wwPDB EM Validation Summary Report

Aug 8, 2023 – 12:50 PM JST

PDB ID	:	7YMI
EMDB ID	:	EMD-33929
Title	:	PSII-Pcb Dimer of Acaryochloris Marina
Authors	:	Shen, L.L.; Gao, Y.Z.; Wang, W.D.; Zhang, X.; Shen, J.R.; Wang, P.Y.; Han, G.Y.
Deposited on	:	2022-07-28
Resolution	:	3.30 Å(reported)

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

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

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

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

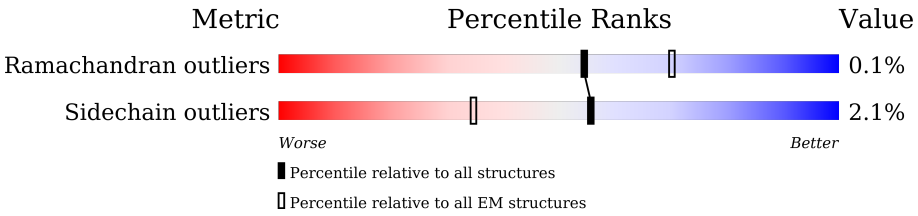
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.30 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	360	8% 78% · 21%
1	a	360	8% 78% · 21%
2	B	506	12% 93% · 5%
2	b	506	12% 93% · 5%
3	C	490	17% 84% · 14%
3	c	490	17% 84% · 14%
4	D	351	8% 91% · 8%
4	d	351	8% 91% · 8%
5	E	83	47% 77% · 22%

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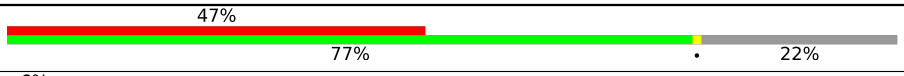
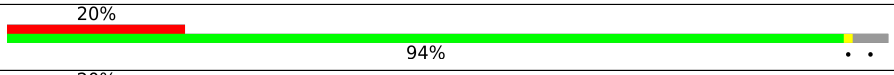
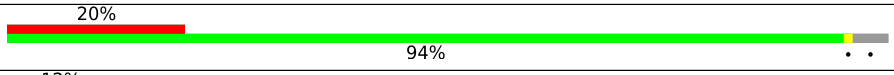
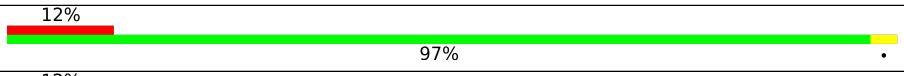
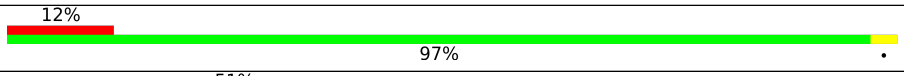
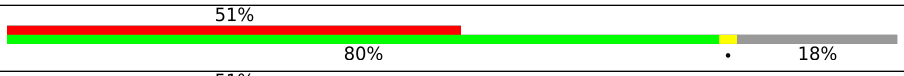
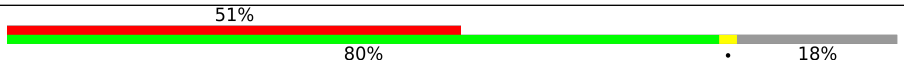
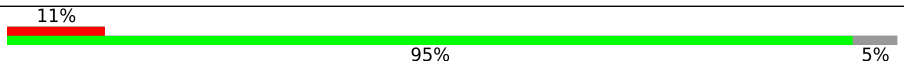
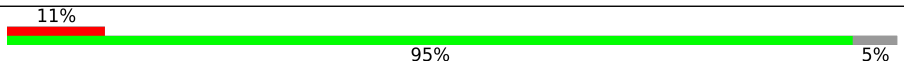
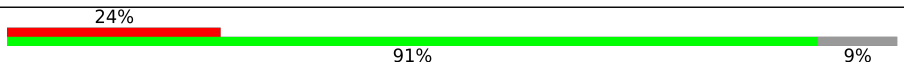
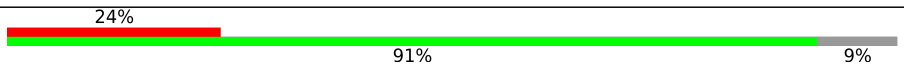
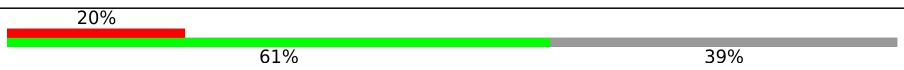
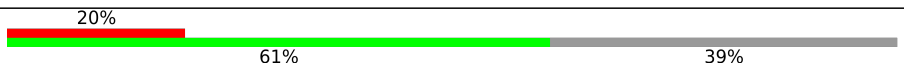
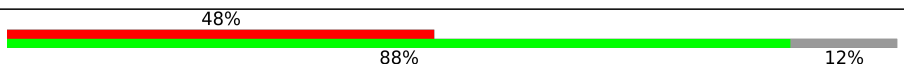
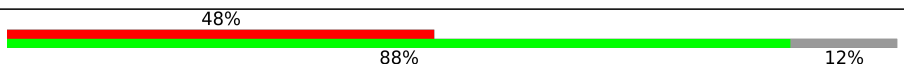
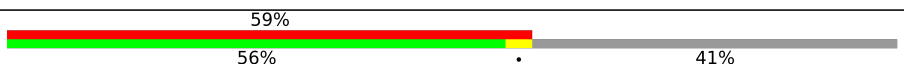
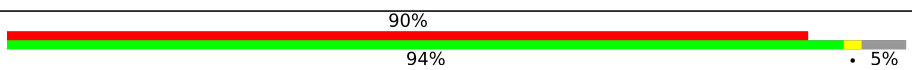
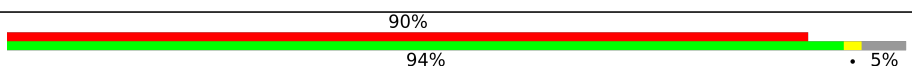
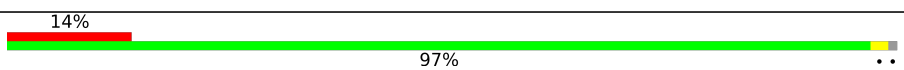
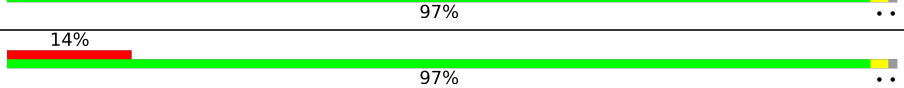
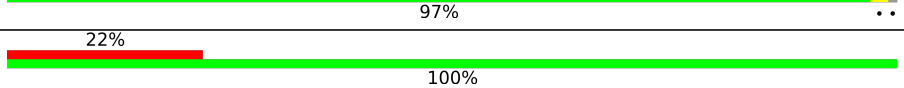
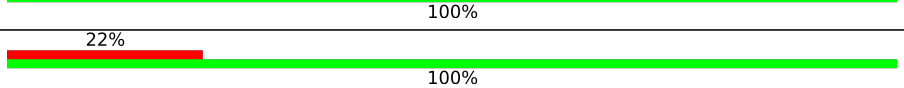
Mol	Chain	Length	Quality of chain
5	e	83	
6	F	99	
6	f	99	
7	H	71	
7	h	71	
8	I	34	
8	i	34	
9	K	45	
9	k	45	
10	L	38	
10	l	38	
11	M	34	
11	m	34	
12	T	46	
12	t	46	
13	X	40	
13	x	40	
14	Y	39	
14	y	39	
15	Z	62	
15	z	62	
16	2	352	
16	6	352	
17	G	41	
17	g	41	

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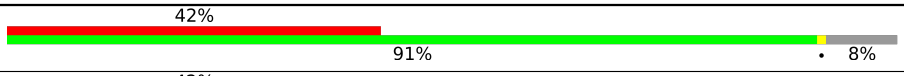
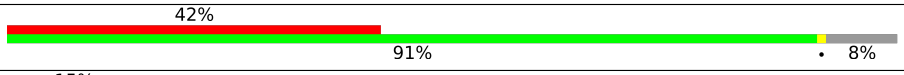
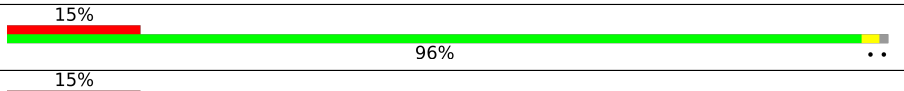
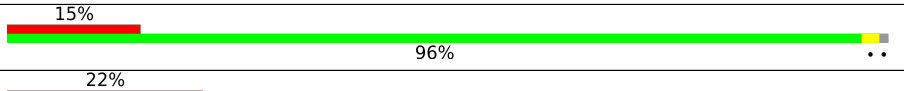
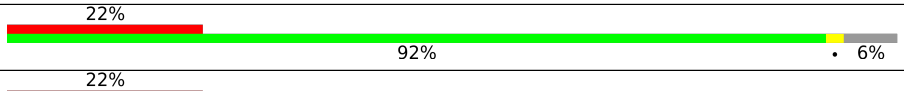
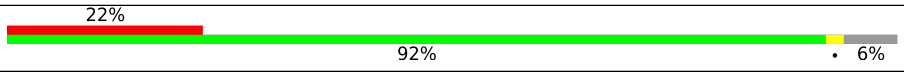
Mol	Chain	Length	Quality of chain
18	1	356	
18	5	356	
19	3	349	
19	7	349	
20	4	353	
20	8	353	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	1	402	X	-	-	-
21	CL7	1	403	X	-	-	-
21	CL7	1	404	X	-	-	-
21	CL7	1	405	X	-	-	-
21	CL7	1	406	X	-	-	-
21	CL7	1	407	X	-	-	-
21	CL7	1	408	X	-	-	-
21	CL7	1	409	X	-	-	-
21	CL7	1	410	X	-	-	-
21	CL7	1	411	X	-	-	-
21	CL7	1	412	X	-	-	-
21	CL7	1	413	X	-	-	-
21	CL7	1	414	X	-	-	-
21	CL7	1	415	X	-	-	-
21	CL7	1	416	X	-	-	-
21	CL7	1	417	X	-	-	-
21	CL7	1	418	X	-	-	-
21	CL7	1	419	X	-	-	-
21	CL7	1	420	X	-	-	-
21	CL7	2	501	X	-	-	-
21	CL7	2	502	X	-	-	-
21	CL7	2	503	X	-	-	-
21	CL7	2	504	X	-	-	-
21	CL7	2	505	X	-	-	-
21	CL7	2	506	X	-	-	-
21	CL7	2	507	X	-	-	-
21	CL7	2	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	2	509	X	-	-	-
21	CL7	2	510	X	-	-	-
21	CL7	2	511	X	-	-	-
21	CL7	2	512	X	-	-	-
21	CL7	2	513	X	-	-	-
21	CL7	2	514	X	-	-	-
21	CL7	2	515	X	-	-	-
21	CL7	2	516	X	-	-	-
21	CL7	2	517	X	-	-	-
21	CL7	2	518	X	-	-	-
21	CL7	3	501	X	-	-	-
21	CL7	3	502	X	-	-	-
21	CL7	3	503	X	-	-	-
21	CL7	3	504	X	-	-	-
21	CL7	3	505	X	-	-	-
21	CL7	3	506	X	-	-	-
21	CL7	3	507	X	-	-	-
21	CL7	3	508	X	-	-	-
21	CL7	3	509	X	-	-	-
21	CL7	3	510	X	-	-	-
21	CL7	3	511	X	-	-	-
21	CL7	3	512	X	-	-	-
21	CL7	3	513	X	-	-	-
21	CL7	3	514	X	-	-	-
21	CL7	3	515	X	-	-	-
21	CL7	3	516	X	-	-	-
21	CL7	3	517	X	-	-	-
21	CL7	3	518	X	-	-	-
21	CL7	4	404	X	-	-	-
21	CL7	4	405	X	-	-	-
21	CL7	4	406	X	-	-	-
21	CL7	4	407	X	-	-	-
21	CL7	4	408	X	-	-	-
21	CL7	4	409	X	-	-	-
21	CL7	4	410	X	-	-	-
21	CL7	4	411	X	-	-	-
21	CL7	4	412	X	-	-	-
21	CL7	4	413	X	-	-	-
21	CL7	4	414	X	-	-	-
21	CL7	4	415	X	-	-	-
21	CL7	4	416	X	-	-	-
21	CL7	4	417	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	5	402	X	-	-	-
21	CL7	5	403	X	-	-	-
21	CL7	5	404	X	-	-	-
21	CL7	5	405	X	-	-	-
21	CL7	5	406	X	-	-	-
21	CL7	5	407	X	-	-	-
21	CL7	5	408	X	-	-	-
21	CL7	5	409	X	-	-	-
21	CL7	5	410	X	-	-	-
21	CL7	5	411	X	-	-	-
21	CL7	5	412	X	-	-	-
21	CL7	5	413	X	-	-	-
21	CL7	5	414	X	-	-	-
21	CL7	5	415	X	-	-	-
21	CL7	5	416	X	-	-	-
21	CL7	5	417	X	-	-	-
21	CL7	5	418	X	-	-	-
21	CL7	5	419	X	-	-	-
21	CL7	5	420	X	-	-	-
21	CL7	6	501	X	-	-	-
21	CL7	6	502	X	-	-	-
21	CL7	6	503	X	-	-	-
21	CL7	6	504	X	-	-	-
21	CL7	6	505	X	-	-	-
21	CL7	6	506	X	-	-	-
21	CL7	6	507	X	-	-	-
21	CL7	6	508	X	-	-	-
21	CL7	6	509	X	-	-	-
21	CL7	6	510	X	-	-	-
21	CL7	6	511	X	-	-	-
21	CL7	6	512	X	-	-	-
21	CL7	6	513	X	-	-	-
21	CL7	6	514	X	-	-	-
21	CL7	6	515	X	-	-	-
21	CL7	6	516	X	-	-	-
21	CL7	6	517	X	-	-	-
21	CL7	6	518	X	-	-	-
21	CL7	7	501	X	-	-	-
21	CL7	7	502	X	-	-	-
21	CL7	7	503	X	-	-	-
21	CL7	7	504	X	-	-	-
21	CL7	7	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	7	506	X	-	-	-
21	CL7	7	507	X	-	-	-
21	CL7	7	508	X	-	-	-
21	CL7	7	509	X	-	-	-
21	CL7	7	510	X	-	-	-
21	CL7	7	511	X	-	-	-
21	CL7	7	512	X	-	-	-
21	CL7	7	513	X	-	-	-
21	CL7	7	514	X	-	-	-
21	CL7	7	515	X	-	-	-
21	CL7	7	516	X	-	-	-
21	CL7	7	517	X	-	-	-
21	CL7	7	518	X	-	-	-
21	CL7	8	404	X	-	-	-
21	CL7	8	405	X	-	-	-
21	CL7	8	406	X	-	-	-
21	CL7	8	407	X	-	-	-
21	CL7	8	408	X	-	-	-
21	CL7	8	409	X	-	-	-
21	CL7	8	410	X	-	-	-
21	CL7	8	411	X	-	-	-
21	CL7	8	412	X	-	-	-
21	CL7	8	413	X	-	-	-
21	CL7	8	414	X	-	-	-
21	CL7	8	415	X	-	-	-
21	CL7	8	416	X	-	-	-
21	CL7	8	417	X	-	-	-
21	CL7	A	401	X	-	-	-
21	CL7	A	403	X	-	-	-
21	CL7	A	406	X	-	-	-
21	CL7	B	601	X	-	-	-
21	CL7	B	602	X	-	-	-
21	CL7	B	603	X	-	-	-
21	CL7	B	604	X	-	-	-
21	CL7	B	605	X	-	-	-
21	CL7	B	606	X	-	-	-
21	CL7	B	607	X	-	-	-
21	CL7	B	608	X	-	-	-
21	CL7	B	609	X	-	-	-
21	CL7	B	610	X	-	-	-
21	CL7	B	611	X	-	-	-
21	CL7	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	B	613	X	-	-	-
21	CL7	B	614	X	-	-	-
21	CL7	B	615	X	-	-	-
21	CL7	B	616	X	-	-	-
21	CL7	B	622	X	-	-	-
21	CL7	C	502	X	-	-	-
21	CL7	C	503	X	-	-	-
21	CL7	C	504	X	-	-	-
21	CL7	C	505	X	-	-	-
21	CL7	C	506	X	-	-	-
21	CL7	C	507	X	-	-	-
21	CL7	C	508	X	-	-	-
21	CL7	C	509	X	-	-	-
21	CL7	C	510	X	-	-	-
21	CL7	C	511	X	-	-	-
21	CL7	C	512	X	-	-	-
21	CL7	C	513	X	-	-	-
21	CL7	C	514	X	-	-	-
21	CL7	C	518	X	-	-	-
21	CL7	D	402	X	-	-	-
21	CL7	D	404	X	-	-	-
21	CL7	D	405	X	-	-	-
21	CL7	a	401	X	-	-	-
21	CL7	a	403	X	-	-	-
21	CL7	a	405	X	-	-	-
21	CL7	b	602	X	-	-	-
21	CL7	b	603	X	-	-	-
21	CL7	b	604	X	-	-	-
21	CL7	b	605	X	-	-	-
21	CL7	b	606	X	-	-	-
21	CL7	b	607	X	-	-	-
21	CL7	b	608	X	-	-	-
21	CL7	b	609	X	-	-	-
21	CL7	b	610	X	-	-	-
21	CL7	b	611	X	-	-	-
21	CL7	b	612	X	-	-	-
21	CL7	b	613	X	-	-	-
21	CL7	b	614	X	-	-	-
21	CL7	b	615	X	-	-	-
21	CL7	b	616	X	-	-	-
21	CL7	b	617	X	-	-	-
21	CL7	b	623	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	c	502	X	-	-	-
21	CL7	c	503	X	-	-	-
21	CL7	c	504	X	-	-	-
21	CL7	c	505	X	-	-	-
21	CL7	c	506	X	-	-	-
21	CL7	c	507	X	-	-	-
21	CL7	c	508	X	-	-	-
21	CL7	c	509	X	-	-	-
21	CL7	c	510	X	-	-	-
21	CL7	c	511	X	-	-	-
21	CL7	c	512	X	-	-	-
21	CL7	c	513	X	-	-	-
21	CL7	c	514	X	-	-	-
21	CL7	c	518	X	-	-	-
21	CL7	d	402	X	-	-	-
21	CL7	d	404	X	-	-	-
21	CL7	d	405	X	-	-	-

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 68428 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		
1	a	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		
2	b	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		
3	c	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		

- Molecule 4 is a protein called Photosystem II D2 protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		
4	d	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		
5	e	65	Total	C	N	O	S	0	0
			538	354	87	96	1		

- Molecule 6 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	f	30	Total	C	N	O	S	0	0
			242	166	39	36	1		

- Molecule 7 is a protein called Photosystem II 10 kDa phosphoprotein PsbH.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		
7	h	68	Total	C	N	O	S	0	0
			519	342	83	91	3		

- Molecule 8 is a protein called Photosystem II protein PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		
8	i	34	Total	C	N	O	S	0	0
			281	194	41	45	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		
9	k	37	Total	C	N	O	S	0	0
			292	205	41	45	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	36	Total	C	N	O	0	0
			288	194	45	49		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	36	Total 288	C 194	N 45	O 49	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total 232	C 156	N 36	O 39	S 1	0	0
11	m	31	Total 232	C 156	N 36	O 39	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	28	Total 231	C 163	N 32	O 34	S 2	0	0
12	t	28	Total 231	C 163	N 32	O 34	S 2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	X	35	Total 269	C 185	N 39	O 45	0	0
13	x	35	Total 269	C 185	N 39	O 45	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	23	Total 164	C 111	N 27	O 25	S 1	0	0
14	y	23	Total 164	C 111	N 27	O 25	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	59	Total 429	C 290	N 64	O 73	S 2	0	0
15	z	59	Total 429	C 290	N 64	O 73	S 2	0	0

- Molecule 16 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		
16	6	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		

- Molecule 17 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	G	41	Total	C	N	O	0	0
			205	123	41	41		
17	g	41	Total	C	N	O	0	0
			205	123	41	41		

- Molecule 18 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		
18	5	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		

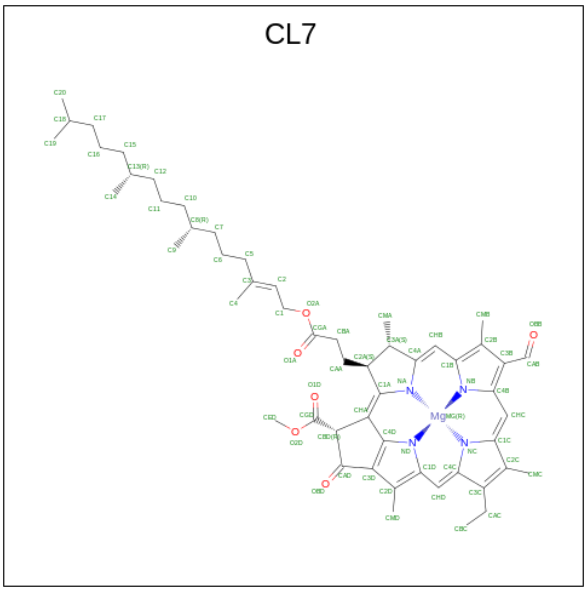
- Molecule 19 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		
19	7	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		

- Molecule 20 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		
20	8	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		

- Molecule 21 is CHLOROPHYLL D (three-letter code: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	D	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	D	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	D	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	3	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	a	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	a	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	a	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	b	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	b	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	c	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	c	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	c	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
21	d	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	d	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	d	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	6	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			58	47	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	7	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	7	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	8	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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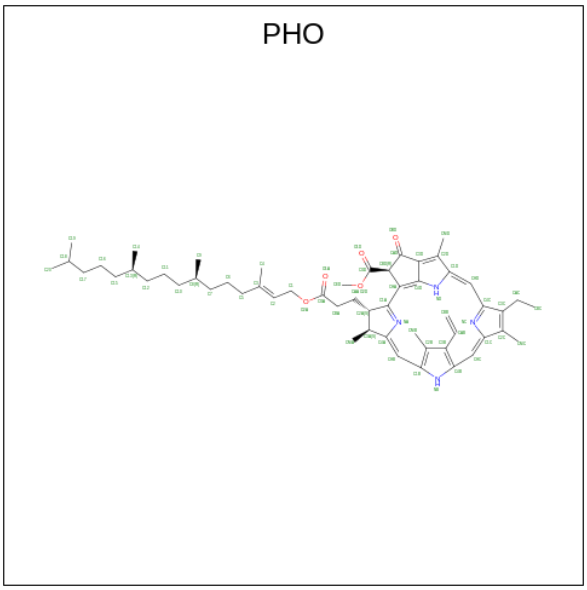
Mol	Chain	Residues	Atoms					AltConf
21	8	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	8	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 22 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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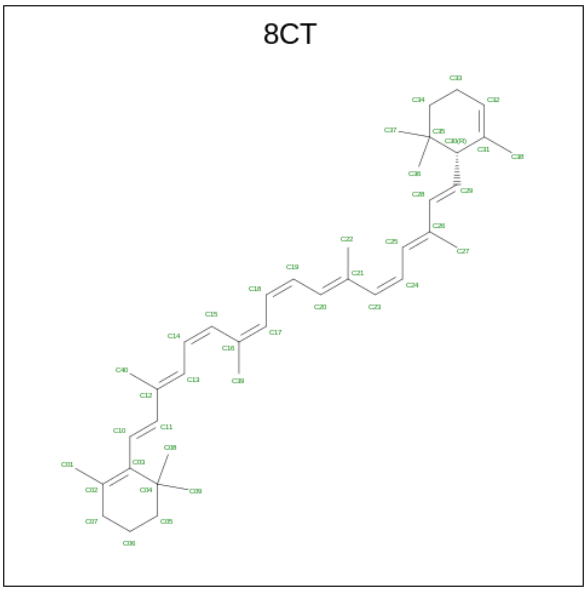
Mol	Chain	Residues	Atoms	AltConf
22	a	1	Total C N O 64 55 4 5	0
22	d	1	Total C N O 64 55 4 5	0

- Molecule 23 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (three-letter code: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	D	1	Total C 40 40	0

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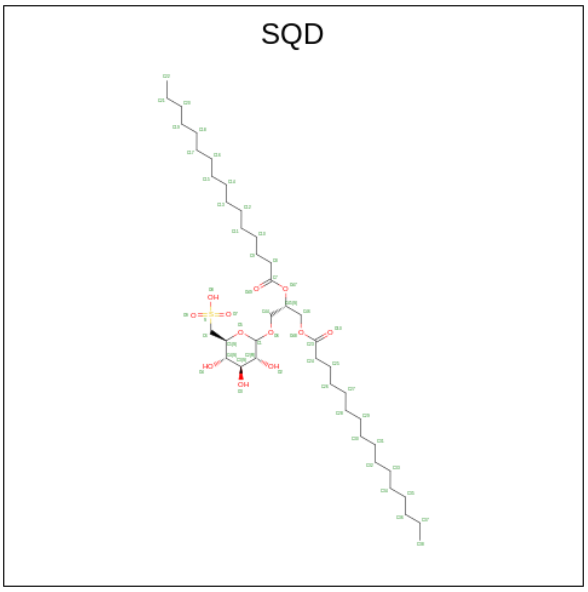
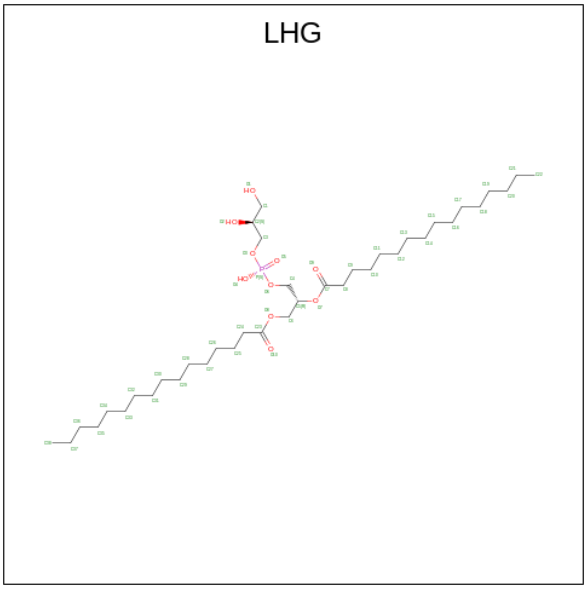
Mol	Chain	Residues	Atoms	AltConf
23	K	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	a	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	c	1	Total C 40 40	0
23	c	1	Total C 40 40	0
23	c	1	Total C 40 40	0
23	d	1	Total C 40 40	0
23	k	1	Total C 40 40	0
23	8	1	Total C 40 40	0

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



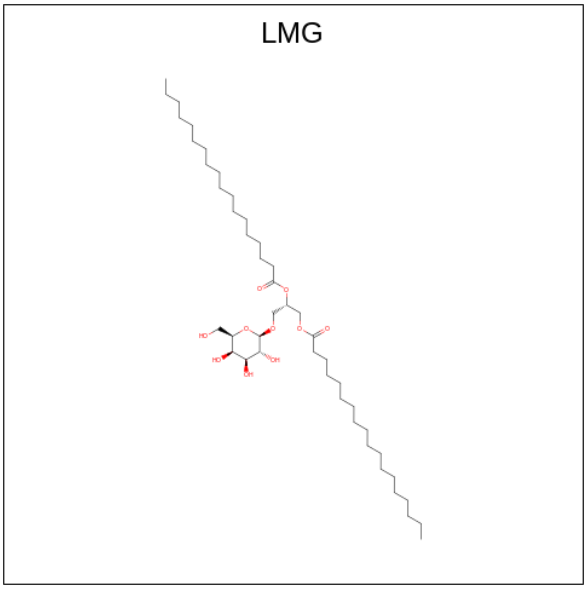
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	S	0
			34	21	12	1	
24	B	1	Total	C	O	S	0
			54	41	12	1	
24	B	1	Total	C	O	S	0
			34	21	12	1	
24	2	1	Total	C	O	S	0
			50	37	12	1	
24	2	1	Total	C	O	S	0
			41	28	12	1	
24	1	1	Total	C	O	S	0
			32	19	12	1	
24	3	1	Total	C	O	S	0
			46	33	12	1	
24	3	1	Total	C	O	S	0
			50	37	12	1	
24	b	1	Total	C	O	S	0
			54	41	12	1	
24	6	1	Total	C	O	S	0
			50	37	12	1	
24	6	1	Total	C	O	S	0
			41	28	12	1	
24	5	1	Total	C	O	S	0
			32	19	12	1	
24	7	1	Total	C	O	S	0
			46	33	12	1	
24	7	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



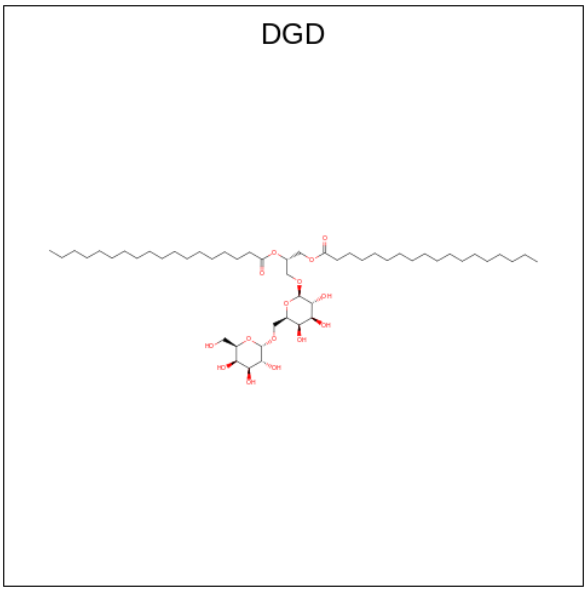
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			46	35	10	1	
25	B	1	Total	C	O	P	0
			45	34	10	1	
25	B	1	Total	C	O	P	0
			49	38	10	1	
25	D	1	Total	C	O	P	0
			49	38	10	1	
25	3	1	Total	C	O	P	0
			36	25	10	1	
25	4	1	Total	C	O	P	0
			49	38	10	1	
25	a	1	Total	C	O	P	0
			46	35	10	1	
25	b	1	Total	C	O	P	0
			45	34	10	1	
25	b	1	Total	C	O	P	0
			49	38	10	1	
25	d	1	Total	C	O	P	0
			49	38	10	1	
25	7	1	Total	C	O	P	0
			36	25	10	1	
25	8	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total C O 51 41 10	0
26	C	1	Total C O 50 40 10	0
26	D	1	Total C O 33 23 10	0
26	1	1	Total C O 51 41 10	0
26	b	1	Total C O 51 41 10	0
26	c	1	Total C O 50 40 10	0
26	d	1	Total C O 33 23 10	0
26	5	1	Total C O 51 41 10	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

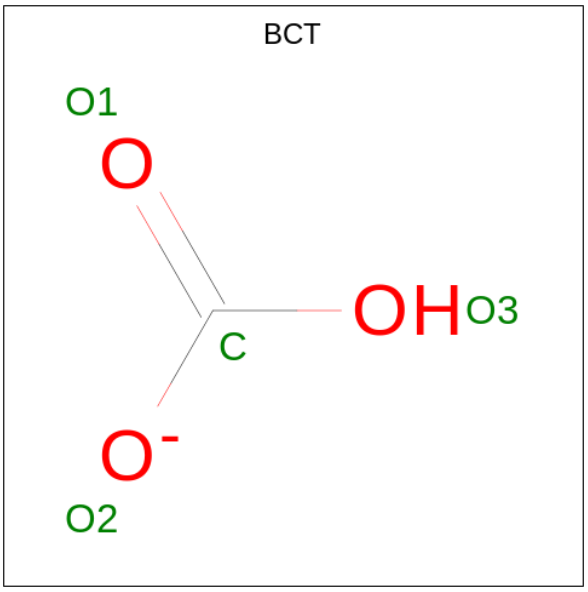


Mol	Chain	Residues	Atoms	AltConf
27	B	1	Total C O 62 47 15	0
27	C	1	Total C O 62 47 15	0
27	b	1	Total C O 62 47 15	0
27	c	1	Total C O 62 47 15	0

- Molecule 28 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

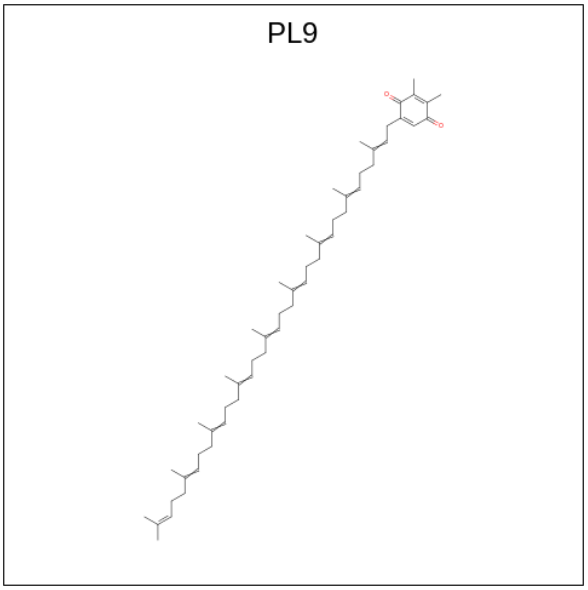
Mol	Chain	Residues	Atoms	AltConf
28	D	1	Total Fe 1 1	0
28	d	1	Total Fe 1 1	0

- Molecule 29 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



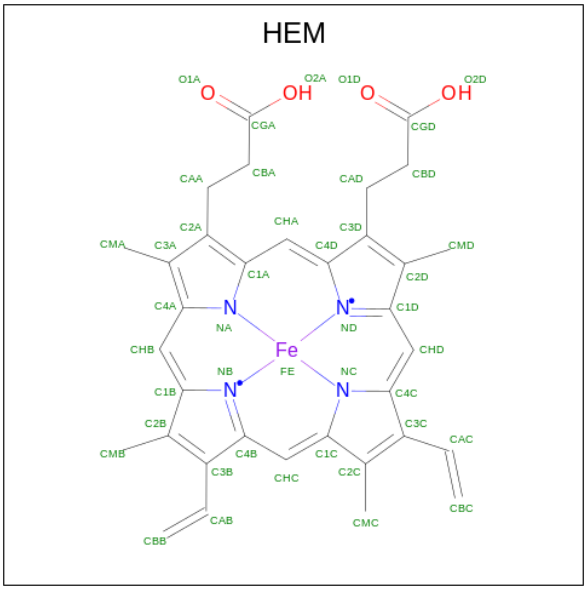
Mol	Chain	Residues	Atoms			AltConf
29	D	1	Total	C	O	0
			4	1	3	
29	d	1	Total	C	O	0
			4	1	3	

- Molecule 30 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: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



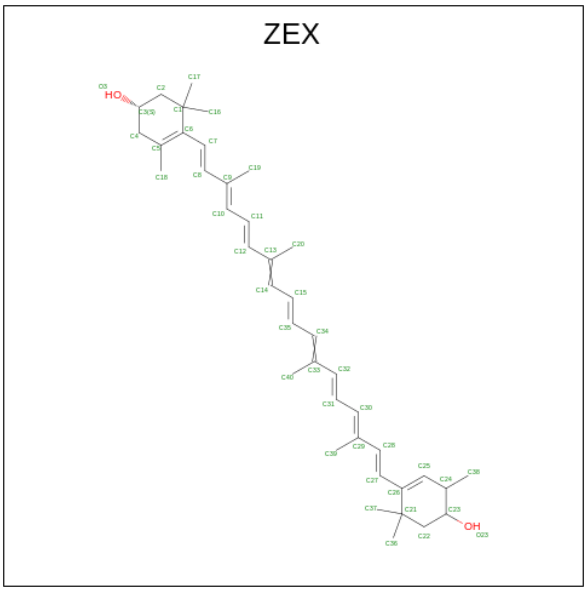
Mol	Chain	Residues	Atoms			AltConf
30	D	1	Total	C	O	0
			55	53	2	
30	d	1	Total	C	O	0
			55	53	2	

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 32 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
32	2	1	Total C O 42 40 2	0
32	2	1	Total C O 42 40 2	0
32	2	1	Total C O 42 40 2	0
32	2	1	Total C O 42 40 2	0
32	2	1	Total C O 42 40 2	0
32	1	1	Total C O 42 40 2	0
32	1	1	Total C O 42 40 2	0
32	3	1	Total C O 42 40 2	0
32	3	1	Total C O 42 40 2	0
32	3	1	Total C O 42 40 2	0
32	3	1	Total C O 42 40 2	0
32	4	1	Total C O 42 40 2	0
32	4	1	Total C O 42 40 2	0
32	4	1	Total C O 42 40 2	0

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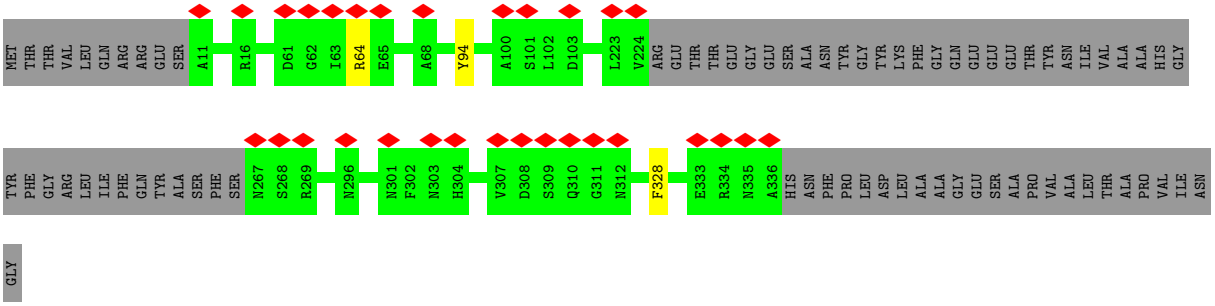
Mol	Chain	Residues	Atoms			AltConf
32	4	1	Total	C	O	0
			42	40	2	
32	6	1	Total	C	O	0
			42	40	2	
32	6	1	Total	C	O	0
			42	40	2	
32	6	1	Total	C	O	0
			42	40	2	
32	6	1	Total	C	O	0
			42	40	2	
32	5	1	Total	C	O	0
			42	40	2	
32	5	1	Total	C	O	0
			42	40	2	
32	7	1	Total	C	O	0
			42	40	2	
32	7	1	Total	C	O	0
			42	40	2	
32	7	1	Total	C	O	0
			42	40	2	
32	8	1	Total	C	O	0
			42	40	2	
32	8	1	Total	C	O	0
			42	40	2	
32	8	1	Total	C	O	0
			42	40	2	
32	8	1	Total	C	O	0
			42	40	2	

3 Residue-property plots

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

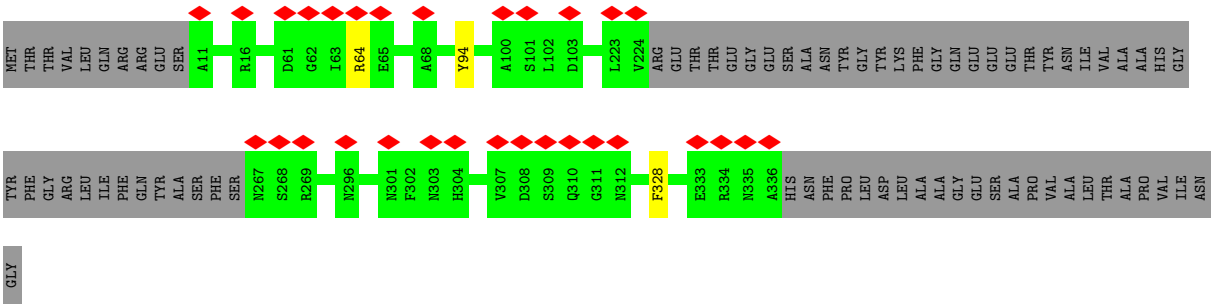
• Molecule 1: Photosystem II protein D1 2

Chain A:



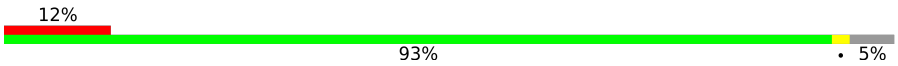
• Molecule 1: Photosystem II protein D1 2

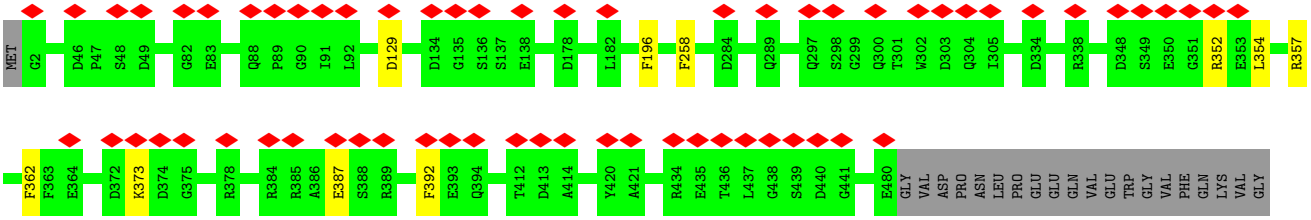
Chain a:



• Molecule 2: Photosystem II CP47 reaction center protein

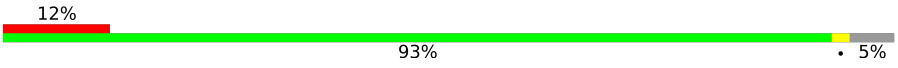
Chain B:

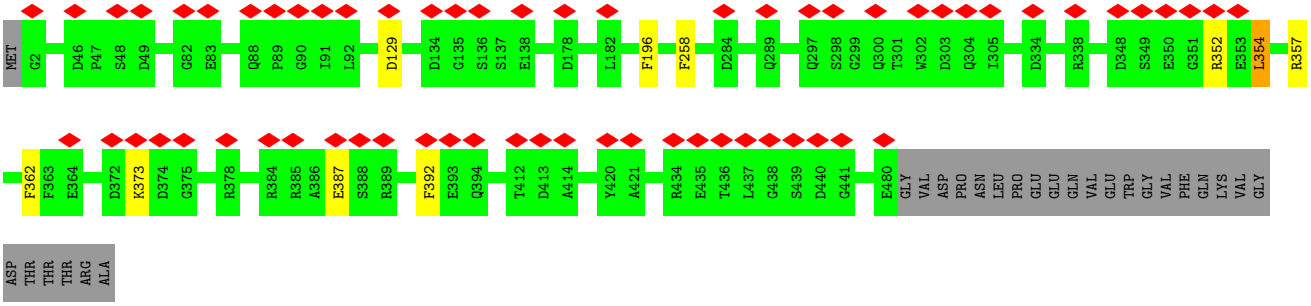




• Molecule 2: Photosystem II CP47 reaction center protein

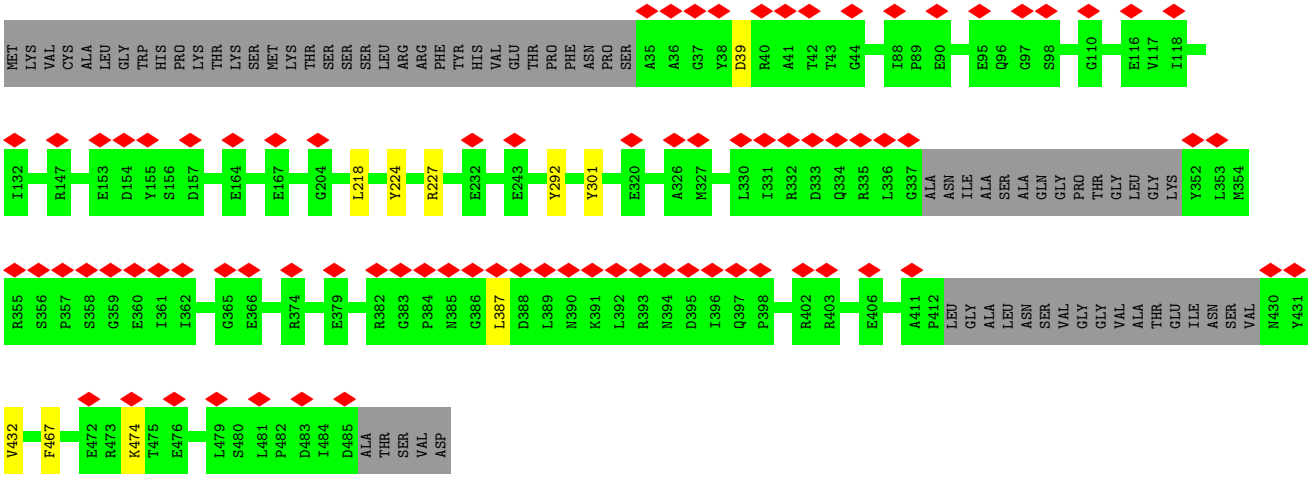
Chain b:





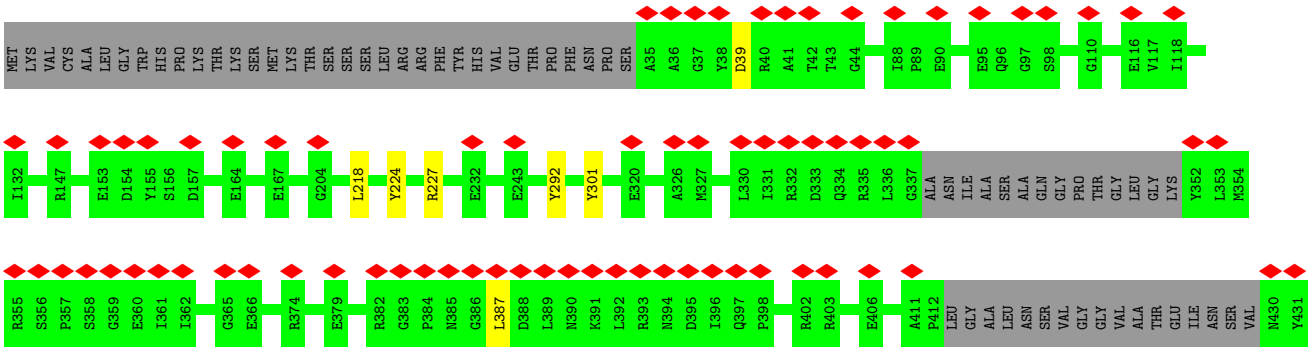
• Molecule 3: Photosystem II CP43 reaction center protein

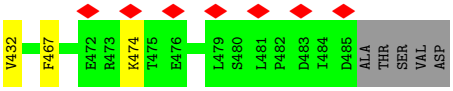
Chain C:



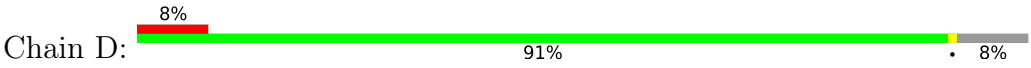
• Molecule 3: Photosystem II CP43 reaction center protein

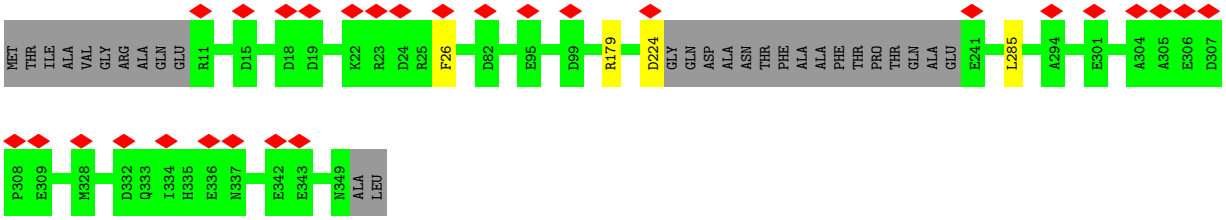
Chain c:



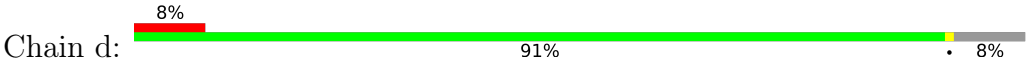


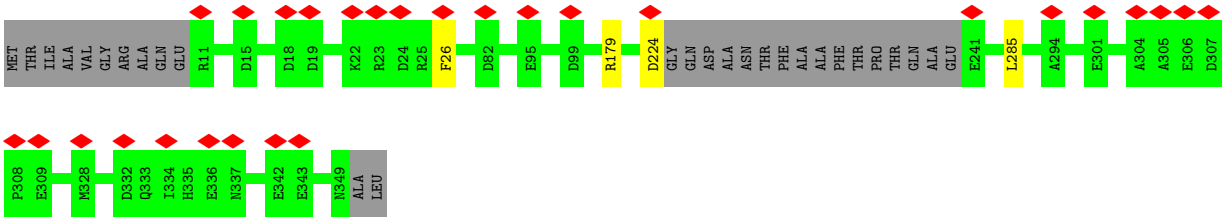
• Molecule 4: Photosystem II D2 protein 1



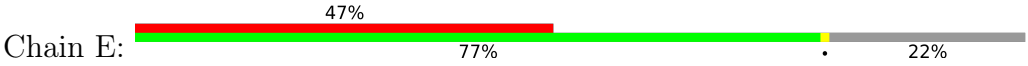


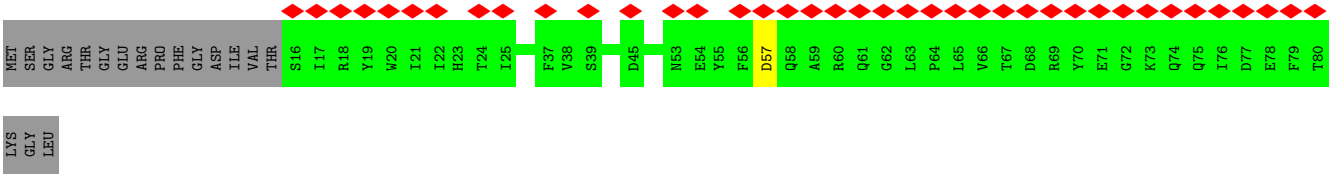
• Molecule 4: Photosystem II D2 protein 1



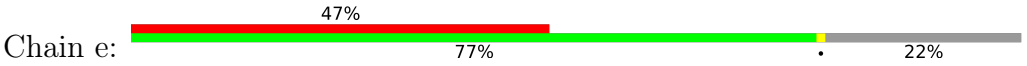


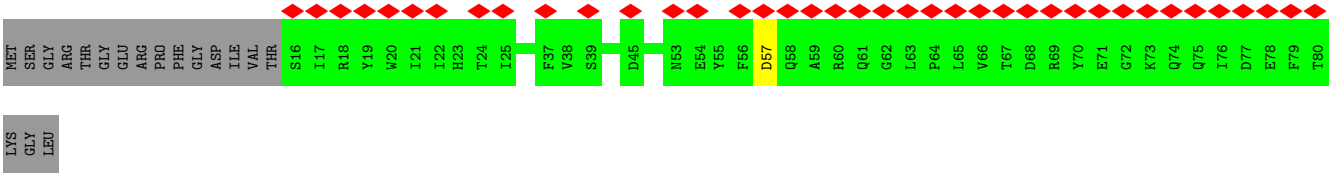
• Molecule 5: Cytochrome b559 subunit alpha



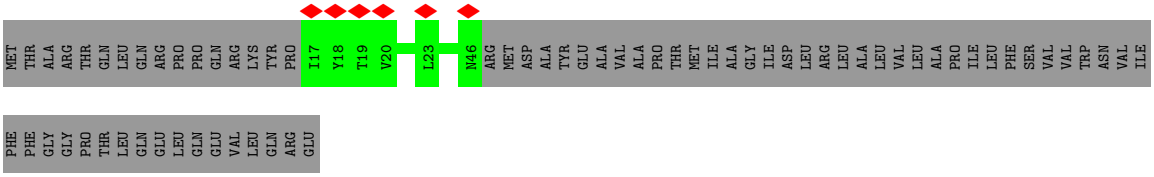


• Molecule 5: Cytochrome b559 subunit alpha

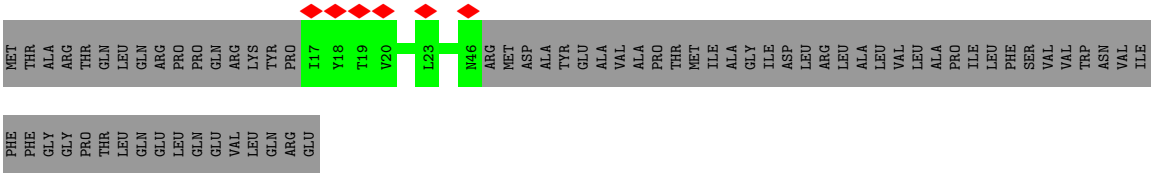




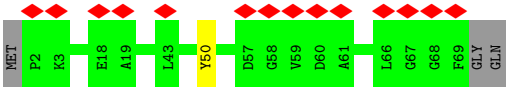
• Molecule 6: Photosystem II protein Y



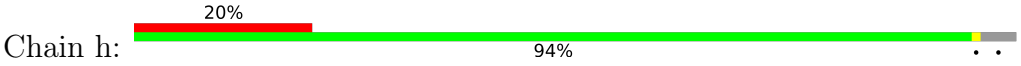
• Molecule 6: Photosystem II protein Y

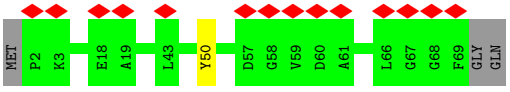


• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH

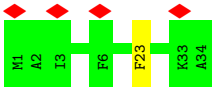


• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH

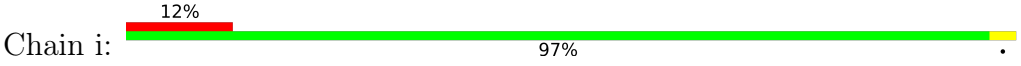


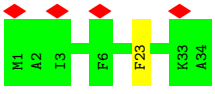


• Molecule 8: Photosystem II protein PsbI

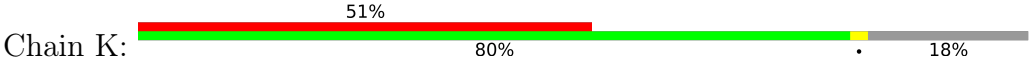


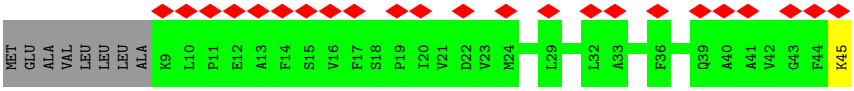
• Molecule 8: Photosystem II protein PsbI



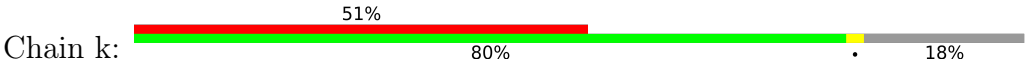


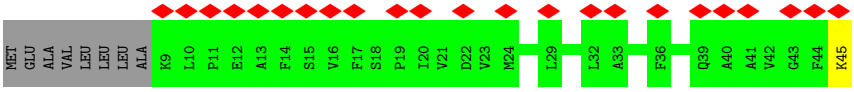
• Molecule 9: Photosystem II reaction center protein K



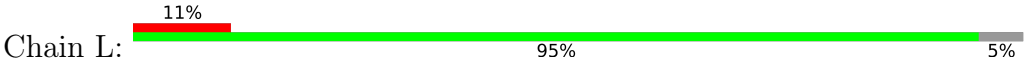


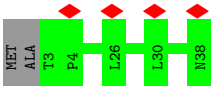
• Molecule 9: Photosystem II reaction center protein K



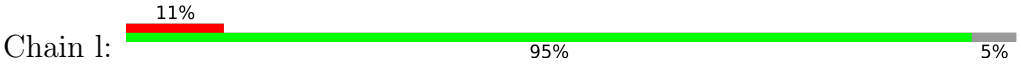


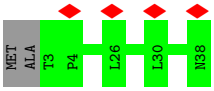
• Molecule 10: Photosystem II reaction center protein L



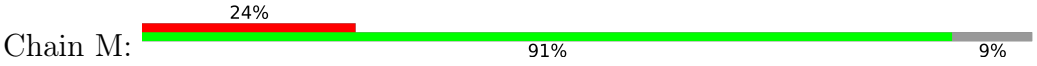


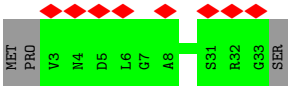
• Molecule 10: Photosystem II reaction center protein L



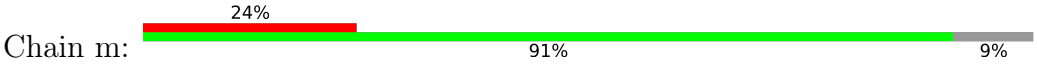


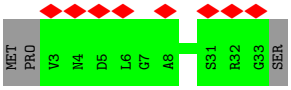
• Molecule 11: Photosystem II reaction center protein M



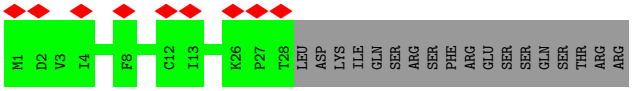


• Molecule 11: Photosystem II reaction center protein M



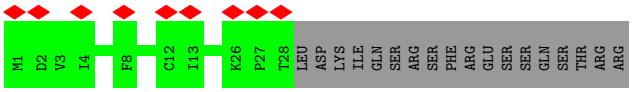


• Molecule 12: Photosystem II reaction center protein T



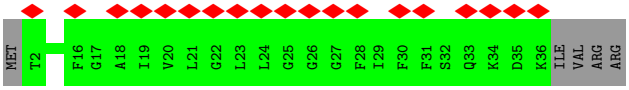
• Molecule 12: Photosystem II reaction center protein T

Chain t:



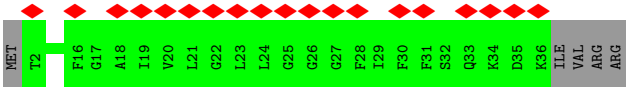
• Molecule 13: Photosystem II reaction center X protein

Chain X:



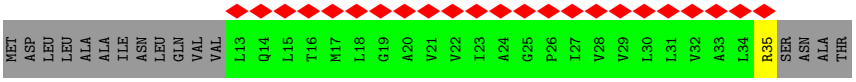
• Molecule 13: Photosystem II reaction center X protein

Chain x:



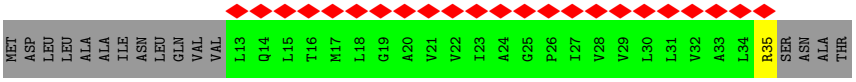
• Molecule 14: Photosystem II reaction center protein Ycf12

Chain Y:



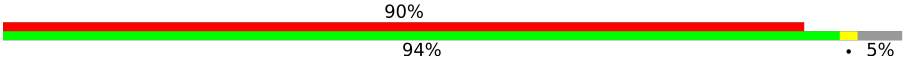
• Molecule 14: Photosystem II reaction center protein Ycf12

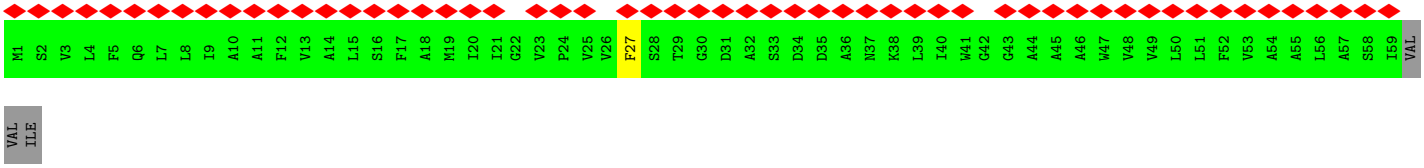
Chain y:



• Molecule 15: Photosystem II reaction center protein Z

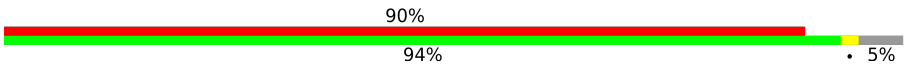
Chain Z:

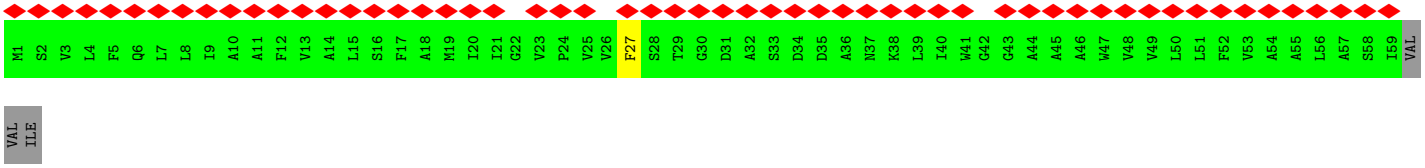




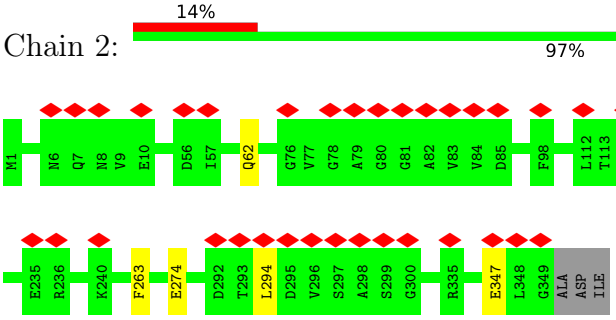
• Molecule 15: Photosystem II reaction center protein Z

Chain z:

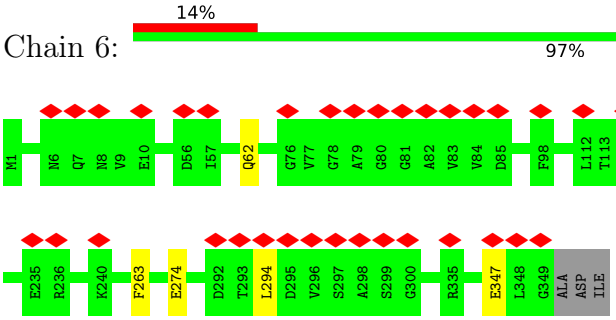




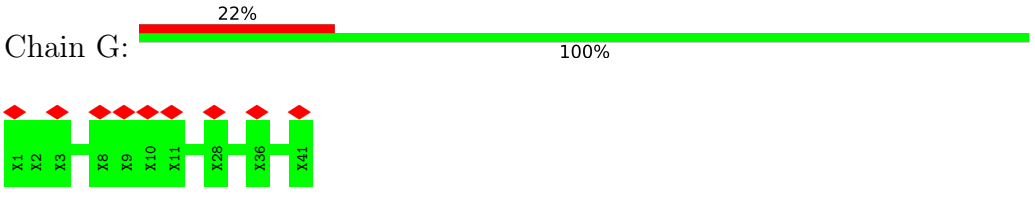
• Molecule 16: High light inducible protein



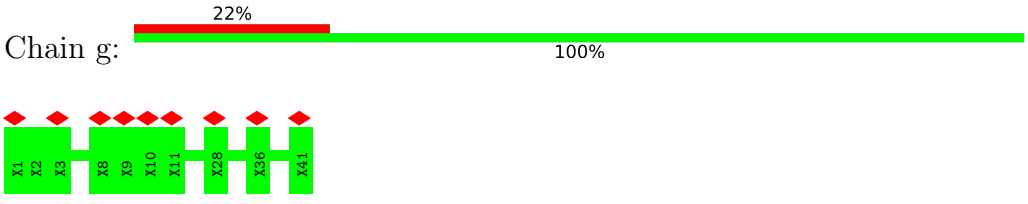
• Molecule 16: High light inducible protein



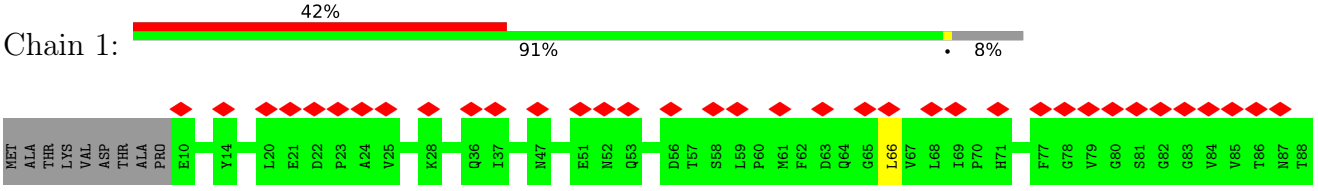
• Molecule 17: Unknown protein

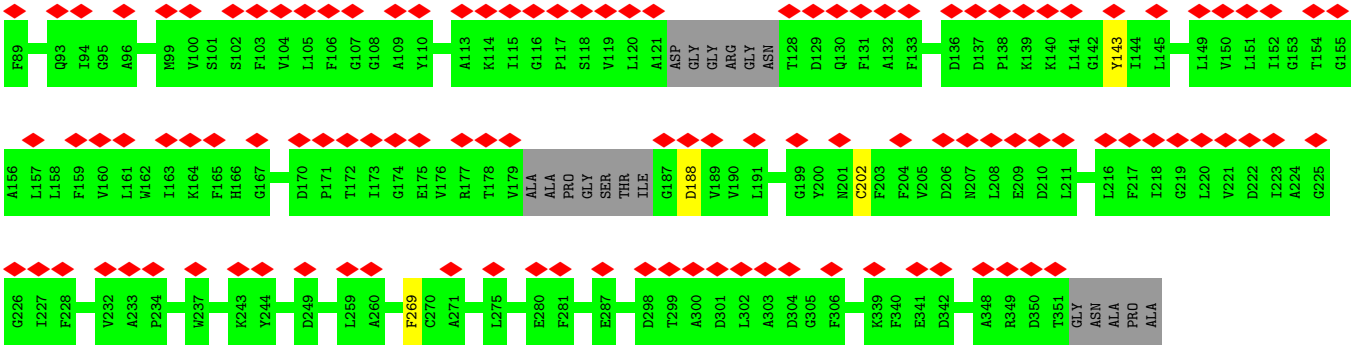


• Molecule 17: Unknown protein



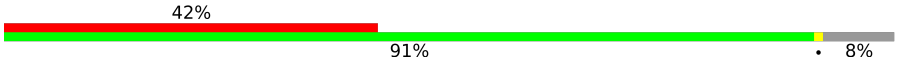
• Molecule 18: High light inducible protein

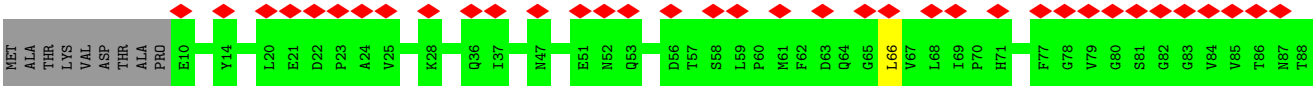


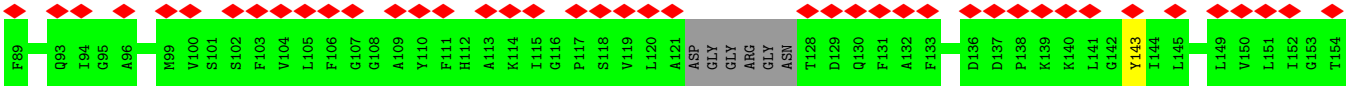


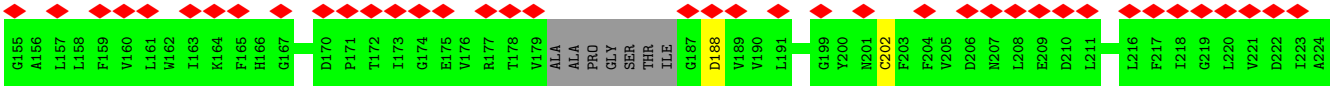
• Molecule 18: High light inducible protein

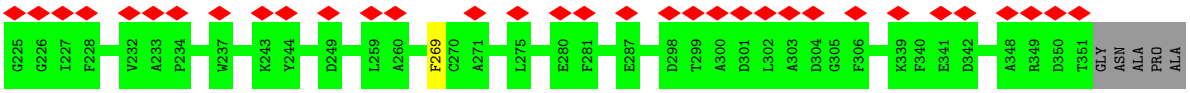
Chain 5:





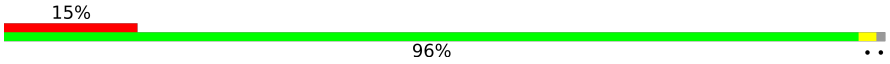


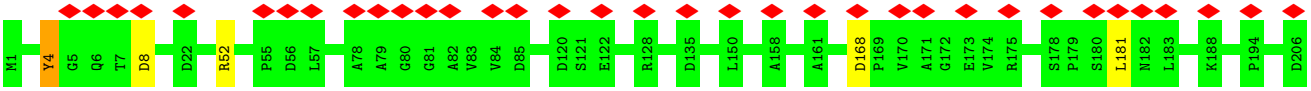


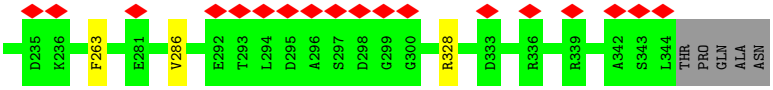


• Molecule 19: High light inducible protein

Chain 3:

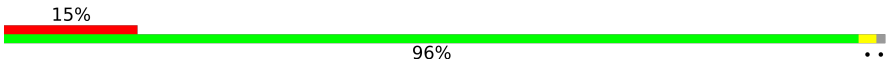


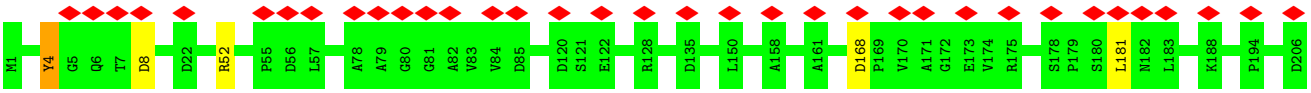


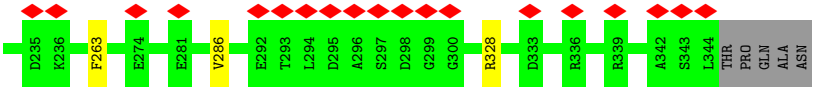


• Molecule 19: High light inducible protein

Chain 7:

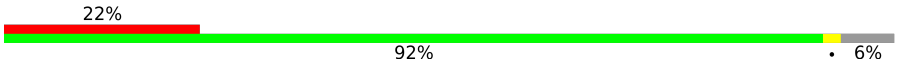


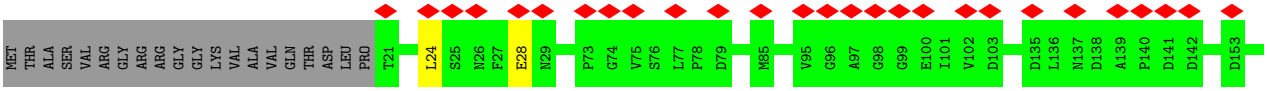


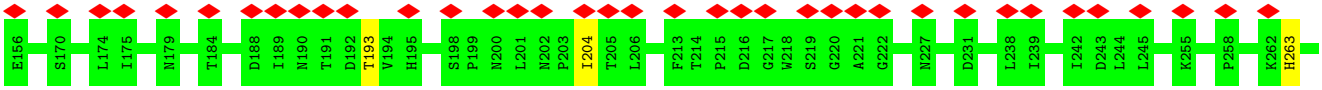


• Molecule 20: High light inducible protein

Chain 4:

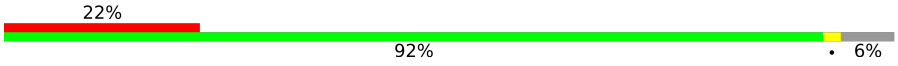


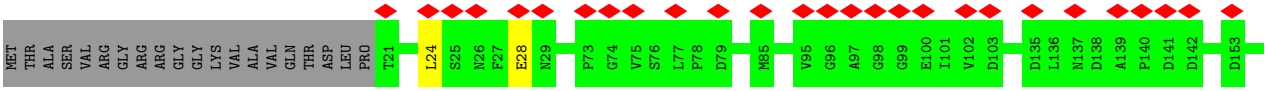


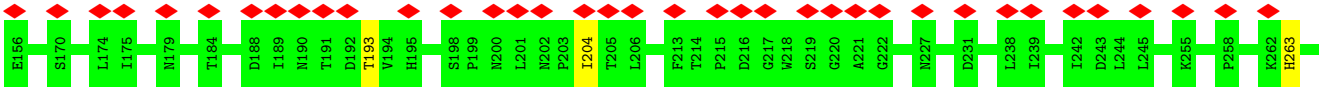


• Molecule 20: High light inducible protein

Chain 8:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0188	Depositor
Map size (Å)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: BCT, SQD, ZEX, PL9, HEM, FE2, 8CT, PHO, CL7, LMG, DGD, LHG

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	0.47	0/2280	0.48	0/3112
1	a	0.47	0/2280	0.48	0/3112
2	B	0.46	0/3929	0.47	0/5360
2	b	0.46	0/3929	0.47	1/5360 (0.0%)
3	C	0.43	0/3431	0.48	1/4669 (0.0%)
3	c	0.43	0/3431	0.48	1/4669 (0.0%)
4	D	0.45	0/2672	0.47	0/3641
4	d	0.45	0/2672	0.47	0/3641
5	E	0.35	0/555	0.44	0/757
5	e	0.35	0/555	0.44	0/757
6	F	0.37	0/250	0.42	0/343
6	f	0.37	0/250	0.42	0/343
7	H	0.37	0/534	0.49	0/729
7	h	0.37	0/534	0.49	0/729
8	I	0.49	0/290	0.43	0/391
8	i	0.49	0/290	0.43	0/391
9	K	0.35	0/303	0.43	0/413
9	k	0.35	0/303	0.43	0/413
10	L	0.44	0/295	0.45	0/401
10	l	0.44	0/295	0.45	0/401
11	M	0.40	0/236	0.48	0/322
11	m	0.40	0/236	0.48	0/322
12	T	0.42	0/238	0.43	0/321
12	t	0.42	0/238	0.43	0/321
13	X	0.34	0/276	0.40	0/370
13	x	0.34	0/276	0.40	0/370
14	Y	0.26	0/164	0.42	0/224
14	y	0.26	0/164	0.42	0/224
15	Z	0.29	0/438	0.38	0/599
15	z	0.29	0/438	0.38	0/599
16	2	0.44	0/2830	0.47	0/3855
16	6	0.44	0/2830	0.47	0/3855

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
18	1	0.37	0/2652	0.45	0/3618
18	5	0.37	0/2652	0.45	0/3618
19	3	0.46	0/2814	0.48	0/3841
19	7	0.46	0/2814	0.48	0/3841
20	4	0.38	0/2590	0.47	0/3537
20	8	0.39	0/2590	0.47	0/3537
All	All	0.43	0/53554	0.47	3/73006 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	387	LEU	CA-CB-CG	5.61	128.20	115.30
3	C	387	LEU	CA-CB-CG	5.59	128.16	115.30
2	b	354	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

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	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
1	a	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
2	B	477/506 (94%)	452 (95%)	25 (5%)	0	100	100
2	b	477/506 (94%)	451 (94%)	26 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
3	c	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
4	D	319/351 (91%)	309 (97%)	10 (3%)	0	100	100
4	d	319/351 (91%)	310 (97%)	9 (3%)	0	100	100
5	E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
5	e	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
6	F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
6	f	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
7	H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
7	h	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
8	I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	i	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
9	K	35/45 (78%)	35 (100%)	0	0	100	100
9	k	35/45 (78%)	35 (100%)	0	0	100	100
10	L	34/38 (90%)	34 (100%)	0	0	100	100
10	l	34/38 (90%)	34 (100%)	0	0	100	100
11	M	29/34 (85%)	29 (100%)	0	0	100	100
11	m	29/34 (85%)	29 (100%)	0	0	100	100
12	T	26/46 (56%)	26 (100%)	0	0	100	100
12	t	26/46 (56%)	26 (100%)	0	0	100	100
13	X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
13	x	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
14	Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
14	y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
15	Z	57/62 (92%)	57 (100%)	0	0	100	100
15	z	57/62 (92%)	57 (100%)	0	0	100	100
16	2	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
16	6	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
18	1	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	41	71
18	5	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	41	71
19	3	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	41	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	7	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	41 71
20	4	329/353 (93%)	306 (93%)	23 (7%)	0	100 100
20	8	329/353 (93%)	306 (93%)	23 (7%)	0	100 100
All	All	6510/7416 (88%)	6206 (95%)	300 (5%)	4 (0%)	54 81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	3	4	TYR
19	7	4	TYR
18	1	202	CYS
18	5	202	CYS

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	232/292 (80%)	229 (99%)	3 (1%)	69 82
1	a	232/292 (80%)	229 (99%)	3 (1%)	69 82
2	B	395/418 (94%)	385 (98%)	10 (2%)	47 72
2	b	395/418 (94%)	385 (98%)	10 (2%)	47 72
3	C	322/378 (85%)	313 (97%)	9 (3%)	43 70
3	c	322/378 (85%)	313 (97%)	9 (3%)	43 70
4	D	265/284 (93%)	261 (98%)	4 (2%)	65 81
4	d	265/284 (93%)	261 (98%)	4 (2%)	65 81
5	E	57/71 (80%)	56 (98%)	1 (2%)	59 78
5	e	57/71 (80%)	56 (98%)	1 (2%)	59 78
6	F	25/84 (30%)	25 (100%)	0	100 100
6	f	25/84 (30%)	25 (100%)	0	100 100
7	H	55/57 (96%)	54 (98%)	1 (2%)	59 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	55/57 (96%)	54 (98%)	1 (2%)	59	78
8	I	30/30 (100%)	29 (97%)	1 (3%)	38	66
8	i	30/30 (100%)	29 (97%)	1 (3%)	38	66
9	K	31/37 (84%)	30 (97%)	1 (3%)	39	67
9	k	31/37 (84%)	30 (97%)	1 (3%)	39	67
10	L	33/34 (97%)	33 (100%)	0	100	100
10	l	33/34 (97%)	33 (100%)	0	100	100
11	M	24/27 (89%)	24 (100%)	0	100	100
11	m	24/27 (89%)	24 (100%)	0	100	100
12	T	24/42 (57%)	24 (100%)	0	100	100
12	t	24/42 (57%)	24 (100%)	0	100	100
13	X	28/33 (85%)	28 (100%)	0	100	100
13	x	28/33 (85%)	28 (100%)	0	100	100
14	Y	18/31 (58%)	17 (94%)	1 (6%)	21	52
14	y	18/31 (58%)	17 (94%)	1 (6%)	21	52
15	Z	43/46 (94%)	42 (98%)	1 (2%)	50	73
15	z	43/46 (94%)	42 (98%)	1 (2%)	50	73
16	2	276/278 (99%)	270 (98%)	6 (2%)	52	74
16	6	276/278 (99%)	270 (98%)	6 (2%)	52	74
18	1	262/278 (94%)	258 (98%)	4 (2%)	65	81
18	5	262/278 (94%)	258 (98%)	4 (2%)	65	81
19	3	269/273 (98%)	261 (97%)	8 (3%)	41	68
19	7	269/273 (98%)	261 (97%)	8 (3%)	41	68
20	4	260/277 (94%)	254 (98%)	6 (2%)	50	73
20	8	260/277 (94%)	254 (98%)	6 (2%)	50	73
All	All	5298/5940 (89%)	5186 (98%)	112 (2%)	56	75

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	94	TYR
20	8	263	HIS
3	c	224	TYR

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Mol	Chain	Res	Type
20	8	204	ILE
19	7	8	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
18	5	215	HIS
19	7	34	GLN
20	8	280	ASN
20	8	195	HIS
20	4	280	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 312 ligands modelled in this entry, 2 are monoatomic - leaving 310 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	$\#\|Z\| > 2$
23	8CT	c	516	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	SQD	6	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	b	615	-	61,68,73	2.30	14 (22%)	59,107,113	2.37	18 (30%)
21	CL7	C	511	-	66,73,73	2.23	11 (16%)	65,113,113	2.19	17 (26%)
21	CL7	3	502	-	59,66,73	2.36	13 (22%)	56,104,113	2.26	17 (30%)
32	ZEX	8	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	8	415	-	46,53,73	2.60	15 (32%)	41,89,113	2.88	15 (36%)
25	LHG	b	624	-	44,44,48	0.31	0	47,50,54	0.39	0
21	CL7	4	404	-	66,73,73	2.22	13 (19%)	65,113,113	2.21	16 (24%)
21	CL7	7	512	-	56,63,73	2.39	13 (23%)	53,101,113	2.45	18 (33%)
21	CL7	6	517	16	66,73,73	2.18	12 (18%)	65,113,113	2.20	17 (26%)
21	CL7	8	408	-	46,53,73	2.66	15 (32%)	41,89,113	2.66	13 (31%)
32	ZEX	3	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	6	501	-	66,73,73	2.17	12 (18%)	65,113,113	2.23	15 (23%)
21	CL7	D	404	-	59,66,73	2.33	14 (23%)	56,104,113	2.36	17 (30%)
25	LHG	7	524	-	35,35,48	0.34	0	38,41,54	0.47	0
25	LHG	3	524	-	35,35,48	0.34	0	38,41,54	0.47	0
32	ZEX	7	519	-	42,43,43	1.02	3 (7%)	55,60,60	2.58	17 (30%)
21	CL7	5	418	18	66,73,73	2.18	12 (18%)	65,113,113	2.31	20 (30%)
21	CL7	6	514	-	46,53,73	2.63	14 (30%)	41,89,113	2.68	12 (29%)
21	CL7	c	511	-	66,73,73	2.23	11 (16%)	65,113,113	2.20	17 (26%)
32	ZEX	7	520	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	c	504	-	66,73,73	2.20	14 (21%)	65,113,113	2.22	17 (26%)
21	CL7	2	510	16	66,73,73	2.18	13 (19%)	65,113,113	2.24	18 (27%)
24	SQD	A	405	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
23	8CT	C	516	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	7	514	-	46,53,73	2.63	14 (30%)	41,89,113	2.80	14 (34%)
21	CL7	3	501	-	66,73,73	2.22	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	5	416	-	42,49,73	2.73	10 (23%)	36,84,113	2.76	14 (38%)
21	CL7	3	506	-	46,53,73	2.58	14 (30%)	41,89,113	2.72	14 (34%)
32	ZEX	8	419	-	42,43,43	0.99	3 (7%)	55,60,60	2.43	25 (45%)
21	CL7	3	508	-	66,73,73	2.20	14 (21%)	65,113,113	2.23	18 (27%)
26	LMG	B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
23	8CT	c	515	-	40,41,41	4.64	22 (55%)	50,56,56	2.40	23 (46%)
32	ZEX	6	524	-	42,43,43	1.03	4 (9%)	55,60,60	2.51	17 (30%)
21	CL7	1	406	-	63,70,73	2.26	12 (19%)	61,109,113	2.30	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	5	420	18	46,53,73	2.63	12 (26%)	41,89,113	2.74	14 (34%)
21	CL7	3	514	-	46,53,73	2.63	14 (30%)	41,89,113	2.80	14 (34%)
21	CL7	5	406	-	63,70,73	2.26	12 (19%)	61,109,113	2.29	14 (22%)
21	CL7	b	608	-	61,68,73	2.30	13 (21%)	59,107,113	2.27	16 (27%)
25	LHG	a	406	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	C	509	-	66,73,73	2.22	13 (19%)	65,113,113	2.28	21 (32%)
21	CL7	4	406	-	66,73,73	2.21	12 (18%)	65,113,113	2.22	17 (26%)
32	ZEX	4	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
21	CL7	7	511	19	66,73,73	2.18	15 (22%)	65,113,113	2.43	19 (29%)
21	CL7	b	613	-	66,73,73	2.15	13 (19%)	65,113,113	2.28	18 (27%)
21	CL7	C	502	-	66,73,73	2.18	13 (19%)	65,113,113	2.19	15 (23%)
21	CL7	6	516	-	66,73,73	2.20	13 (19%)	65,113,113	2.23	19 (29%)
23	8CT	C	515	-	40,41,41	4.64	21 (52%)	50,56,56	2.40	23 (46%)
25	LHG	4	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	2	502	-	66,73,73	2.19	13 (19%)	65,113,113	2.26	18 (27%)
32	ZEX	4	418	-	42,43,43	0.85	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	5	403	-	61,68,73	2.29	13 (21%)	59,107,113	2.38	15 (25%)
29	BCT	D	403	28	2,3,3	1.00	0	2,3,3	1.67	1 (50%)
21	CL7	6	511	16	61,68,73	2.33	11 (18%)	59,107,113	2.21	15 (25%)
25	LHG	b	626	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	6	504	-	46,53,73	2.62	13 (28%)	41,89,113	2.63	14 (34%)
21	CL7	3	518	19	46,53,73	2.68	12 (26%)	41,89,113	2.66	14 (34%)
21	CL7	3	512	-	56,63,73	2.38	13 (23%)	53,101,113	2.45	18 (33%)
21	CL7	b	614	-	56,63,73	2.38	14 (25%)	53,101,113	2.41	17 (32%)
24	SQD	B	626	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
32	ZEX	8	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
27	DGD	c	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
23	8CT	4	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
21	CL7	C	507	-	61,68,73	2.31	13 (21%)	59,107,113	2.39	18 (30%)
21	CL7	7	517	19	51,58,73	2.49	13 (25%)	47,95,113	2.55	14 (29%)
25	LHG	B	625	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	2	517	16	66,73,73	2.18	12 (18%)	65,113,113	2.20	17 (26%)
32	ZEX	2	525	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
30	PL9	d	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.62	1 (1%)
21	CL7	b	612	-	66,73,73	2.19	14 (21%)	65,113,113	2.26	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	7	507	-	66,73,73	2.16	13 (19%)	65,113,113	2.30	18 (27%)
21	CL7	2	507	-	66,73,73	2.19	14 (21%)	65,113,113	2.31	17 (26%)
21	CL7	8	409	-	61,68,73	2.27	14 (22%)	59,107,113	2.50	20 (33%)
32	ZEX	5	422	-	42,43,43	0.95	1 (2%)	55,60,60	2.24	18 (32%)
21	CL7	7	505	-	66,73,73	2.16	13 (19%)	65,113,113	2.34	15 (23%)
21	CL7	5	405	-	46,53,73	2.62	13 (28%)	41,89,113	2.59	12 (29%)
32	ZEX	8	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
21	CL7	1	403	-	61,68,73	2.29	13 (21%)	59,107,113	2.39	15 (25%)
21	CL7	d	402	-	51,58,73	2.55	12 (23%)	47,95,113	2.47	15 (31%)
21	CL7	B	610	-	66,73,73	2.16	13 (19%)	65,113,113	2.31	15 (23%)
26	LMG	b	622	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	3	516	19	56,63,73	2.42	13 (23%)	53,101,113	2.43	19 (35%)
21	CL7	5	408	-	66,73,73	2.19	13 (19%)	65,113,113	2.31	19 (29%)
21	CL7	c	510	-	66,73,73	2.22	14 (21%)	65,113,113	2.23	16 (24%)
21	CL7	5	419	-	46,53,73	2.65	12 (26%)	41,89,113	2.58	13 (31%)
21	CL7	7	502	-	59,66,73	2.36	13 (22%)	56,104,113	2.26	17 (30%)
26	LMG	5	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
21	CL7	5	413	-	42,49,73	2.64	10 (23%)	36,84,113	2.94	15 (41%)
21	CL7	A	406	-	66,73,73	2.24	13 (19%)	65,113,113	2.30	16 (24%)
21	CL7	4	407	-	42,49,73	2.66	10 (23%)	36,84,113	2.86	14 (38%)
21	CL7	7	504	-	66,73,73	2.21	13 (19%)	65,113,113	2.24	17 (26%)
21	CL7	B	611	-	66,73,73	2.18	14 (21%)	65,113,113	2.26	16 (24%)
21	CL7	a	405	-	66,73,73	2.24	13 (19%)	65,113,113	2.29	16 (24%)
21	CL7	b	606	-	66,73,73	2.23	14 (21%)	65,113,113	2.22	15 (23%)
21	CL7	1	407	-	42,49,73	2.66	11 (26%)	36,84,113	2.81	15 (41%)
22	PHO	a	402	-	51,69,69	0.74	2 (3%)	47,99,99	0.74	1 (2%)
21	CL7	c	503	-	61,68,73	2.30	14 (22%)	59,107,113	2.30	15 (25%)
24	SQD	3	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	C	508	-	66,73,73	2.17	14 (21%)	65,113,113	2.26	18 (27%)
21	CL7	1	411	-	46,53,73	2.64	12 (26%)	41,89,113	2.61	14 (34%)
21	CL7	b	617	-	46,53,73	2.62	14 (30%)	41,89,113	2.60	16 (39%)
21	CL7	A	403	-	56,63,73	2.40	14 (25%)	53,101,113	2.59	18 (33%)
21	CL7	c	506	-	66,73,73	2.21	14 (21%)	65,113,113	2.25	17 (26%)
21	CL7	C	514	-	46,53,73	2.63	12 (26%)	41,89,113	2.69	14 (34%)
24	SQD	1	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	LMG	c	501	-	50,50,55	0.91	2 (4%)	58,58,63	1.21	5 (8%)
32	ZEX	1	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	B	622	-	46,53,73	2.67	12 (26%)	41,89,113	2.58	13 (31%)
24	SQD	5	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	8	410	-	46,53,73	2.61	12 (26%)	41,89,113	2.65	13 (31%)
24	SQD	2	524	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	7	501	-	66,73,73	2.22	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	2	501	-	66,73,73	2.17	12 (18%)	65,113,113	2.23	15 (23%)
21	CL7	D	402	-	51,58,73	2.55	12 (23%)	47,95,113	2.46	15 (31%)
21	CL7	7	508	-	66,73,73	2.20	14 (21%)	65,113,113	2.24	18 (27%)
21	CL7	3	517	19	51,58,73	2.49	13 (25%)	47,95,113	2.54	14 (29%)
21	CL7	8	405	-	66,73,73	2.21	14 (21%)	65,113,113	2.31	20 (30%)
27	DGD	b	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
23	8CT	B	627	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
32	ZEX	6	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	B	607	-	61,68,73	2.30	13 (21%)	59,107,113	2.27	16 (27%)
21	CL7	7	510	-	66,73,73	2.18	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	5	410	-	66,73,73	2.24	13 (19%)	65,113,113	2.17	16 (24%)
24	SQD	7	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	3	510	-	66,73,73	2.18	13 (19%)	65,113,113	2.22	18 (27%)
21	CL7	7	518	19	46,53,73	2.68	13 (28%)	41,89,113	2.66	14 (34%)
21	CL7	2	518	16	66,73,73	2.23	12 (18%)	65,113,113	2.17	17 (26%)
29	BCT	d	403	28	2,3,3	1.00	0	2,3,3	1.67	1 (50%)
21	CL7	7	509	-	66,73,73	2.20	11 (16%)	65,113,113	2.19	16 (24%)
31	HEM	F	101	-	41,50,50	1.41	6 (14%)	45,82,82	2.03	11 (24%)
32	ZEX	6	520	-	42,43,43	0.98	3 (7%)	55,60,60	2.19	17 (30%)
21	CL7	b	610	-	66,73,73	2.24	14 (21%)	65,113,113	2.15	15 (23%)
21	CL7	1	415	-	42,49,73	2.70	12 (28%)	36,84,113	2.91	14 (38%)
32	ZEX	2	520	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	4	417	20	43,50,73	2.67	11 (25%)	36,85,113	2.89	13 (36%)
23	8CT	b	620	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
23	8CT	8	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
32	ZEX	7	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	4	409	-	61,68,73	2.27	14 (22%)	59,107,113	2.50	20 (33%)
23	8CT	b	619	-	40,41,41	4.69	20 (50%)	50,56,56	2.67	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	3	509	-	66,73,73	2.20	11 (16%)	65,113,113	2.19	16 (24%)
21	CL7	4	413	20	61,68,73	2.27	14 (22%)	59,107,113	2.32	16 (27%)
21	CL7	1	418	18	66,73,73	2.17	12 (18%)	65,113,113	2.31	20 (30%)
21	CL7	C	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.25	17 (26%)
21	CL7	C	505	-	56,63,73	2.43	12 (21%)	53,101,113	2.38	14 (26%)
21	CL7	3	504	-	66,73,73	2.20	13 (19%)	65,113,113	2.24	17 (26%)
23	8CT	B	618	-	40,41,41	4.69	21 (52%)	50,56,56	2.67	20 (40%)
32	ZEX	4	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	7	516	19	56,63,73	2.41	13 (23%)	53,101,113	2.42	19 (35%)
21	CL7	b	602	-	42,49,73	2.67	11 (26%)	36,84,113	2.82	12 (33%)
21	CL7	D	405	-	46,53,73	2.57	13 (28%)	41,89,113	2.73	16 (39%)
21	CL7	1	416	-	42,49,73	2.73	10 (23%)	36,84,113	2.76	14 (38%)
23	8CT	b	601	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	C	513	-	42,49,73	2.56	9 (21%)	36,84,113	2.89	14 (38%)
21	CL7	6	503	-	66,73,73	2.19	15 (22%)	65,113,113	2.38	19 (29%)
26	LMG	C	501	-	50,50,55	0.92	2 (4%)	58,58,63	1.22	5 (8%)
21	CL7	b	611	-	66,73,73	2.15	13 (19%)	65,113,113	2.32	15 (23%)
21	CL7	B	606	-	56,63,73	2.43	14 (25%)	53,101,113	2.48	16 (30%)
21	CL7	1	414	-	42,49,73	2.73	10 (23%)	36,84,113	2.92	15 (41%)
21	CL7	c	509	-	66,73,73	2.21	13 (19%)	65,113,113	2.29	21 (32%)
21	CL7	5	412	-	46,53,73	2.59	12 (26%)	41,89,113	2.71	14 (34%)
21	CL7	5	409	-	46,53,73	2.61	13 (28%)	41,89,113	2.62	15 (36%)
21	CL7	2	516	-	66,73,73	2.20	13 (19%)	65,113,113	2.23	19 (29%)
21	CL7	1	408	-	66,73,73	2.19	13 (19%)	65,113,113	2.31	19 (29%)
21	CL7	B	615	-	51,58,73	2.44	14 (27%)	47,95,113	2.63	16 (34%)
21	CL7	1	420	18	46,53,73	2.63	12 (26%)	41,89,113	2.74	14 (34%)
21	CL7	B	605	-	66,73,73	2.24	14 (21%)	65,113,113	2.22	15 (23%)
23	8CT	k	101	-	40,41,41	4.75	24 (60%)	50,56,56	2.65	16 (32%)
25	LHG	B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
32	ZEX	1	422	-	42,43,43	0.95	1 (2%)	55,60,60	2.24	18 (32%)
21	CL7	5	417	18	56,63,73	2.42	14 (25%)	53,101,113	2.41	15 (28%)
24	SQD	6	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
31	HEM	f	101	-	41,50,50	1.41	6 (14%)	45,82,82	2.03	11 (24%)
21	CL7	8	406	-	66,73,73	2.21	13 (19%)	65,113,113	2.22	17 (26%)
32	ZEX	2	519	-	42,43,43	1.06	3 (7%)	55,60,60	2.50	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	b	607	-	56,63,73	2.43	14 (25%)	53,101,113	2.48	16 (30%)
24	SQD	3	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	a	403	-	56,63,73	2.40	14 (25%)	53,101,113	2.58	18 (33%)
23	8CT	c	519	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
21	CL7	2	503	-	66,73,73	2.18	15 (22%)	65,113,113	2.38	19 (29%)
21	CL7	1	413	-	42,49,73	2.64	10 (23%)	36,84,113	2.94	15 (41%)
21	CL7	B	603	-	66,73,73	2.22	13 (19%)	65,113,113	2.22	17 (26%)
21	CL7	6	505	-	66,73,73	2.22	13 (19%)	65,113,113	2.40	19 (29%)
23	8CT	b	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	5	404	-	66,73,73	2.27	12 (18%)	65,113,113	2.25	16 (24%)
23	8CT	a	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
21	CL7	C	503	-	61,68,73	2.30	14 (22%)	59,107,113	2.30	15 (25%)
21	CL7	5	402	-	61,68,73	2.31	14 (22%)	59,107,113	2.37	15 (25%)
21	CL7	1	405	-	46,53,73	2.63	13 (28%)	41,89,113	2.59	12 (29%)
23	8CT	B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.91	18 (36%)
21	CL7	3	511	19	66,73,73	2.18	15 (22%)	65,113,113	2.43	19 (29%)
21	CL7	1	419	-	46,53,73	2.65	12 (26%)	41,89,113	2.58	13 (31%)
21	CL7	2	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.19	16 (24%)
21	CL7	1	410	-	66,73,73	2.24	13 (19%)	65,113,113	2.17	16 (24%)
21	CL7	4	412	-	66,73,73	2.22	12 (18%)	65,113,113	2.20	18 (27%)
22	PHO	d	408	-	51,69,69	1.68	7 (13%)	47,99,99	1.66	11 (23%)
21	CL7	4	405	-	66,73,73	2.21	14 (21%)	65,113,113	2.31	20 (30%)
21	CL7	b	623	-	46,53,73	2.67	12 (26%)	41,89,113	2.57	13 (31%)
21	CL7	2	515	-	46,53,73	2.62	12 (26%)	41,89,113	2.66	15 (36%)
21	CL7	8	411	-	66,73,73	2.22	12 (18%)	65,113,113	2.20	17 (26%)
21	CL7	B	608	-	66,73,73	2.19	13 (19%)	65,113,113	2.17	14 (21%)
21	CL7	c	508	-	66,73,73	2.17	14 (21%)	65,113,113	2.26	18 (27%)
21	CL7	5	414	-	42,49,73	2.74	10 (23%)	36,84,113	2.92	15 (41%)
21	CL7	3	513	-	46,53,73	2.66	15 (32%)	41,89,113	2.67	13 (31%)
21	CL7	d	405	-	46,53,73	2.57	13 (28%)	41,89,113	2.74	16 (39%)
21	CL7	b	605	-	66,73,73	2.15	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	B	602	-	61,68,73	2.32	12 (19%)	59,107,113	2.39	18 (30%)
21	CL7	6	507	-	66,73,73	2.19	14 (21%)	65,113,113	2.31	17 (26%)
24	SQD	7	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	C	518	-	42,49,73	2.62	10 (23%)	36,84,113	2.83	14 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	B	614	-	61,68,73	2.30	14 (22%)	59,107,113	2.37	18 (30%)
26	LMG	d	410	-	33,33,55	0.28	0	41,41,63	0.33	0
25	LHG	8	401	-	48,48,48	0.28	0	51,54,54	0.34	0
22	PHO	A	402	-	51,69,69	0.74	2 (3%)	47,99,99	0.74	1 (2%)
23	8CT	C	519	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
22	PHO	D	408	-	51,69,69	1.67	7 (13%)	47,99,99	1.66	11 (23%)
21	CL7	c	514	-	46,53,73	2.62	12 (26%)	41,89,113	2.68	14 (34%)
23	8CT	d	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
24	SQD	B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
32	ZEX	3	520	-	42,43,43	0.94	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	4	410	-	46,53,73	2.62	12 (26%)	41,89,113	2.64	13 (31%)
32	ZEX	3	519	-	42,43,43	1.02	4 (9%)	55,60,60	2.58	17 (30%)
21	CL7	6	518	16	66,73,73	2.23	12 (18%)	65,113,113	2.17	16 (24%)
21	CL7	b	603	-	61,68,73	2.32	12 (19%)	59,107,113	2.39	18 (30%)
21	CL7	4	408	-	46,53,73	2.65	15 (32%)	41,89,113	2.67	13 (31%)
21	CL7	3	503	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	18 (27%)
21	CL7	2	509	-	66,73,73	2.22	14 (21%)	65,113,113	2.17	15 (23%)
21	CL7	C	512	3	43,50,73	2.70	11 (25%)	36,85,113	2.79	12 (33%)
21	CL7	4	415	-	46,53,73	2.60	15 (32%)	41,89,113	2.88	14 (34%)
21	CL7	B	609	-	66,73,73	2.24	14 (21%)	65,113,113	2.15	15 (23%)
21	CL7	c	507	-	61,68,73	2.32	13 (21%)	59,107,113	2.40	18 (30%)
21	CL7	8	407	-	42,49,73	2.64	10 (23%)	36,84,113	2.85	14 (38%)
32	ZEX	2	523	-	42,43,43	1.04	4 (9%)	55,60,60	2.47	16 (29%)
21	CL7	4	411	-	66,73,73	2.22	12 (18%)	65,113,113	2.20	17 (26%)
21	CL7	B	612	-	66,73,73	2.15	13 (19%)	65,113,113	2.28	18 (27%)
21	CL7	8	416	-	42,49,73	2.69	10 (23%)	36,84,113	2.90	15 (41%)
21	CL7	c	512	3	43,50,73	2.69	11 (25%)	36,85,113	2.78	13 (36%)
32	ZEX	2	521	-	42,43,43	0.98	3 (7%)	55,60,60	2.19	17 (30%)
21	CL7	c	505	-	56,63,73	2.43	13 (23%)	53,101,113	2.38	14 (26%)
21	CL7	c	513	-	42,49,73	2.56	10 (23%)	36,84,113	2.89	14 (38%)
26	LMG	D	410	-	33,33,55	0.28	0	41,41,63	0.33	0
21	CL7	A	401	-	66,73,73	2.27	15 (22%)	65,113,113	2.34	19 (29%)
21	CL7	6	508	-	46,53,73	2.59	14 (30%)	41,89,113	2.65	14 (34%)
21	CL7	4	414	-	54,61,73	2.39	13 (24%)	50,98,113	2.53	16 (32%)
21	CL7	B	616	-	46,53,73	2.62	14 (30%)	41,89,113	2.60	16 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	8CT	D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	2	504	-	46,53,73	2.62	13 (28%)	41,89,113	2.63	14 (34%)
21	CL7	8	417	20	43,50,73	2.66	11 (25%)	36,85,113	2.89	13 (36%)
21	CL7	8	404	-	66,73,73	2.22	13 (19%)	65,113,113	2.20	16 (24%)
21	CL7	2	514	-	46,53,73	2.63	13 (28%)	41,89,113	2.68	12 (29%)
23	8CT	A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
21	CL7	c	502	-	66,73,73	2.18	13 (19%)	65,113,113	2.20	15 (23%)
27	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	2	512	-	66,73,73	2.17	11 (16%)	65,113,113	2.28	17 (26%)
21	CL7	b	604	-	66,73,73	2.22	13 (19%)	65,113,113	2.22	17 (26%)
25	LHG	A	407	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	B	604	-	66,73,73	2.15	13 (19%)	65,113,113	2.23	18 (27%)
32	ZEX	3	525	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	5	415	-	42,49,73	2.70	12 (28%)	36,84,113	2.91	14 (38%)
21	CL7	a	401	-	66,73,73	2.27	15 (22%)	65,113,113	2.34	19 (29%)
21	CL7	C	510	-	66,73,73	2.22	14 (21%)	65,113,113	2.23	16 (24%)
21	CL7	8	412	-	66,73,73	2.21	13 (19%)	65,113,113	2.20	18 (27%)
21	CL7	B	601	-	42,49,73	2.67	11 (26%)	36,84,113	2.81	12 (33%)
21	CL7	5	407	-	42,49,73	2.65	11 (26%)	36,84,113	2.81	16 (44%)
24	SQD	b	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
23	8CT	B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	2	511	16	61,68,73	2.33	12 (19%)	59,107,113	2.22	15 (25%)
21	CL7	5	411	-	46,53,73	2.64	12 (26%)	41,89,113	2.62	14 (34%)
27	DGD	B	624	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
21	CL7	1	412	-	46,53,73	2.59	12 (26%)	41,89,113	2.70	14 (34%)
21	CL7	B	613	-	56,63,73	2.38	14 (25%)	53,101,113	2.42	17 (32%)
21	CL7	7	515	-	42,49,73	2.66	10 (23%)	36,84,113	2.86	15 (41%)
25	LHG	d	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	2	508	-	46,53,73	2.60	14 (30%)	41,89,113	2.65	14 (34%)
21	CL7	1	409	-	46,53,73	2.61	13 (28%)	41,89,113	2.61	15 (36%)
21	CL7	6	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.19	16 (24%)
21	CL7	6	512	-	66,73,73	2.17	11 (16%)	65,113,113	2.28	17 (26%)
32	ZEX	4	419	-	42,43,43	0.99	3 (7%)	55,60,60	2.43	25 (45%)
21	CL7	1	402	-	61,68,73	2.31	14 (22%)	59,107,113	2.37	15 (25%)
21	CL7	1	417	18	56,63,73	2.42	14 (25%)	53,101,113	2.41	15 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	3	505	-	66,73,73	2.16	13 (19%)	65,113,113	2.33	15 (23%)
21	CL7	6	510	16	66,73,73	2.18	13 (19%)	65,113,113	2.24	18 (27%)
21	CL7	6	515	-	46,53,73	2.62	12 (26%)	41,89,113	2.66	15 (36%)
21	CL7	d	404	-	59,66,73	2.33	14 (23%)	56,104,113	2.36	17 (30%)
21	CL7	7	506	-	46,53,73	2.59	14 (30%)	41,89,113	2.73	14 (34%)
25	LHG	D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
30	PL9	D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	7	503	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	18 (27%)
21	CL7	c	518	-	42,49,73	2.62	10 (23%)	36,84,113	2.83	14 (38%)
21	CL7	2	505	-	66,73,73	2.22	13 (19%)	65,113,113	2.42	19 (29%)
21	CL7	7	513	-	46,53,73	2.66	15 (32%)	41,89,113	2.67	13 (31%)
21	CL7	2	513	-	46,53,73	2.65	13 (28%)	41,89,113	2.66	15 (36%)
24	SQD	2	522	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	C	504	-	66,73,73	2.20	14 (21%)	65,113,113	2.22	17 (26%)
21	CL7	6	502	-	66,73,73	2.19	13 (19%)	65,113,113	2.26	17 (26%)
21	CL7	6	509	-	66,73,73	2.21	14 (21%)	65,113,113	2.17	15 (23%)
26	LMG	1	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
32	ZEX	5	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	3	507	-	66,73,73	2.16	13 (19%)	65,113,113	2.30	18 (27%)
21	CL7	b	616	-	51,58,73	2.44	14 (27%)	47,95,113	2.63	16 (34%)
21	CL7	8	414	-	54,61,73	2.39	14 (25%)	50,98,113	2.53	16 (32%)
32	ZEX	6	522	-	42,43,43	1.05	4 (9%)	55,60,60	2.47	16 (29%)
21	CL7	6	513	-	46,53,73	2.65	13 (28%)	41,89,113	2.67	15 (36%)
21	CL7	1	404	-	66,73,73	2.27	12 (18%)	65,113,113	2.25	16 (24%)
21	CL7	4	416	-	42,49,73	2.69	10 (23%)	36,84,113	2.89	15 (41%)
21	CL7	b	609	-	66,73,73	2.19	13 (19%)	65,113,113	2.17	14 (21%)
21	CL7	3	515	-	42,49,73	2.65	10 (23%)	36,84,113	2.86	15 (41%)
23	8CT	K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.65	16 (32%)
21	CL7	8	413	20	61,68,73	2.27	14 (22%)	59,107,113	2.32	16 (27%)

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
23	8CT	c	516	-	-	10/29/63/63	0/2/2/2
24	SQD	6	521	-	-	7/45/65/69	0/1/1/1
21	CL7	b	615	-	2/2/14/20	12/31/109/115	-
21	CL7	C	511	-	2/2/15/20	20/37/115/115	-
21	CL7	3	502	-	2/2/13/20	10/29/107/115	-
32	ZEX	8	403	-	-	10/29/67/67	0/2/2/2
21	CL7	8	415	-	2/2/11/20	10/13/91/115	-
25	LHG	b	624	-	-	3/49/49/53	-
21	CL7	4	404	-	2/2/15/20	14/37/115/115	-
21	CL7	7	512	-	2/2/13/20	12/25/103/115	-
21	CL7	6	517	16	2/2/15/20	19/37/115/115	-
21	CL7	8	408	-	2/2/11/20	2/13/91/115	-
32	ZEX	3	522	-	-	5/29/67/67	0/2/2/2
21	CL7	6	501	-	2/2/15/20	15/37/115/115	-
21	CL7	D	404	-	2/2/13/20	11/29/107/115	-
25	LHG	7	524	-	-	3/40/40/53	-
25	LHG	3	524	-	-	3/40/40/53	-
32	ZEX	7	519	-	-	10/29/67/67	0/2/2/2
21	CL7	5	418	18	2/2/15/20	20/37/115/115	-
21	CL7	6	514	-	2/2/11/20	7/13/91/115	-
21	CL7	c	511	-	2/2/15/20	20/37/115/115	-
32	ZEX	7	520	-	-	10/29/67/67	0/2/2/2
21	CL7	c	504	-	2/2/15/20	17/37/115/115	-
21	CL7	2	510	16	2/2/15/20	20/37/115/115	-
24	SQD	A	405	-	-	3/29/49/69	0/1/1/1
23	8CT	C	516	-	-	10/29/63/63	0/2/2/2
21	CL7	7	514	-	2/2/11/20	5/13/91/115	-
21	CL7	3	501	-	2/2/15/20	19/37/115/115	-
21	CL7	5	416	-	2/2/10/20	2/8/86/115	-
21	CL7	3	506	-	2/2/11/20	11/13/91/115	-
32	ZEX	8	419	-	-	9/29/67/67	0/2/2/2
21	CL7	3	508	-	2/2/15/20	14/37/115/115	-
26	LMG	B	621	-	-	7/46/66/70	0/1/1/1
23	8CT	c	515	-	-	14/29/63/63	0/2/2/2
32	ZEX	6	524	-	-	11/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	1	406	-	2/2/14/20	11/34/112/115	-
21	CL7	5	420	18	2/2/11/20	4/13/91/115	-
21	CL7	3	514	-	2/2/11/20	5/13/91/115	-
21	CL7	5	406	-	2/2/14/20	11/34/112/115	-
21	CL7	b	608	-	2/2/14/20	9/31/109/115	-
25	LHG	a	406	-	-	5/50/50/53	-
21	CL7	C	509	-	2/2/15/20	15/37/115/115	-
21	CL7	4	406	-	2/2/15/20	22/37/115/115	-
32	ZEX	4	420	-	-	12/29/67/67	0/2/2/2
21	CL7	7	511	19	2/2/15/20	17/37/115/115	-
21	CL7	b	613	-	2/2/15/20	15/37/115/115	-
21	CL7	C	502	-	2/2/15/20	18/37/115/115	-
21	CL7	6	516	-	2/2/15/20	14/37/115/115	-
23	8CT	C	515	-	-	14/29/63/63	0/2/2/2
25	LHG	4	401	-	-	8/53/53/53	-
21	CL7	2	502	-	2/2/15/20	15/37/115/115	-
32	ZEX	4	418	-	-	9/29/67/67	0/2/2/2
21	CL7	5	403	-	2/2/14/20	9/31/109/115	-
21	CL7	6	511	16	2/2/14/20	14/31/109/115	-
25	LHG	b	626	-	-	6/53/53/53	-
21	CL7	6	504	-	2/2/11/20	4/13/91/115	-
21	CL7	3	518	19	2/2/11/20	5/13/91/115	-
21	CL7	3	512	-	2/2/13/20	12/25/103/115	-
21	CL7	b	614	-	2/2/13/20	4/25/103/115	-
24	SQD	B	626	-	-	3/29/49/69	0/1/1/1
32	ZEX	8	418	-	-	9/29/67/67	0/2/2/2
27	DGD	c	517	-	-	9/51/91/95	0/2/2/2
23	8CT	4	402	-	-	4/29/63/63	0/2/2/2
21	CL7	C	507	-	2/2/14/20	13/31/109/115	-
21	CL7	7	517	19	2/2/12/20	7/19/97/115	-
25	LHG	B	625	-	-	6/53/53/53	-
21	CL7	2	517	16	2/2/15/20	19/37/115/115	-
32	ZEX	2	525	-	-	11/29/67/67	0/2/2/2
30	PL9	d	407	-	-	9/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	b	612	-	2/2/15/20	15/37/115/115	-
21	CL7	7	507	-	2/2/15/20	13/37/115/115	-
21	CL7	2	507	-	2/2/15/20	18/37/115/115	-
21	CL7	8	409	-	2/2/14/20	15/31/109/115	-
32	ZEX	5	422	-	-	6/29/67/67	0/2/2/2
21	CL7	7	505	-	2/2/15/20	14/37/115/115	-
21	CL7	5	405	-	2/2/11/20	9/13/91/115	-
32	ZEX	8	420	-	-	12/29/67/67	0/2/2/2
21	CL7	1	403	-	2/2/14/20	9/31/109/115	-
21	CL7	d	402	-	2/2/12/20	7/19/97/115	-
21	CL7	B	610	-	2/2/15/20	11/37/115/115	-
26	LMG	b	622	-	-	7/46/66/70	0/1/1/1
21	CL7	3	516	19	2/2/13/20	14/25/103/115	-
21	CL7	5	408	-	2/2/15/20	14/37/115/115	-
21	CL7	c	510	-	2/2/15/20	18/37/115/115	-
21	CL7	5	419	-	2/2/11/20	7/13/91/115	-
21	CL7	7	502	-	2/2/13/20	10/29/107/115	-
26	LMG	5	401	-	-	5/46/66/70	0/1/1/1
21	CL7	5	413	-	2/2/10/20	2/8/86/115	-
21	CL7	A	406	-	2/2/15/20	14/37/115/115	-
21	CL7	4	407	-	2/2/10/20	1/8/86/115	-
21	CL7	7	504	-	2/2/15/20	14/37/115/115	-
21	CL7	B	611	-	2/2/15/20	15/37/115/115	-
21	CL7	a	405	-	2/2/15/20	14/37/115/115	-
21	CL7	b	606	-	2/2/15/20	16/37/115/115	-
21	CL7	1	407	-	2/2/10/20	2/8/86/115	-
22	PHO	a	402	-	-	3/37/103/103	0/5/6/6
21	CL7	c	503	-	2/2/14/20	10/31/109/115	-
24	SQD	3	521	-	-	3/41/61/69	0/1/1/1
21	CL7	C	508	-	2/2/15/20	15/37/115/115	-
21	CL7	1	411	-	2/2/11/20	5/13/91/115	-
21	CL7	b	617	-	2/2/11/20	4/13/91/115	-
21	CL7	A	403	-	2/2/13/20	9/25/103/115	-
21	CL7	c	506	-	2/2/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	C	514	-	2/2/11/20	6/13/91/115	-
24	SQD	1	423	-	-	3/27/47/69	0/1/1/1
26	LMG	c	501	-	-	16/45/65/70	0/1/1/1
32	ZEX	1	421	-	-	14/29/67/67	0/2/2/2
21	CL7	B	622	-	2/2/11/20	6/13/91/115	-
24	SQD	5	423	-	-	3/27/47/69	0/1/1/1
21	CL7	8	410	-	2/2/11/20	7/13/91/115	-
24	SQD	2	524	-	-	0/36/56/69	0/1/1/1
21	CL7	7	501	-	2/2/15/20	19/37/115/115	-
21	CL7	2	501	-	2/2/15/20	15/37/115/115	-
21	CL7	D	402	-	2/2/12/20	7/19/97/115	-
21	CL7	7	508	-	2/2/15/20	14/37/115/115	-
21	CL7	3	517	19	2/2/12/20	7/19/97/115	-
21	CL7	8	405	-	2/2/15/20	16/37/115/115	-
27	DGD	b	625	-	-	7/51/91/95	0/2/2/2
23	8CT	B	627	-	-	10/29/63/63	0/2/2/2
32	ZEX	6	519	-	-	11/29/67/67	0/2/2/2
21	CL7	B	607	-	2/2/14/20	9/31/109/115	-
21	CL7	7	510	-	2/2/15/20	13/37/115/115	-
21	CL7	5	410	-	2/2/15/20	15/37/115/115	-
24	SQD	7	523	-	-	7/45/65/69	0/1/1/1
21	CL7	3	510	-	2/2/15/20	13/37/115/115	-
21	CL7	7	518	19	2/2/11/20	5/13/91/115	-
21	CL7	2	518	16	2/2/15/20	10/37/115/115	-
21	CL7	7	509	-	2/2/15/20	15/37/115/115	-
31	HEM	F	101	-	-	6/12/54/54	-
32	ZEX	6	520	-	-	6/29/67/67	0/2/2/2
21	CL7	b	610	-	2/2/15/20	12/37/115/115	-
21	CL7	1	415	-	2/2/10/20	5/8/86/115	-
32	ZEX	2	520	-	-	7/29/67/67	0/2/2/2
21	CL7	4	417	20	2/2/10/20	4/10/88/115	-
23	8CT	b	620	-	-	4/29/63/63	0/2/2/2
23	8CT	8	402	-	-	4/29/63/63	0/2/2/2
32	ZEX	7	522	-	-	5/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	4	409	-	2/2/14/20	15/31/109/115	-
23	8CT	b	619	-	-	10/29/63/63	0/2/2/2
21	CL7	3	509	-	2/2/15/20	15/37/115/115	-
21	CL7	4	413	20	2/2/14/20	7/31/109/115	-
21	CL7	1	418	18	2/2/15/20	20/37/115/115	-
21	CL7	C	506	-	2/2/15/20	14/37/115/115	-
21	CL7	C	505	-	2/2/13/20	11/25/103/115	-
21	CL7	3	504	-	2/2/15/20	14/37/115/115	-
23	8CT	B	618	-	-	10/29/63/63	0/2/2/2
32	ZEX	4	403	-	-	10/29/67/67	0/2/2/2
21	CL7	7	516	19	2/2/13/20	14/25/103/115	-
21	CL7	b	602	-	2/2/10/20	4/8/86/115	-
21	CL7	D	405	-	2/2/11/20	6/13/91/115	-
21	CL7	1	416	-	2/2/10/20	2/8/86/115	-
23	8CT	b	601	-	-	10/29/63/63	0/2/2/2
21	CL7	C	513	-	2/2/10/20	2/8/86/115	-
21	CL7	6	503	-	2/2/15/20	17/37/115/115	-
26	LMG	C	501	-	-	16/45/65/70	0/1/1/1
21	CL7	b	611	-	2/2/15/20	11/37/115/115	-
21	CL7	B	606	-	2/2/13/20	4/25/103/115	-
21	CL7	1	414	-	2/2/10/20	1/8/86/115	-
21	CL7	c	509	-	2/2/15/20	15/37/115/115	-
21	CL7	5	412	-	2/2/11/20	8/13/91/115	-
21	CL7	5	409	-	2/2/11/20	4/13/91/115	-
21	CL7	2	516	-	2/2/15/20	14/37/115/115	-
21	CL7	1	408	-	2/2/15/20	14/37/115/115	-
21	CL7	B	615	-	2/2/12/20	8/19/97/115	-
21	CL7	1	420	18	2/2/11/20	4/13/91/115	-
21	CL7	B	605	-	2/2/15/20	16/37/115/115	-
23	8CT	k	101	-	-	10/29/63/63	0/2/2/2
25	LHG	B	623	-	-	3/49/49/53	-
32	ZEX	1	422	-	-	6/29/67/67	0/2/2/2
21	CL7	5	417	18	2/2/13/20	7/25/103/115	-
24	SQD	6	523	-	-	0/36/56/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	HEM	f	101	-	-	6/12/54/54	-
21	CL7	8	406	-	2/2/15/20	22/37/115/115	-
32	ZEX	2	519	-	-	11/29/67/67	0/2/2/2
21	CL7	b	607	-	2/2/13/20	4/25/103/115	-
24	SQD	3	523	-	-	7/45/65/69	0/1/1/1
21	CL7	a	403	-	2/2/13/20	9/25/103/115	-
23	8CT	c	519	-	-	8/29/63/63	0/2/2/2
21	CL7	2	503	-	2/2/15/20	17/37/115/115	-
21	CL7	1	413	-	2/2/10/20	2/8/86/115	-
21	CL7	B	603	-	2/2/15/20	12/37/115/115	-
21	CL7	6	505	-	2/2/15/20	16/37/115/115	-
23	8CT	b	618	-	-	7/29/63/63	0/2/2/2
21	CL7	5	404	-	2/2/15/20	13/37/115/115	-
23	8CT	a	404	-	-	5/29/63/63	0/2/2/2
21	CL7	C	503	-	2/2/14/20	10/31/109/115	-
21	CL7	5	402	-	2/2/14/20	14/31/109/115	-
21	CL7	1	405	-	2/2/11/20	9/13/91/115	-
23	8CT	B	619	-	-	4/29/63/63	0/2/2/2
21	CL7	3	511	19	2/2/15/20	17/37/115/115	-
21	CL7	1	419	-	2/2/11/20	7/13/91/115	-
21	CL7	2	506	-	2/2/15/20	12/37/115/115	-
21	CL7	1	410	-	2/2/15/20	15/37/115/115	-
21	CL7	4	412	-	2/2/15/20	17/37/115/115	-
22	PHO	d	408	-	-	5/37/103/103	0/5/6/6
21	CL7	4	405	-	2/2/15/20	16/37/115/115	-
21	CL7	b	623	-	2/2/11/20	6/13/91/115	-
21	CL7	2	515	-	2/2/11/20	6/13/91/115	-
21	CL7	8	411	-	2/2/15/20	12/37/115/115	-
21	CL7	B	608	-	2/2/15/20	15/37/115/115	-
21	CL7	c	508	-	2/2/15/20	15/37/115/115	-
21	CL7	5	414	-	2/2/10/20	1/8/86/115	-
21	CL7	3	513	-	2/2/11/20	7/13/91/115	-
21	CL7	d	405	-	2/2/11/20	6/13/91/115	-
21	CL7	b	605	-	2/2/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	B	602	-	2/2/14/20	7/31/109/115	-
21	CL7	6	507	-	2/2/15/20	18/37/115/115	-
24	SQD	7	521	-	-	3/41/61/69	0/1/1/1
21	CL7	C	518	-	2/2/10/20	3/8/86/115	-
21	CL7	B	614	-	2/2/14/20	12/31/109/115	-
26	LMG	d	410	-	-	6/28/48/70	0/1/1/1
25	LHG	8	401	-	-	8/53/53/53	-
22	PHO	A	402	-	-	3/37/103/103	0/5/6/6
23	8CT	C	519	-	-	8/29/63/63	0/2/2/2
22	PHO	D	408	-	-	5/37/103/103	0/5/6/6
21	CL7	c	514	-	2/2/11/20	6/13/91/115	-
23	8CT	d	406	-	-	10/29/63/63	0/2/2/2
24	SQD	B	620	-	-	5/49/69/69	0/1/1/1
32	ZEX	3	520	-	-	10/29/67/67	0/2/2/2
21	CL7	4	410	-	2/2/11/20	7/13/91/115	-
32	ZEX	3	519	-	-	10/29/67/67	0/2/2/2
21	CL7	6	518	16	2/2/15/20	10/37/115/115	-
21	CL7	b	603	-	2/2/14/20	7/31/109/115	-
21	CL7	4	408	-	2/2/11/20	2/13/91/115	-
21	CL7	3	503	-	2/2/15/20	18/37/115/115	-
21	CL7	2	509	-	2/2/15/20	14/37/115/115	-
21	CL7	C	512	3	2/2/10/20	3/10/88/115	-
21	CL7	4	415	-	2/2/11/20	10/13/91/115	-
21	CL7	B	609	-	2/2/15/20	12/37/115/115	-
21	CL7	c	507	-	2/2/14/20	13/31/109/115	-
21	CL7	8	407	-	2/2/10/20	1/8/86/115	-
32	ZEX	2	523	-	-	6/29/67/67	0/2/2/2
21	CL7	4	411	-	2/2/15/20	12/37/115/115	-
21	CL7	B	612	-	2/2/15/20	15/37/115/115	-
21	CL7	8	416	-	2/2/10/20	5/8/86/115	-
21	CL7	c	512	3	2/2/10/20	3/10/88/115	-
32	ZEX	2	521	-	-	6/29/67/67	0/2/2/2
21	CL7	c	505	-	2/2/13/20	11/25/103/115	-
21	CL7	c	513	-	2/2/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	A	401	-	2/2/15/20	16/37/115/115	-
21	CL7	6	508	-	2/2/11/20	3/13/91/115	-
21	CL7	4	414	-	2/2/12/20	6/23/101/115	-
21	CL7	B	616	-	2/2/11/20	4/13/91/115	-
23	8CT	D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	2	504	-	2/2/11/20	4/13/91/115	-
21	CL7	8	417	20	2/2/10/20	4/10/88/115	-
21	CL7	8	404	-	2/2/15/20	14/37/115/115	-
21	CL7	2	514	-	2/2/11/20	7/13/91/115	-
23	8CT	A	404	-	-	5/29/63/63	0/2/2/2
21	CL7	c	502	-	2/2/15/20	18/37/115/115	-
27	DGD	C	517	-	-	9/51/91/95	0/2/2/2
21	CL7	2	512	-	2/2/15/20	16/37/115/115	-
21	CL7	b	604	-	2/2/15/20	12/37/115/115	-
25	LHG	A	407	-	-	5/50/50/53	-
21	CL7	B	604	-	2/2/15/20	15/37/115/115	-
32	ZEX	3	525	-	-	7/29/67/67	0/2/2/2
21	CL7	5	415	-	2/2/10/20	5/8/86/115	-
21	CL7	a	401	-	2/2/15/20	16/37/115/115	-
21	CL7	C	510	-	2/2/15/20	18/37/115/115	-
21	CL7	8	412	-	2/2/15/20	17/37/115/115	-
21	CL7	B	601	-	2/2/10/20	4/8/86/115	-
21	CL7	5	407	-	2/2/10/20	2/8/86/115	-
24	SQD	b	621	-	-	5/49/69/69	0/1/1/1
23	8CT	B	617	-	-	7/29/63/63	0/2/2/2
21	CL7	2	511	16	2/2/14/20	14/31/109/115	-
21	CL7	5	411	-	2/2/11/20	5/13/91/115	-
27	DGD	B	624	-	-	7/51/91/95	0/2/2/2
21	CL7	1	412	-	2/2/11/20	8/13/91/115	-
21	CL7	B	613	-	2/2/13/20	4/25/103/115	-
21	CL7	7	515	-	2/2/10/20	0/8/86/115	-
25	LHG	d	409	-	-	7/53/53/53	-
21	CL7	2	508	-	2/2/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	1	409	-	2/2/11/20	4/13/91/115	-
21	CL7	6	506	-	2/2/15/20	12/37/115/115	-
21	CL7	6	512	-	2/2/15/20	16/37/115/115	-
32	ZEX	4	419	-	-	9/29/67/67	0/2/2/2
21	CL7	1	402	-	2/2/14/20	14/31/109/115	-
21	CL7	1	417	18	2/2/13/20	7/25/103/115	-
21	CL7	3	505	-	2/2/15/20	14/37/115/115	-
21	CL7	6	510	16	2/2/15/20	20/37/115/115	-
21	CL7	6	515	-	2/2/11/20	6/13/91/115	-
21	CL7	d	404	-	2/2/13/20	11/29/107/115	-
21	CL7	7	506	-	2/2/11/20	11/13/91/115	-
25	LHG	D	409	-	-	7/53/53/53	-
30	PL9	D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	7	503	-	2/2/15/20	18/37/115/115	-
21	CL7	c	518	-	2/2/10/20	3/8/86/115	-
21	CL7	2	505	-	2/2/15/20	16/37/115/115	-
21	CL7	7	513	-	2/2/11/20	7/13/91/115	-
21	CL7	2	513	-	2/2/11/20	6/13/91/115	-
24	SQD	2	522	-	-	7/45/65/69	0/1/1/1
21	CL7	C	504	-	2/2/15/20	17/37/115/115	-
21	CL7	6	502	-	2/2/15/20	15/37/115/115	-
21	CL7	6	509	-	2/2/15/20	14/37/115/115	-
26	LMG	1	401	-	-	5/46/66/70	0/1/1/1
32	ZEX	5	421	-	-	14/29/67/67	0/2/2/2
21	CL7	3	507	-	2/2/15/20	13/37/115/115	-
21	CL7	b	616	-	2/2/12/20	8/19/97/115	-
21	CL7	8	414	-	2/2/12/20	6/23/101/115	-
32	ZEX	6	522	-	-	6/29/67/67	0/2/2/2
21	CL7	6	513	-	2/2/11/20	6/13/91/115	-
21	CL7	1	404	-	2/2/15/20	13/37/115/115	-
21	CL7	4	416	-	2/2/10/20	5/8/86/115	-
21	CL7	b	609	-	2/2/15/20	15/37/115/115	-
21	CL7	3	515	-	2/2/10/20	0/8/86/115	-
23	8CT	K	101	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	8	413	20	2/2/14/20	7/31/109/115	-

The worst 5 of 3338 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	627	8CT	C02-C03	14.81	1.60	1.34
23	b	601	8CT	C02-C03	14.81	1.60	1.34
23	B	618	8CT	C02-C03	14.76	1.60	1.34
23	b	619	8CT	C02-C03	14.76	1.60	1.34
23	C	519	8CT	C02-C03	14.59	1.59	1.34

The worst 5 of 4416 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	403	CL7	C3C-C4C-NC	10.55	117.83	110.18
21	a	403	CL7	C3C-C4C-NC	10.50	117.79	110.18
21	7	505	CL7	C3C-C4C-NC	10.29	117.64	110.18
21	3	505	CL7	C3C-C4C-NC	10.28	117.63	110.18
23	8	402	8CT	C33-C32-C31	-10.15	115.12	124.85

5 of 424 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	401	CL7	NA
21	A	401	CL7	NC
21	A	403	CL7	NA
21	A	403	CL7	NC
21	A	406	CL7	NA

5 of 2944 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	403	CL7	O1A-CGA-O2A-C1
21	A	403	CL7	CBA-CGA-O2A-C1
21	A	403	CL7	C1A-C2A-CAA-CBA
21	A	403	CL7	C3A-C2A-CAA-CBA
21	A	406	CL7	C1A-C2A-CAA-CBA

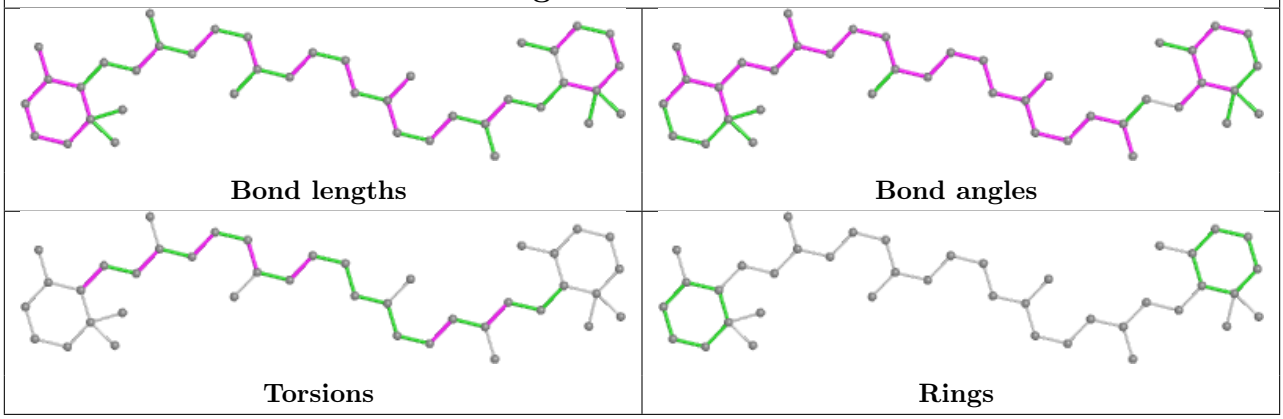
There are no ring outliers.

No monomer is involved in short contacts.

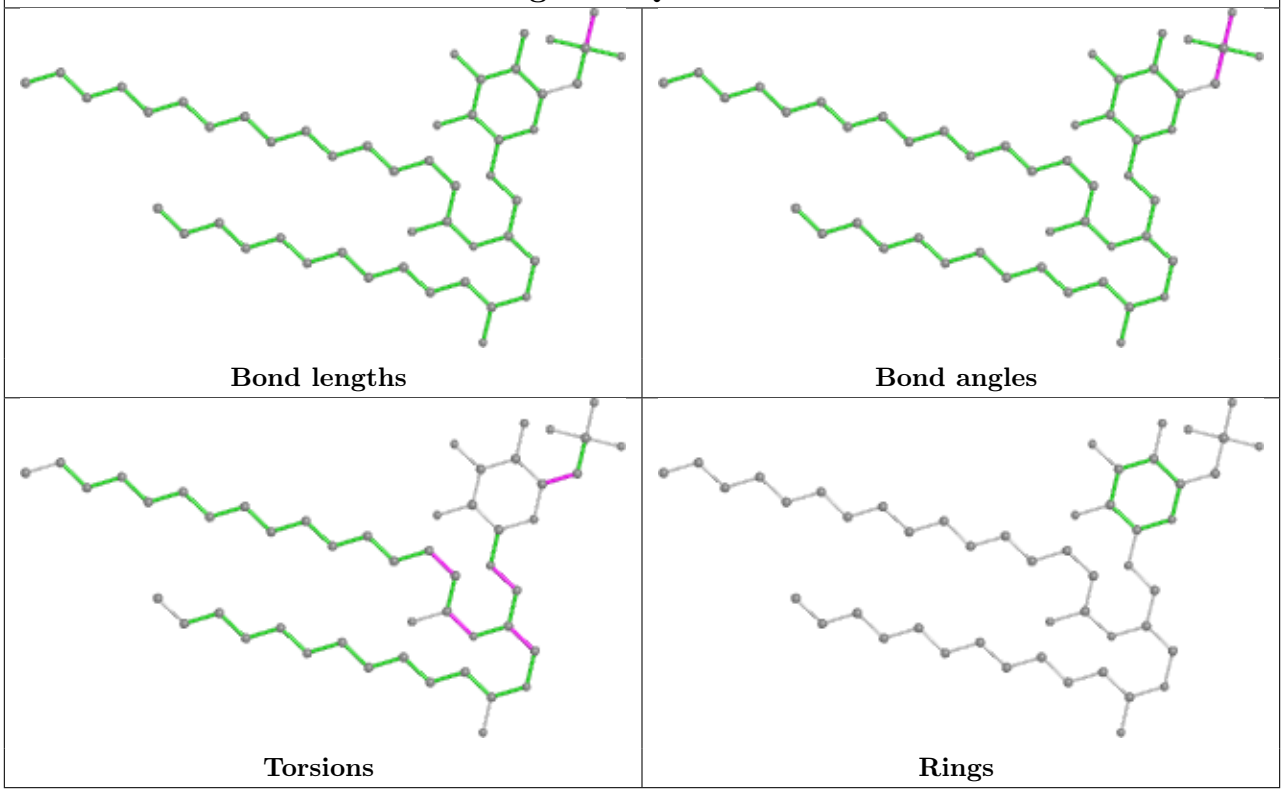
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

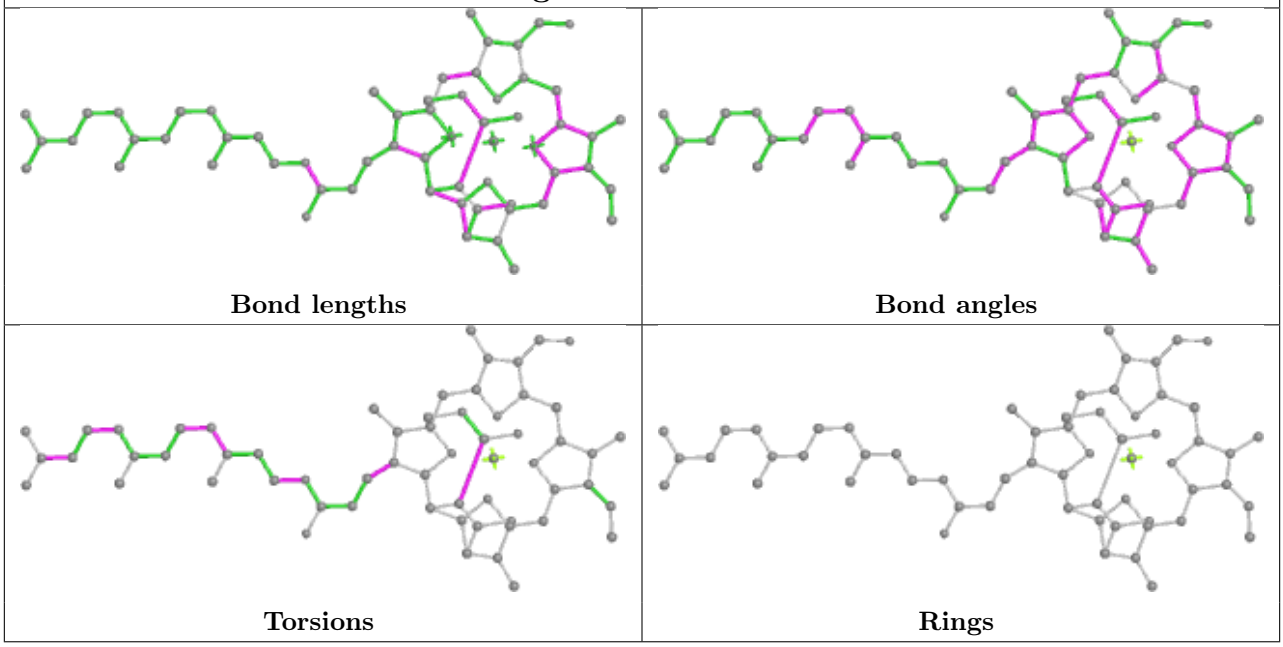
Ligand 8CT c 516



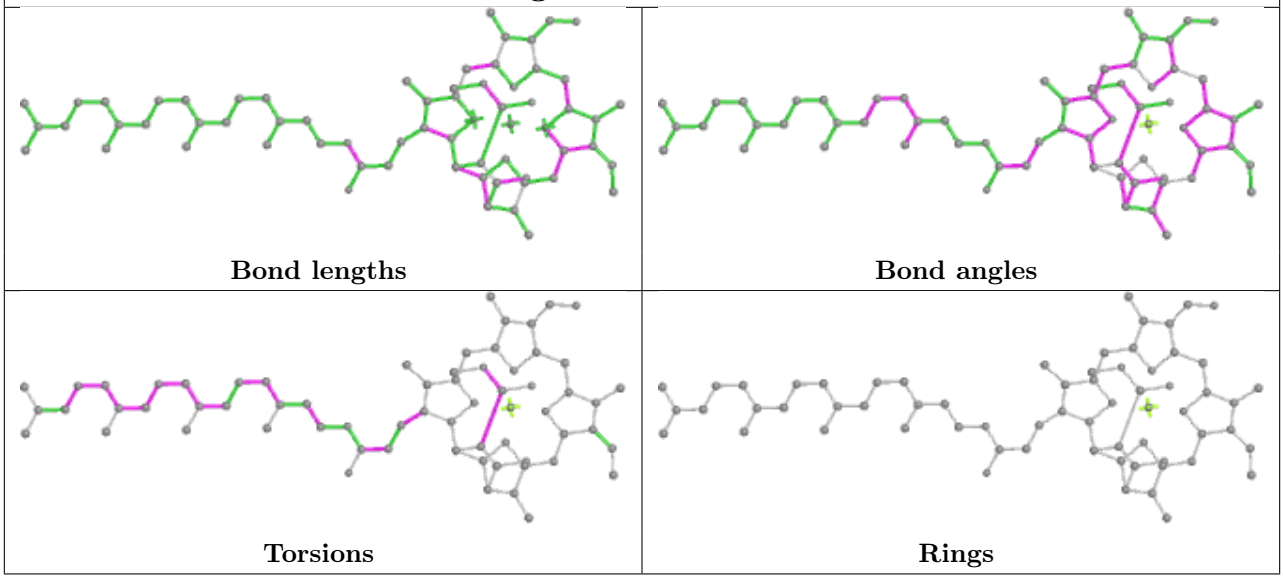
Ligand SQD 6 521



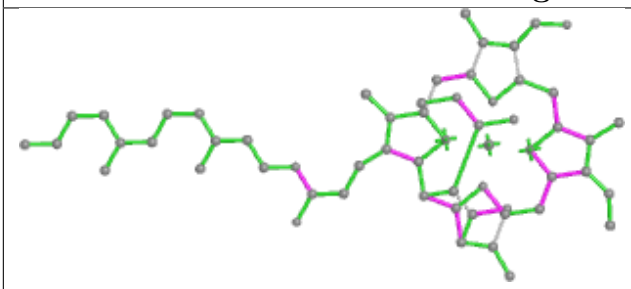
Ligand CL7 b 615



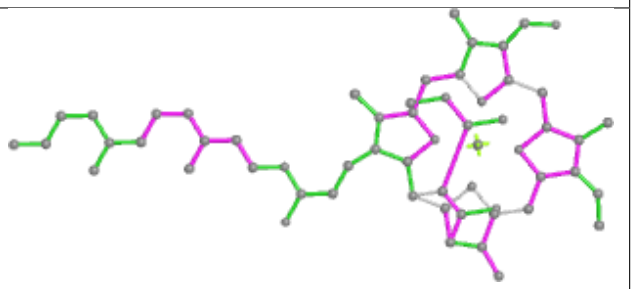
Ligand CL7 C 511



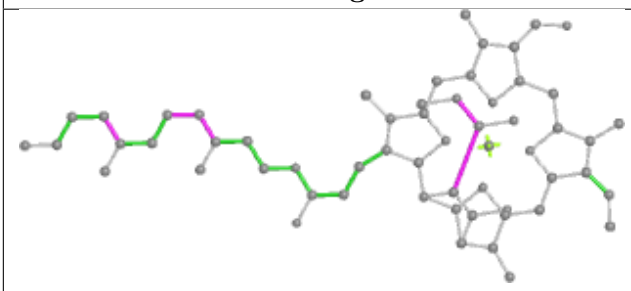
Ligand CL7 3 502



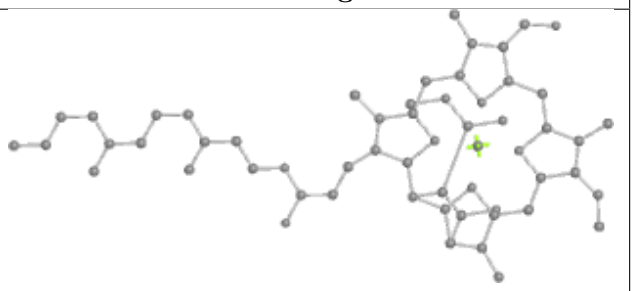
Bond lengths



Bond angles

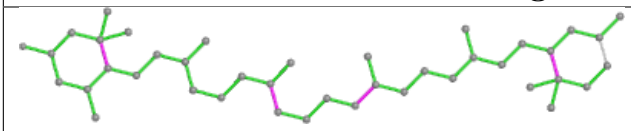


Torsions

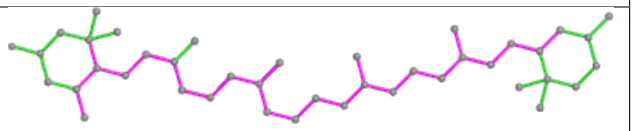


Rings

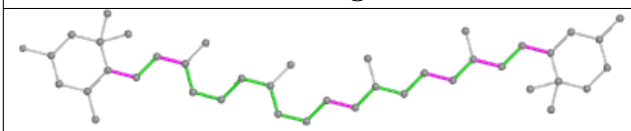
Ligand ZEX 8 403



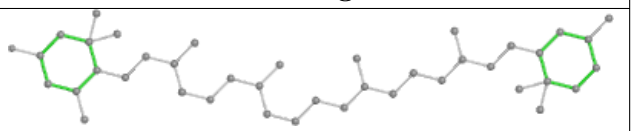
Bond lengths



Bond angles

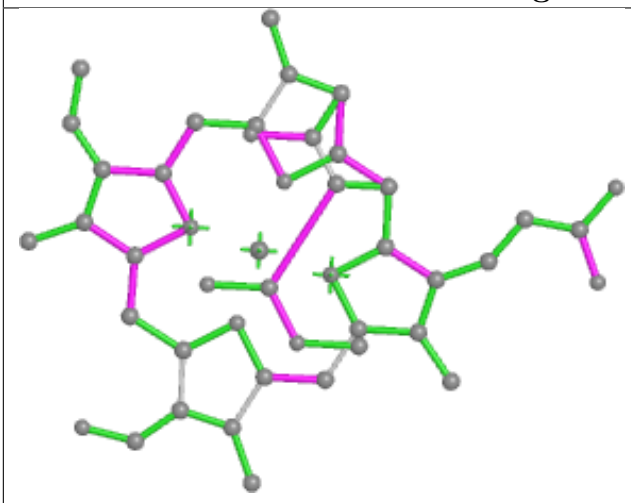


Torsions

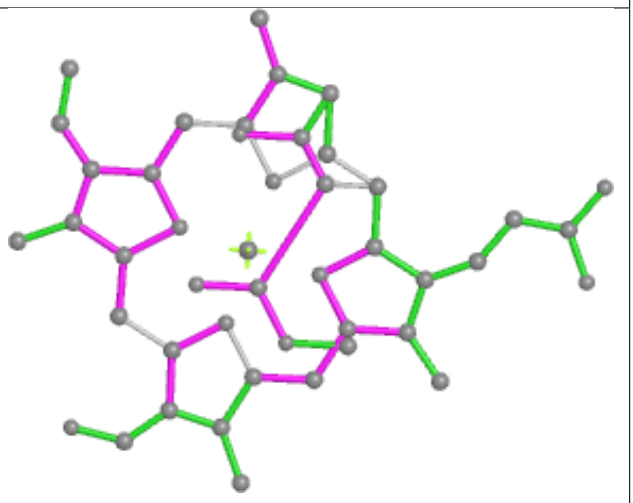


Rings

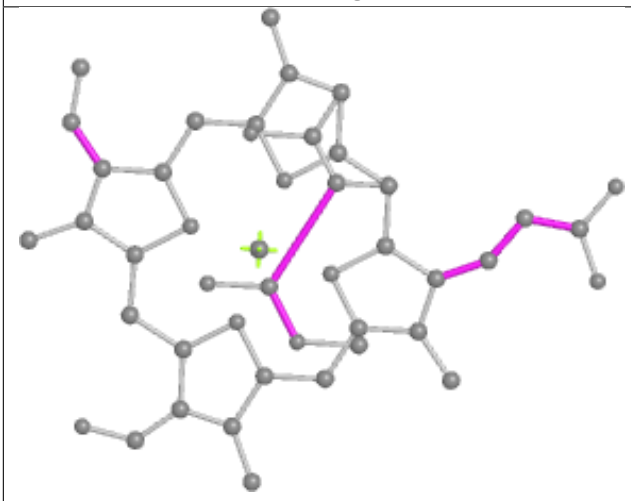
Ligand CL7 8 415



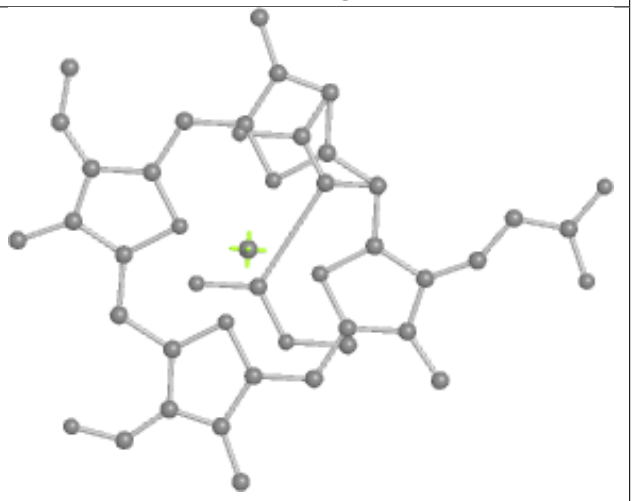
Bond lengths



Bond angles

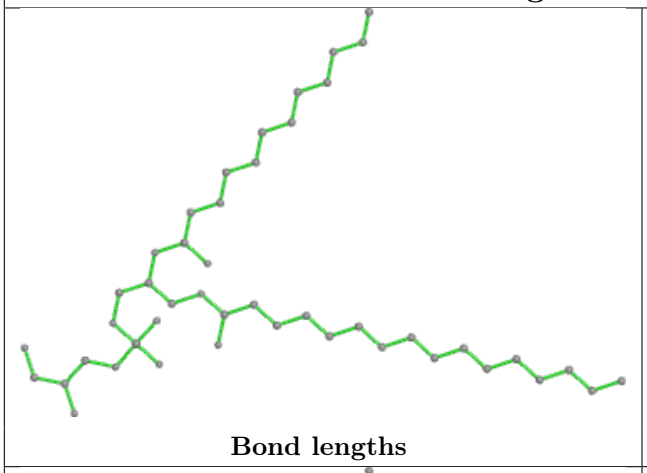


Torsions

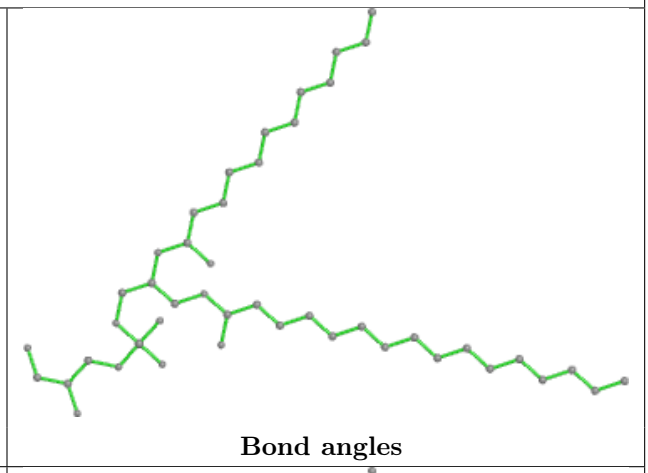


Rings

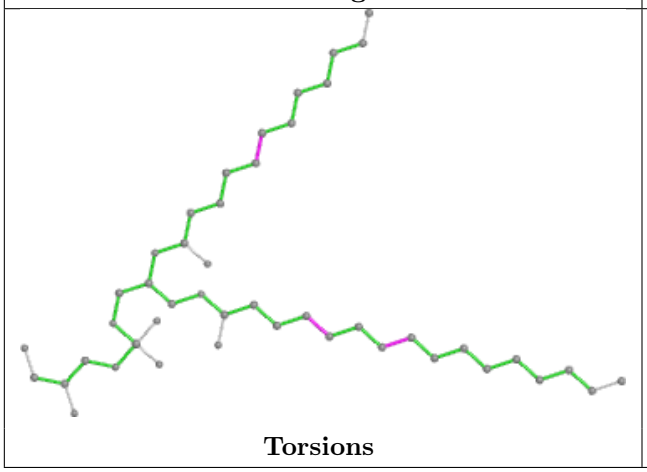
Ligand LHG b 624



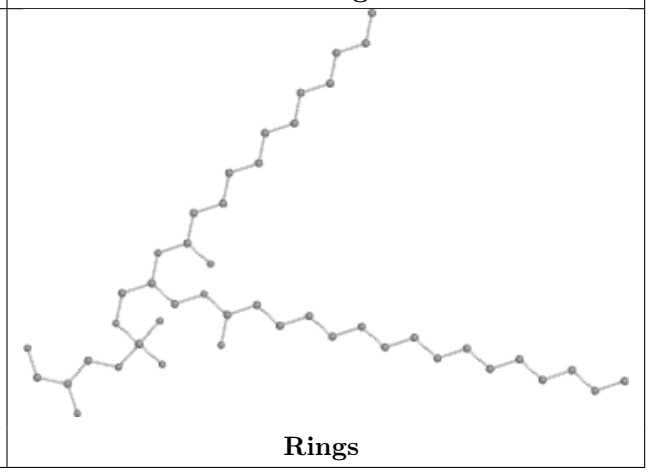
Bond lengths



Bond angles

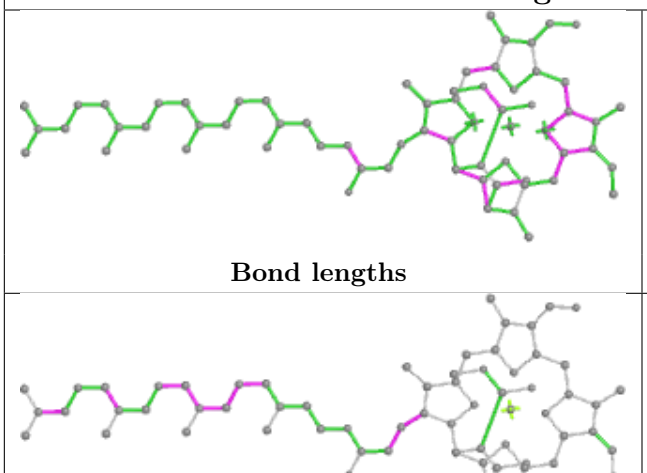


Torsions

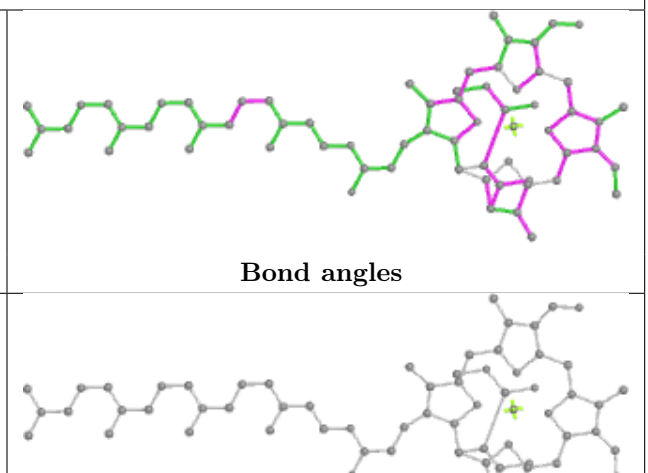


Rings

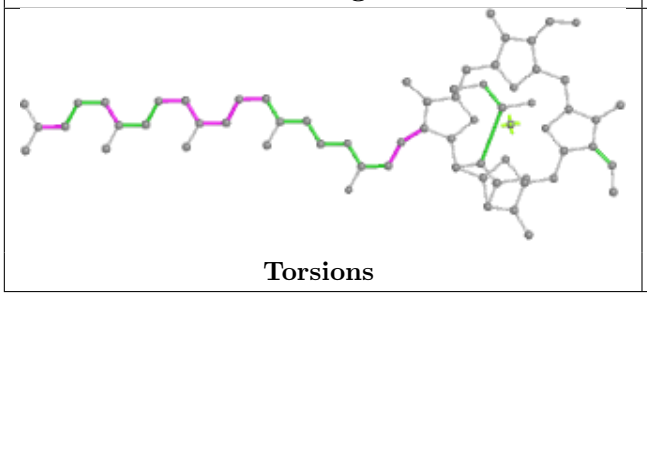
Ligand CL7 4 404



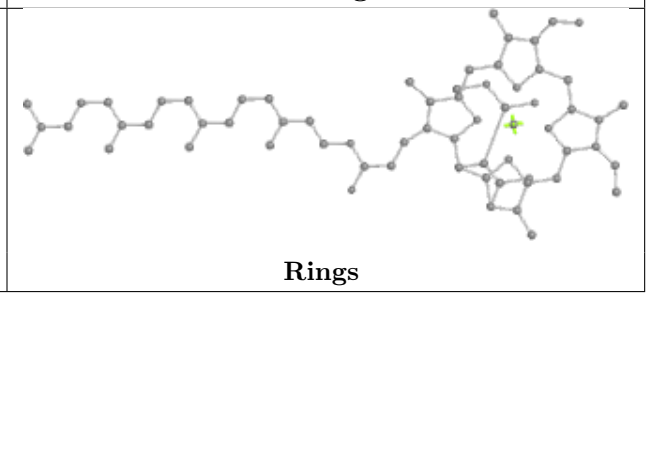
Bond lengths



Bond angles

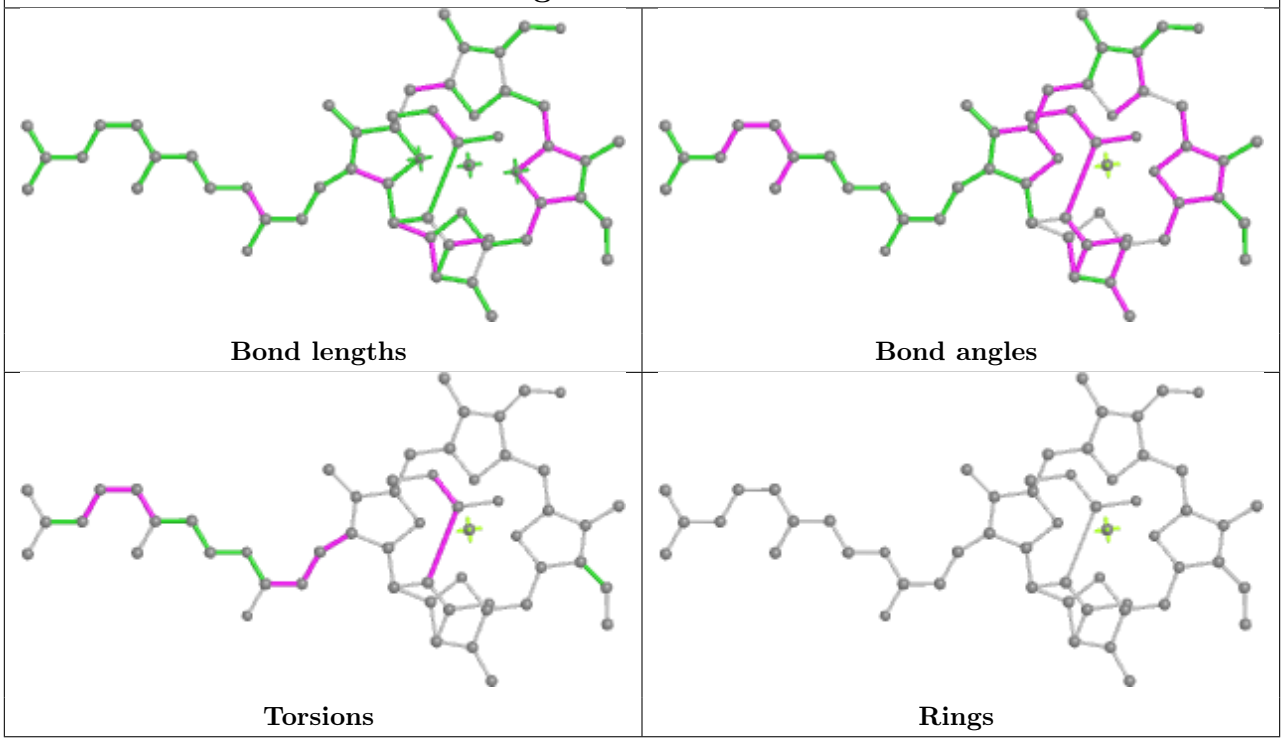


Torsions

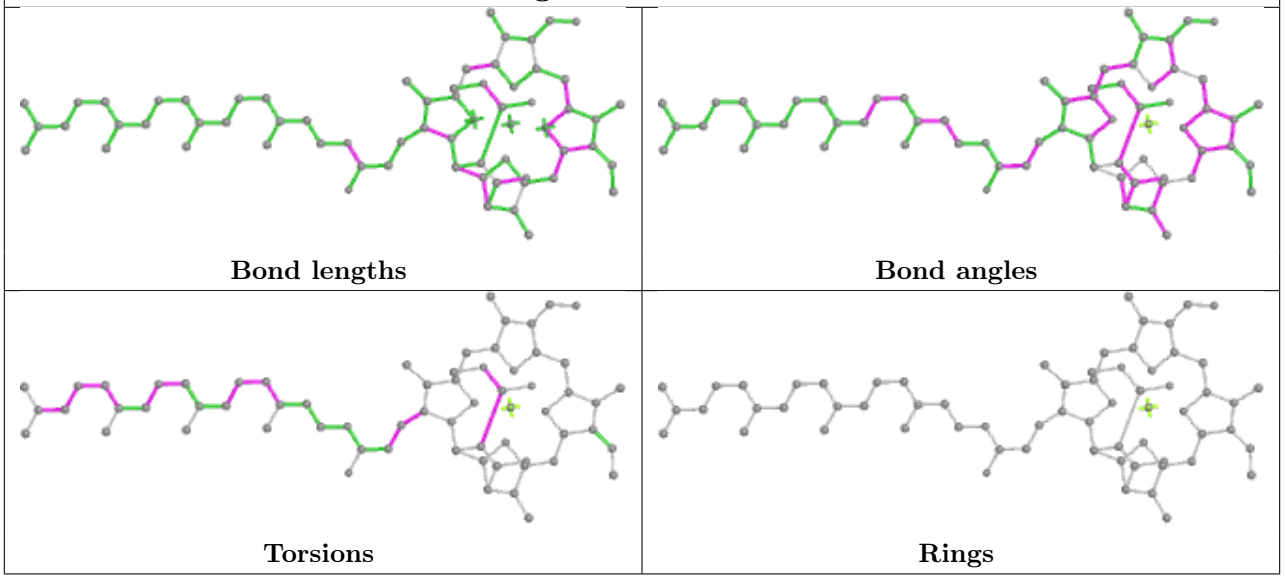


Rings

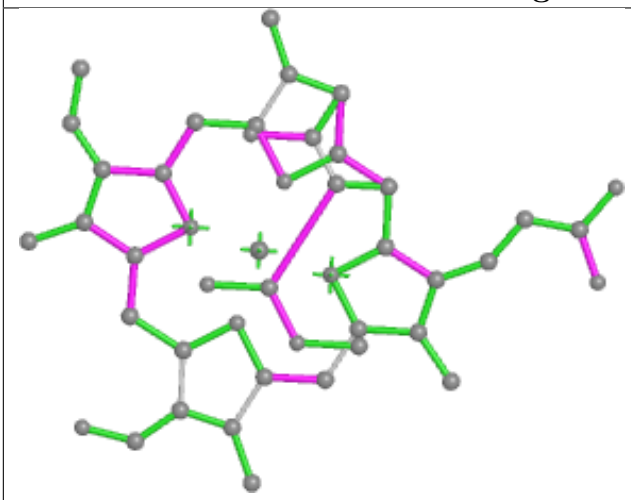
Ligand CL7 7 512



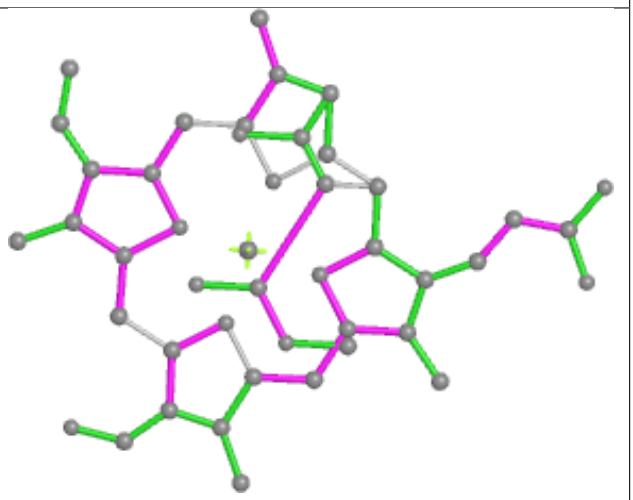
Ligand CL7 6 517



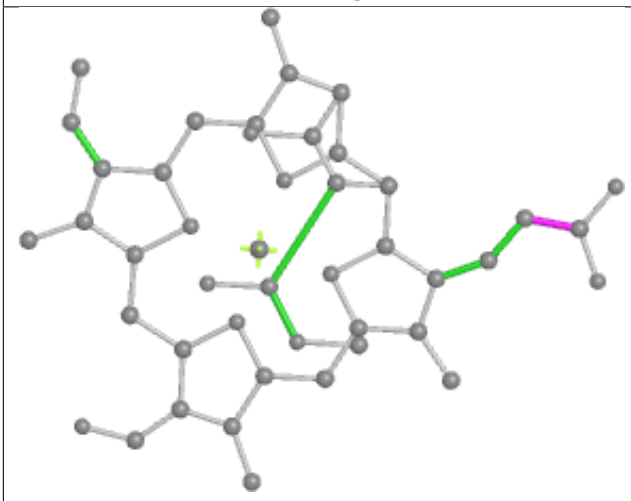
Ligand CL7 8 408



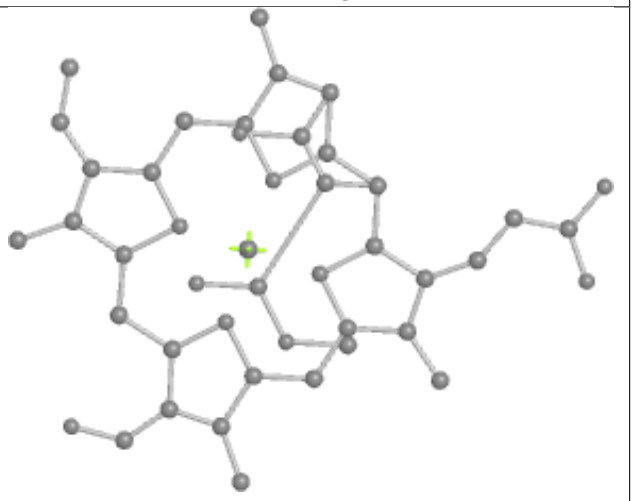
Bond lengths



Bond angles

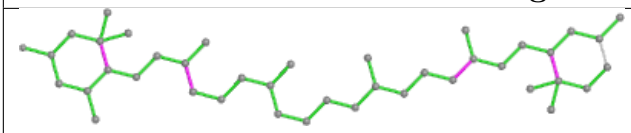


Torsions

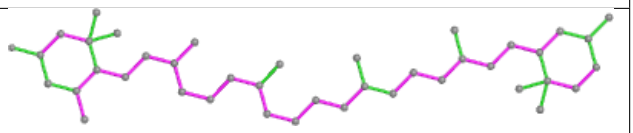


Rings

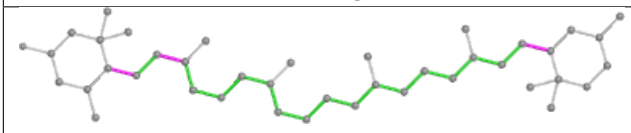
Ligand ZEX 3 522



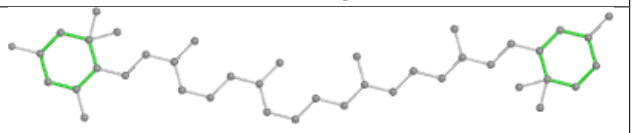
Bond lengths



Bond angles

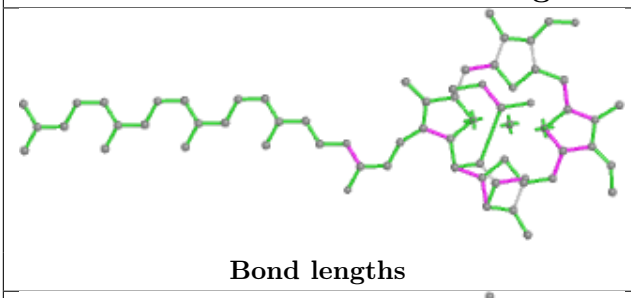


Torsions

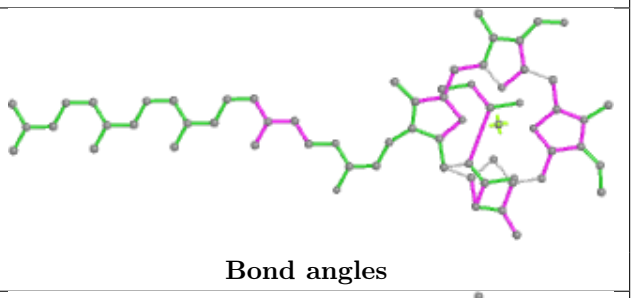


Rings

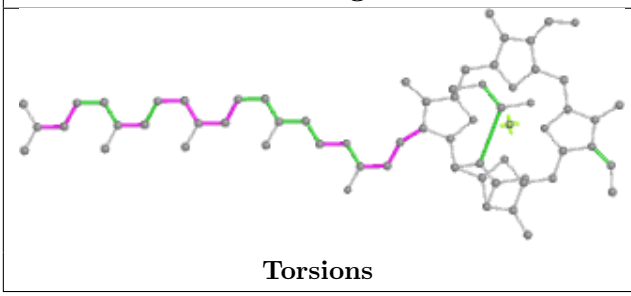
Ligand CL7 6 501



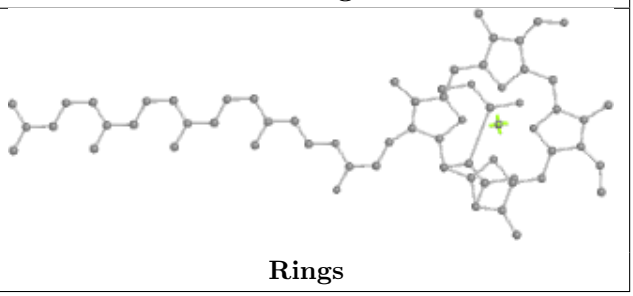
Bond lengths



Bond angles

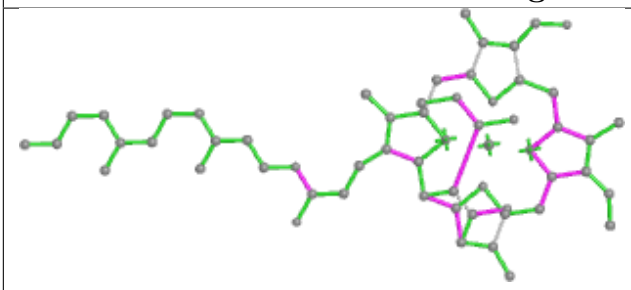


Torsions

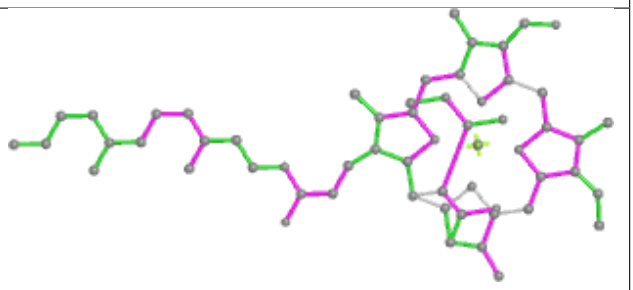


Rings

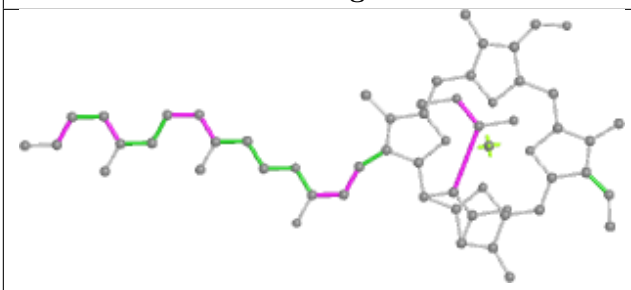
Ligand CL7 D 404



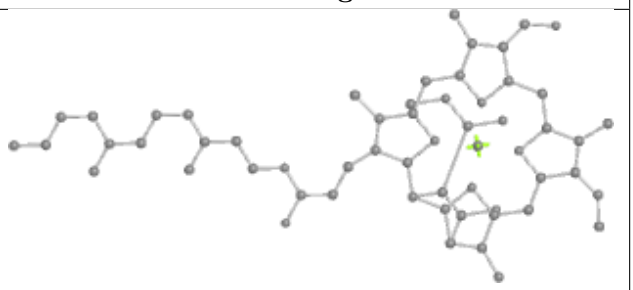
Bond lengths



Bond angles

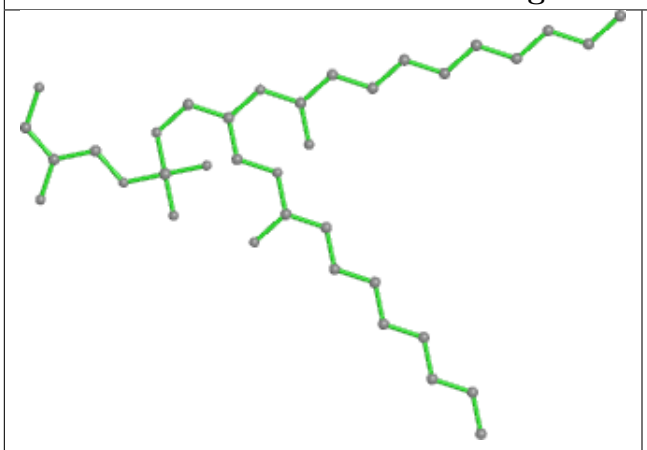


Torsions



Rings

Ligand LHG 7 524



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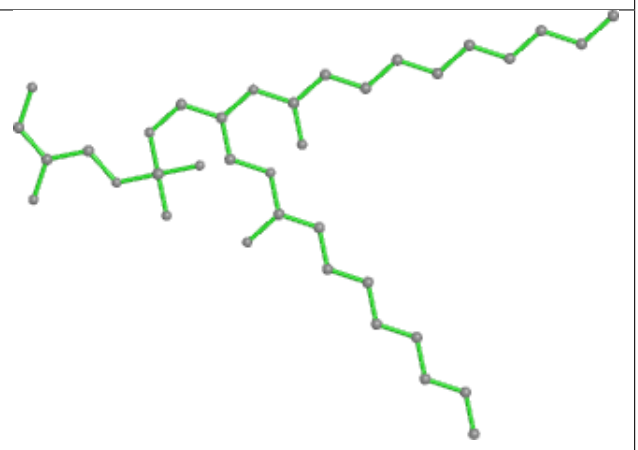
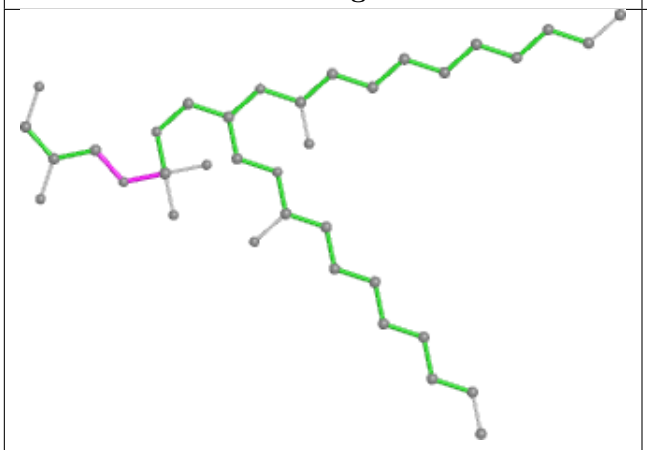
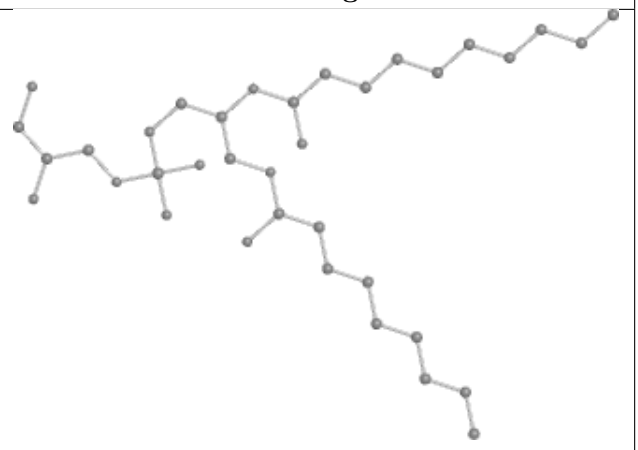


Bond angles

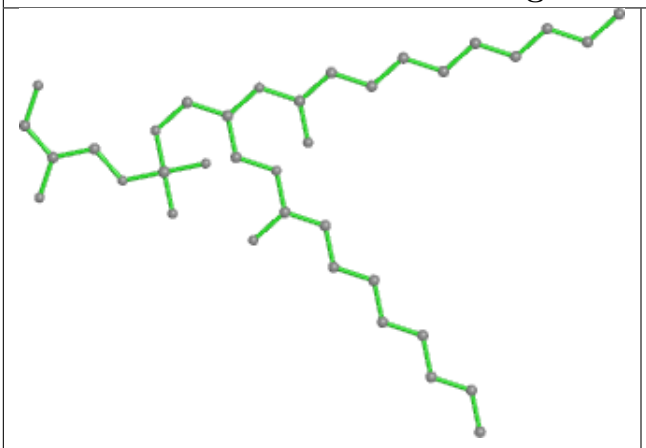


Torsions

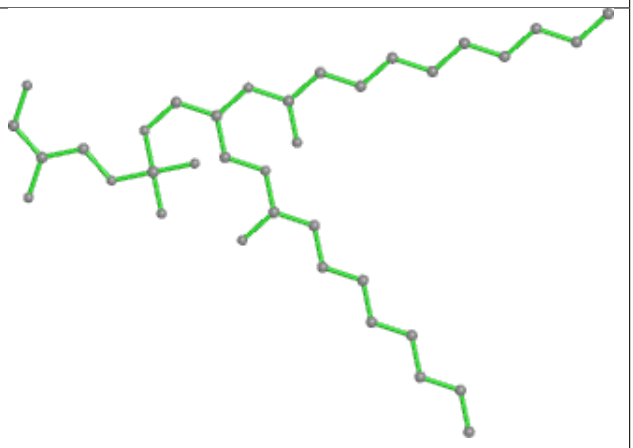


Rings

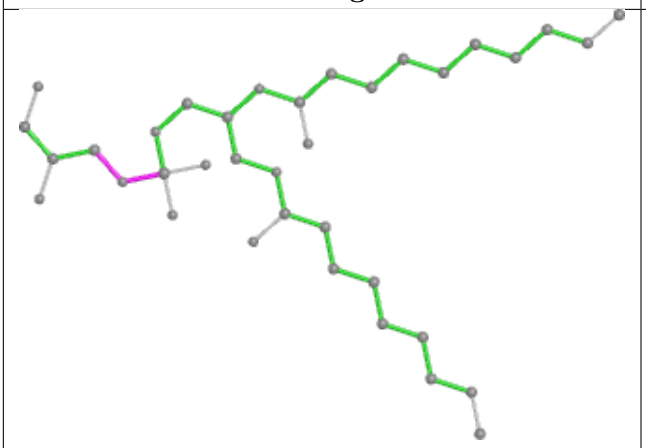
Ligand LHG 3 524



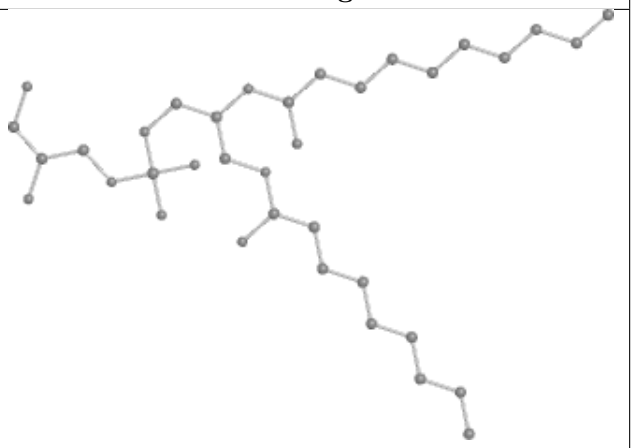
Bond lengths



Bond angles

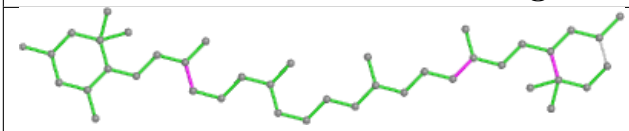


Torsions



Rings

Ligand ZEX 7 519



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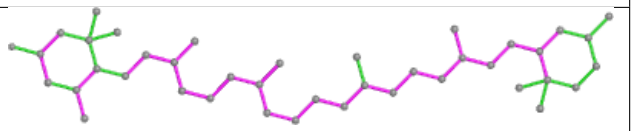
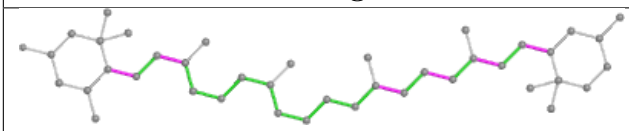
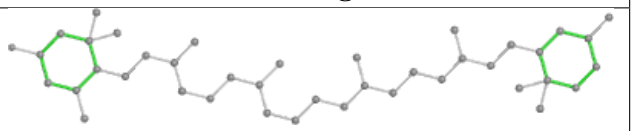


Bond angles

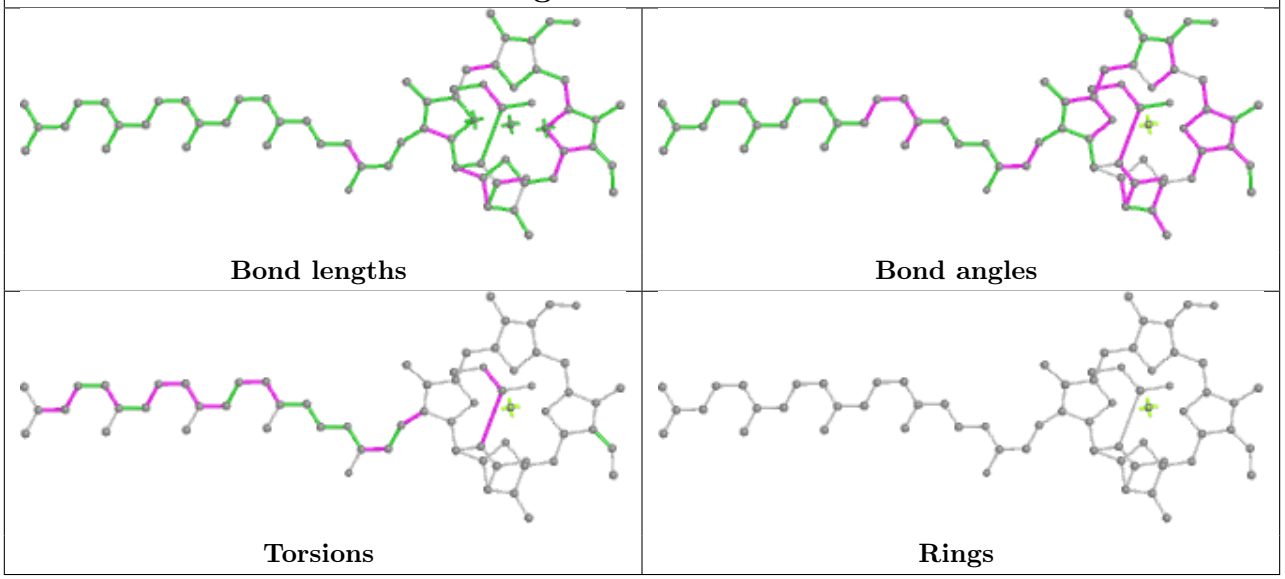


Torsions

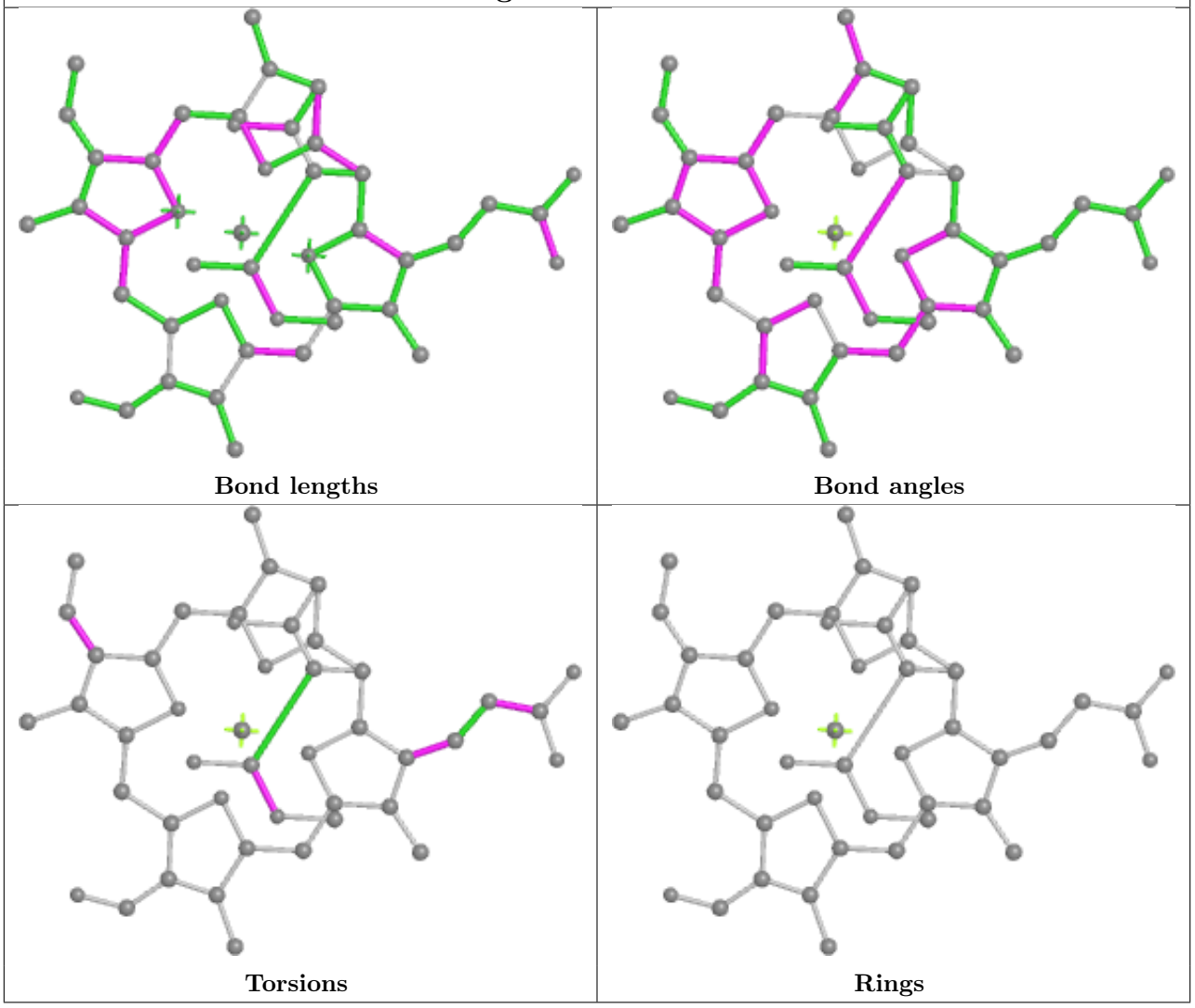


Rings

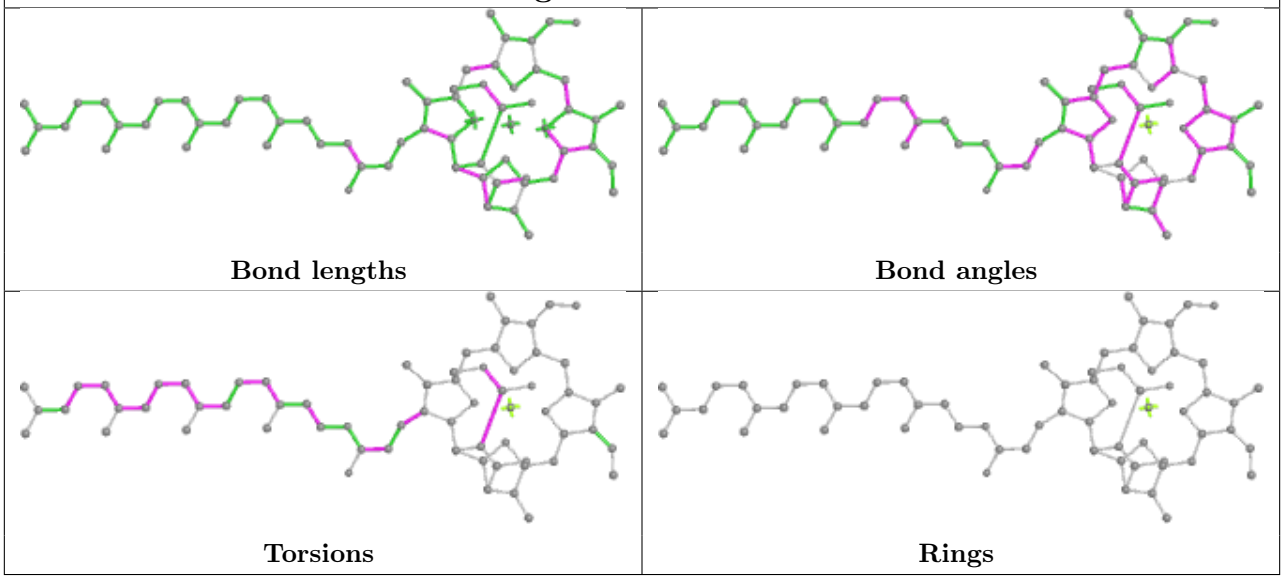
Ligand CL7 5 418



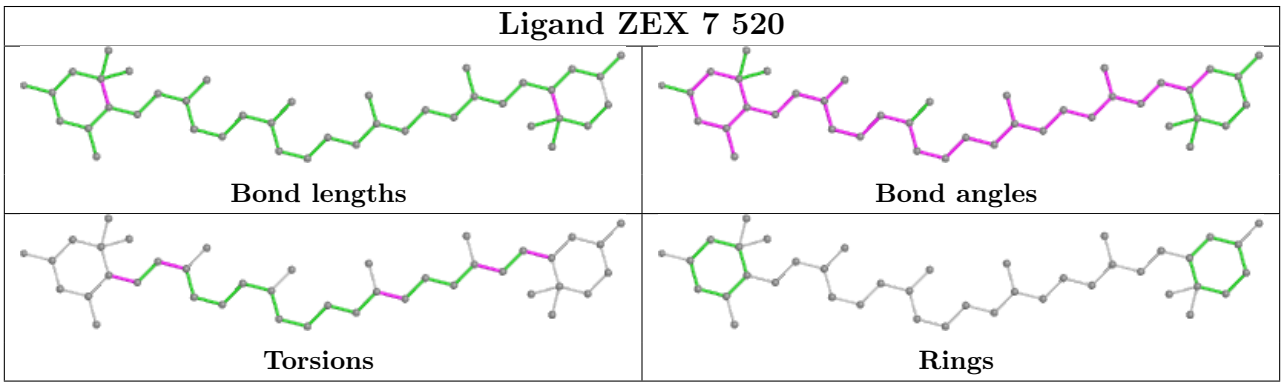
Ligand CL7 6 514



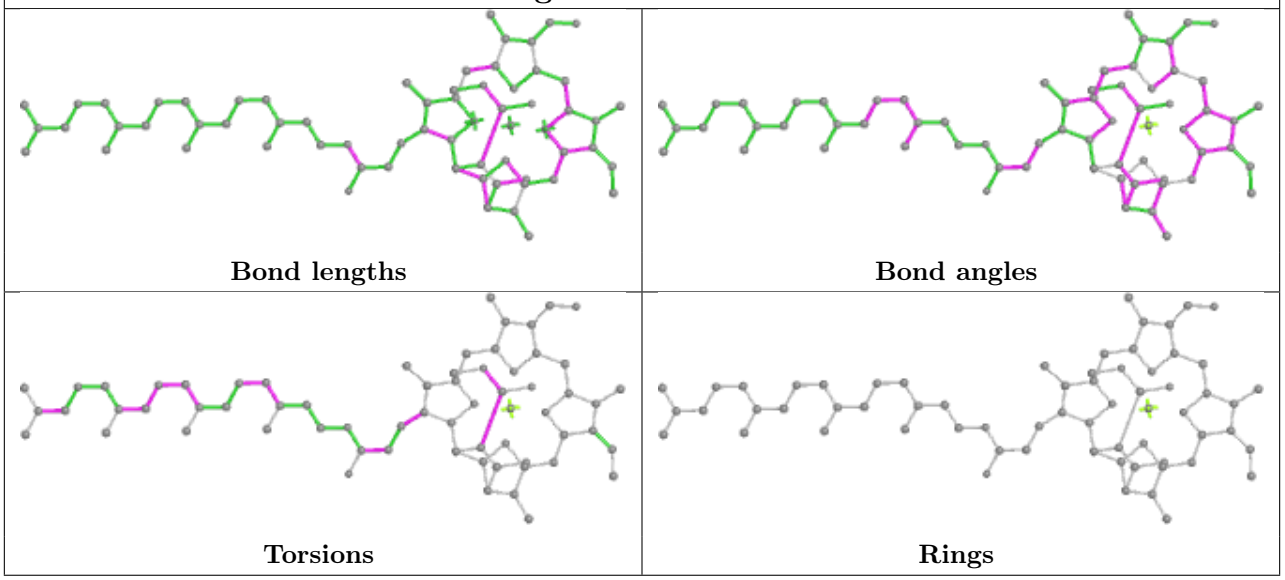
Ligand CL7 c 511



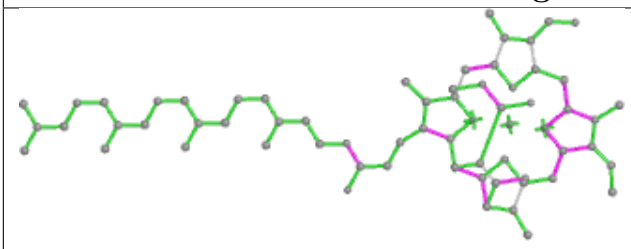
Ligand ZEX 7 520



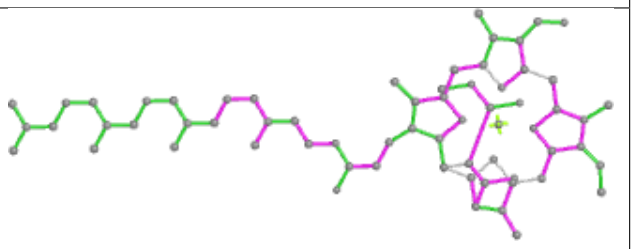
Ligand CL7 c 504



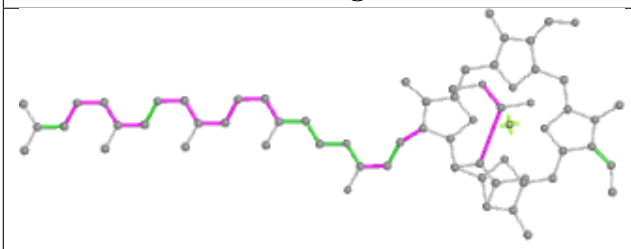
Ligand CL7 2 510



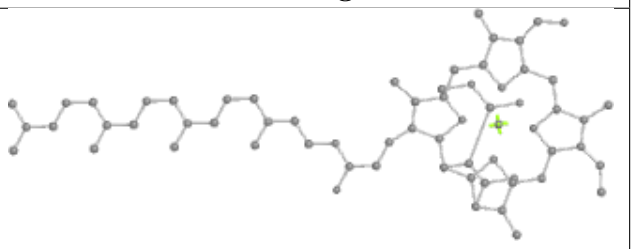
Bond lengths



Bond angles

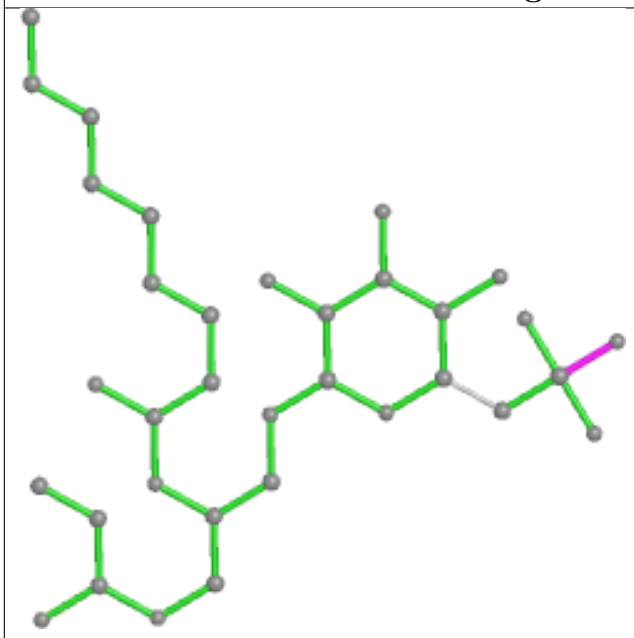


Torsions

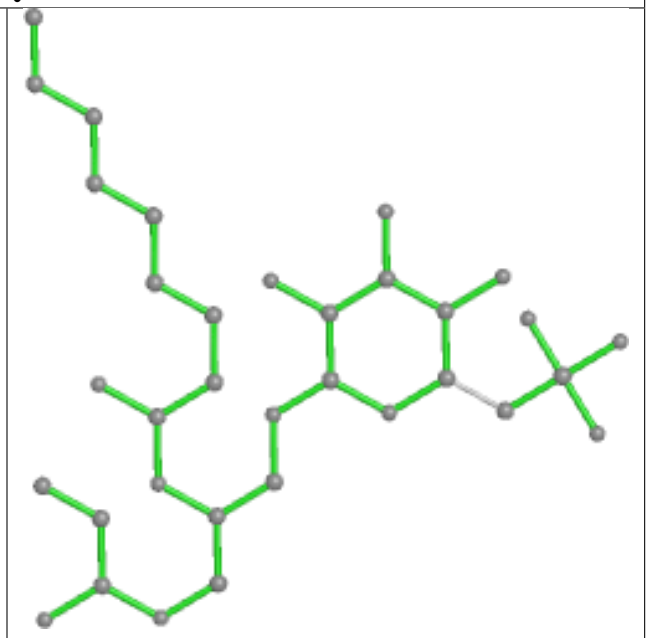


Rings

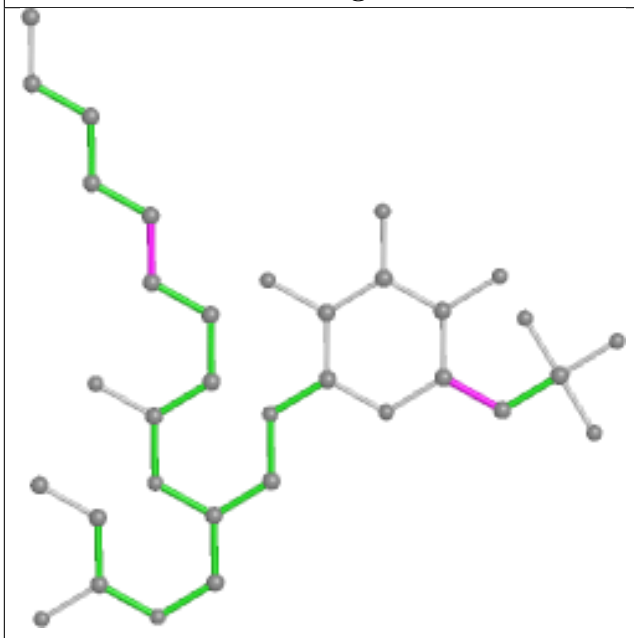
Ligand SQD A 405



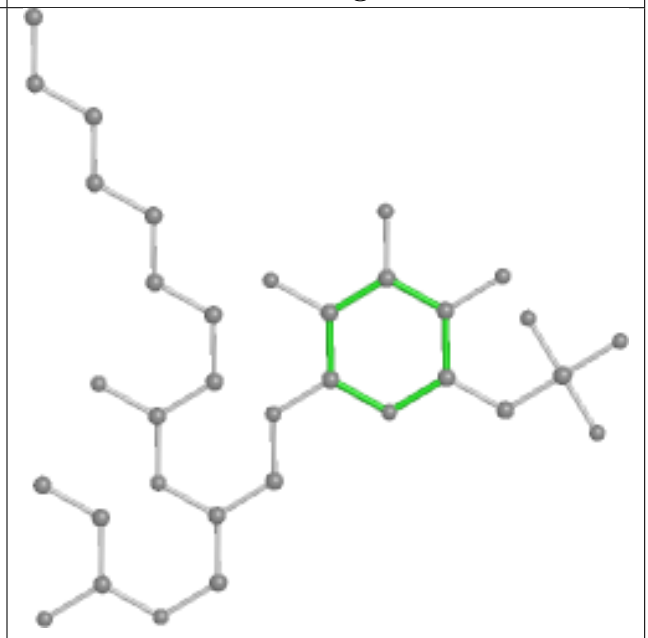
Bond lengths



Bond angles

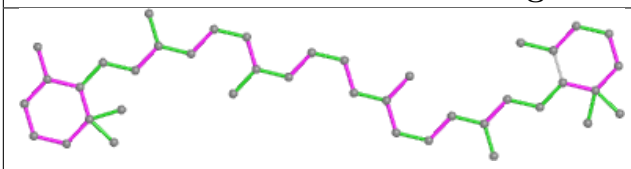


Torsions

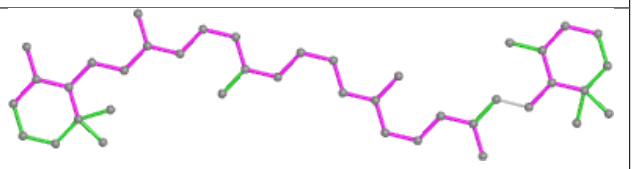


Rings

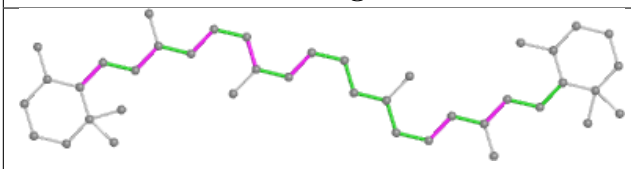
Ligand 8CT C 516



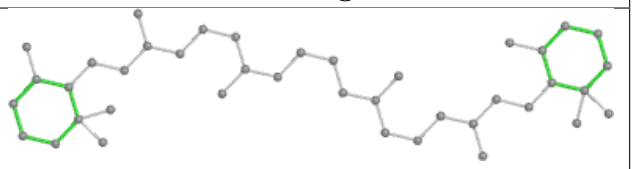
Bond lengths



Bond angles

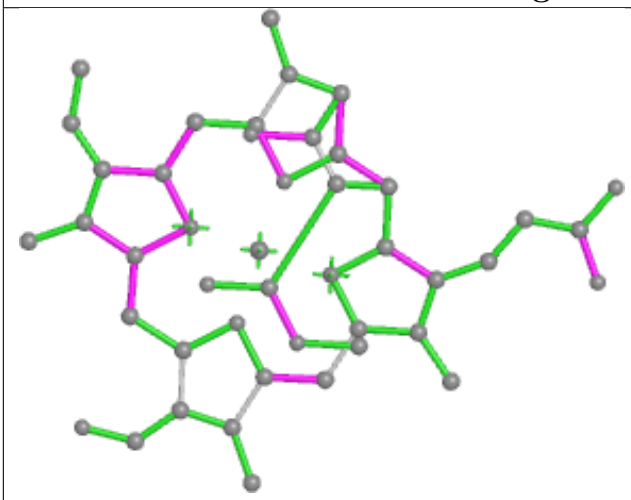


Torsions

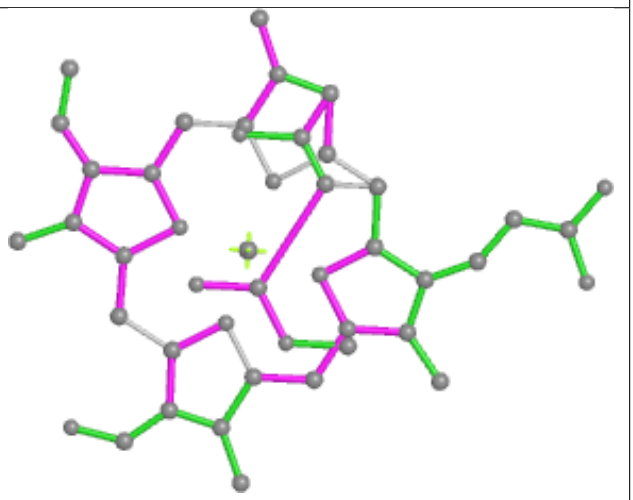


Rings

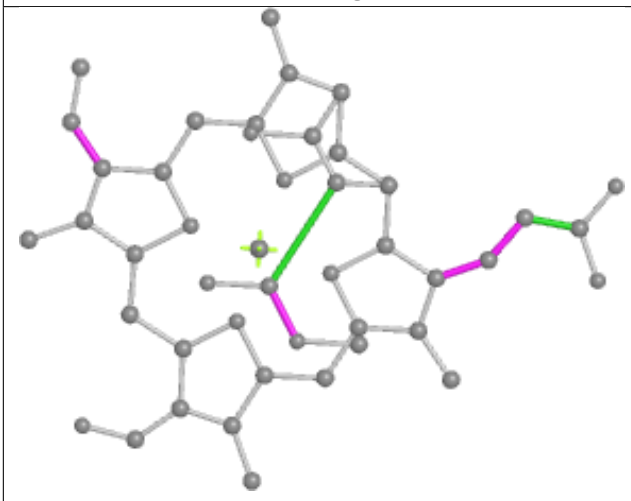
Ligand CL7 7 514



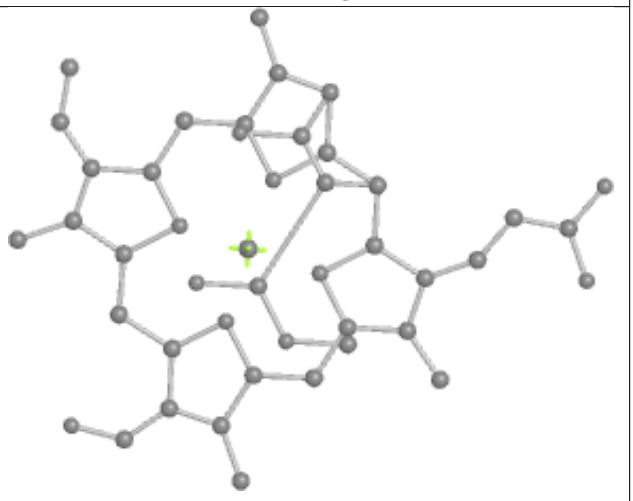
Bond lengths



Bond angles

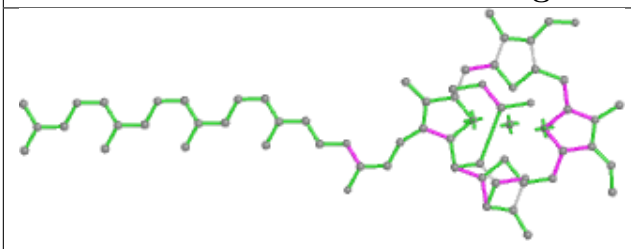


Torsions

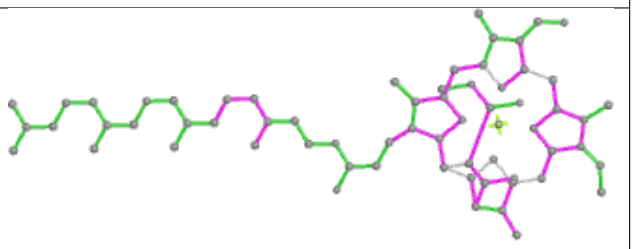


Rings

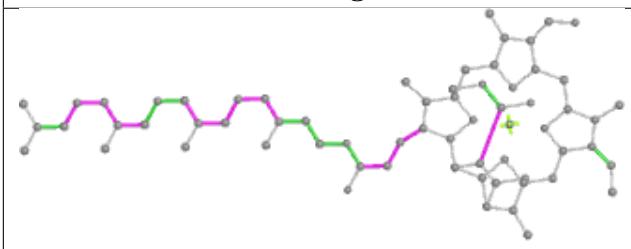
Ligand CL7 3 501



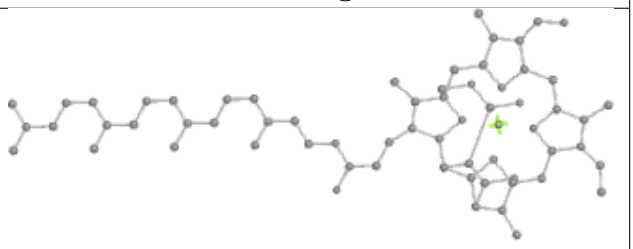
Bond lengths



Bond angles

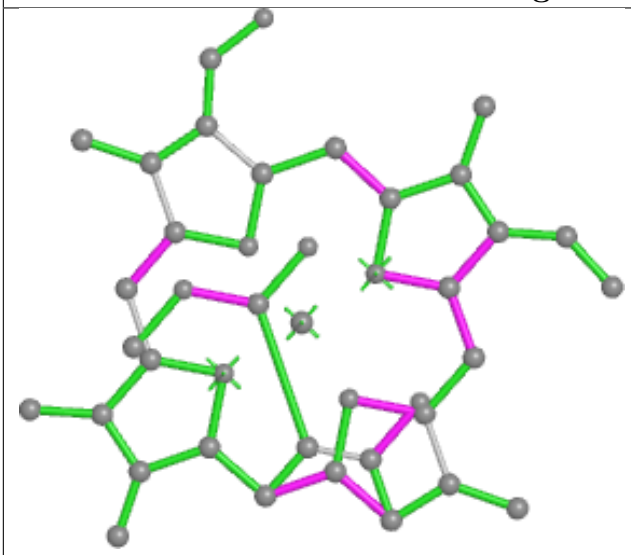


Torsions

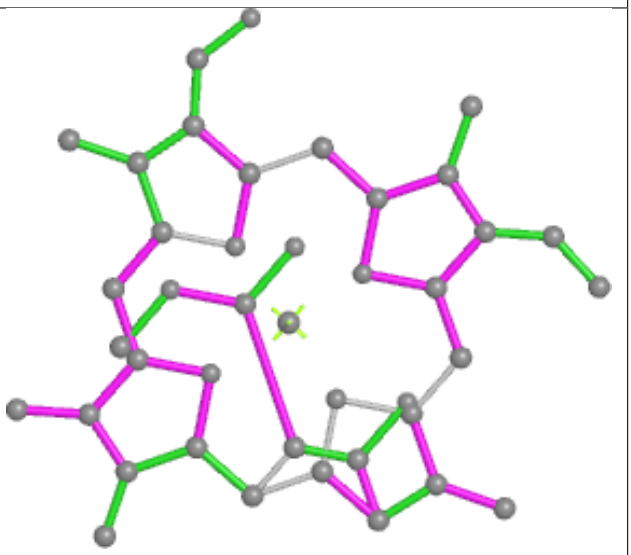


Rings

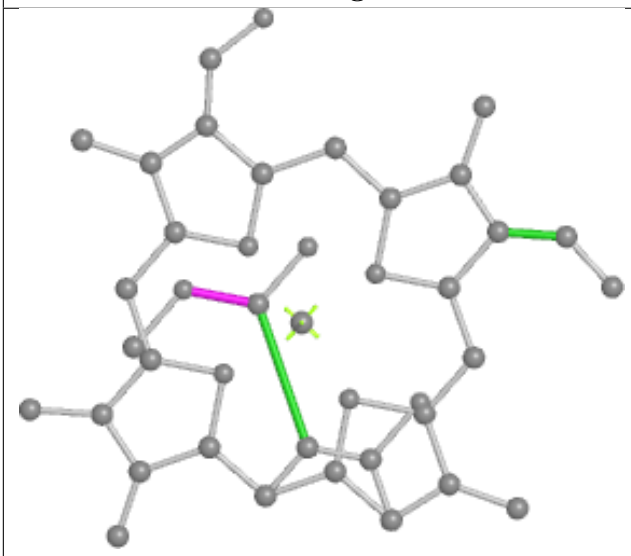
Ligand CL7 5 416



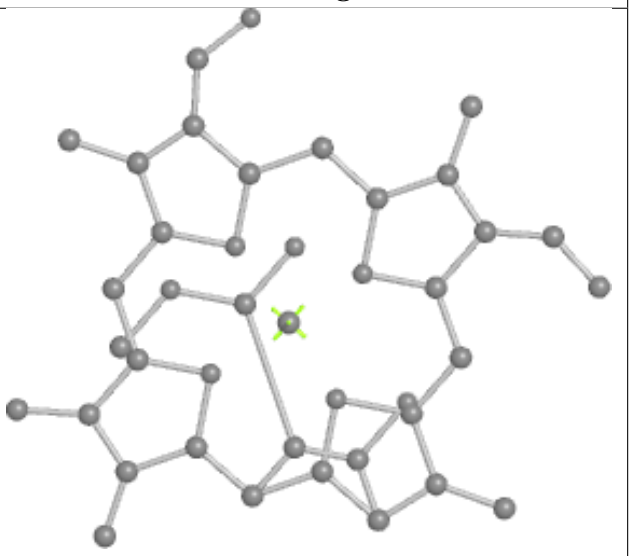
Bond lengths



Bond angles

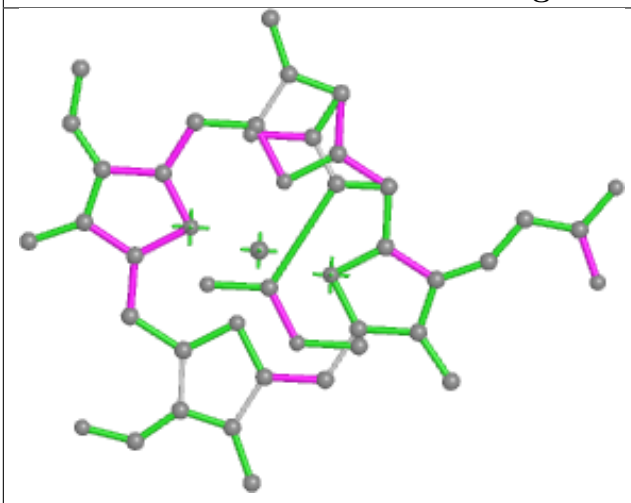


Torsions

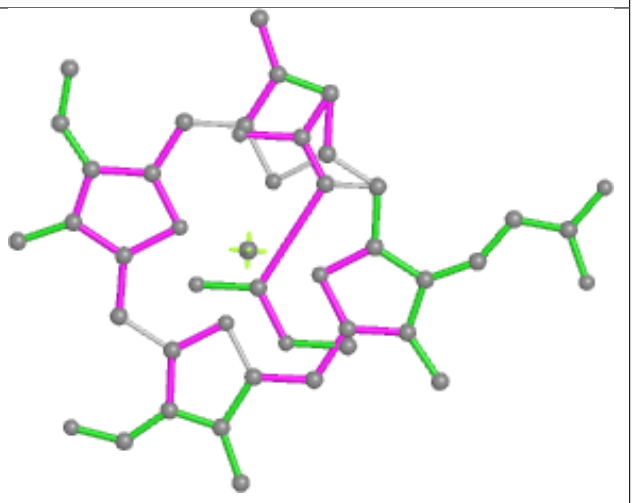


Rings

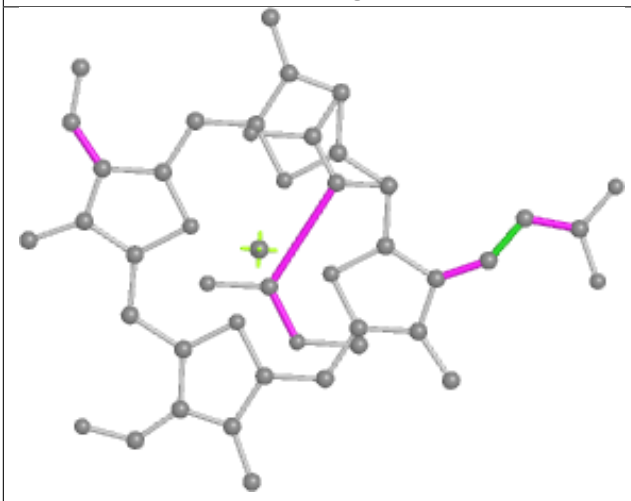
Ligand CL7 3 506



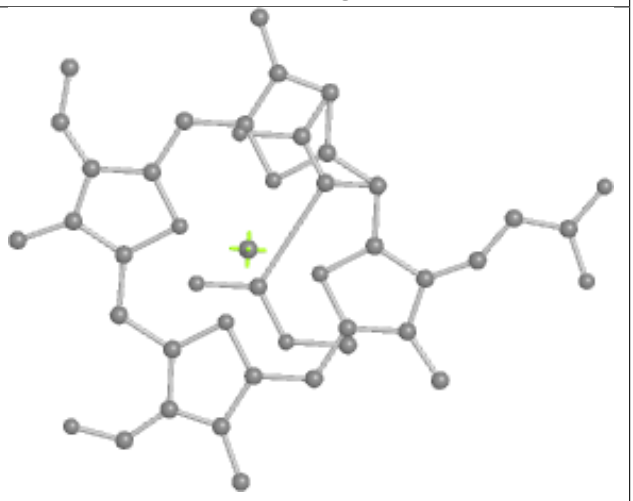
Bond lengths



Bond angles

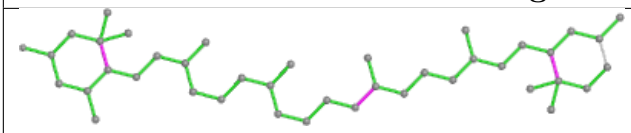


Torsions

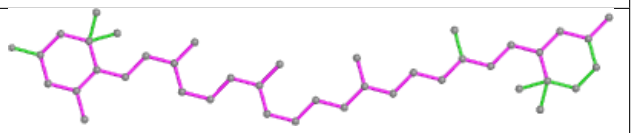


Rings

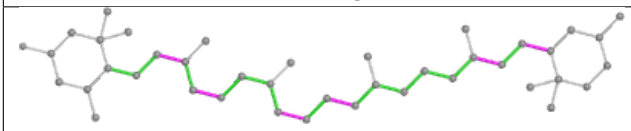
Ligand ZEX 8 419



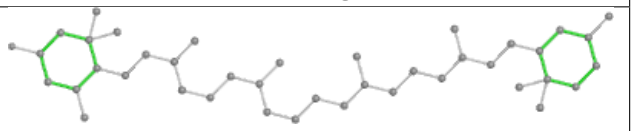
Bond lengths



Bond angles

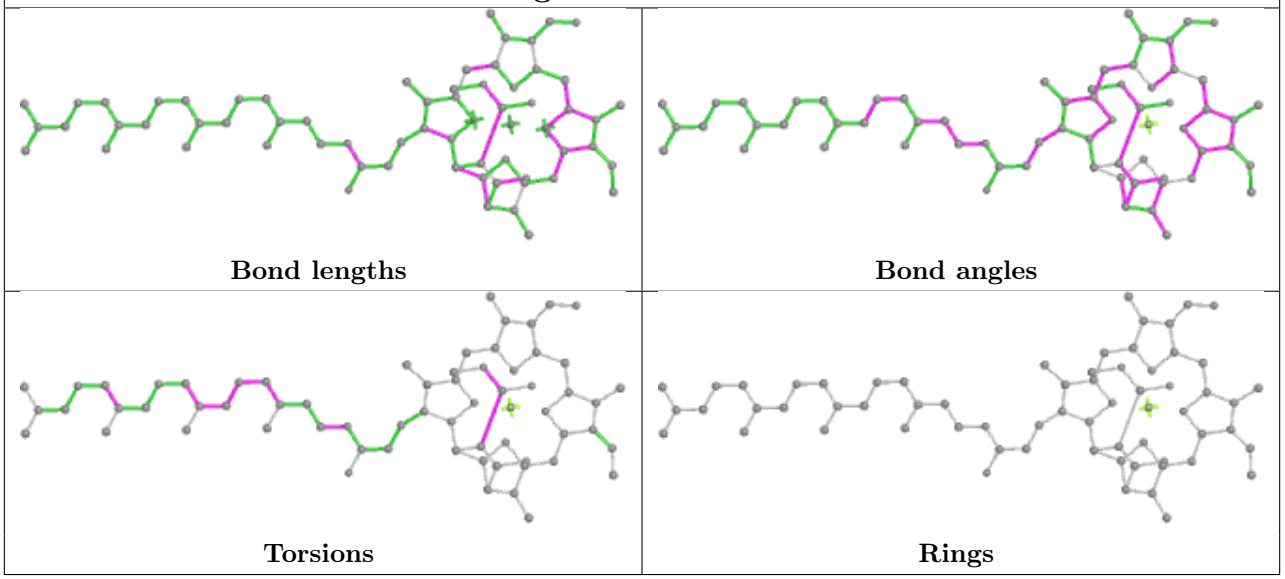


Torsions

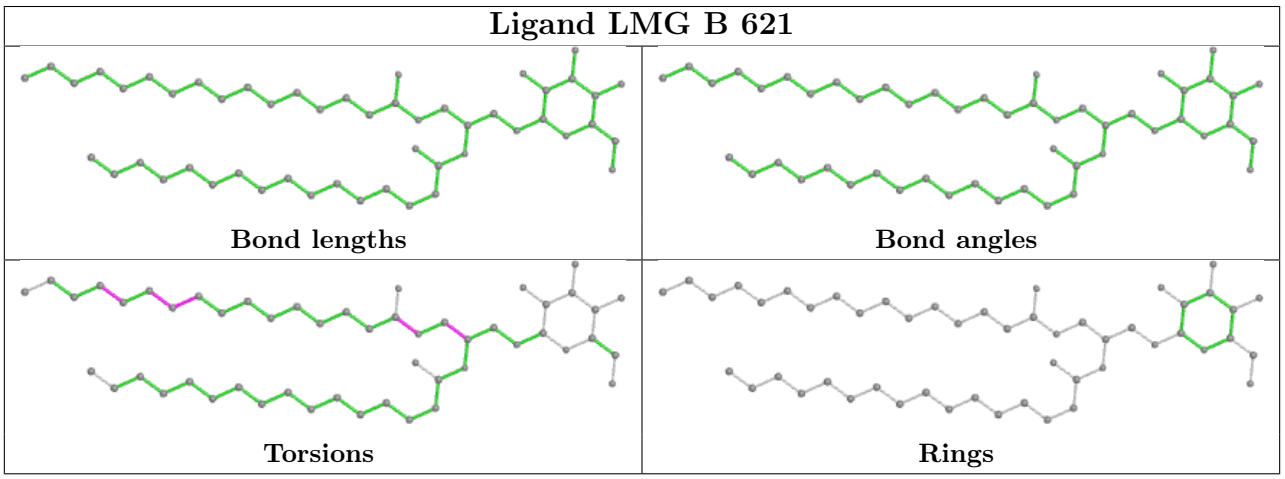


Rings

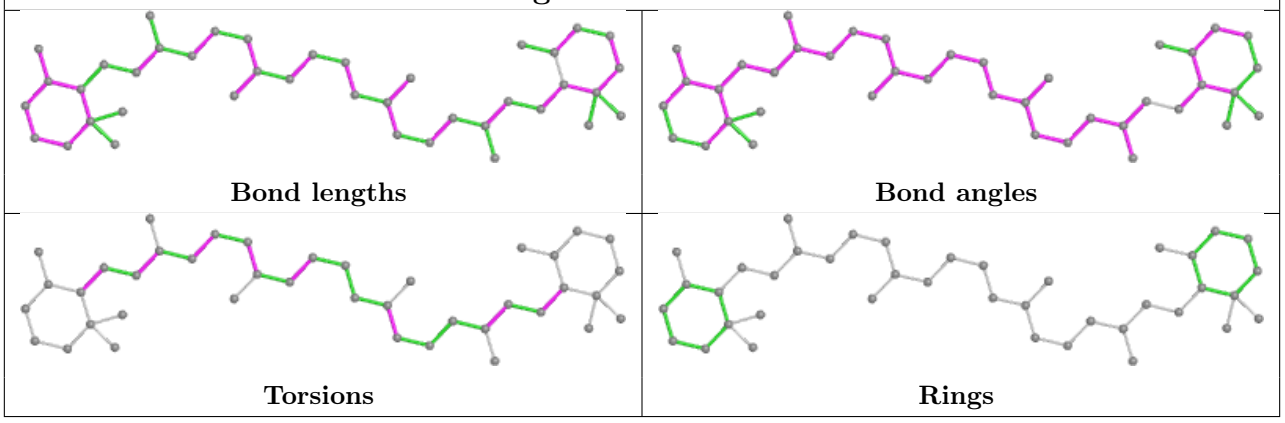
Ligand CL7 3 508



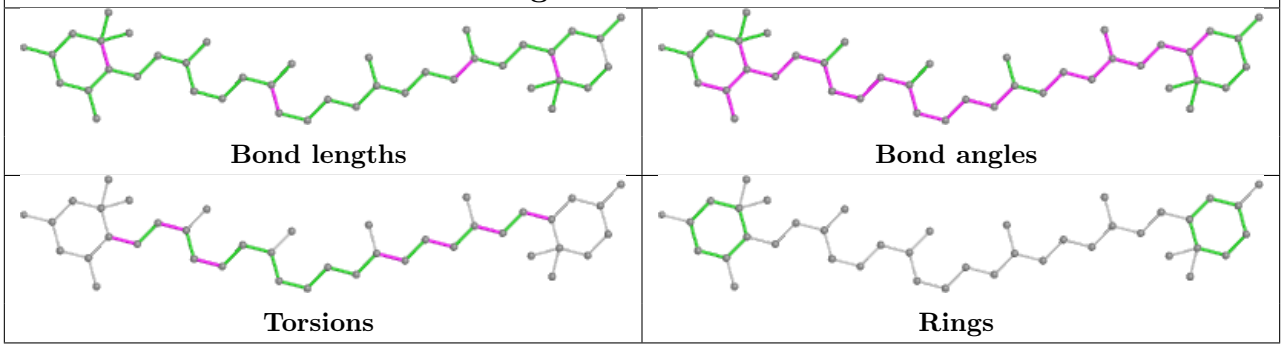
Ligand LMG B 621



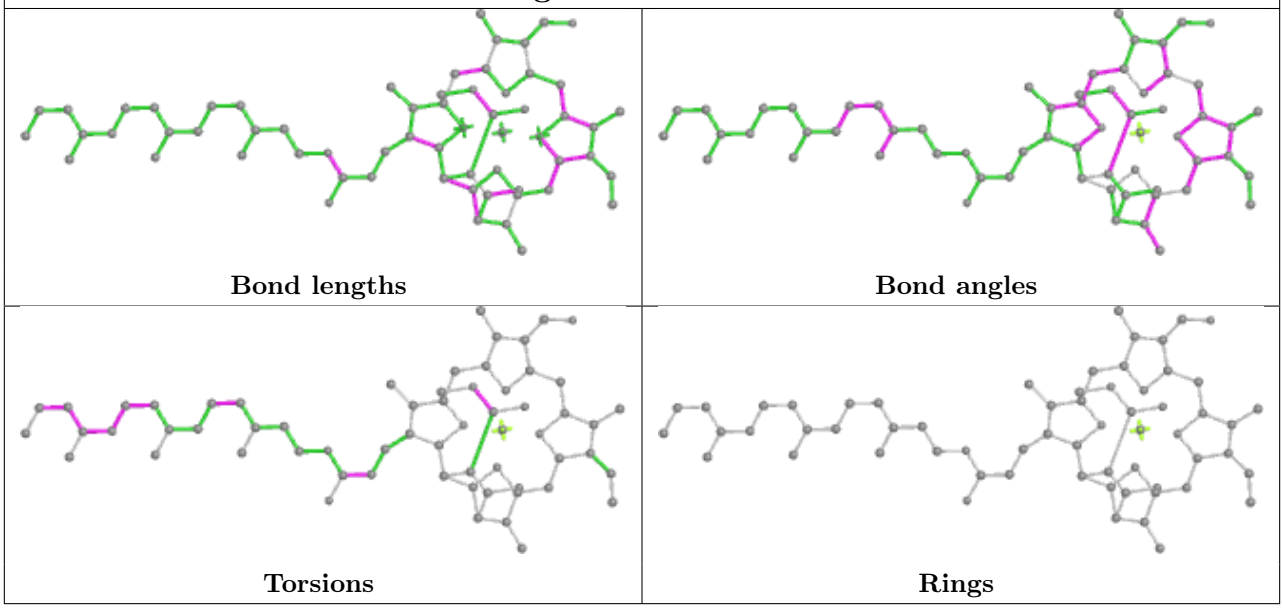
Ligand 8CT c 515



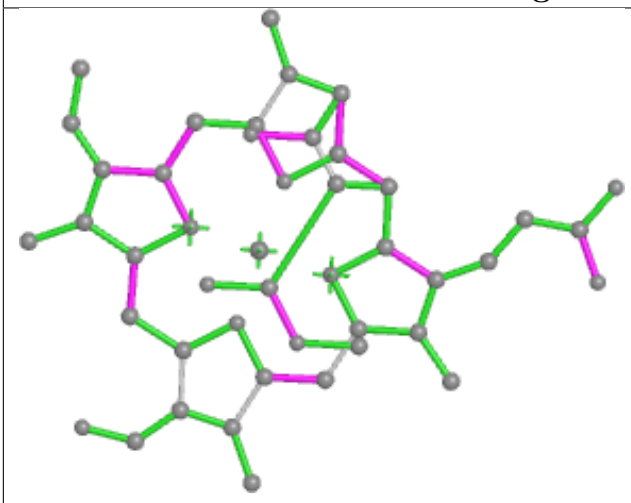
Ligand ZEX 6 524



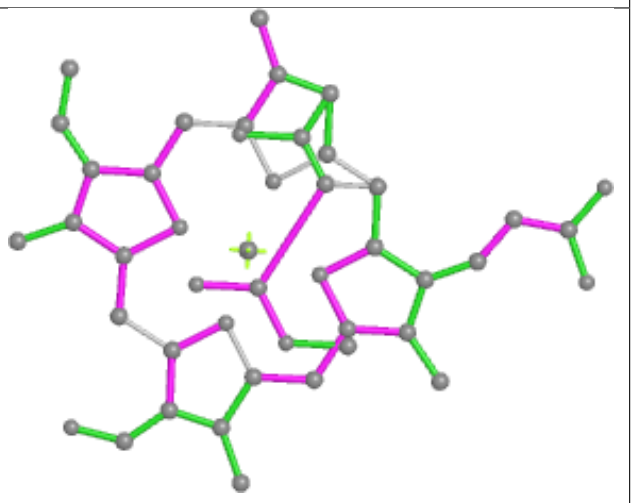
Ligand CL7 1 406



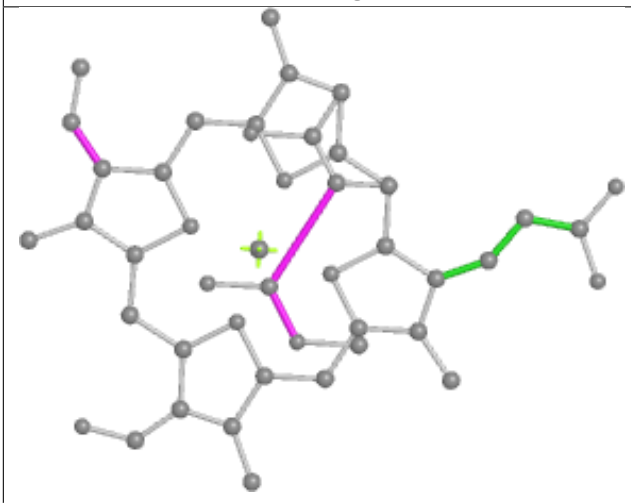
Ligand CL7 5 420



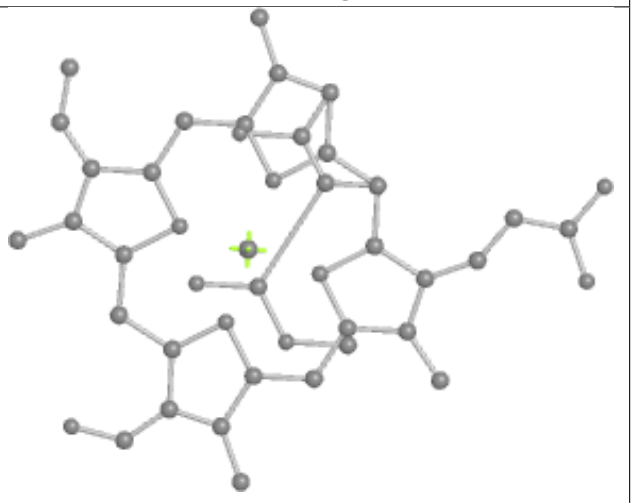
Bond lengths



Bond angles

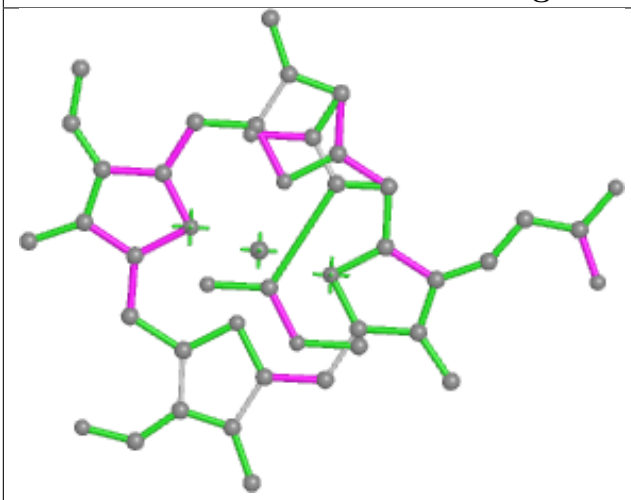


Torsions

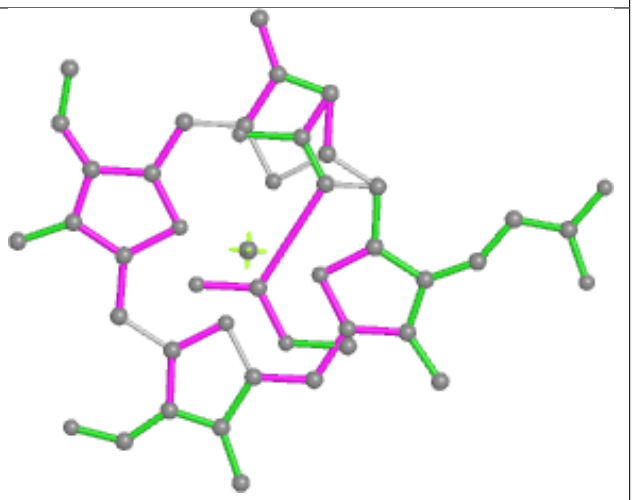


Rings

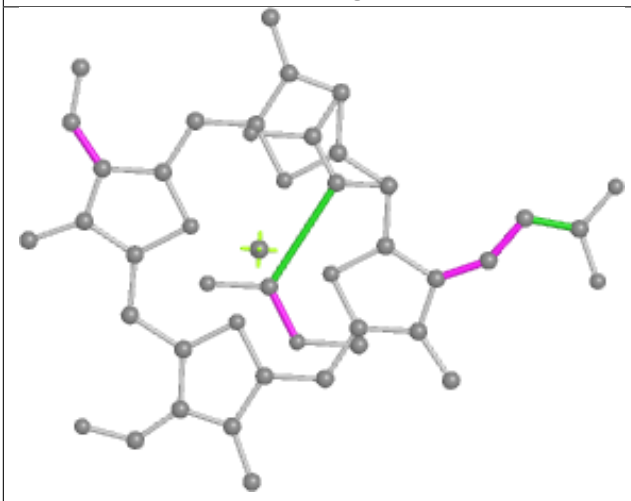
Ligand CL7 3 514



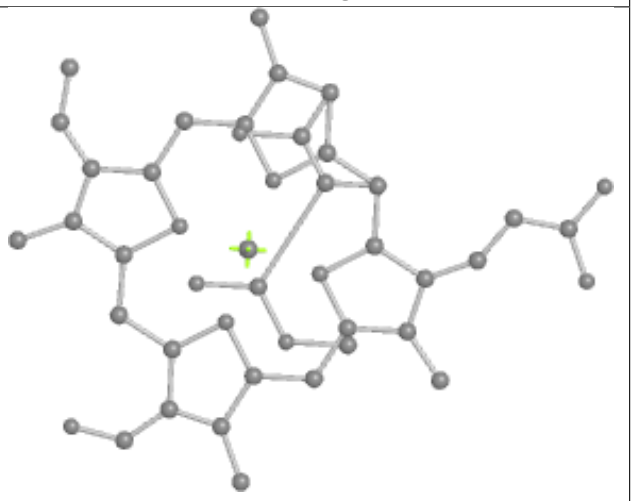
Bond lengths



Bond angles

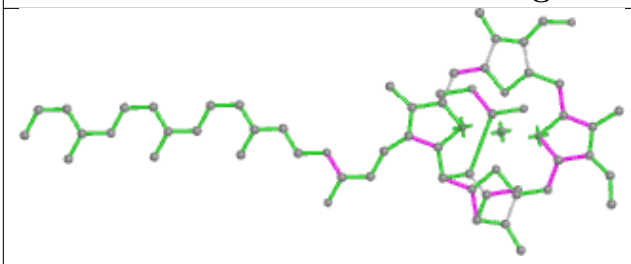


Torsions

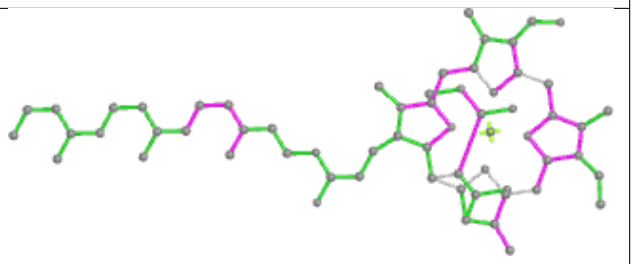


Rings

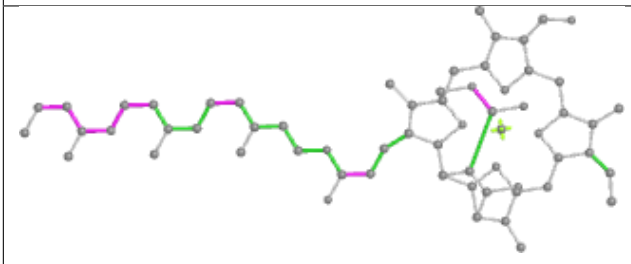
Ligand CL7 5 406



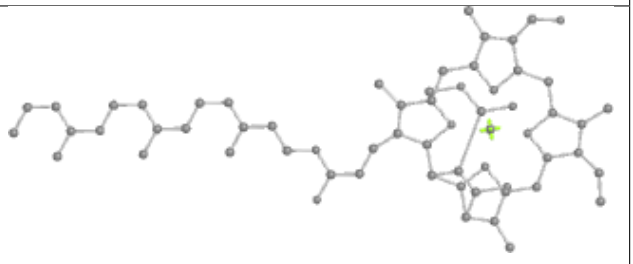
Bond lengths



Bond angles

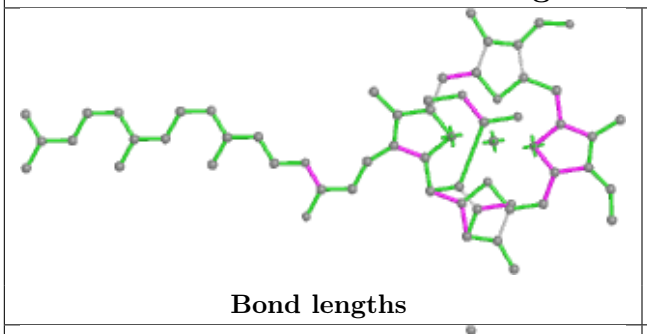


Torsions

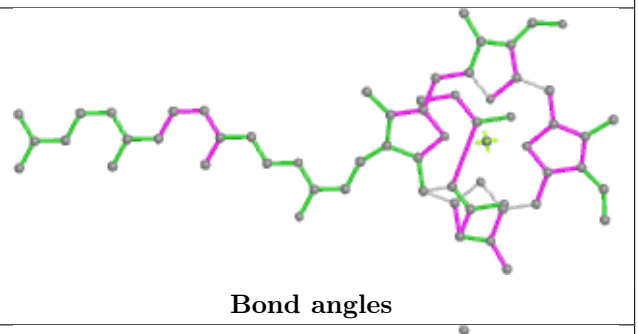


Rings

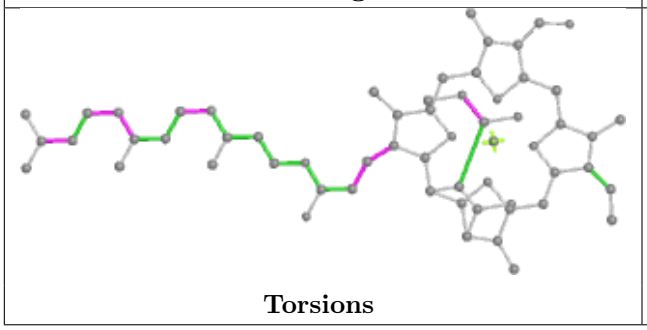
Ligand CL7 b 608



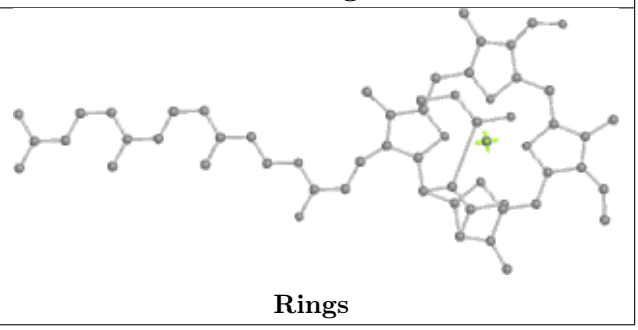
Bond lengths



Bond angles

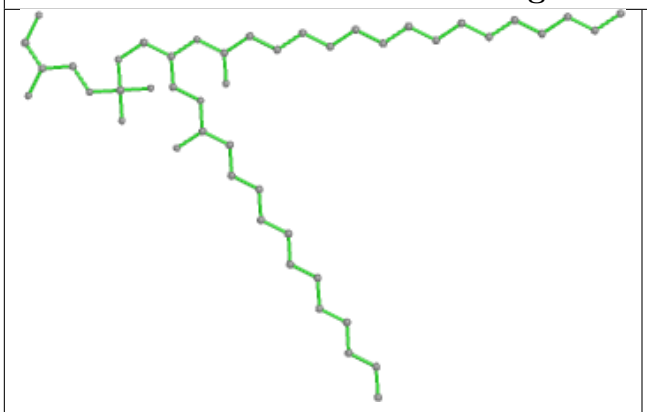


Torsions

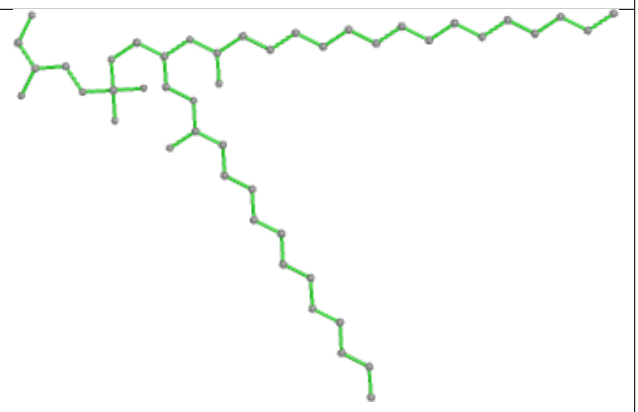


Rings

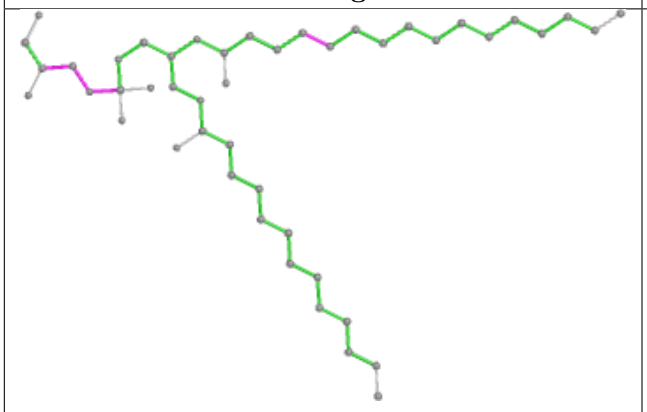
Ligand LHG a 406



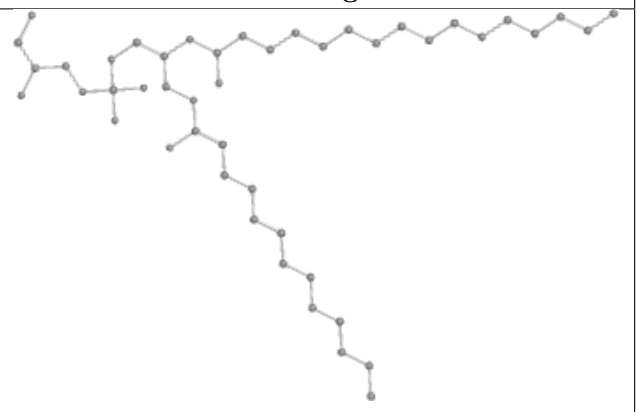
Bond lengths



Bond angles

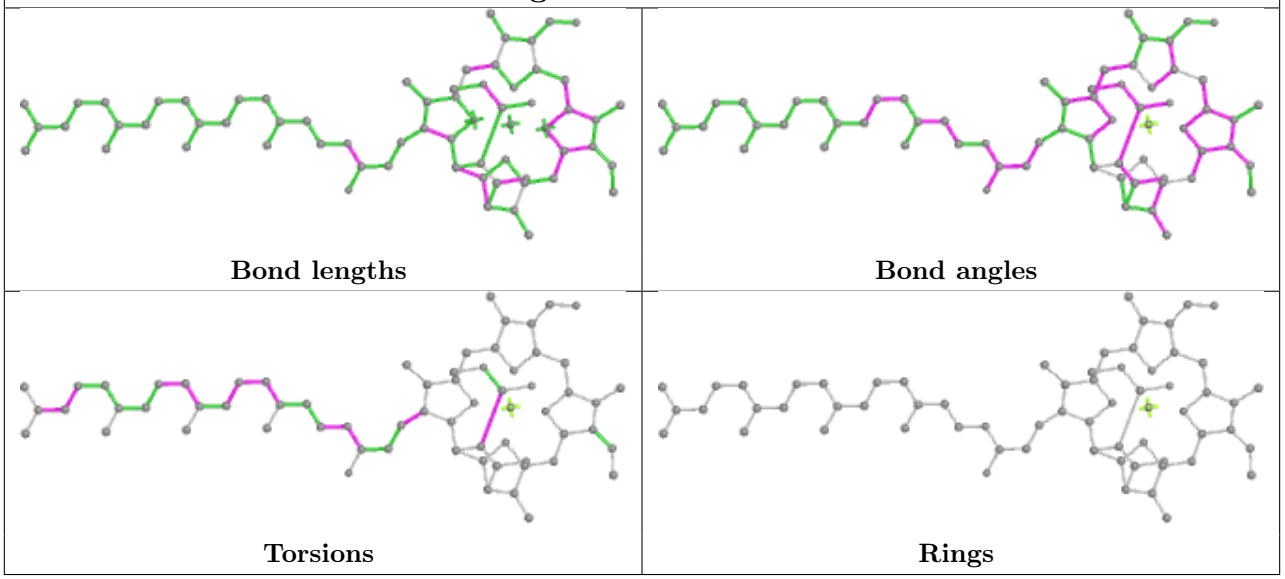


Torsions

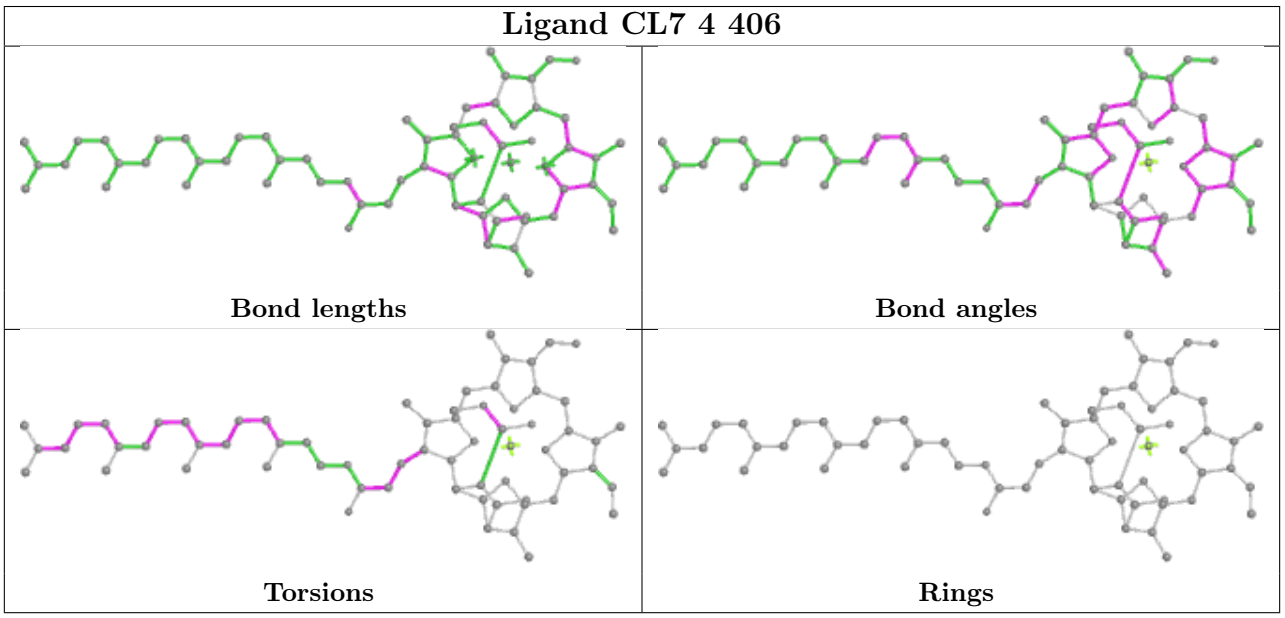


Rings

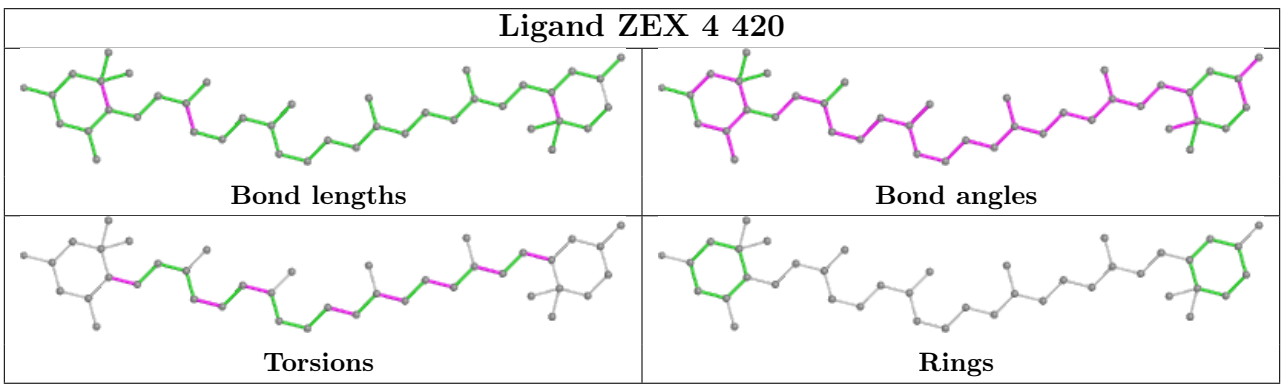
Ligand CL7 C 509



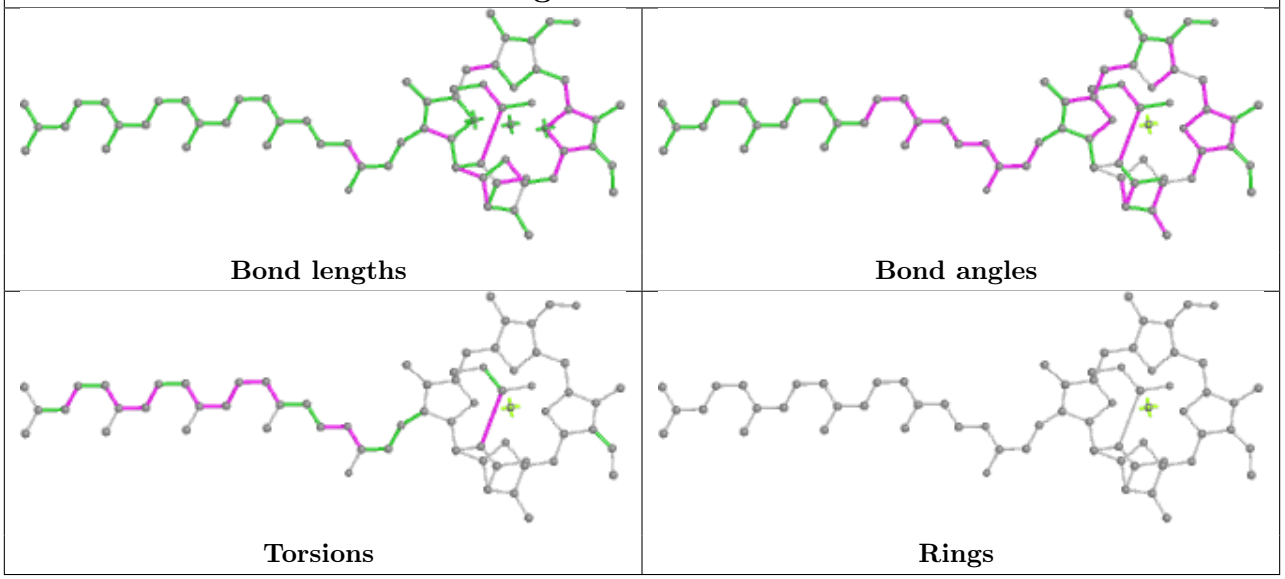
Ligand CL7 4 406



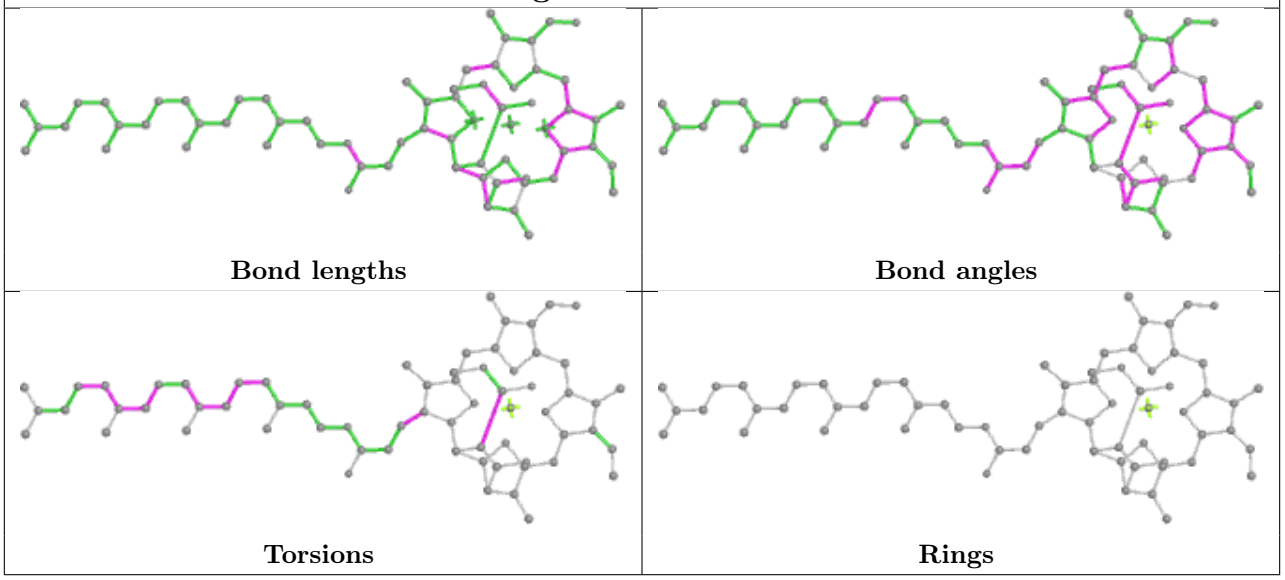
Ligand ZEX 4 420



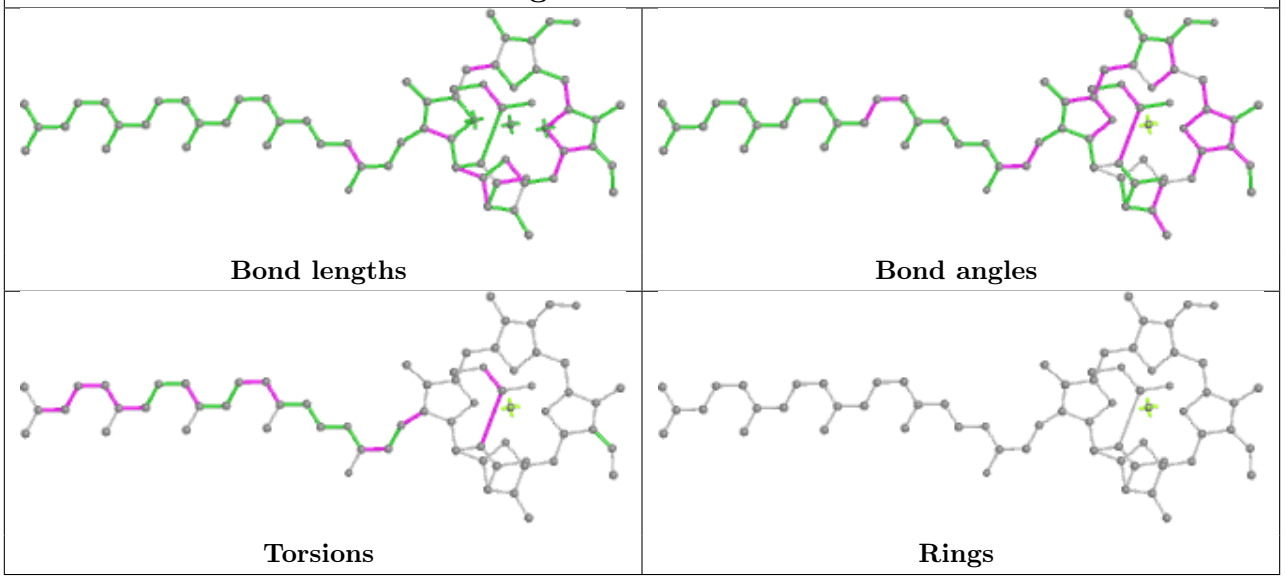
Ligand CL7 7 511



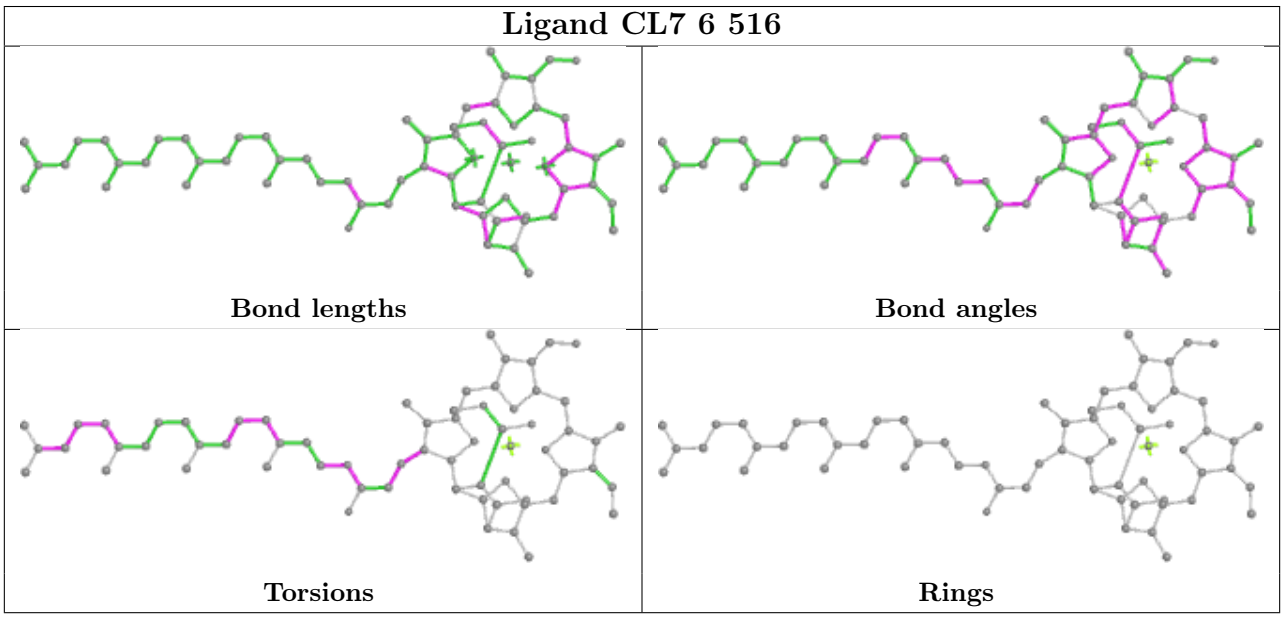
Ligand CL7 b 613



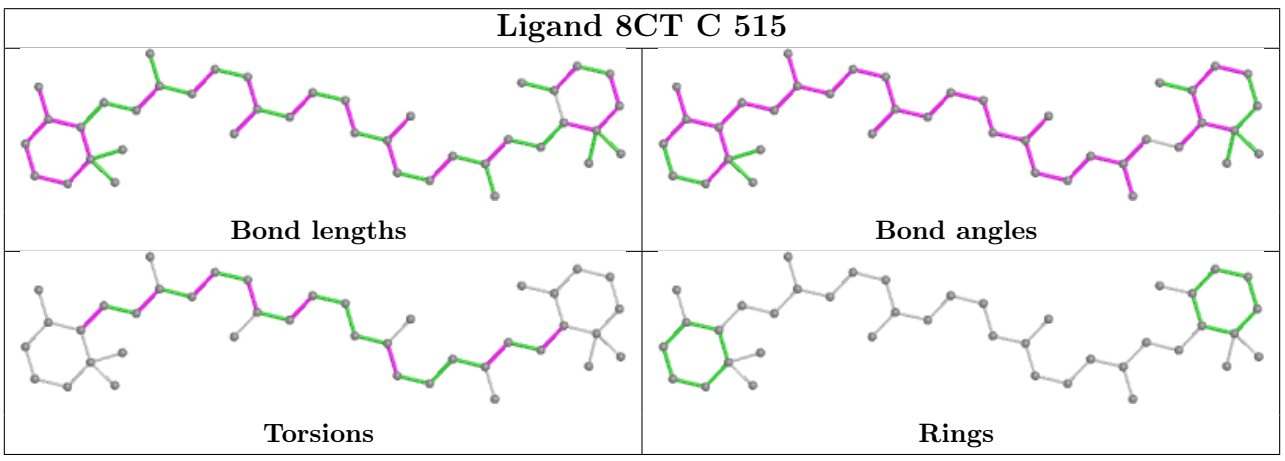
Ligand CL7 C 502



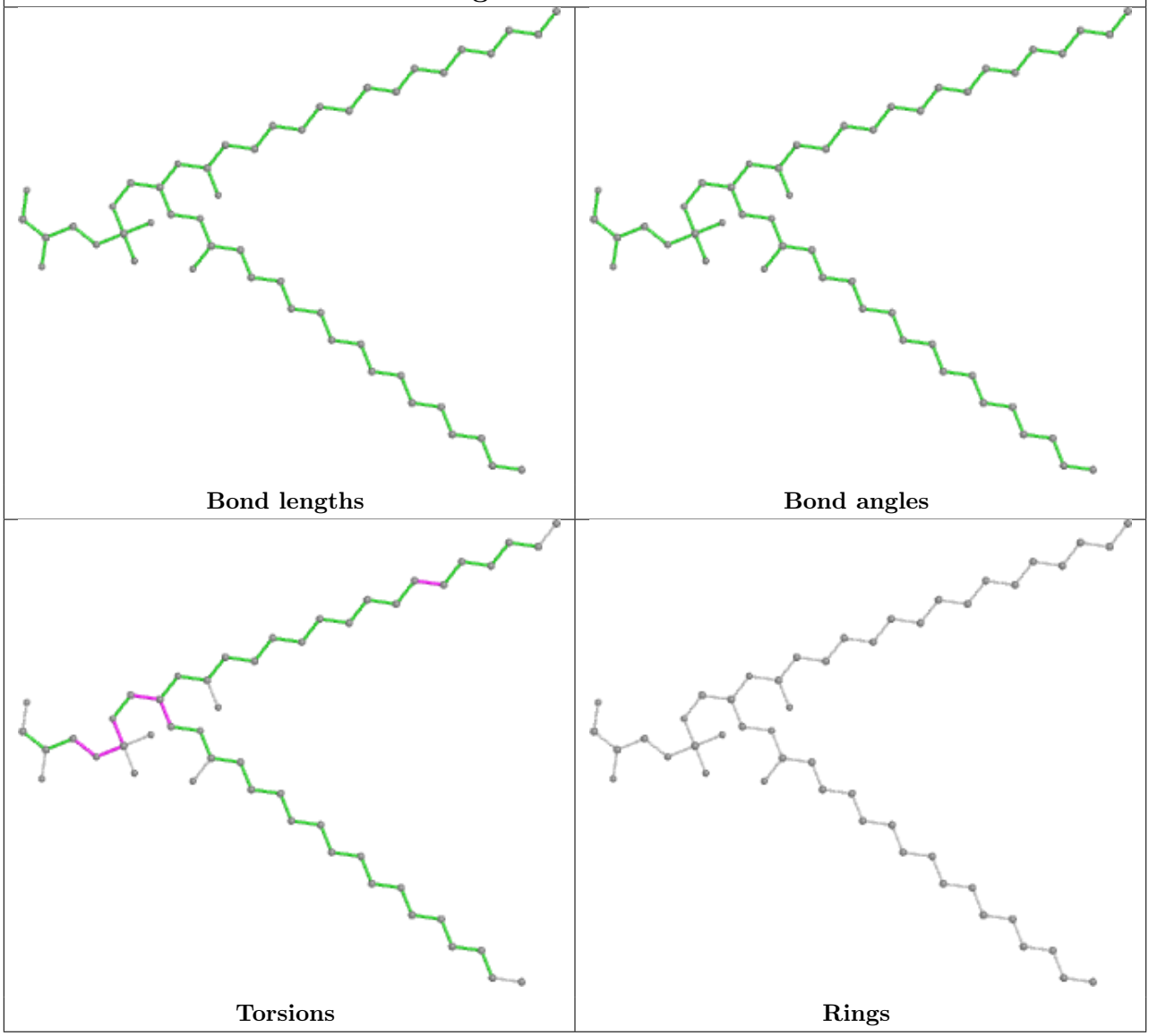
Ligand CL7 6 516



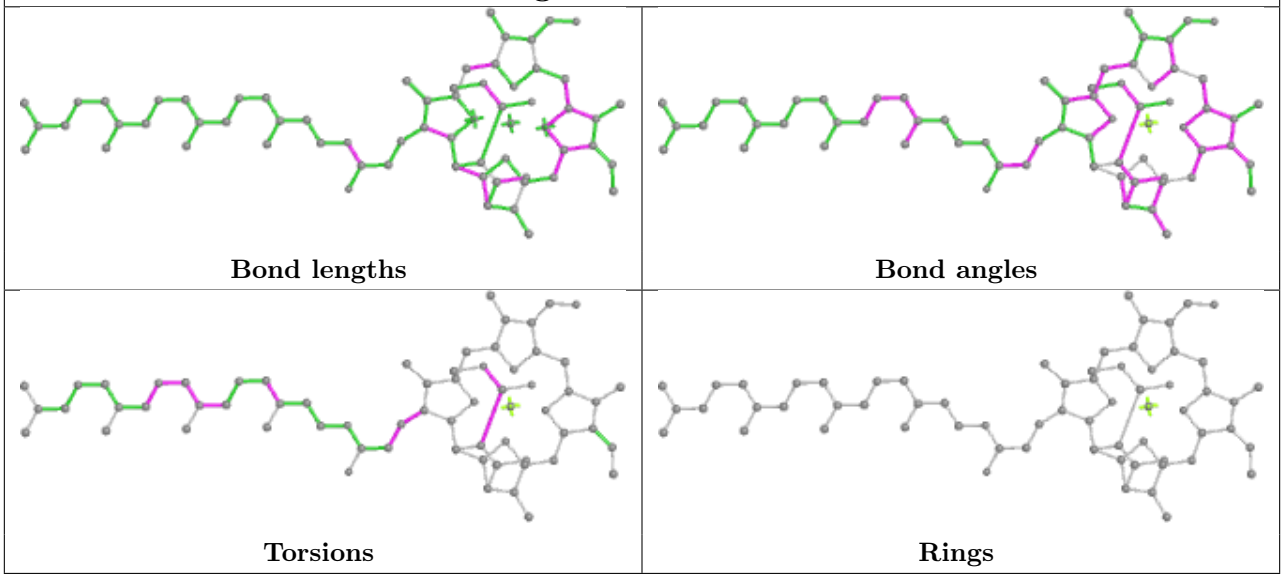
Ligand 8CT C 515



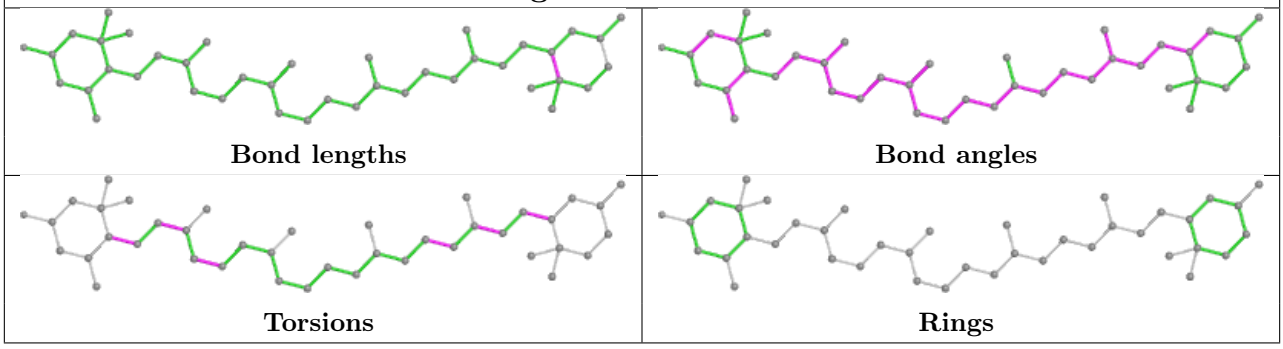
Ligand LHG 4 401



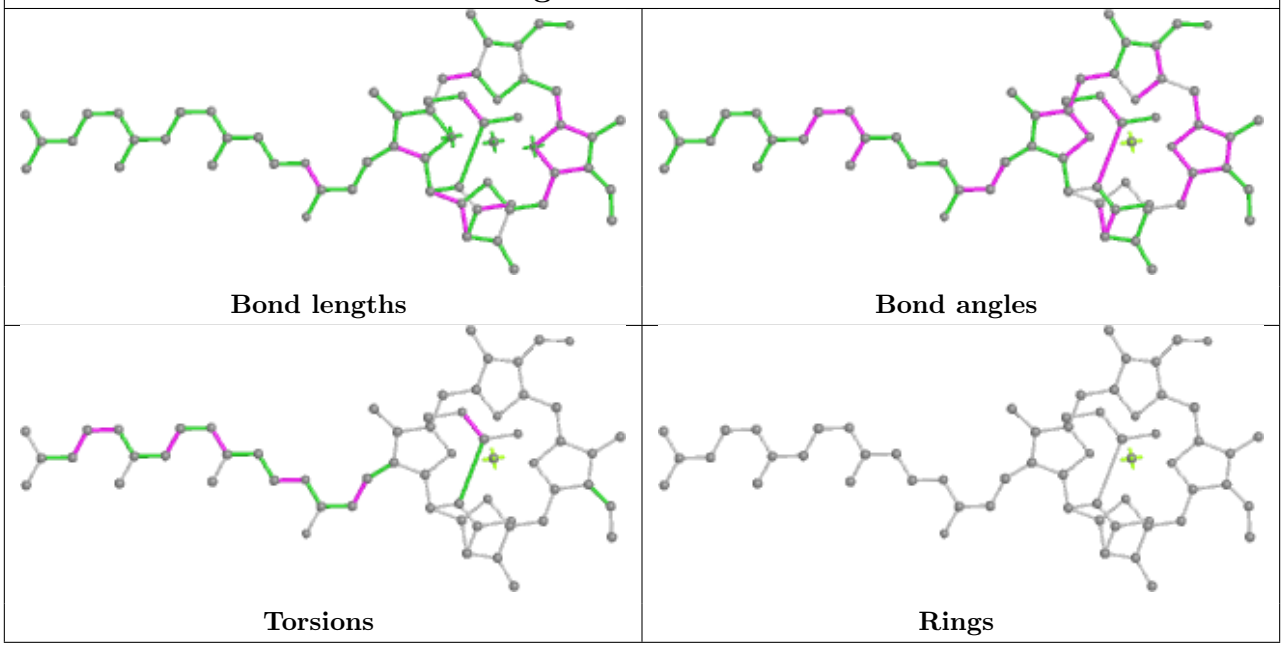
Ligand CL7 2 502



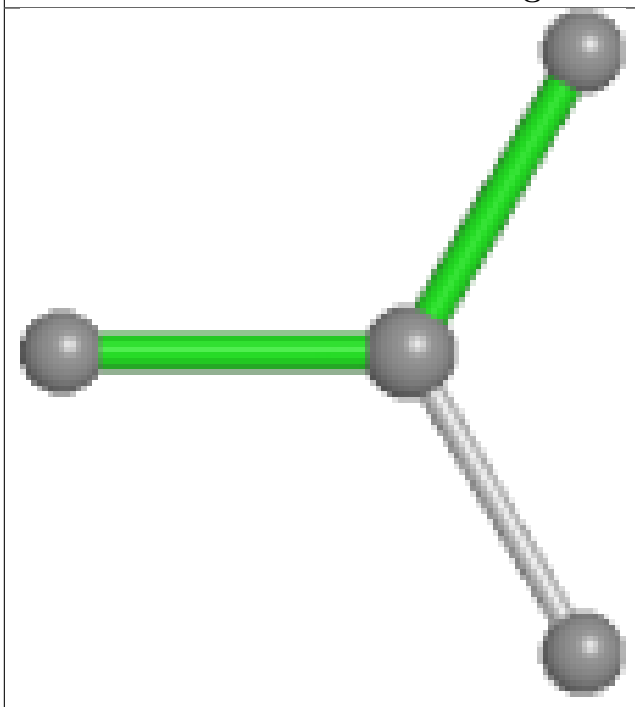
Ligand ZEX 4 418



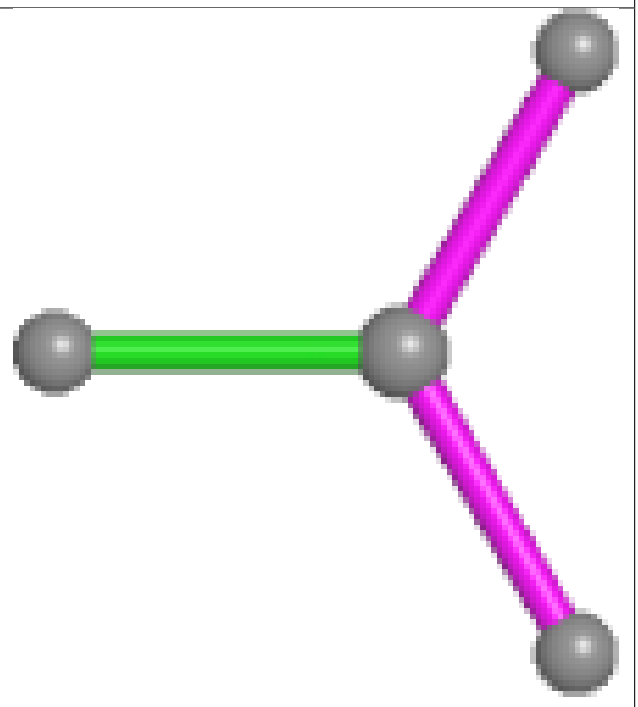
Ligand CL7 5 403



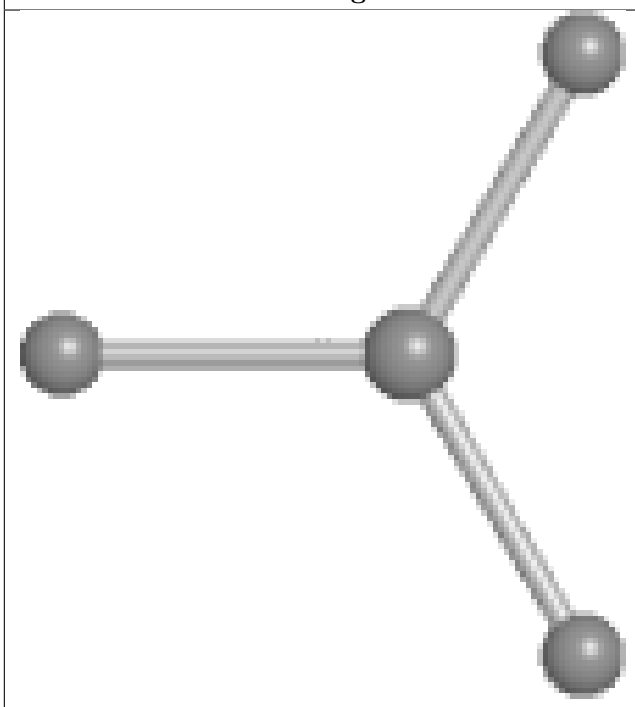
Ligand BCT D 403



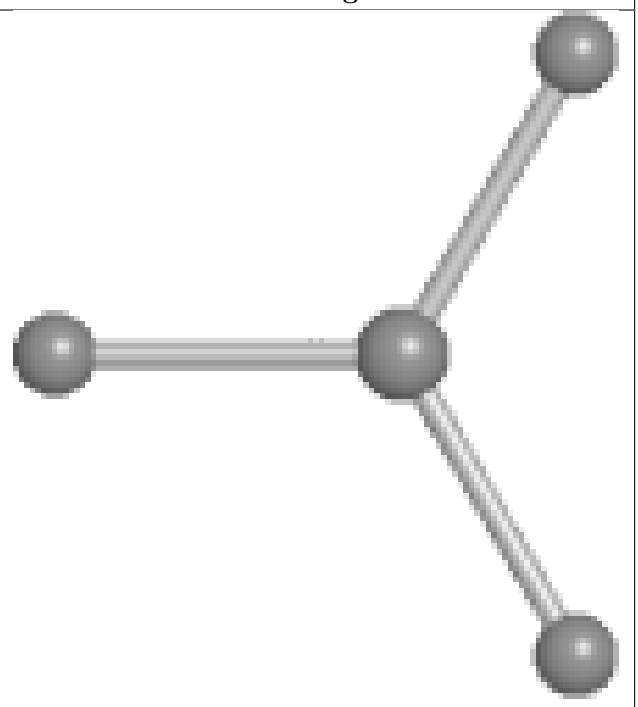
Bond lengths



Bond angles

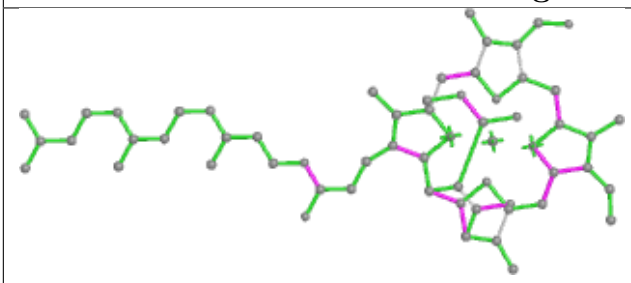


Torsions

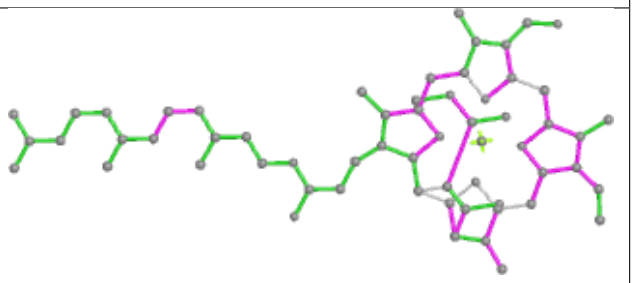


Rings

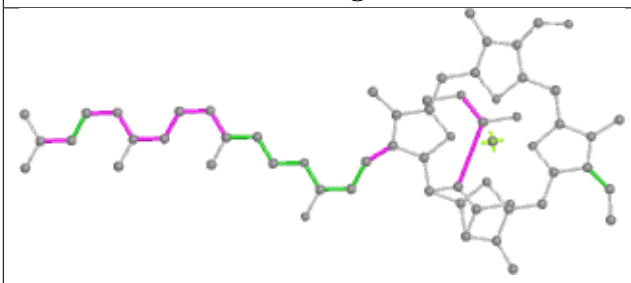
Ligand CL7 6 511



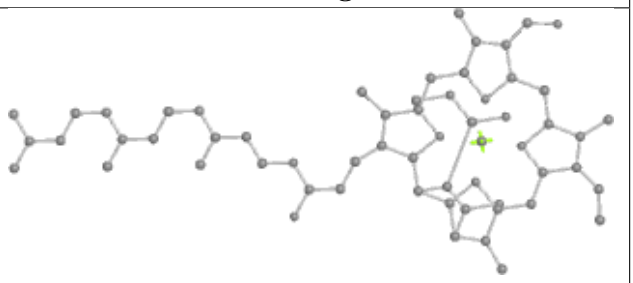
Bond lengths



Bond angles

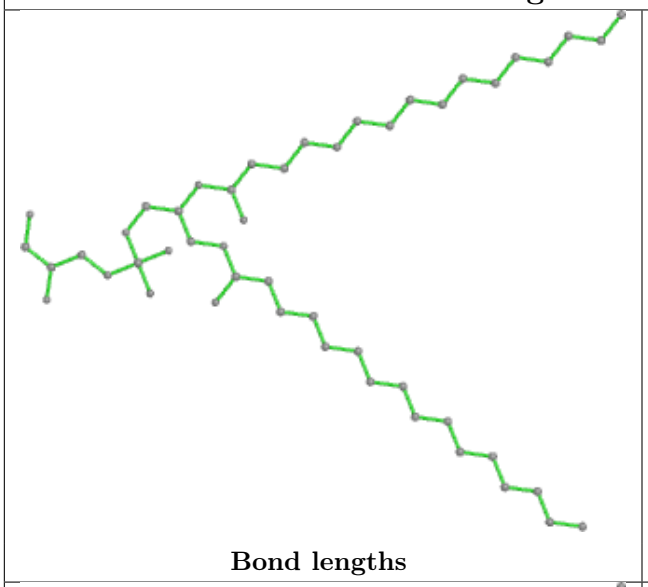


Torsions

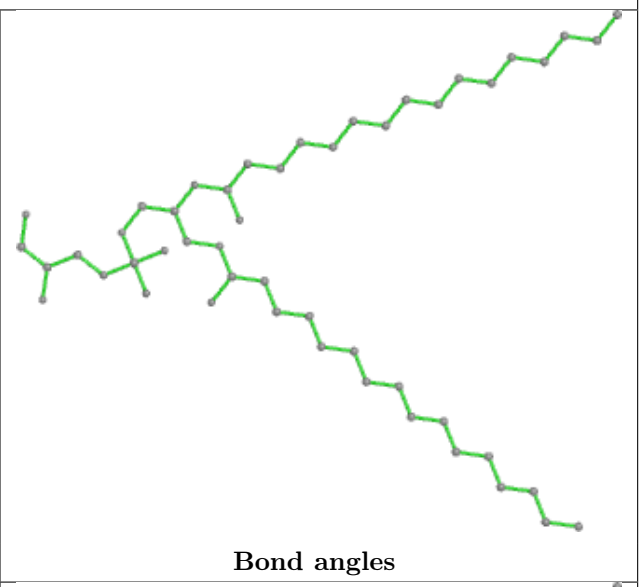


Rings

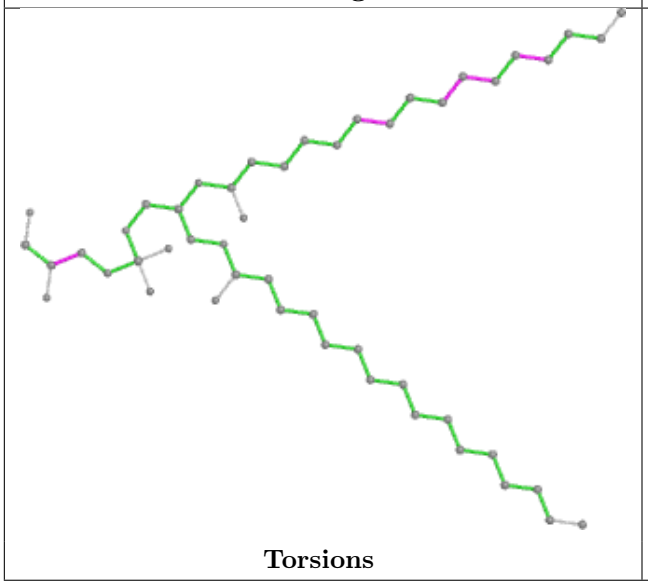
Ligand LHG b 626



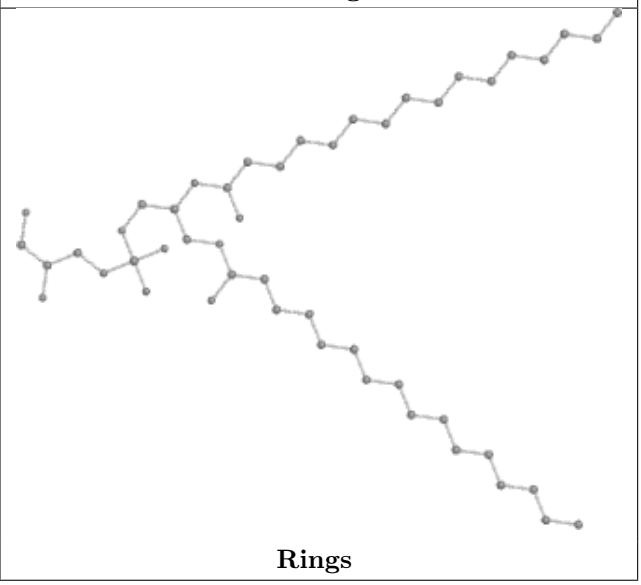
Bond lengths



Bond angles

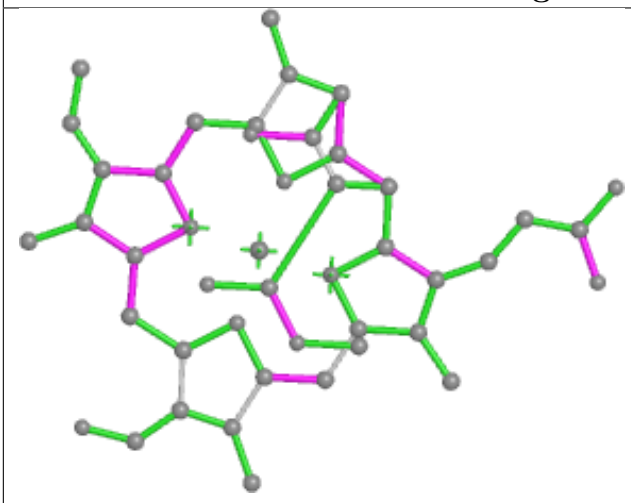


Torsions

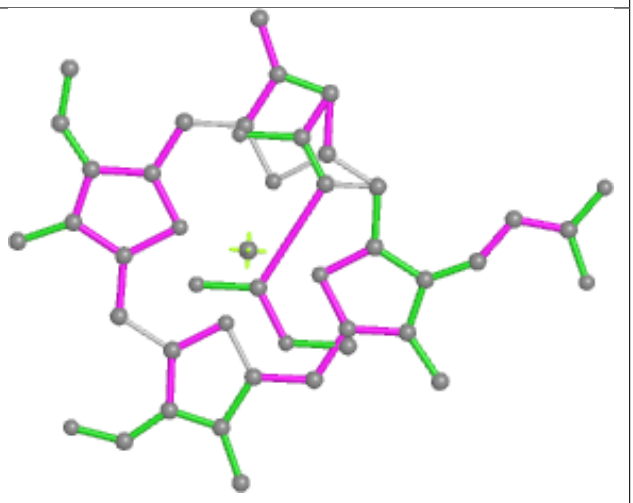


Rings

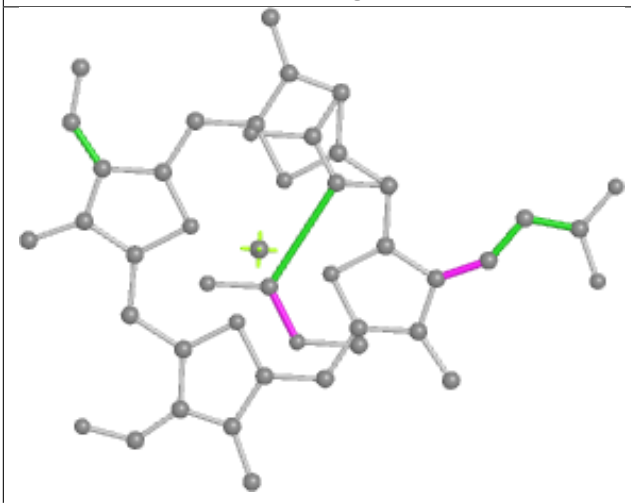
Ligand CL7 6 504



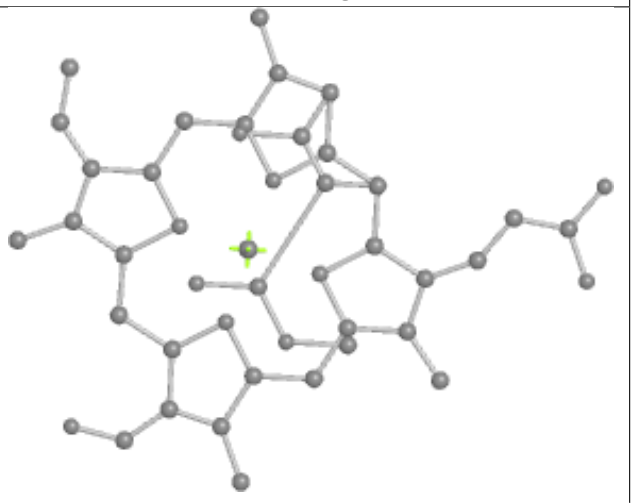
Bond lengths



Bond angles

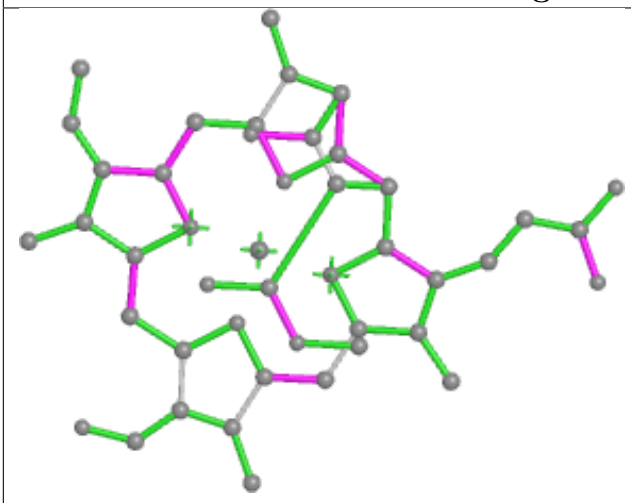


Torsions

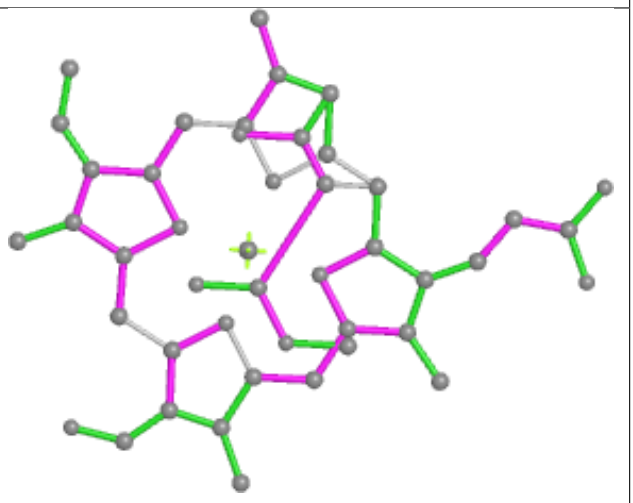


Rings

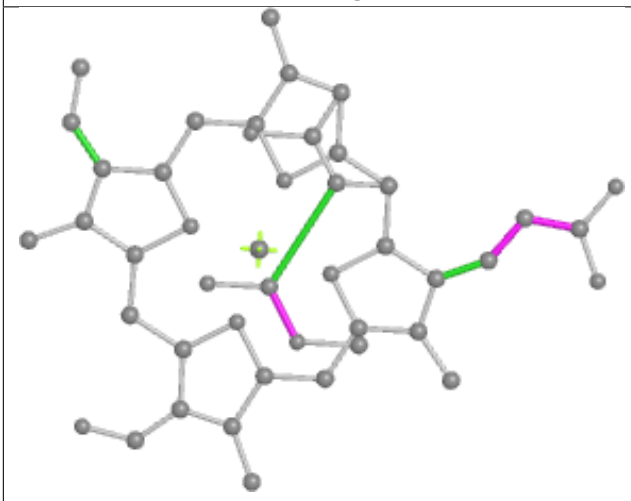
Ligand CL7 3 518



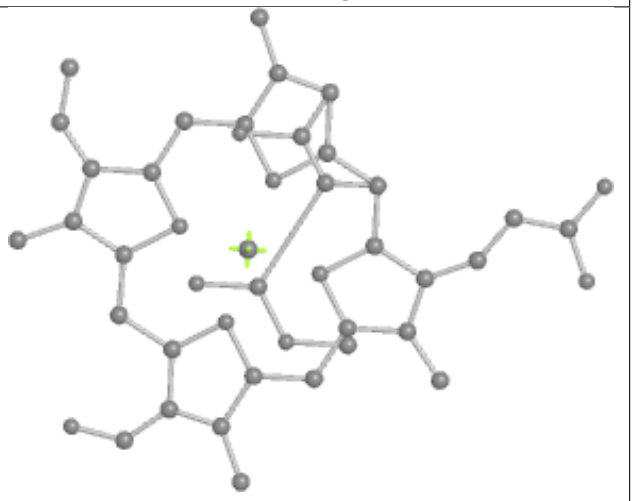
Bond lengths



Bond angles

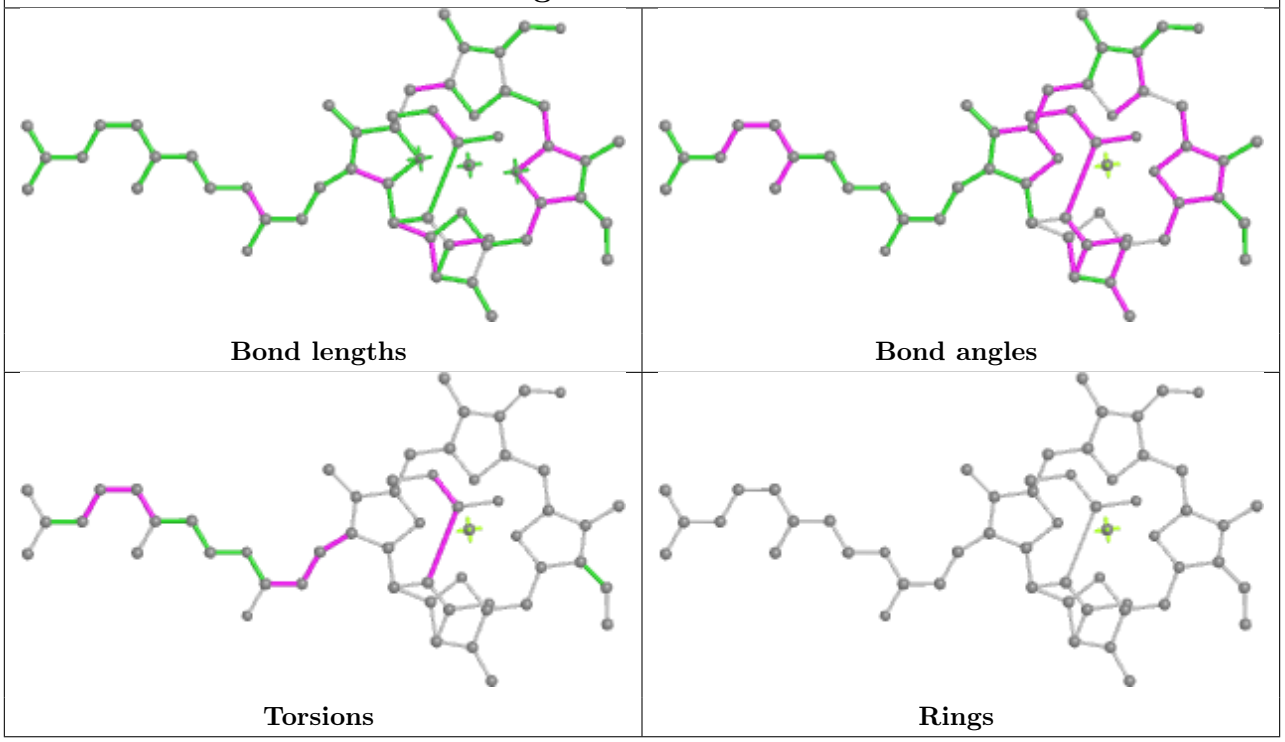


Torsions

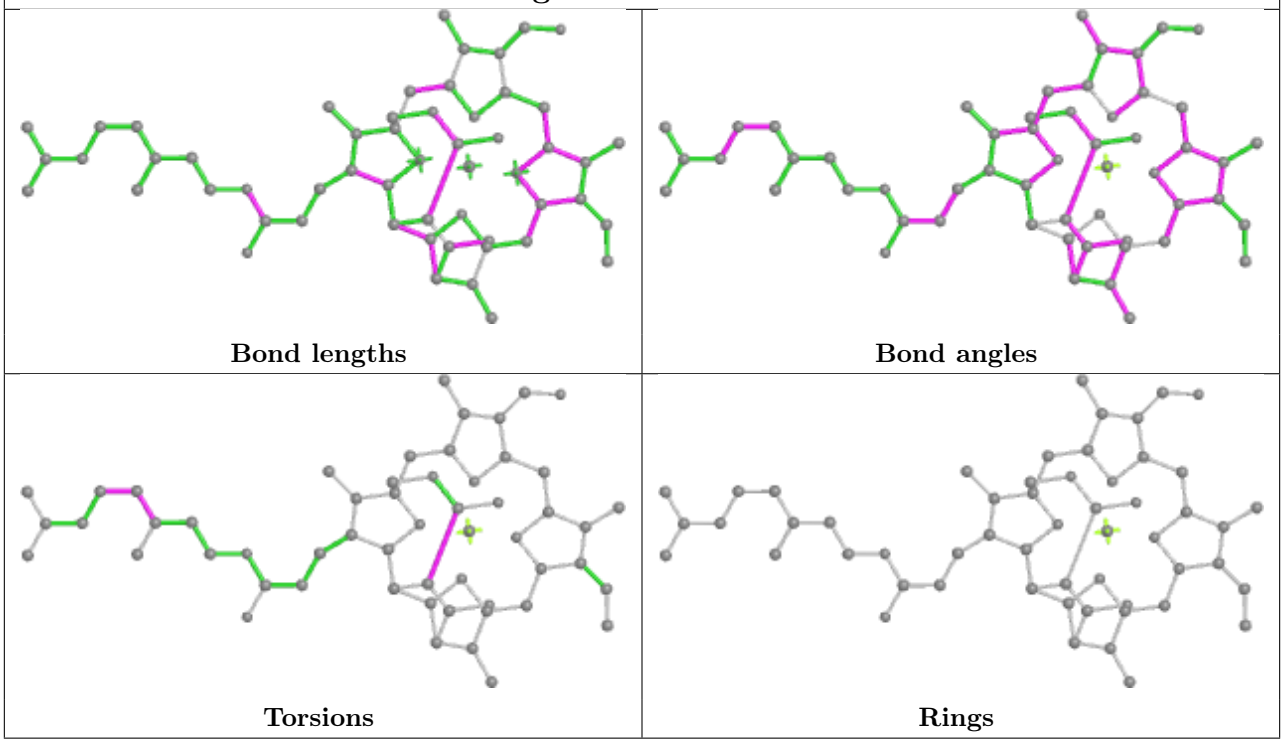


Rings

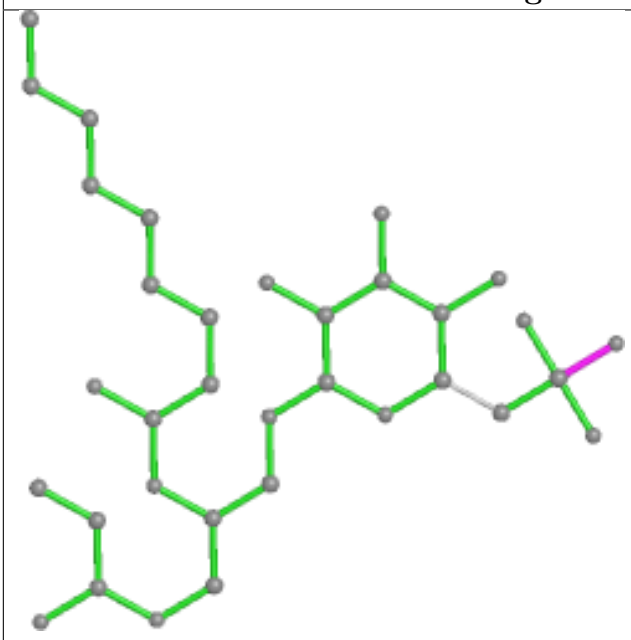
Ligand CL7 3 512



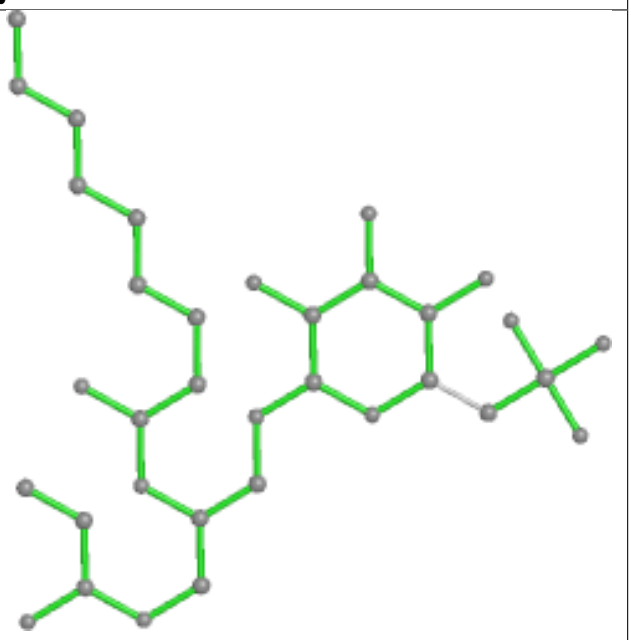
Ligand CL7 b 614



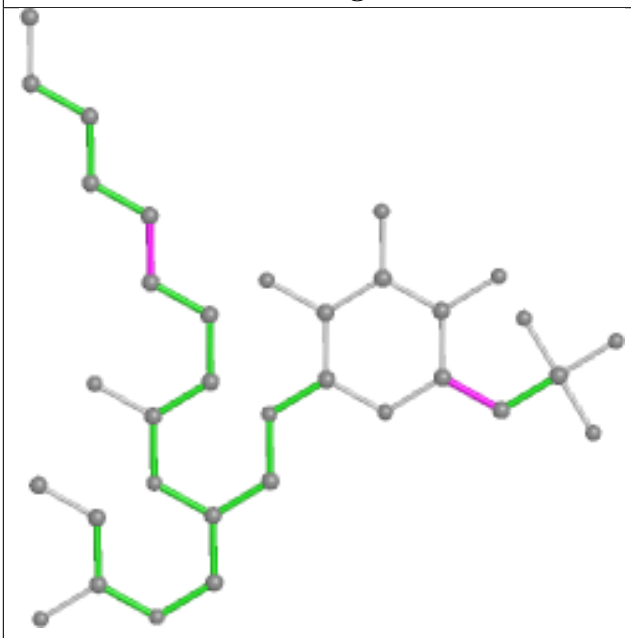
Ligand SQD B 626



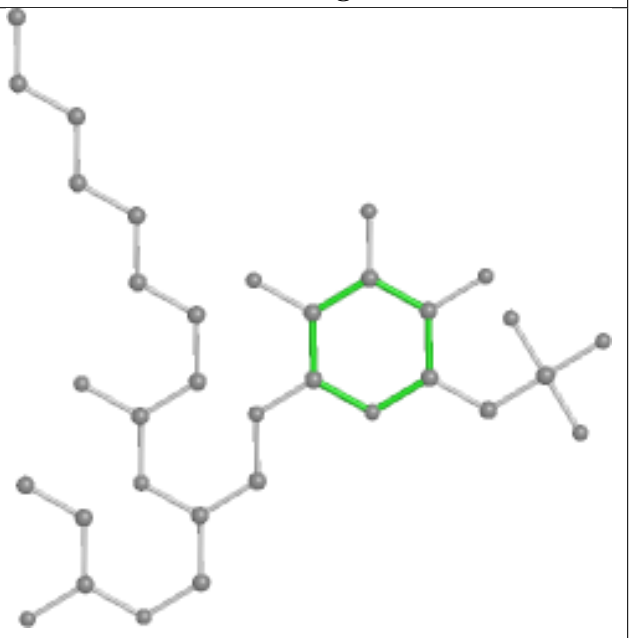
Bond lengths



Bond angles

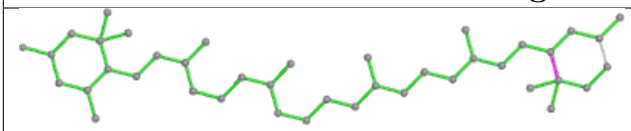


Torsions

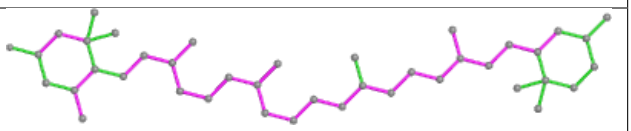


Rings

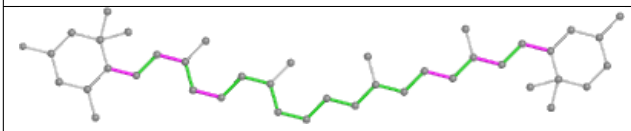
Ligand ZEX 8 418



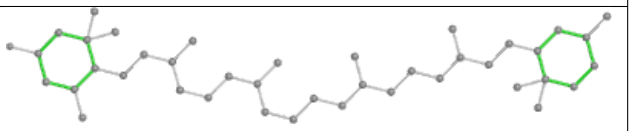
Bond lengths



Bond angles

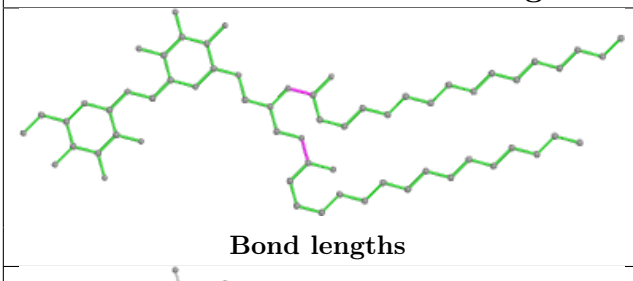


Torsions

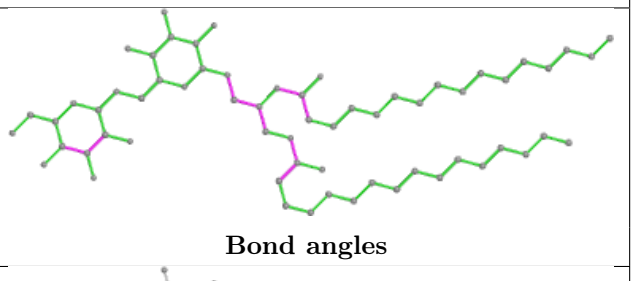


Rings

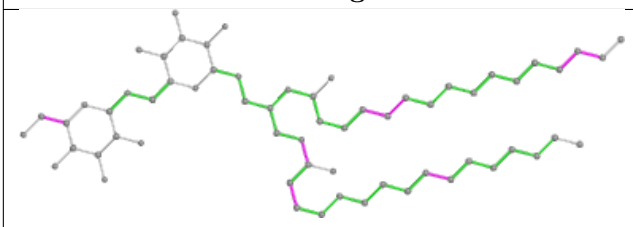
Ligand DGD c 517



Bond lengths



Bond angles



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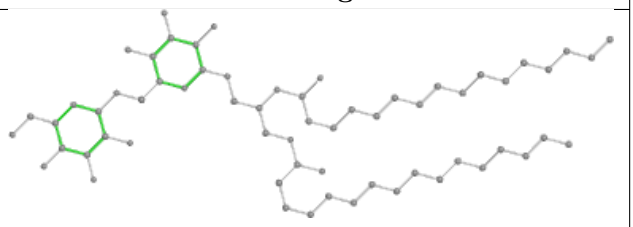
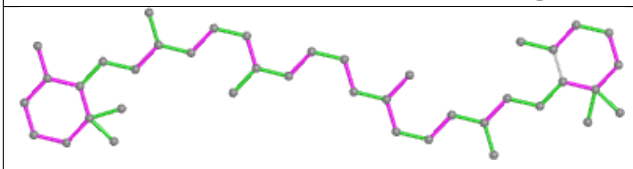
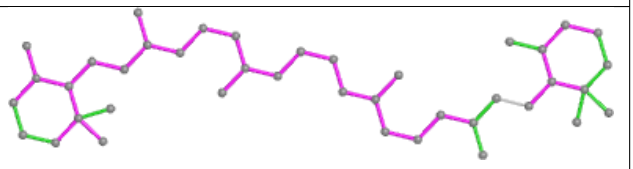


Rings

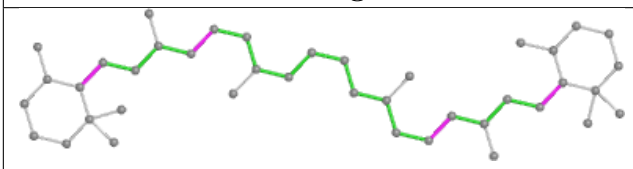
Ligand 8CT 4 402



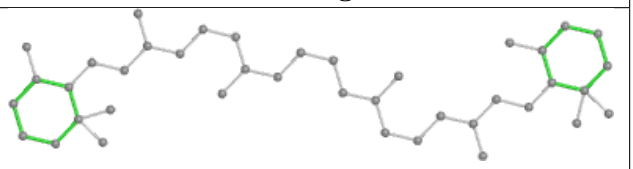
Bond lengths



Bond angles

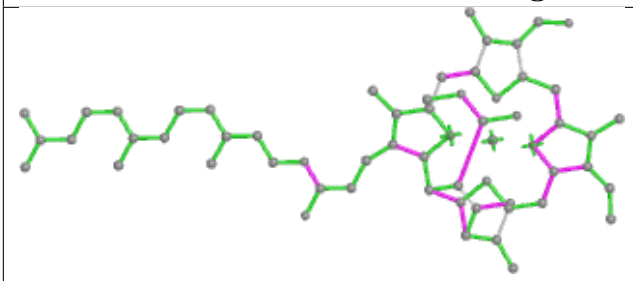


Torsions

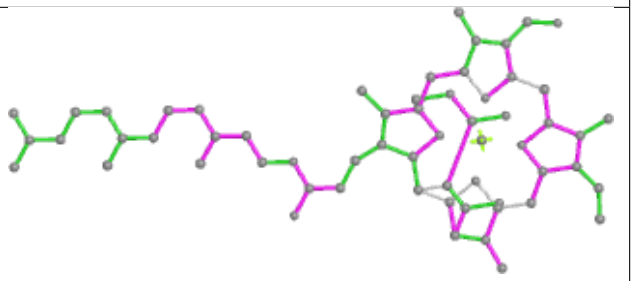


Rings

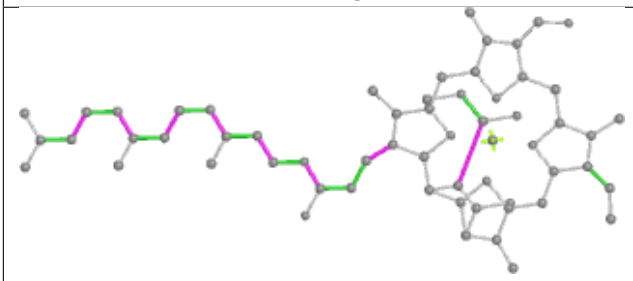
Ligand CL7 C 507



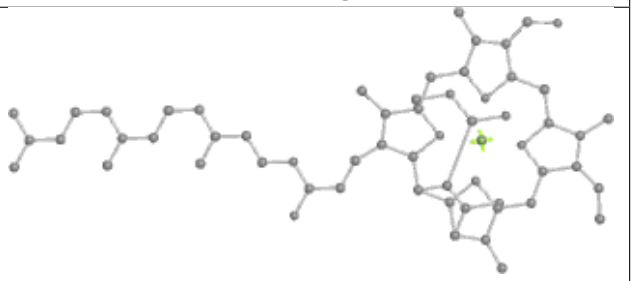
Bond lengths



Bond angles

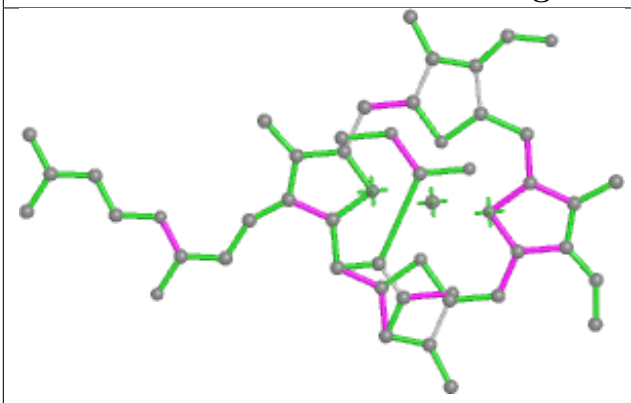


Torsions

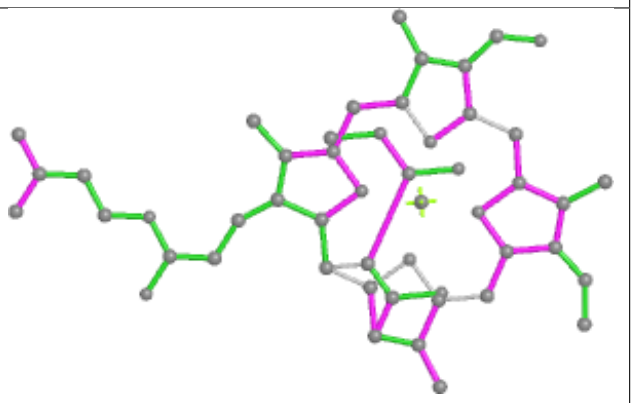


Rings

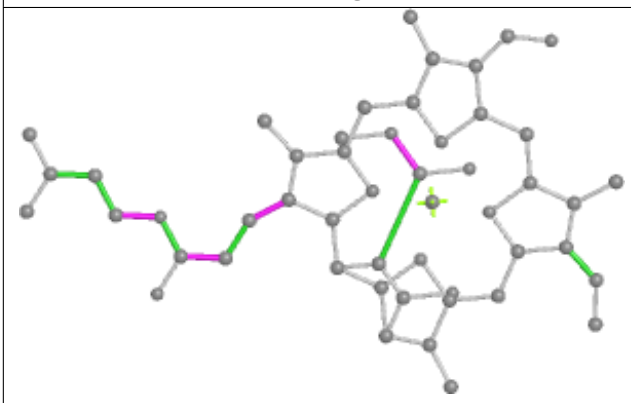
Ligand CL7 7 517



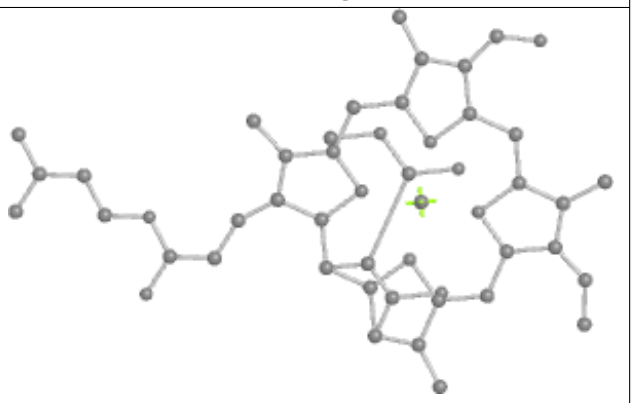
Bond lengths



Bond angles

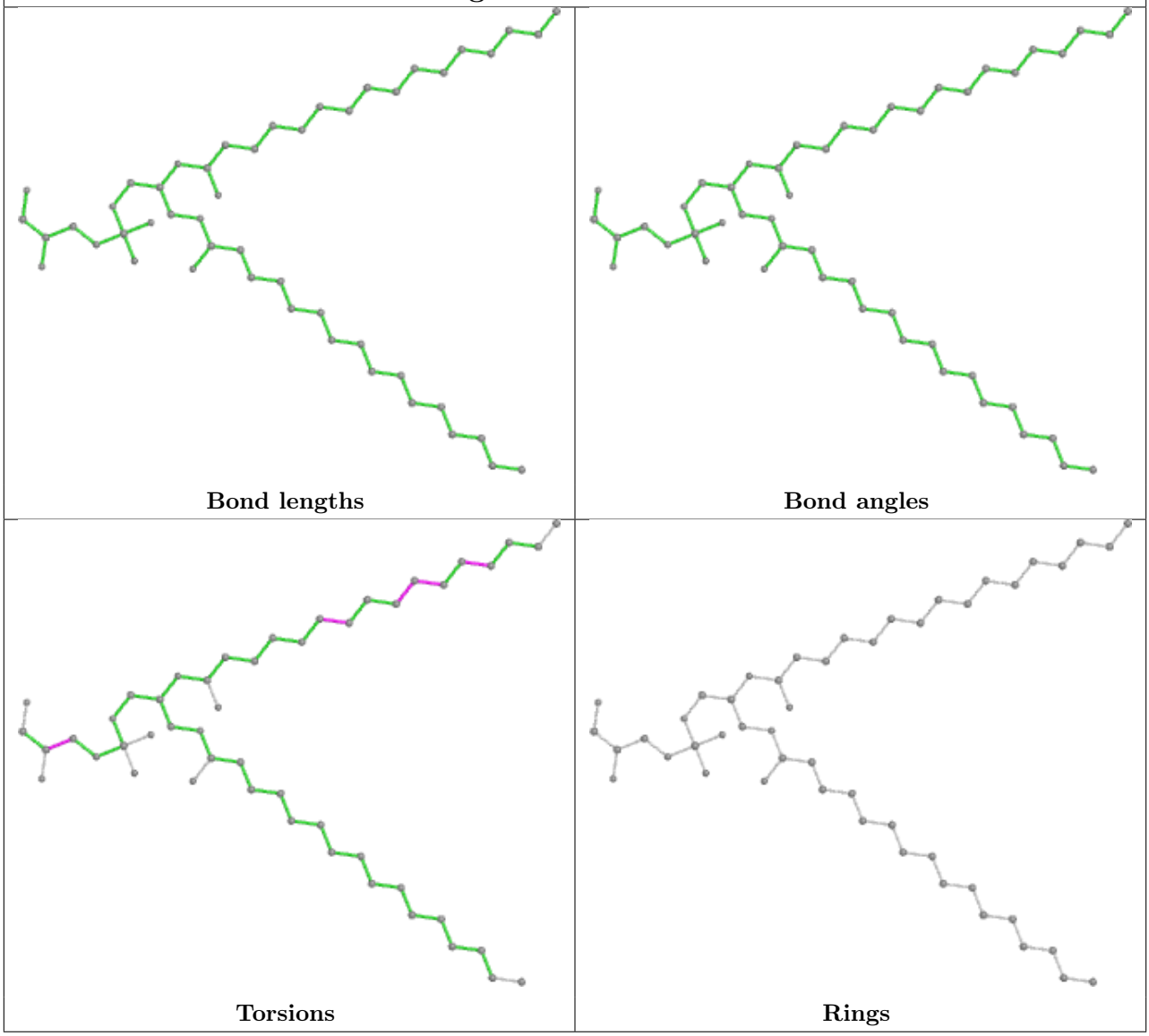


Torsions

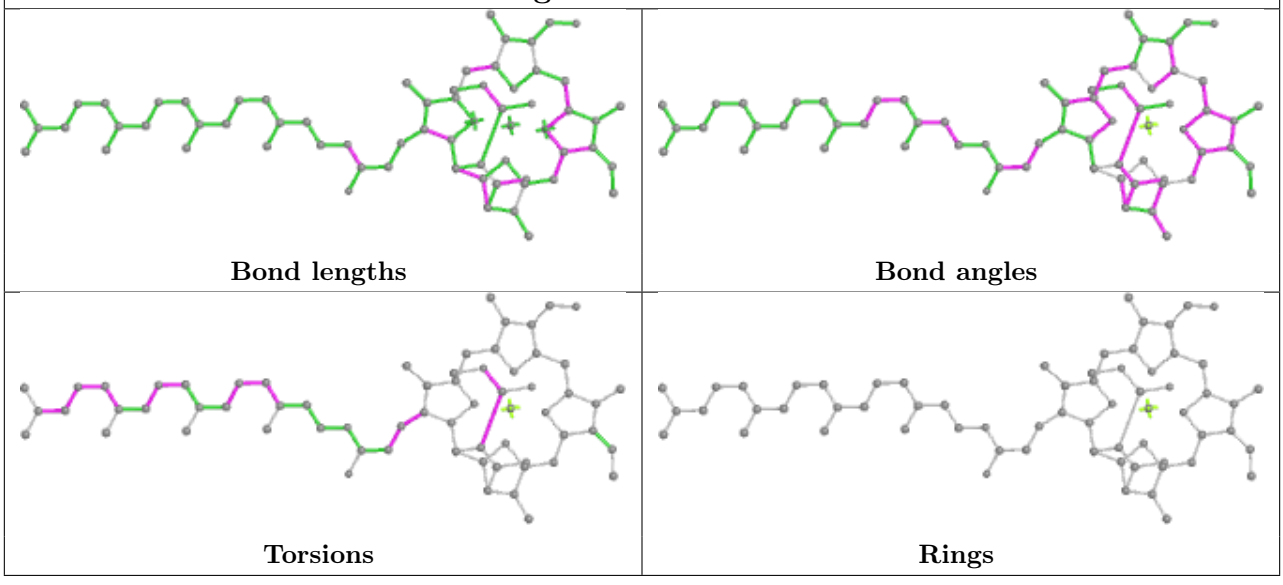


Rings

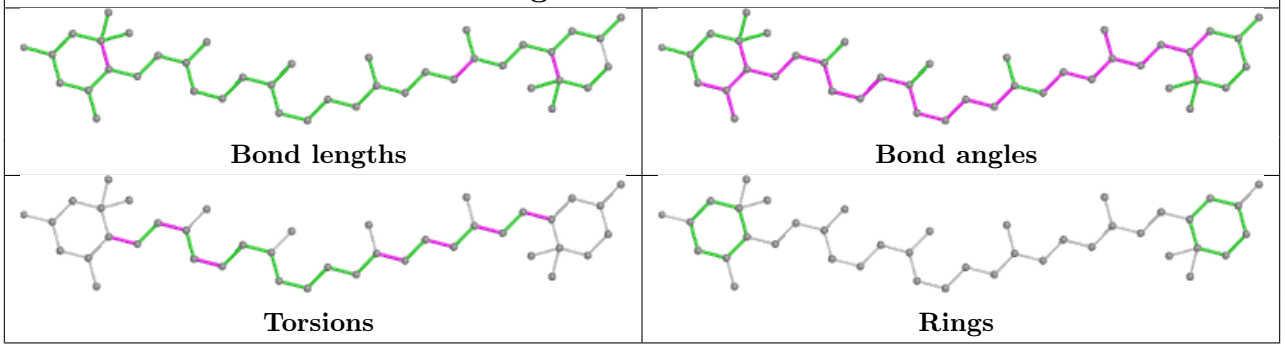
Ligand LHG B 625



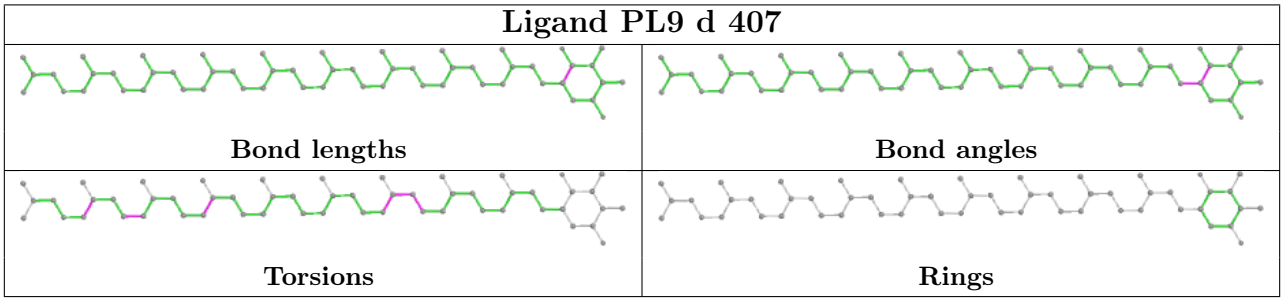
Ligand CL7 2 517



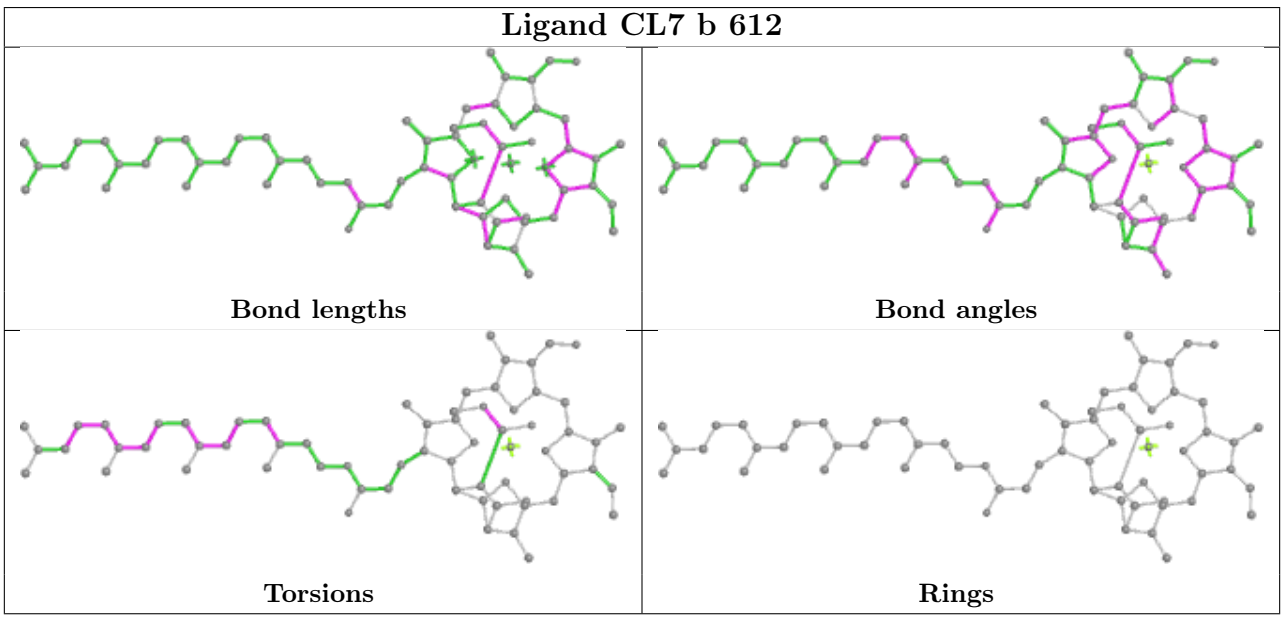
Ligand ZEX 2 525



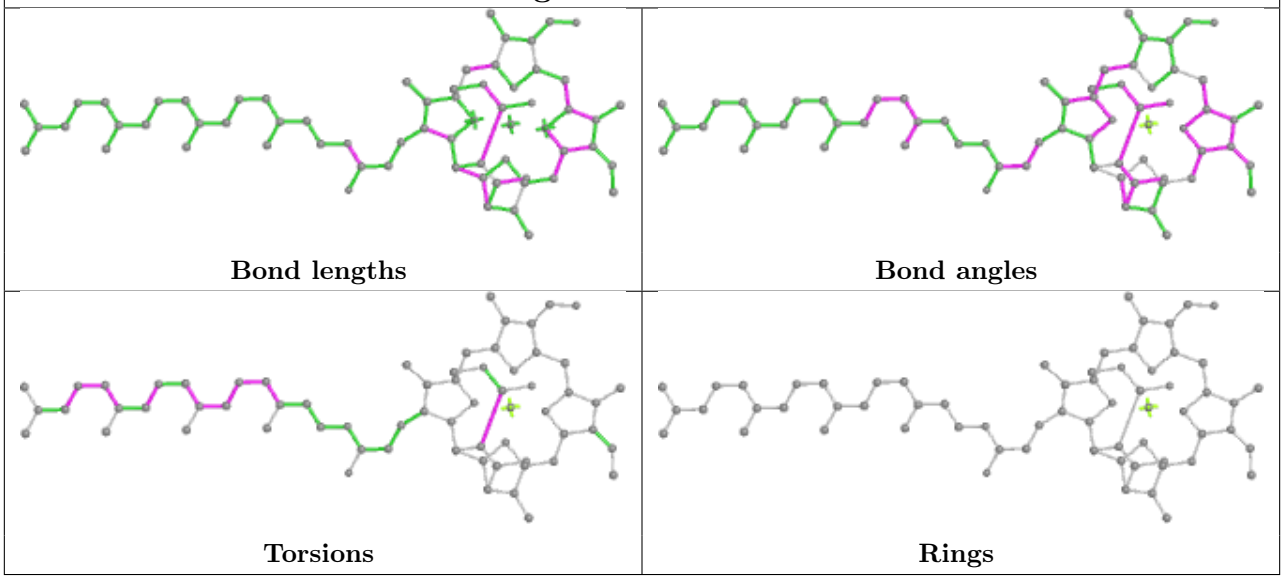
Ligand PL9 d 407



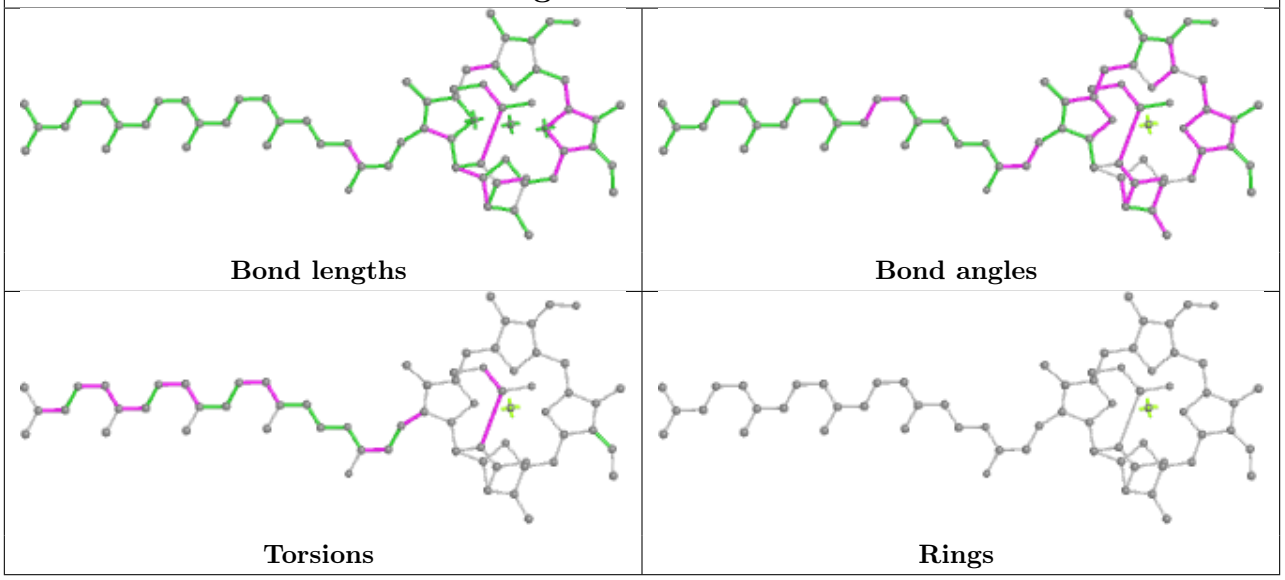
Ligand CL7 b 612



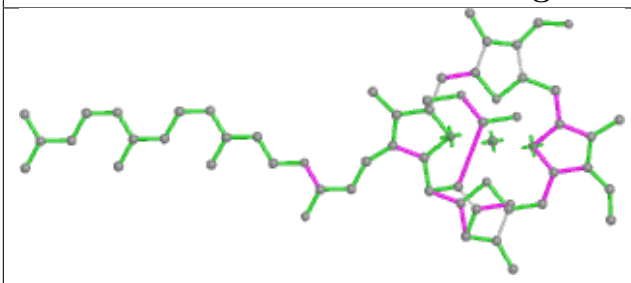
Ligand CL7 7 507



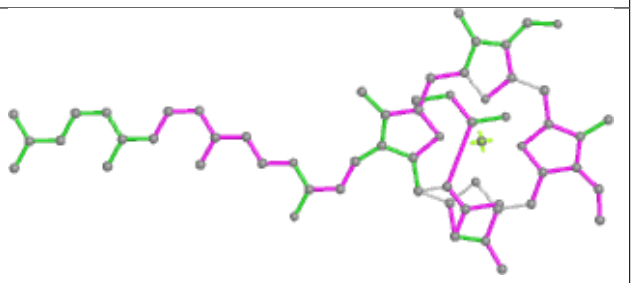
Ligand CL7 2 507



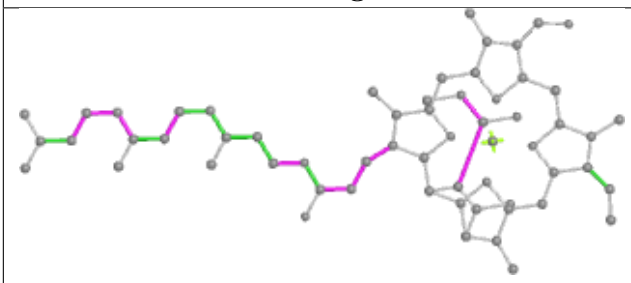
Ligand CL7 8 409



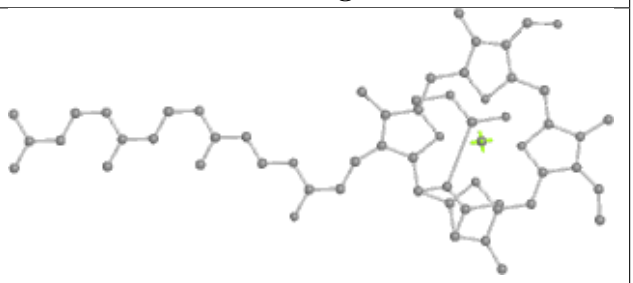
Bond lengths



Bond angles

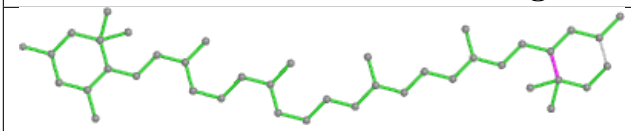


Torsions

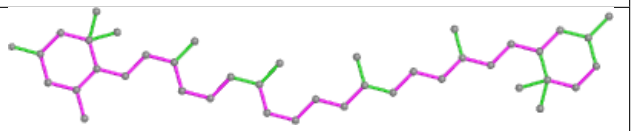


Rings

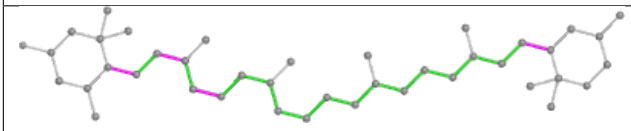
Ligand ZEX 5 422



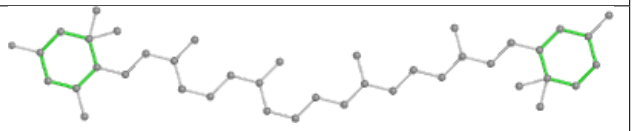
Bond lengths



Bond angles

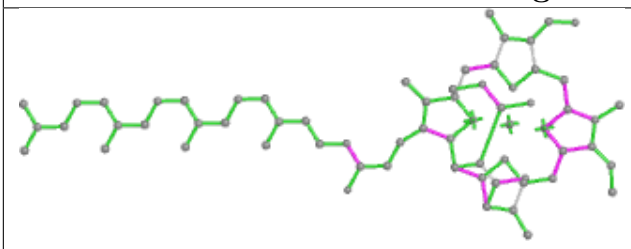


Torsions

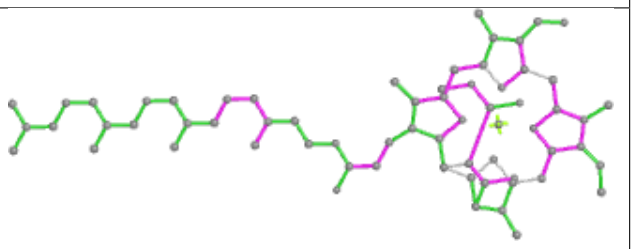


Rings

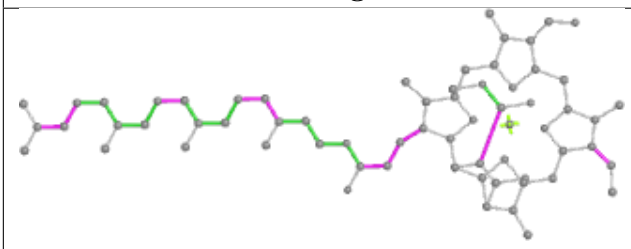
Ligand CL7 7 505



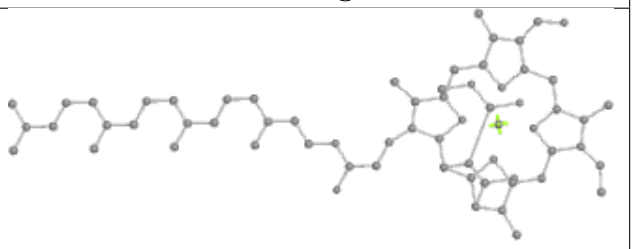
Bond lengths



Bond angles

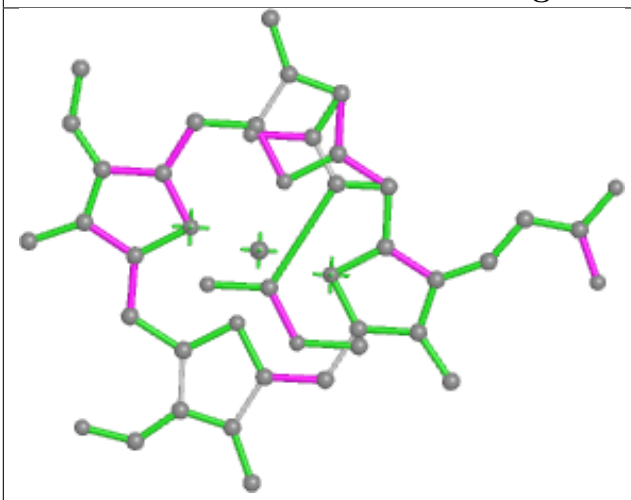


Torsions

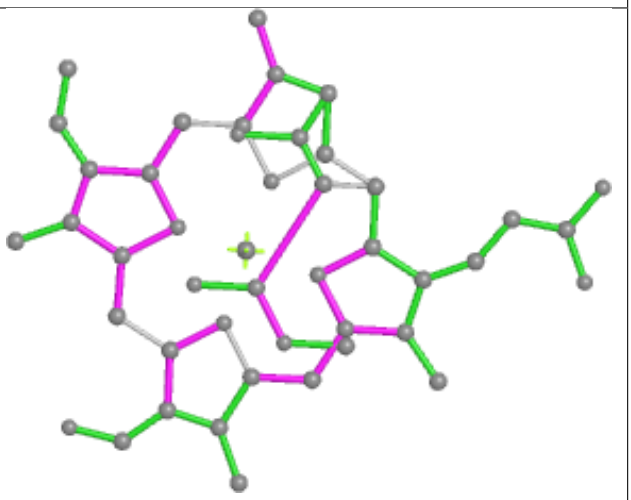


Rings

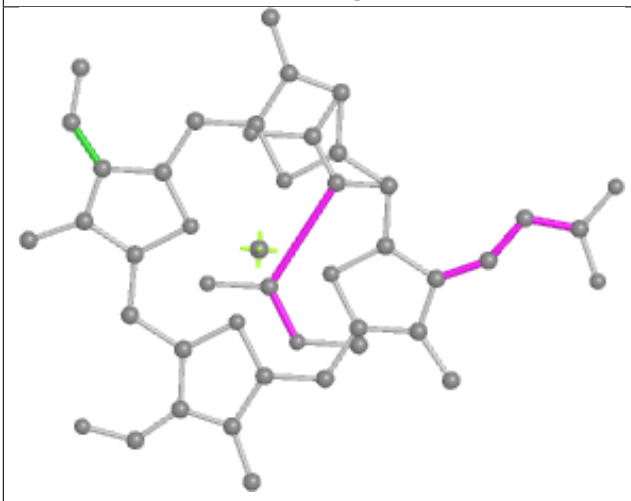
Ligand CL7 5 405



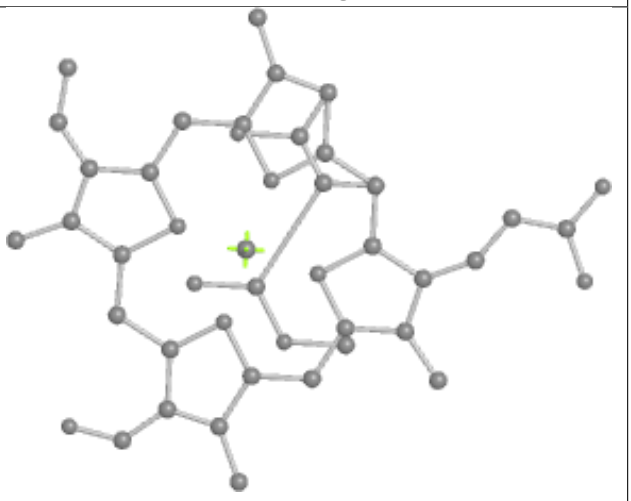
Bond lengths



Bond angles

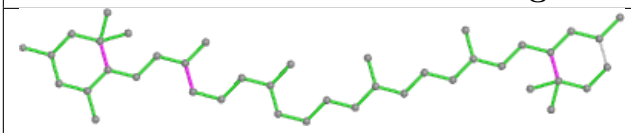


Torsions

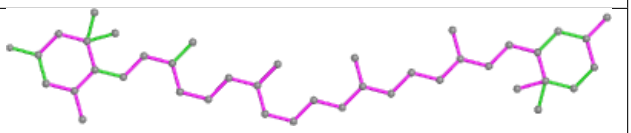


Rings

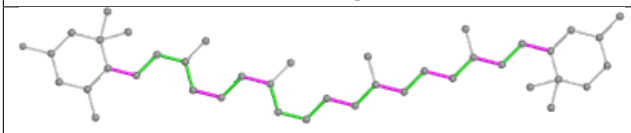
Ligand ZEX 8 420



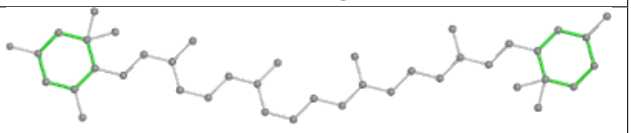
Bond lengths



Bond angles

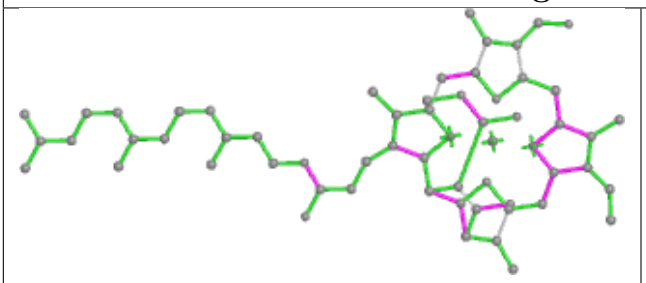


Torsions

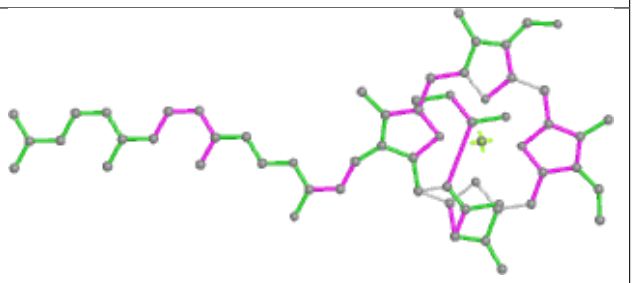


Rings

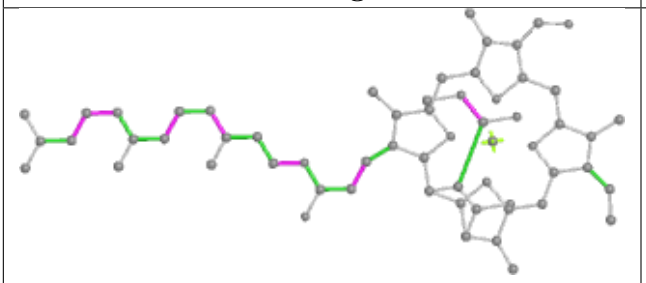
Ligand CL7 1 403



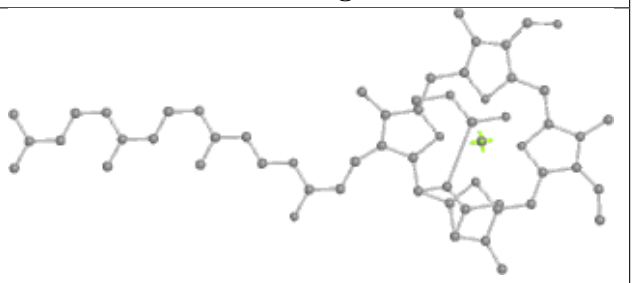
Bond lengths



Bond angles

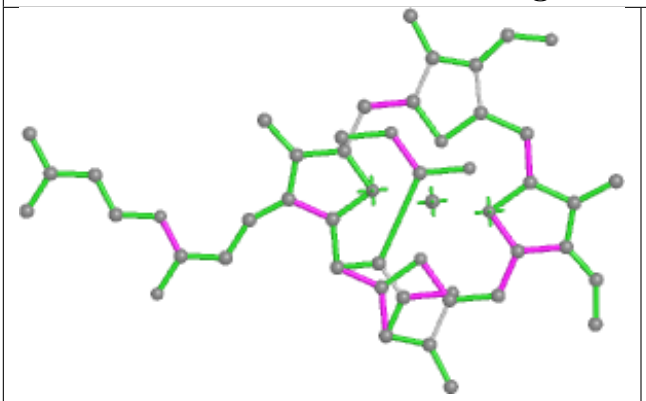


Torsions

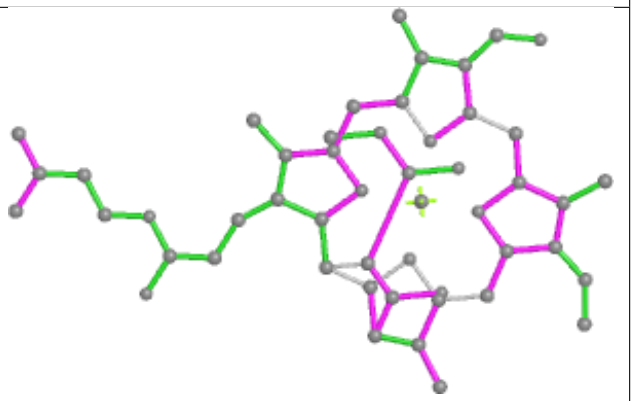


Rings

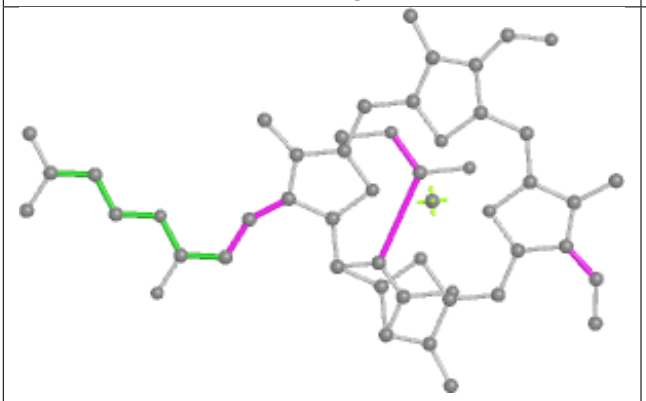
Ligand CL7 d 402



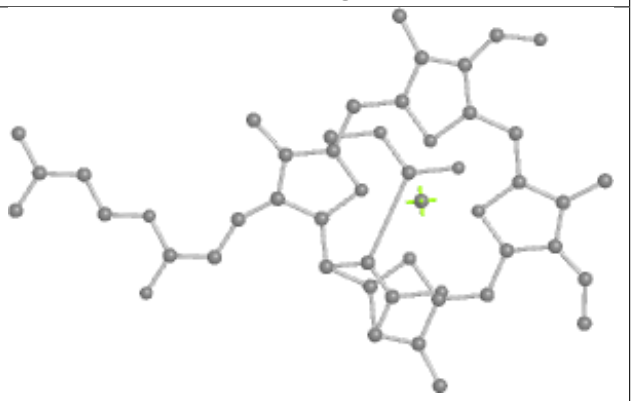
Bond lengths



Bond angles

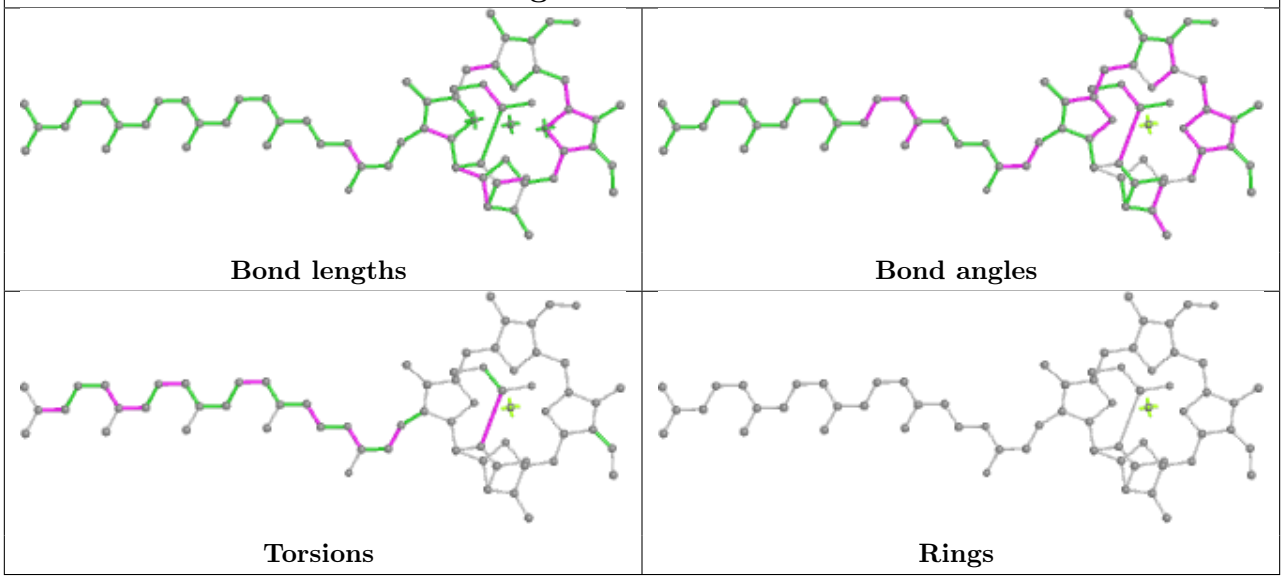


Torsions

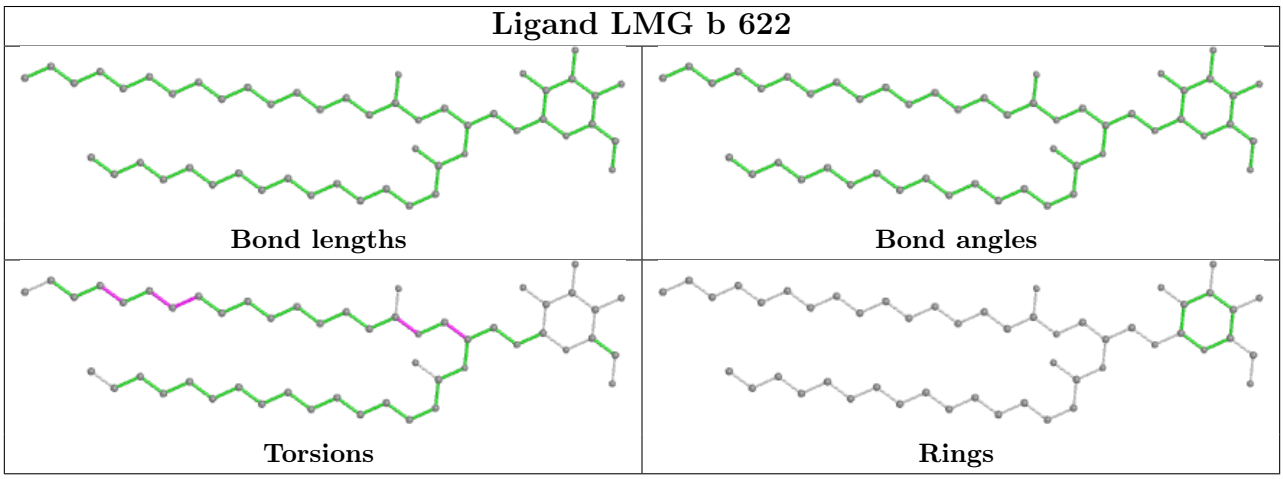


Rings

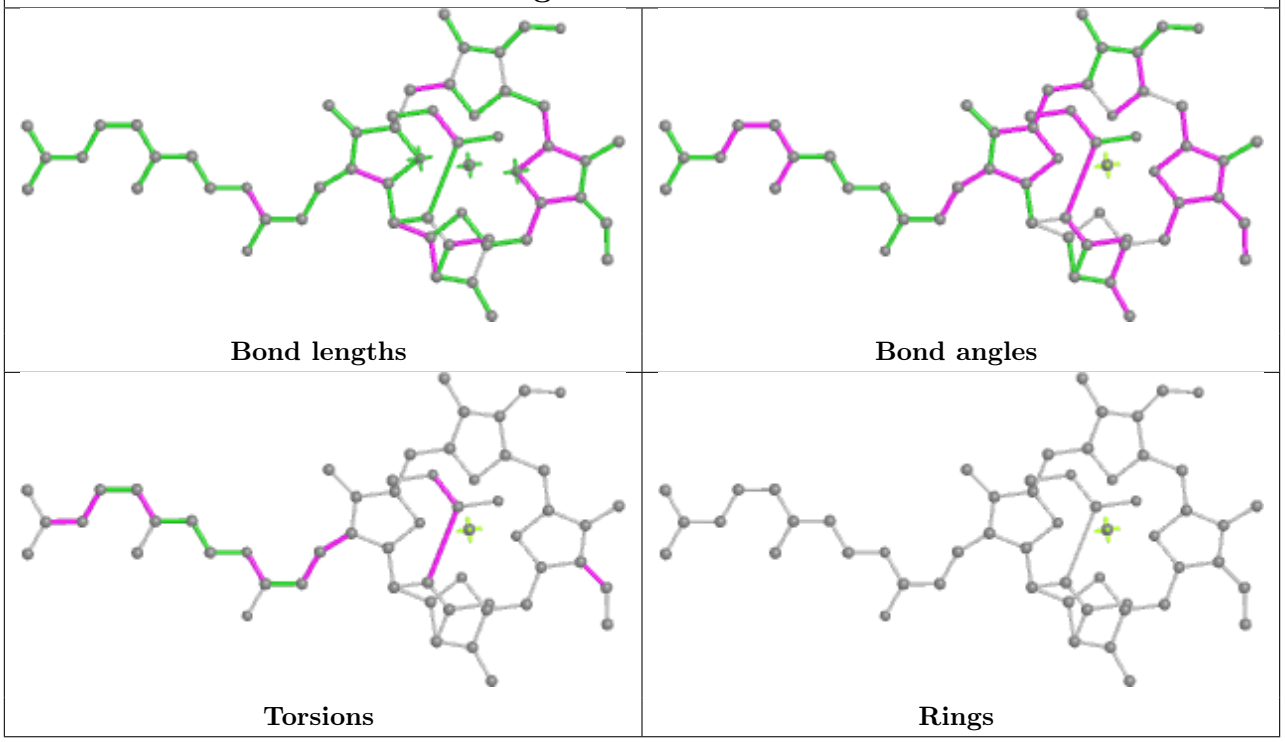
Ligand CL7 B 610



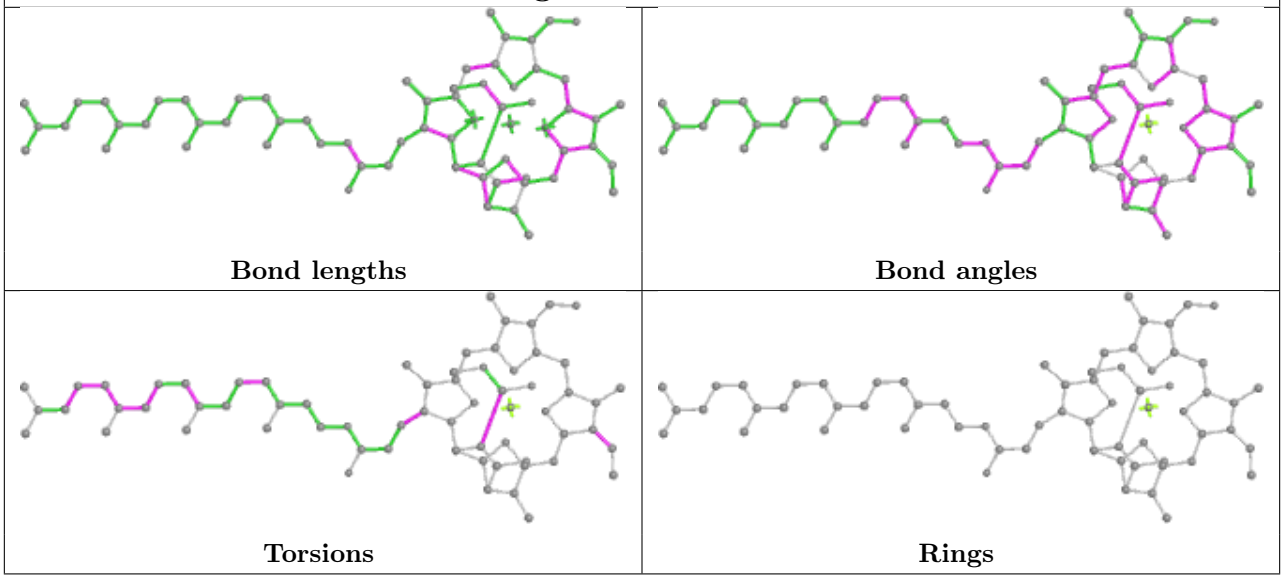
Ligand LMG b 622



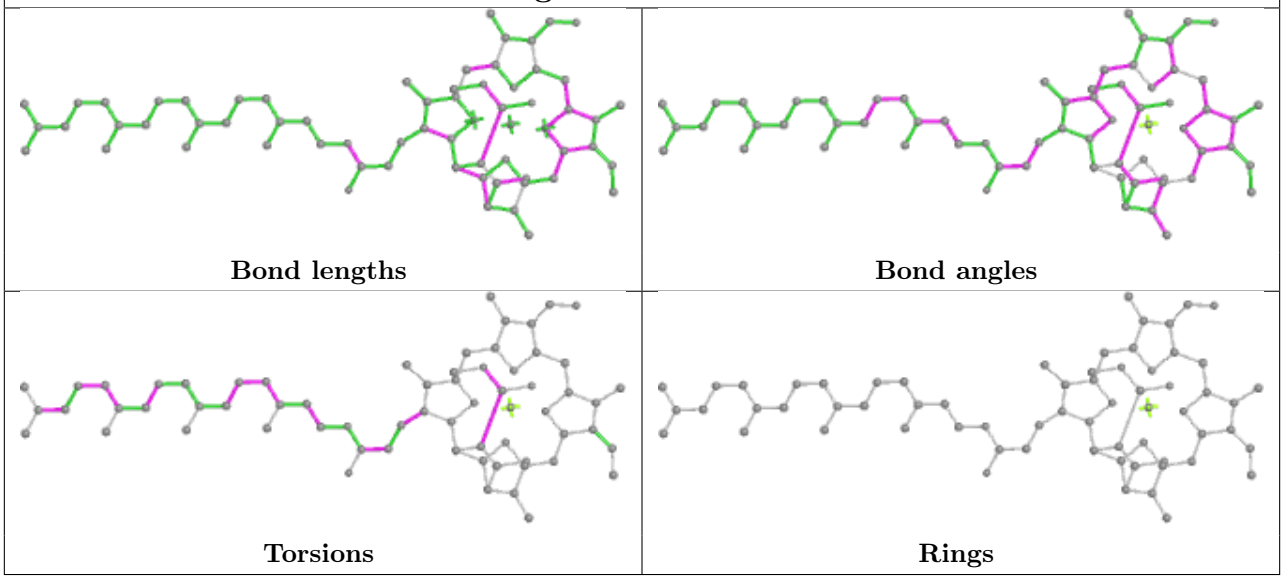
Ligand CL7 3 516



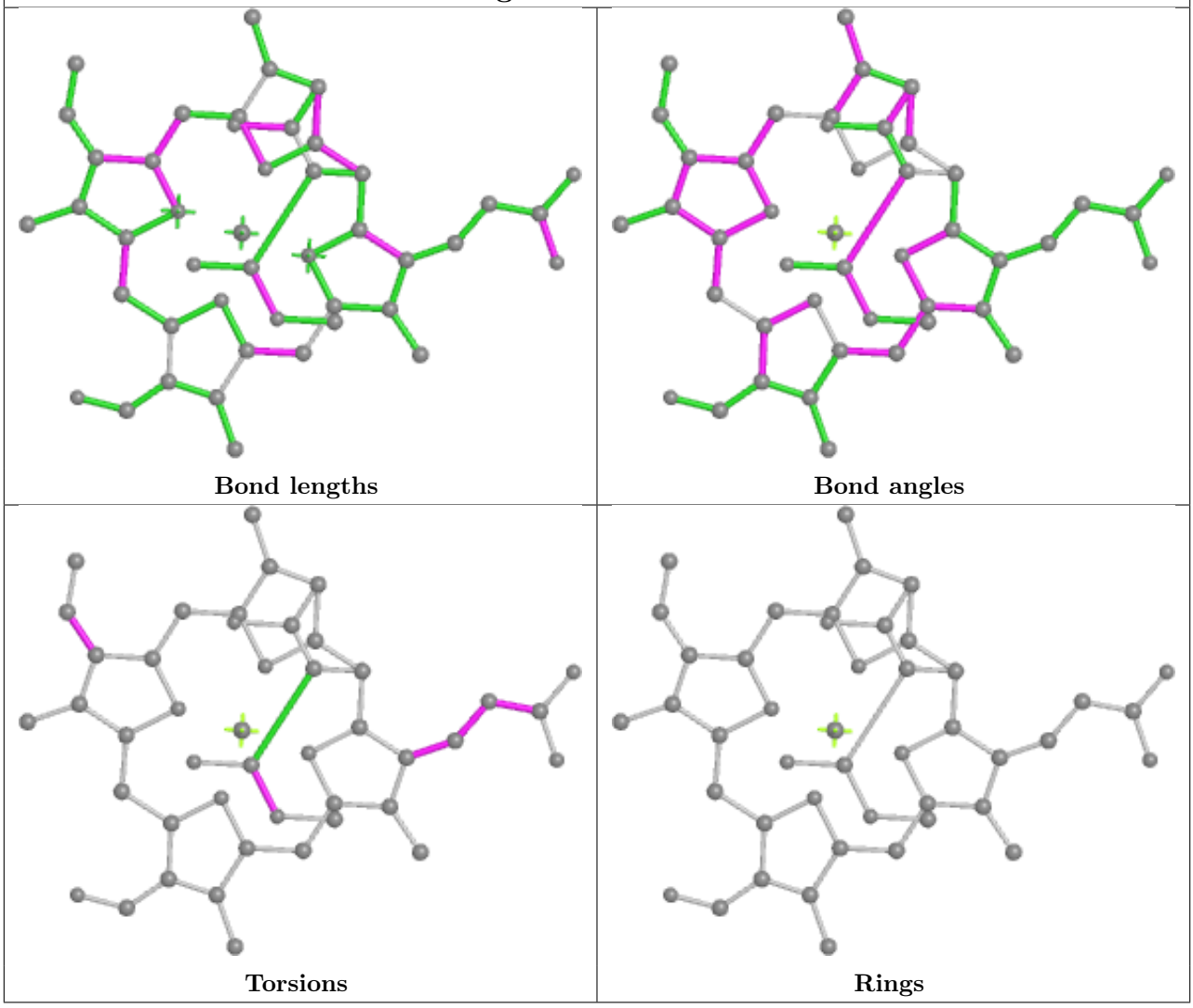
Ligand CL7 5 408



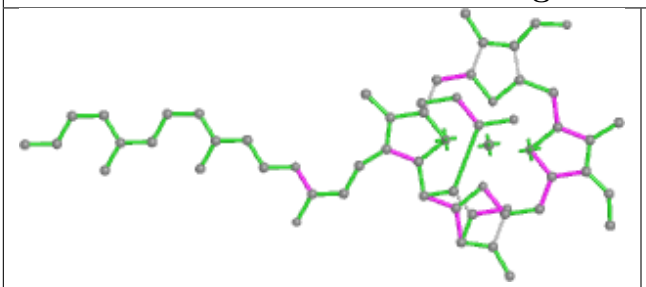
Ligand CL7 c 510



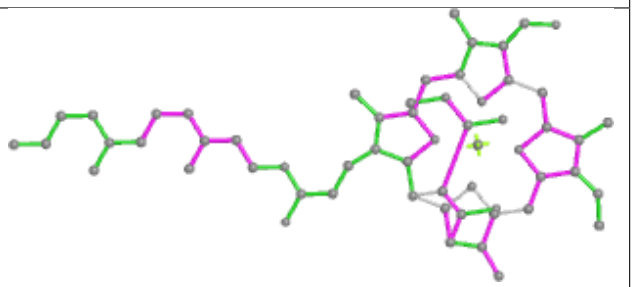
Ligand CL7 5 419



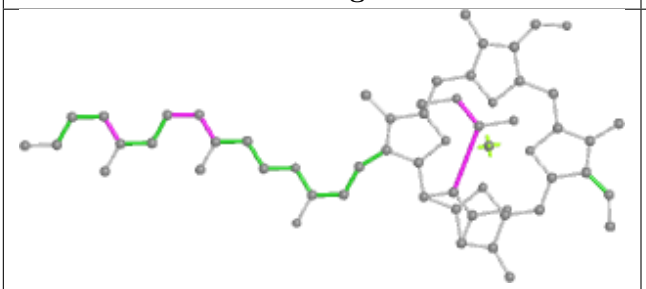
Ligand CL7 7 502



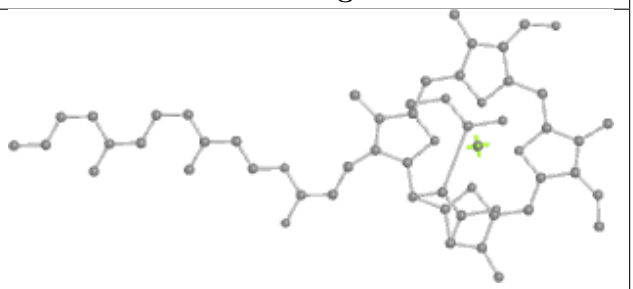
Bond lengths



Bond angles

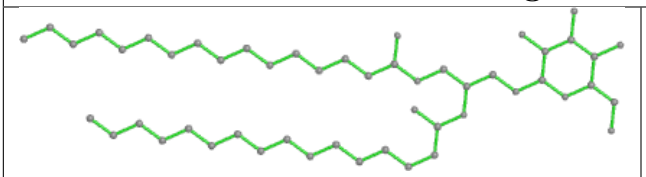


Torsions

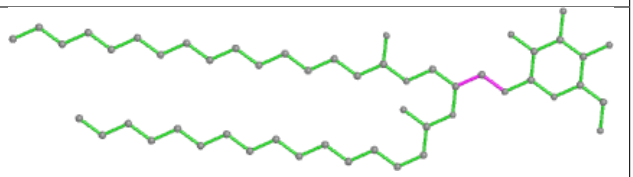


Rings

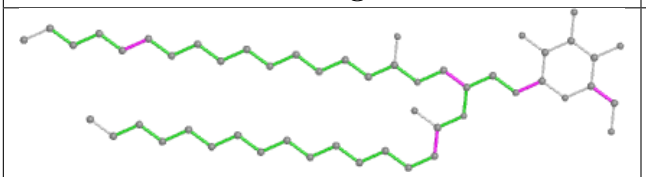
Ligand LMG 5 401



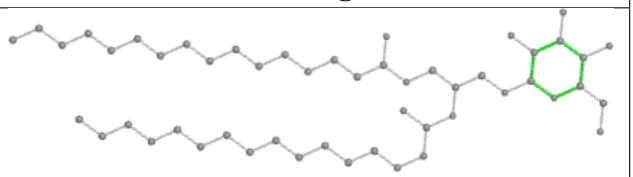
Bond lengths



Bond angles

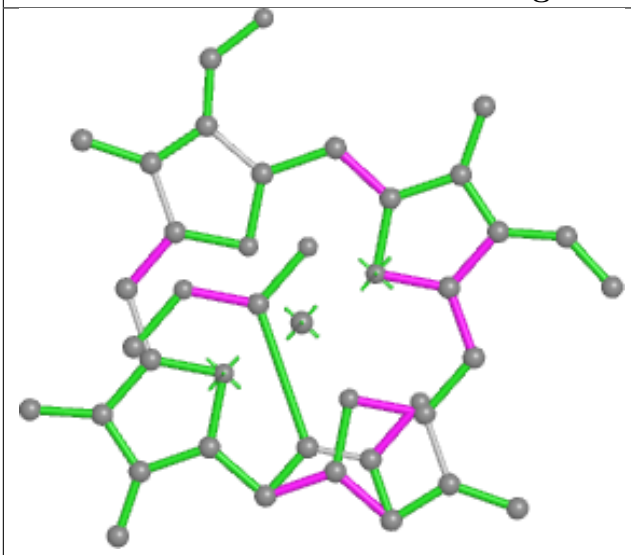


Torsions

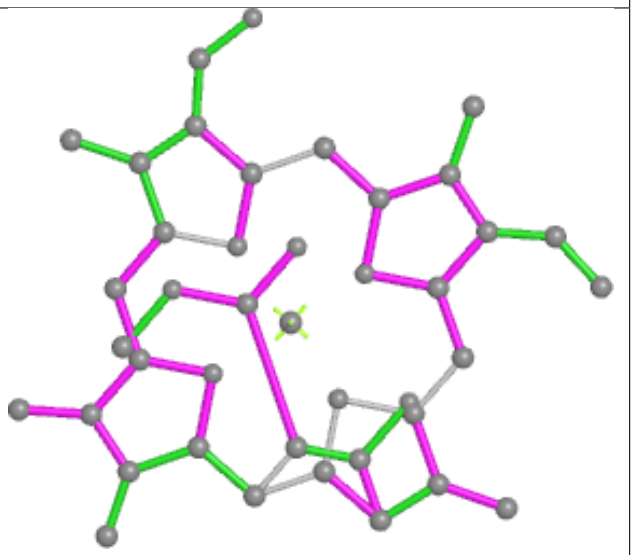


Rings

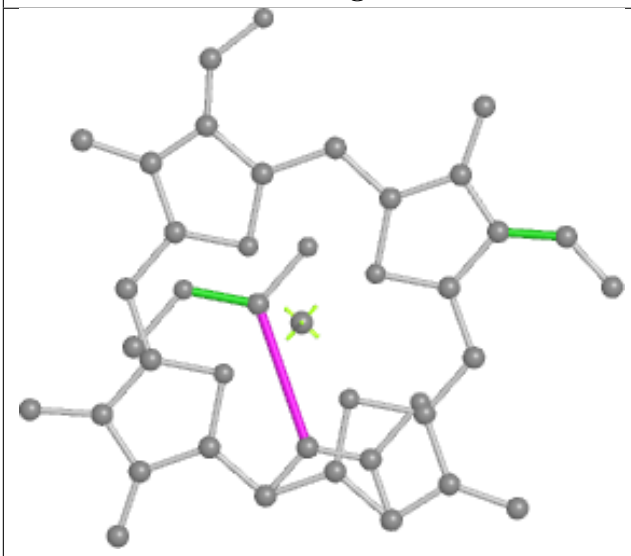
Ligand CL7 5 413



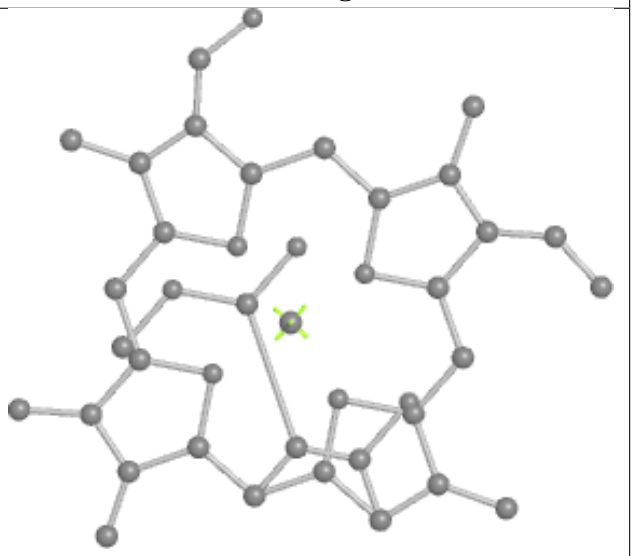
Bond lengths



Bond angles

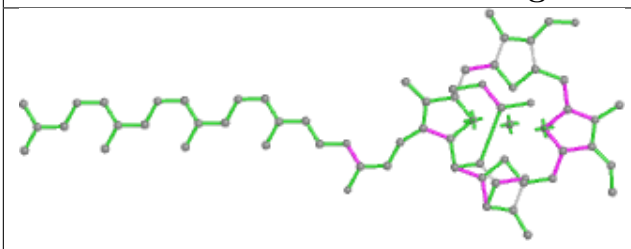


Torsions

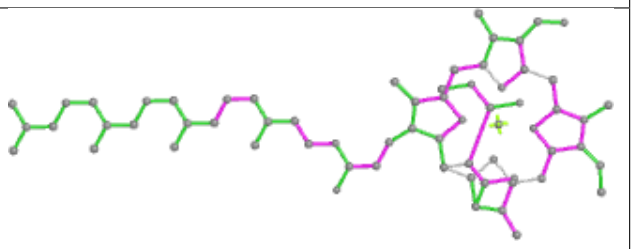


Rings

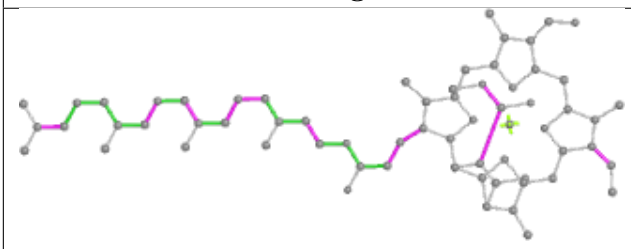
Ligand CL7 A 406



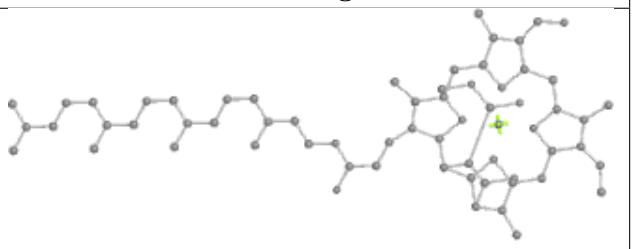
Bond lengths



Bond angles

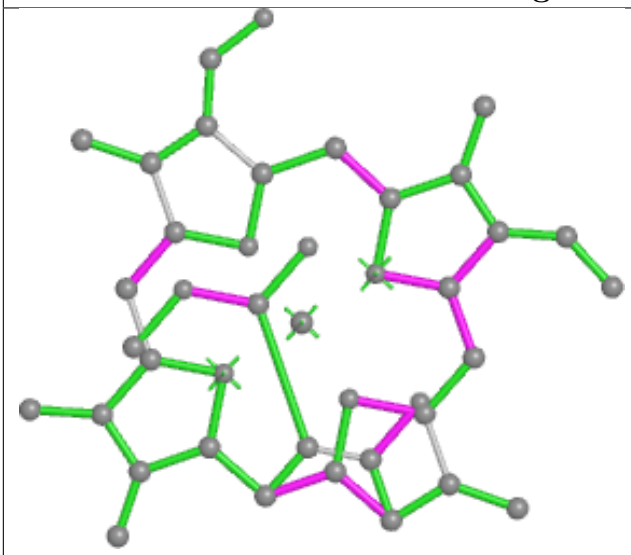


Torsions

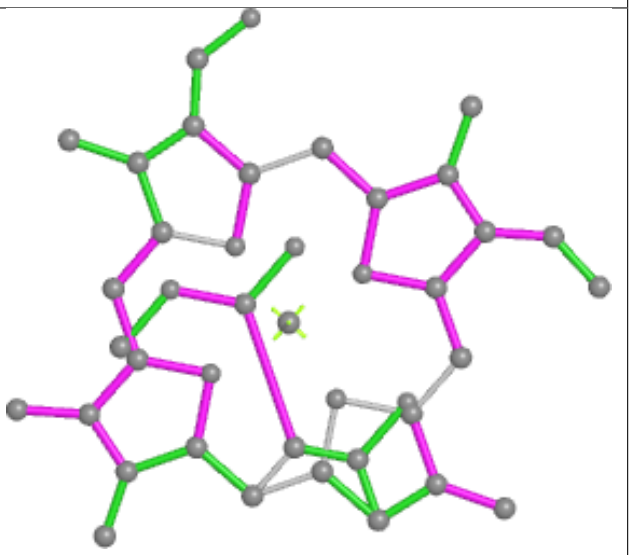


Rings

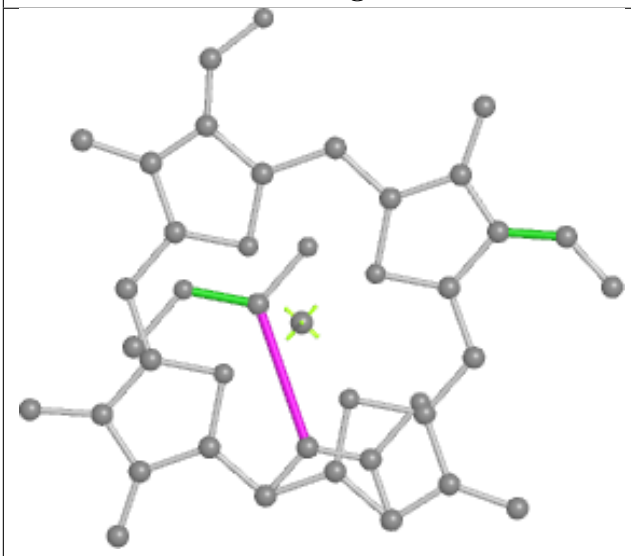
Ligand CL7 4 407



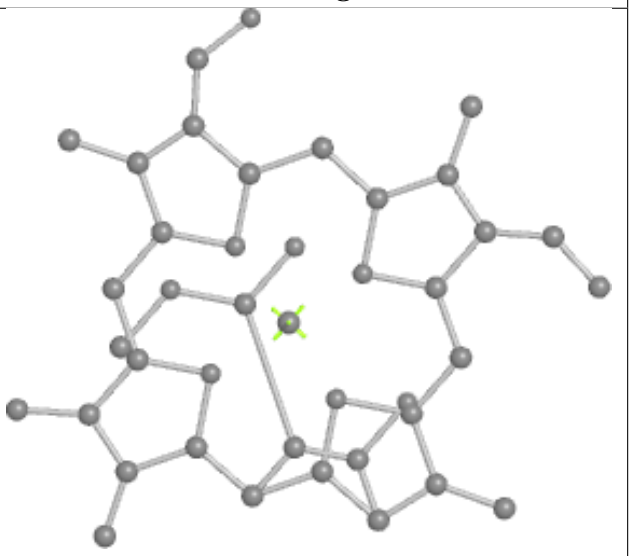
Bond lengths



Bond angles

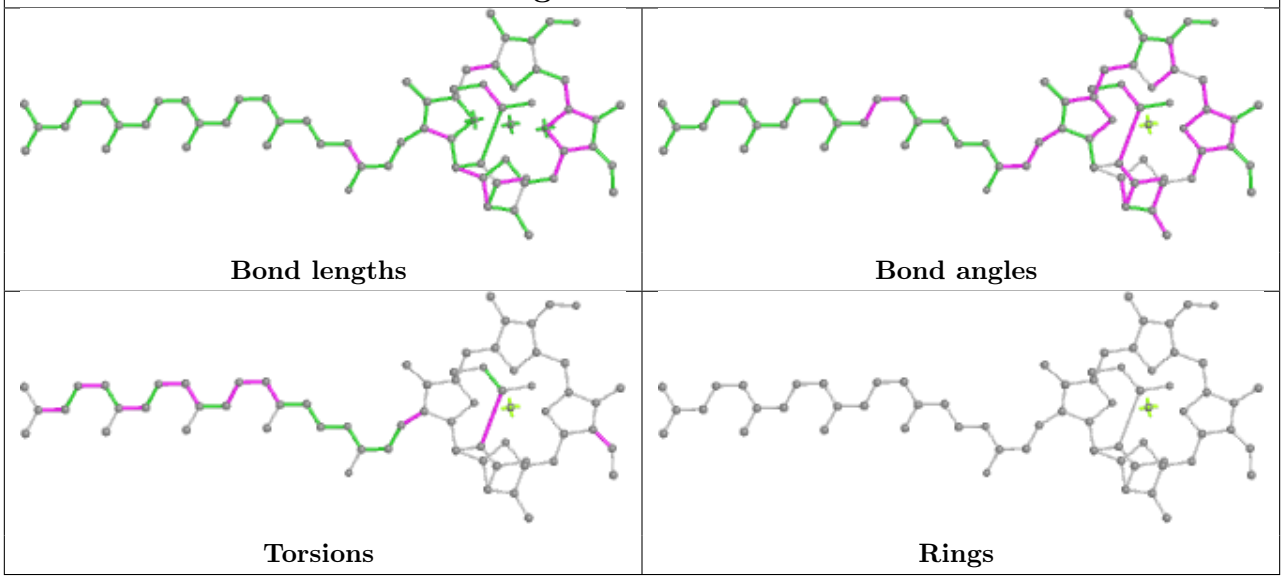


Torsions

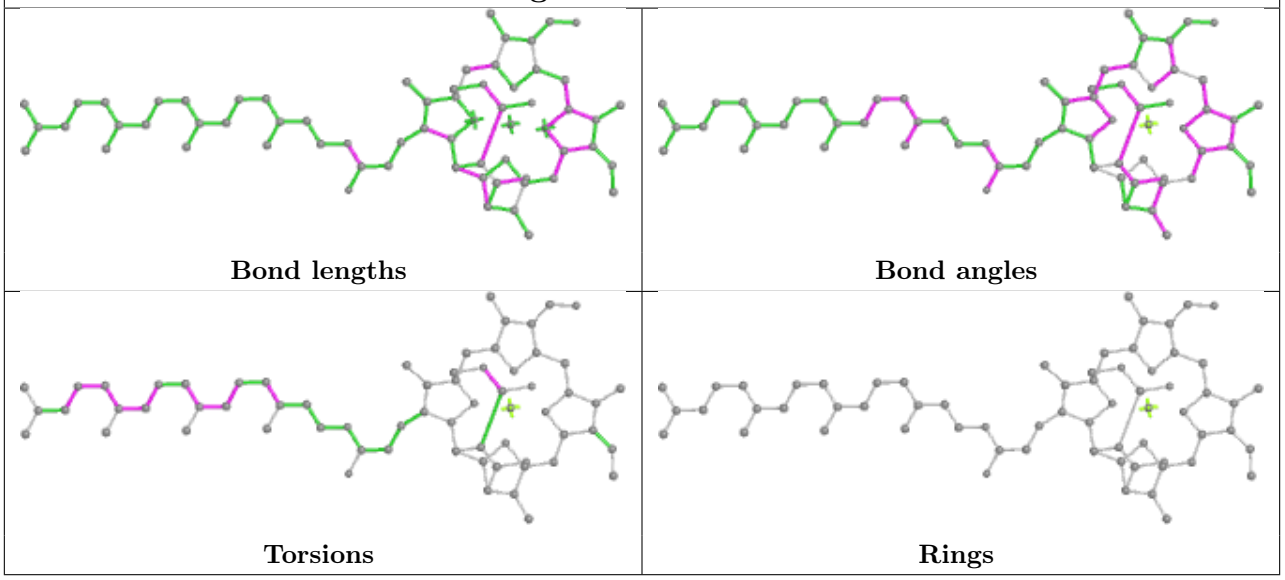


Rings

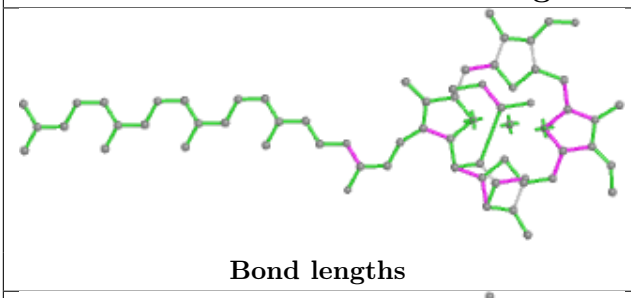
Ligand CL7 7 504



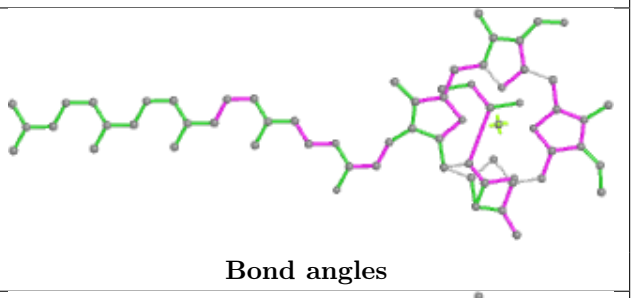
Ligand CL7 B 611



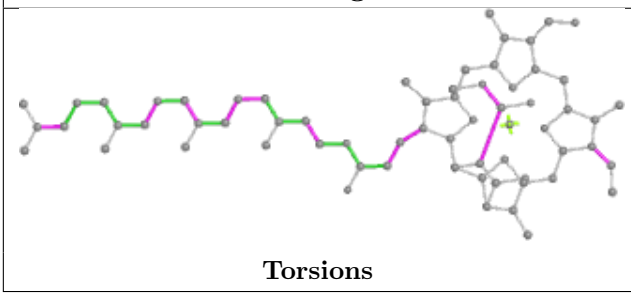
Ligand CL7 a 405



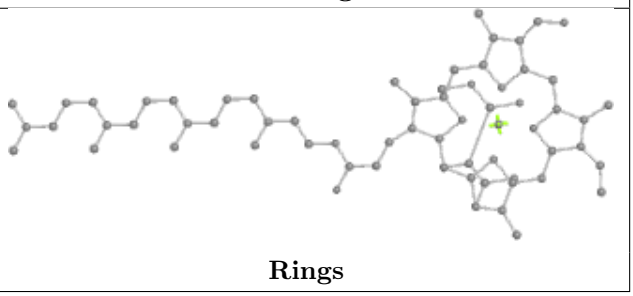
Bond lengths



Bond angles

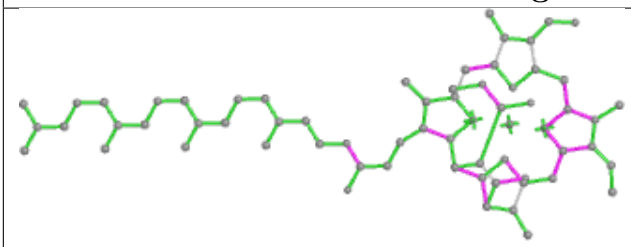


Torsions

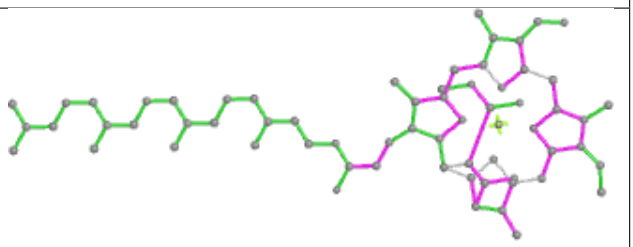


Rings

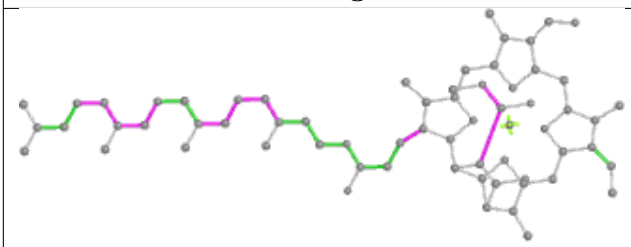
Ligand CL7 b 606



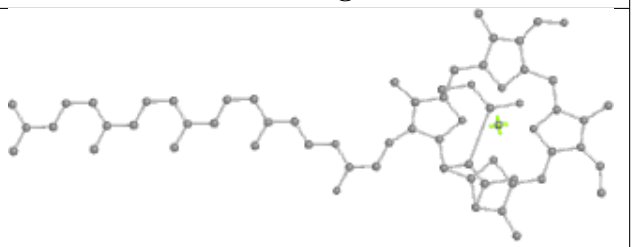
Bond lengths



Bond angles

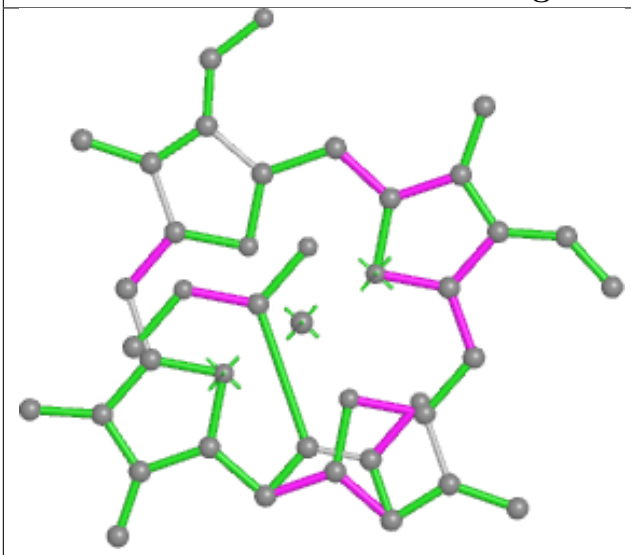


Torsions

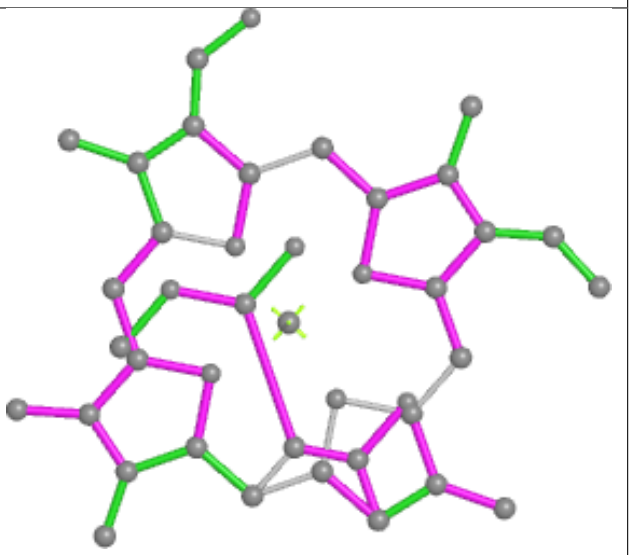


Rings

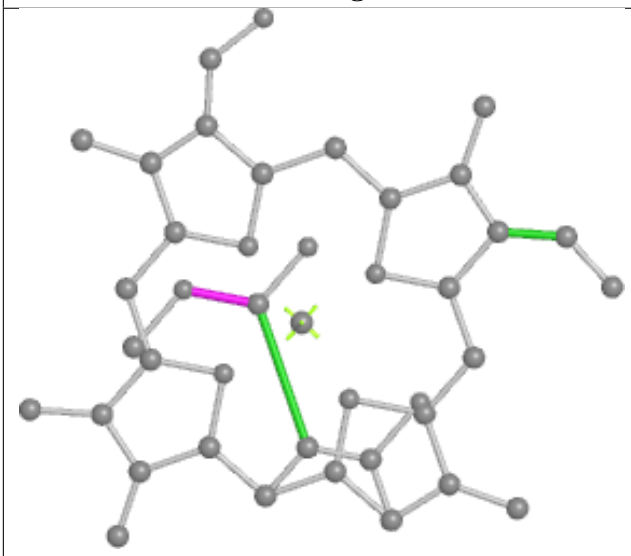
Ligand CL7 1 407



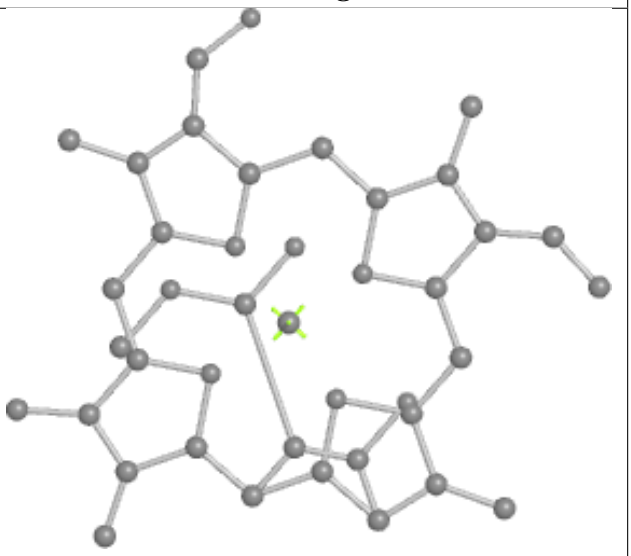
Bond lengths



Bond angles

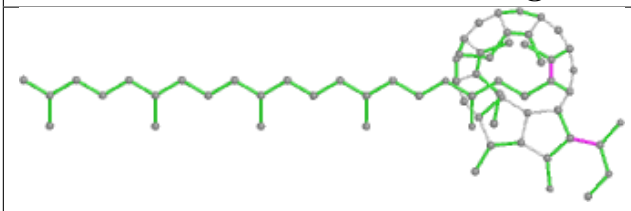


Torsions

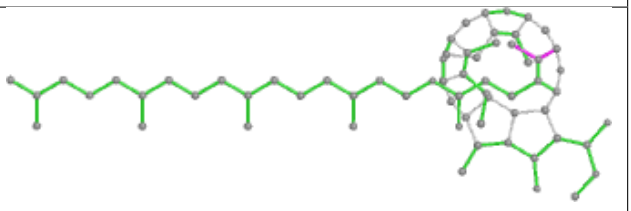


Rings

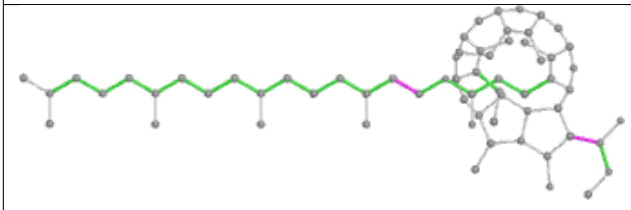
Ligand PHO a 402



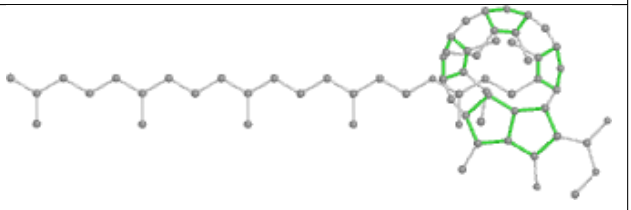
Bond lengths



Bond angles

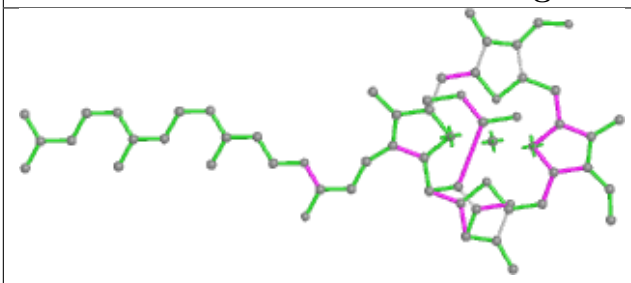


Torsions

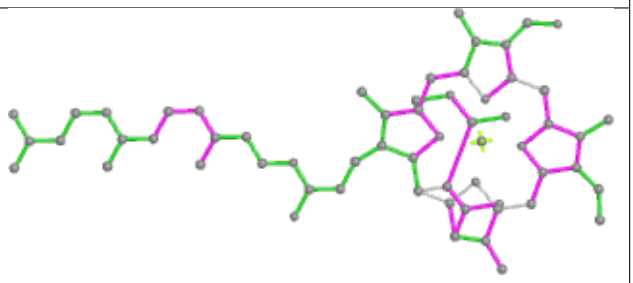


Rings

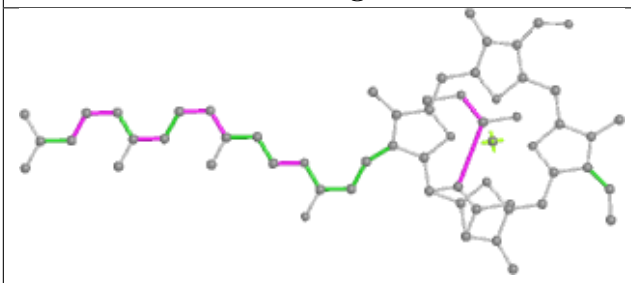
Ligand CL7 c 503



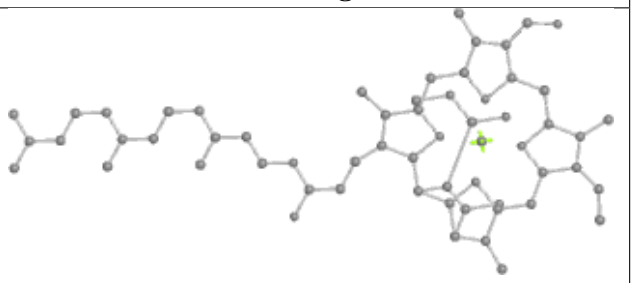
Bond lengths



Bond angles

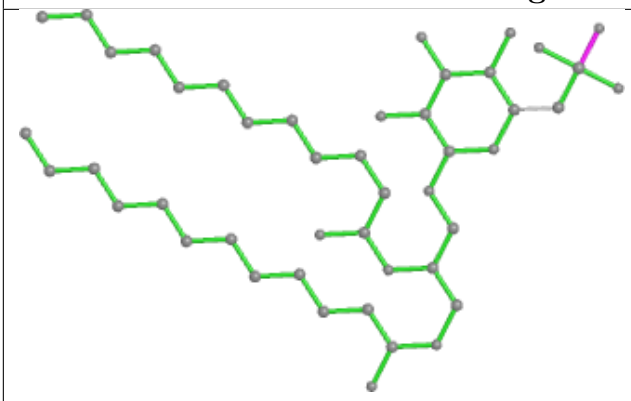


Torsions

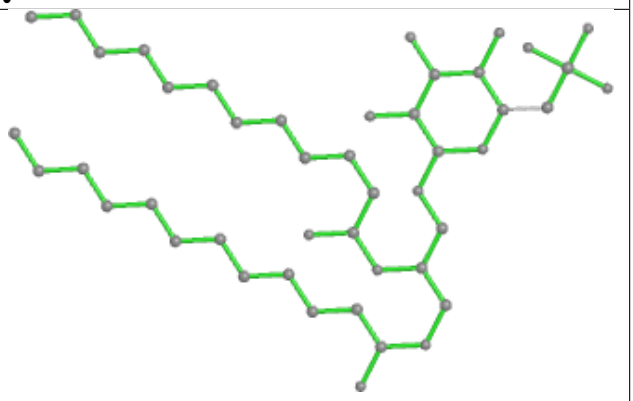


Rings

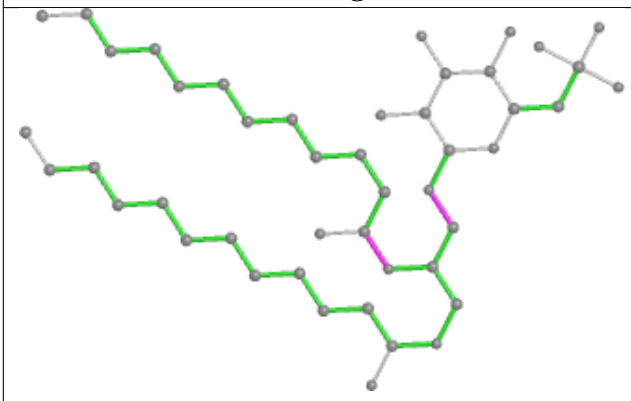
Ligand SQD 3 521



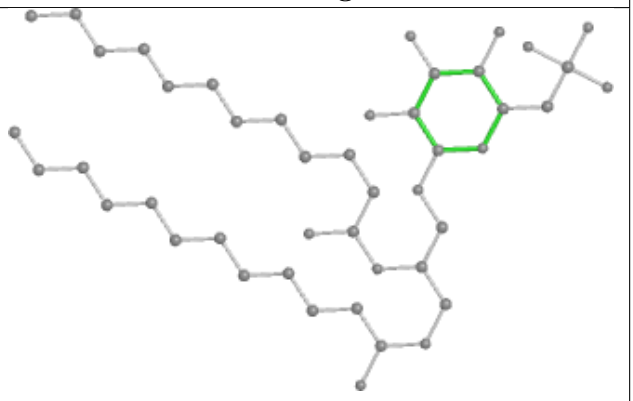
Bond lengths



Bond angles

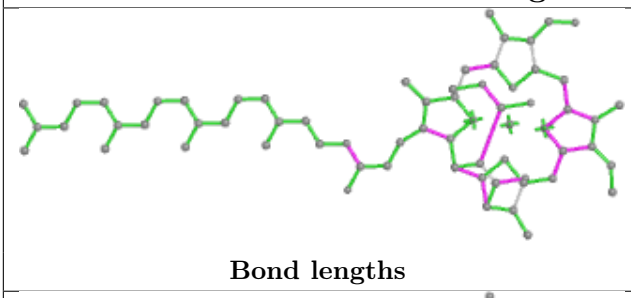


Torsions

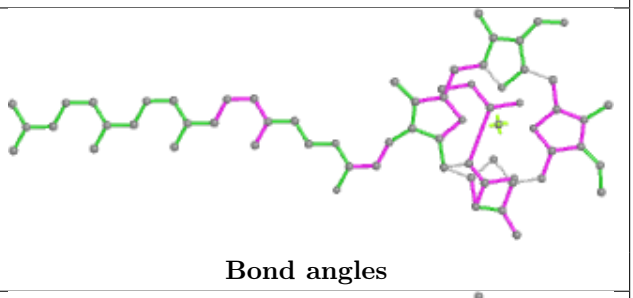


Rings

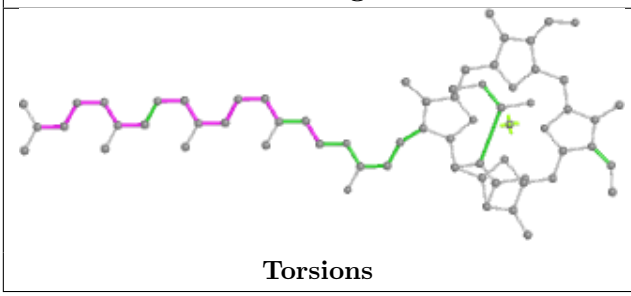
Ligand CL7 C 508



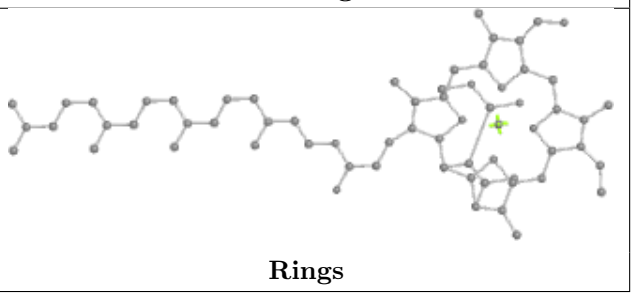
Bond lengths



Bond angles

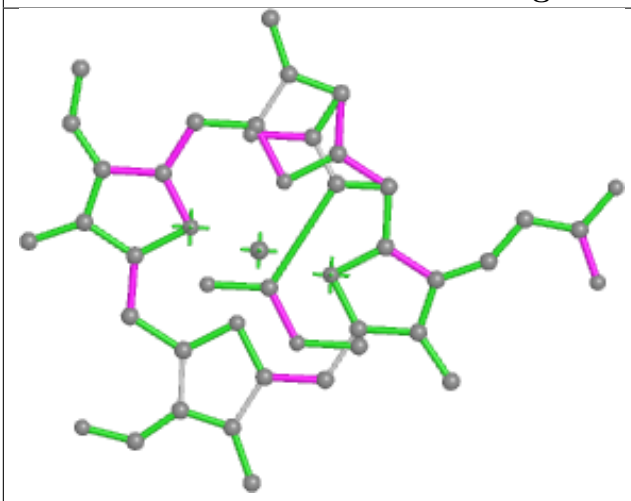


Torsions



Rings

Ligand CL7 1 411



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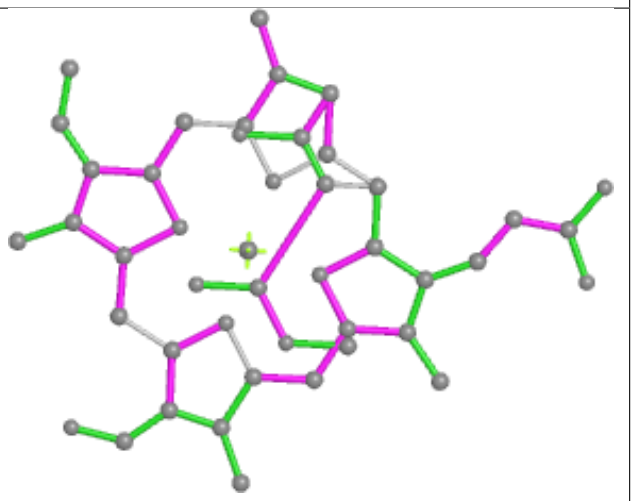
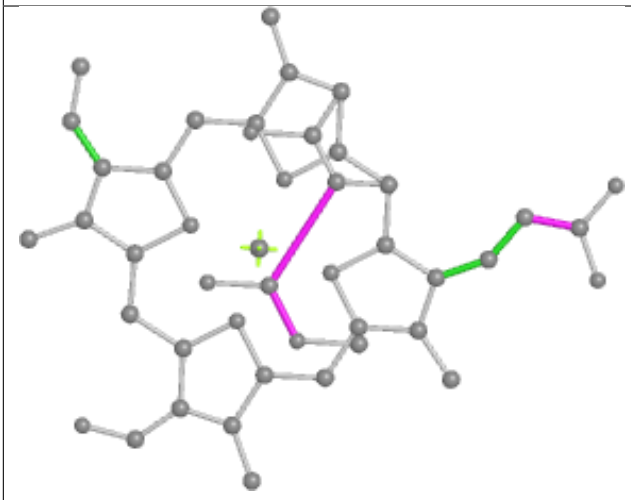
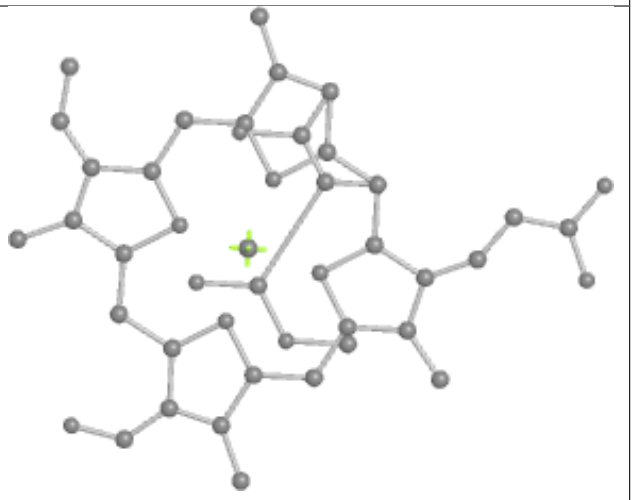


Bond angles

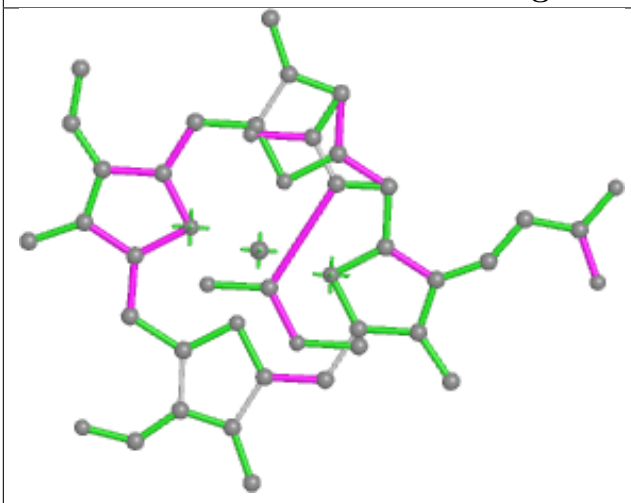


Torsions



Rings

Ligand CL7 b 617



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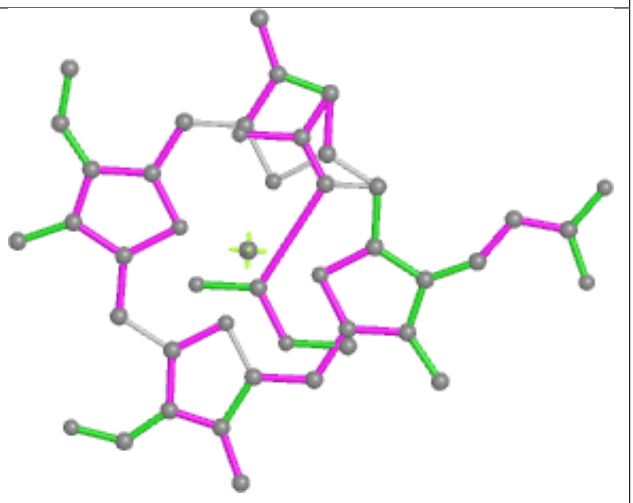
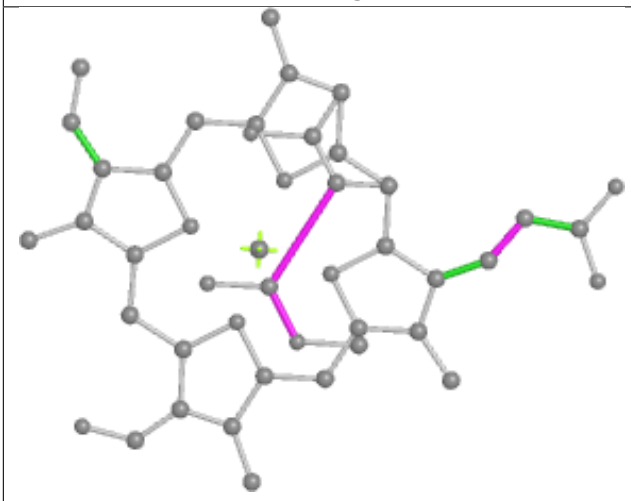
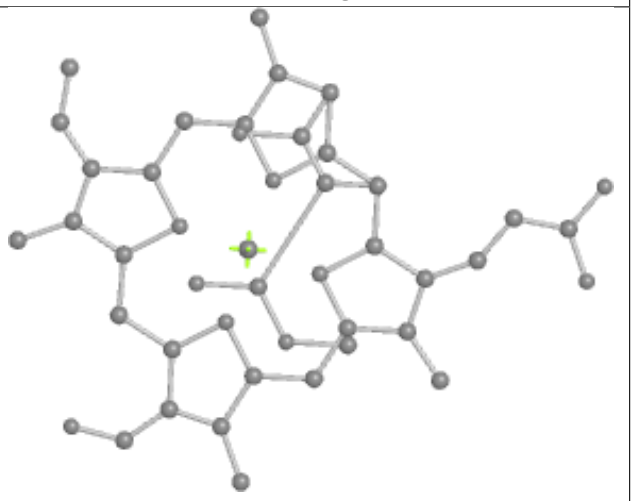


Bond angles

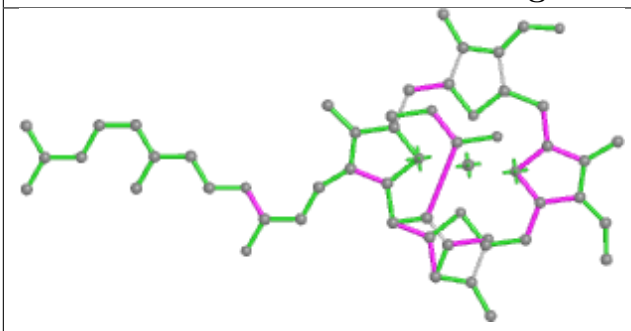


Torsions

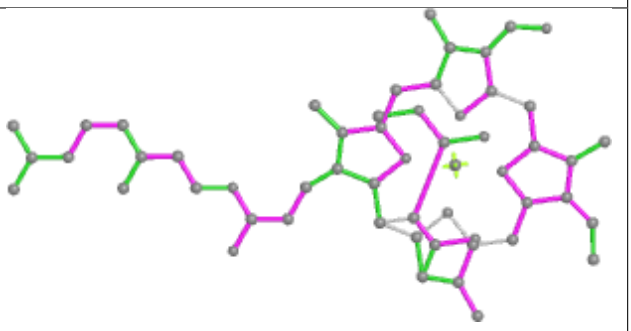


Rings

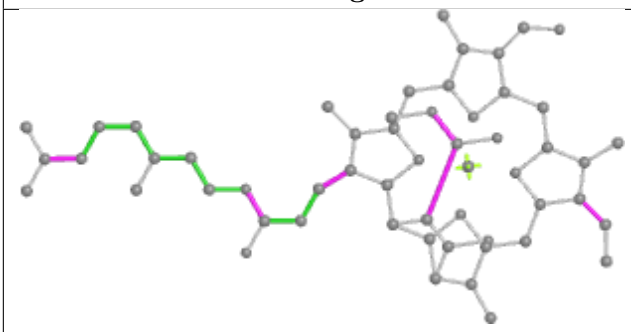
Ligand CL7 A 403



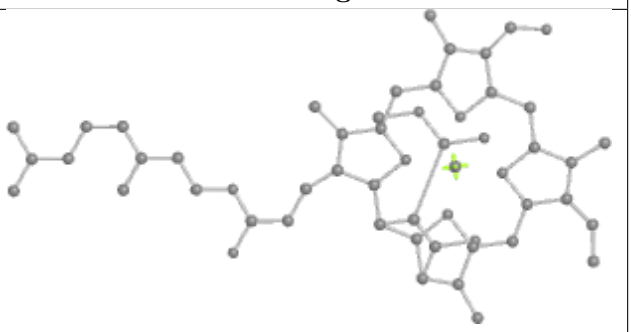
Bond lengths



Bond angles

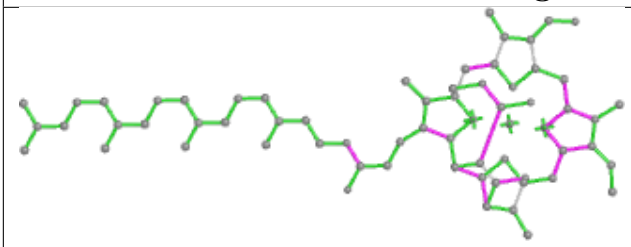


Torsions



Rings

Ligand CL7 c 506



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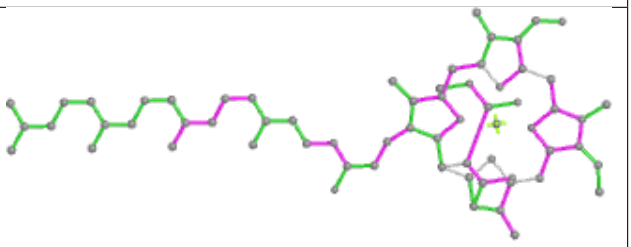
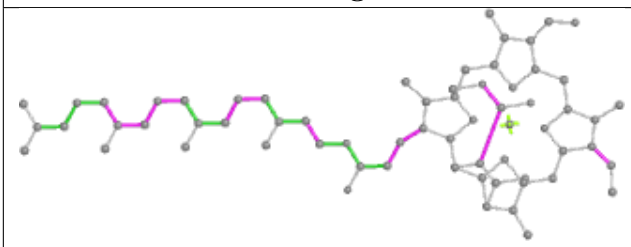


Bond angles



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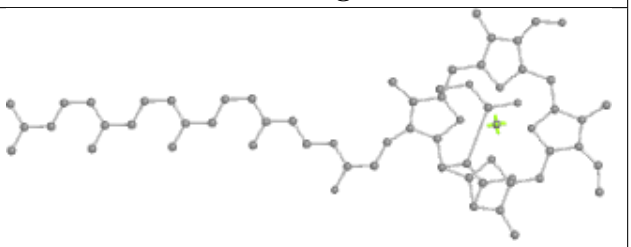
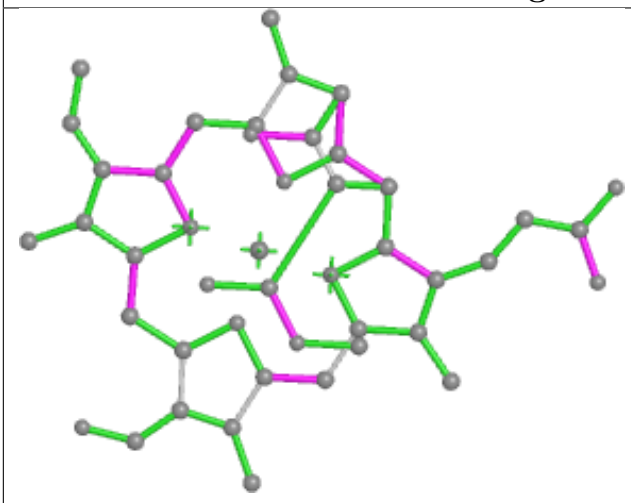
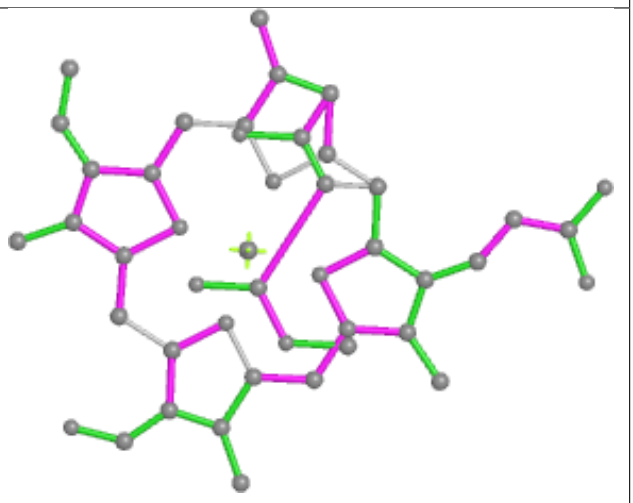


Rings

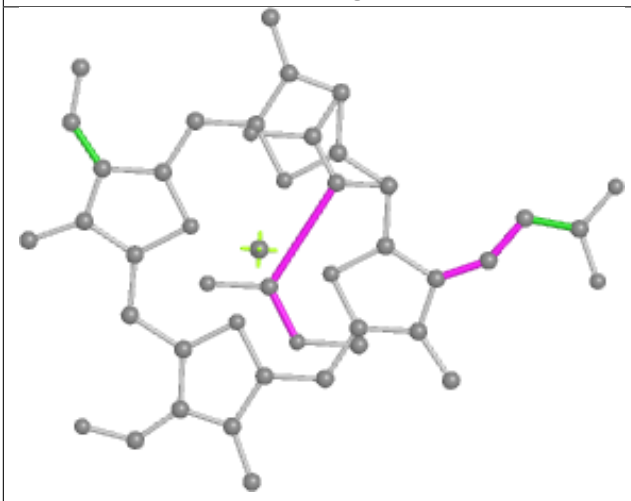
Ligand CL7 C 514



Bond lengths



Bond angles



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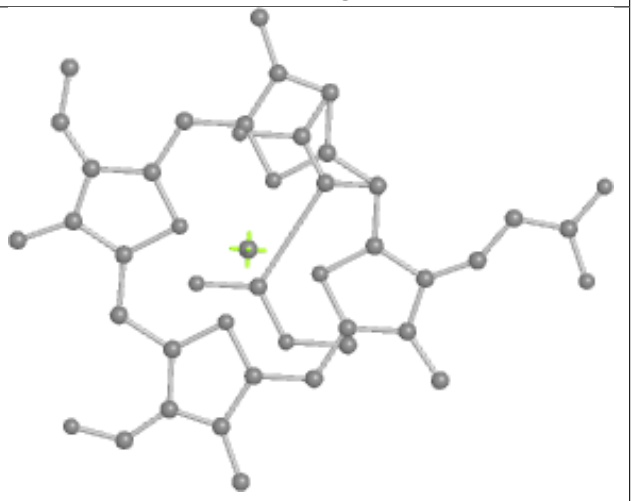
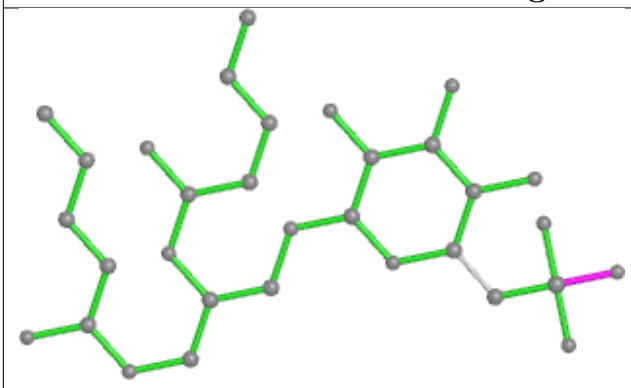
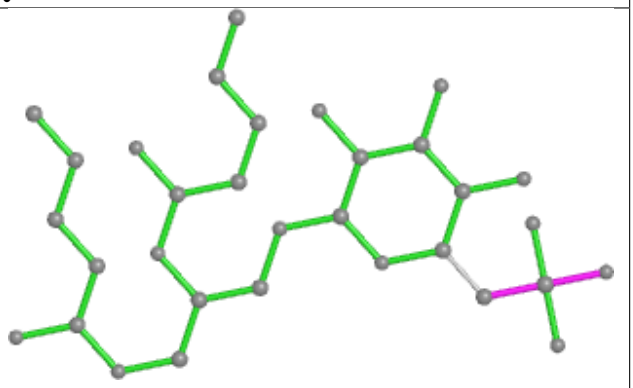


Rings

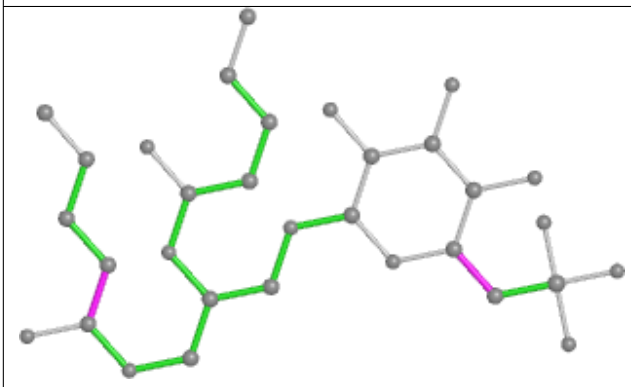
Ligand SQD 1 423



Bond lengths



Bond angles



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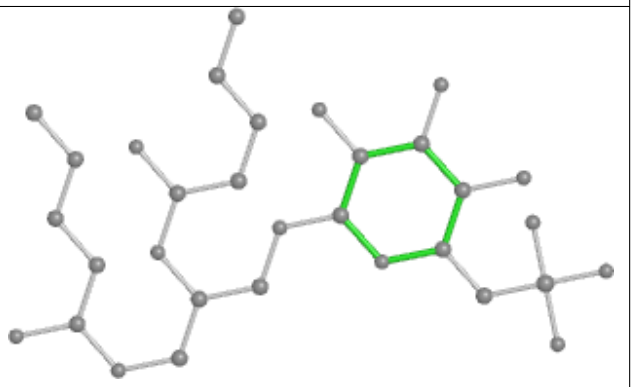
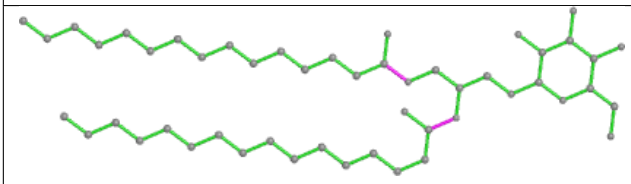
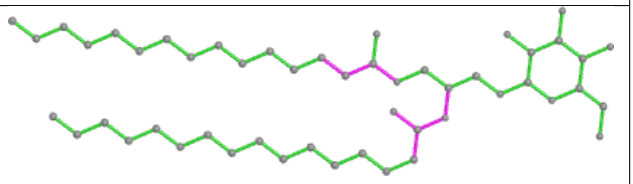


Rings

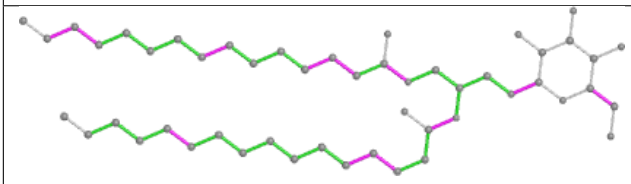
Ligand LMG c 501



Bond lengths



Bond angles



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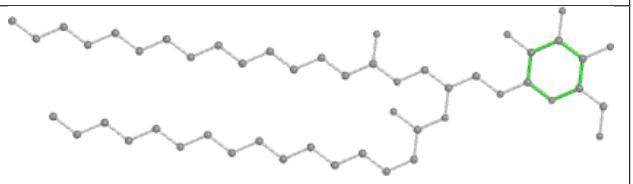
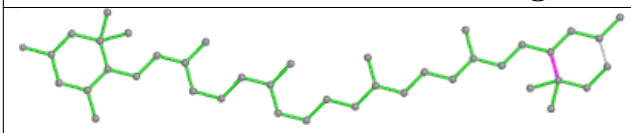
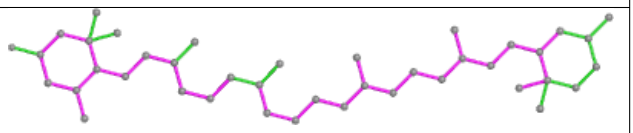


Rings

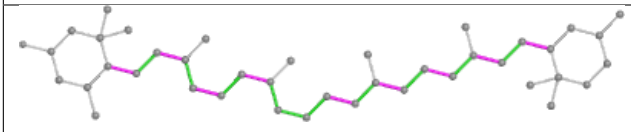
Ligand ZEX 1 421



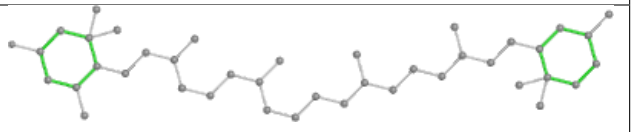
Bond lengths



Bond angles

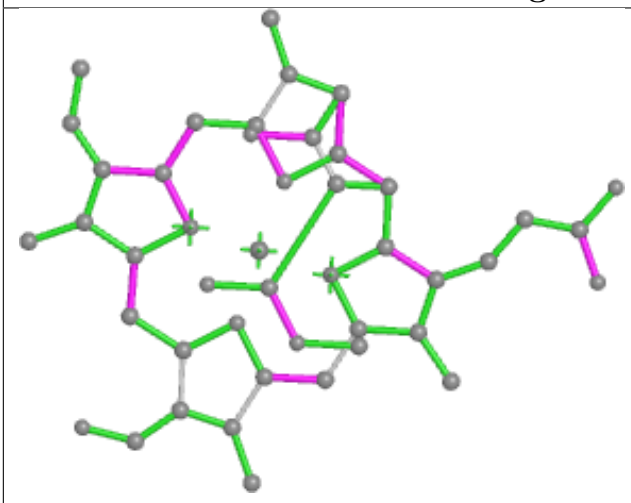


Torsions

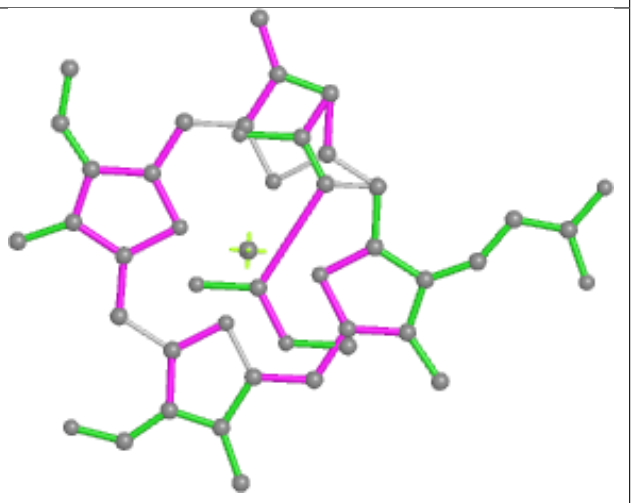


Rings

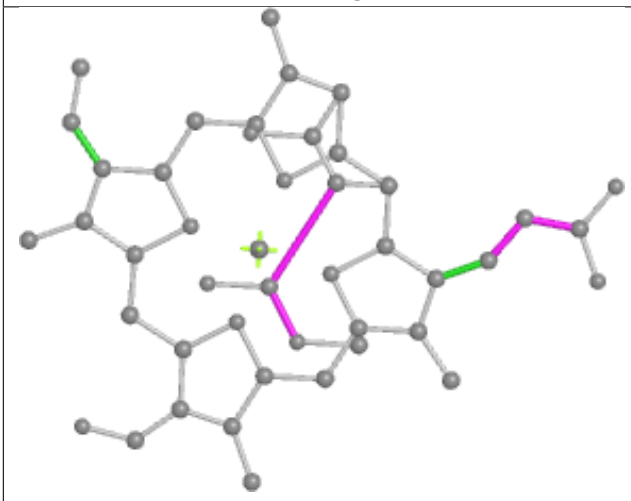
Ligand CL7 B 622



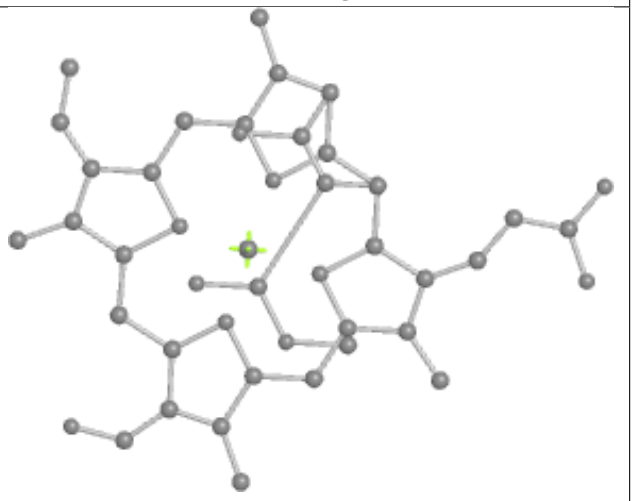
Bond lengths



Bond angles

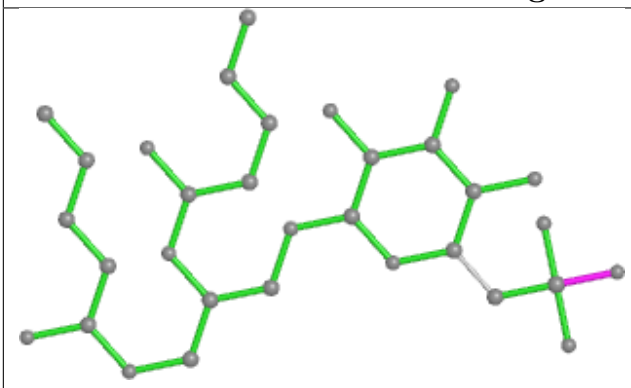


Torsions

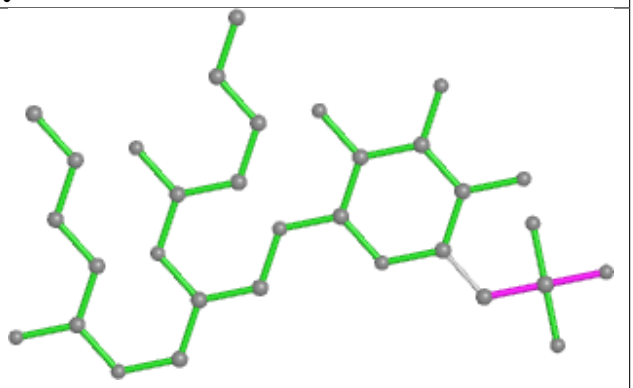


Rings

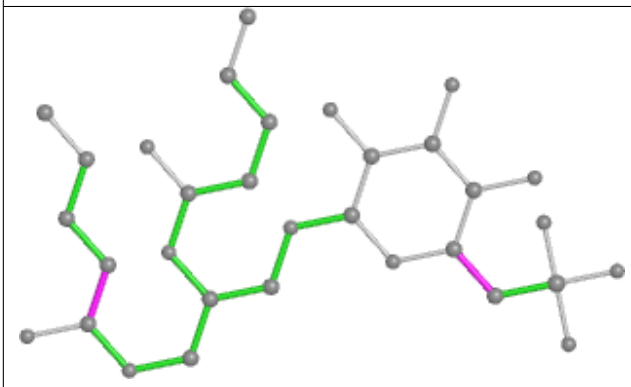
Ligand SQD 5 423



Bond lengths



Bond angles



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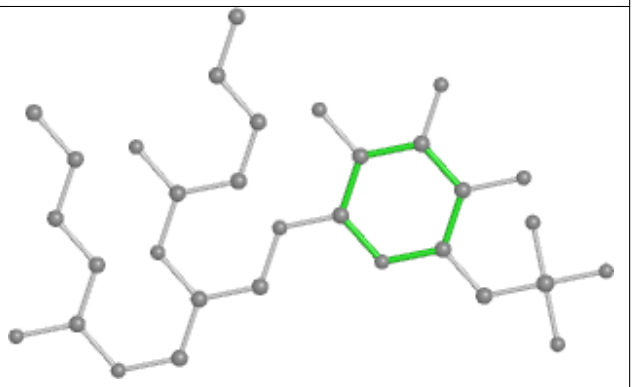
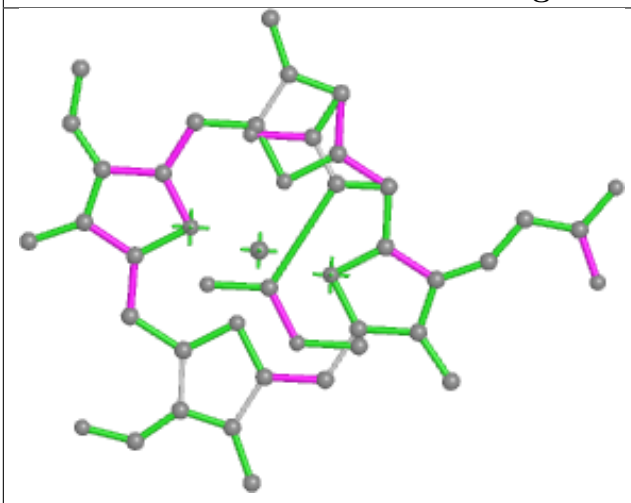


Rings

Ligand CL7 8 410



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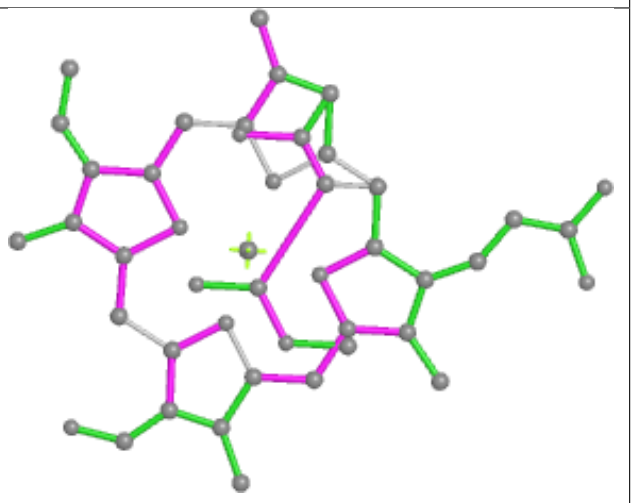
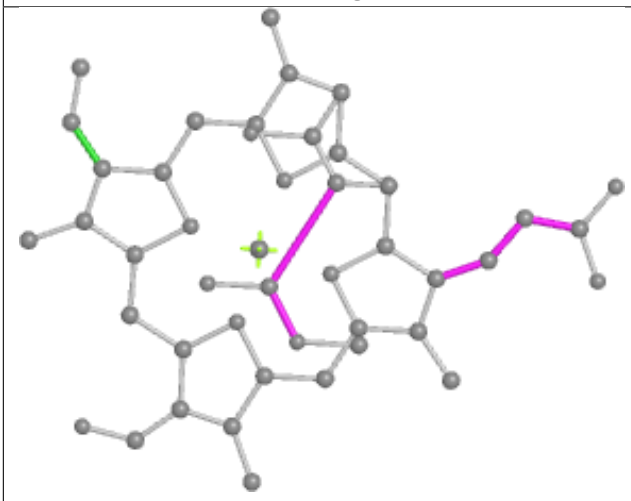


Bond angles



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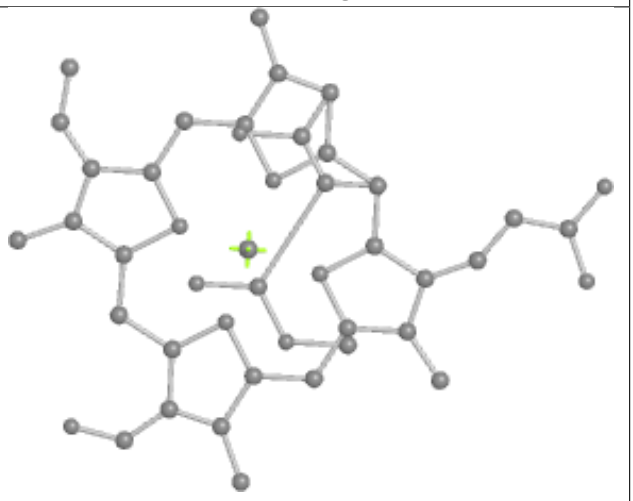
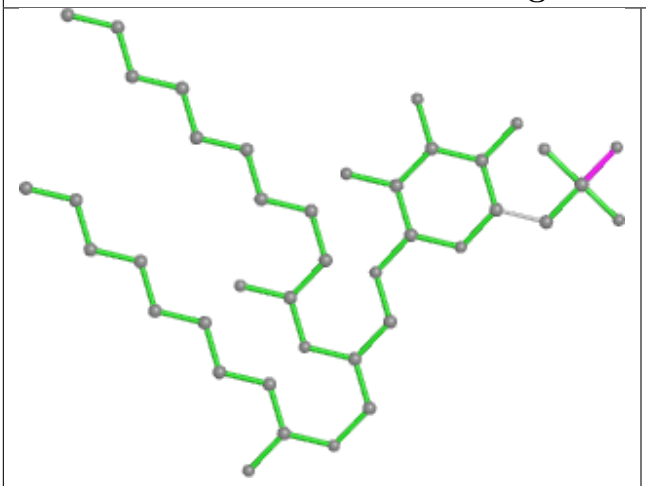
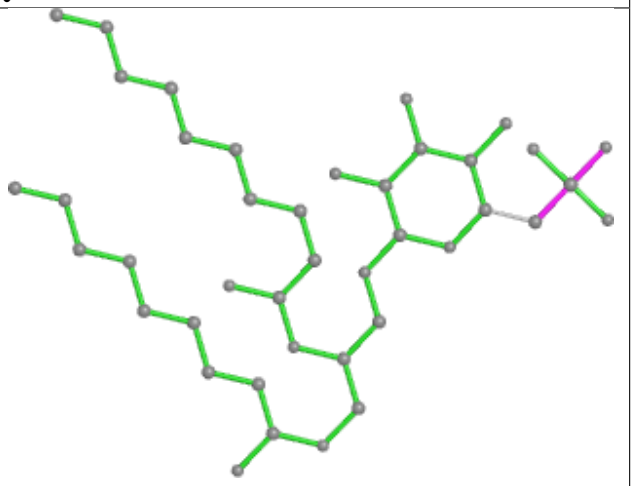


Rings

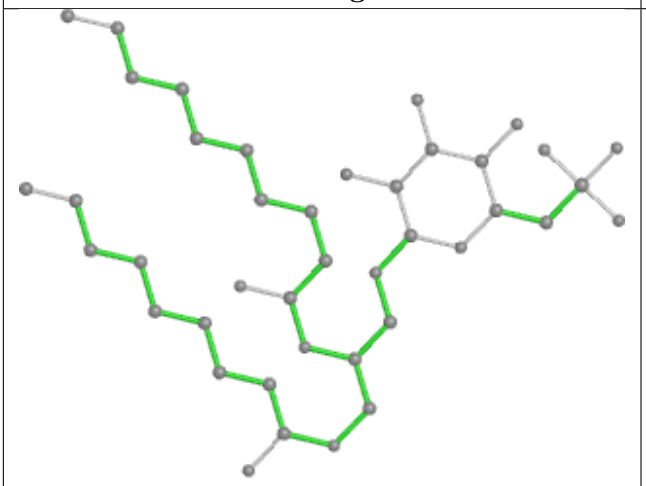
Ligand SQD 2 524



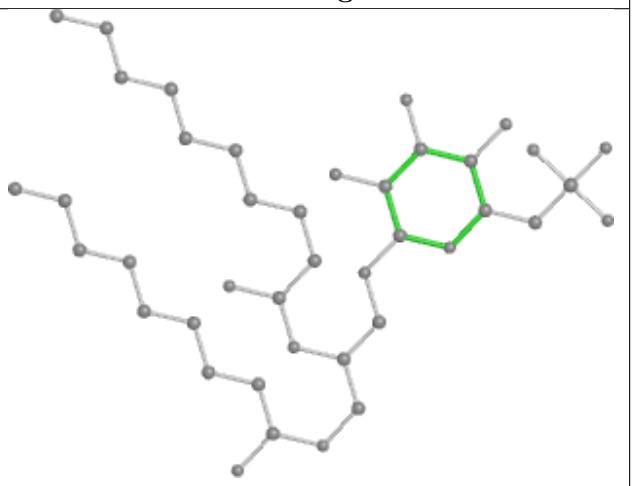
Bond lengths



Bond angles

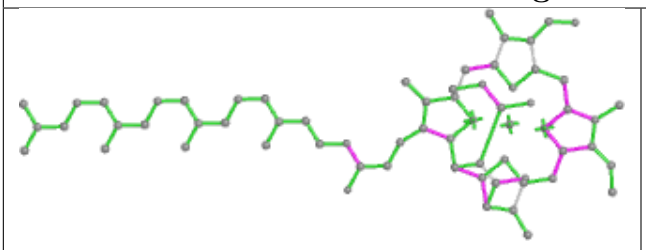


Torsions

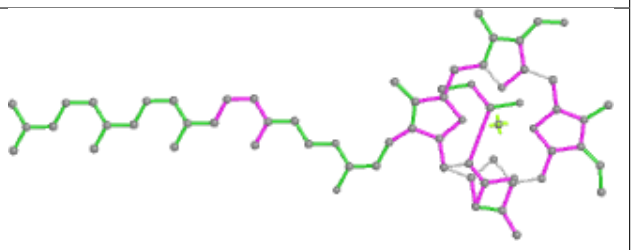


Rings

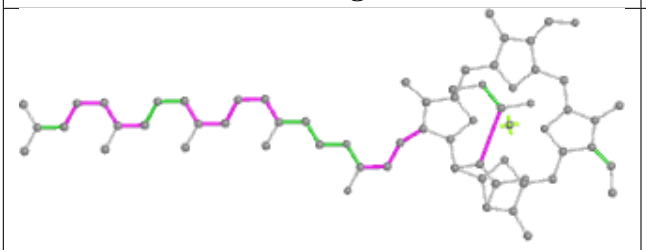
Ligand CL7 7 501



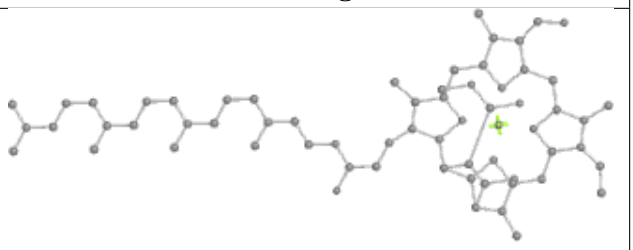
Bond lengths



Bond angles

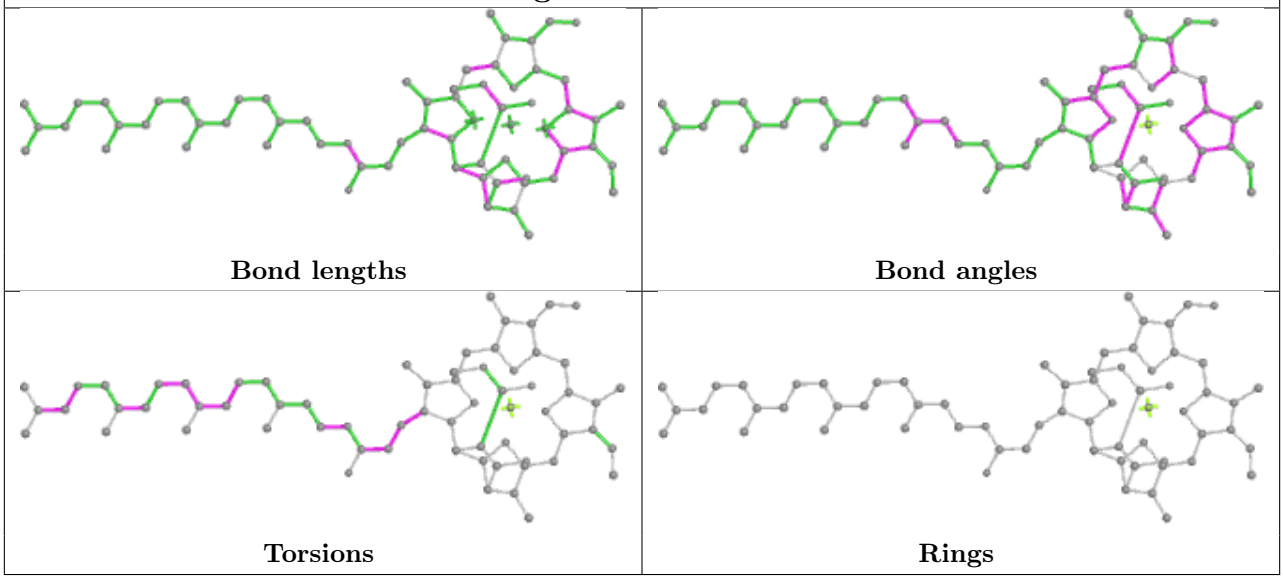


Torsions

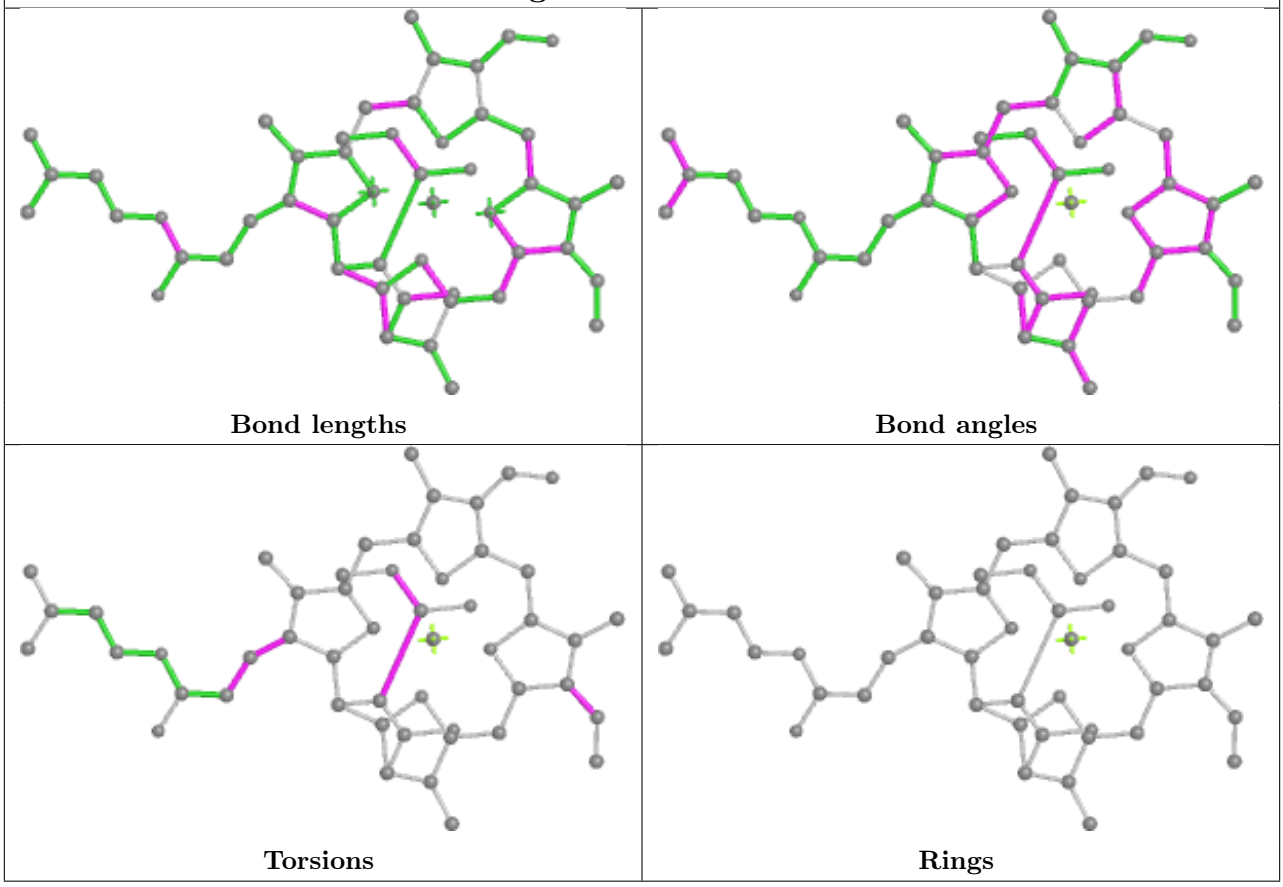


Rings

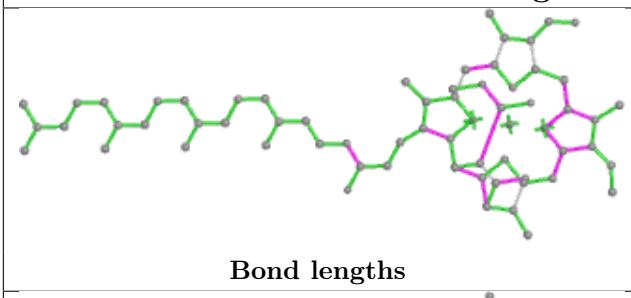
Ligand CL7 2 501



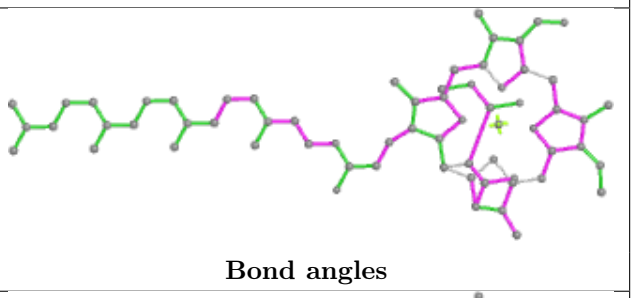
Ligand CL7 D 402



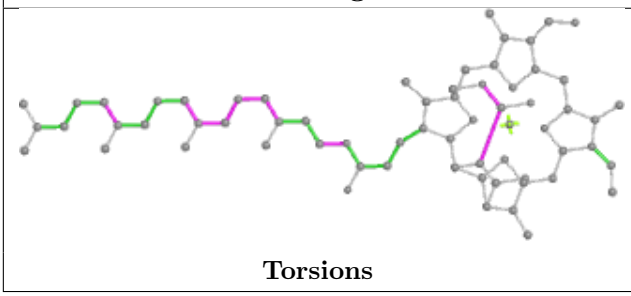
Ligand CL7 7 508



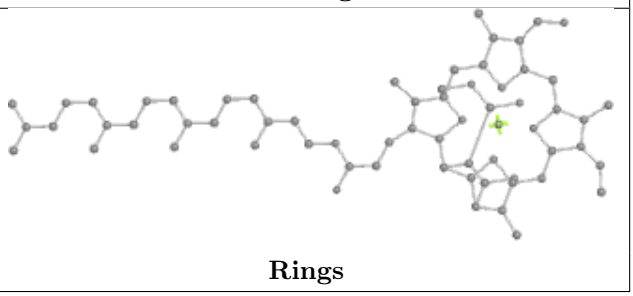
Bond lengths



Bond angles

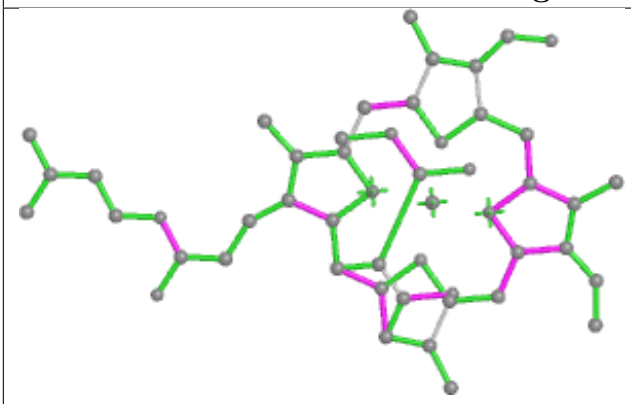


Torsions

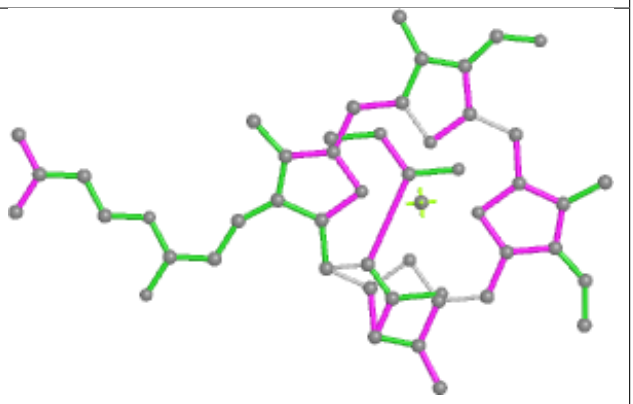


Rings

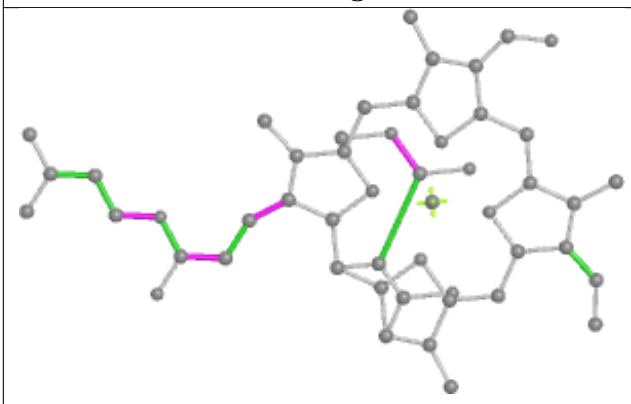
Ligand CL7 3 517



Bond lengths



Bond angles



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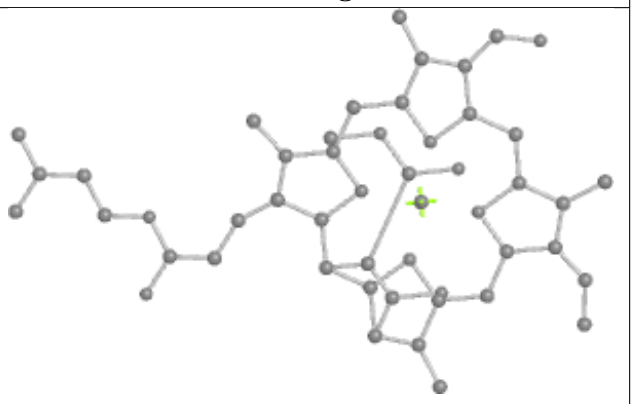
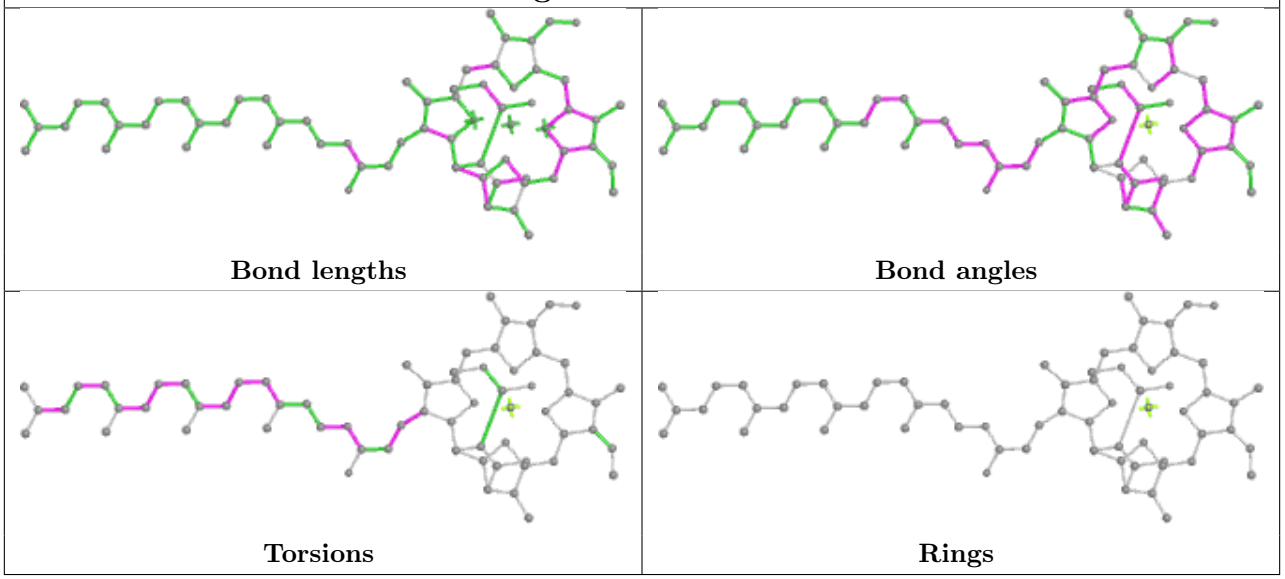
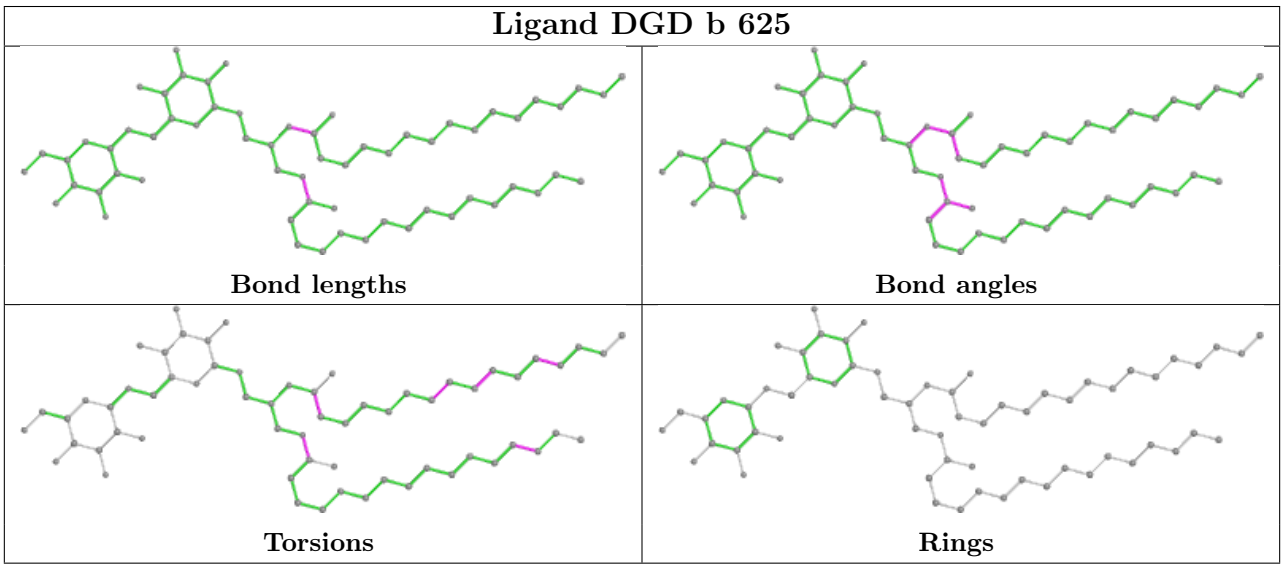


Rings

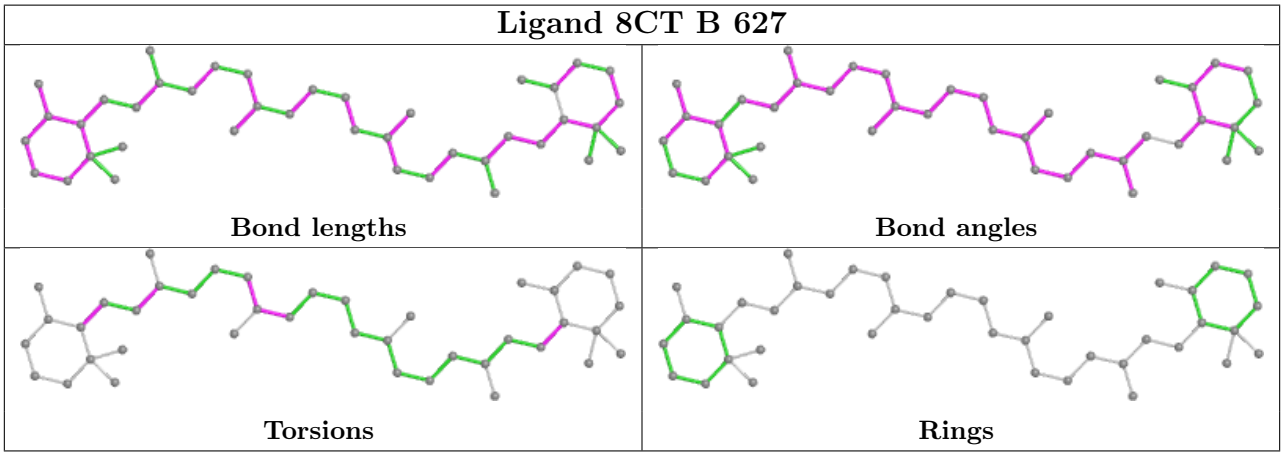
Ligand CL7 8 405



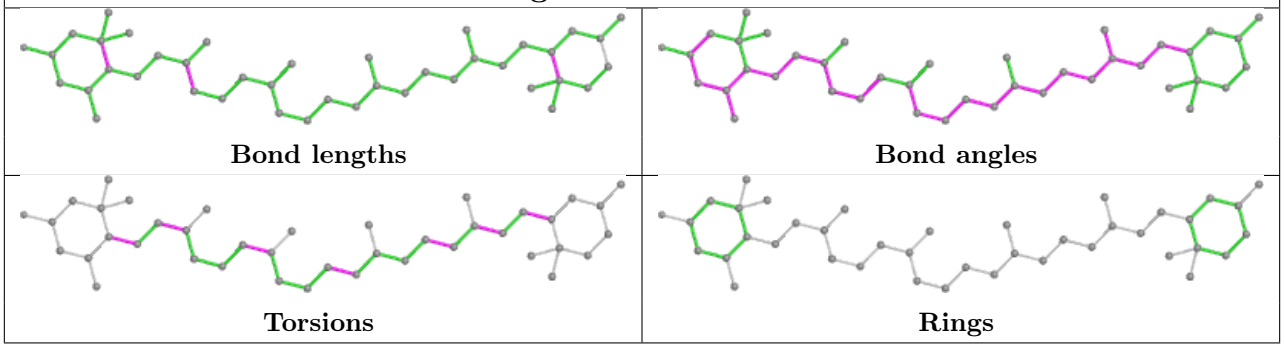
Ligand DGD b 625



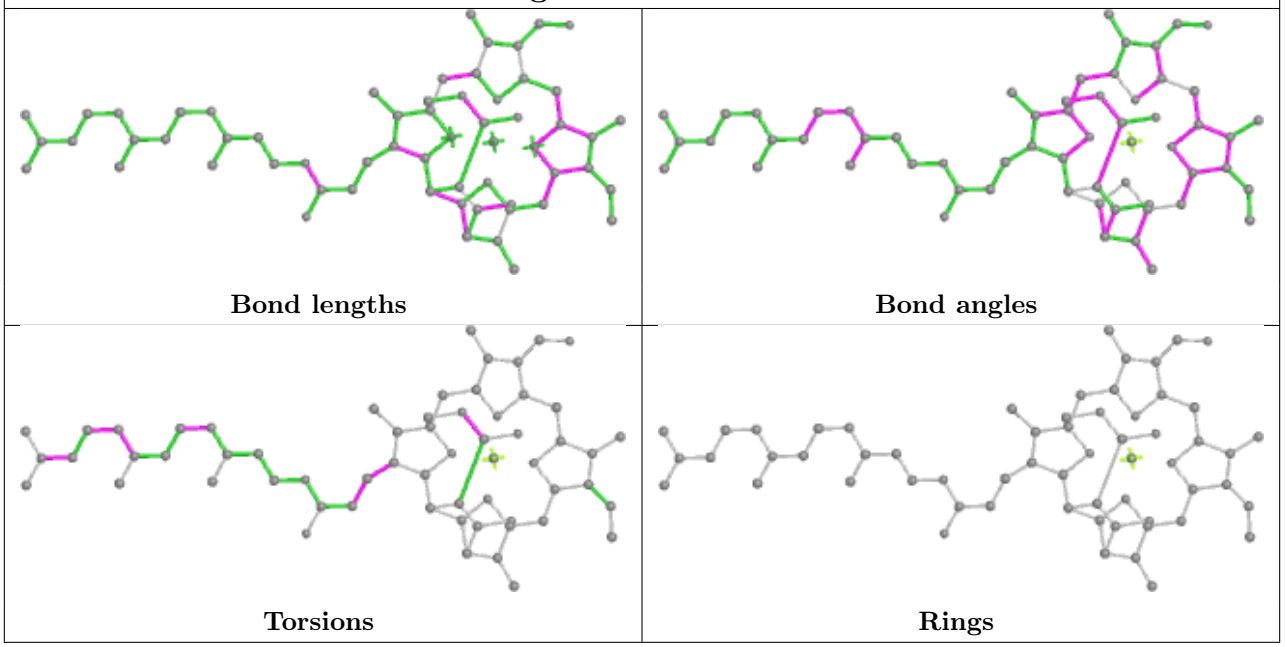
Ligand 8CT B 627



Ligand ZEX 6 519



Ligand CL7 B 607



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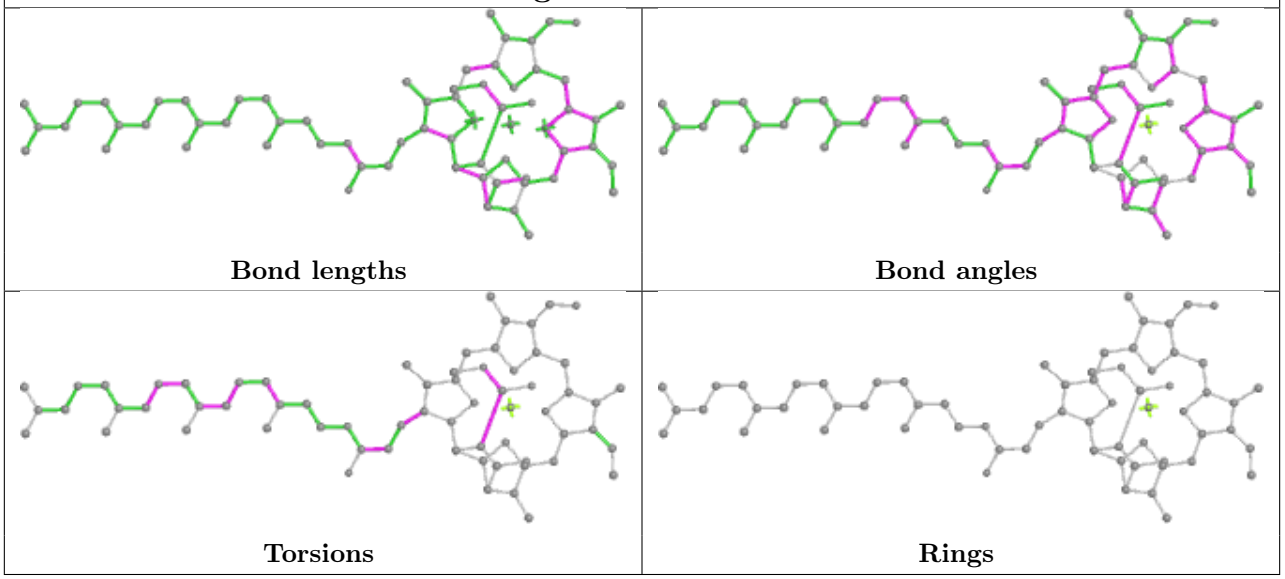
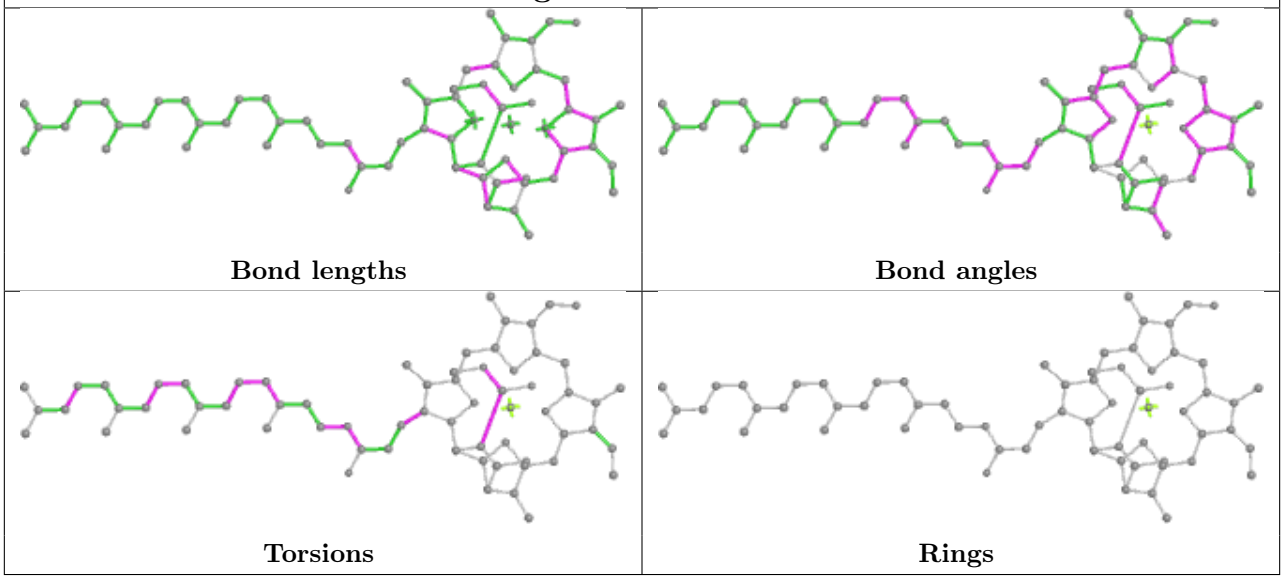
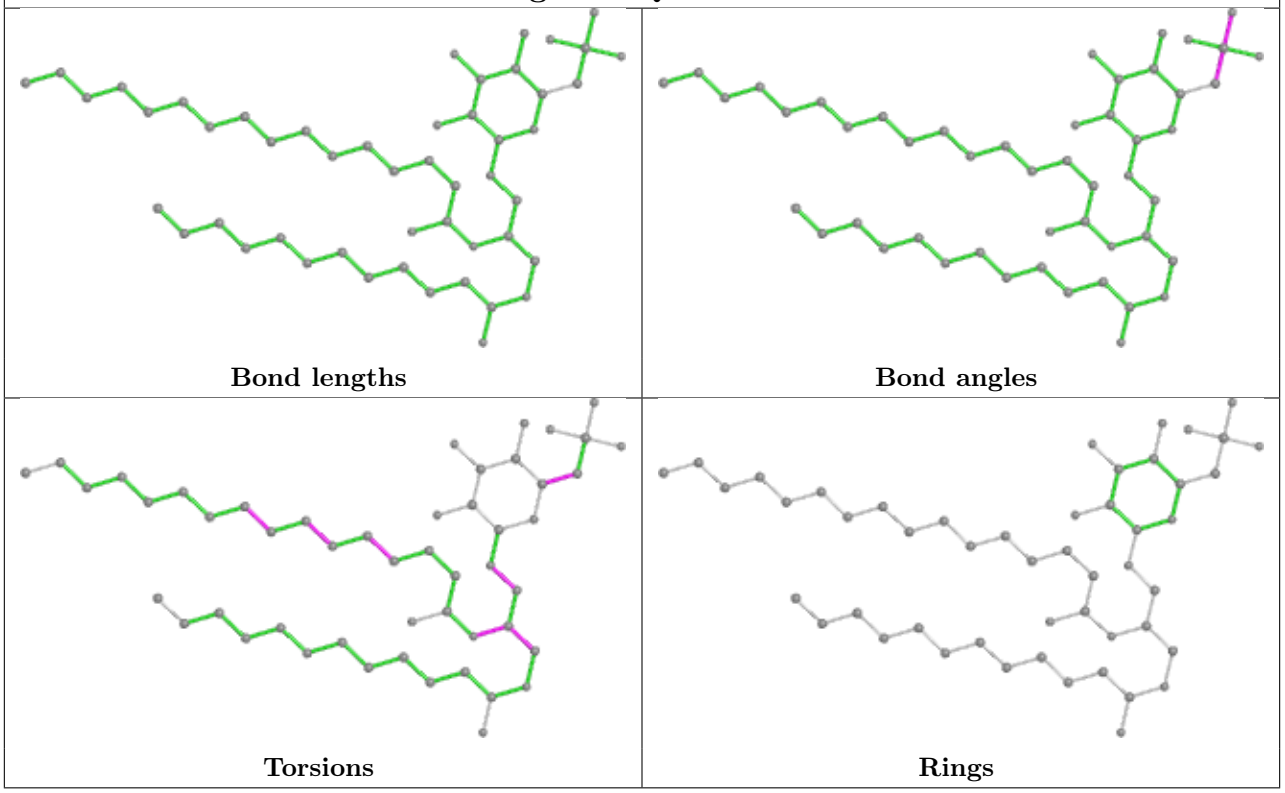


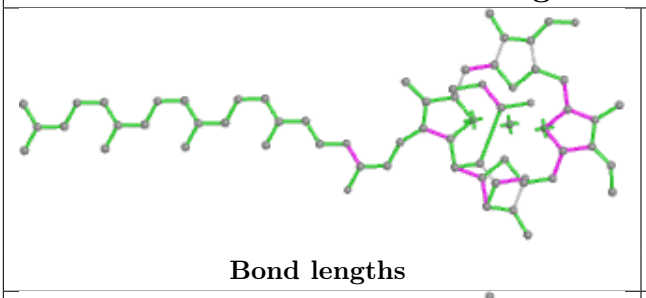
Ligand CL7 5 410



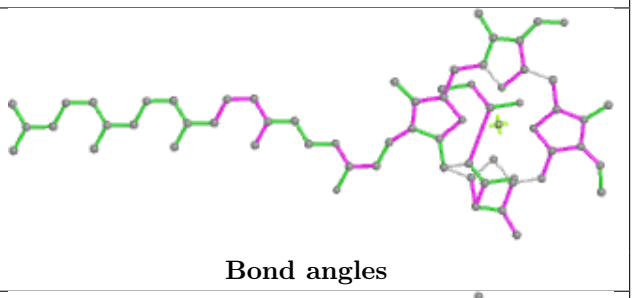
Ligand SQD 7 523



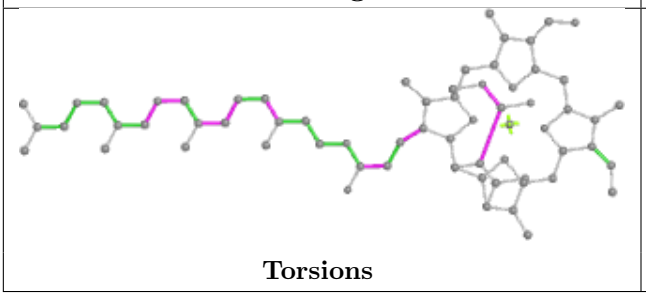
Ligand CL7 3 510



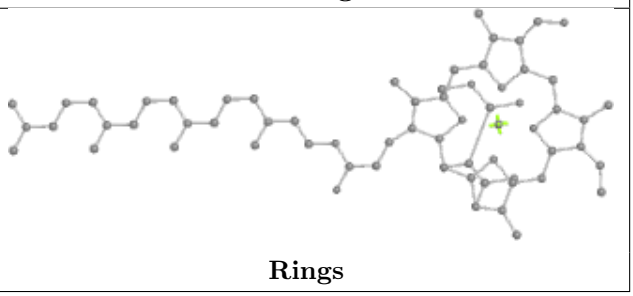
Bond lengths



Bond angles

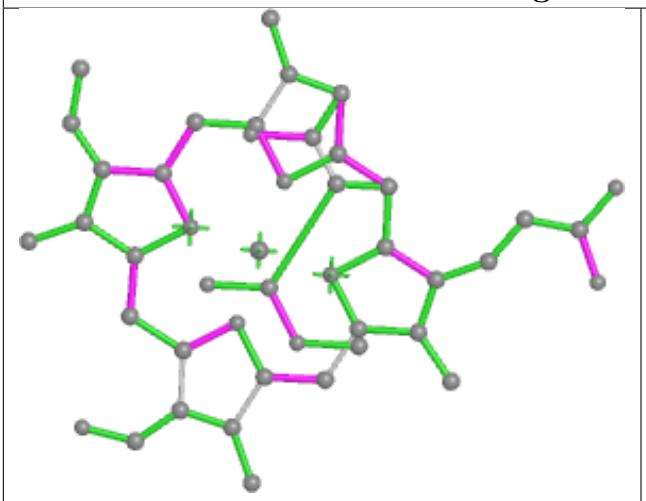


Torsions

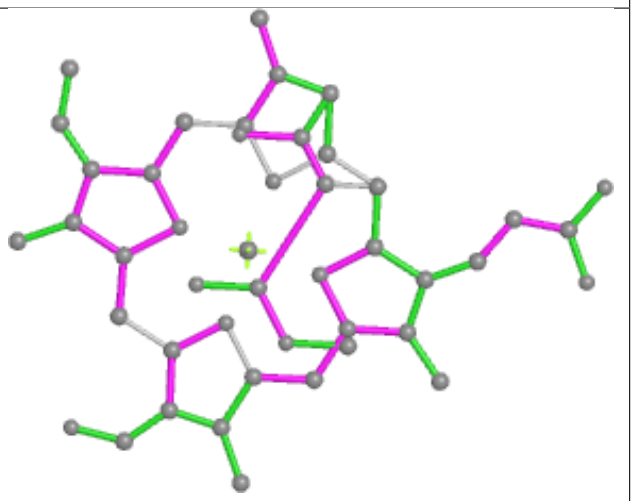


Rings

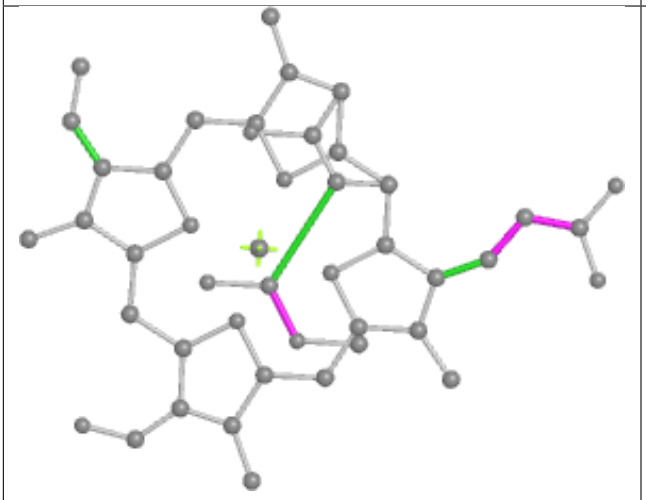
Ligand CL7 7 518



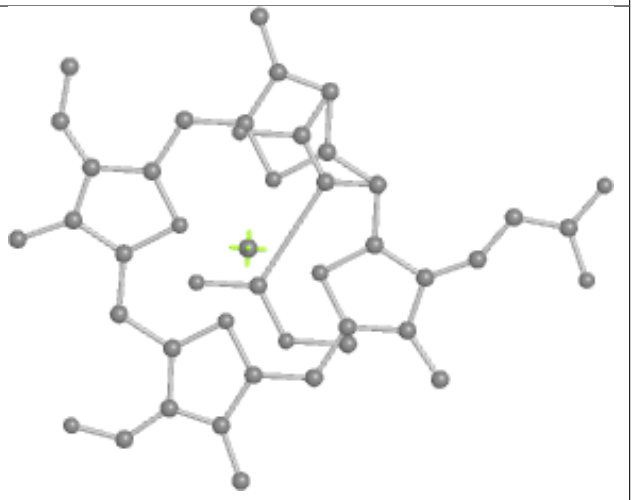
Bond lengths



Bond angles

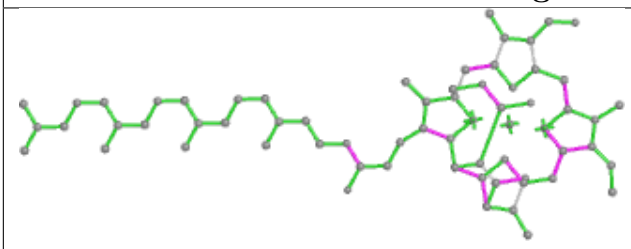


Torsions

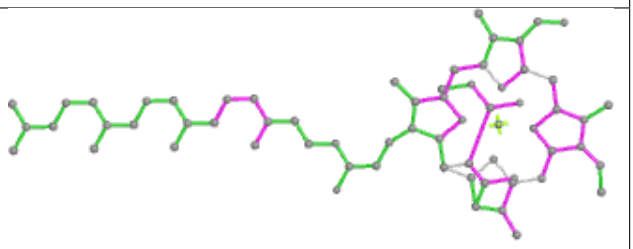


Rings

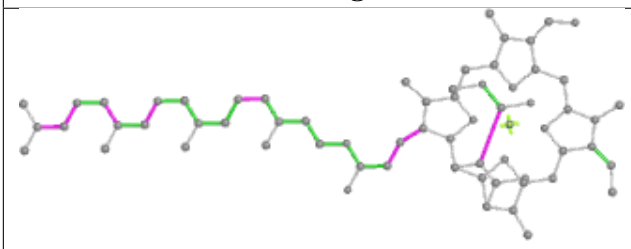
Ligand CL7 2 518



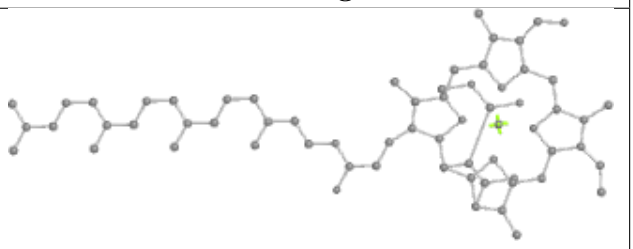
Bond lengths



Bond angles

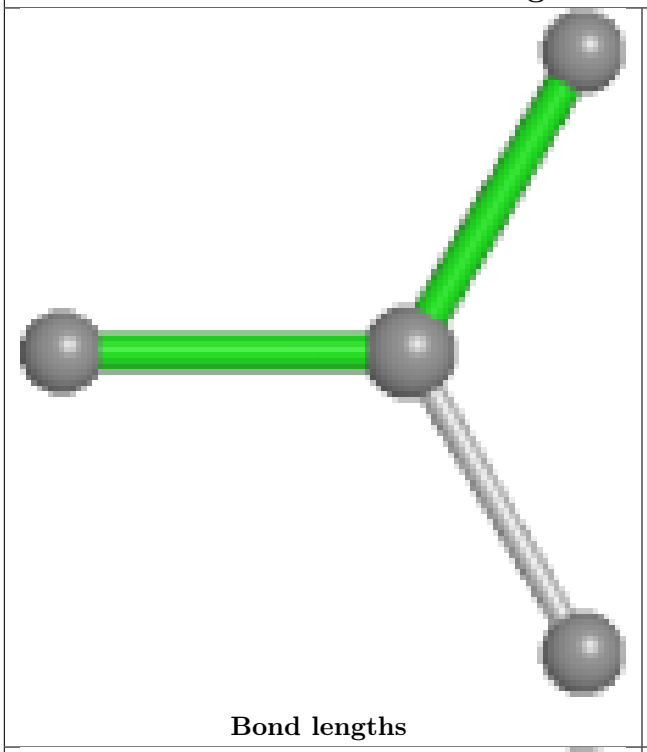


Torsions

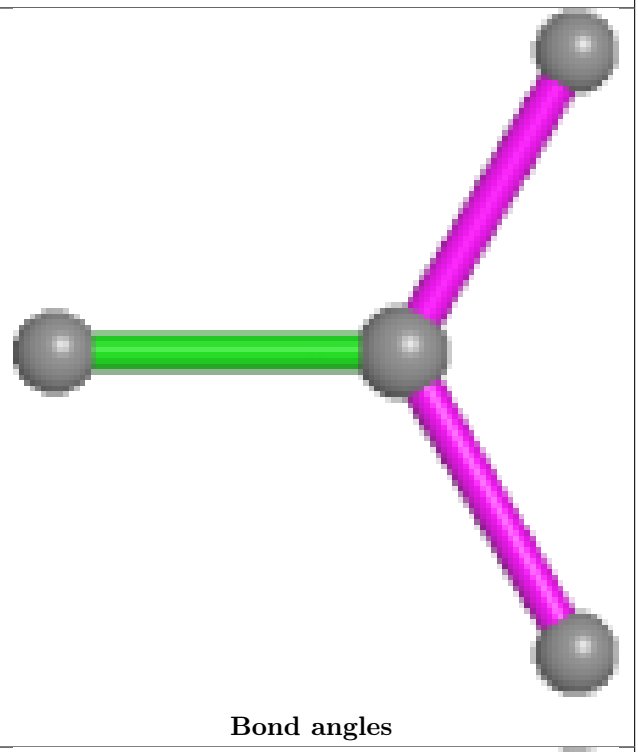


Rings

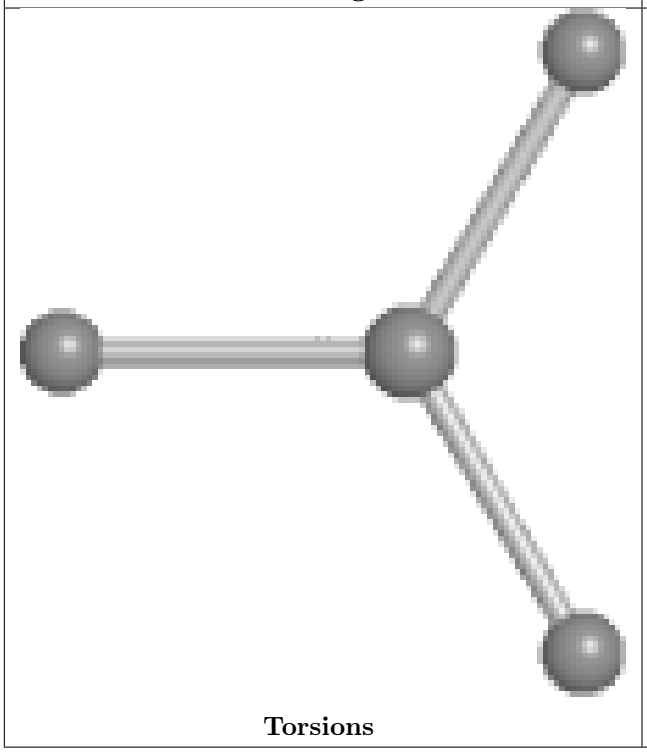
Ligand BCT d 403



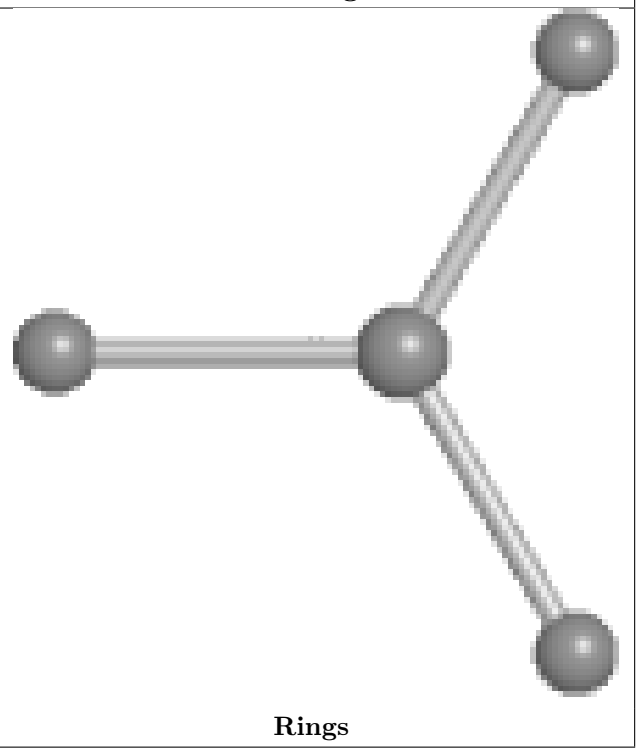
Bond lengths



Bond angles

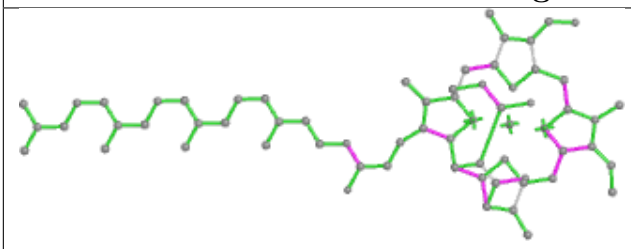


Torsions

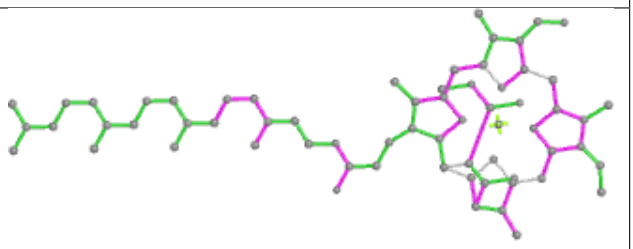


Rings

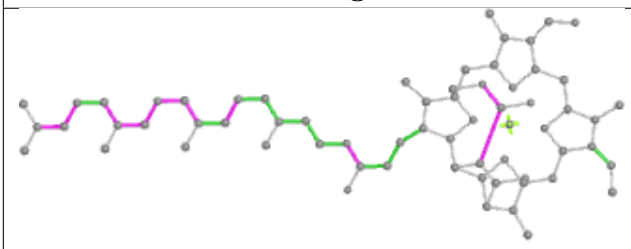
Ligand CL7 7 509



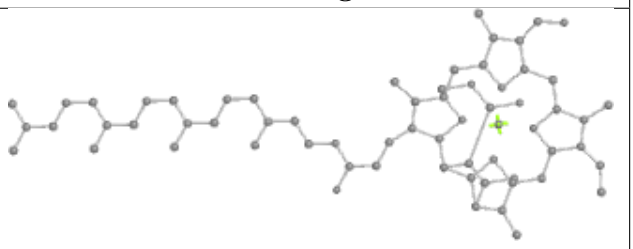
Bond lengths



Bond angles

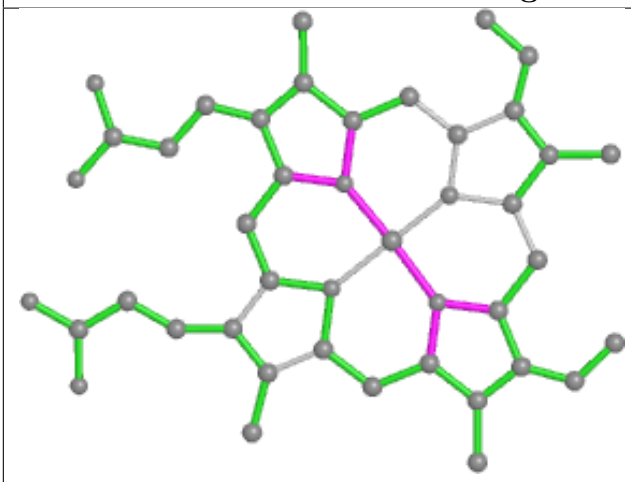


Torsions

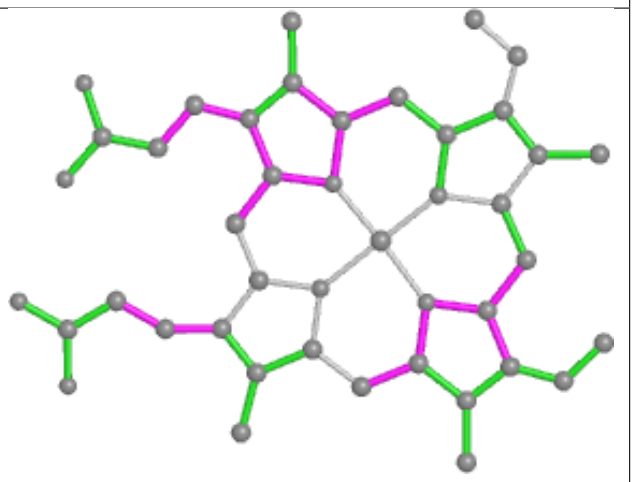


Rings

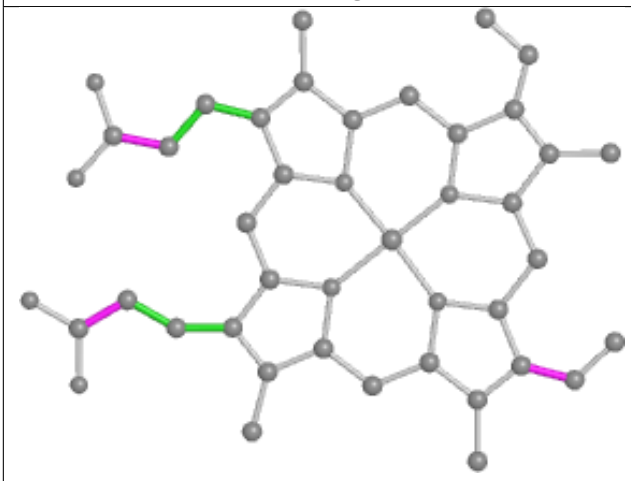
Ligand HEM F 101



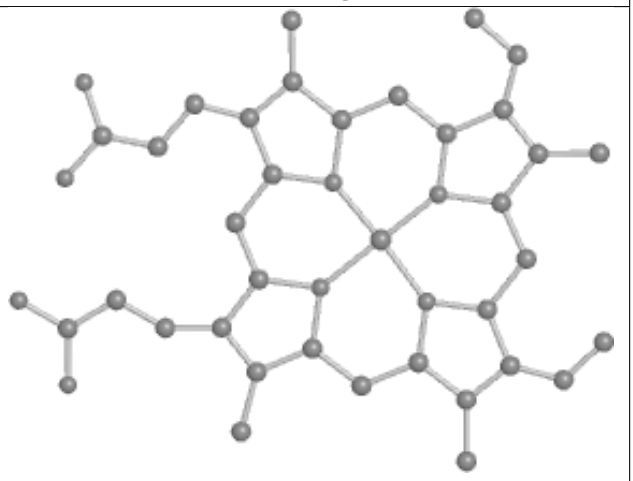
Bond lengths



Bond angles

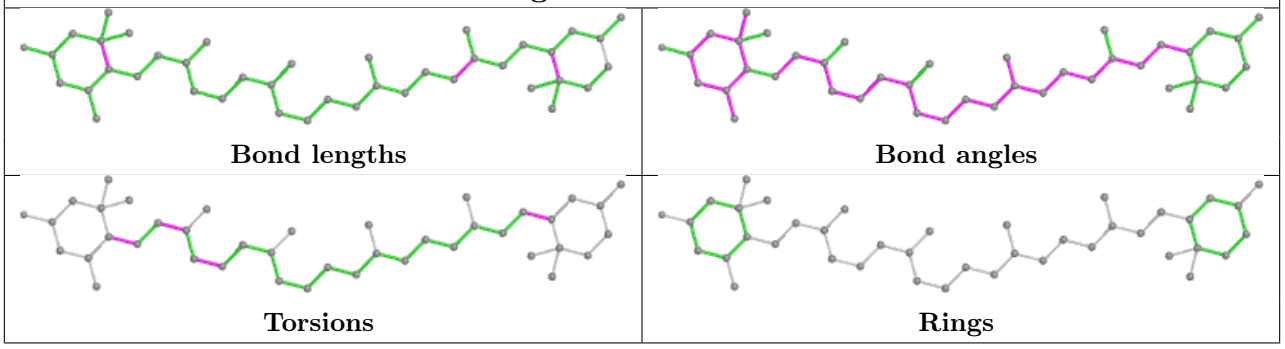


Torsions

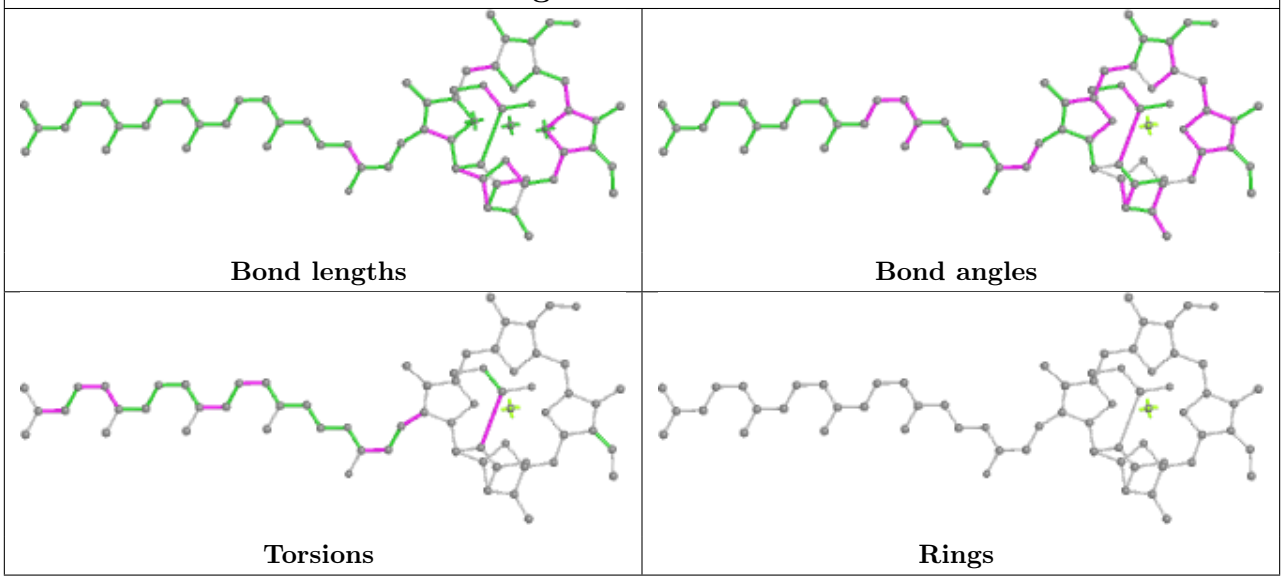


Rings

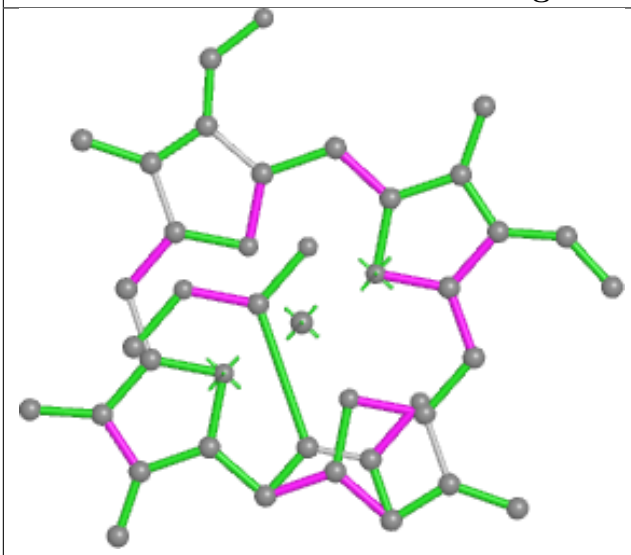
Ligand ZEX 6 520



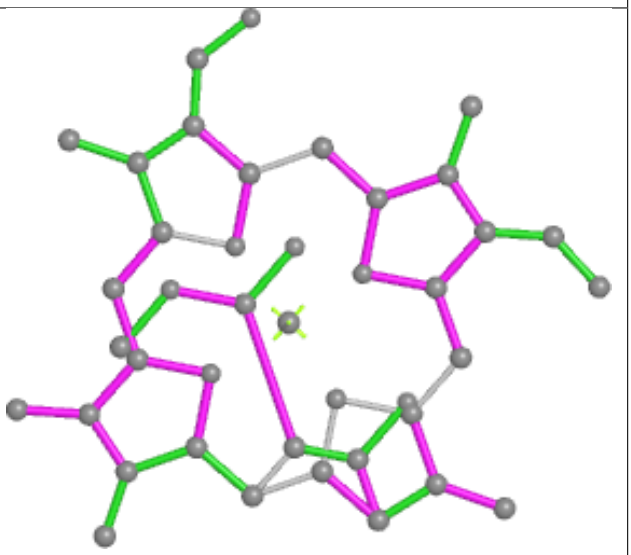
Ligand CL7 b 610



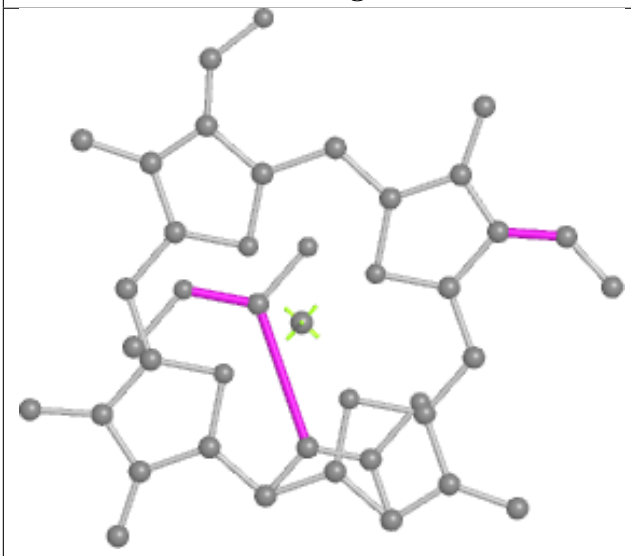
Ligand CL7 1 415



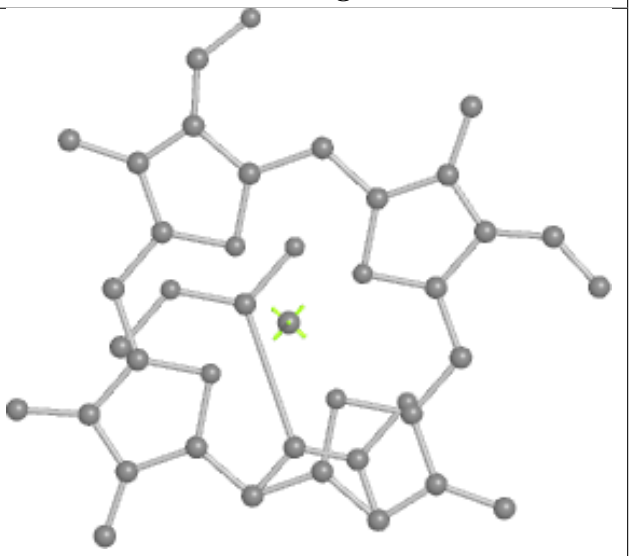
Bond lengths



Bond angles

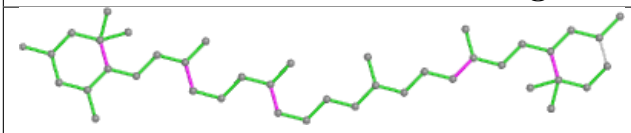


Torsions

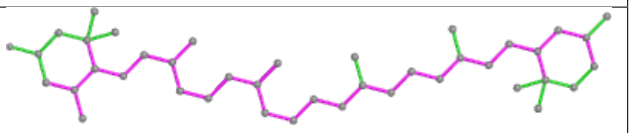


Rings

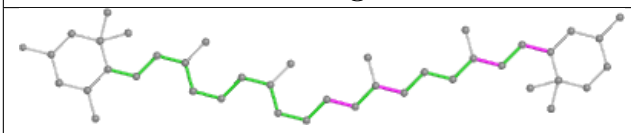
Ligand ZEX 2 520



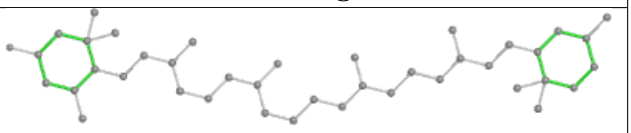
Bond lengths



Bond angles

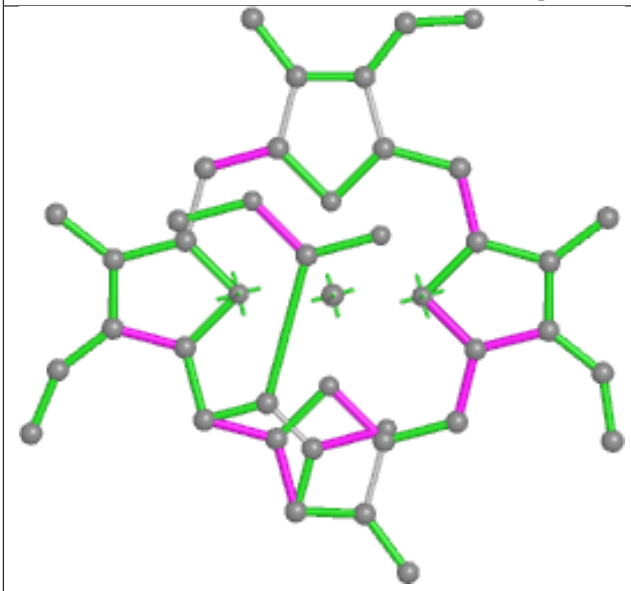


Torsions

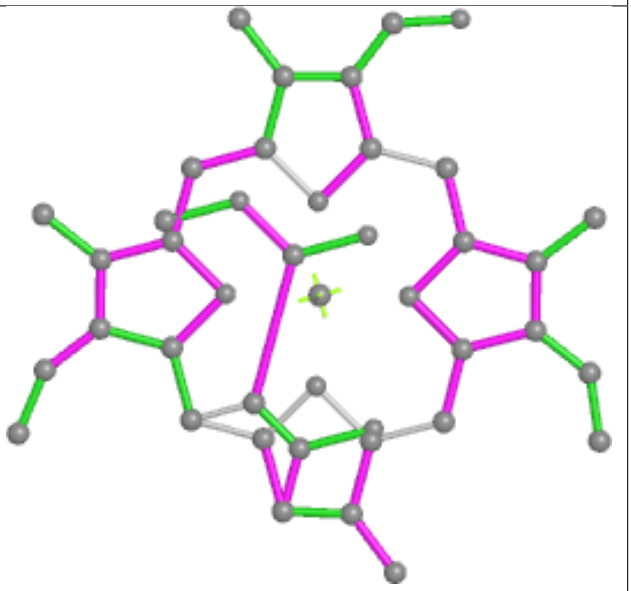


Rings

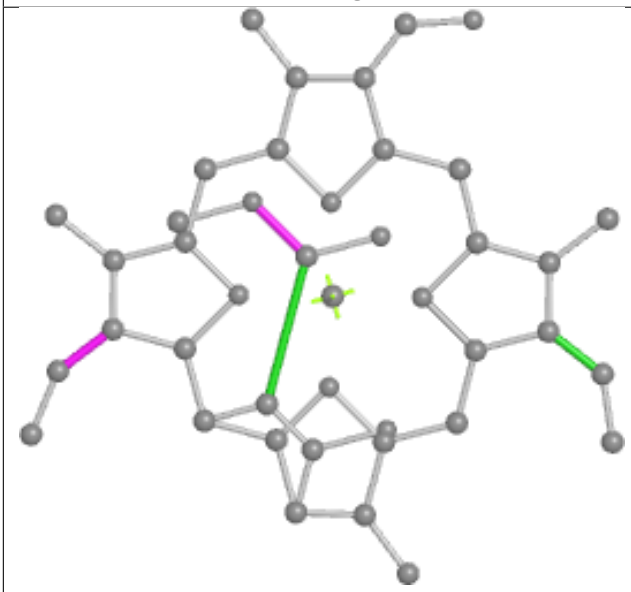
Ligand CL7 4 417



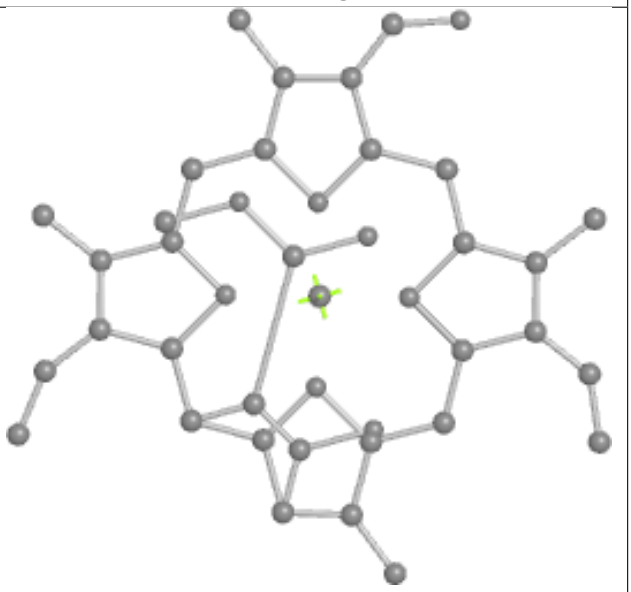
Bond lengths



Bond angles

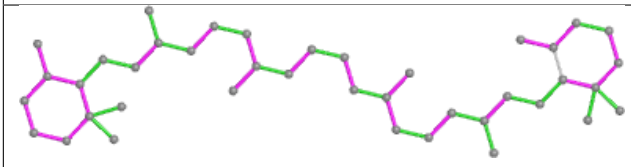


Torsions

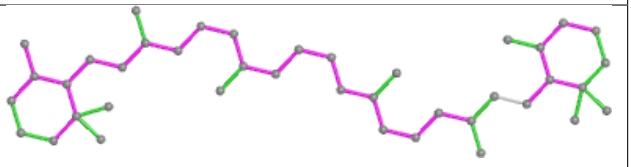


Rings

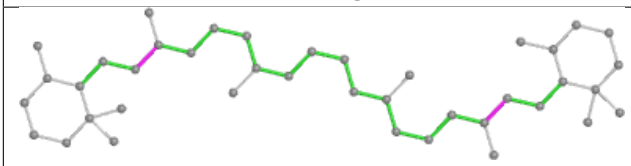
Ligand 8CT b 620



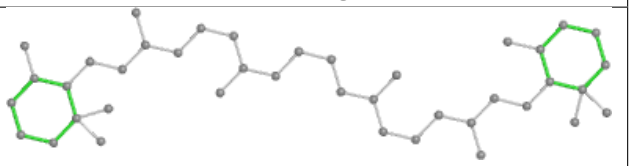
Bond lengths



Bond angles

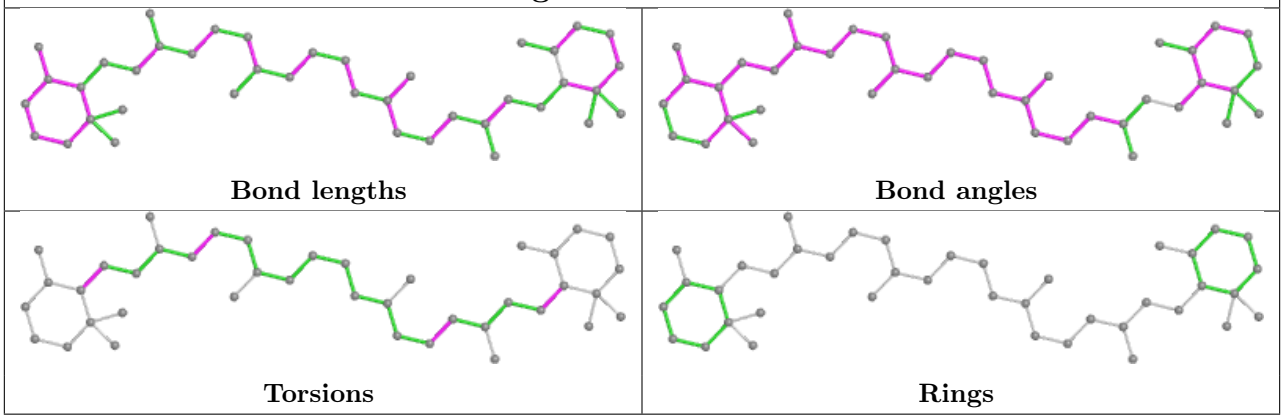


Torsions

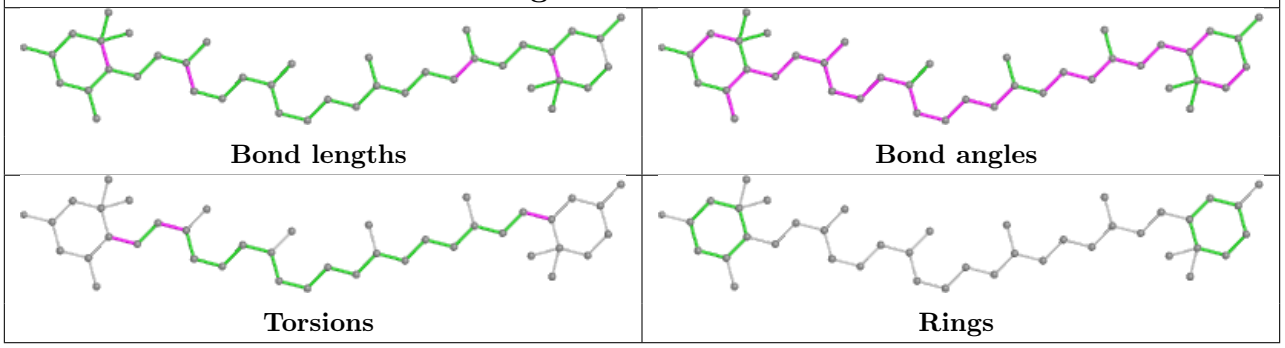


Rings

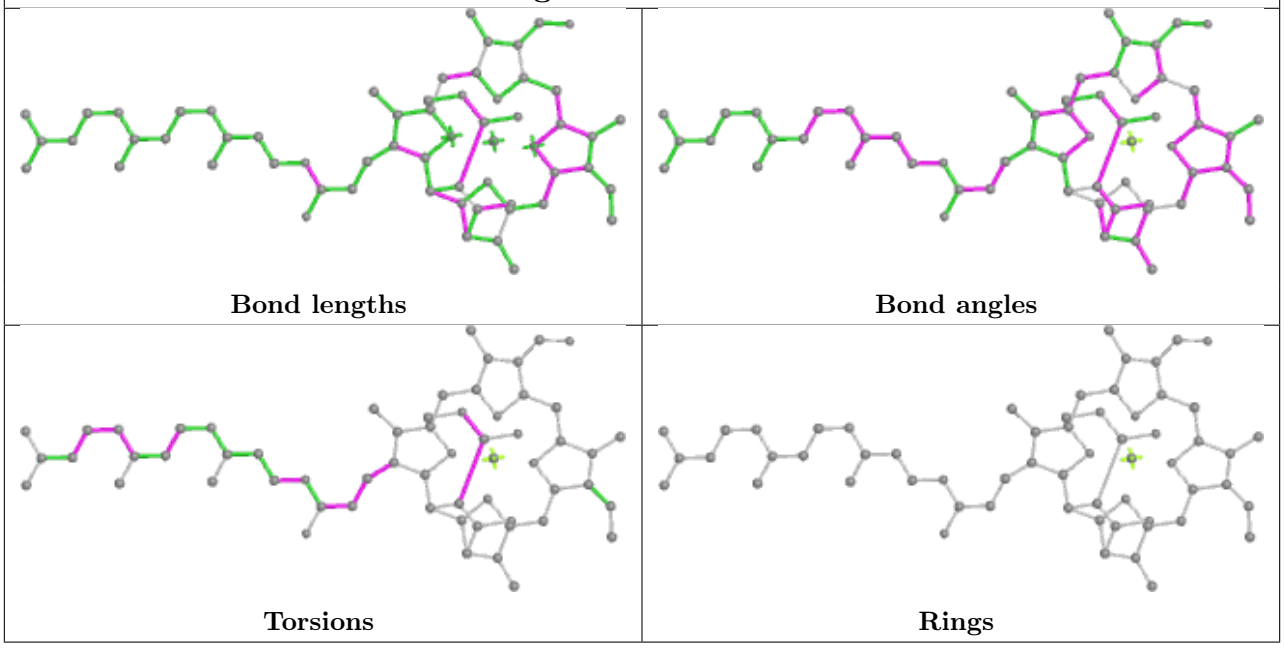
Ligand 8CT 8 402



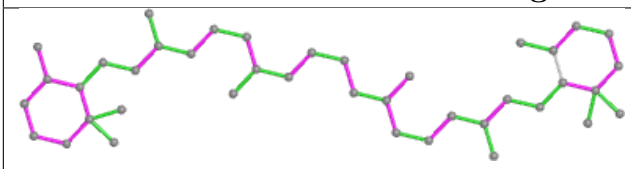
Ligand ZEX 7 522



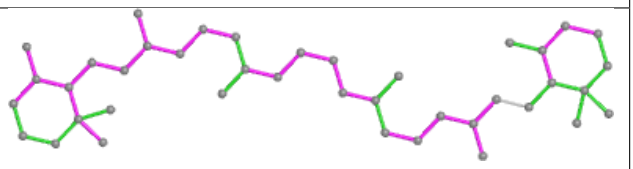
Ligand CL7 4 409



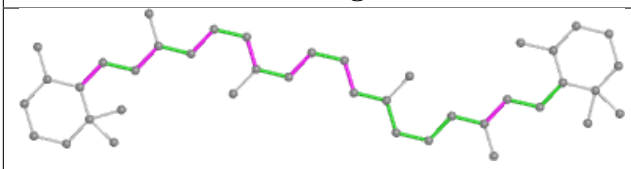
Ligand 8CT b 619



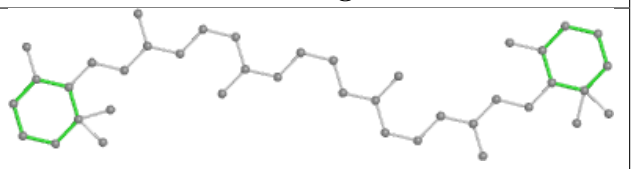
Bond lengths



Bond angles

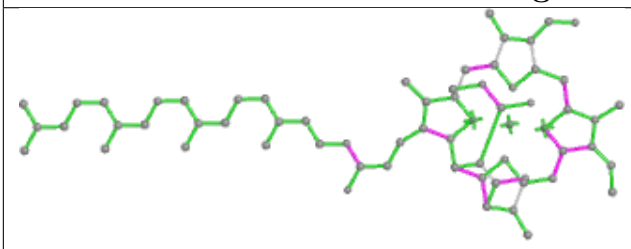


Torsions

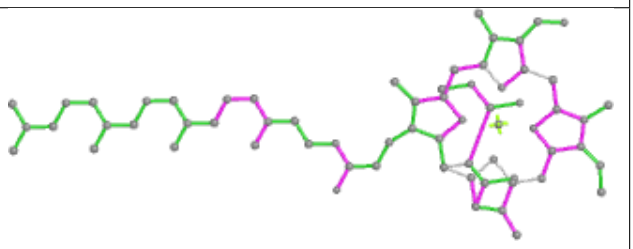


Rings

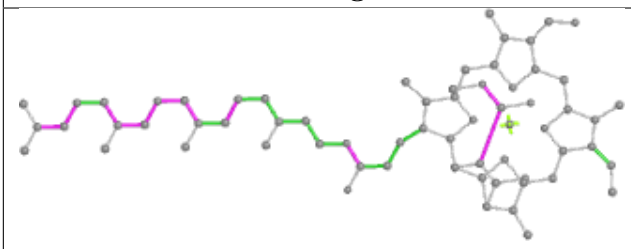
Ligand CL7 3 509



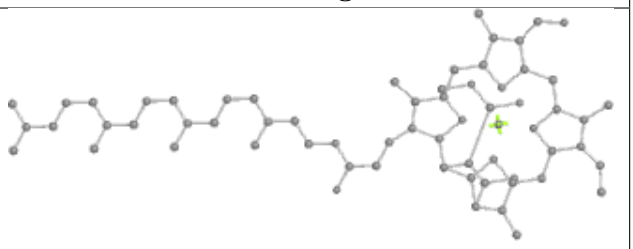
Bond lengths



Bond angles

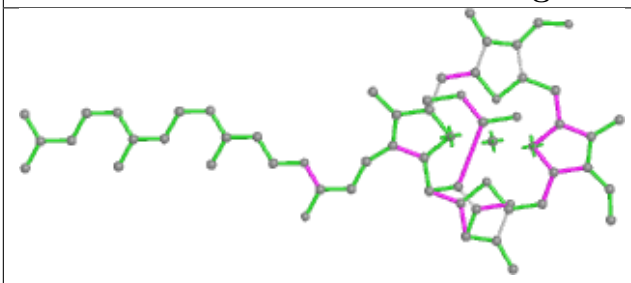


Torsions

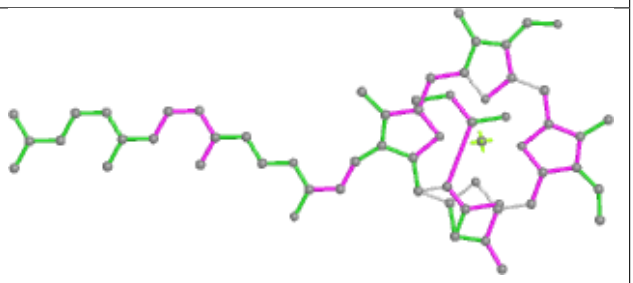


Rings

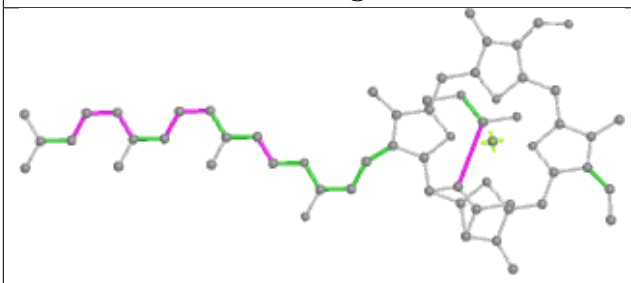
Ligand CL7 4 413



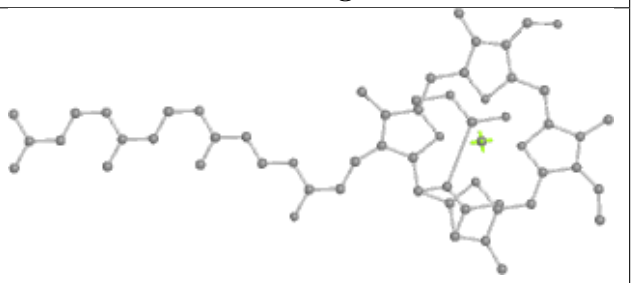
Bond lengths



Bond angles

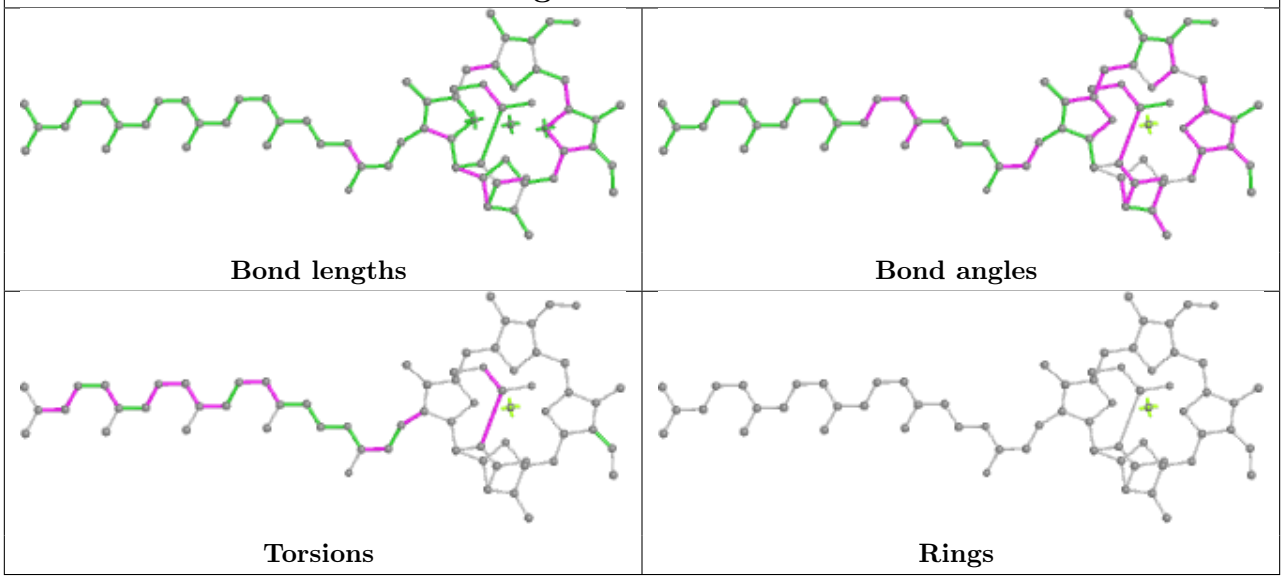


Torsions

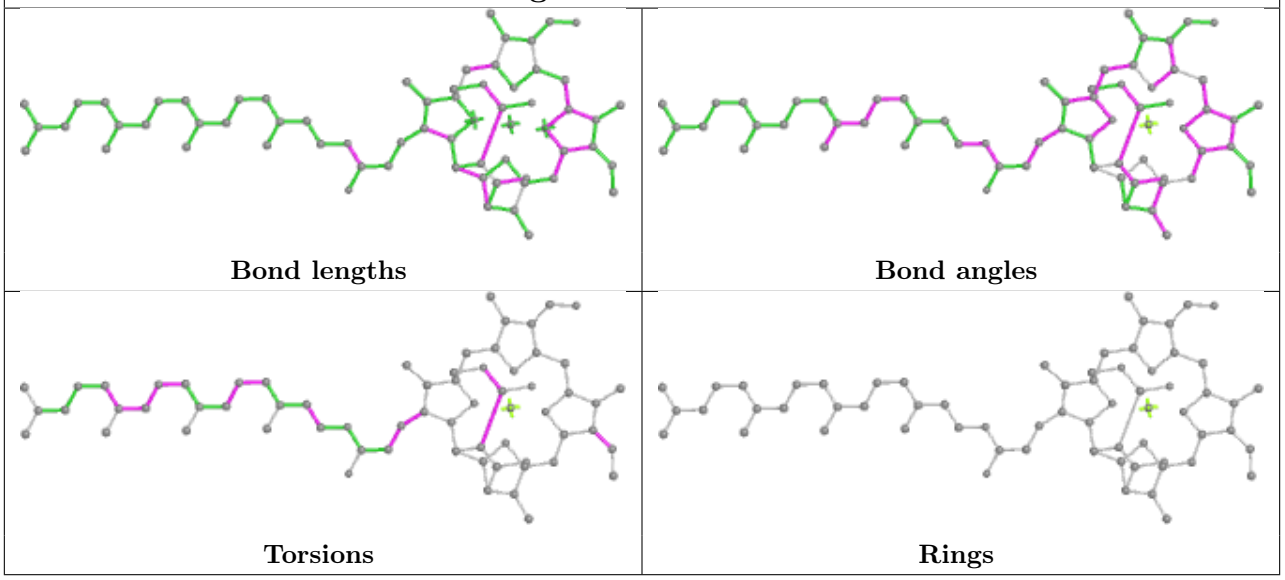


Rings

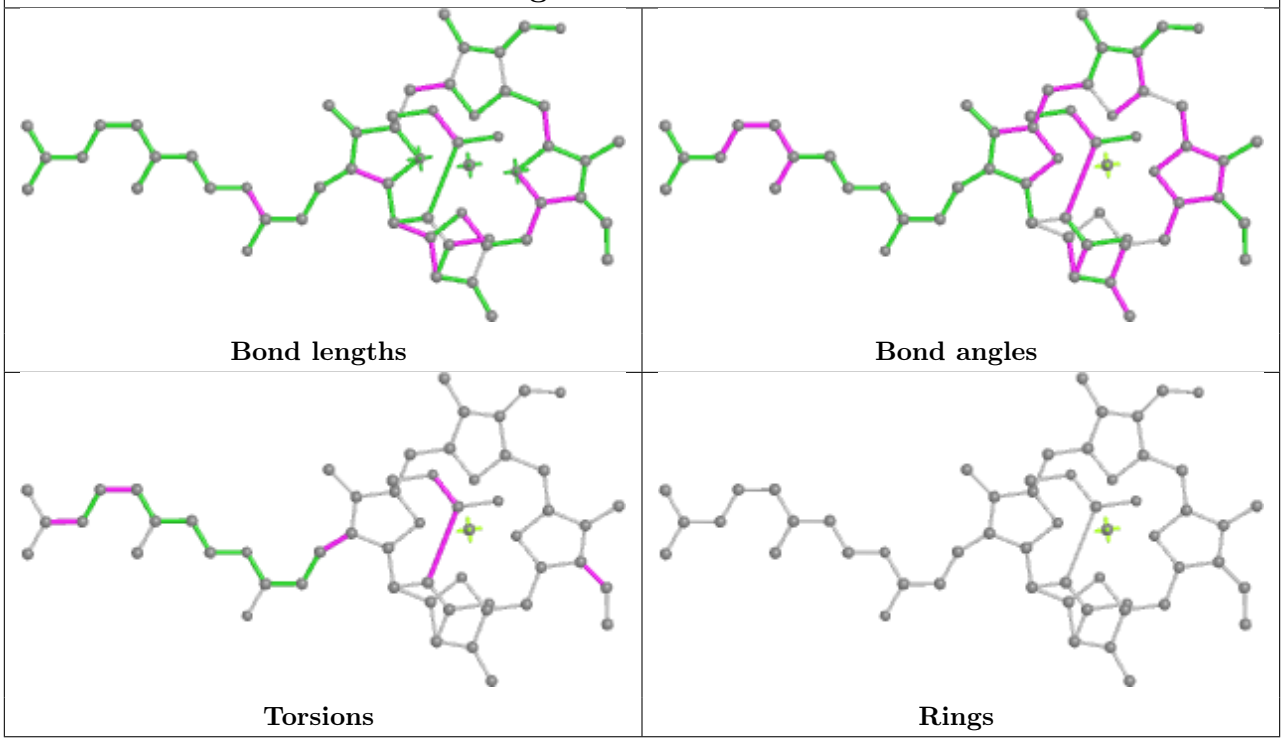
Ligand CL7 1 418



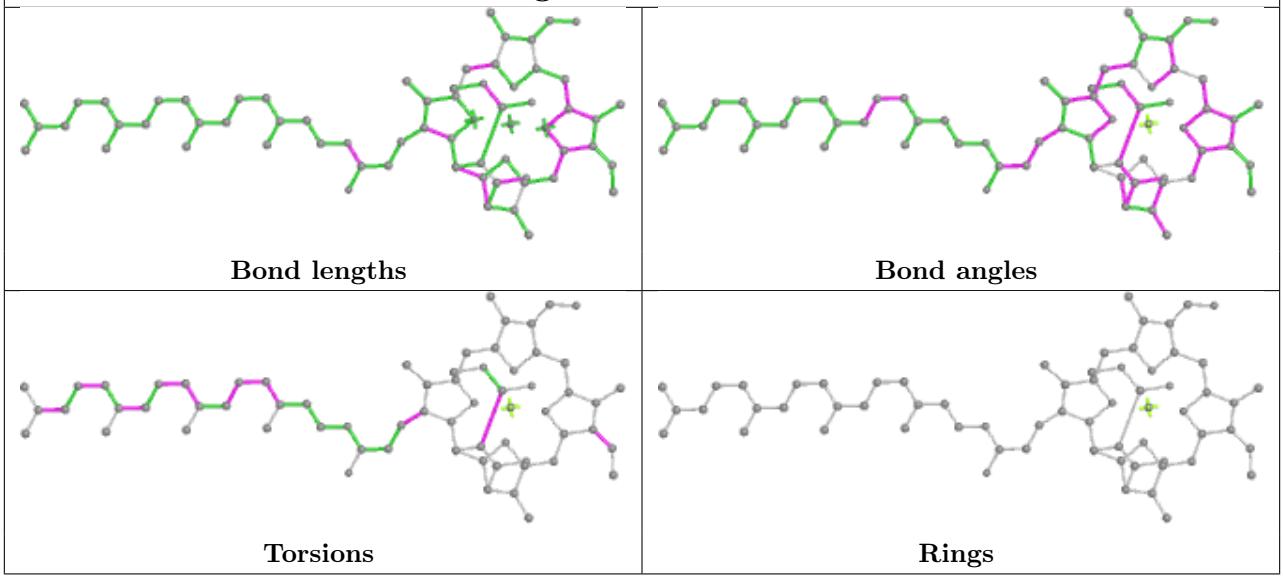
Ligand CL7 C 506



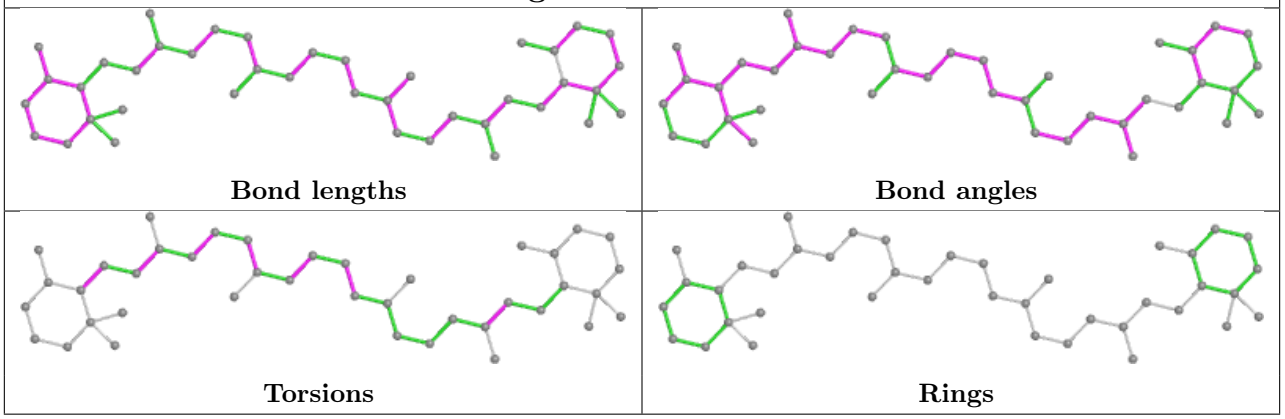
Ligand CL7 C 505



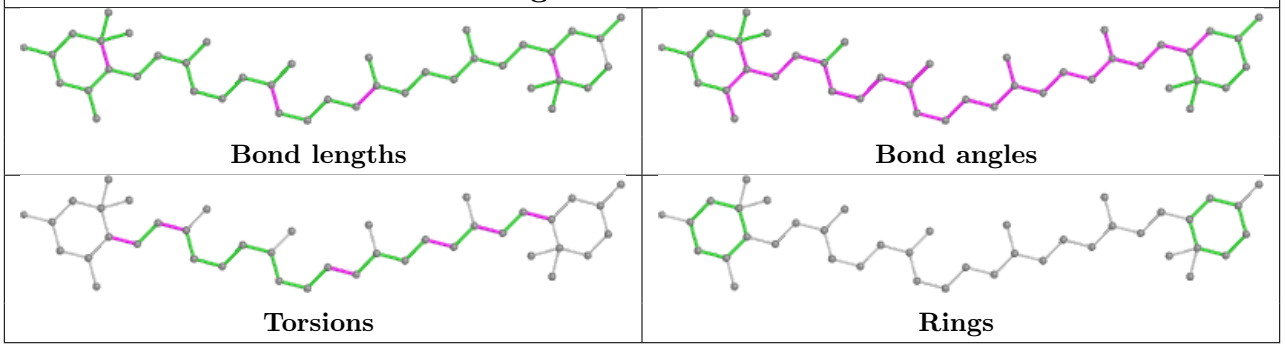
Ligand CL7 3 504



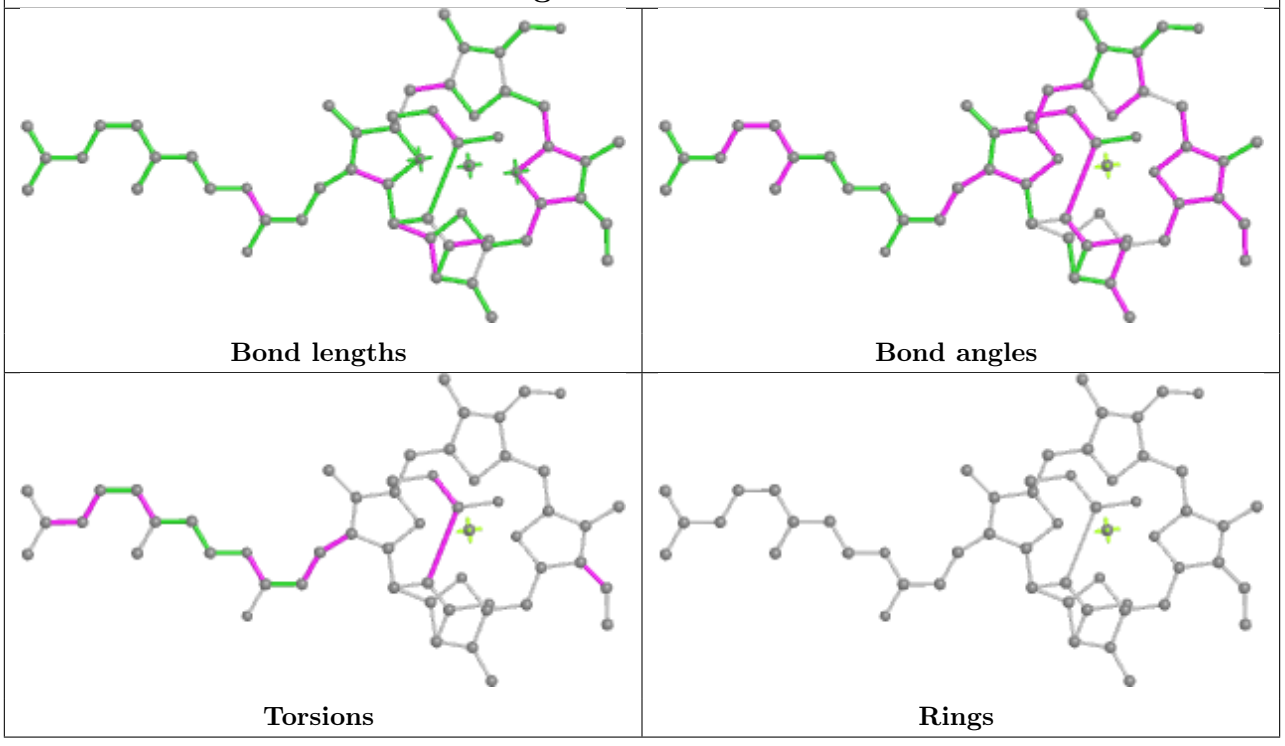
Ligand 8CT B 618



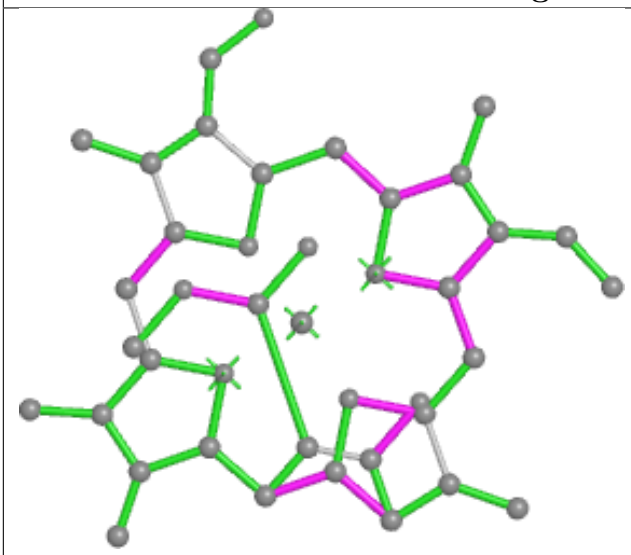
Ligand ZEX 4 403



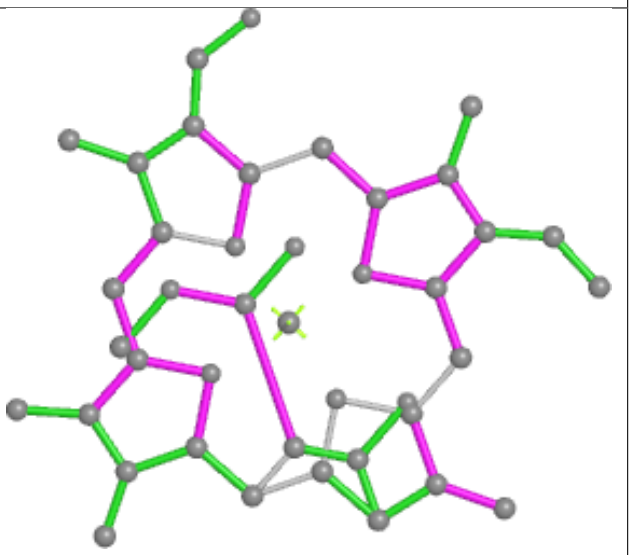
Ligand CL7 7 516



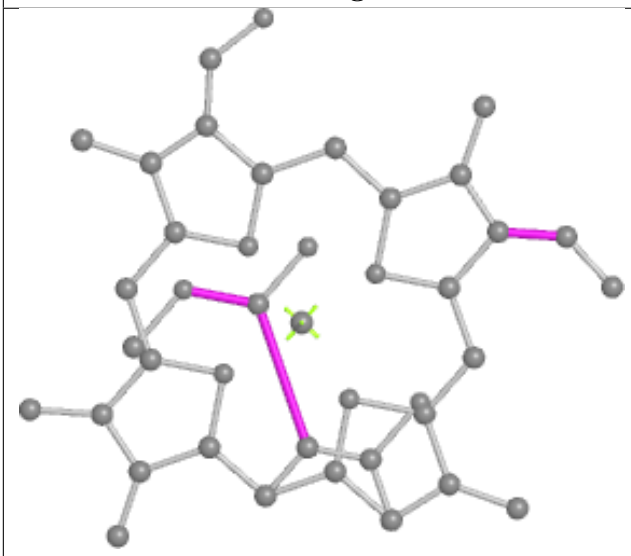
Ligand CL7 b 602



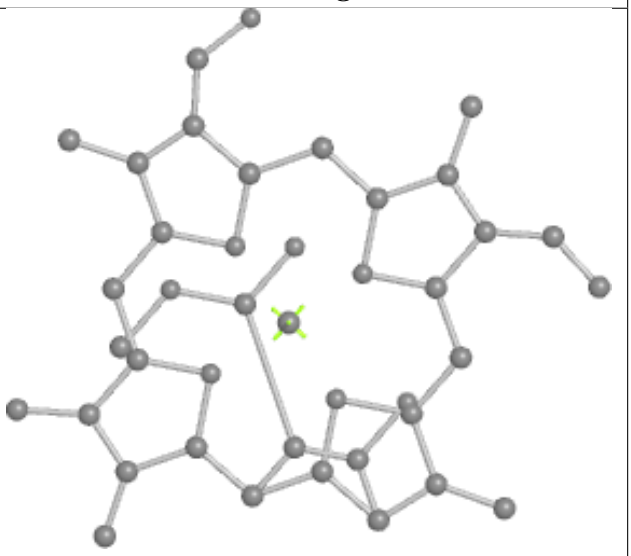
Bond lengths



Bond angles

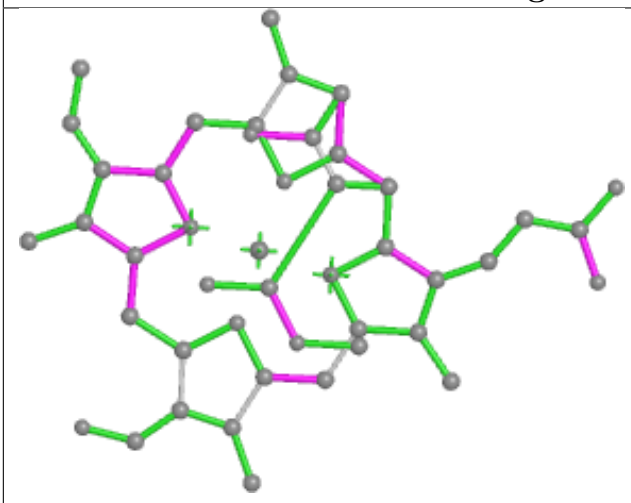


Torsions

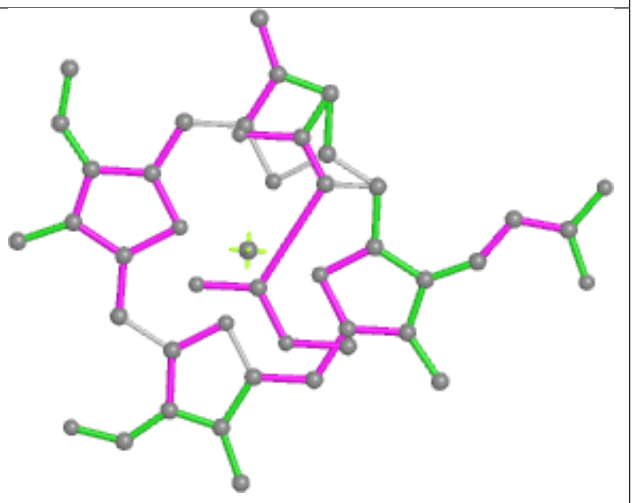


Rings

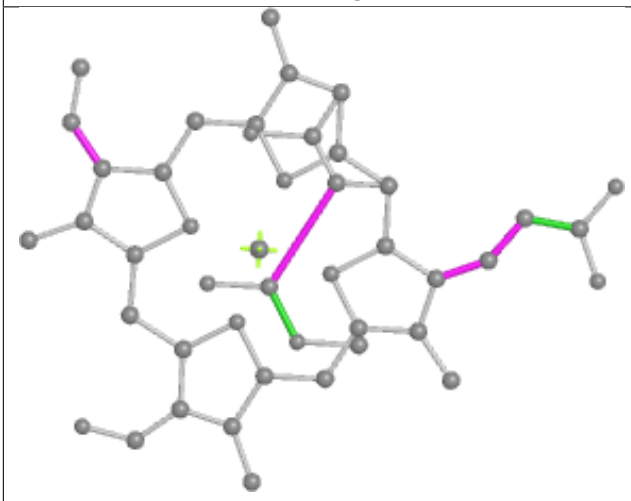
Ligand CL7 D 405



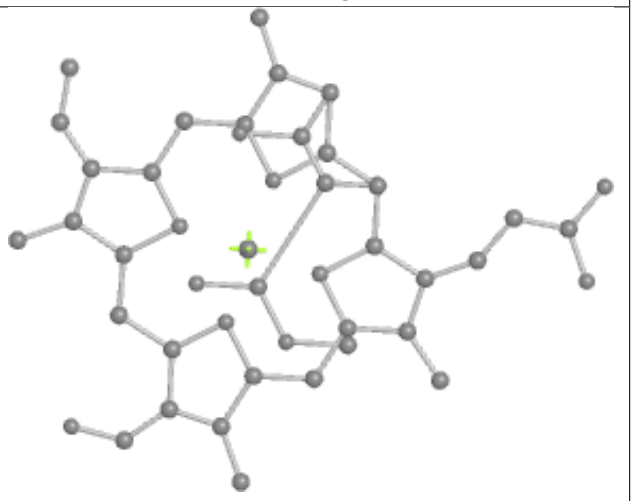
Bond lengths



Bond angles

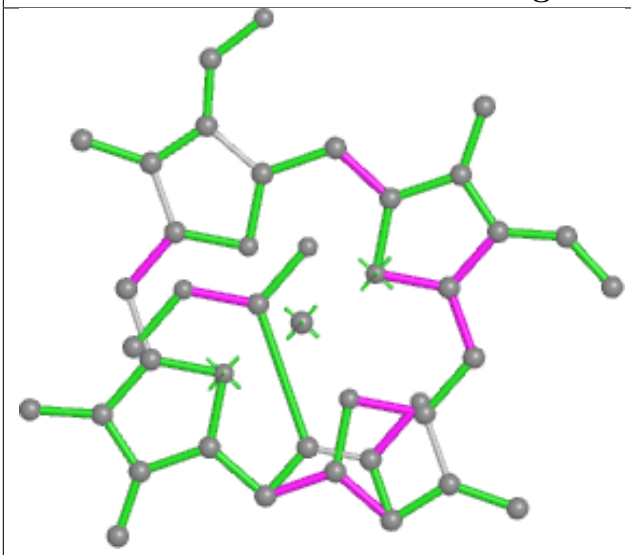


Torsions

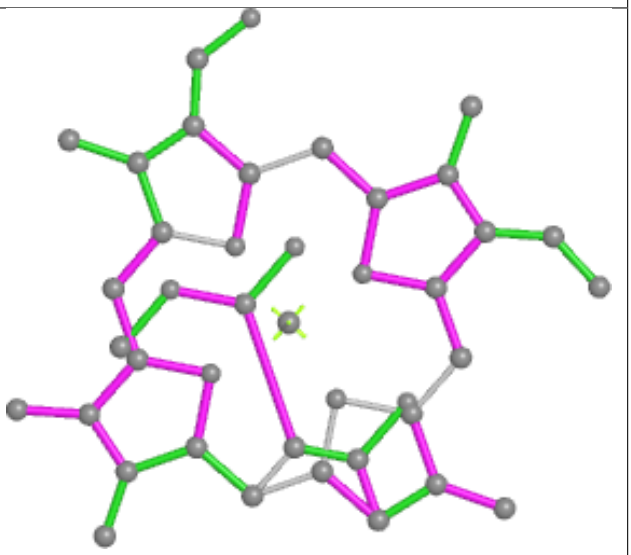


Rings

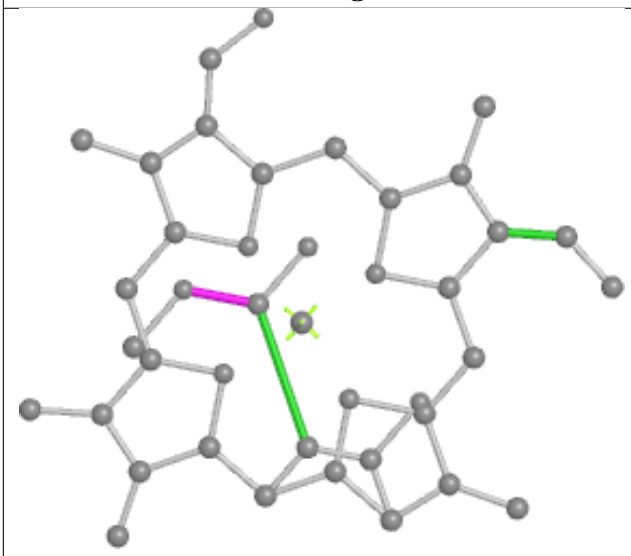
Ligand CL7 1 416



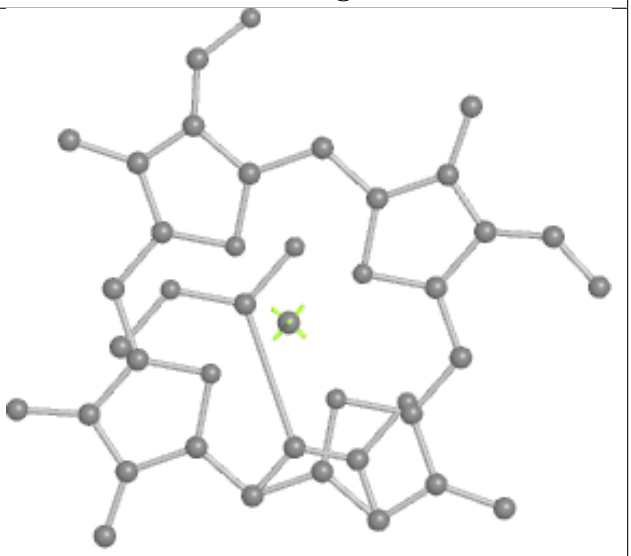
Bond lengths



Bond angles

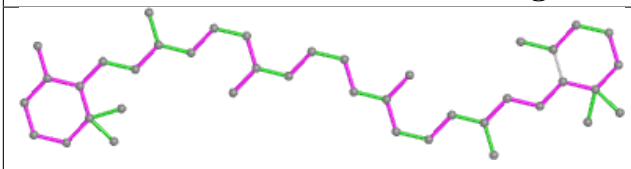


Torsions

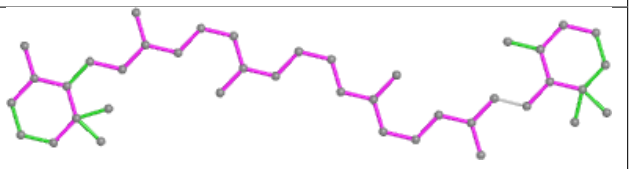


Rings

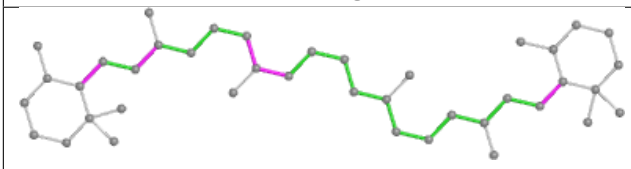
Ligand 8CT b 601



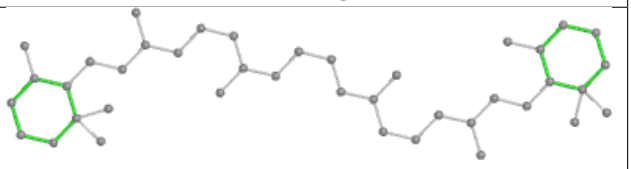
Bond lengths



Bond angles

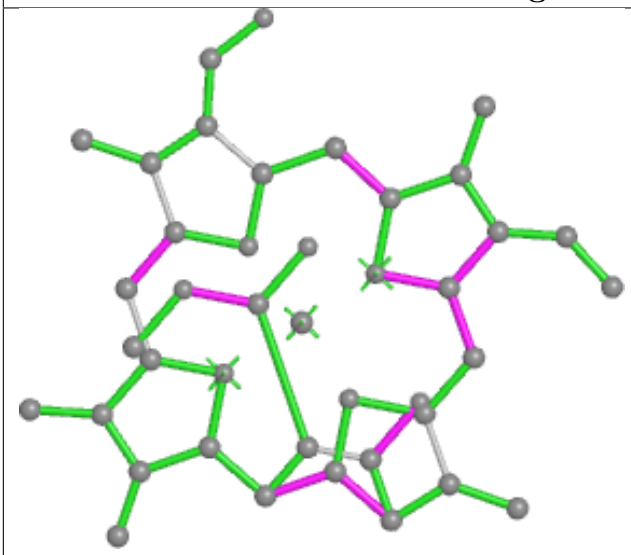


Torsions

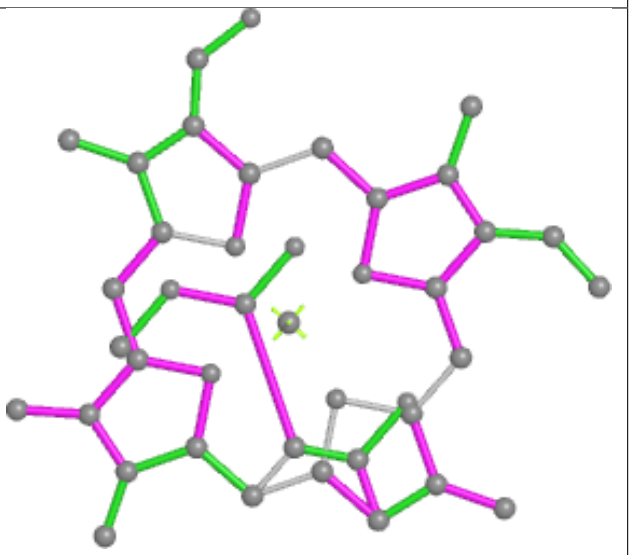


Rings

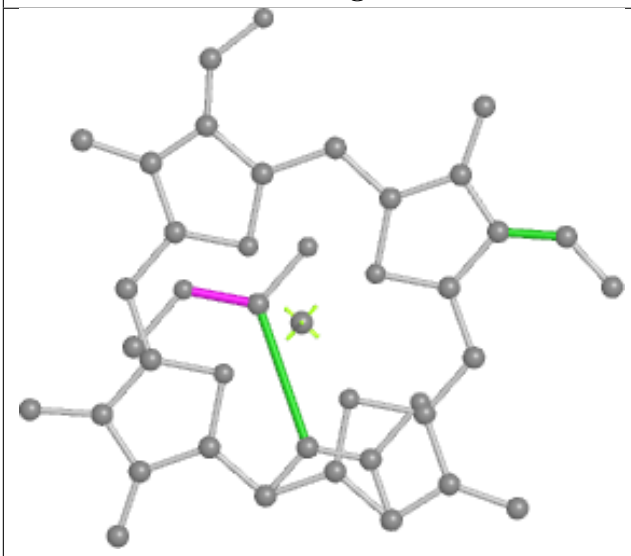
Ligand CL7 C 513



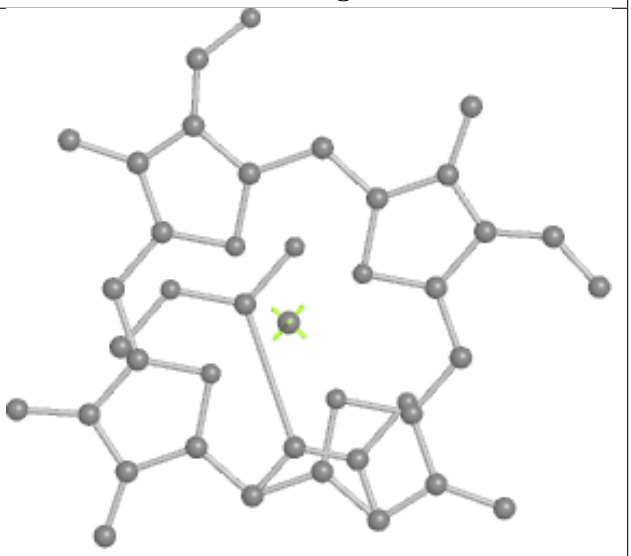
Bond lengths



Bond angles

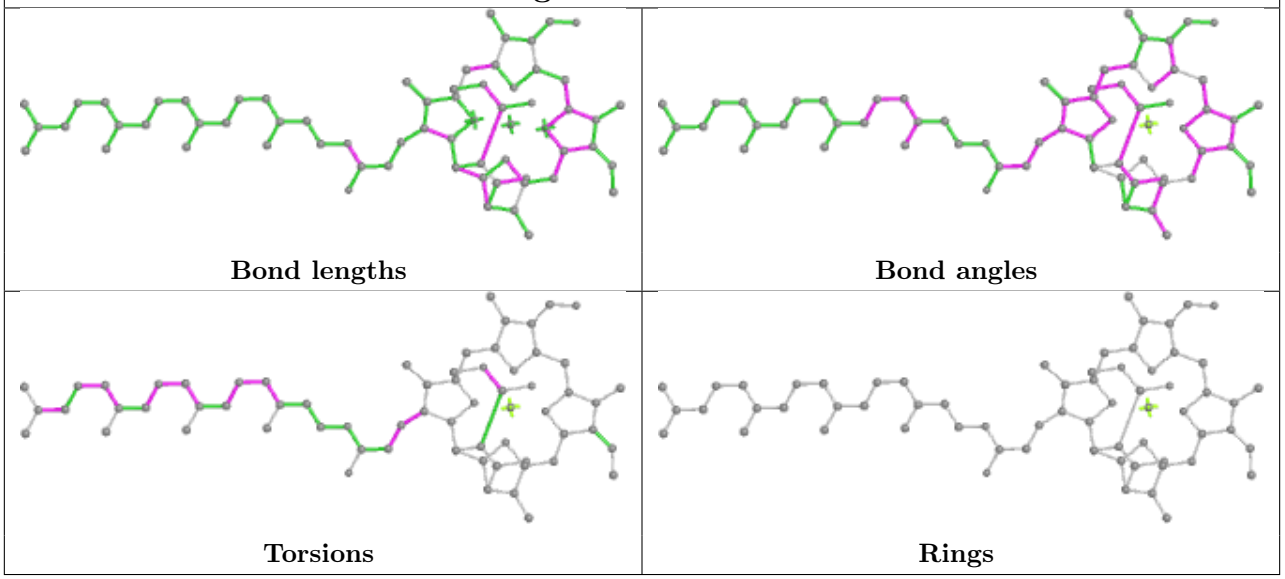


Torsions

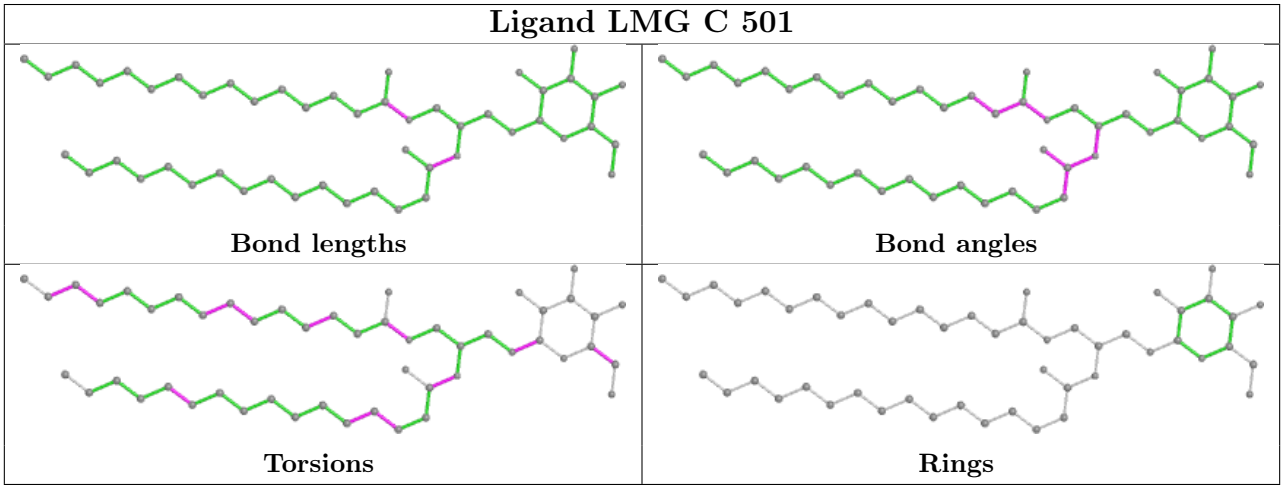


Rings

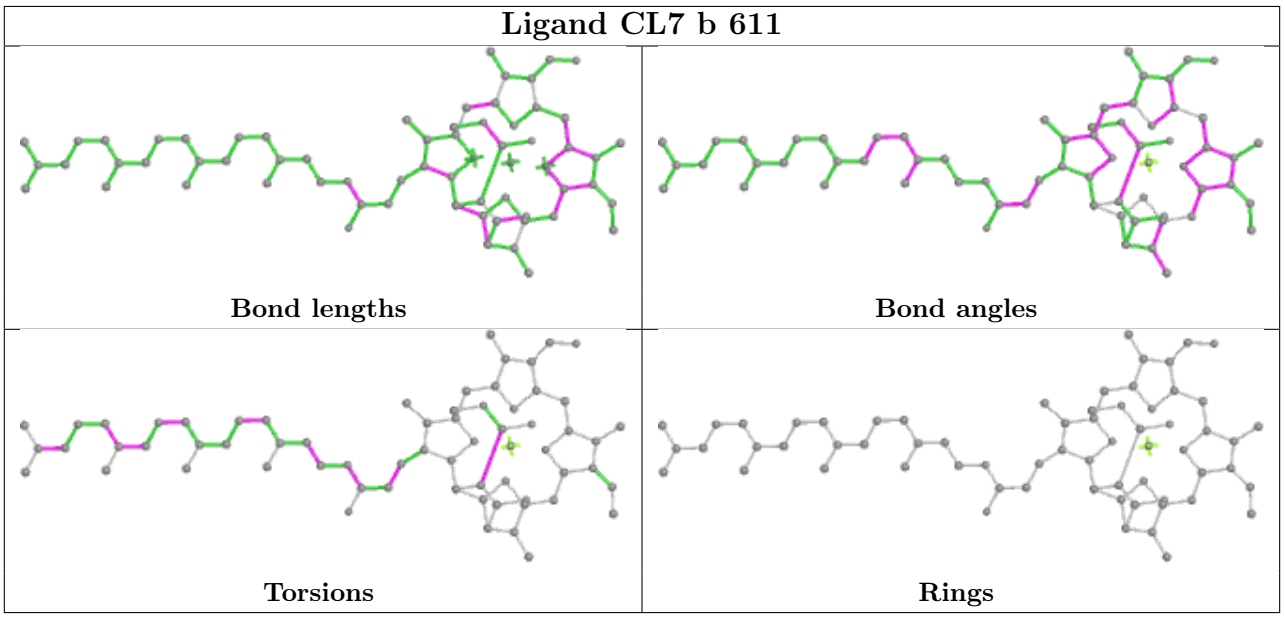
Ligand CL7 6 503



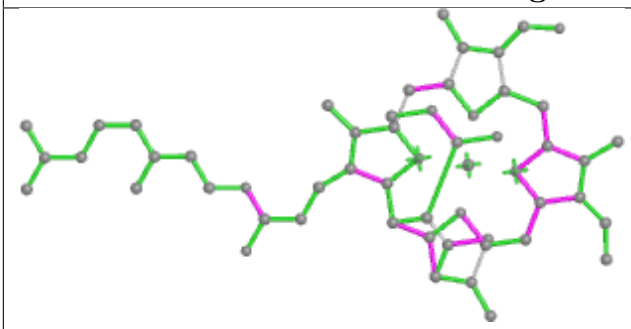
Ligand LMG C 501



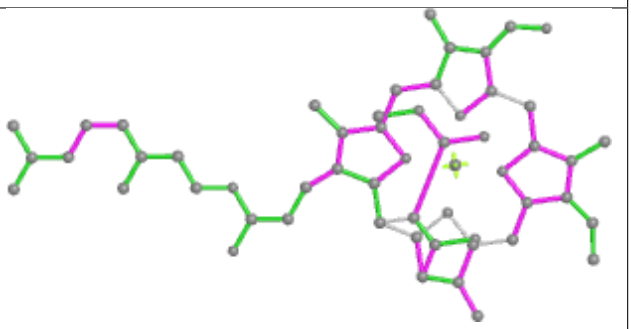
Ligand CL7 b 611



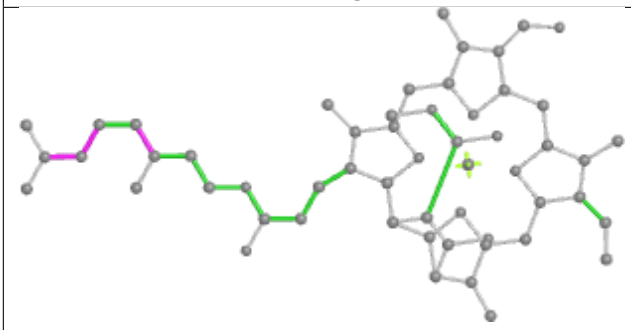
Ligand CL7 B 606



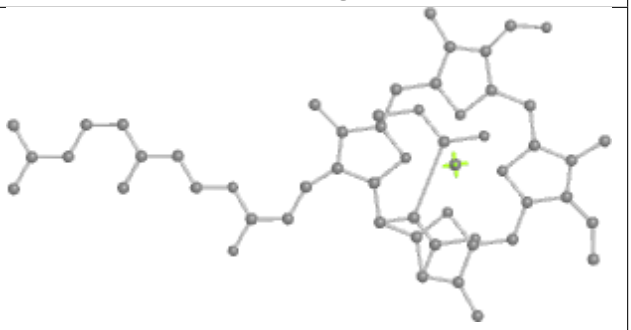
Bond lengths



Bond angles

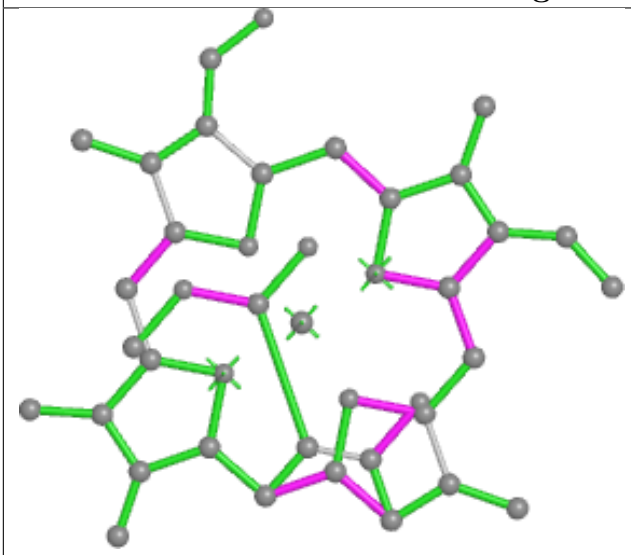


Torsions

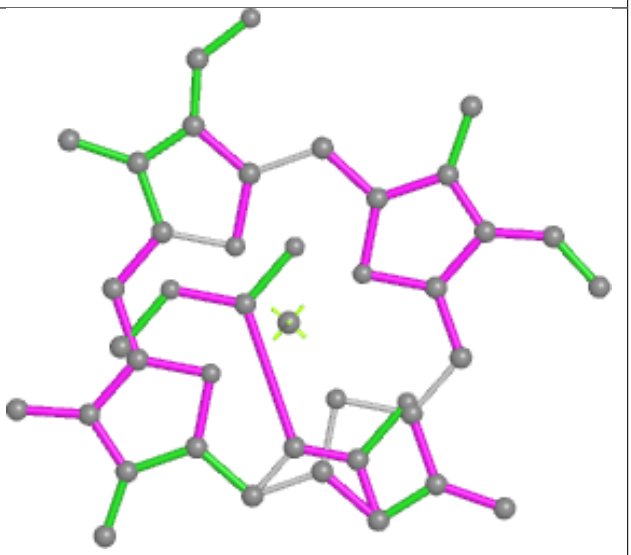


Rings

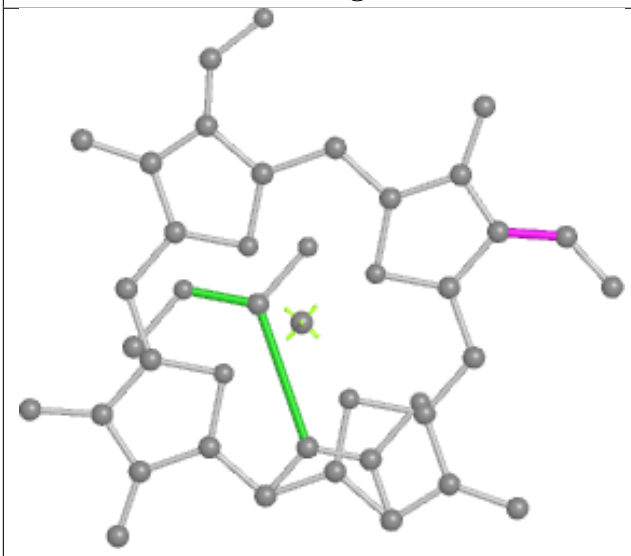
Ligand CL7 1 414



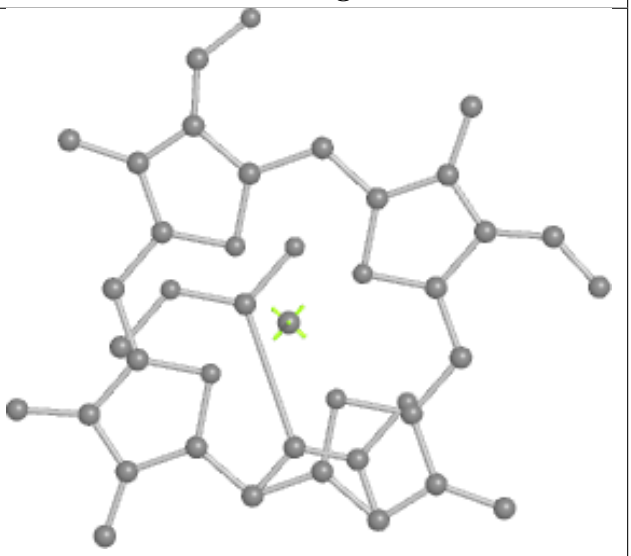
Bond lengths



Bond angles

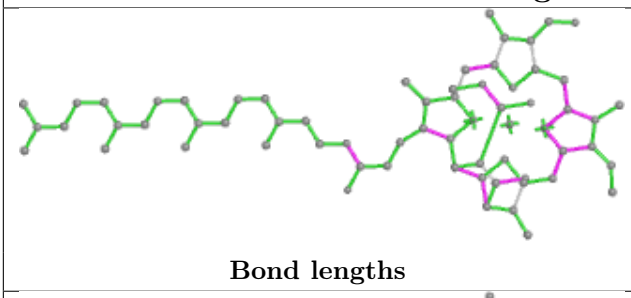


Torsions

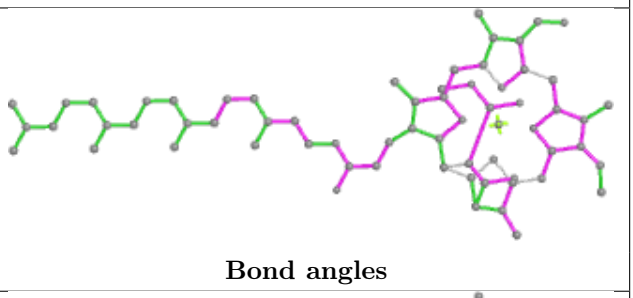


Rings

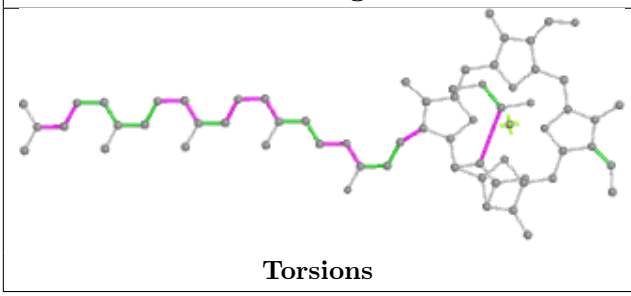
Ligand CL7 c 509



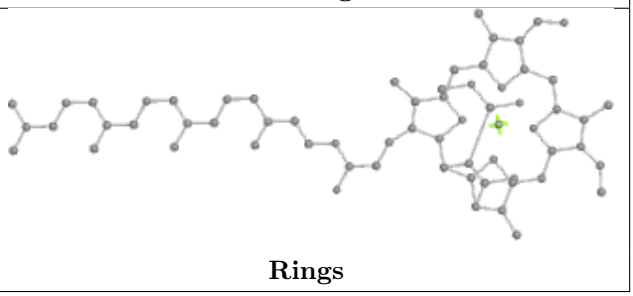
Bond lengths



Bond angles

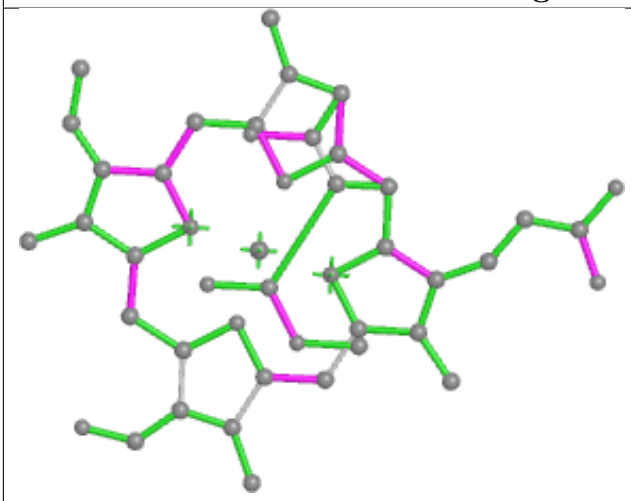


Torsions

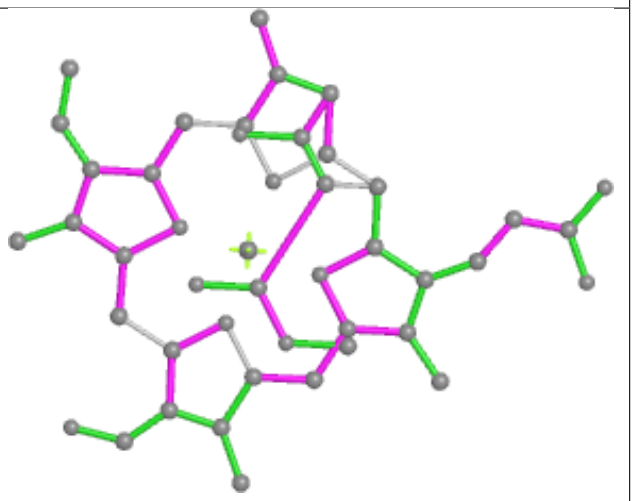


Rings

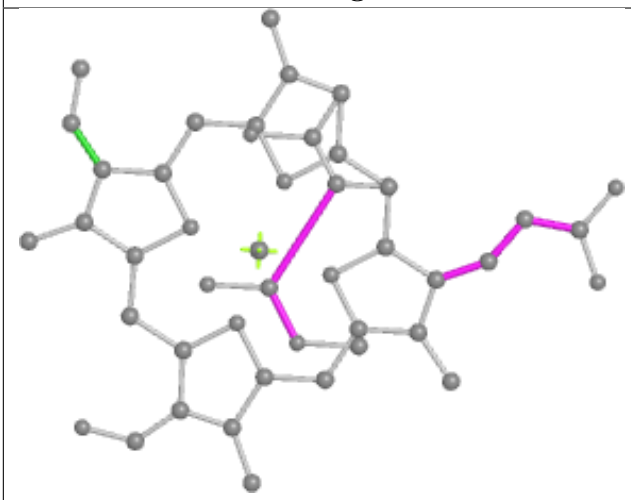
Ligand CL7 5 412



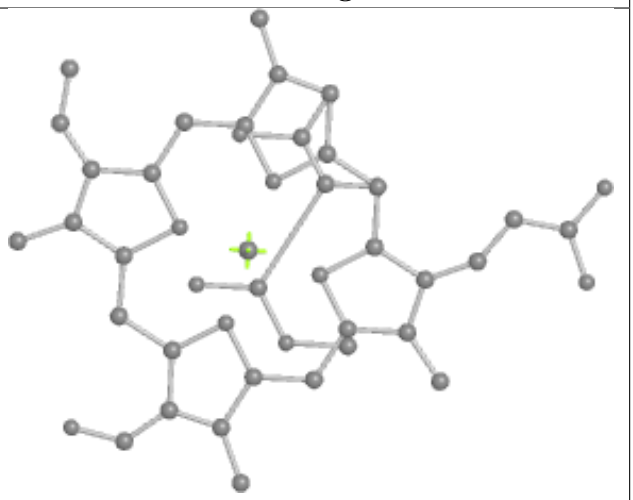
Bond lengths



Bond angles

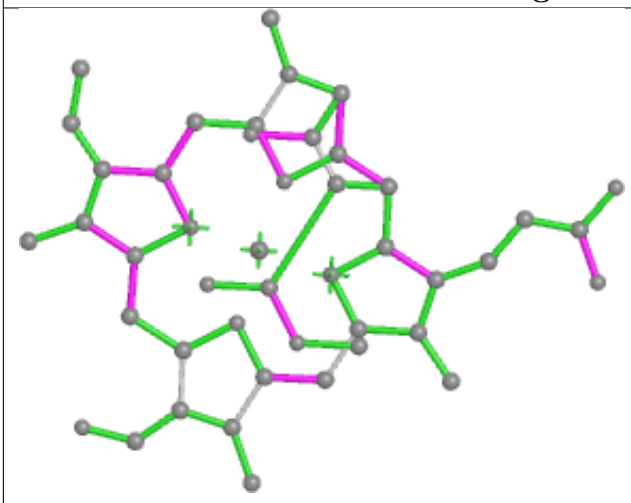


Torsions

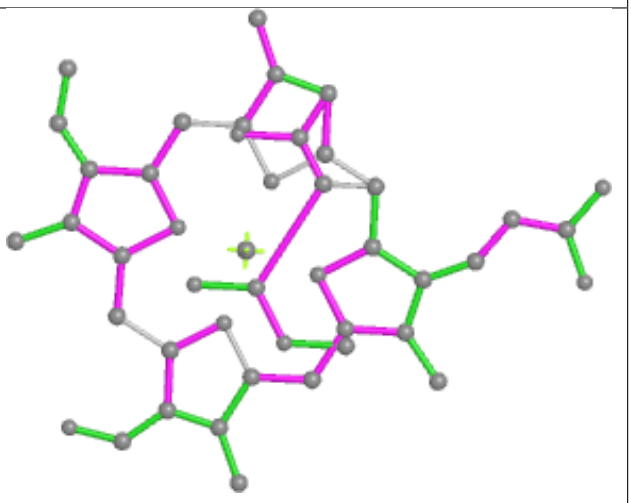


Rings

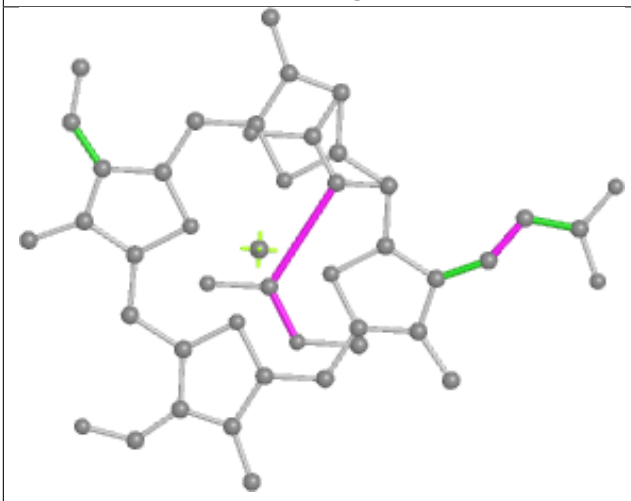
Ligand CL7 5 409



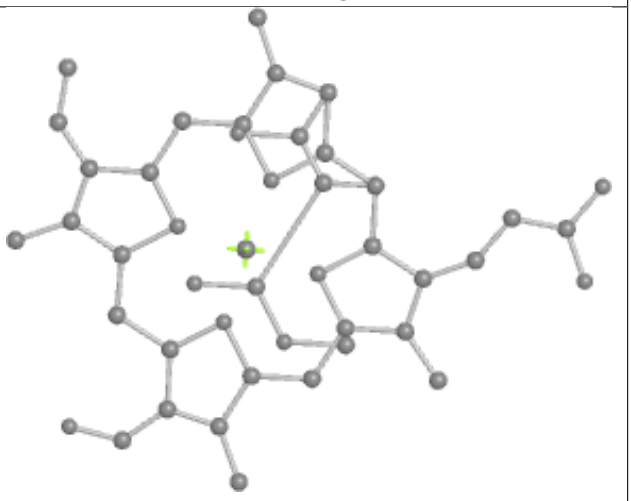
Bond lengths



Bond angles

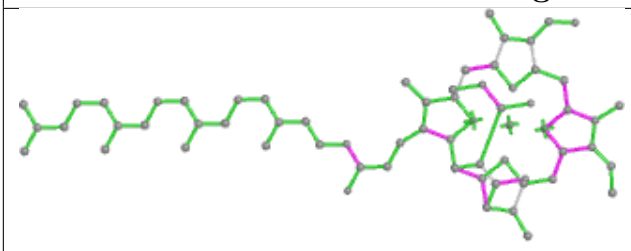


Torsions

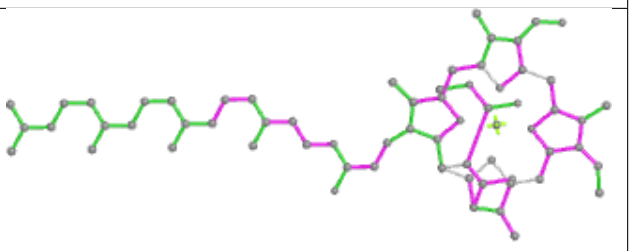


Rings

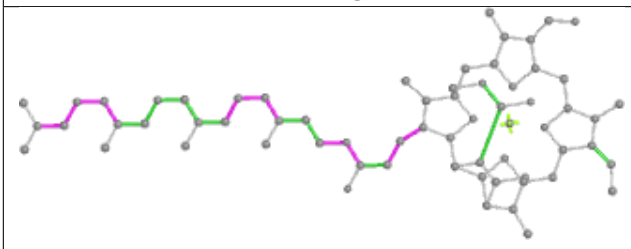
Ligand CL7 2 516



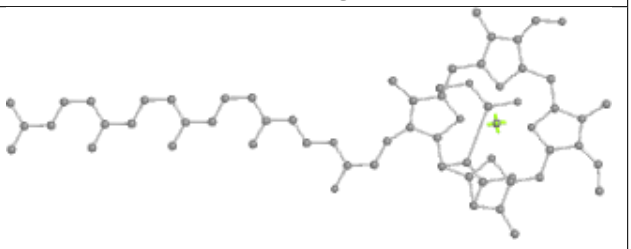
Bond lengths



Bond angles

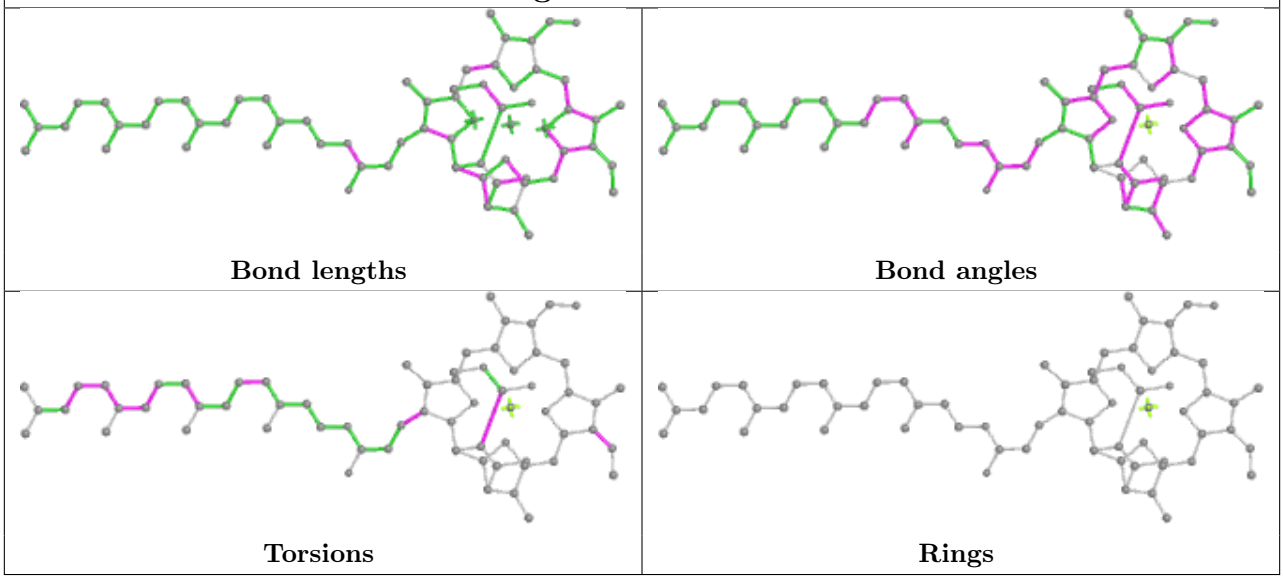


Torsions

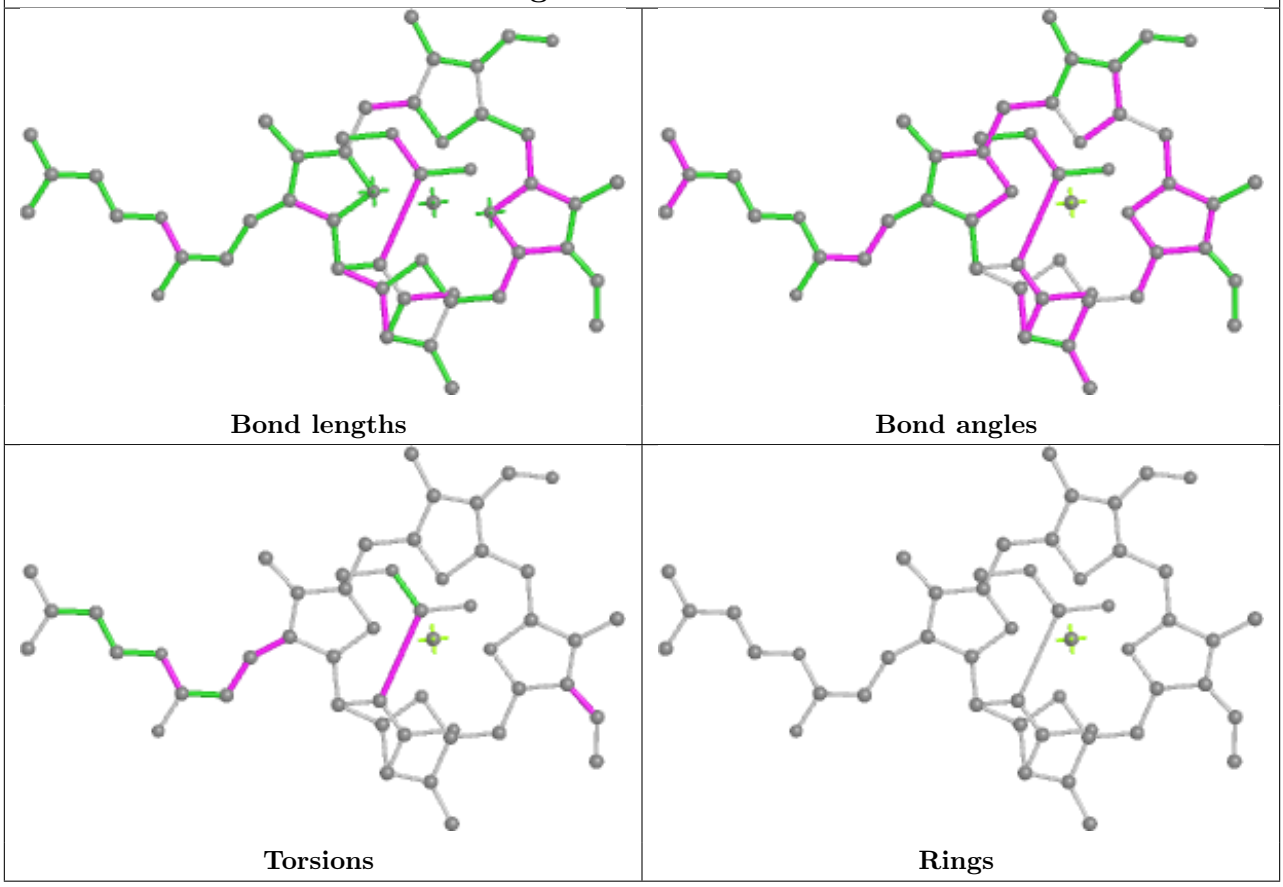


Rings

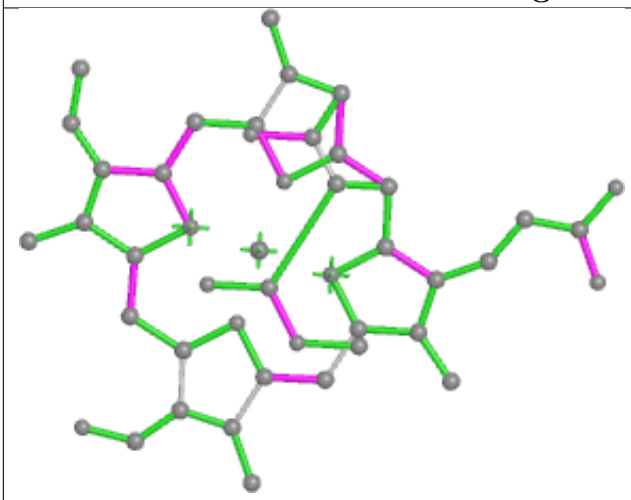
Ligand CL7 1 408



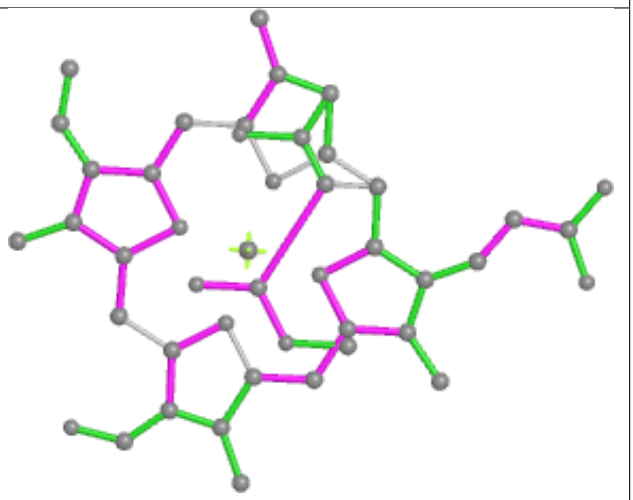
Ligand CL7 B 615



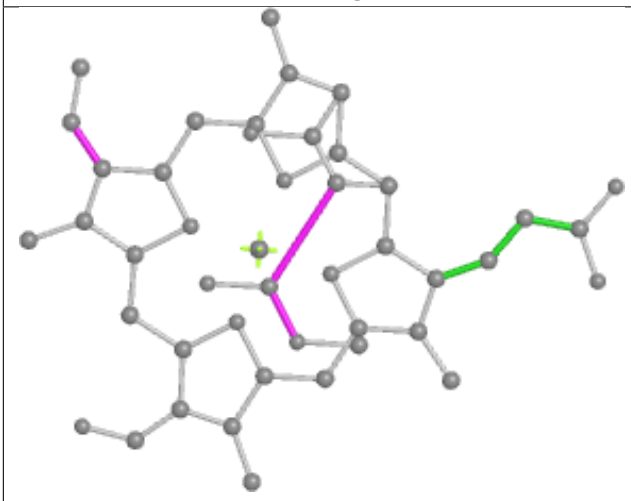
Ligand CL7 1 420



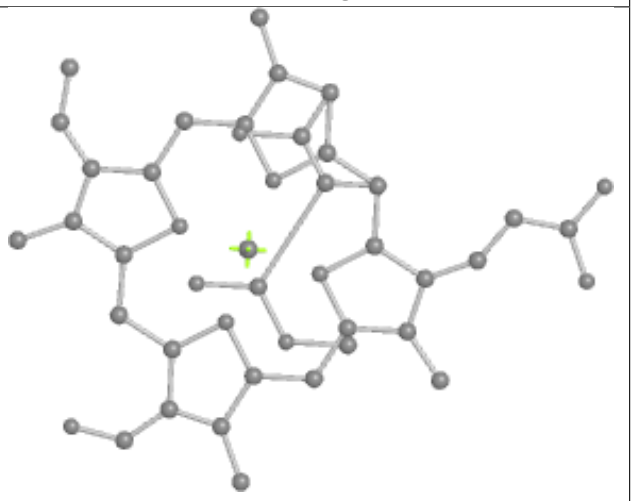
Bond lengths



Bond angles

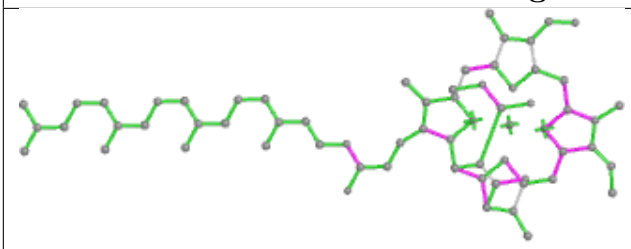


Torsions

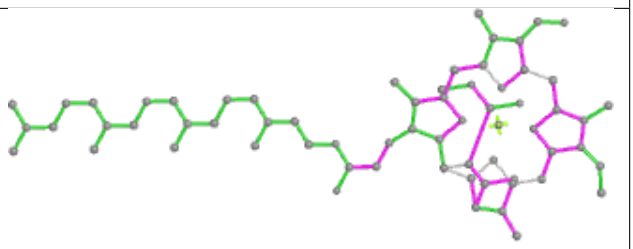


Rings

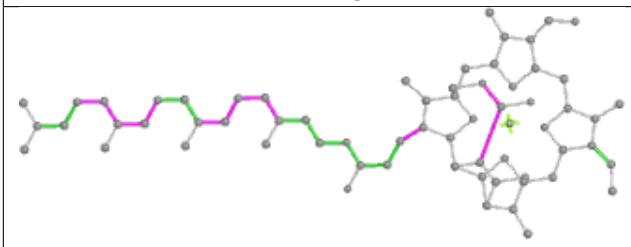
Ligand CL7 B 605



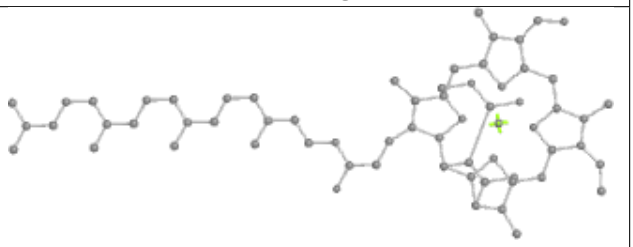
Bond lengths



Bond angles

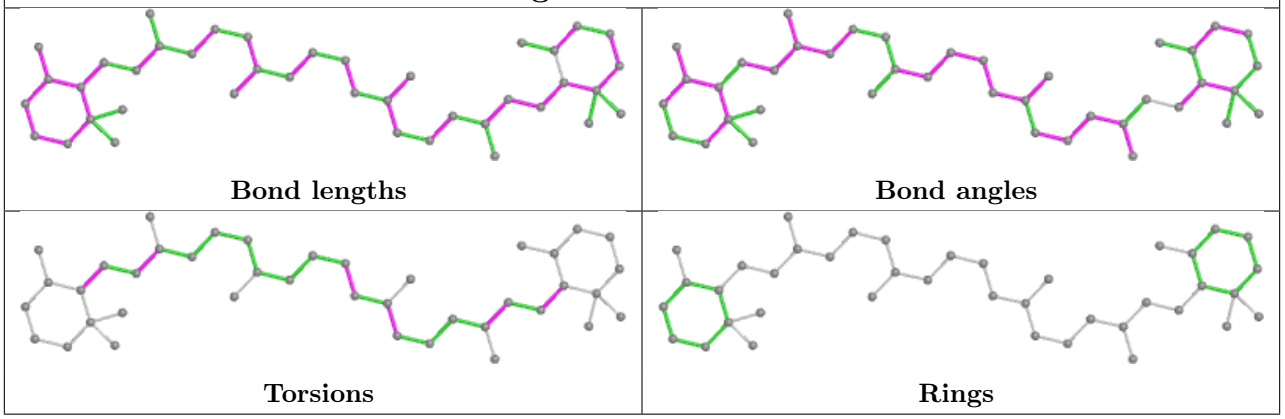


Torsions

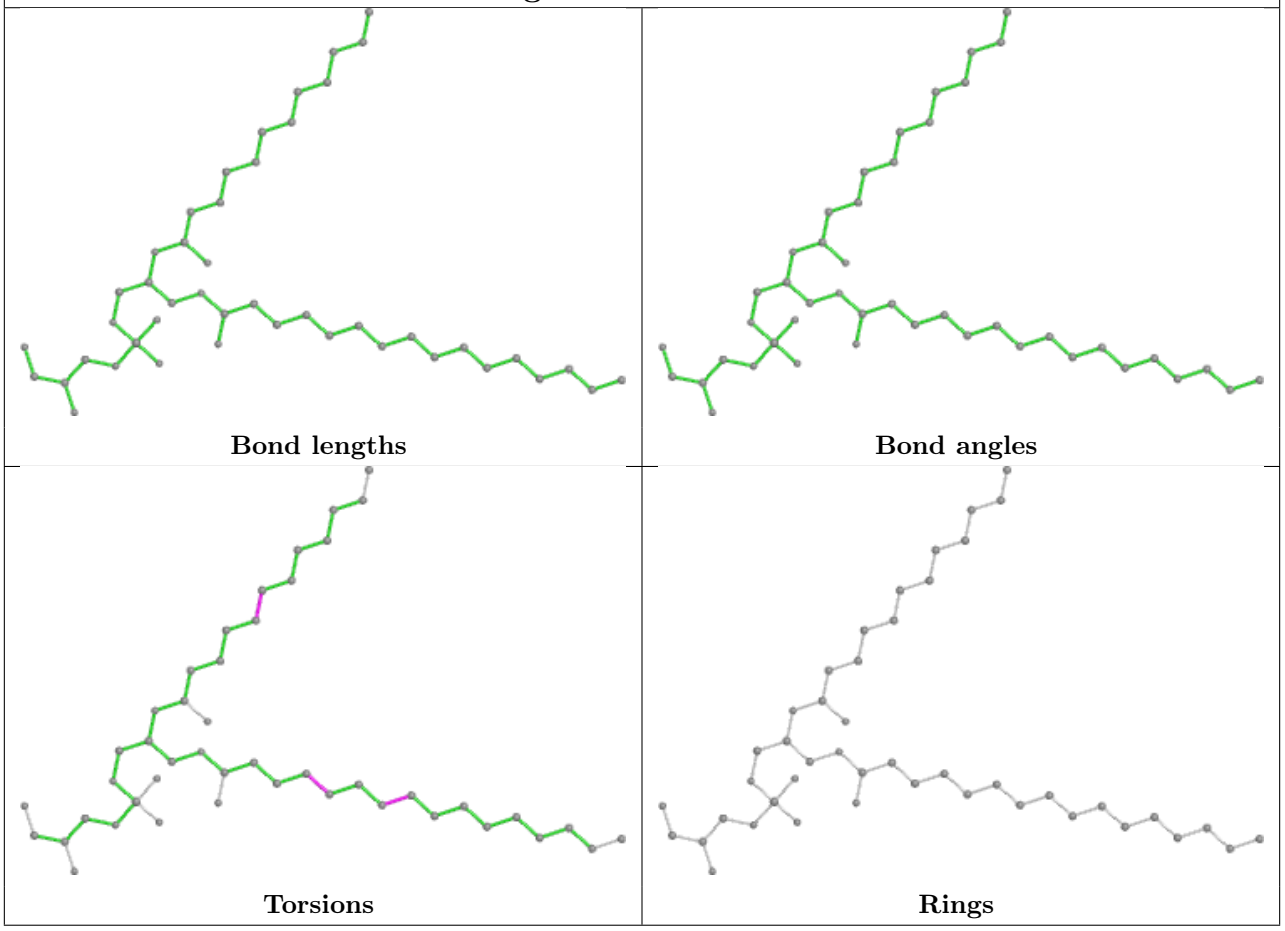


Rings

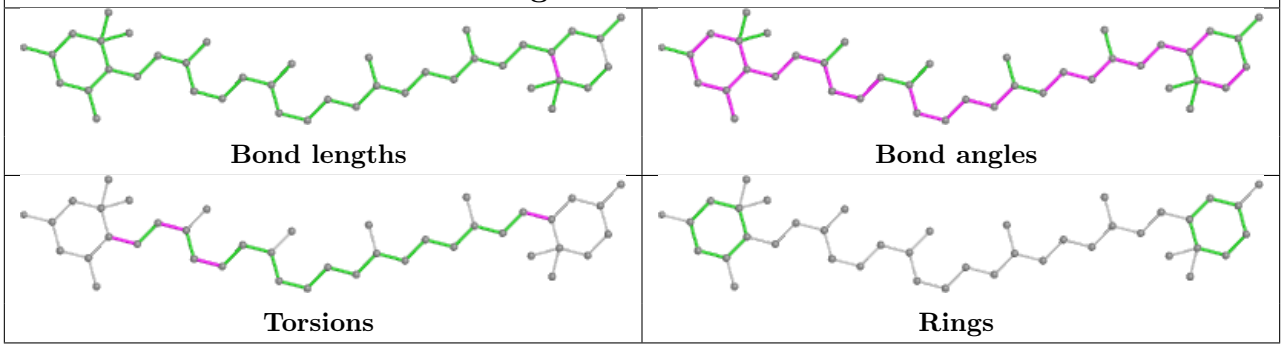
Ligand 8CT k 101



Ligand LHG B 623



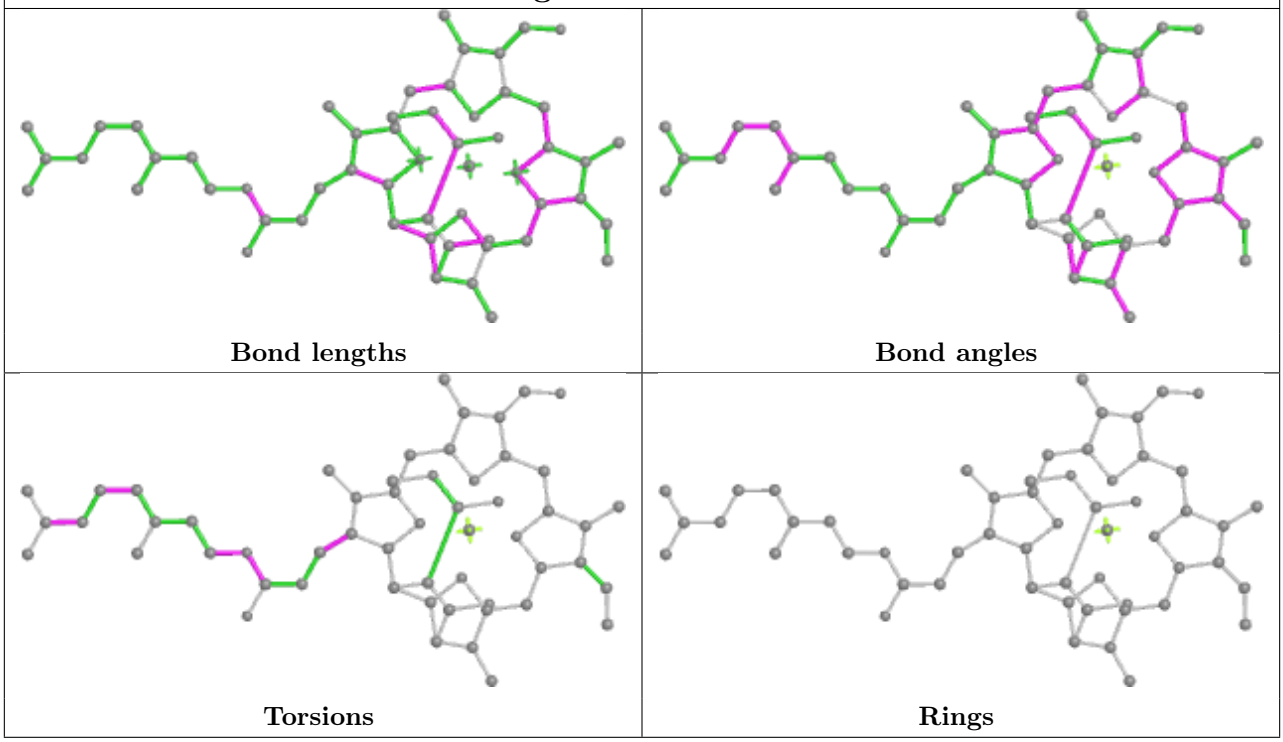
Ligand ZEX 1 422



Bond lengths | Bond angles

Torsions | Rings

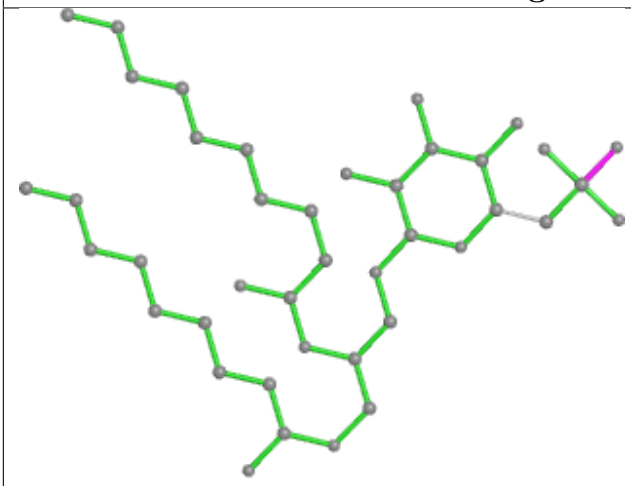
Ligand CL7 5 417



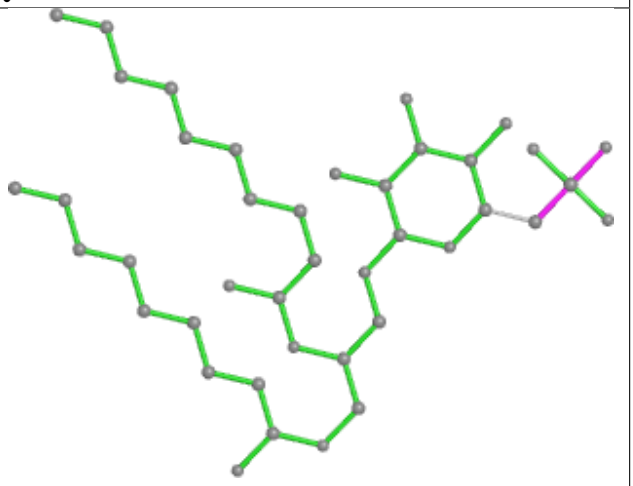
Bond lengths | Bond angles

Torsions | Rings

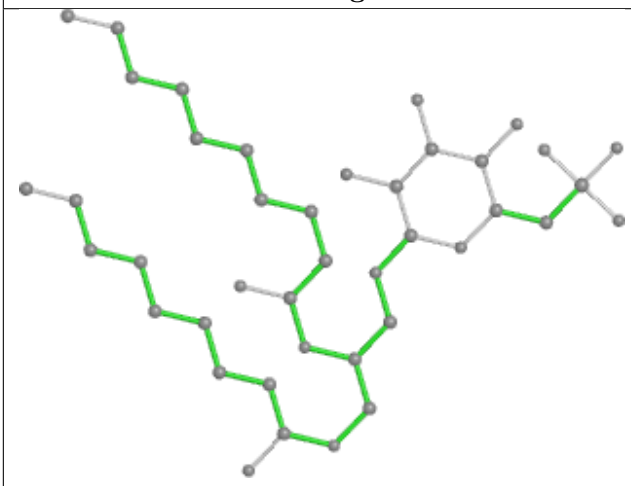
Ligand SQD 6 523



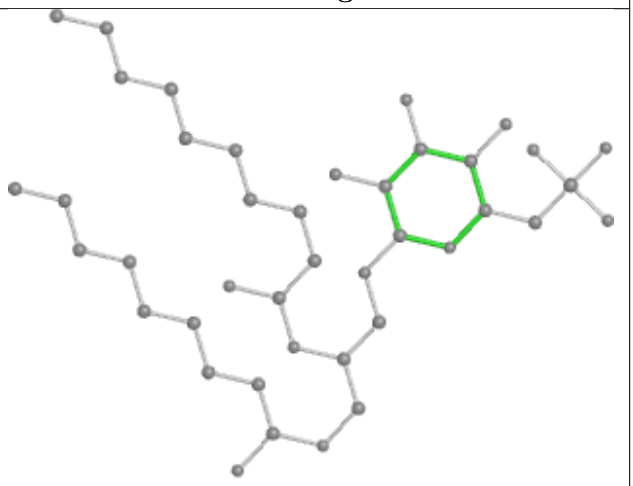
Bond lengths



Bond angles

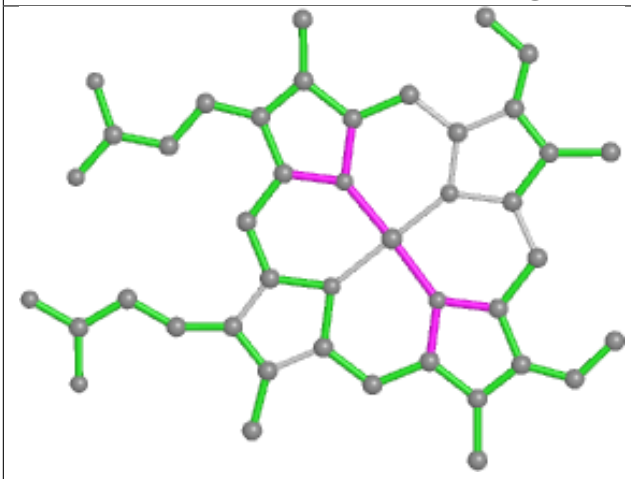


Torsions

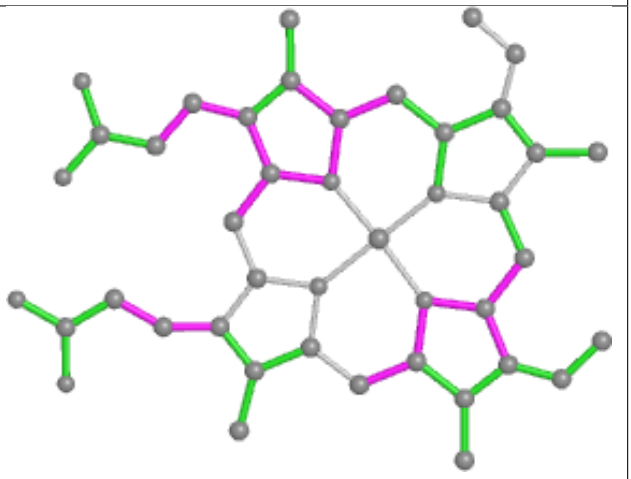


Rings

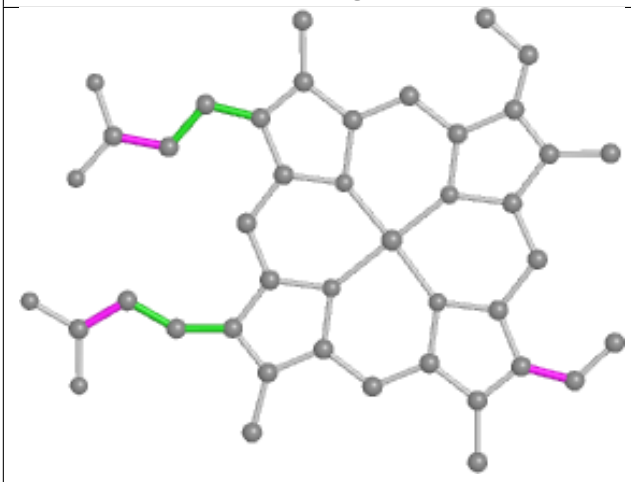
Ligand HEM f 101



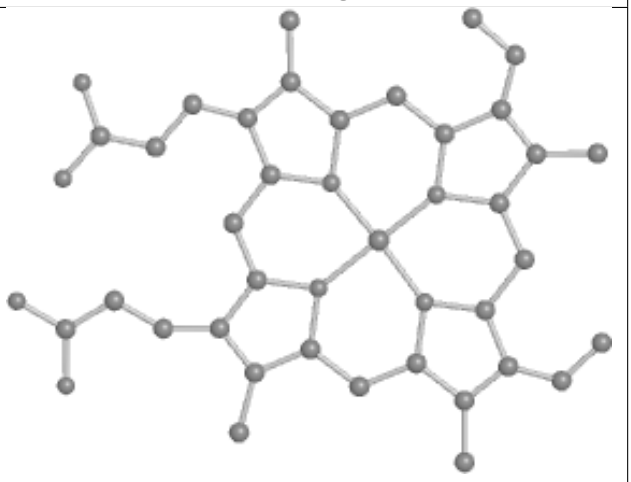
Bond lengths



Bond angles

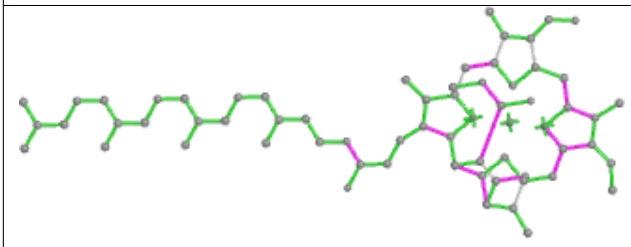


Torsions

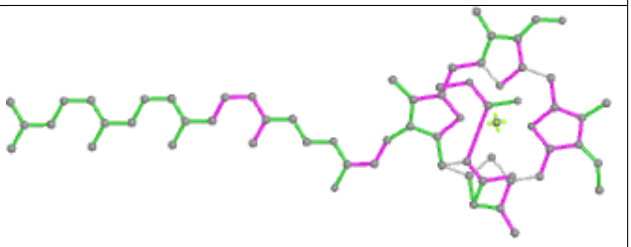


Rings

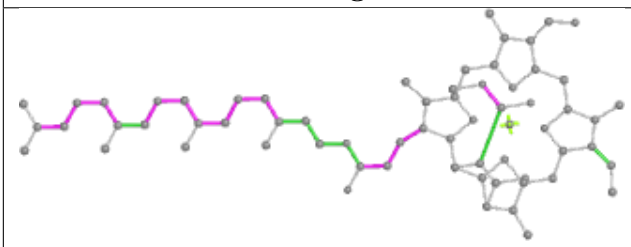
Ligand CL7 8 406



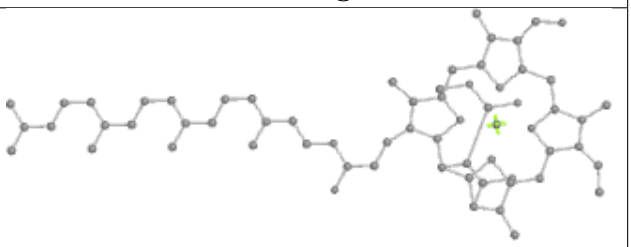
Bond lengths



Bond angles

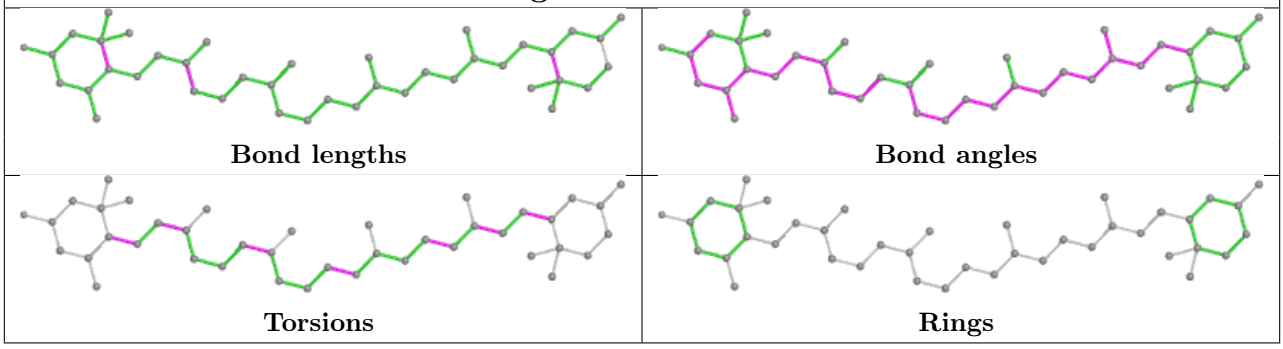


Torsions



Rings

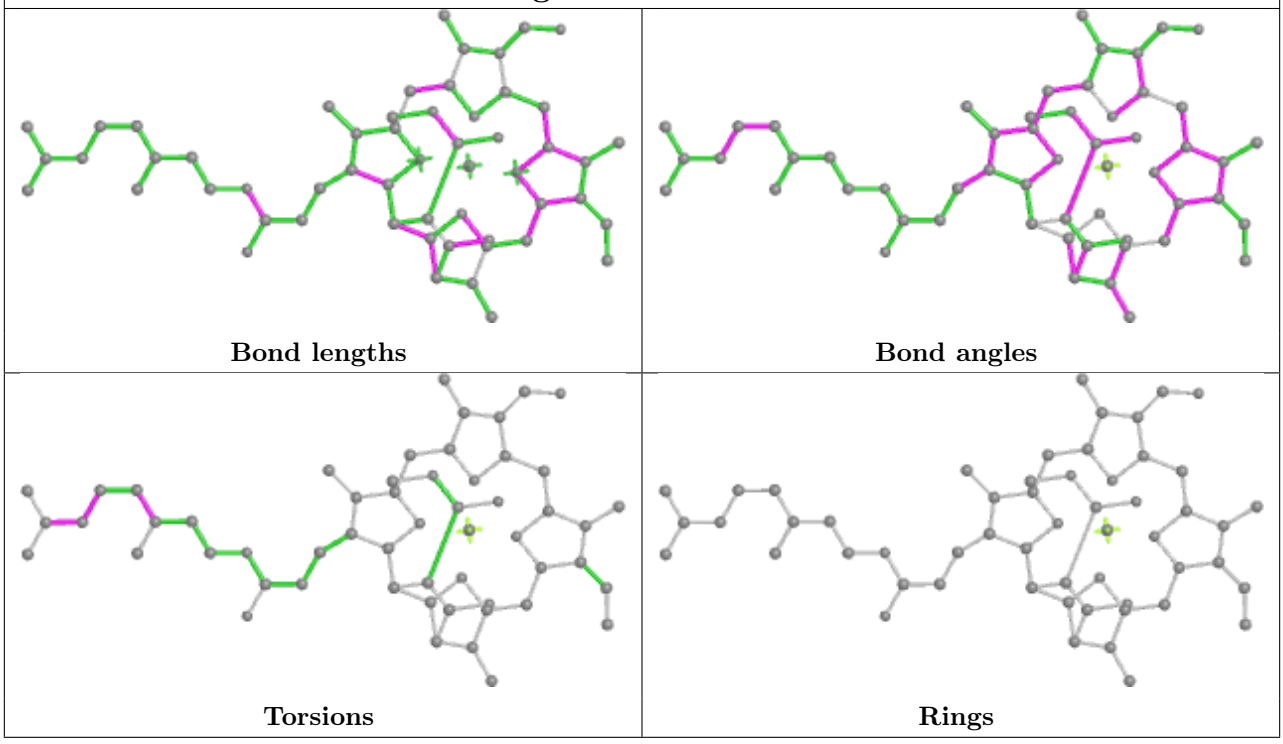
Ligand ZEX 2 519



Bond lengths | Bond angles

Torsions | Rings

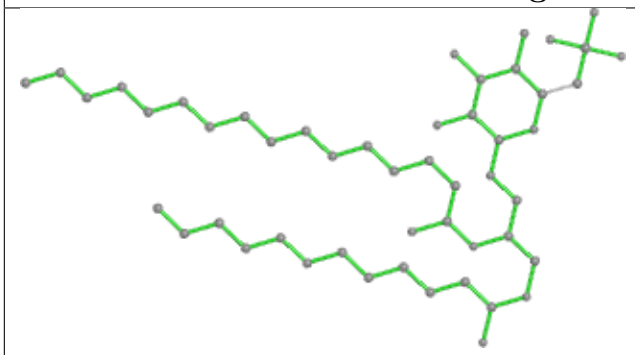
Ligand CL7 b 607



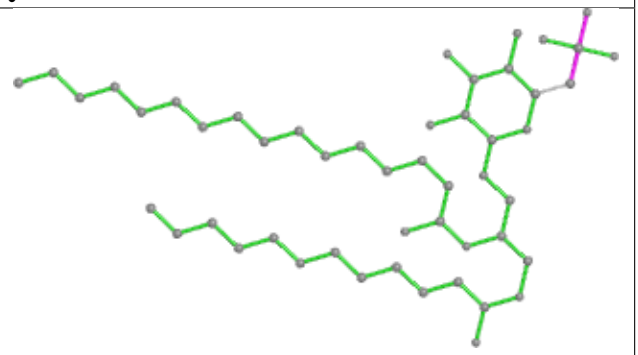
Bond lengths | Bond angles

Torsions | Rings

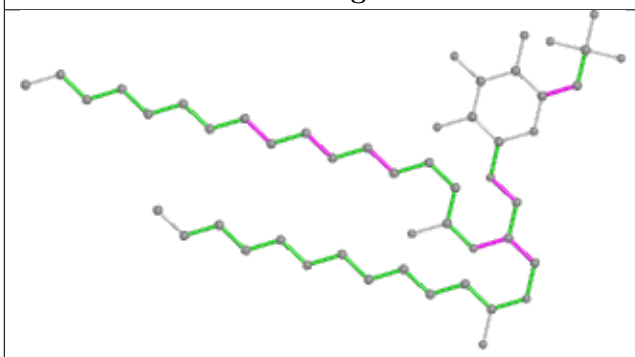
Ligand SQD 3 523



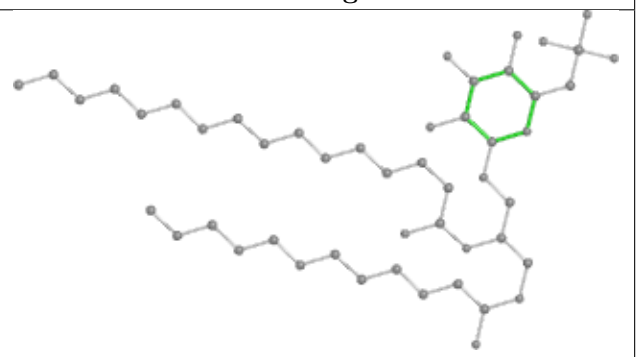
Bond lengths



Bond angles

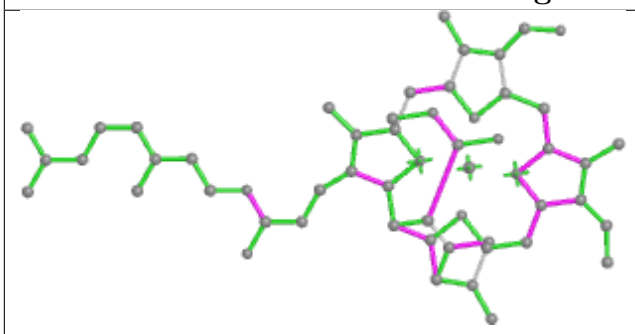


Torsions

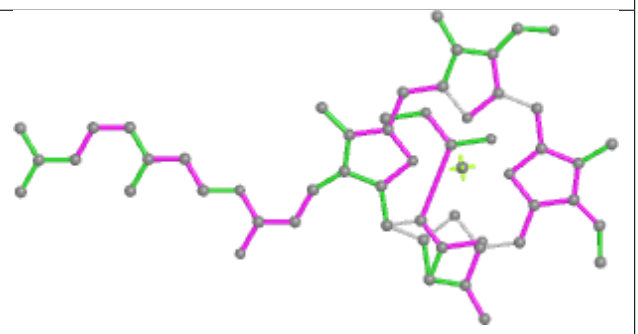


Rings

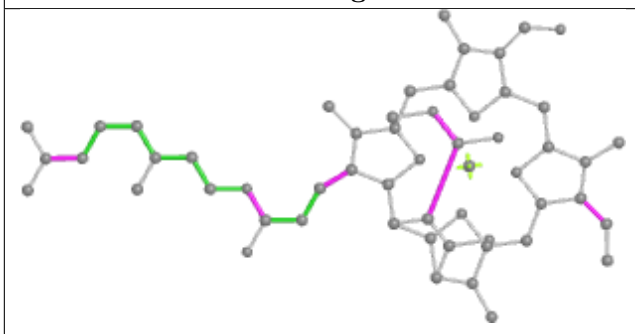
Ligand CL7 a 403



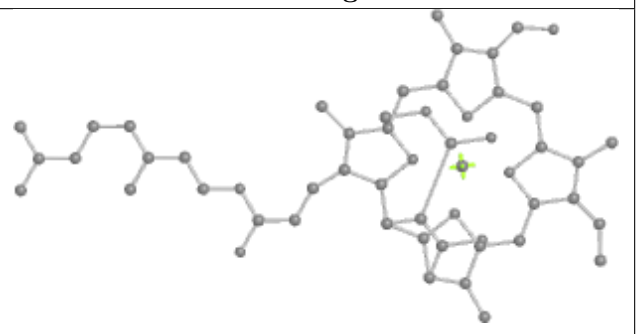
Bond lengths



Bond angles

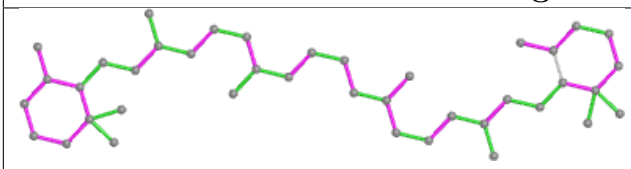


Torsions

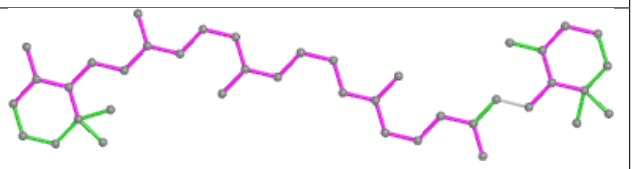


Rings

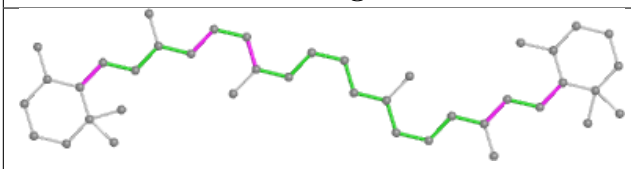
Ligand 8CT c 519



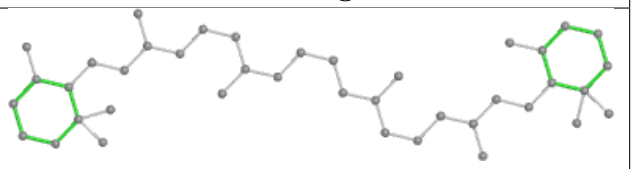
Bond lengths



Bond angles

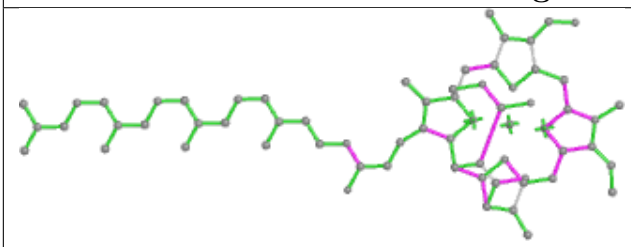


Torsions

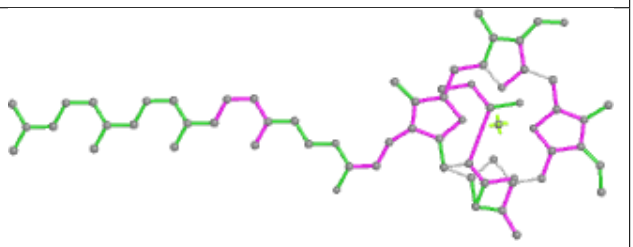


Rings

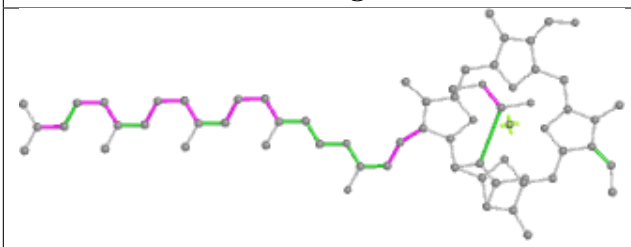
Ligand CL7 2 503



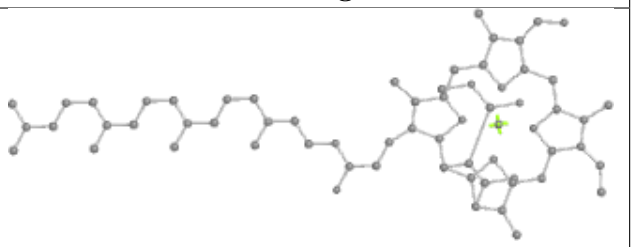
Bond lengths



Bond angles

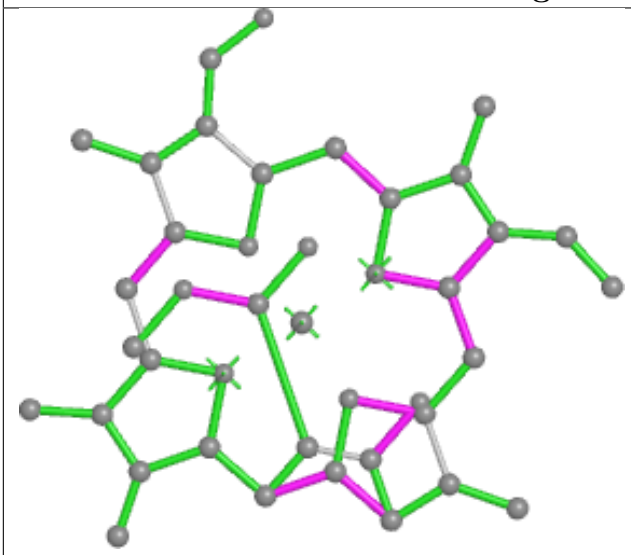


Torsions

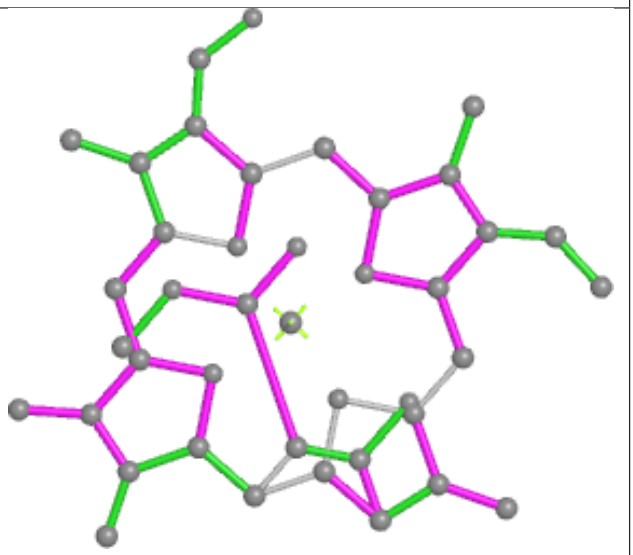


Rings

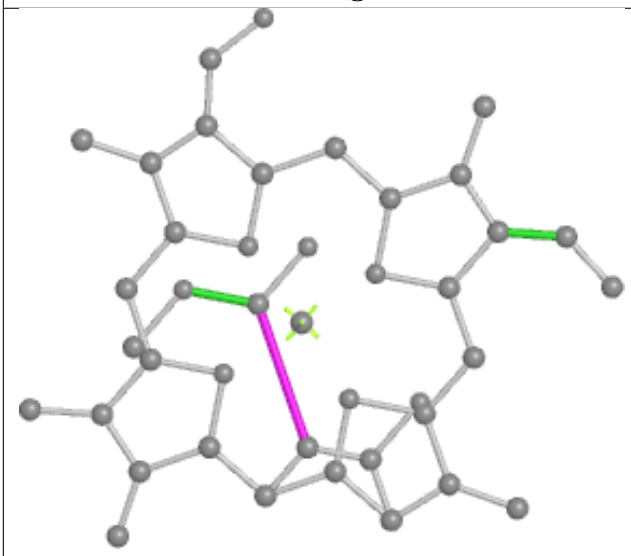
Ligand CL7 1 413



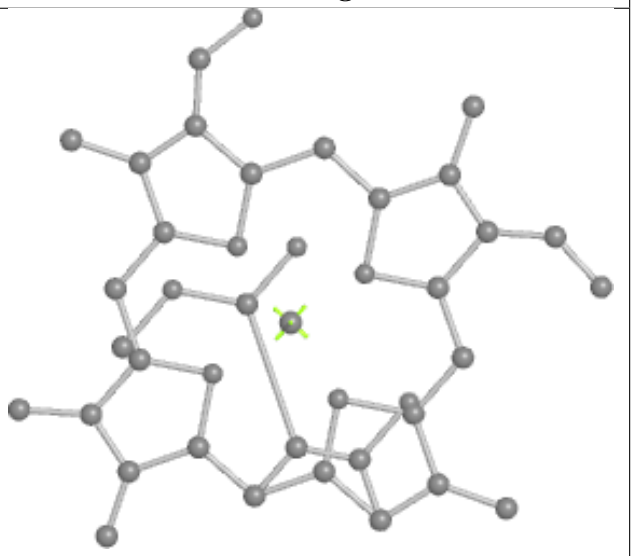
Bond lengths



Bond angles

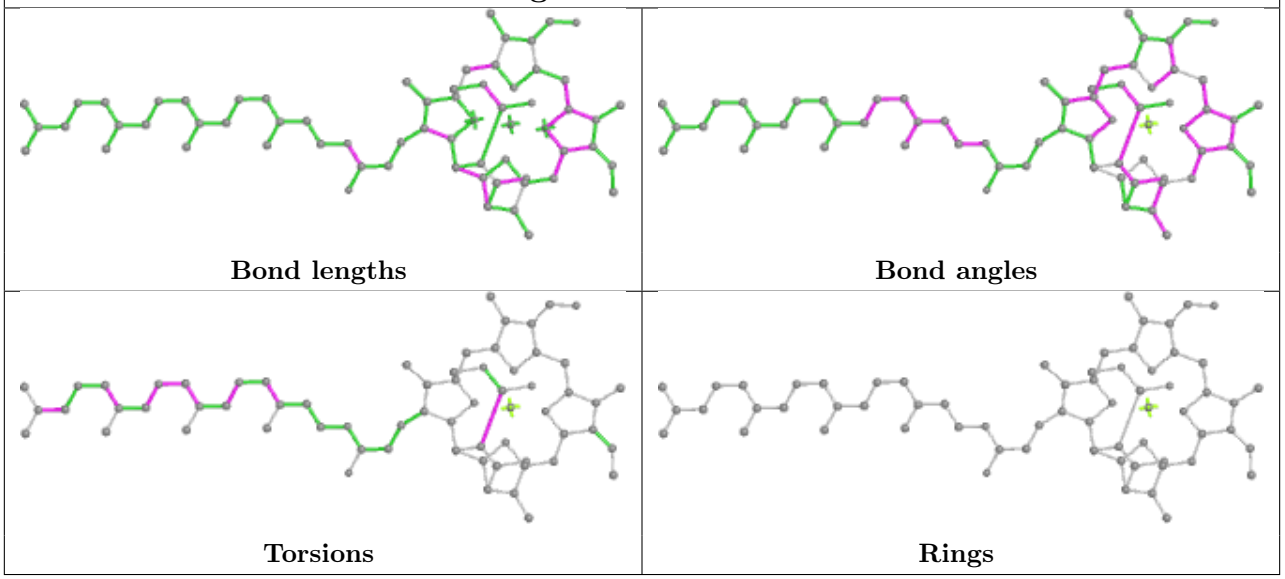


Torsions

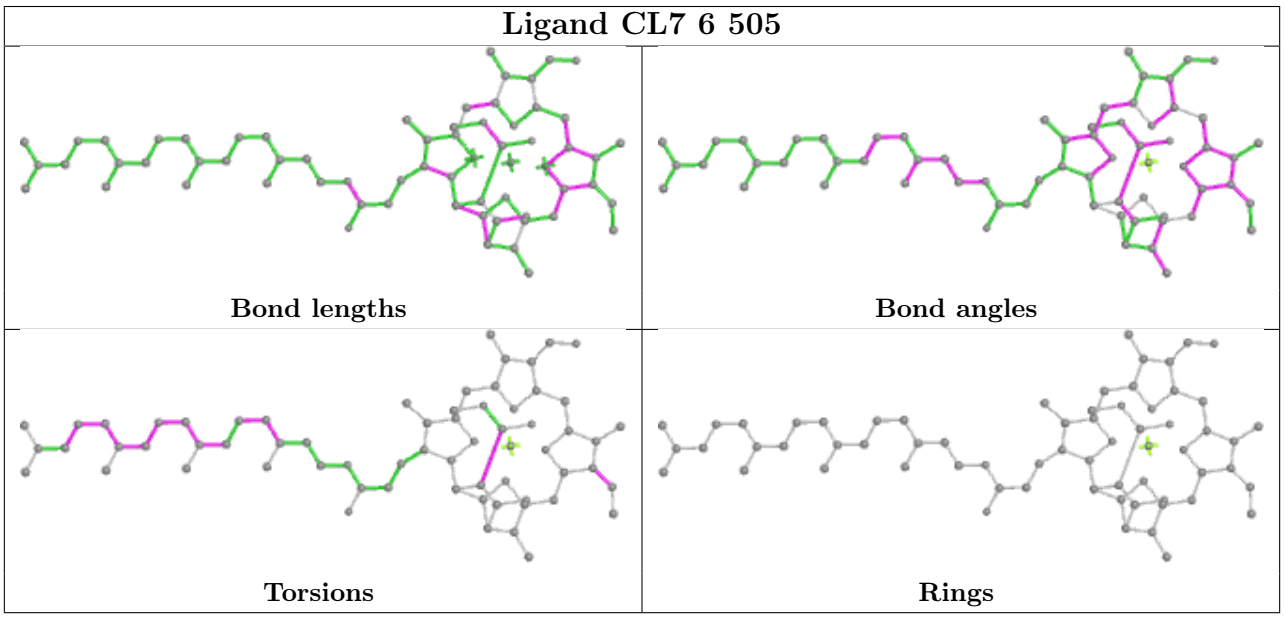


Rings

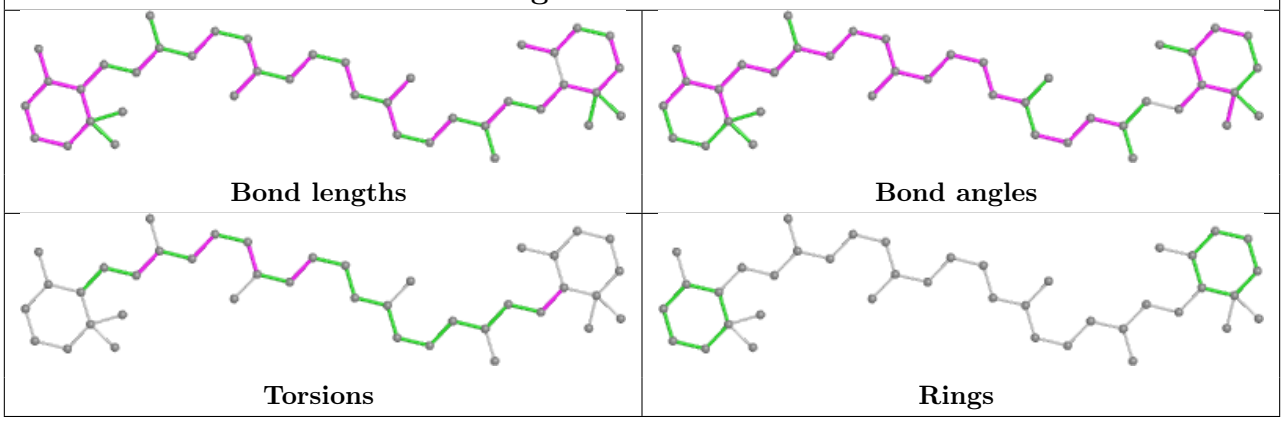
Ligand CL7 B 603



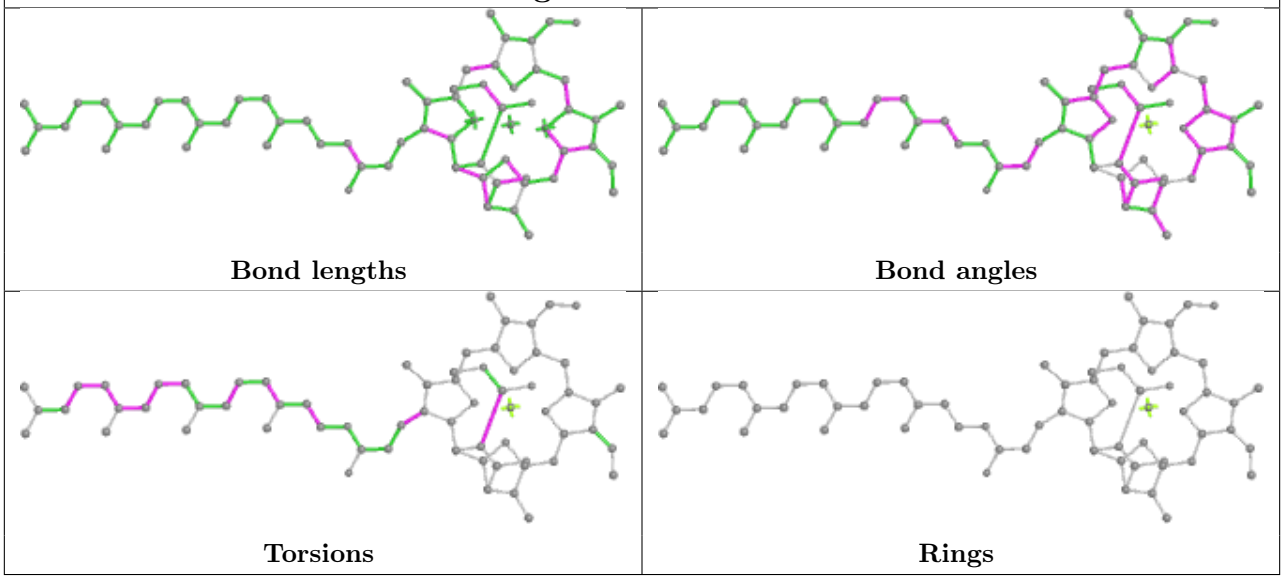
Ligand CL7 6 505



Ligand 8CT b 618



Ligand CL7 5 404



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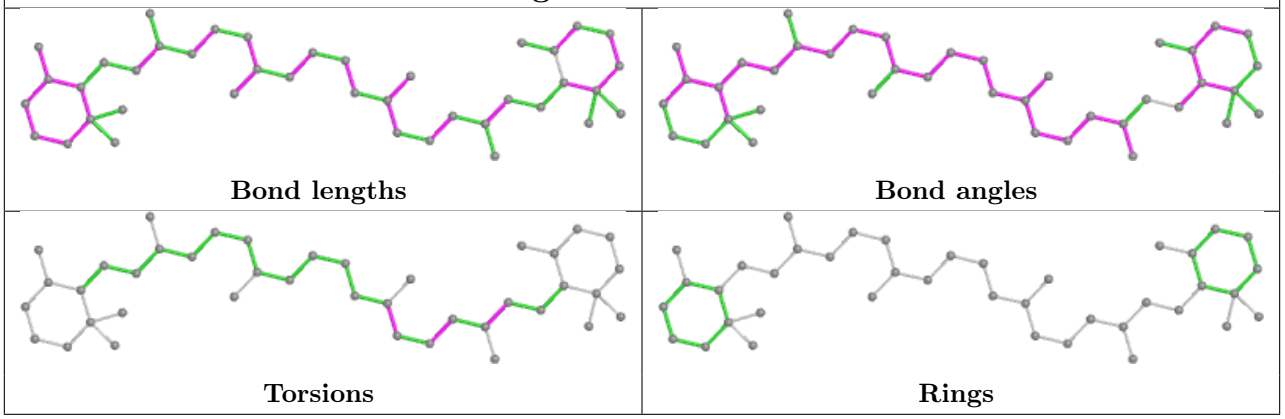
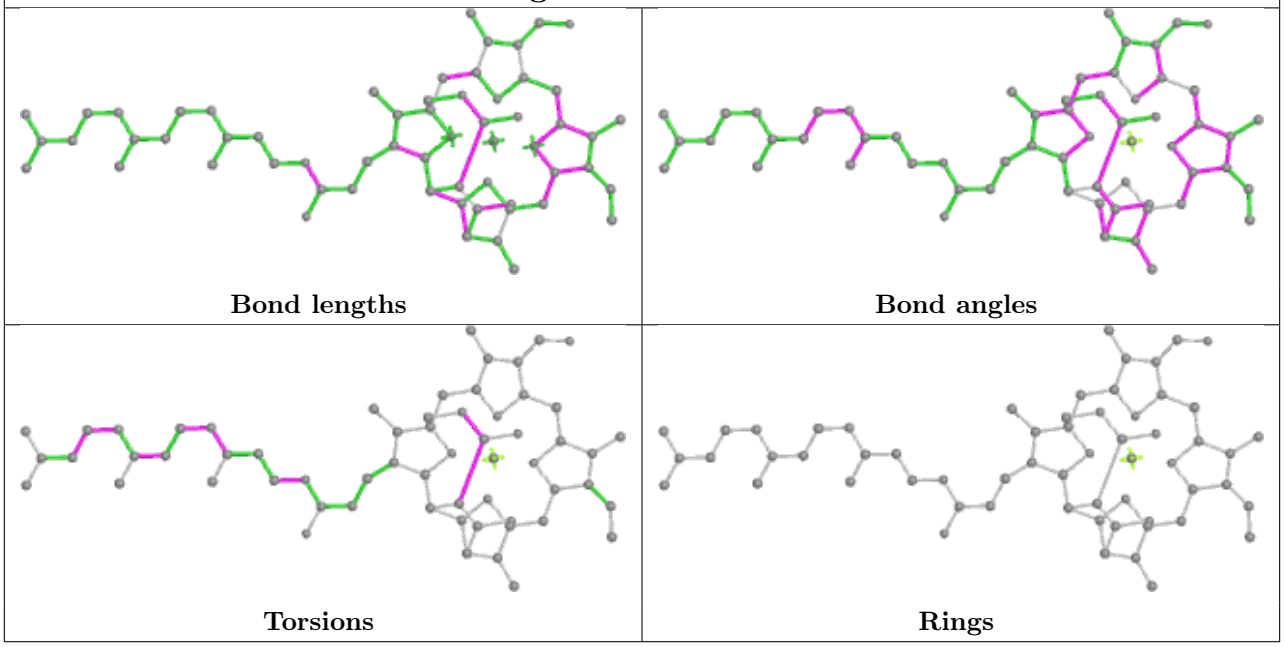
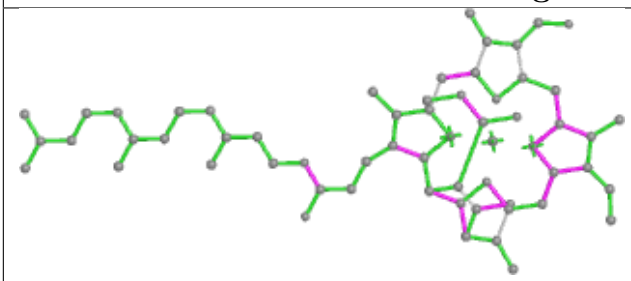


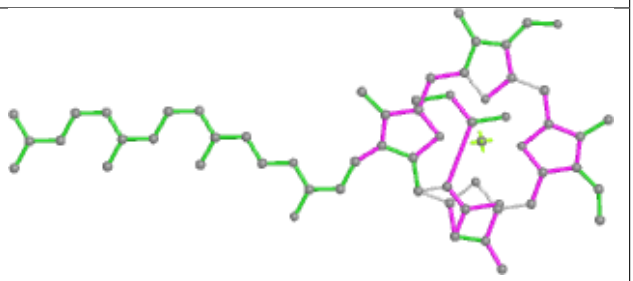
Ligand CL7 C 503



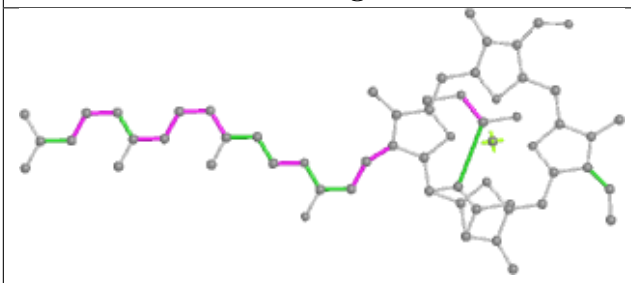
Ligand CL7 5 402



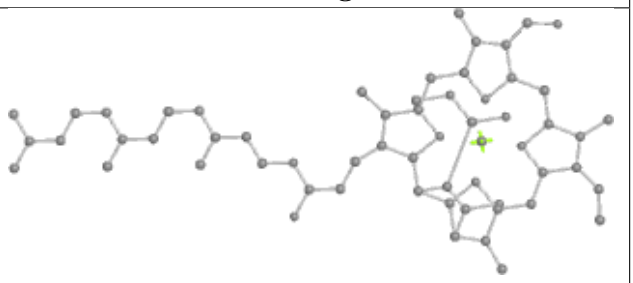
Bond lengths



Bond angles

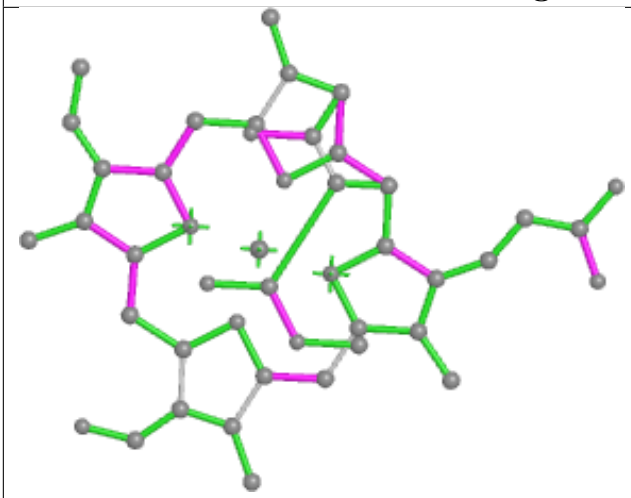


Torsions

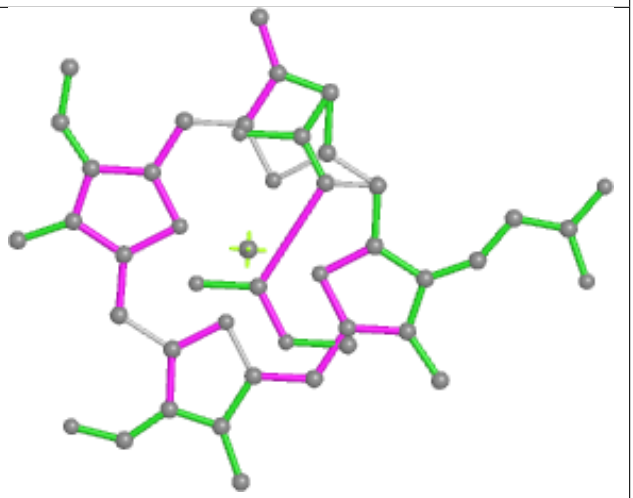


Rings

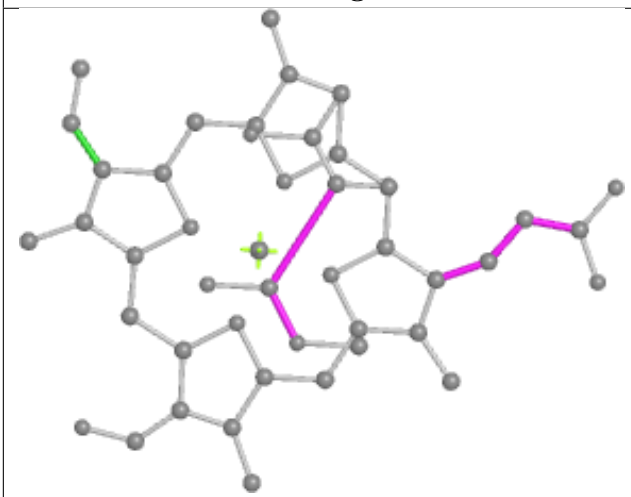
Ligand CL7 1 405



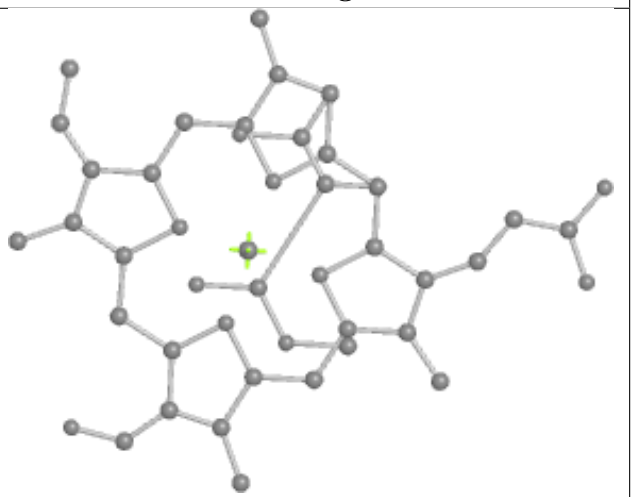
Bond lengths



Bond angles

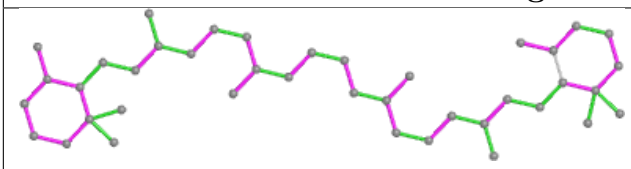


Torsions

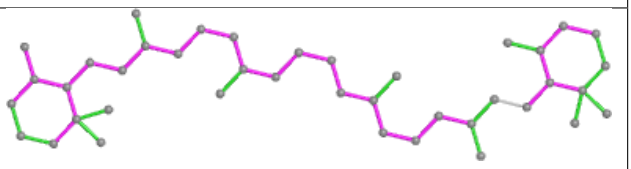


Rings

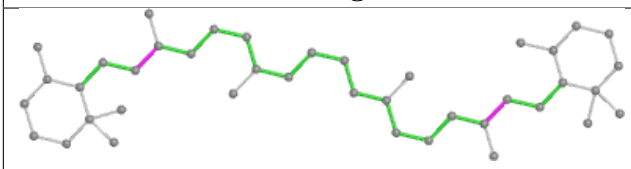
Ligand 8CT B 619



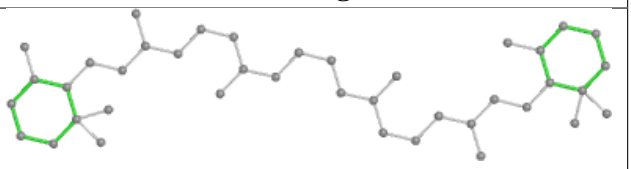
Bond lengths



Bond angles

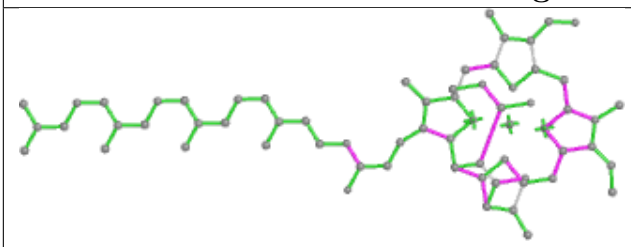


Torsions

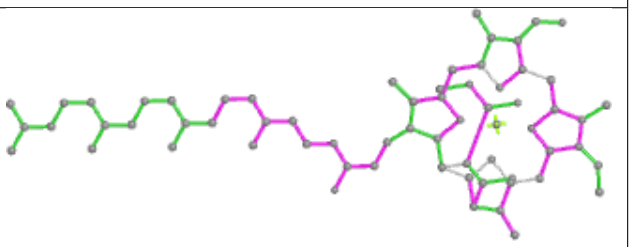


Rings

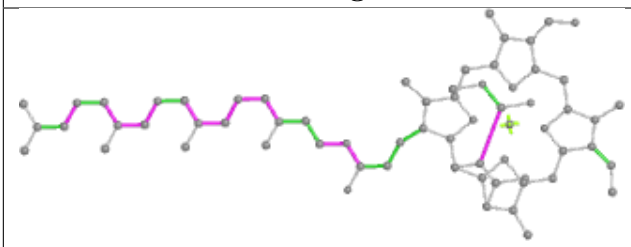
Ligand CL7 3 511



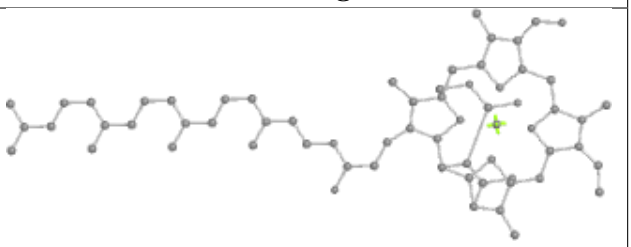
Bond lengths



Bond angles

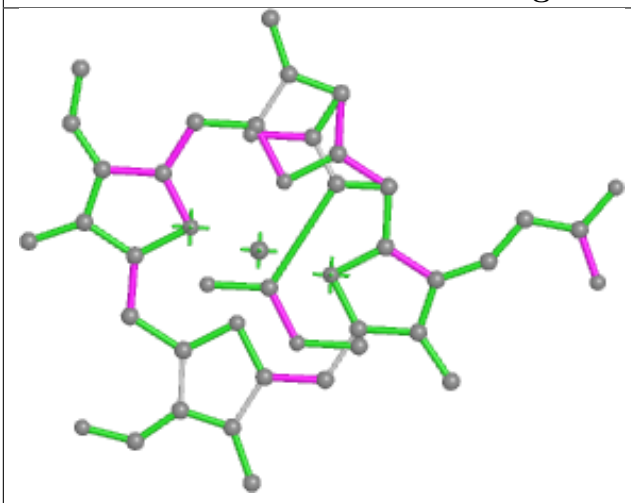


Torsions

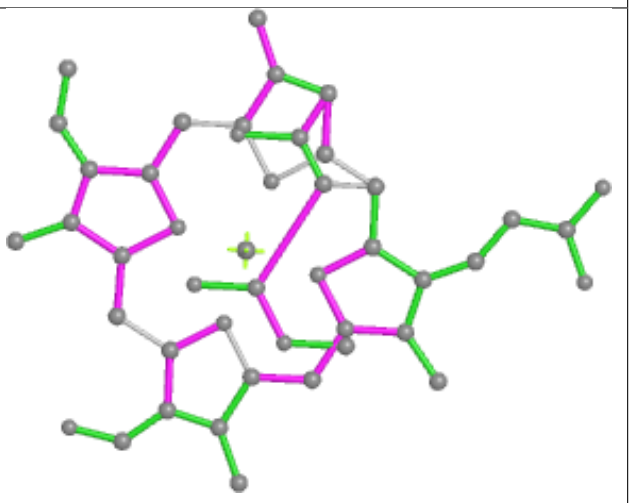


Rings

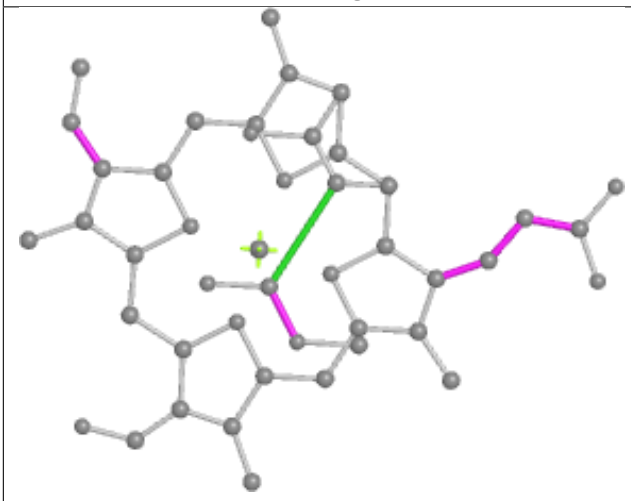
Ligand CL7 1 419



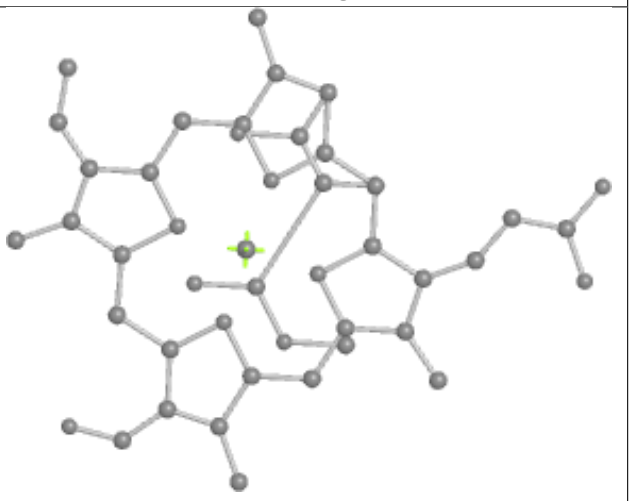
Bond lengths



Bond angles

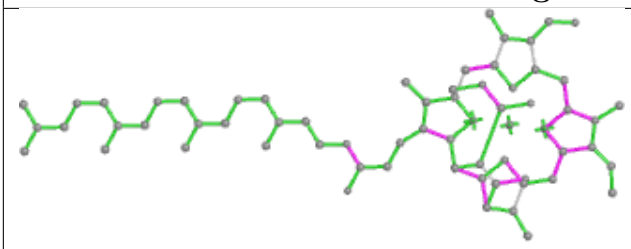


Torsions



Rings

Ligand CL7 2 506



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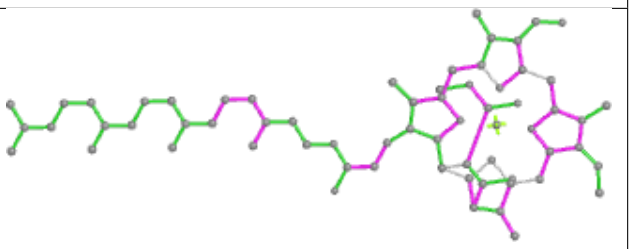
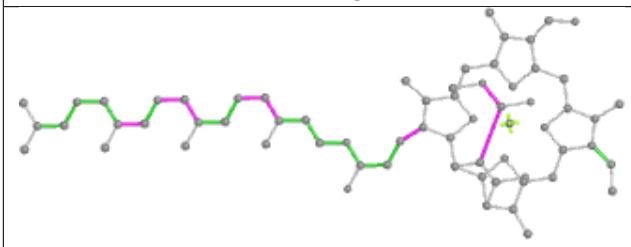


Bond angles



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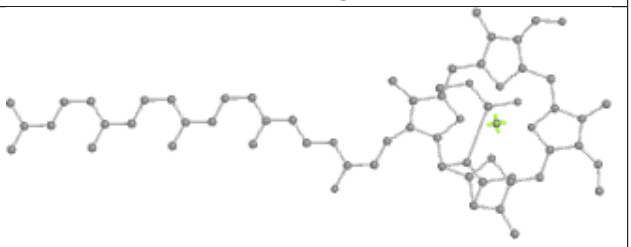
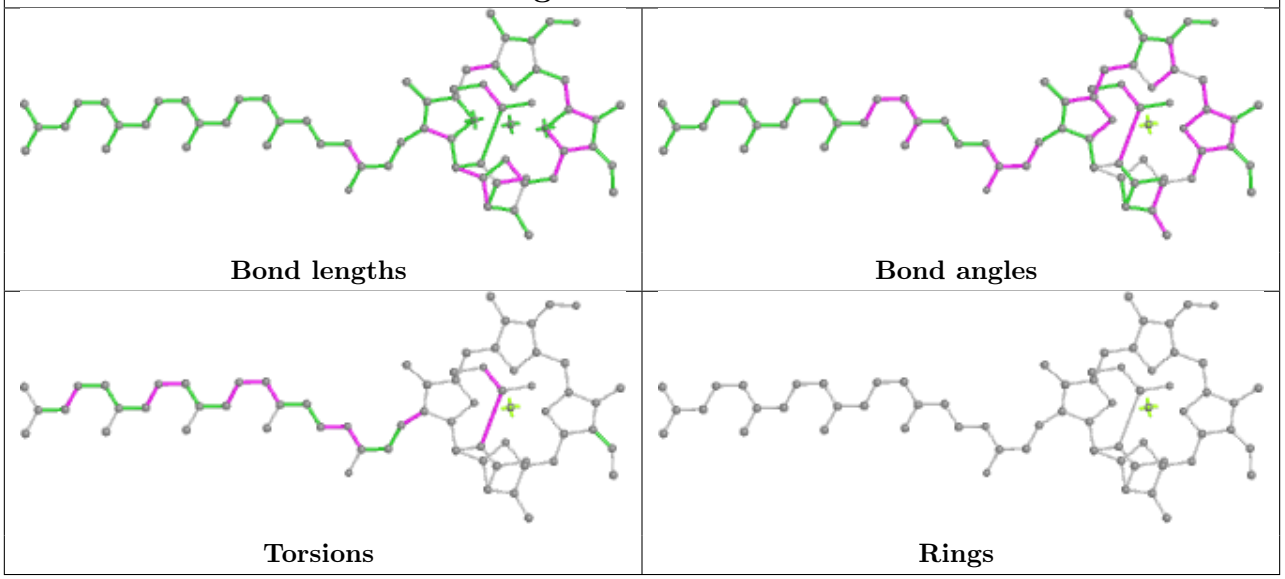
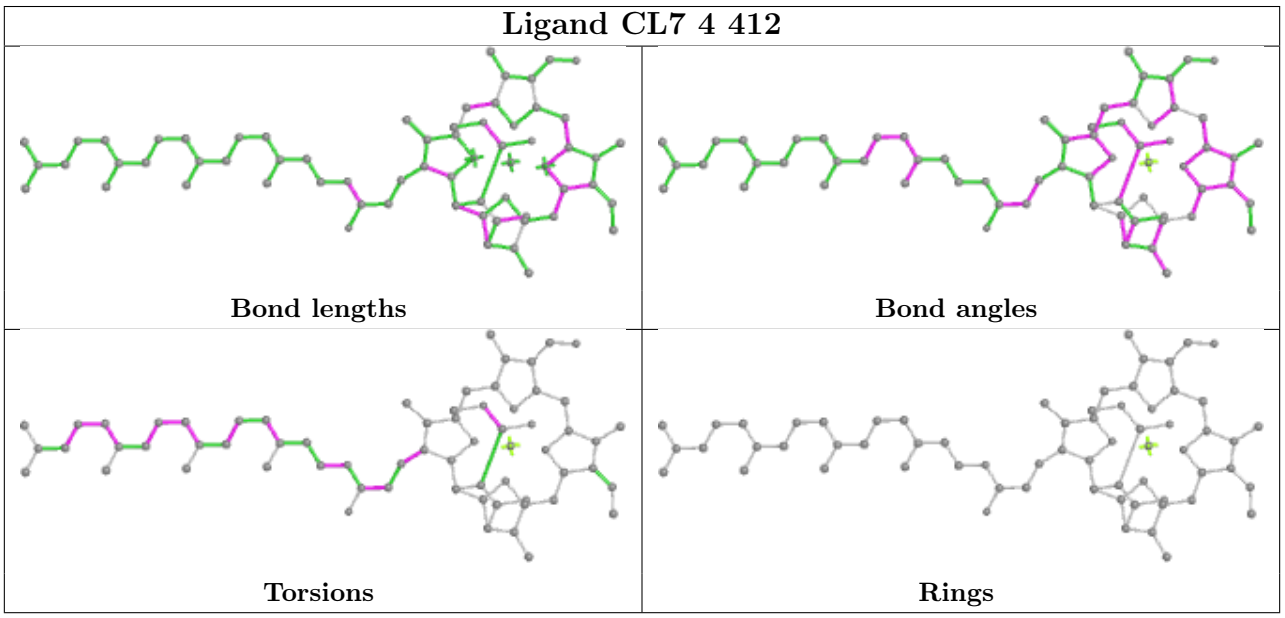


Rings

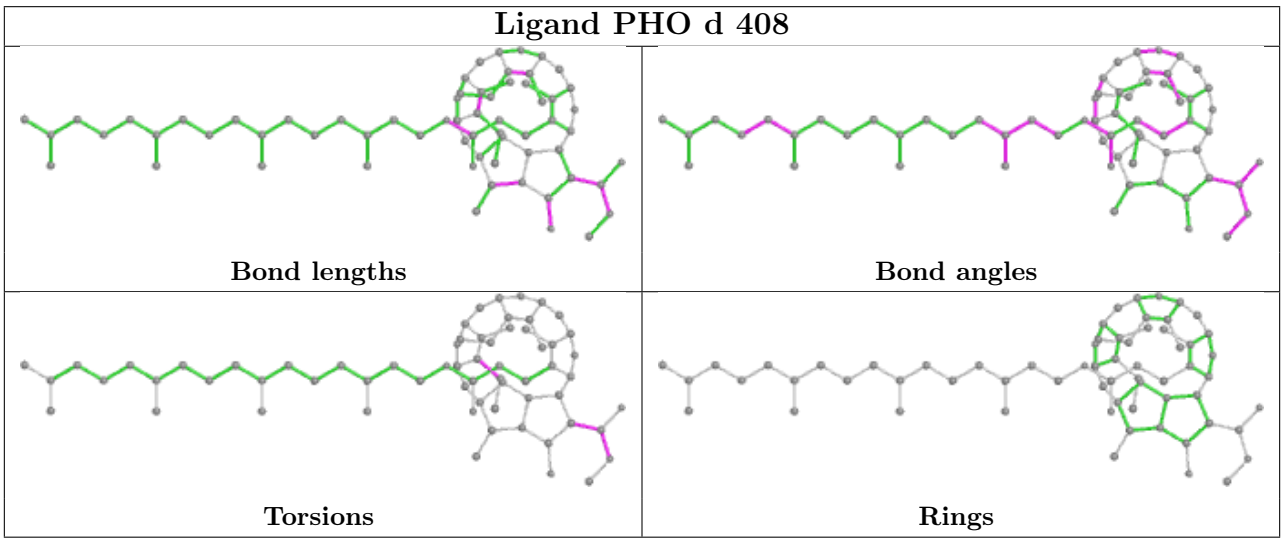
Ligand CL7 1 410



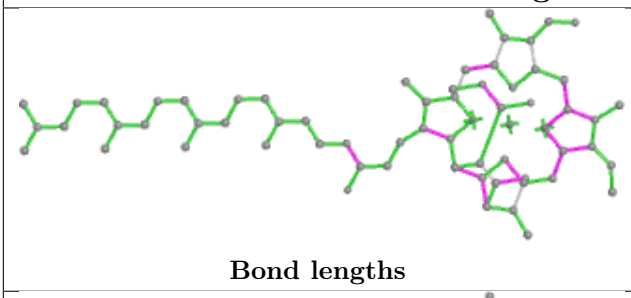
Ligand CL7 4 412



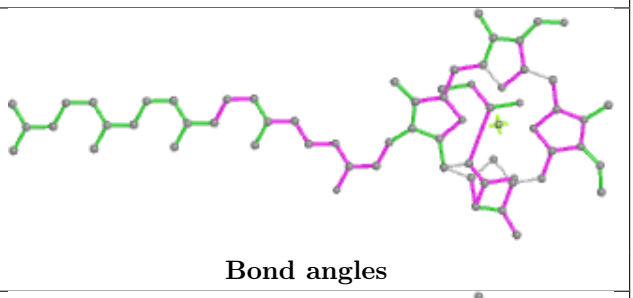
Ligand PHO d 408



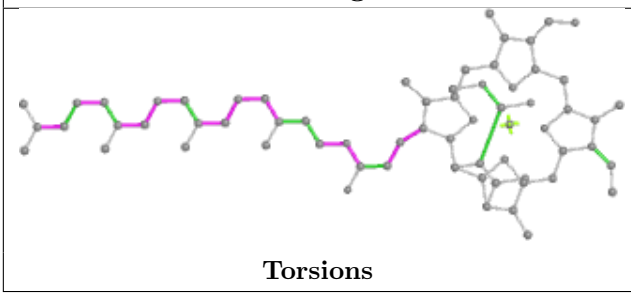
Ligand CL7 4 405



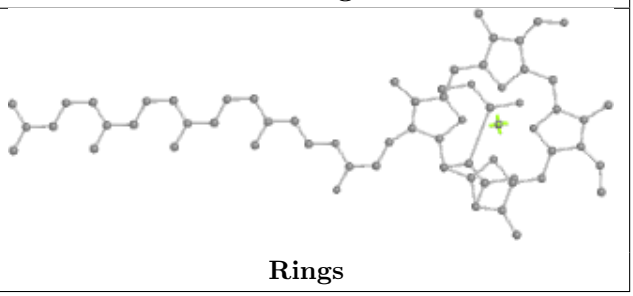
Bond lengths



Bond angles

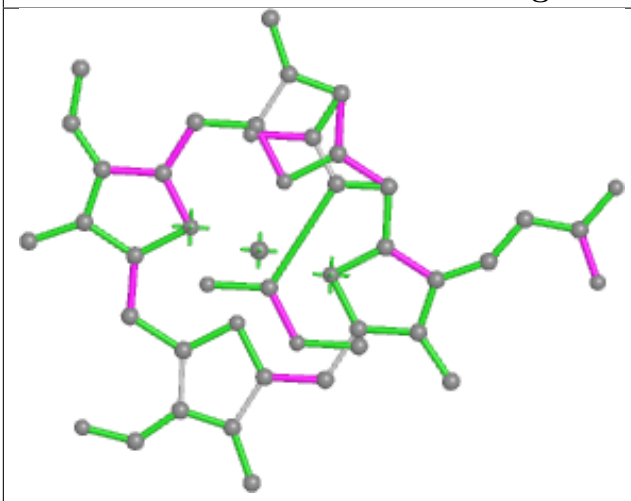


Torsions

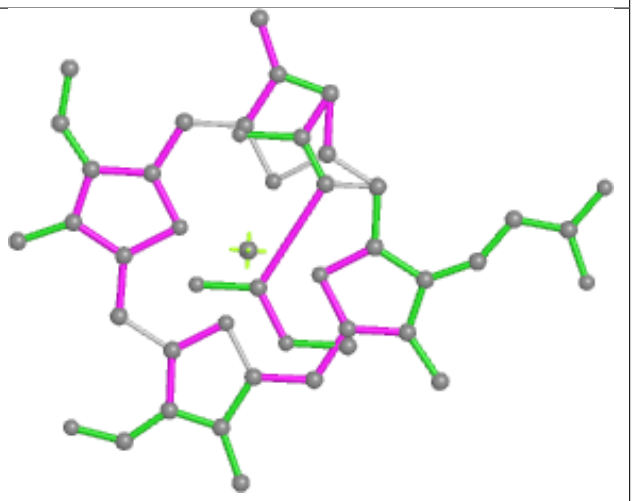


Rings

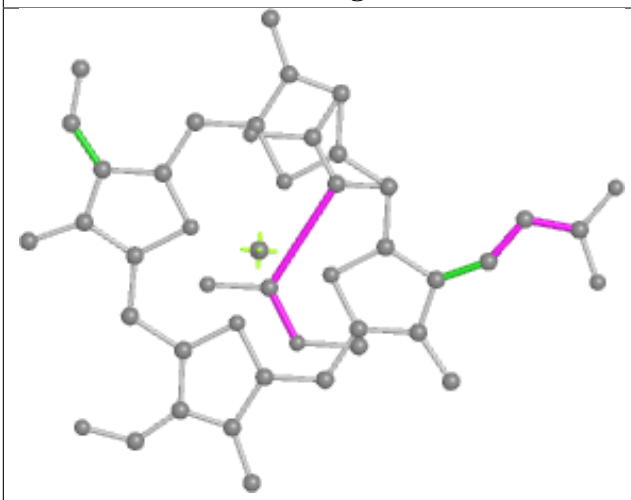
Ligand CL7 b 623



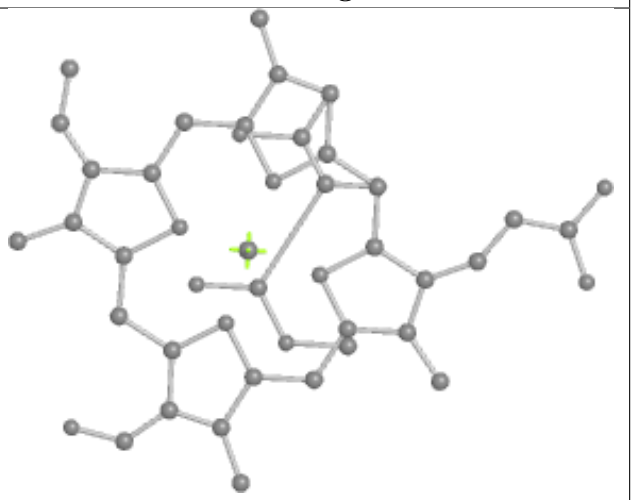
Bond lengths



Bond angles

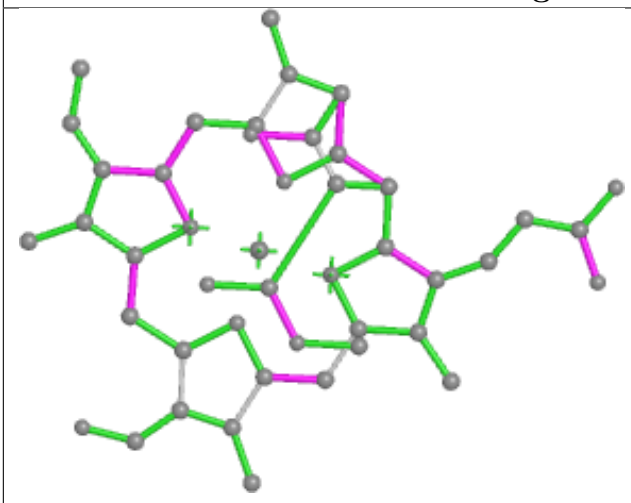


Torsions

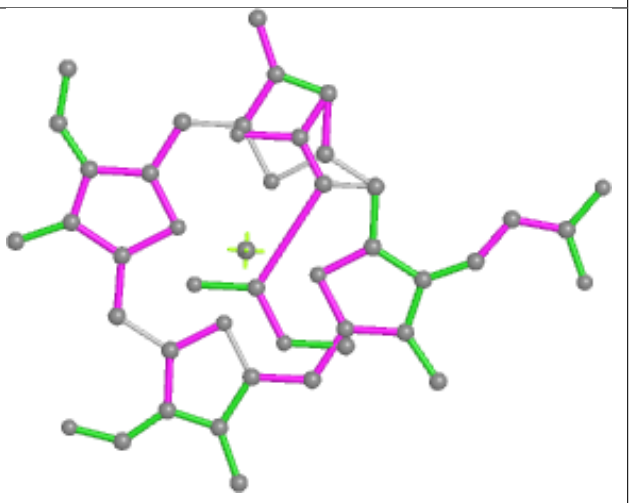


Rings

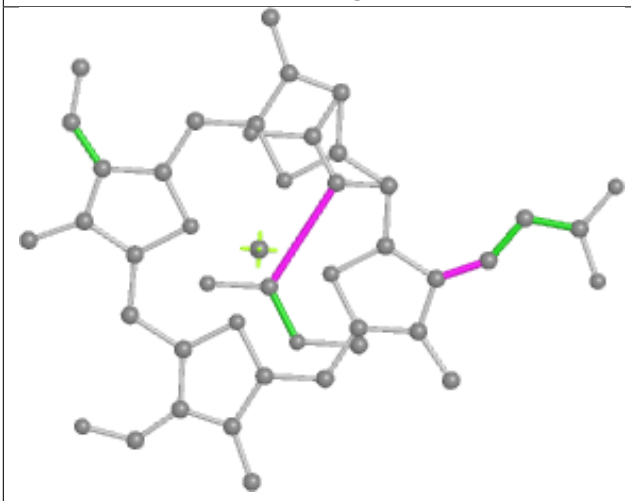
Ligand CL7 2 515



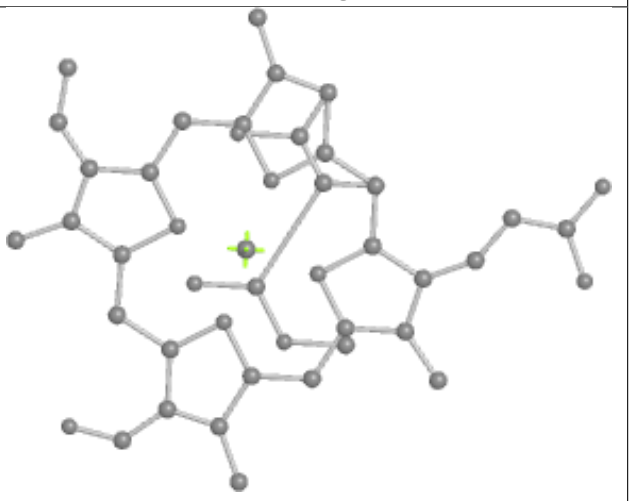
Bond lengths



Bond angles

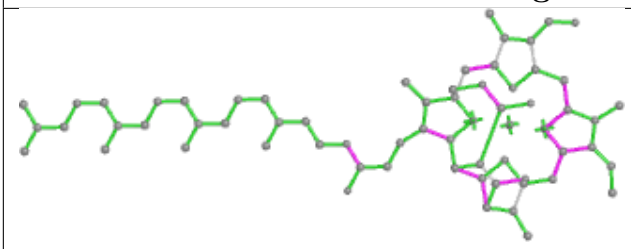


Torsions

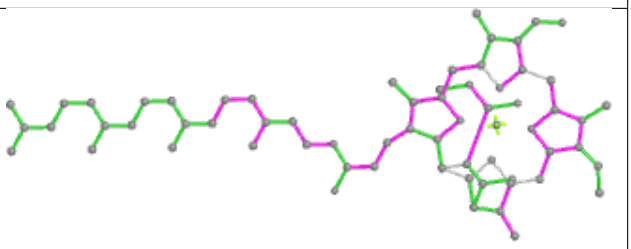


Rings

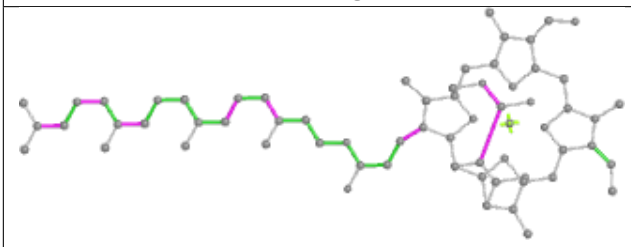
Ligand CL7 8 411



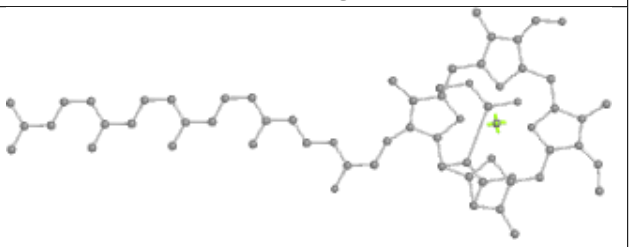
Bond lengths



Bond angles

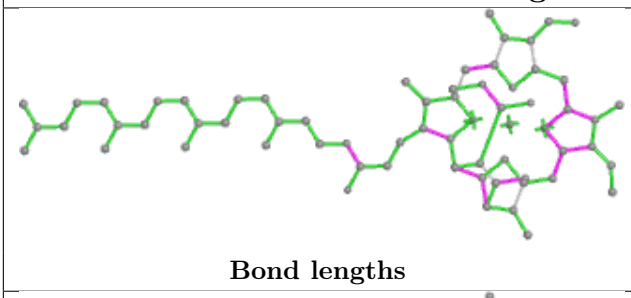


Torsions

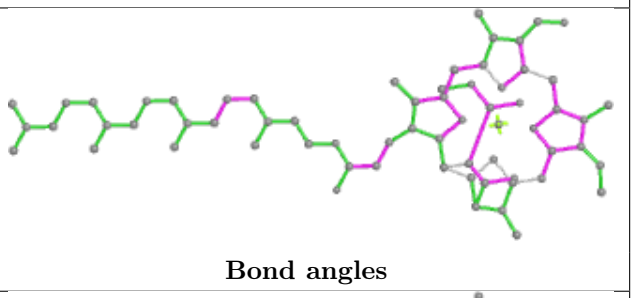


Rings

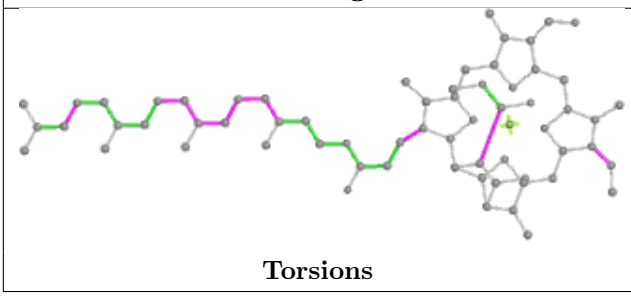
Ligand CL7 B 608



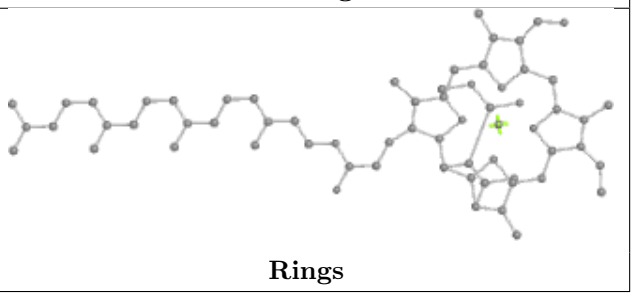
Bond lengths



Bond angles

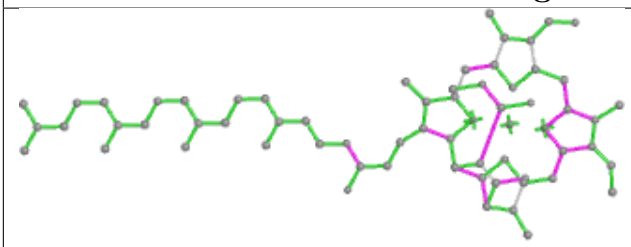


Torsions

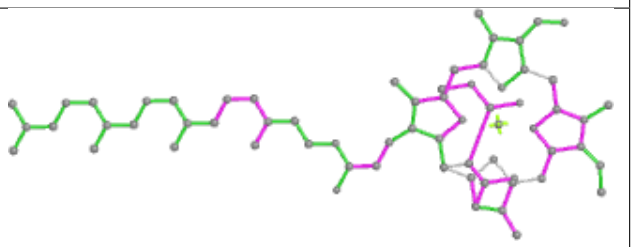


Rings

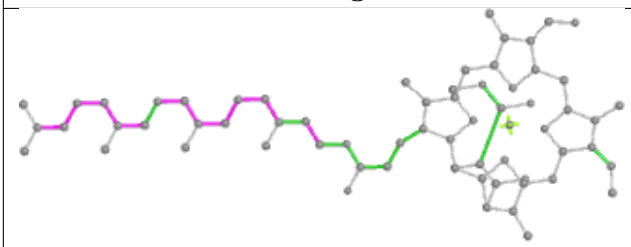
Ligand CL7 c 508



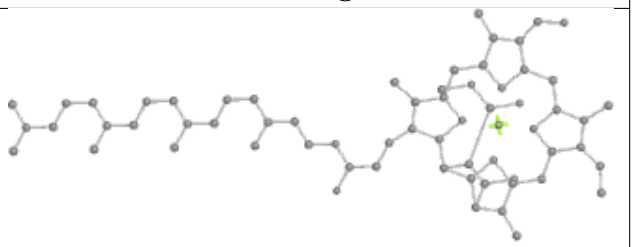
Bond lengths



Bond angles

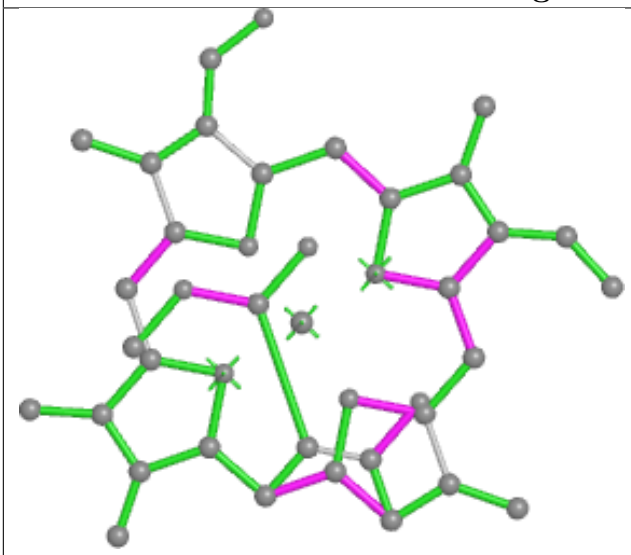


Torsions

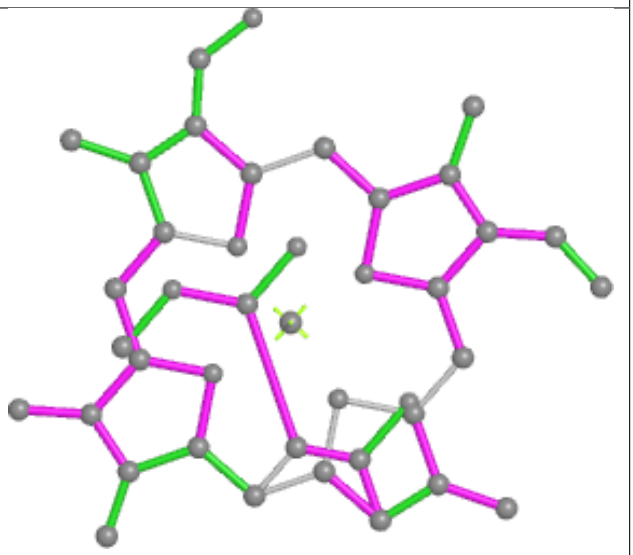


Rings

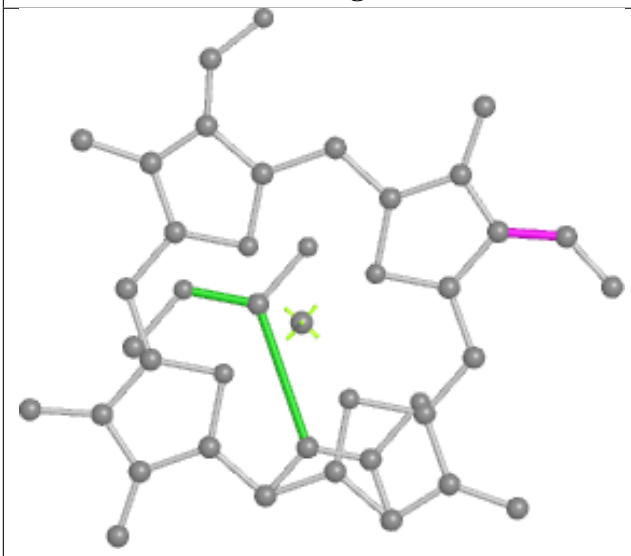
Ligand CL7 5 414



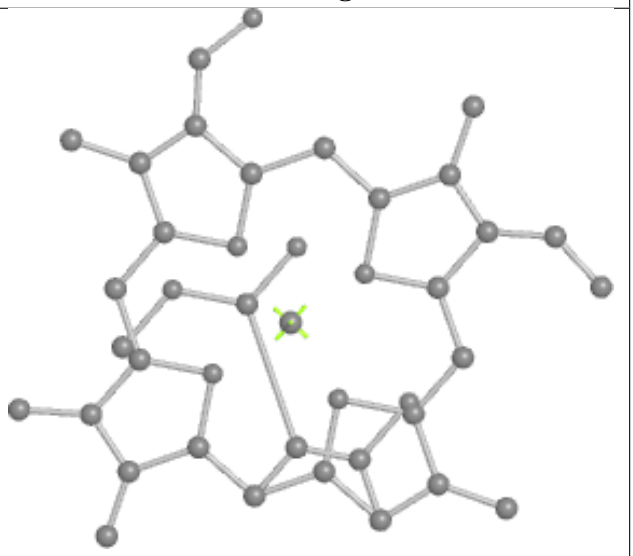
Bond lengths



Bond angles

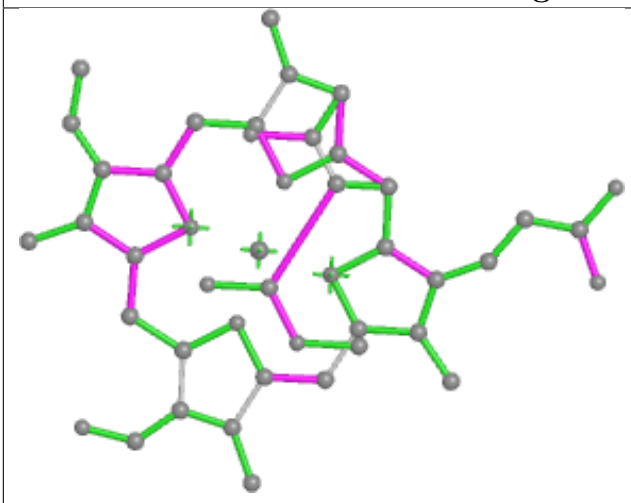


Torsions



Rings

Ligand CL7 3 513



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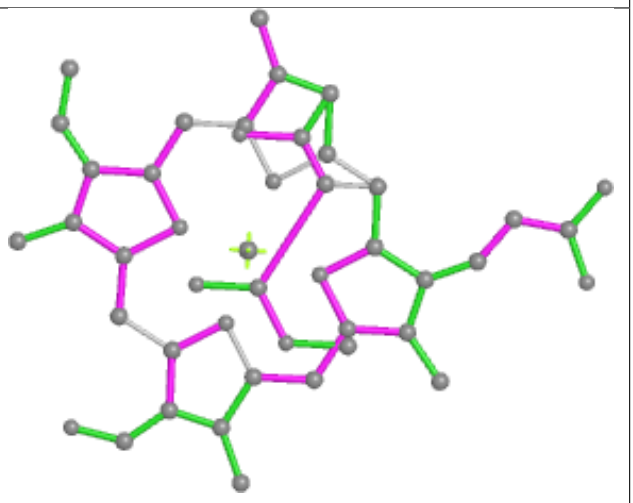
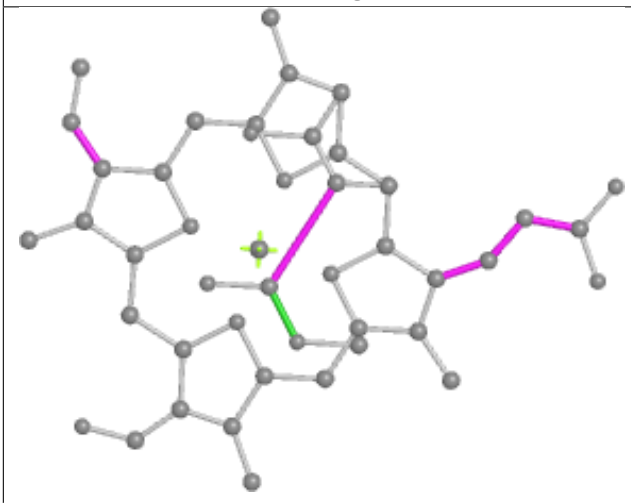
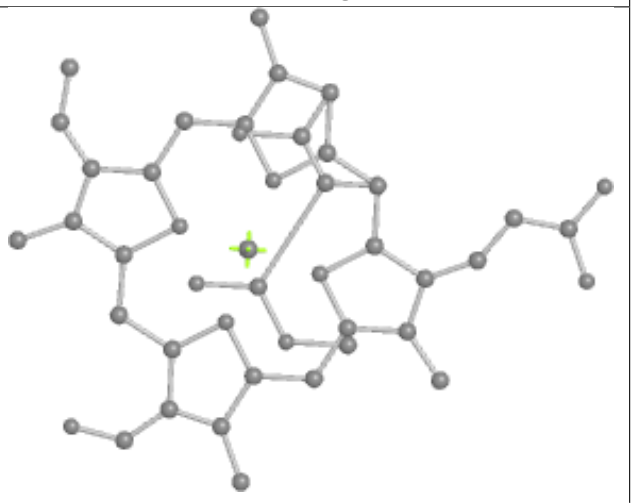


Bond angles

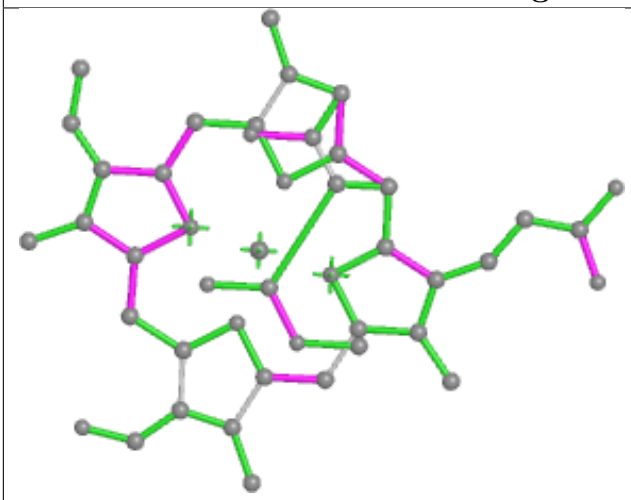


Torsions

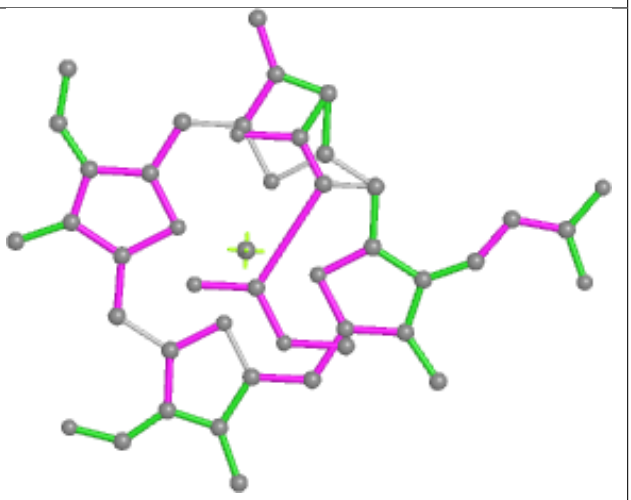


Rings

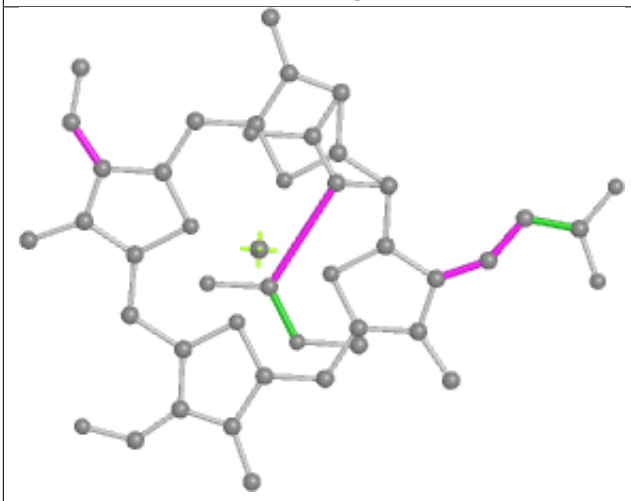
Ligand CL7 d 405



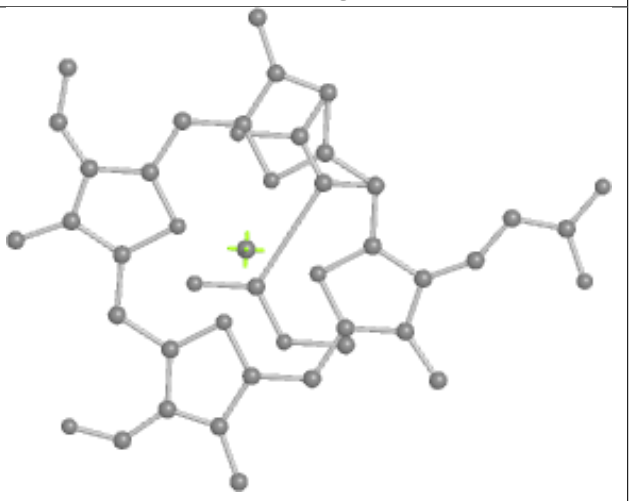
Bond lengths



Bond angles

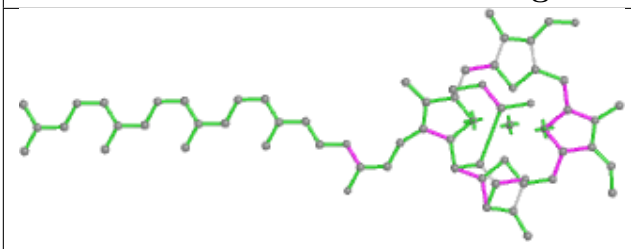


Torsions

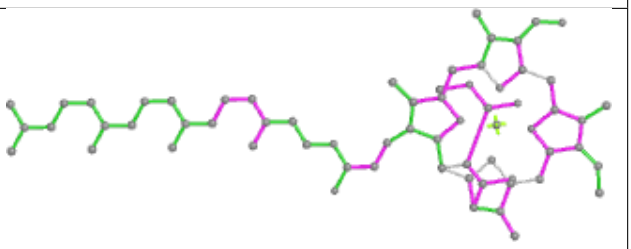


Rings

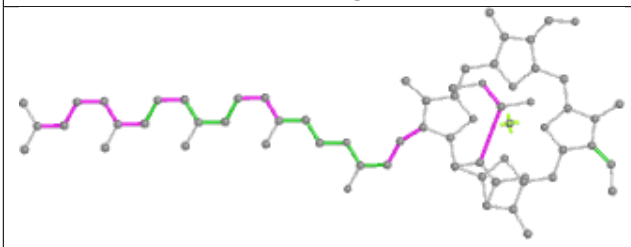
Ligand CL7 b 605



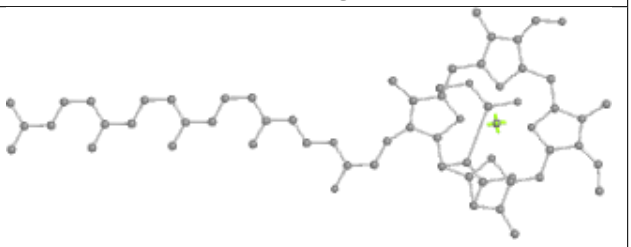
Bond lengths



Bond angles

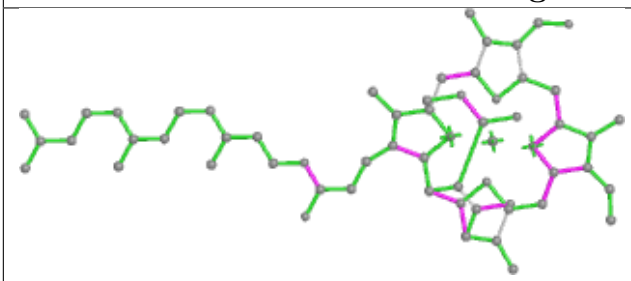


Torsions

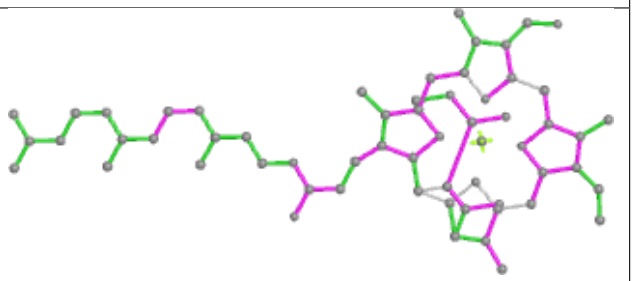


Rings

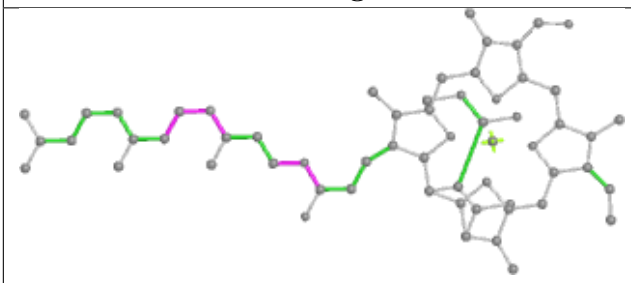
Ligand CL7 B 602



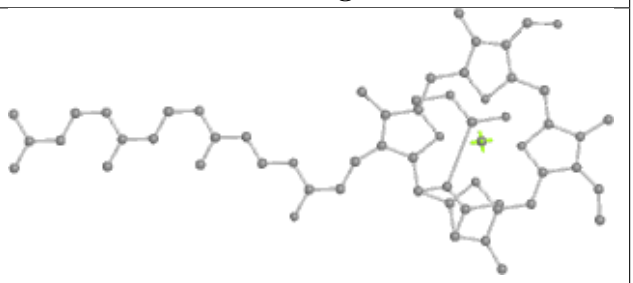
Bond lengths



Bond angles

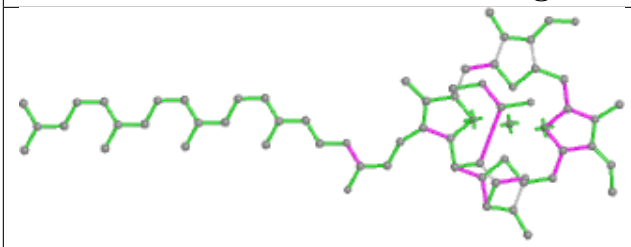


Torsions

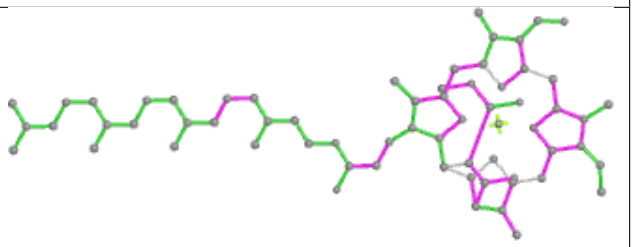


Rings

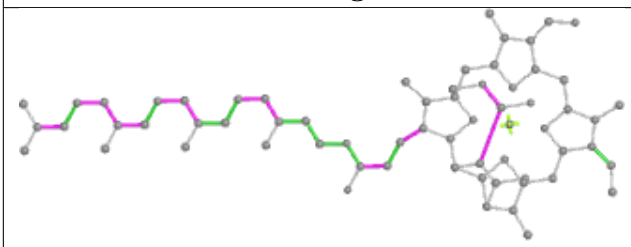
Ligand CL7 6 507



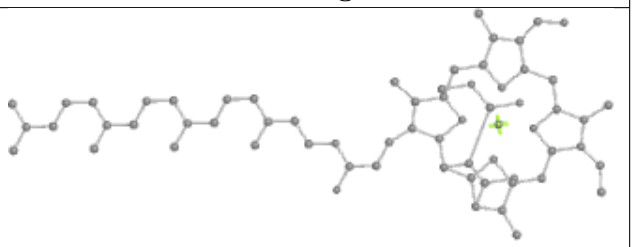
Bond lengths



Bond angles

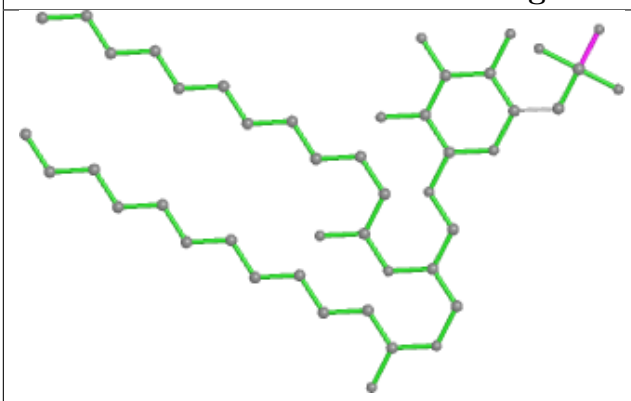


Torsions

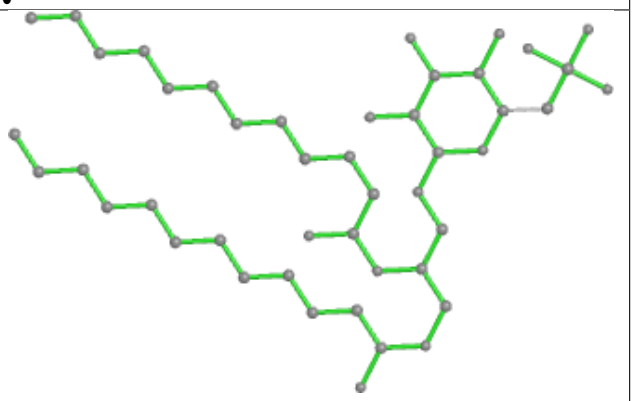


Rings

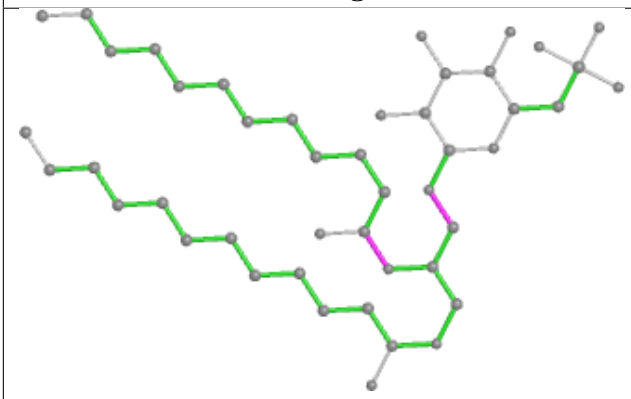
Ligand SQD 7 521



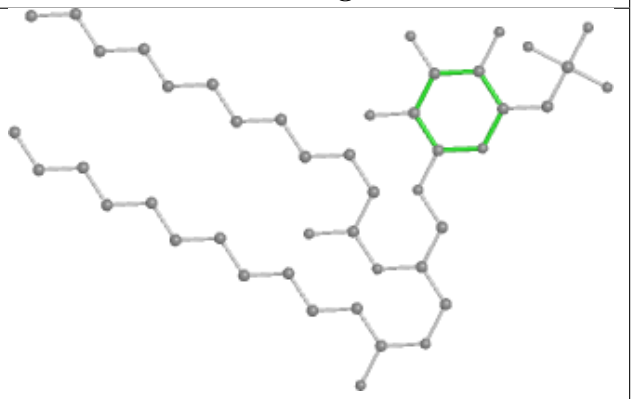
Bond lengths



Bond angles

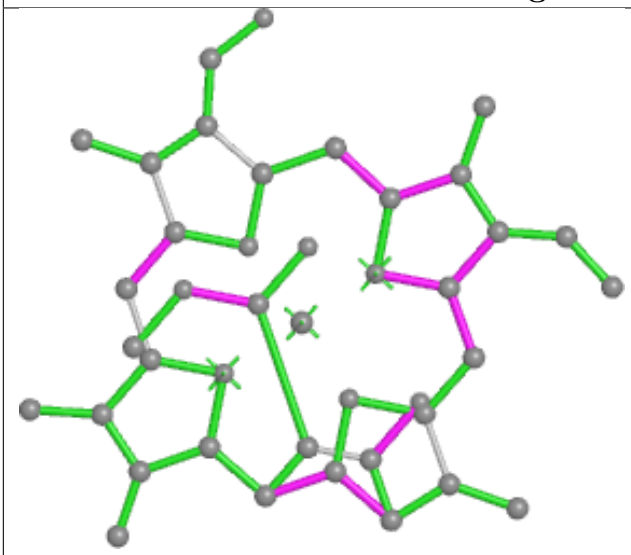


Torsions

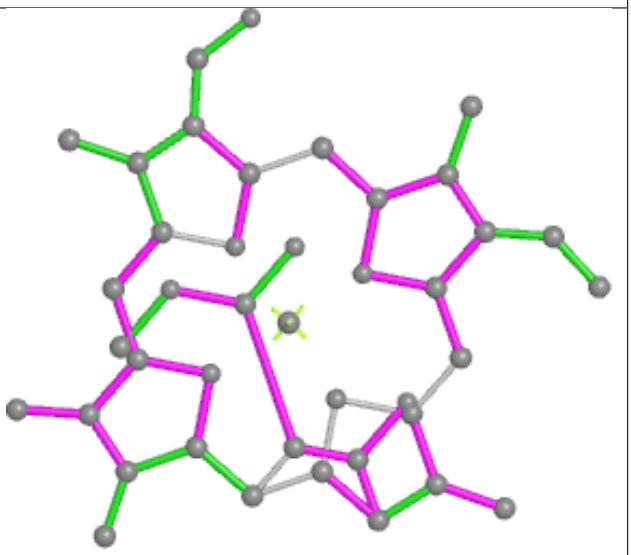


Rings

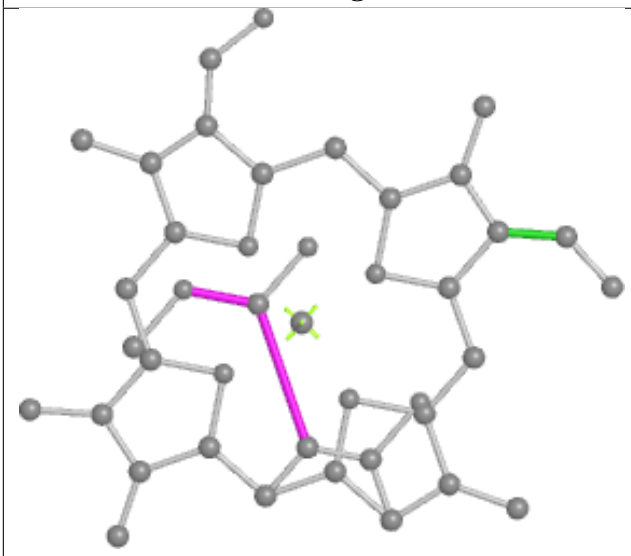
Ligand CL7 C 518



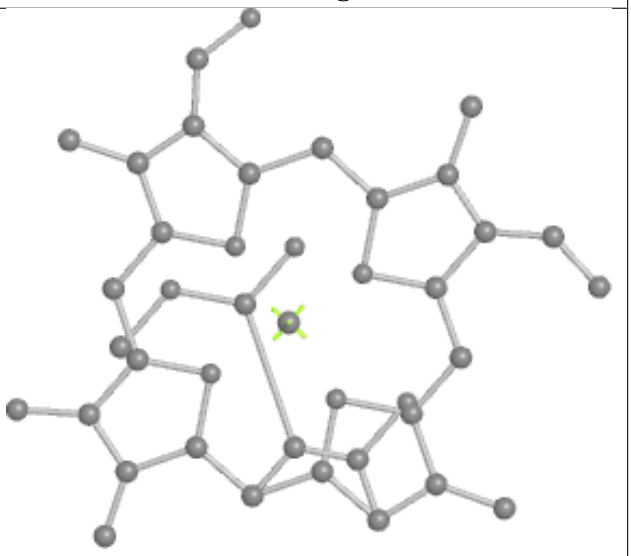
Bond lengths



Bond angles

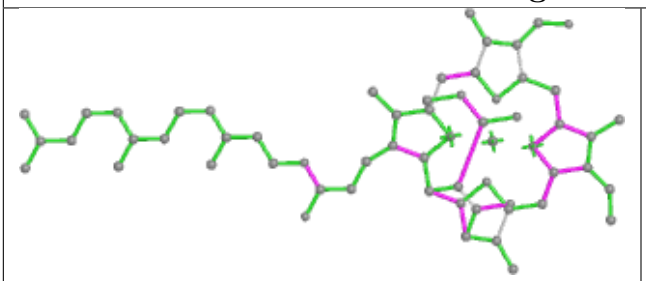


Torsions

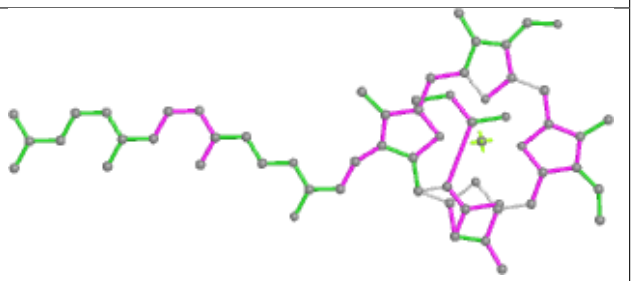


Rings

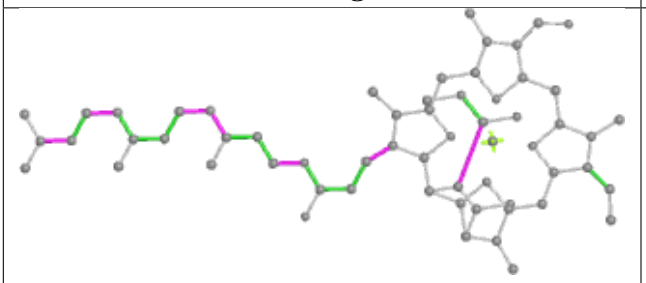
Ligand CL7 B 614



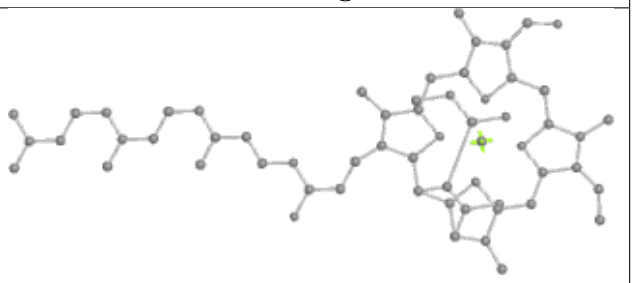
Bond lengths



Bond angles

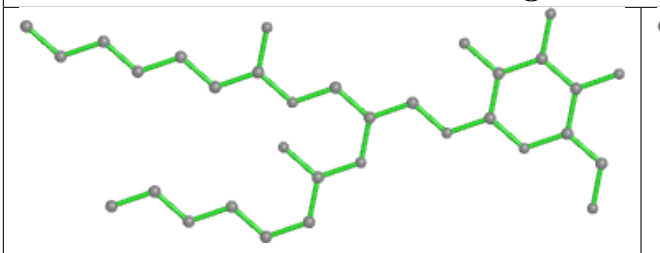


Torsions

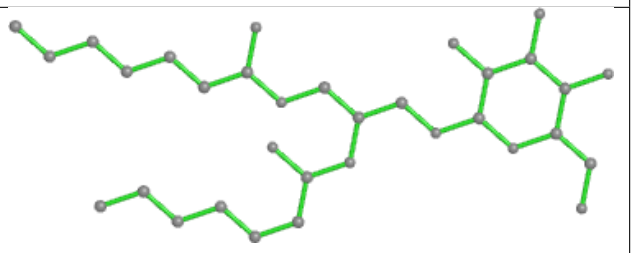


Rings

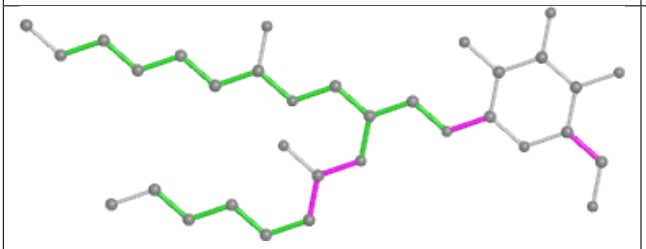
Ligand LMG d 410



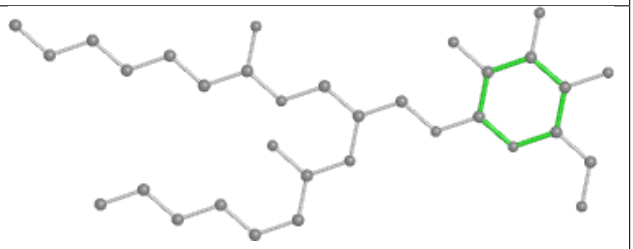
Bond lengths



Bond angles

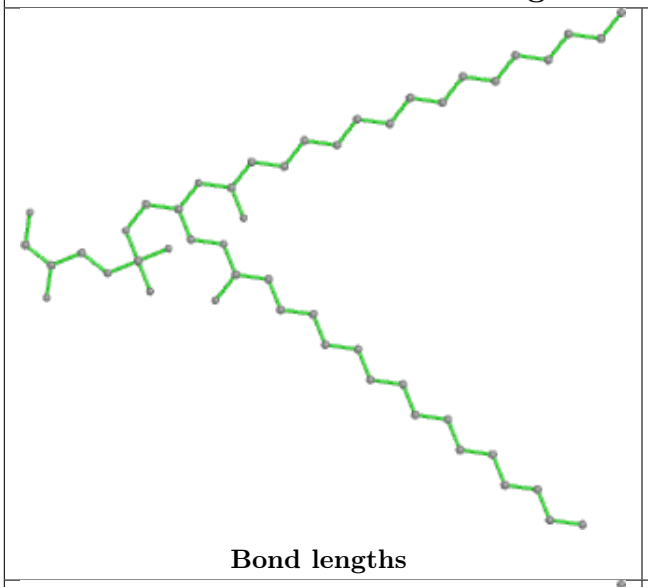


Torsions

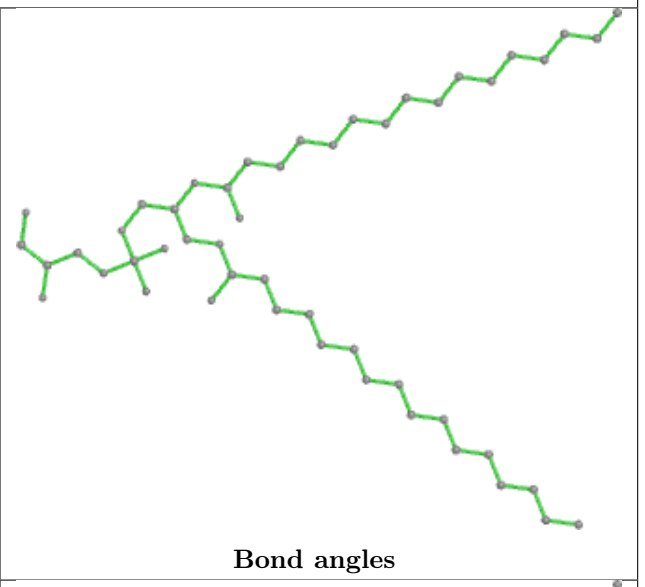


Rings

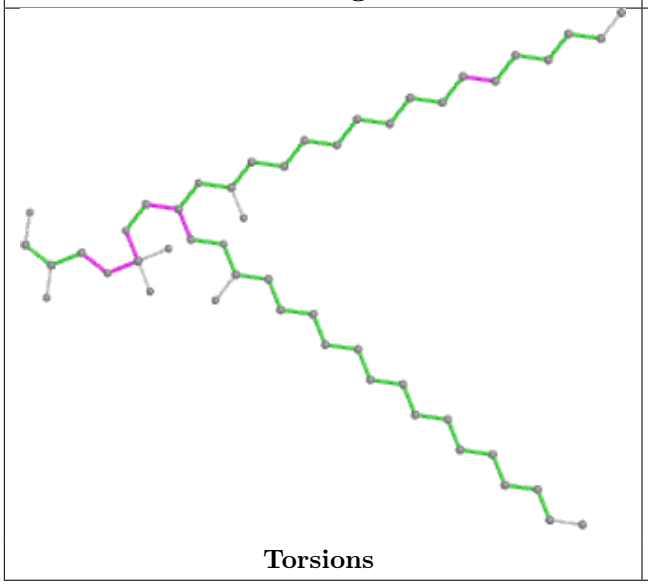
Ligand LHG 8 401



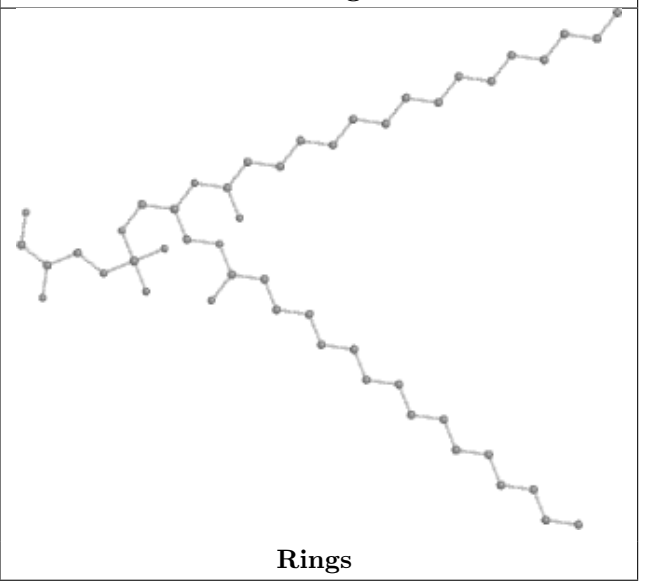
Bond lengths



Bond angles

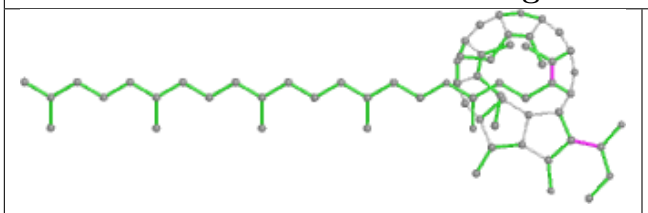


Torsions

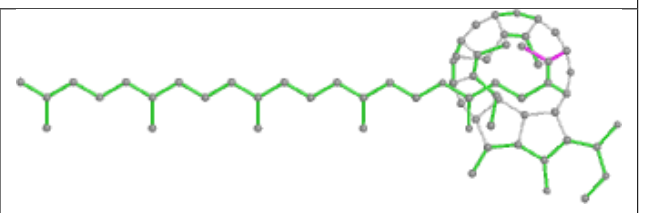


Rings

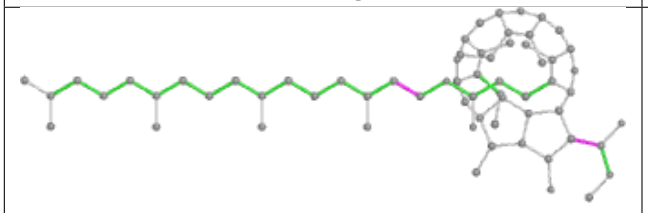
Ligand PHO A 402



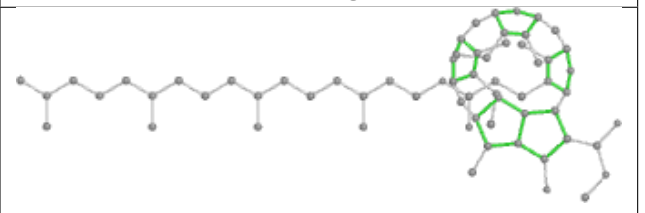
Bond lengths



Bond angles

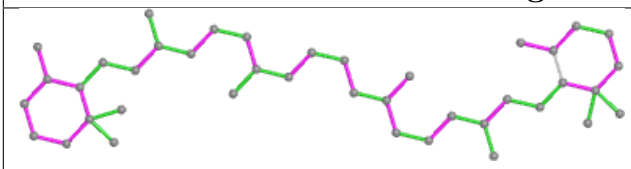


Torsions

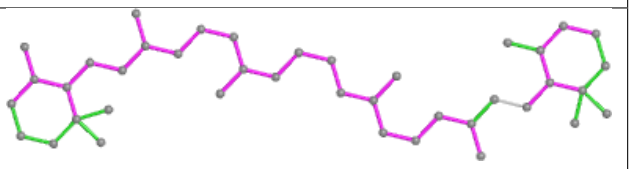


Rings

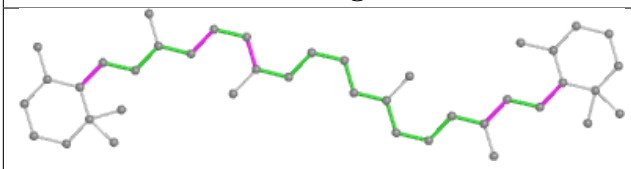
Ligand 8CT C 519



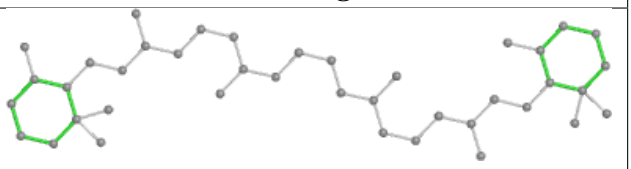
Bond lengths



Bond angles

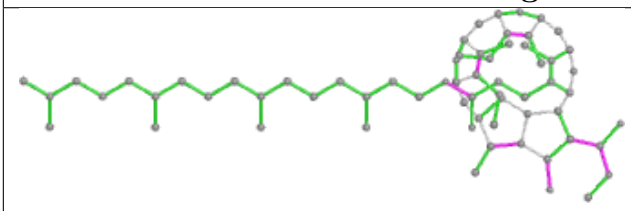


Torsions

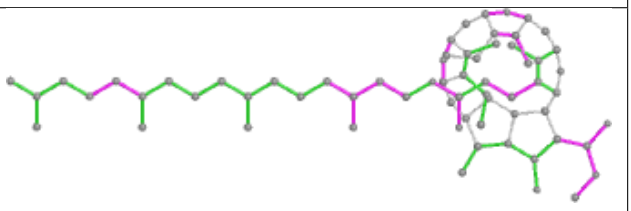


Rings

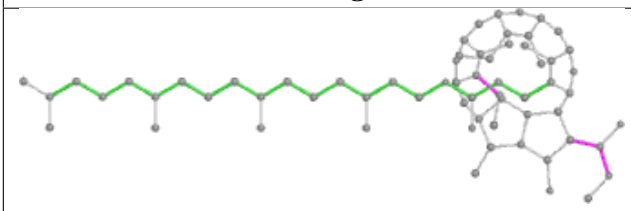
Ligand PHO D 408



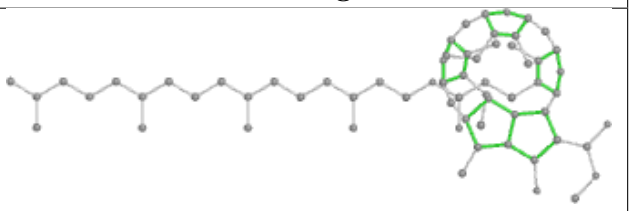
Bond lengths



Bond angles

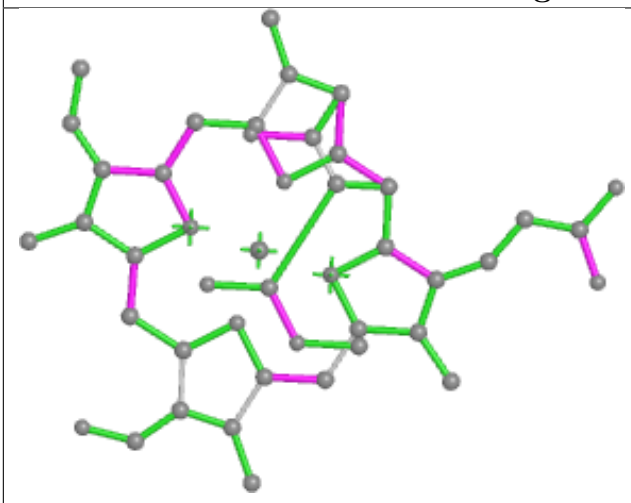


Torsions

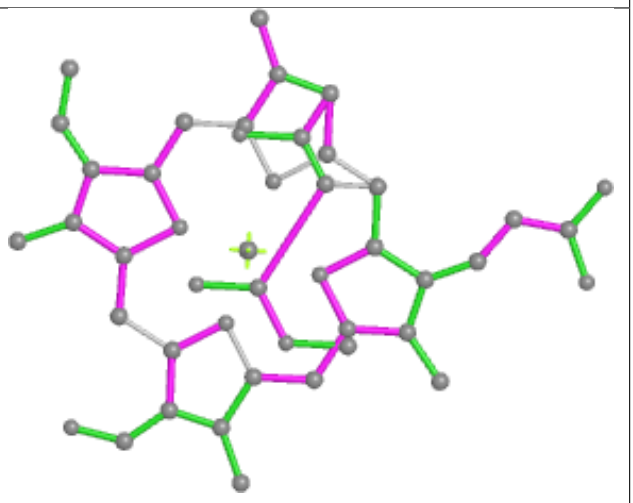


Rings

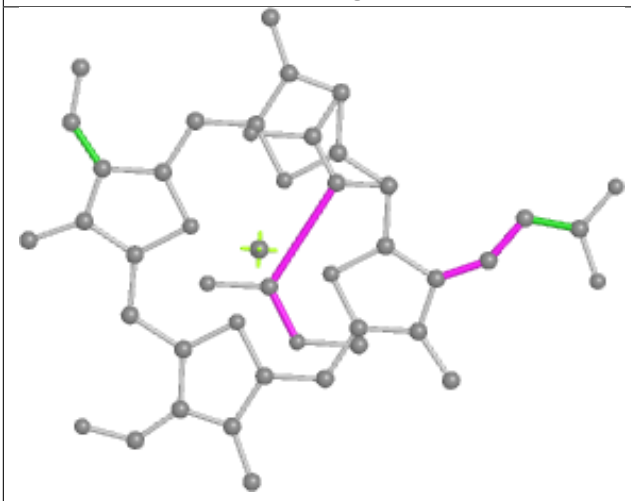
Ligand CL7 c 514



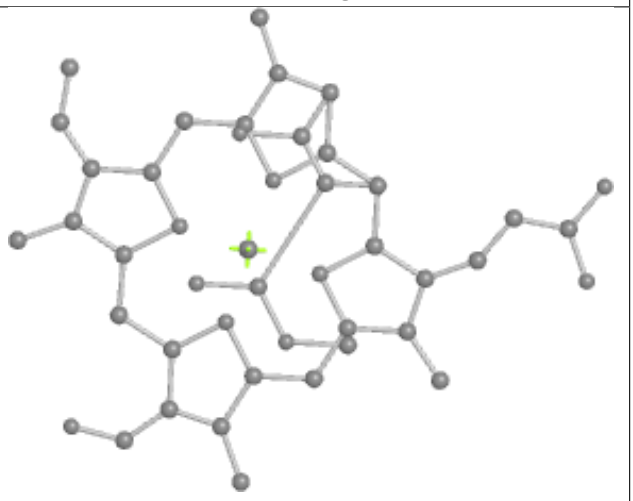
Bond lengths



Bond angles

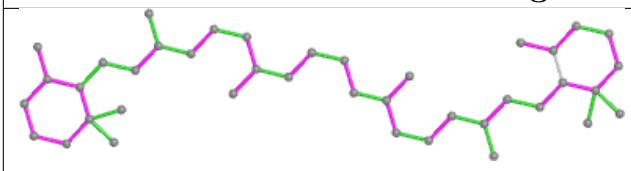


Torsions

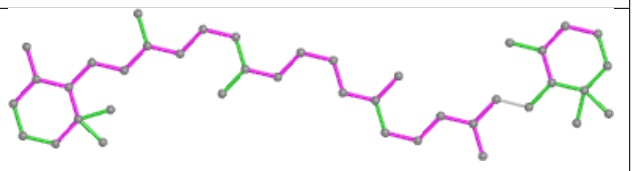


Rings

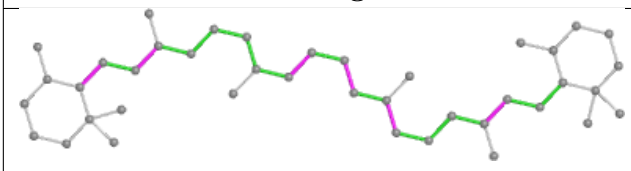
Ligand 8CT d 406



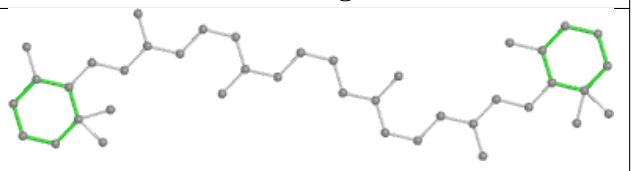
Bond lengths



Bond angles

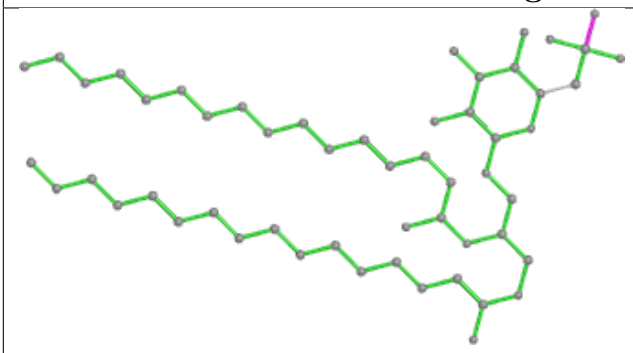


Torsions



Rings

Ligand SQD B 620



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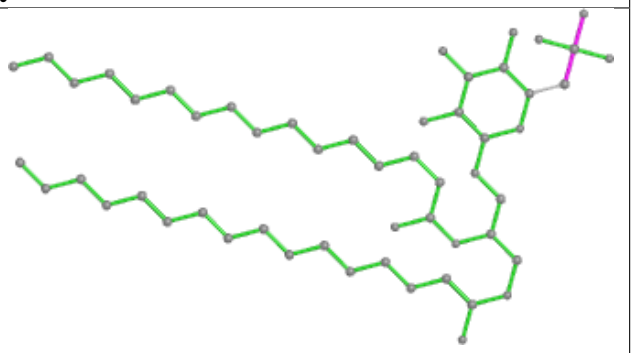

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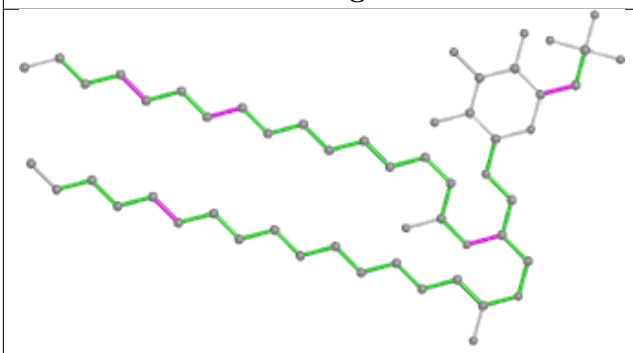

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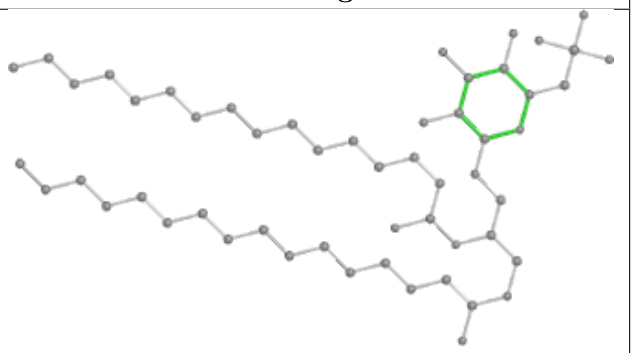
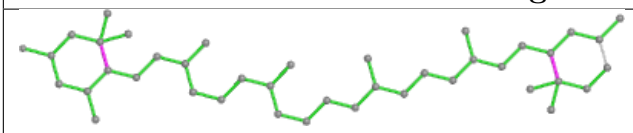


Rings

Ligand ZEX 3 520



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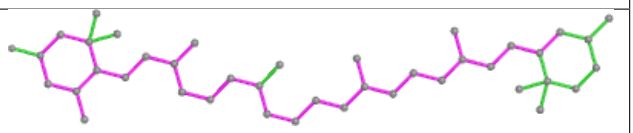
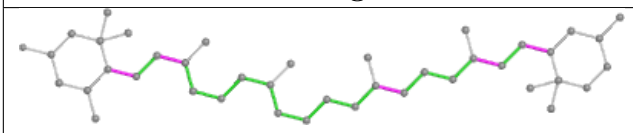


Bond angles



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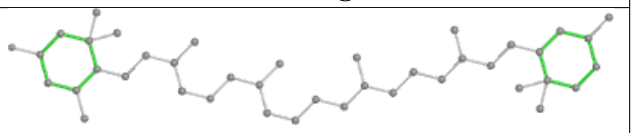
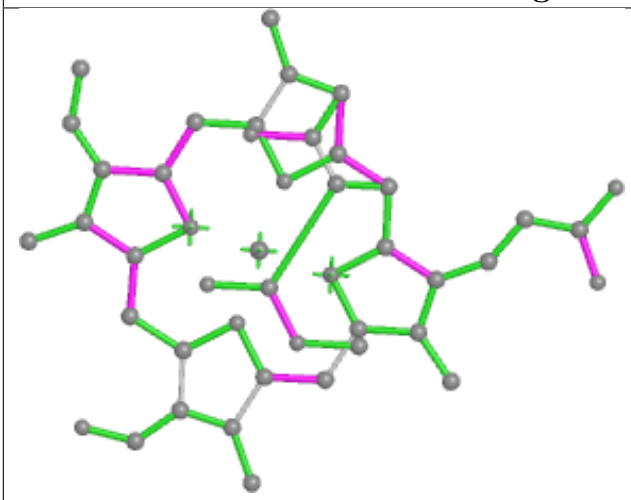


Rings

Ligand CL7 4 410



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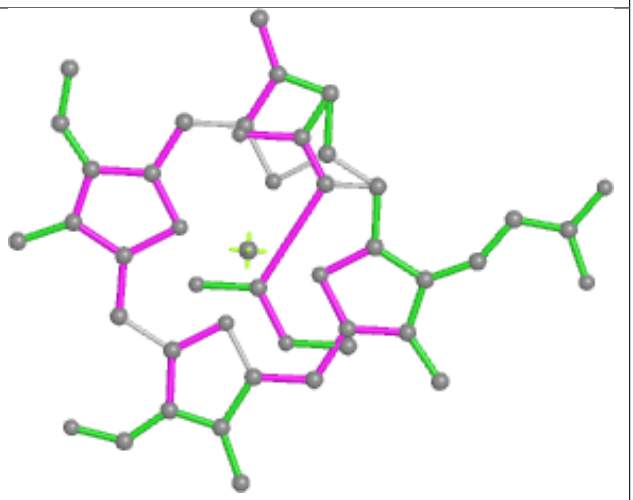
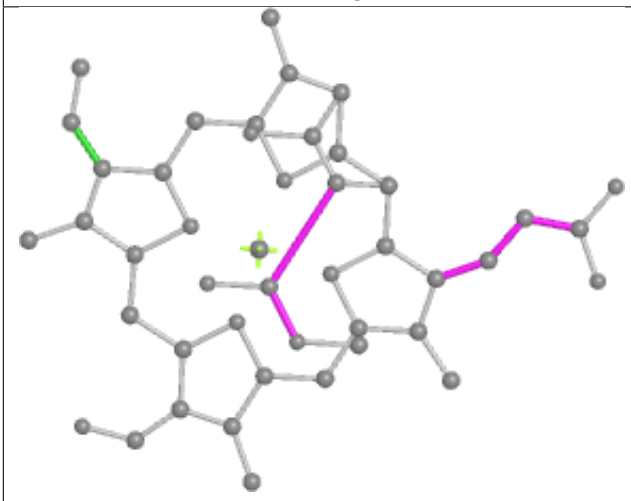


Bond angles



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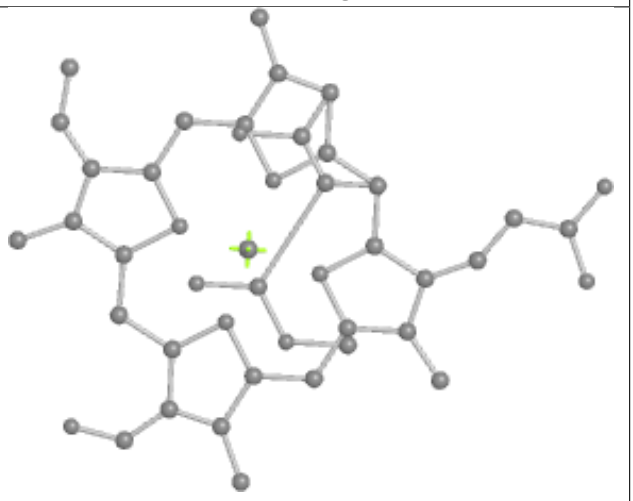
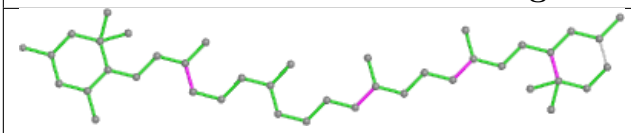


Rings

Ligand ZEX 3 519



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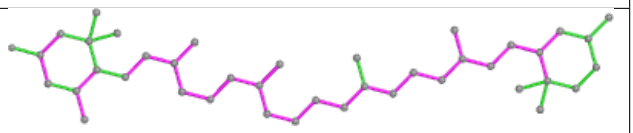

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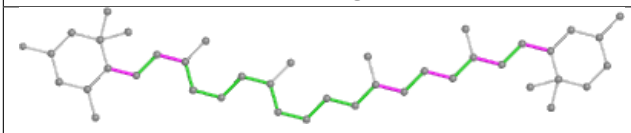

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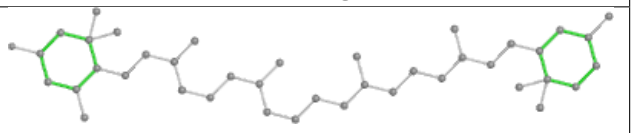
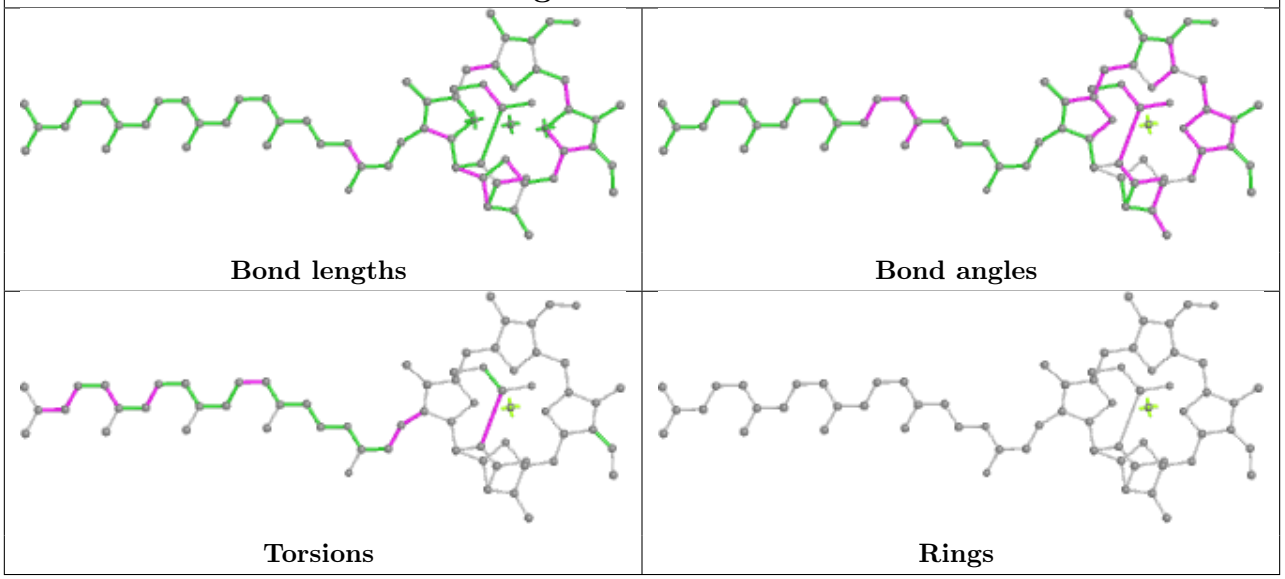
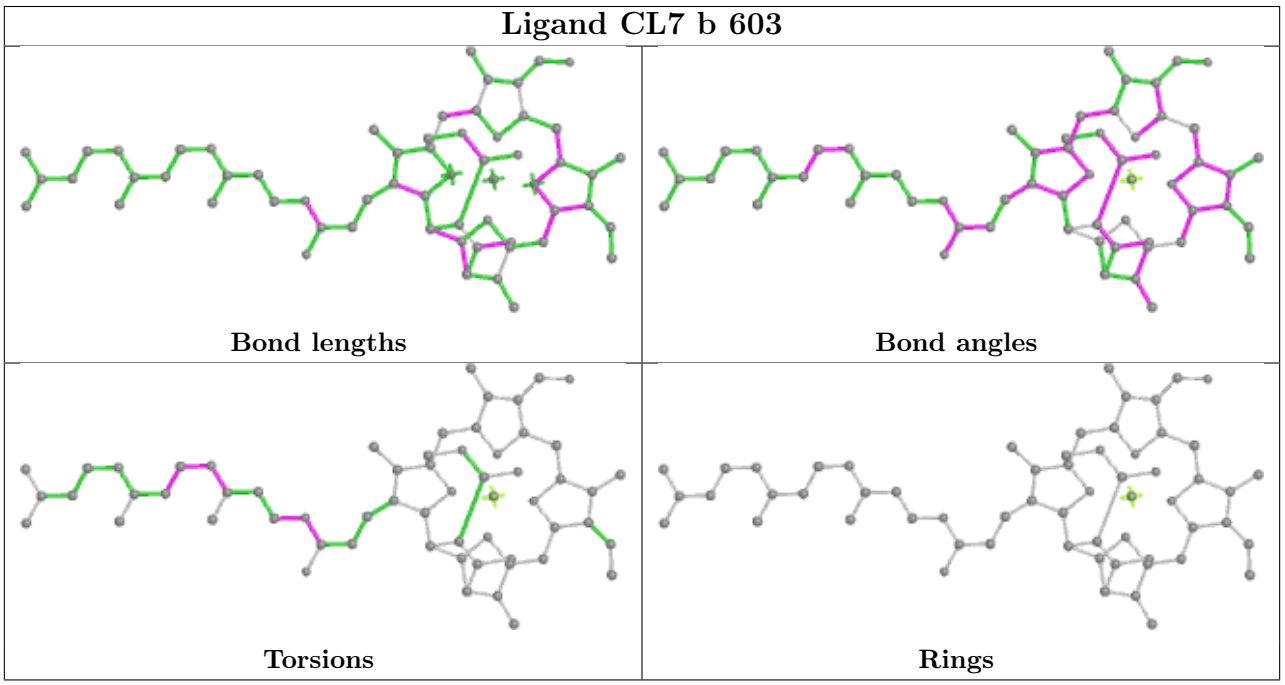


Rings

Ligand CL7 6 518



Ligand CL7 b 603



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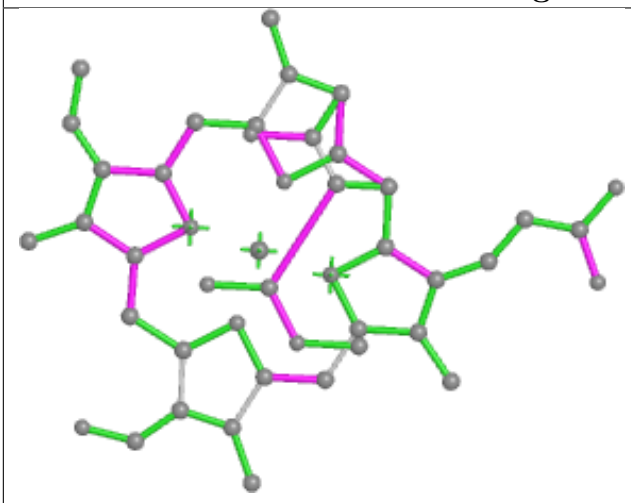

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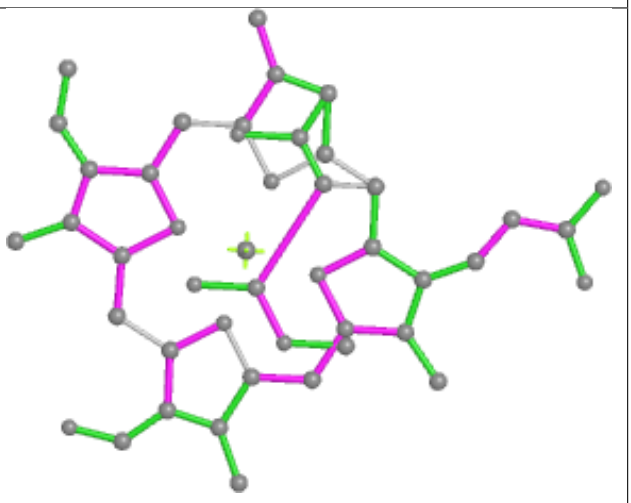
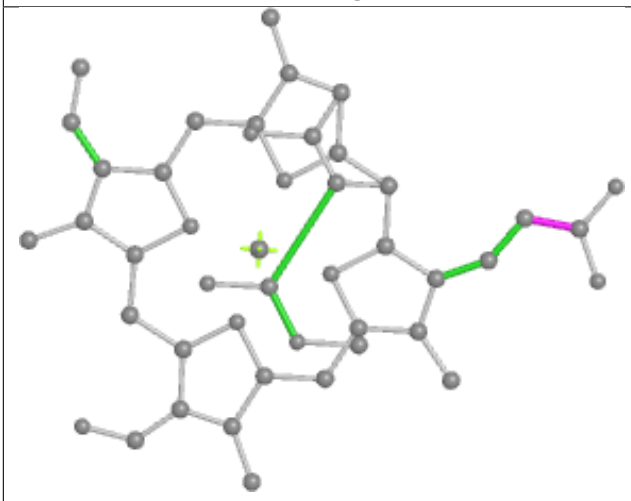


Bond angles



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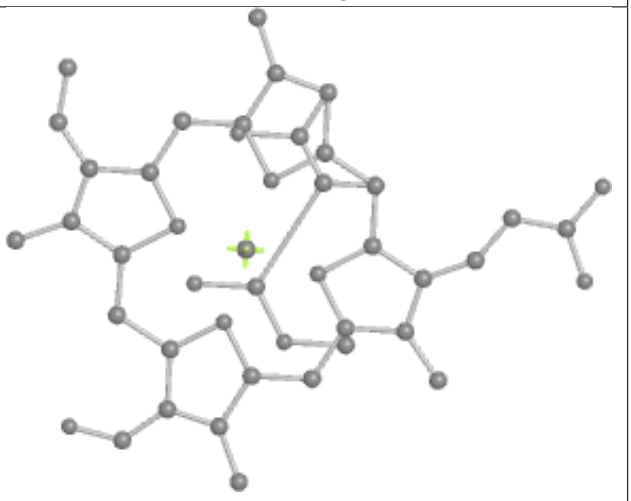
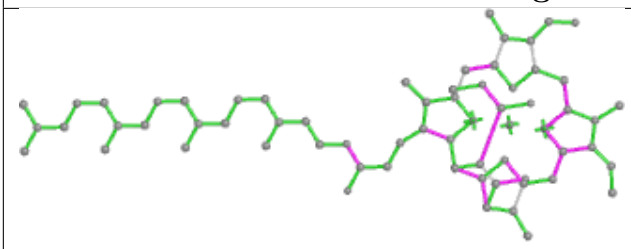


Rings

Ligand CL7 3 503



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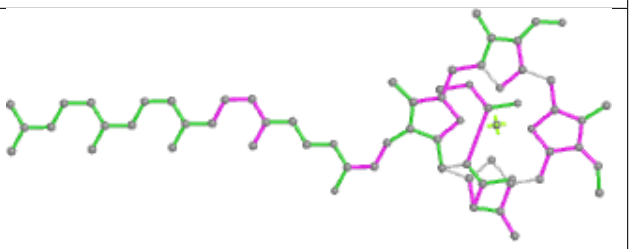
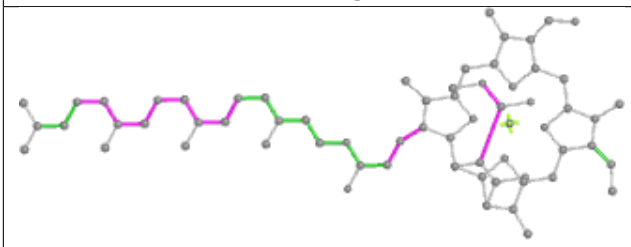


Bond angles



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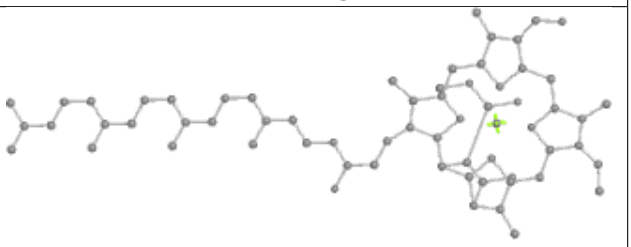
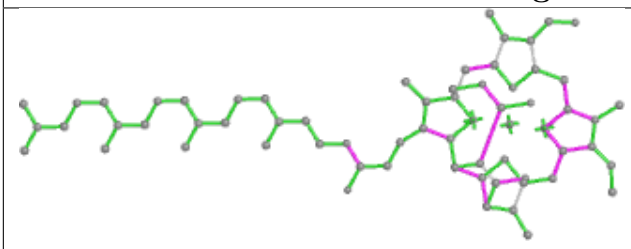


Rings

Ligand CL7 2 509



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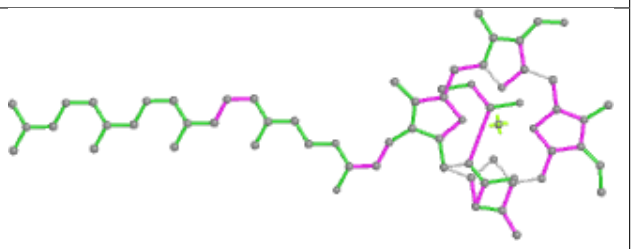
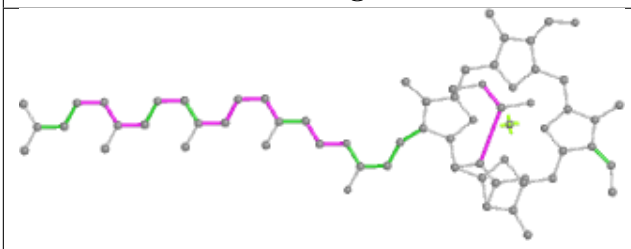
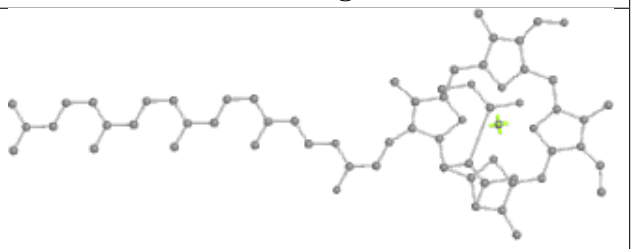


Bond angles

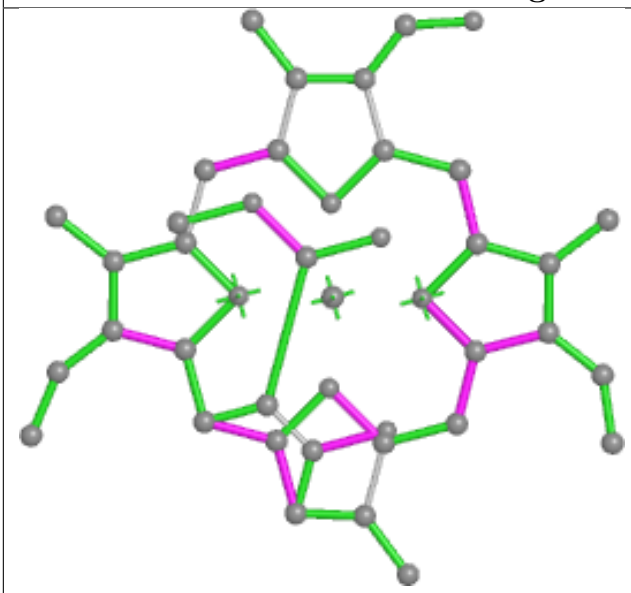


Torsions

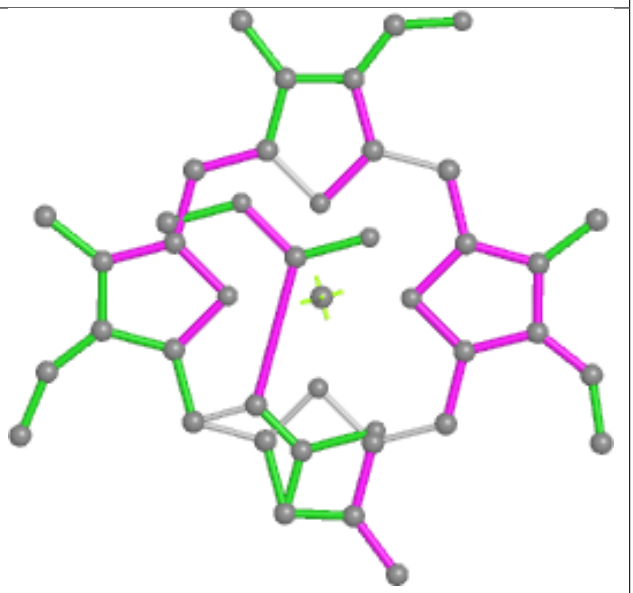


Rings

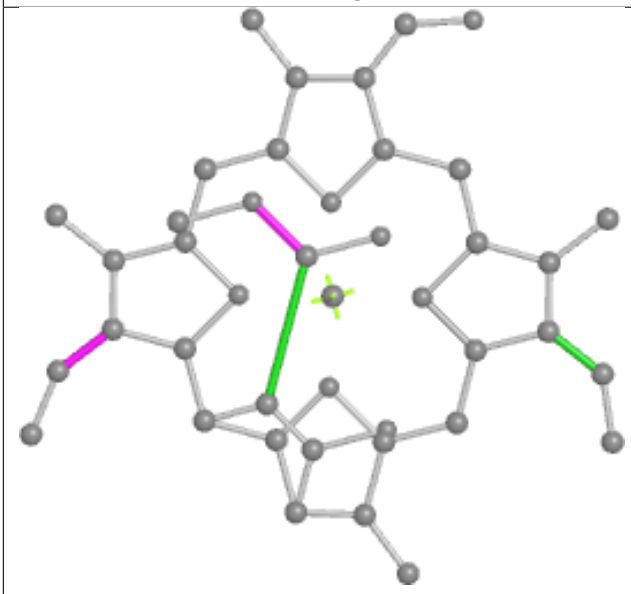
Ligand CL7 C 512



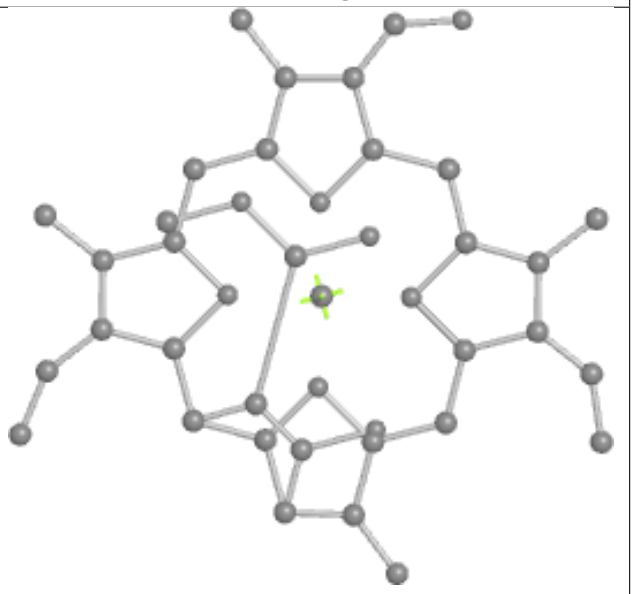
Bond lengths



Bond angles

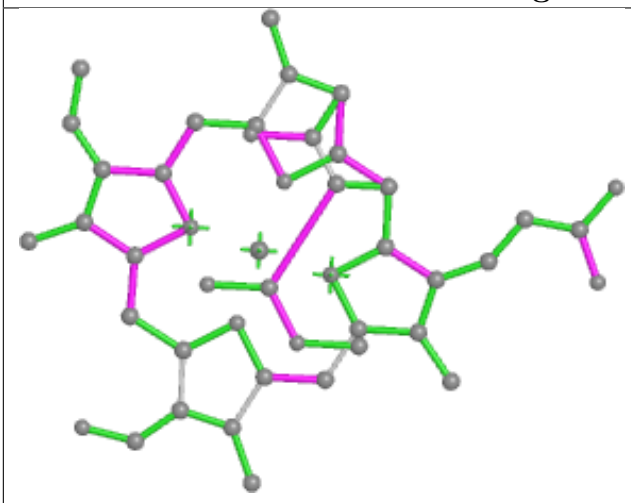


Torsions

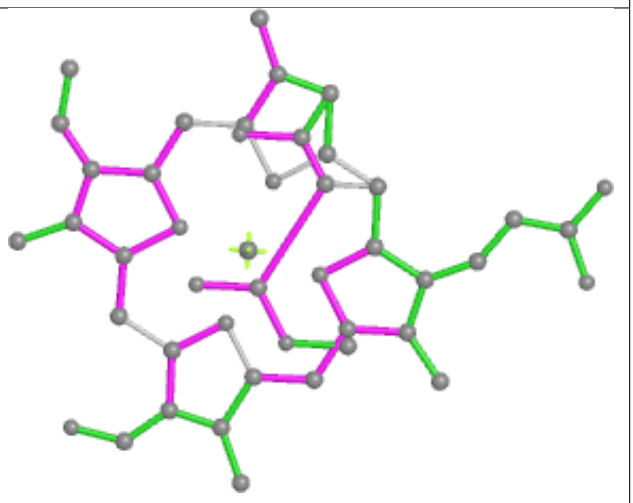


Rings

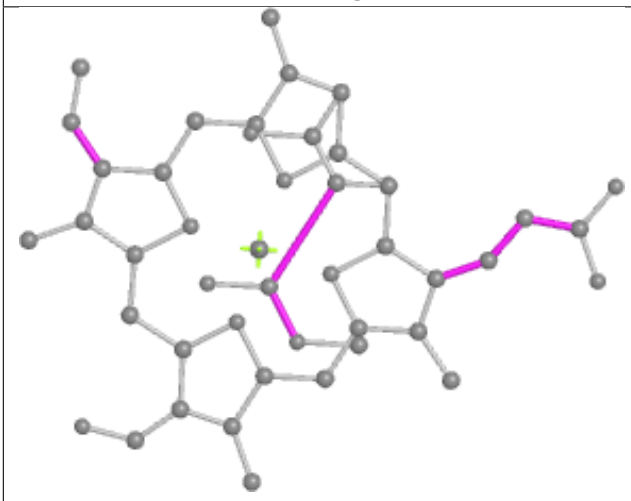
Ligand CL7 4 415



Bond lengths



Bond angles



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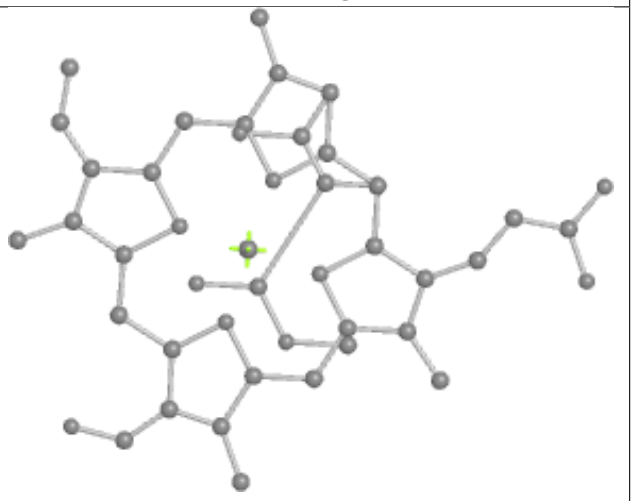
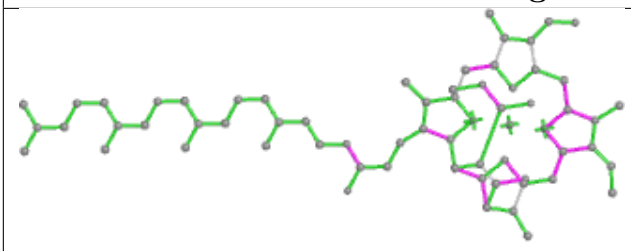


Rings

Ligand CL7 B 609



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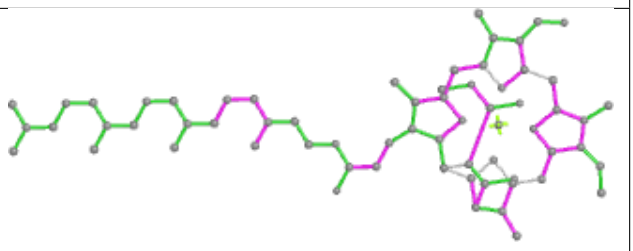
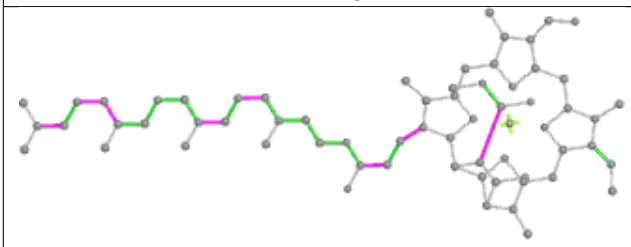


Bond angles



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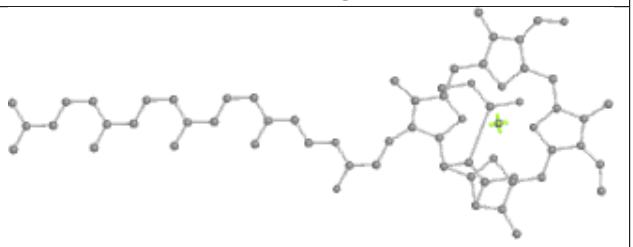
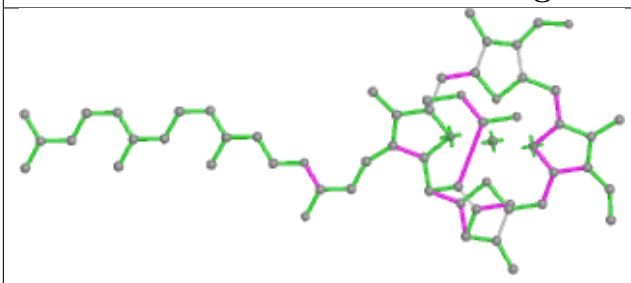


Rings

Ligand CL7 c 507



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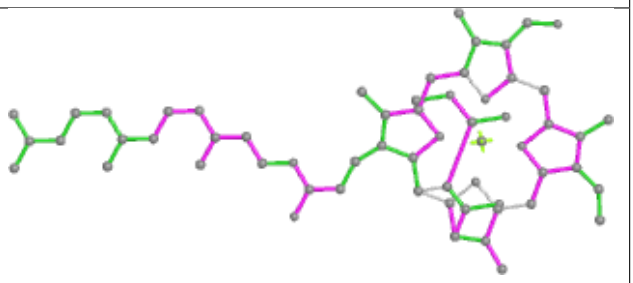
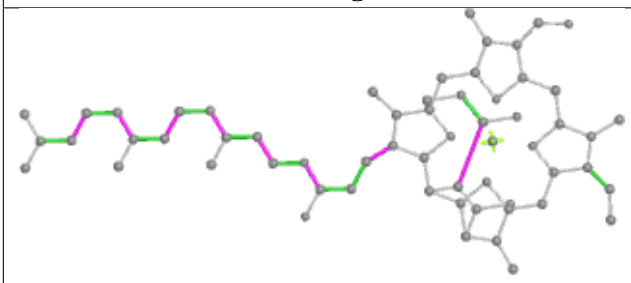


Bond angles



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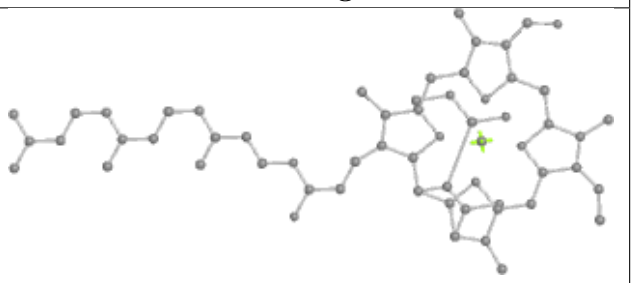
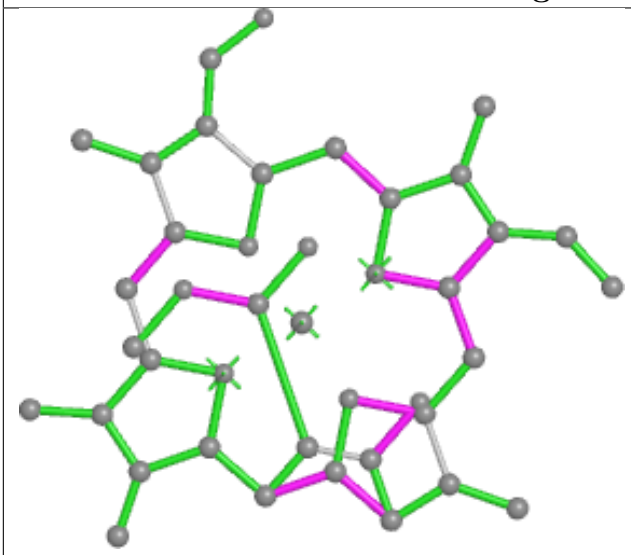
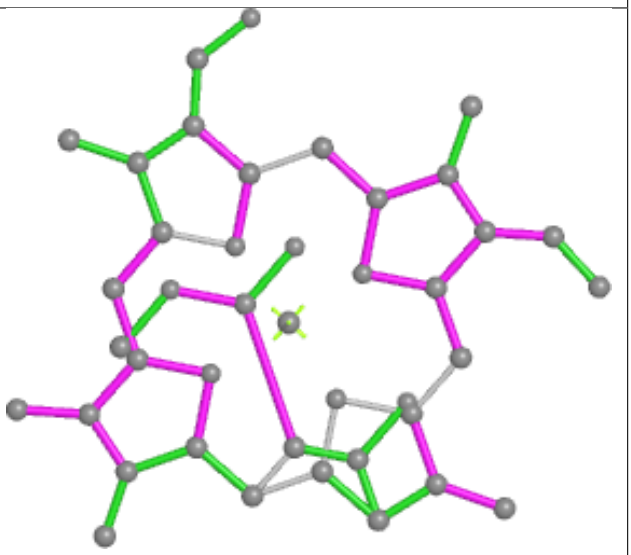


Rings

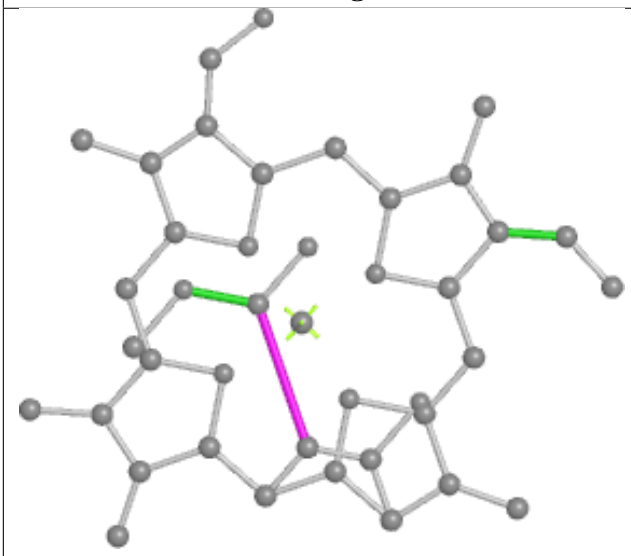
Ligand CL7 8 407



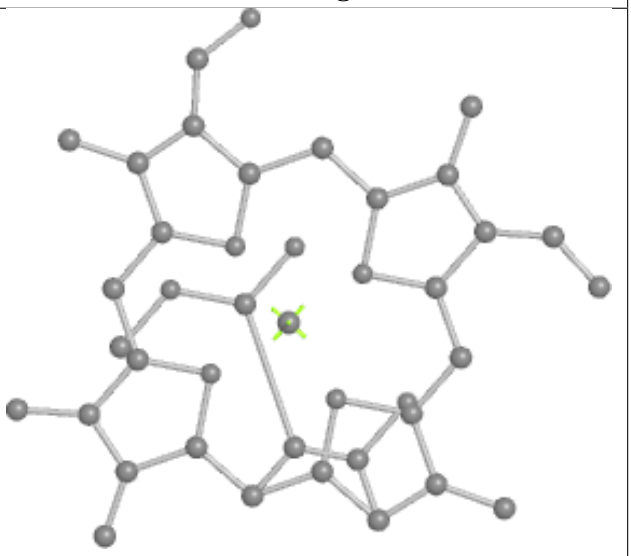
Bond lengths



Bond angles

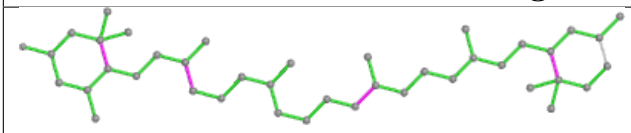


Torsions

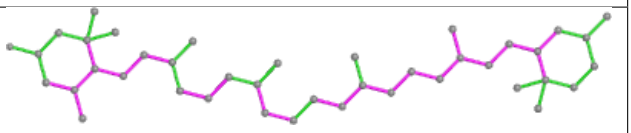


Rings

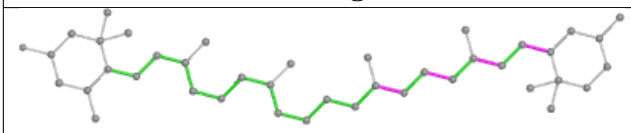
Ligand ZEX 2 523



Bond lengths



Bond angles



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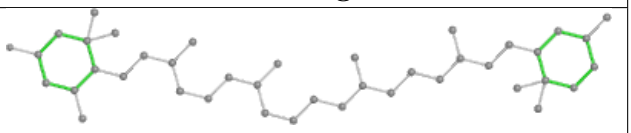
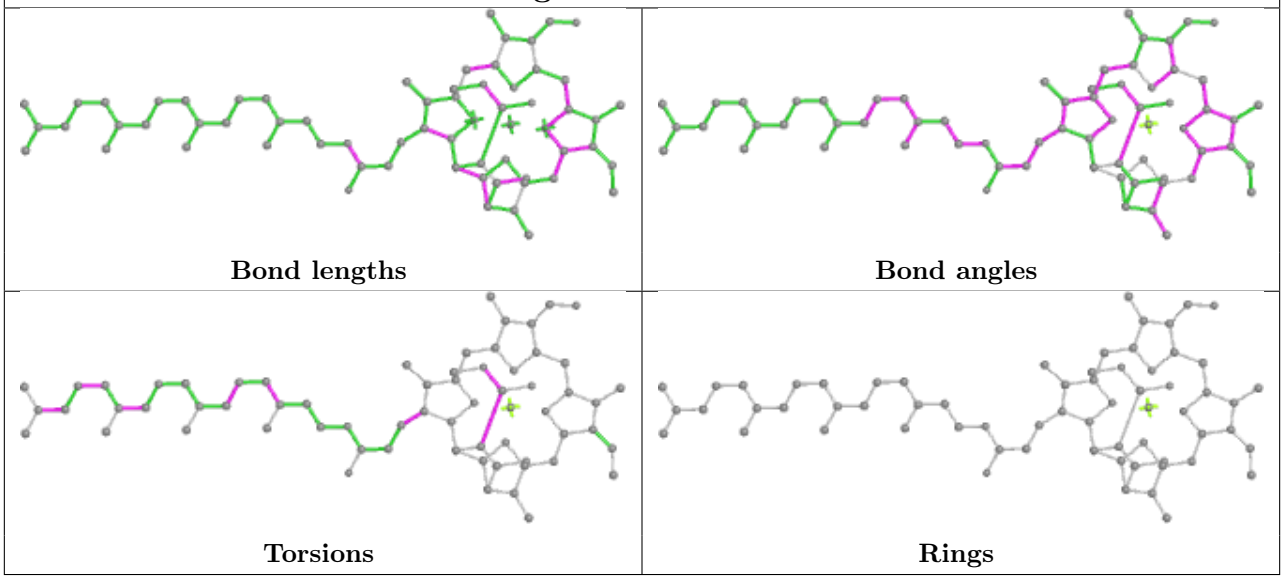
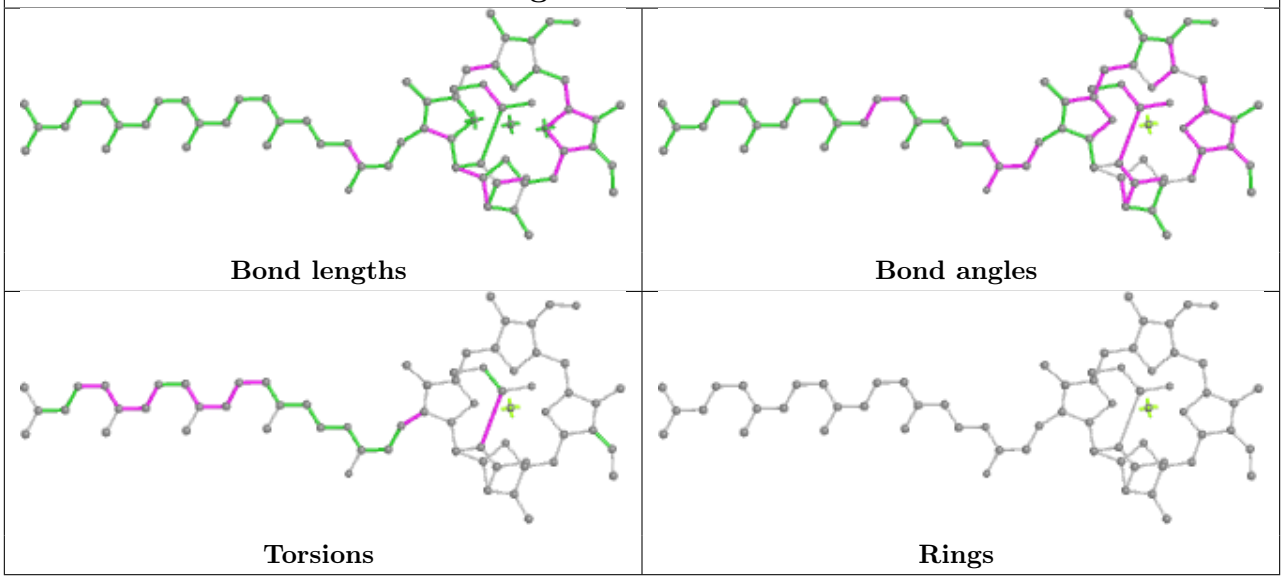


Rings

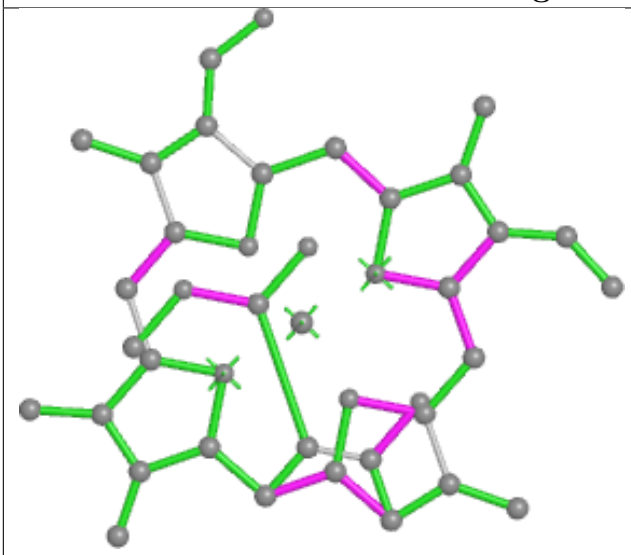
Ligand CL7 4 411



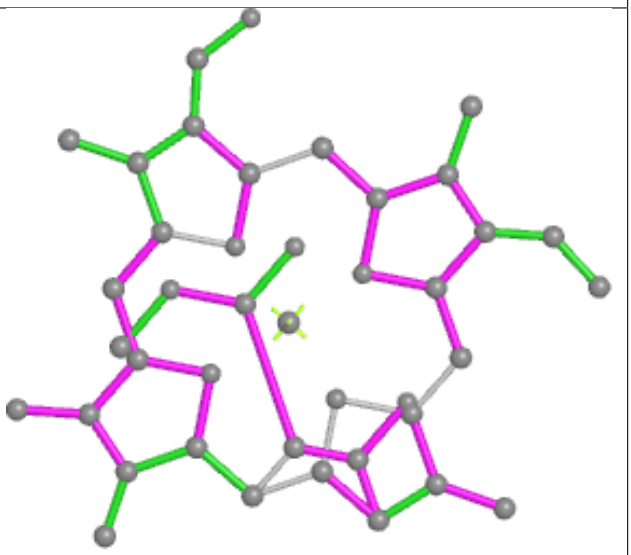
Ligand CL7 B 612



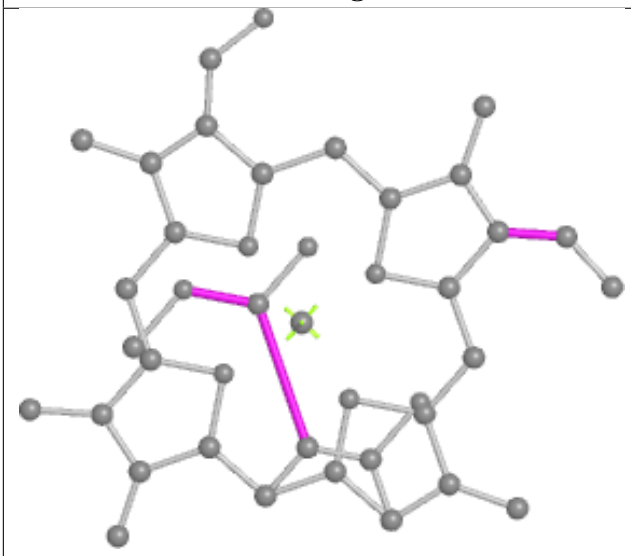
Ligand CL7 8 416



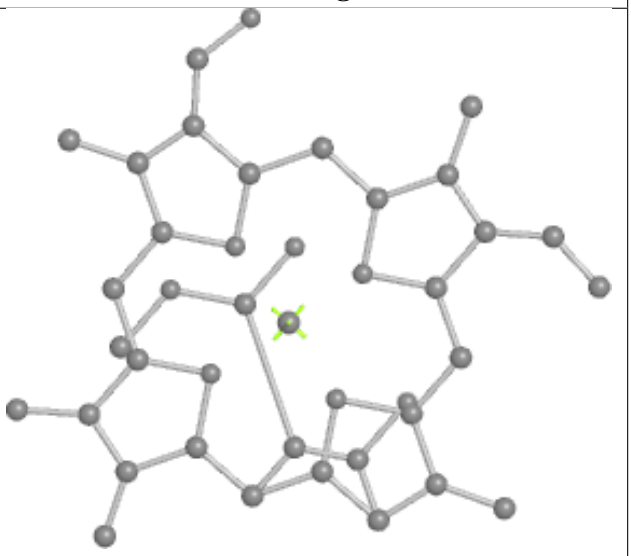
Bond lengths



Bond angles

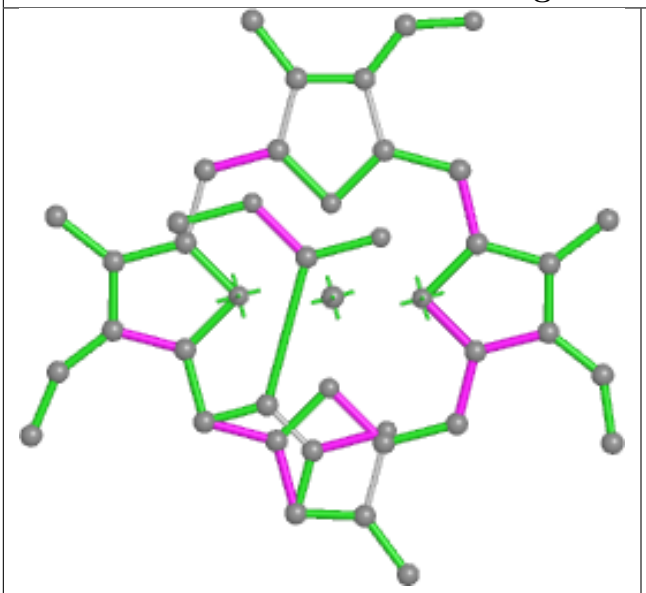


Torsions



Rings

Ligand CL7 c 512



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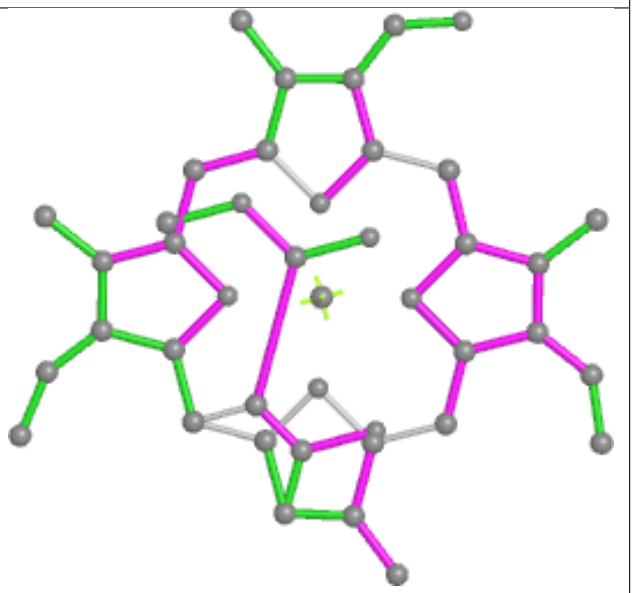
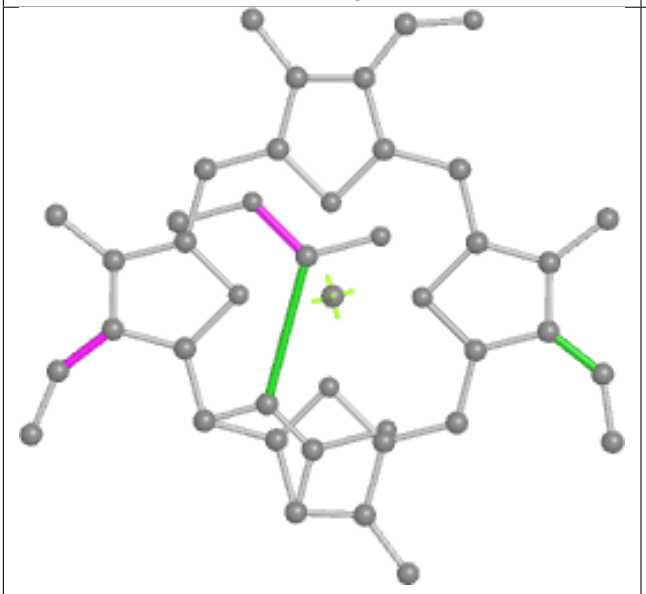
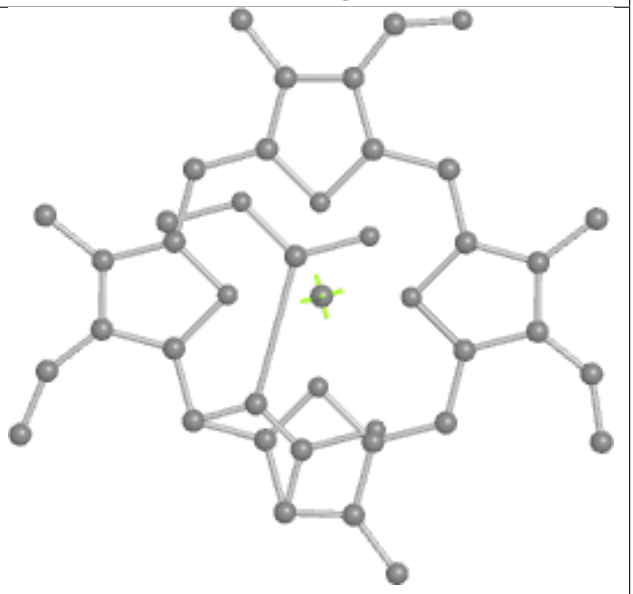


Bond angles

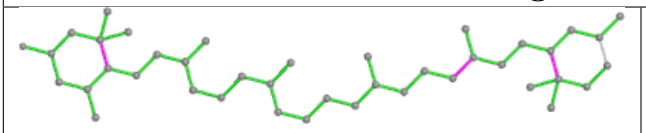


Torsions

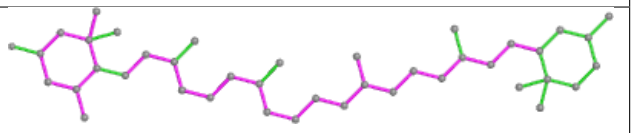


Rings

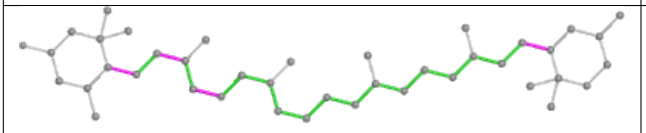
Ligand ZEX 2 521



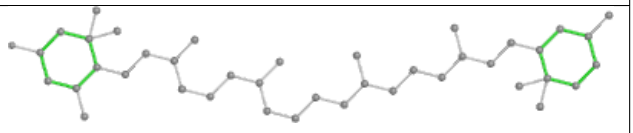
Bond lengths



Bond angles

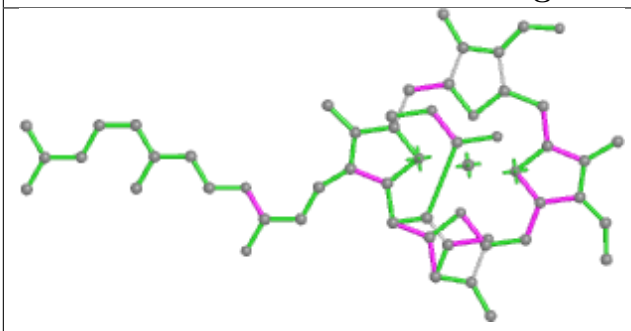


Torsions

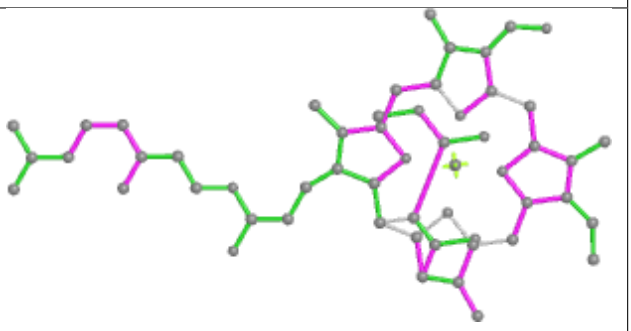


Rings

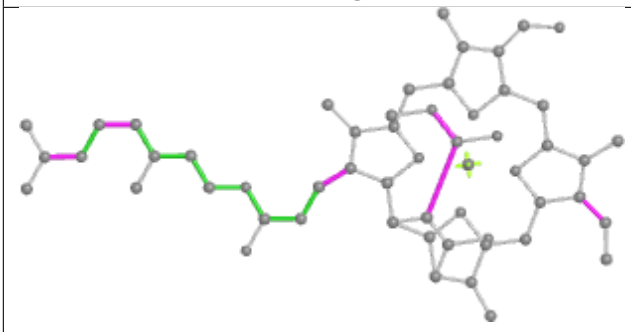
Ligand CL7 c 505



Bond lengths



Bond angles



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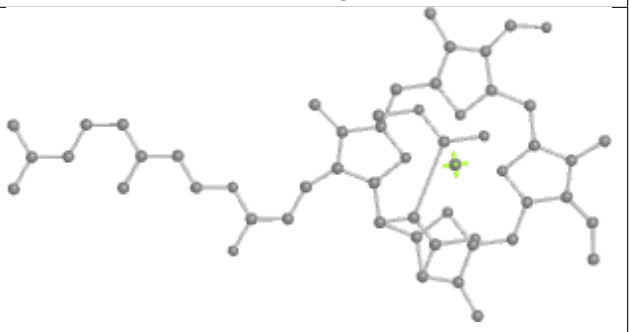
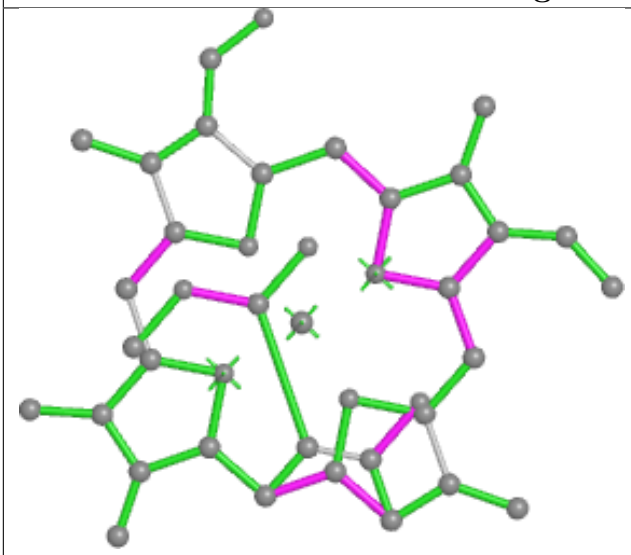


Rings

Ligand CL7 c 513



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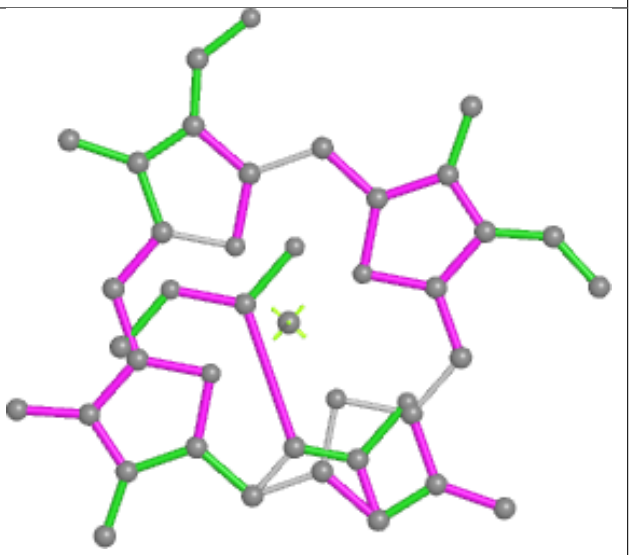
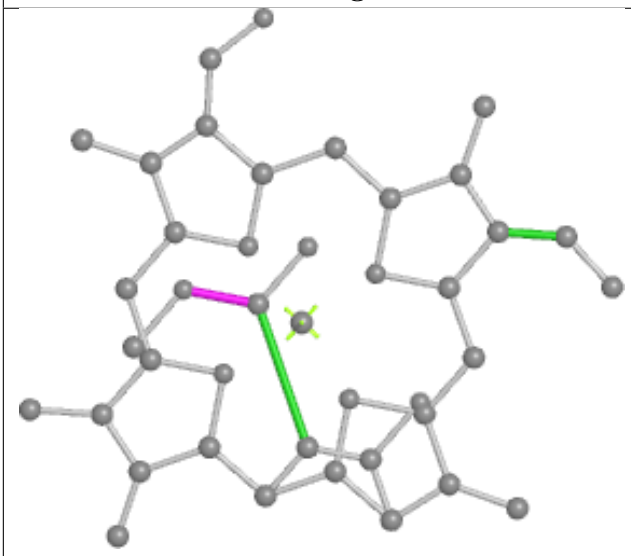


Bond angles



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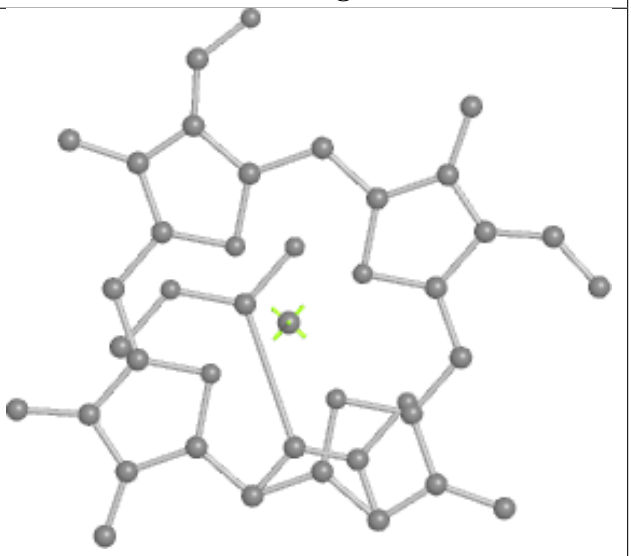
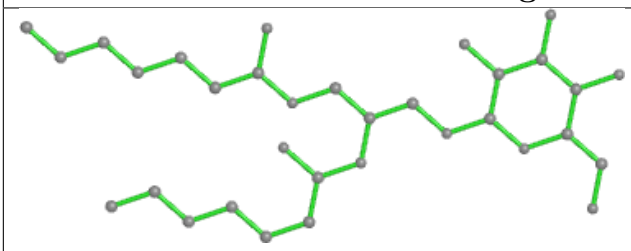
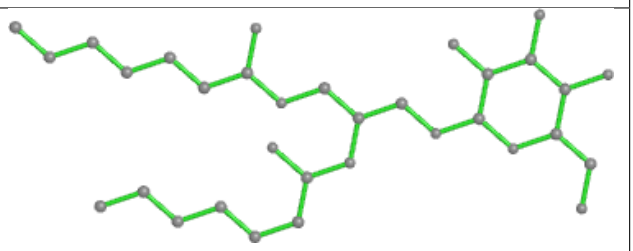


Rings

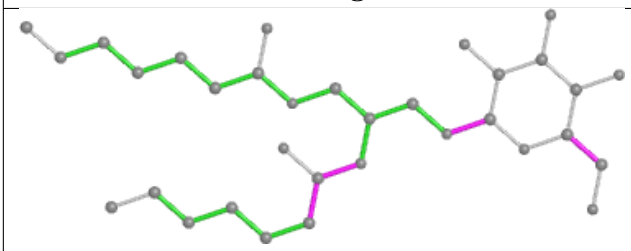
Ligand LMG D 410



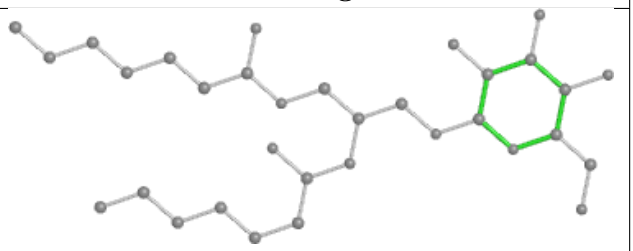
Bond lengths



Bond angles

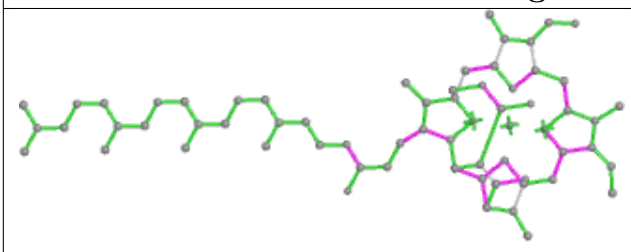


Torsions

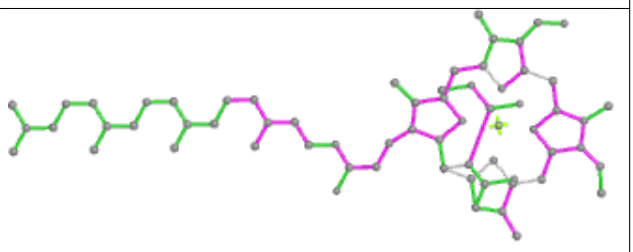


Rings

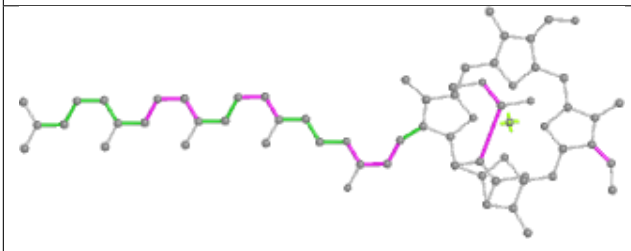
Ligand CL7 A 401



Bond lengths



Bond angles



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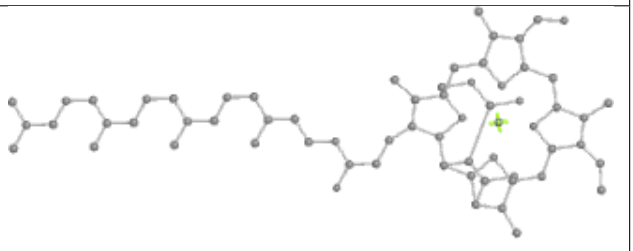
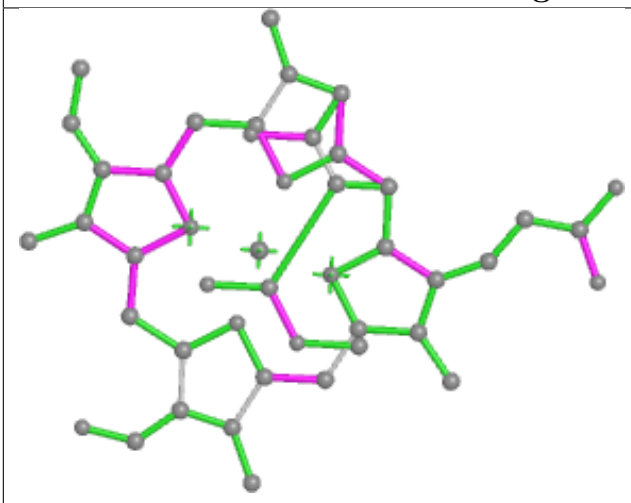


Rings

Ligand CL7 6 508



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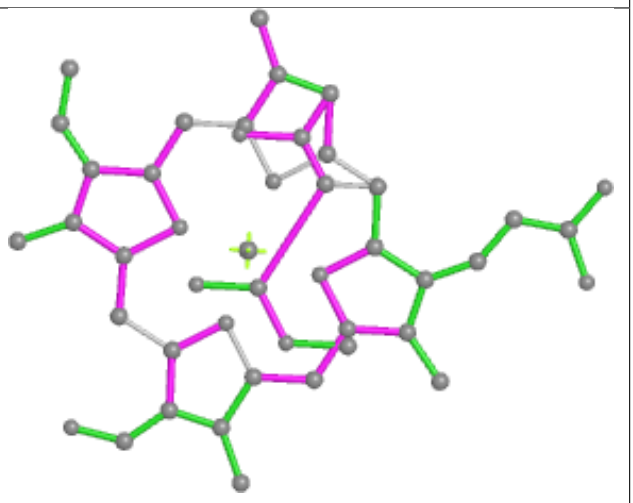
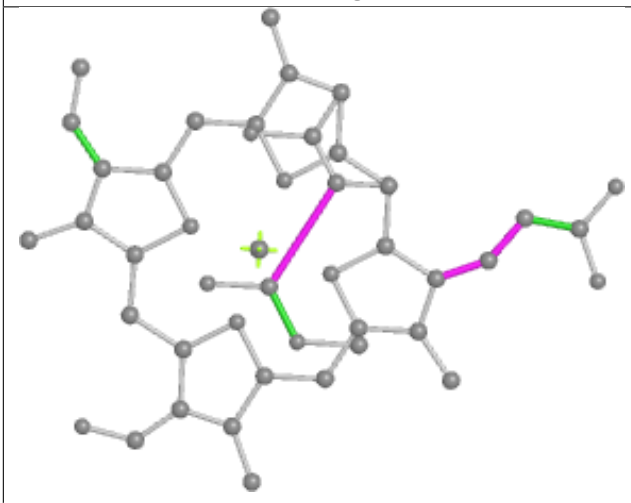
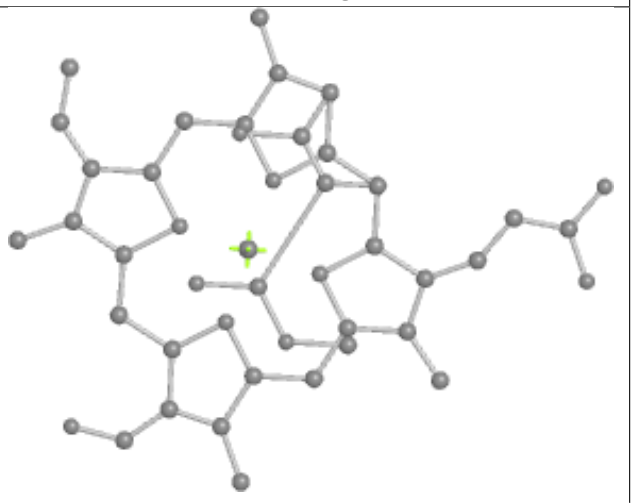


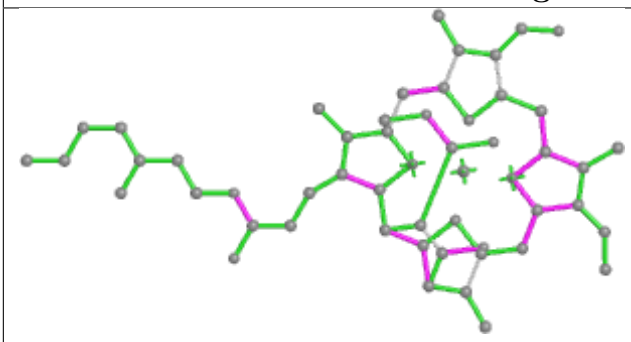
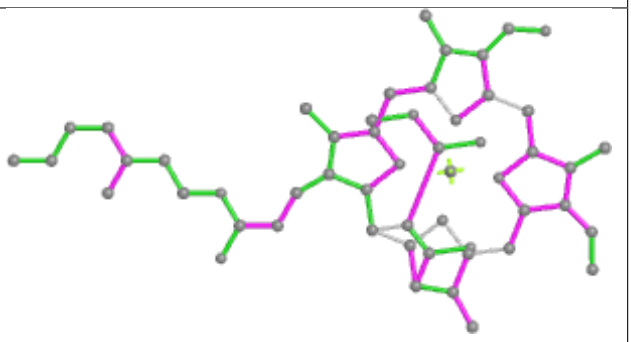
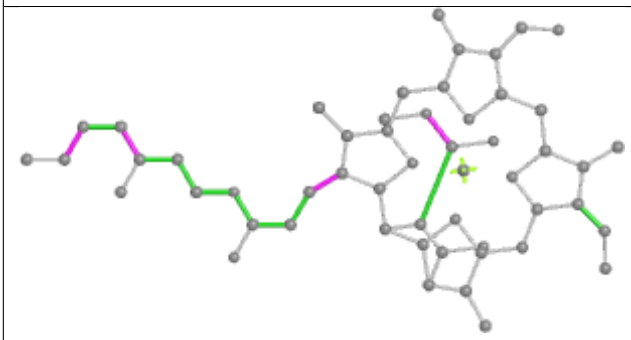
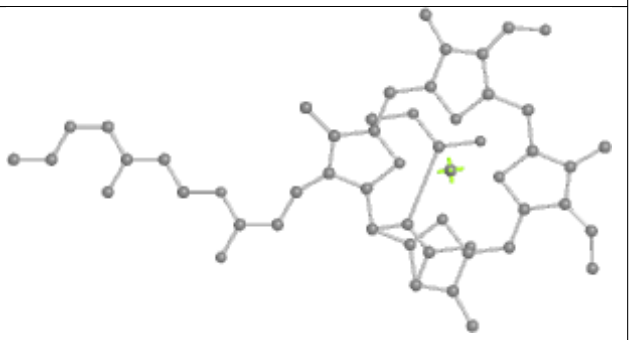
Bond angles



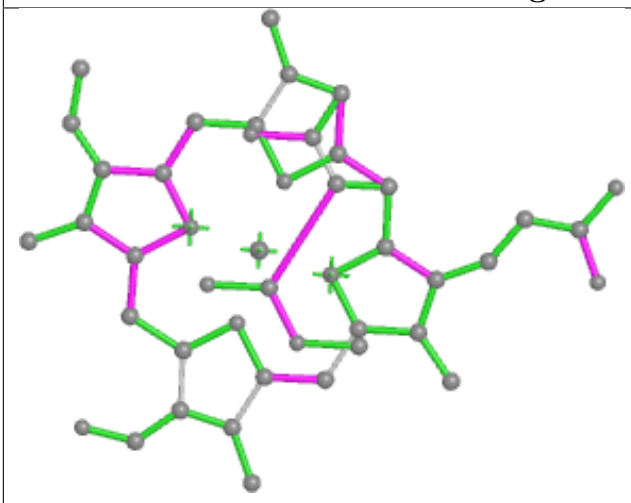
Torsions



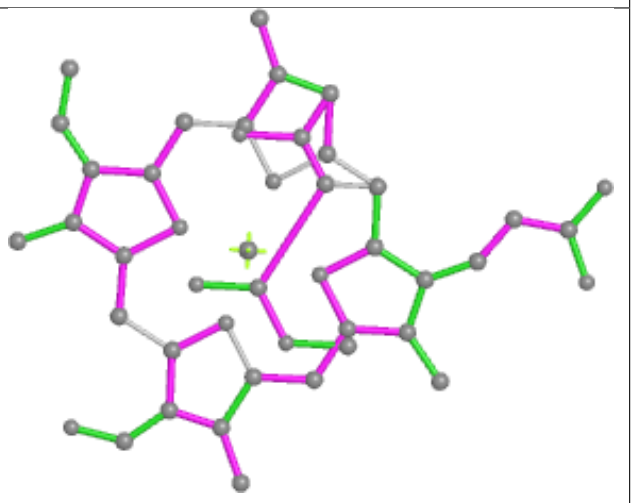
Rings

Ligand CL7 4 414	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

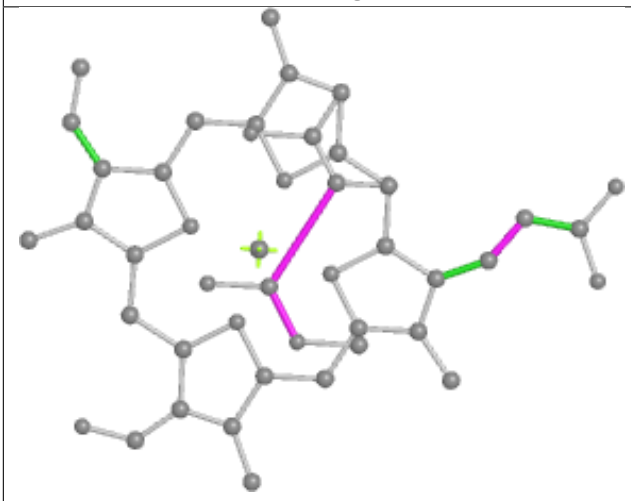
Ligand CL7 B 616



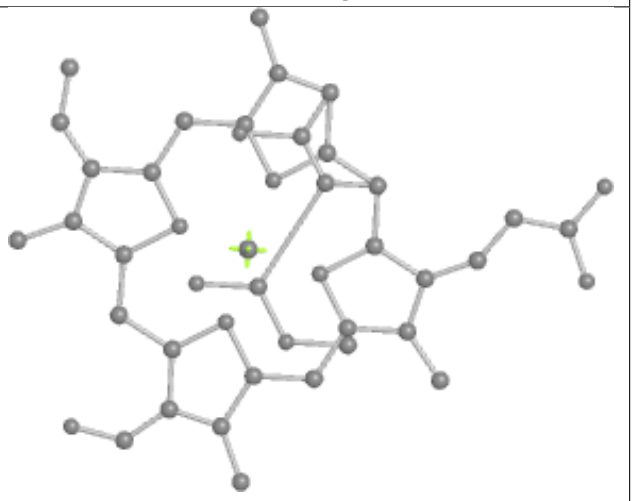
Bond lengths



Bond angles

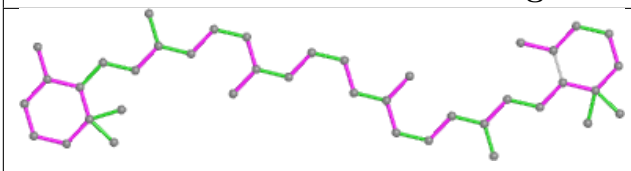


Torsions

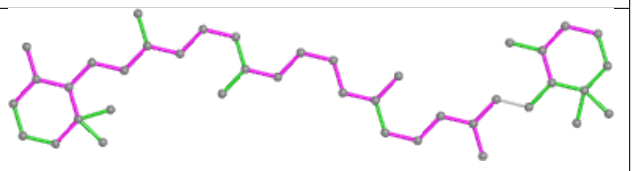


Rings

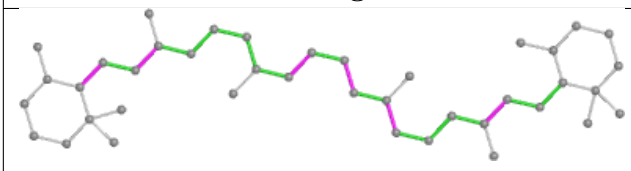
Ligand 8CT D 406



Bond lengths



Bond angles



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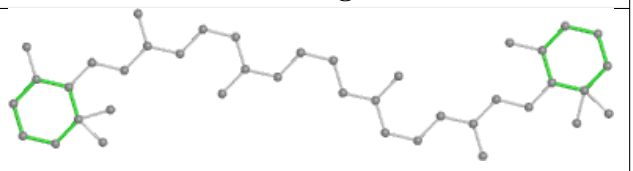
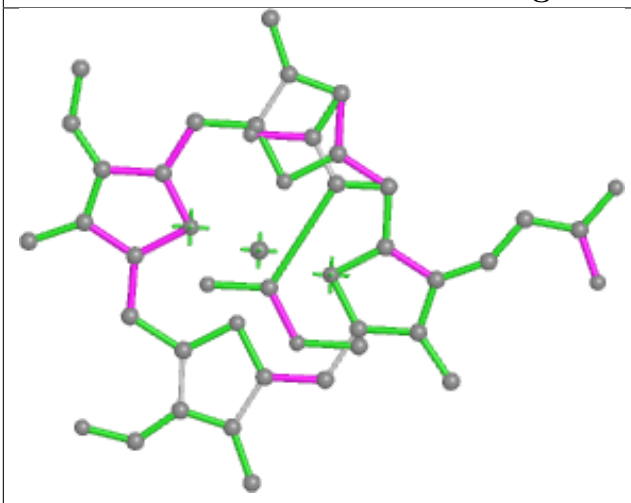
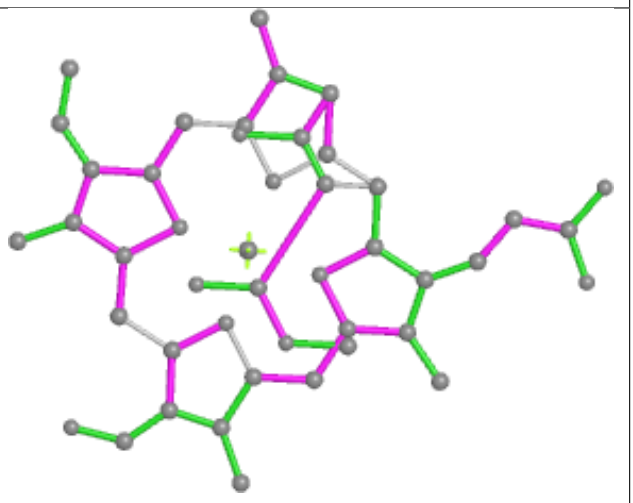


Rings

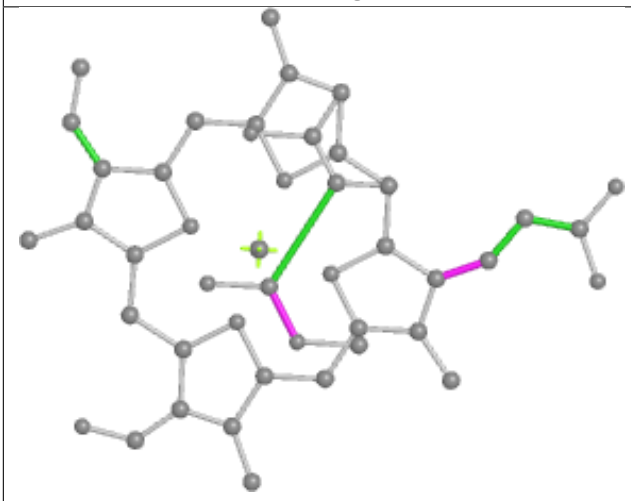
Ligand CL7 2 504



Bond lengths



Bond angles



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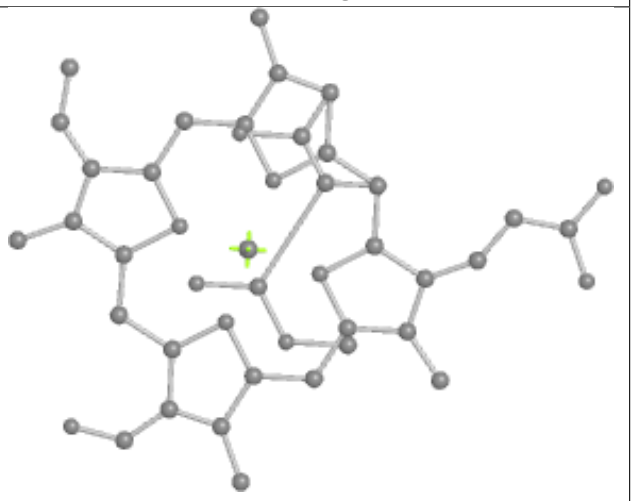
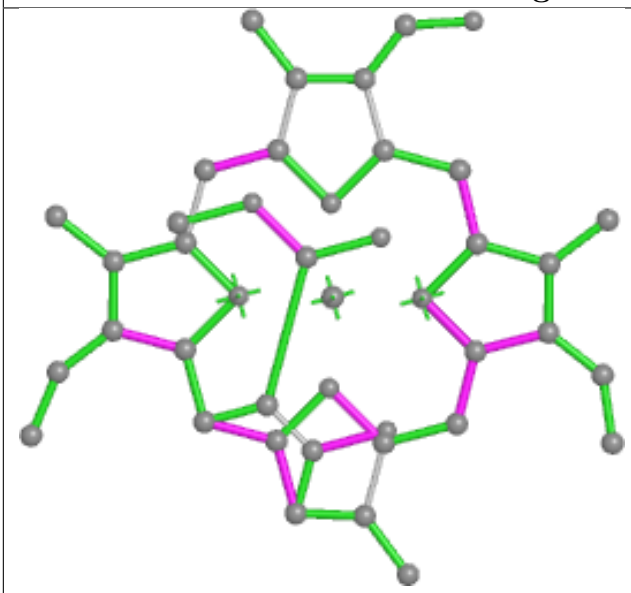
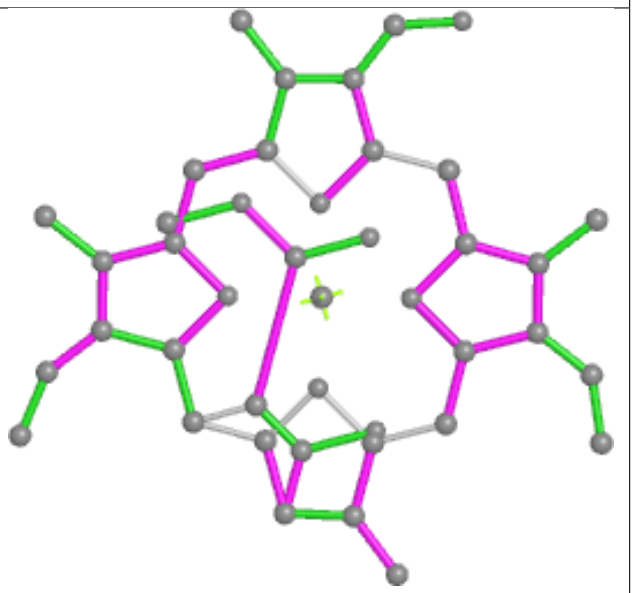


Rings

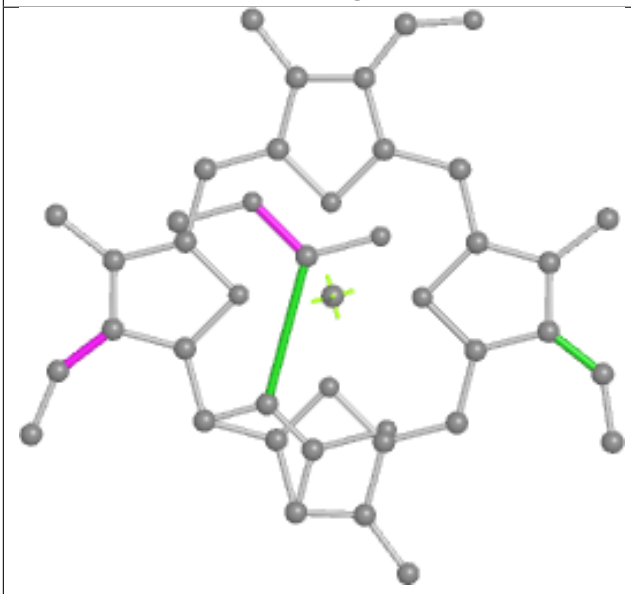
Ligand CL7 8 417



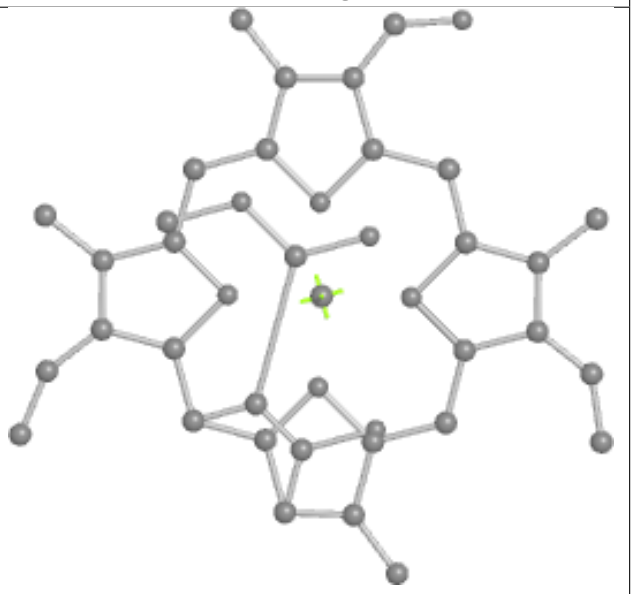
Bond lengths



Bond angles

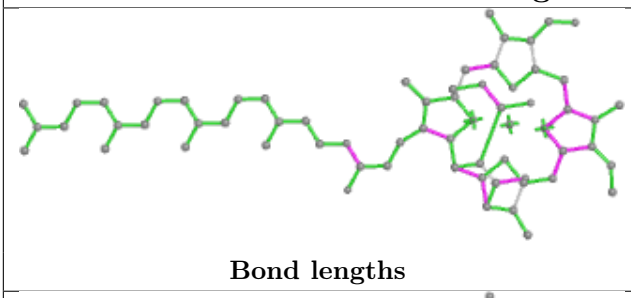


Torsions

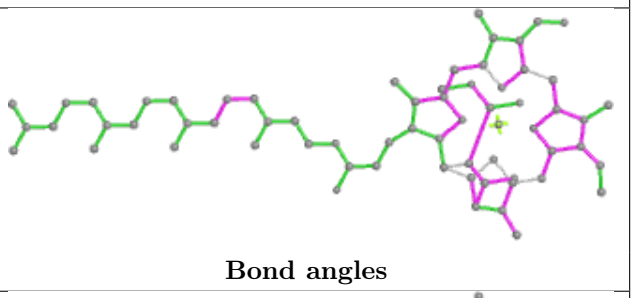


Rings

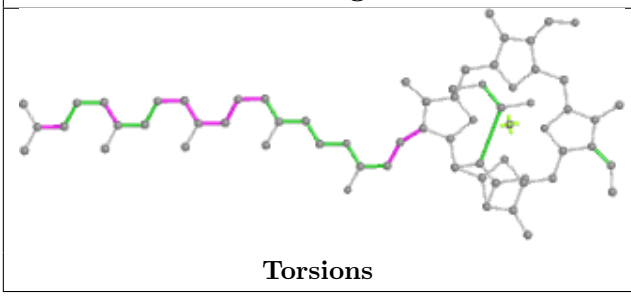
Ligand CL7 8 404



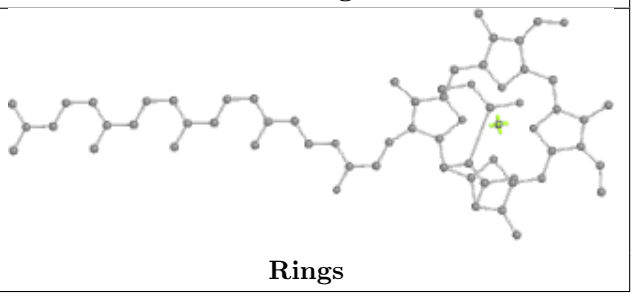
Bond lengths



Bond angles

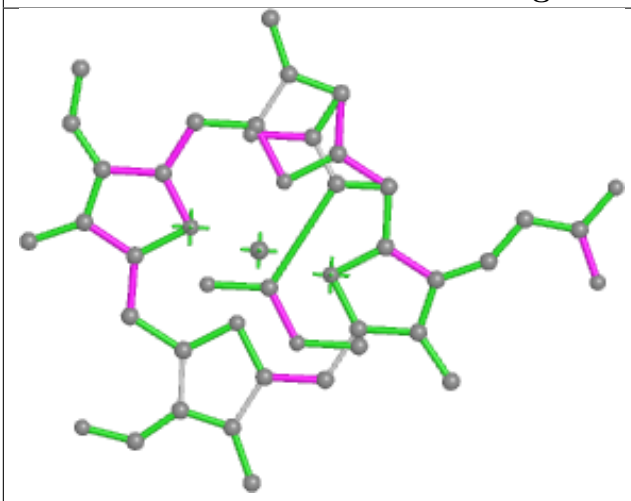


Torsions

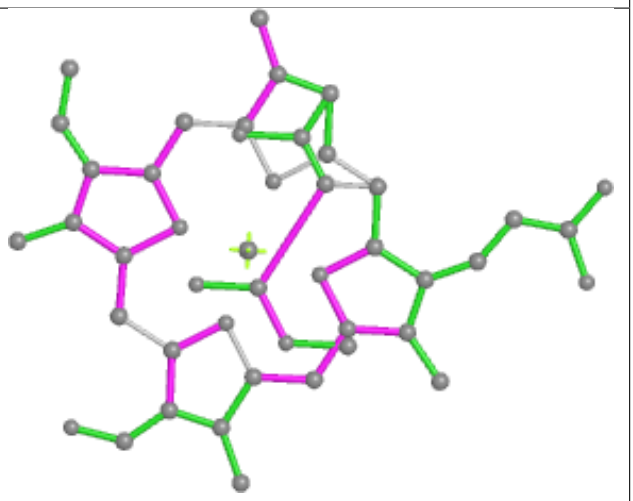


Rings

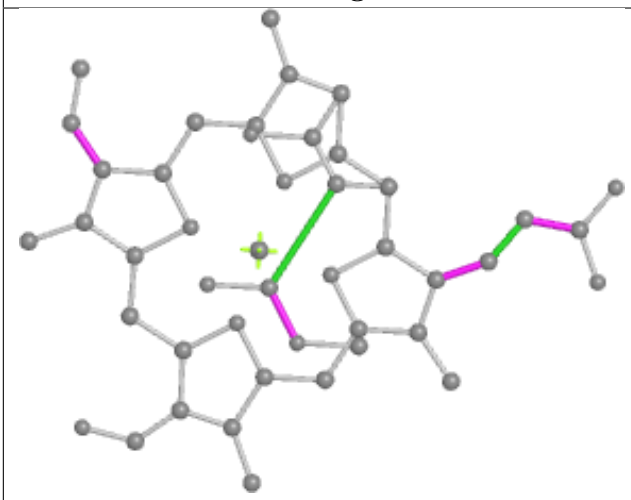
Ligand CL7 2 514



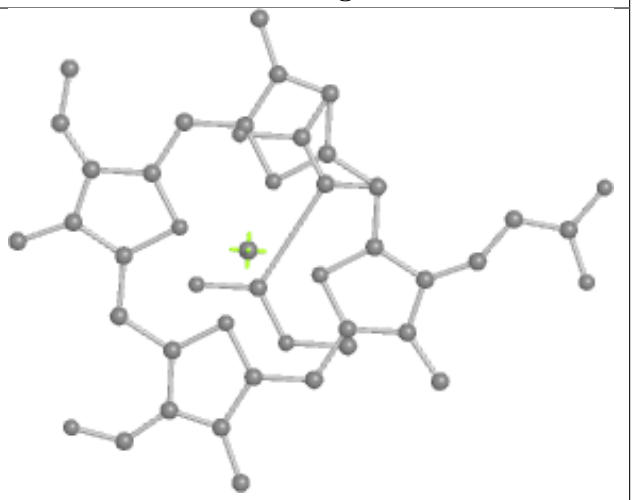
Bond lengths



Bond angles

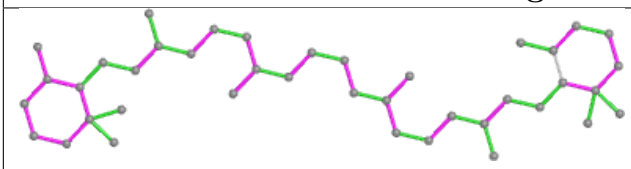


Torsions

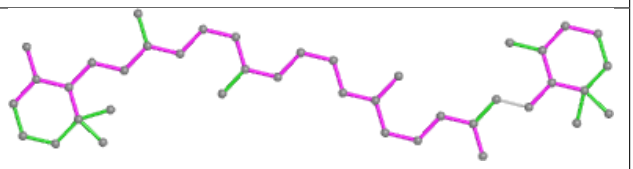


Rings

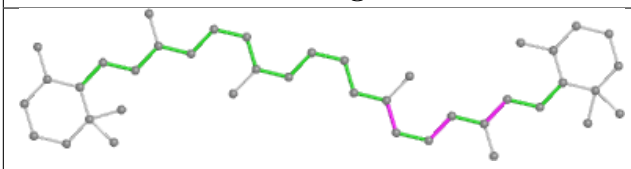
Ligand 8CT A 404



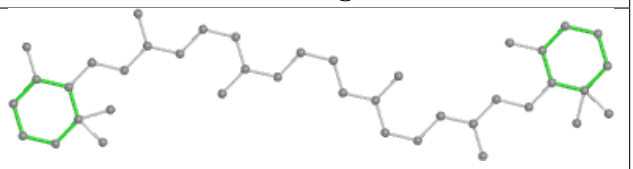
Bond lengths



Bond angles

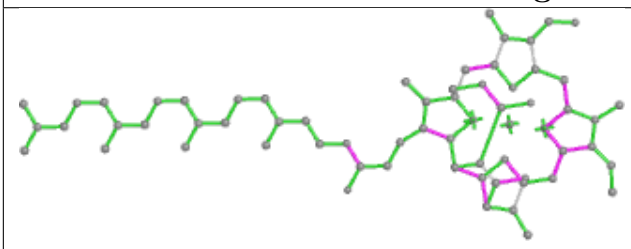


Torsions

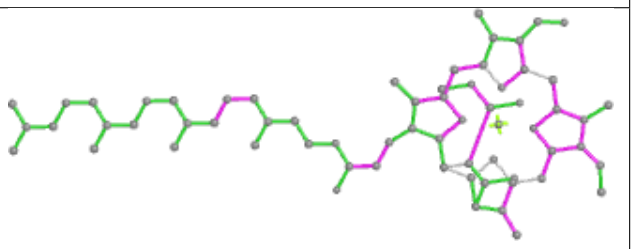


Rings

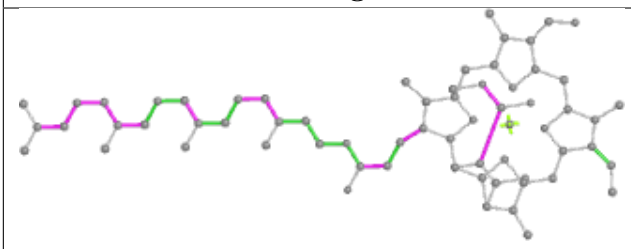
Ligand CL7 c 502



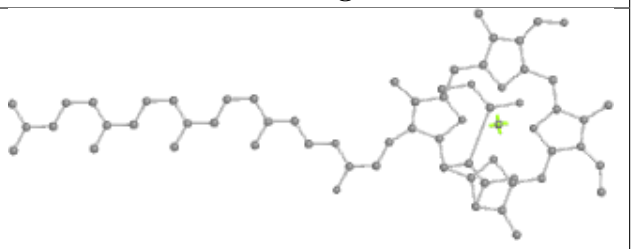
Bond lengths



Bond angles

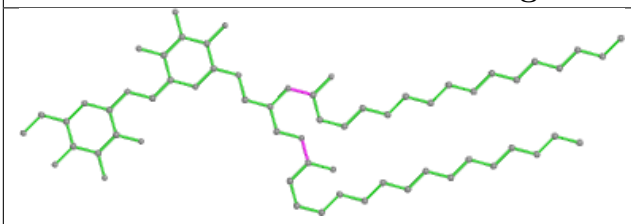


Torsions

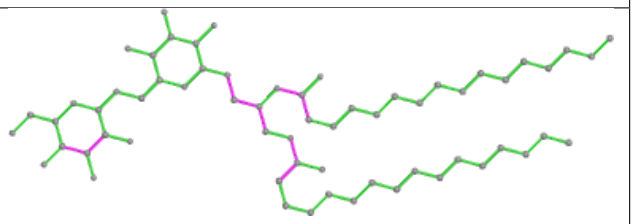


Rings

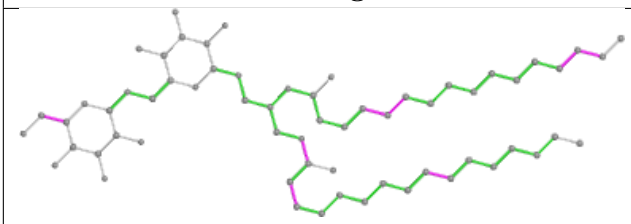
Ligand DGD C 517



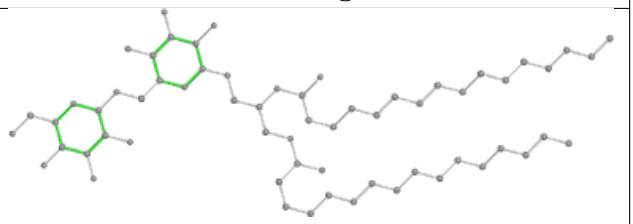
Bond lengths



Bond angles

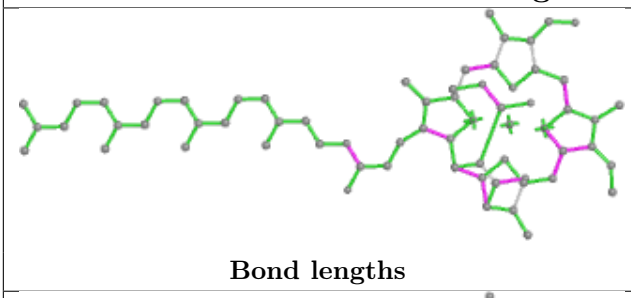


Torsions

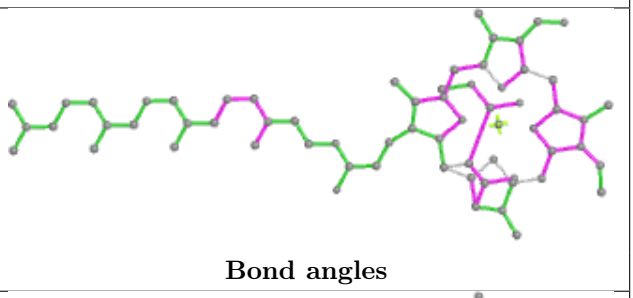


Rings

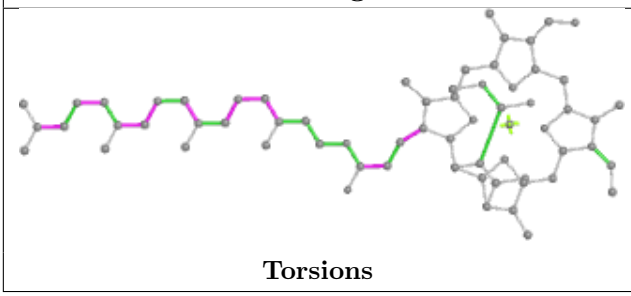
Ligand CL7 2 512



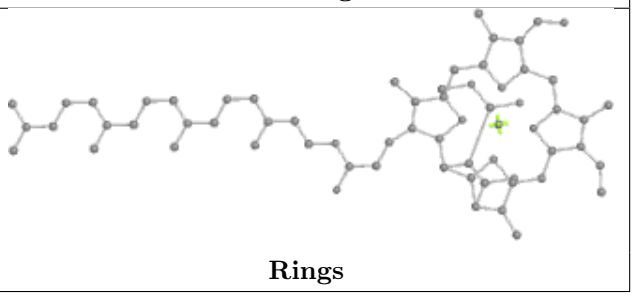
Bond lengths



Bond angles

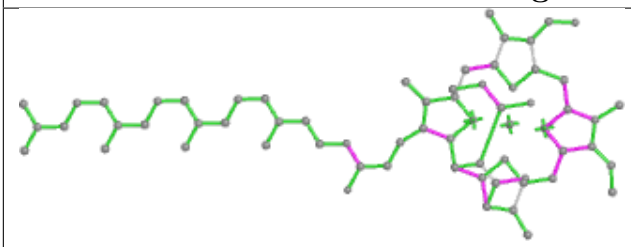


Torsions

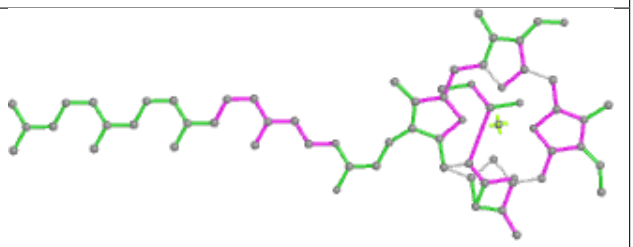


Rings

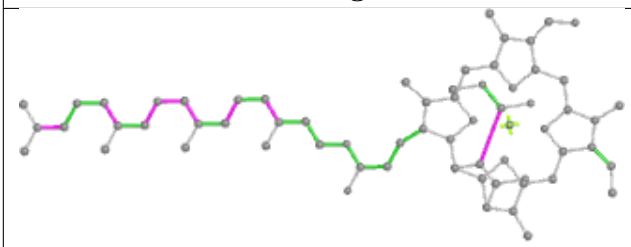
Ligand CL7 b 604



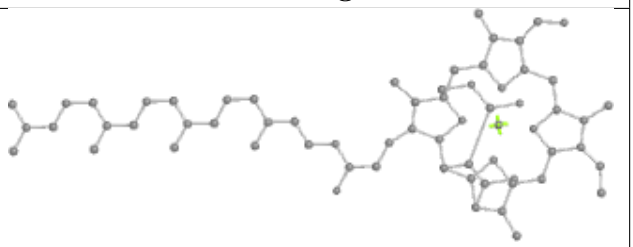
Bond lengths



Bond angles

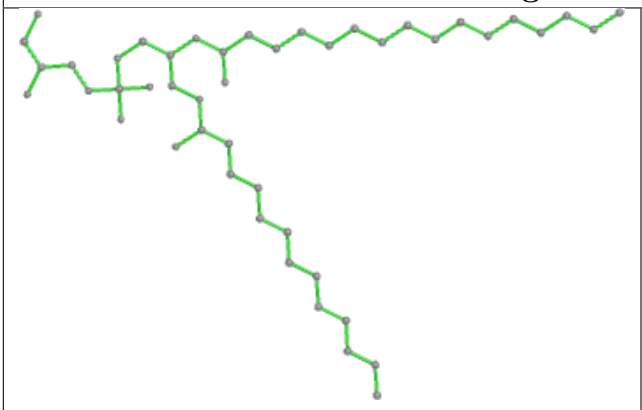


Torsions

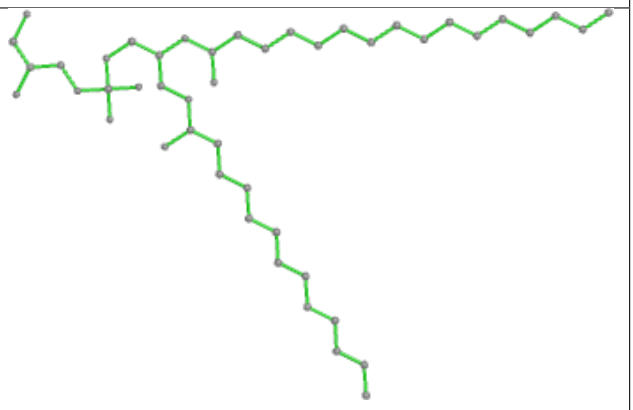


Rings

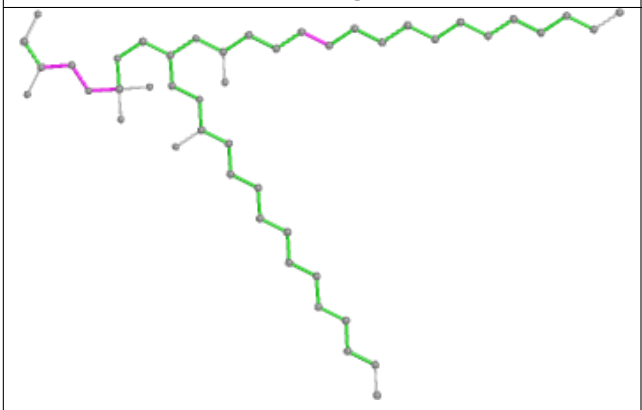
Ligand LHG A 407



Bond lengths



Bond angles



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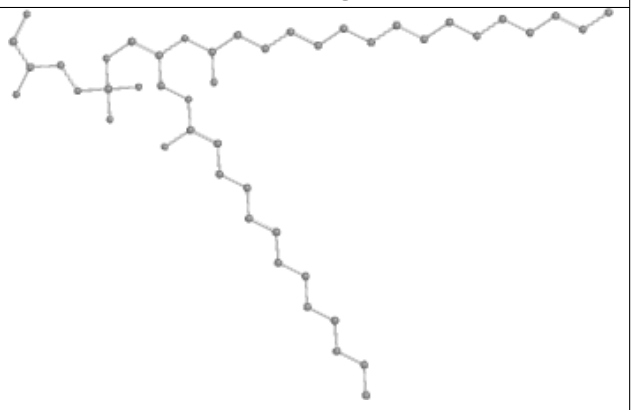
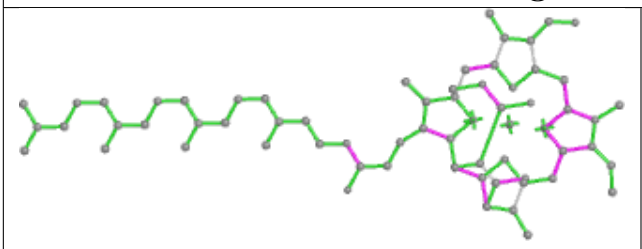
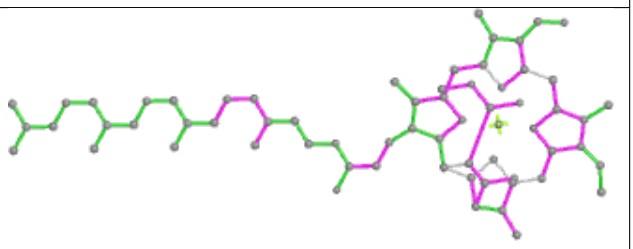


Rings

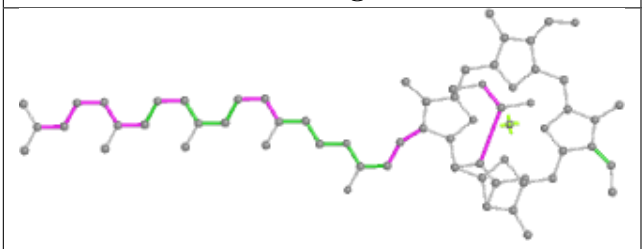
Ligand CL7 B 604



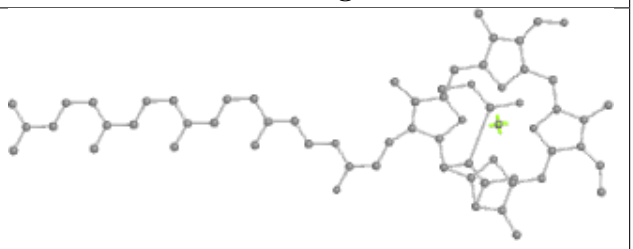
Bond lengths



Bond angles

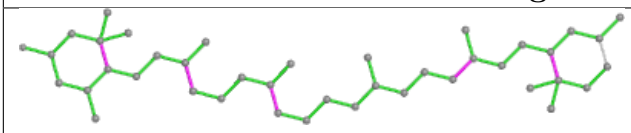


Torsions

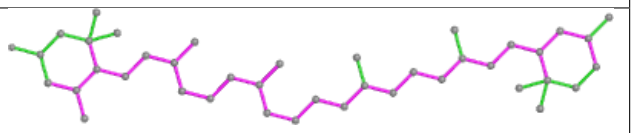


Rings

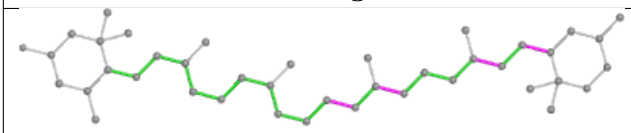
Ligand ZEX 3 525



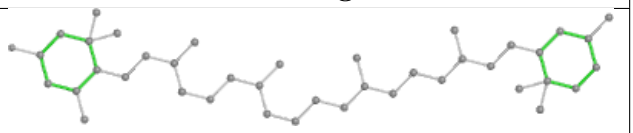
Bond lengths



Bond angles

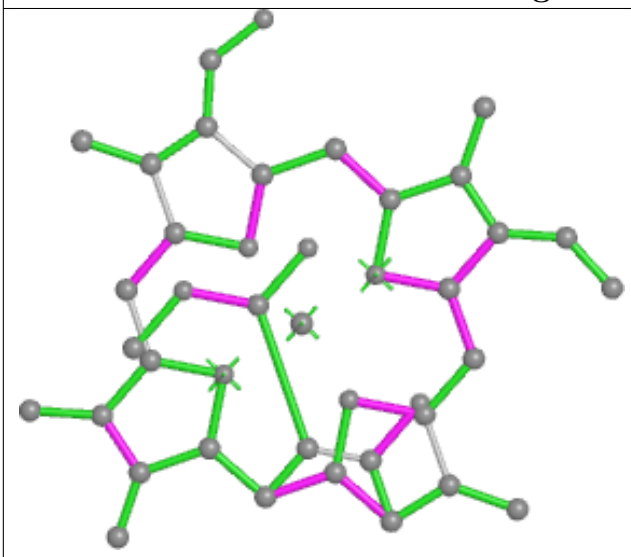


Torsions

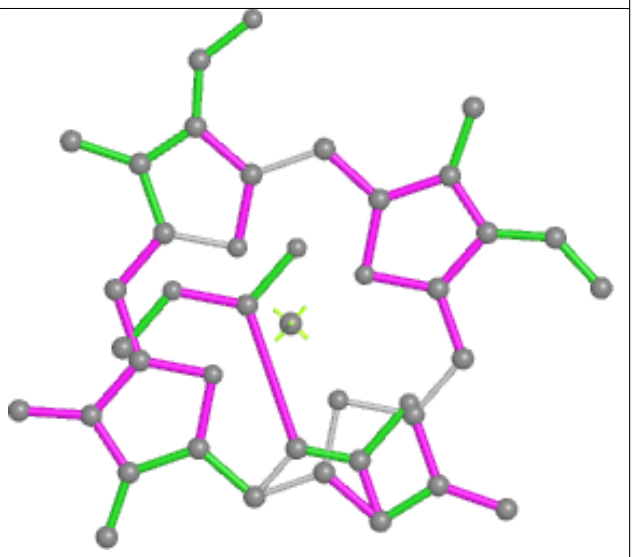


Rings

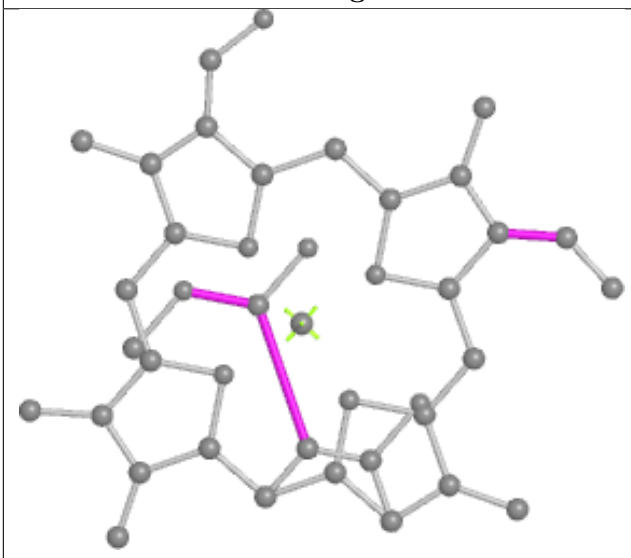
Ligand CL7 5 415



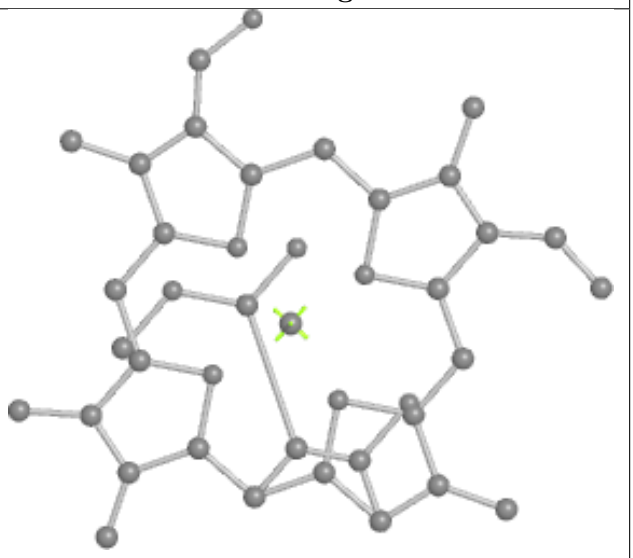
Bond lengths



Bond angles

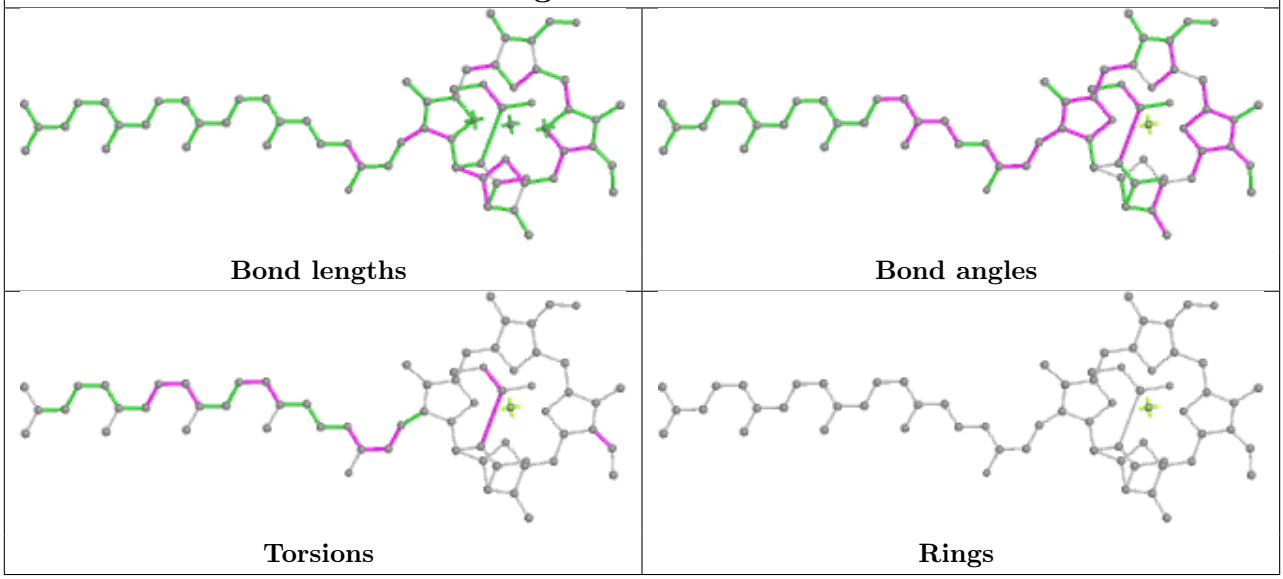


Torsions

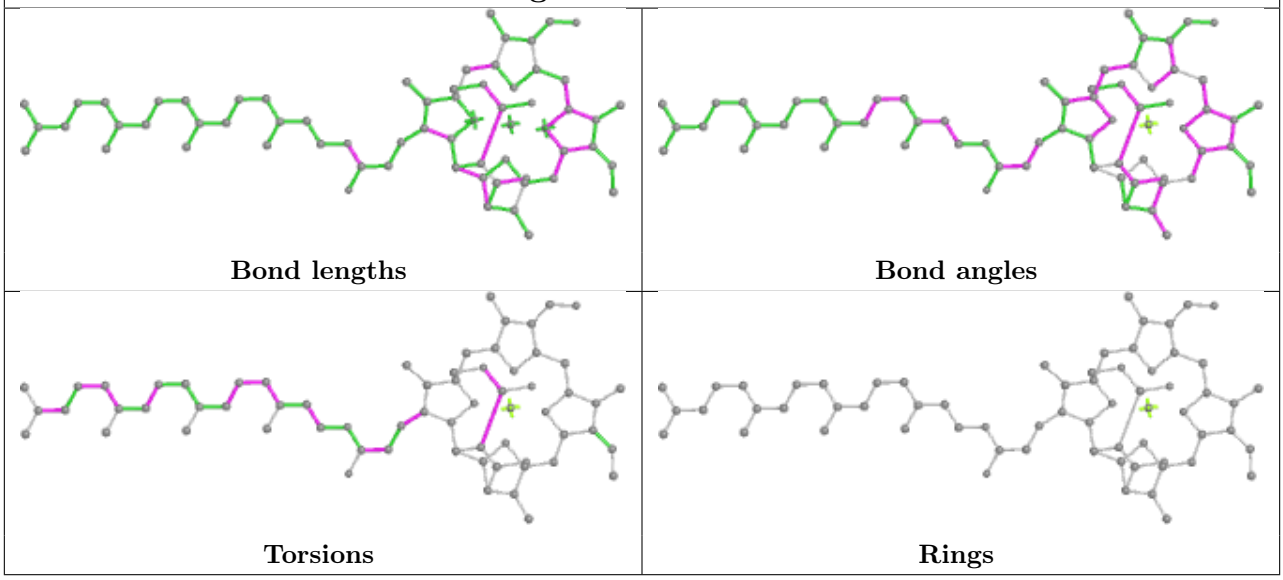


Rings

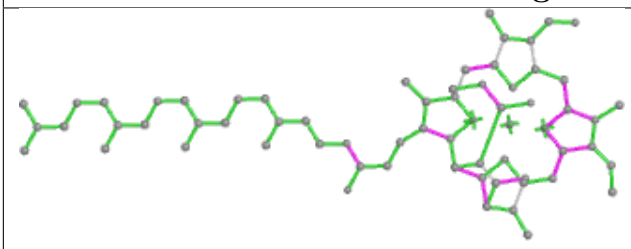
Ligand CL7 a 401



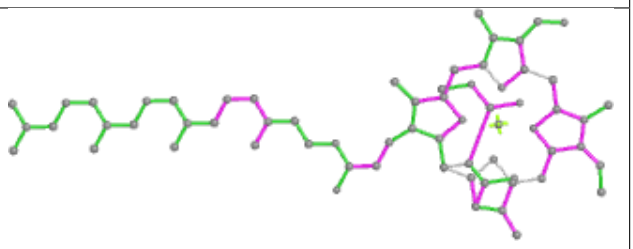
Ligand CL7 C 510



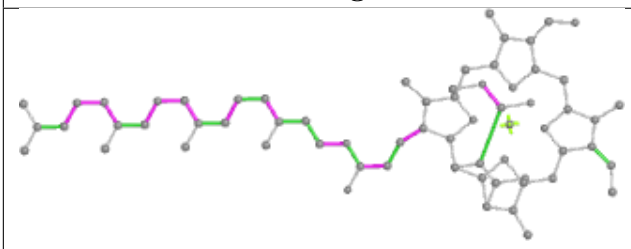
Ligand CL7 8 412



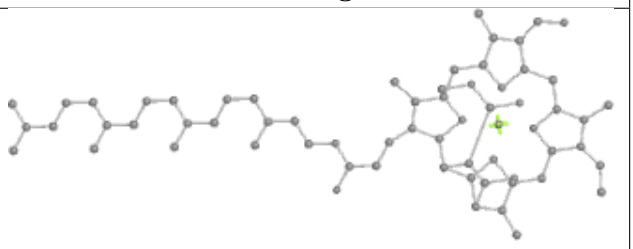
Bond lengths



Bond angles

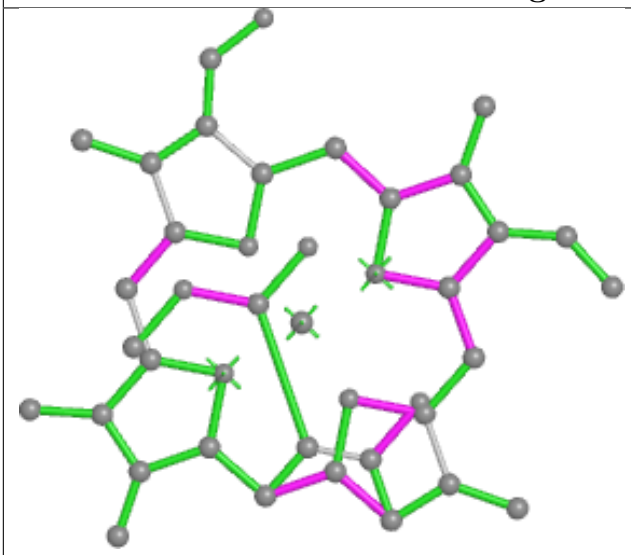


Torsions

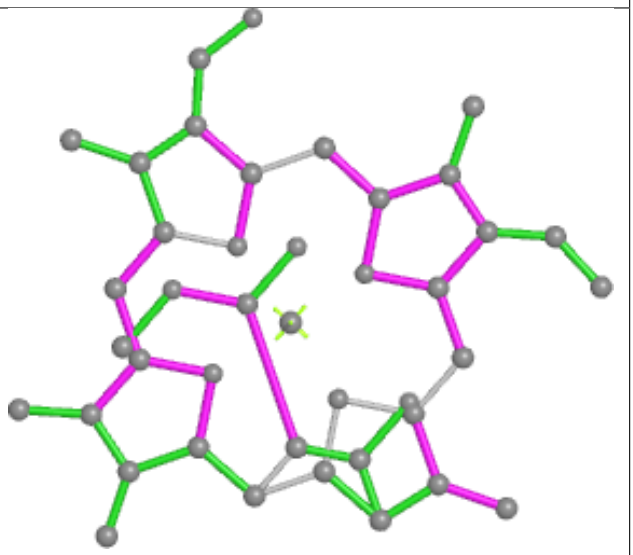


Rings

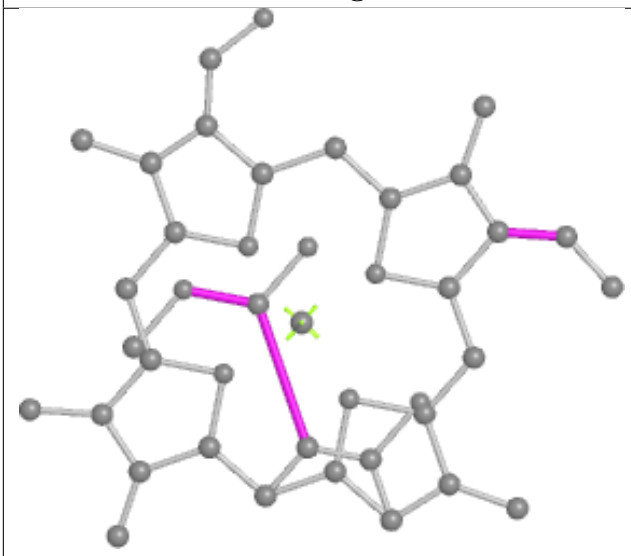
Ligand CL7 B 601



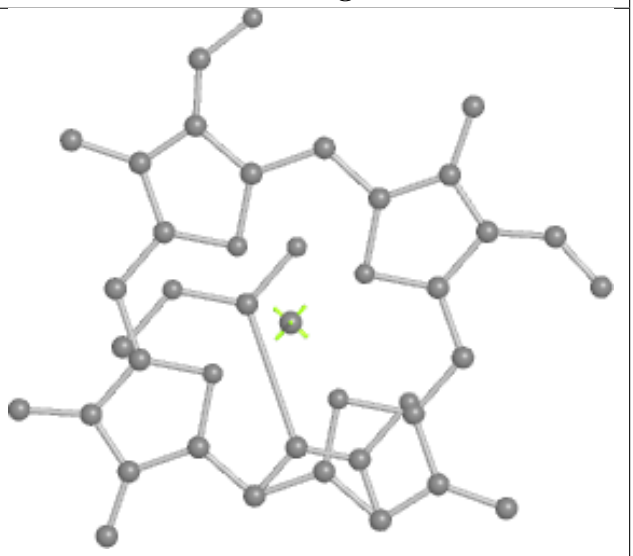
Bond lengths



Bond angles

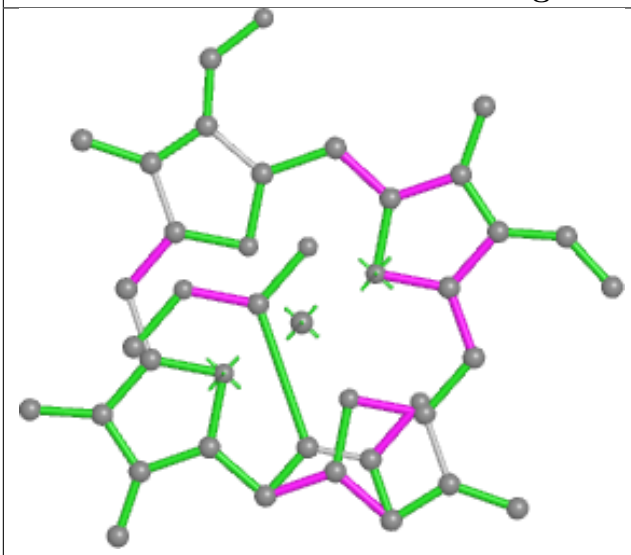


Torsions

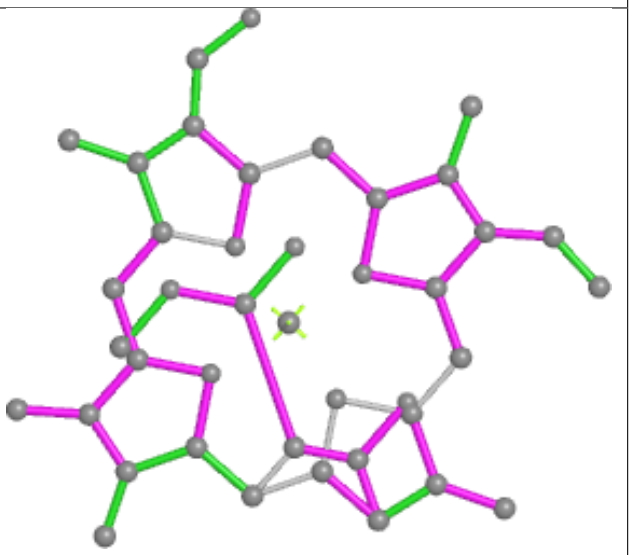


Rings

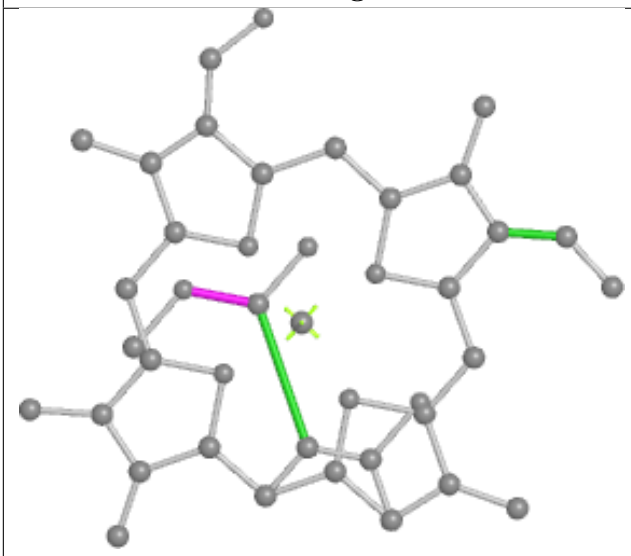
Ligand CL7 5 407



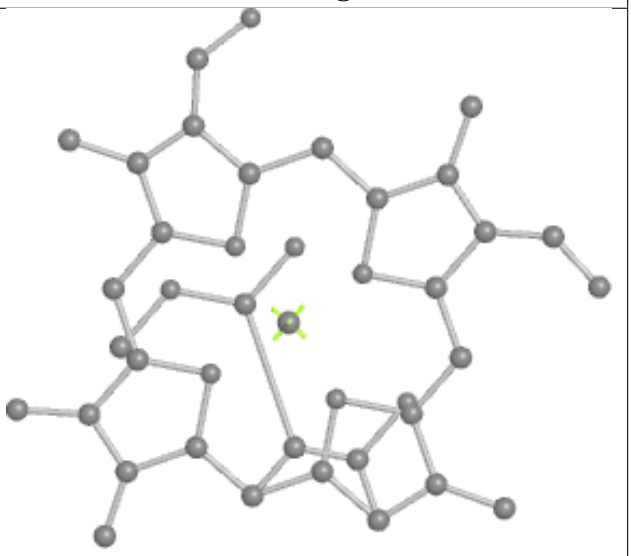
Bond lengths



Bond angles

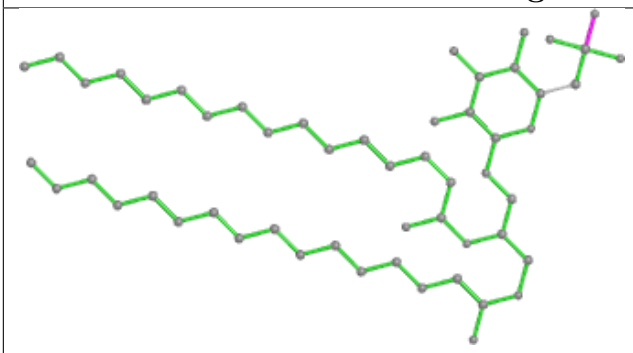


Torsions

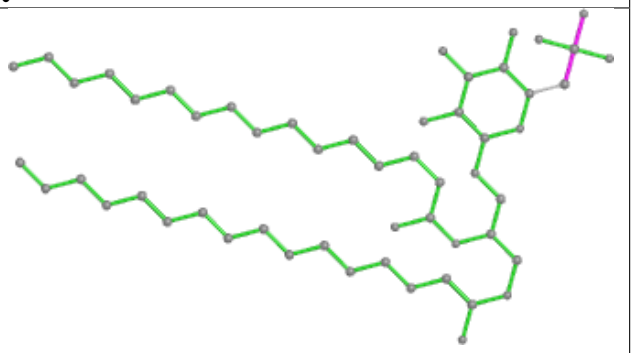


Rings

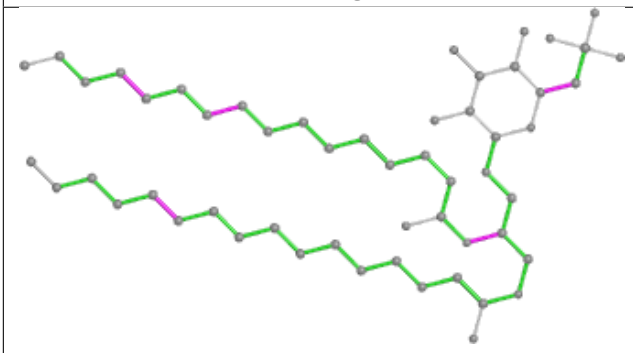
Ligand SQD b 621



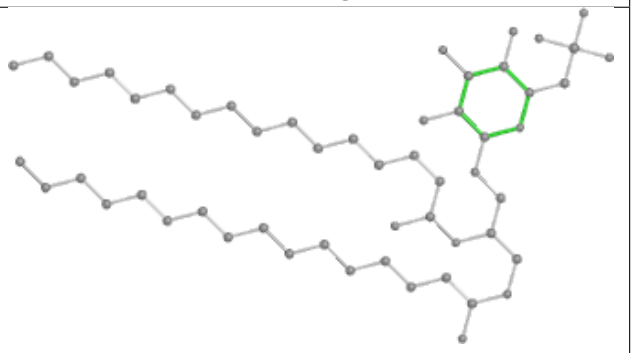
Bond lengths



Bond angles

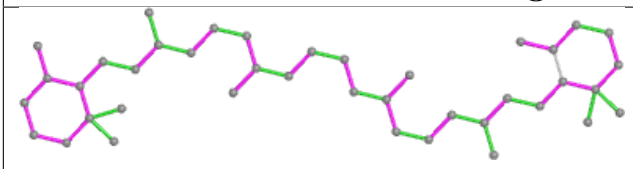


Torsions

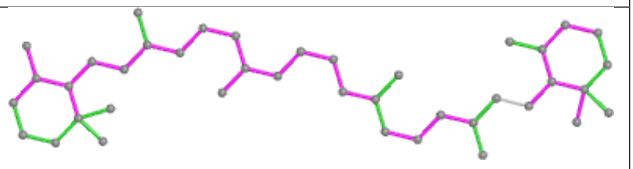


Rings

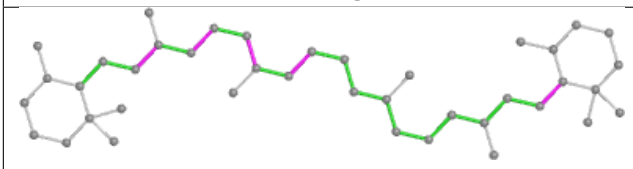
Ligand 8CT B 617



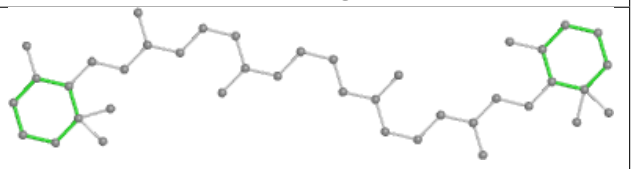
Bond lengths



Bond angles

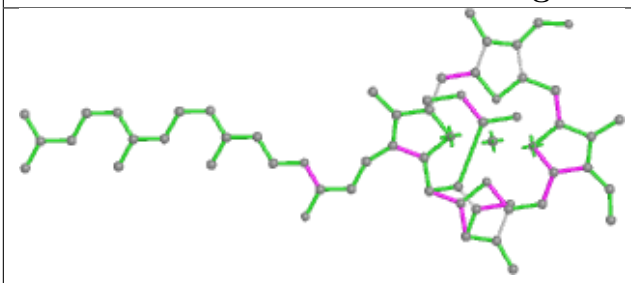


Torsions

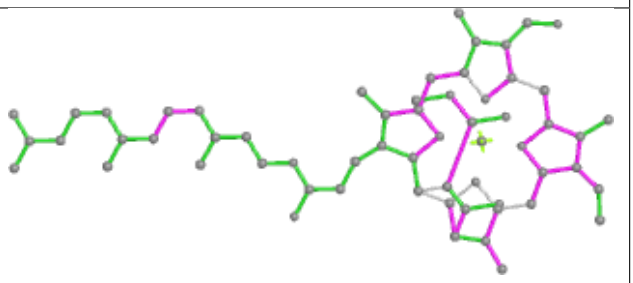


Rings

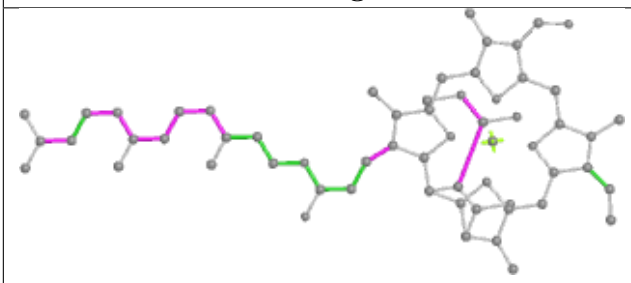
Ligand CL7 2 511



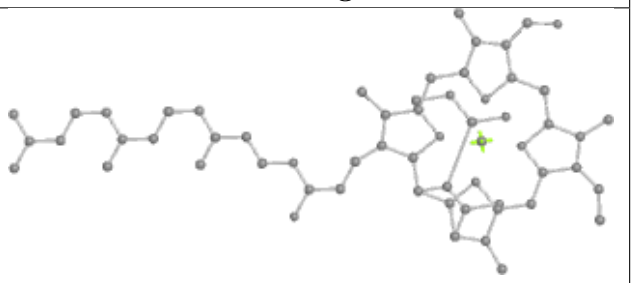
Bond lengths



Bond angles

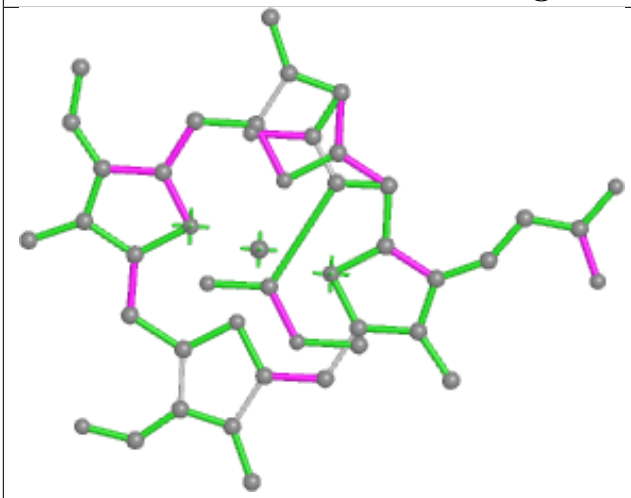


Torsions

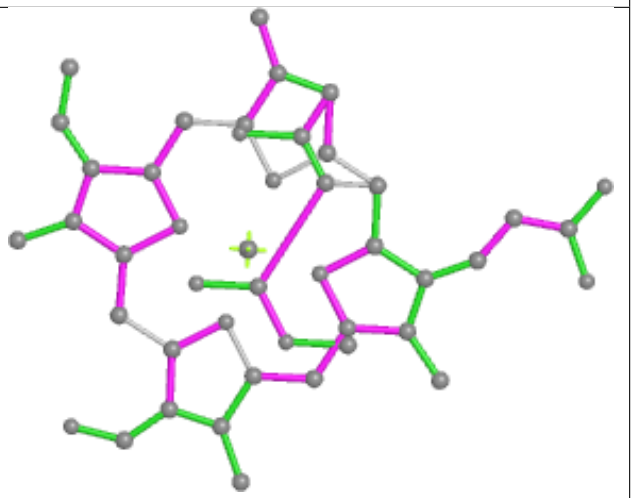


Rings

Ligand CL7 5 411



Bond lengths



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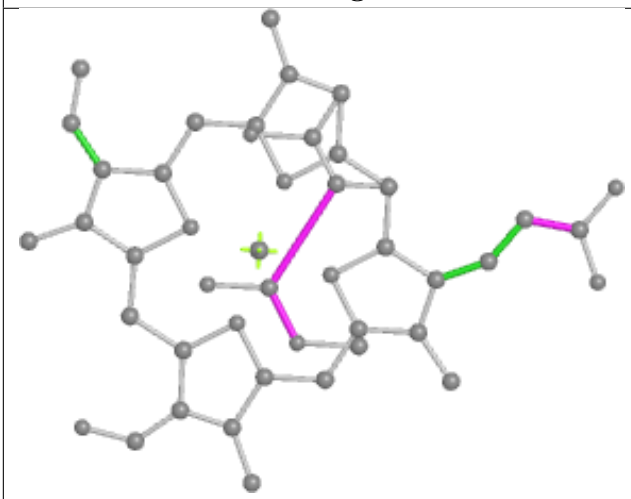
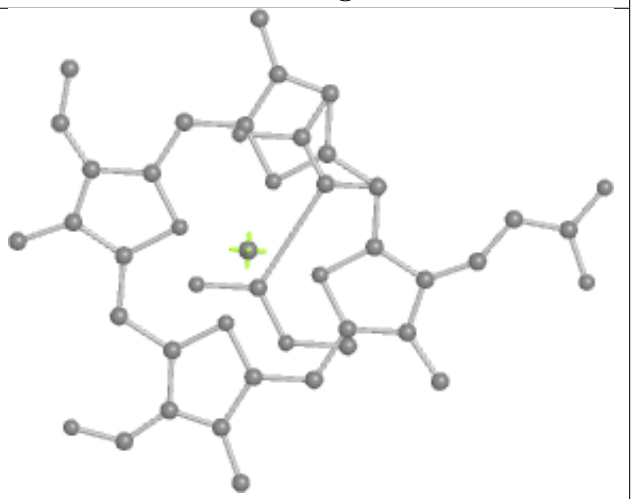
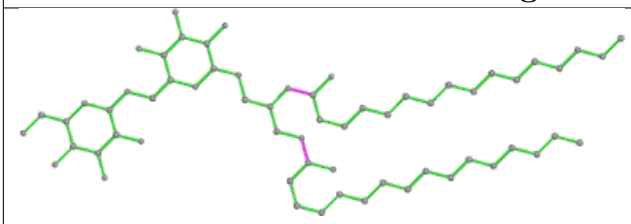


Torsions

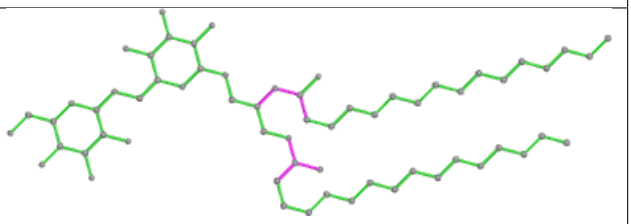


Rings

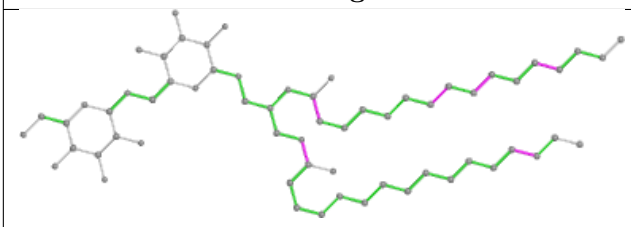
Ligand DGD B 624



Bond lengths



Bond angles



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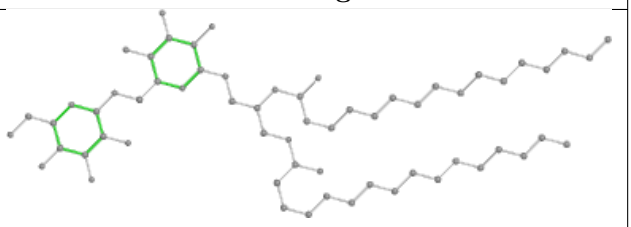
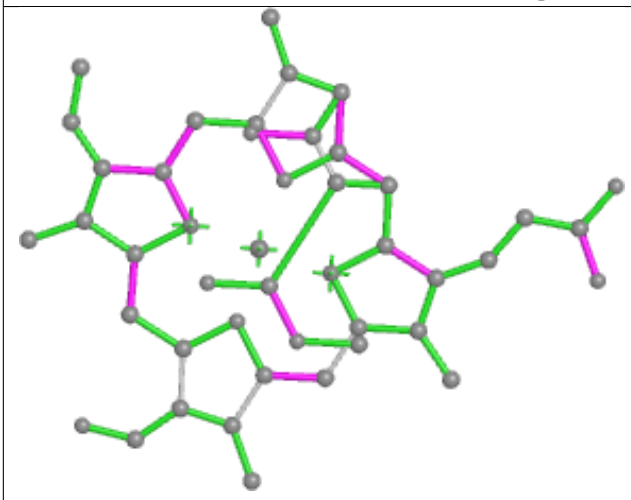


Rings

Ligand CL7 1 412



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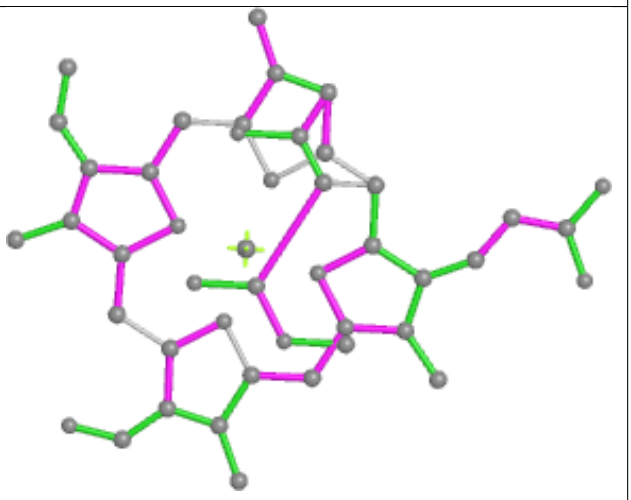
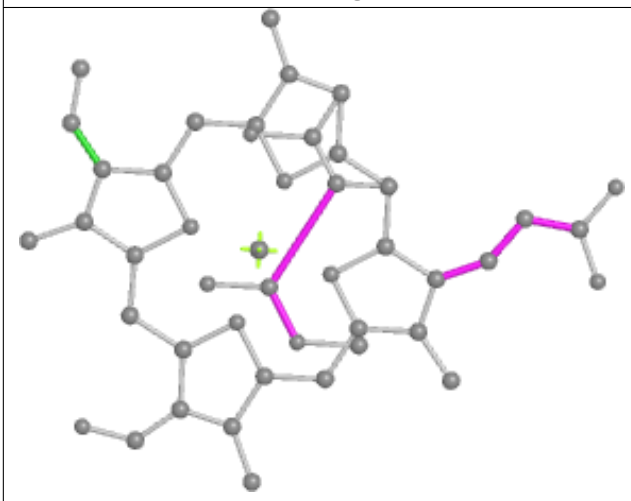


Bond angles



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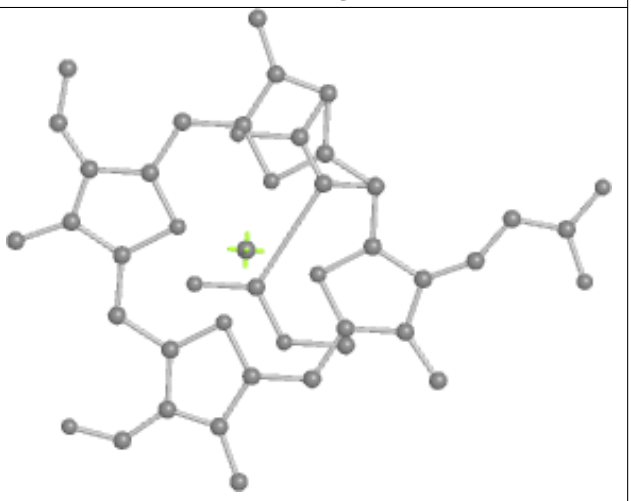
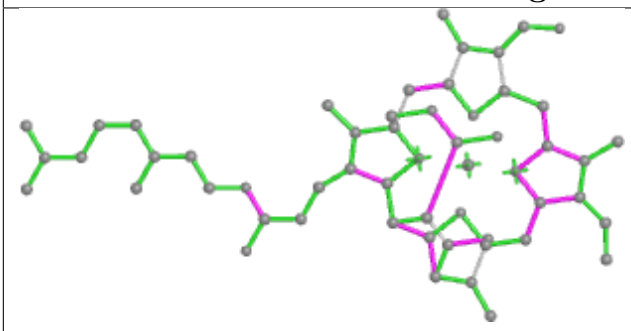


Rings

Ligand CL7 B 613



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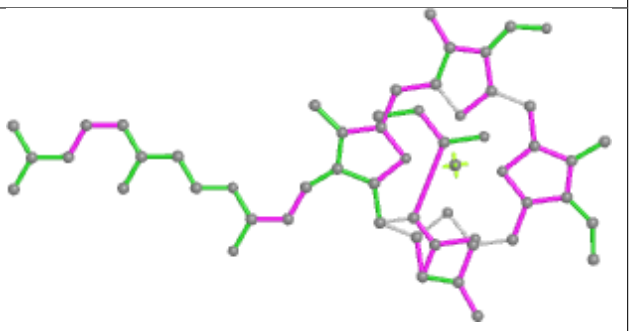
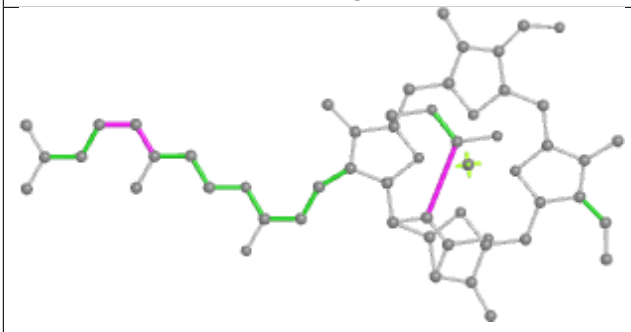
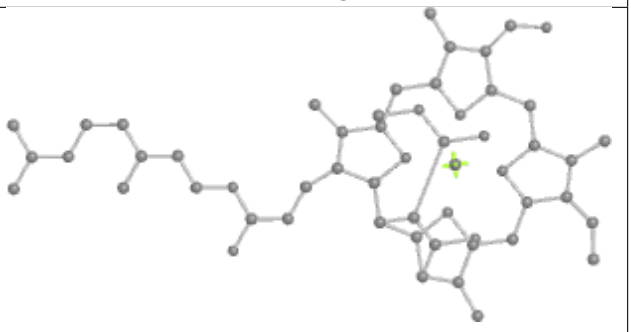


Bond angles

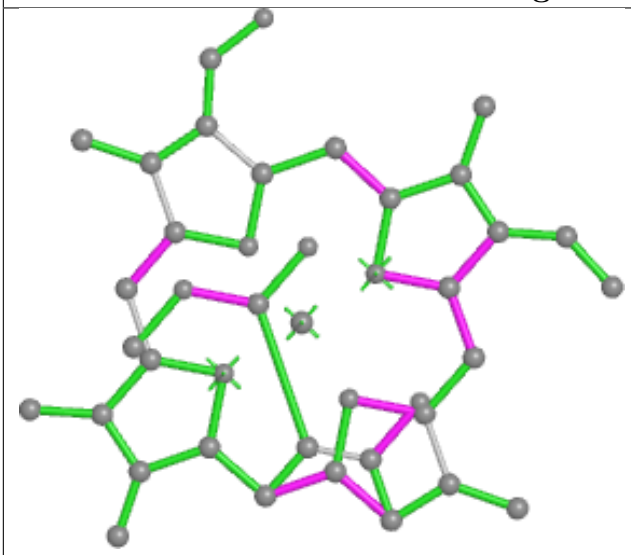


Torsions



Rings

Ligand CL7 7 515



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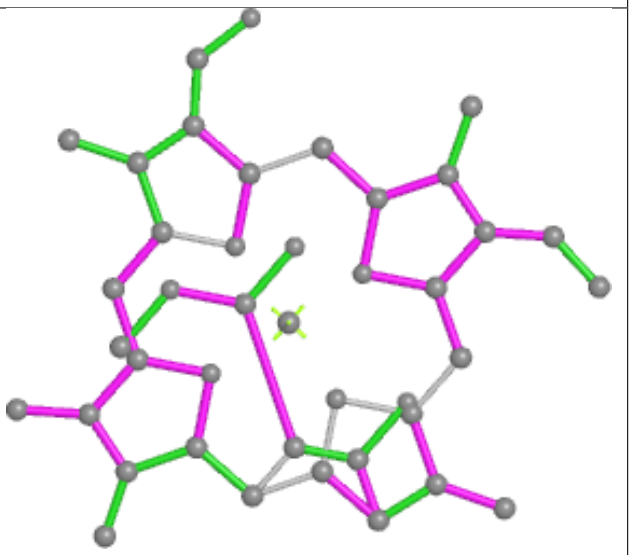
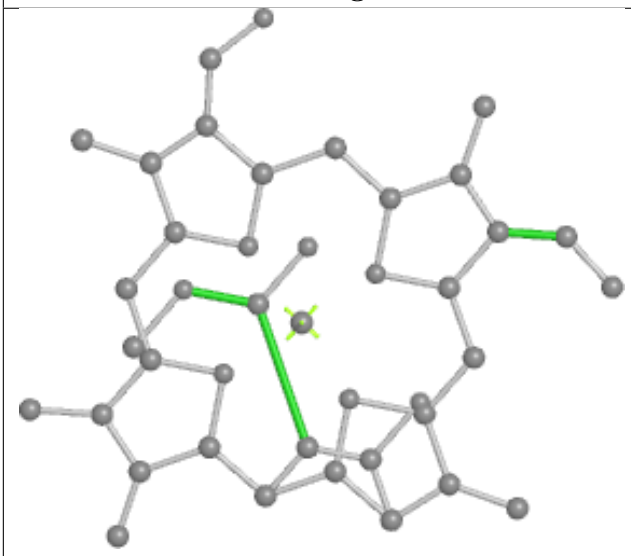


Bond angles



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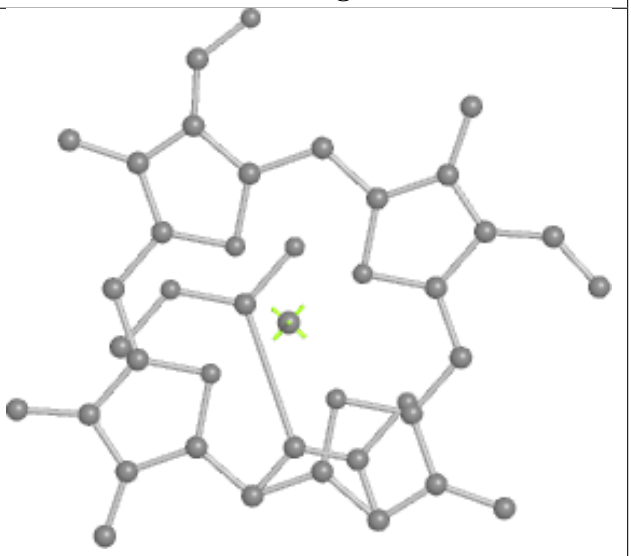
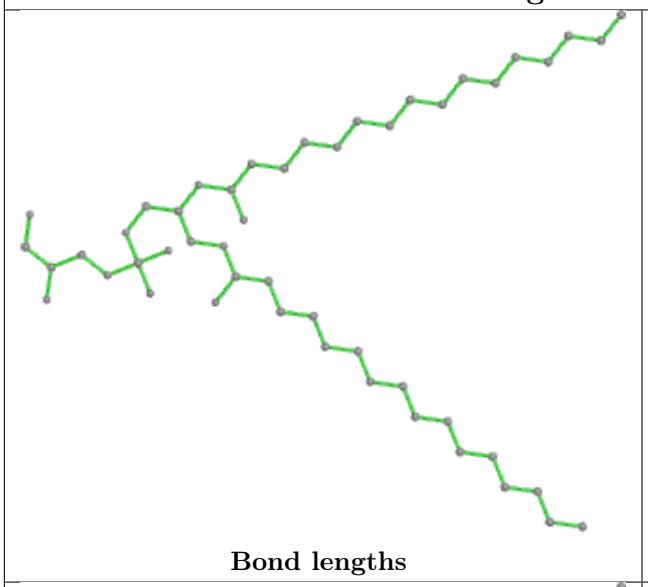


Rings

Ligand LHG d 409



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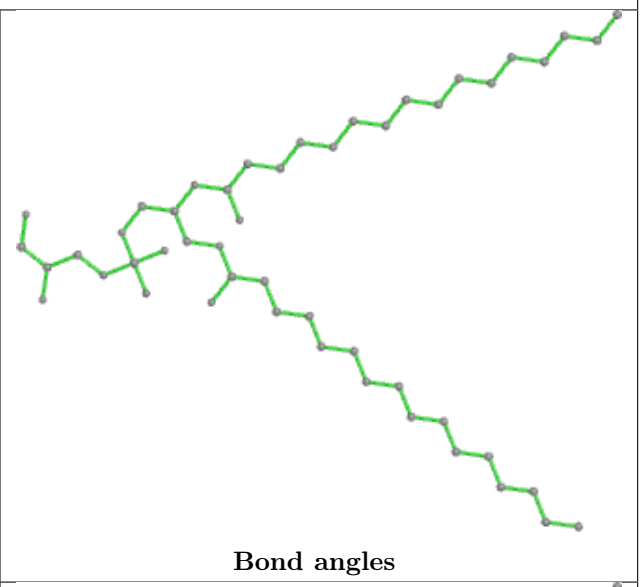
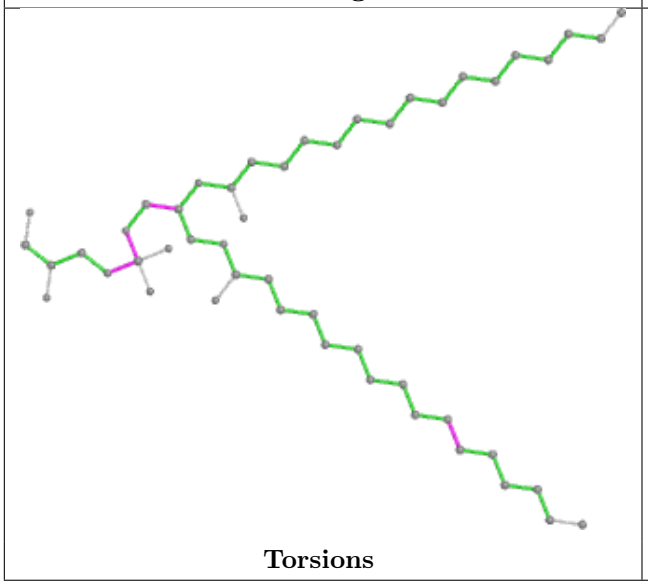


Bond angles



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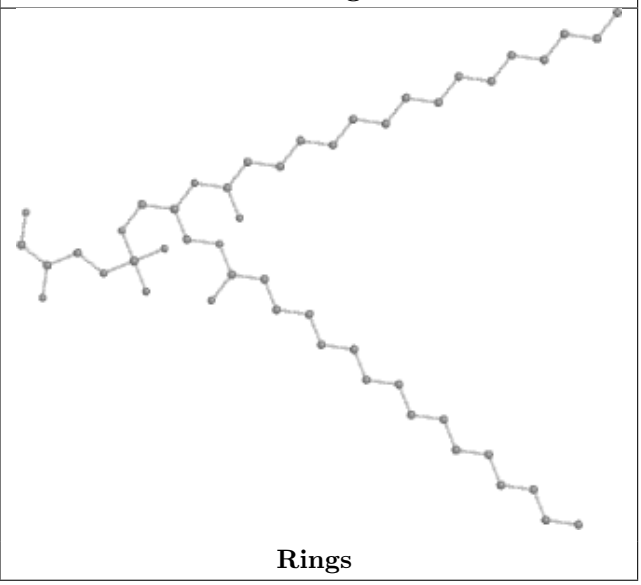
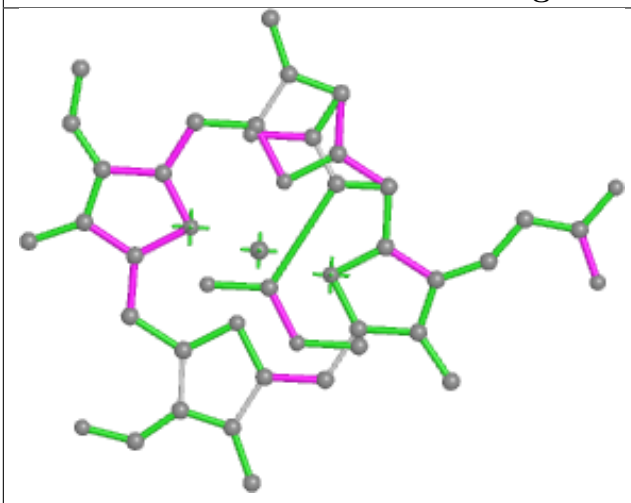


Rings

Ligand CL7 2 508



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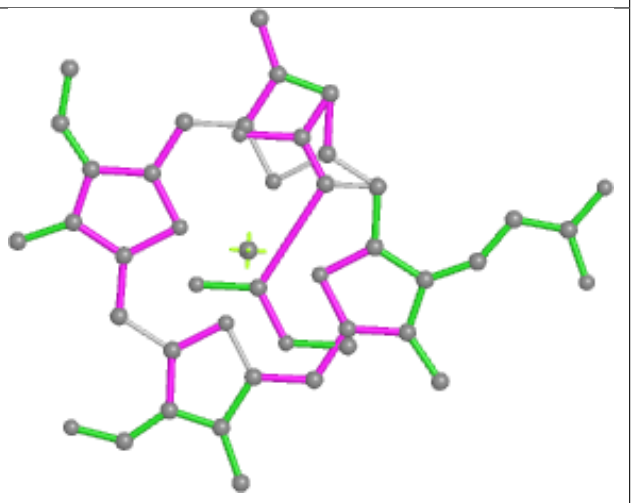
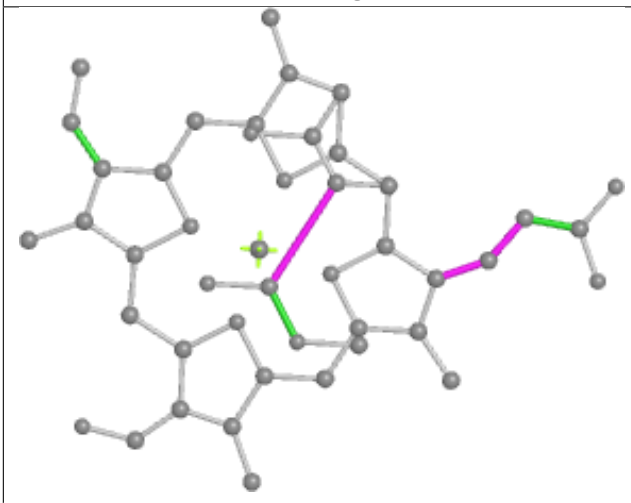


Bond angles



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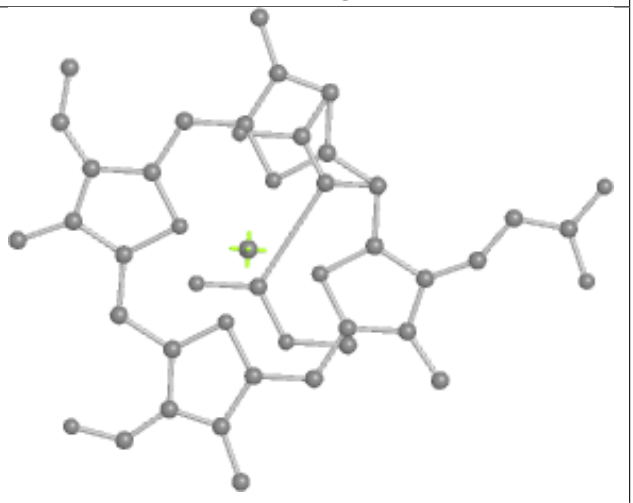
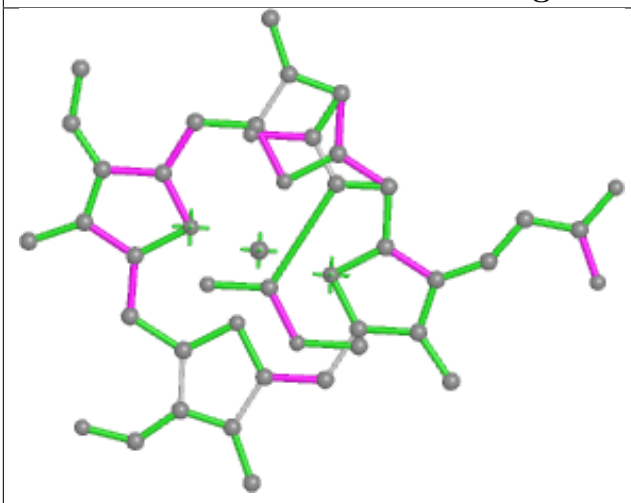
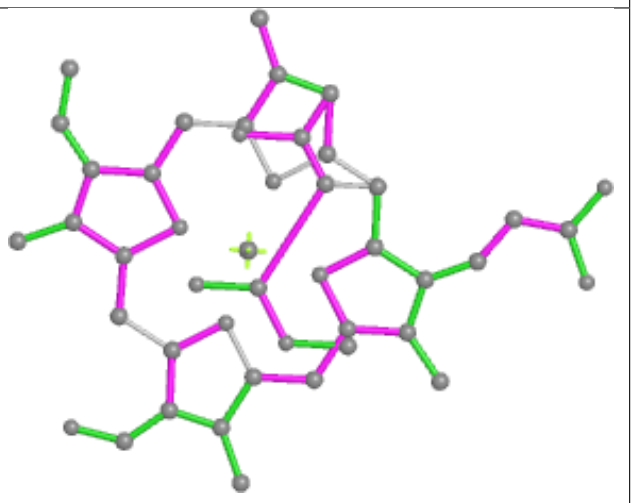


Rings

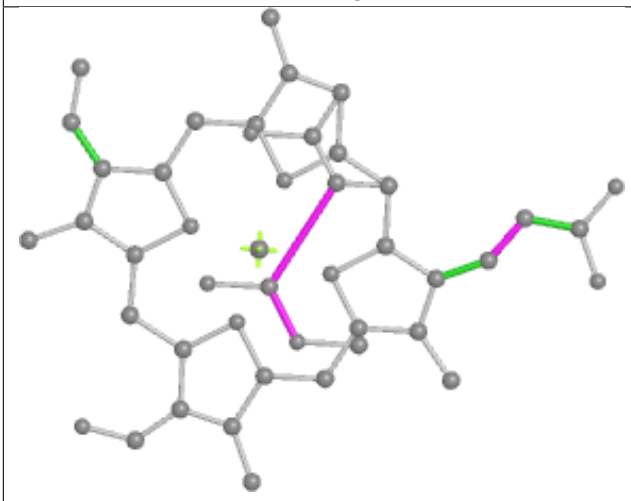
Ligand CL7 1 409



Bond lengths



Bond angles



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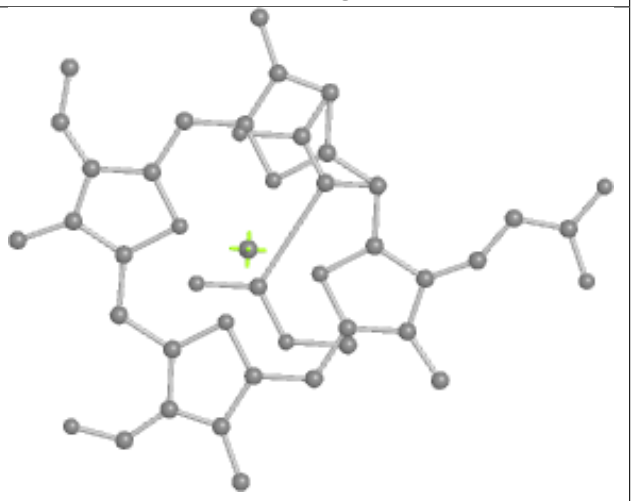
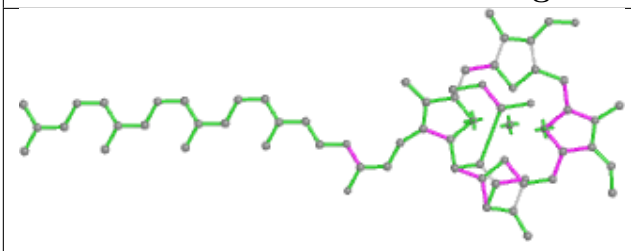
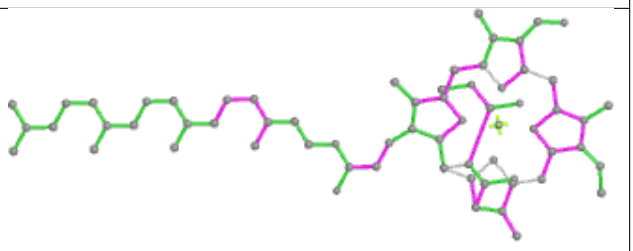


Rings

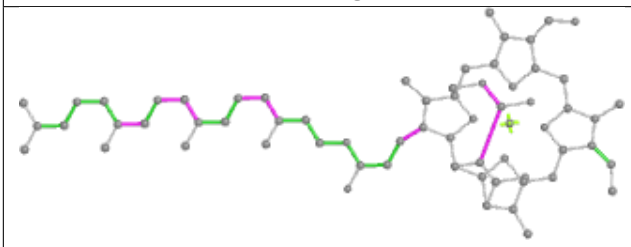
Ligand CL7 6 506



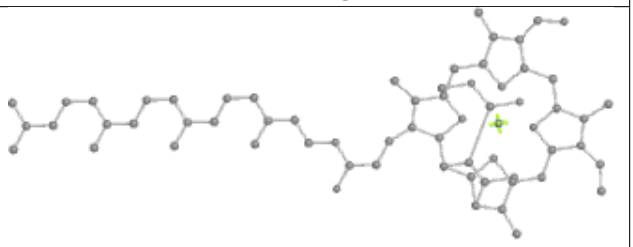
Bond lengths



Bond angles

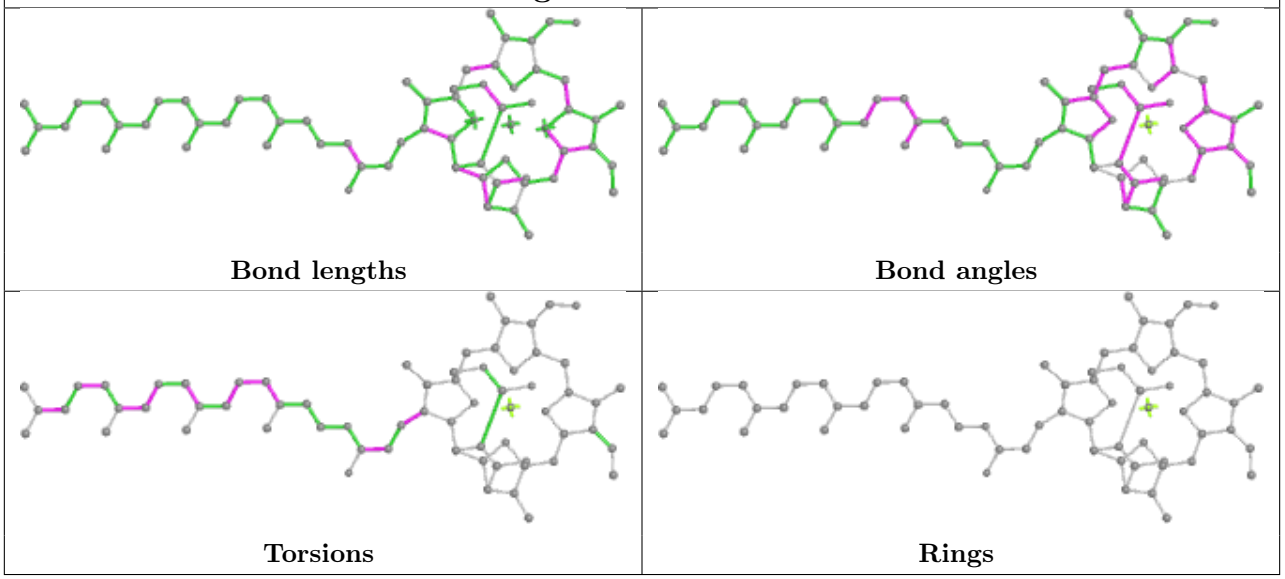


Torsions

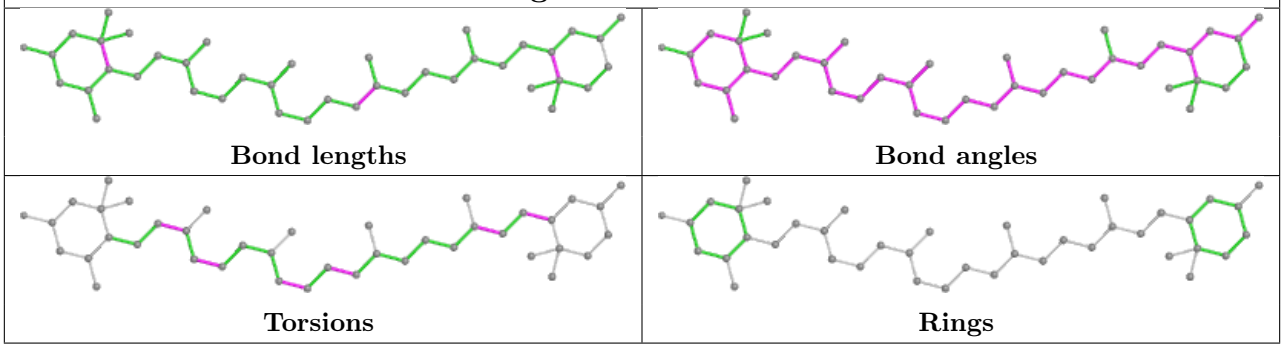


Rings

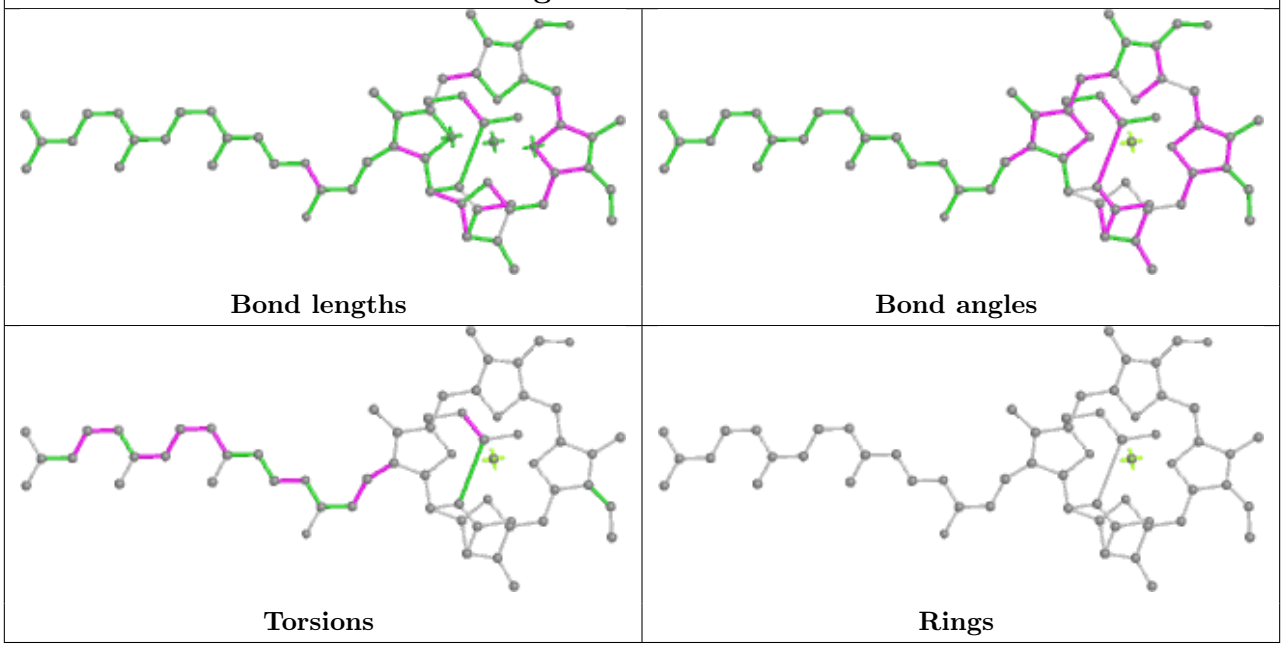
Ligand CL7 6 512



Ligand ZEX 4 419



Ligand CL7 1 402



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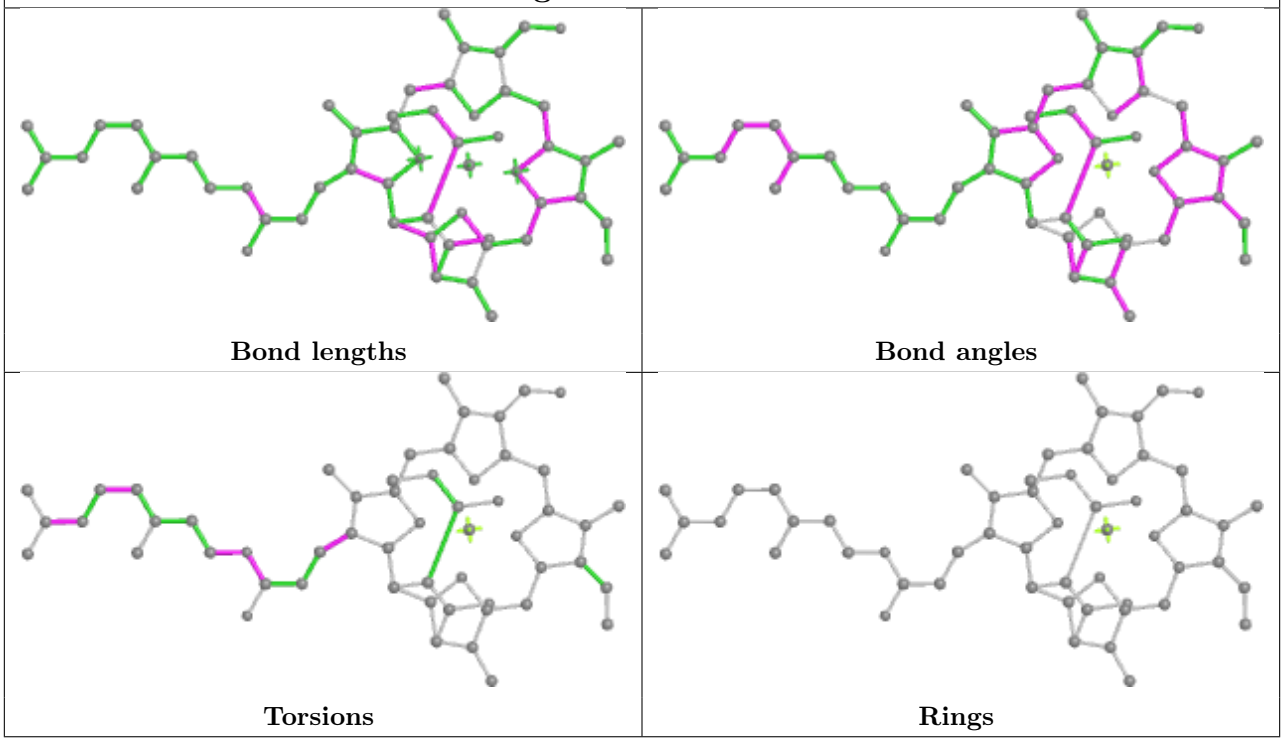
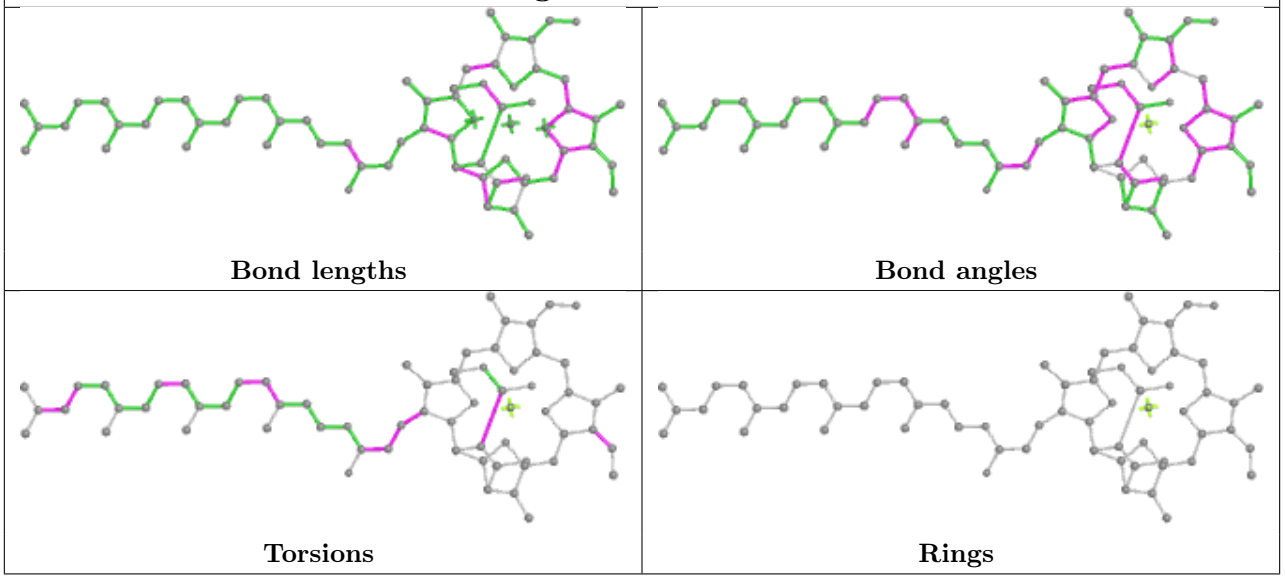
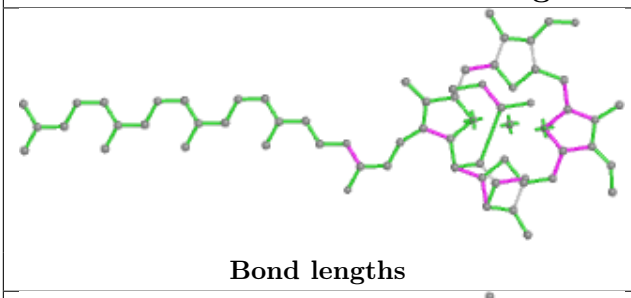


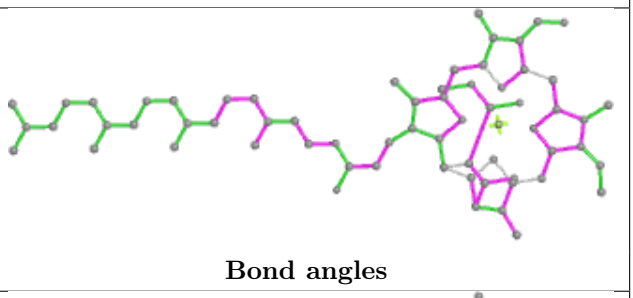
Ligand CL7 3 505



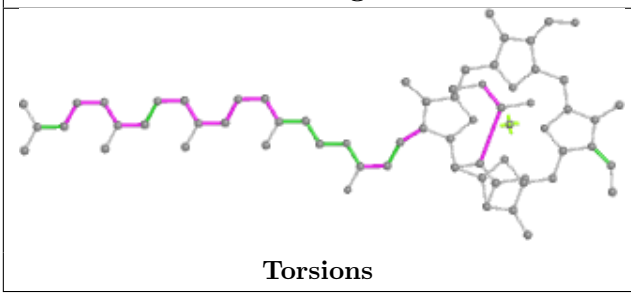
Ligand CL7 6 510



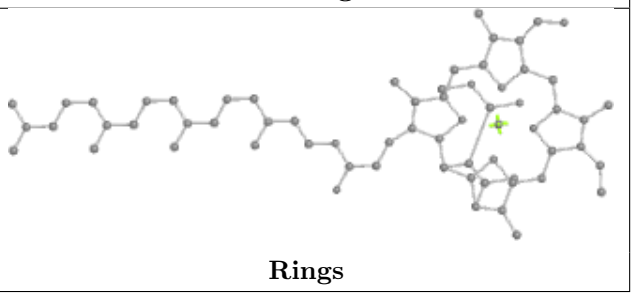
Bond lengths



Bond angles

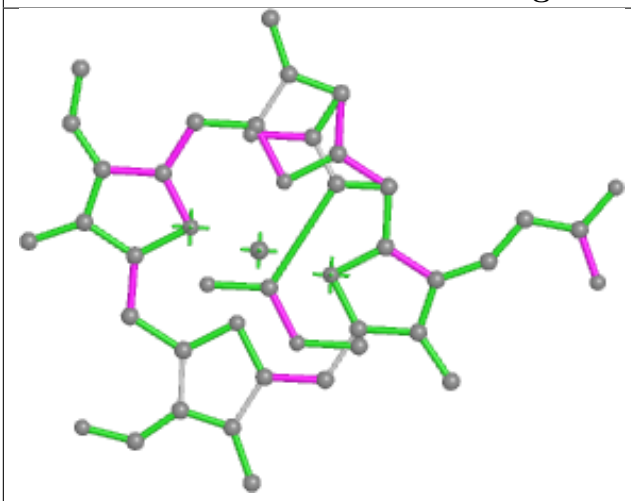


Torsions

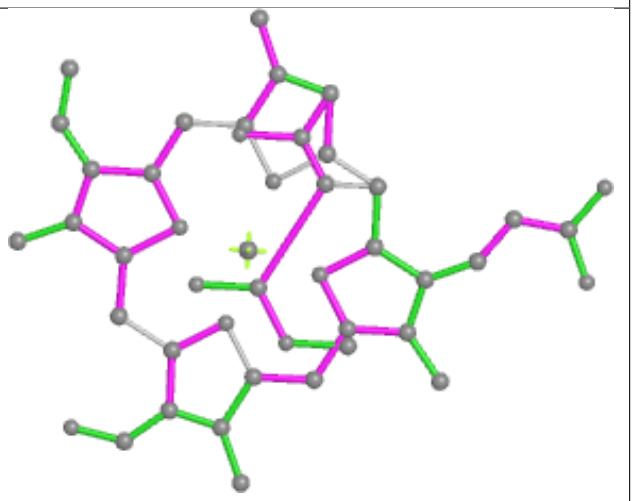


Rings

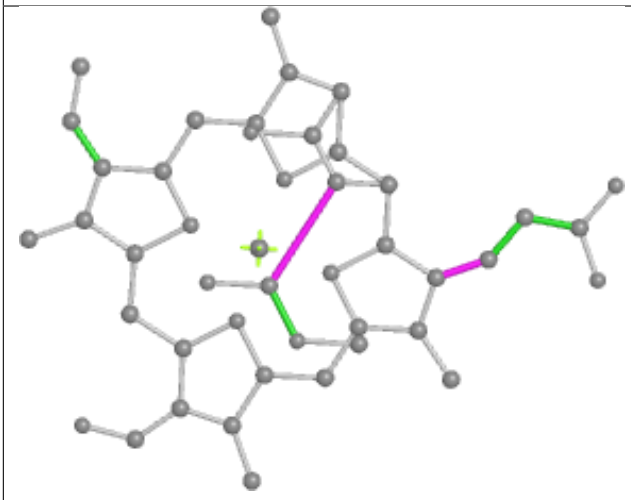
Ligand CL7 6 515



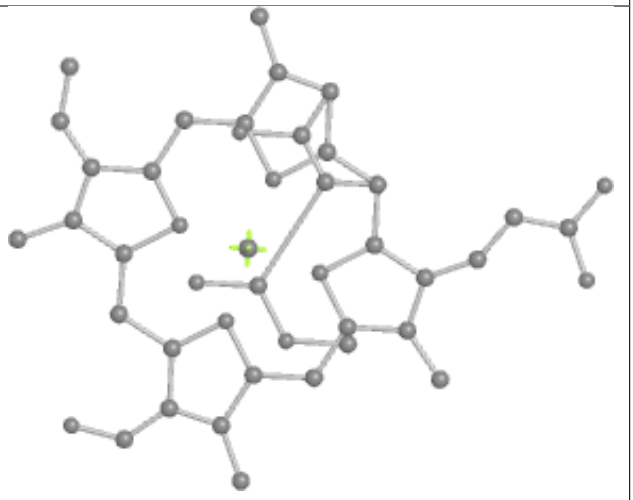
Bond lengths



Bond angles

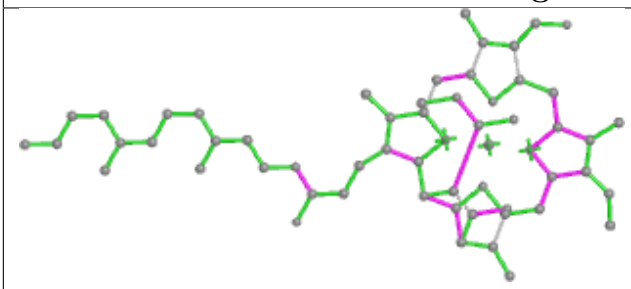


Torsions

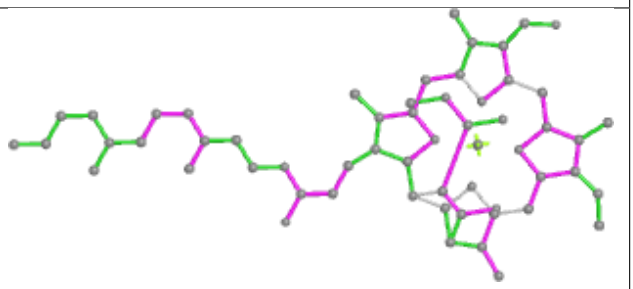


Rings

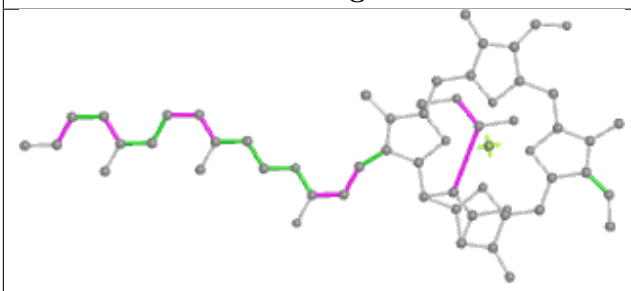
Ligand CL7 d 404



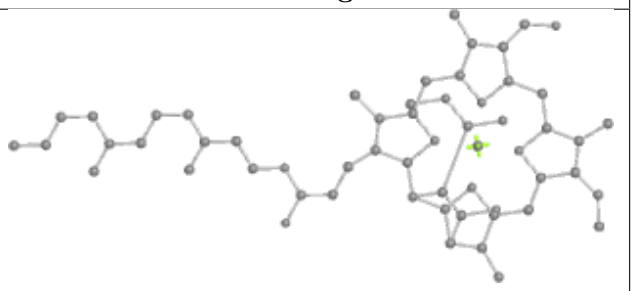
Bond lengths



Bond angles

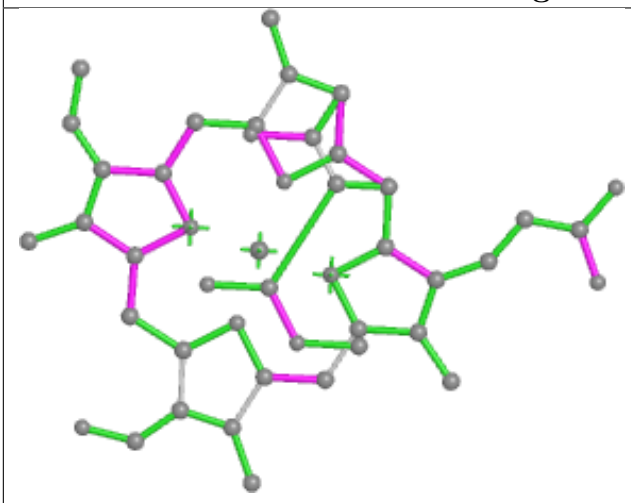


Torsions

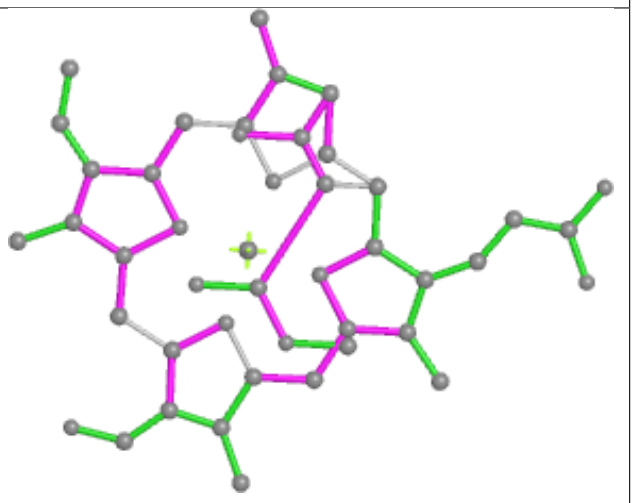


Rings

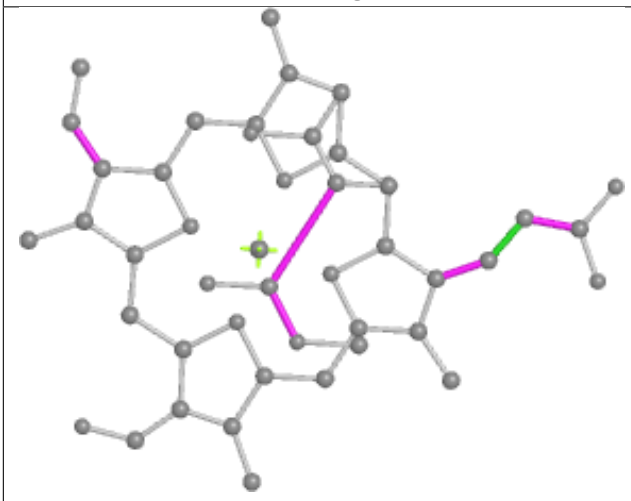
Ligand CL7 7 506



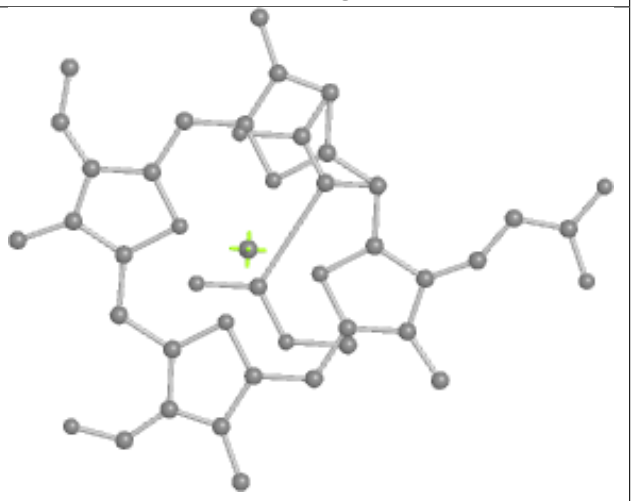
Bond lengths



Bond angles

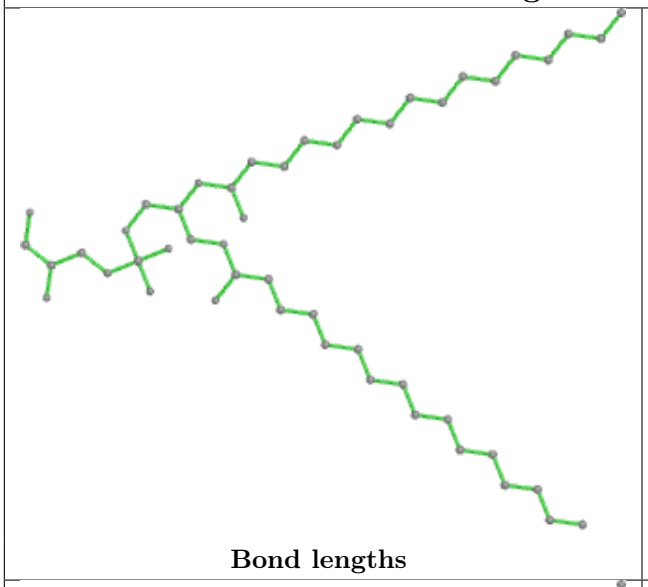


Torsions

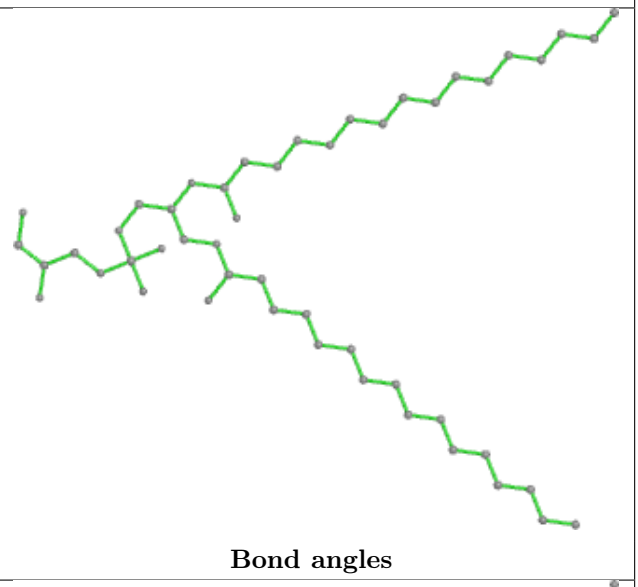


Rings

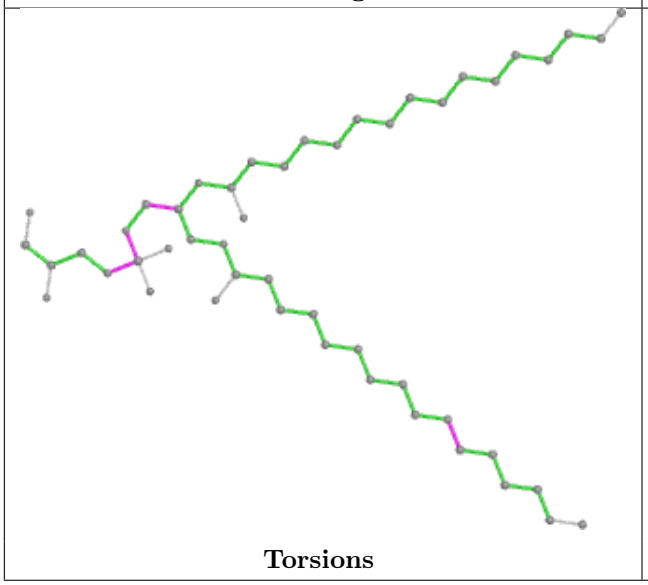
Ligand LHG D 409



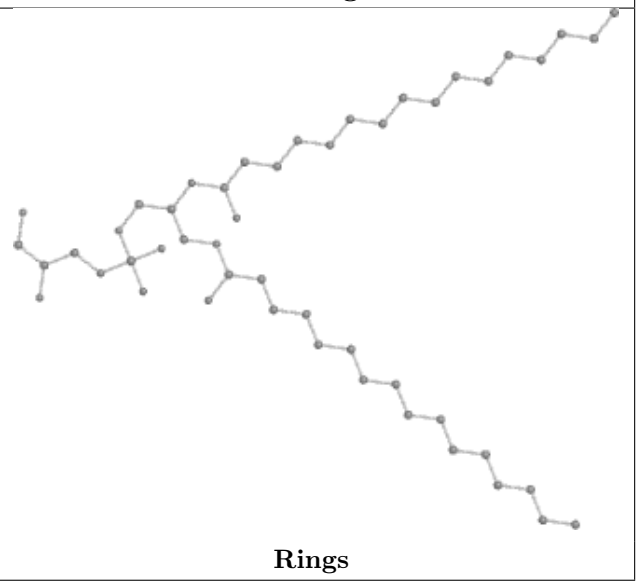
Bond lengths



Bond angles

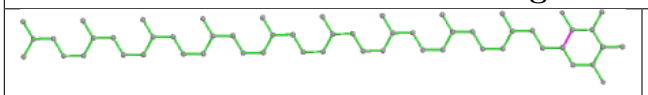


Torsions

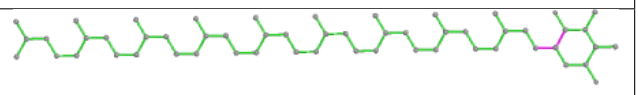


Rings

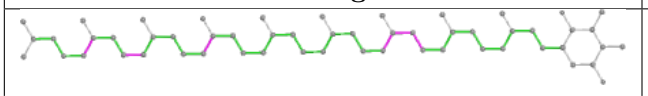
Ligand PL9 D 407



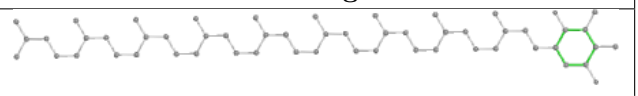
Bond lengths



Bond angles

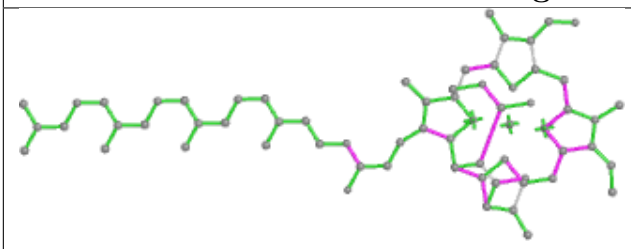


Torsions



Rings

Ligand CL7 7 503



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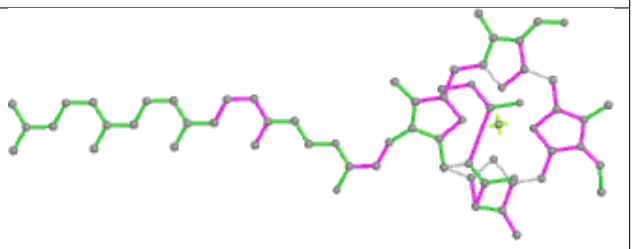
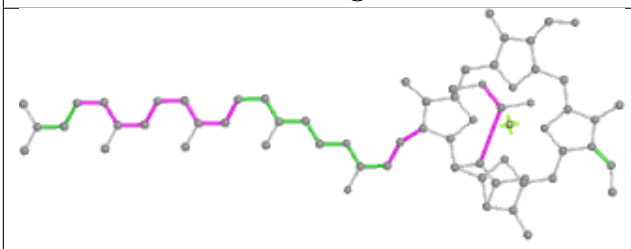
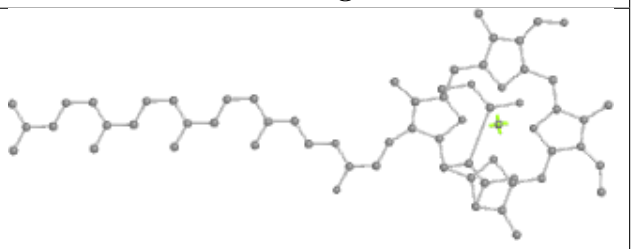


Bond angles

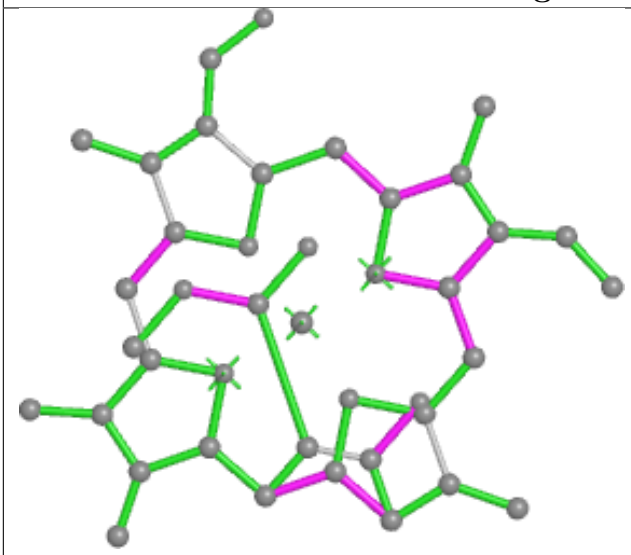


Torsions



Rings

Ligand CL7 c 518



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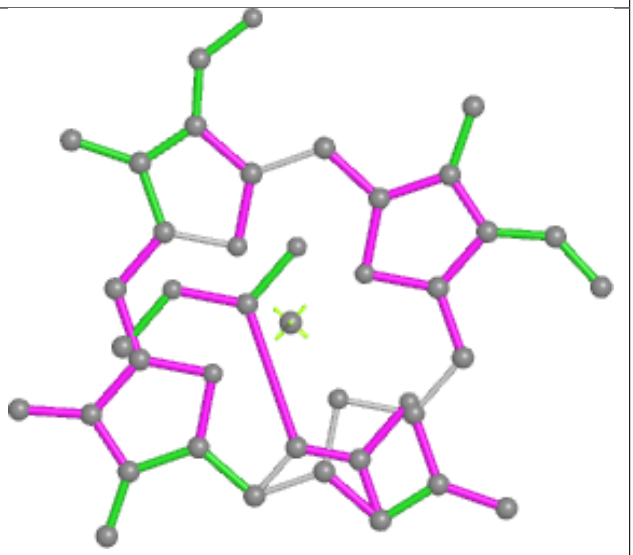
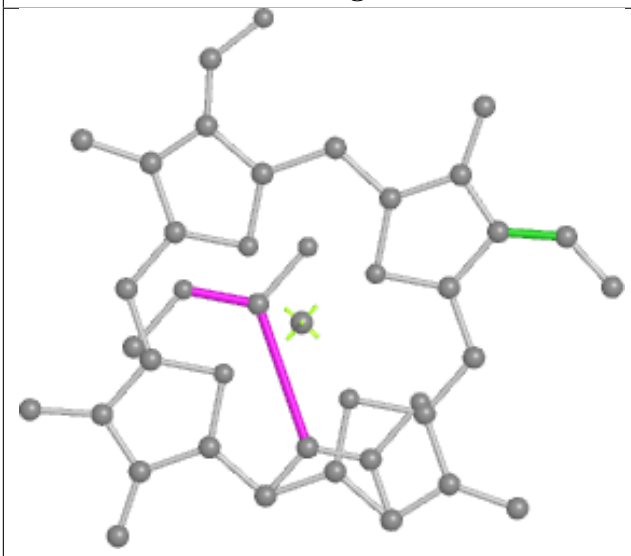
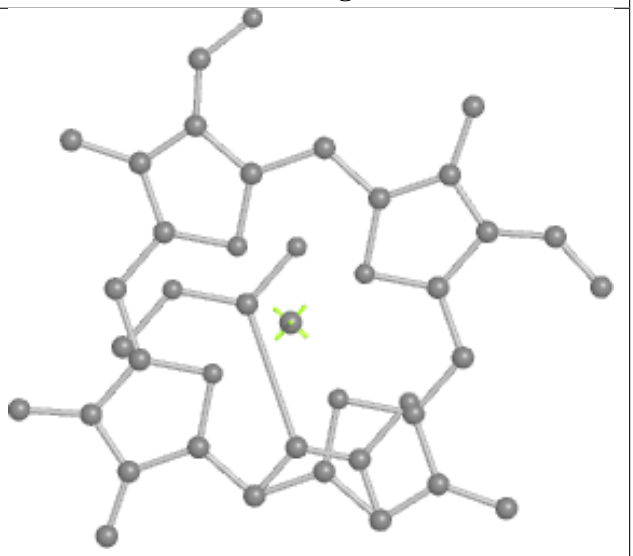


Bond angles

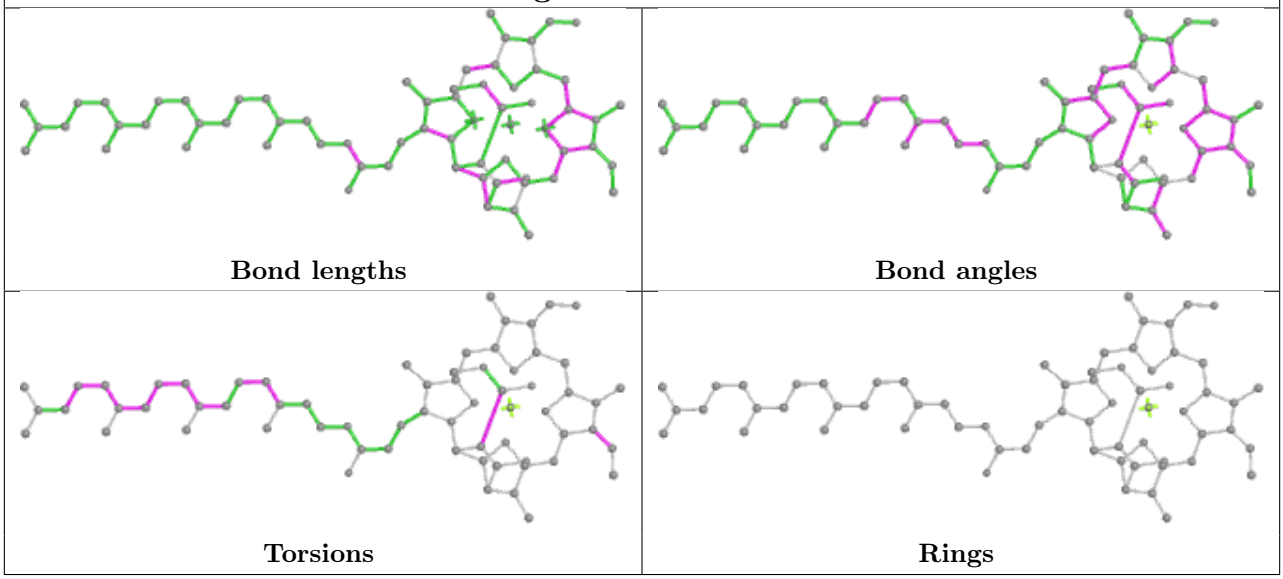


Torsions

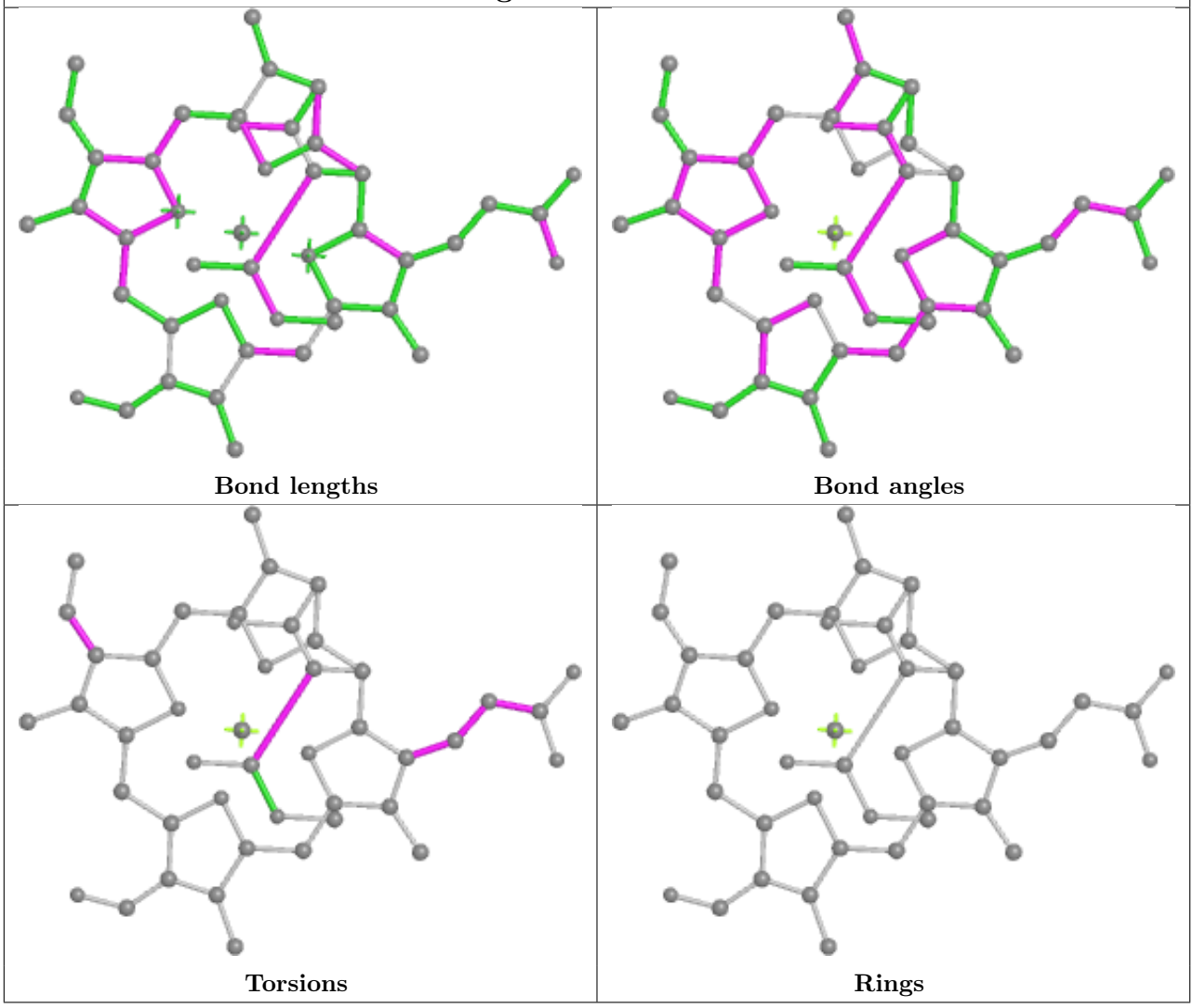


Rings

Ligand CL7 2 505



Ligand CL7 7 513



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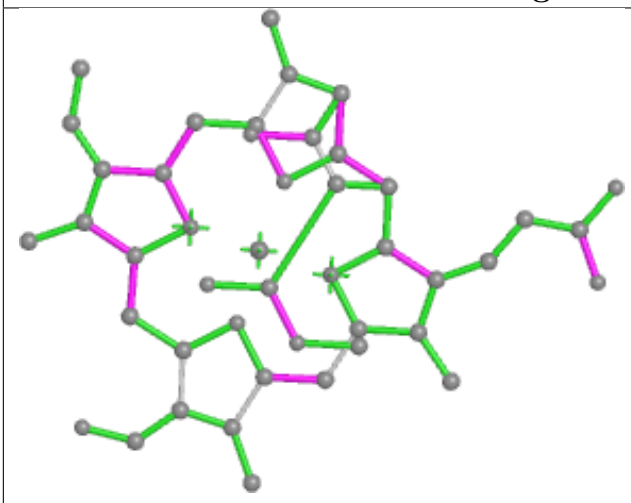

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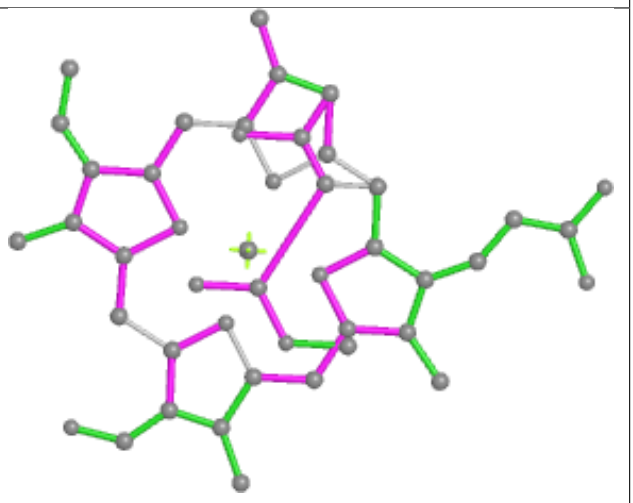
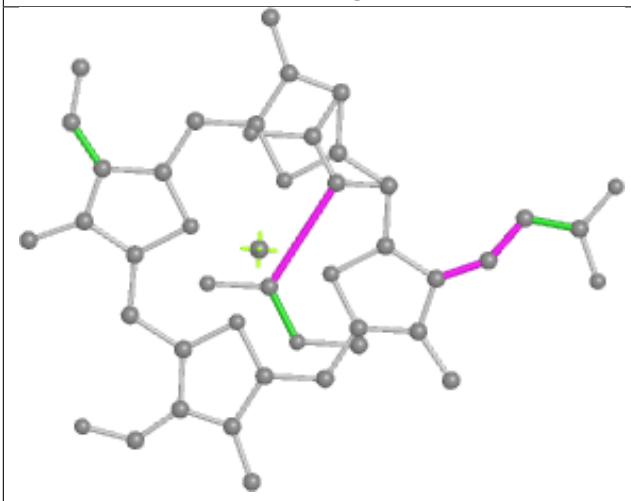


Bond angles



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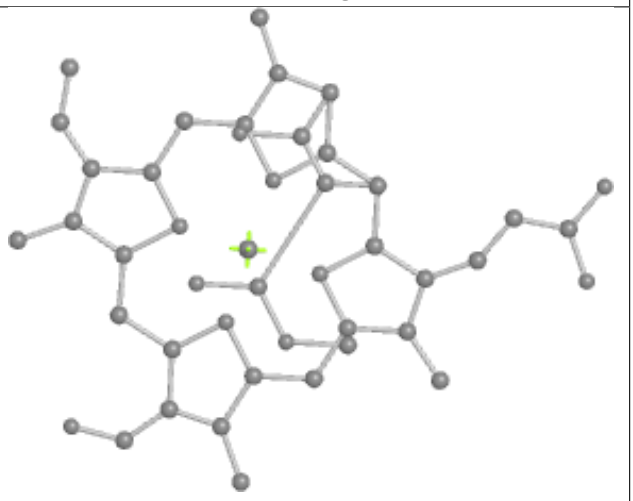
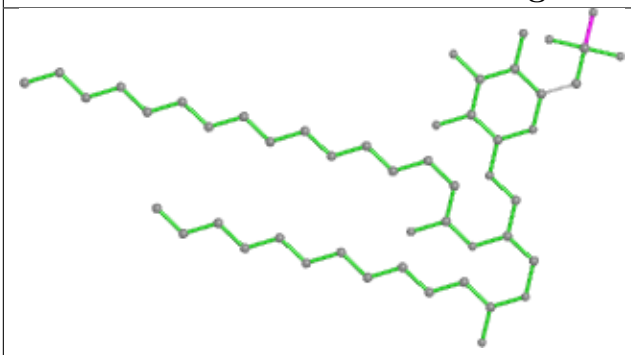
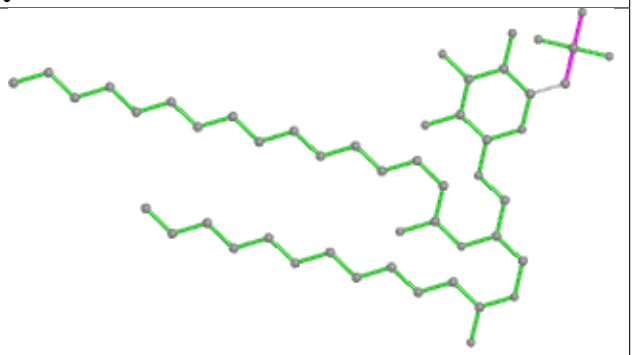


Rings

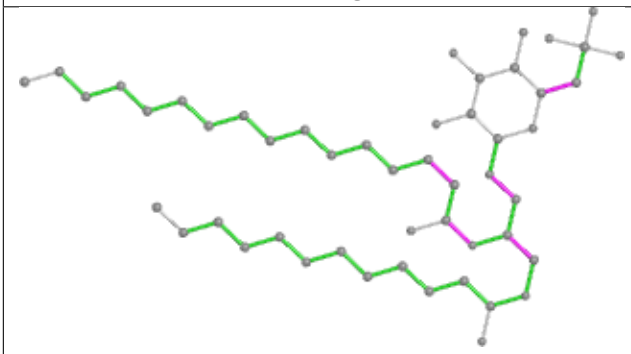
Ligand SQD 2 522



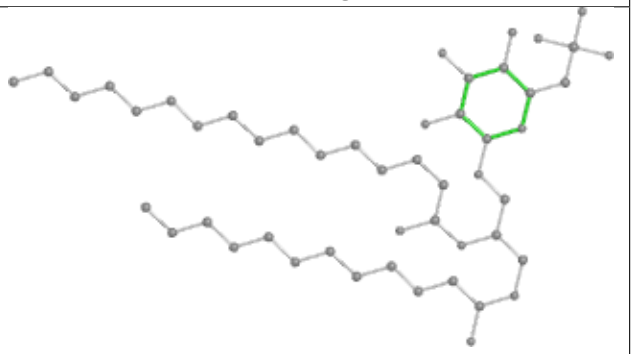
Bond lengths



Bond angles

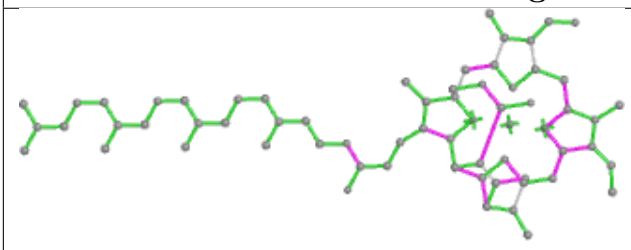


Torsions



Rings

Ligand CL7 C 504



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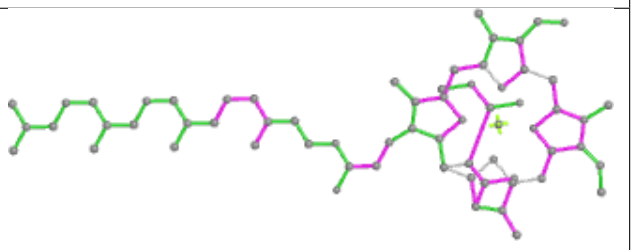
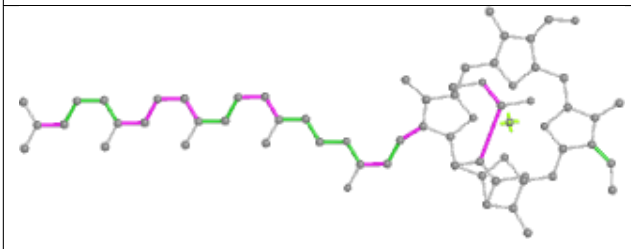


Bond angles



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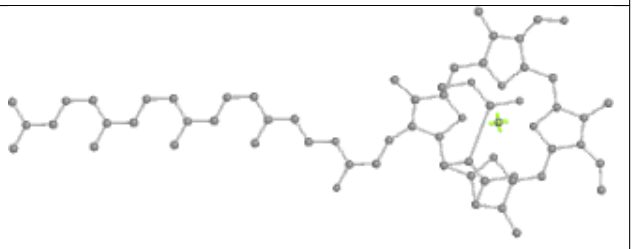
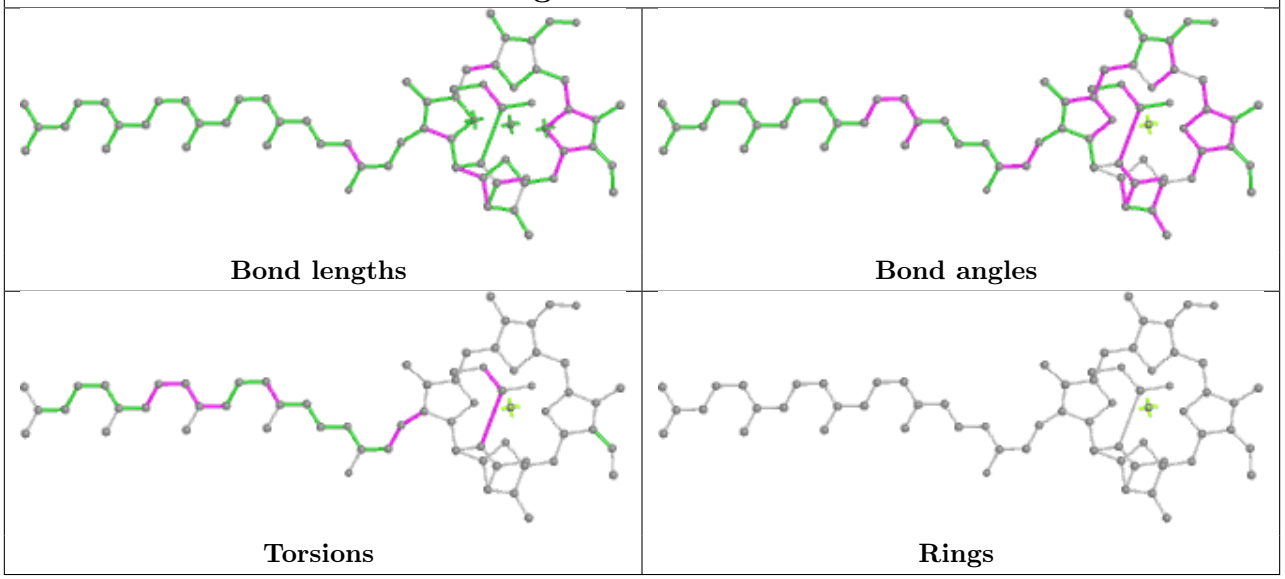
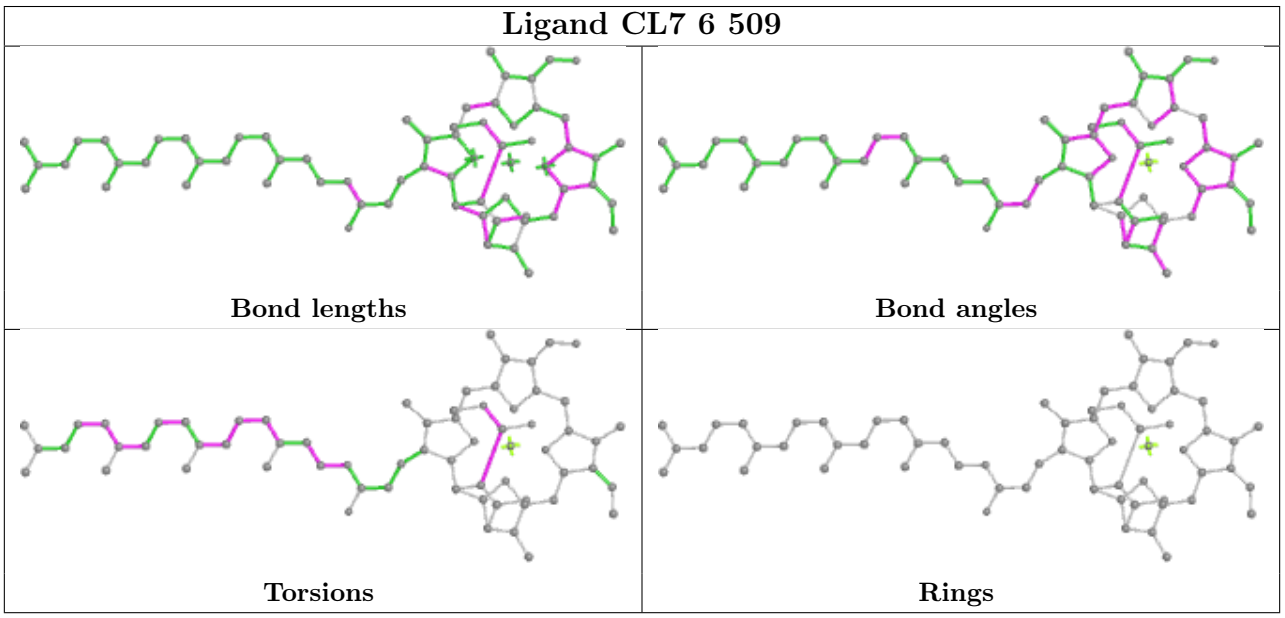


Rings

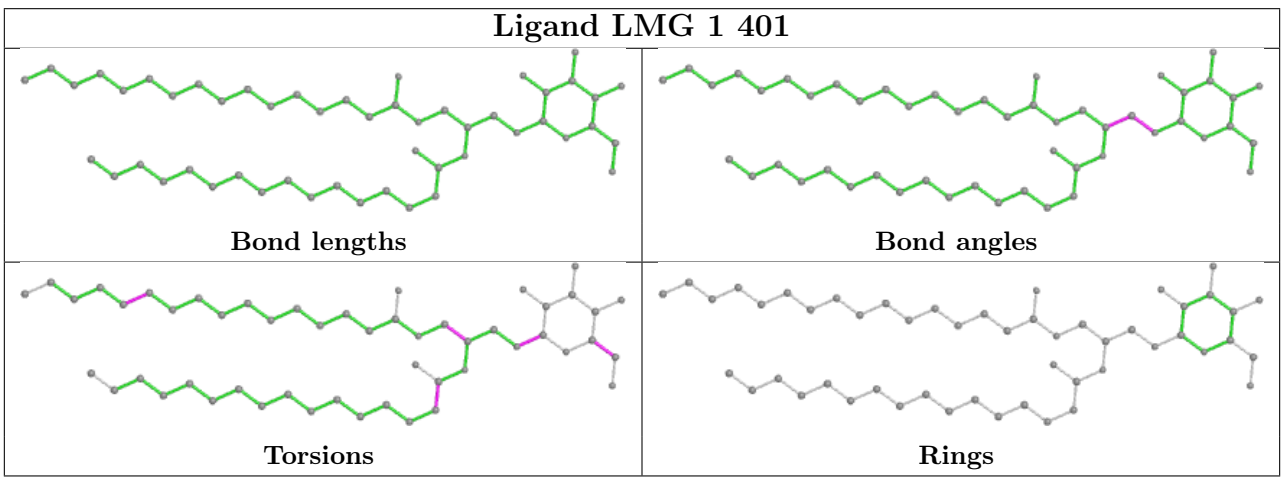
Ligand CL7 6 502



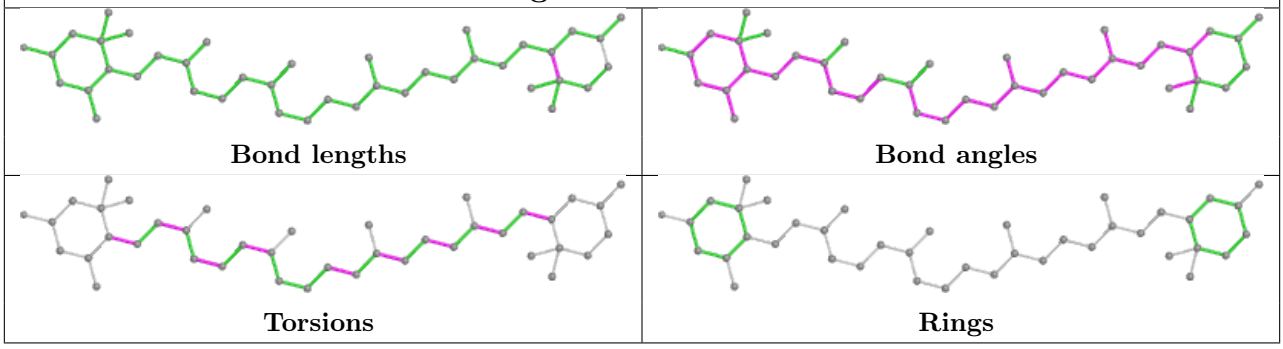
Ligand CL7 6 509



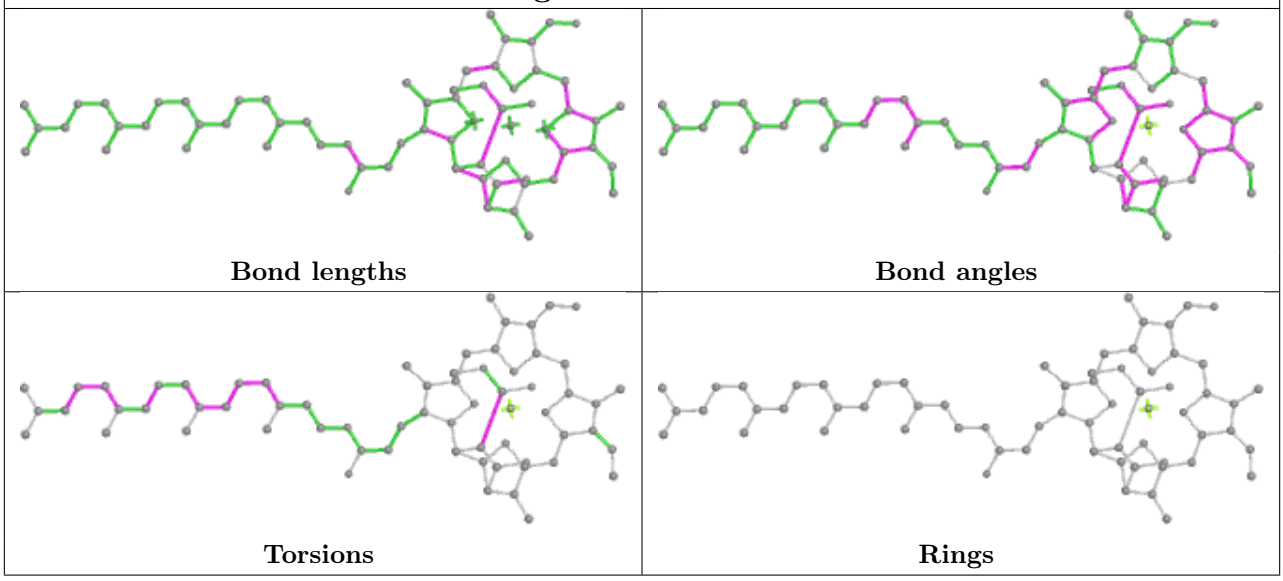
Ligand LMG 1 401



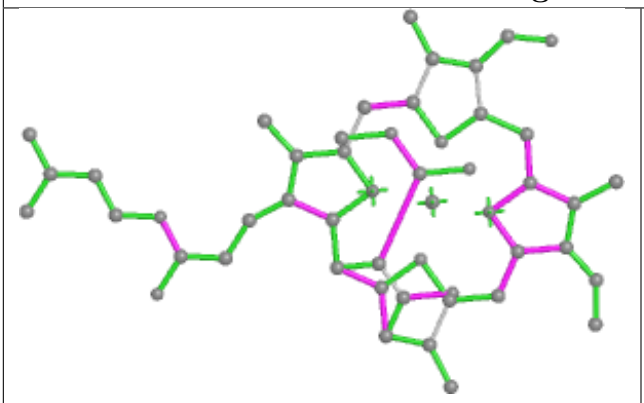
Ligand ZEX 5 421



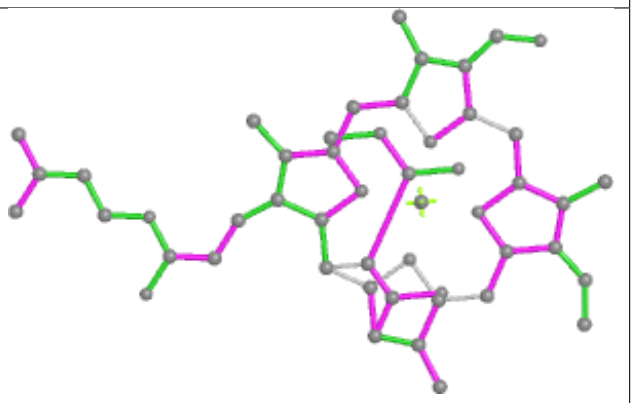
Ligand CL7 3 507



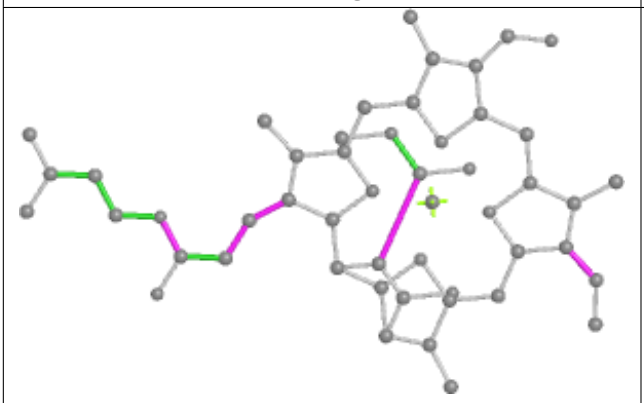
Ligand CL7 b 616



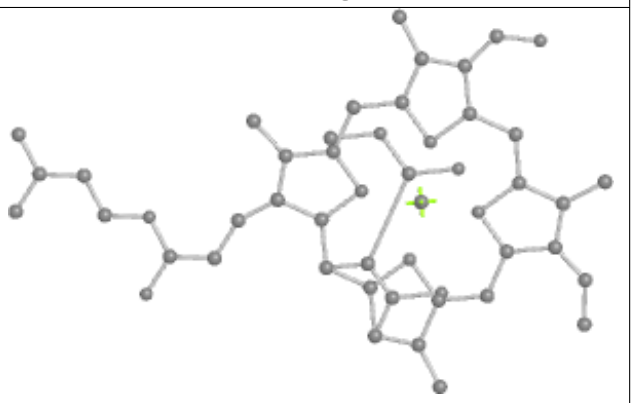
Bond lengths



Bond angles

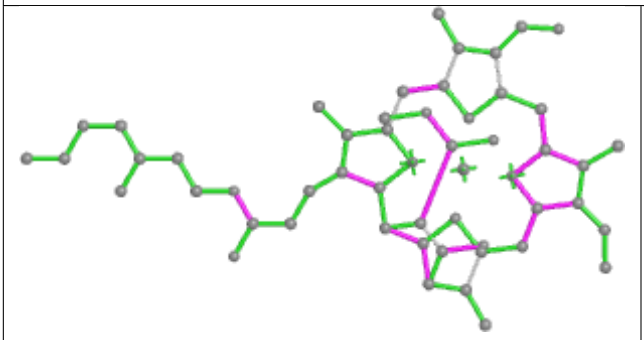


Torsions

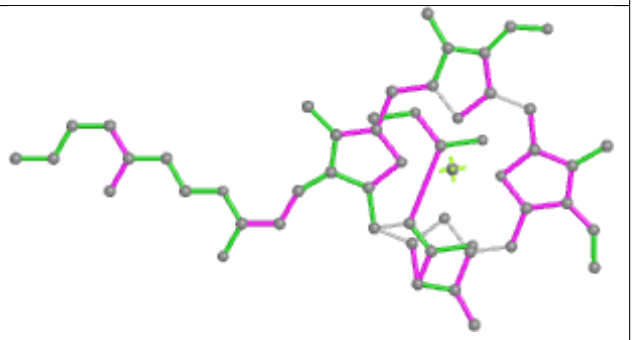


Rings

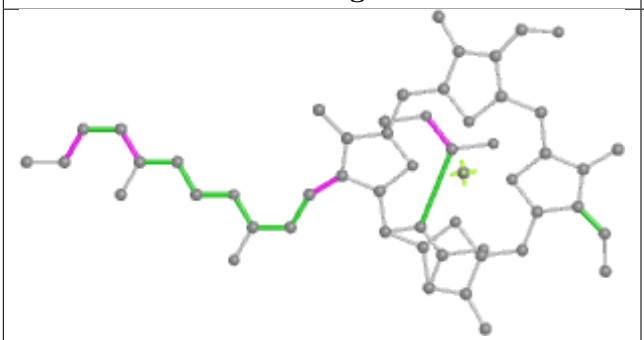
Ligand CL7 8 414



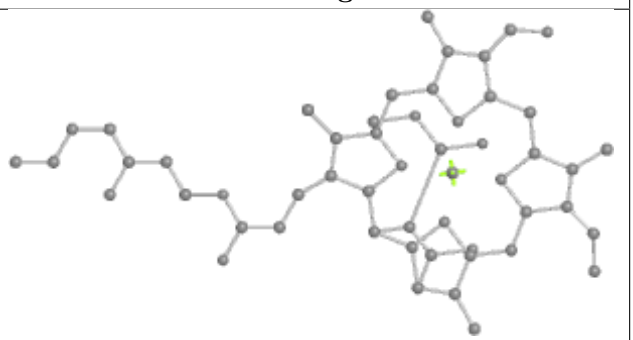
Bond lengths



Bond angles

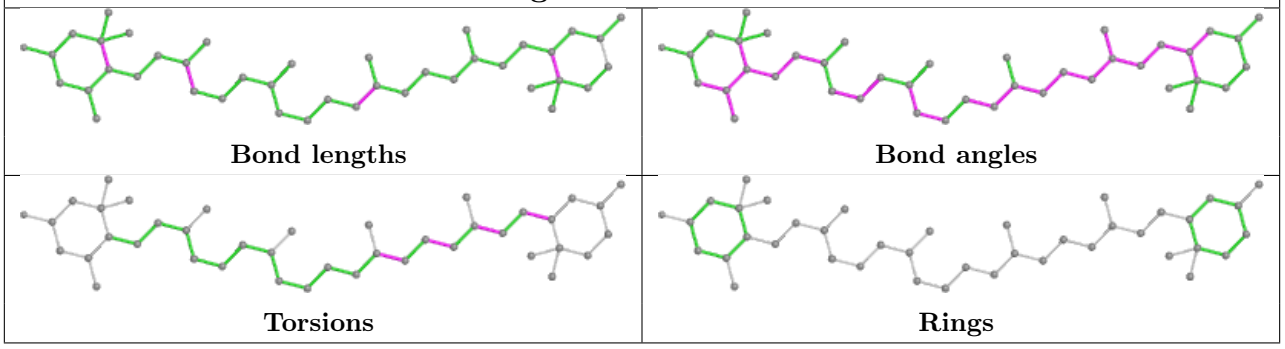


Torsions

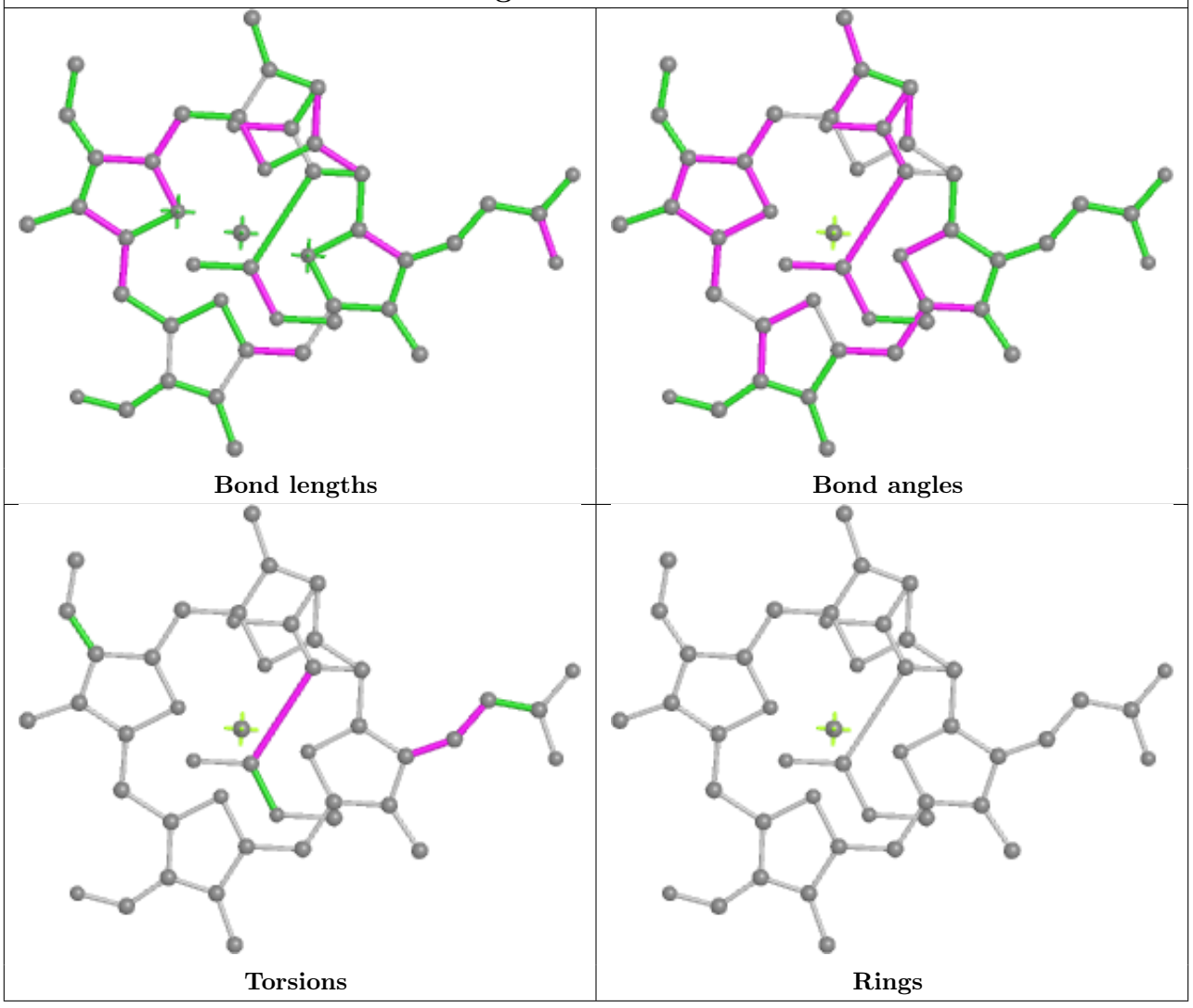


Rings

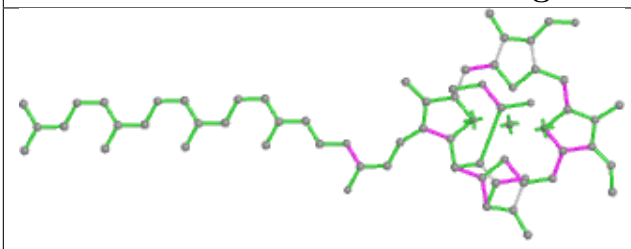
Ligand ZEX 6 522



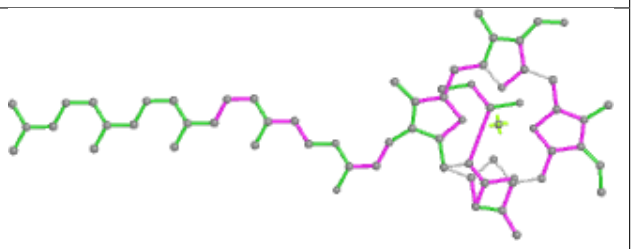
Ligand CL7 6 513



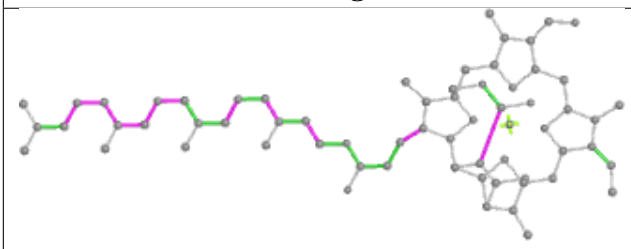
Ligand CL7 1 404



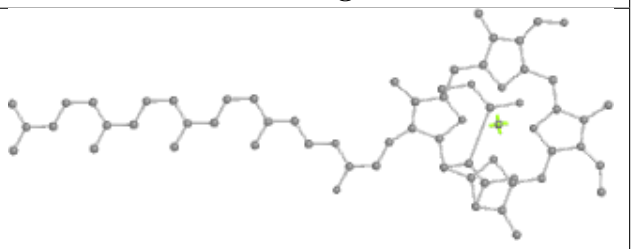
Bond lengths



Bond angles

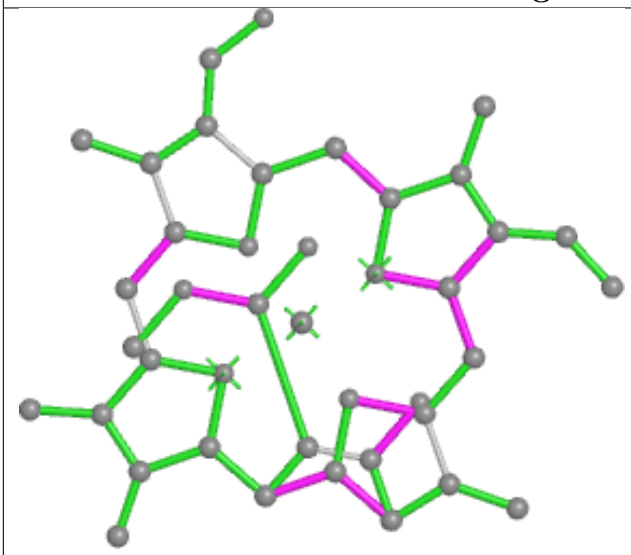


Torsions

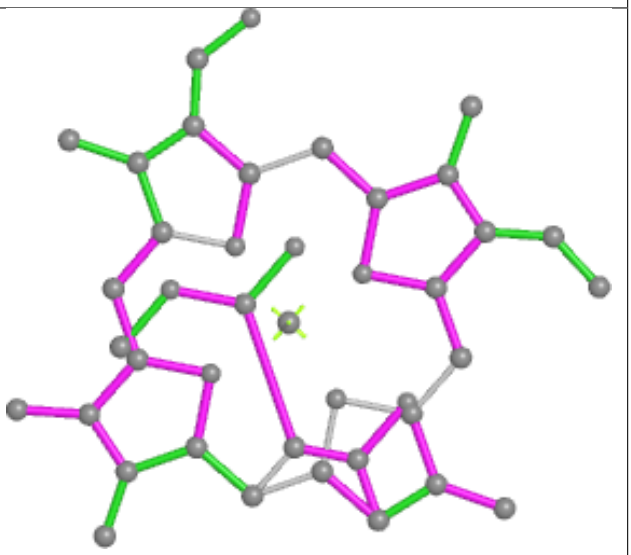


Rings

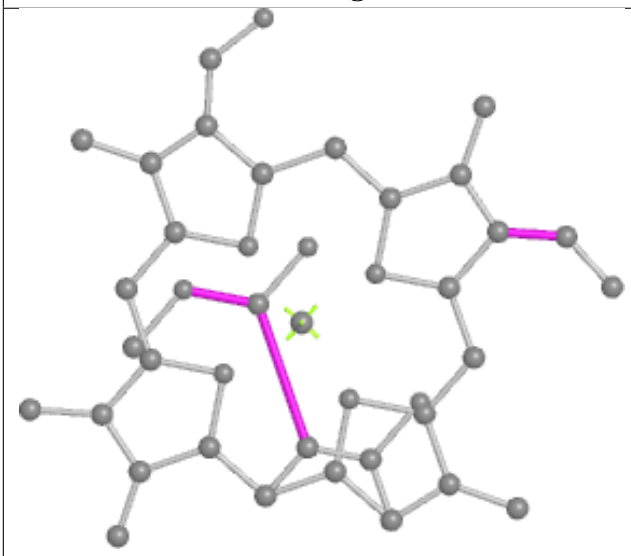
Ligand CL7 4 416



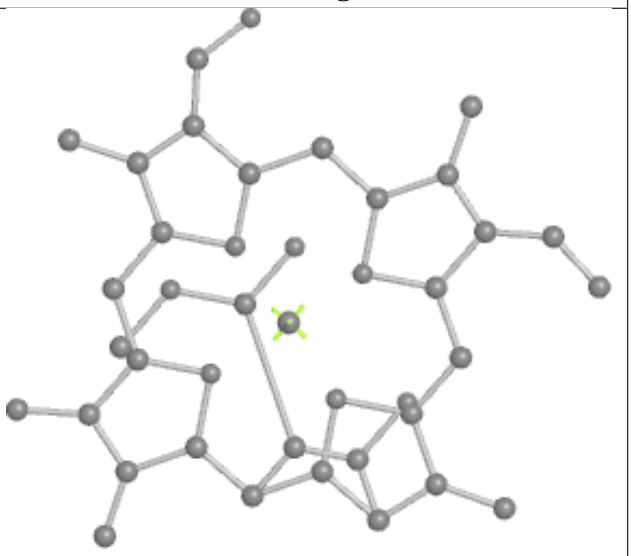
Bond lengths



Bond angles

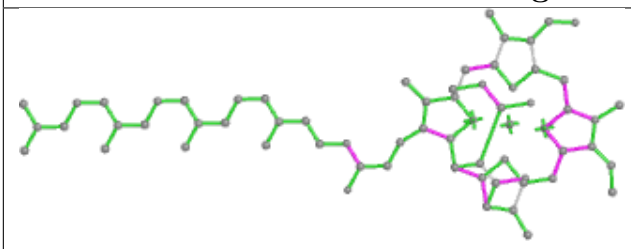


Torsions

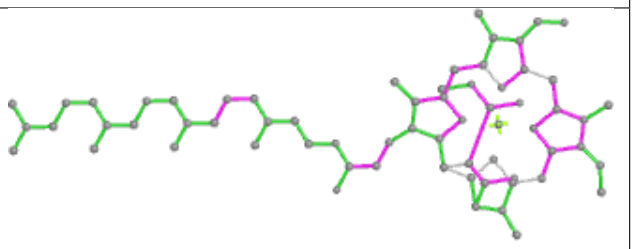


Rings

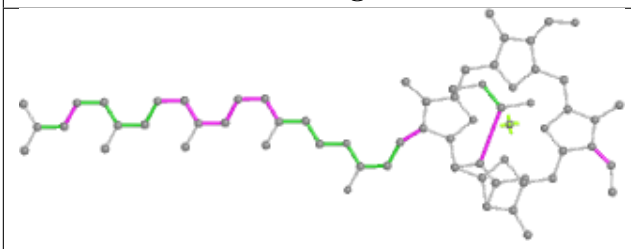
Ligand CL7 b 609



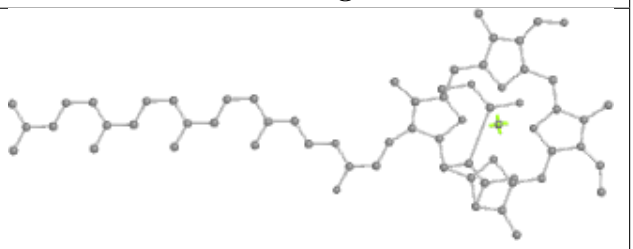
Bond lengths



Bond angles

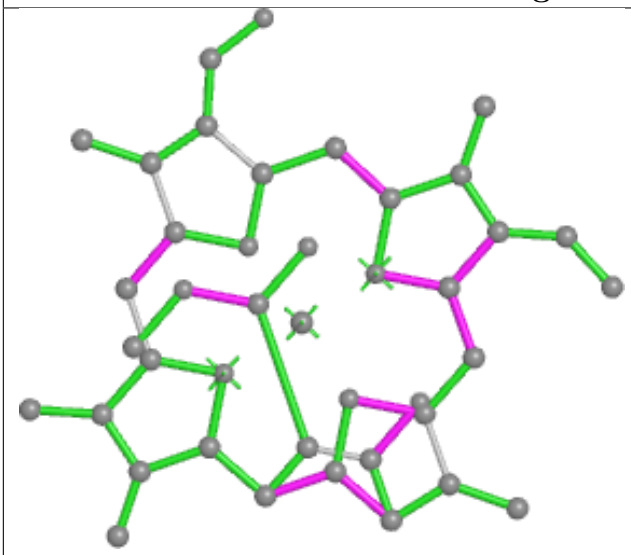


Torsions

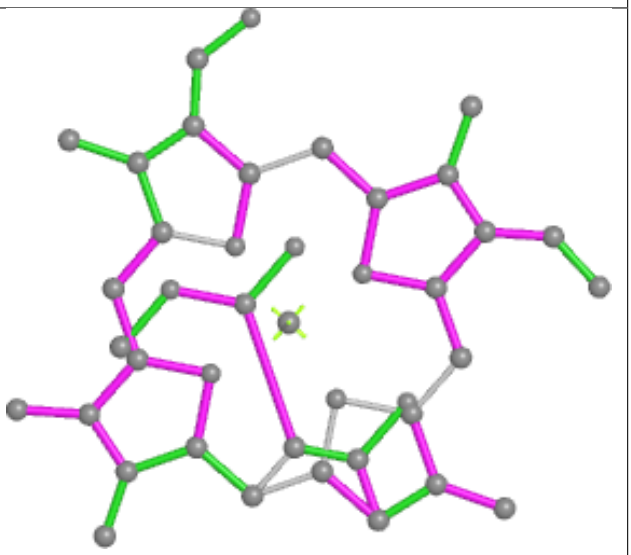


Rings

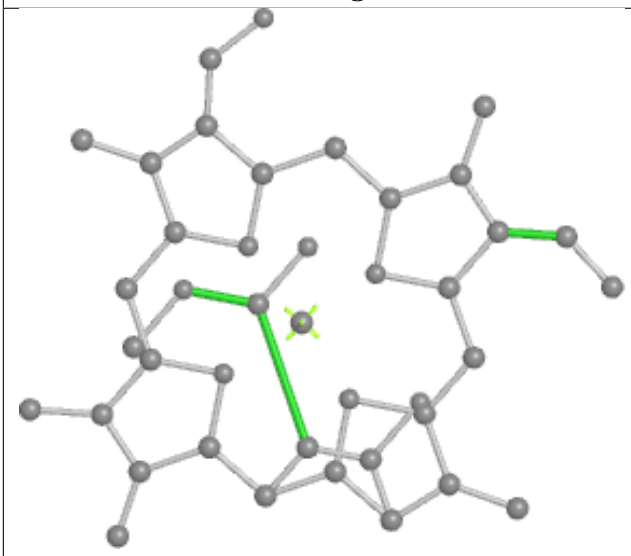
Ligand CL7 3 515



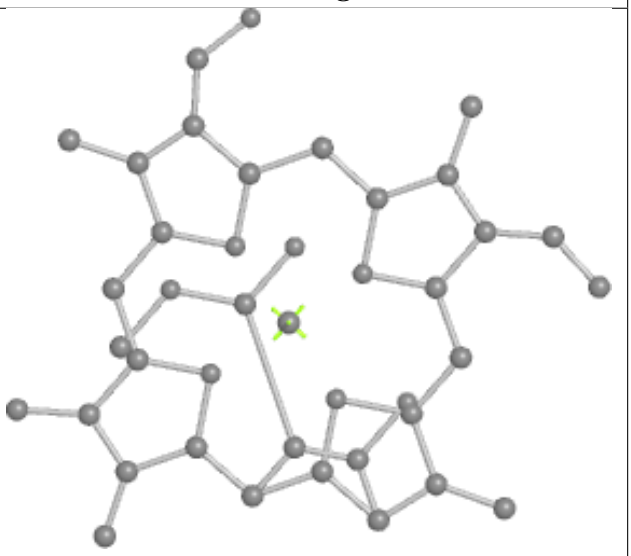
Bond lengths



Bond angles

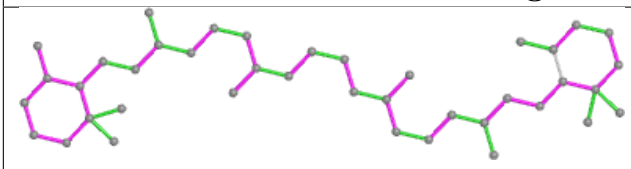


Torsions

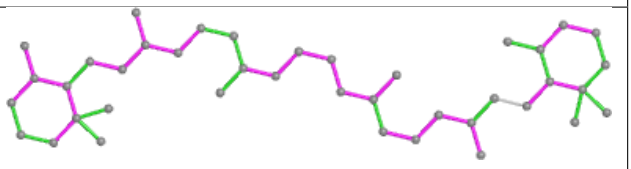


Rings

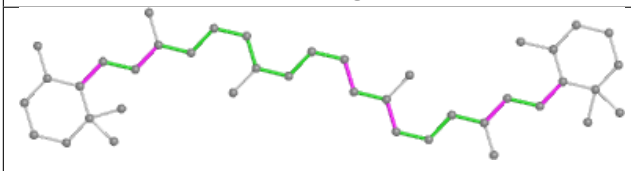
Ligand 8CT K 101



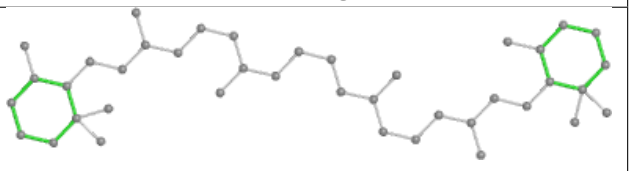
Bond lengths



Bond angles

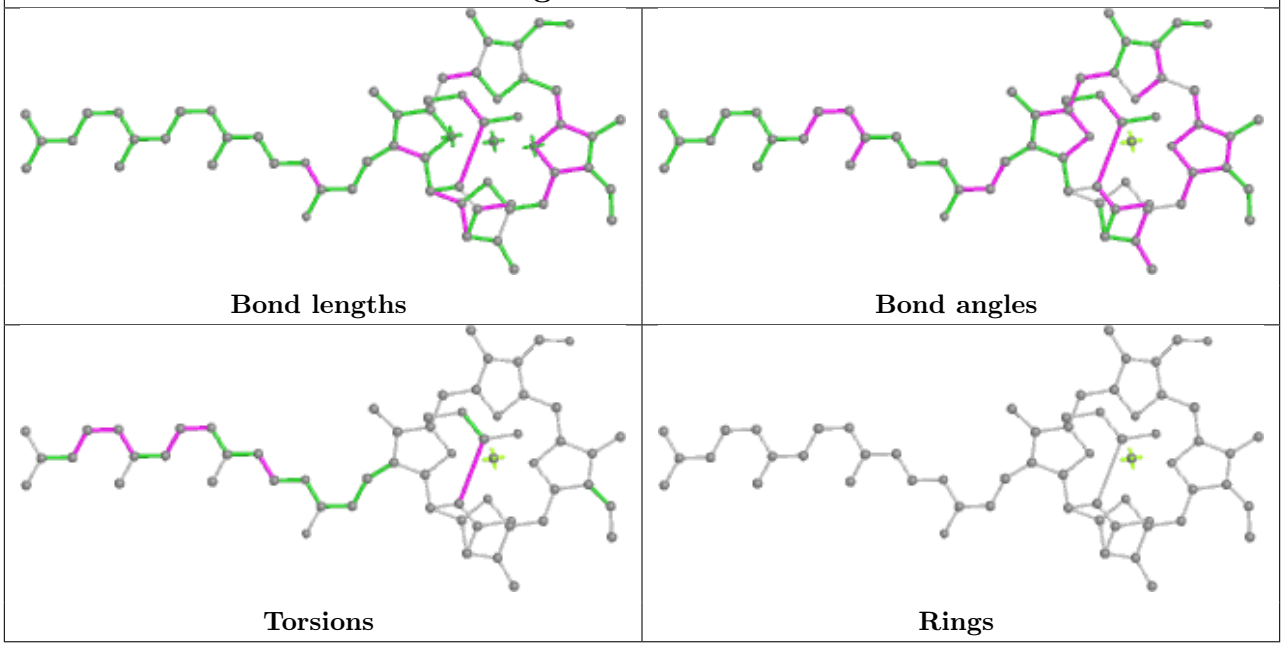


Torsions



Rings

Ligand CL7 8 413



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.

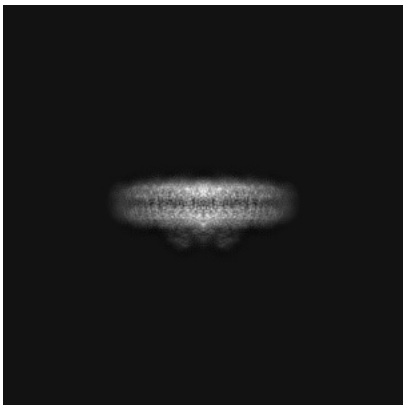
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33929. These allow visual inspection of the internal detail of the map and identification of artifacts.

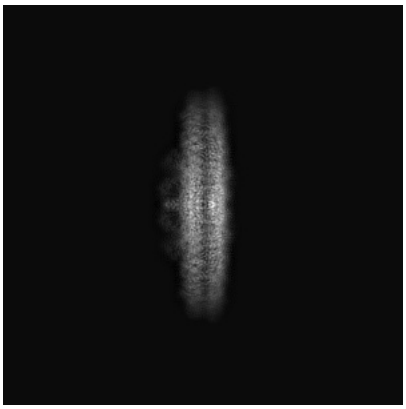
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

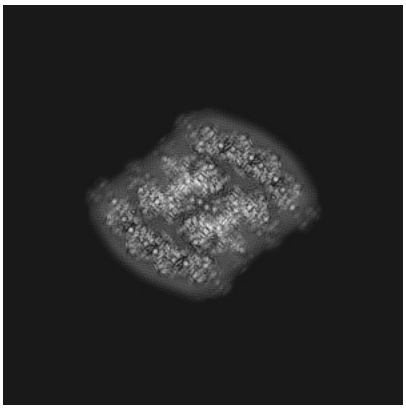
6.1.1 Primary map



X

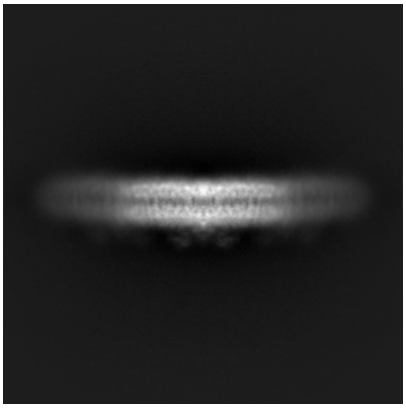


Y

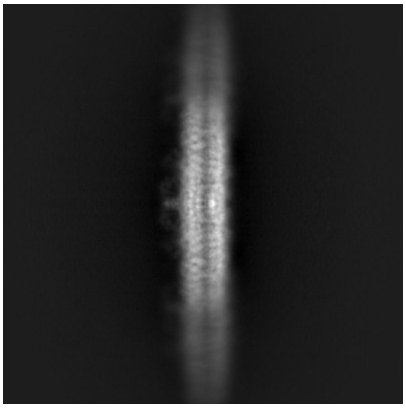


Z

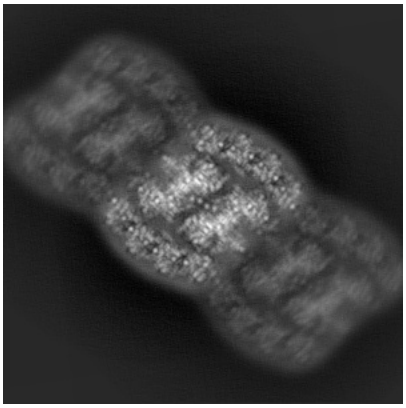
6.1.2 Raw map



X



Y

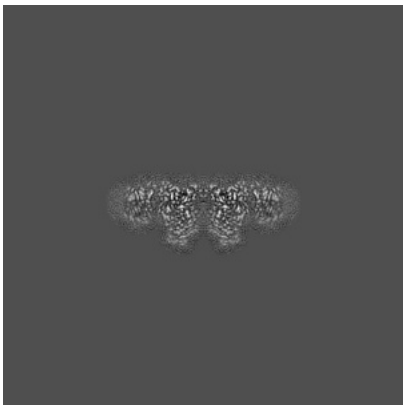


Z

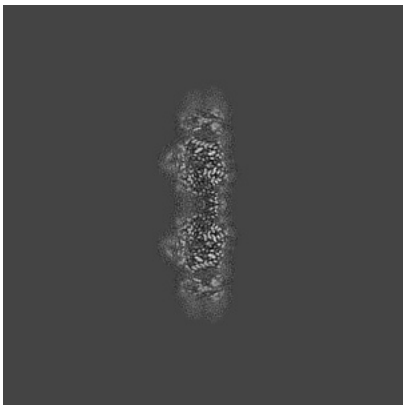
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

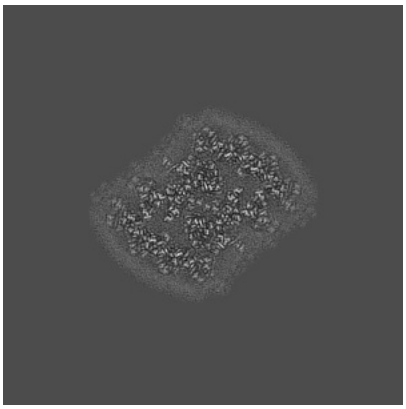
6.2.1 Primary map



X Index: 240

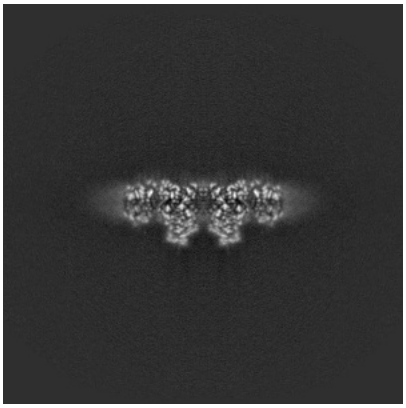


Y Index: 240

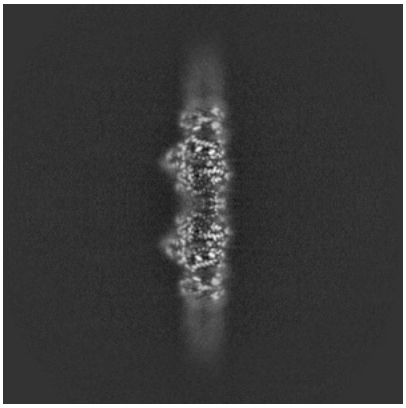


Z Index: 240

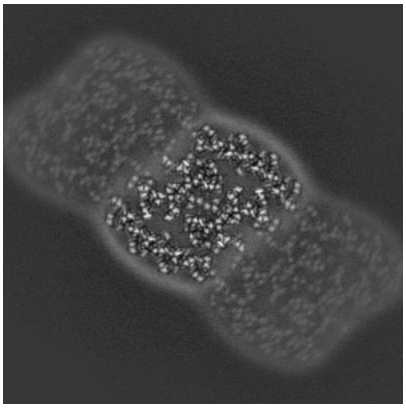
6.2.2 Raw map



X Index: 240



Y Index: 240



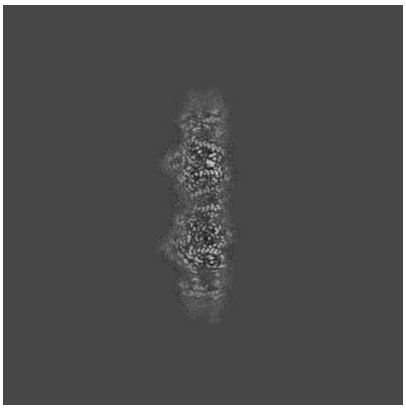
Z Index: 240

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

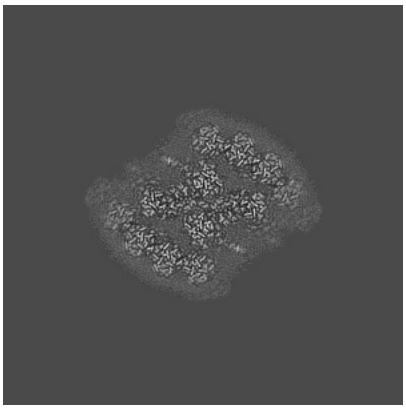
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 237



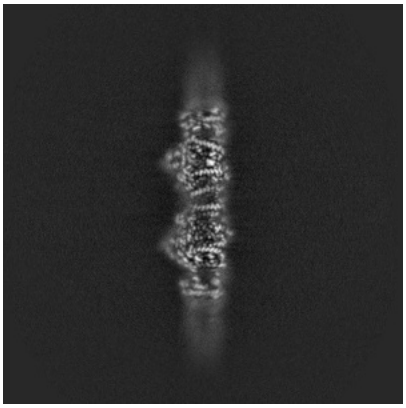
Y Index: 242



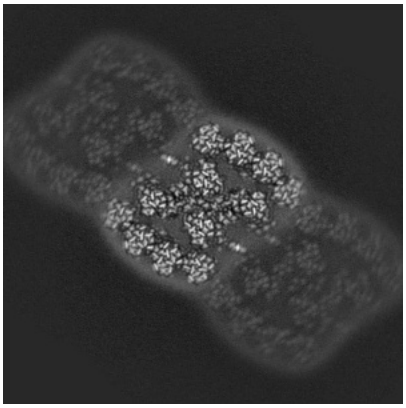
Z Index: 251

6.3.2 Raw map

X Index: 237



Y Index: 242

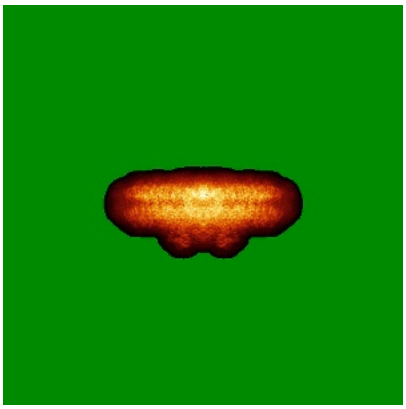


Z Index: 251

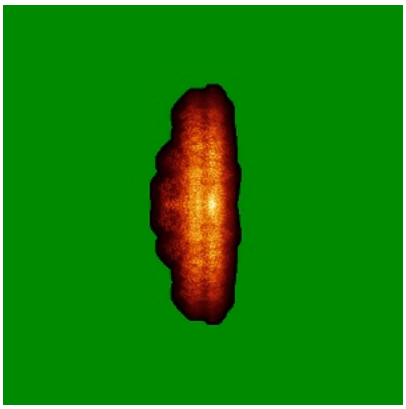
The images above show the largest variance slices of the map in three orthogonal directions.

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

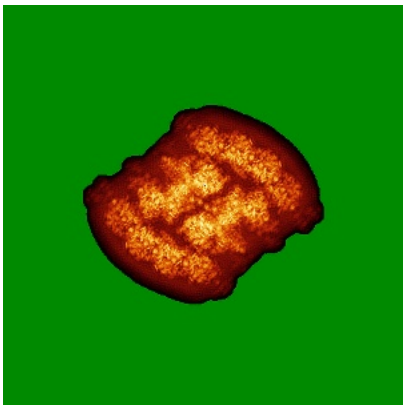
6.4.1 Primary map



X

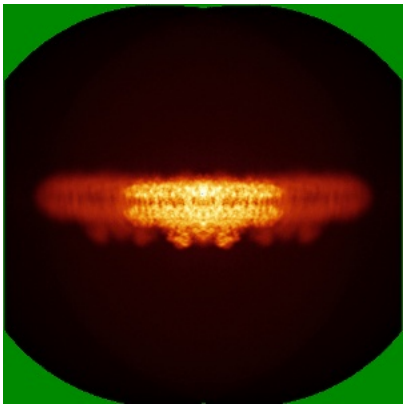


Y

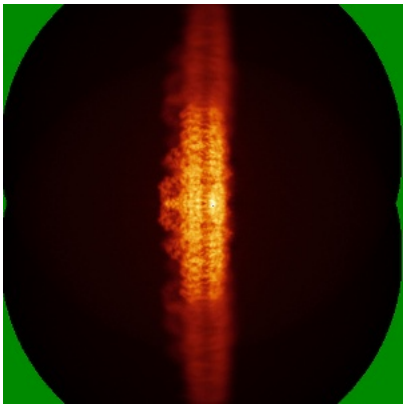


Z

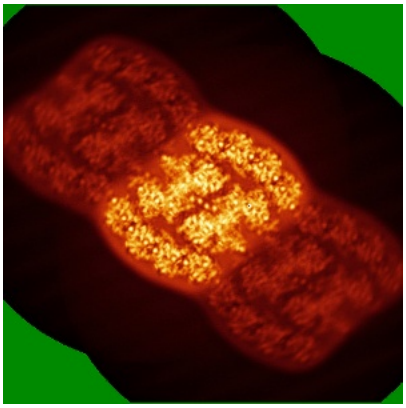
6.4.2 Raw map



X



Y

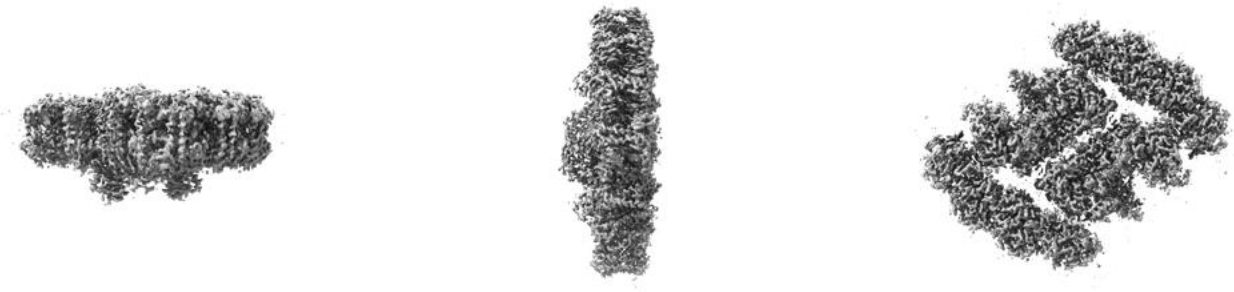


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0188. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

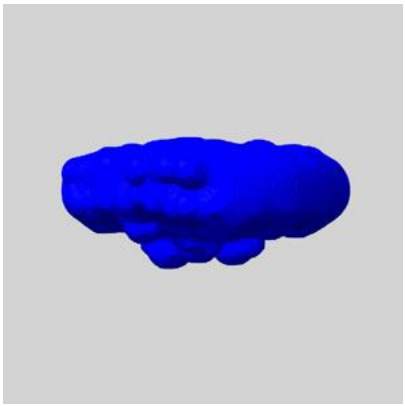
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

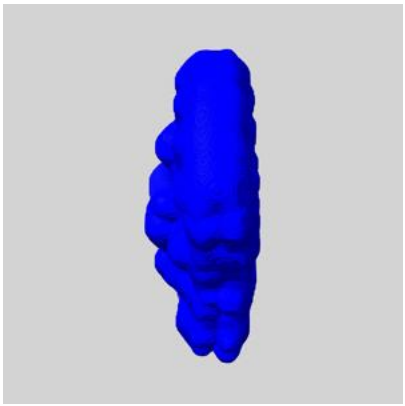
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

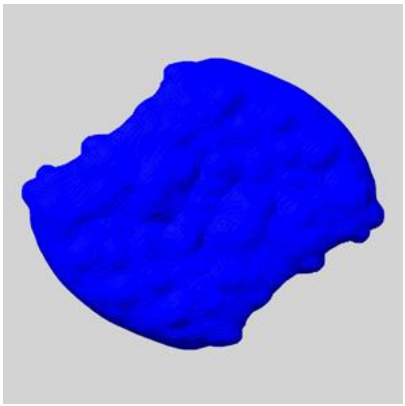
6.6.1 emd_33929_msk_1.map



X



Y

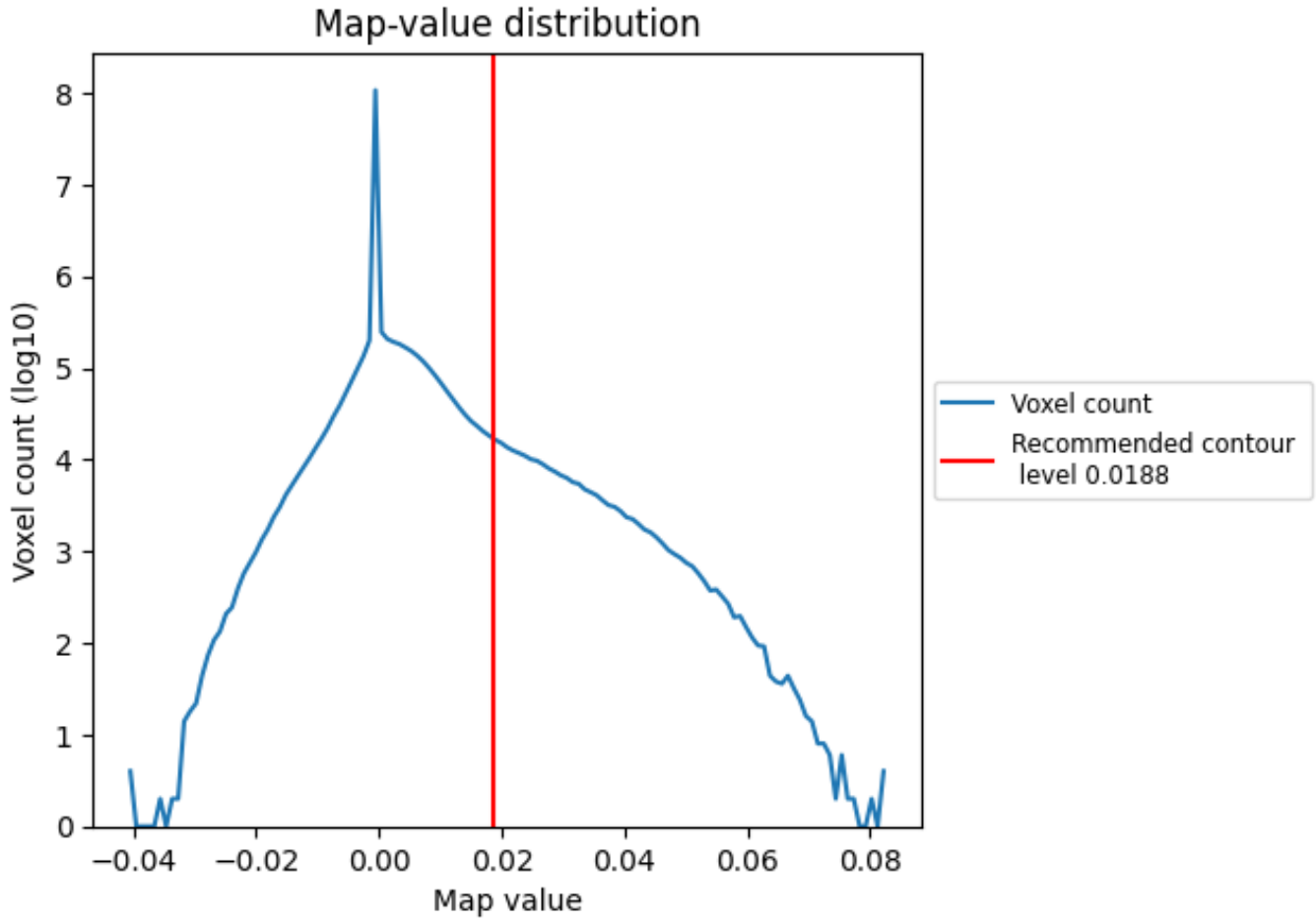


Z

7 Map analysis

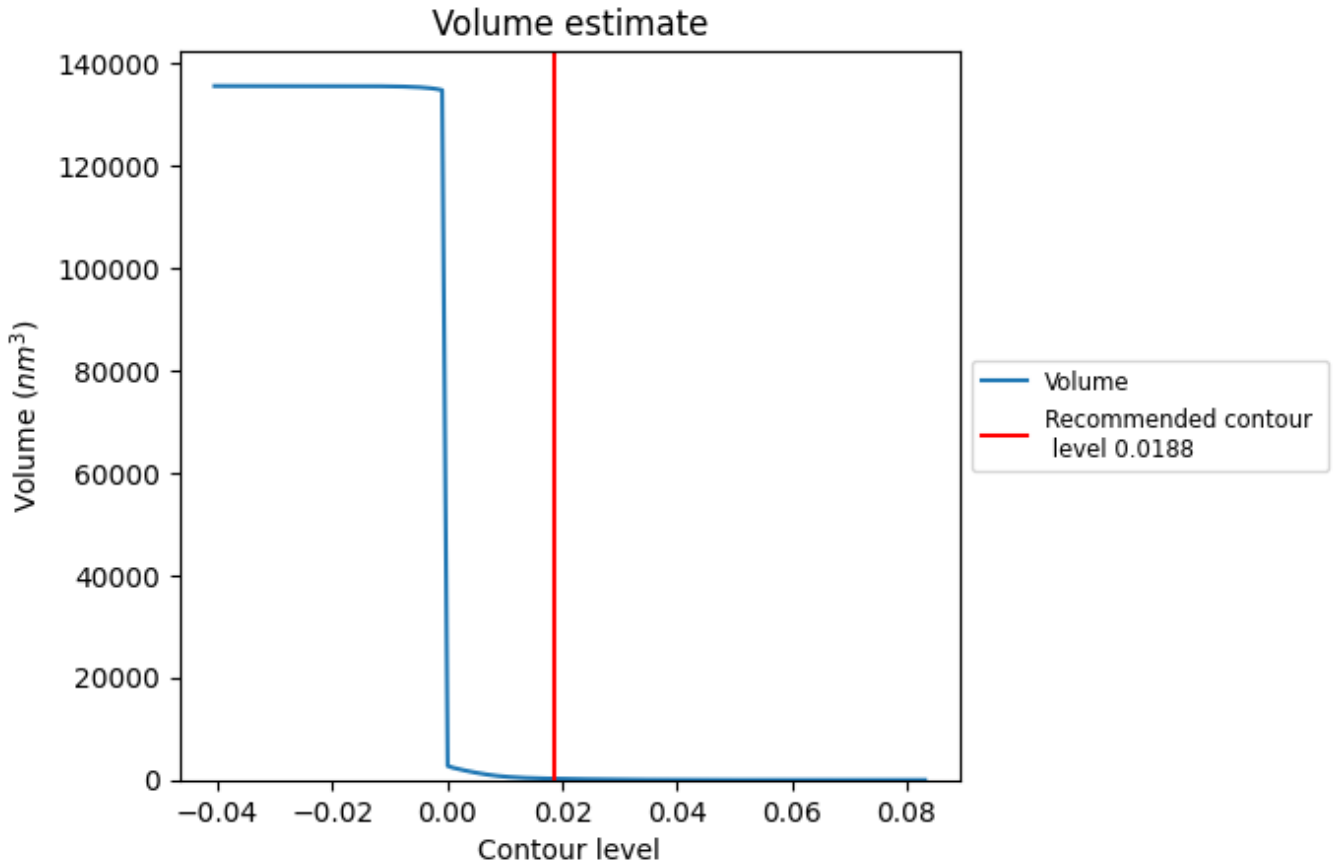
This section contains the results of statistical analysis of the map.

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.

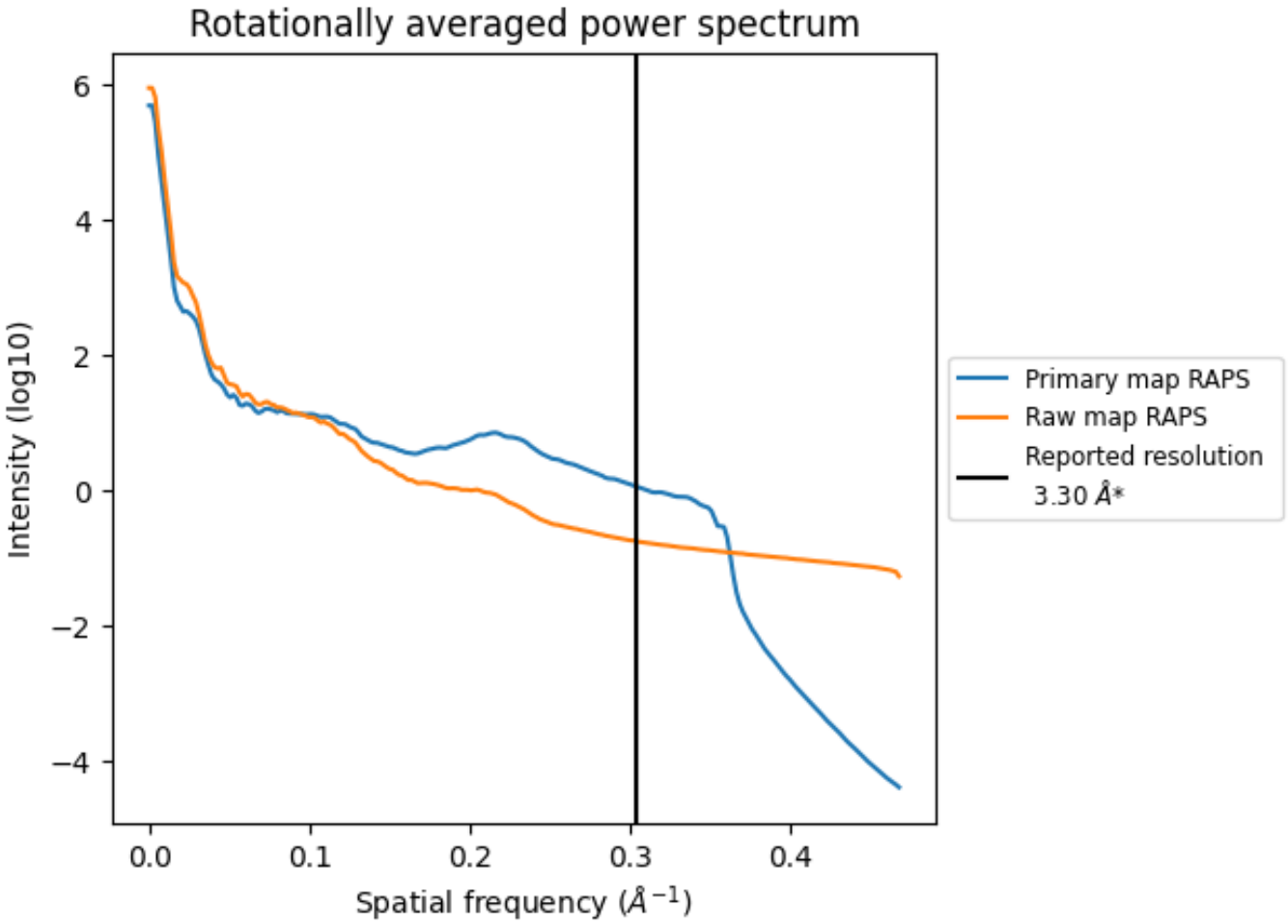
7.2 Volume estimate (i)



The volume at the recommended contour level is 243 nm^3; this corresponds to an approximate mass of 219 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

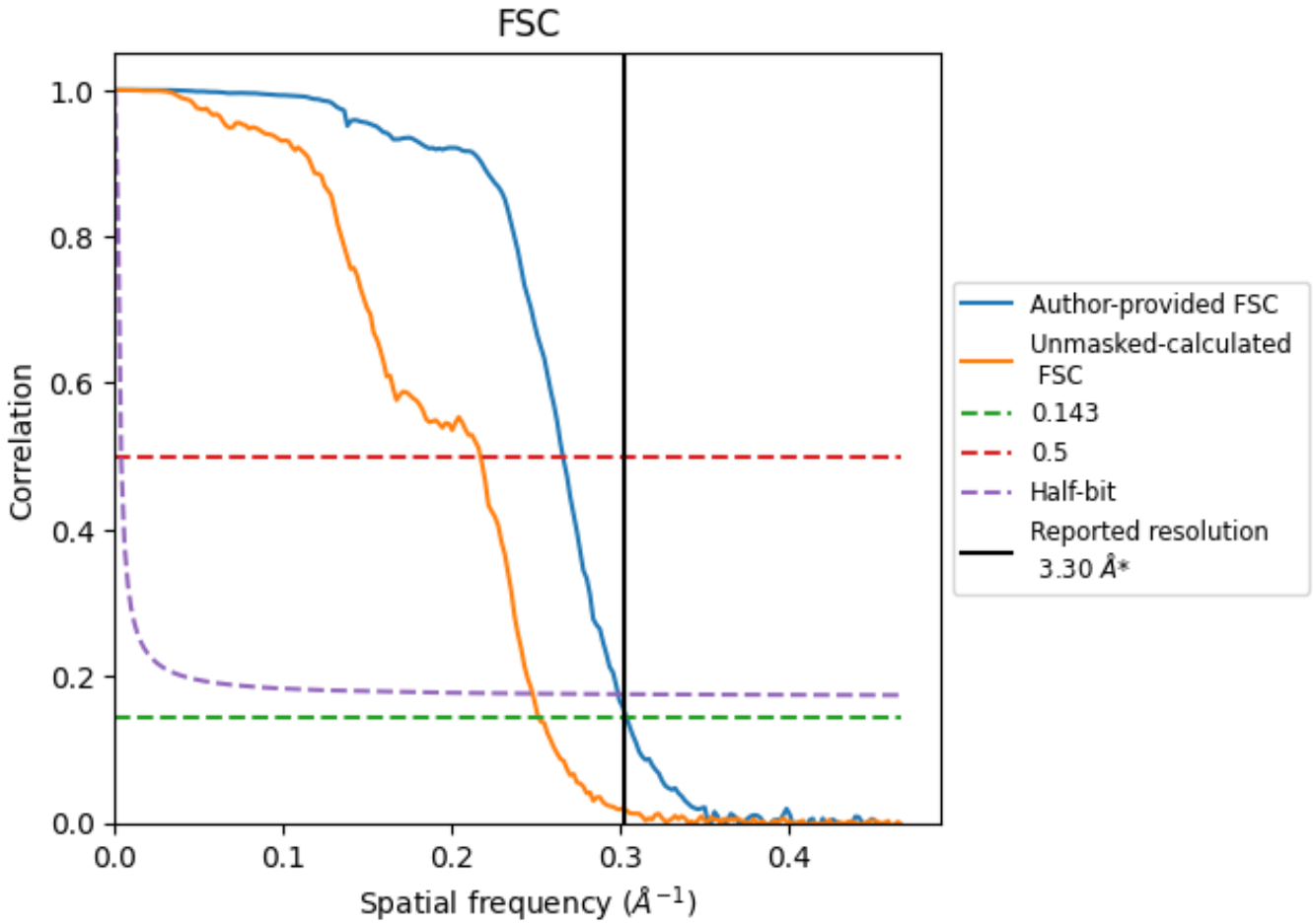


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

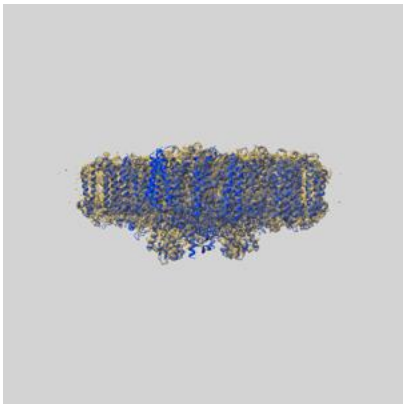
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.76	3.34
Unmasked-calculated*	3.97	4.60	4.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.97 differs from the reported value 3.3 by more than 10 %

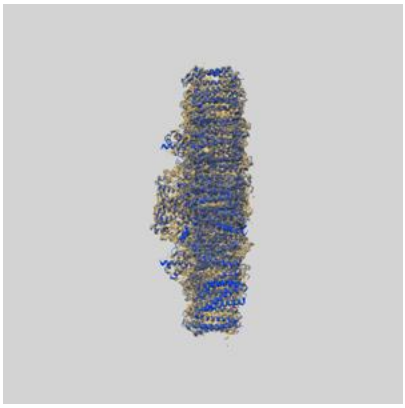
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33929 and PDB model 7YMI. Per-residue inclusion information can be found in section 3 on page 35.

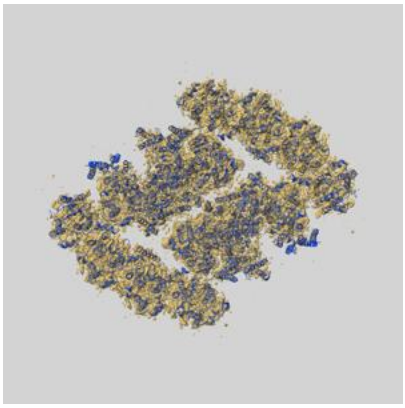
9.1 Map-model overlay



X



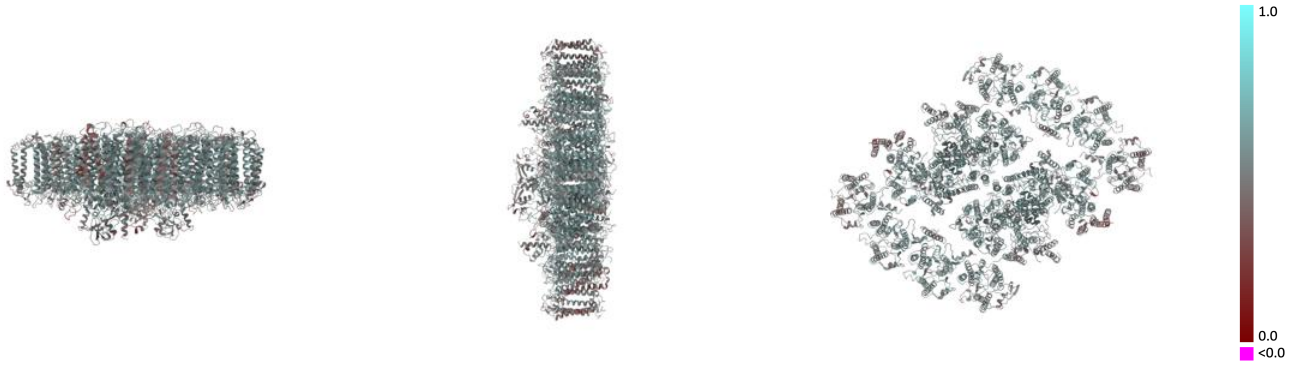
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0188 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.

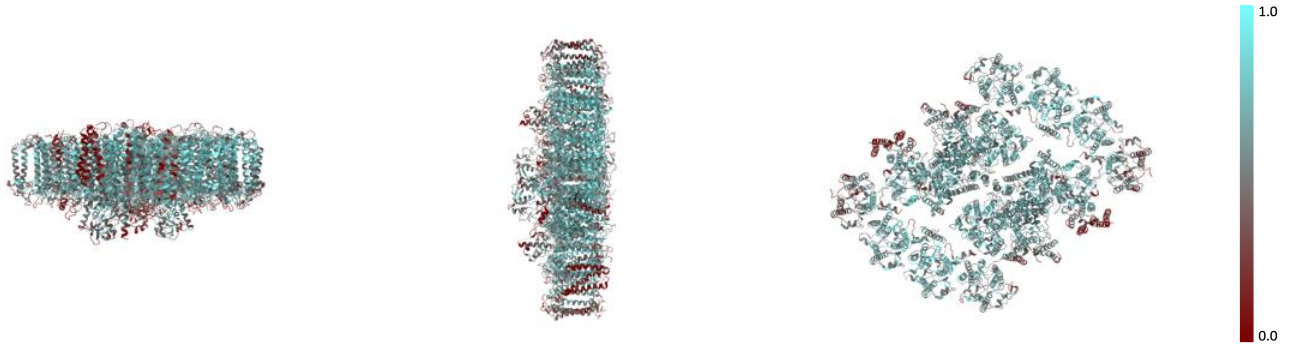
9.2 Q-score mapped to coordinate model



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.

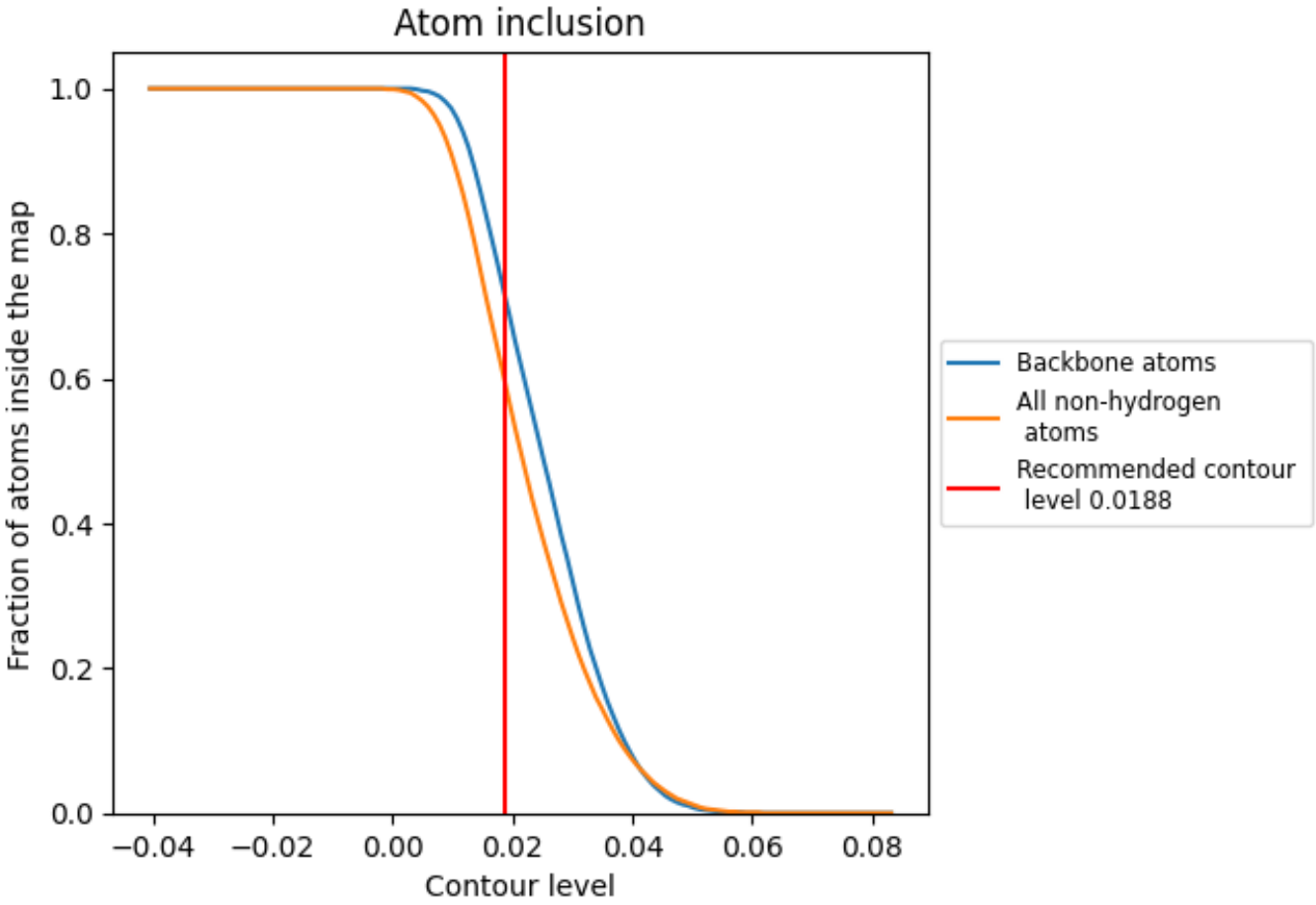
9.3 Atom inclusion mapped to coordinate model



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 (0.0188).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 59% 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 (0.0188) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5910	0.5380
1	0.4760	0.5010
2	0.6300	0.5500
3	0.6430	0.5510
4	0.5670	0.5290
5	0.4770	0.5000
6	0.6280	0.5490
7	0.6410	0.5510
8	0.5670	0.5310
A	0.6660	0.5610
B	0.6550	0.5590
C	0.5910	0.5410
D	0.6720	0.5710
E	0.3170	0.4380
F	0.4820	0.4780
G	0.5660	0.4670
H	0.5860	0.5430
I	0.6350	0.5470
K	0.3050	0.4820
L	0.6320	0.5700
M	0.5240	0.5200
T	0.5130	0.5430
X	0.3360	0.4910
Y	0.0560	0.4000
Z	0.1340	0.3830
a	0.6740	0.5610
b	0.6590	0.5590
c	0.5920	0.5410
d	0.6720	0.5700
e	0.3190	0.4380
f	0.4820	0.4720
g	0.5660	0.4590
h	0.5880	0.5420
i	0.6350	0.5490
k	0.3050	0.4810

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
l	0.6280	0.5630
m	0.5240	0.5180
t	0.5130	0.5400
x	0.3360	0.4860
y	0.0560	0.3990
z	0.1340	0.3810