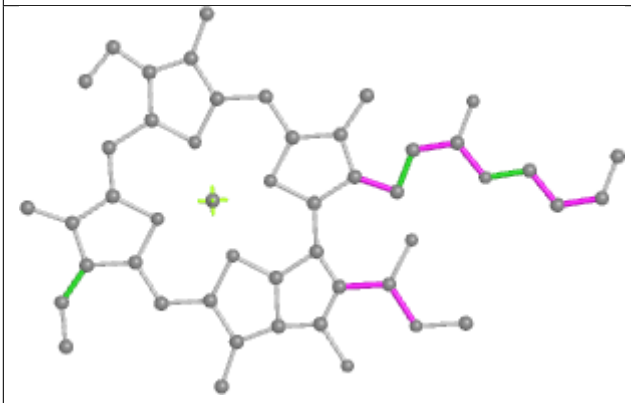
Ligand CLA S 603



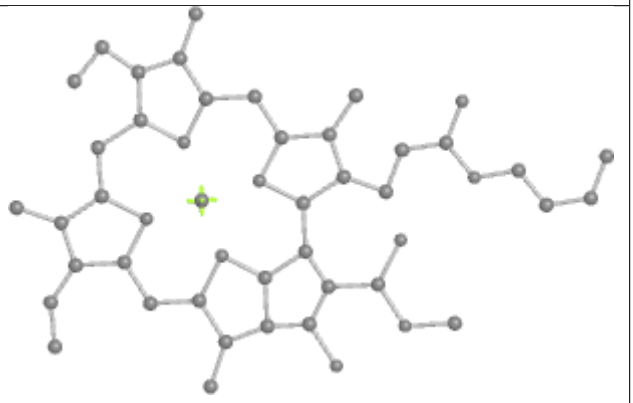
Bond lengths



Bond angles

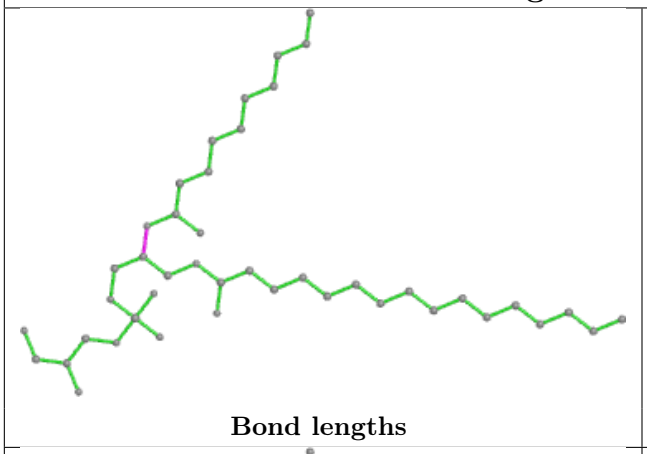


Torsions



Rings

Ligand LHG d 408



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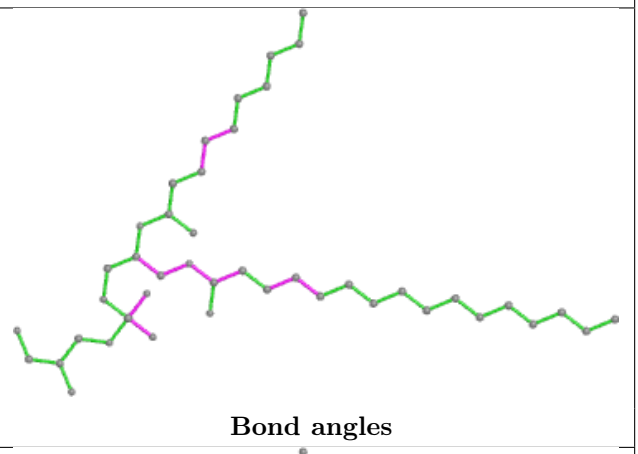
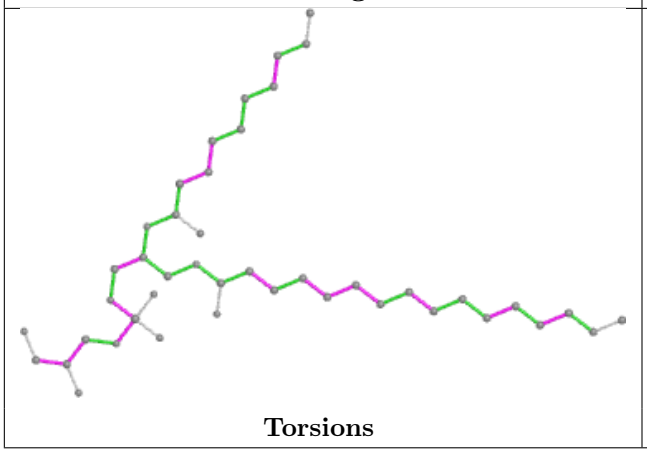


Bond angles



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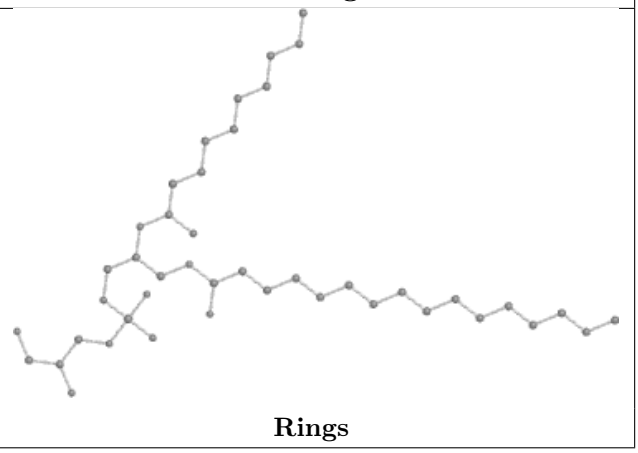
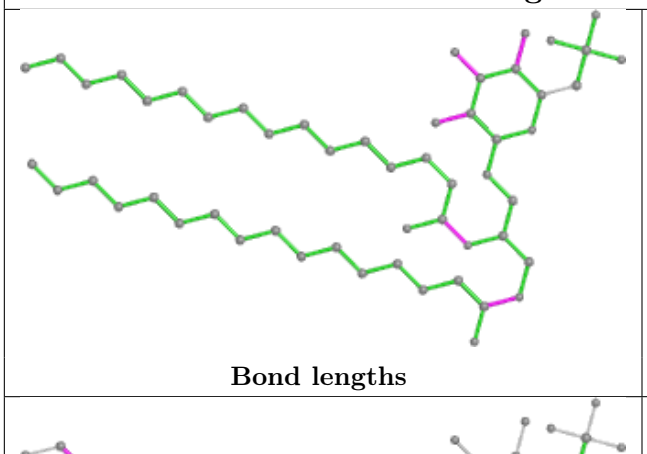


Rings

Ligand SQD A 412



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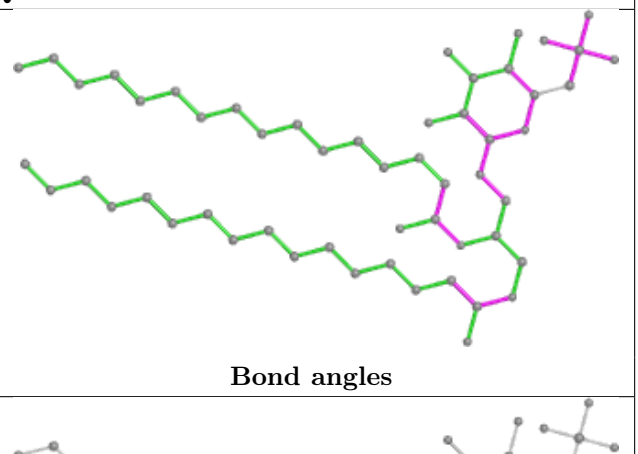
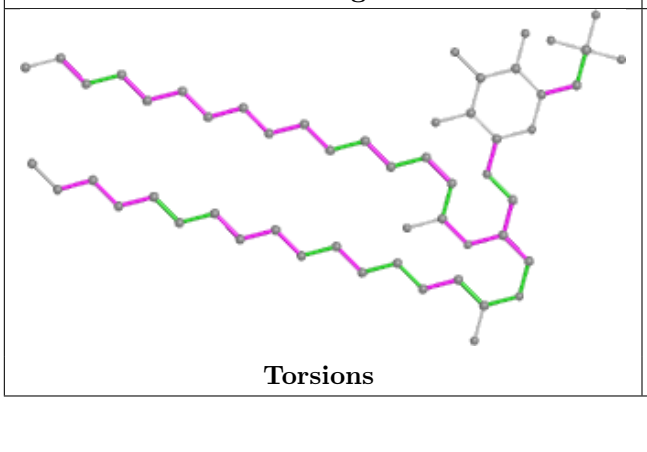
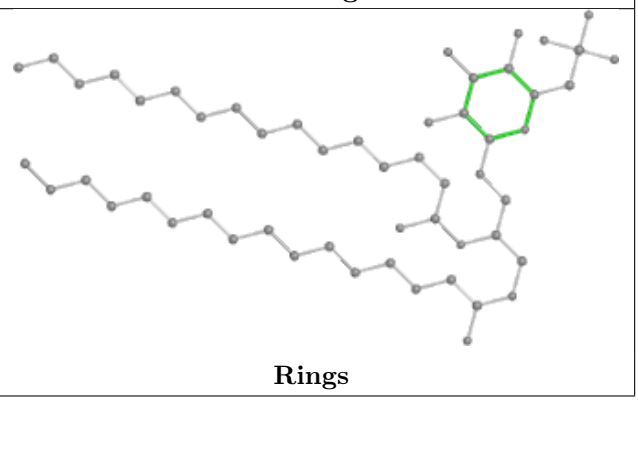


Bond angles

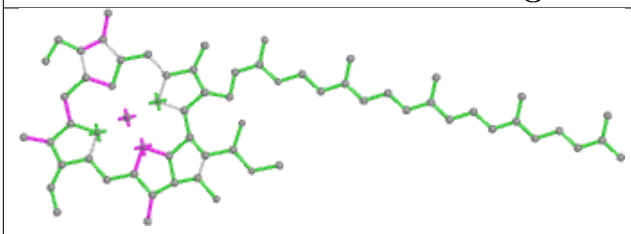


Torsions

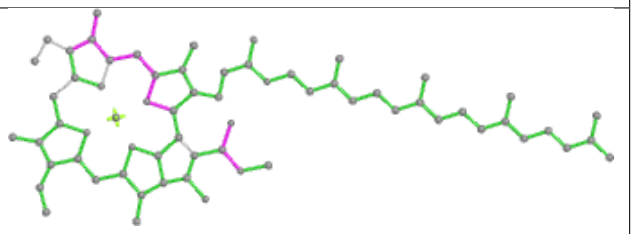


Rings

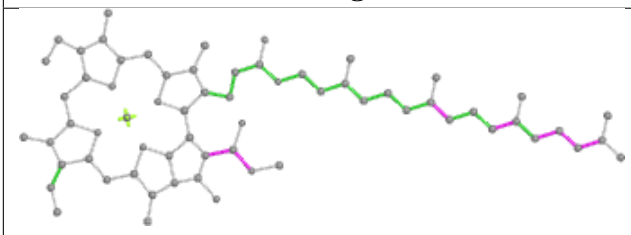
Ligand CLA B 616



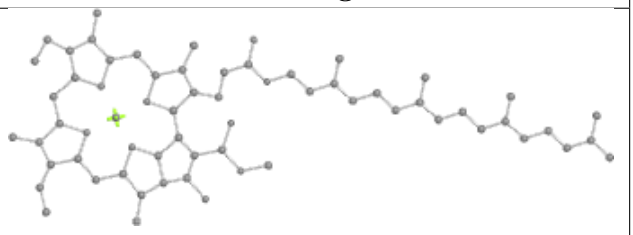
Bond lengths



Bond angles

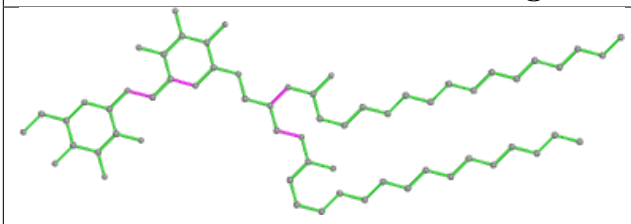


Torsions



Rings

Ligand DGD c 520



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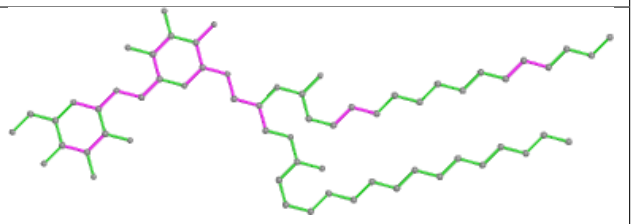
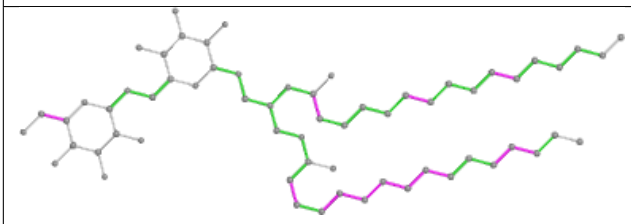
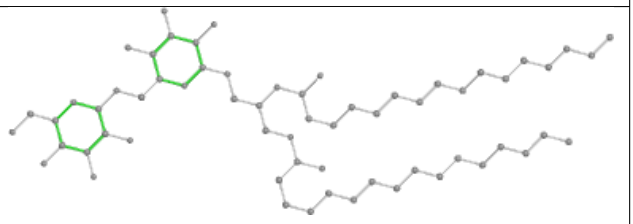


Bond angles

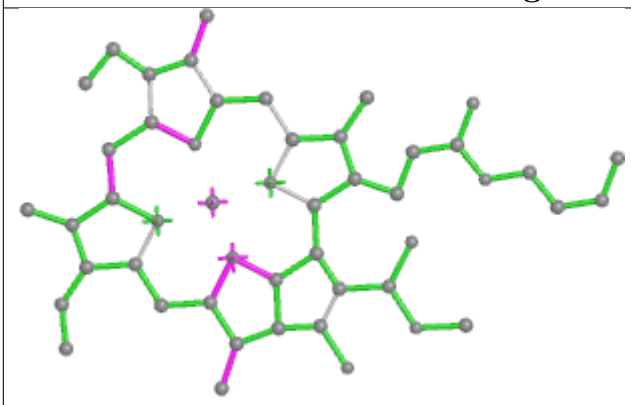


Torsions

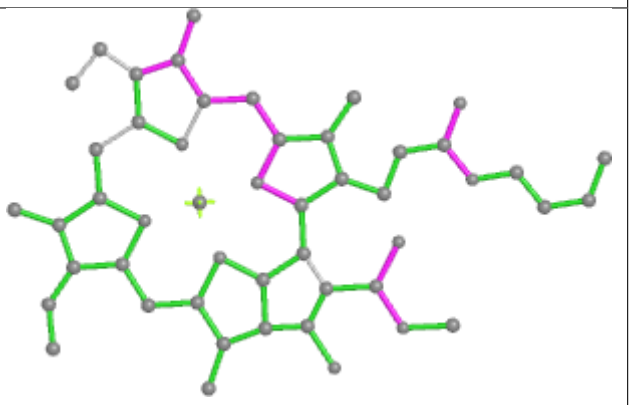


Rings

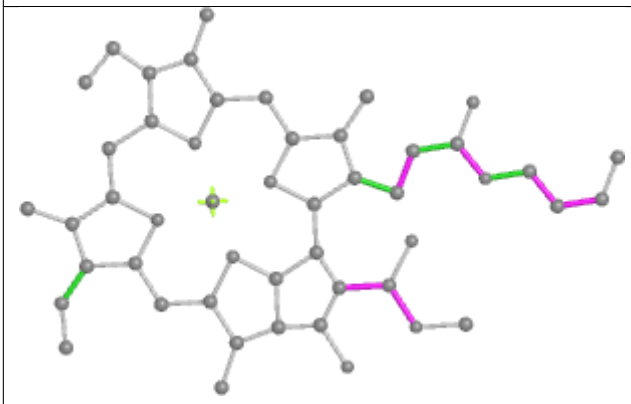
Ligand CLA N 614



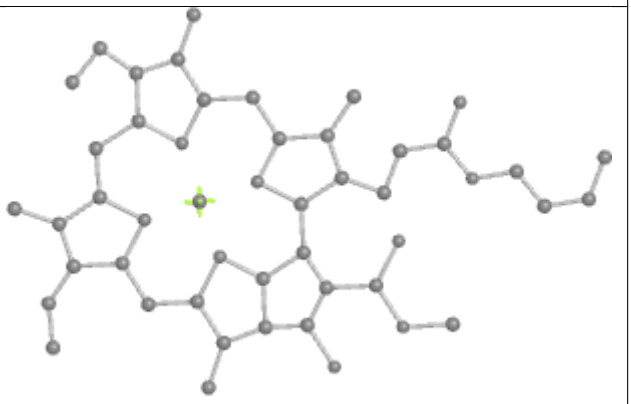
Bond lengths



Bond angles

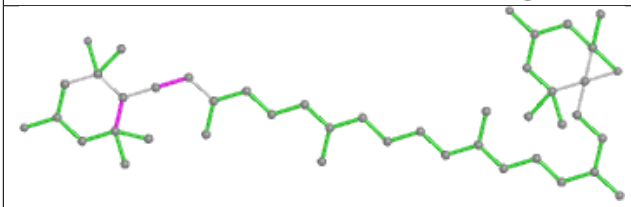


Torsions

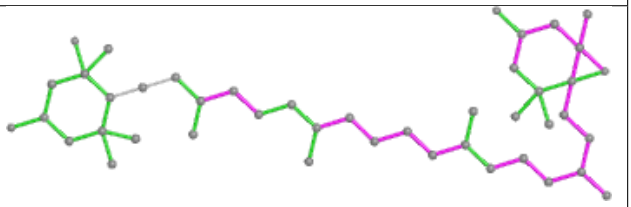


Rings

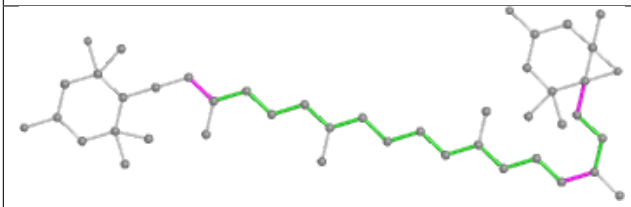
Ligand NEX s 1623



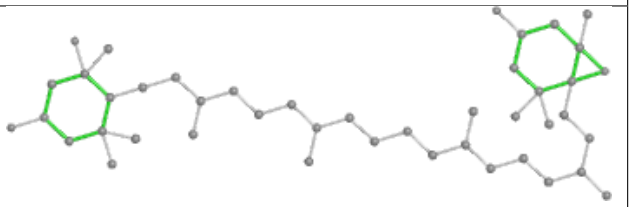
Bond lengths



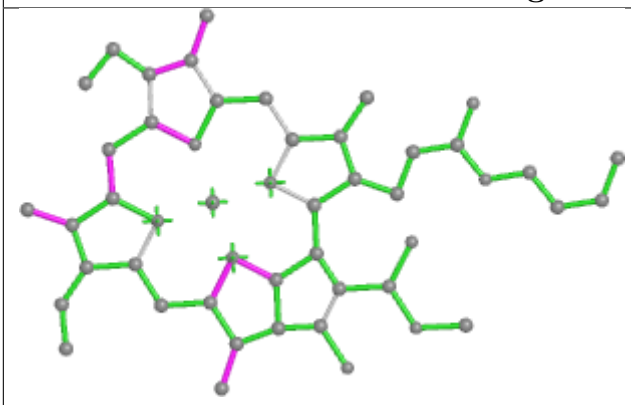
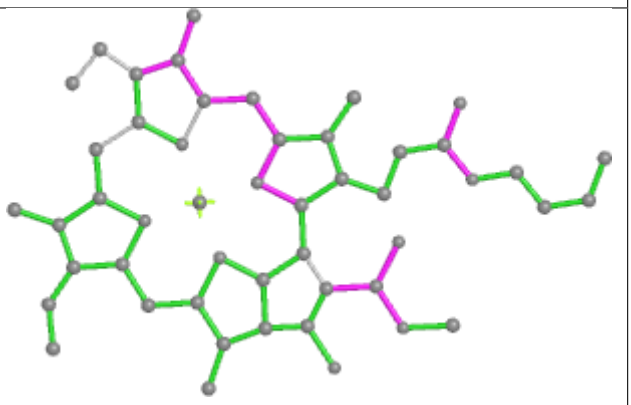
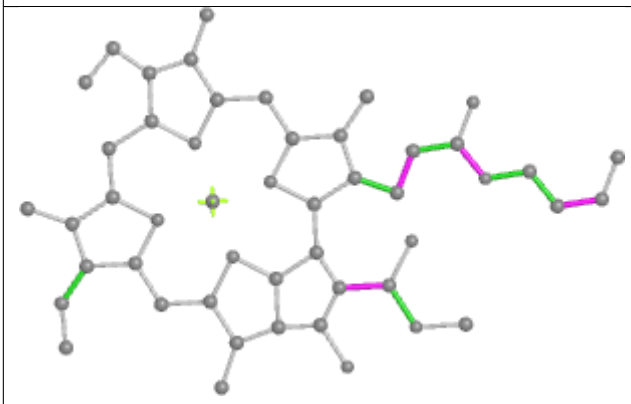
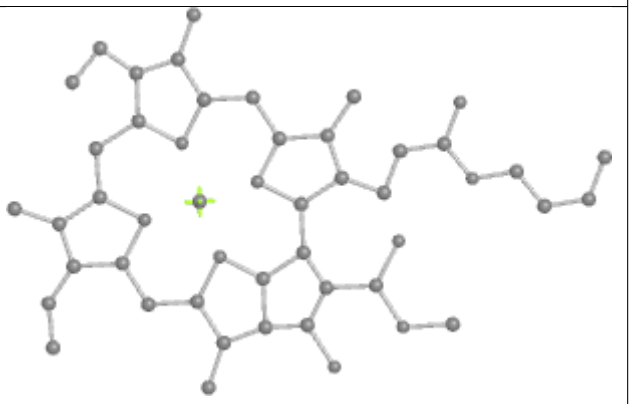
Bond angles

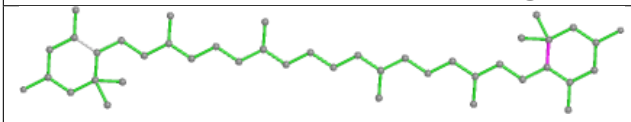
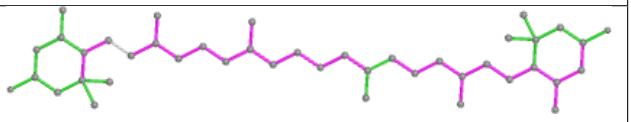
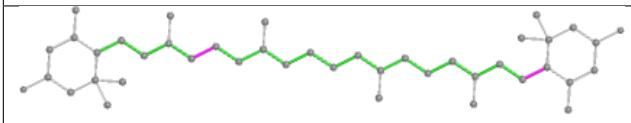
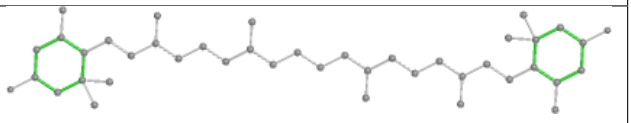


Torsions

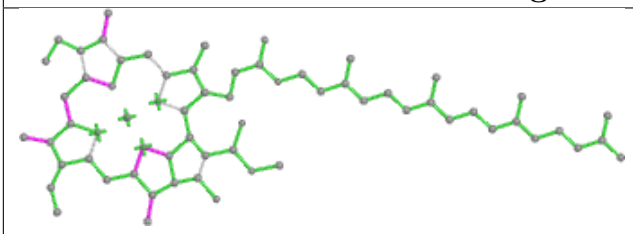


Rings

Ligand CLA n 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT s 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 610



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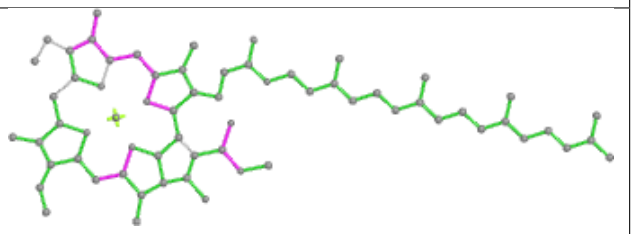
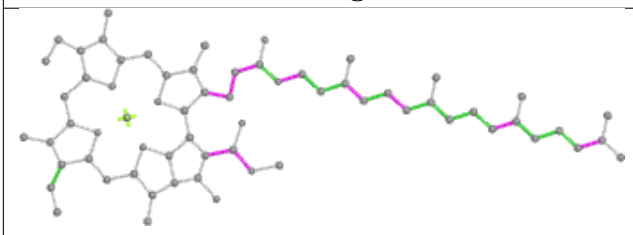


Bond angles



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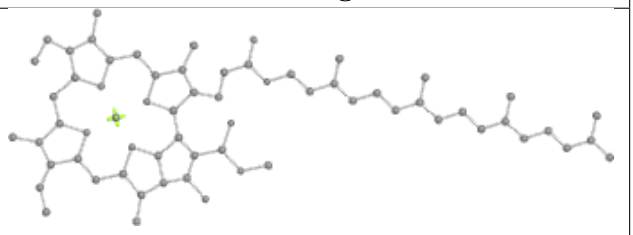
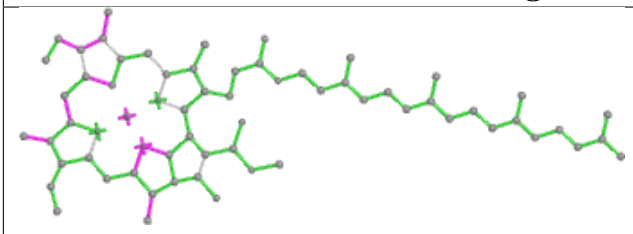


Rings

Ligand CLA B 606



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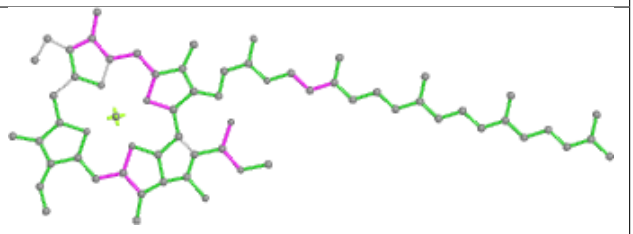
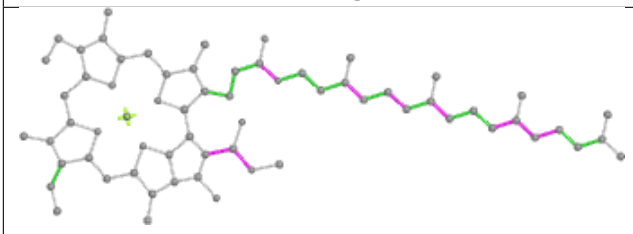
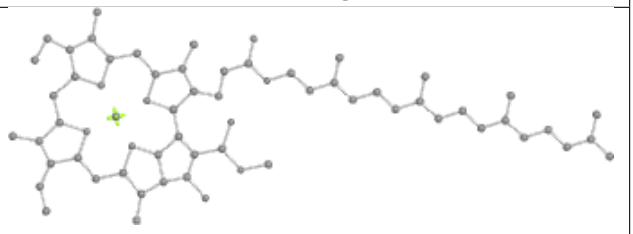


Bond angles

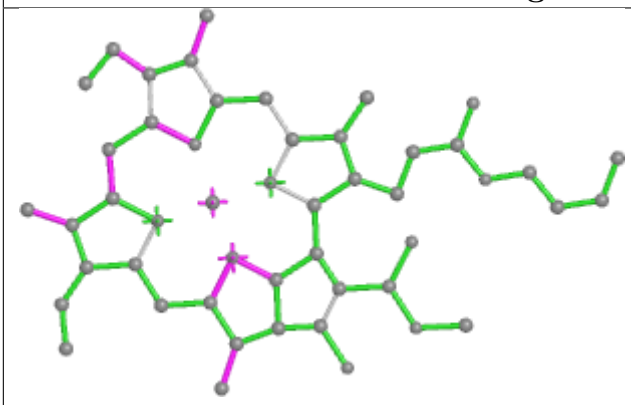


Torsions



Rings

Ligand CLA S 613



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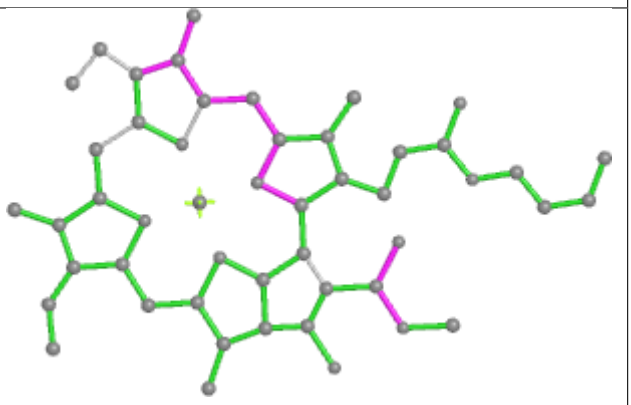
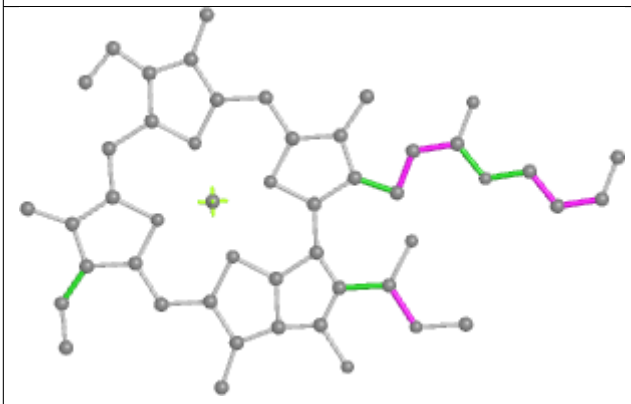


Bond angles



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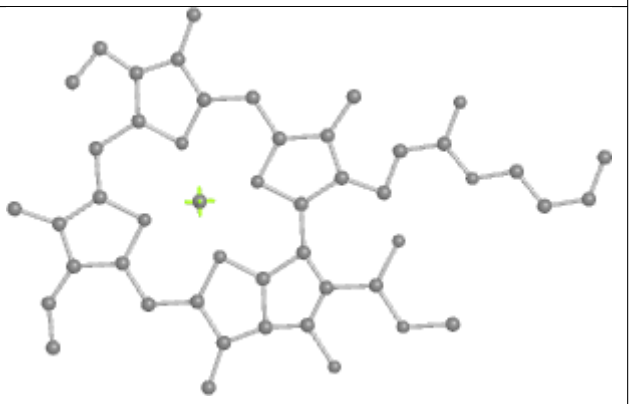
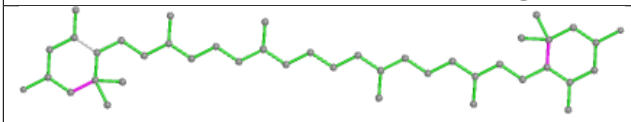


Rings

Ligand LUT Y 1620



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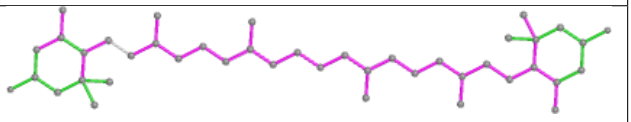
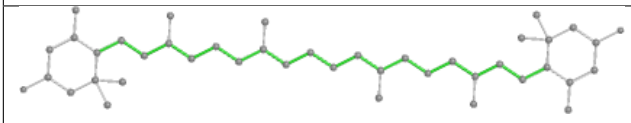


Bond angles



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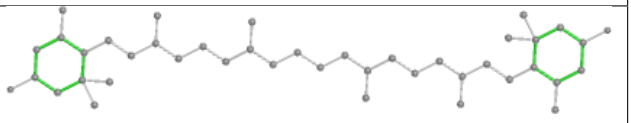
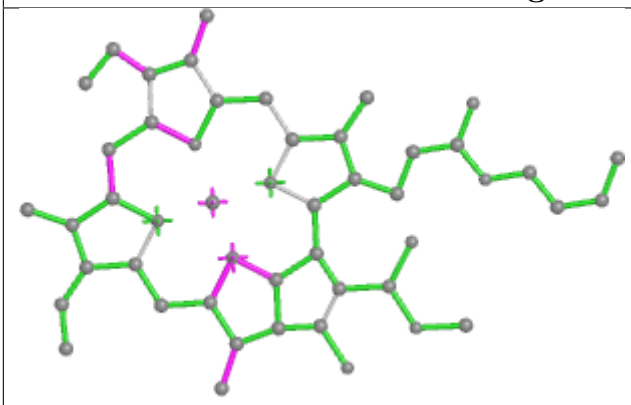


Rings

Ligand CLA y 614



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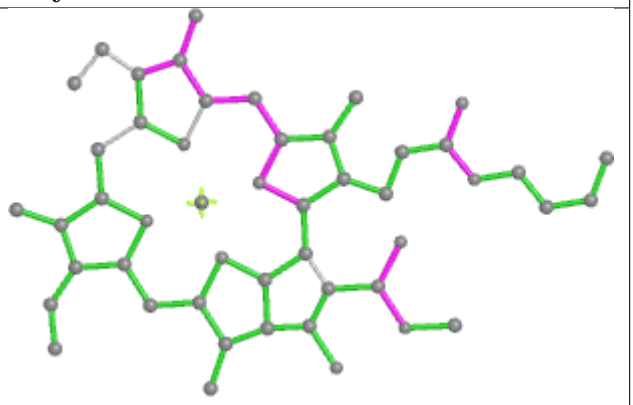
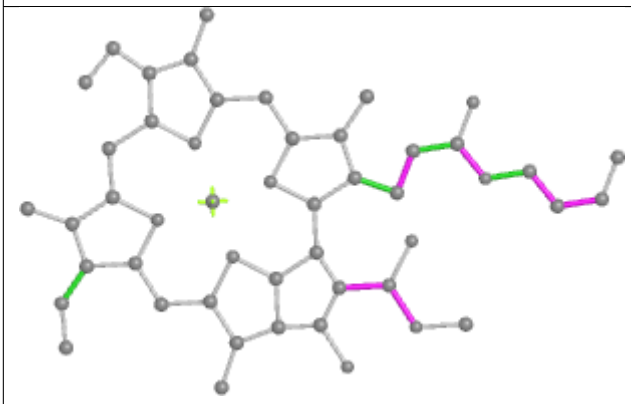


Bond angles



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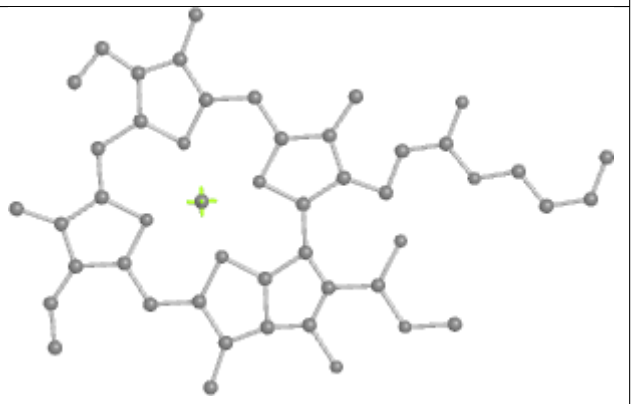
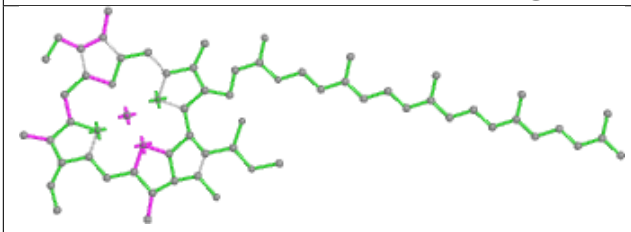


Rings

Ligand CLA b 607



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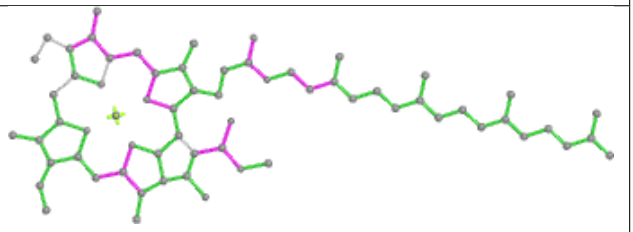

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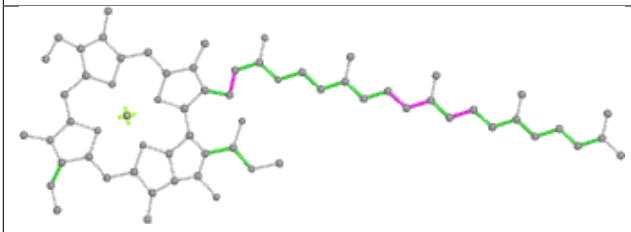

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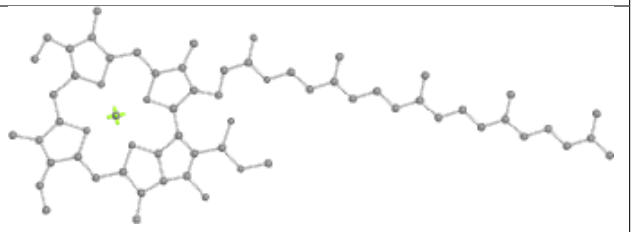
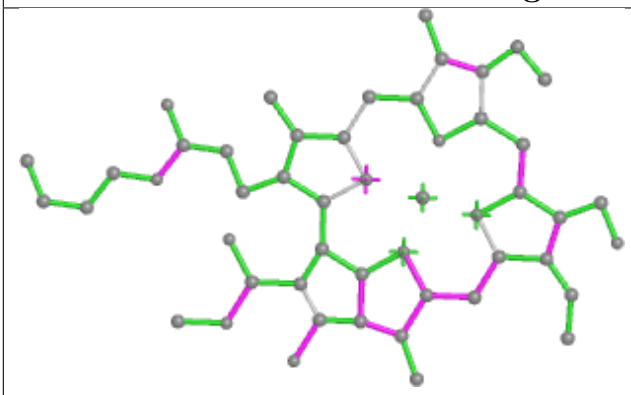


Rings

Ligand CHL Y 608



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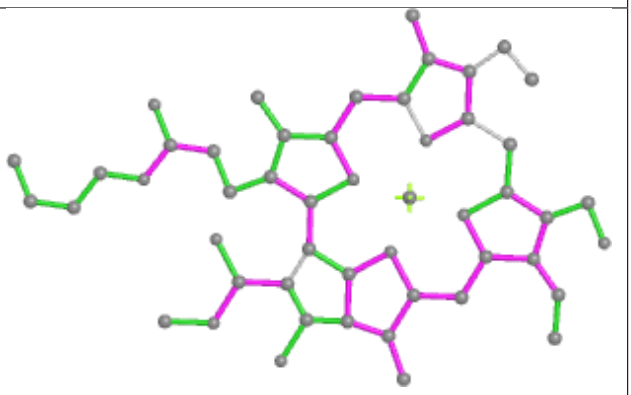
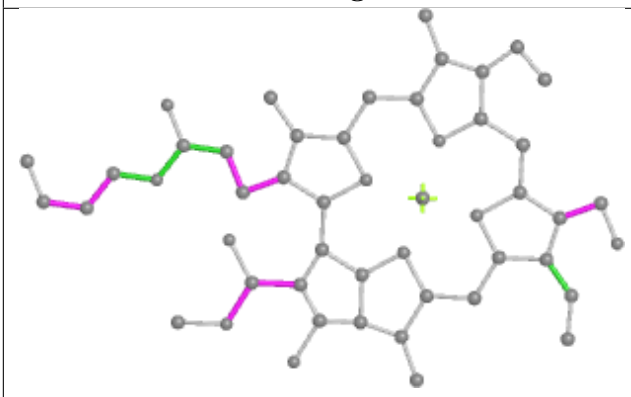


Bond angles



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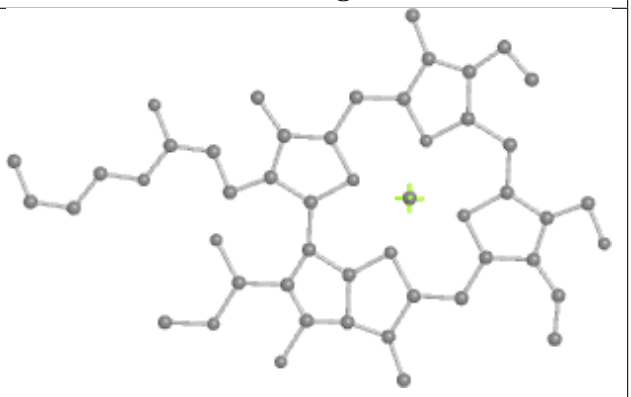
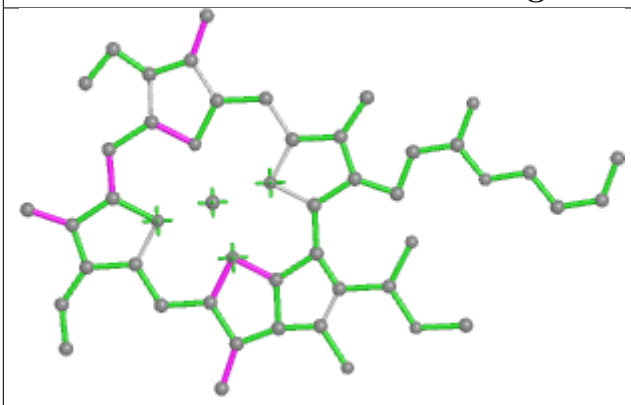


Rings

Ligand CLA S 610



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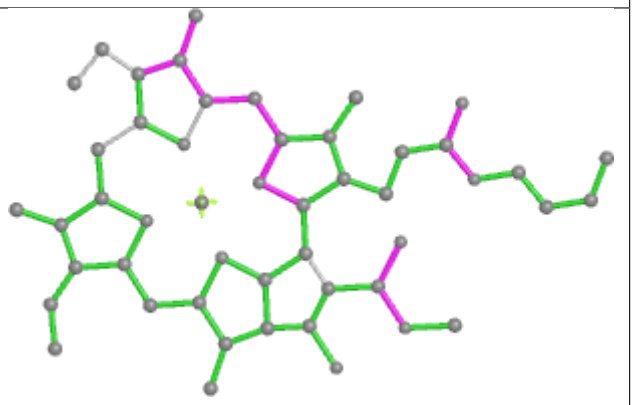

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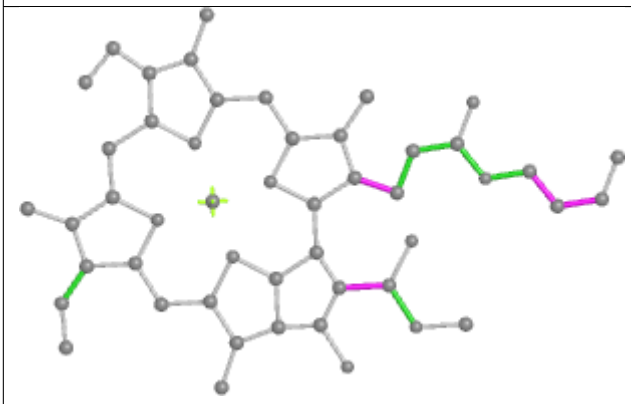
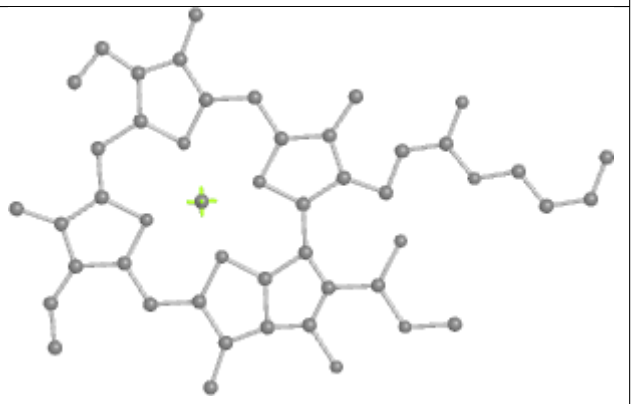
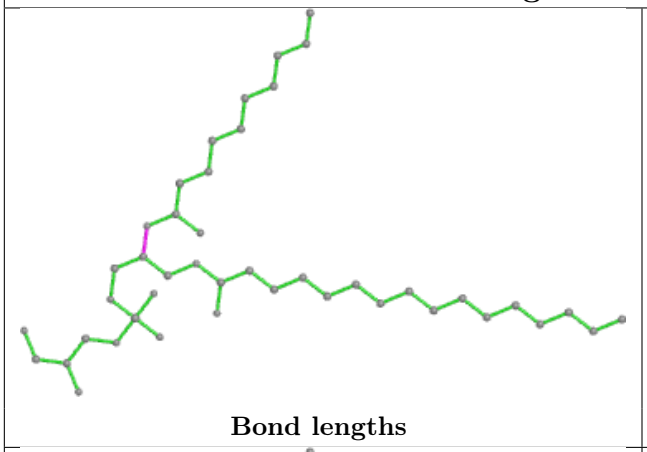


Torsions

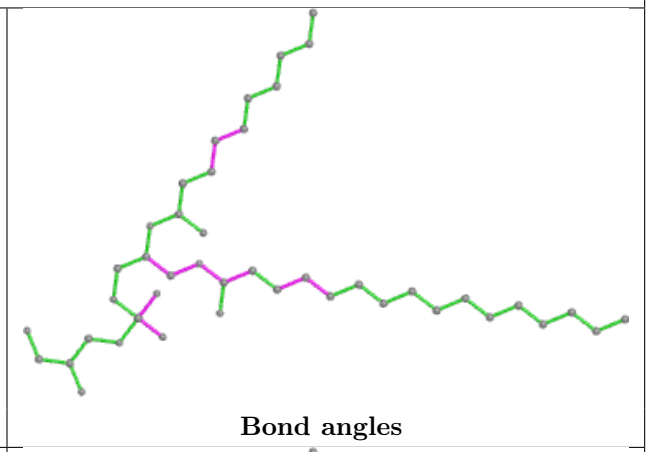


Rings

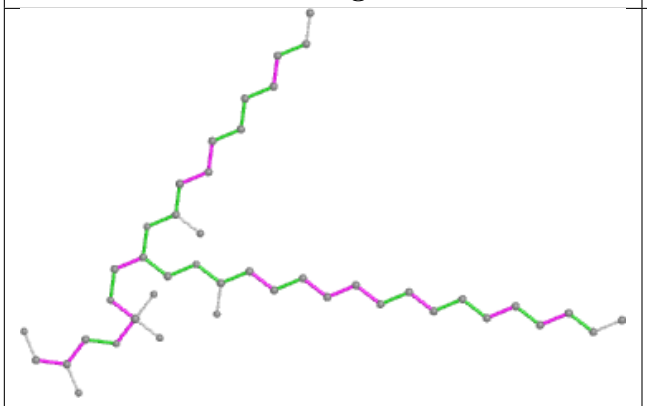
Ligand LHG D 408



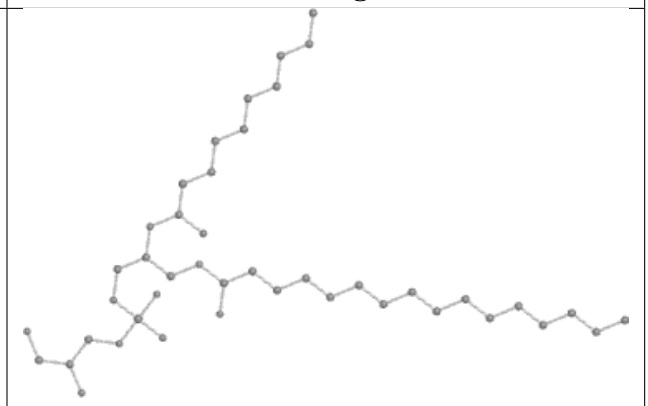
Bond lengths



Bond angles

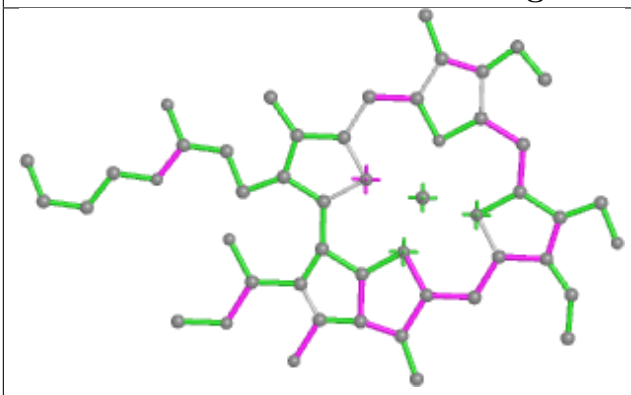


Torsions



Rings

Ligand CHL S 606



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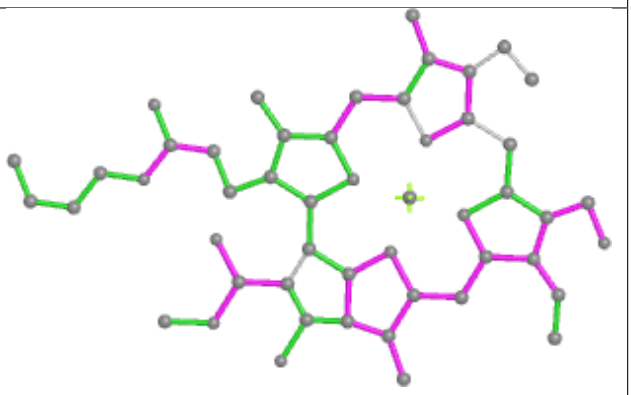
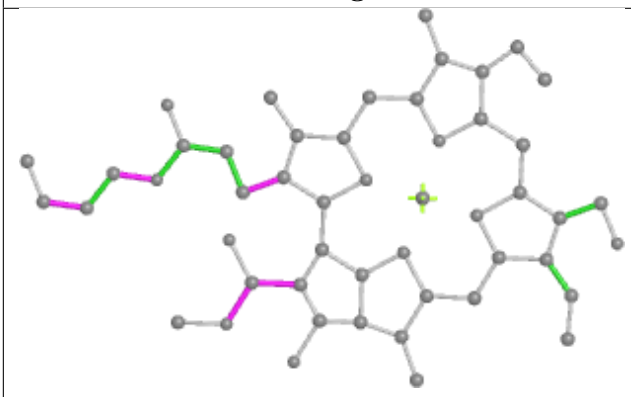


Bond angles



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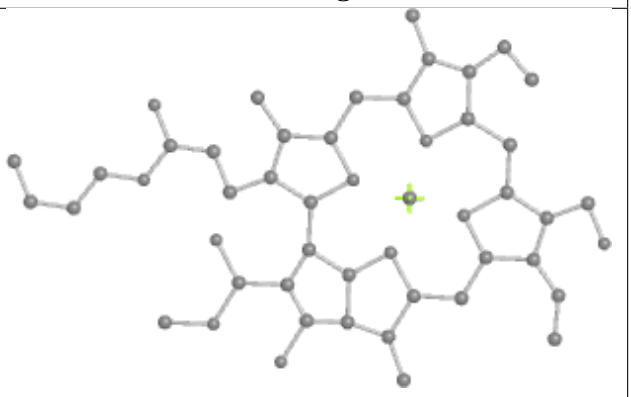
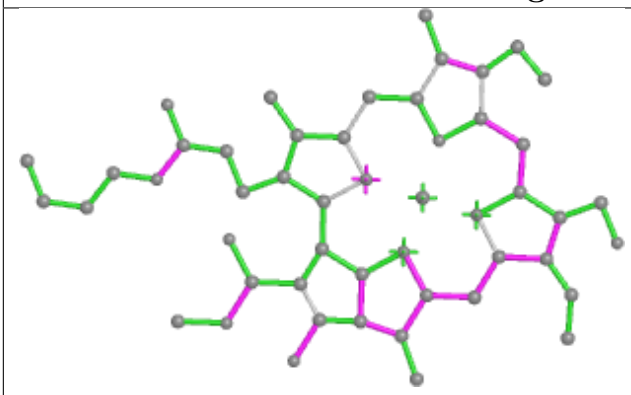


Rings

Ligand CHL g 606



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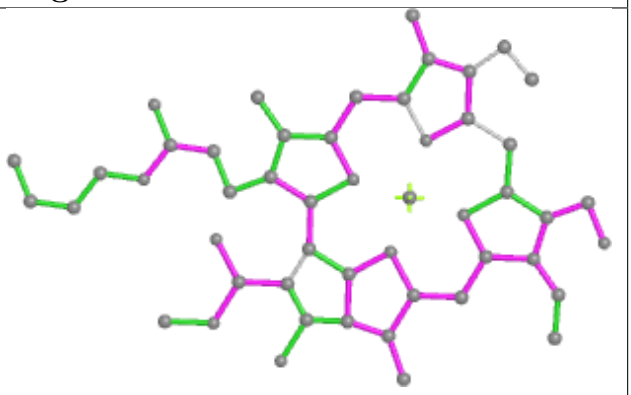
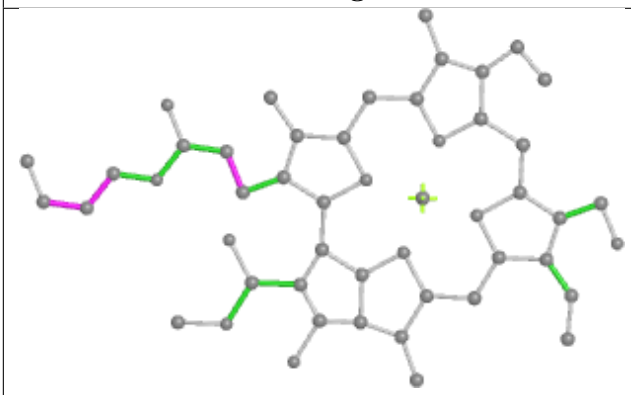
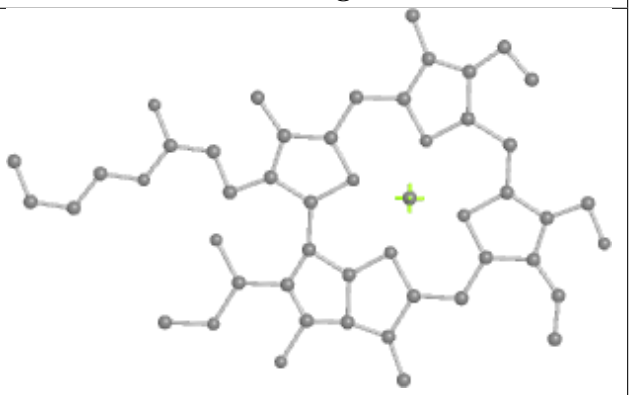


Bond angles

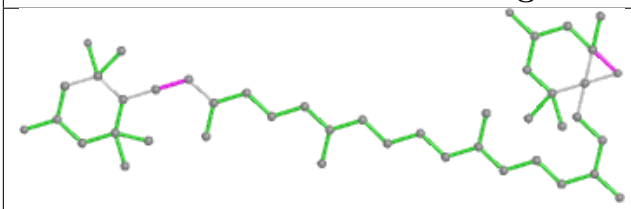


Torsions

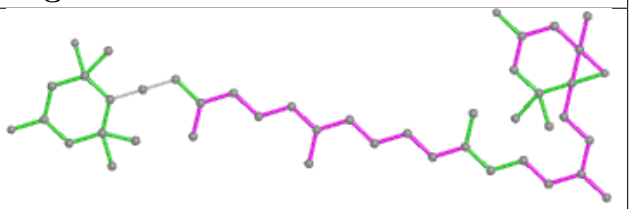


Rings

Ligand NEX g 1623



Bond lengths

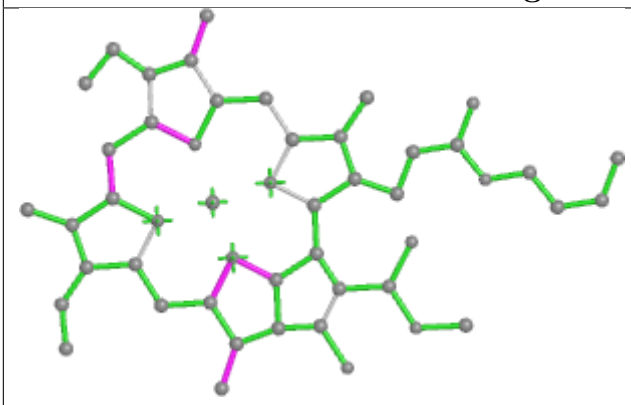


Bond angles

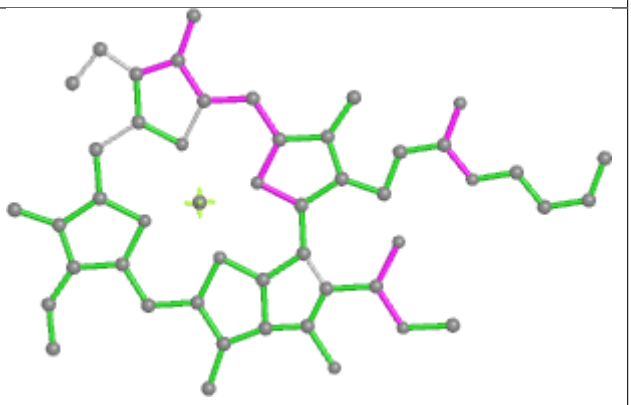
Torsions

Rings

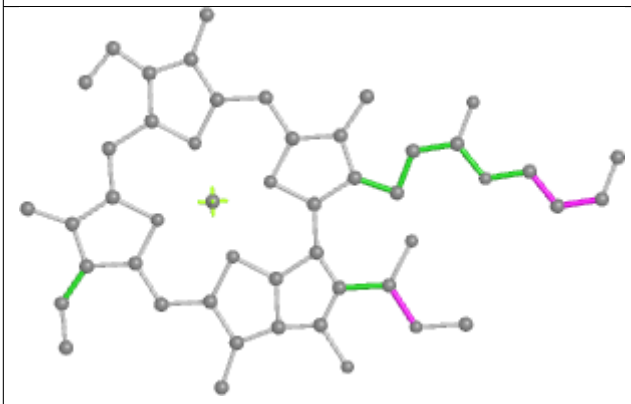
Ligand CLA R 612



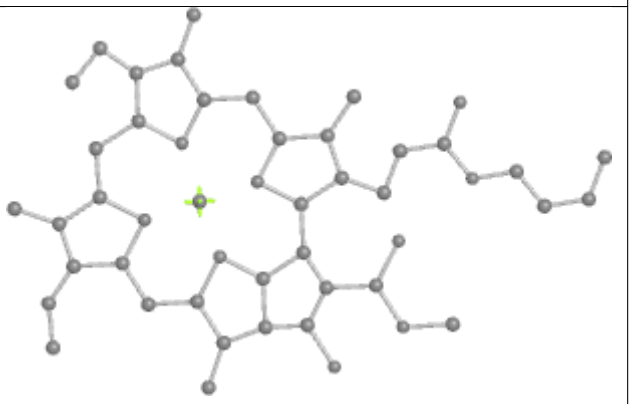
Bond lengths



Bond angles

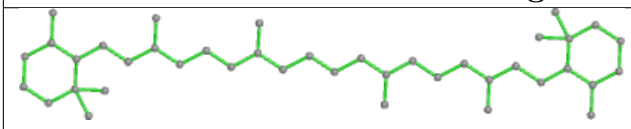


Torsions

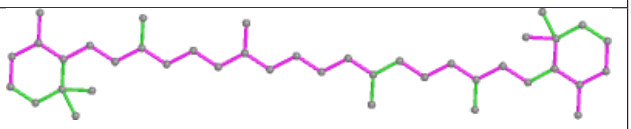


Rings

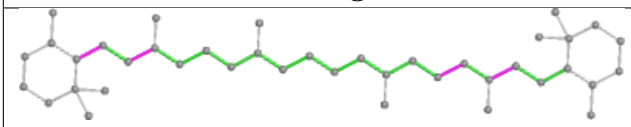
Ligand BCR c 516



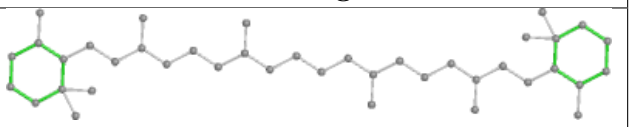
Bond lengths



Bond angles

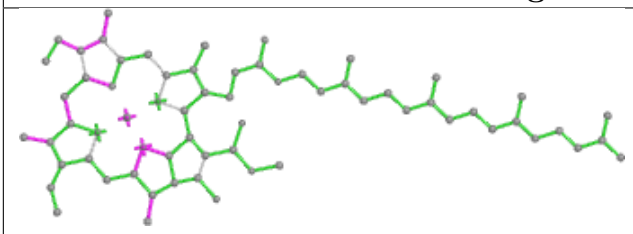


Torsions

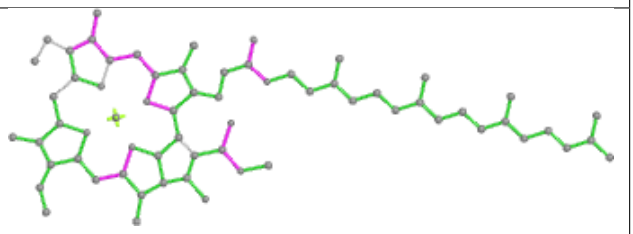


Rings

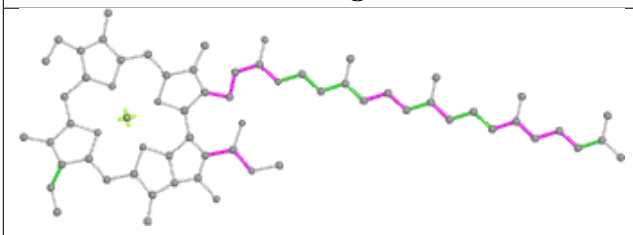
Ligand CLA b 602



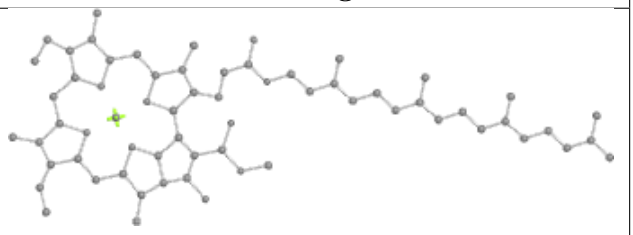
Bond lengths



Bond angles

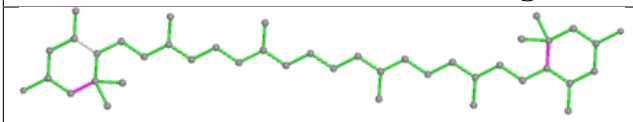


Torsions

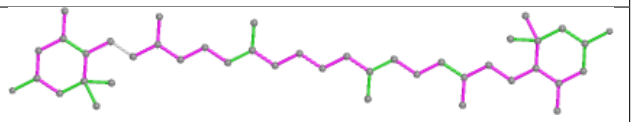


Rings

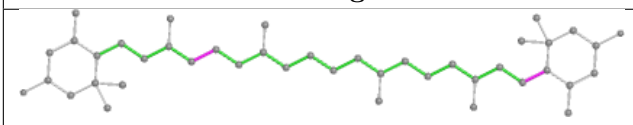
Ligand LUT n 1621



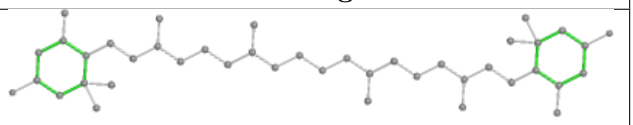
Bond lengths



Bond angles

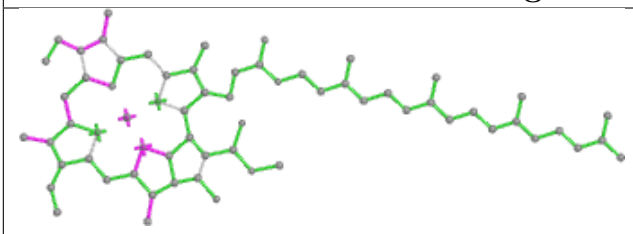


Torsions



Rings

Ligand CLA B 603



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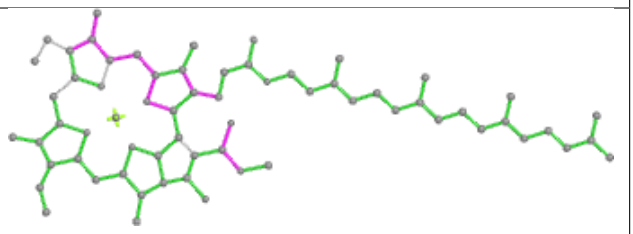
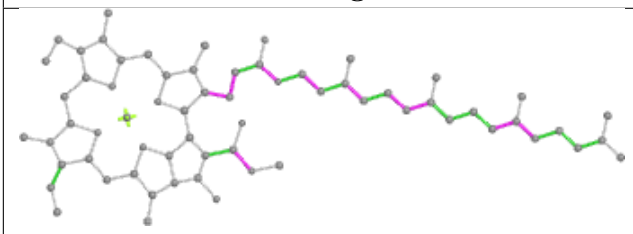
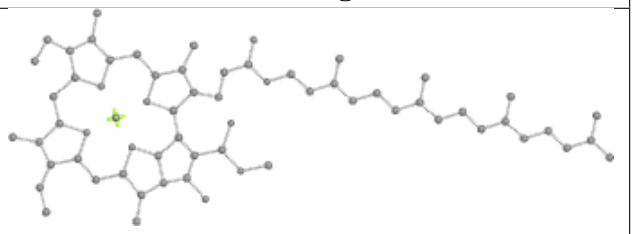


Bond angles

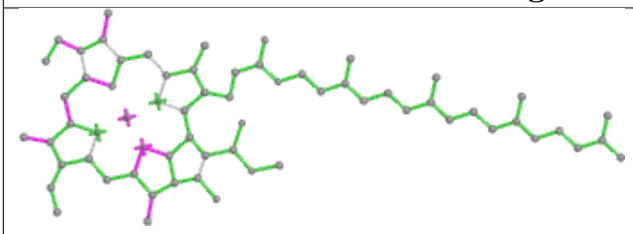


Torsions

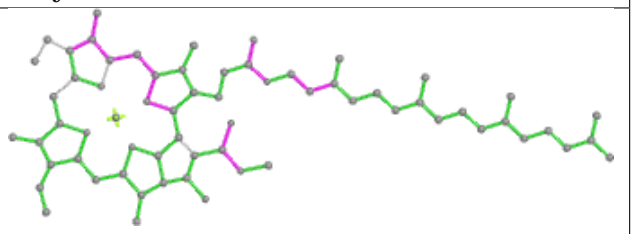


Rings

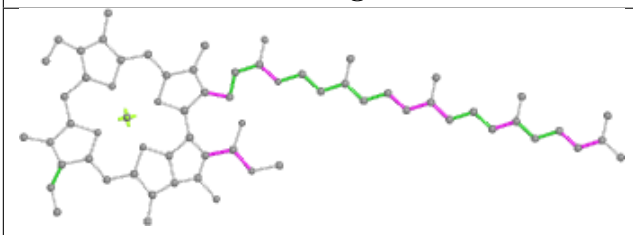
Ligand CLA y 610



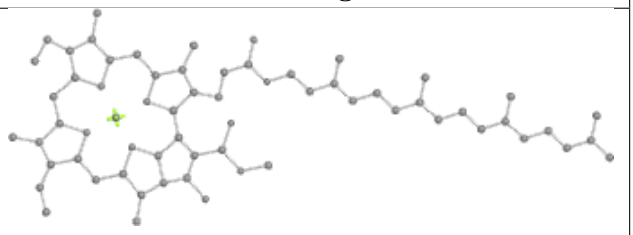
Bond lengths



Bond angles

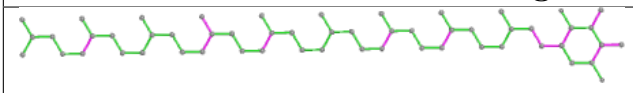


Torsions



Rings

Ligand PL9 d 405



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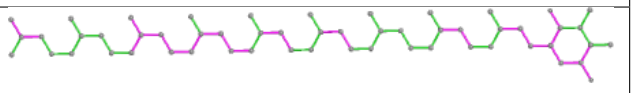
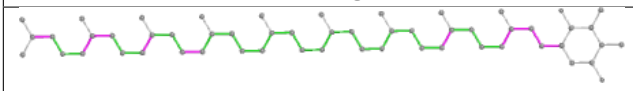


Bond angles



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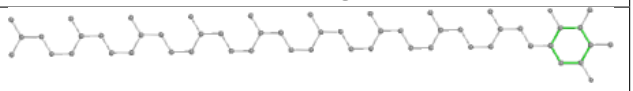
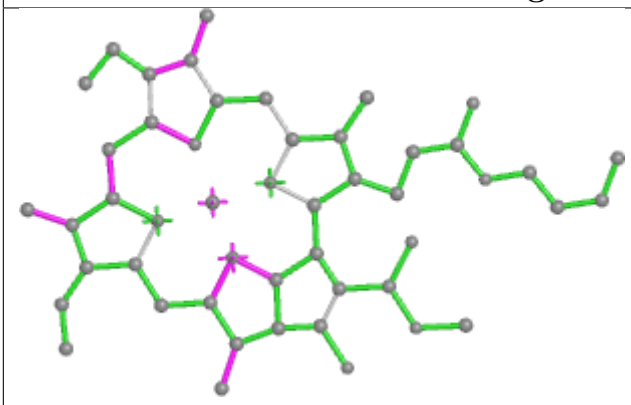


Rings

Ligand CLA y 603



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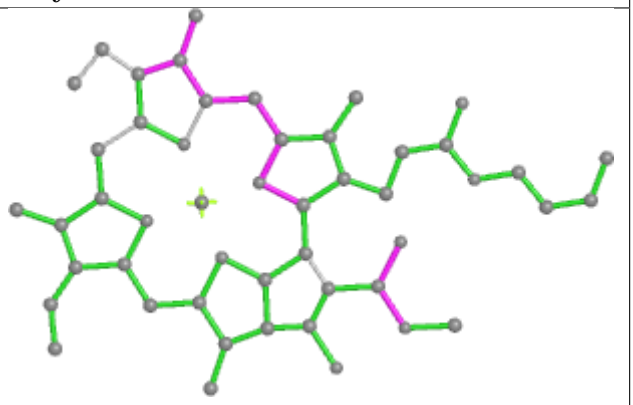
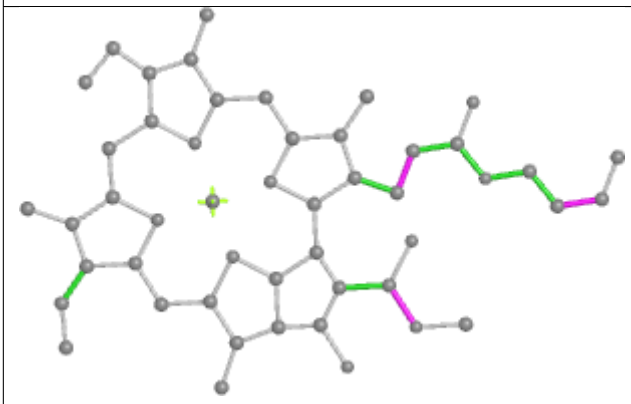


Bond angles



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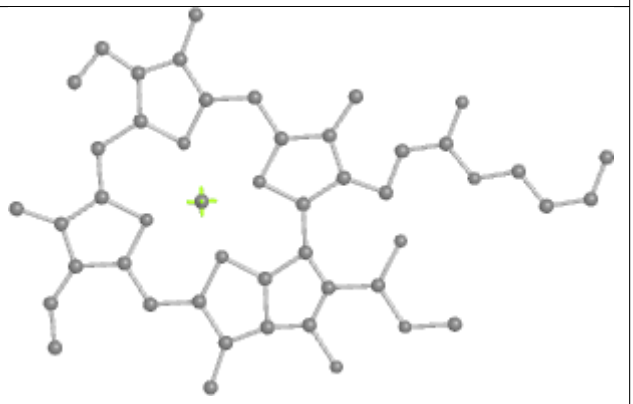
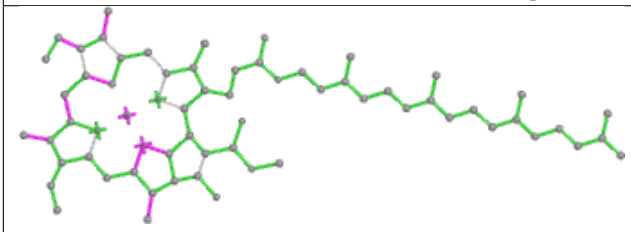


Rings

Ligand CLA C 505



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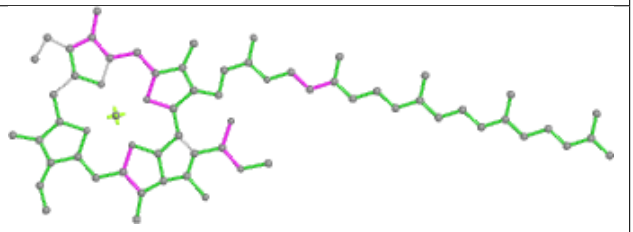
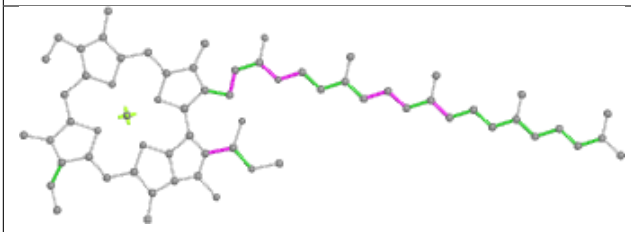


Bond angles



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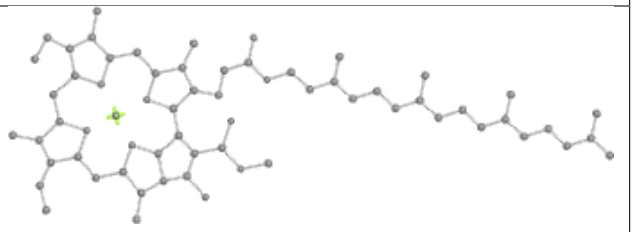
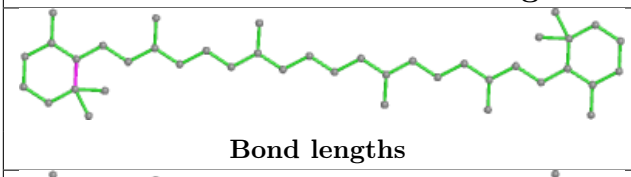


Rings

Ligand BCR H 101



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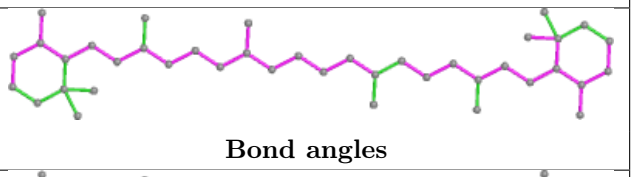
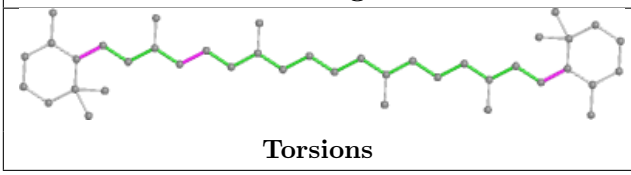
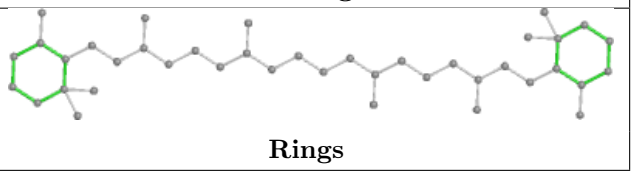


Bond angles

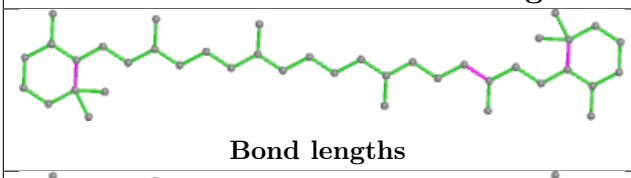


Torsions



Rings

Ligand BCR b 618



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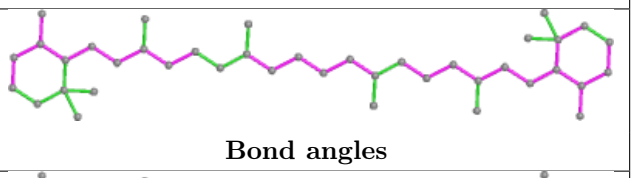
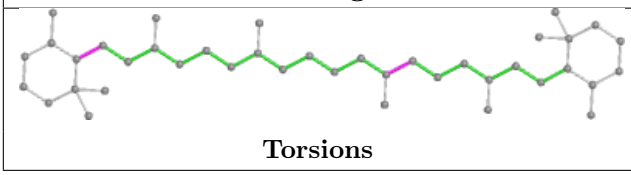
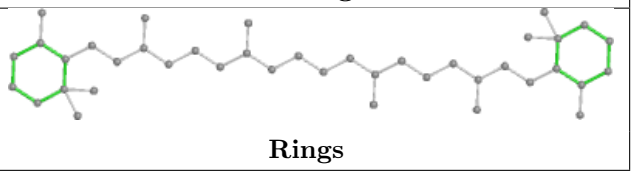


Bond angles

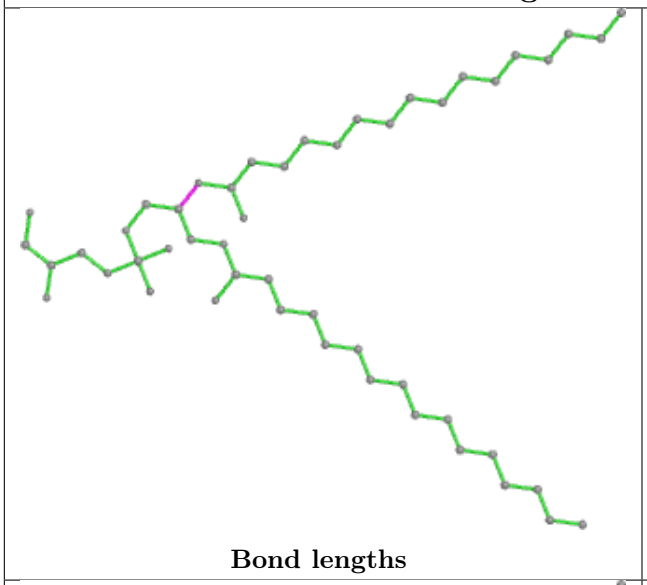


Torsions



Rings

Ligand LHG r 2630



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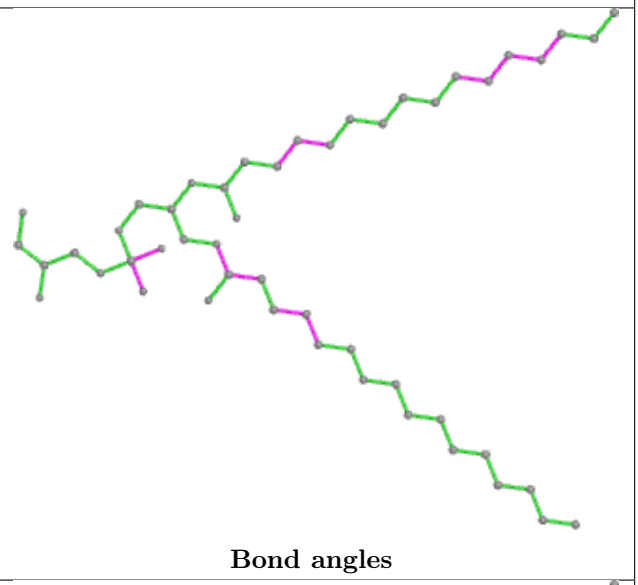
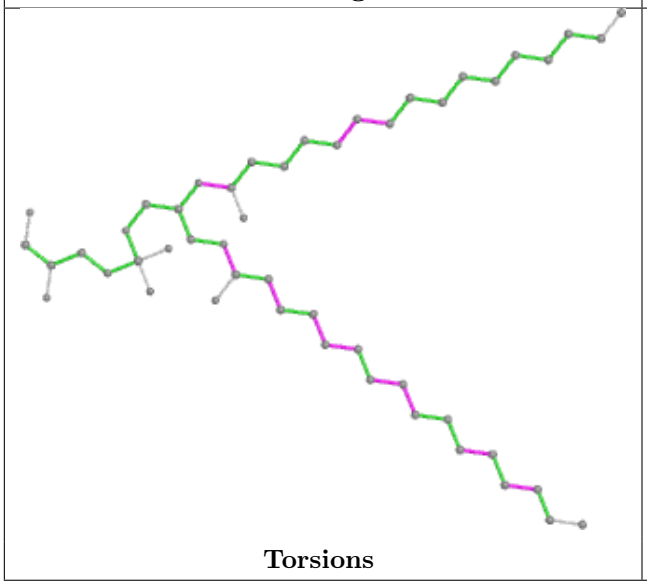
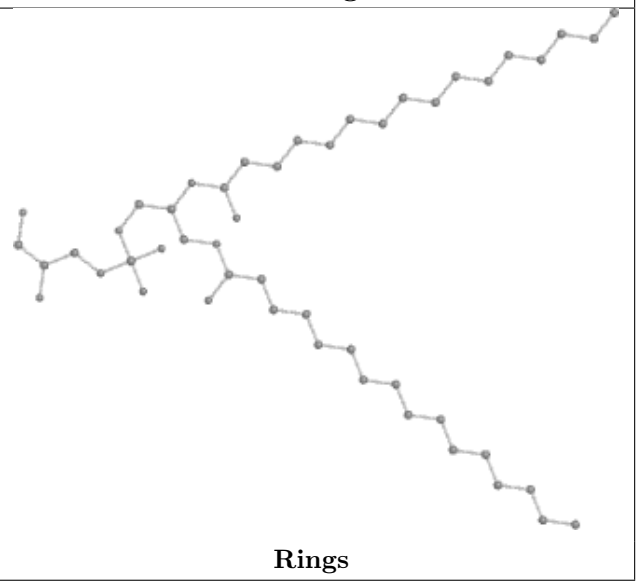


Bond angles

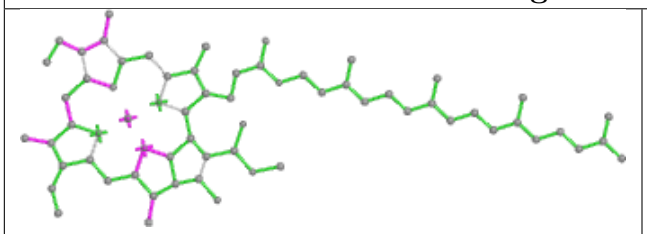


Torsions



Rings

Ligand CLA c 502



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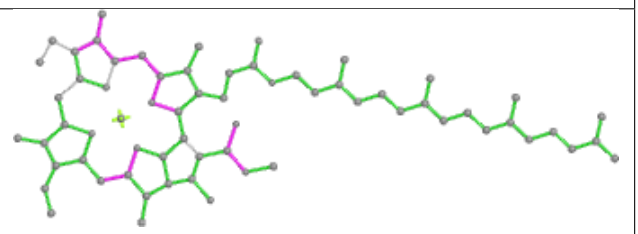
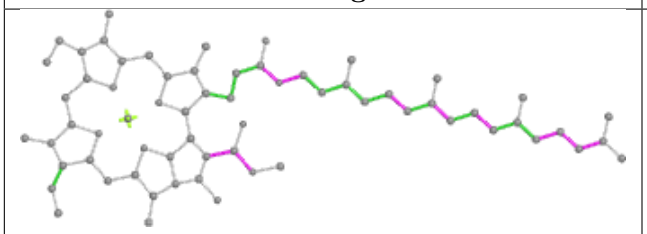


Bond angles



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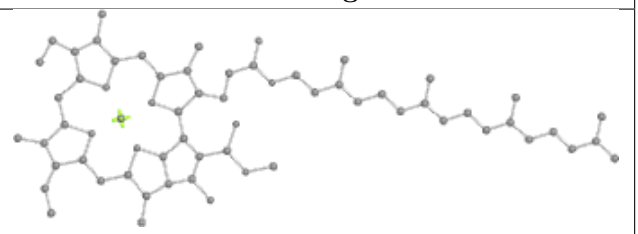
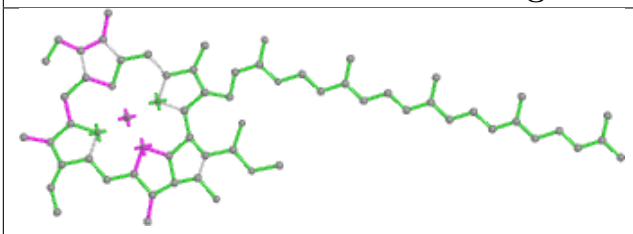
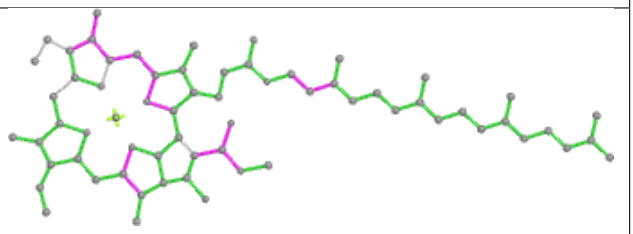


Rings

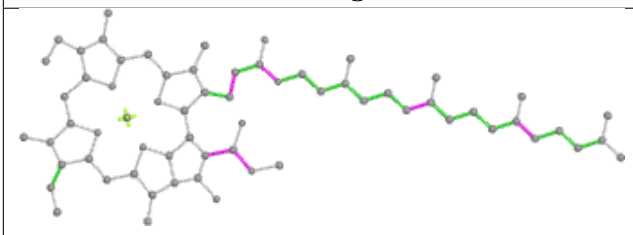
Ligand CLA b 608



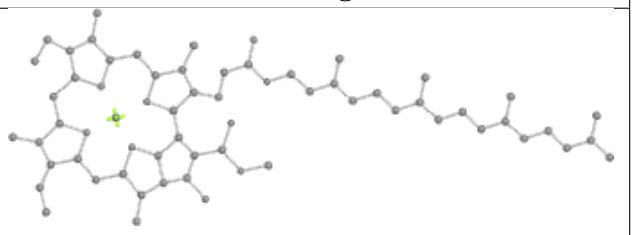
Bond lengths



Bond angles

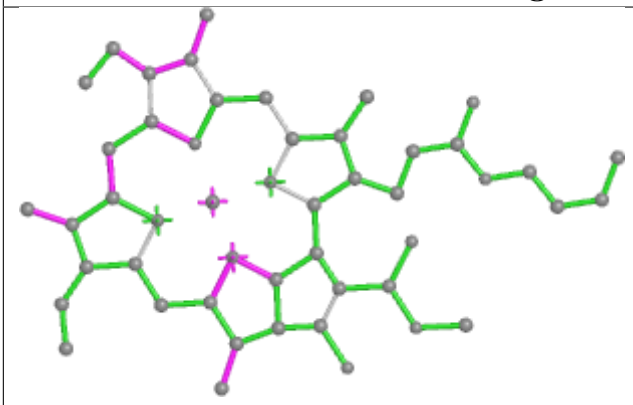


Torsions

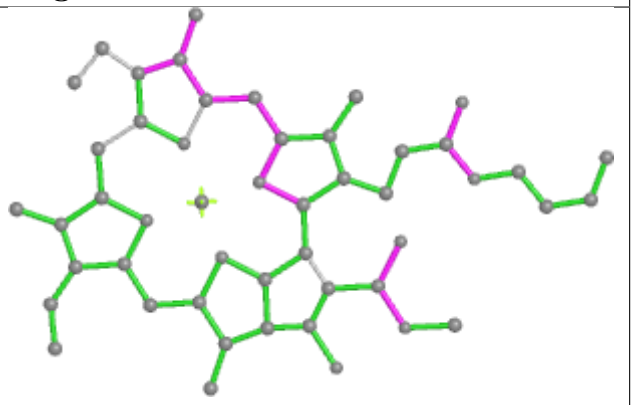


Rings

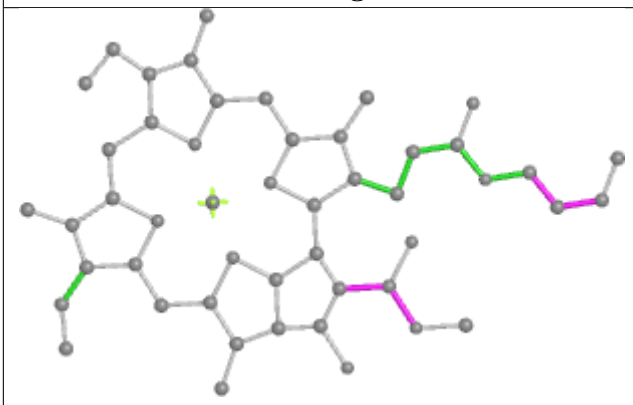
Ligand CLA g 612



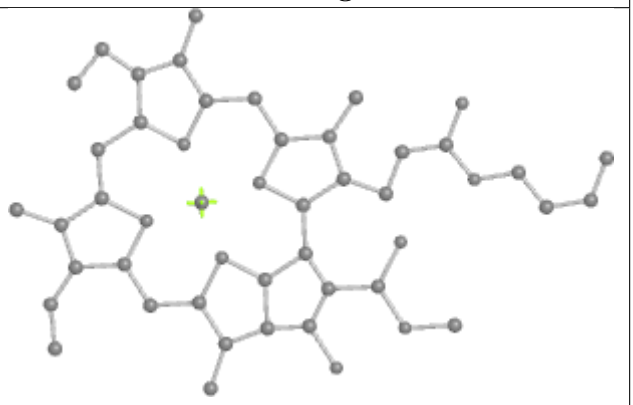
Bond lengths



Bond angles

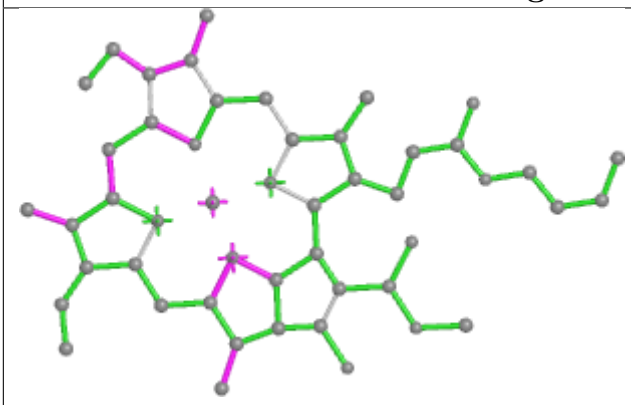


Torsions

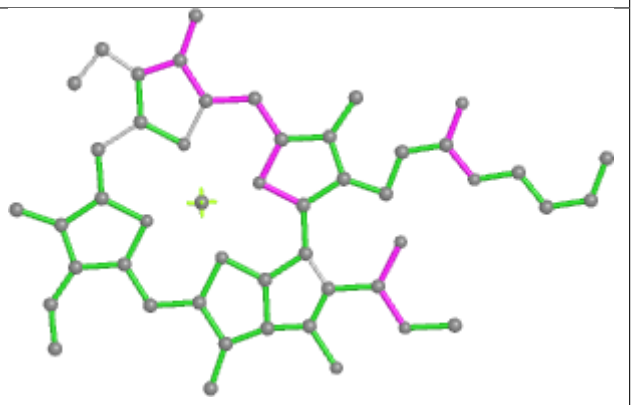


Rings

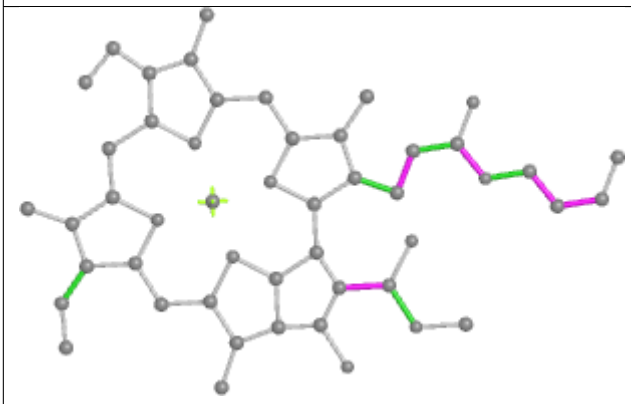
Ligand CLA S 611



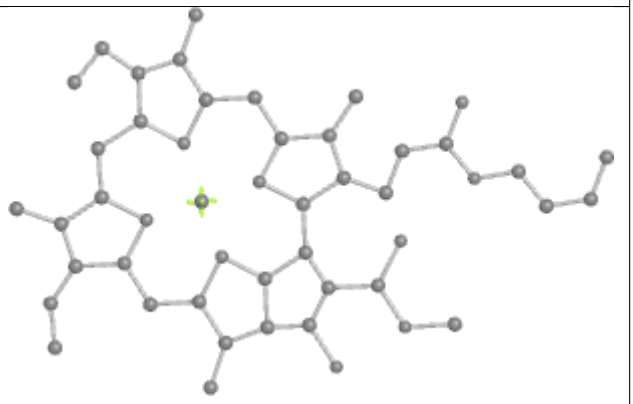
Bond lengths



Bond angles

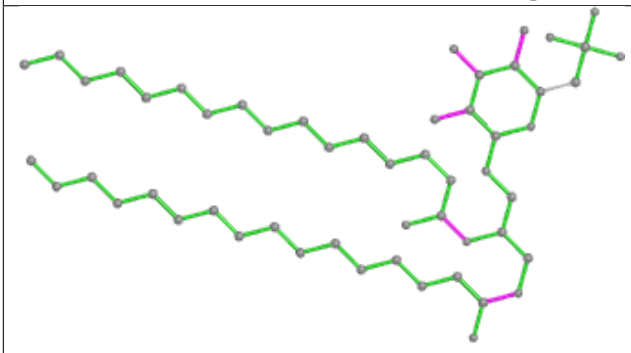


Torsions

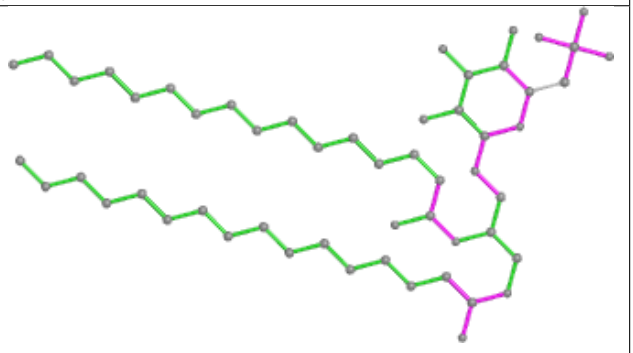


Rings

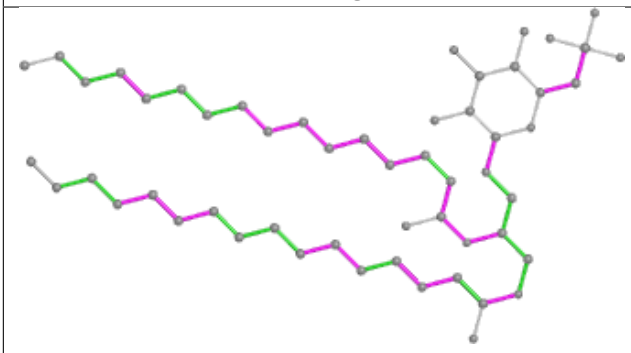
Ligand SQD B 621



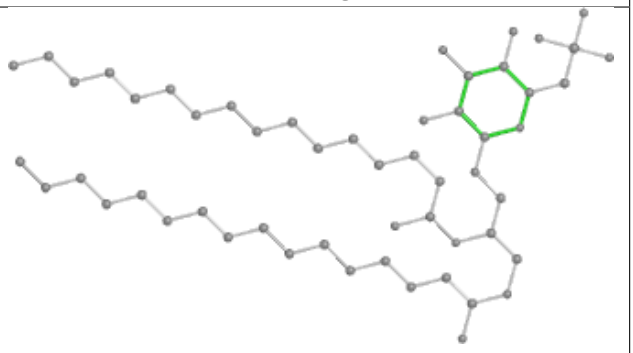
Bond lengths



Bond angles

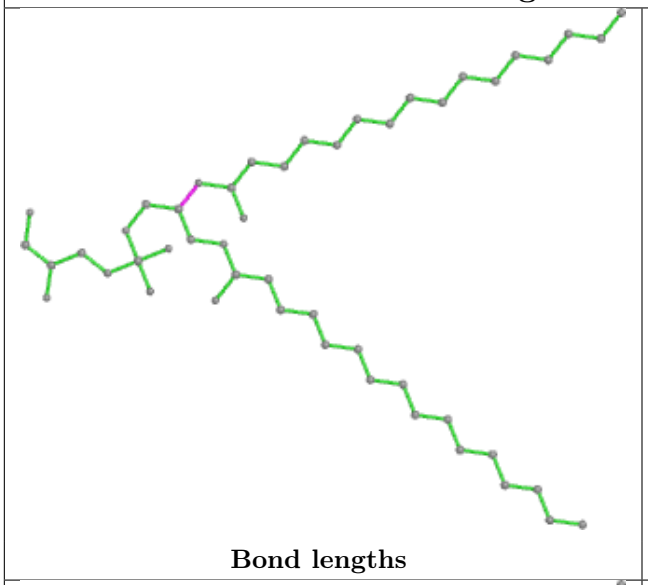


Torsions

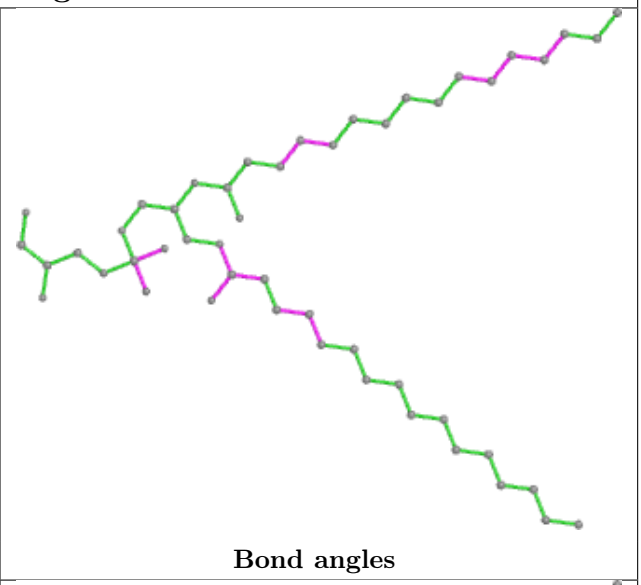


Rings

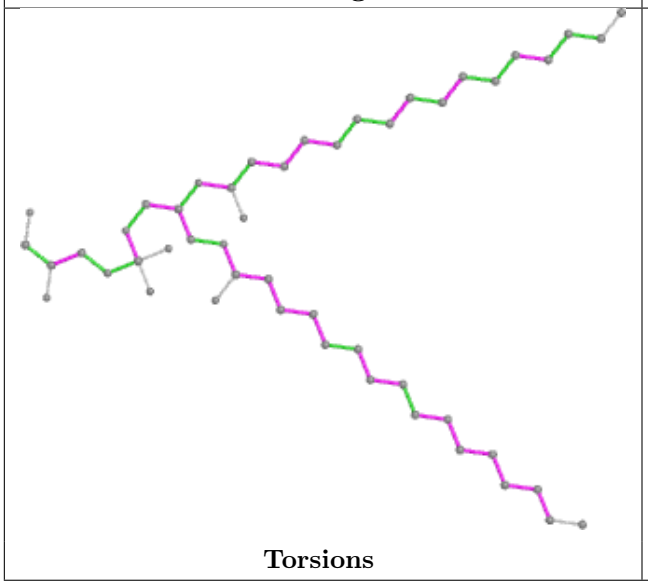
Ligand LHG g 2630



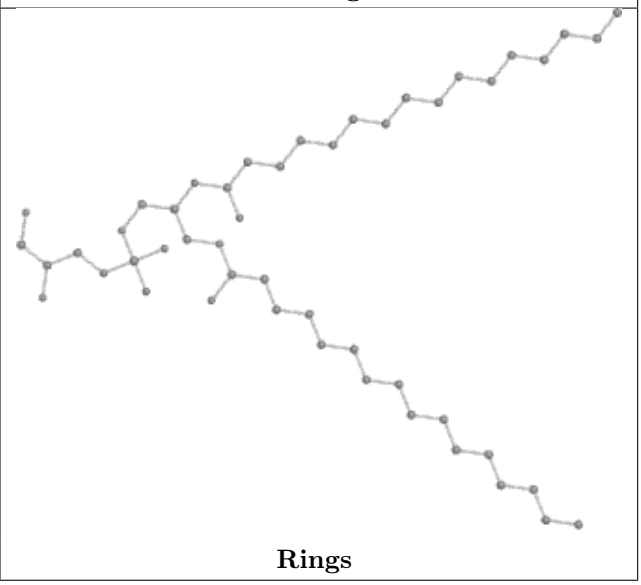
Bond lengths



Bond angles

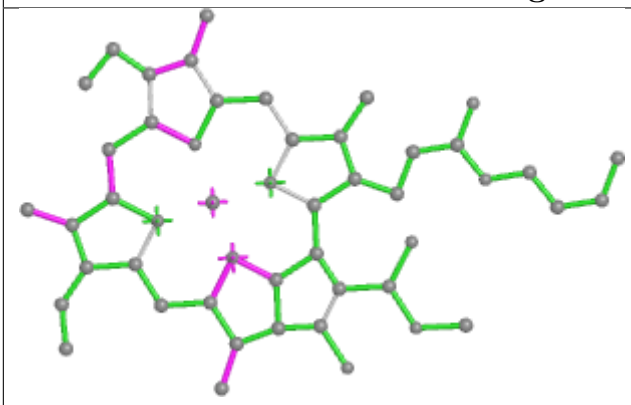


Torsions

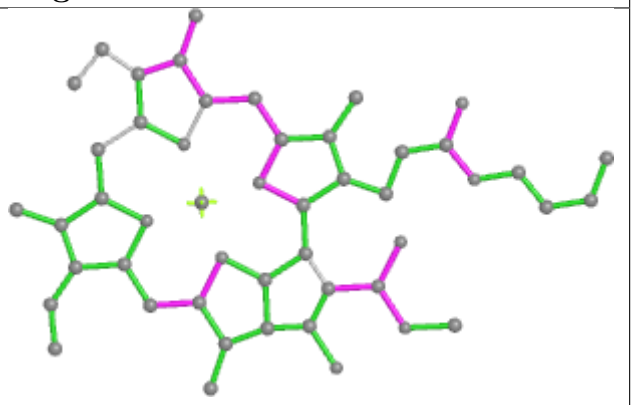


Rings

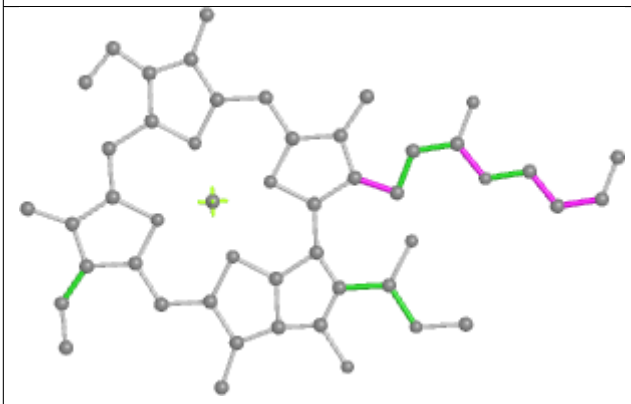
Ligand CLA g 611



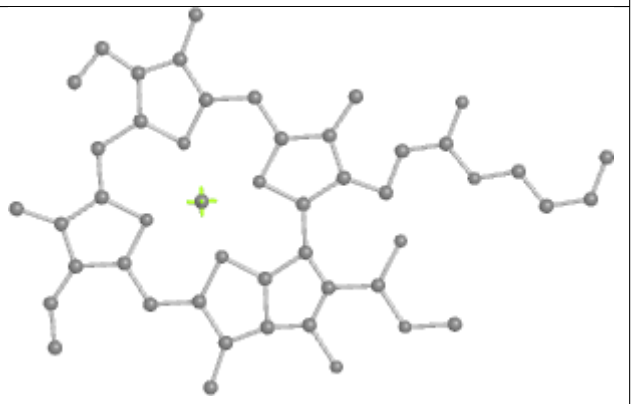
Bond lengths



Bond angles

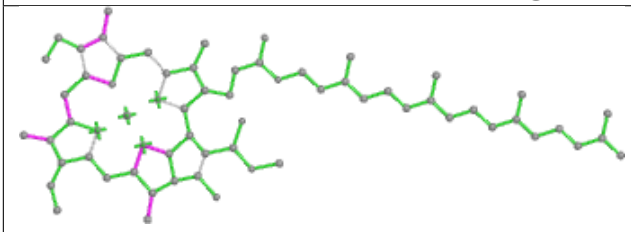


Torsions



Rings

Ligand CLA n 602



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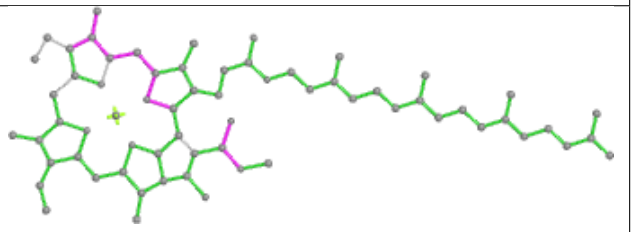
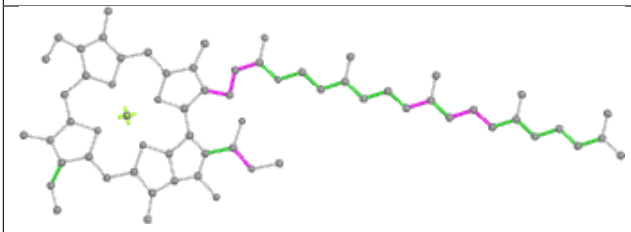
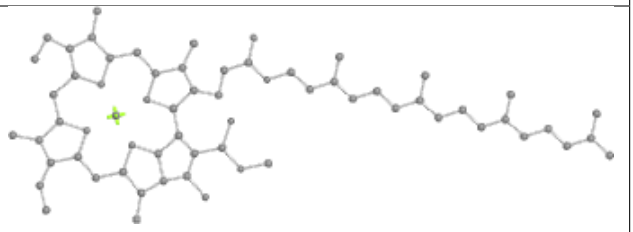


Bond angles

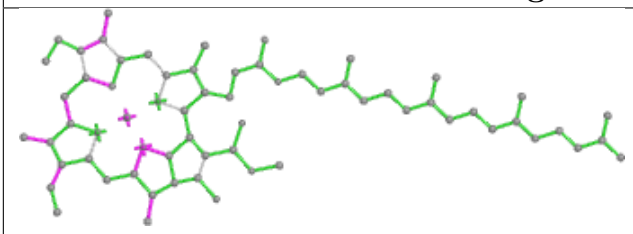


Torsions



Rings

Ligand CLA b 612



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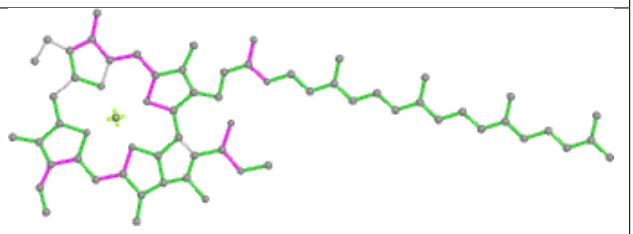
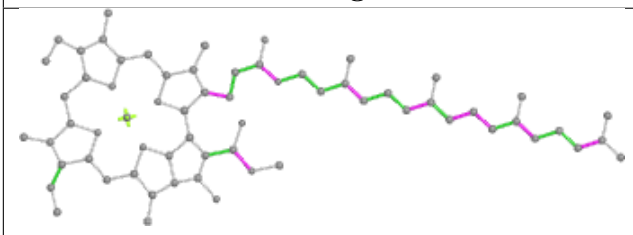
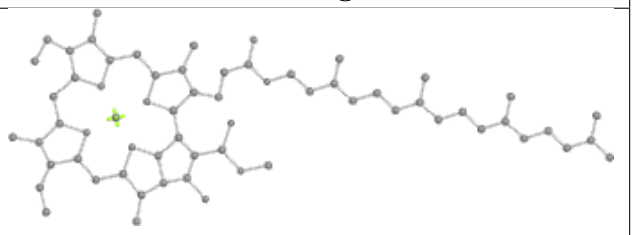


Bond angles

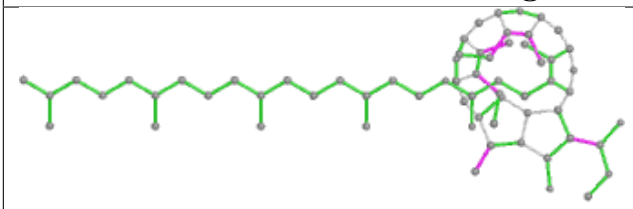


Torsions



Rings

Ligand PHO A 409



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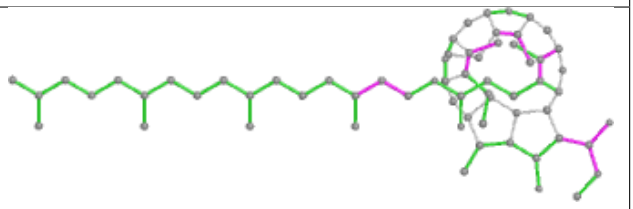
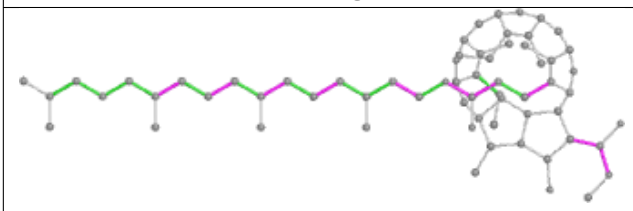
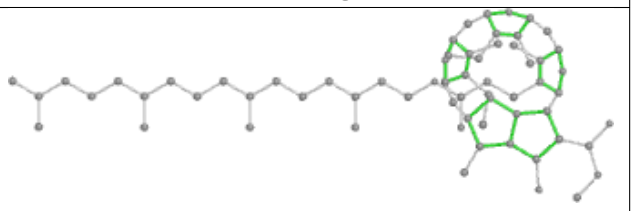


Bond angles

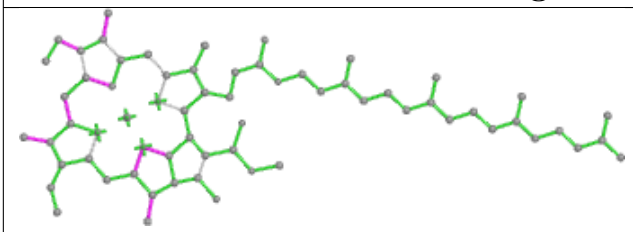


Torsions



Rings

Ligand CLA r 602



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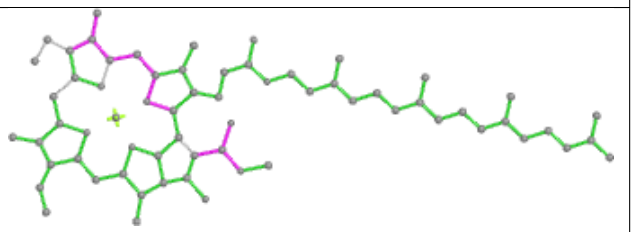
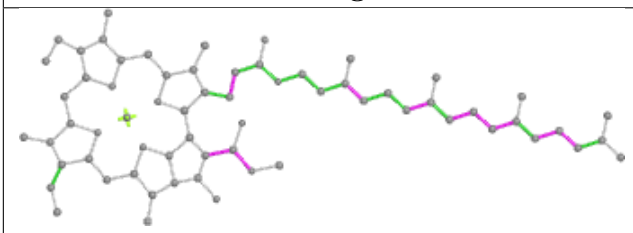


Bond angles



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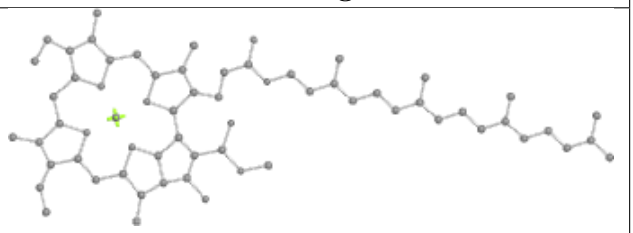
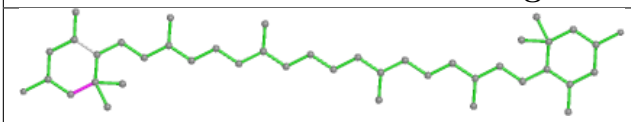


Rings

Ligand LUT R 620



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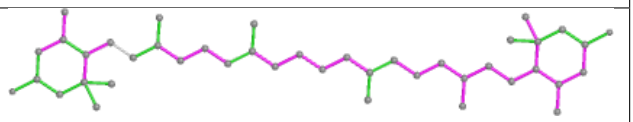
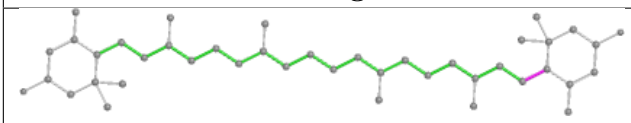
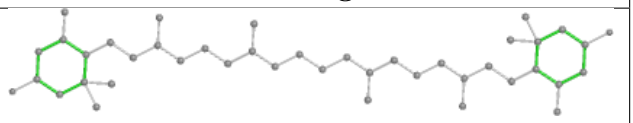


Bond angles

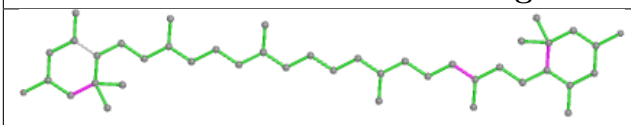


Torsions

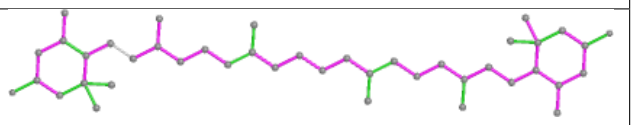


Rings

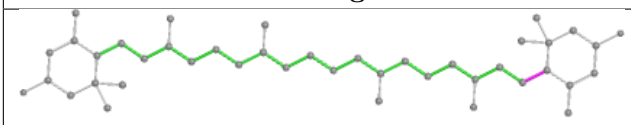
Ligand LUT Y 1621



Bond lengths



Bond angles



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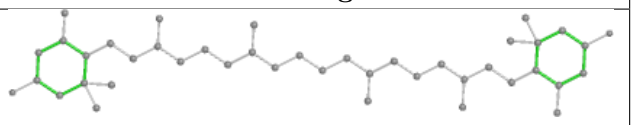
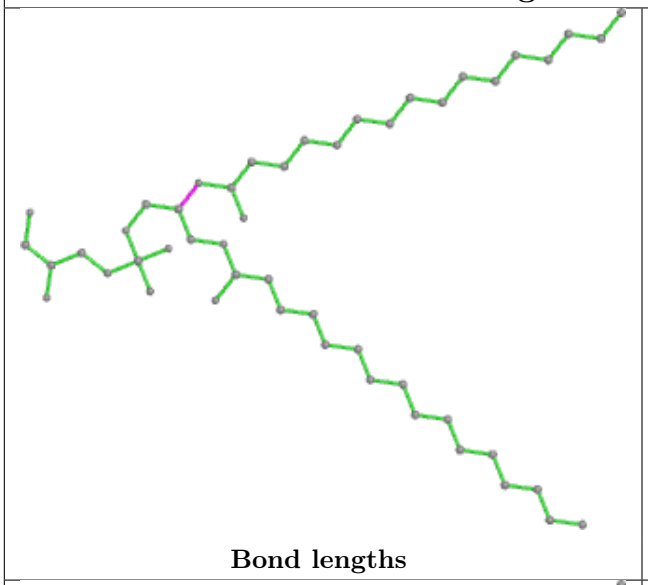


Rings

Ligand LHG y 2630



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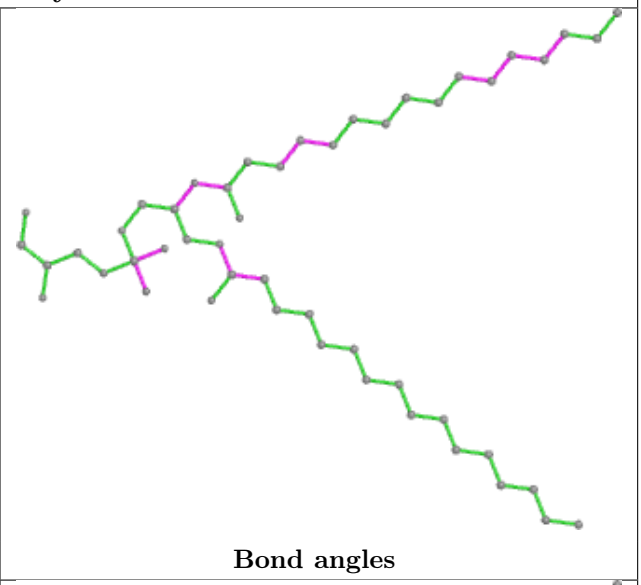
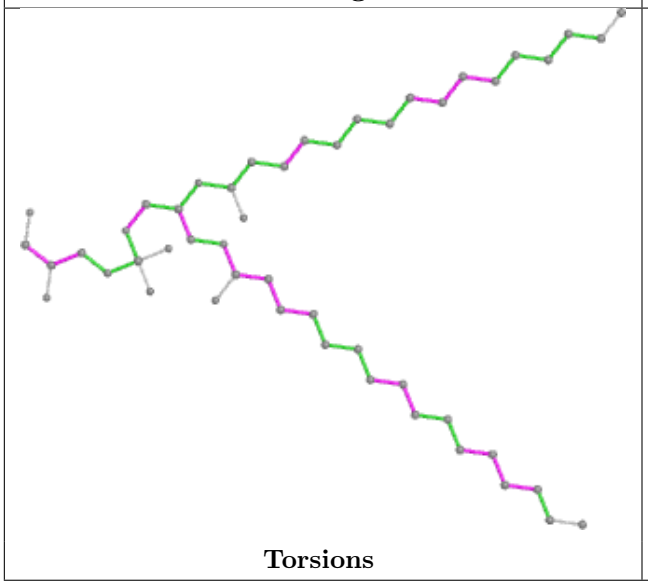
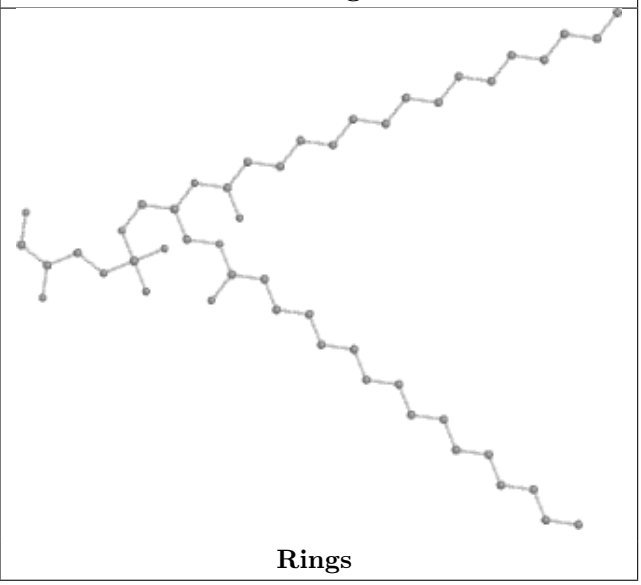


Bond angles

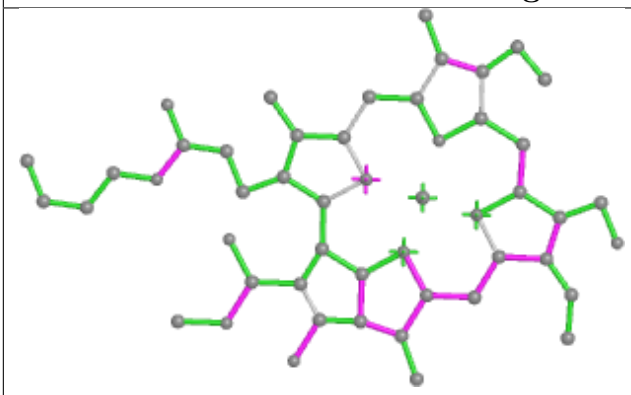


Torsions



Rings

Ligand CHL G 607



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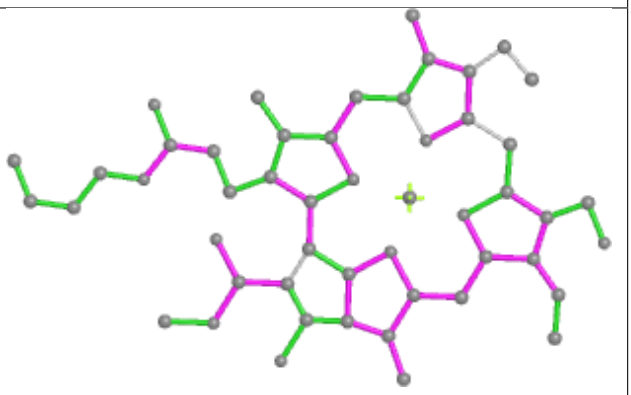
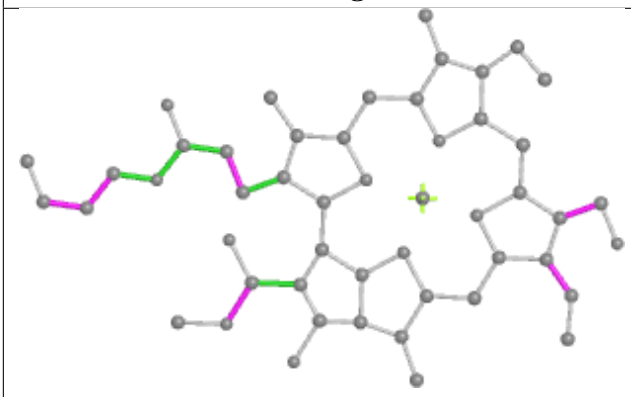
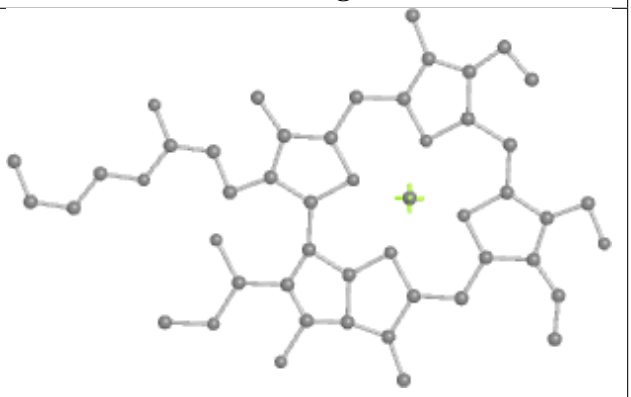


Bond angles

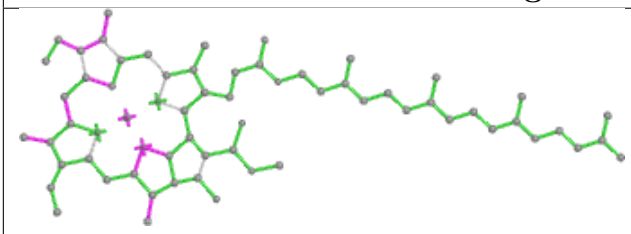


Torsions

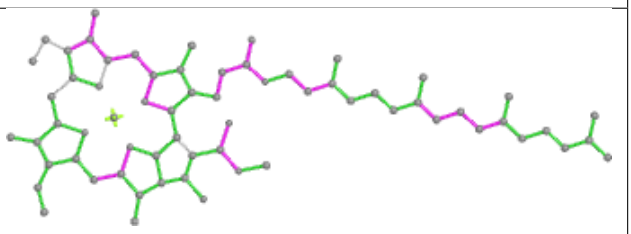


Rings

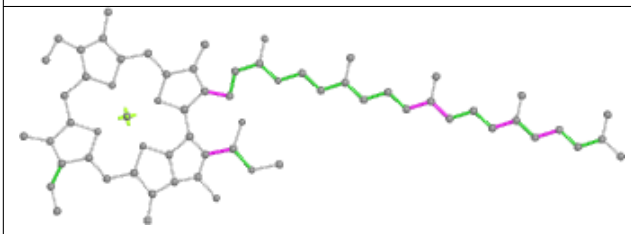
Ligand CLA C 509



Bond lengths



Bond angles



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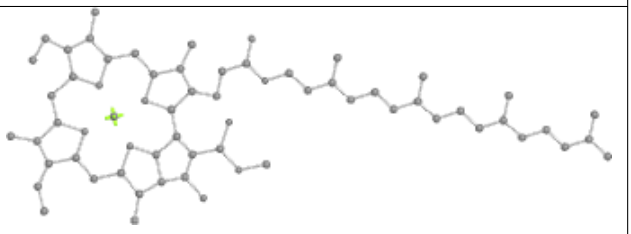
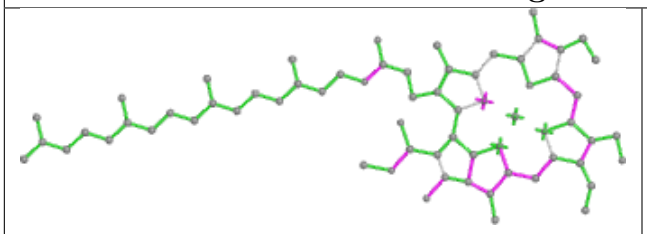
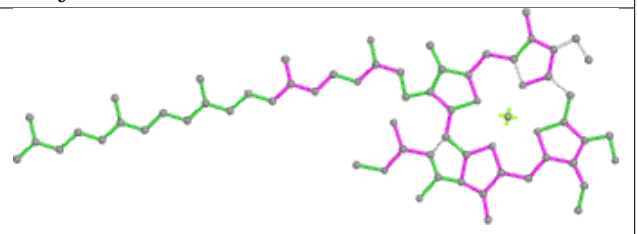


Rings

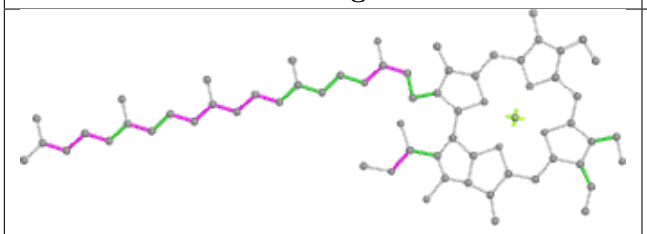
Ligand CHL y 601



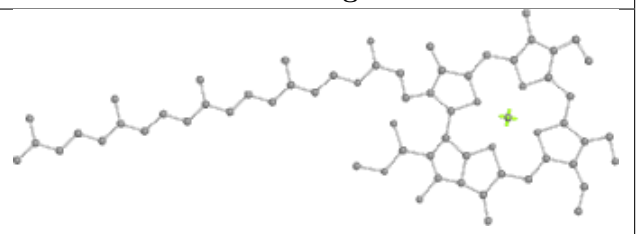
Bond lengths



Bond angles

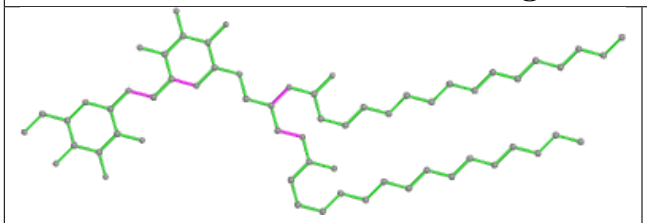


Torsions

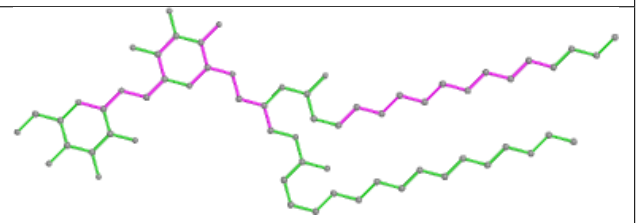


Rings

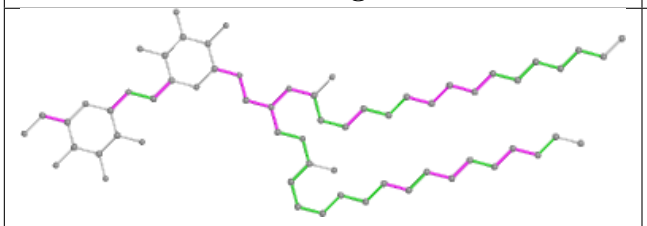
Ligand DGD C 519



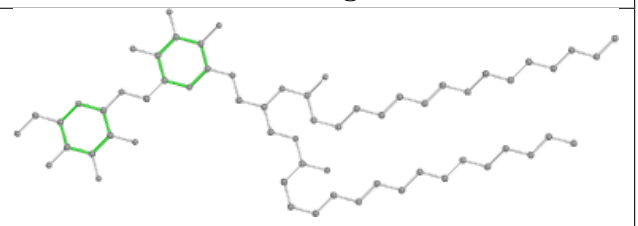
Bond lengths



Bond angles

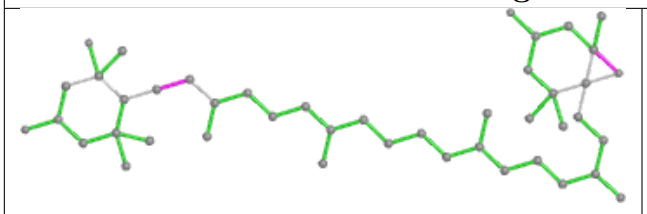


Torsions

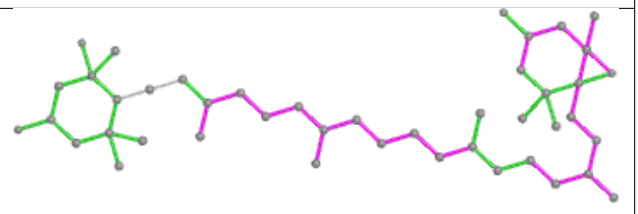


Rings

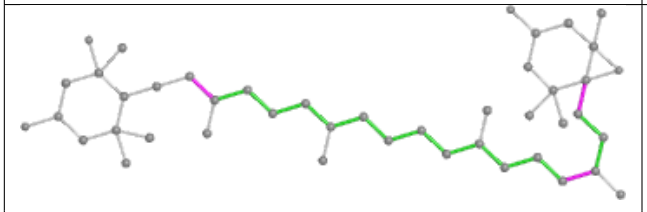
Ligand NEX G 1623



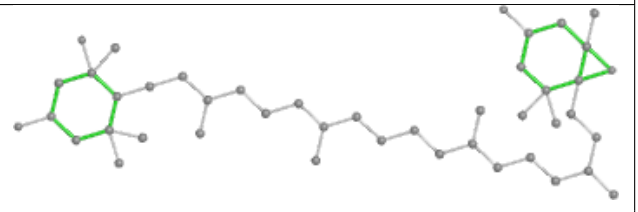
Bond lengths



Bond angles

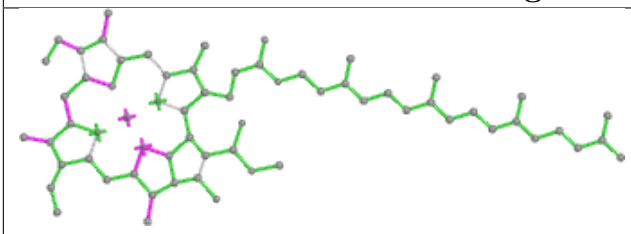


Torsions

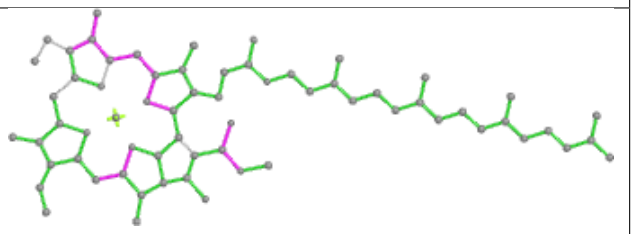


Rings

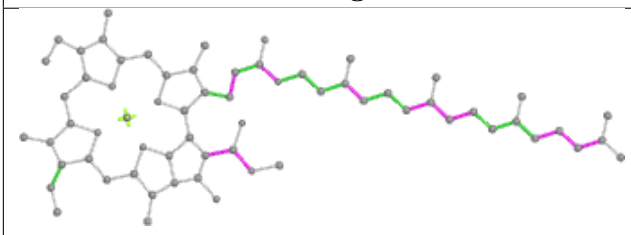
Ligand CLA C 510



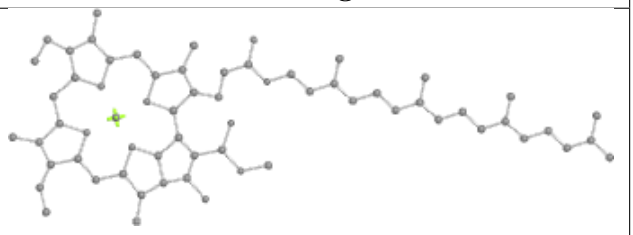
Bond lengths



Bond angles

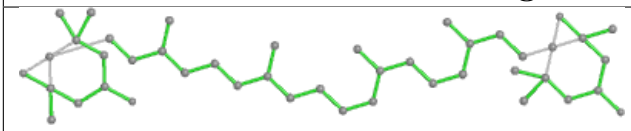


Torsions

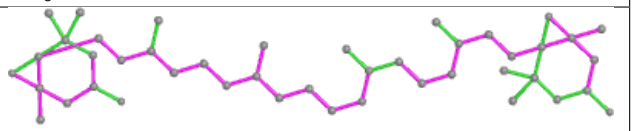


Rings

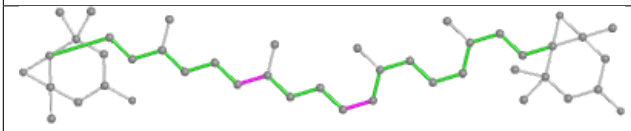
Ligand XAT y 1622



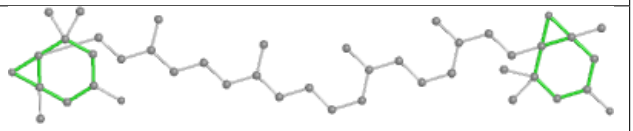
Bond lengths



Bond angles

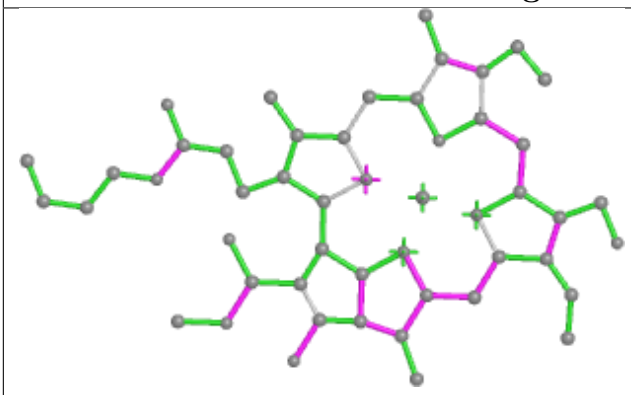


Torsions



Rings

Ligand CHL N 608



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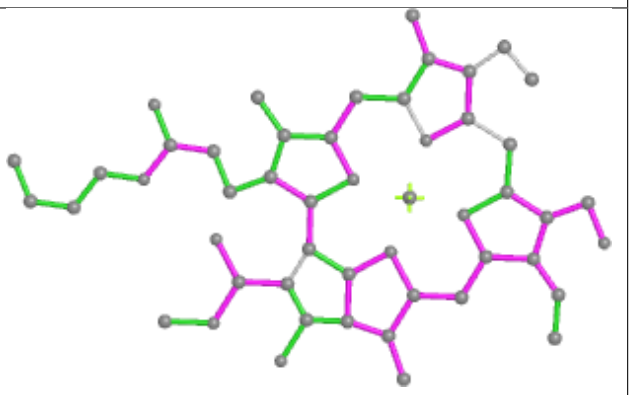
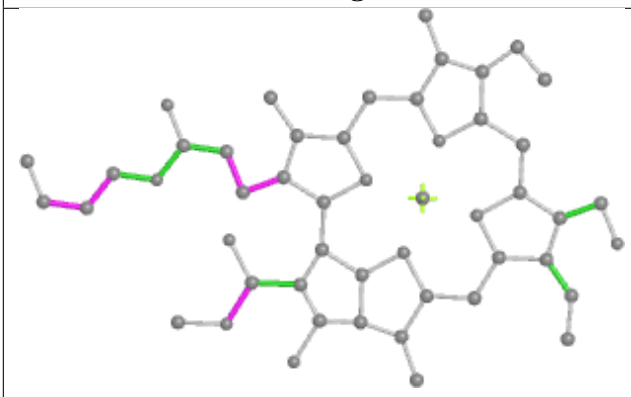
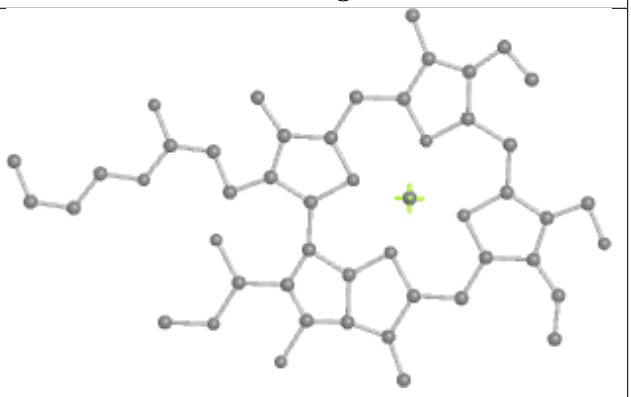


Bond angles

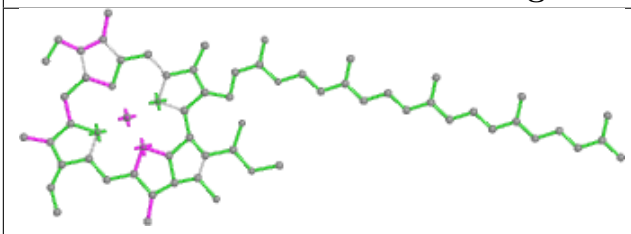


Torsions

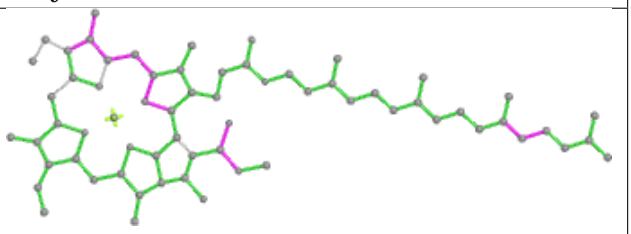


Rings

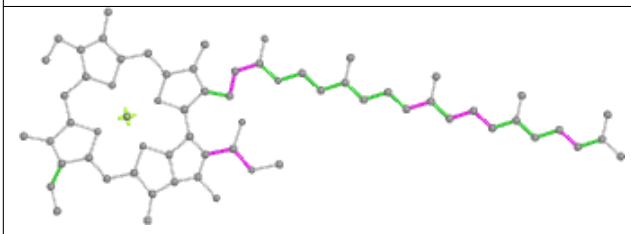
Ligand CLA y 602



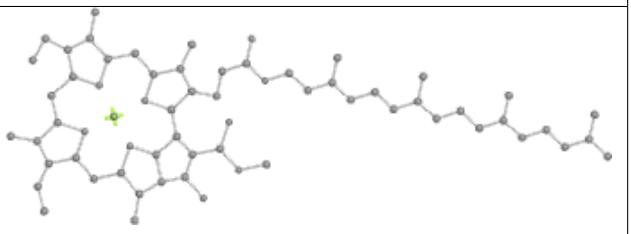
Bond lengths



Bond angles

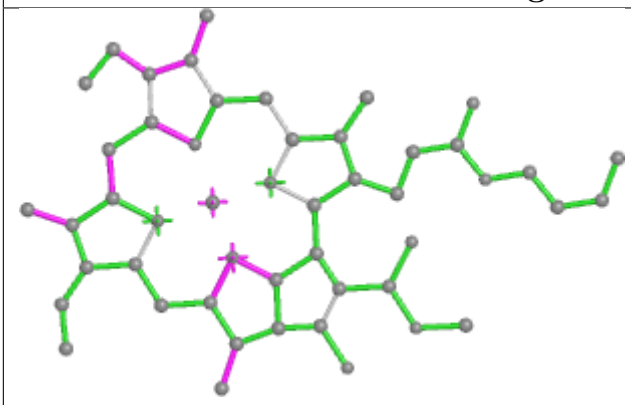


Torsions

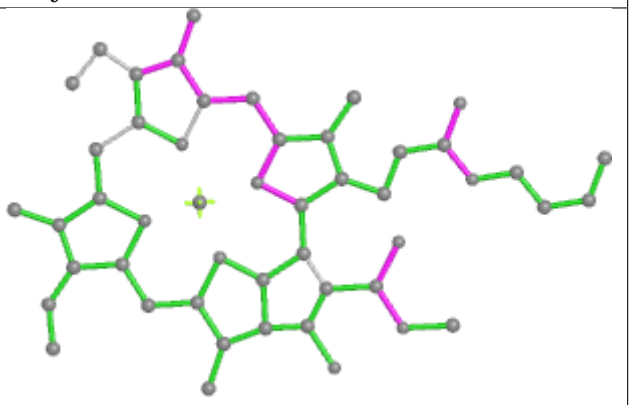


Rings

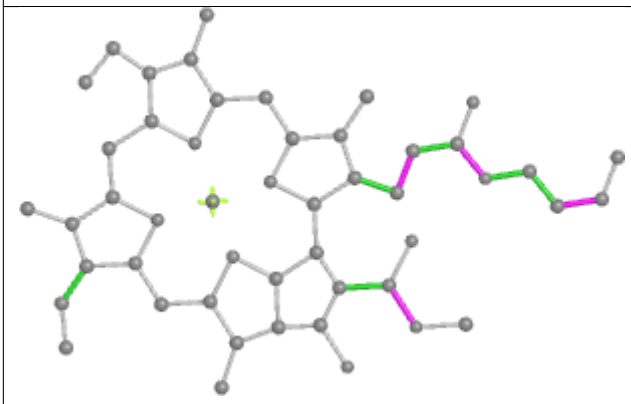
Ligand CLA y 604



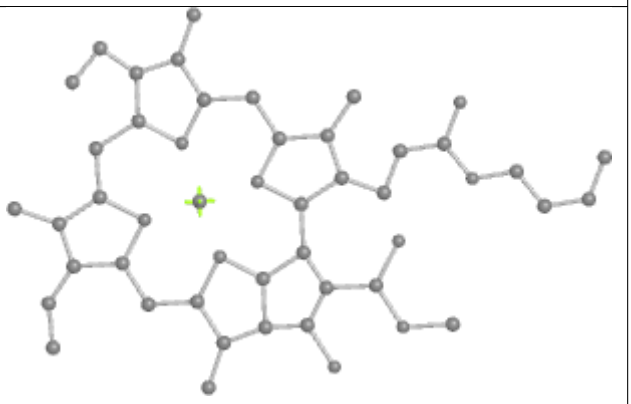
Bond lengths



Bond angles

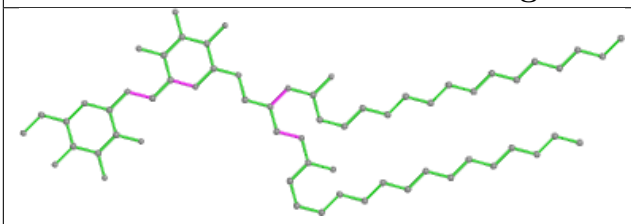


Torsions



Rings

Ligand DGD C 520



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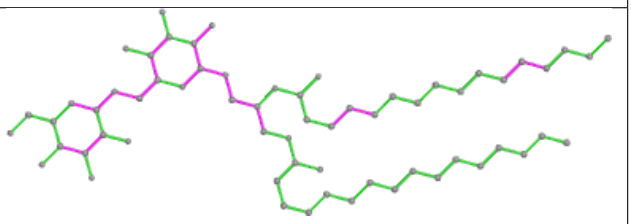
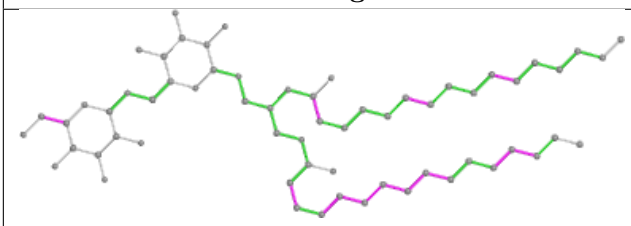


Bond angles



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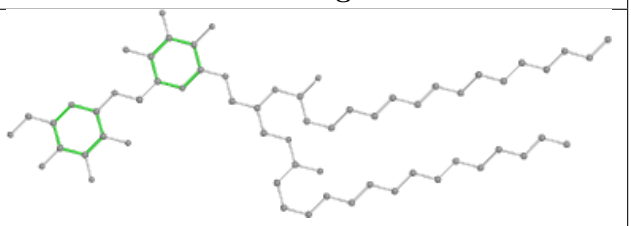
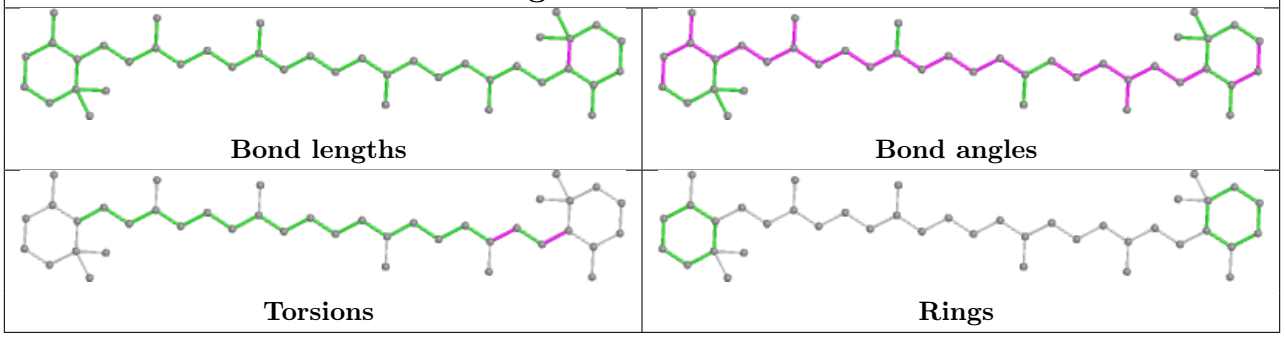
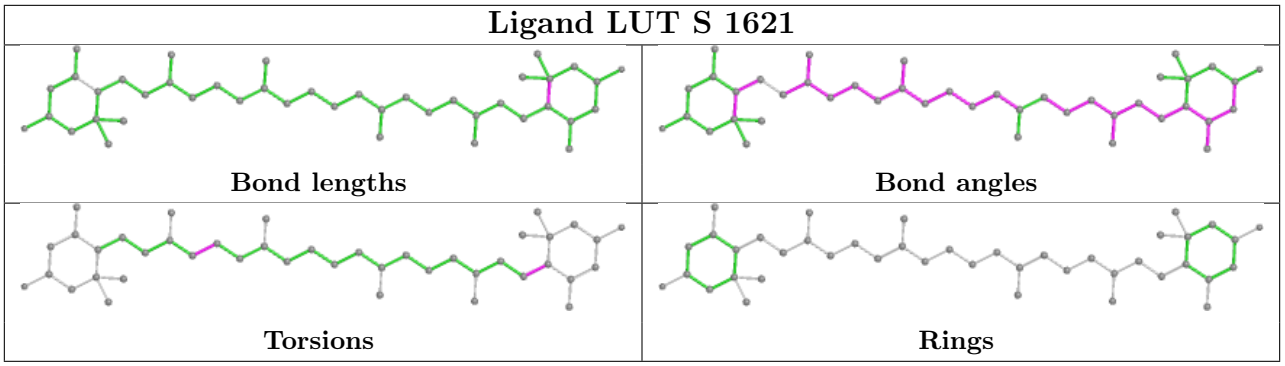


Rings

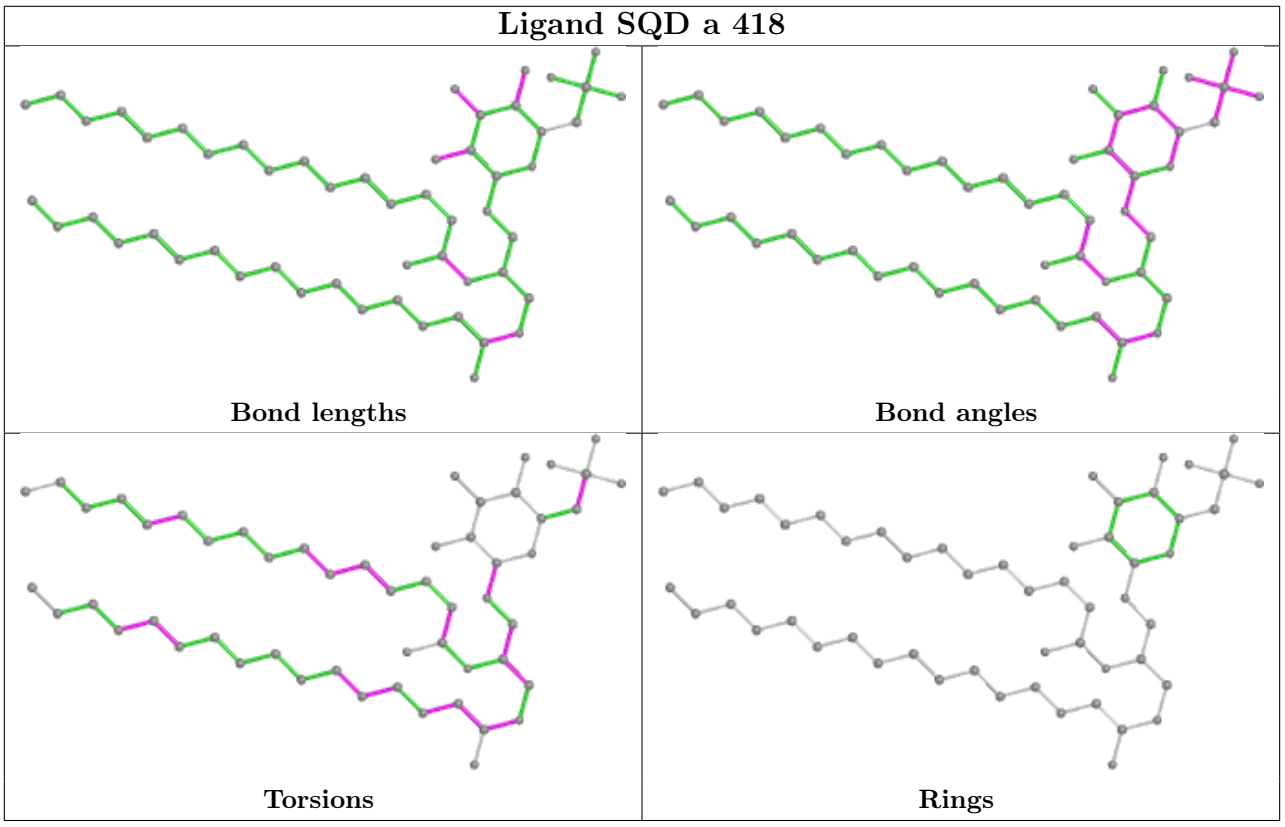
Ligand BCR c 514



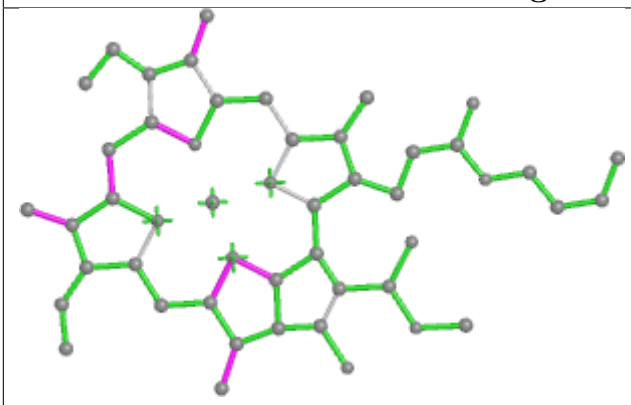
Ligand LUT S 1621



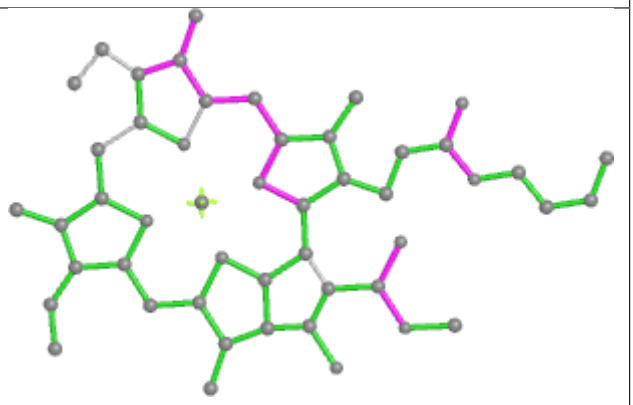
Ligand SQD a 418



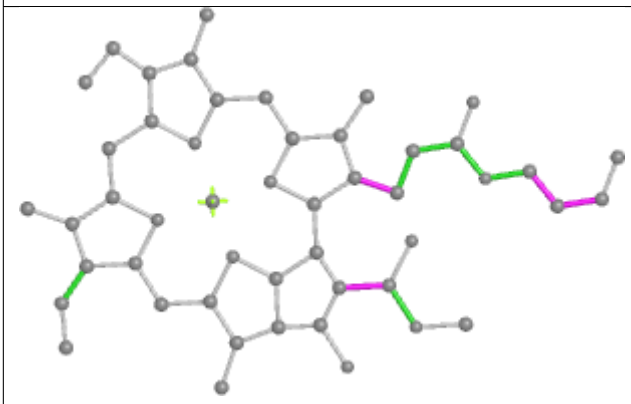
Ligand CLA s 610



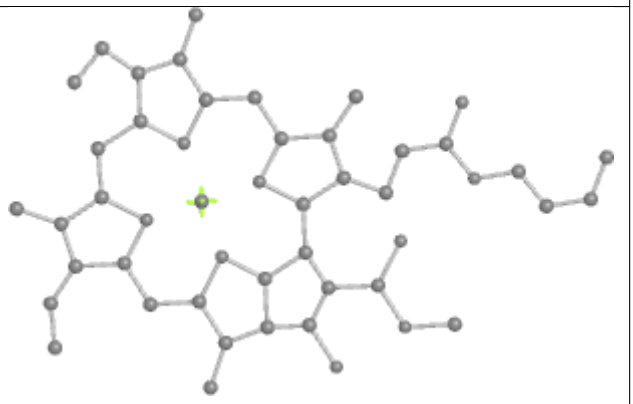
Bond lengths



Bond angles

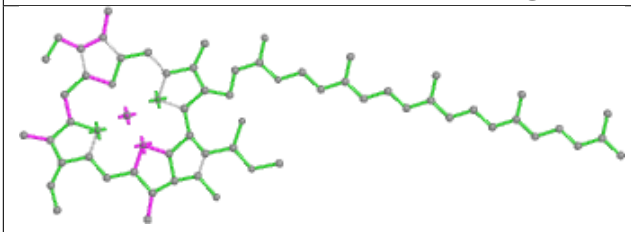


Torsions

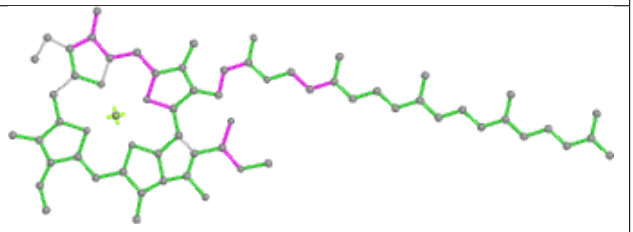


Rings

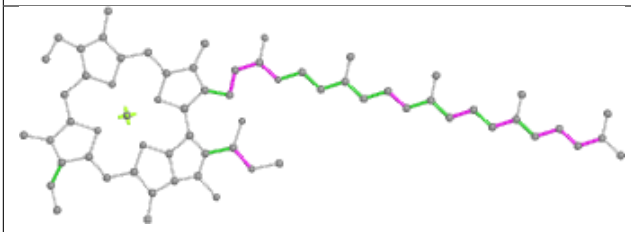
Ligand CLA A 405



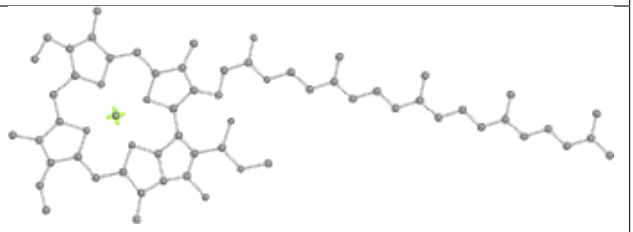
Bond lengths



Bond angles

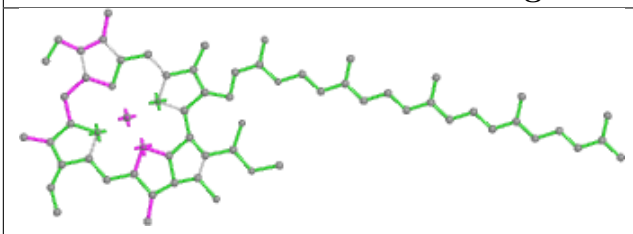


Torsions

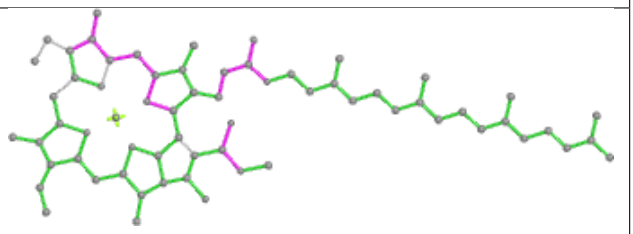


Rings

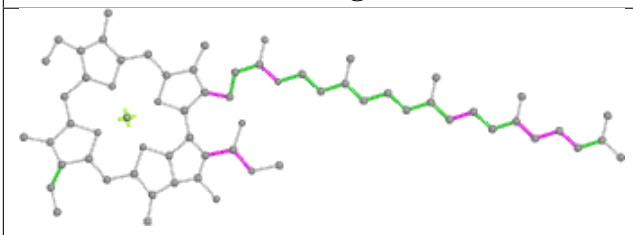
Ligand CLA C 503



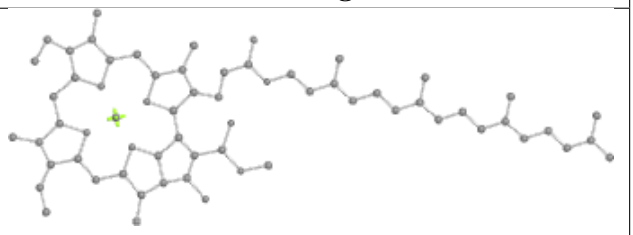
Bond lengths



Bond angles

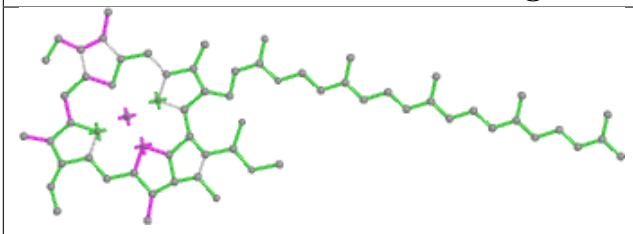


Torsions

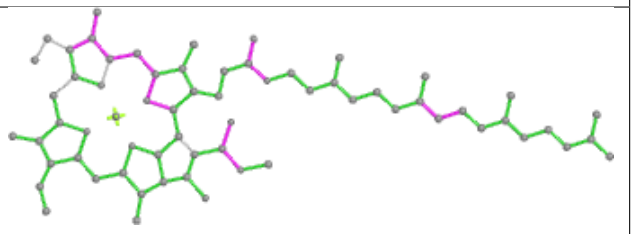


Rings

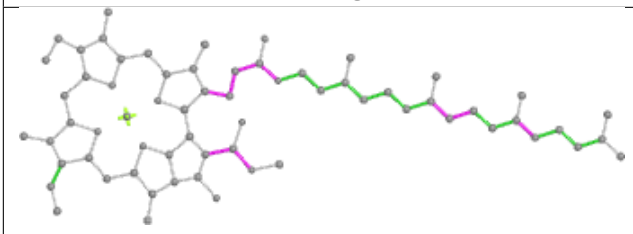
Ligand CLA C 501



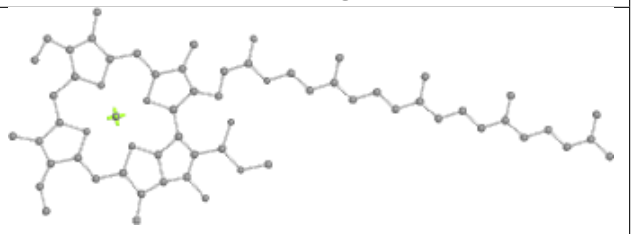
Bond lengths



Bond angles

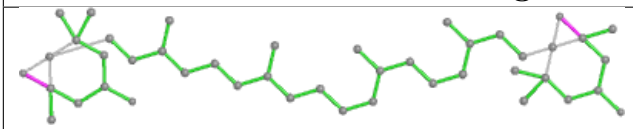


Torsions



Rings

Ligand XAT G 1622



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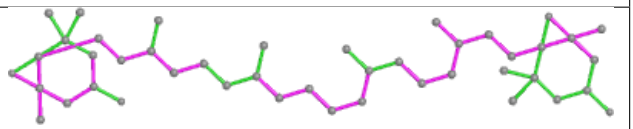
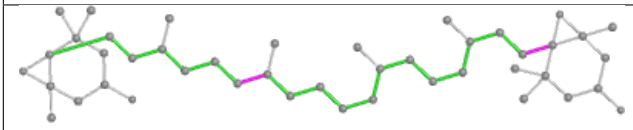
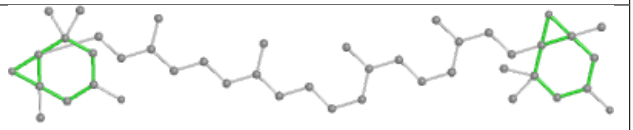


Bond angles

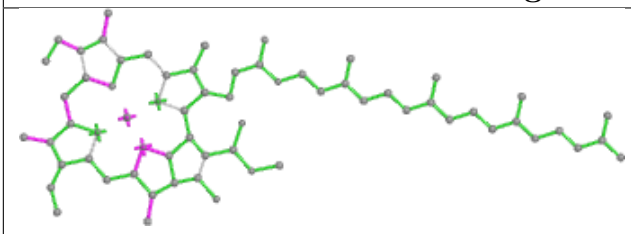


Torsions

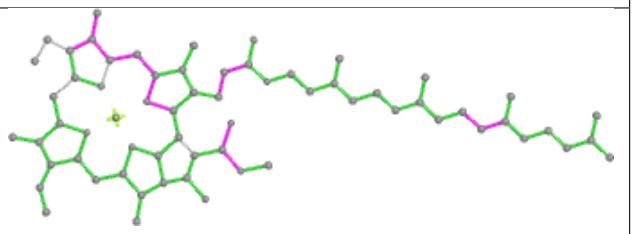


Rings

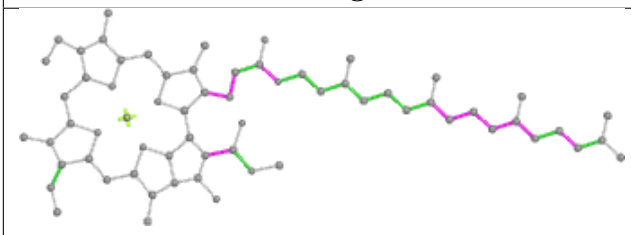
Ligand CLA B 613



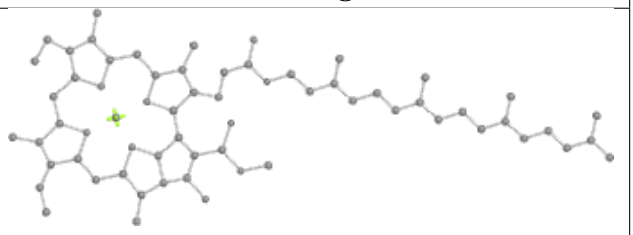
Bond lengths



Bond angles

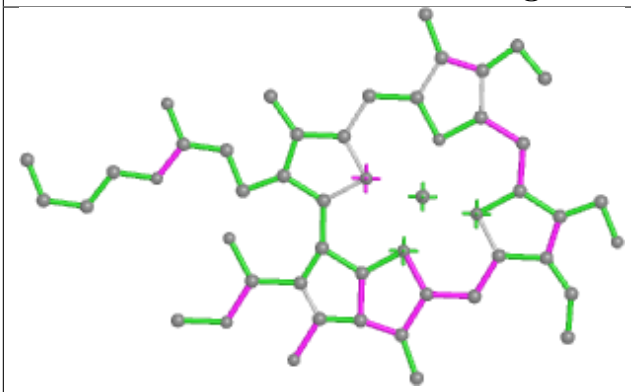


Torsions

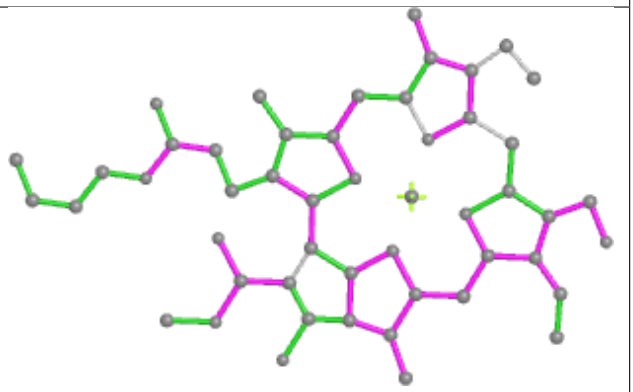


Rings

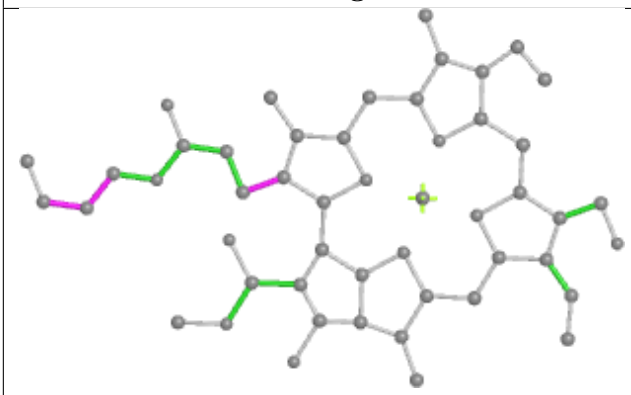
Ligand CHL N 606



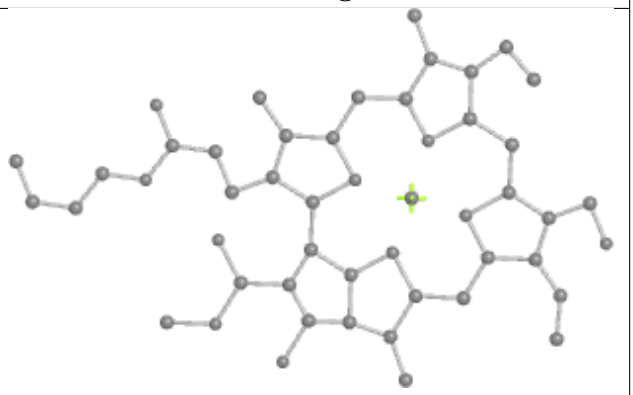
Bond lengths



Bond angles

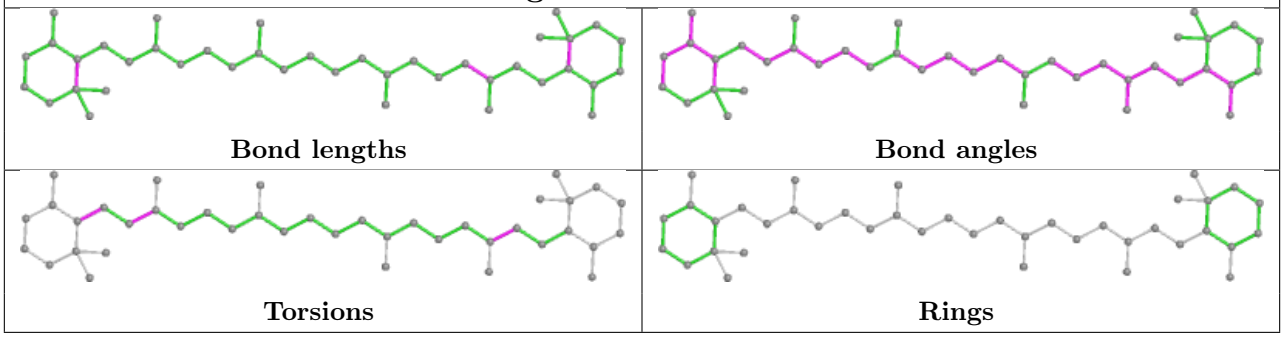


Torsions

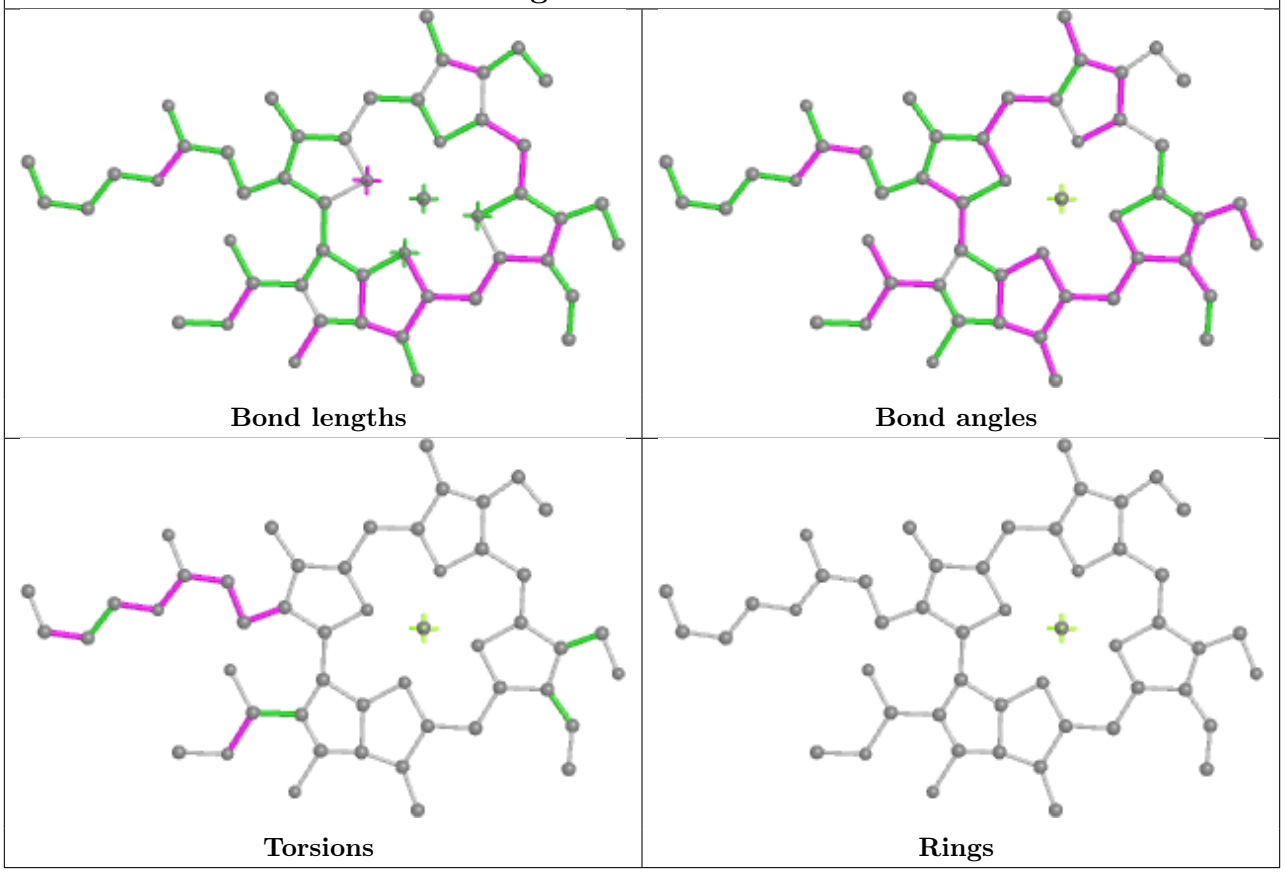


Rings

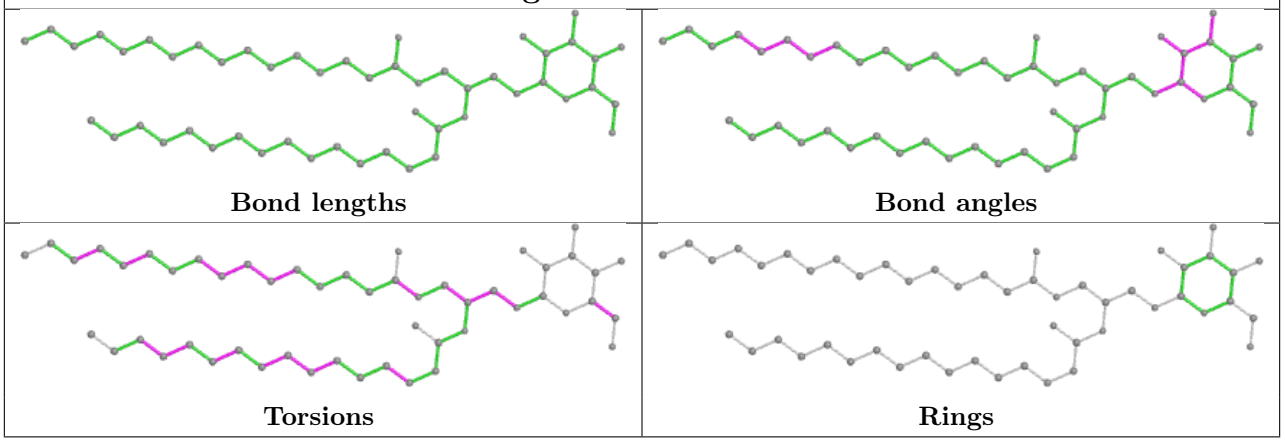
Ligand BCR b 620



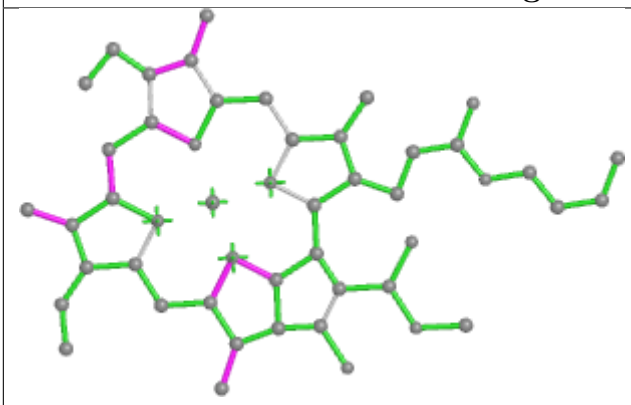
Ligand CHL r 607



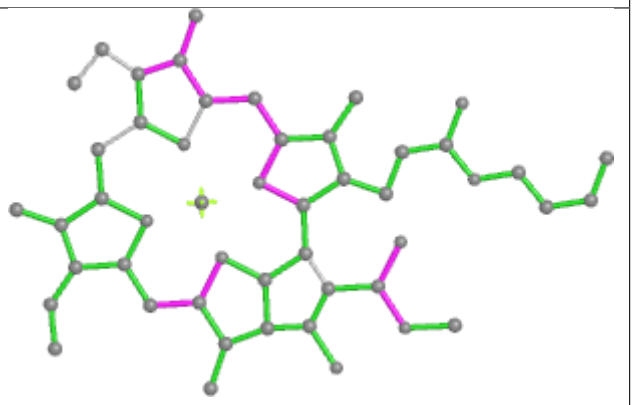
Ligand LMG Z 101



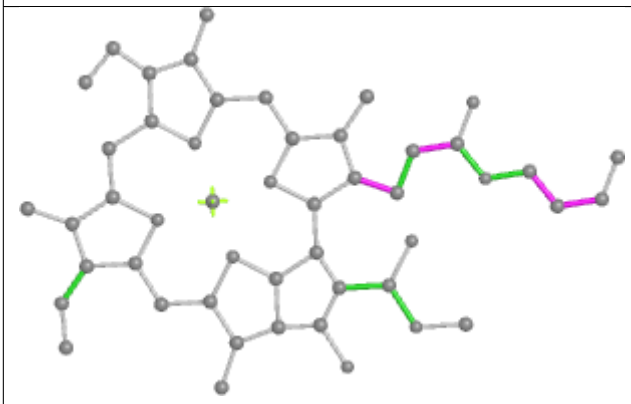
Ligand CLA G 603



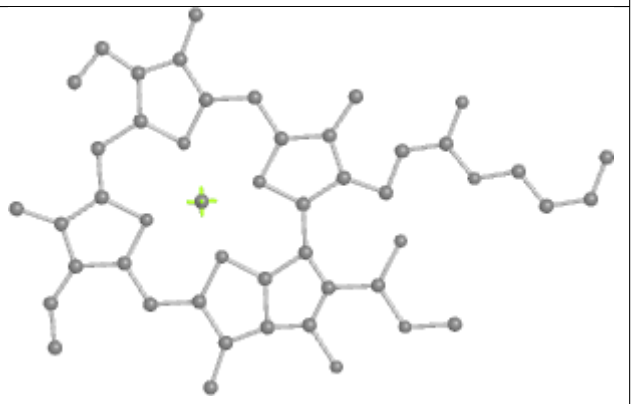
Bond lengths



Bond angles

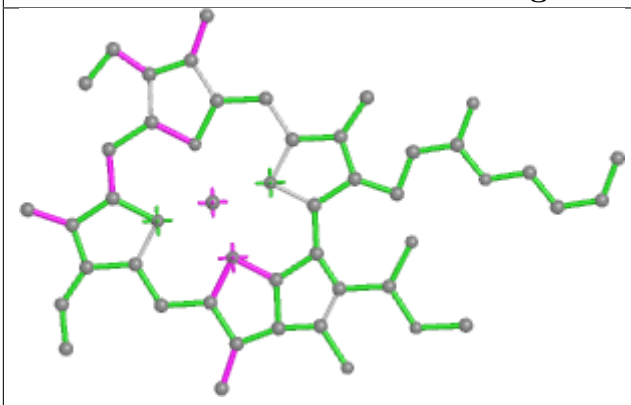


Torsions

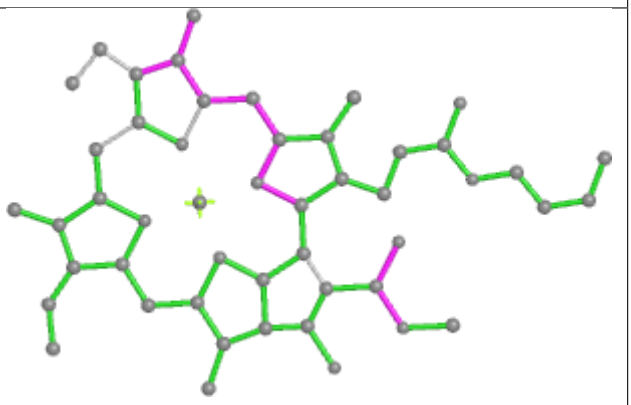


Rings

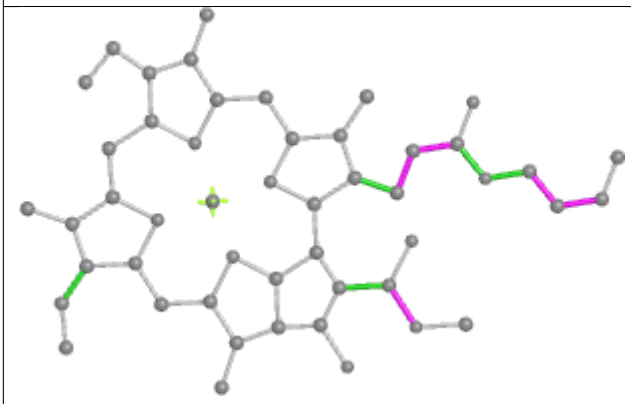
Ligand CLA s 613



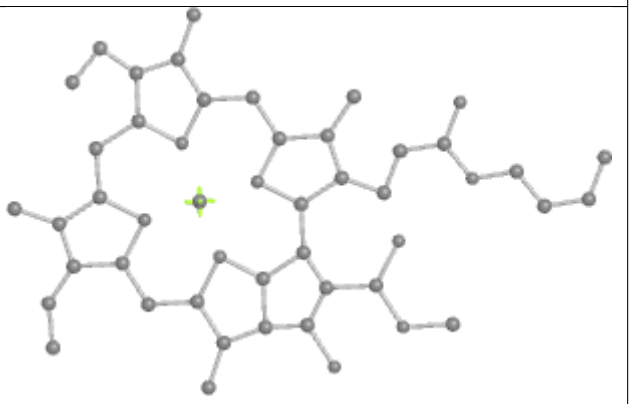
Bond lengths



Bond angles

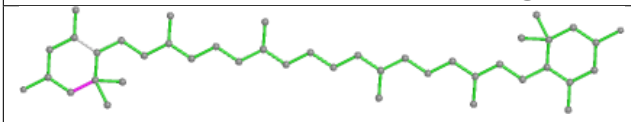


Torsions

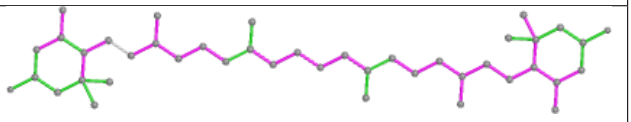


Rings

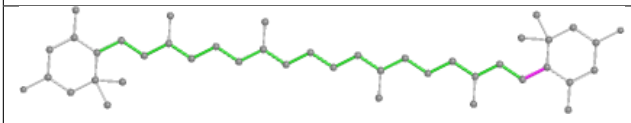
Ligand LUT n 1620



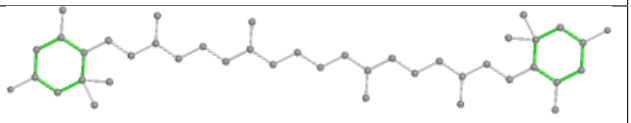
Bond lengths



Bond angles

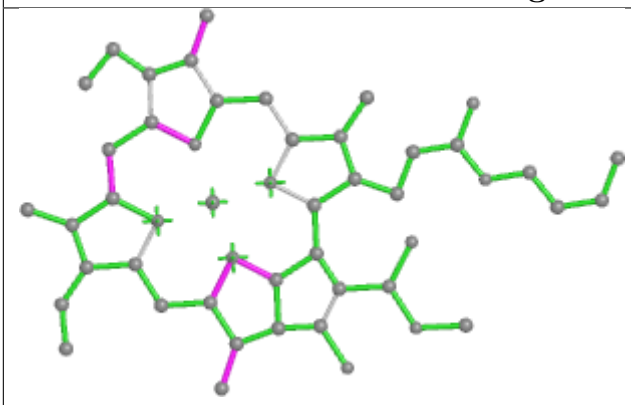


Torsions

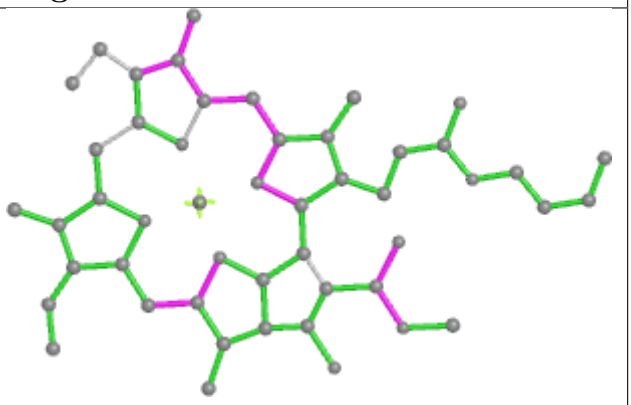


Rings

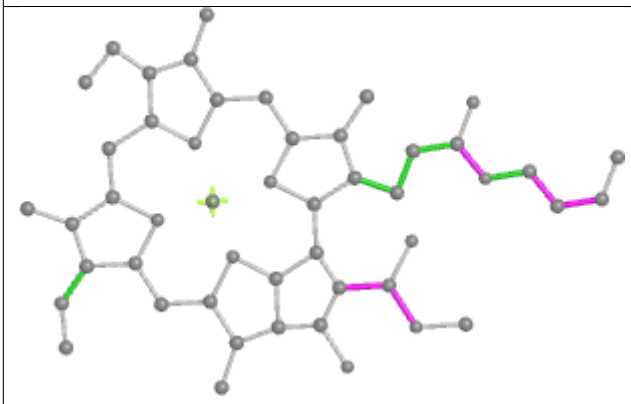
Ligand CLA g 614



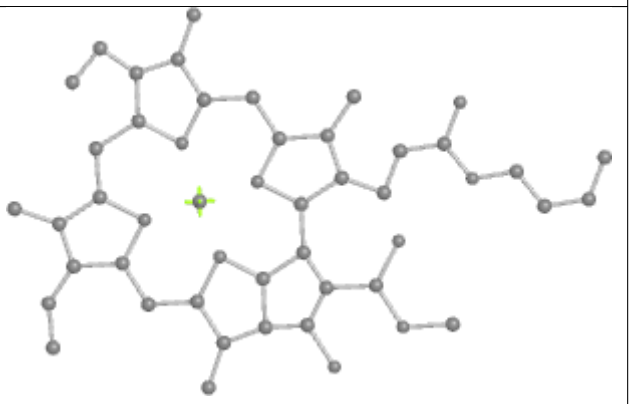
Bond lengths



Bond angles

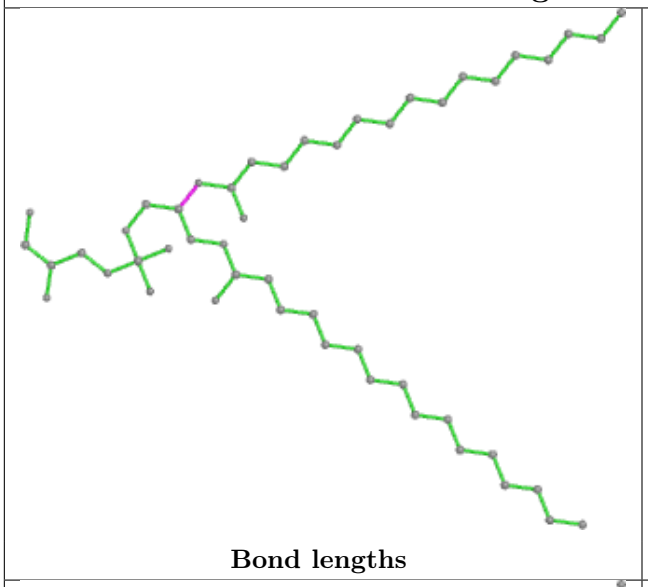


Torsions

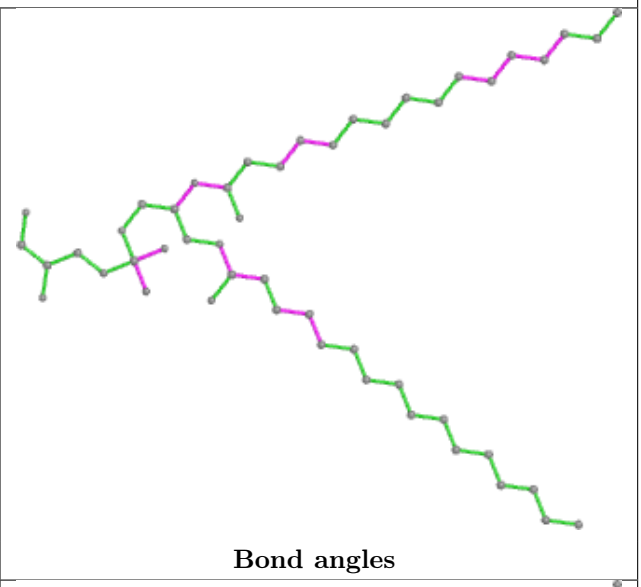


Rings

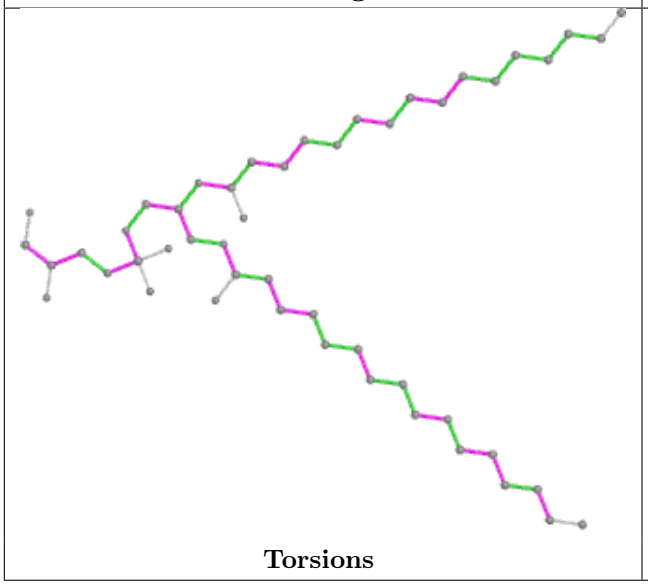
Ligand LHG l 101



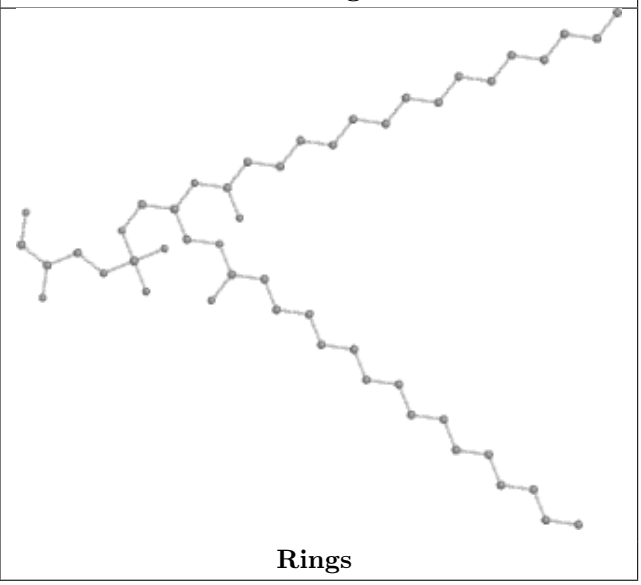
Bond lengths



Bond angles

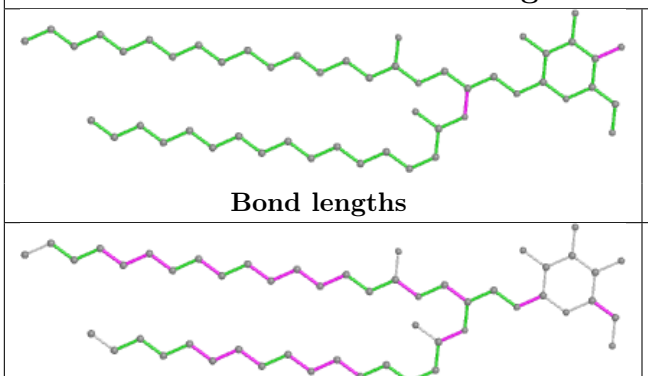


Torsions

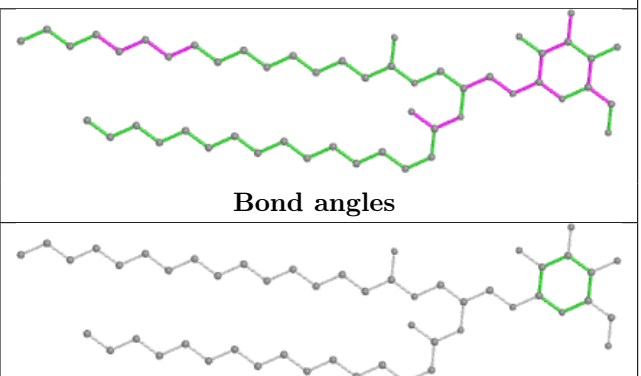


Rings

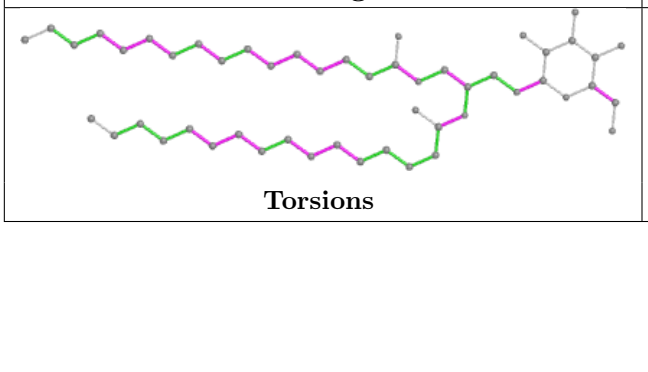
Ligand LMG B 622



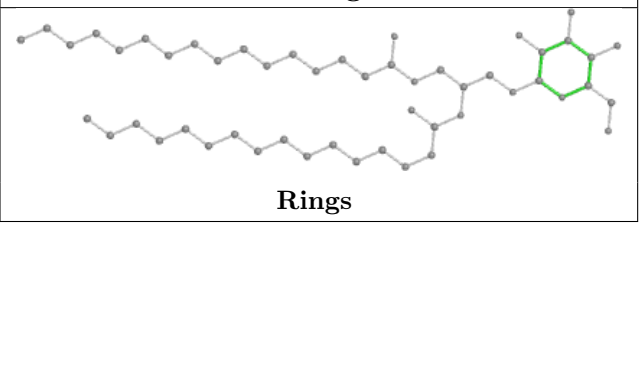
Bond lengths



Bond angles

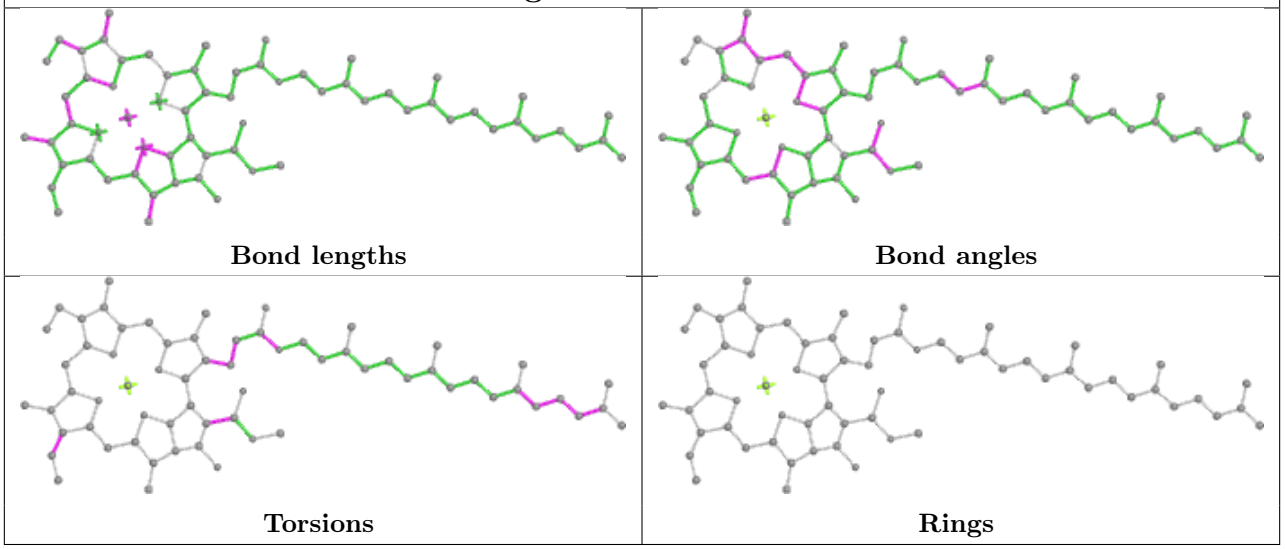


Torsions

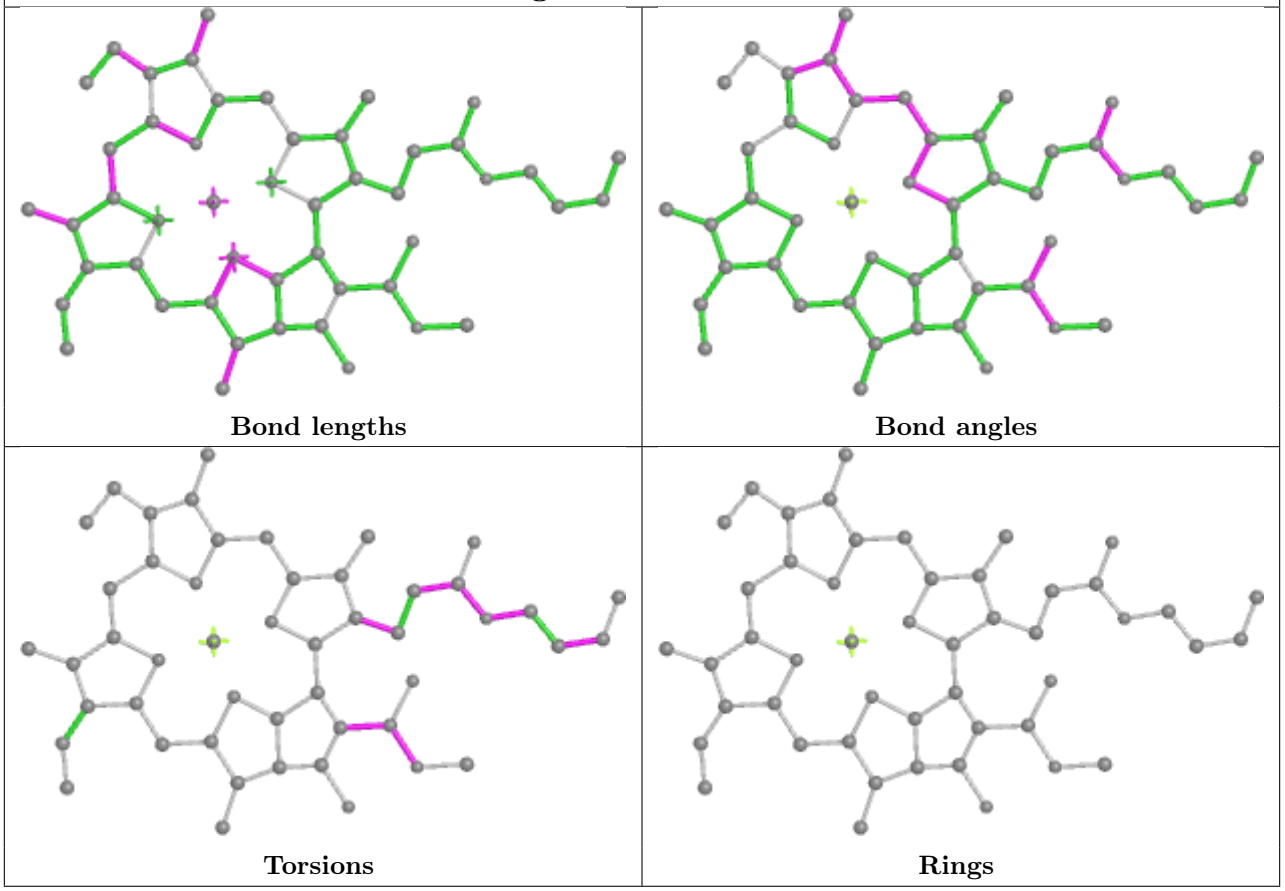


Rings

Ligand CLA A 406



Ligand CLA s 604



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

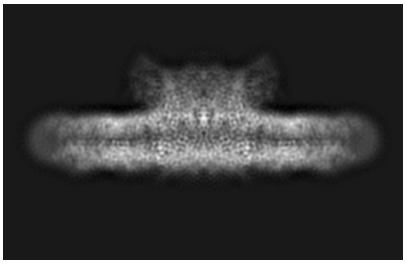
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6617. These allow visual inspection of the internal detail of the map and identification of artifacts.

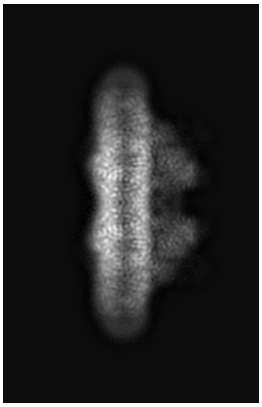
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

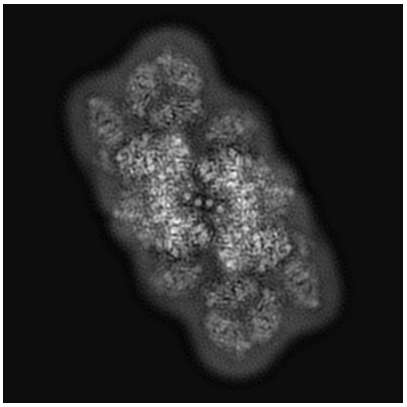
6.1.1 Primary map



X



Y

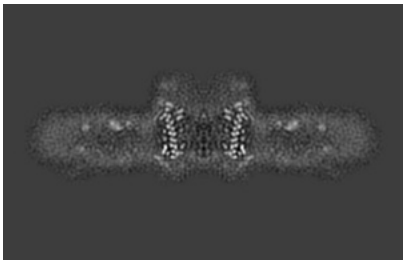


Z

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

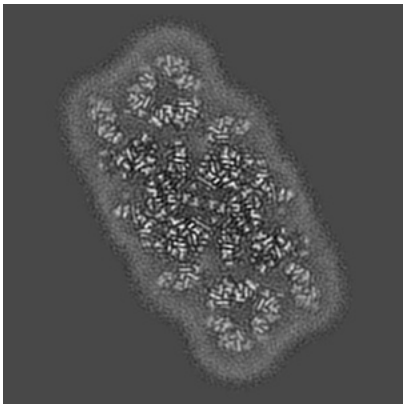
6.2 Central slices

6.2.1 Primary map



X Index: 125

Y Index: 125



Z Index: 80

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: 146 Y Index: 147 Z Index: 69

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

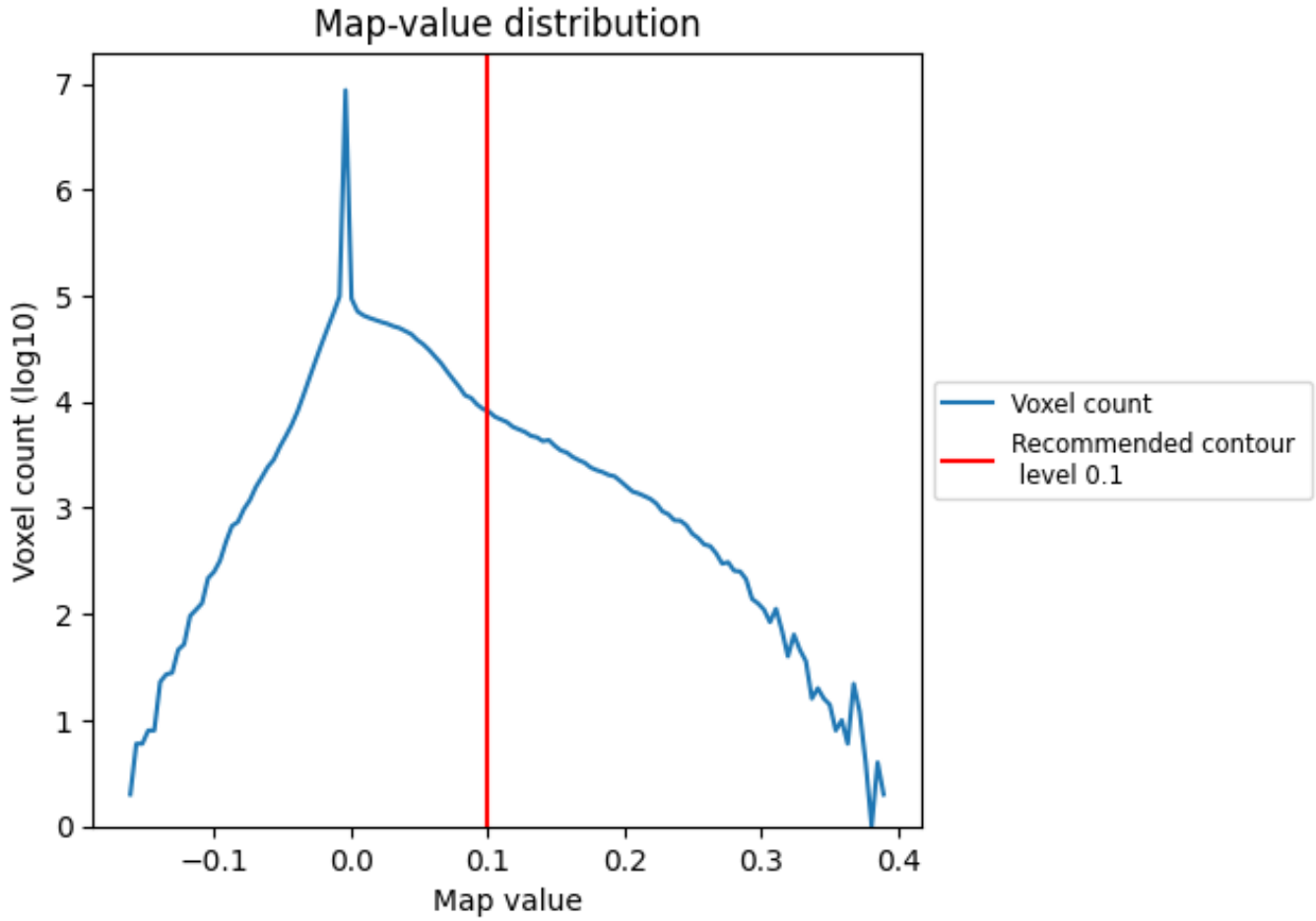
6.5 Mask visualisation (i)

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

7 Map analysis

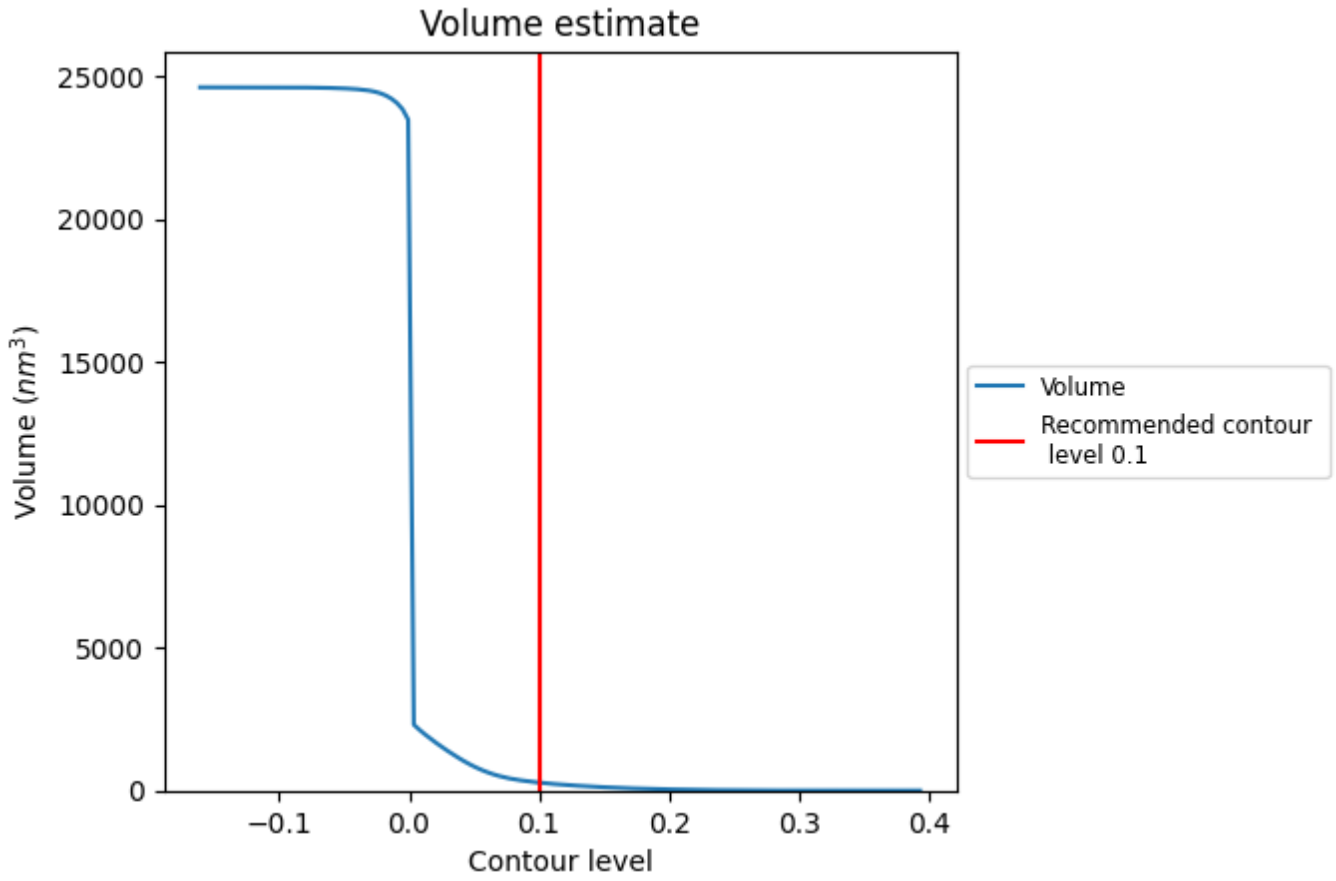
This section contains the results of statistical analysis of the map.

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 279 nm^3; this corresponds to an approximate mass of 252 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

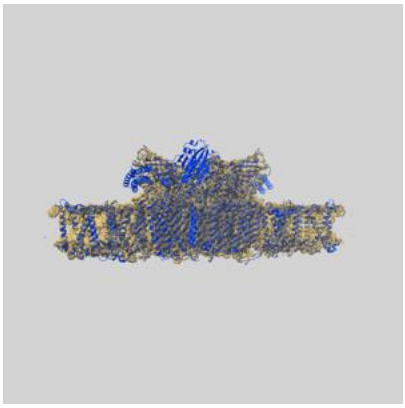
8 Fourier-Shell correlation

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

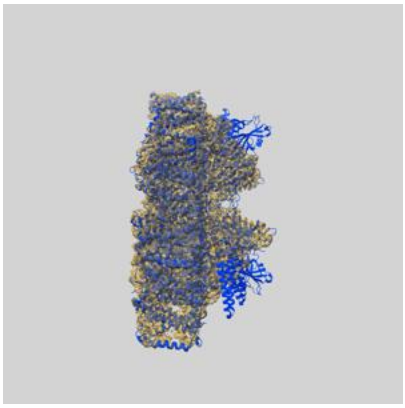
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6617 and PDB model 3JCU. Per-residue inclusion information can be found in section 3 on page 39.

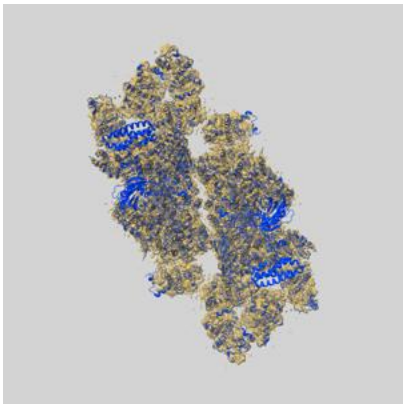
9.1 Map-model overlay



X



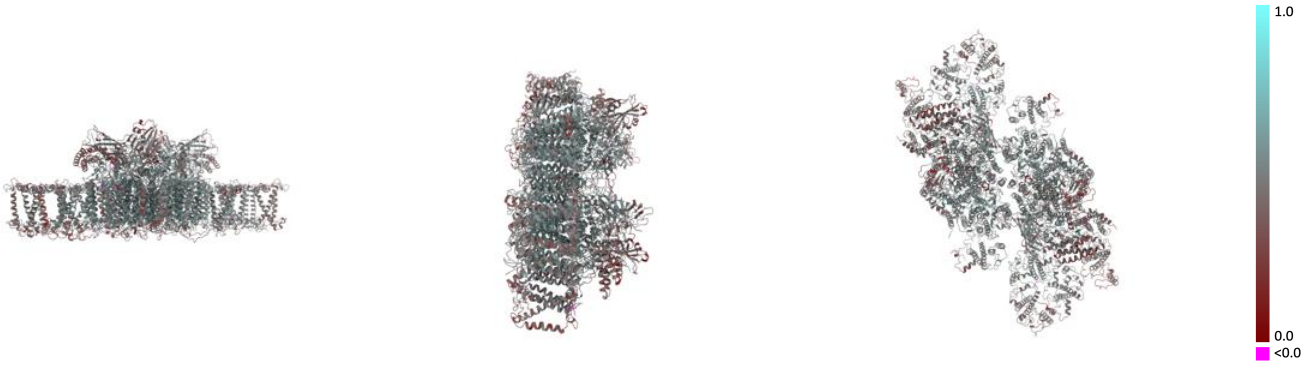
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

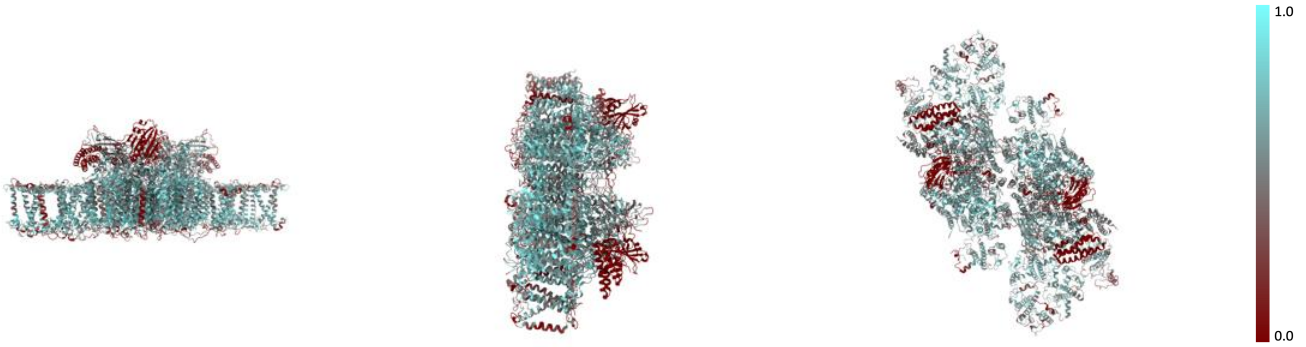
9.2 Q-score mapped to coordinate model



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.

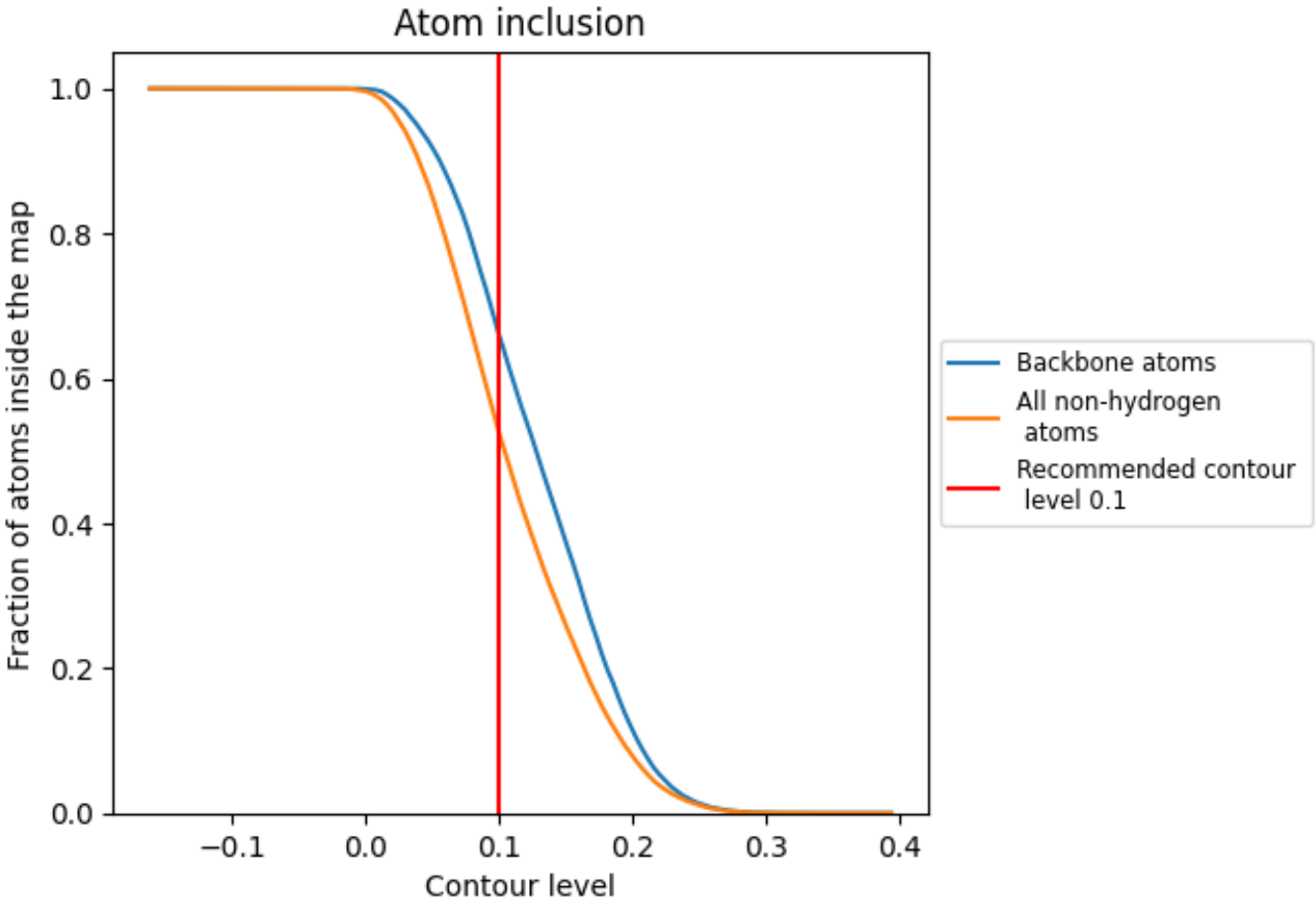
9.3 Atom inclusion mapped to coordinate model



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 53% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5257	0.4830
A	0.6232	0.5310
B	0.6539	0.5350
C	0.6198	0.5220
D	0.6447	0.5370
E	0.5347	0.4210
F	0.5601	0.4540
G	0.5187	0.4420
H	0.5947	0.5320
I	0.6192	0.5090
J	0.1116	0.3960
K	0.5578	0.4630
L	0.5746	0.5270
M	0.4669	0.4960
N	0.5451	0.4720
O	0.3670	0.4340
P	0.0023	0.3960
Q	0.0044	0.3390
R	0.4518	0.4510
S	0.4441	0.3950
T	0.5579	0.5170
U	0.6310	0.4660
W	0.4915	0.4880
X	0.4959	0.4600
Y	0.6293	0.5190
Z	0.3897	0.4340
a	0.6235	0.5310
b	0.6543	0.5350
c	0.6185	0.5210
d	0.6450	0.5360
e	0.5363	0.4210
f	0.5601	0.4530
g	0.5175	0.4440
h	0.5947	0.5310
i	0.6192	0.5140

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Continued from previous page...

Chain	Atom inclusion	Q-score
j	0.1116	0.3980
k	0.5611	0.4620
l	0.5746	0.5280
m	0.4669	0.4950
n	0.5427	0.4720
o	0.3664	0.4350
p	0.0023	0.3950
q	0.0044	0.3370
r	0.4518	0.4510
s	0.4441	0.3940
t	0.5579	0.5200
u	0.6310	0.4680
w	0.4939	0.4870
x	0.4959	0.4640
y	0.6297	0.5180
z	0.3897	0.4340