wwPDB EM Validation Summary Report

Nov 22, 2022 – 01:04 AM JST

PDB ID	:	7DWQ
EMDB ID	:	EMD-30882
Title	:	Photosystem I from a chlorophyll d-containing cyanobacterium Acaryochloris marina
Authors	:	Chen, J.H.; Zhang, X.; Shen, J.R.
Deposited on	:	2021-01-17
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:

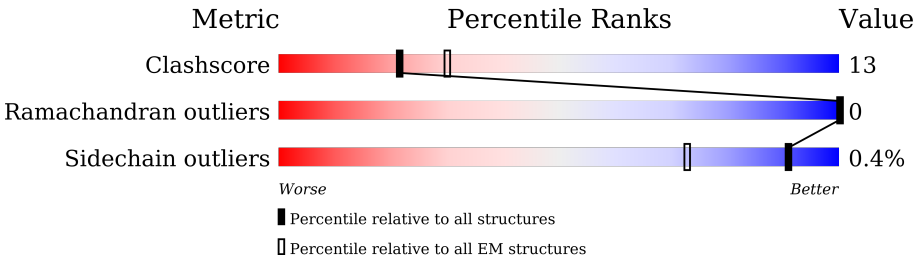
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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)
Clashscore	158937	4297
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	D	139	55% 12% 32%
2	A	753	71% 25% .
3	B	736	66% 24% 10%
4	C	81	77% 22% .
5	E	89	53% 12% 35%
6	F	167	44% 17% . 38%
7	J	51	25% 16% 59%
8	L	153	78% 16% 6%

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Mol	Chain	Length	Quality of chain
9	M	31	
10	W	34	

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
11	CL7	A	1022	X	-	-	-
11	CL7	A	1101	X	-	-	-
11	CL7	A	1102	X	-	-	-
11	CL7	A	1103	X	-	-	-
11	CL7	A	1104	X	-	-	-
11	CL7	A	1105	X	-	-	-
11	CL7	A	1106	X	-	-	-
11	CL7	A	1107	X	-	-	-
11	CL7	A	1109	X	-	-	-
11	CL7	A	1110	X	-	-	-
11	CL7	A	1111	X	-	-	-
11	CL7	A	1112	X	-	-	-
11	CL7	A	1113	X	-	-	-
11	CL7	A	1114	X	-	-	-
11	CL7	A	1115	X	-	-	-
11	CL7	A	1116	X	-	-	-
11	CL7	A	1117	X	-	-	-
11	CL7	A	1118	X	-	-	-
11	CL7	A	1119	X	-	-	-
11	CL7	A	1120	X	-	-	-
11	CL7	A	1121	X	-	-	-
11	CL7	A	1122	X	-	-	-
11	CL7	A	1123	X	-	-	-
11	CL7	A	1124	X	-	-	-
11	CL7	A	1125	X	-	-	-
11	CL7	A	1126	X	-	-	-
11	CL7	A	1127	X	-	-	-
11	CL7	A	1128	X	-	-	-
11	CL7	A	1129	X	-	-	-
11	CL7	A	1130	X	-	-	-
11	CL7	A	1131	X	-	-	-
11	CL7	A	1132	X	-	-	-
11	CL7	A	1135	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CL7	A	1136	X	-	-	-
11	CL7	A	1137	X	-	-	-
11	CL7	A	1138	X	-	-	-
11	CL7	A	1139	X	-	-	-
11	CL7	A	1140	X	-	-	-
11	CL7	A	1237	X	-	-	-
11	CL7	A	1801	X	-	-	-
11	CL7	A	1802	X	-	-	-
11	CL7	B	1012	X	-	-	-
11	CL7	B	1021	X	-	-	-
11	CL7	B	1201	X	-	-	-
11	CL7	B	1202	X	-	-	-
11	CL7	B	1203	X	-	-	-
11	CL7	B	1204	X	-	-	-
11	CL7	B	1205	X	-	-	-
11	CL7	B	1206	X	-	-	-
11	CL7	B	1207	X	-	-	-
11	CL7	B	1208	X	-	-	-
11	CL7	B	1210	X	-	-	-
11	CL7	B	1211	X	-	-	-
11	CL7	B	1212	X	-	-	-
11	CL7	B	1213	X	-	-	-
11	CL7	B	1214	X	-	-	-
11	CL7	B	1215	X	-	-	-
11	CL7	B	1222	X	-	-	-
11	CL7	B	1223	X	-	-	-
11	CL7	B	1224	X	-	-	-
11	CL7	B	1225	X	-	-	-
11	CL7	B	1226	X	-	-	-
11	CL7	B	1228	X	-	-	-
11	CL7	B	1229	X	-	-	-
11	CL7	B	1230	X	-	-	-
11	CL7	B	1234	X	-	-	-
11	CL7	B	1235	X	-	-	-
11	CL7	B	1236	X	-	-	-
11	CL7	B	1238	X	-	-	-
11	CL7	B	1239	X	-	-	-
11	CL7	F	1301	X	-	-	-
11	CL7	J	1302	X	-	-	-
11	CL7	L	1501	X	-	-	-
11	CL7	L	1502	X	-	-	-
11	CL7	L	1503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CL7	W	2601	X	-	-	-
14	LHG	A	5001	-	X	-	-
14	LHG	A	5003	-	X	-	-
15	G9R	A	1011	X	-	-	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 19961 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 I protein PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	94	725	459	123	139	4	0	0

- Molecule 2 is a protein called Photosystem I P740 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	726	5715	3734	977	975	29	0	0

- Molecule 3 is a protein called Photosystem I P740 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	659	5252	3458	878	896	20	0	0

- Molecule 4 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	80	599	367	103	118	11	0	0

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	58	452	283	83	85	1	0	0

- Molecule 6 is a protein called Photosystem I protein PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	103	775	484	143	143	5	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	21	Total	C	N	O	0	0
			162	111	25	26		

- Molecule 8 is a protein called Photosystem I protein PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	144	Total	C	N	O	S	0	0
			1008	643	169	192	4		

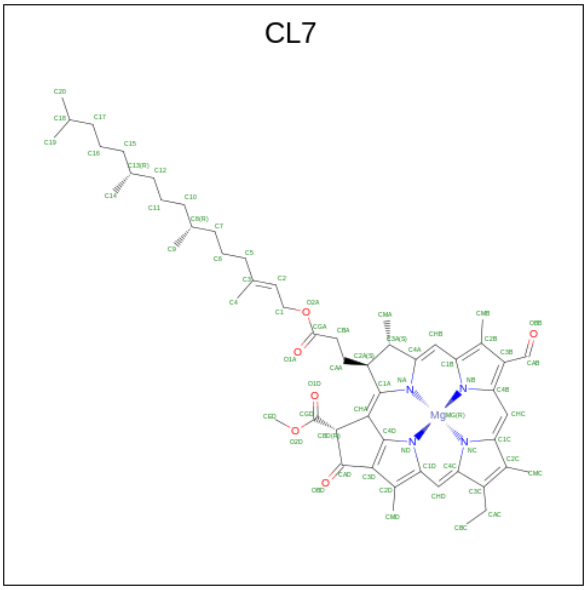
- Molecule 9 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	30	Total	C	N	O	S	0	0
			213	141	32	39	1		

- Molecule 10 is a protein called Photosystem I protein Psa27.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	28	Total	C	N	O	S	0	0
			208	142	28	36	2		

- Molecule 11 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
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0

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Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	A	1	Total 2145	C 1694	Mg 41	N 164	O 246	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0

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Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0
11	B	1	Total 1445	C 1126	Mg 29	N 116	O 174	0

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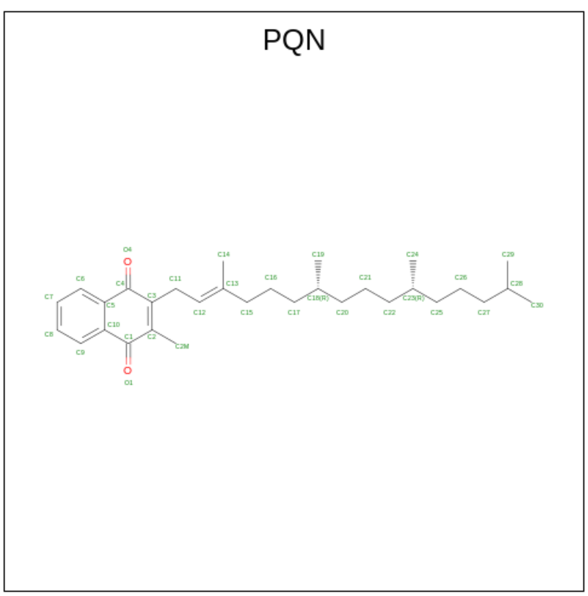
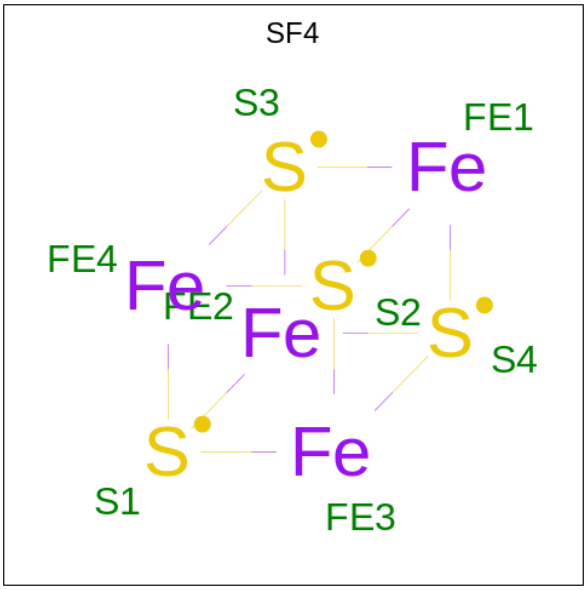
Mol	Chain	Residues	Atoms	AltConf
11	B	1	Total C Mg N O 1445 1126 29 116 174	0
11	B	1	Total C Mg N O 1445 1126 29 116 174	0
11	B	1	Total C Mg N O 1445 1126 29 116 174	0
11	B	1	Total C Mg N O 1445 1126 29 116 174	0
11	B	1	Total C Mg N O 1445 1126 29 116 174	0
11	B	1	Total C Mg N O 1445 1126 29 116 174	0
11	F	1	Total C Mg N O 45 34 1 4 6	0
11	J	1	Total C Mg N O 45 34 1 4 6	0
11	L	1	Total C Mg N O 175 142 3 12 18	0
11	L	1	Total C Mg N O 175 142 3 12 18	0
11	L	1	Total C Mg N O 175 142 3 12 18	0
11	W	1	Total C Mg N O 45 34 1 4 6	0

- Molecule 12 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



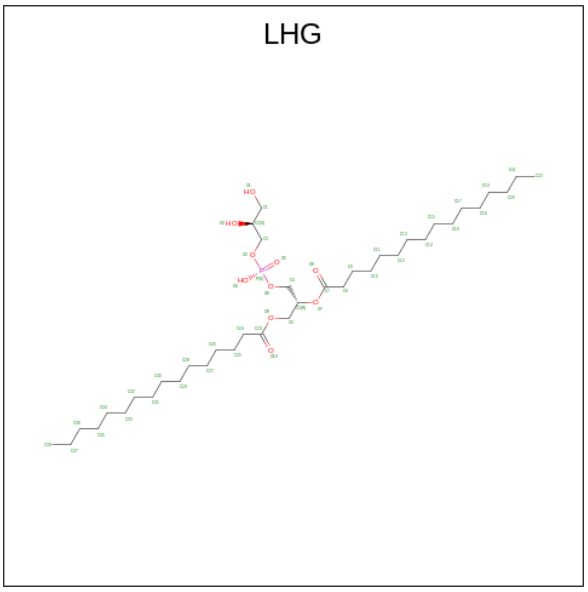
Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total C O 33 31 2	0
12	B	1	Total C O 33 31 2	0

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



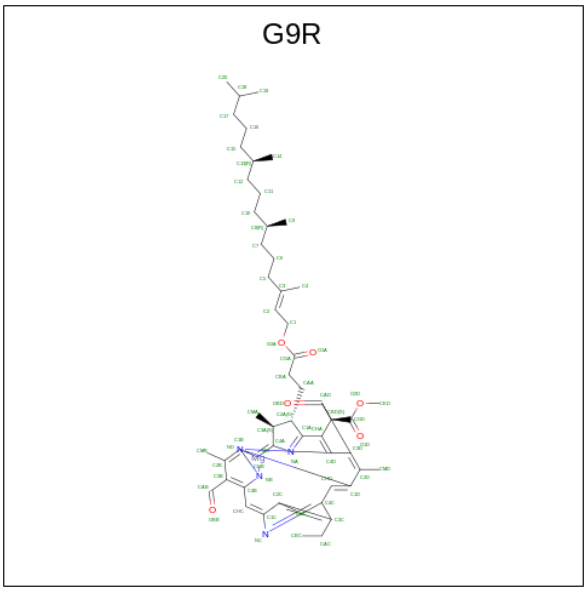
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total Fe S 8 4 4	0
13	C	1	Total Fe S 16 8 8	0
13	C	1	Total Fe S 16 8 8	0

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



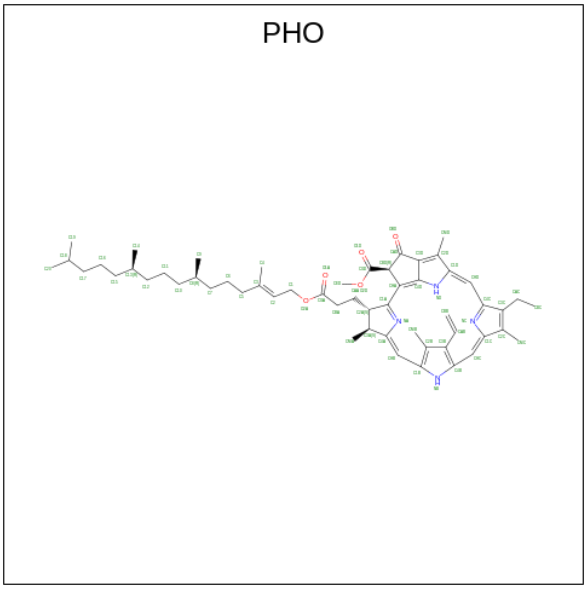
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O	P	0
			98	76	20	2	
14	A	1	Total	C	O	P	0
			98	76	20	2	

- Molecule 15 is CHLOROPHYLL D ISOMER (three-letter code: G9R) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



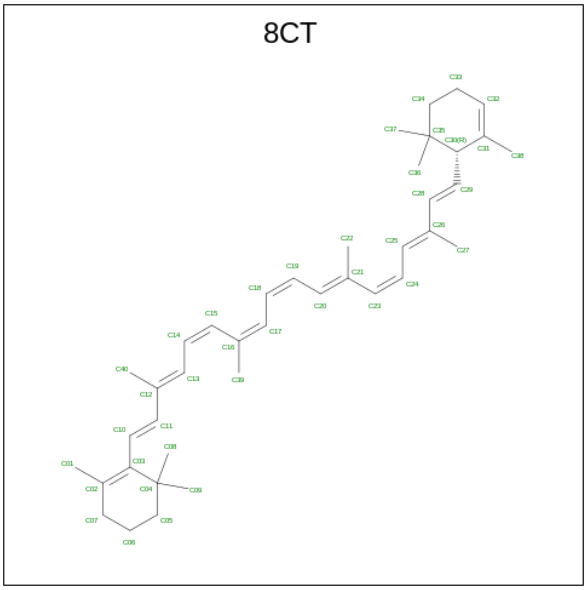
Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 16 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



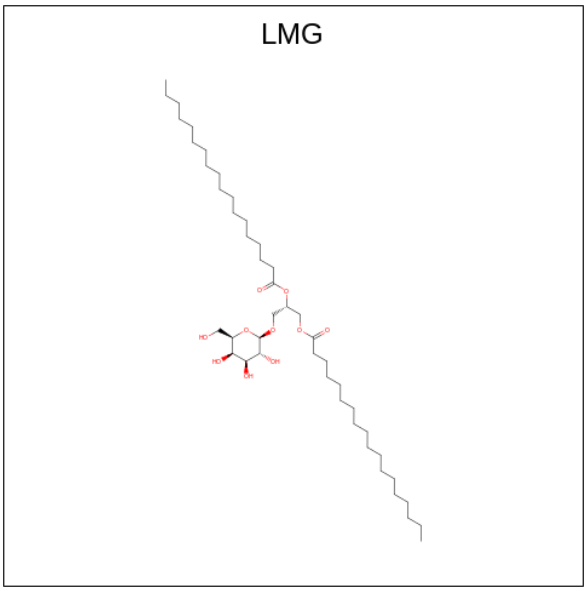
Mol	Chain	Residues	Atoms				AltConf
16	A	1	Total	C	N	O	0
			64	55	4	5	
16	B	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 17 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
17	A	1	Total C 120 120	0
17	A	1	Total C 120 120	0
17	A	1	Total C 120 120	0
17	B	1	Total C 120 120	0
17	B	1	Total C 120 120	0
17	B	1	Total C 120 120	0
17	J	1	Total C 80 80	0
17	J	1	Total C 80 80	0
17	L	1	Total C 80 80	0
17	L	1	Total C 80 80	0
17	M	1	Total C 40 40	0
17	W	1	Total C 80 80	0
17	W	1	Total C 80 80	0

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



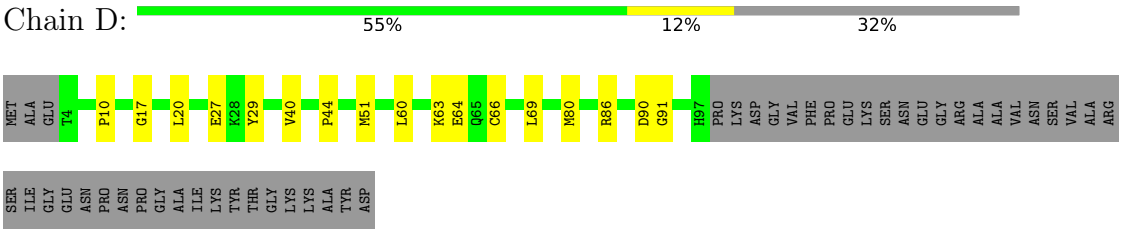
Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	C	O	0
			51	41	10	

3 Residue-property plots (i)

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

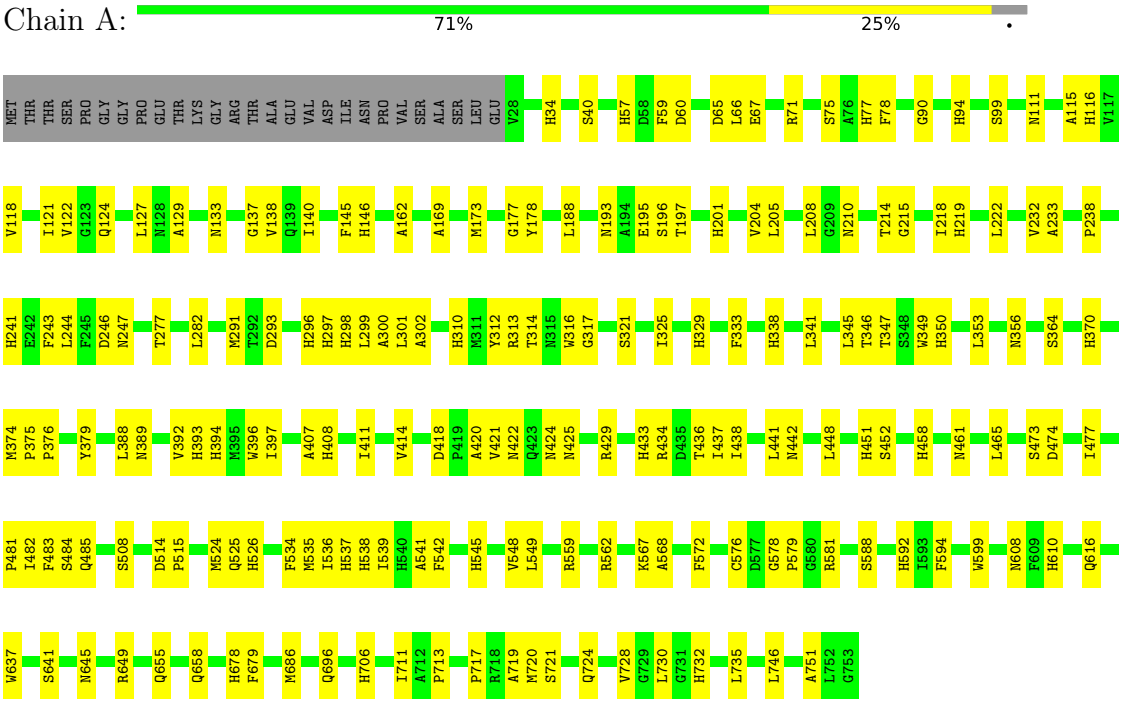
• Molecule 1: Photosystem I protein PsaD

Chain D:



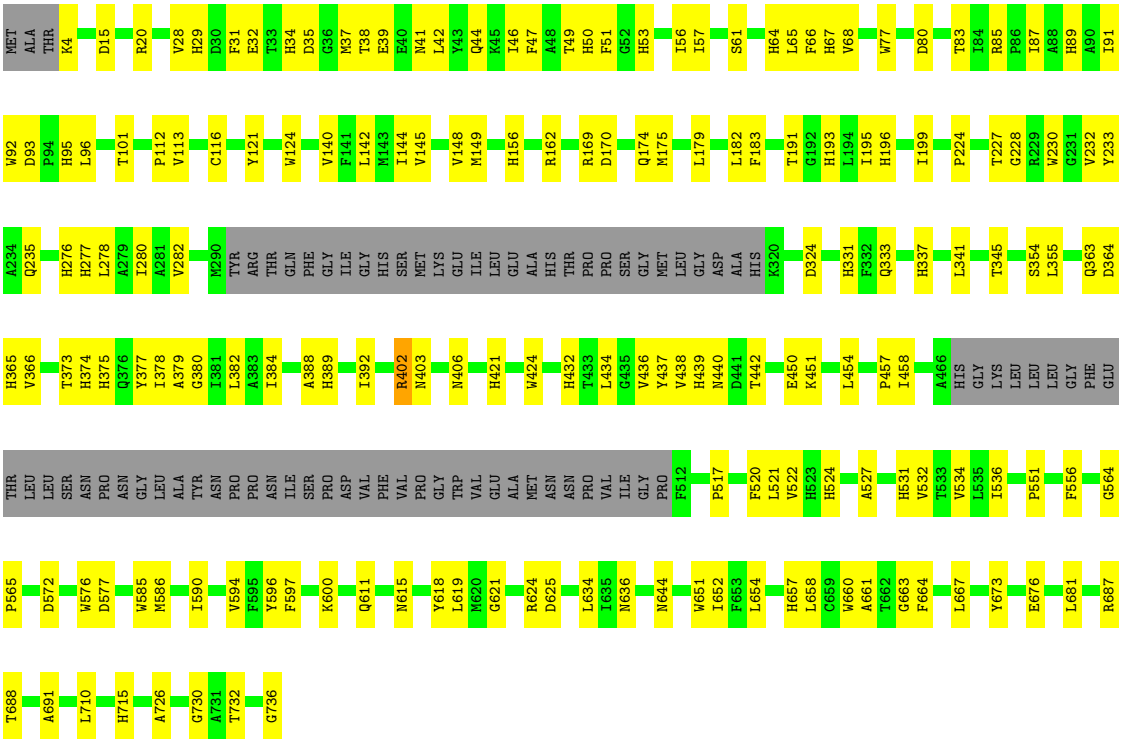
• Molecule 2: Photosystem I P740 chlorophyll a apoprotein A1

Chain A:



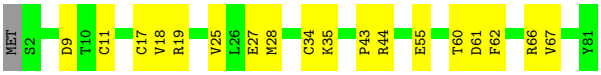
• Molecule 3: Photosystem I P740 chlorophyll a apoprotein A2

Chain B:



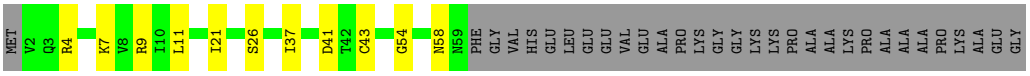
• Molecule 4: Photosystem I iron-sulfur center

Chain C:



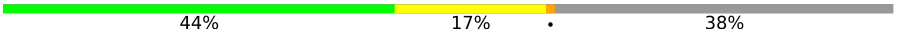
• Molecule 5: Photosystem I reaction center subunit IV

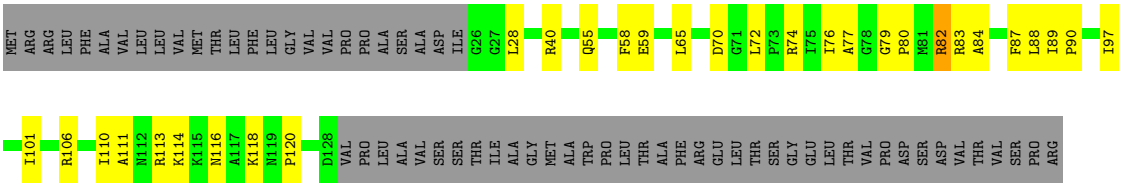
Chain E:



• Molecule 6: Photosystem I protein PsaF

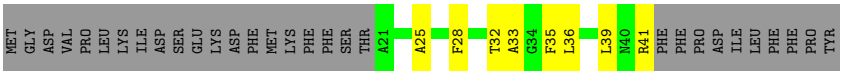
Chain F:





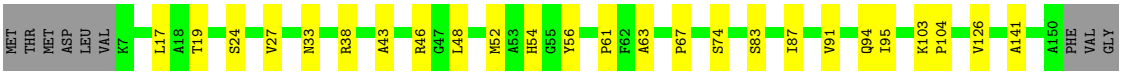
• Molecule 7: Photosystem I reaction center subunit IX

Chain J:



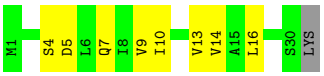
• Molecule 8: Photosystem I protein PsaL

Chain L:



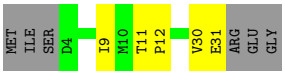
• Molecule 9: Photosystem I reaction center subunit XII

Chain M:



• Molecule 10: Photosystem I protein Psa27

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	240880	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	38244	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.061	Depositor
Minimum map value	-1.735	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.171	Depositor
Map size (Å)	522.8, 522.8, 522.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3069999, 1.3069999, 1.3069999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PHO, LHG, CL7, 8CT, LMG, PQN, SF4, G9R

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	D	0.25	0/737	0.50	0/995
2	A	0.26	0/5909	0.45	0/8049
3	B	0.26	0/5446	0.44	0/7439
4	C	0.25	0/609	0.54	0/825
5	E	0.27	0/460	0.56	0/623
6	F	0.28	0/790	0.56	0/1061
7	J	0.26	0/165	0.56	0/225
8	L	0.26	0/1030	0.45	0/1403
9	M	0.29	0/213	0.65	0/291
10	W	0.27	0/213	0.43	0/291
All	All	0.26	0/15572	0.47	0/21202

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	725	0	737	13	0
2	A	5715	0	5546	172	0
3	B	5252	0	5015	164	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	599	0	577	12	0
5	E	452	0	447	6	0
6	F	775	0	773	27	0
7	J	162	0	172	7	0
8	L	1008	0	1012	19	0
9	M	213	0	244	6	0
10	W	208	0	213	3	0
11	A	2145	0	1844	143	0
11	B	1445	0	1163	95	0
11	F	45	0	31	5	0
11	J	45	0	31	1	0
11	L	175	0	169	6	0
11	W	45	0	31	2	0
12	A	33	0	46	3	0
12	B	33	0	46	1	0
13	A	8	0	0	1	0
13	C	16	0	0	1	0
14	A	98	0	148	3	0
15	A	65	0	0	1	0
16	A	64	0	72	9	0
16	B	64	0	74	9	0
17	A	120	0	0	0	0
17	B	120	0	0	0	0
17	J	80	0	0	1	0
17	L	80	0	0	0	0
17	M	40	0	0	0	0
17	W	80	0	0	0	0
18	B	51	0	75	3	0
All	All	19961	0	18466	501	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 501 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1013:PHO:H3A	16:A:1013:PHO:H2	1.33	1.06
2:A:408:HIS:HE1	11:A:1128:CL7:NA	1.65	0.94
3:B:276:HIS:HE2	11:B:1215:CL7:HMB3	1.35	0.90
2:A:57:HIS:HE1	11:A:1102:CL7:NB	1.69	0.90
2:A:706:HIS:HE1	11:A:1138:CL7:ND	1.78	0.80

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	92/139 (66%)	90 (98%)	2 (2%)	0	100	100
2	A	724/753 (96%)	687 (95%)	37 (5%)	0	100	100
3	B	653/736 (89%)	631 (97%)	22 (3%)	0	100	100
4	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
5	E	56/89 (63%)	53 (95%)	3 (5%)	0	100	100
6	F	101/167 (60%)	96 (95%)	5 (5%)	0	100	100
7	J	19/51 (37%)	19 (100%)	0	0	100	100
8	L	142/153 (93%)	137 (96%)	5 (4%)	0	100	100
9	M	28/31 (90%)	28 (100%)	0	0	100	100
10	W	26/34 (76%)	23 (88%)	3 (12%)	0	100	100
All	All	1919/2234 (86%)	1838 (96%)	81 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	78/112 (70%)	78 (100%)	0	100	100
2	A	584/606 (96%)	584 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	B	531/594 (89%)	530 (100%)	1 (0%)	93 97
4	C	68/69 (99%)	67 (98%)	1 (2%)	65 81
5	E	49/69 (71%)	47 (96%)	2 (4%)	30 61
6	F	79/133 (59%)	78 (99%)	1 (1%)	69 82
7	J	17/46 (37%)	16 (94%)	1 (6%)	19 49
8	L	104/112 (93%)	104 (100%)	0	100 100
9	M	24/25 (96%)	24 (100%)	0	100 100
10	W	21/26 (81%)	21 (100%)	0	100 100
All	All	1555/1792 (87%)	1549 (100%)	6 (0%)	91 95

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	7	LYS
6	F	82	ARG
7	J	41	ARG
4	C	19	ARG
3	B	402	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	442	ASN
2	A	540	HIS
3	B	174	GLN
3	B	275	HIS
6	F	109	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

100 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	CL7	A	1118	-	46,53,73	2.68	13 (28%)	41,89,113	2.55	12 (29%)
11	CL7	B	1206	3	46,53,73	2.65	13 (28%)	41,89,113	2.56	11 (26%)
13	SF4	C	3003	4	0,12,12	-	-	-		
11	CL7	A	1120	-	46,53,73	2.68	13 (28%)	41,89,113	2.58	13 (31%)
11	CL7	A	1137	-	46,53,73	2.62	13 (28%)	41,89,113	2.64	14 (34%)
16	PHO	B	1023	-	51,69,69	0.95	4 (7%)	47,99,99	1.20	5 (10%)
11	CL7	B	1238	-	66,73,73	2.25	13 (19%)	65,113,113	2.13	15 (23%)
17	8CT	B	4014	-	40,41,41	4.75	25 (62%)	50,56,56	2.42	15 (30%)
11	CL7	A	1138	-	46,53,73	2.67	13 (28%)	41,89,113	2.55	12 (29%)
14	LHG	A	5003	-	48,48,48	2.47	35 (72%)	51,54,54	1.62	7 (13%)
11	CL7	B	1021	-	66,73,73	2.21	12 (18%)	65,113,113	2.19	15 (23%)
11	CL7	B	1205	-	46,53,73	2.66	13 (28%)	41,89,113	2.51	11 (26%)
12	PQN	B	2002	-	34,34,34	3.53	16 (47%)	42,45,45	2.20	3 (7%)
11	CL7	B	1203	-	66,73,73	2.25	12 (18%)	65,113,113	2.14	15 (23%)
11	CL7	A	1139	-	46,53,73	2.70	14 (30%)	41,89,113	2.52	12 (29%)
11	CL7	B	1224	-	46,53,73	2.65	13 (28%)	41,89,113	2.51	11 (26%)
13	SF4	A	3001	2,3	0,12,12	-	-	-		
11	CL7	A	1802	-	46,53,73	2.69	13 (28%)	41,89,113	2.55	13 (31%)
17	8CT	A	4008	-	40,41,41	4.72	24 (60%)	50,56,56	3.57	23 (46%)
11	CL7	B	1212	-	46,53,73	2.69	13 (28%)	41,89,113	2.55	13 (31%)
17	8CT	J	4015	-	40,41,41	4.74	25 (62%)	50,56,56	2.71	19 (38%)
11	CL7	F	1301	-	46,53,73	2.70	13 (28%)	41,89,113	2.56	12 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CL7	B	1012	-	66,73,73	2.23	13 (19%)	65,113,113	2.14	14 (21%)
11	CL7	B	1213	-	46,53,73	2.69	13 (28%)	41,89,113	2.56	13 (31%)
12	PQN	A	2001	-	34,34,34	3.52	17 (50%)	42,45,45	2.12	3 (7%)
11	CL7	B	1202	-	46,53,73	2.65	13 (28%)	41,89,113	2.56	11 (26%)
11	CL7	A	1104	-	66,73,73	2.24	14 (21%)	65,113,113	2.13	14 (21%)
11	CL7	B	1223	-	46,53,73	2.67	13 (28%)	41,89,113	2.57	13 (31%)
11	CL7	A	1103	-	66,73,73	2.26	13 (19%)	65,113,113	2.11	15 (23%)
11	CL7	A	1111	-	46,53,73	2.69	13 (28%)	41,89,113	2.51	11 (26%)
11	CL7	W	2601	-	46,53,73	2.66	13 (28%)	41,89,113	2.56	11 (26%)
11	CL7	A	1101	-	66,73,73	2.26	13 (19%)	65,113,113	2.13	14 (21%)
11	CL7	A	1110	-	46,53,73	2.65	13 (28%)	41,89,113	2.65	13 (31%)
11	CL7	A	1128	-	66,73,73	2.27	13 (19%)	65,113,113	2.17	15 (23%)
17	8CT	A	4007	-	40,41,41	4.73	25 (62%)	50,56,56	3.21	21 (42%)
11	CL7	A	1106	-	66,73,73	2.25	13 (19%)	65,113,113	2.13	14 (21%)
11	CL7	A	1113	-	46,53,73	2.67	13 (28%)	41,89,113	2.57	13 (31%)
11	CL7	B	1228	-	46,53,73	2.68	13 (28%)	41,89,113	2.53	13 (31%)
11	CL7	B	1234	-	46,53,73	2.67	13 (28%)	41,89,113	2.57	11 (26%)
11	CL7	B	1211	-	46,53,73	2.68	13 (28%)	41,89,113	2.51	12 (29%)
11	CL7	A	1112	-	46,53,73	2.67	13 (28%)	41,89,113	2.53	12 (29%)
11	CL7	A	1022	-	66,73,73	2.24	14 (21%)	65,113,113	2.14	16 (24%)
11	CL7	A	1121	-	46,53,73	2.66	13 (28%)	41,89,113	2.55	12 (29%)
11	CL7	B	1208	-	46,53,73	2.67	13 (28%)	41,89,113	2.56	13 (31%)
11	CL7	A	1237	-	66,73,73	2.24	13 (19%)	65,113,113	2.13	15 (23%)
11	CL7	A	1125	-	66,73,73	2.25	12 (18%)	65,113,113	2.16	15 (23%)
11	CL7	B	1214	-	46,53,73	2.66	14 (30%)	41,89,113	2.71	13 (31%)
11	CL7	A	1126	-	66,73,73	2.27	13 (19%)	65,113,113	2.09	14 (21%)
11	CL7	B	1226	-	66,73,73	2.25	13 (19%)	65,113,113	2.19	16 (24%)
17	8CT	J	4013	-	40,41,41	4.78	25 (62%)	50,56,56	2.53	18 (36%)
11	CL7	A	1140	-	66,73,73	2.24	13 (19%)	65,113,113	2.12	14 (21%)
11	CL7	A	1117	-	66,73,73	2.24	13 (19%)	65,113,113	2.09	13 (20%)
11	CL7	A	1114	-	46,53,73	2.75	14 (30%)	41,89,113	2.56	13 (31%)
11	CL7	A	1116	-	46,53,73	2.68	13 (28%)	41,89,113	2.53	12 (29%)
11	CL7	A	1132	-	66,73,73	2.26	14 (21%)	65,113,113	2.08	16 (24%)
11	CL7	B	1235	-	46,53,73	2.66	13 (28%)	41,89,113	2.53	13 (31%)
11	CL7	A	1801	-	46,53,73	2.66	13 (28%)	41,89,113	2.55	12 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CL7	B	1229	-	46,53,73	2.69	13 (28%)	41,89,113	2.54	13 (31%)
11	CL7	B	1222	-	46,53,73	2.67	13 (28%)	41,89,113	2.53	14 (34%)
11	CL7	B	1230	-	46,53,73	2.65	13 (28%)	41,89,113	2.54	11 (26%)
11	CL7	A	1122	-	46,53,73	2.65	13 (28%)	41,89,113	2.54	12 (29%)
17	8CT	M	4021	-	40,41,41	4.76	25 (62%)	50,56,56	2.87	18 (36%)
11	CL7	B	1236	-	46,53,73	2.66	13 (28%)	41,89,113	2.59	12 (29%)
11	CL7	B	1225	-	66,73,73	2.24	14 (21%)	65,113,113	2.11	15 (23%)
15	G9R	A	1011	-	65,71,71	2.35	10 (15%)	71,104,104	1.88	19 (26%)
11	CL7	J	1302	-	46,53,73	2.68	13 (28%)	41,89,113	2.55	12 (29%)
11	CL7	B	1201	-	46,53,73	2.65	13 (28%)	41,89,113	2.54	13 (31%)
11	CL7	L	1503	-	46,53,73	2.66	13 (28%)	41,89,113	2.56	12 (29%)
11	CL7	L	1502	-	66,73,73	2.25	13 (19%)	65,113,113	2.14	15 (23%)
17	8CT	B	4017	-	40,41,41	4.73	25 (62%)	50,56,56	3.46	24 (48%)
18	LMG	B	5002	-	51,51,55	2.84	30 (58%)	59,59,63	0.95	2 (3%)
11	CL7	A	1115	-	46,53,73	2.68	13 (28%)	41,89,113	2.59	13 (31%)
11	CL7	A	1130	-	46,53,73	2.67	13 (28%)	41,89,113	2.58	14 (34%)
16	PHO	A	1013	-	51,69,69	0.95	4 (7%)	47,99,99	1.22	4 (8%)
17	8CT	A	4011	-	40,41,41	4.74	25 (62%)	50,56,56	2.86	18 (36%)
17	8CT	L	4020	-	40,41,41	4.73	25 (62%)	50,56,56	2.55	17 (34%)
11	CL7	B	1207	-	46,53,73	2.65	13 (28%)	41,89,113	2.57	12 (29%)
11	CL7	B	1239	-	66,73,73	2.24	13 (19%)	65,113,113	2.14	14 (21%)
11	CL7	A	1129	-	46,53,73	2.67	13 (28%)	41,89,113	2.51	12 (29%)
11	CL7	B	1204	-	46,53,73	2.67	13 (28%)	41,89,113	2.58	14 (34%)
13	SF4	C	3002	4	0,12,12	-	-	-		
11	CL7	A	1102	11	46,53,73	2.67	13 (28%)	41,89,113	2.58	14 (34%)
11	CL7	L	1501	8	66,73,73	2.24	13 (19%)	65,113,113	2.13	16 (24%)
17	8CT	W	4018	-	40,41,41	4.76	25 (62%)	50,56,56	2.57	20 (40%)
11	CL7	A	1109	11	46,53,73	2.67	13 (28%)	41,89,113	2.53	12 (29%)
11	CL7	B	1215	-	46,53,73	2.65	13 (28%)	41,89,113	2.59	13 (31%)
11	CL7	A	1105	-	46,53,73	2.68	13 (28%)	41,89,113	2.71	12 (29%)
14	LHG	A	5001	-	48,48,48	2.47	34 (70%)	51,54,54	1.62	7 (13%)
11	CL7	A	1124	-	46,53,73	2.65	13 (28%)	41,89,113	2.56	14 (34%)
17	8CT	B	4006	-	40,41,41	4.74	25 (62%)	50,56,56	2.58	16 (32%)
11	CL7	A	1107	2	46,53,73	2.66	13 (28%)	41,89,113	2.56	13 (31%)
11	CL7	A	1123	-	66,73,73	2.25	13 (19%)	65,113,113	2.14	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	8CT	L	4019	-	40,41,41	4.76	24 (60%)	50,56,56	2.40	18 (36%)
11	CL7	A	1127	-	46,53,73	2.68	13 (28%)	41,89,113	2.54	14 (34%)
11	CL7	B	1210	-	46,53,73	2.68	13 (28%)	41,89,113	2.57	12 (29%)
17	8CT	W	4020	-	40,41,41	4.72	25 (62%)	50,56,56	2.46	18 (36%)
11	CL7	A	1135	-	46,53,73	2.67	13 (28%)	41,89,113	2.58	12 (29%)
11	CL7	A	1131	-	66,73,73	2.24	13 (19%)	65,113,113	2.15	15 (23%)
11	CL7	A	1119	-	46,53,73	2.64	14 (30%)	41,89,113	2.60	12 (29%)
11	CL7	A	1136	-	66,73,73	2.28	13 (19%)	65,113,113	2.14	15 (23%)

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
11	CL7	A	1118	-	2/2/11/20	4/13/91/115	-
11	CL7	B	1206	3	2/2/11/20	8/13/91/115	-
13	SF4	C	3003	4	-	-	0/6/5/5
11	CL7	A	1120	-	2/2/11/20	3/13/91/115	-
11	CL7	A	1137	-	2/2/11/20	6/13/91/115	-
16	PHO	B	1023	-	-	14/37/103/103	0/5/6/6
11	CL7	B	1238	-	2/2/15/20	14/37/115/115	-
17	8CT	B	4014	-	-	6/29/63/63	0/2/2/2
11	CL7	A	1138	-	2/2/11/20	6/13/91/115	-
14	LHG	A	5003	-	-	30/53/53/53	-
11	CL7	B	1021	-	2/2/15/20	22/37/115/115	-
11	CL7	B	1205	-	2/2/11/20	4/13/91/115	-
12	PQN	B	2002	-	-	13/23/43/43	0/2/2/2
11	CL7	B	1203	-	2/2/15/20	23/37/115/115	-
11	CL7	A	1139	-	2/2/11/20	5/13/91/115	-
11	CL7	B	1224	-	2/2/11/20	5/13/91/115	-
13	SF4	A	3001	2,3	-	-	0/6/5/5
11	CL7	A	1802	-	2/2/11/20	7/13/91/115	-
17	8CT	A	4008	-	-	3/29/63/63	0/2/2/2
11	CL7	B	1212	-	2/2/11/20	7/13/91/115	-
17	8CT	J	4015	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CL7	F	1301	-	2/2/11/20	5/13/91/115	-
11	CL7	B	1012	-	2/2/15/20	15/37/115/115	-
11	CL7	B	1213	-	2/2/11/20	7/13/91/115	-
11	CL7	B	1202	-	2/2/11/20	6/13/91/115	-
12	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
11	CL7	A	1104	-	2/2/15/20	16/37/115/115	-
11	CL7	B	1223	-	2/2/11/20	6/13/91/115	-
11	CL7	A	1103	-	2/2/15/20	14/37/115/115	-
11	CL7	A	1111	-	2/2/11/20	7/13/91/115	-
11	CL7	W	2601	-	2/2/11/20	5/13/91/115	-
11	CL7	A	1101	-	2/2/15/20	13/37/115/115	-
11	CL7	A	1110	-	2/2/11/20	5/13/91/115	-
11	CL7	A	1128	-	2/2/15/20	14/37/115/115	-
17	8CT	A	4007	-	-	6/29/63/63	0/2/2/2
11	CL7	A	1106	-	2/2/15/20	18/37/115/115	-
11	CL7	A	1113	-	2/2/11/20	5/13/91/115	-
11	CL7	B	1228	-	2/2/11/20	6/13/91/115	-
11	CL7	B	1234	-	2/2/11/20	3/13/91/115	-
11	CL7	B	1211	-	2/2/11/20	7/13/91/115	-
11	CL7	A	1112	-	2/2/11/20	6/13/91/115	-
11	CL7	A	1022	-	2/2/15/20	12/37/115/115	-
11	CL7	A	1121	-	2/2/11/20	5/13/91/115	-
11	CL7	B	1208	-	2/2/11/20	5/13/91/115	-
11	CL7	A	1237	-	2/2/15/20	16/37/115/115	-
11	CL7	A	1125	-	2/2/15/20	15/37/115/115	-
11	CL7	B	1214	-	2/2/11/20	4/13/91/115	-
11	CL7	A	1126	-	2/2/15/20	16/37/115/115	-
11	CL7	B	1226	-	2/2/15/20	20/37/115/115	-
17	8CT	J	4013	-	-	11/29/63/63	0/2/2/2
11	CL7	A	1140	-	2/2/15/20	12/37/115/115	-
11	CL7	A	1117	-	2/2/15/20	17/37/115/115	-
11	CL7	A	1114	-	2/2/11/20	4/13/91/115	-
11	CL7	A	1116	-	2/2/11/20	3/13/91/115	-
11	CL7	A	1132	-	2/2/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CL7	B	1235	-	2/2/11/20	5/13/91/115	-
11	CL7	A	1801	-	2/2/11/20	8/13/91/115	-
11	CL7	B	1229	-	2/2/11/20	5/13/91/115	-
11	CL7	B	1222	-	2/2/11/20	5/13/91/115	-
11	CL7	B	1230	-	2/2/11/20	6/13/91/115	-
11	CL7	A	1122	-	2/2/11/20	4/13/91/115	-
17	8CT	M	4021	-	-	10/29/63/63	0/2/2/2
11	CL7	B	1236	-	2/2/11/20	5/13/91/115	-
11	CL7	B	1225	-	2/2/15/20	15/37/115/115	-
15	G9R	A	1011	-	1/1/17/22	18/48/107/107	-
11	CL7	J	1302	-	2/2/11/20	8/13/91/115	-
11	CL7	B	1201	-	2/2/11/20	5/13/91/115	-
11	CL7	L	1503	-	2/2/11/20	5/13/91/115	-
11	CL7	L	1502	-	2/2/15/20	15/37/115/115	-
17	8CT	B	4017	-	-	9/29/63/63	0/2/2/2
18	LMG	B	5002	-	-	18/46/66/70	0/1/1/1
11	CL7	A	1115	-	2/2/11/20	7/13/91/115	-
11	CL7	A	1130	-	2/2/11/20	5/13/91/115	-
16	PHO	A	1013	-	-	18/37/103/103	0/5/6/6
17	8CT	A	4011	-	-	14/29/63/63	0/2/2/2
17	8CT	L	4020	-	-	7/29/63/63	0/2/2/2
11	CL7	B	1207	-	2/2/11/20	4/13/91/115	-
11	CL7	B	1239	-	2/2/15/20	13/37/115/115	-
11	CL7	A	1129	-	2/2/11/20	6/13/91/115	-
11	CL7	B	1204	-	2/2/11/20	5/13/91/115	-
13	SF4	C	3002	4	-	-	0/6/5/5
11	CL7	A	1102	11	2/2/11/20	6/13/91/115	-
11	CL7	L	1501	8	2/2/15/20	14/37/115/115	-
17	8CT	W	4018	-	-	9/29/63/63	0/2/2/2
11	CL7	A	1109	11	2/2/11/20	5/13/91/115	-
11	CL7	B	1215	-	2/2/11/20	4/13/91/115	-
11	CL7	A	1105	-	2/2/11/20	7/13/91/115	-
14	LHG	A	5001	-	-	21/53/53/53	-
11	CL7	A	1124	-	2/2/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	8CT	B	4006	-	-	12/29/63/63	0/2/2/2
11	CL7	A	1107	2	2/2/11/20	3/13/91/115	-
11	CL7	A	1123	-	2/2/15/20	12/37/115/115	-
17	8CT	L	4019	-	-	3/29/63/63	0/2/2/2
11	CL7	A	1127	-	2/2/11/20	5/13/91/115	-
11	CL7	B	1210	-	2/2/11/20	5/13/91/115	-
17	8CT	W	4020	-	-	11/29/63/63	0/2/2/2
11	CL7	A	1135	-	2/2/11/20	9/13/91/115	-
11	CL7	A	1131	-	2/2/15/20	18/37/115/115	-
11	CL7	A	1119	-	2/2/11/20	4/13/91/115	-
11	CL7	A	1136	-	2/2/15/20	16/37/115/115	-

The worst 5 of 1466 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1011	G9R	CHC-C1C	15.37	1.48	1.35
17	J	4013	8CT	C02-C03	14.95	1.60	1.34
17	L	4019	8CT	C02-C03	14.91	1.60	1.34
17	W	4018	8CT	C02-C03	14.87	1.60	1.34
17	M	4021	8CT	C02-C03	14.86	1.60	1.34

The worst 5 of 1298 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	4008	8CT	C19-C20-C21	-10.91	111.73	127.31
17	A	4008	8CT	C24-C25-C26	-10.14	112.83	127.31
11	A	1105	CL7	C3C-C4C-NC	10.05	117.46	110.18
17	J	4015	8CT	C33-C32-C31	-9.65	115.60	124.85
11	B	1226	CL7	C3C-C4C-NC	9.49	117.05	110.18

5 of 153 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	1022	CL7	NA
11	A	1022	CL7	NC
11	A	1101	CL7	NA
11	A	1101	CL7	NC
11	A	1102	CL7	NA

5 of 906 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1101	CL7	C1A-C2A-CAA-CBA
11	A	1101	CL7	C3A-C2A-CAA-CBA
11	A	1102	CL7	C1A-C2A-CAA-CBA
11	A	1103	CL7	C4-C3-C5-C6
11	A	1104	CL7	C1A-C2A-CAA-CBA

There are no ring outliers.

83 monomers are involved in 277 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1118	CL7	5	0
11	B	1206	CL7	4	0
13	C	3003	SF4	1	0
11	A	1137	CL7	3	0
16	B	1023	PHO	9	0
11	B	1238	CL7	5	0
11	A	1138	CL7	3	0
14	A	5003	LHG	2	0
11	B	1021	CL7	8	0
11	B	1205	CL7	5	0
12	B	2002	PQN	1	0
11	B	1203	CL7	6	0
11	A	1139	CL7	2	0
11	B	1224	CL7	3	0
13	A	3001	SF4	1	0
11	A	1802	CL7	1	0
11	B	1212	CL7	2	0
17	J	4015	8CT	1	0
11	F	1301	CL7	5	0
11	B	1012	CL7	8	0
11	B	1213	CL7	4	0
12	A	2001	PQN	3	0
11	B	1202	CL7	1	0
11	A	1104	CL7	6	0
11	B	1223	CL7	2	0
11	A	1103	CL7	6	0
11	A	1111	CL7	7	0
11	W	2601	CL7	2	0
11	A	1101	CL7	3	0
11	A	1110	CL7	3	0
11	A	1128	CL7	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1106	CL7	5	0
11	A	1113	CL7	4	0
11	B	1228	CL7	2	0
11	B	1234	CL7	2	0
11	B	1211	CL7	1	0
11	A	1112	CL7	2	0
11	A	1022	CL7	8	0
11	A	1121	CL7	2	0
11	B	1208	CL7	2	0
11	A	1237	CL7	4	0
11	A	1125	CL7	2	0
11	B	1214	CL7	4	0
11	A	1126	CL7	7	0
11	B	1226	CL7	4	0
11	A	1140	CL7	6	0
11	A	1117	CL7	6	0
11	A	1114	CL7	6	0
11	A	1116	CL7	3	0
11	A	1132	CL7	8	0
11	B	1235	CL7	3	0
11	B	1229	CL7	3	0
11	B	1222	CL7	1	0
11	B	1230	CL7	5	0
11	A	1122	CL7	3	0
11	B	1236	CL7	3	0
11	B	1225	CL7	4	0
15	A	1011	G9R	1	0
11	J	1302	CL7	1	0
11	B	1201	CL7	2	0
11	L	1502	CL7	3	0
18	B	5002	LMG	3	0
11	A	1115	CL7	4	0
11	A	1130	CL7	3	0
16	A	1013	PHO	9	0
11	B	1207	CL7	2	0
11	B	1239	CL7	2	0
11	A	1129	CL7	4	0
11	B	1204	CL7	5	0
11	A	1102	CL7	7	0
11	L	1501	CL7	3	0
11	A	1109	CL7	3	0
11	B	1215	CL7	4	0

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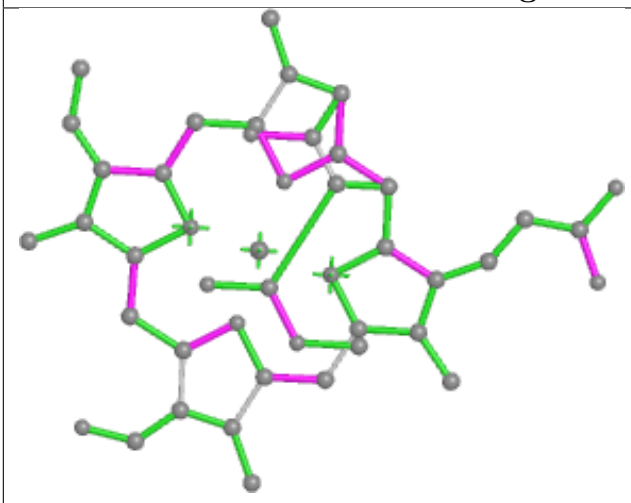
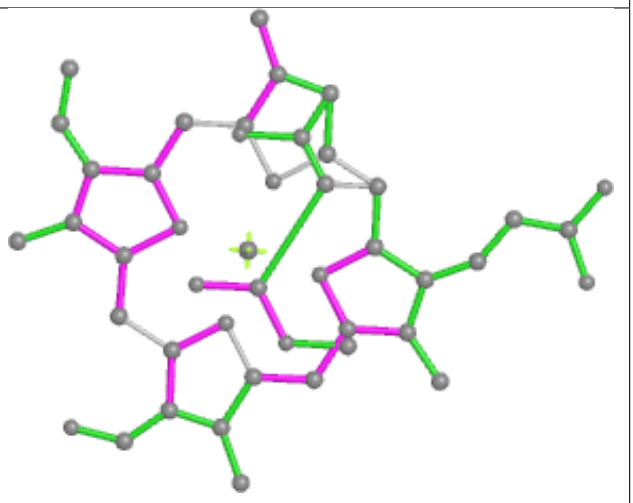
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1105	CL7	2	0
14	A	5001	LHG	1	0
11	A	1107	CL7	3	0
11	A	1123	CL7	3	0
11	A	1127	CL7	2	0
11	B	1210	CL7	1	0
11	A	1135	CL7	4	0
11	A	1131	CL7	5	0
11	A	1119	CL7	3	0
11	A	1136	CL7	8	0

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

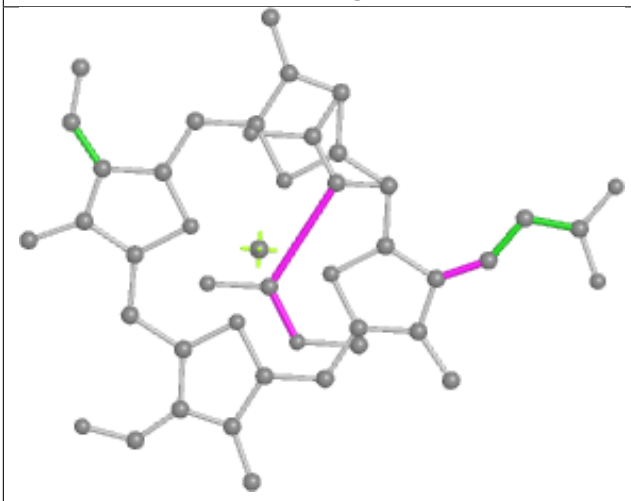
Ligand CL7 A 1118



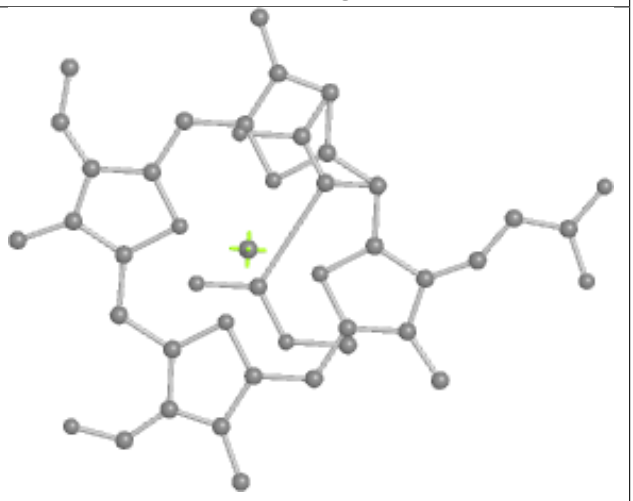
Bond lengths



Bond angles

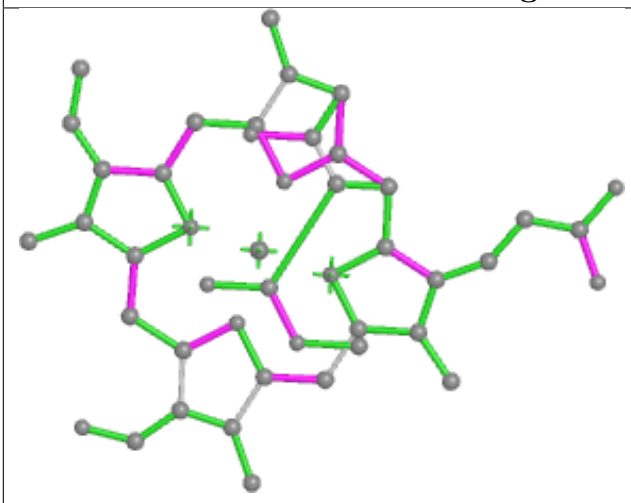


Torsions

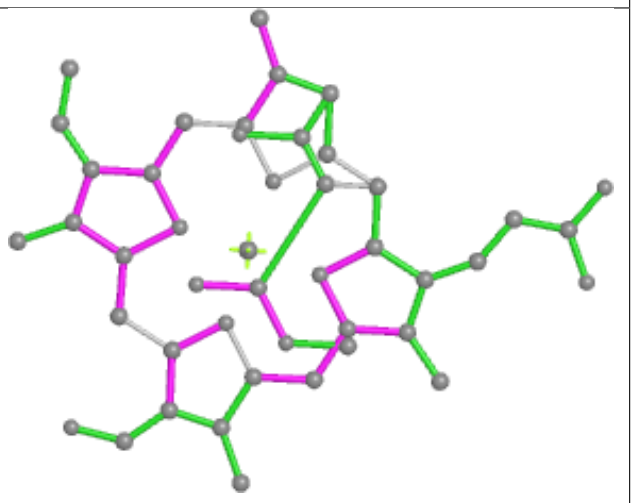


Rings

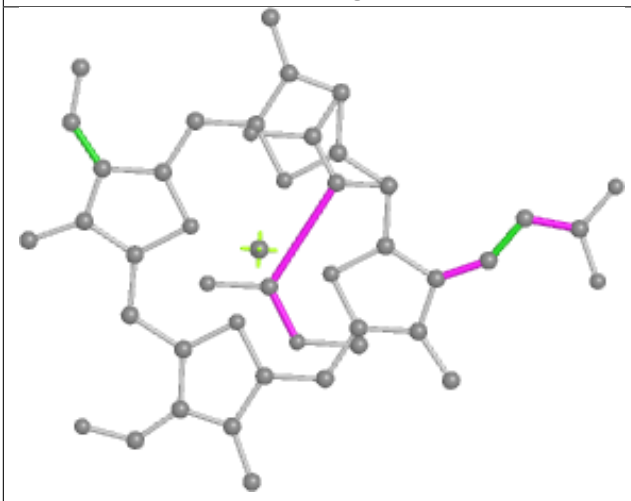
Ligand CL7 B 1206



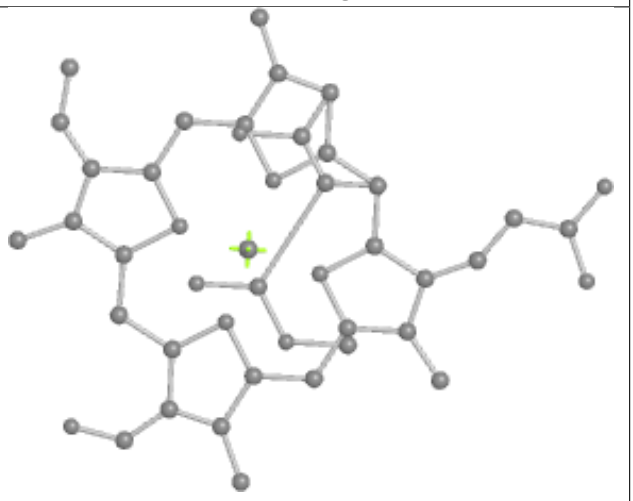
Bond lengths



Bond angles

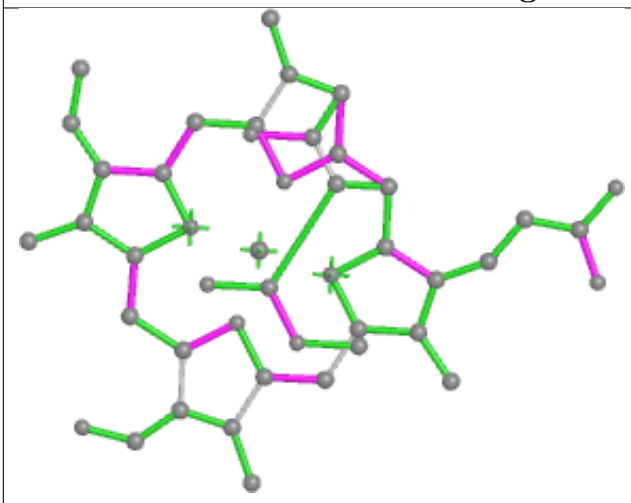


Torsions

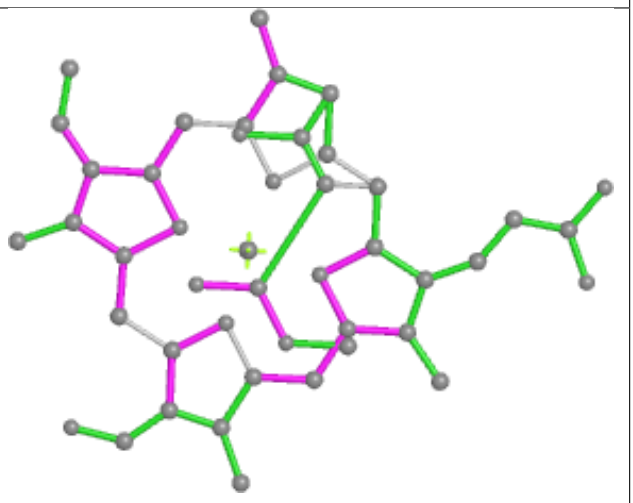


Rings

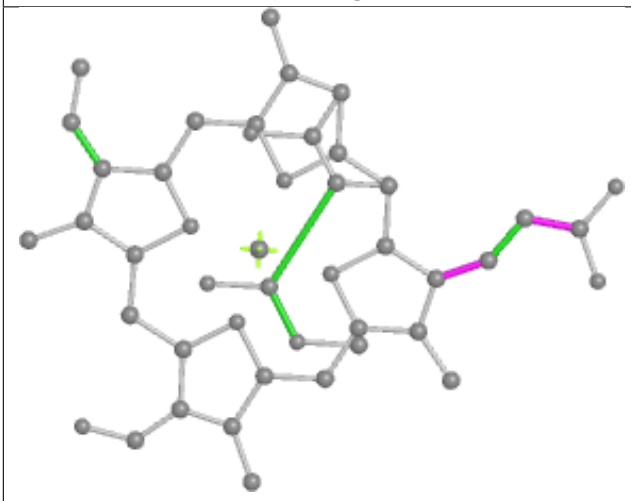
Ligand CL7 A 1120



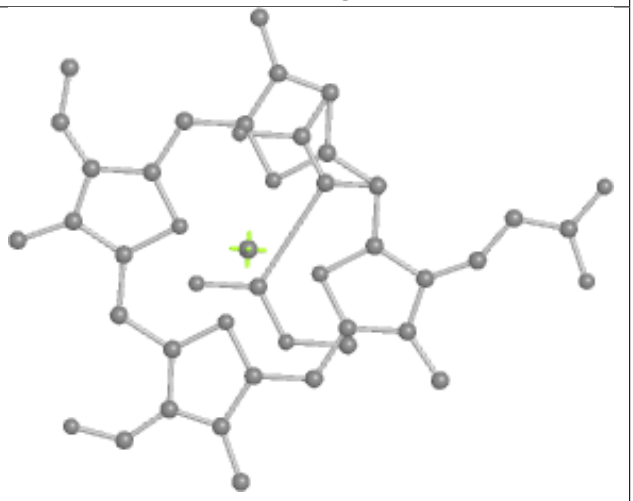
Bond lengths



Bond angles

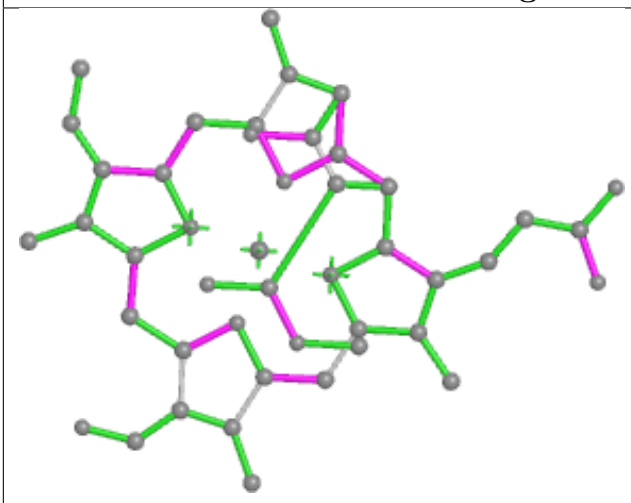


Torsions

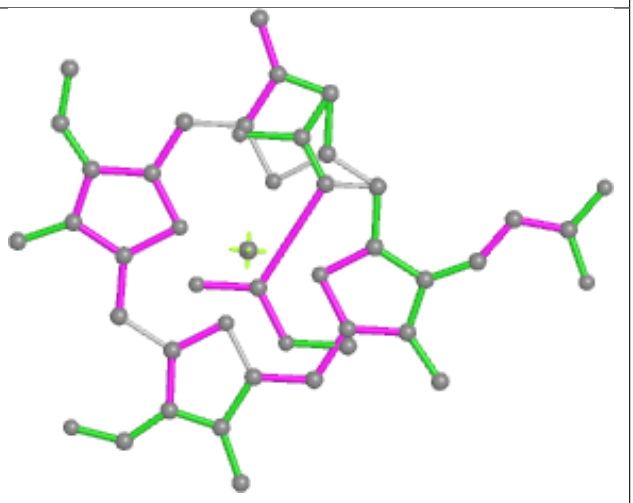


Rings

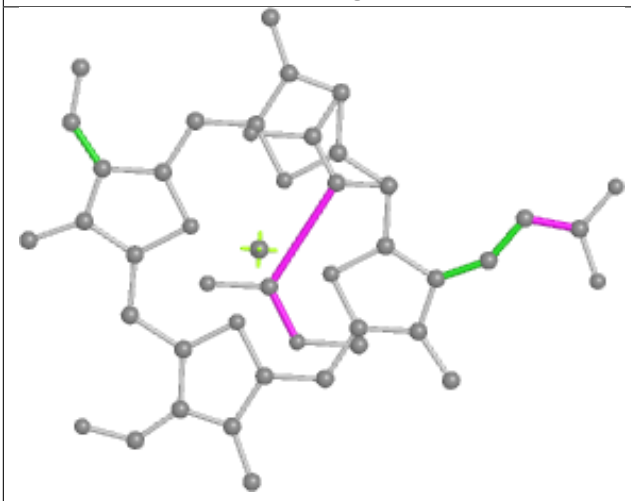
Ligand CL7 A 1137



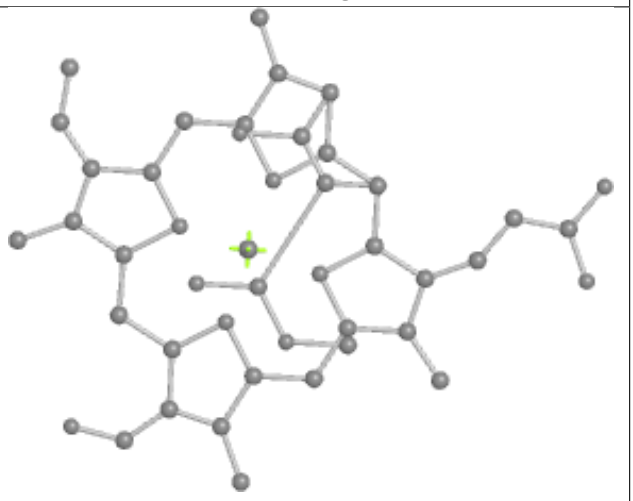
Bond lengths



Bond angles

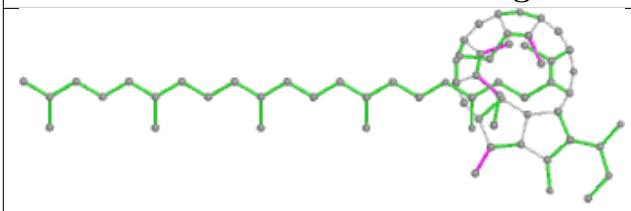


Torsions

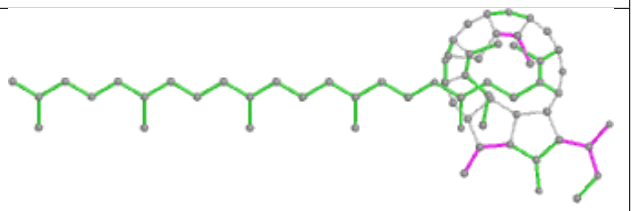


Rings

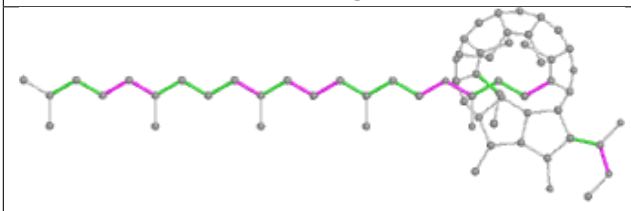
Ligand PHO B 1023



Bond lengths



Bond angles



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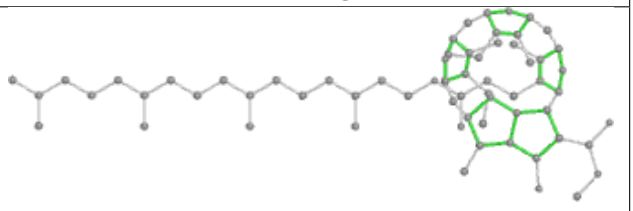
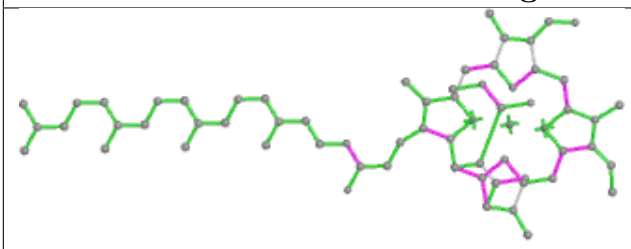


Rings

Ligand CL7 B 1238



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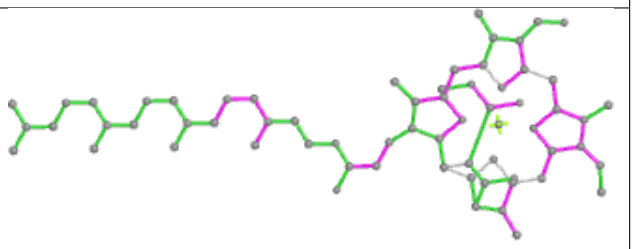

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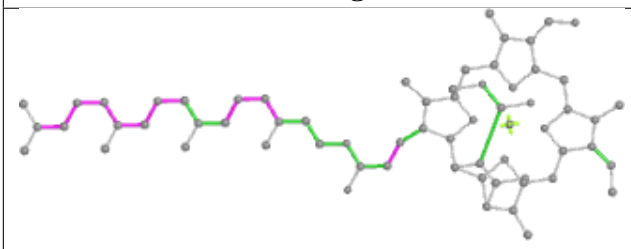
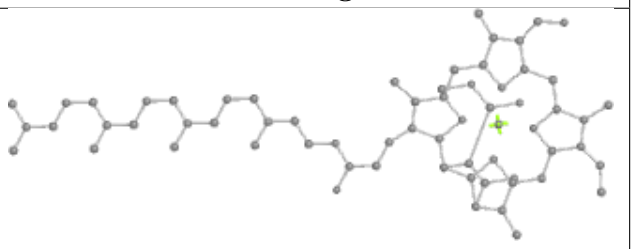
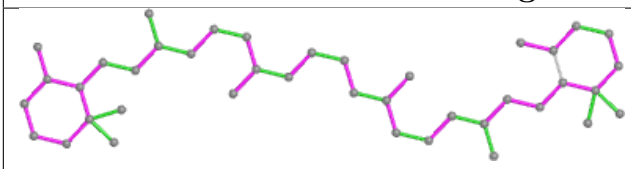


Torsions



Rings

Ligand 8CT B 4014



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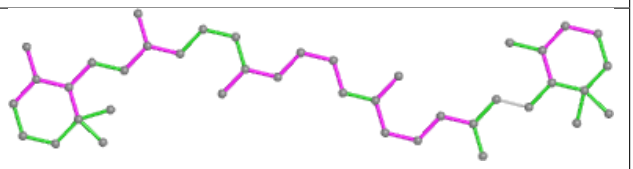

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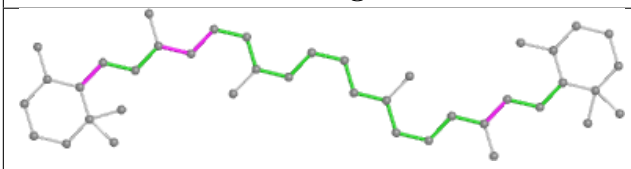

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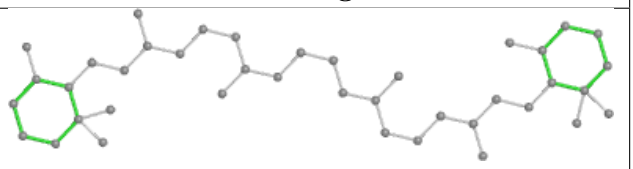
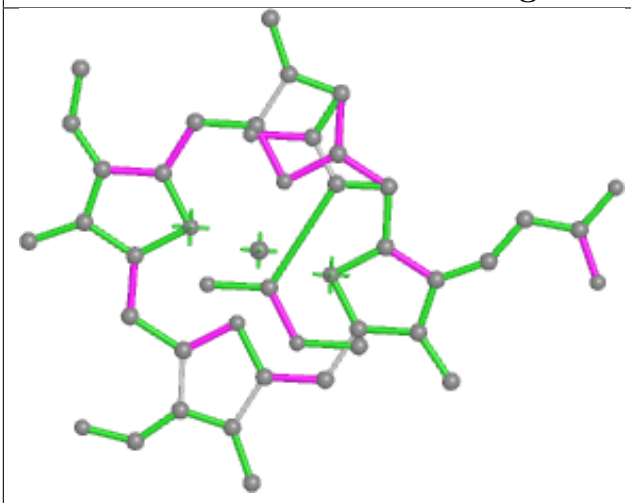


Rings

Ligand CL7 A 1138



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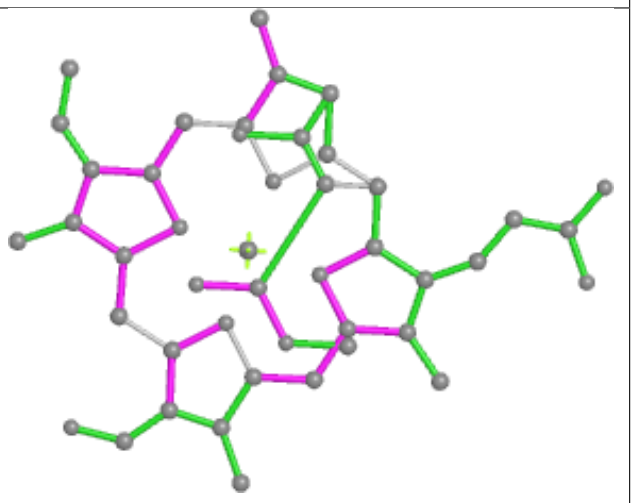
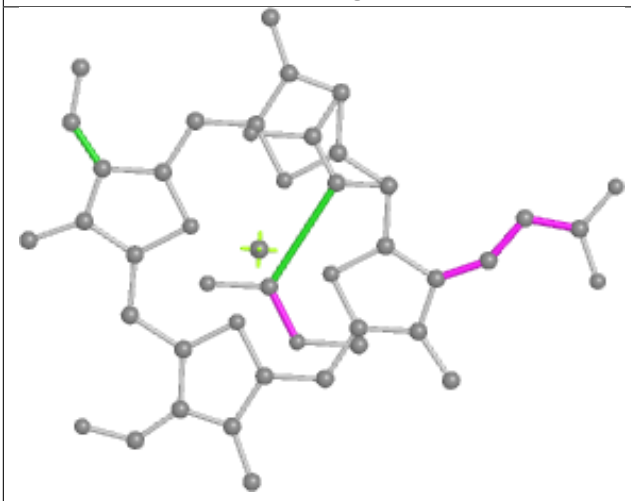


Bond angles



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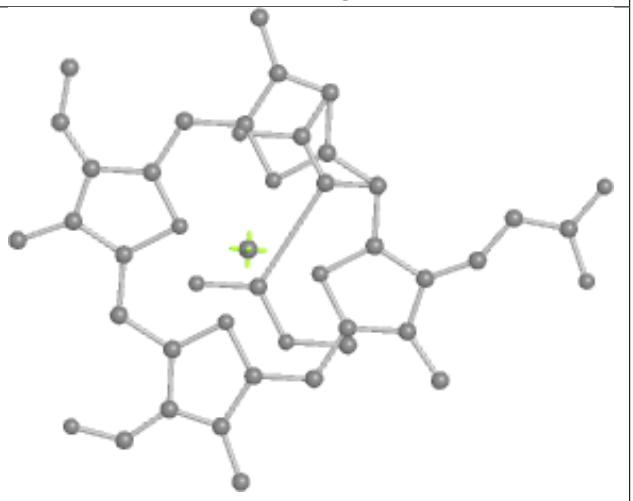
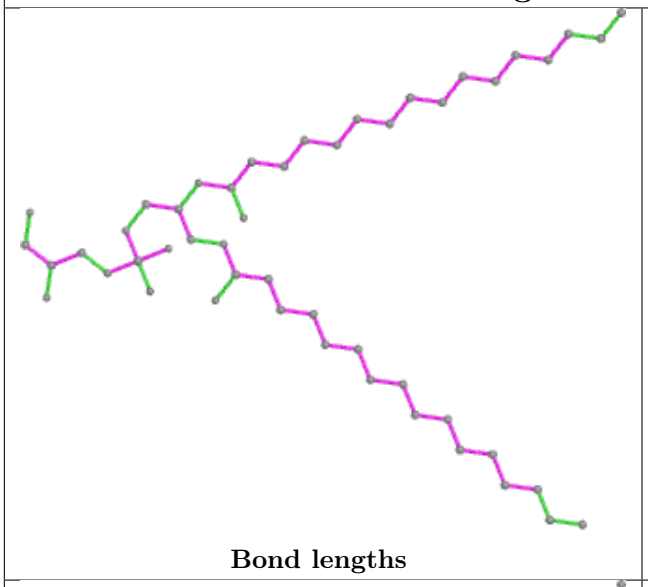


Rings

Ligand LHG A 5003



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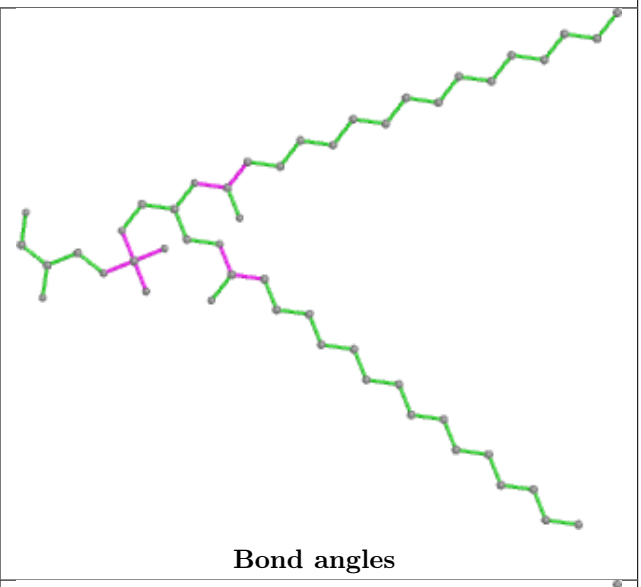
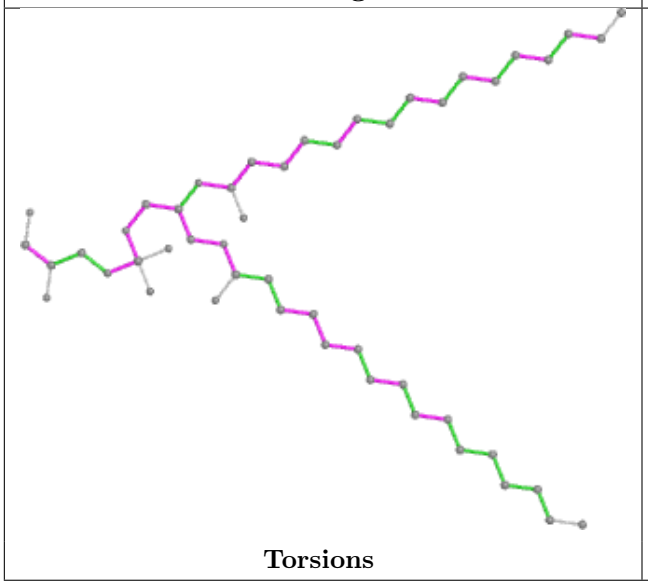


Bond angles



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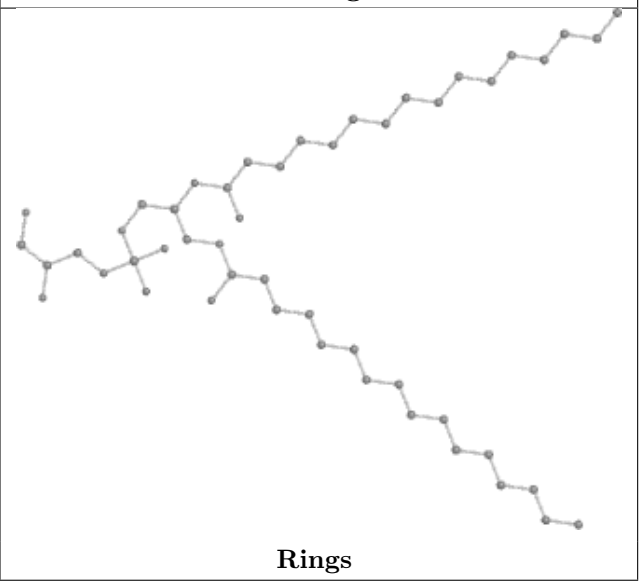
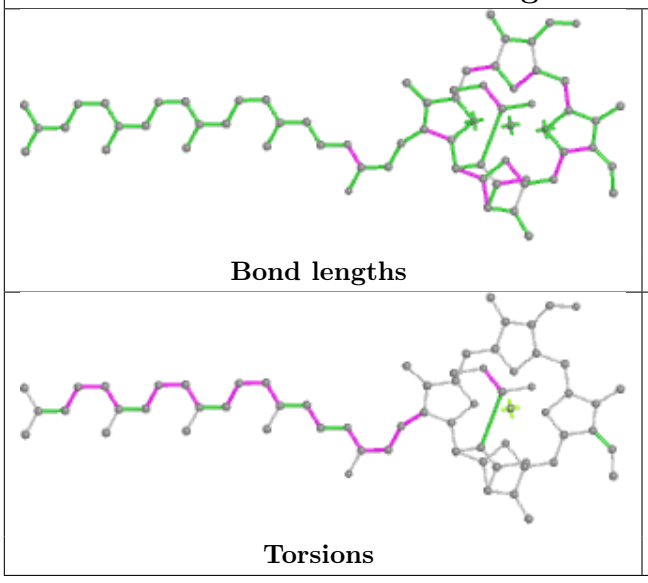


Rings

Ligand CL7 B 1021



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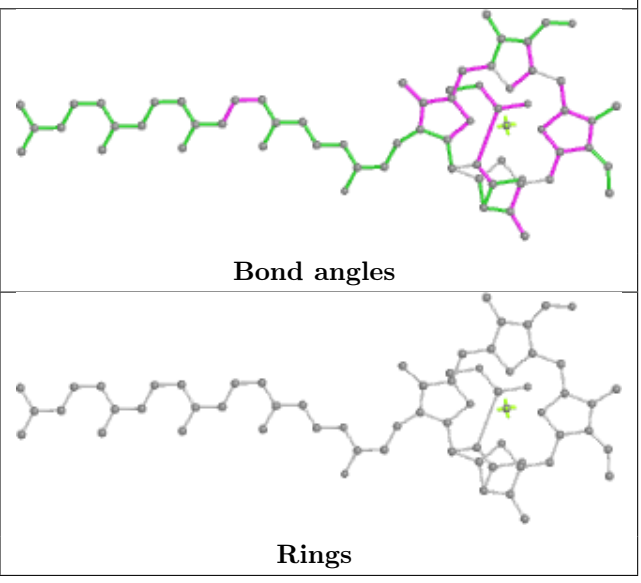
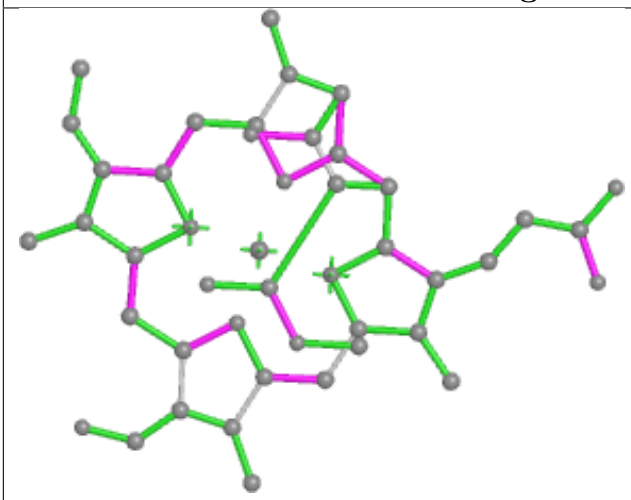


Bond angles

Torsions

Rings

Ligand CL7 B 1205



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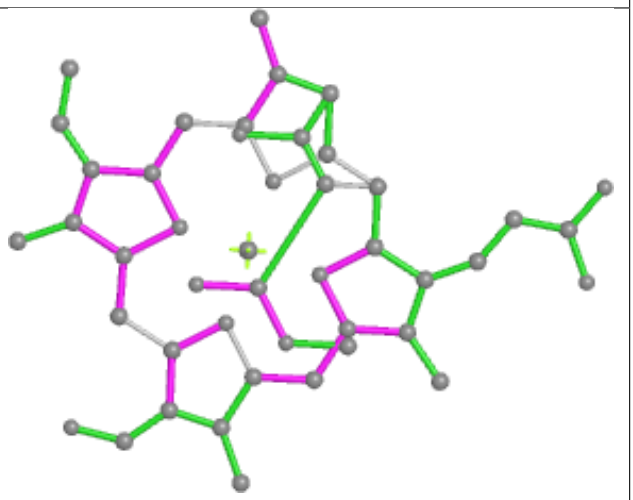
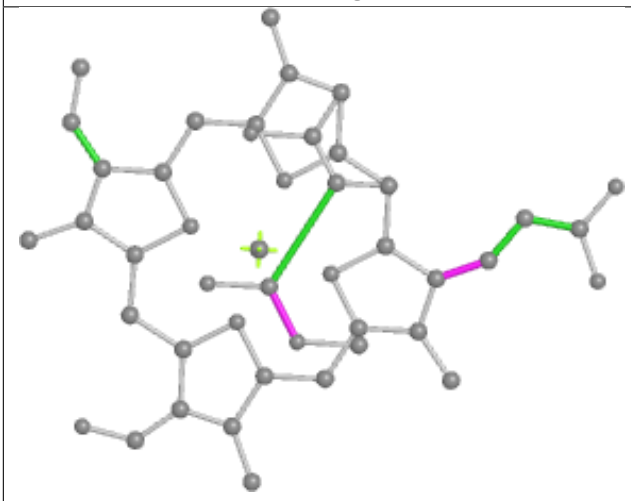


Bond angles



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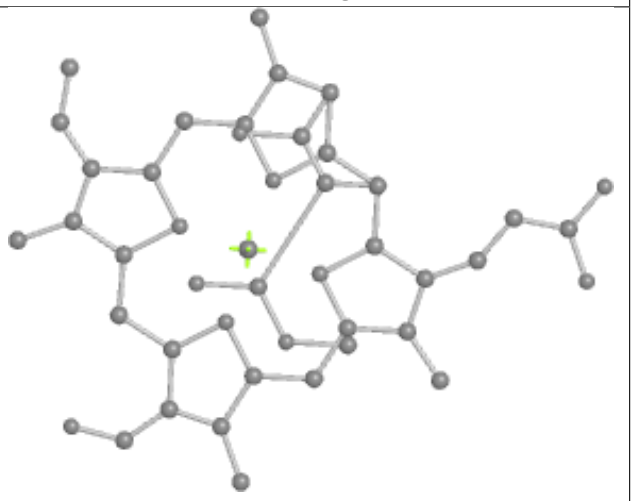
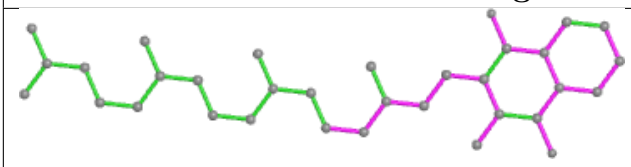


Rings

Ligand PQN B 2002



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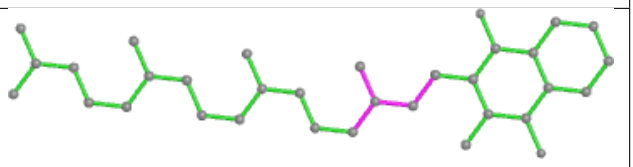

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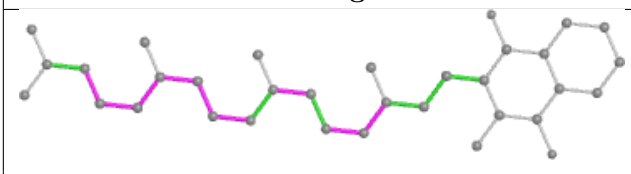

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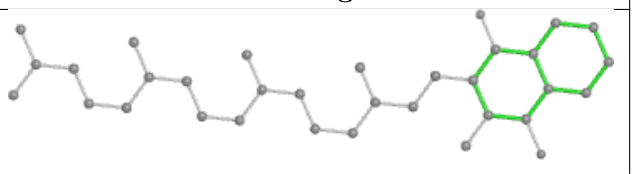
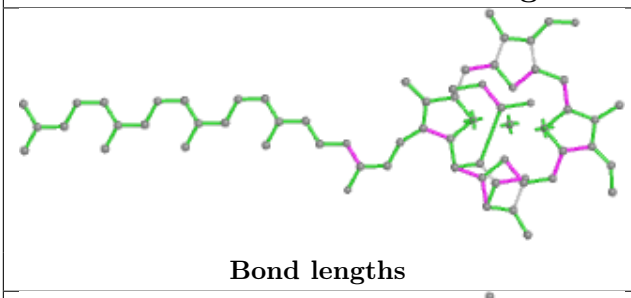


Rings

Ligand CL7 B 1203



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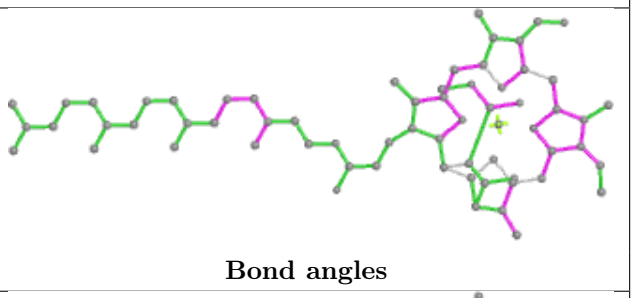
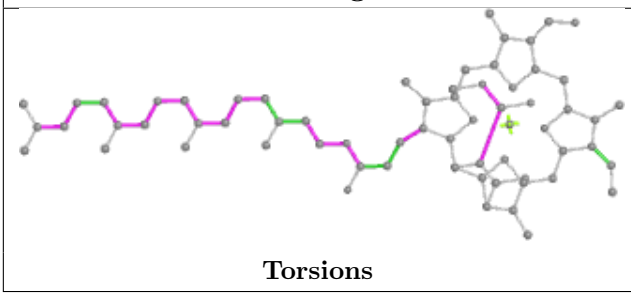


Bond angles



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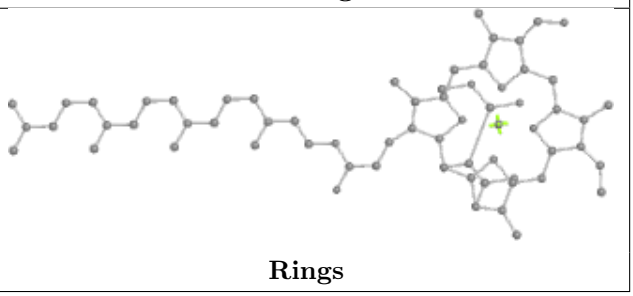
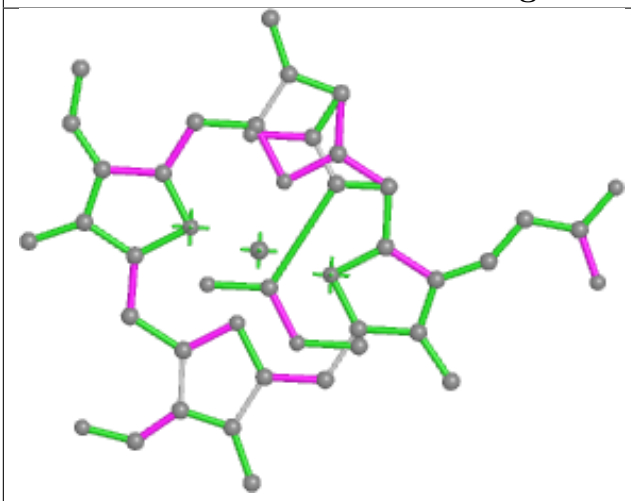


Rings

Ligand CL7 A 1139



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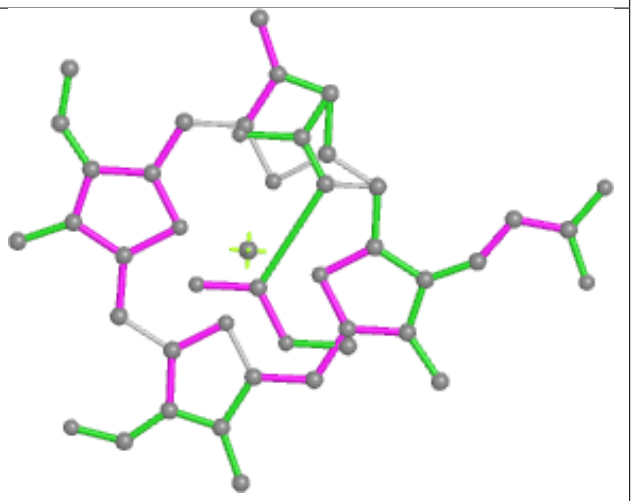
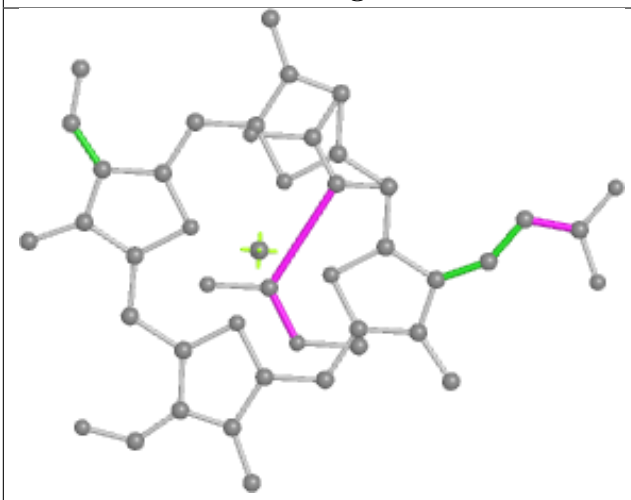
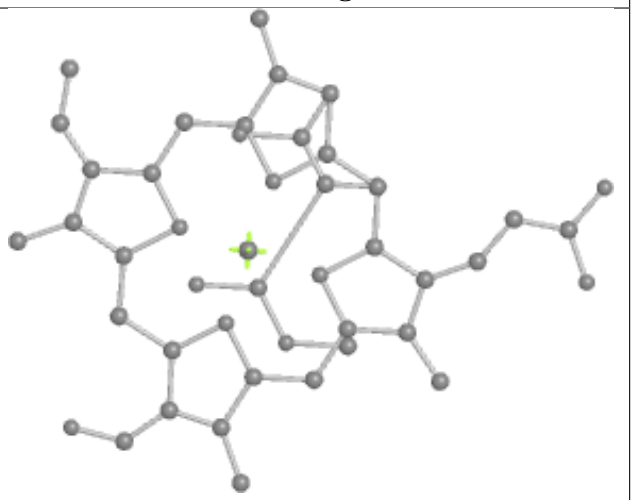


Bond angles

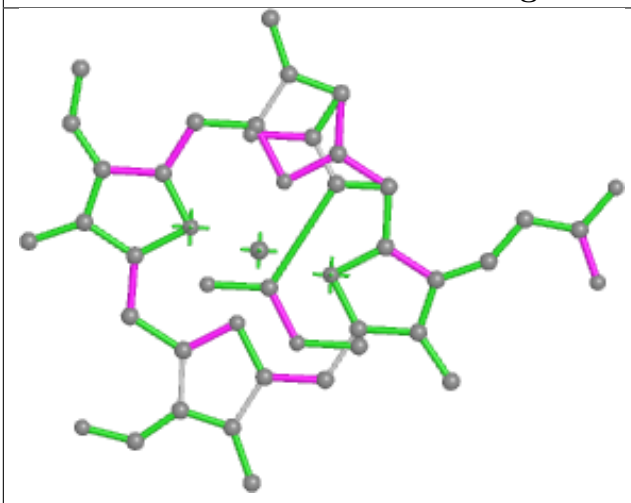


Torsions



Rings

Ligand CL7 B 1224



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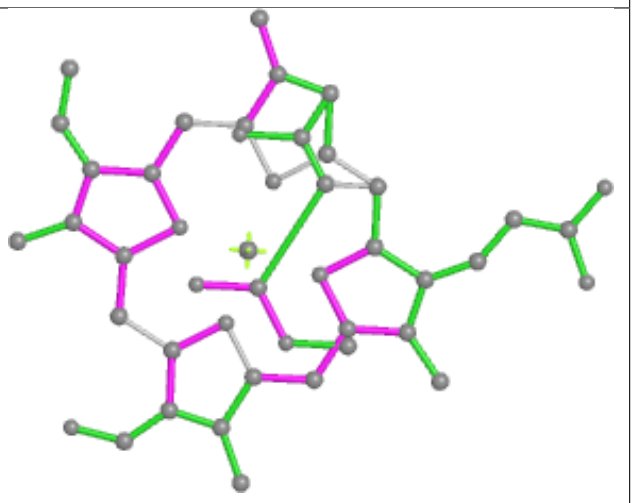
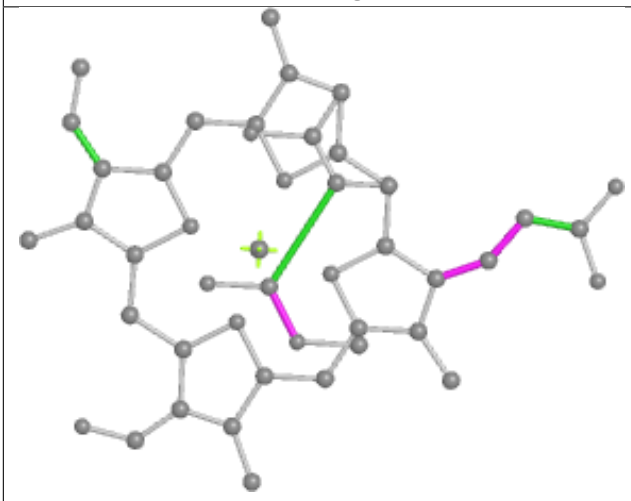
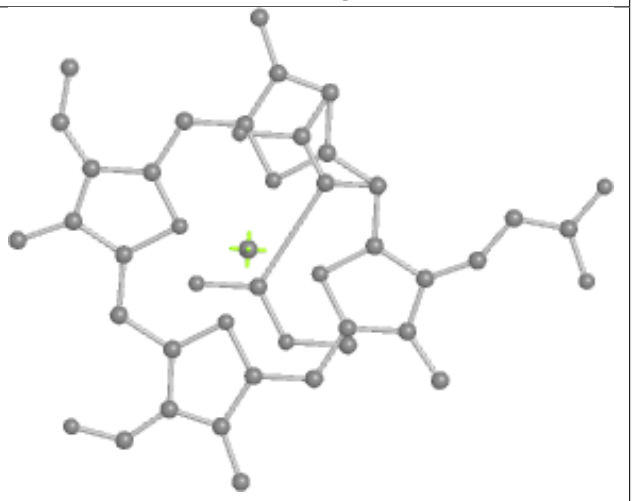


Bond angles

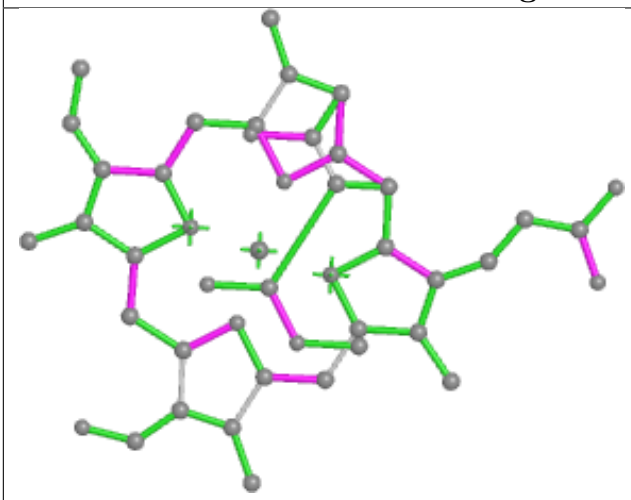


Torsions



Rings

Ligand CL7 A 1802



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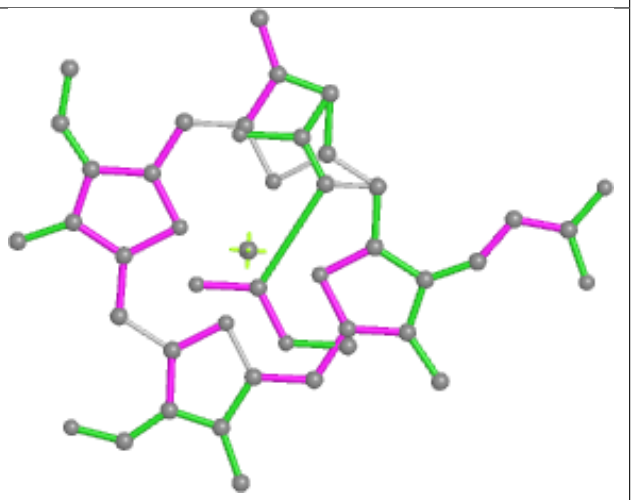
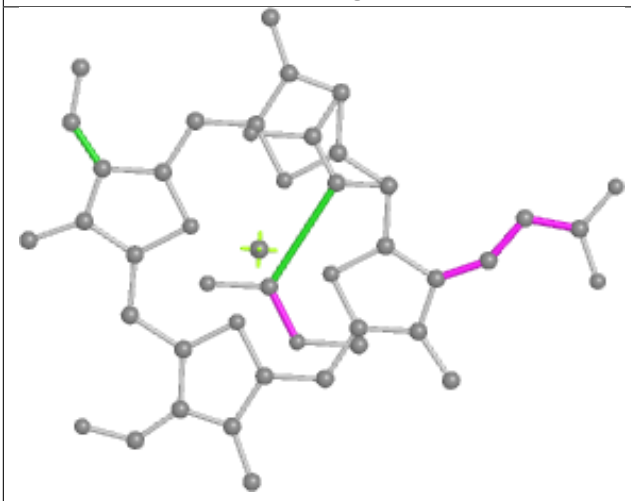
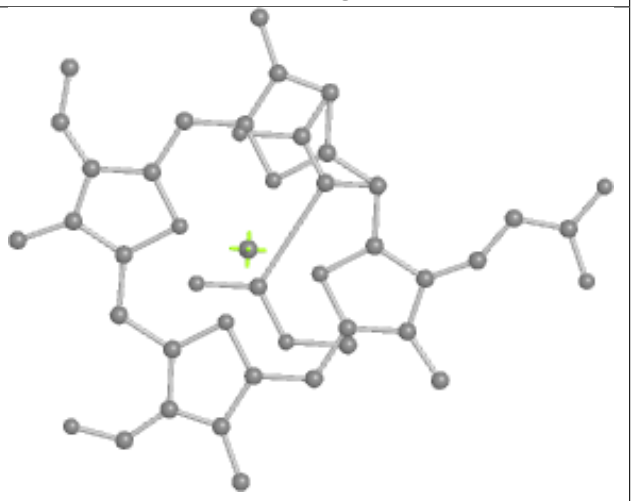


Bond angles

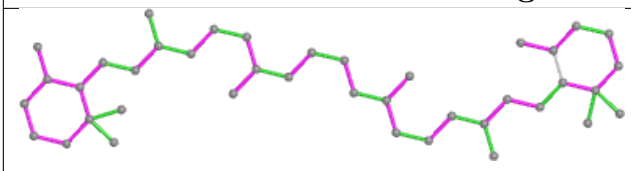


Torsions



Rings

Ligand 8CT A 4008



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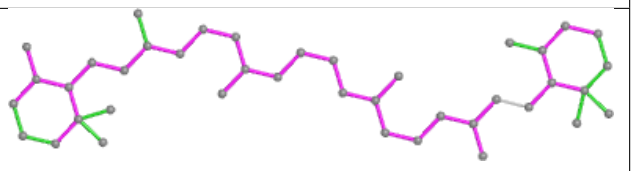
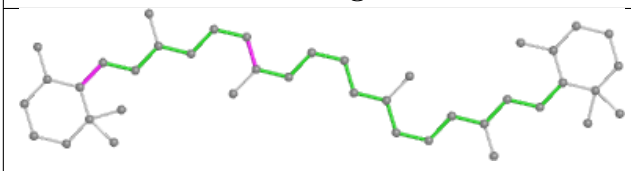
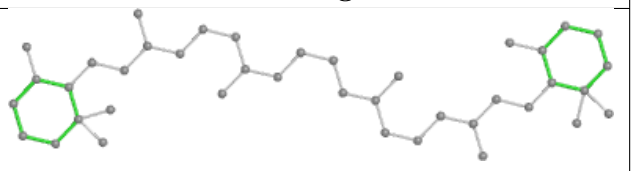


Bond angles

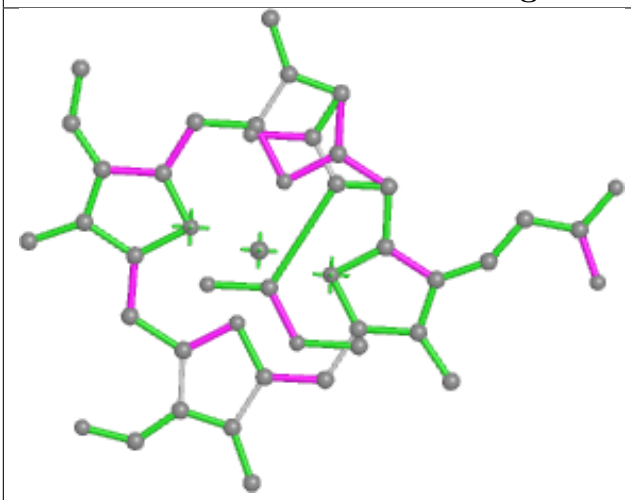


Torsions

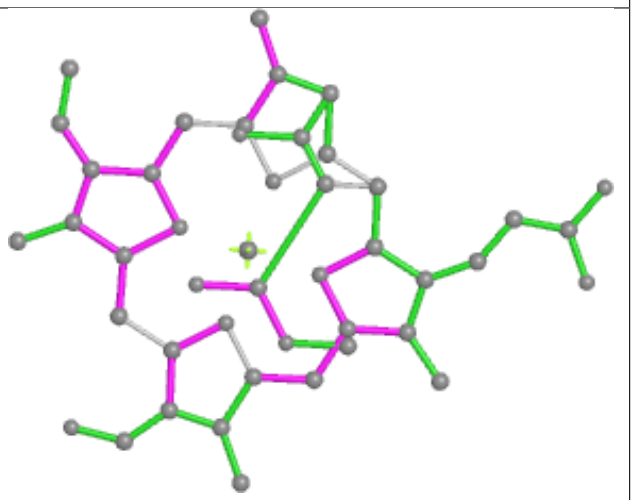


Rings

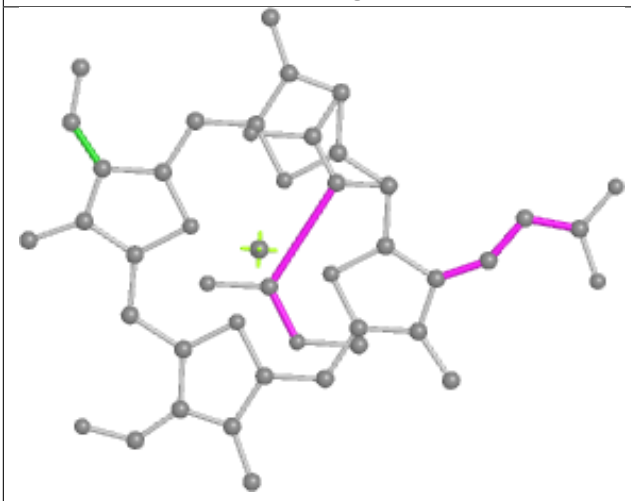
Ligand CL7 B 1212



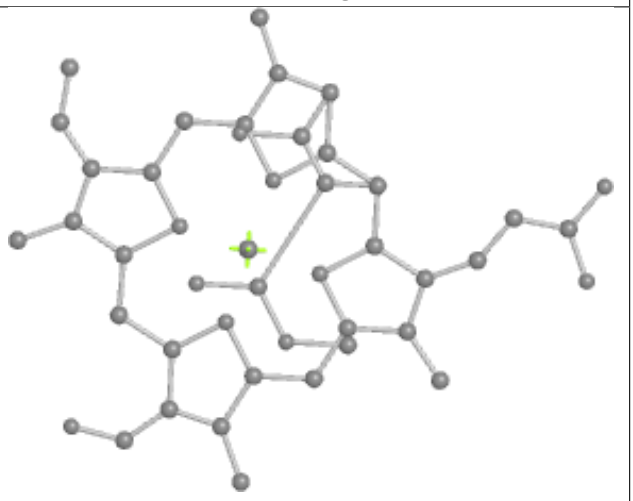
Bond lengths



Bond angles

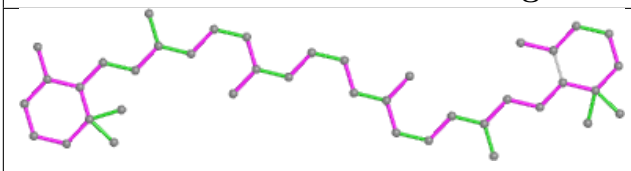


Torsions

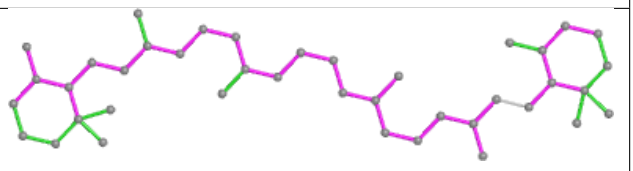


Rings

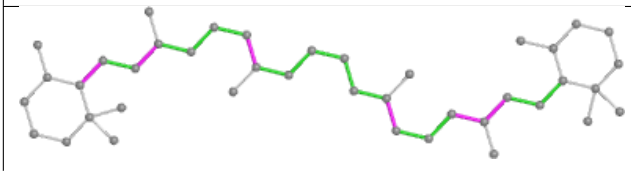
Ligand 8CT J 4015



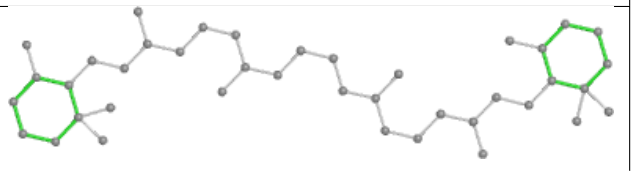
Bond lengths



Bond angles

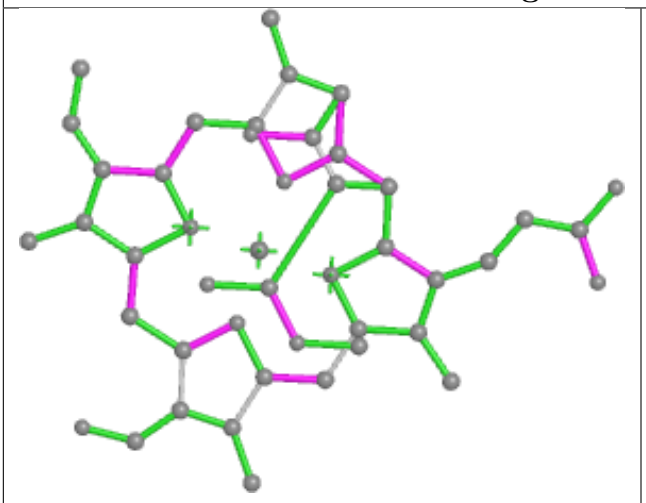


Torsions

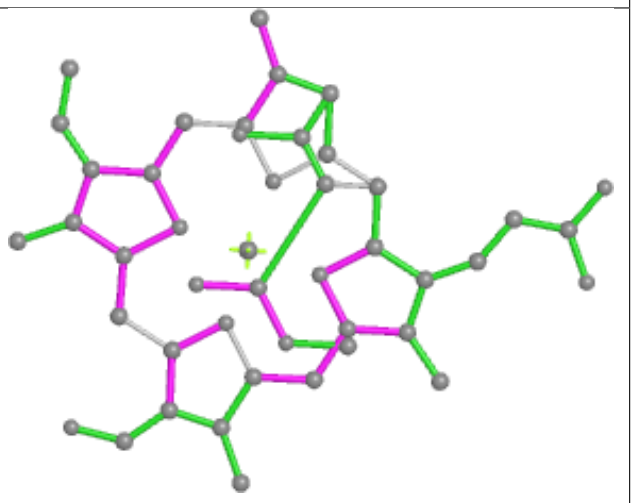


Rings

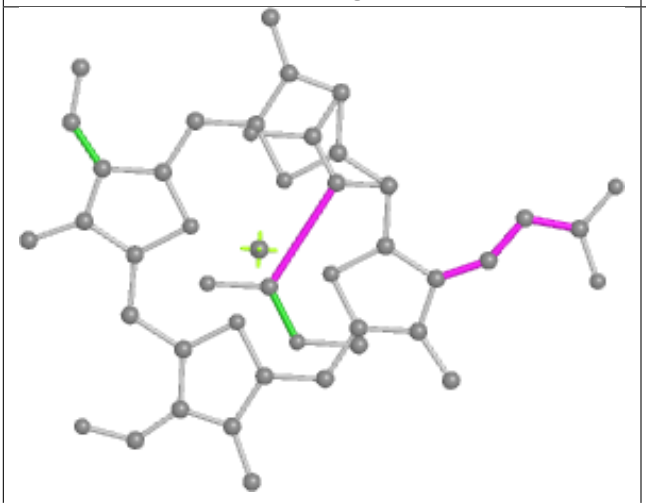
Ligand CL7 F 1301



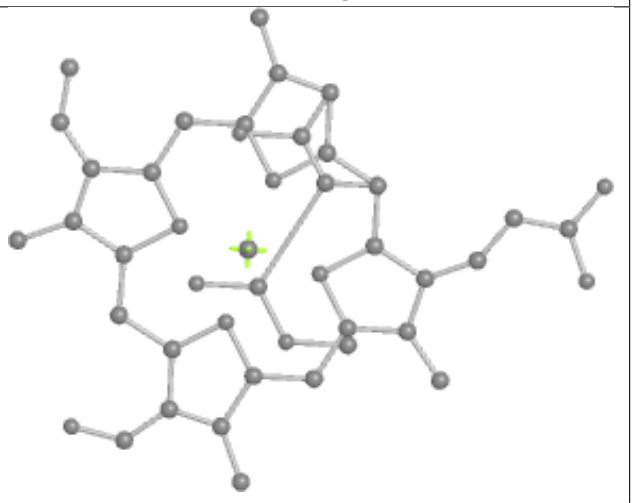
Bond lengths



Bond angles

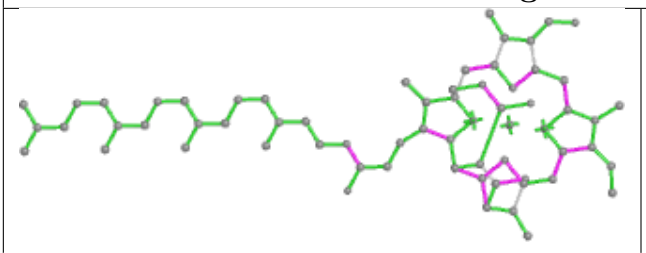


Torsions

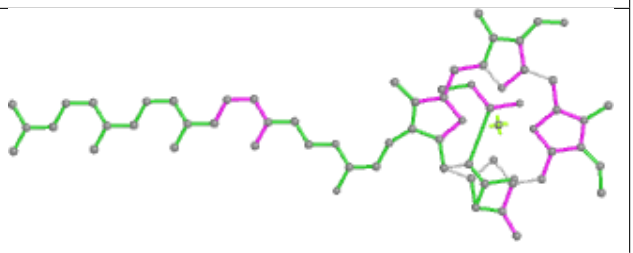


Rings

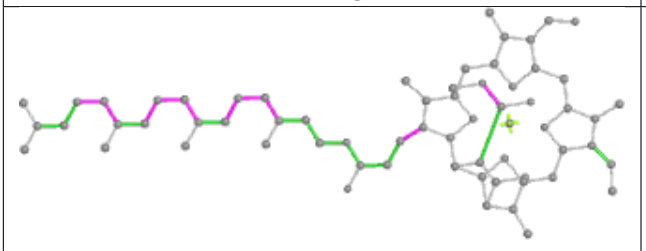
Ligand CL7 B 1012



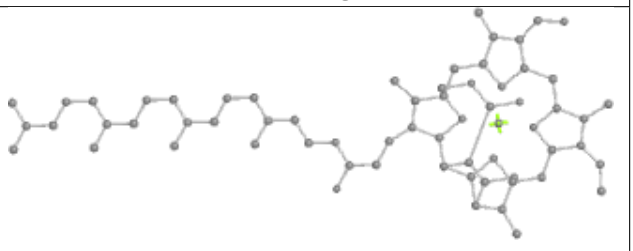
Bond lengths



Bond angles

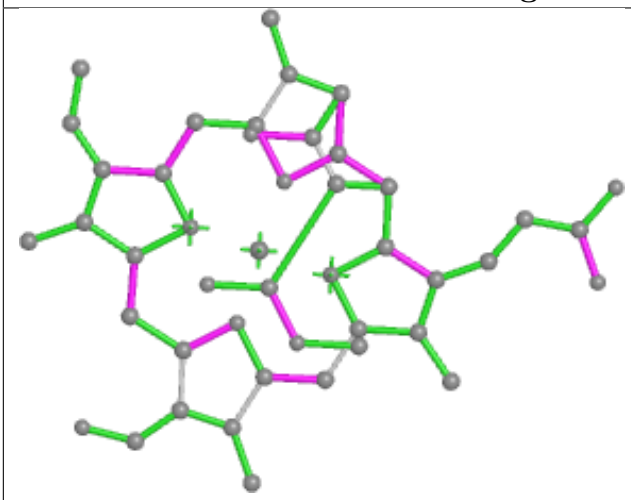


Torsions

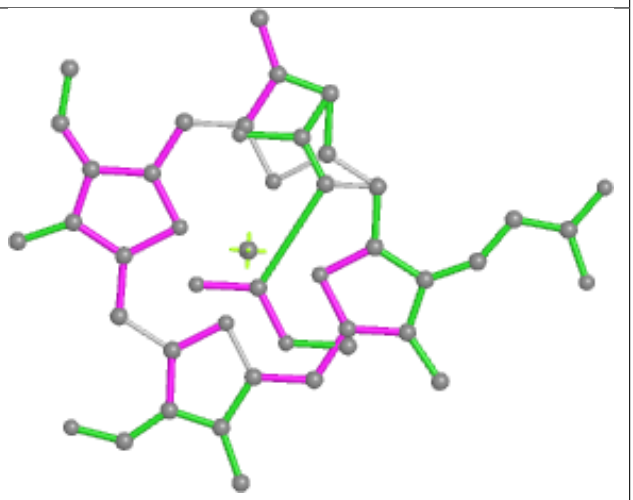


Rings

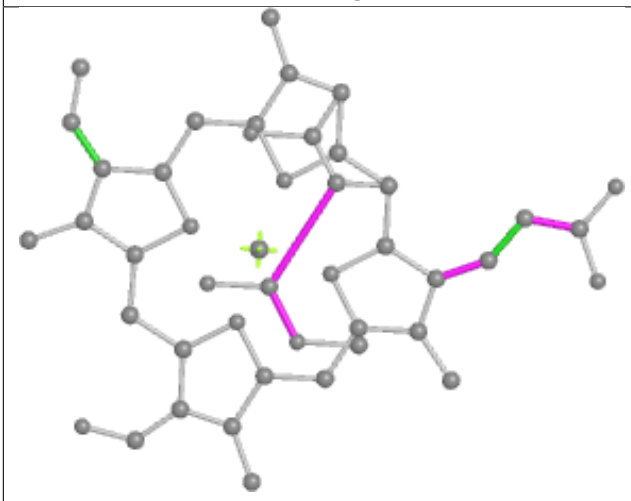
Ligand CL7 B 1213



Bond lengths



Bond angles



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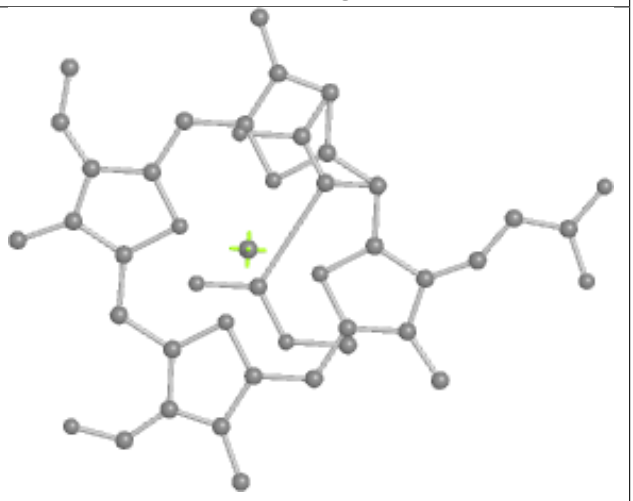
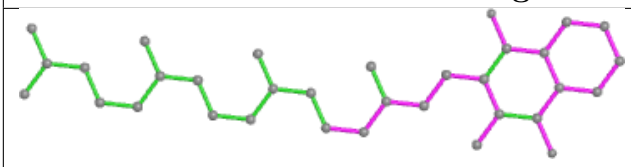


Rings

Ligand PQN A 2001



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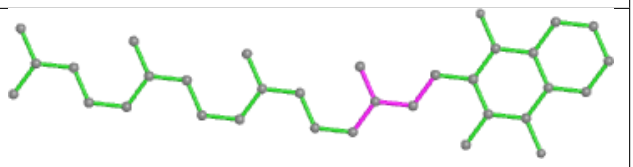
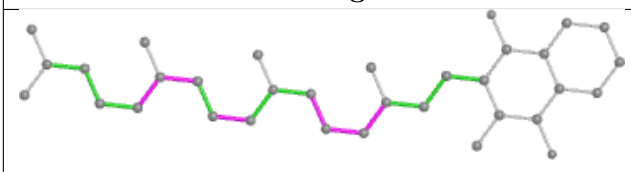


Bond angles



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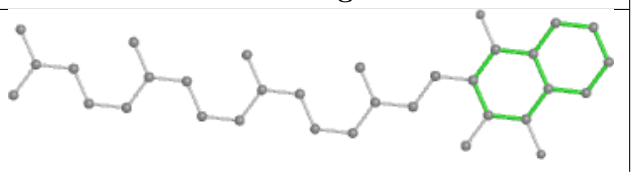
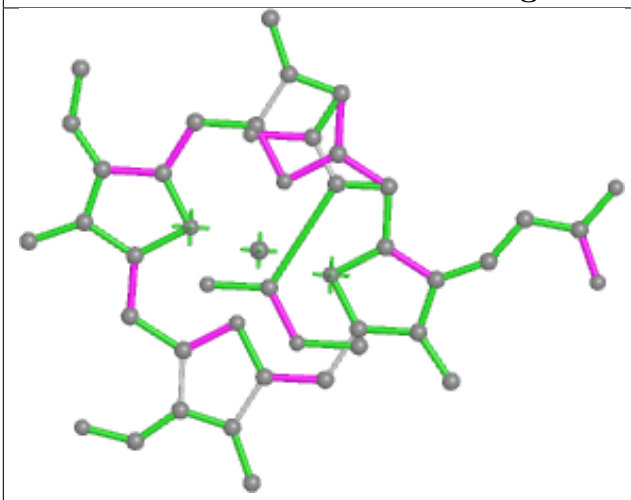
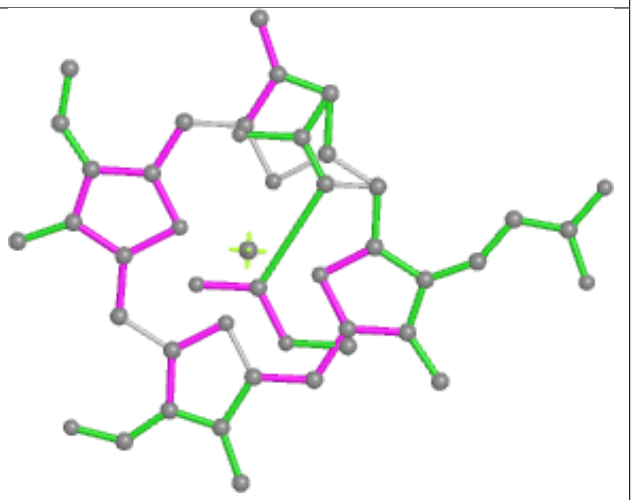


Rings

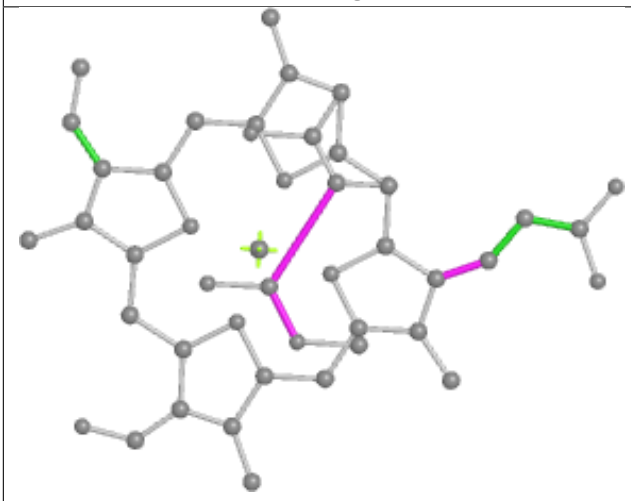
Ligand CL7 B 1202



Bond lengths



Bond angles



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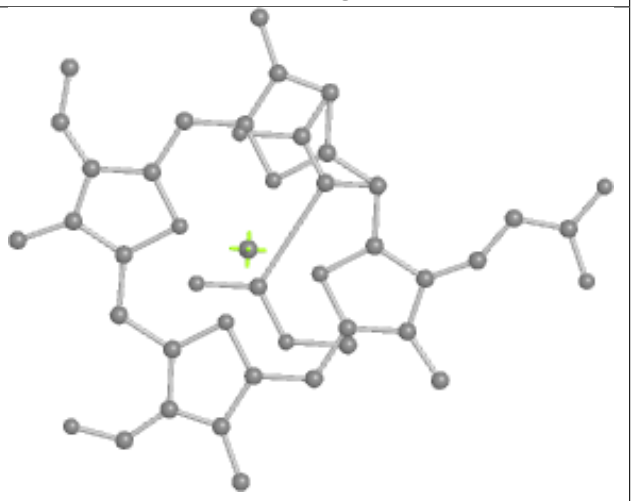
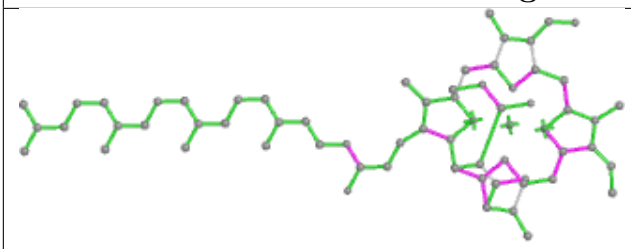


Rings

Ligand CL7 A 1104



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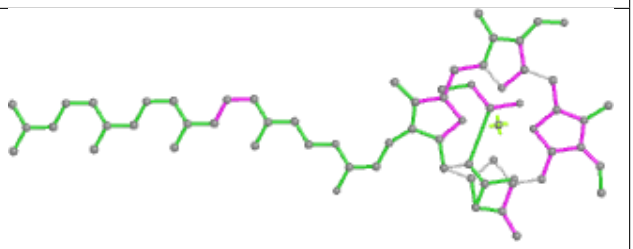
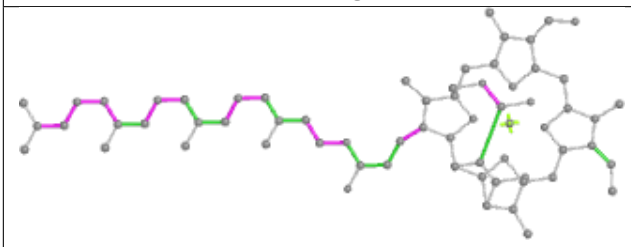
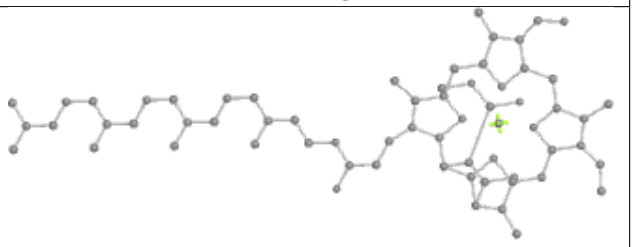


Bond angles

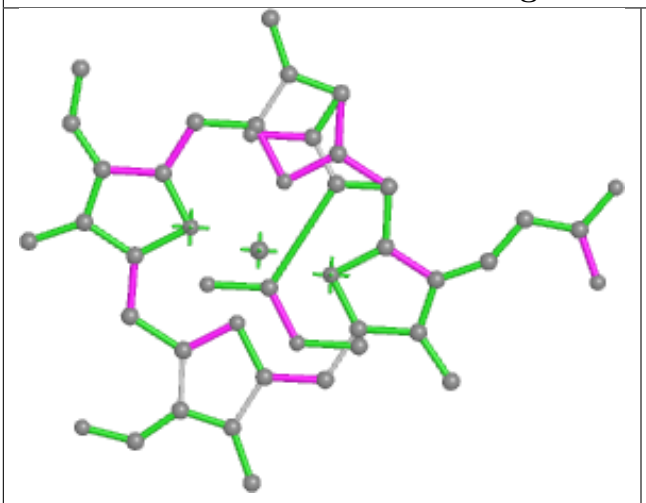


Torsions

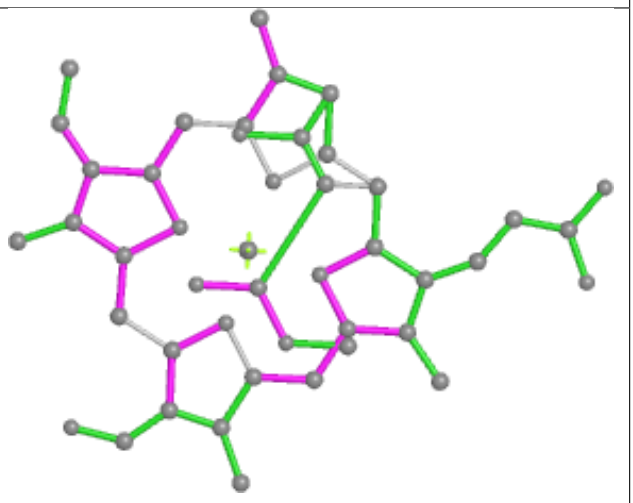


Rings

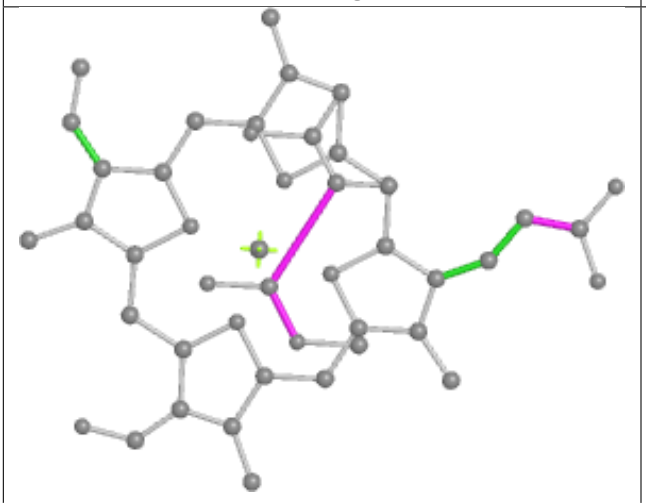
Ligand CL7 B 1223



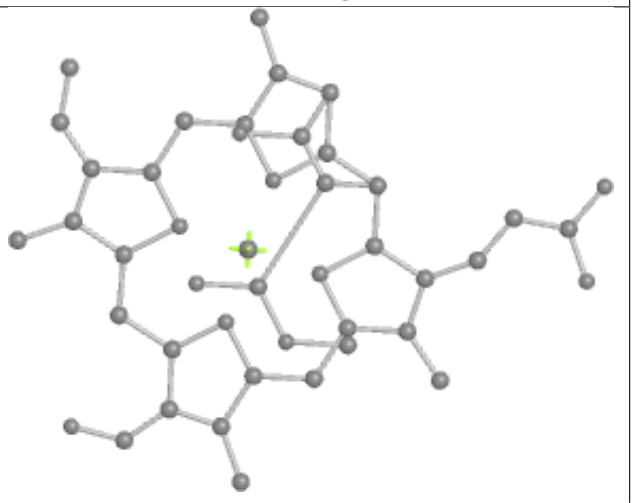
Bond lengths



Bond angles

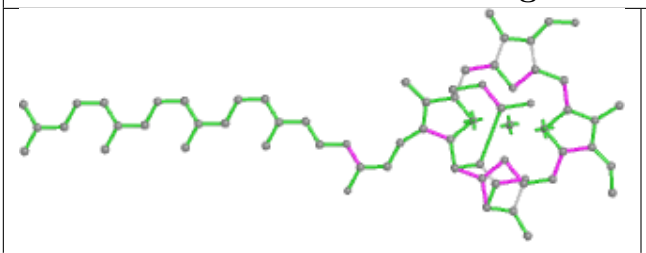


Torsions



Rings

Ligand CL7 A 1103



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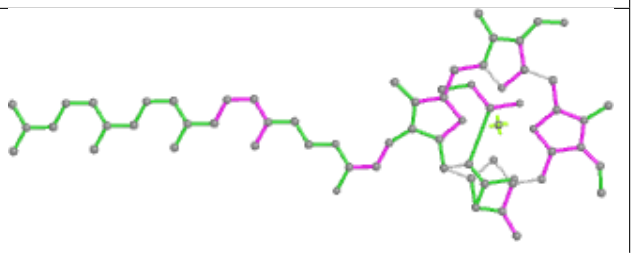
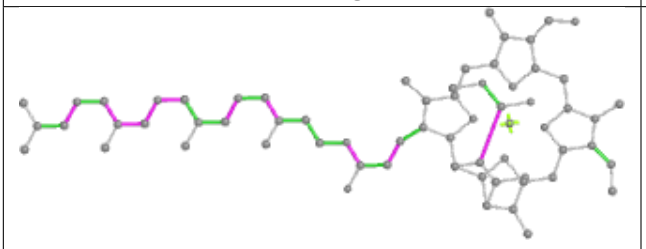
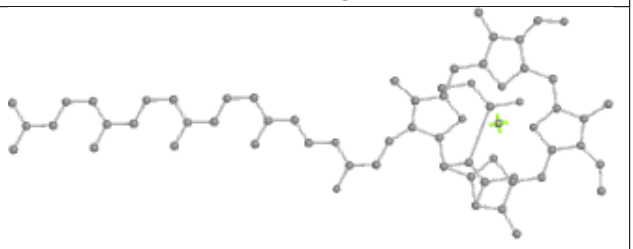


Bond angles

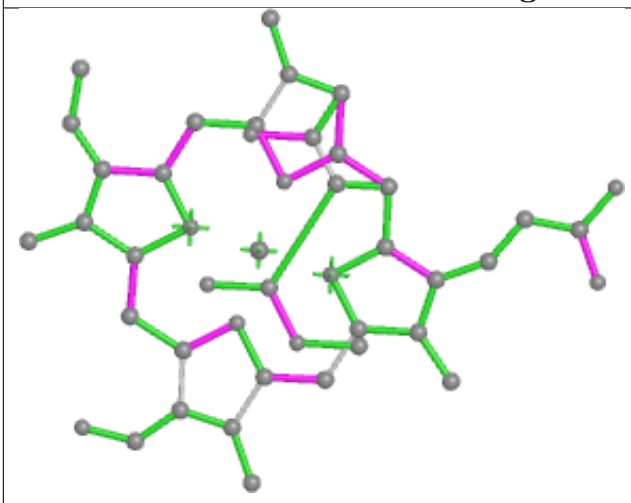


Torsions



Rings

Ligand CL7 A 1111



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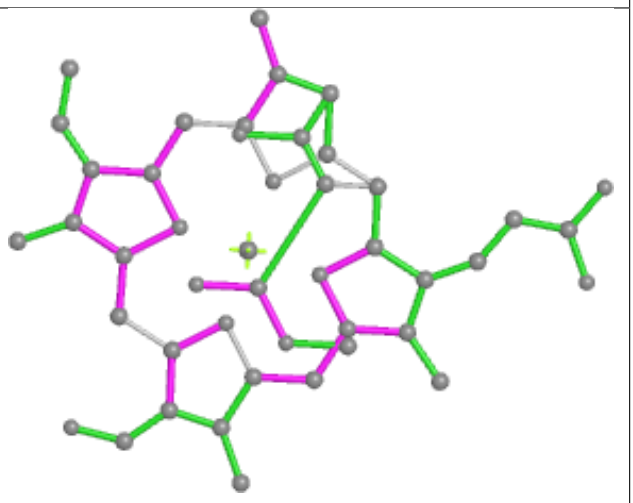
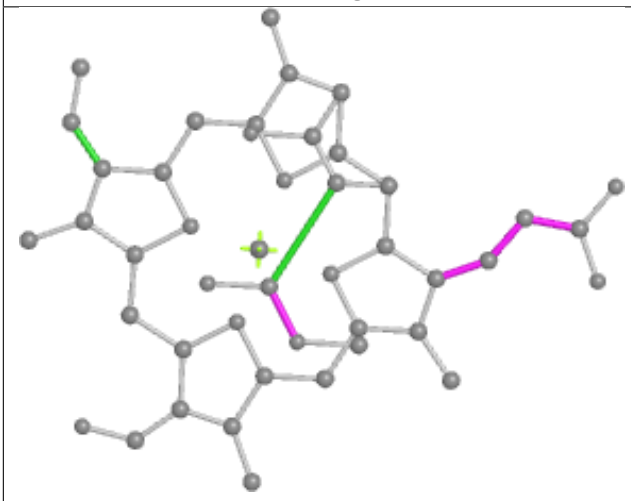


Bond angles



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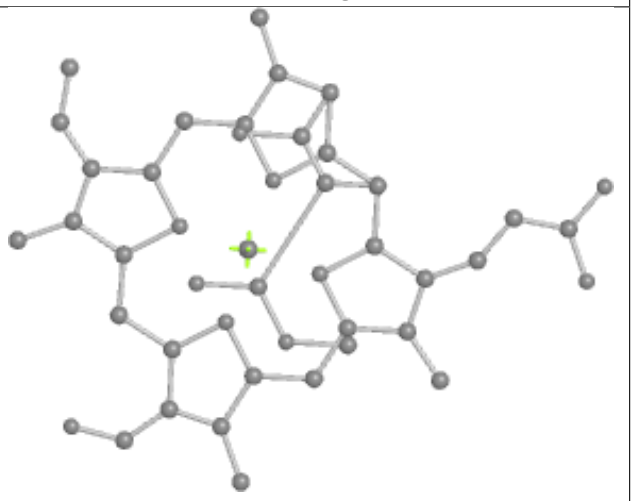
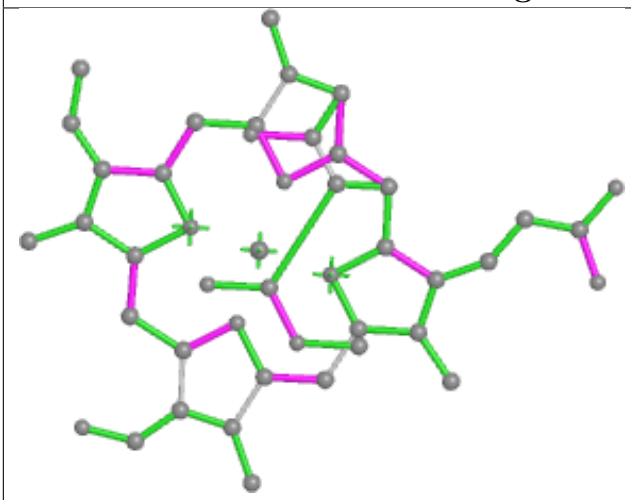


Rings

Ligand CL7 W 2601



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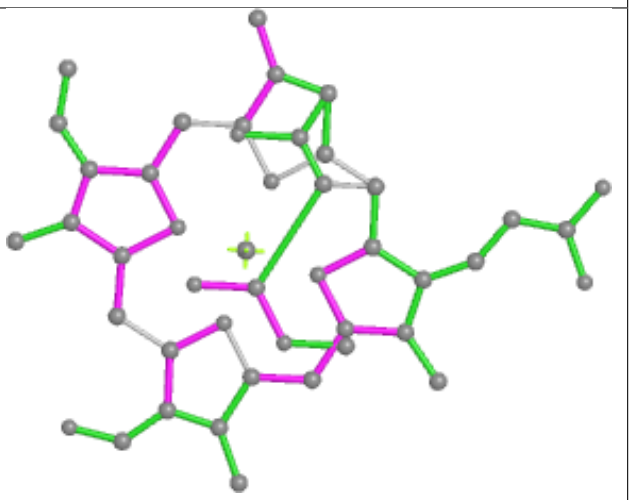
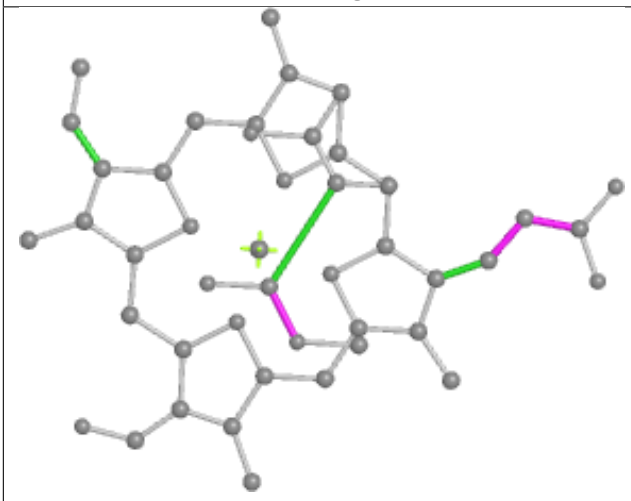


Bond angles



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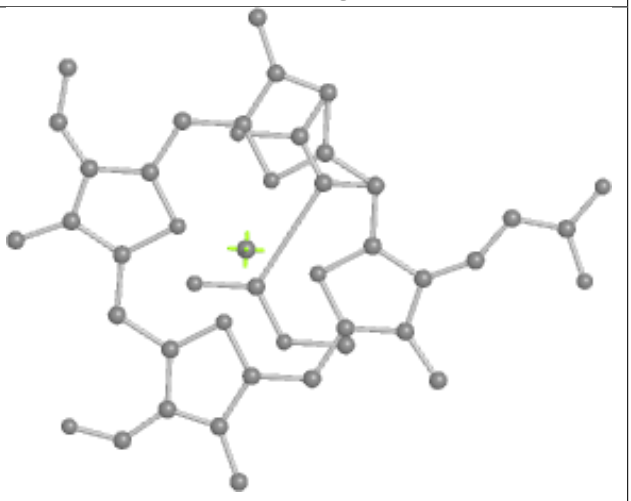
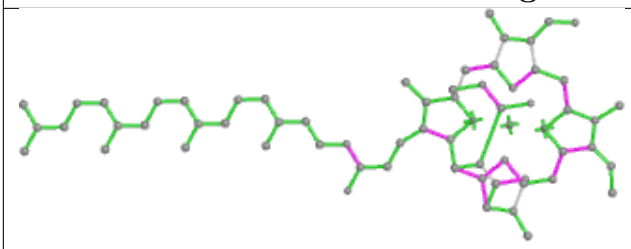


Rings

Ligand CL7 A 1101



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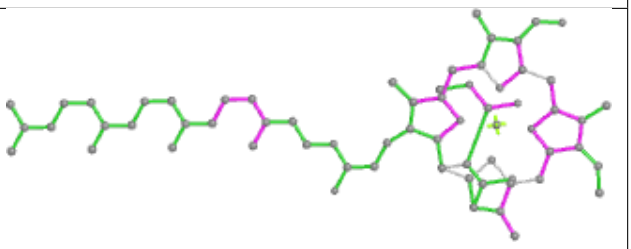
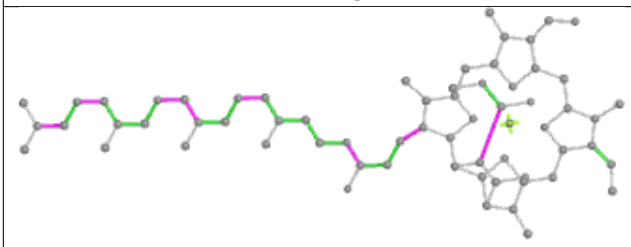


Bond angles



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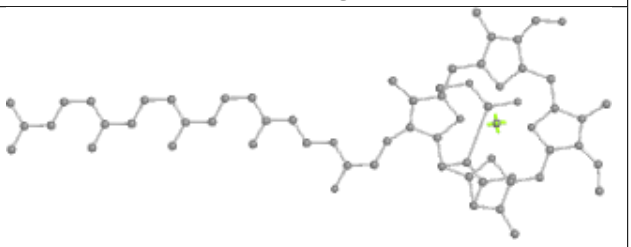
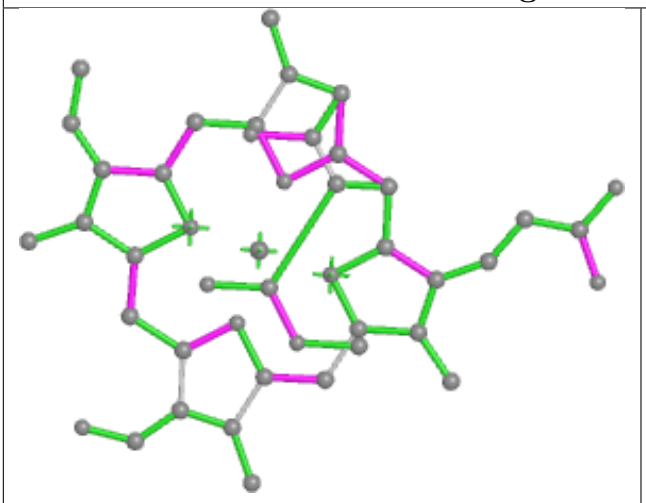
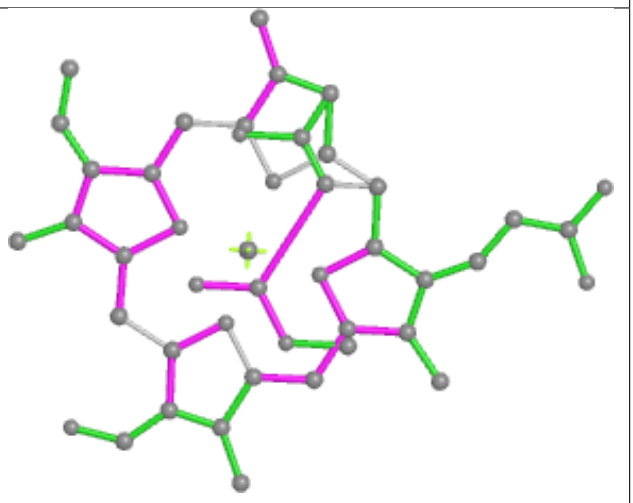


Rings

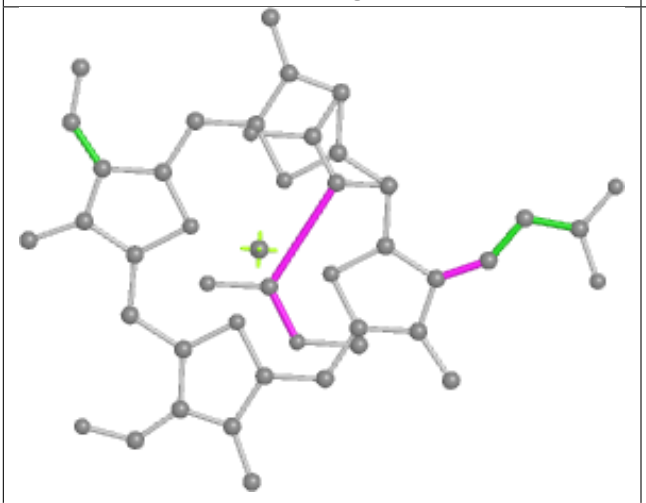
Ligand CL7 A 1110



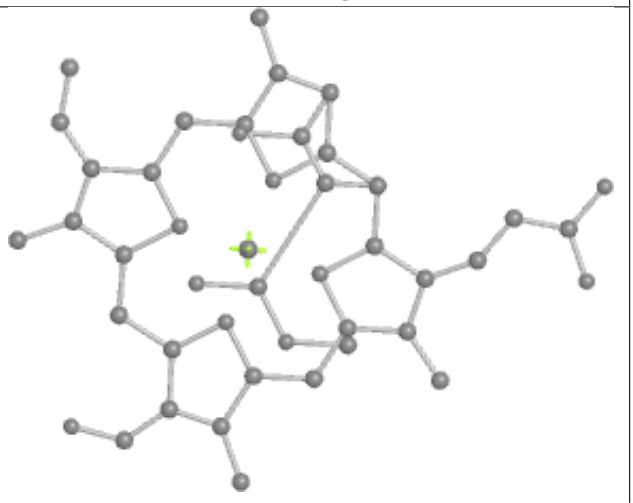
Bond lengths



Bond angles

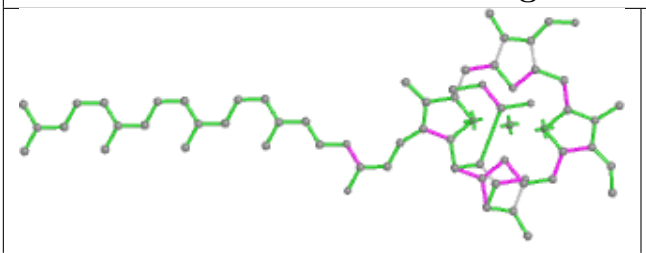


Torsions

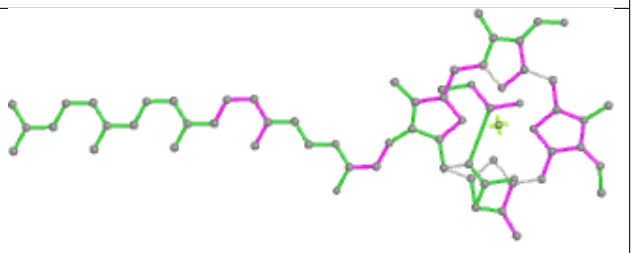


Rings

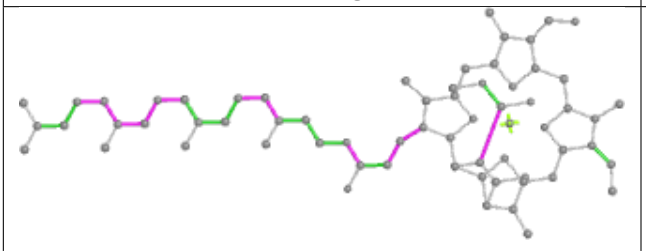
Ligand CL7 A 1128



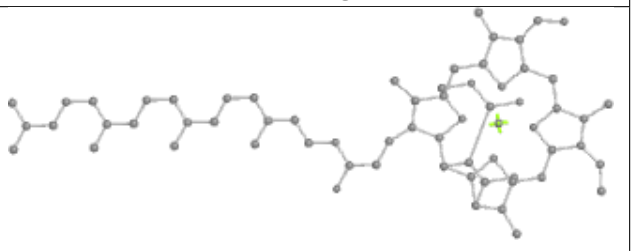
Bond lengths



Bond angles

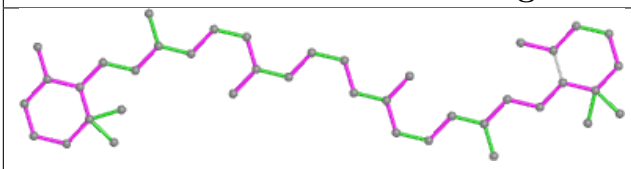


Torsions

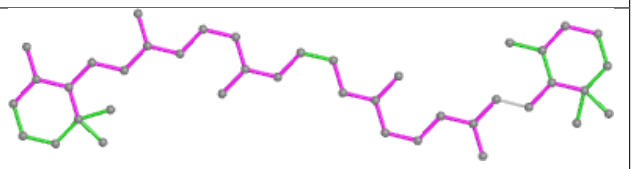


Rings

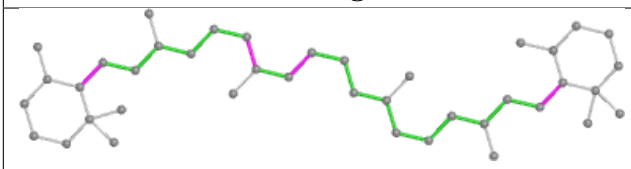
Ligand 8CT A 4007



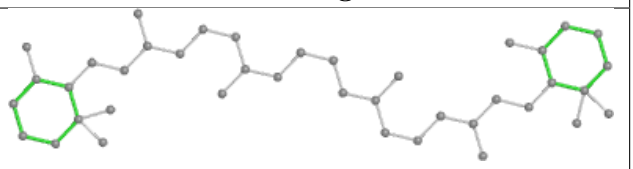
Bond lengths



Bond angles

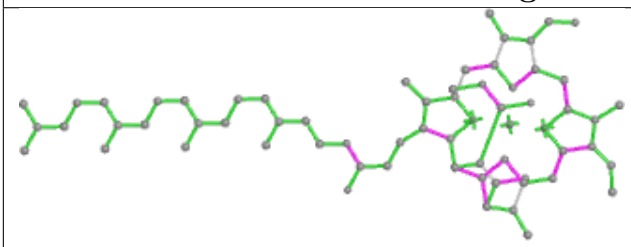


Torsions

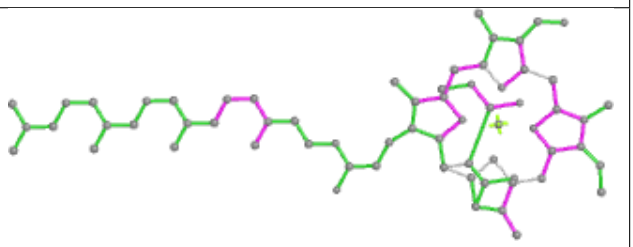


Rings

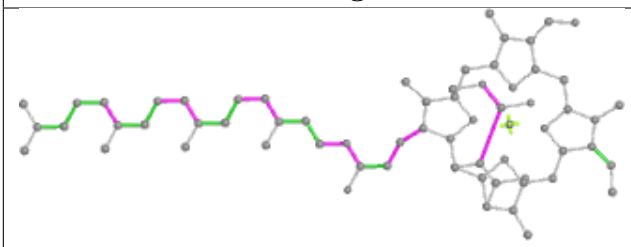
Ligand CL7 A 1106



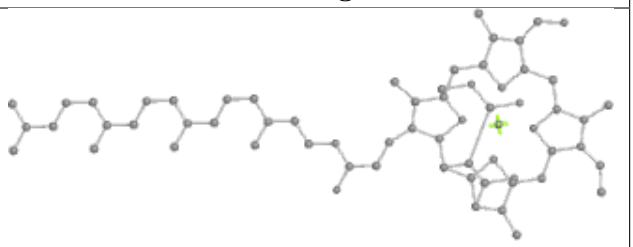
Bond lengths



Bond angles

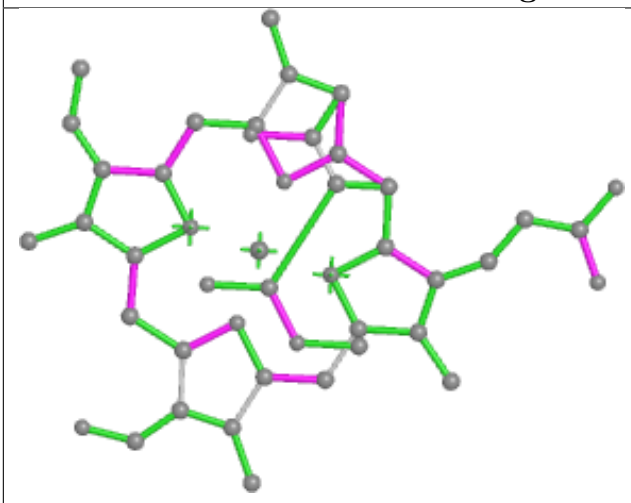


Torsions

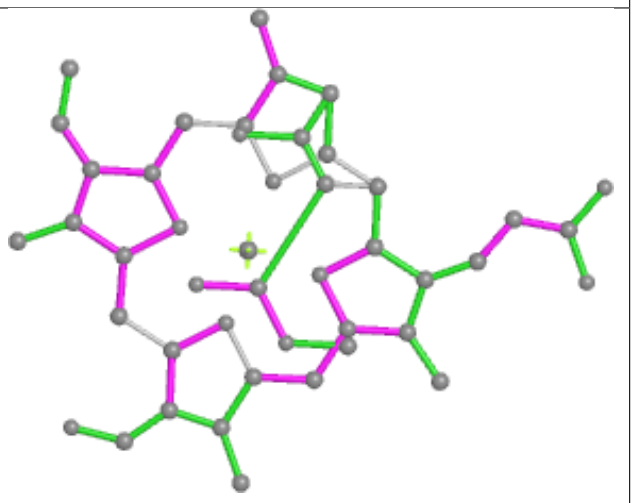


Rings

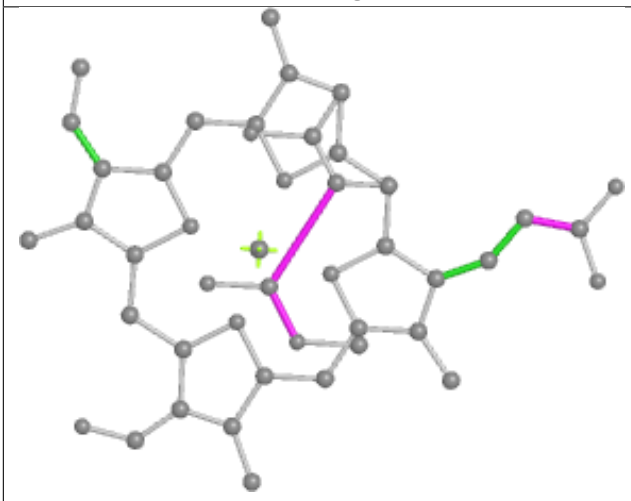
Ligand CL7 A 1113



Bond lengths



Bond angles



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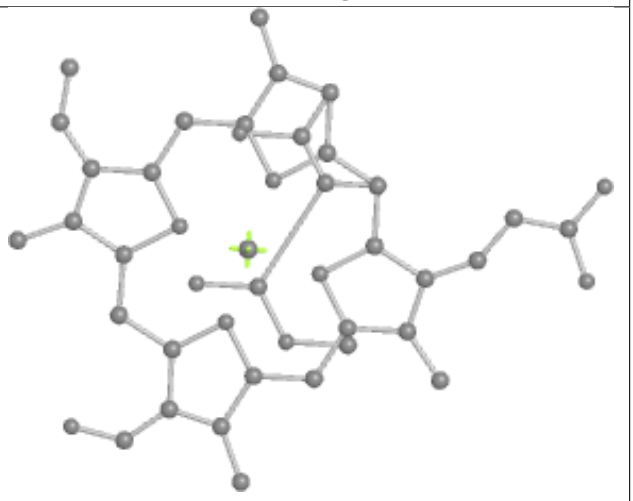
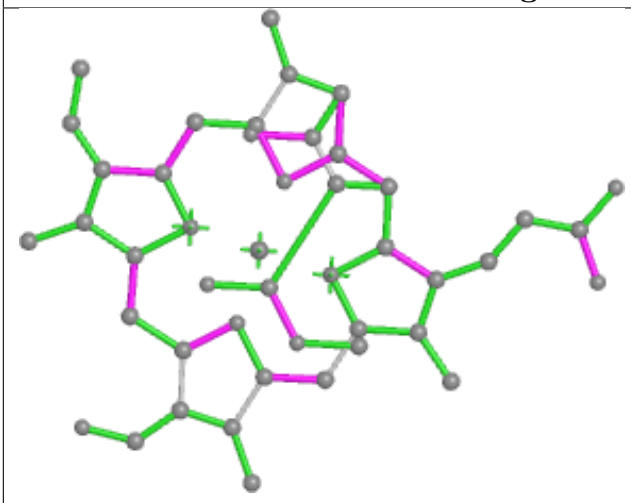


Rings

Ligand CL7 B 1228



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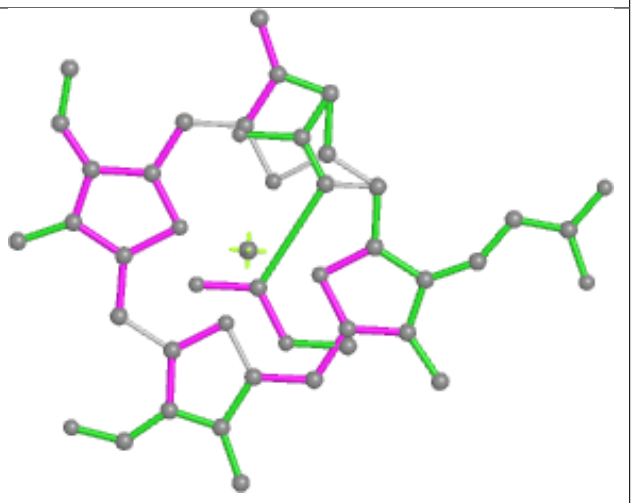
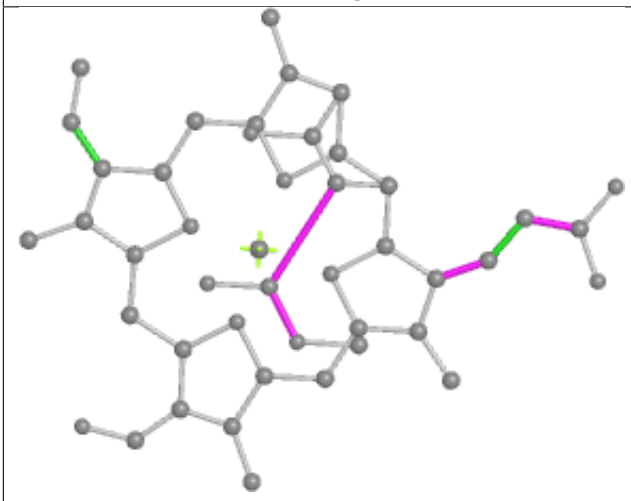
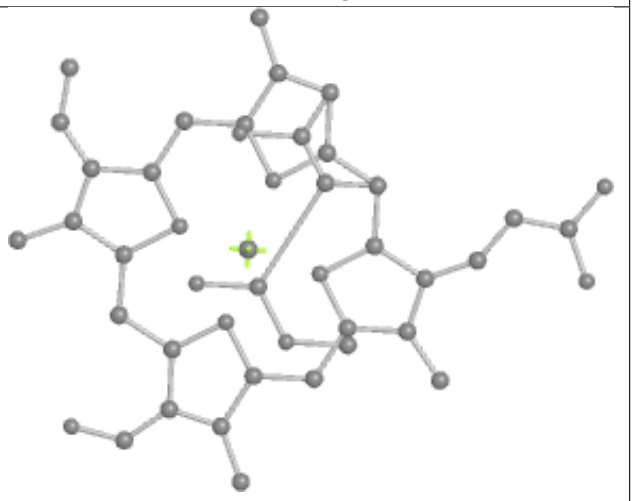


Bond angles

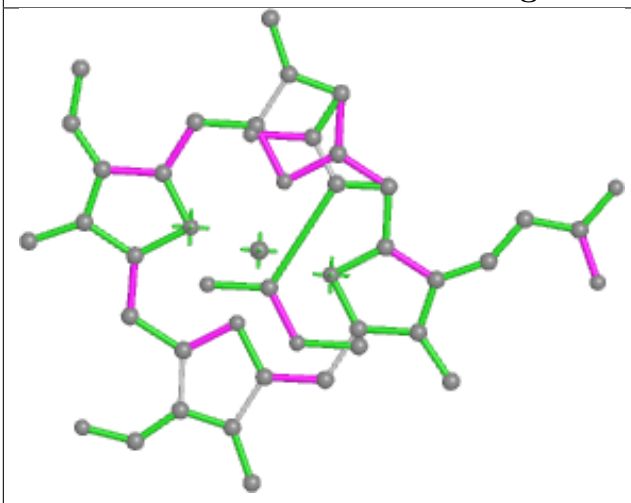


Torsions

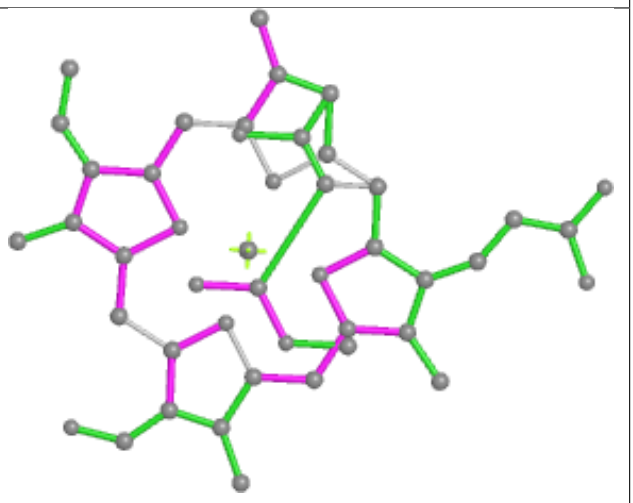


Rings

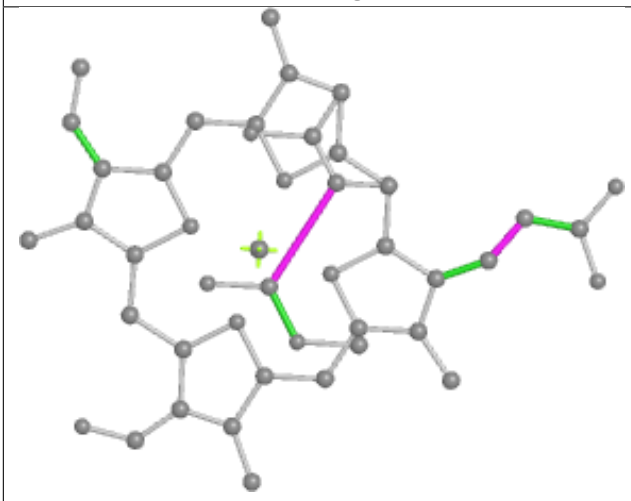
Ligand CL7 B 1234



Bond lengths



Bond angles



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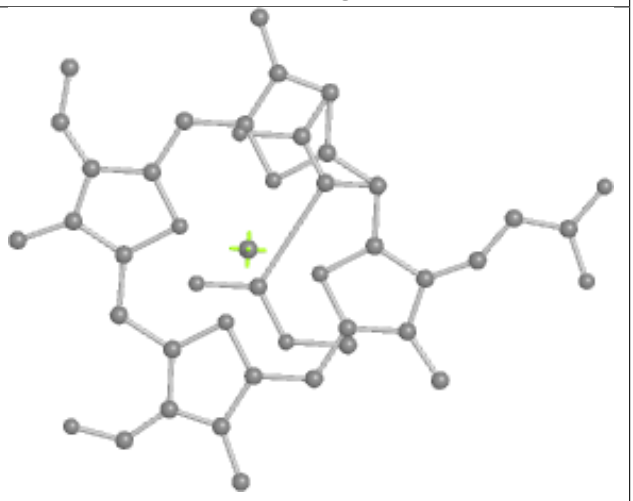
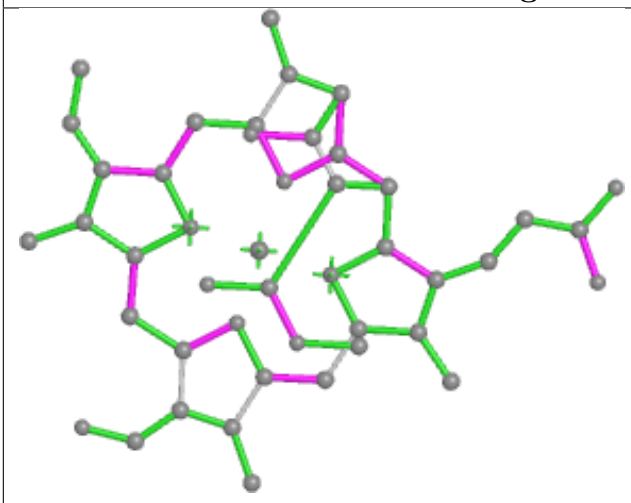
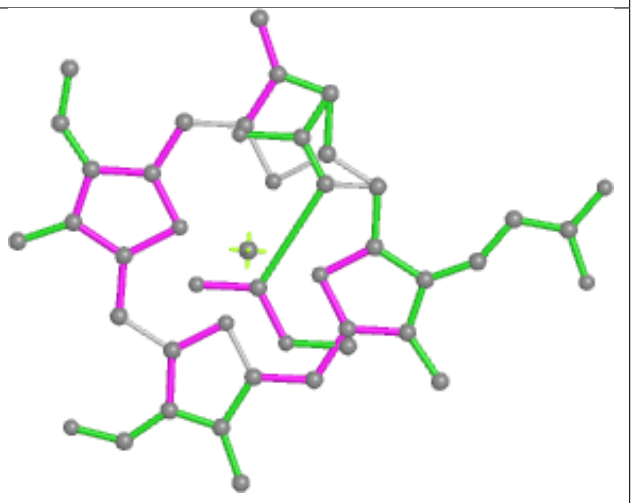


Rings

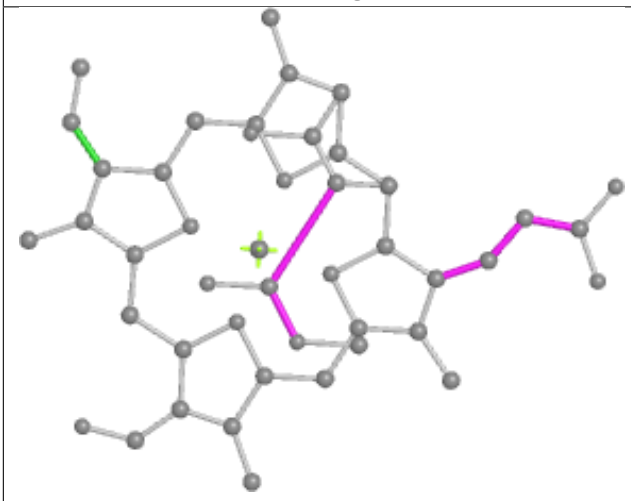
Ligand CL7 B 1211



Bond lengths



Bond angles



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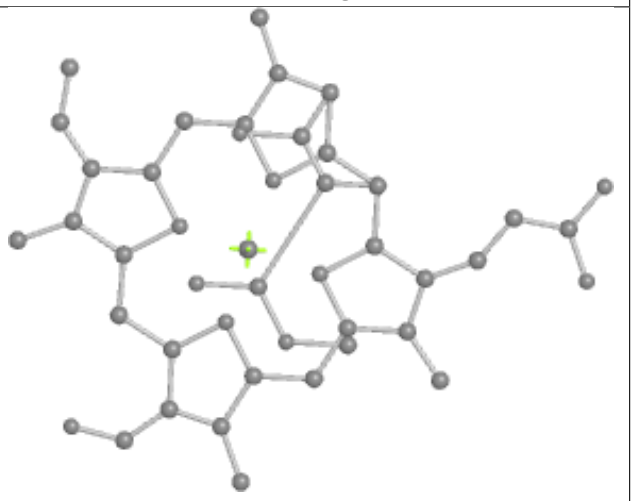
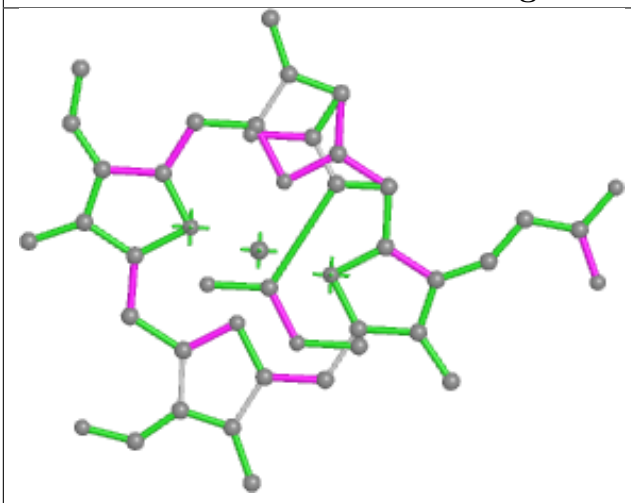
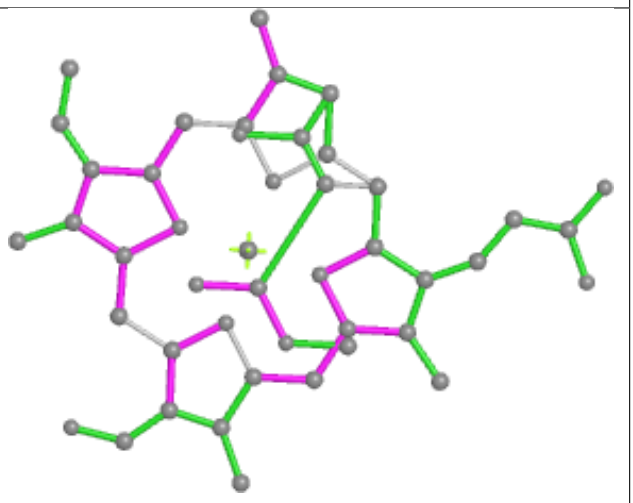


Rings

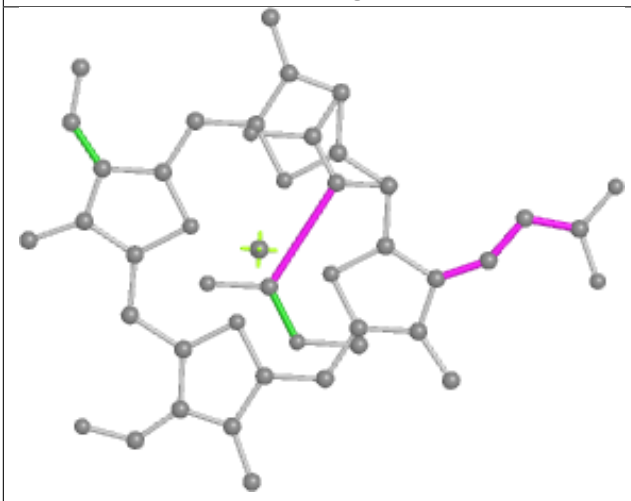
Ligand CL7 A 1112



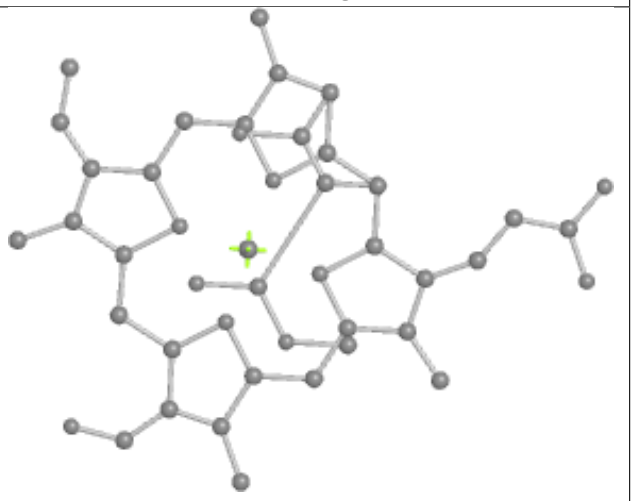
Bond lengths



Bond angles

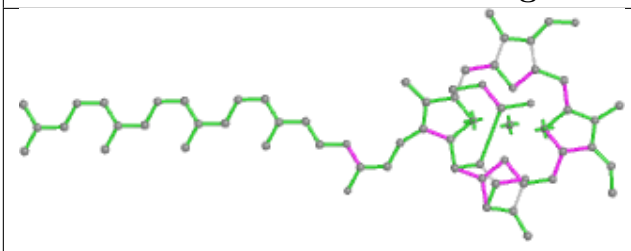


Torsions



Rings

Ligand CL7 A 1022



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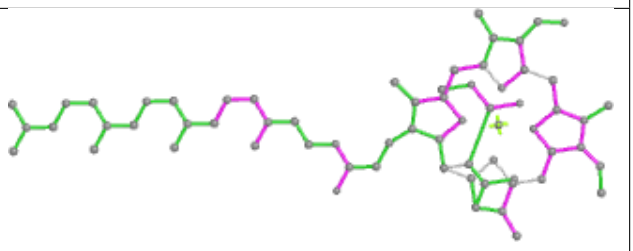
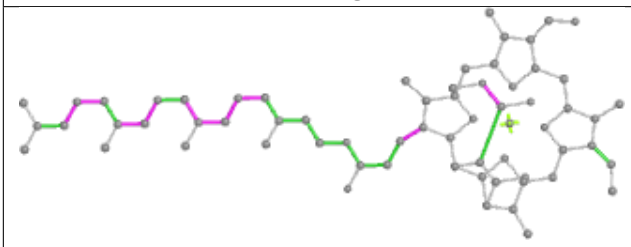
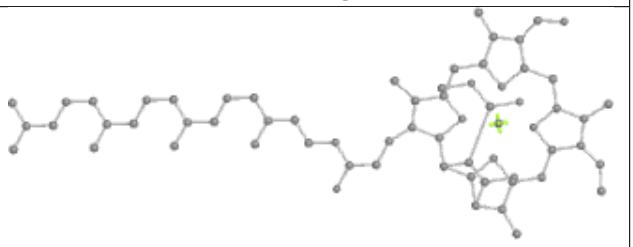


Bond angles

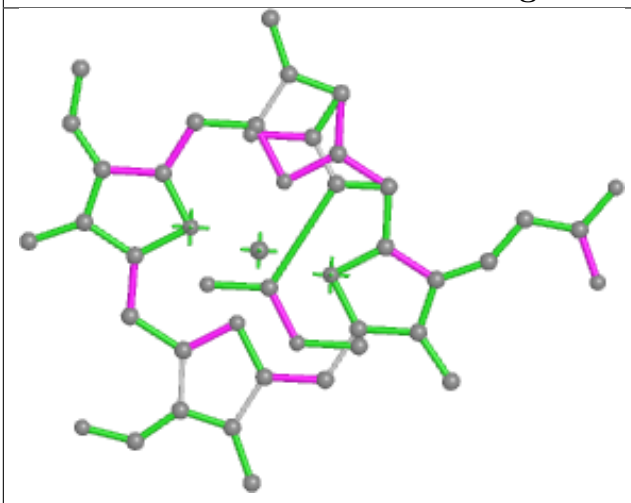


Torsions

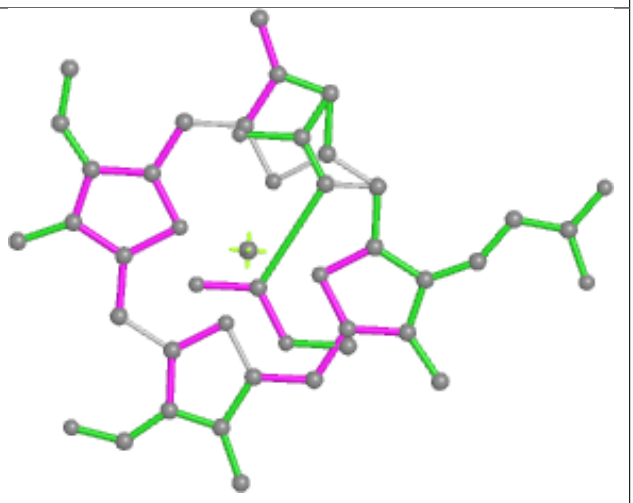


Rings

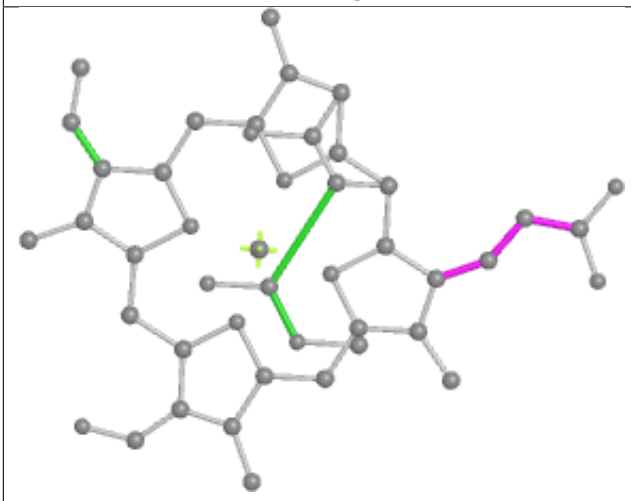
Ligand CL7 A 1121



Bond lengths



Bond angles



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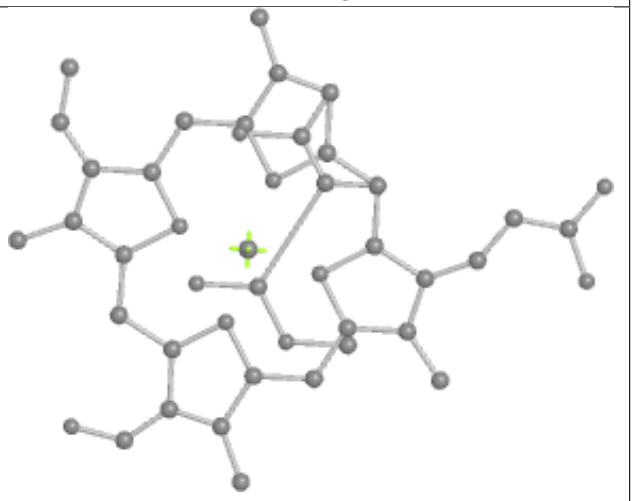
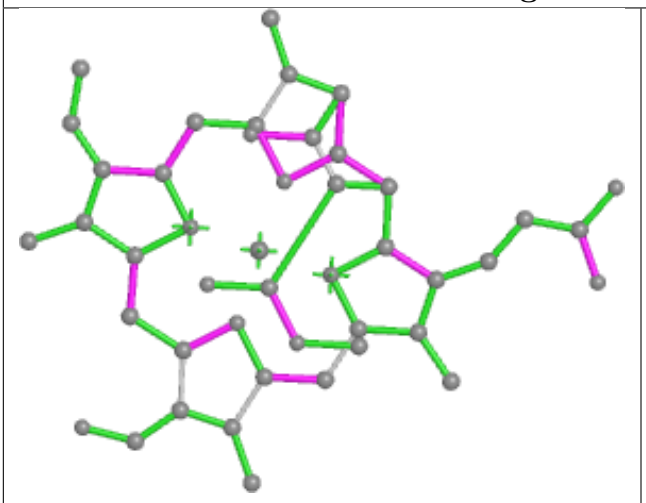
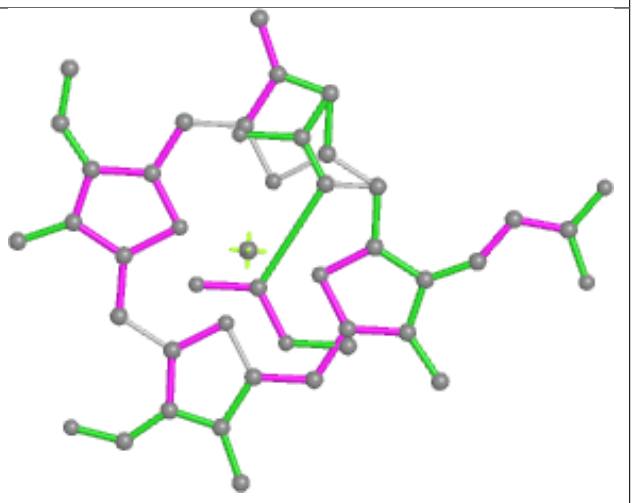


Rings

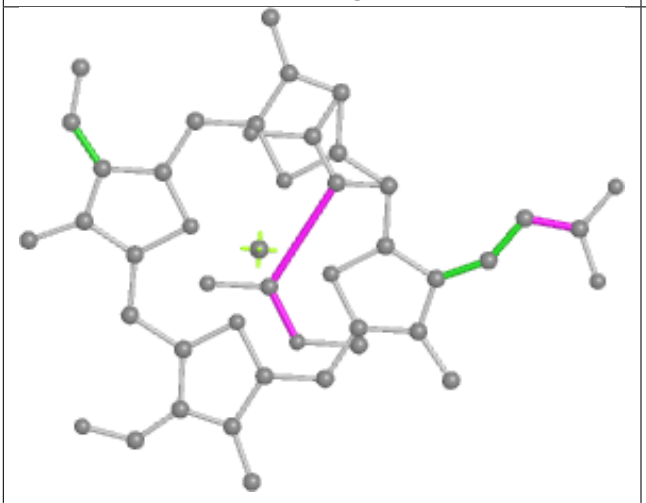
Ligand CL7 B 1208



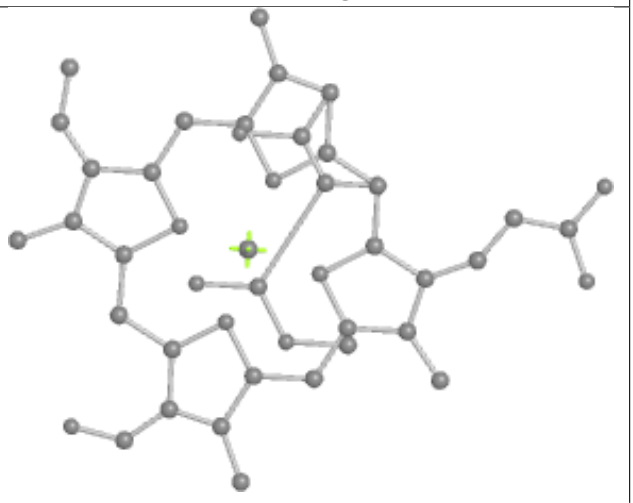
Bond lengths



Bond angles

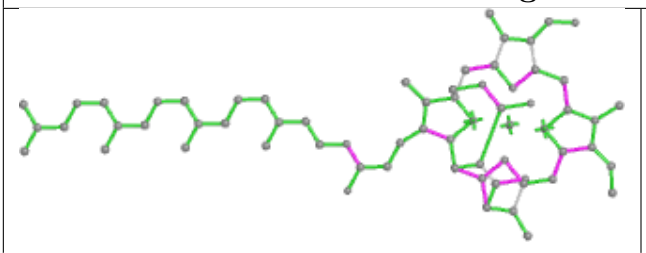


Torsions

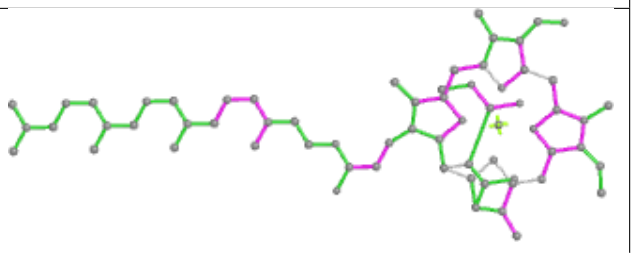


Rings

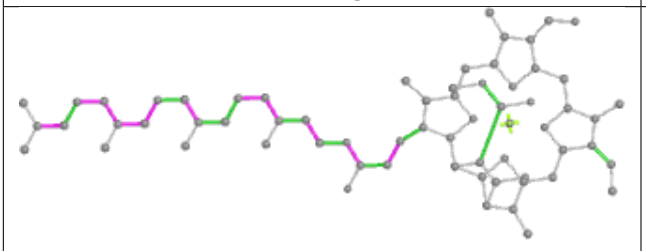
Ligand CL7 A 1237



Bond lengths



Bond angles



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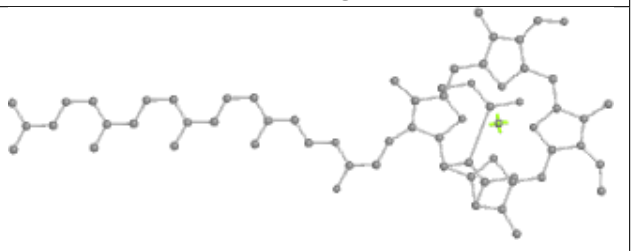
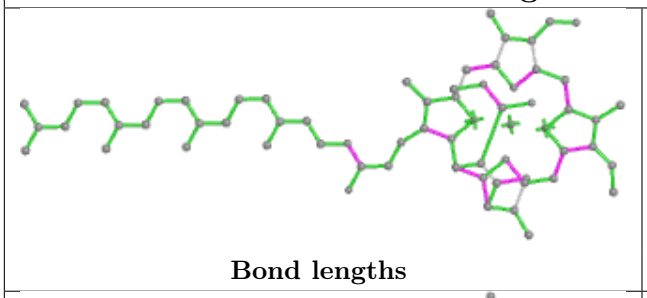
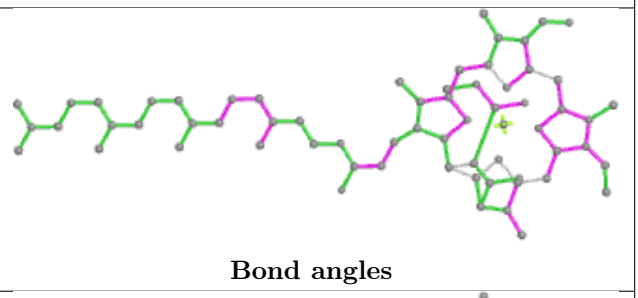


Rings

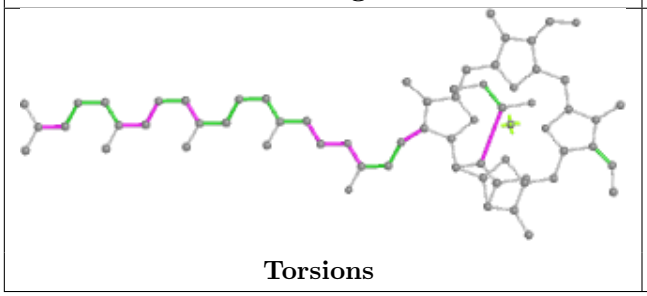
Ligand CL7 A 1125



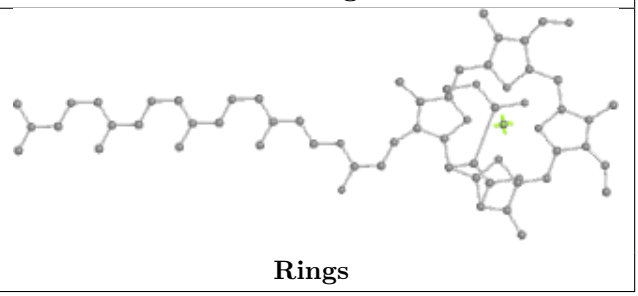
Bond lengths



Bond angles

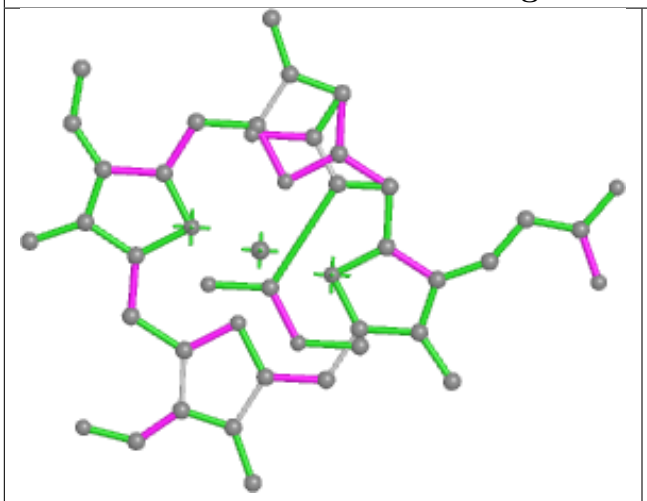


Torsions

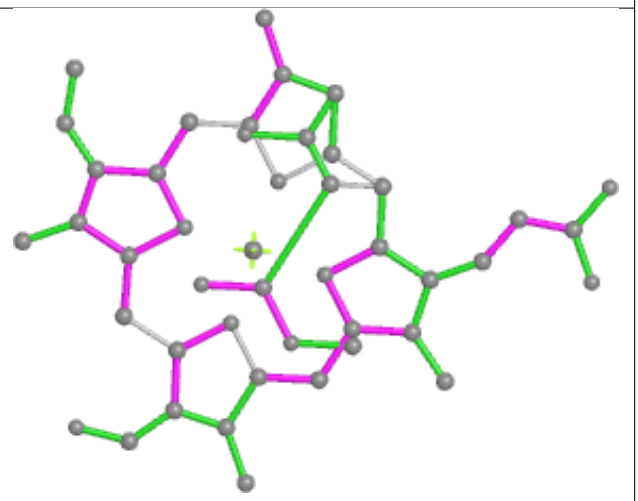


Rings

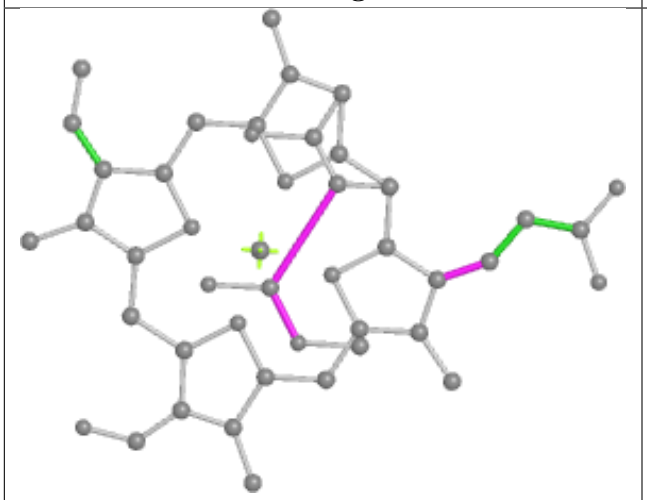
Ligand CL7 B 1214



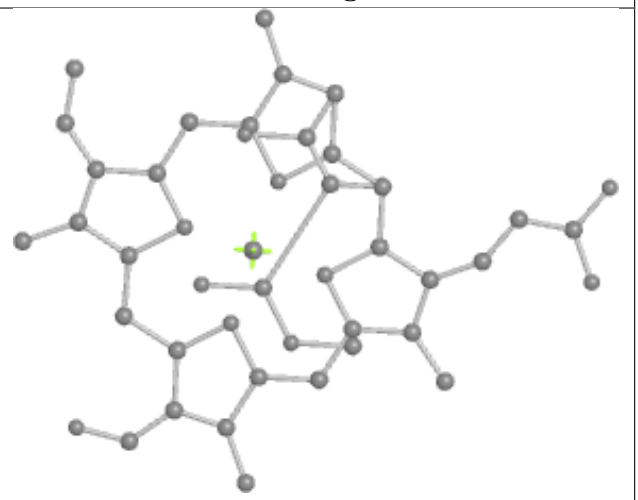
Bond lengths



Bond angles

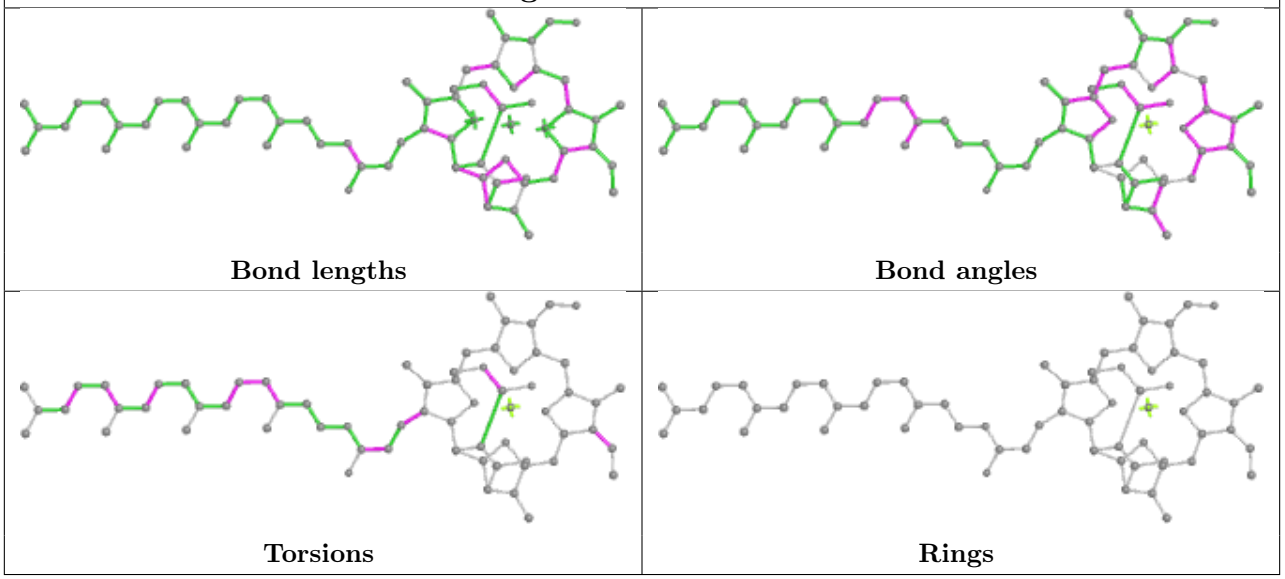


Torsions

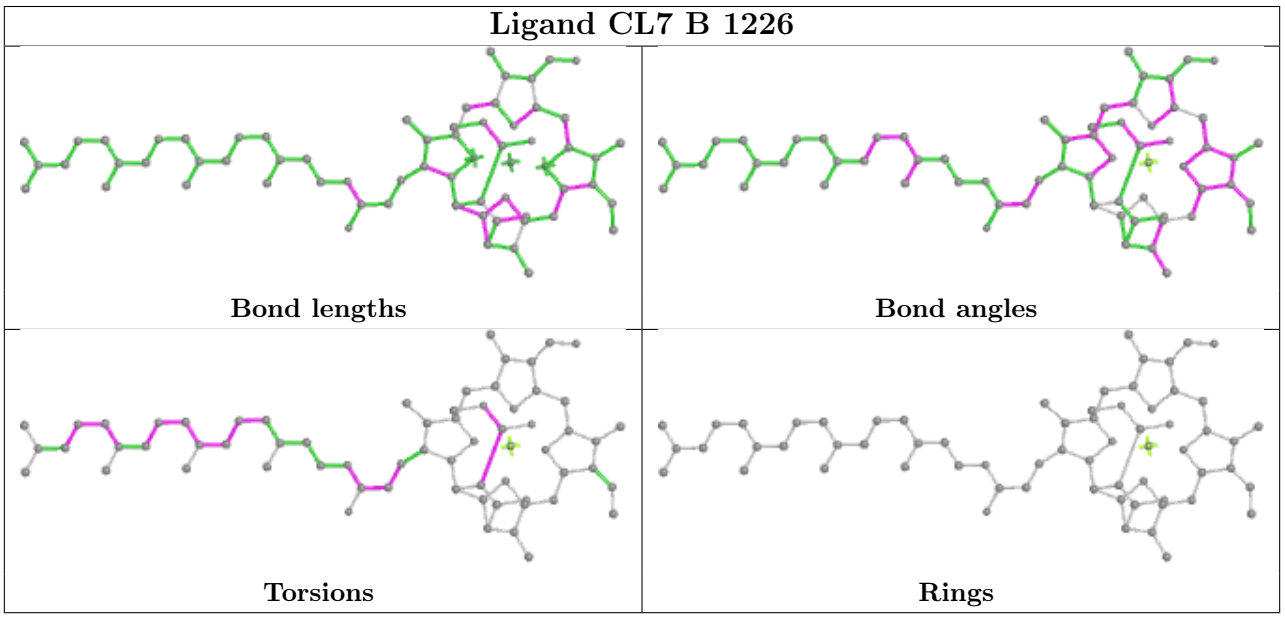


Rings

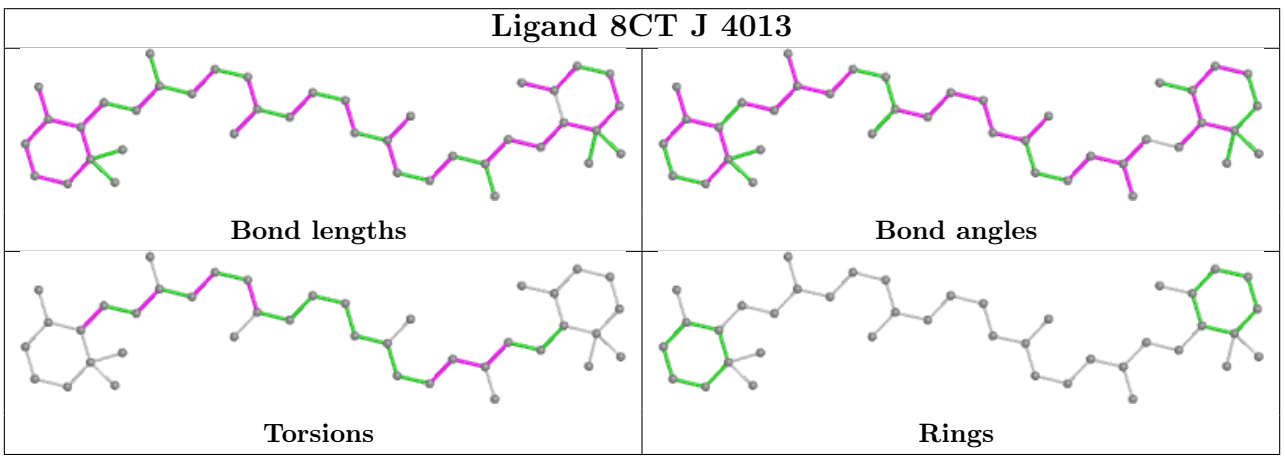
Ligand CL7 A 1126



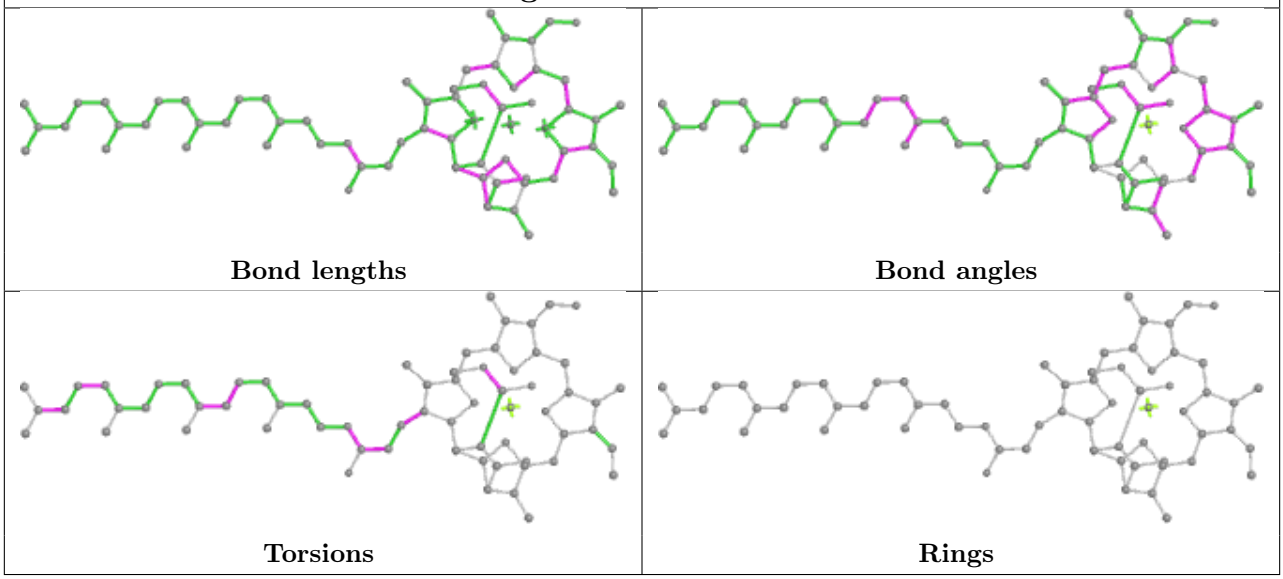
Ligand CL7 B 1226



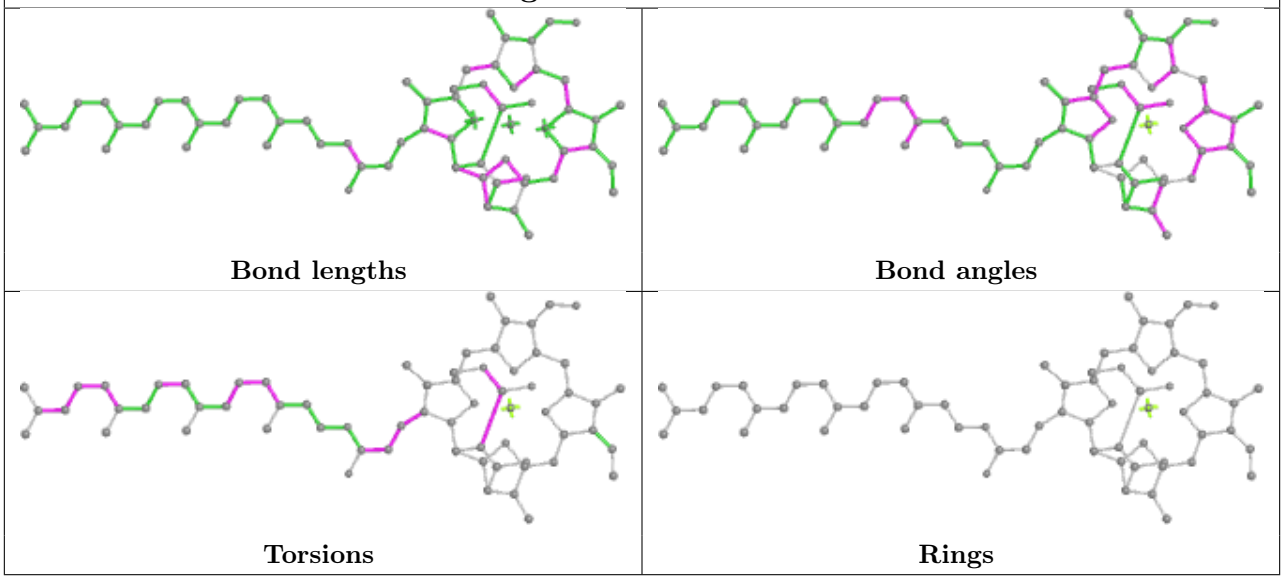
Ligand 8CT J 4013



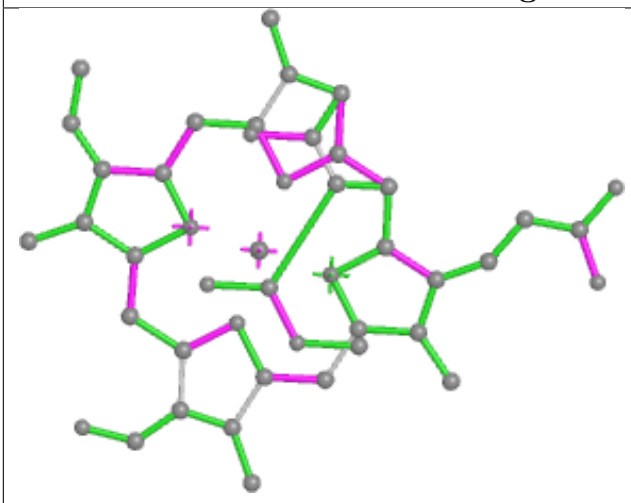
Ligand CL7 A 1140



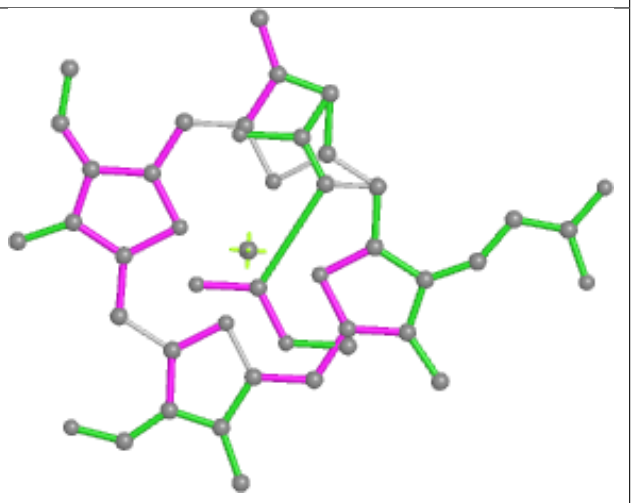
Ligand CL7 A 1117



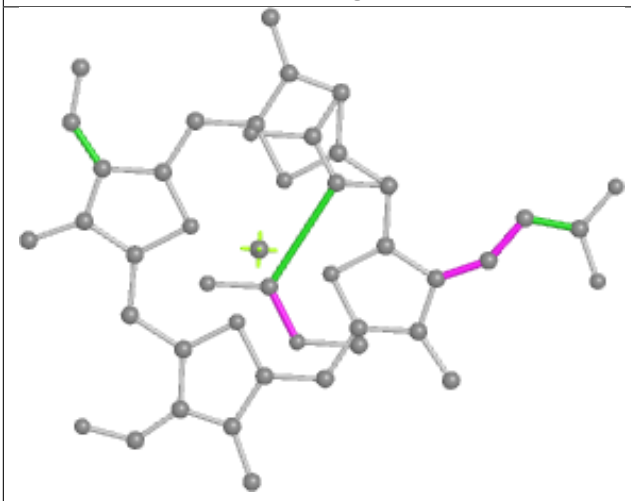
Ligand CL7 A 1114



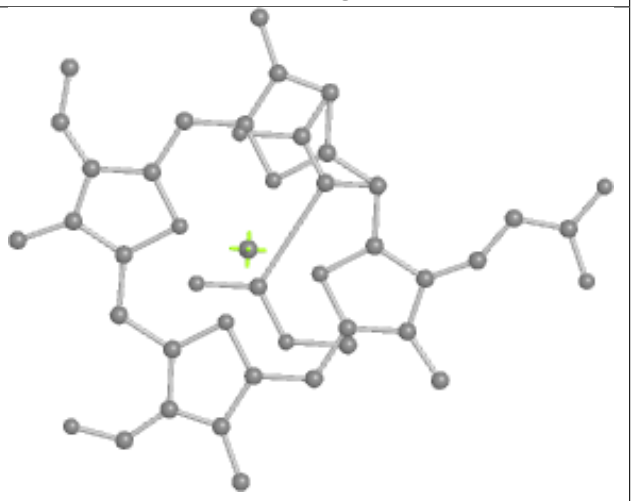
Bond lengths



Bond angles

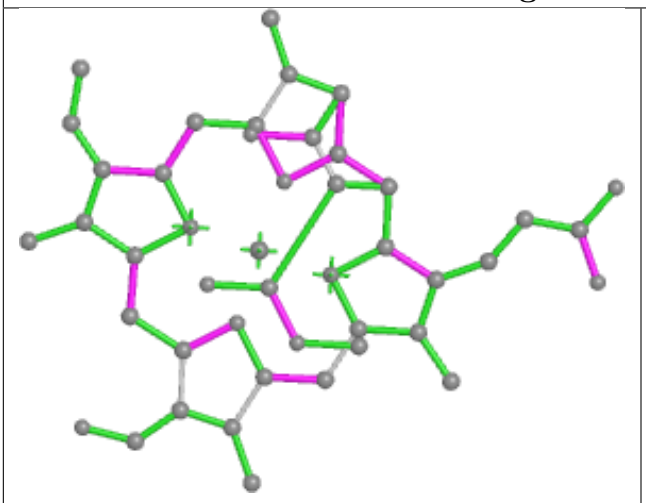


Torsions

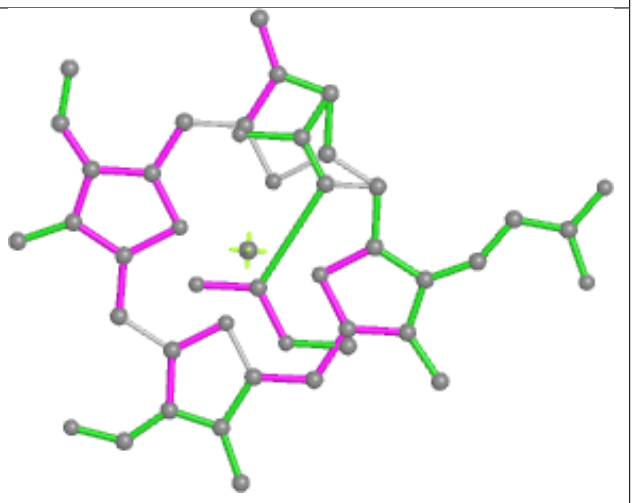


Rings

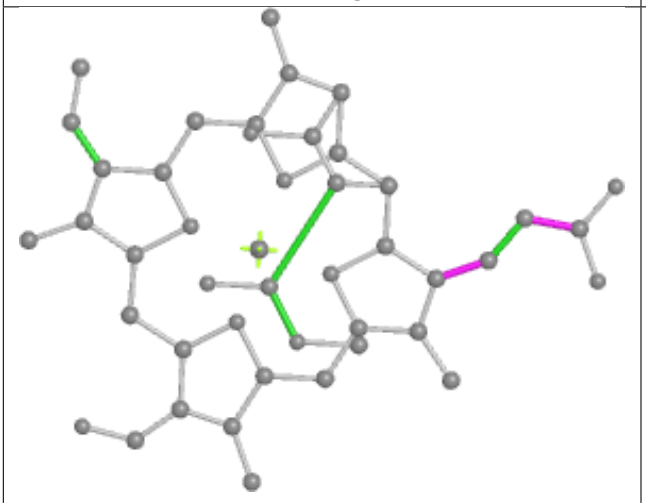
Ligand CL7 A 1116



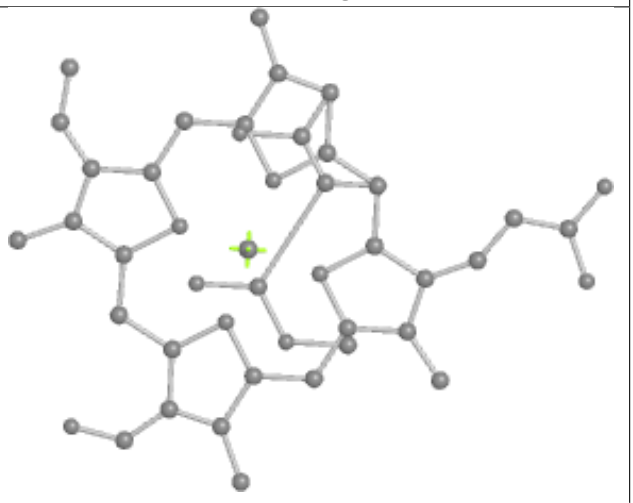
Bond lengths



Bond angles

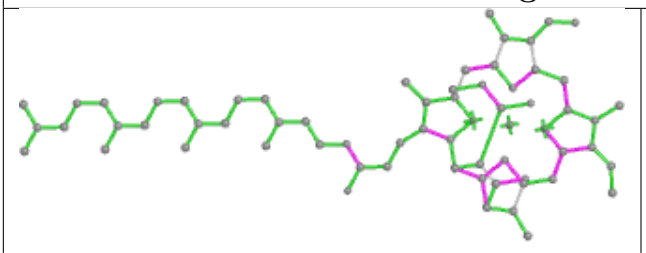


Torsions

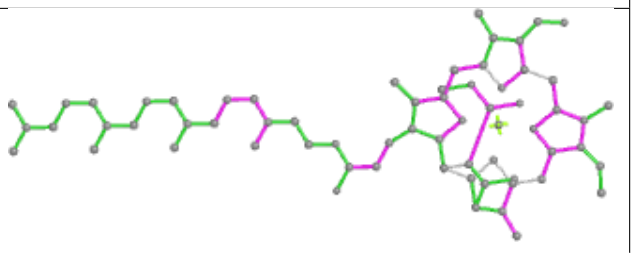


Rings

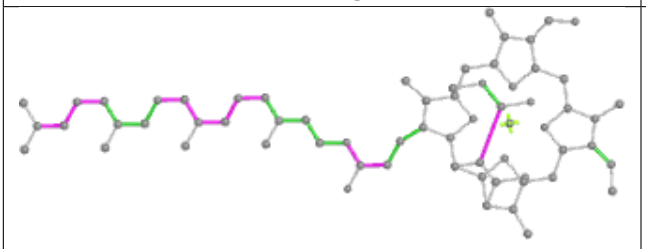
Ligand CL7 A 1132



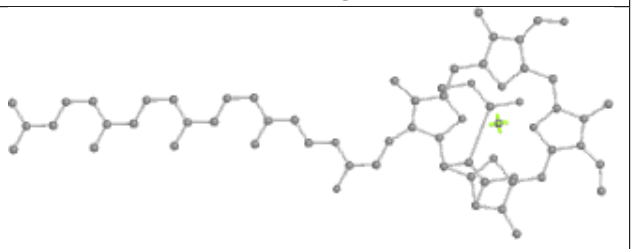
Bond lengths



Bond angles

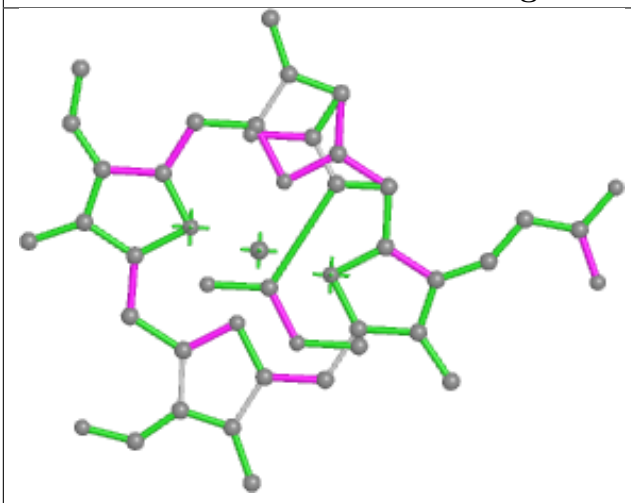


Torsions

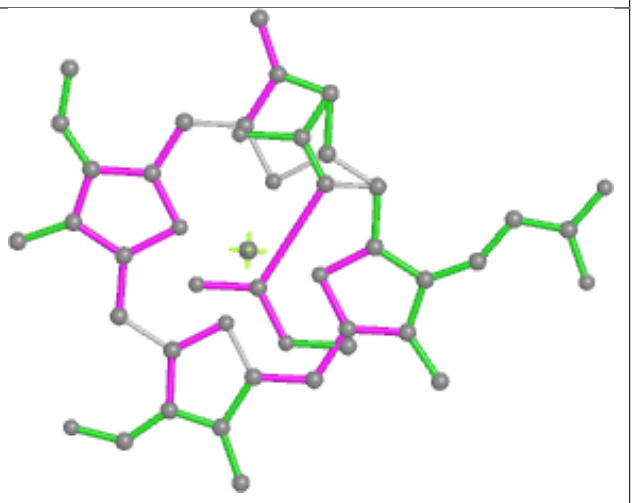


Rings

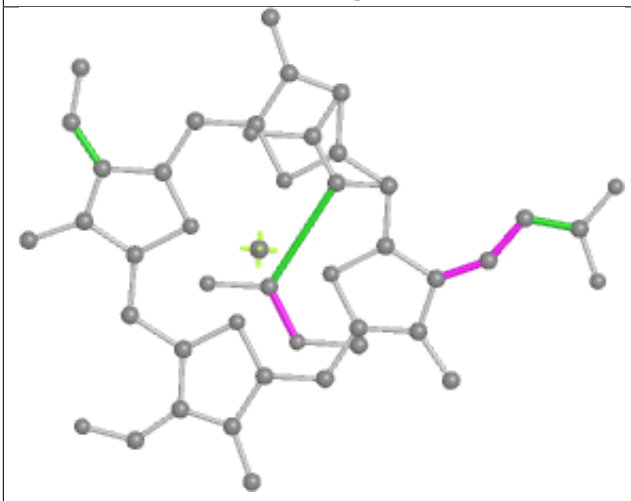
Ligand CL7 B 1235



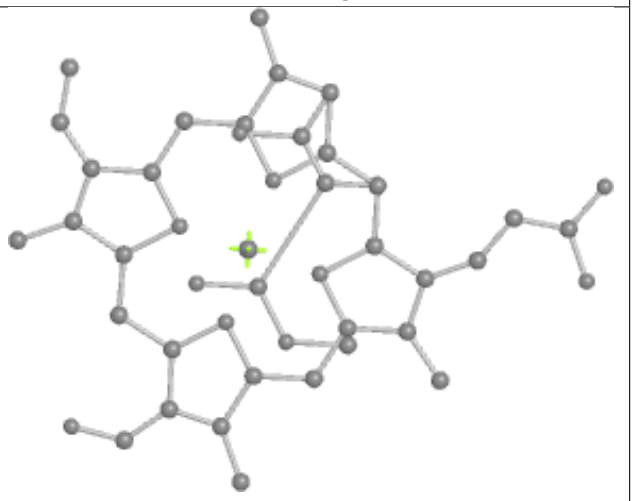
Bond lengths



Bond angles

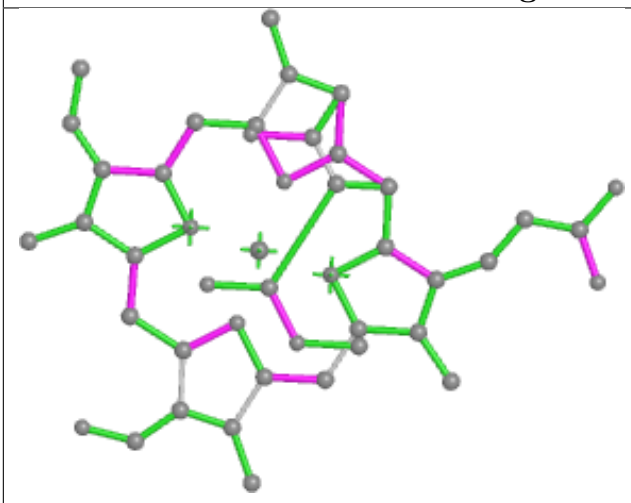


Torsions

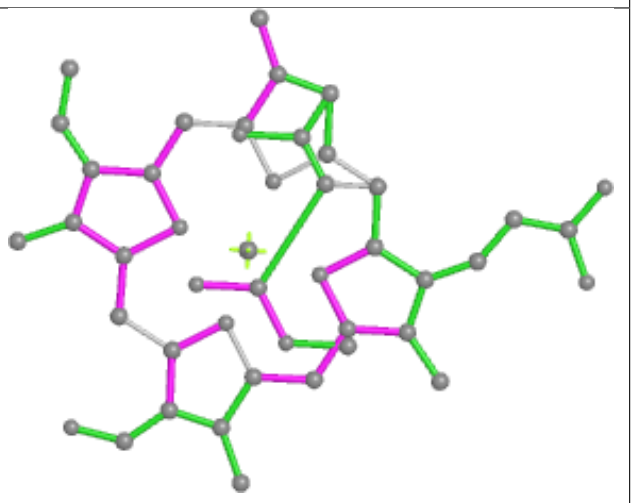


Rings

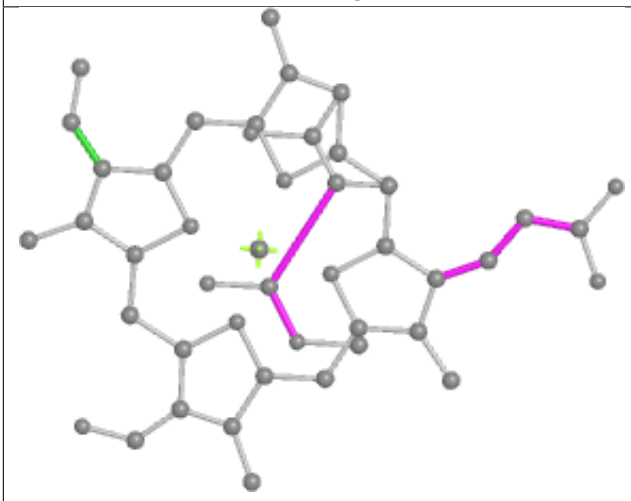
Ligand CL7 A 1801



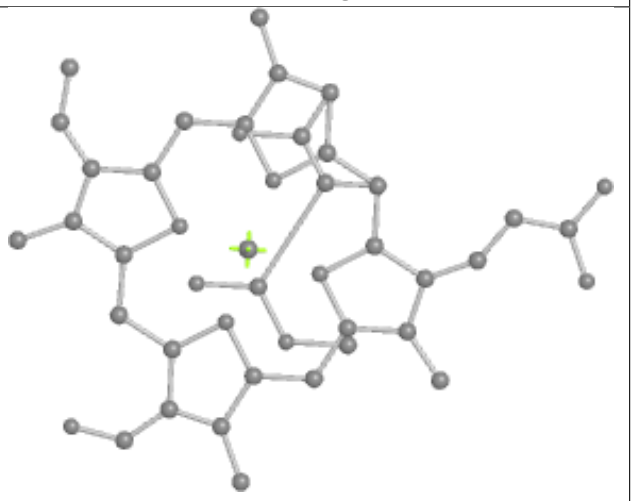
Bond lengths



Bond angles

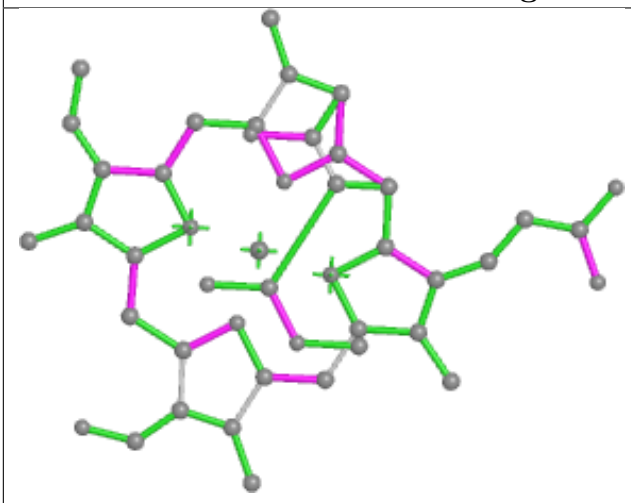


Torsions

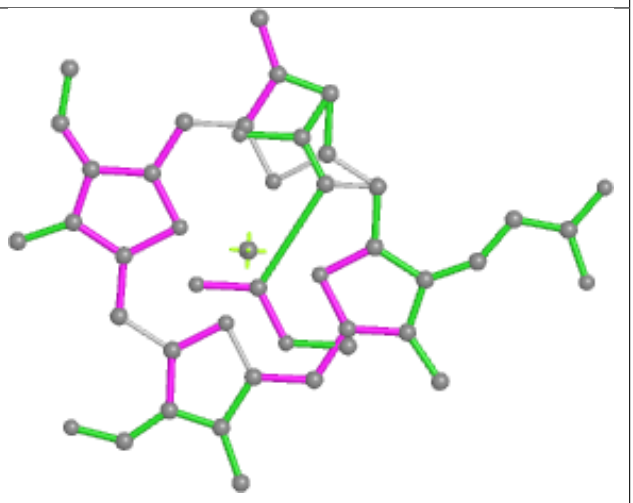


Rings

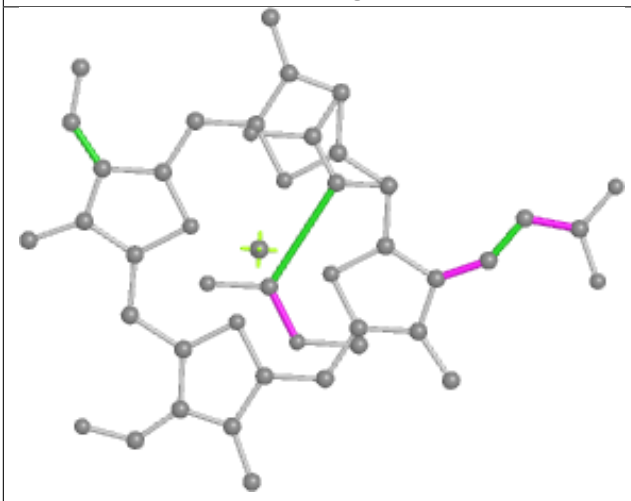
Ligand CL7 B 1229



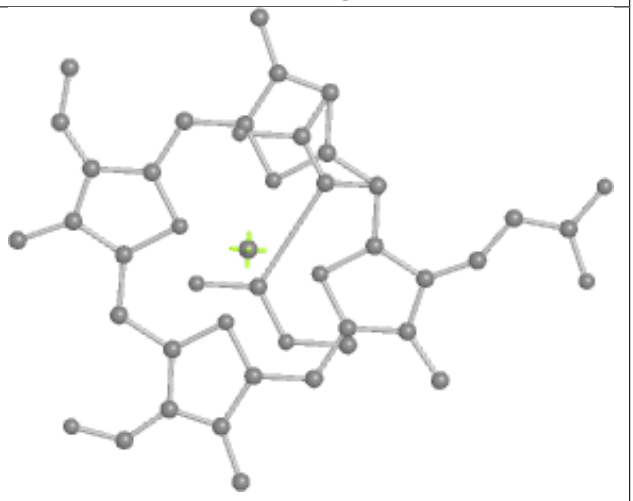
Bond lengths



Bond angles

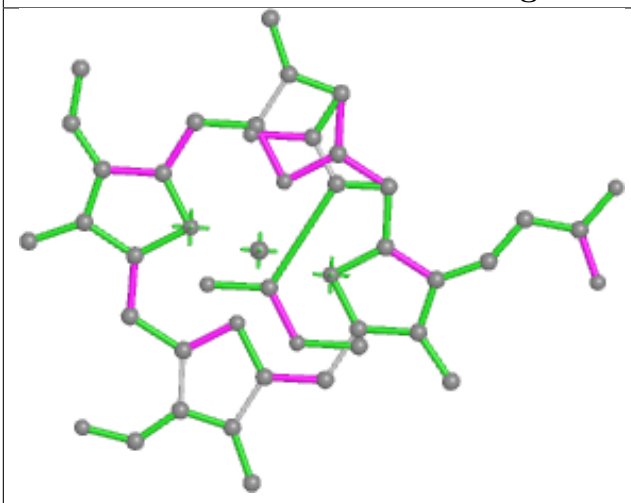


Torsions

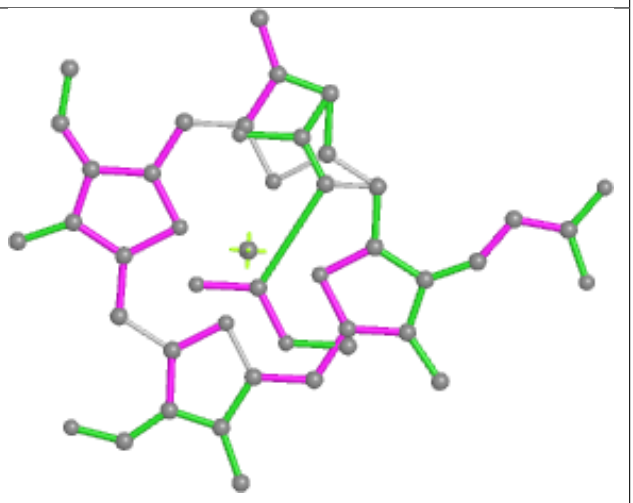


Rings

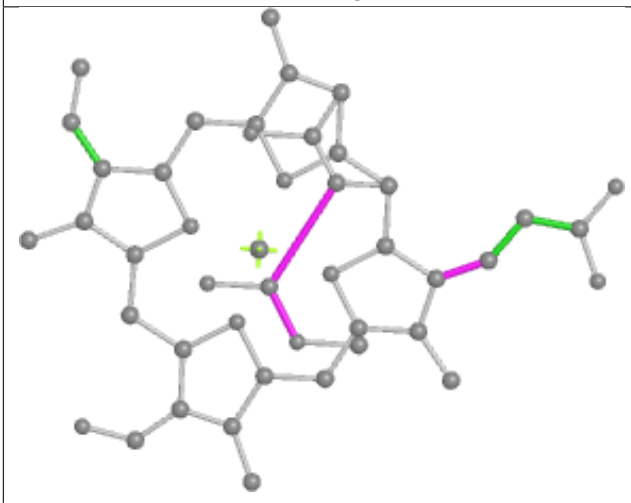
Ligand CL7 B 1222



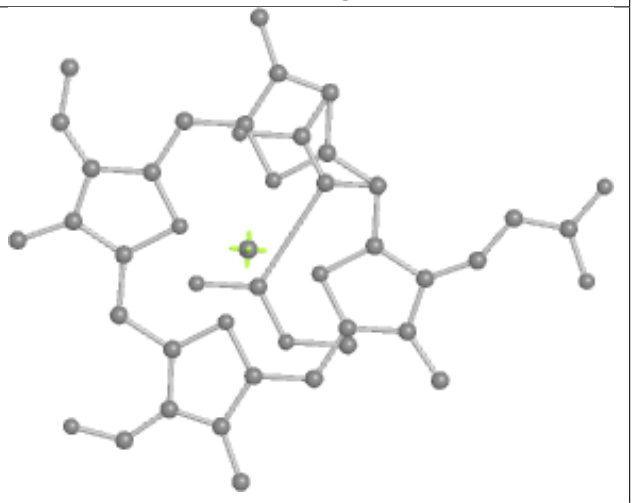
Bond lengths



Bond angles

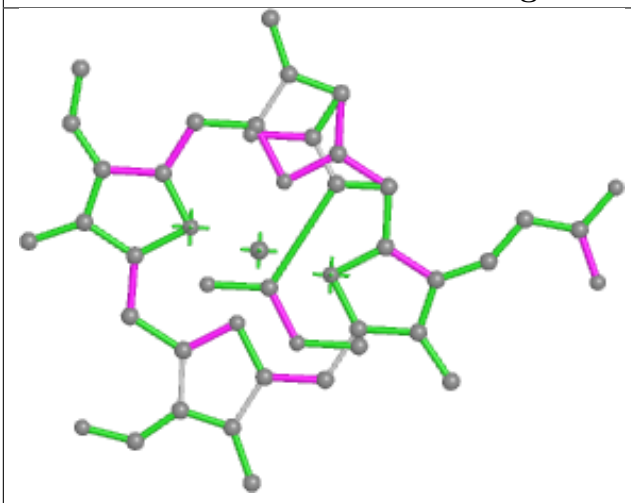


Torsions

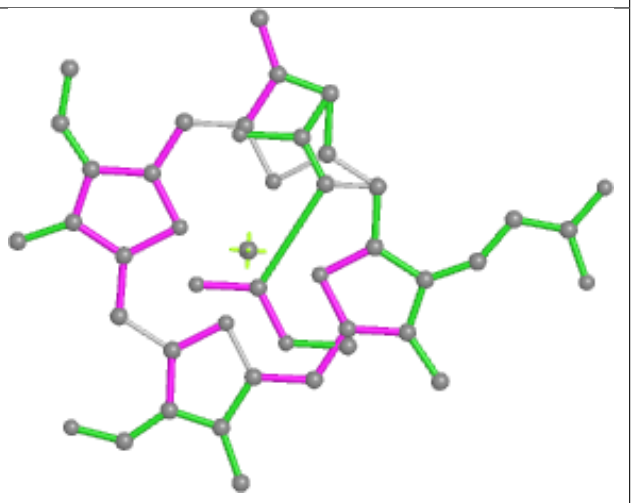


Rings

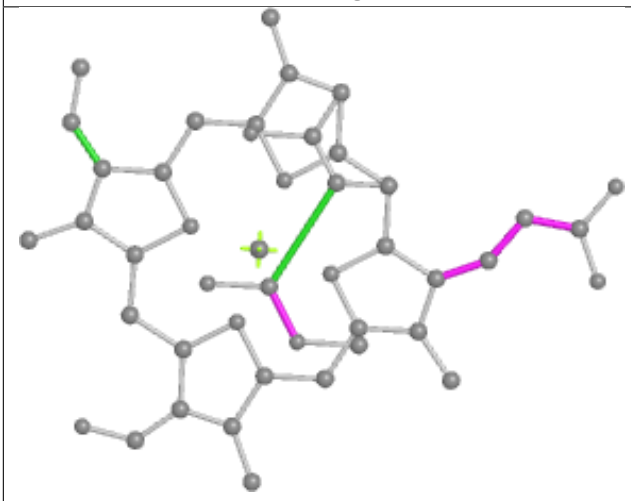
Ligand CL7 B 1230



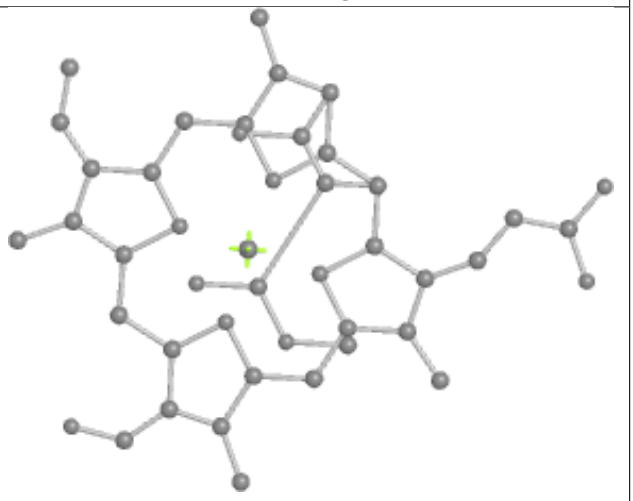
Bond lengths



Bond angles

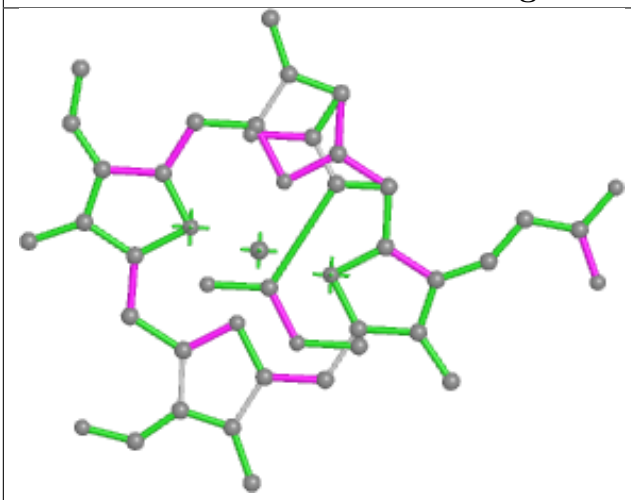


Torsions

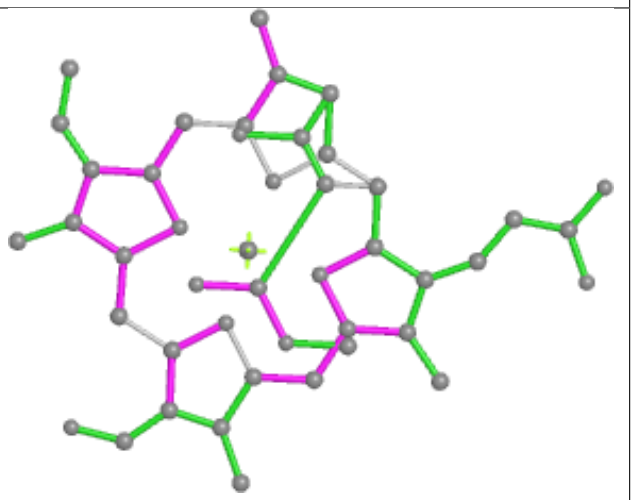


Rings

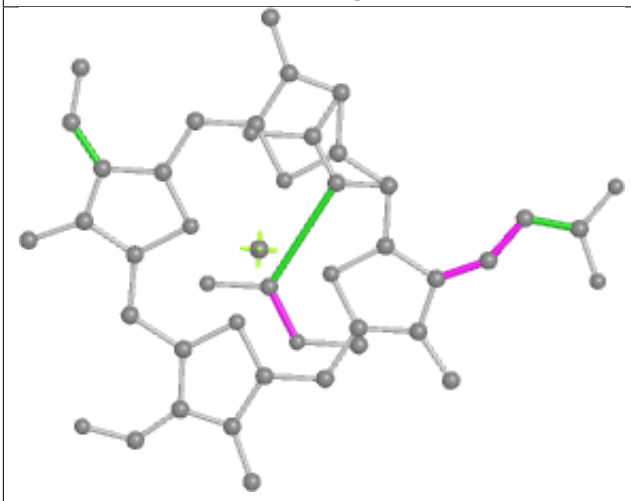
Ligand CL7 A 1122



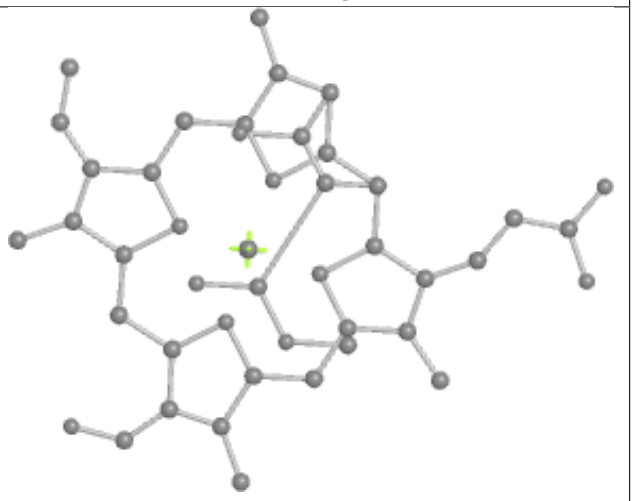
Bond lengths



Bond angles

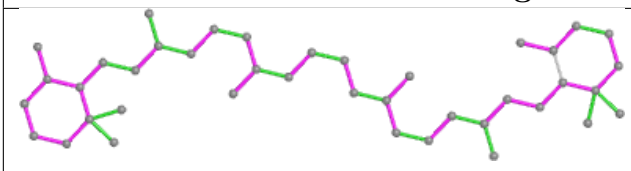


Torsions

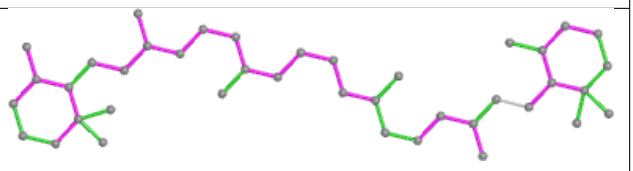


Rings

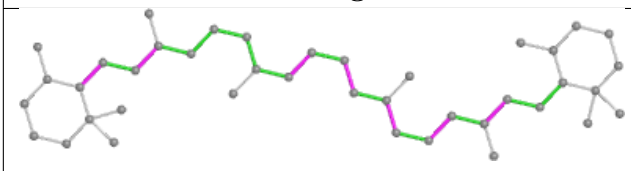
Ligand 8CT M 4021



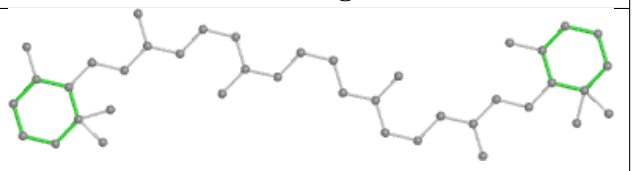
Bond lengths



Bond angles

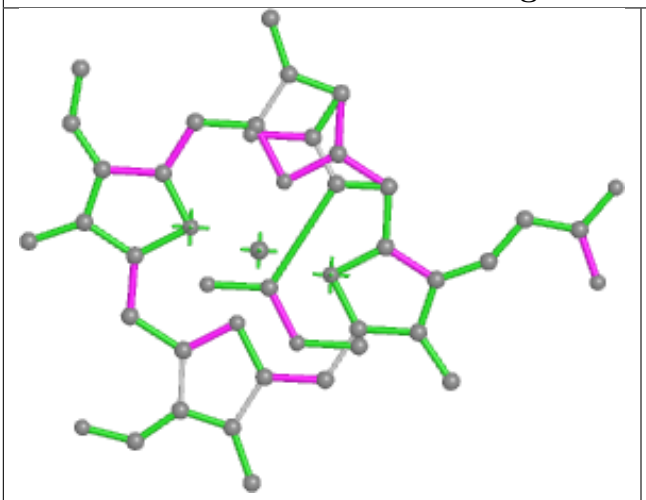


Torsions

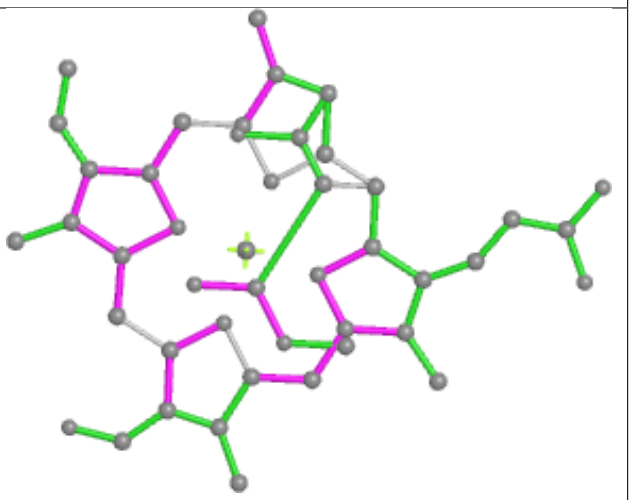


Rings

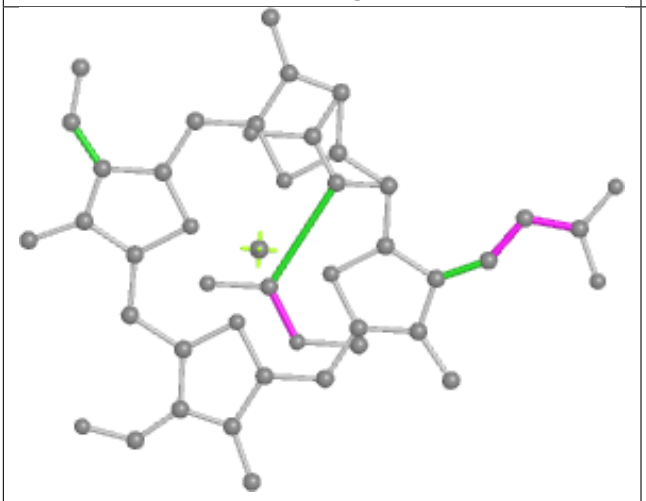
Ligand CL7 B 1236



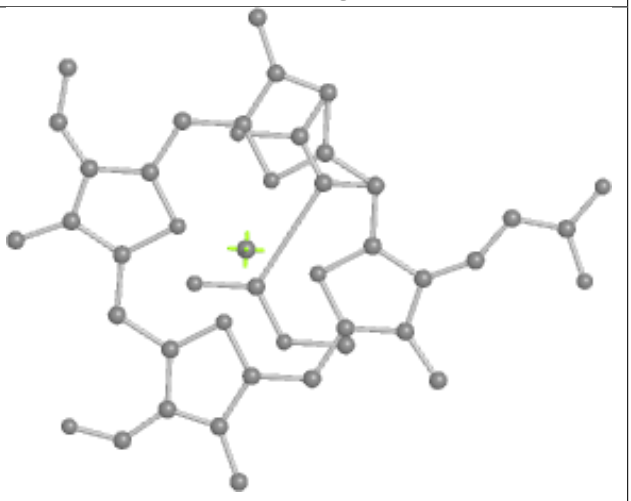
Bond lengths



Bond angles

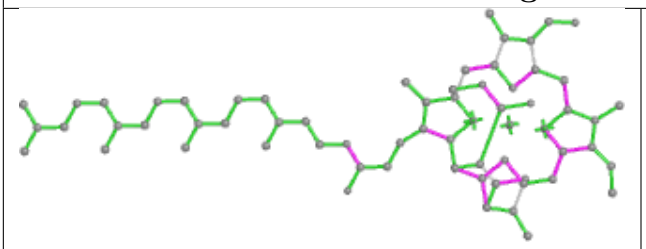


Torsions

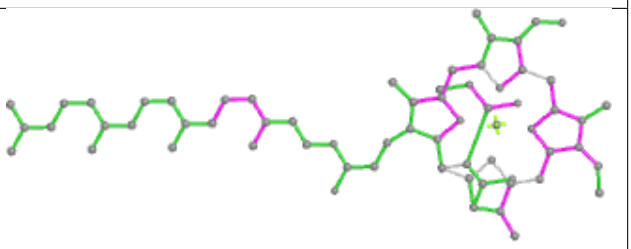


Rings

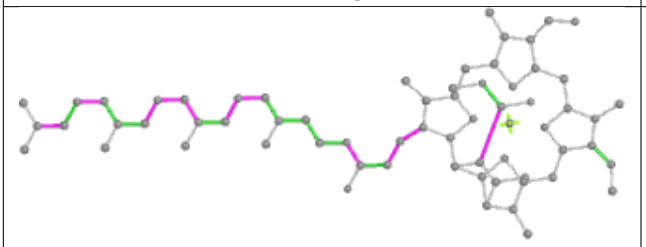
Ligand CL7 B 1225



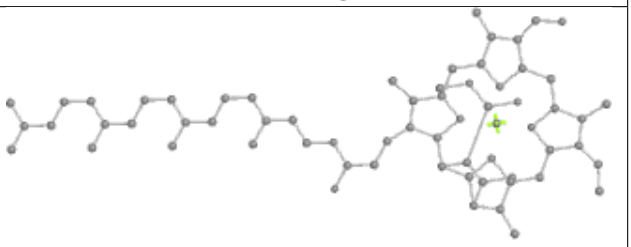
Bond lengths



Bond angles

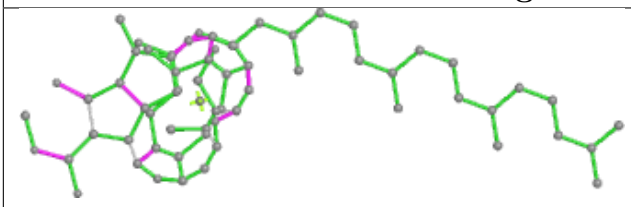


Torsions

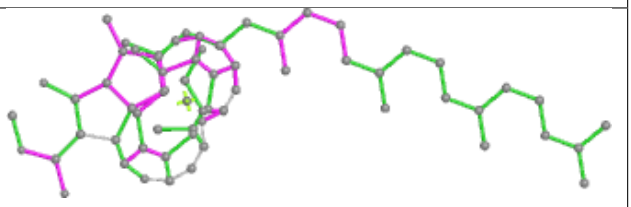


Rings

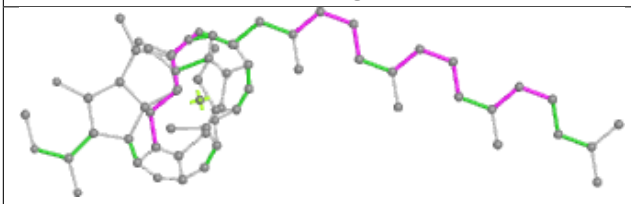
Ligand G9R A 1011



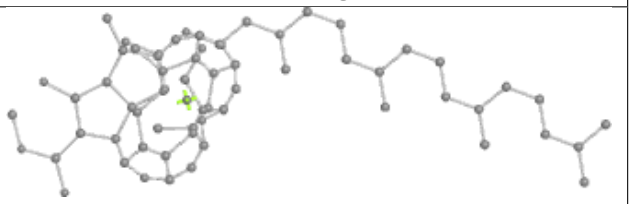
Bond lengths



Bond angles

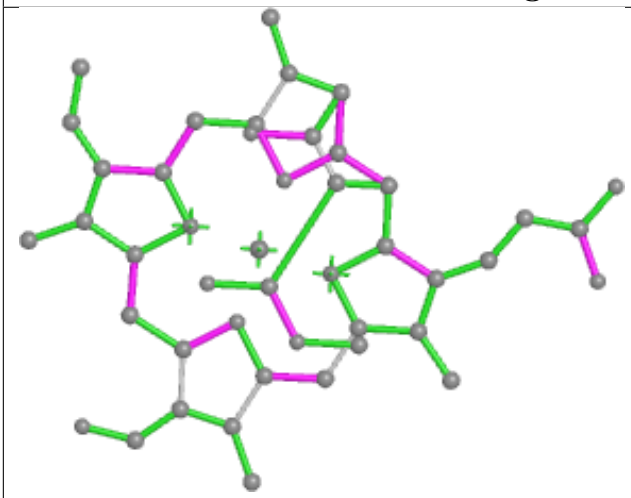


Torsions

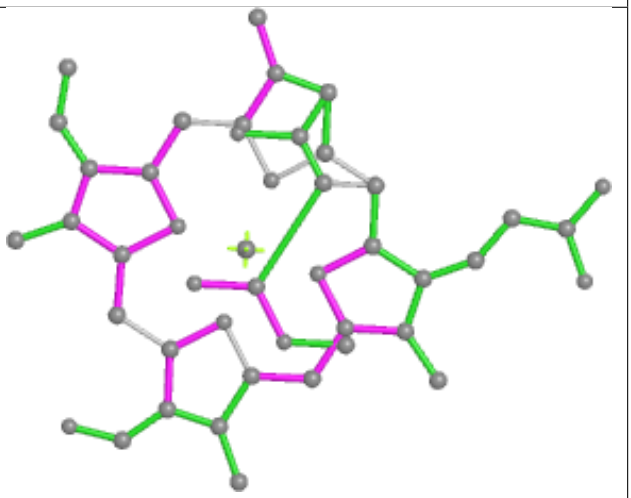


Rings

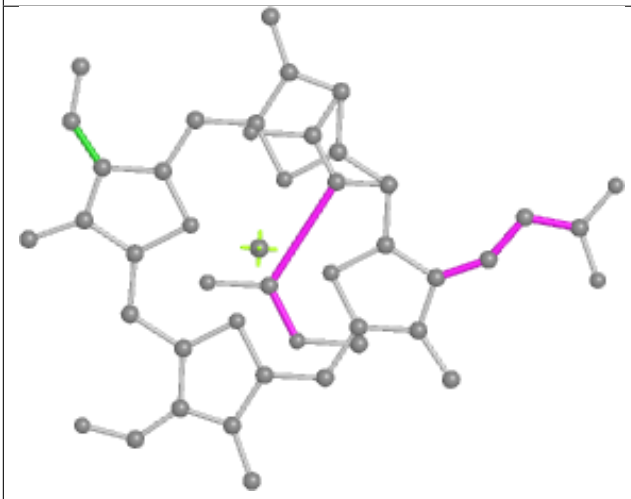
Ligand CL7 J 1302



Bond lengths



Bond angles



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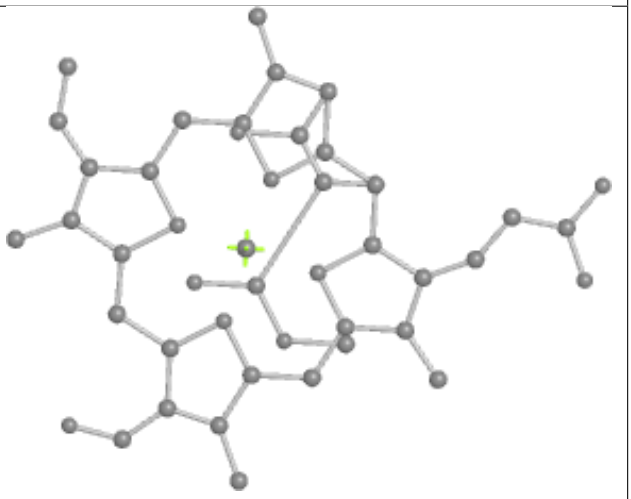
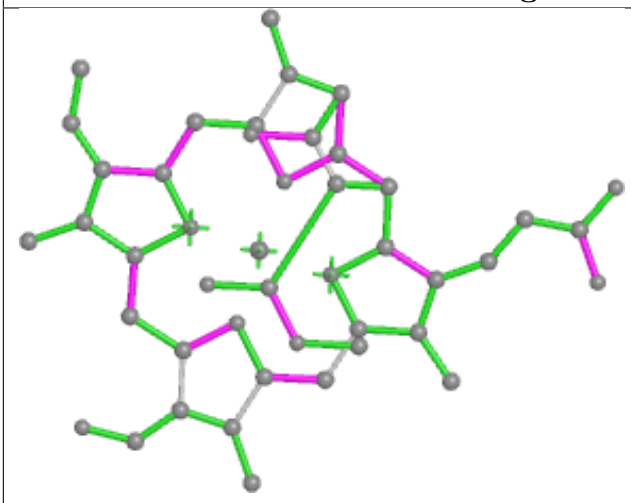
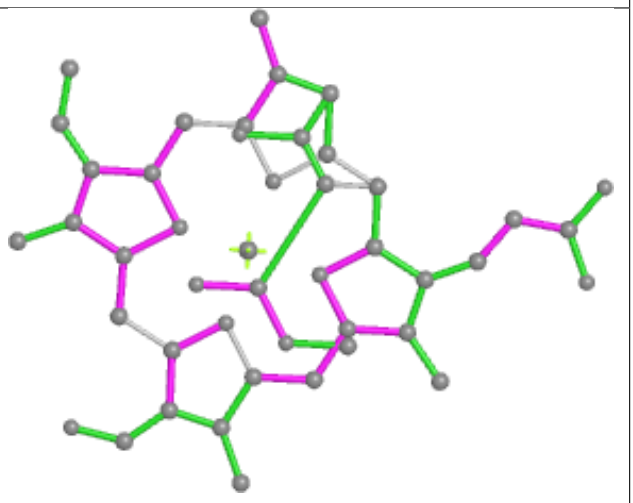


Rings

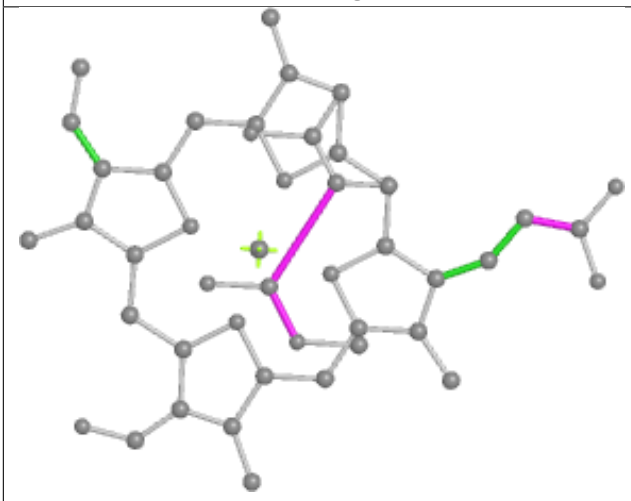
Ligand CL7 B 1201



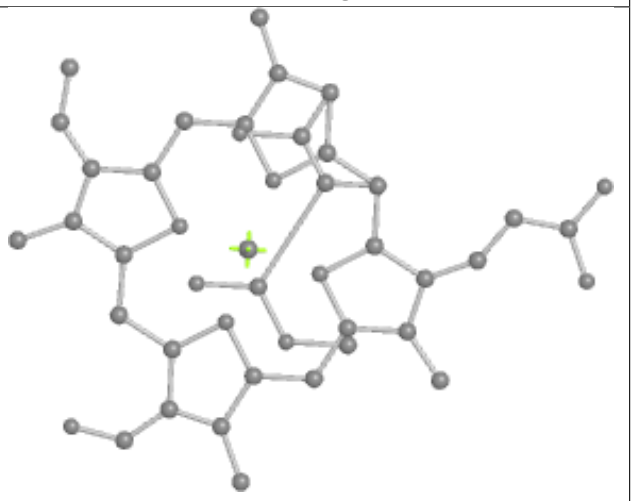
Bond lengths



Bond angles

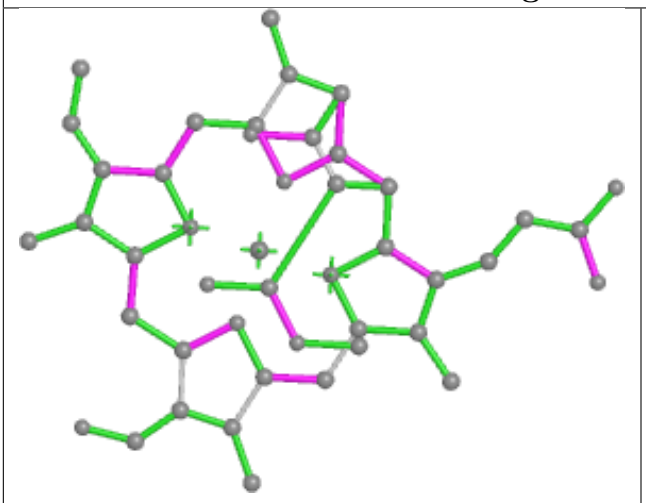


Torsions

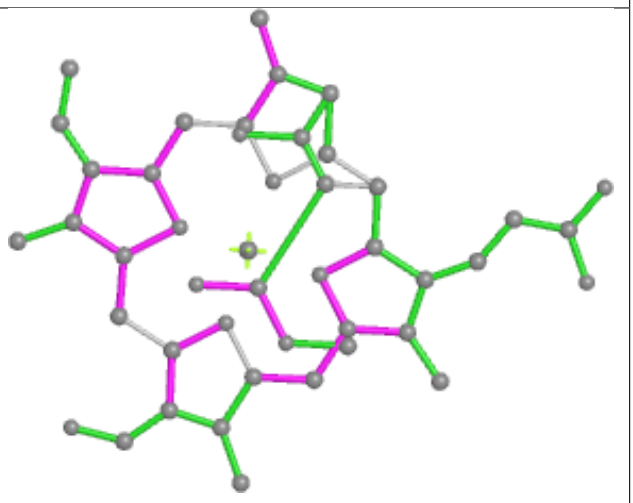


Rings

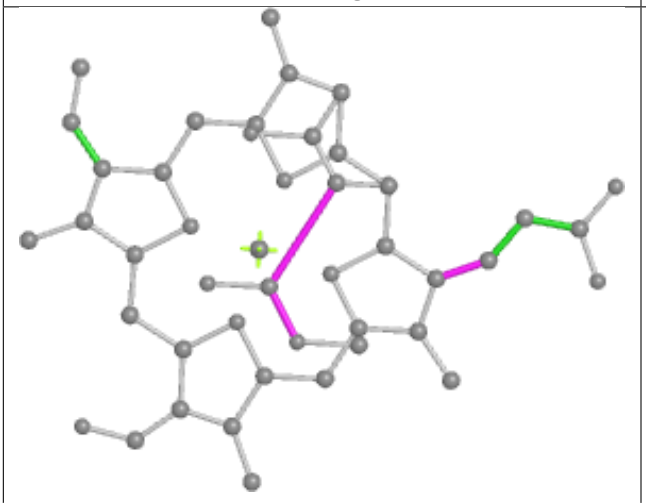
Ligand CL7 L 1503



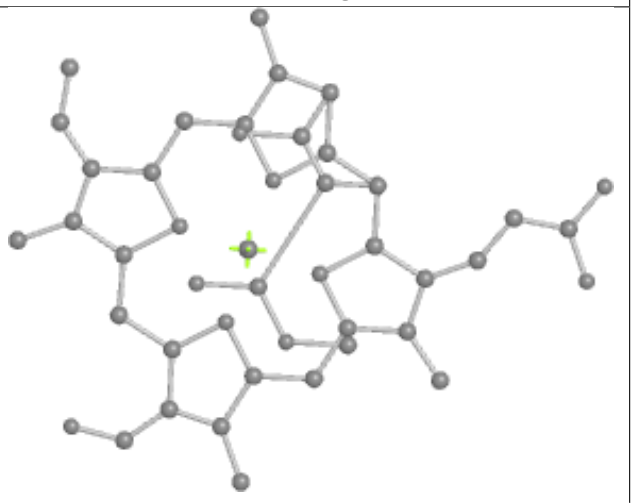
Bond lengths



Bond angles

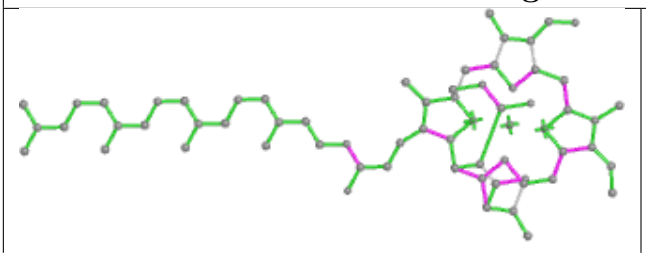


Torsions



Rings

Ligand CL7 L 1502



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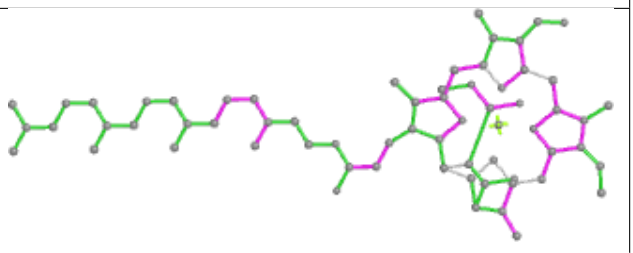
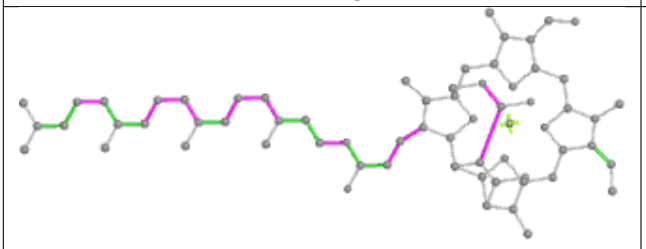


Bond angles



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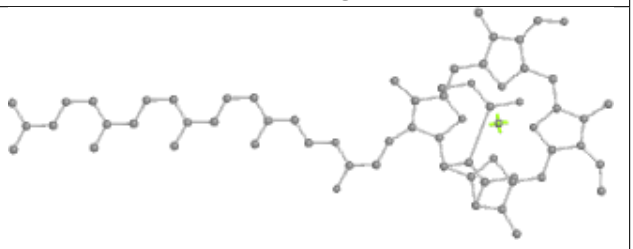
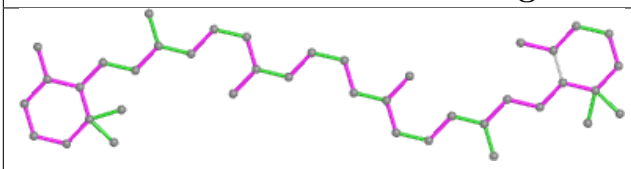


Rings

Ligand 8CT B 4017



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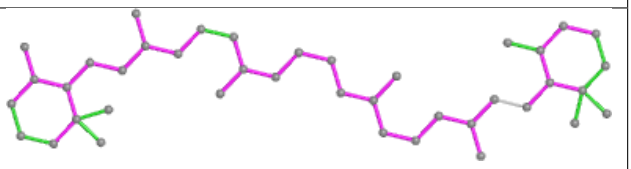
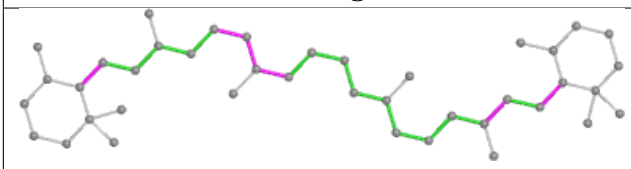
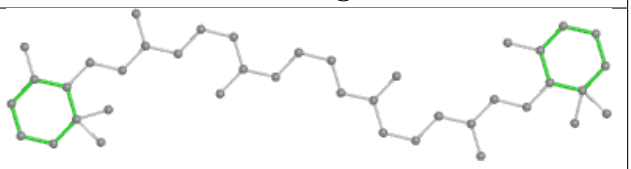


Bond angles

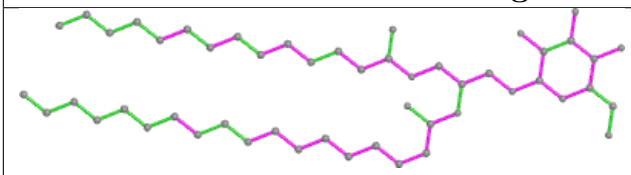


Torsions

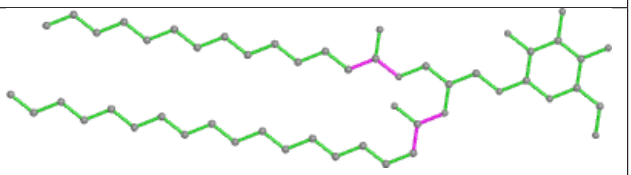


Rings

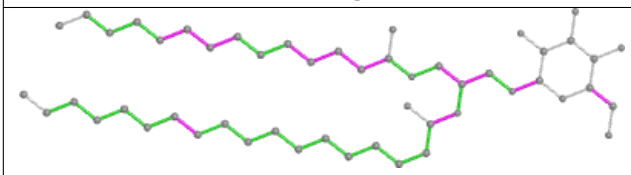
Ligand LMG B 5002



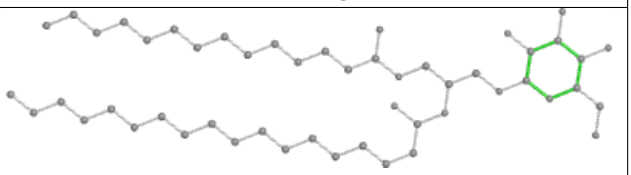
Bond lengths



Bond angles

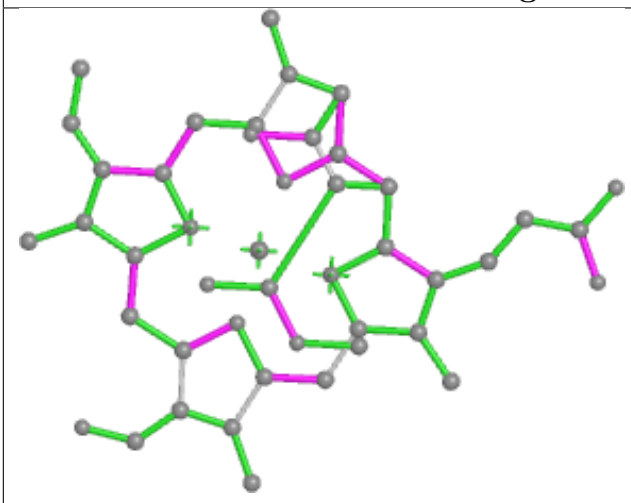


Torsions

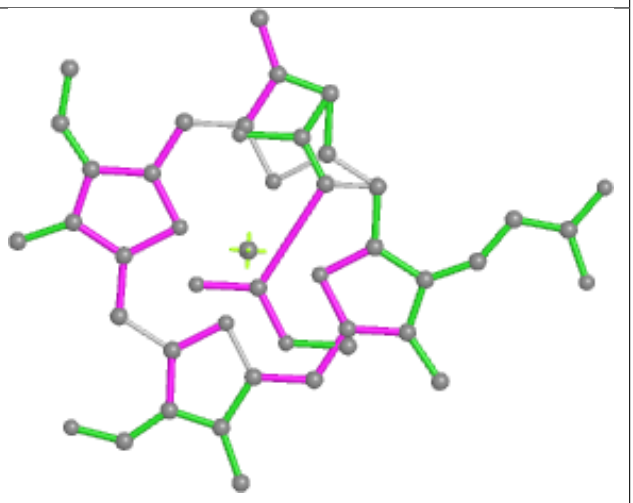


Rings

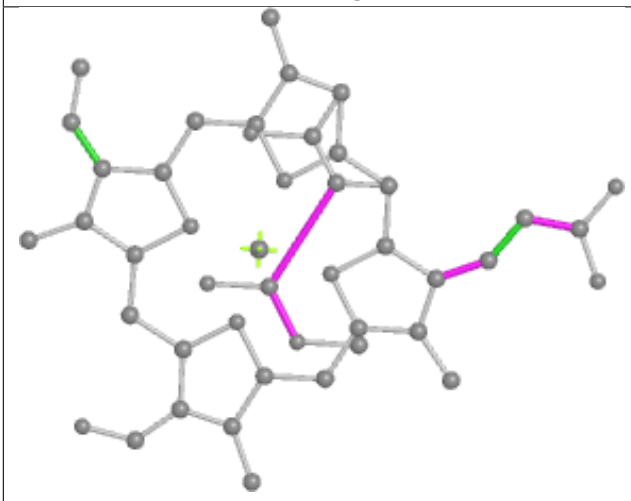
Ligand CL7 A 1115



Bond lengths



Bond angles



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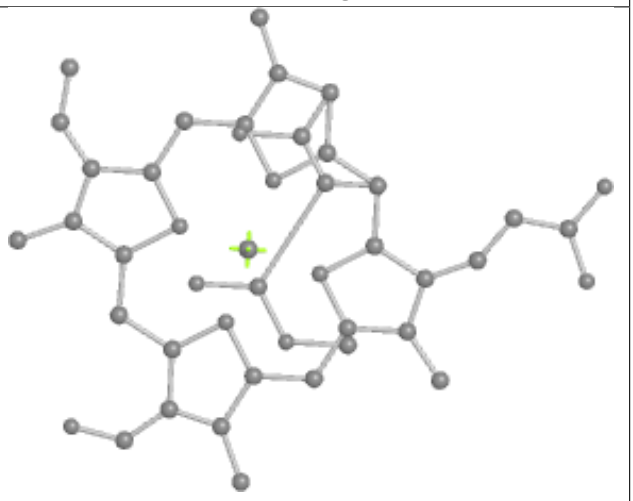
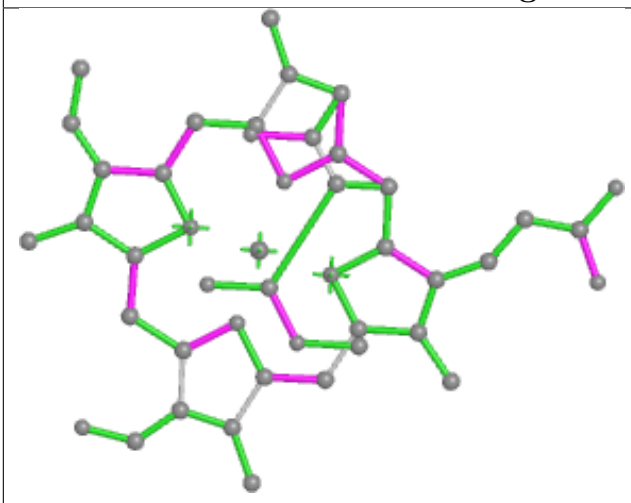
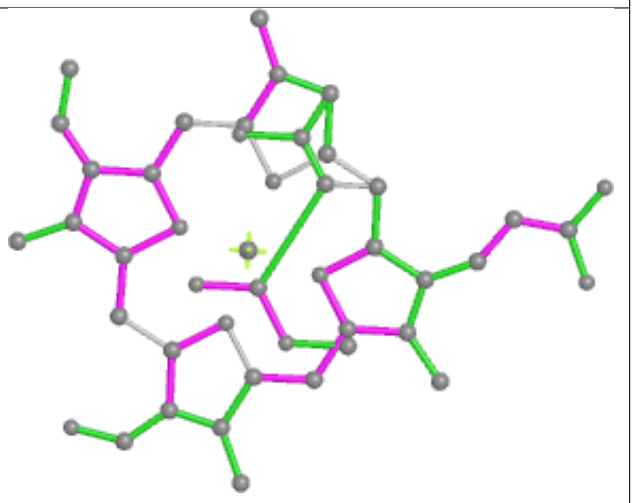


Rings

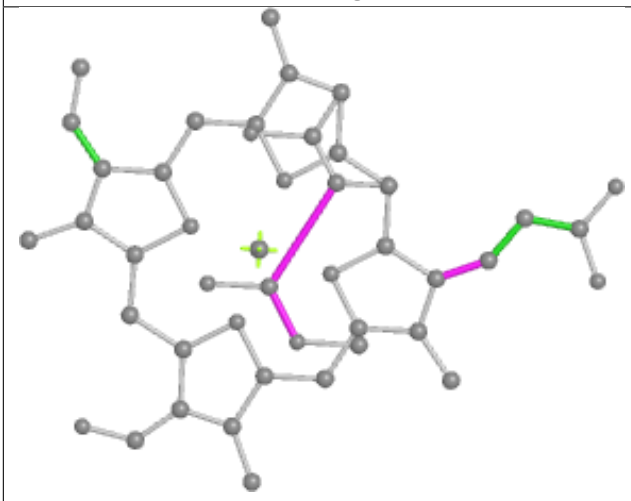
Ligand CL7 A 1130



Bond lengths



Bond angles



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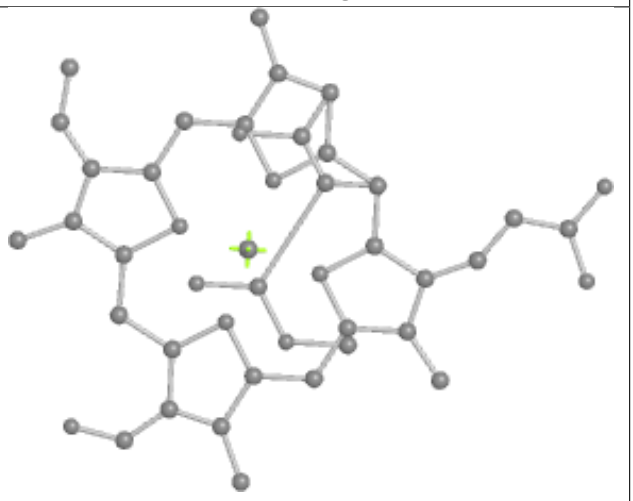
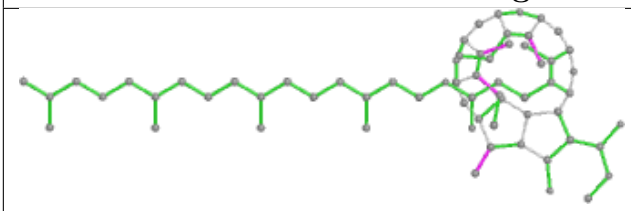
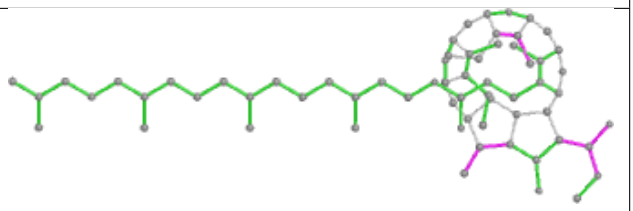


Rings

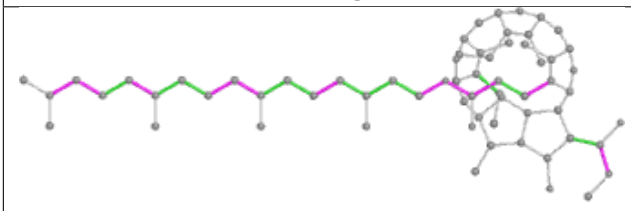
Ligand PHO A 1013



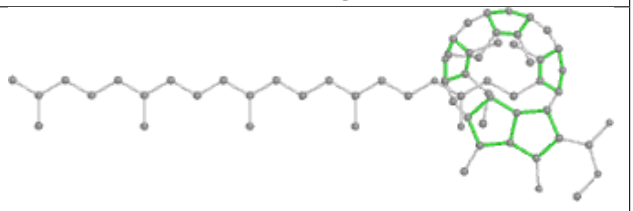
Bond lengths



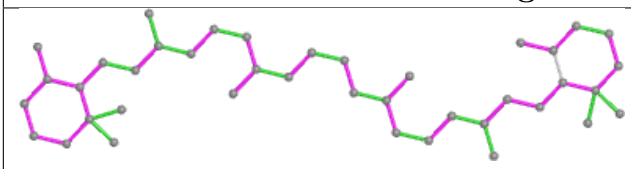
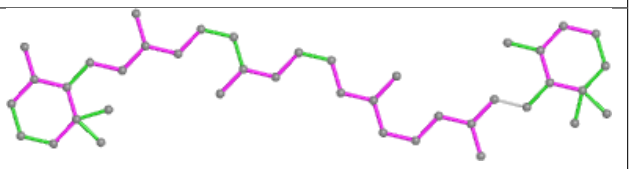
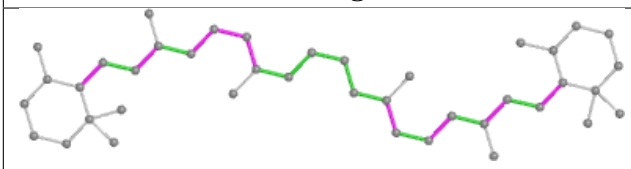
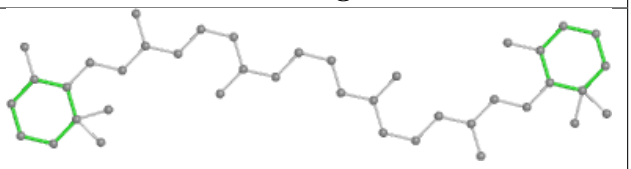
Bond angles

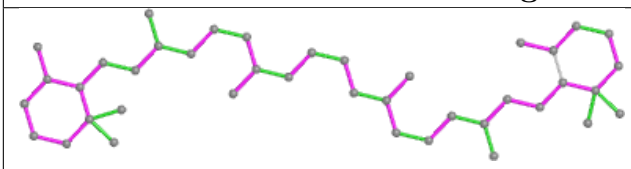
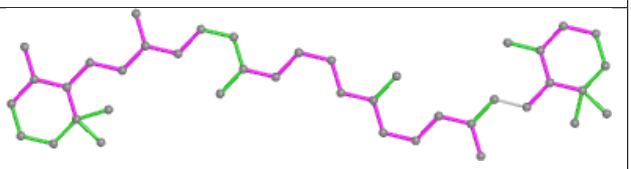
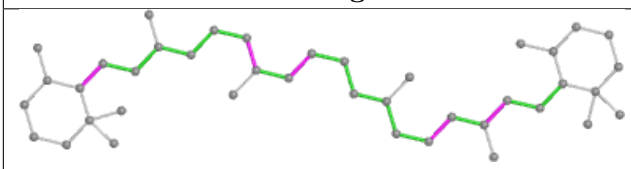
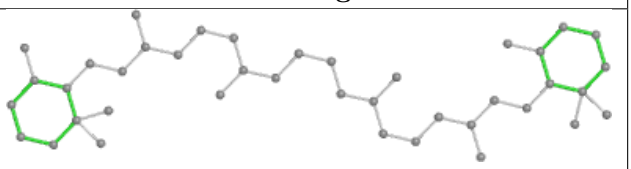


Torsions

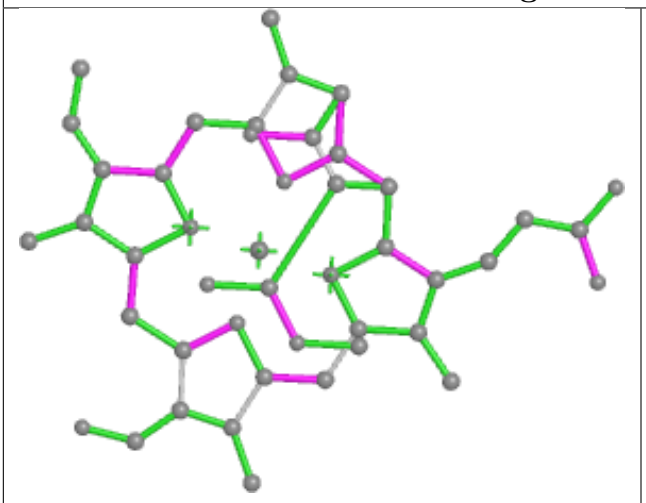


Rings

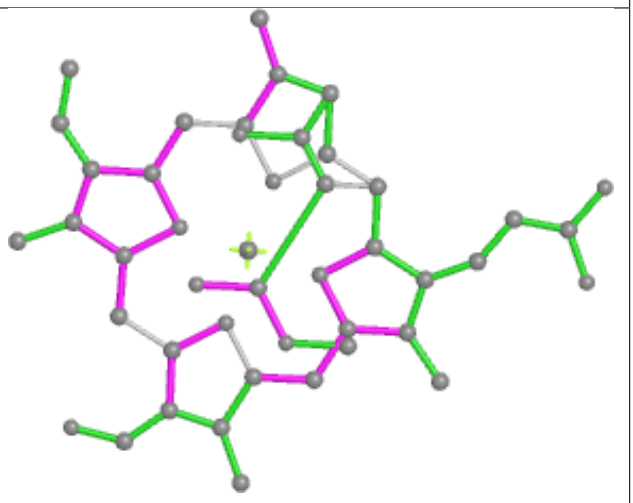
Ligand 8CT A 4011	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT L 4020	
 Bond lengths	 Bond angles
 Torsions	 Rings

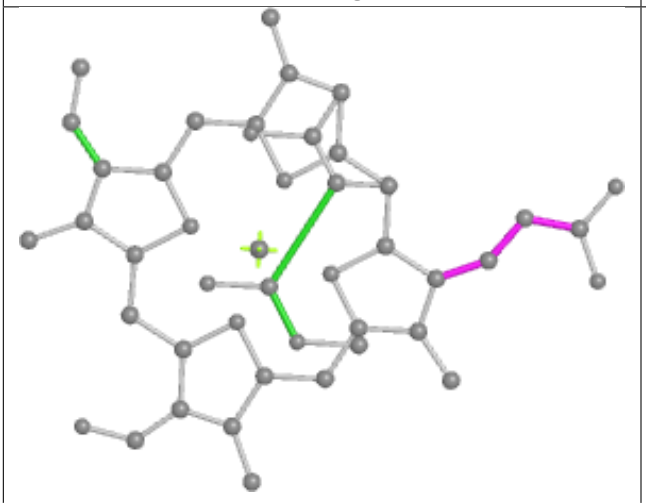
Ligand CL7 B 1207



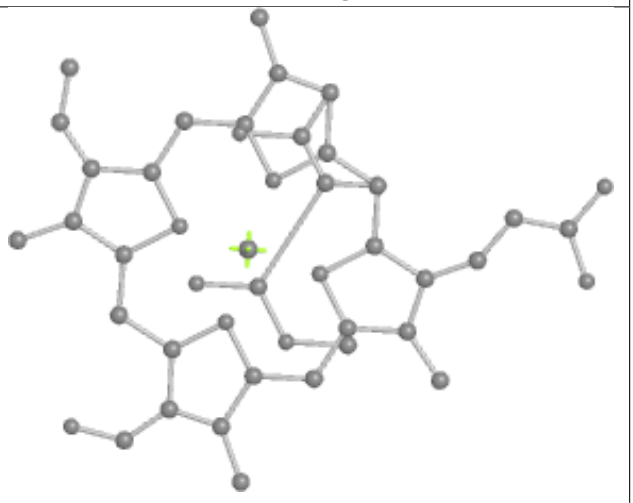
Bond lengths



Bond angles

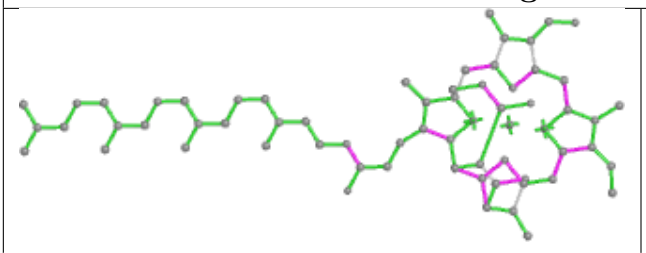


Torsions



Rings

Ligand CL7 B 1239



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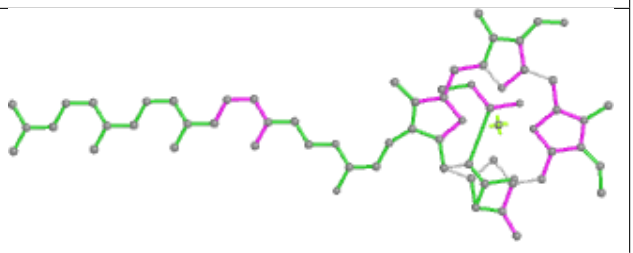
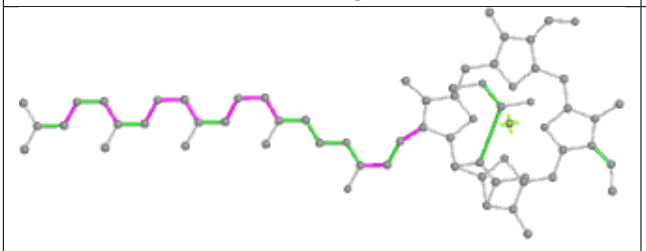
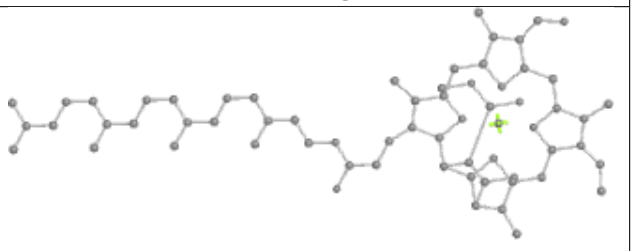


Bond angles

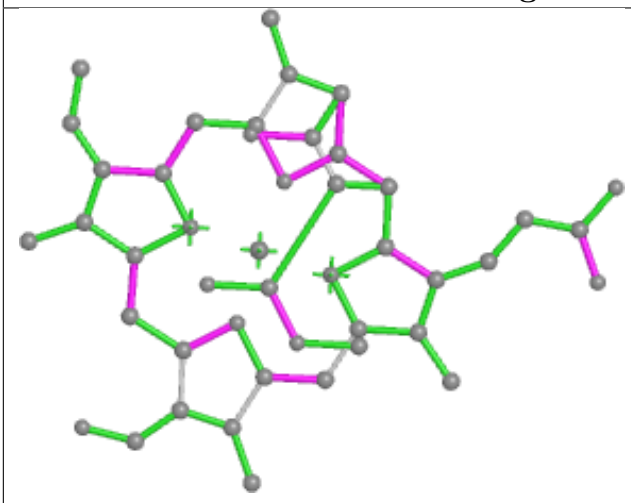


Torsions



Rings

Ligand CL7 A 1129



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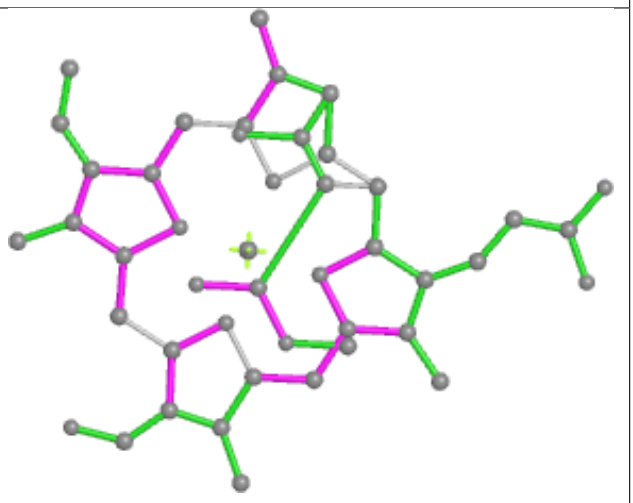
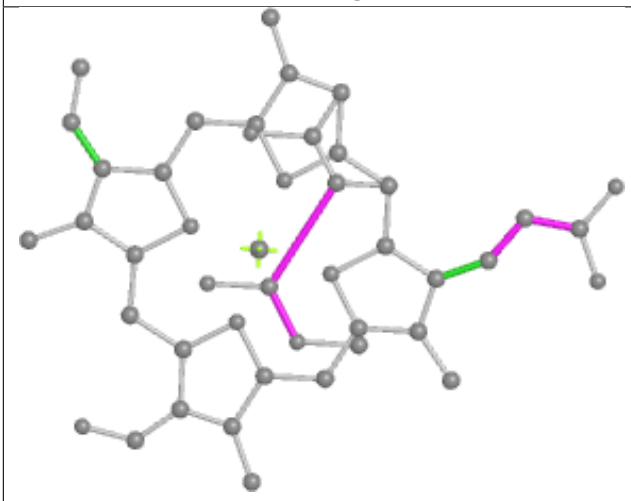


Bond angles



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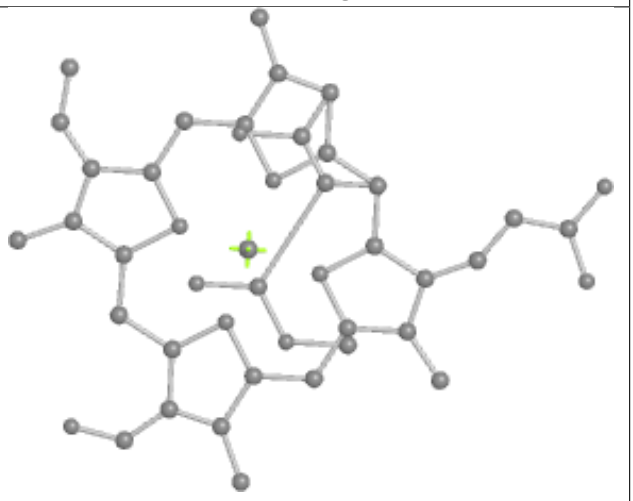
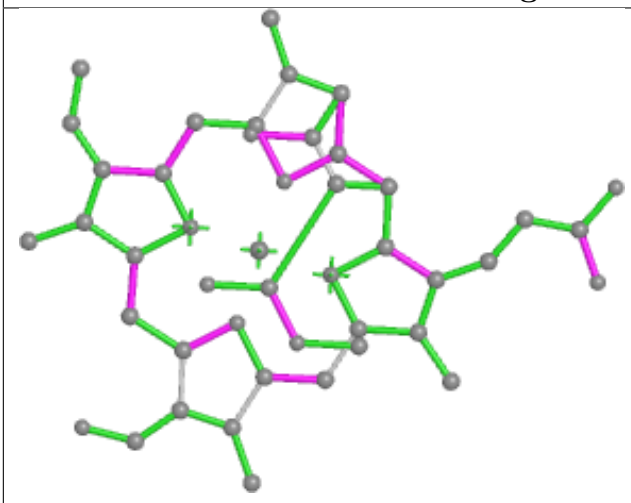


Rings

Ligand CL7 B 1204



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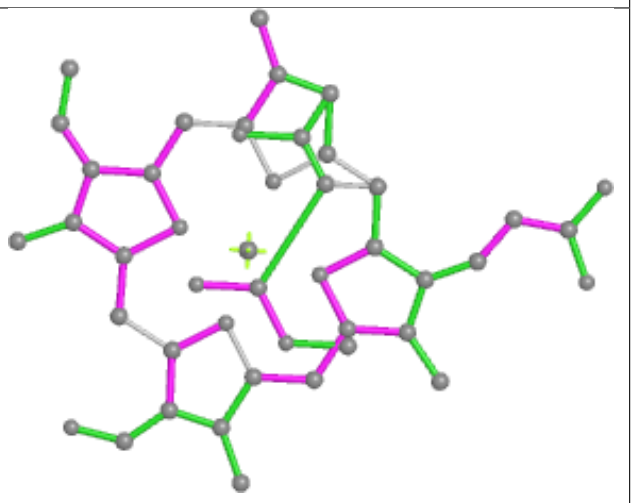
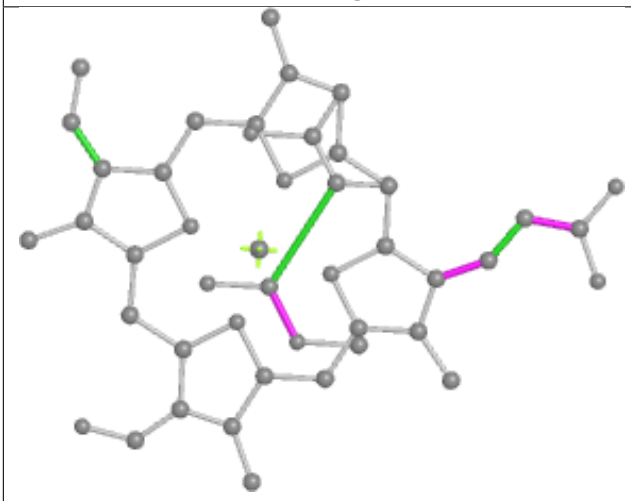


Bond angles



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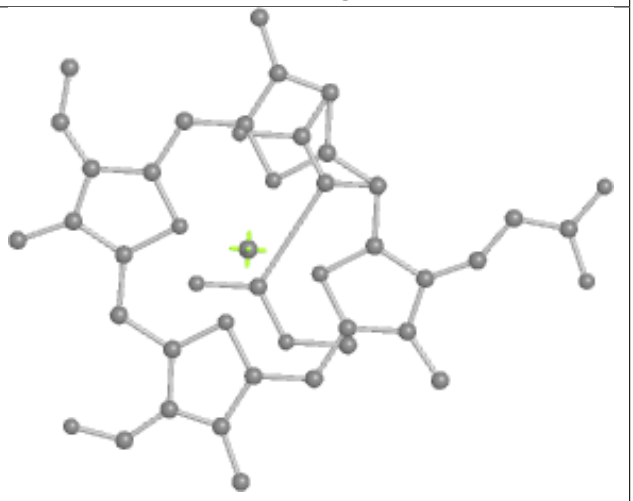
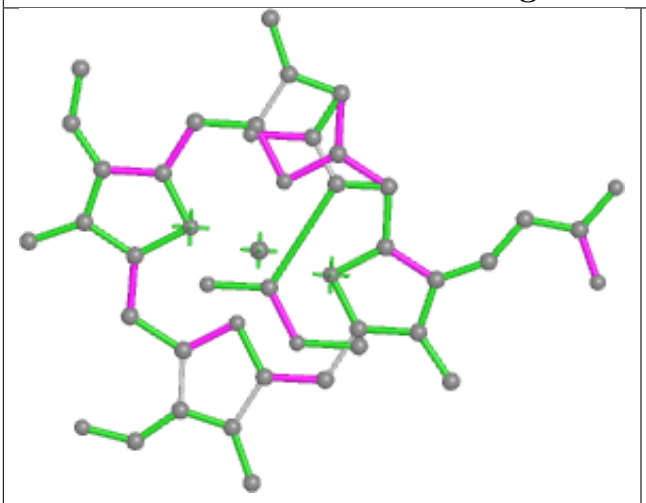


Rings

Ligand CL7 A 1102



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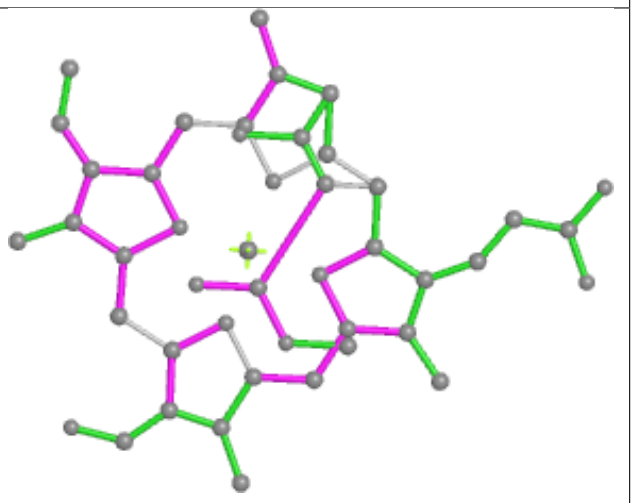
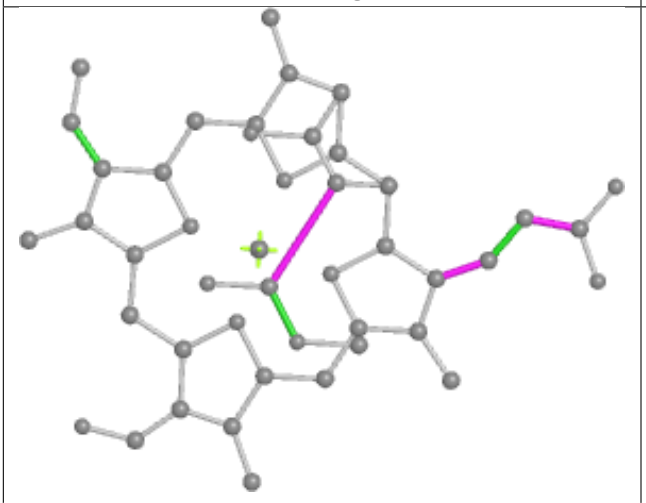


Bond angles



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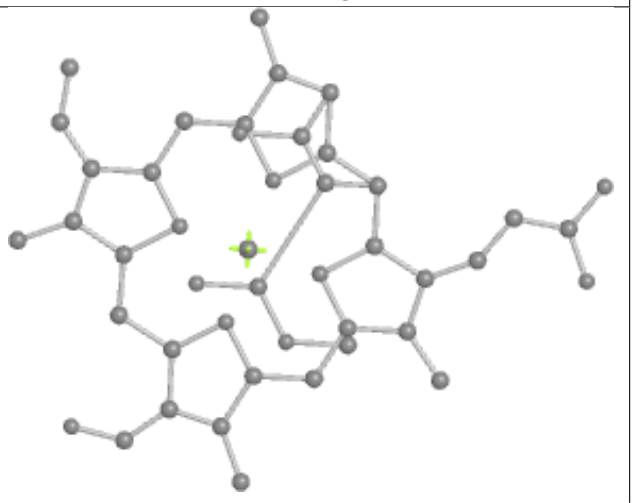
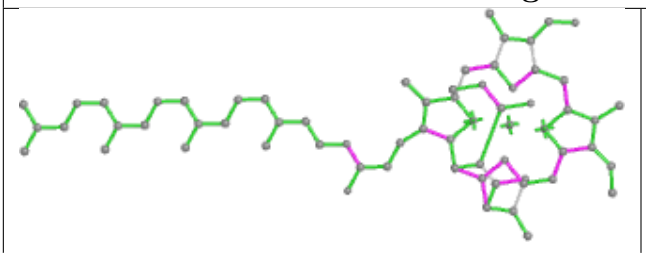


Rings

Ligand CL7 L 1501



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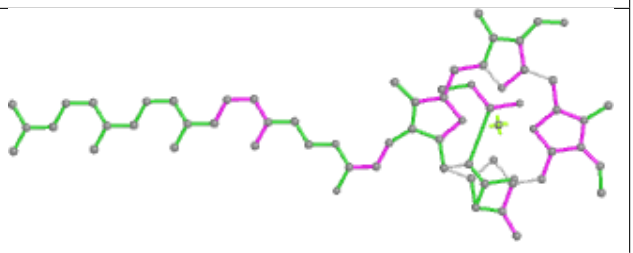
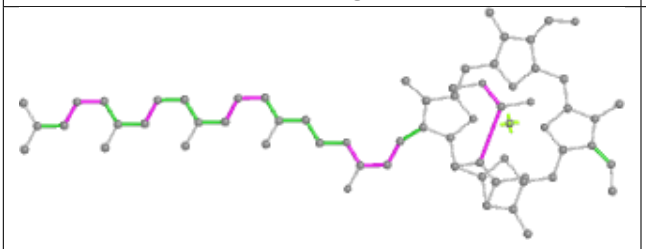


Bond angles



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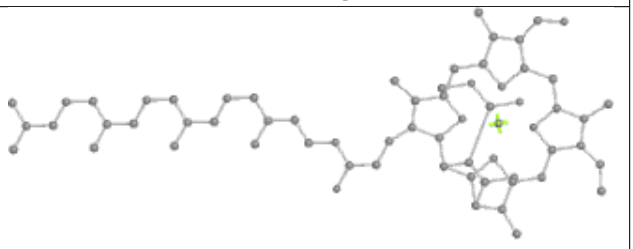
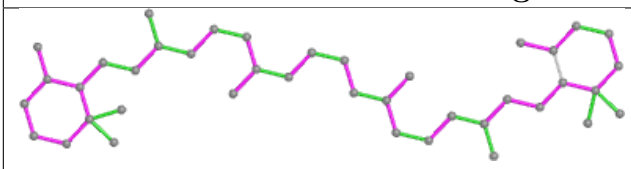


Rings

Ligand 8CT W 4018



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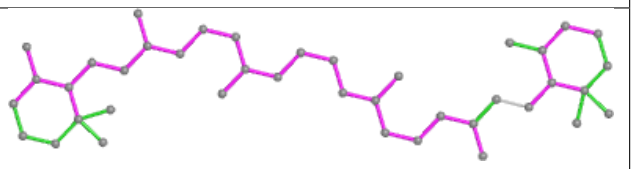
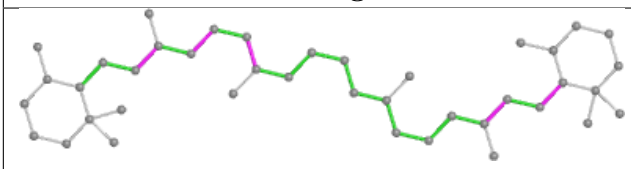


Bond angles



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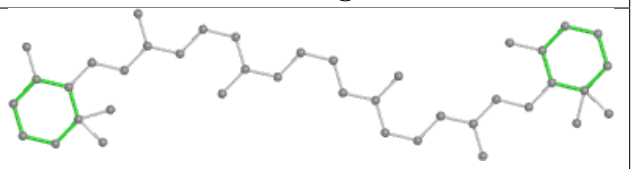
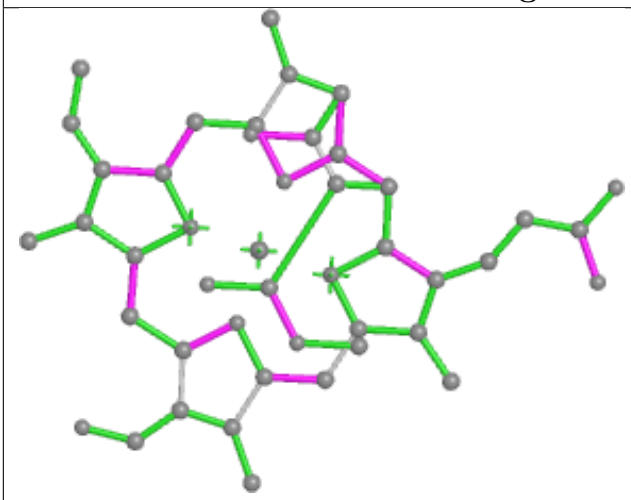


Rings

Ligand CL7 A 1109



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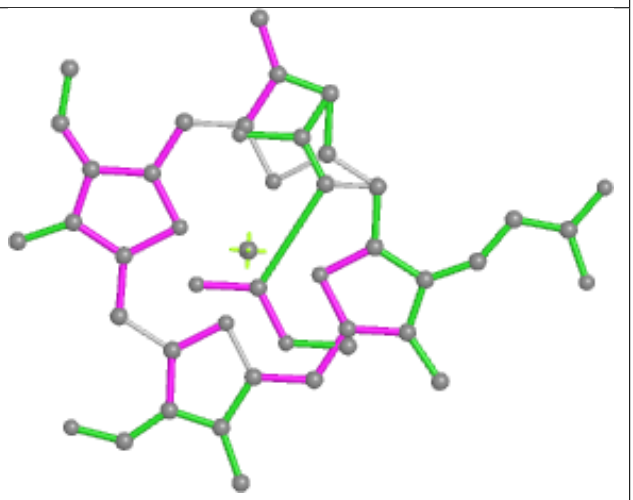
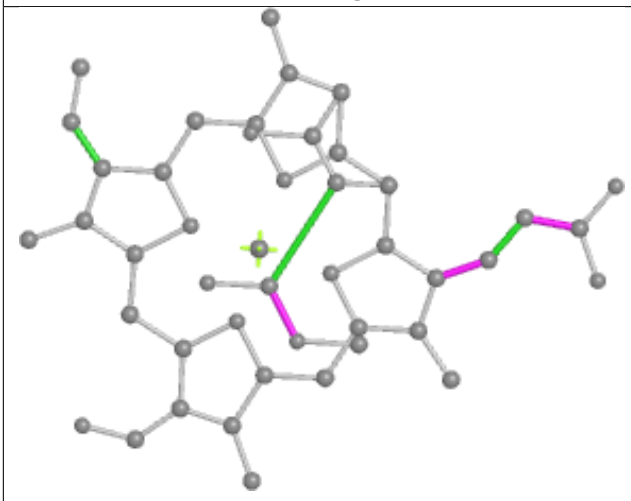
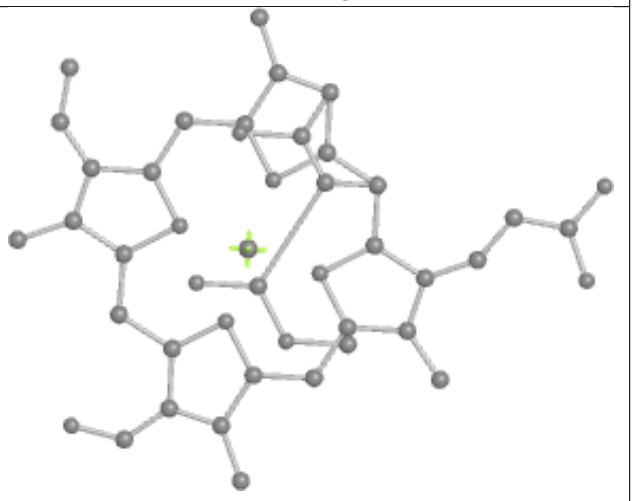


Bond angles

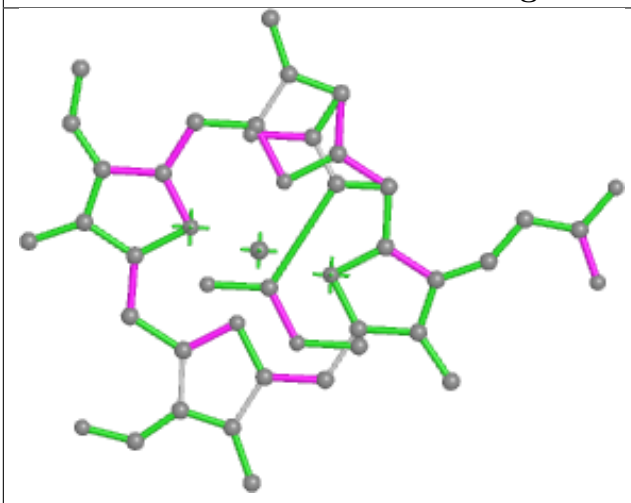


Torsions



Rings

Ligand CL7 B 1215



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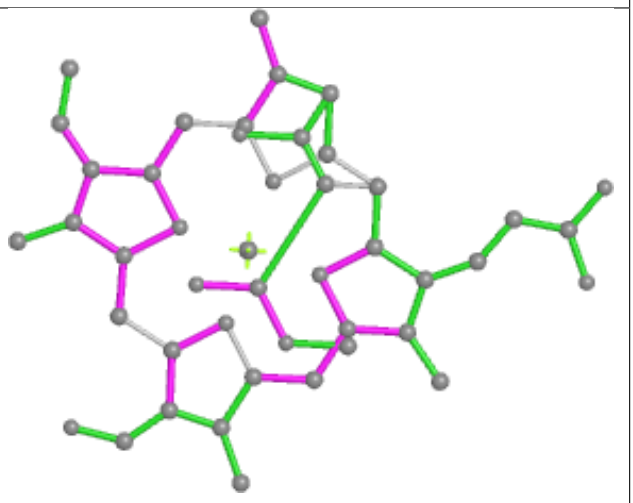
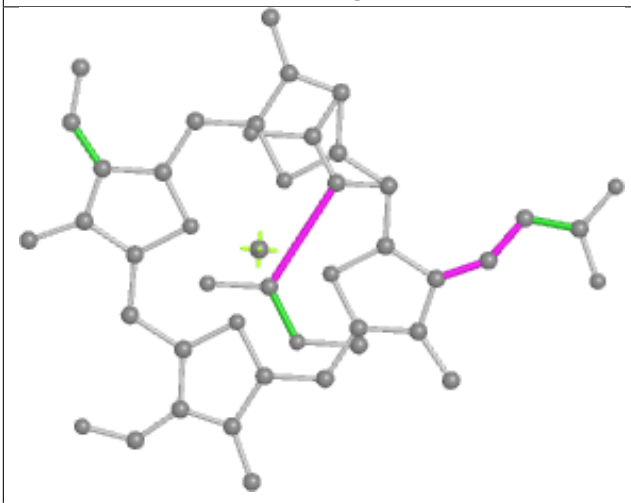


Bond angles



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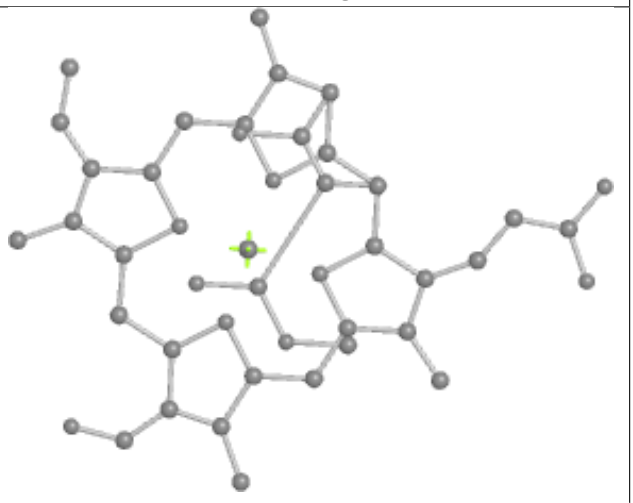
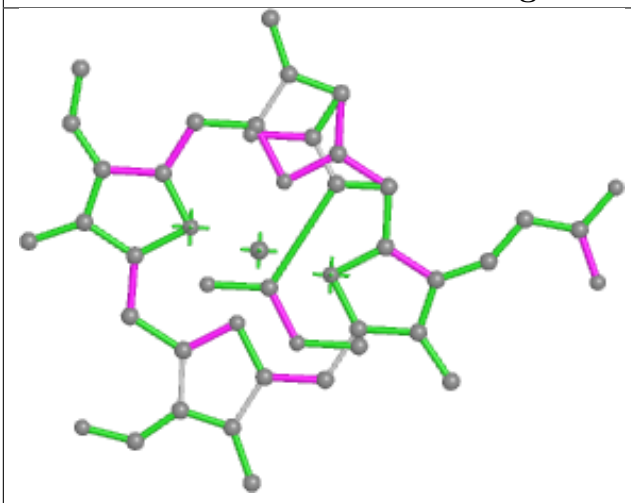


Rings

Ligand CL7 A 1105



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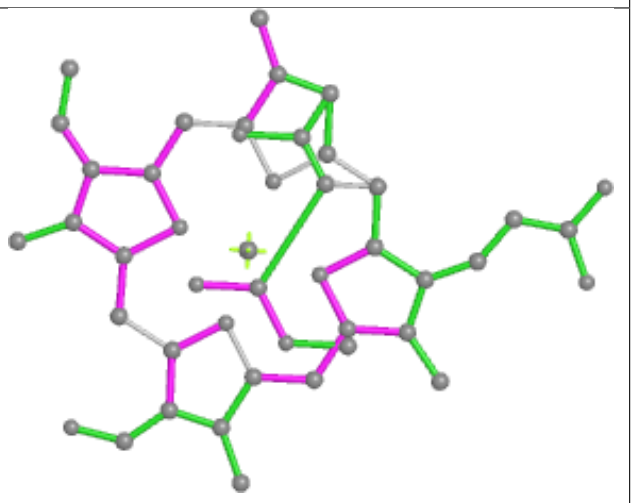
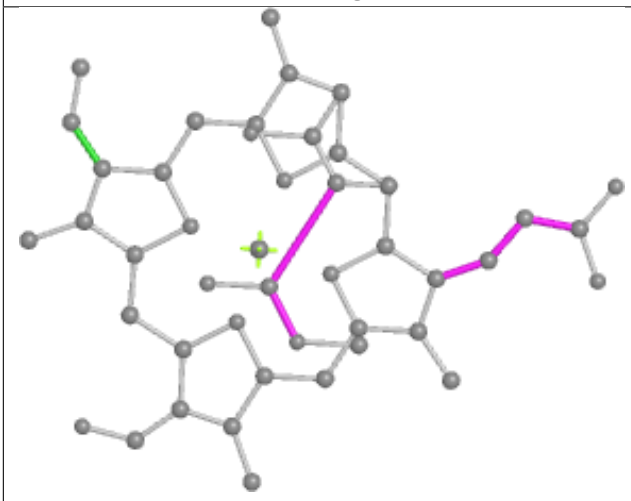


Bond angles



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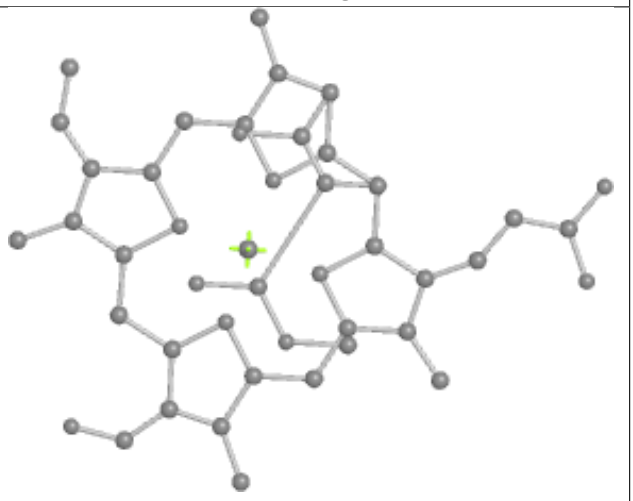
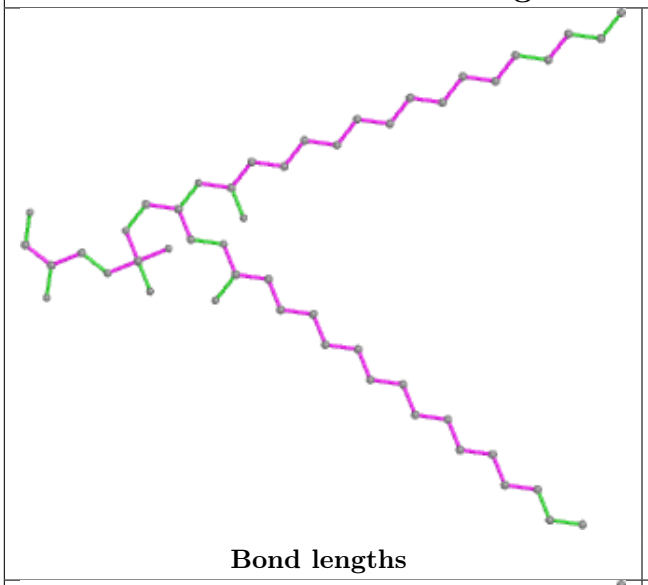


Rings

Ligand LHG A 5001



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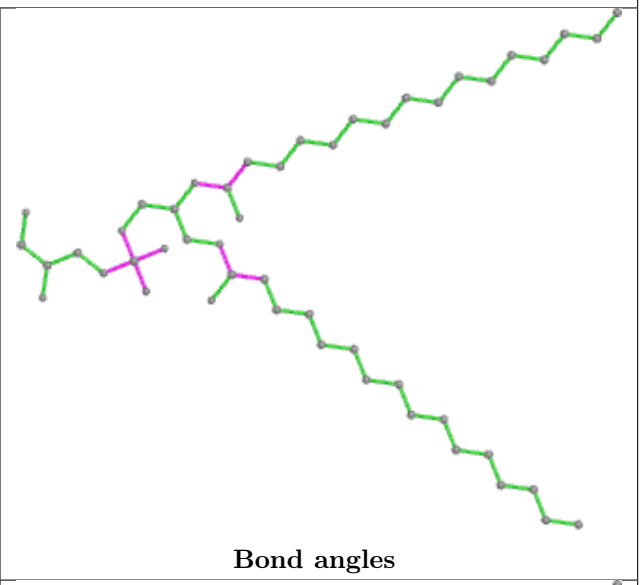
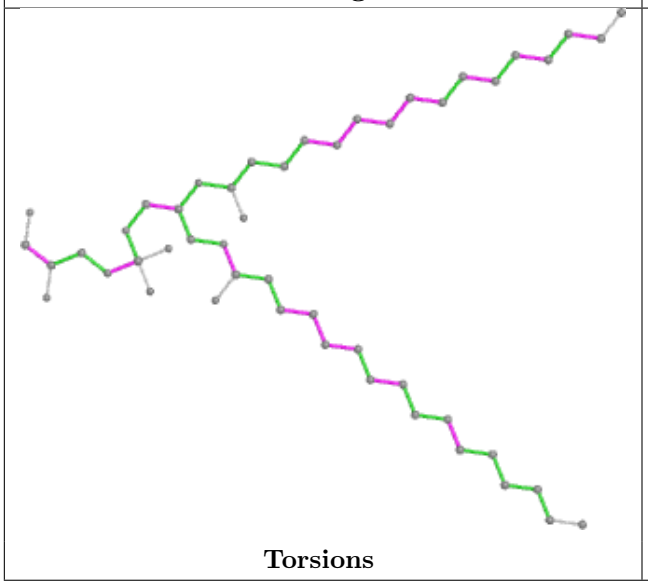


Bond angles



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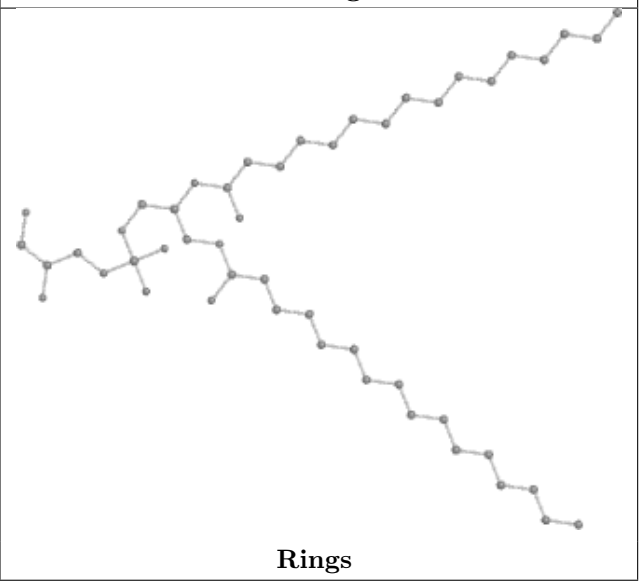
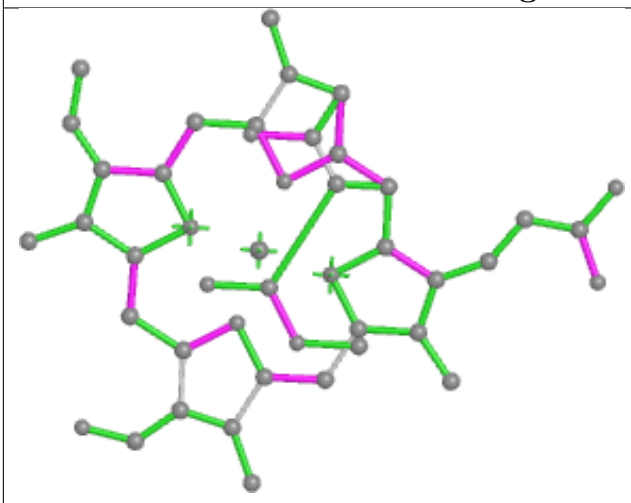


Rings

Ligand CL7 A 1124



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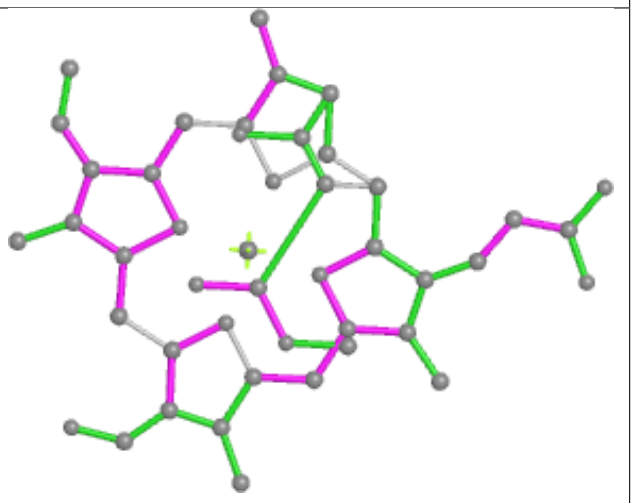

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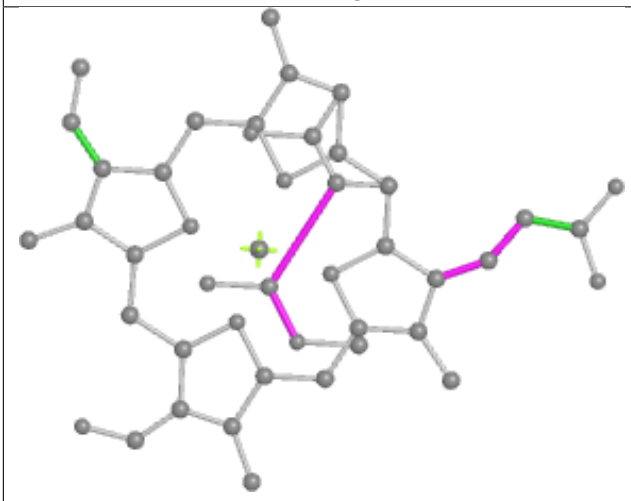

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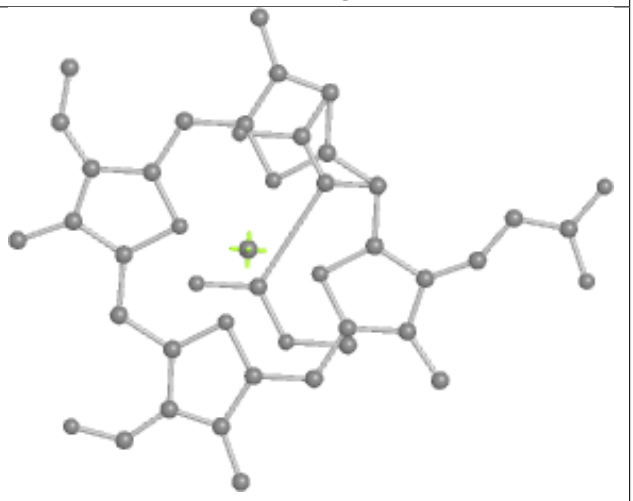
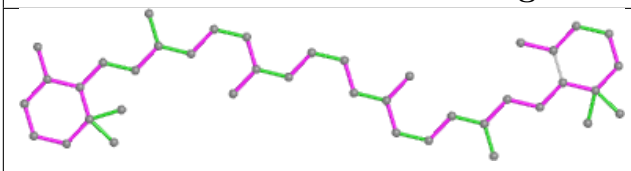


Rings

Ligand 8CT B 4006



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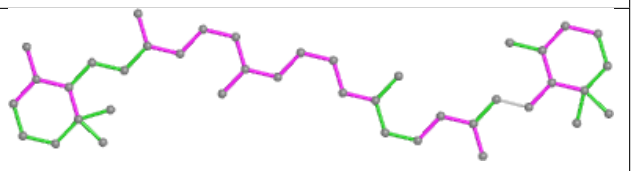
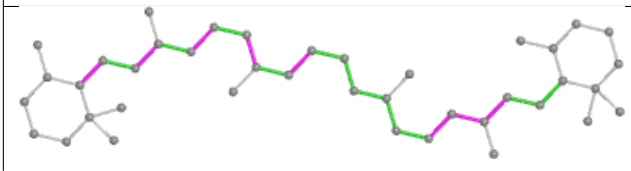


Bond angles



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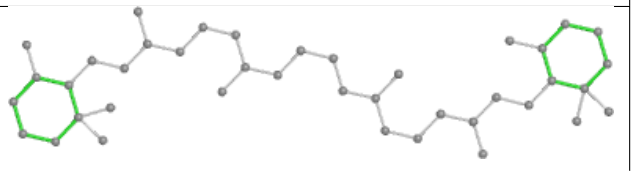
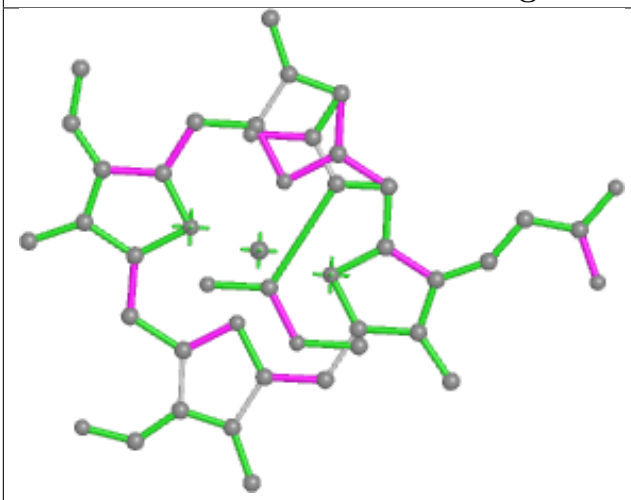
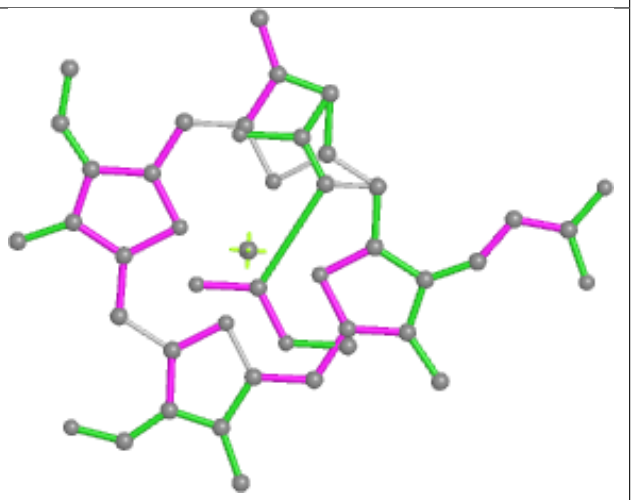


Rings

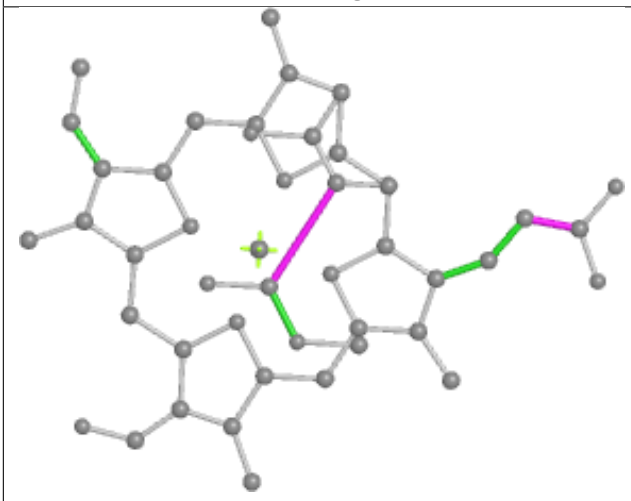
Ligand CL7 A 1107



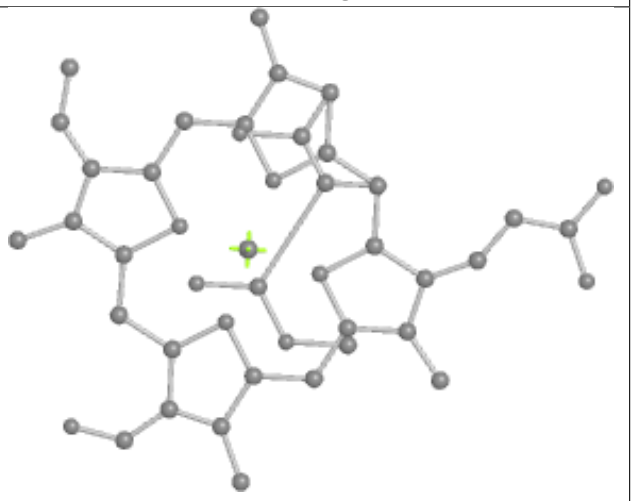
Bond lengths



Bond angles

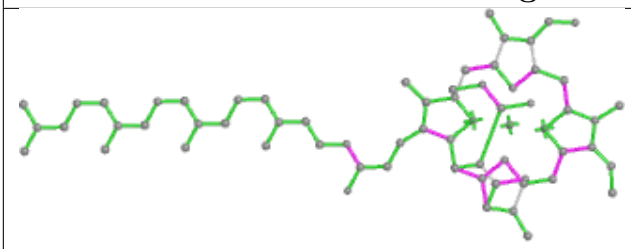


Torsions

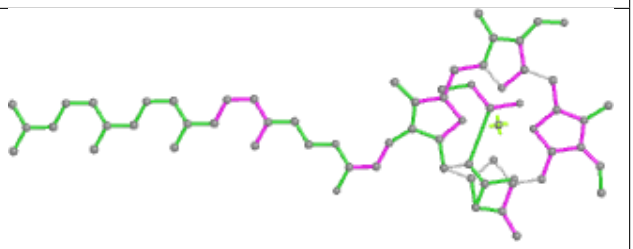


Rings

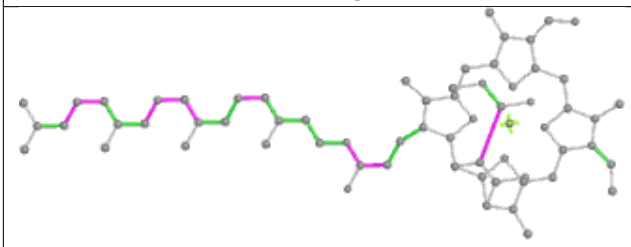
Ligand CL7 A 1123



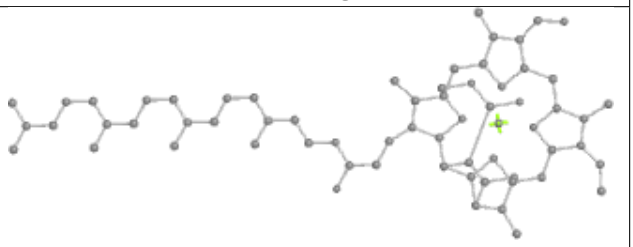
Bond lengths



Bond angles

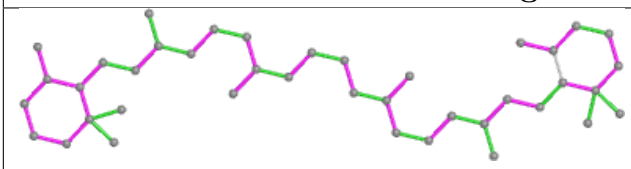


Torsions

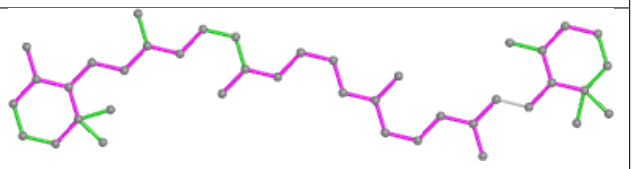


Rings

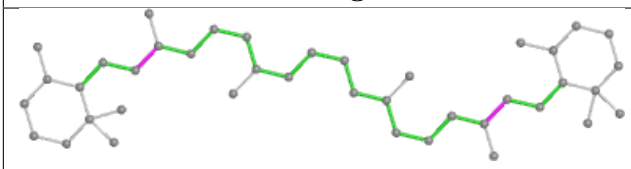
Ligand 8CT L 4019



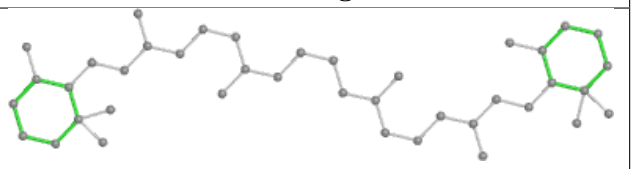
Bond lengths



Bond angles

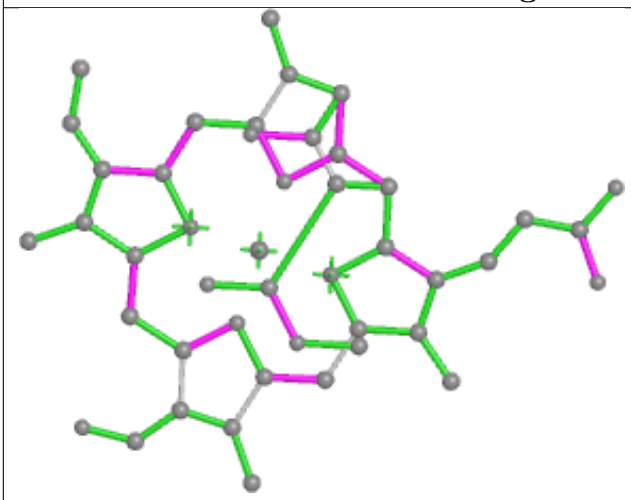


Torsions

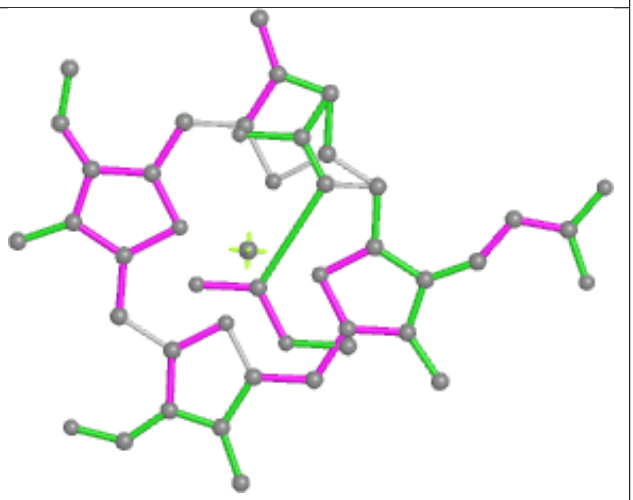


Rings

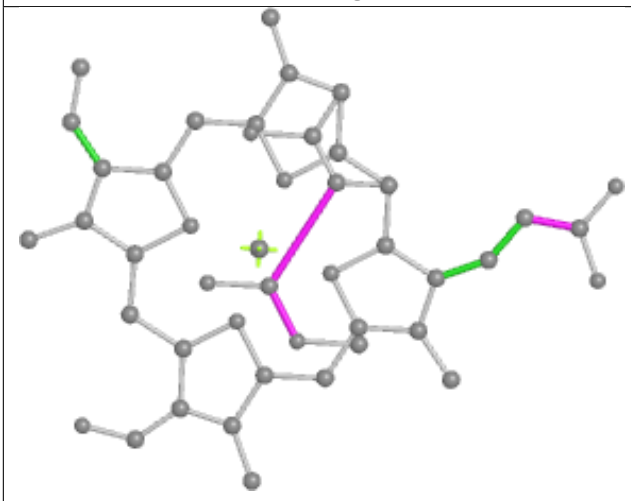
Ligand CL7 A 1127



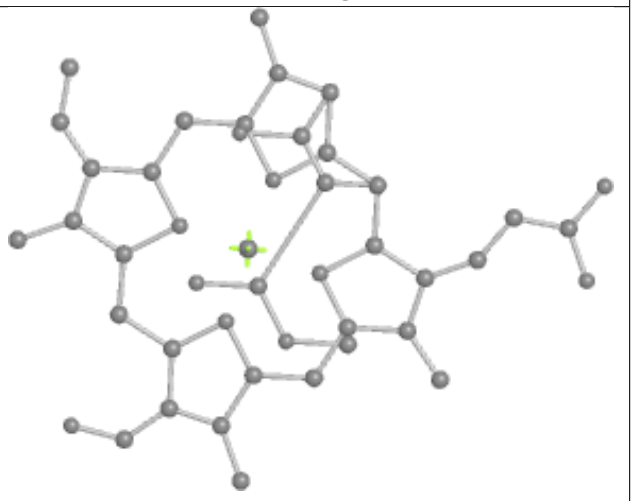
Bond lengths



Bond angles

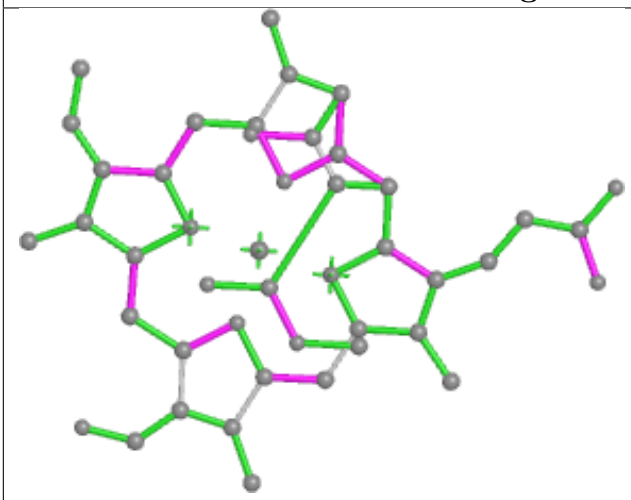


Torsions

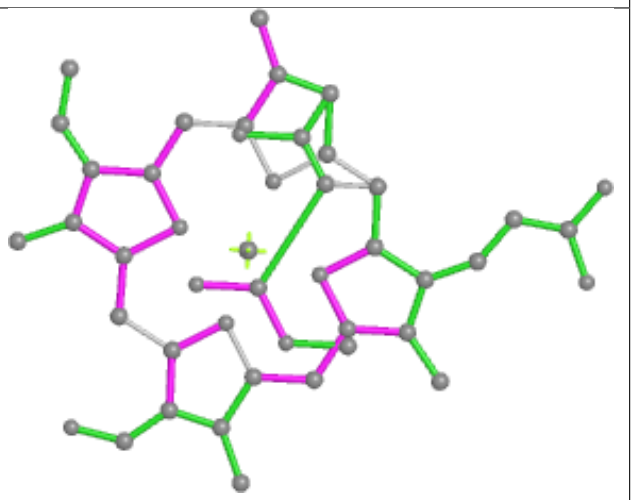


Rings

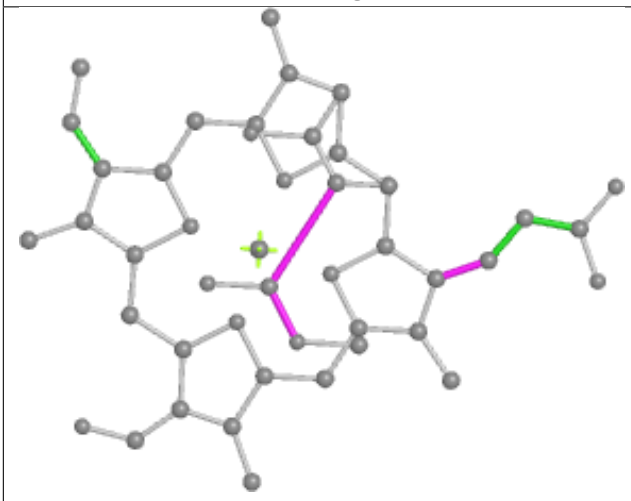
Ligand CL7 B 1210



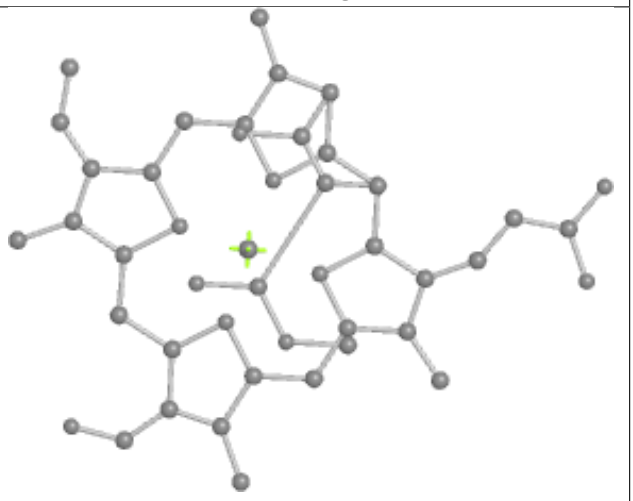
Bond lengths



Bond angles

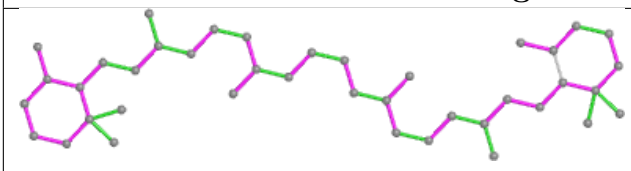


Torsions

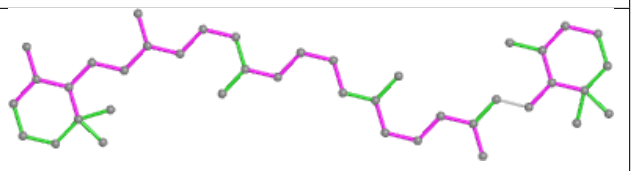


Rings

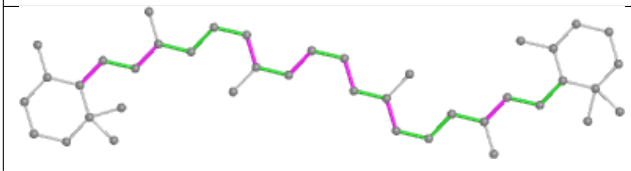
Ligand 8CT W 4020



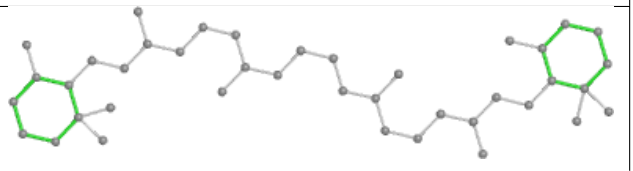
Bond lengths



Bond angles

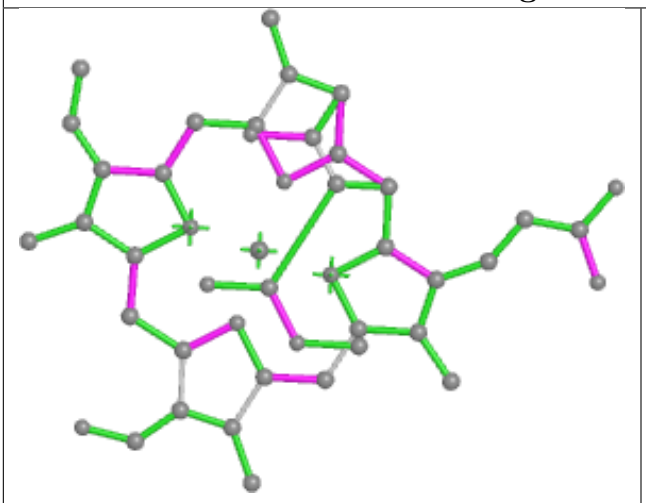


Torsions

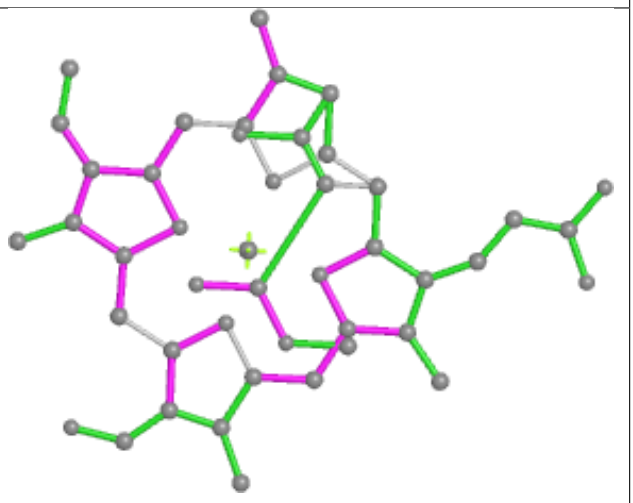


Rings

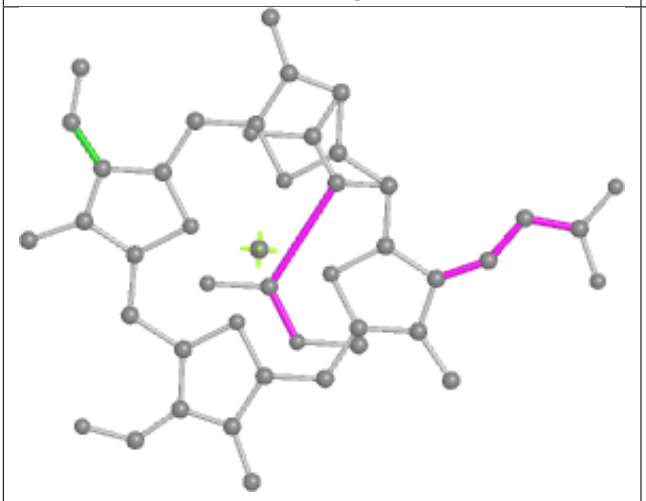
Ligand CL7 A 1135



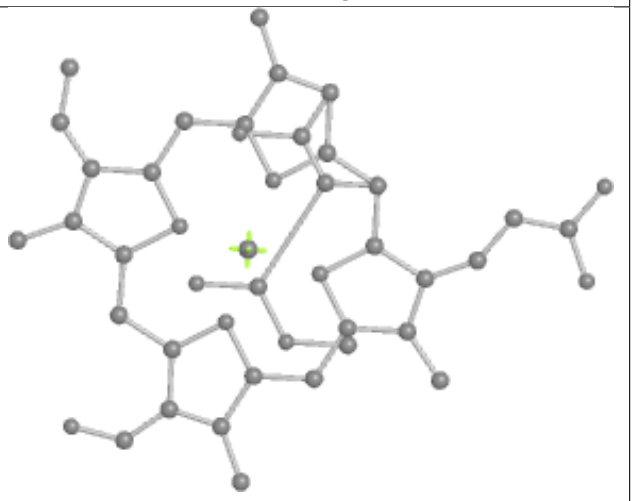
Bond lengths



Bond angles

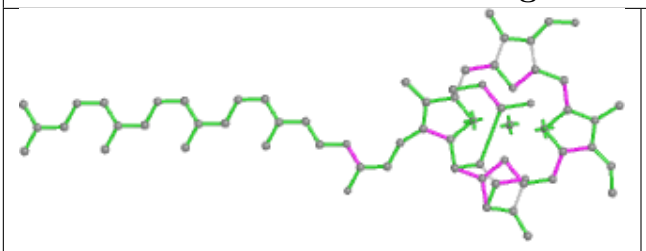


Torsions

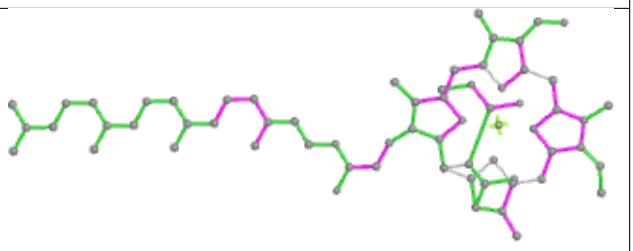


Rings

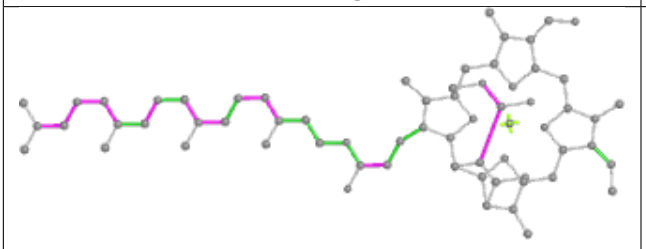
Ligand CL7 A 1131



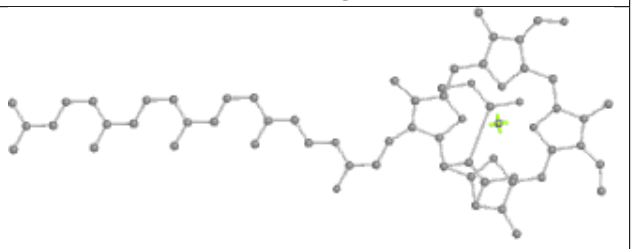
Bond lengths



Bond angles

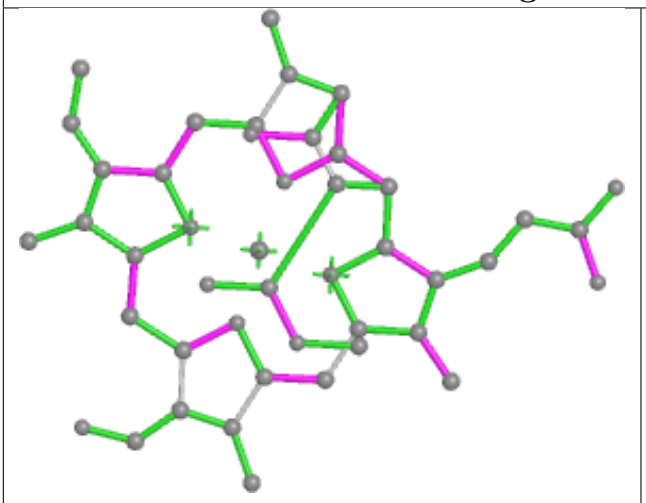


Torsions

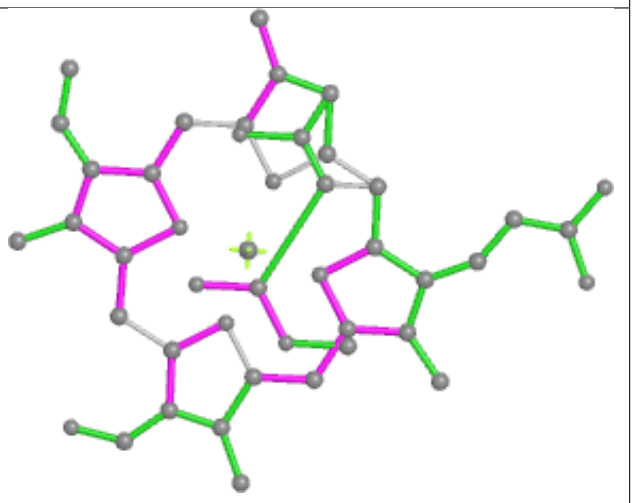


Rings

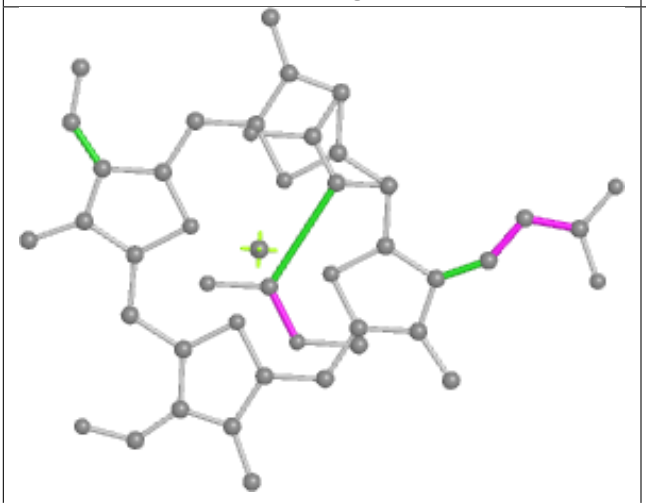
Ligand CL7 A 1119



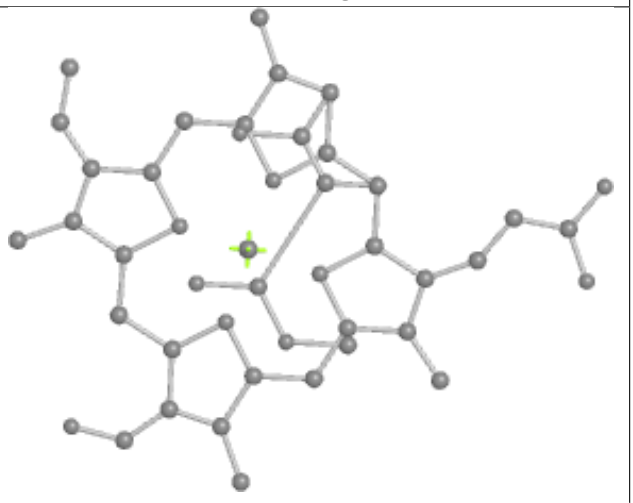
Bond lengths



Bond angles

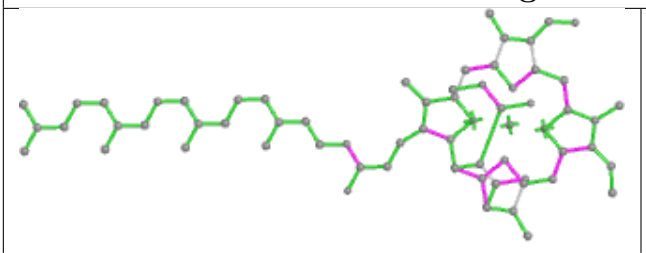


Torsions

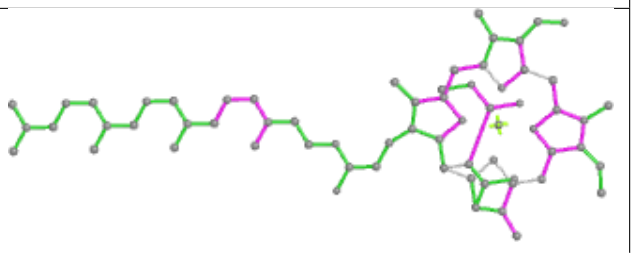


Rings

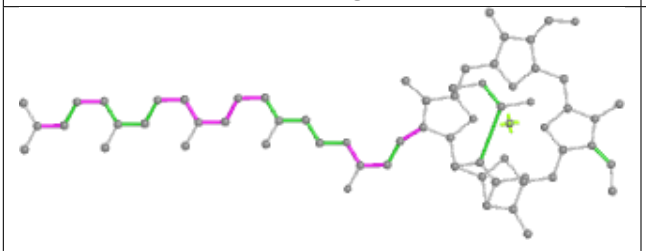
Ligand CL7 A 1136



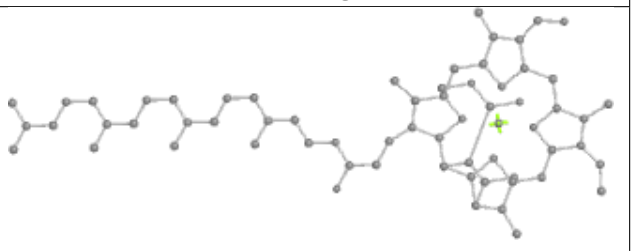
Bond lengths



Bond angles



Torsions



Rings

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.

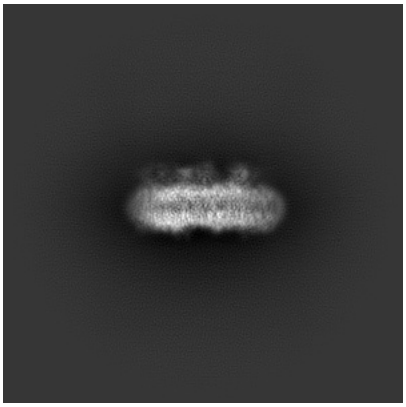
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30882. These allow visual inspection of the internal detail of the map and identification of artifacts.

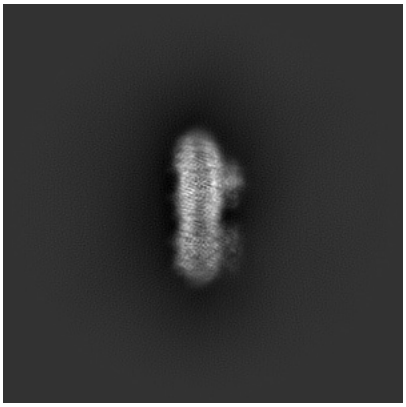
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

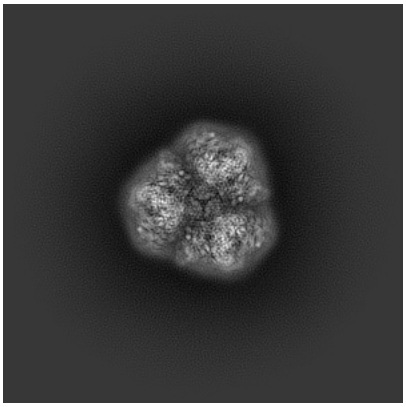
6.1.1 Primary map



X



Y

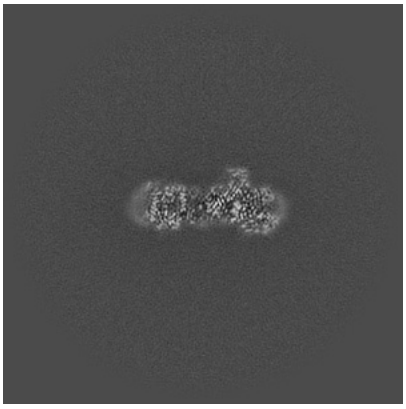


Z

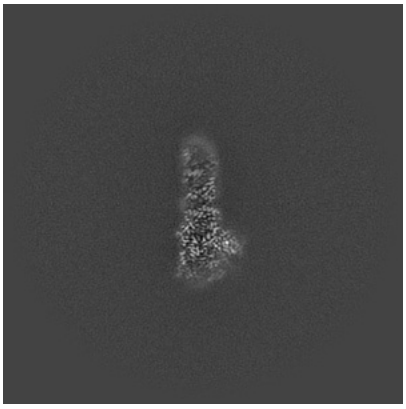
The images above show the map projected in three orthogonal directions.

6.2 Central slices

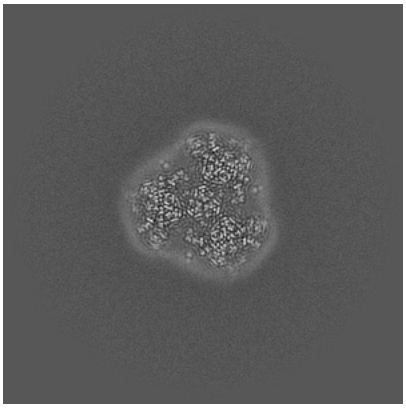
6.2.1 Primary map



X Index: 200



Y Index: 200

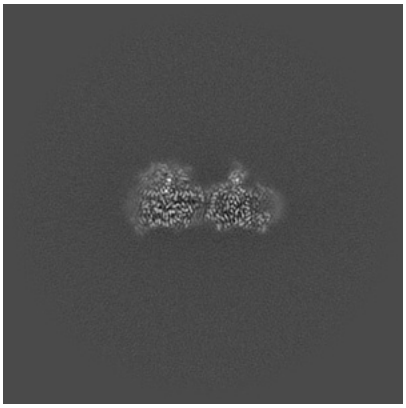


Z Index: 200

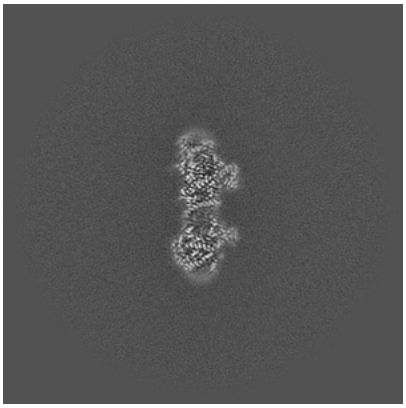
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

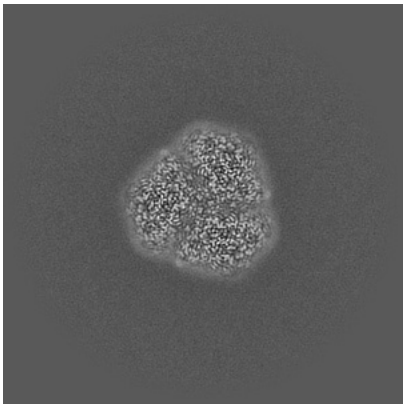
6.3.1 Primary map



X Index: 219



Y Index: 180

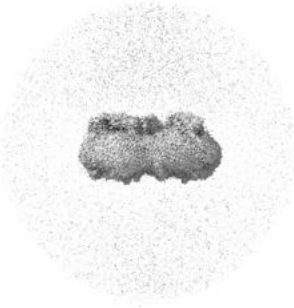


Z Index: 188

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.171. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

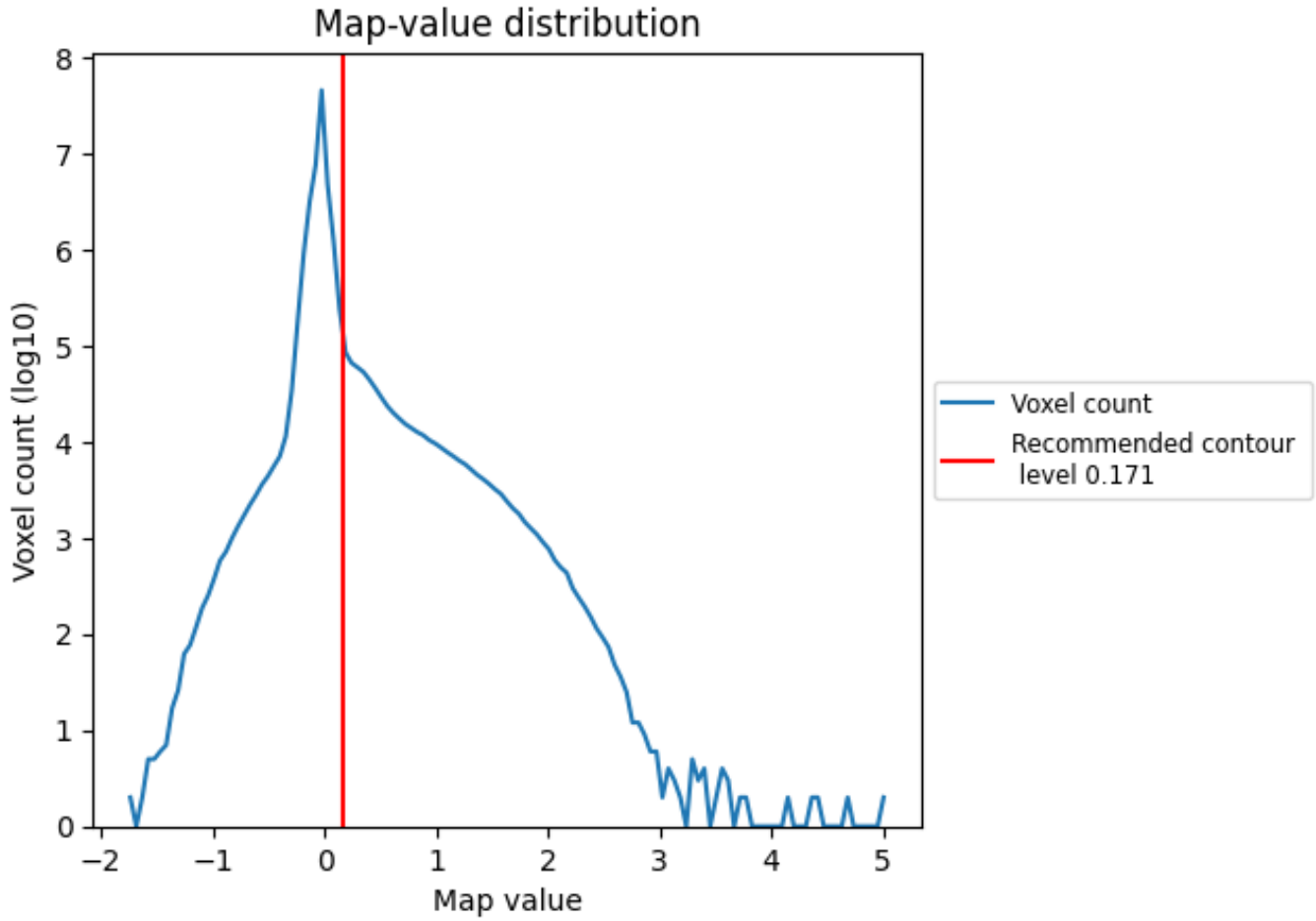
6.5 Mask visualisation (i)

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

7 Map analysis

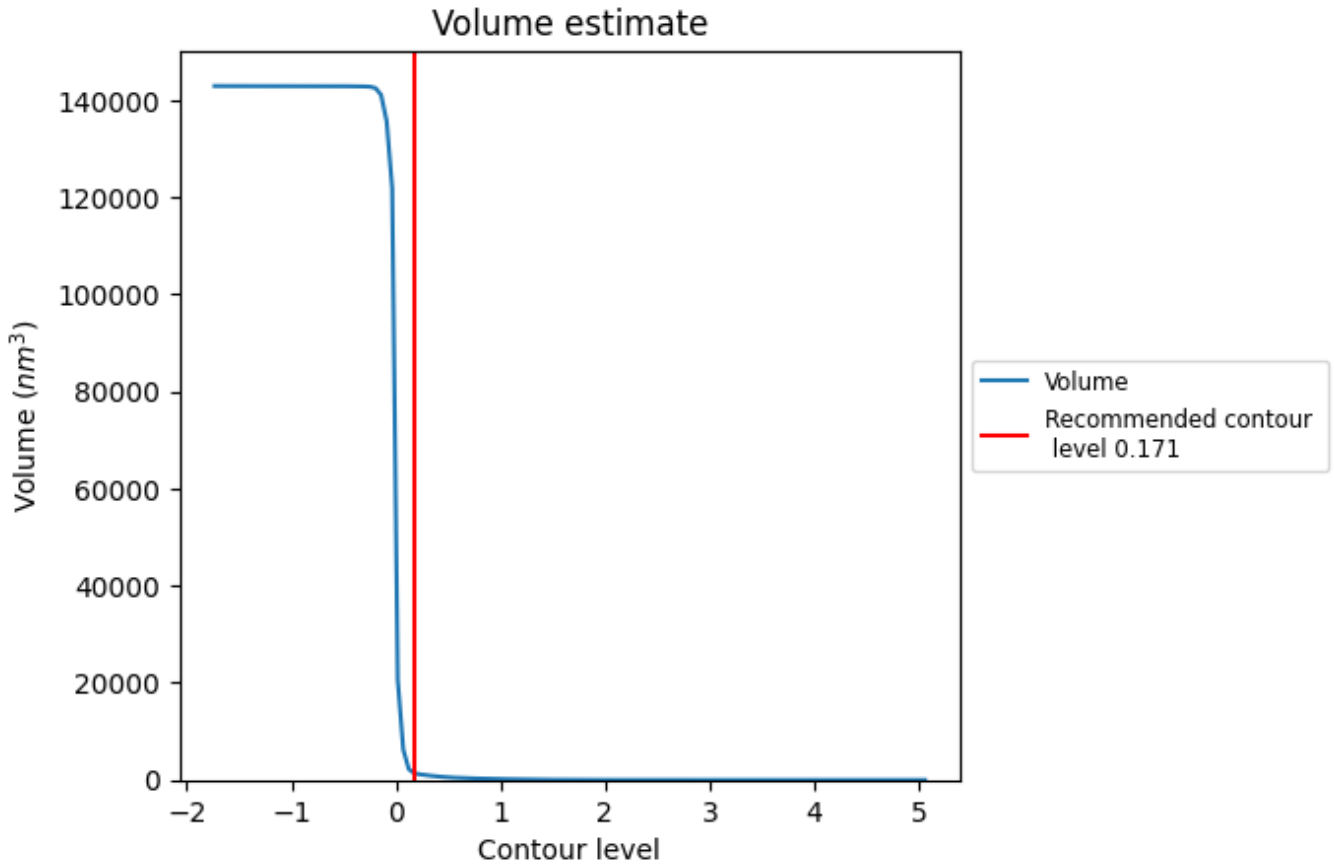
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

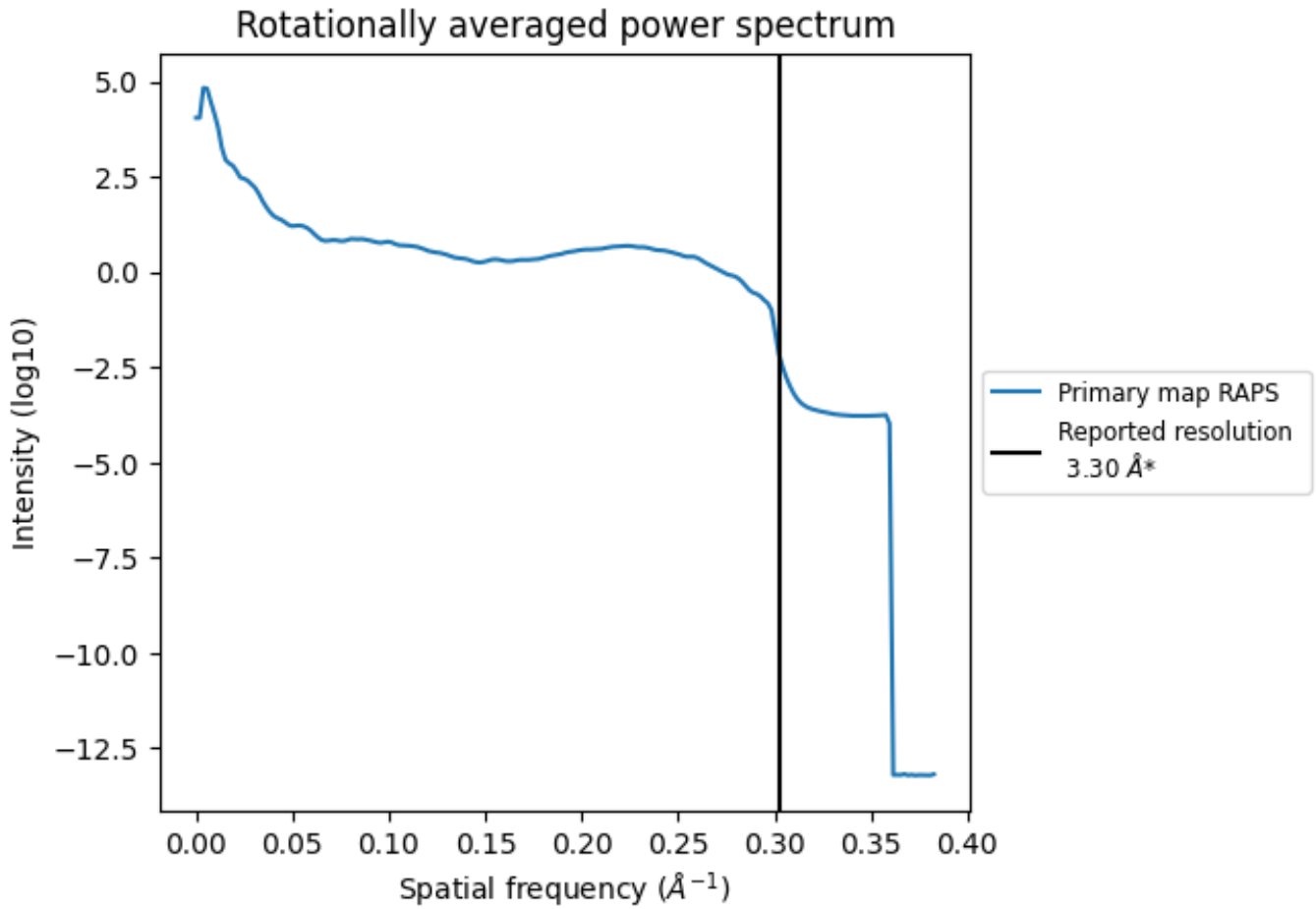
7.2 Volume estimate



The volume at the recommended contour level is 1462 nm^3; this corresponds to an approximate mass of 1320 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

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

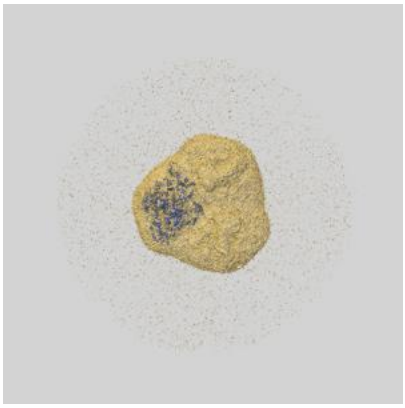
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30882 and PDB model 7DWQ. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay

X

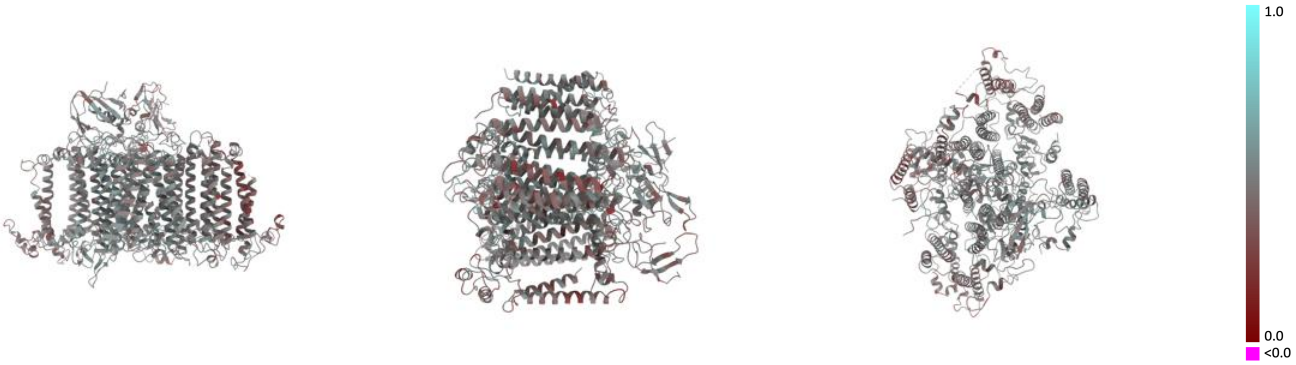
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.171 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.

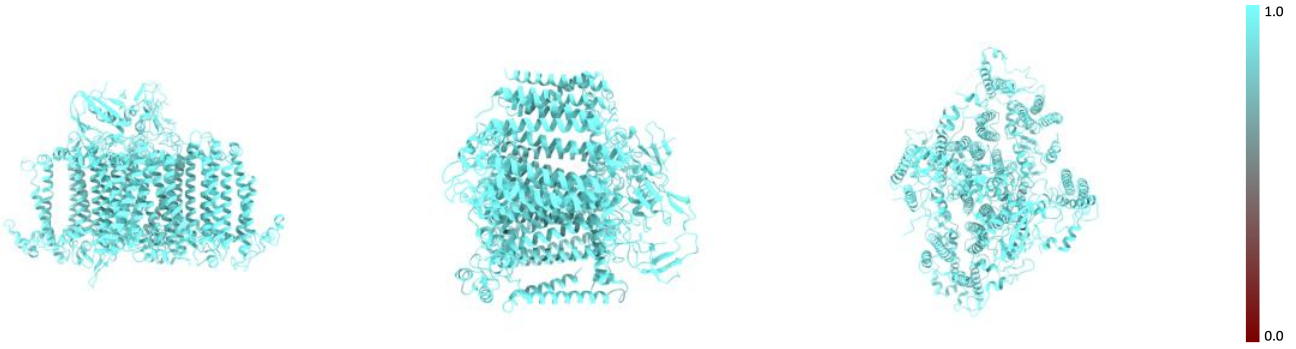
9.2 Q-score mapped to coordinate model



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.

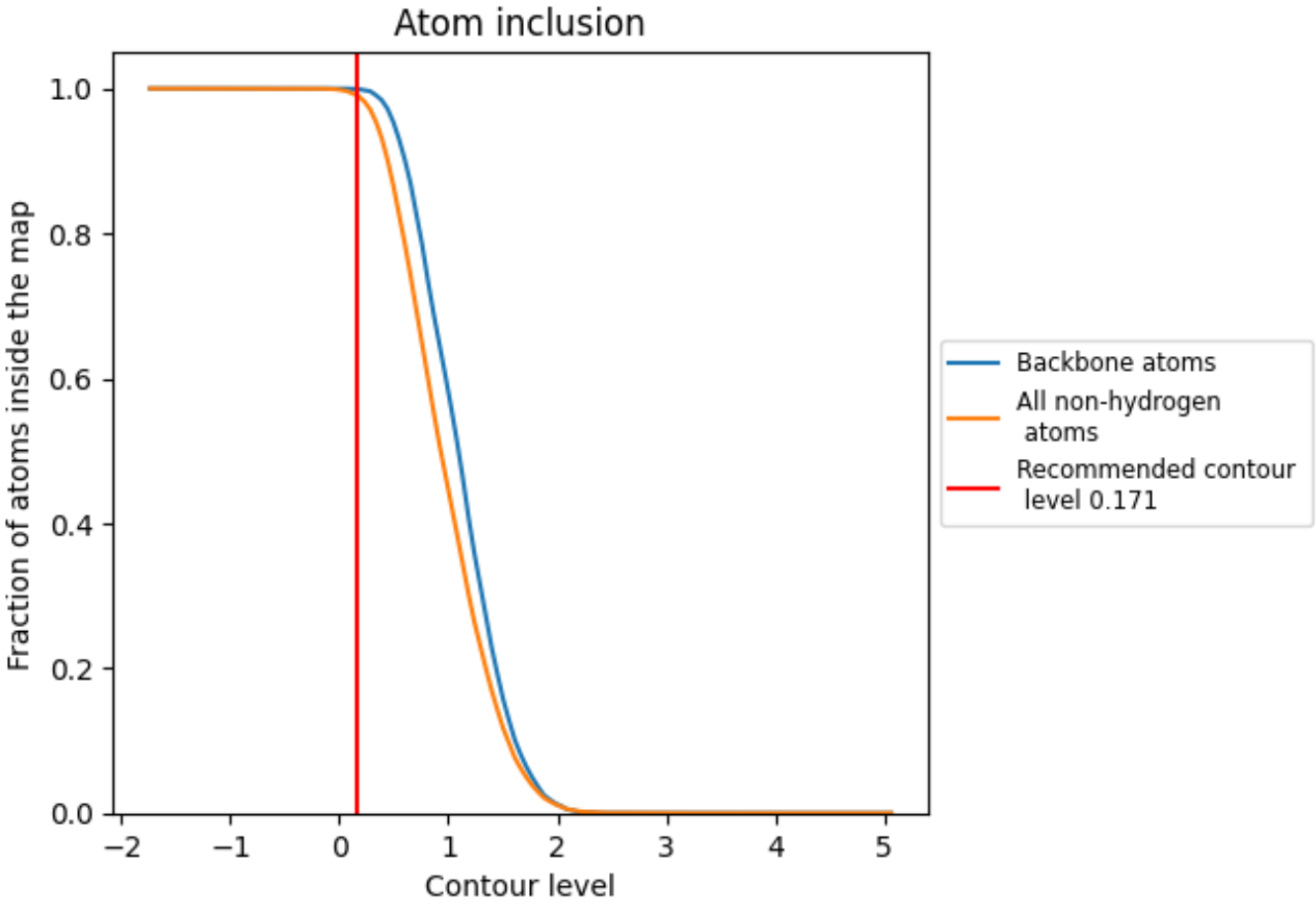
9.3 Atom inclusion mapped to coordinate model



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 (0.171).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.171) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9901	0.4690
A	0.9921	0.4790
B	0.9910	0.4710
C	1.0000	0.4540
D	0.9986	0.4810
E	0.9909	0.4300
F	0.9636	0.3750
J	0.9609	0.3970
L	0.9943	0.4920
M	0.9565	0.4250
W	0.9847	0.4930