wwPDB X-ray Structure Validation Summary Report (i)

Nov 23, 2023 – 03:16 AM JST

PDB ID	:	8H2U
Title	:	X-ray Structure of photosystem I-LHCI super complex from Chlamydomonas reinhardtii.
Authors	:	Tanaka, H.; Kubota-Kawai, H.; Misumi, Y.; Kurisu, G.
Deposited on	:	2022-10-07
Resolution	:	3.40 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

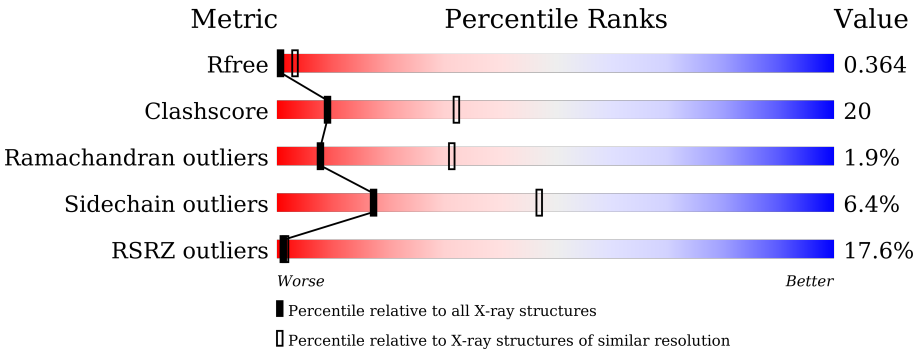
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	11% 72% 25%
2	B	735	15% 68% 29%
3	C	81	35% 70% 26%
4	D	196	22% 63% 9% 28%
5	E	97	21% 54% 9% 37%
6	F	227	4% 57% 8% 34%

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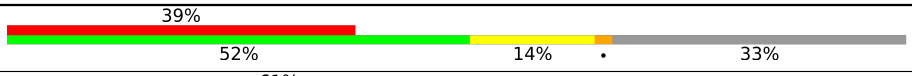
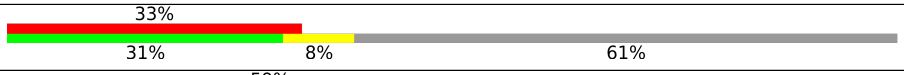
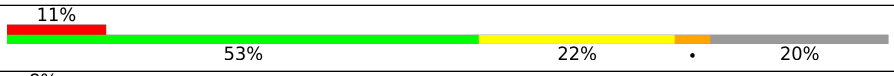
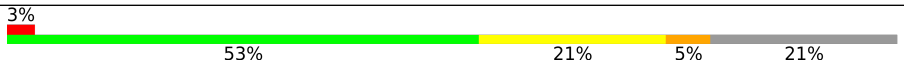
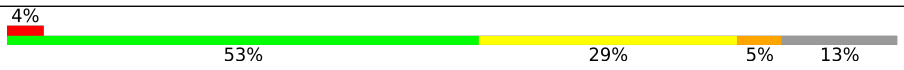
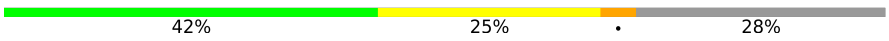
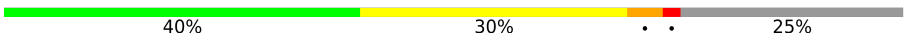
Mol	Chain	Length	Quality of chain
7	G	126	
8	H	130	
9	I	106	
10	J	41	
11	K	113	
12	L	196	
13	0	228	
13	1	228	
14	8	243	
15	7	241	
16	3	298	
17	4	264	
18	6	257	
19	5	257	

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
20	CLA	0	301	X	-	-	-
20	CLA	0	305	X	-	-	-
20	CLA	0	306	X	-	-	-
20	CLA	0	307	X	-	-	-
20	CLA	0	308	X	-	-	-
20	CLA	0	309	X	-	-	-
20	CLA	0	310	X	-	-	-
20	CLA	0	311	X	-	-	-
20	CLA	0	312	X	-	-	-
20	CLA	0	313	X	-	-	-
20	CLA	0	316	X	-	-	-
20	CLA	1	1003	X	-	-	-
20	CLA	1	1004	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	1	1005	X	-	-	-
20	CLA	1	1006	X	-	-	-
20	CLA	1	1007	X	-	-	-
20	CLA	1	1008	X	-	-	-
20	CLA	1	1009	X	-	-	-
20	CLA	1	1010	X	-	-	-
20	CLA	1	1011	X	-	-	-
20	CLA	1	1014	X	-	-	-
20	CLA	1	1017	X	-	-	-
20	CLA	3	1005	X	-	-	-
20	CLA	3	1006	X	-	-	-
20	CLA	3	1007	X	-	-	-
20	CLA	3	1008	X	-	-	-
20	CLA	3	1009	X	-	-	-
20	CLA	3	1010	X	-	-	-
20	CLA	3	1011	X	-	-	-
20	CLA	3	1012	X	-	-	-
20	CLA	3	1013	X	-	-	-
20	CLA	3	1015	X	-	-	-
20	CLA	3	1016	X	-	-	-
20	CLA	3	1017	X	-	-	-
20	CLA	4	304	X	-	-	-
20	CLA	4	305	X	-	-	-
20	CLA	4	306	X	-	-	-
20	CLA	4	307	X	-	-	-
20	CLA	4	308	X	-	-	-
20	CLA	4	309	X	-	-	-
20	CLA	4	310	X	-	-	-
20	CLA	4	311	X	-	-	-
20	CLA	4	314	X	-	-	-
20	CLA	5	301	X	-	-	-
20	CLA	5	304	X	-	-	-
20	CLA	5	305	X	-	-	-
20	CLA	5	306	X	-	-	-
20	CLA	5	307	X	-	-	-
20	CLA	5	308	X	-	-	-
20	CLA	5	309	X	-	-	-
20	CLA	5	310	X	-	-	-
20	CLA	5	311	X	-	-	-
20	CLA	5	312	X	-	-	-
20	CLA	5	315	X	-	-	-
20	CLA	5	318	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	5	321	X	-	-	-
20	CLA	5	322	X	-	-	-
20	CLA	5	323	X	-	-	-
20	CLA	6	301	X	-	-	-
20	CLA	6	305	X	-	-	-
20	CLA	6	306	X	-	-	-
20	CLA	6	307	X	-	-	-
20	CLA	6	308	X	-	-	-
20	CLA	6	309	X	-	-	-
20	CLA	6	310	X	-	-	-
20	CLA	6	311	X	-	-	-
20	CLA	6	312	X	-	-	-
20	CLA	6	315	X	-	-	-
20	CLA	6	318	X	-	-	-
20	CLA	6	320	X	-	-	-
20	CLA	7	1004	X	-	-	-
20	CLA	7	1005	X	-	-	-
20	CLA	7	1006	X	-	-	-
20	CLA	7	1007	X	-	-	-
20	CLA	7	1008	X	-	-	-
20	CLA	7	1009	X	-	-	-
20	CLA	7	1010	X	-	-	-
20	CLA	7	1011	X	-	-	-
20	CLA	7	1014	X	-	-	-
20	CLA	8	305	X	-	-	-
20	CLA	8	306	X	-	-	-
20	CLA	8	307	X	-	-	-
20	CLA	8	308	X	-	-	-
20	CLA	8	309	X	-	-	-
20	CLA	8	310	X	-	-	-
20	CLA	8	311	X	-	-	-
20	CLA	8	312	X	-	-	-
20	CLA	8	313	X	-	-	-
20	CLA	8	316	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	802	X	-	-	-
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	-	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	-	-
20	CLA	A	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	809	X	-	-	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	816	X	-	-	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	-	-
20	CLA	A	819	X	-	-	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-
20	CLA	A	823	X	-	-	-
20	CLA	A	824	X	-	-	-
20	CLA	A	825	X	-	-	-
20	CLA	A	826	X	-	-	-
20	CLA	A	827	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	-	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	-	-
20	CLA	A	839	X	-	-	-
20	CLA	A	840	X	-	-	-
20	CLA	A	851	X	-	-	-
20	CLA	A	852	X	-	-	-
20	CLA	B	801	X	-	-	-
20	CLA	B	802	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	825	X	-	-	-
20	CLA	B	826	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	-	-
20	CLA	B	837	X	-	-	-
20	CLA	B	838	X	-	-	-
20	CLA	B	839	X	-	-	-
20	CLA	B	840	X	-	-	-
20	CLA	B	841	X	-	-	-
20	CLA	B	850	X	-	-	-
20	CLA	F	302	X	-	-	-
20	CLA	F	303	X	-	-	-
20	CLA	F	305	X	-	-	-
20	CLA	G	201	X	-	-	X
20	CLA	G	202	X	-	-	X
20	CLA	G	203	X	-	-	X
20	CLA	J	102	X	-	-	-
20	CLA	K	201	X	-	-	X
20	CLA	K	202	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	L	201	X	-	-	-
20	CLA	L	202	X	-	-	X
20	CLA	L	203	X	-	-	X
20	CLA	L	204	X	-	-	X
21	SF4	C	1002	-	-	X	-
22	PQN	B	842	-	-	-	X
23	LHG	3	1019	-	-	-	X
24	BCR	1	1001	-	-	-	X
24	BCR	A	844	-	-	-	X
24	BCR	A	845	-	-	-	X
24	BCR	A	846	-	-	-	X
24	BCR	A	850	-	-	-	X
24	BCR	B	804	-	-	-	X
24	BCR	B	845	-	-	-	X
24	BCR	B	847	-	-	-	X
24	BCR	G	204	-	-	-	X
24	BCR	G	205	-	-	-	X
24	BCR	H	201	-	-	-	X
24	BCR	I	201	-	-	-	X
26	LMT	3	1018	-	-	-	X
26	LMT	B	849	-	-	-	X
27	LMG	0	303	-	-	X	X
27	LMG	4	318	-	-	X	-
27	LMG	6	319	-	-	-	X
27	LMG	8	319	-	-	-	X
27	LMG	J	101	-	-	-	X
28	LUT	1	1002	-	-	-	X
29	CHL	0	314	X	-	-	-
29	CHL	0	315	X	-	-	-
29	CHL	0	317	X	-	-	X
29	CHL	1	1012	X	-	-	-
29	CHL	1	1013	X	-	-	-
29	CHL	1	1015	X	-	-	X
29	CHL	3	1014	X	-	-	-
29	CHL	4	312	X	-	-	-
29	CHL	4	313	X	-	-	-
29	CHL	4	315	X	-	-	-
29	CHL	4	316	X	-	-	-
29	CHL	5	313	X	-	-	-
29	CHL	5	314	X	-	-	-
29	CHL	5	316	X	-	-	-
29	CHL	5	317	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CHL	6	313	X	-	-	-
29	CHL	6	314	X	-	-	-
29	CHL	6	316	X	-	-	-
29	CHL	6	317	X	-	-	-
29	CHL	7	1012	X	-	-	-
29	CHL	7	1013	X	-	-	-
29	CHL	7	1015	X	-	-	-
29	CHL	7	1017	X	-	-	-
29	CHL	8	314	X	-	-	-
29	CHL	8	315	X	-	-	-
29	CHL	8	317	X	-	-	-

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 42070 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	0	0
			5799	3792	989	996	22			

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	728	Total	C	N	O	S	0	0	0
			5786	3801	969	998	18			

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			600	369	103	116	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1101	703	196	195	7			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	61	Total	C	N	O	0	0	0
			480	306	85	89			

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	150	Total	C	N	O	S	0	0	0
			1150	745	192	210	3			

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	85	Total	C	N	O	0	0	0
			620	398	108	114			

- Molecule 8 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	90	Total	C	N	O	S	0	0	0
			694	433	120	139	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total	C	N	O	S	0	0	0
			221	153	31	36	1			

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	39	Total	C	N	O	S	0	0	0
			320	219	45	55	1			

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	44	Total	C	N	O	S	0	0	0
			295	191	47	55	2			

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	150	Total	C	N	O	S	0	0	0
			1082	703	178	198	3			

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	0	182	Total	C	N	O	S	0	0	0
			1361	887	226	245	3			
13	1	182	Total	C	N	O	S	0	0	0
			1362	886	226	247	3			

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	8	193	Total	C	N	O	S	0	0	0
			1466	953	251	258	4			

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	7	209	Total	C	N	O	S	0	0	0
			1622	1051	271	294	6			

- Molecule 16 is a protein called Lhca3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3	201	Total	C	N	O	S	0	0	0
			1542	1008	250	276	8			

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4	202	Total	C	N	O	S	0	0	0
			1571	1031	254	281	5			

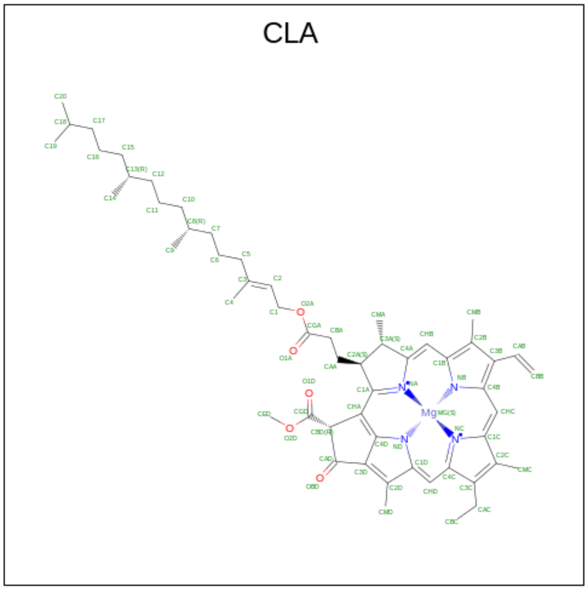
- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	6	184	Total	C	N	O	S	0	0	0
			1431	945	235	247	4			

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	5	193	Total	C	N	O	S	0	0	0
			1510	984	255	264	7			

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 40 32 1 4 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	A	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 44 34 1 4 5	0	0
20	B	1	Total C Mg N O 43 33 1 4 5	0	0
20	F	1	Total C Mg N O 44 34 1 4 5	0	0
20	F	1	Total C Mg N O 44 34 1 4 5	0	0
20	F	1	Total C Mg N O 44 34 1 4 5	0	0
20	G	1	Total C Mg N O 44 34 1 4 5	0	0
20	G	1	Total C Mg N O 44 34 1 4 5	0	0
20	G	1	Total C Mg N O 44 34 1 4 5	0	0
20	J	1	Total C Mg N O 44 34 1 4 5	0	0
20	K	1	Total C Mg N O 44 34 1 4 5	0	0
20	K	1	Total C Mg N 27 22 1 4	0	0
20	L	1	Total C Mg N O 44 34 1 4 5	0	0
20	L	1	Total C Mg N O 44 34 1 4 5	0	0
20	L	1	Total C Mg N O 44 34 1 4 5	0	0
20	L	1	Total C Mg N O 44 34 1 4 5	0	0
20	0	1	Total C Mg N O 44 34 1 4 5	0	0
20	0	1	Total C Mg N O 44 34 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	0	1	Total C Mg N O 44 34 1 4 5	0	0
20	0	1	Total C Mg N O 44 34 1 4 5	0	0
20	0	1	Total C Mg N O 44 34 1 4 5	0	0
20	0	1	Total C Mg N O 44 34 1 4 5	0	0
20	0	1	Total C Mg N O 44 34 1 4 5	0	0
20	0	1	Total C Mg N O 44 34 1 4 5	0	0
20	0	1	Total C Mg N O 44 34 1 4 5	0	0
20	0	1	Total C Mg N O 44 34 1 4 5	0	0
20	0	1	Total C Mg N O 44 34 1 4 5	0	0
20	8	1	Total C Mg N O 44 34 1 4 5	0	0
20	8	1	Total C Mg N O 44 34 1 4 5	0	0
20	8	1	Total C Mg N O 44 34 1 4 5	0	0
20	8	1	Total C Mg N O 44 34 1 4 5	0	0
20	8	1	Total C Mg N O 44 34 1 4 5	0	0
20	8	1	Total C Mg N O 44 34 1 4 5	0	0
20	8	1	Total C Mg N O 44 34 1 4 5	0	0
20	8	1	Total C Mg N O 44 34 1 4 5	0	0
20	8	1	Total C Mg N O 44 34 1 4 5	0	0
20	8	1	Total C Mg N O 44 34 1 4 5	0	0
20	7	1	Total C Mg N O 44 34 1 4 5	0	0
20	7	1	Total C Mg N O 44 34 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	7	1	Total C Mg N O 44 34 1 4 5	0	0
20	7	1	Total C Mg N O 44 34 1 4 5	0	0
20	7	1	Total C Mg N O 44 34 1 4 5	0	0
20	7	1	Total C Mg N O 44 34 1 4 5	0	0
20	7	1	Total C Mg N O 44 34 1 4 5	0	0
20	7	1	Total C Mg N O 44 34 1 4 5	0	0
20	7	1	Total C Mg N O 44 34 1 4 5	0	0
20	3	1	Total C Mg N O 44 34 1 4 5	0	0
20	3	1	Total C Mg N O 44 34 1 4 5	0	0
20	3	1	Total C Mg N O 44 34 1 4 5	0	0
20	3	1	Total C Mg N O 44 34 1 4 5	0	0
20	3	1	Total C Mg N O 44 34 1 4 5	0	0
20	3	1	Total C Mg N O 44 34 1 4 5	0	0
20	3	1	Total C Mg N O 40 32 1 4 3	0	0
20	3	1	Total C Mg N O 44 34 1 4 5	0	0
20	3	1	Total C Mg N O 44 34 1 4 5	0	0
20	3	1	Total C Mg N O 44 34 1 4 5	0	0
20	3	1	Total C Mg N O 44 34 1 4 5	0	0
20	3	1	Total C Mg N O 44 34 1 4 5	0	0
20	1	1	Total C Mg N O 44 34 1 4 5	0	0
20	1	1	Total C Mg N O 44 34 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	1	1	Total C Mg N O 44 34 1 4 5	0	0
20	1	1	Total C Mg N O 44 34 1 4 5	0	0
20	1	1	Total C Mg N O 44 34 1 4 5	0	0
20	1	1	Total C Mg N O 44 34 1 4 5	0	0
20	1	1	Total C Mg N O 44 34 1 4 5	0	0
20	1	1	Total C Mg N O 44 34 1 4 5	0	0
20	1	1	Total C Mg N O 44 34 1 4 5	0	0
20	1	1	Total C Mg N O 44 34 1 4 5	0	0
20	1	1	Total C Mg N O 44 34 1 4 5	0	0
20	4	1	Total C Mg N O 44 34 1 4 5	0	0
20	4	1	Total C Mg N O 44 34 1 4 5	0	0
20	4	1	Total C Mg N O 44 34 1 4 5	0	0
20	4	1	Total C Mg N O 44 34 1 4 5	0	0
20	4	1	Total C Mg N O 44 34 1 4 5	0	0
20	4	1	Total C Mg N O 44 34 1 4 5	0	0
20	4	1	Total C Mg N O 44 34 1 4 5	0	0
20	4	1	Total C Mg N O 44 34 1 4 5	0	0
20	4	1	Total C Mg N O 44 34 1 4 5	0	0
20	6	1	Total C Mg N O 44 34 1 4 5	0	0
20	6	1	Total C Mg N O 44 34 1 4 5	0	0
20	6	1	Total C Mg N O 44 34 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	6	1	Total C Mg N O 44 34 1 4 5	0	0
20	6	1	Total C Mg N O 44 34 1 4 5	0	0
20	6	1	Total C Mg N O 44 34 1 4 5	0	0
20	6	1	Total C Mg N O 44 34 1 4 5	0	0
20	6	1	Total C Mg N O 44 34 1 4 5	0	0
20	6	1	Total C Mg N O 44 34 1 4 5	0	0
20	6	1	Total C Mg N O 44 34 1 4 5	0	0
20	6	1	Total C Mg N O 44 34 1 4 5	0	0
20	6	1	Total C Mg N O 44 34 1 4 5	0	0
20	5	1	Total C Mg N O 44 34 1 4 5	0	0
20	5	1	Total C Mg N O 44 34 1 4 5	0	0
20	5	1	Total C Mg N O 44 34 1 4 5	0	0
20	5	1	Total C Mg N O 44 34 1 4 5	0	0
20	5	1	Total C Mg N O 44 34 1 4 5	0	0
20	5	1	Total C Mg N O 44 34 1 4 5	0	0
20	5	1	Total C Mg N O 44 34 1 4 5	0	0
20	5	1	Total C Mg N O 44 34 1 4 5	0	0
20	5	1	Total C Mg N O 44 34 1 4 5	0	0
20	5	1	Total C Mg N O 44 34 1 4 5	0	0
20	5	1	Total C Mg N O 44 34 1 4 5	0	0
20	5	1	Total C Mg N O 44 34 1 4 5	0	0

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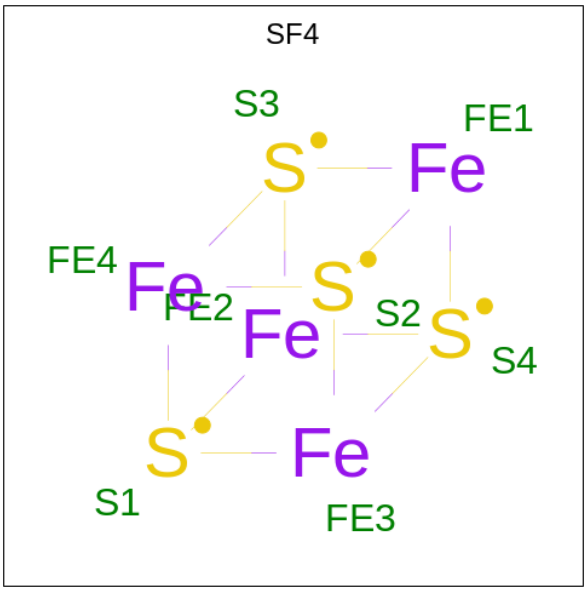
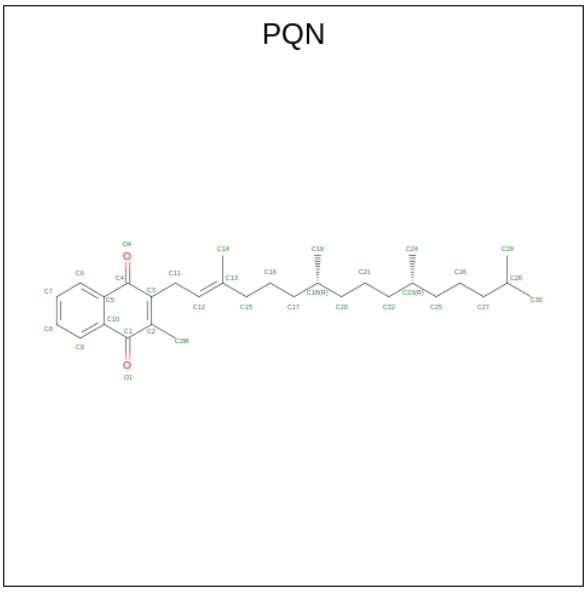
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



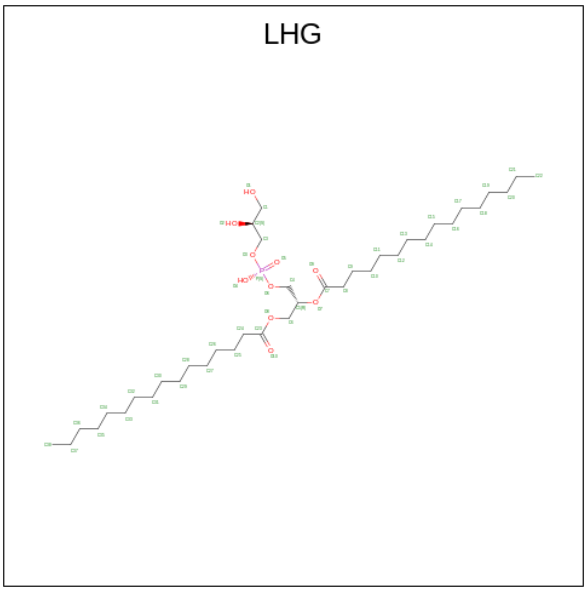
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Fe	S		0	0
			8	4	4			
21	C	1	Total	Fe	S		0	0
			8	4	4			
21	C	1	Total	Fe	S		0	0
			8	4	4			

- Molecule 22 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O P 40 29 10 1	0	0

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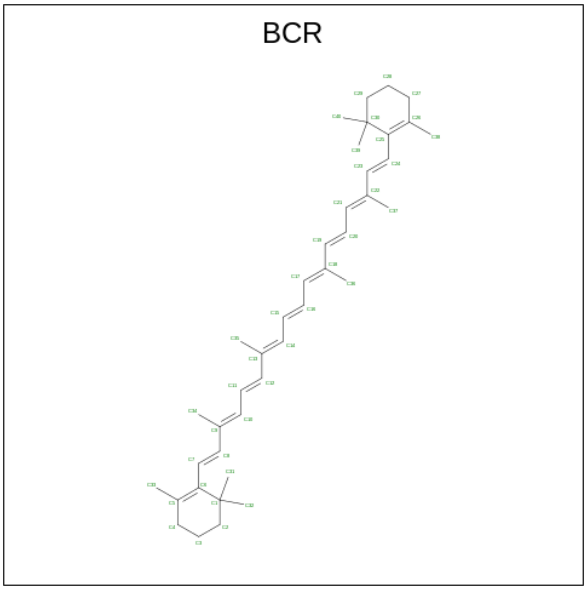
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O P 49 38 10 1	0	0
23	0	1	Total C O P 21 10 10 1	0	0
23	8	1	Total C O P 49 38 10 1	0	0
23	7	1	Total C O P 35 24 10 1	0	0
23	3	1	Total C O P 20 10 9 1	0	0
23	4	1	Total C O P 49 38 10 1	0	0

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0
24	A	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	G	1	Total C 40 40	0	0
24	G	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	I	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	8	1	Total C 40 40	0	0
24	7	1	Total C 40 40	0	0
24	3	1	Total C 40 40	0	0
24	3	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	4	1	Total C 40 40	0	0
24	6	1	Total C 40 40	0	0

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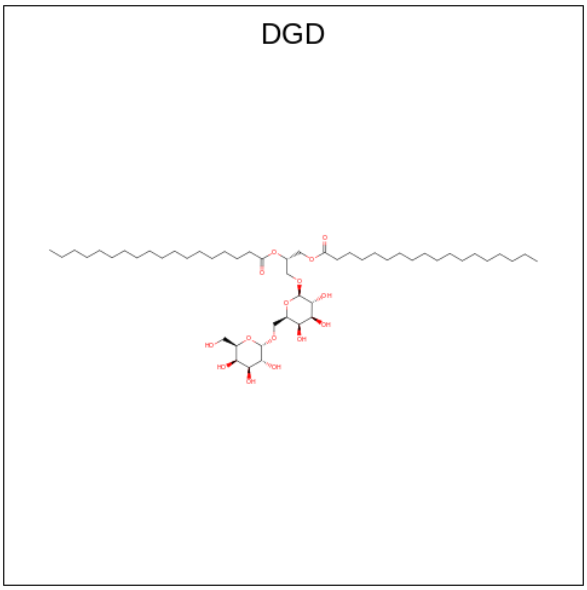
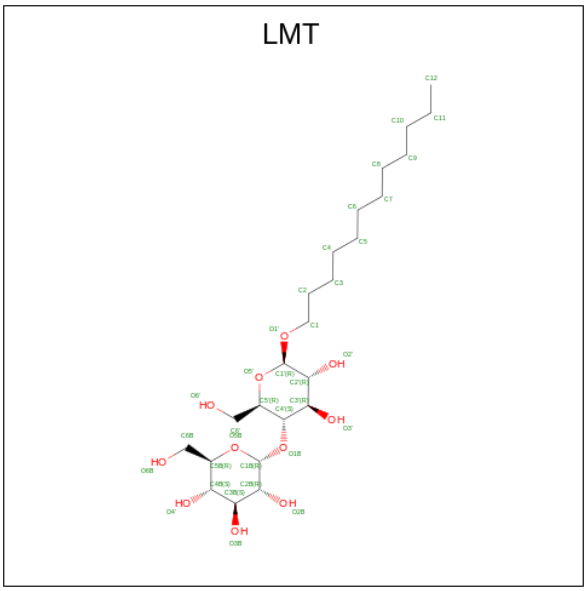
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	5	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



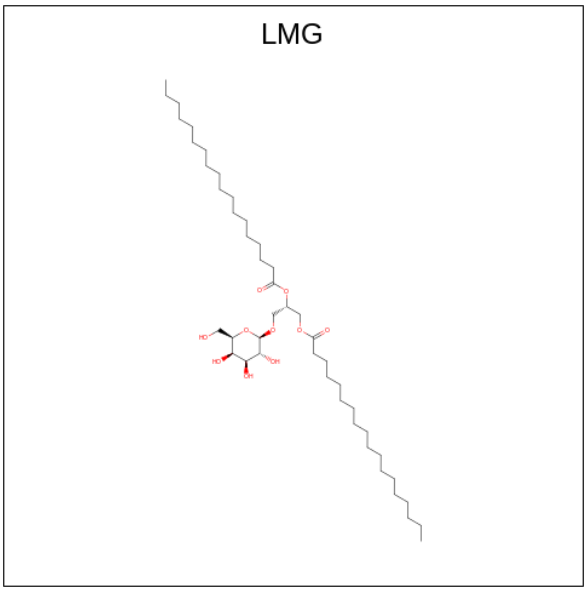
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C O 61 46 15	0	0
25	5	1	Total C O 51 36 15	0	0

- Molecule 26 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	B	1	Total C O 31 20 11	0	0
26	3	1	Total C O 31 20 11	0	0

- Molecule 27 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	ZeroOcc	AltConf
27	J	1	Total C O 30 20 10	0	0

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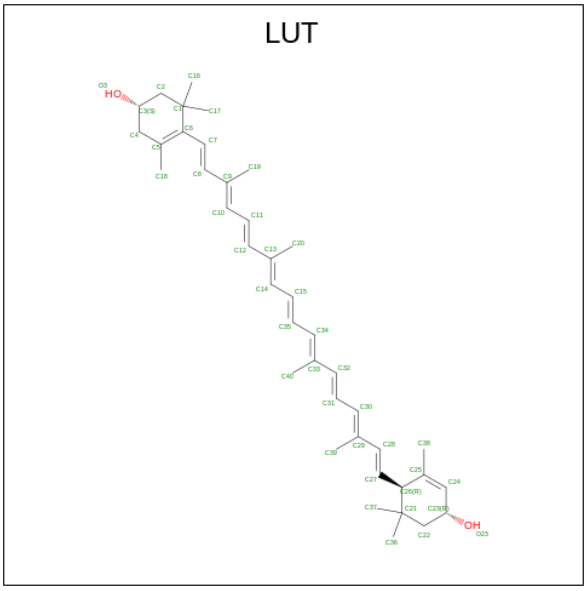
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	0	1	Total C O 50 40 10	0	0
27	8	1	Total C O 28 18 10	0	0
27	8	1	Total C O 44 34 10	0	0
27	4	1	Total C O 34 24 10	0	0
27	6	1	Total C O 44 34 10	0	0
27	5	1	Total C O 45 35 10	0	0

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	J	1	Total C O 42 40 2	0	0
28	0	1	Total C O 42 40 2	0	0
28	0	1	Total C O 42 40 2	0	0
28	8	1	Total C O 42 40 2	0	0

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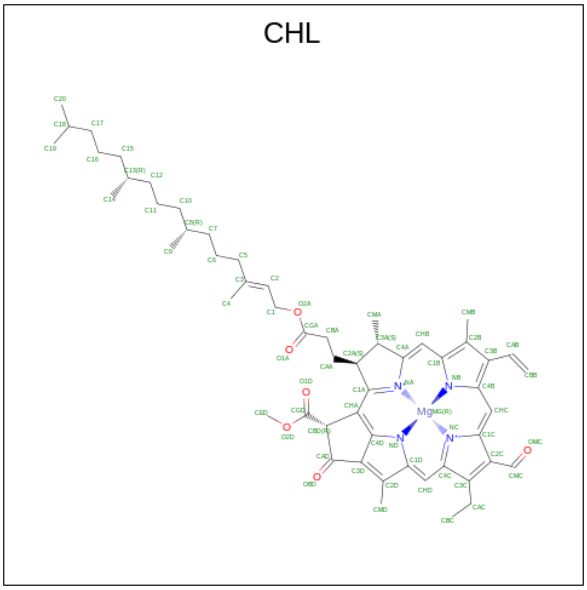
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	7	1	Total C O 42 40 2	0	0
28	3	1	Total C O 42 40 2	0	0
28	3	1	Total C O 42 40 2	0	0
28	1	1	Total C O 42 40 2	0	0
28	1	1	Total C O 42 40 2	0	0
28	4	1	Total C O 42 40 2	0	0
28	6	1	Total C O 42 40 2	0	0
28	5	1	Total C O 42 40 2	0	0

- Molecule 29 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	0	1	Total C Mg N O 47 36 1 4 6	0	0
29	0	1	Total C Mg N O 51 40 1 4 6	0	0
29	0	1	Total C Mg N O 61 50 1 4 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	8	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	8	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
29	8	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	7	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	7	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
29	7	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
29	7	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
29	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	1	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
29	1	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
29	4	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
29	6	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	6	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
29	6	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	6	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
29	5	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	5	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		

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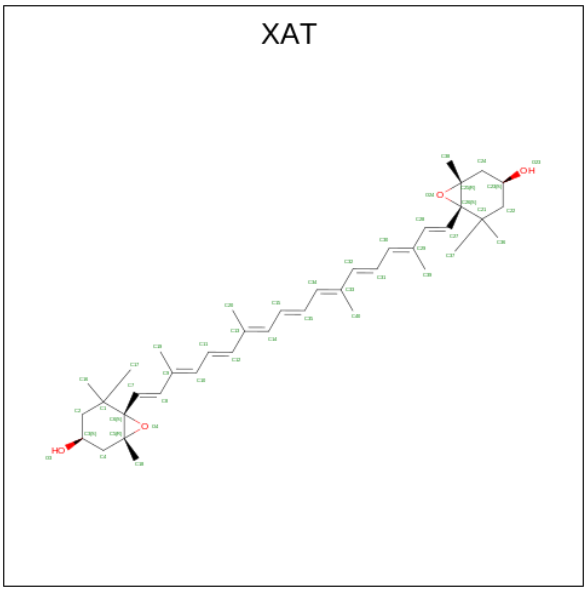
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	5	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	5	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

- Molecule 30 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



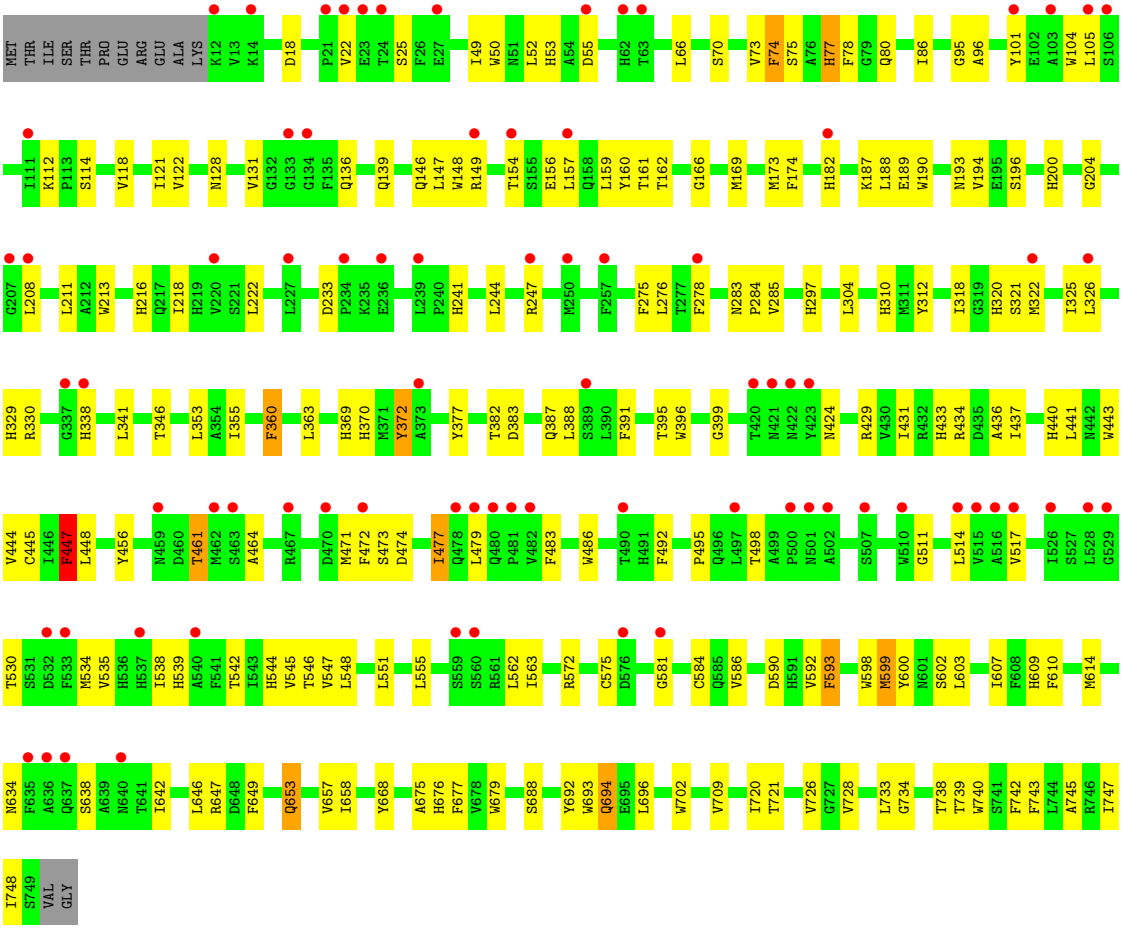
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	8	1	Total	C	O	0	0
			44	40	4		
30	7	1	Total	C	O	0	0
			44	40	4		
30	4	1	Total	C	O	0	0
			44	40	4		
30	6	1	Total	C	O	0	0
			44	40	4		
30	5	1	Total	C	O	0	0
			44	40	4		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

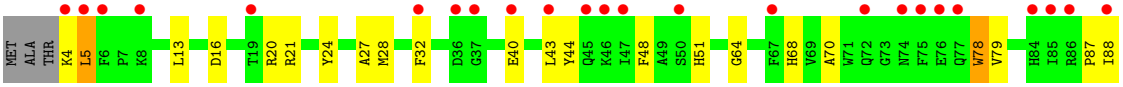
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

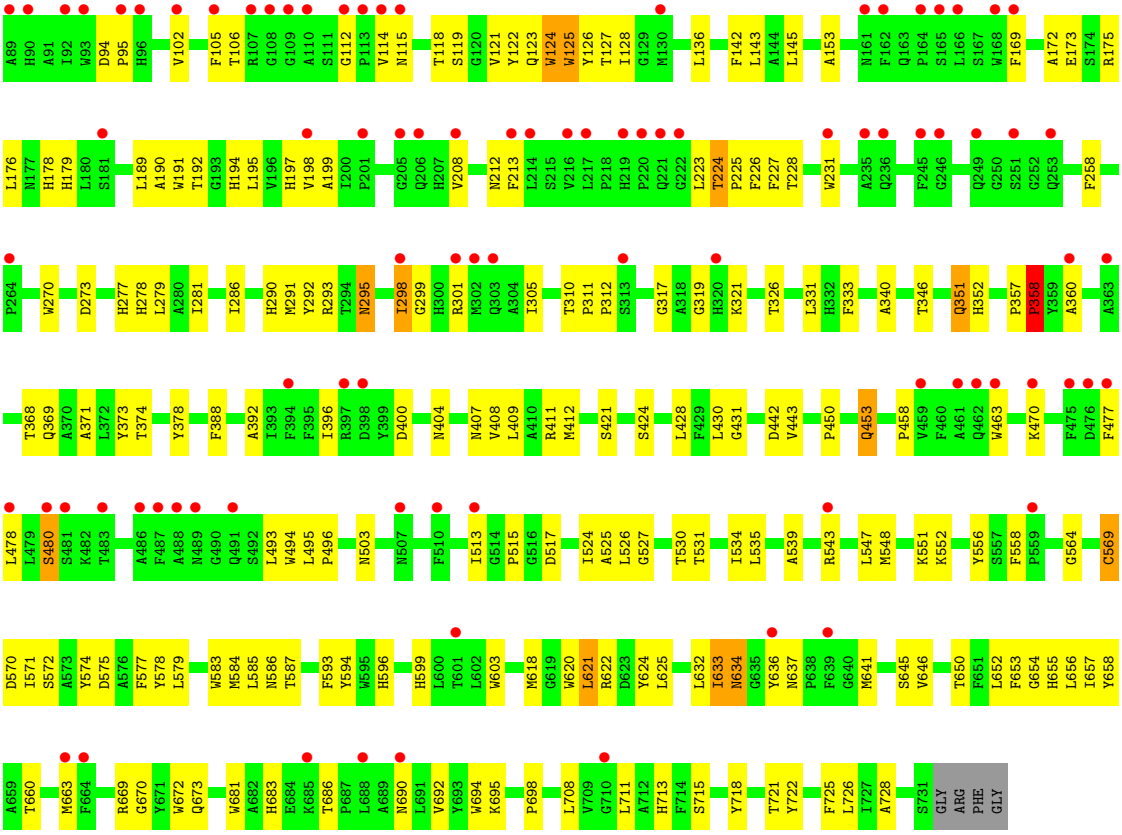
Chain A:



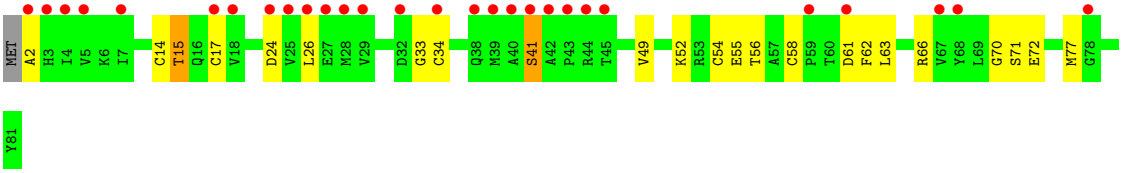
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

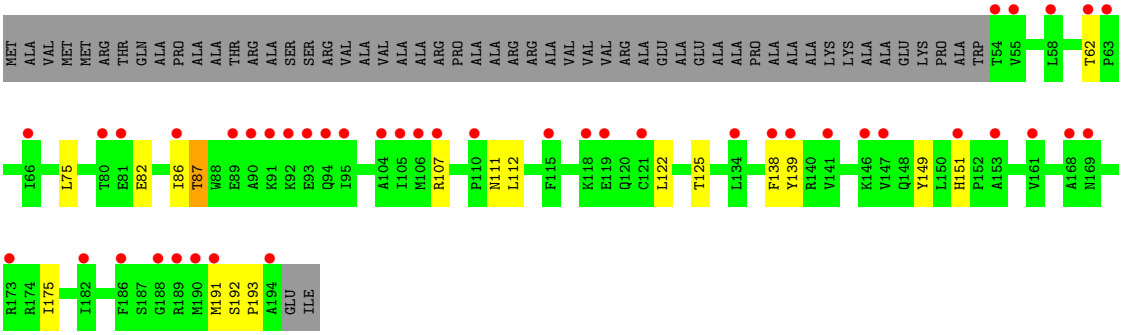




• Molecule 3: Photosystem I iron-sulfur center

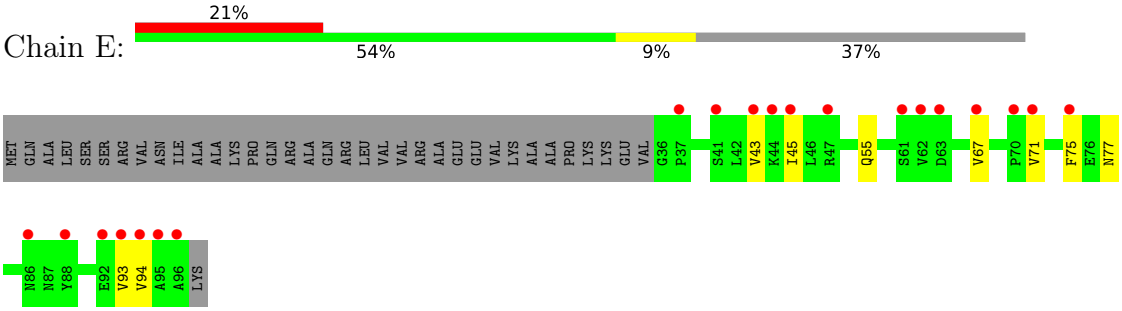


• Molecule 4: Photosystem I reaction center subunit II, chloroplastic



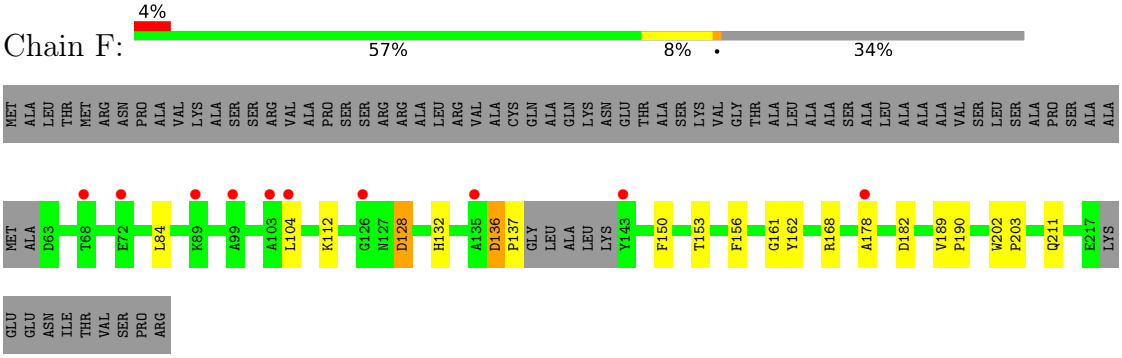
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



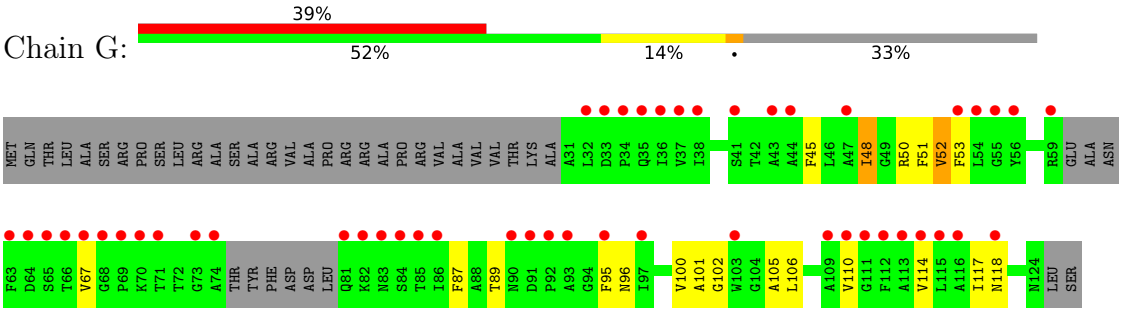
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:



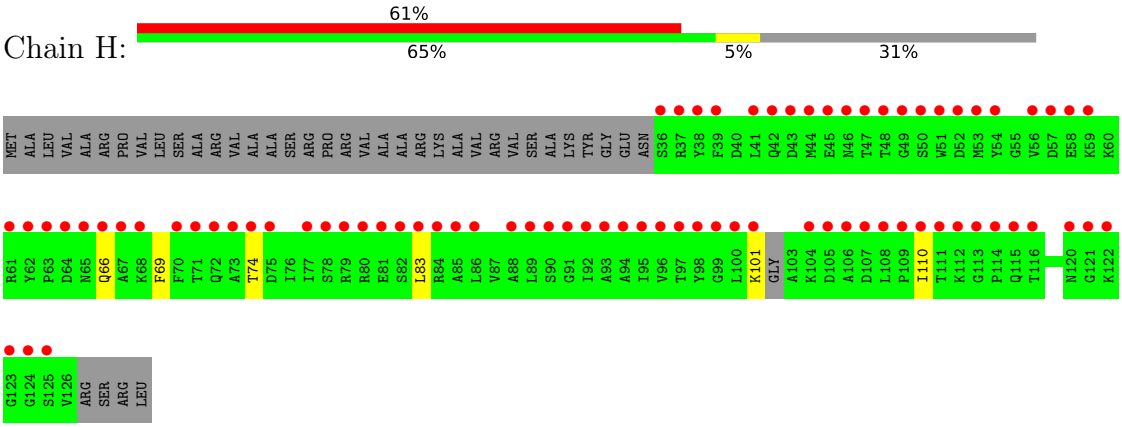
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:



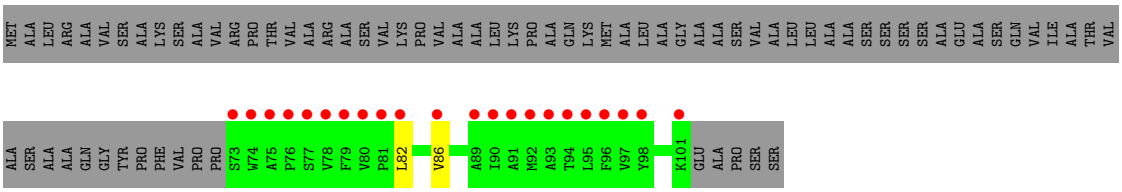
• Molecule 8: Photosystem I reaction center subunit VI, chloroplastic

Chain H:



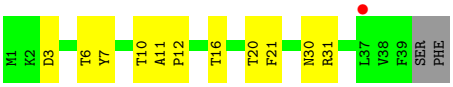
• Molecule 9: Photosystem I reaction center subunit VIII

Chain I:



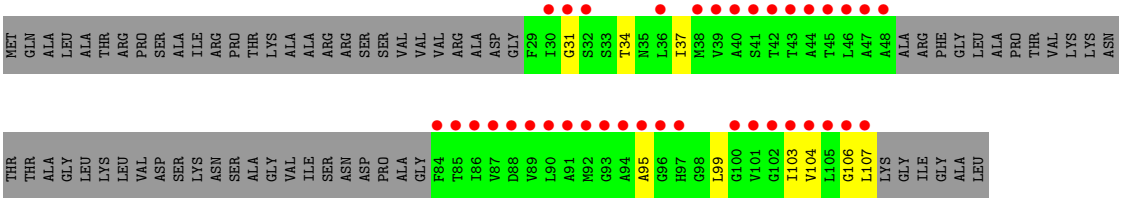
• Molecule 10: Photosystem I reaction center subunit IX

Chain J:



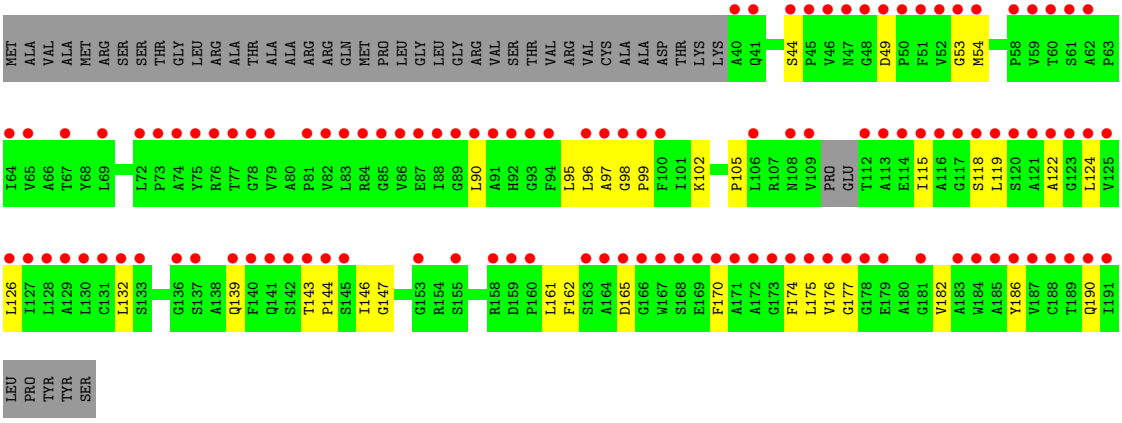
• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:



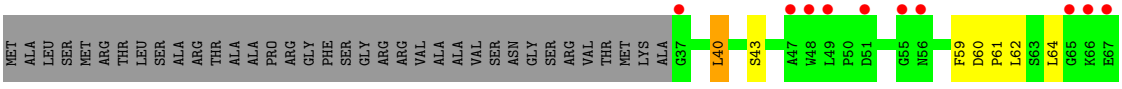
• Molecule 12: PSI subunit V

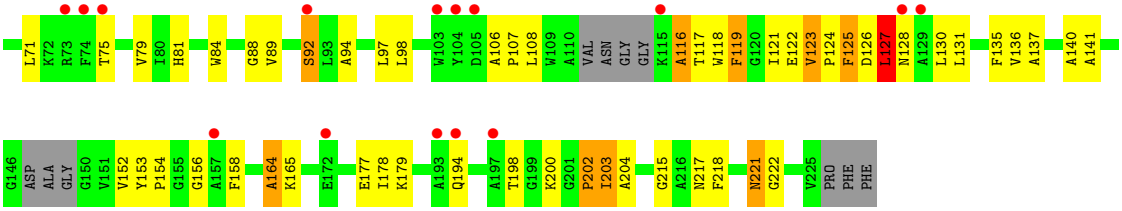
Chain L:



• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

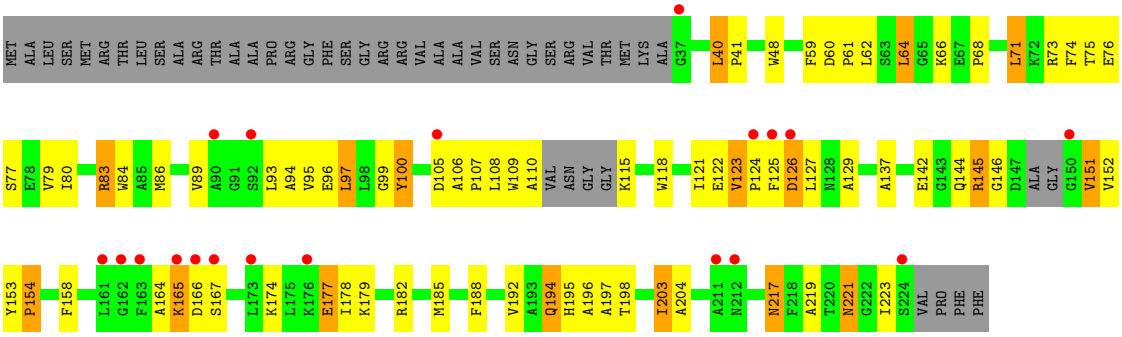
Chain 0:





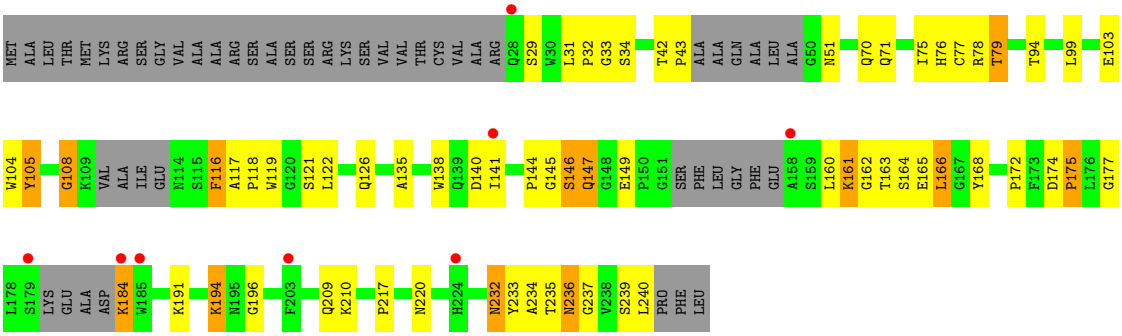
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



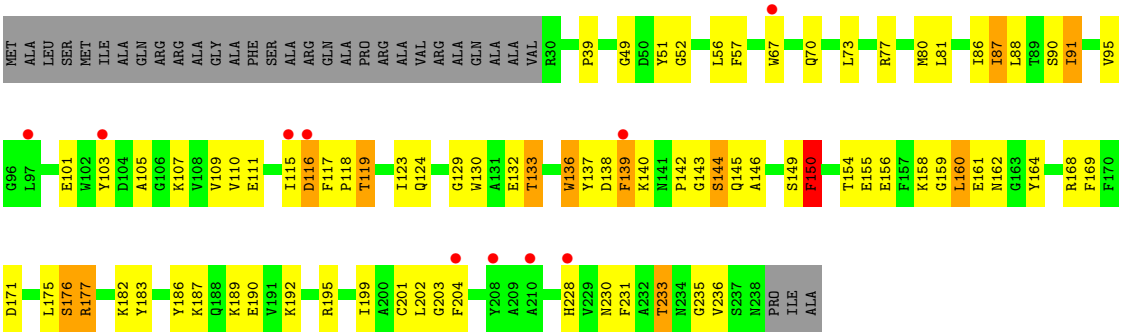
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



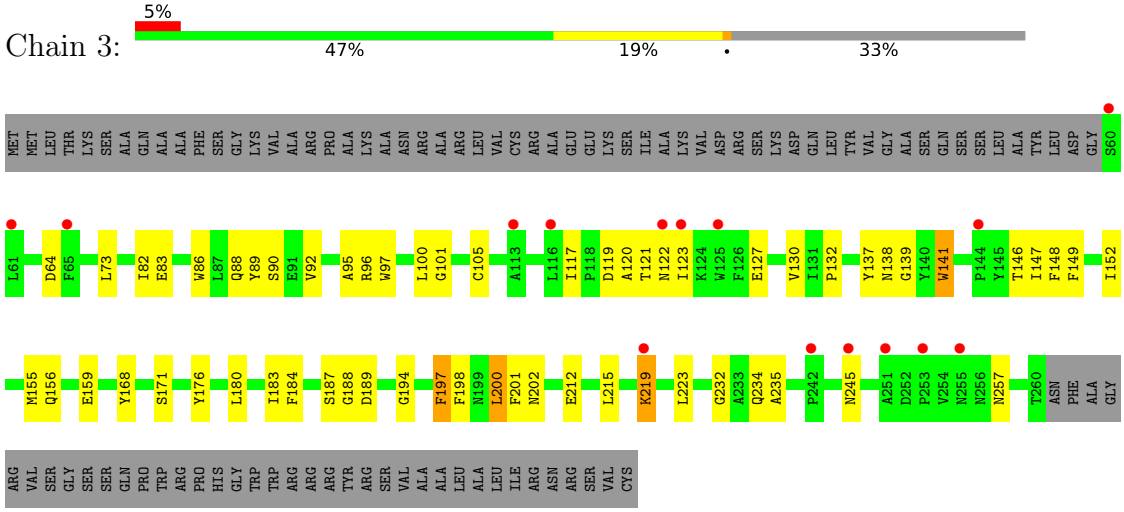
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



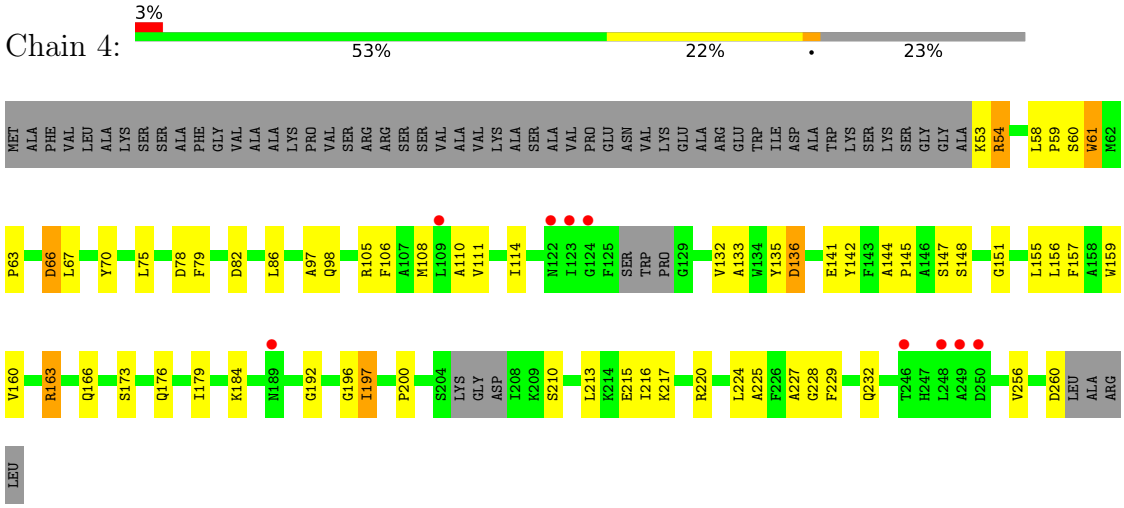
• Molecule 16: Lhca3

Chain 3:



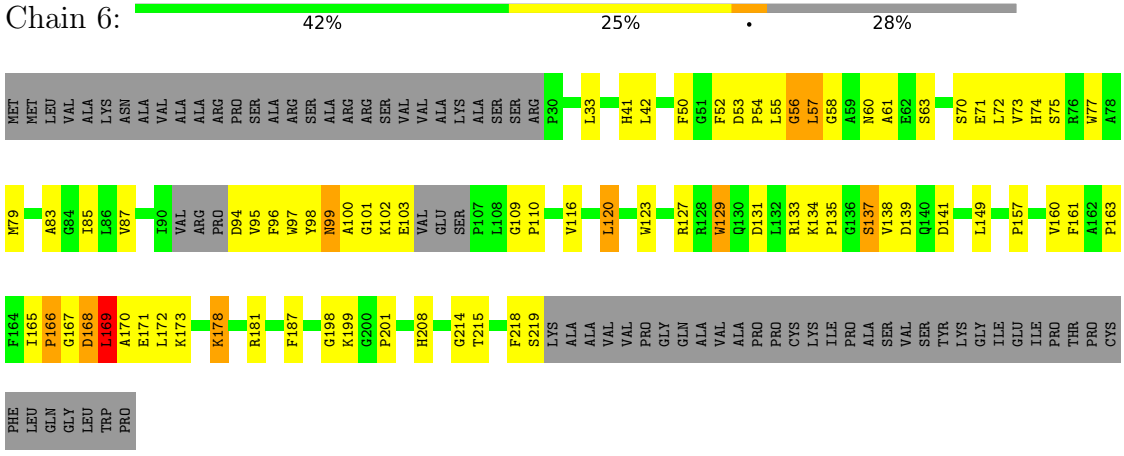
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



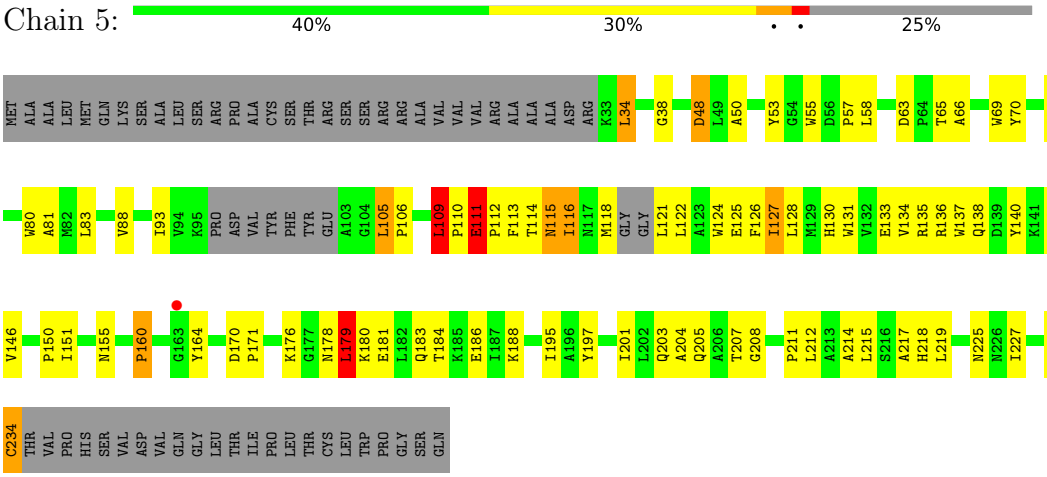
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 5:


40%
30%
25%
MET ALA ALA LEU MET GLN LYS SER ALA LEU SER ARG PRO ALA CYS SER THR ARG SER SER ARG ARG ALA VAL VAL VAL ARG ALA ALA ALA ASP ARG K33 L34 G38 D48 L49 A50 Y53 G54 W55 D56 P57 L58 D63 P64 T65 A66 W69 Y70 S73 Q76 H77
W80 A81 M82 L83 V88 I93 V94 K95 PRO ASP VAL TYR PHE TYR GLU A103 G104 L105 P106 L109 P110 E111 P112 F113 T114 N115 I116 N117 M118 GLY GLY L121 L122 A123 W124 E125 F126 I127 L128 M129 H130 W131 V132 E133 V134 R135 R136 W137 Q138 D139 Y140 K141 N142 F143 G144 S145
V146 P150 I151 N155 P160 G163 Y164 D170 P171 K176 G177 N178 L179 K180 E181 L182 Q183 T184 K185 E186 I187 K188 I195 A196 Y197 I201 L202 Q203 A204 Q205 A206 T207 G208 P211 L212 A213 A214 L215 S216 A217 H218 L219 N225 N226 I227 N230 I231 G232 T233
C234 THR VAL PRO HIS SER VAL ASP VAL GLN GLY LEU THR ILE PRO LEU THR CYS LEU TRP PRO GLY SER GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	194.57Å 98.12Å 210.13Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	47.74 – 3.40 47.74 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.74-3.40) 99.1 (47.74-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.291 , 0.359 0.300 , 0.364	Depositor DCC
R_{free} test set	5416 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	108.0	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 103.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	42070	wwPDB-VP
Average B, all atoms (Å^2)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, DGD, SF4, LUT, LMG, LMT, CLA, XAT, LHG, CHL, PQN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.62	0/5995	0.68	0/8175
2	B	0.60	0/5997	0.68	0/8190
3	C	0.55	0/610	0.68	0/826
4	D	0.65	0/1127	0.73	0/1521
5	E	0.68	0/490	0.73	0/667
6	F	0.66	0/1174	0.74	0/1588
7	G	0.70	0/631	0.74	0/855
8	H	0.70	0/704	0.73	0/947
9	I	0.69	0/228	0.69	0/314
10	J	0.64	0/331	0.72	0/454
11	K	0.76	0/296	0.75	0/401
12	L	0.70	0/1106	0.74	0/1512
13	0	0.67	0/1402	0.81	0/1906
13	1	0.66	0/1403	0.80	0/1907
14	8	0.67	0/1509	0.82	0/2050
15	7	0.67	0/1673	0.82	0/2270
16	3	0.66	0/1587	0.77	0/2154
17	4	0.65	0/1621	0.77	0/2206
18	6	0.66	0/1479	0.82	0/2012
19	5	0.65	0/1553	0.83	0/2107
All	All	0.64	0/30916	0.74	0/42062

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
13	0	0	3
13	1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	8	0	1
19	5	0	2
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	0	125	PHE	Peptide
13	0	164	ALA	Peptide
13	0	198	THR	Peptide
14	8	232	ASN	Peptide
1	A	447	PHE	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5799	0	5646	193	0
2	B	5786	0	5542	221	0
3	C	600	0	583	19	0
4	D	1101	0	1123	10	0
5	E	480	0	476	7	0
6	F	1150	0	1174	17	0
7	G	620	0	612	43	0
8	H	694	0	682	6	0
9	I	221	0	234	1	0
10	J	320	0	322	9	0
11	K	295	0	312	11	0
12	L	1082	0	1103	27	0
13	0	1361	0	1318	63	0
13	1	1362	0	1313	86	0
14	8	1466	0	1444	72	0
15	7	1622	0	1552	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	3	1542	0	1511	75	0
17	4	1571	0	1529	86	0
18	6	1431	0	1415	67	0
19	5	1510	0	1499	108	0
20	0	484	0	330	34	0
20	1	484	0	330	43	0
20	3	524	0	356	26	0
20	4	396	0	270	46	0
20	5	660	0	450	67	0
20	6	528	0	360	45	0
20	7	396	0	270	31	0
20	8	440	0	300	35	0
20	A	1844	0	1256	120	0
20	B	1803	0	1225	129	0
20	F	132	0	90	10	0
20	G	132	0	90	11	0
20	J	44	0	30	3	0
20	K	71	0	33	6	0
20	L	176	0	120	11	0
21	A	8	0	0	1	0
21	C	16	0	0	2	0
22	A	33	0	46	4	0
22	B	33	0	46	3	0
23	0	21	0	12	3	0
23	3	20	0	14	5	0
23	4	49	0	74	15	0
23	7	35	0	40	6	0
23	8	49	0	74	0	0
23	A	89	0	127	6	0
24	1	40	0	56	8	0
24	3	80	0	112	8	0
24	4	40	0	56	5	0
24	5	40	0	56	17	0
24	6	40	0	56	15	0
24	7	40	0	56	2	0
24	8	40	0	56	6	0
24	A	240	0	336	25	0
24	B	240	0	336	32	0
24	F	80	0	112	7	0
24	G	80	0	112	25	0
24	H	40	0	56	2	0
24	I	40	0	56	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	J	40	0	56	0	0
25	5	51	0	60	17	0
25	B	61	0	83	2	0
26	3	31	0	35	8	0
26	B	31	0	35	3	0
27	0	50	0	70	27	0
27	4	34	0	38	38	0
27	5	45	0	60	7	0
27	6	44	0	61	9	0
27	8	72	0	86	9	0
27	J	30	0	30	0	0
28	0	84	0	112	16	0
28	1	84	0	112	20	0
28	3	84	0	112	6	0
28	4	42	0	56	3	0
28	5	42	0	56	6	0
28	6	42	0	56	4	0
28	7	42	0	56	5	0
28	8	42	0	56	4	0
28	J	42	0	56	10	0
29	0	159	0	124	21	0
29	1	159	0	124	18	0
29	3	47	0	31	4	0
29	4	202	0	153	21	0
29	5	202	0	153	17	0
29	6	202	0	154	14	0
29	7	207	0	164	16	0
29	8	159	0	124	10	0
30	4	44	0	56	2	0
30	5	44	0	56	7	0
30	6	44	0	56	10	0
30	7	44	0	56	0	0
30	8	44	0	56	1	0
All	All	42070	0	39382	1635	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 20.

The worst 5 of 1635 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)
1:A:738:THR:OG1	20:A:801:CLA:O2D	1.57	1.22
17:4:54:ARG:HB3	17:4:67:LEU:O	1.45	1.17
1:A:473:SER:O	1:A:477:ILE:O	1.64	1.14
20:1:1007:CLA:HBC1	20:1:1014:CLA:HBC2	1.26	1.14
20:4:307:CLA:HAC1	27:4:318:LMG:H151	1.22	1.14

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	736/751 (98%)	683 (93%)	51 (7%)	2 (0%)	41 72
2	B	726/735 (99%)	668 (92%)	54 (7%)	4 (1%)	25 57
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100 100
4	D	139/196 (71%)	121 (87%)	18 (13%)	0	100 100
5	E	59/97 (61%)	52 (88%)	7 (12%)	0	100 100
6	F	146/227 (64%)	128 (88%)	15 (10%)	3 (2%)	7 30
7	G	79/126 (63%)	69 (87%)	9 (11%)	1 (1%)	12 39
8	H	86/130 (66%)	74 (86%)	12 (14%)	0	100 100
9	I	27/106 (26%)	23 (85%)	4 (15%)	0	100 100
10	J	37/41 (90%)	34 (92%)	3 (8%)	0	100 100
11	K	40/113 (35%)	34 (85%)	5 (12%)	1 (2%)	5 26
12	L	146/196 (74%)	125 (86%)	19 (13%)	2 (1%)	11 37
13	0	176/228 (77%)	136 (77%)	28 (16%)	12 (7%)	1 8
13	1	176/228 (77%)	133 (76%)	37 (21%)	6 (3%)	3 21
14	8	183/243 (75%)	142 (78%)	34 (19%)	7 (4%)	3 19
15	7	207/241 (86%)	168 (81%)	31 (15%)	8 (4%)	3 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	3	199/298 (67%)	165 (83%)	32 (16%)	2 (1%)	15 46
17	4	196/264 (74%)	159 (81%)	35 (18%)	2 (1%)	15 46
18	6	178/257 (69%)	152 (85%)	14 (8%)	12 (7%)	1 8
19	5	187/257 (73%)	134 (72%)	42 (22%)	11 (6%)	1 11
All	All	3801/4815 (79%)	3276 (86%)	452 (12%)	73 (2%)	8 31

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	136	ASP
13	0	165	LYS
14	8	146	SER
15	7	150	PHE
13	1	165	LYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	599/610 (98%)	570 (95%)	29 (5%)	25 56
2	B	593/597 (99%)	562 (95%)	31 (5%)	23 53
3	C	69/70 (99%)	65 (94%)	4 (6%)	20 50
4	D	118/152 (78%)	114 (97%)	4 (3%)	37 65
5	E	52/81 (64%)	51 (98%)	1 (2%)	57 78
6	F	114/169 (68%)	110 (96%)	4 (4%)	36 65
7	G	61/94 (65%)	59 (97%)	2 (3%)	38 66
8	H	73/102 (72%)	72 (99%)	1 (1%)	67 83
9	I	24/76 (32%)	24 (100%)	0	100 100
10	J	35/37 (95%)	35 (100%)	0	100 100
11	K	30/80 (38%)	30 (100%)	0	100 100
12	L	112/148 (76%)	107 (96%)	5 (4%)	27 58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	0	130/162 (80%)	114 (88%)	16 (12%)	4 17
13	1	130/162 (80%)	112 (86%)	18 (14%)	3 14
14	8	146/183 (80%)	132 (90%)	14 (10%)	8 29
15	7	161/181 (89%)	141 (88%)	20 (12%)	4 17
16	3	154/230 (67%)	147 (96%)	7 (4%)	27 58
17	4	159/205 (78%)	148 (93%)	11 (7%)	15 45
18	6	146/203 (72%)	131 (90%)	15 (10%)	7 26
19	5	154/206 (75%)	141 (92%)	13 (8%)	11 36
All	All	3060/3748 (82%)	2865 (94%)	195 (6%)	17 47

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	7	111	GLU
13	1	97	LEU
15	7	133	THR
15	7	177	ARG
13	1	151	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
13	0	217	ASN
19	5	72	GLN
14	8	232	ASN
18	6	140	GLN
19	5	138	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)

278 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	$\#\|Z\| > 2$
20	CLA	6	312	18	43,52,73	2.73	9 (20%)	49,88,113	1.60	8 (16%)
24	BCR	B	845	-	41,41,41	0.54	0	56,56,56	0.94	3 (5%)
23	LHG	4	301	20	48,48,48	0.31	0	51,54,54	0.48	0
29	CHL	5	316	-	61,69,74	2.22	11 (18%)	67,108,114	1.55	11 (16%)
20	CLA	A	810	20	43,52,73	2.84	7 (16%)	49,88,113	1.42	7 (14%)
20	CLA	7	1005	15	43,52,73	2.95	8 (18%)	49,88,113	1.58	6 (12%)
20	CLA	A	829	-	43,52,73	2.74	9 (20%)	49,88,113	1.32	8 (16%)
20	CLA	A	836	-	43,52,73	2.72	8 (18%)	49,88,113	1.47	8 (16%)
20	CLA	7	1004	15	43,52,73	2.59	8 (18%)	49,88,113	1.45	10 (20%)
20	CLA	3	1007	-	43,52,73	2.85	9 (20%)	49,88,113	1.41	8 (16%)
20	CLA	0	309	-	43,52,73	2.78	8 (18%)	49,88,113	1.43	6 (12%)
20	CLA	B	821	-	43,52,73	2.86	8 (18%)	49,88,113	1.46	8 (16%)
20	CLA	3	1010	-	43,52,73	2.78	8 (18%)	49,88,113	1.36	7 (14%)
23	LHG	A	849	-	48,48,48	0.25	0	51,54,54	0.33	0
20	CLA	A	809	-	43,52,73	2.76	9 (20%)	49,88,113	1.28	8 (16%)
24	BCR	A	844	-	41,41,41	0.34	0	56,56,56	0.55	0
20	CLA	8	305	14	43,52,73	2.51	7 (16%)	49,88,113	1.29	6 (12%)
24	BCR	H	201	-	41,41,41	0.86	3 (7%)	56,56,56	1.22	6 (10%)
28	LUT	3	1001	-	42,43,43	0.26	0	51,60,60	0.44	0
29	CHL	5	314	-	51,59,74	2.57	9 (17%)	55,96,114	1.55	7 (12%)
30	XAT	5	303	-	39,47,47	0.26	0	54,74,74	1.11	3 (5%)
20	CLA	B	839	-	43,52,73	2.73	8 (18%)	49,88,113	1.44	8 (16%)
20	CLA	B	841	-	43,52,73	2.95	7 (16%)	49,88,113	1.46	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	840	-	43,52,73	2.61	8 (18%)	49,88,113	1.41	6 (12%)
20	CLA	G	203	-	43,52,73	3.04	8 (18%)	49,88,113	1.26	7 (14%)
24	BCR	A	846	-	41,41,41	0.64	0	56,56,56	0.89	2 (3%)
20	CLA	8	316	14	43,52,73	2.42	9 (20%)	49,88,113	1.42	6 (12%)
20	CLA	A	812	-	43,52,73	2.87	8 (18%)	49,88,113	1.31	7 (14%)
20	CLA	B	830	-	43,52,73	2.63	7 (16%)	49,88,113	1.36	6 (12%)
20	CLA	L	204	-	43,52,73	3.11	8 (18%)	49,88,113	1.32	6 (12%)
20	CLA	7	1009	-	43,52,73	2.75	9 (20%)	49,88,113	1.40	5 (10%)
20	CLA	A	815	-	43,52,73	2.68	8 (18%)	49,88,113	1.42	6 (12%)
20	CLA	1	1003	-	43,52,73	2.77	8 (18%)	49,88,113	1.35	8 (16%)
20	CLA	A	804	-	43,52,73	2.93	9 (20%)	49,88,113	1.51	7 (14%)
20	CLA	0	310	-	43,52,73	3.20	8 (18%)	49,88,113	1.40	7 (14%)
29	CHL	1	1013	-	51,59,74	2.39	7 (13%)	55,96,114	1.55	9 (16%)
25	DGD	5	319	-	52,52,67	1.07	3 (5%)	66,66,81	1.44	8 (12%)
20	CLA	3	1012	-	43,52,73	2.88	8 (18%)	49,88,113	1.33	8 (16%)
20	CLA	3	1005	16	43,52,73	2.65	9 (20%)	49,88,113	1.27	7 (14%)
29	CHL	5	317	19	43,51,74	2.47	9 (20%)	45,86,114	1.52	6 (13%)
20	CLA	B	832	-	43,52,73	2.81	9 (20%)	49,88,113	1.33	8 (16%)
20	CLA	5	304	19	43,52,73	2.98	8 (18%)	49,88,113	1.34	8 (16%)
20	CLA	7	1011	-	43,52,73	2.94	9 (20%)	49,88,113	1.29	8 (16%)
20	CLA	3	1016	-	43,52,73	2.70	8 (18%)	49,88,113	1.48	8 (16%)
24	BCR	F	301	-	41,41,41	0.54	1 (2%)	56,56,56	0.63	1 (1%)
20	CLA	6	309	-	43,52,73	2.84	8 (18%)	49,88,113	1.41	7 (14%)
24	BCR	3	1003	-	41,41,41	0.60	0	56,56,56	0.90	2 (3%)
27	LMG	4	318	-	34,34,55	0.32	0	42,42,63	0.95	3 (7%)
20	CLA	F	305	-	43,52,73	2.85	8 (18%)	49,88,113	1.42	8 (16%)
20	CLA	1	1009	23	43,52,73	2.62	9 (20%)	49,88,113	1.20	5 (10%)
20	CLA	5	305	19	43,52,73	3.06	7 (16%)	49,88,113	1.41	8 (16%)
20	CLA	B	805	-	43,52,73	2.67	8 (18%)	49,88,113	1.30	7 (14%)
20	CLA	8	308	14	43,52,73	2.83	10 (23%)	49,88,113	1.55	9 (18%)
20	CLA	7	1007	15	43,52,73	2.98	9 (20%)	49,88,113	1.61	9 (18%)
20	CLA	5	318	-	43,52,73	2.79	8 (18%)	49,88,113	1.50	10 (20%)
20	CLA	4	307	17	43,52,73	3.04	9 (20%)	49,88,113	1.98	10 (20%)
22	PQN	B	842	-	34,34,34	0.31	0	42,45,45	0.31	0
20	CLA	8	310	-	43,52,73	2.78	8 (18%)	49,88,113	1.36	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	839	-	43,52,73	2.84	9 (20%)	49,88,113	1.27	6 (12%)
24	BCR	3	1004	-	41,41,41	0.65	1 (2%)	56,56,56	1.02	3 (5%)
20	CLA	B	829	-	43,52,73	2.67	8 (18%)	49,88,113	1.45	8 (16%)
23	LHG	3	1019	20	19,19,48	0.71	1 (5%)	21,24,54	0.51	0
20	CLA	8	313	14	43,52,73	2.89	8 (18%)	49,88,113	1.46	9 (18%)
20	CLA	7	1010	23	43,52,73	2.63	8 (18%)	49,88,113	1.24	6 (12%)
24	BCR	B	844	-	41,41,41	0.42	0	56,56,56	0.56	0
29	CHL	0	314	-	47,55,74	2.48	10 (21%)	50,91,114	1.44	6 (12%)
28	LUT	4	317	-	42,43,43	0.35	0	51,60,60	0.53	1 (1%)
20	CLA	B	809	-	43,52,73	2.93	8 (18%)	49,88,113	1.38	8 (16%)
20	CLA	B	834	-	43,52,73	2.60	9 (20%)	49,88,113	1.22	6 (12%)
20	CLA	5	322	-	43,52,73	2.79	8 (18%)	49,88,113	1.40	9 (18%)
20	CLA	6	307	-	43,52,73	2.77	7 (16%)	49,88,113	1.40	7 (14%)
20	CLA	B	807	-	43,52,73	2.80	9 (20%)	49,88,113	1.36	8 (16%)
24	BCR	B	847	-	41,41,41	0.17	0	56,56,56	0.63	0
20	CLA	A	819	-	43,52,73	2.85	8 (18%)	49,88,113	1.30	6 (12%)
29	CHL	0	317	-	61,69,74	2.11	10 (16%)	67,108,114	1.51	8 (11%)
20	CLA	5	306	-	43,52,73	2.84	9 (20%)	49,88,113	1.39	8 (16%)
26	LMT	B	849	-	32,32,36	0.20	0	43,43,47	0.47	0
29	CHL	7	1013	-	48,56,74	2.40	9 (18%)	51,92,114	1.89	7 (13%)
20	CLA	A	837	-	43,52,73	2.75	9 (20%)	49,88,113	1.46	7 (14%)
20	CLA	B	827	-	43,52,73	2.76	9 (20%)	49,88,113	1.44	8 (16%)
20	CLA	A	823	-	43,52,73	2.78	8 (18%)	49,88,113	1.37	6 (12%)
20	CLA	3	1015	16	43,52,73	2.96	9 (20%)	49,88,113	1.32	8 (16%)
29	CHL	0	315	-	51,59,74	2.39	9 (17%)	55,96,114	1.54	7 (12%)
20	CLA	A	822	-	43,52,73	2.94	8 (18%)	49,88,113	1.41	8 (16%)
20	CLA	1	1007	-	43,52,73	2.86	8 (18%)	49,88,113	1.55	8 (16%)
20	CLA	4	311	17	43,52,73	2.87	7 (16%)	49,88,113	1.42	8 (16%)
22	PQN	A	842	-	34,34,34	0.32	0	42,45,45	0.50	1 (2%)
20	CLA	1	1004	13	43,52,73	2.85	9 (20%)	49,88,113	1.41	8 (16%)
20	CLA	G	201	-	43,52,73	2.92	7 (16%)	49,88,113	1.40	9 (18%)
29	CHL	1	1015	-	61,69,74	1.95	10 (16%)	67,108,114	1.64	10 (14%)
23	LHG	8	301	20	48,48,48	0.27	0	51,54,54	0.29	0
24	BCR	J	103	-	41,41,41	0.32	0	56,56,56	0.41	0
20	CLA	A	802	-	43,52,73	2.80	9 (20%)	49,88,113	1.41	8 (16%)
23	LHG	7	1016	20	34,34,48	0.42	0	37,40,54	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	5	301	-	43,52,73	3.17	9 (20%)	49,88,113	1.58	9 (18%)
24	BCR	1	1001	-	41,41,41	0.52	1 (2%)	56,56,56	1.08	5 (8%)
20	CLA	A	817	-	43,52,73	2.91	6 (13%)	49,88,113	1.51	9 (18%)
20	CLA	B	824	-	43,52,73	2.72	8 (18%)	49,88,113	1.53	9 (18%)
20	CLA	7	1006	-	43,52,73	2.58	7 (16%)	49,88,113	1.44	7 (14%)
24	BCR	F	304	-	41,41,41	0.32	0	56,56,56	0.64	0
20	CLA	B	812	2	43,52,73	2.96	7 (16%)	49,88,113	1.37	7 (14%)
20	CLA	1	1005	-	43,52,73	2.87	8 (18%)	49,88,113	1.34	7 (14%)
24	BCR	7	1003	-	41,41,41	0.69	1 (2%)	56,56,56	1.56	6 (10%)
20	CLA	6	311	-	43,52,73	2.64	9 (20%)	49,88,113	1.21	5 (10%)
20	CLA	B	815	-	43,52,73	3.11	8 (18%)	49,88,113	1.44	7 (14%)
28	LUT	0	304	-	42,43,43	0.25	0	51,60,60	0.56	1 (1%)
20	CLA	A	806	-	43,52,73	2.70	8 (18%)	49,88,113	1.52	9 (18%)
27	LMG	6	319	-	44,44,55	0.37	0	52,52,63	0.61	1 (1%)
20	CLA	7	1008	-	43,52,73	2.77	8 (18%)	49,88,113	1.33	6 (12%)
20	CLA	B	837	-	43,52,73	3.11	7 (16%)	49,88,113	1.40	7 (14%)
20	CLA	0	313	13	43,52,73	2.90	7 (16%)	49,88,113	1.33	9 (18%)
27	LMG	8	318	-	28,28,55	0.30	0	36,36,63	0.49	0
20	CLA	B	811	-	43,52,73	2.92	8 (18%)	49,88,113	1.39	7 (14%)
20	CLA	K	201	-	43,52,73	3.04	7 (16%)	49,88,113	1.31	5 (10%)
29	CHL	4	316	17	43,51,74	2.33	9 (20%)	45,86,114	1.59	6 (13%)
24	BCR	4	302	-	41,41,41	0.49	1 (2%)	56,56,56	1.14	5 (8%)
20	CLA	4	314	17	43,52,73	2.57	8 (18%)	49,88,113	1.38	9 (18%)
28	LUT	0	318	-	42,43,43	0.41	0	51,60,60	0.53	0
23	LHG	0	302	20	20,20,48	0.34	0	23,26,54	1.79	4 (17%)
20	CLA	A	820	-	43,52,73	2.83	8 (18%)	49,88,113	1.43	8 (16%)
20	CLA	B	802	-	43,52,73	2.71	9 (20%)	49,88,113	1.45	10 (20%)
29	CHL	6	317	18	43,51,74	2.70	9 (20%)	45,86,114	1.59	7 (15%)
20	CLA	A	818	-	43,52,73	2.72	8 (18%)	49,88,113	1.36	8 (16%)
28	LUT	1	1016	-	42,43,43	0.24	0	51,60,60	0.52	0
20	CLA	5	309	19	43,52,73	2.77	8 (18%)	49,88,113	1.61	10 (20%)
30	XAT	4	303	-	39,47,47	0.19	0	54,74,74	0.85	3 (5%)
20	CLA	5	323	-	43,52,73	2.81	7 (16%)	49,88,113	1.36	9 (18%)
20	CLA	6	305	18	43,52,73	2.61	9 (20%)	49,88,113	1.35	6 (12%)
20	CLA	A	830	-	43,52,73	2.97	8 (18%)	49,88,113	1.36	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	B	840	-	43,52,73	2.81	8 (18%)	49,88,113	1.30	6 (12%)
24	BCR	I	201	-	41,41,41	0.58	0	56,56,56	0.93	3 (5%)
20	CLA	0	311	23	43,52,73	2.86	8 (18%)	49,88,113	1.22	6 (12%)
20	CLA	L	201	-	43,52,73	2.76	8 (18%)	49,88,113	1.35	6 (12%)
20	CLA	K	202	-	29,35,73	3.95	12 (41%)	28,60,113	2.60	10 (35%)
20	CLA	A	801	-	43,52,73	2.89	8 (18%)	49,88,113	1.55	9 (18%)
28	LUT	6	303	-	42,43,43	0.33	0	51,60,60	0.51	0
28	LUT	1	1002	-	42,43,43	0.36	0	51,60,60	0.59	0
20	CLA	A	833	1	43,52,73	2.82	9 (20%)	49,88,113	1.50	7 (14%)
24	BCR	B	843	-	41,41,41	1.04	3 (7%)	56,56,56	1.48	9 (16%)
20	CLA	B	836	-	43,52,73	2.73	9 (20%)	49,88,113	1.39	9 (18%)
20	CLA	B	850	-	40,49,73	4.56	8 (20%)	38,80,113	1.55	7 (18%)
20	CLA	A	803	20	43,52,73	2.91	8 (18%)	49,88,113	1.40	7 (14%)
27	LMG	0	303	-	50,50,55	0.30	0	58,58,63	0.53	1 (1%)
20	CLA	A	828	-	43,52,73	2.75	9 (20%)	49,88,113	1.45	9 (18%)
20	CLA	A	831	-	43,52,73	3.06	8 (18%)	49,88,113	1.31	7 (14%)
29	CHL	7	1012	-	47,55,74	2.48	9 (19%)	50,91,114	1.71	7 (14%)
29	CHL	6	314	-	51,59,74	2.16	10 (19%)	55,96,114	1.75	8 (14%)
20	CLA	A	835	-	43,52,73	2.82	8 (18%)	49,88,113	1.44	6 (12%)
23	LHG	A	843	-	39,39,48	0.29	0	42,45,54	0.26	0
20	CLA	B	833	-	43,52,73	2.73	7 (16%)	49,88,113	1.38	9 (18%)
29	CHL	4	312	-	47,55,74	2.48	10 (21%)	50,91,114	1.73	9 (18%)
20	CLA	B	818	-	43,52,73	2.69	8 (18%)	49,88,113	1.25	8 (16%)
20	CLA	6	315	18	43,52,73	2.76	9 (20%)	49,88,113	1.40	7 (14%)
20	CLA	B	816	-	43,52,73	2.96	8 (18%)	49,88,113	1.37	7 (14%)
20	CLA	A	838	-	43,52,73	2.66	7 (16%)	49,88,113	1.45	6 (12%)
20	CLA	0	308	13	43,52,73	2.62	9 (20%)	49,88,113	1.37	6 (12%)
20	CLA	0	312	-	43,52,73	2.91	6 (13%)	49,88,113	1.47	8 (16%)
20	CLA	L	202	-	43,52,73	2.84	8 (18%)	49,88,113	1.38	6 (12%)
20	CLA	0	306	13	43,52,73	2.79	8 (18%)	49,88,113	1.43	8 (16%)
20	CLA	4	304	17	43,52,73	2.61	8 (18%)	49,88,113	1.38	7 (14%)
24	BCR	B	804	-	41,41,41	0.56	1 (2%)	56,56,56	1.88	12 (21%)
20	CLA	B	825	-	43,52,73	2.76	9 (20%)	49,88,113	1.37	8 (16%)
30	XAT	8	304	-	39,47,47	1.75	6 (15%)	54,74,74	1.71	11 (20%)
20	CLA	A	808	-	43,52,73	2.92	8 (18%)	49,88,113	1.35	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	827	-	43,52,73	2.59	8 (18%)	49,88,113	1.38	7 (14%)
20	CLA	3	1011	23	39,48,73	3.13	9 (23%)	44,83,113	1.50	8 (18%)
20	CLA	A	826	-	43,52,73	3.04	8 (18%)	49,88,113	1.31	8 (16%)
20	CLA	3	1006	-	43,52,73	2.96	8 (18%)	49,88,113	1.52	9 (18%)
29	CHL	5	313	-	47,55,74	2.97	11 (23%)	50,91,114	1.78	7 (14%)
20	CLA	B	822	-	43,52,73	2.66	9 (20%)	49,88,113	1.45	8 (16%)
28	LUT	J	104	-	42,43,43	0.48	0	51,60,60	0.62	0
27	LMG	5	324	-	45,45,55	0.44	0	53,53,63	0.64	1 (1%)
20	CLA	5	321	-	43,52,73	2.72	8 (18%)	49,88,113	1.46	8 (16%)
20	CLA	B	828	-	43,52,73	2.72	9 (20%)	49,88,113	1.43	7 (14%)
20	CLA	A	851	-	43,52,73	2.78	8 (18%)	49,88,113	1.34	8 (16%)
20	CLA	B	813	-	43,52,73	3.25	8 (18%)	49,88,113	1.48	8 (16%)
20	CLA	8	307	14	43,52,73	2.35	9 (20%)	49,88,113	1.38	5 (10%)
20	CLA	A	811	-	43,52,73	3.00	7 (16%)	49,88,113	1.48	8 (16%)
20	CLA	A	813	-	43,52,73	3.04	7 (16%)	49,88,113	1.42	9 (18%)
30	XAT	7	1002	-	39,47,47	1.77	7 (17%)	54,74,74	1.80	12 (22%)
28	LUT	3	1002	-	42,43,43	0.41	0	51,60,60	0.64	1 (1%)
30	XAT	6	304	-	39,47,47	0.31	0	54,74,74	0.89	2 (3%)
20	CLA	1	1017	-	43,52,73	2.82	7 (16%)	49,88,113	1.46	7 (14%)
20	CLA	B	835	-	43,52,73	2.83	8 (18%)	49,88,113	1.42	7 (14%)
24	BCR	A	848	-	41,41,41	0.20	0	56,56,56	0.55	0
20	CLA	0	301	23	43,52,73	2.93	8 (18%)	49,88,113	1.36	7 (14%)
20	CLA	0	316	-	43,52,73	2.78	7 (16%)	49,88,113	1.50	8 (16%)
20	CLA	B	814	-	43,52,73	2.92	8 (18%)	49,88,113	1.35	8 (16%)
20	CLA	6	310	-	43,52,73	2.56	9 (20%)	49,88,113	1.50	8 (16%)
20	CLA	3	1017	-	43,52,73	2.94	9 (20%)	49,88,113	1.38	7 (14%)
20	CLA	4	308	17	43,52,73	2.90	7 (16%)	49,88,113	1.50	8 (16%)
21	SF4	C	1002	3	0,12,12	-	-	-		
20	CLA	A	832	-	43,52,73	2.72	8 (18%)	49,88,113	1.36	8 (16%)
20	CLA	6	318	-	43,52,73	2.96	9 (20%)	49,88,113	1.53	9 (18%)
28	LUT	7	1001	-	42,43,43	0.46	0	51,60,60	0.75	2 (3%)
20	CLA	5	315	19	43,52,73	2.62	9 (20%)	49,88,113	1.38	5 (10%)
29	CHL	8	315	-	51,59,74	2.35	9 (17%)	55,96,114	1.75	11 (20%)
29	CHL	4	313	-	51,59,74	2.29	8 (15%)	55,96,114	1.69	10 (18%)
20	CLA	8	309	27	43,52,73	3.19	9 (20%)	49,88,113	1.60	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	8	312	-	43,52,73	2.78	9 (20%)	49,88,113	1.42	7 (14%)
20	CLA	A	821	-	43,52,73	2.99	9 (20%)	49,88,113	1.53	9 (18%)
20	CLA	A	805	-	43,52,73	2.88	8 (18%)	49,88,113	1.30	7 (14%)
25	DGD	B	848	-	62,62,67	0.86	2 (3%)	76,76,81	1.13	6 (7%)
20	CLA	L	203	-	43,52,73	2.98	8 (18%)	49,88,113	1.37	8 (16%)
20	CLA	0	305	-	43,52,73	2.74	9 (20%)	49,88,113	1.42	9 (18%)
20	CLA	0	307	-	43,52,73	2.98	9 (20%)	49,88,113	1.29	7 (14%)
20	CLA	1	1010	-	43,52,73	2.68	8 (18%)	49,88,113	1.40	8 (16%)
20	CLA	5	311	-	43,52,73	3.08	7 (16%)	49,88,113	1.56	8 (16%)
24	BCR	A	845	-	41,41,41	0.65	0	56,56,56	1.61	9 (16%)
29	CHL	6	313	-	47,55,74	2.67	8 (17%)	50,91,114	1.48	7 (14%)
20	CLA	B	823	-	43,52,73	3.12	8 (18%)	49,88,113	1.37	7 (14%)
20	CLA	B	817	-	43,52,73	2.84	8 (18%)	49,88,113	1.43	7 (14%)
24	BCR	A	850	-	41,41,41	0.39	0	56,56,56	0.79	1 (1%)
20	CLA	6	306	18	43,52,73	2.64	9 (20%)	49,88,113	1.41	9 (18%)
24	BCR	5	320	-	41,41,41	0.37	0	56,56,56	0.67	1 (1%)
20	CLA	4	306	-	43,52,73	2.72	8 (18%)	49,88,113	1.29	6 (12%)
29	CHL	6	316	-	61,69,74	2.03	9 (14%)	67,108,114	1.32	7 (10%)
20	CLA	A	814	-	39,48,73	3.10	9 (23%)	44,83,113	1.54	9 (20%)
20	CLA	B	819	-	43,52,73	2.84	9 (20%)	49,88,113	1.36	8 (16%)
20	CLA	3	1013	16	43,52,73	2.72	7 (16%)	49,88,113	1.49	7 (14%)
20	CLA	G	202	-	43,52,73	2.98	8 (18%)	49,88,113	1.36	7 (14%)
20	CLA	J	102	-	43,52,73	2.94	9 (20%)	49,88,113	1.30	8 (16%)
24	BCR	6	302	-	41,41,41	0.52	1 (2%)	56,56,56	1.23	3 (5%)
29	CHL	4	315	-	61,69,74	2.13	9 (14%)	67,108,114	1.35	8 (11%)
20	CLA	1	1006	13	43,52,73	2.68	7 (16%)	49,88,113	1.46	6 (12%)
20	CLA	B	831	-	43,52,73	2.94	8 (18%)	49,88,113	1.45	7 (14%)
24	BCR	B	846	-	41,41,41	0.34	0	56,56,56	0.47	0
20	CLA	B	820	-	43,52,73	2.91	8 (18%)	49,88,113	1.53	8 (16%)
20	CLA	7	1014	15	43,52,73	2.79	9 (20%)	49,88,113	1.43	6 (12%)
20	CLA	6	301	-	43,52,73	2.74	9 (20%)	49,88,113	1.37	8 (16%)
20	CLA	4	305	17	43,52,73	3.25	9 (20%)	49,88,113	1.40	8 (16%)
29	CHL	3	1014	-	47,55,74	2.30	9 (19%)	50,91,114	1.76	6 (12%)
20	CLA	F	303	6	43,52,73	2.81	9 (20%)	49,88,113	1.41	7 (14%)
20	CLA	A	824	-	43,52,73	2.95	8 (18%)	49,88,113	1.48	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CHL	7	1017	15	66,74,74	2.03	9 (13%)	73,114,114	1.45	10 (13%)
20	CLA	1	1014	-	43,52,73	2.91	7 (16%)	49,88,113	1.47	9 (18%)
24	BCR	G	204	-	41,41,41	0.60	0	56,56,56	1.03	4 (7%)
20	CLA	5	312	19	43,52,73	2.79	8 (18%)	49,88,113	1.51	9 (18%)
20	CLA	A	852	-	43,52,73	2.90	7 (16%)	49,88,113	1.41	8 (16%)
20	CLA	8	311	-	43,52,73	2.64	6 (13%)	49,88,113	1.33	8 (16%)
20	CLA	4	309	-	43,52,73	2.79	8 (18%)	49,88,113	1.38	7 (14%)
27	LMG	8	319	20	44,44,55	0.29	0	52,52,63	0.83	1 (1%)
20	CLA	B	806	-	43,52,73	2.76	8 (18%)	49,88,113	1.31	6 (12%)
20	CLA	A	807	-	43,52,73	2.67	9 (20%)	49,88,113	1.42	8 (16%)
29	CHL	1	1012	-	47,55,74	2.37	11 (23%)	50,91,114	1.58	5 (10%)
29	CHL	8	314	-	47,55,74	2.50	9 (19%)	50,91,114	1.57	8 (16%)
20	CLA	A	834	-	43,52,73	2.93	8 (18%)	49,88,113	1.51	7 (14%)
20	CLA	F	302	-	43,52,73	2.78	9 (20%)	49,88,113	1.41	10 (20%)
20	CLA	A	816	-	43,52,73	2.85	8 (18%)	49,88,113	1.34	7 (14%)
24	BCR	8	302	-	41,41,41	0.52	0	56,56,56	1.28	5 (8%)
20	CLA	5	308	-	43,52,73	2.70	10 (23%)	49,88,113	1.47	10 (20%)
29	CHL	8	317	-	61,69,74	2.22	10 (16%)	67,108,114	1.47	8 (11%)
20	CLA	B	810	-	43,52,73	2.75	9 (20%)	49,88,113	1.45	7 (14%)
21	SF4	A	841	2,1	0,12,12	-	-	-		
20	CLA	B	808	-	43,52,73	2.98	7 (16%)	49,88,113	1.40	7 (14%)
20	CLA	5	310	-	43,52,73	2.85	9 (20%)	49,88,113	1.27	4 (8%)
20	CLA	5	307	19	43,52,73	2.81	9 (20%)	49,88,113	1.56	8 (16%)
27	LMG	J	101	-	30,30,55	0.24	0	38,38,63	0.24	0
20	CLA	1	1011	13	43,52,73	2.87	8 (18%)	49,88,113	1.45	9 (18%)
28	LUT	5	302	-	42,43,43	0.34	0	51,60,60	0.56	0
20	CLA	B	826	-	43,52,73	2.97	8 (18%)	49,88,113	1.48	8 (16%)
20	CLA	3	1009	-	43,52,73	2.92	9 (20%)	49,88,113	1.40	7 (14%)
20	CLA	8	306	14	43,52,73	2.84	11 (25%)	49,88,113	1.53	7 (14%)
20	CLA	B	803	-	43,52,73	2.85	8 (18%)	49,88,113	1.53	9 (18%)
20	CLA	1	1008	-	43,52,73	2.90	9 (20%)	49,88,113	1.42	7 (14%)
20	CLA	4	310	-	43,52,73	2.83	6 (13%)	49,88,113	1.43	6 (12%)
21	SF4	C	1001	3	0,12,12	-	-	-		
29	CHL	7	1015	-	46,54,74	2.77	11 (23%)	49,90,114	1.65	8 (16%)
20	CLA	A	825	-	43,52,73	2.92	8 (18%)	49,88,113	1.38	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	6	320	-	43,52,73	2.86	7 (16%)	49,88,113	1.57	11 (22%)
28	LUT	8	303	-	42,43,43	0.31	0	51,60,60	0.48	0
24	BCR	A	847	-	41,41,41	0.40	0	56,56,56	0.78	2 (3%)
20	CLA	3	1008	16	43,52,73	2.93	8 (18%)	49,88,113	1.56	10 (20%)
20	CLA	B	801	-	43,52,73	2.74	8 (18%)	49,88,113	1.36	7 (14%)
26	LMT	3	1018	-	32,32,36	0.30	0	43,43,47	0.69	1 (2%)
24	BCR	G	205	-	41,41,41	0.50	1 (2%)	56,56,56	1.20	4 (7%)
20	CLA	B	838	-	43,52,73	2.89	8 (18%)	49,88,113	1.45	7 (14%)
20	CLA	6	308	-	43,52,73	3.05	8 (18%)	49,88,113	1.52	10 (20%)

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
20	CLA	6	312	18	1/1/11/20	0/11/89/115	-
24	BCR	B	845	-	-	10/29/63/63	0/2/2/2
29	CHL	5	316	-	3/3/19/26	15/33/131/137	-
23	LHG	4	301	20	-	21/53/53/53	-
20	CLA	A	810	20	1/1/11/20	5/11/89/115	-
20	CLA	7	1005	15	1/1/11/20	2/11/89/115	-
20	CLA	A	829	-	1/1/11/20	4/11/89/115	-
20	CLA	A	836	-	1/1/11/20	5/11/89/115	-
20	CLA	7	1004	15	1/1/11/20	6/11/89/115	-
20	CLA	3	1007	-	1/1/11/20	4/11/89/115	-
20	CLA	0	309	-	1/1/11/20	5/11/89/115	-
20	CLA	B	821	-	1/1/11/20	3/11/89/115	-
20	CLA	3	1010	-	1/1/11/20	3/11/89/115	-
29	CHL	8	314	-	3/3/16/26	4/17/115/137	-
20	CLA	A	809	-	1/1/11/20	0/11/89/115	-
24	BCR	A	844	-	-	2/29/63/63	0/2/2/2
20	CLA	8	305	14	1/1/11/20	3/11/89/115	-
24	BCR	H	201	-	-	12/29/63/63	0/2/2/2
29	CHL	5	314	-	3/3/17/26	3/21/119/137	-
28	LUT	3	1001	-	-	3/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	XAT	5	303	-	-	2/31/93/93	0/4/4/4
20	CLA	B	839	-	1/1/11/20	4/11/89/115	-
20	CLA	B	841	-	1/1/11/20	6/11/89/115	-
20	CLA	A	840	-	1/1/11/20	3/11/89/115	-
20	CLA	G	203	-	1/1/11/20	6/11/89/115	-
24	BCR	A	846	-	-	6/29/63/63	0/2/2/2
20	CLA	8	316	14	1/1/11/20	2/11/89/115	-
20	CLA	A	812	-	1/1/11/20	4/11/89/115	-
20	CLA	B	830	-	1/1/11/20	3/11/89/115	-
20	CLA	L	204	-	1/1/11/20	3/11/89/115	-
20	CLA	7	1009	-	1/1/11/20	3/11/89/115	-
20	CLA	A	815	-	1/1/11/20	5/11/89/115	-
20	CLA	1	1003	-	1/1/11/20	3/11/89/115	-
20	CLA	A	804	-	1/1/11/20	4/11/89/115	-
20	CLA	0	310	-	1/1/11/20	7/11/89/115	-
29	CHL	1	1013	-	3/3/17/26	1/21/119/137	-
25	DGD	5	319	-	-	19/40/80/95	0/2/2/2
20	CLA	3	1012	-	1/1/11/20	3/11/89/115	-
20	CLA	3	1005	16	1/1/11/20	6/11/89/115	-
29	CHL	5	317	19	3/3/15/26	2/12/110/137	-
20	CLA	B	832	-	1/1/11/20	1/11/89/115	-
20	CLA	5	304	19	1/1/11/20	2/11/89/115	-
20	CLA	7	1011	-	1/1/11/20	5/11/89/115	-
20	CLA	3	1016	-	1/1/11/20	8/11/89/115	-
24	BCR	F	301	-	-	5/29/63/63	0/2/2/2
20	CLA	6	309	-	1/1/11/20	7/11/89/115	-
24	BCR	3	1003	-	-	11/29/63/63	0/2/2/2
27	LMG	4	318	-	-	10/29/49/70	0/1/1/1
20	CLA	F	305	-	1/1/11/20	0/11/89/115	-
20	CLA	1	1009	23	1/1/11/20	2/11/89/115	-
20	CLA	5	305	19	1/1/11/20	4/11/89/115	-
20	CLA	B	805	-	1/1/11/20	2/11/89/115	-
20	CLA	8	308	14	1/1/11/20	2/11/89/115	-
20	CLA	7	1007	15	1/1/11/20	3/11/89/115	-
20	CLA	5	318	-	1/1/11/20	1/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	307	17	1/1/11/20	4/11/89/115	-
22	PQN	B	842	-	-	9/23/43/43	0/2/2/2
20	CLA	8	310	-	1/1/11/20	4/11/89/115	-
20	CLA	A	839	-	1/1/11/20	2/11/89/115	-
24	BCR	3	1004	-	-	8/29/63/63	0/2/2/2
20	CLA	B	829	-	1/1/11/20	4/11/89/115	-
23	LHG	3	1019	20	-	12/23/23/53	-
20	CLA	8	313	14	1/1/11/20	2/11/89/115	-
20	CLA	7	1010	23	1/1/11/20	0/11/89/115	-
29	CHL	0	314	-	3/3/16/26	2/17/115/137	-
24	BCR	B	844	-	-	10/29/63/63	0/2/2/2
28	LUT	4	317	-	-	0/29/67/67	0/2/2/2
20	CLA	B	809	-	1/1/11/20	3/11/89/115	-
20	CLA	B	834	-	1/1/11/20	2/11/89/115	-
20	CLA	5	322	-	1/1/11/20	1/11/89/115	-
20	CLA	6	307	-	1/1/11/20	1/11/89/115	-
20	CLA	B	807	-	1/1/11/20	2/11/89/115	-
29	CHL	0	317	-	3/3/19/26	14/33/131/137	-
20	CLA	A	819	-	1/1/11/20	5/11/89/115	-
24	BCR	B	847	-	-	5/29/63/63	0/2/2/2
20	CLA	5	306	-	1/1/11/20	3/11/89/115	-
26	LMT	B	849	-	-	5/17/57/61	0/2/2/2
29	CHL	7	1013	-	3/3/16/26	3/18/116/137	-
20	CLA	A	837	-	1/1/11/20	4/11/89/115	-
20	CLA	B	827	-	1/1/11/20	3/11/89/115	-
20	CLA	A	823	-	1/1/11/20	1/11/89/115	-
20	CLA	3	1015	16	1/1/11/20	2/11/89/115	-
29	CHL	0	315	-	3/3/17/26	3/21/119/137	-
20	CLA	A	822	-	1/1/11/20	2/11/89/115	-
20	CLA	1	1007	-	1/1/11/20	5/11/89/115	-
20	CLA	4	311	17	1/1/11/20	2/11/89/115	-
22	PQN	A	842	-	-	6/23/43/43	0/2/2/2
20	CLA	1	1004	13	1/1/11/20	4/11/89/115	-
20	CLA	G	201	-	1/1/11/20	3/11/89/115	-
29	CHL	1	1015	-	3/3/19/26	12/33/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	8	301	20	-	17/53/53/53	-
24	BCR	J	103	-	-	4/29/63/63	0/2/2/2
20	CLA	A	802	-	1/1/11/20	2/11/89/115	-
23	LHG	7	1016	20	-	13/39/39/53	-
20	CLA	5	301	-	1/1/11/20	7/11/89/115	-
24	BCR	1	1001	-	-	8/29/63/63	0/2/2/2
20	CLA	A	817	-	1/1/11/20	4/11/89/115	-
20	CLA	B	824	-	1/1/11/20	0/11/89/115	-
20	CLA	7	1006	-	1/1/11/20	4/11/89/115	-
29	CHL	4	315	-	3/3/19/26	17/33/131/137	-
20	CLA	B	812	2	1/1/11/20	3/11/89/115	-
20	CLA	1	1005	-	1/1/11/20	1/11/89/115	-
24	BCR	F	304	-	-	4/29/63/63	0/2/2/2
20	CLA	6	311	-	1/1/11/20	2/11/89/115	-
20	CLA	B	815	-	1/1/11/20	3/11/89/115	-
24	BCR	7	1003	-	-	16/29/63/63	0/2/2/2
20	CLA	A	806	-	1/1/11/20	5/11/89/115	-
27	LMG	6	319	-	-	11/39/59/70	0/1/1/1
28	LUT	0	304	-	-	6/29/67/67	0/2/2/2
20	CLA	7	1008	-	1/1/11/20	4/11/89/115	-
20	CLA	B	837	-	1/1/11/20	4/11/89/115	-
20	CLA	0	313	13	1/1/11/20	2/11/89/115	-
27	LMG	8	318	-	-	5/22/42/70	0/1/1/1
20	CLA	B	811	-	1/1/11/20	0/11/89/115	-
20	CLA	K	201	-	1/1/11/20	6/11/89/115	-
29	CHL	4	316	17	3/3/15/26	2/12/110/137	-
24	BCR	4	302	-	-	7/29/63/63	0/2/2/2
20	CLA	4	314	17	1/1/11/20	3/11/89/115	-
28	LUT	0	318	-	-	2/29/67/67	0/2/2/2
23	LHG	0	302	20	-	9/23/23/53	-
20	CLA	A	820	-	1/1/11/20	5/11/89/115	-
20	CLA	B	802	-	1/1/11/20	4/11/89/115	-
29	CHL	6	317	18	3/3/15/26	4/12/110/137	-
20	CLA	A	818	-	1/1/11/20	4/11/89/115	-
28	LUT	1	1016	-	-	1/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	5	309	19	1/1/11/20	9/11/89/115	-
30	XAT	4	303	-	-	2/31/93/93	0/4/4/4
20	CLA	5	323	-	1/1/11/20	5/11/89/115	-
20	CLA	6	305	18	1/1/11/20	2/11/89/115	-
20	CLA	A	830	-	1/1/11/20	3/11/89/115	-
20	CLA	B	840	-	1/1/11/20	4/11/89/115	-
24	BCR	I	201	-	-	11/29/63/63	0/2/2/2
20	CLA	0	311	23	1/1/11/20	2/11/89/115	-
20	CLA	L	201	-	1/1/11/20	3/11/89/115	-
20	CLA	K	202	-	1/1/5/20	-	-
20	CLA	A	801	-	1/1/11/20	3/11/89/115	-
28	LUT	6	303	-	-	2/29/67/67	0/2/2/2
28	LUT	1	1002	-	-	5/29/67/67	0/2/2/2
20	CLA	A	833	1	1/1/11/20	3/11/89/115	-
24	BCR	B	843	-	-	9/29/63/63	0/2/2/2
20	CLA	B	836	-	1/1/11/20	0/11/89/115	-
20	CLA	B	850	-	1/1/11/20	4/11/86/115	-
20	CLA	A	803	20	1/1/11/20	6/11/89/115	-
27	LMG	0	303	-	-	21/45/65/70	0/1/1/1
20	CLA	A	828	-	1/1/11/20	4/11/89/115	-
20	CLA	A	831	-	1/1/11/20	2/11/89/115	-
29	CHL	7	1012	-	3/3/16/26	4/17/115/137	-
29	CHL	6	314	-	3/3/17/26	5/21/119/137	-
20	CLA	A	835	-	1/1/11/20	2/11/89/115	-
29	CHL	4	312	-	3/3/16/26	3/17/115/137	-
20	CLA	B	833	-	1/1/11/20	3/11/89/115	-
23	LHG	A	843	-	-	21/44/44/53	-
20	CLA	B	818	-	1/1/11/20	2/11/89/115	-
20	CLA	6	315	18	1/1/11/20	0/11/89/115	-
20	CLA	B	816	-	1/1/11/20	7/11/89/115	-
20	CLA	A	838	-	1/1/11/20	1/11/89/115	-
20	CLA	0	308	13	1/1/11/20	3/11/89/115	-
20	CLA	0	312	-	1/1/11/20	4/11/89/115	-
20	CLA	L	202	-	1/1/11/20	2/11/89/115	-
20	CLA	0	306	13	1/1/11/20	4/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	304	17	1/1/11/20	3/11/89/115	-
24	BCR	B	804	-	-	6/29/63/63	0/2/2/2
20	CLA	B	825	-	1/1/11/20	4/11/89/115	-
30	XAT	8	304	-	-	12/31/93/93	0/4/4/4
20	CLA	A	808	-	1/1/11/20	3/11/89/115	-
20	CLA	A	827	-	1/1/11/20	3/11/89/115	-
20	CLA	3	1011	23	1/1/10/20	0/6/84/115	-
20	CLA	A	826	-	1/1/11/20	0/11/89/115	-
20	CLA	3	1006	-	1/1/11/20	4/11/89/115	-
29	CHL	5	313	-	3/3/16/26	6/17/115/137	-
20	CLA	B	822	-	1/1/11/20	0/11/89/115	-
28	LUT	J	104	-	-	7/29/67/67	0/2/2/2
27	LMG	5	324	-	-	26/40/60/70	0/1/1/1
20	CLA	5	321	-	1/1/11/20	4/11/89/115	-
20	CLA	B	828	-	1/1/11/20	3/11/89/115	-
20	CLA	A	851	-	1/1/11/20	2/11/89/115	-
20	CLA	B	813	-	1/1/11/20	2/11/89/115	-
20	CLA	8	307	14	1/1/11/20	2/11/89/115	-
20	CLA	A	811	-	1/1/11/20	5/11/89/115	-
20	CLA	A	813	-	1/1/11/20	4/11/89/115	-
30	XAT	7	1002	-	-	6/31/93/93	0/4/4/4
28	LUT	3	1002	-	-	8/29/67/67	0/2/2/2
30	XAT	6	304	-	-	5/31/93/93	0/4/4/4
20	CLA	1	1017	-	1/1/11/20	1/11/89/115	-
20	CLA	B	835	-	1/1/11/20	0/11/89/115	-
24	BCR	A	848	-	-	9/29/63/63	0/2/2/2
20	CLA	0	301	23	1/1/11/20	2/11/89/115	-
20	CLA	0	316	-	1/1/11/20	2/11/89/115	-
20	CLA	B	814	-	1/1/11/20	0/11/89/115	-
20	CLA	6	310	-	1/1/11/20	7/11/89/115	-
20	CLA	3	1017	-	1/1/11/20	4/11/89/115	-
20	CLA	4	308	17	1/1/11/20	5/11/89/115	-
21	SF4	C	1002	3	-	-	0/6/5/5
20	CLA	A	832	-	1/1/11/20	2/11/89/115	-
20	CLA	6	318	-	1/1/11/20	3/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	7	1001	-	-	5/29/67/67	0/2/2/2
20	CLA	5	315	19	1/1/11/20	0/11/89/115	-
29	CHL	8	315	-	3/3/17/26	1/21/119/137	-
29	CHL	4	313	-	3/3/17/26	3/21/119/137	-
20	CLA	8	309	27	1/1/11/20	7/11/89/115	-
20	CLA	8	312	-	1/1/11/20	3/11/89/115	-
20	CLA	A	821	-	1/1/11/20	2/11/89/115	-
20	CLA	A	805	-	1/1/11/20	4/11/89/115	-
25	DGD	B	848	-	-	18/50/90/95	0/2/2/2
20	CLA	L	203	-	1/1/11/20	3/11/89/115	-
20	CLA	0	305	-	1/1/11/20	3/11/89/115	-
20	CLA	0	307	-	1/1/11/20	3/11/89/115	-
20	CLA	1	1010	-	1/1/11/20	6/11/89/115	-
20	CLA	5	311	-	1/1/11/20	3/11/89/115	-
24	BCR	A	845	-	-	9/29/63/63	0/2/2/2
29	CHL	6	313	-	3/3/16/26	5/17/115/137	-
20	CLA	B	823	-	1/1/11/20	3/11/89/115	-
20	CLA	B	817	-	1/1/11/20	2/11/89/115	-
29	CHL	6	316	-	3/3/19/26	13/33/131/137	-
20	CLA	6	306	18	1/1/11/20	2/11/89/115	-
24	BCR	A	850	-	-	7/29/63/63	0/2/2/2
20	CLA	4	306	-	1/1/11/20	4/11/89/115	-
24	BCR	5	320	-	-	5/29/63/63	0/2/2/2
20	CLA	A	814	-	1/1/10/20	2/6/84/115	-
20	CLA	B	819	-	1/1/11/20	3/11/89/115	-
20	CLA	3	1013	16	1/1/11/20	4/11/89/115	-
20	CLA	G	202	-	1/1/11/20	4/11/89/115	-
20	CLA	J	102	-	1/1/11/20	4/11/89/115	-
24	BCR	6	302	-	-	7/29/63/63	0/2/2/2
20	CLA	1	1006	13	1/1/11/20	2/11/89/115	-
20	CLA	B	831	-	1/1/11/20	1/11/89/115	-
24	BCR	B	846	-	-	2/29/63/63	0/2/2/2
20	CLA	B	820	-	1/1/11/20	2/11/89/115	-
20	CLA	7	1014	15	1/1/11/20	0/11/89/115	-
20	CLA	6	301	-	1/1/11/20	6/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	A	849	-	-	20/53/53/53	-
20	CLA	4	305	17	1/1/11/20	4/11/89/115	-
29	CHL	3	1014	-	3/3/16/26	6/17/115/137	-
20	CLA	F	303	6	1/1/11/20	3/11/89/115	-
20	CLA	A	824	-	1/1/11/20	4/11/89/115	-
29	CHL	7	1017	15	3/3/20/26	9/39/137/137	-
20	CLA	1	1014	-	1/1/11/20	2/11/89/115	-
24	BCR	G	204	-	-	2/29/63/63	0/2/2/2
20	CLA	5	312	19	1/1/11/20	2/11/89/115	-
20	CLA	A	852	-	1/1/11/20	2/11/89/115	-
20	CLA	8	311	-	1/1/11/20	3/11/89/115	-
20	CLA	4	309	-	1/1/11/20	9/11/89/115	-
27	LMG	8	319	20	-	12/39/59/70	0/1/1/1
20	CLA	B	806	-	1/1/11/20	2/11/89/115	-
20	CLA	A	807	-	1/1/11/20	5/11/89/115	-
29	CHL	1	1012	-	3/3/16/26	5/17/115/137	-
20	CLA	A	834	-	1/1/11/20	2/11/89/115	-
20	CLA	F	302	-	1/1/11/20	2/11/89/115	-
20	CLA	A	816	-	1/1/11/20	0/11/89/115	-
24	BCR	8	302	-	-	7/29/63/63	0/2/2/2
20	CLA	5	308	-	1/1/11/20	3/11/89/115	-
29	CHL	8	317	-	3/3/19/26	17/33/131/137	-
20	CLA	B	810	-	1/1/11/20	2/11/89/115	-
21	SF4	A	841	2,1	-	-	0/6/5/5
20	CLA	B	808	-	1/1/11/20	4/11/89/115	-
20	CLA	5	310	-	1/1/11/20	4/11/89/115	-
20	CLA	5	307	19	1/1/11/20	2/11/89/115	-
27	LMG	J	101	-	-	6/25/45/70	0/1/1/1
20	CLA	1	1011	13	1/1/11/20	2/11/89/115	-
28	LUT	5	302	-	-	3/29/67/67	0/2/2/2
20	CLA	B	826	-	1/1/11/20	6/11/89/115	-
20	CLA	3	1009	-	1/1/11/20	7/11/89/115	-
20	CLA	8	306	14	1/1/11/20	3/11/89/115	-
20	CLA	B	803	-	1/1/11/20	3/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	1008	-	1/1/11/20	9/11/89/115	-
20	CLA	4	310	-	1/1/11/20	4/11/89/115	-
29	CHL	7	1015	-	3/3/16/26	8/15/113/137	-
21	SF4	C	1001	3	-	-	0/6/5/5
20	CLA	A	825	-	1/1/11/20	0/11/89/115	-
20	CLA	6	320	-	1/1/11/20	1/11/89/115	-
28	LUT	8	303	-	-	2/29/67/67	0/2/2/2
24	BCR	A	847	-	-	9/29/63/63	0/2/2/2
20	CLA	3	1008	16	1/1/11/20	3/11/89/115	-
20	CLA	B	801	-	1/1/11/20	1/11/89/115	-
26	LMT	3	1018	-	-	4/17/57/61	0/2/2/2
24	BCR	G	205	-	-	7/29/63/63	0/2/2/2
20	CLA	B	838	-	1/1/11/20	5/11/89/115	-
20	CLA	6	308	-	1/1/11/20	2/11/89/115	-

The worst 5 of 1792 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	850	CLA	C4C-NC	21.89	1.46	1.30
20	5	301	CLA	C4B-NB	17.13	1.50	1.35
20	6	308	CLA	C4B-NB	16.83	1.50	1.35
20	B	837	CLA	C4B-NB	16.69	1.50	1.35
20	8	309	CLA	C4B-NB	16.66	1.50	1.35

The worst 5 of 1753 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	7	1013	CHL	C4A-NA-C1A	-9.89	102.26	106.71
29	6	314	CHL	C4A-NA-C1A	-9.07	102.63	106.71
29	1	1015	CHL	C4A-NA-C1A	-9.04	102.64	106.71
20	K	202	CLA	C1C-NC-C4C	-8.95	102.68	106.71
29	5	313	CHL	C4A-NA-C1A	-8.26	102.99	106.71

5 of 263 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	801	CLA	ND
20	A	802	CLA	ND
20	A	803	CLA	ND

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Mol	Chain	Res	Type	Atom
20	A	804	CLA	ND
20	A	805	CLA	ND

5 of 1279 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	803	CLA	C1A-C2A-CAA-CBA
20	A	807	CLA	C1A-C2A-CAA-CBA
20	A	807	CLA	C3A-C2A-CAA-CBA
20	A	810	CLA	C1A-C2A-CAA-CBA
20	A	810	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

255 monomers are involved in 952 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	6	312	CLA	15	0
24	B	845	BCR	8	0
23	4	301	LHG	15	0
29	5	316	CHL	4	0
20	7	1005	CLA	2	0
20	A	829	CLA	2	0
20	A	836	CLA	2	0
20	7	1004	CLA	12	0
20	3	1007	CLA	3	0
20	0	309	CLA	7	0
20	B	821	CLA	6	0
23	A	849	LHG	3	0
20	A	809	CLA	1	0
24	A	844	BCR	7	0
20	8	305	CLA	3	0
24	H	201	BCR	2	0
28	3	1001	LUT	4	0
29	5	314	CHL	3	0
30	5	303	XAT	7	0
20	B	839	CLA	2	0
20	A	840	CLA	11	0
20	G	203	CLA	8	0
24	A	846	BCR	5	0
20	8	316	CLA	3	0
20	A	812	CLA	4	0
20	B	830	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	L	204	CLA	5	0
20	A	815	CLA	10	0
20	1	1003	CLA	6	0
20	A	804	CLA	4	0
20	0	310	CLA	4	0
29	1	1013	CHL	5	0
25	5	319	DGD	17	0
20	3	1012	CLA	1	0
20	3	1005	CLA	5	0
29	5	317	CHL	9	0
20	B	832	CLA	3	0
20	5	304	CLA	6	0
20	7	1011	CLA	1	0
20	3	1016	CLA	3	0
24	F	301	BCR	6	0
20	6	309	CLA	2	0
24	3	1003	BCR	3	0
27	4	318	LMG	38	0
20	F	305	CLA	1	0
20	1	1009	CLA	3	0
20	5	305	CLA	2	0
20	B	805	CLA	4	0
20	8	308	CLA	3	0
20	7	1007	CLA	1	0
20	5	318	CLA	3	0
20	4	307	CLA	18	0
22	B	842	PQN	3	0
20	8	310	CLA	4	0
20	A	839	CLA	1	0
24	3	1004	BCR	5	0
20	B	829	CLA	5	0
23	3	1019	LHG	5	0
20	8	313	CLA	4	0
20	7	1010	CLA	8	0
24	B	844	BCR	2	0
29	0	314	CHL	10	0
28	4	317	LUT	3	0
20	B	809	CLA	1	0
20	B	834	CLA	7	0
20	6	307	CLA	1	0
24	B	847	BCR	3	0
20	A	819	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	0	317	CHL	7	0
20	5	306	CLA	1	0
26	B	849	LMT	3	0
29	7	1013	CHL	3	0
20	A	837	CLA	1	0
20	B	827	CLA	2	0
20	A	823	CLA	4	0
20	3	1015	CLA	5	0
29	0	315	CHL	5	0
20	A	822	CLA	1	0
20	1	1007	CLA	7	0
20	4	311	CLA	8	0
22	A	842	PQN	4	0
20	G	201	CLA	2	0
29	1	1015	CHL	12	0
20	A	802	CLA	6	0
23	7	1016	LHG	6	0
20	5	301	CLA	3	0
24	1	1001	BCR	8	0
20	A	817	CLA	5	0
20	B	824	CLA	4	0
20	7	1006	CLA	2	0
24	F	304	BCR	1	0
20	B	812	CLA	6	0
20	1	1005	CLA	2	0
24	7	1003	BCR	2	0
20	6	311	CLA	4	0
28	0	304	LUT	12	0
20	A	806	CLA	1	0
27	6	319	LMG	9	0
20	7	1008	CLA	2	0
20	B	837	CLA	1	0
20	0	313	CLA	5	0
27	8	318	LMG	3	0
20	B	811	CLA	7	0
20	K	201	CLA	6	0
29	4	316	CHL	6	0
24	4	302	BCR	5	0
28	0	318	LUT	4	0
23	0	302	LHG	3	0
20	A	820	CLA	1	0
20	B	802	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	6	317	CHL	5	0
20	A	818	CLA	2	0
28	1	1016	LUT	3	0
20	5	309	CLA	6	0
30	4	303	XAT	2	0
20	5	323	CLA	7	0
20	6	305	CLA	3	0
20	B	840	CLA	4	0
24	I	201	BCR	17	0
20	0	311	CLA	4	0
20	L	201	CLA	5	0
20	A	801	CLA	10	0
28	6	303	LUT	4	0
28	1	1002	LUT	17	0
20	A	833	CLA	6	0
24	B	843	BCR	12	0
20	B	836	CLA	5	0
20	B	850	CLA	10	0
27	0	303	LMG	27	0
20	A	828	CLA	2	0
20	A	831	CLA	7	0
29	7	1012	CHL	6	0
29	6	314	CHL	5	0
20	A	835	CLA	4	0
23	A	843	LHG	3	0
29	4	312	CHL	1	0
20	B	818	CLA	5	0
20	6	315	CLA	2	0
20	B	816	CLA	3	0
20	A	838	CLA	6	0
20	0	308	CLA	2	0
20	0	312	CLA	1	0
20	L	202	CLA	1	0
20	4	304	CLA	3	0
24	B	804	BCR	6	0
20	B	825	CLA	5	0
30	8	304	XAT	1	0
20	A	808	CLA	2	0
20	A	827	CLA	1	0
20	3	1011	CLA	2	0
20	A	826	CLA	2	0
20	3	1006	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	5	313	CHL	4	0
20	B	822	CLA	3	0
28	J	104	LUT	10	0
27	5	324	LMG	7	0
20	5	321	CLA	4	0
20	B	828	CLA	2	0
20	A	851	CLA	5	0
20	B	813	CLA	8	0
20	8	307	CLA	2	0
20	A	811	CLA	1	0
20	A	813	CLA	8	0
28	3	1002	LUT	2	0
30	6	304	XAT	10	0
20	1	1017	CLA	8	0
20	B	835	CLA	3	0
24	A	848	BCR	3	0
20	0	301	CLA	3	0
20	0	316	CLA	5	0
20	B	814	CLA	1	0
20	6	310	CLA	8	0
20	4	308	CLA	1	0
21	C	1002	SF4	2	0
20	A	832	CLA	1	0
20	6	318	CLA	1	0
28	7	1001	LUT	5	0
20	5	315	CLA	6	0
29	8	315	CHL	3	0
29	4	313	CHL	1	0
20	8	309	CLA	6	0
20	8	312	CLA	2	0
20	A	821	CLA	3	0
25	B	848	DGD	2	0
20	L	203	CLA	2	0
20	0	305	CLA	7	0
20	0	307	CLA	2	0
20	1	1010	CLA	1	0
24	A	845	BCR	3	0
29	6	313	CHL	2	0
20	B	823	CLA	3	0
20	B	817	CLA	11	0
24	A	850	BCR	6	0
20	6	306	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	5	320	BCR	17	0
20	4	306	CLA	5	0
29	6	316	CHL	3	0
20	A	814	CLA	1	0
20	B	819	CLA	3	0
20	3	1013	CLA	3	0
20	G	202	CLA	1	0
20	J	102	CLA	3	0
24	6	302	BCR	15	0
29	4	315	CHL	19	0
20	1	1006	CLA	7	0
20	B	831	CLA	7	0
24	B	846	BCR	1	0
20	B	820	CLA	2	0
20	7	1014	CLA	4	0
20	6	301	CLA	1	0
20	4	305	CLA	1	0
29	3	1014	CHL	4	0
20	F	303	CLA	1	0
20	A	824	CLA	3	0
29	7	1017	CHL	6	0
20	1	1014	CLA	5	0
24	G	204	BCR	6	0
20	5	312	CLA	18	0
20	A	852	CLA	8	0
20	8	311	CLA	8	0
20	4	309	CLA	5	0
27	8	319	LMG	6	0
20	A	807	CLA	2	0
29	1	1012	CHL	4	0
29	8	314	CHL	3	0
20	A	834	CLA	5	0
20	F	302	CLA	8	0
20	A	816	CLA	1	0
24	8	302	BCR	6	0
20	5	308	CLA	8	0
29	8	317	CHL	4	0
20	B	810	CLA	4	0
21	A	841	SF4	1	0
20	B	808	CLA	7	0
20	5	310	CLA	6	0
20	5	307	CLA	4	0

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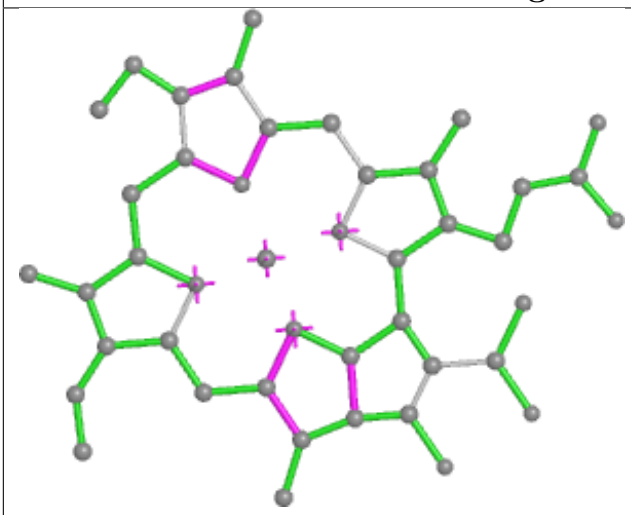
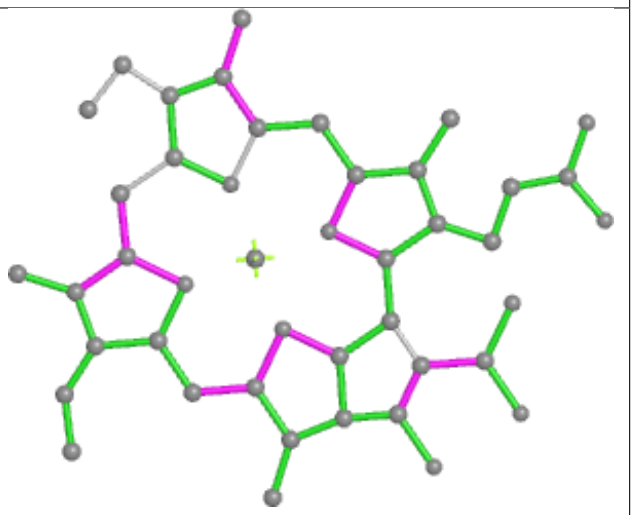
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	1011	CLA	4	0
28	5	302	LUT	6	0
20	B	826	CLA	1	0
20	3	1009	CLA	2	0
20	8	306	CLA	2	0
20	B	803	CLA	2	0
20	1	1008	CLA	7	0
20	4	310	CLA	5	0
29	7	1015	CHL	1	0
20	A	825	CLA	3	0
20	6	320	CLA	4	0
28	8	303	LUT	4	0
24	A	847	BCR	7	0
20	3	1008	CLA	2	0
20	B	801	CLA	7	0
26	3	1018	LMT	8	0
24	G	205	BCR	19	0
20	B	838	CLA	3	0
20	6	308	CLA	7	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.

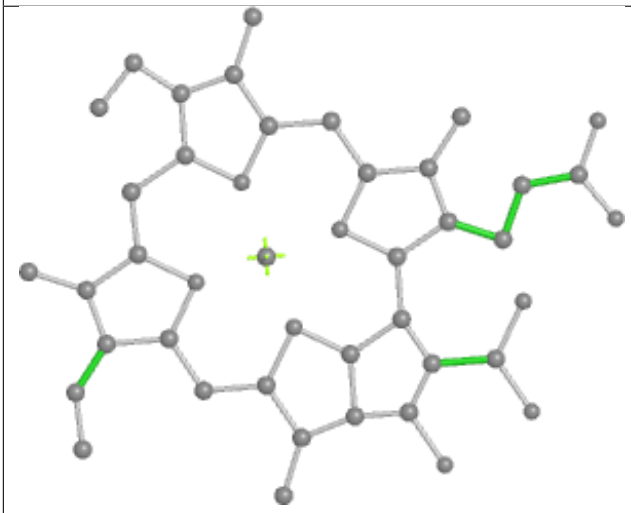
Ligand CLA 6 312



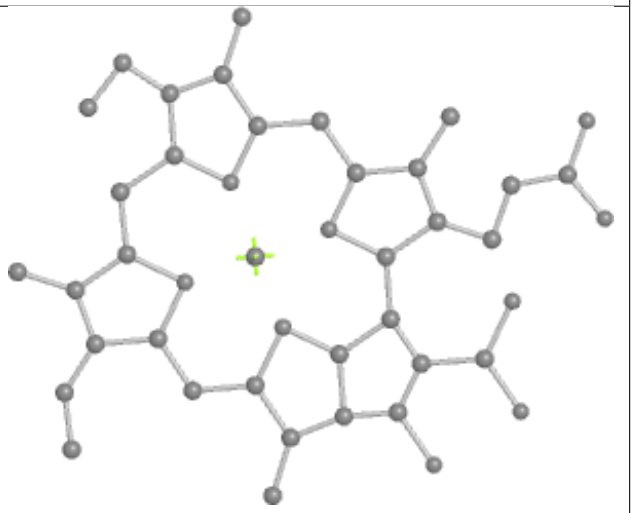
Bond lengths



Bond angles

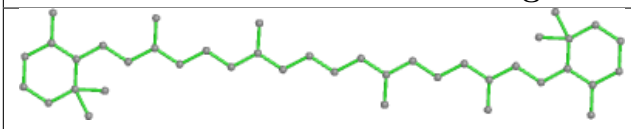


Torsions



Rings

Ligand BCR B 845



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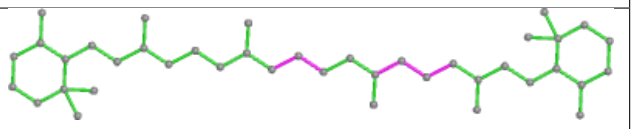
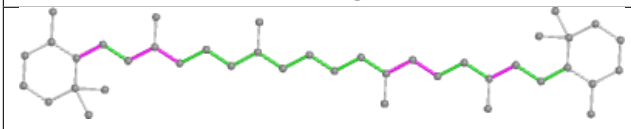


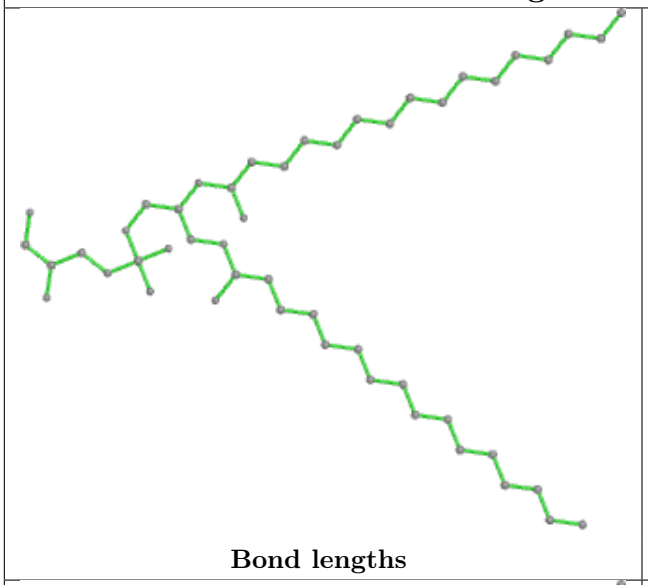
Bond angles



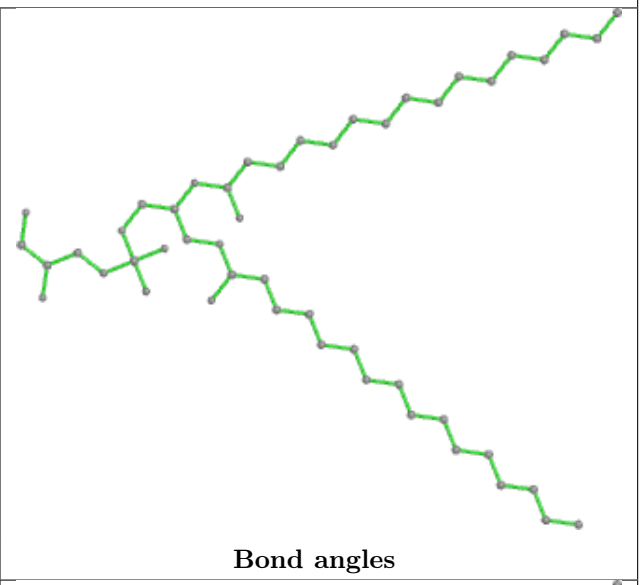
Torsions

Rings

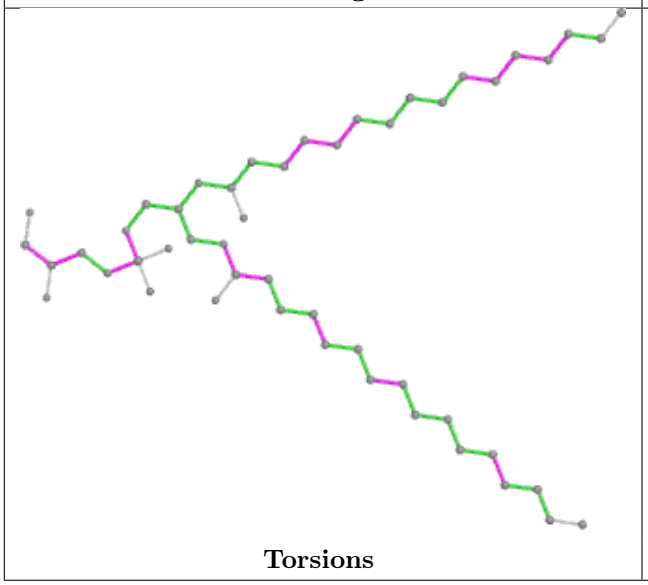
Ligand LHG 4 301



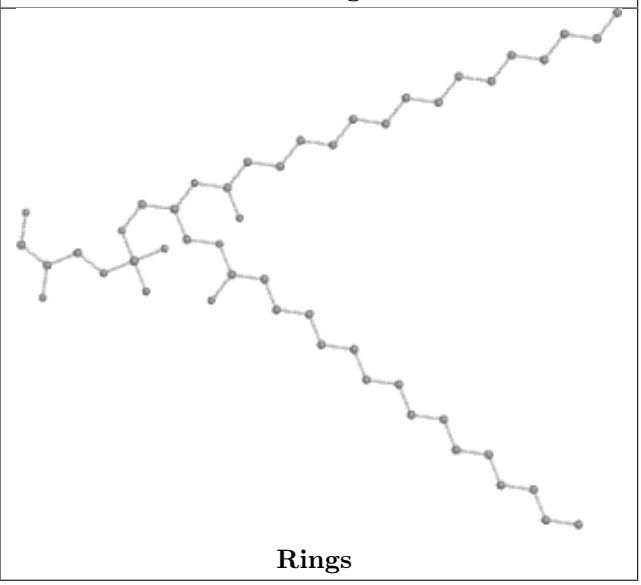
Bond lengths



Bond angles

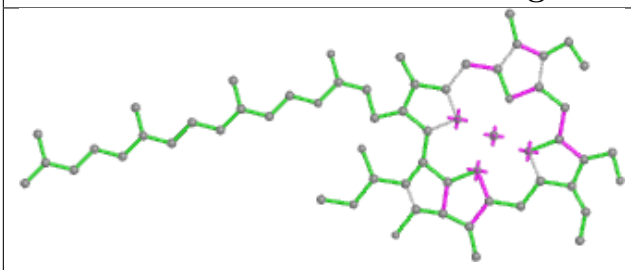


Torsions

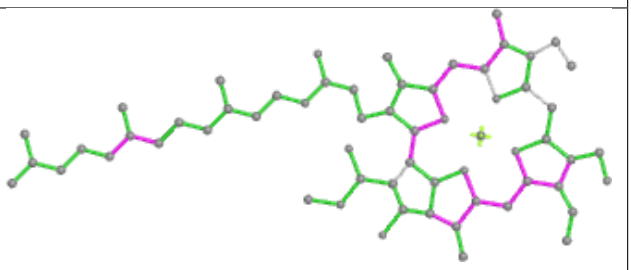


Rings

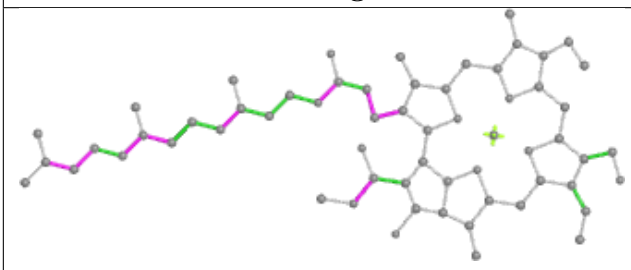
Ligand CHL 5 316



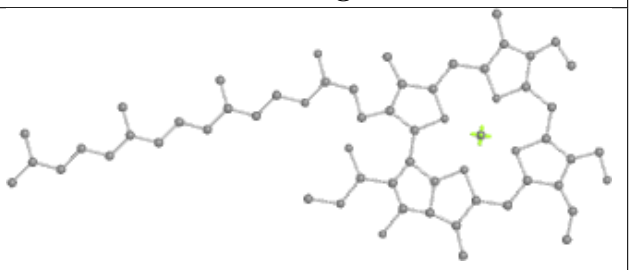
Bond lengths



Bond angles

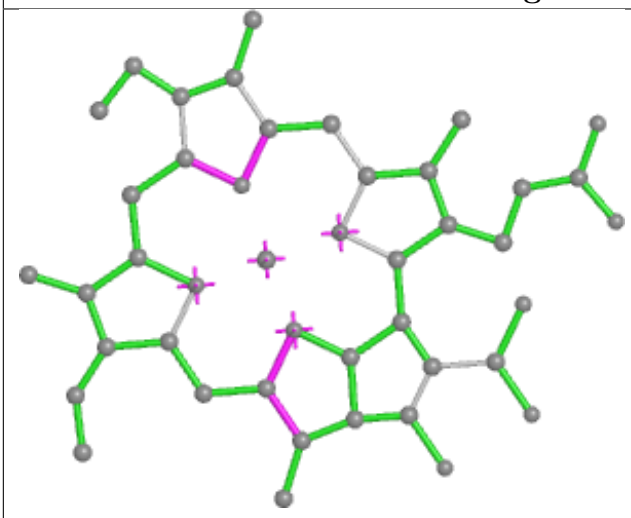


Torsions

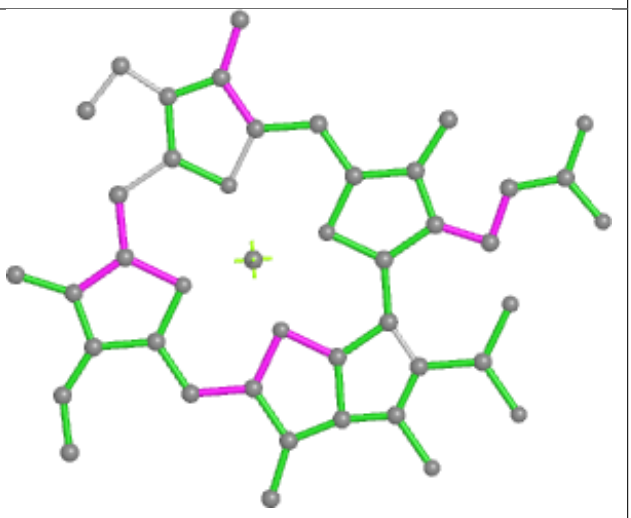


Rings

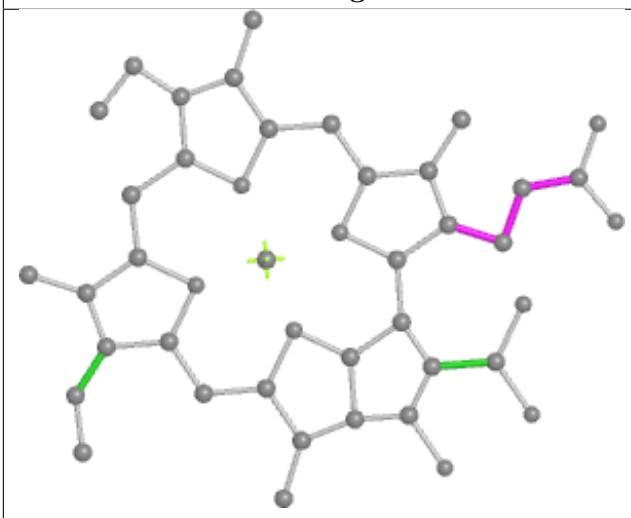
Ligand CLA A 810



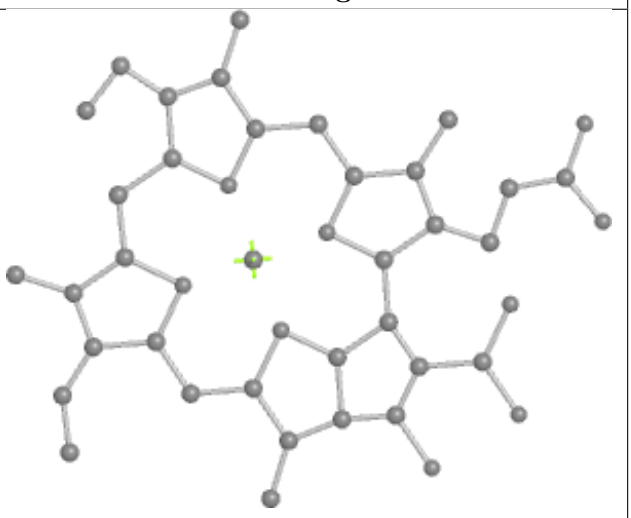
Bond lengths



Bond angles

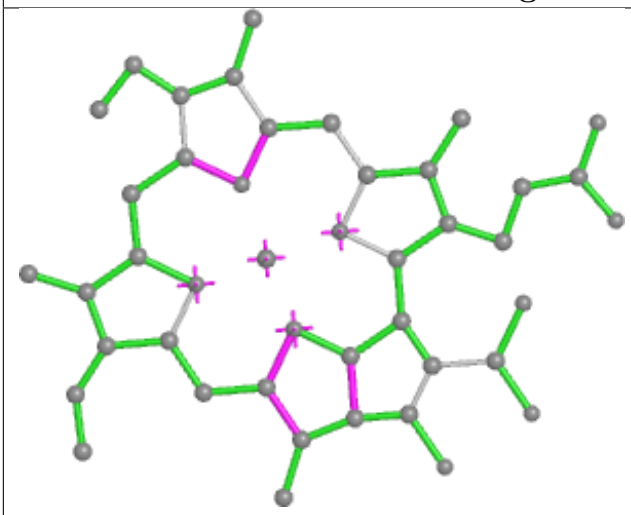


Torsions



Rings

Ligand CLA 7 1005



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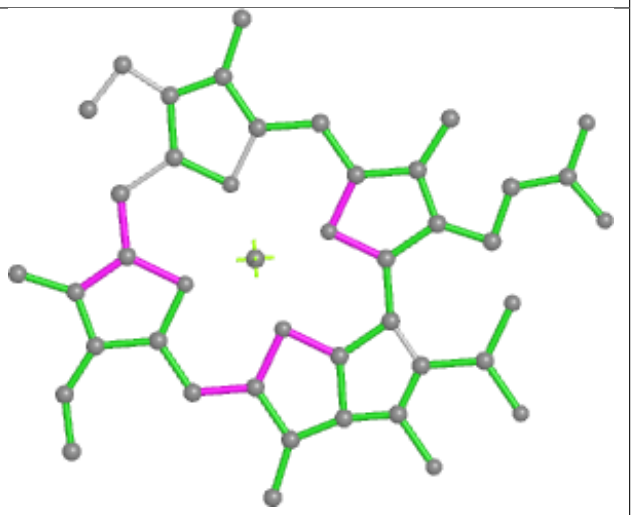

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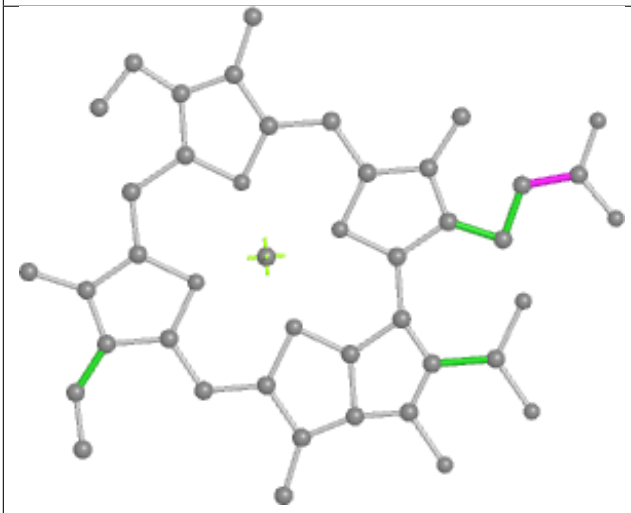

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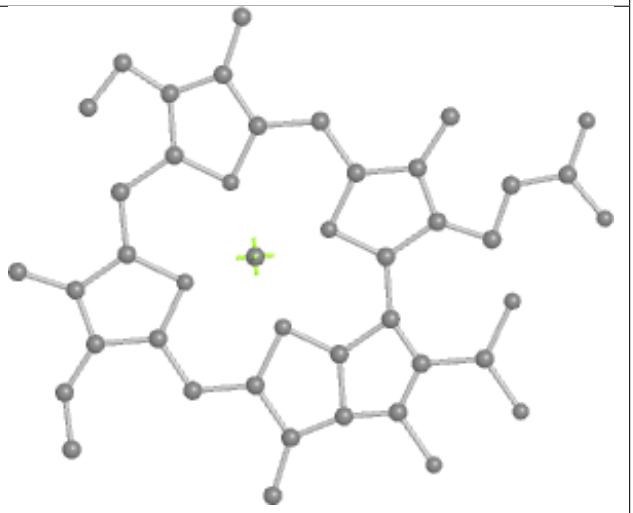
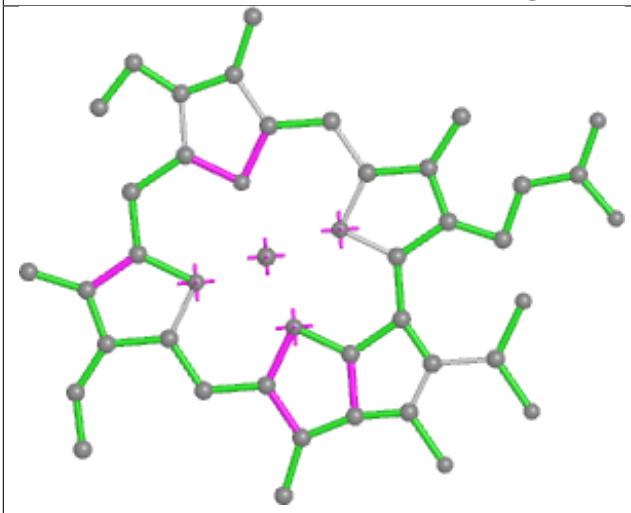


Rings

Ligand CLA A 829



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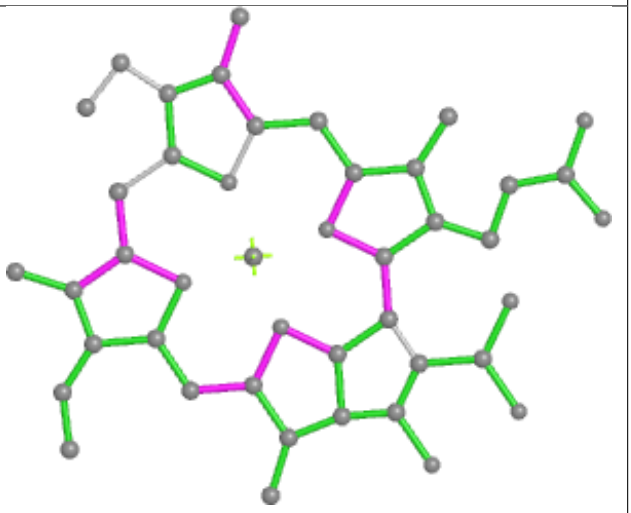
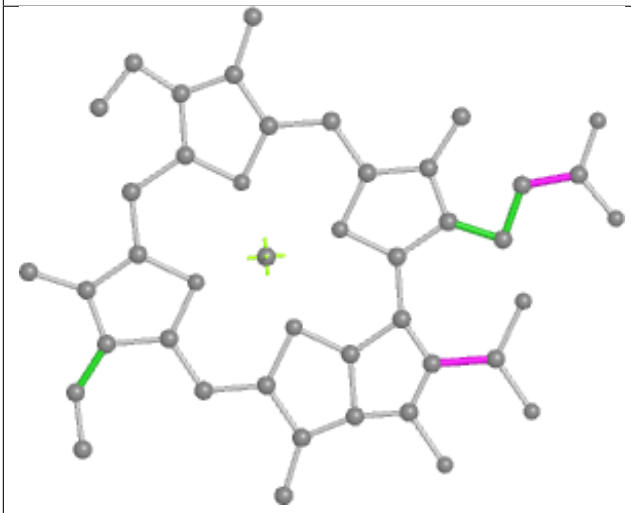


Bond angles



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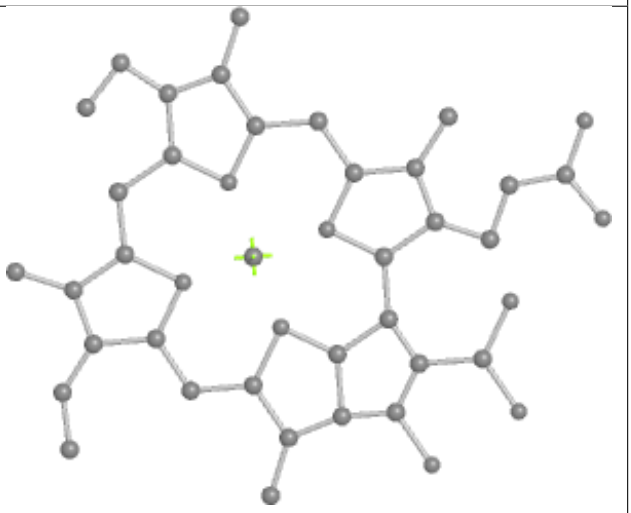
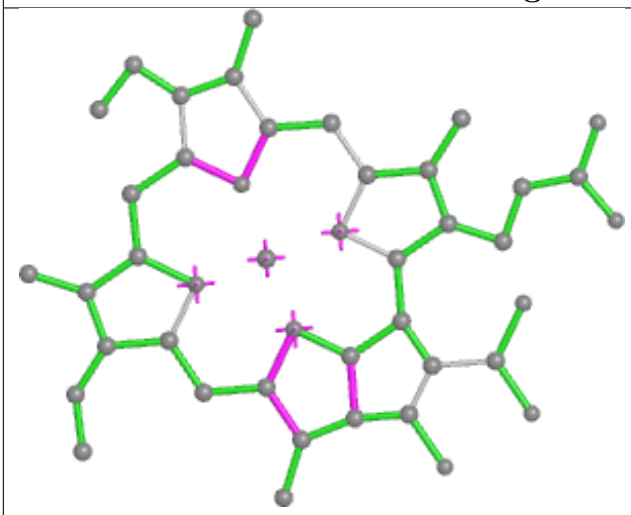
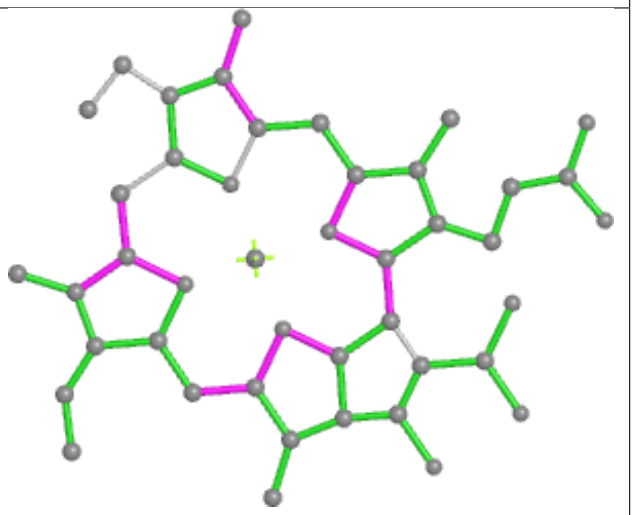


Rings

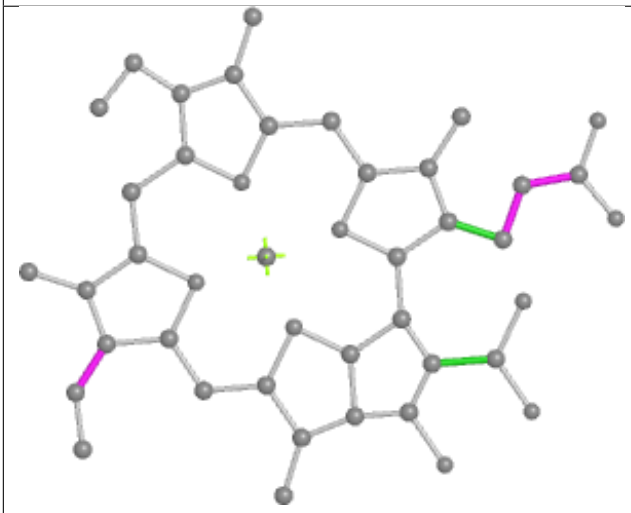
Ligand CLA A 836



Bond lengths



Bond angles



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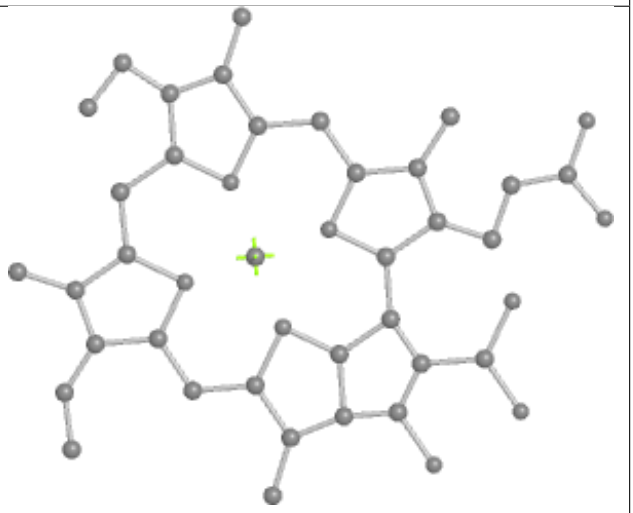
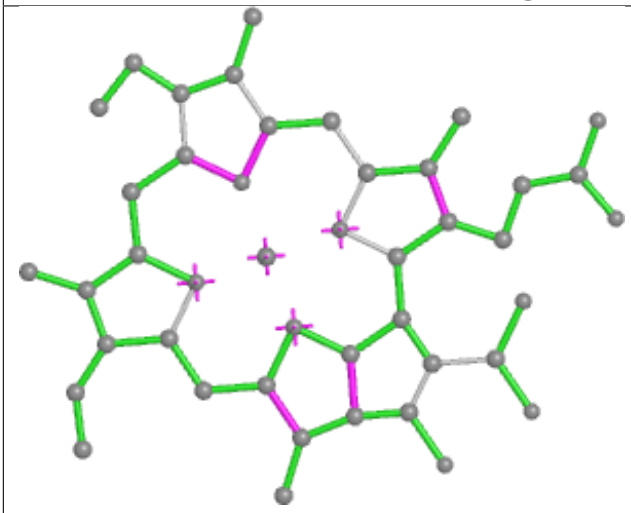
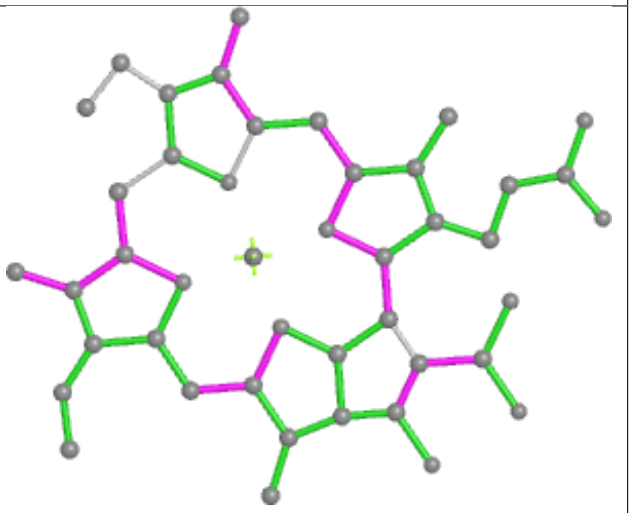


Rings

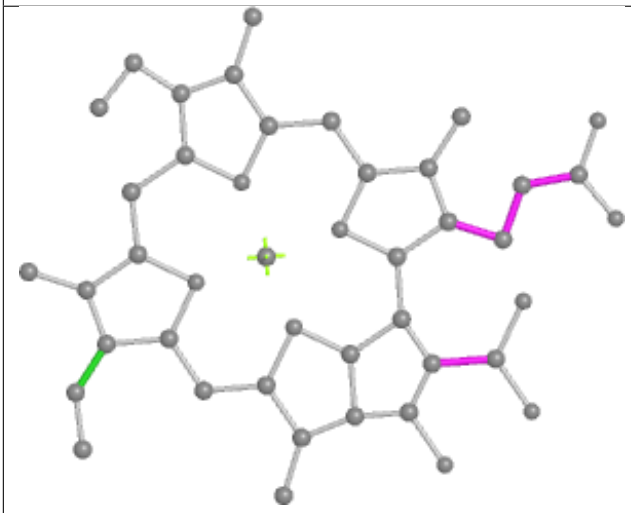
Ligand CLA 7 1004



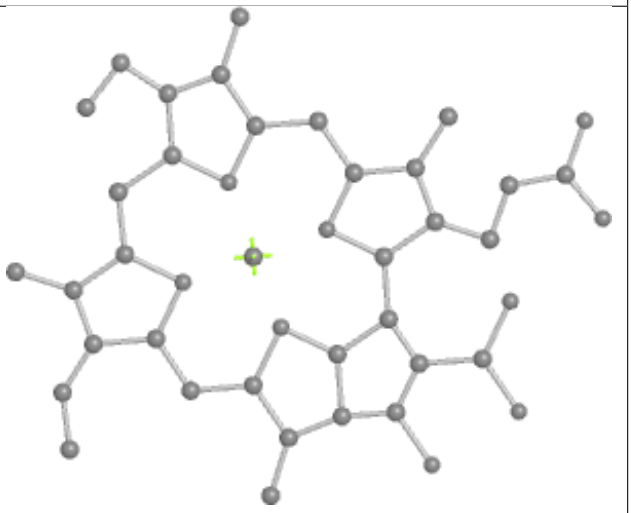
Bond lengths



Bond angles

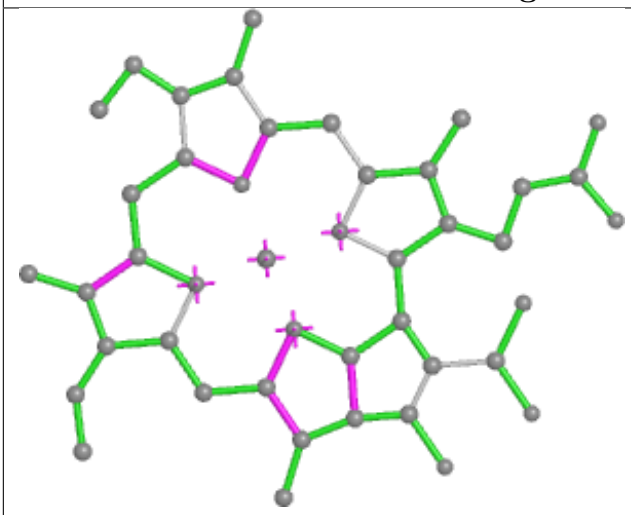


Torsions

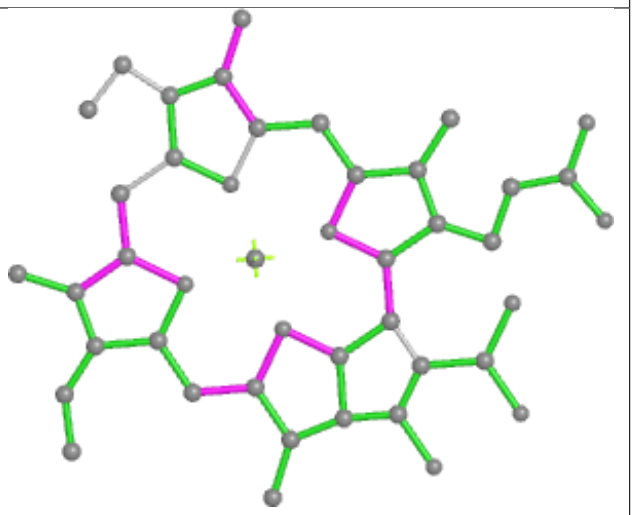


Rings

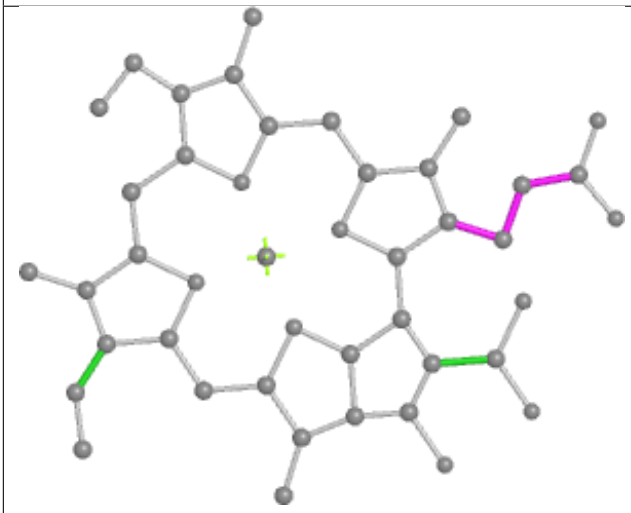
Ligand CLA 3 1007



Bond lengths



Bond angles



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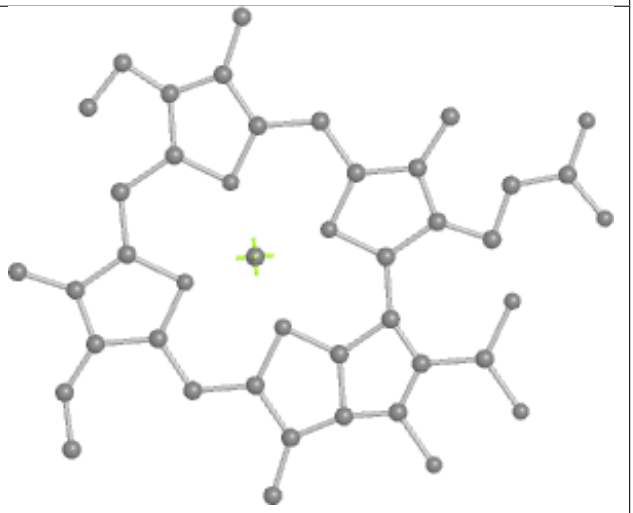
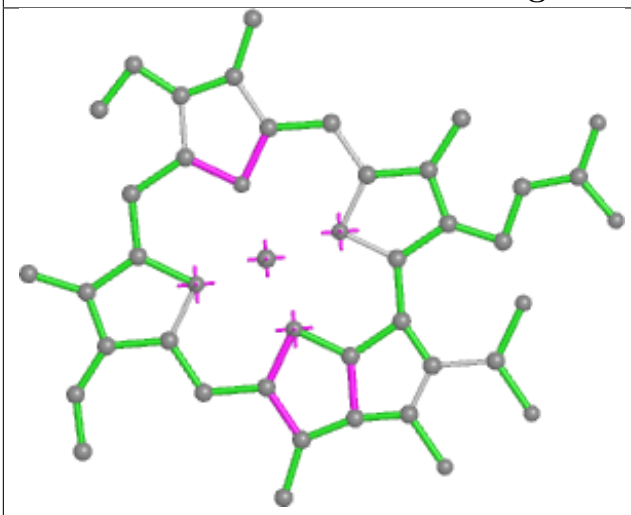
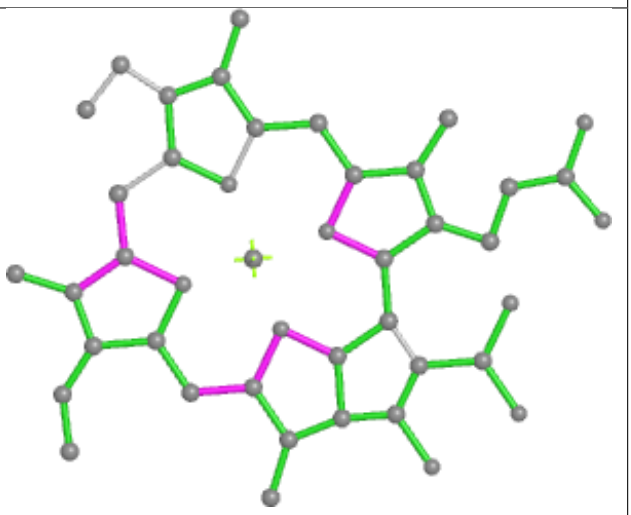


Rings

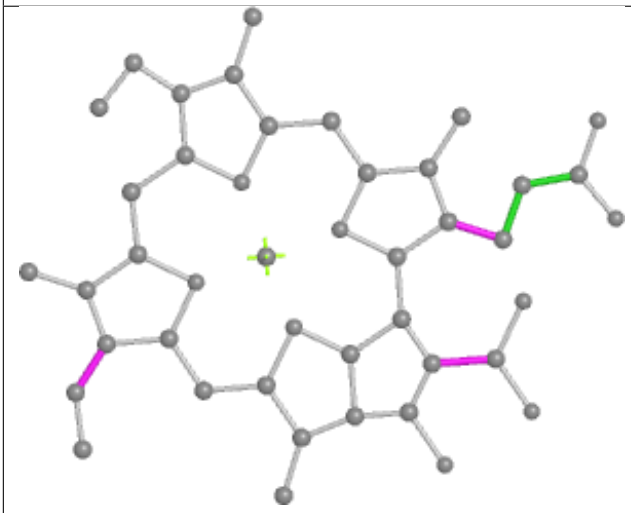
Ligand CLA 0 309



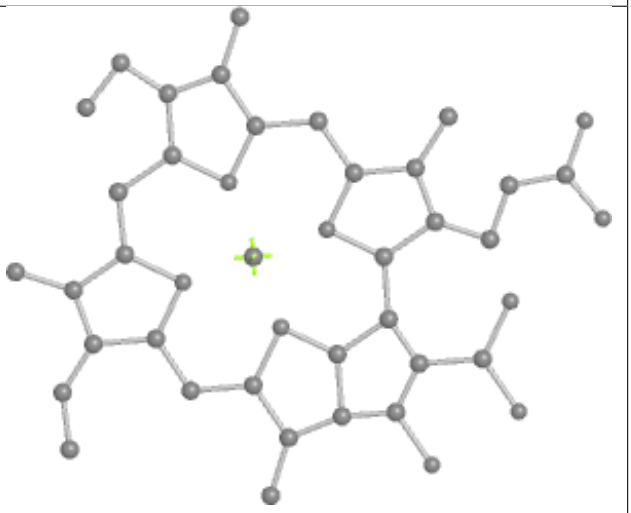
Bond lengths



Bond angles

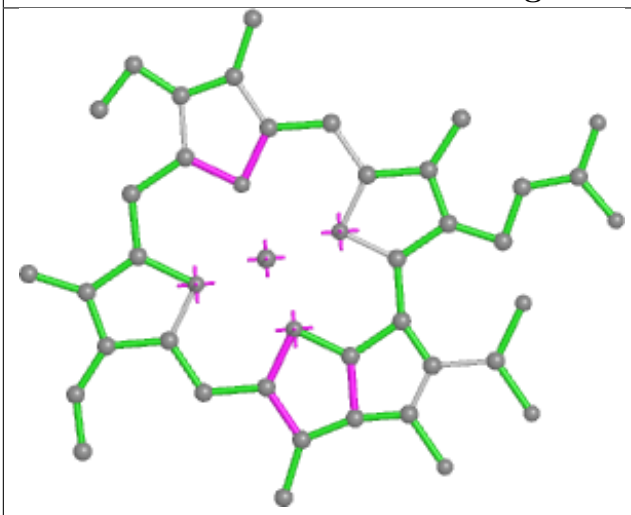


Torsions



Rings

Ligand CLA B 821



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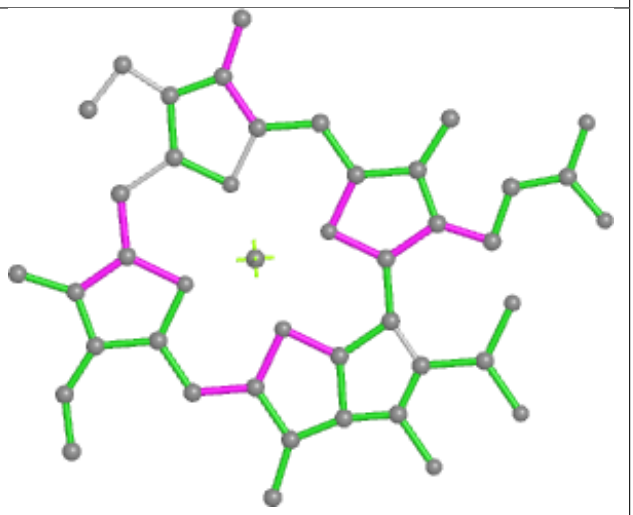
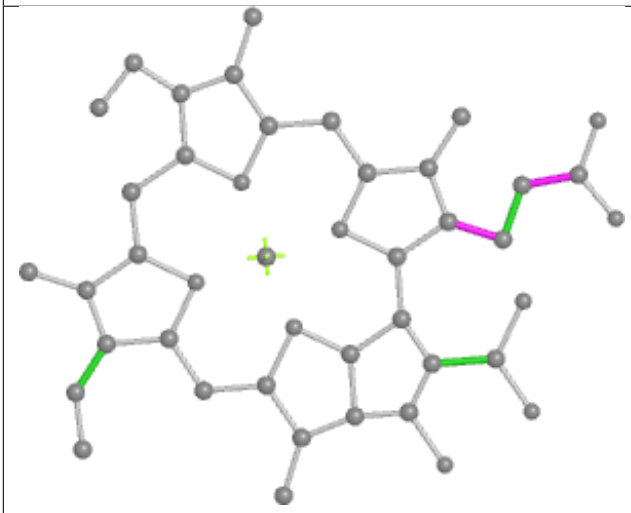
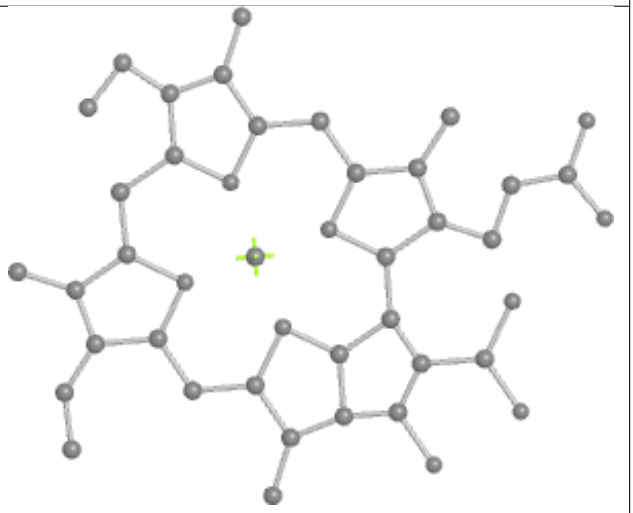


Bond angles

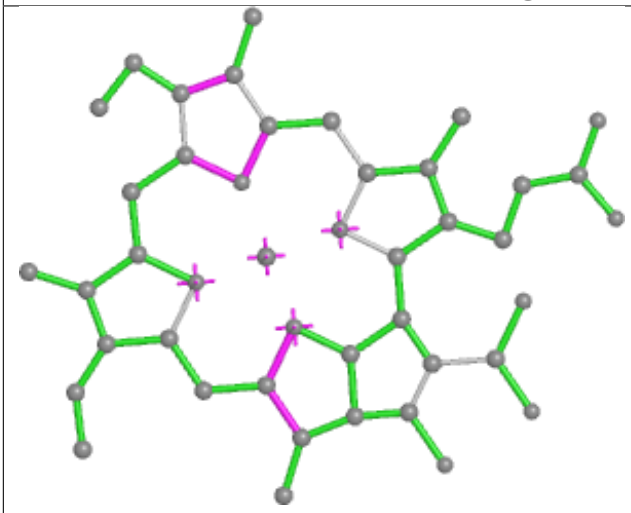


Torsions



Rings

Ligand CLA 3 1010



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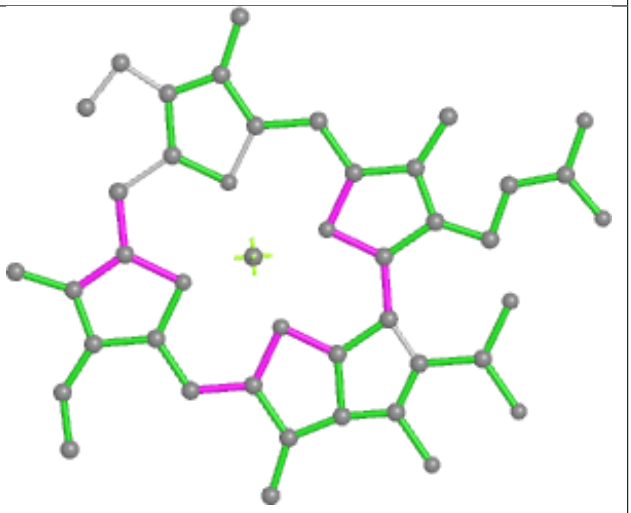
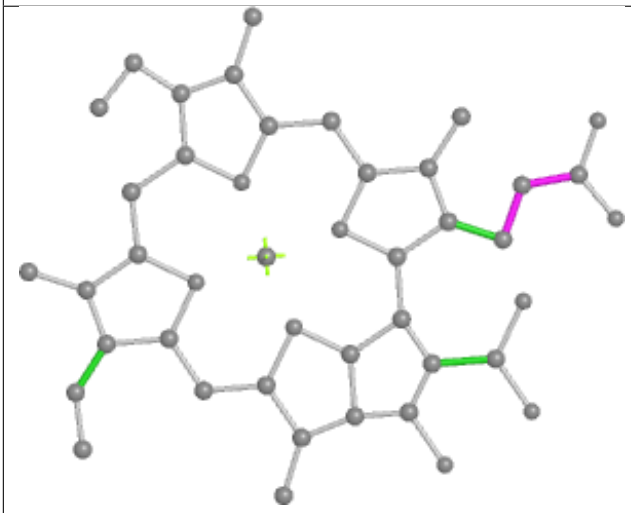
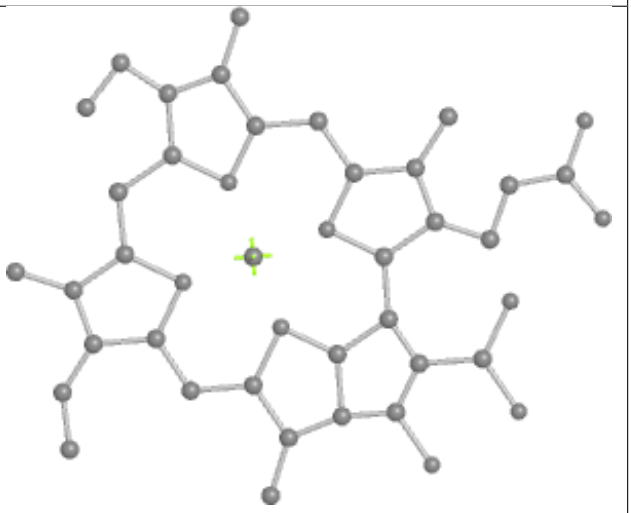


Bond angles

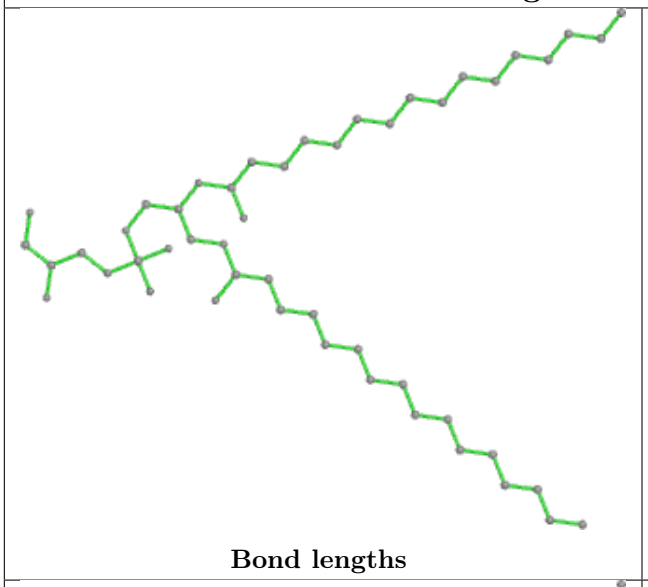


Torsions



Rings

Ligand LHG A 849



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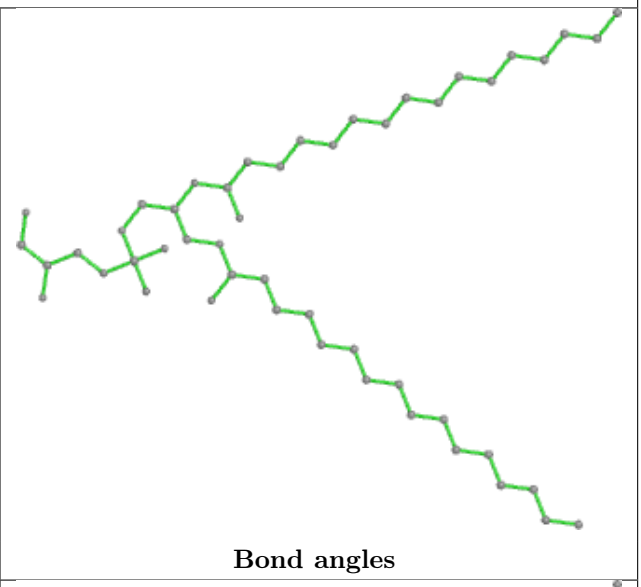
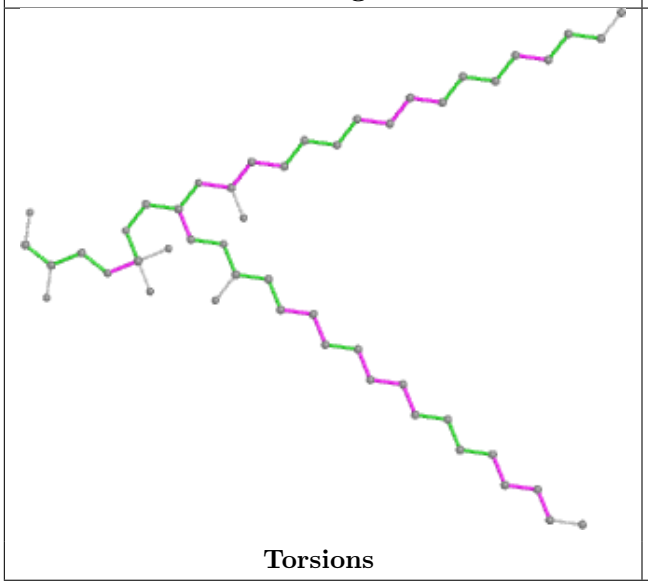


Bond angles



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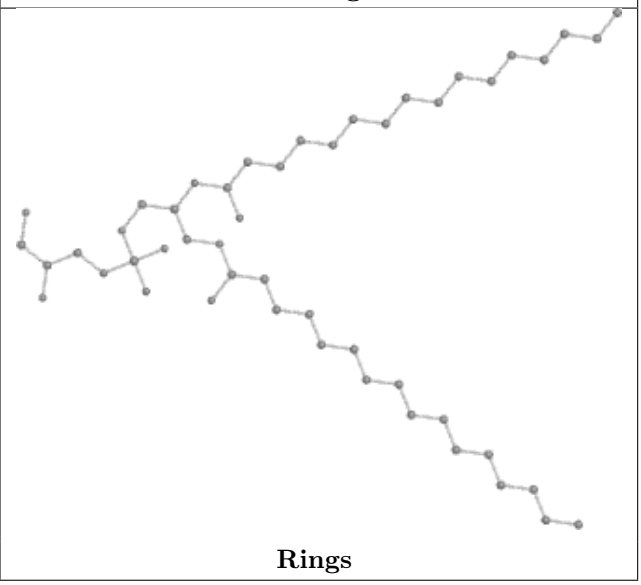
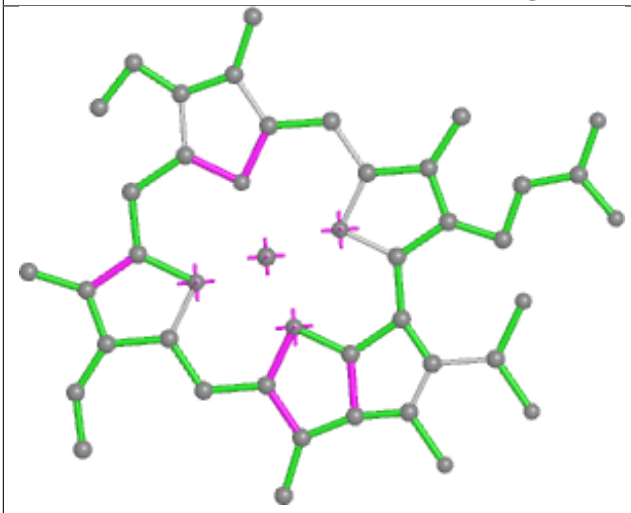


Rings

Ligand CLA A 809



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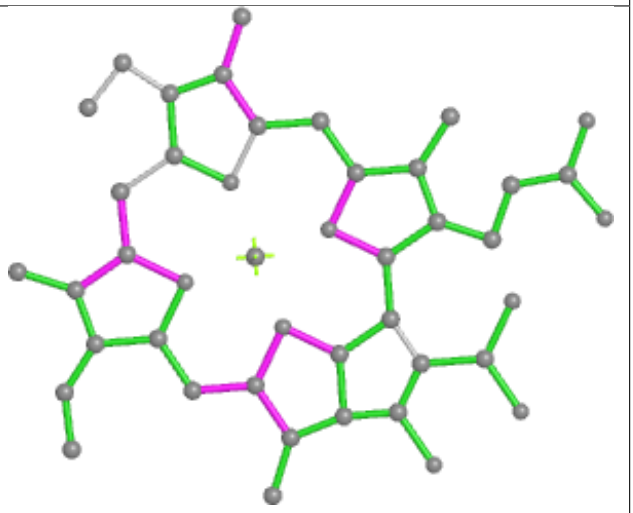
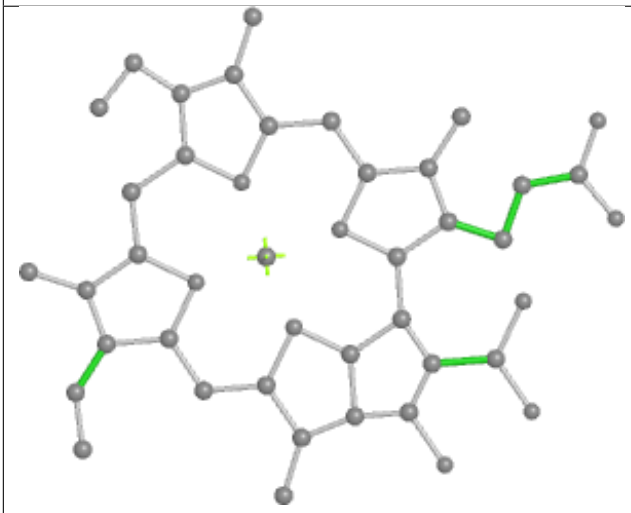


Bond angles



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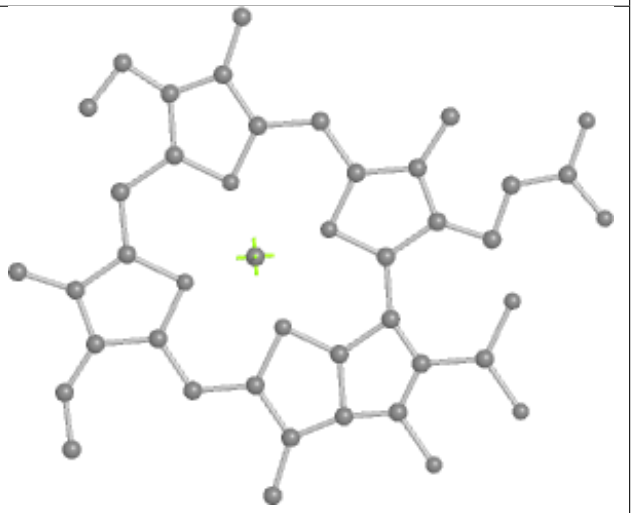
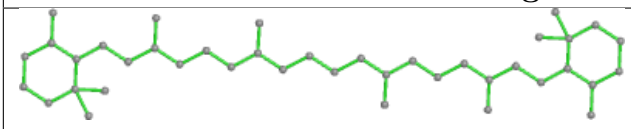


Rings

Ligand BCR A 844



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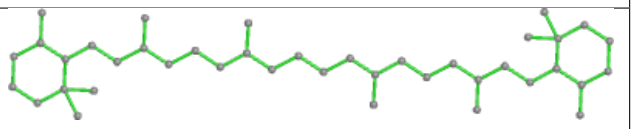
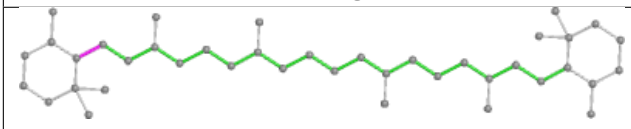


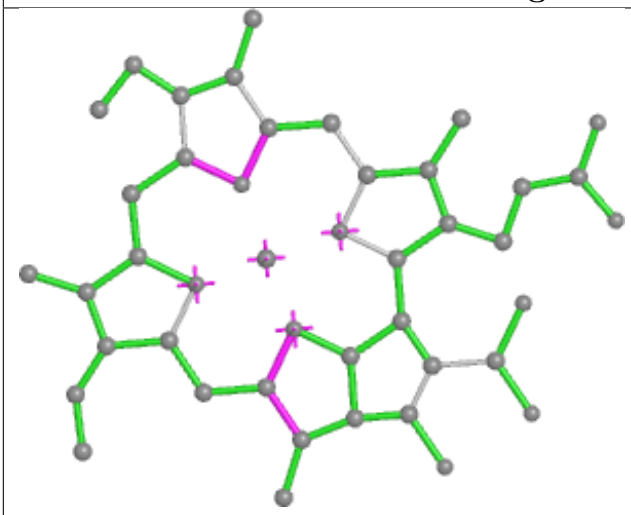
Bond angles



Torsions

Rings

Ligand CLA 8 305



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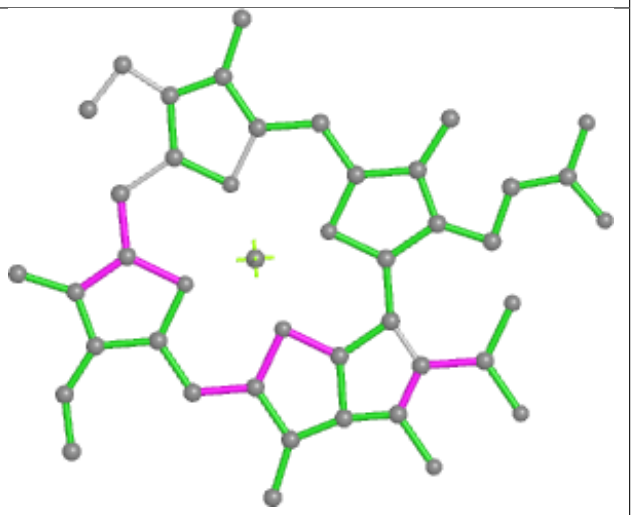
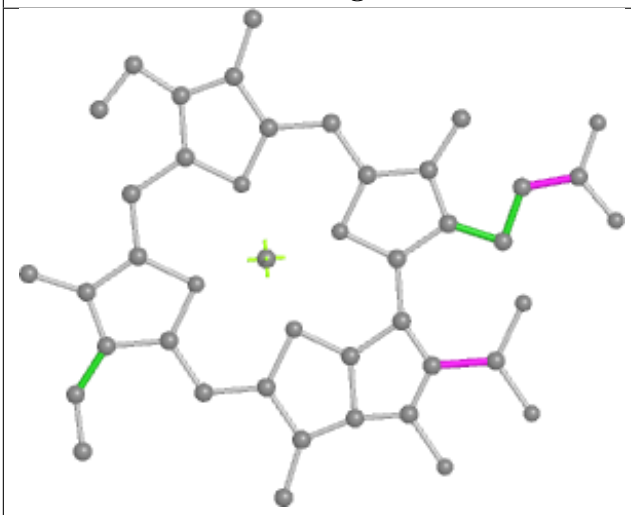


Bond angles



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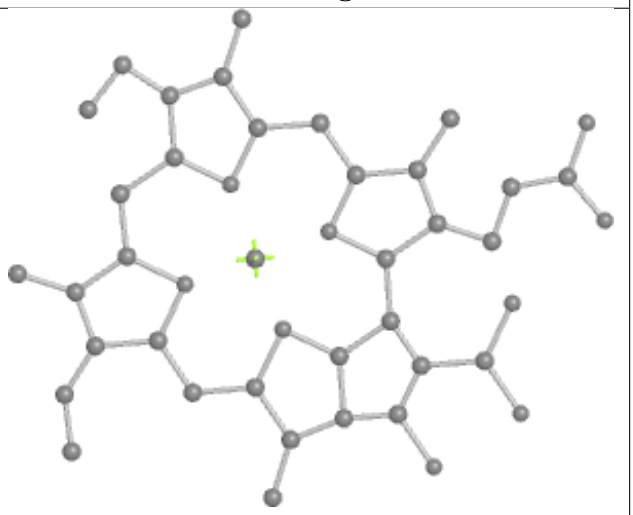
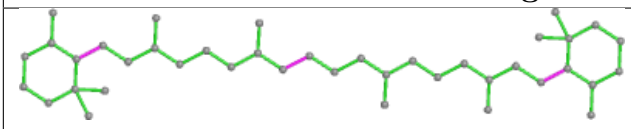


Rings

Ligand BCR H 201



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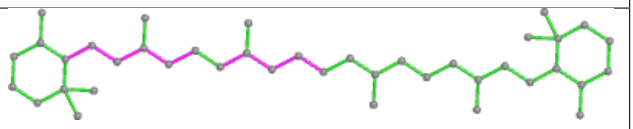
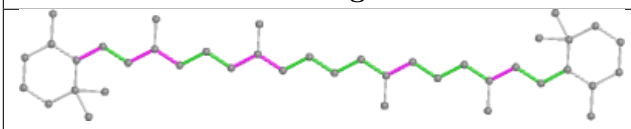
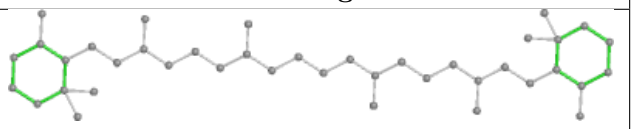


Bond angles

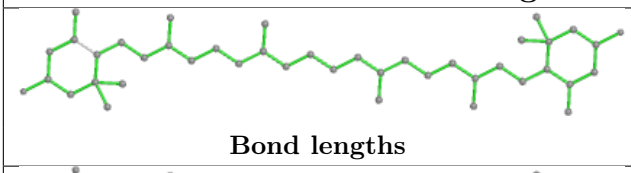


Torsions

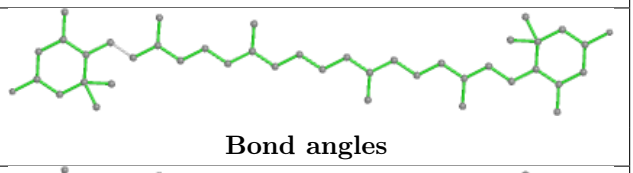


Rings

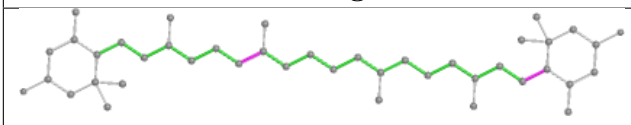
Ligand LUT 3 1001



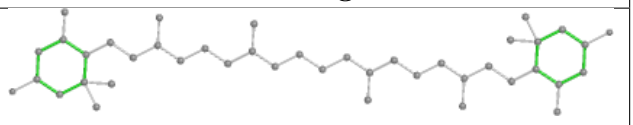
Bond lengths



Bond angles

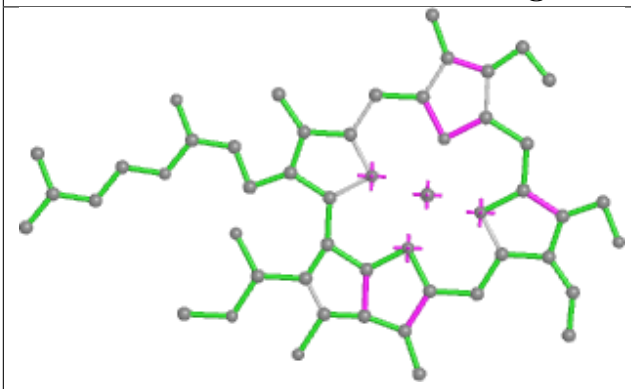


Torsions

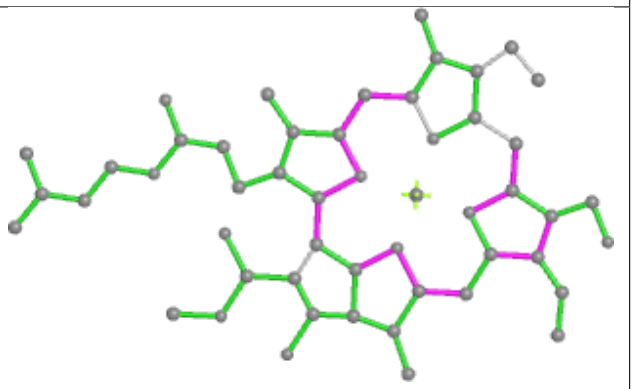


Rings

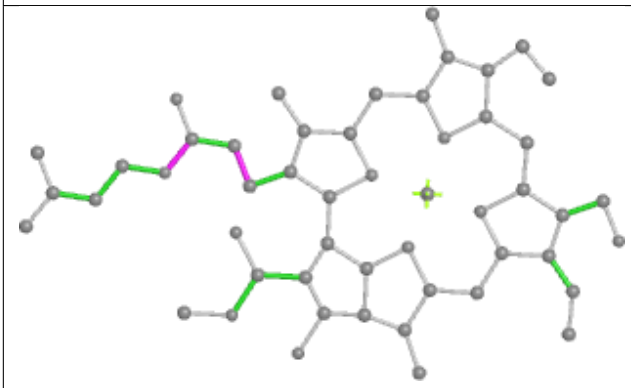
Ligand CHL 5 314



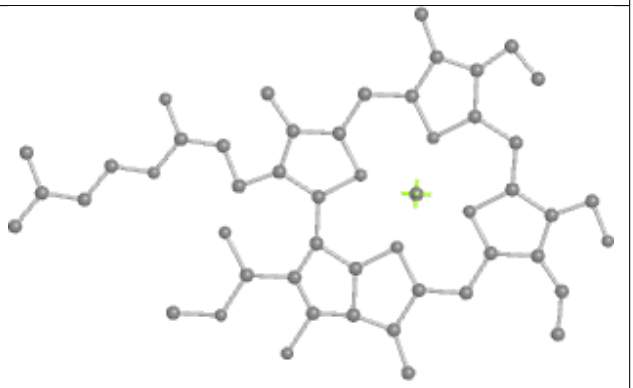
Bond lengths



Bond angles

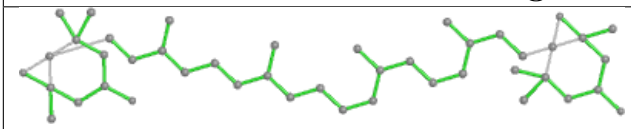


Torsions



Rings

Ligand XAT 5 303



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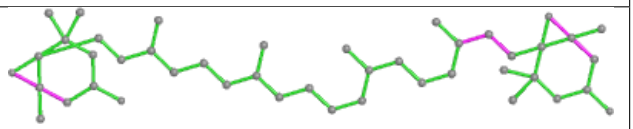
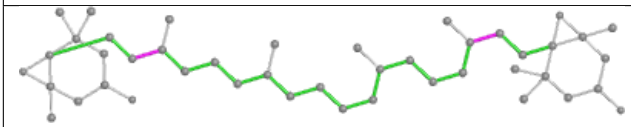


Bond angles



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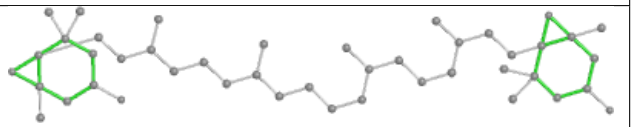
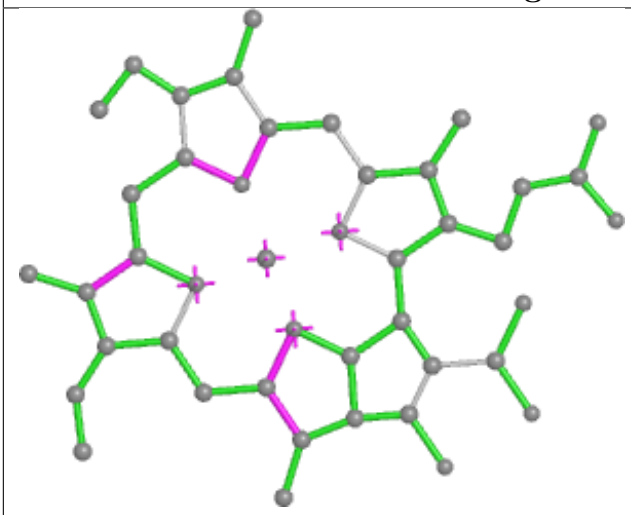


Rings

Ligand CLA B 839



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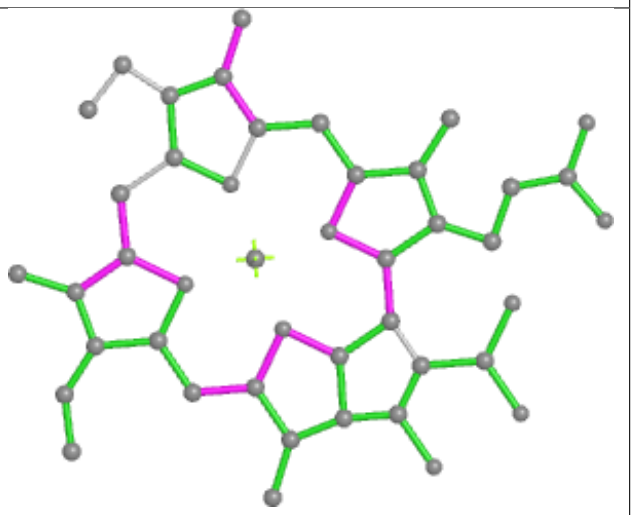
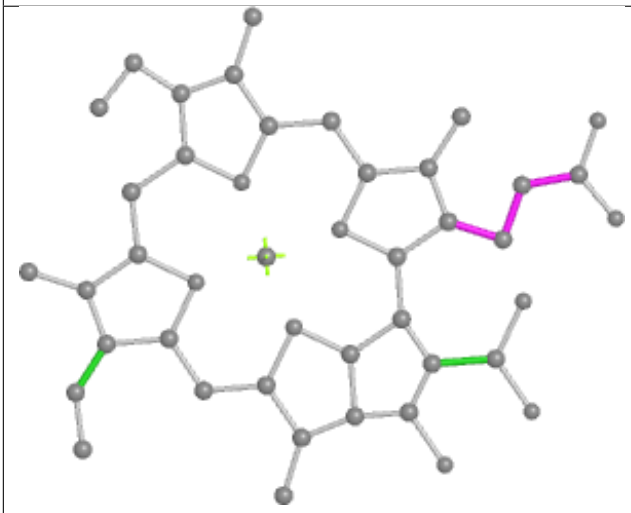


Bond angles



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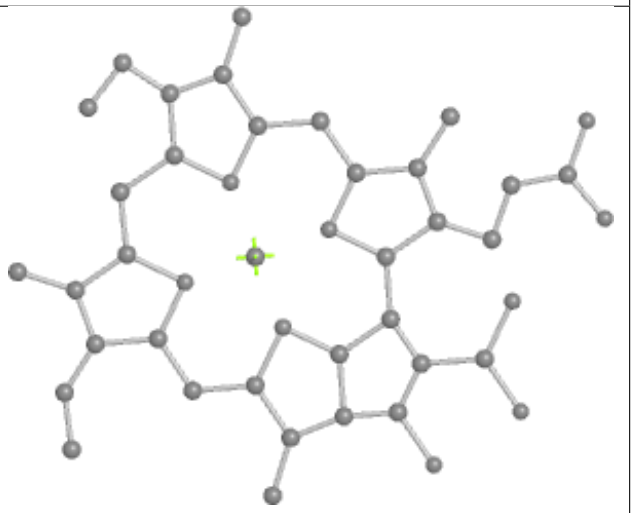
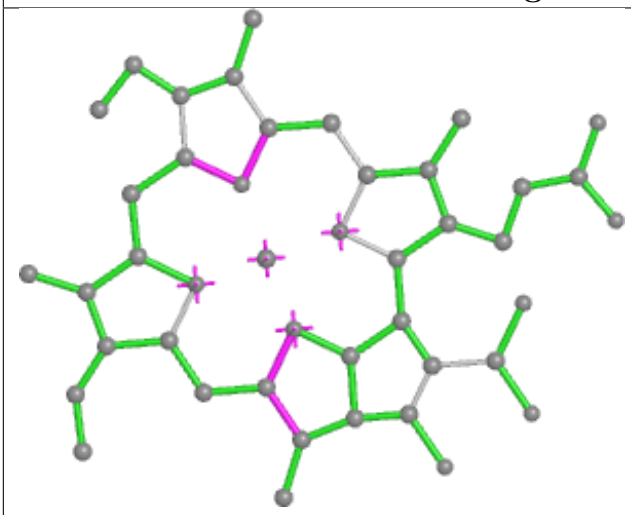
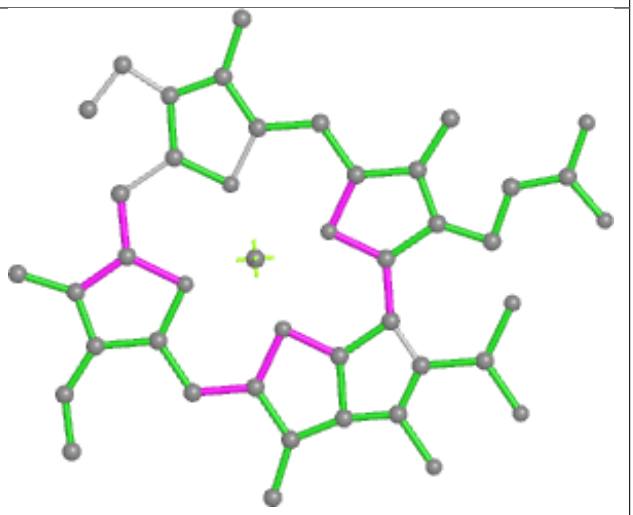


Rings

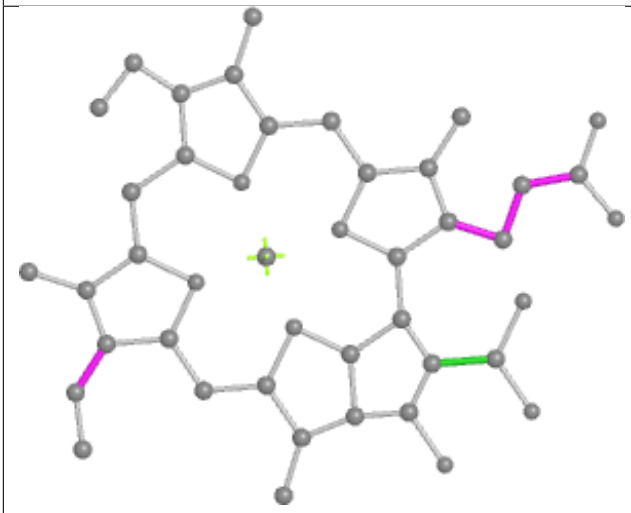
Ligand CLA B 841



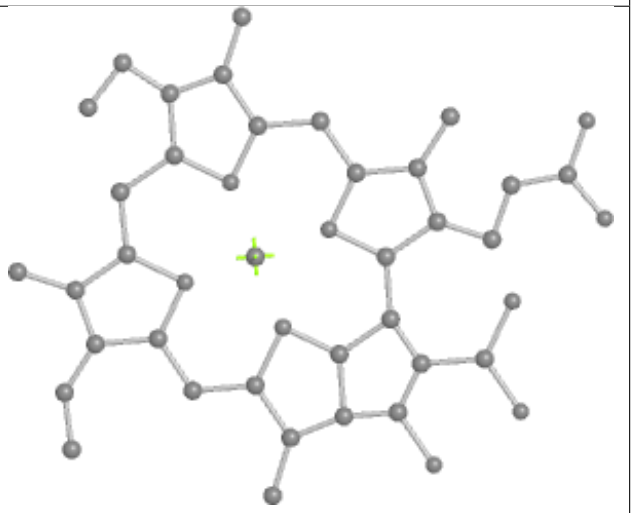
Bond lengths



Bond angles

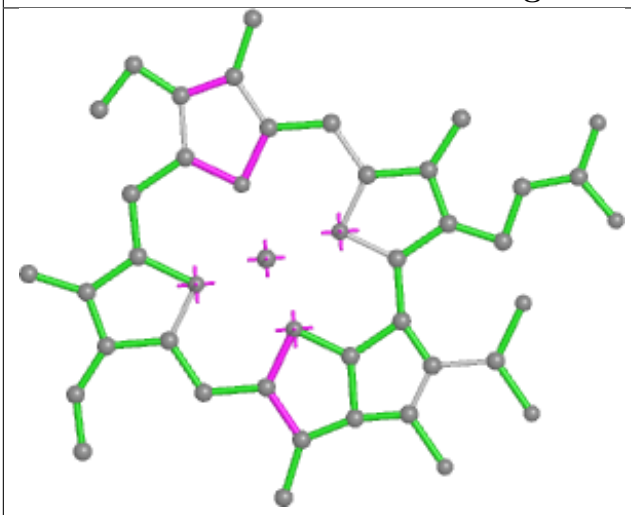


Torsions

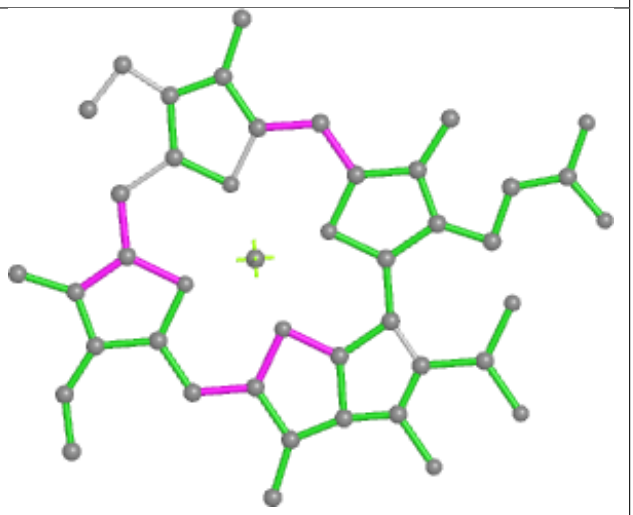


Rings

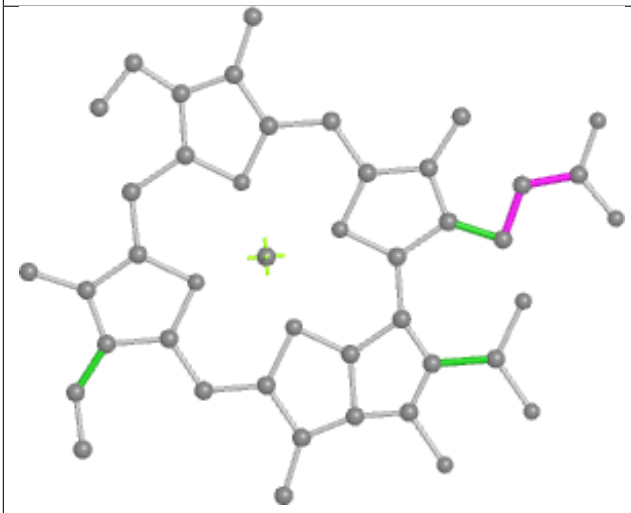
Ligand CLA A 840



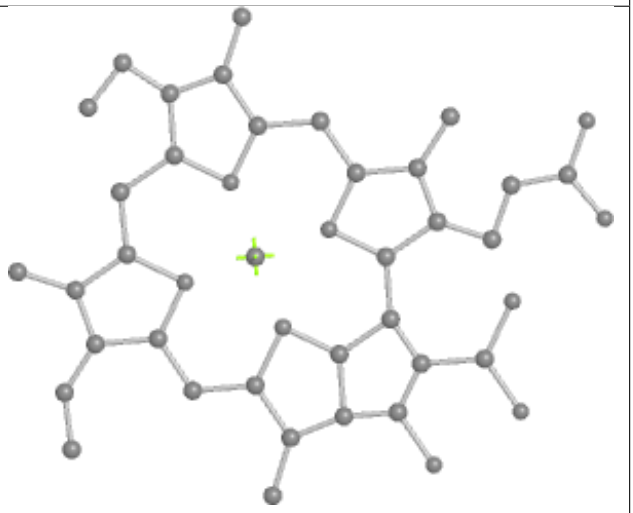
Bond lengths



Bond angles

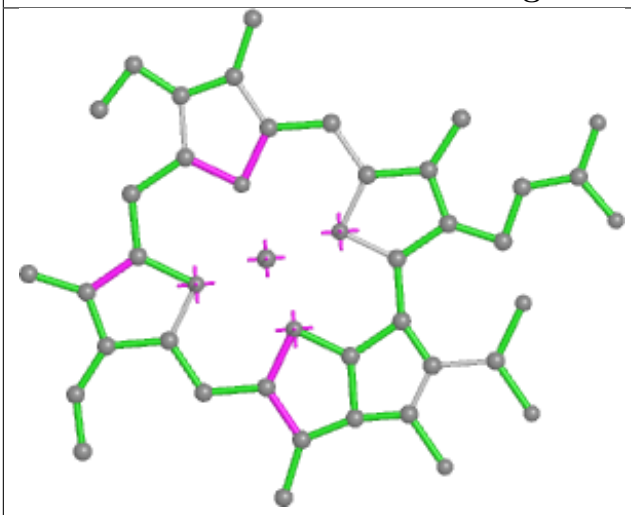


Torsions

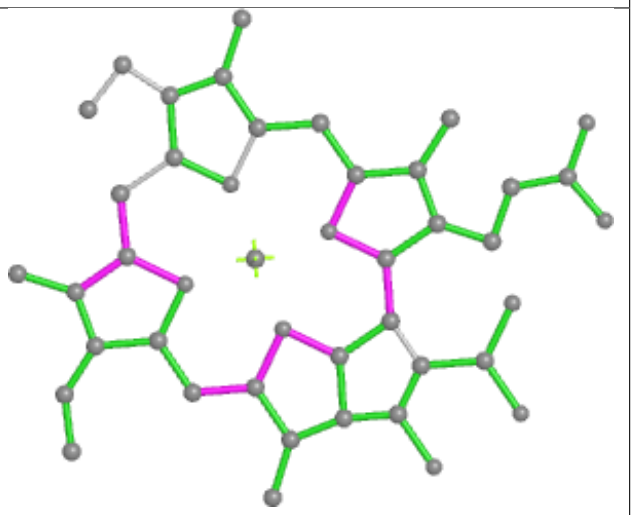


Rings

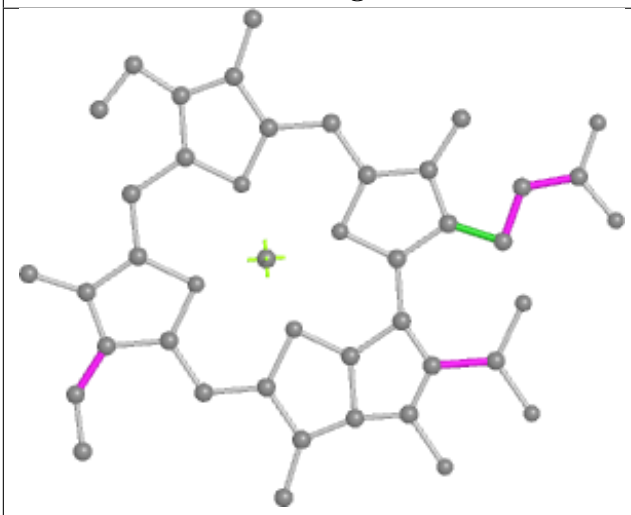
Ligand CLA G 203



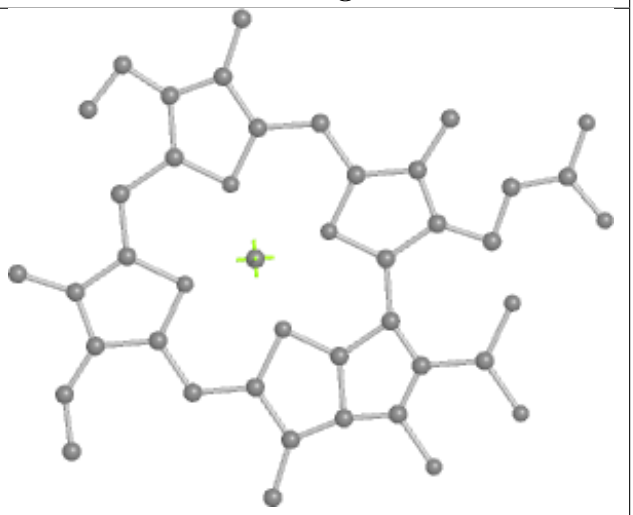
Bond lengths



Bond angles

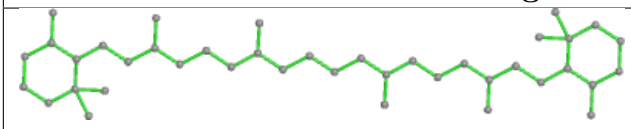


Torsions

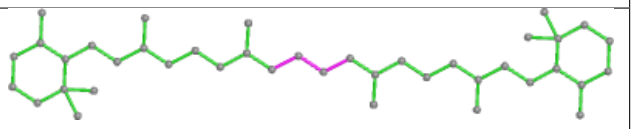


Rings

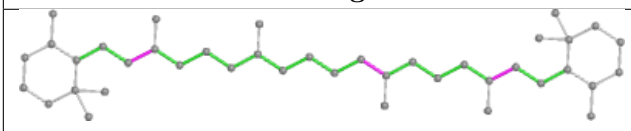
Ligand BCR A 846



Bond lengths



Bond angles



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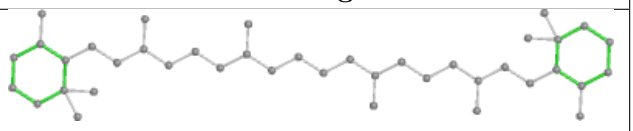
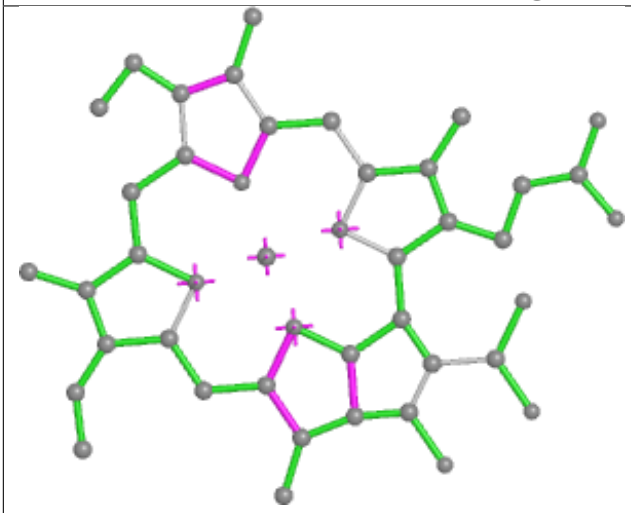


Rings

Ligand CLA 8 316



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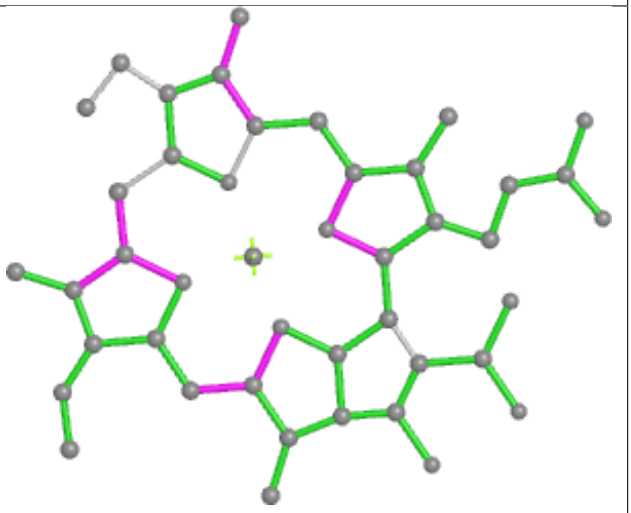

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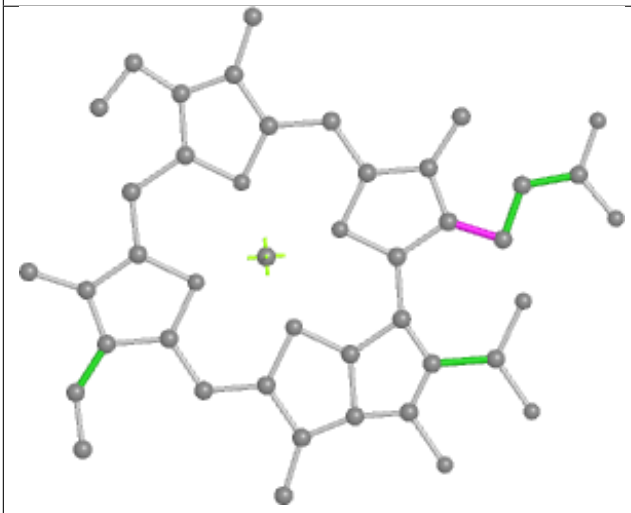

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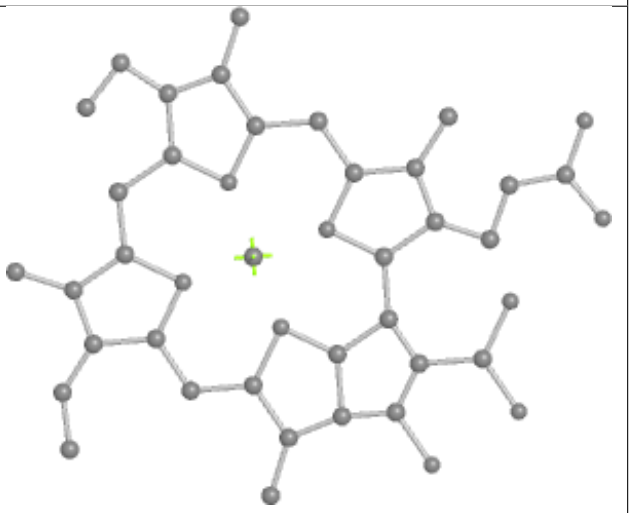
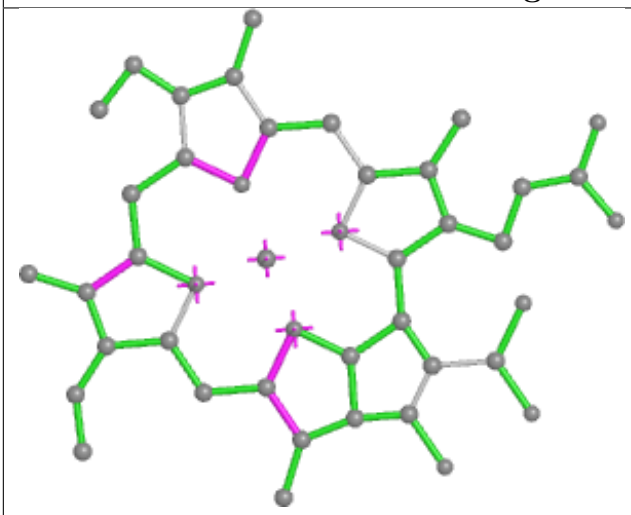


Rings

Ligand CLA A 812



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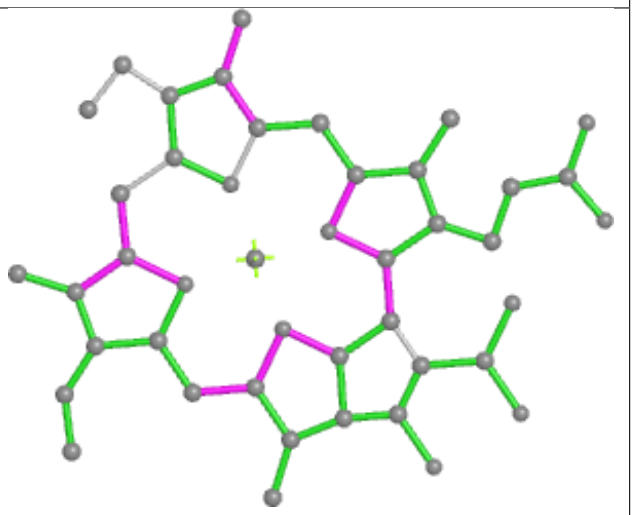

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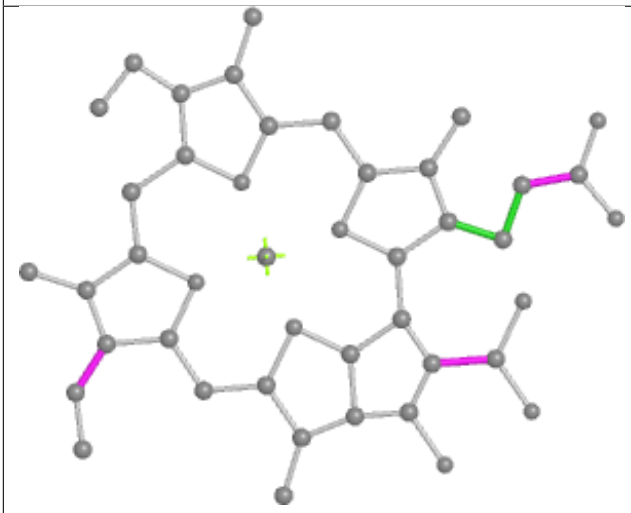

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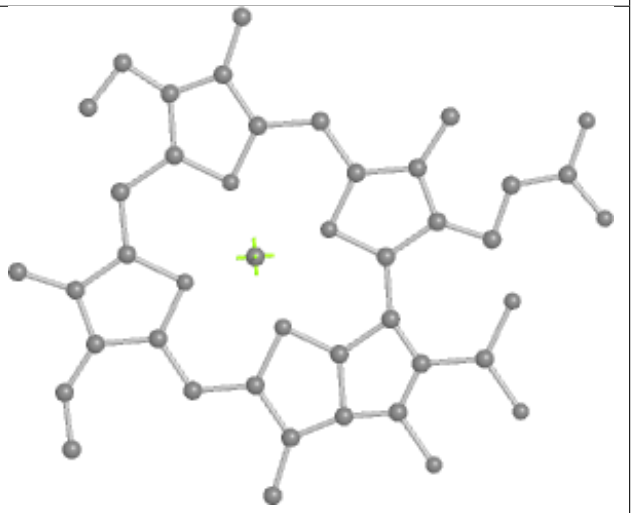
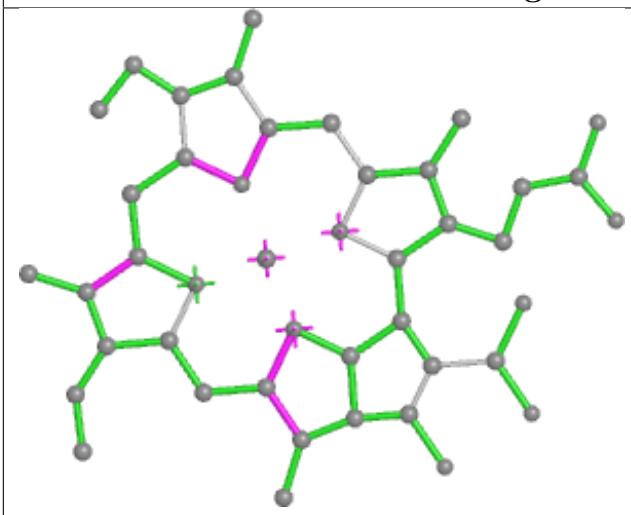


Rings

Ligand CLA B 830



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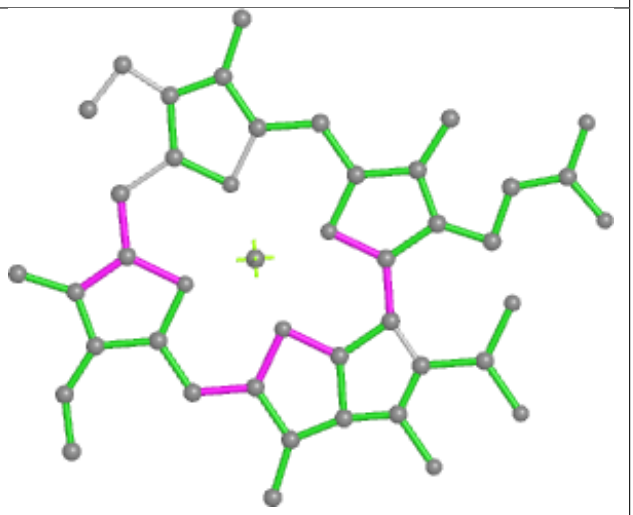

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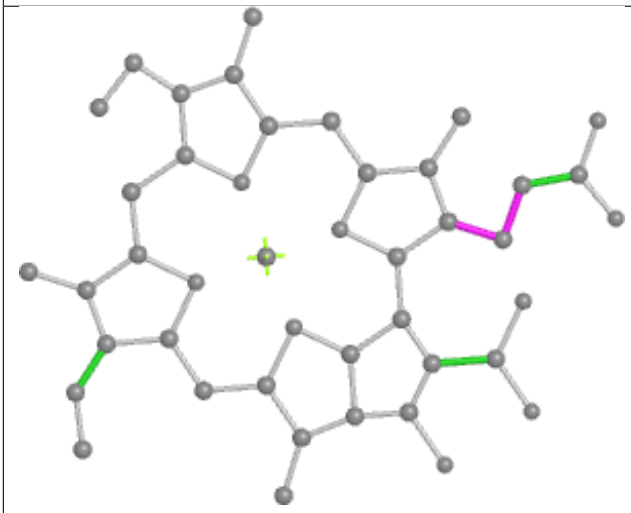

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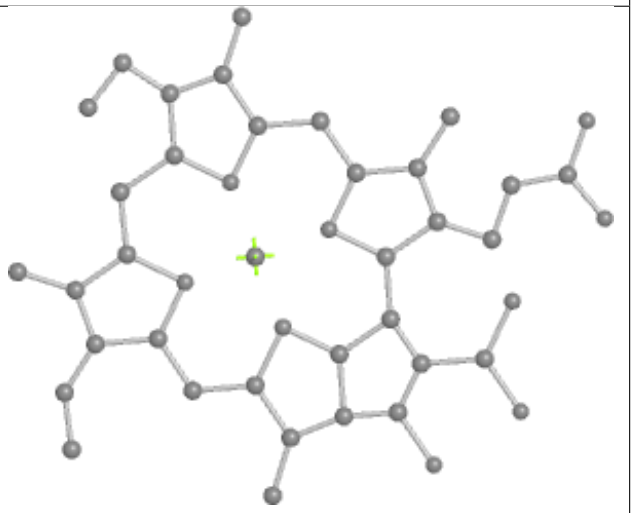
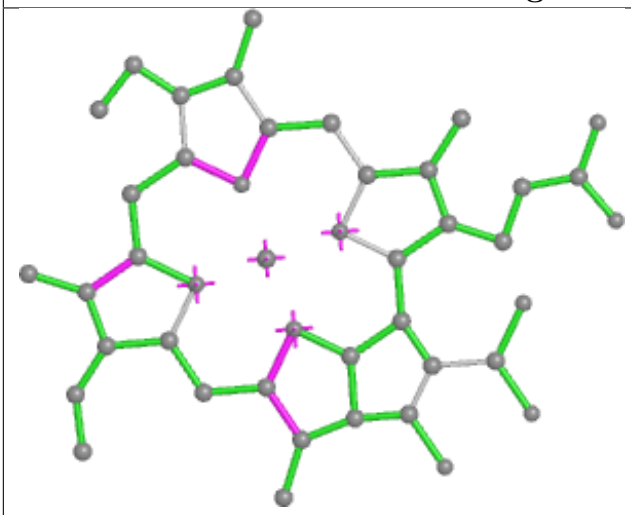


Rings

Ligand CLA L 204



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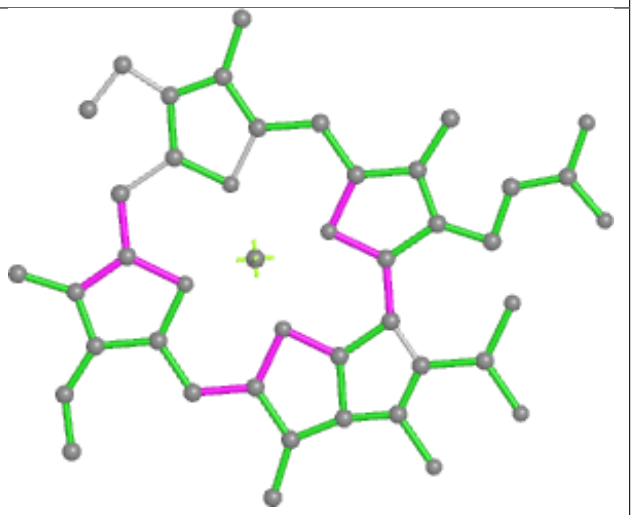

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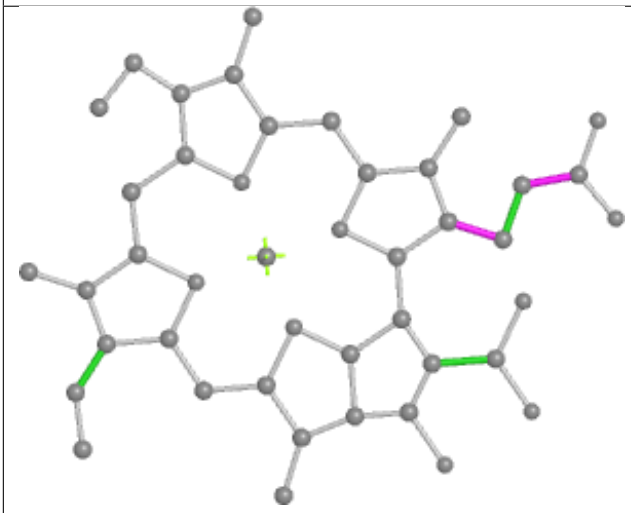

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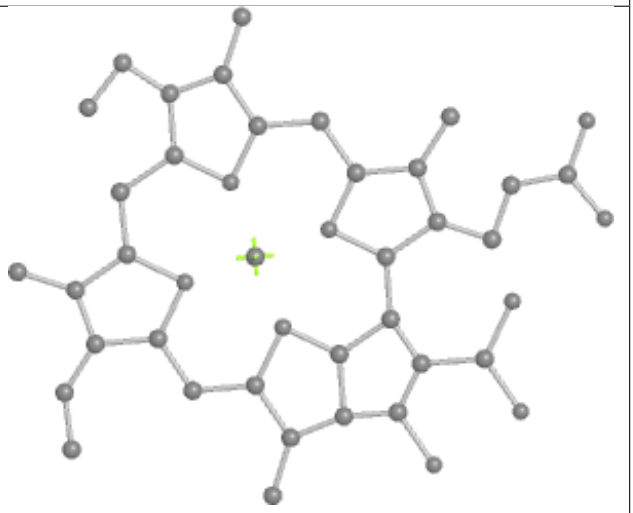
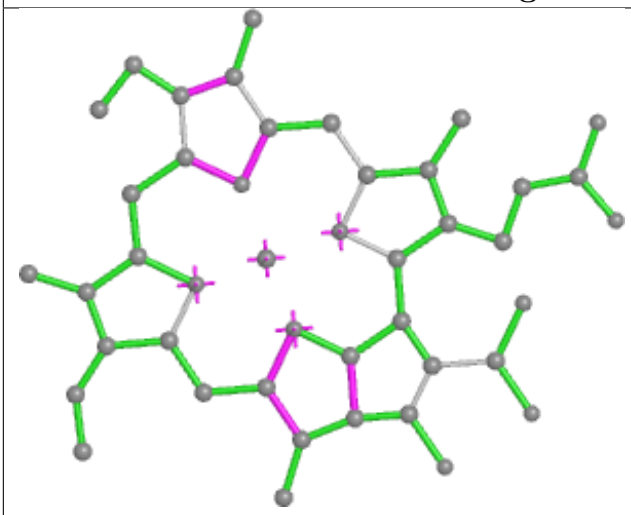


Rings

Ligand CLA 7 1009



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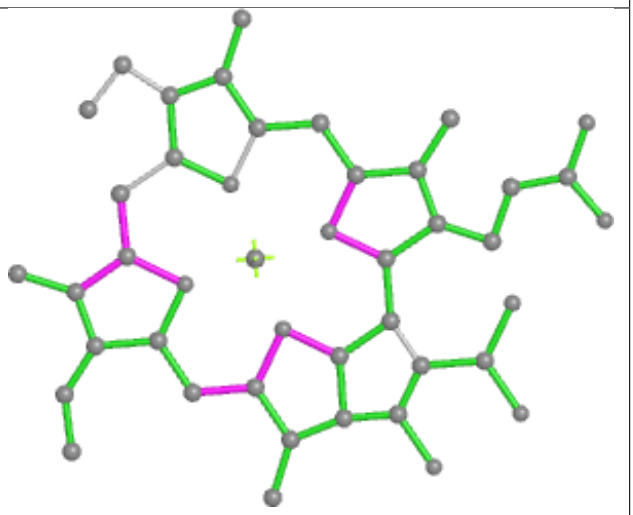
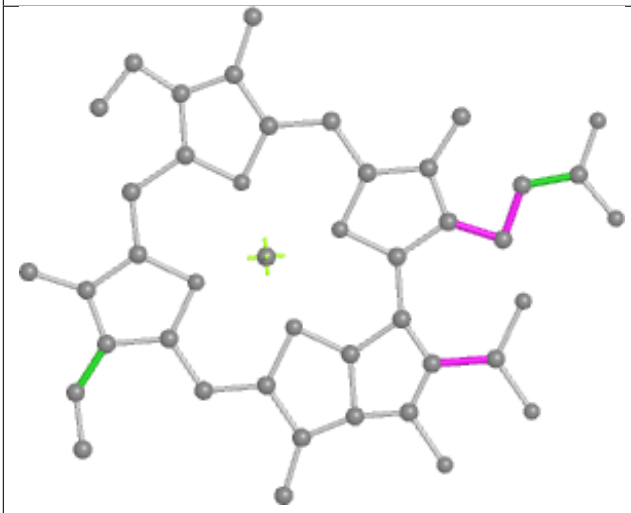


Bond angles



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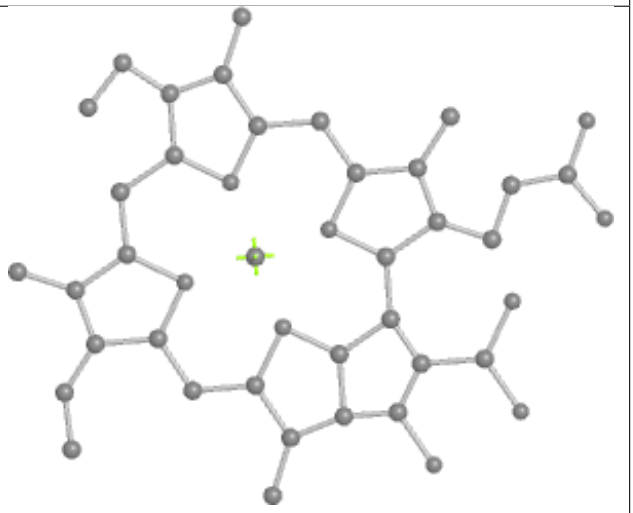
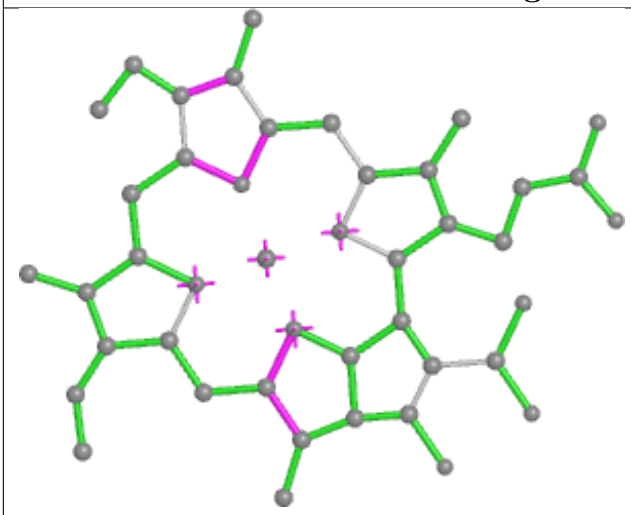


Rings

Ligand CLA A 815



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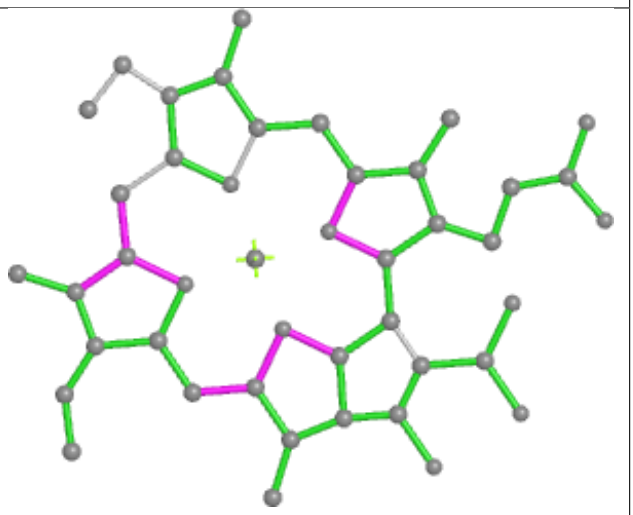

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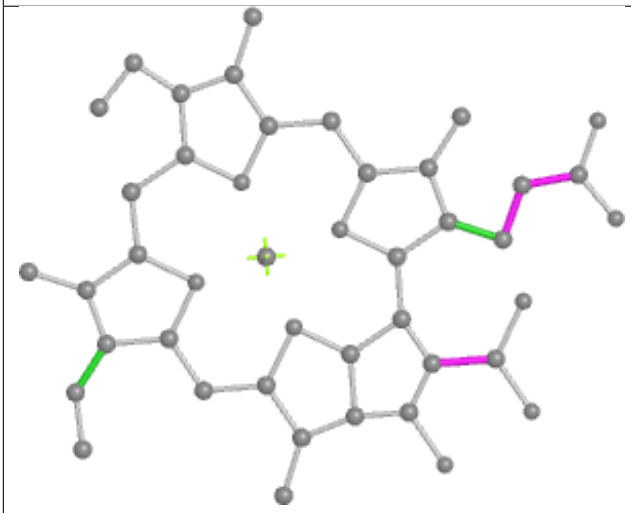

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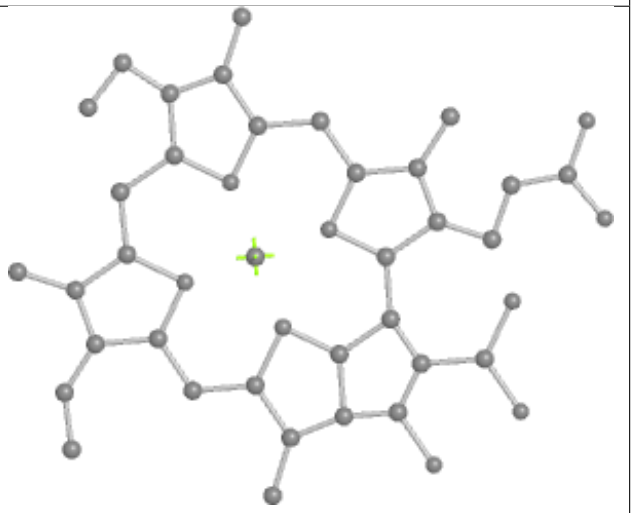
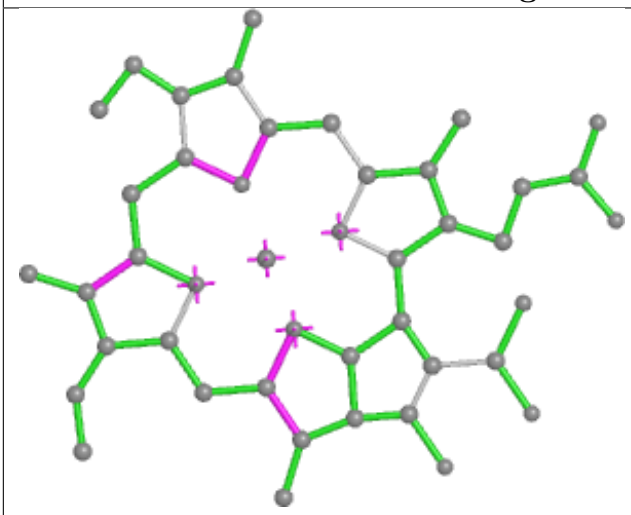


Rings

Ligand CLA 1 1003



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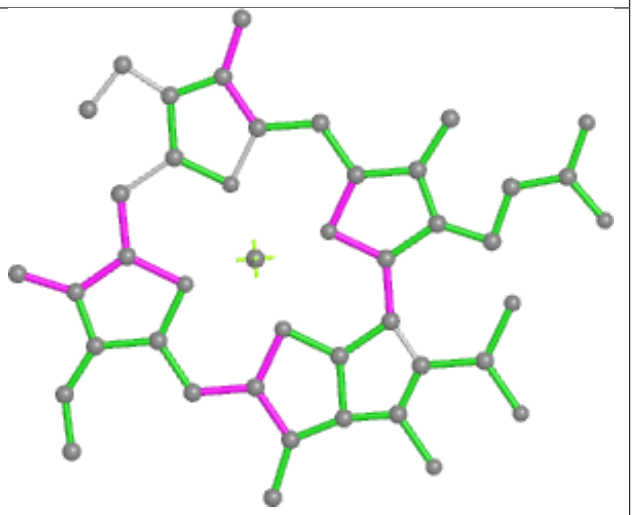
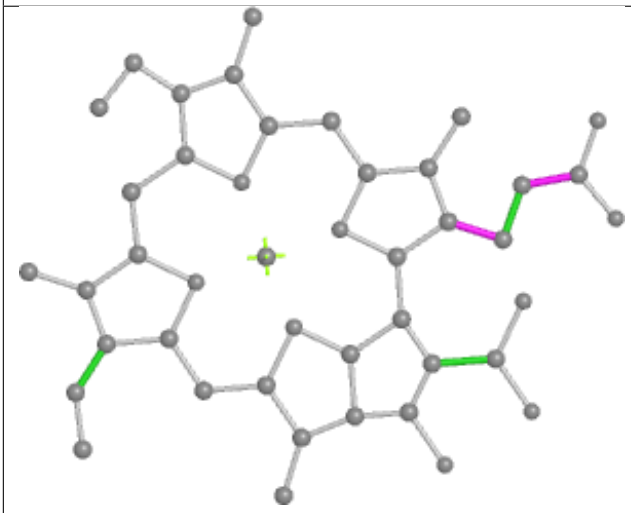


Bond angles



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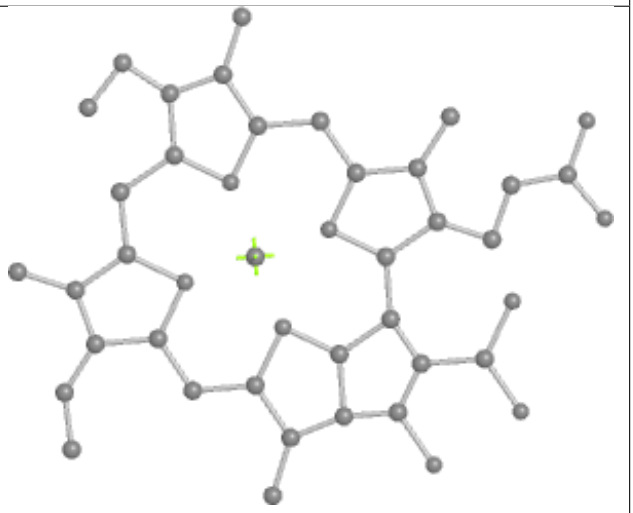
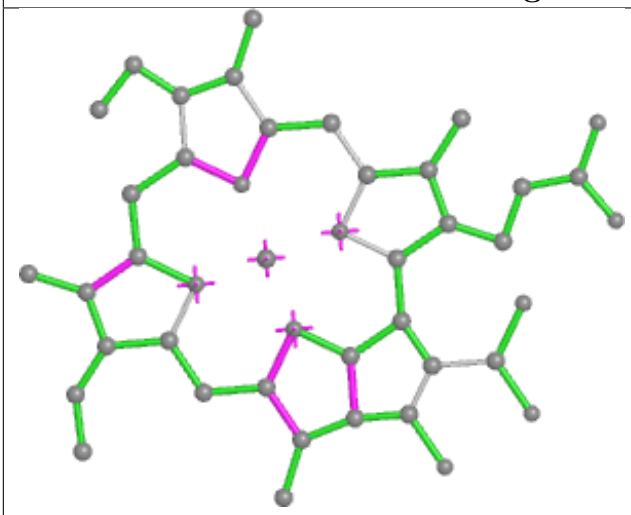


Rings

Ligand CLA A 804



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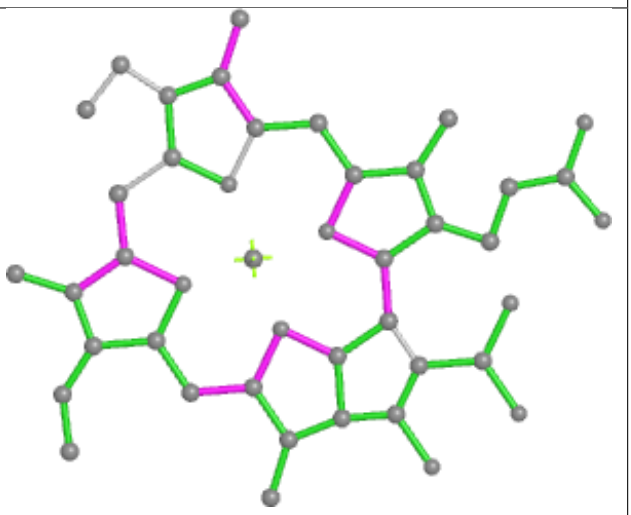
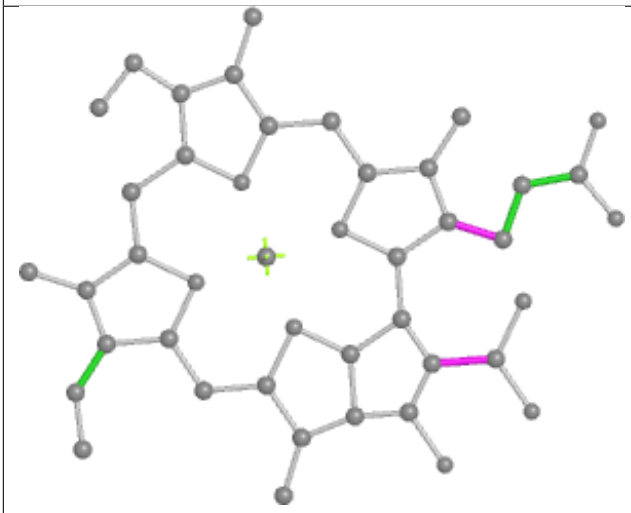


Bond angles



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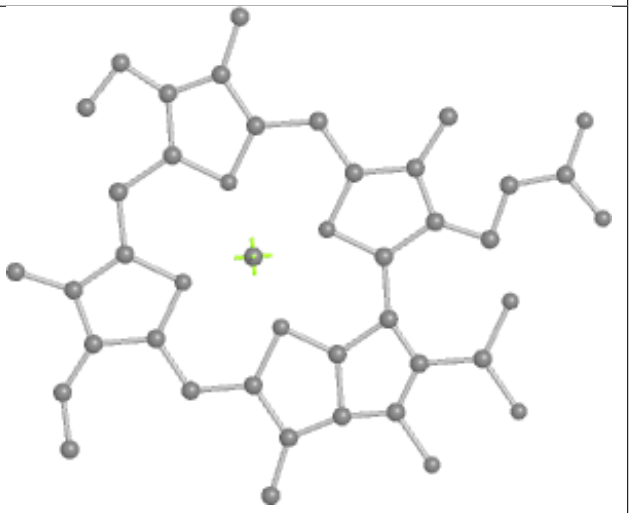
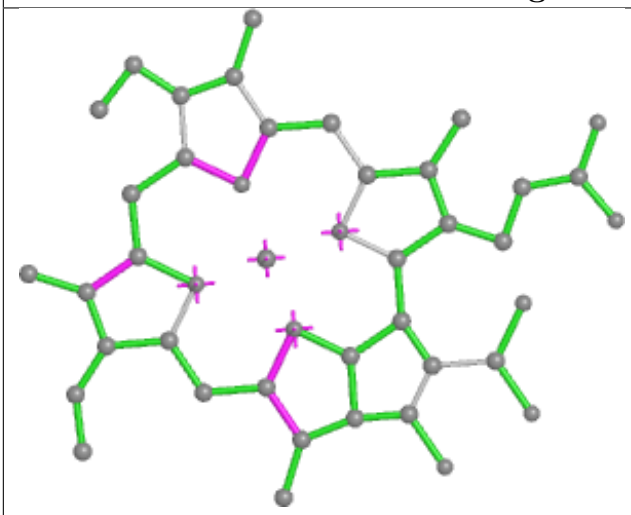


Rings

Ligand CLA 0 310



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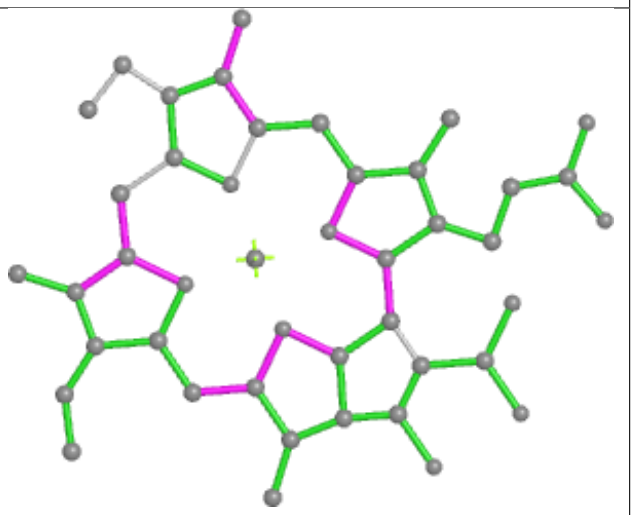
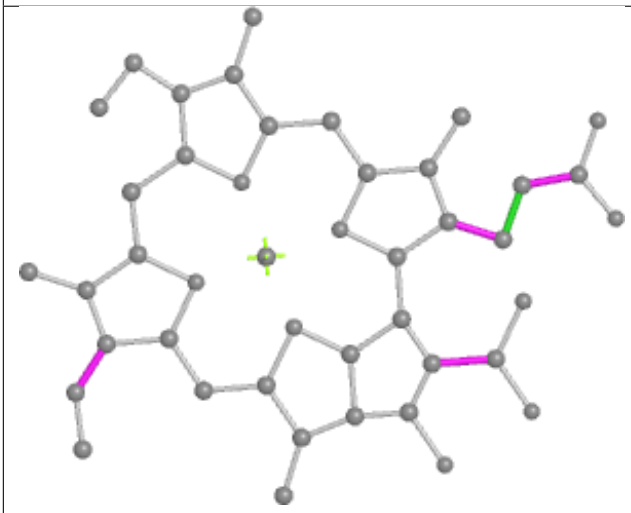


Bond angles



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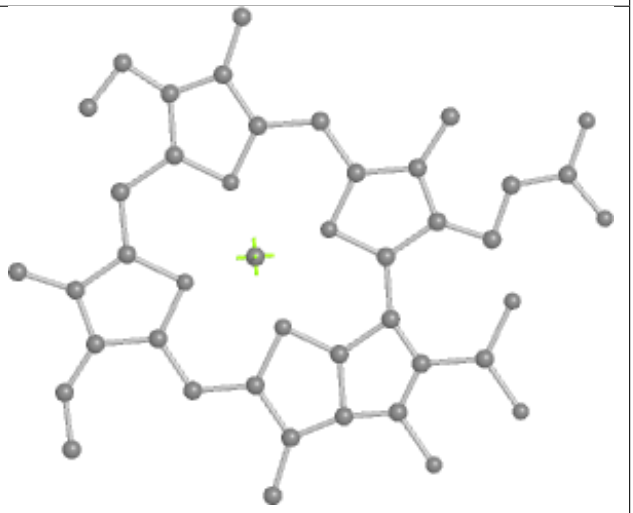
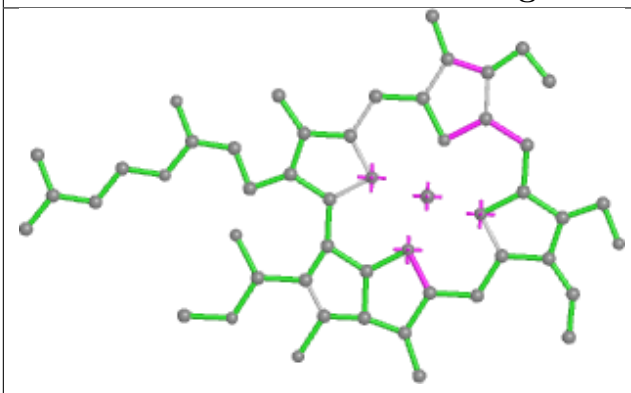


Rings

Ligand CHL 1 1013



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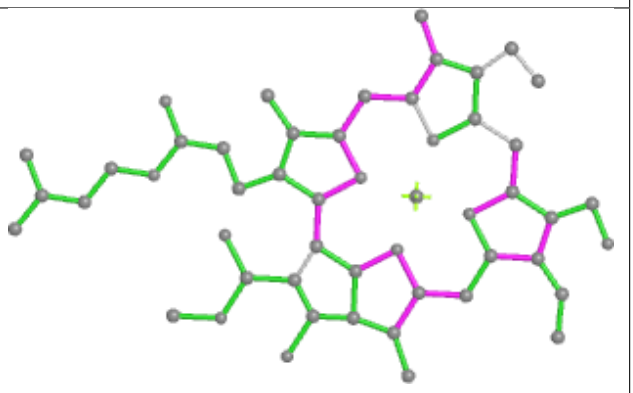

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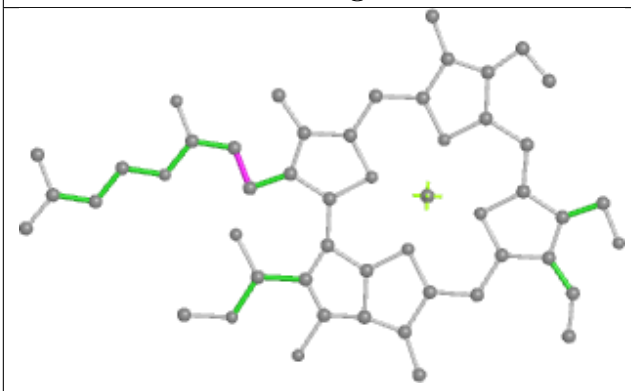

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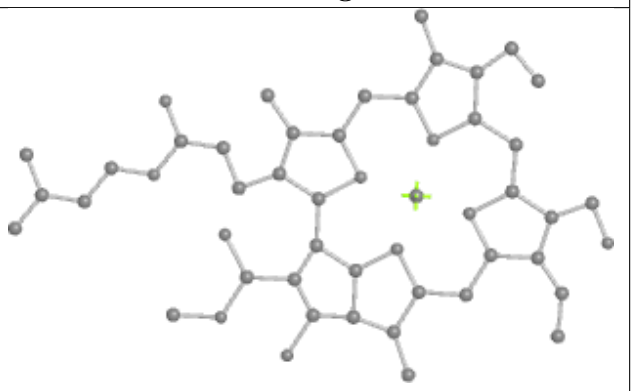
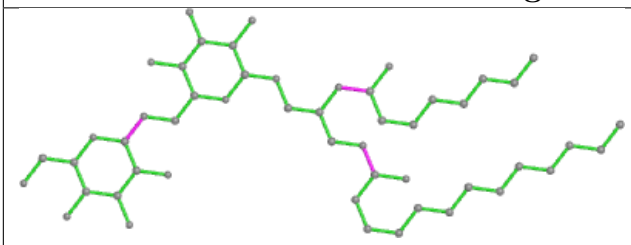


Rings

Ligand DGD 5 319



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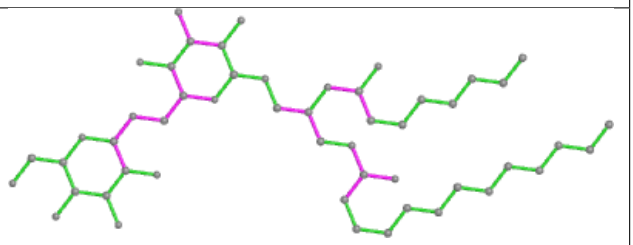
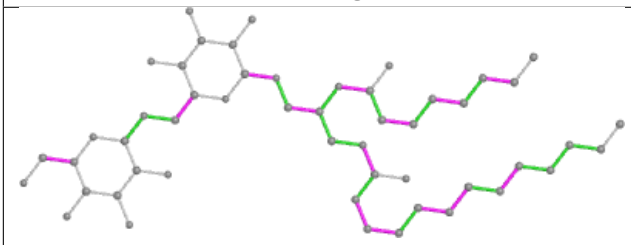


Bond angles



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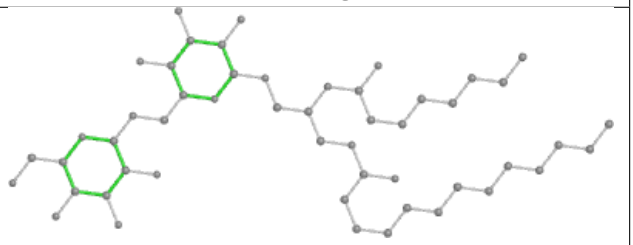
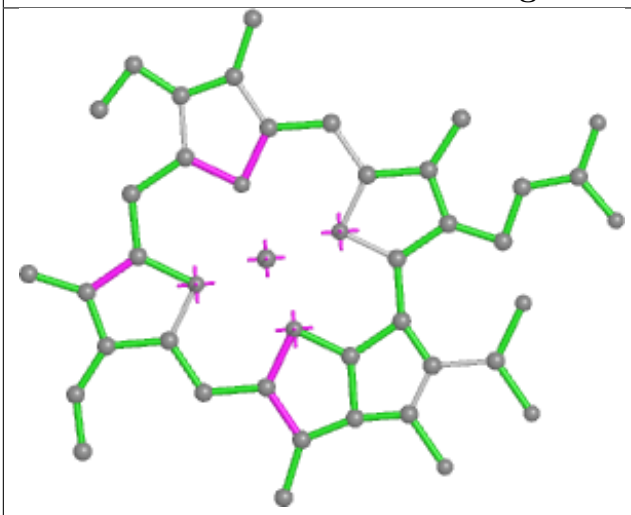


Rings

Ligand CLA 3 1012



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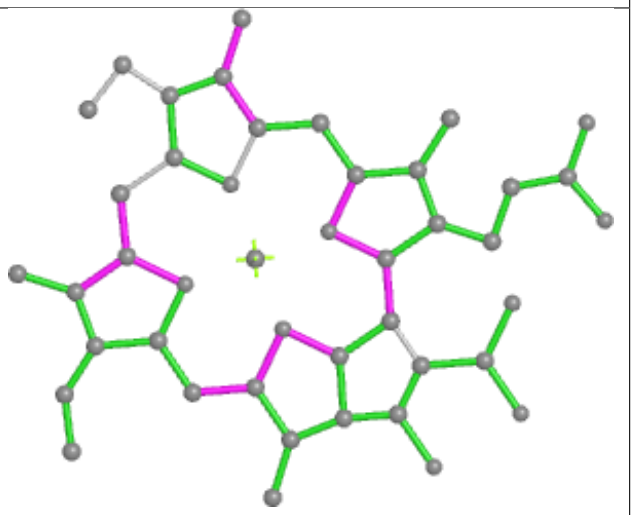
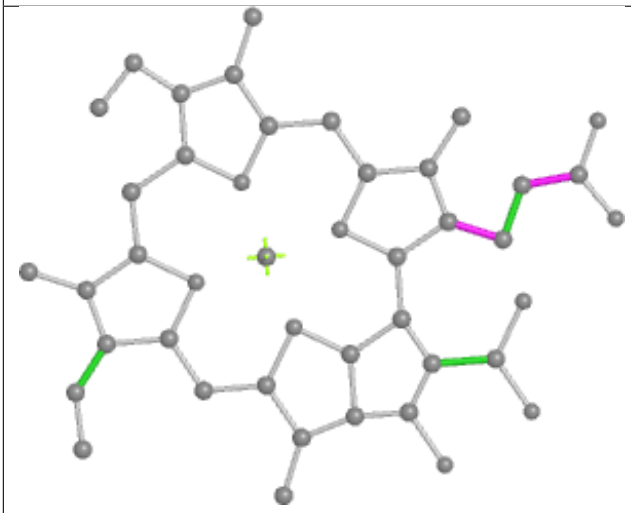


Bond angles



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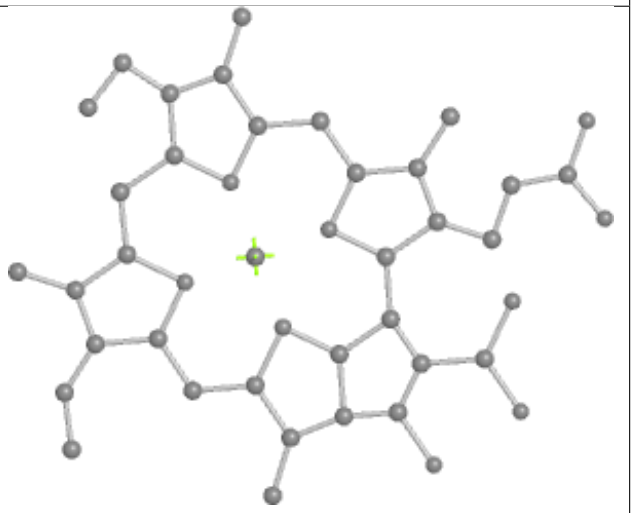
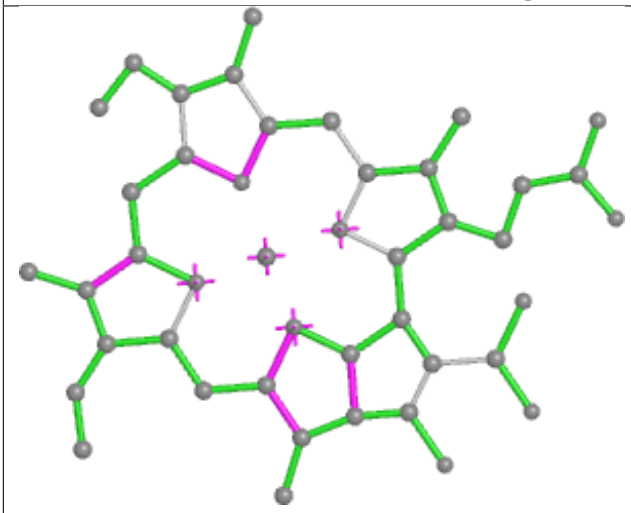


Rings

Ligand CLA 3 1005



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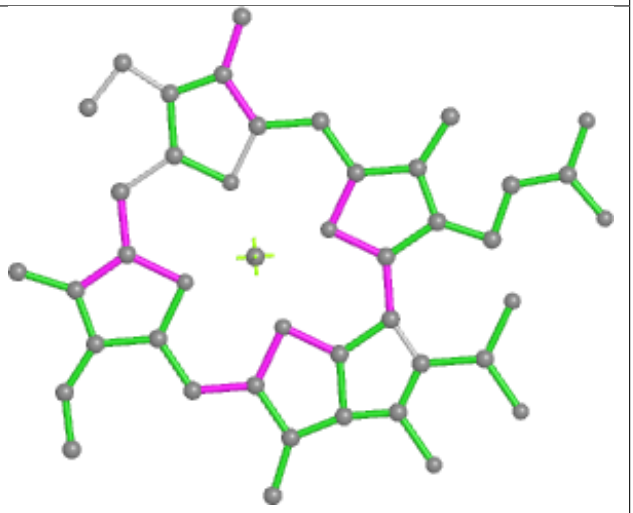
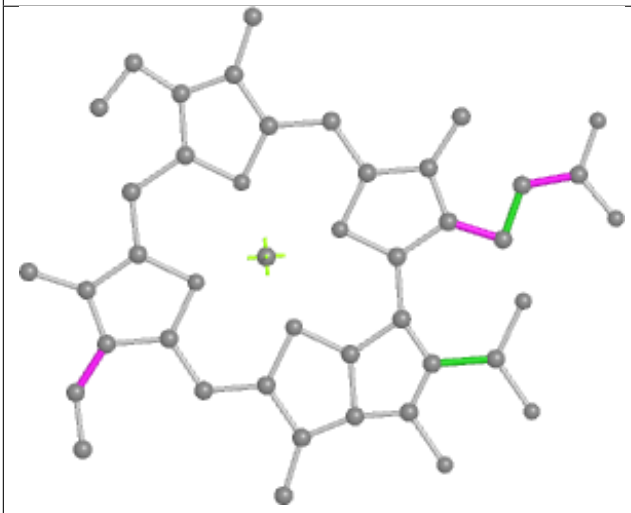


Bond angles



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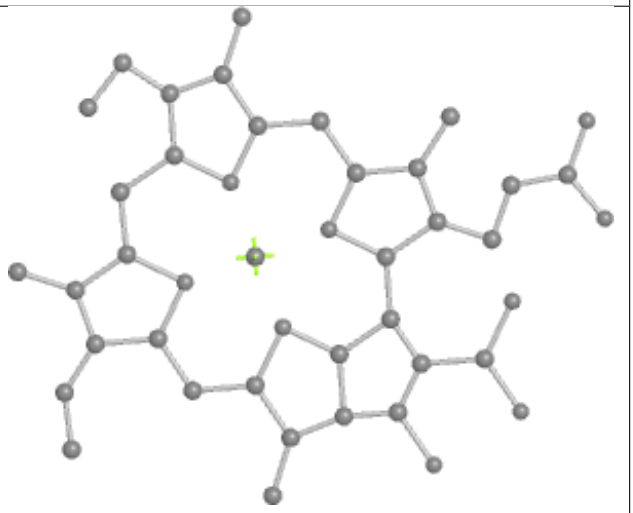
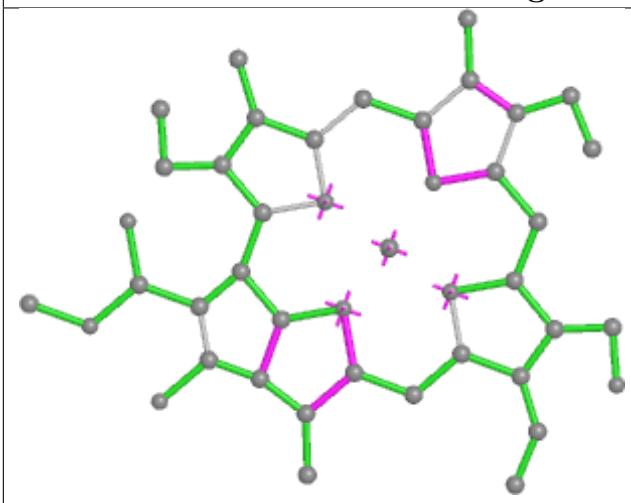


Rings

Ligand CHL 5 317



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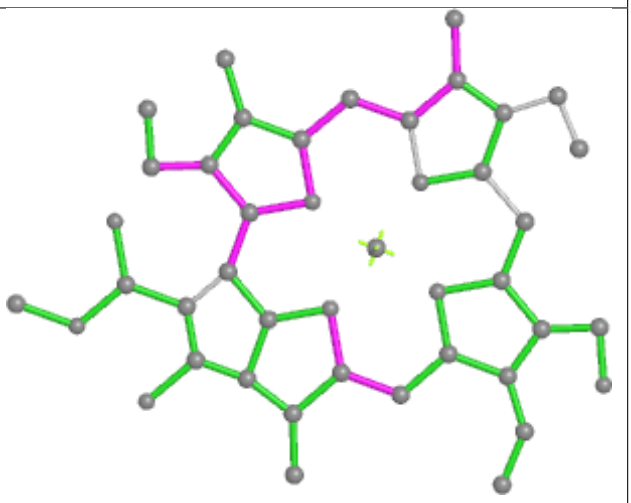
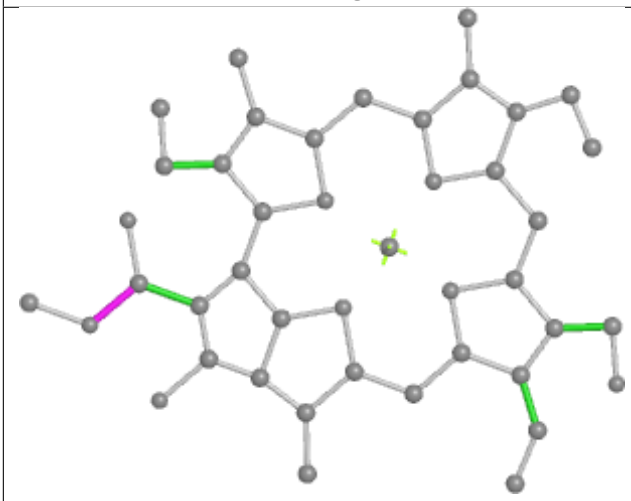
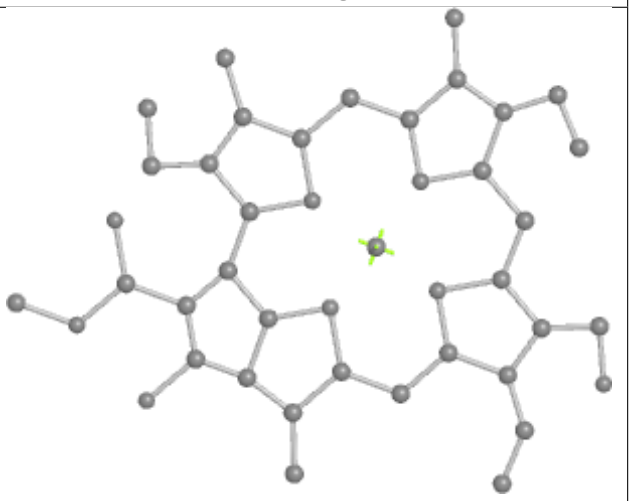


Bond angles

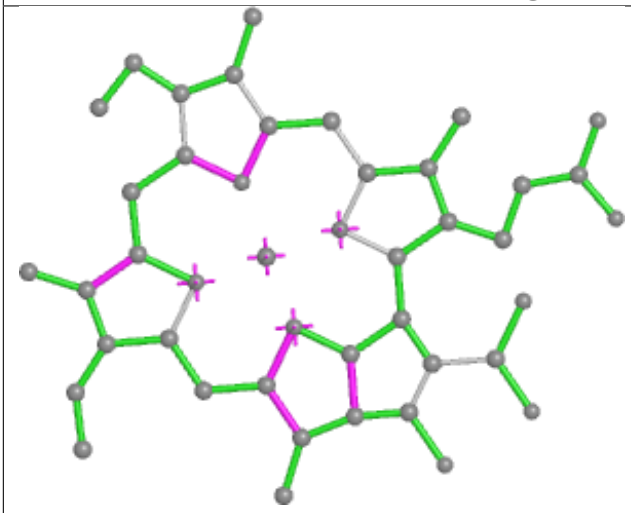


Torsions



Rings

Ligand CLA B 832



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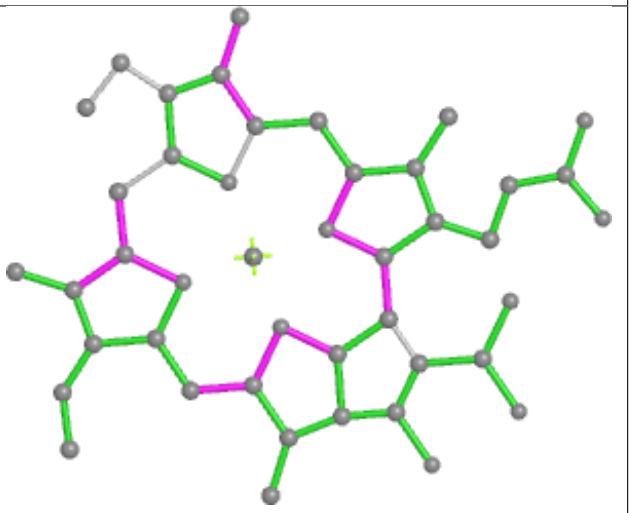

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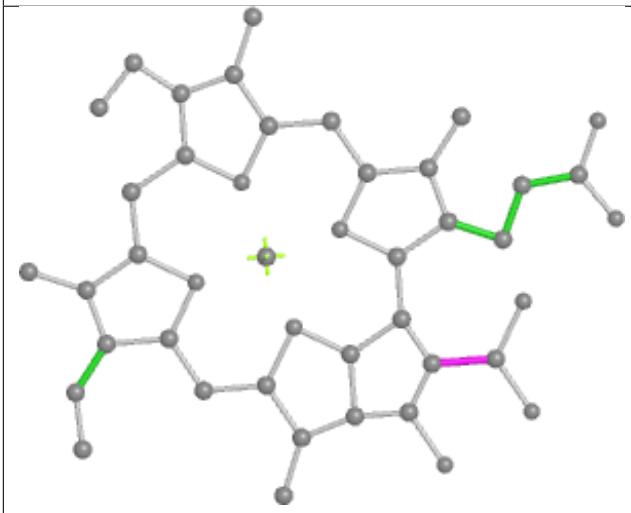

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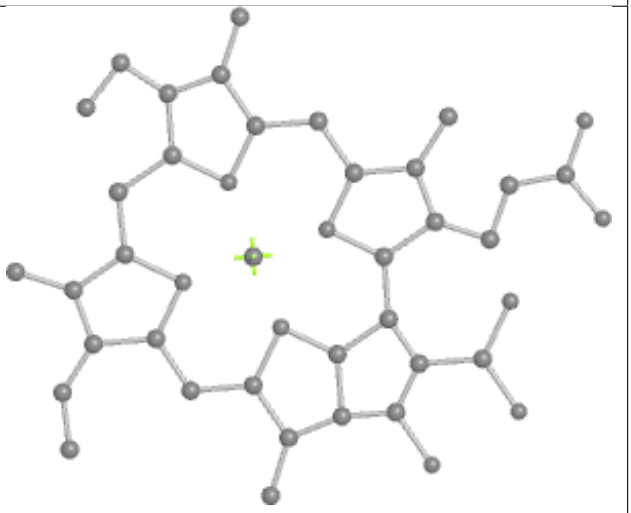
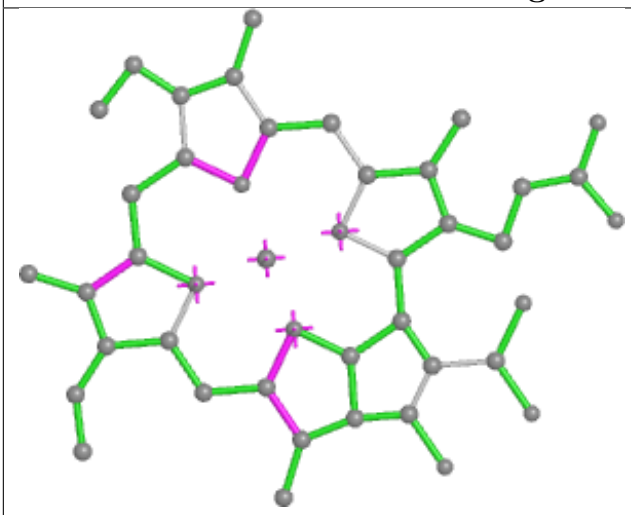


Rings

Ligand CLA 5 304



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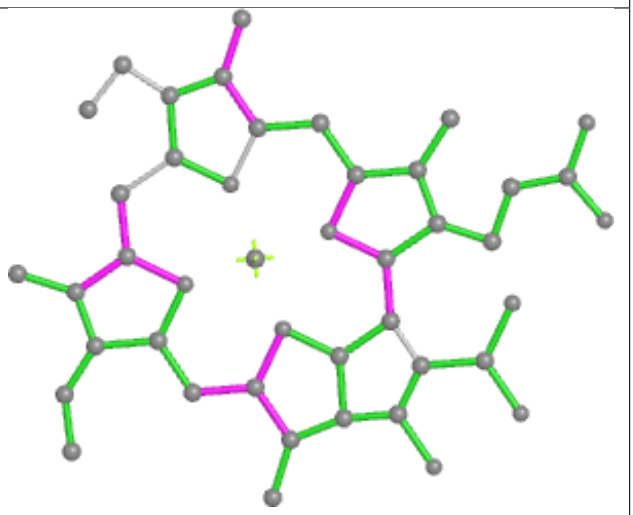
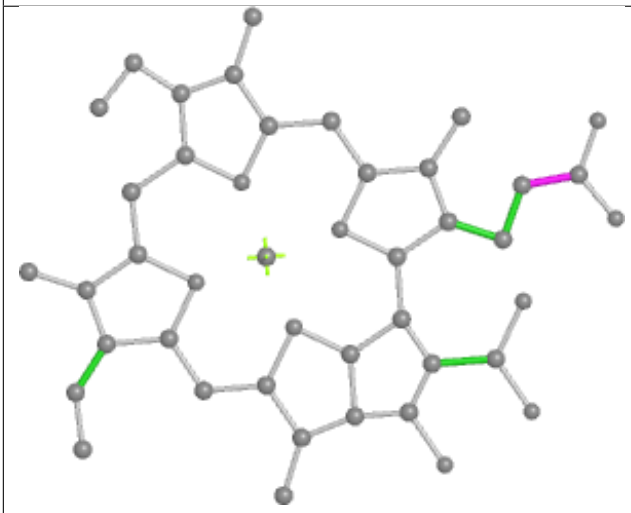


Bond angles



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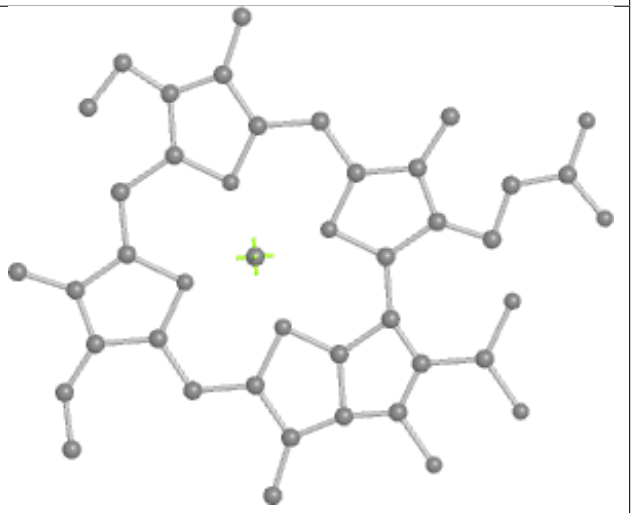
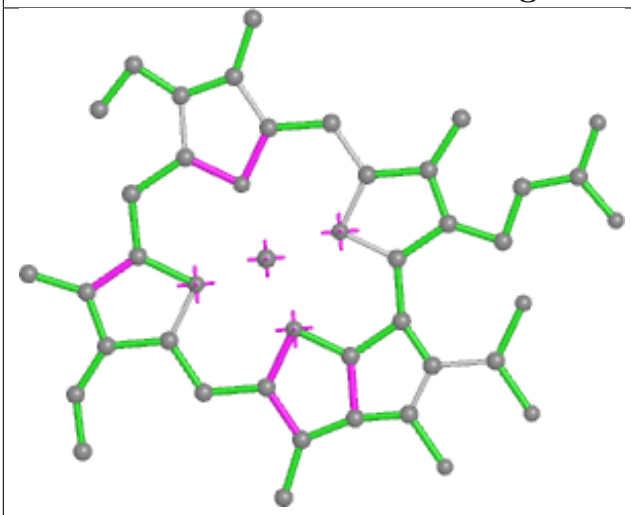


Rings

Ligand CLA 7 1011



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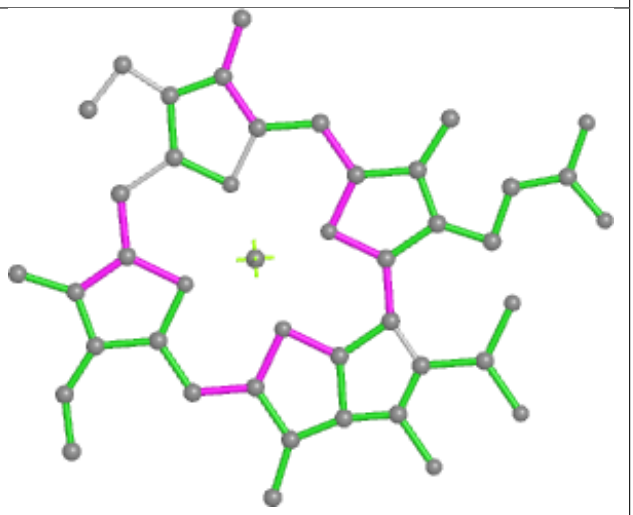

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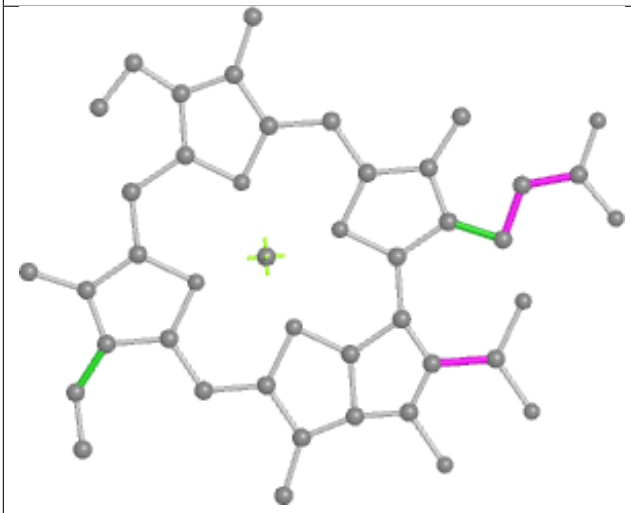

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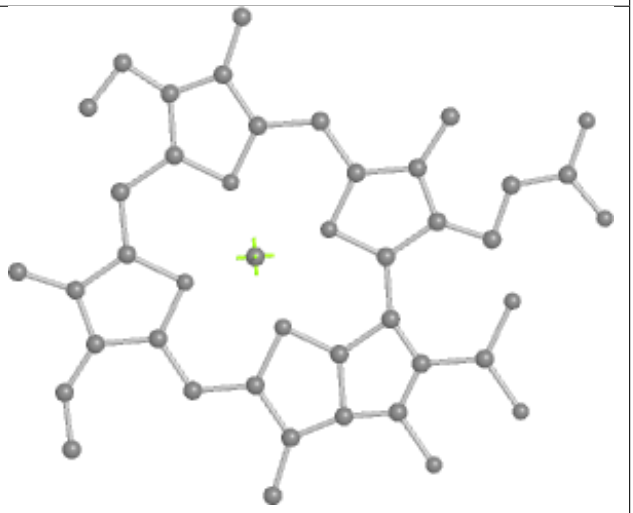
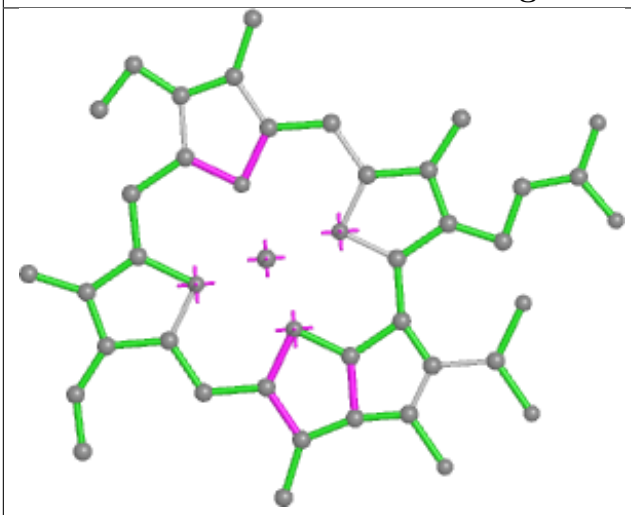


Rings

Ligand CLA 3 1016



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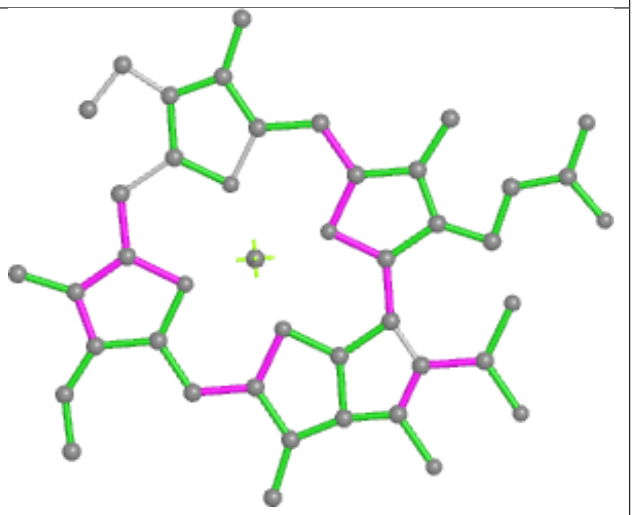

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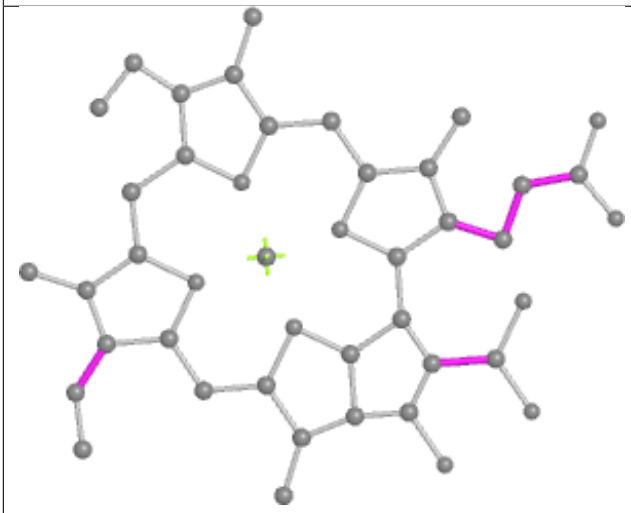

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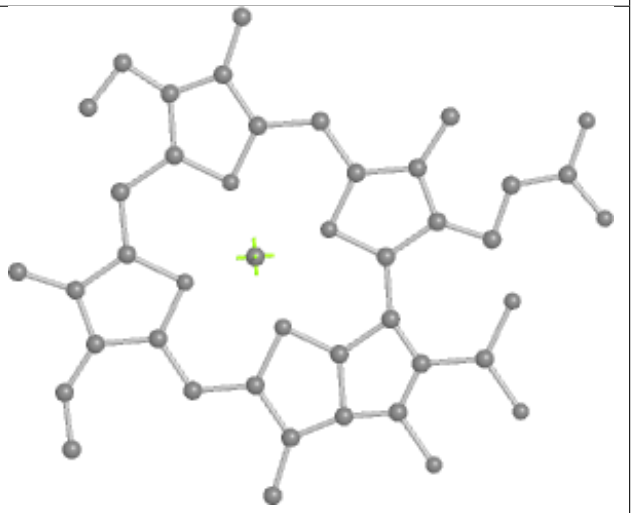
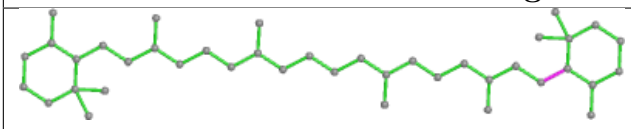


Rings

Ligand BCR F 301



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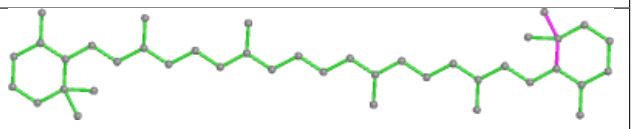

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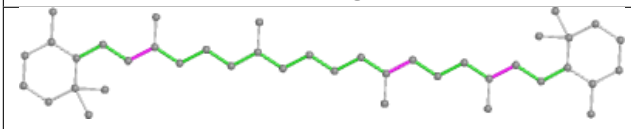
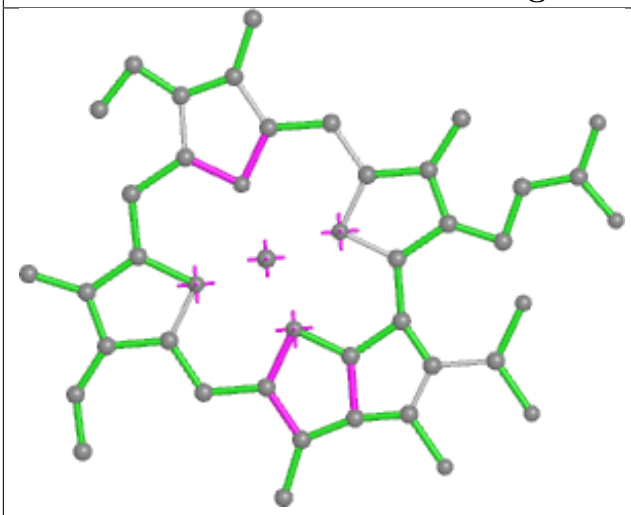


Torsions

Rings

Ligand CLA 6 309



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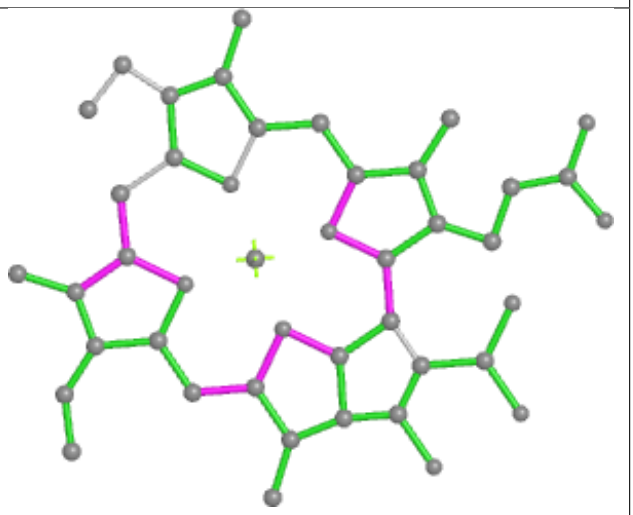

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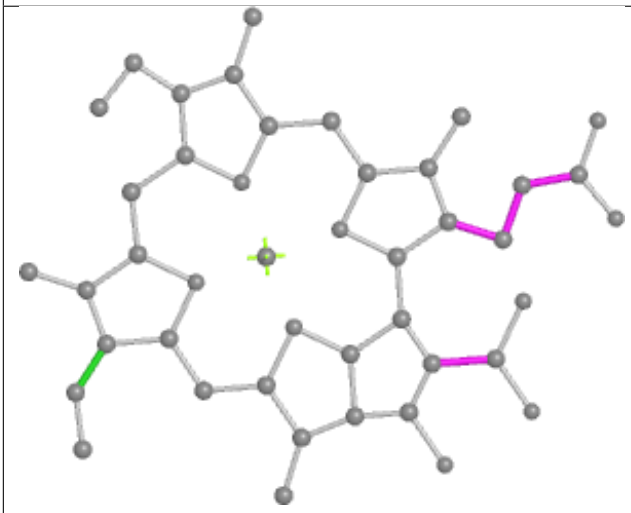

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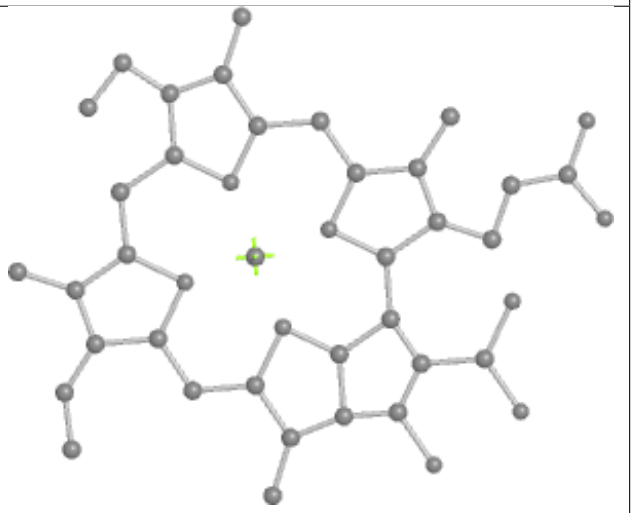
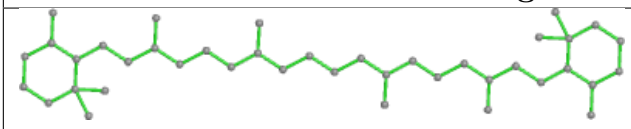


Rings

Ligand BCR 3 1003



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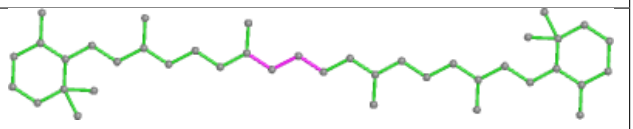

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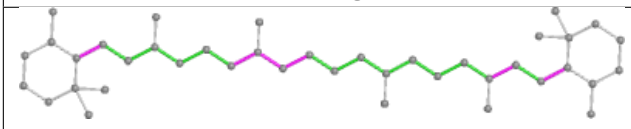
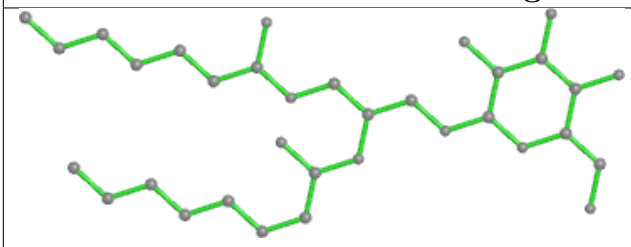


Torsions

Rings

Ligand LMG 4 318



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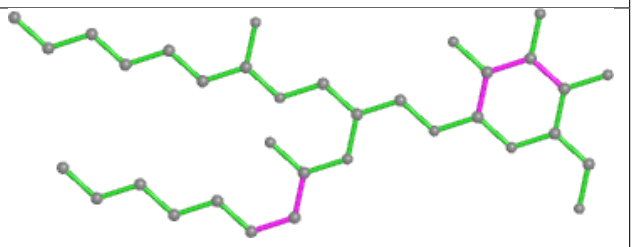

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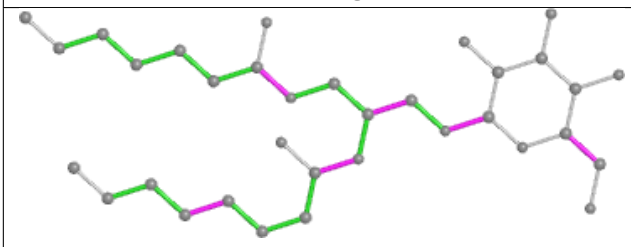

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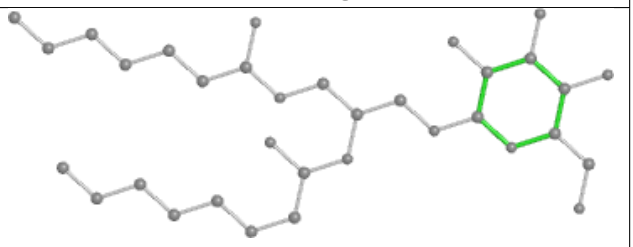
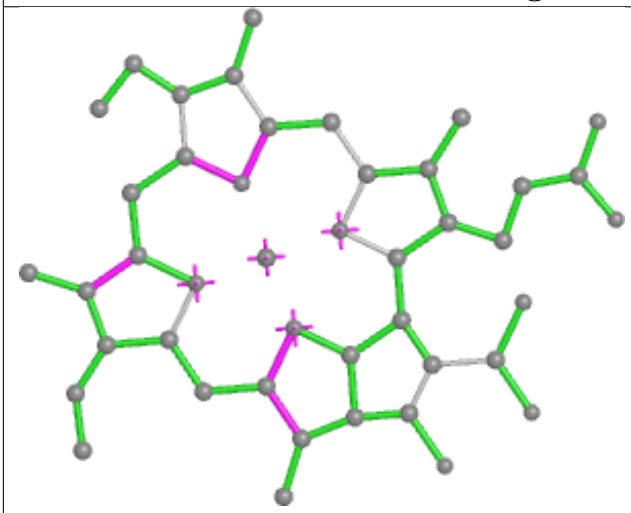


Rings

Ligand CLA F 305



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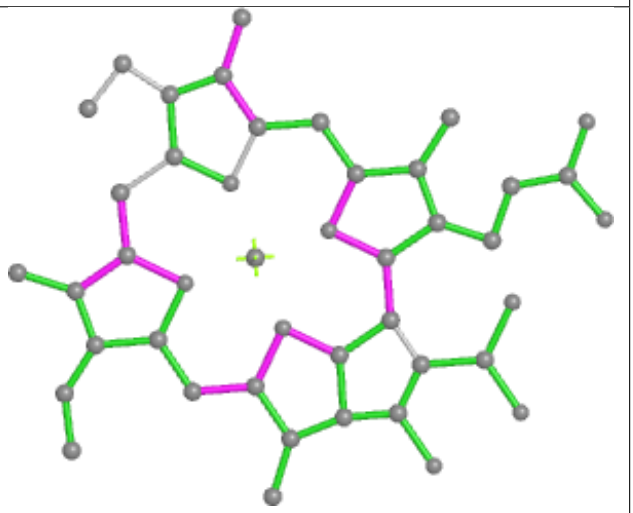
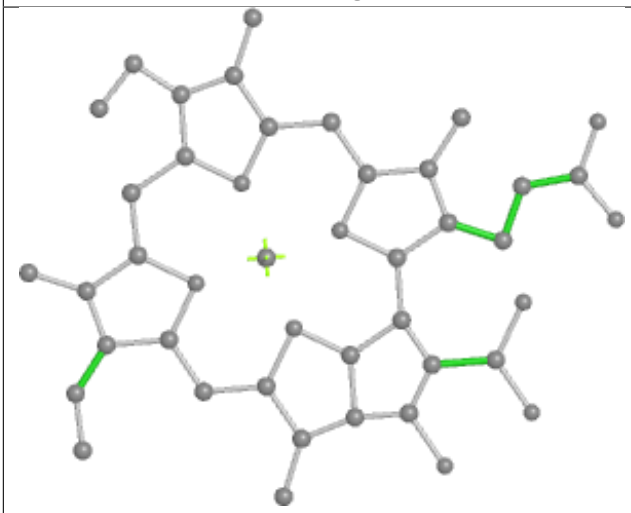


Bond angles



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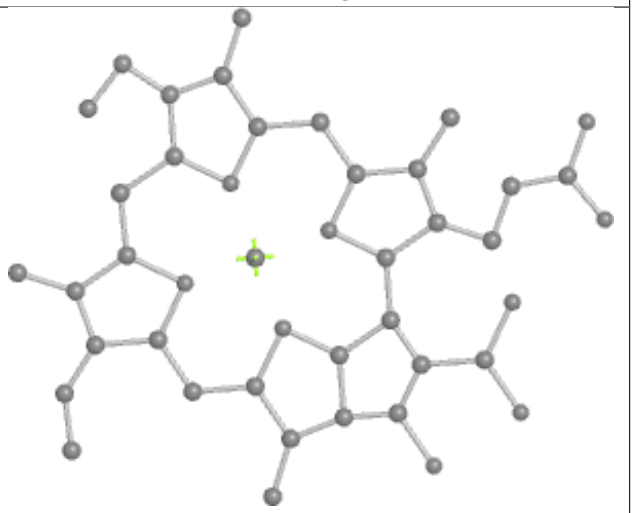
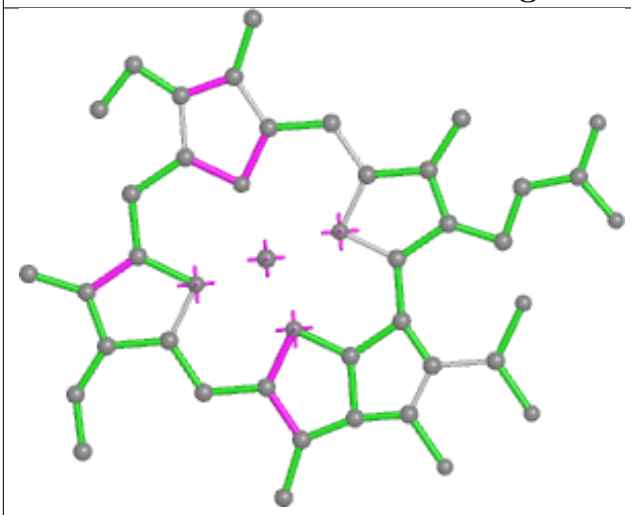


Rings

Ligand CLA 1 1009



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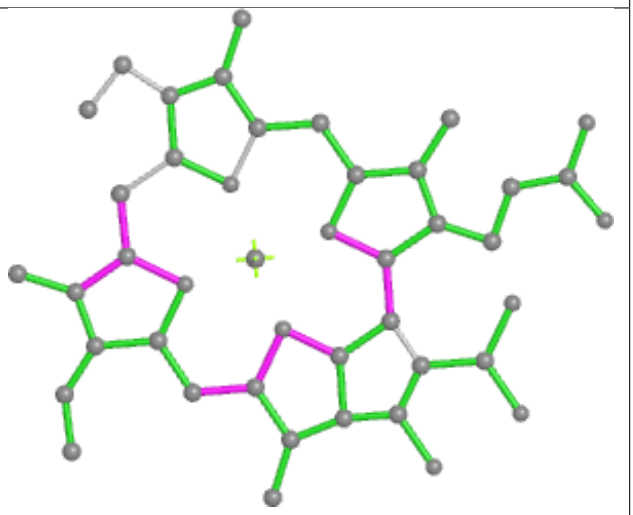

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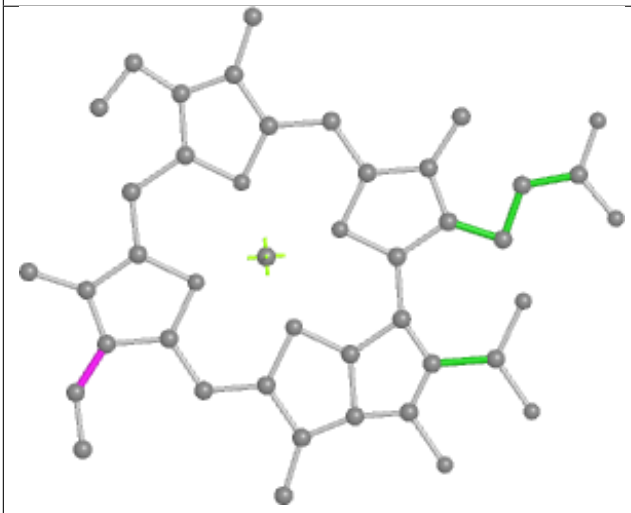

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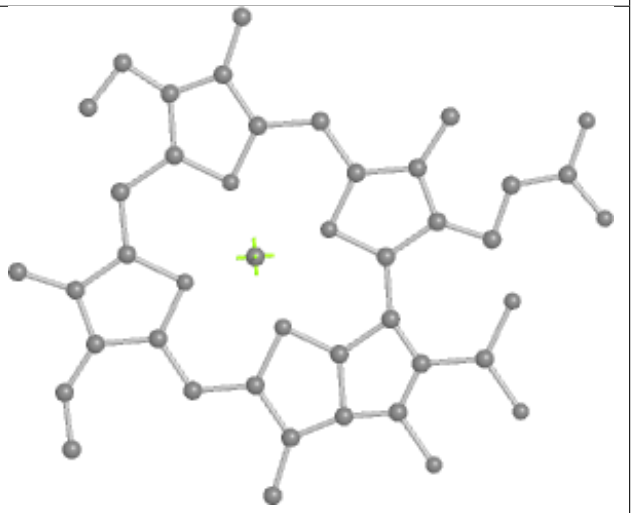
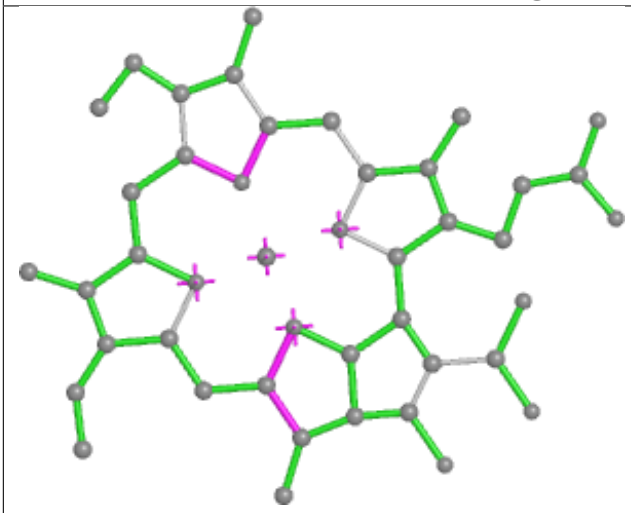


Rings

Ligand CLA 5 305



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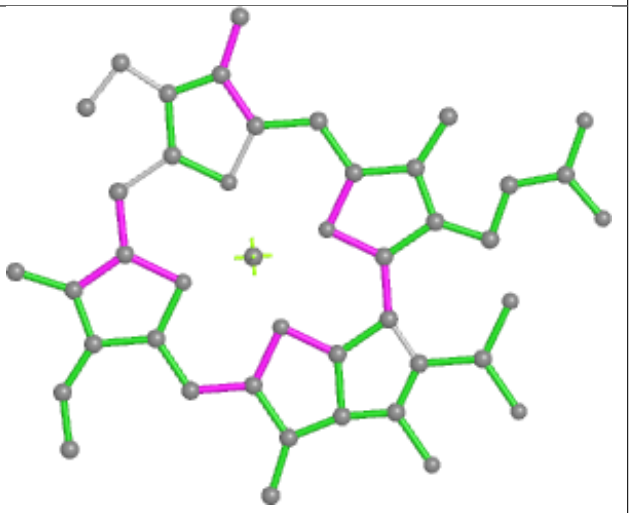

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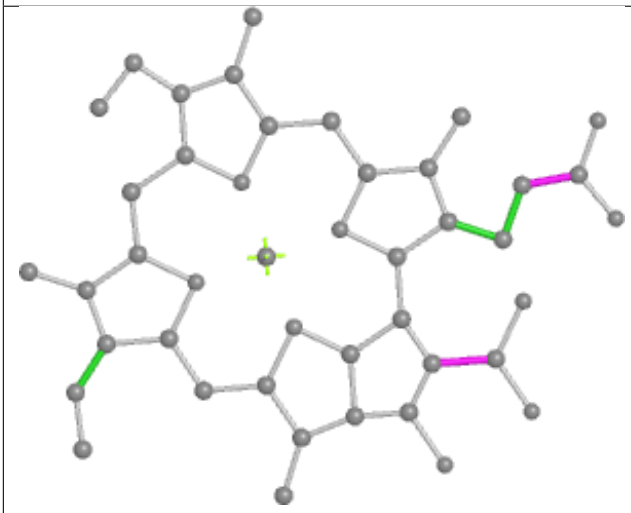

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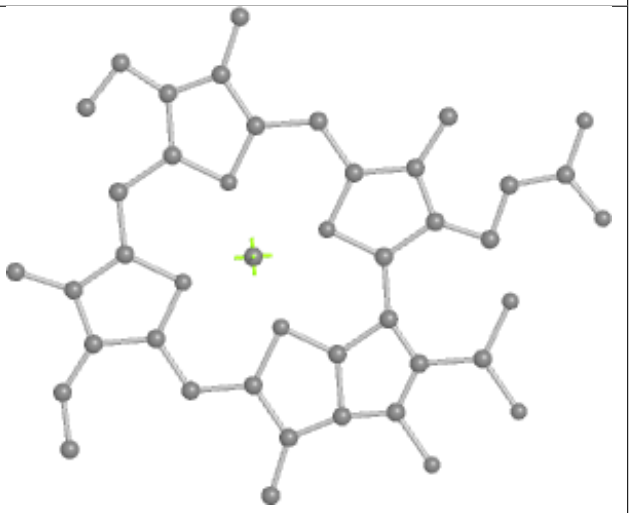
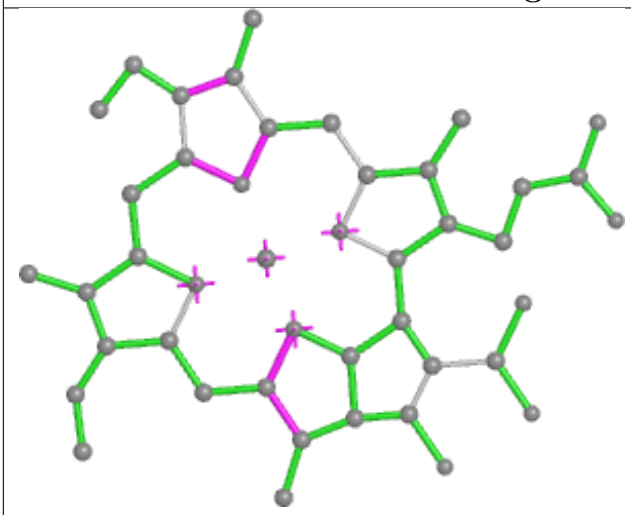


Rings

Ligand CLA B 805



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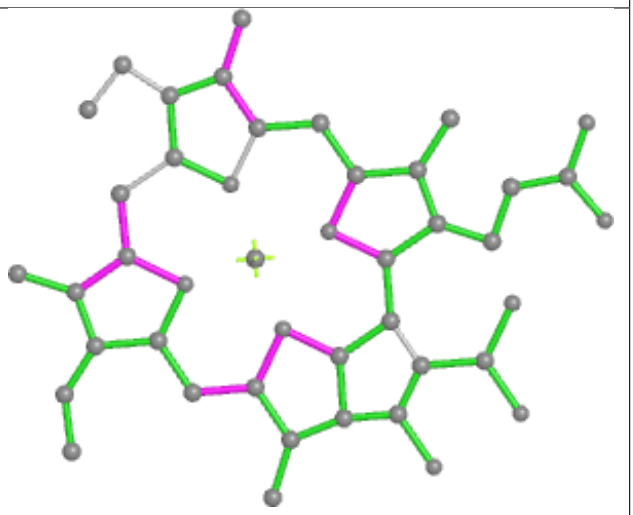
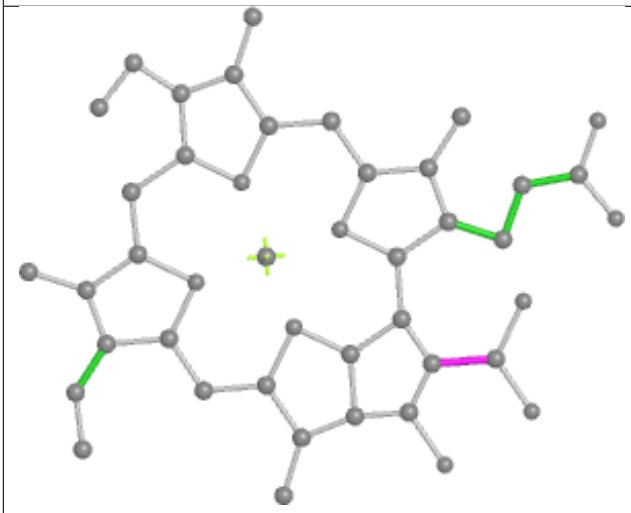
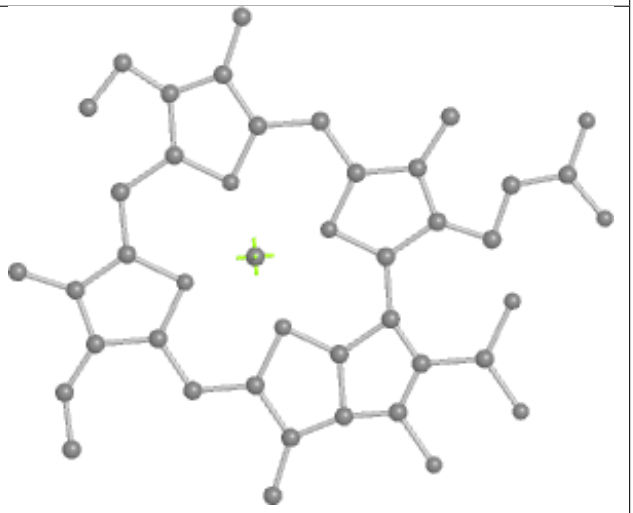


Bond angles

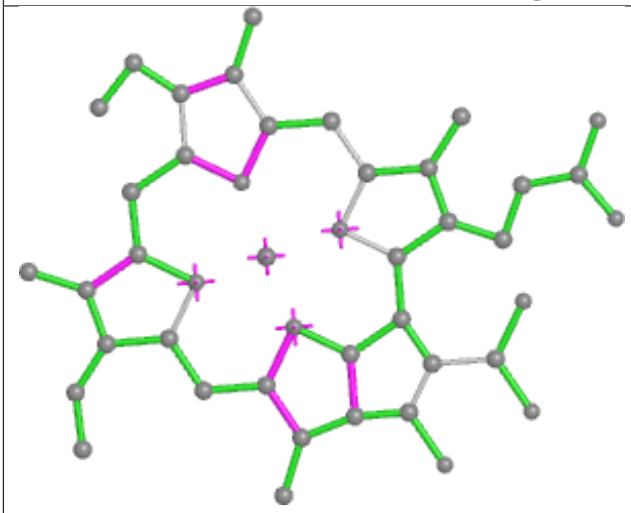


Torsions



Rings

Ligand CLA 8 308



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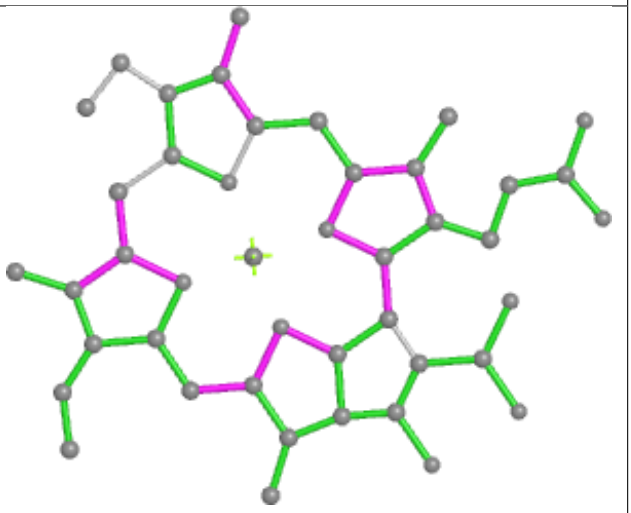
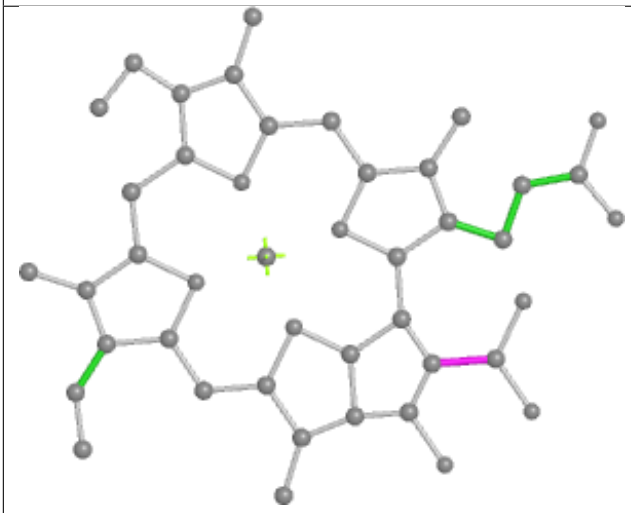


Bond angles



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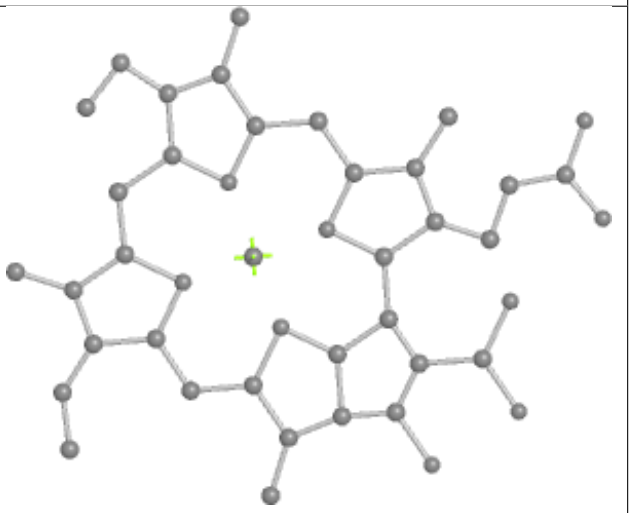
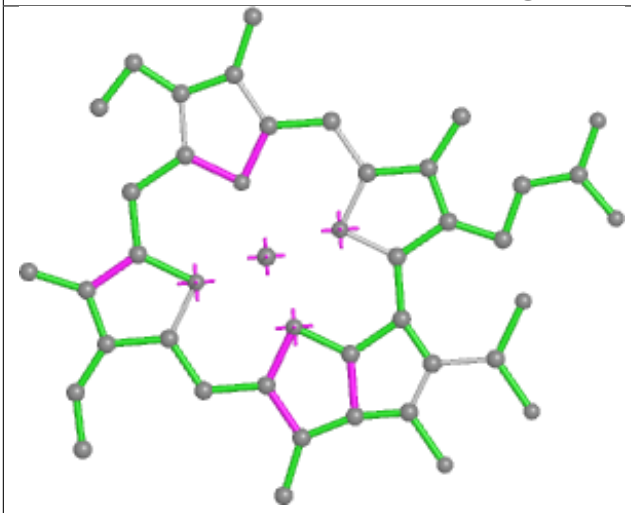
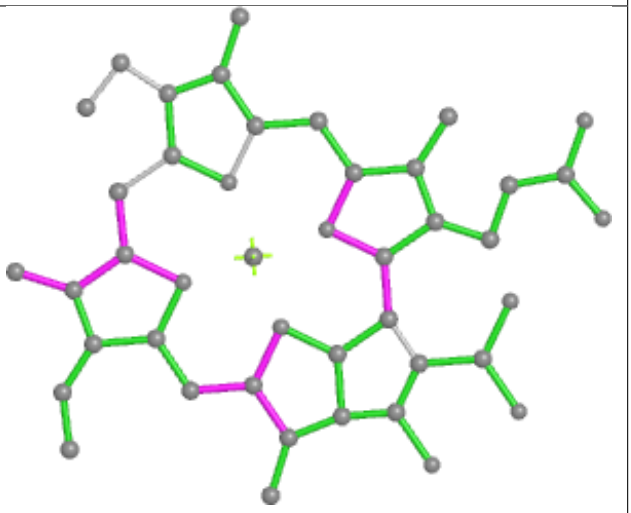


Rings

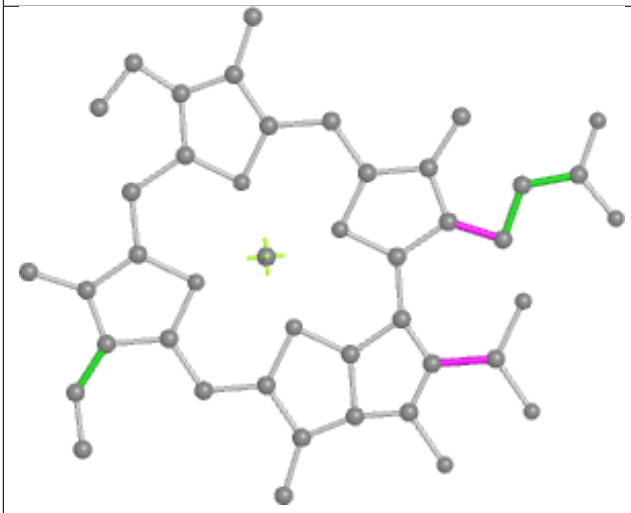
Ligand CLA 7 1007



Bond lengths



Bond angles



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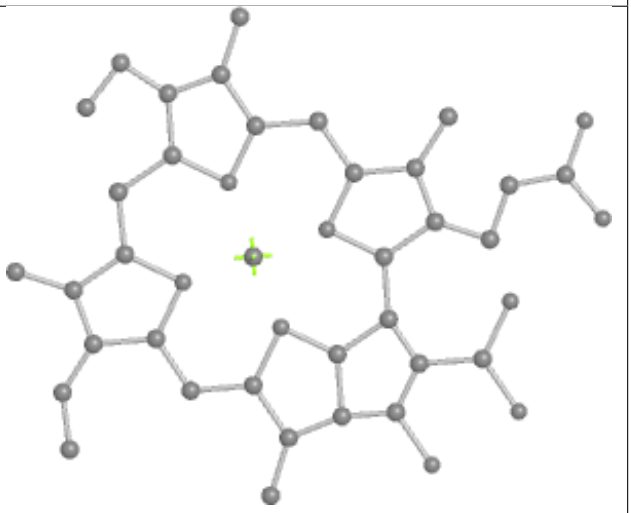
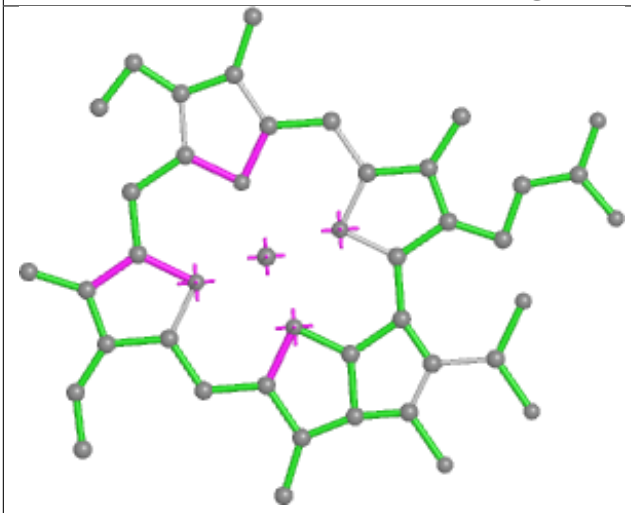
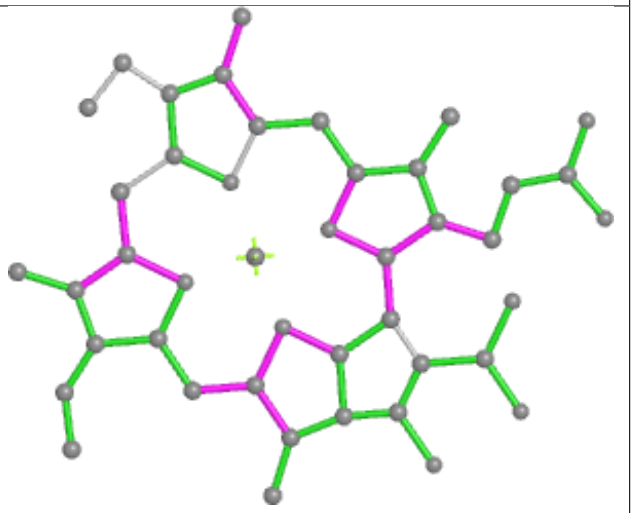


Rings

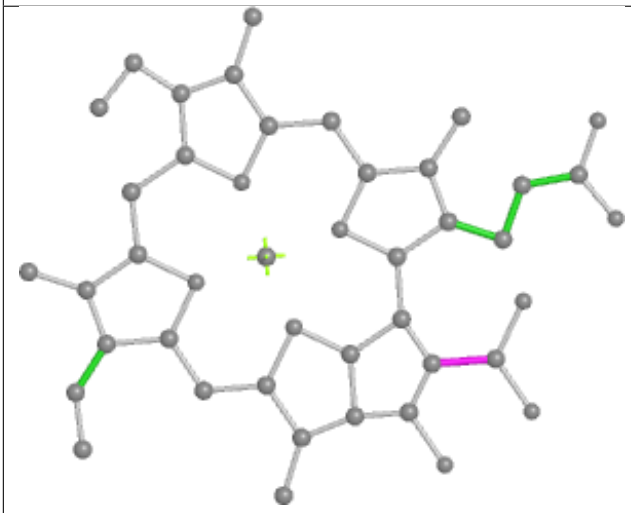
Ligand CLA 5 318



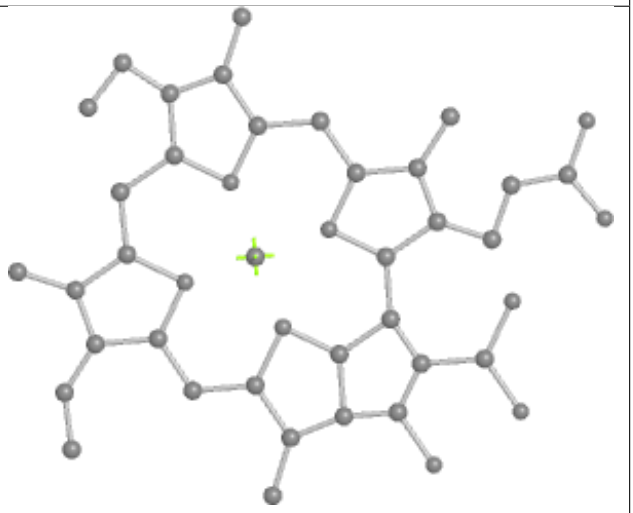
Bond lengths



Bond angles

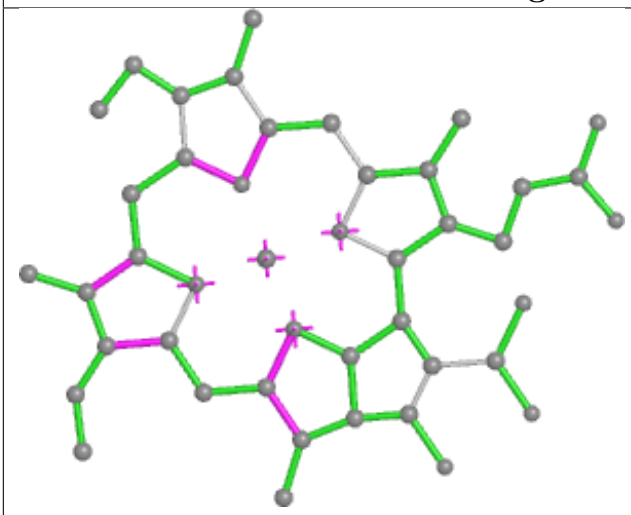


Torsions



Rings

Ligand CLA 4 307



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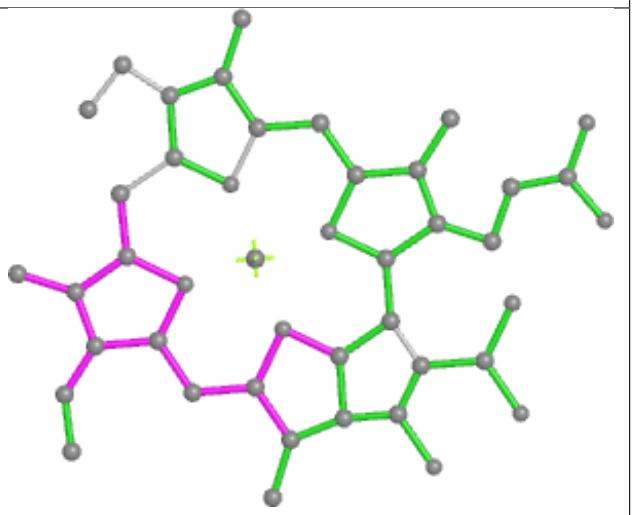

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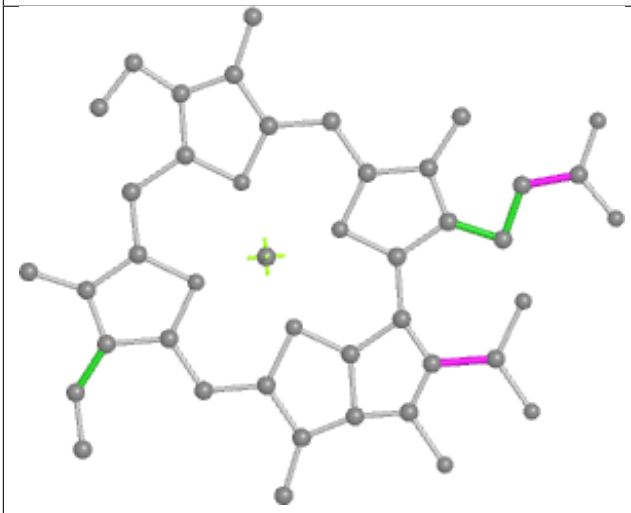
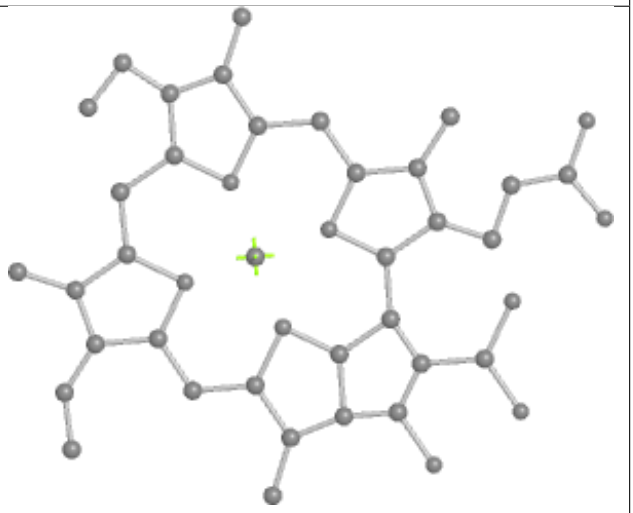
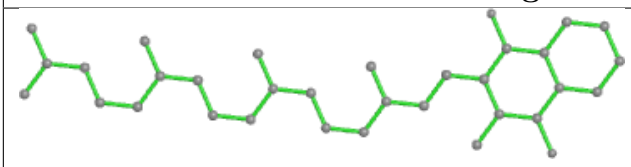


Torsions



Rings

Ligand PQN B 842



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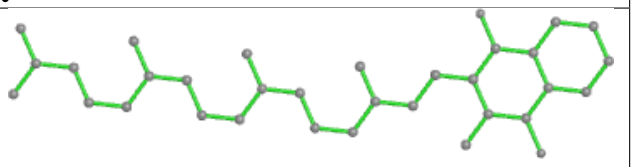
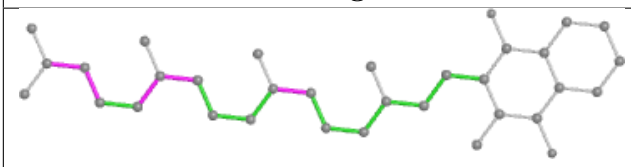


Bond angles



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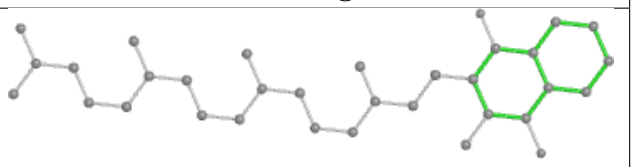
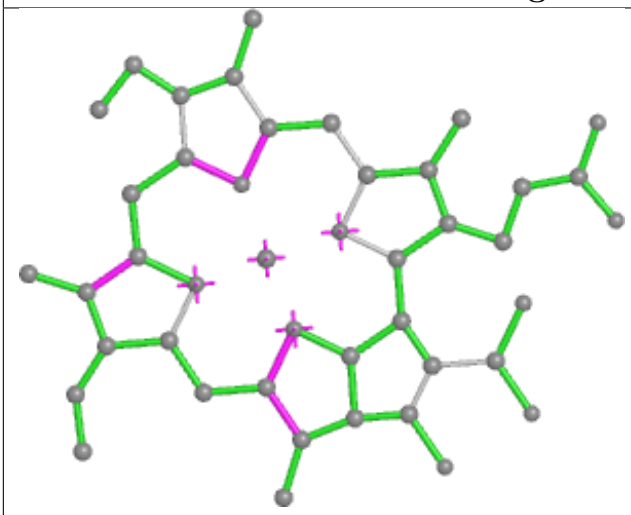


Rings

Ligand CLA 8 310



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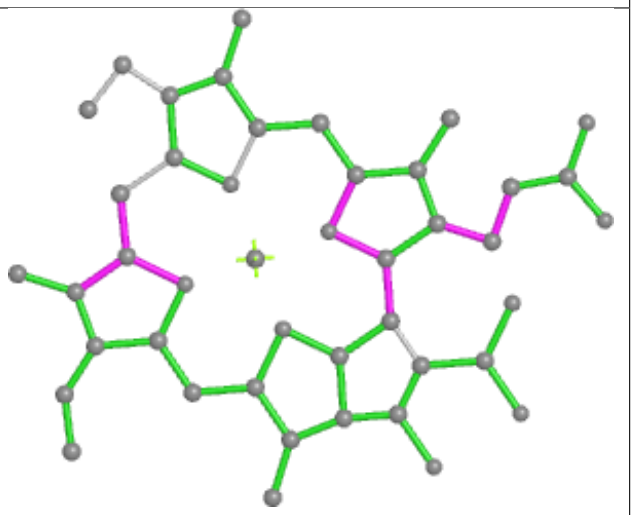

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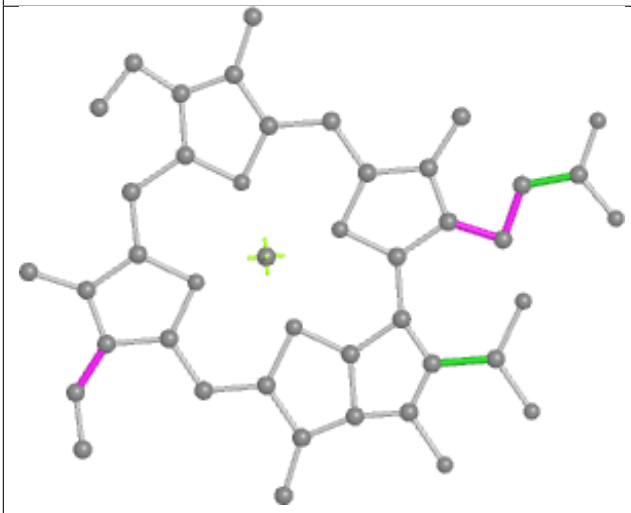

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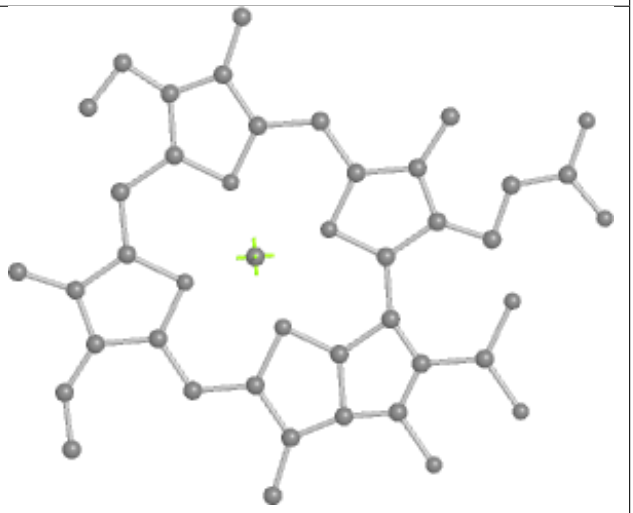
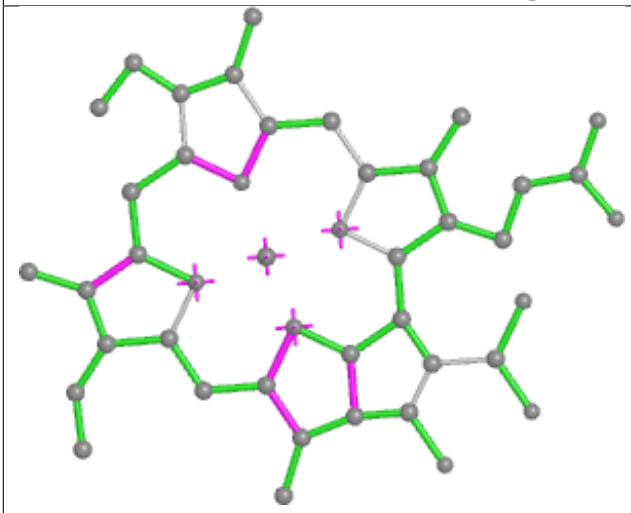
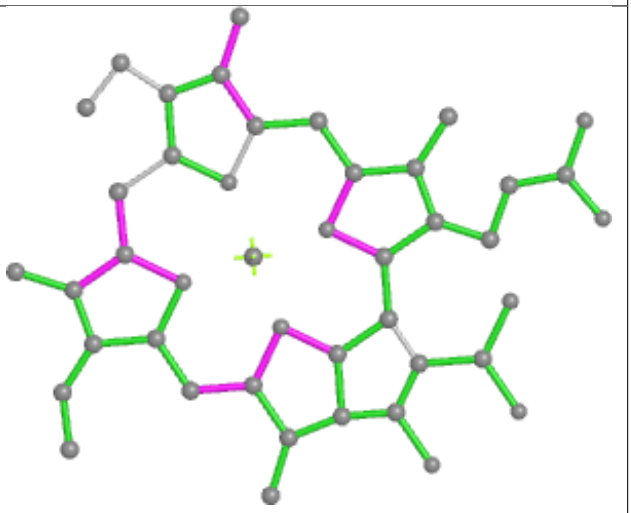


Rings

Ligand CLA A 839



Bond lengths



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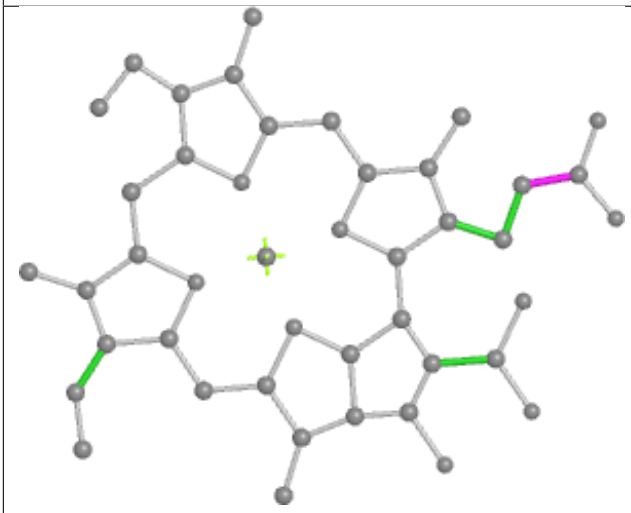

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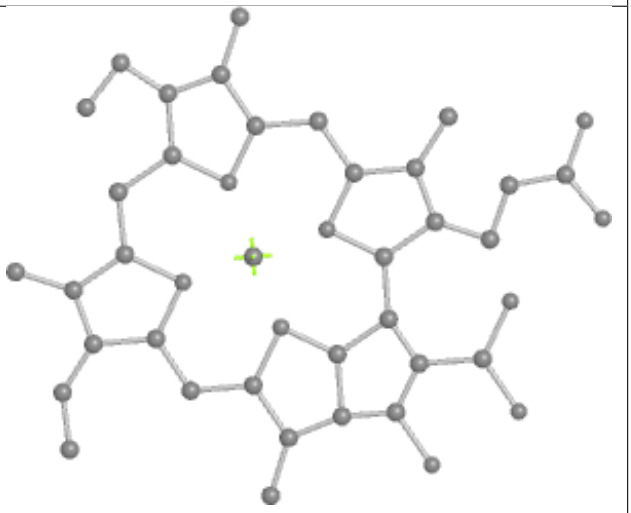
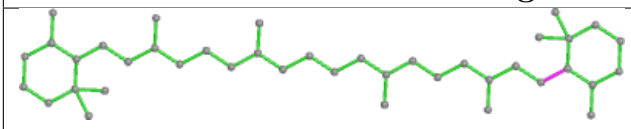


Rings

Ligand BCR 3 1004



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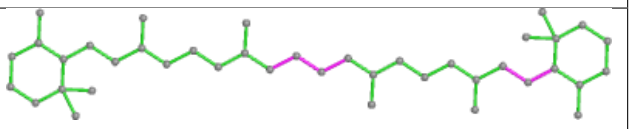
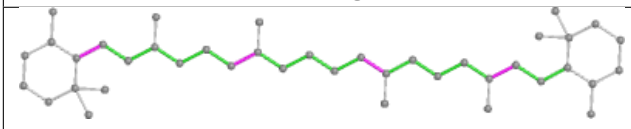


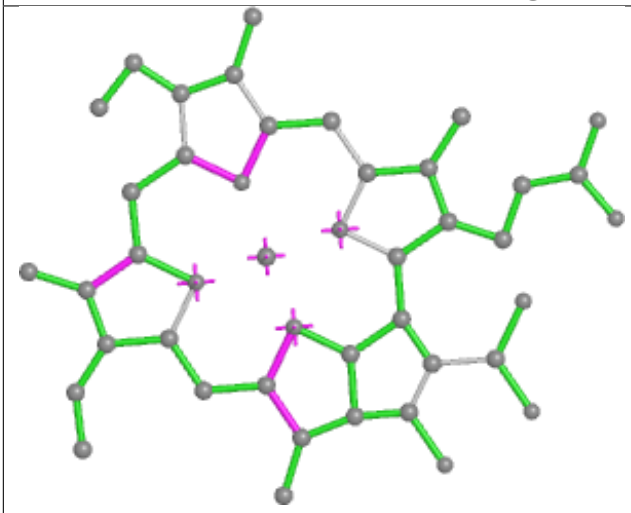
Bond angles



Torsions

Rings

Ligand CLA B 829



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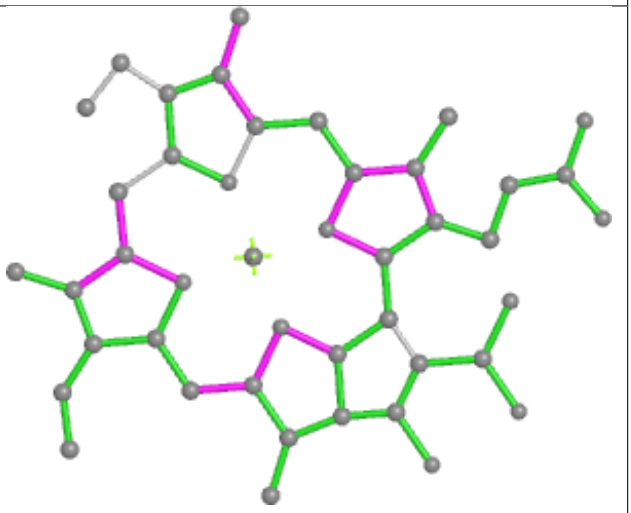
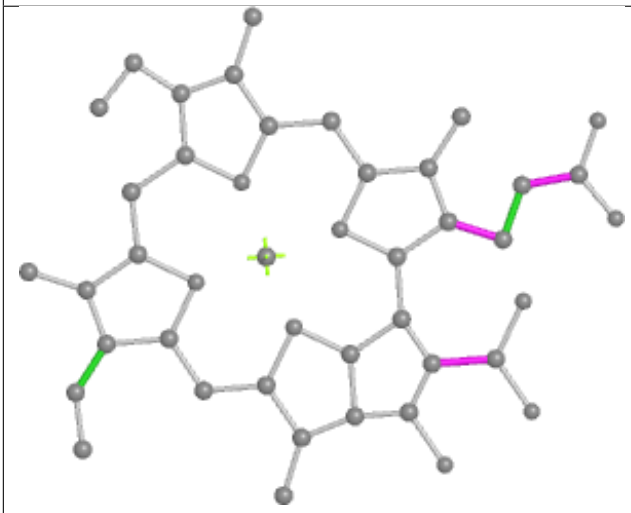


Bond angles



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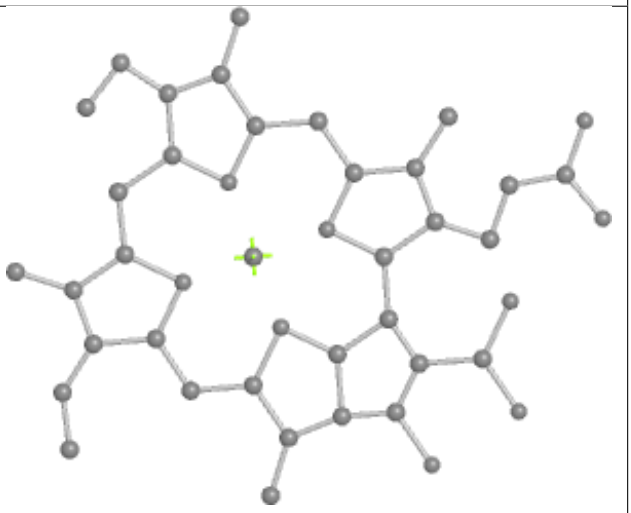
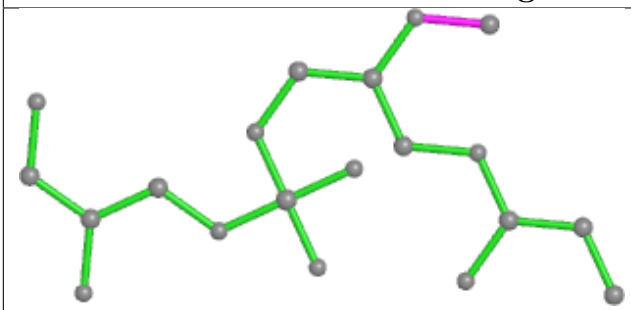


Rings

Ligand LHG 3 1019



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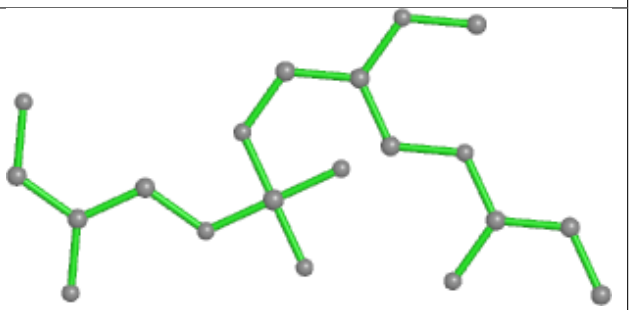

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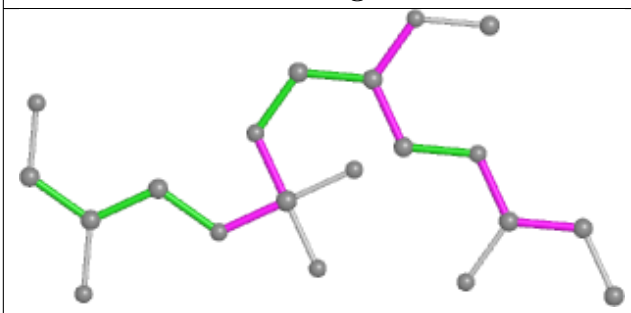

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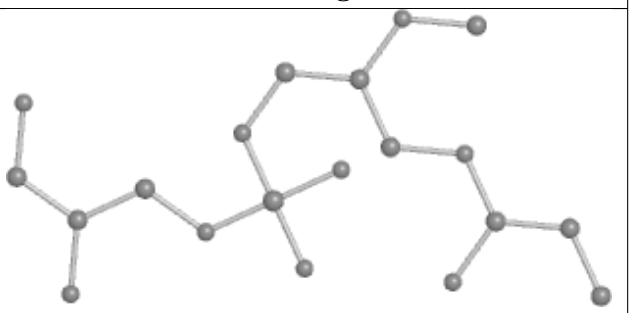
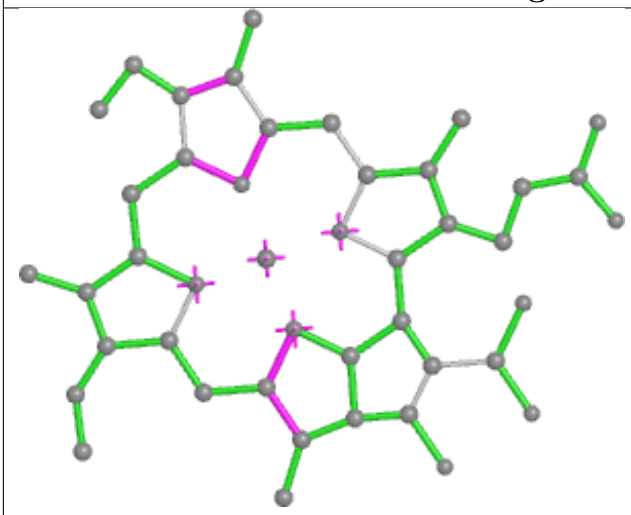
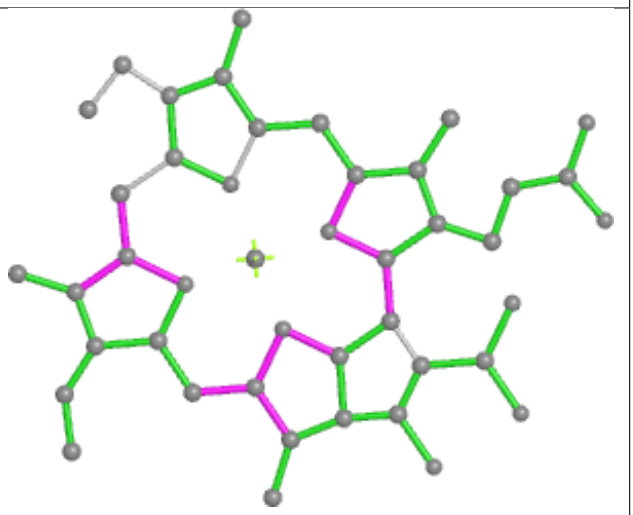


Rings

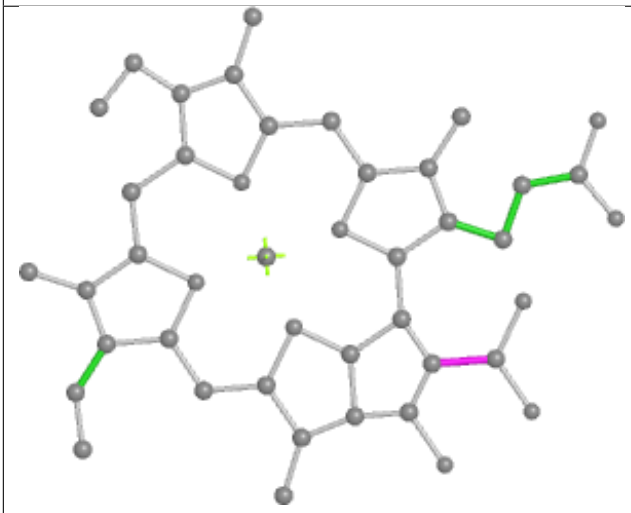
Ligand CLA 8 313



Bond lengths



Bond angles



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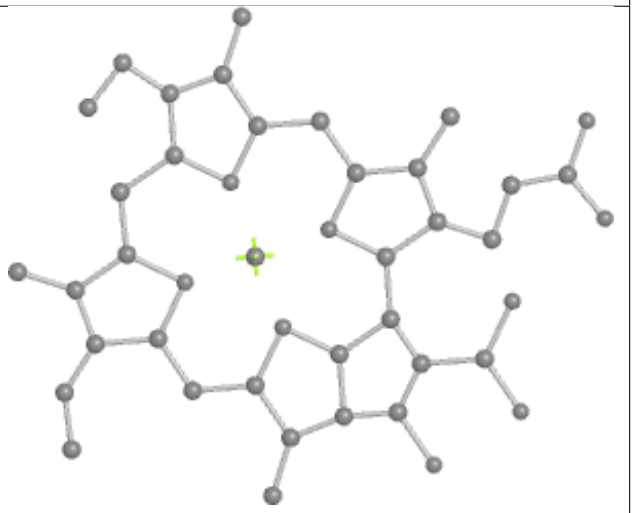
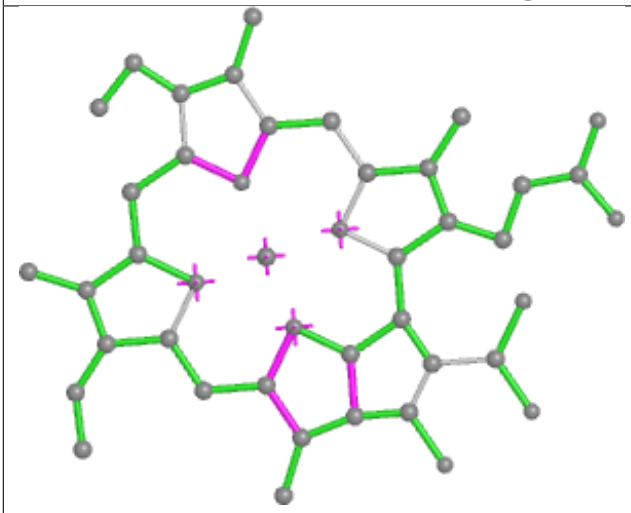


Rings

Ligand CLA 7 1010



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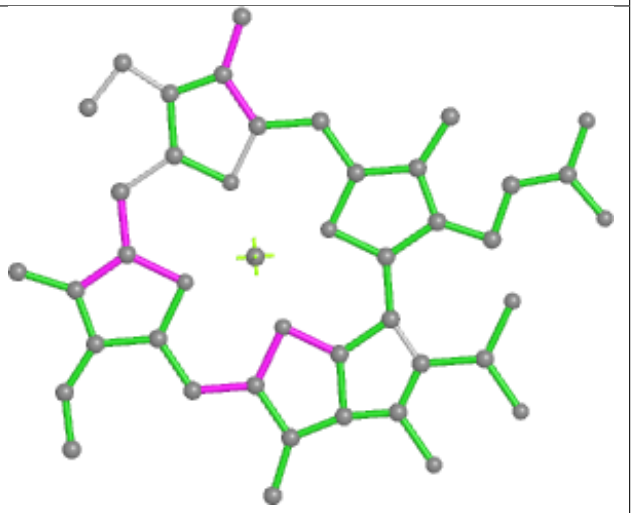

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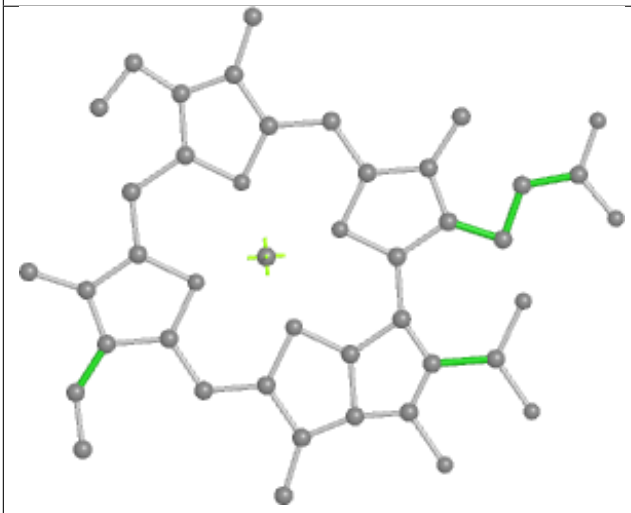

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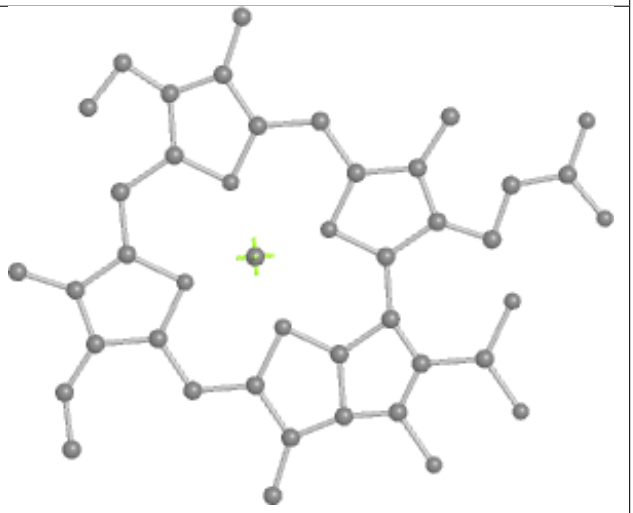
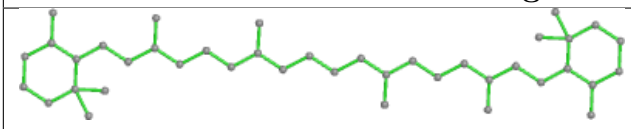


Rings

Ligand BCR B 844



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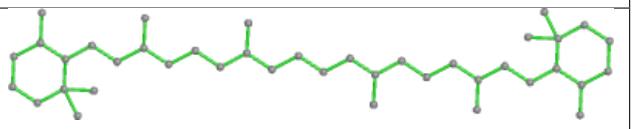

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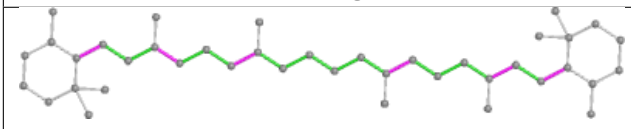
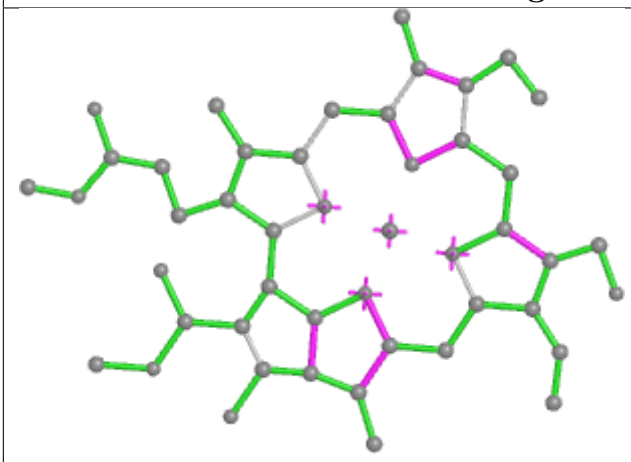


Torsions

Rings

Ligand CHL 0 314



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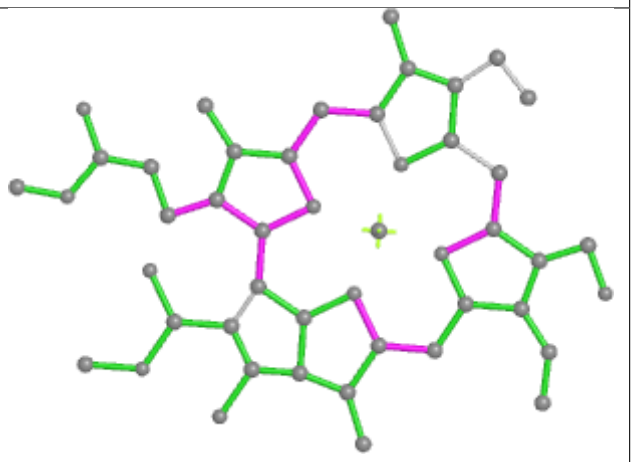
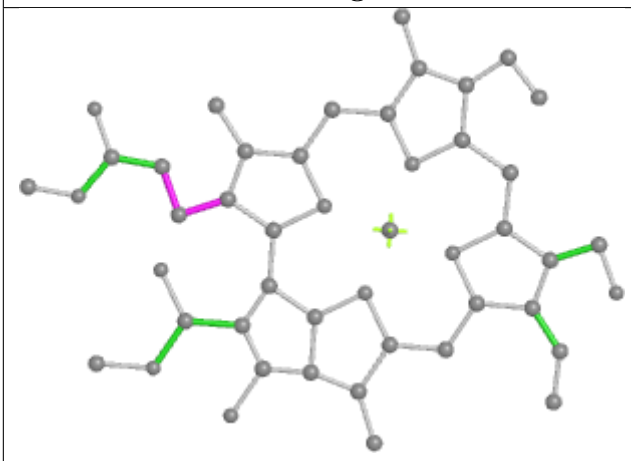
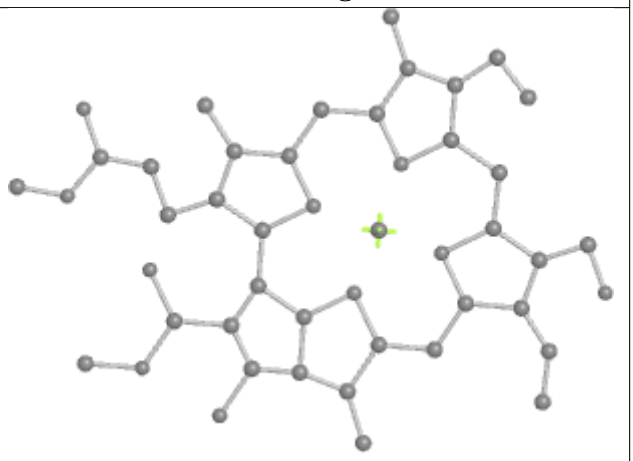


Bond angles

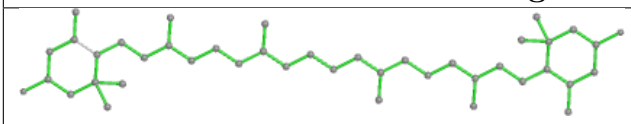


Torsions



Rings

Ligand LUT 4 317



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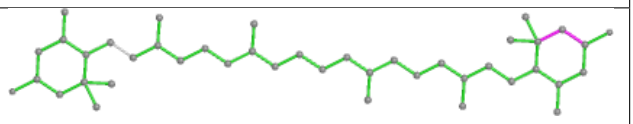
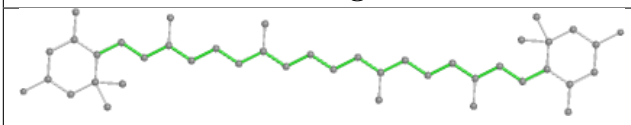


Bond angles



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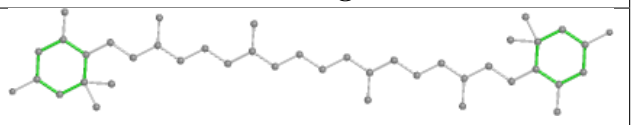
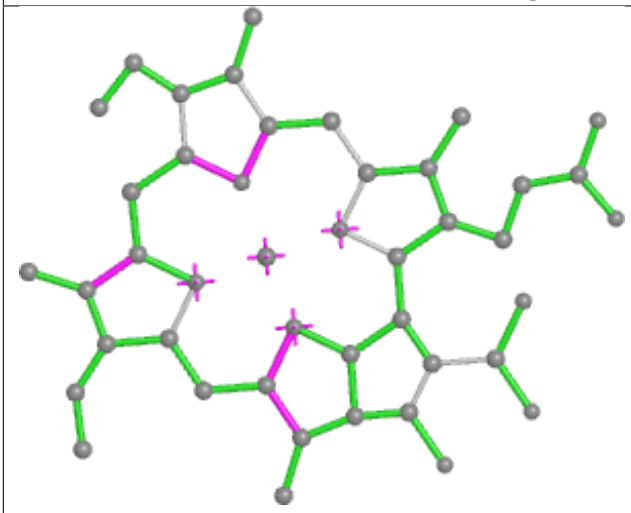
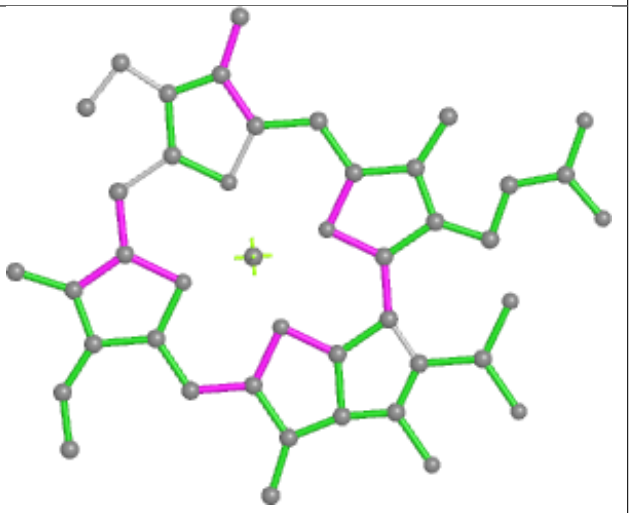


Rings

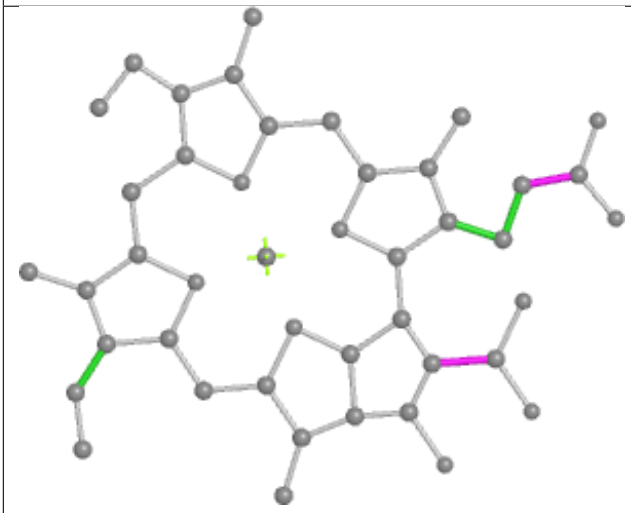
Ligand CLA B 809



Bond lengths



Bond angles



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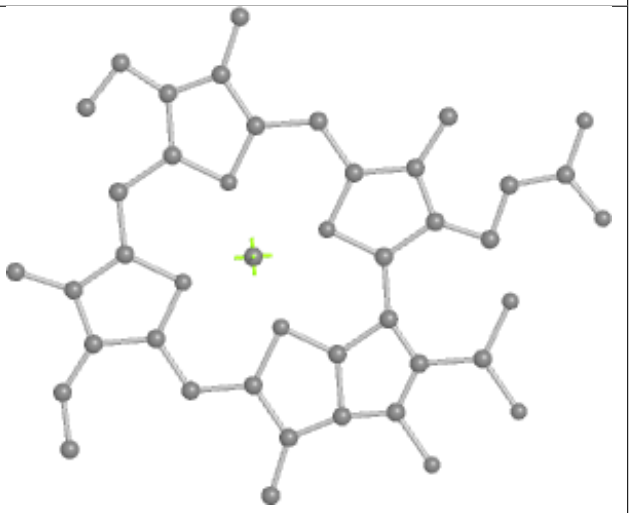
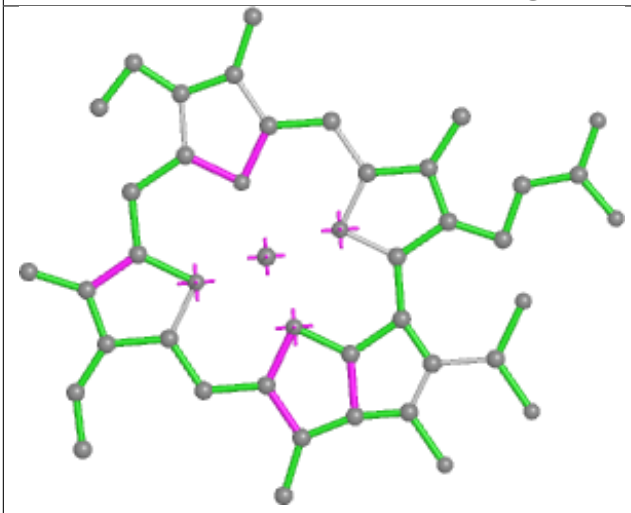
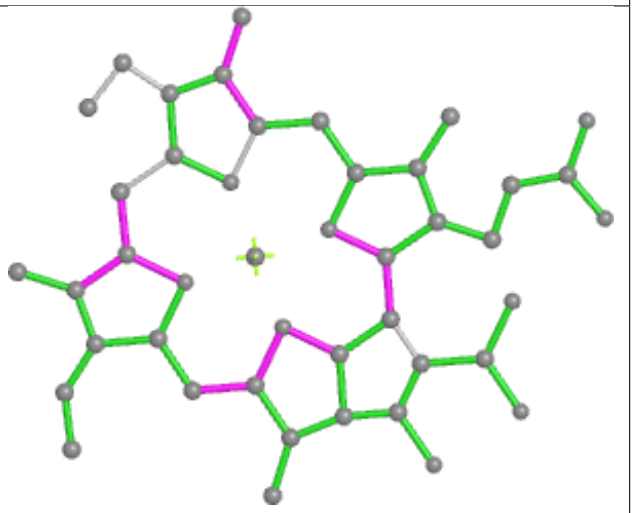


Rings

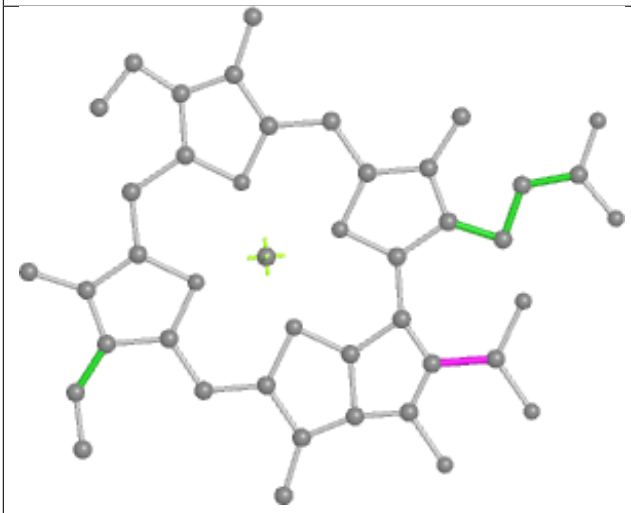
Ligand CLA B 834



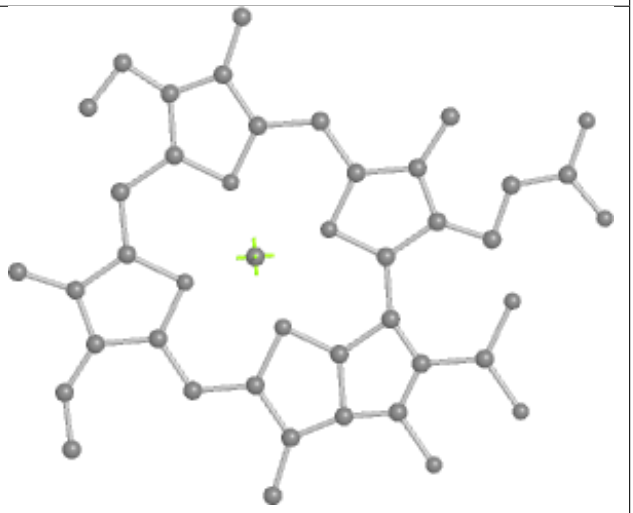
Bond lengths



Bond angles

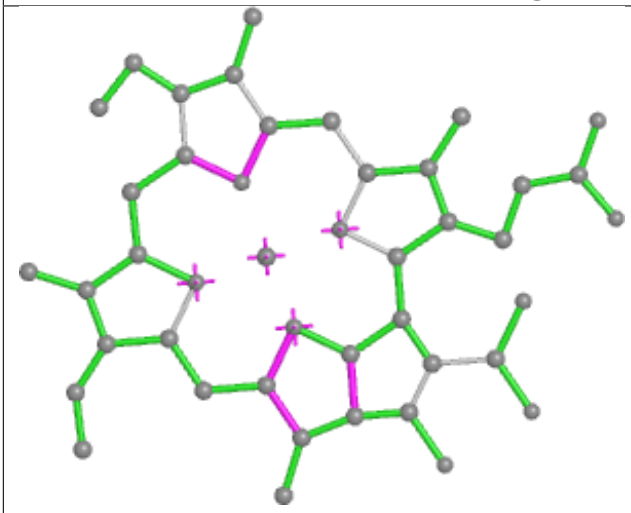


Torsions

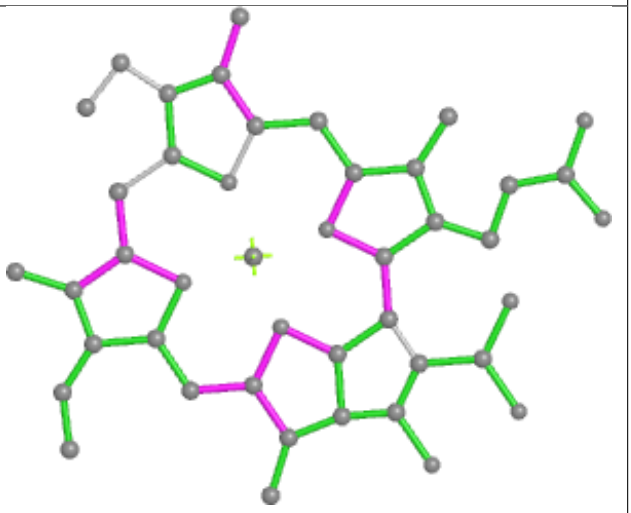


Rings

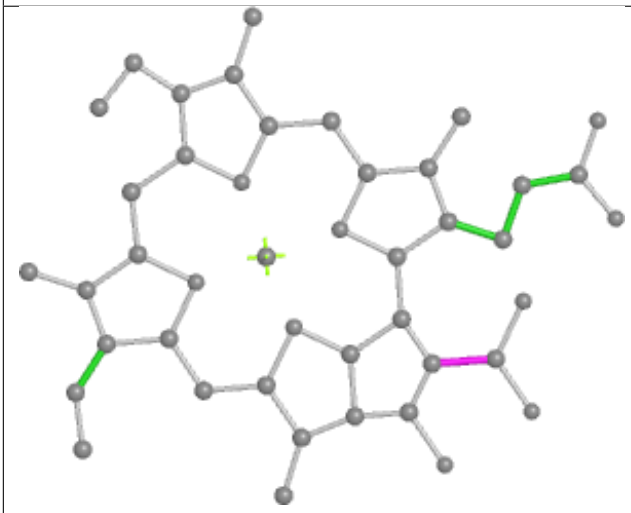
Ligand CLA 5 322



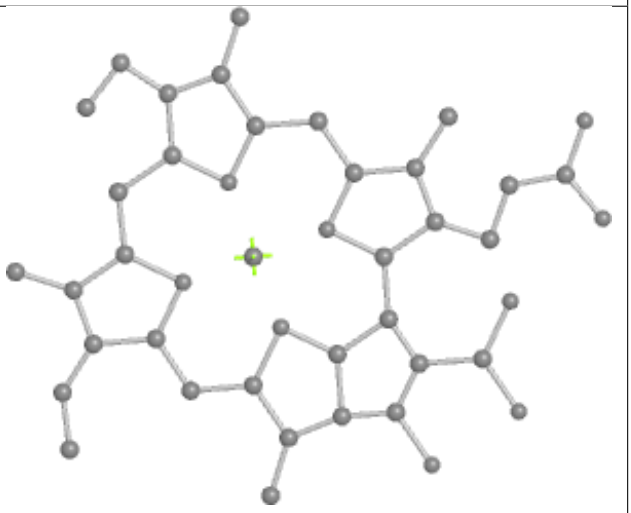
Bond lengths



Bond angles

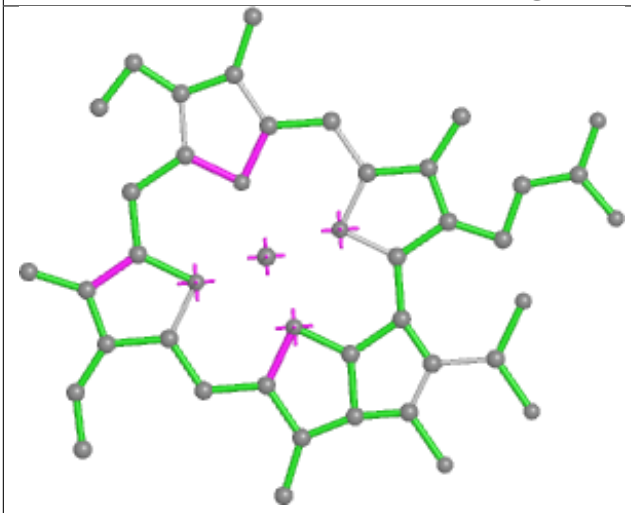


Torsions



Rings

Ligand CLA 6 307



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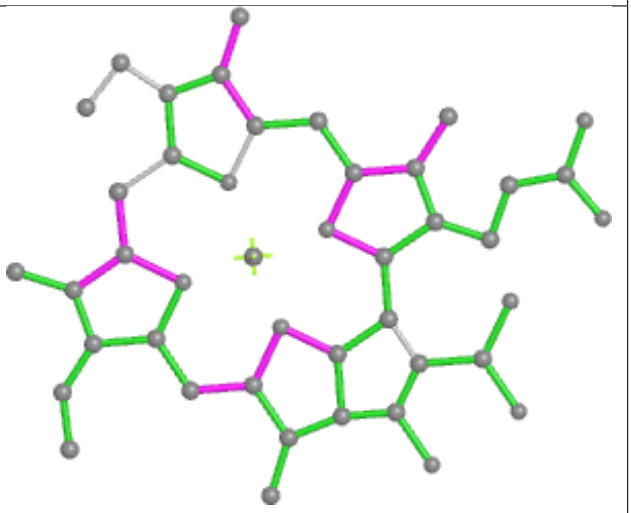

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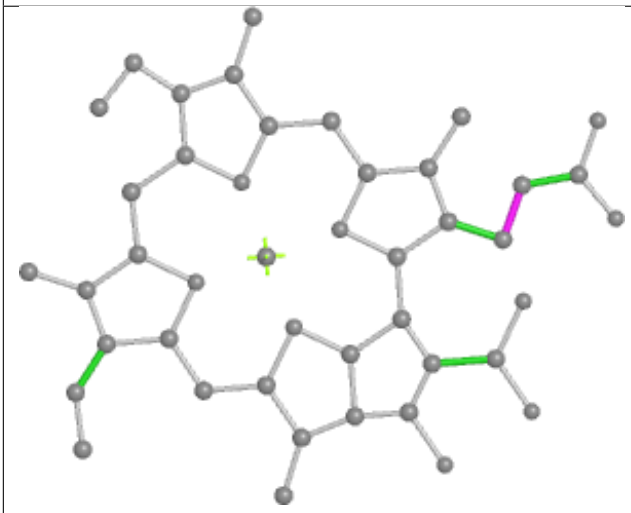

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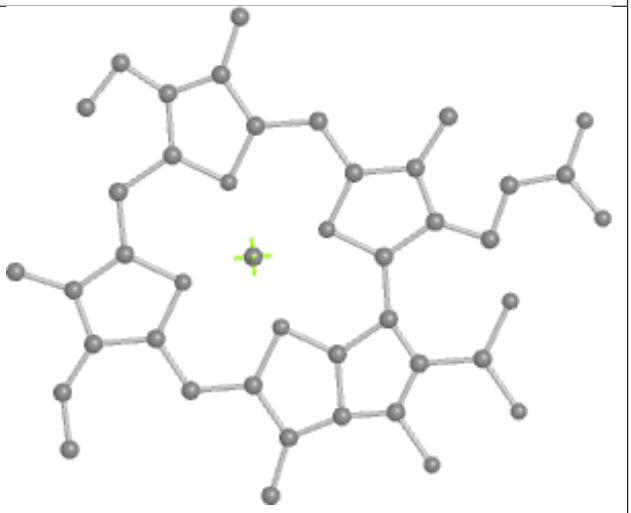
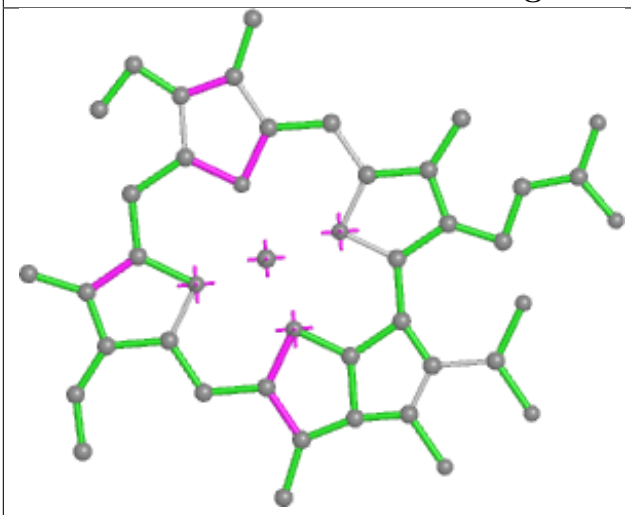


Rings

Ligand CLA B 807



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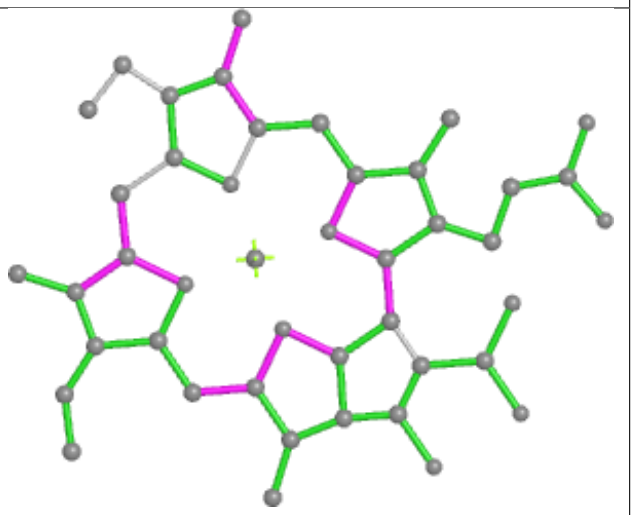

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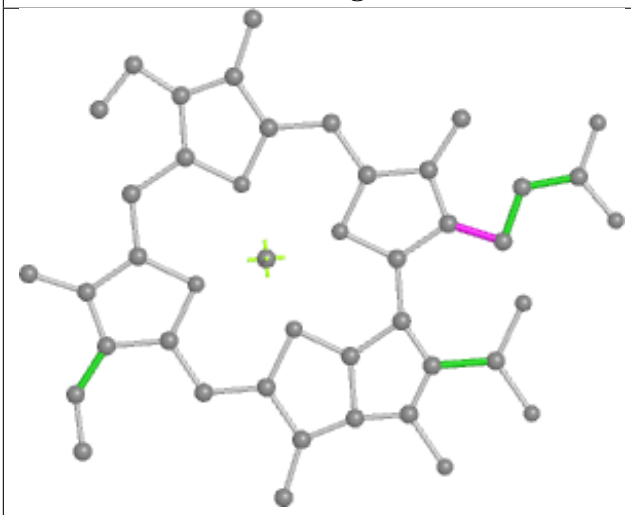

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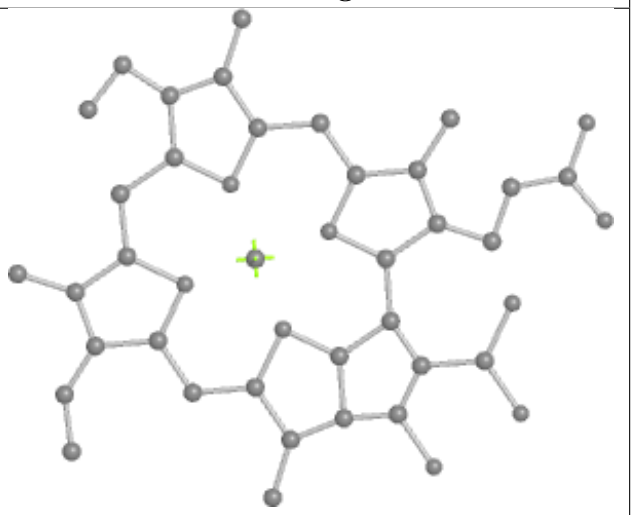
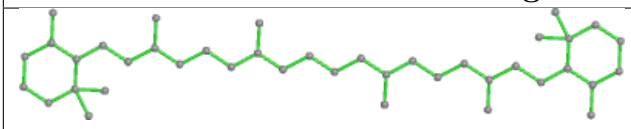


Rings

Ligand BCR B 847



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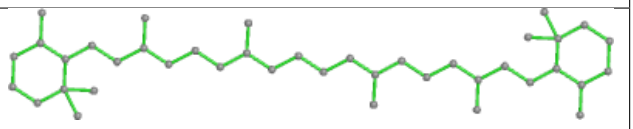

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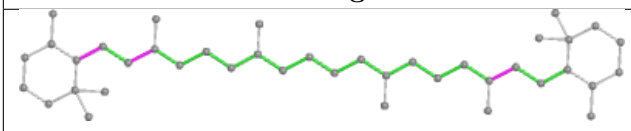

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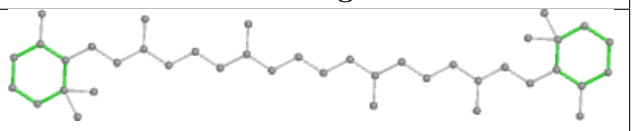
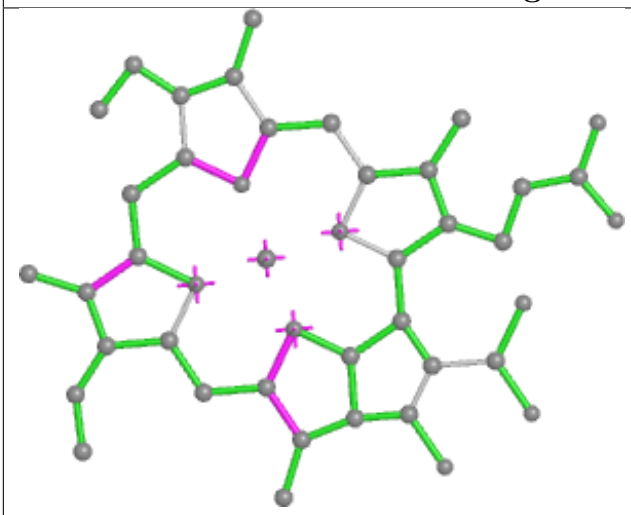


Rings

Ligand CLA A 819



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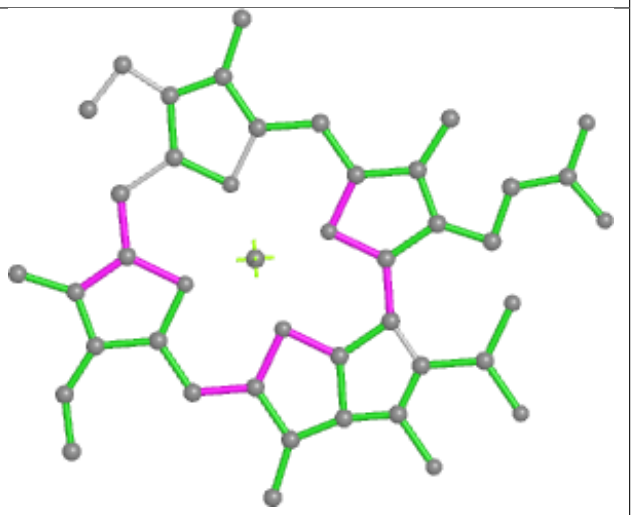

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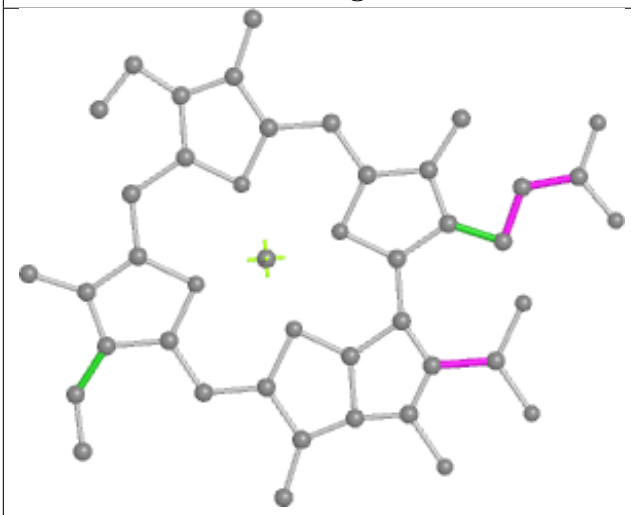

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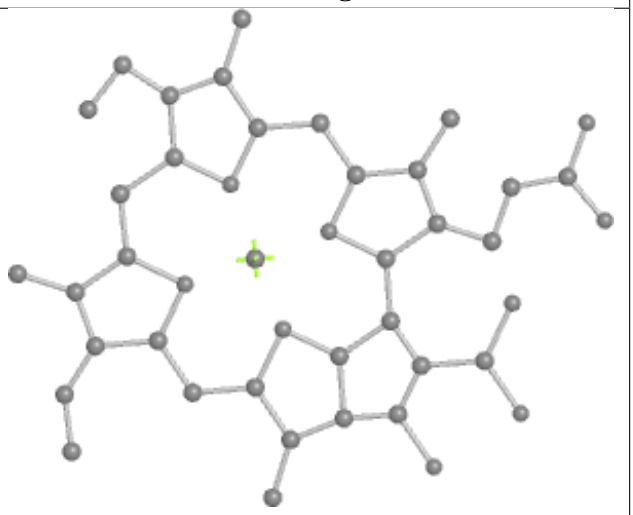
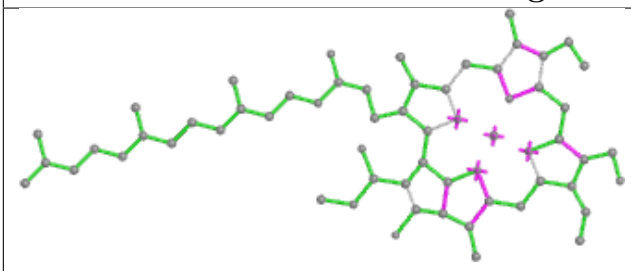


Rings

Ligand CHL 0 317



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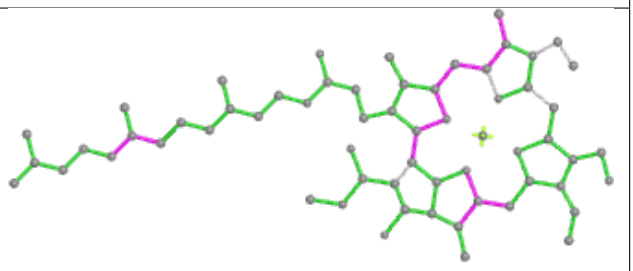
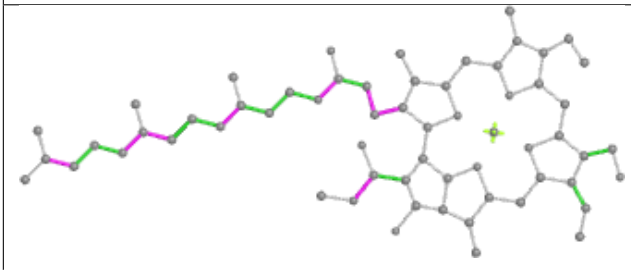


Bond angles



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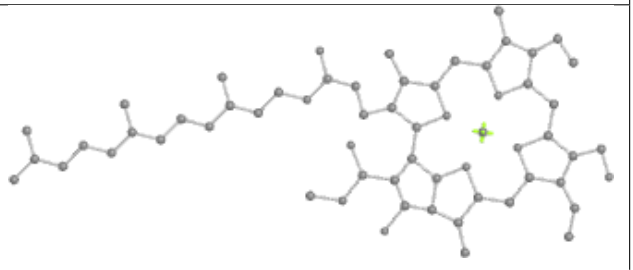
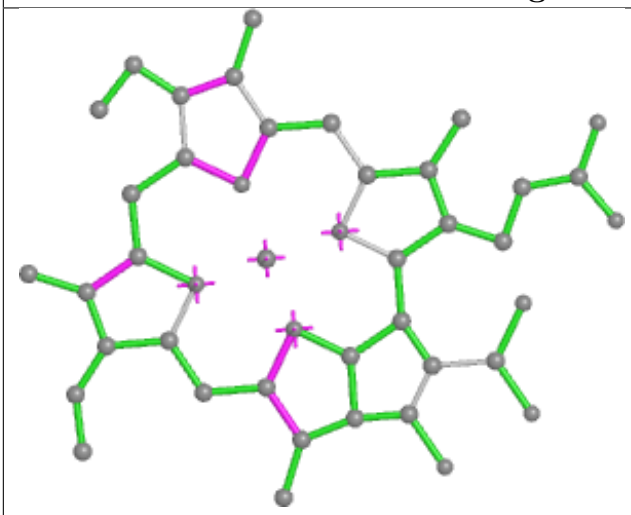


Rings

Ligand CLA 5 306



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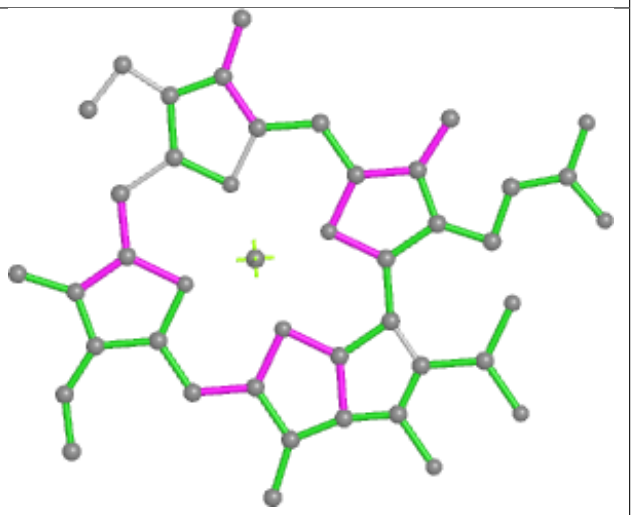

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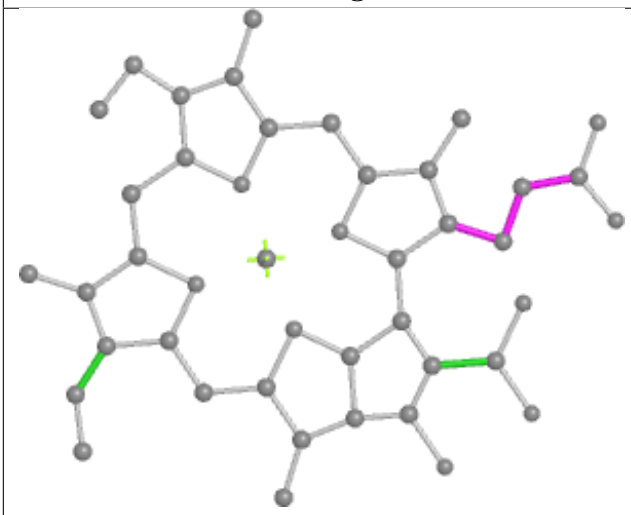

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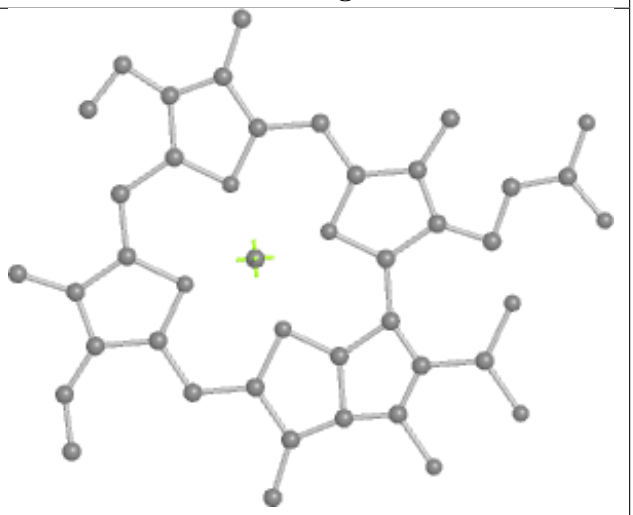
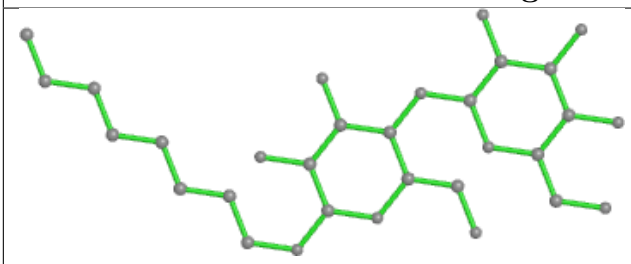


Rings

Ligand LMT B 849



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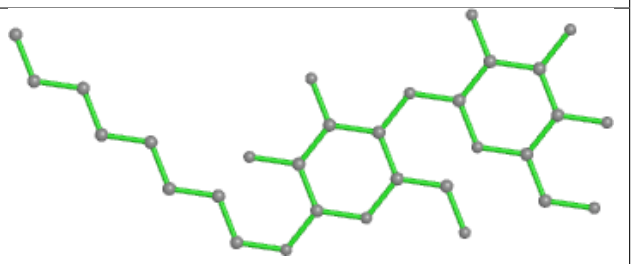
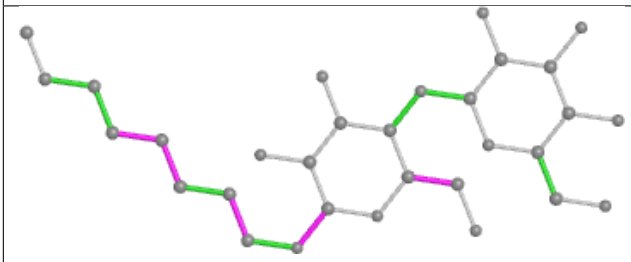


Bond angles



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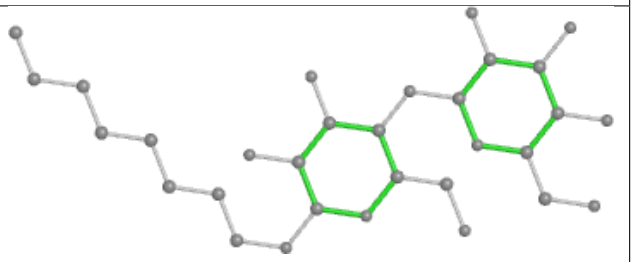
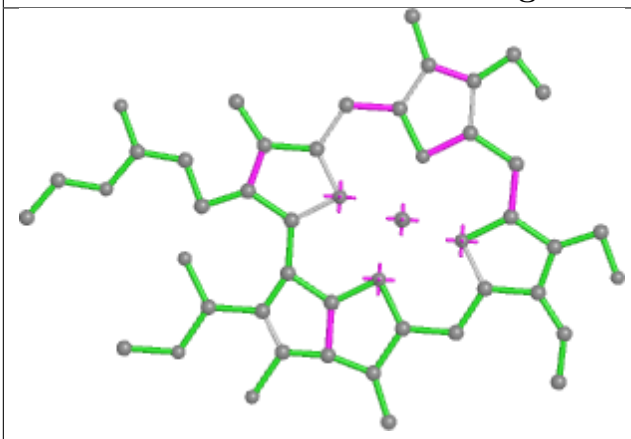


Rings

Ligand CHL 7 1013



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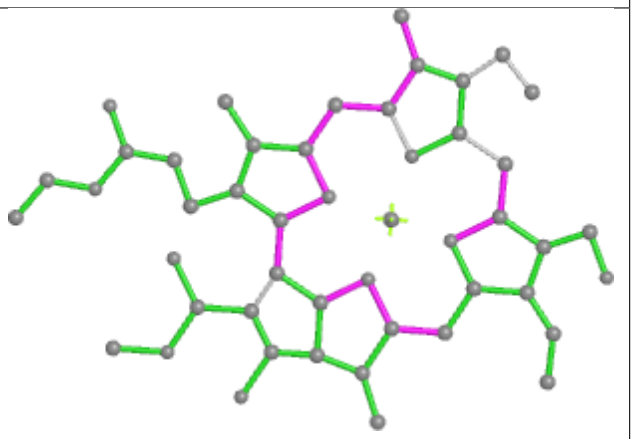
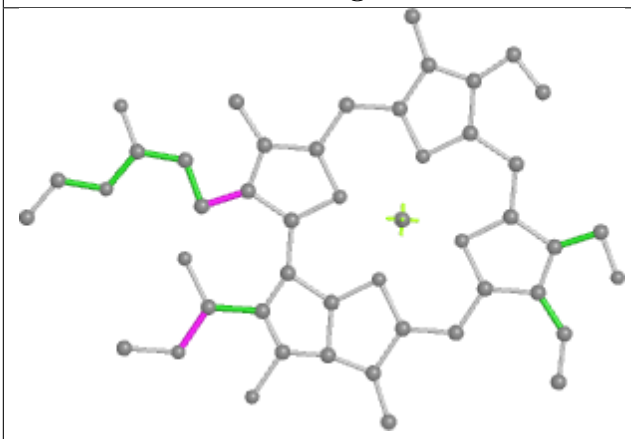


Bond angles



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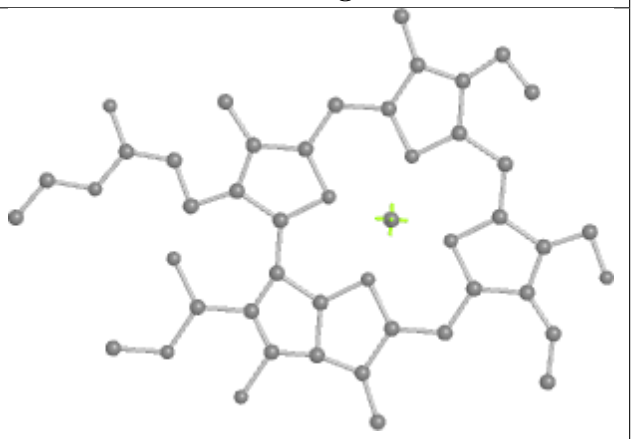
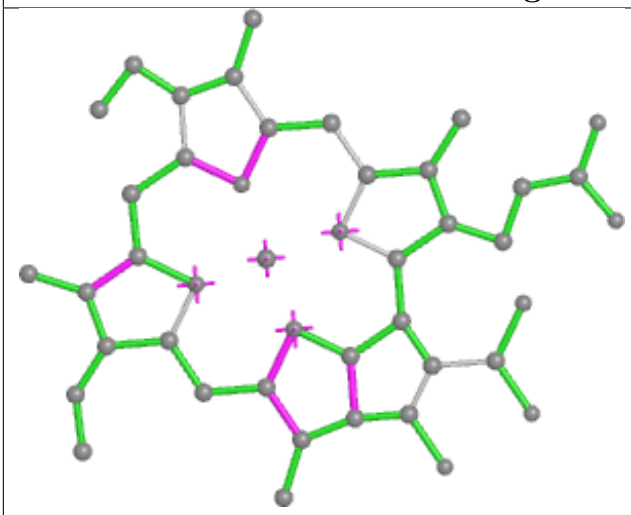


Rings

Ligand CLA A 837



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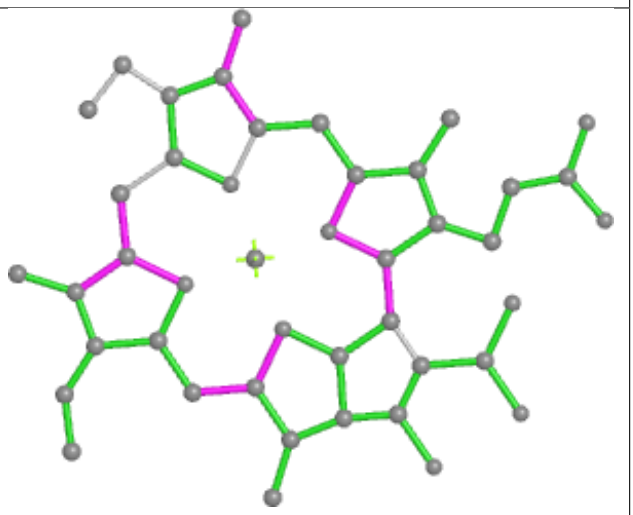
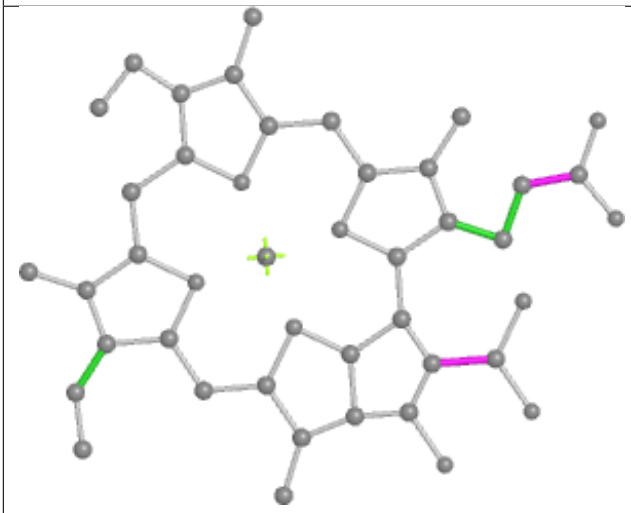
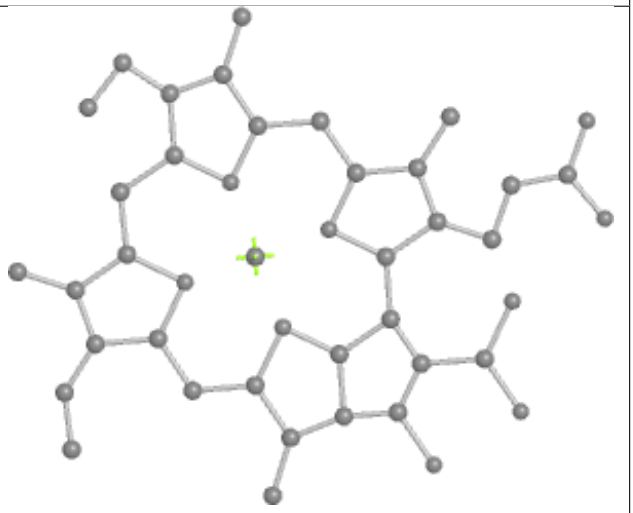


Bond angles

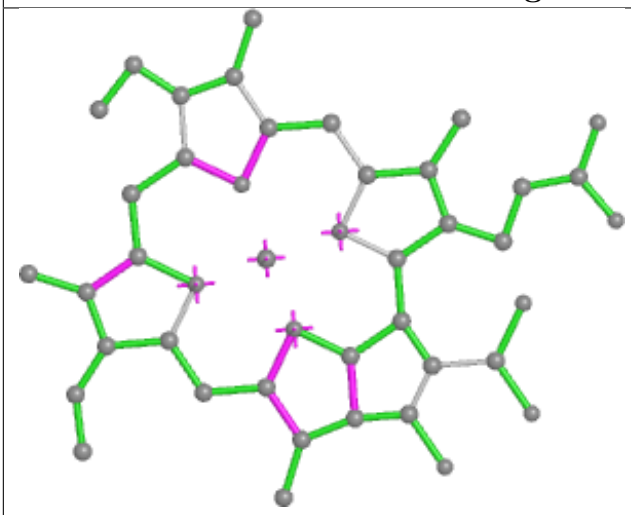


Torsions



Rings

Ligand CLA B 827



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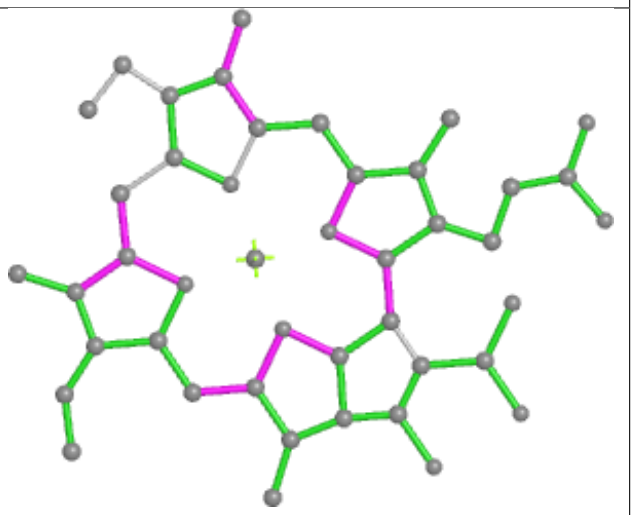
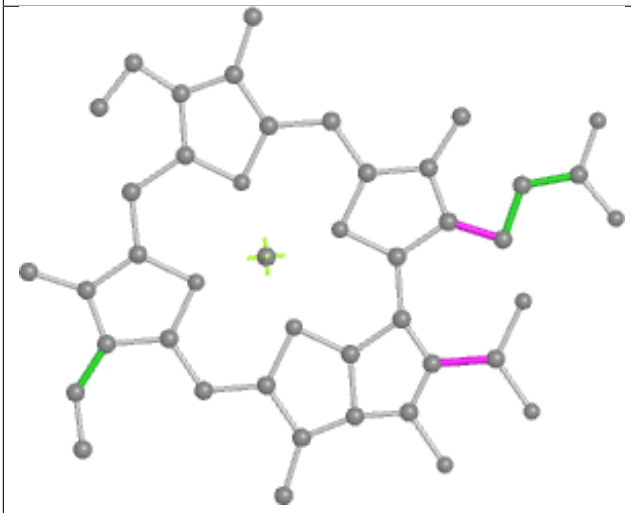
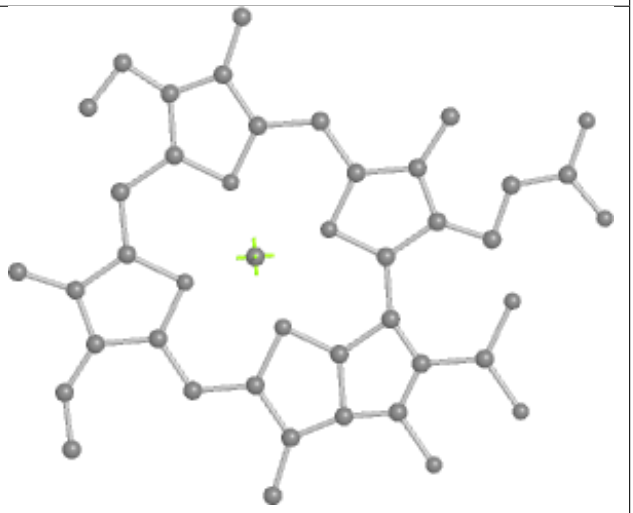


Bond angles

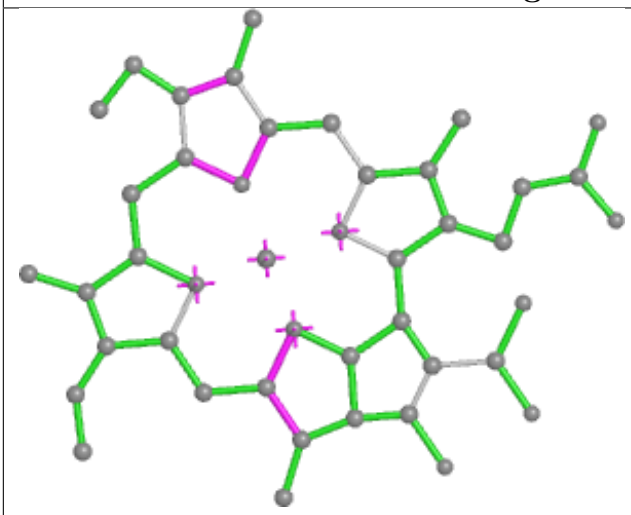


Torsions



Rings

Ligand CLA A 823



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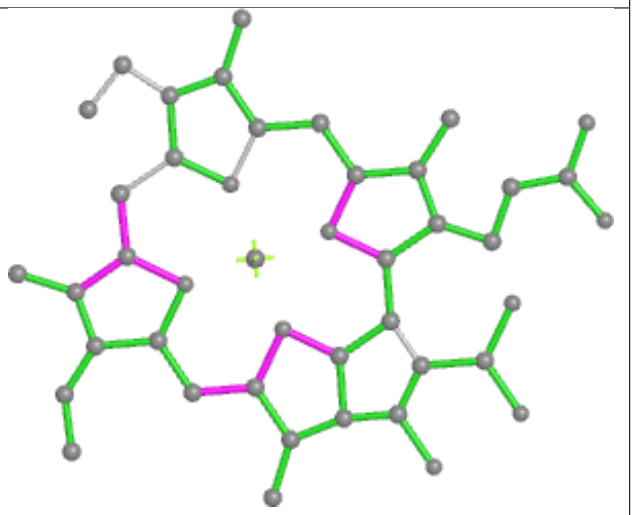
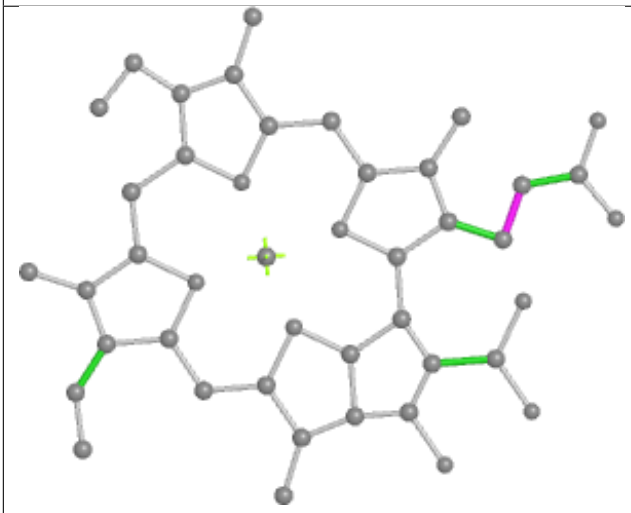
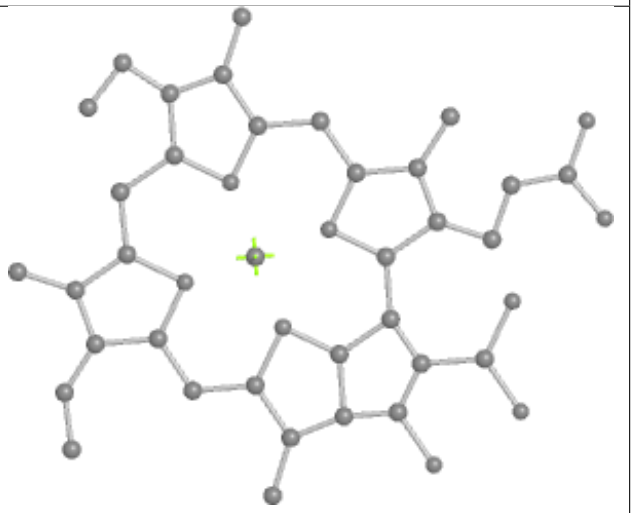


Bond angles

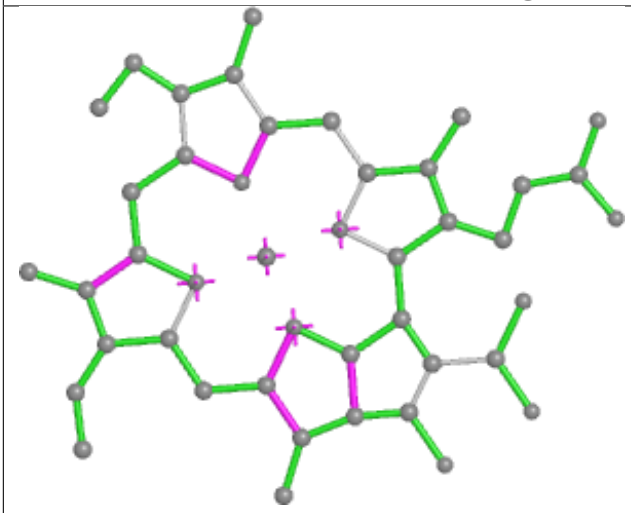


Torsions

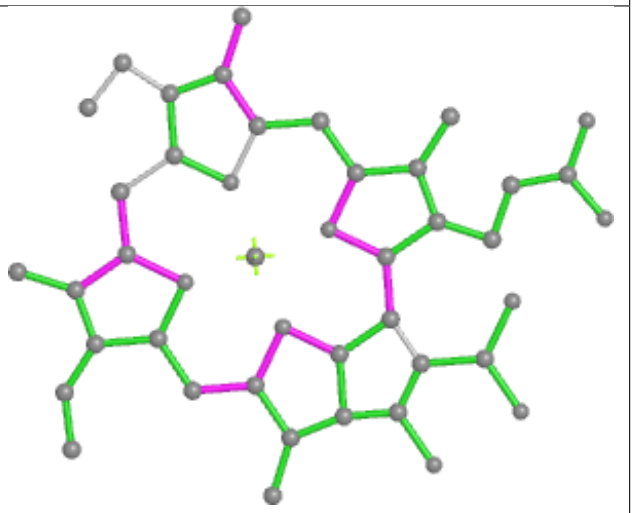


Rings

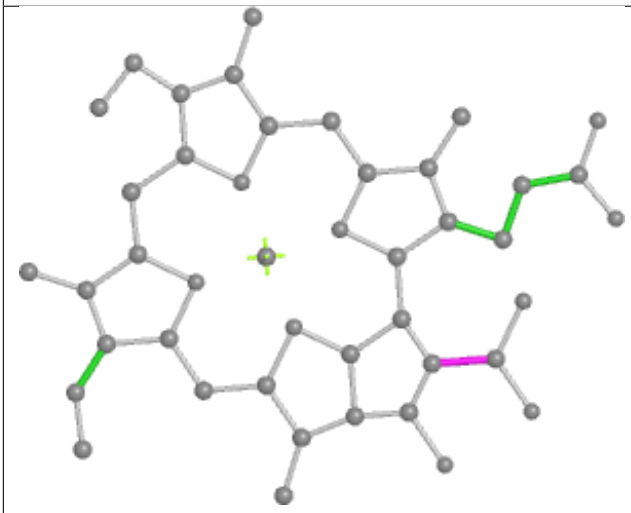
Ligand CLA 3 1015



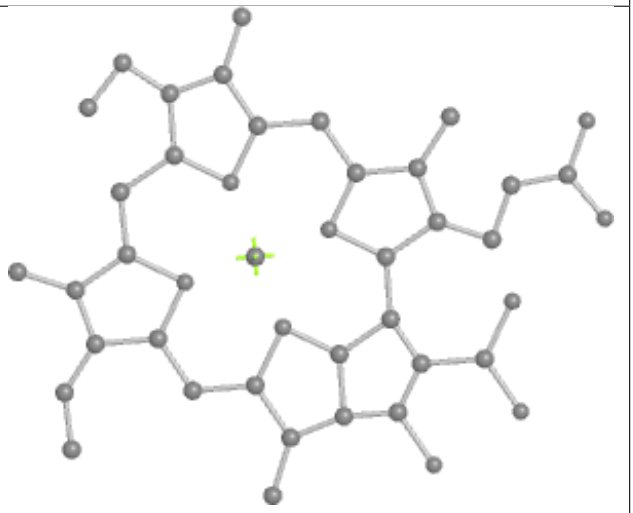
Bond lengths



Bond angles

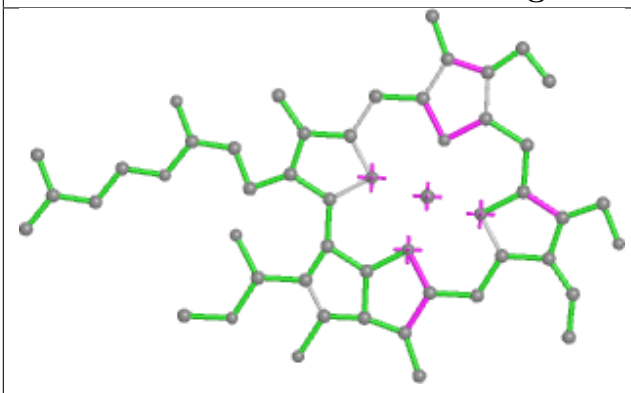


Torsions

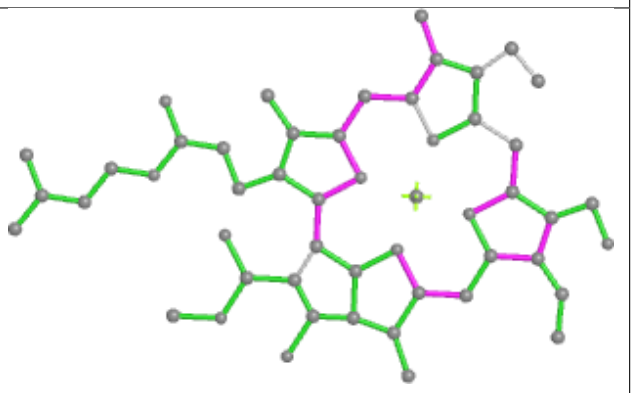


Rings

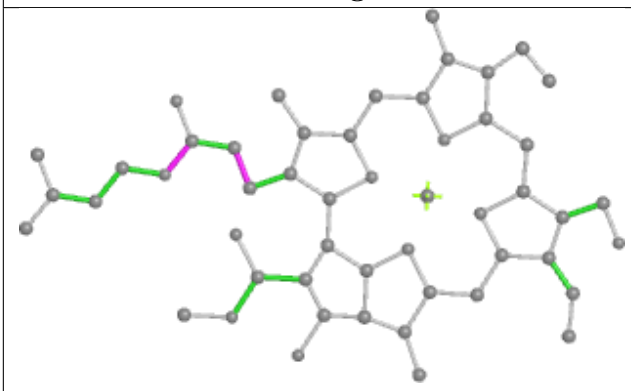
Ligand CHL 0 315



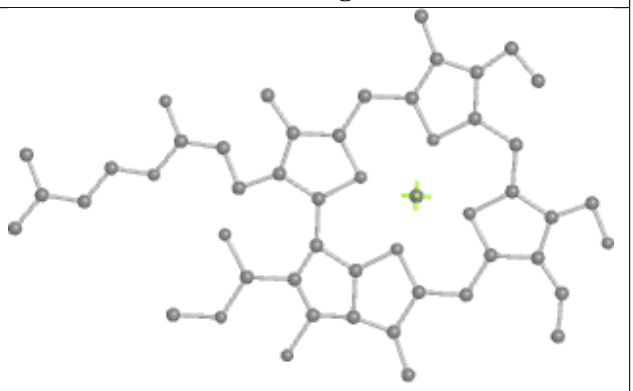
Bond lengths



Bond angles

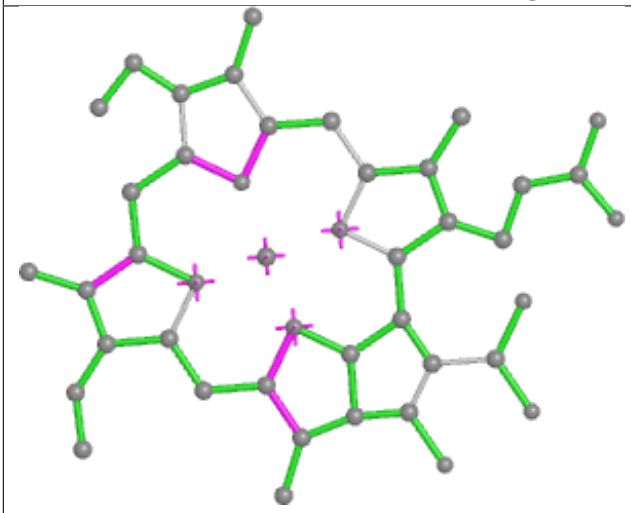


Torsions

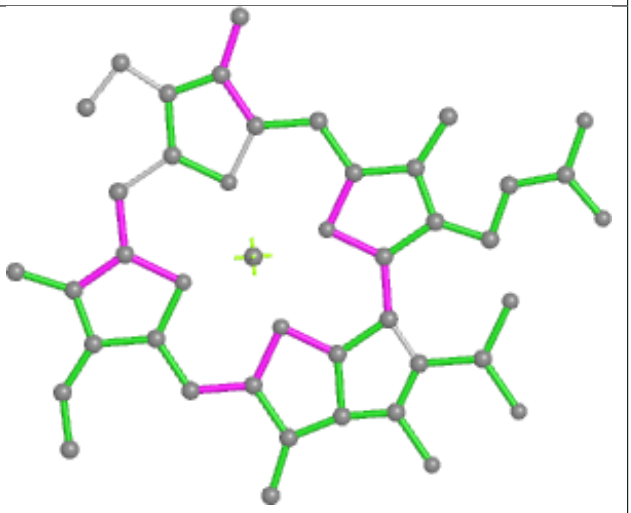


Rings

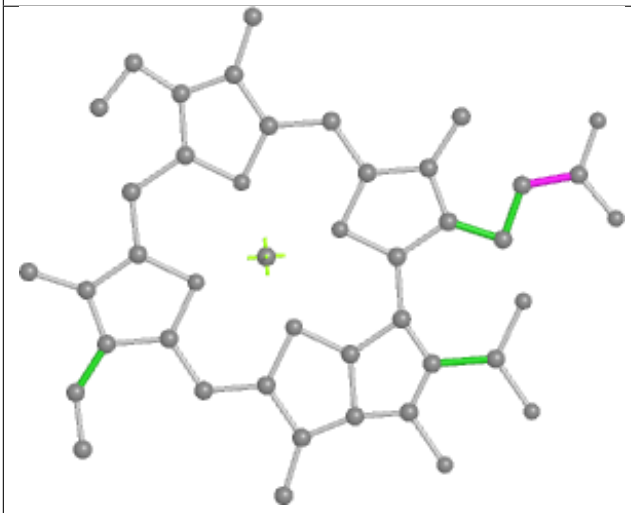
Ligand CLA A 822



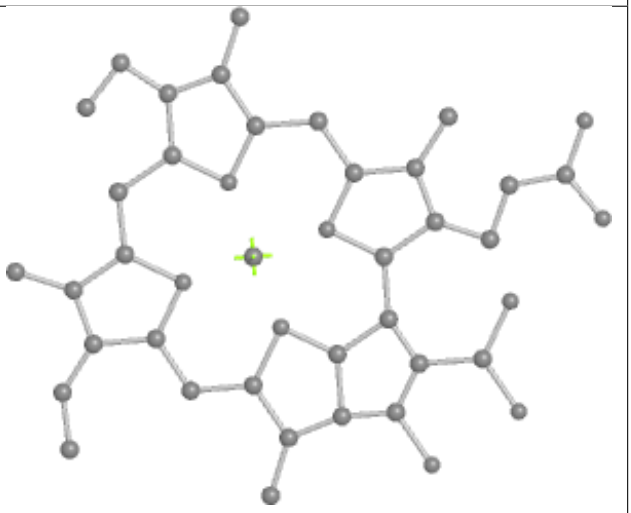
Bond lengths



Bond angles

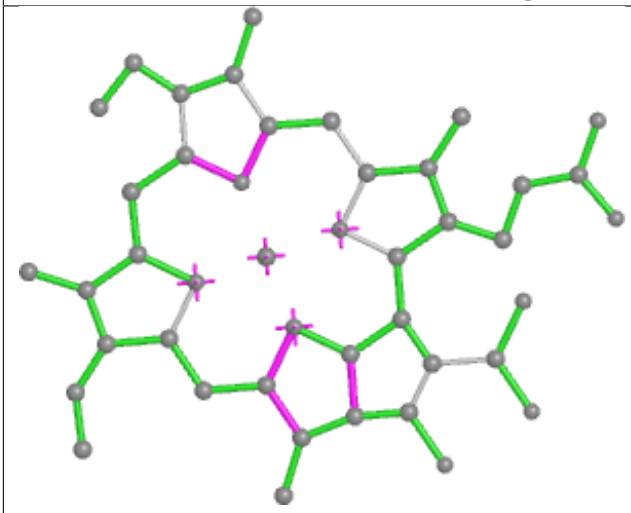


Torsions



Rings

Ligand CLA 1 1007



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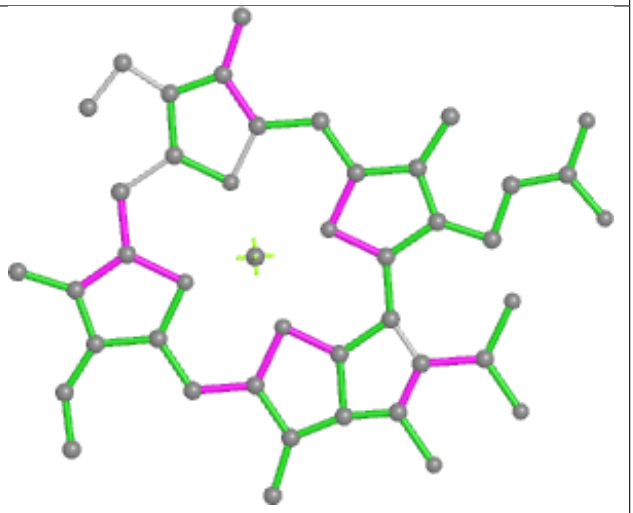

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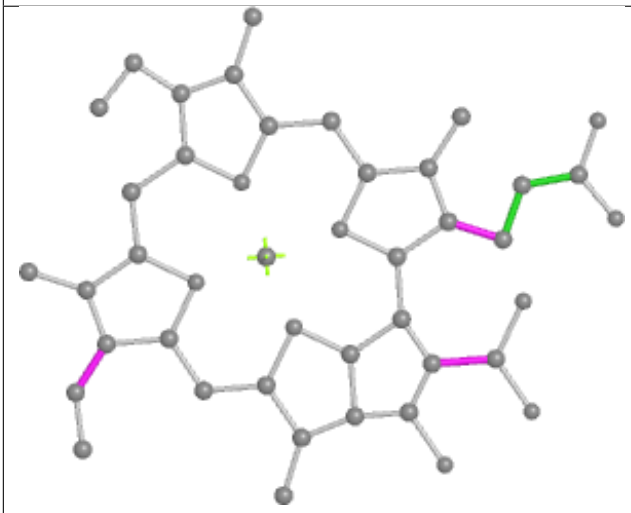

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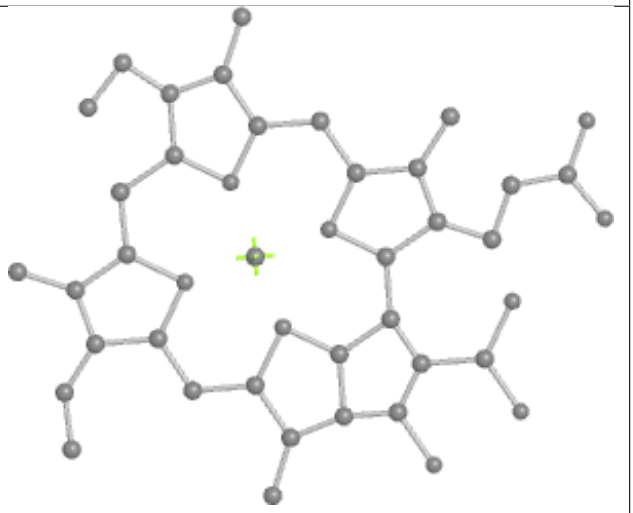
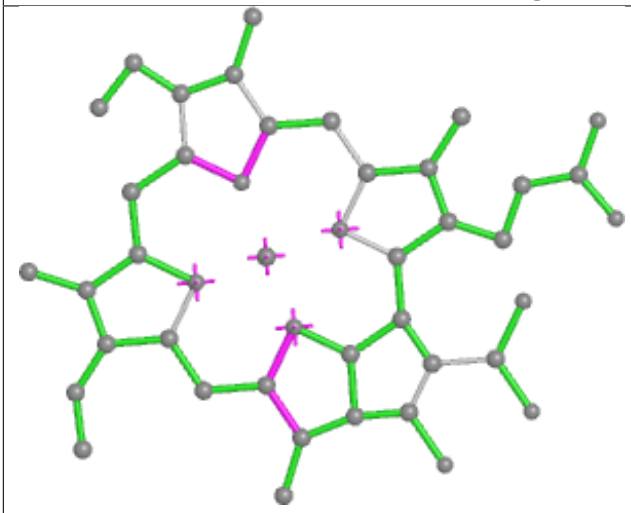


Rings

Ligand CLA 4 311



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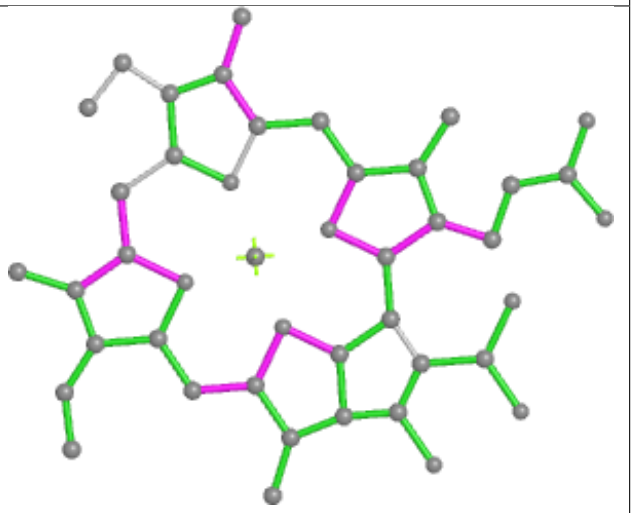

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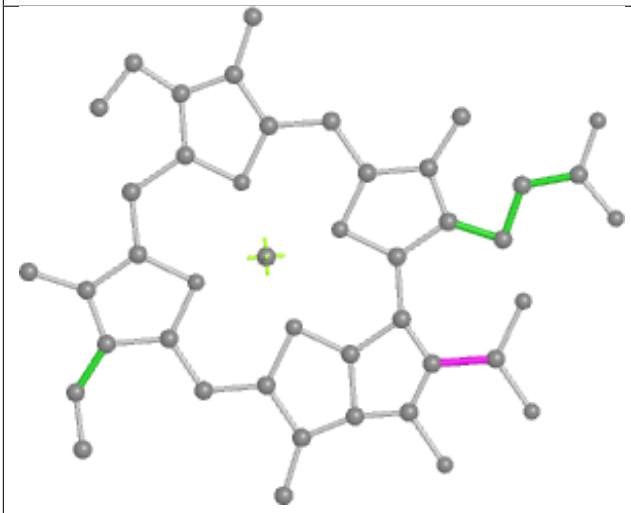

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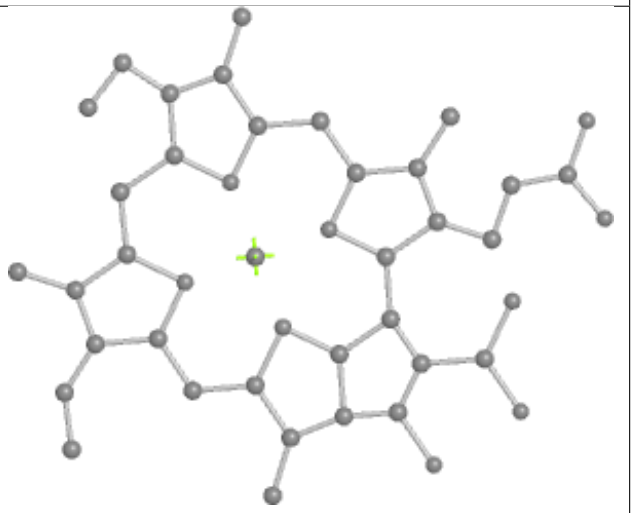
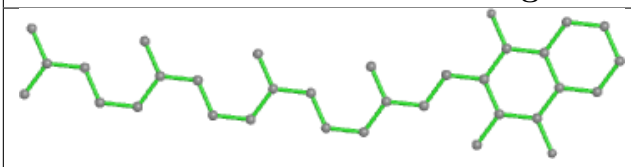


Rings

Ligand PQN A 842



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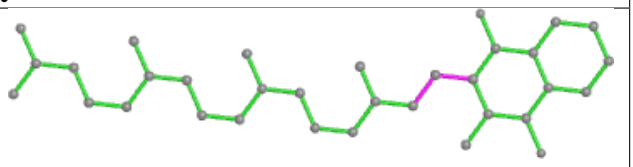

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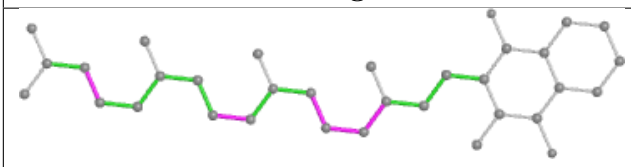
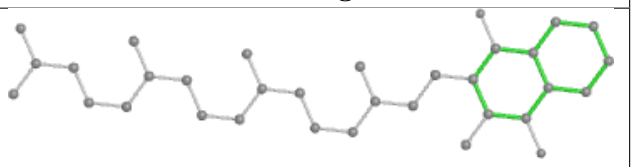
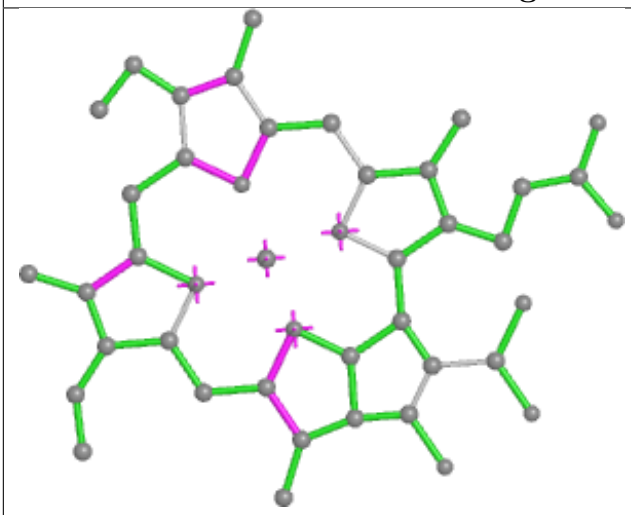


Torsions



Rings

Ligand CLA 1 1004



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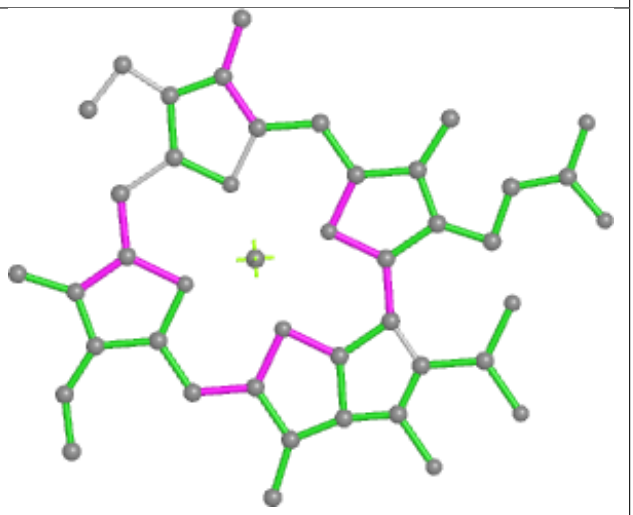
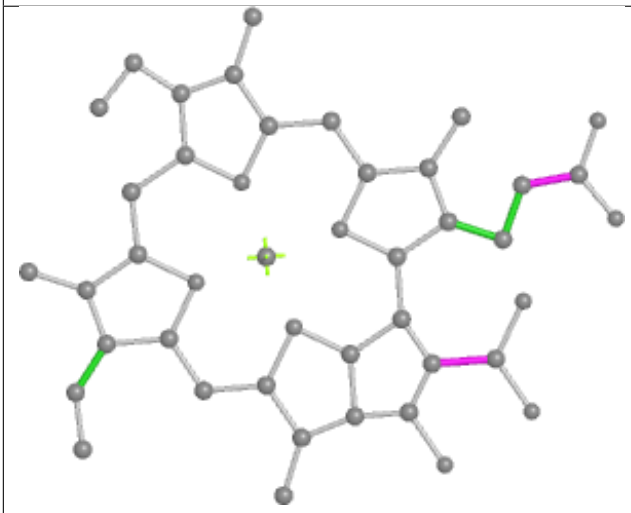


Bond angles



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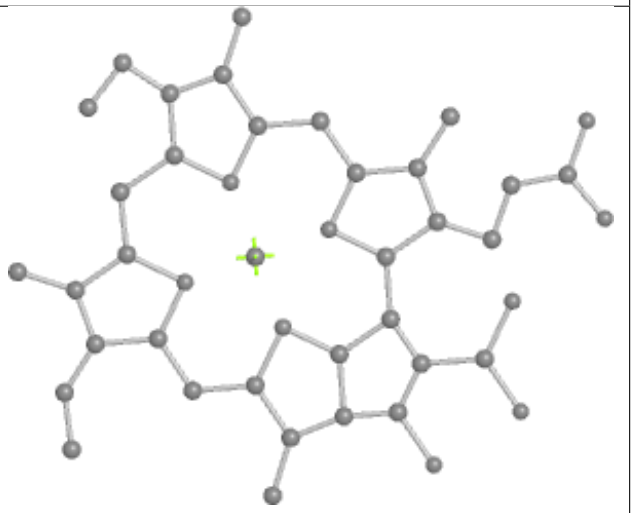
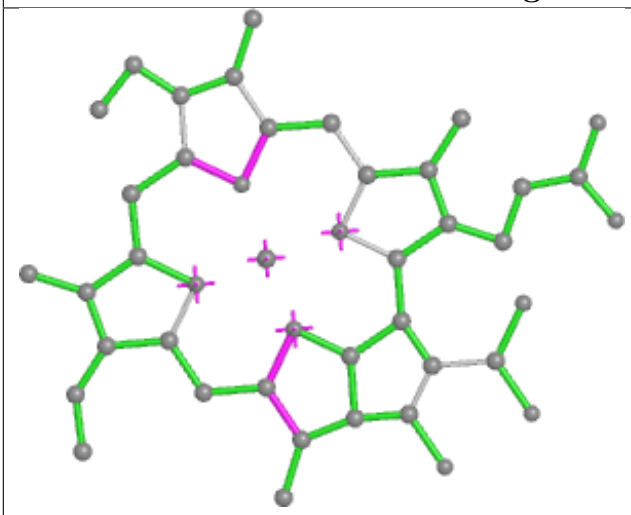


Rings

Ligand CLA G 201



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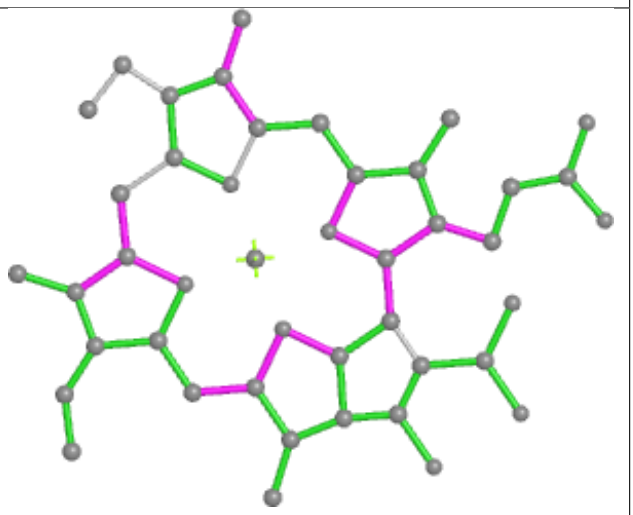

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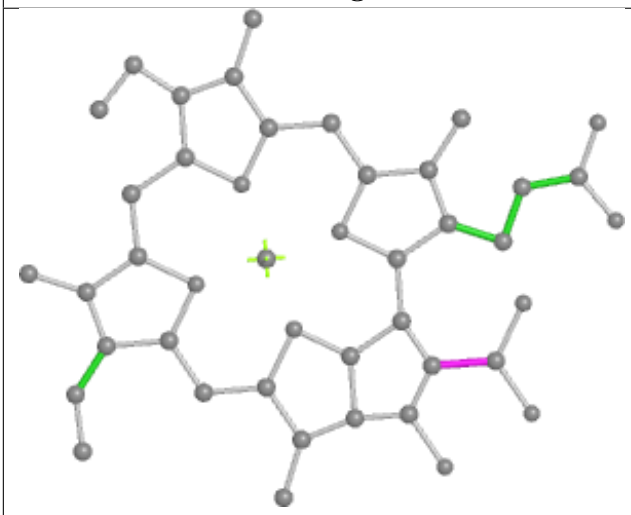

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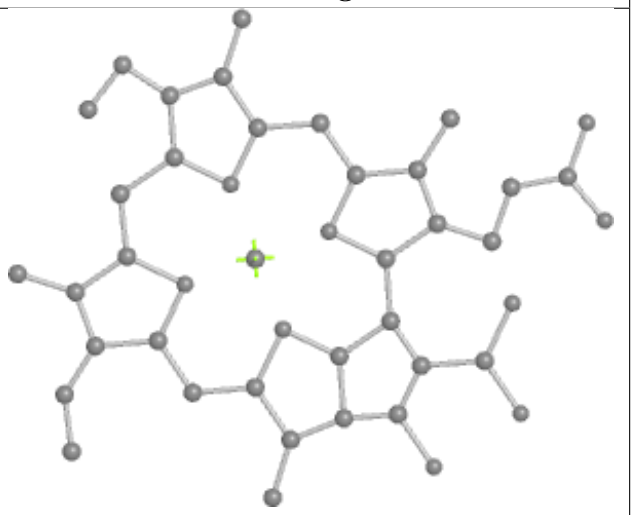
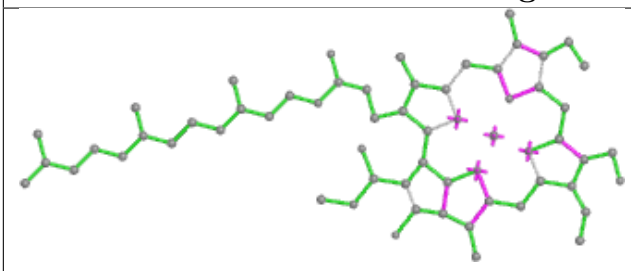


Rings

Ligand CHL 1 1015



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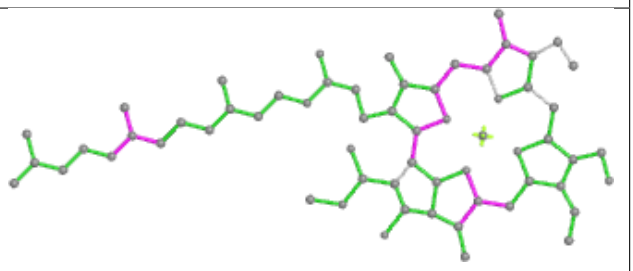
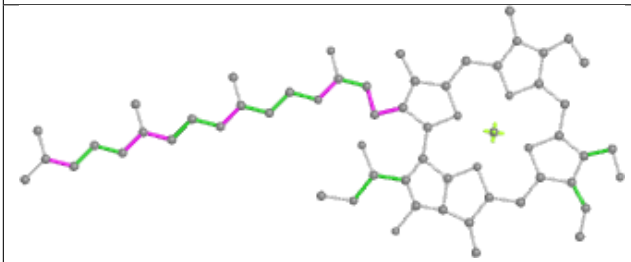


Bond angles



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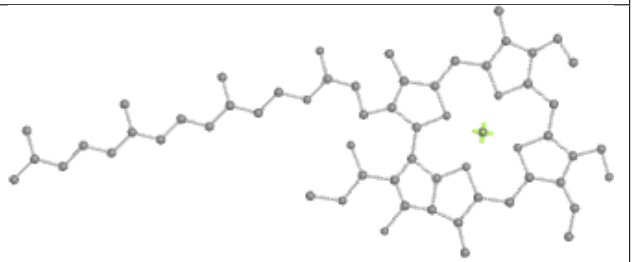
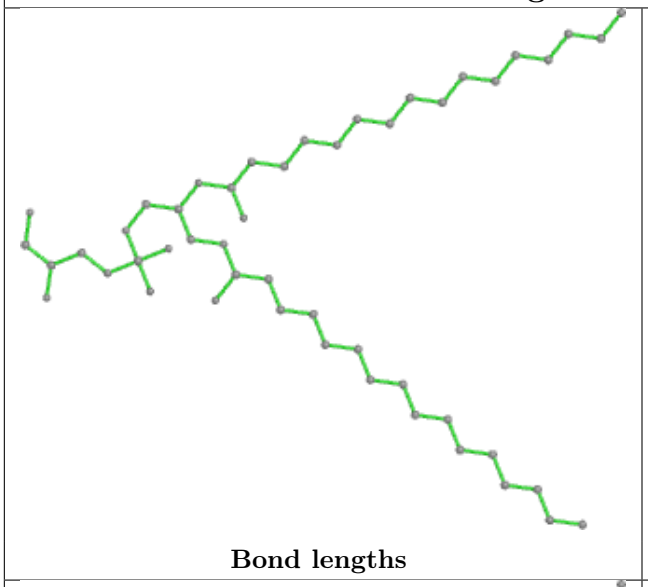


Rings

Ligand LHG 8 301



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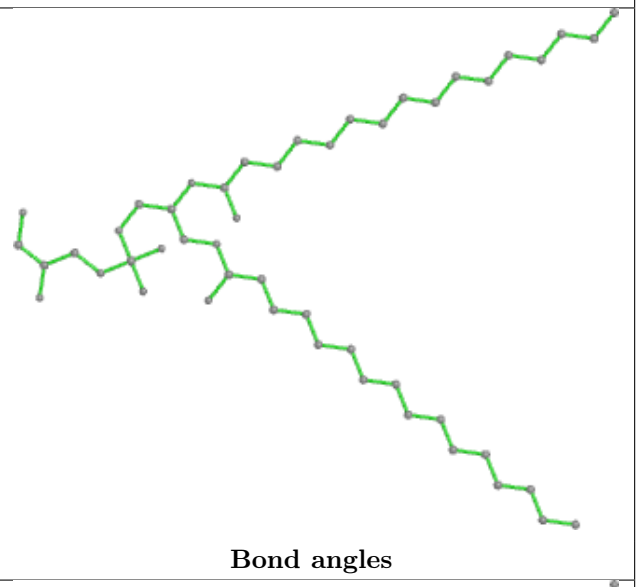
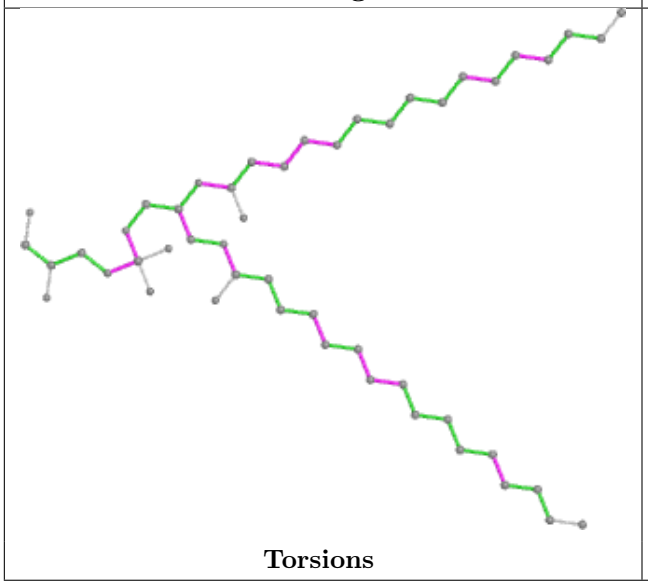


Bond angles



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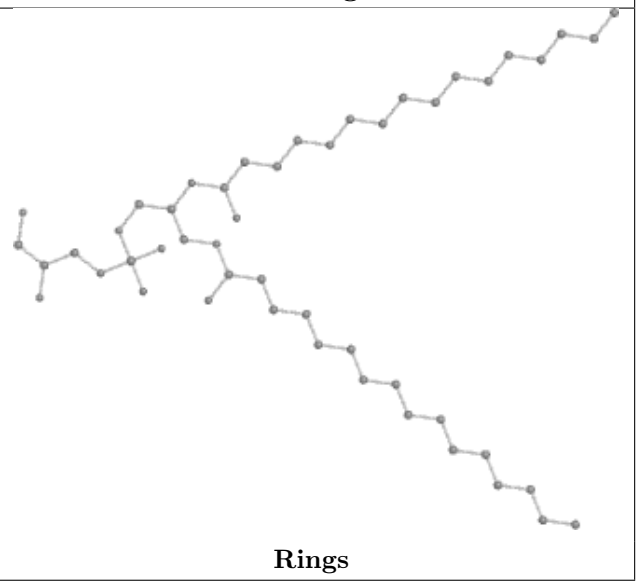
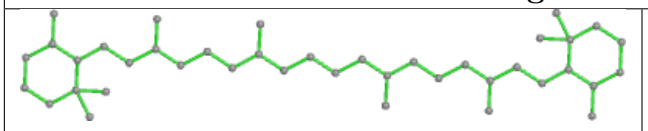


Rings

Ligand BCR J 103



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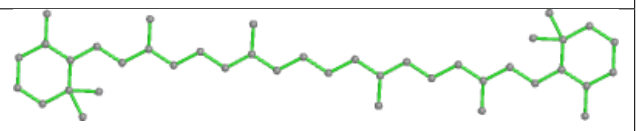
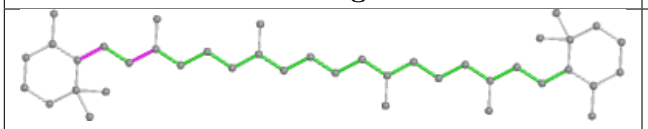


Bond angles



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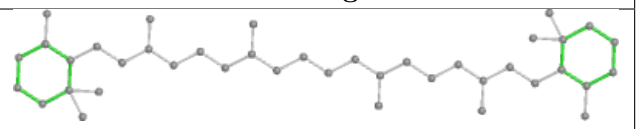
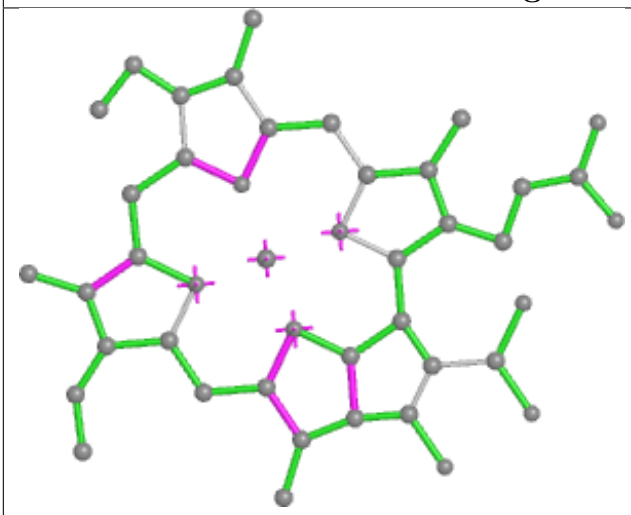


Rings

Ligand CLA A 802



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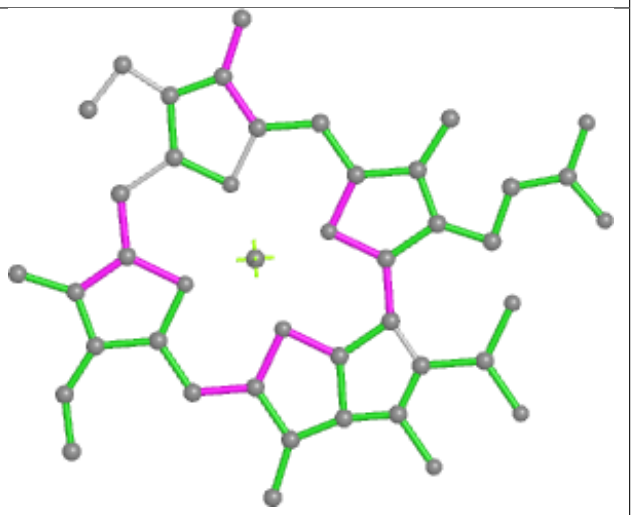
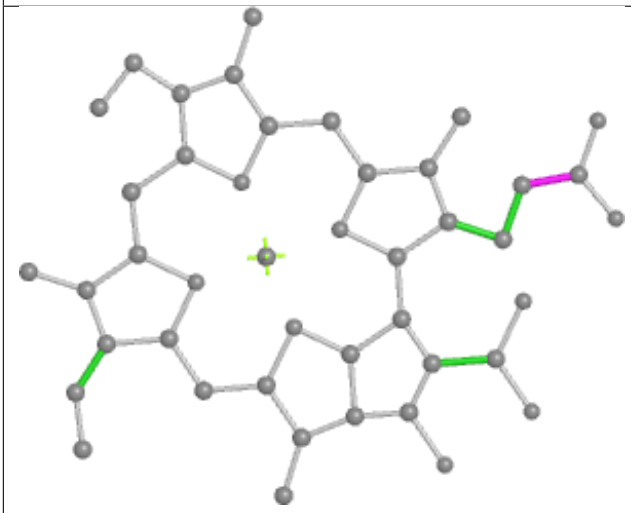
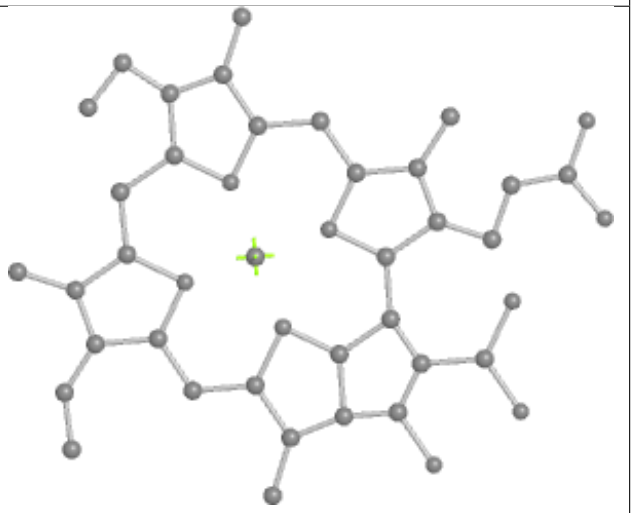


Bond angles

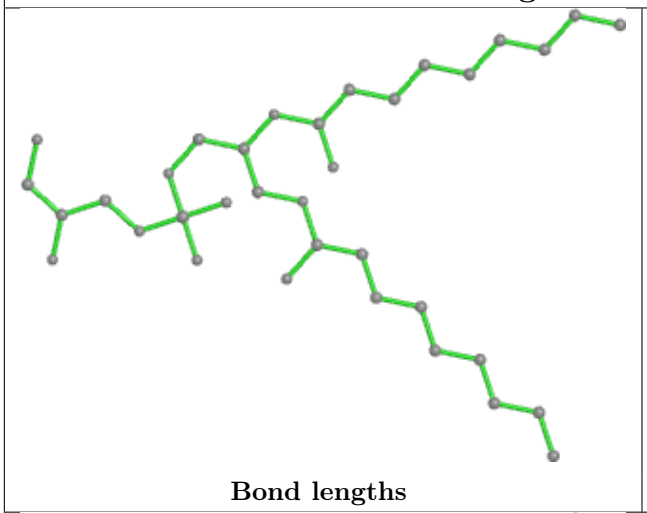


Torsions



Rings

Ligand LHG 7 1016



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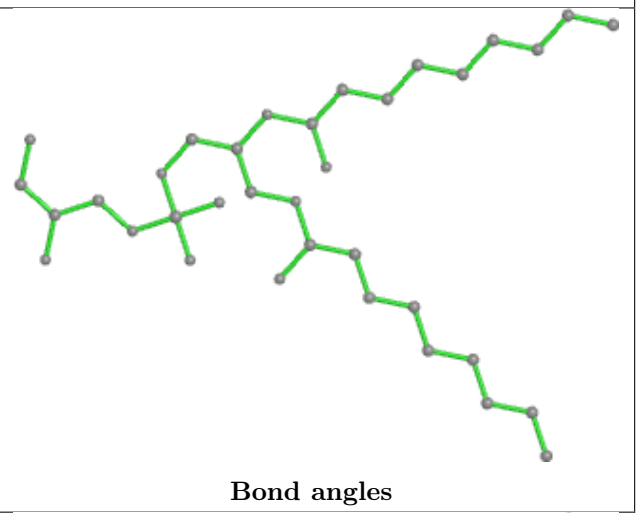

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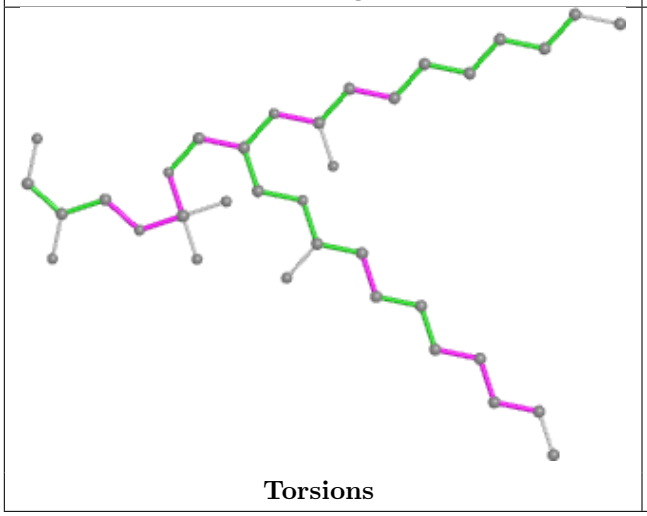

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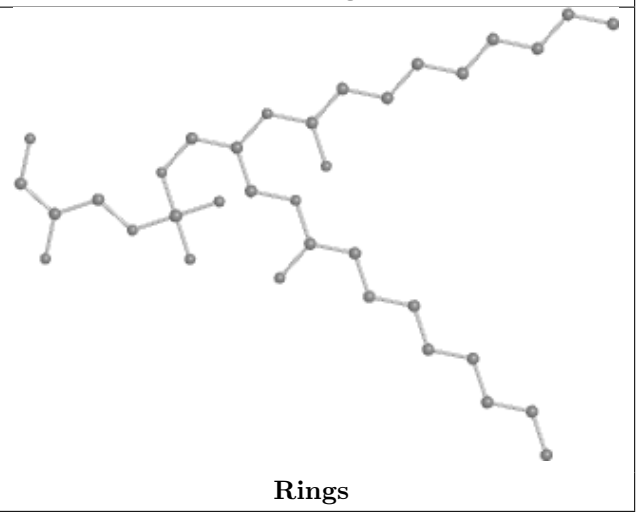
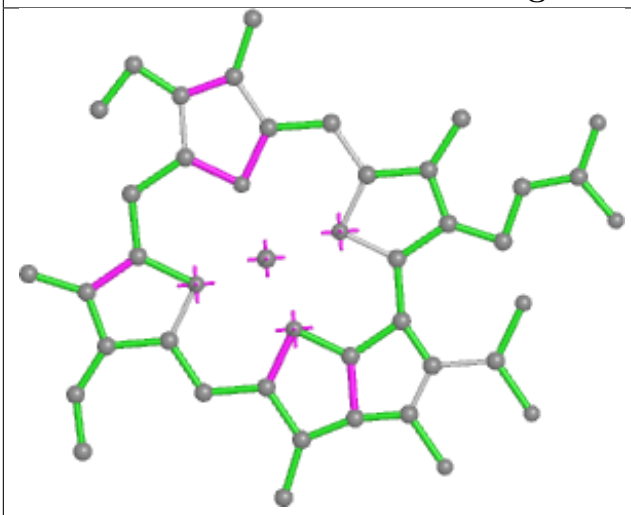


Rings

Ligand CLA 5 301



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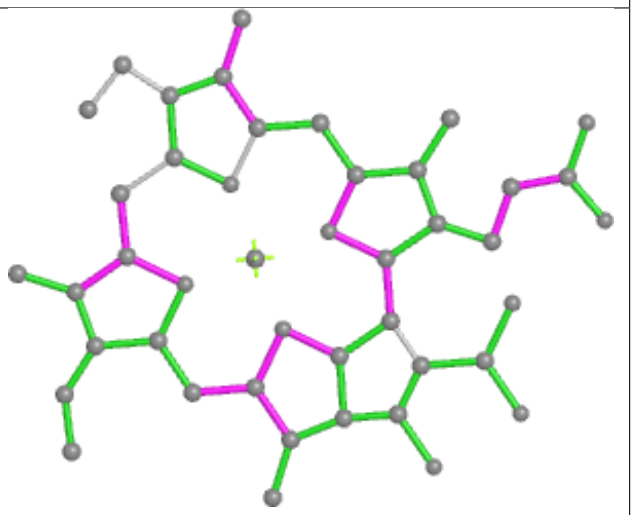

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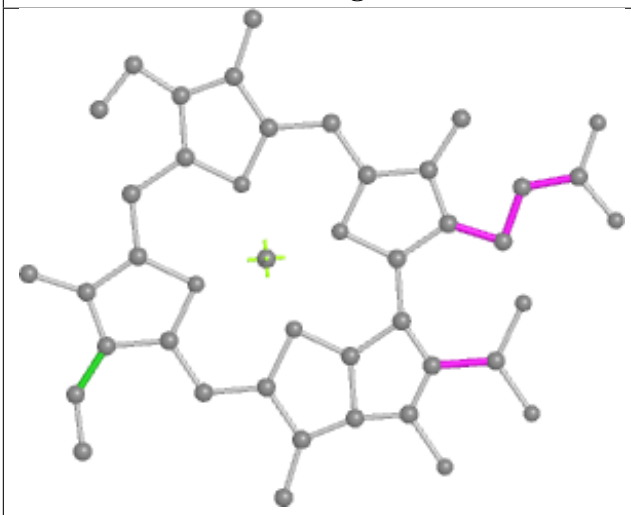

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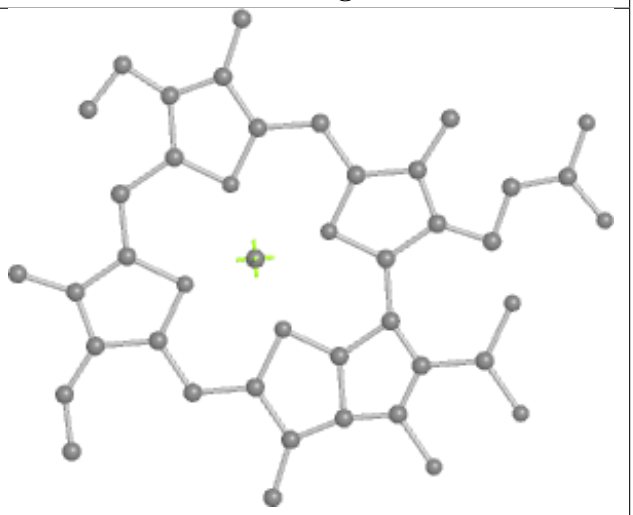
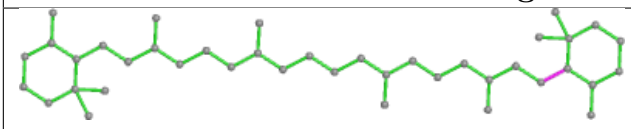


Rings

Ligand BCR 1 1001



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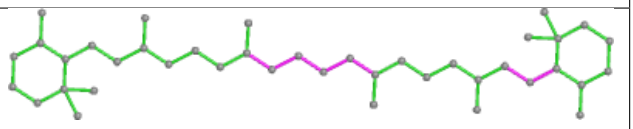
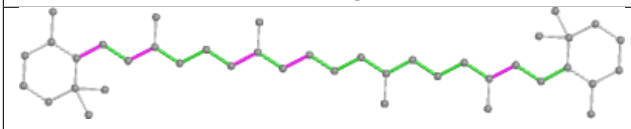


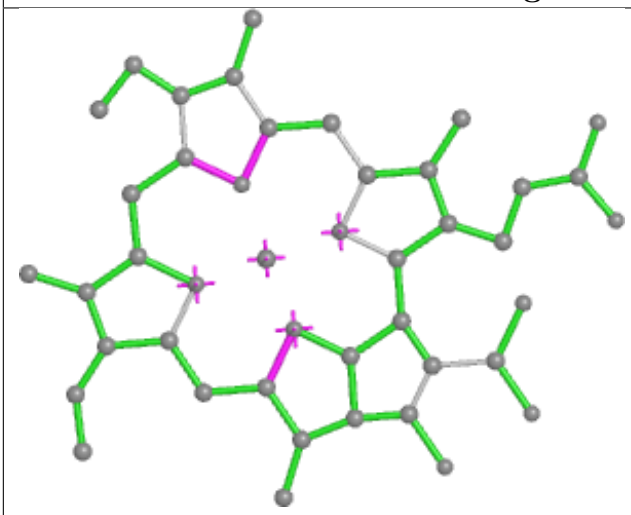
Bond angles



Torsions

Rings

Ligand CLA A 817



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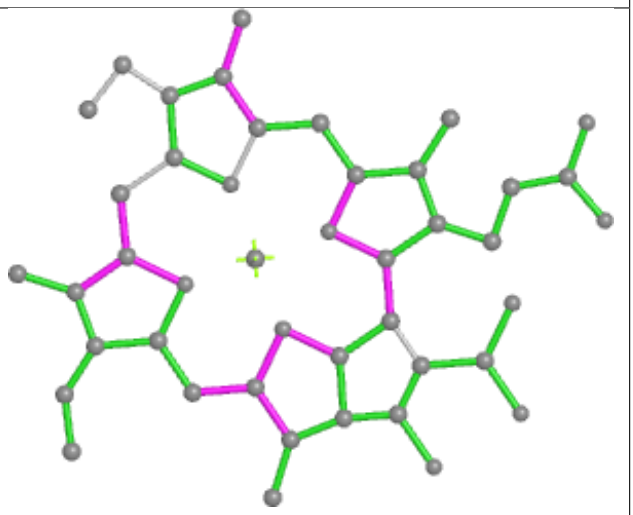
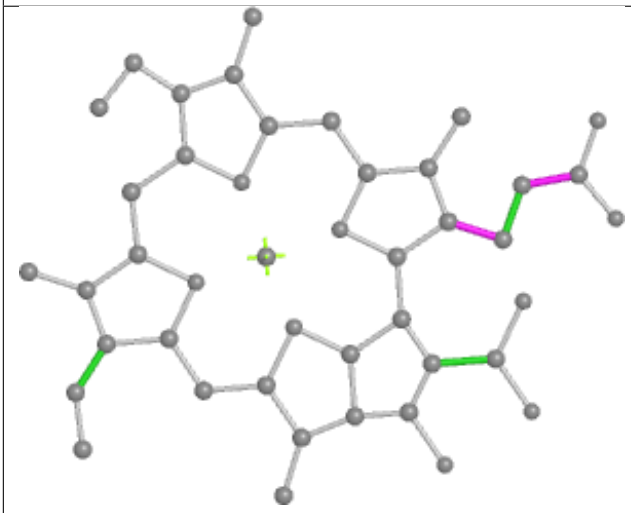
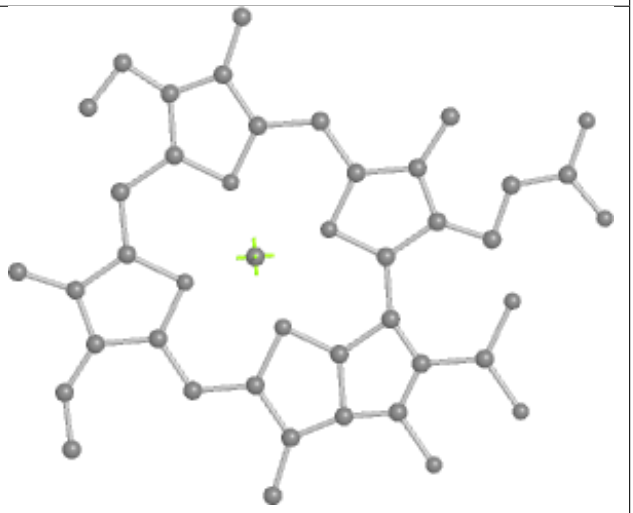


Bond angles

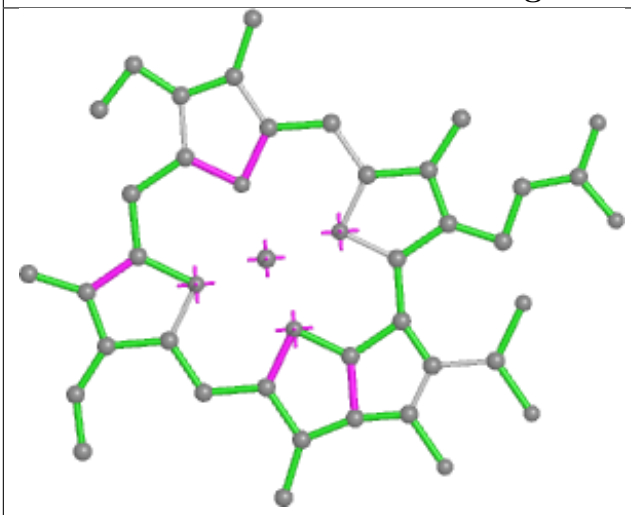


Torsions

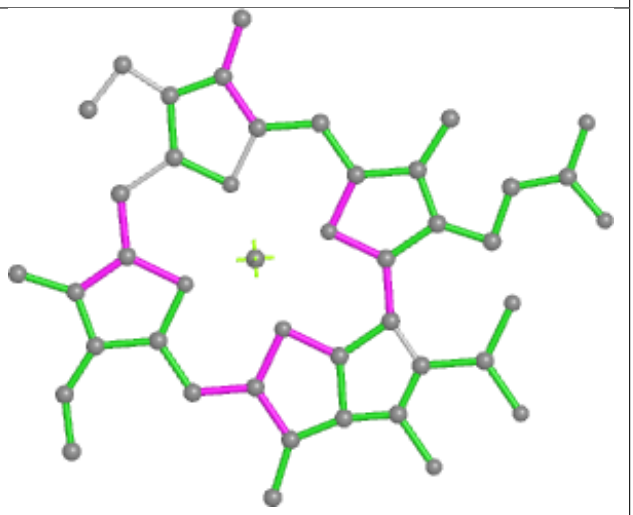


Rings

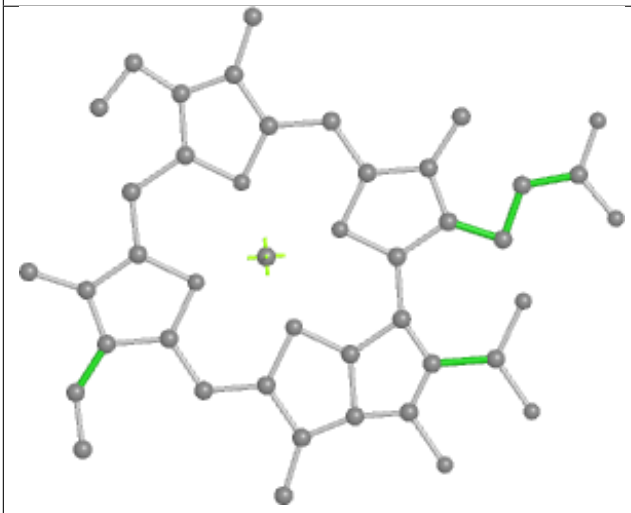
Ligand CLA B 824



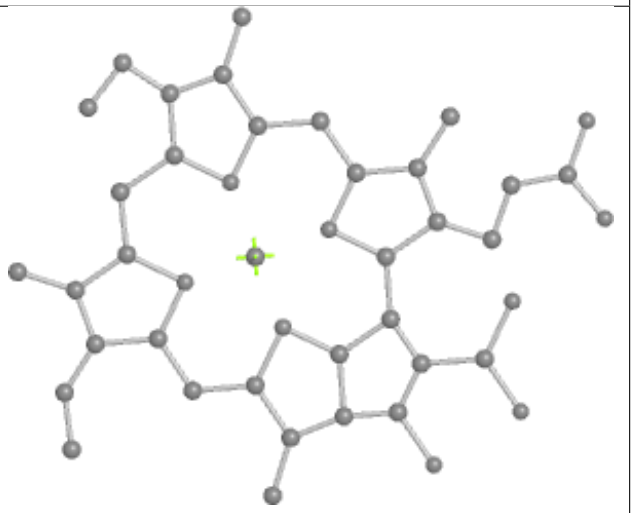
Bond lengths



Bond angles

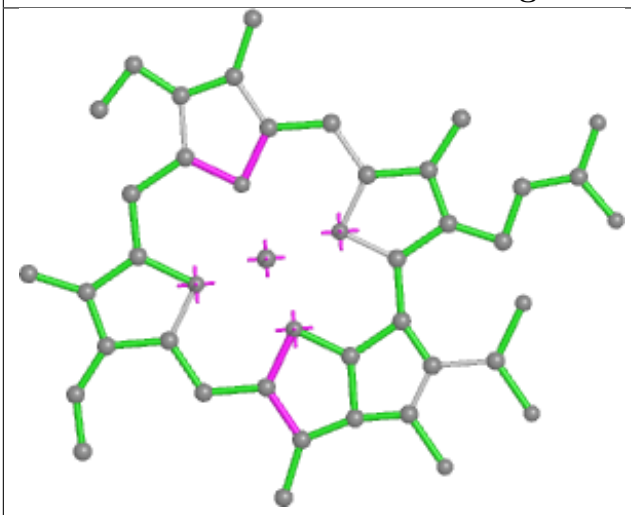


Torsions

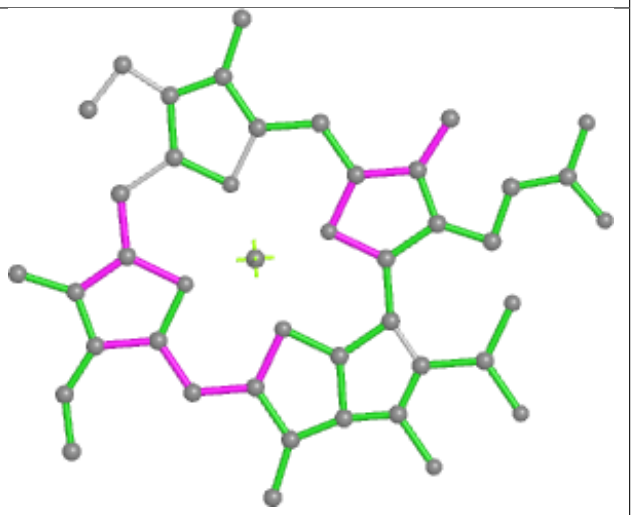


Rings

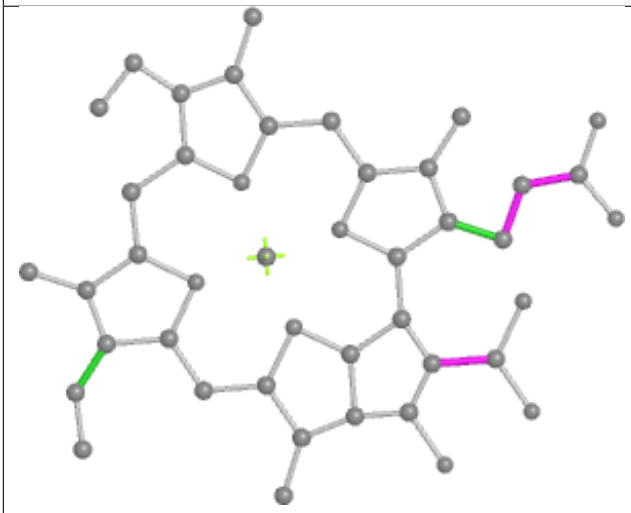
Ligand CLA 7 1006



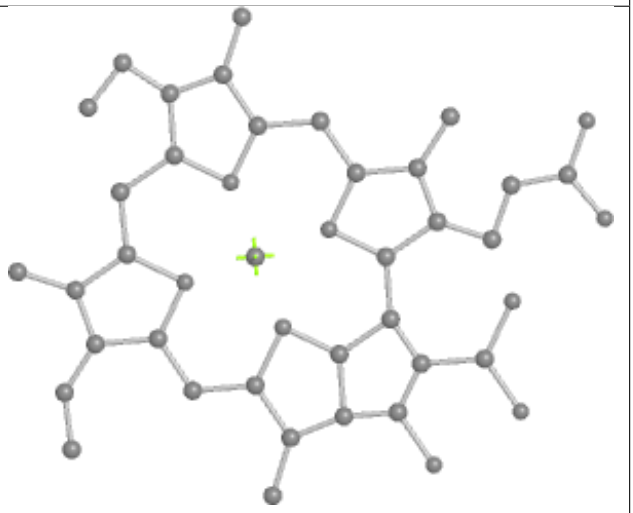
Bond lengths



Bond angles

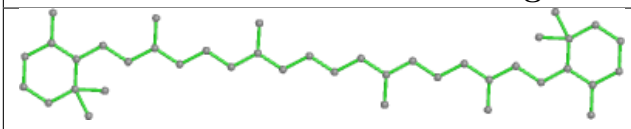


Torsions



Rings

Ligand BCR F 304



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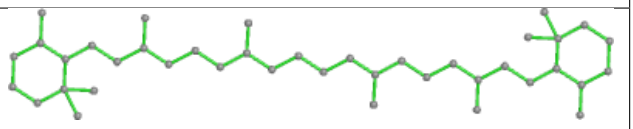
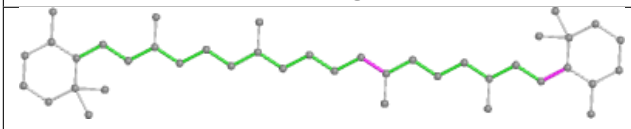


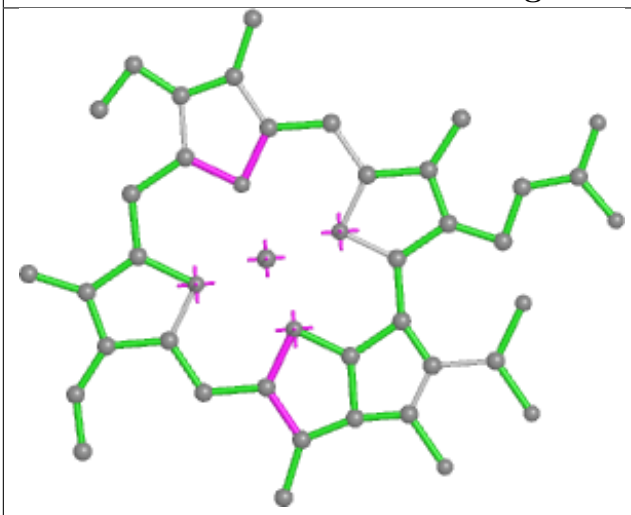
Bond angles



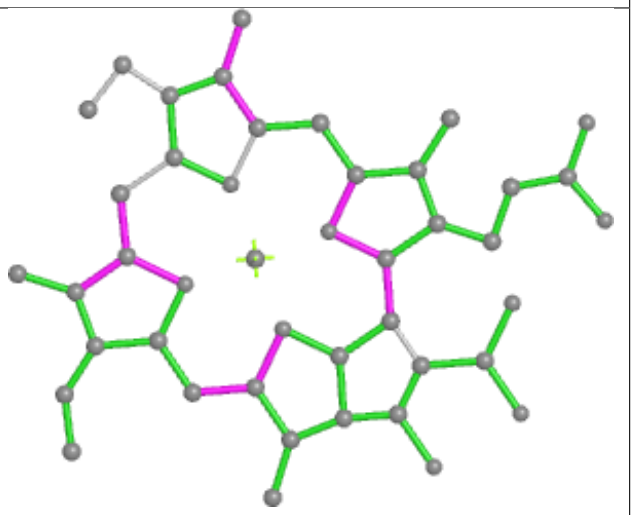
Torsions

Rings

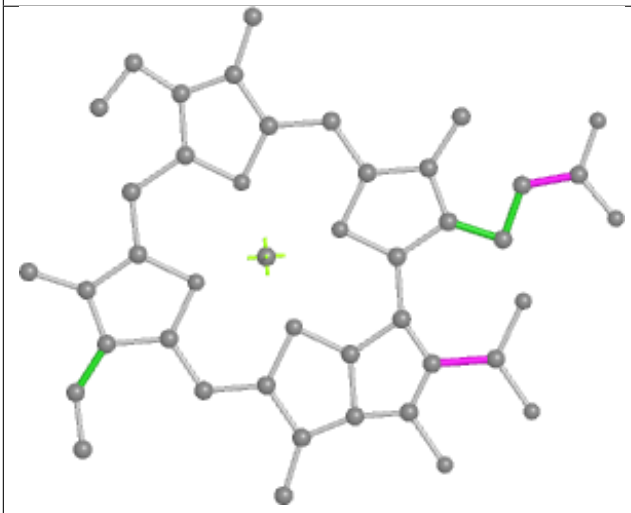
Ligand CLA B 812



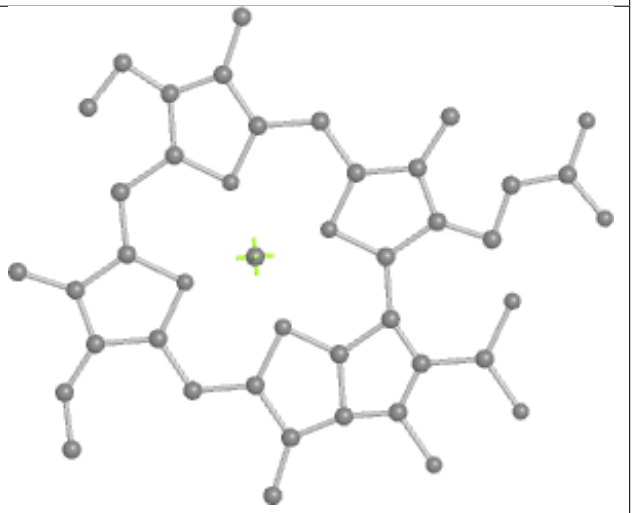
Bond lengths



Bond angles

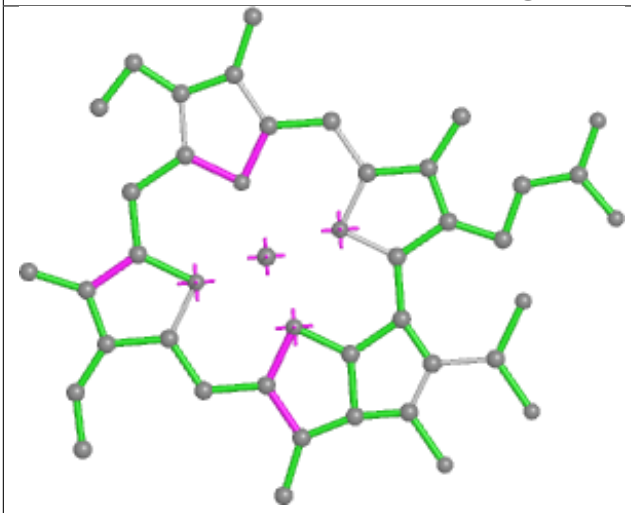


Torsions



Rings

Ligand CLA 1 1005



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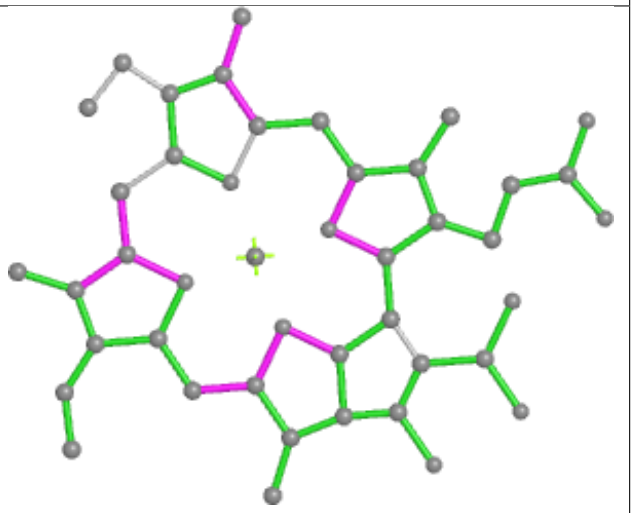
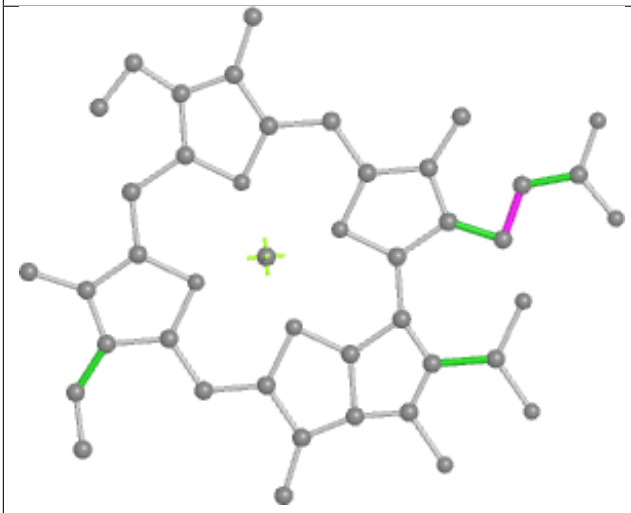
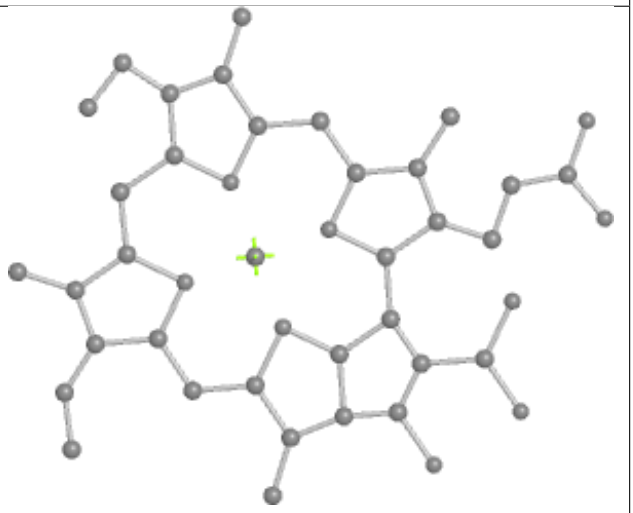


Bond angles

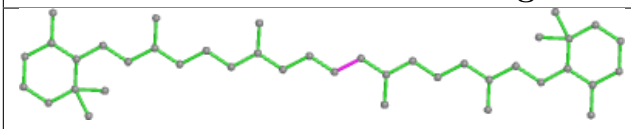


Torsions



Rings

Ligand BCR 7 1003



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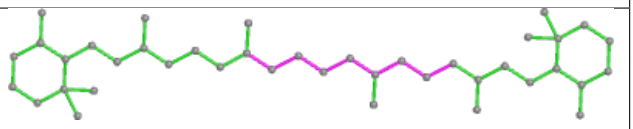
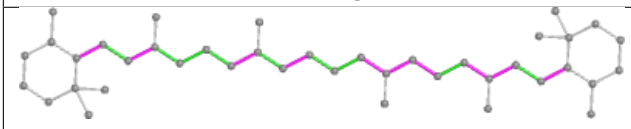


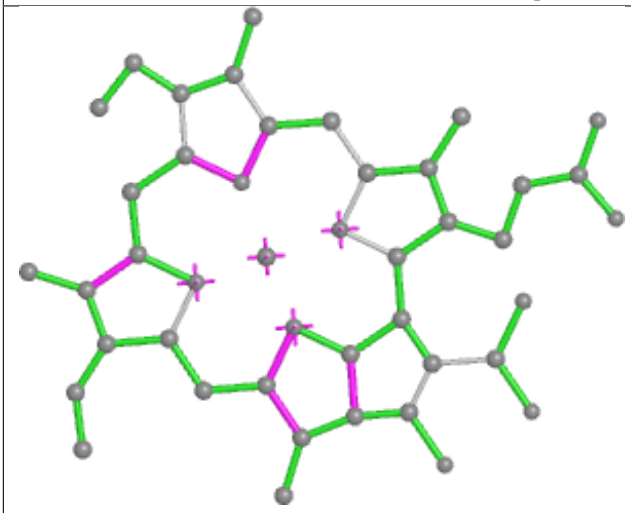
Bond angles



Torsions

Rings

Ligand CLA 6 311



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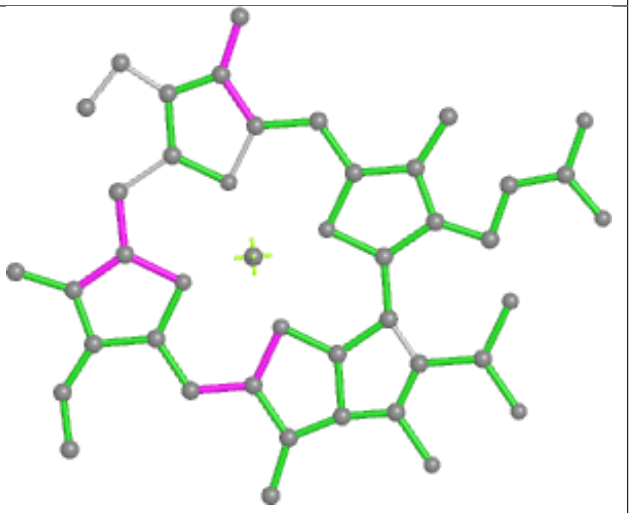
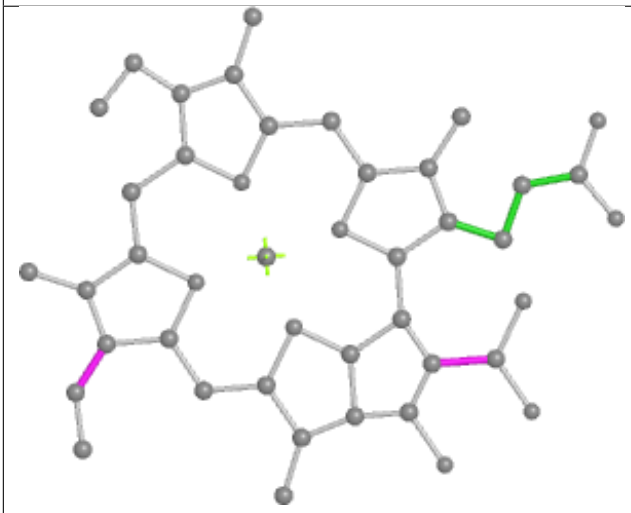


Bond angles



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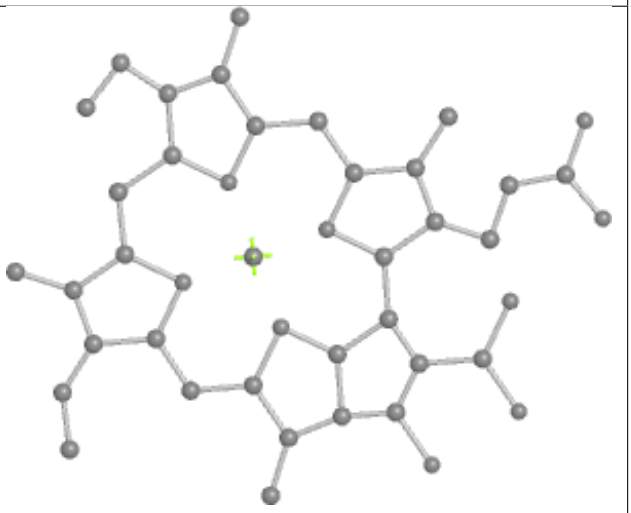
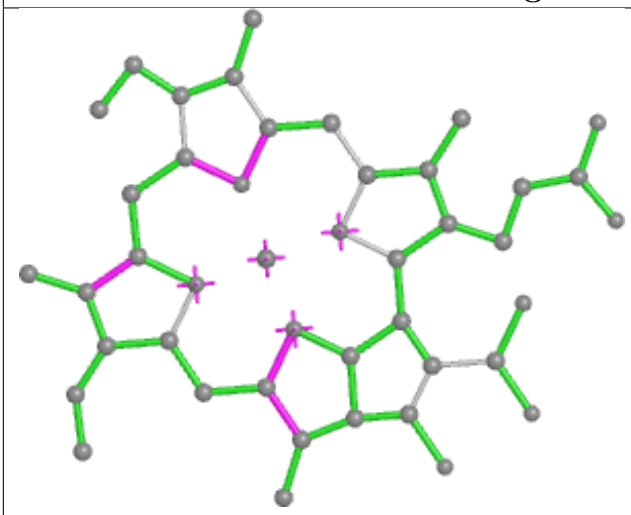


Rings

Ligand CLA B 815



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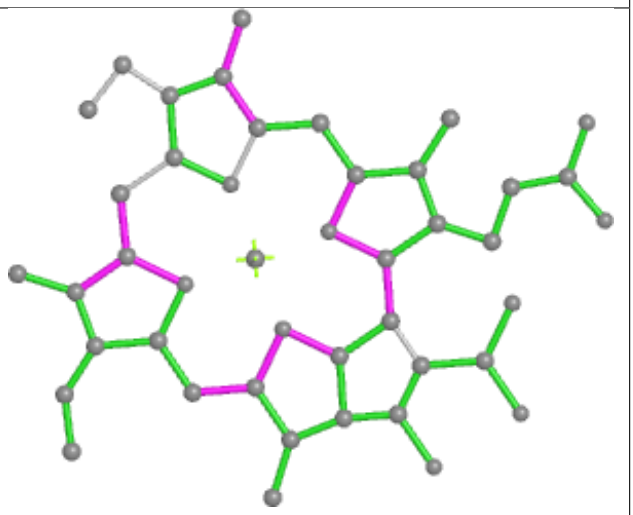
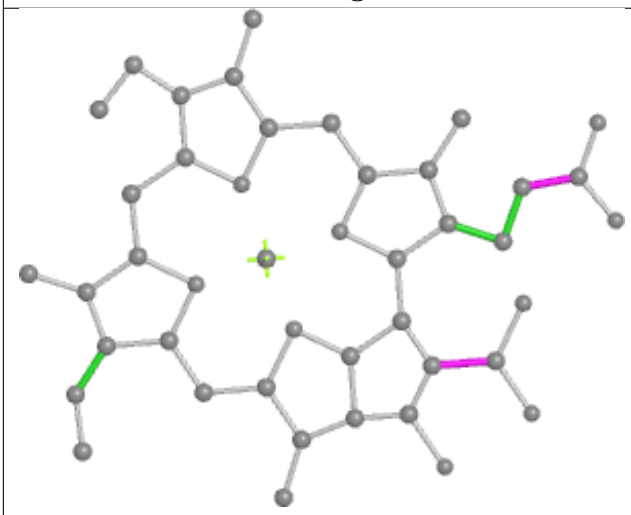
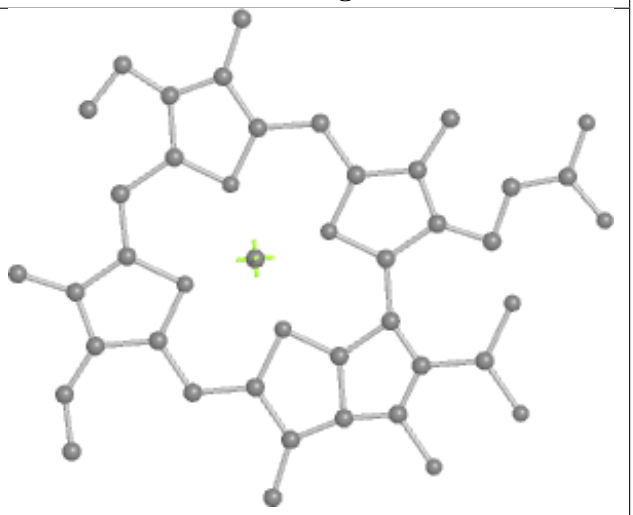


Bond angles

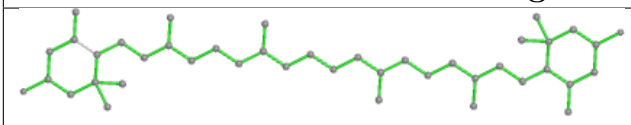


Torsions



Rings

Ligand LUT 0 304



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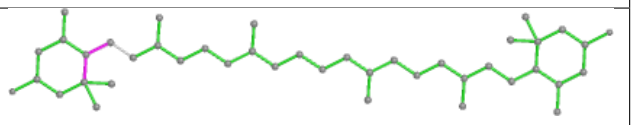
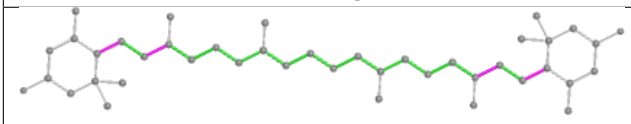


Bond angles



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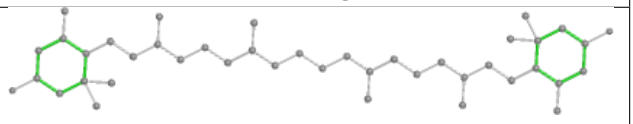
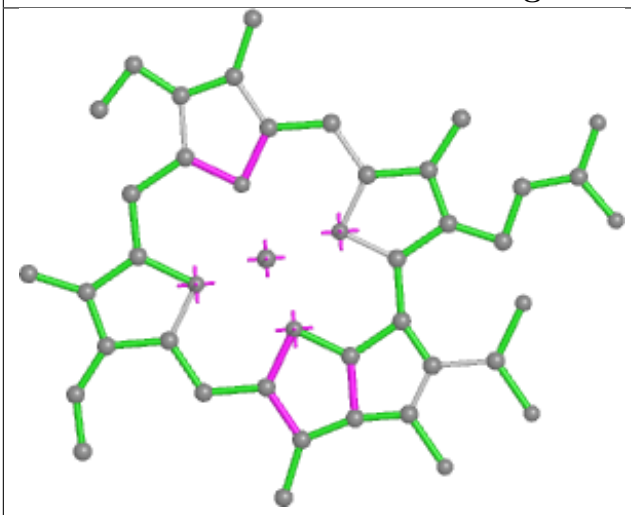


Rings

Ligand CLA A 806



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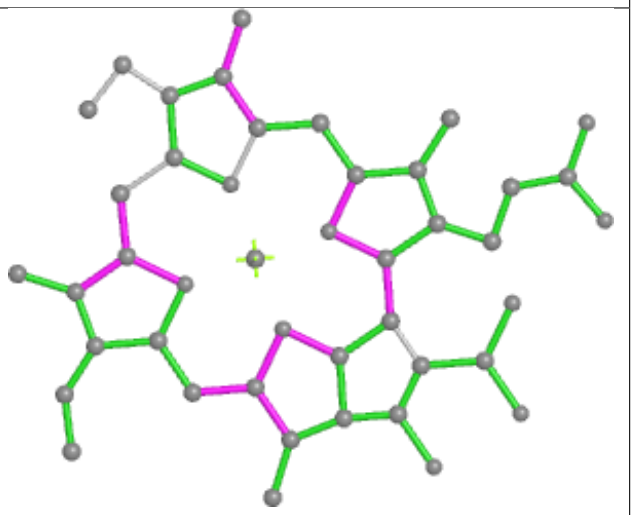
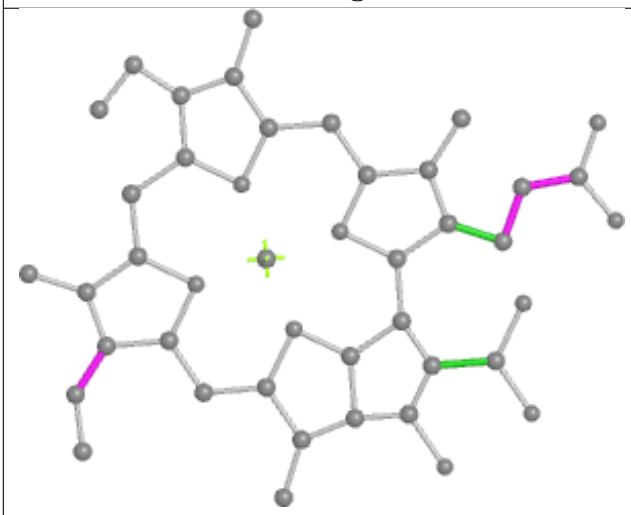
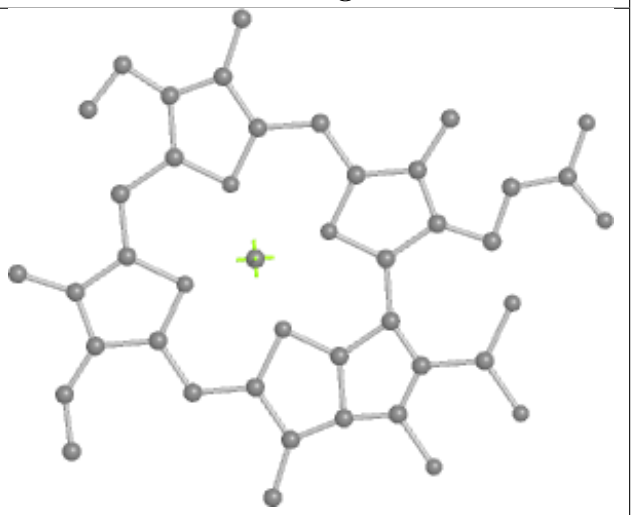


Bond angles

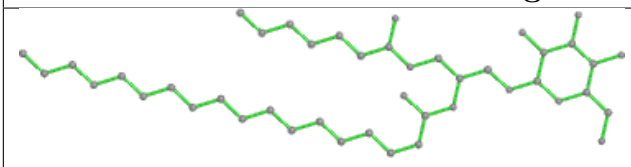


Torsions



Rings

Ligand LMG 6 319



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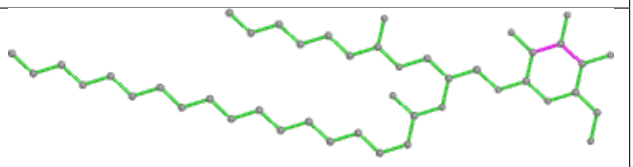
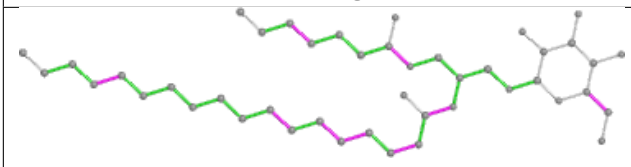
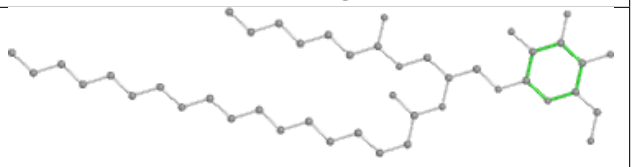


Bond angles

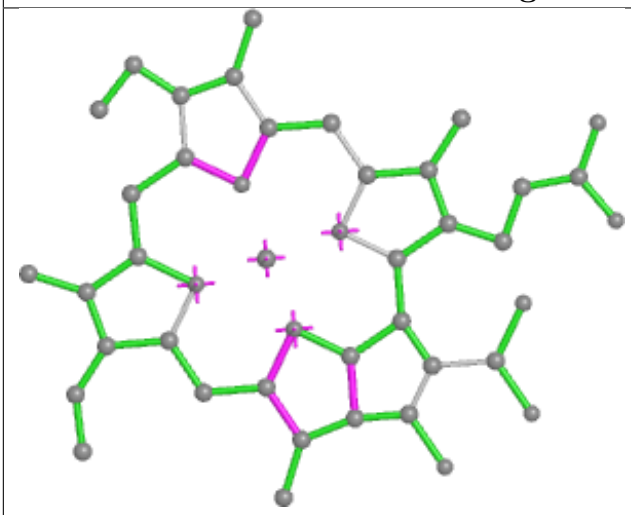


Torsions



Rings

Ligand CLA 7 1008



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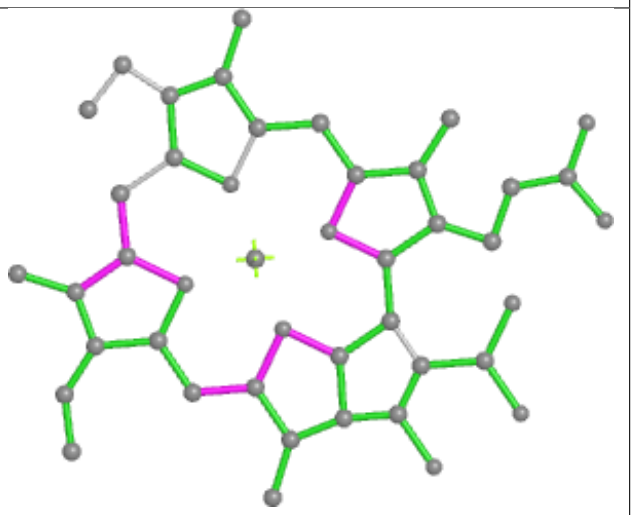
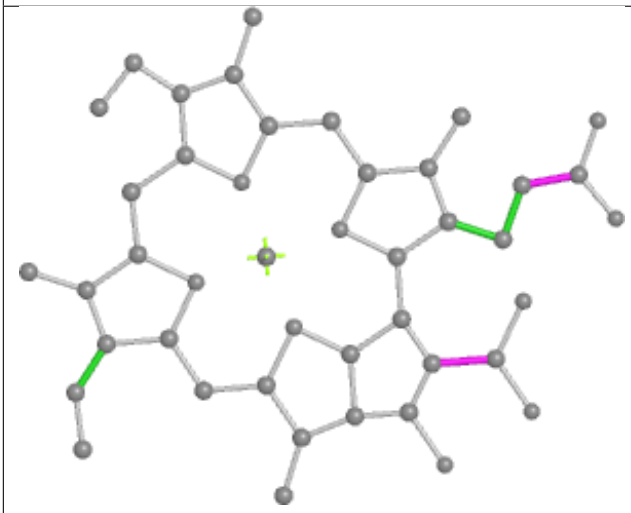


Bond angles



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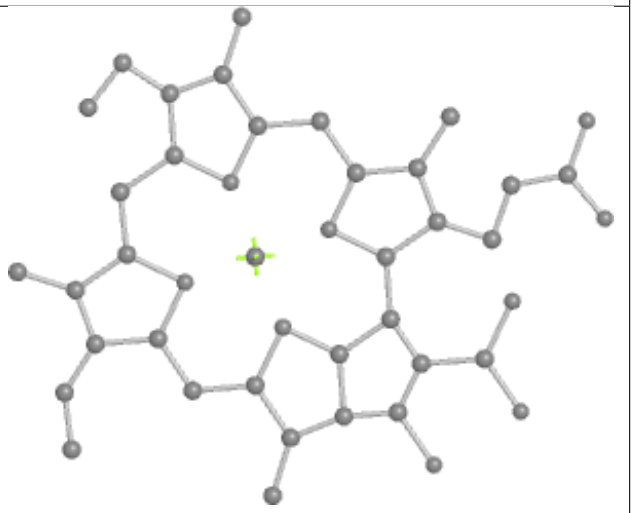
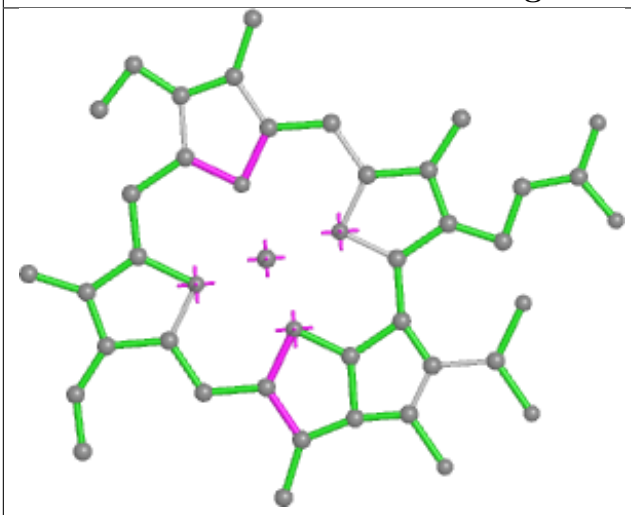


Rings

Ligand CLA B 837



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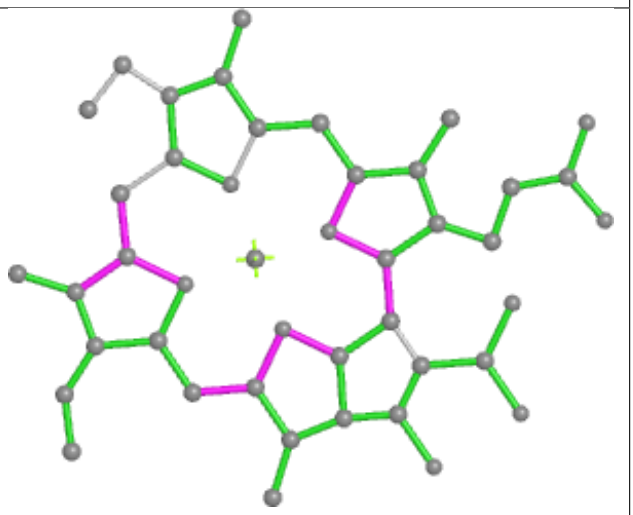
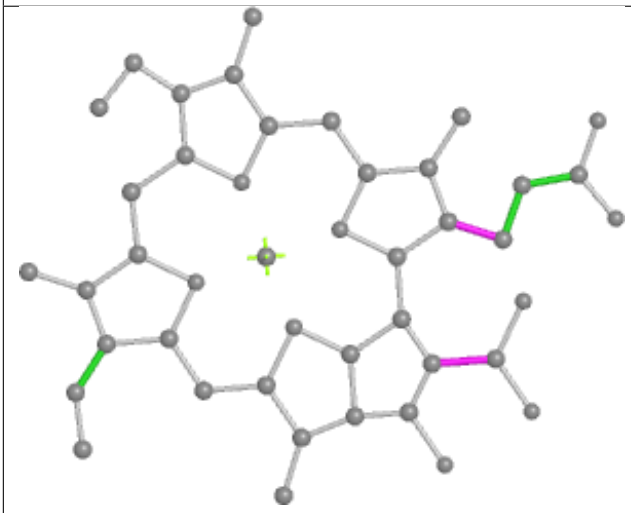


Bond angles



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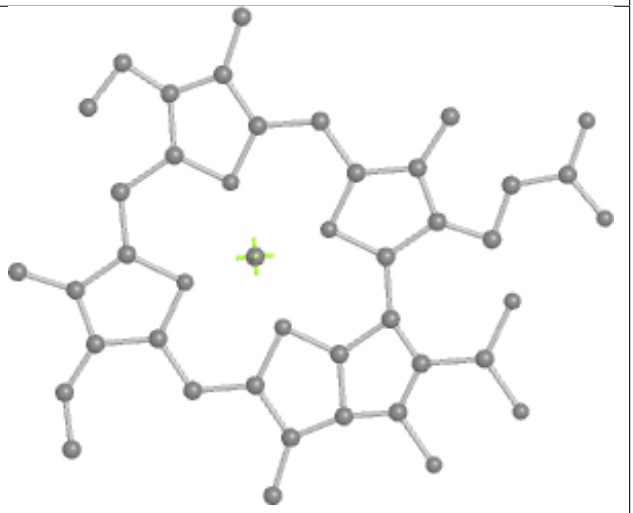
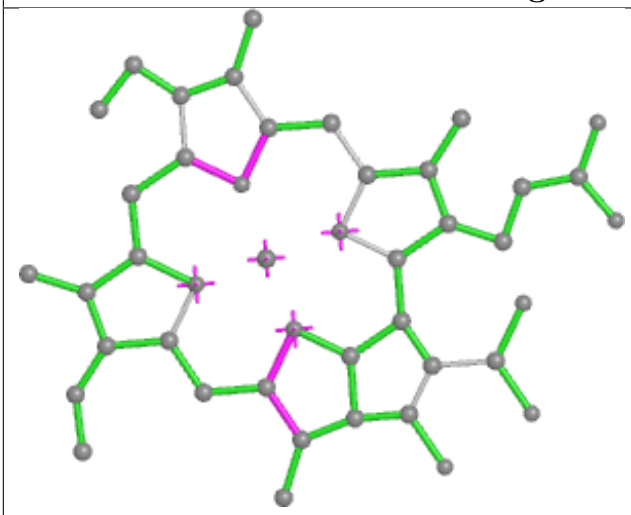


Rings

Ligand CLA 0 313



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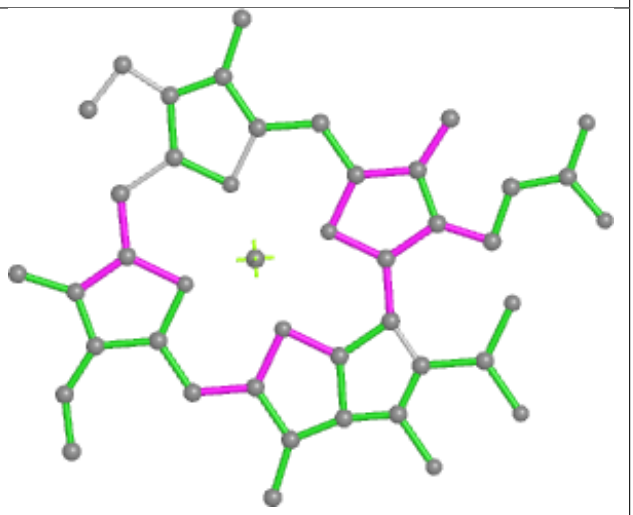
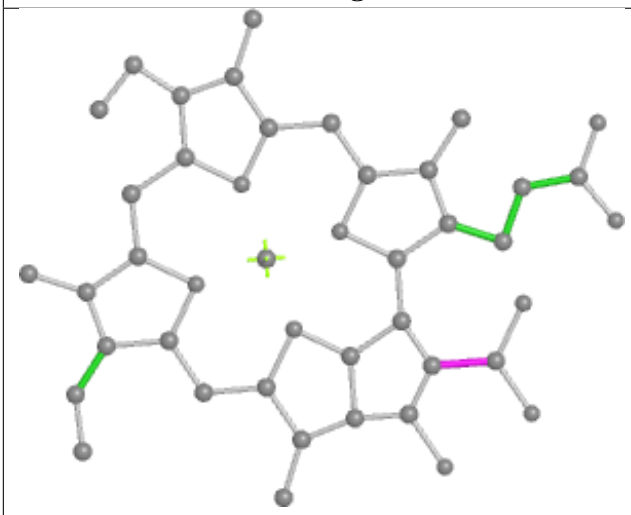


Bond angles



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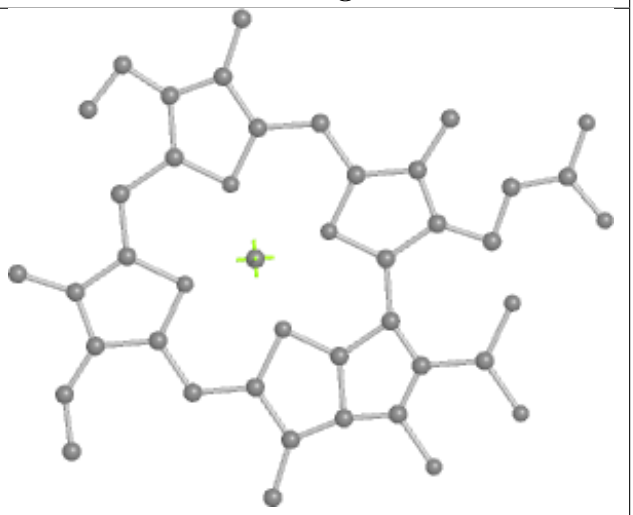
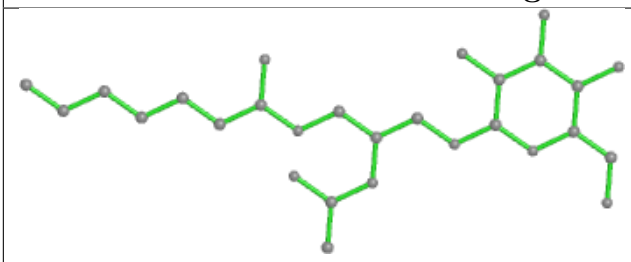


Rings

Ligand LMG 8 318



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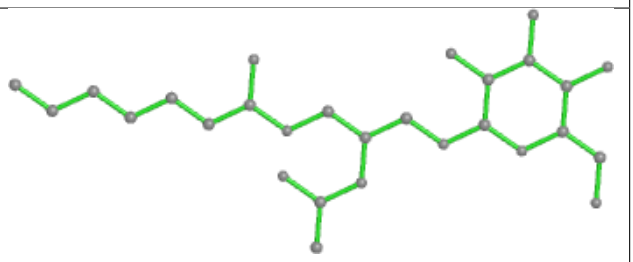
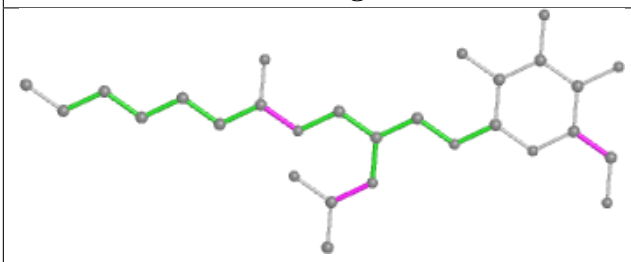
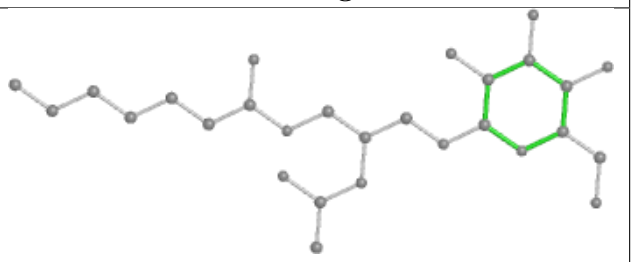


Bond angles

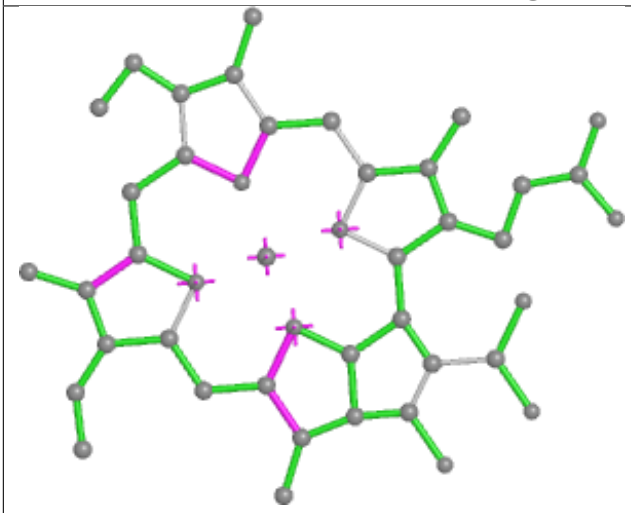


Torsions

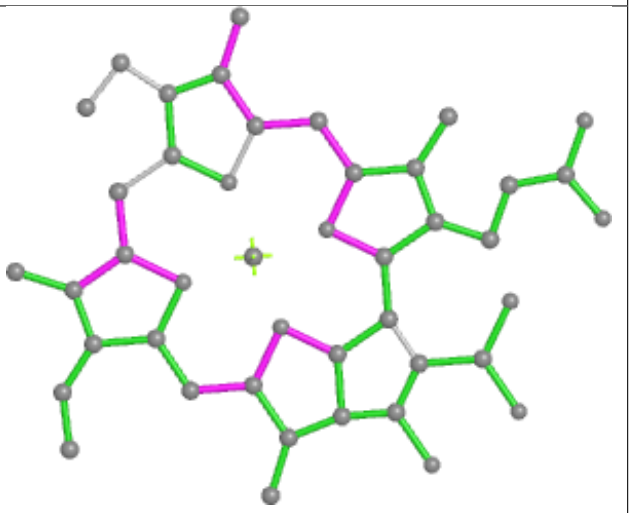


Rings

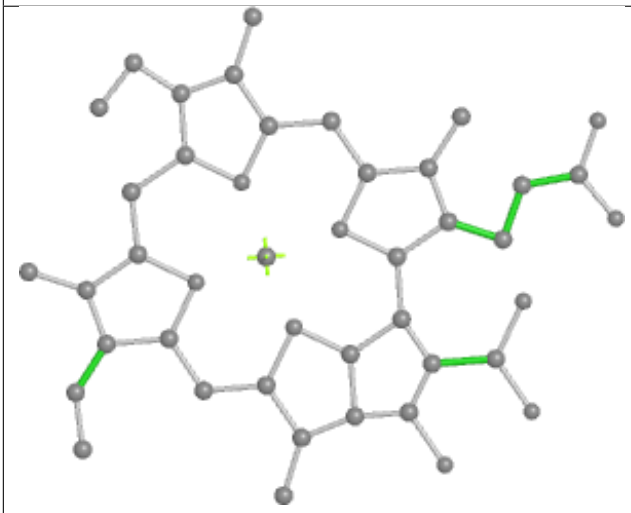
Ligand CLA B 811



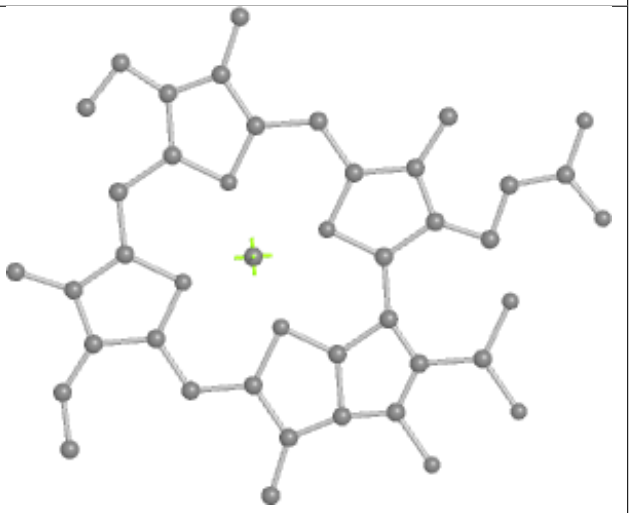
Bond lengths



Bond angles

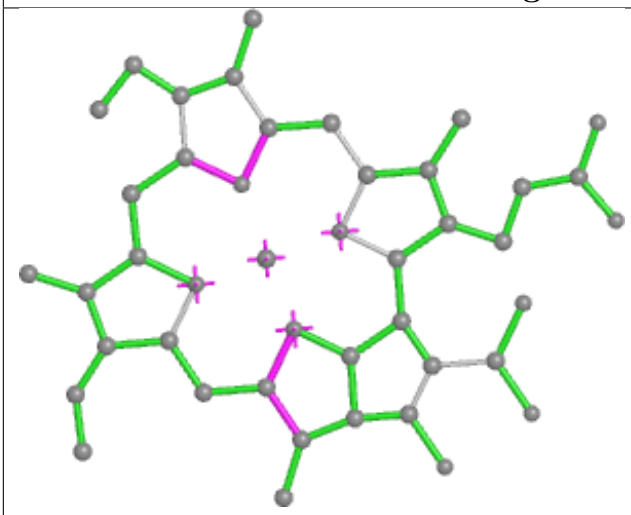


Torsions

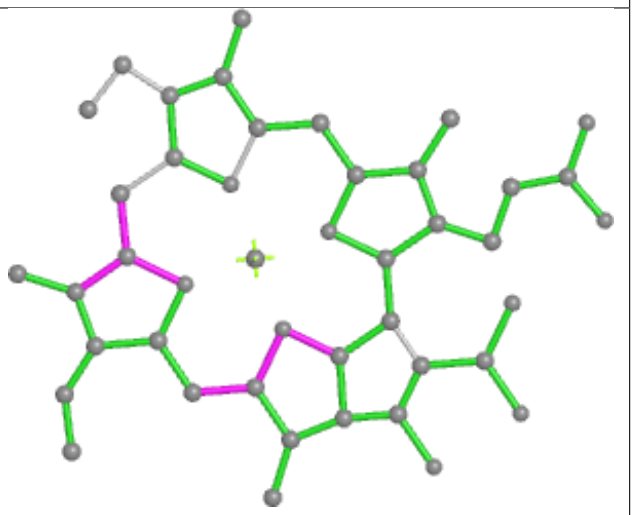


Rings

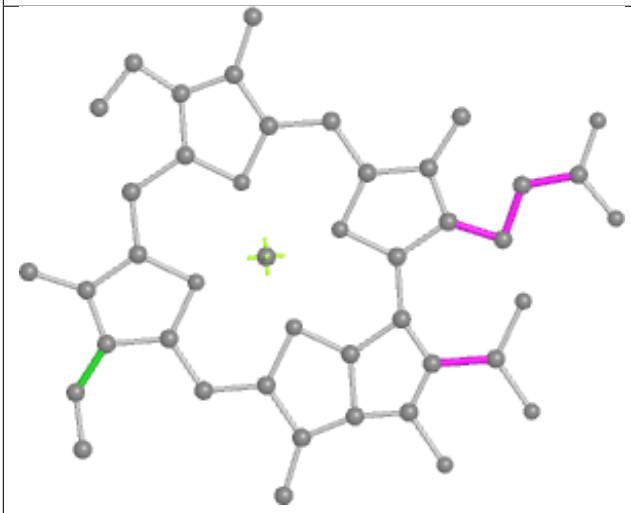
Ligand CLA K 201



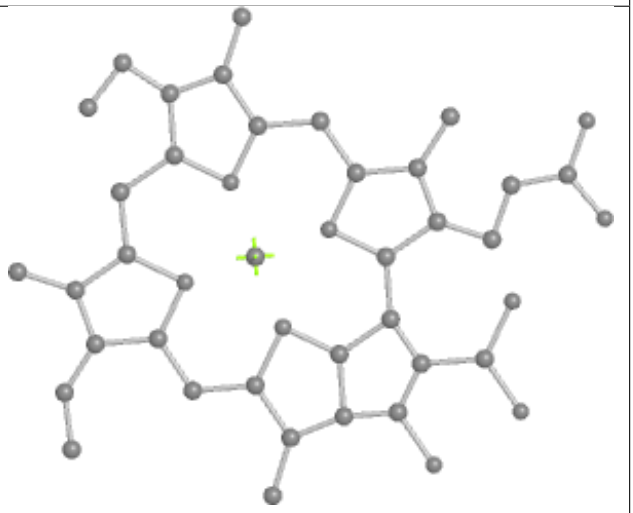
Bond lengths



Bond angles

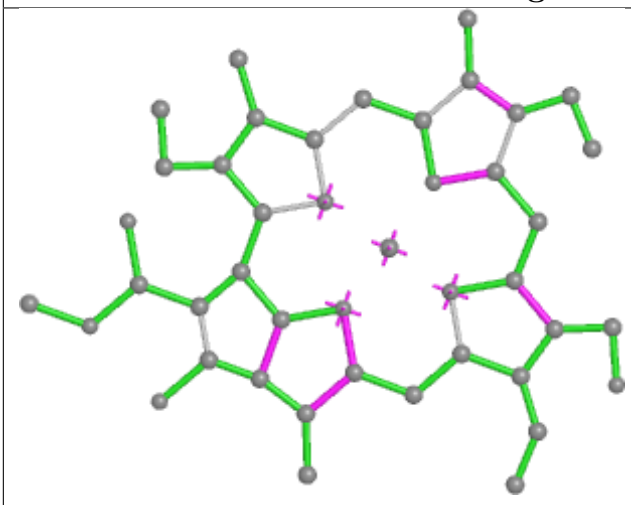


Torsions



Rings

Ligand CHL 4 316



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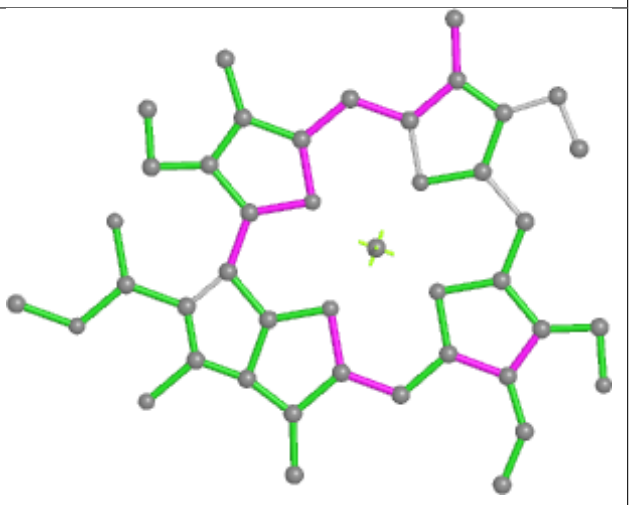

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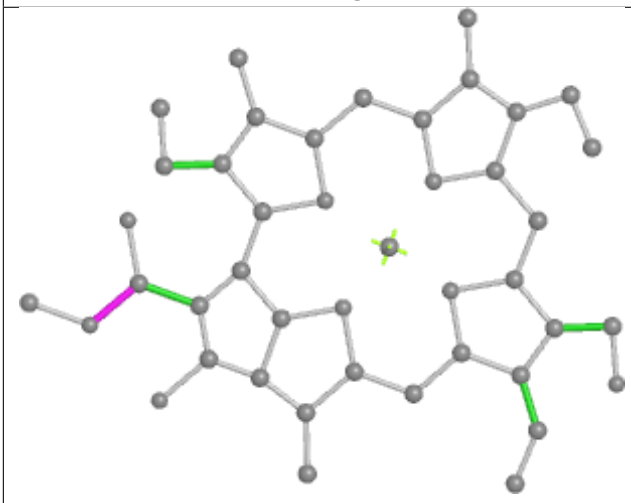

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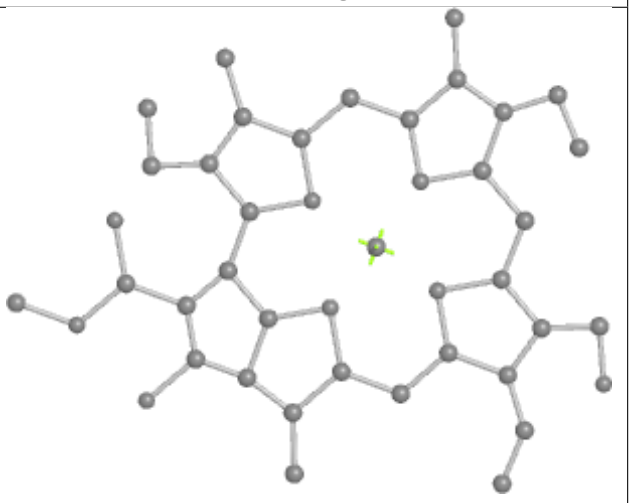
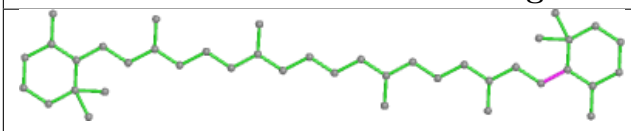


Rings

Ligand BCR 4 302



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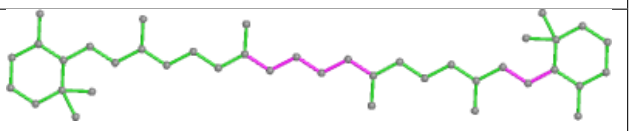
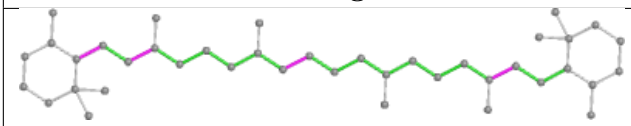


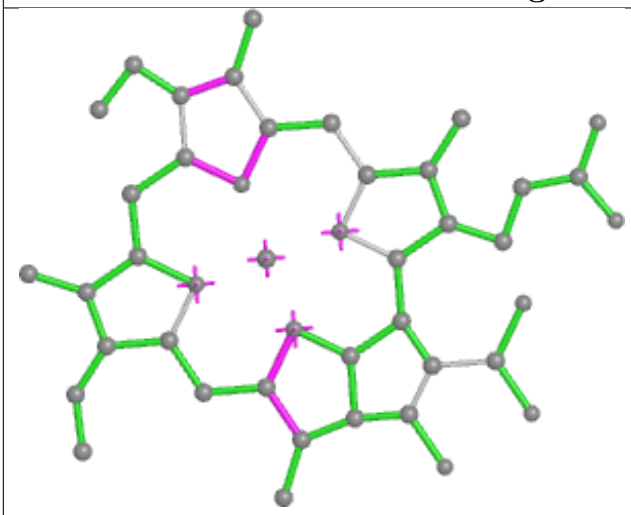
Bond angles



Torsions

Rings

Ligand CLA 4 314



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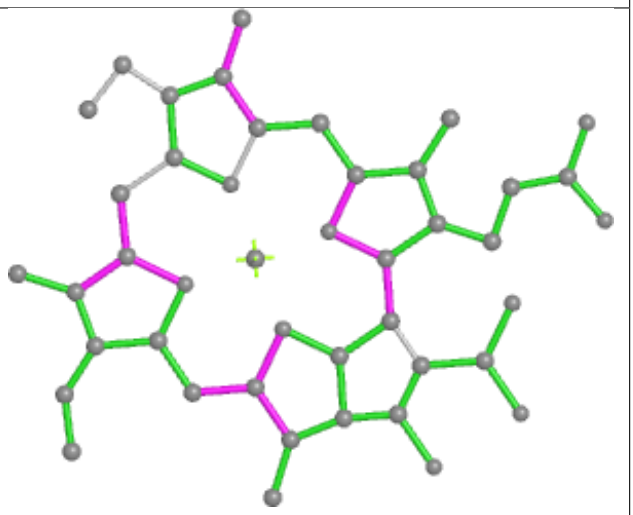

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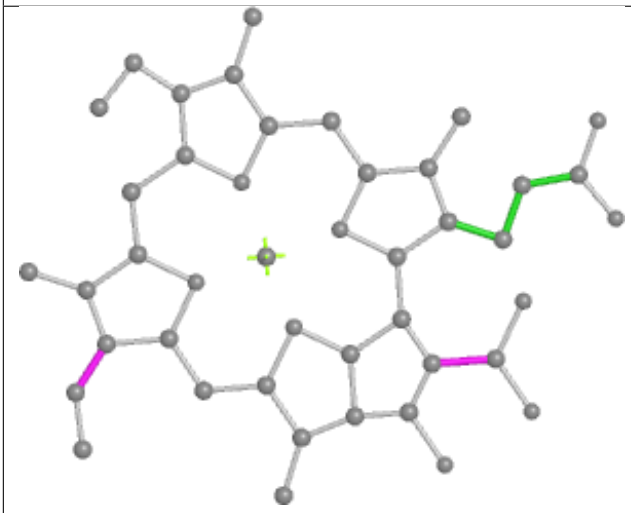

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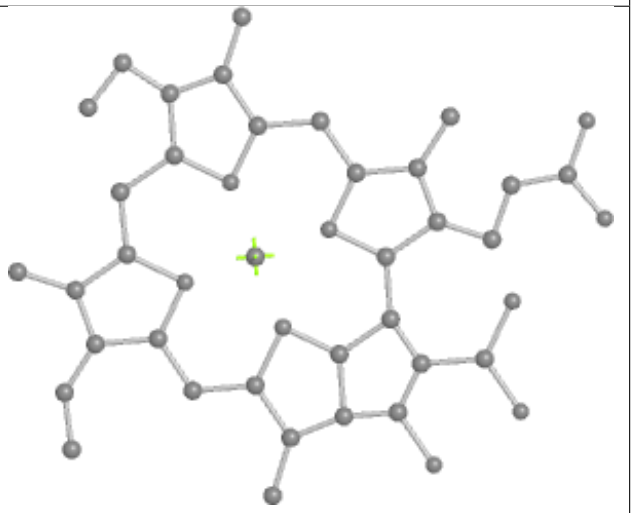
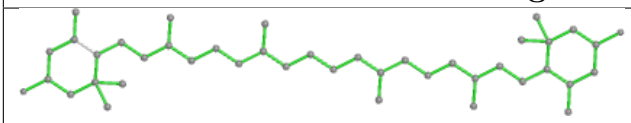


Rings

Ligand LUT 0 318



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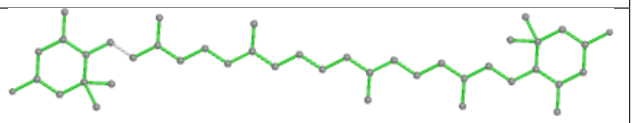

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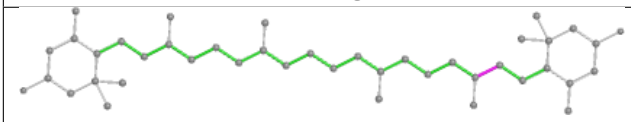

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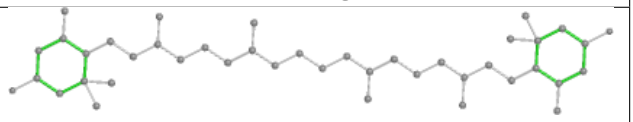
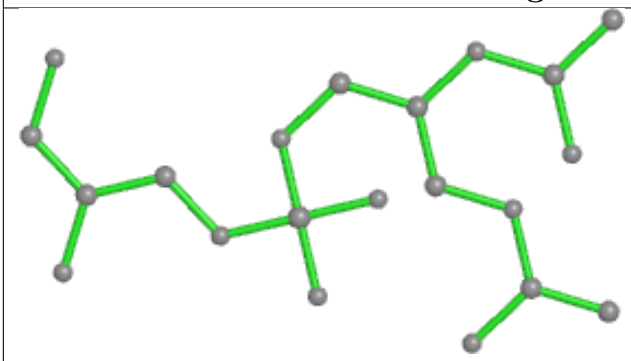


Rings

Ligand LHG 0 302



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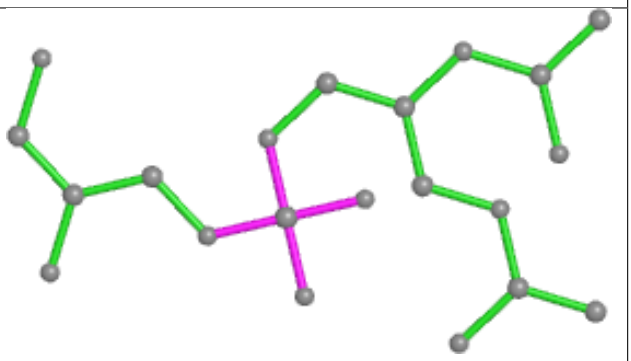

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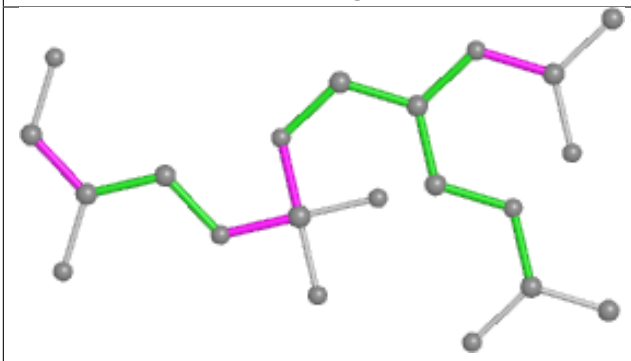

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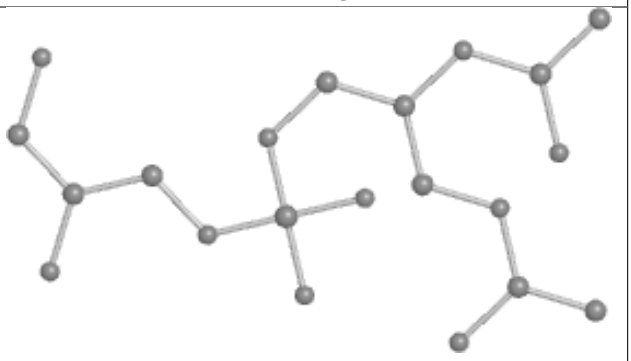
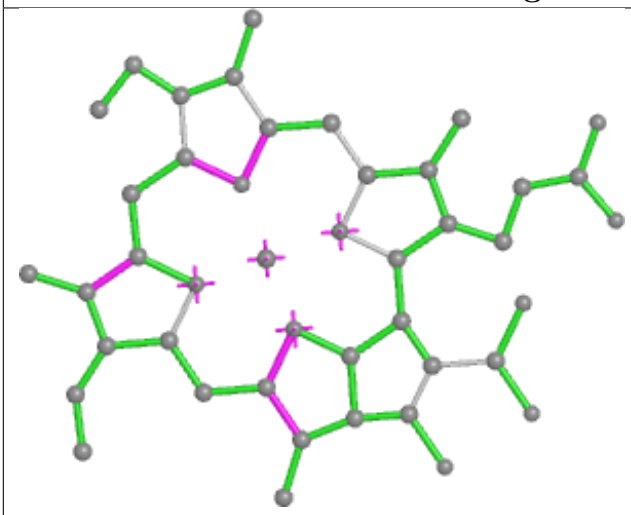


Rings

Ligand CLA A 820



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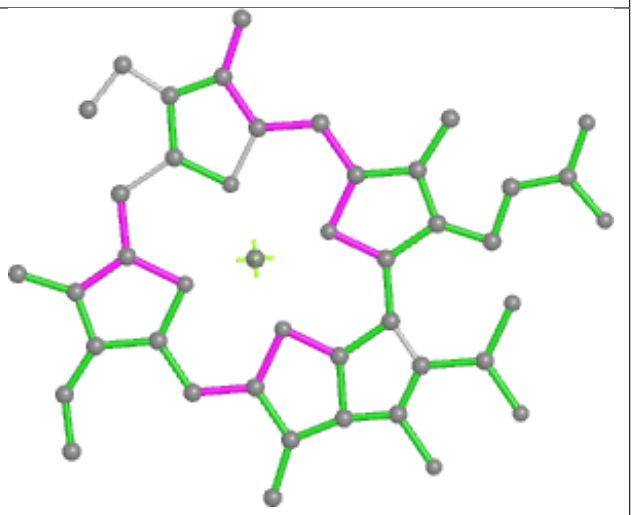

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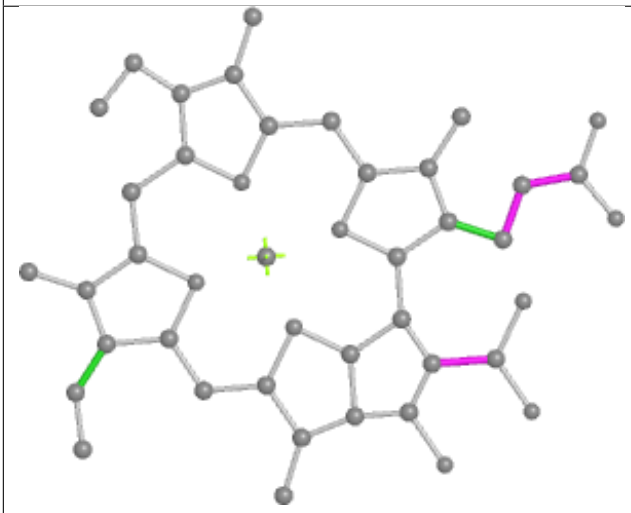

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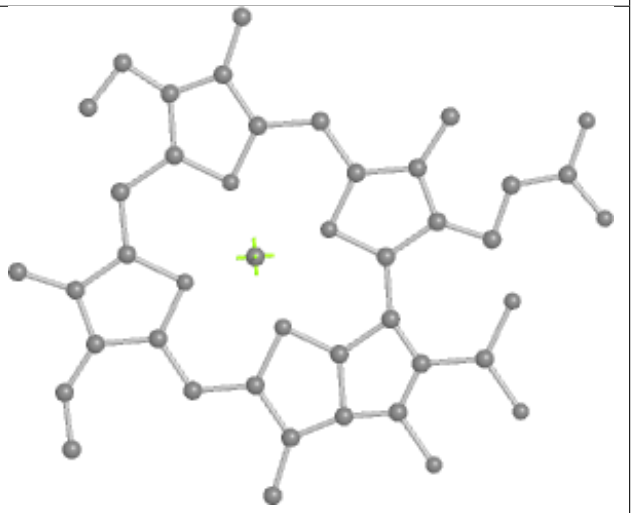
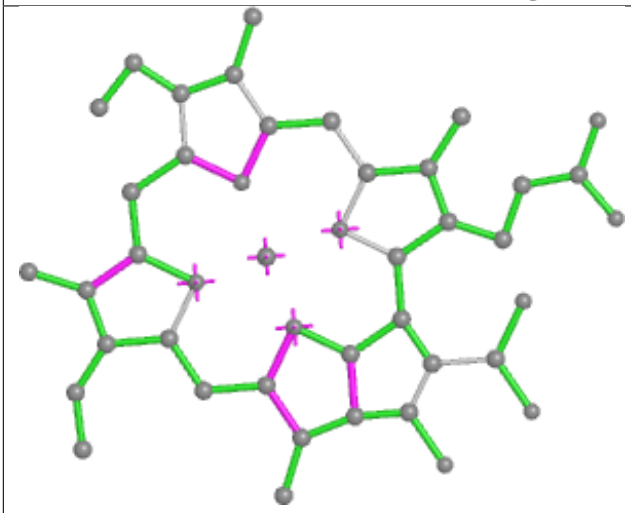


Rings

Ligand CLA B 802



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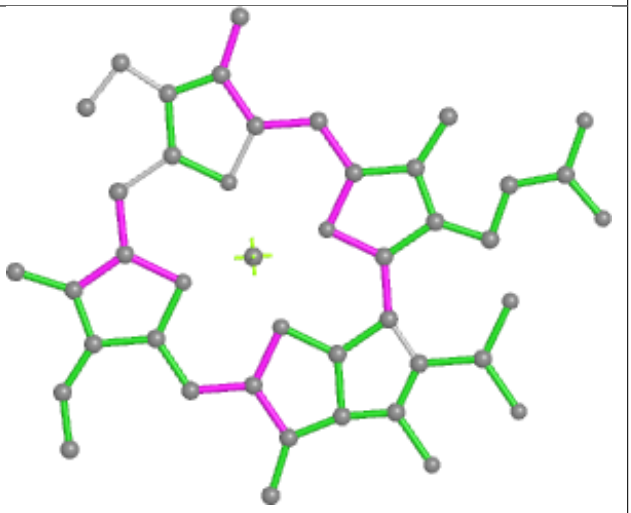

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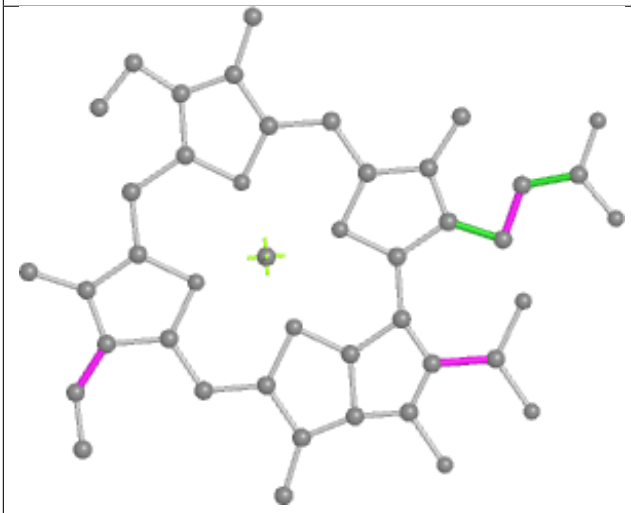

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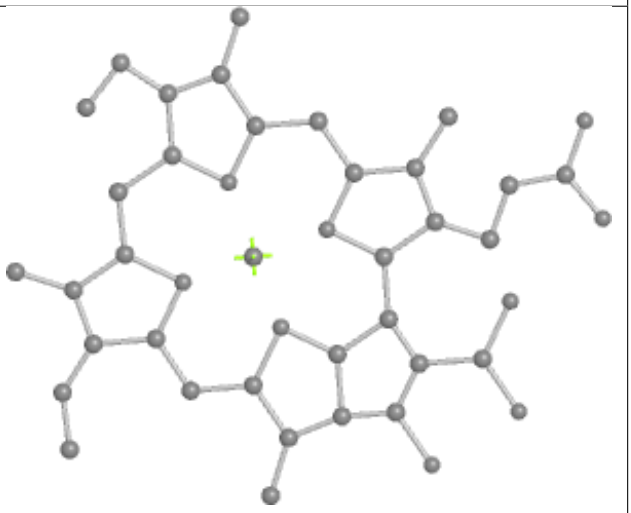
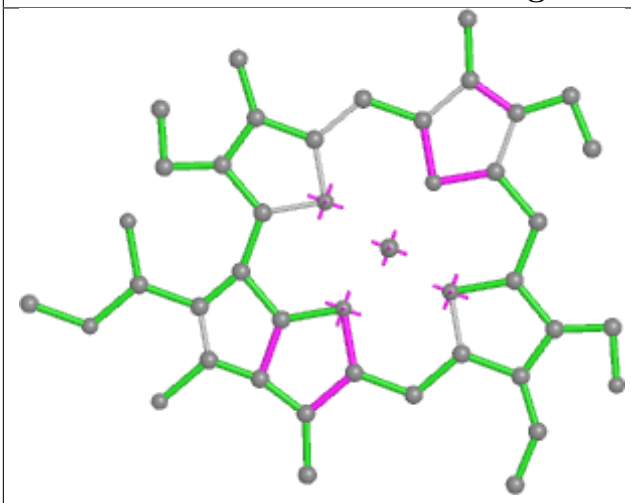


Rings

Ligand CHL 6 317



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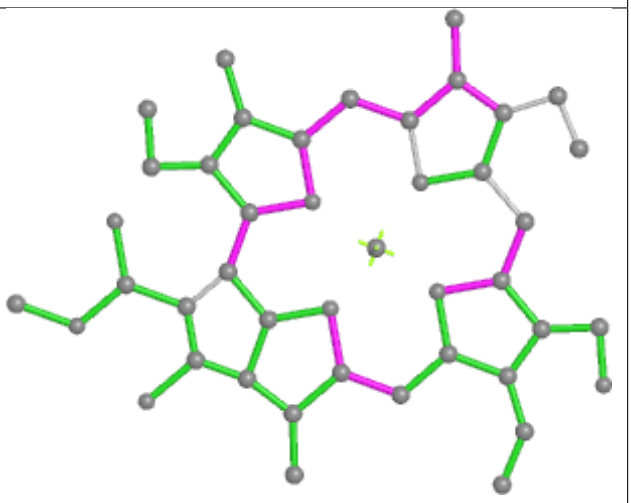

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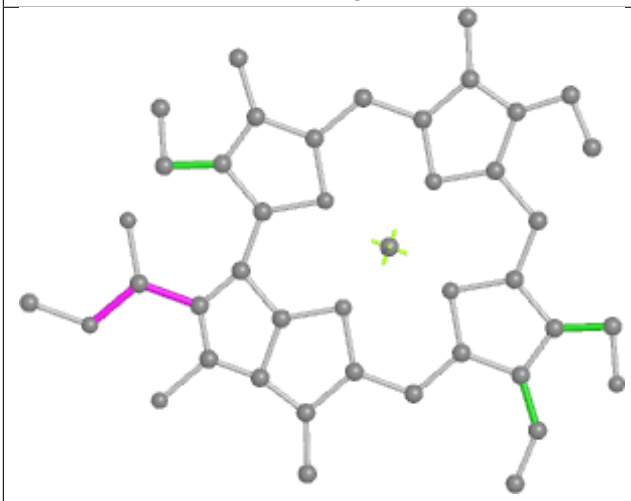

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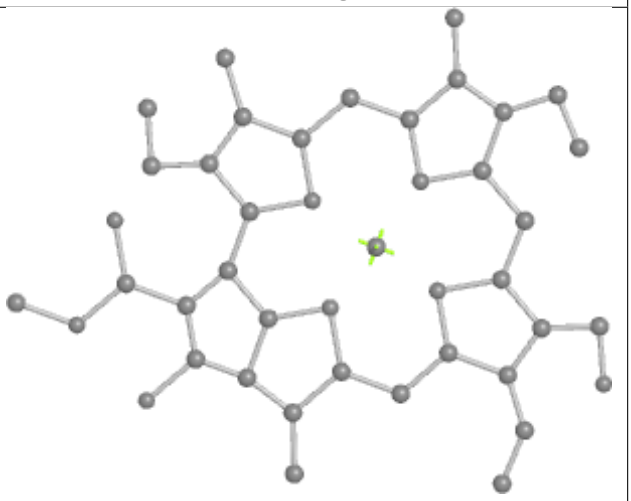
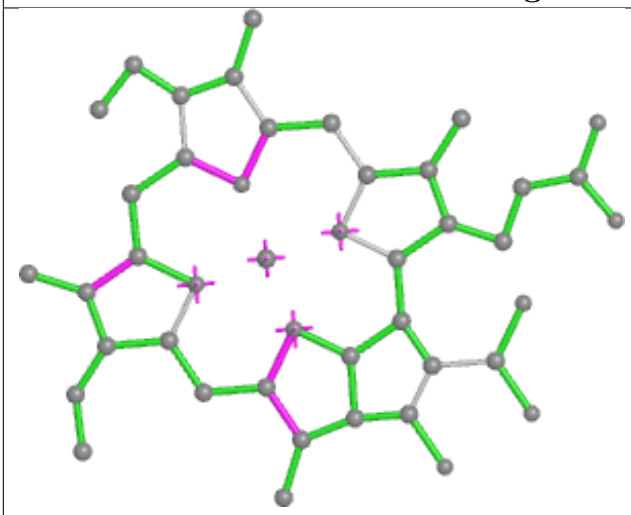


Rings

Ligand CLA A 818



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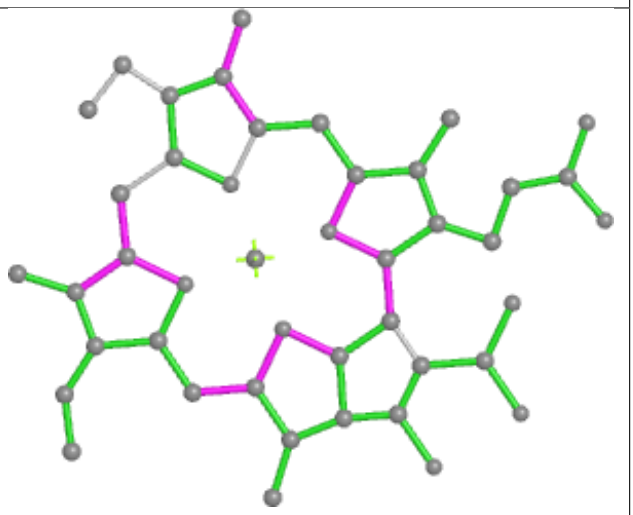

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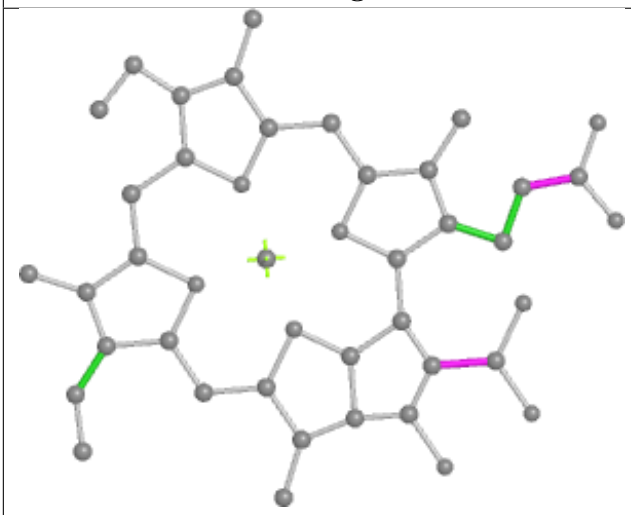

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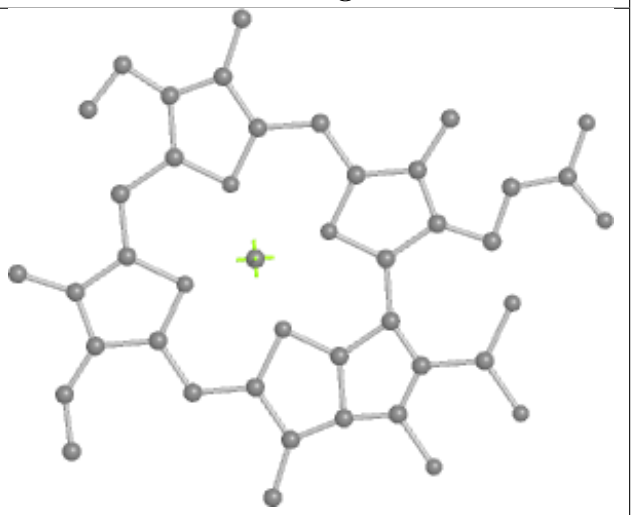
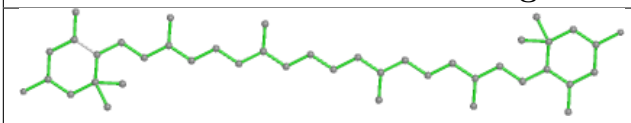


Rings

Ligand LUT 1 1016



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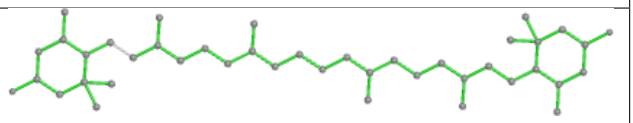

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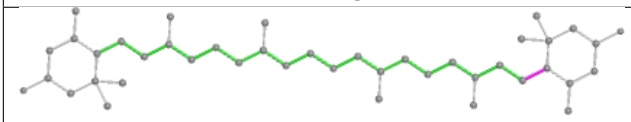

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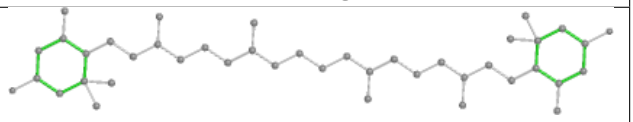
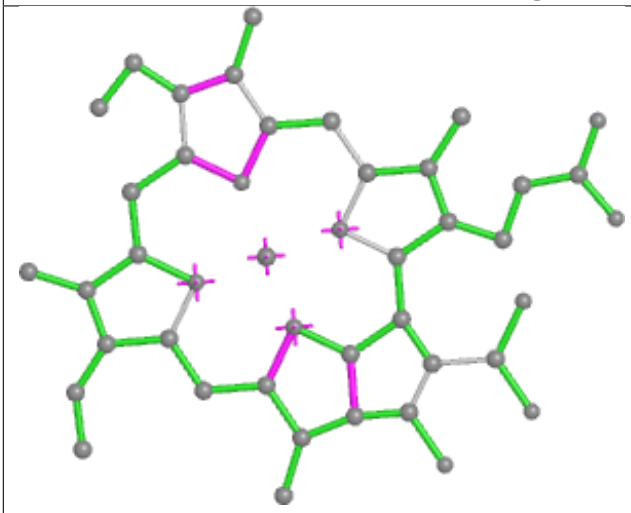


Rings

Ligand CLA 5 309



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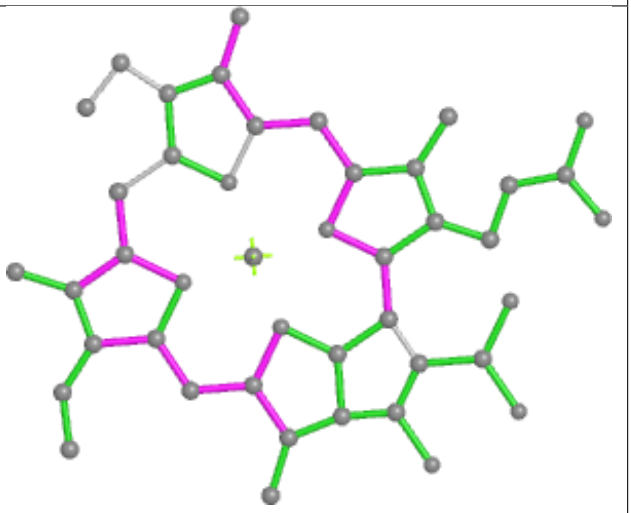

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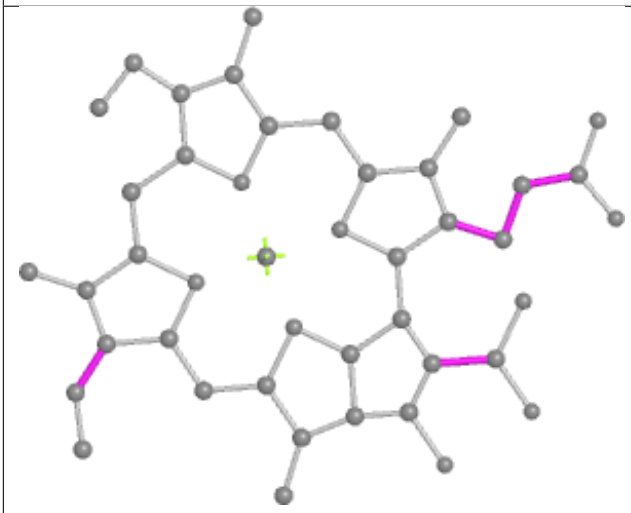

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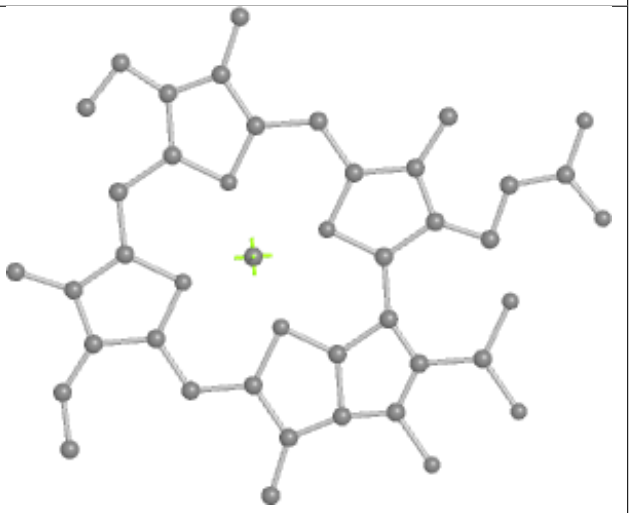
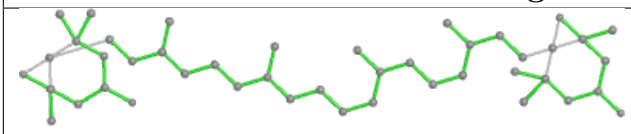


Rings

Ligand XAT 4 303



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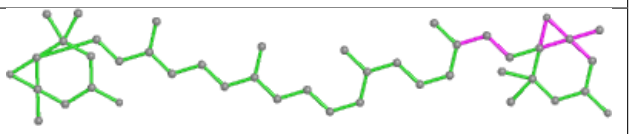
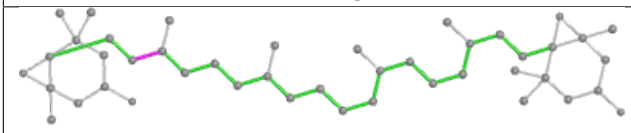


Bond angles



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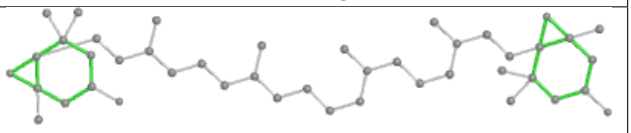
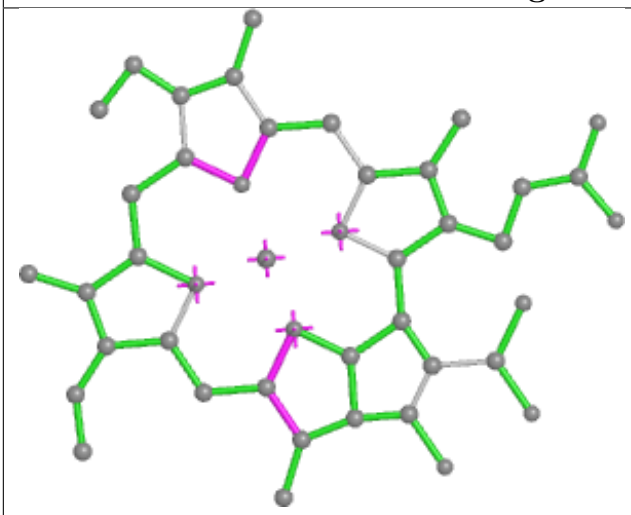


Rings

Ligand CLA 5 323



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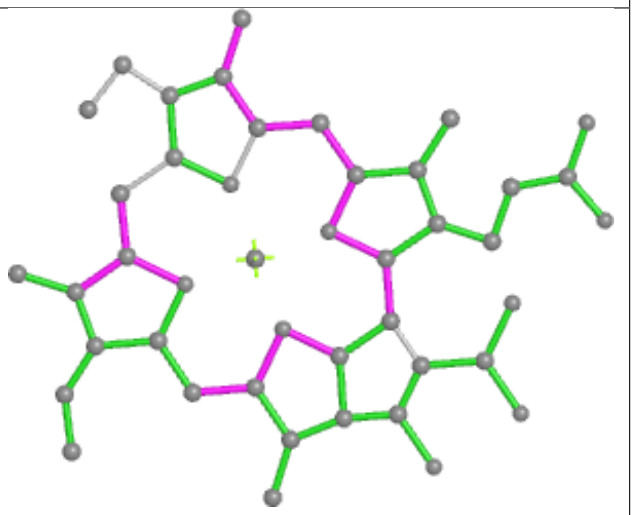
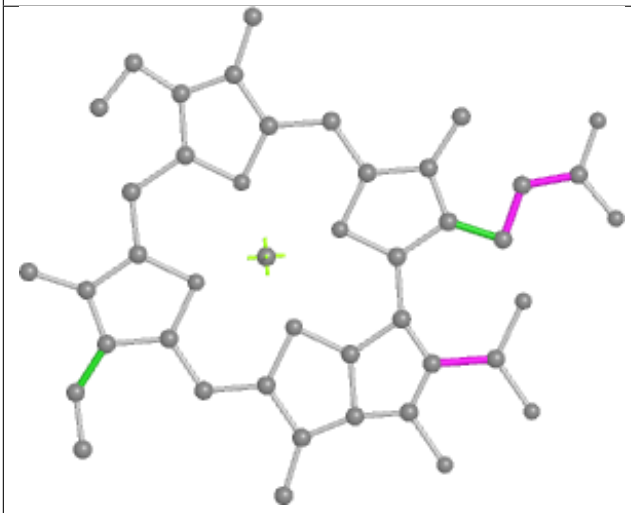


Bond angles



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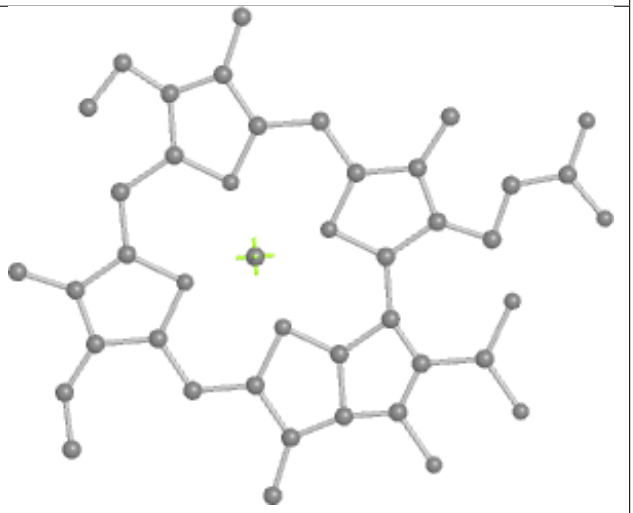
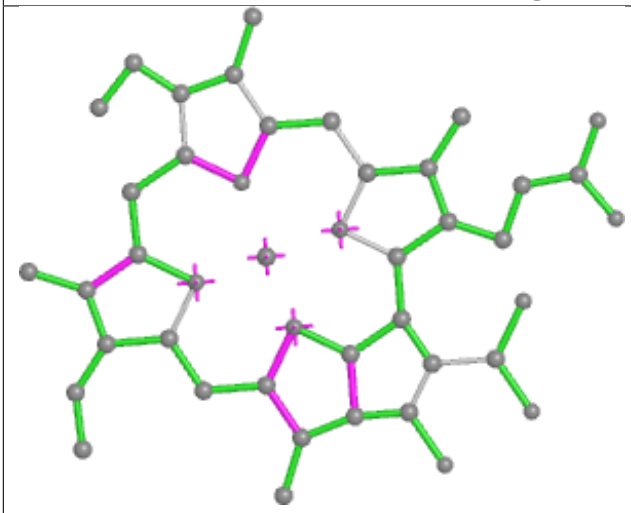
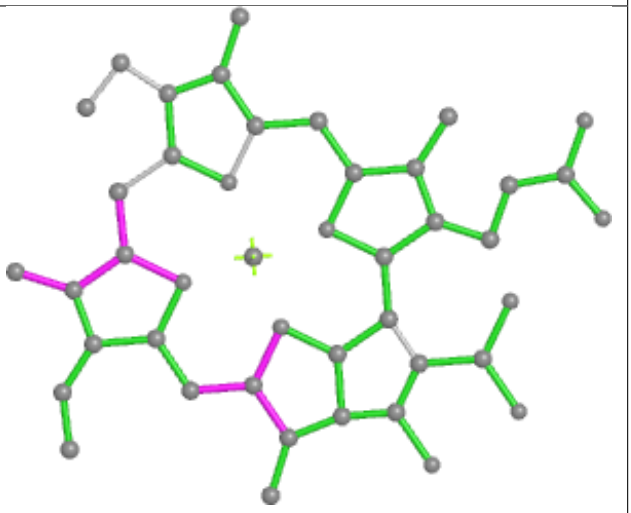


Rings

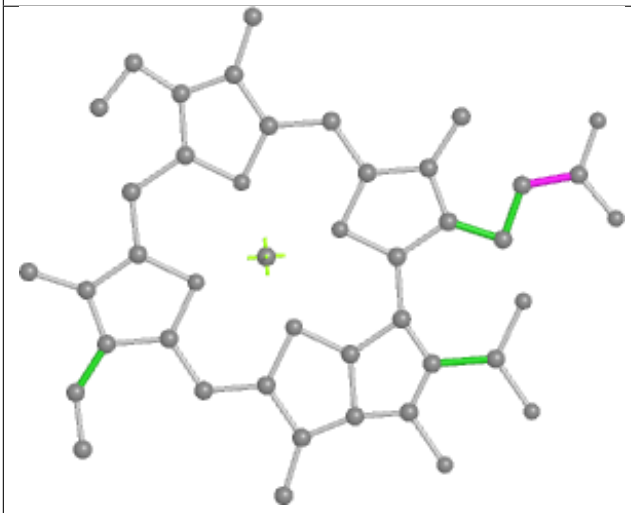
Ligand CLA 6 305



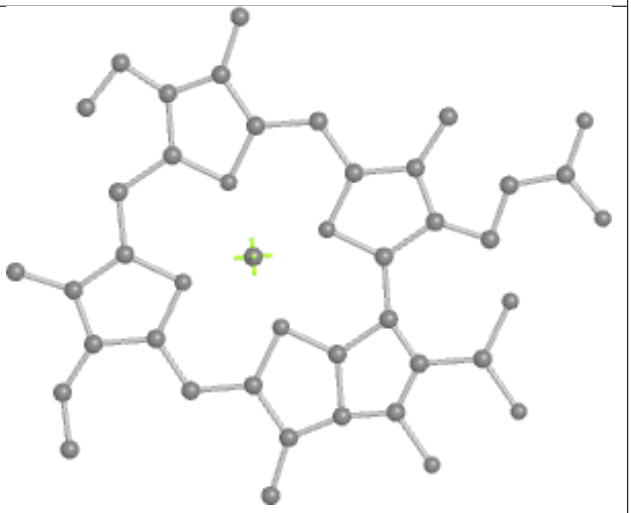
Bond lengths



Bond angles

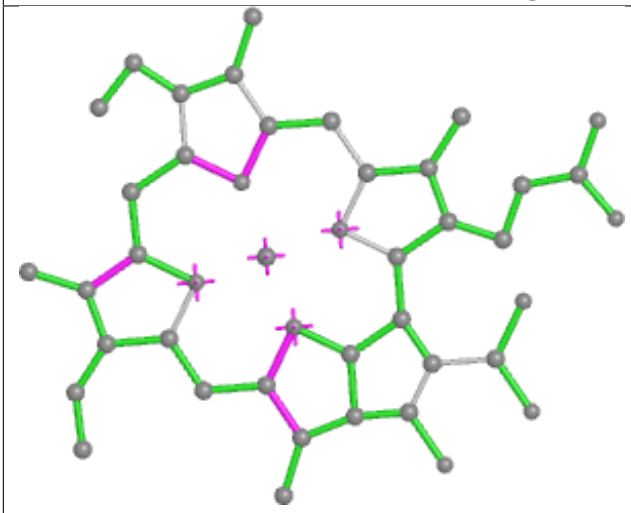


Torsions

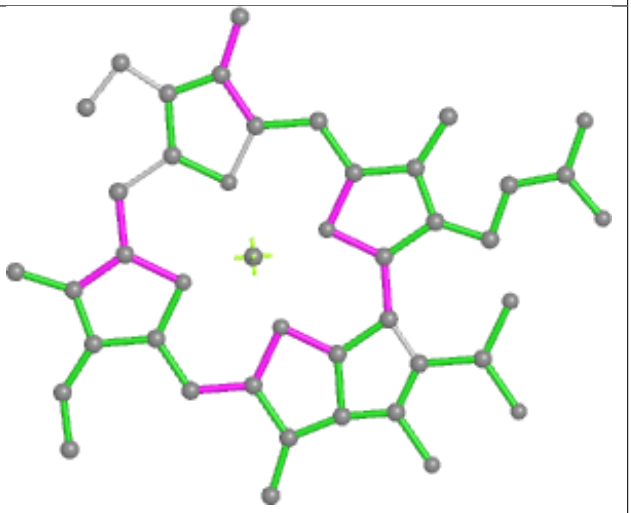


Rings

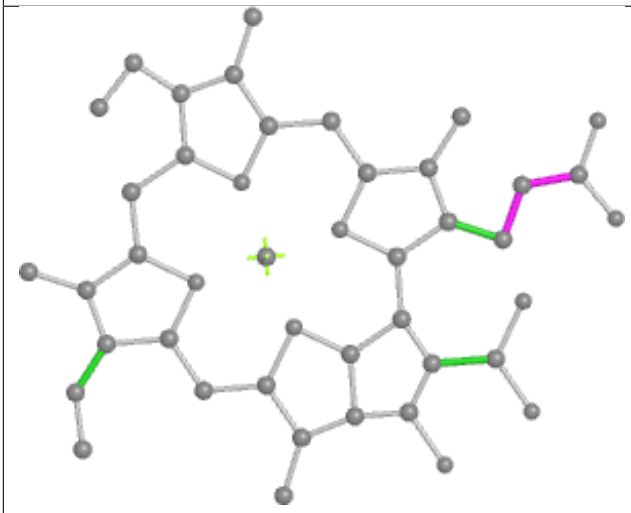
Ligand CLA A 830



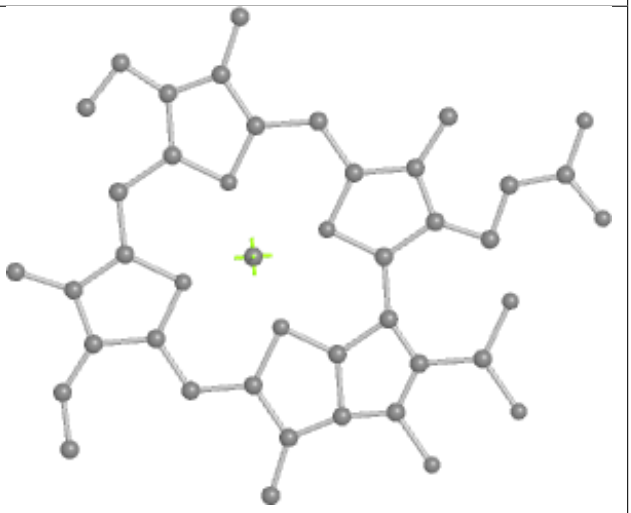
Bond lengths



Bond angles

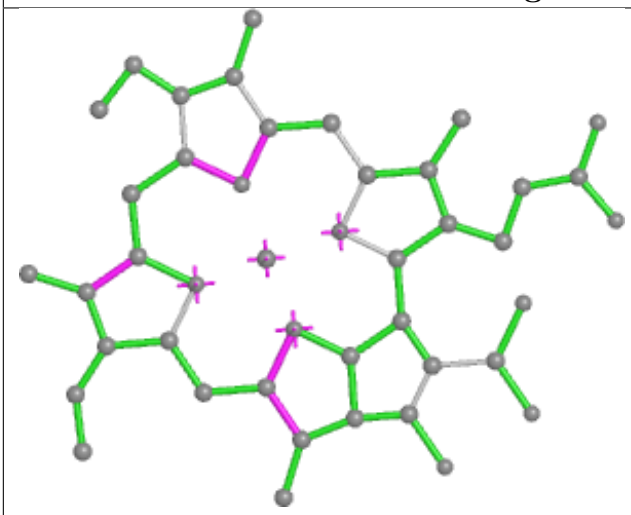


Torsions



Rings

Ligand CLA B 840



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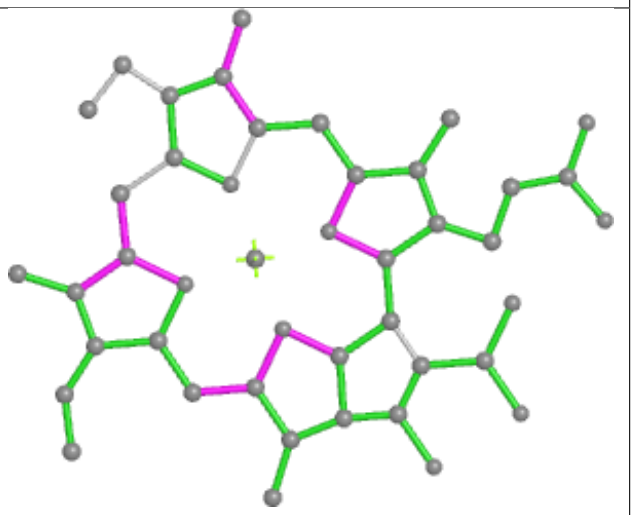

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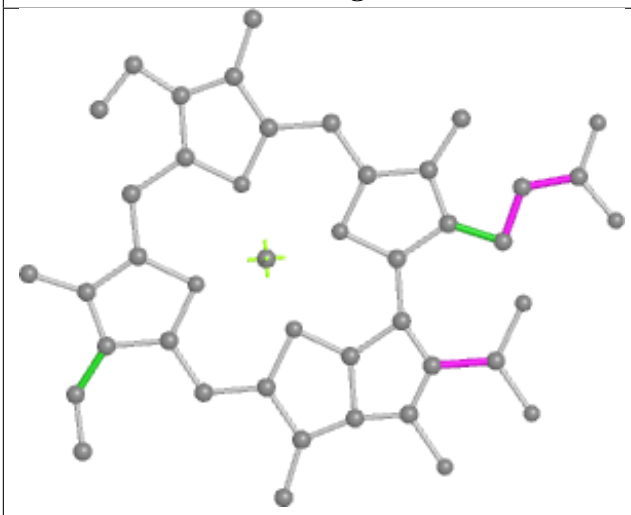

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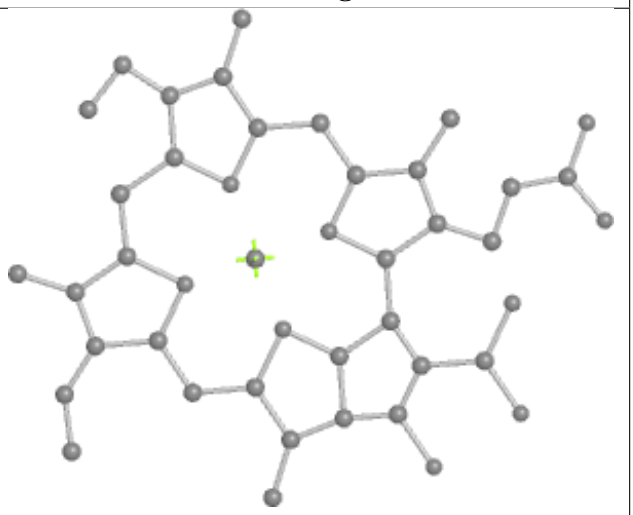
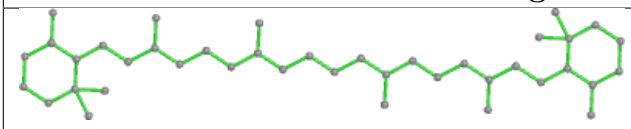


Rings

Ligand BCR I 201



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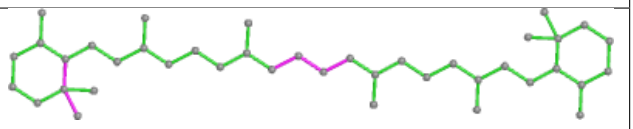

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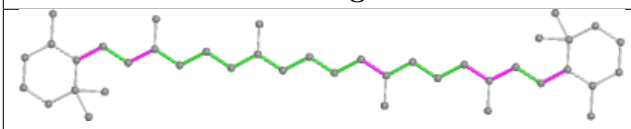

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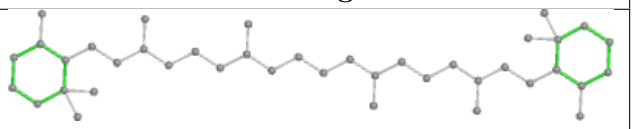
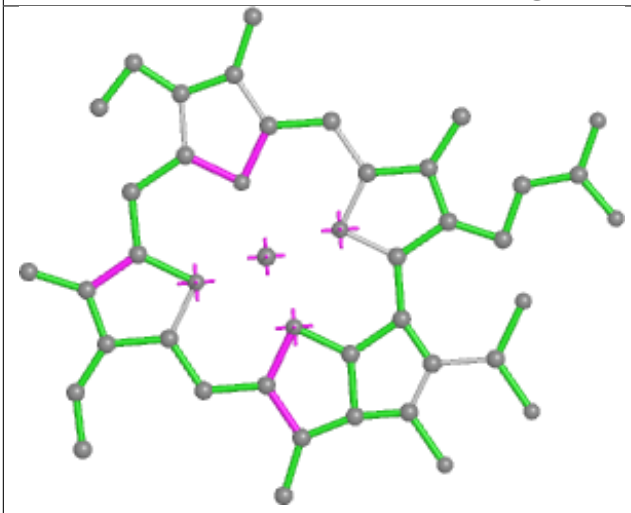


Rings

Ligand CLA 0 311



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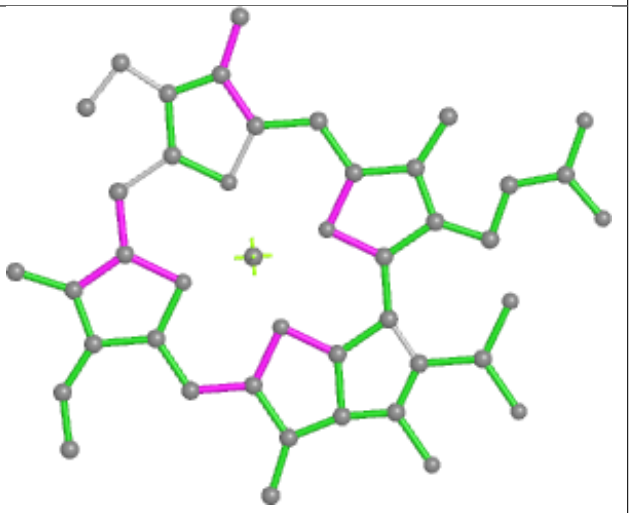
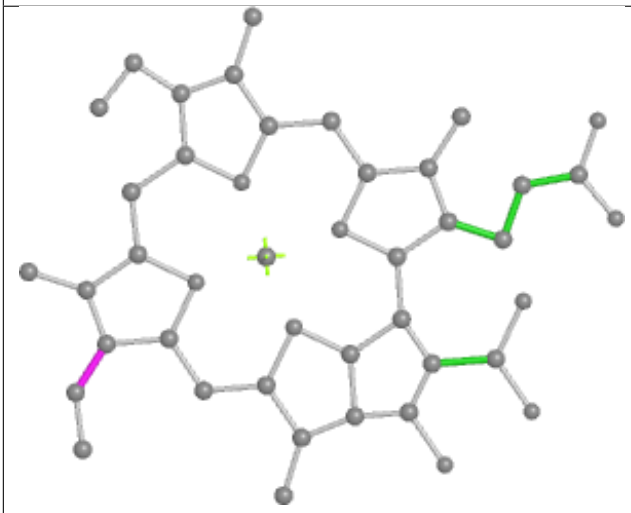


Bond angles



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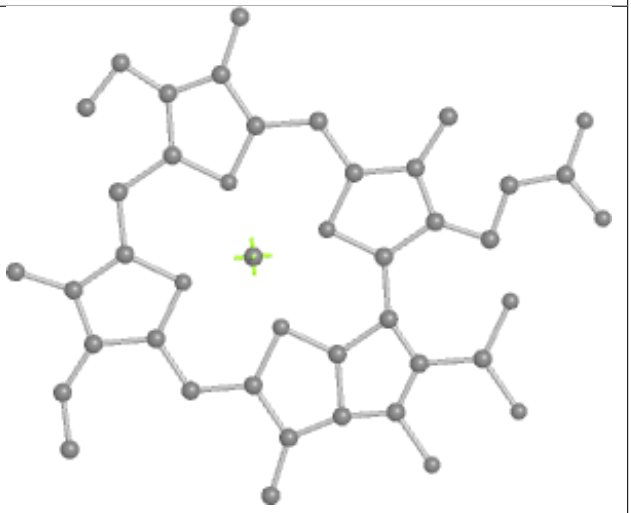
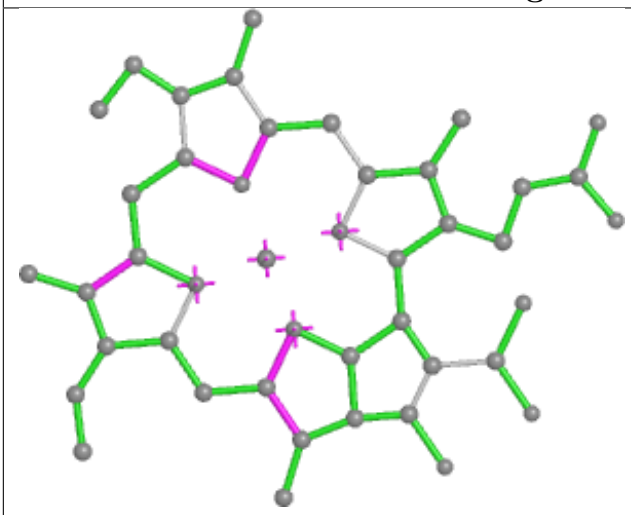


Rings

Ligand CLA L 201



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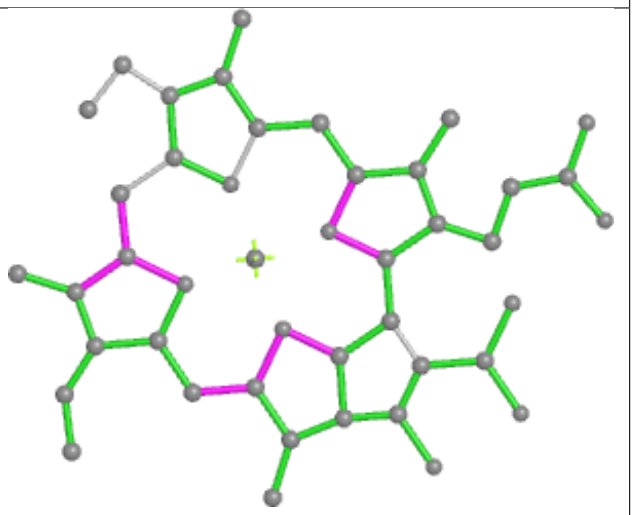
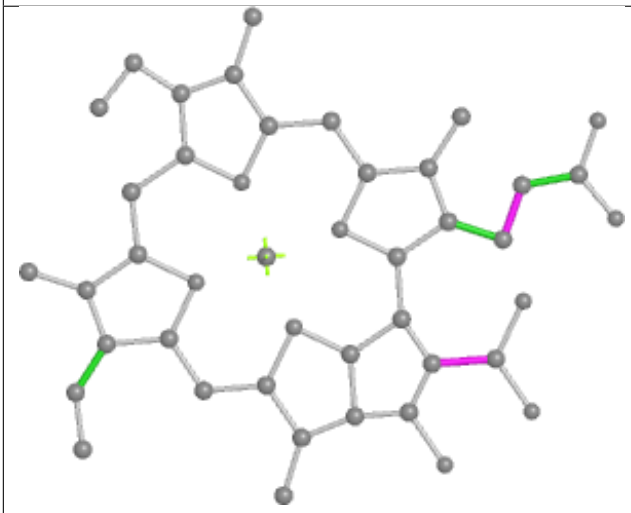


Bond angles



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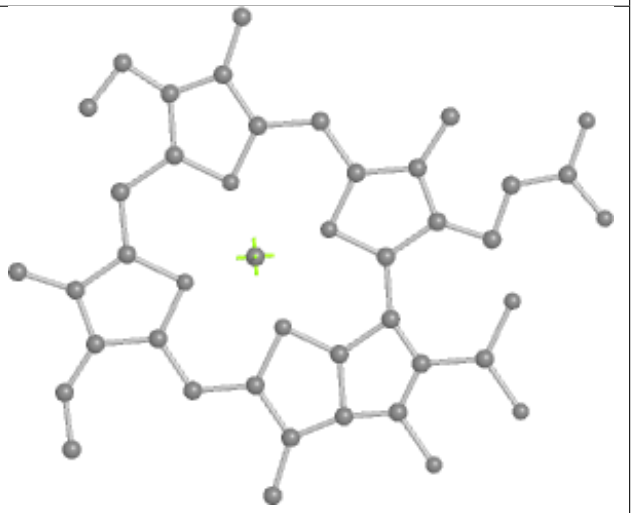
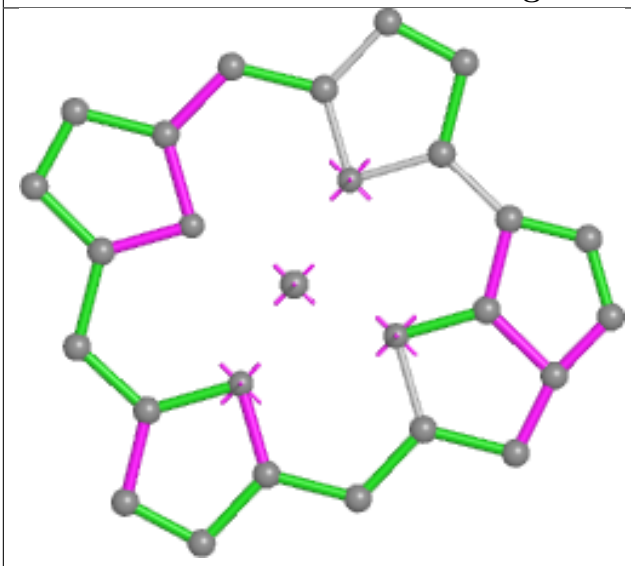


Rings

Ligand CLA K 202



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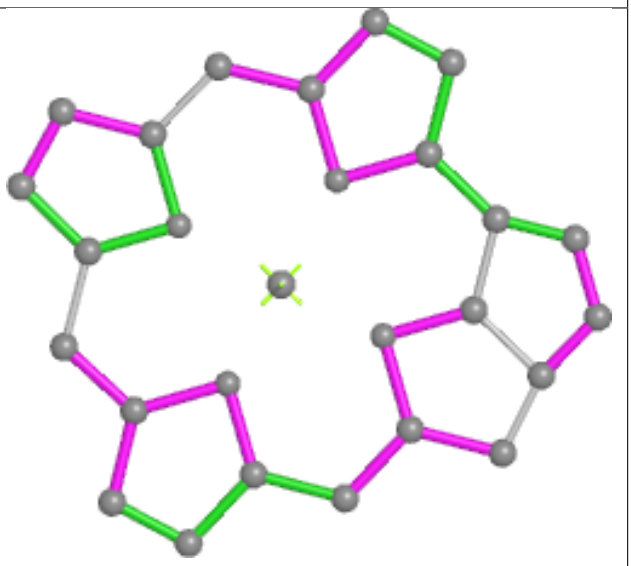
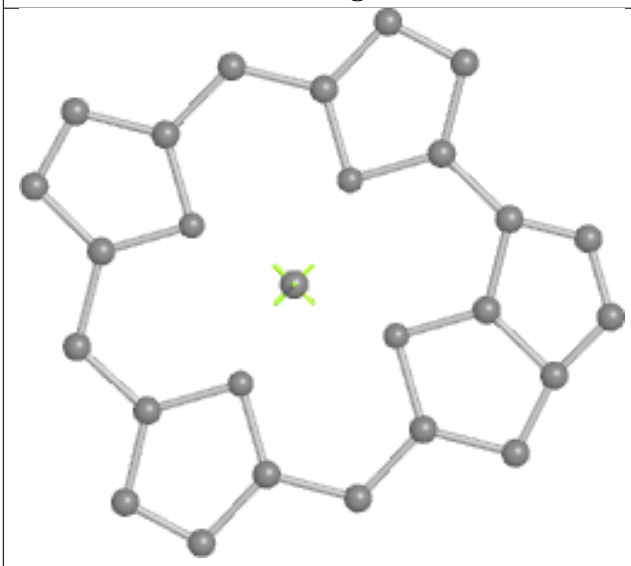


Bond angles



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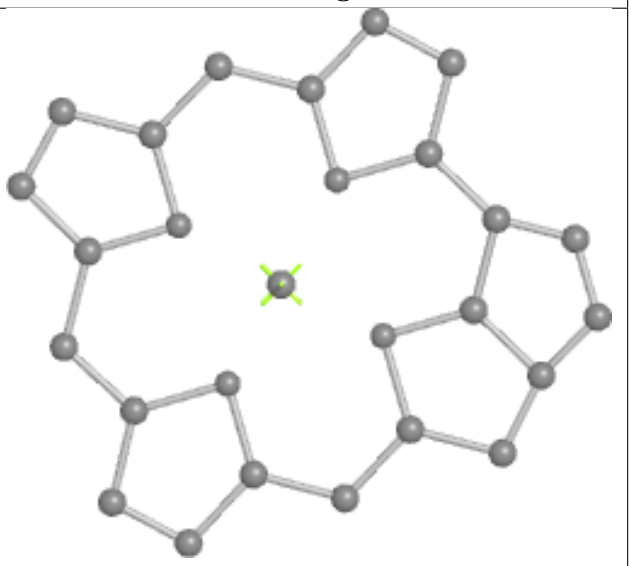
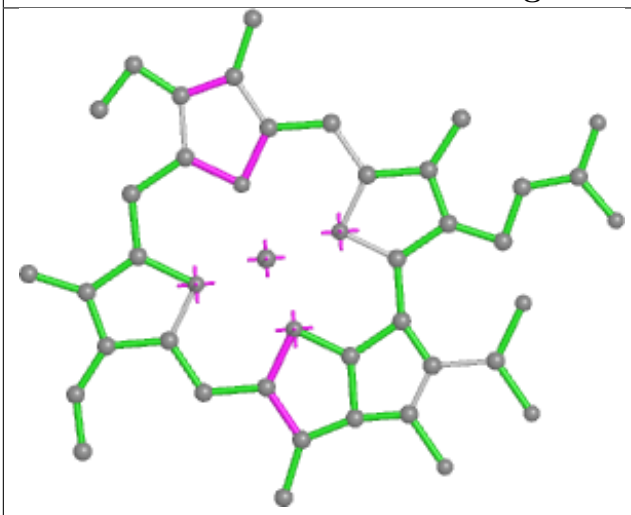


Rings

Ligand CLA A 801



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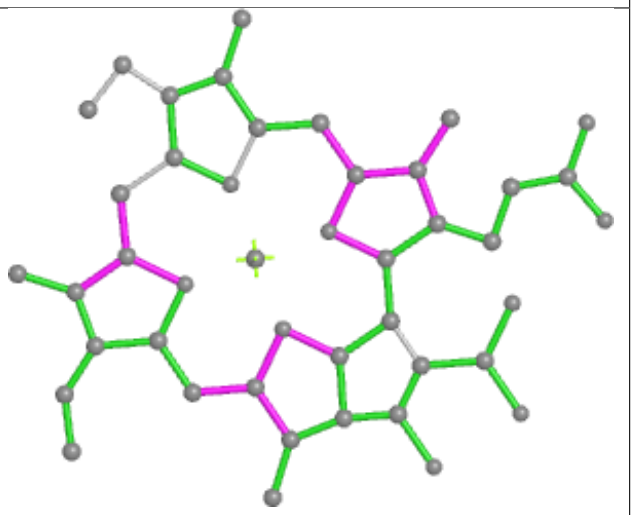
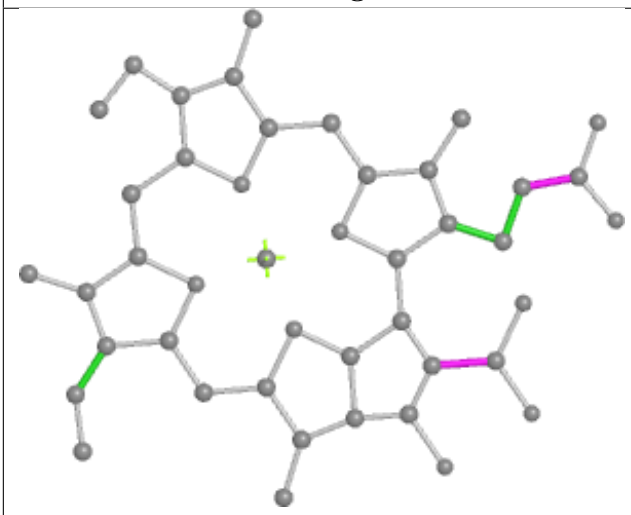


Bond angles



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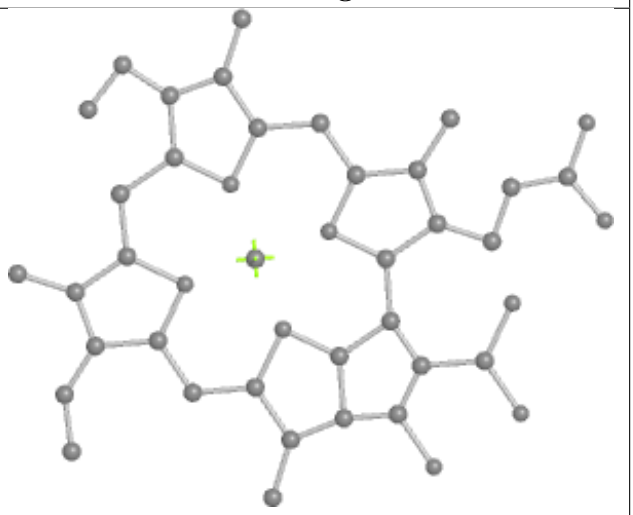
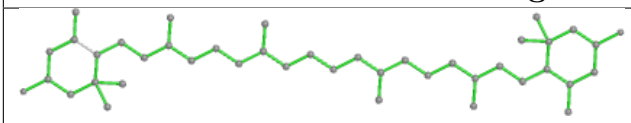


Rings

Ligand LUT 6 303



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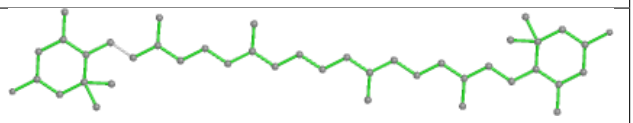
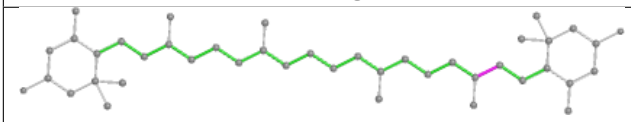


Bond angles



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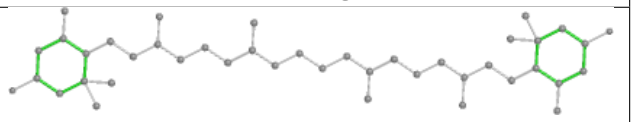
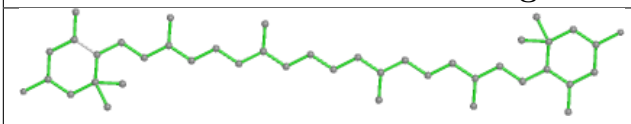


Rings

Ligand LUT 1 1002



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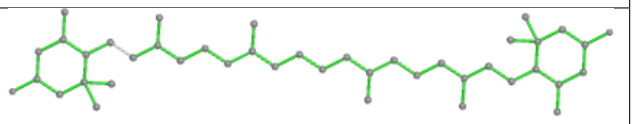
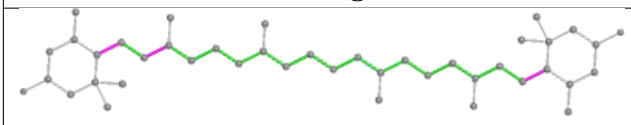


Bond angles



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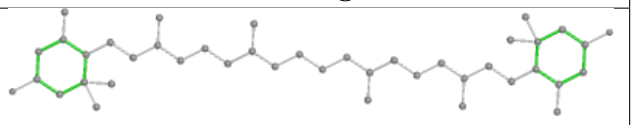
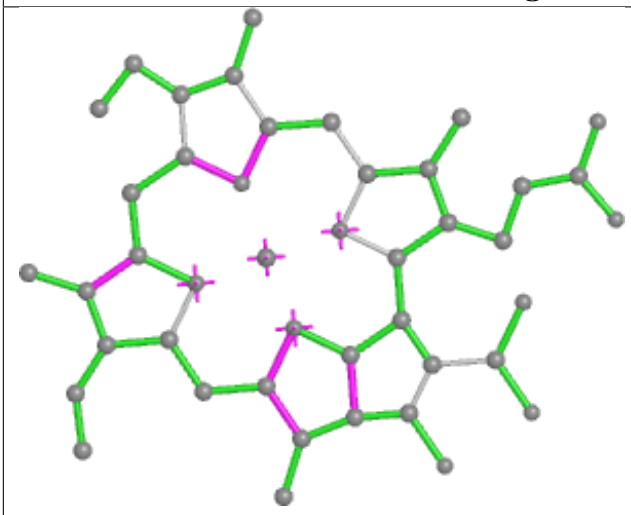


Rings

Ligand CLA A 833



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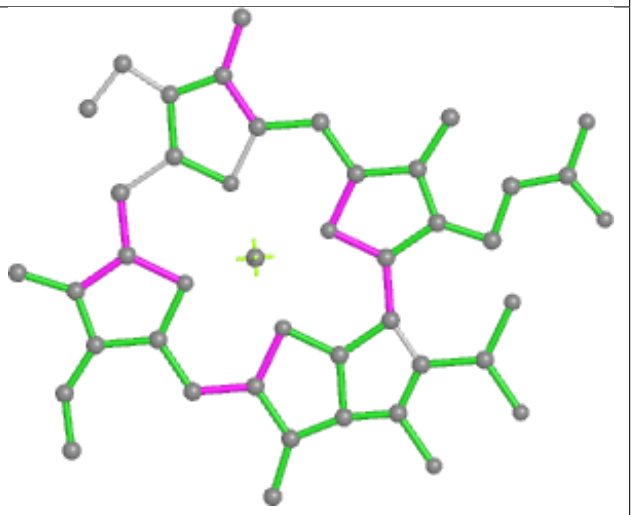
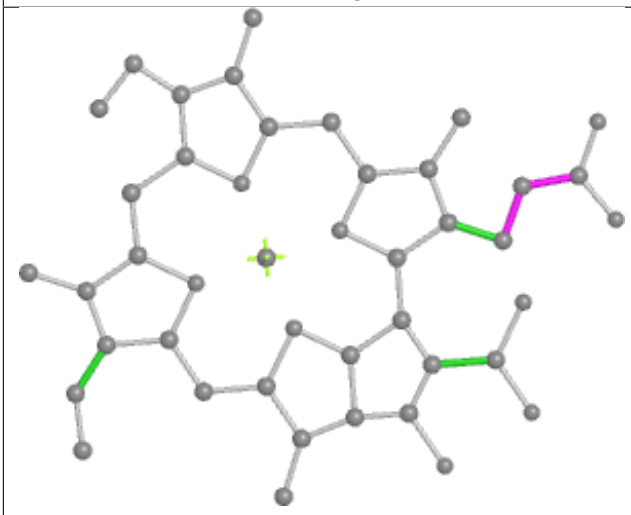


Bond angles



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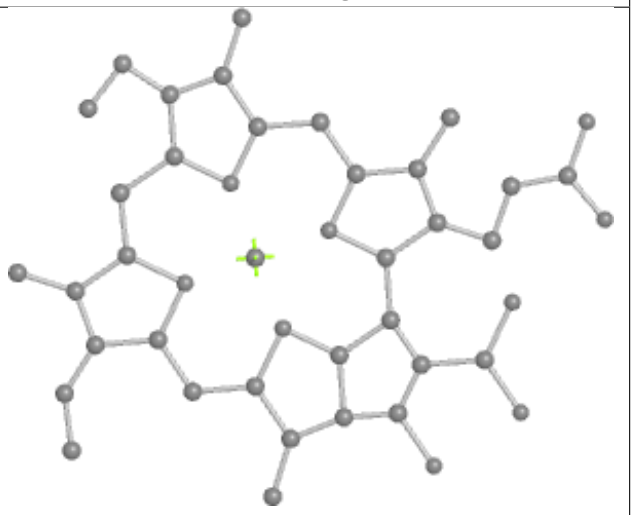
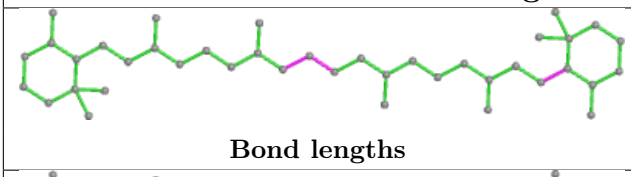
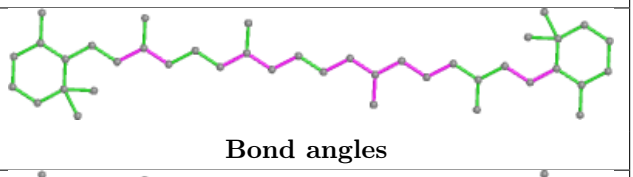


Rings

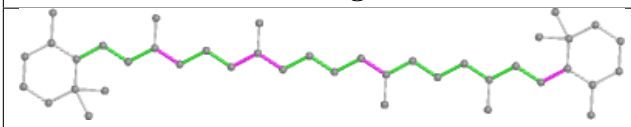
Ligand BCR B 843



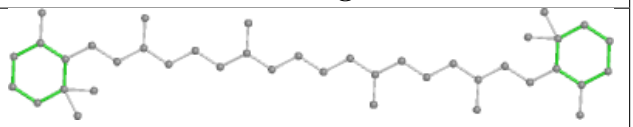
Bond lengths



Bond angles

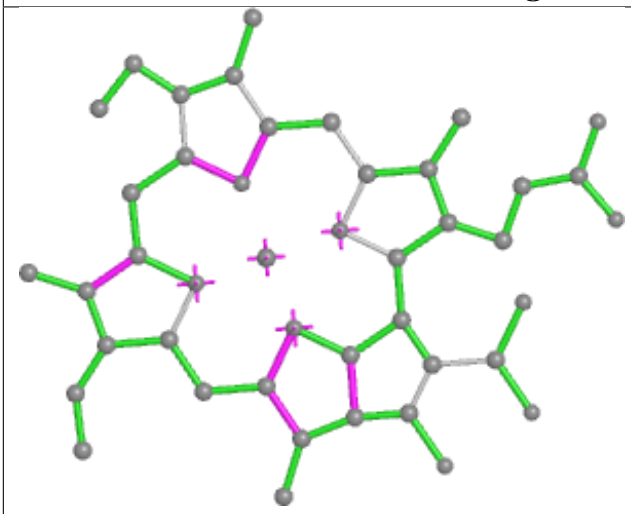


Torsions



Rings

Ligand CLA B 836



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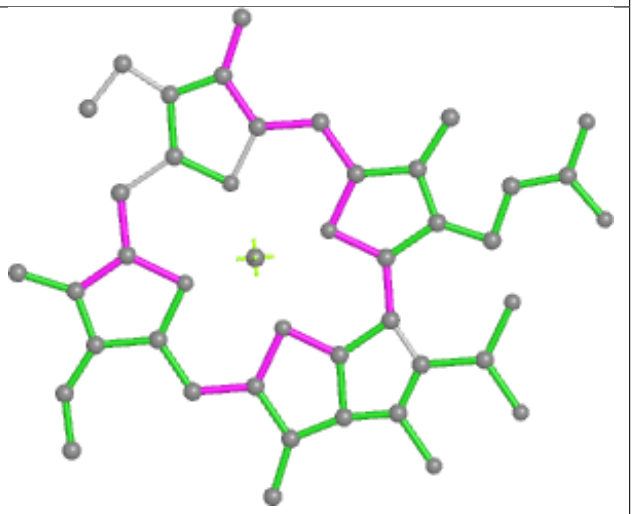
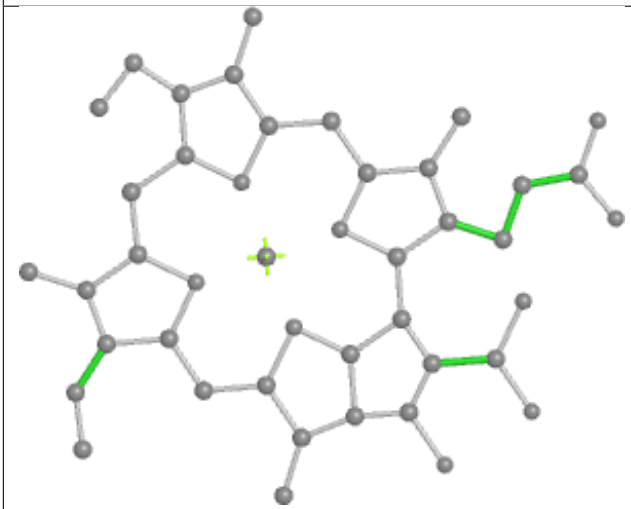


Bond angles



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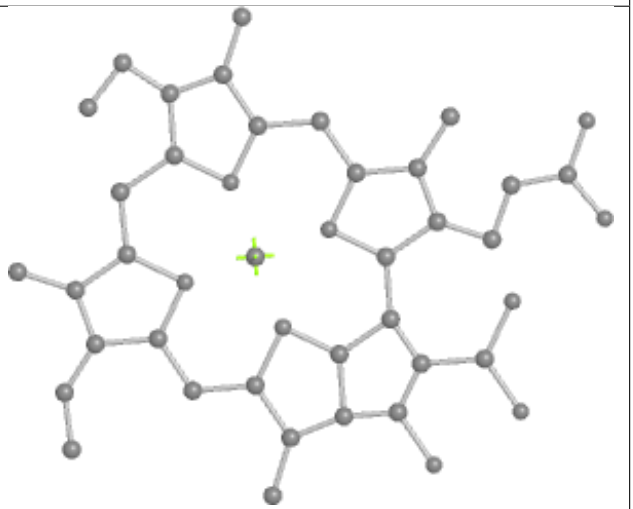
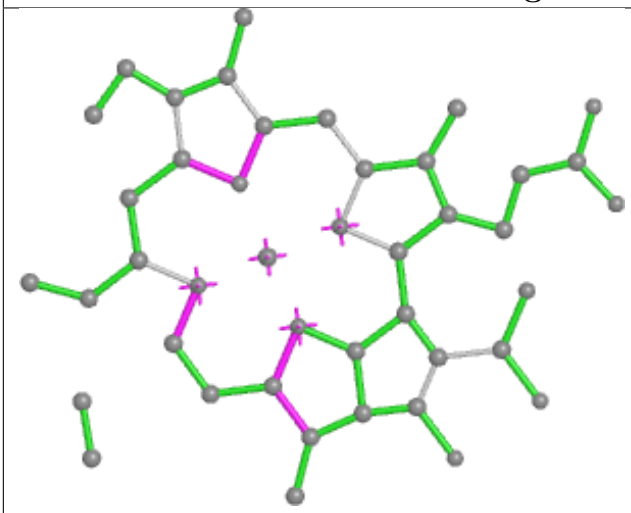


Rings

Ligand CLA B 850



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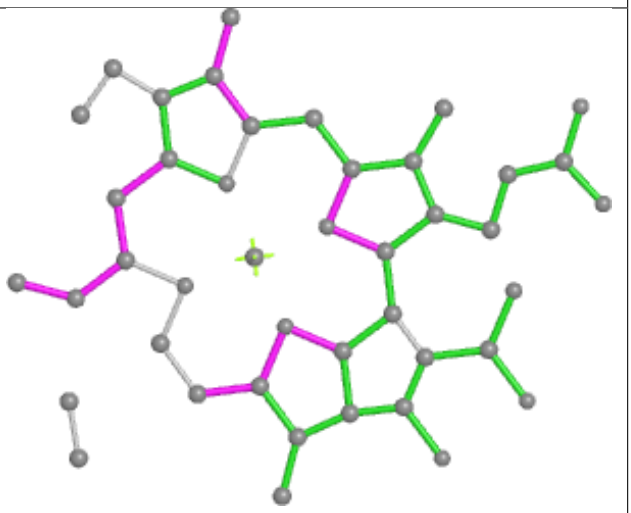
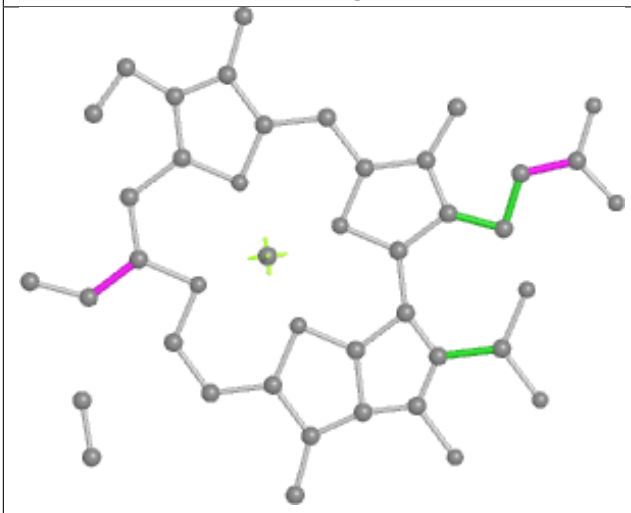


Bond angles



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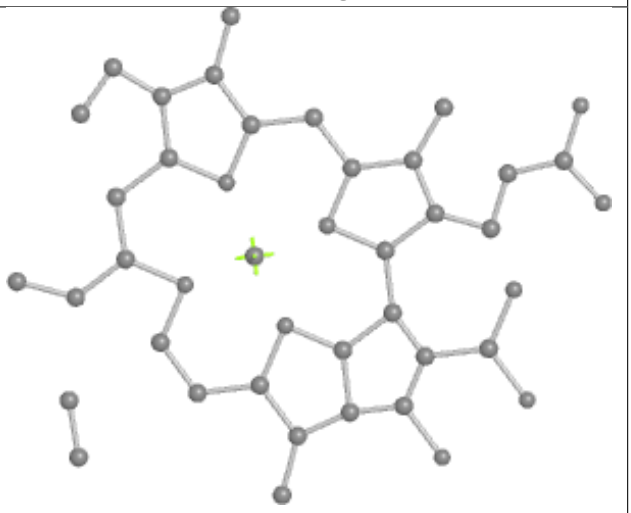
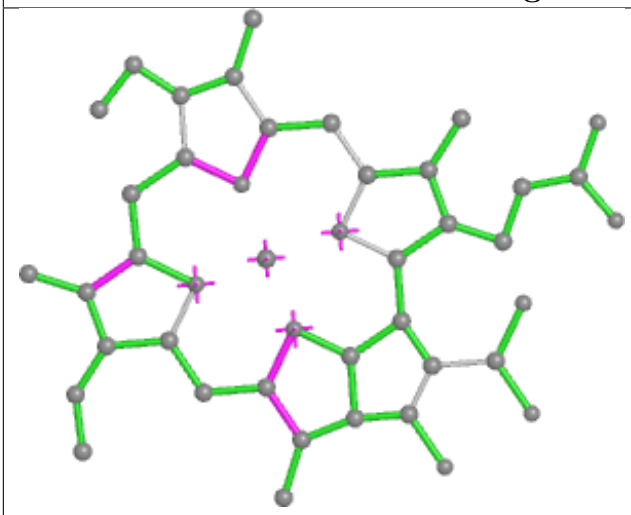
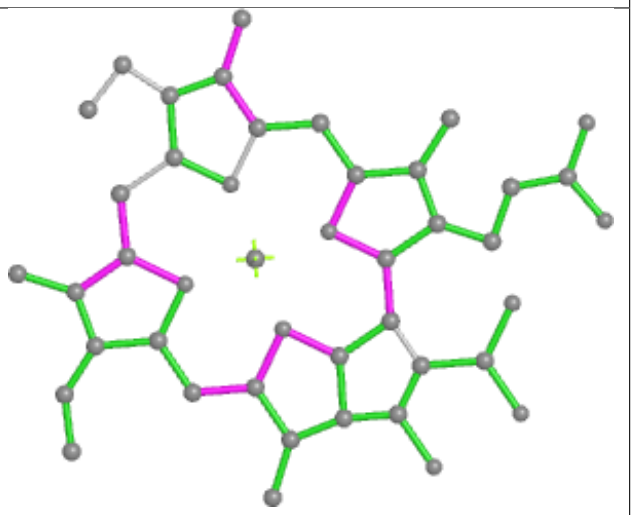


Rings

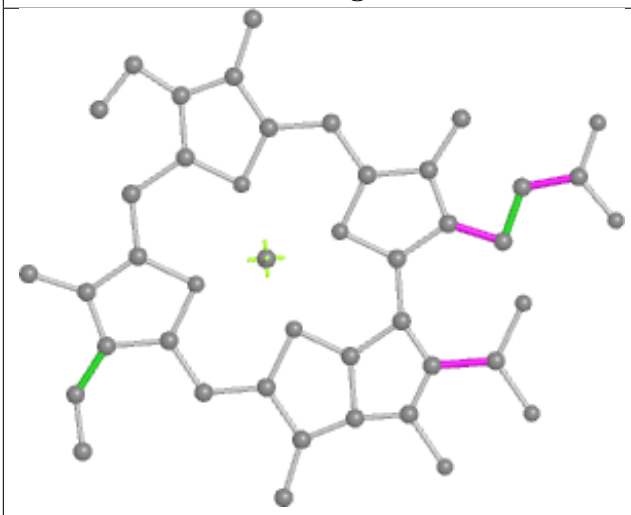
Ligand CLA A 803



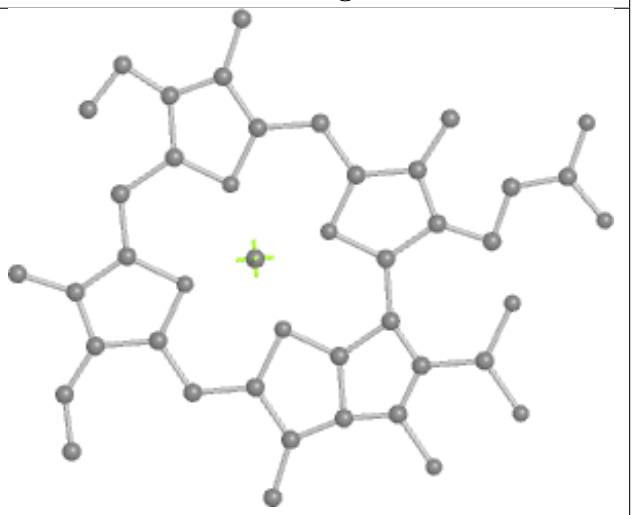
Bond lengths



Bond angles

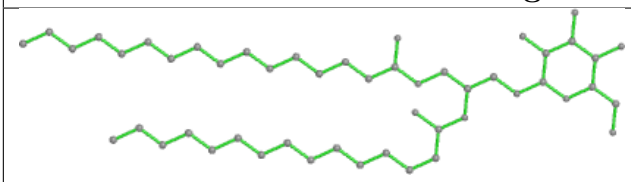


Torsions

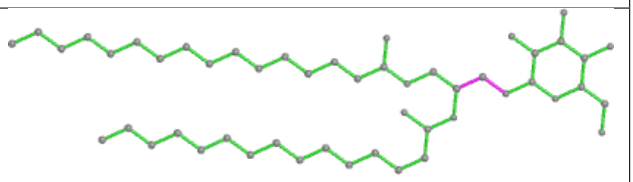


Rings

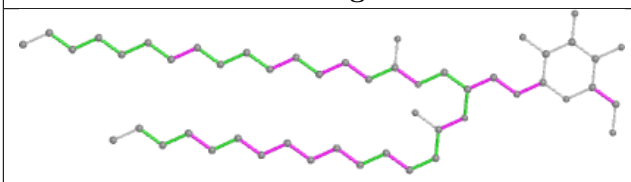
Ligand LMG 0 303



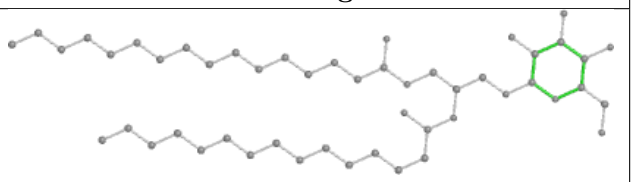
Bond lengths



Bond angles

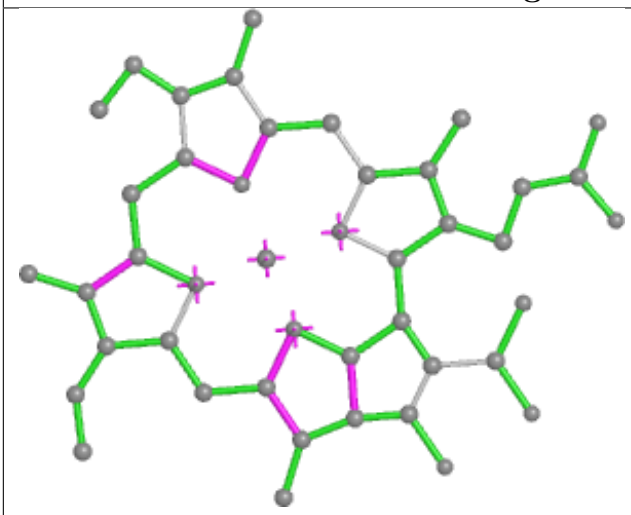


Torsions



Rings

Ligand CLA A 828



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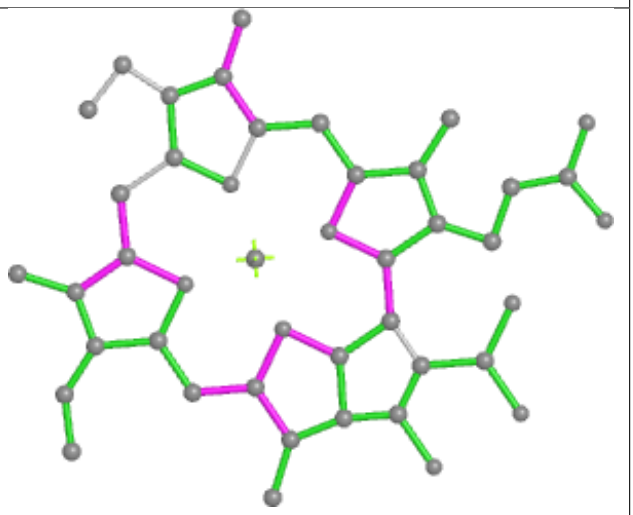
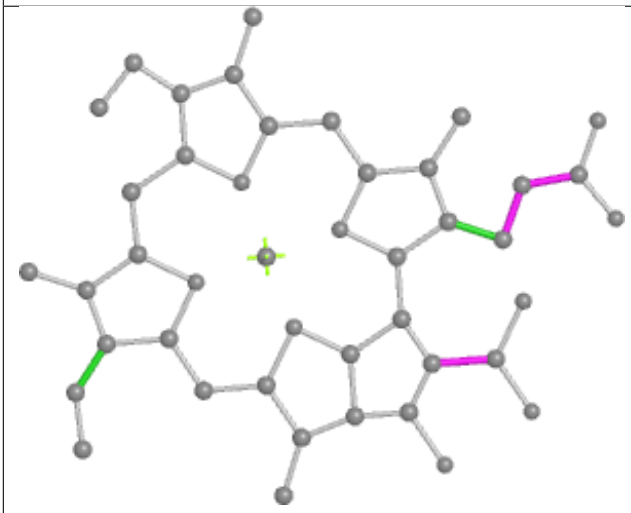


Bond angles



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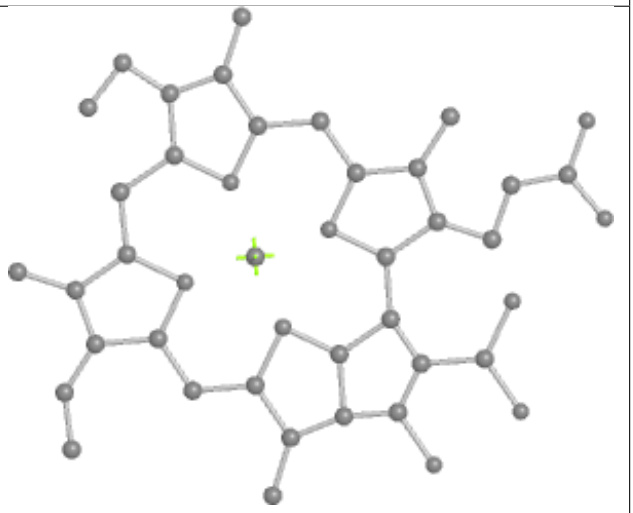
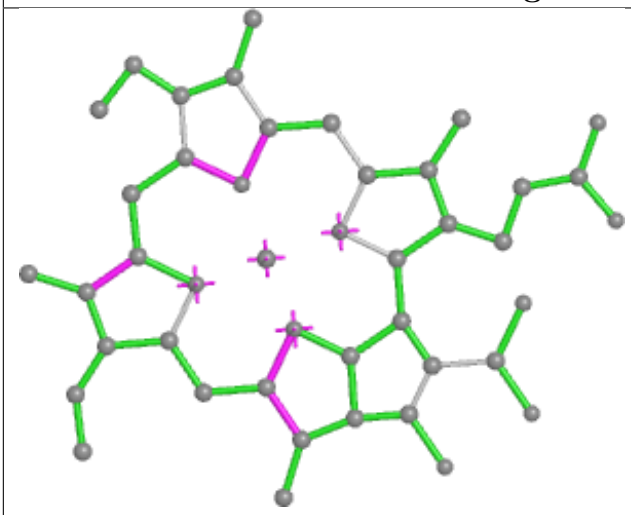


Rings

Ligand CLA A 831



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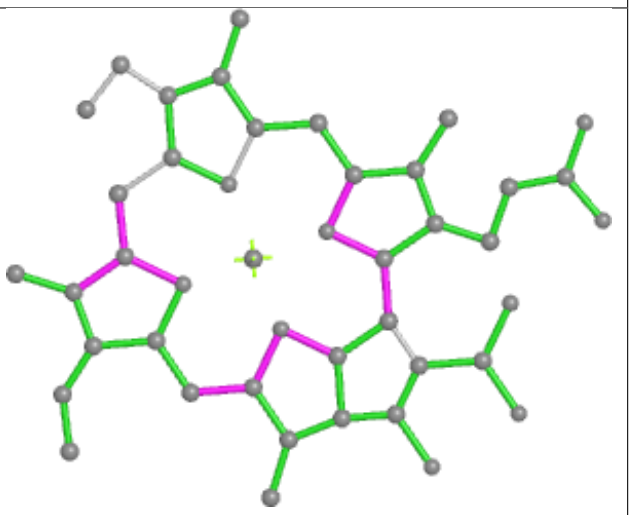
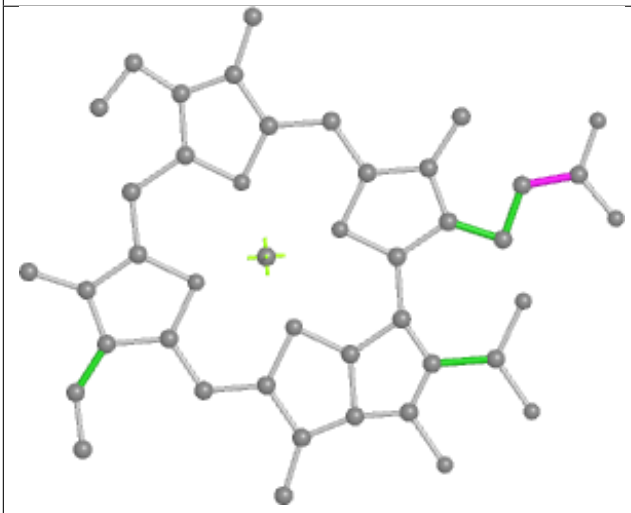
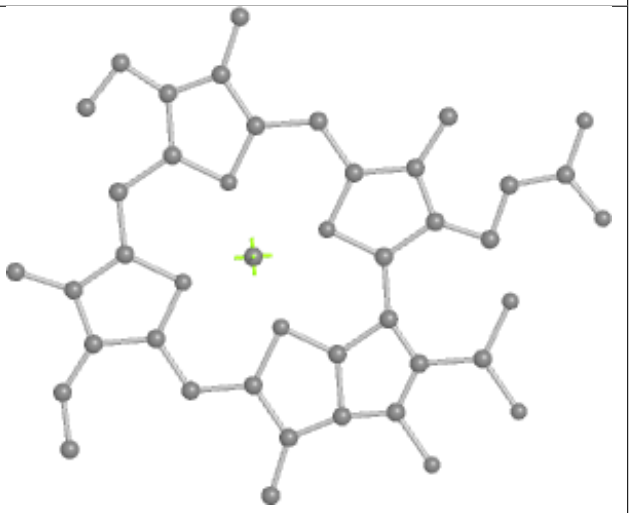


Bond angles

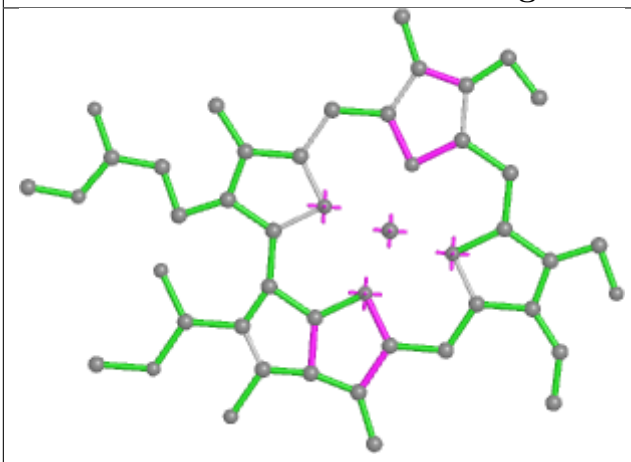


Torsions



Rings

Ligand CHL 7 1012



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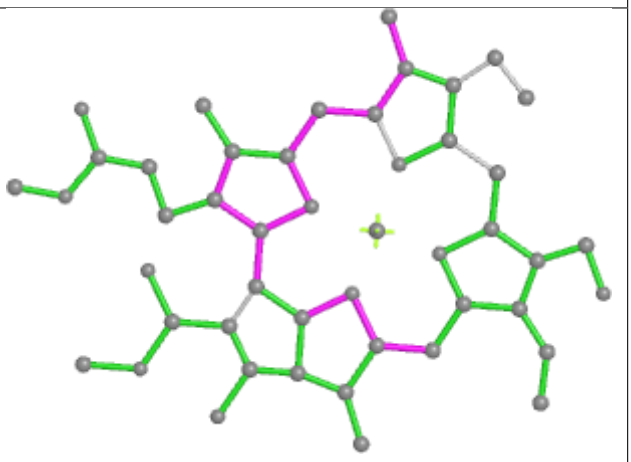
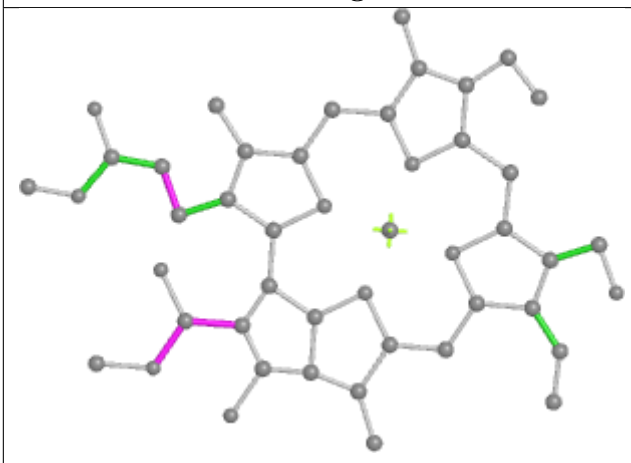


Bond angles



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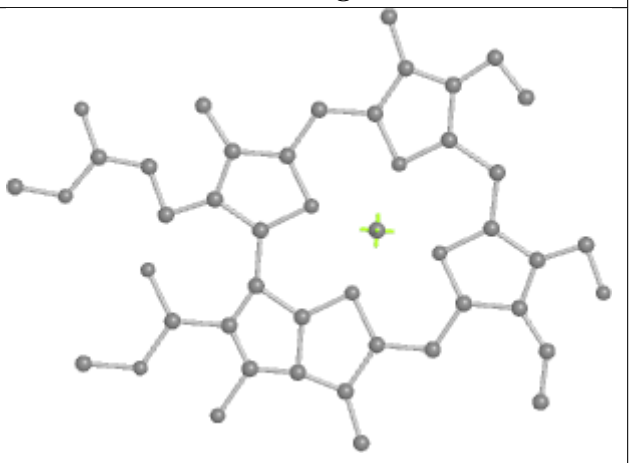
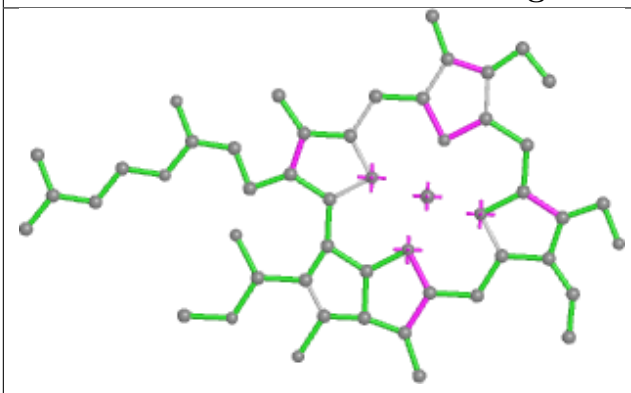


Rings

Ligand CHL 6 314



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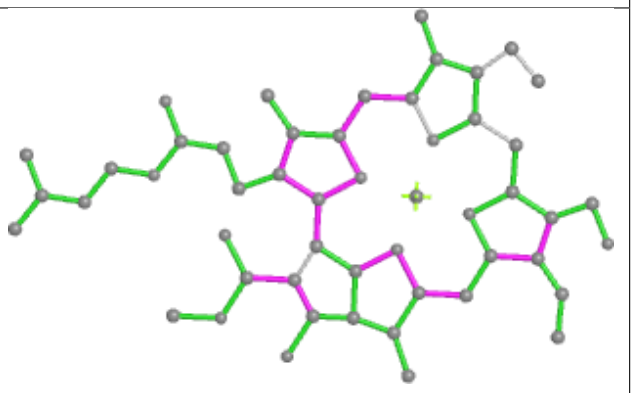
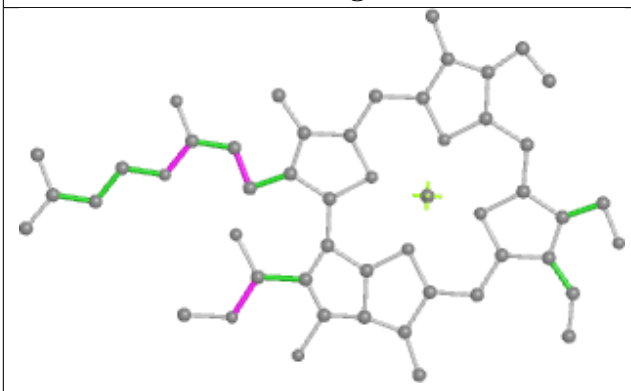


Bond angles



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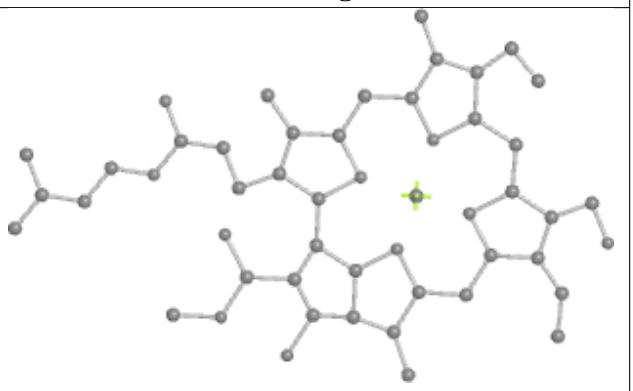
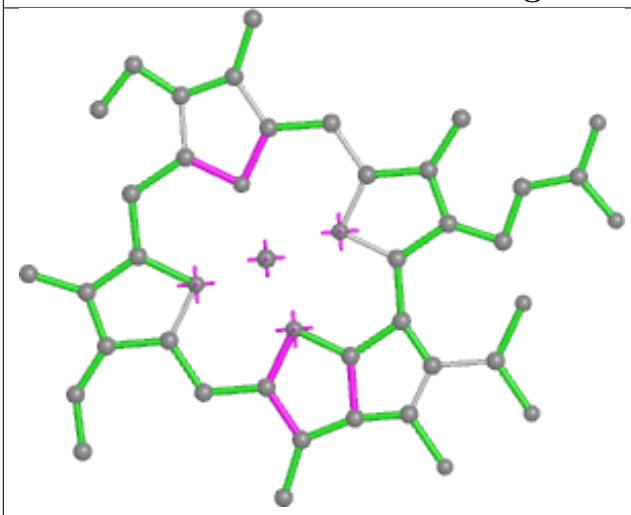


Rings

Ligand CLA A 835



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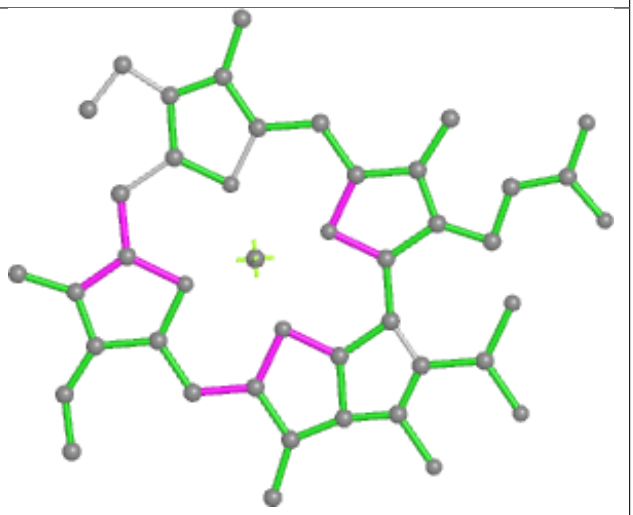
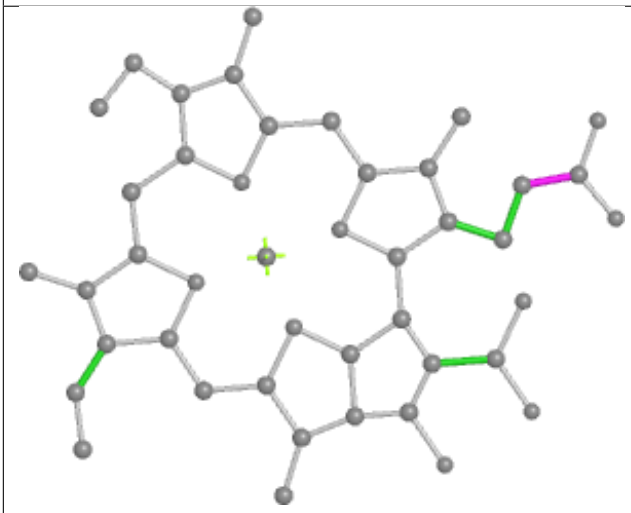
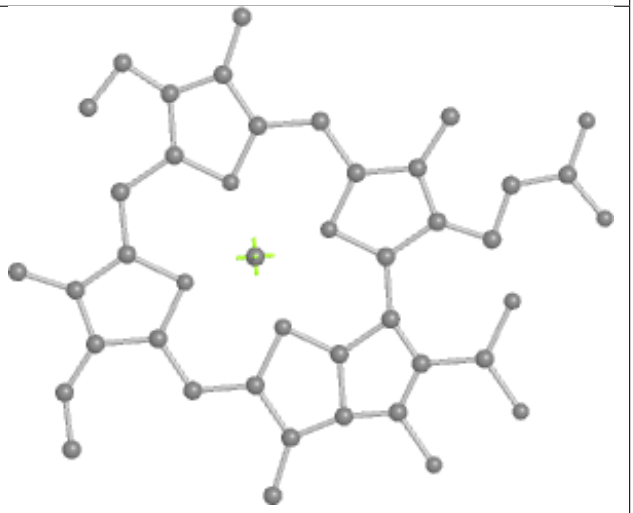


Bond angles

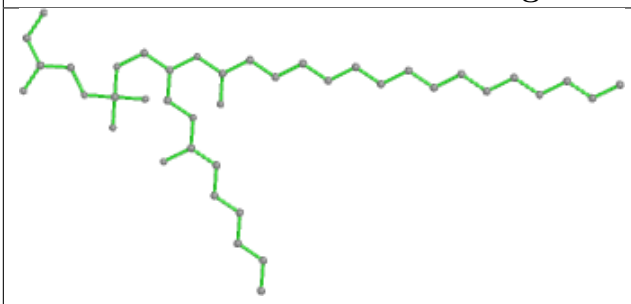


Torsions



Rings

Ligand LHG A 843



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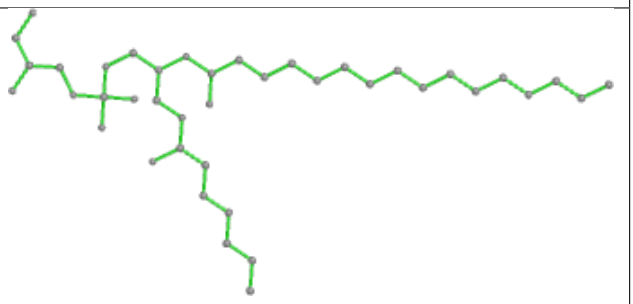

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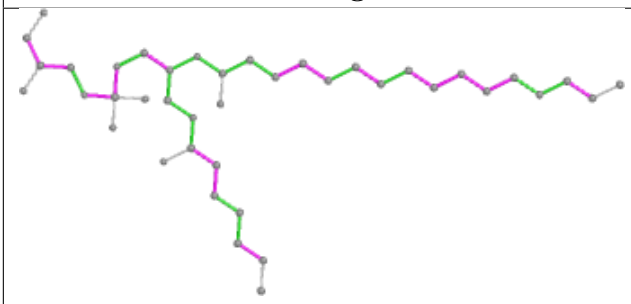

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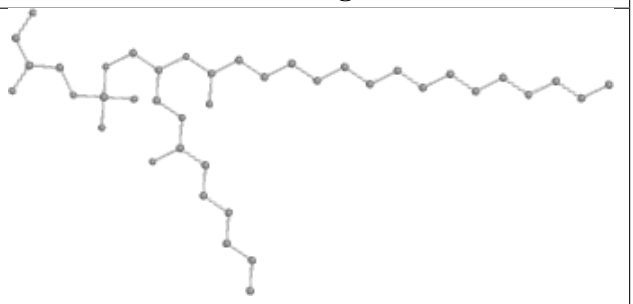
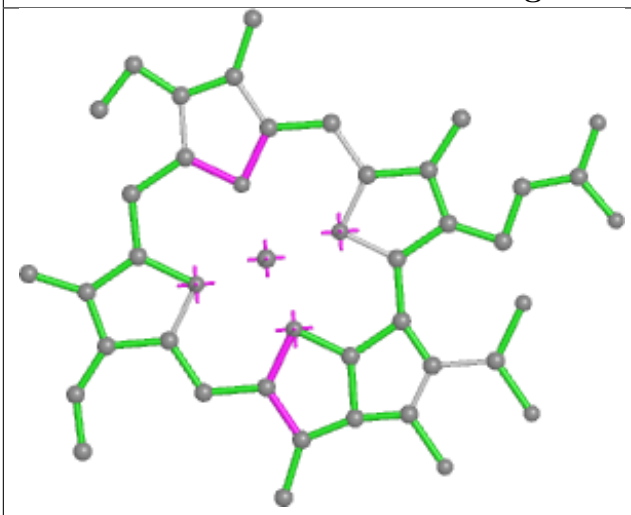
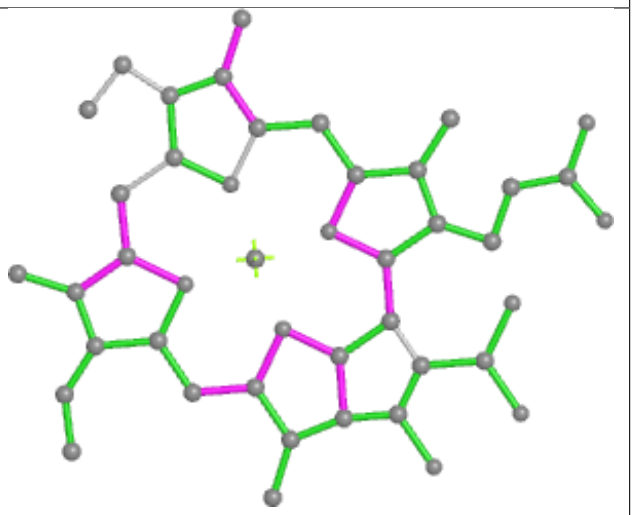


Rings

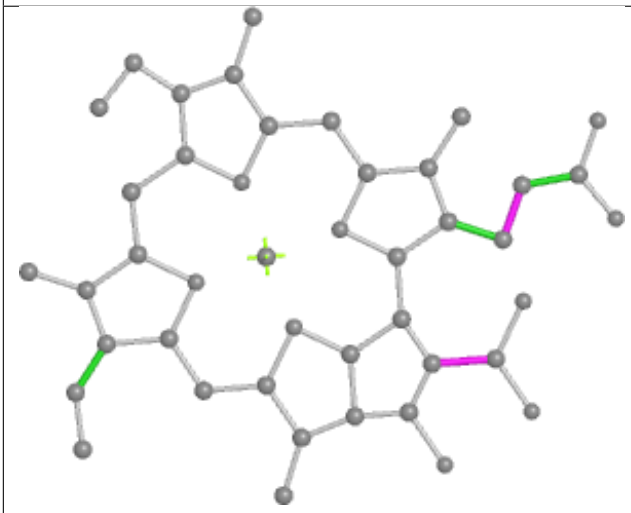
Ligand CLA B 833



Bond lengths



Bond angles



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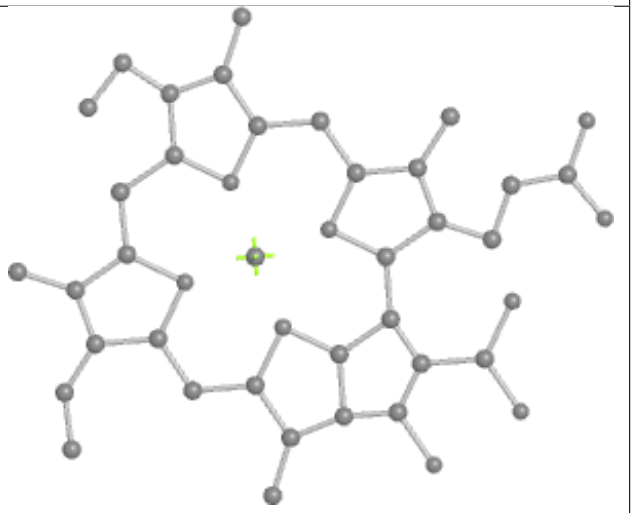
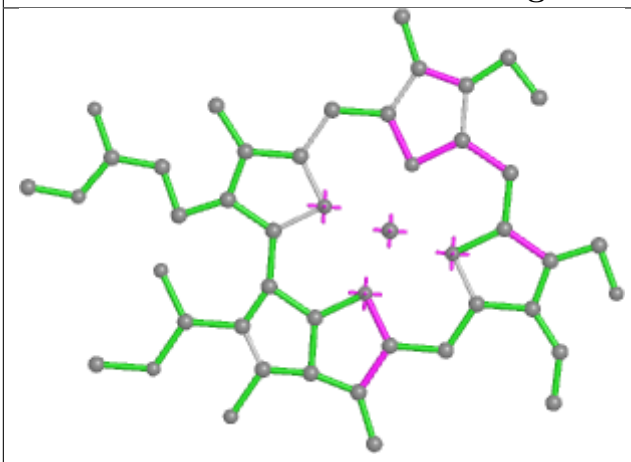


Rings

Ligand CHL 4 312



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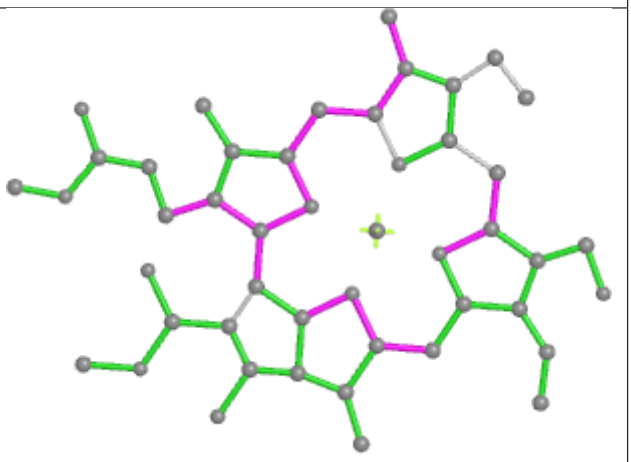
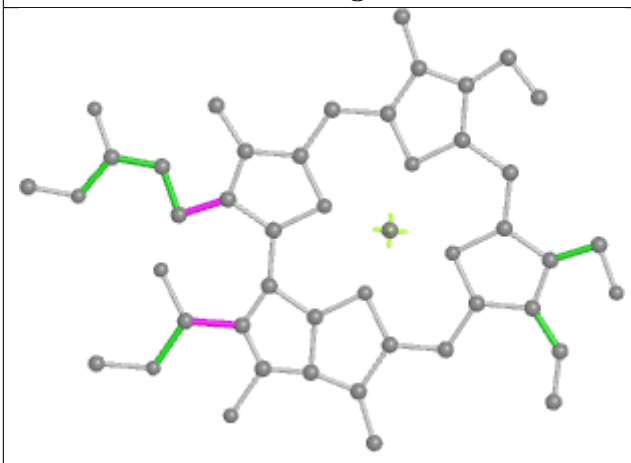
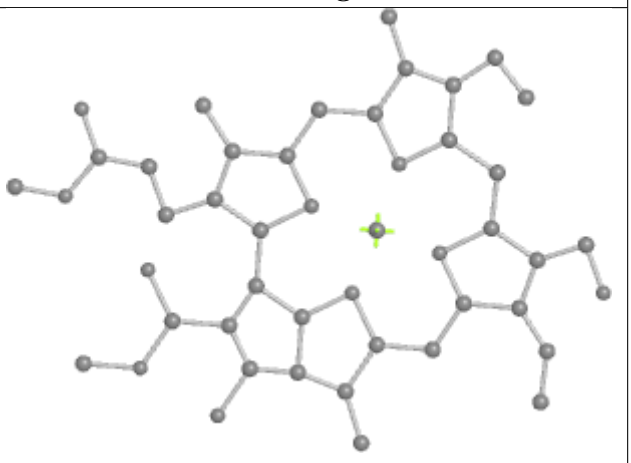


Bond angles

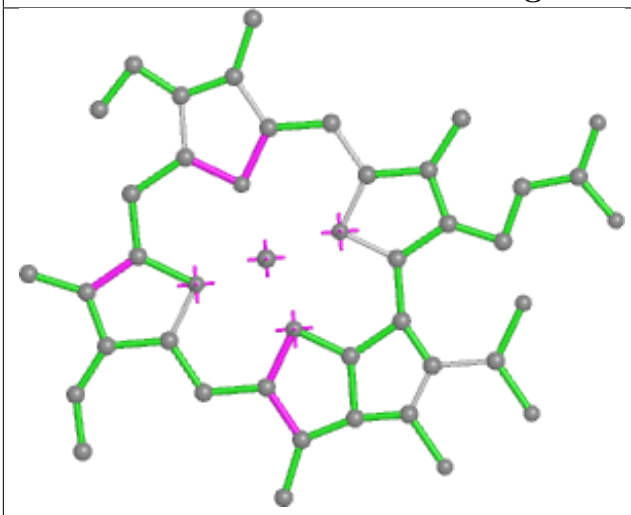


Torsions



Rings

Ligand CLA B 818



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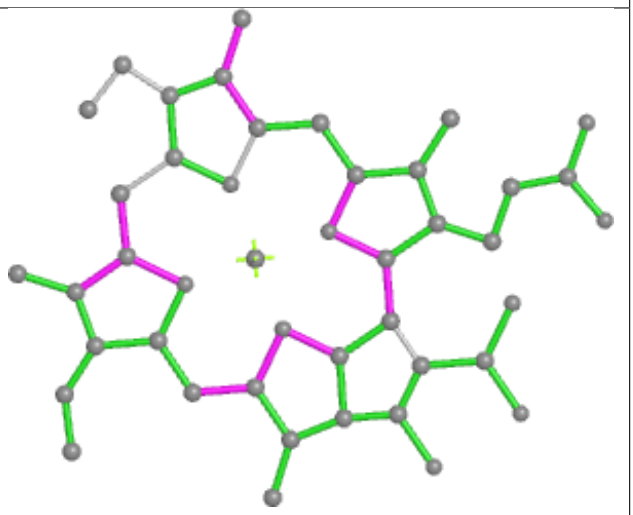
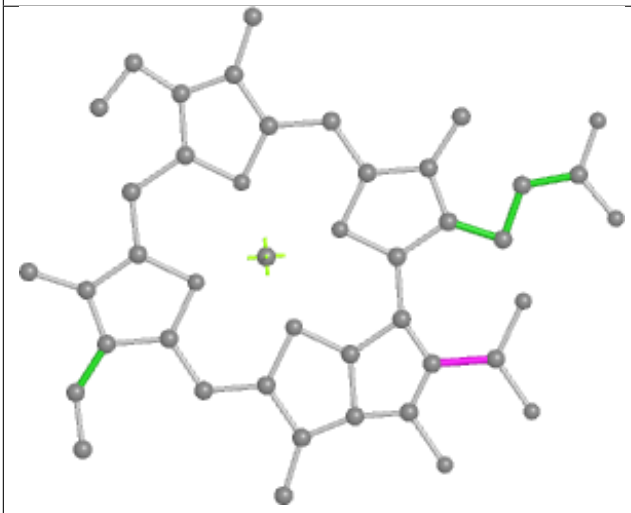


Bond angles



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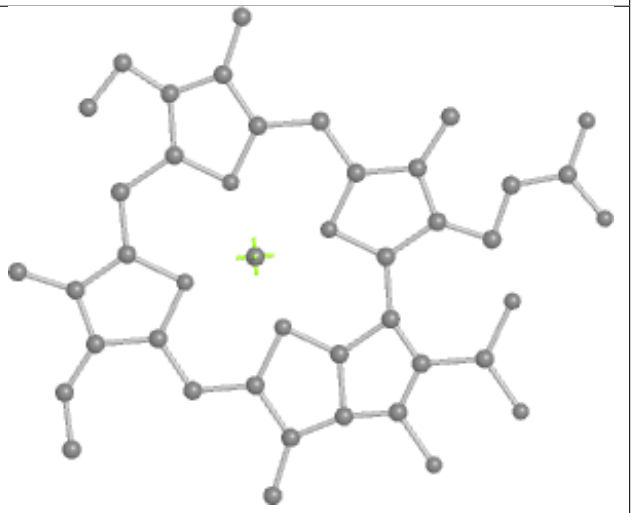
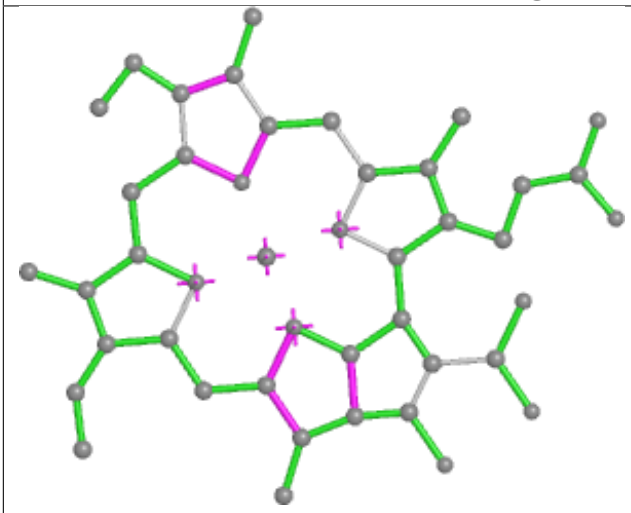


Rings

Ligand CLA 6 315



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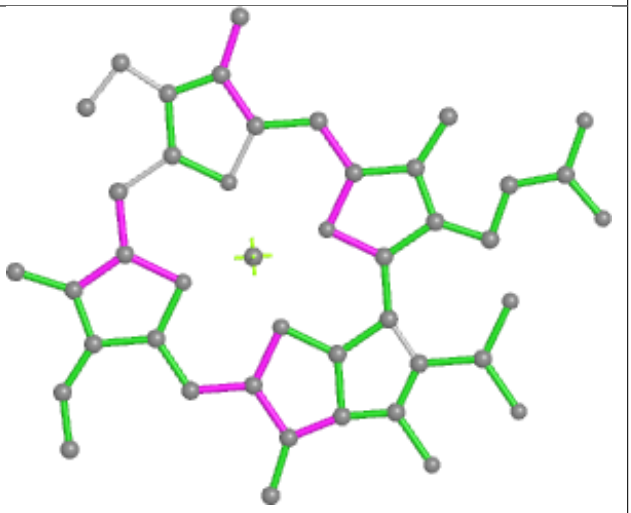
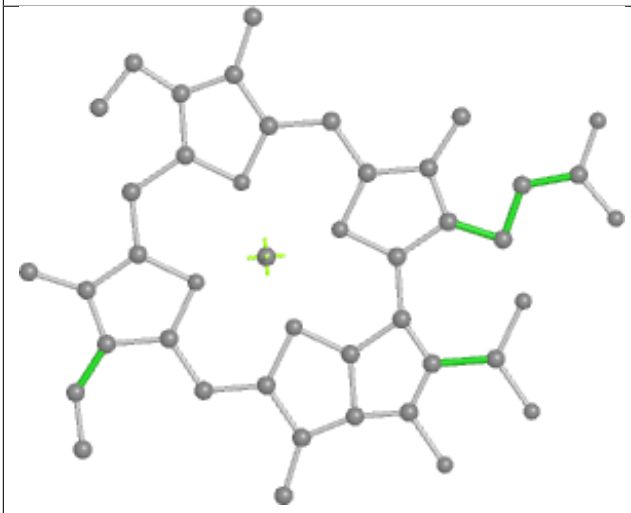


Bond angles



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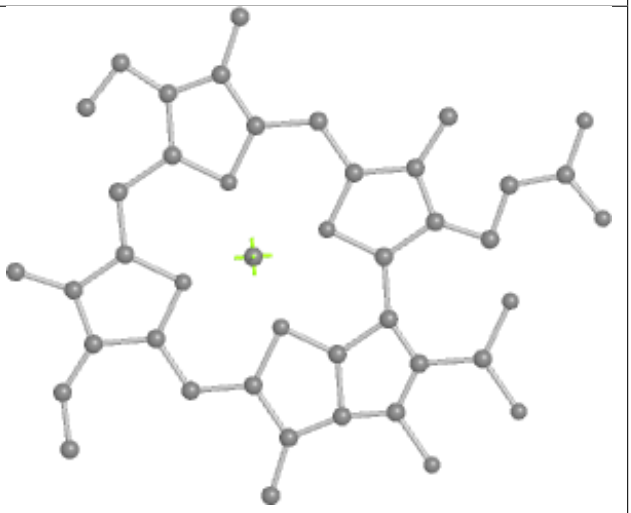
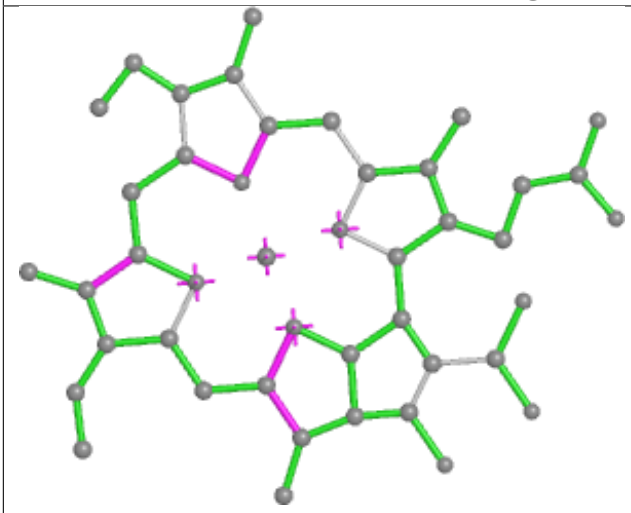


Rings

Ligand CLA B 816



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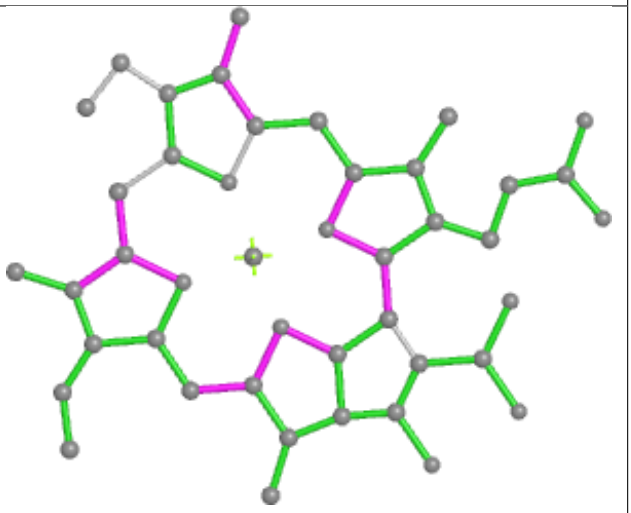
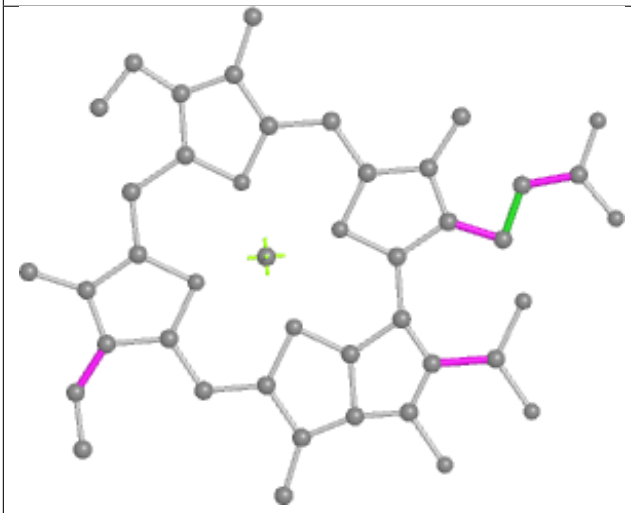


Bond angles



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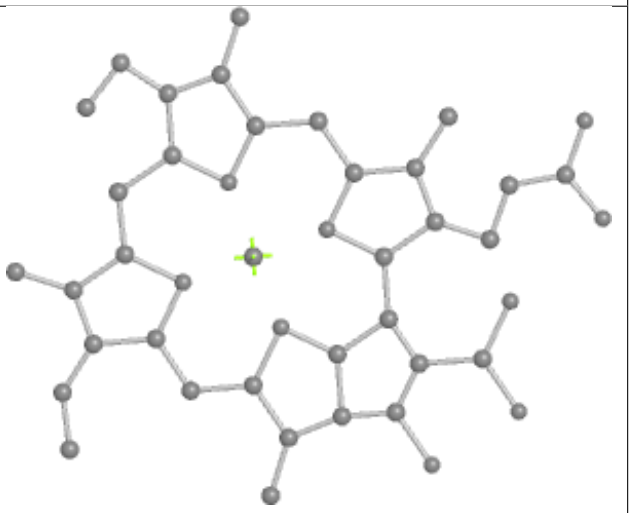
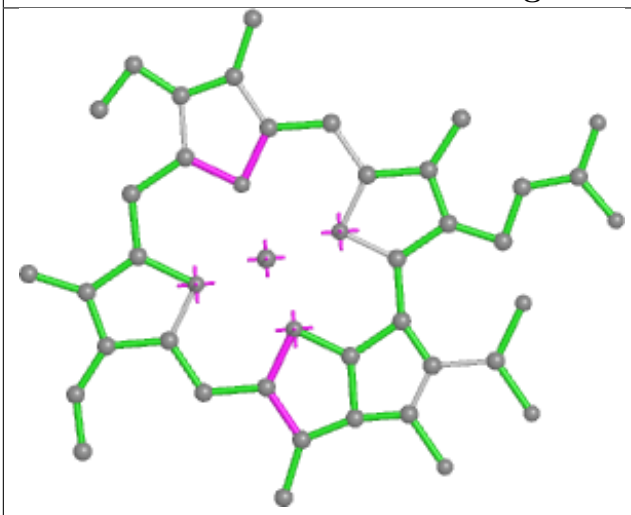
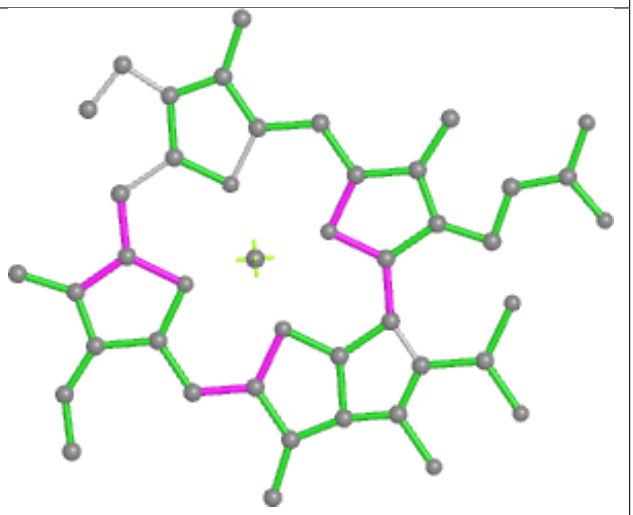


Rings

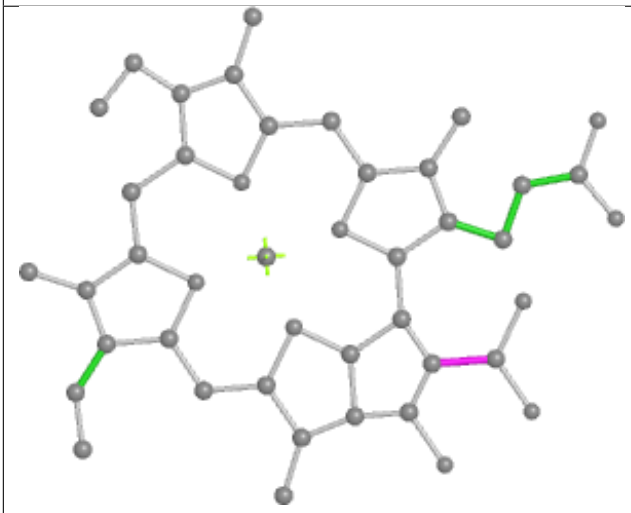
Ligand CLA A 838



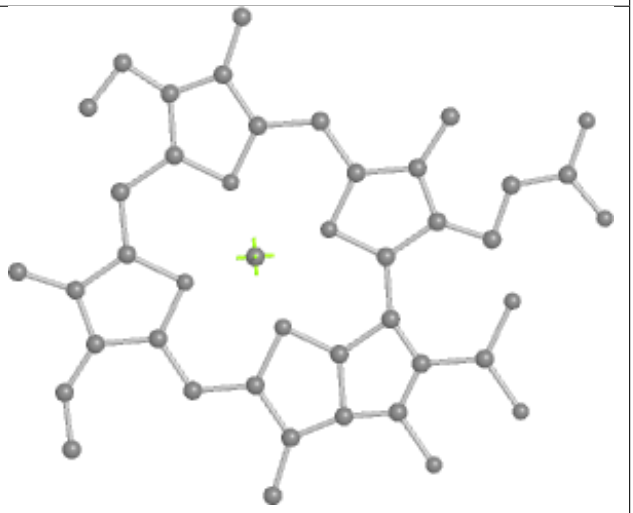
Bond lengths



Bond angles

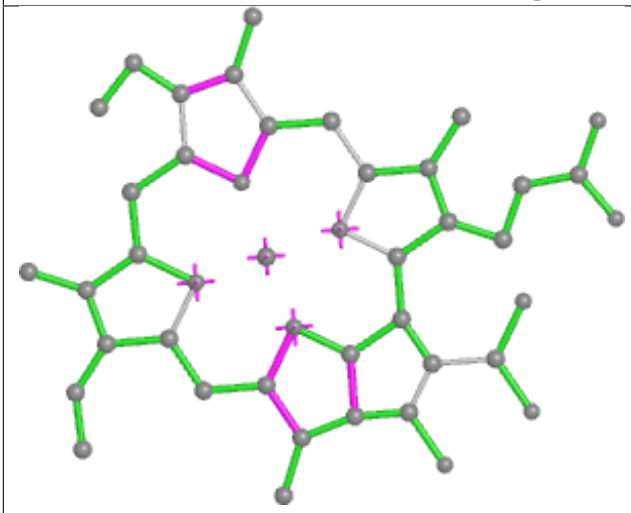


Torsions

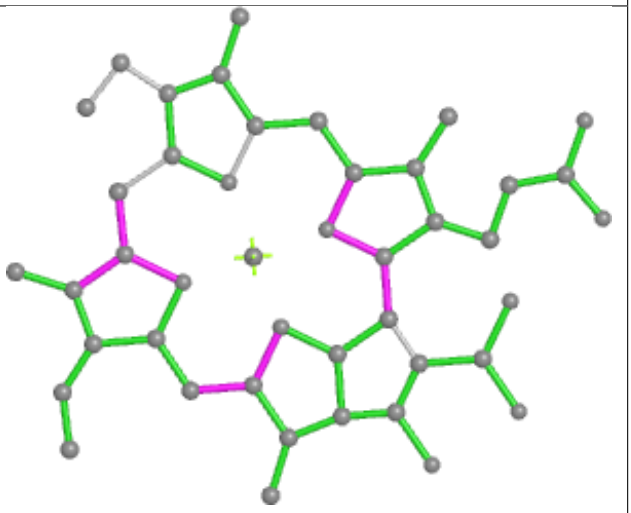


Rings

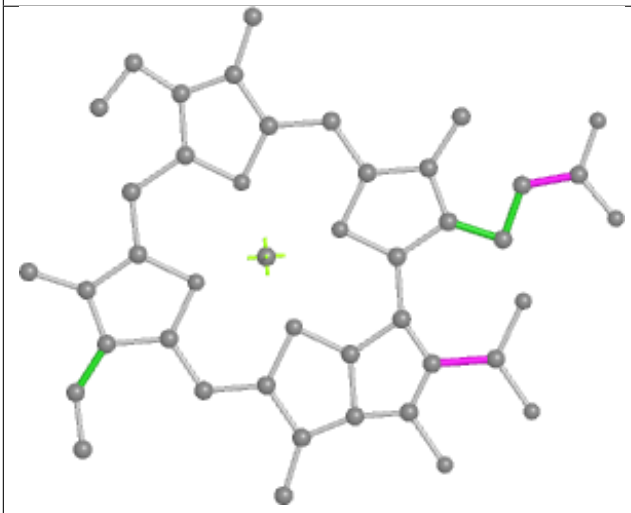
Ligand CLA 0 308



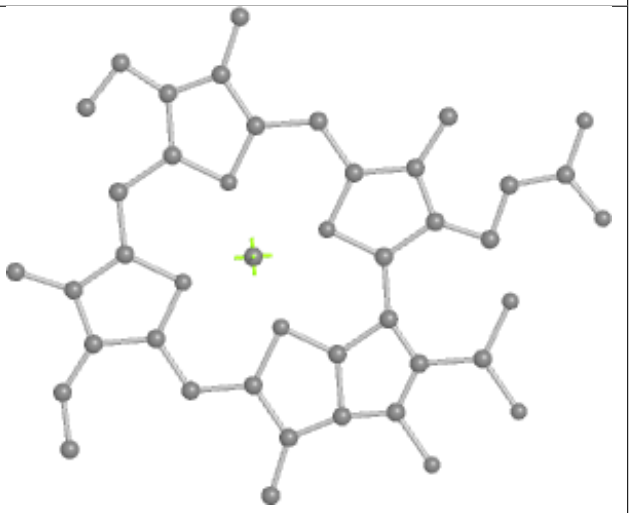
Bond lengths



Bond angles

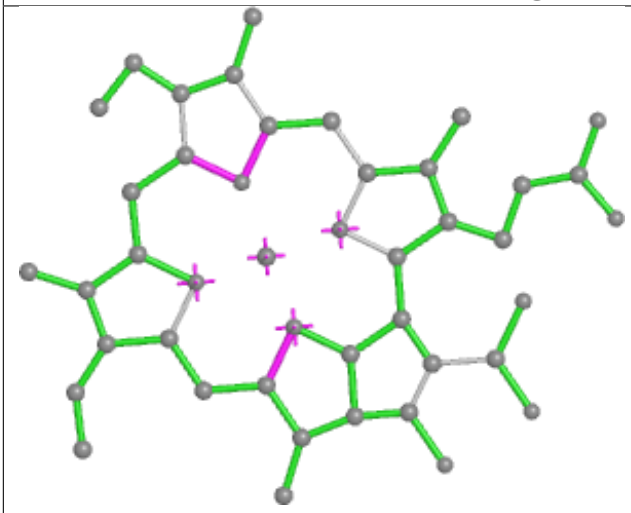


Torsions

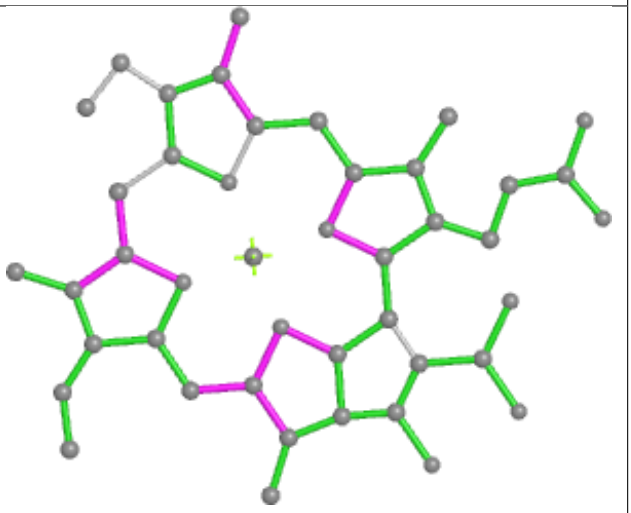


Rings

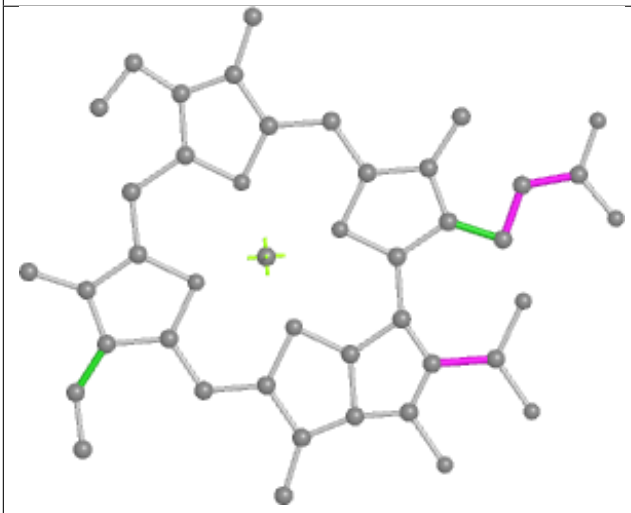
Ligand CLA 0 312



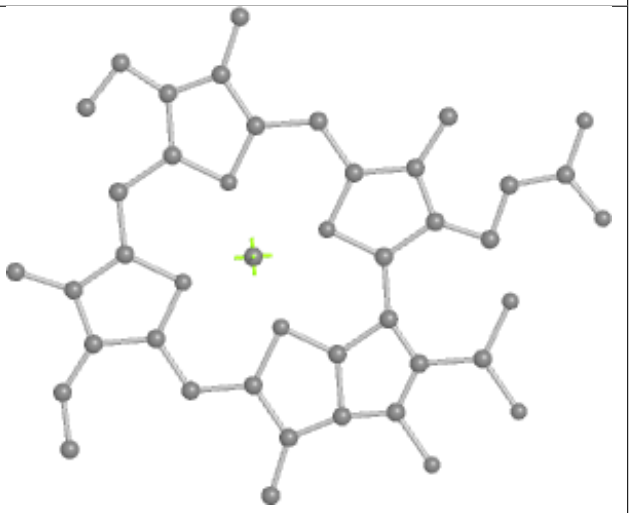
Bond lengths



Bond angles

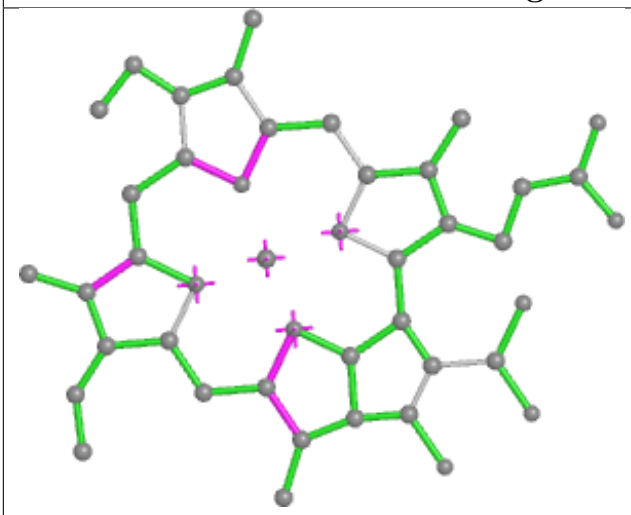


Torsions



Rings

Ligand CLA L 202



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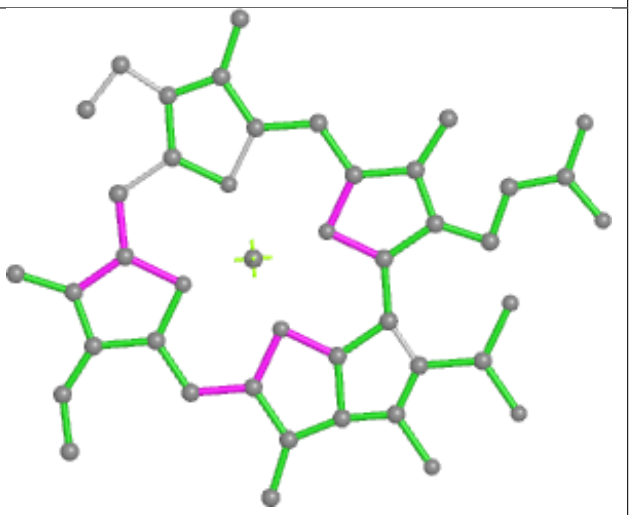
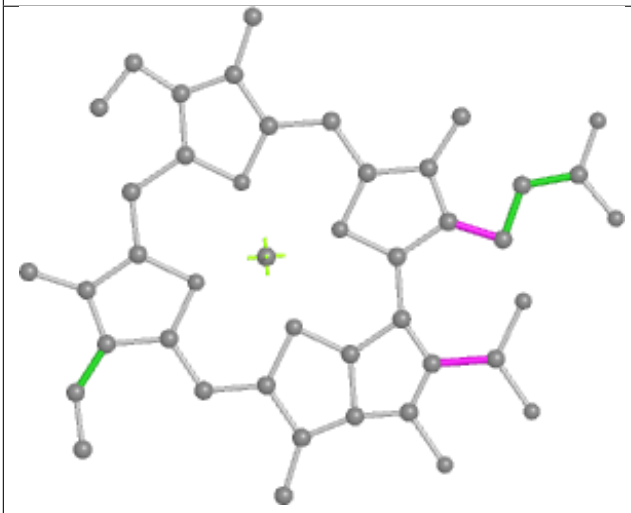


Bond angles



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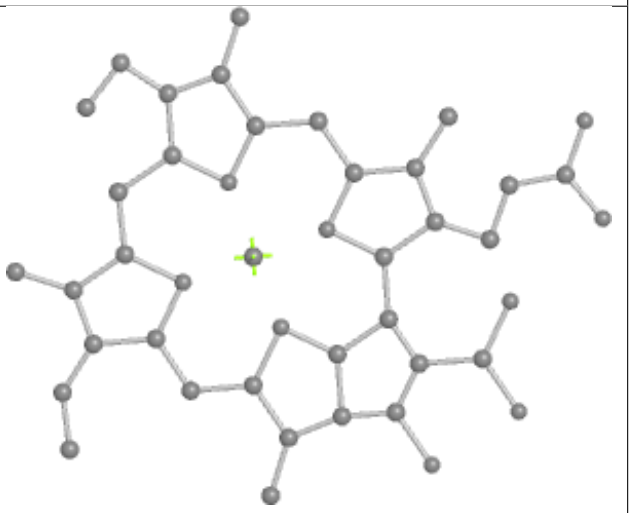
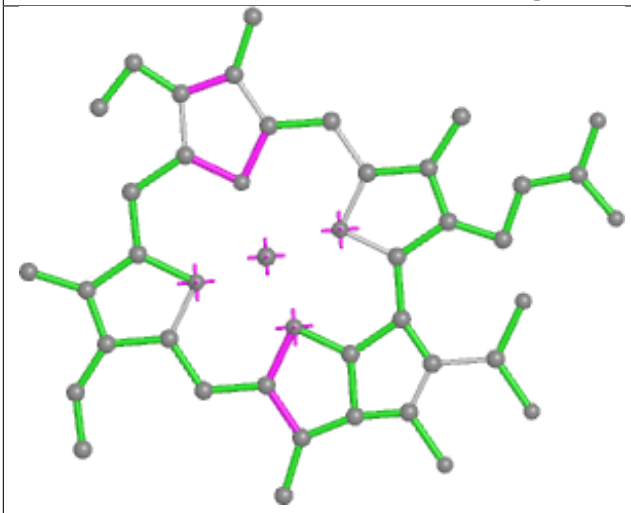


Rings

Ligand CLA 0 306



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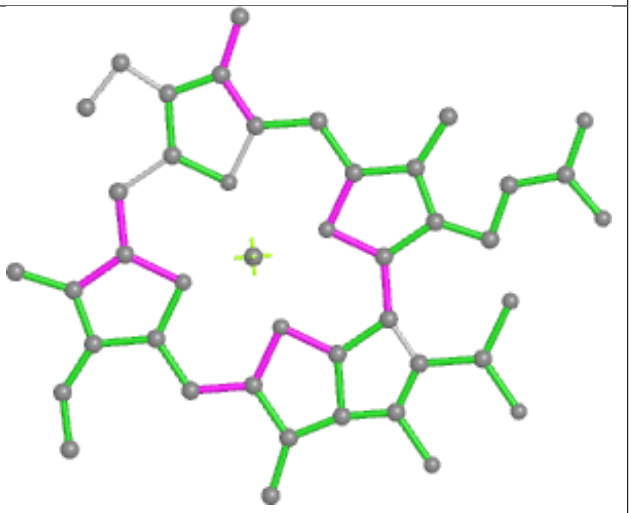
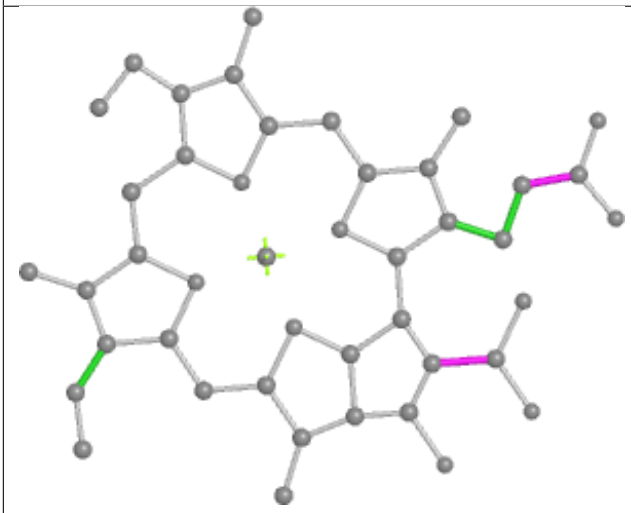


Bond angles



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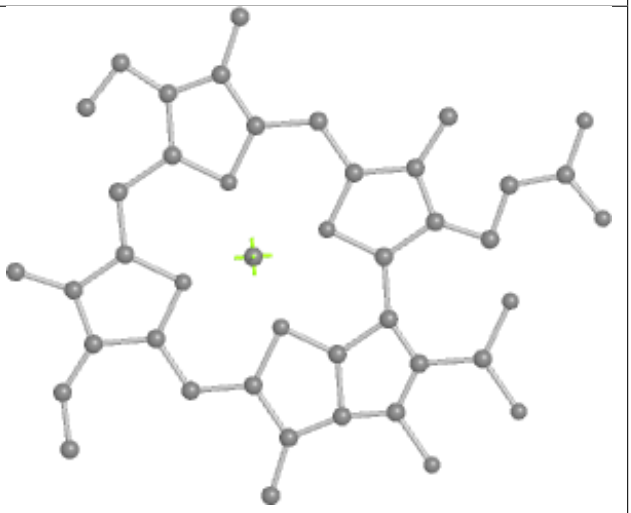
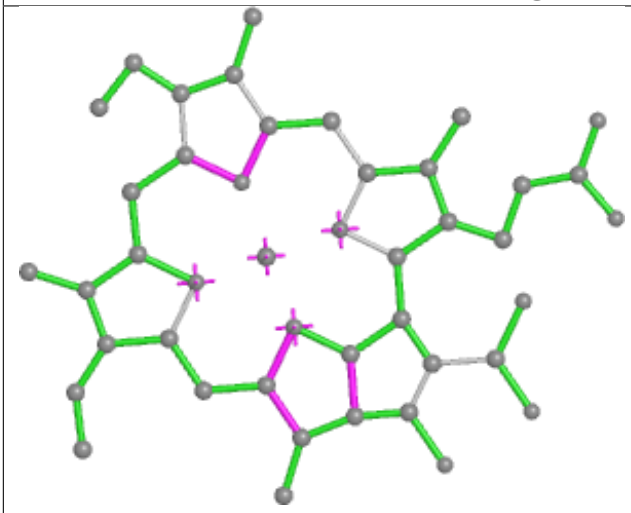


Rings

Ligand CLA 4 304



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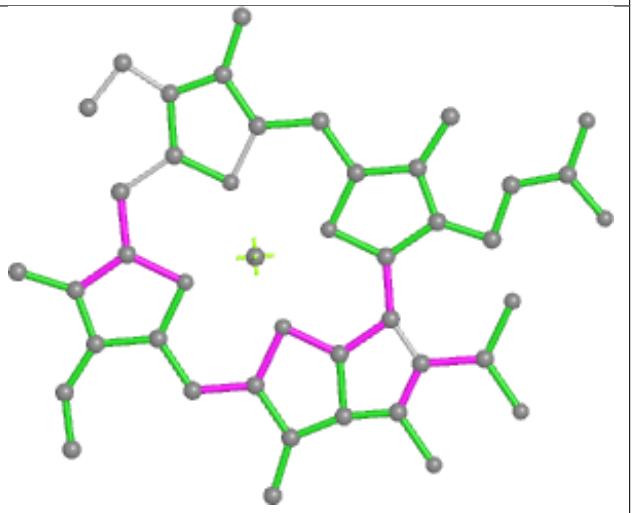

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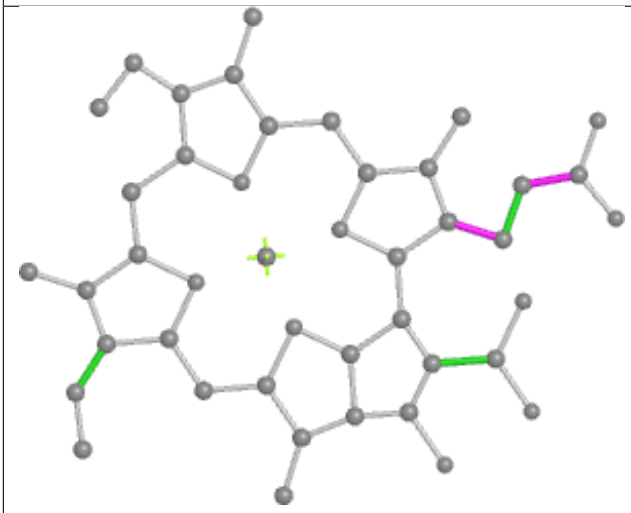

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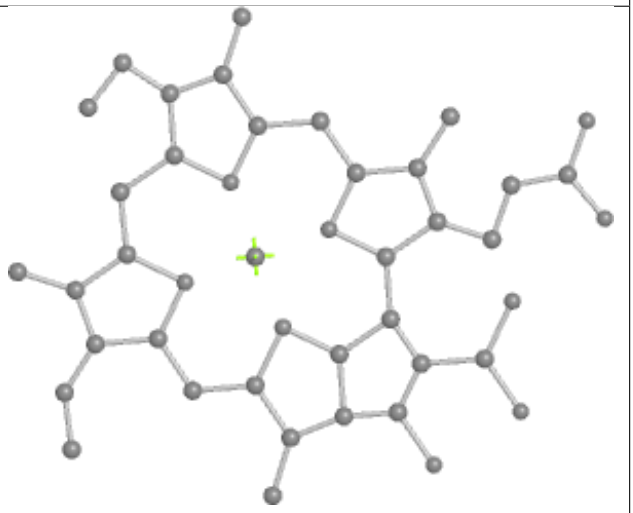
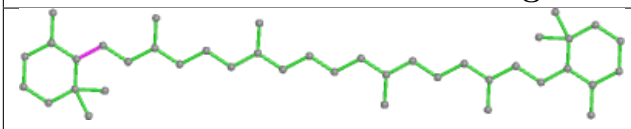


Rings

Ligand BCR B 804



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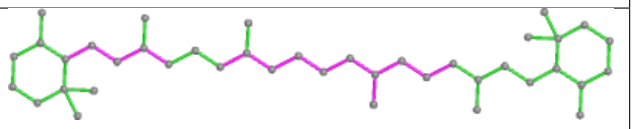

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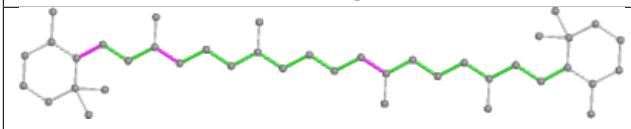
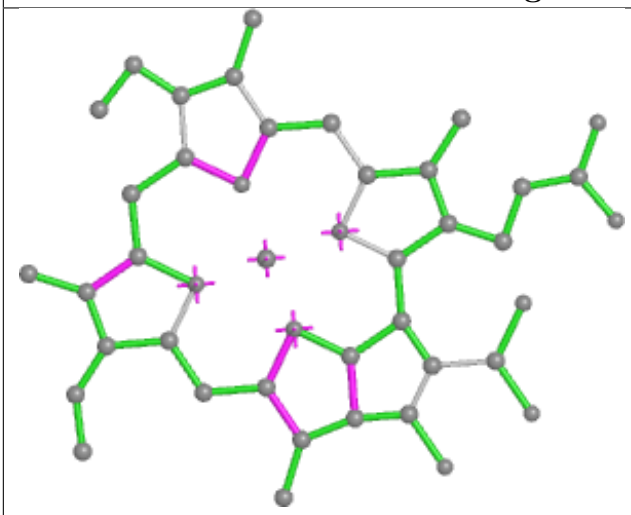


Torsions

Rings

Ligand CLA B 825



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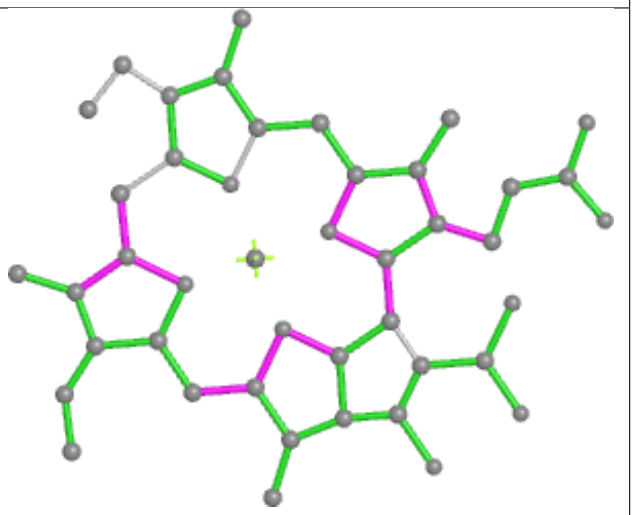
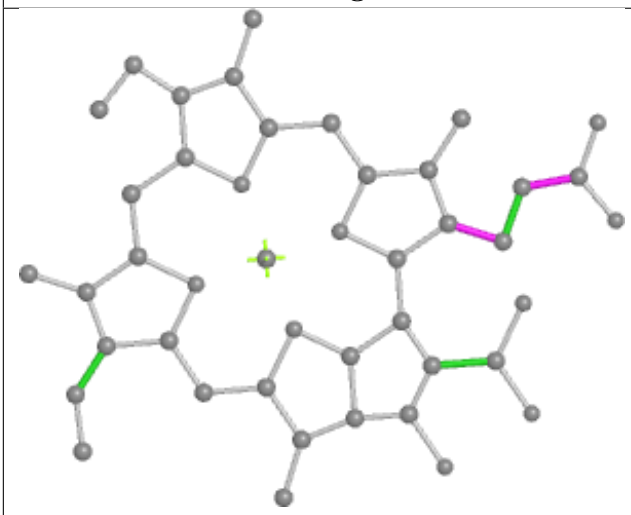


Bond angles



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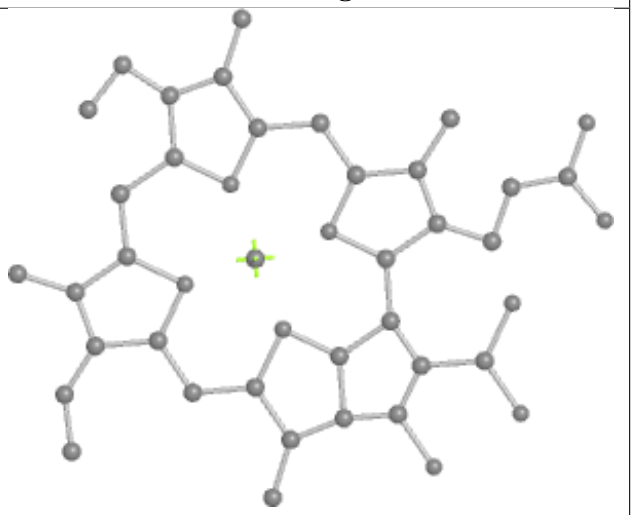
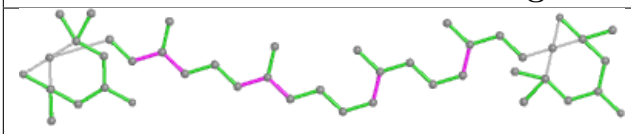


Rings

Ligand XAT 8 304



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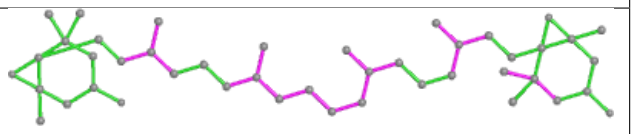

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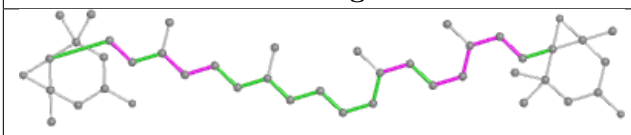

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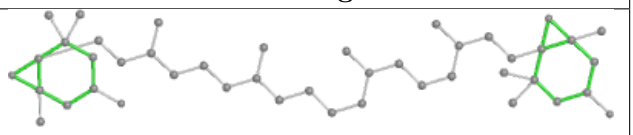
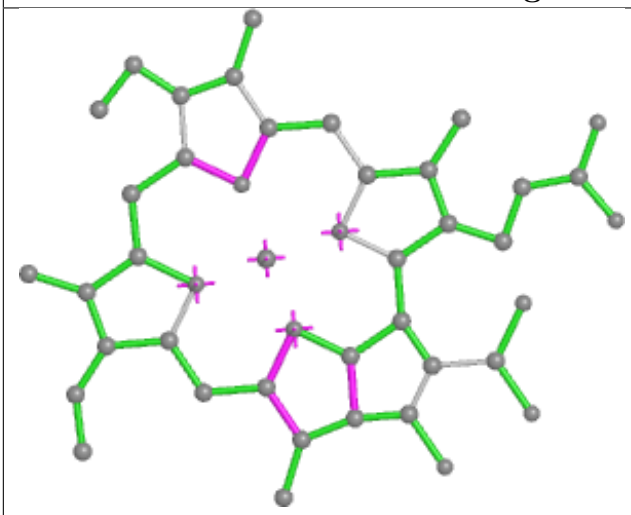


Rings

Ligand CLA A 808



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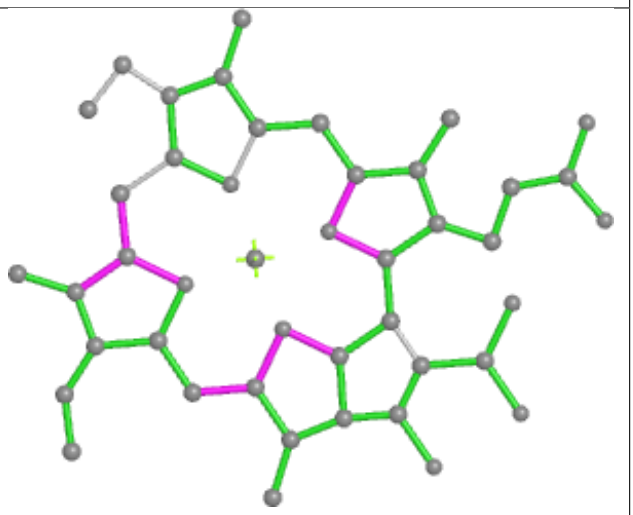
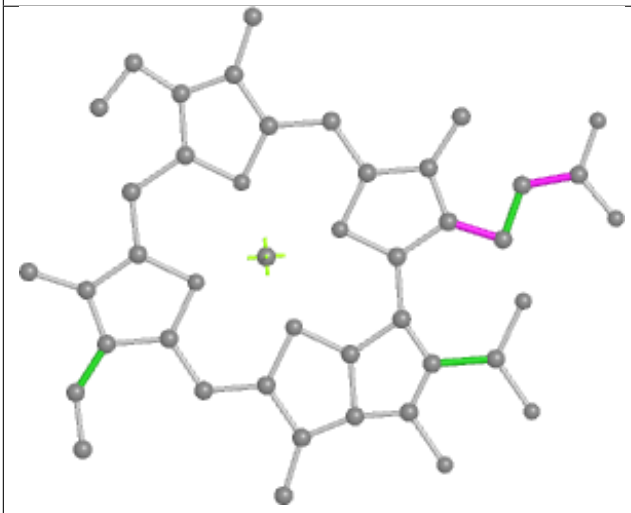


Bond angles



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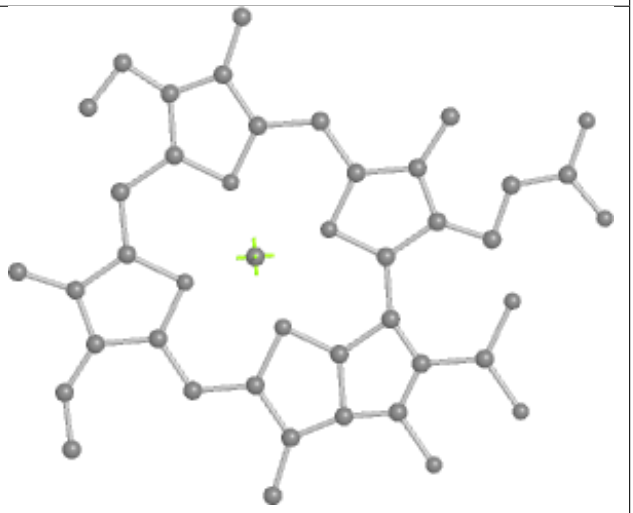
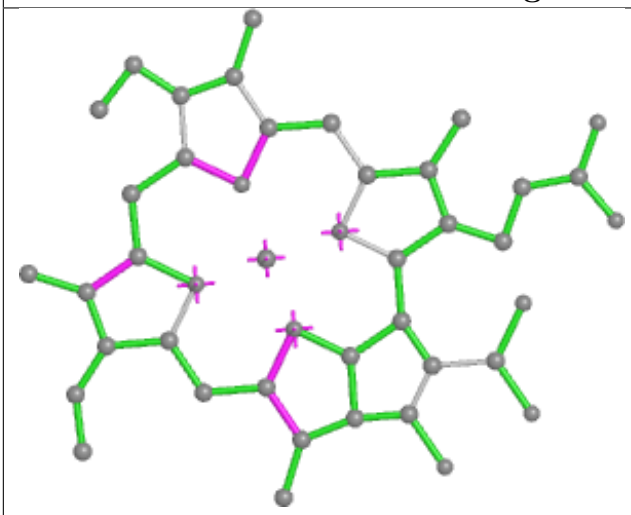


Rings

Ligand CLA A 827



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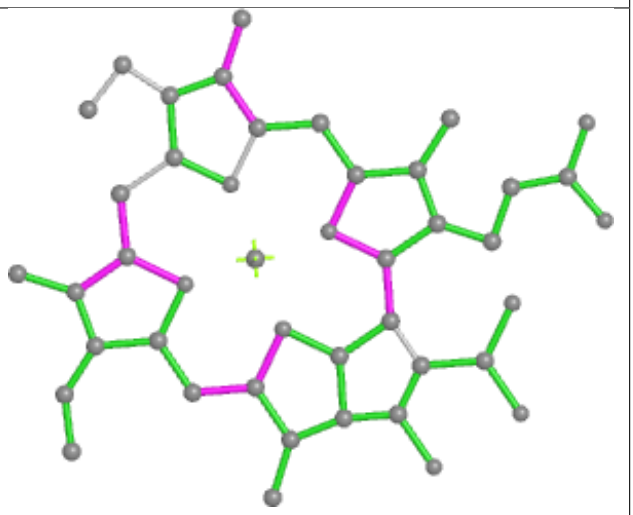
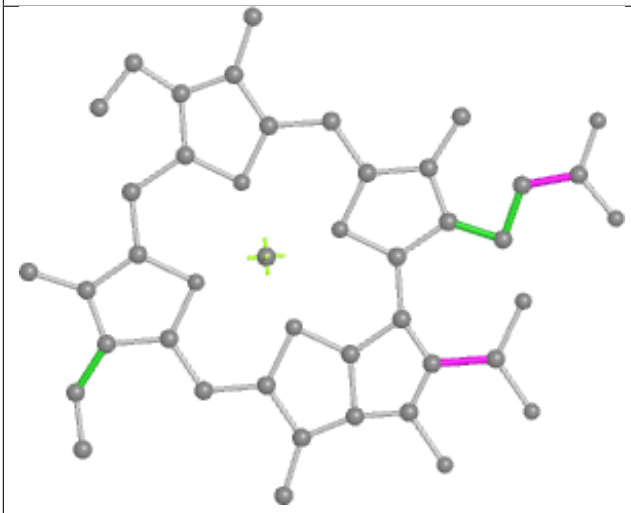


Bond angles



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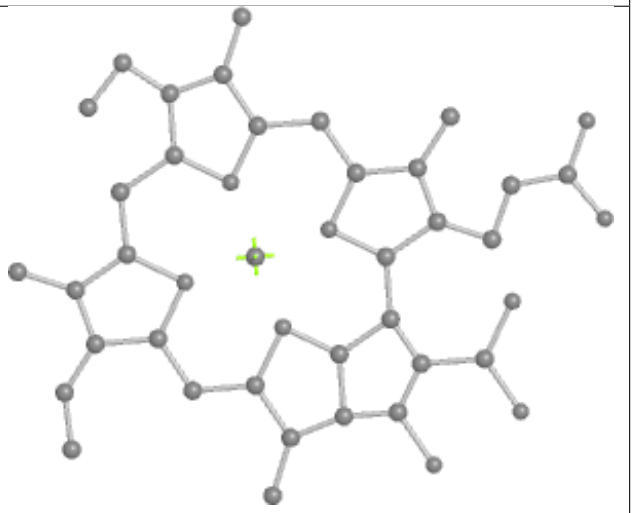
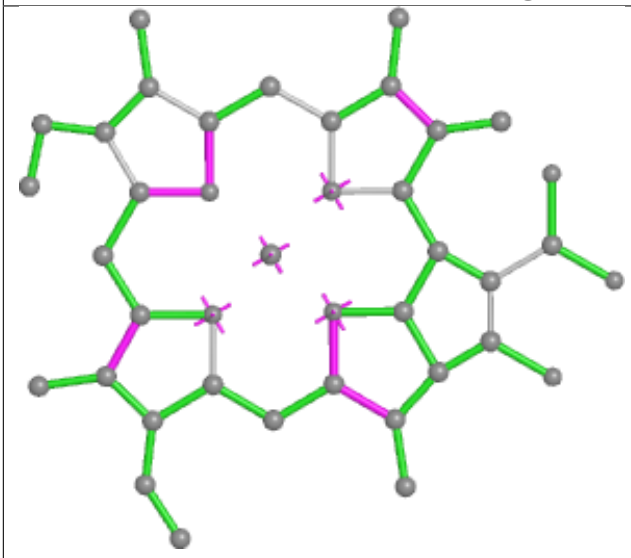


Rings

Ligand CLA 3 1011



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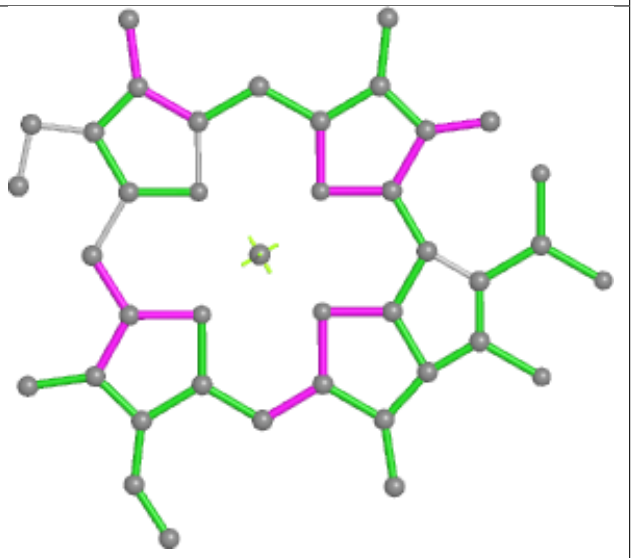
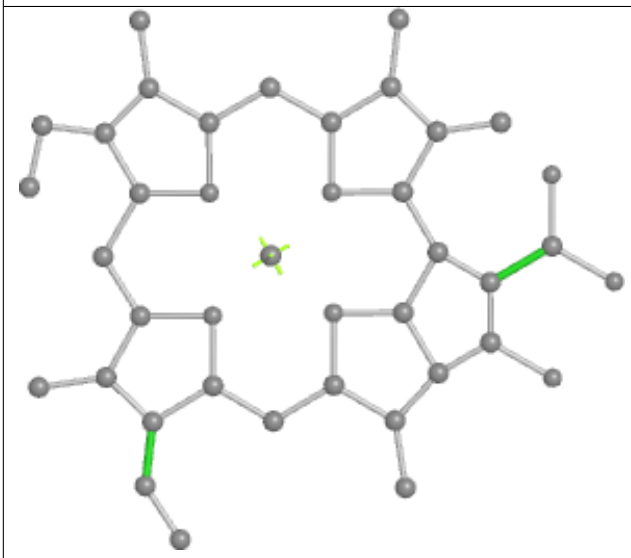


Bond angles



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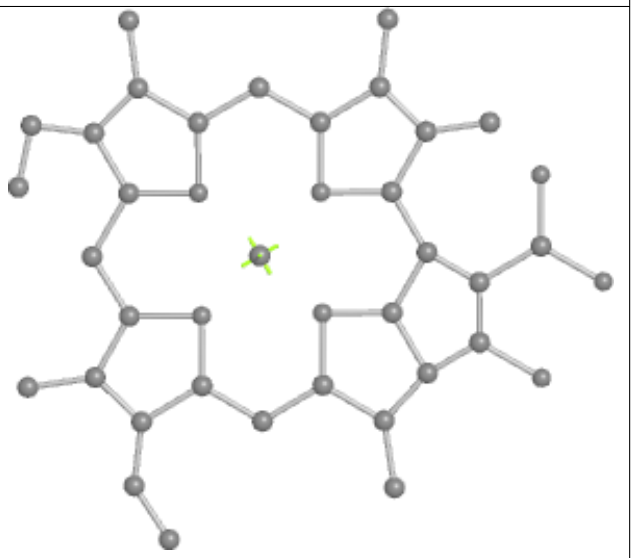
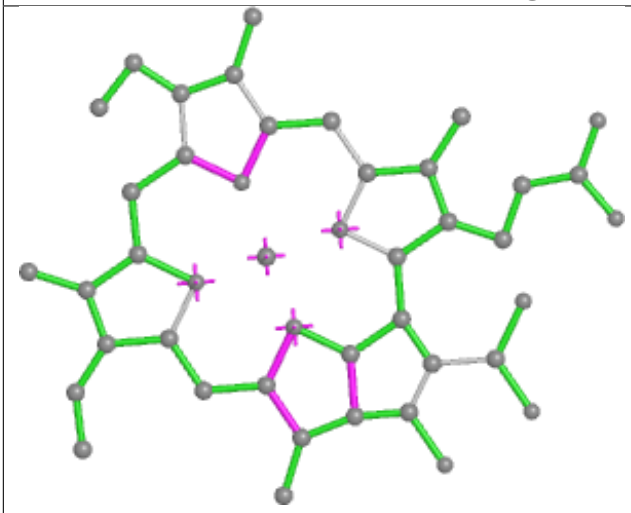


Rings

Ligand CLA A 826



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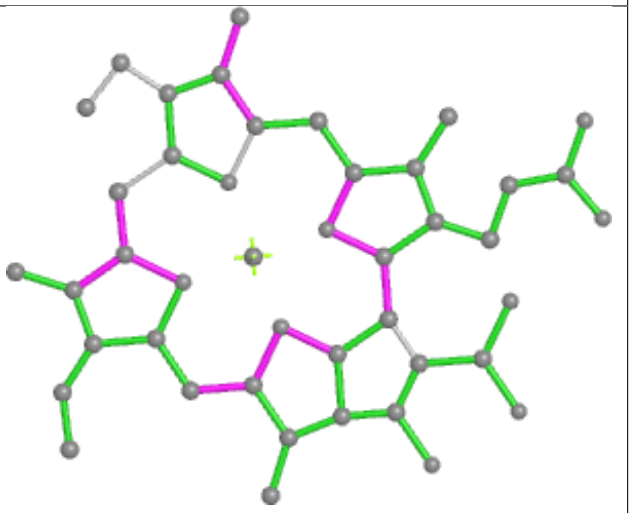

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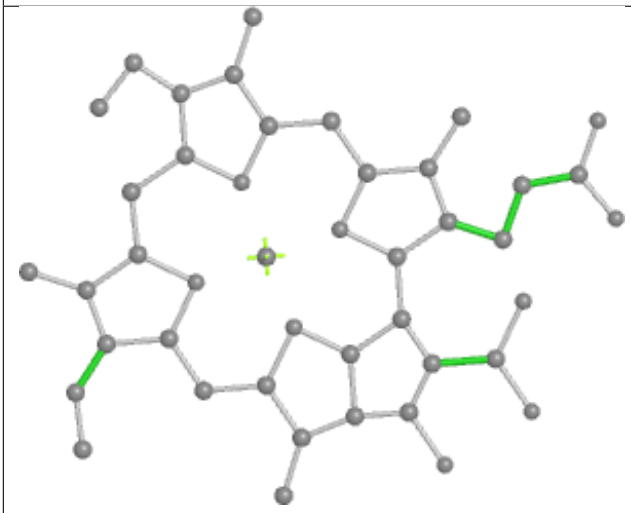

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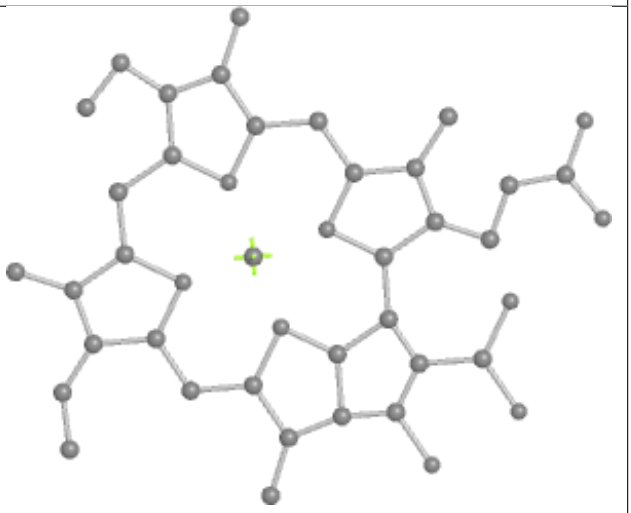
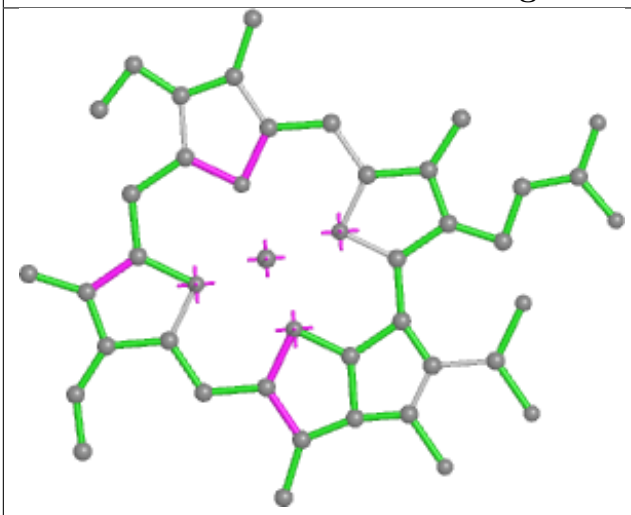


Rings

Ligand CLA 3 1006



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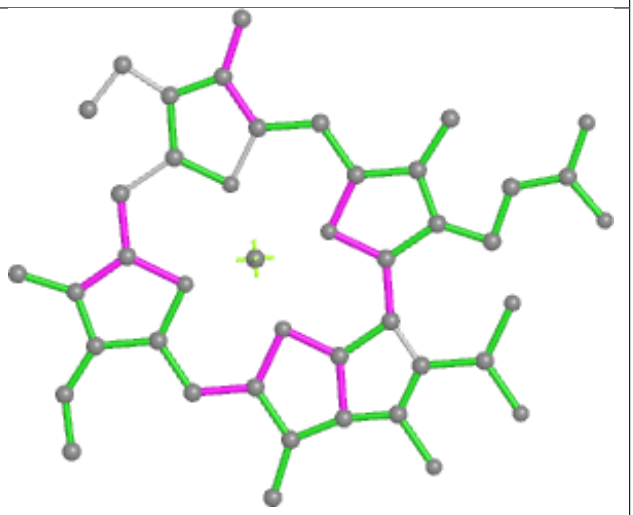

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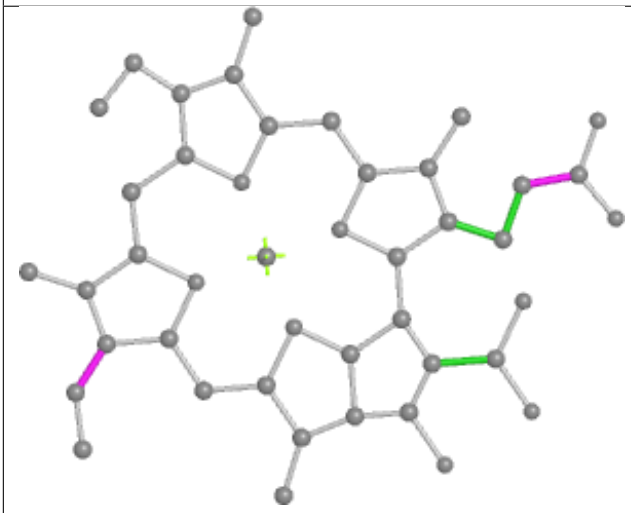

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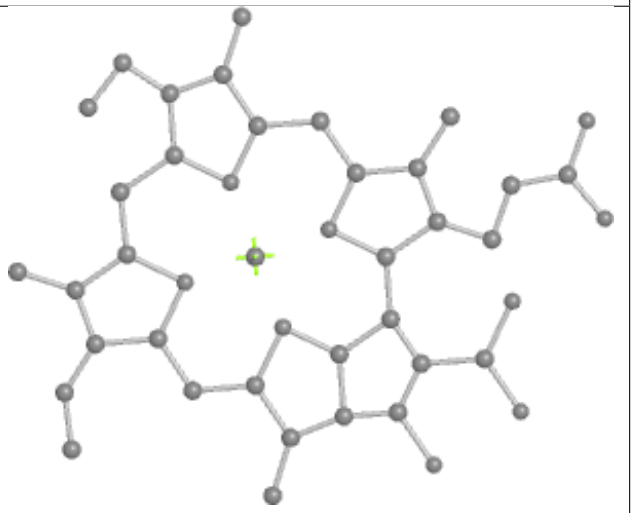
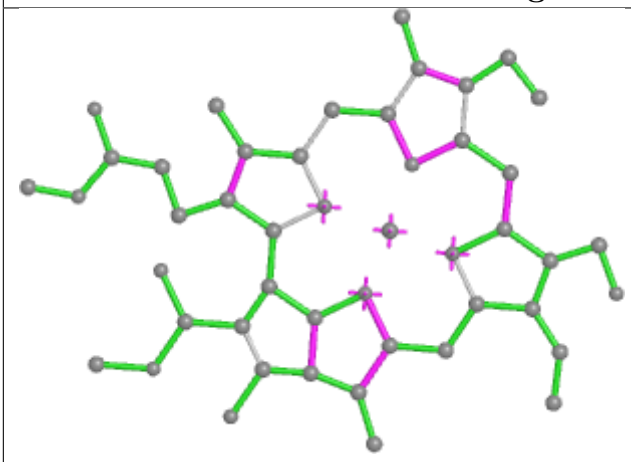


Rings

Ligand CHL 5 313



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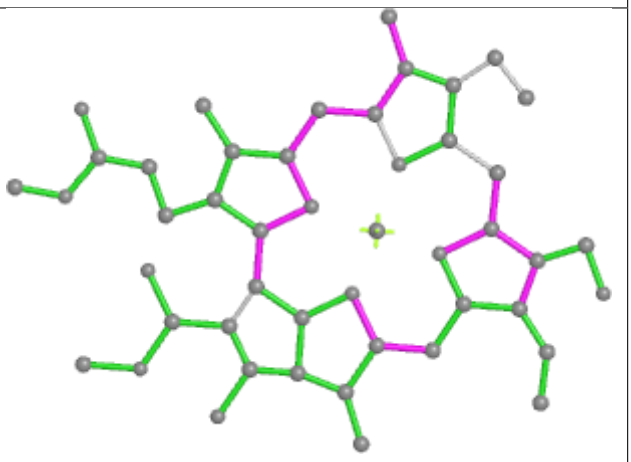
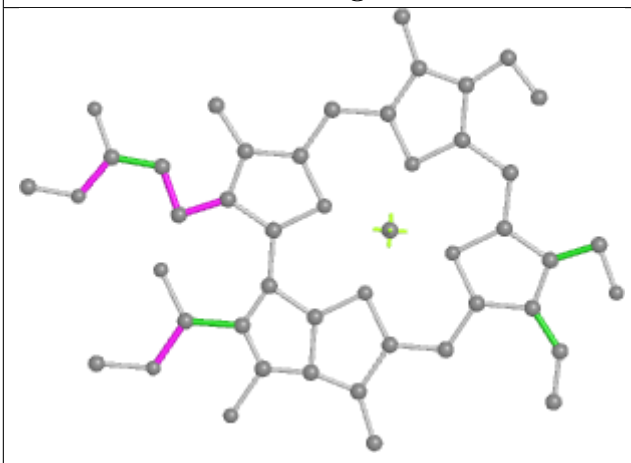


Bond angles



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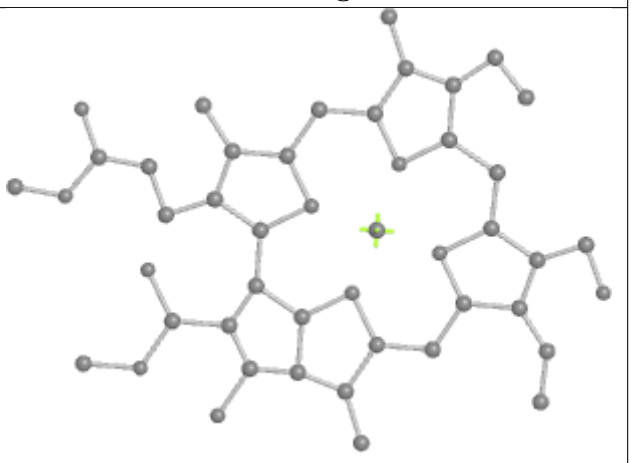
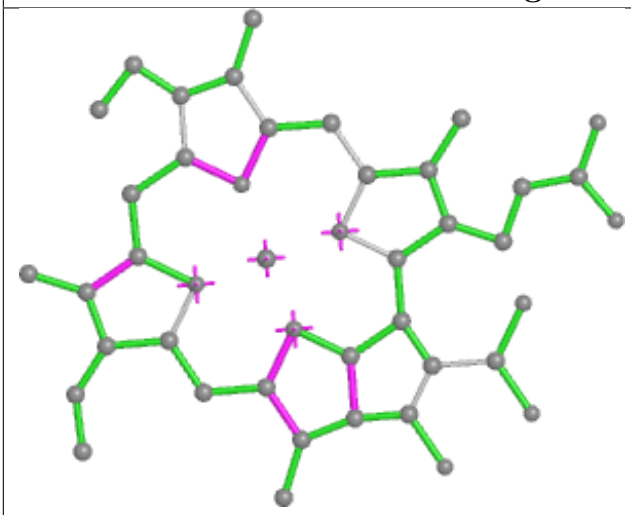
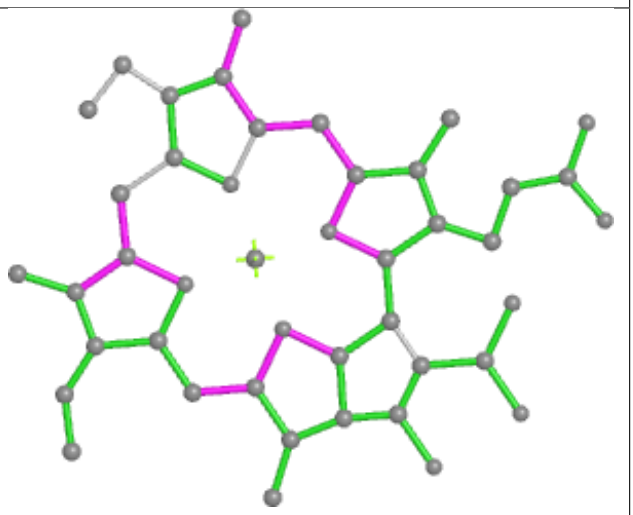


Rings

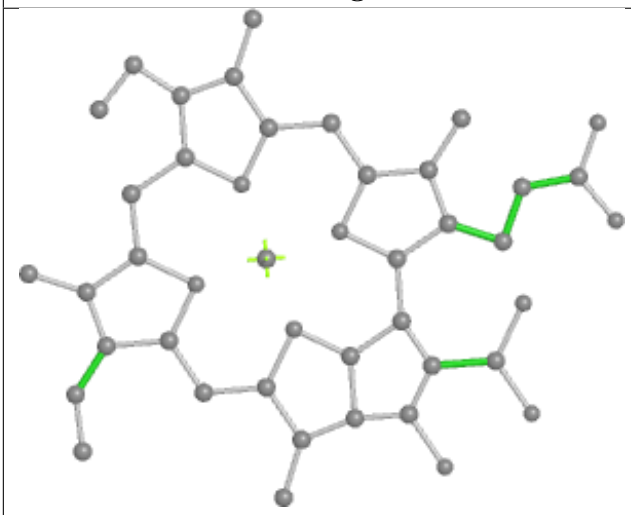
Ligand CLA B 822



Bond lengths



Bond angles



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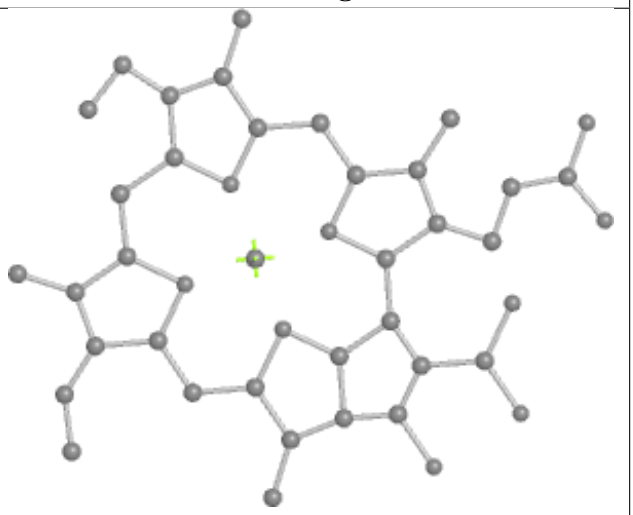
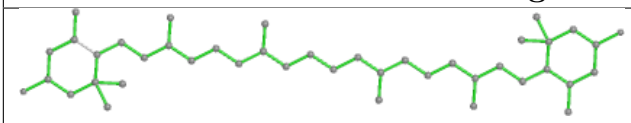
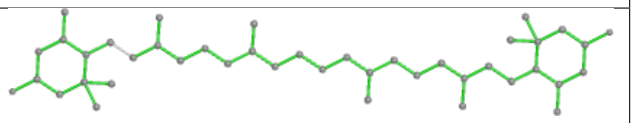


Rings

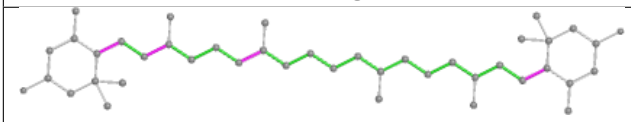
Ligand LUT J 104



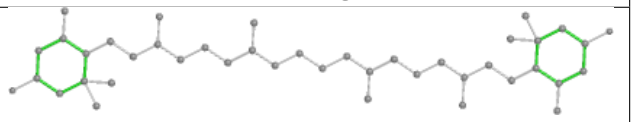
Bond lengths



Bond angles

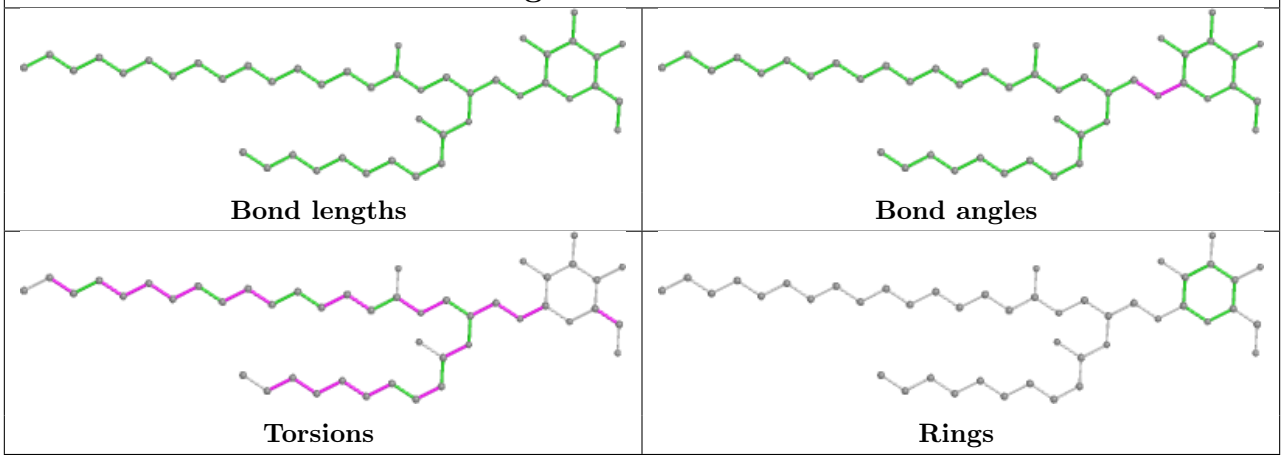


Torsions

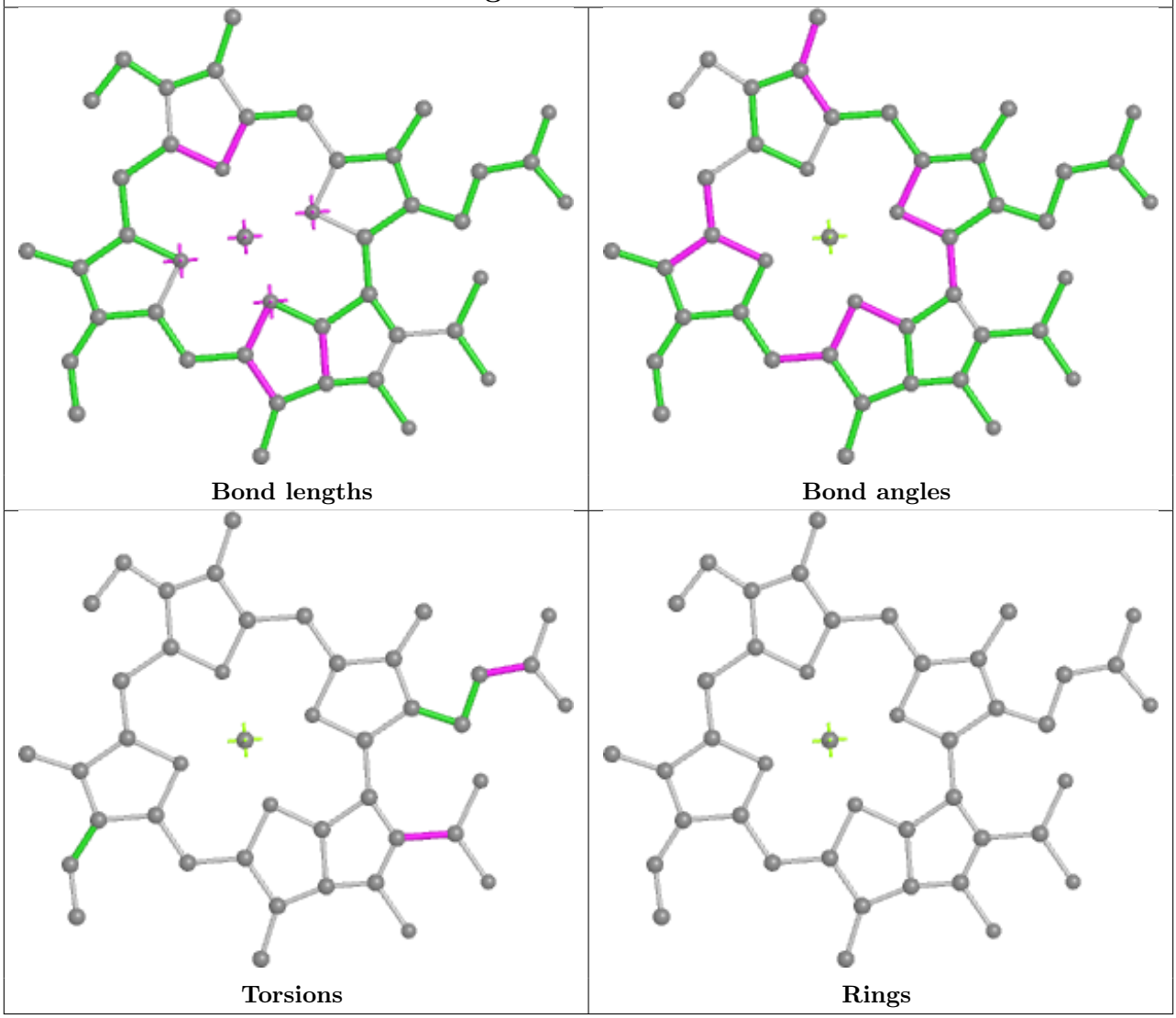


Rings

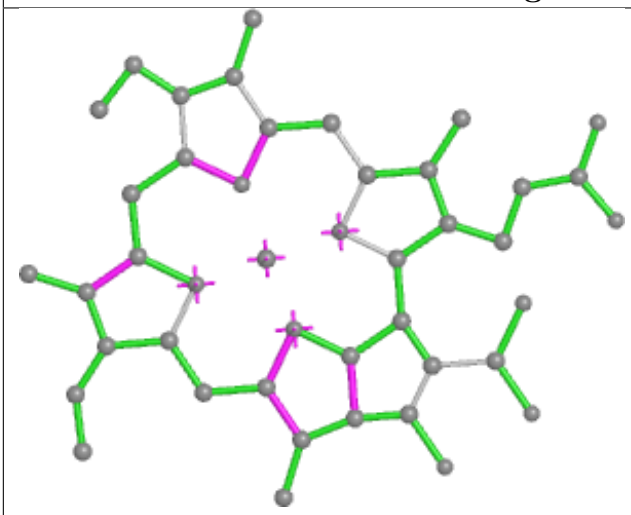
Ligand LMG 5 324



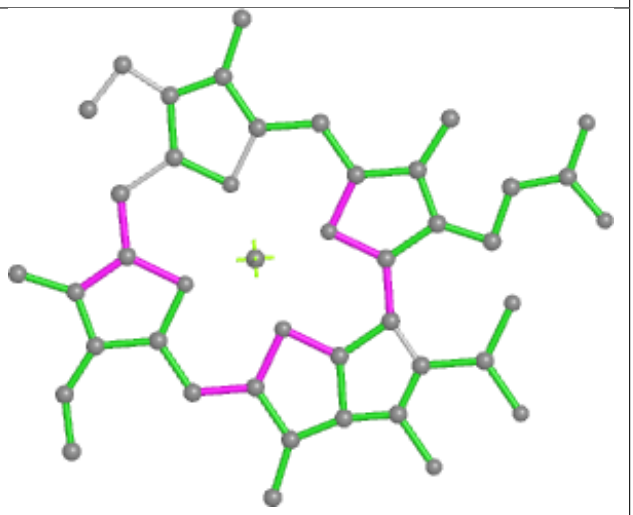
Ligand CLA 5 321



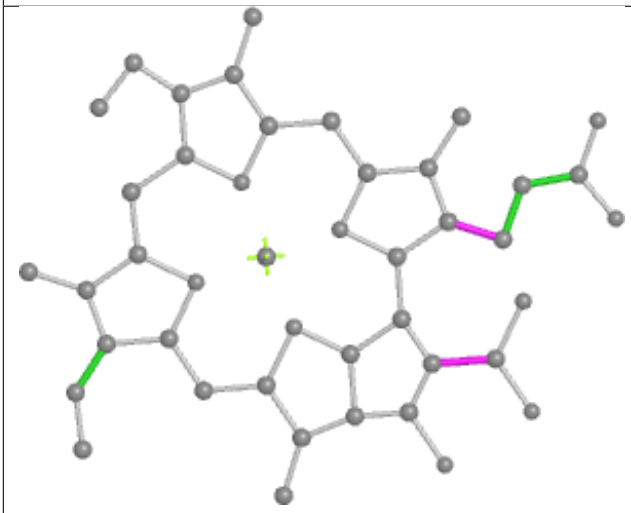
Ligand CLA B 828



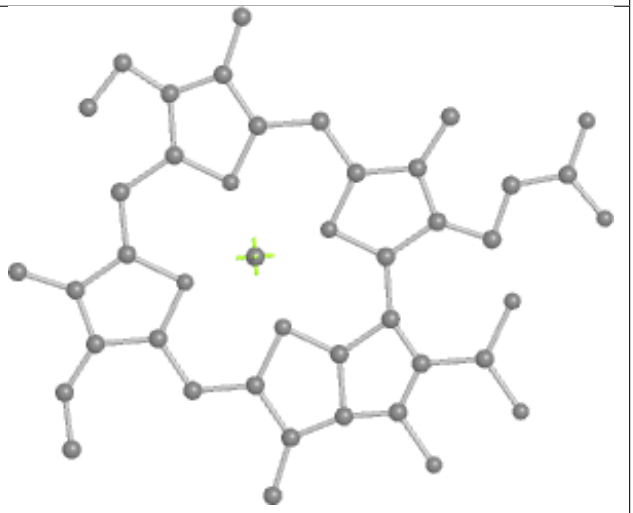
Bond lengths



Bond angles

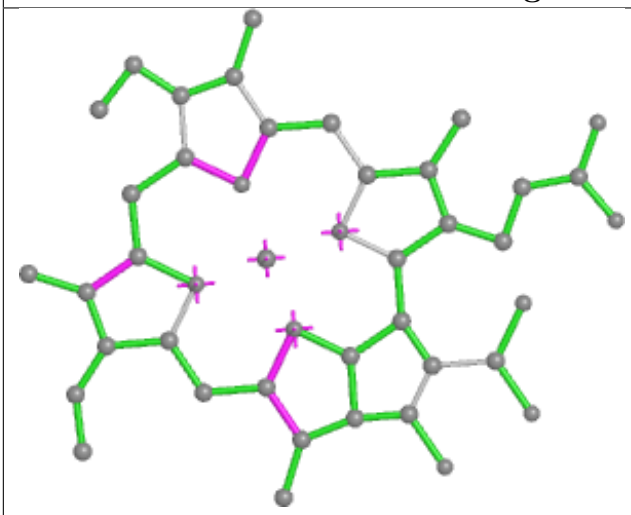


Torsions



Rings

Ligand CLA A 851



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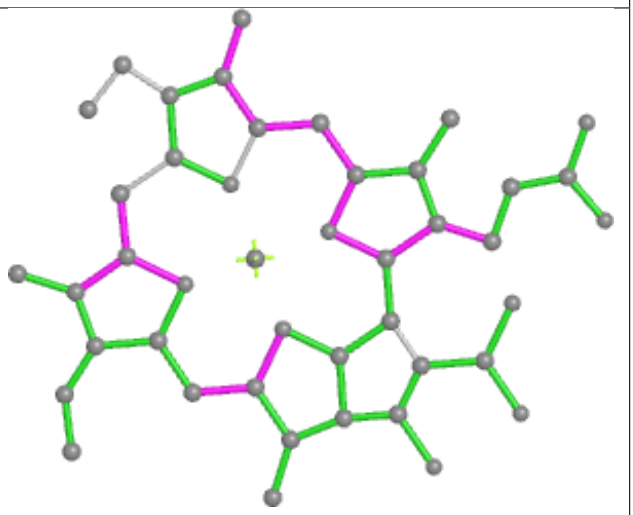
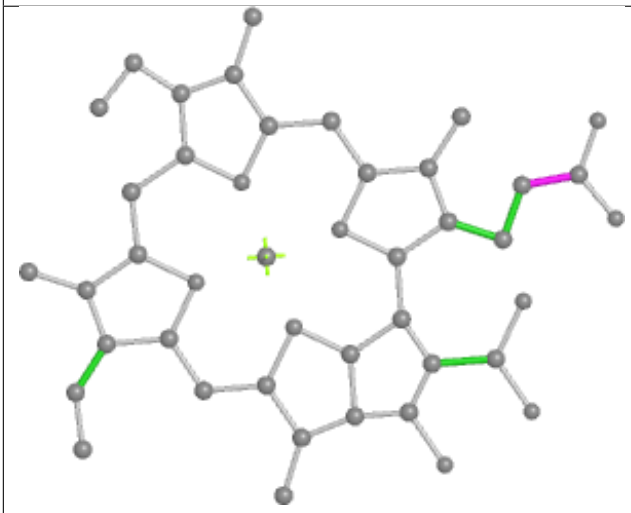


Bond angles



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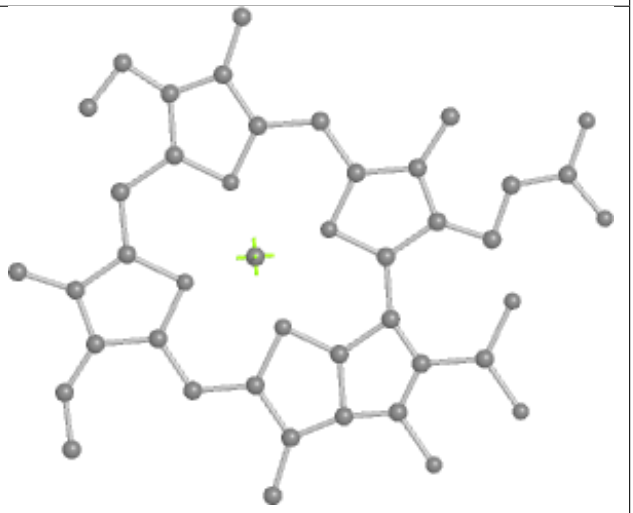
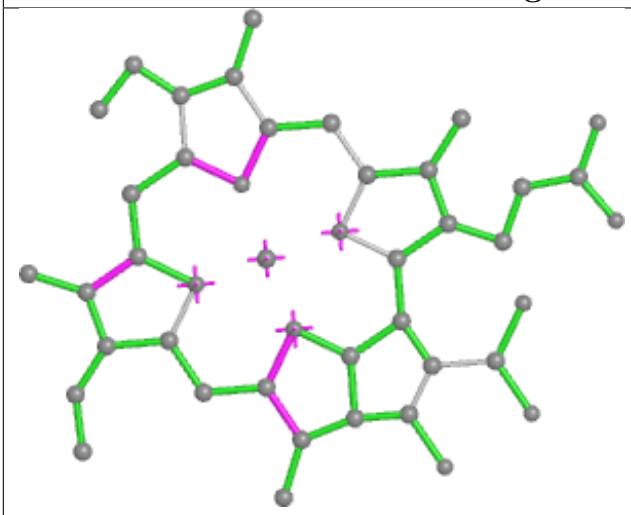


Rings

Ligand CLA B 813



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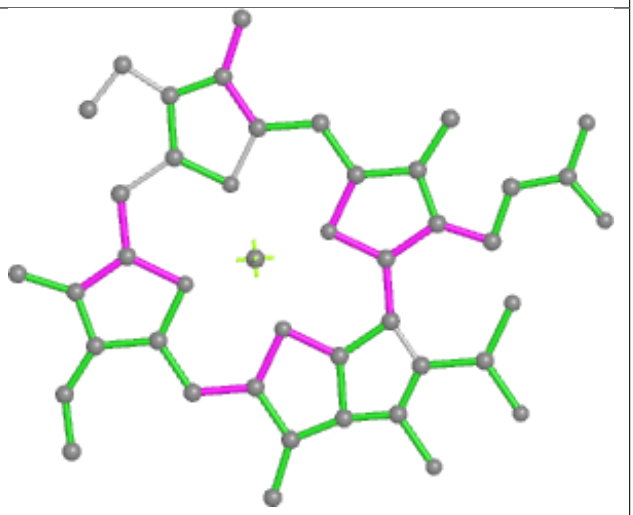
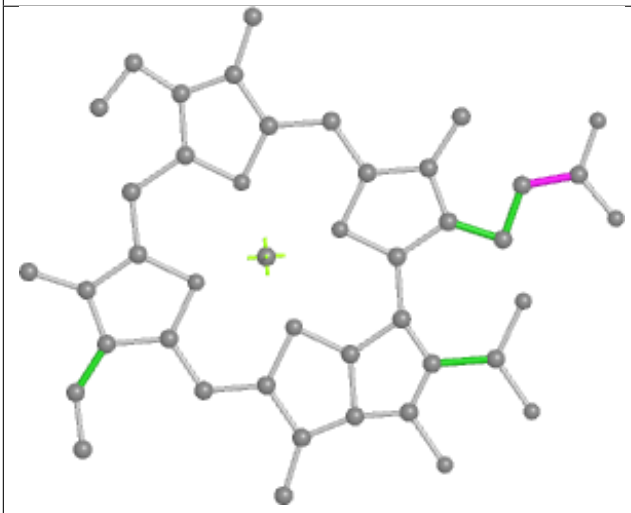
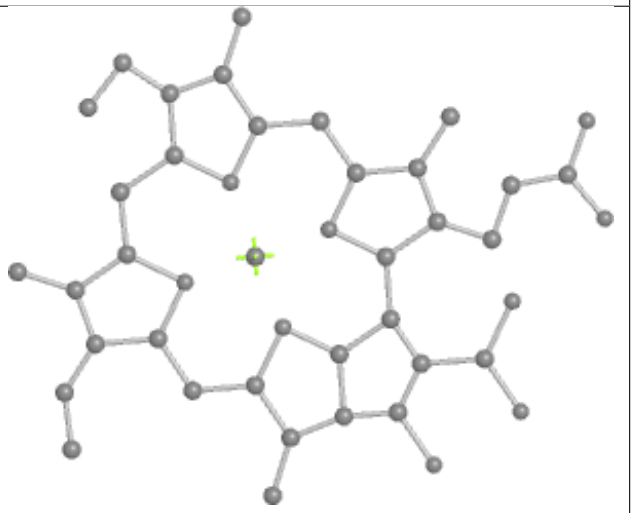


Bond angles

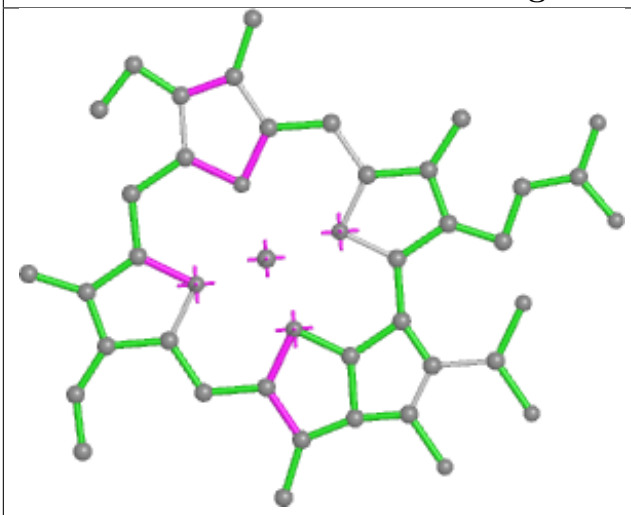


Torsions



Rings

Ligand CLA 8 307



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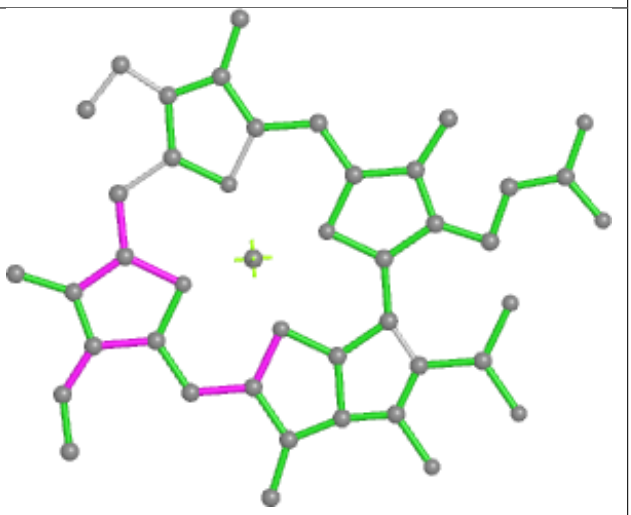
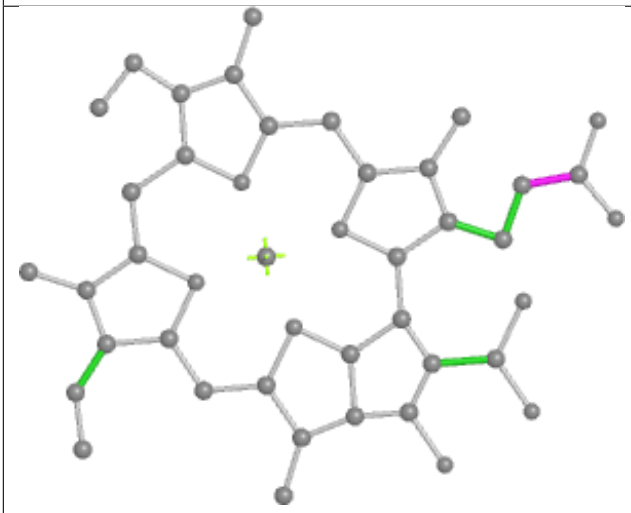


Bond angles



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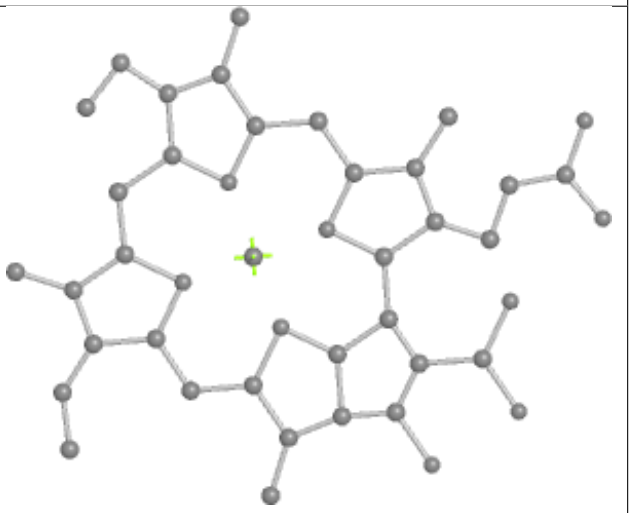
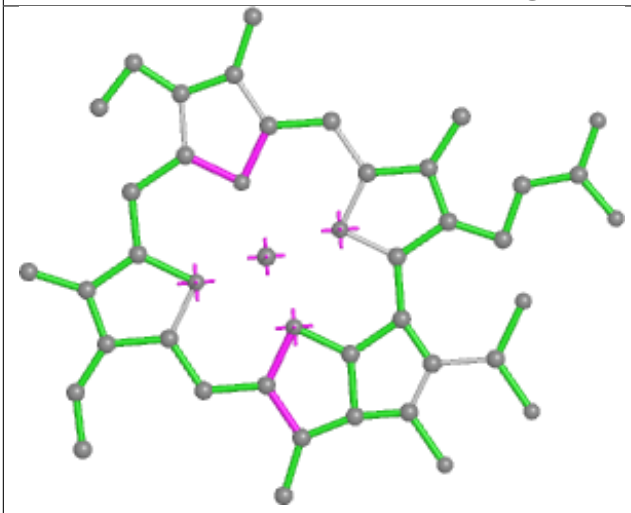


Rings

Ligand CLA A 811



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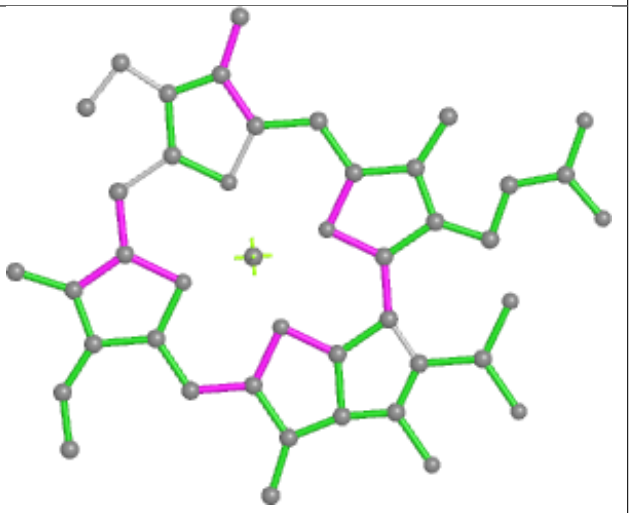

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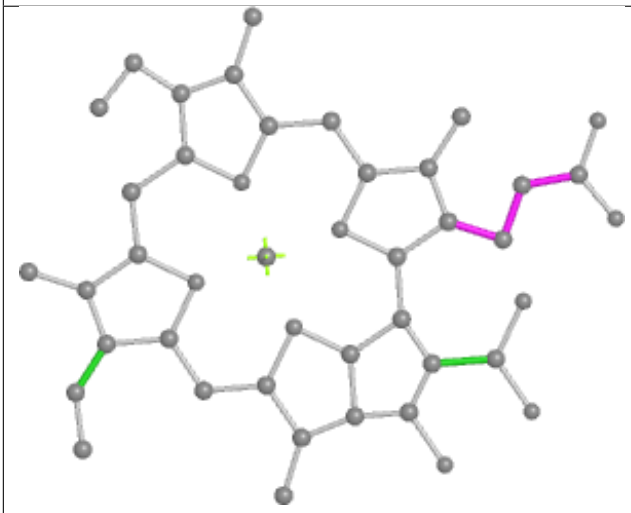

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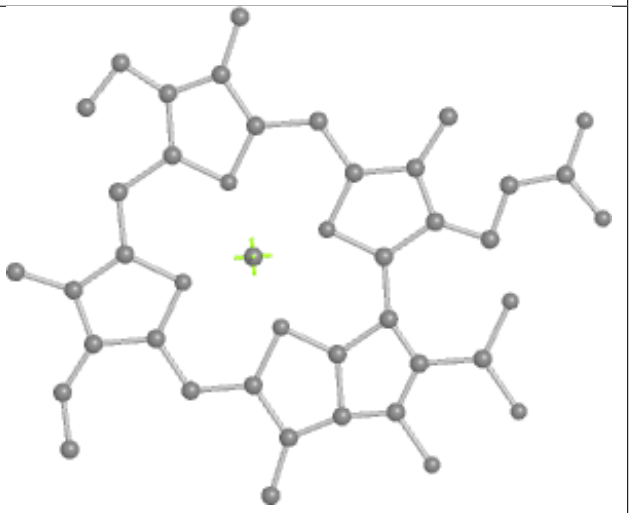
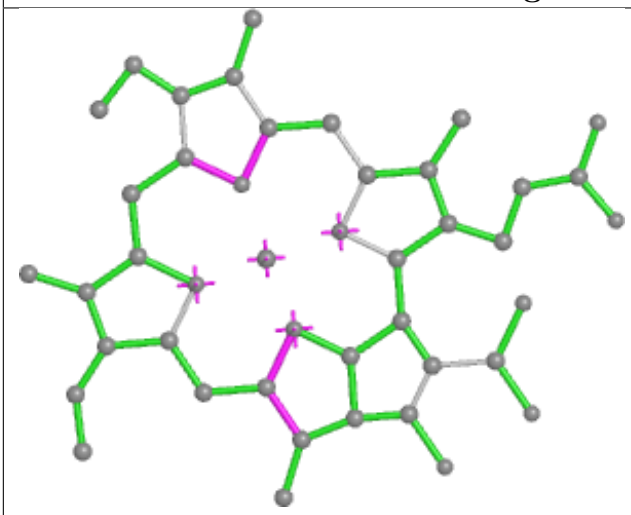


Rings

Ligand CLA A 813



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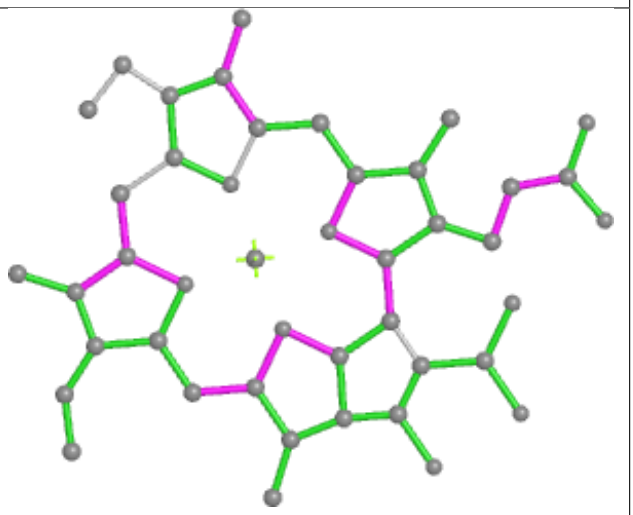

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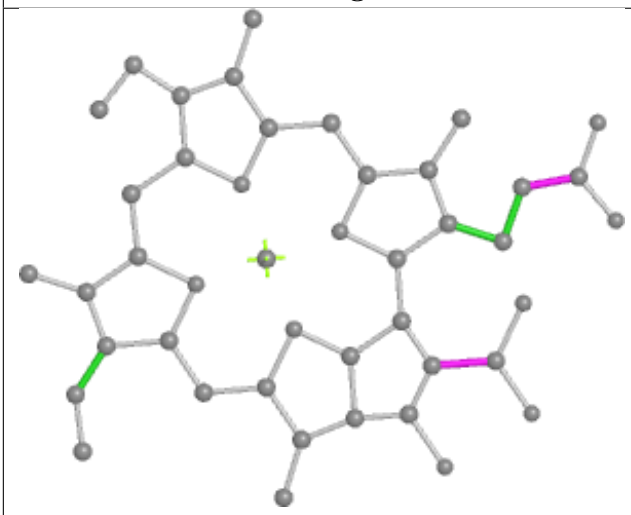

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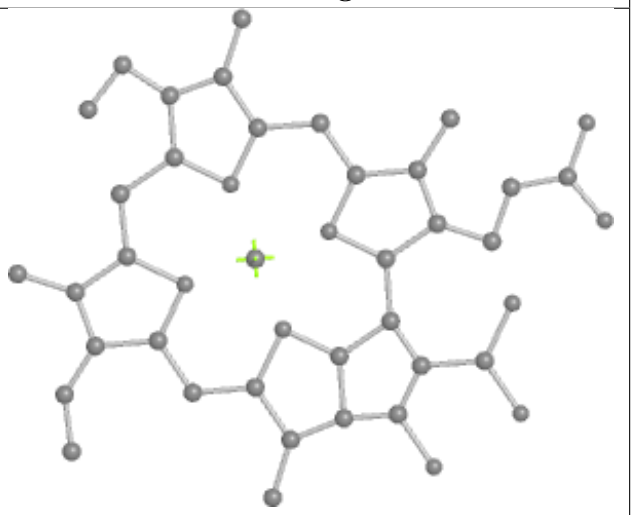
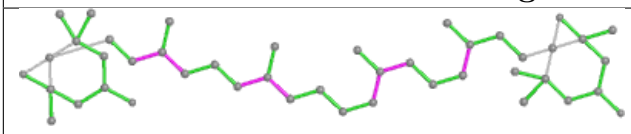


Rings

Ligand XAT 7 1002



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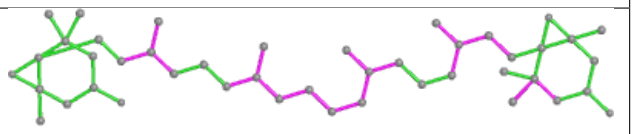
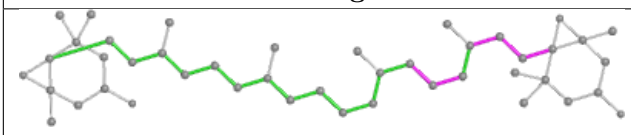


Bond angles



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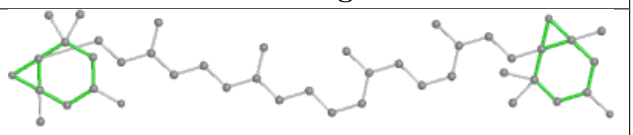
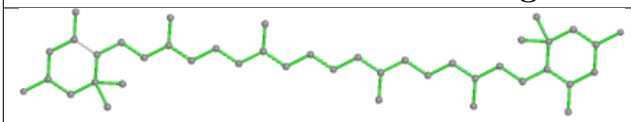
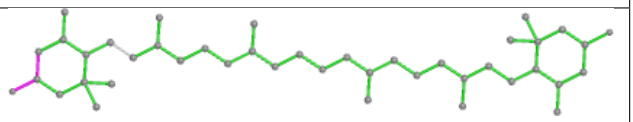


Rings

Ligand LUT 3 1002



Bond lengths



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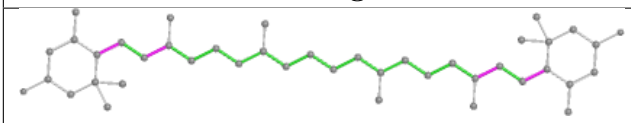

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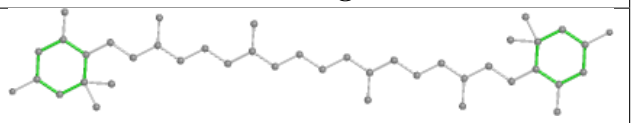
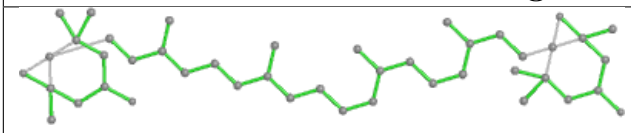


Rings

Ligand XAT 6 304



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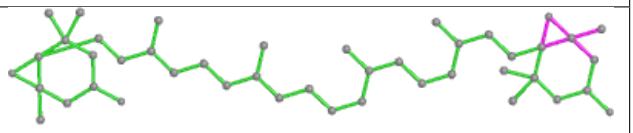
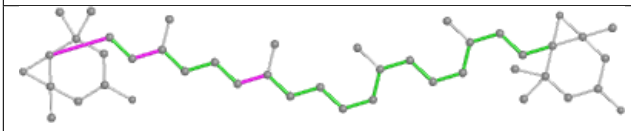


Bond angles



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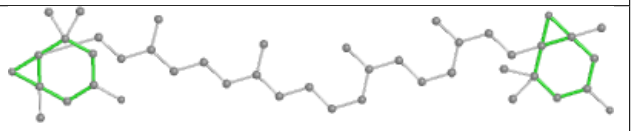
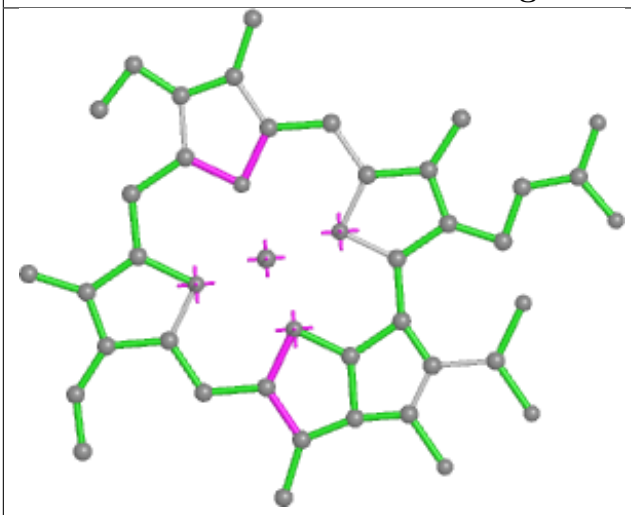


Rings

Ligand CLA 1 1017



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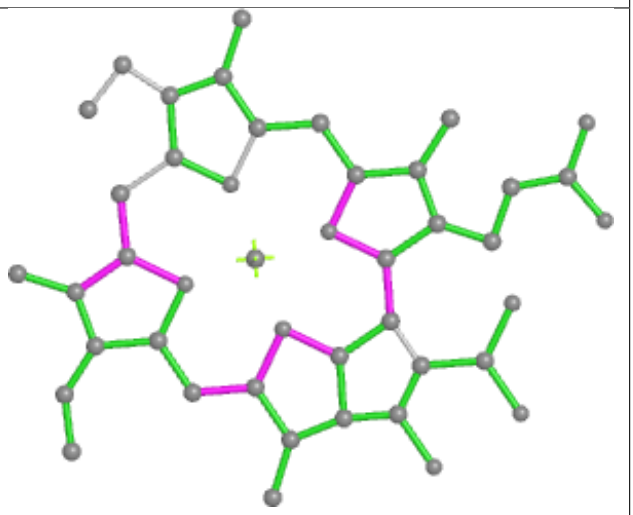

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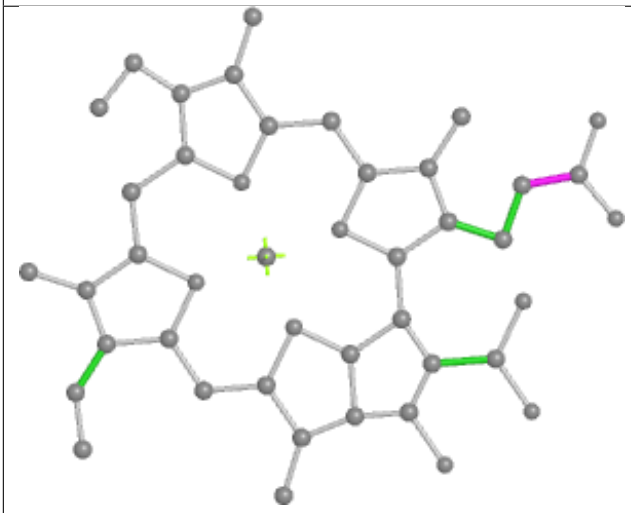

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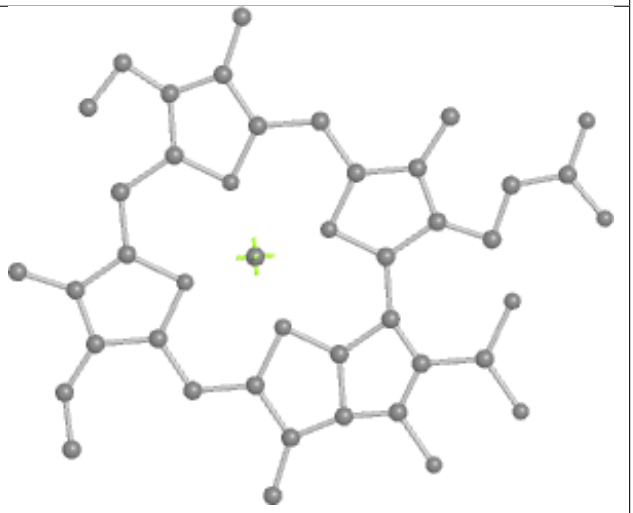
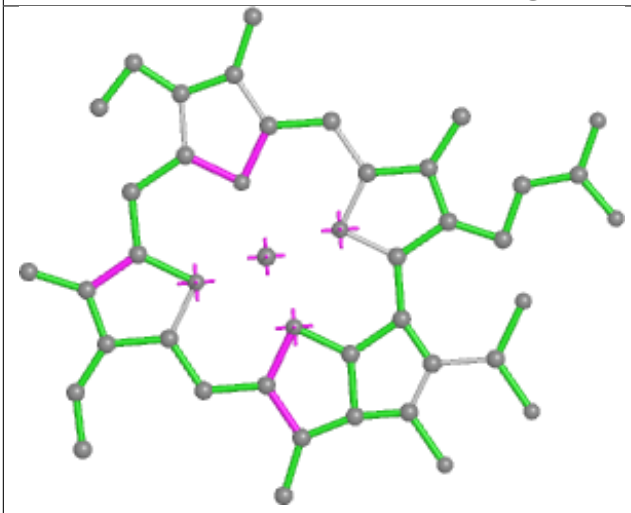


Rings

Ligand CLA B 835



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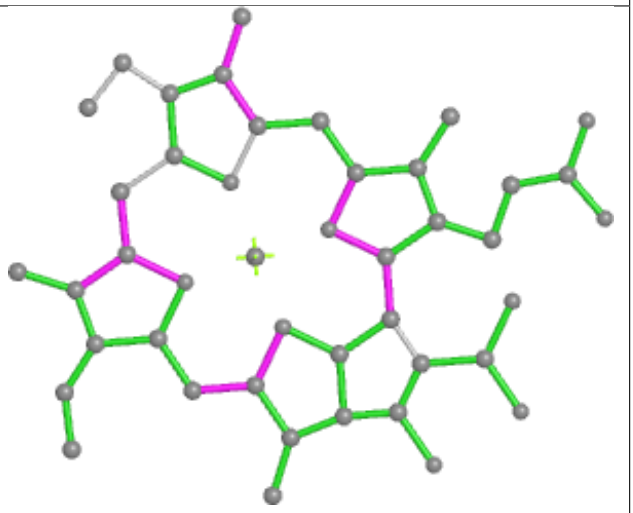

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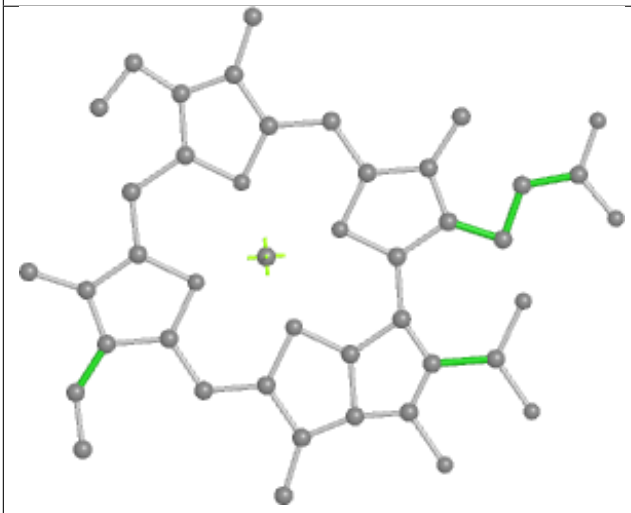

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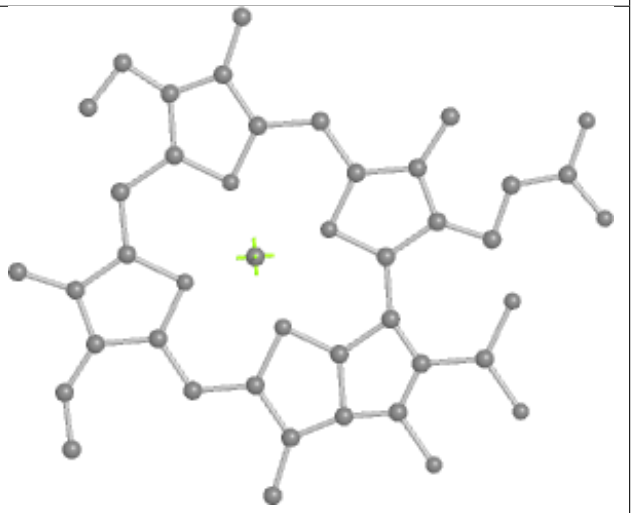
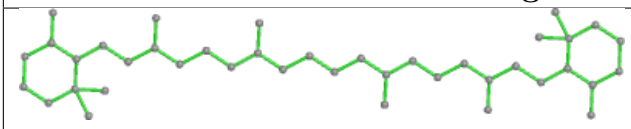


Rings

Ligand BCR A 848



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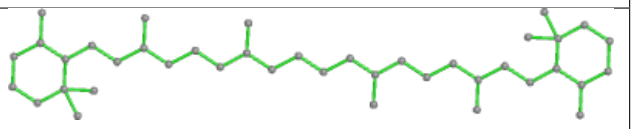
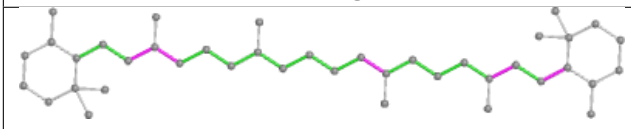


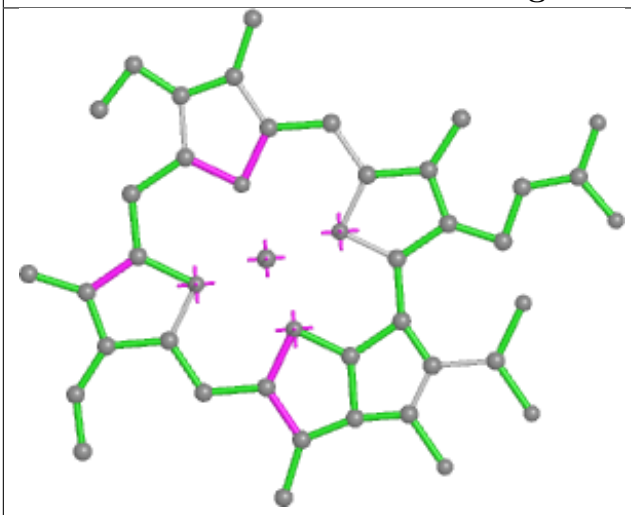
Bond angles



Torsions

Rings

Ligand CLA 0 301



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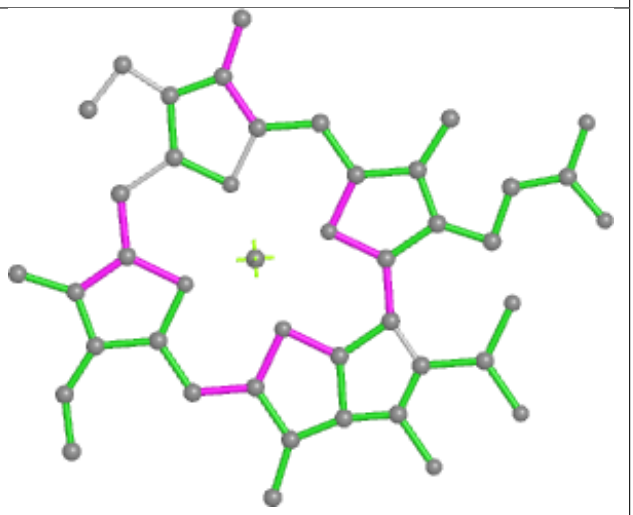
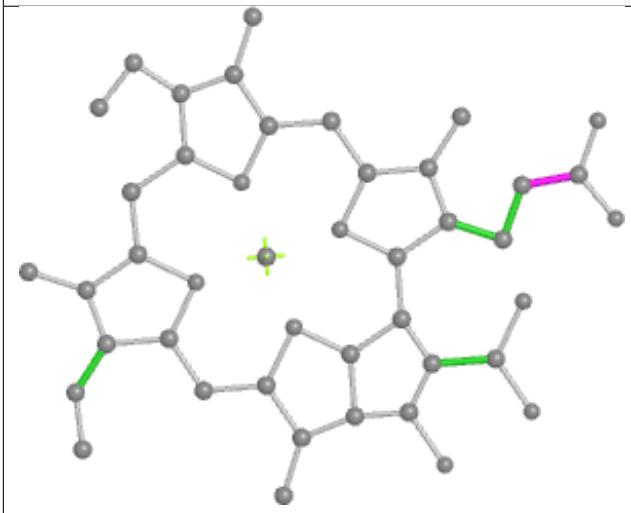
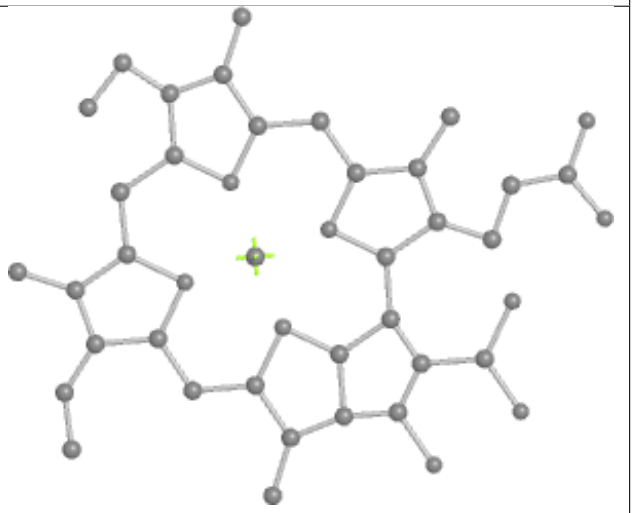


Bond angles

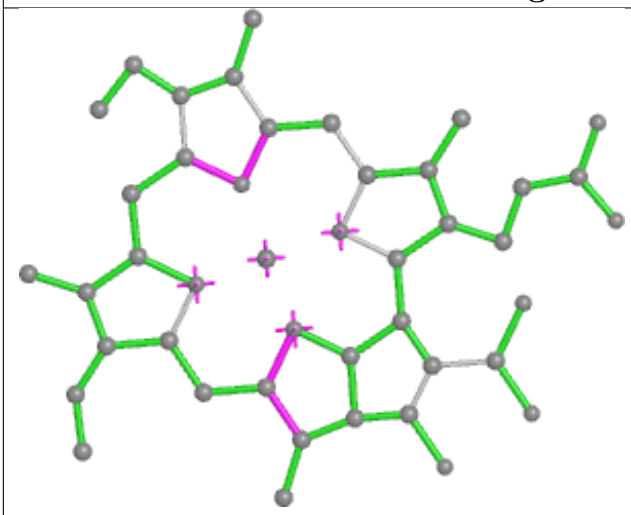


Torsions

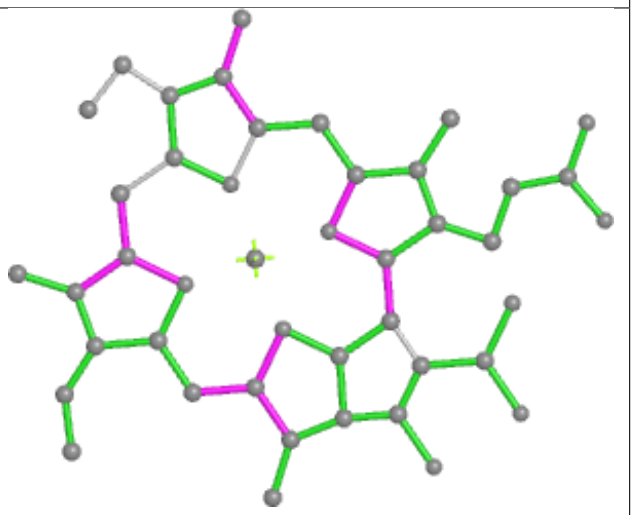


Rings

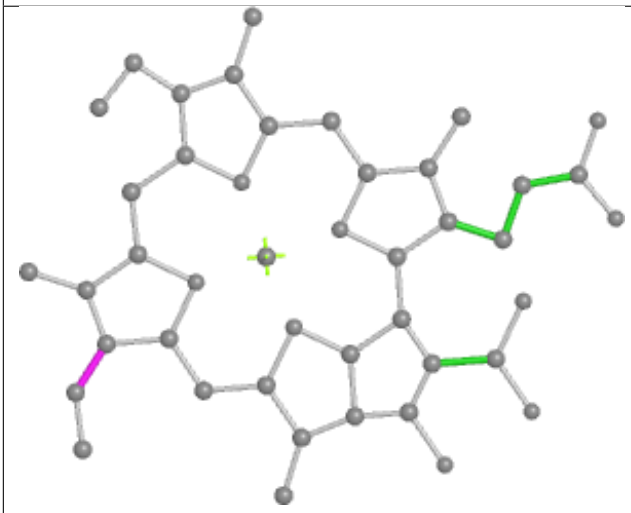
Ligand CLA 0 316



Bond lengths



Bond angles



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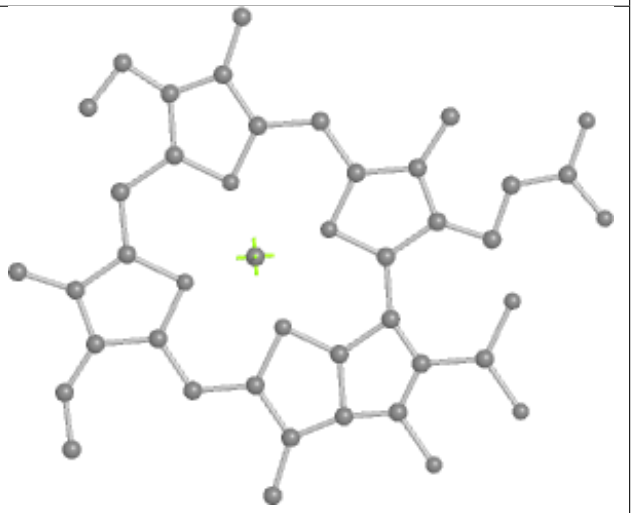
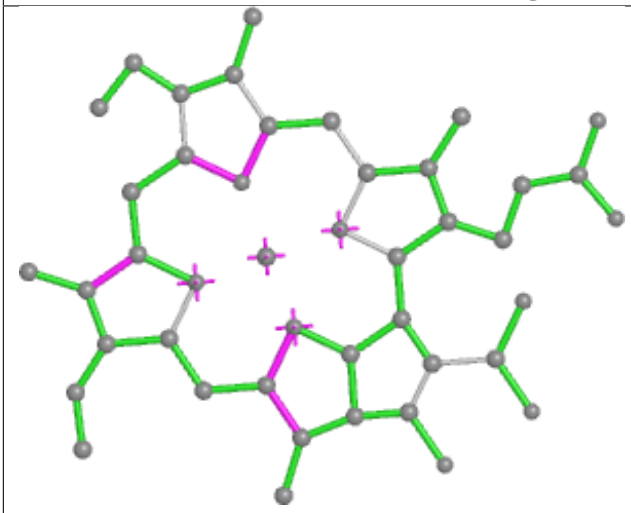
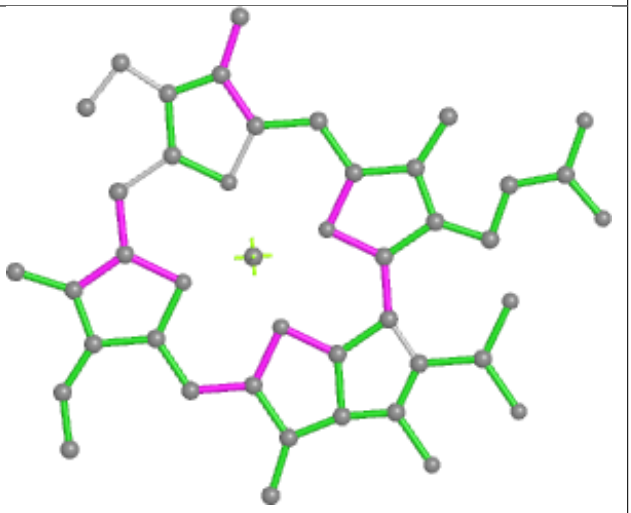


Rings

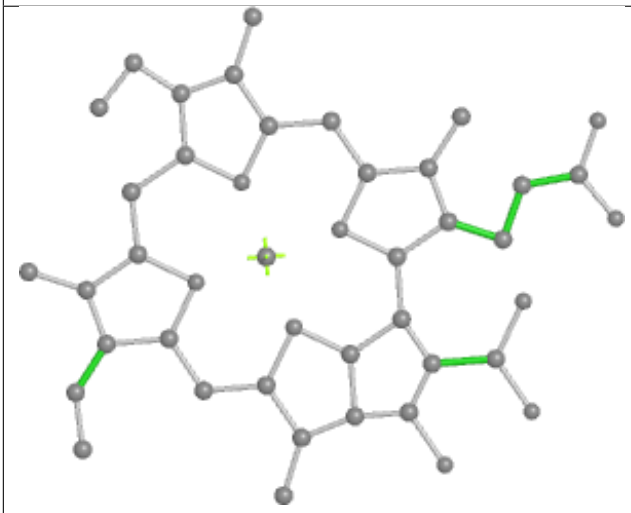
Ligand CLA B 814



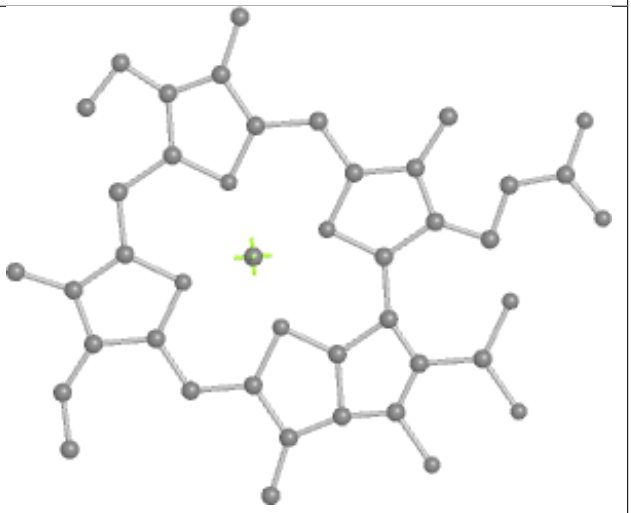
Bond lengths



Bond angles

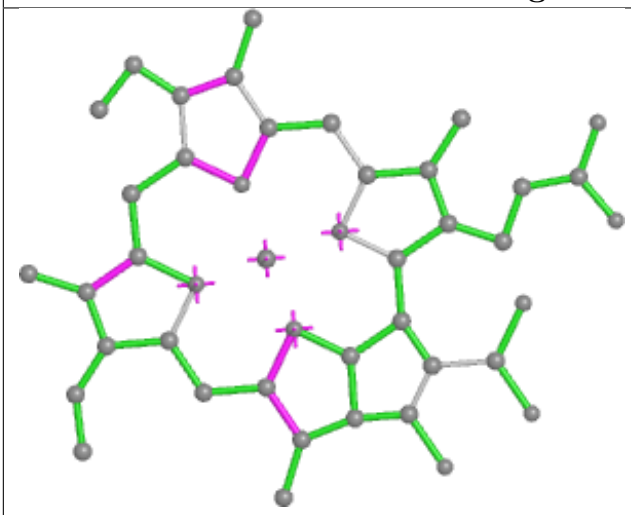


Torsions



Rings

Ligand CLA 6 310



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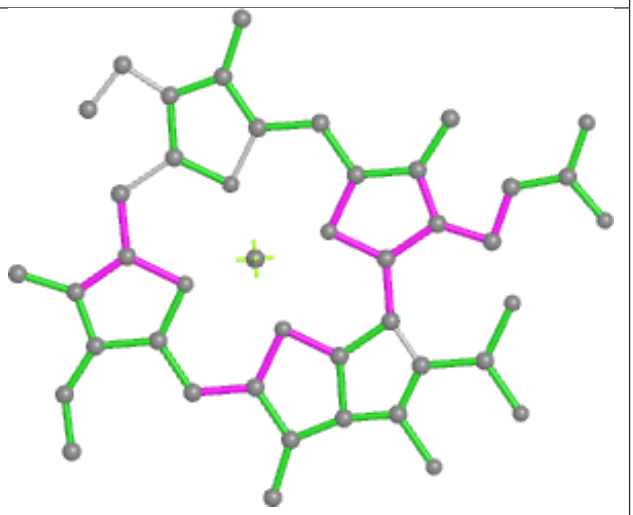

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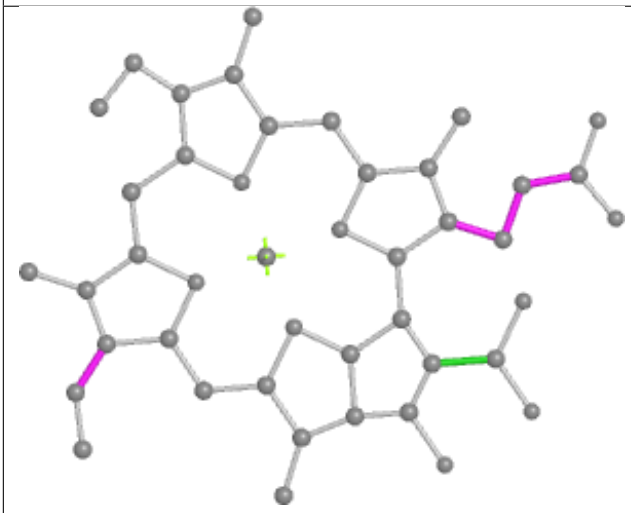

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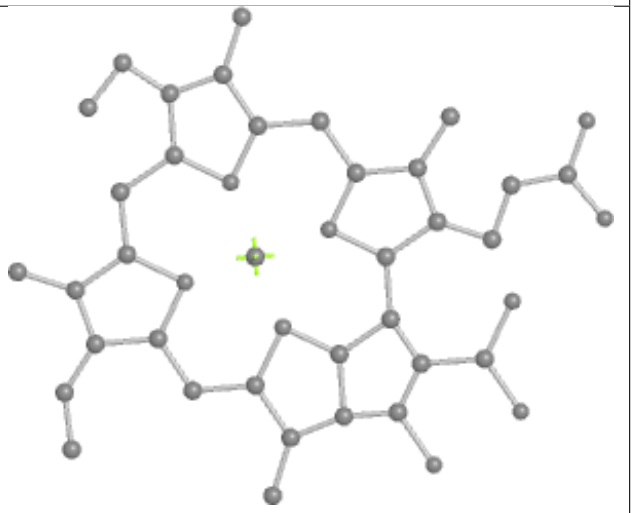
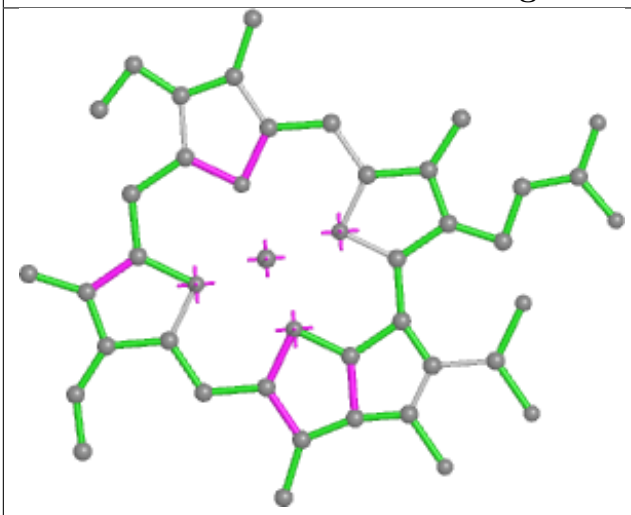


Rings

Ligand CLA 3 1017



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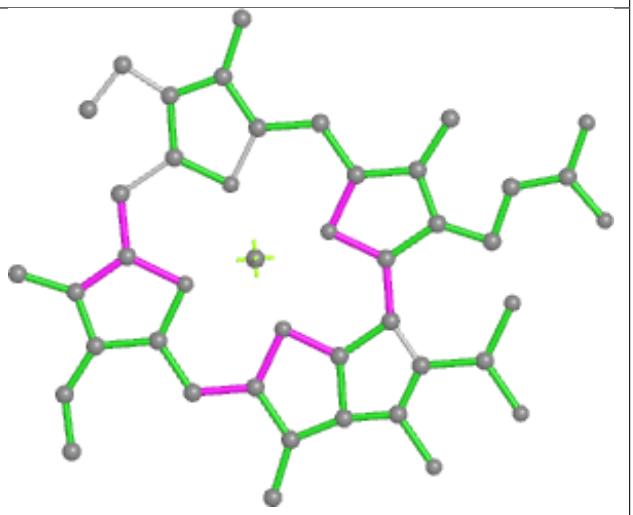

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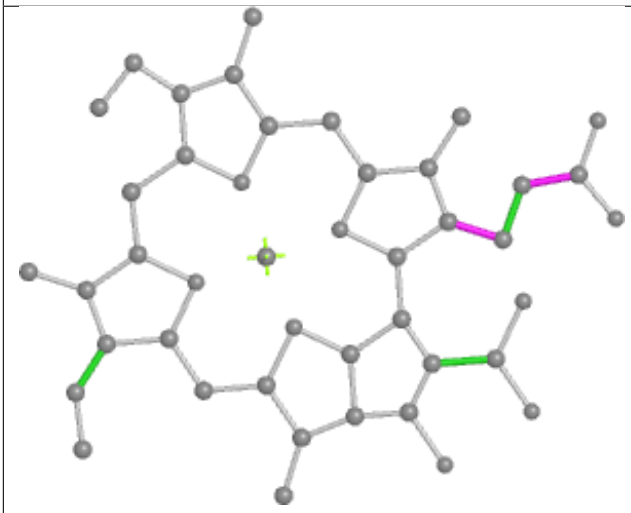

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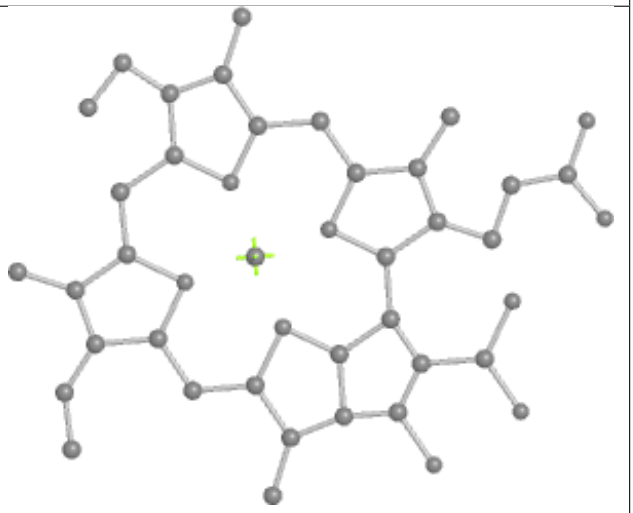
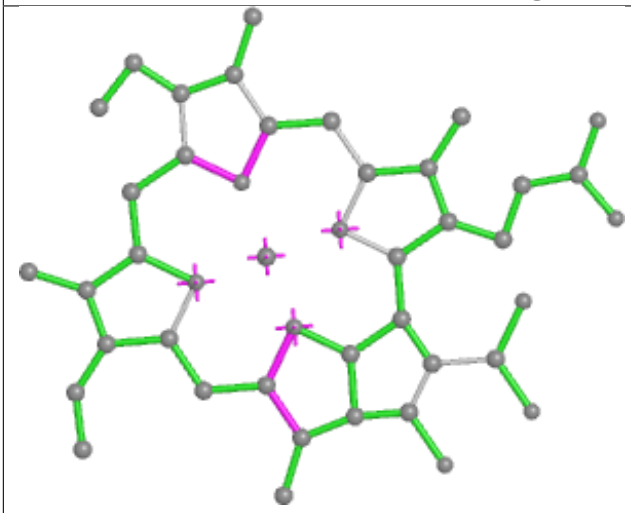


Rings

Ligand CLA 4 308



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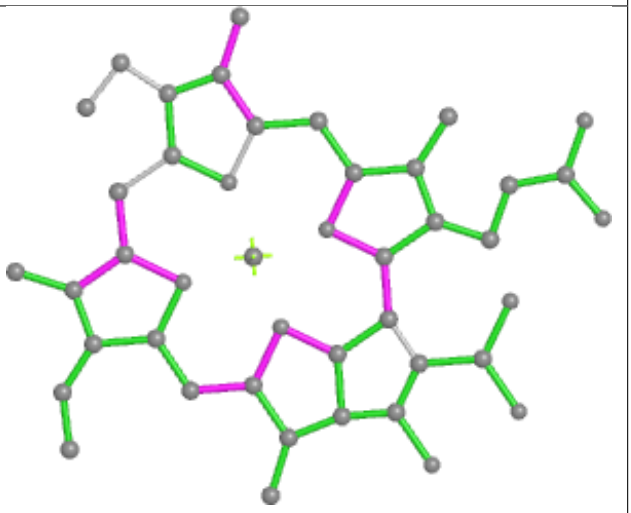

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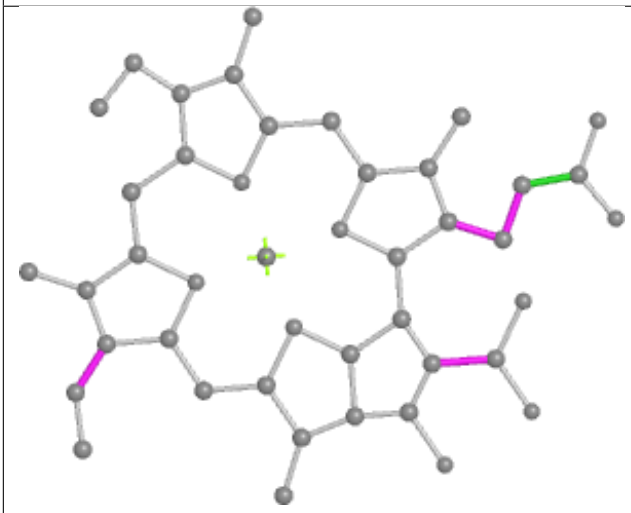
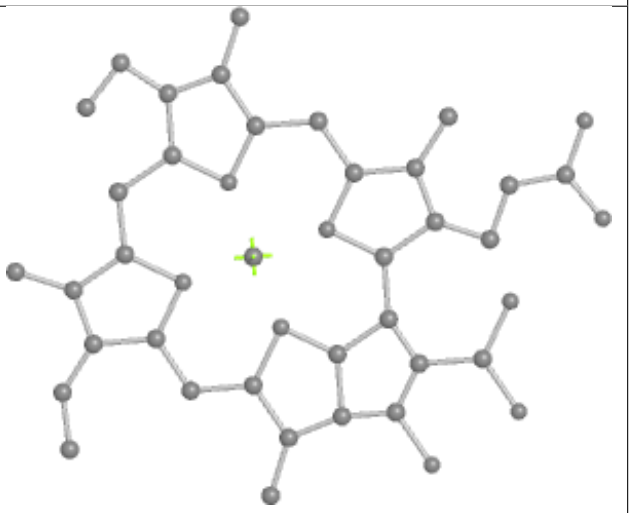
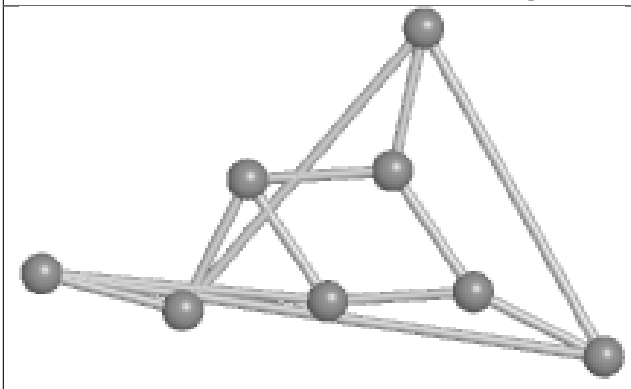


Torsions

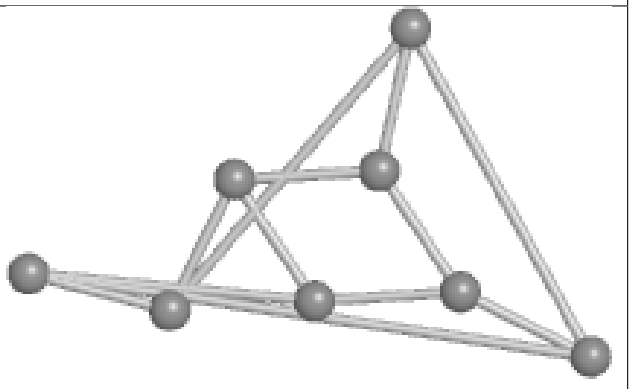


Rings

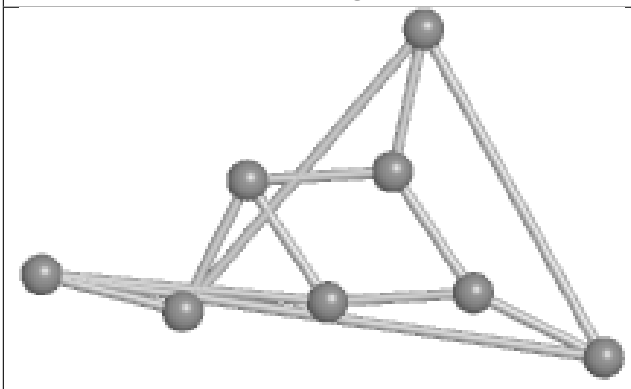
Ligand SF4 C 1002



Bond lengths



Bond angles



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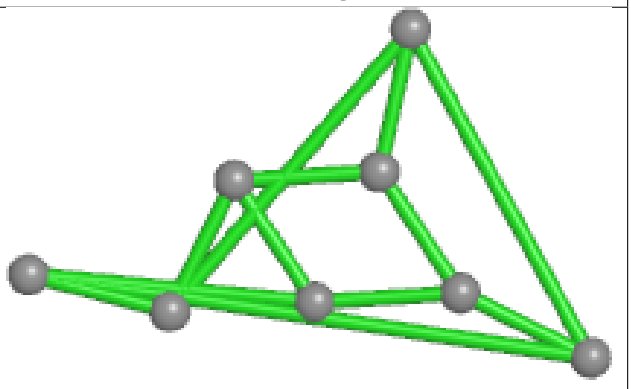
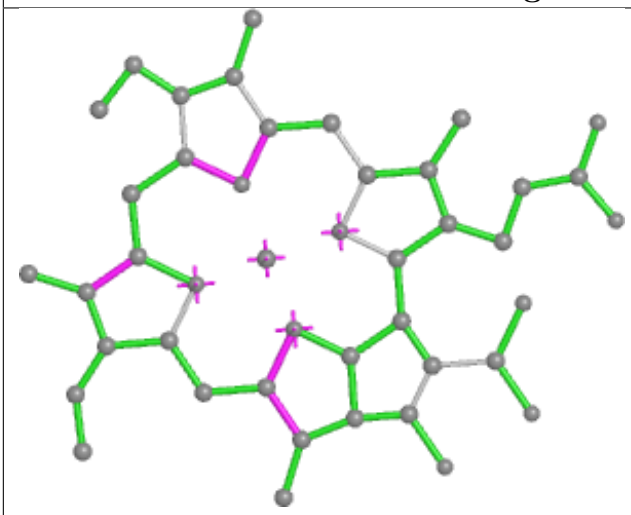


Rings

Ligand CLA A 832



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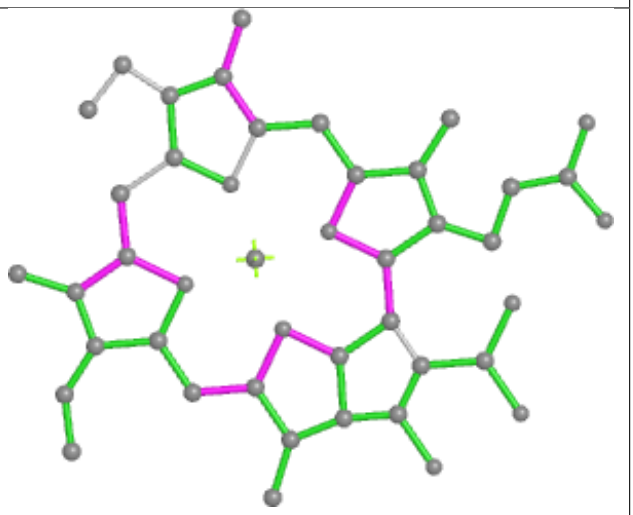
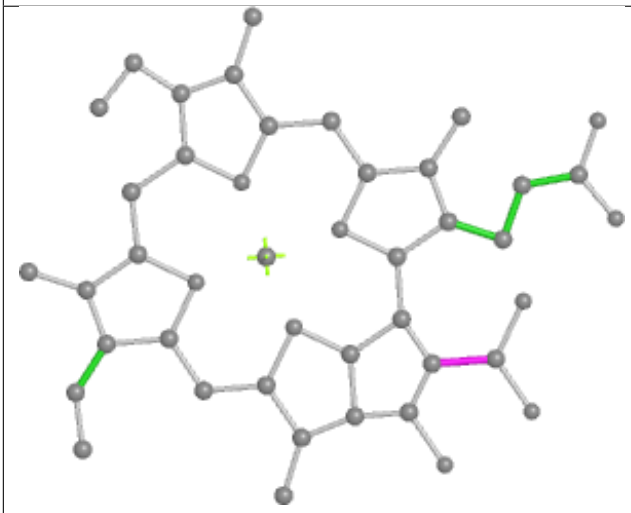


Bond angles



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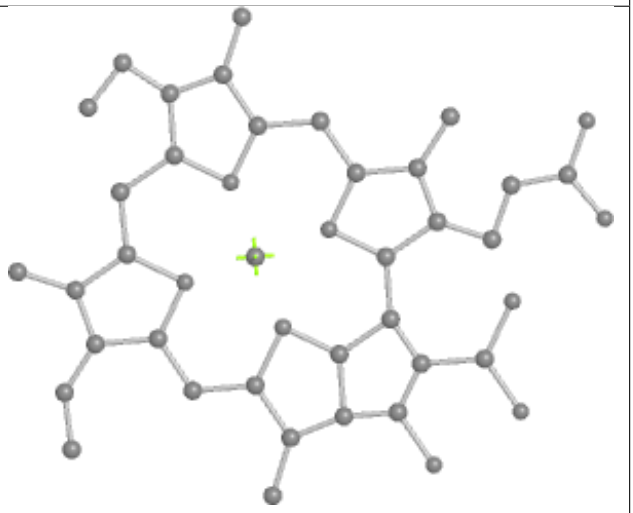
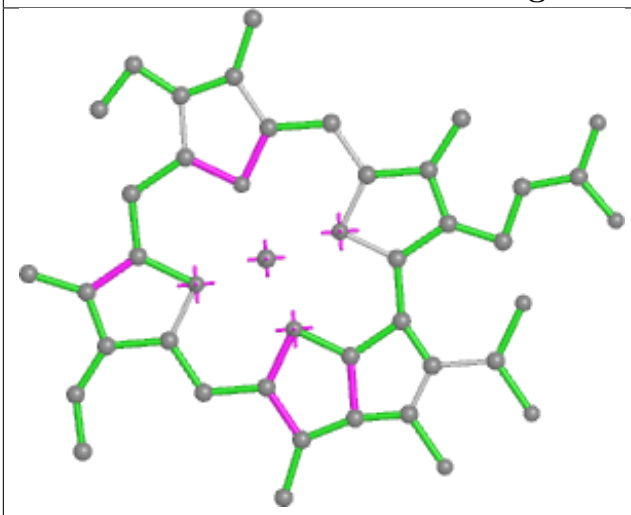


Rings

Ligand CLA 6 318



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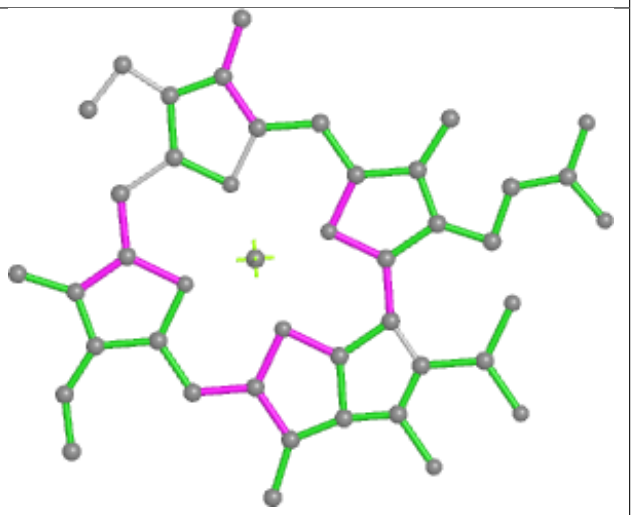
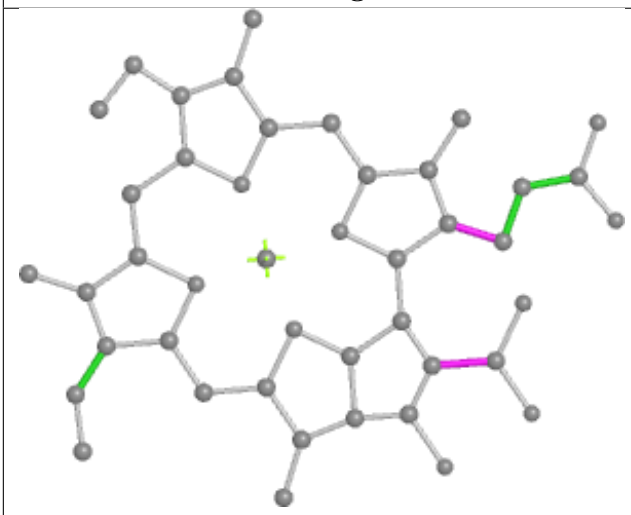


Bond angles



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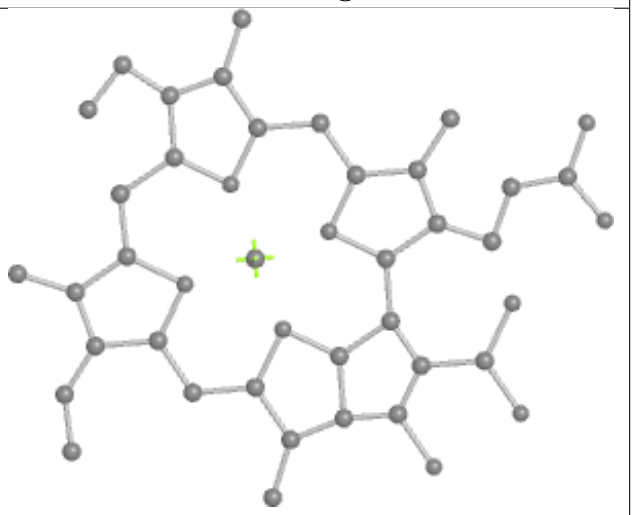
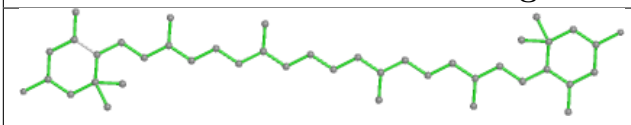


Rings

Ligand LUT 7 1001



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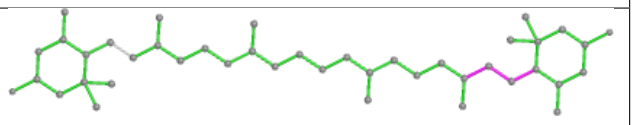
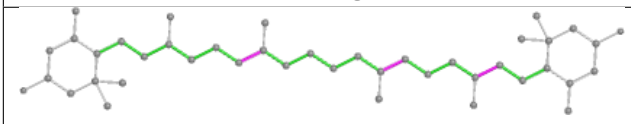


Bond angles



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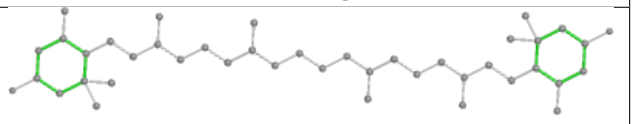
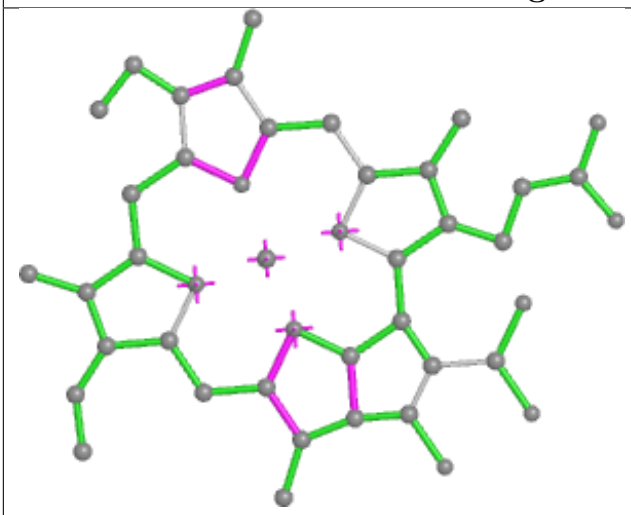


Rings

Ligand CLA 5 315



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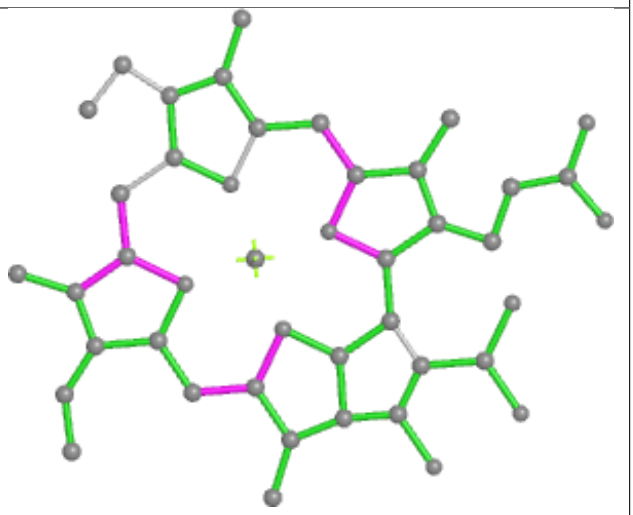
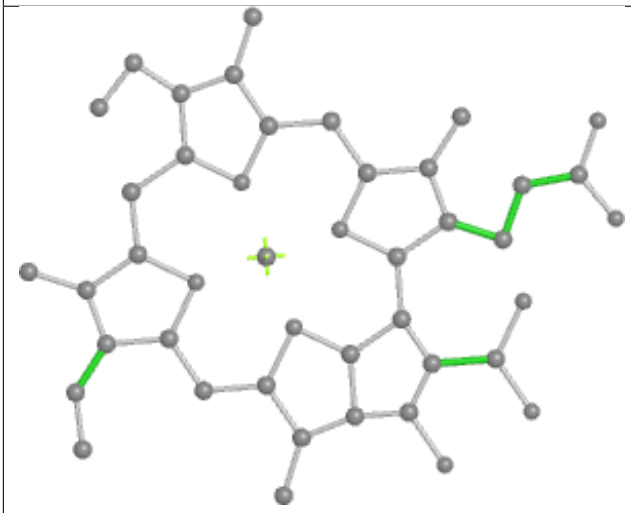
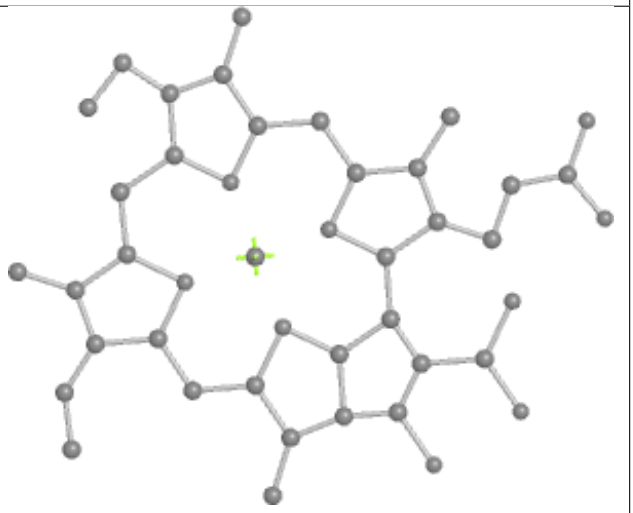


Bond angles

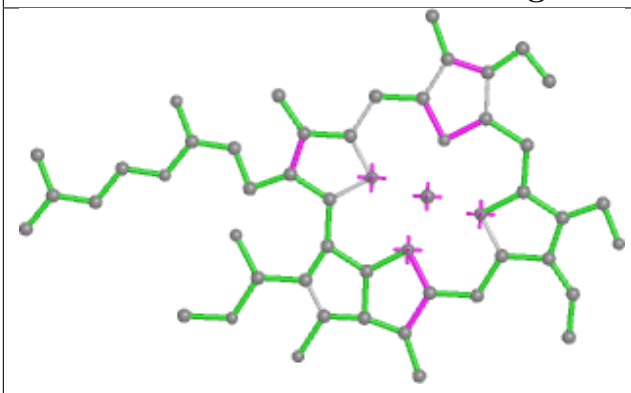


Torsions



Rings

Ligand CHL 8 315



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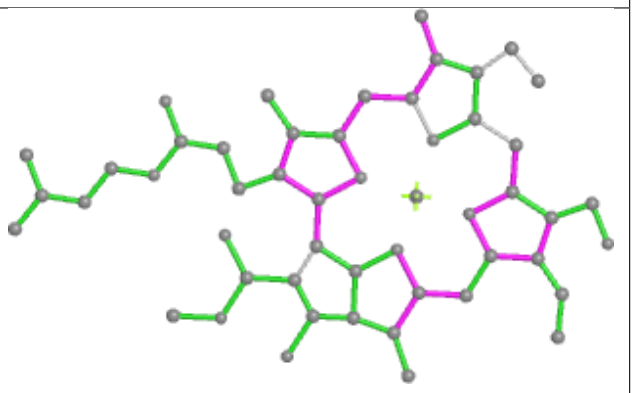
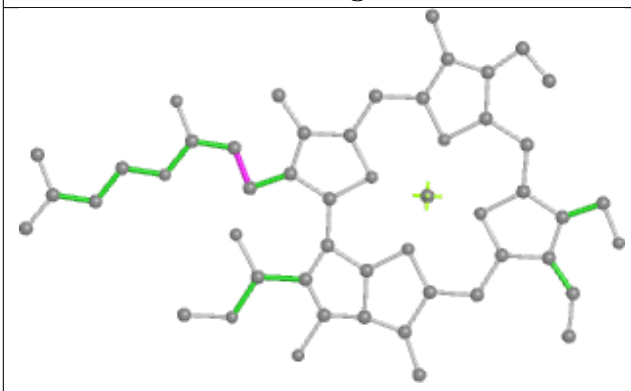


Bond angles



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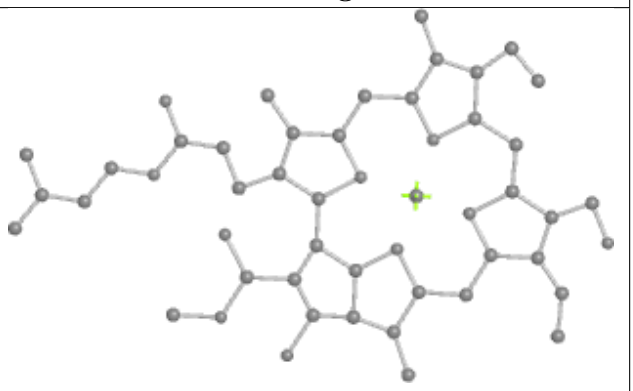
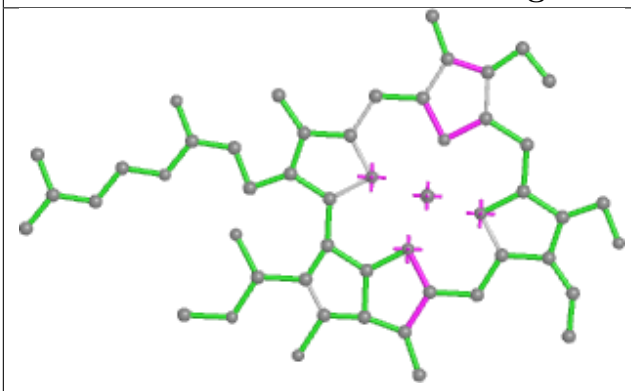


Rings

Ligand CHL 4 313



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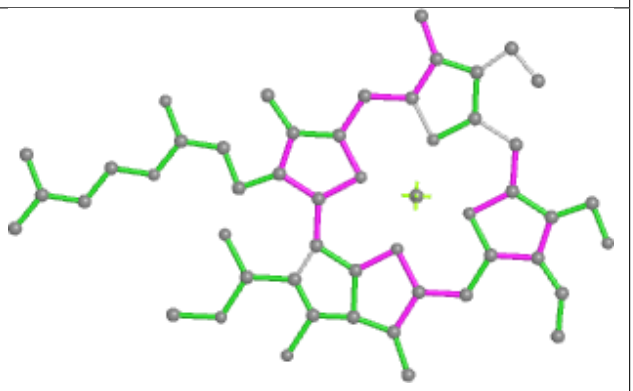
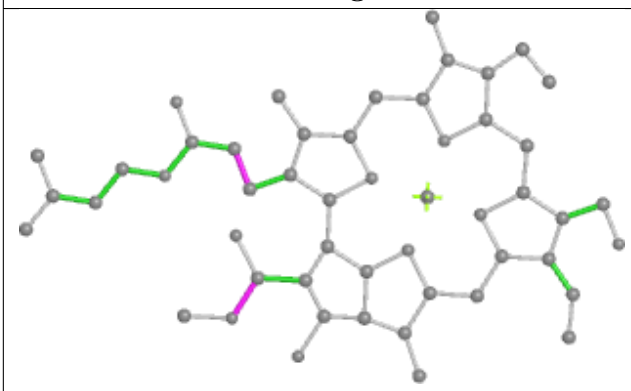


Bond angles



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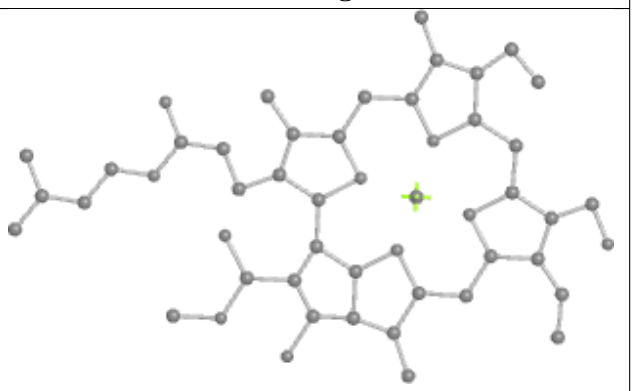
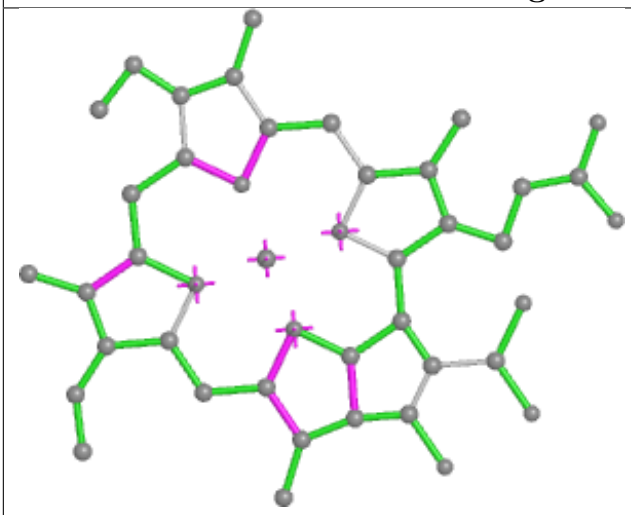


Rings

Ligand CLA 8 309



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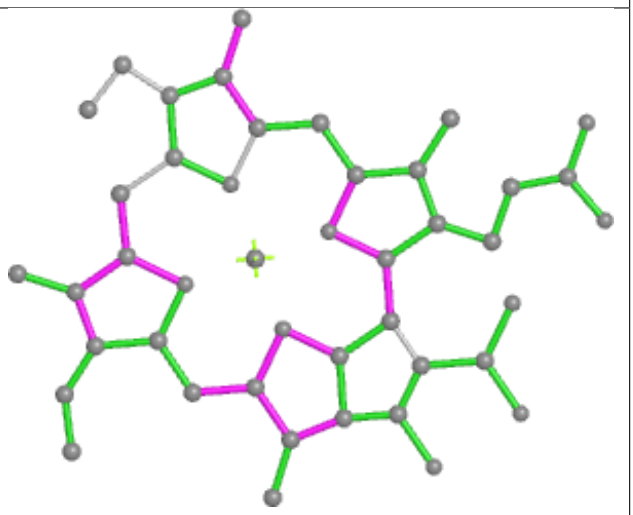
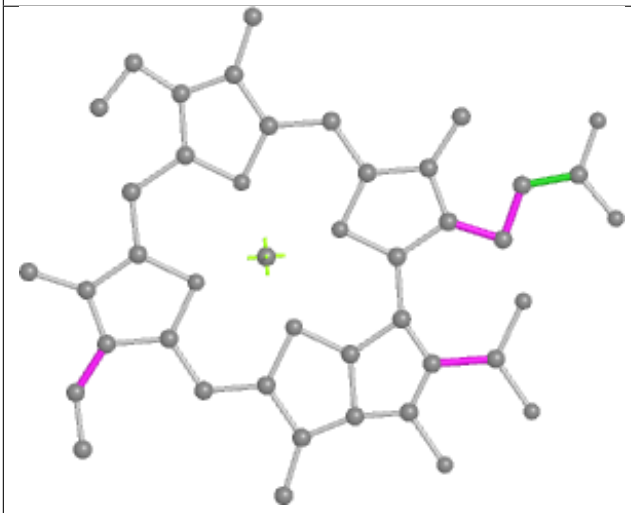


Bond angles



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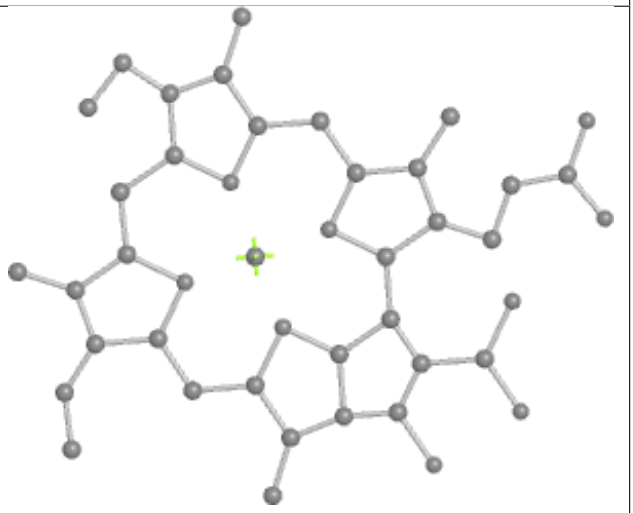
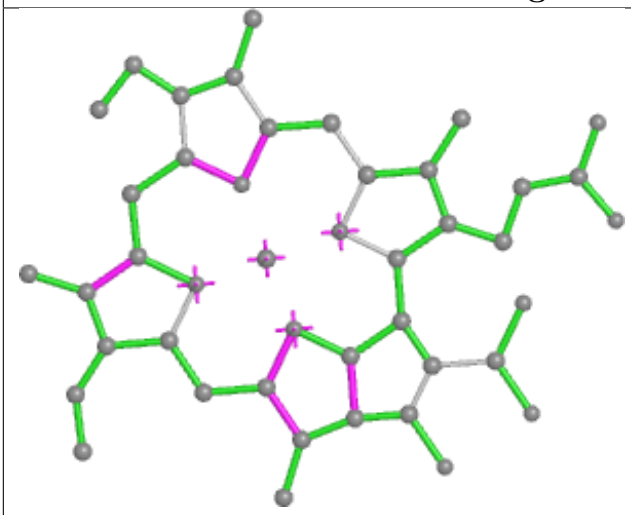


Rings

Ligand CLA 8 312



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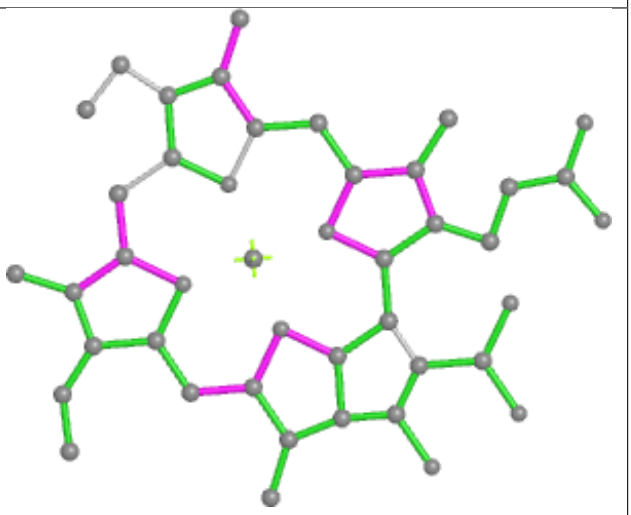
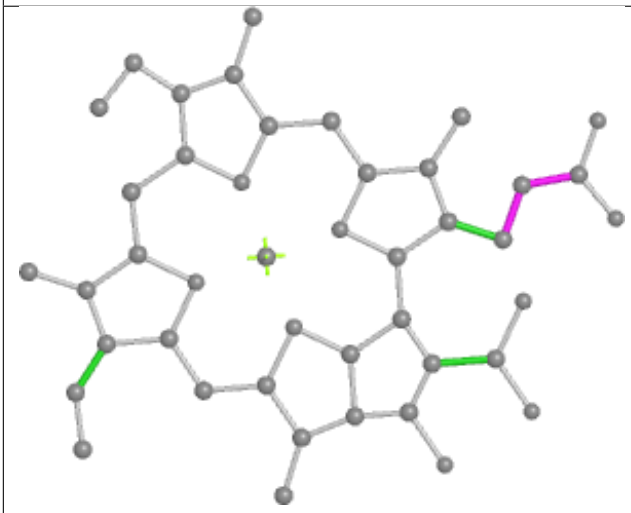


Bond angles



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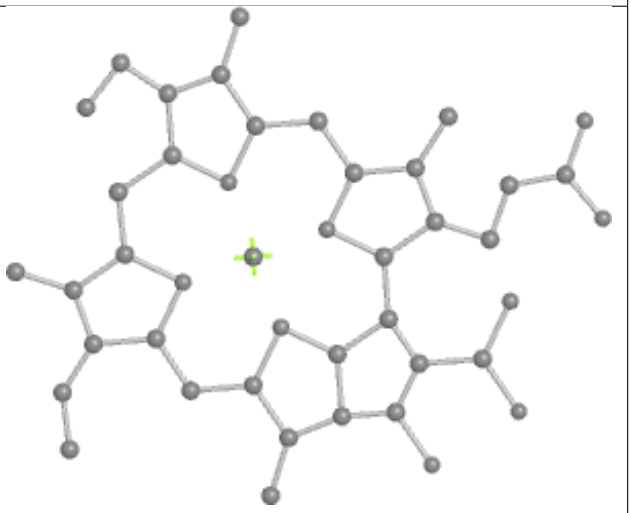
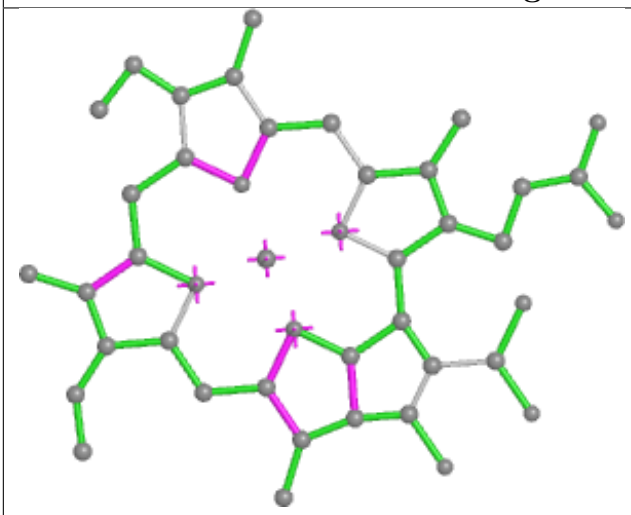


Rings

Ligand CLA A 821



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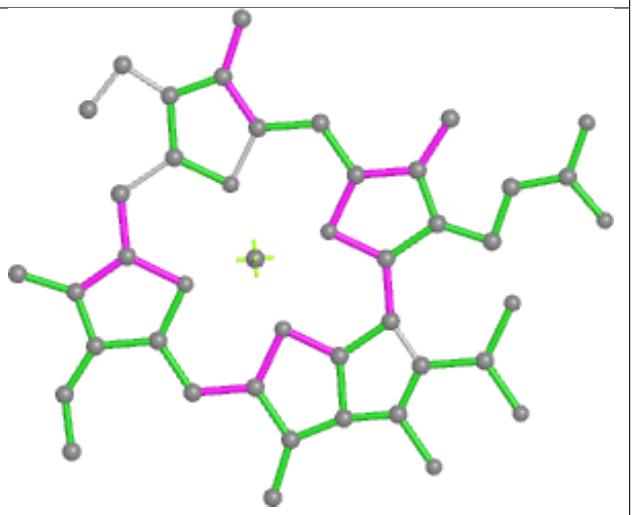
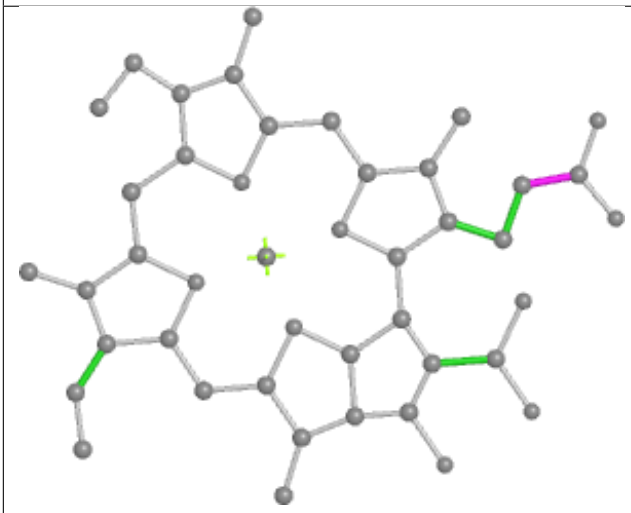
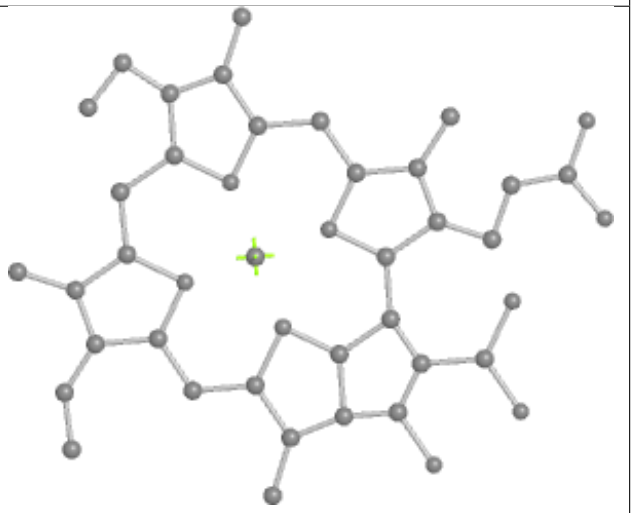


Bond angles

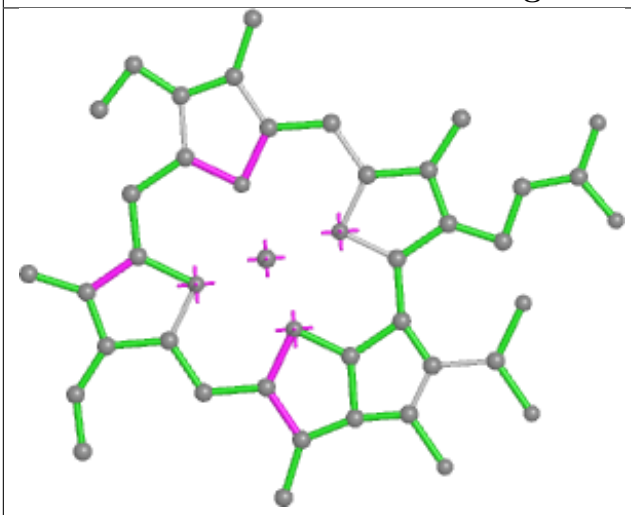


Torsions

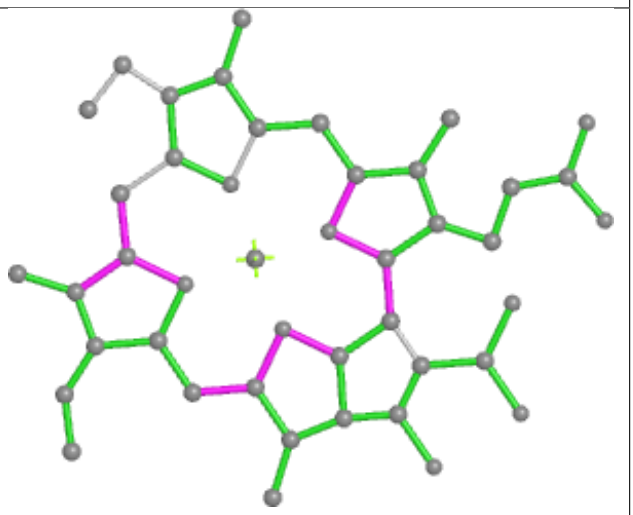


Rings

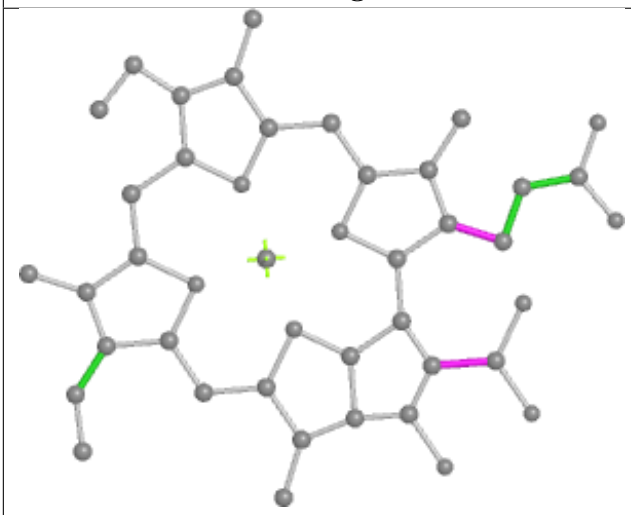
Ligand CLA A 805



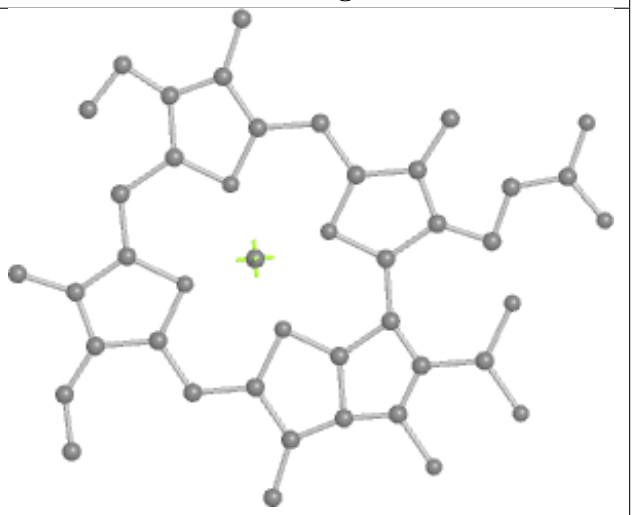
Bond lengths



Bond angles

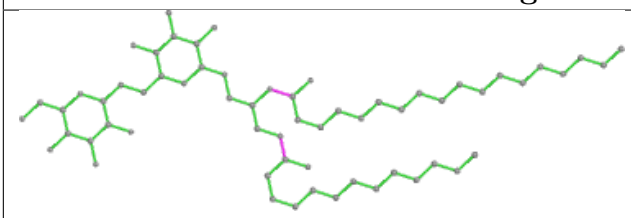


Torsions

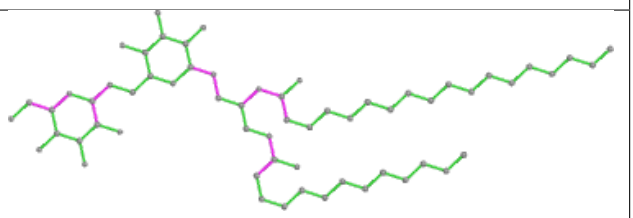


Rings

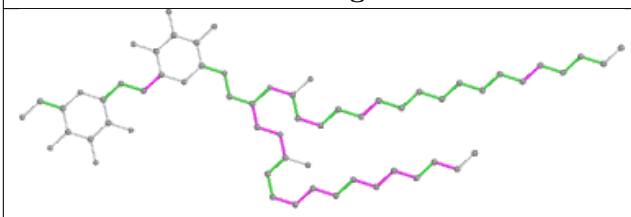
Ligand DGD B 848



Bond lengths



Bond angles



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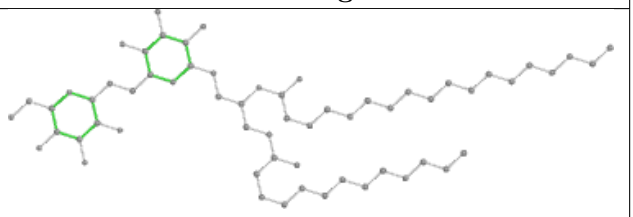
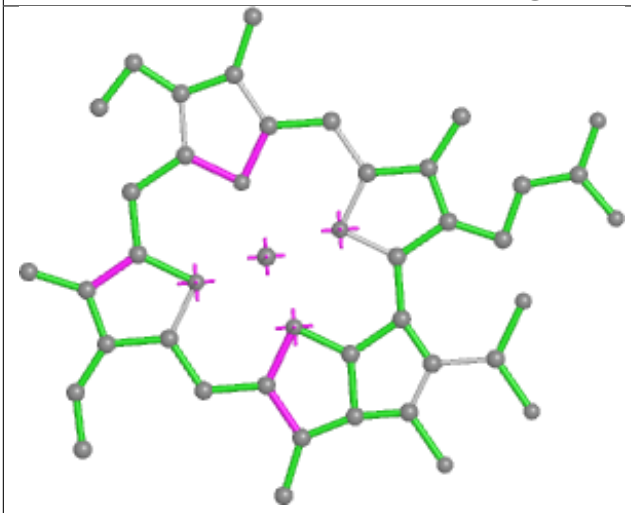
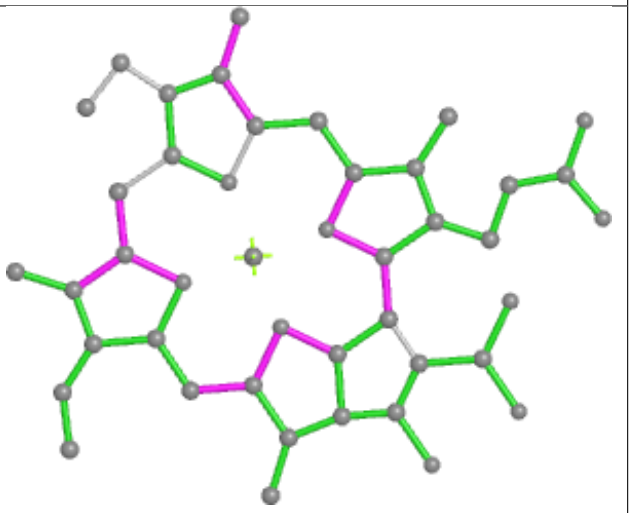


Rings

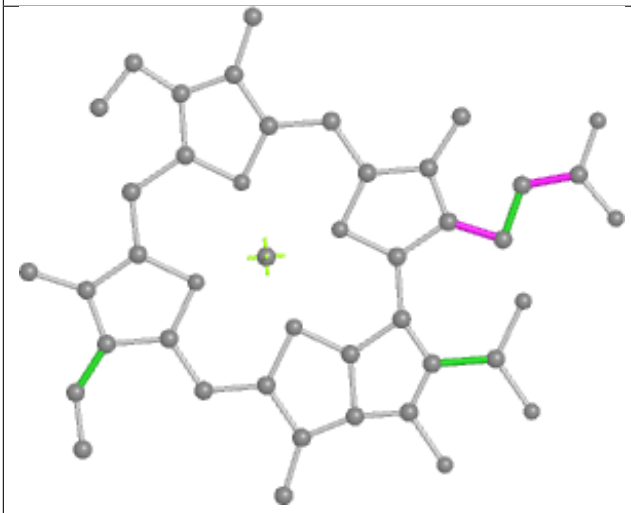
Ligand CLA L 203



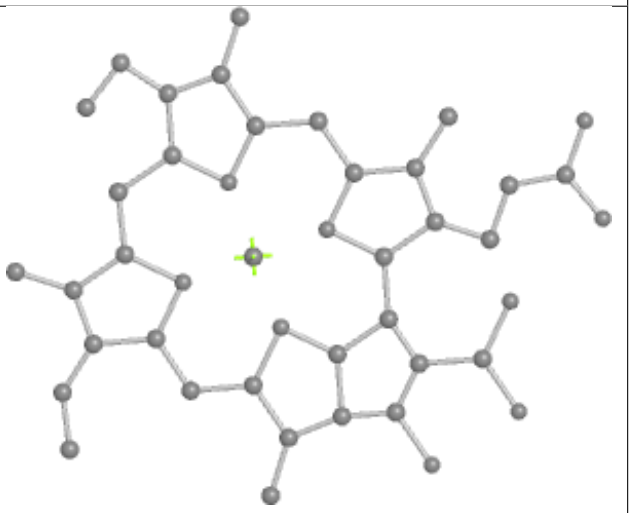
Bond lengths



Bond angles

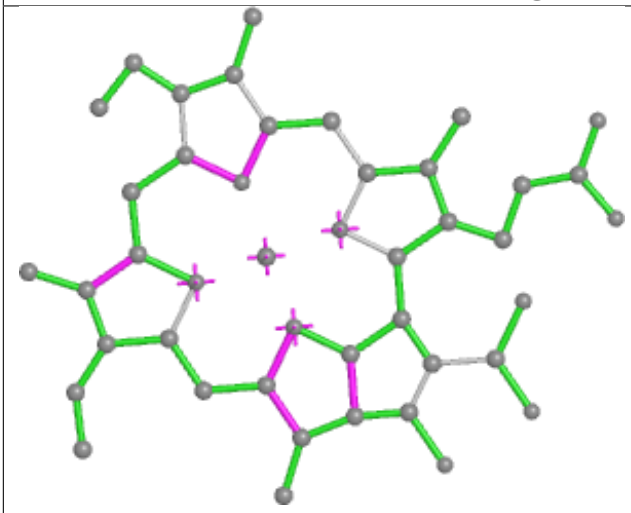


Torsions



Rings

Ligand CLA 0 305



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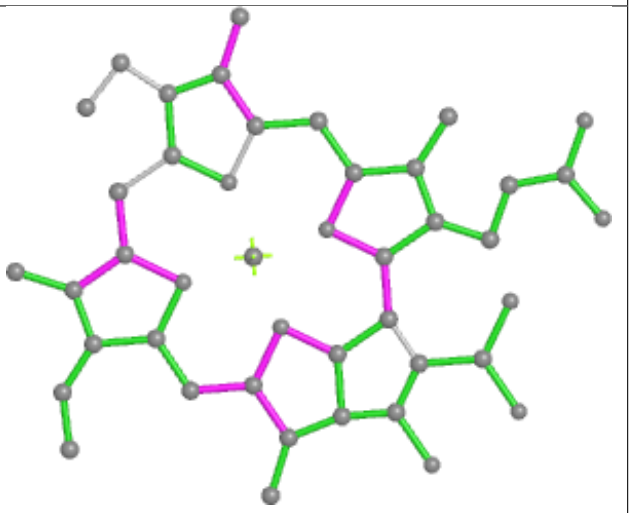
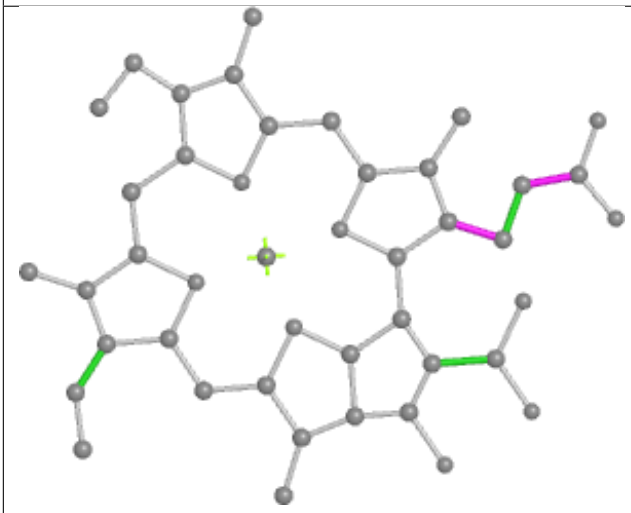


Bond angles



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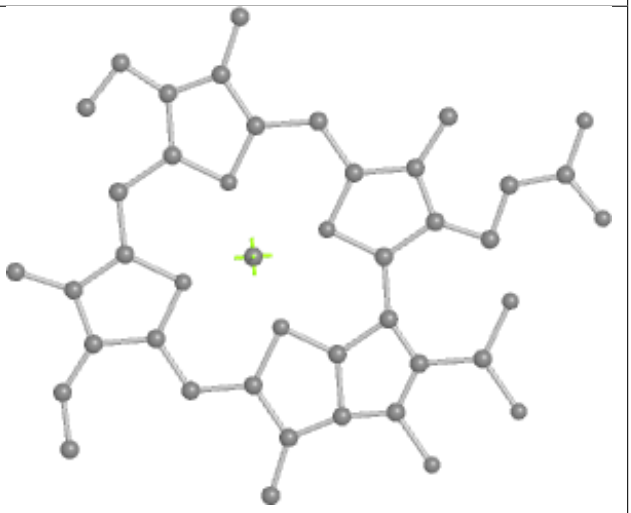
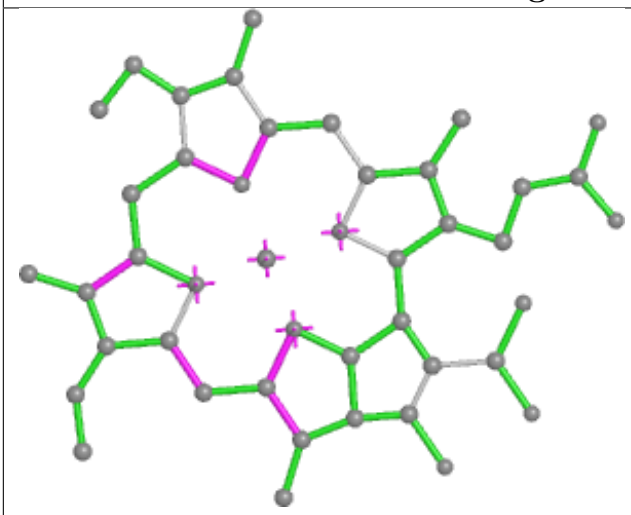


Rings

Ligand CLA 0 307



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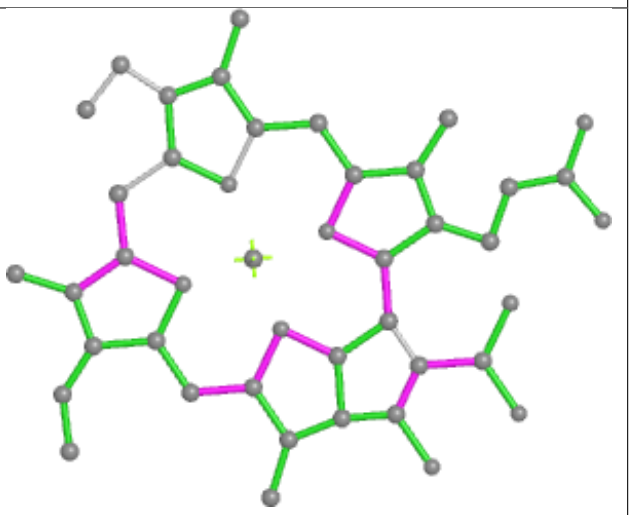
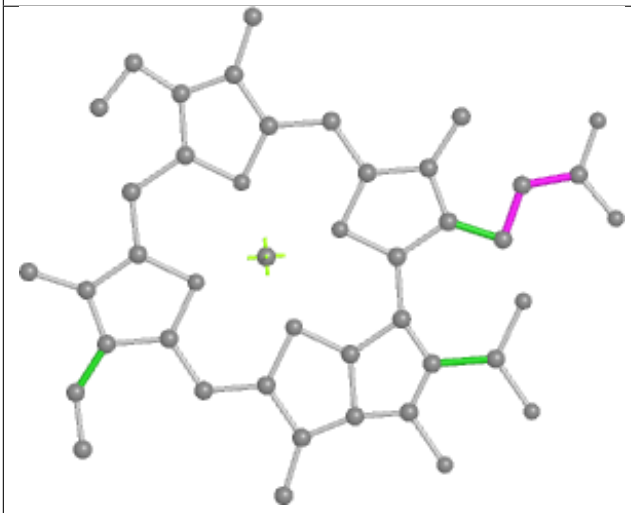


Bond angles



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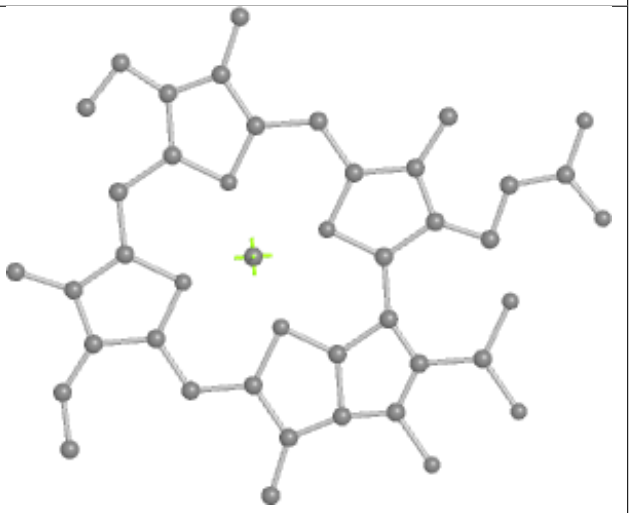
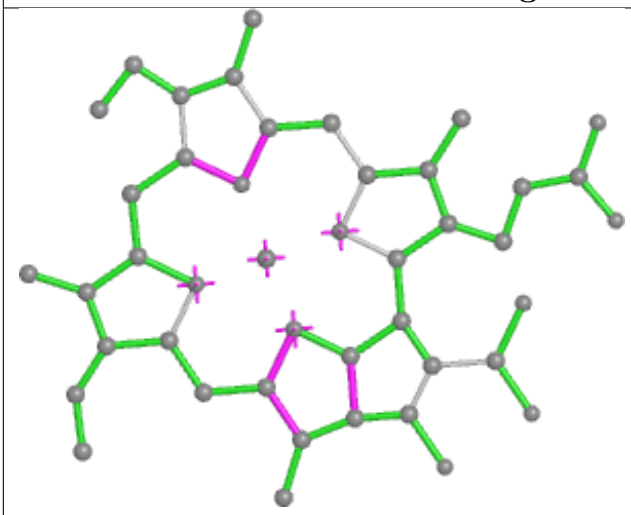


Rings

Ligand CLA 1 1010



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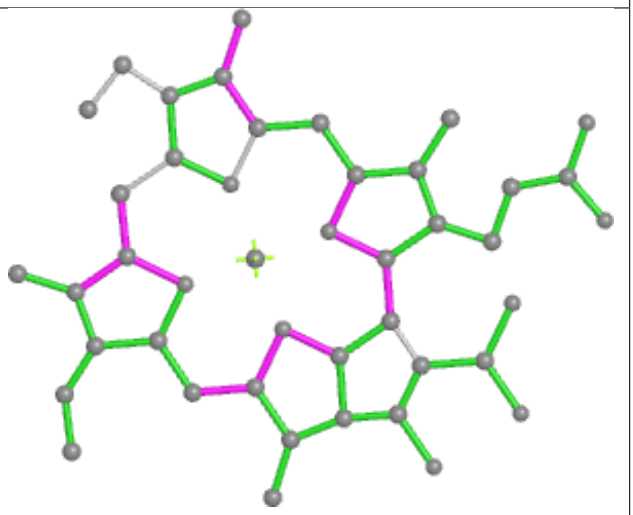

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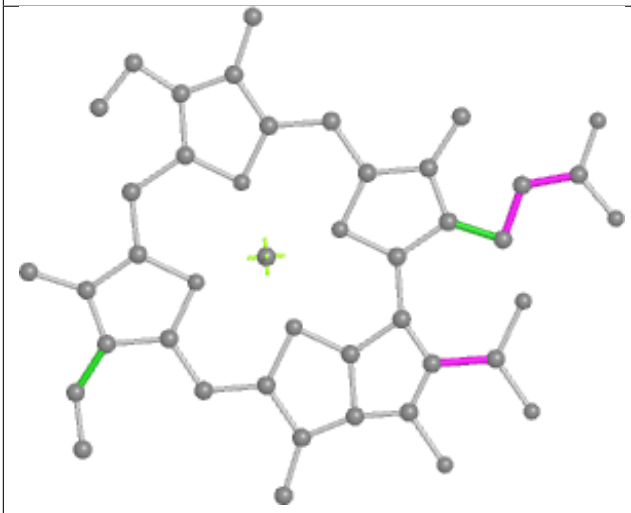

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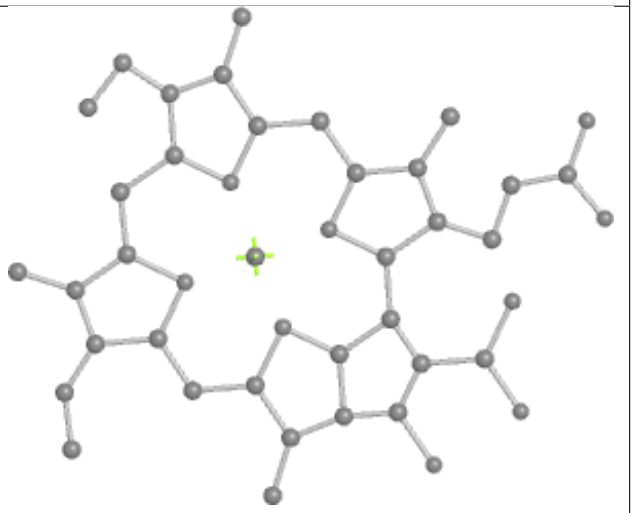
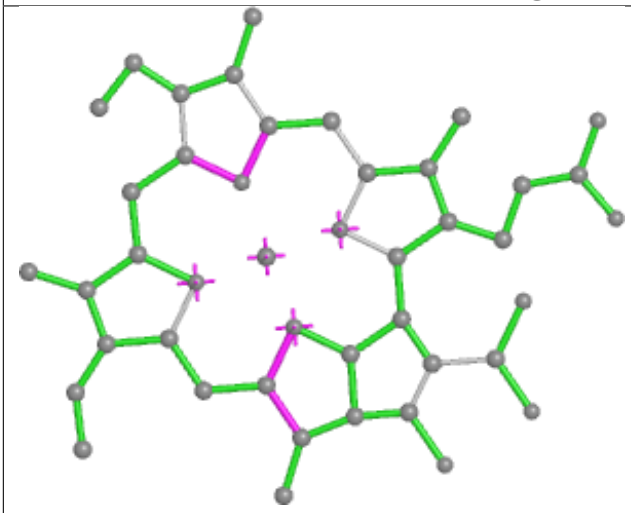


Rings

Ligand CLA 5 311



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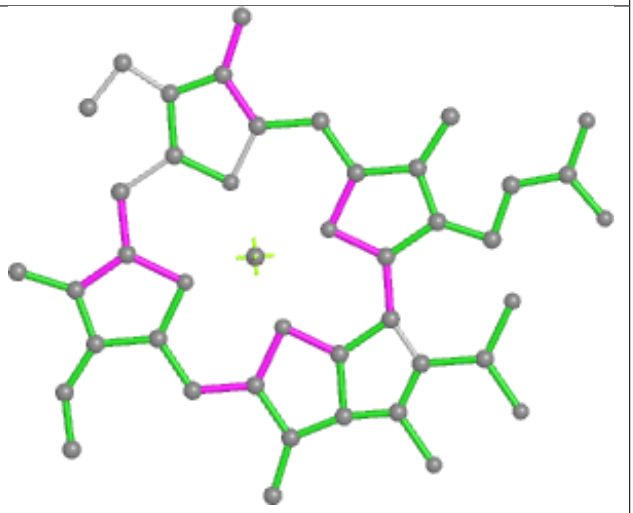
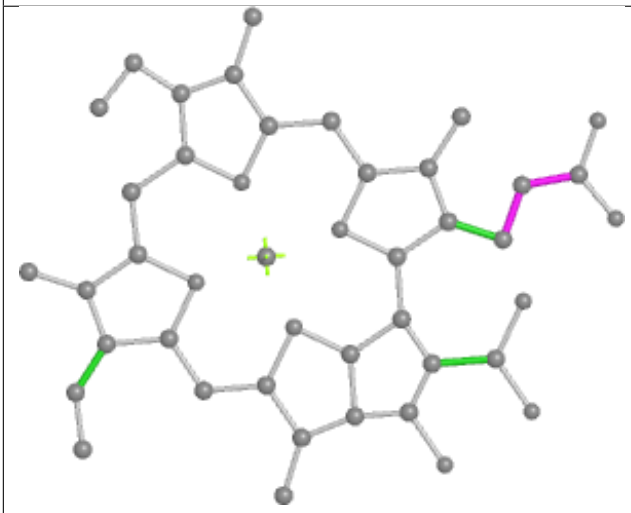


Bond angles



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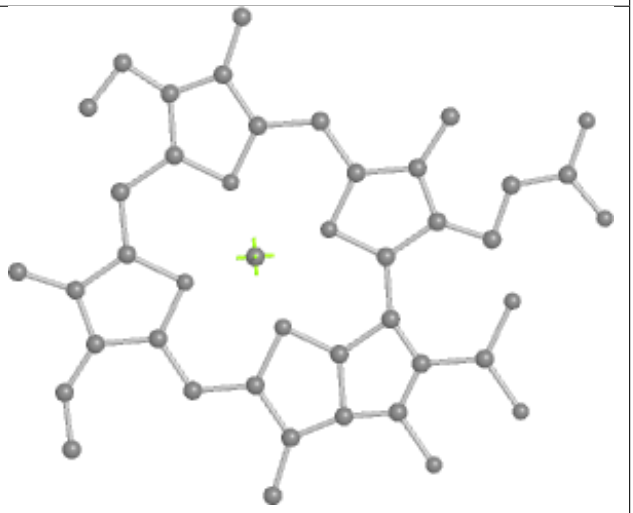
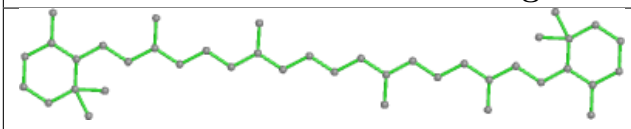


Rings

Ligand BCR A 845



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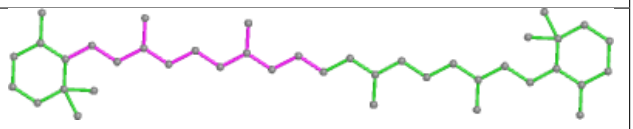

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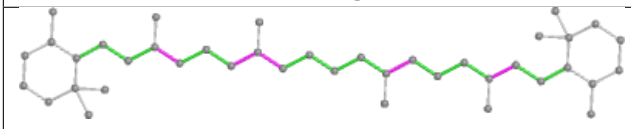
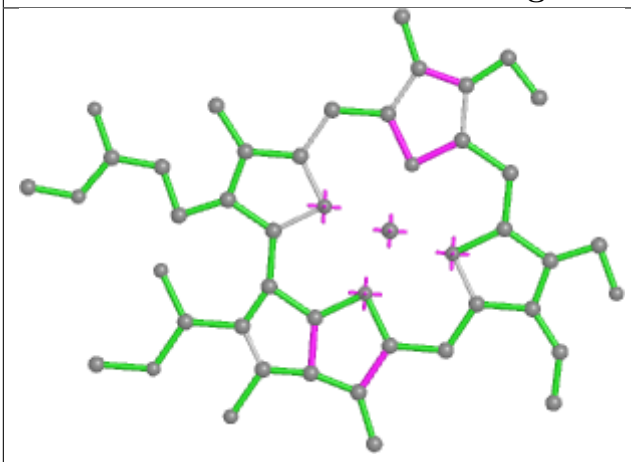


Torsions

Rings

Ligand CHL 6 313



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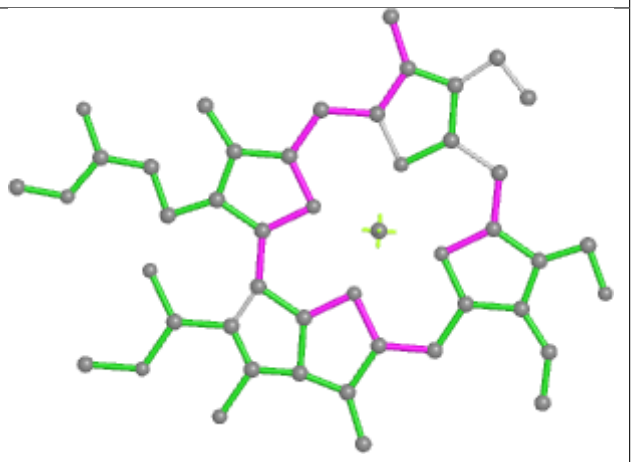

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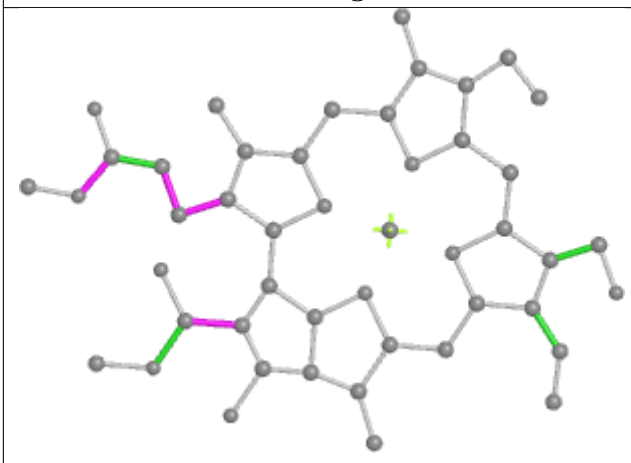

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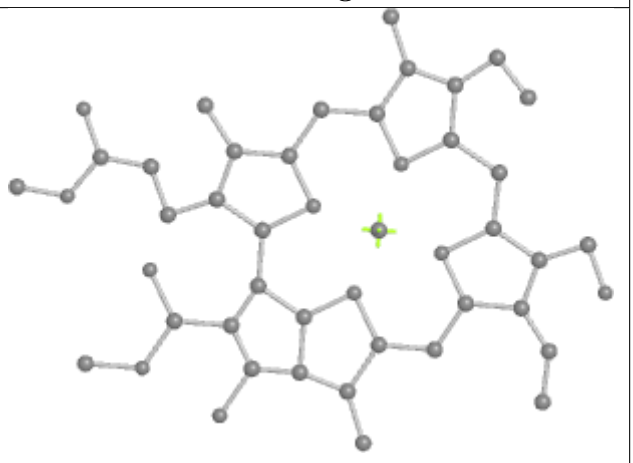
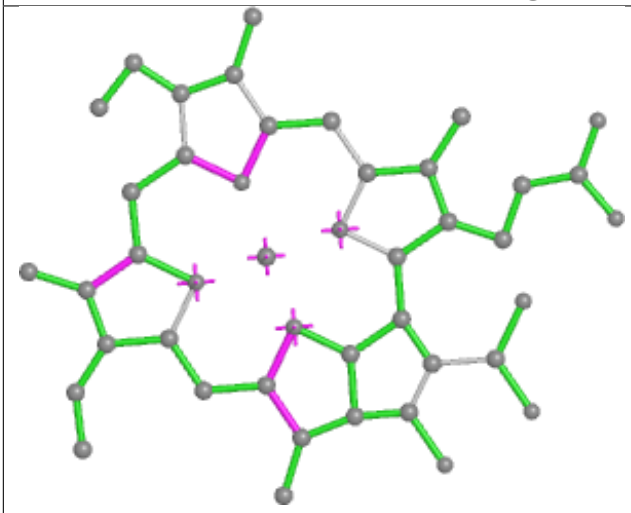
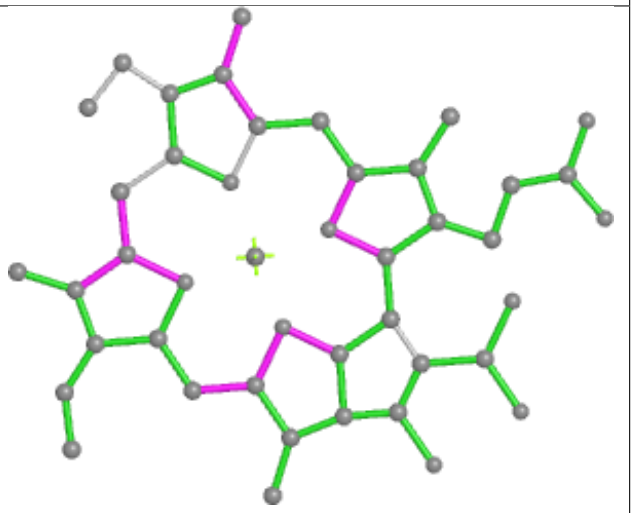


Rings

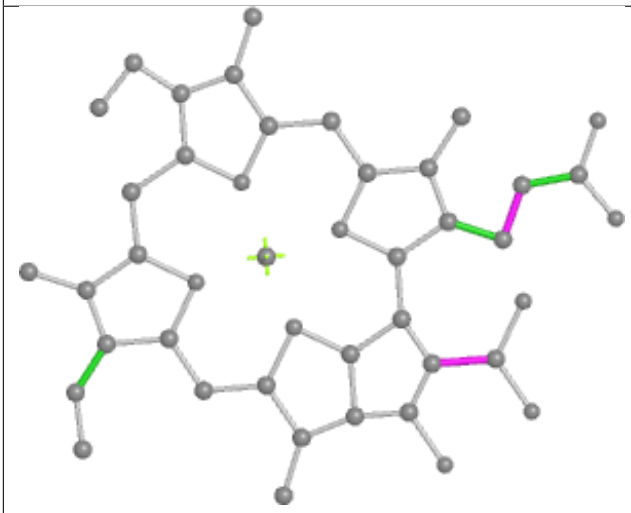
Ligand CLA B 823



Bond lengths



Bond angles



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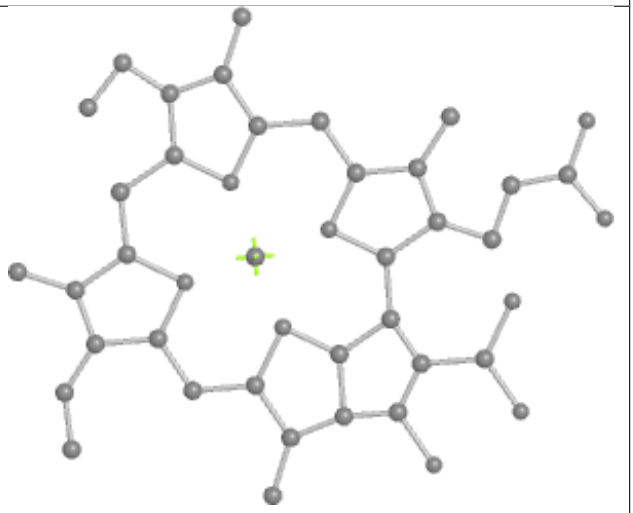
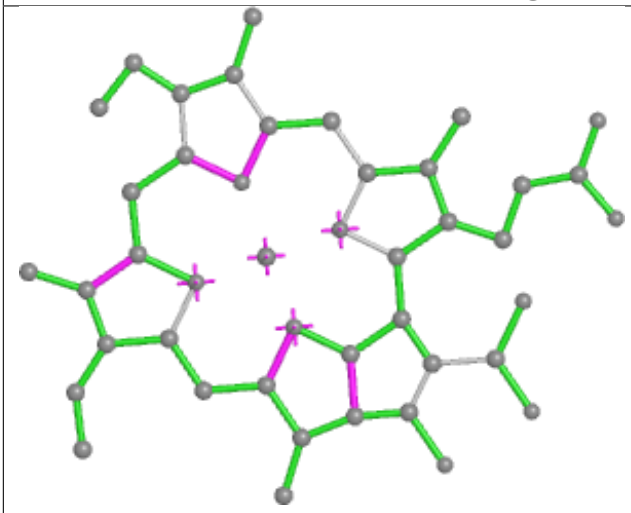


Rings

Ligand CLA B 817



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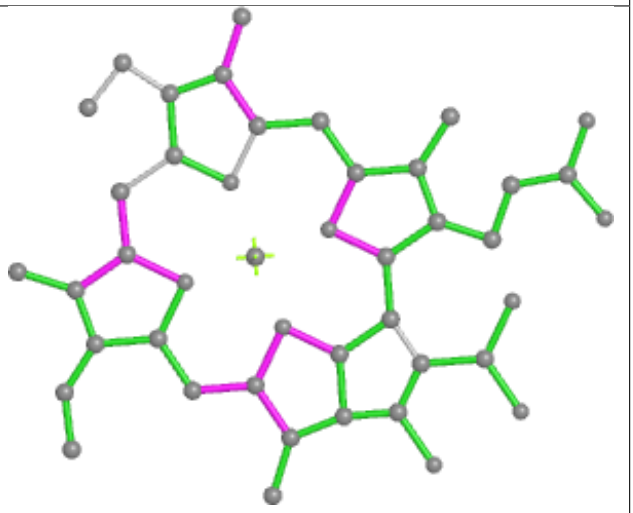

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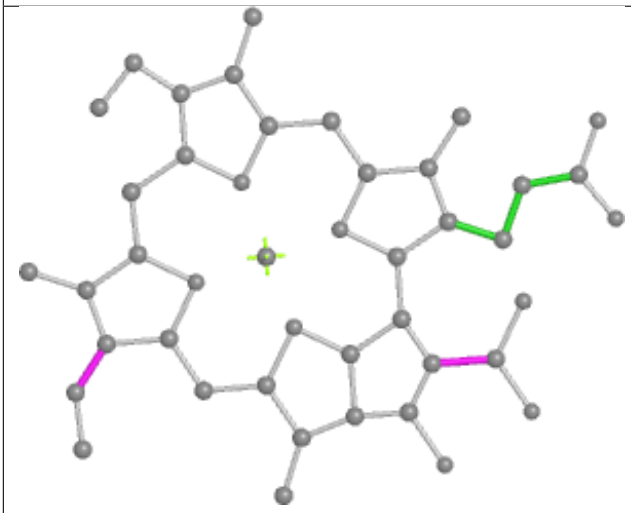

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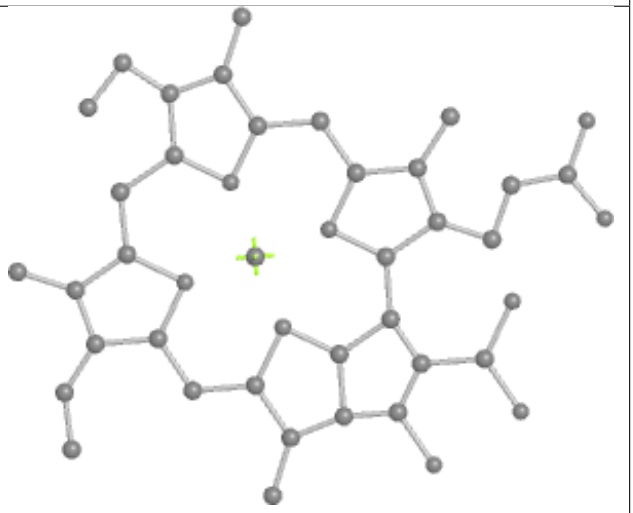
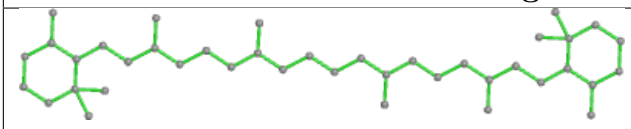


Rings

Ligand BCR A 850



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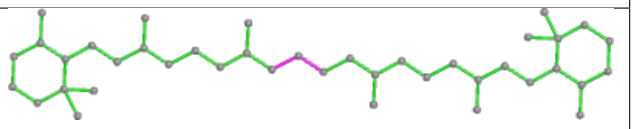
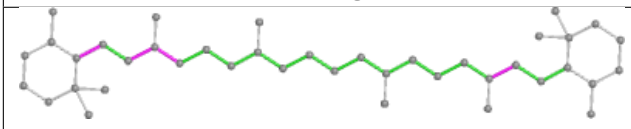


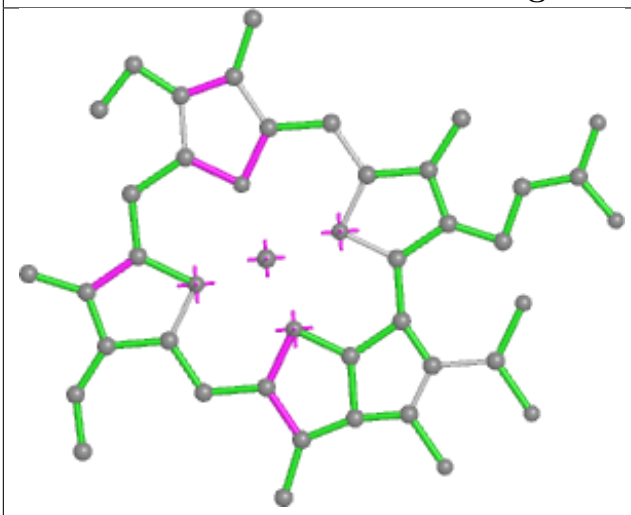
Bond angles



Torsions

Rings

Ligand CLA 6 306



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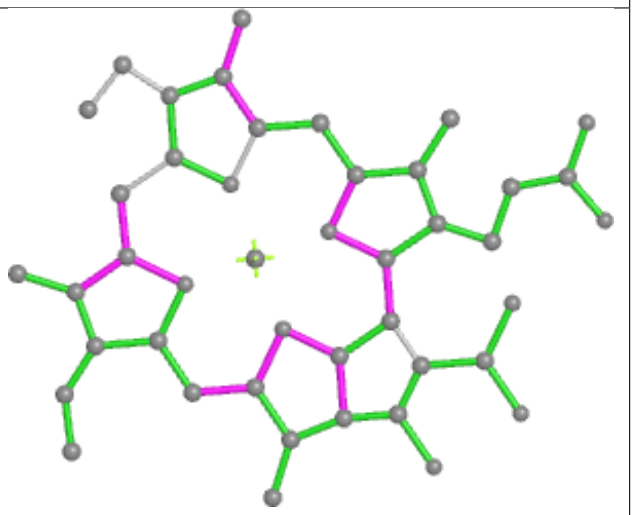
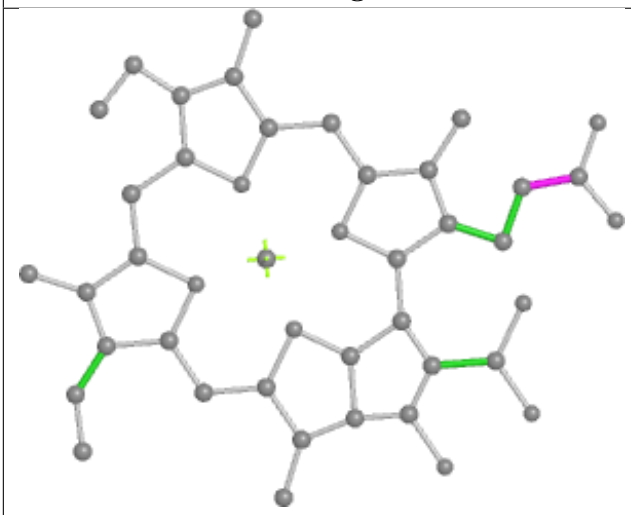


Bond angles



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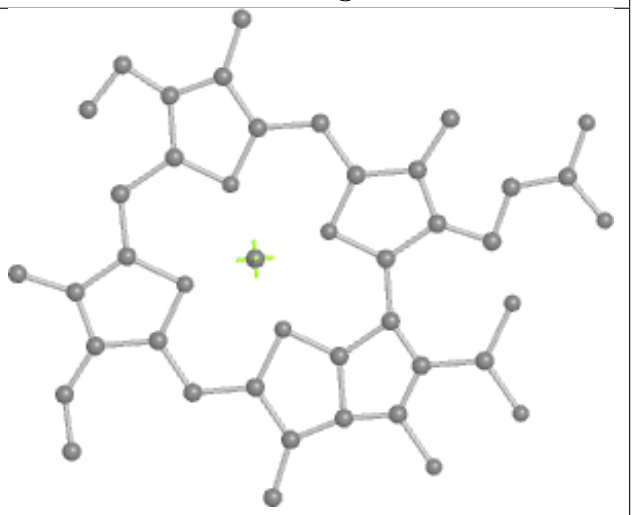
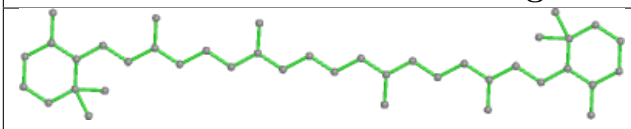


Rings

Ligand BCR 5 320



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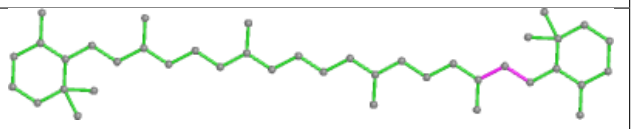
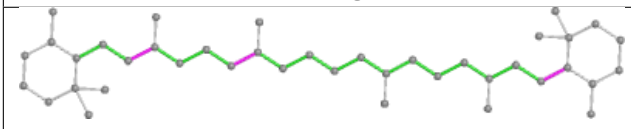


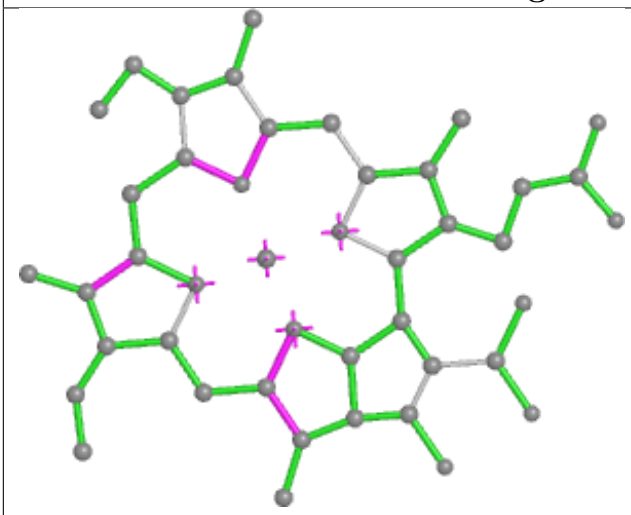
Bond angles



Torsions

Rings

Ligand CLA 4 306



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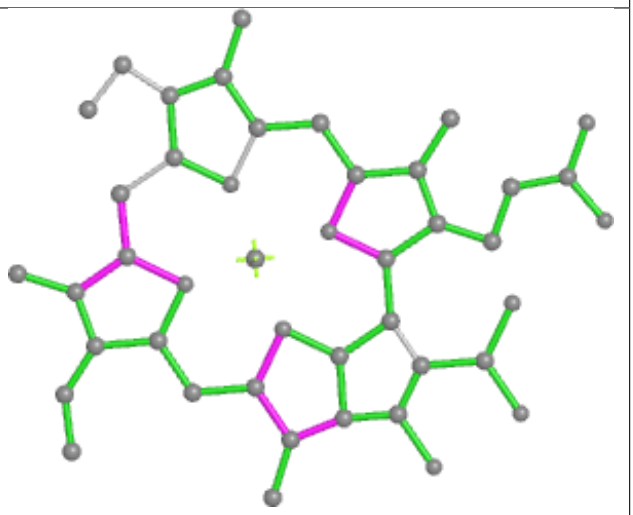
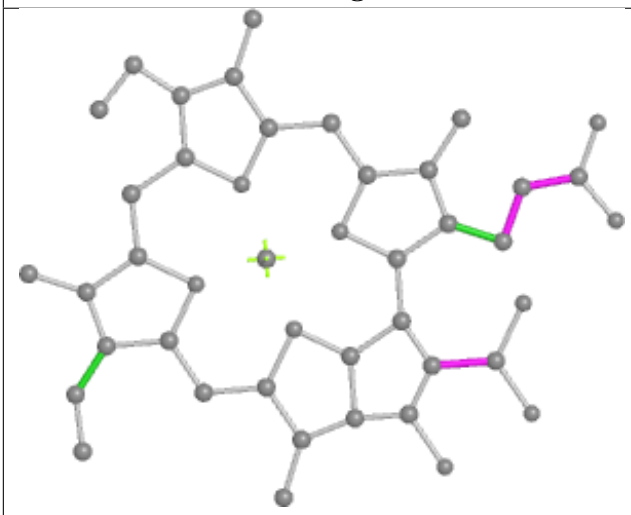
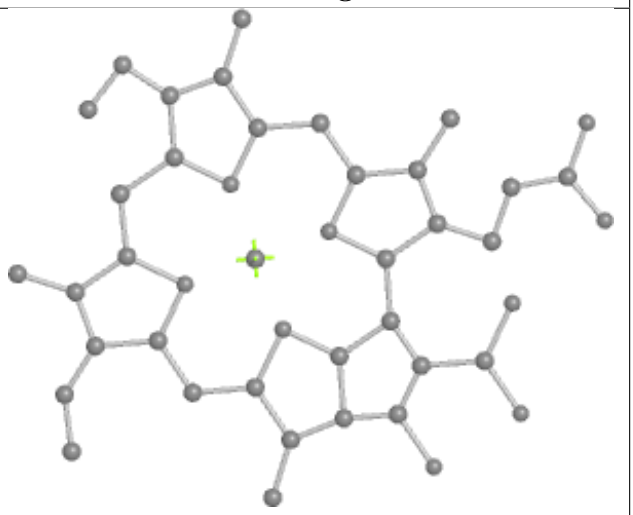


Bond angles

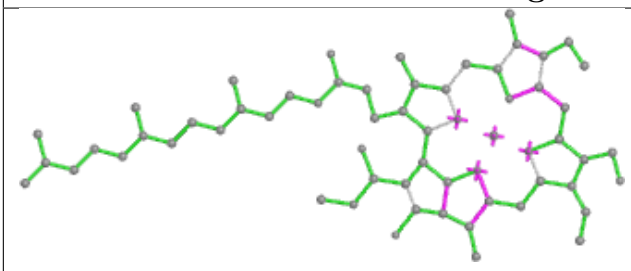


Torsions



Rings

Ligand CHL 6 316



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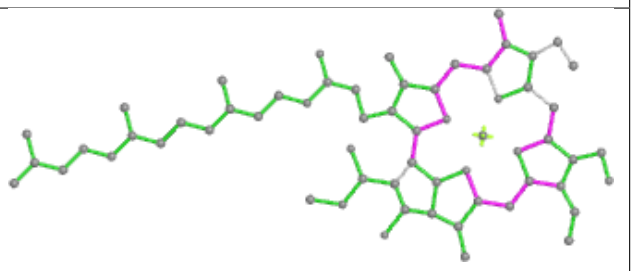
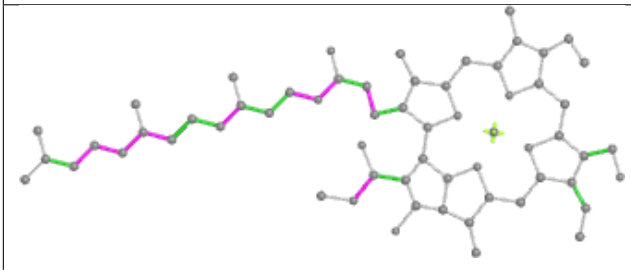
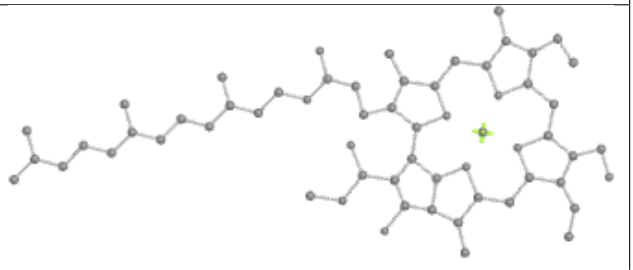


Bond angles

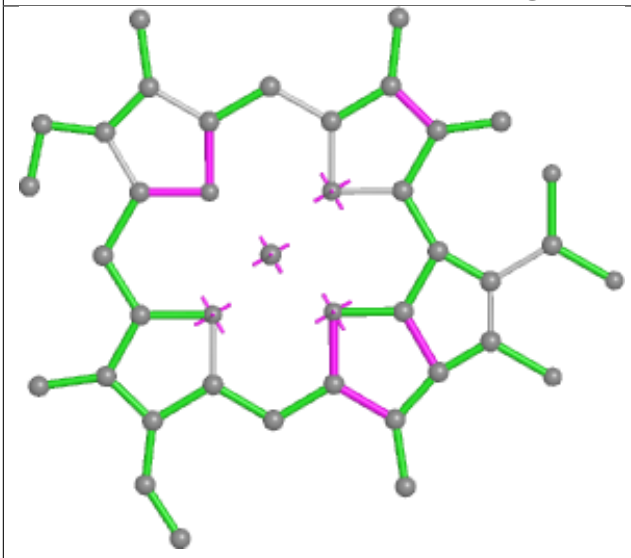


Torsions

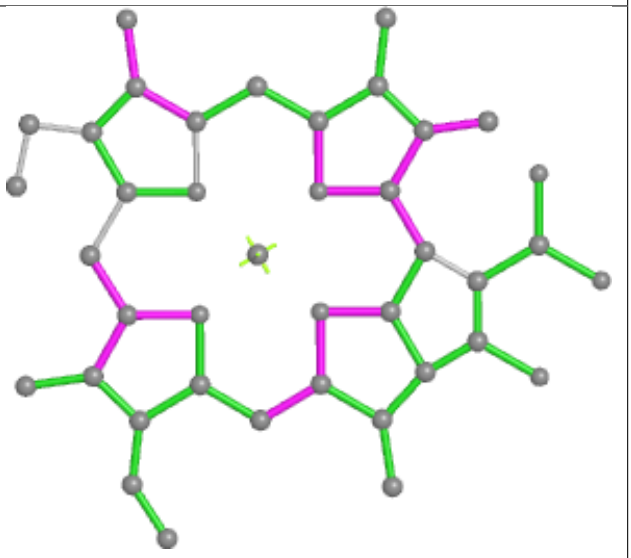


Rings

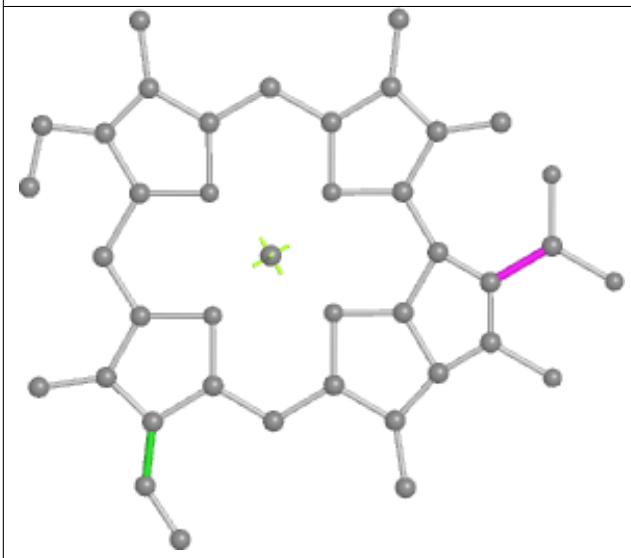
Ligand CLA A 814



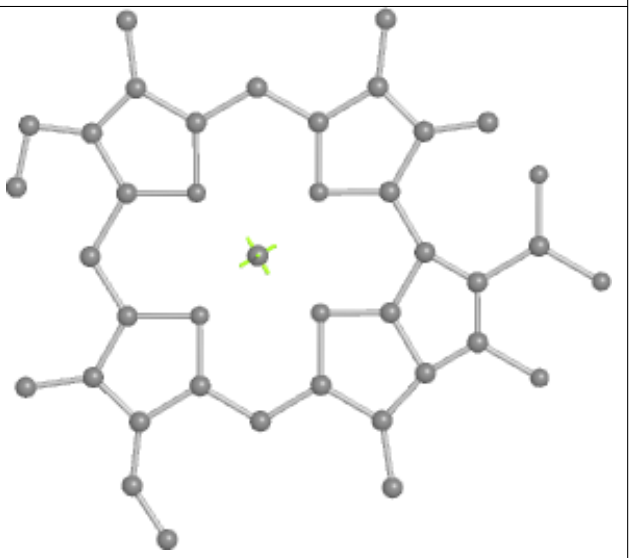
Bond lengths



Bond angles

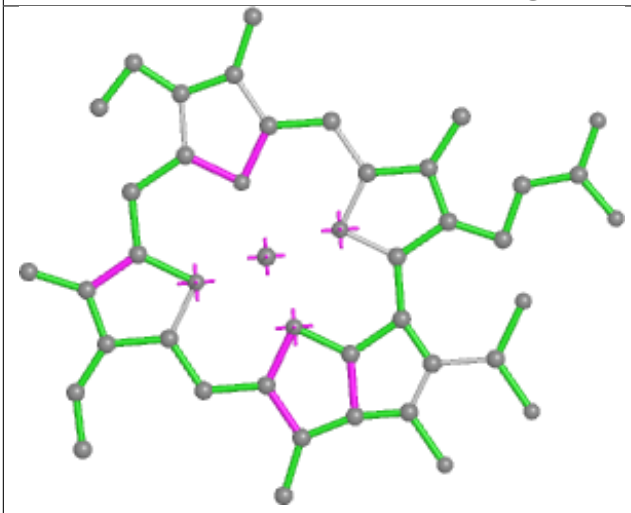


Torsions

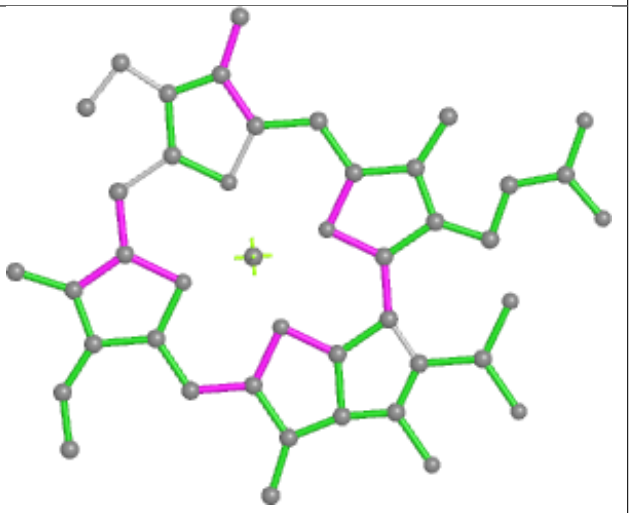


Rings

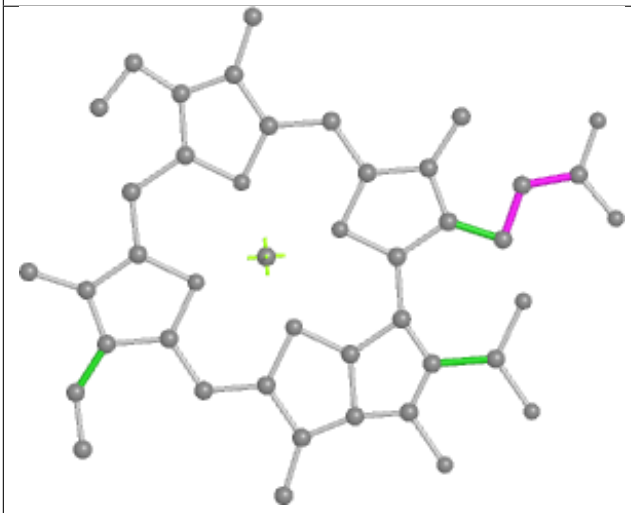
Ligand CLA B 819



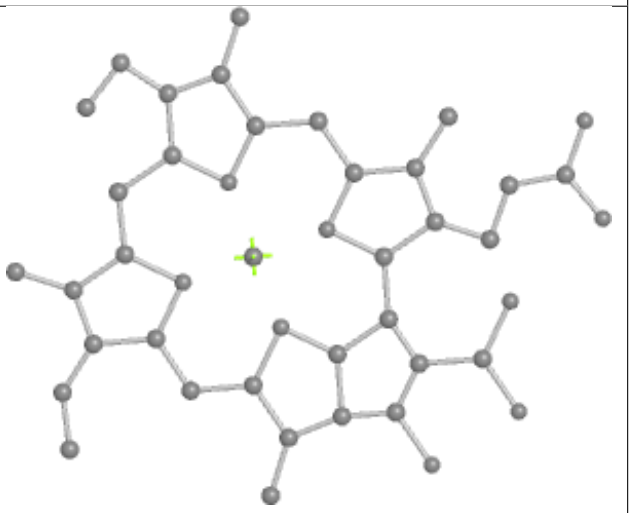
Bond lengths



Bond angles

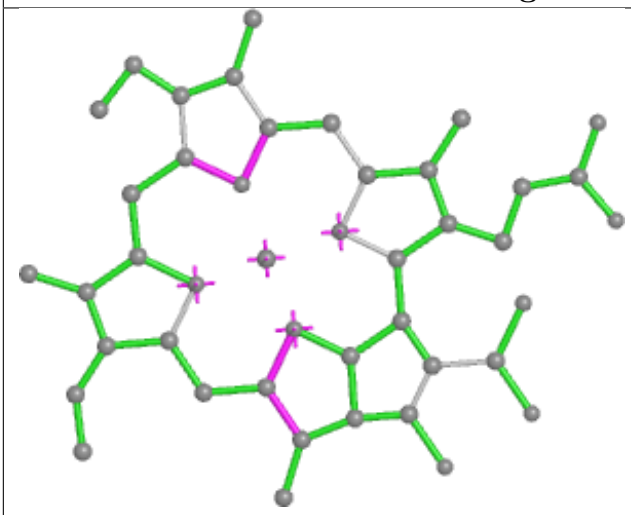


Torsions



Rings

Ligand CLA 3 1013



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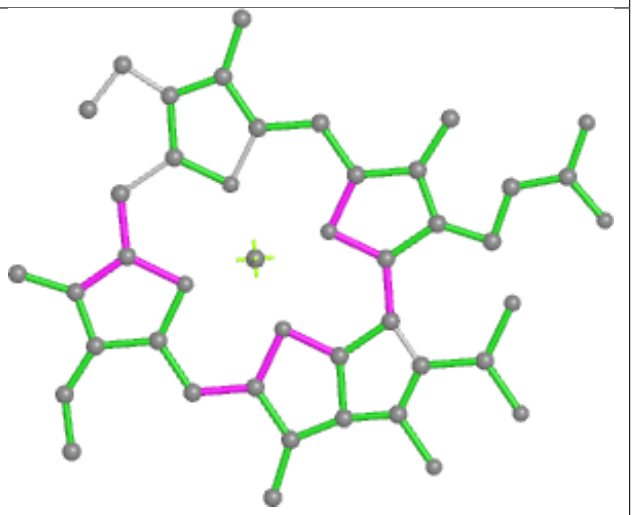
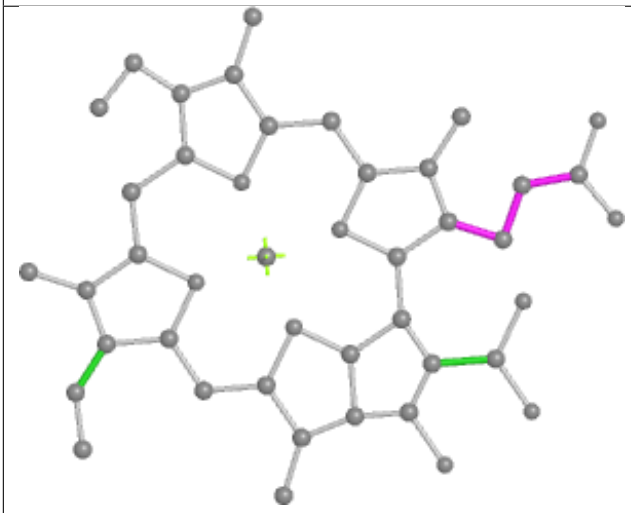
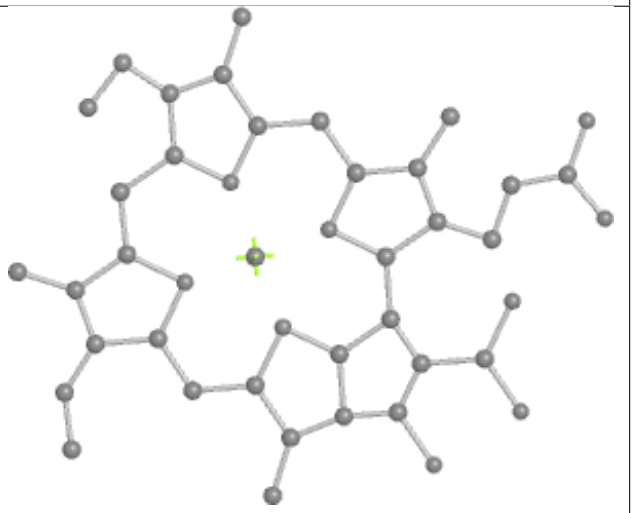


Bond angles

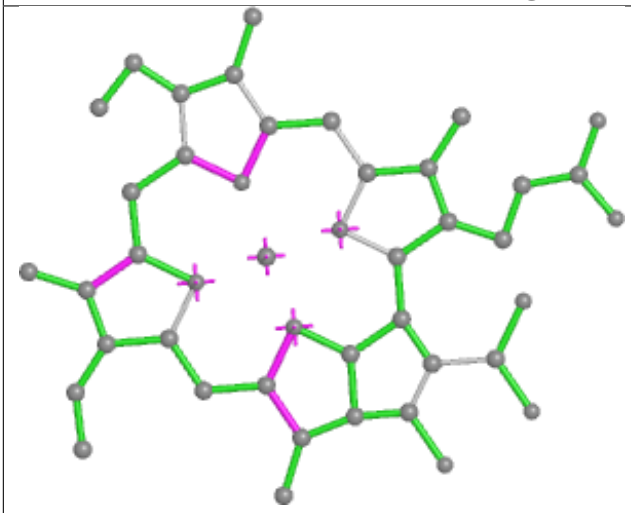


Torsions

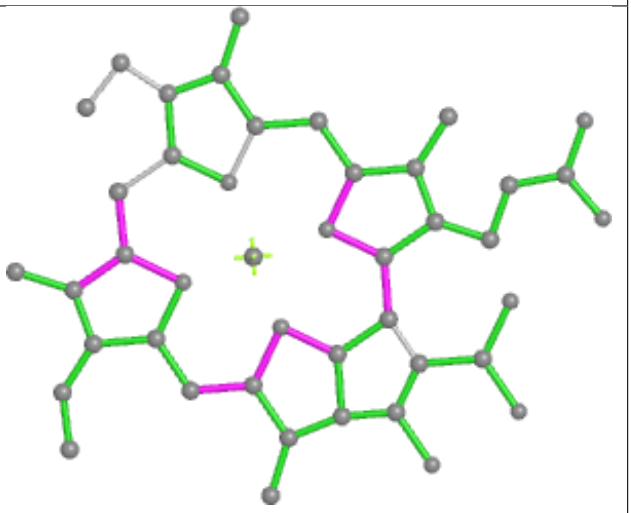


Rings

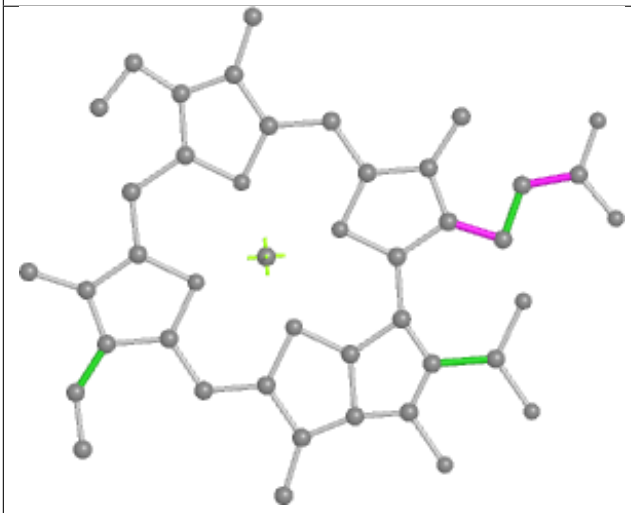
Ligand CLA G 202



Bond lengths



Bond angles



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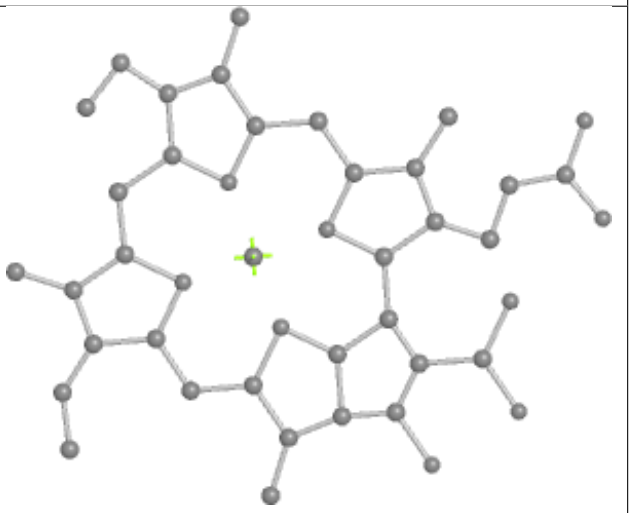
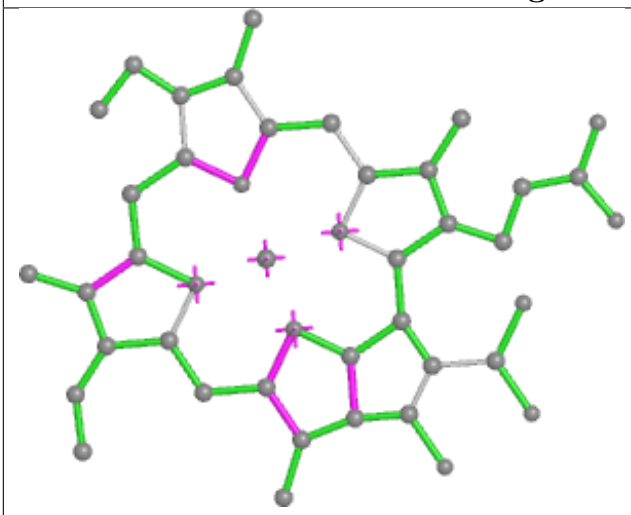


Rings

Ligand CLA J 102



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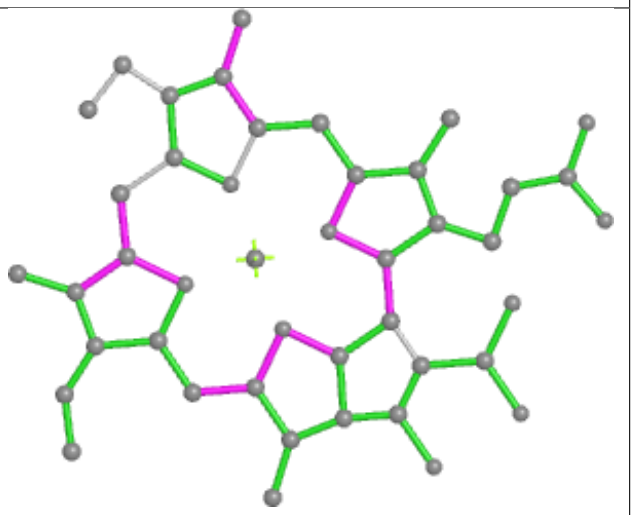
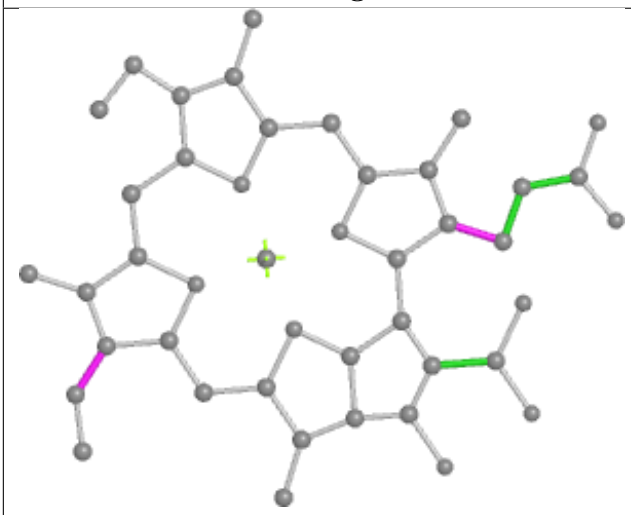


Bond angles



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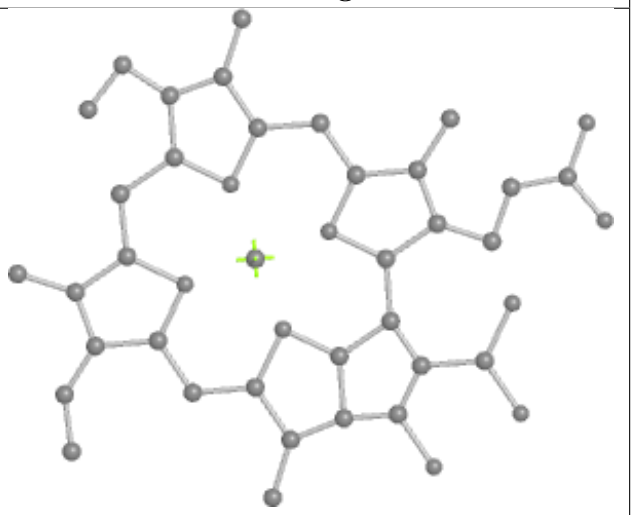
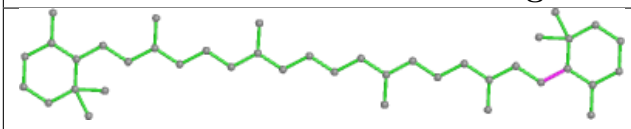


Rings

Ligand BCR 6 302



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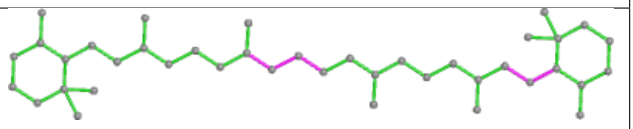
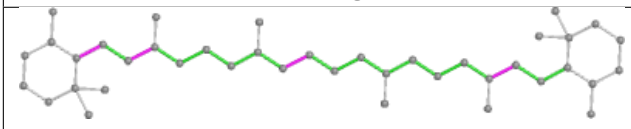


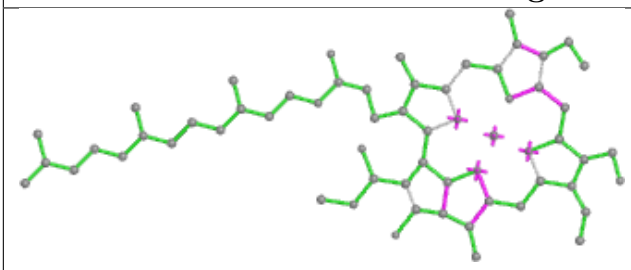
Bond angles



Torsions

Rings

Ligand CHL 4 315



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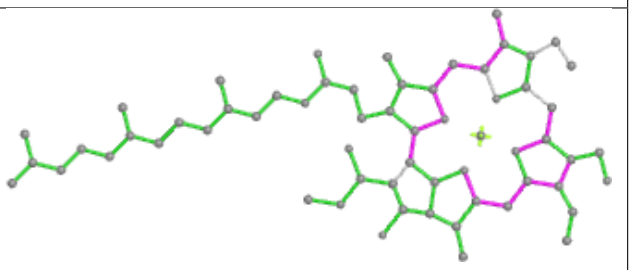

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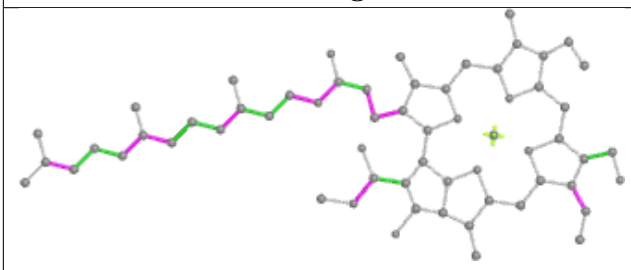

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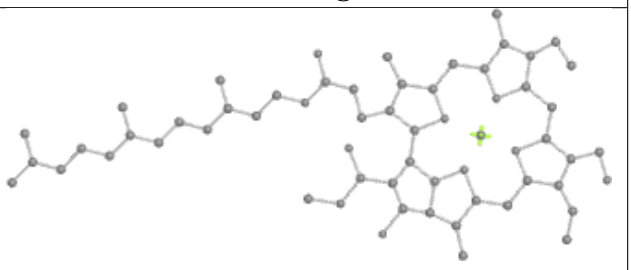
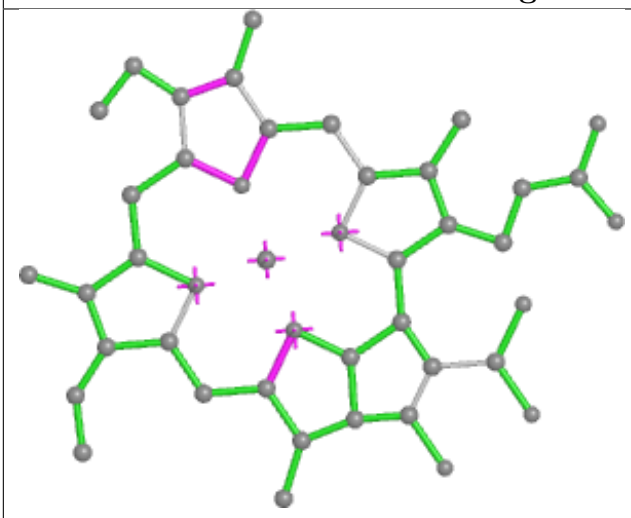


Rings

Ligand CLA 1 1006



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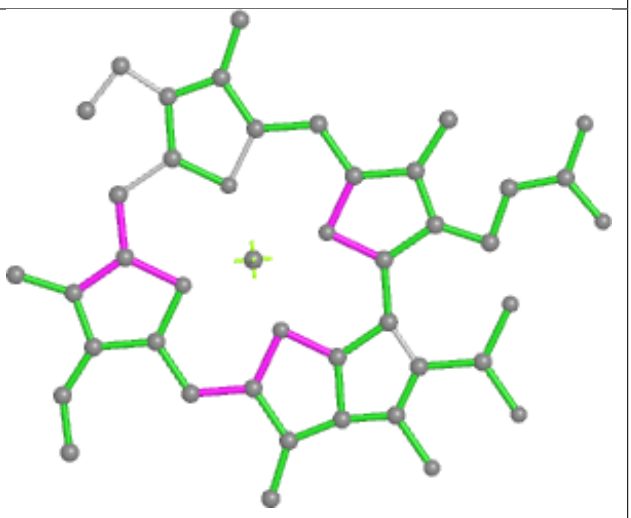
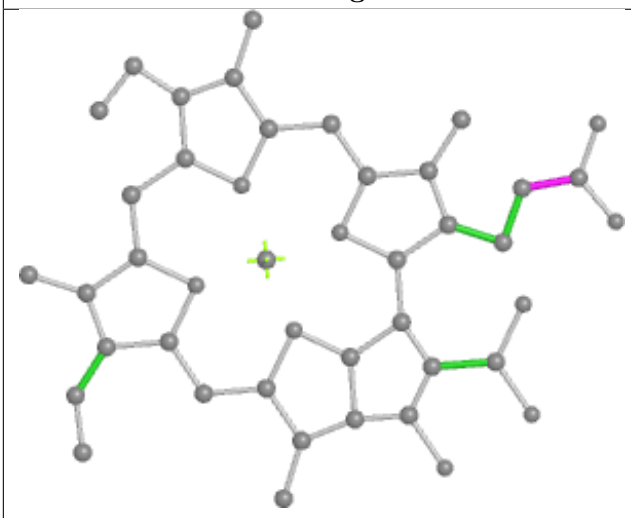


Bond angles



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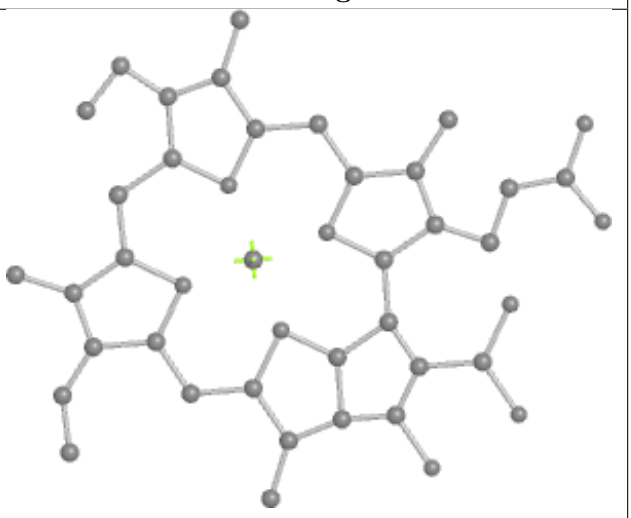
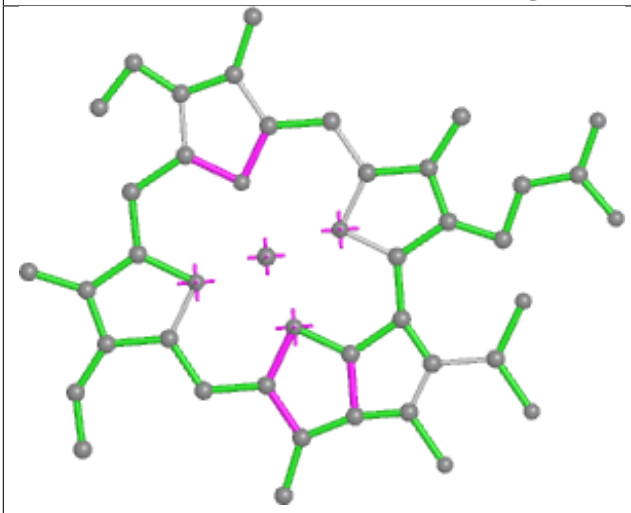
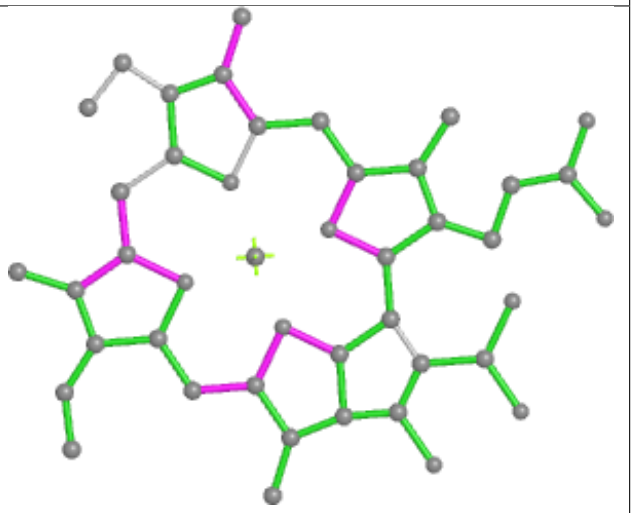


Rings

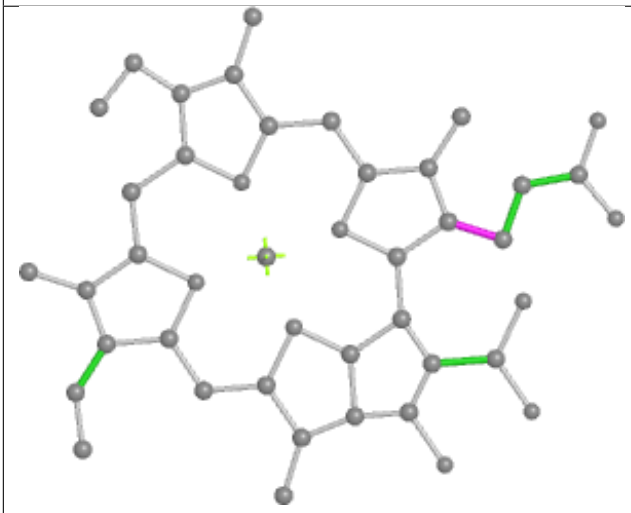
Ligand CLA B 831



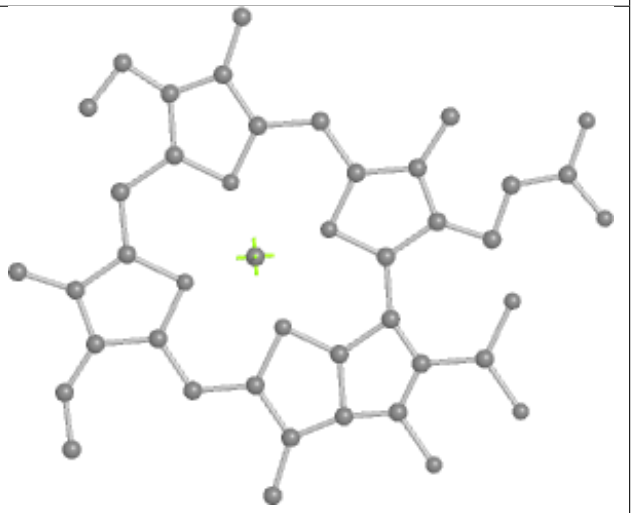
Bond lengths



Bond angles

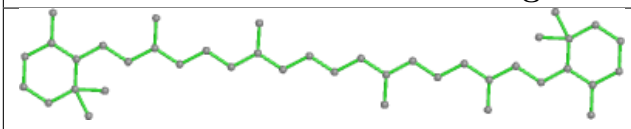


Torsions



Rings

Ligand BCR B 846



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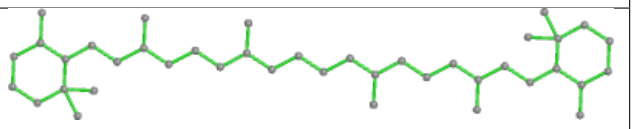
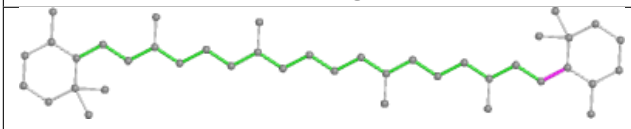


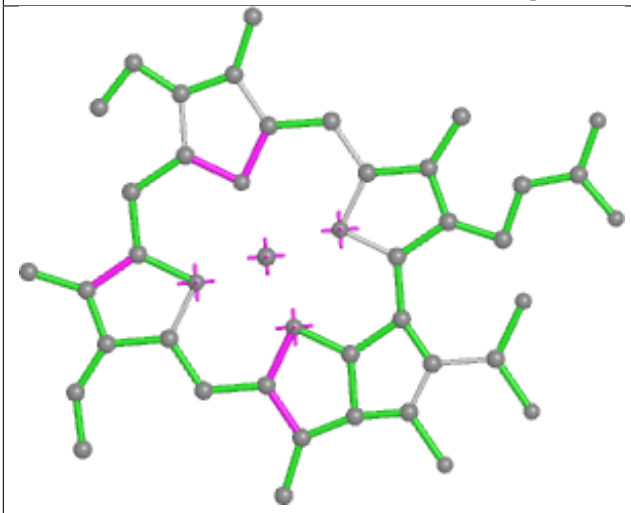
Bond angles



Torsions

Rings

Ligand CLA B 820



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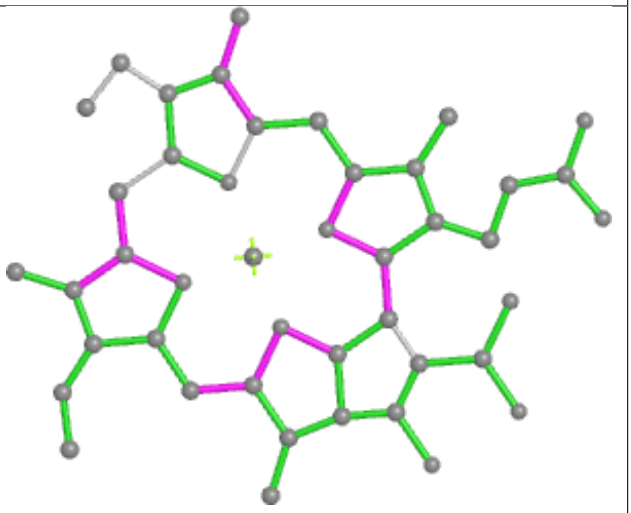
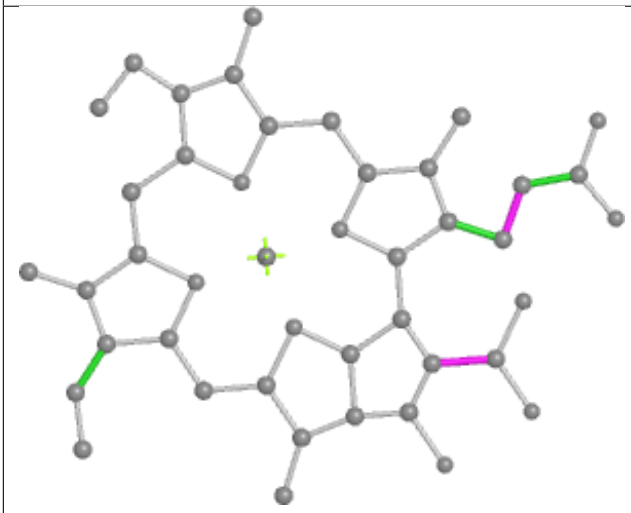


Bond angles



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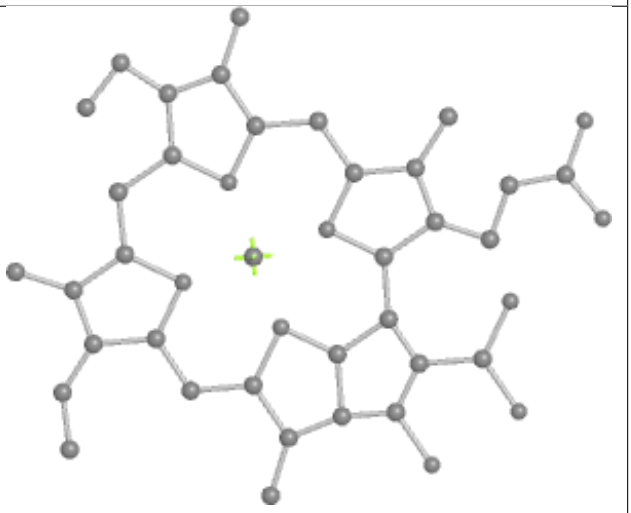
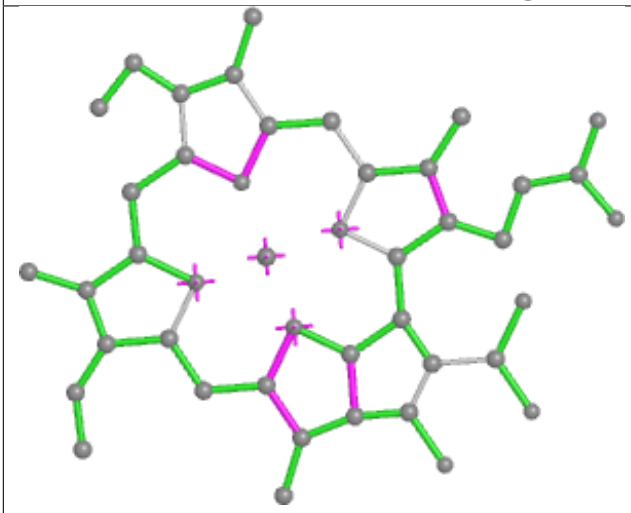


Rings

Ligand CLA 7 1014



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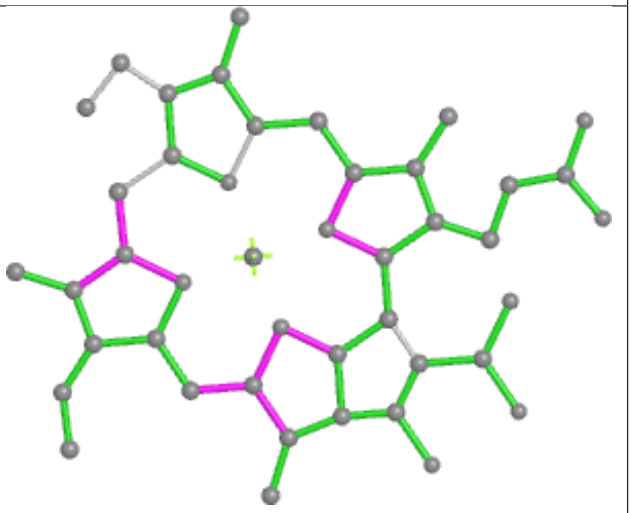
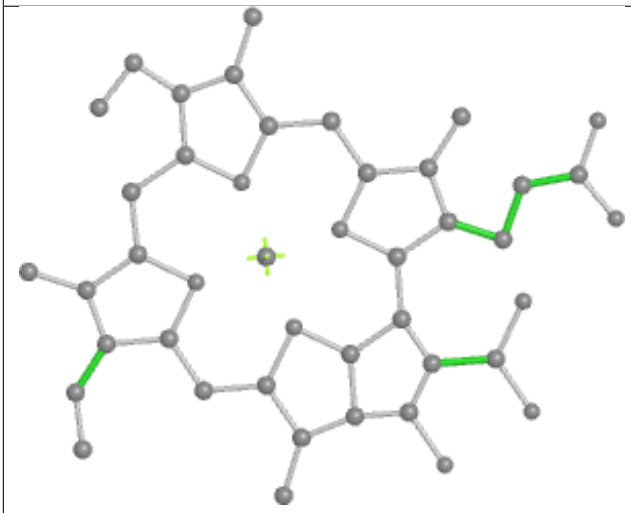


Bond angles



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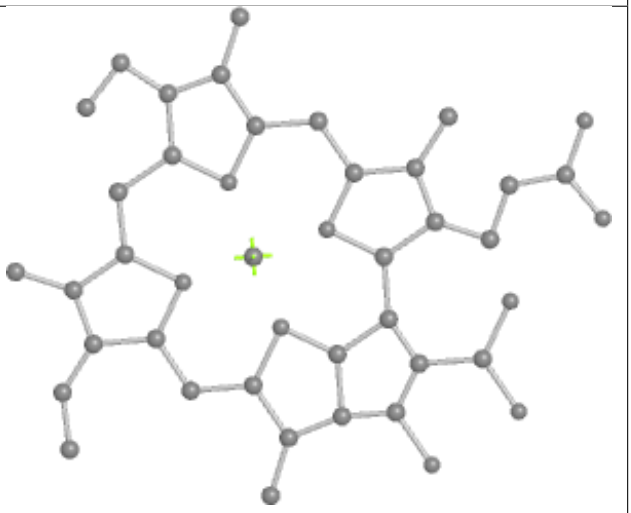
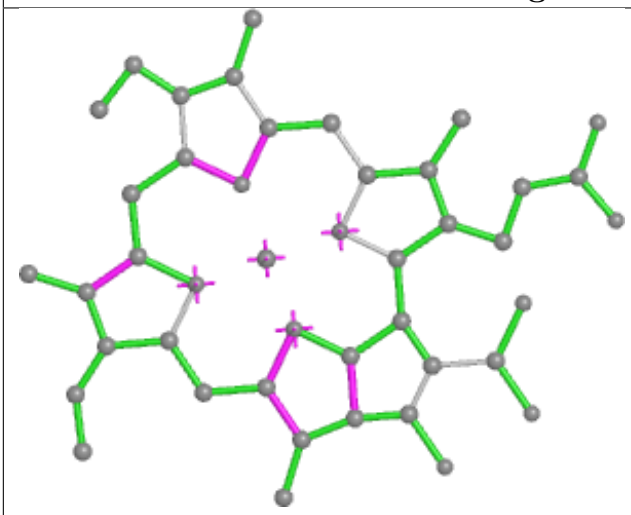
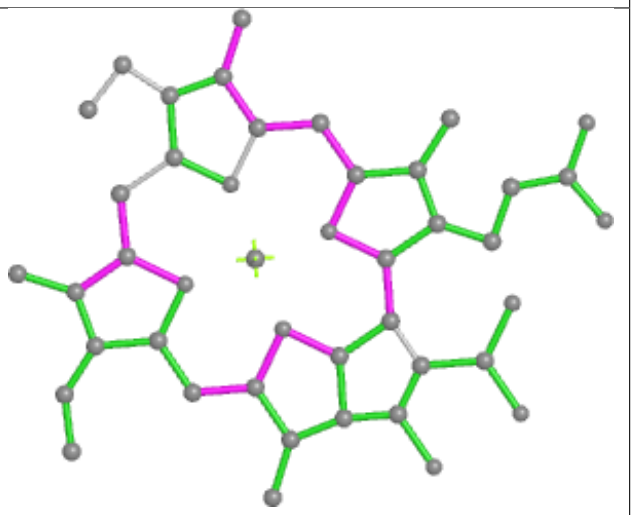


Rings

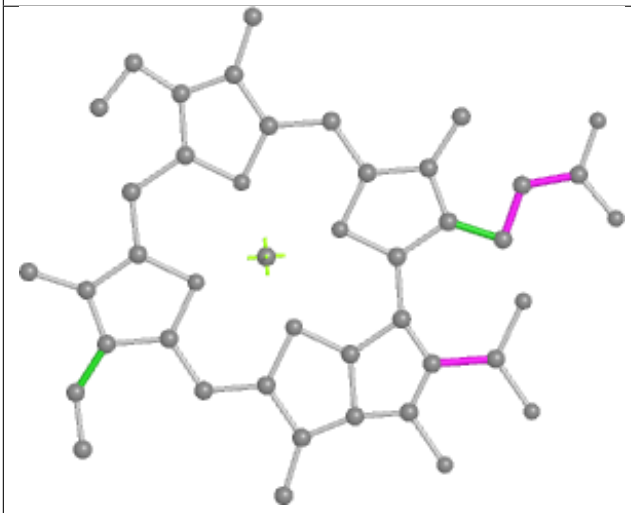
Ligand CLA 6 301



Bond lengths



Bond angles



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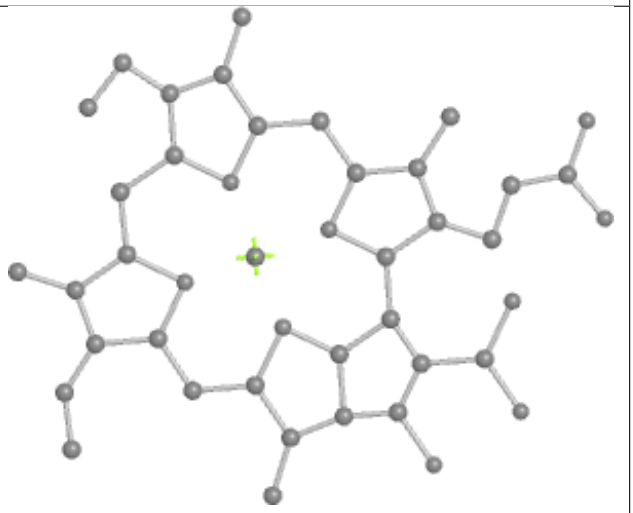
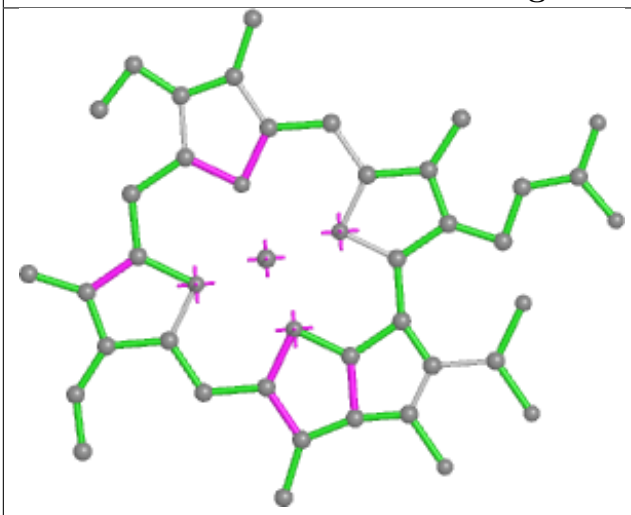
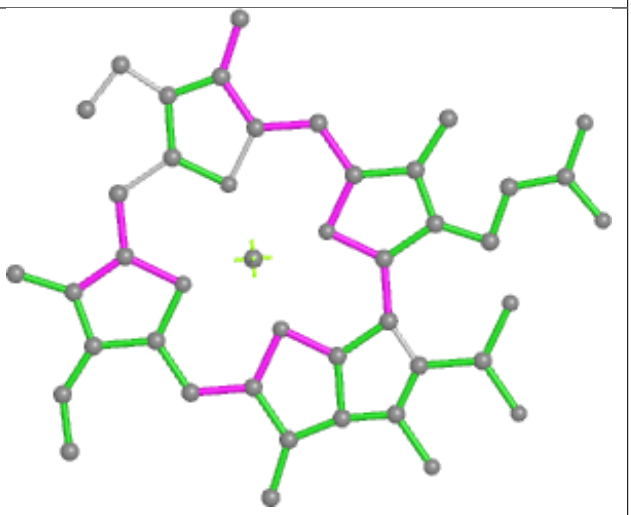


Rings

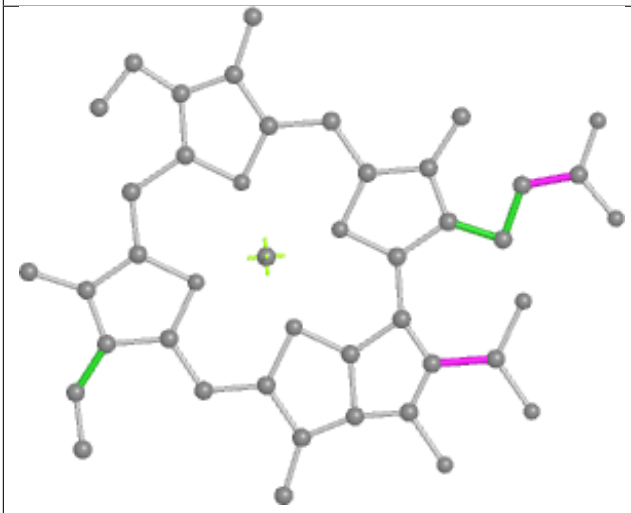
Ligand CLA 4 305



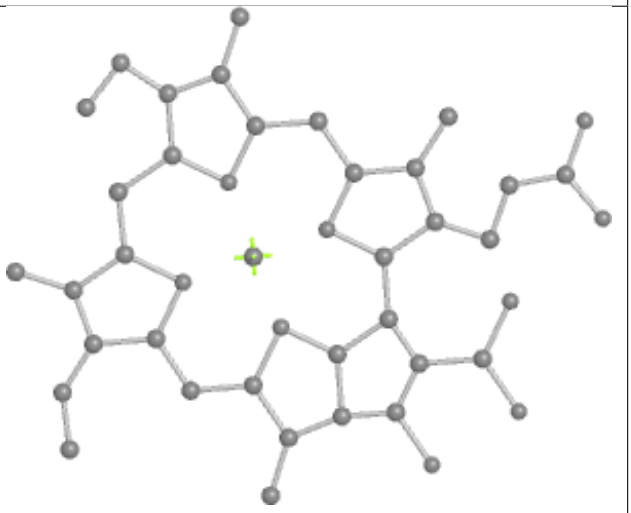
Bond lengths



Bond angles

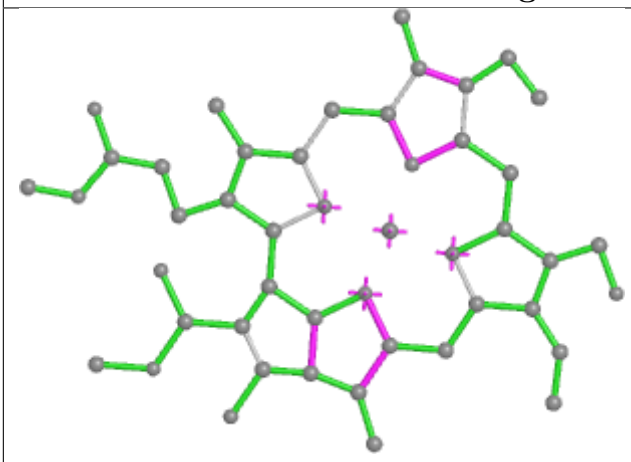


Torsions

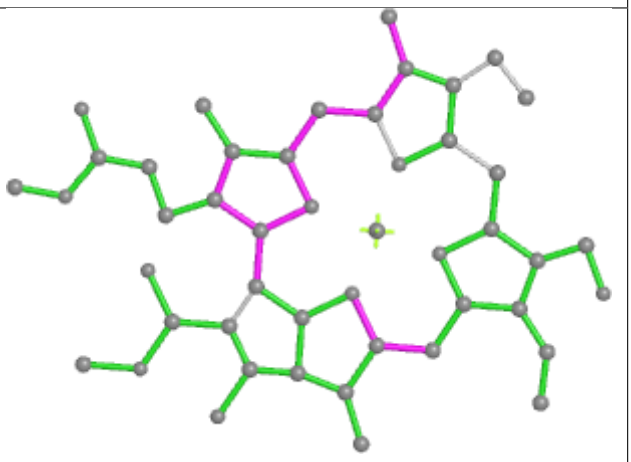


Rings

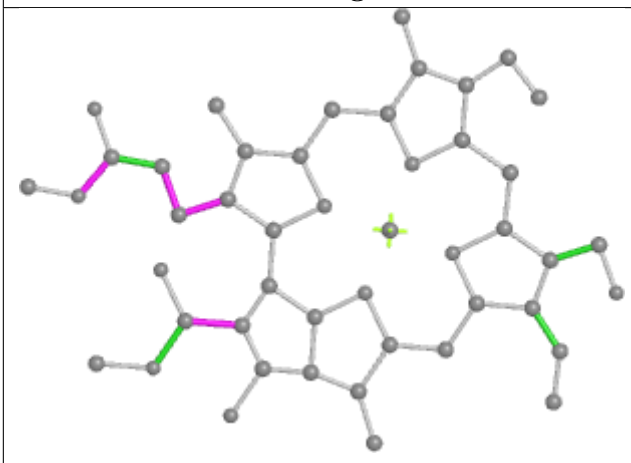
Ligand CHL 3 1014



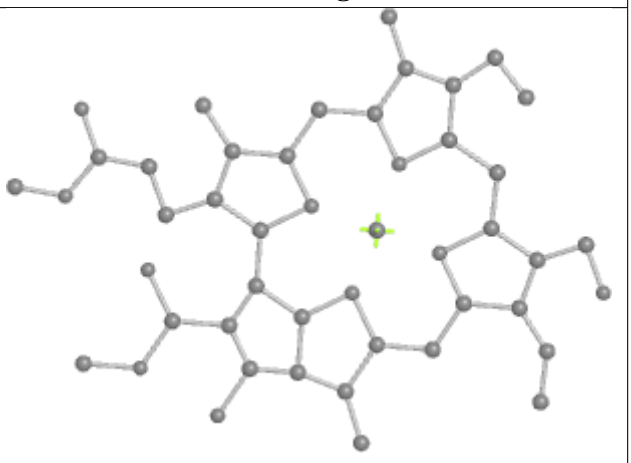
Bond lengths



Bond angles

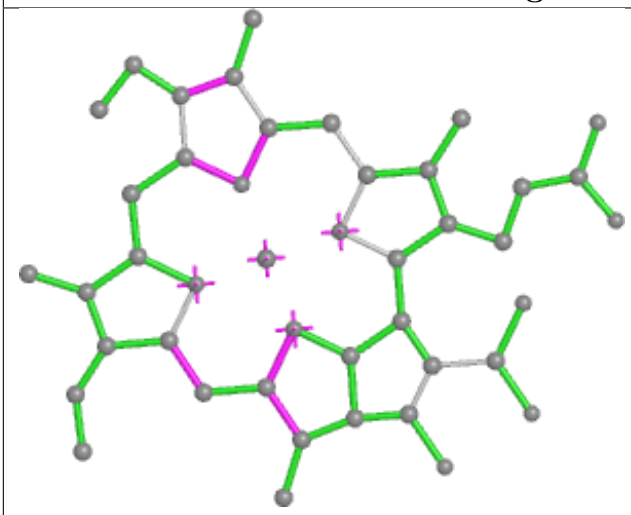


Torsions



Rings

Ligand CLA F 303



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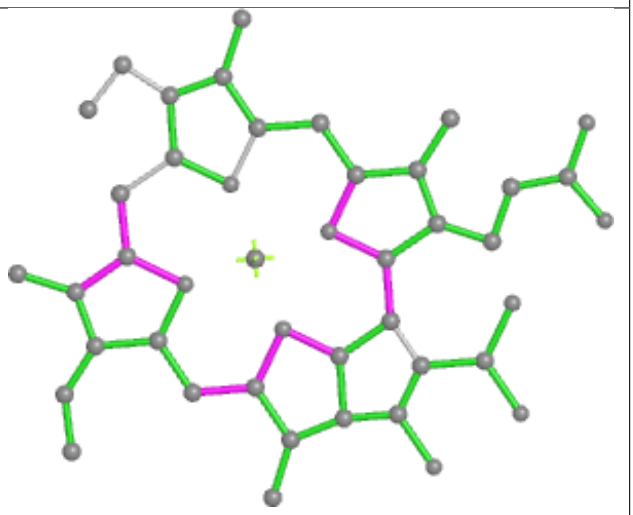
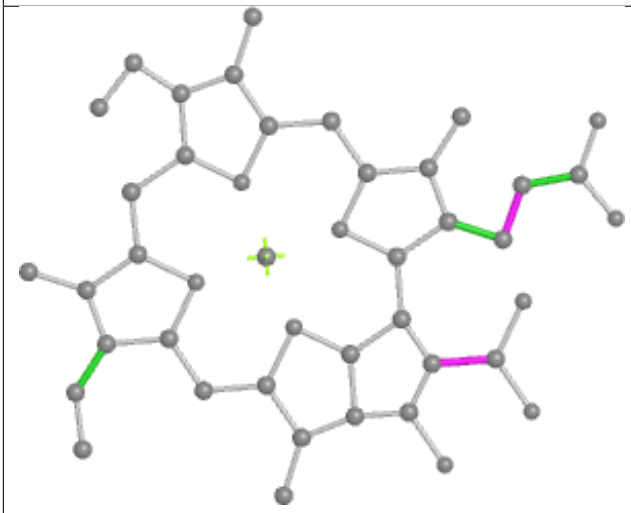


Bond angles



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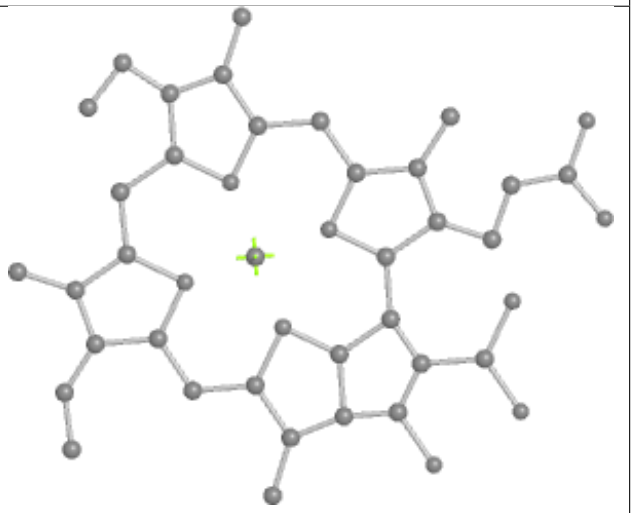
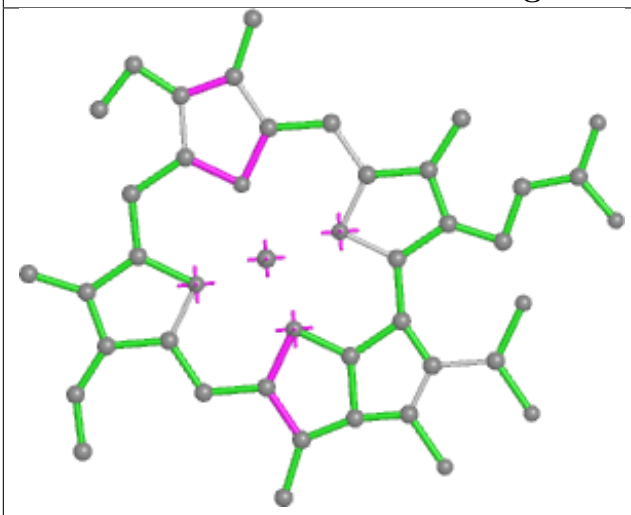


Rings

Ligand CLA A 824



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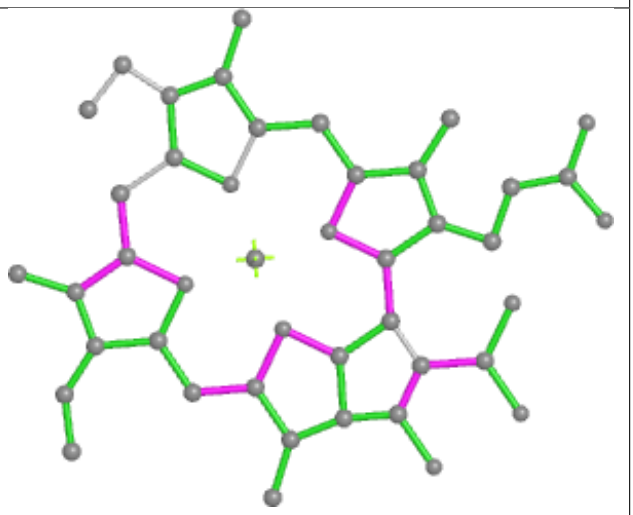
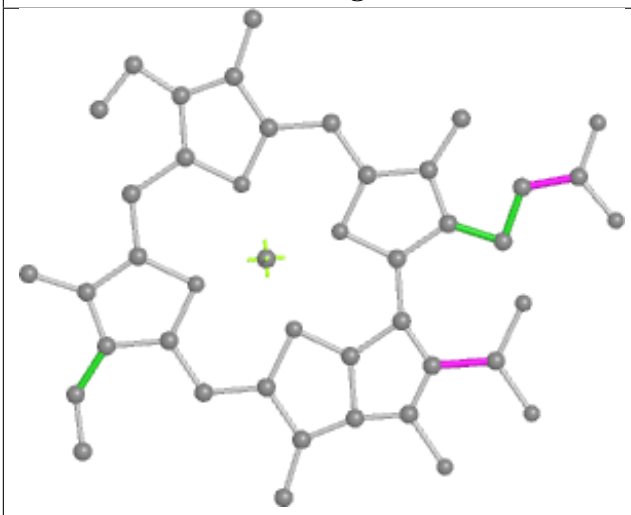


Bond angles



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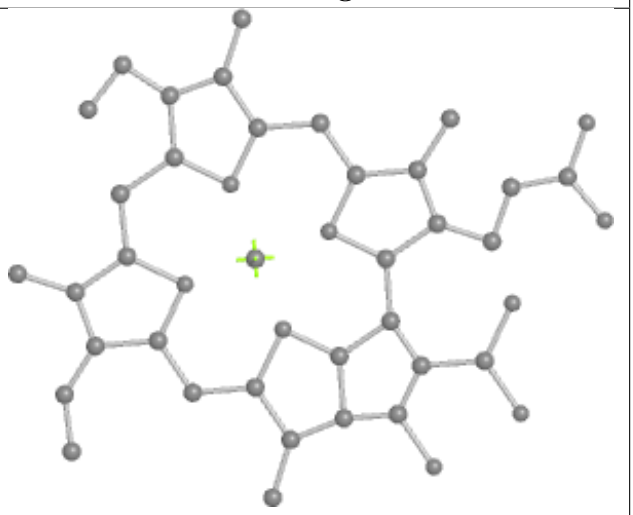
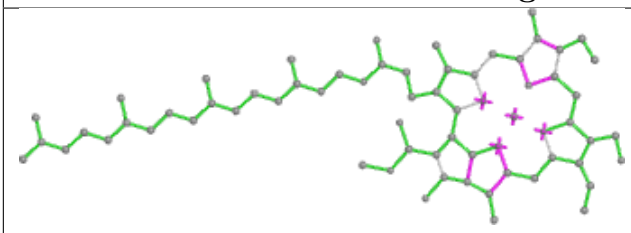


Rings

Ligand CHL 7 1017



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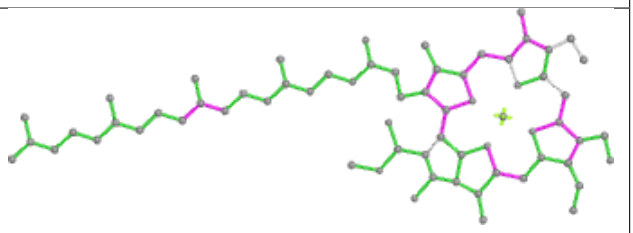
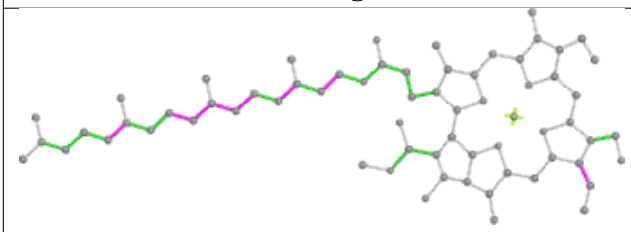


Bond angles



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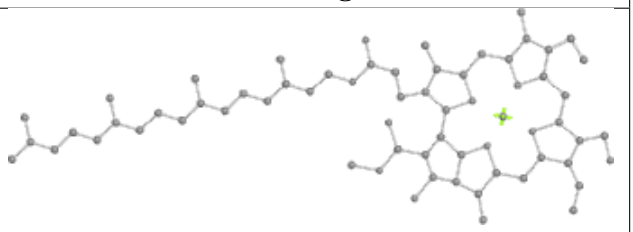
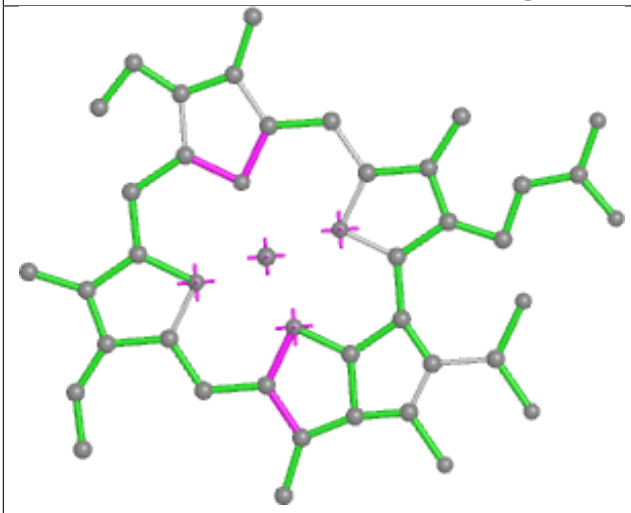
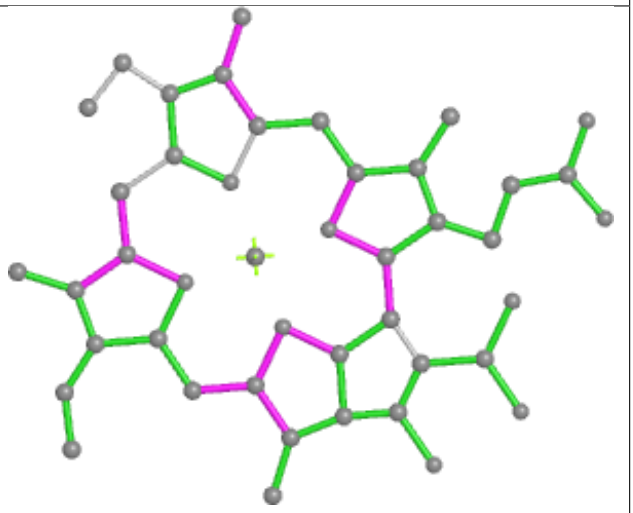


Rings

Ligand CLA 1 1014



Bond lengths



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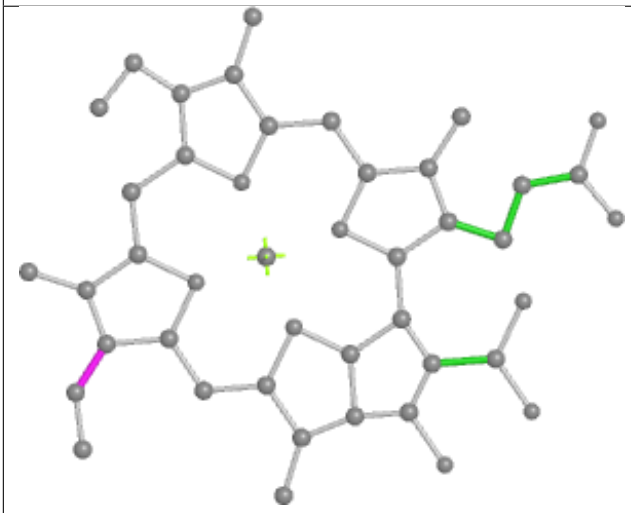

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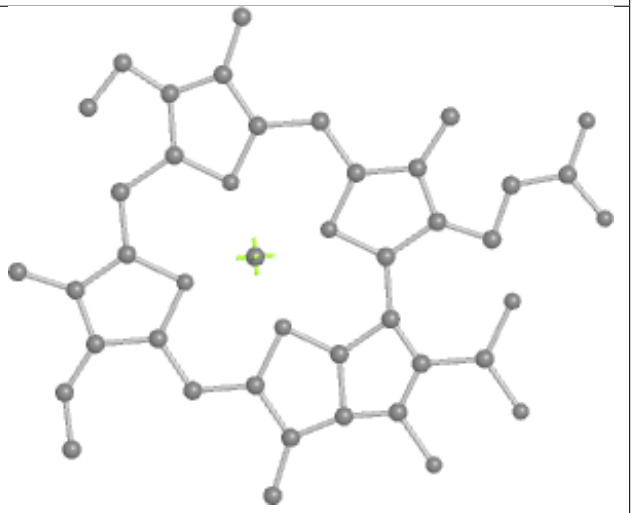
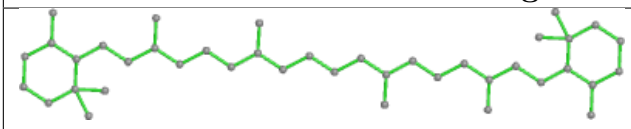


Rings

Ligand BCR G 204



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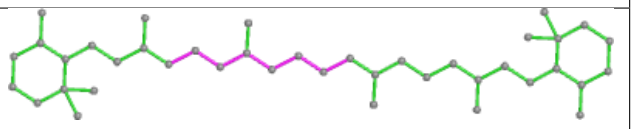

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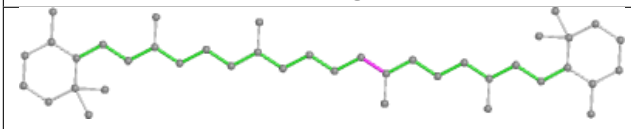
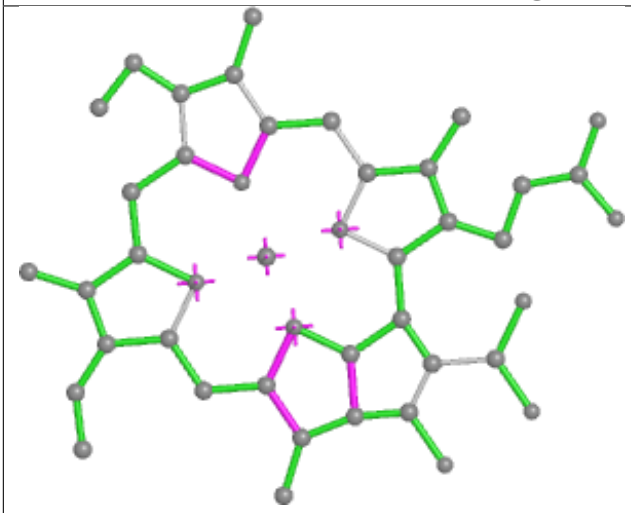


Torsions

Rings

Ligand CLA 5 312



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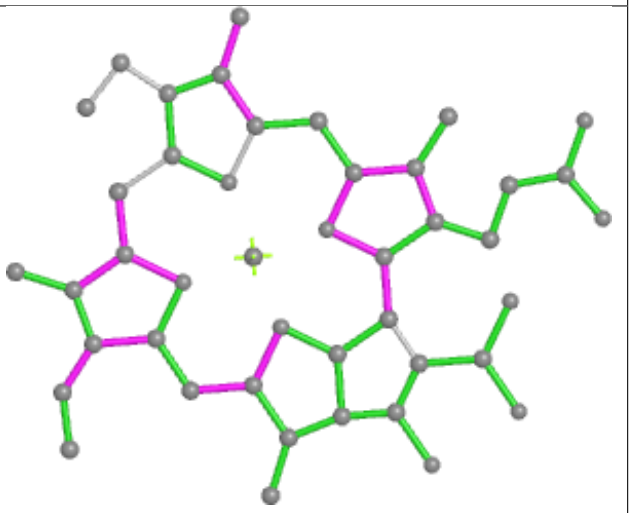

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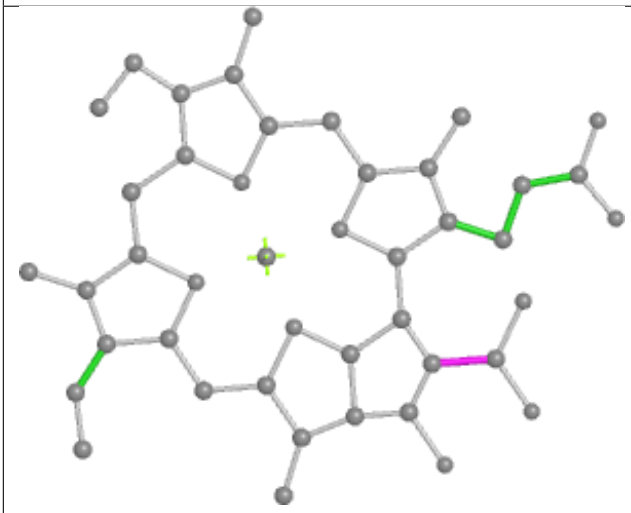

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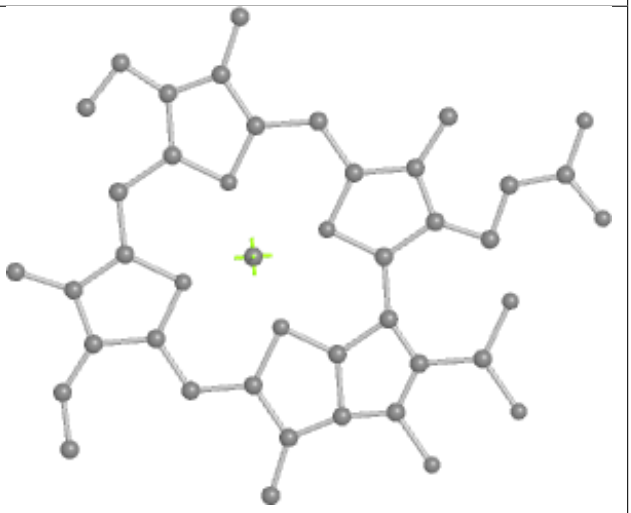
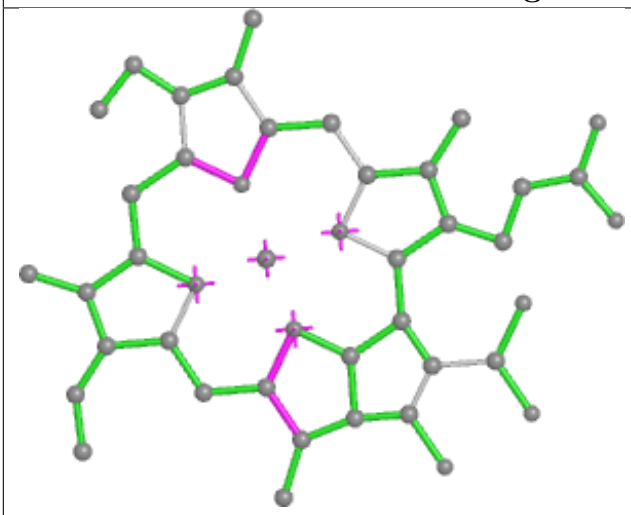


Rings

Ligand CLA A 852



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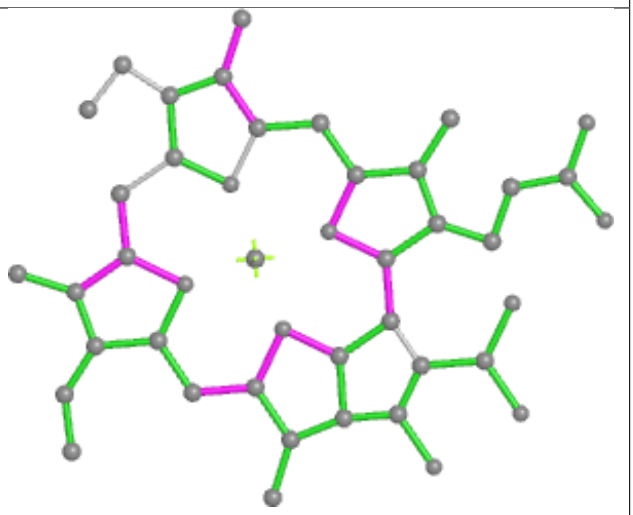

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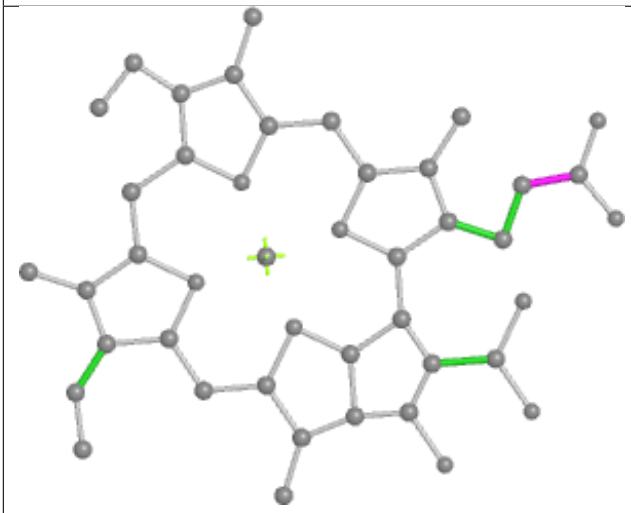

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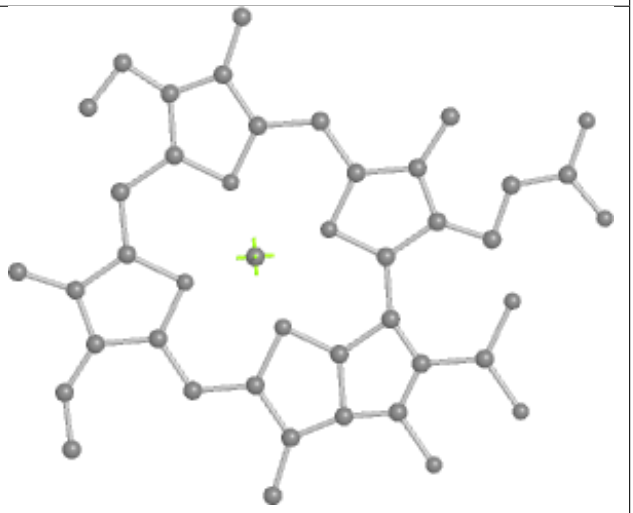
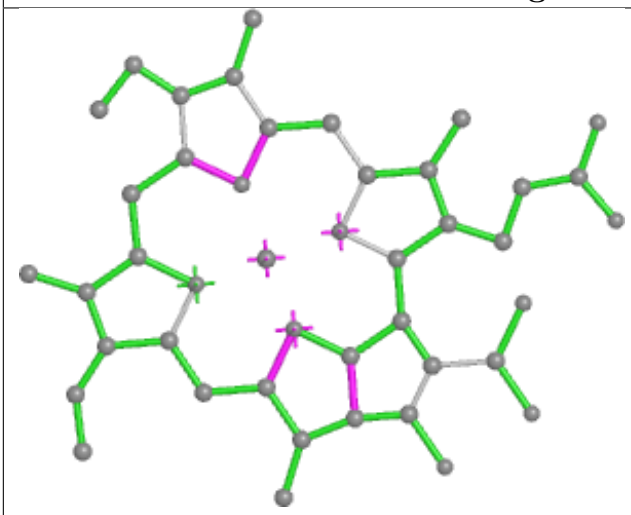


Rings

Ligand CLA 8 311



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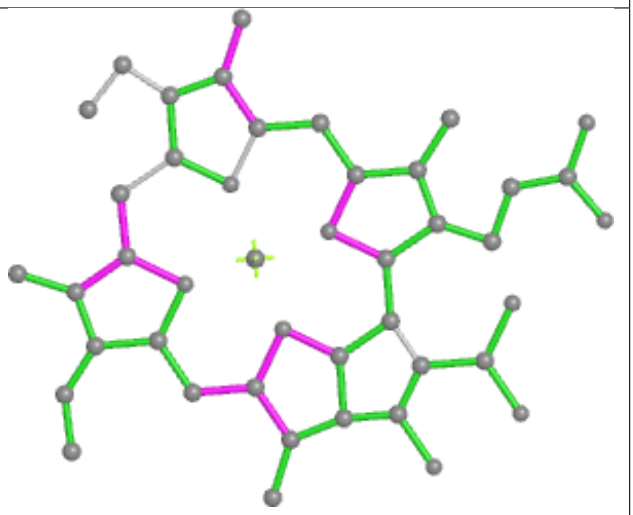
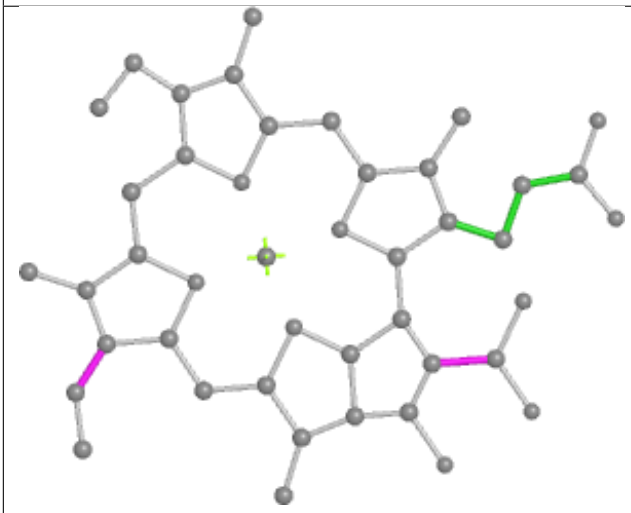


Bond angles



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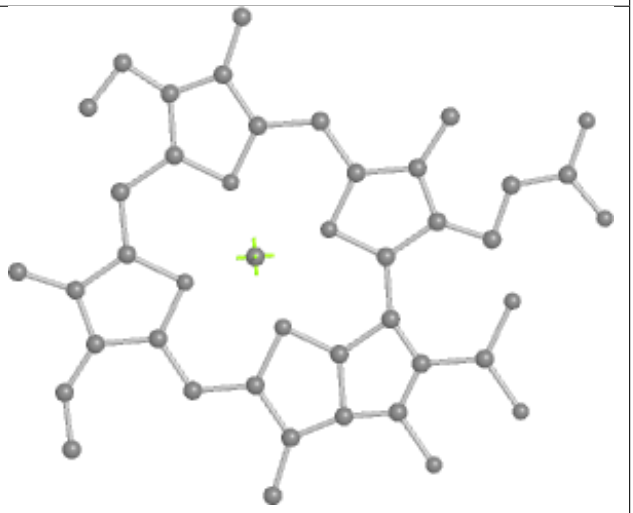
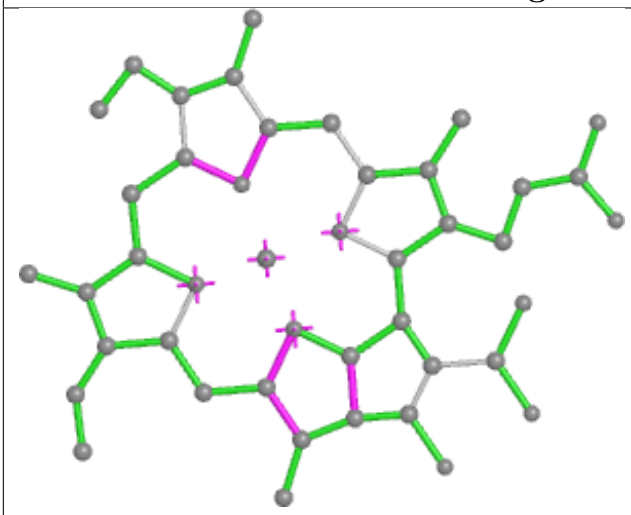
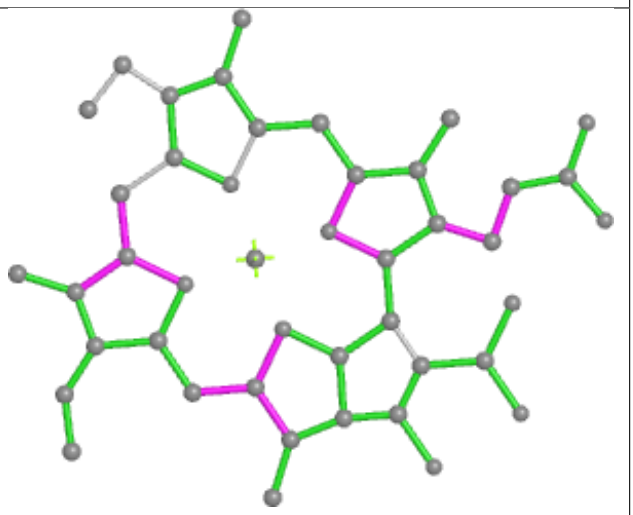


Rings

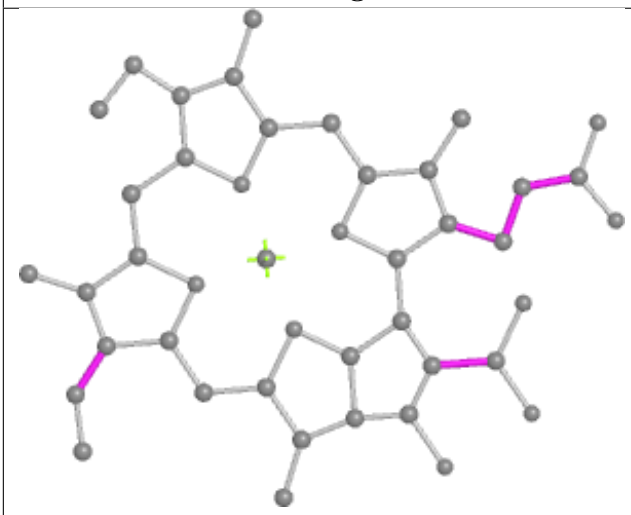
Ligand CLA 4 309



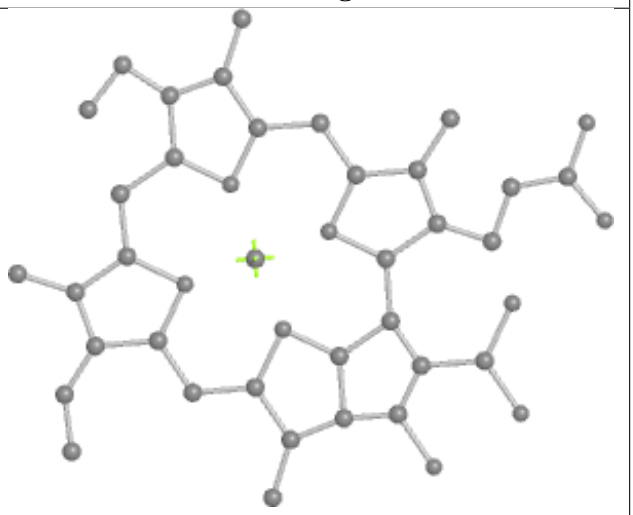
Bond lengths



Bond angles

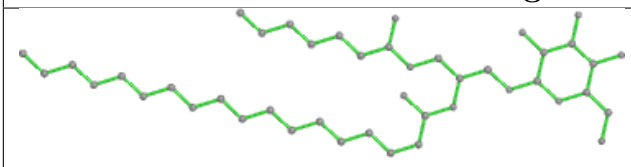


Torsions



Rings

Ligand LMG 8 319



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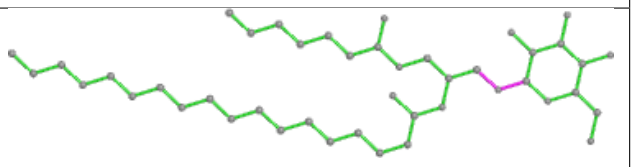

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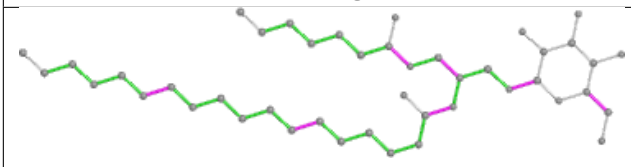

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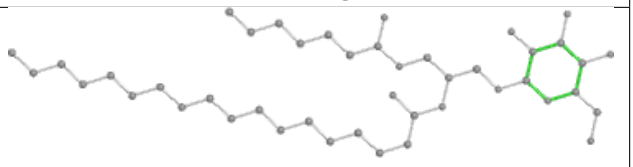
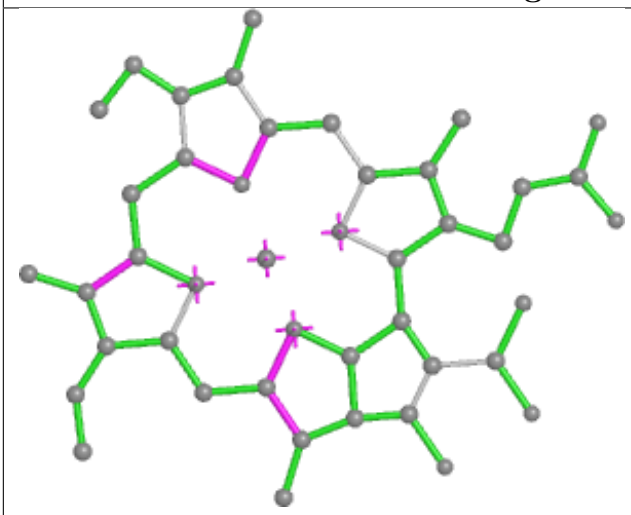


Rings

Ligand CLA B 806



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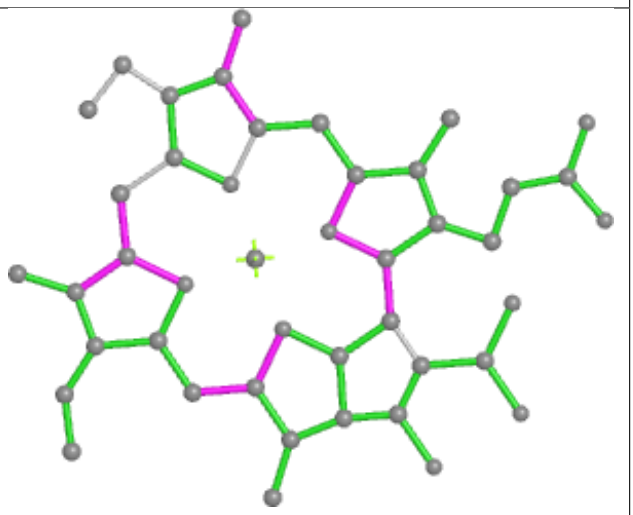
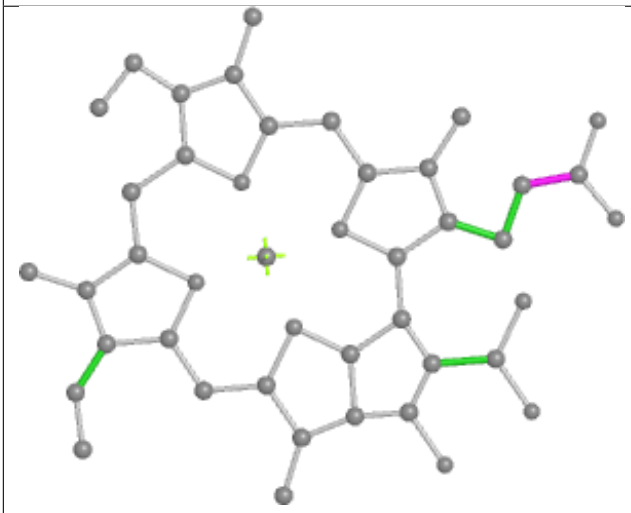


Bond angles



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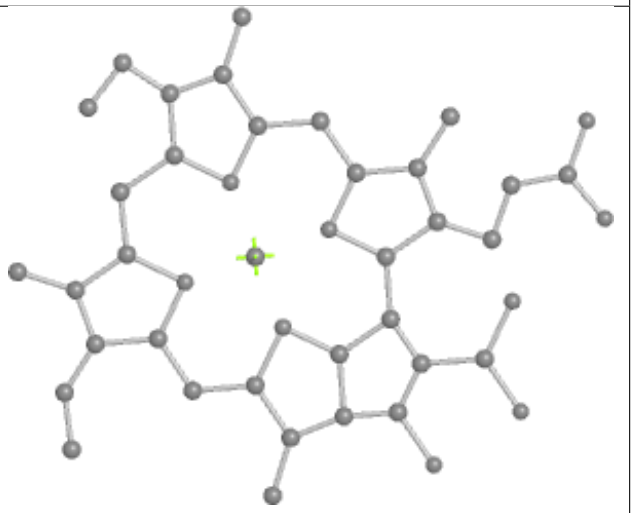
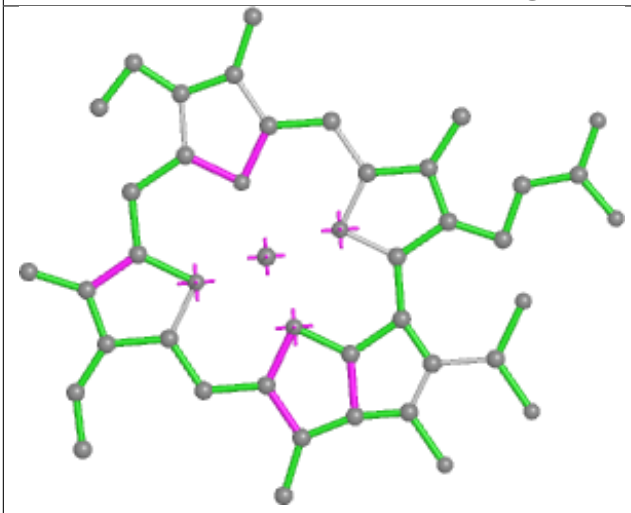


Rings

Ligand CLA A 807



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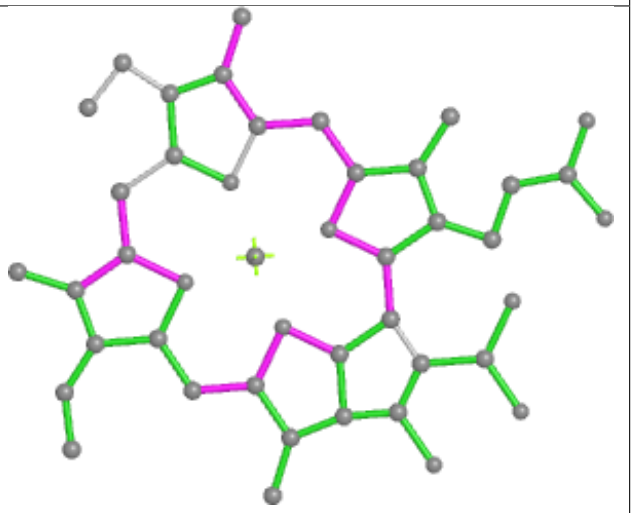
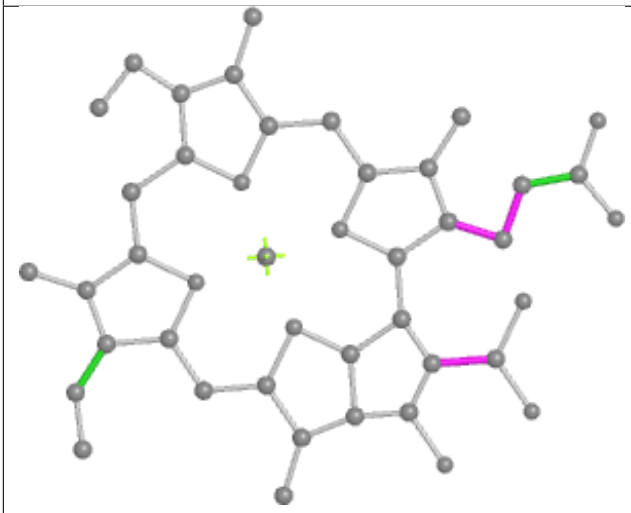


Bond angles



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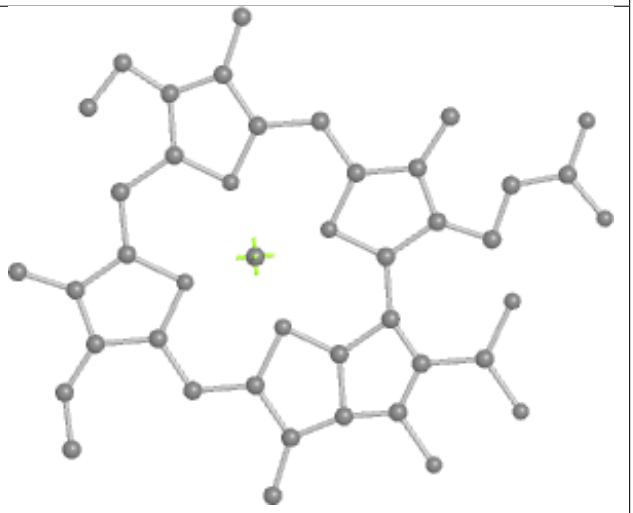
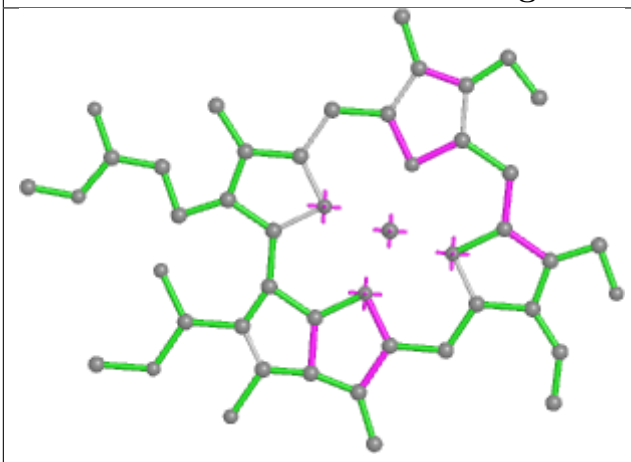


Rings

Ligand CHL 1 1012



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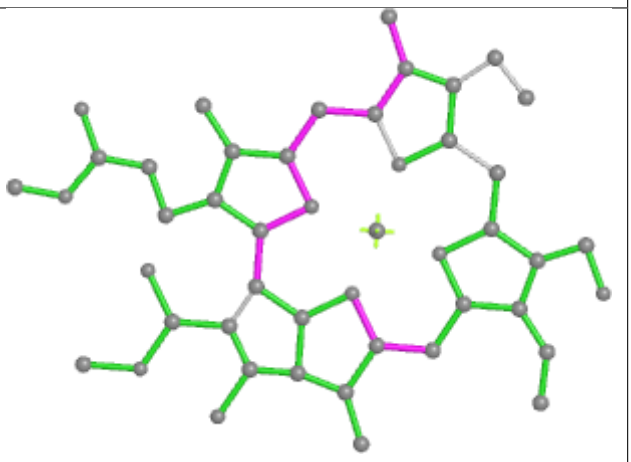
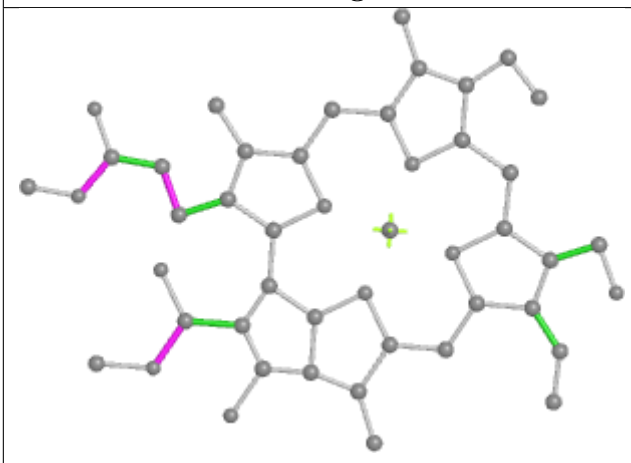
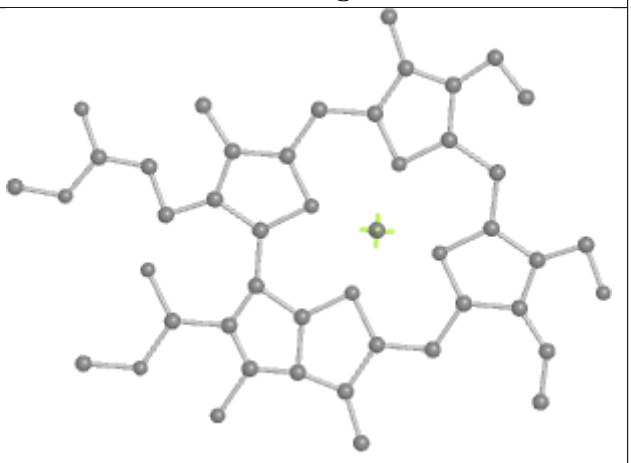


Bond angles

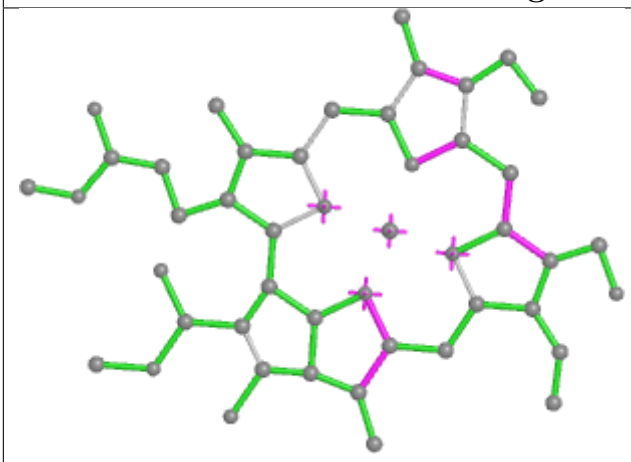


Torsions



Rings

Ligand CHL 8 314



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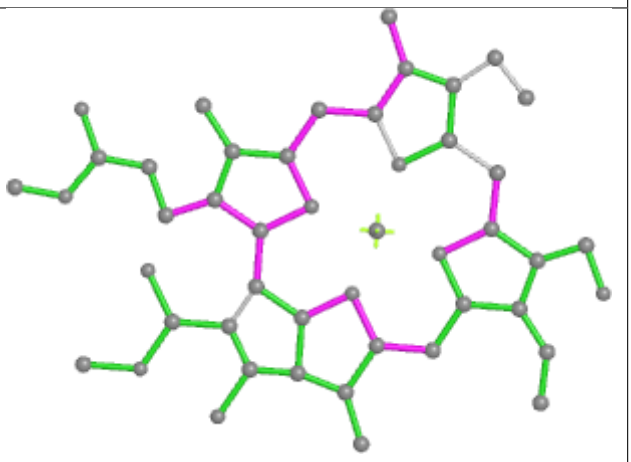
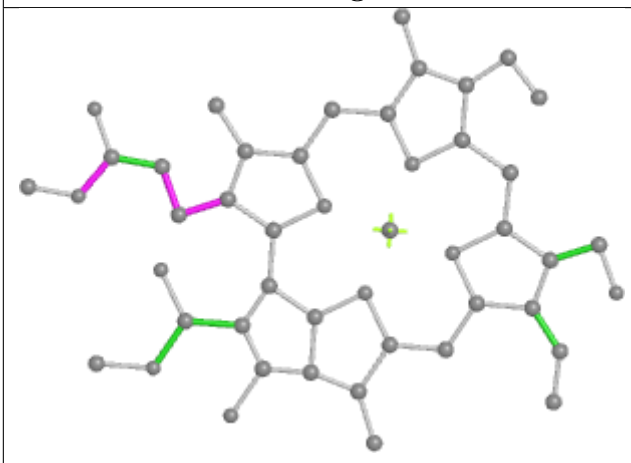
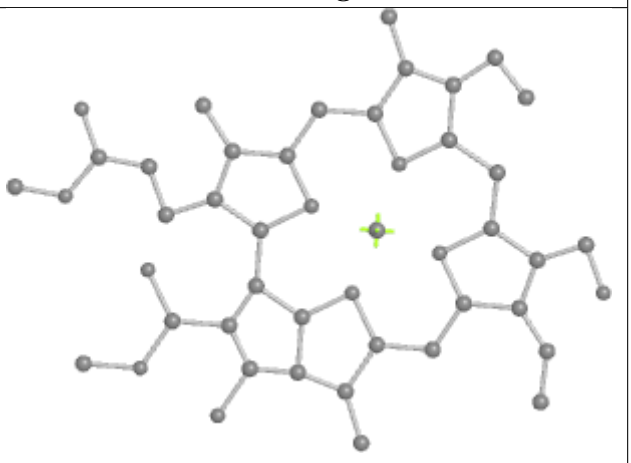


Bond angles

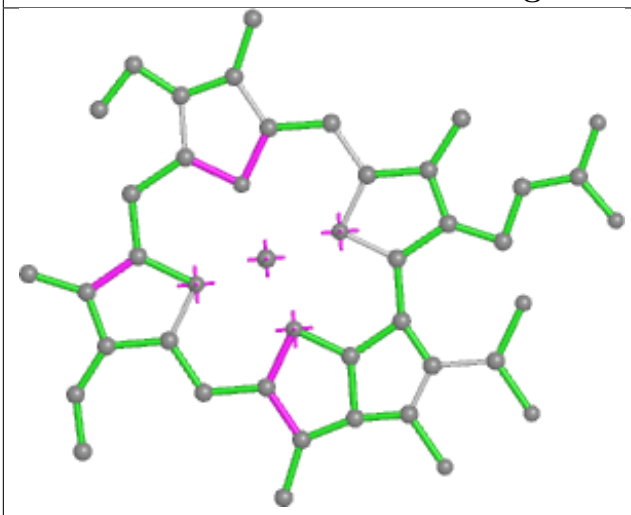


Torsions

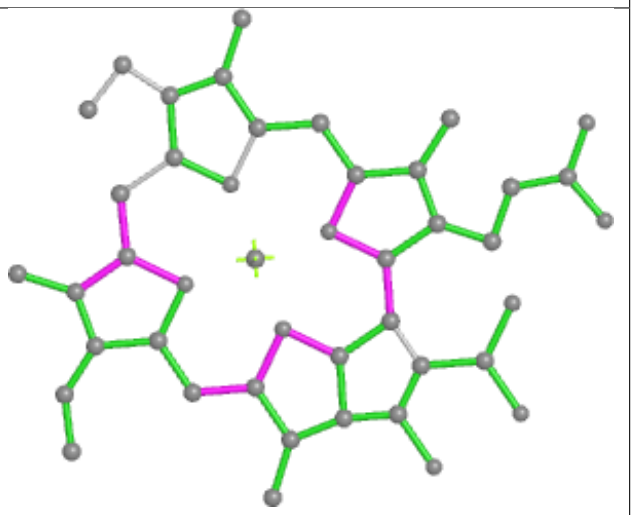


Rings

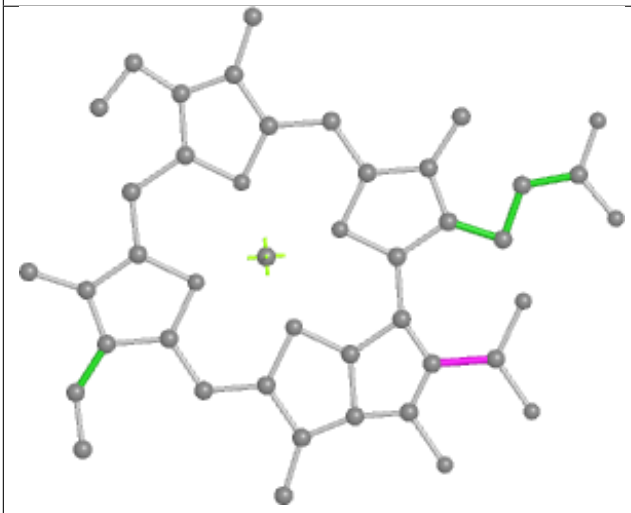
Ligand CLA A 834



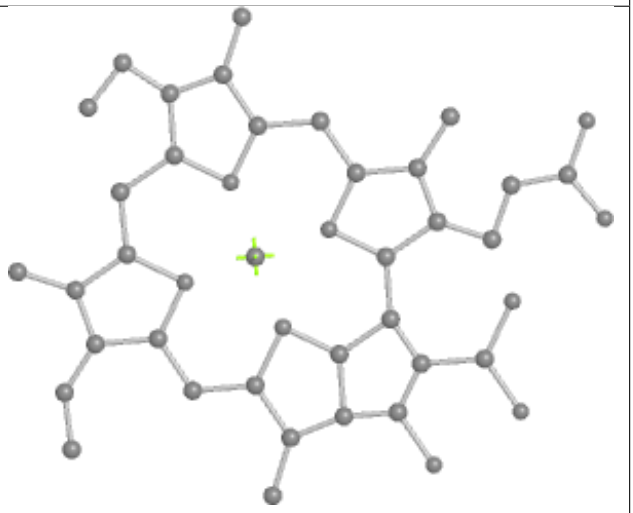
Bond lengths



Bond angles

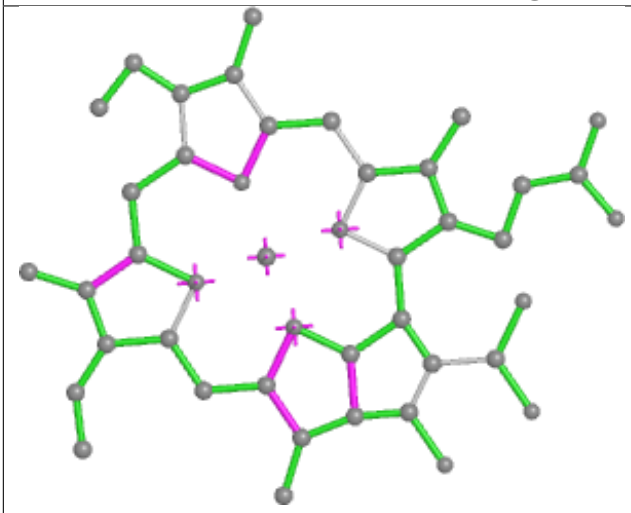


Torsions



Rings

Ligand CLA F 302



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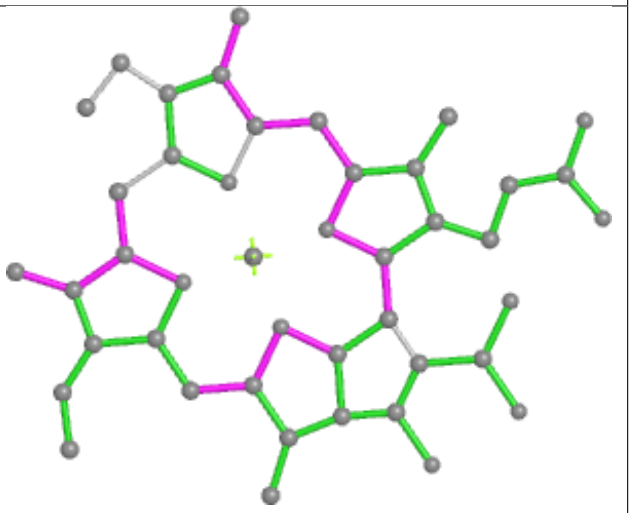

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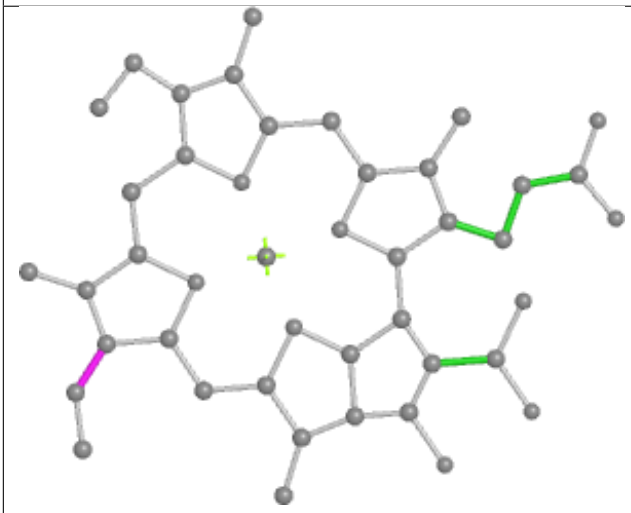

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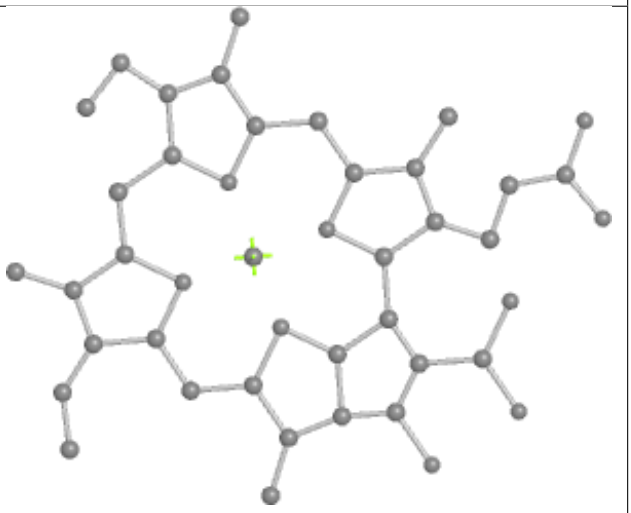
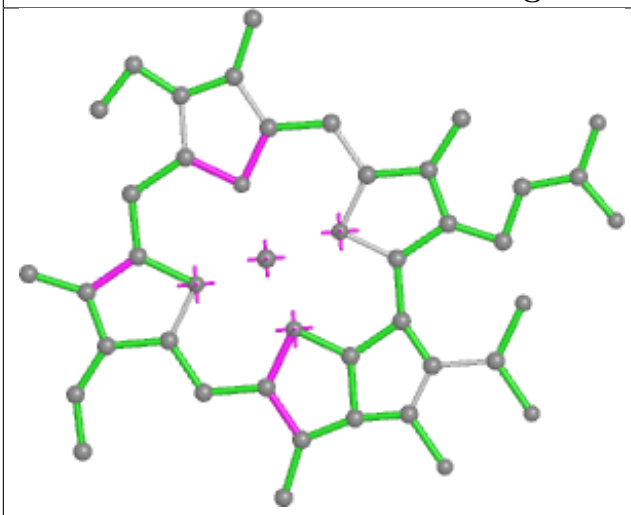


Rings

Ligand CLA A 816



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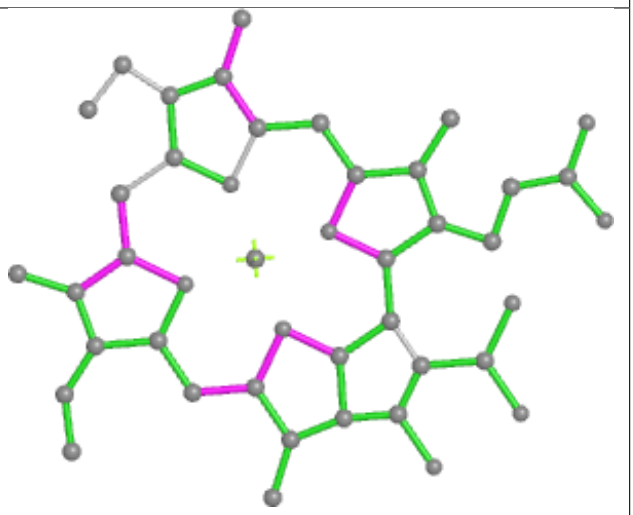

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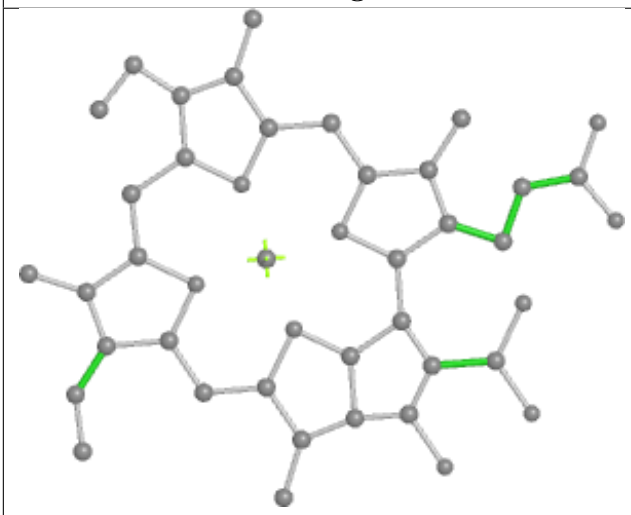

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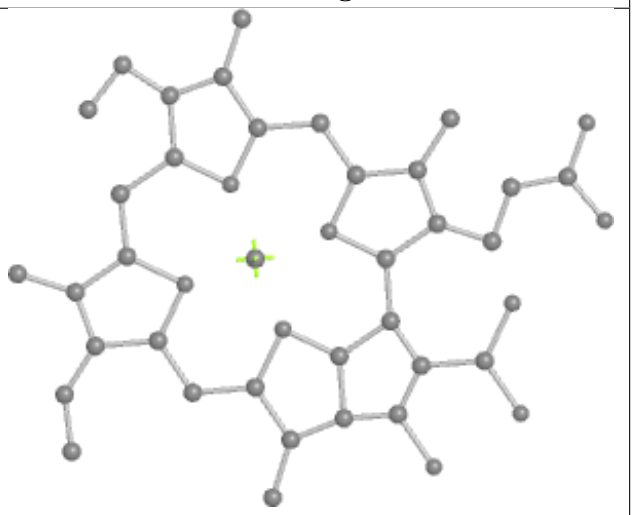
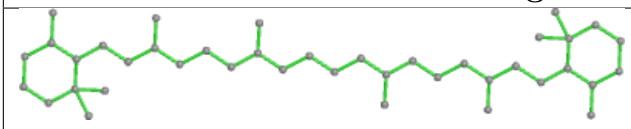


Rings

Ligand BCR 8 302



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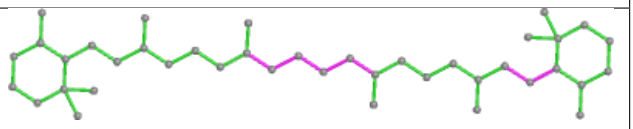
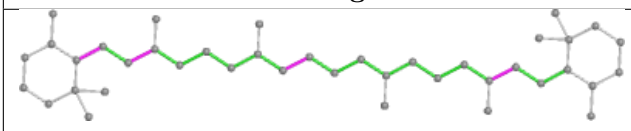


Bond angles



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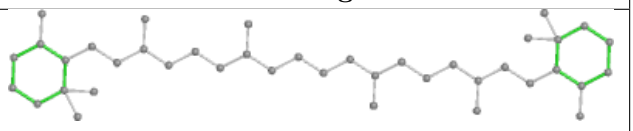
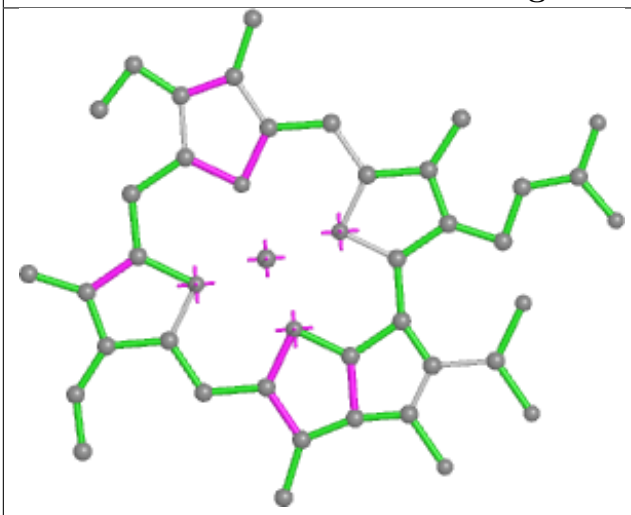


Rings

Ligand CLA 5 308



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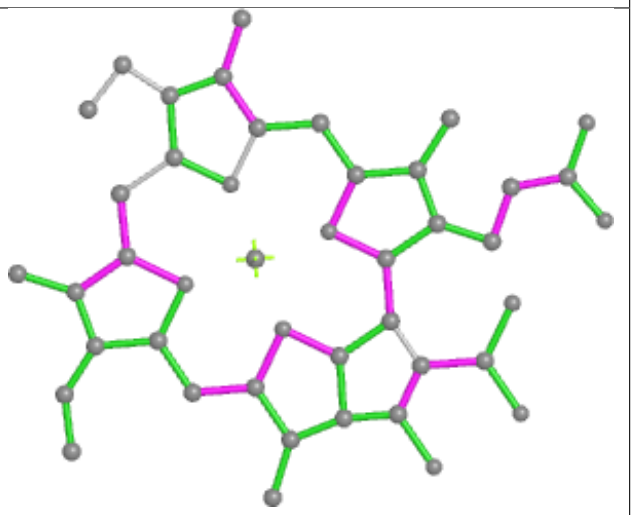

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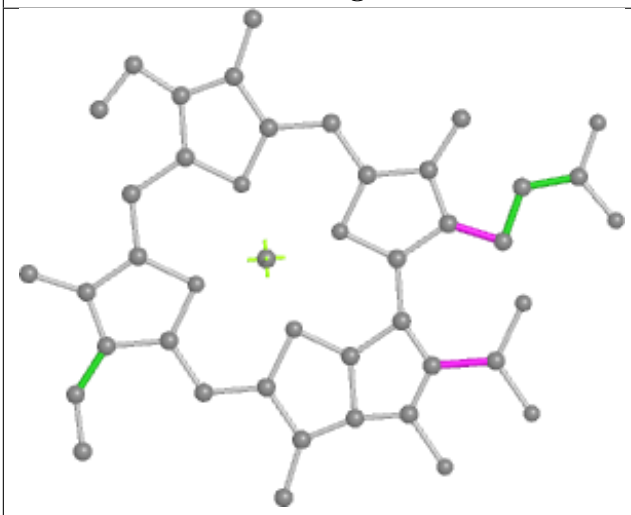

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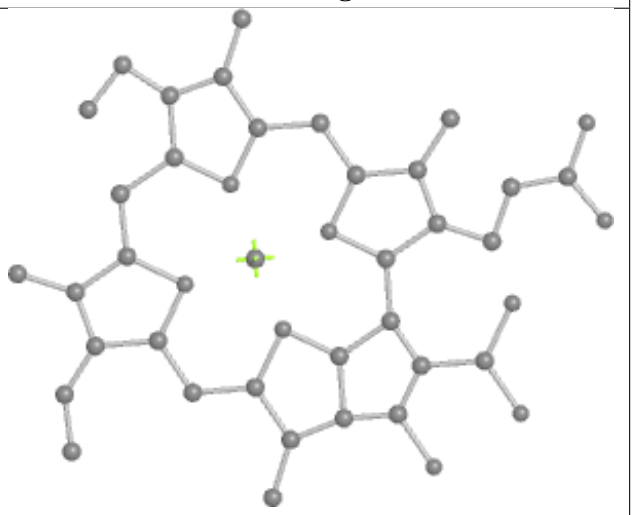
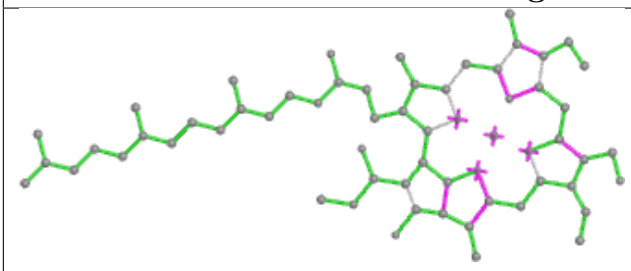


Rings

Ligand CHL 8 317



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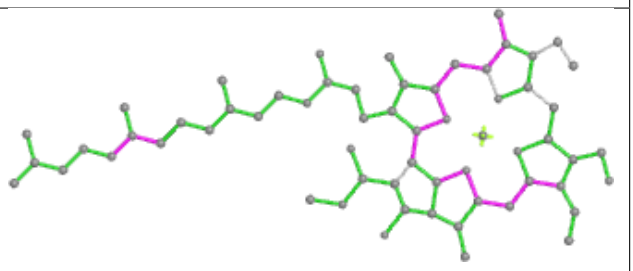
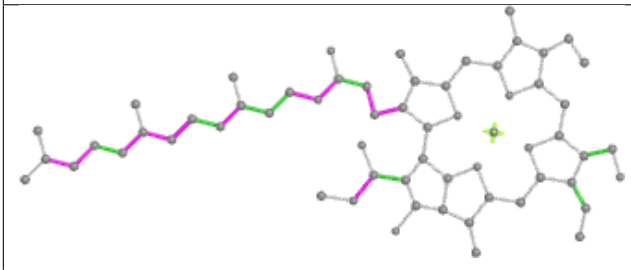


Bond angles



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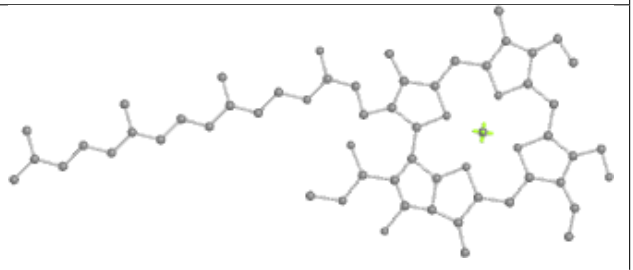
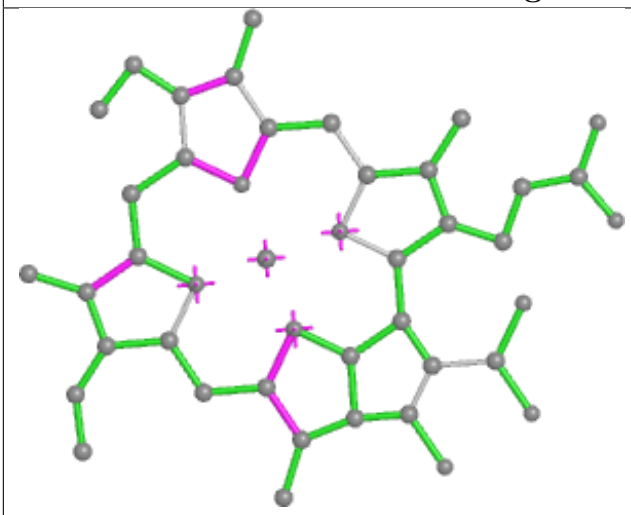


Rings

Ligand CLA B 810



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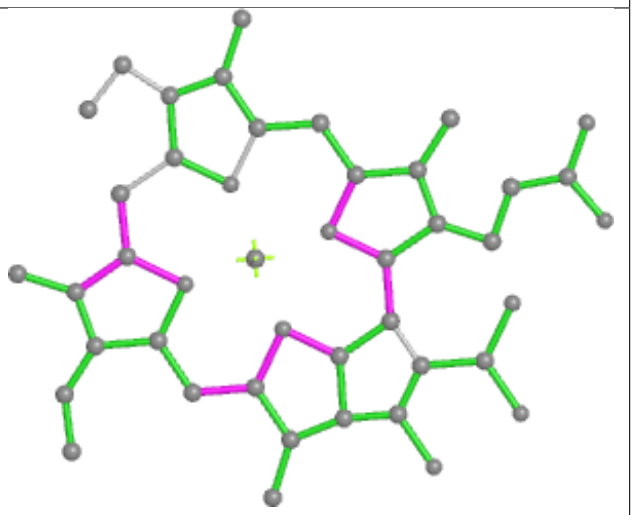
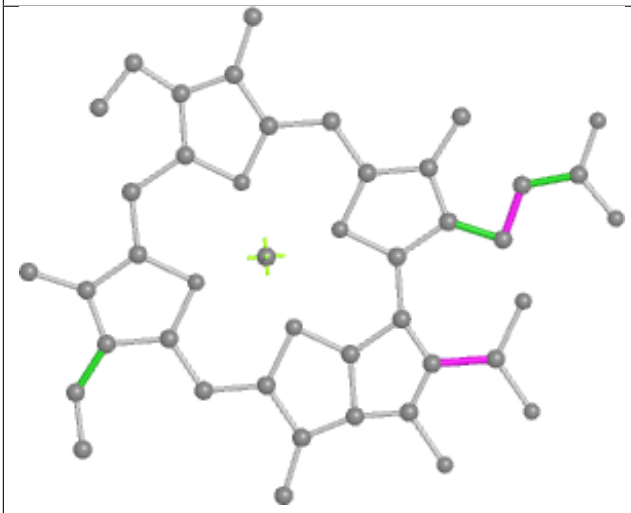


Bond angles



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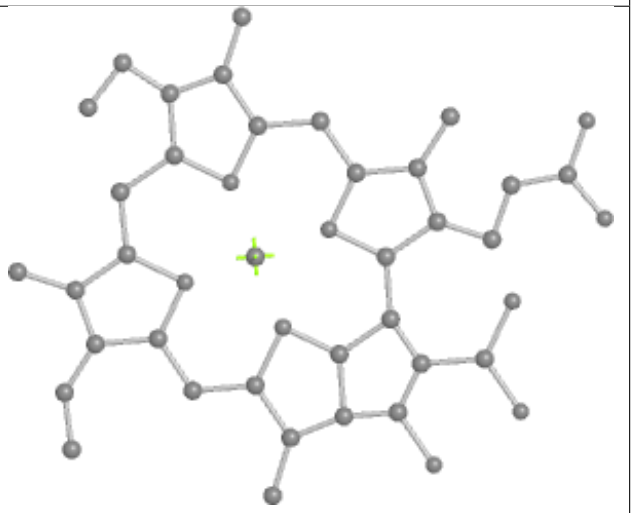
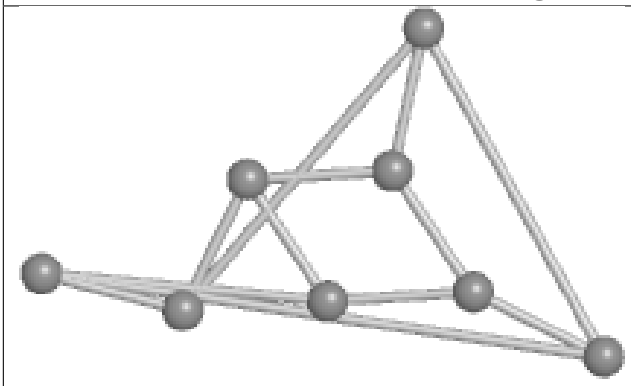


Rings

Ligand SF4 A 841



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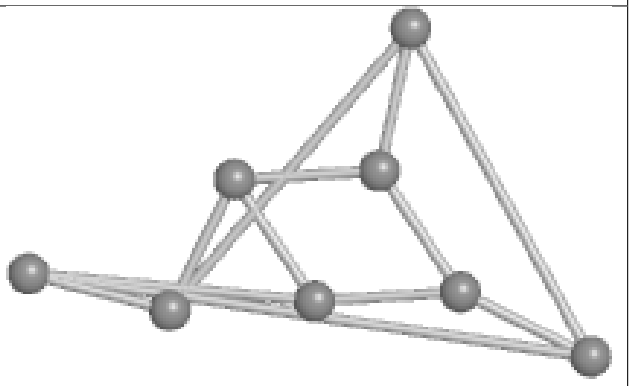

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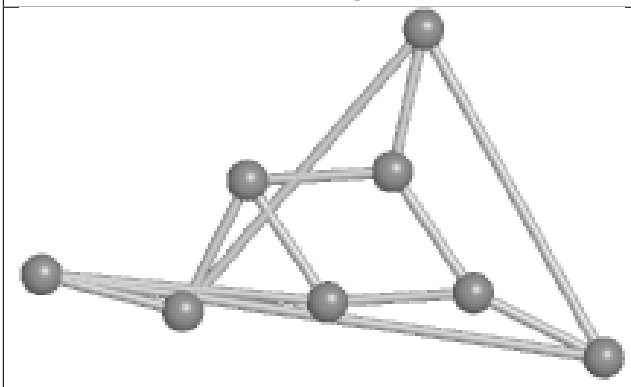

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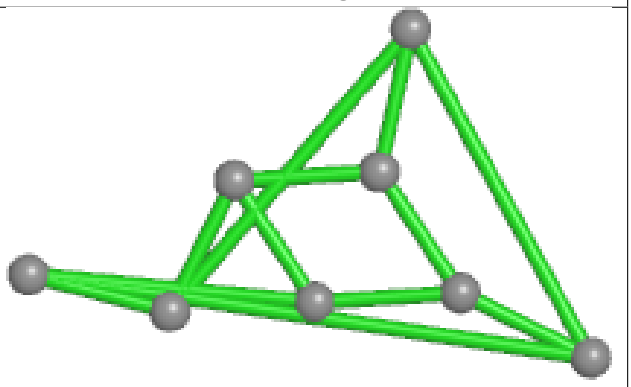
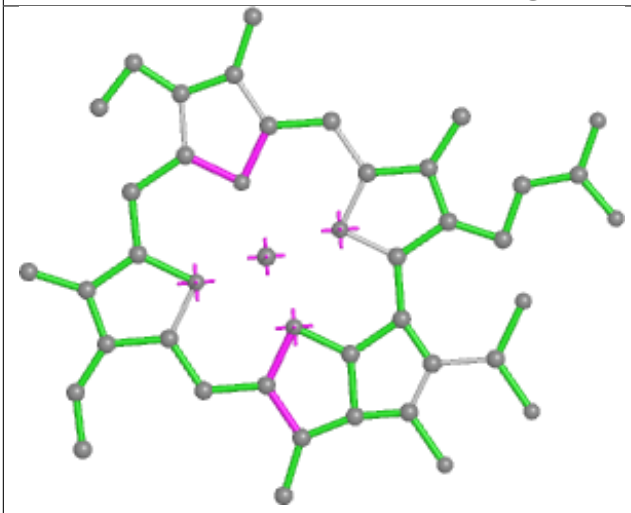


Rings

Ligand CLA B 808



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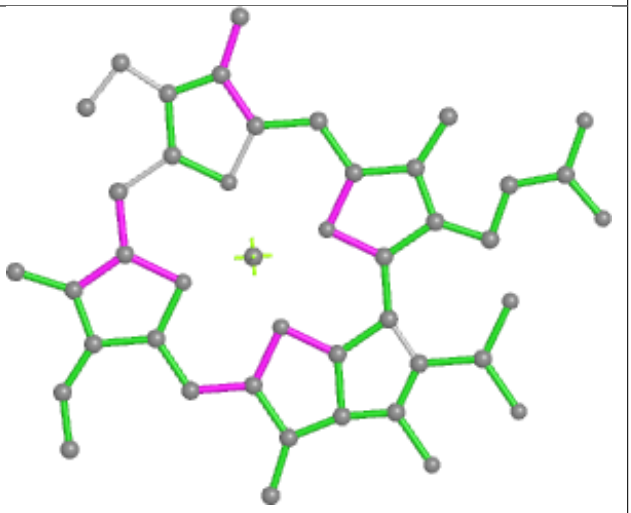

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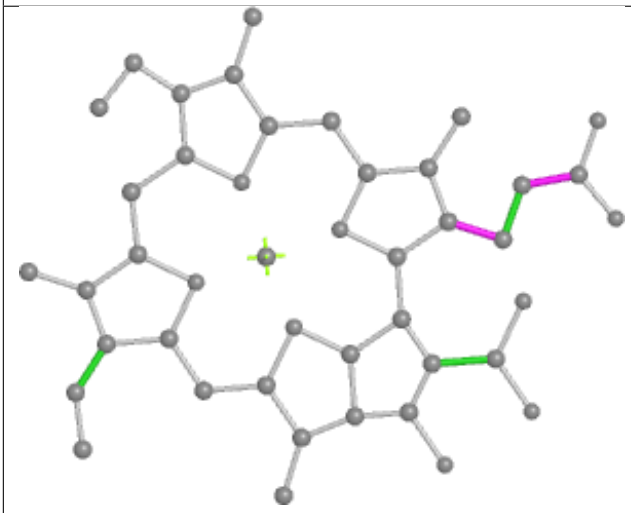

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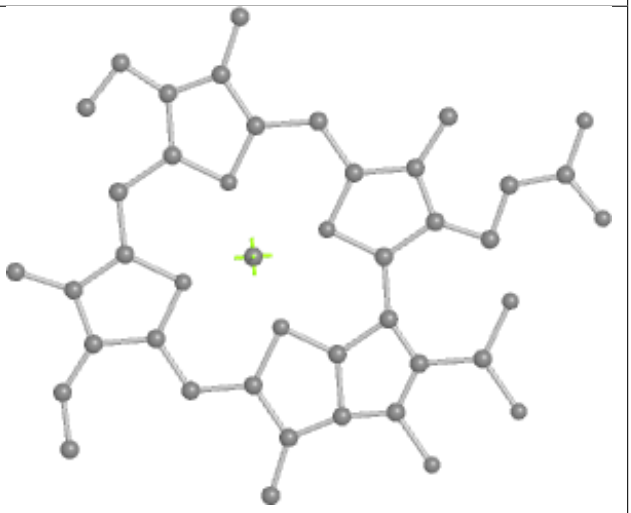
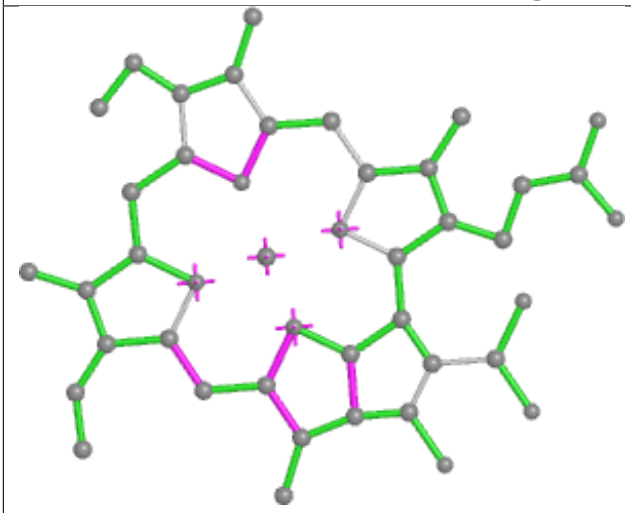


Rings

Ligand CLA 5 310



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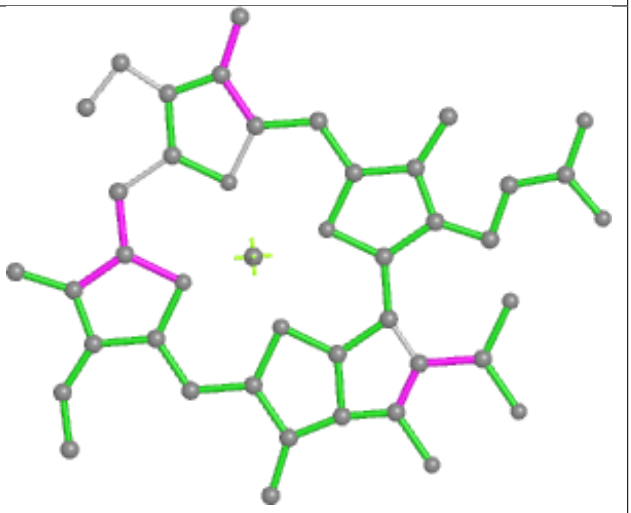
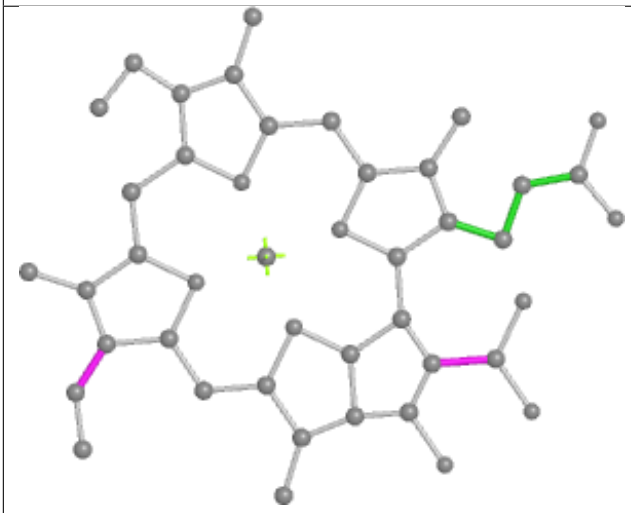


Bond angles



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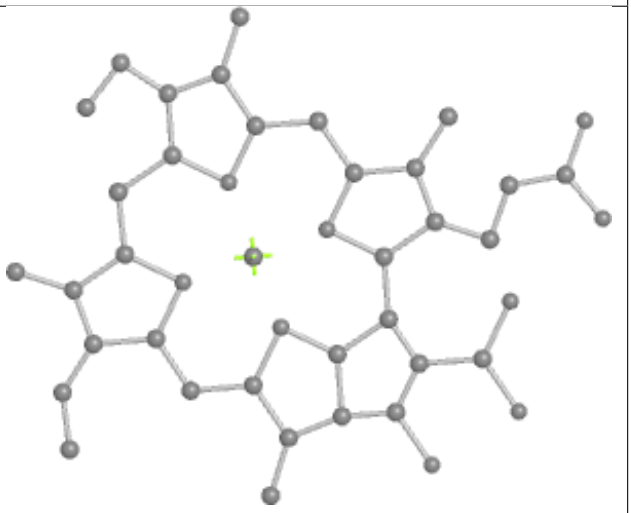
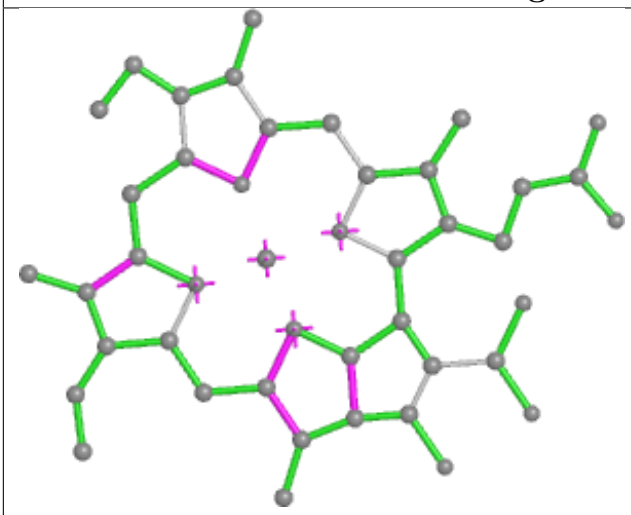


Rings

Ligand CLA 5 307



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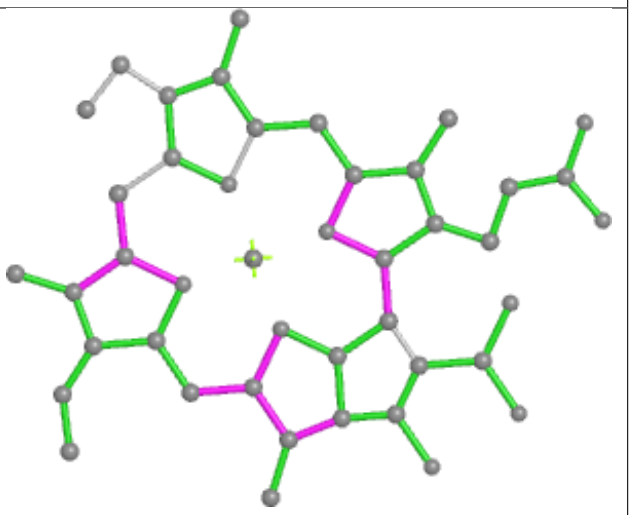
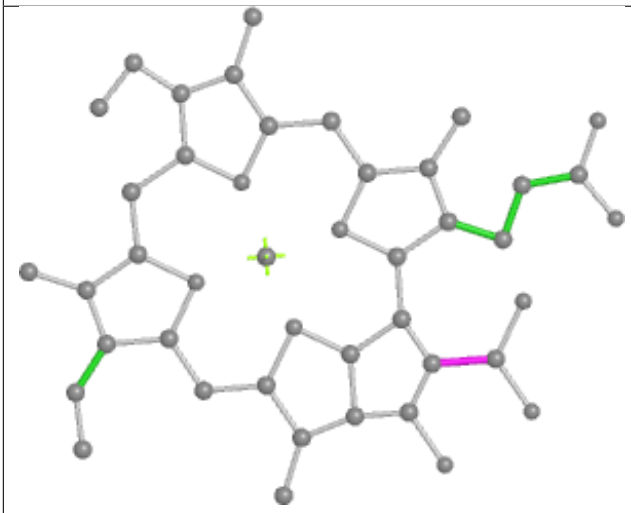


Bond angles



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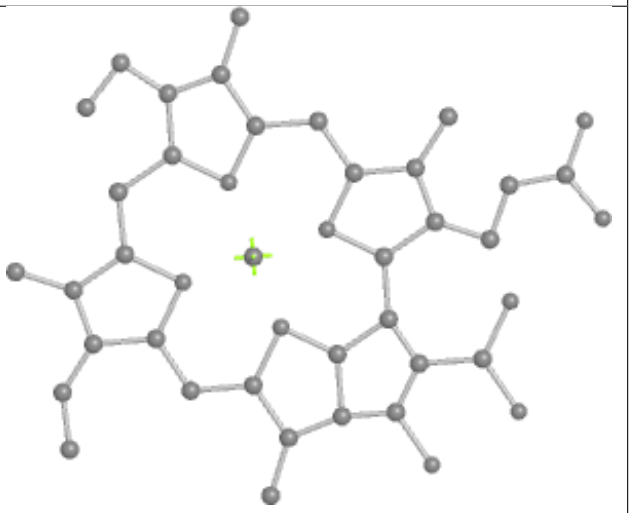
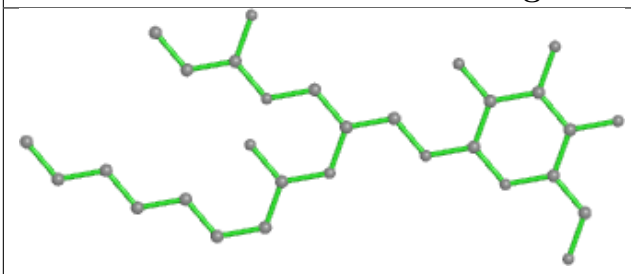


Rings

Ligand LMG J 101



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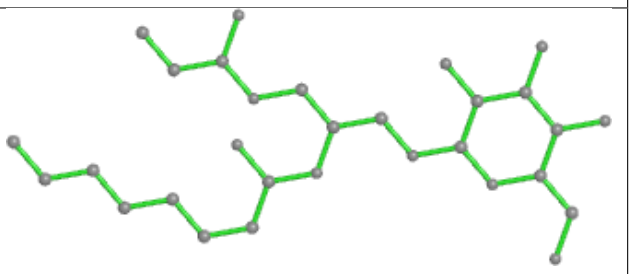
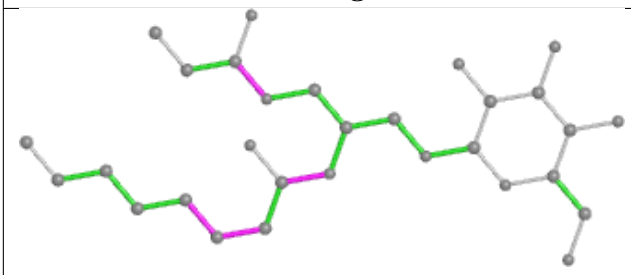


Bond angles



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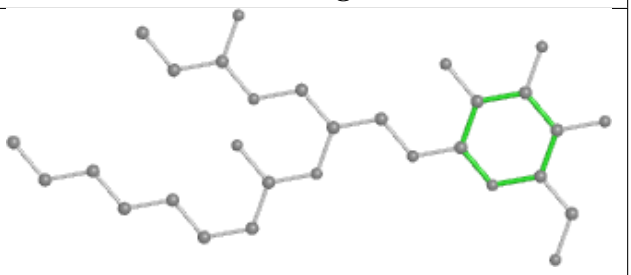
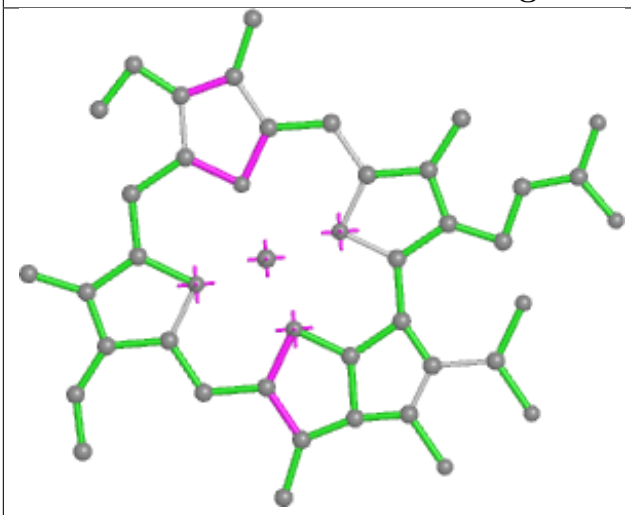


Rings

Ligand CLA 1 1011



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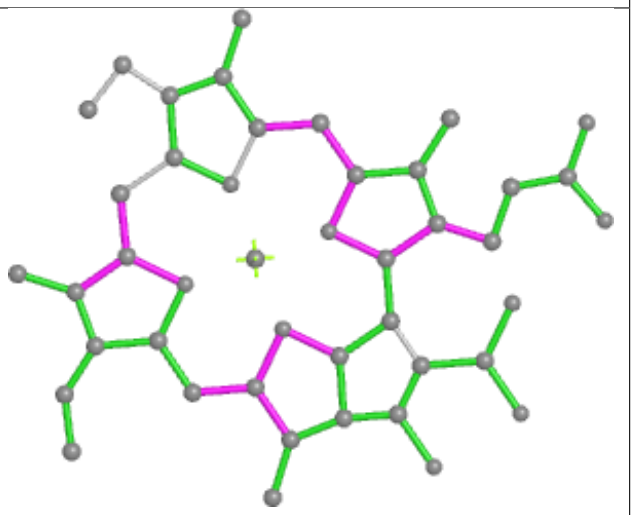
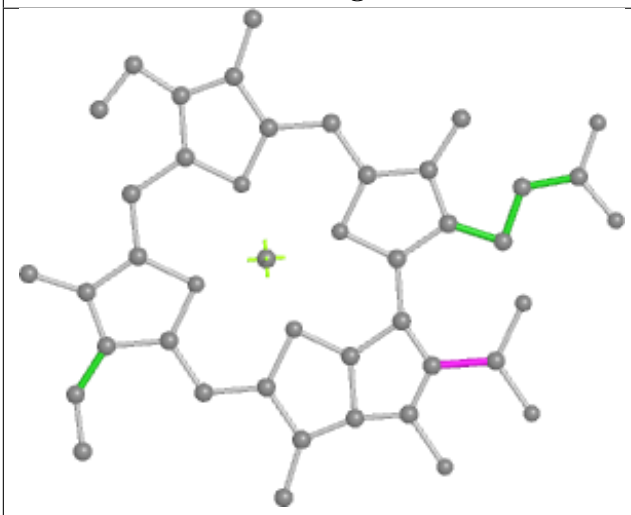


Bond angles



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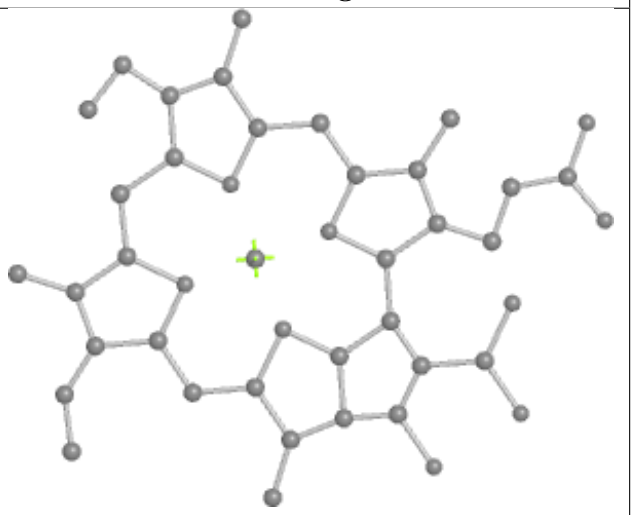
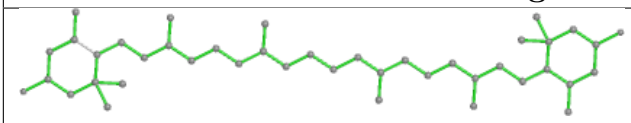


Rings

Ligand LUT 5 302



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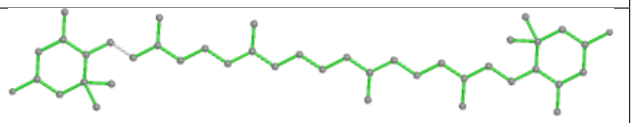
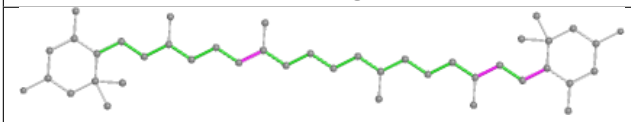


Bond angles



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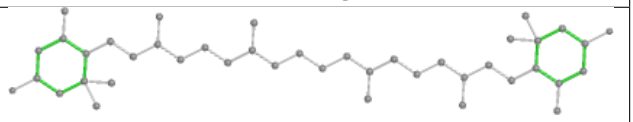
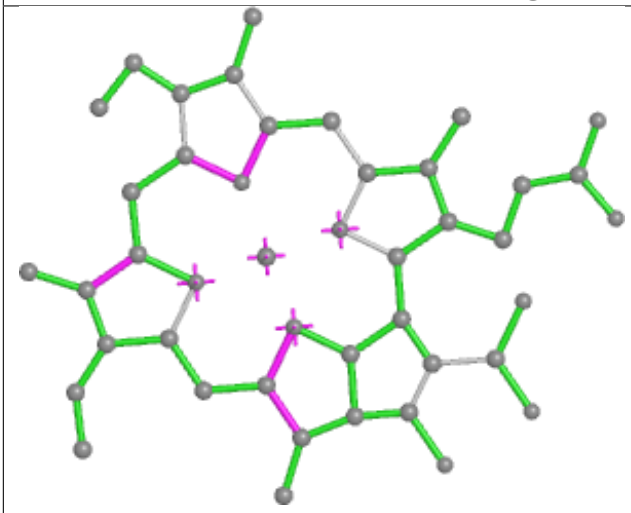
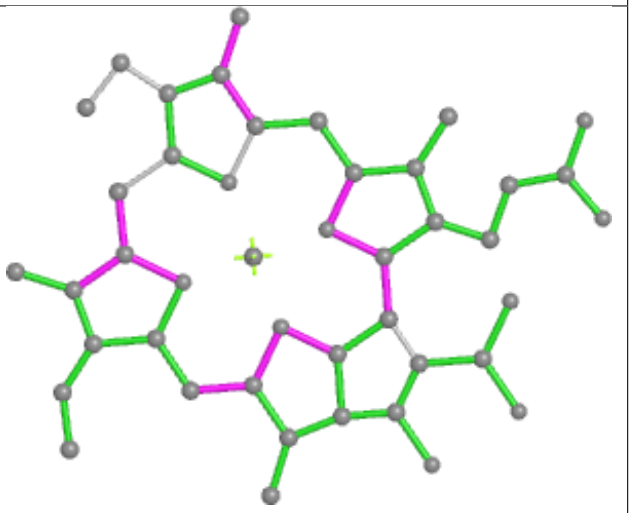


Rings

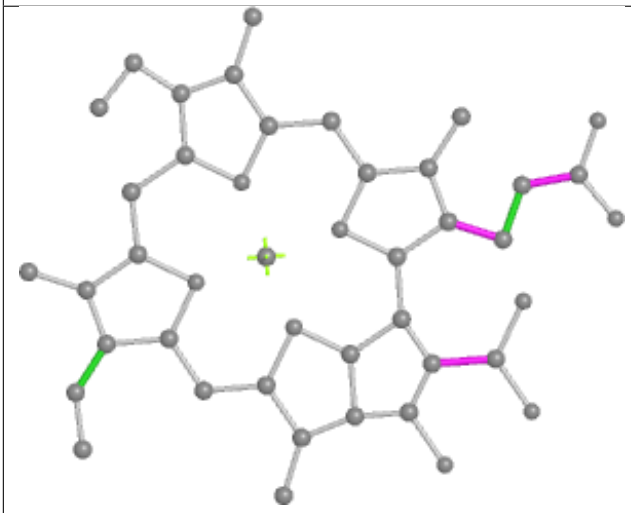
Ligand CLA B 826



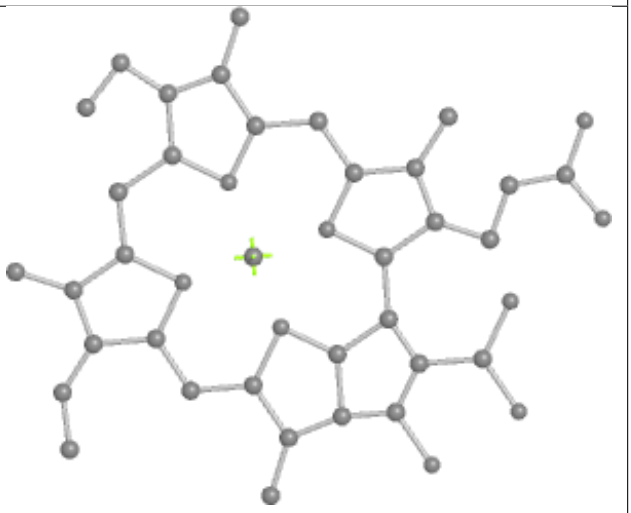
Bond lengths



Bond angles

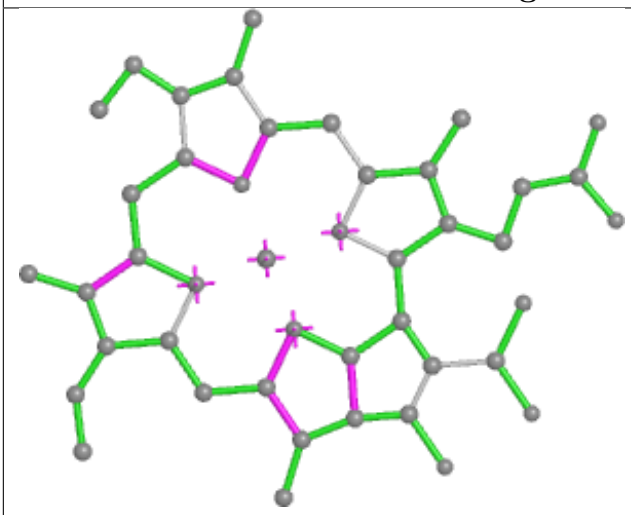


Torsions

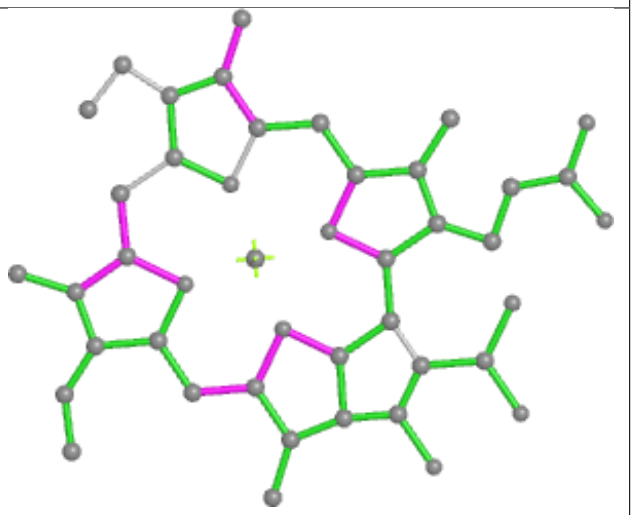


Rings

Ligand CLA 3 1009



Bond lengths



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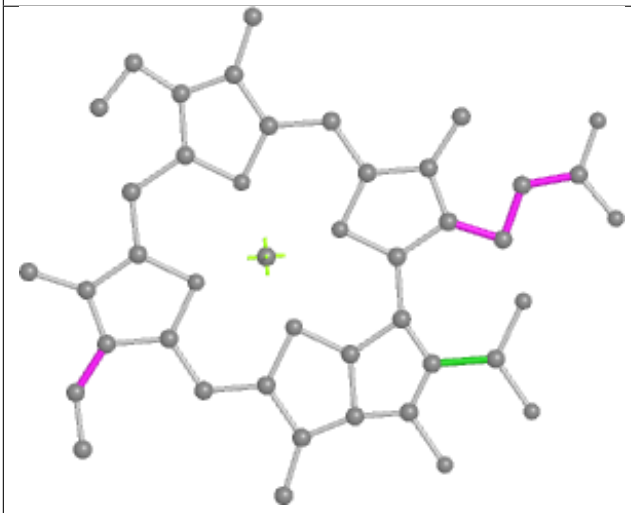

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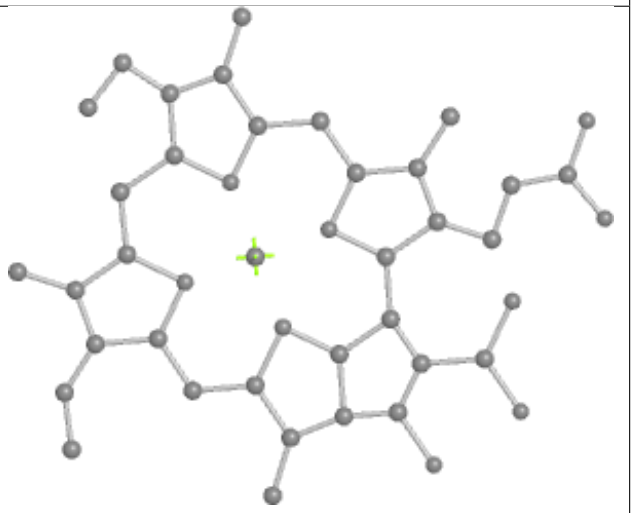
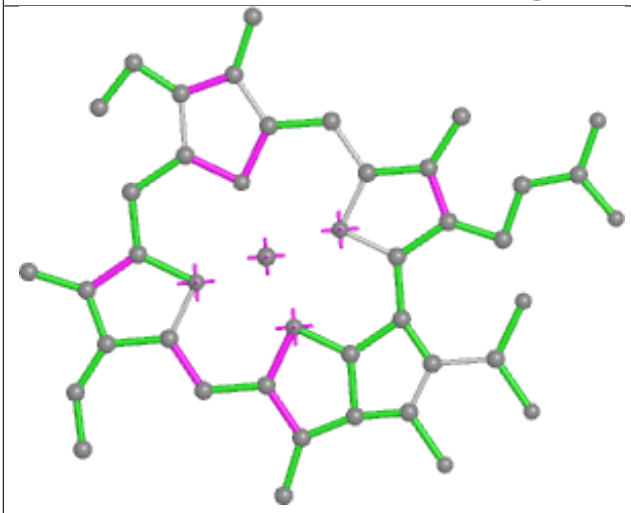


Rings

Ligand CLA 8 306



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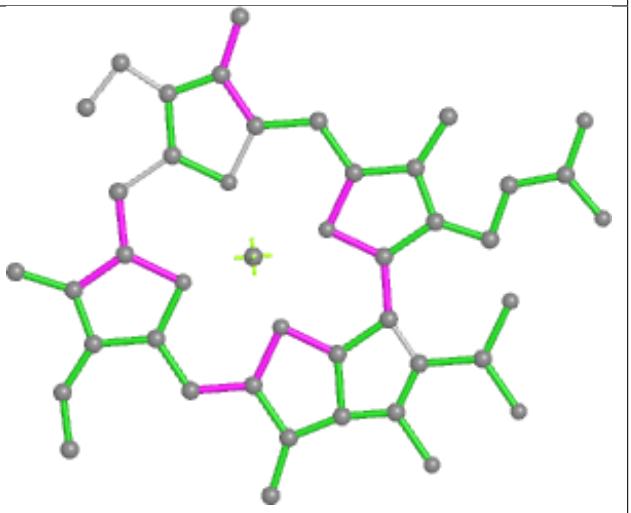
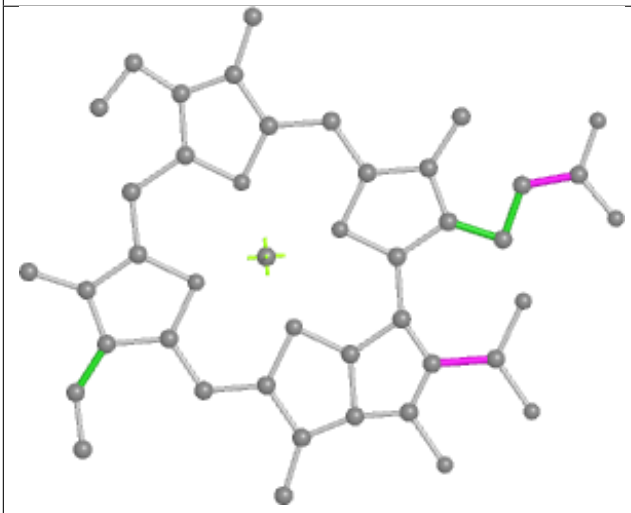


Bond angles



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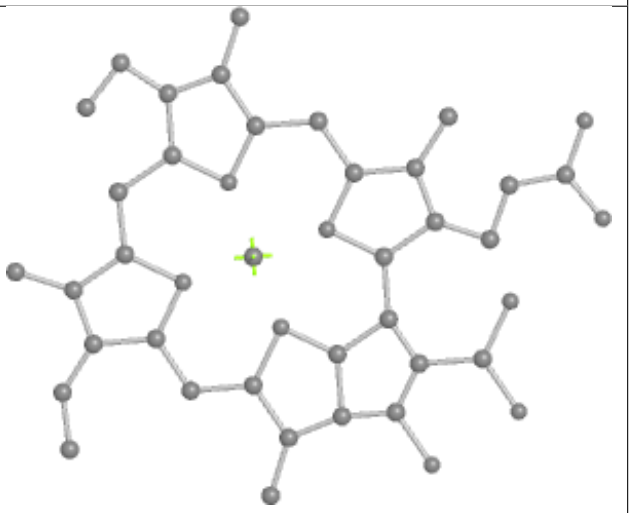
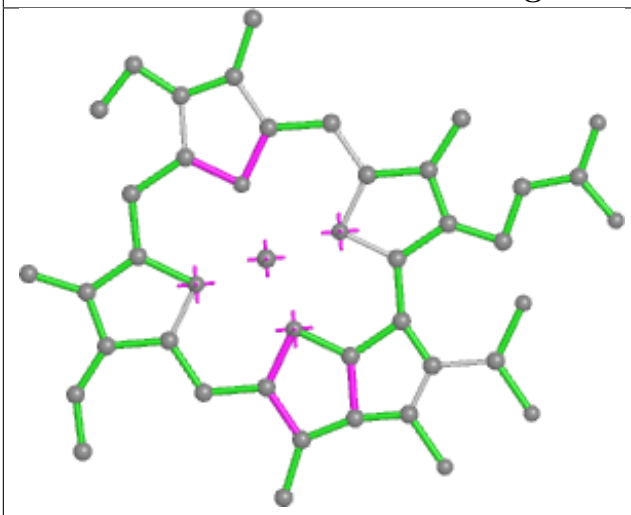
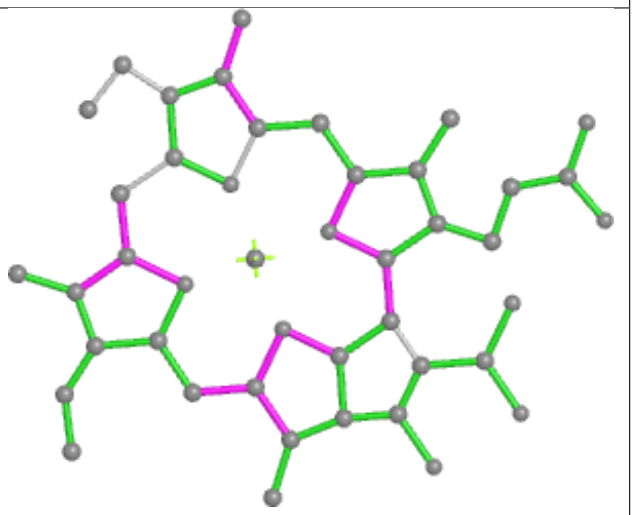


Rings

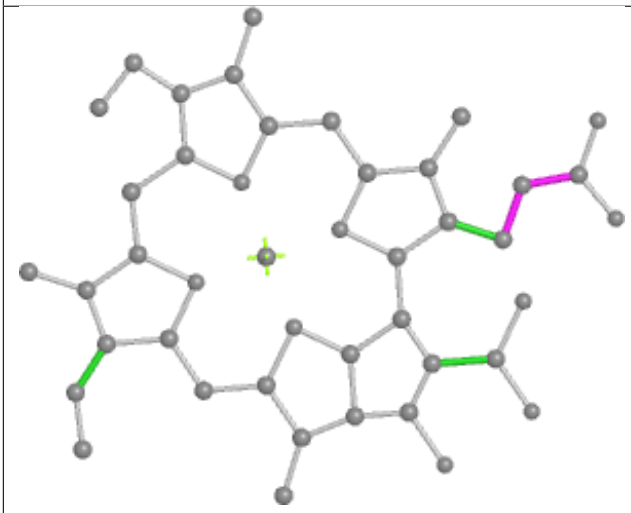
Ligand CLA B 803



Bond lengths



Bond angles



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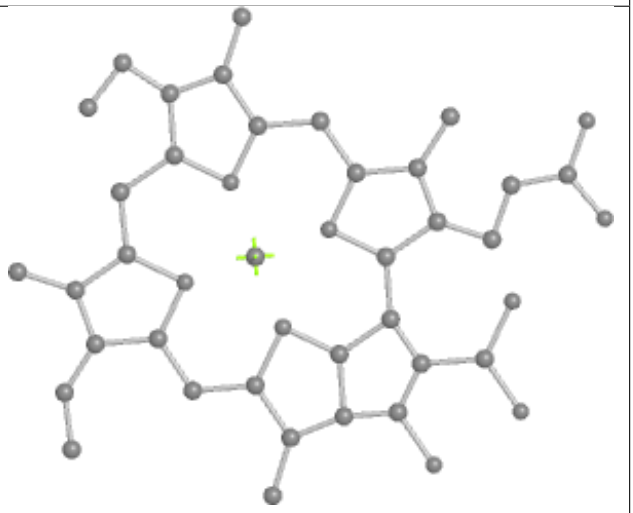
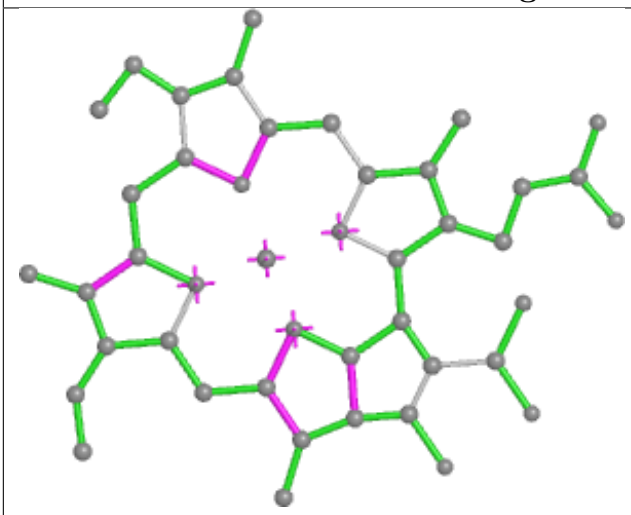


Rings

Ligand CLA 1 1008



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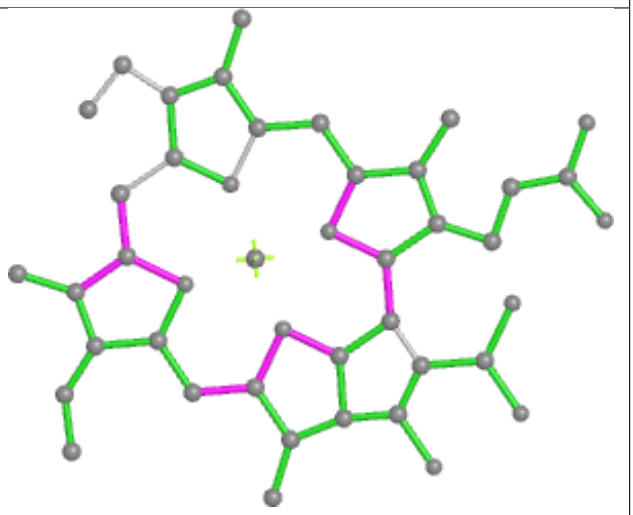
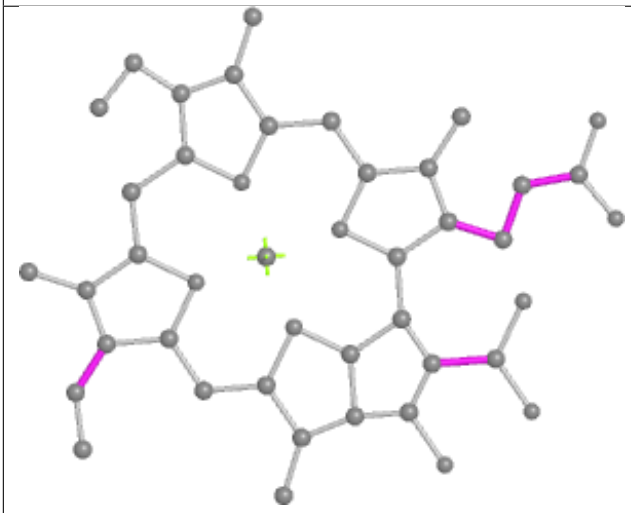


Bond angles



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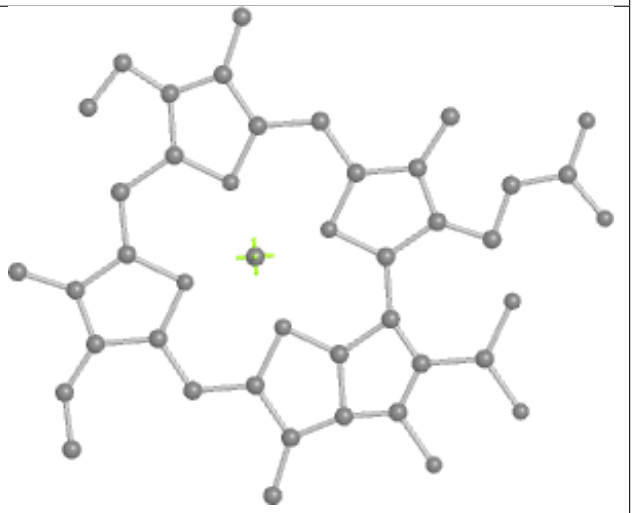
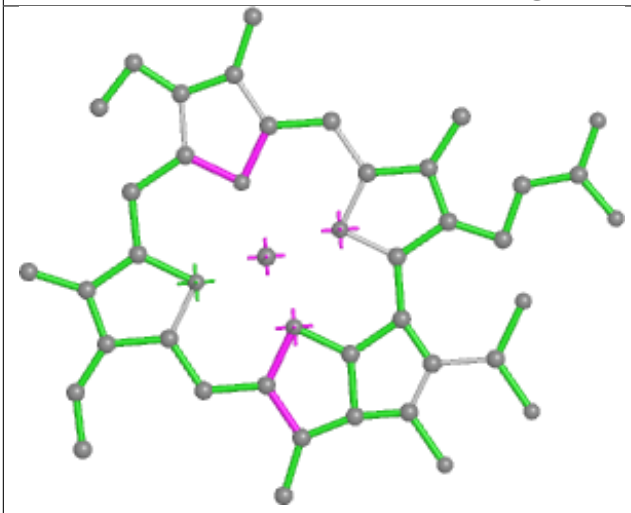


Rings

Ligand CLA 4 310



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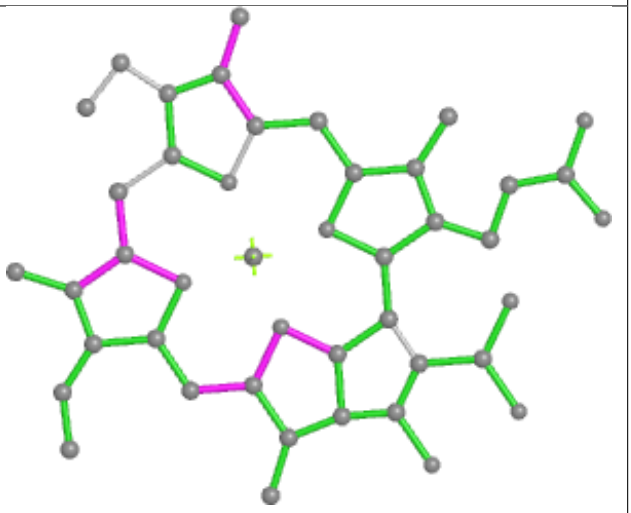
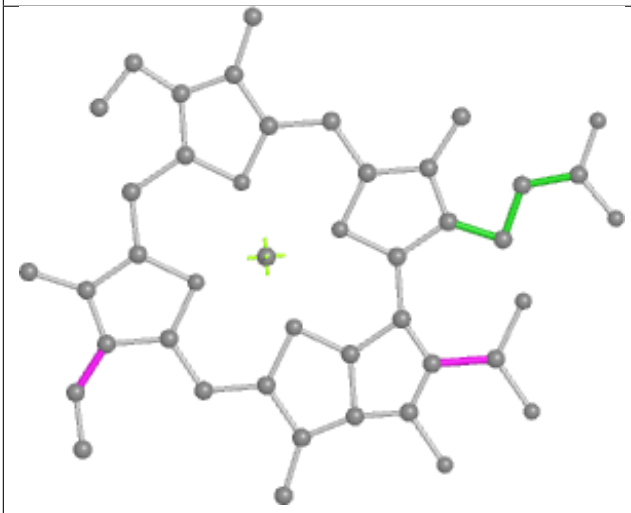


Bond angles



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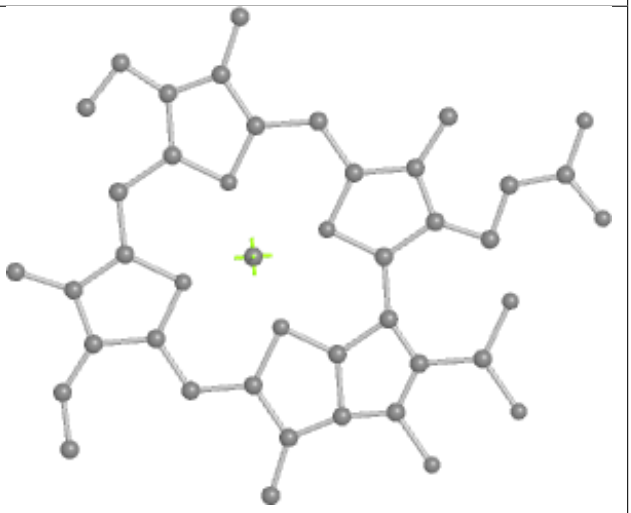
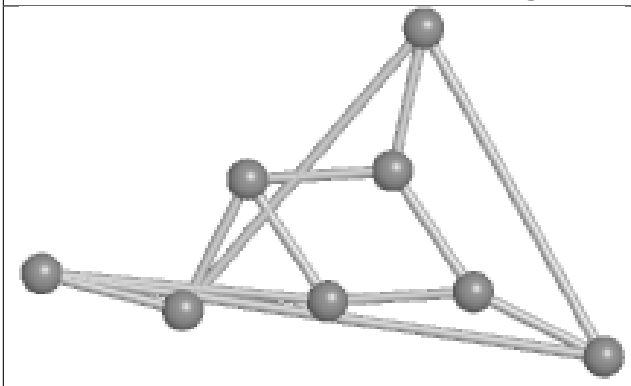


Rings

Ligand SF4 C 1001



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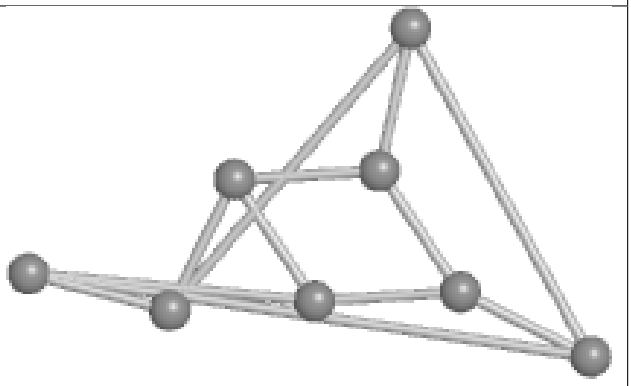
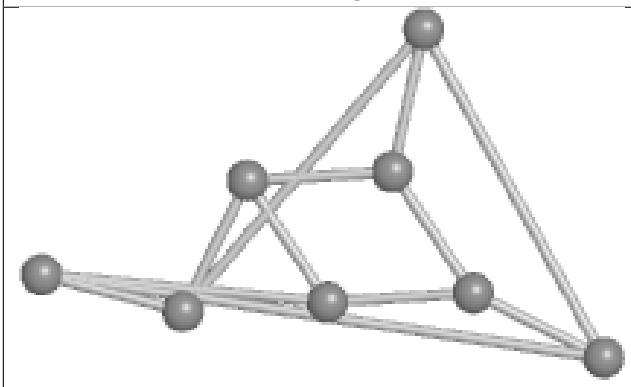


Bond angles



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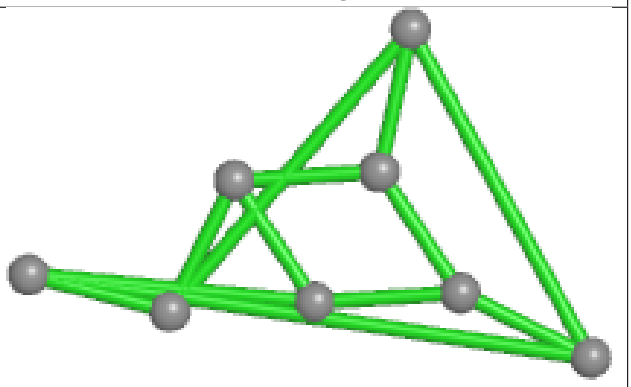
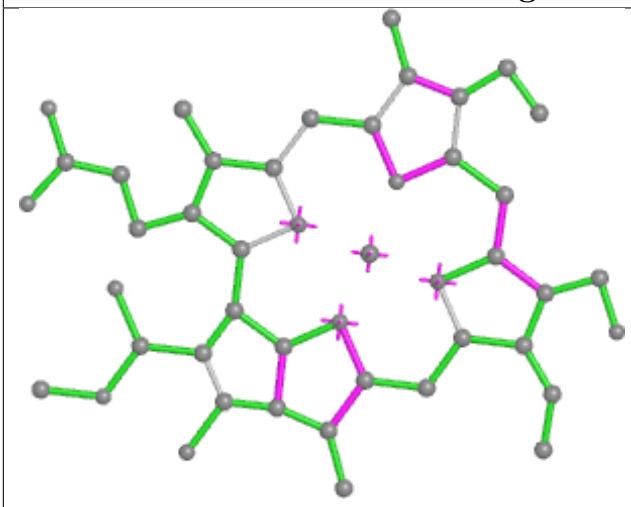


Rings

Ligand CHL 7 1015



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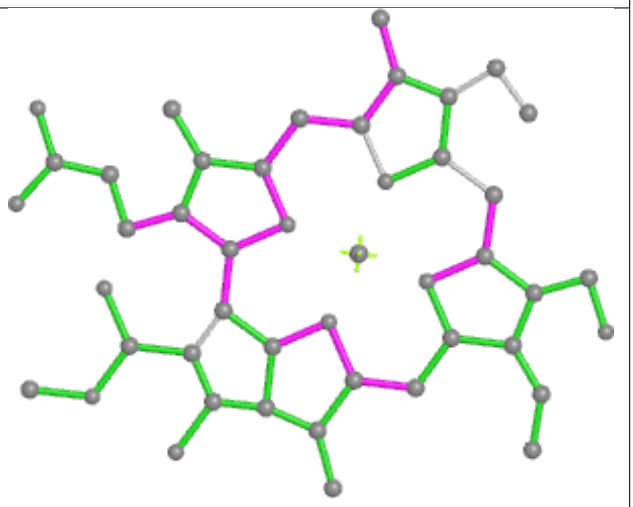
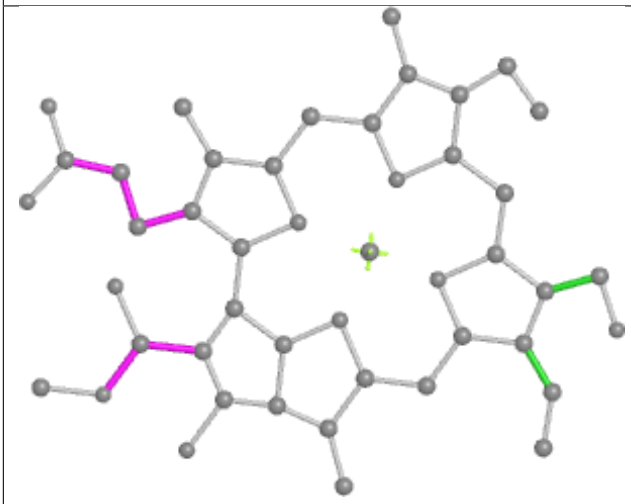


Bond angles



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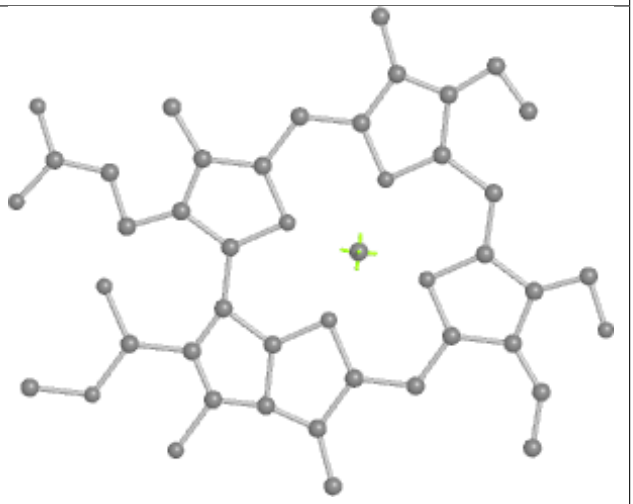
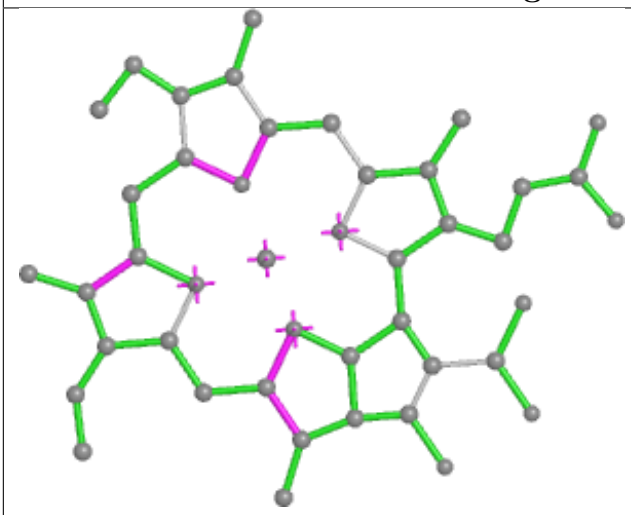


Rings

Ligand CLA A 825



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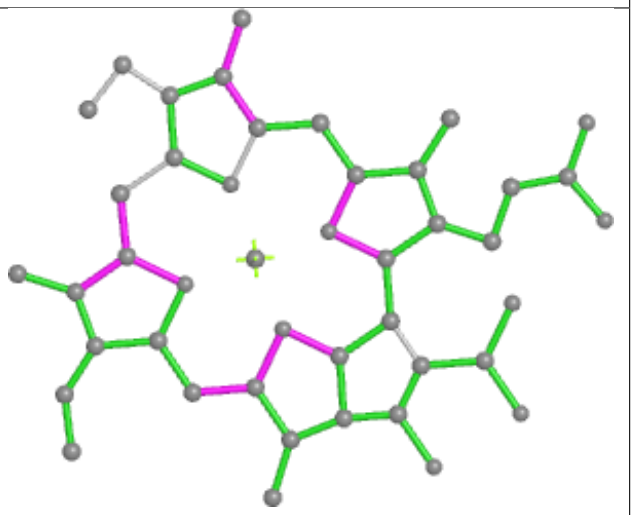
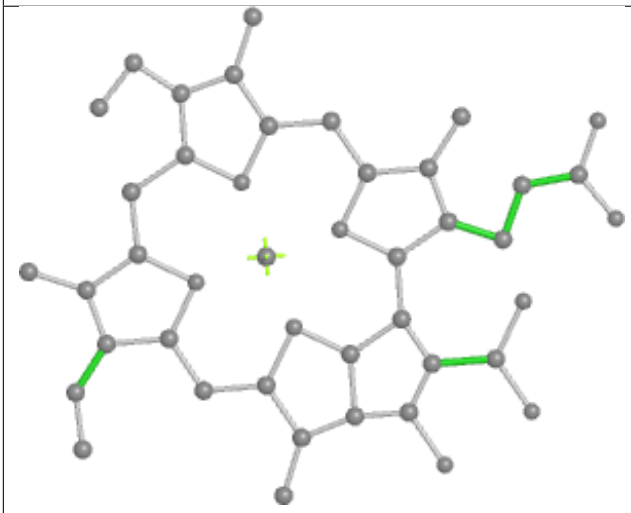
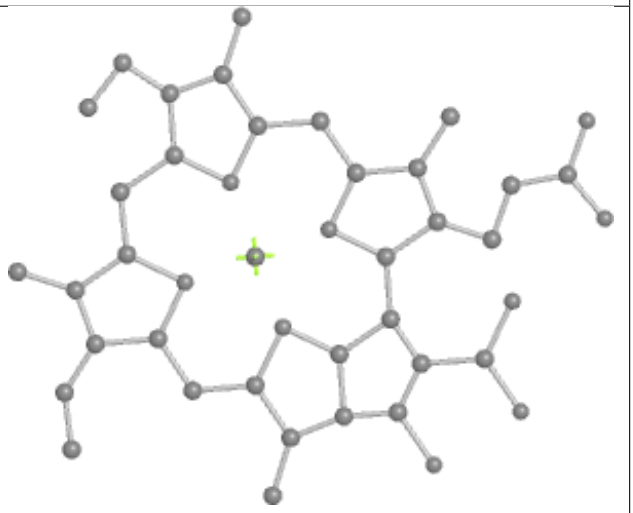


Bond angles

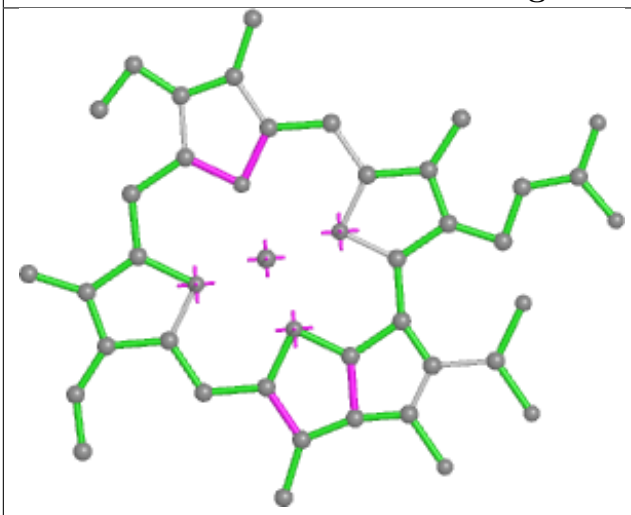


Torsions



Rings

Ligand CLA 6 320



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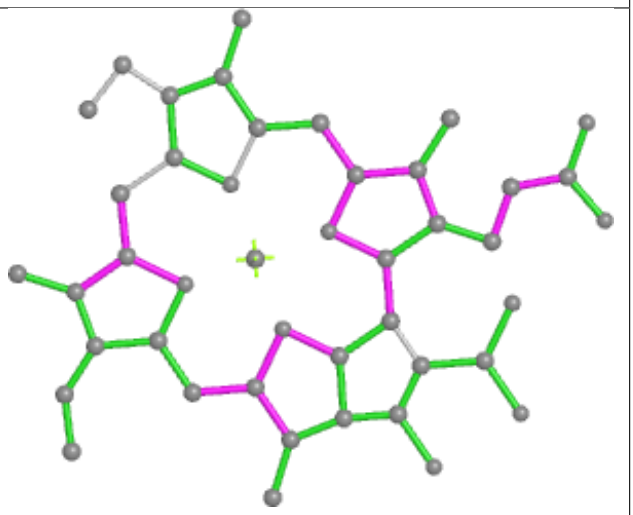
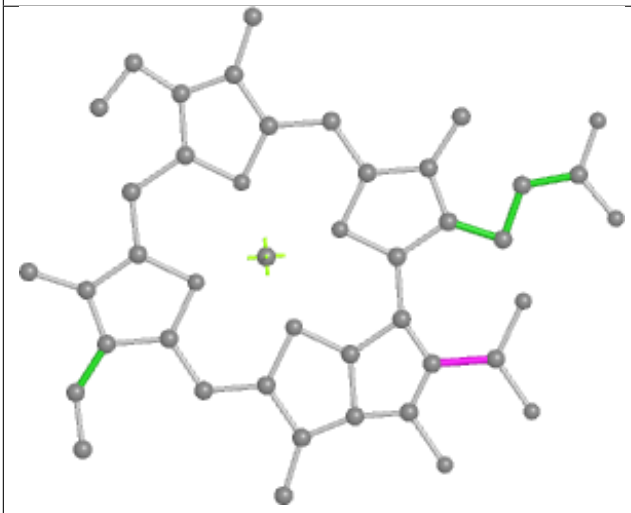
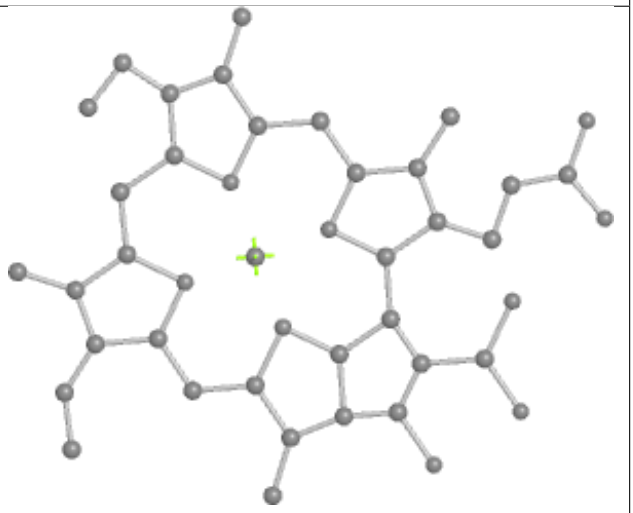


Bond angles

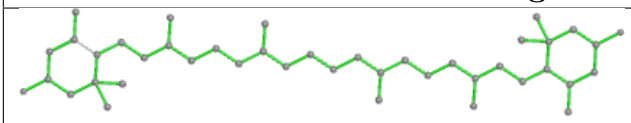


Torsions



Rings

Ligand LUT 8 303



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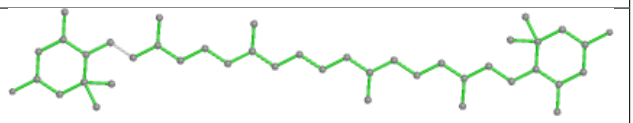
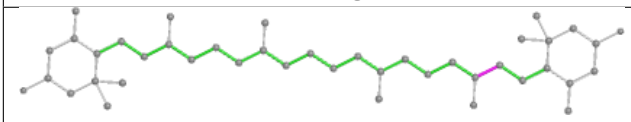


Bond angles



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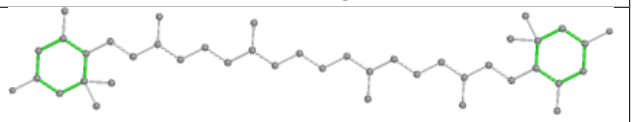
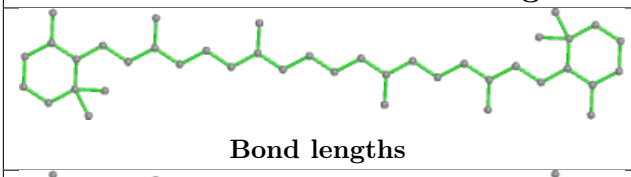


Rings

Ligand BCR A 847



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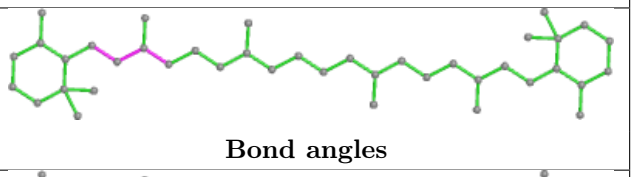
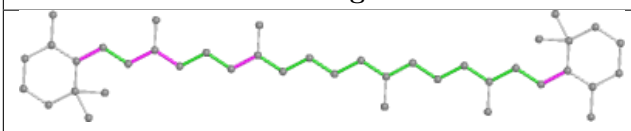


Bond angles



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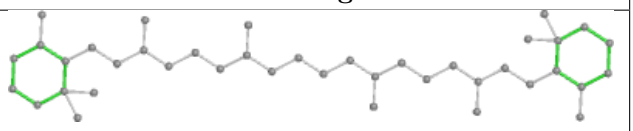
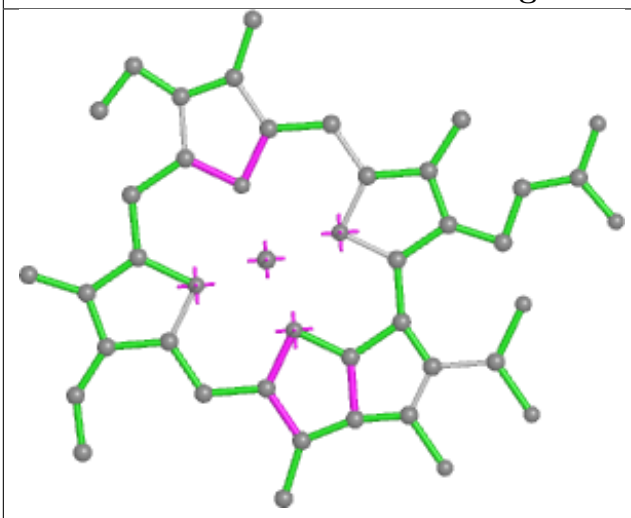
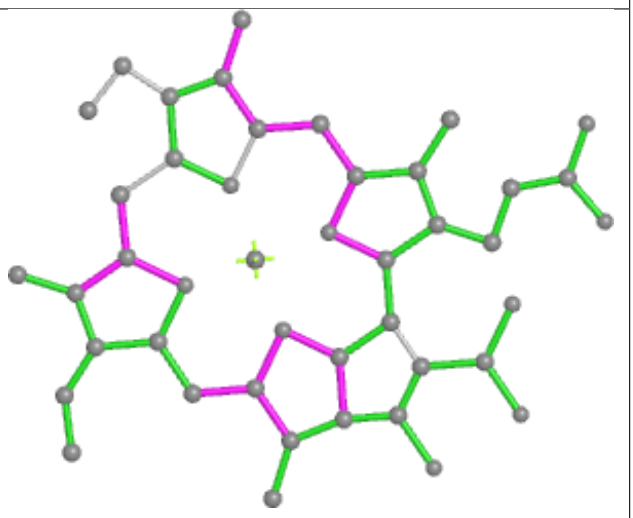


Rings

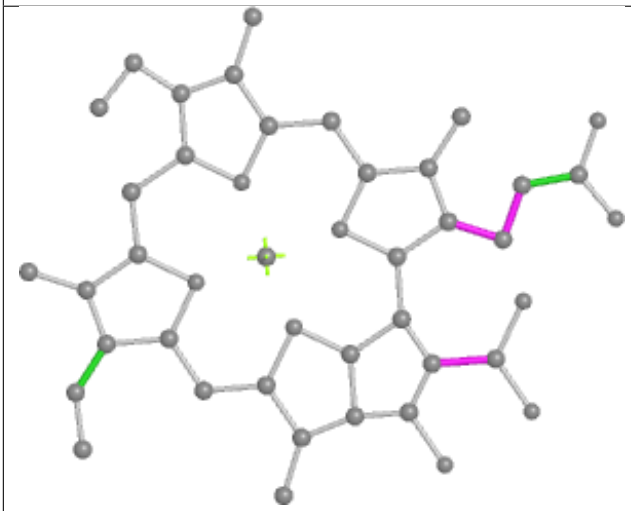
Ligand CLA 3 1008



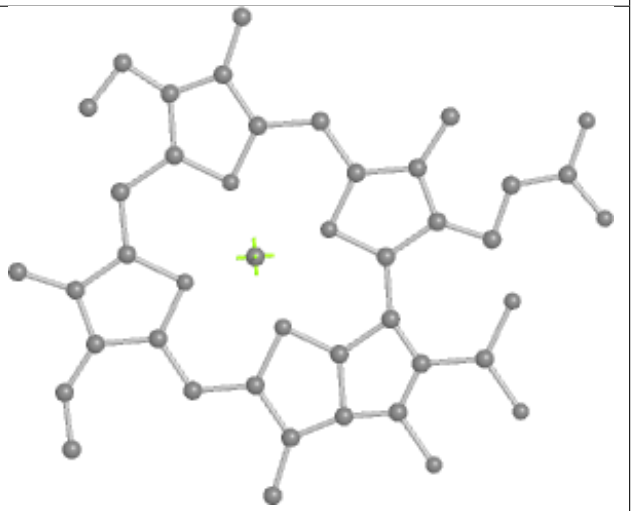
Bond lengths



Bond angles

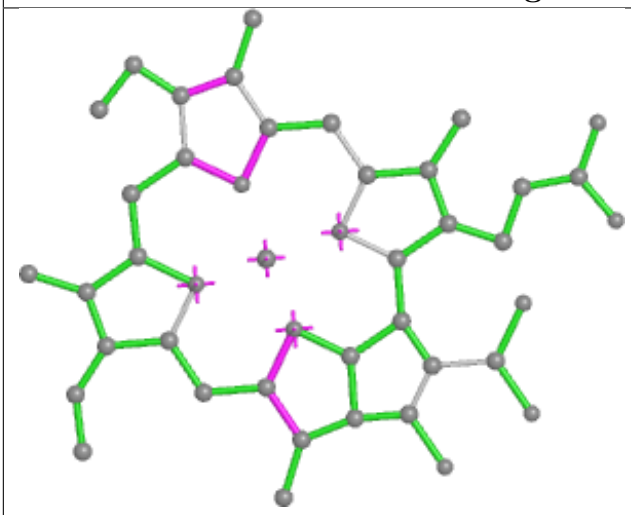


Torsions

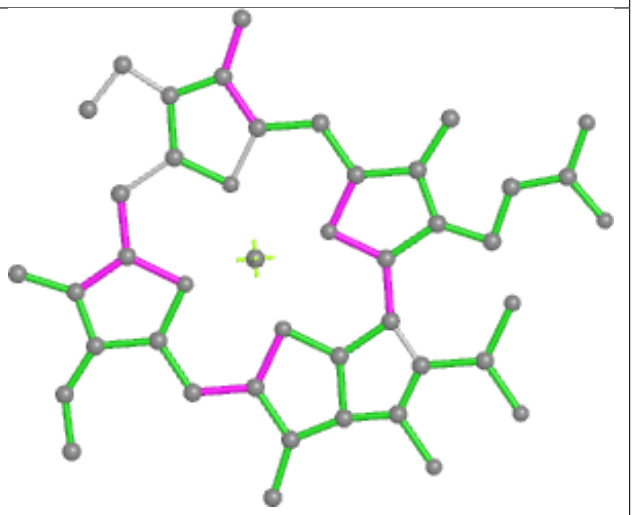


Rings

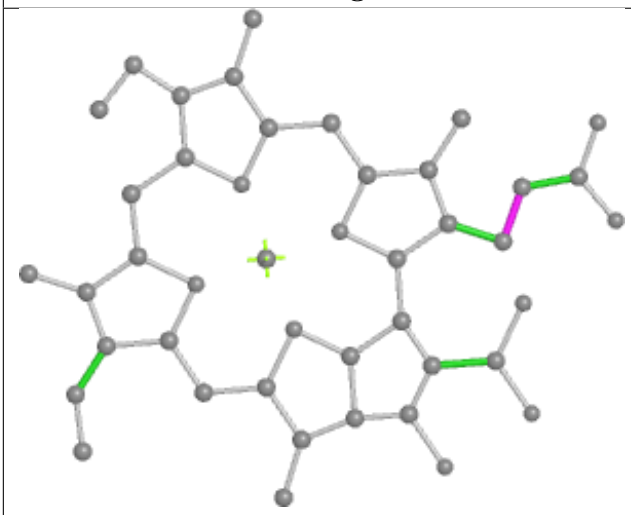
Ligand CLA B 801



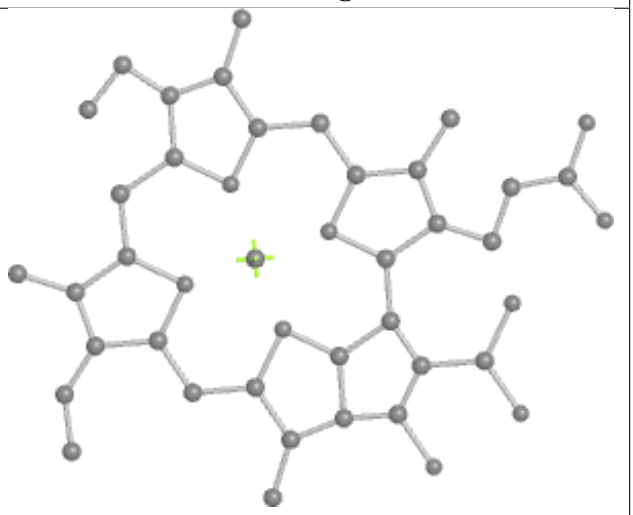
Bond lengths



Bond angles

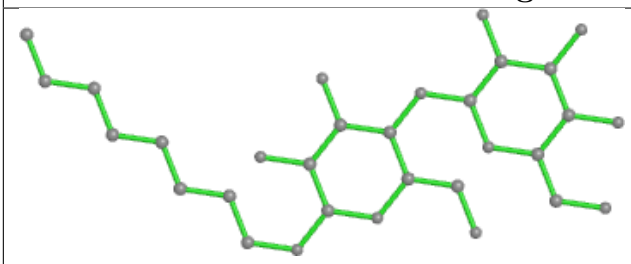


Torsions

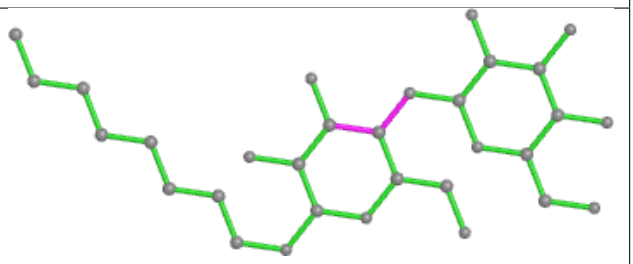


Rings

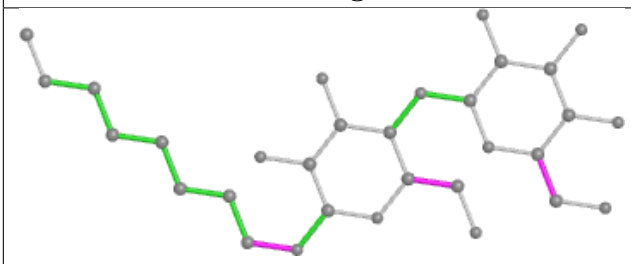
Ligand LMT 3 1018



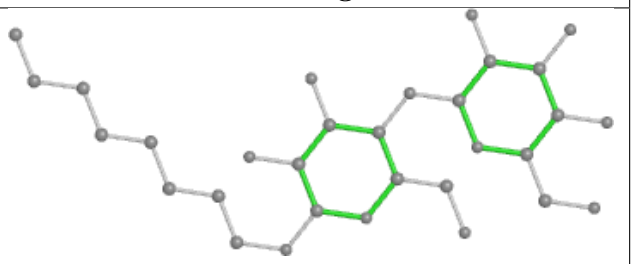
Bond lengths



Bond angles

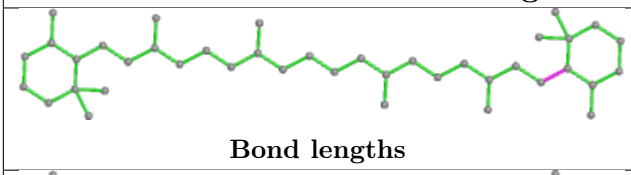


Torsions

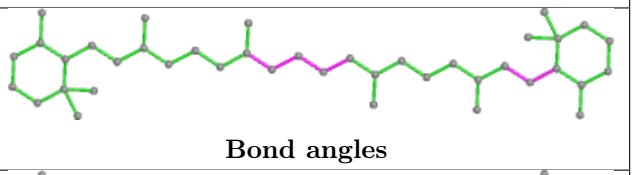


Rings

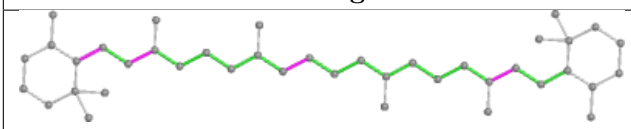
Ligand BCR G 205



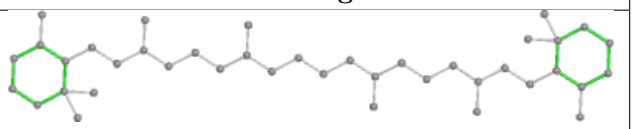
Bond lengths



Bond angles

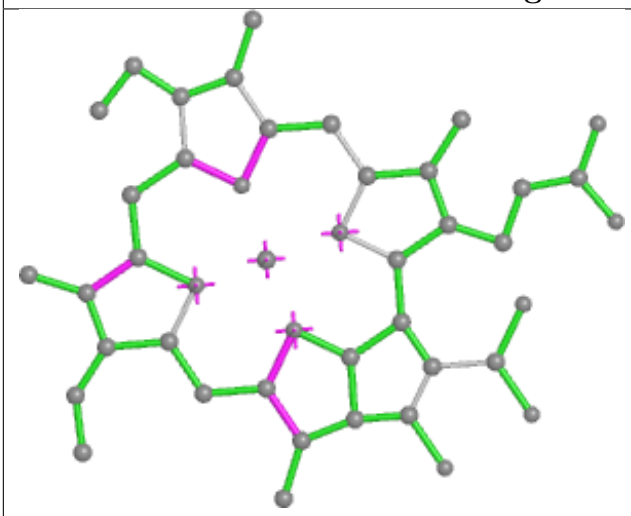


Torsions

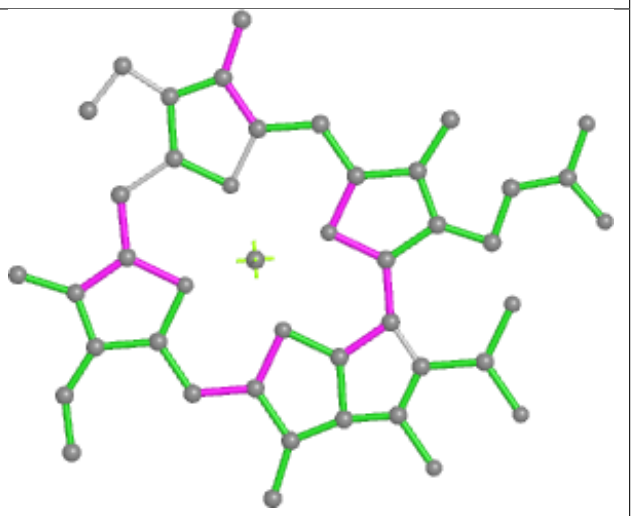


Rings

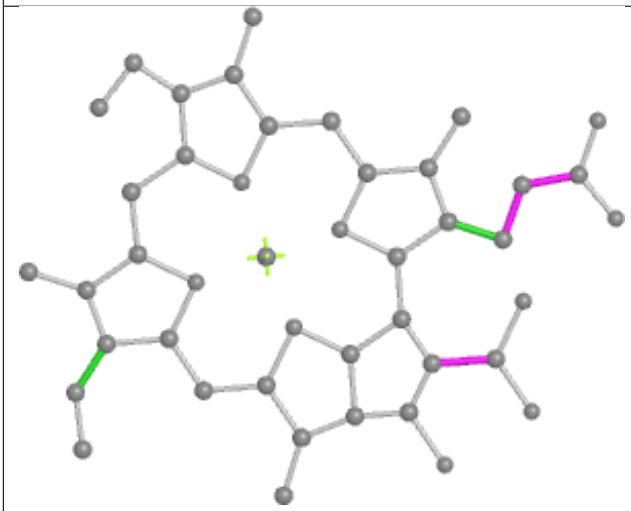
Ligand CLA B 838



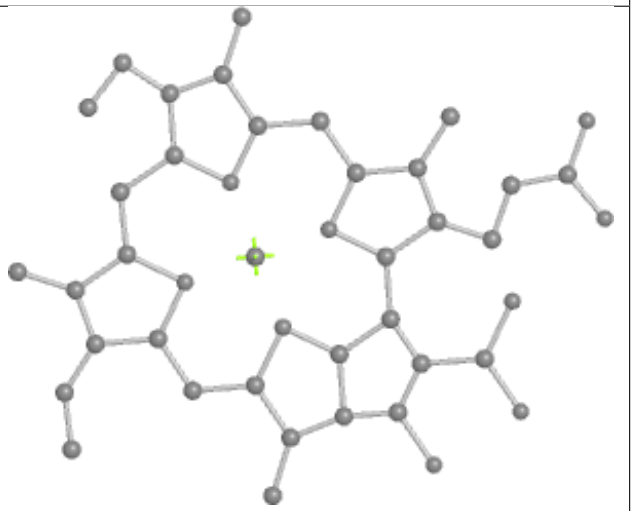
Bond lengths



Bond angles

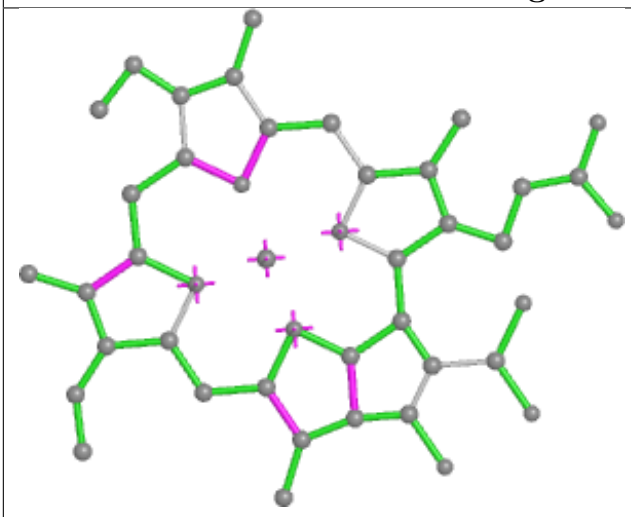


Torsions

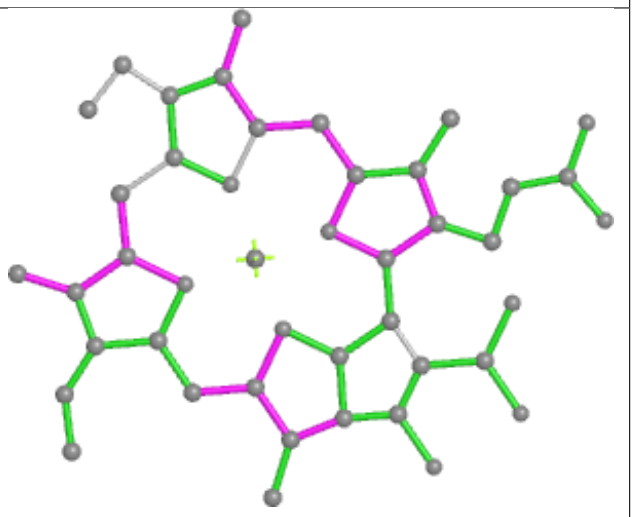


Rings

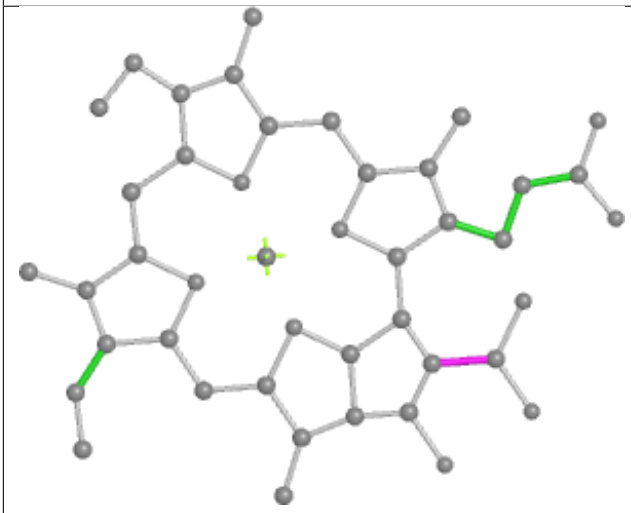
Ligand CLA 6 308



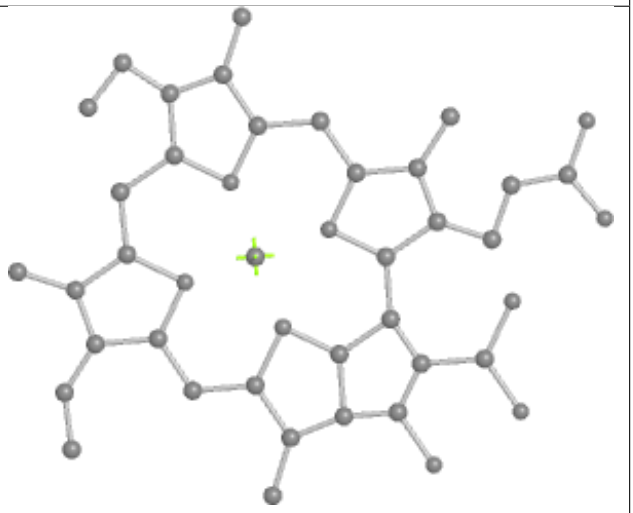
Bond lengths



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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	738/751 (98%)	0.68	79 (10%) 6 7	91, 155, 210, 250	0
2	B	728/735 (99%)	0.88	113 (15%) 2 2	106, 177, 229, 279	0
3	C	80/81 (98%)	1.68	28 (35%) 0 0	136, 172, 199, 219	0
4	D	141/196 (71%)	1.55	44 (31%) 0 0	132, 182, 217, 255	0
5	E	61/97 (62%)	1.44	20 (32%) 0 0	111, 159, 184, 195	0
6	F	150/227 (66%)	0.48	10 (6%) 17 19	89, 138, 175, 204	0
7	G	85/126 (67%)	3.78	49 (57%) 0 0	175, 261, 344, 421	0
8	H	90/130 (69%)	4.91	79 (87%) 0 0	197, 283, 367, 430	0
9	I	29/106 (27%)	3.40	22 (75%) 0 0	204, 305, 350, 396	0
10	J	39/41 (95%)	-0.08	1 (2%) 56 54	107, 131, 165, 179	0
11	K	44/113 (38%)	4.50	37 (84%) 0 0	195, 342, 432, 470	0
12	L	150/196 (76%)	5.09	115 (76%) 0 0	185, 331, 501, 579	0
13	0	182/228 (79%)	0.73	25 (13%) 3 3	101, 152, 203, 245	0
13	1	182/228 (79%)	0.44	19 (10%) 6 8	80, 119, 167, 195	0
14	8	193/243 (79%)	0.11	8 (4%) 37 36	61, 100, 129, 158	0
15	7	209/241 (86%)	0.20	10 (4%) 30 31	55, 89, 126, 164	0
16	3	201/298 (67%)	0.29	15 (7%) 14 16	73, 122, 160, 195	0
17	4	202/264 (76%)	0.23	9 (4%) 33 33	70, 106, 141, 170	0
18	6	184/257 (71%)	-0.07	0 100 100	43, 90, 128, 185	0
19	5	193/257 (75%)	0.07	1 (0%) 91 90	56, 95, 137, 166	0
All	All	3881/4815 (80%)	1.00	684 (17%) 1 1	43, 147, 298, 579	0

The worst 5 of 684 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	36	SER	25.8
12	L	112	THR	22.5
12	L	113	ALA	21.3
12	L	78	GLY	20.8
12	L	109	VAL	19.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	L	204	44/65	0.33	0.79	210,255,268,270	0
24	BCR	A	850	40/40	0.41	0.74	177,223,310,313	0
24	BCR	H	201	40/40	0.46	1.03	189,232,262,263	0
20	CLA	G	203	44/65	0.50	0.43	155,244,268,275	0
20	CLA	L	203	44/65	0.53	0.59	225,282,298,301	0
24	BCR	B	845	40/40	0.56	0.83	142,194,236,238	0
24	BCR	I	201	40/40	0.57	0.51	194,224,242,243	0
20	CLA	L	202	44/65	0.63	0.63	240,279,308,311	0
20	CLA	K	201	44/65	0.65	0.42	212,242,252,254	0
24	BCR	G	205	40/40	0.67	0.86	119,205,273,275	0
24	BCR	B	804	40/40	0.67	0.51	122,142,155,163	0
20	CLA	K	202	27/65	0.67	0.91	214,233,244,248	0
26	LMT	3	1018	31/35	0.67	0.45	111,185,218,227	0
24	BCR	G	204	40/40	0.68	0.56	206,227,250,259	0
27	LMG	0	303	50/55	0.68	0.41	196,217,237,261	0
24	BCR	A	846	40/40	0.71	0.52	134,183,205,209	0
20	CLA	B	813	44/65	0.71	0.35	195,214,224,228	0
24	BCR	B	847	40/40	0.71	0.43	137,156,174,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	LHG	3	1019	20/49	0.73	0.80	202,256,264,269	0
20	CLA	B	850	43/65	0.74	0.32	183,226,244,260	0
25	DGD	B	848	61/66	0.74	0.40	120,168,217,250	0
24	BCR	A	844	40/40	0.75	0.43	123,155,197,200	0
22	PQN	B	842	33/33	0.76	0.48	121,166,191,200	0
25	DGD	5	319	51/66	0.76	0.38	96,147,186,192	0
20	CLA	B	826	44/65	0.76	0.34	161,182,190,192	0
20	CLA	G	202	44/65	0.76	0.44	177,217,238,249	0
27	LMG	8	319	44/55	0.76	0.52	151,179,216,229	0
29	CHL	0	317	61/66	0.76	0.52	186,220,246,264	0
20	CLA	B	814	44/65	0.77	0.31	149,201,229,238	0
20	CLA	G	201	44/65	0.77	0.70	201,273,294,301	0
24	BCR	A	845	40/40	0.77	0.56	102,120,156,172	0
29	CHL	1	1015	61/66	0.77	0.51	139,177,205,216	0
24	BCR	B	844	40/40	0.78	0.38	164,196,213,216	0
24	BCR	1	1001	40/40	0.78	0.47	91,137,239,246	0
20	CLA	A	840	44/65	0.78	0.40	173,213,233,245	0
27	LMG	6	319	44/55	0.78	0.46	95,120,158,169	0
20	CLA	A	833	44/65	0.78	0.35	181,193,207,213	0
26	LMT	B	849	31/35	0.78	0.50	164,183,224,228	0
20	CLA	B	816	44/65	0.79	0.39	174,190,199,205	0
20	CLA	A	824	44/65	0.79	0.39	102,147,173,183	0
20	CLA	B	836	44/65	0.79	0.28	142,175,192,198	0
20	CLA	B	840	44/65	0.79	0.34	158,197,210,214	0
27	LMG	J	101	30/55	0.79	0.49	135,158,176,180	0
20	CLA	L	201	44/65	0.80	0.35	149,200,218,235	0
20	CLA	0	316	44/65	0.80	0.31	145,186,199,209	0
20	CLA	B	810	44/65	0.80	0.33	160,186,210,222	0
27	LMG	5	324	45/55	0.80	0.31	46,97,156,183	0
28	LUT	J	104	42/42	0.80	0.46	79,115,162,172	0
28	LUT	1	1002	42/42	0.80	0.54	99,133,171,176	0
24	BCR	B	846	40/40	0.80	0.36	143,161,184,187	0
20	CLA	B	812	44/65	0.80	0.43	140,165,186,188	0
24	BCR	3	1004	40/40	0.81	0.49	111,134,161,169	0
28	LUT	3	1001	42/42	0.81	0.36	89,116,145,156	0
28	LUT	3	1002	42/42	0.81	0.45	97,117,129,142	0
24	BCR	F	304	40/40	0.81	0.38	104,116,140,143	0
29	CHL	0	315	51/66	0.81	0.56	154,226,245,260	0
24	BCR	4	302	40/40	0.81	0.68	99,130,160,164	0
24	BCR	7	1003	40/40	0.81	0.54	92,124,149,156	0
20	CLA	B	822	44/65	0.82	0.36	130,151,188,201	0
24	BCR	8	302	40/40	0.82	0.45	91,102,155,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	LUT	0	318	42/42	0.82	0.48	122,137,164,167	0
23	LHG	A	849	49/49	0.82	0.36	121,149,179,196	0
20	CLA	A	822	44/65	0.82	0.47	170,196,205,216	0
24	BCR	B	843	40/40	0.82	0.37	175,201,216,221	0
29	CHL	0	314	47/66	0.82	0.35	164,201,252,295	0
20	CLA	B	817	44/65	0.82	0.27	148,178,197,209	0
27	LMG	4	318	34/55	0.82	0.60	126,166,215,225	0
29	CHL	8	317	61/66	0.82	0.35	96,109,139,149	0
20	CLA	5	312	44/65	0.82	0.35	106,124,150,154	0
30	XAT	7	1002	44/44	0.82	0.51	69,83,91,97	0
20	CLA	B	835	44/65	0.83	0.32	127,158,171,189	0
24	BCR	A	847	40/40	0.83	0.32	120,138,183,185	0
20	CLA	B	819	44/65	0.83	0.33	171,196,246,285	0
20	CLA	A	820	44/65	0.83	0.27	135,178,186,193	0
29	CHL	4	312	47/66	0.83	0.35	97,120,136,169	0
20	CLA	B	801	44/65	0.83	0.29	118,166,178,191	0
20	CLA	B	811	44/65	0.84	0.30	130,155,170,179	0
20	CLA	B	815	44/65	0.84	0.36	128,158,232,249	0
24	BCR	6	302	40/40	0.84	0.61	98,133,141,150	0
27	LMG	8	318	28/55	0.84	0.31	72,118,150,161	0
20	CLA	B	824	44/65	0.85	0.30	148,171,185,200	0
20	CLA	F	303	44/65	0.85	0.28	118,132,162,189	0
24	BCR	J	103	40/40	0.85	0.44	113,134,148,157	0
20	CLA	3	1011	40/65	0.85	0.45	180,202,216,218	0
30	XAT	5	303	44/44	0.85	0.40	49,77,104,108	0
24	BCR	A	848	40/40	0.86	0.35	102,125,154,157	0
29	CHL	8	314	47/66	0.86	0.38	102,134,169,185	0
20	CLA	A	834	44/65	0.86	0.34	144,167,186,190	0
20	CLA	B	823	44/65	0.86	0.32	153,173,203,206	0
23	LHG	0	302	21/49	0.86	0.26	136,159,173,187	0
20	CLA	A	825	44/65	0.86	0.27	117,135,157,167	0
24	BCR	5	320	40/40	0.86	0.56	81,107,129,134	0
20	CLA	5	323	44/65	0.87	0.25	75,122,154,168	0
22	PQN	A	842	33/33	0.87	0.43	106,115,157,162	0
20	CLA	B	818	44/65	0.87	0.42	214,236,252,260	0
20	CLA	A	804	44/65	0.87	0.33	124,142,150,157	0
20	CLA	B	820	44/65	0.87	0.30	149,174,193,209	0
23	LHG	8	301	49/49	0.87	0.62	111,140,220,230	0
20	CLA	3	1012	44/65	0.87	0.44	139,174,214,234	0
23	LHG	4	301	49/49	0.87	0.43	110,136,193,195	0
20	CLA	1	1010	44/65	0.87	0.27	95,135,156,184	0
24	BCR	F	301	40/40	0.87	0.36	104,125,152,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	5	311	44/65	0.87	0.30	88,107,161,222	0
20	CLA	A	815	44/65	0.87	0.32	120,138,154,165	0
20	CLA	0	309	44/65	0.88	0.26	143,171,200,215	0
20	CLA	B	807	44/65	0.88	0.25	119,158,173,175	0
20	CLA	A	811	44/65	0.88	0.27	110,148,160,171	0
28	LUT	1	1016	42/42	0.88	0.72	105,124,136,145	0
20	CLA	B	831	44/65	0.88	0.24	141,164,178,198	0
20	CLA	1	1005	44/65	0.88	0.25	84,120,130,145	0
20	CLA	A	819	44/65	0.88	0.27	147,180,190,194	0
20	CLA	A	830	44/65	0.88	0.30	161,200,217,226	0
20	CLA	B	838	44/65	0.88	0.32	114,136,149,158	0
29	CHL	7	1017	66/66	0.88	0.40	100,117,150,172	0
29	CHL	1	1012	47/66	0.88	0.26	102,132,156,174	0
20	CLA	A	852	44/65	0.88	0.24	141,151,167,187	0
20	CLA	A	832	44/65	0.88	0.33	155,176,191,202	0
30	XAT	8	304	44/44	0.88	0.46	50,85,95,109	0
28	LUT	0	304	42/42	0.88	0.50	128,147,202,207	0
20	CLA	B	803	44/65	0.88	0.43	170,200,215,220	0
20	CLA	A	821	44/65	0.89	0.28	159,185,199,231	0
23	LHG	A	843	40/49	0.89	0.34	166,193,211,225	0
20	CLA	A	803	44/65	0.89	0.33	80,90,114,117	0
20	CLA	A	812	44/65	0.89	0.27	95,111,124,135	0
20	CLA	A	814	40/65	0.89	0.26	147,160,199,217	0
20	CLA	0	306	44/65	0.89	0.21	123,146,154,163	0
29	CHL	4	315	61/66	0.89	0.33	113,149,173,192	0
29	CHL	6	316	61/66	0.89	0.37	95,112,152,159	0
29	CHL	5	313	47/66	0.89	0.28	65,87,107,125	0
20	CLA	A	835	44/65	0.89	0.28	138,164,192,219	0
20	CLA	0	312	44/65	0.89	0.21	101,128,147,160	0
20	CLA	B	829	44/65	0.89	0.30	155,179,193,196	0
20	CLA	1	1017	44/65	0.90	0.25	92,114,125,136	0
20	CLA	6	301	44/65	0.90	0.29	93,111,124,154	0
20	CLA	A	809	44/65	0.90	0.29	98,121,134,143	0
20	CLA	0	307	44/65	0.90	0.34	90,104,125,144	0
29	CHL	1	1013	51/66	0.90	0.35	111,140,153,172	0
20	CLA	A	831	44/65	0.90	0.21	132,146,202,227	0
20	CLA	B	828	44/65	0.90	0.25	134,151,160,167	0
20	CLA	B	821	44/65	0.90	0.33	133,160,183,185	0
29	CHL	6	313	47/66	0.90	0.27	83,98,121,171	0
20	CLA	3	1007	44/65	0.90	0.29	118,139,154,166	0
20	CLA	B	809	44/65	0.90	0.26	150,162,177,184	0
20	CLA	B	833	44/65	0.90	0.22	94,117,146,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	A	813	44/65	0.90	0.26	112,132,149,155	0
20	CLA	0	305	44/65	0.90	0.28	115,150,185,194	0
20	CLA	5	318	44/65	0.91	0.25	55,72,92,103	0
20	CLA	5	322	44/65	0.91	0.25	95,115,135,153	0
20	CLA	F	305	44/65	0.91	0.25	102,130,154,167	0
28	LUT	4	317	42/42	0.91	0.43	75,98,117,123	0
28	LUT	5	302	42/42	0.91	0.40	68,88,99,105	0
20	CLA	8	311	44/65	0.91	0.26	72,109,143,161	0
20	CLA	A	810	44/65	0.91	0.41	101,123,131,139	0
20	CLA	A	836	44/65	0.91	0.26	143,180,192,207	0
20	CLA	0	301	44/65	0.91	0.32	133,166,178,188	0
20	CLA	1	1004	44/65	0.91	0.29	91,123,152,161	0
29	CHL	7	1012	47/66	0.91	0.30	98,115,161,176	0
20	CLA	B	808	44/65	0.91	0.26	134,145,169,180	0
20	CLA	J	102	44/65	0.91	0.21	121,142,156,168	0
20	CLA	1	1014	44/65	0.91	0.24	86,113,129,136	0
20	CLA	A	816	44/65	0.91	0.25	131,154,200,217	0
20	CLA	4	314	44/65	0.91	0.26	77,98,118,140	0
20	CLA	A	826	44/65	0.91	0.20	104,122,141,146	0
20	CLA	6	311	44/65	0.91	0.30	89,99,113,132	0
24	BCR	3	1003	40/40	0.91	0.34	63,111,123,129	0
20	CLA	0	310	44/65	0.91	0.28	98,110,151,172	0
28	LUT	8	303	42/42	0.91	0.36	60,74,91,96	0
28	LUT	7	1001	42/42	0.91	0.30	56,73,85,91	0
30	XAT	4	303	44/44	0.91	0.37	66,91,98,101	0
30	XAT	6	304	44/44	0.91	0.34	39,78,87,91	0
20	CLA	A	823	44/65	0.91	0.26	155,173,187,192	0
20	CLA	0	311	44/65	0.92	0.22	113,128,159,183	0
20	CLA	1	1003	44/65	0.92	0.29	68,85,114,138	0
20	CLA	B	825	44/65	0.92	0.24	150,176,188,201	0
20	CLA	0	313	44/65	0.92	0.28	90,114,149,162	0
29	CHL	8	315	51/66	0.92	0.31	56,101,126,149	0
20	CLA	1	1007	44/65	0.92	0.27	110,118,130,141	0
20	CLA	1	1008	44/65	0.92	0.36	96,118,156,180	0
20	CLA	1	1009	44/65	0.92	0.24	83,108,131,160	0
20	CLA	F	302	44/65	0.92	0.23	91,99,108,109	0
20	CLA	8	308	44/65	0.92	0.26	53,76,86,92	0
20	CLA	B	830	44/65	0.92	0.27	132,144,168,179	0
20	CLA	4	308	44/65	0.92	0.23	65,82,94,100	0
20	CLA	8	312	44/65	0.92	0.30	78,90,106,124	0
20	CLA	7	1009	44/65	0.92	0.26	62,80,95,104	0
29	CHL	6	314	51/66	0.92	0.31	73,98,112,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	A	801	44/65	0.92	0.26	93,116,157,224	0
20	CLA	6	315	44/65	0.92	0.25	59,82,87,100	0
20	CLA	6	318	44/65	0.92	0.19	79,94,106,123	0
20	CLA	5	306	44/65	0.92	0.23	91,110,117,118	0
20	CLA	5	310	44/65	0.92	0.27	91,112,129,150	0
20	CLA	3	1010	44/65	0.92	0.26	99,114,127,142	0
20	CLA	B	806	44/65	0.92	0.33	166,188,198,201	0
20	CLA	B	839	44/65	0.93	0.23	118,134,148,154	0
20	CLA	5	315	44/65	0.93	0.27	65,89,99,104	0
20	CLA	3	1008	44/65	0.93	0.27	111,129,174,202	0
20	CLA	3	1009	44/65	0.93	0.23	87,120,129,132	0
20	CLA	B	802	44/65	0.93	0.26	99,123,145,168	0
20	CLA	B	841	44/65	0.93	0.32	84,105,159,184	0
20	CLA	0	308	44/65	0.93	0.27	93,113,124,125	0
29	CHL	7	1013	48/66	0.93	0.32	73,86,106,112	0
29	CHL	7	1015	46/66	0.93	0.23	70,81,108,131	0
20	CLA	3	1013	44/65	0.93	0.22	89,133,159,173	0
20	CLA	6	309	44/65	0.93	0.26	64,88,100,134	0
20	CLA	6	310	44/65	0.93	0.23	84,99,108,121	0
20	CLA	3	1017	44/65	0.93	0.22	91,110,140,160	0
23	LHG	7	1016	35/49	0.93	0.36	88,105,127,130	0
20	CLA	A	838	44/65	0.93	0.31	98,111,134,136	0
29	CHL	4	316	43/66	0.93	0.29	93,105,118,145	0
20	CLA	B	837	44/65	0.93	0.32	100,117,128,141	0
20	CLA	6	320	44/65	0.93	0.26	68,87,93,104	0
20	CLA	5	304	44/65	0.93	0.28	69,97,114,125	0
20	CLA	8	316	44/65	0.93	0.26	77,101,116,126	0
20	CLA	5	308	44/65	0.93	0.27	81,90,105,119	0
20	CLA	5	309	44/65	0.93	0.33	84,103,114,120	0
20	CLA	B	834	44/65	0.93	0.21	98,111,121,136	0
28	LUT	6	303	42/42	0.93	0.37	64,81,96,113	0
20	CLA	3	1006	44/65	0.93	0.24	104,132,140,148	0
20	CLA	8	313	44/65	0.94	0.23	71,101,113,120	0
20	CLA	A	828	44/65	0.94	0.33	112,134,146,155	0
20	CLA	7	1005	44/65	0.94	0.19	64,79,92,106	0
20	CLA	7	1006	44/65	0.94	0.22	62,81,91,104	0
20	CLA	7	1008	44/65	0.94	0.21	73,91,104,129	0
20	CLA	A	817	44/65	0.94	0.18	107,120,144,168	0
20	CLA	5	321	44/65	0.94	0.19	60,71,80,82	0
20	CLA	7	1010	44/65	0.94	0.28	85,104,121,130	0
20	CLA	7	1011	44/65	0.94	0.26	73,87,129,156	0
20	CLA	4	305	44/65	0.94	0.22	76,87,106,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	4	306	44/65	0.94	0.25	71,80,88,96	0
20	CLA	4	307	44/65	0.94	0.23	63,79,93,99	0
20	CLA	7	1014	44/65	0.94	0.26	73,91,97,111	0
20	CLA	4	310	44/65	0.94	0.24	85,107,115,129	0
20	CLA	4	311	44/65	0.94	0.27	63,96,112,119	0
20	CLA	B	827	44/65	0.94	0.25	98,109,123,130	0
20	CLA	A	818	44/65	0.94	0.30	113,142,151,156	0
20	CLA	6	307	44/65	0.94	0.22	65,82,89,92	0
20	CLA	6	308	44/65	0.94	0.25	32,39,48,71	0
20	CLA	A	808	44/65	0.94	0.26	102,112,122,129	0
29	CHL	4	313	51/66	0.94	0.32	86,105,120,132	0
20	CLA	A	851	44/65	0.94	0.29	115,135,143,146	0
20	CLA	8	306	44/65	0.94	0.18	59,71,95,103	0
20	CLA	6	312	44/65	0.94	0.27	59,98,130,141	0
20	CLA	8	307	44/65	0.94	0.28	57,65,89,126	0
20	CLA	A	805	44/65	0.94	0.27	102,121,133,140	0
20	CLA	8	310	44/65	0.94	0.26	51,72,106,148	0
20	CLA	5	301	44/65	0.94	0.27	71,78,106,120	0
20	CLA	3	1015	44/65	0.94	0.25	99,108,120,132	0
20	CLA	5	305	44/65	0.94	0.20	66,81,103,125	0
20	CLA	B	832	44/65	0.94	0.26	143,153,171,179	0
20	CLA	A	807	44/65	0.94	0.27	117,131,148,155	0
20	CLA	4	304	44/65	0.95	0.30	74,83,90,101	0
20	CLA	A	802	44/65	0.95	0.22	68,90,128,167	0
20	CLA	A	839	44/65	0.95	0.23	70,83,98,111	0
20	CLA	A	829	44/65	0.95	0.22	90,109,125,128	0
20	CLA	1	1006	44/65	0.95	0.25	56,75,91,94	0
20	CLA	4	309	44/65	0.95	0.21	69,79,107,136	0
20	CLA	A	806	44/65	0.95	0.22	92,115,135,141	0
20	CLA	8	309	44/65	0.95	0.21	75,95,102,114	0
20	CLA	3	1005	44/65	0.95	0.25	78,106,124,128	0
20	CLA	B	805	44/65	0.95	0.27	87,109,132,149	0
20	CLA	5	307	44/65	0.95	0.24	52,64,76,83	0
29	CHL	5	317	43/66	0.95	0.28	80,97,120,132	0
20	CLA	6	306	44/65	0.95	0.20	68,87,93,118	0
20	CLA	1	1011	44/65	0.95	0.30	99,108,125,138	0
20	CLA	3	1016	44/65	0.95	0.24	66,74,123,169	0
20	CLA	7	1007	44/65	0.95	0.25	52,60,67,75	0
29	CHL	3	1014	47/66	0.95	0.27	83,110,124,131	0
29	CHL	5	316	61/66	0.96	0.34	54,73,167,176	0
20	CLA	7	1004	44/65	0.96	0.22	40,58,84,93	0
20	CLA	A	827	44/65	0.96	0.32	110,133,141,161	0

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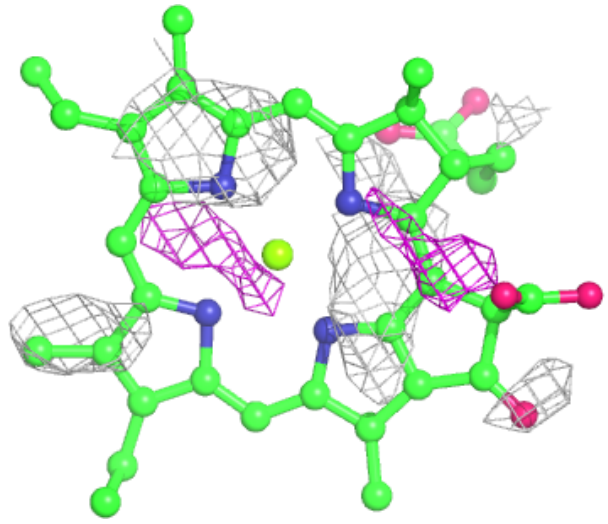
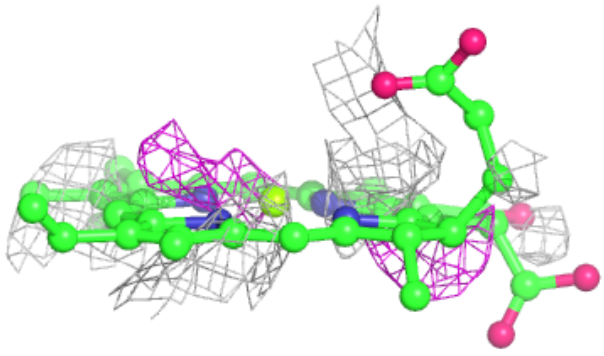
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	A	837	44/65	0.96	0.24	91,107,122,126	0
29	CHL	6	317	43/66	0.96	0.21	85,96,129,160	0
20	CLA	8	305	44/65	0.96	0.26	75,87,99,115	0
29	CHL	5	314	51/66	0.96	0.31	64,82,117,121	0
20	CLA	6	305	44/65	0.97	0.24	44,58,76,90	0
21	SF4	A	841	8/8	0.99	0.25	110,119,124,131	0
21	SF4	C	1001	8/8	0.99	0.13	136,146,148,158	0
21	SF4	C	1002	8/8	0.99	0.09	143,149,158,161	0

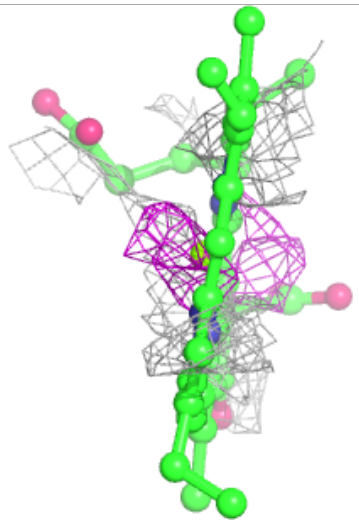
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CLA L 204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

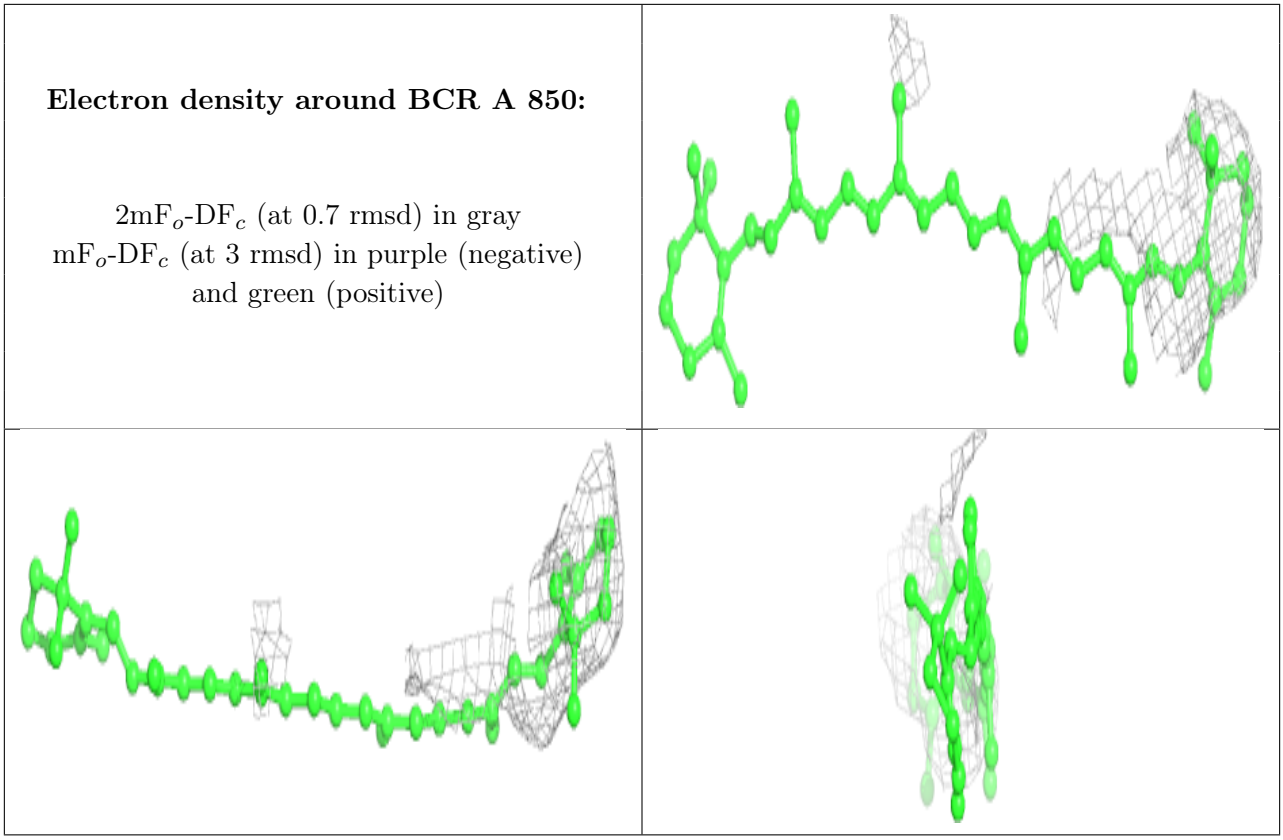






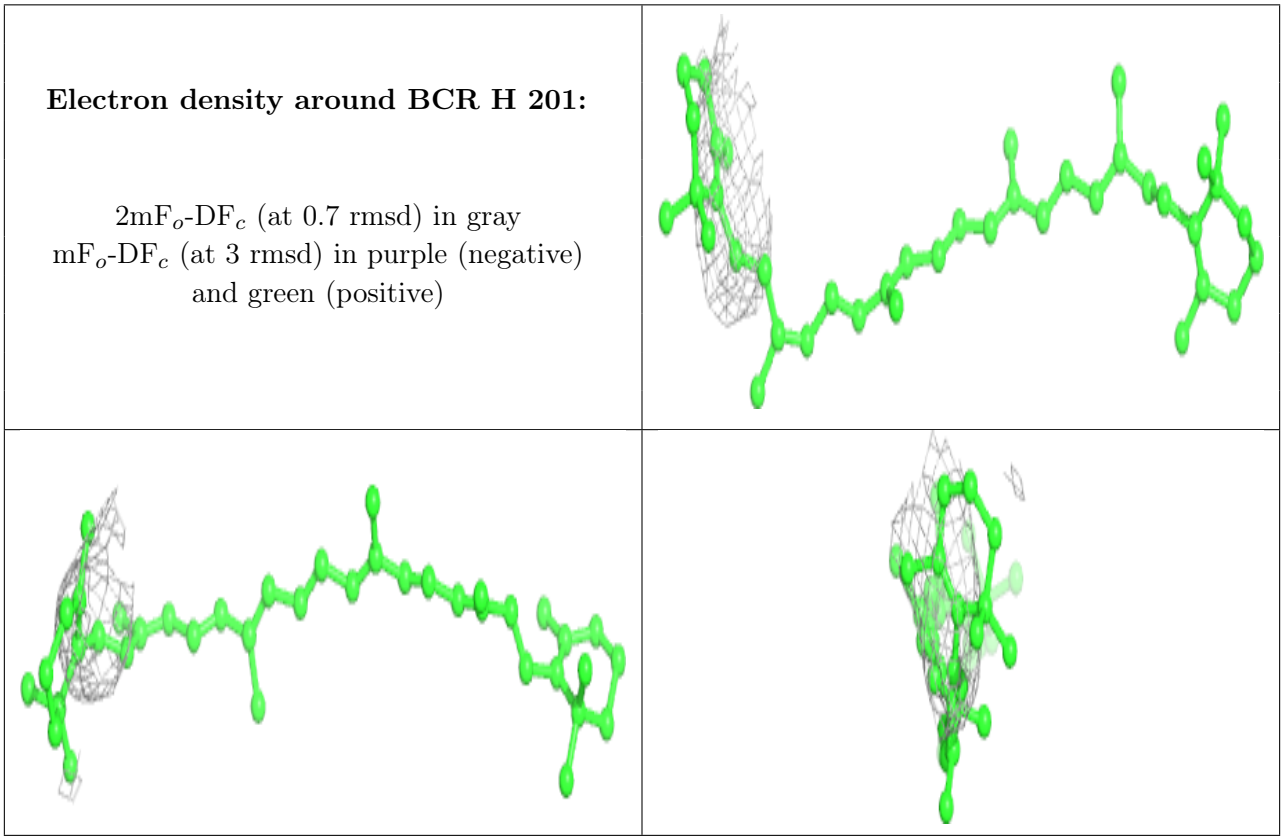
Electron density around BCR A 850:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



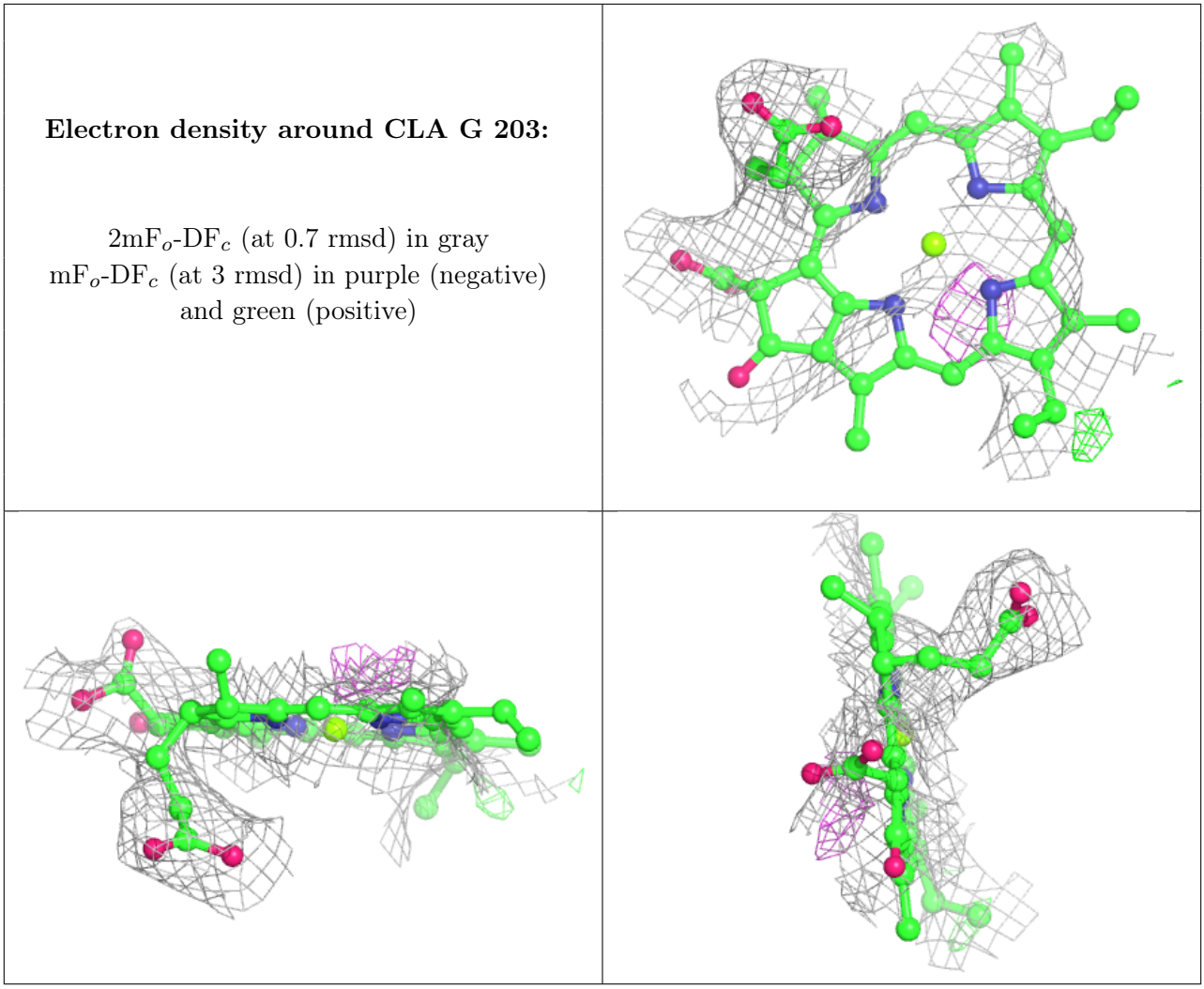
Electron density around BCR H 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



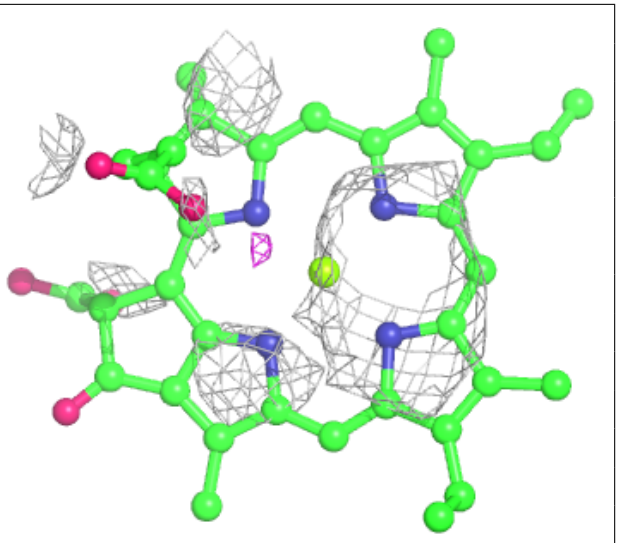
Electron density around CLA G 203:

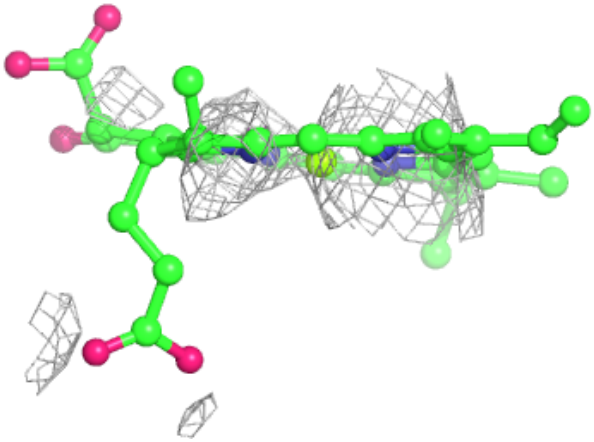
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

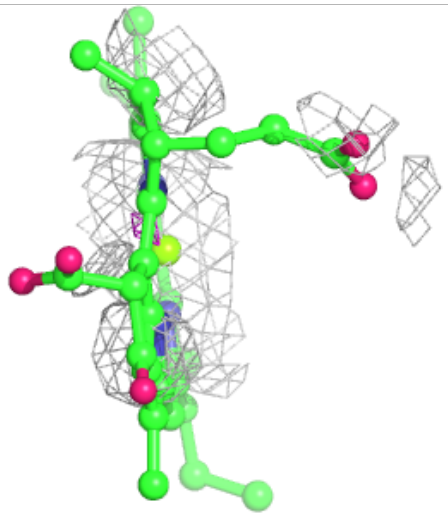


Electron density around CLA L 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

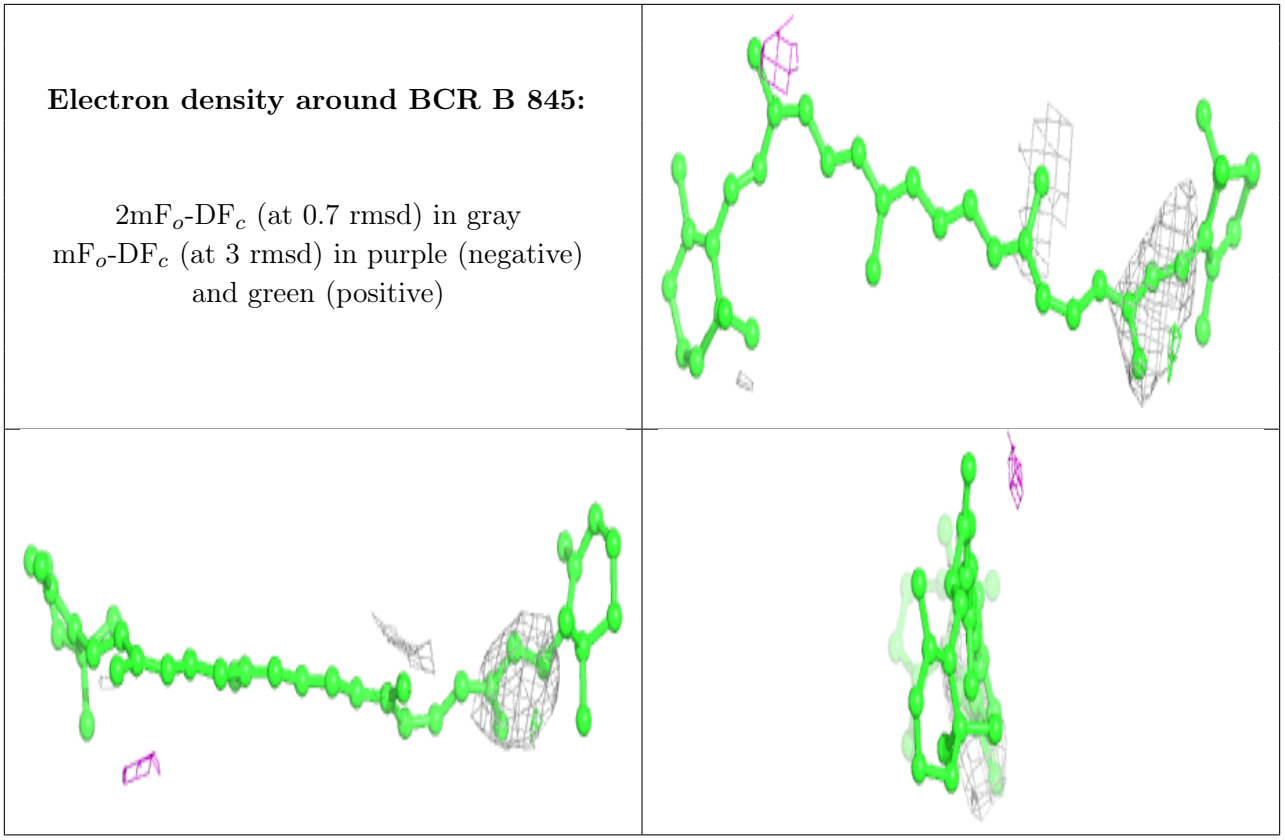






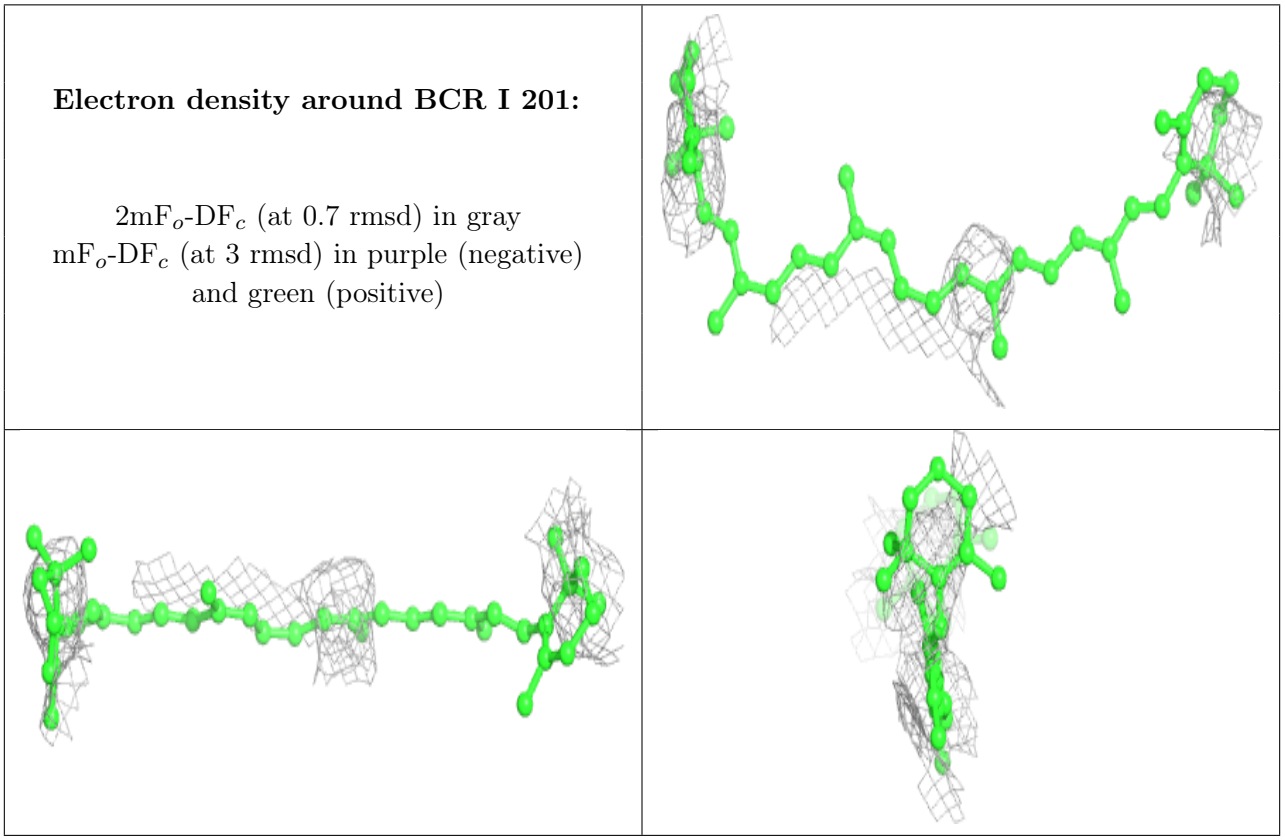
Electron density around BCR B 845:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



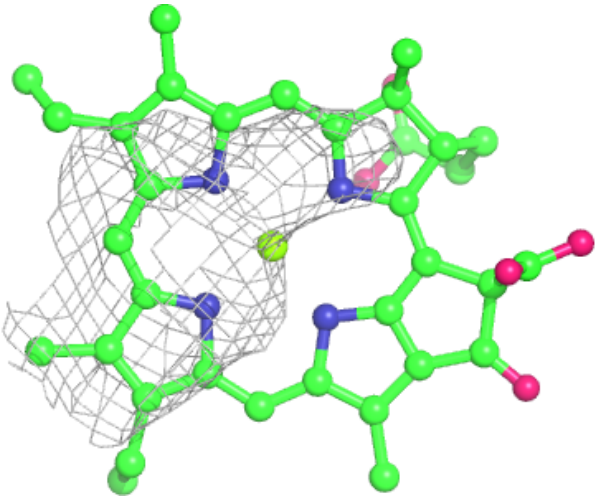
Electron density around BCR I 201:

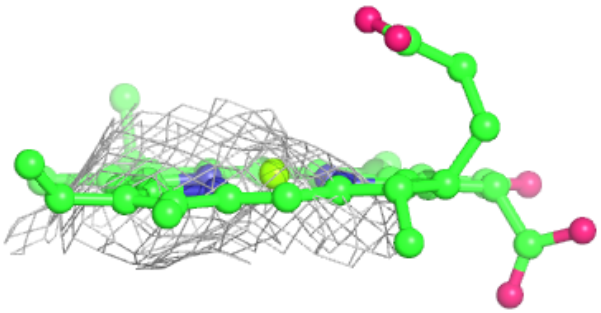
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

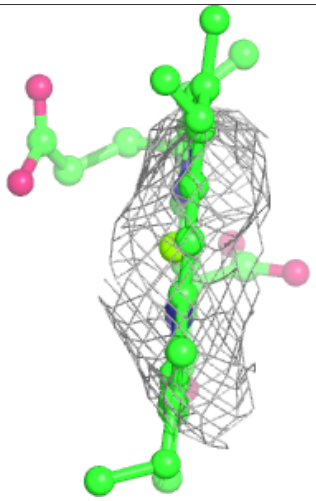


Electron density around CLA L 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

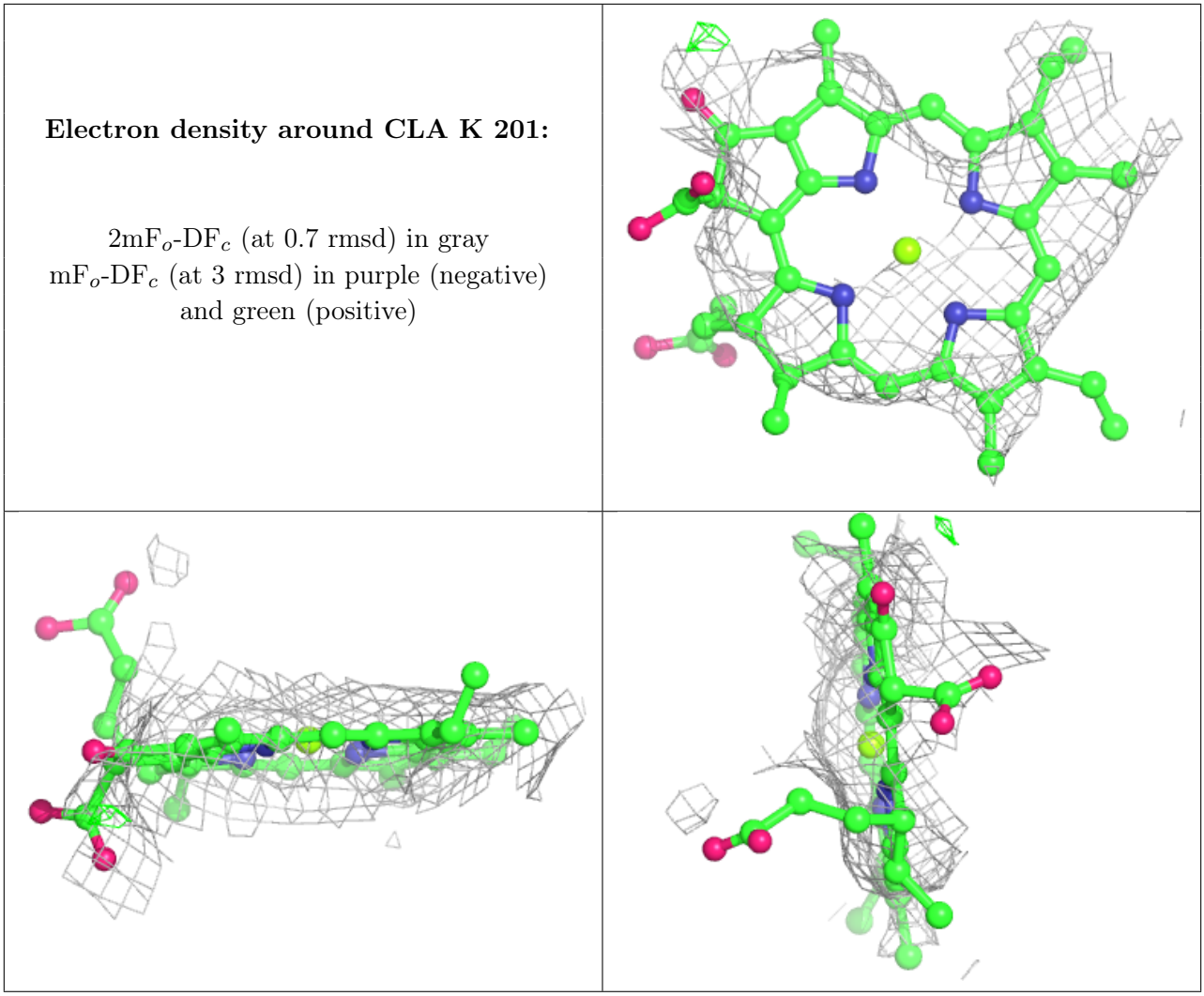






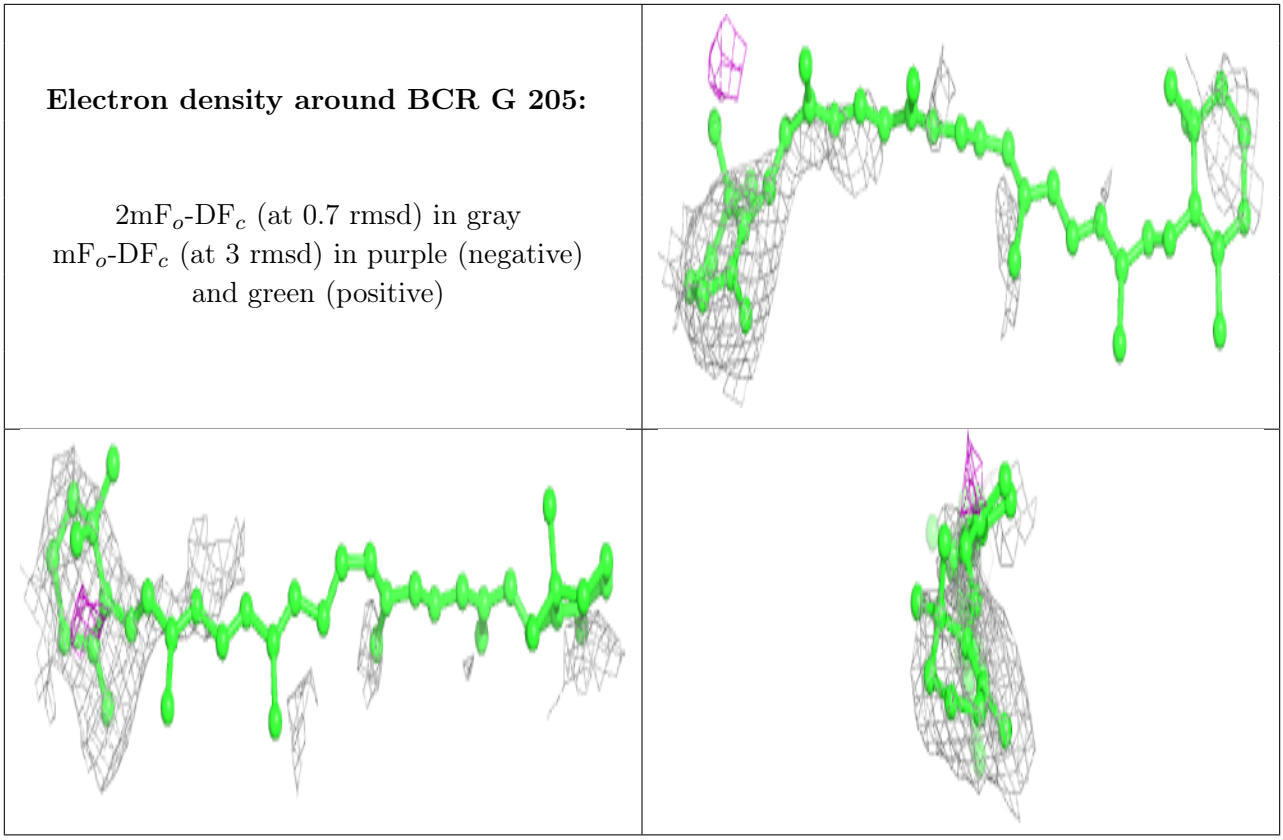
Electron density around CLA K 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



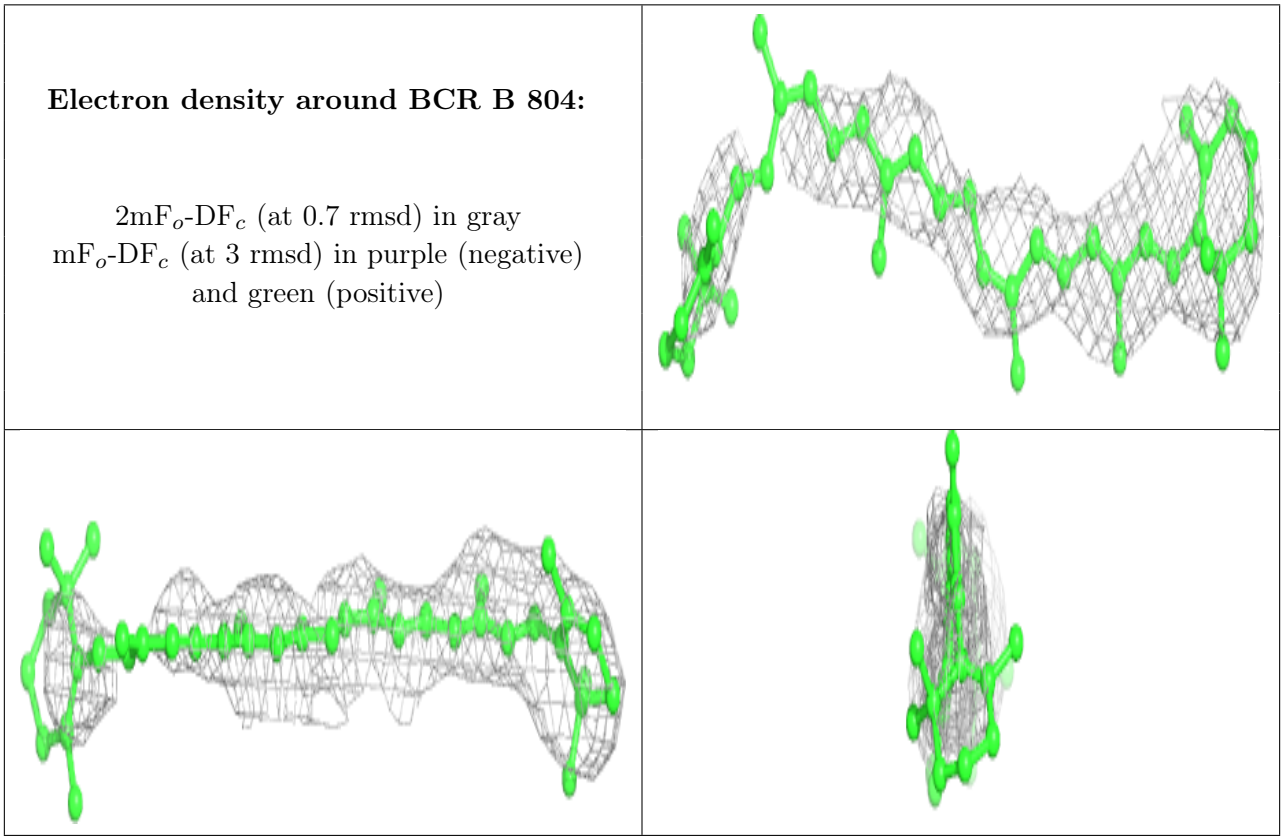
Electron density around BCR G 205:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



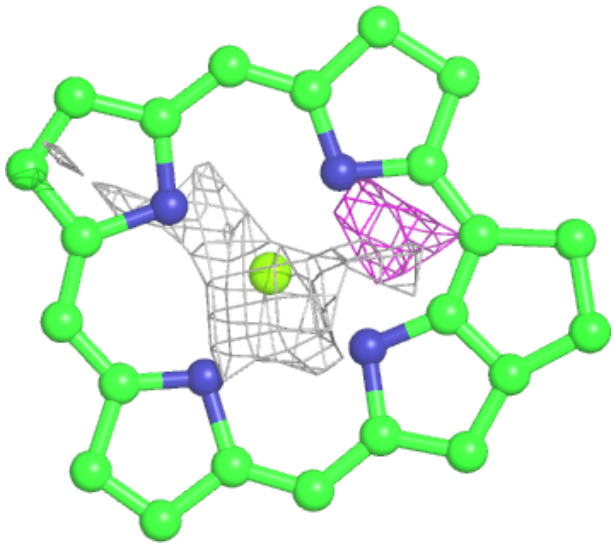
Electron density around BCR B 804:

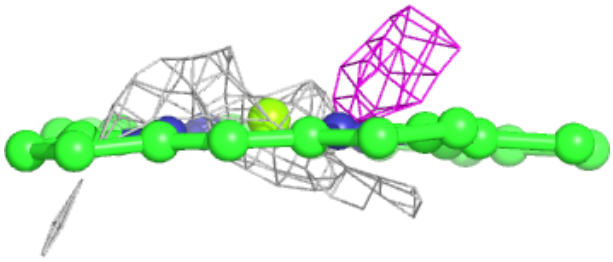
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

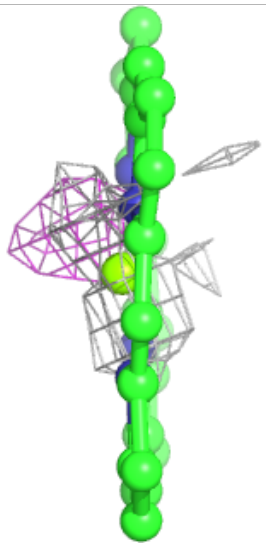


Electron density around CLA K 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

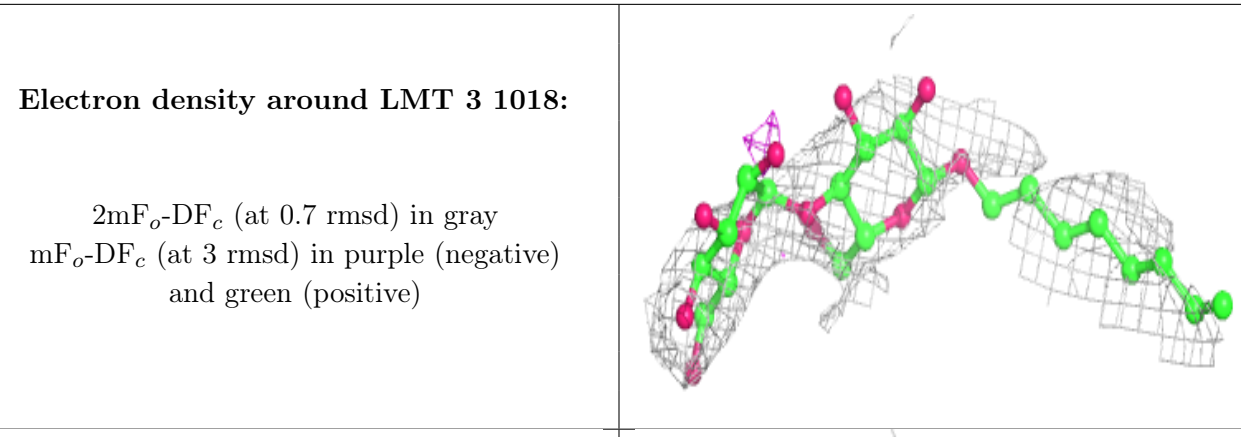






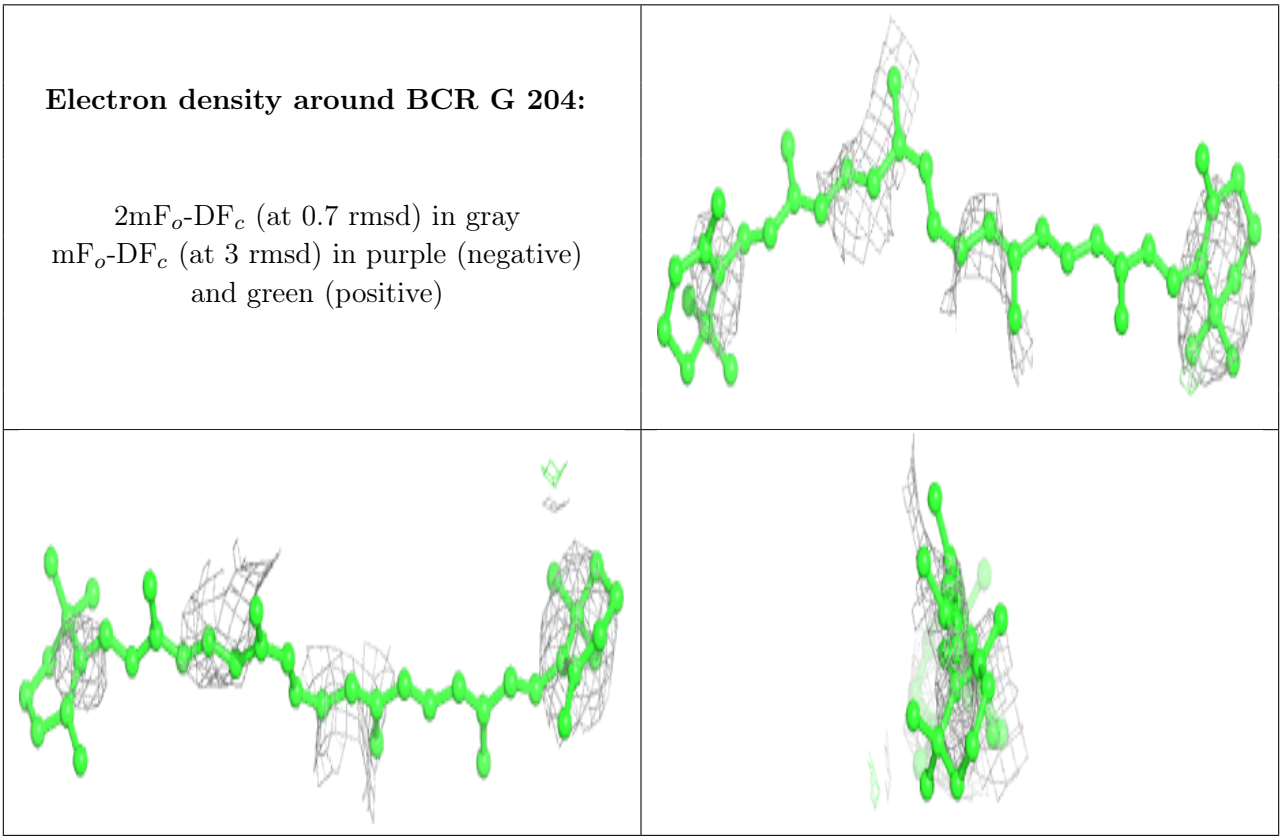
Electron density around LMT 3 1018:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



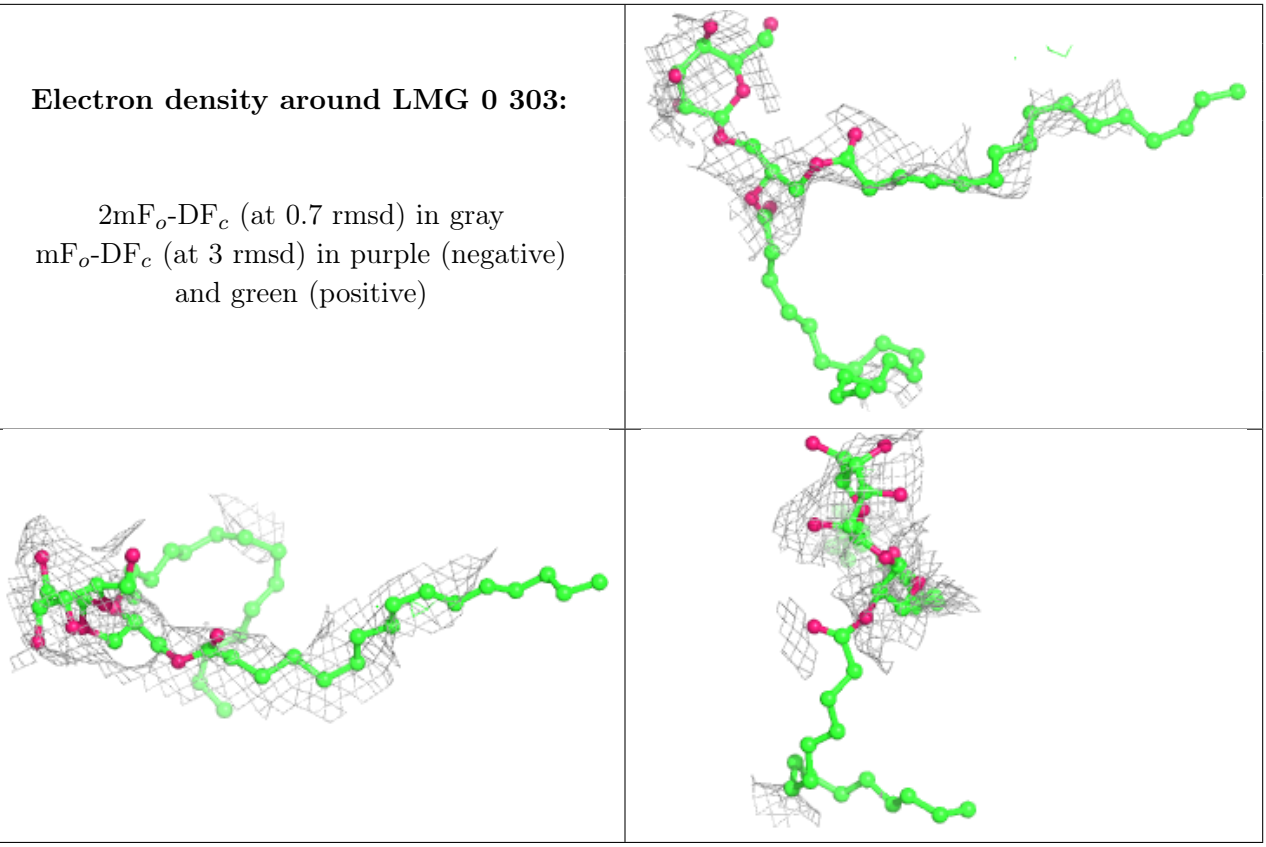
Electron density around BCR G 204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



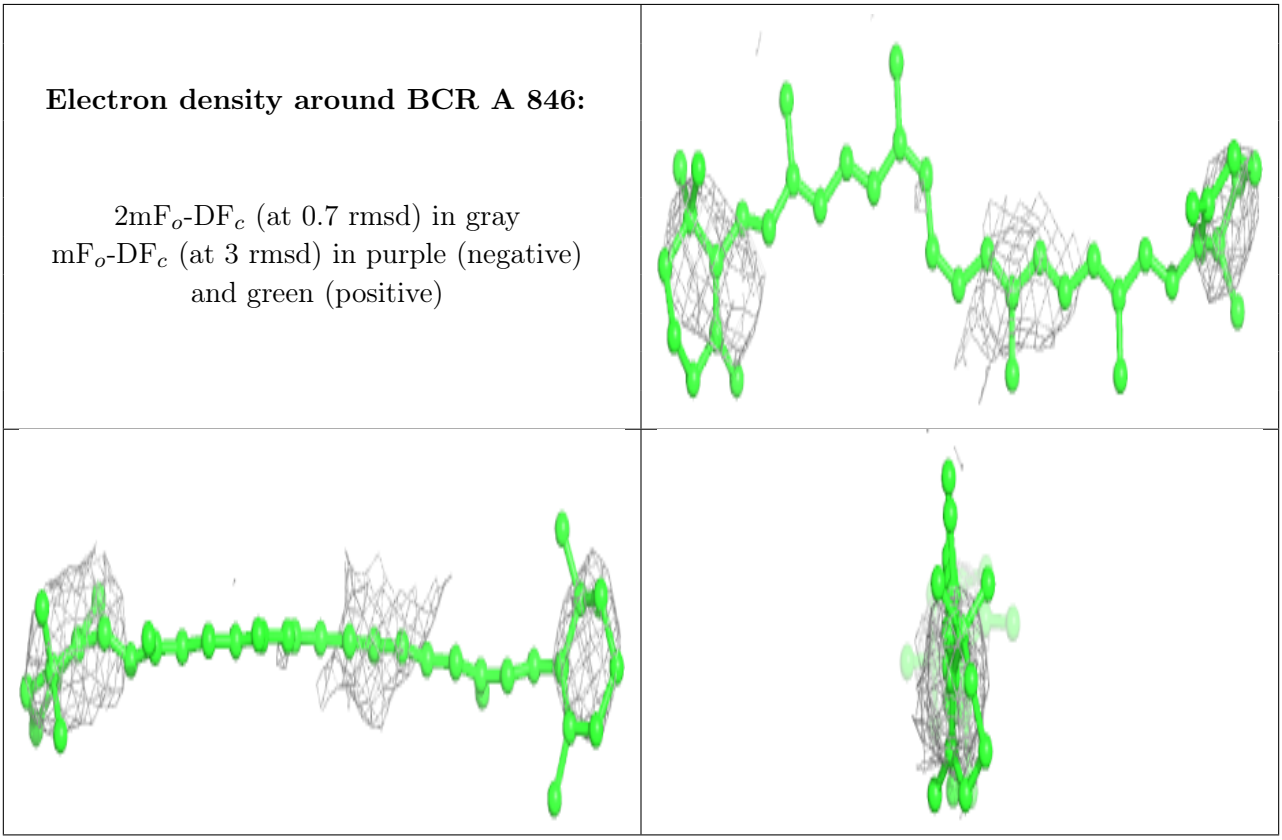
Electron density around LMG 0 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



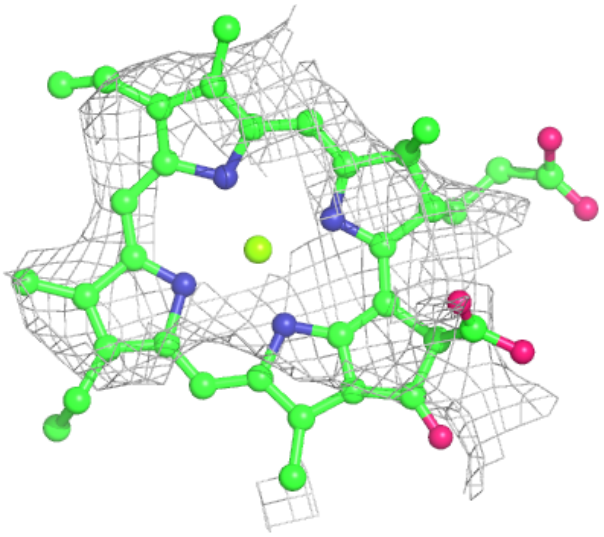
Electron density around BCR A 846:

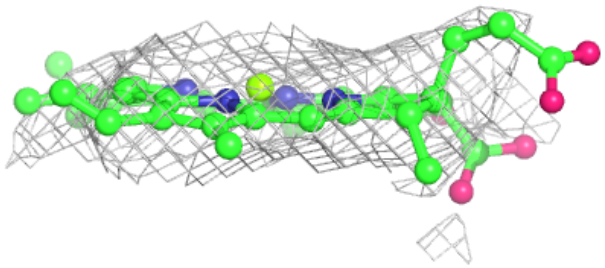
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

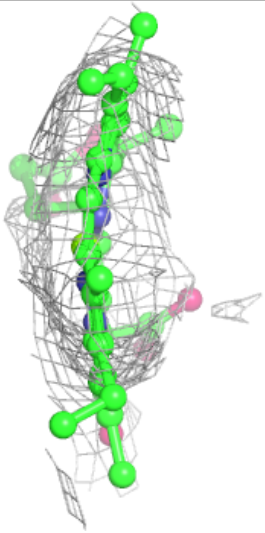


Electron density around CLA B 813:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

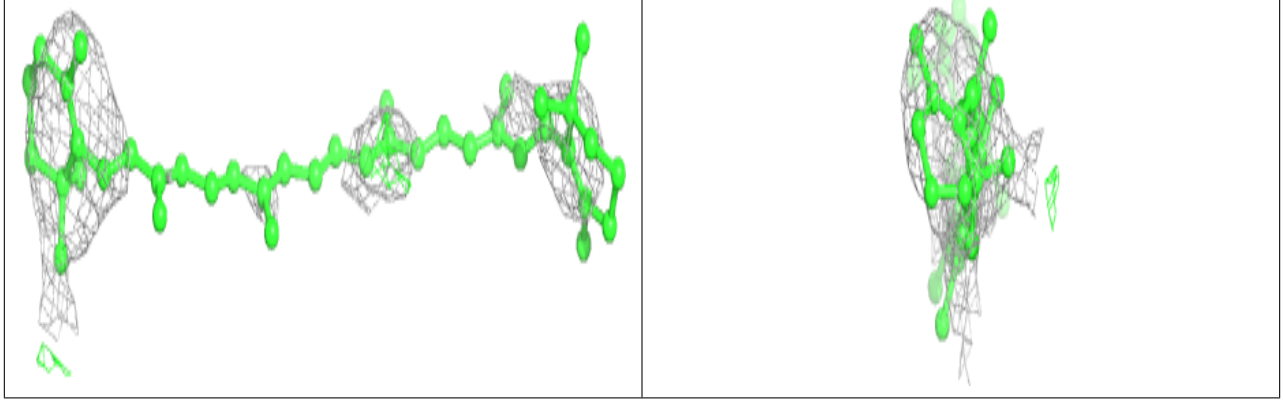






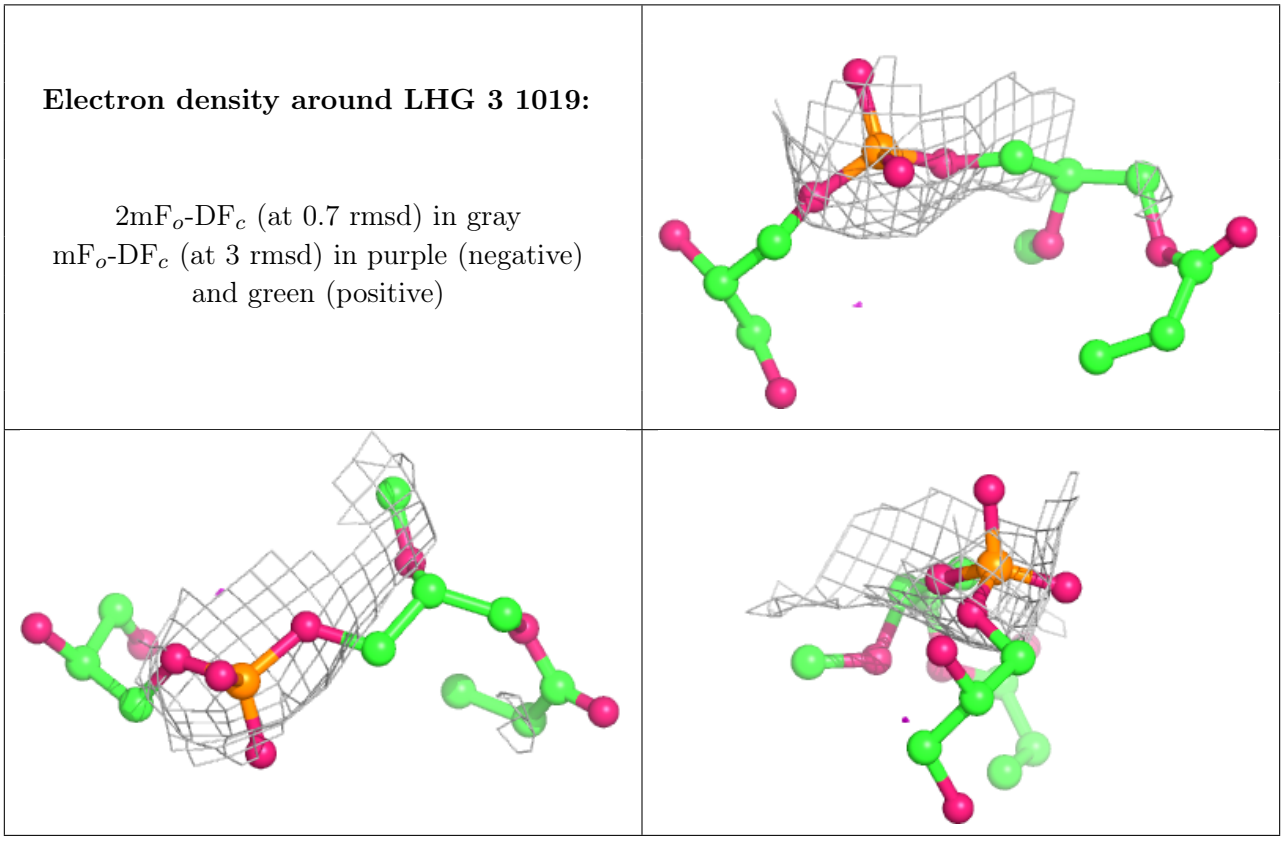
Electron density around BCR B 847:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



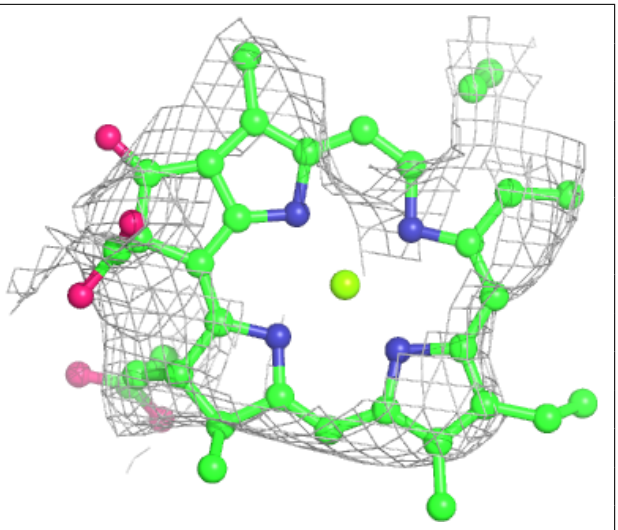
Electron density around LHG 3 1019:

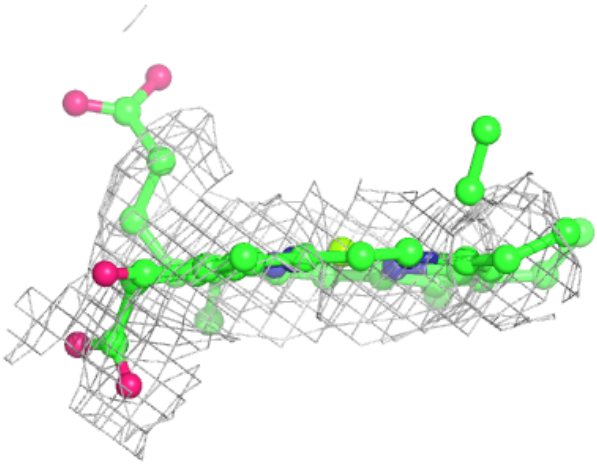
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

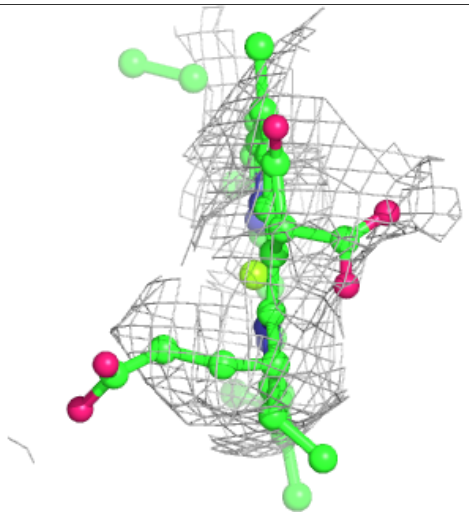


Electron density around CLA B 850:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

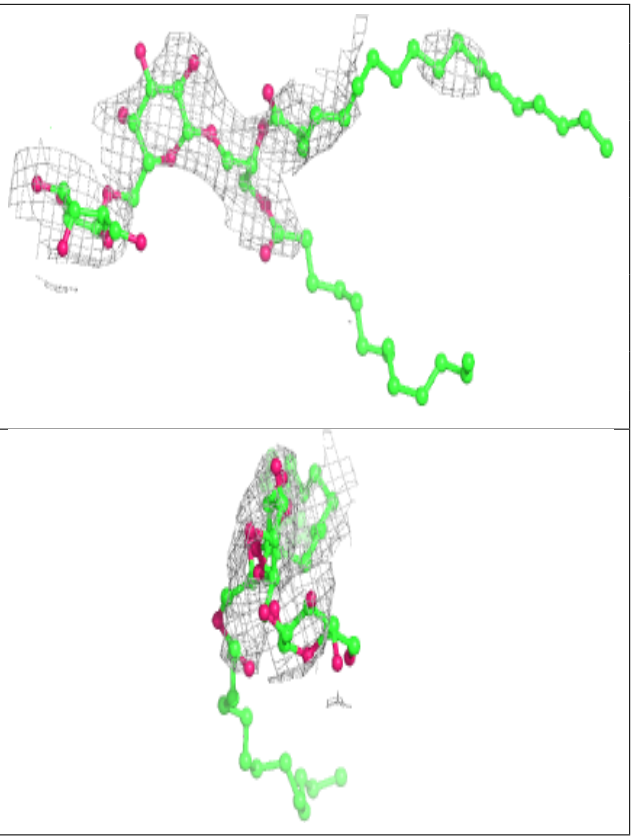






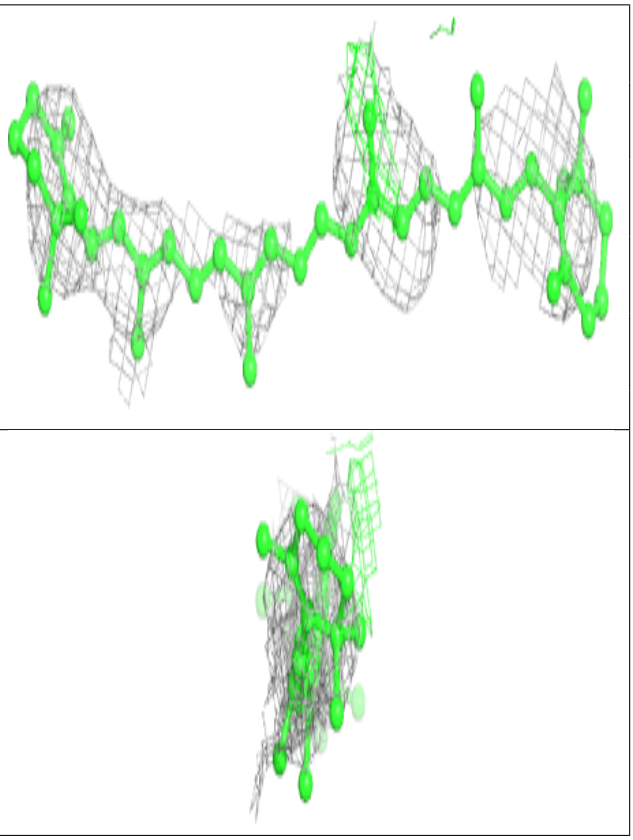
Electron density around DGD B 848:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



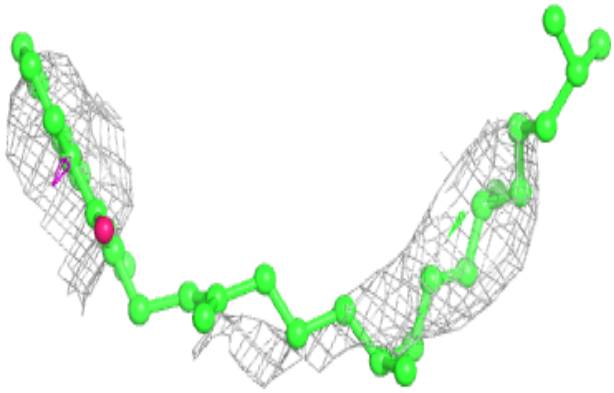
Electron density around BCR A 844:

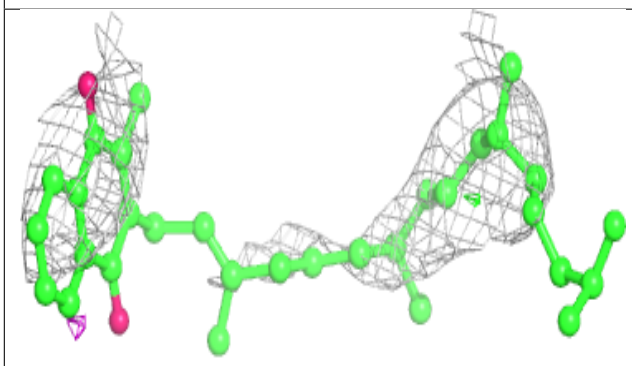
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

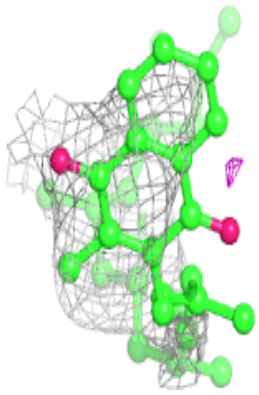


Electron density around PQN B 842:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

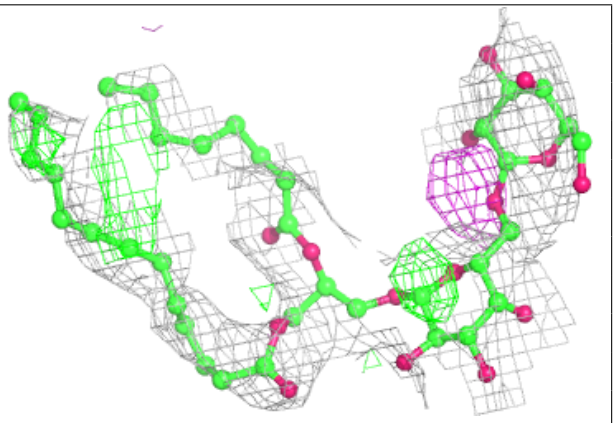


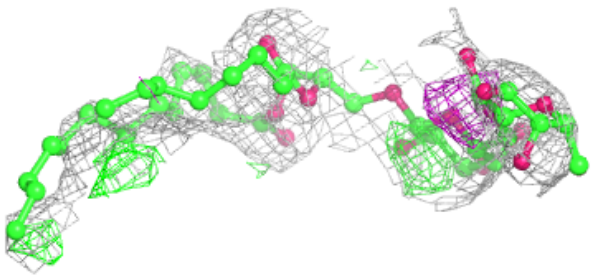


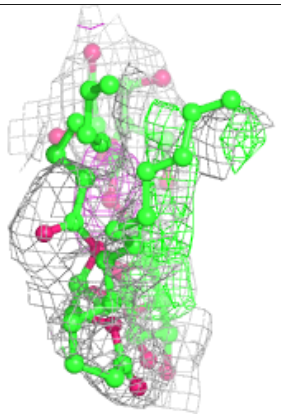


Electron density around DGD 5 319:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

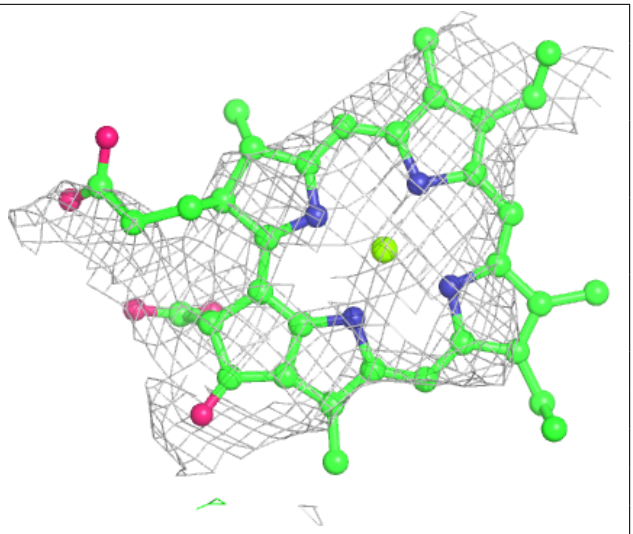


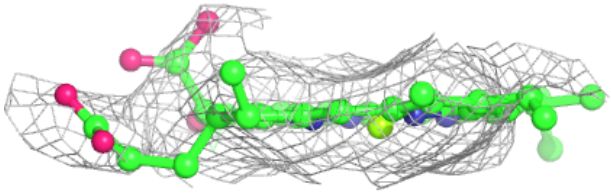


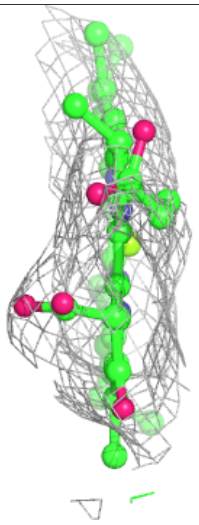


Electron density around CLA B 826:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

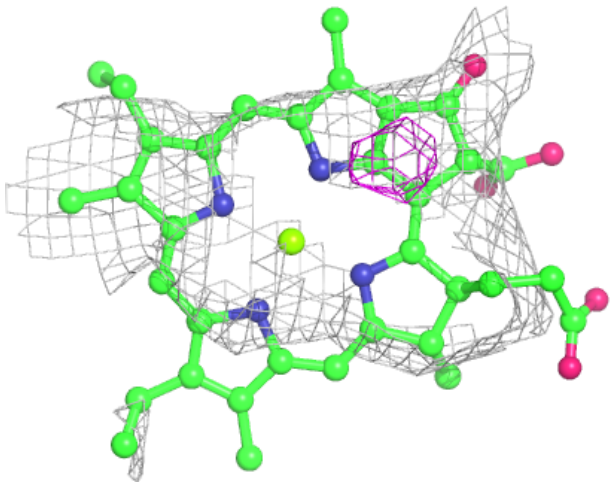


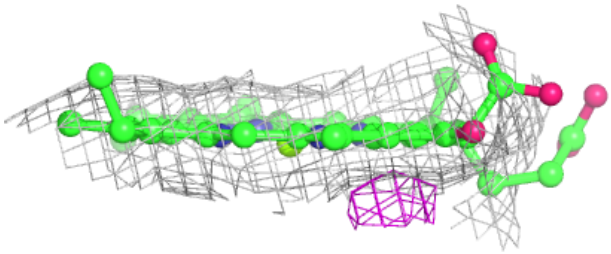


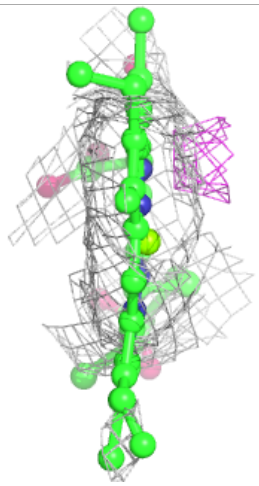


Electron density around CLA G 202:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

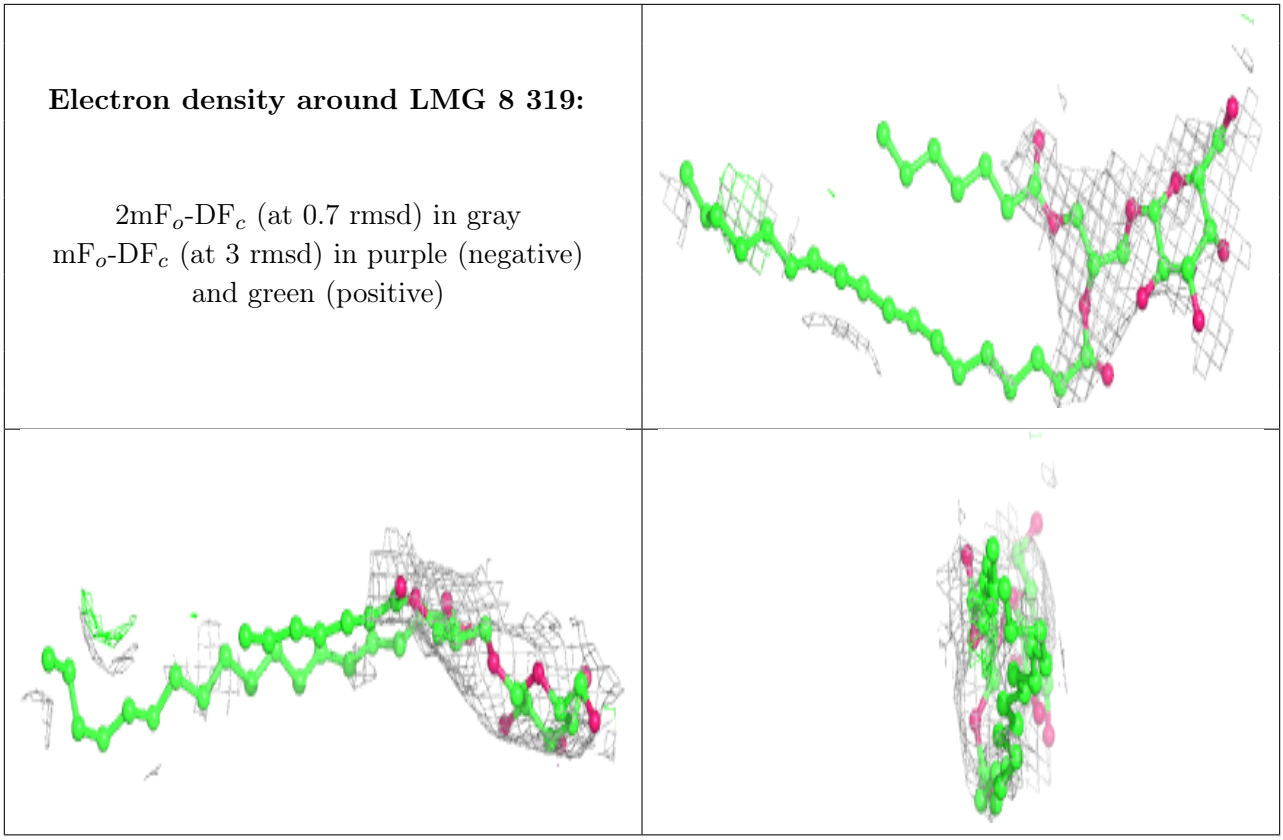






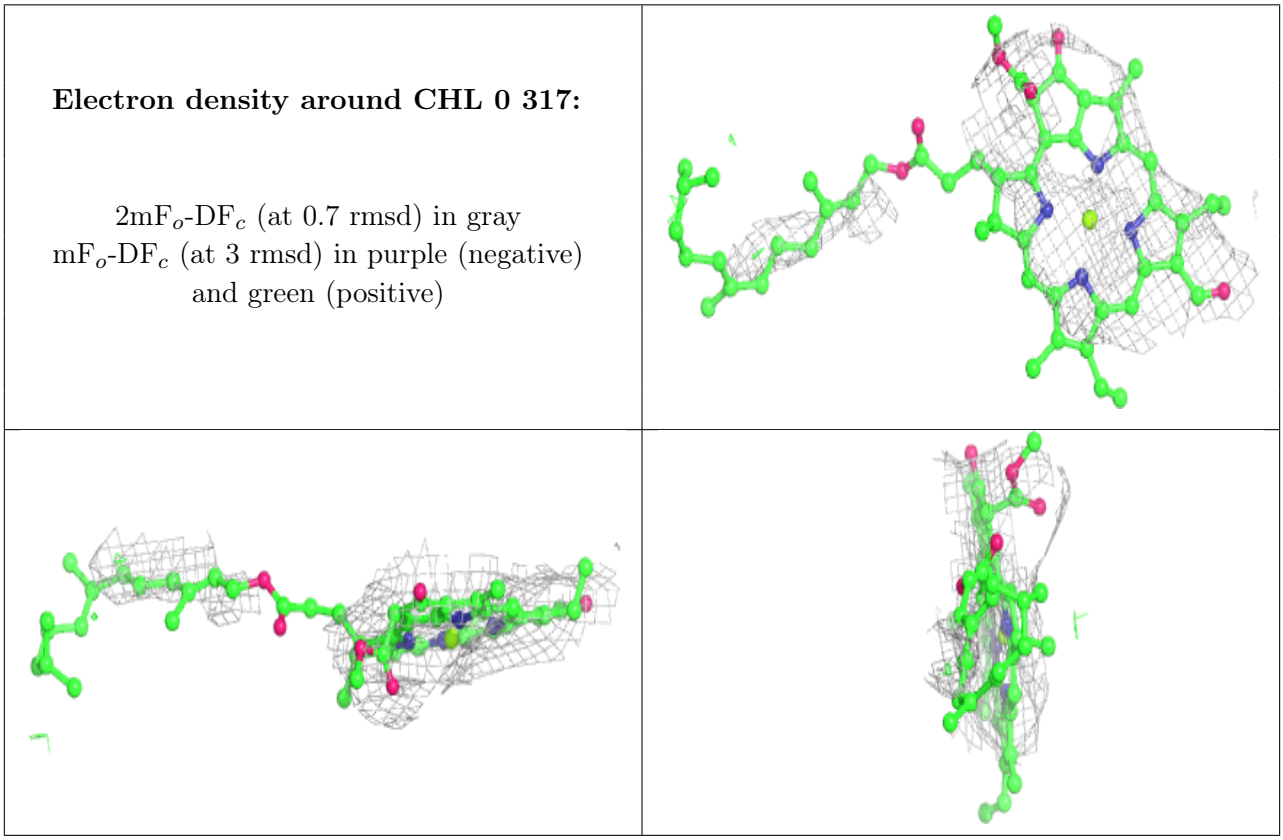
Electron density around LMG 8 319:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



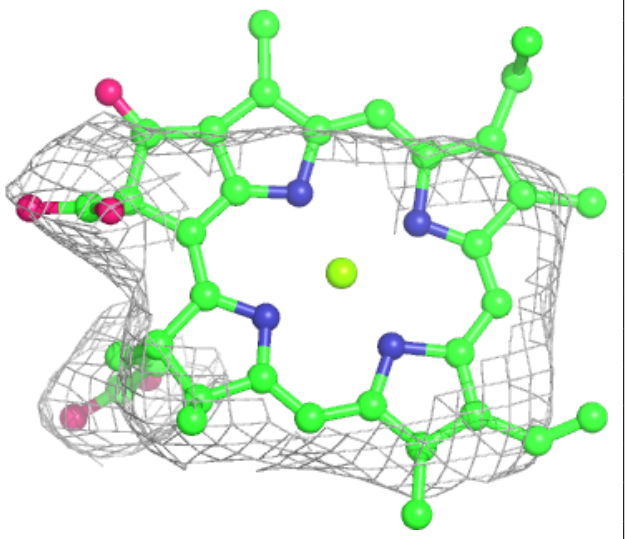
Electron density around CHL 0 317:

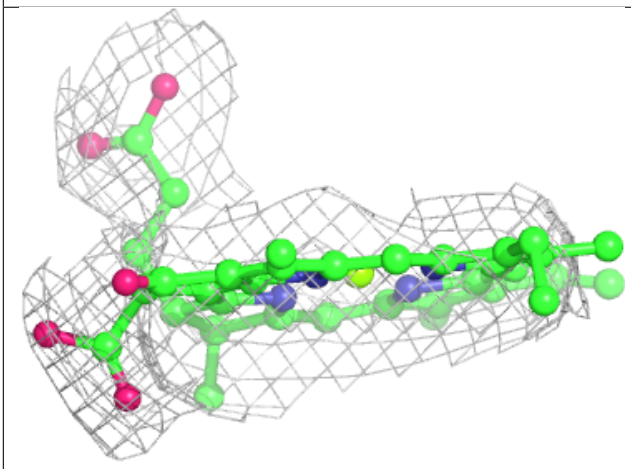
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

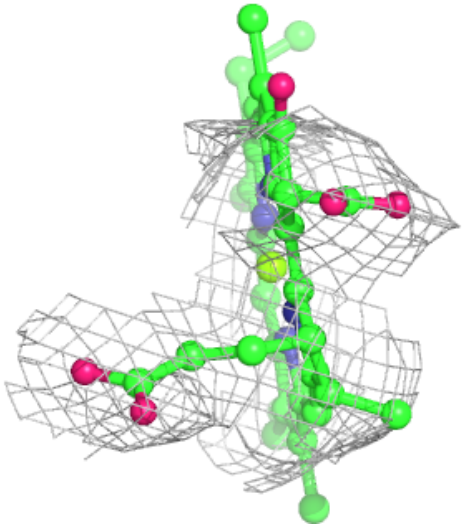


Electron density around CLA B 814:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

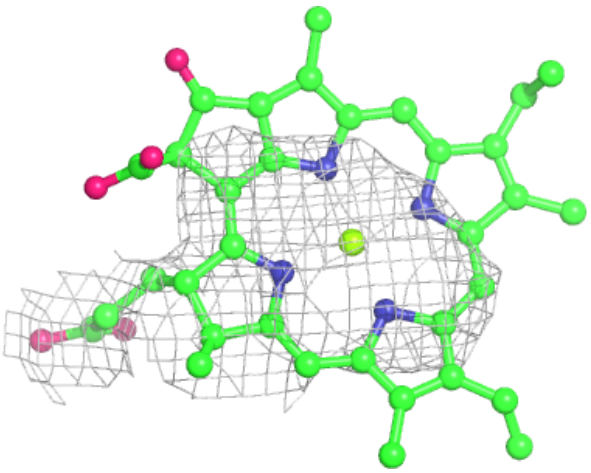


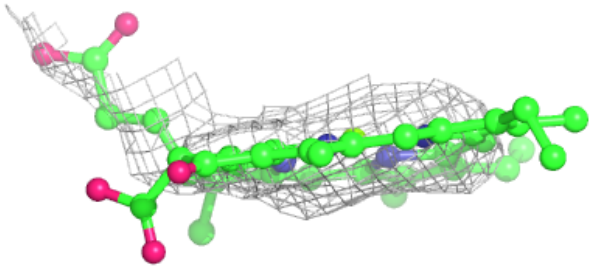


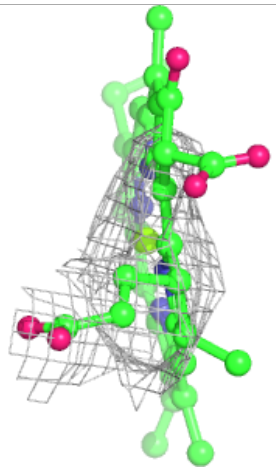


Electron density around CLA G 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

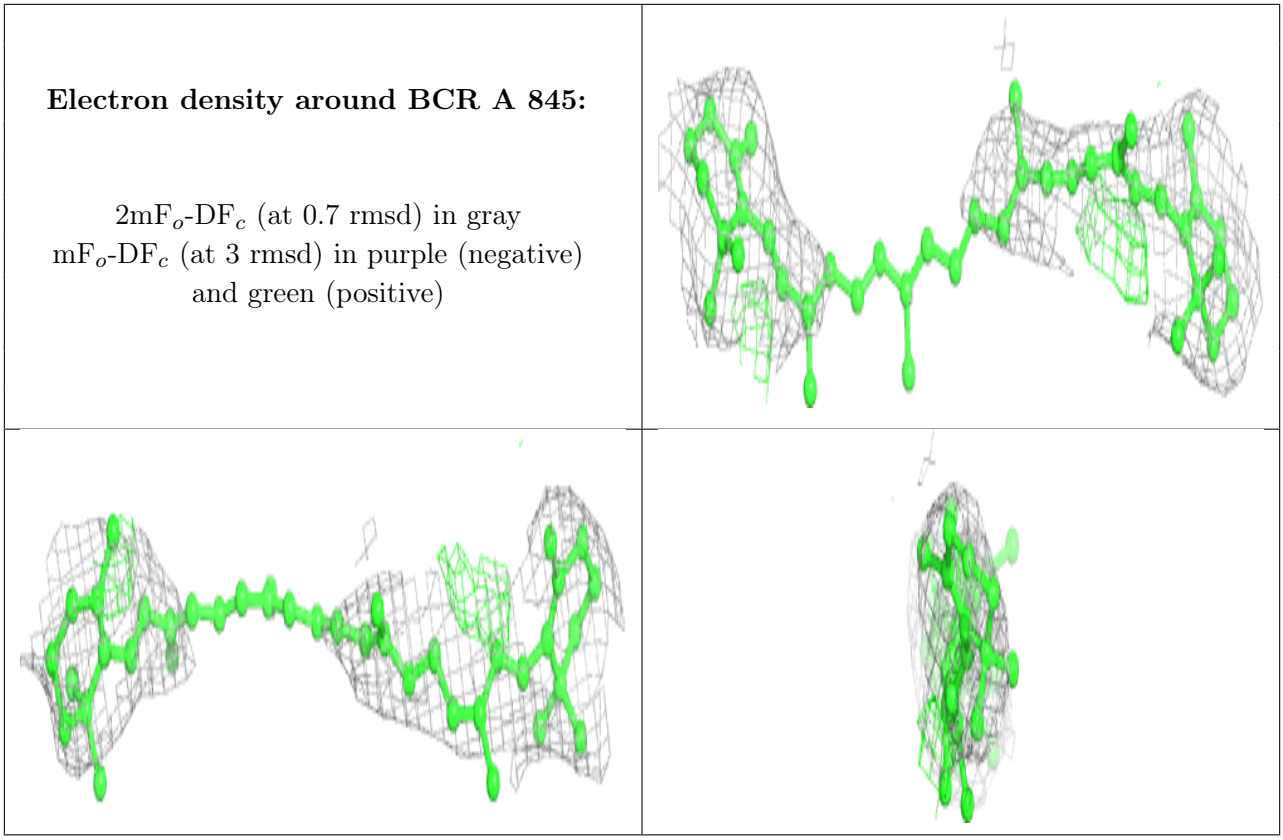






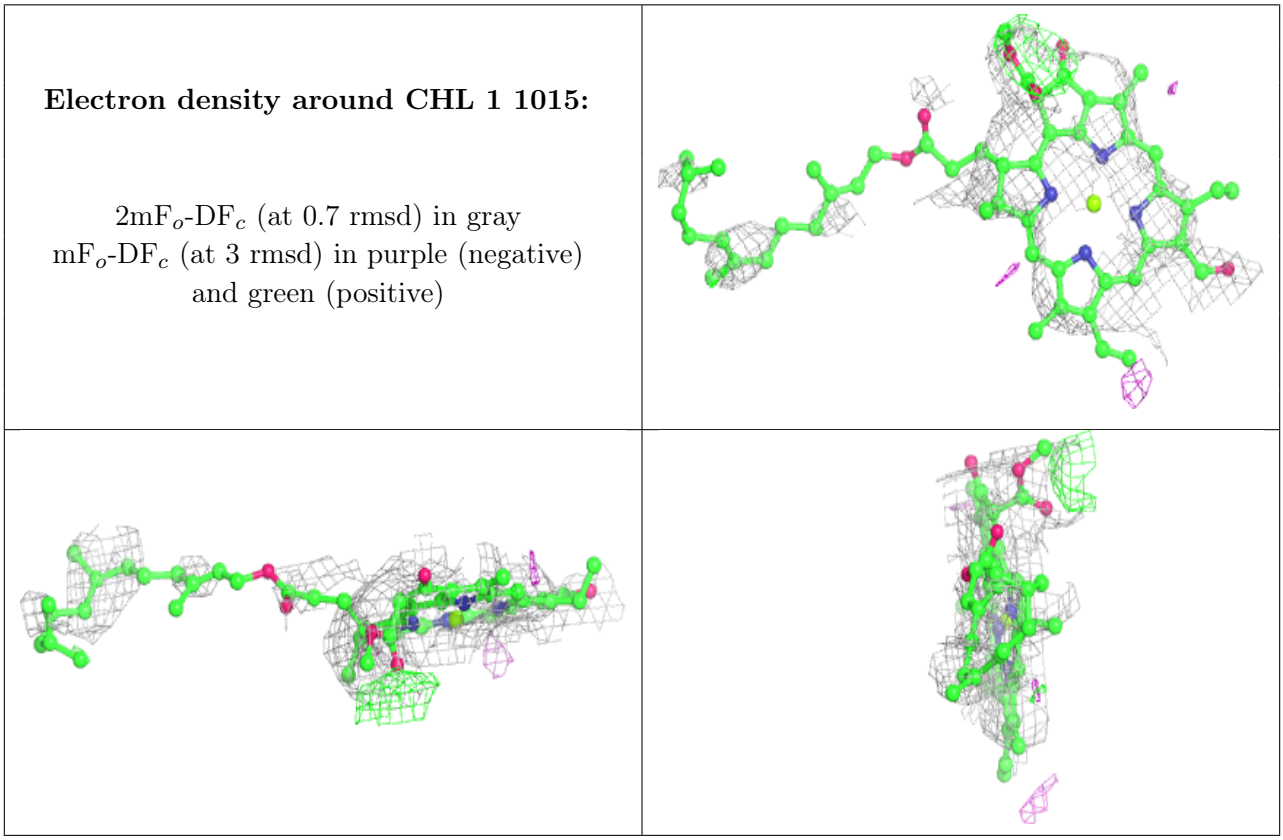
Electron density around BCR A 845:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



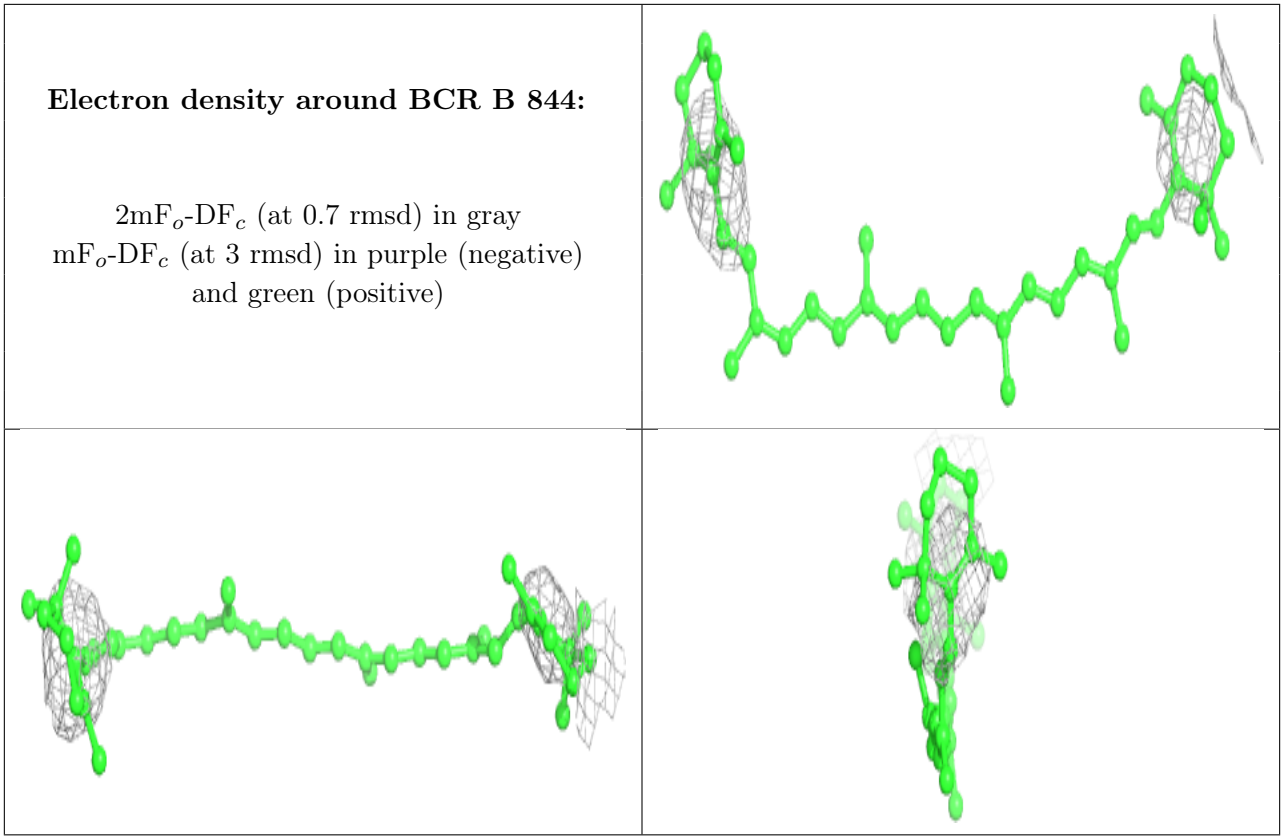
Electron density around CHL 1 1015:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



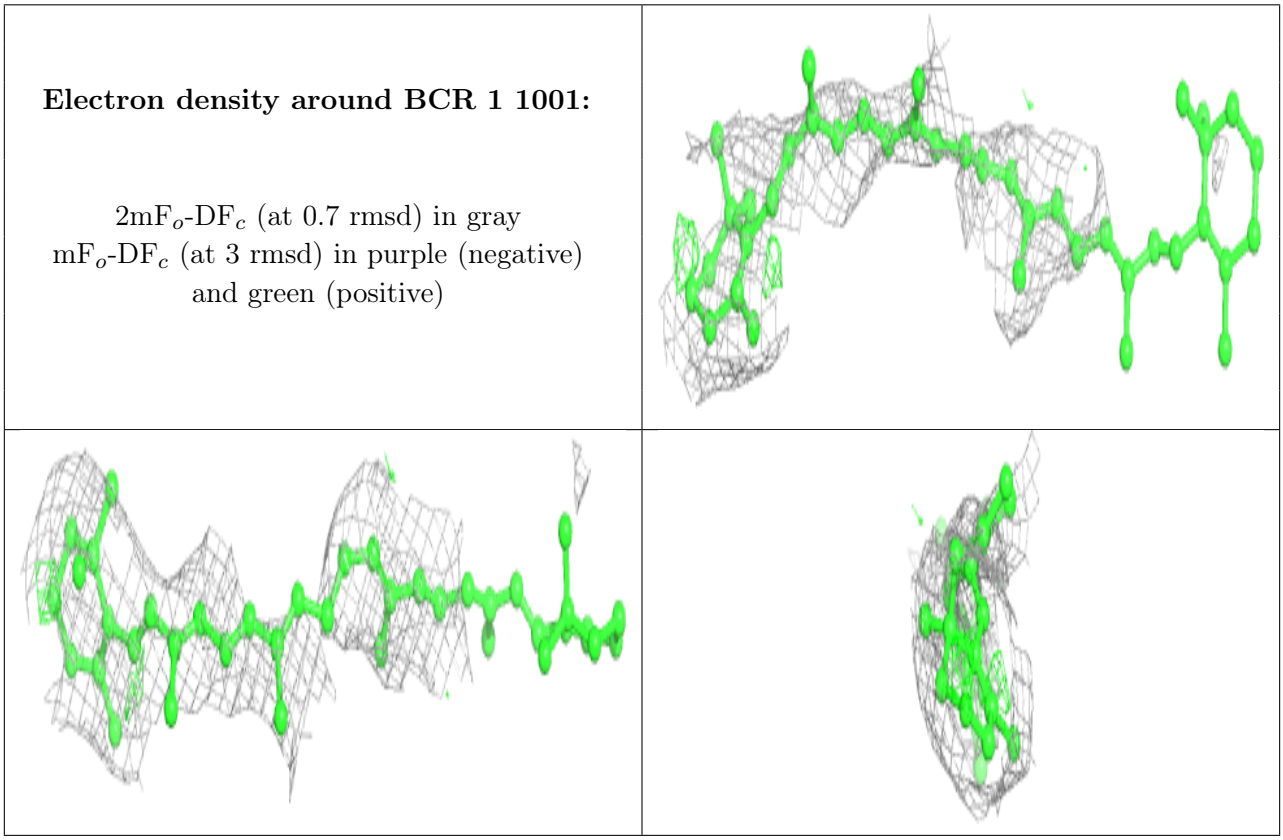
Electron density around BCR B 844:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



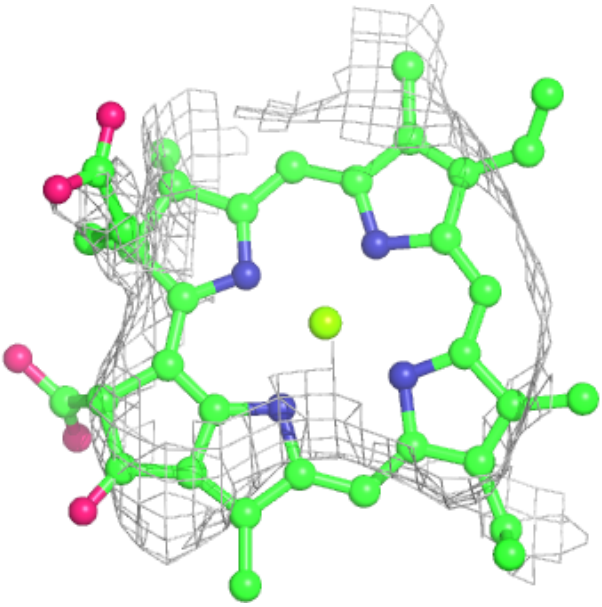
Electron density around BCR 1 1001:

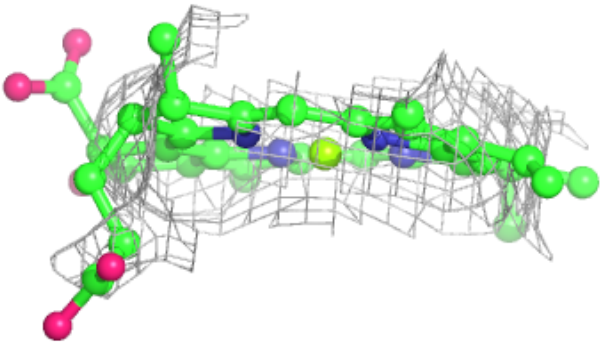
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA A 840:

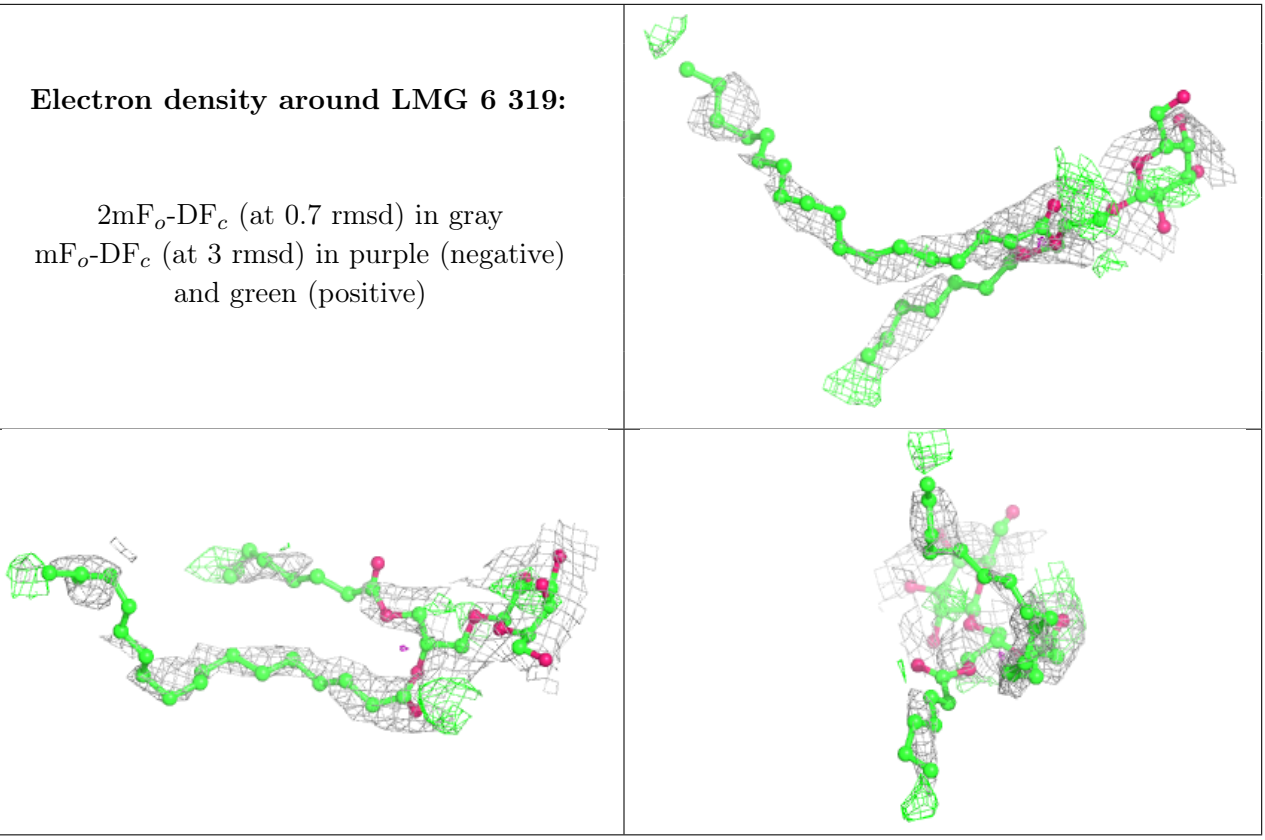
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





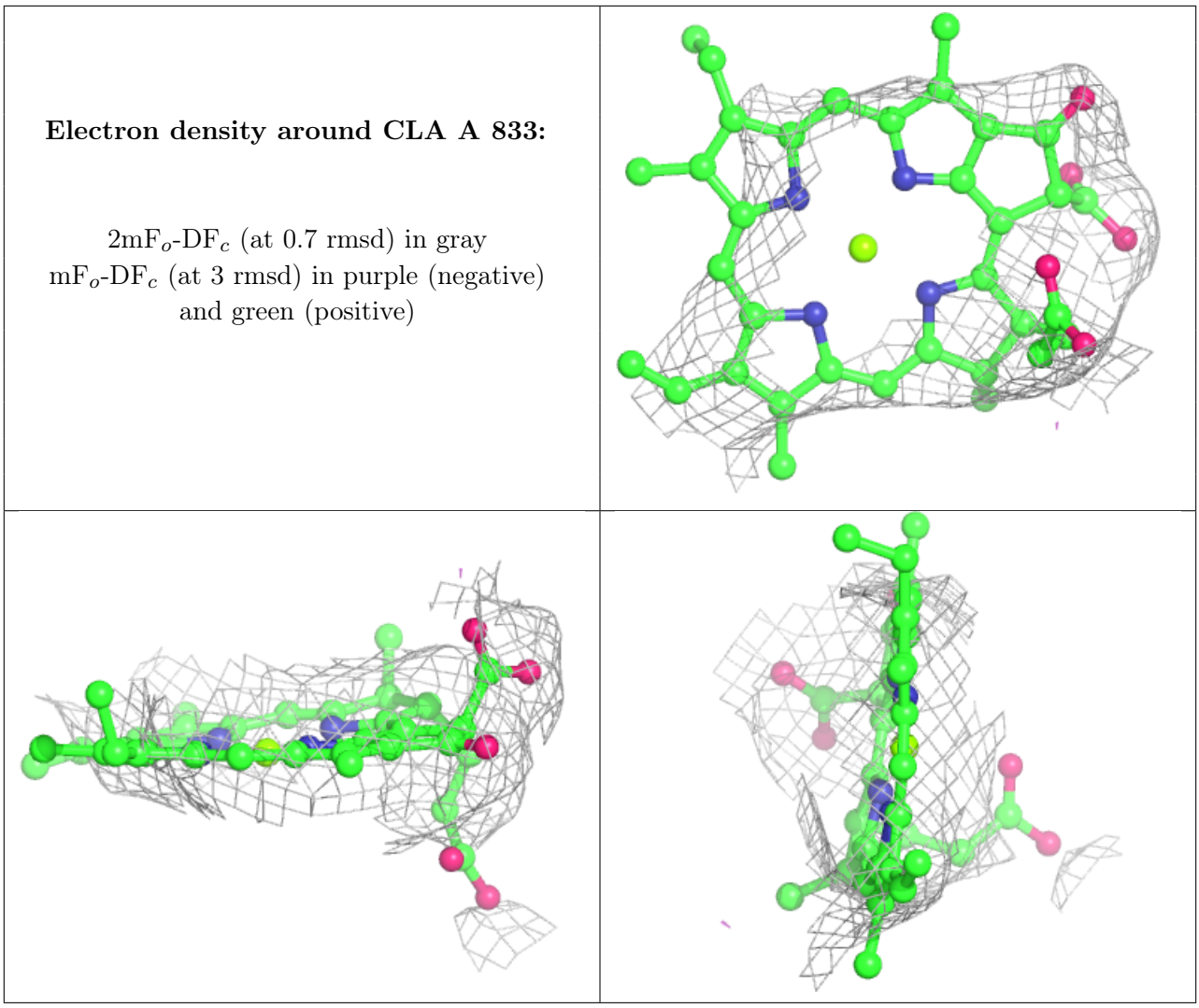
Electron density around LMG 6 319:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



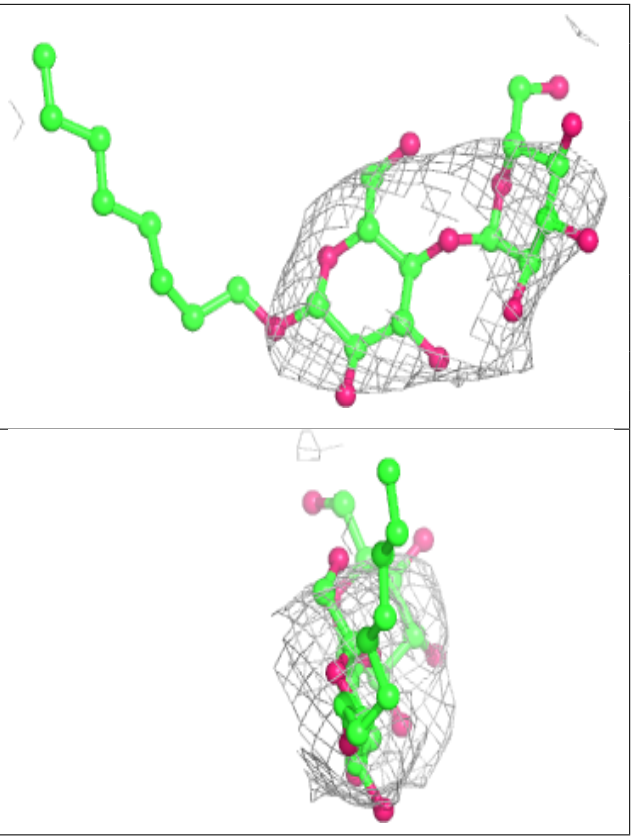
Electron density around CLA A 833:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



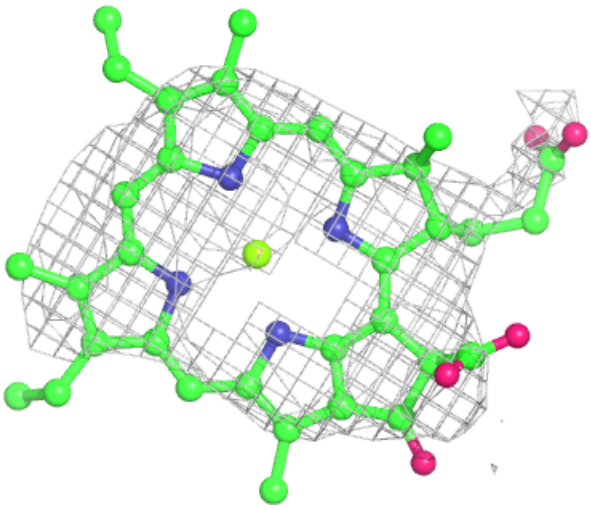
Electron density around LMT B 849:

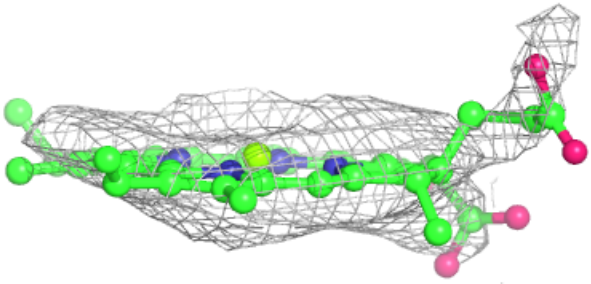
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

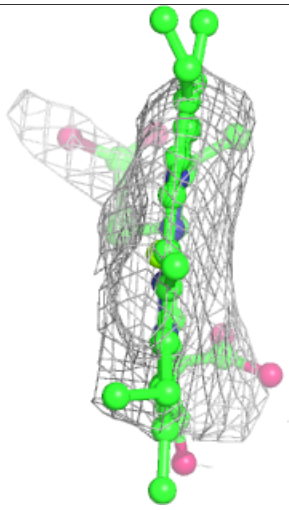


Electron density around CLA B 816:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

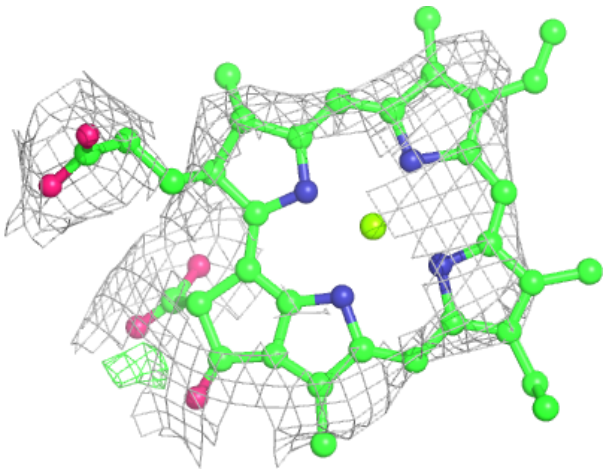


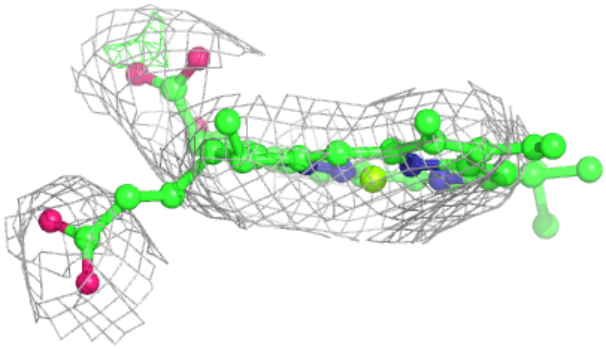


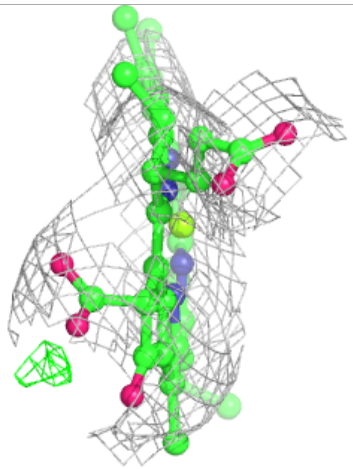


Electron density around CLA A 824:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

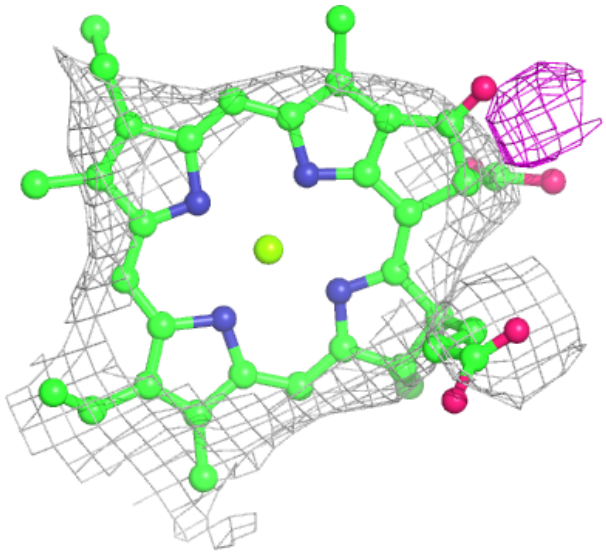


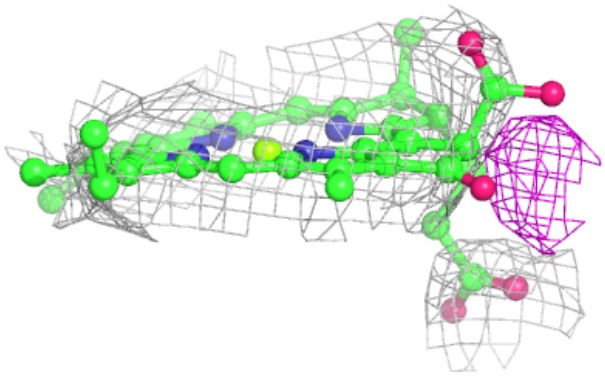


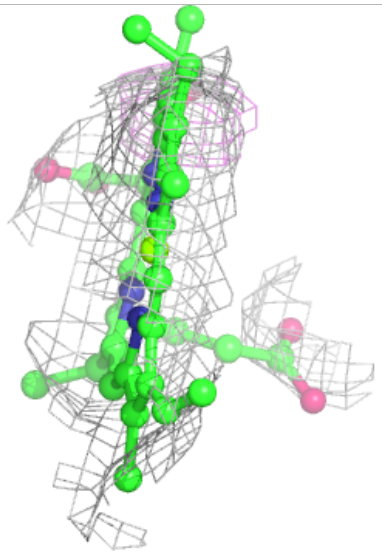


Electron density around CLA B 836:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

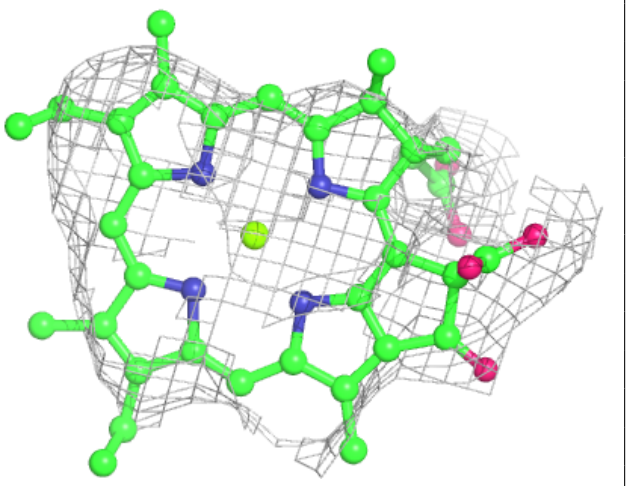


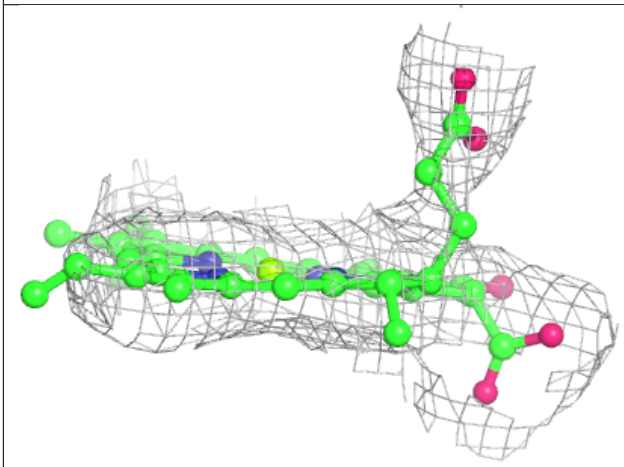


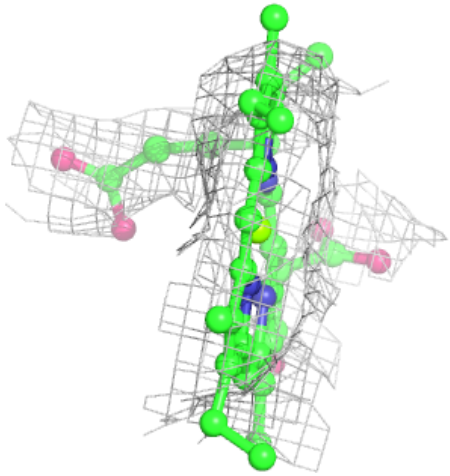


Electron density around CLA B 840:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

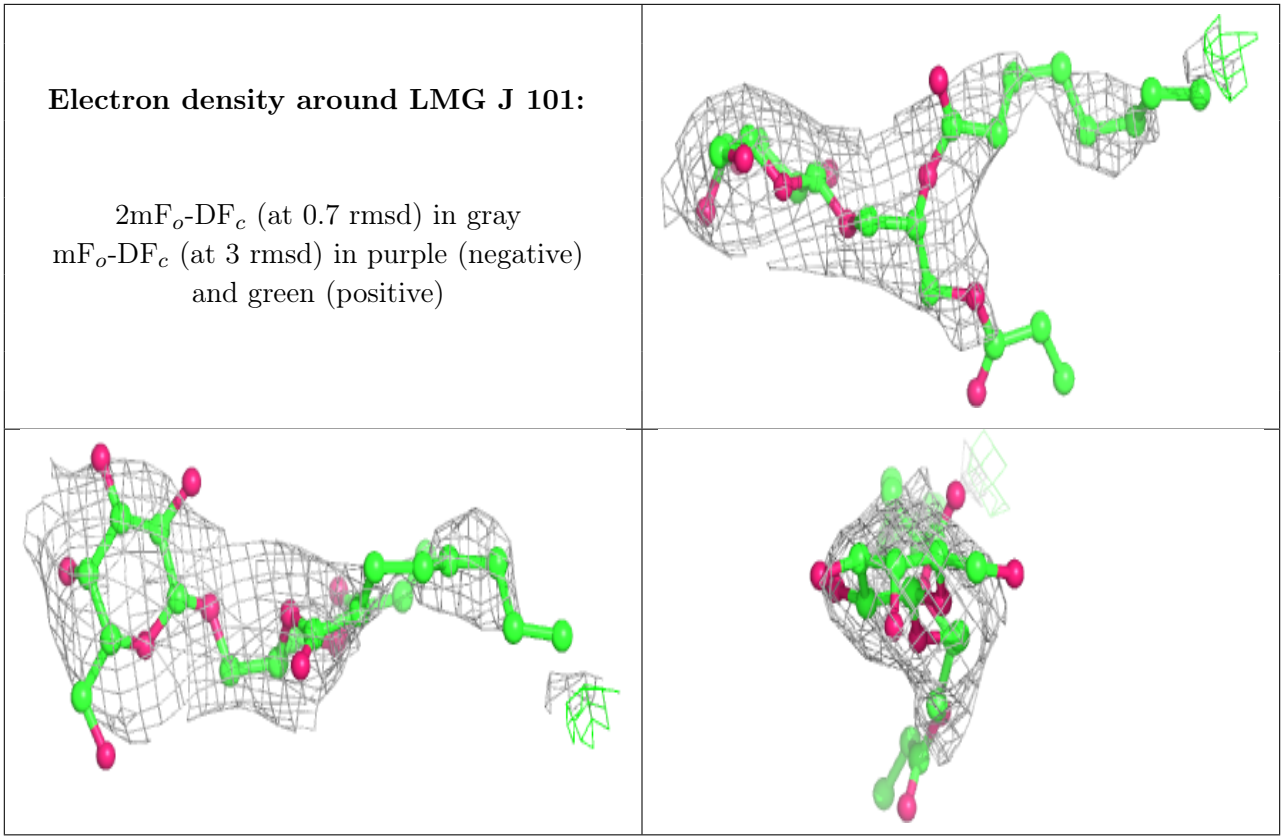






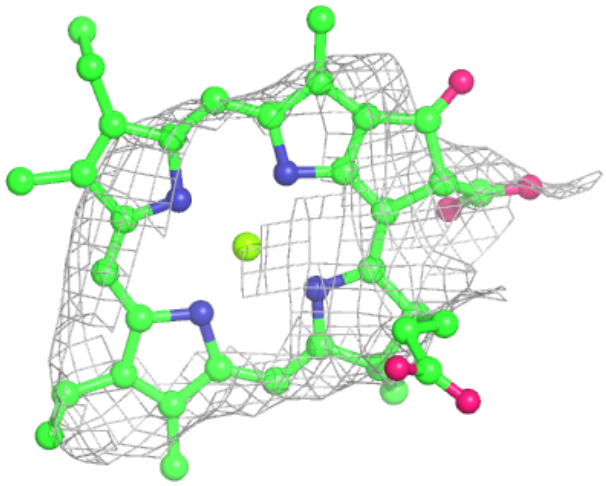
Electron density around LMG J 101:

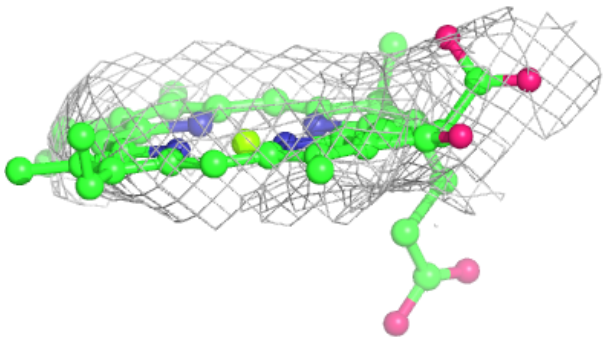
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

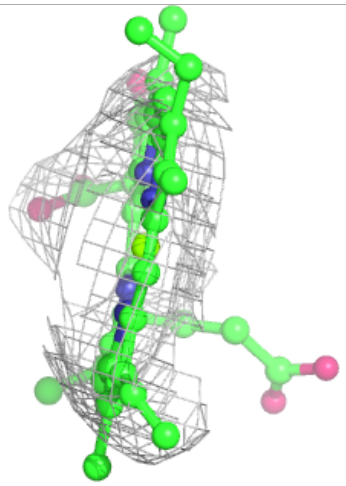


Electron density around CLA L 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

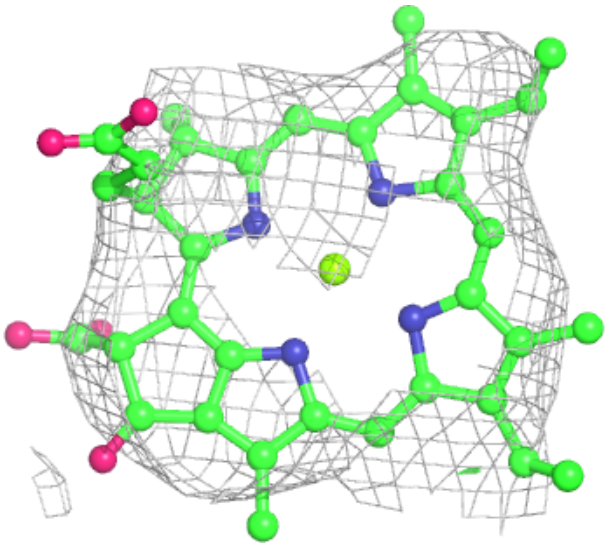


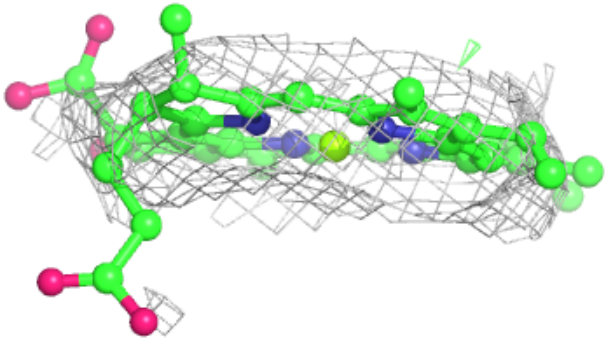


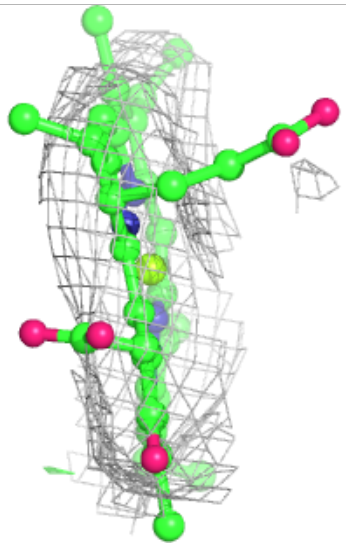


Electron density around CLA 0 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

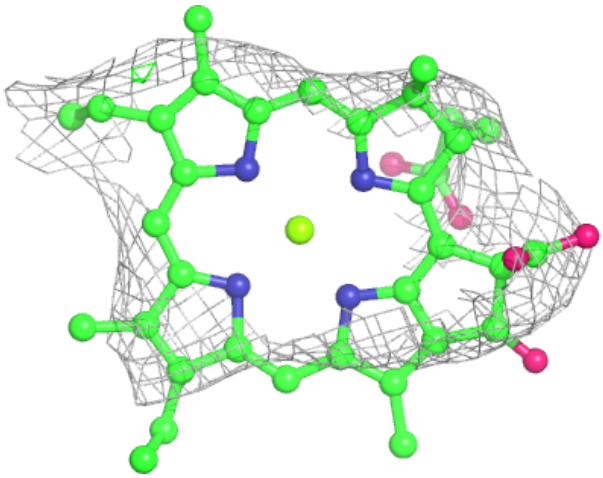


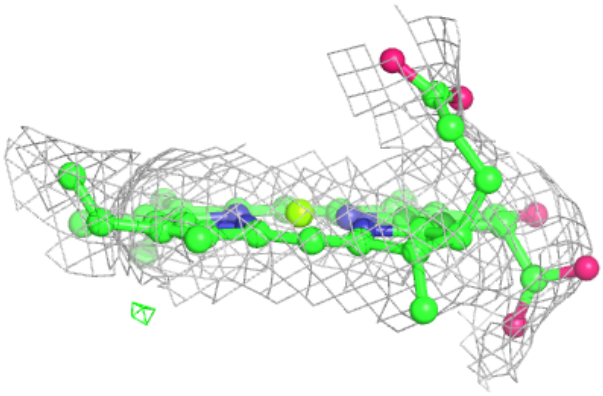


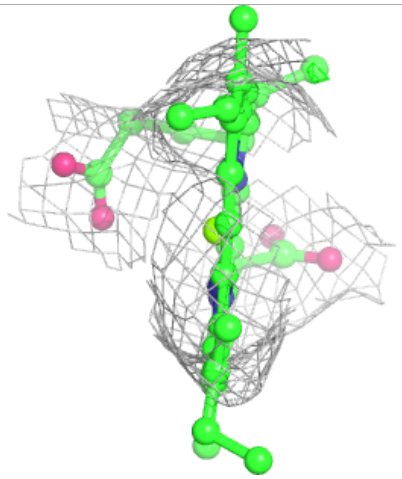


Electron density around CLA B 810:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

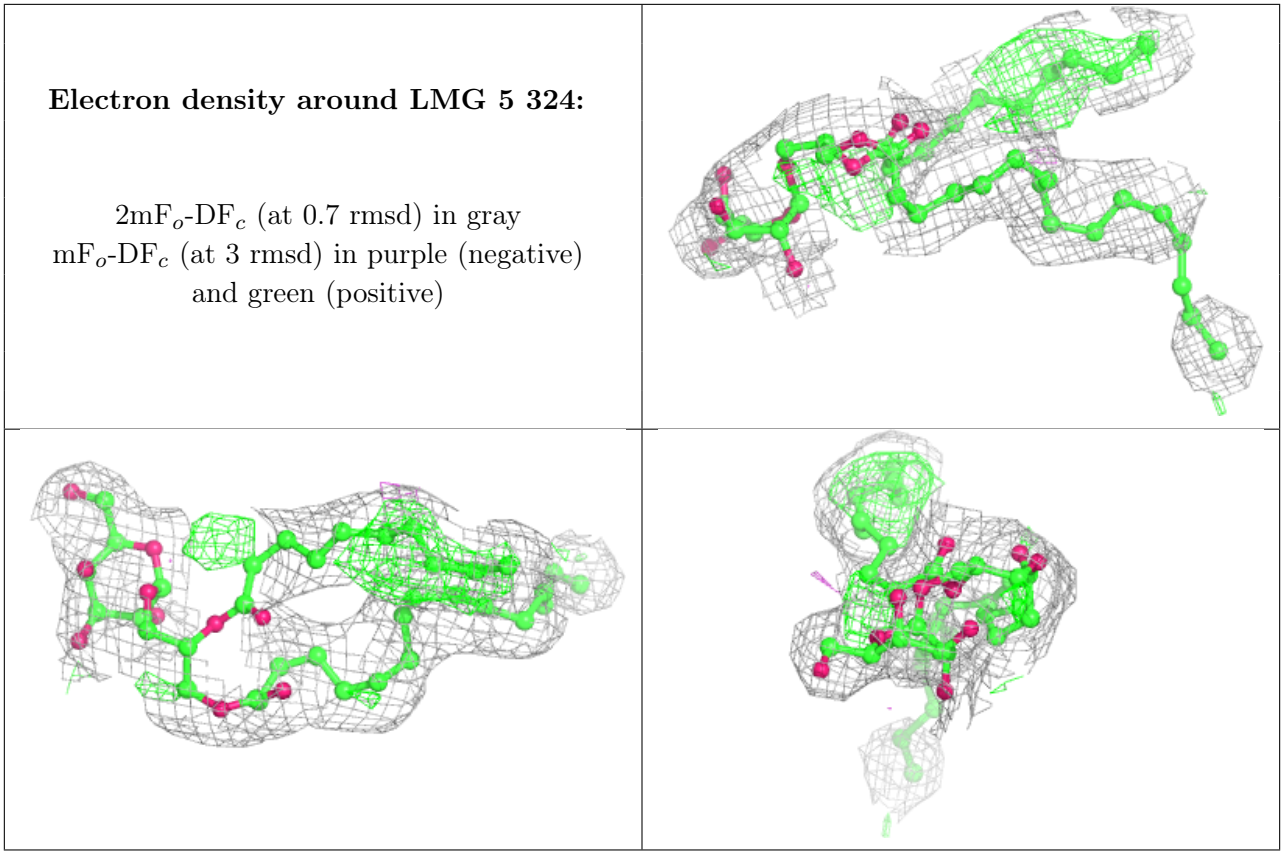






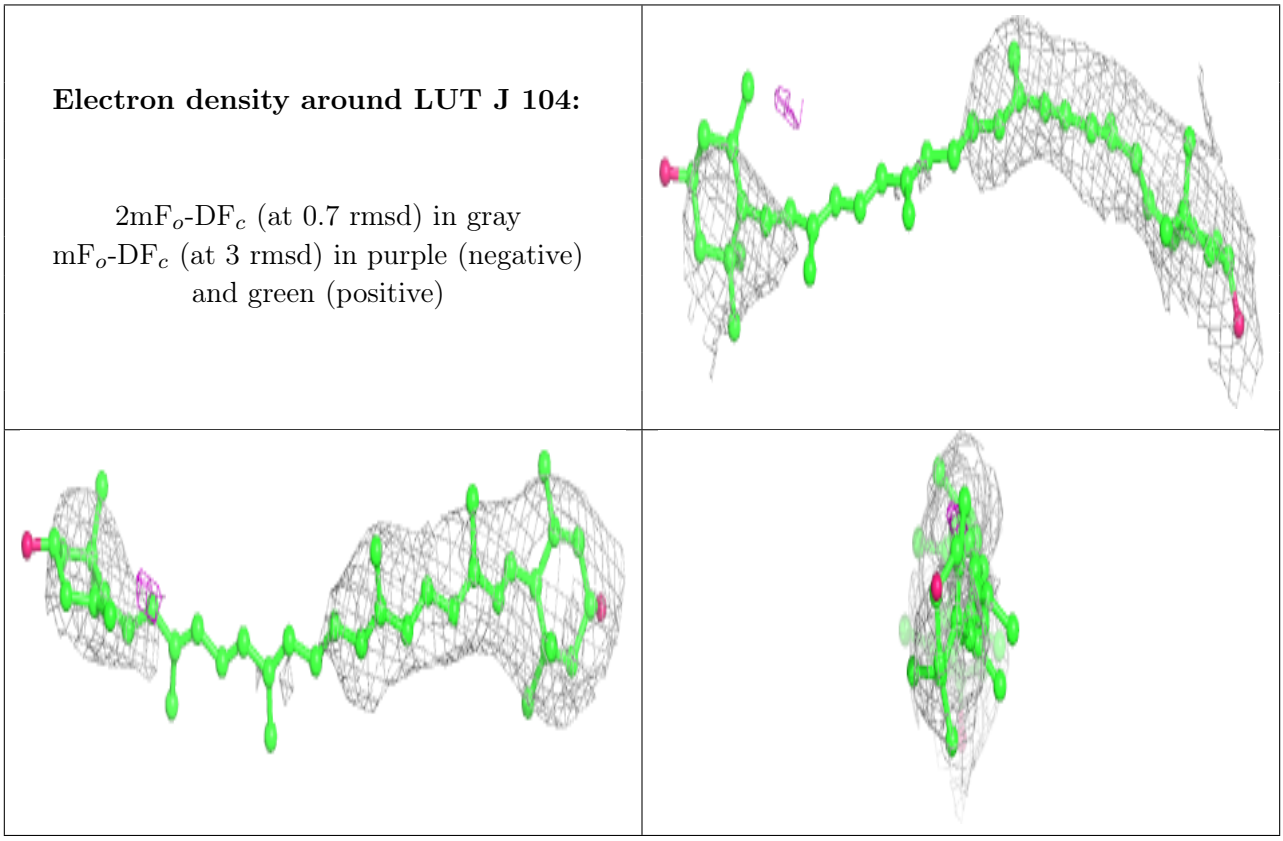
Electron density around LMG 5 324:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



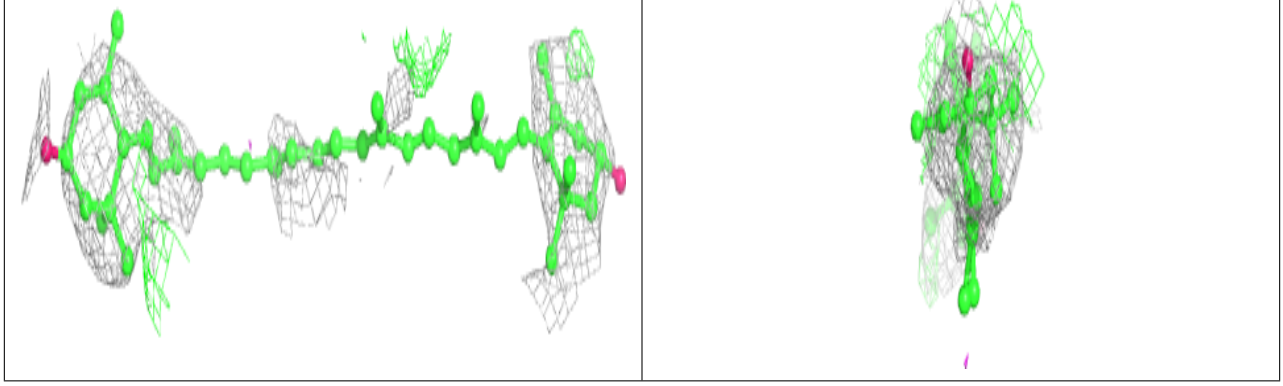
Electron density around LUT J 104:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



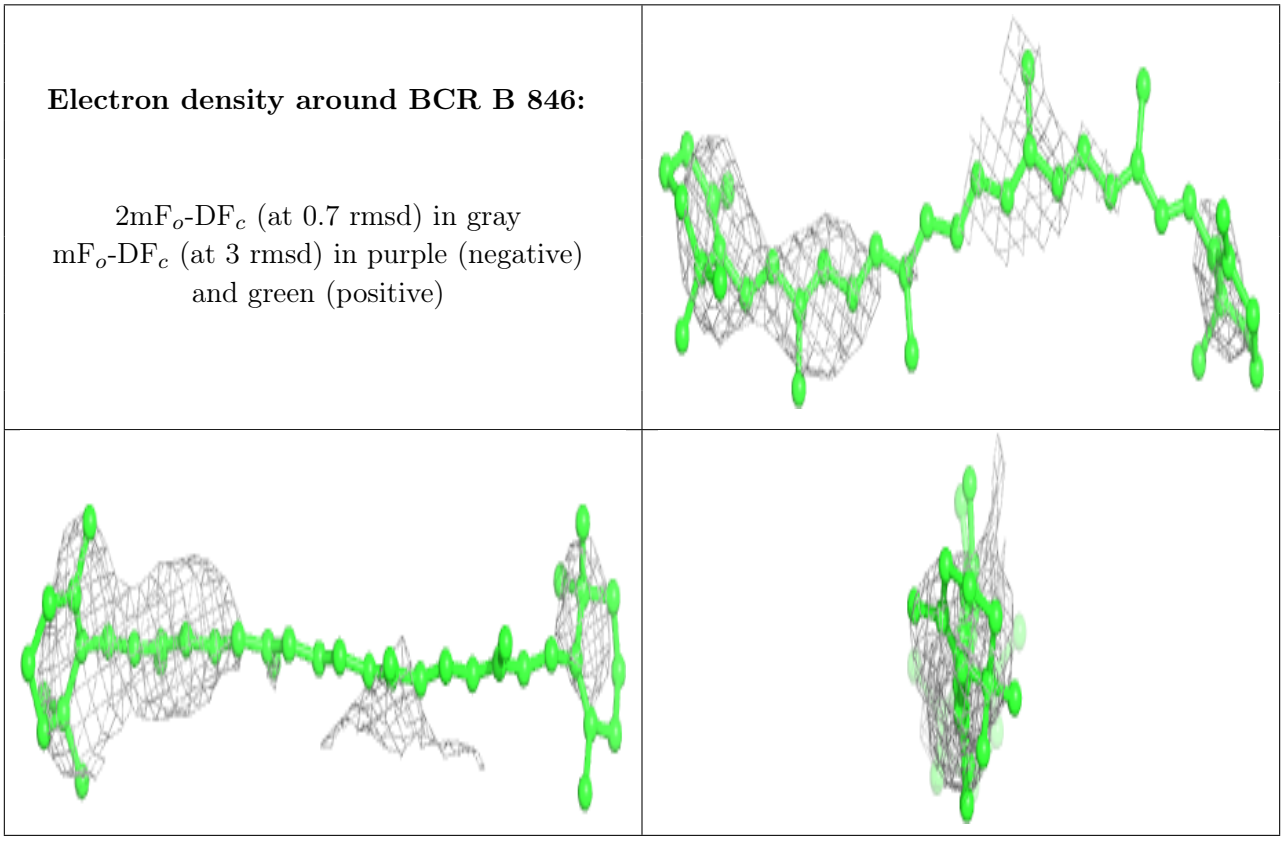
Electron density around LUT 1 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



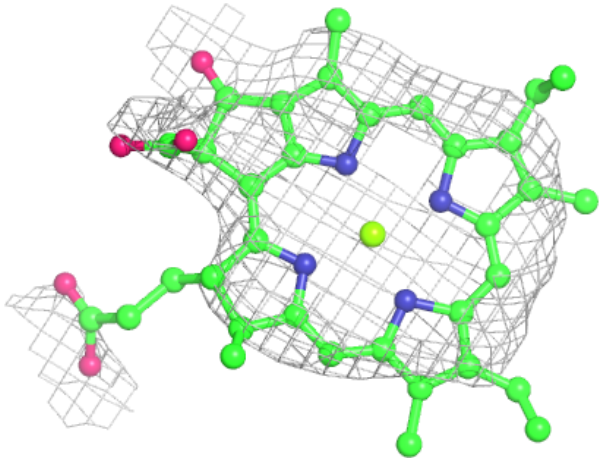
Electron density around BCR B 846:

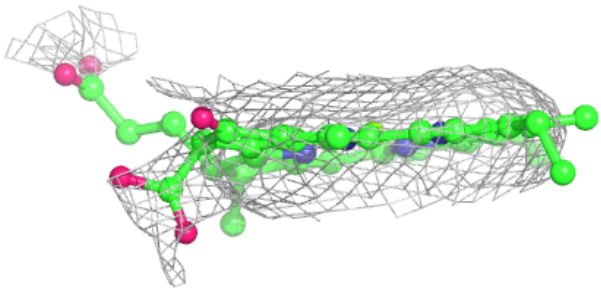
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

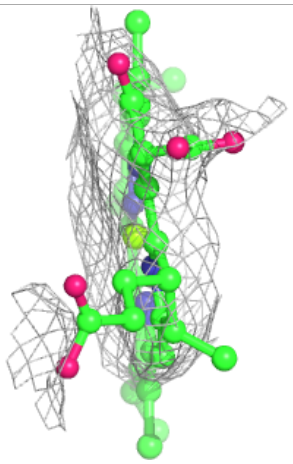


Electron density around CLA B 812:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

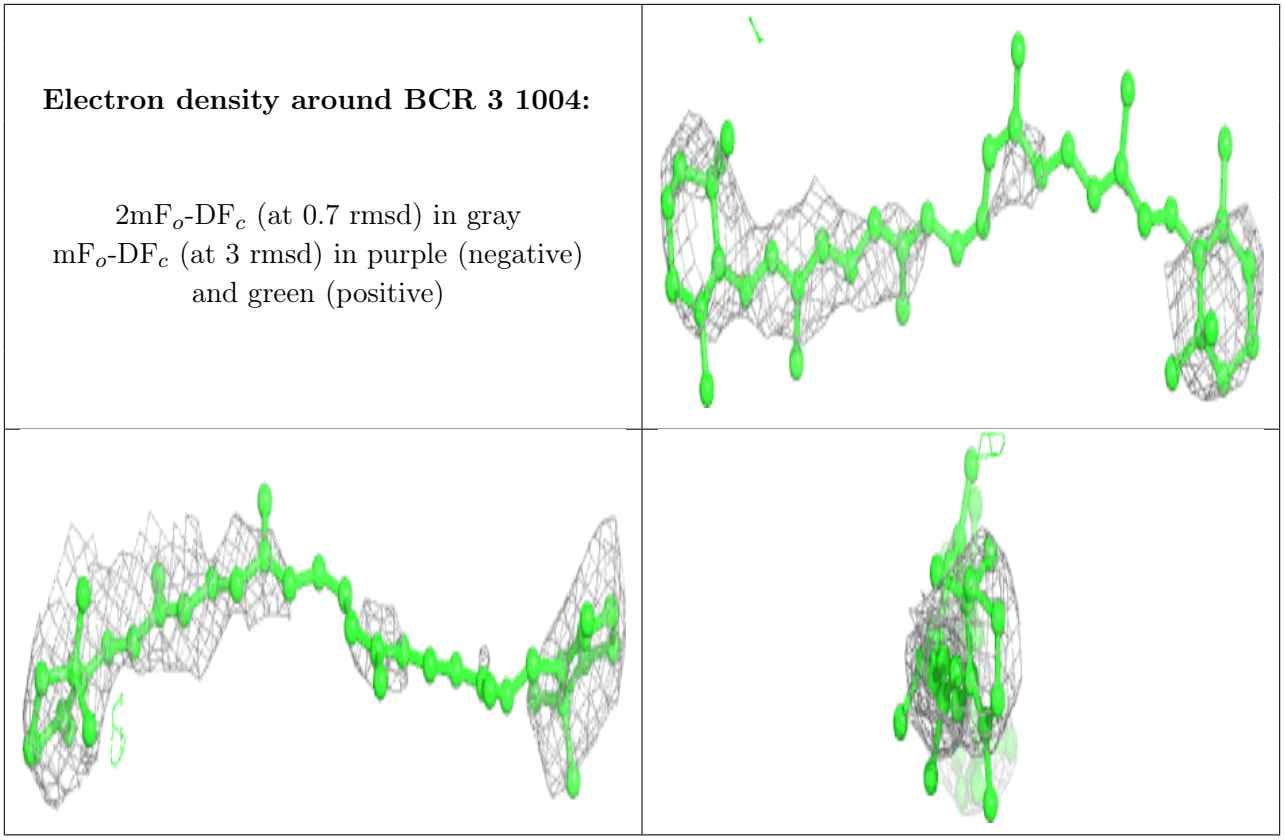






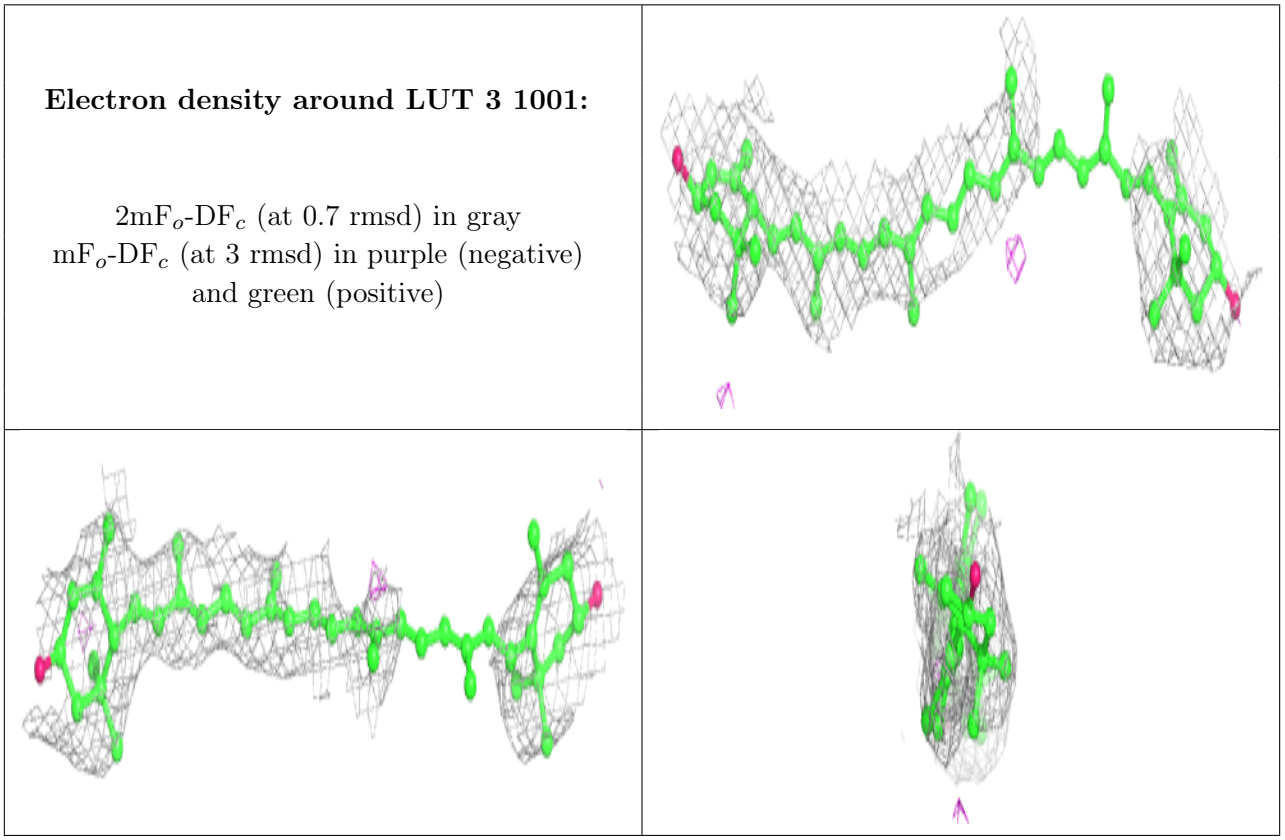
Electron density around BCR 3 1004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



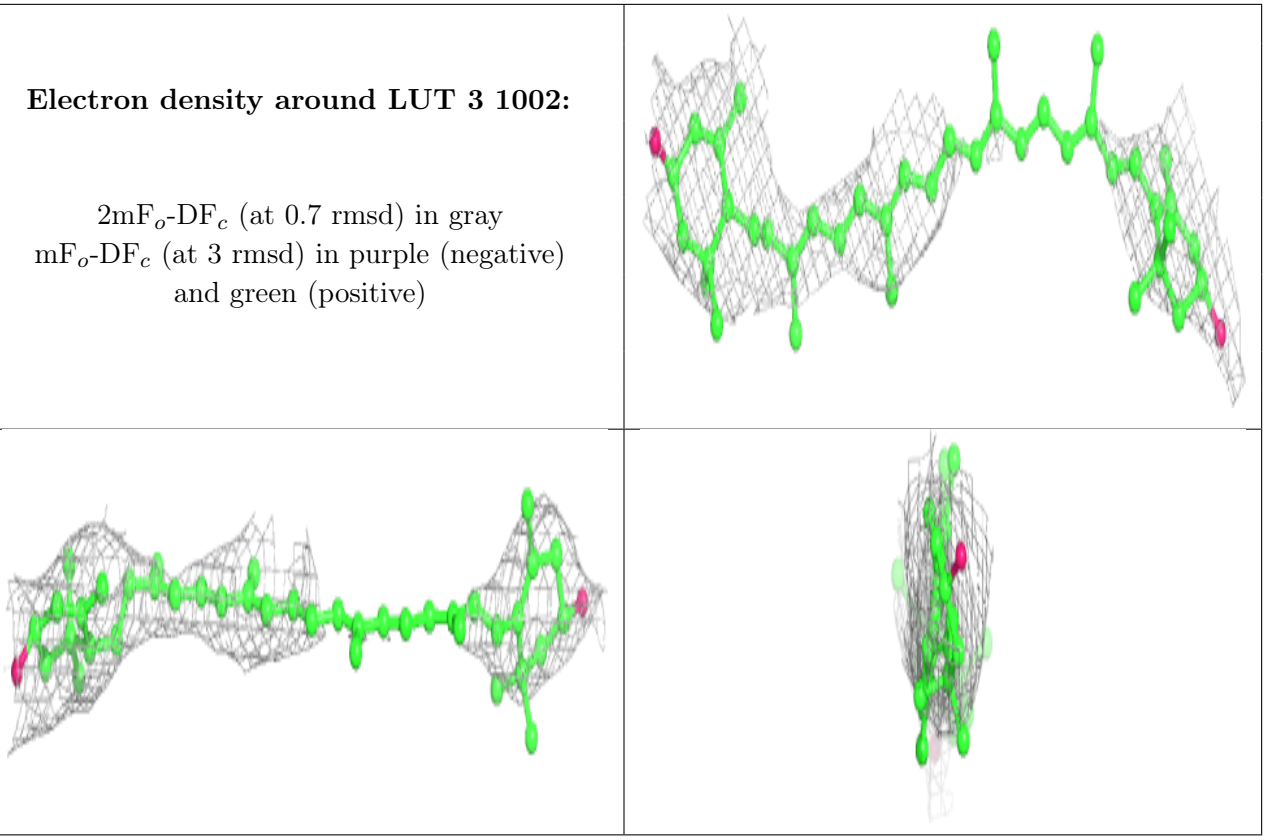
Electron density around LUT 3 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



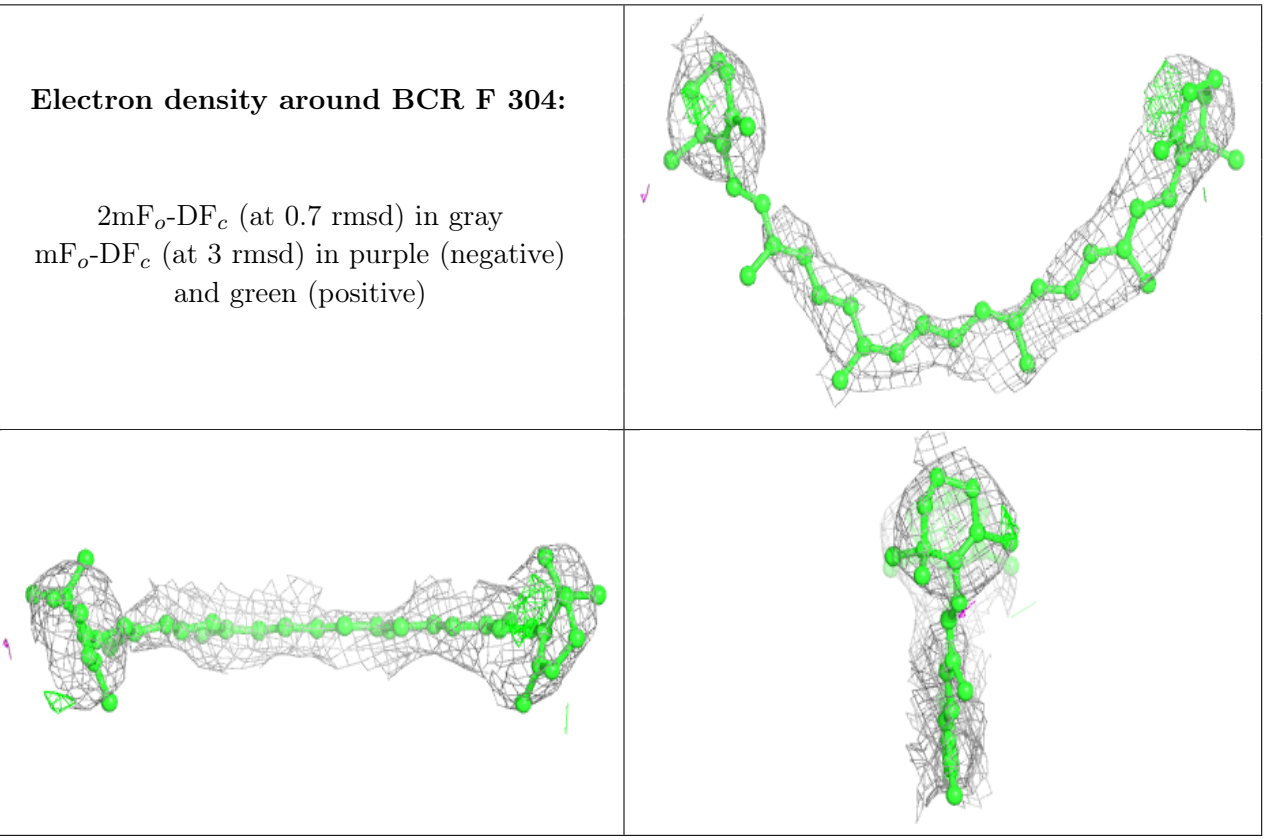
Electron density around LUT 3 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



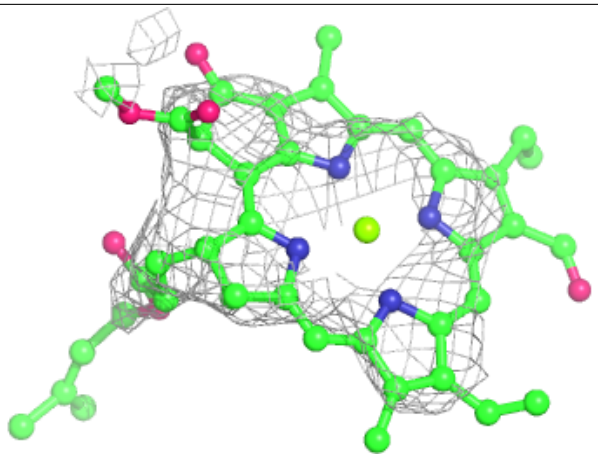
Electron density around BCR F 304:

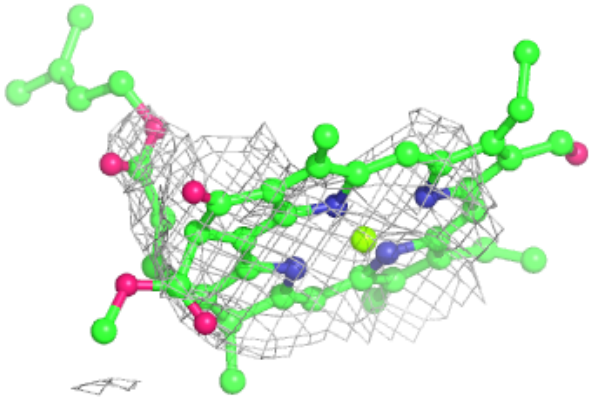
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

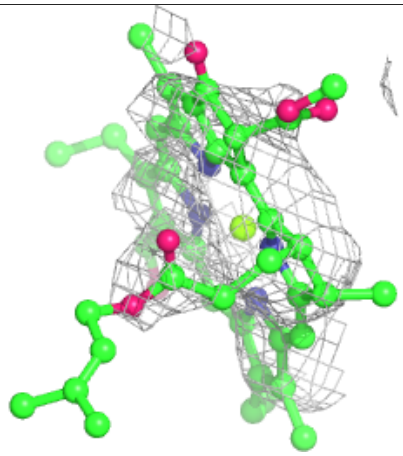


Electron density around CHL 0 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

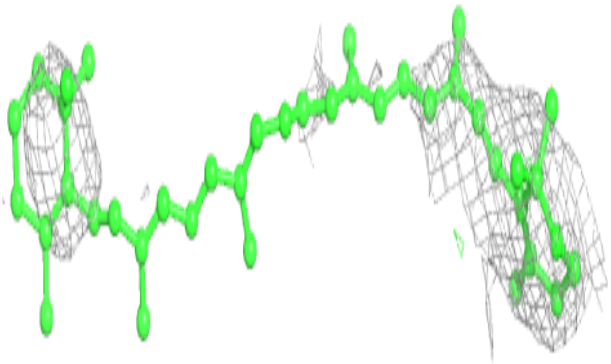


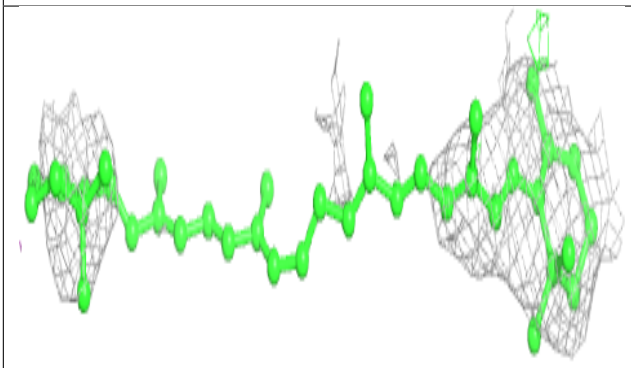


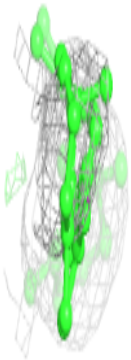


Electron density around BCR 4 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

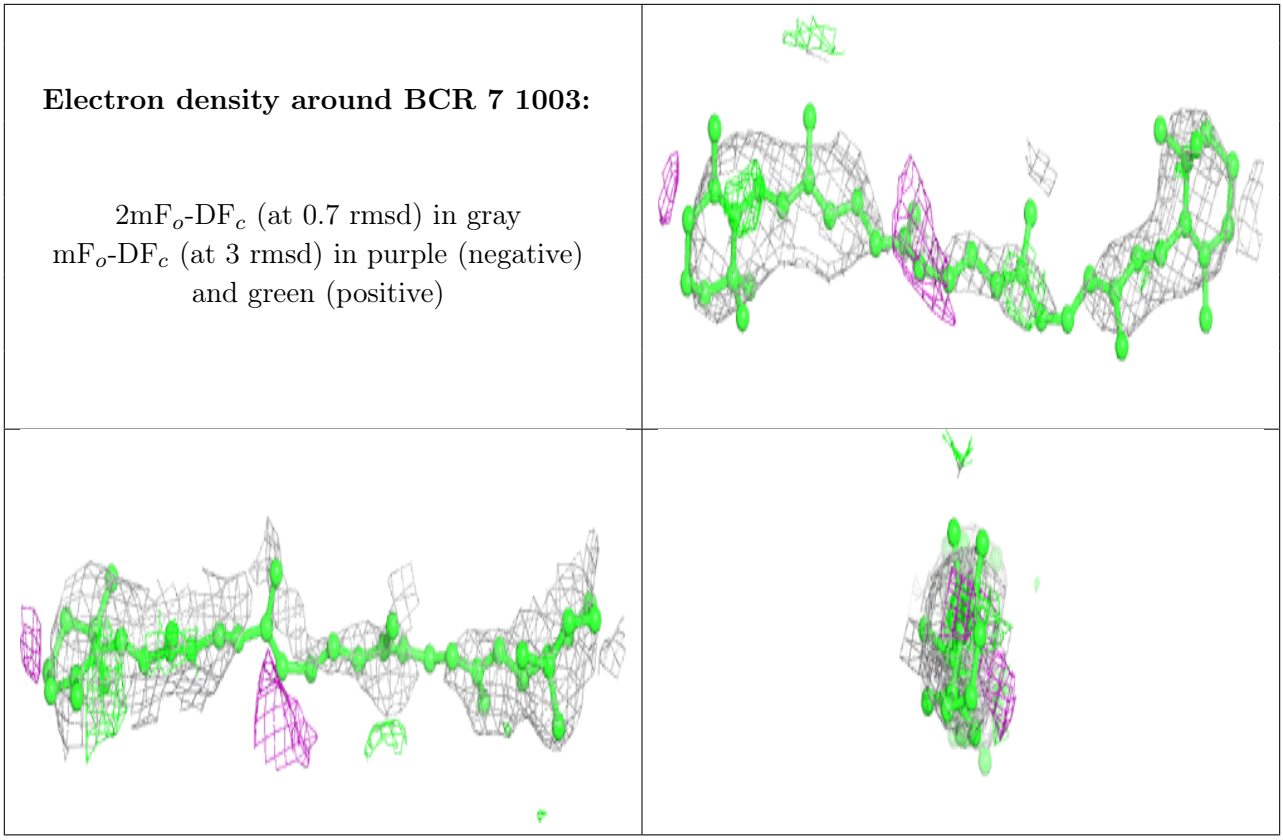






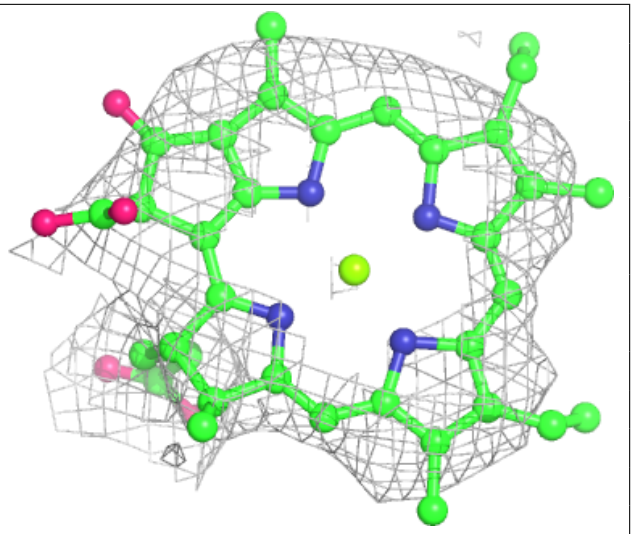
Electron density around BCR 7 1003:

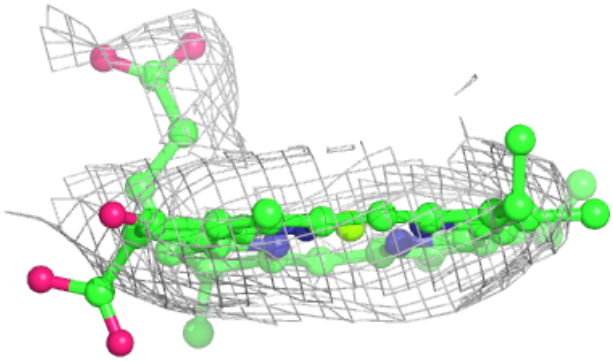
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 822:

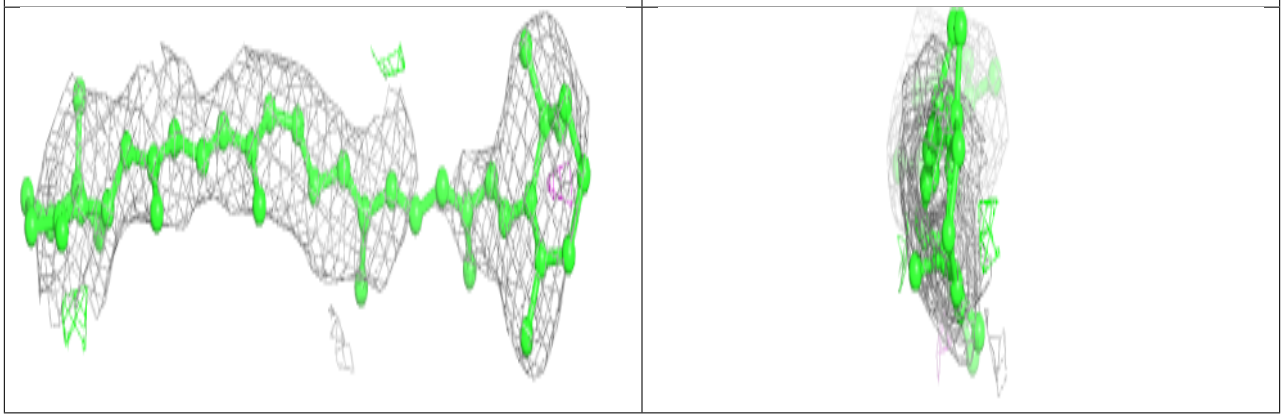
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





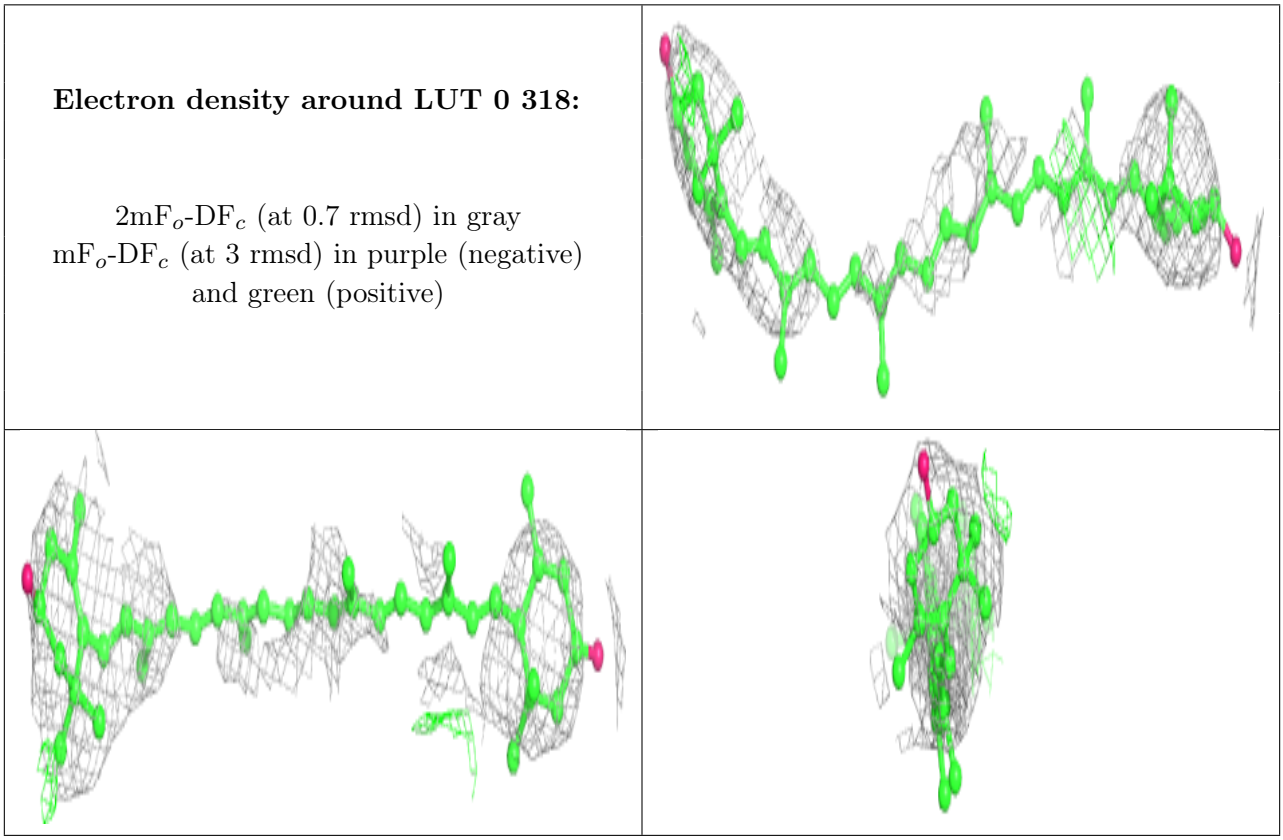
Electron density around BCR 8 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



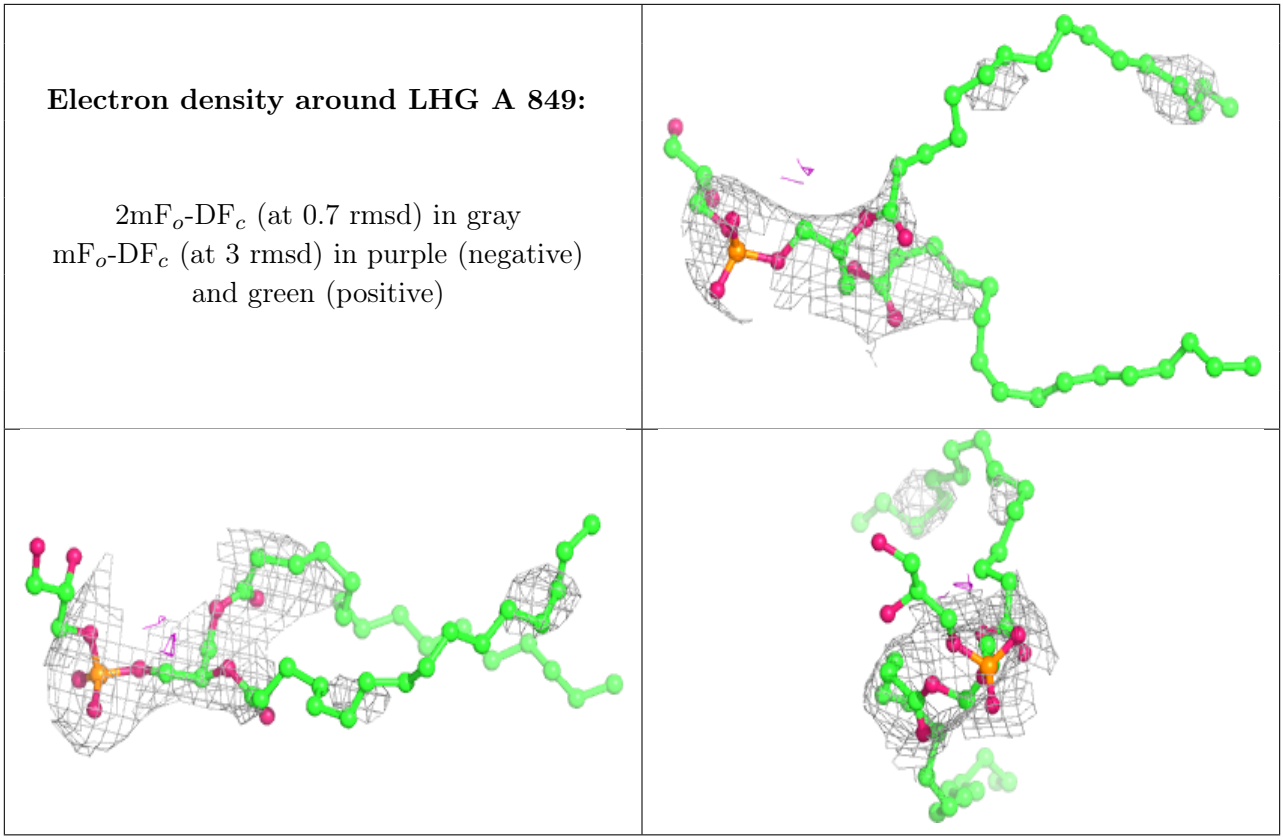
Electron density around LUT 0 318:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



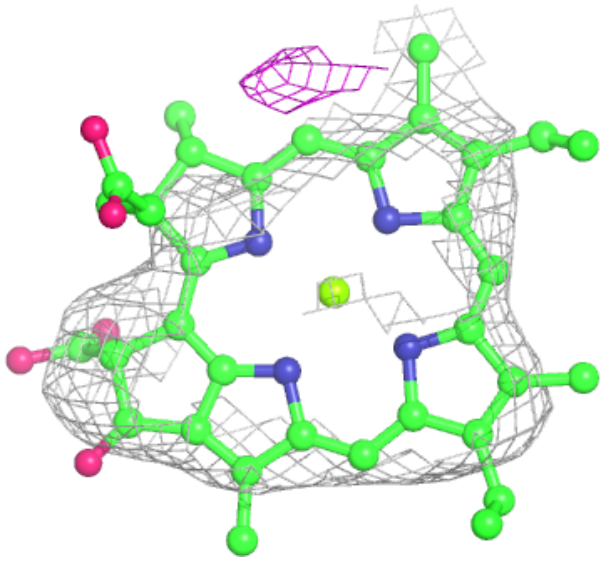
Electron density around LHG A 849:

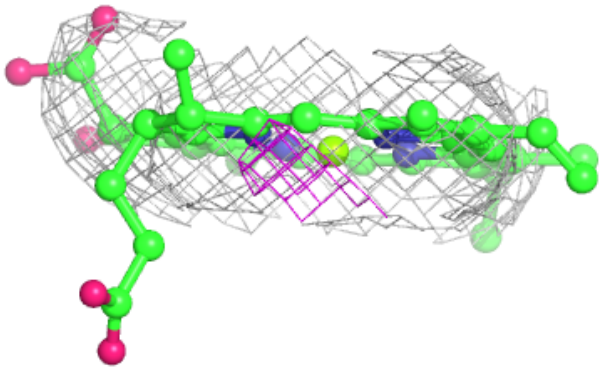
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

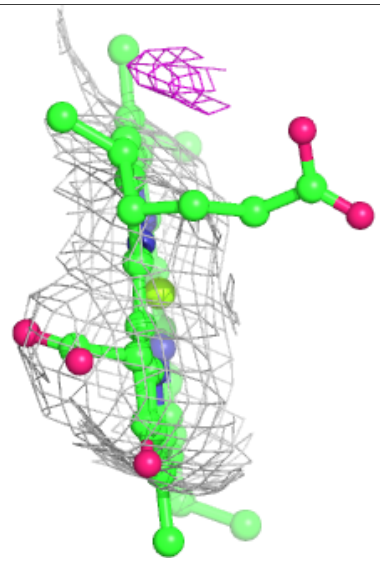


Electron density around CLA A 822:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

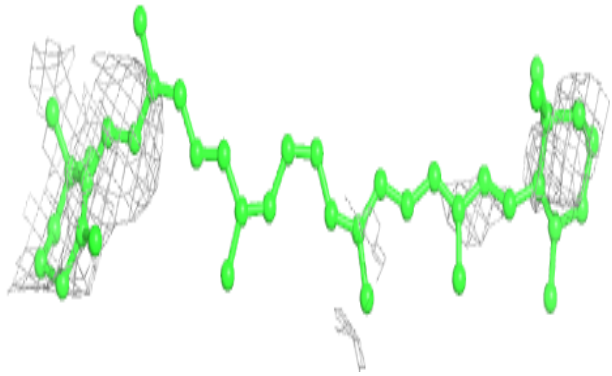


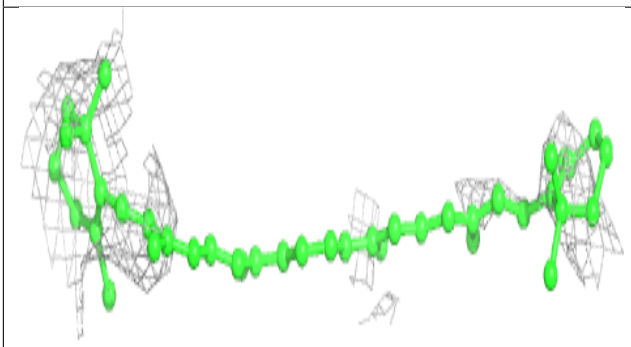


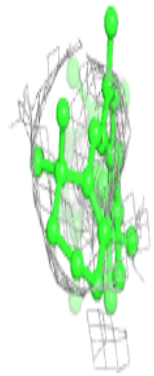


Electron density around BCR B 843:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

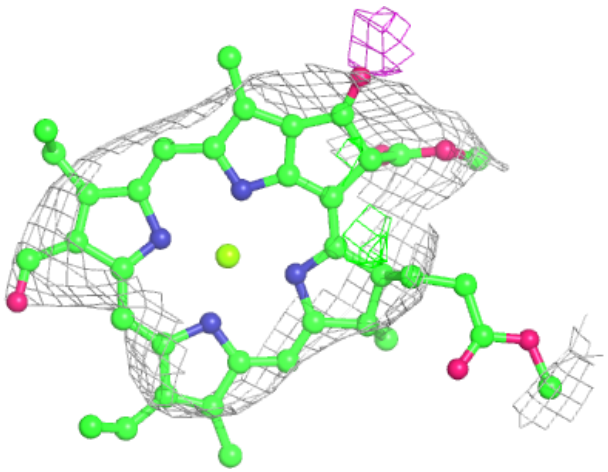


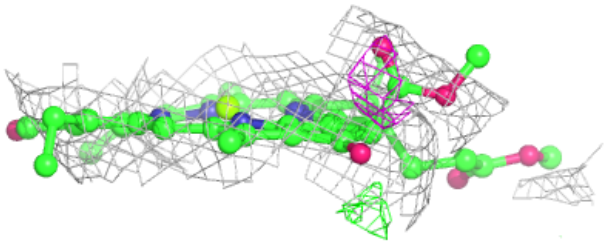


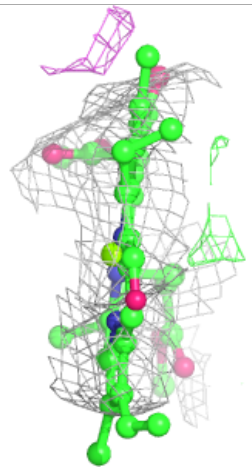


Electron density around CHL 0 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

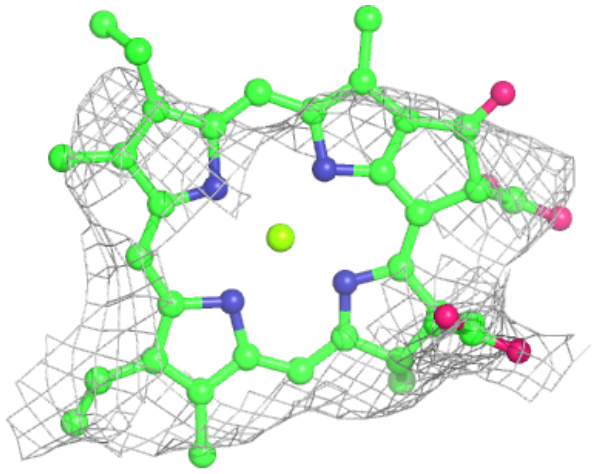


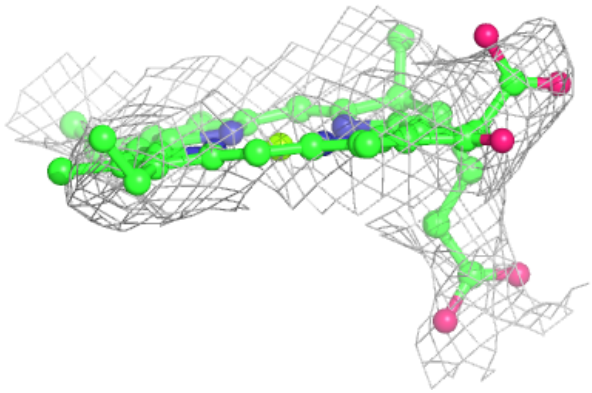


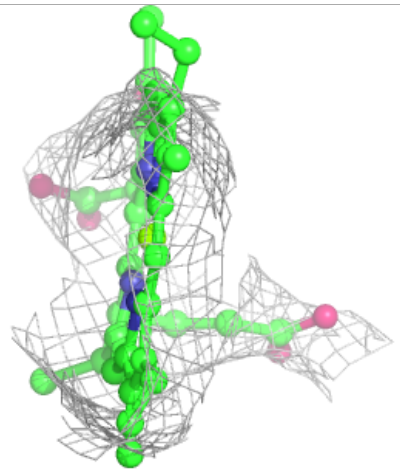


Electron density around CLA B 817:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

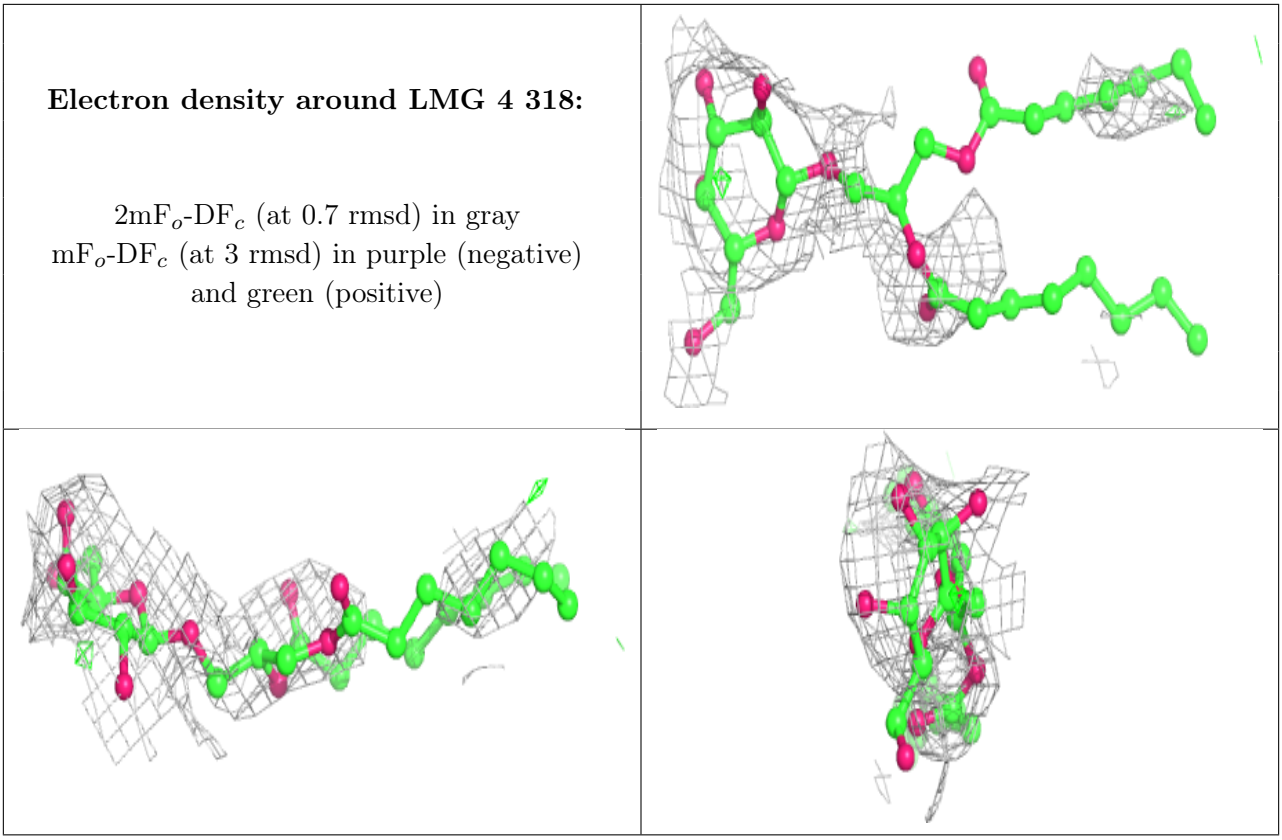






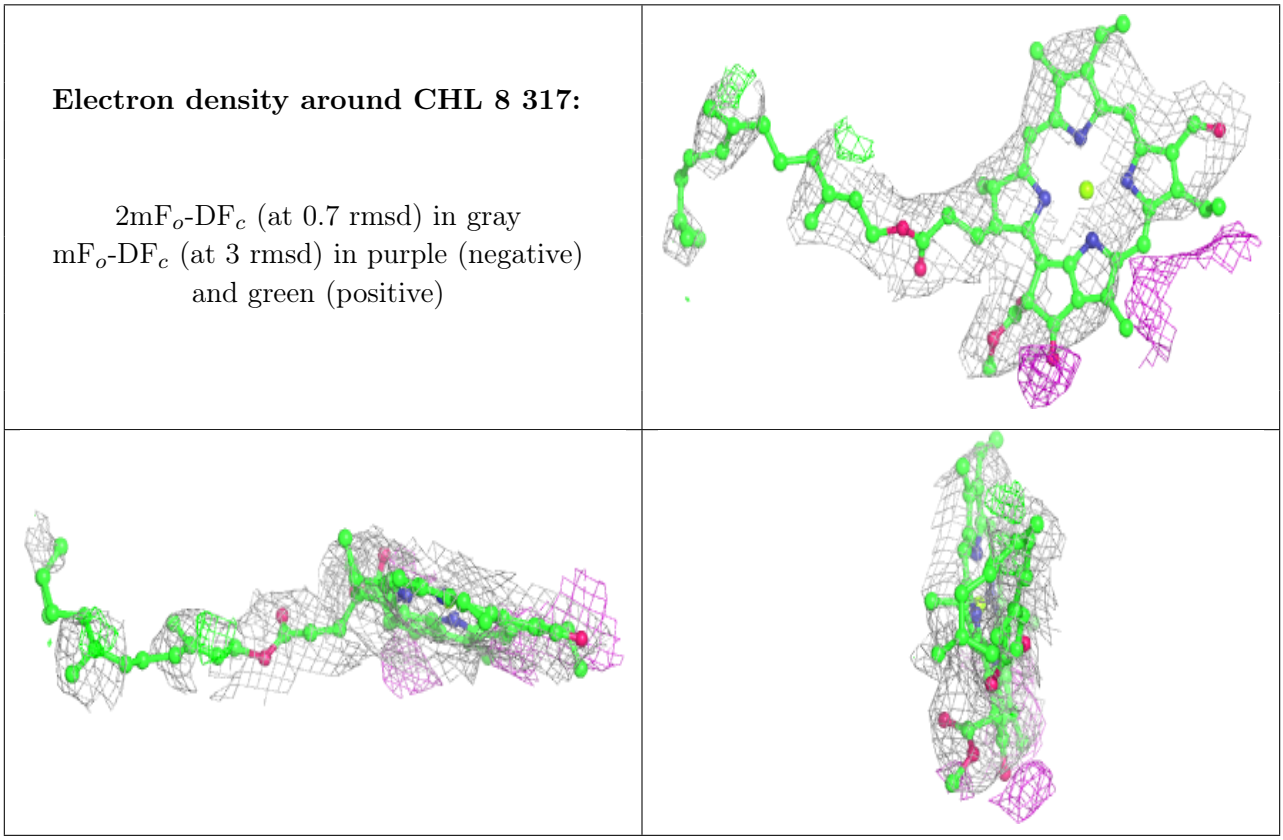
Electron density around LMG 4 318:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



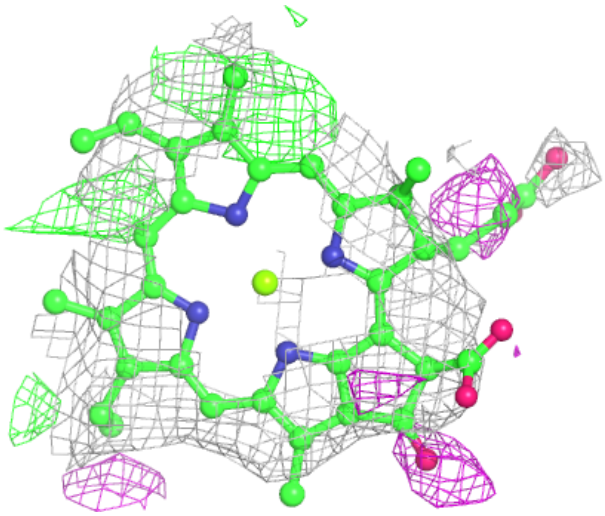
Electron density around CHL 8 317:

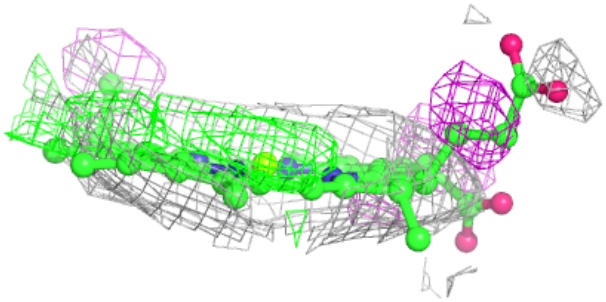
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

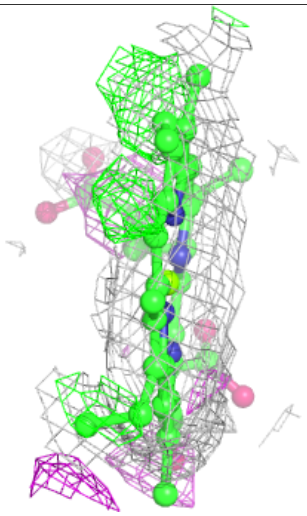


Electron density around CLA 5 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

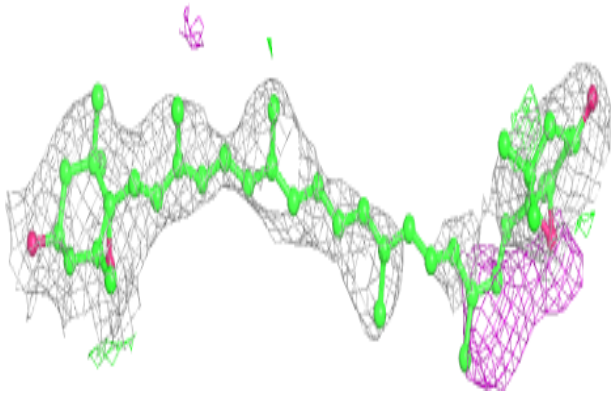


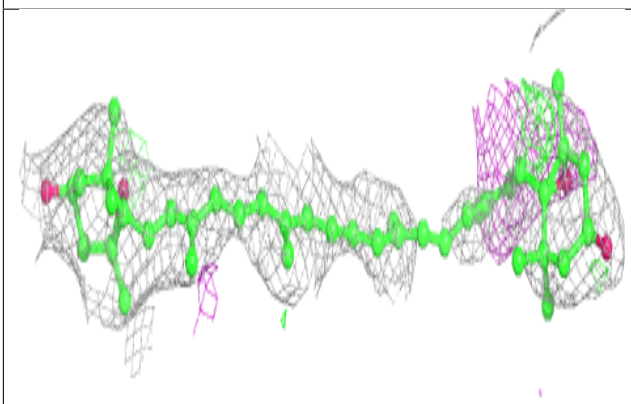


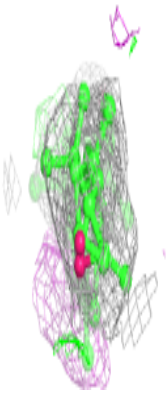


Electron density around XAT 7 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

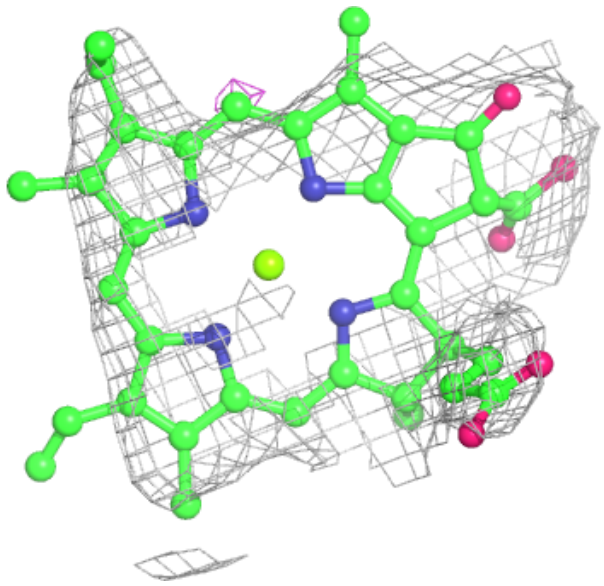


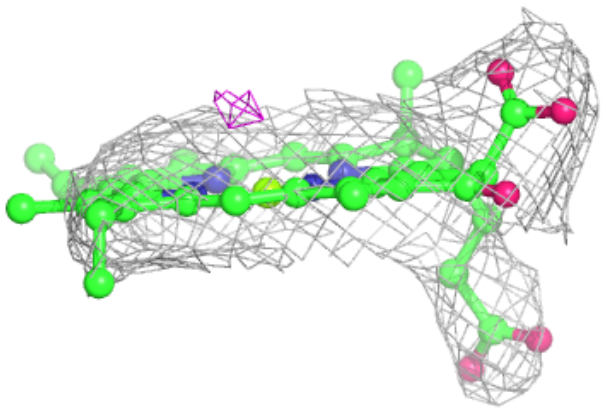


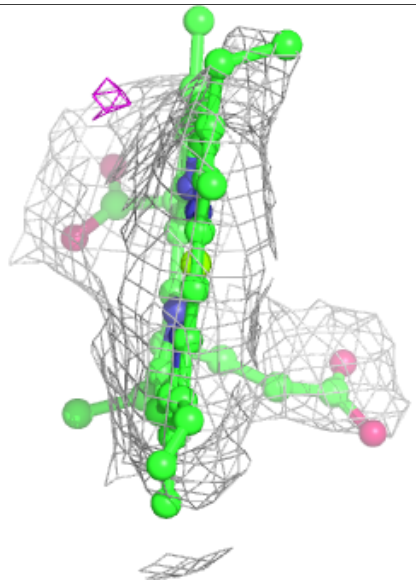


Electron density around CLA B 835:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

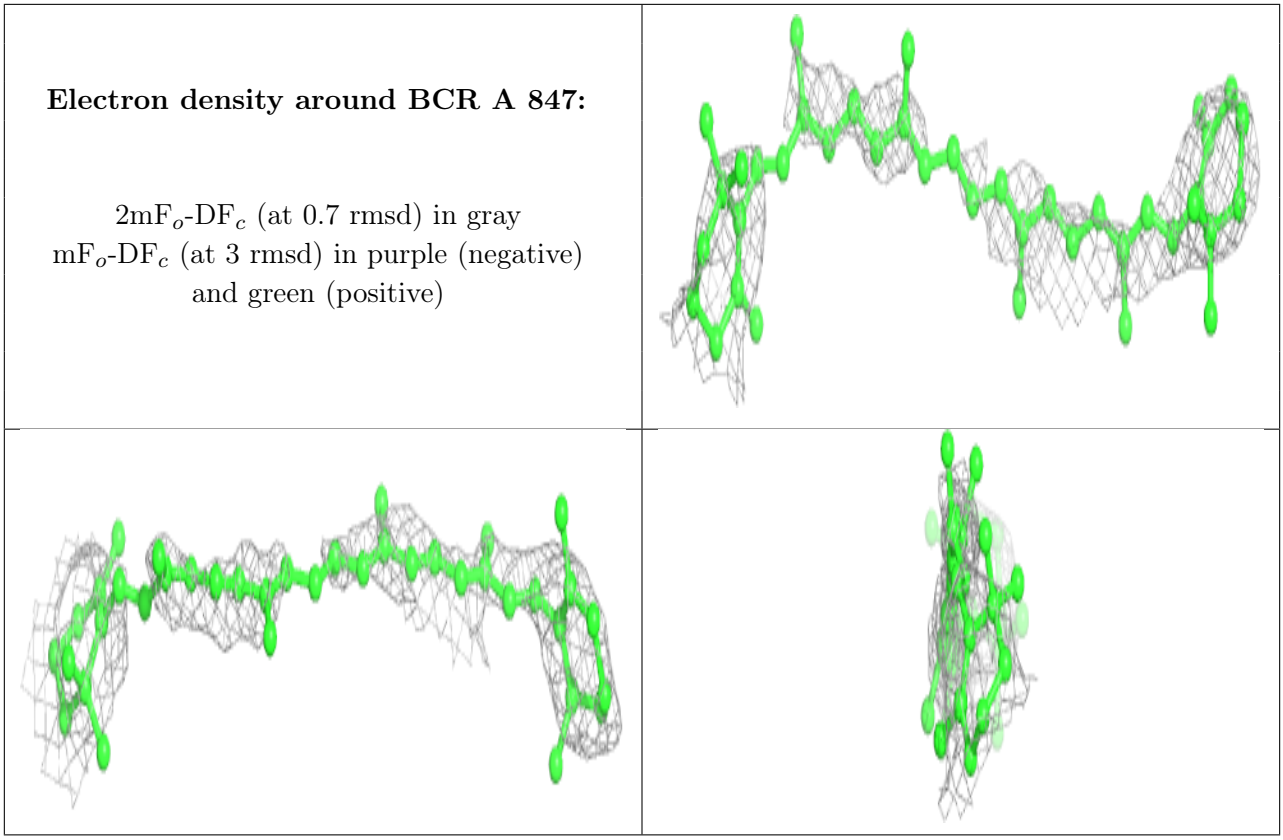






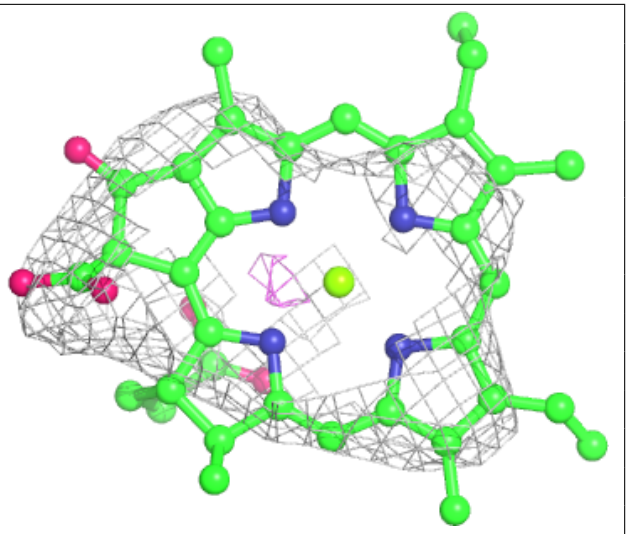
Electron density around BCR A 847:

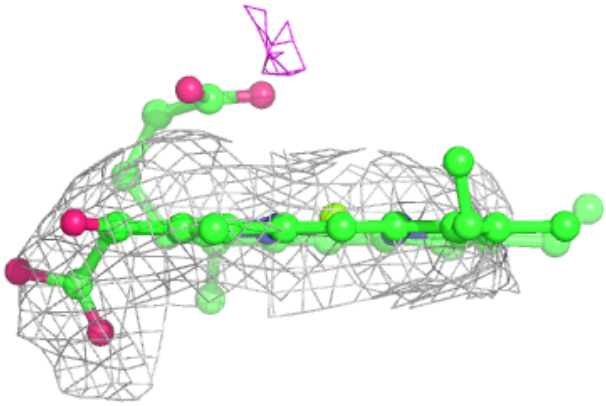
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

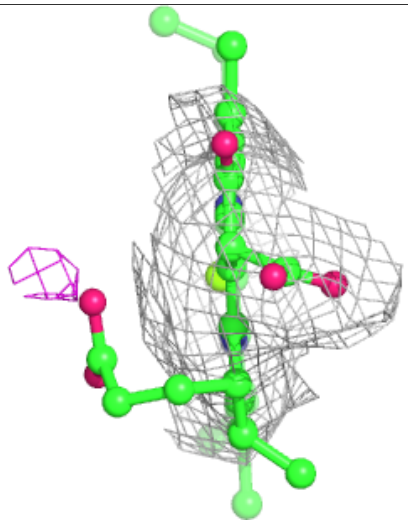


Electron density around CLA B 819:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

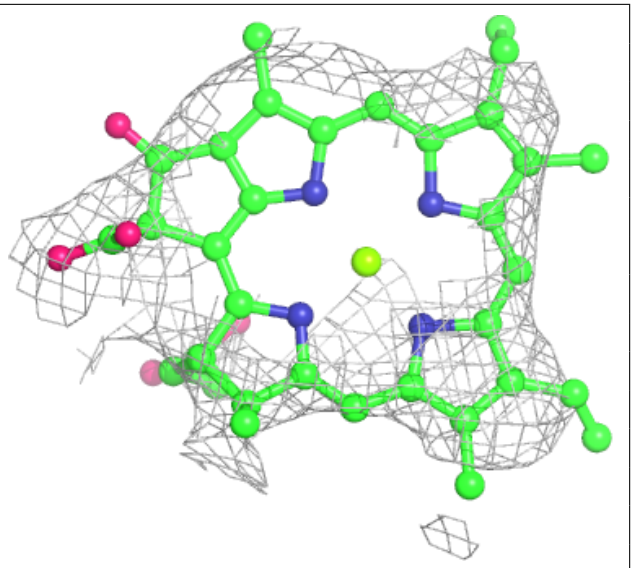


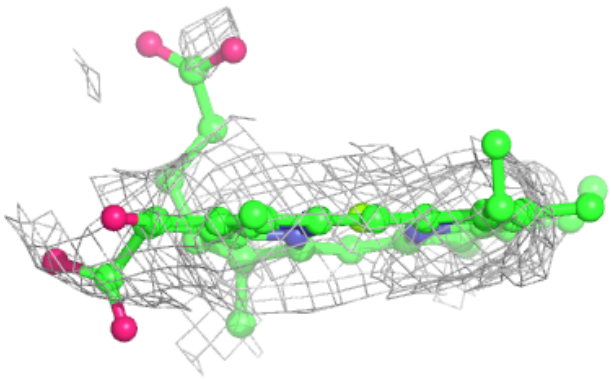


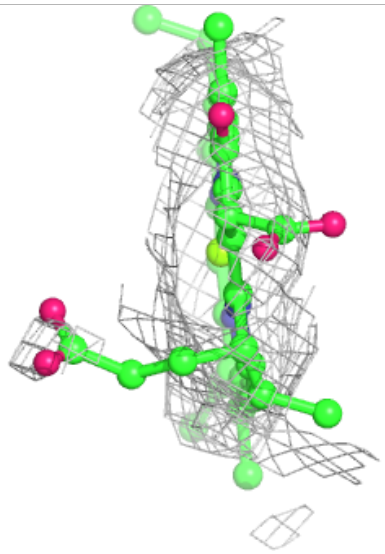


Electron density around CLA A 820:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

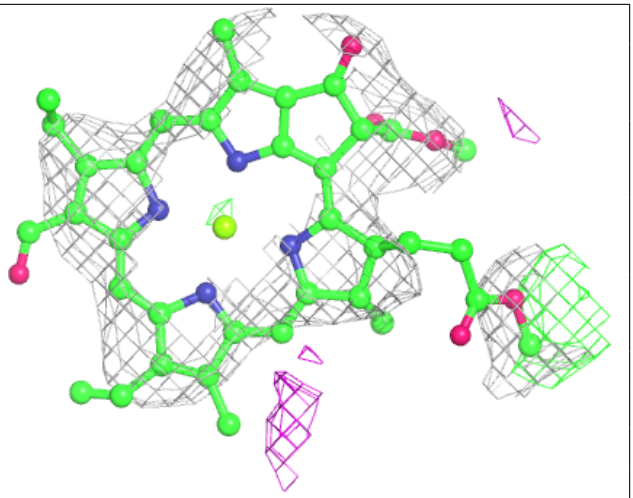


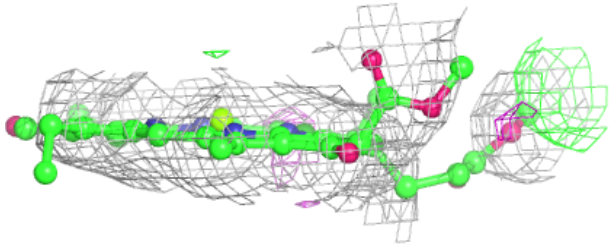


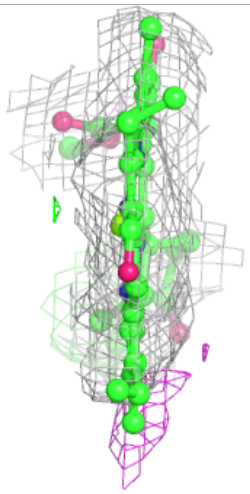


Electron density around CHL 4 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

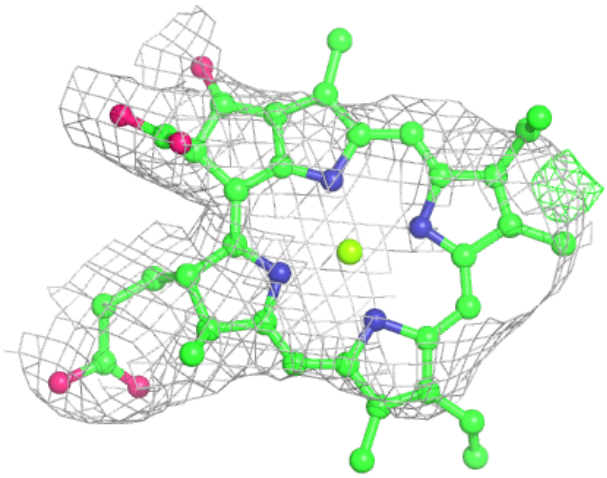


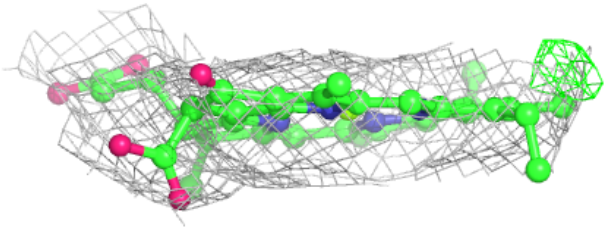


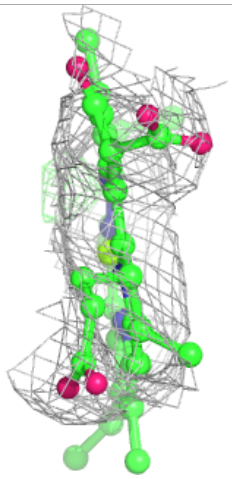


Electron density around CLA B 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

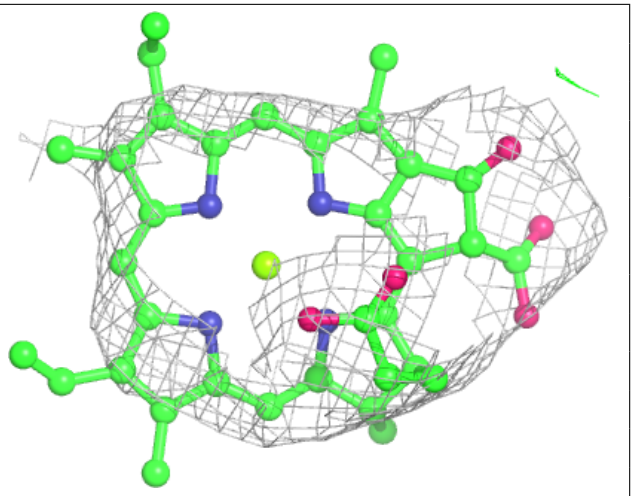


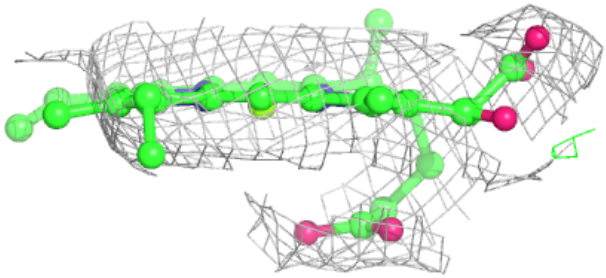


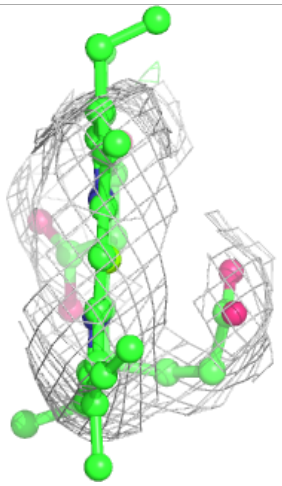


Electron density around CLA B 811:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

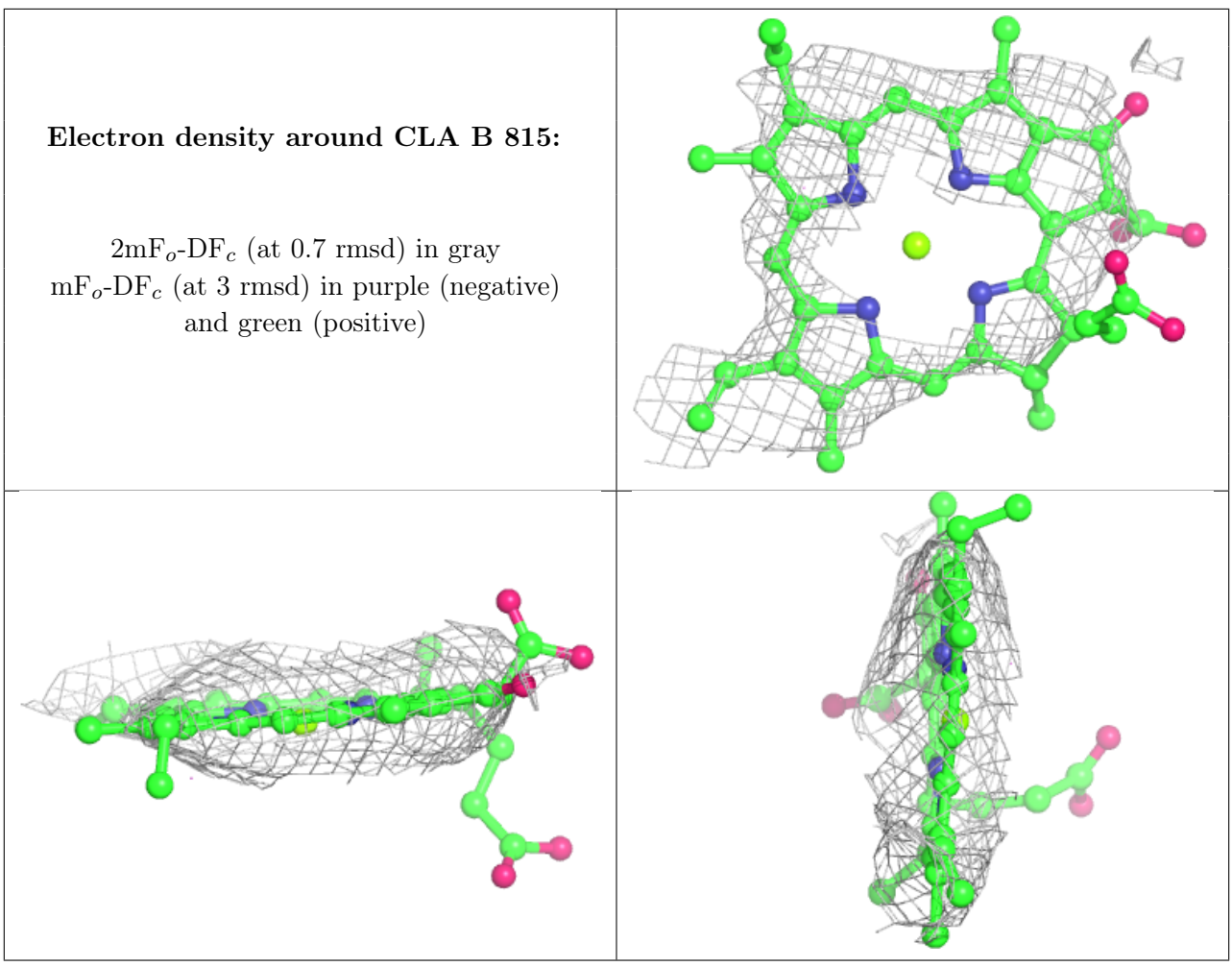






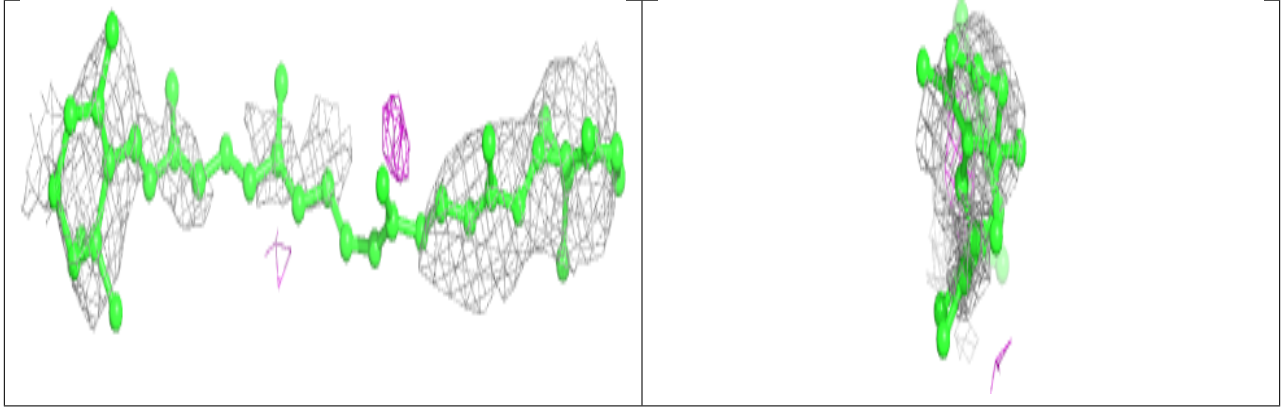
Electron density around CLA B 815:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



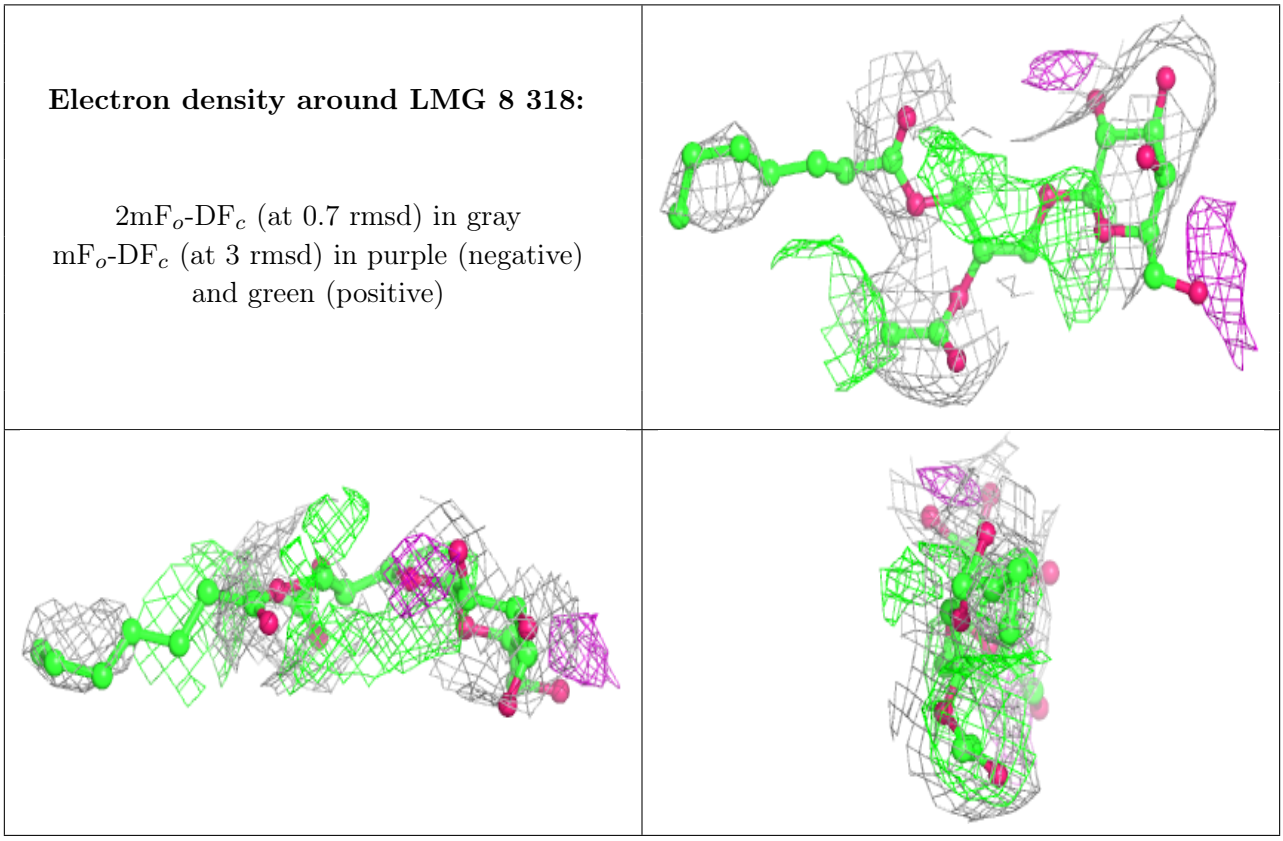
Electron density around BCR 6 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



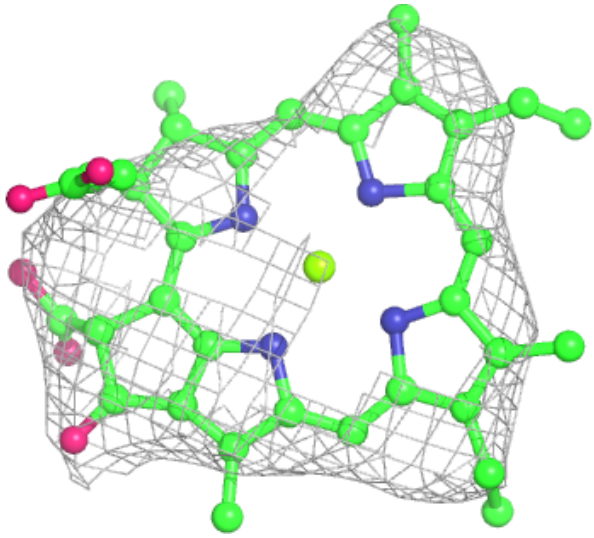
Electron density around LMG 8 318:

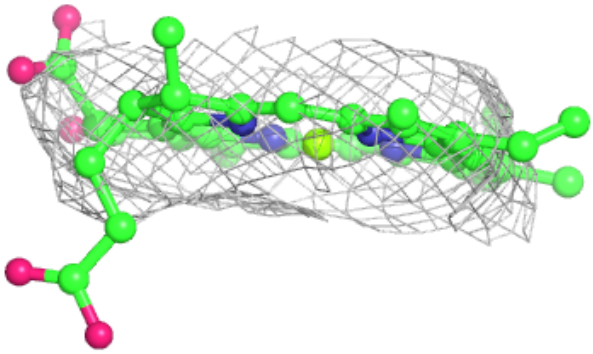
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

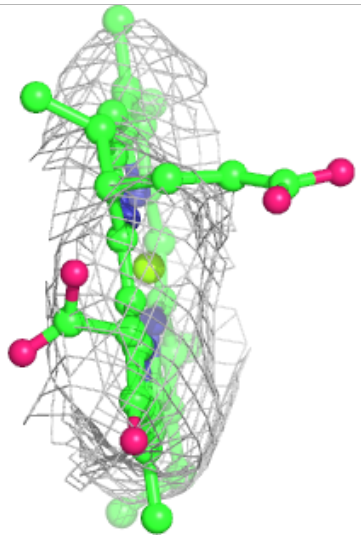


Electron density around CLA B 824:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

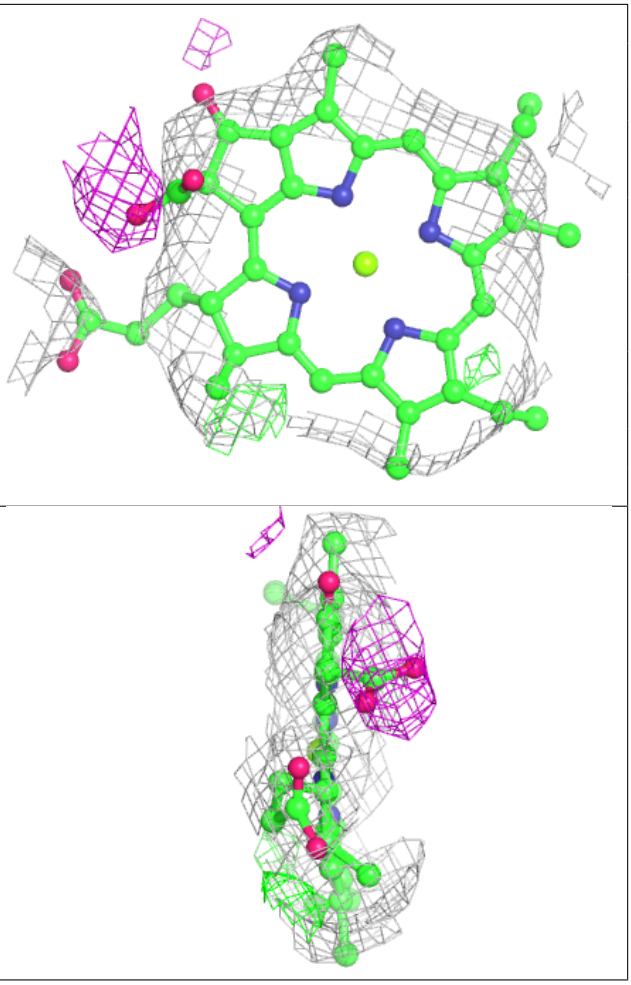


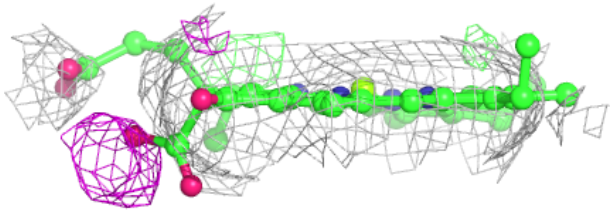




Electron density around CLA F 303:

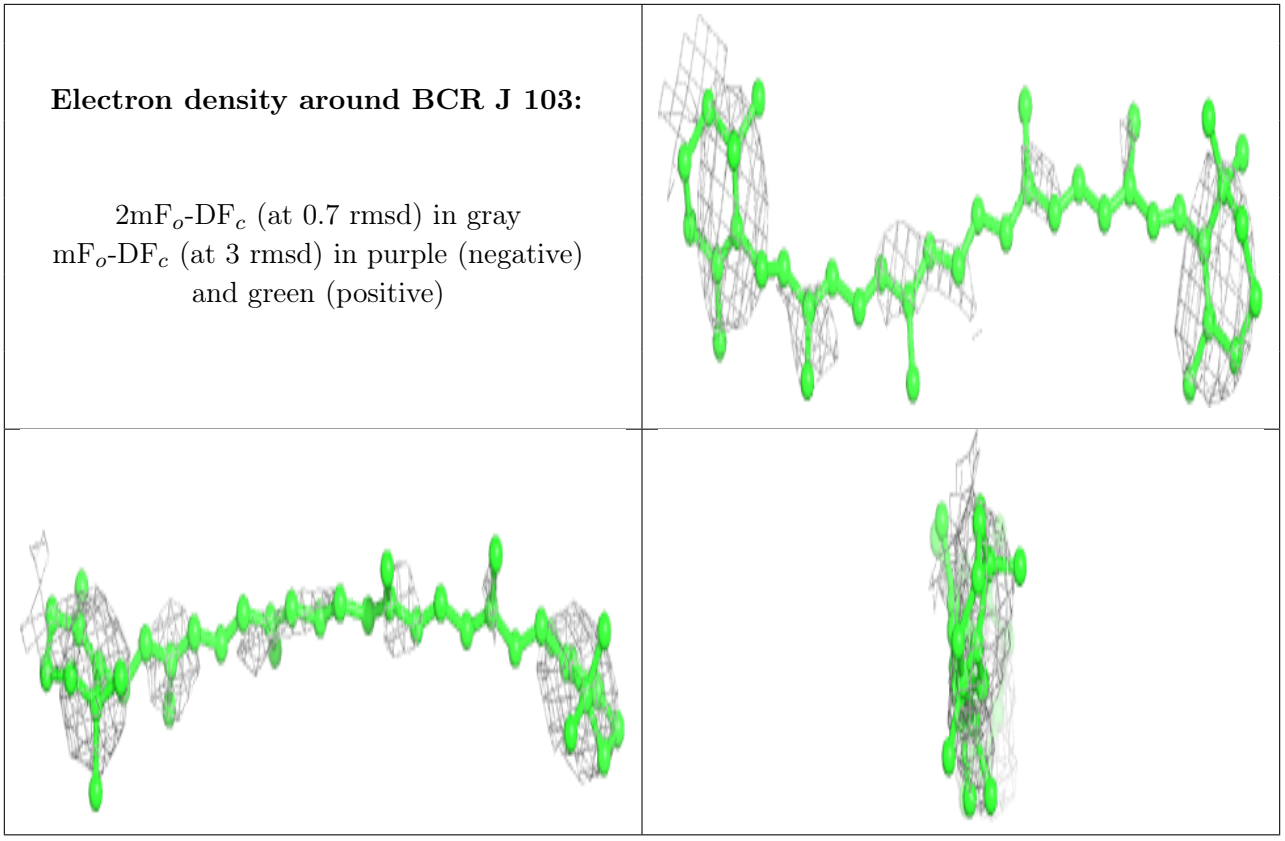
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





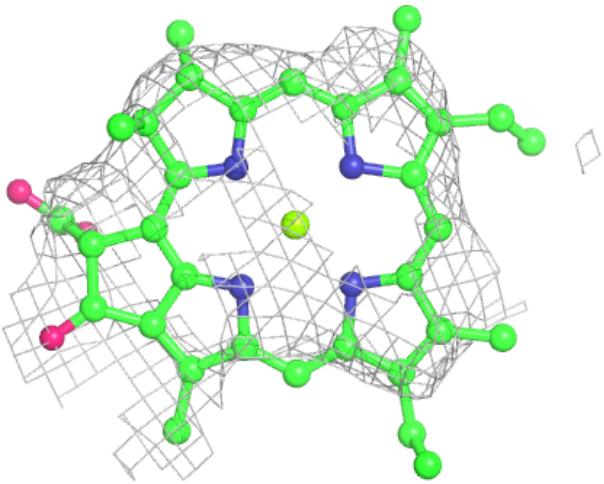
Electron density around BCR J 103:

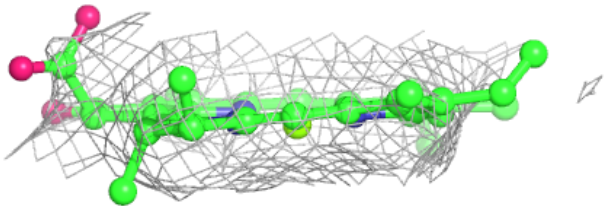
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

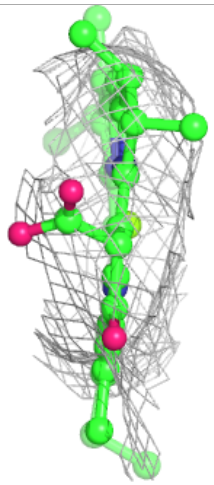


Electron density around CLA 3 1011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

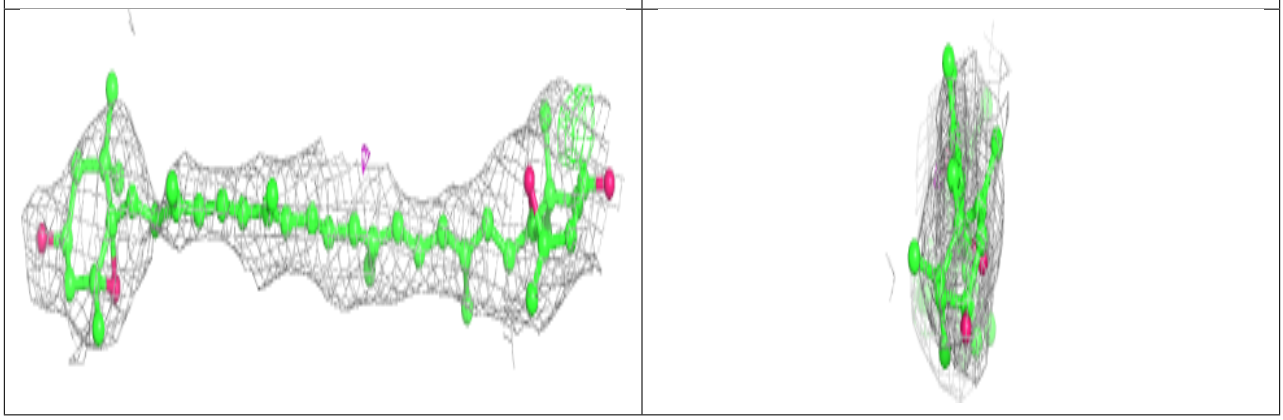






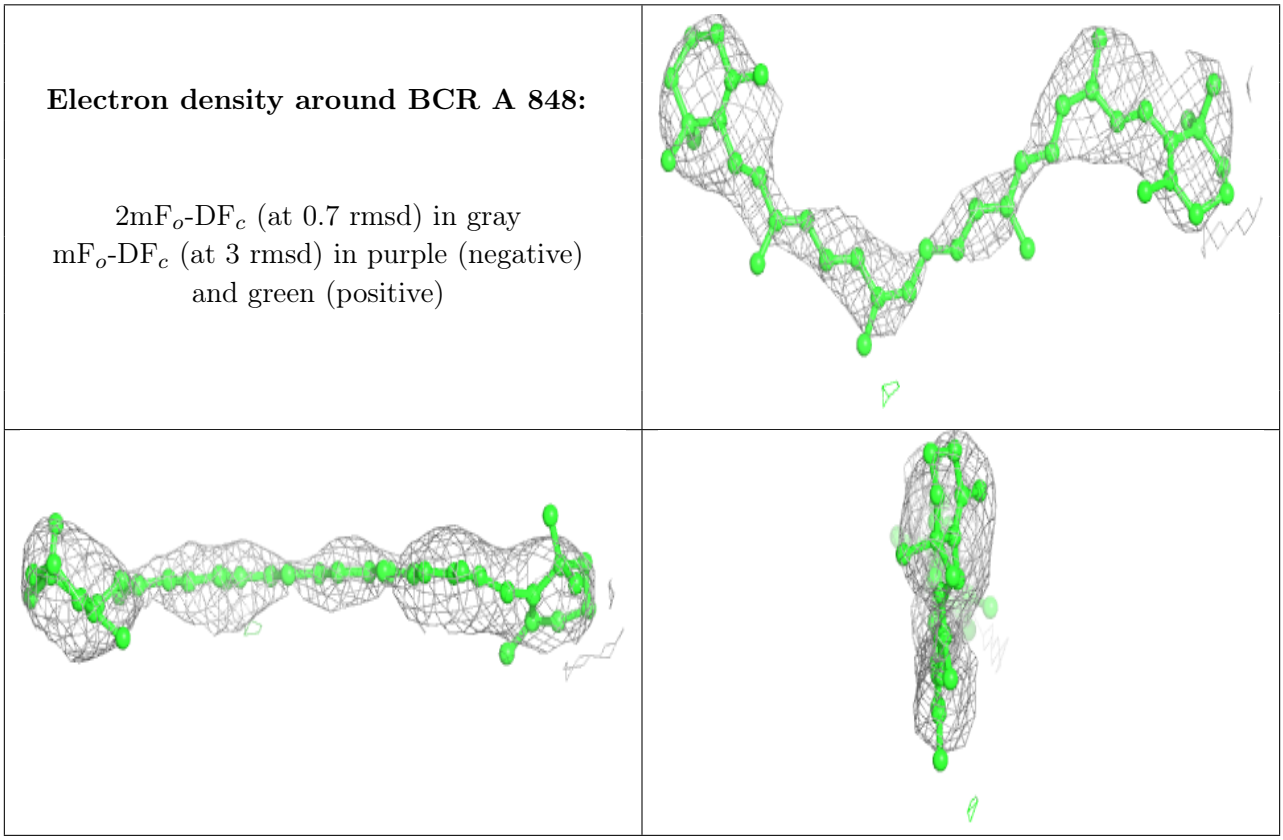
Electron density around XAT 5 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



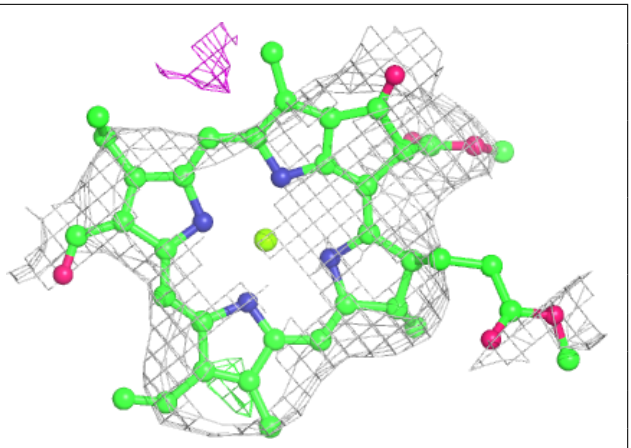
Electron density around BCR A 848:

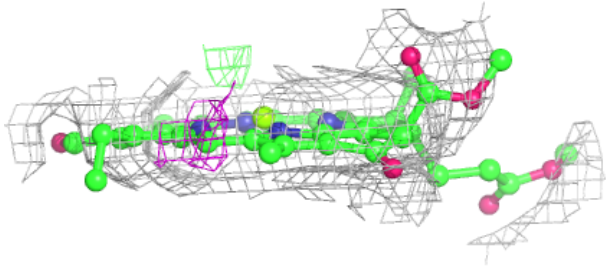
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

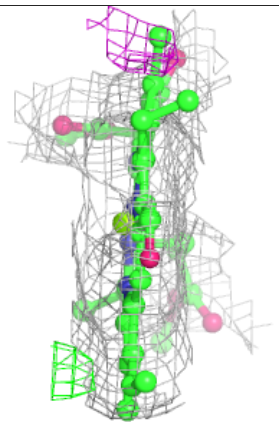


Electron density around CHL 8 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

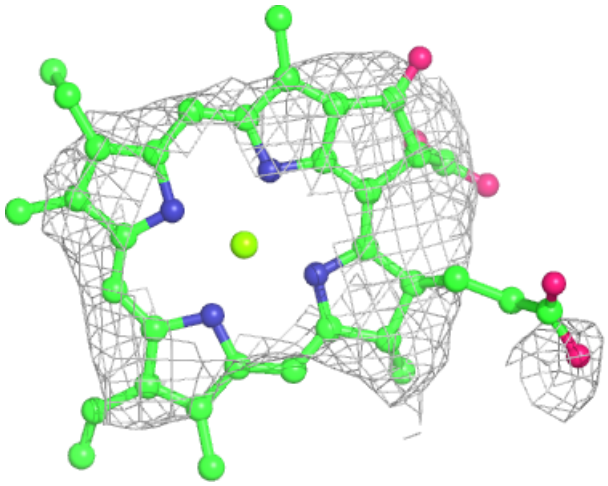


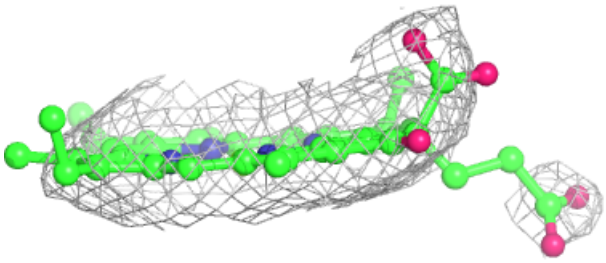


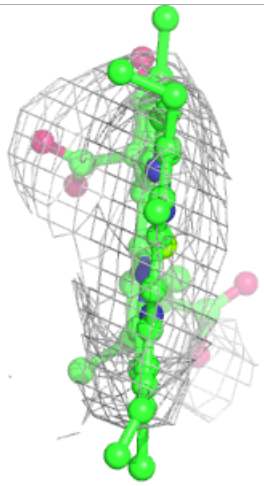


Electron density around CLA A 834:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

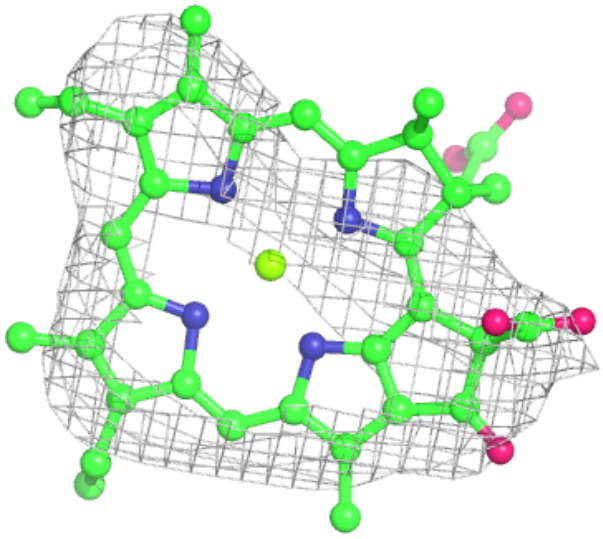


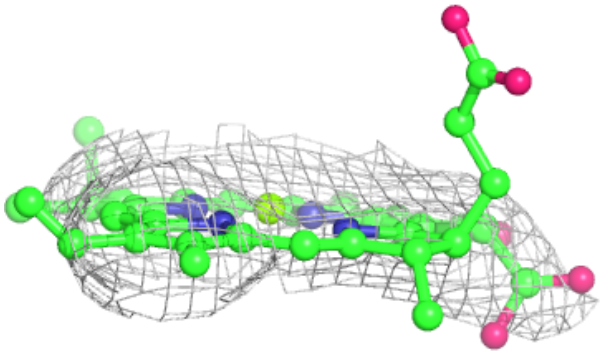


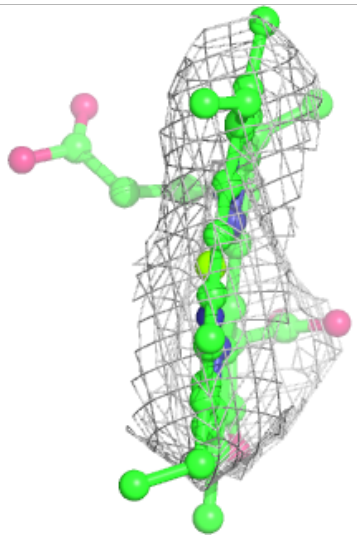


Electron density around CLA B 823:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

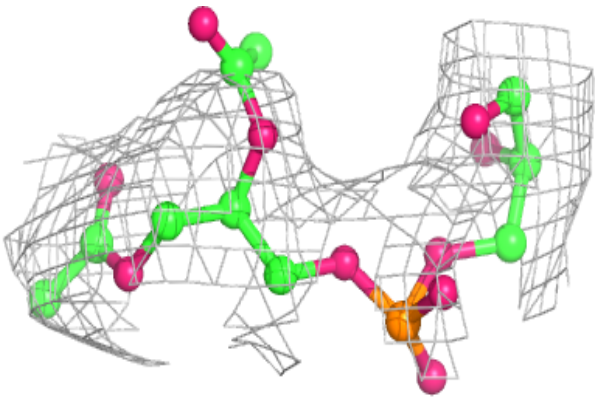


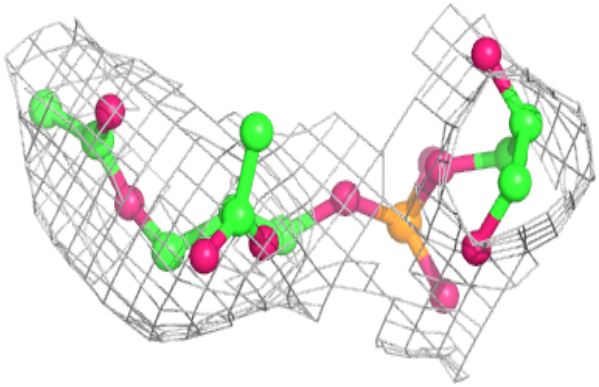


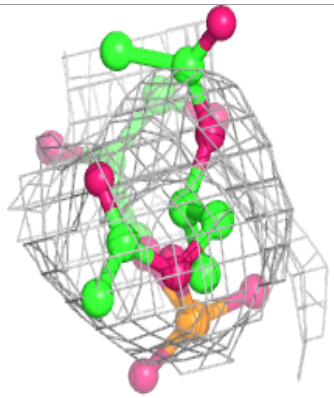


Electron density around LHG 0 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

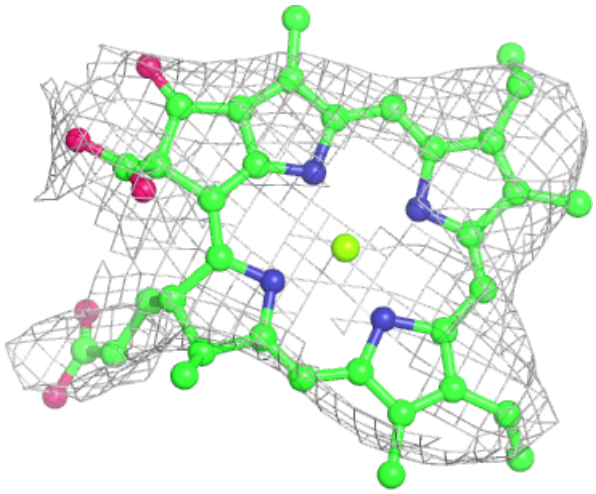


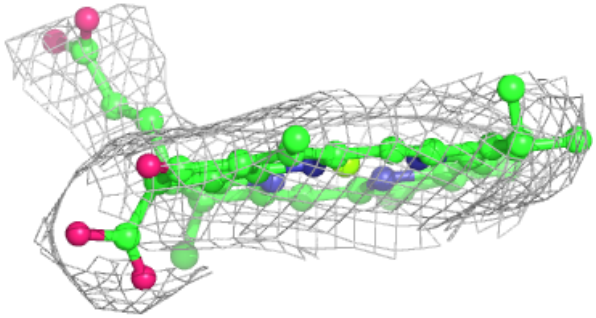


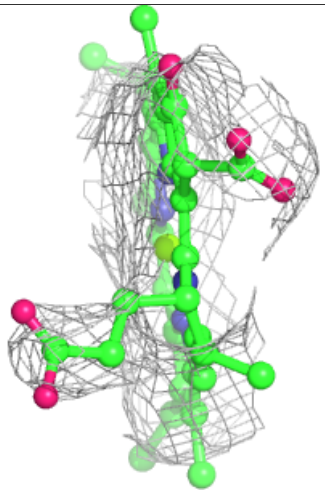


Electron density around CLA A 825:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

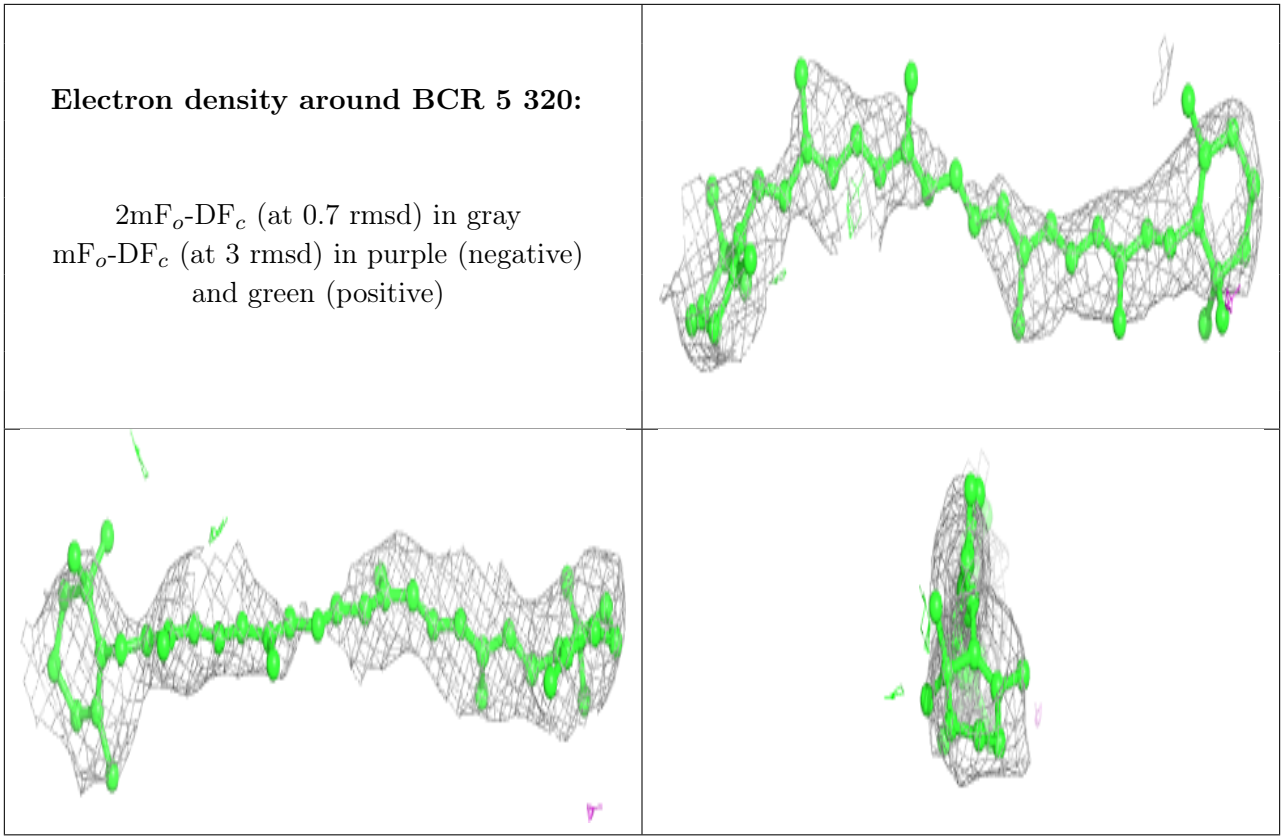






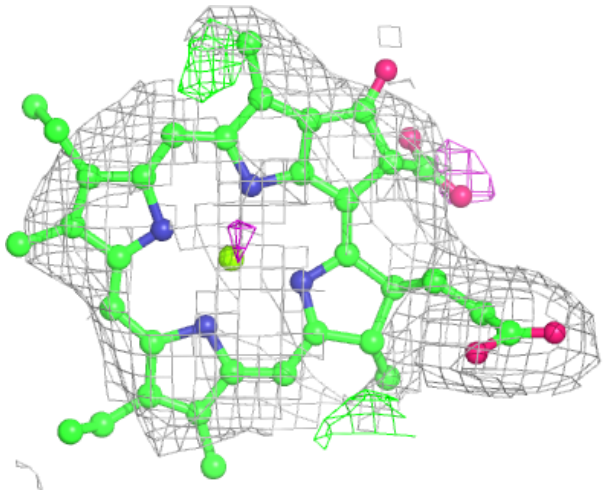
Electron density around BCR 5 320:

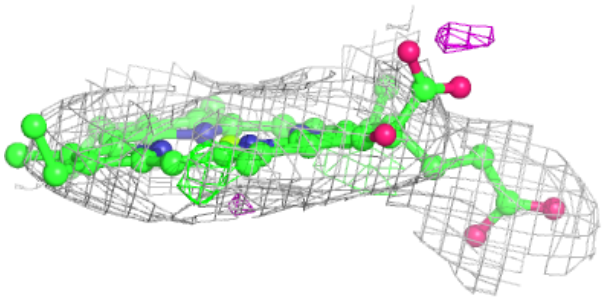
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

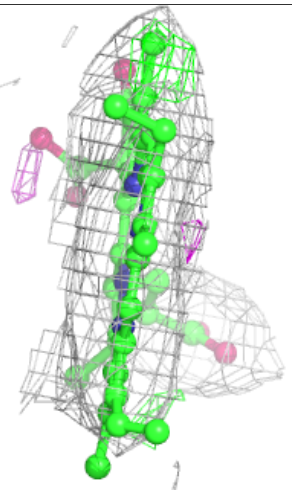


Electron density around CLA 5 323:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

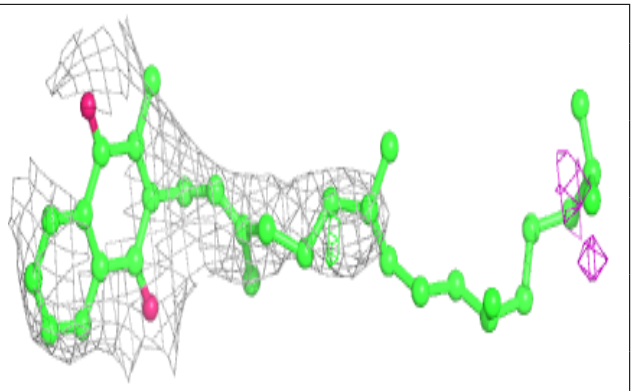


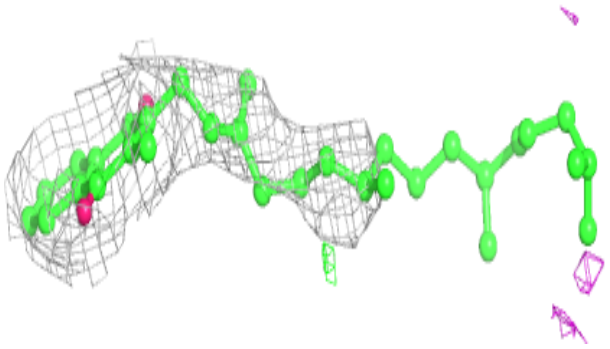


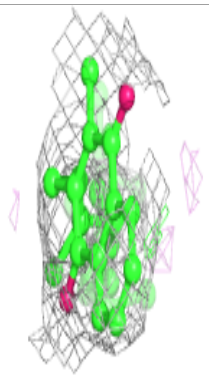


Electron density around PQN A 842:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

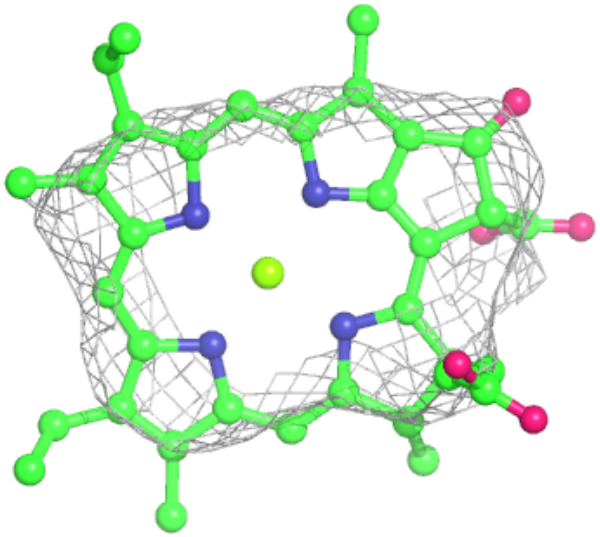


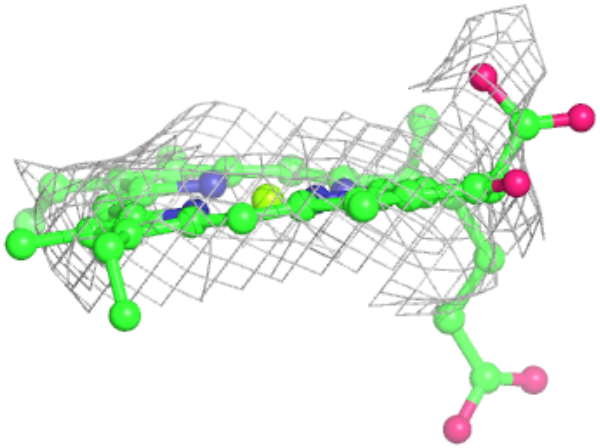


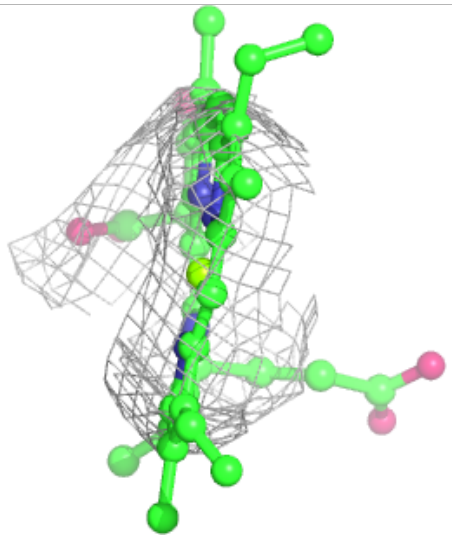


Electron density around CLA B 818:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

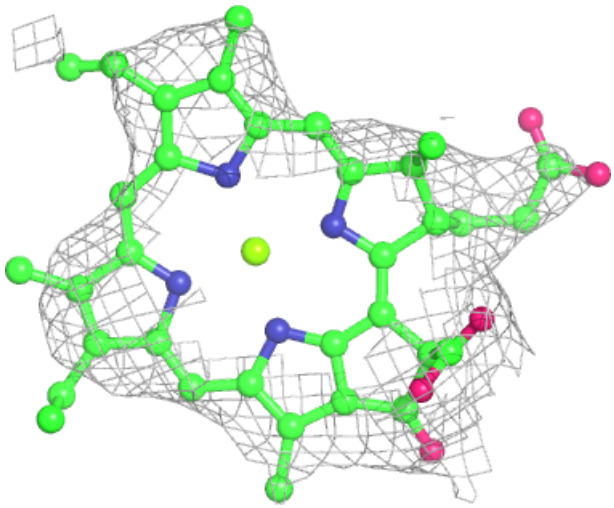


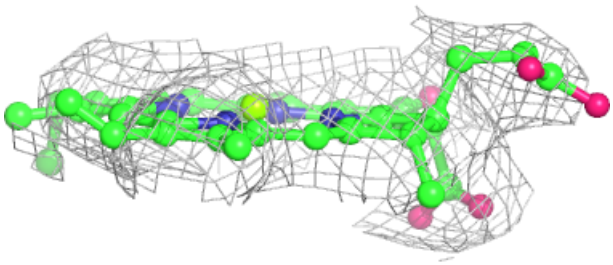


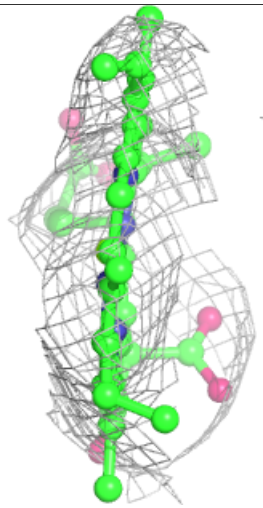


Electron density around CLA A 804:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

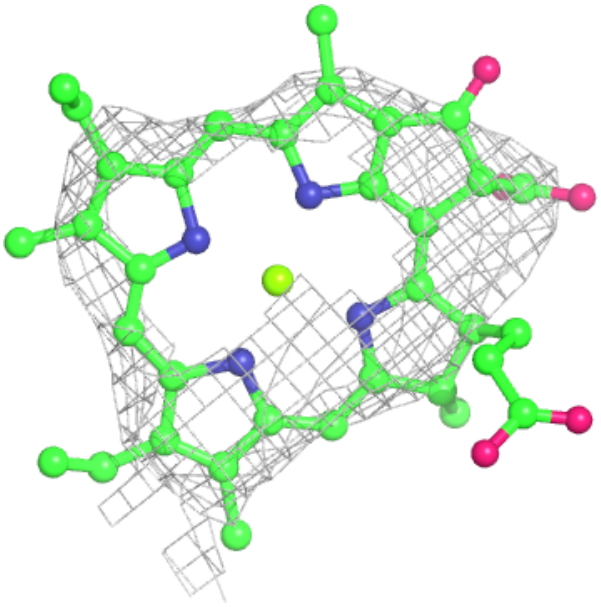


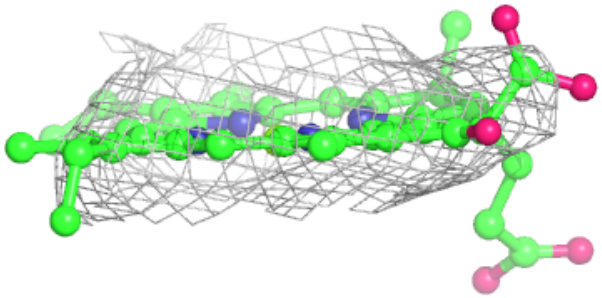


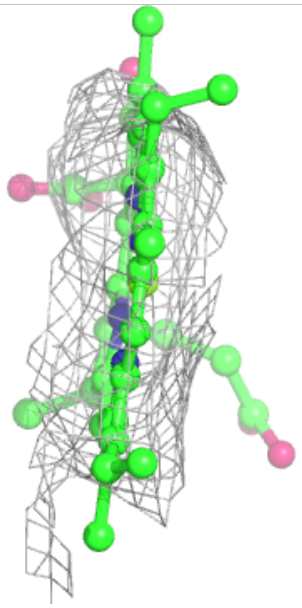


Electron density around CLA B 820:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

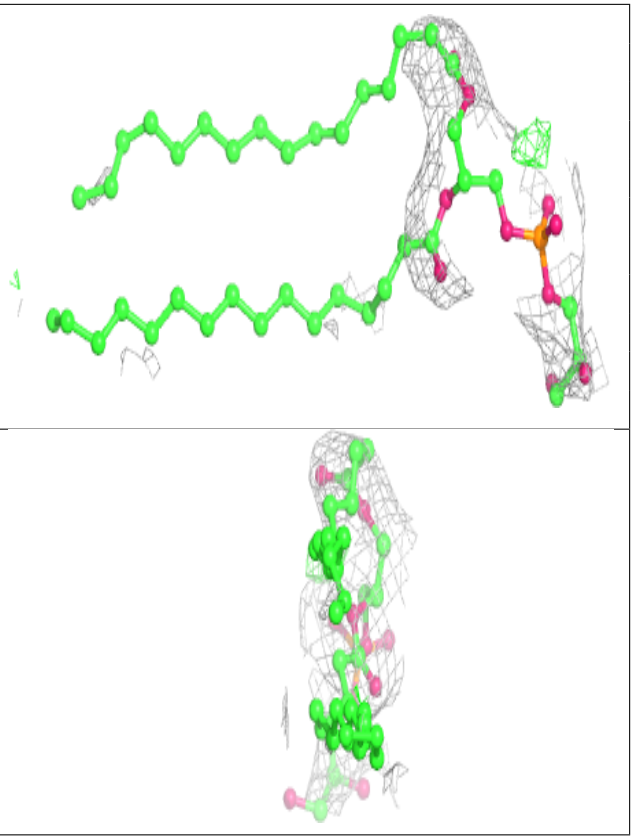


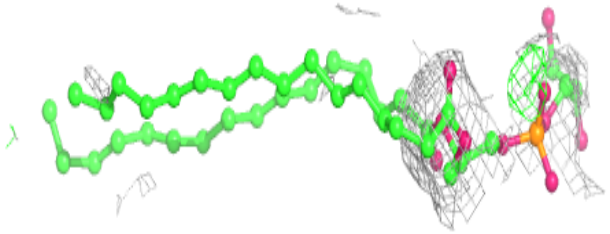




Electron density around LHG 8 301:

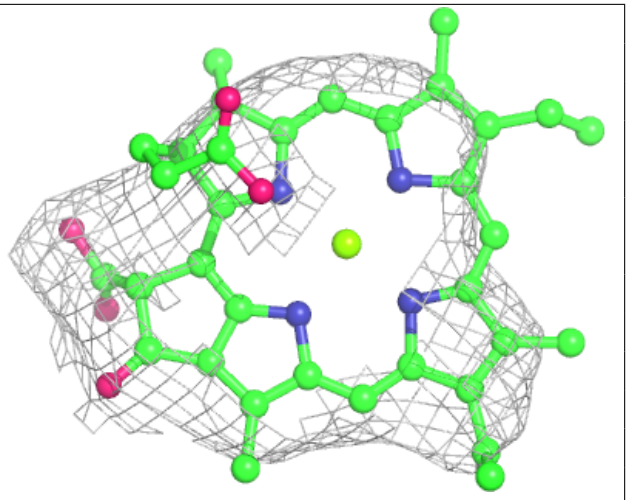
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

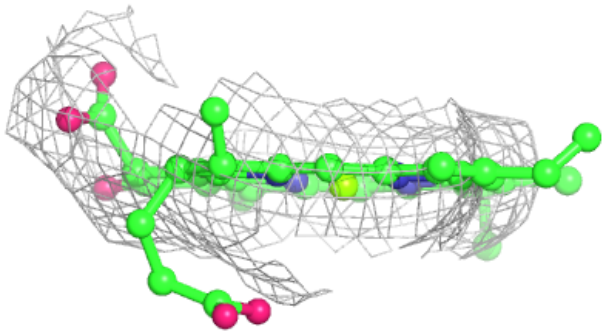


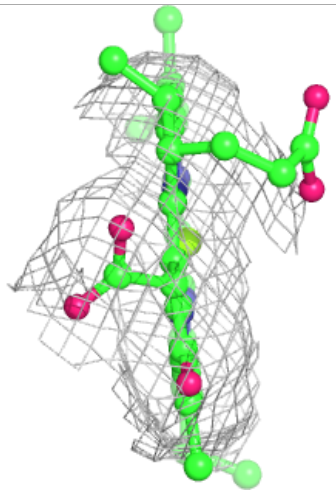


Electron density around CLA 3 1012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

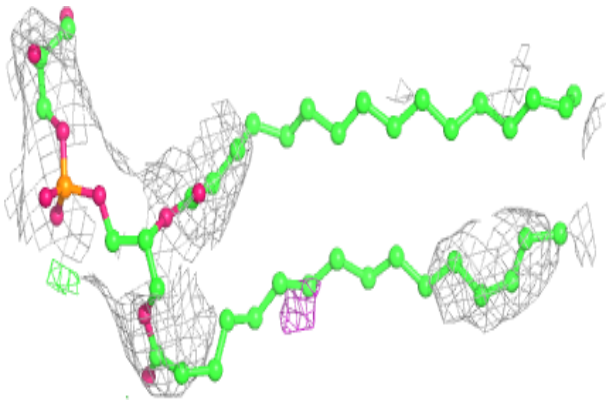


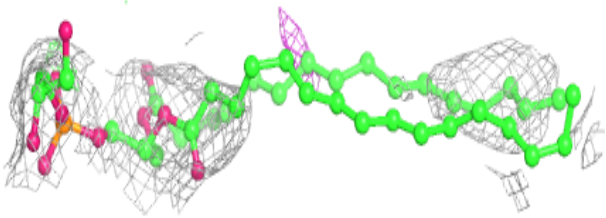




Electron density around LHG 4 301:

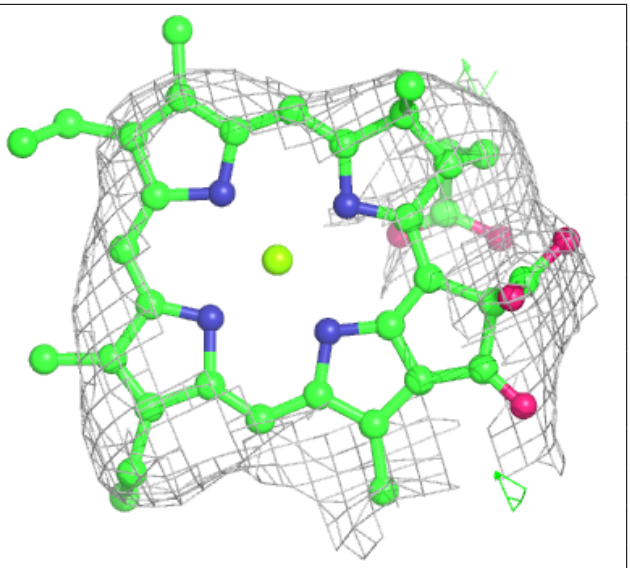
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

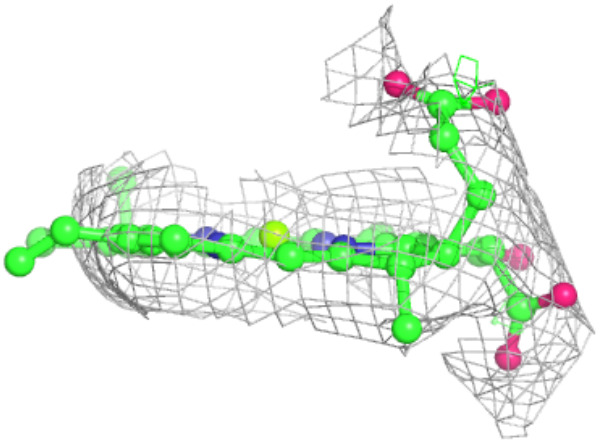


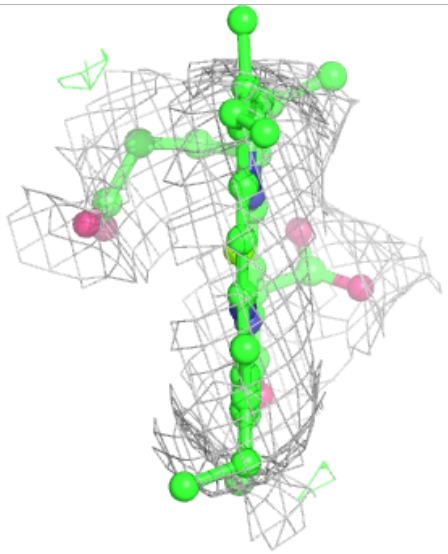


Electron density around CLA 1 1010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

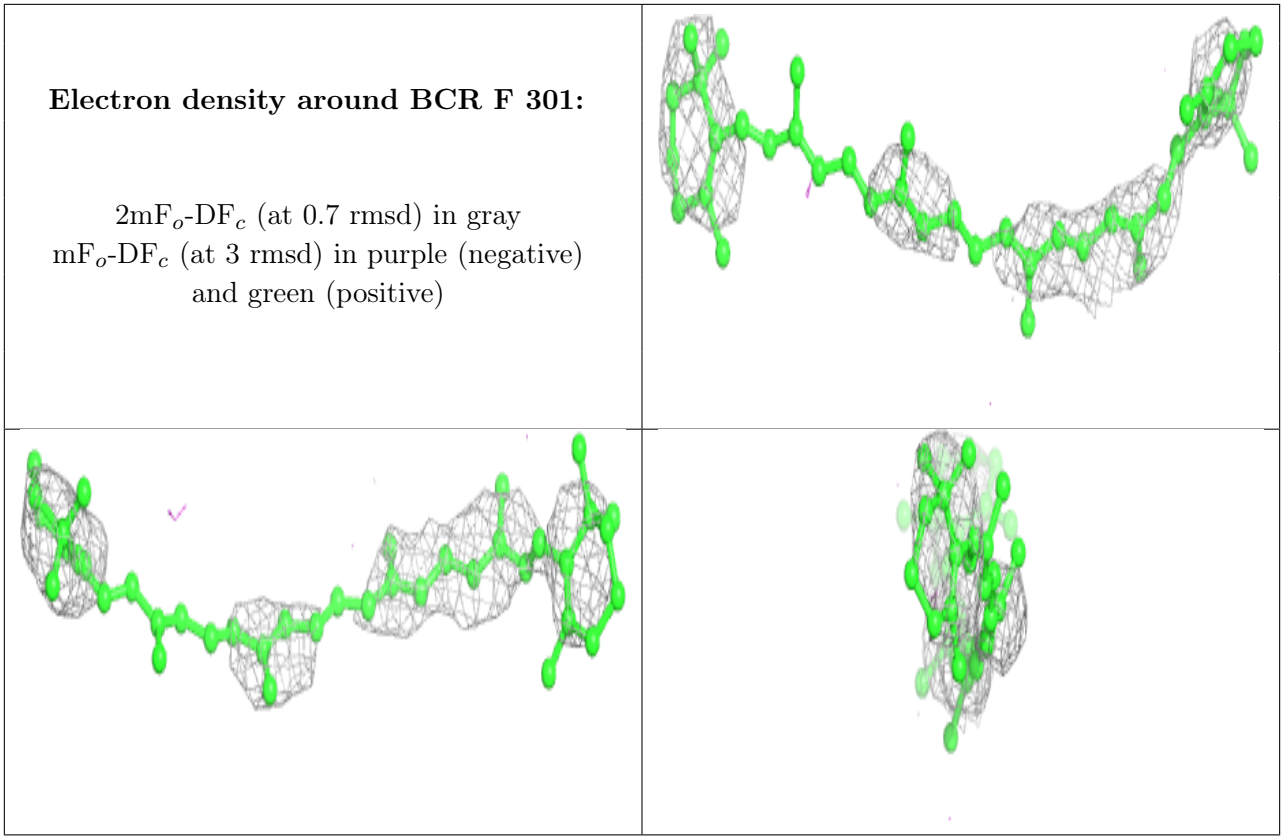






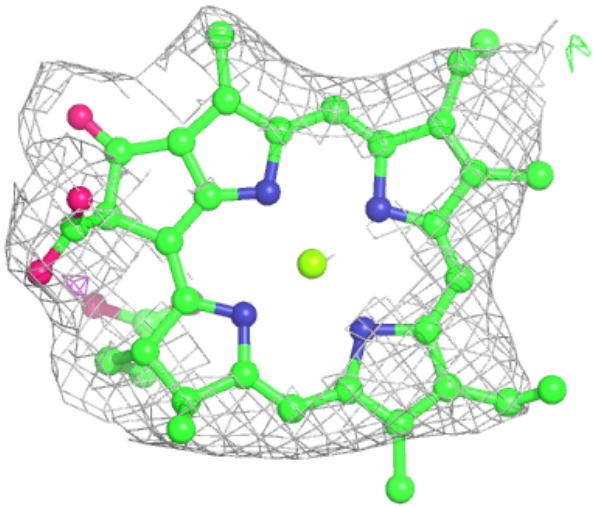
Electron density around BCR F 301:

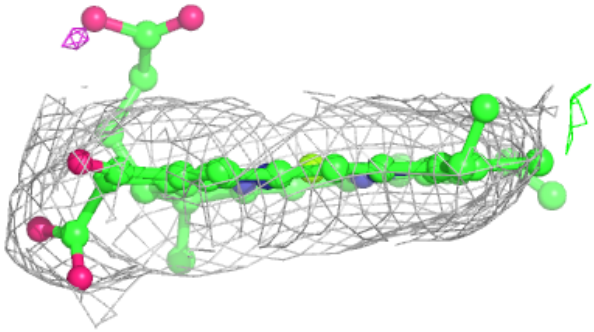
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

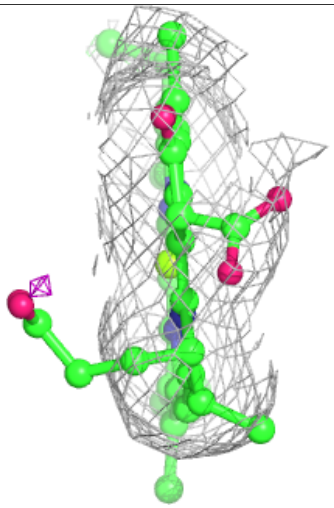


Electron density around CLA 5 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

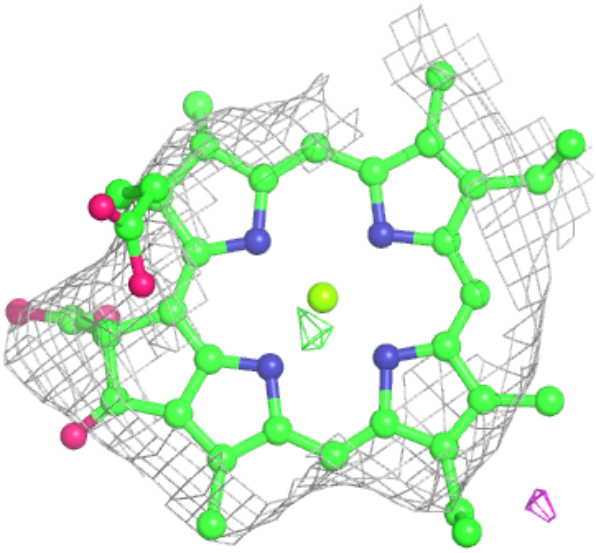


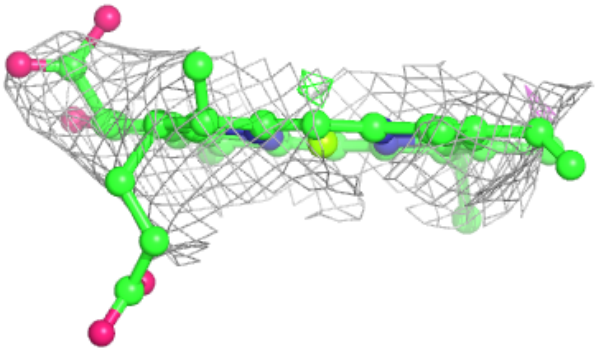


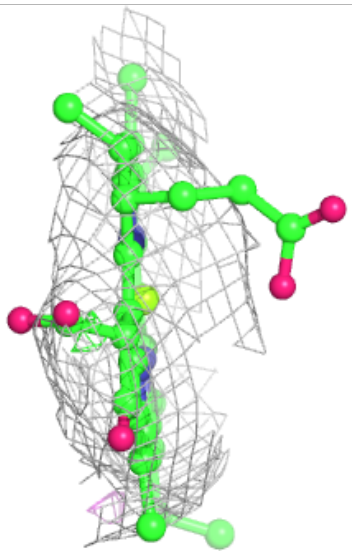


Electron density around CLA A 815:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

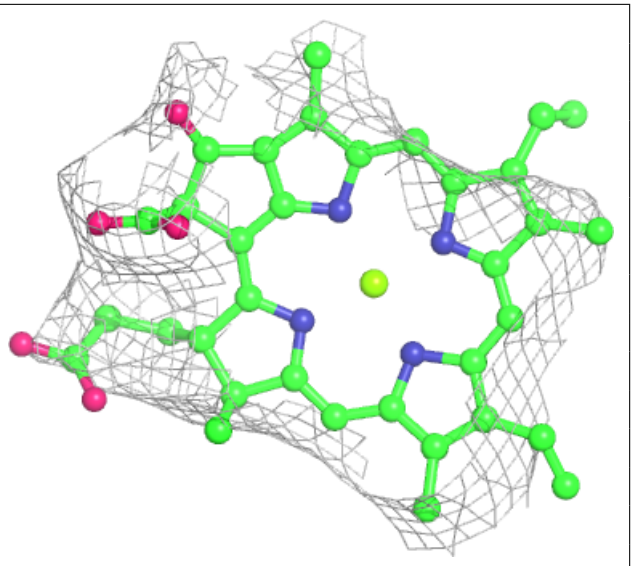


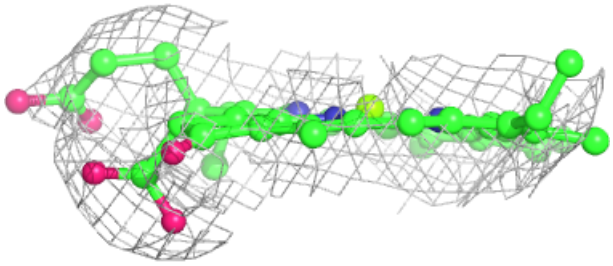


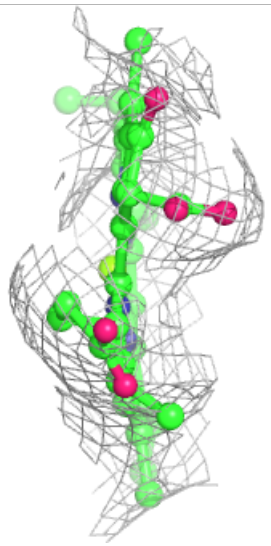


Electron density around CLA 0 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

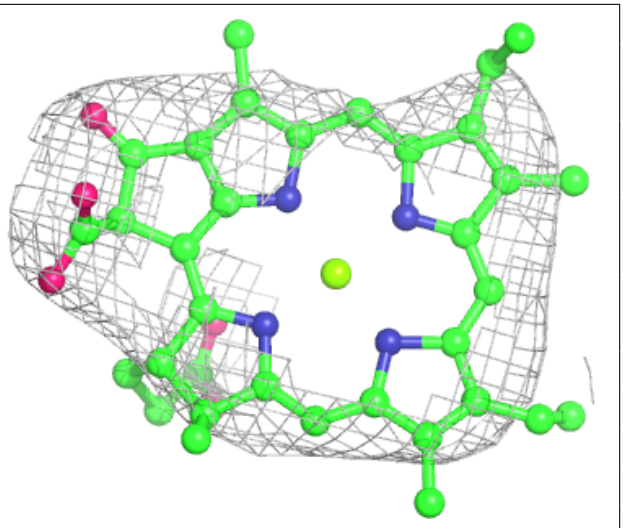


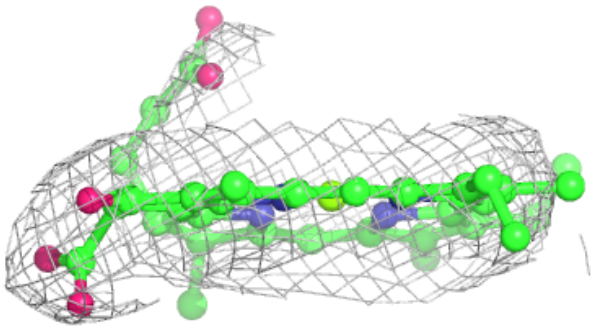


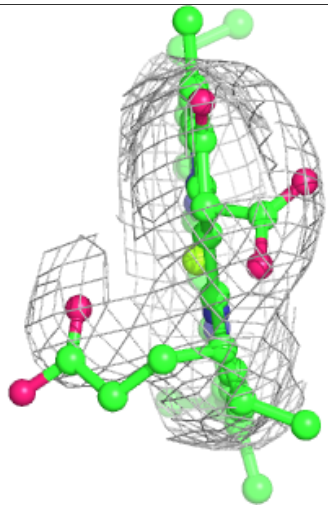


Electron density around CLA B 807:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

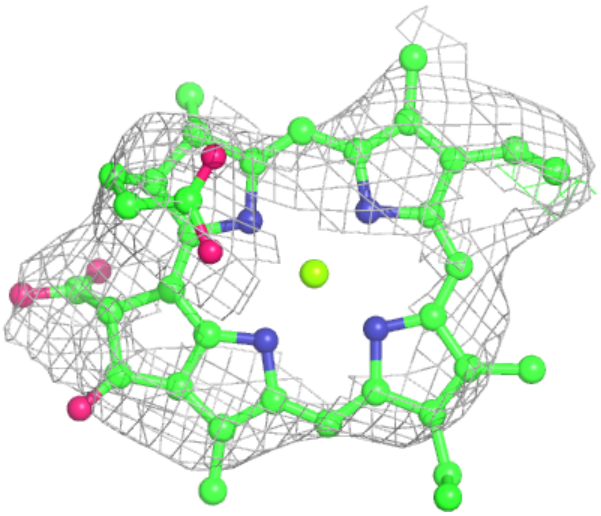


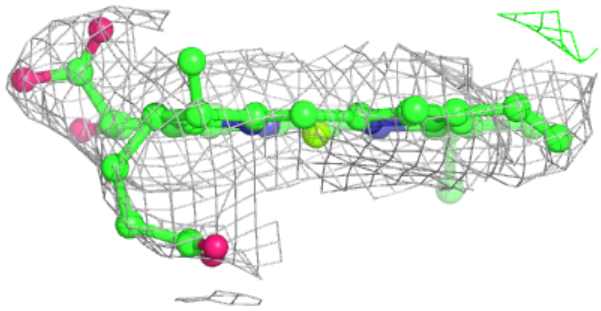


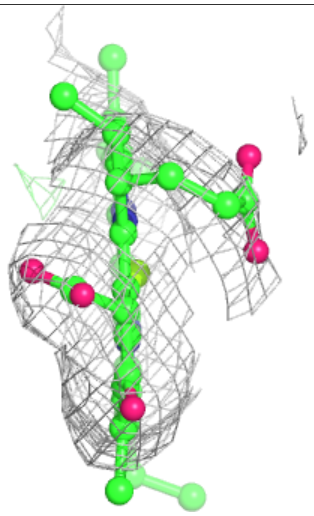


Electron density around CLA A 811:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

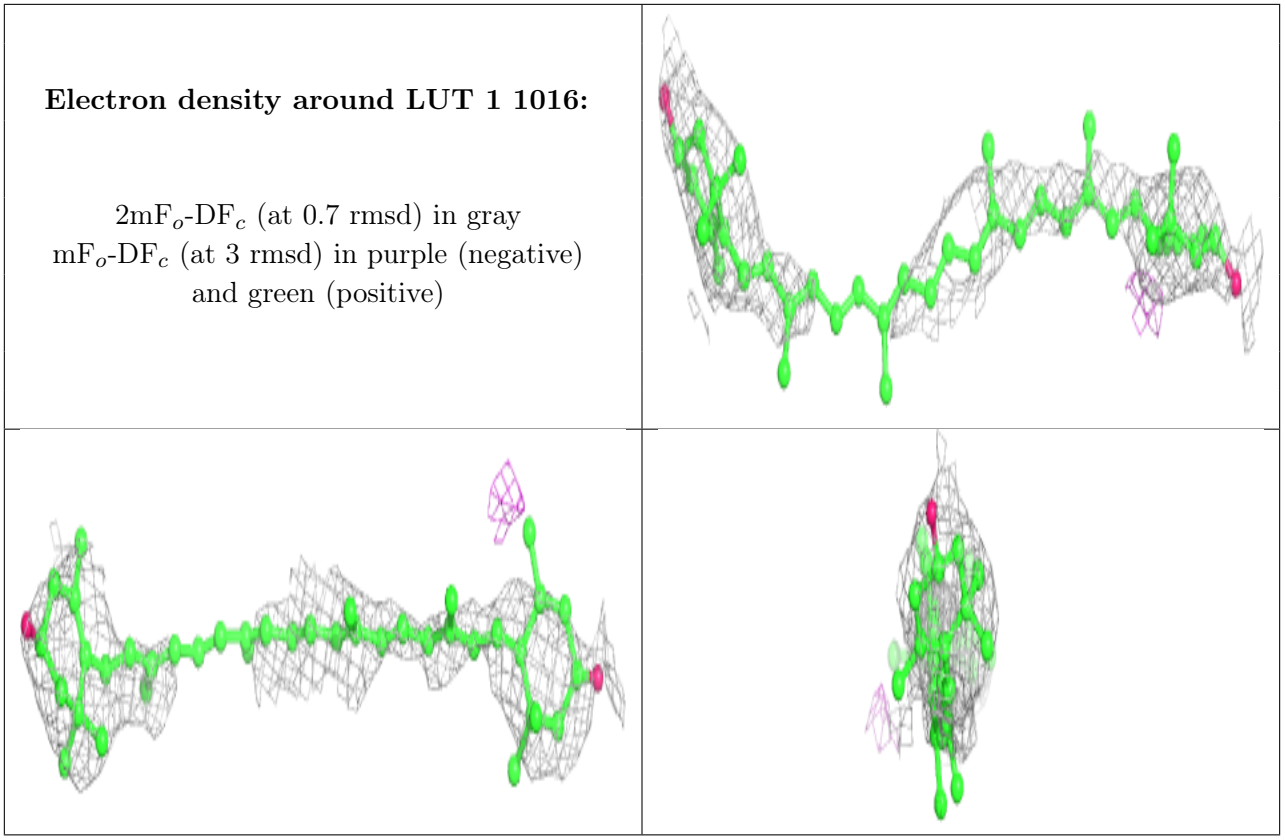






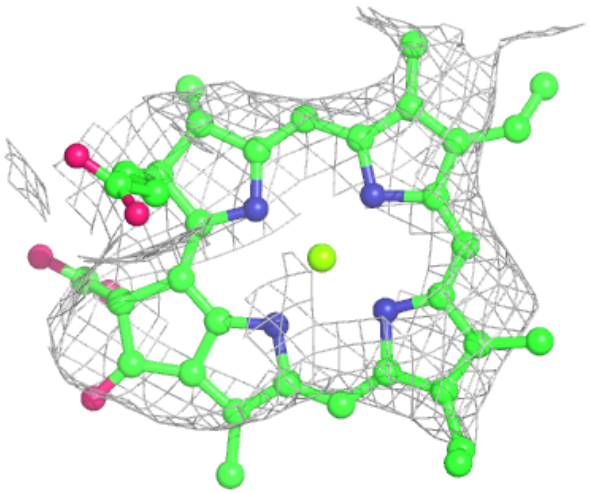
Electron density around LUT 1 1016:

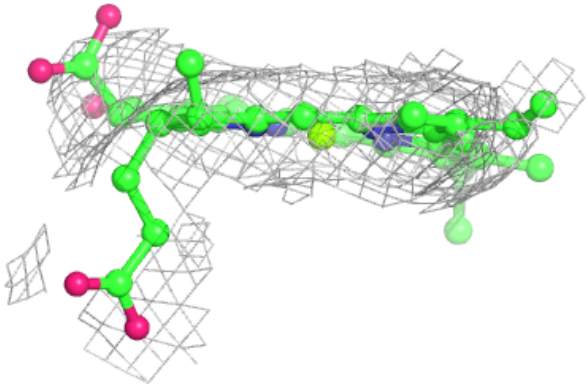
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

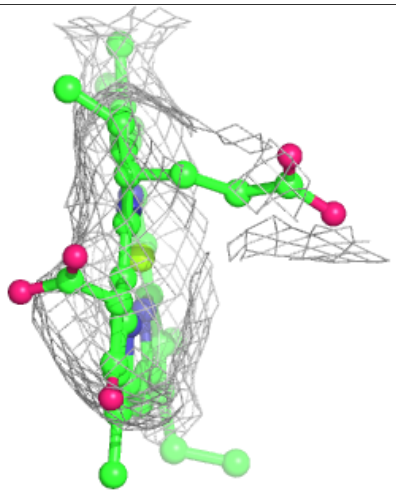


Electron density around CLA B 831:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

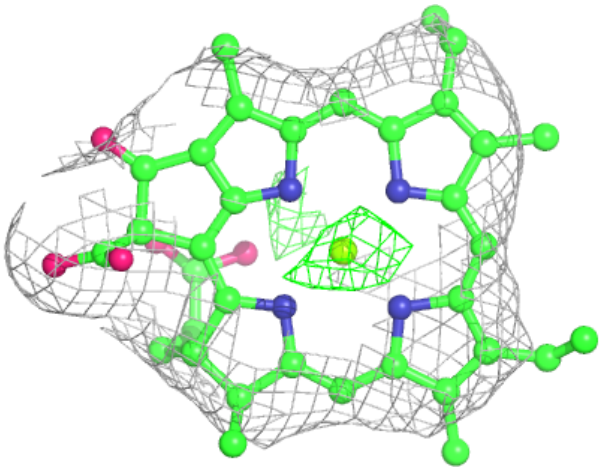


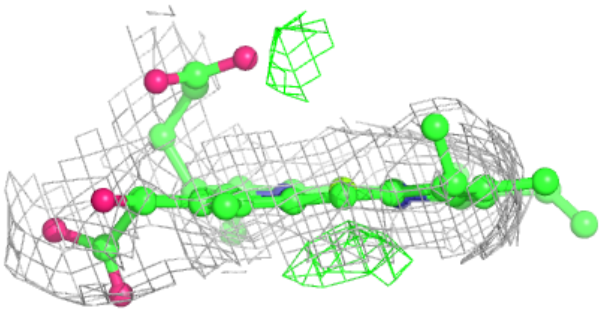


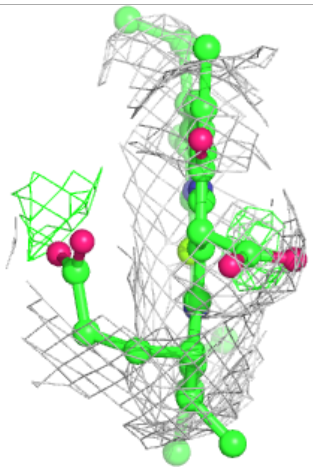


Electron density around CLA 1 1005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

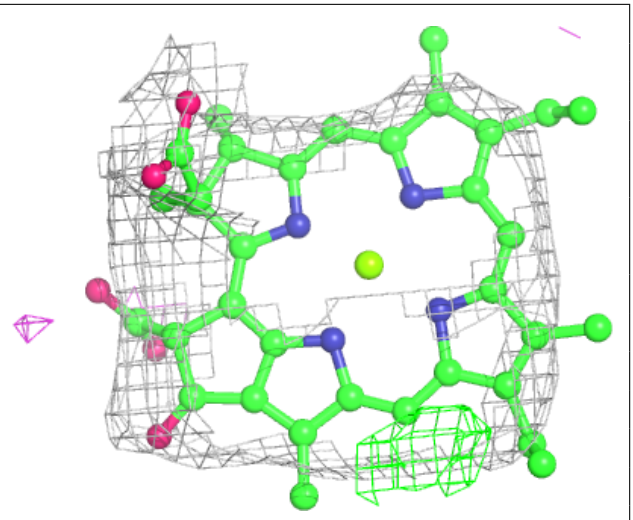


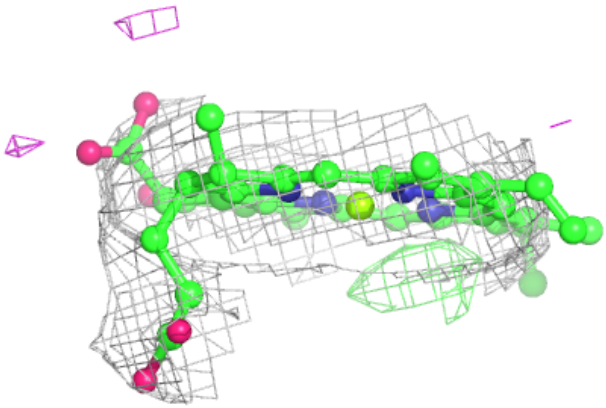


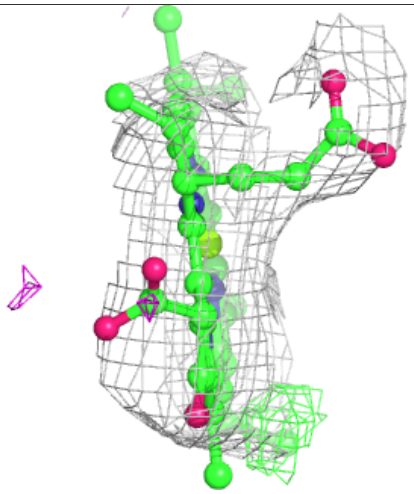


Electron density around CLA A 819:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

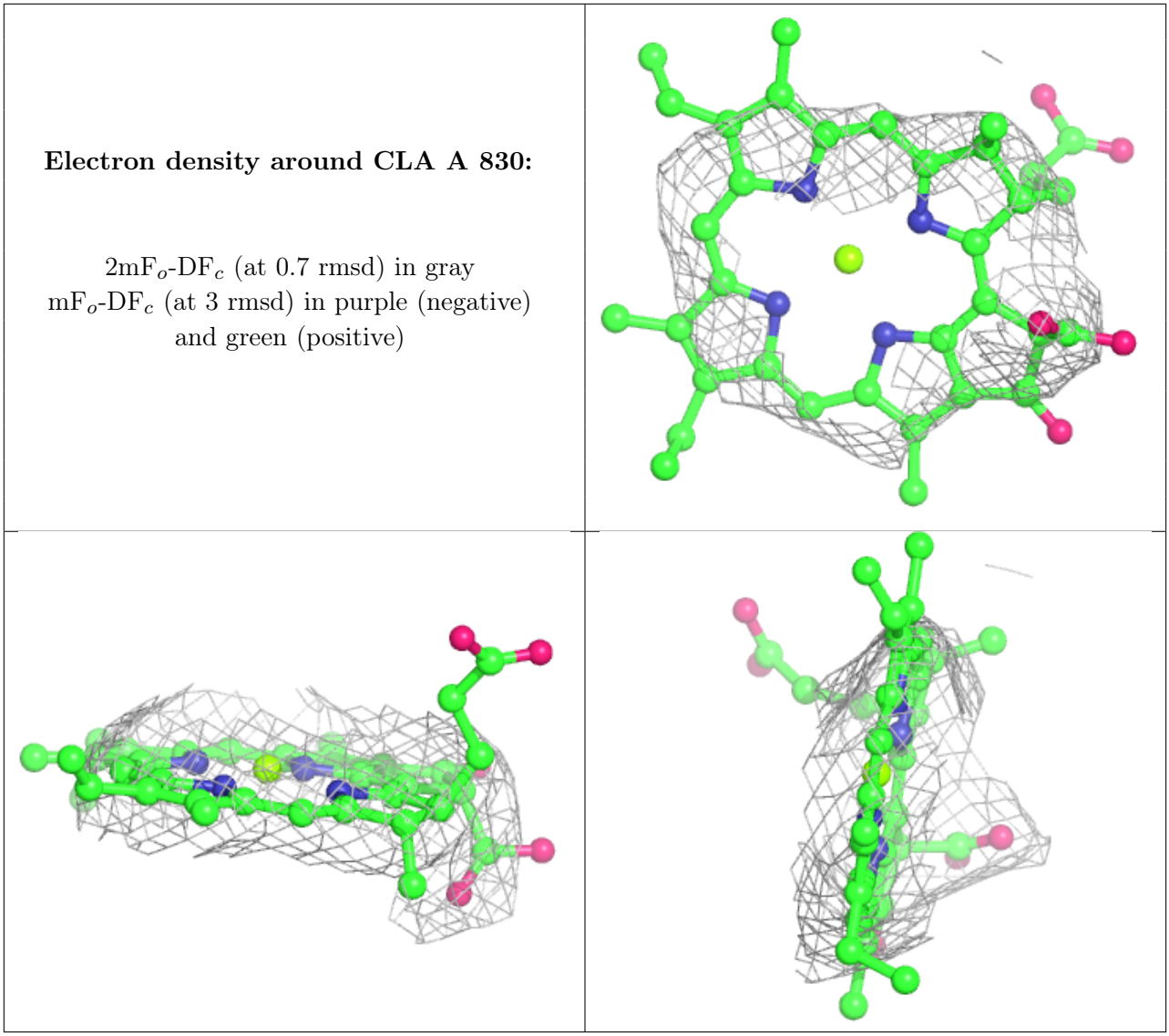






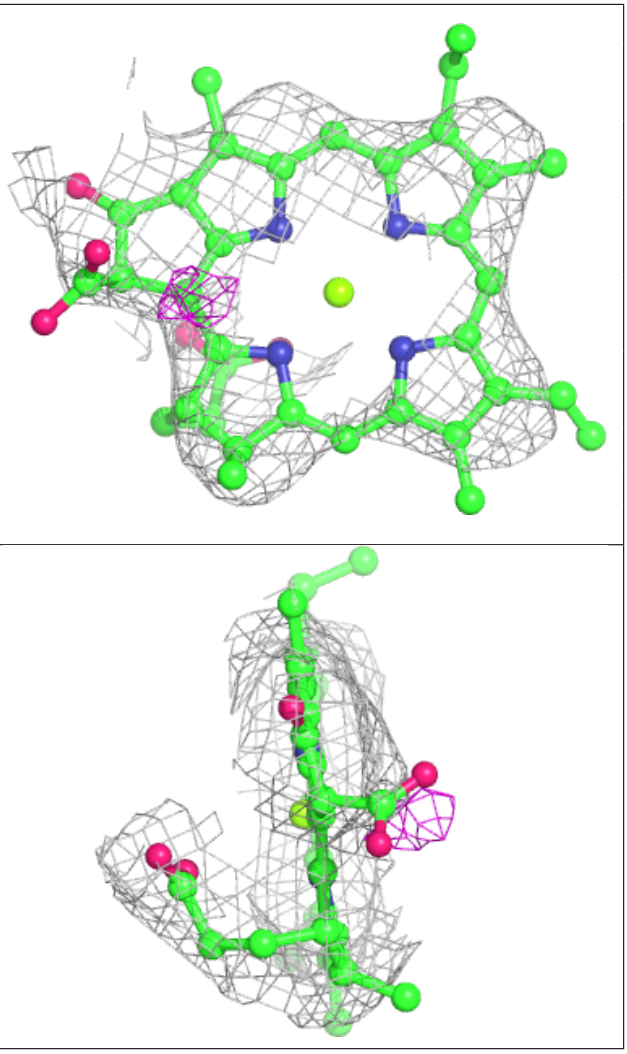
Electron density around CLA A 830:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



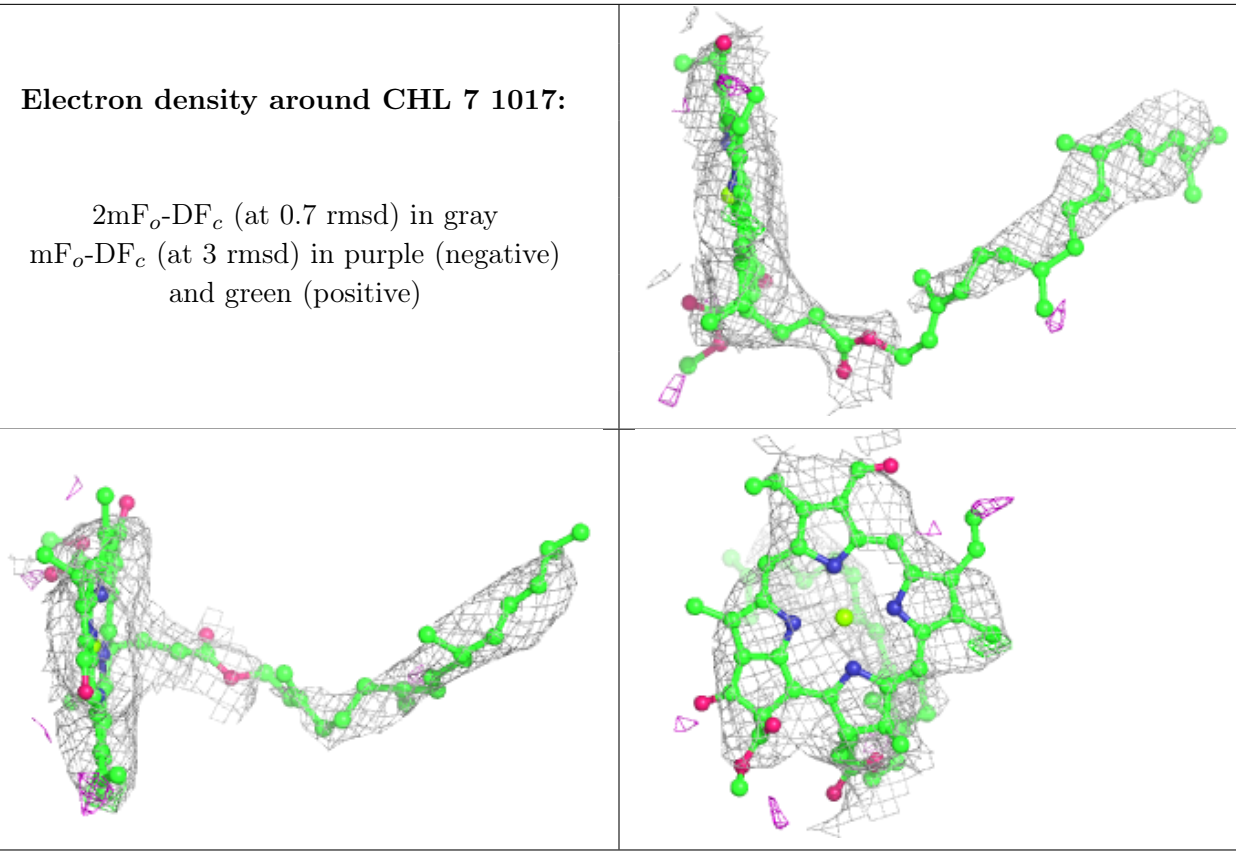
Electron density around CLA B 838:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



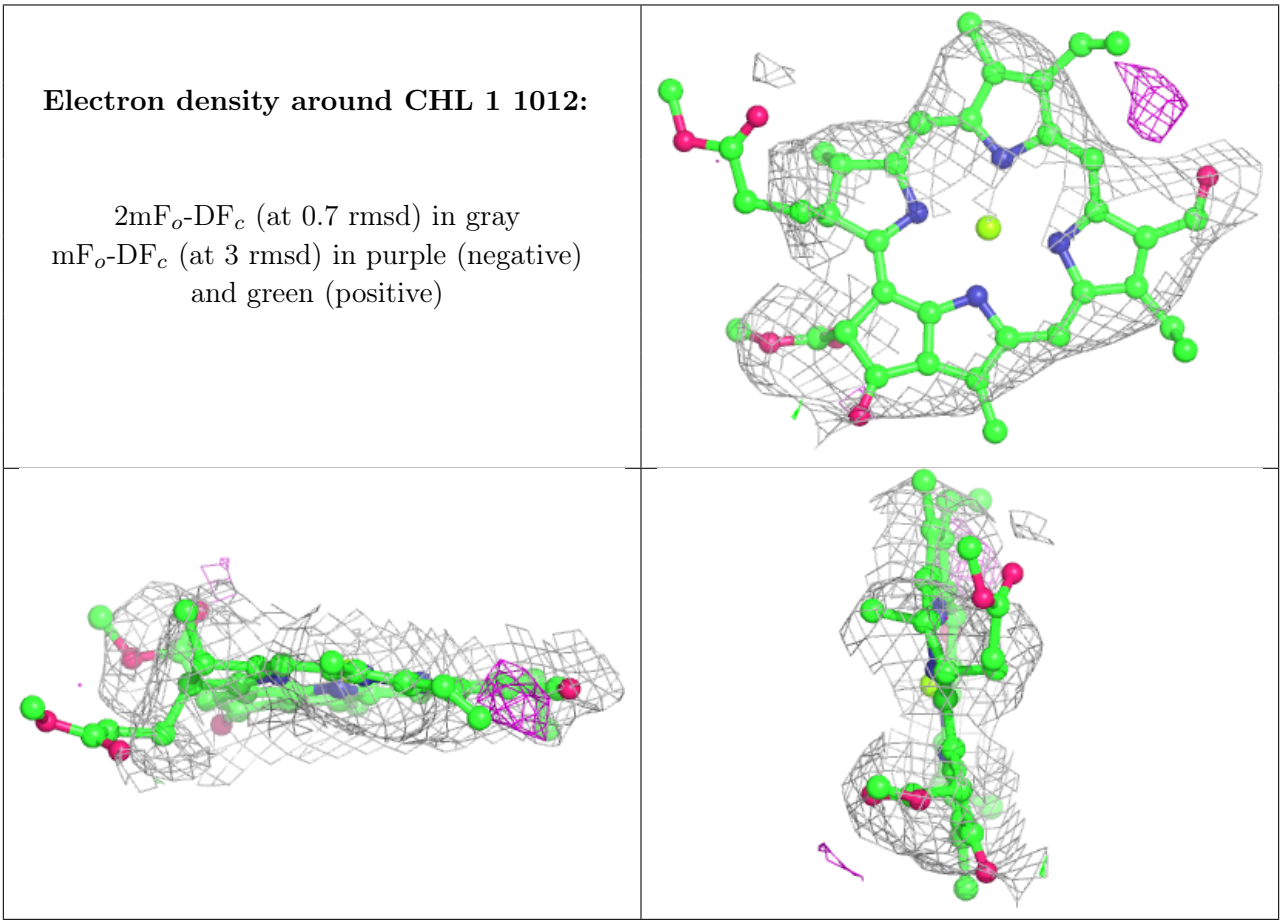
Electron density around CHL 7 1017:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



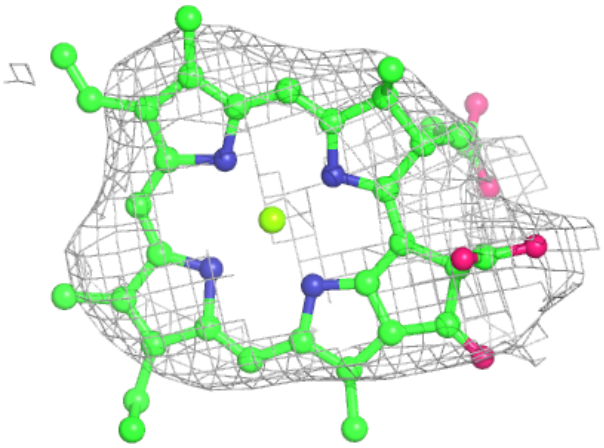
Electron density around CHL 1 1012:

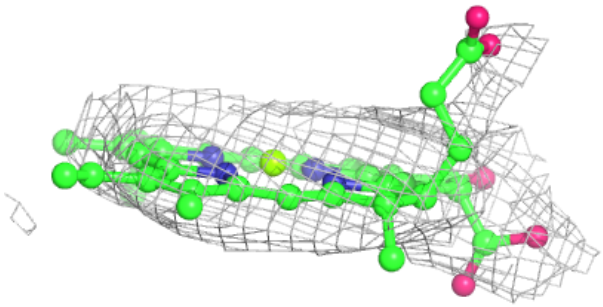
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

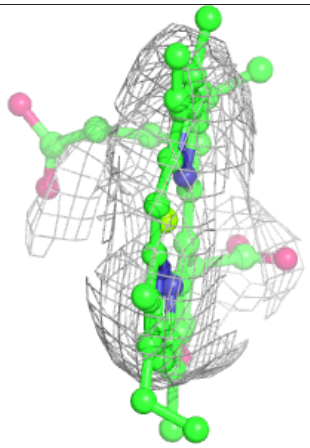


Electron density around CLA A 852:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

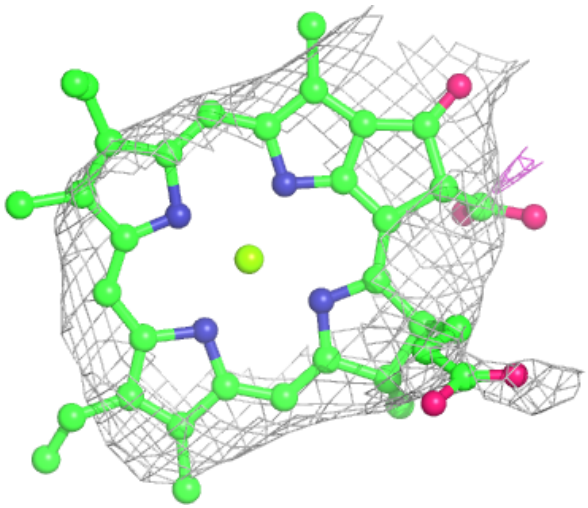


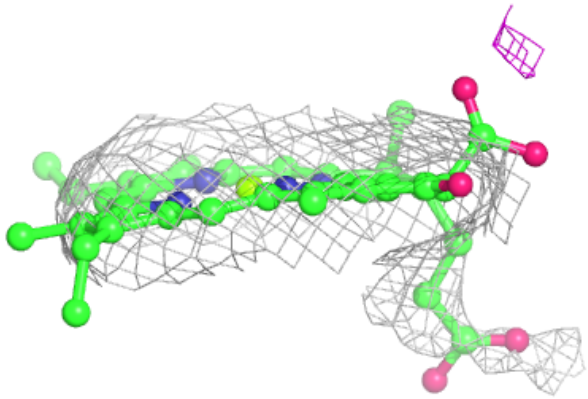


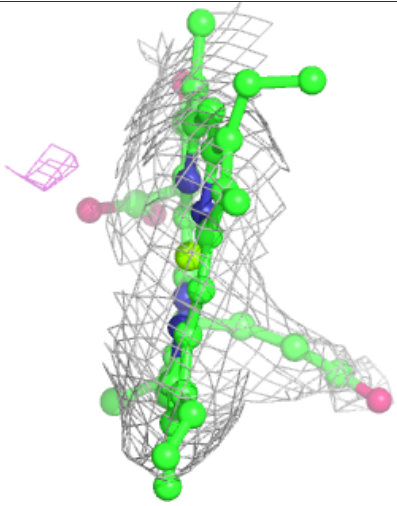


Electron density around CLA A 832:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

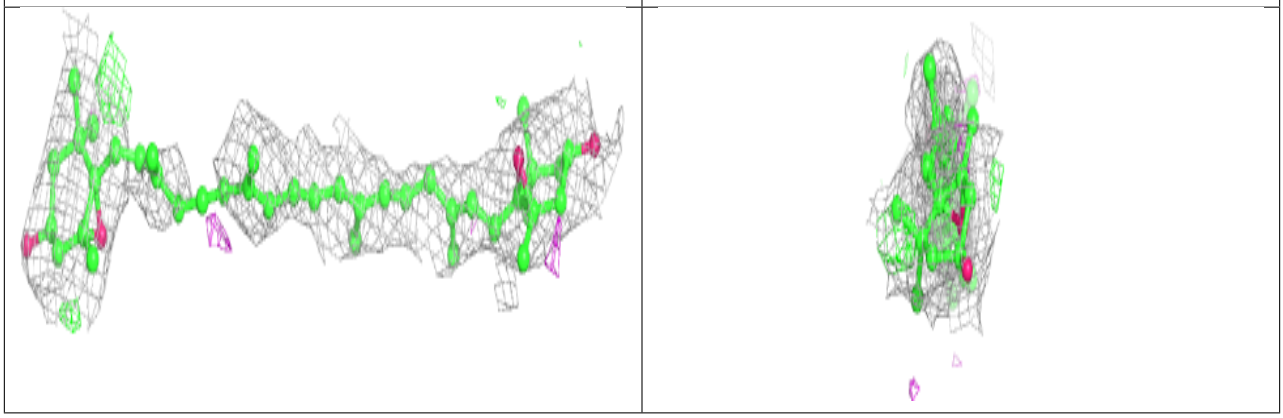






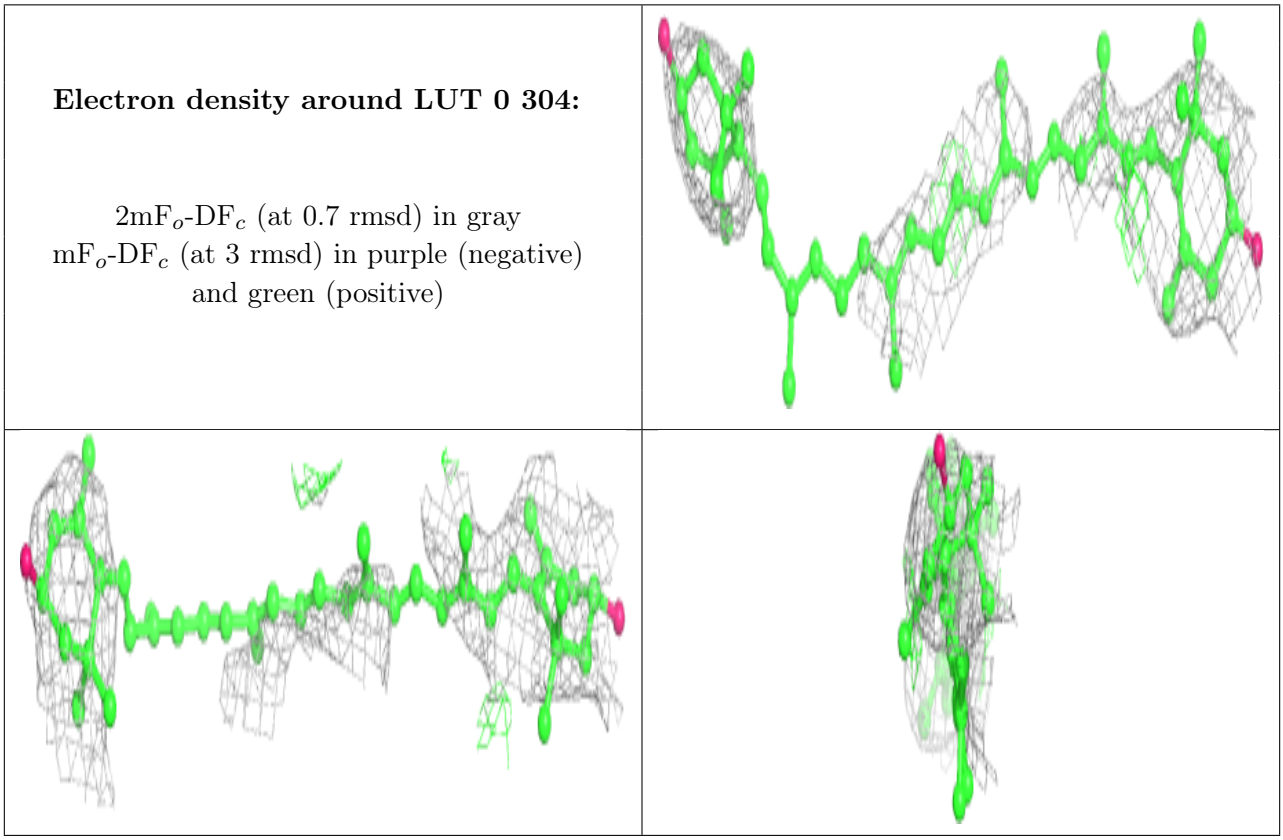
Electron density around XAT 8 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



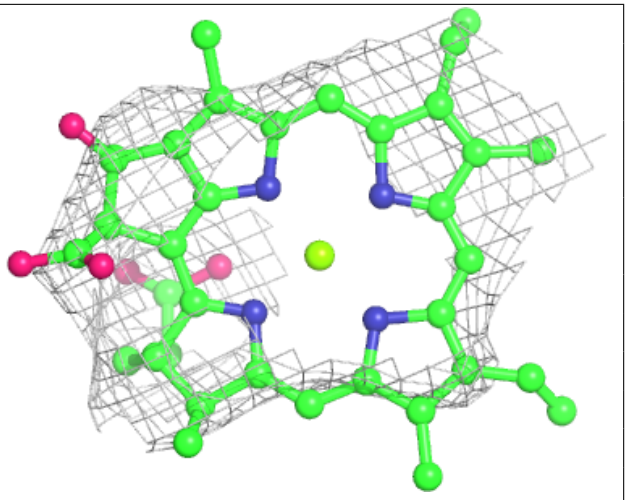
Electron density around LUT 0 304:

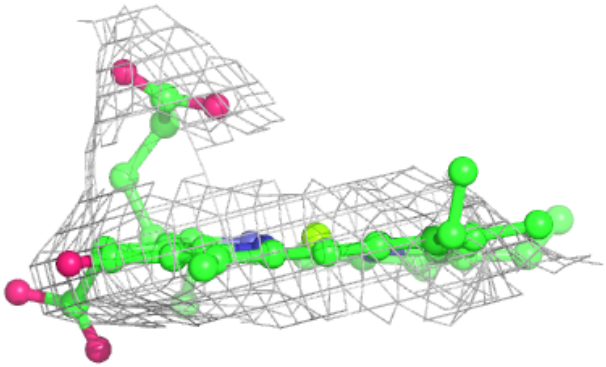
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

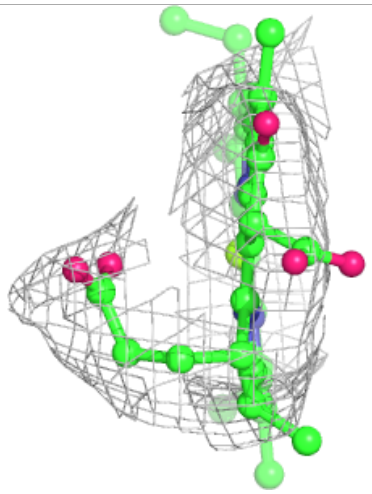


Electron density around CLA B 803:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

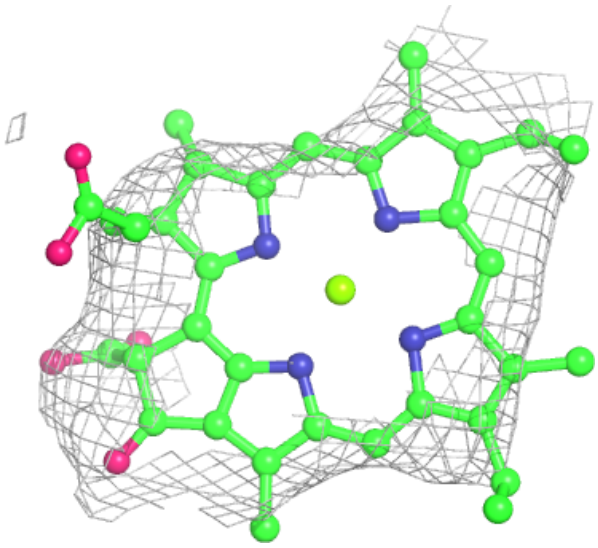


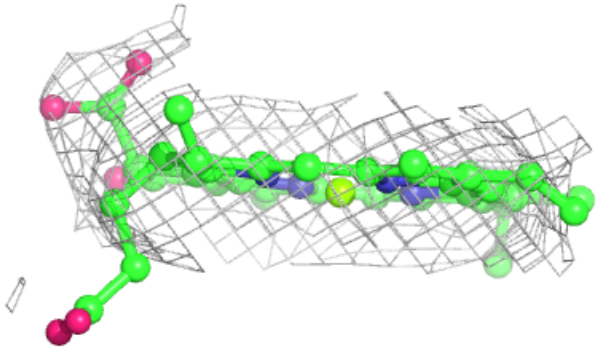


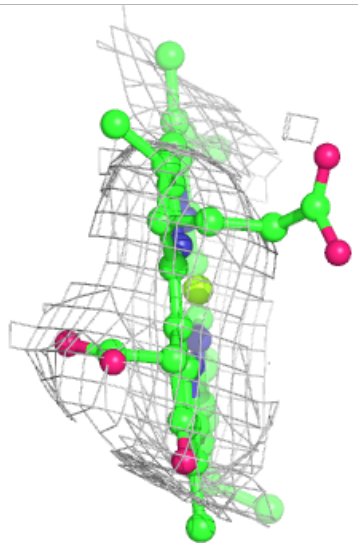


Electron density around CLA A 821:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

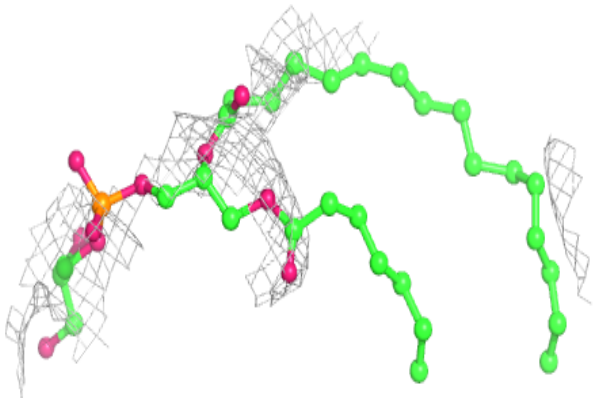


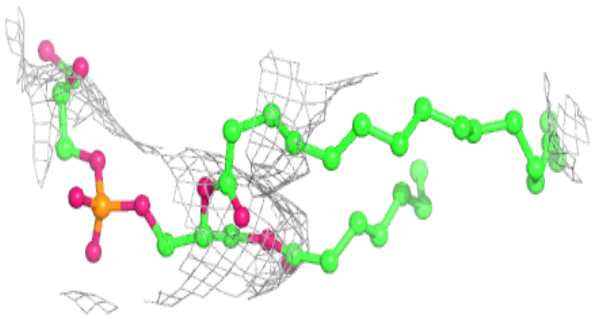


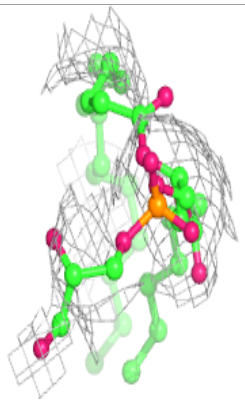


Electron density around LHG A 843:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

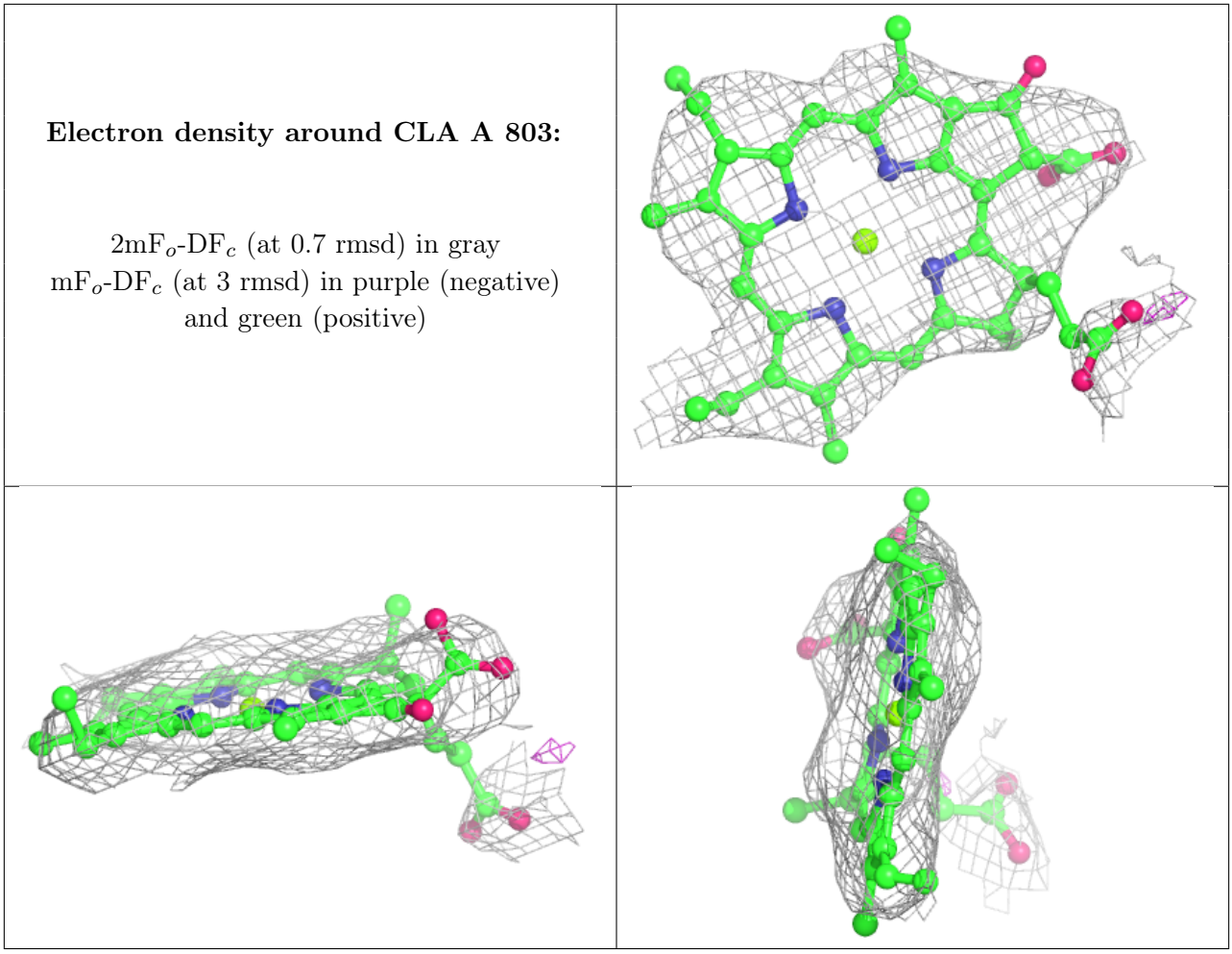






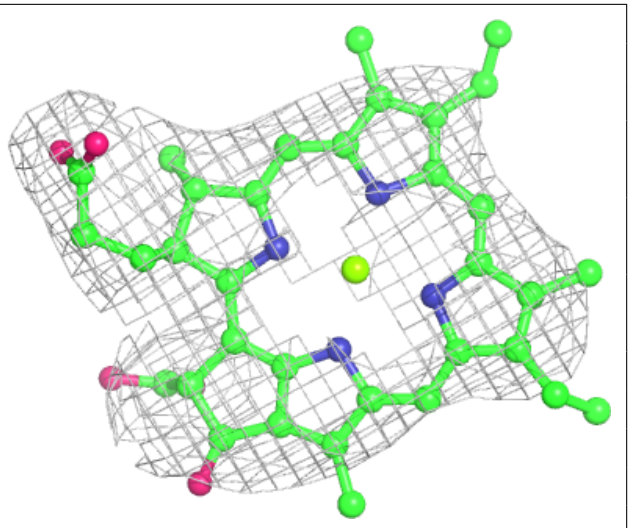
Electron density around CLA A 803:

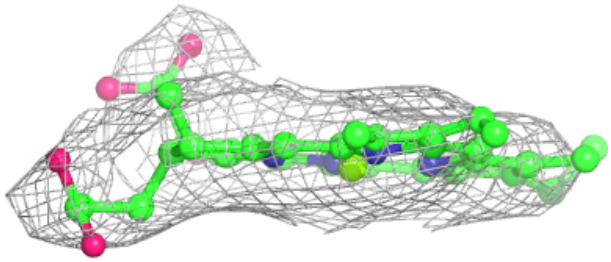
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

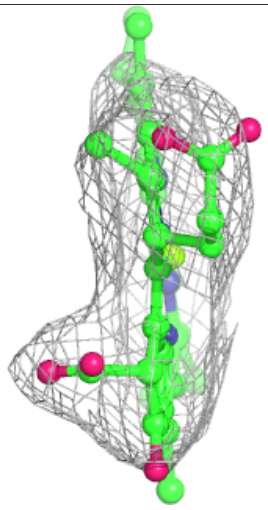


Electron density around CLA A 812:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

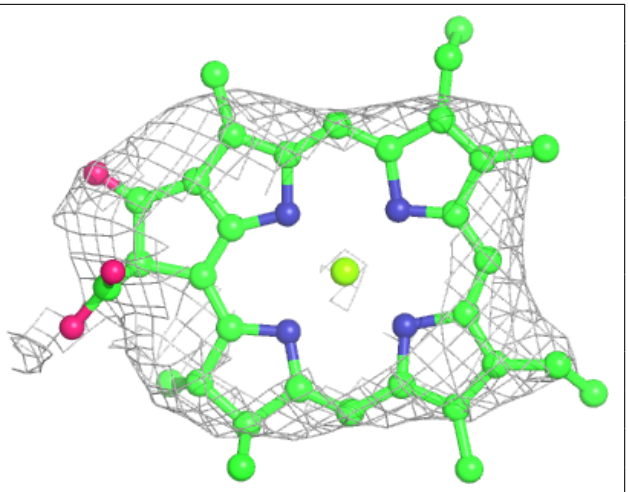


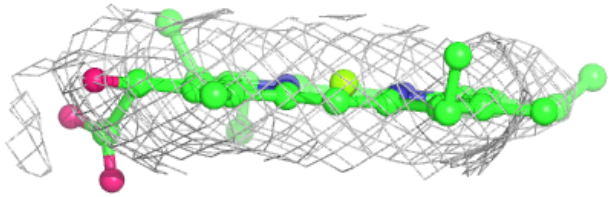


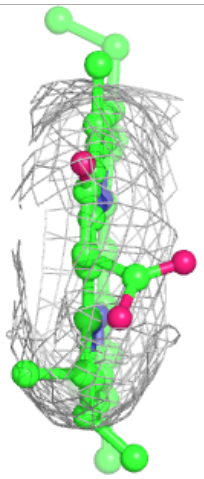


Electron density around CLA A 814:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

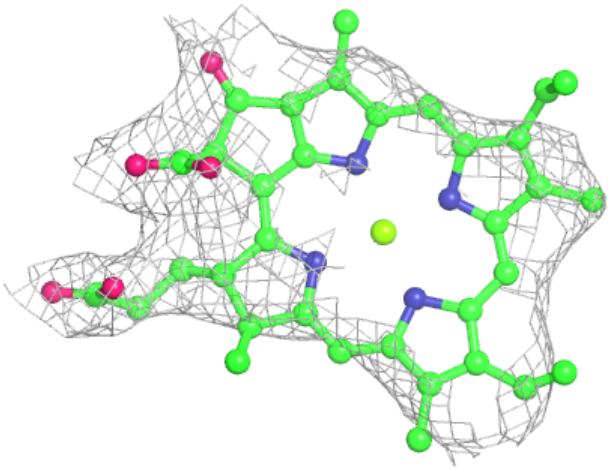


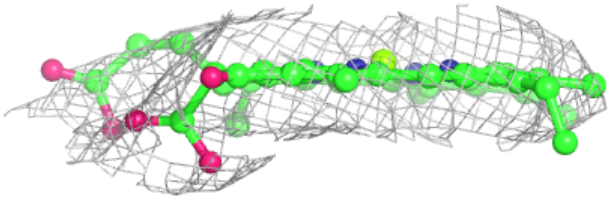


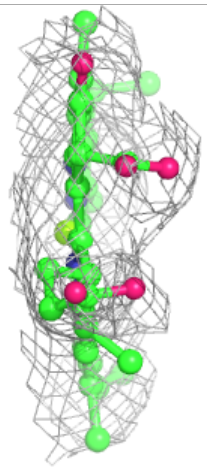


Electron density around CLA 0 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

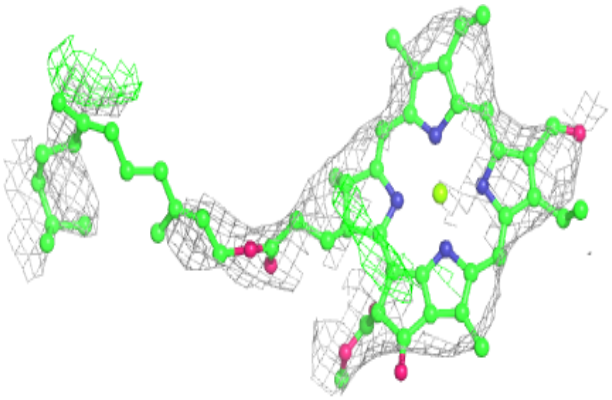


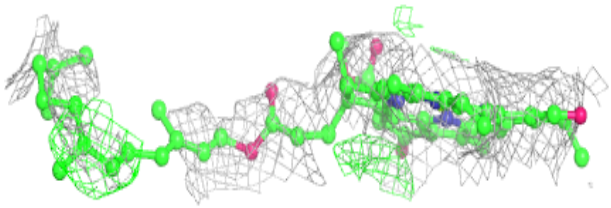


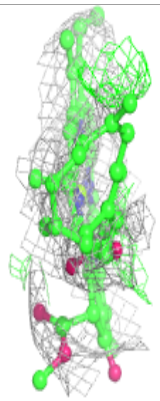


Electron density around CHL 4 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

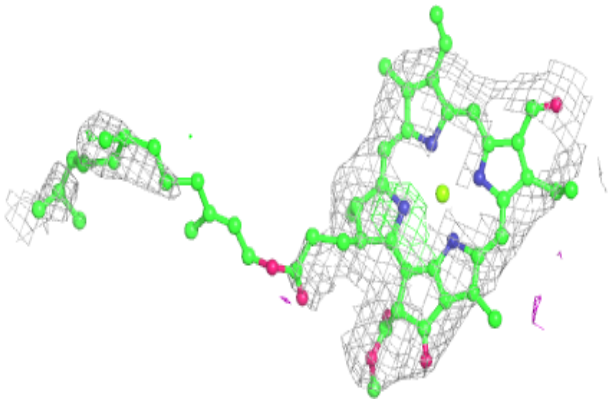


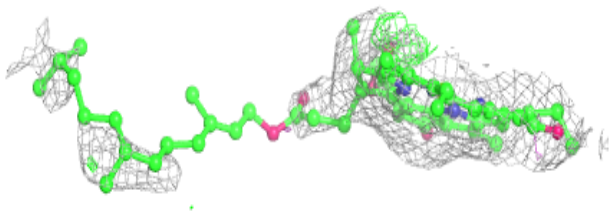


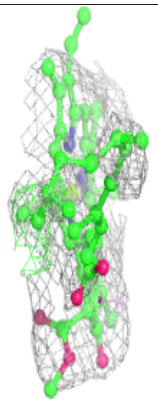


Electron density around CHL 6 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

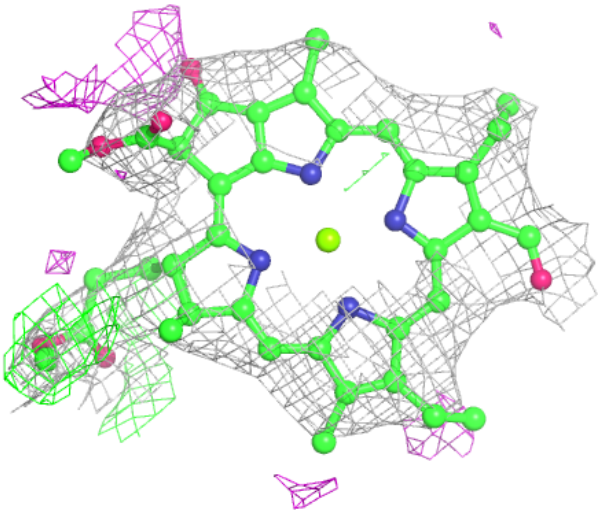


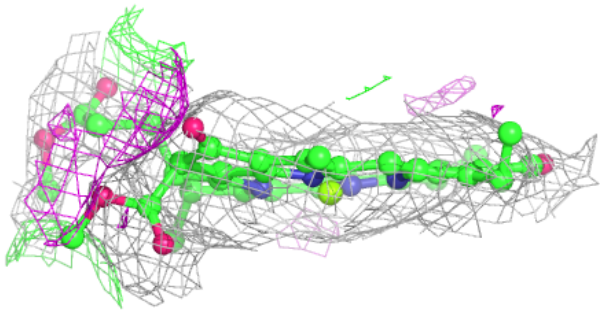


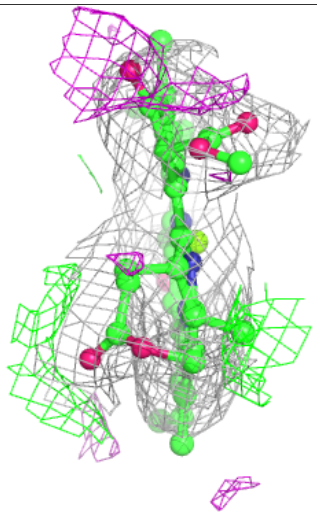


Electron density around CHL 5 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

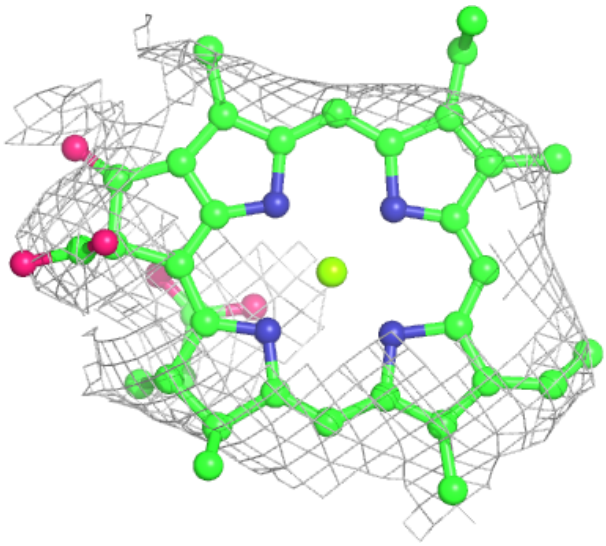


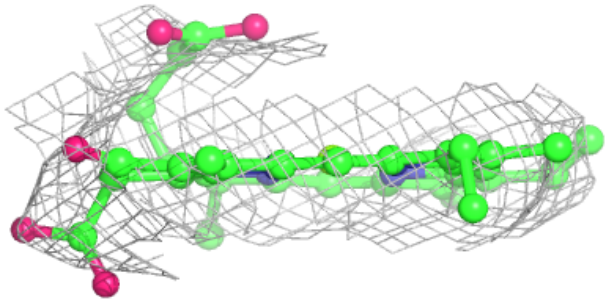


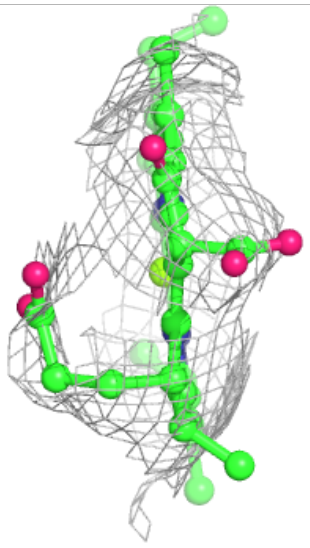


Electron density around CLA A 835:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

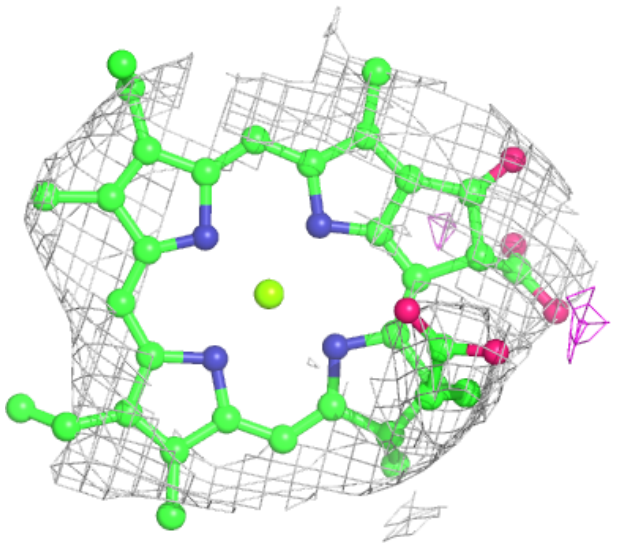


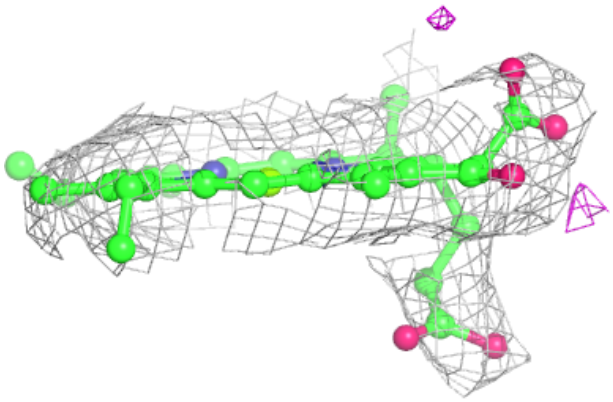


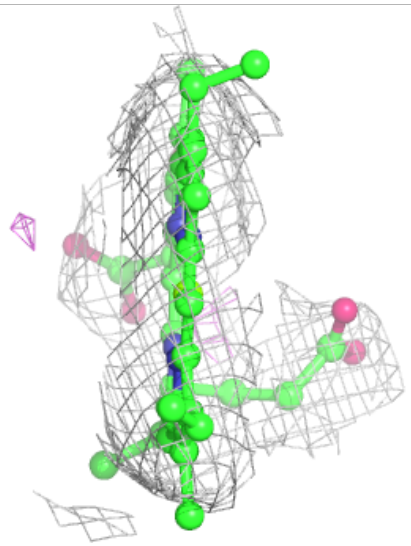


Electron density around CLA 0 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

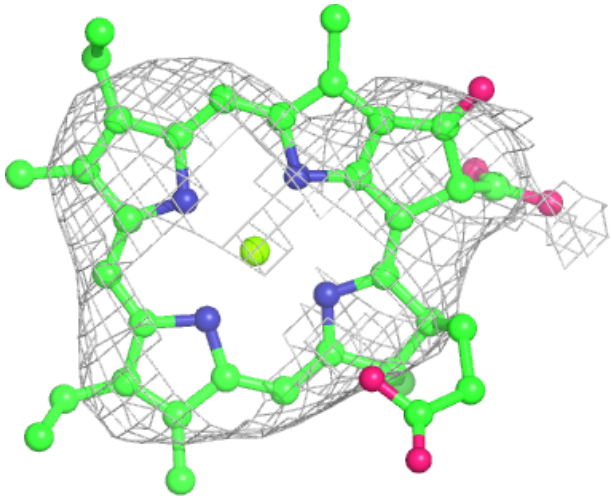


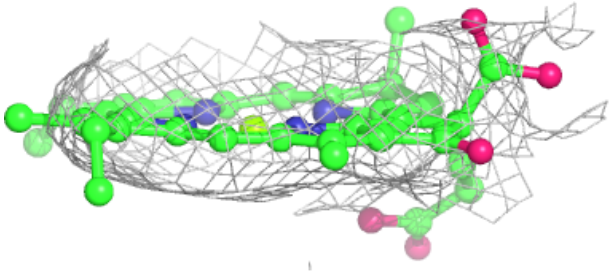


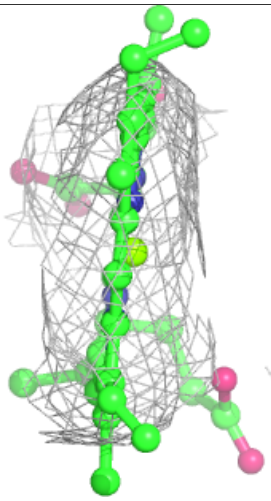


Electron density around CLA B 829:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

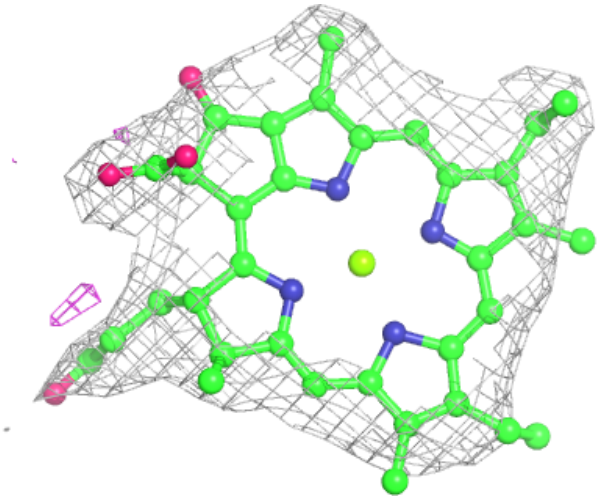


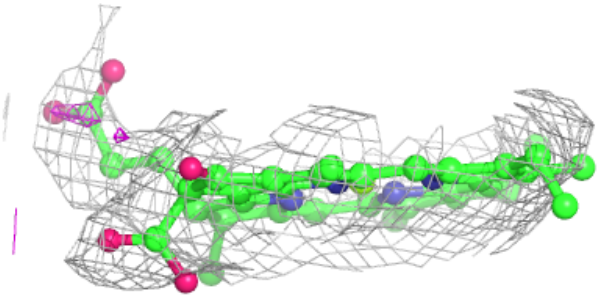


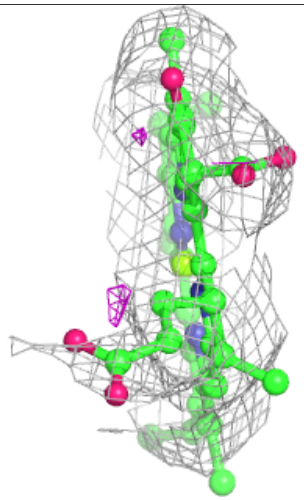


Electron density around CLA 1 1017:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

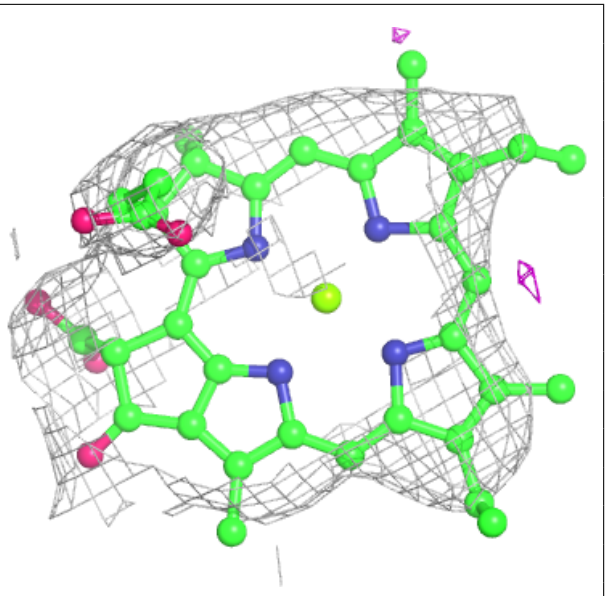


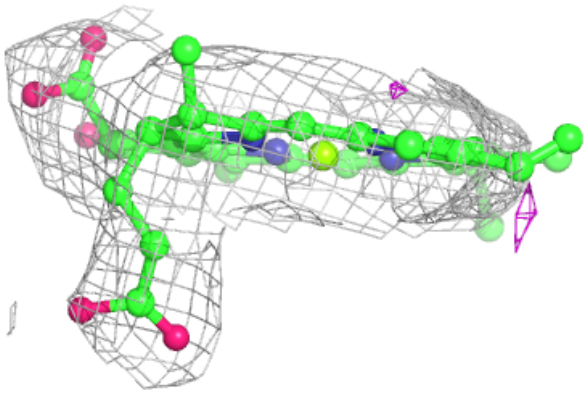


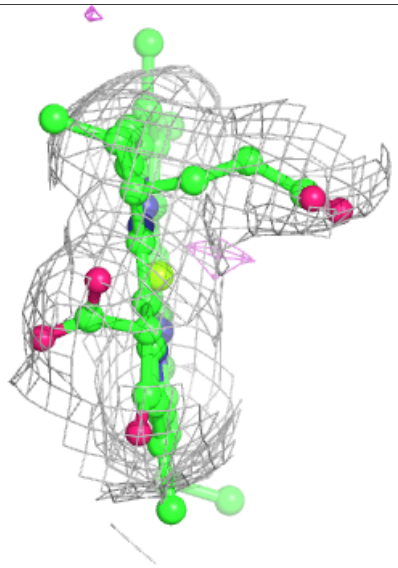


Electron density around CLA 6 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

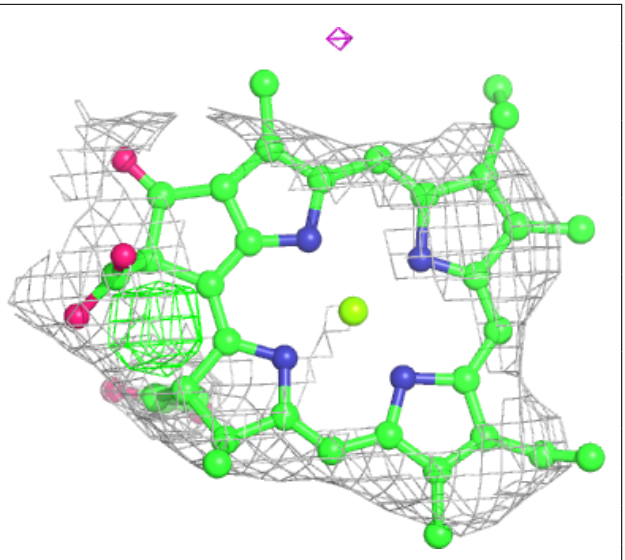


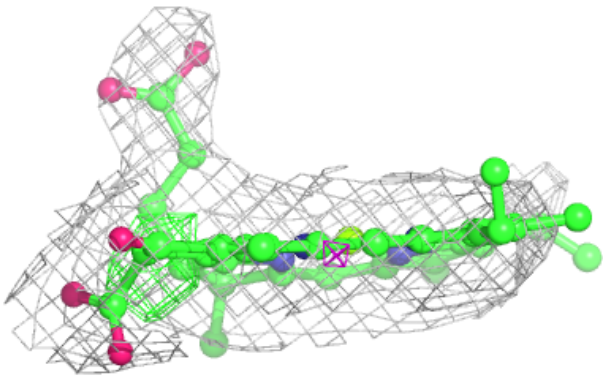


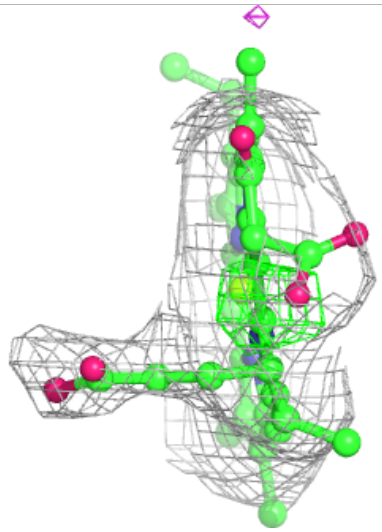


Electron density around CLA A 809:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

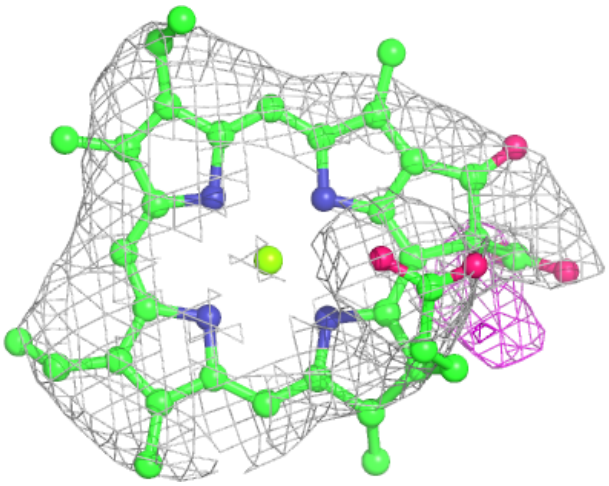


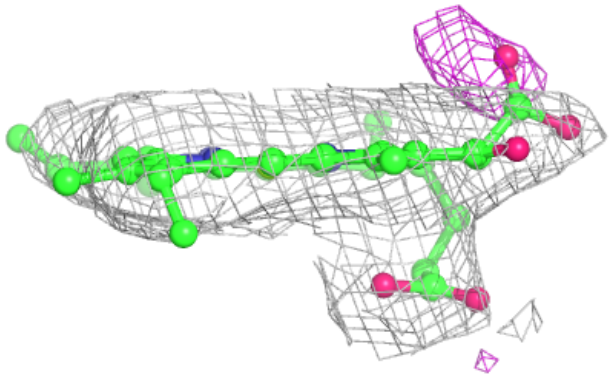


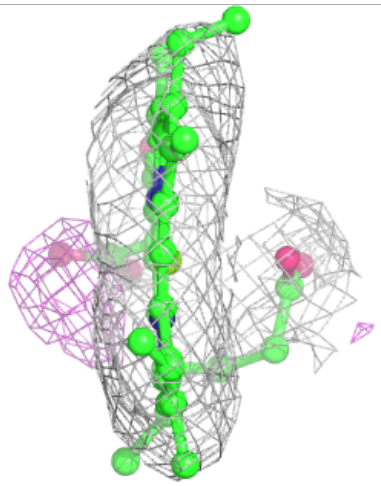


Electron density around CLA 0 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

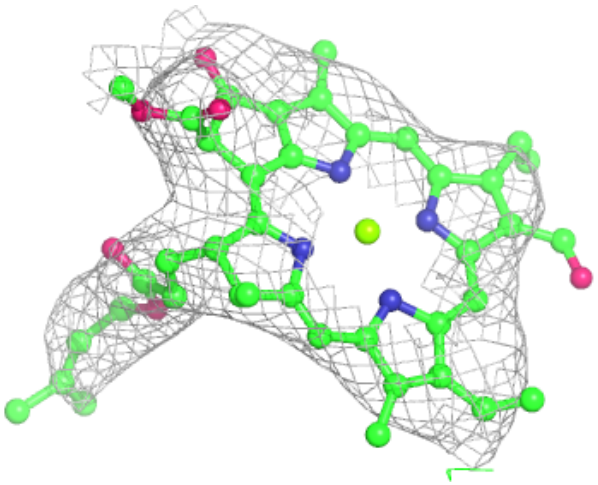


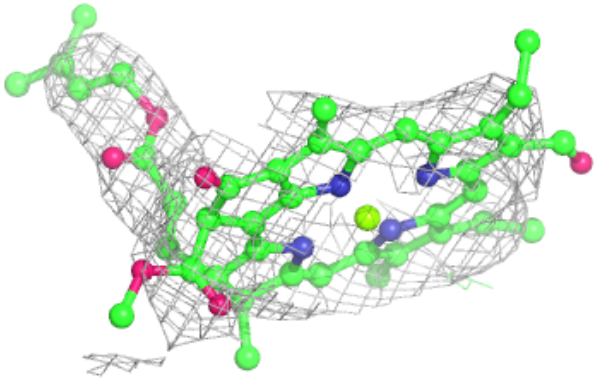


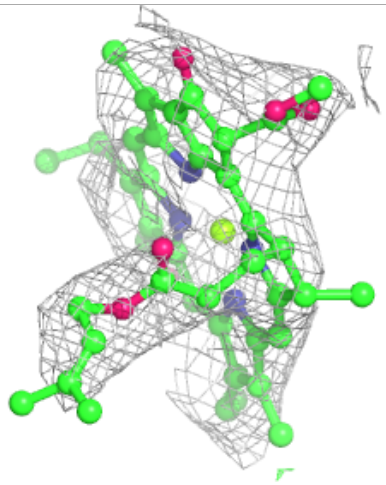


Electron density around CHL 1 1013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

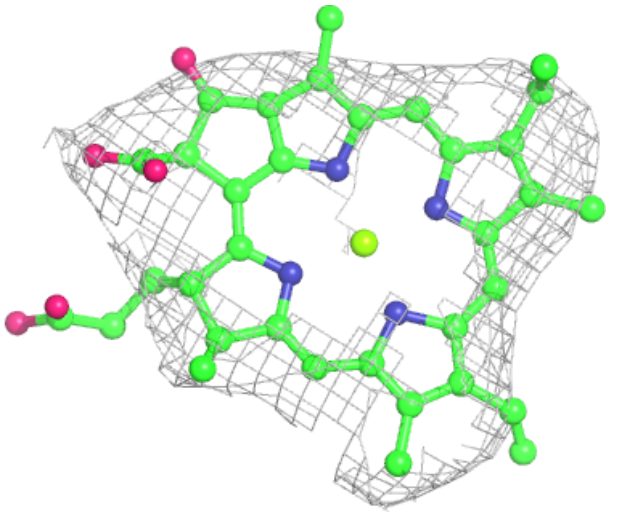


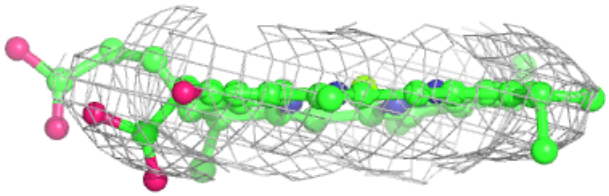


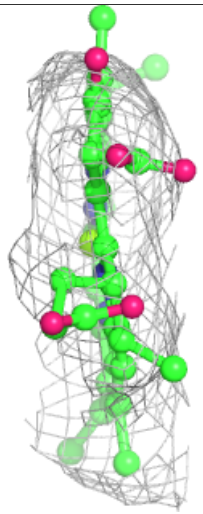


Electron density around CLA A 831:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

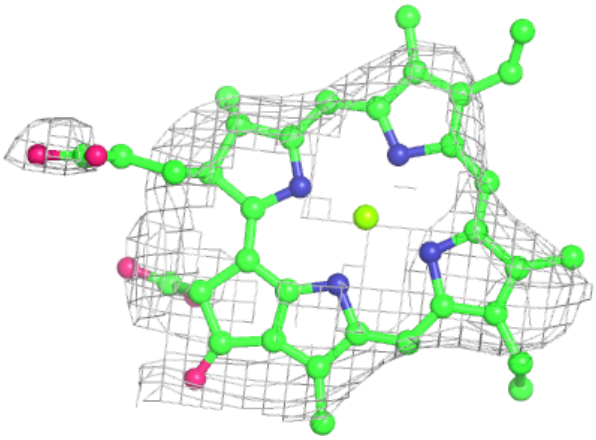


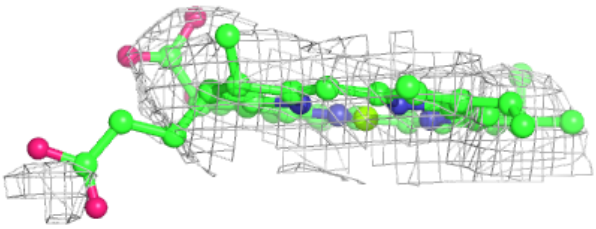


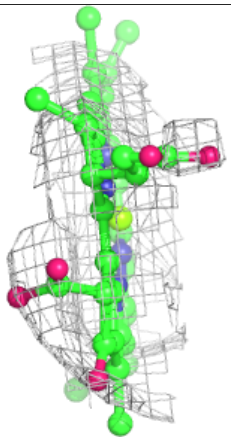


Electron density around CLA B 828:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

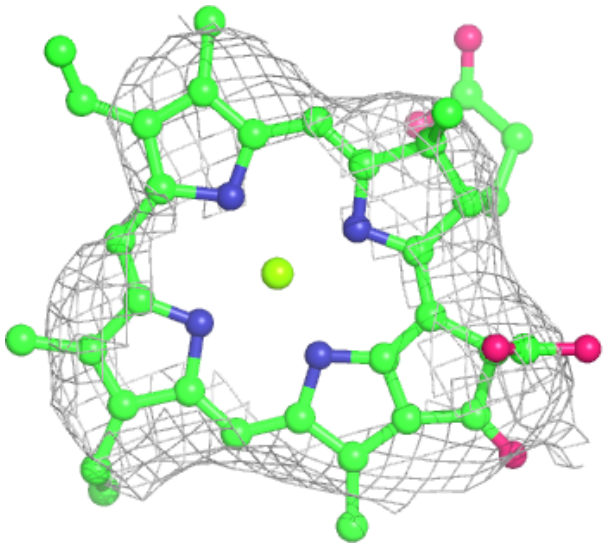


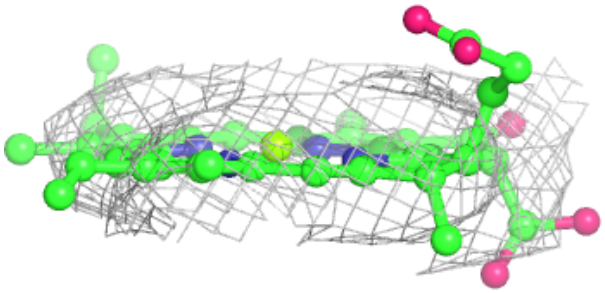


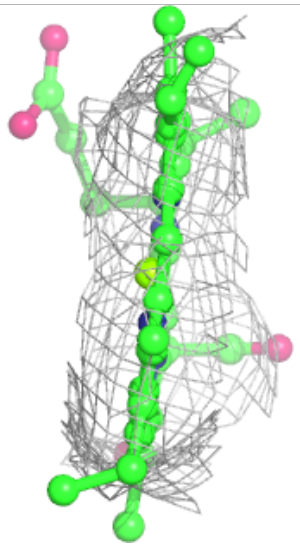


Electron density around CLA B 821:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

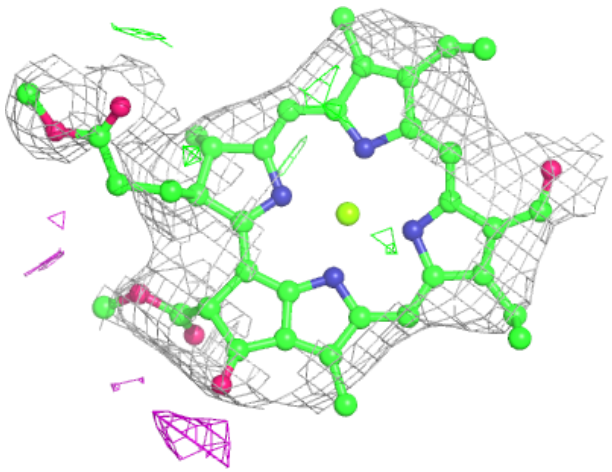


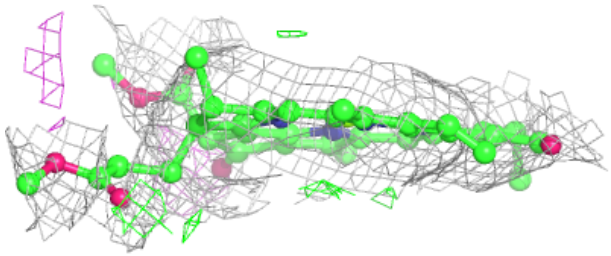




Electron density around CHL 6 313:

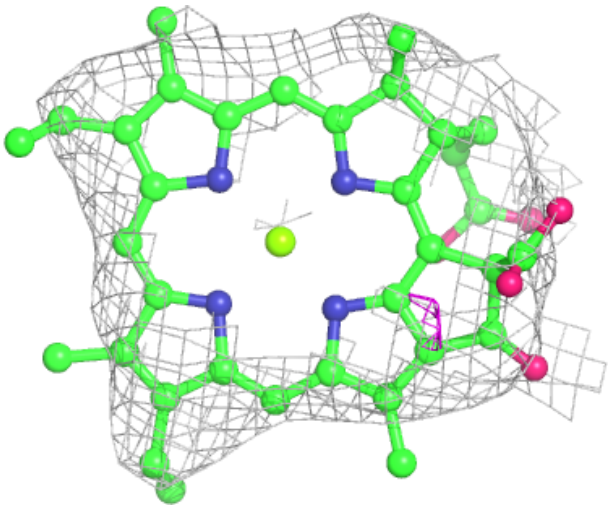
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

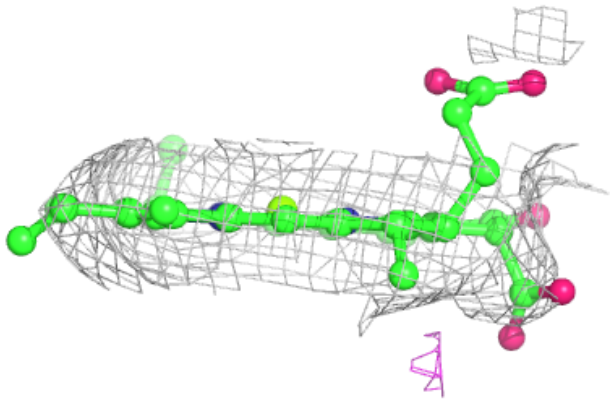


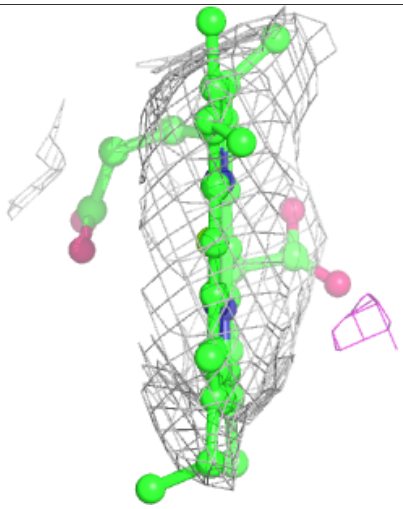


Electron density around CLA 3 1007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

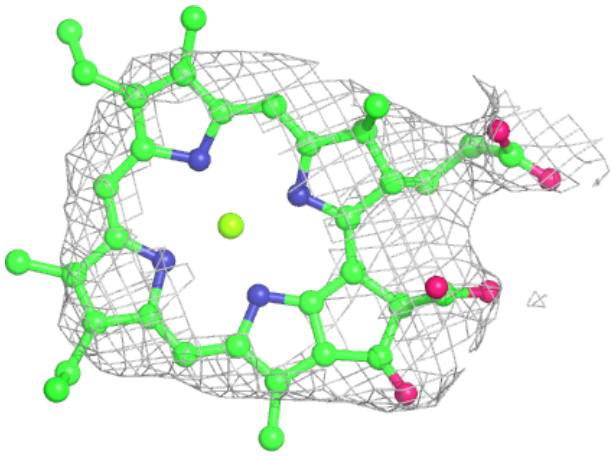


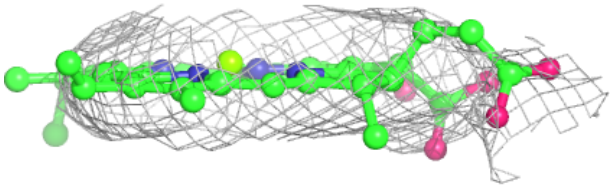


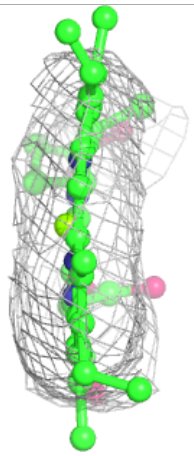


Electron density around CLA B 809:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

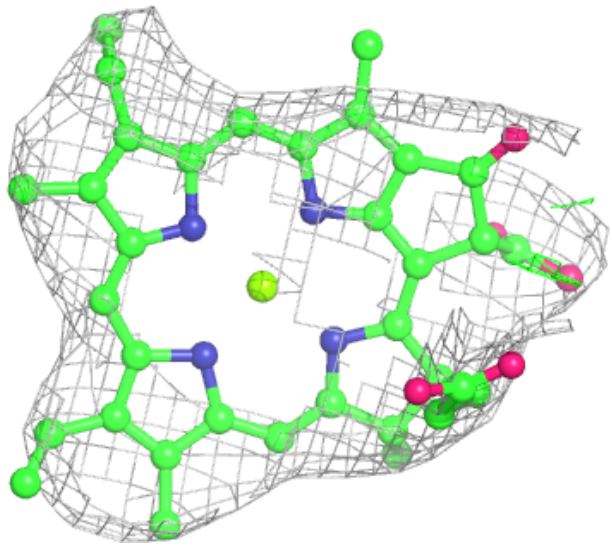


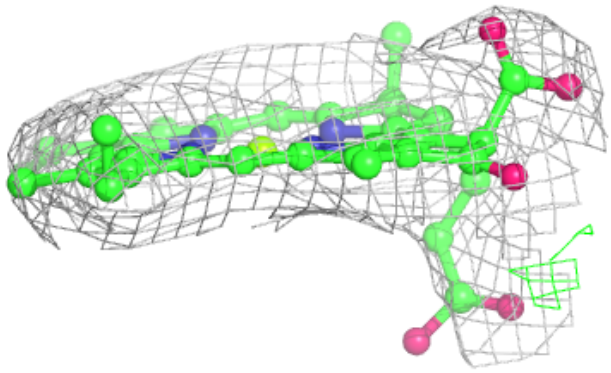


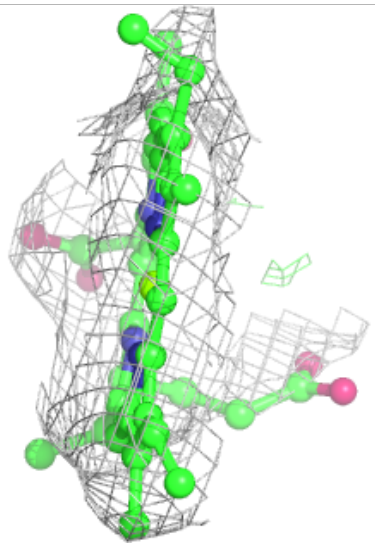


Electron density around CLA B 833:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

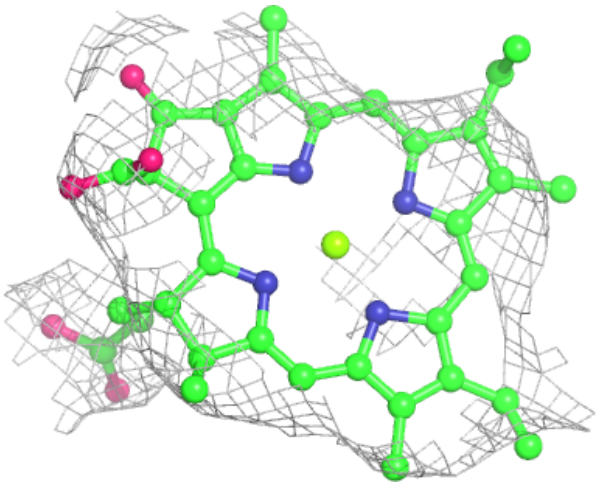


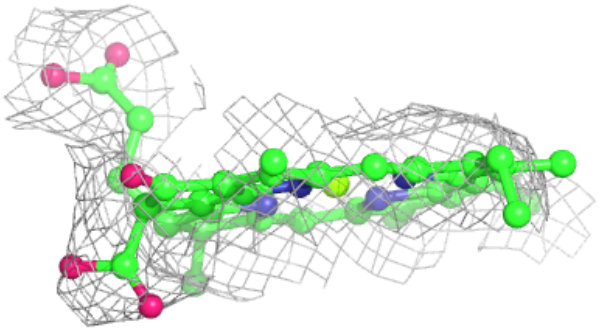


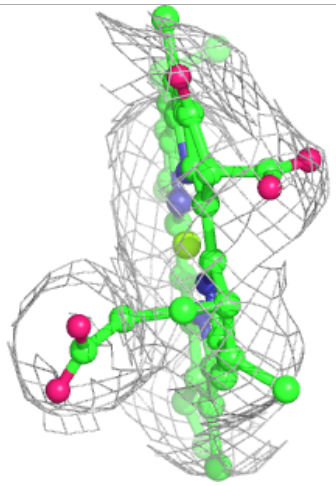


Electron density around CLA A 813:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

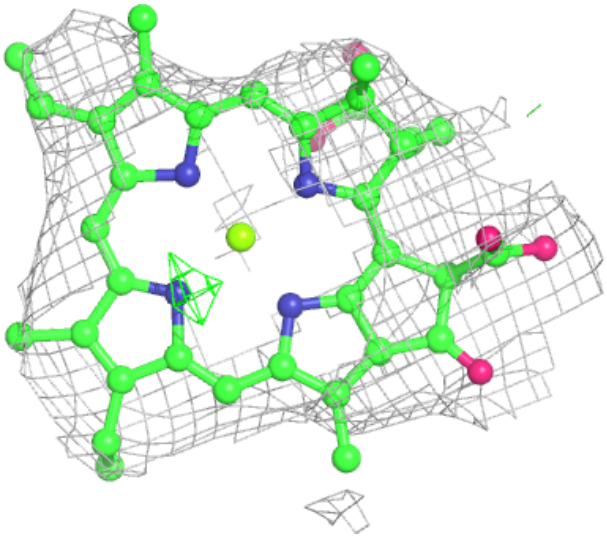


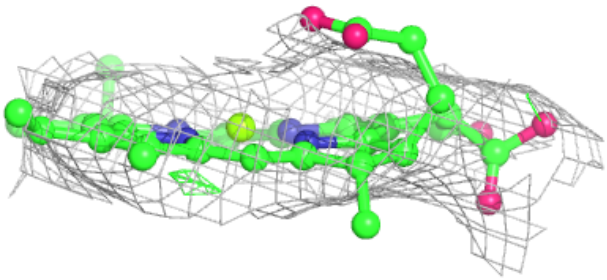


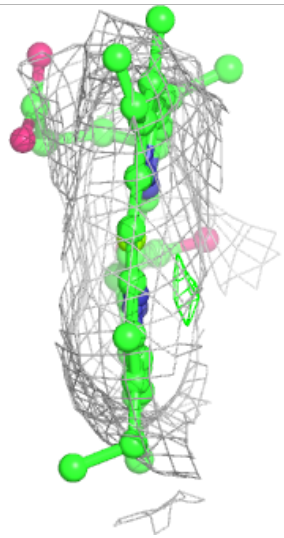


Electron density around CLA 0 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

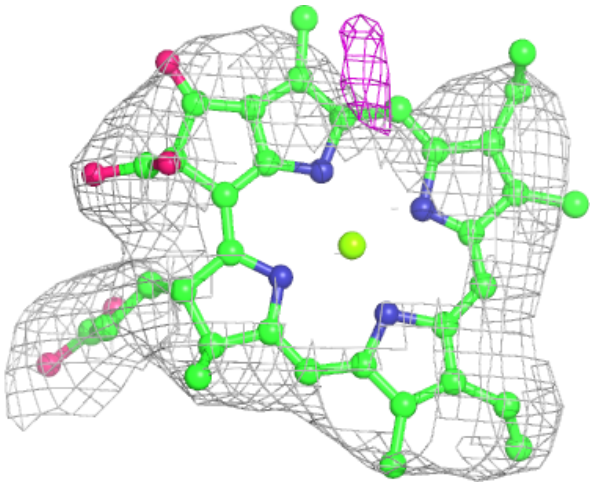


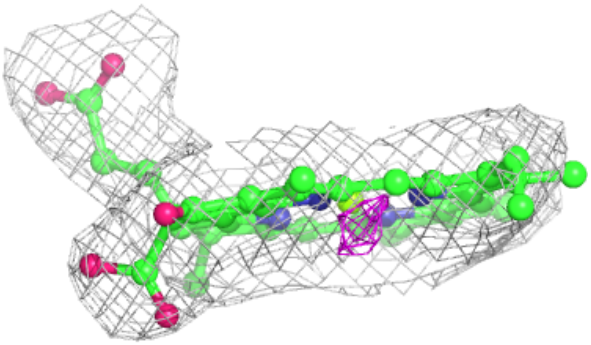


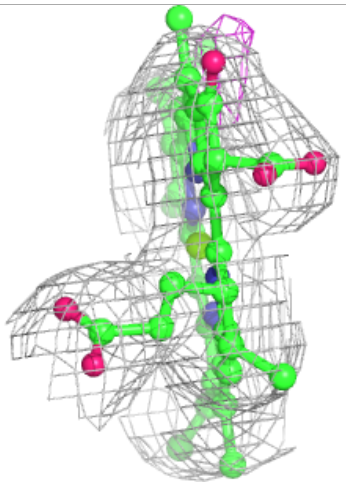


Electron density around CLA 5 318:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

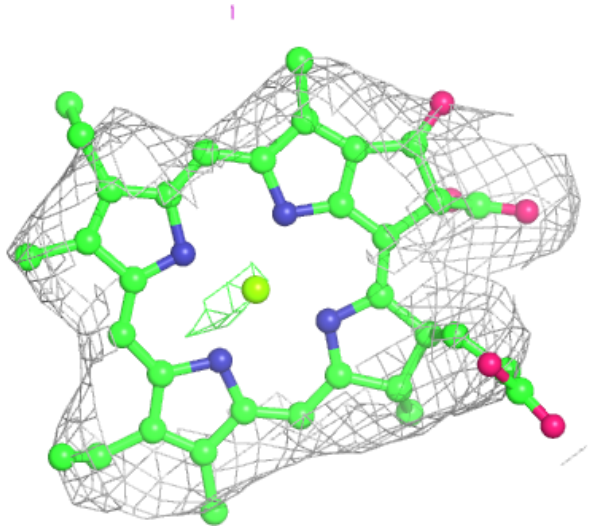


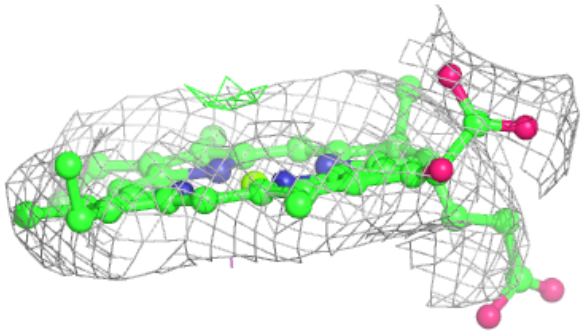


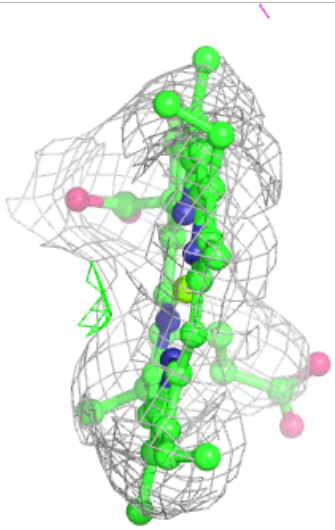


Electron density around CLA 5 322:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

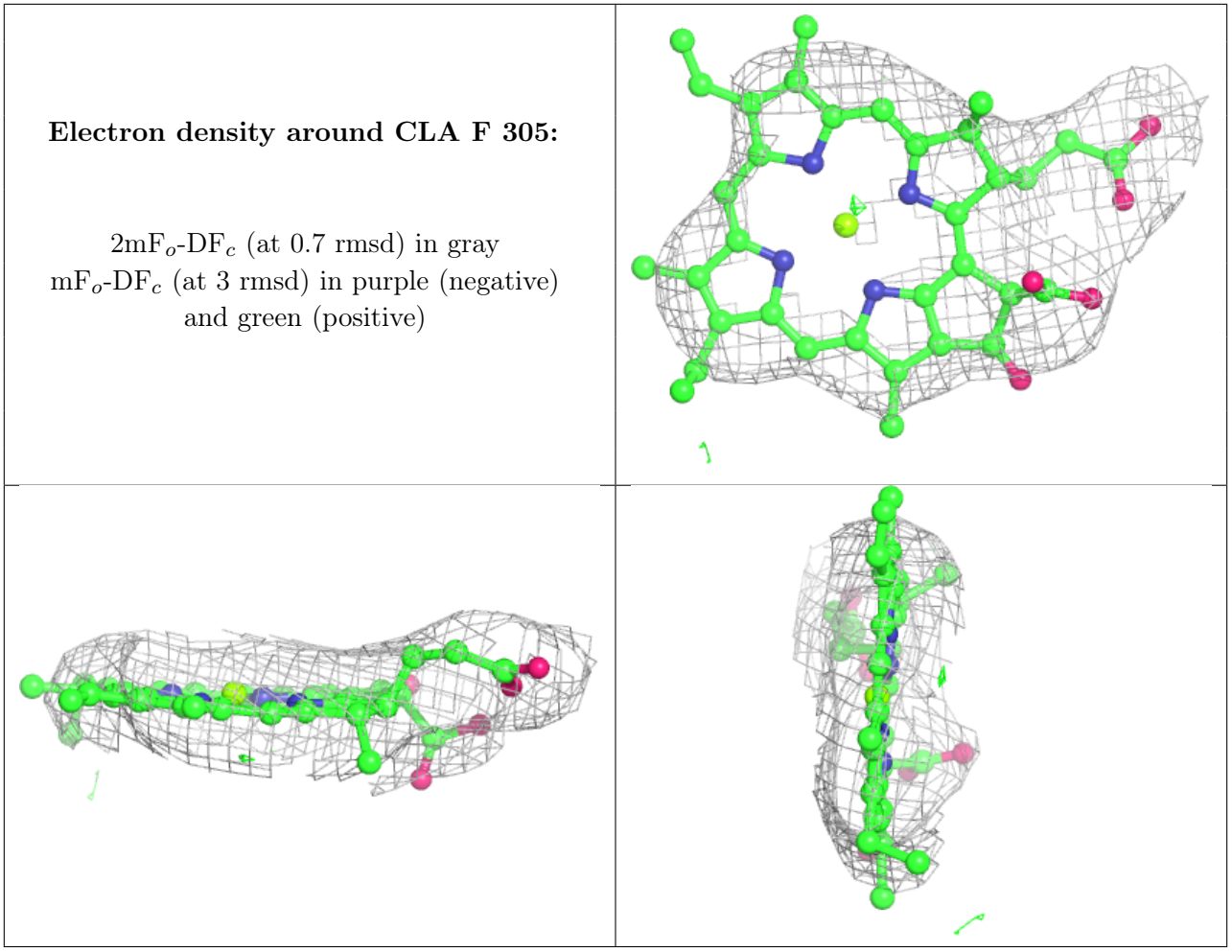






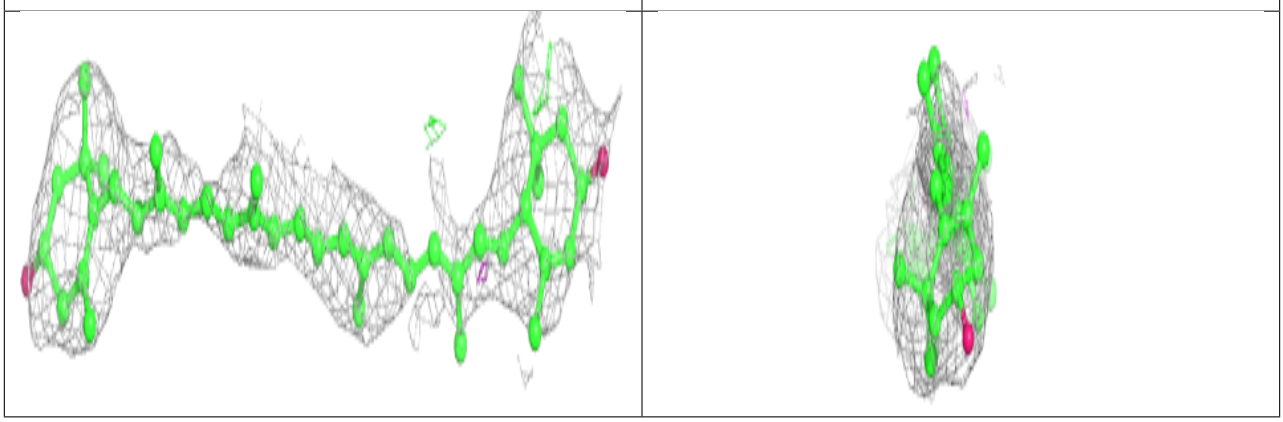
Electron density around CLA F 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



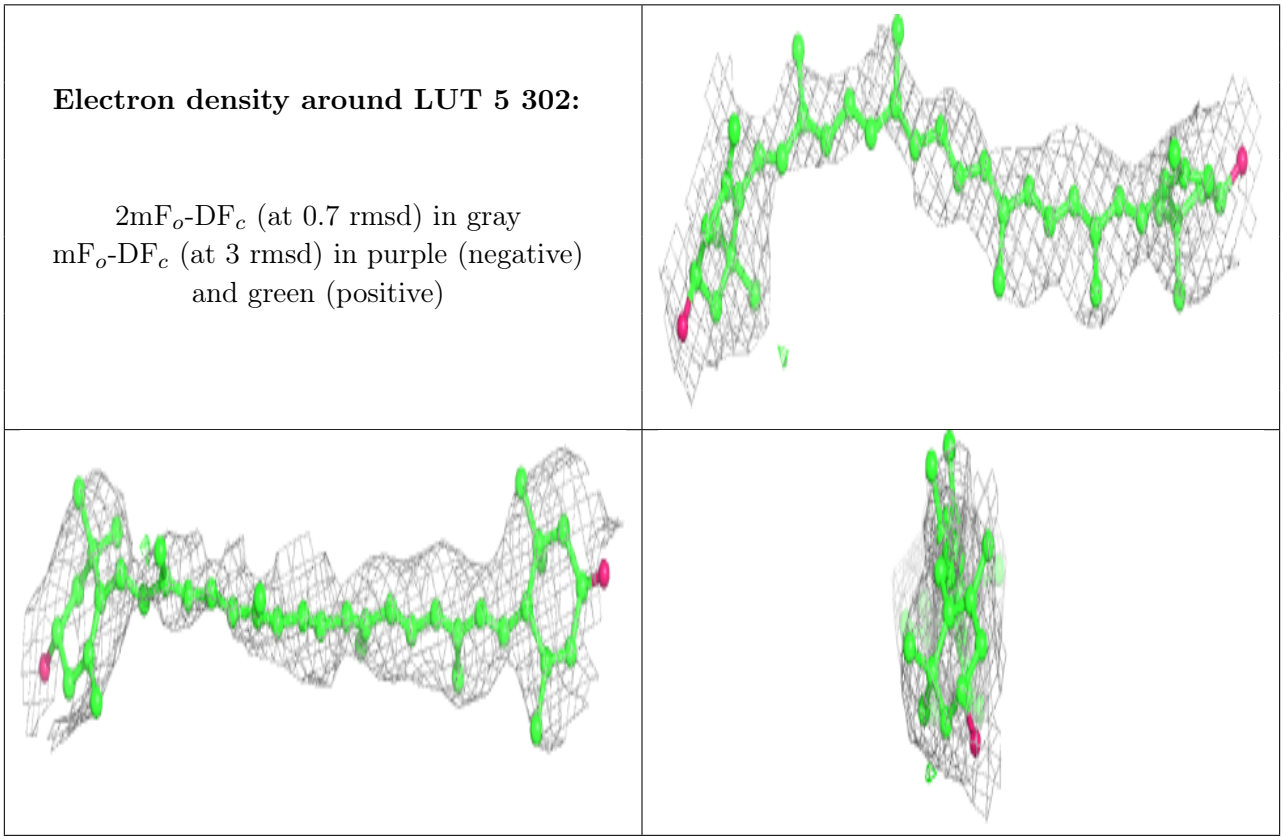
Electron density around LUT 4 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



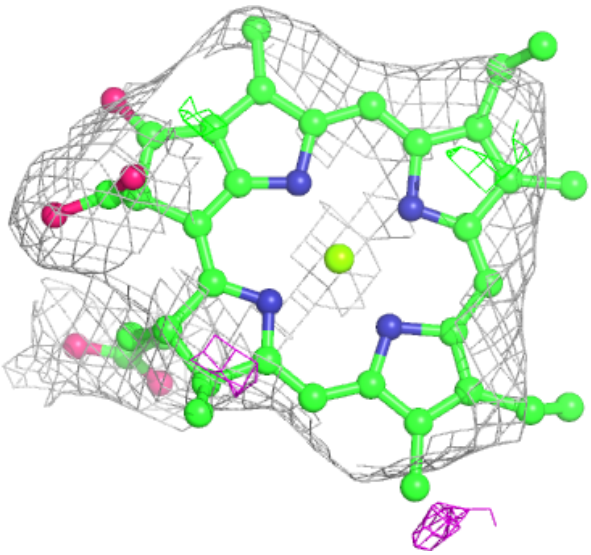
Electron density around LUT 5 302:

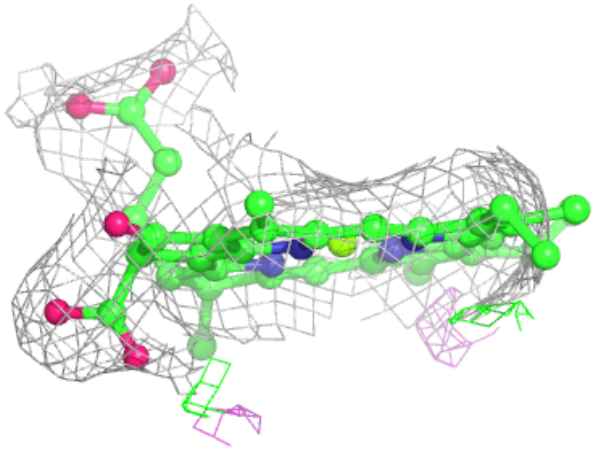
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

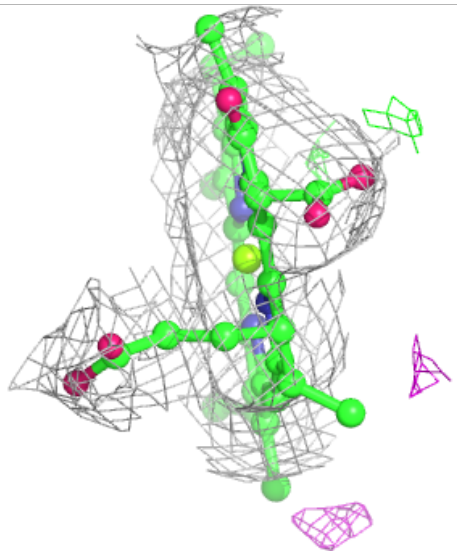


Electron density around CLA 8 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

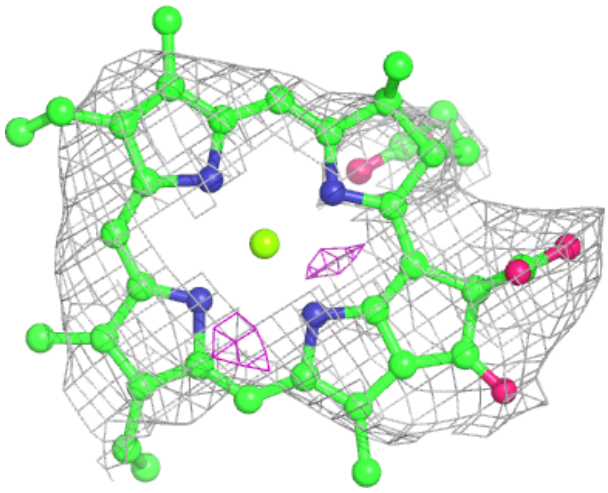


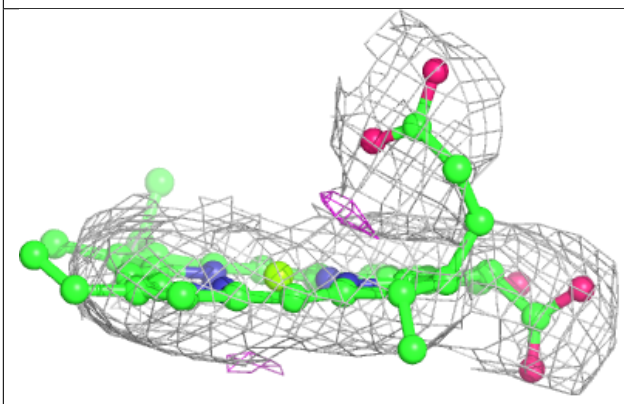


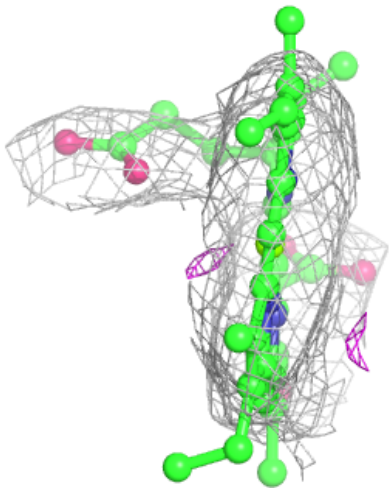


Electron density around CLA A 810:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

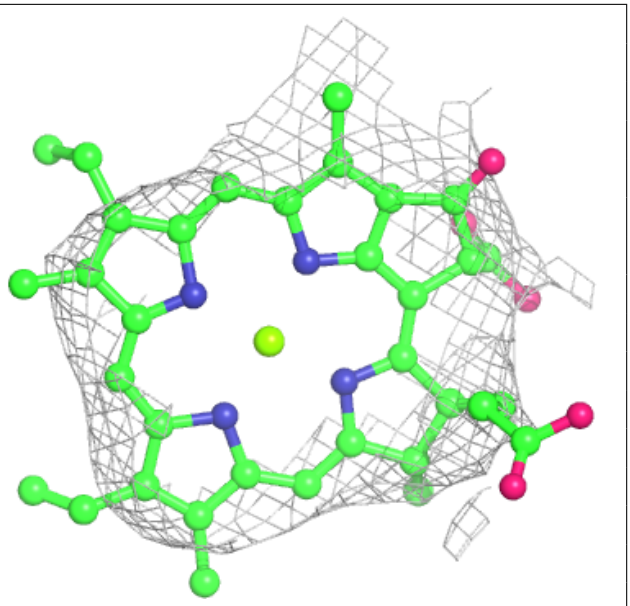


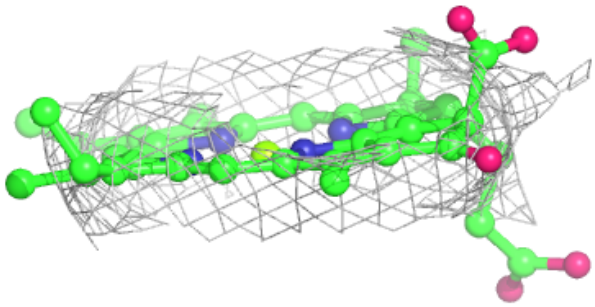


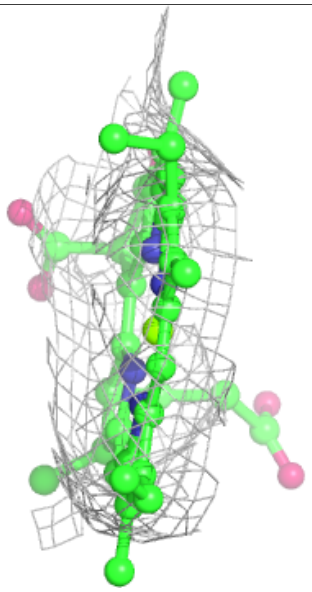


Electron density around CLA A 836:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

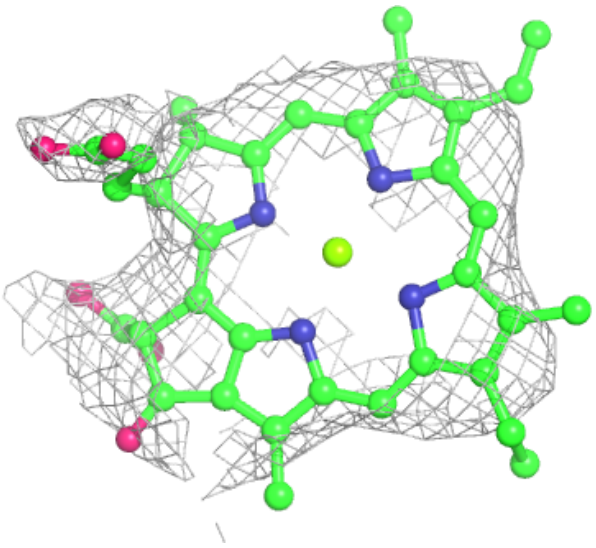


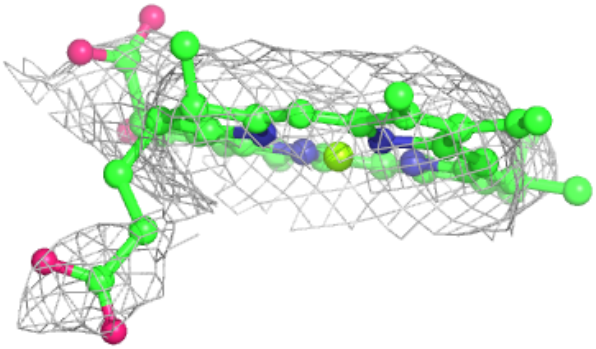


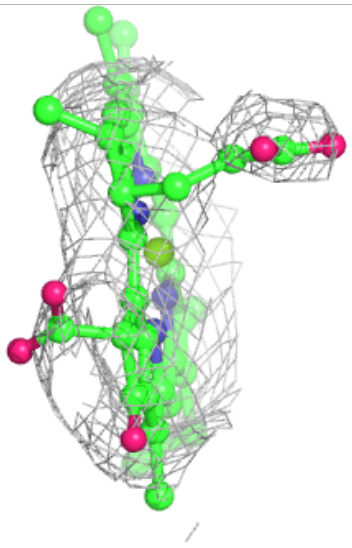


Electron density around CLA 0 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

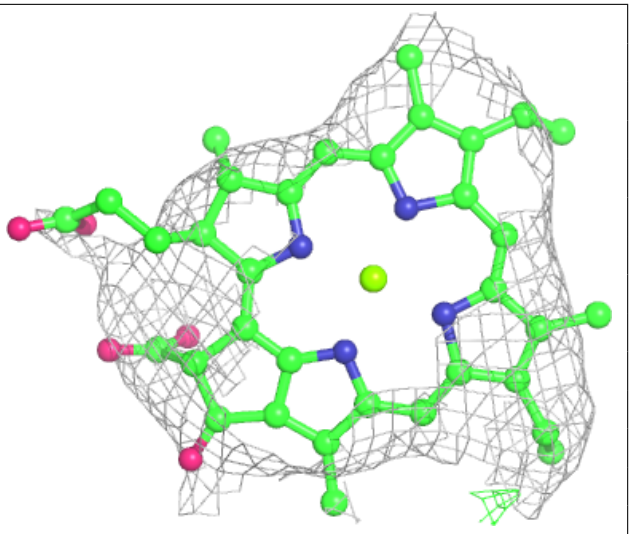


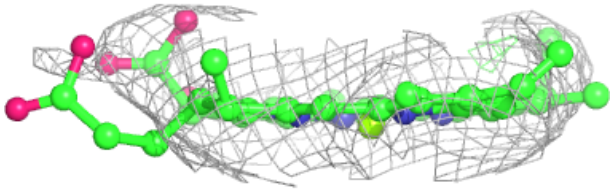


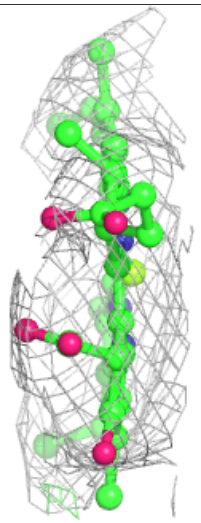


Electron density around CLA 1 1004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

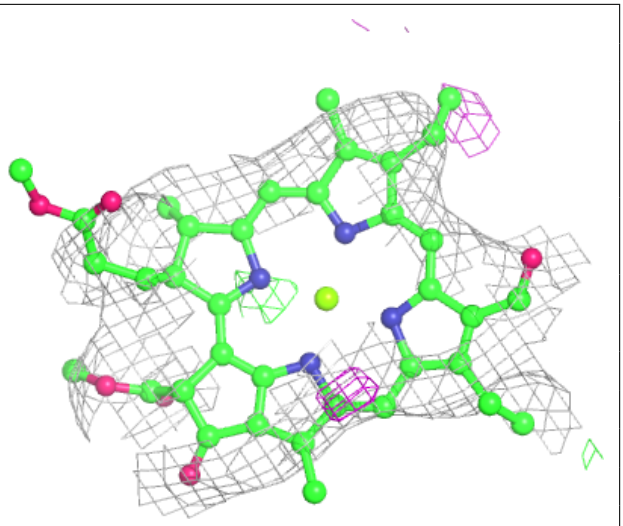


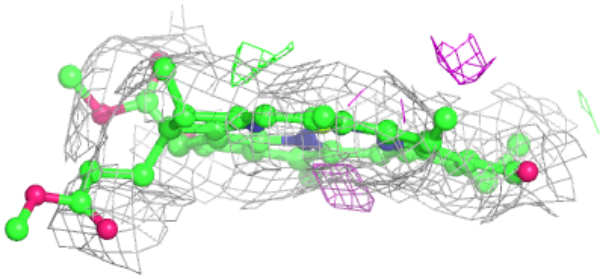


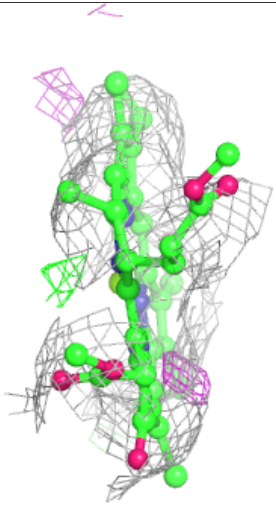


Electron density around CHL 7 1012:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

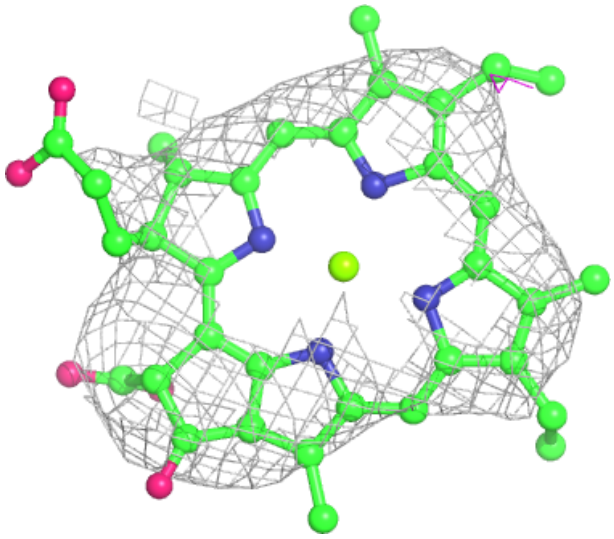


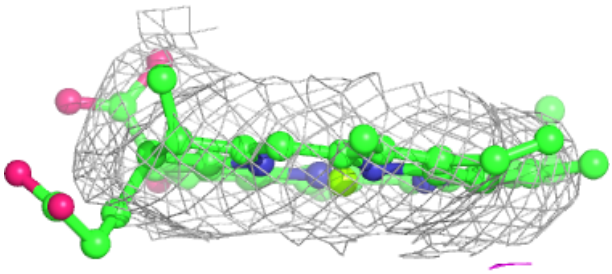


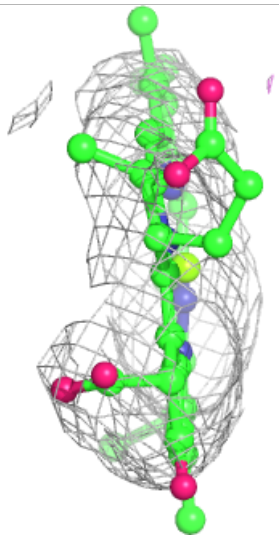


Electron density around CLA B 808:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

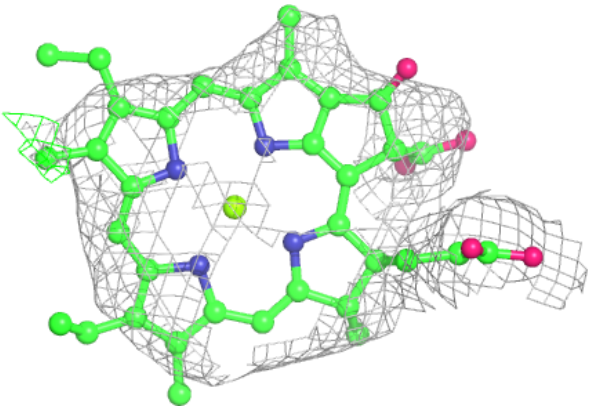


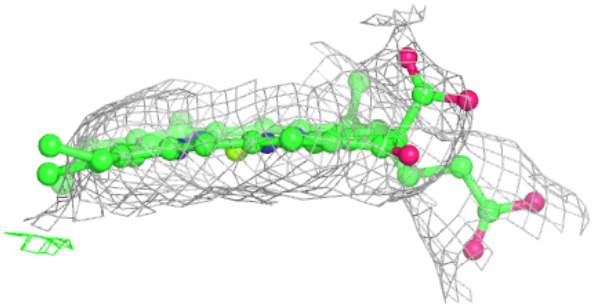


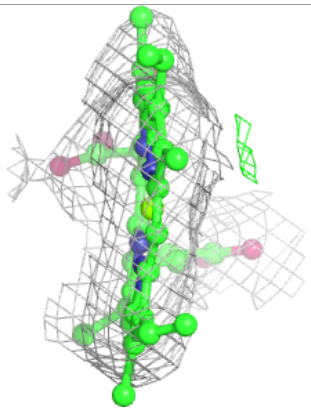


Electron density around CLA J 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

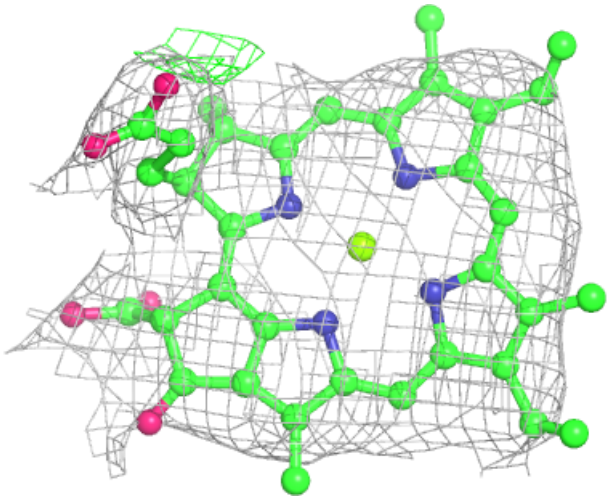


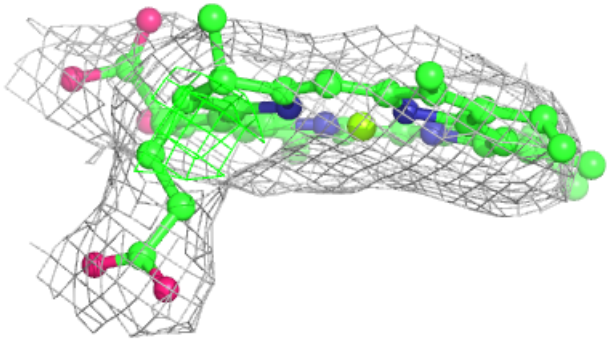


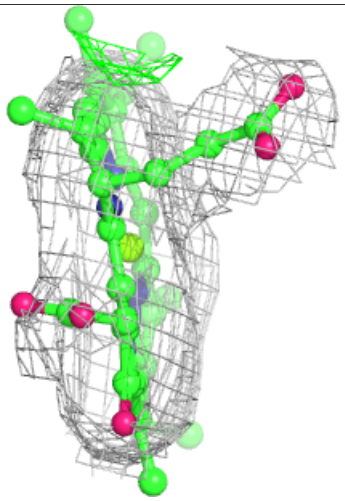


Electron density around CLA 1 1014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

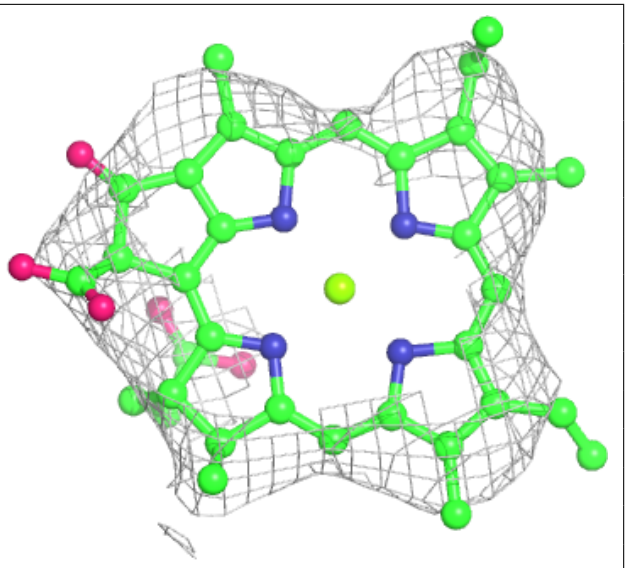


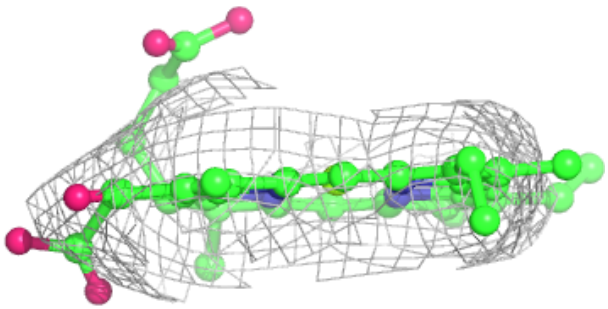


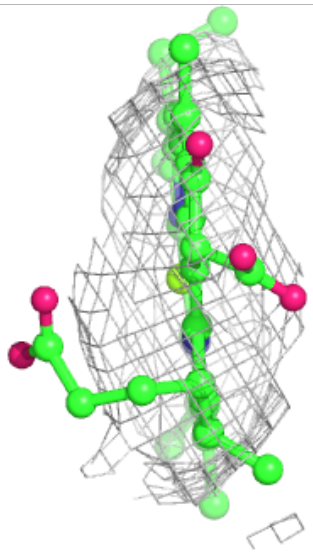


Electron density around CLA A 816:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

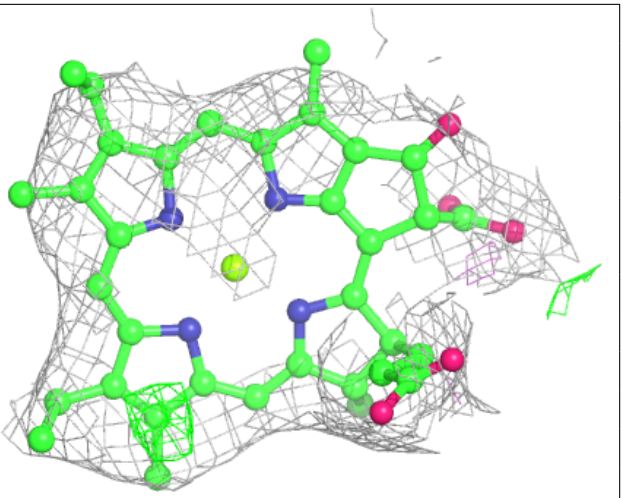


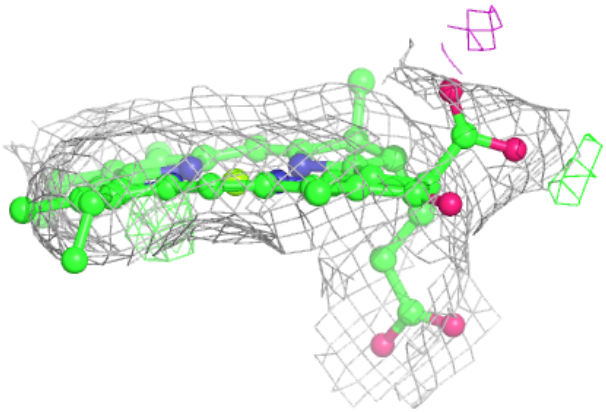


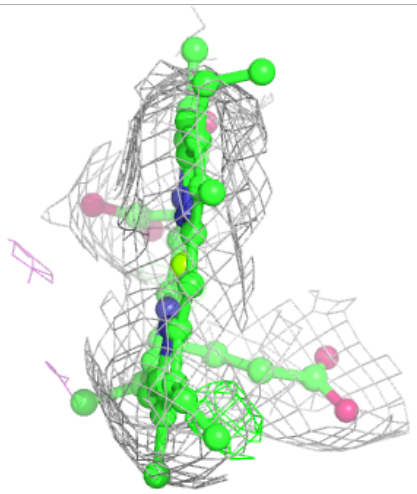


Electron density around CLA 4 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

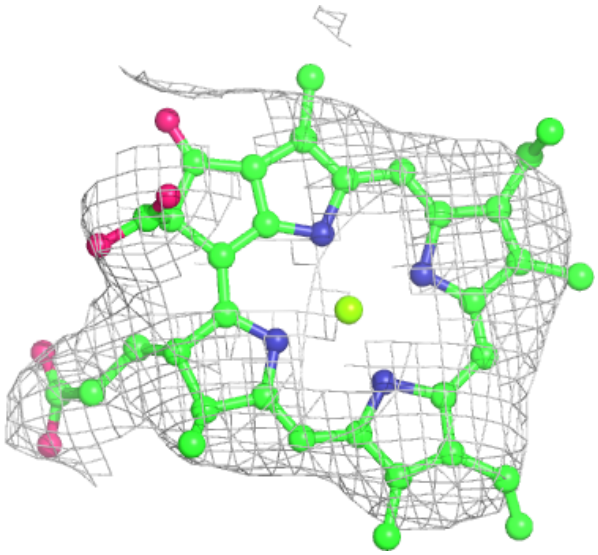


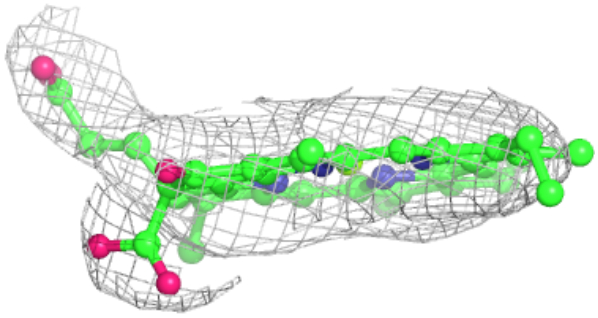


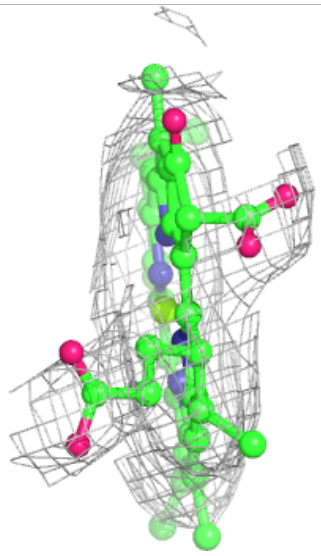


Electron density around CLA A 826:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

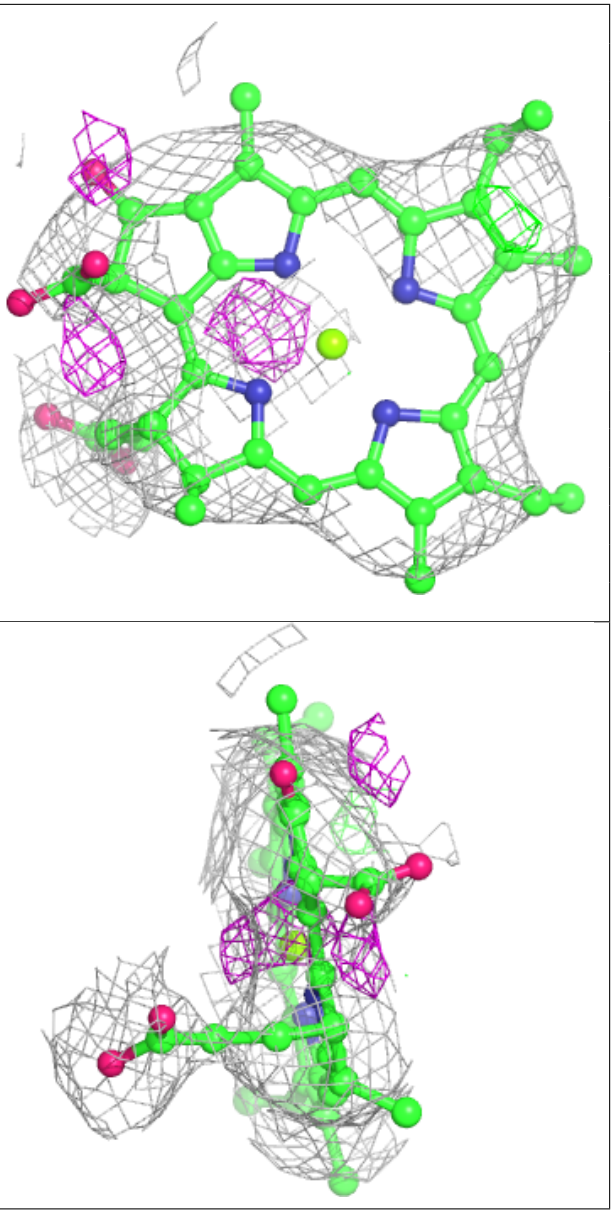


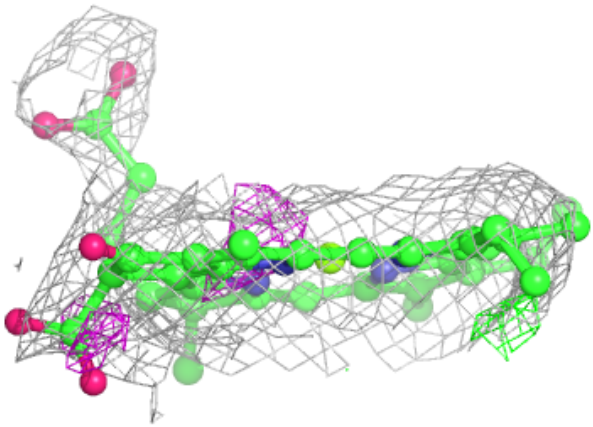




Electron density around CLA 6 311:

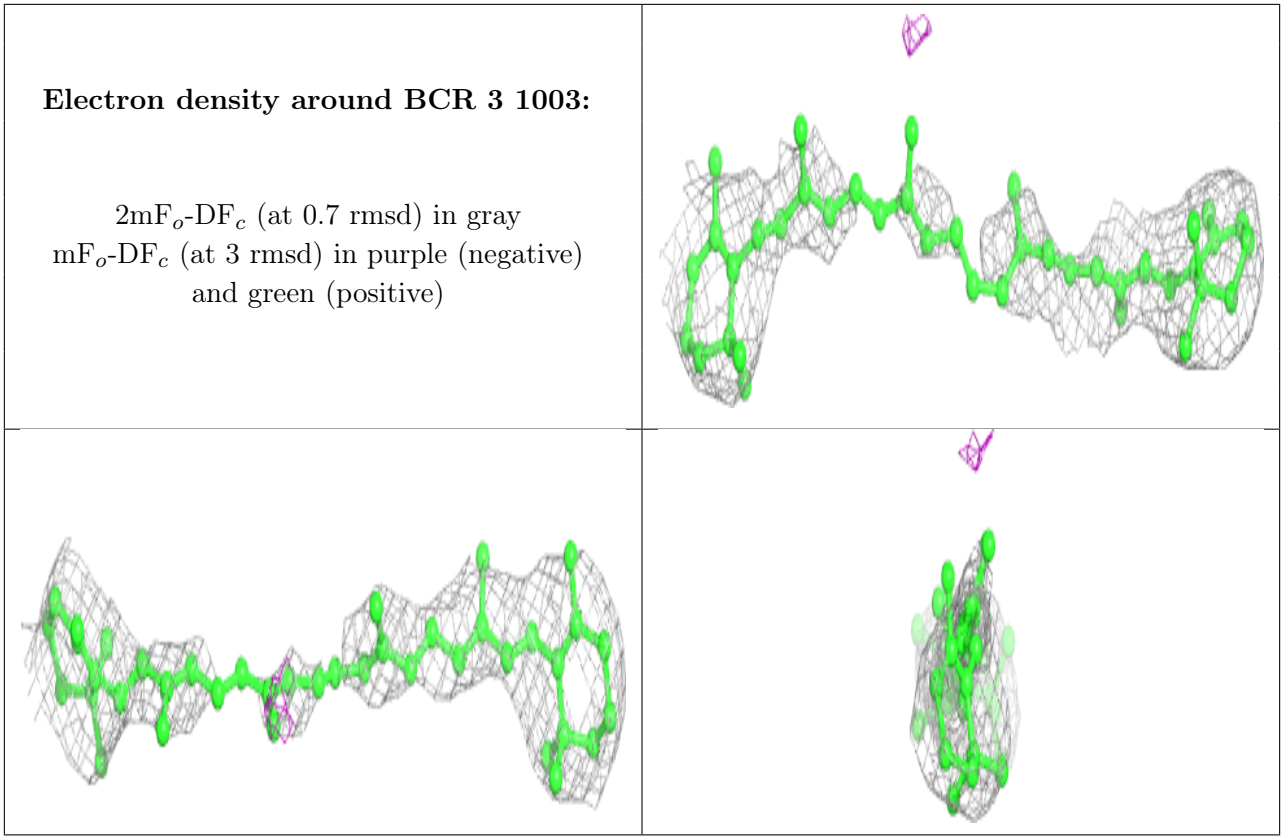
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





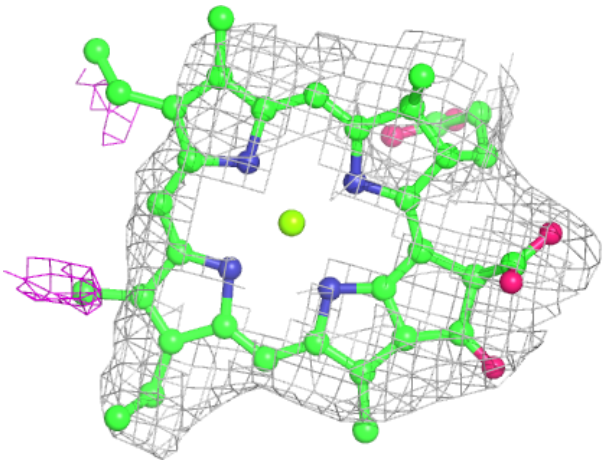
Electron density around BCR 3 1003:

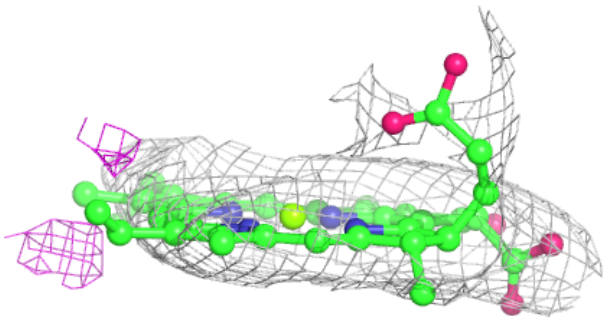
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

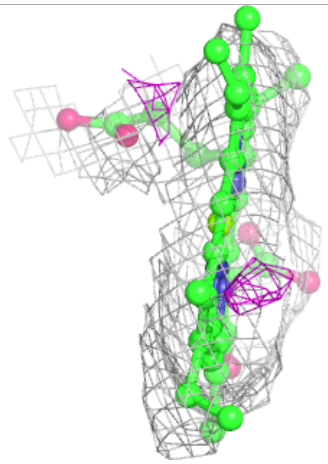


Electron density around CLA 0 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

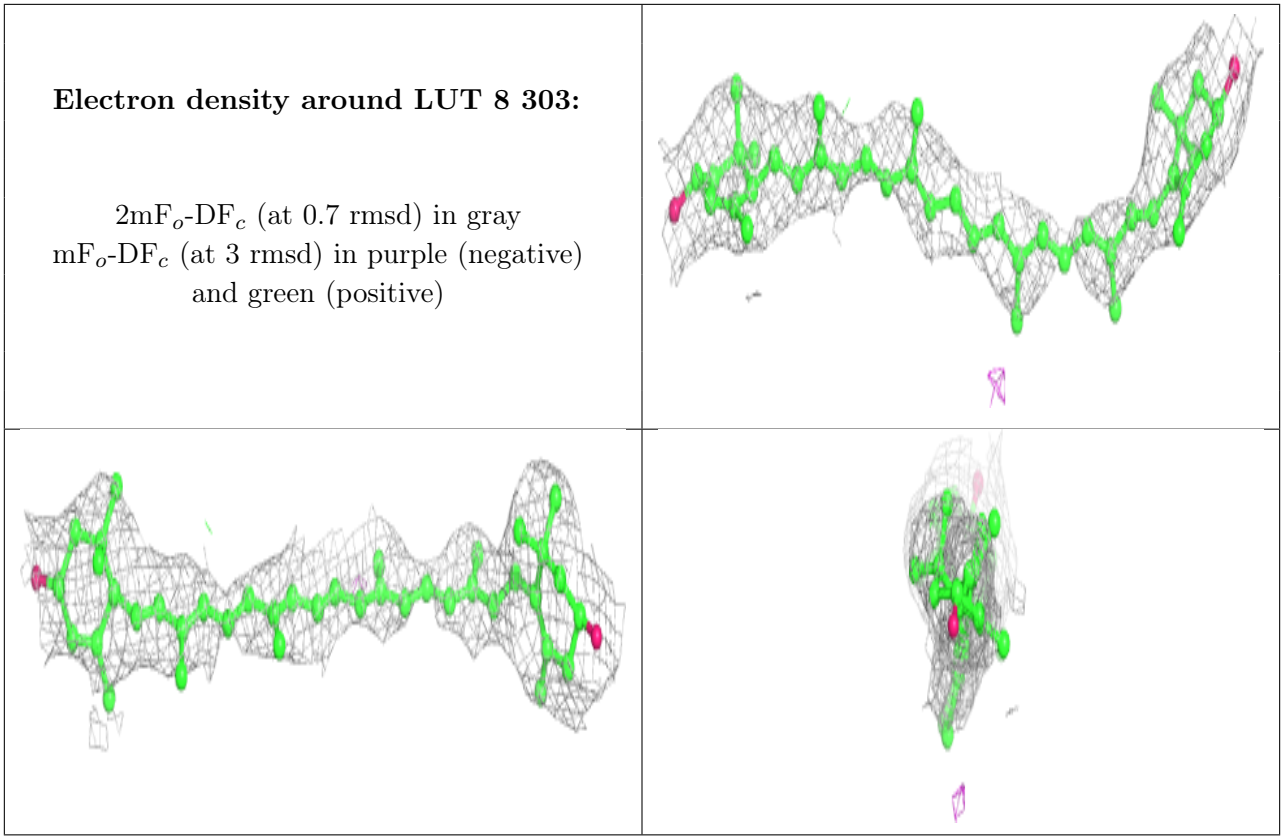






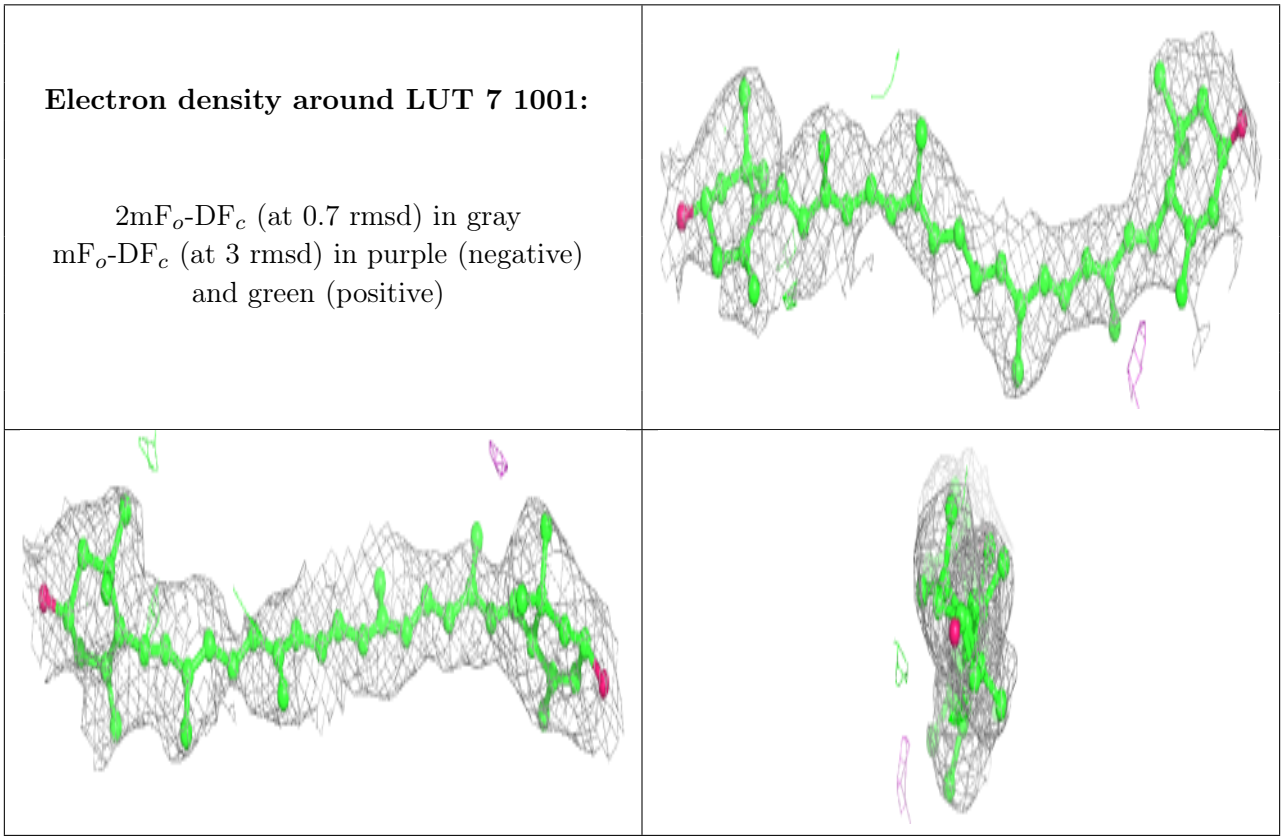
Electron density around LUT 8 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



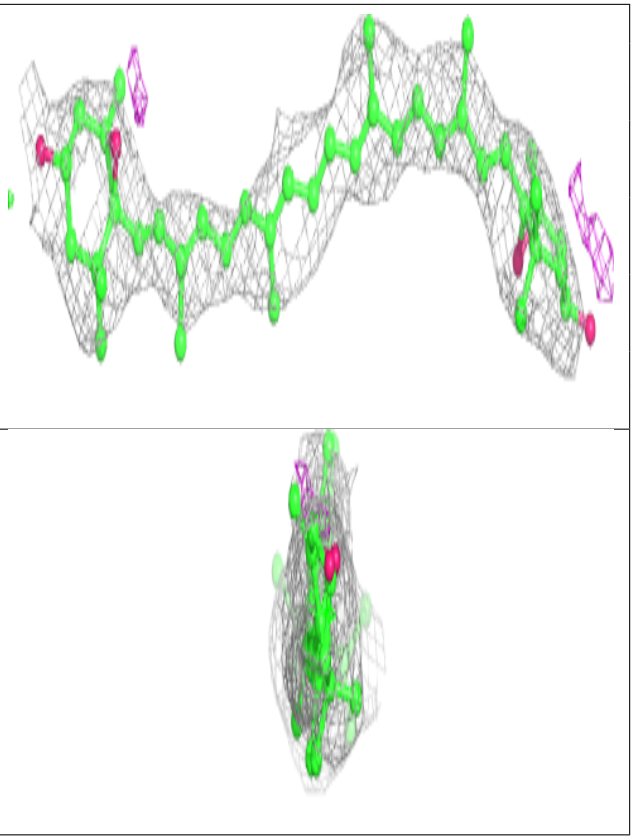
Electron density around LUT 7 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



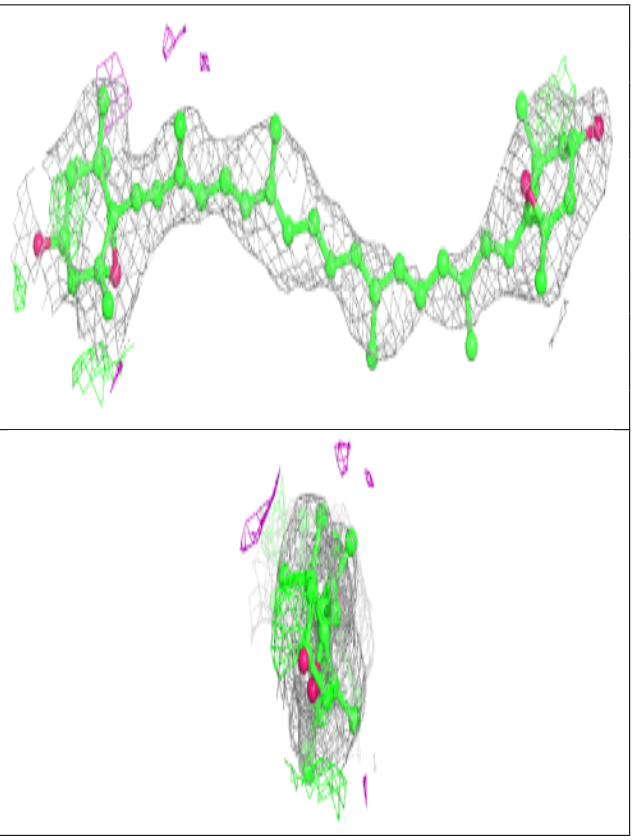
Electron density around XAT 4 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



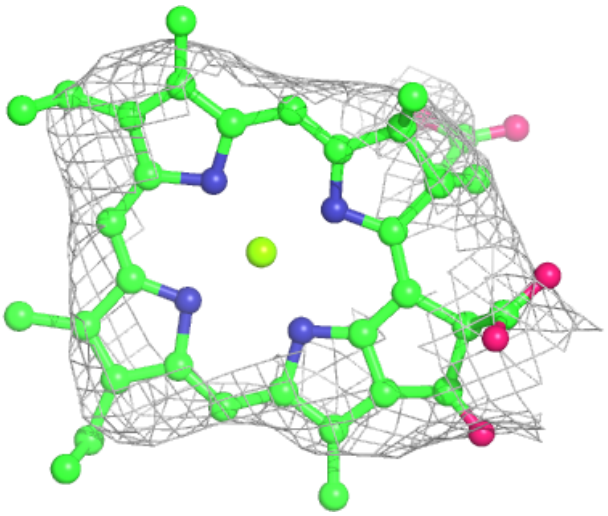
Electron density around XAT 6 304:

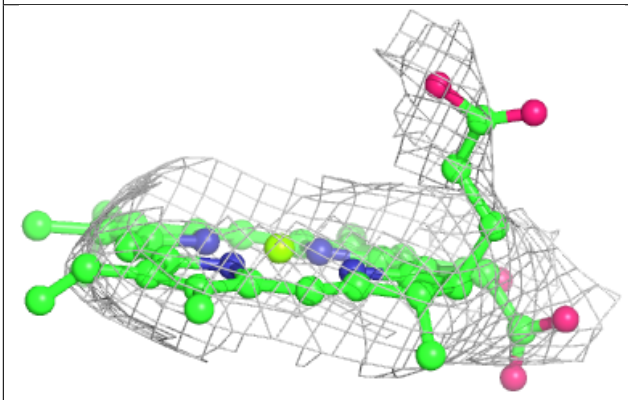
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

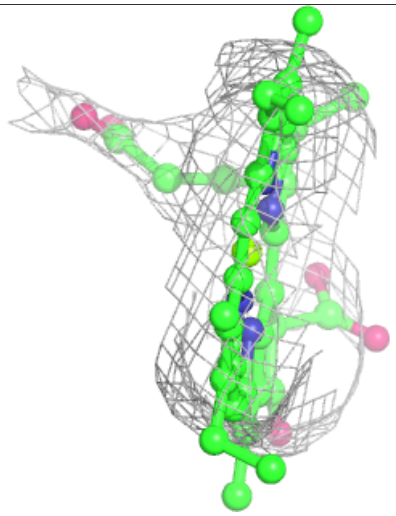


Electron density around CLA A 823:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

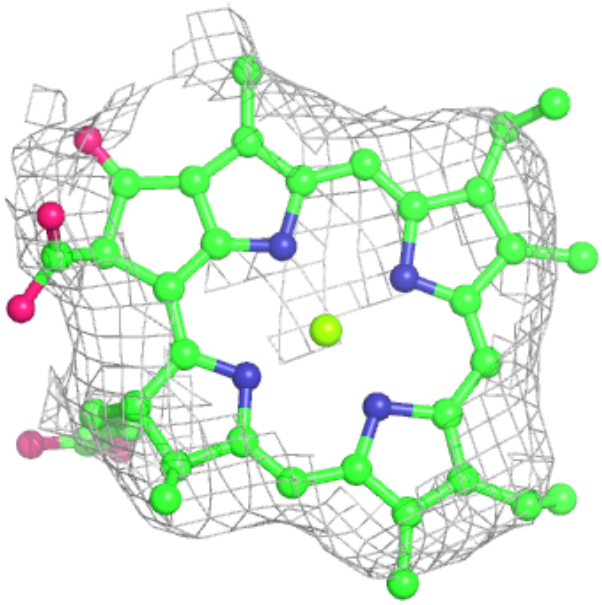


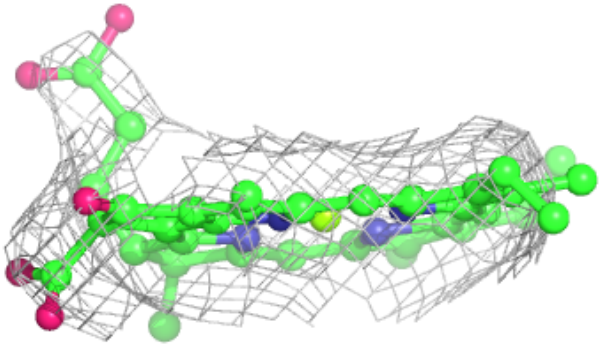


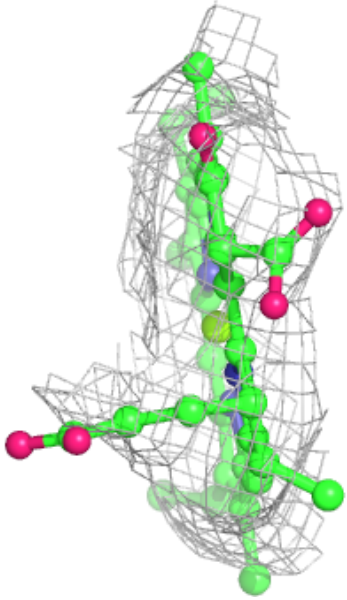


Electron density around CLA 0 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

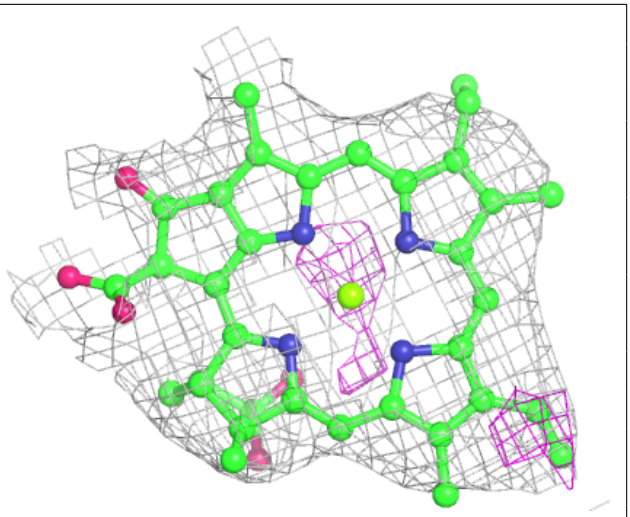


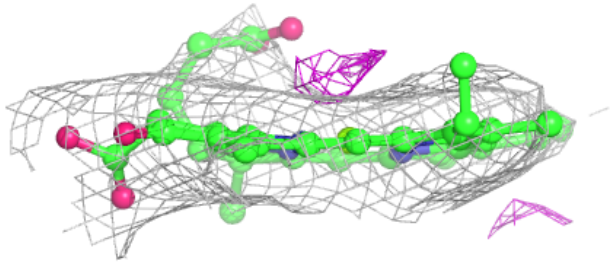


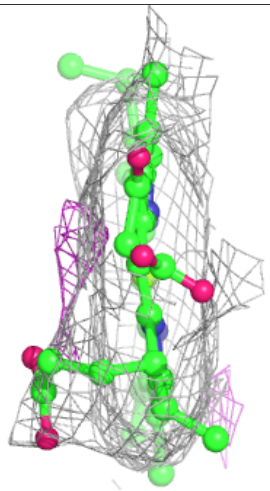


Electron density around CLA 1 1003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

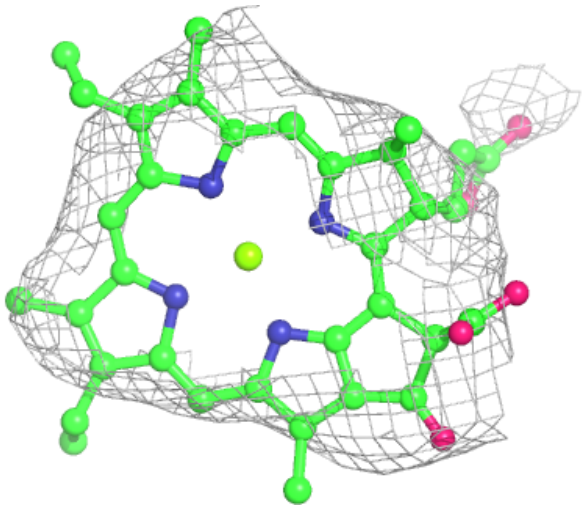


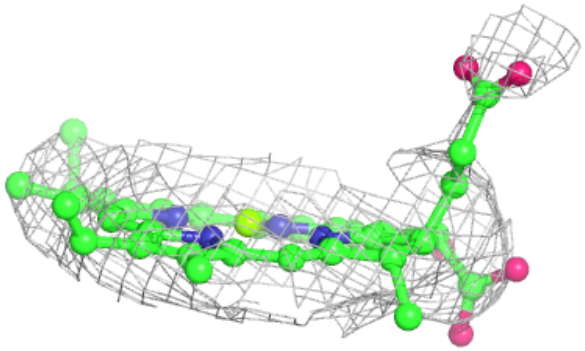


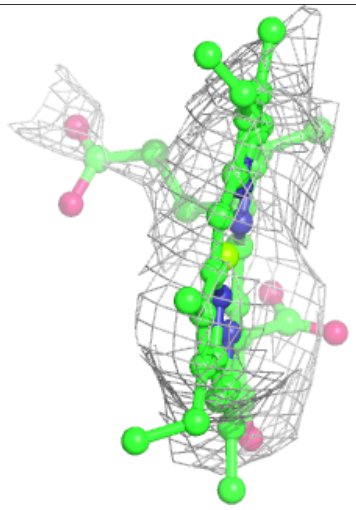


Electron density around CLA B 825:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

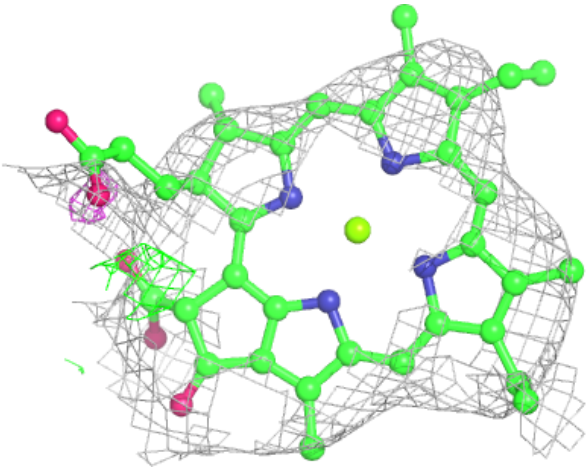


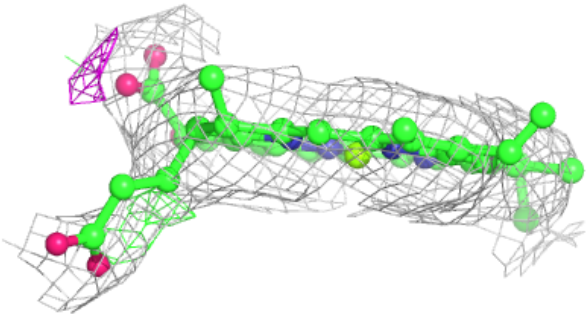


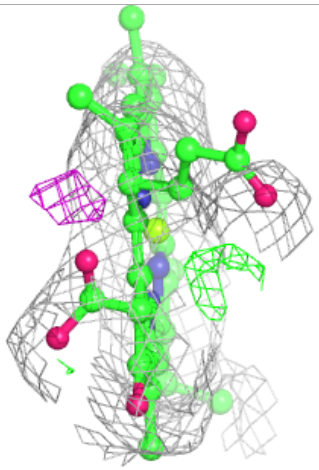


Electron density around CLA 0 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

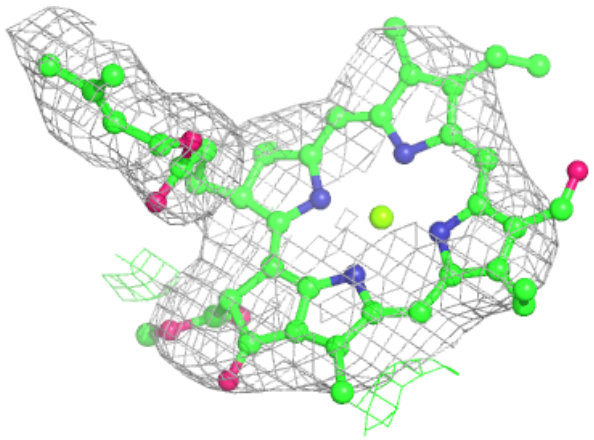


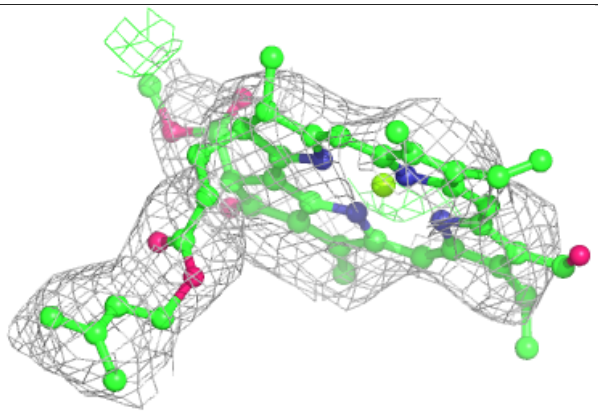


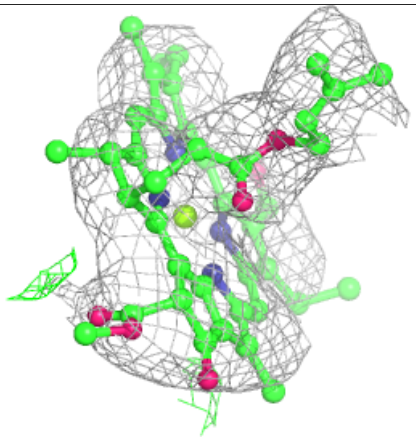


Electron density around CHL 8 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

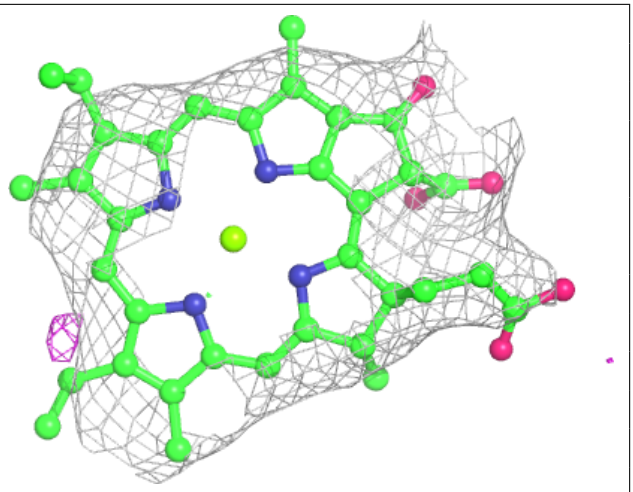


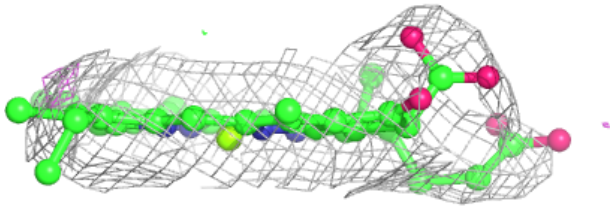


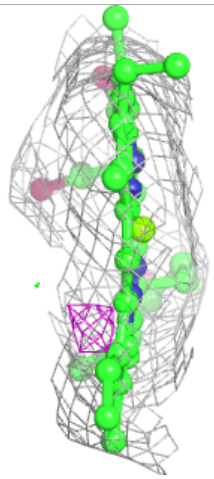


Electron density around CLA 1 1007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

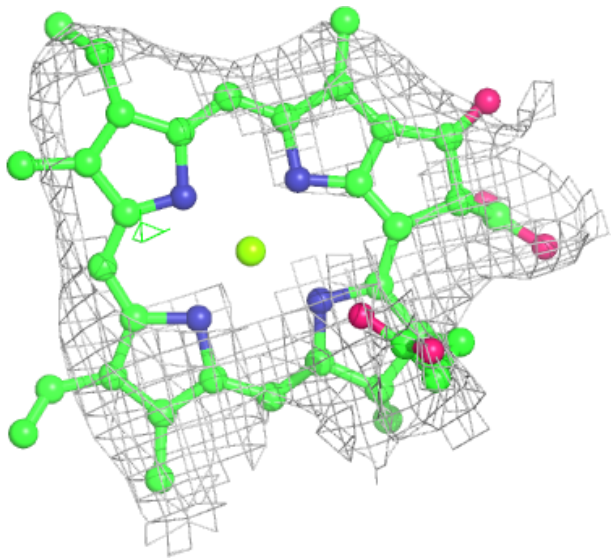


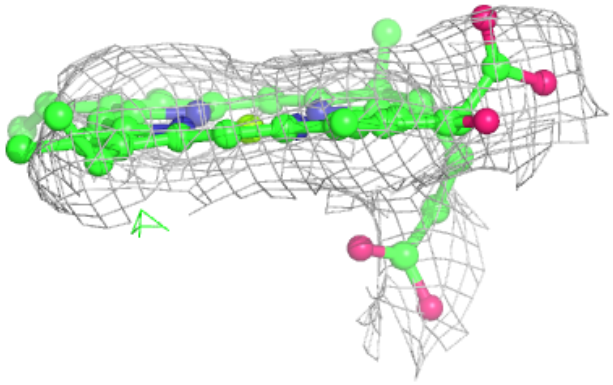


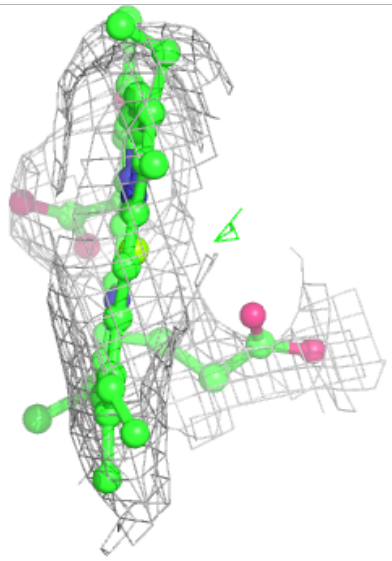


Electron density around CLA 1 1008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

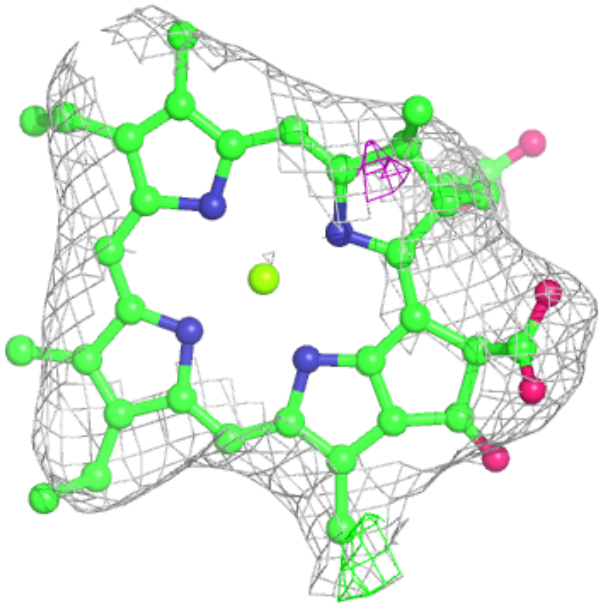


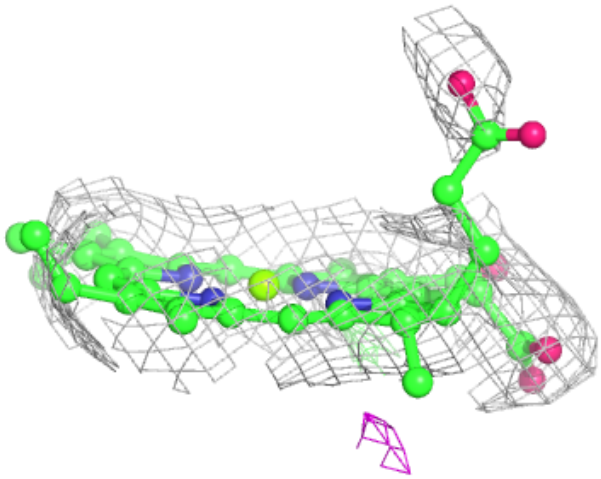


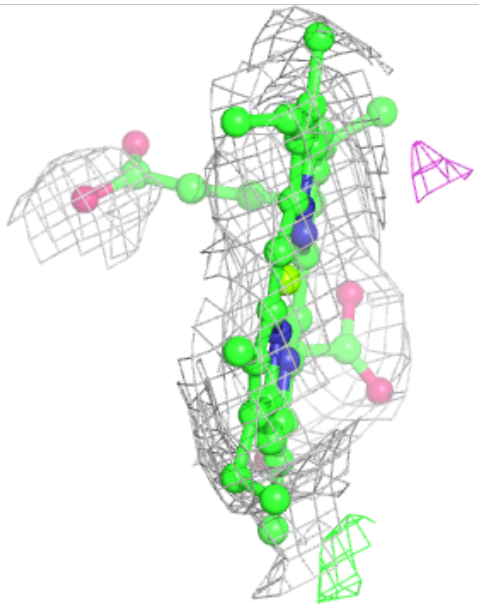


Electron density around CLA 1 1009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

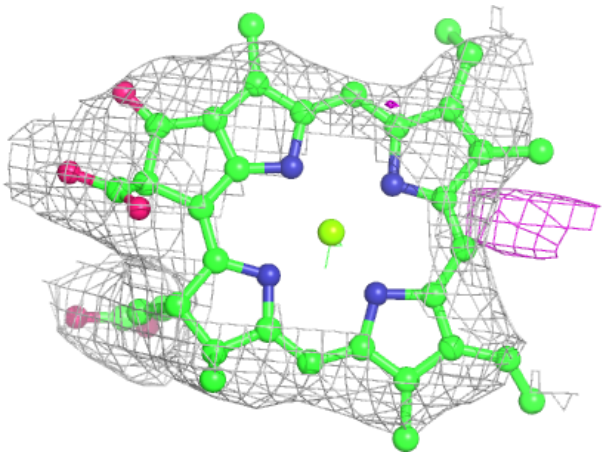


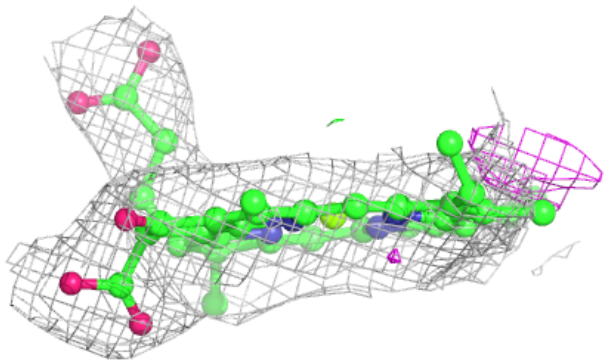


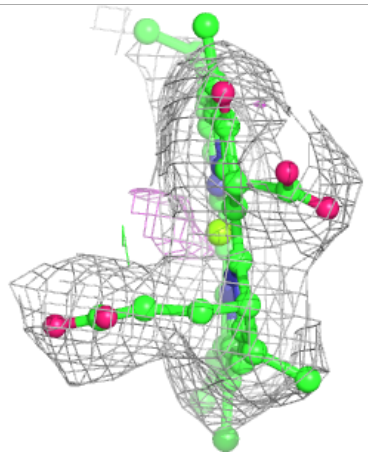


Electron density around CLA F 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

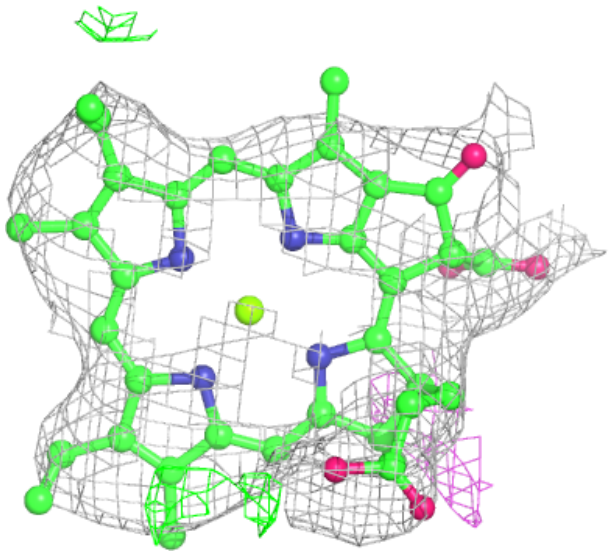


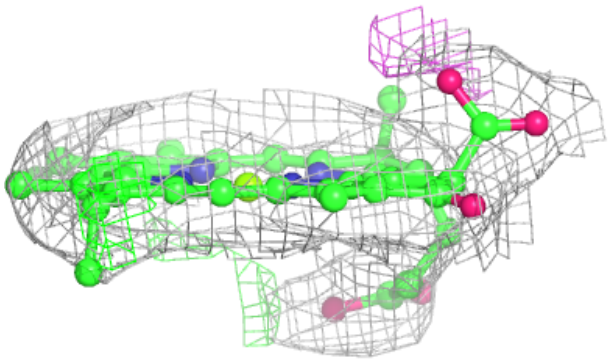


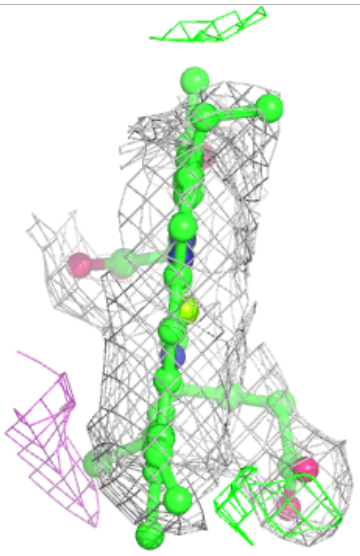


Electron density around CLA 8 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

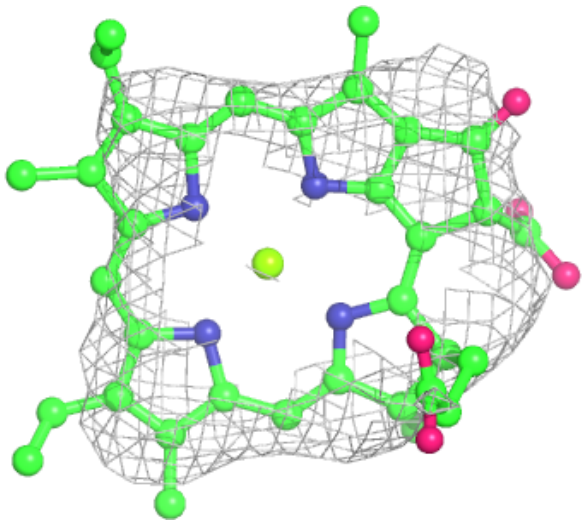


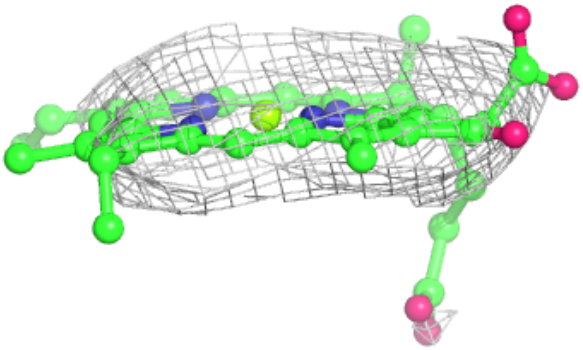


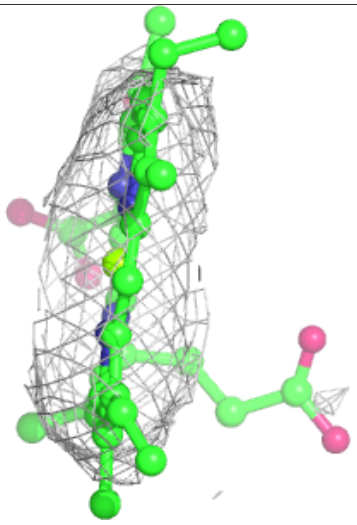


Electron density around CLA B 830:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

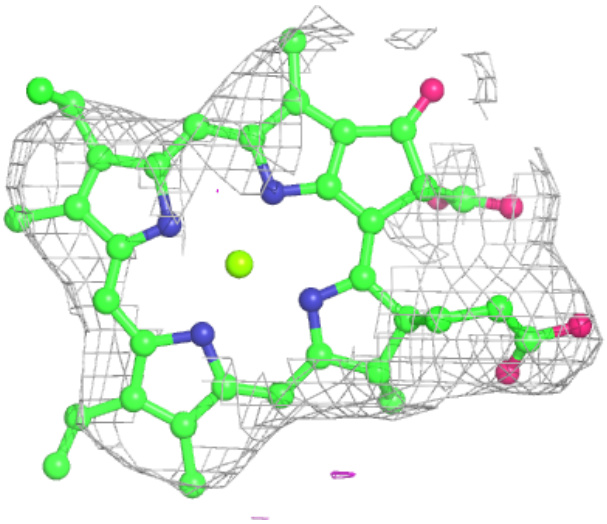


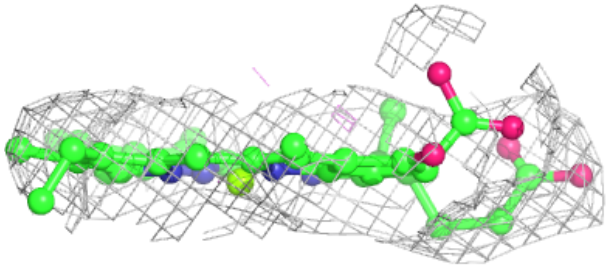


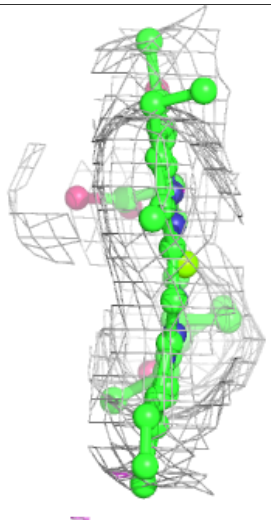


Electron density around CLA 4 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

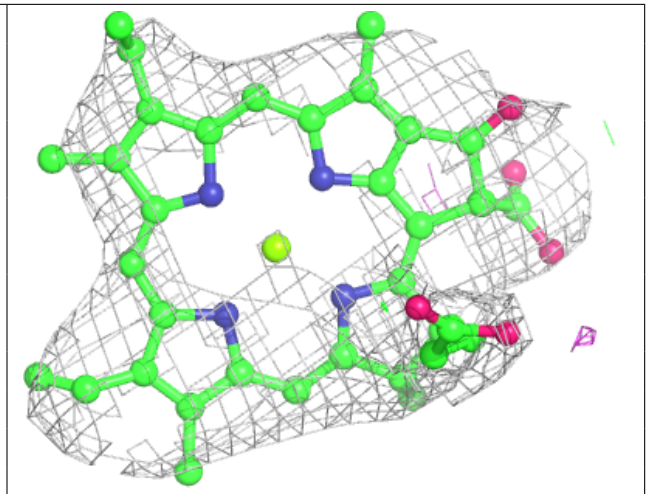


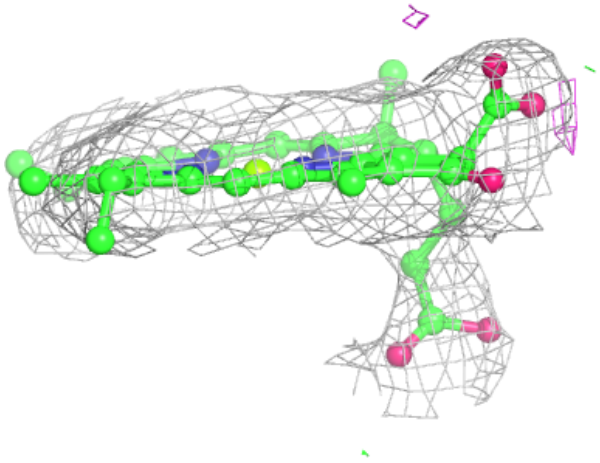


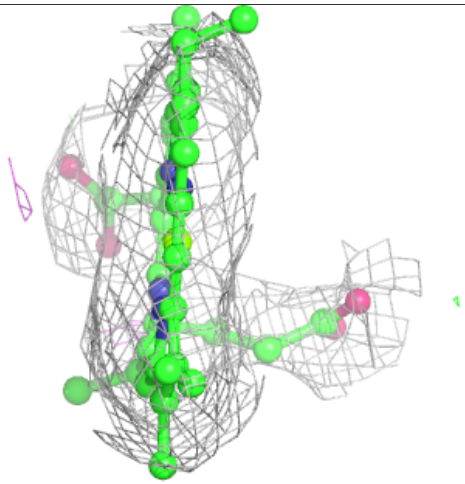


Electron density around CLA 8 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

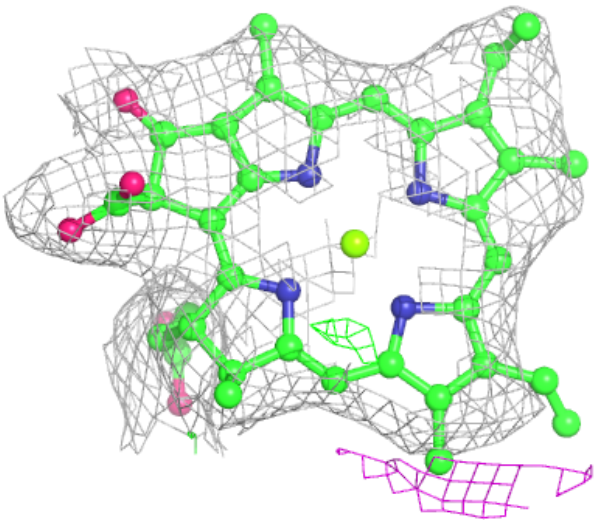


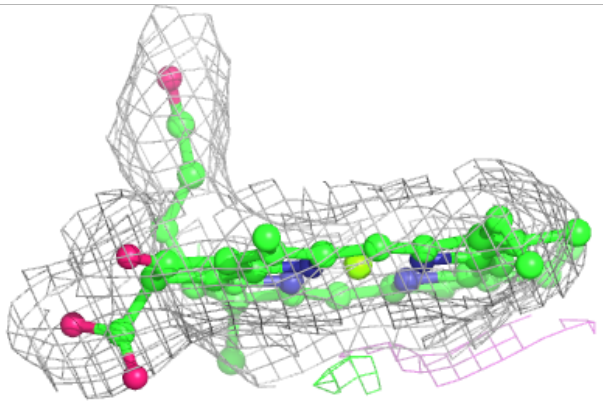


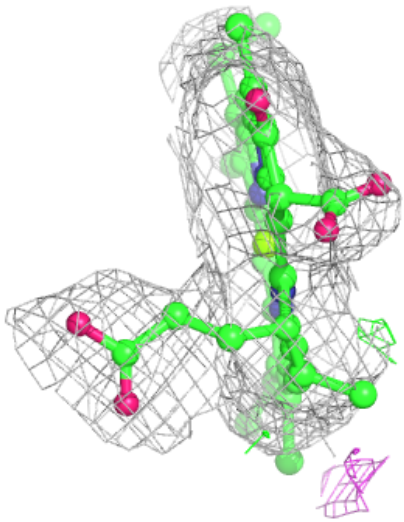


Electron density around CLA 7 1009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

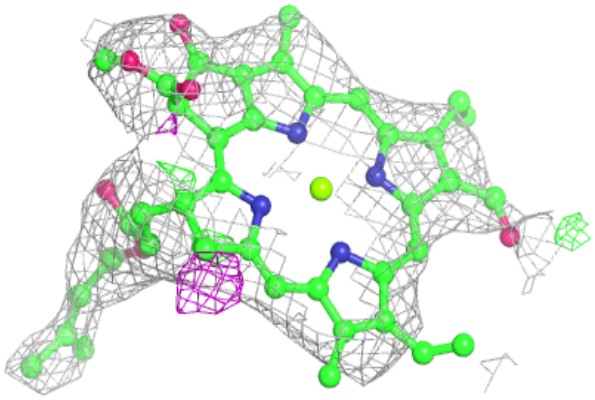


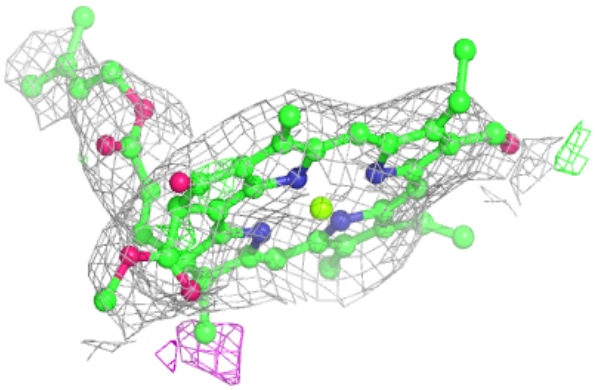


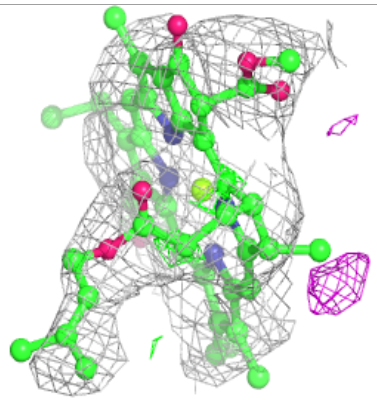


Electron density around CHL 6 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

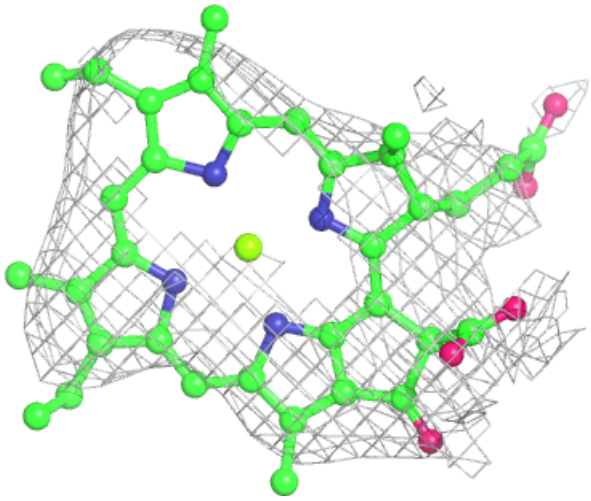


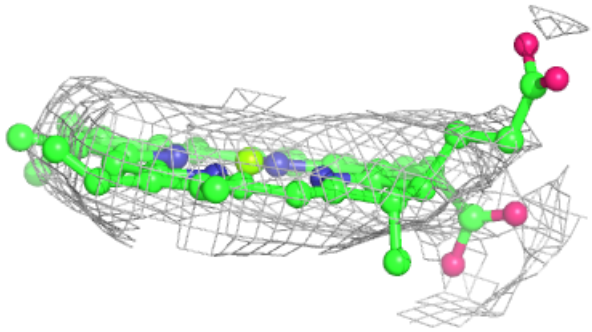


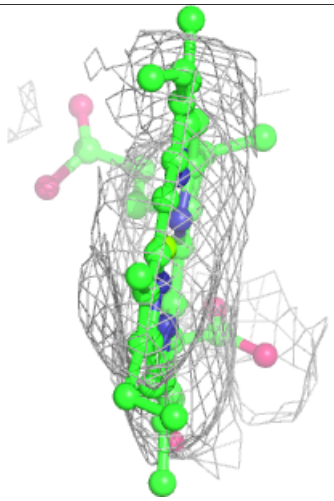


Electron density around CLA A 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

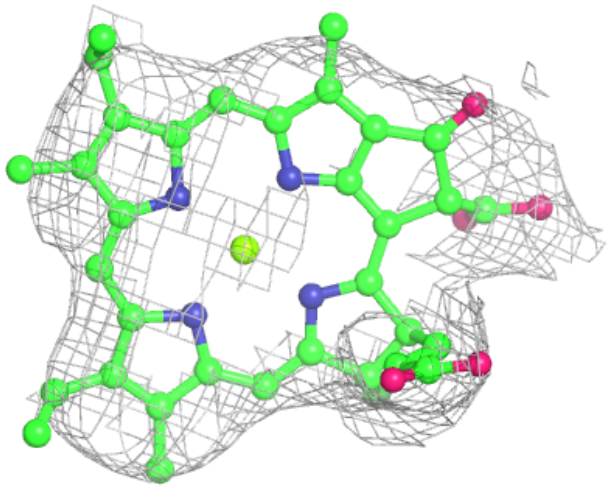


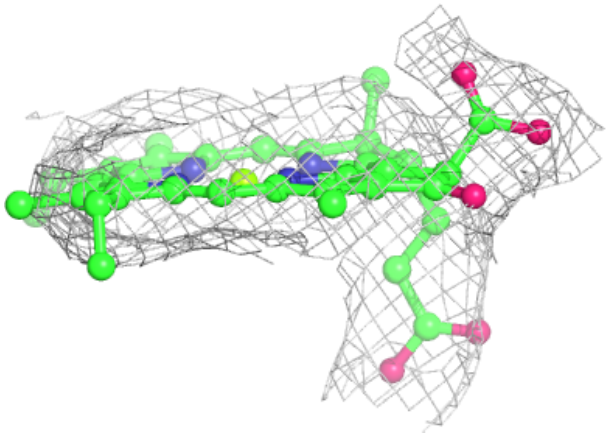


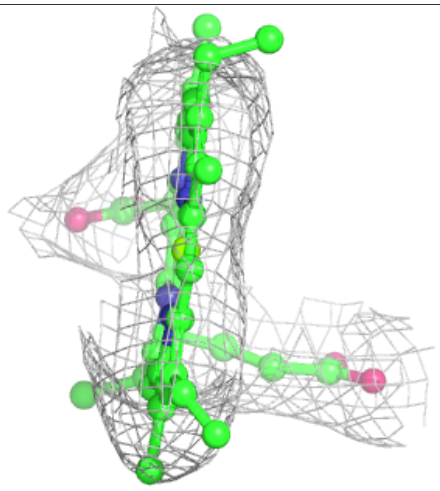


Electron density around CLA 6 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

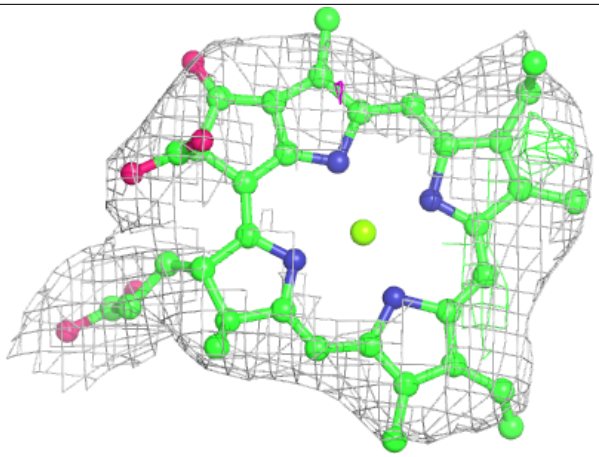


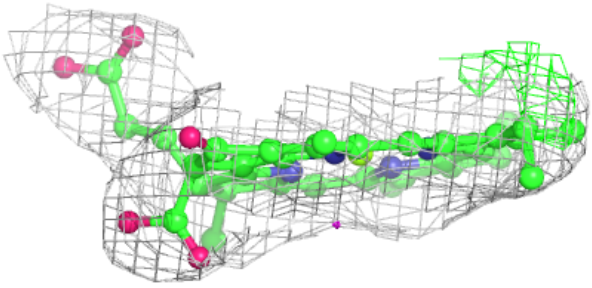


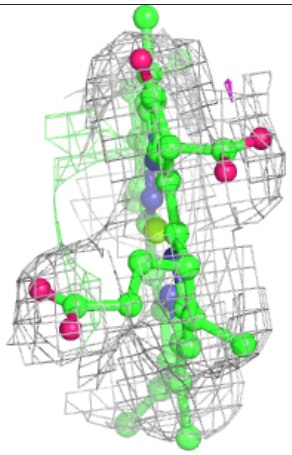


Electron density around CLA 6 318:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

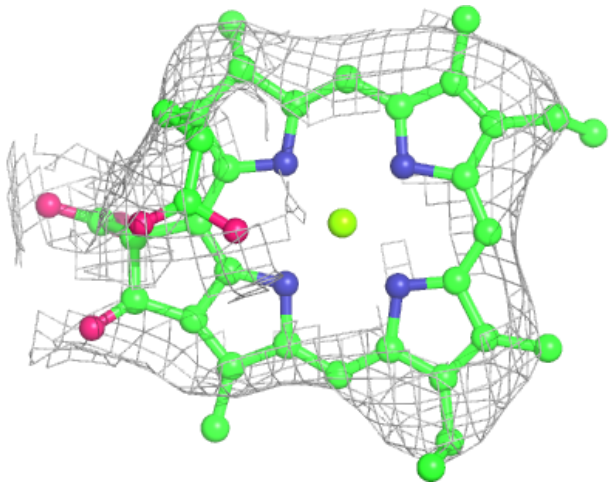


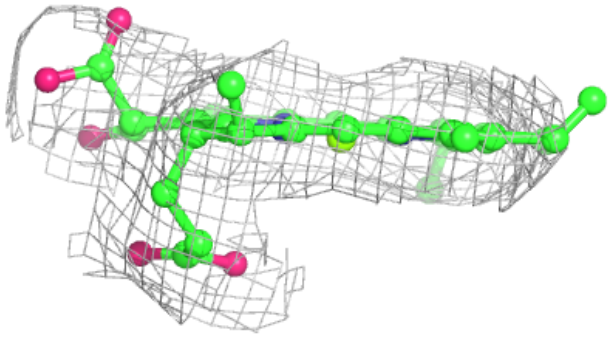


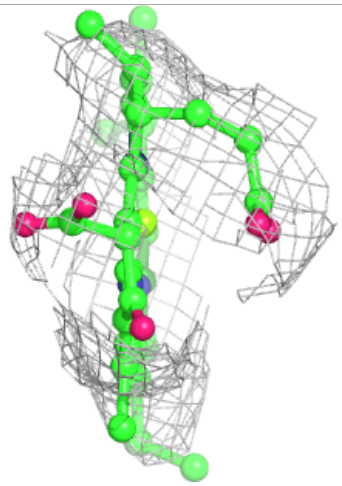


Electron density around CLA 5 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

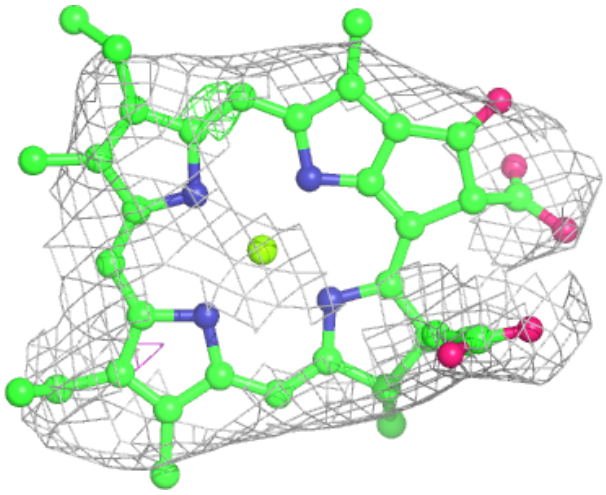


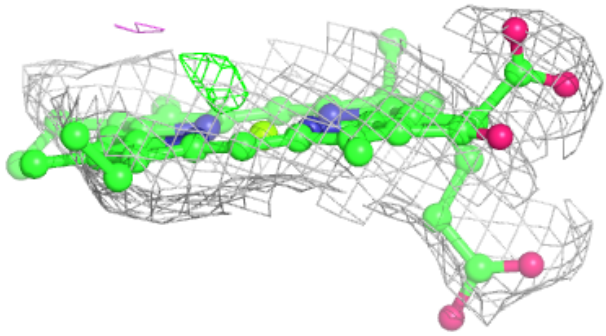


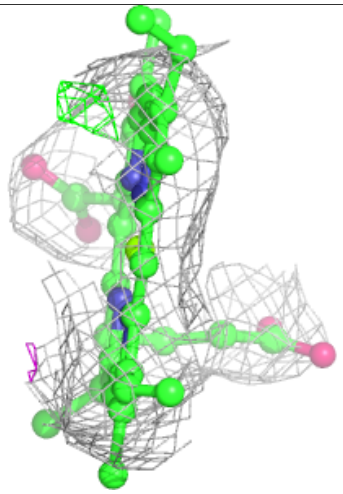


Electron density around CLA 5 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

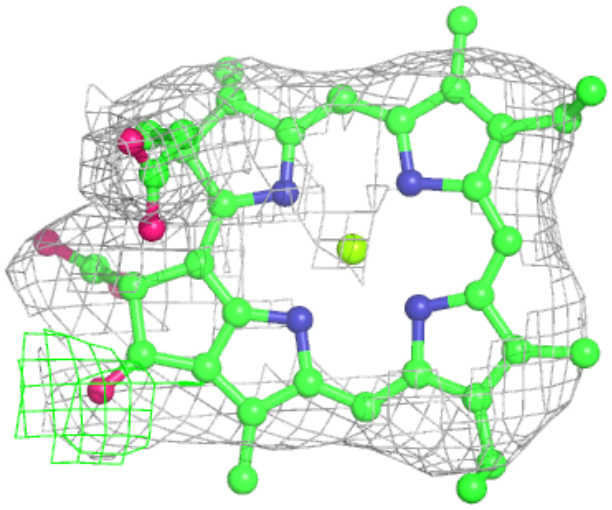


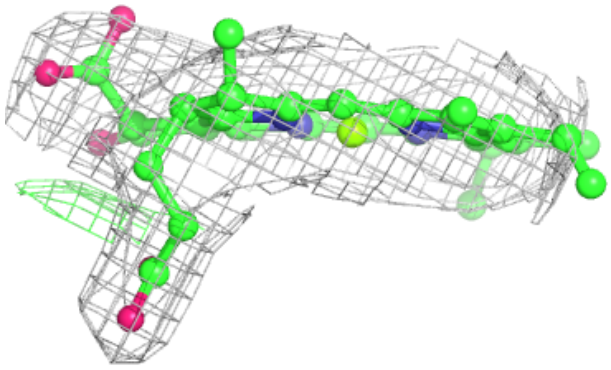


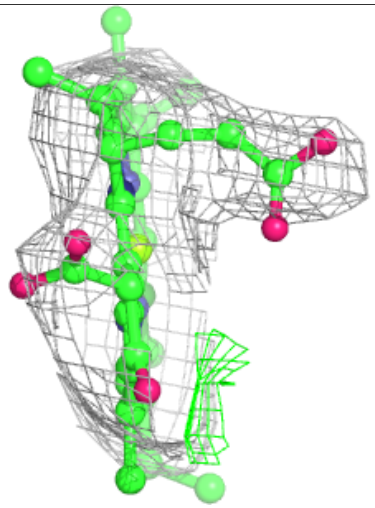


Electron density around CLA 3 1010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

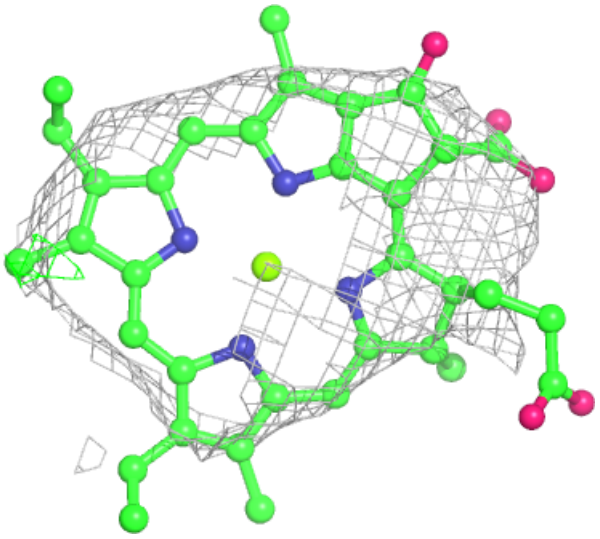


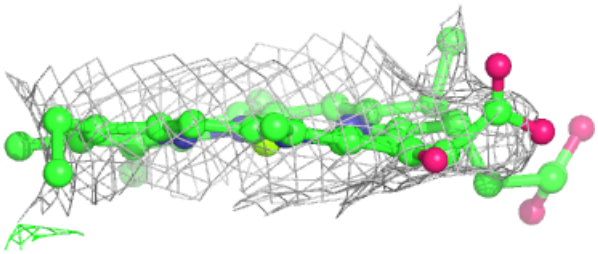


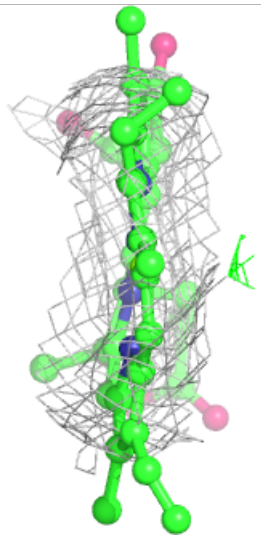


Electron density around CLA B 806:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

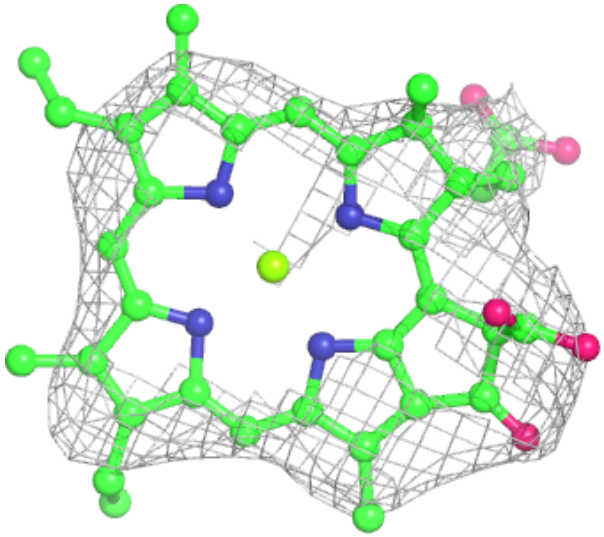


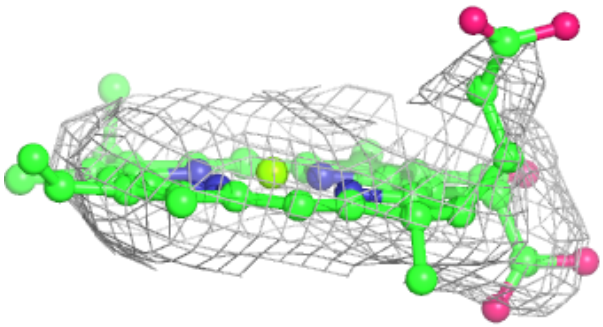


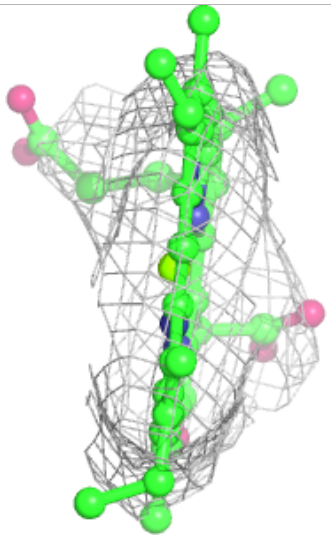


Electron density around CLA B 839:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

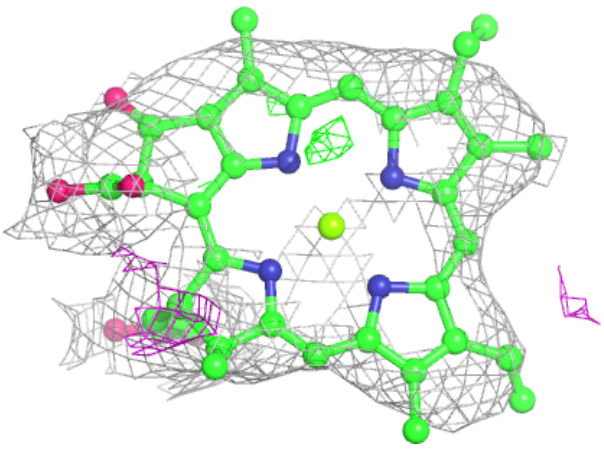


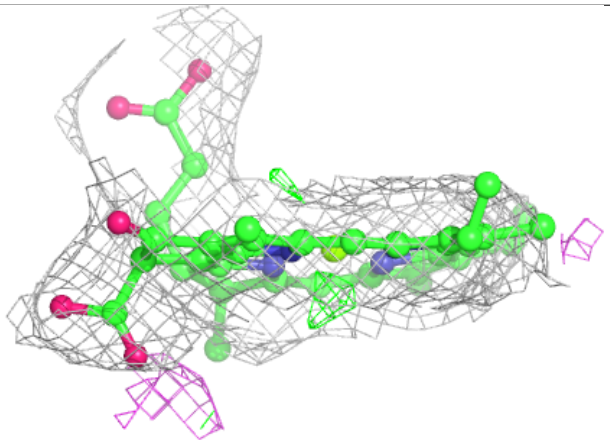


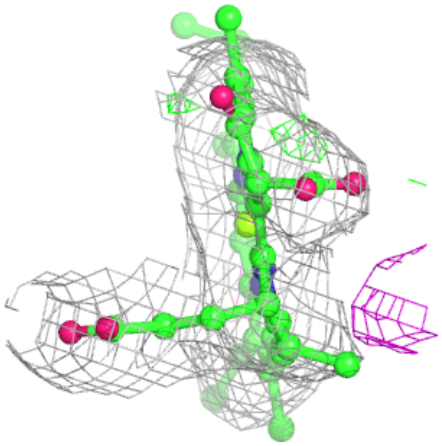


Electron density around CLA 5 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

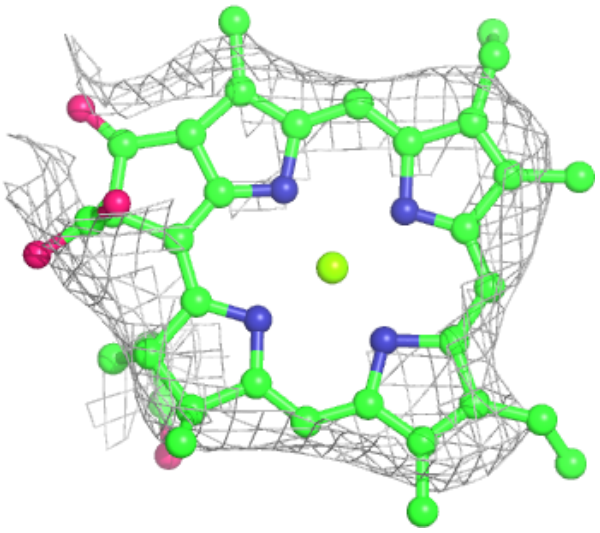


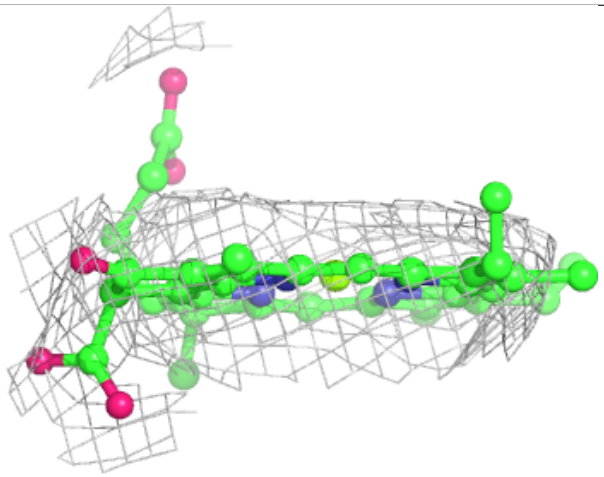


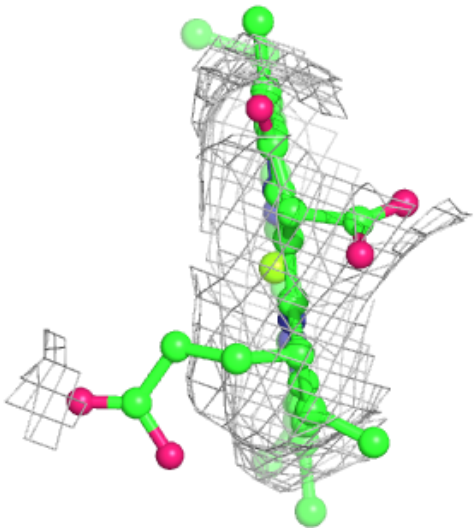


Electron density around CLA 3 1008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

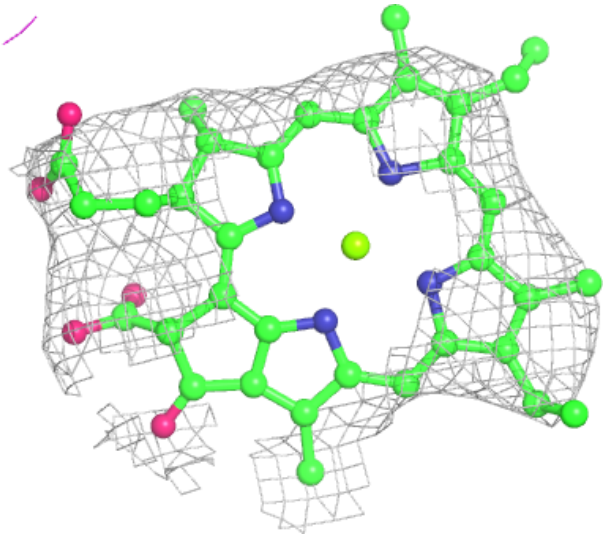


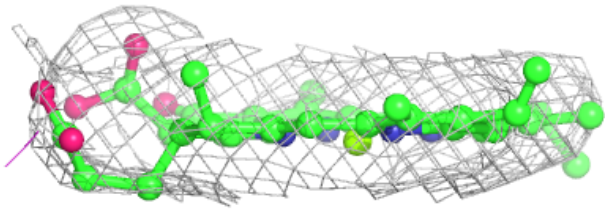


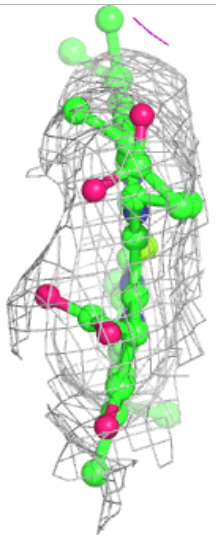


Electron density around CLA 3 1009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

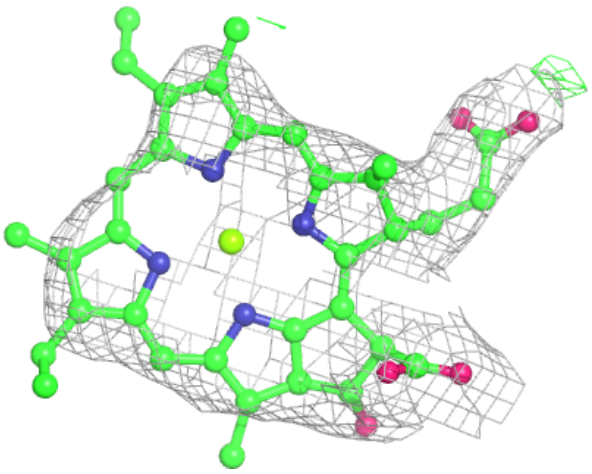


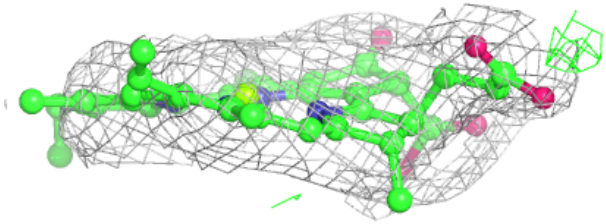


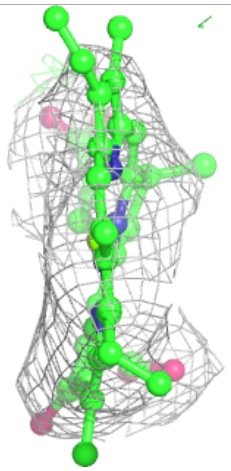


Electron density around CLA B 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

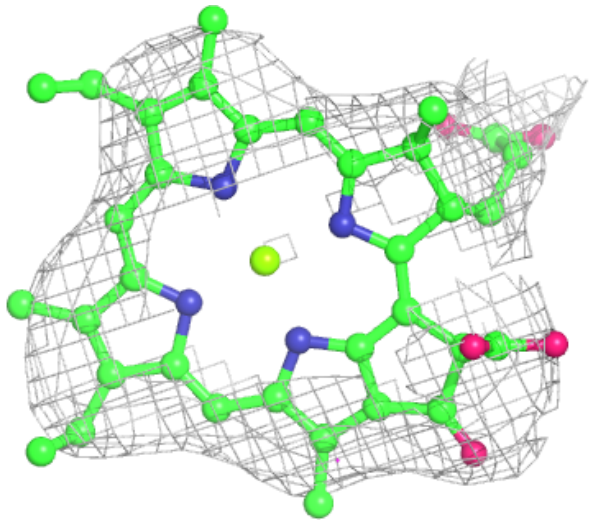


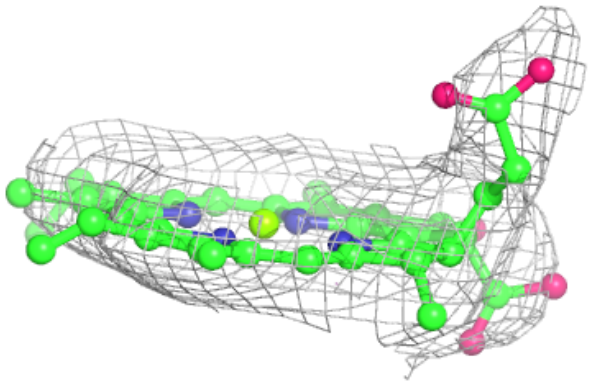


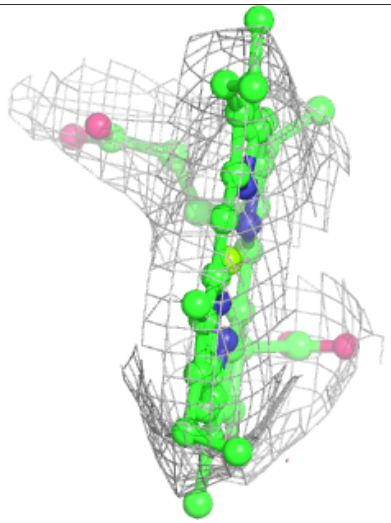


Electron density around CLA B 841:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

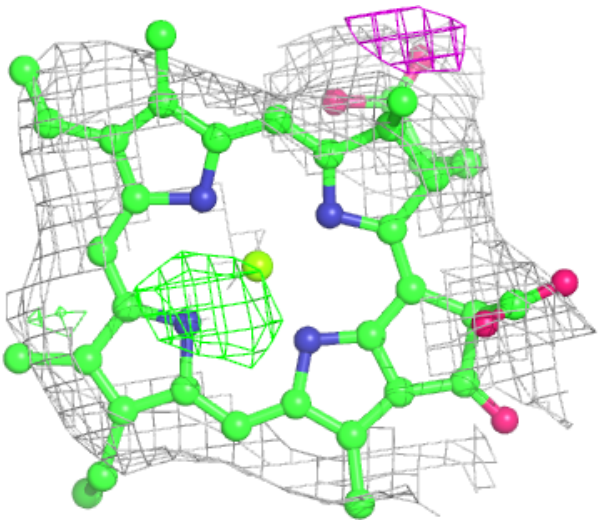


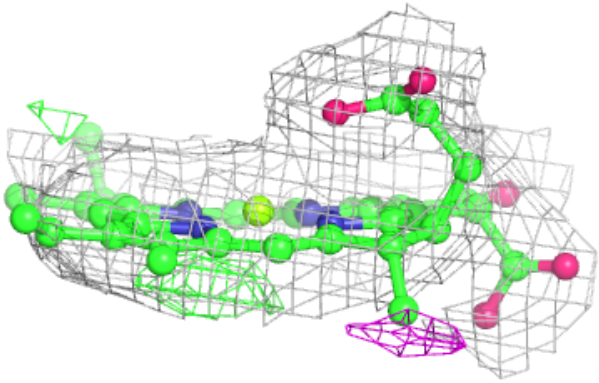




Electron density around CLA 0 308:

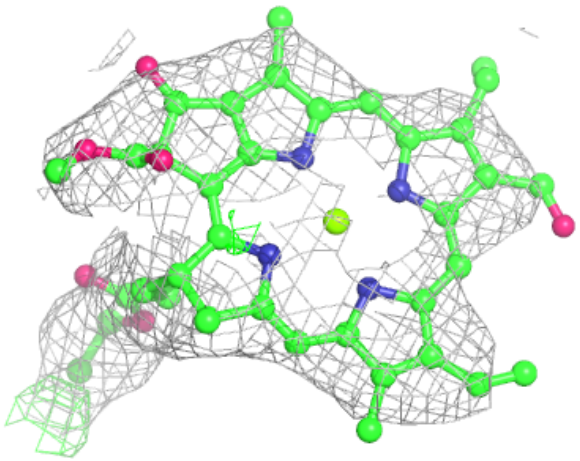
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

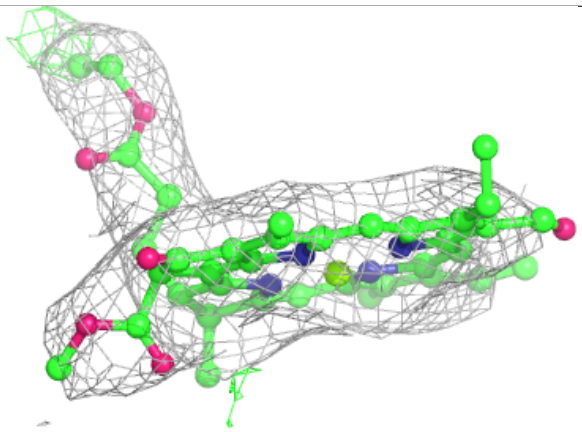


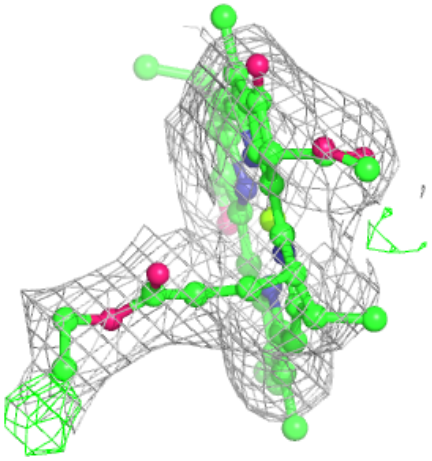


Electron density around CHL 7 1013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

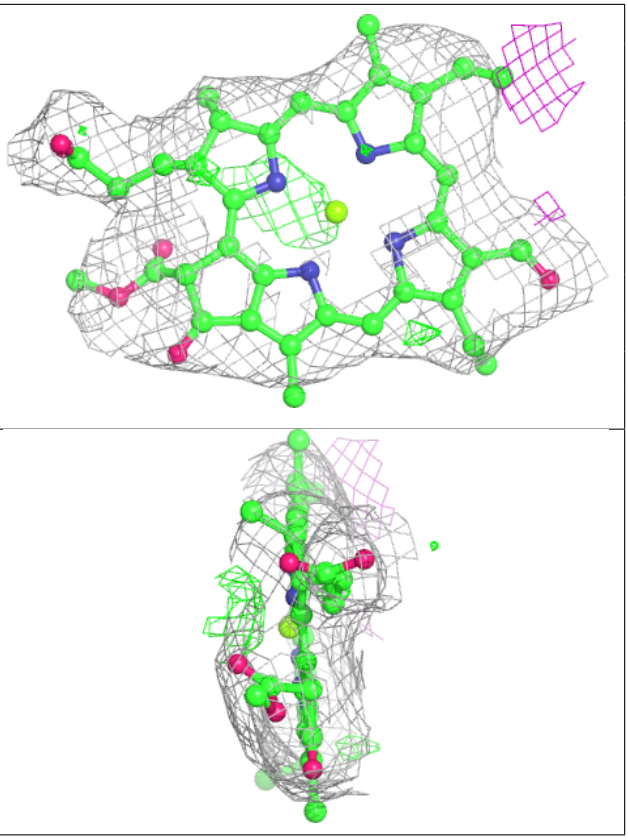


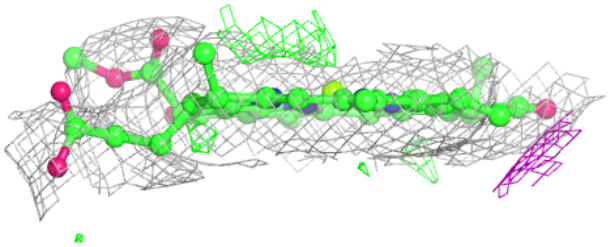




Electron density around CHL 7 1015:

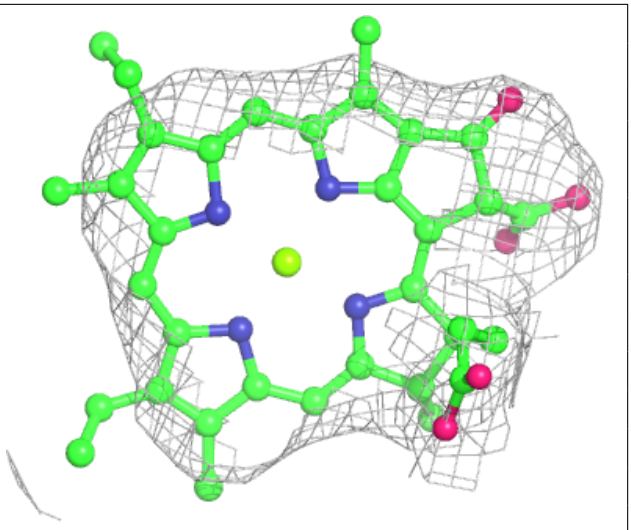
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

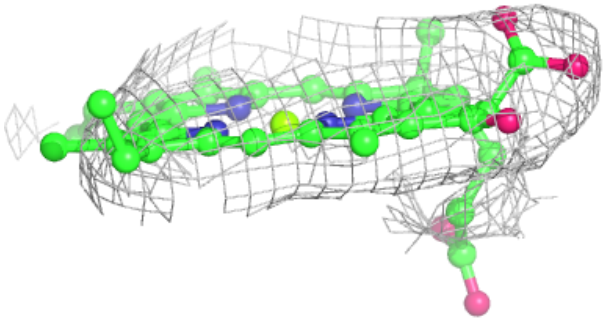


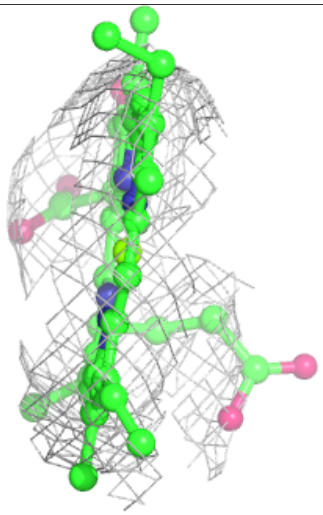


Electron density around CLA 3 1013:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

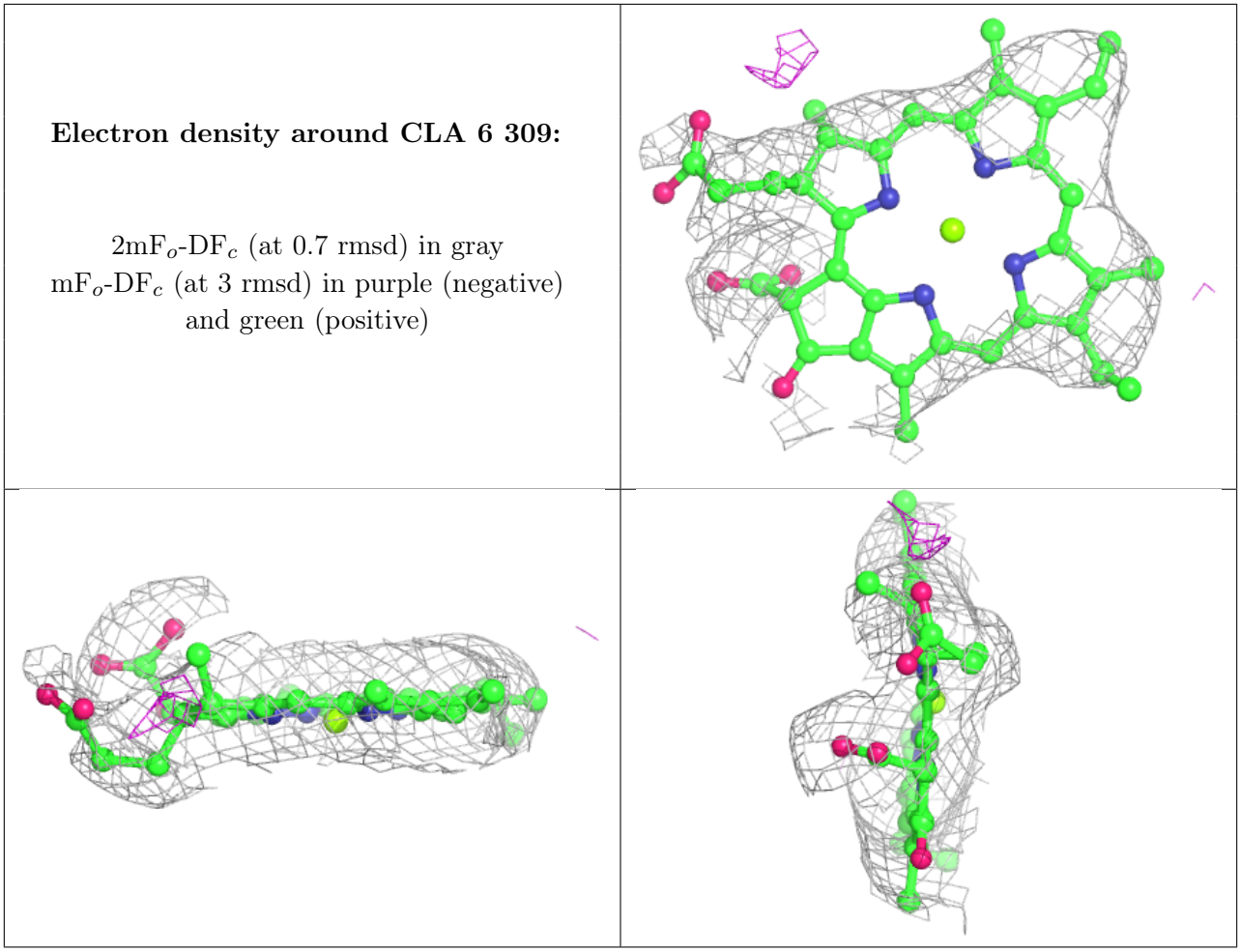






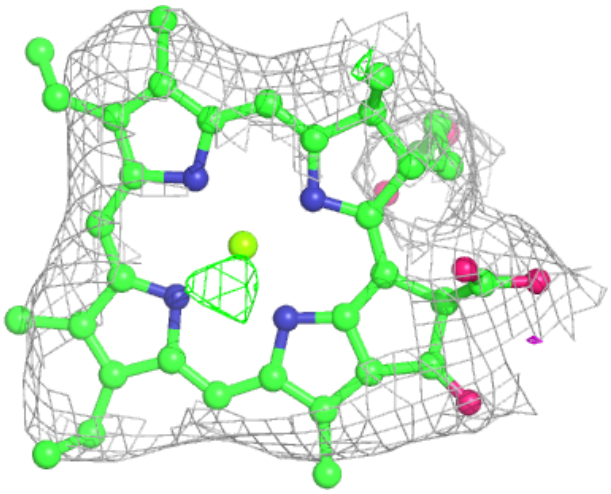
Electron density around CLA 6 309:

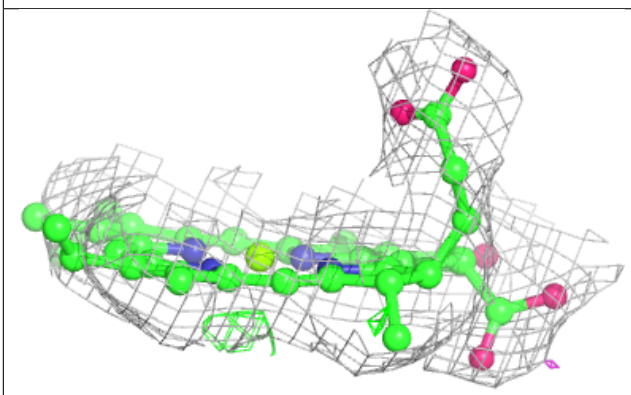
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

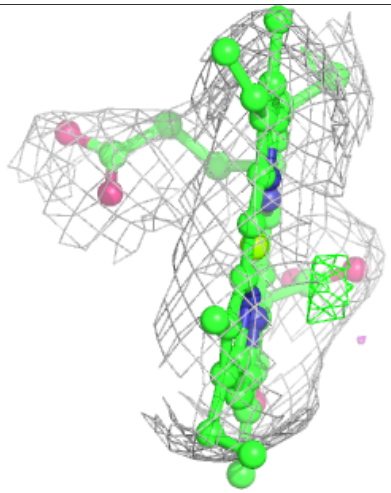


Electron density around CLA 6 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

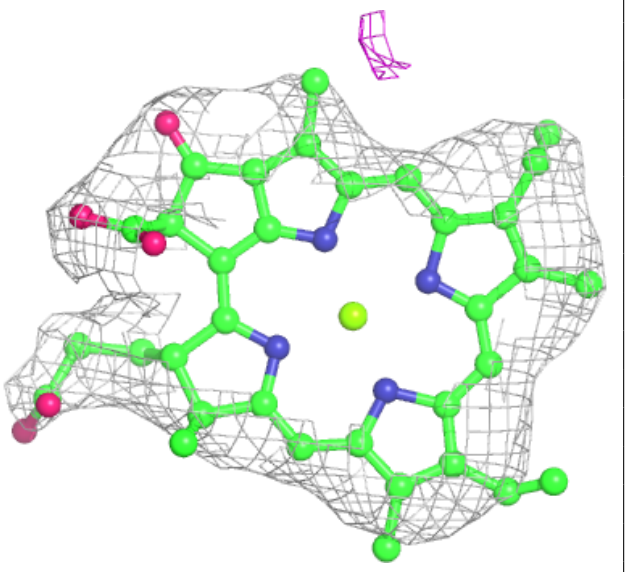


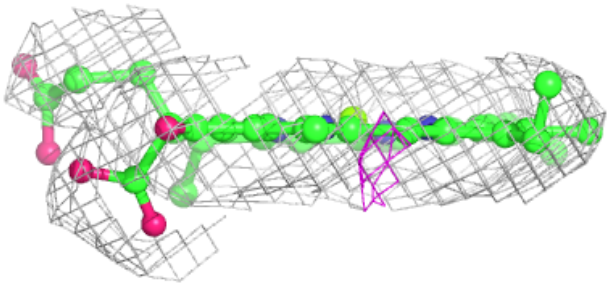


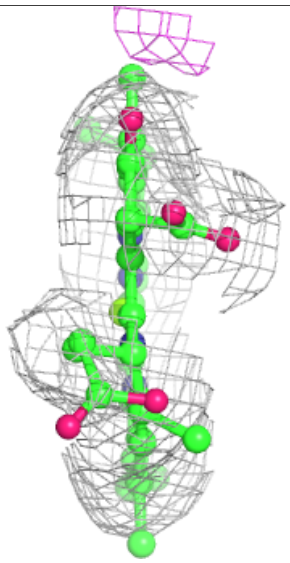


Electron density around CLA 3 1017:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

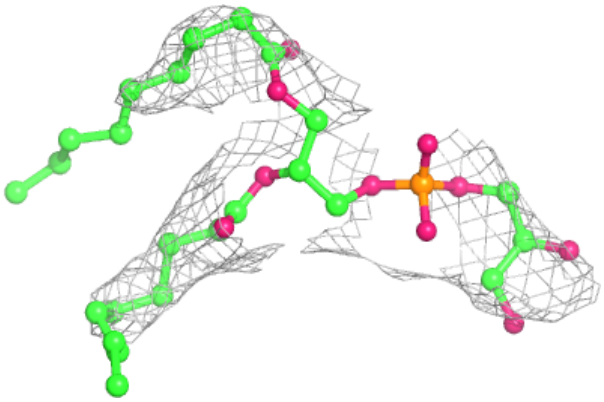


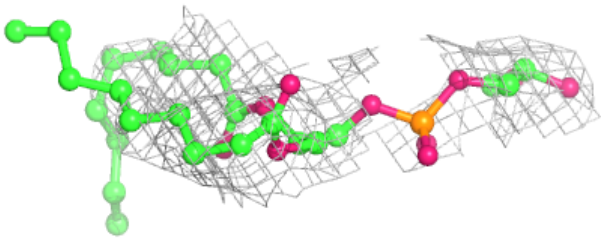


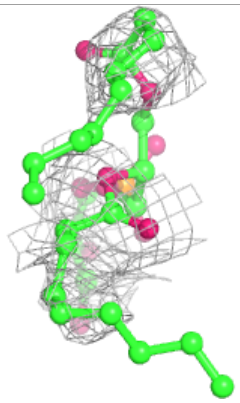


Electron density around LHG 7 1016:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

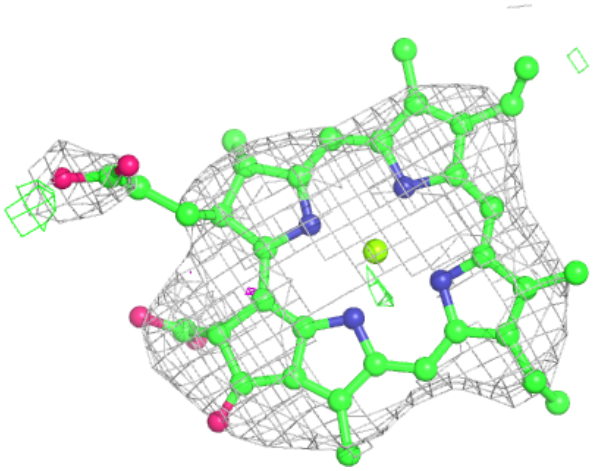


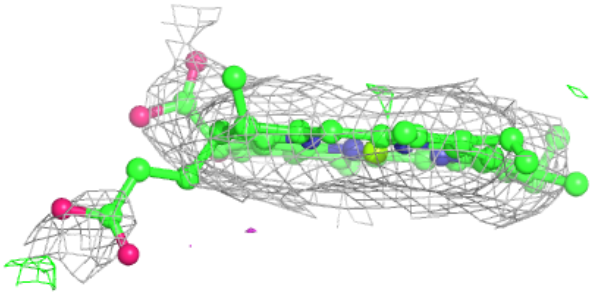


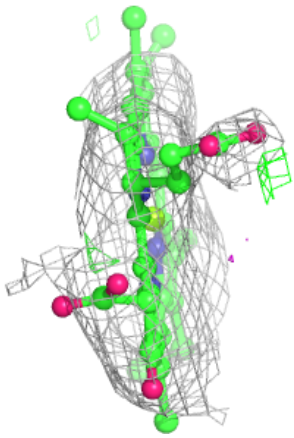


Electron density around CLA A 838:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

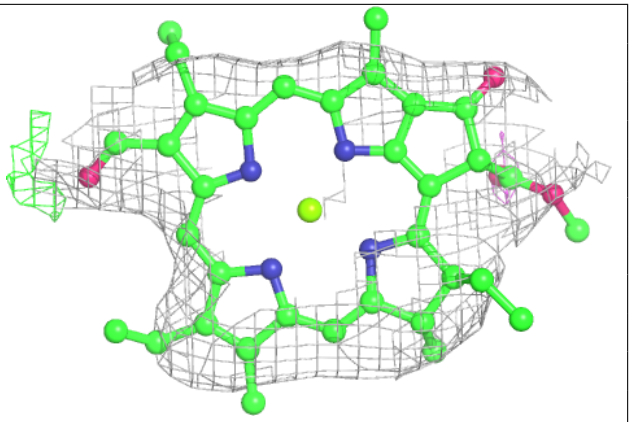


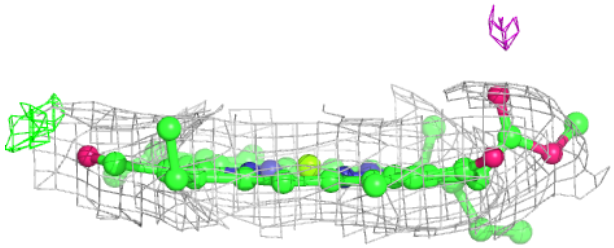


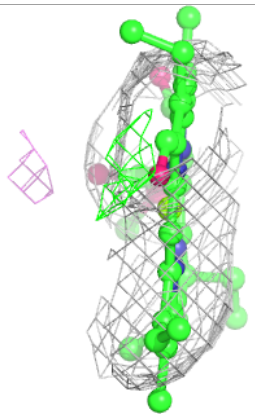


Electron density around CHL 4 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

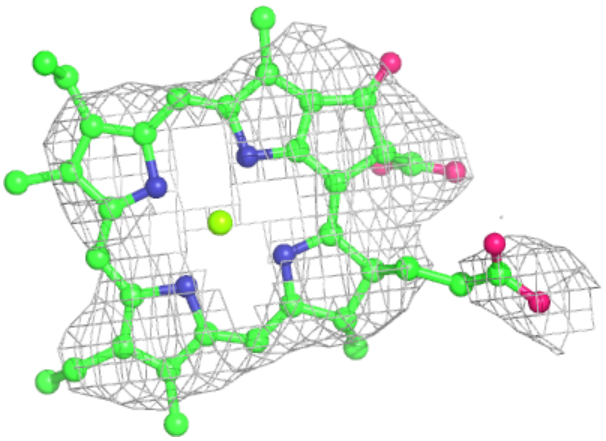


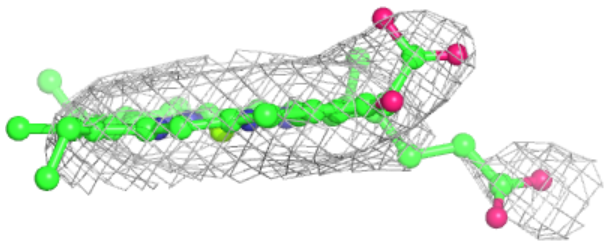


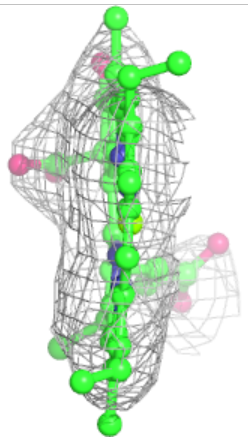


Electron density around CLA B 837:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

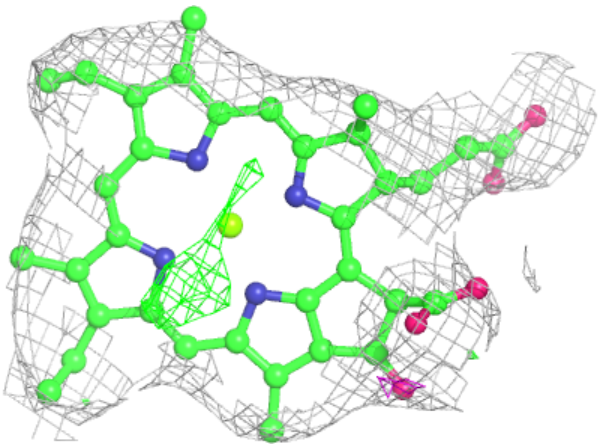


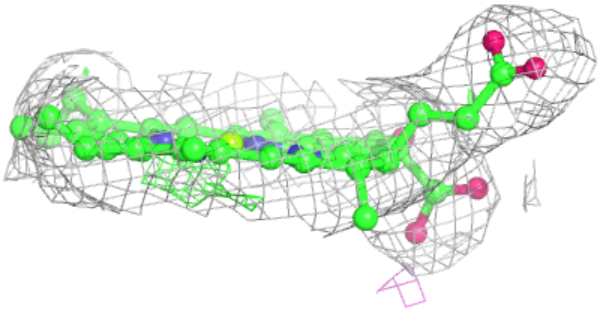




Electron density around CLA 6 320:

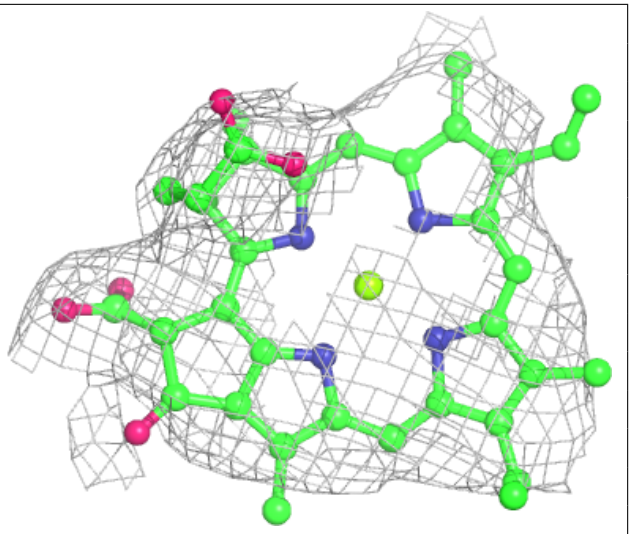
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

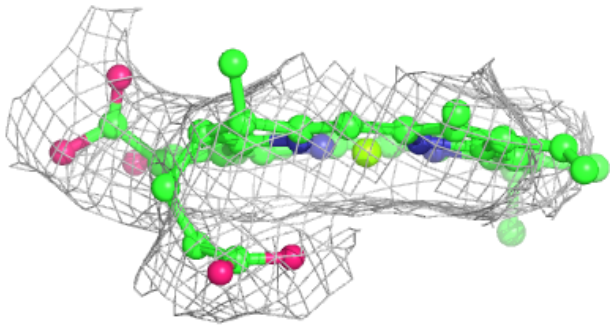


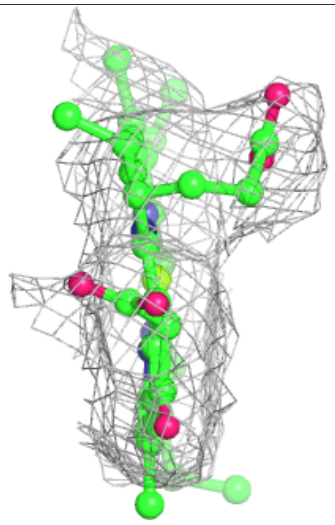


Electron density around CLA 5 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

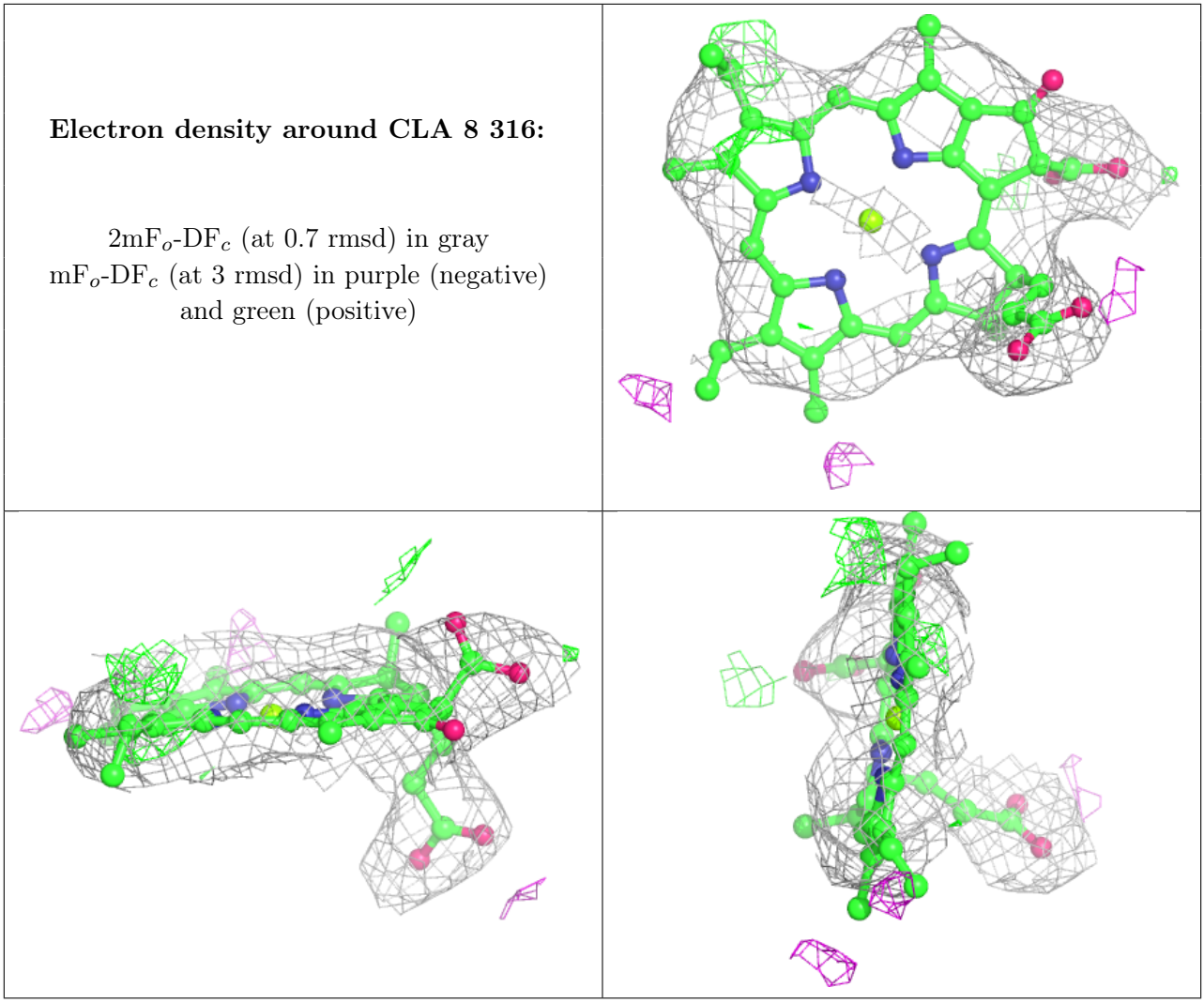






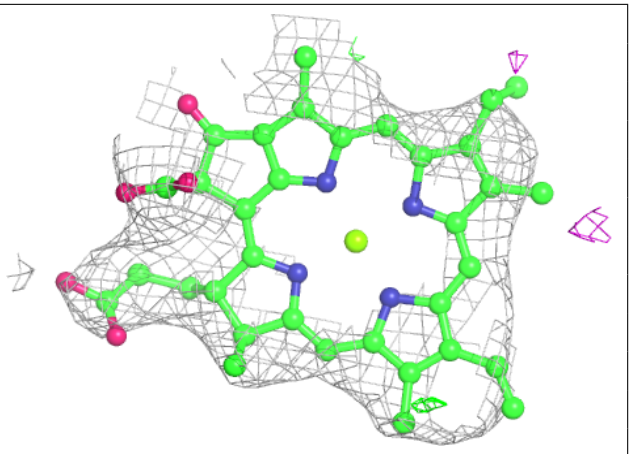
Electron density around CLA 8 316:

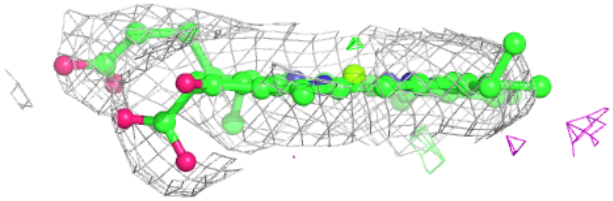
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

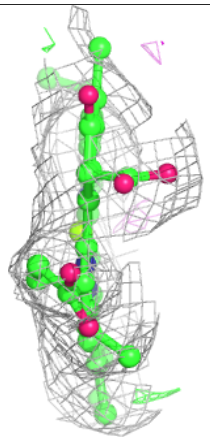


Electron density around CLA 5 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

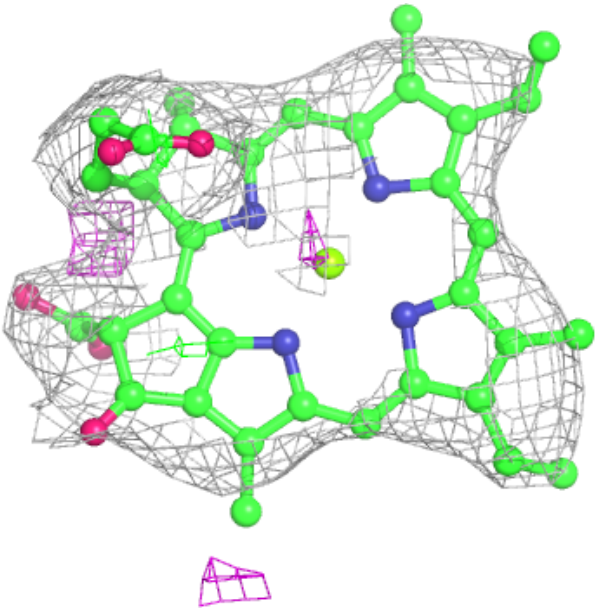


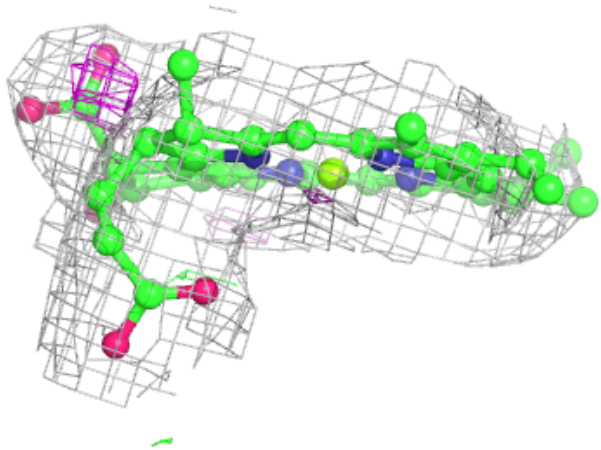


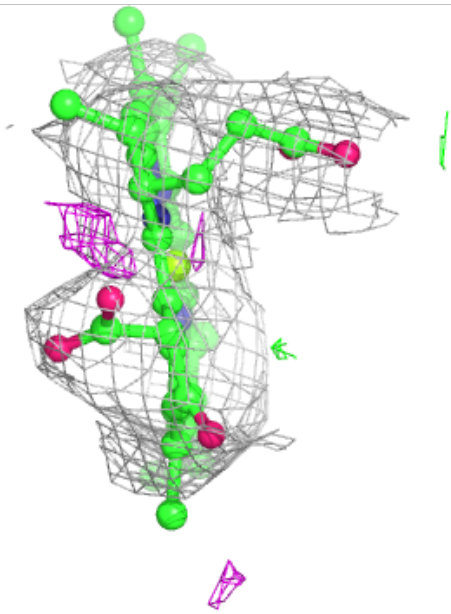


Electron density around CLA 5 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

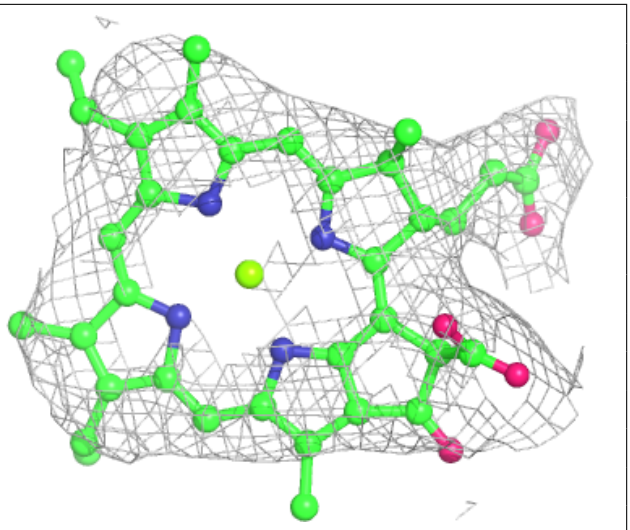


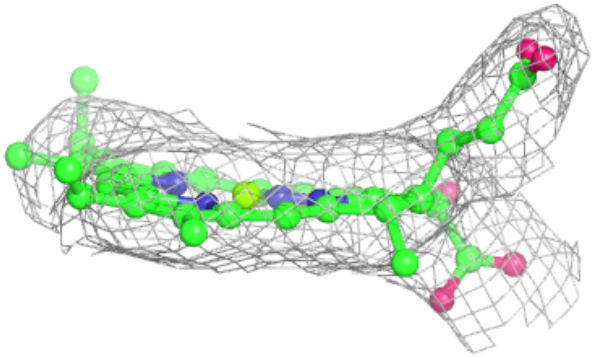




Electron density around CLA B 834:

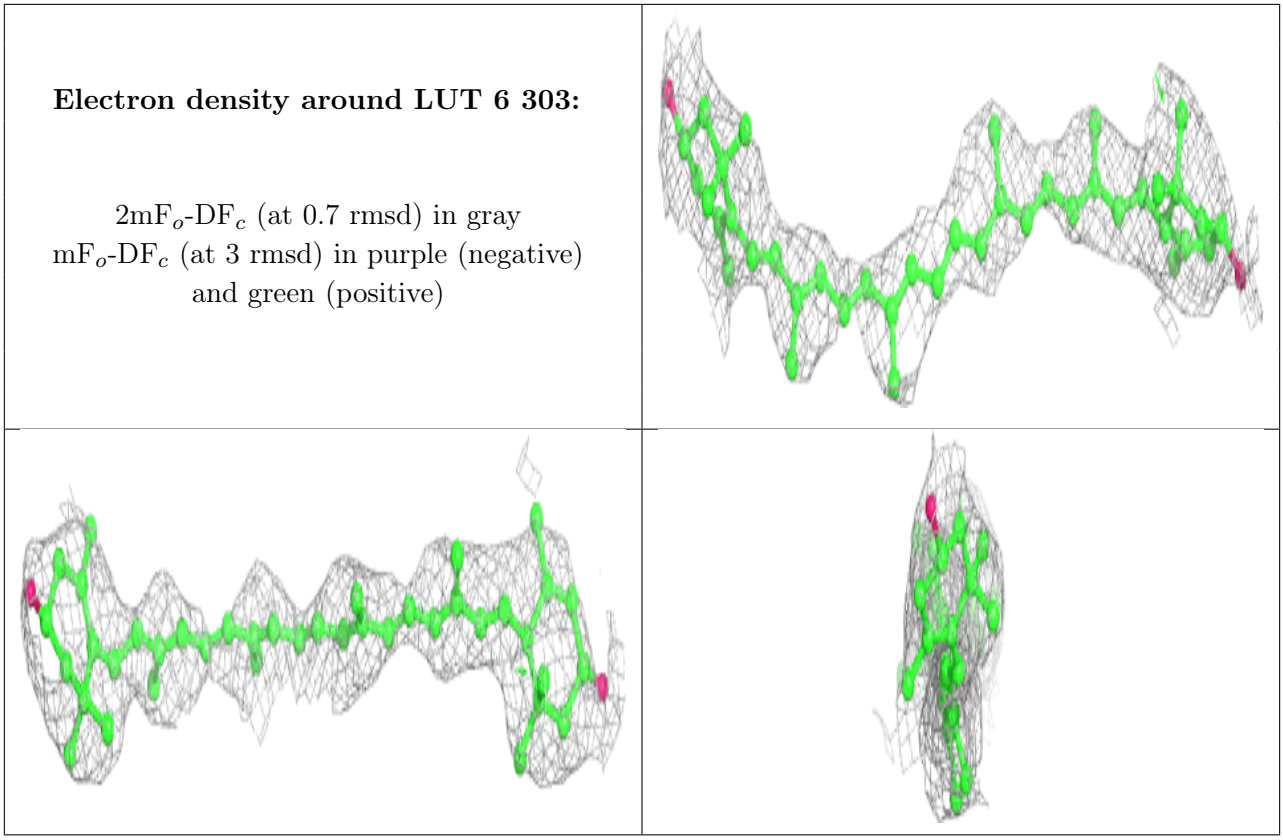
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





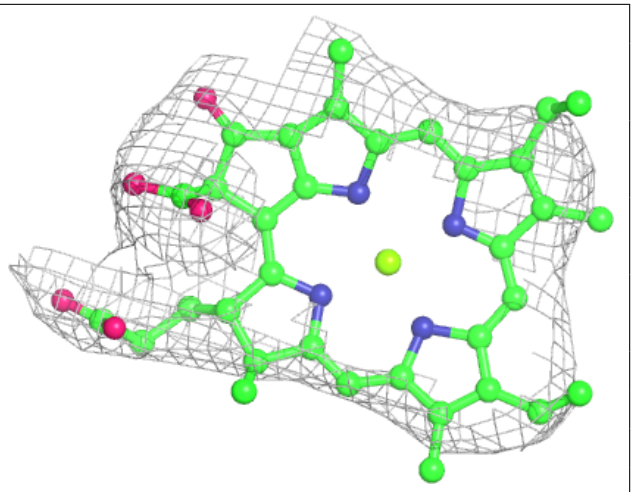
Electron density around LUT 6 303:

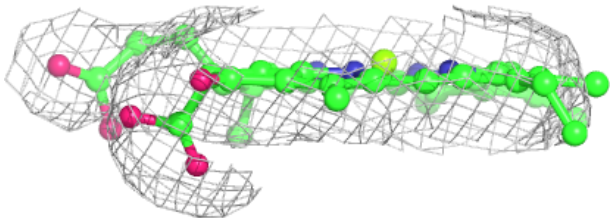
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

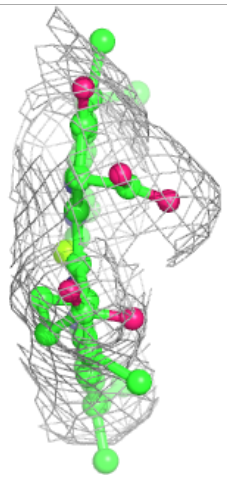


Electron density around CLA 3 1006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

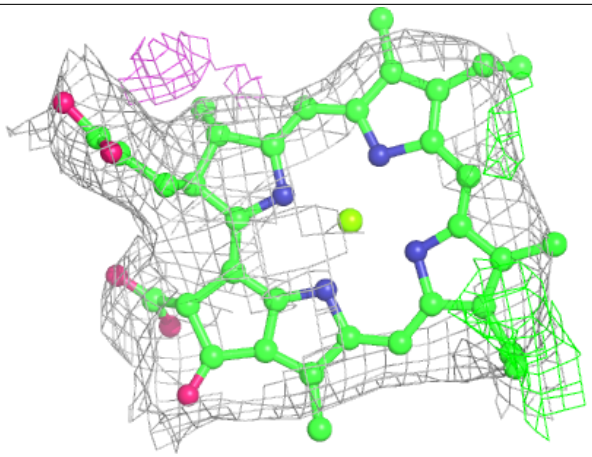


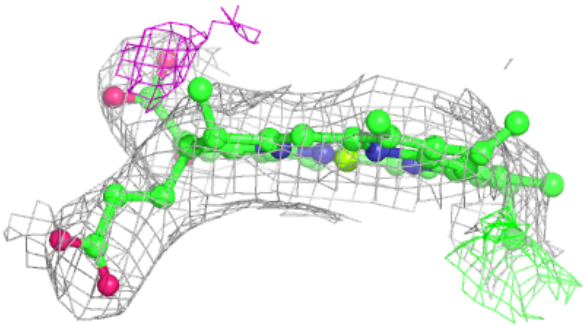


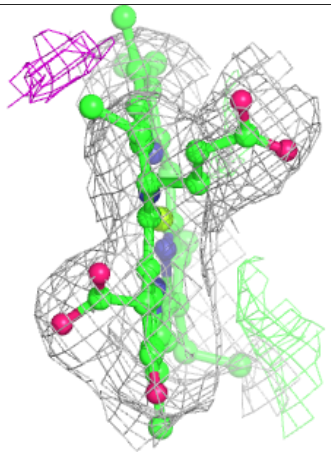


Electron density around CLA 8 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

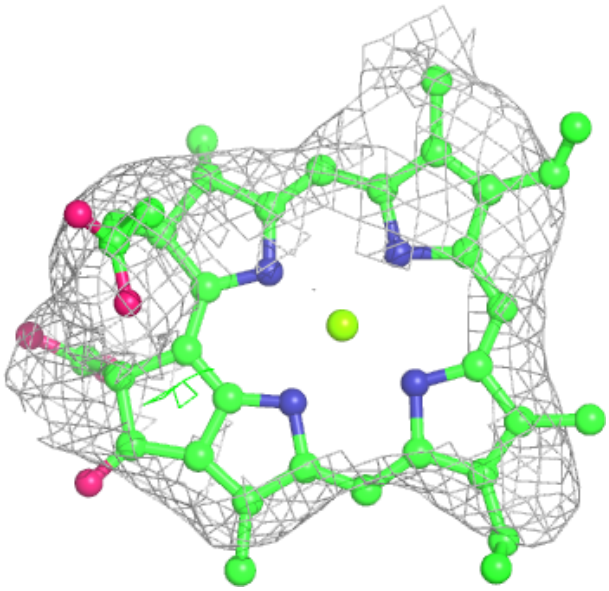


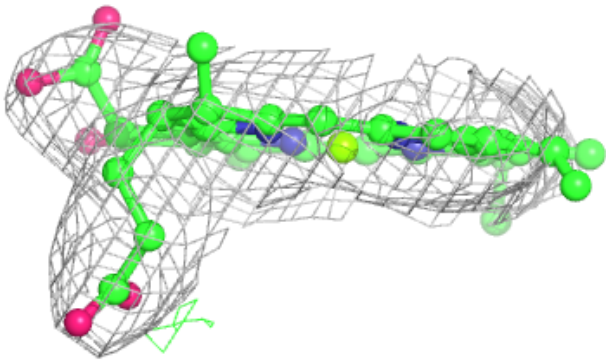


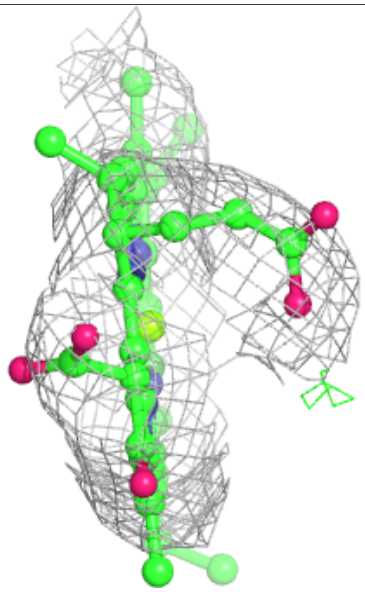


Electron density around CLA A 828:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

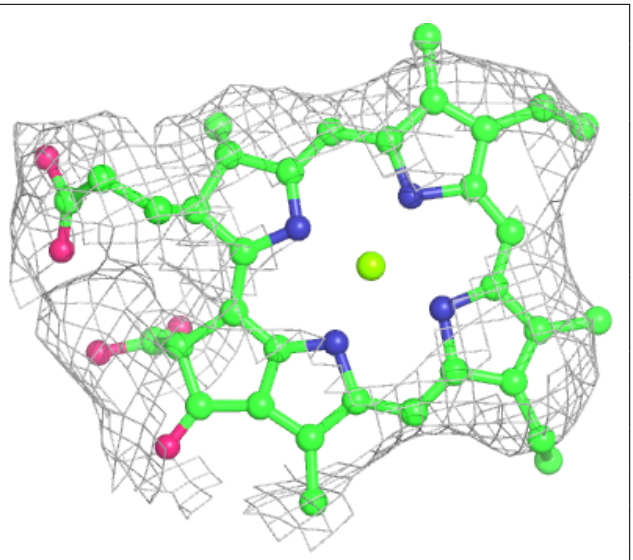


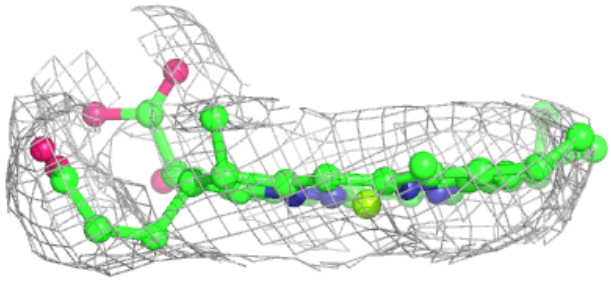


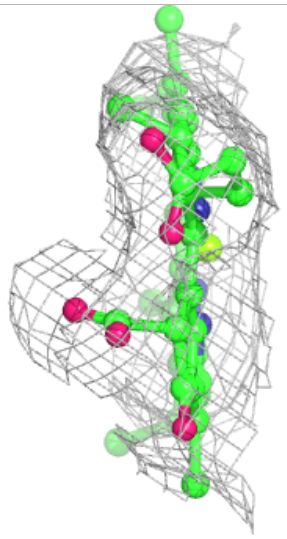


Electron density around CLA 7 1005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

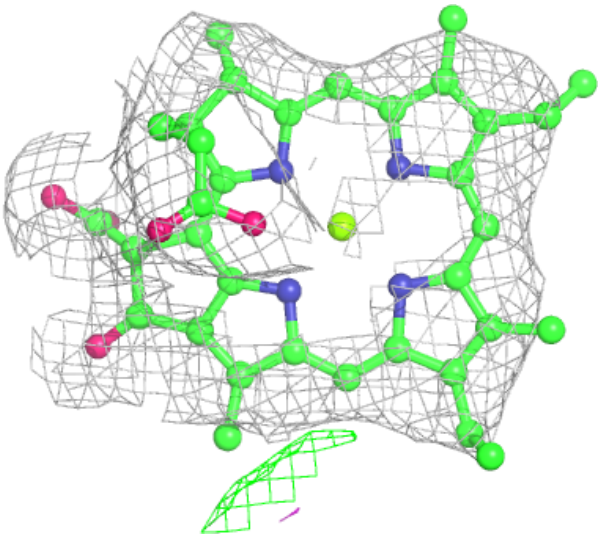


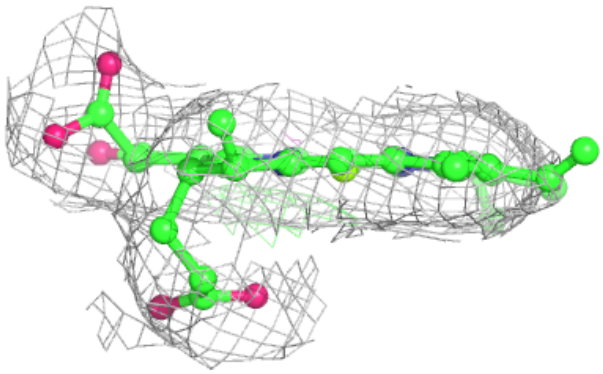


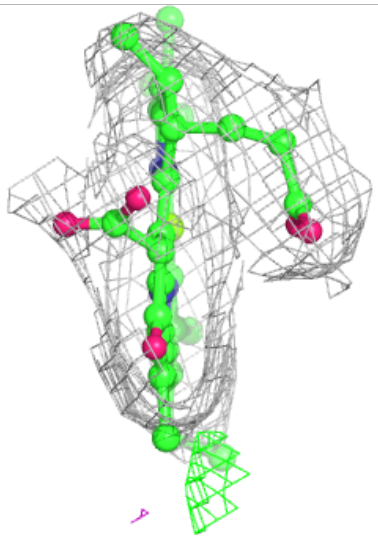


Electron density around CLA 7 1006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

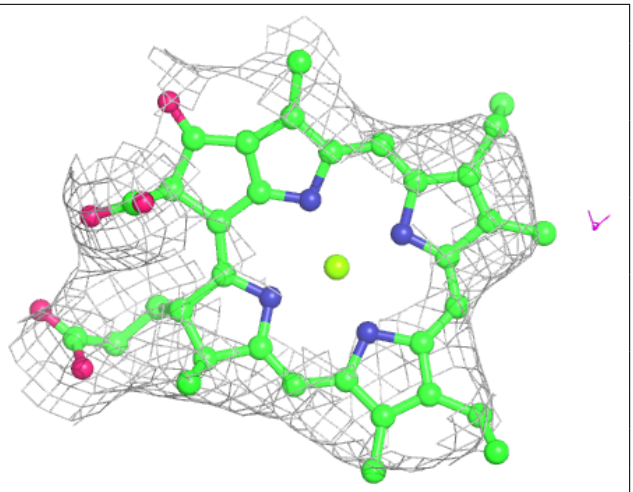


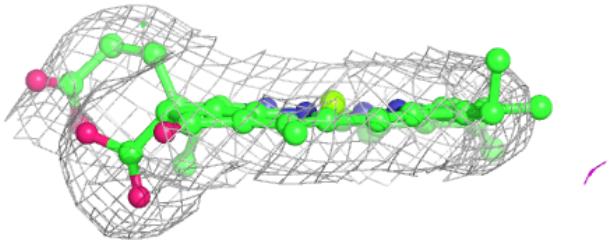


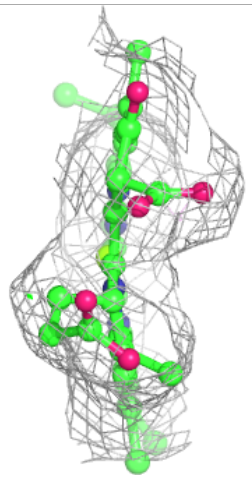


Electron density around CLA 7 1008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

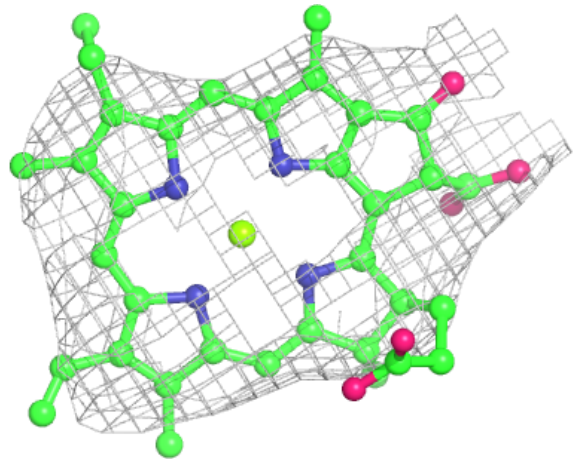


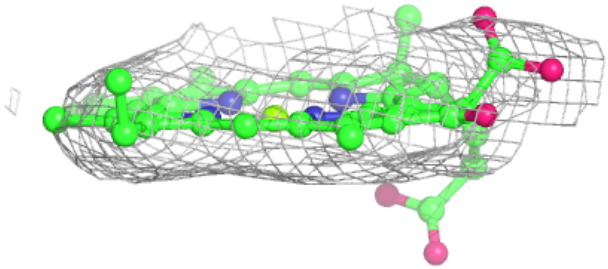


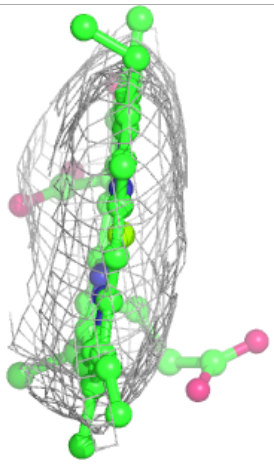


Electron density around CLA A 817:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

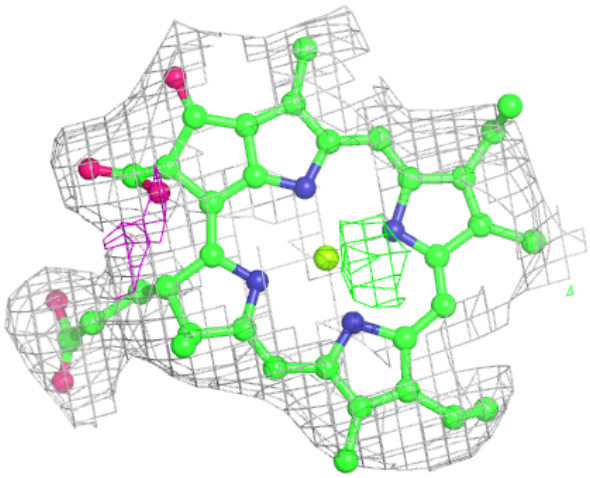


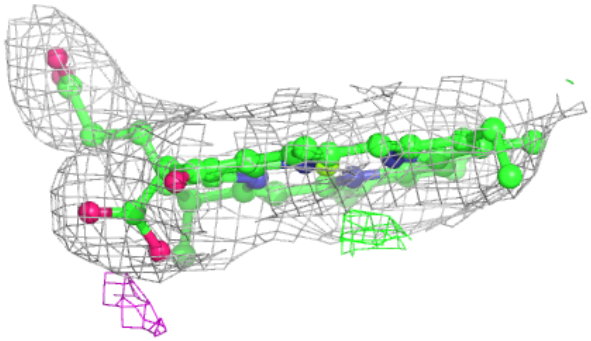


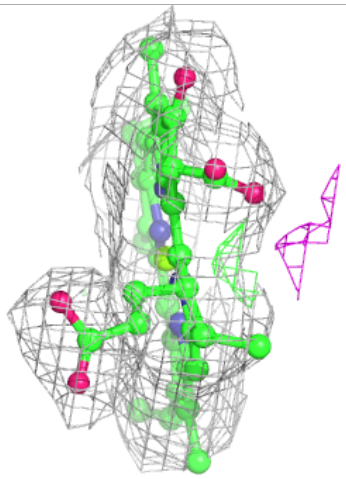


Electron density around CLA 5 321:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

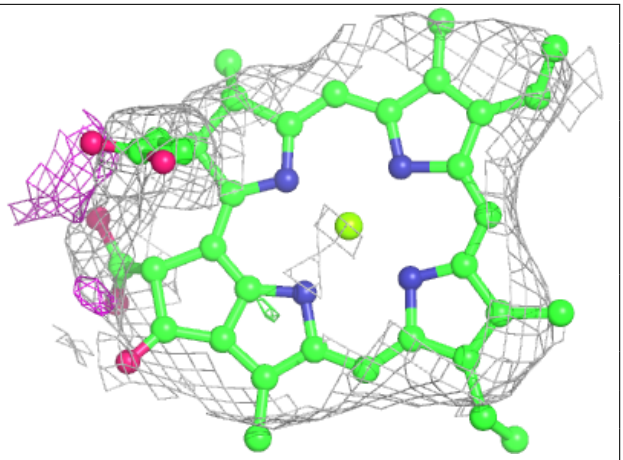


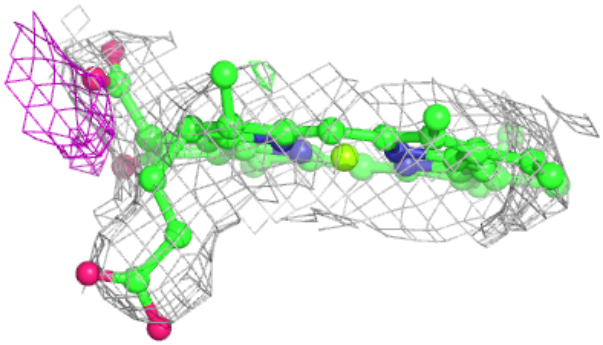


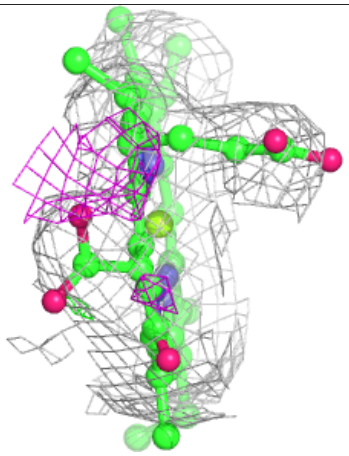


Electron density around CLA 7 1010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

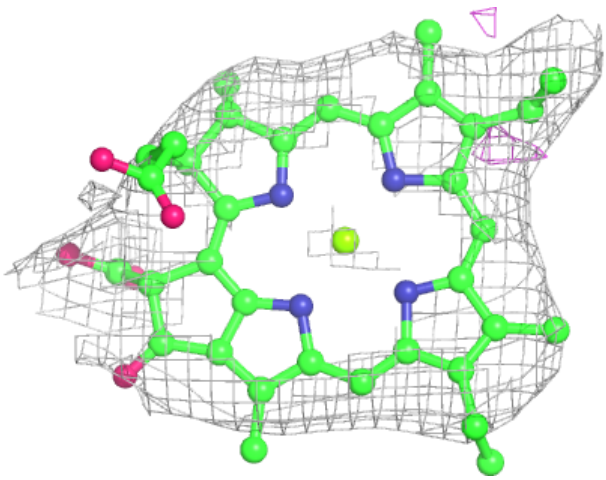


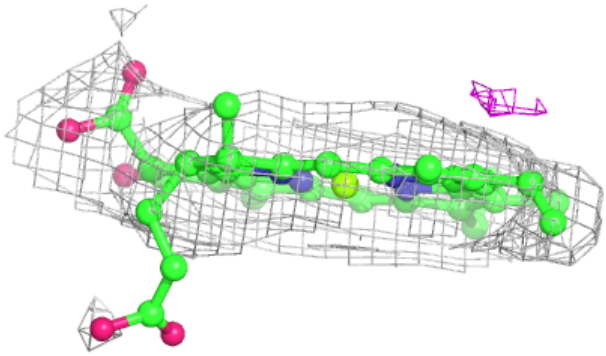


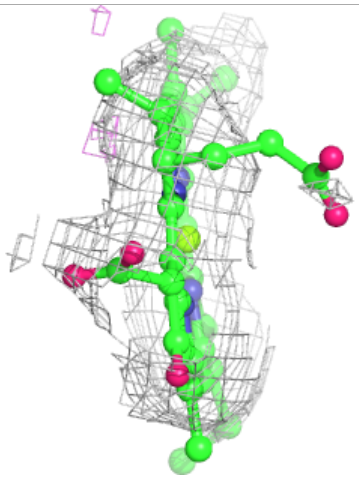


Electron density around CLA 7 1011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

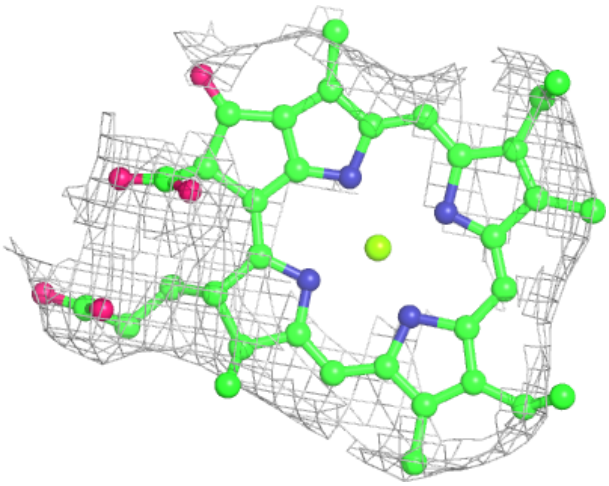


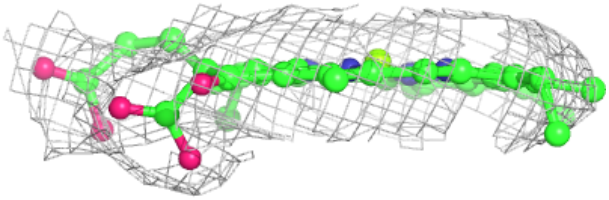


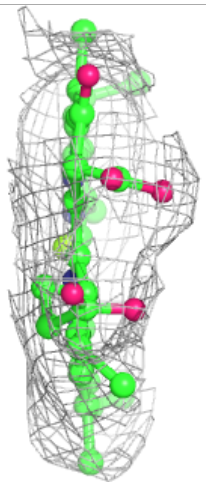


Electron density around CLA 4 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

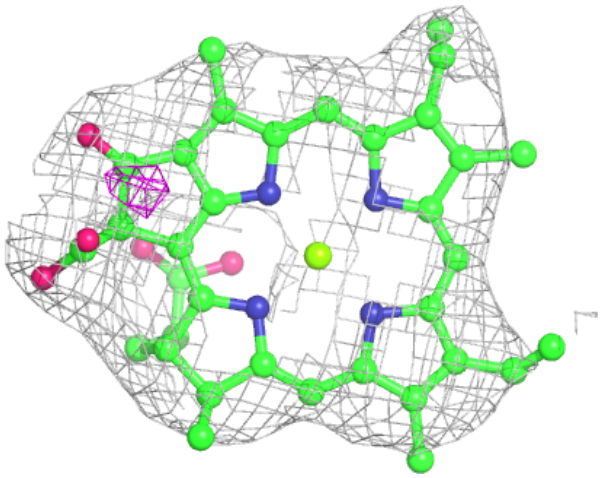


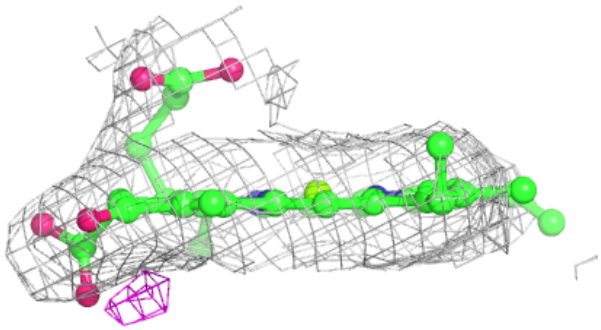


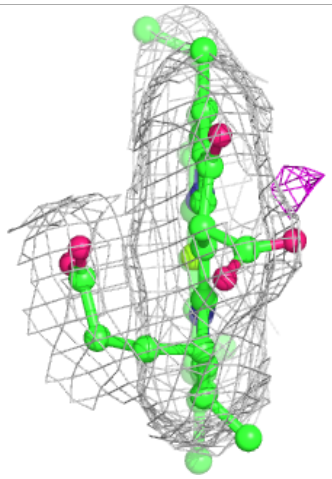


Electron density around CLA 4 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

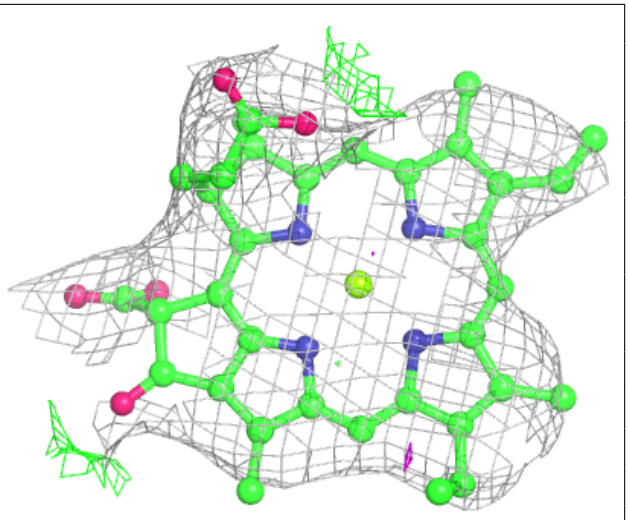


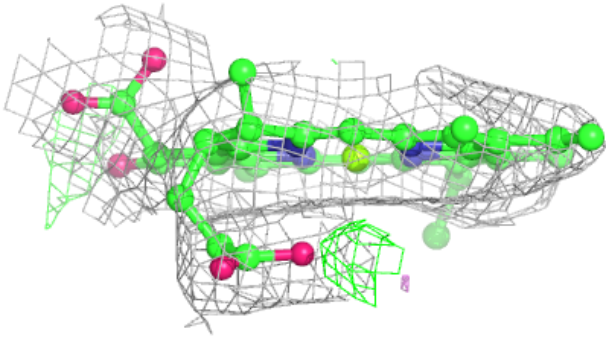


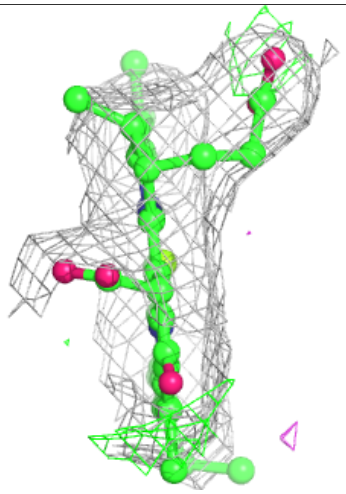


Electron density around CLA 4 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

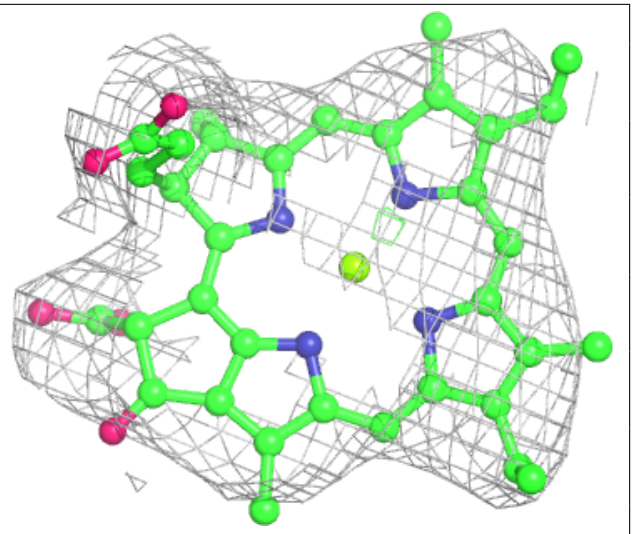


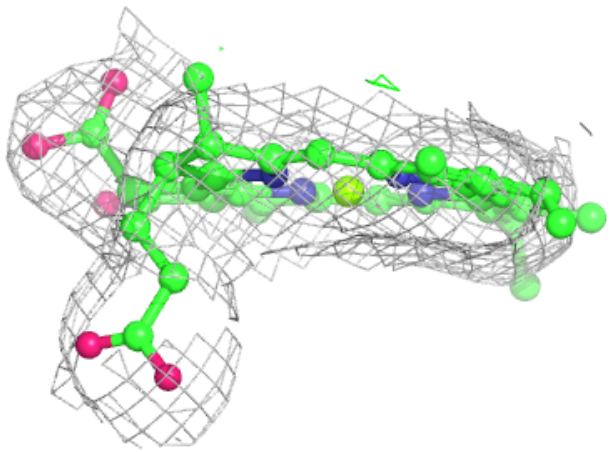




Electron density around CLA 7 1014:

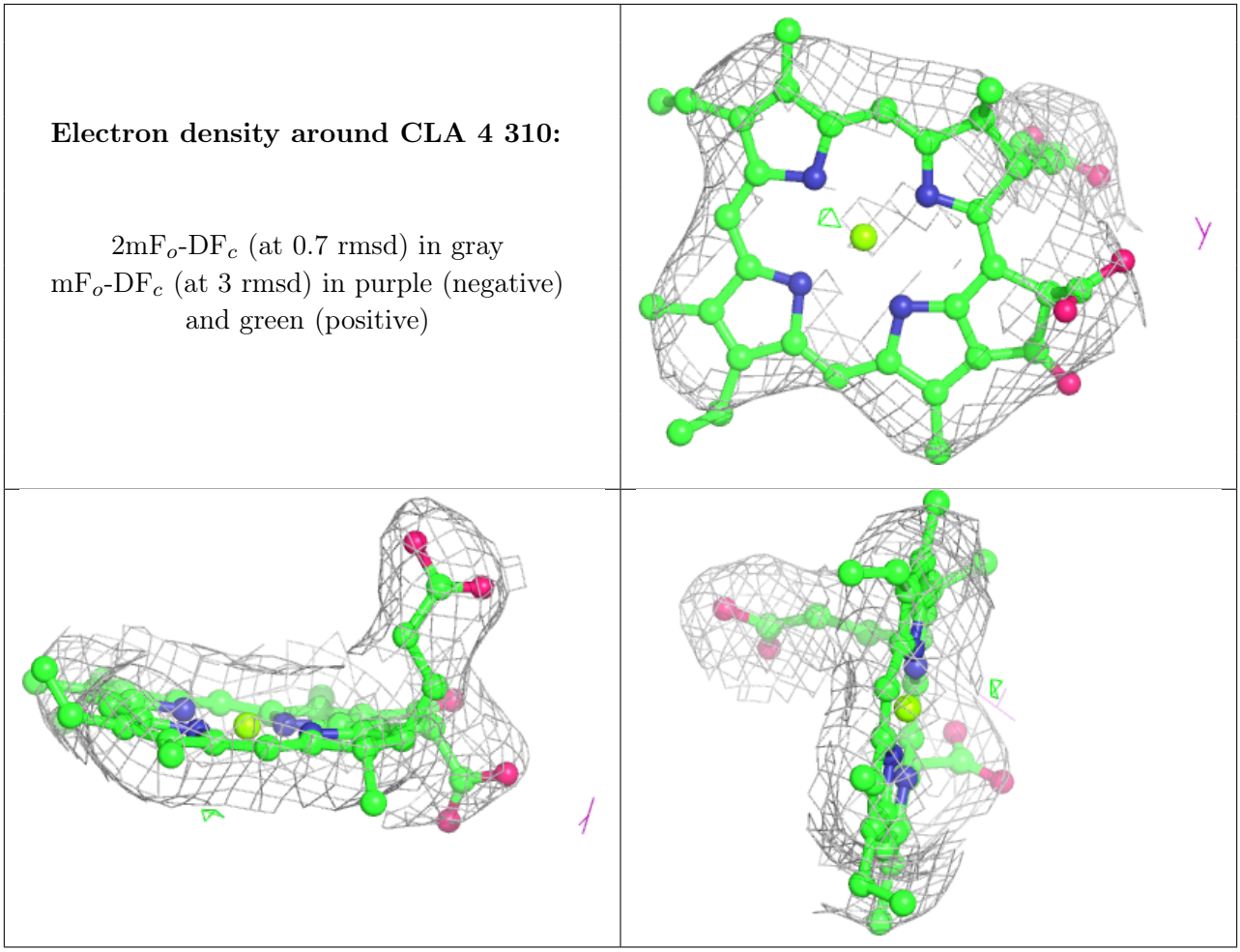
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





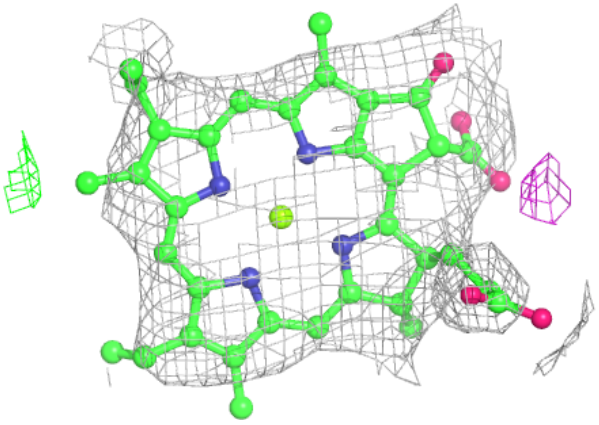
Electron density around CLA 4 310:

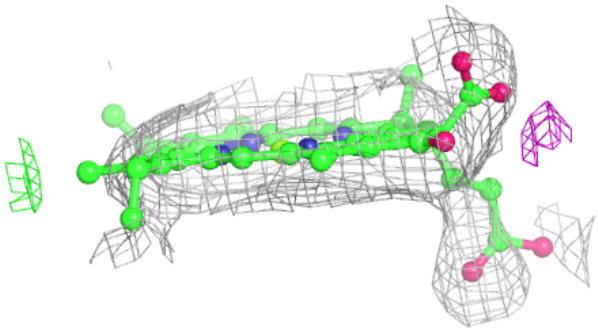
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

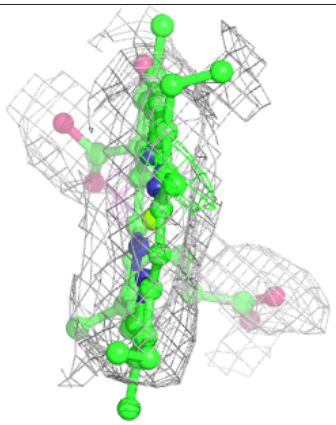


Electron density around CLA 4 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

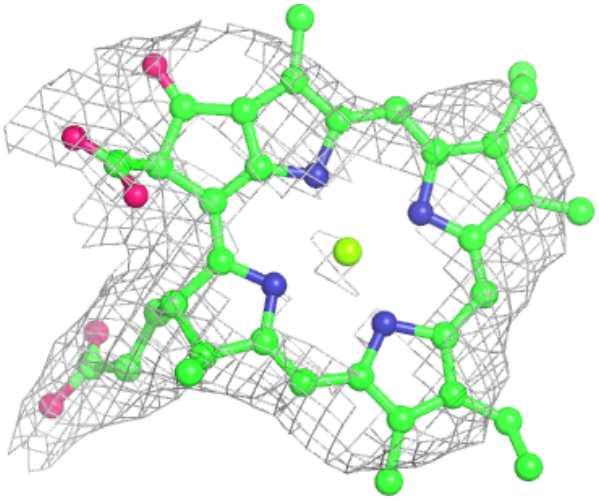


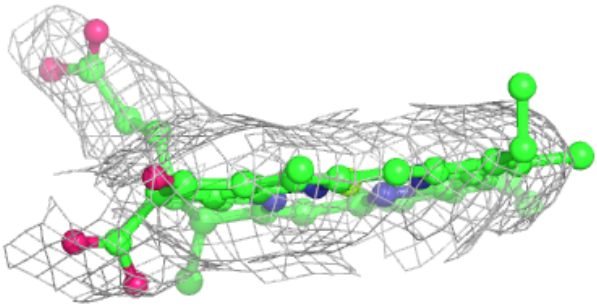


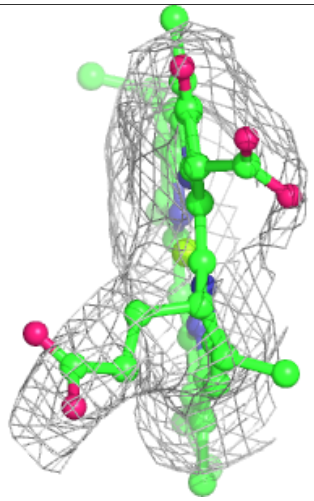


Electron density around CLA B 827:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

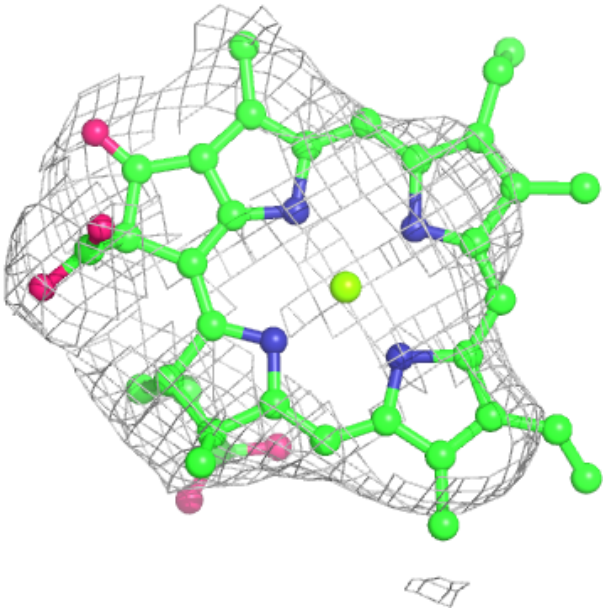


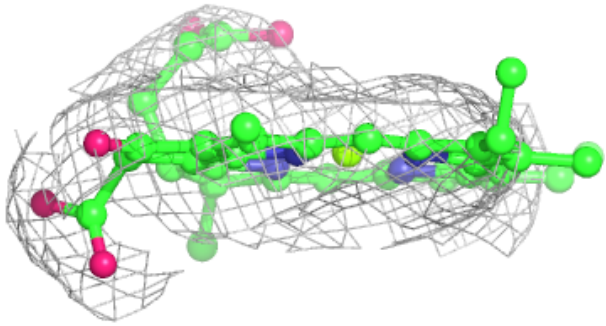


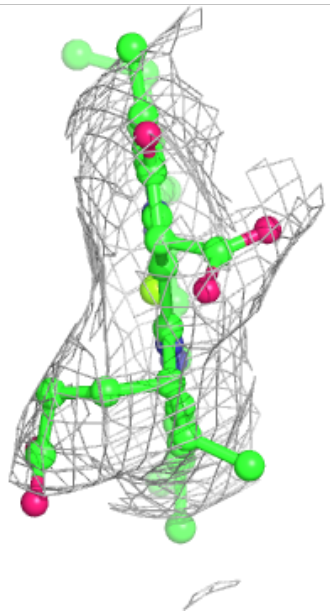


Electron density around CLA A 818:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

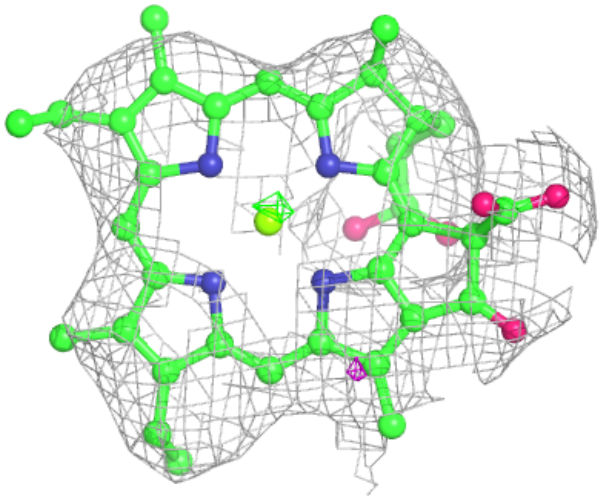


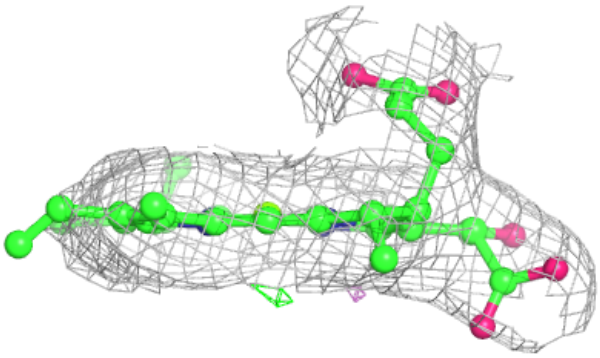


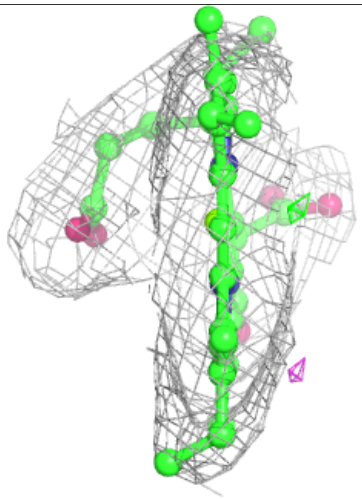


Electron density around CLA 6 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

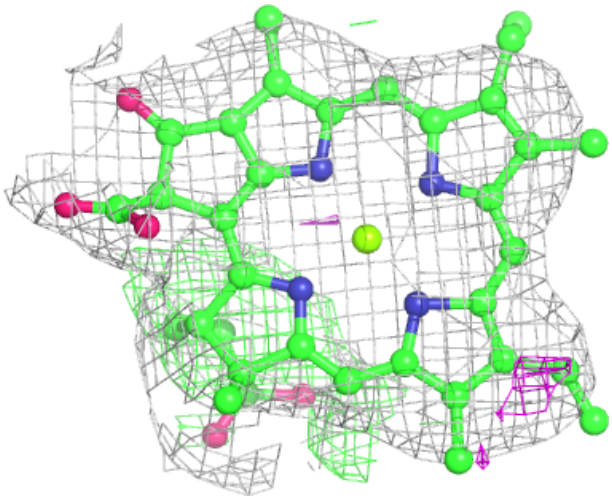


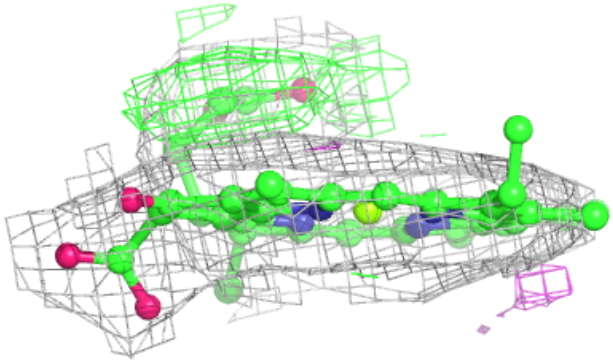


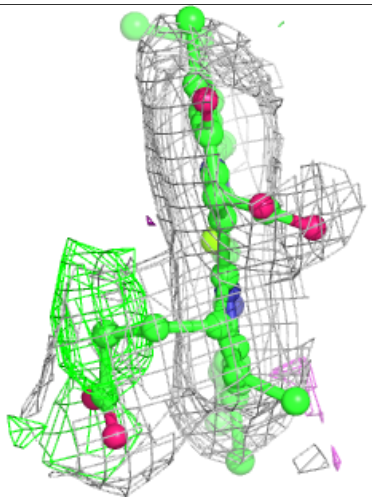


Electron density around CLA 6 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

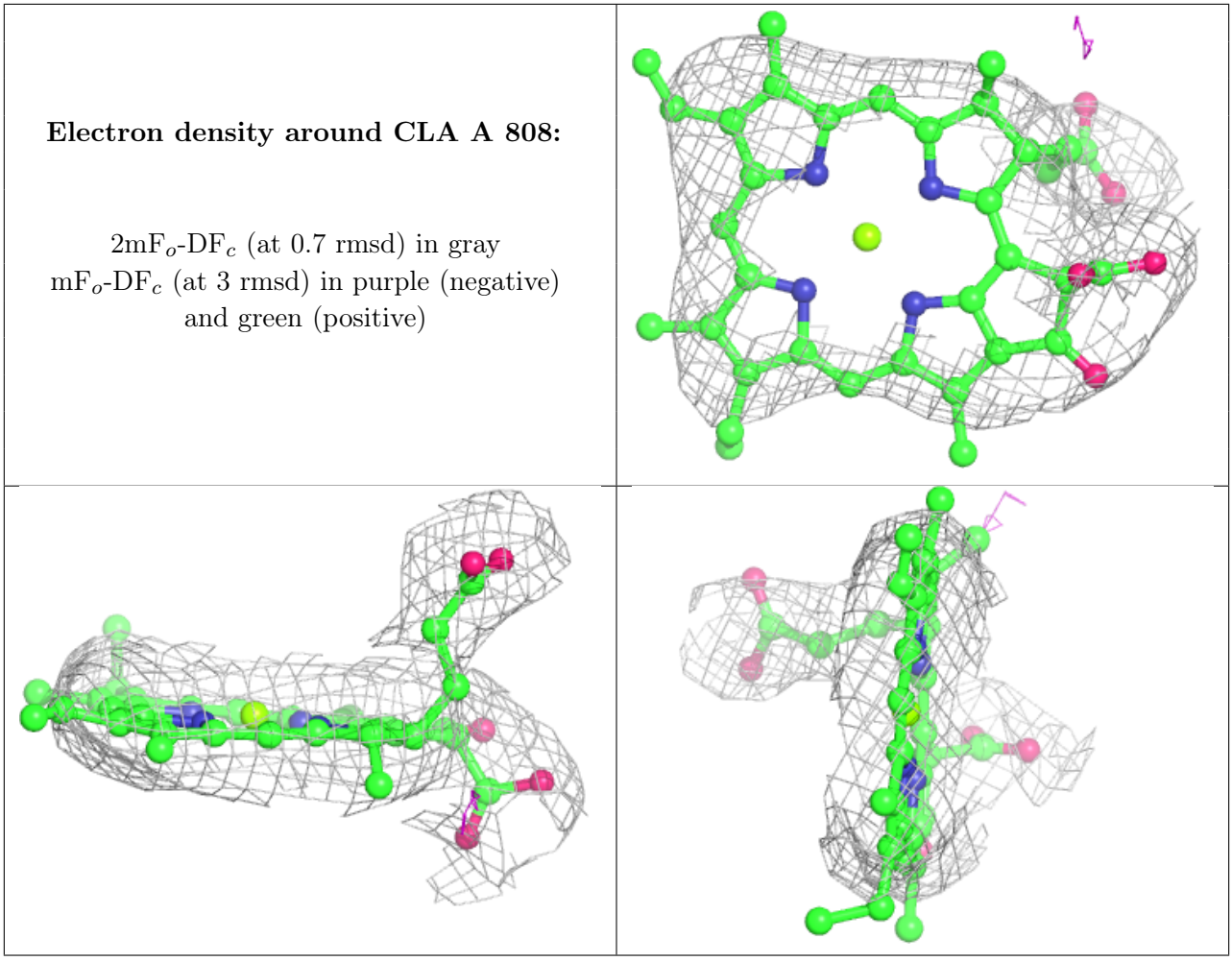






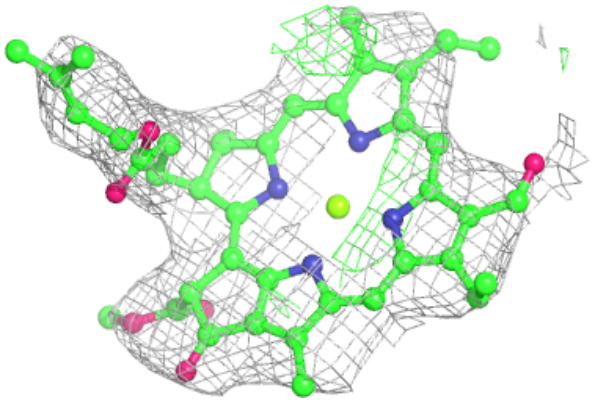
Electron density around CLA A 808:

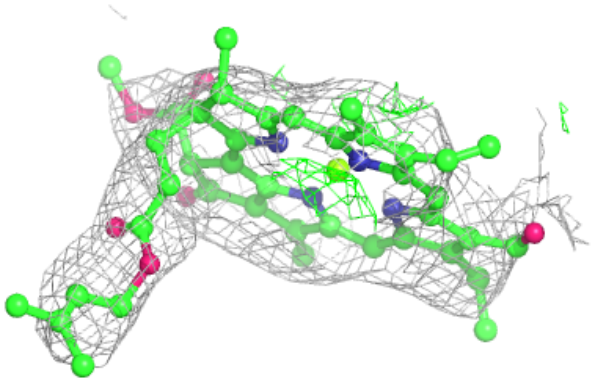
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

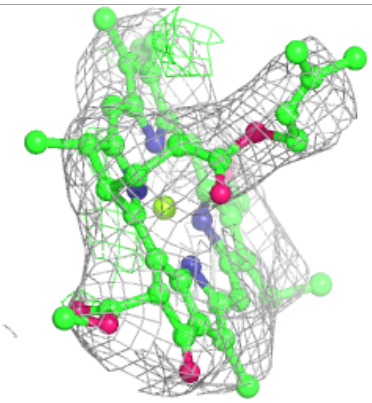


Electron density around CHL 4 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

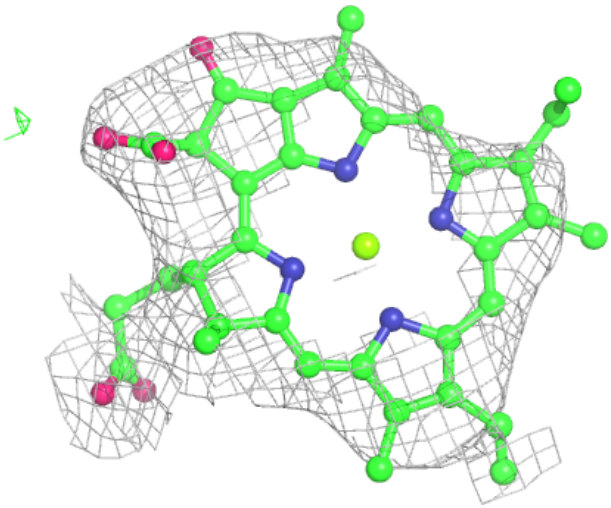


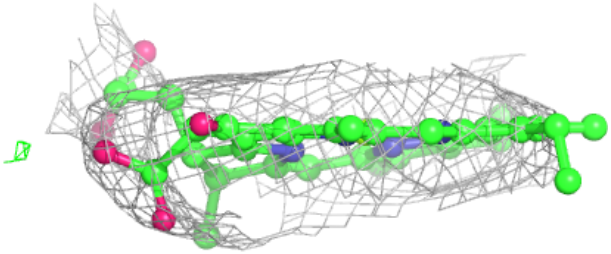


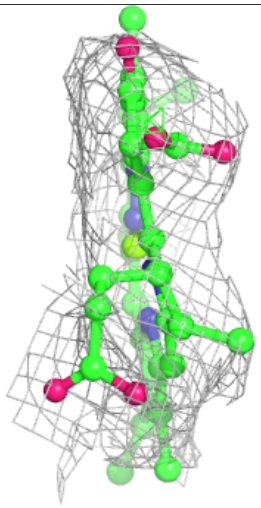


Electron density around CLA A 851:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

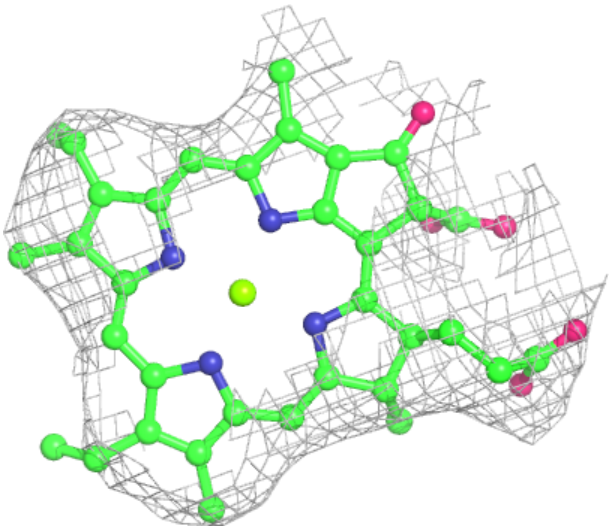


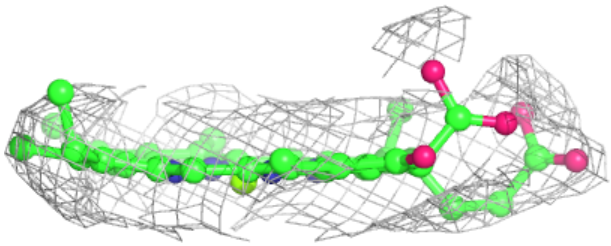


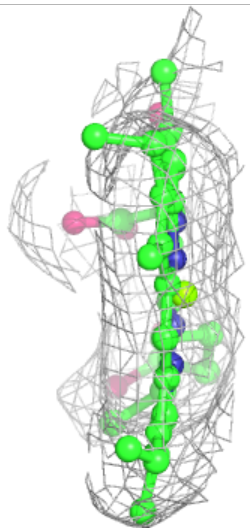


Electron density around CLA 8 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

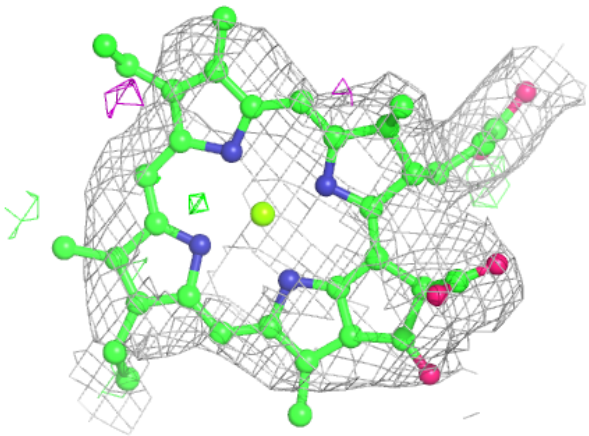


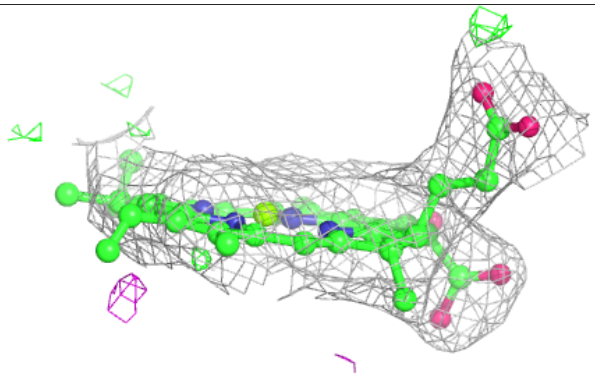


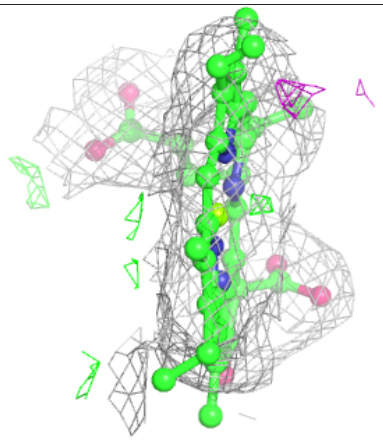


Electron density around CLA 6 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

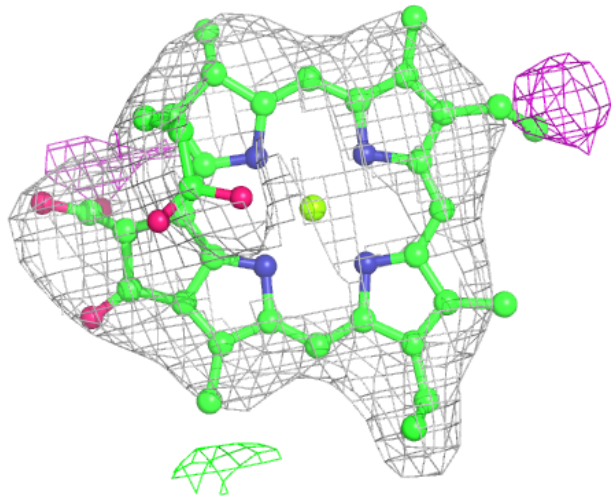


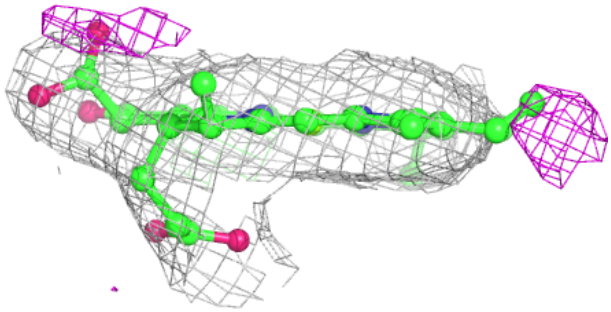


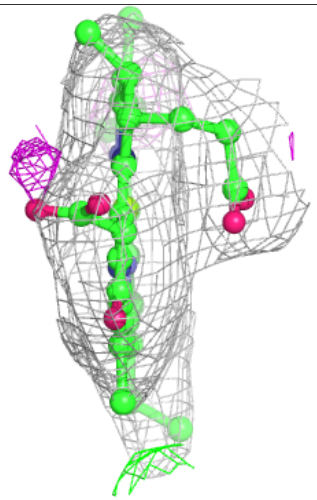


Electron density around CLA 8 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

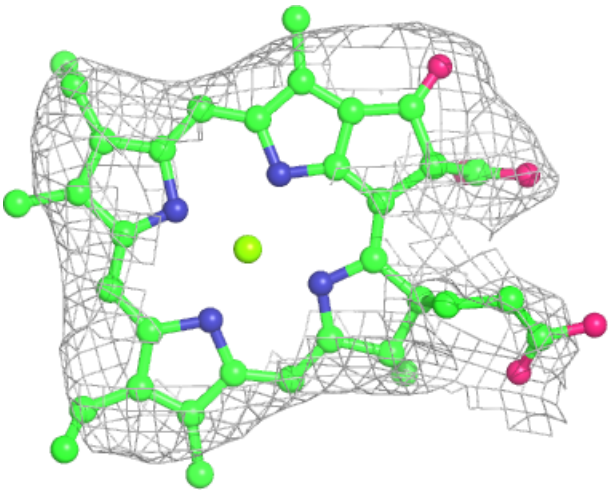


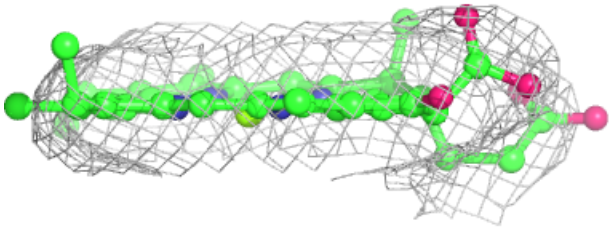


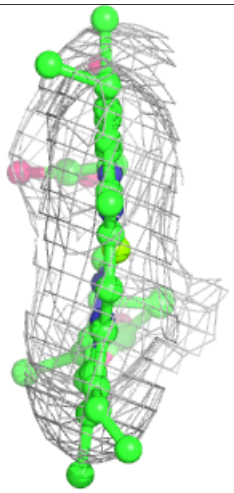


Electron density around CLA A 805:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

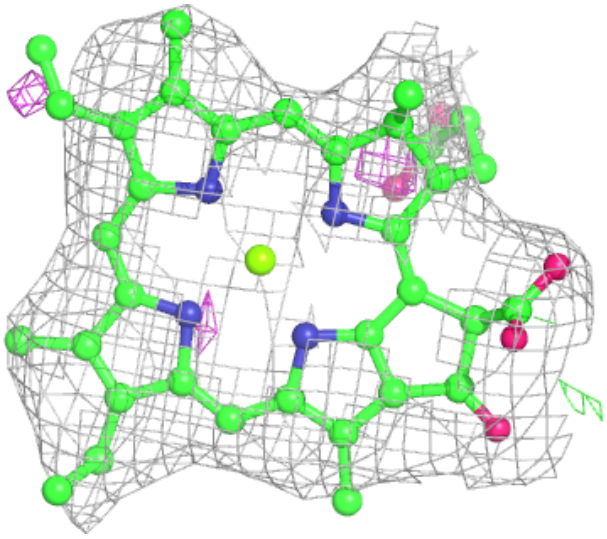


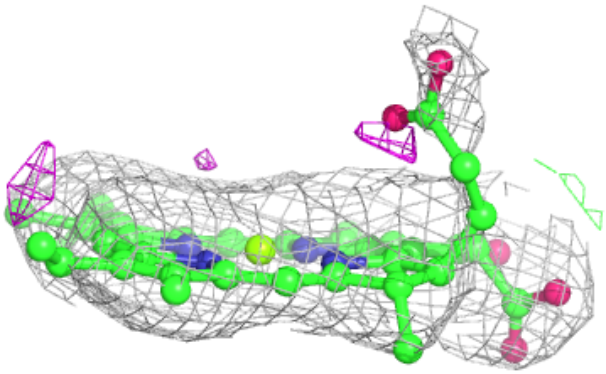


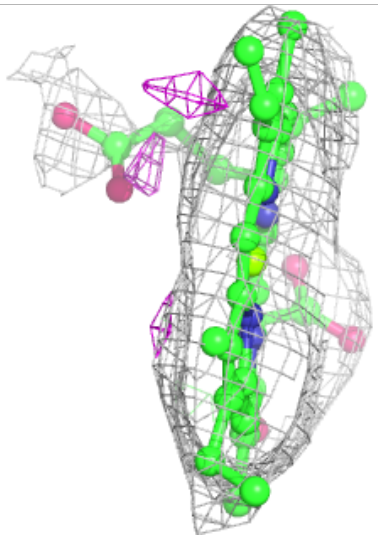


Electron density around CLA 8 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

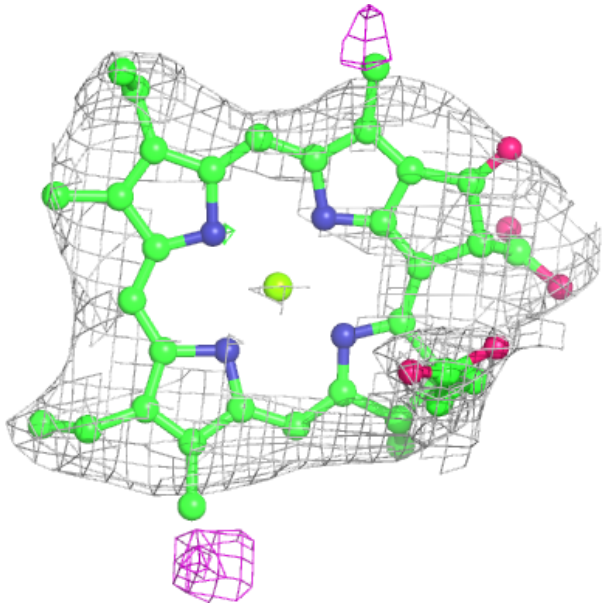


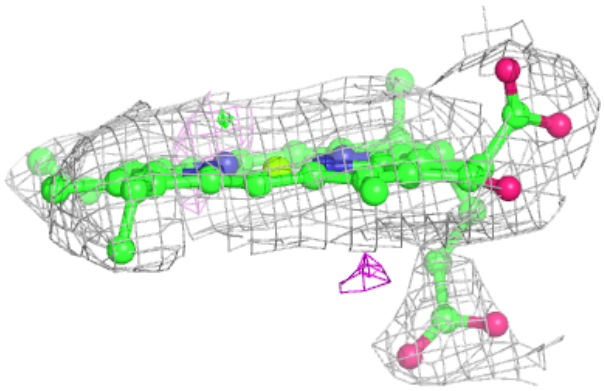


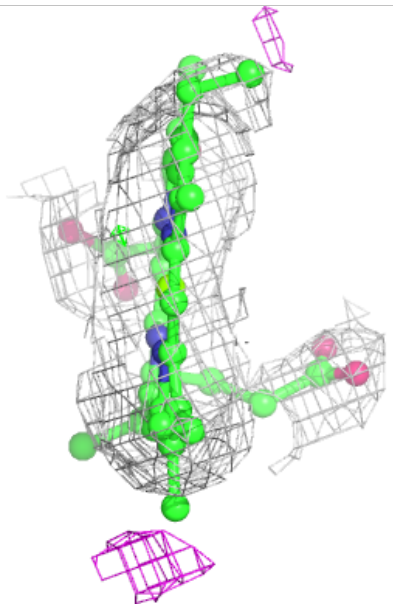


Electron density around CLA 5 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

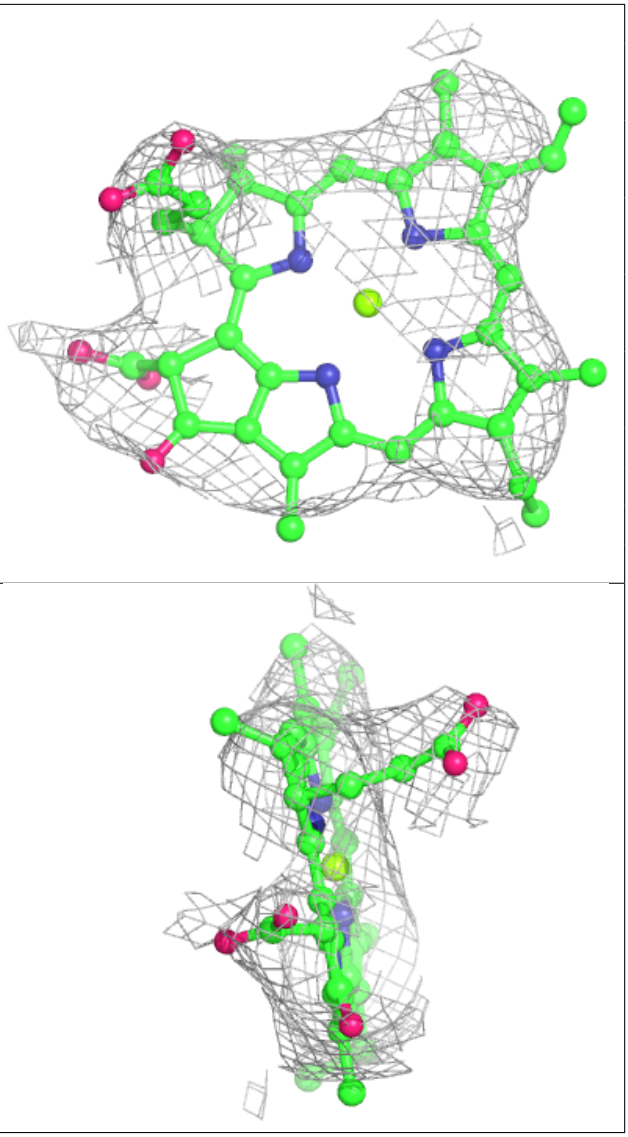






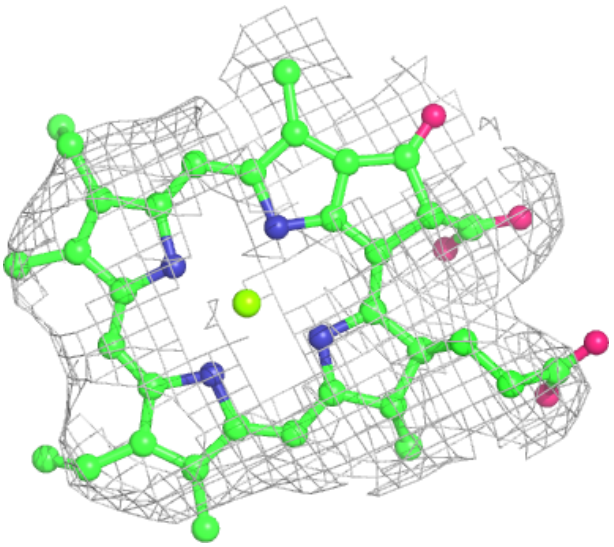
Electron density around CLA 3 1015:

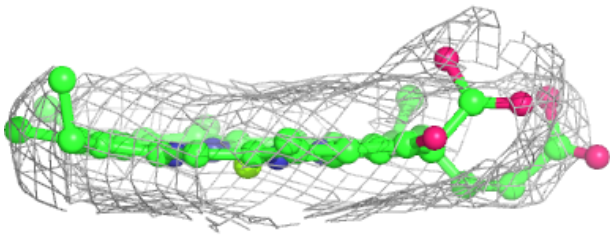
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

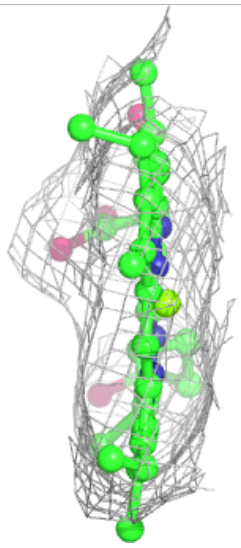


Electron density around CLA 5 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

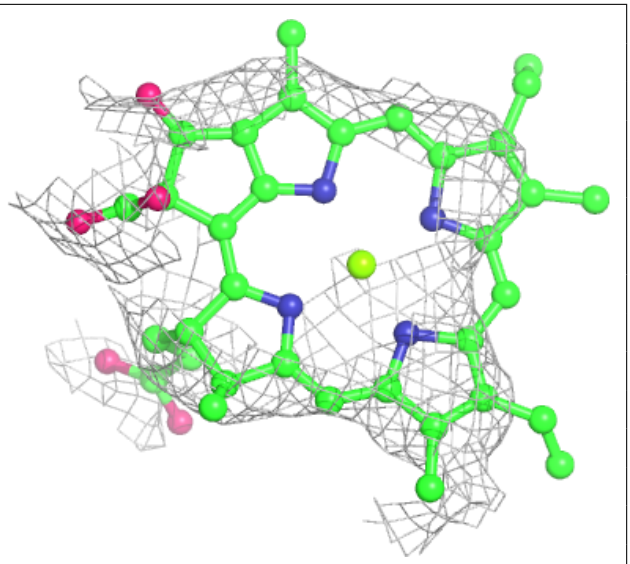


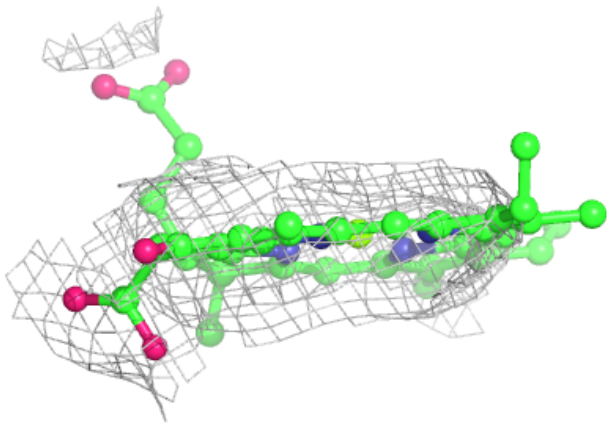


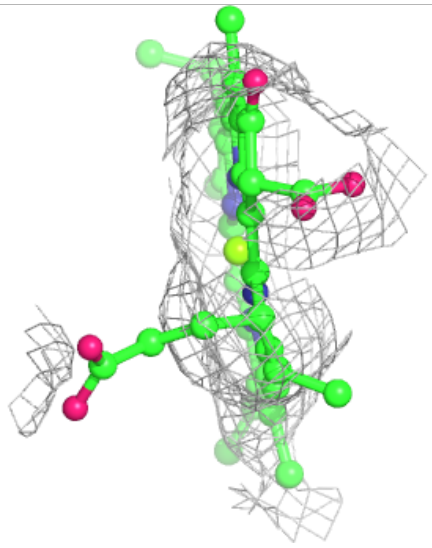


Electron density around CLA B 832:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

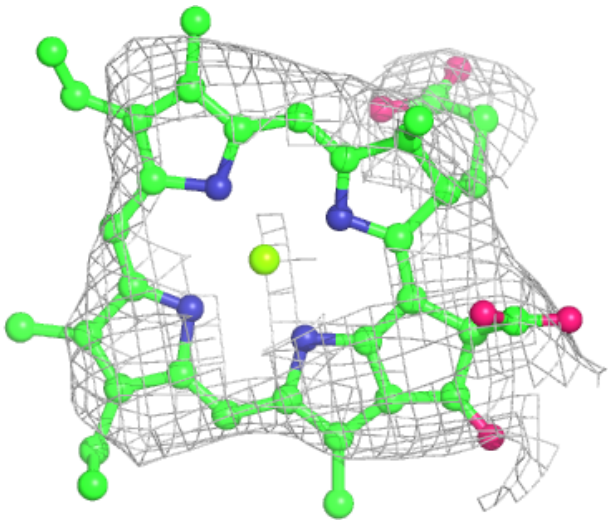


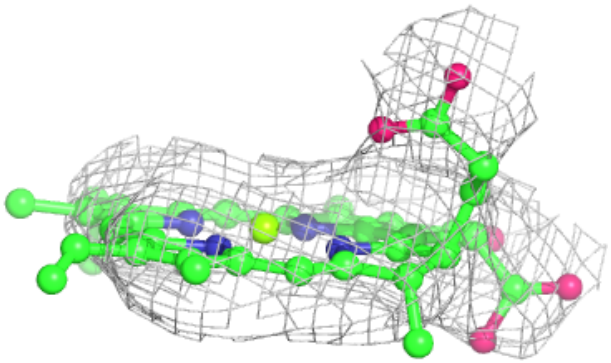


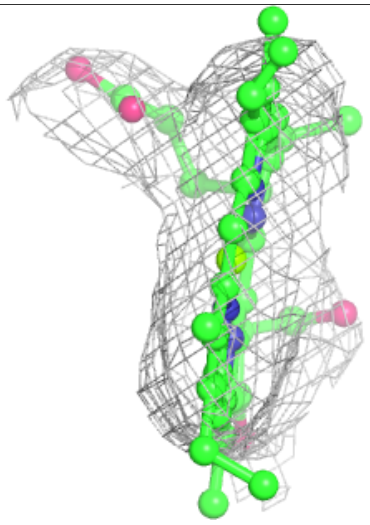


Electron density around CLA A 807:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

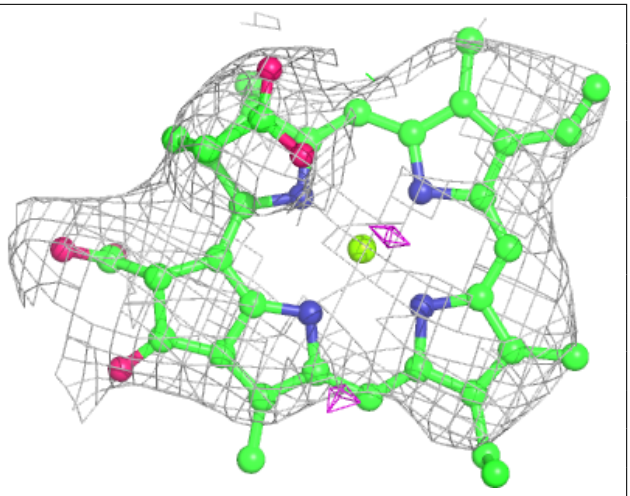


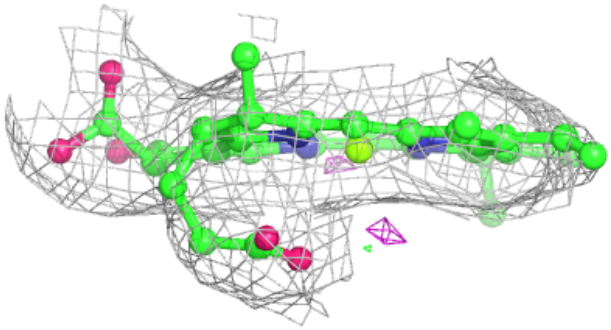


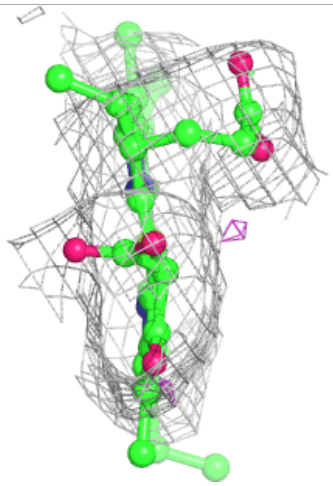


Electron density around CLA 4 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

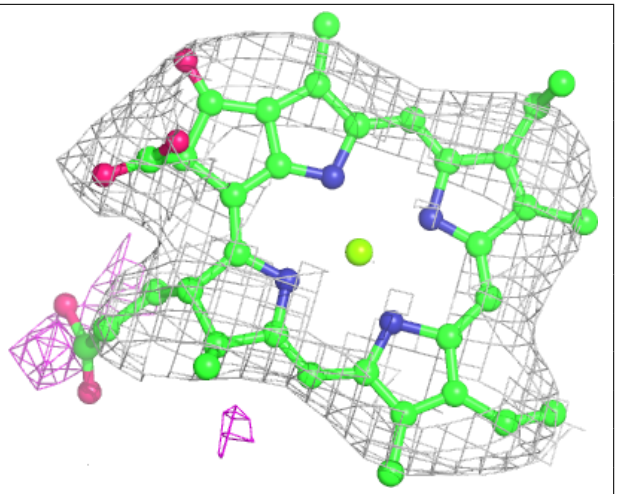


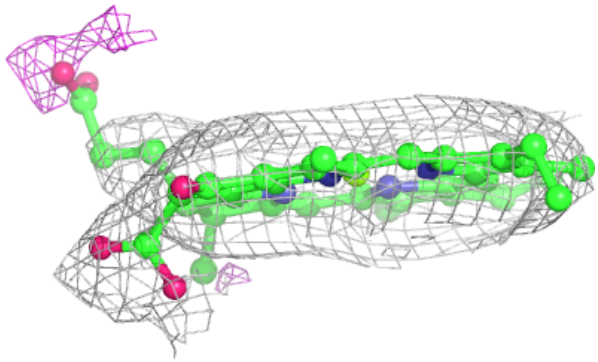


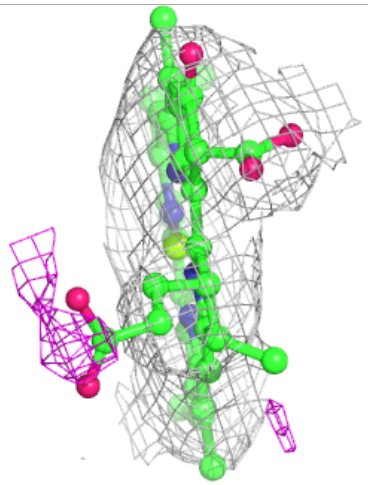


Electron density around CLA A 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

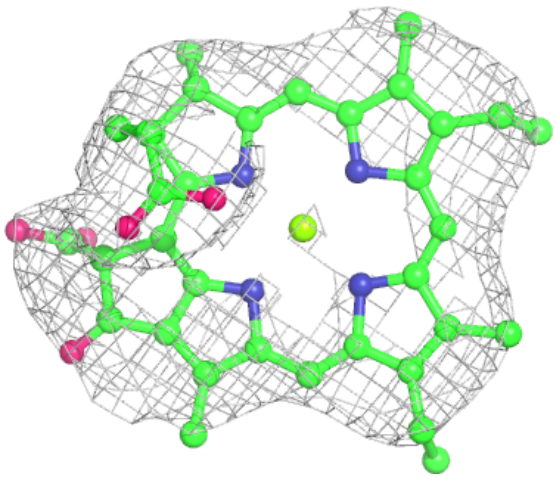


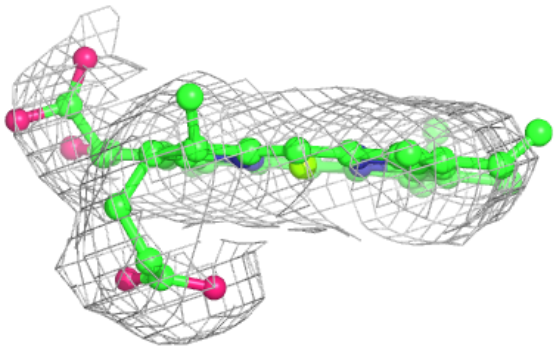


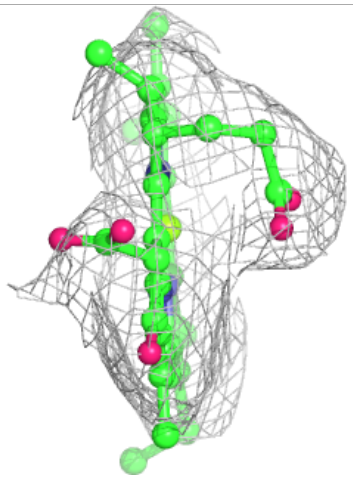


Electron density around CLA A 839:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

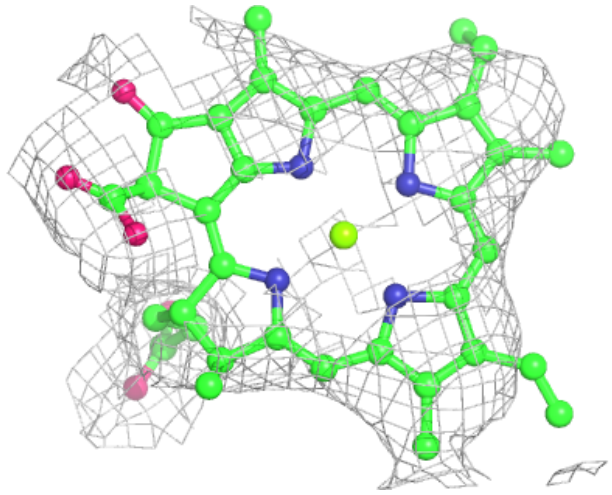


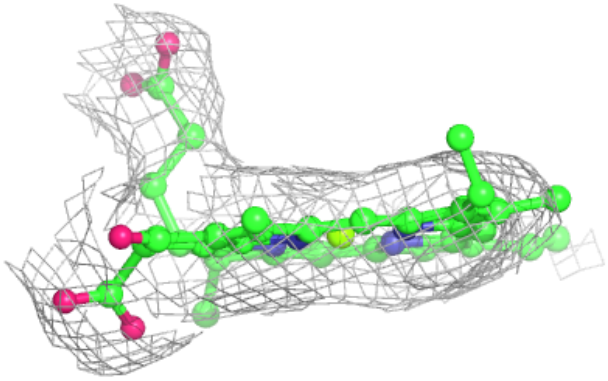


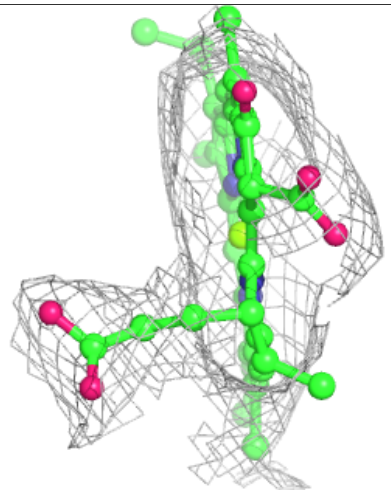


Electron density around CLA A 829:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

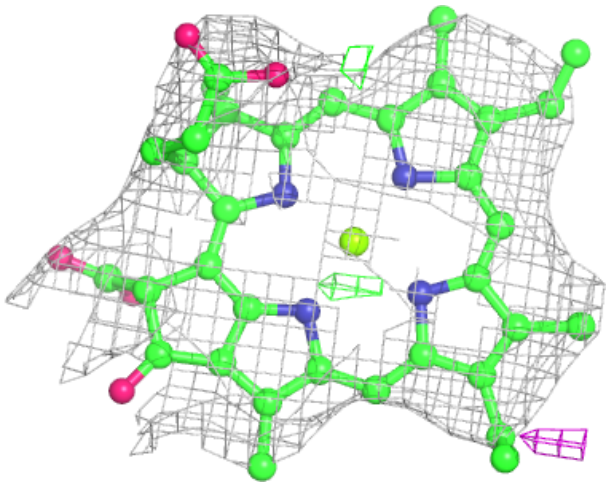


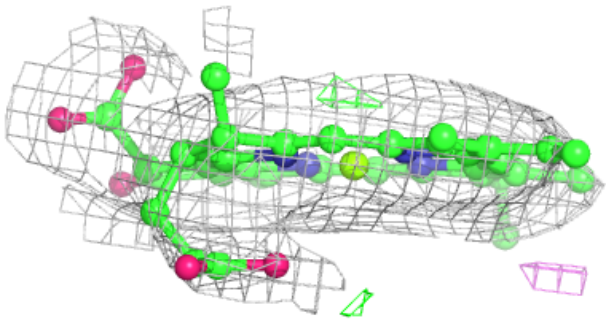


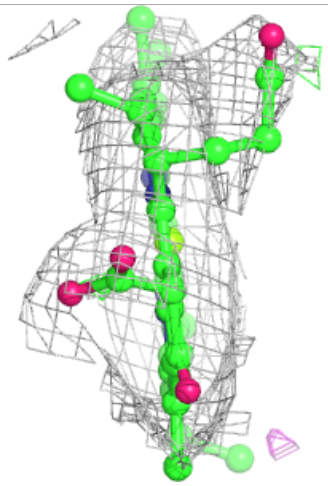


Electron density around CLA 1 1006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

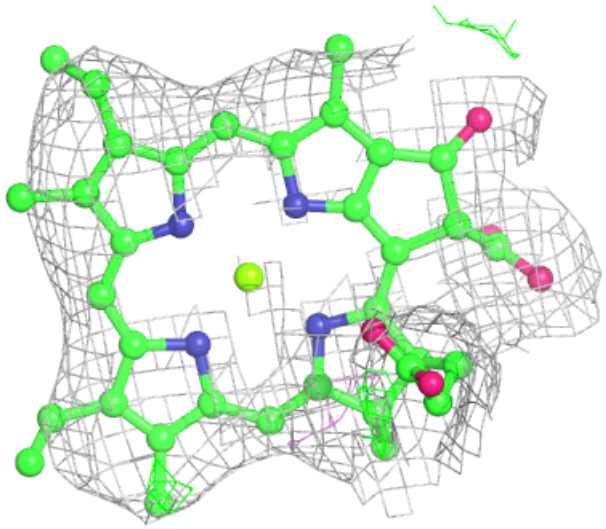


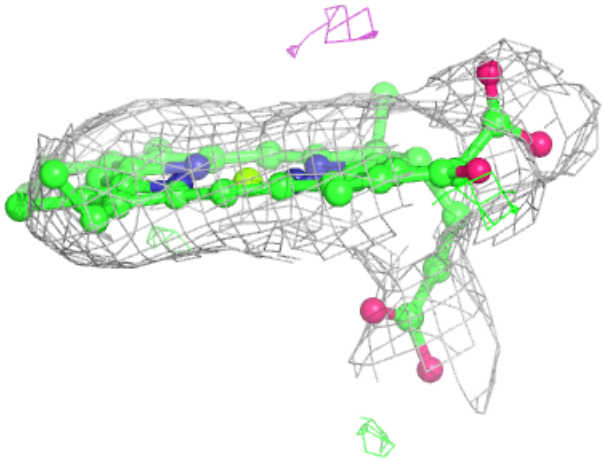


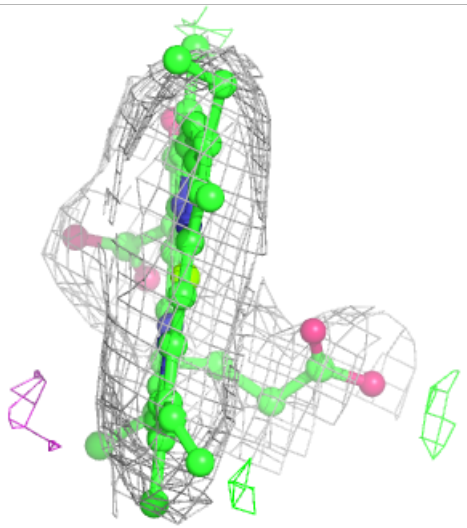


Electron density around CLA 4 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

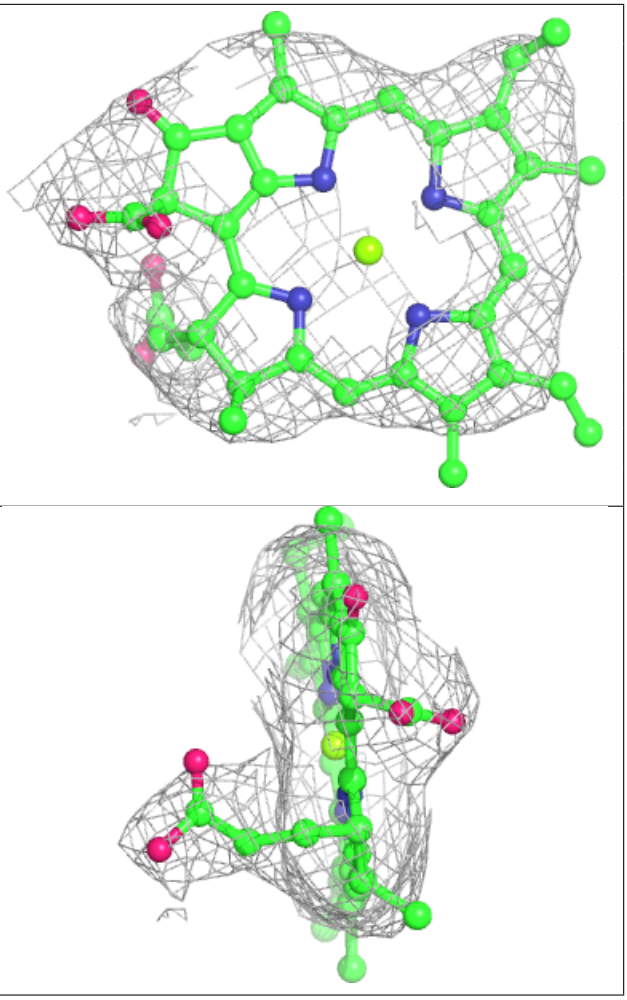






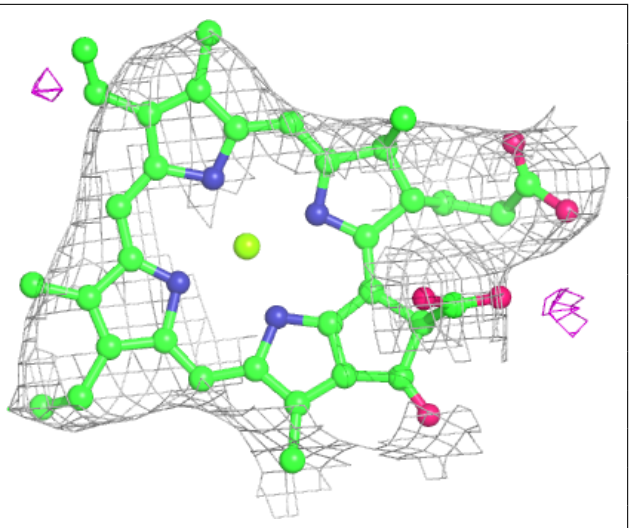
Electron density around CLA A 806:

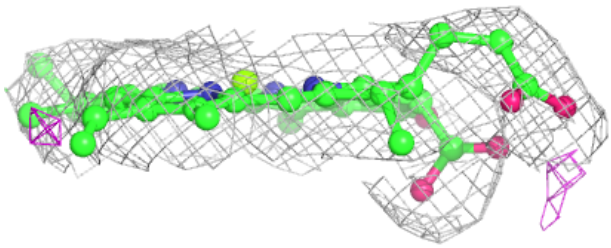
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

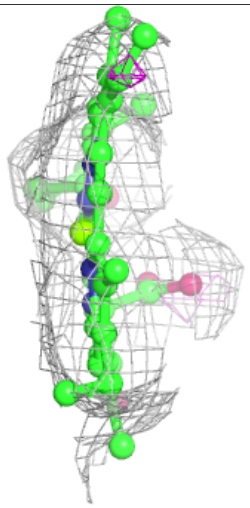


Electron density around CLA 8 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

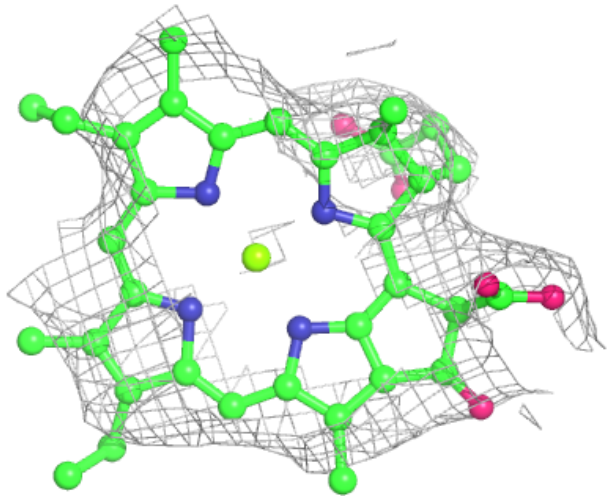


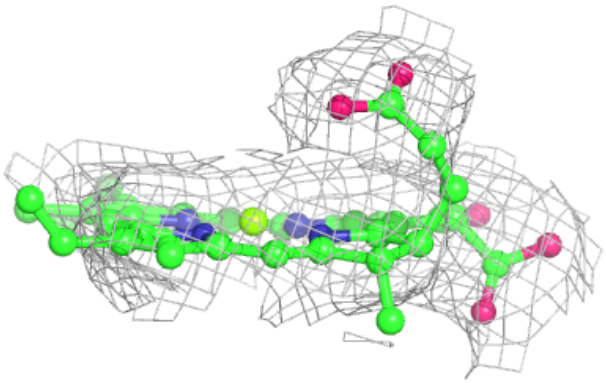


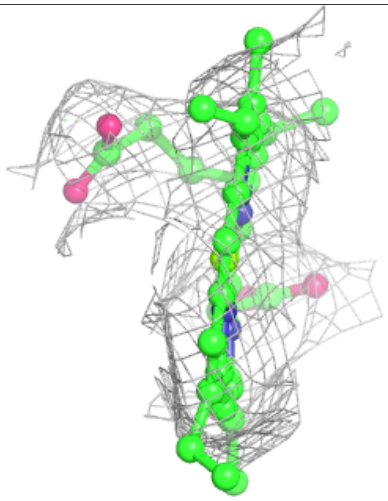


Electron density around CLA 3 1005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

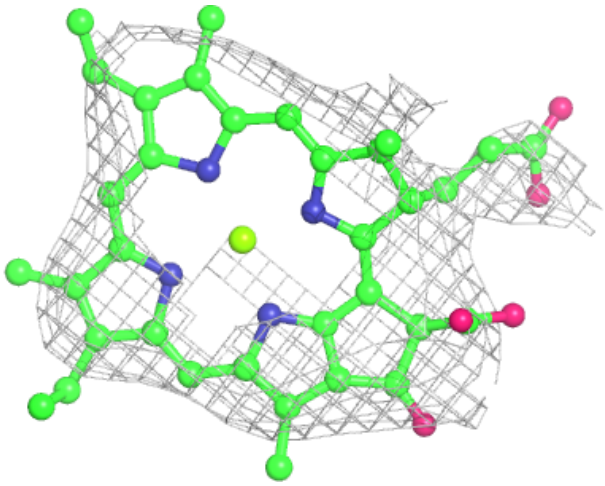


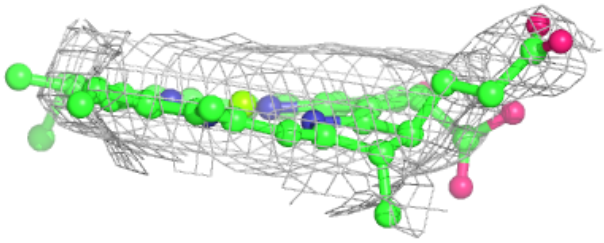


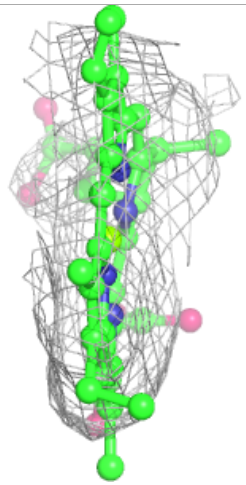


Electron density around CLA B 805:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

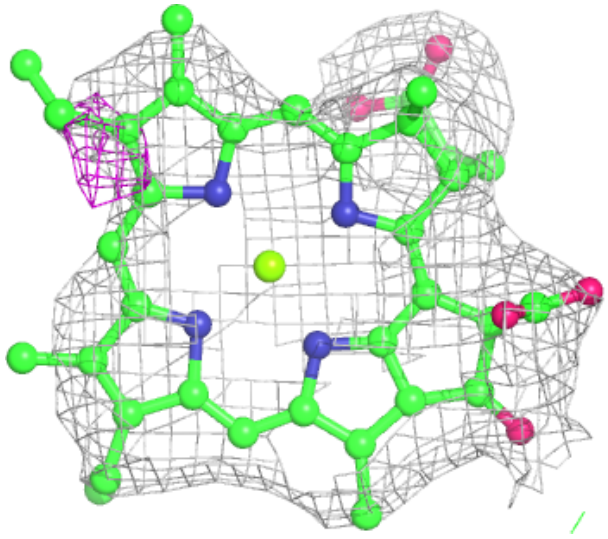


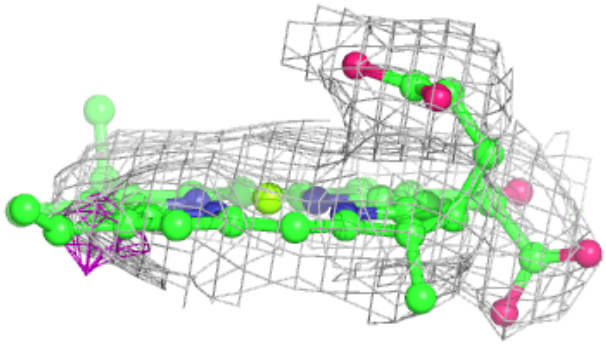


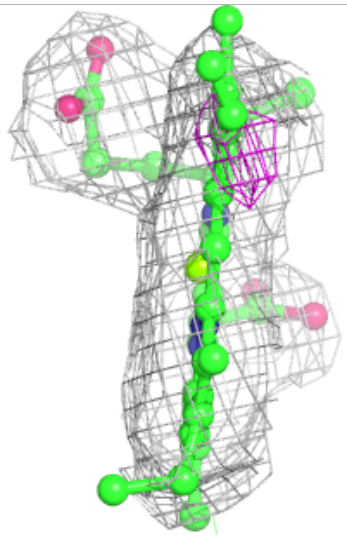


Electron density around CLA 5 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

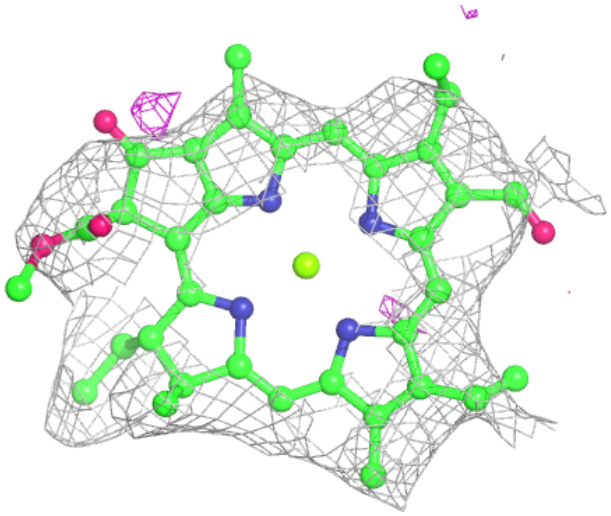


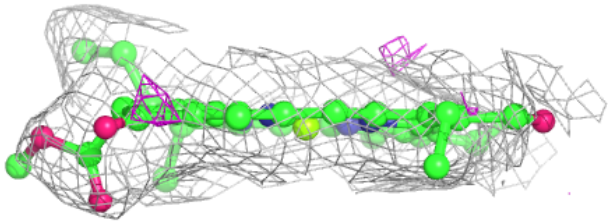


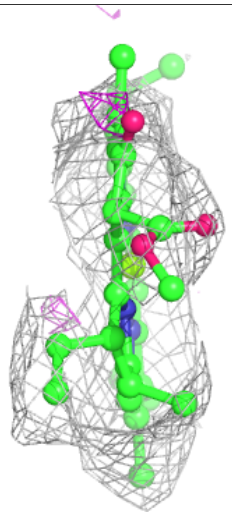


Electron density around CHL 5 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

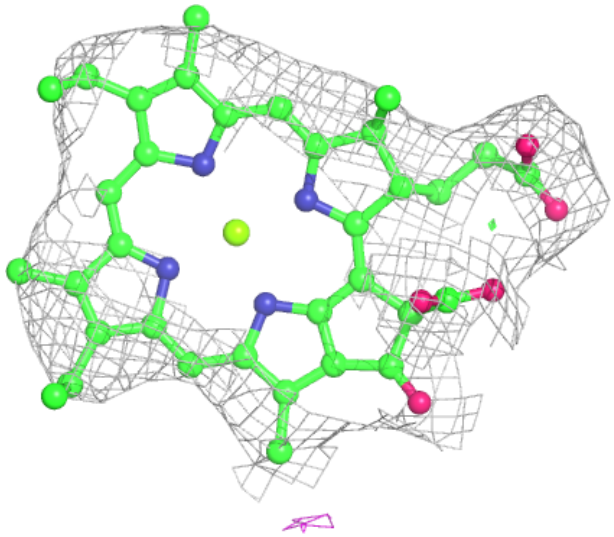


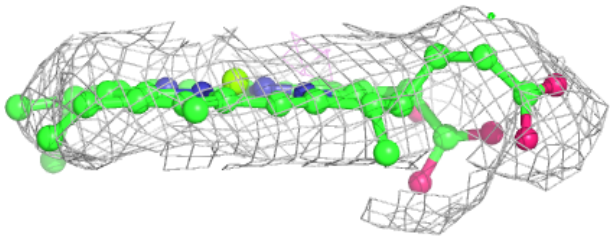


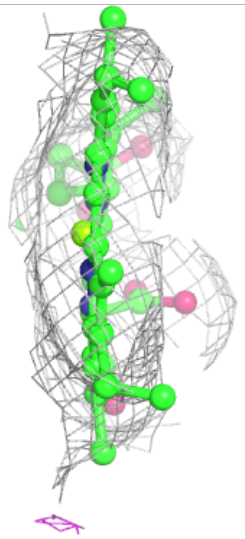


Electron density around CLA 6 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

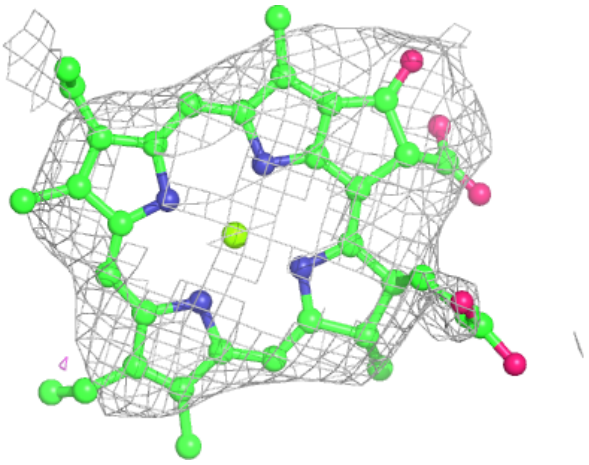


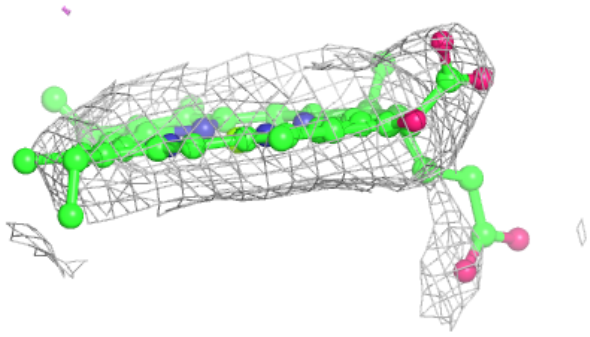


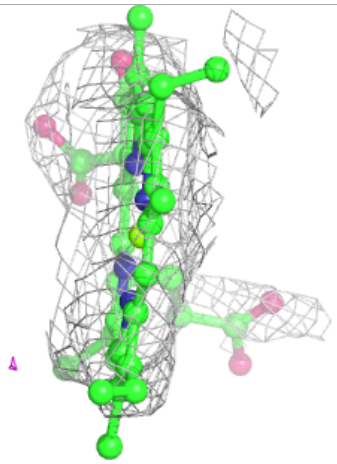


Electron density around CLA 1 1011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

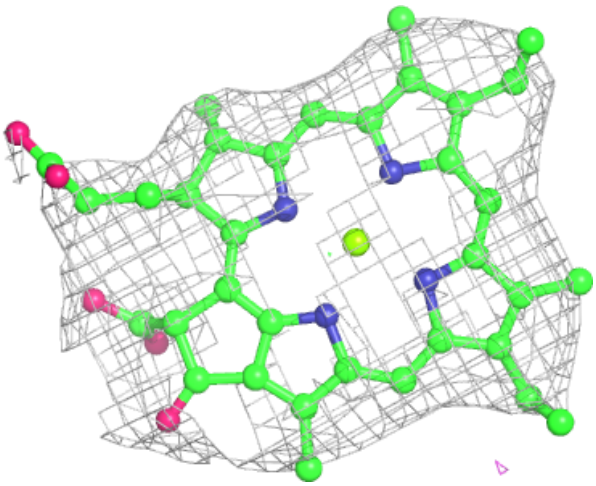


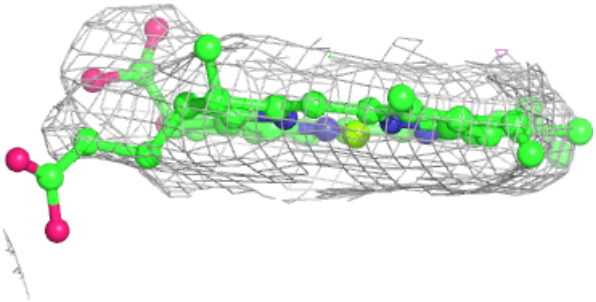


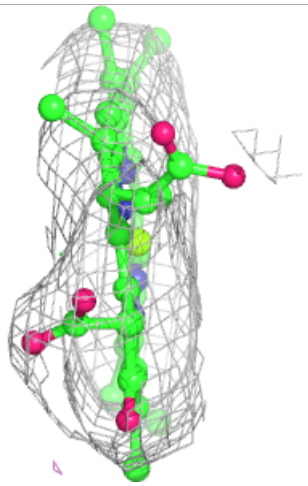


Electron density around CLA 3 1016:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

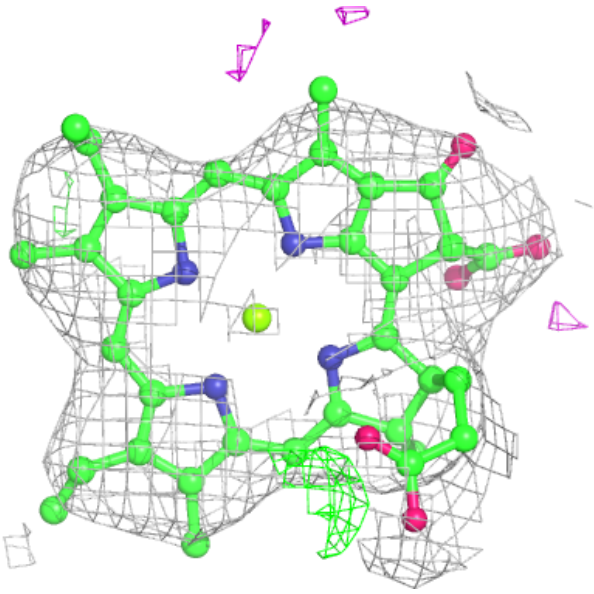


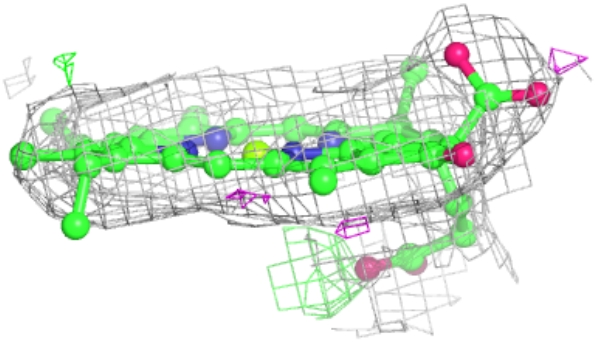


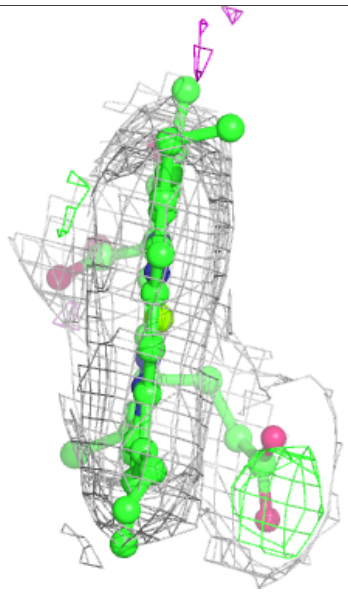


Electron density around CLA 7 1007:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

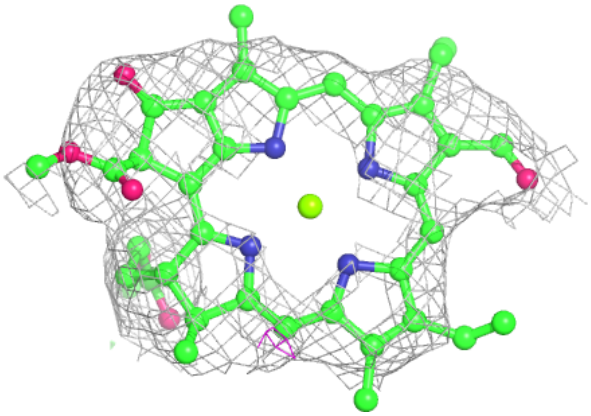


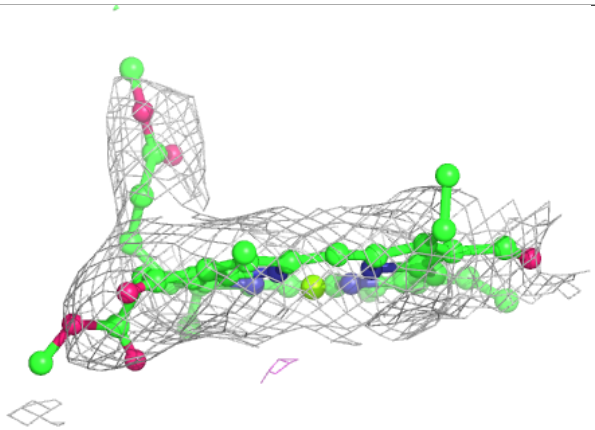


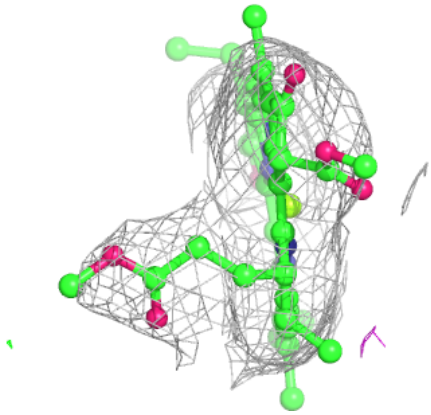


Electron density around CHL 3 1014:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

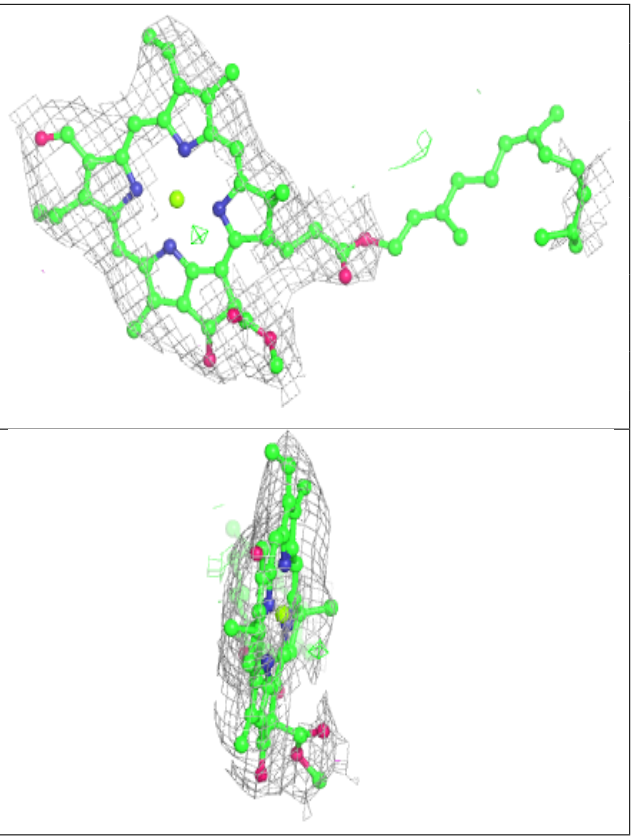


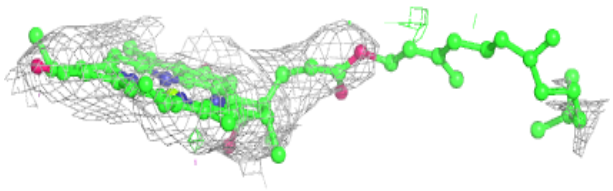




Electron density around CHL 5 316:

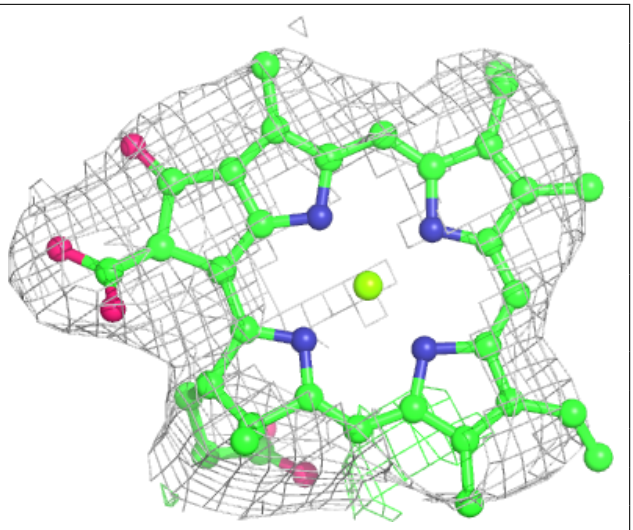
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

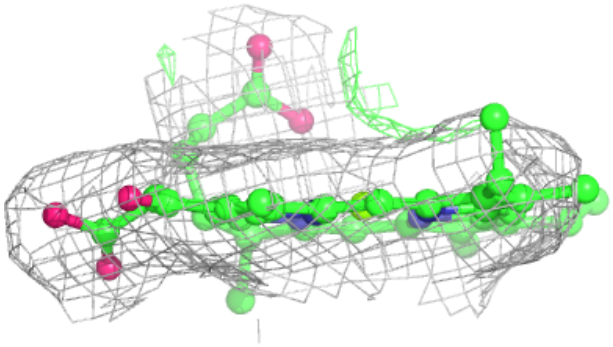


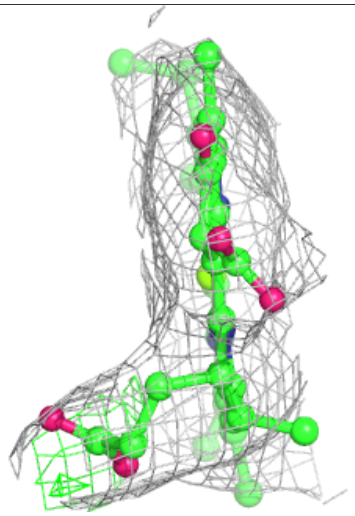


Electron density around CLA 7 1004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

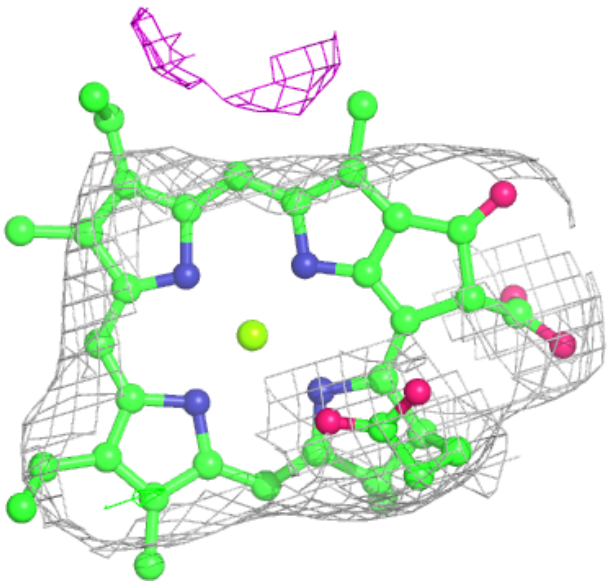


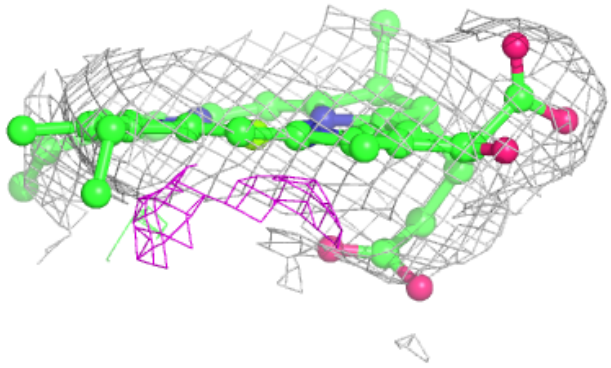


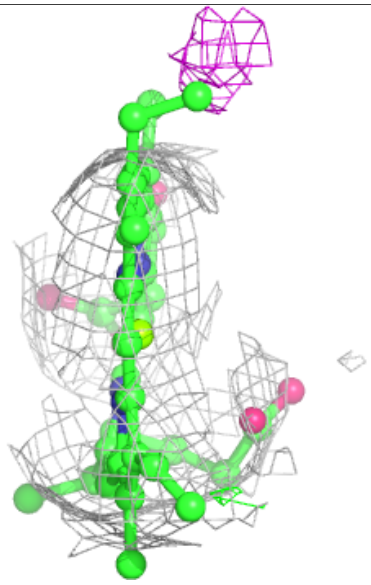


Electron density around CLA A 827:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

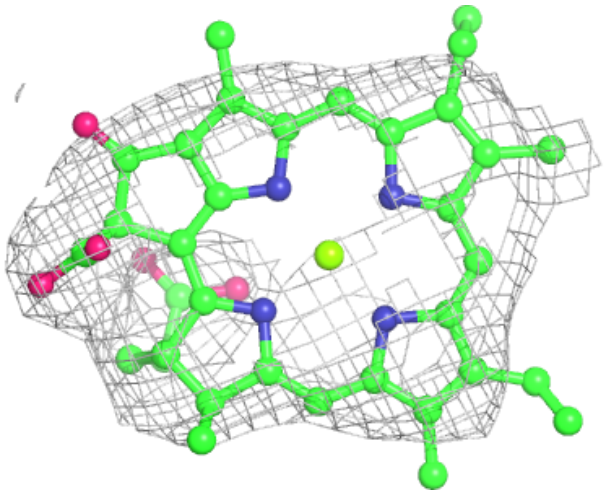


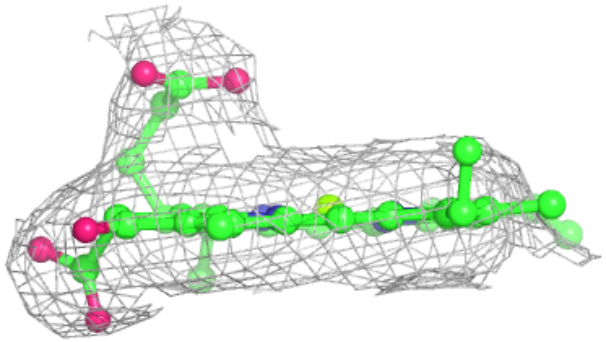


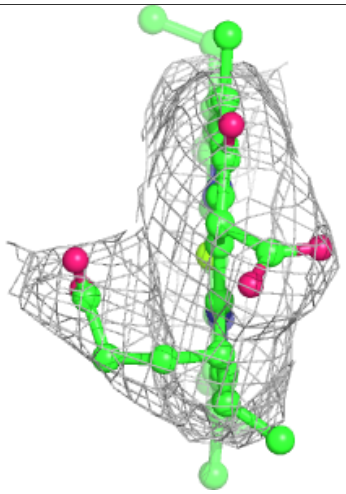


Electron density around CLA A 837:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

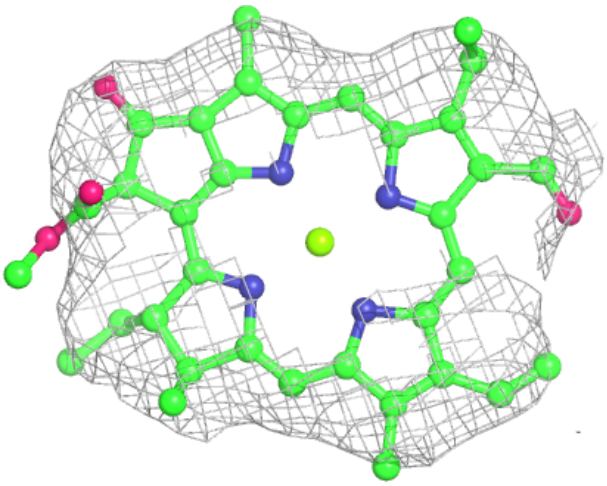


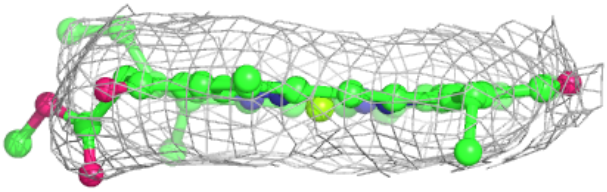


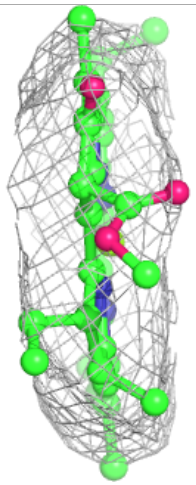


Electron density around CHL 6 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

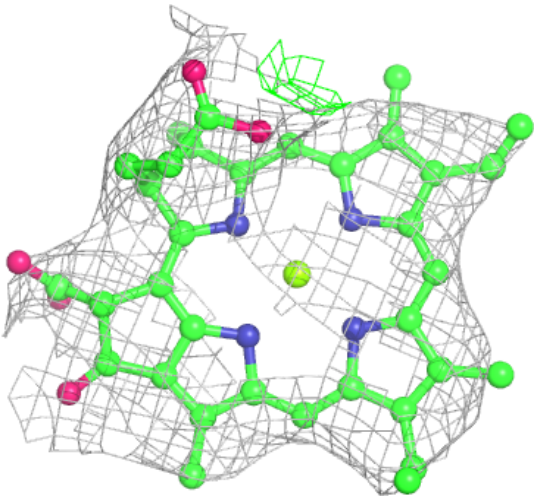


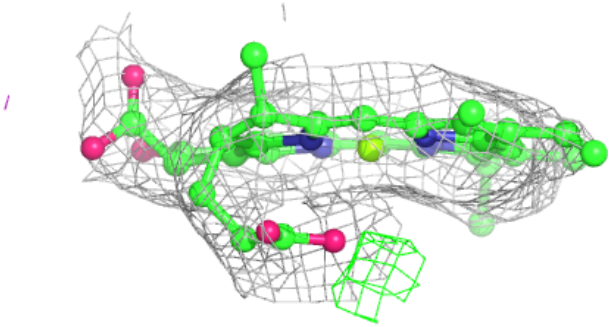


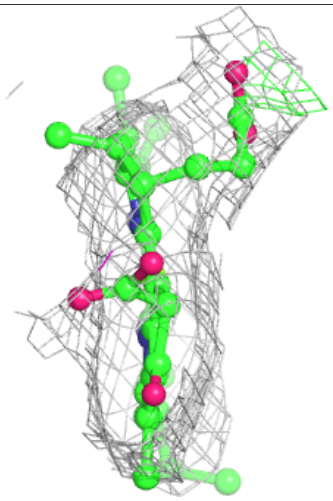


Electron density around CLA 8 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

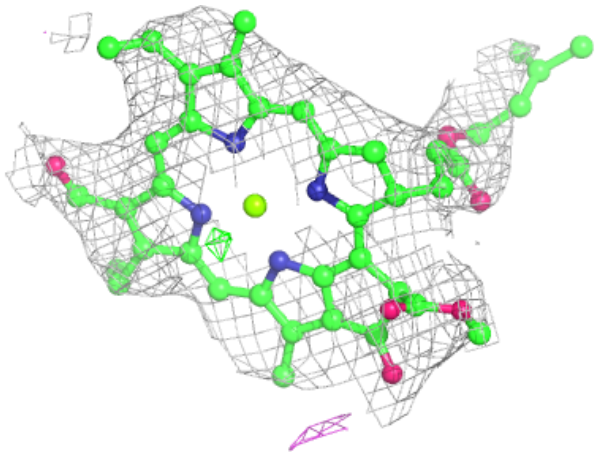


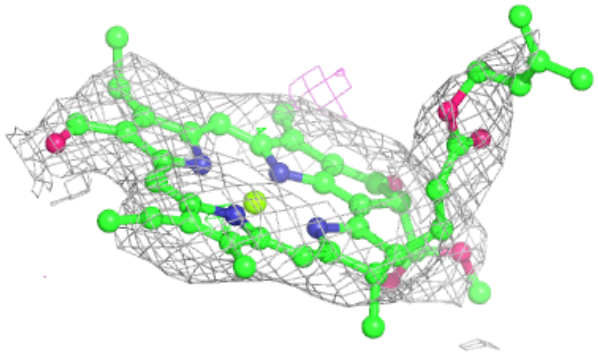


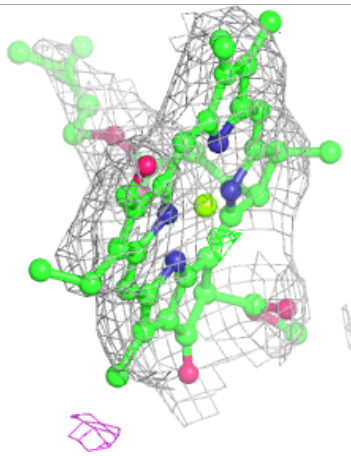


Electron density around CHL 5 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

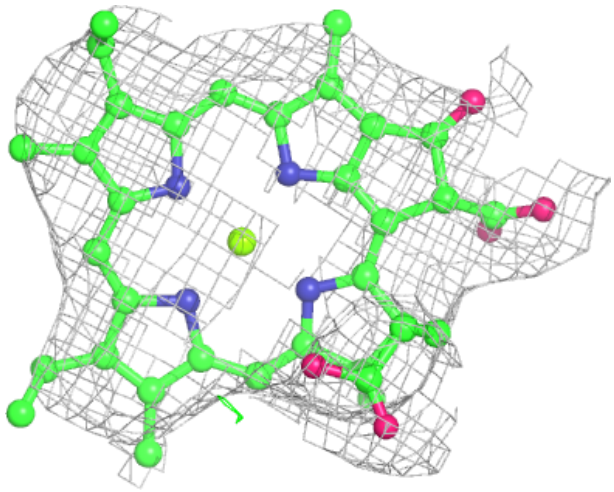


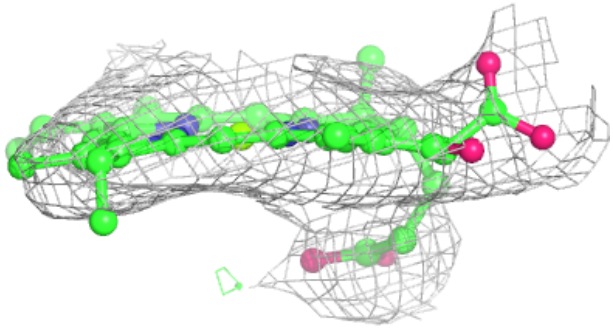


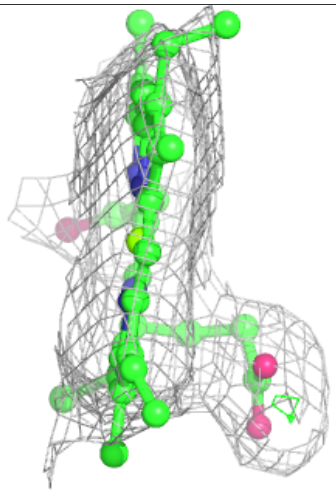


Electron density around CLA 6 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

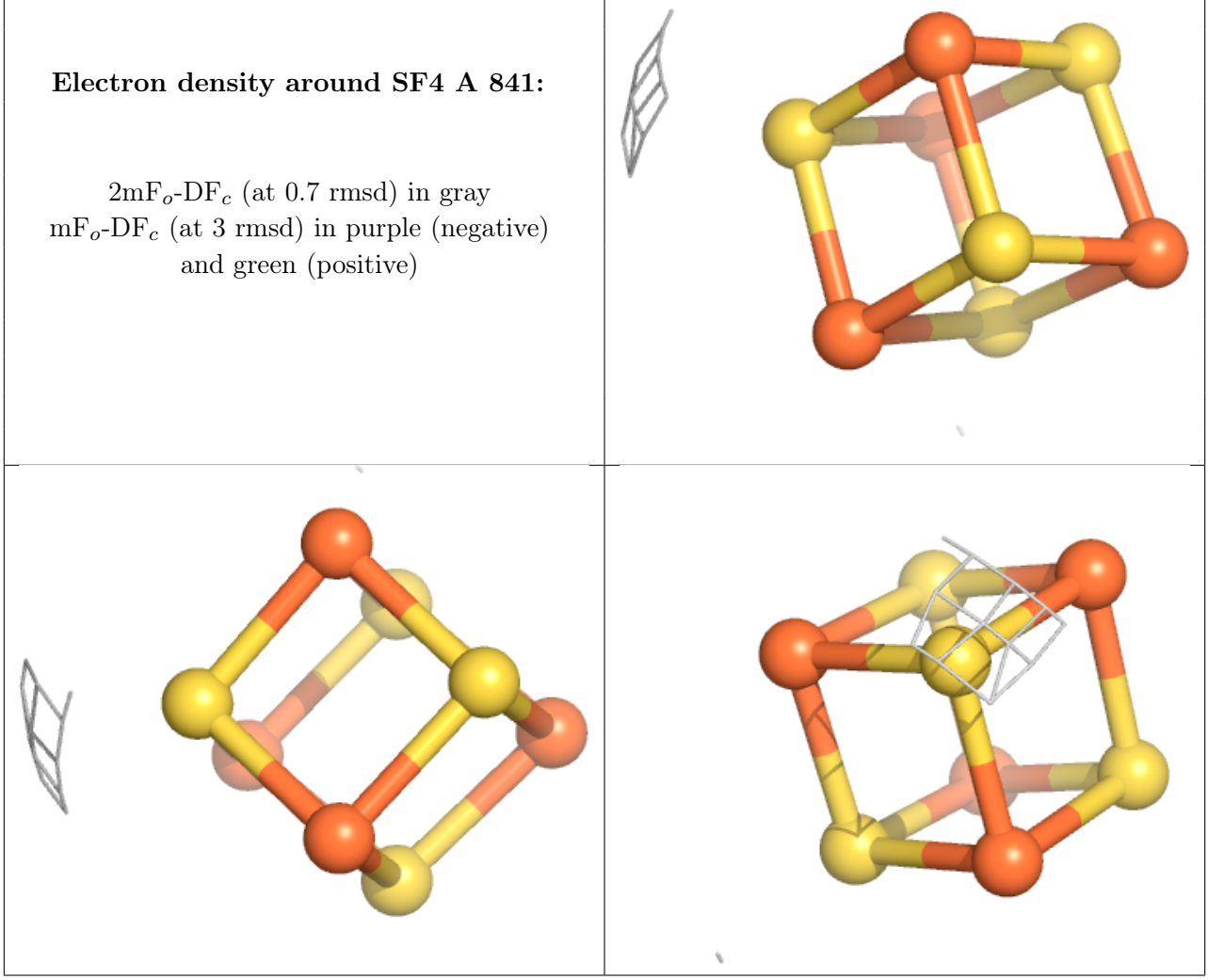






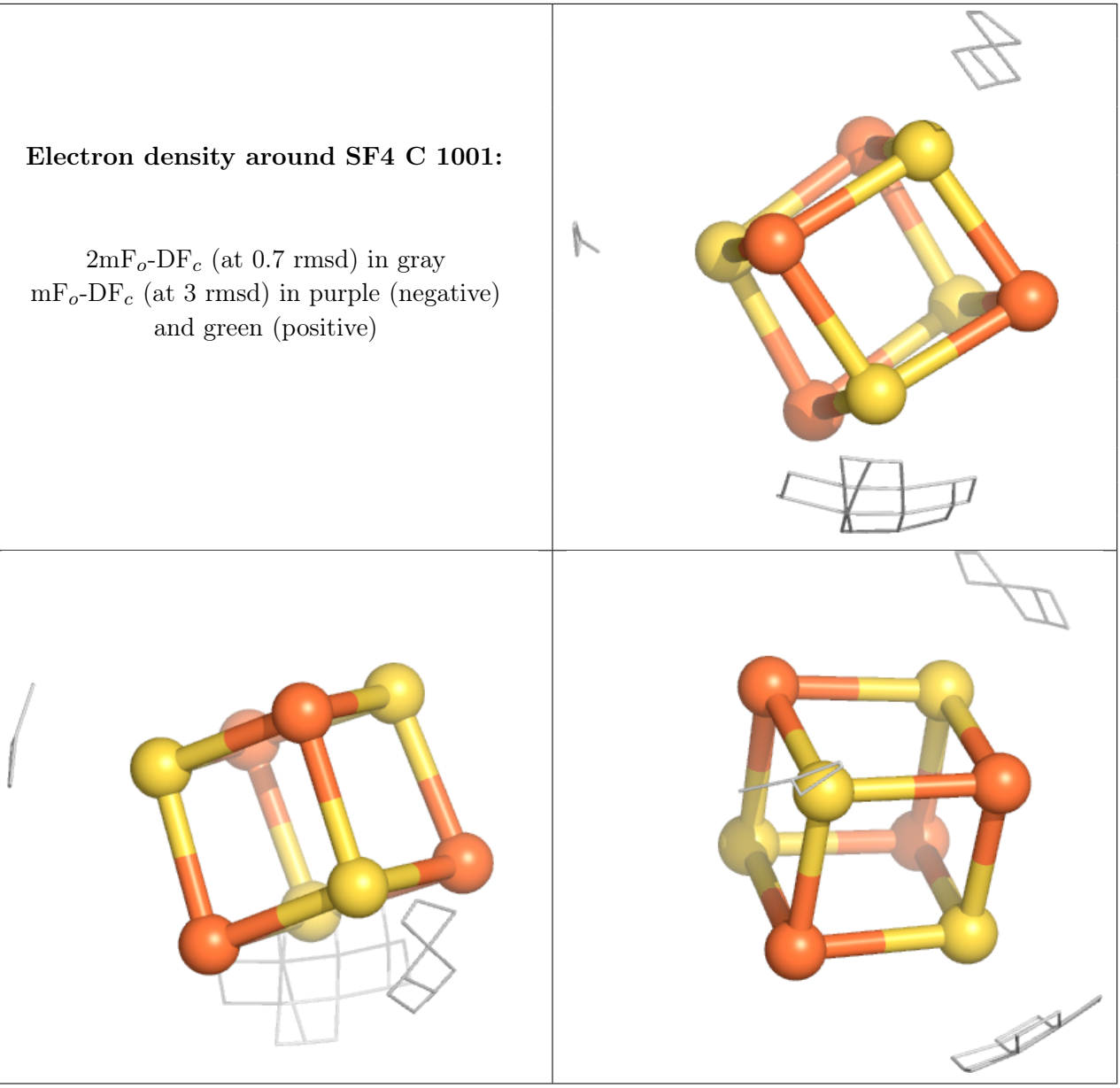
Electron density around SF4 A 841:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



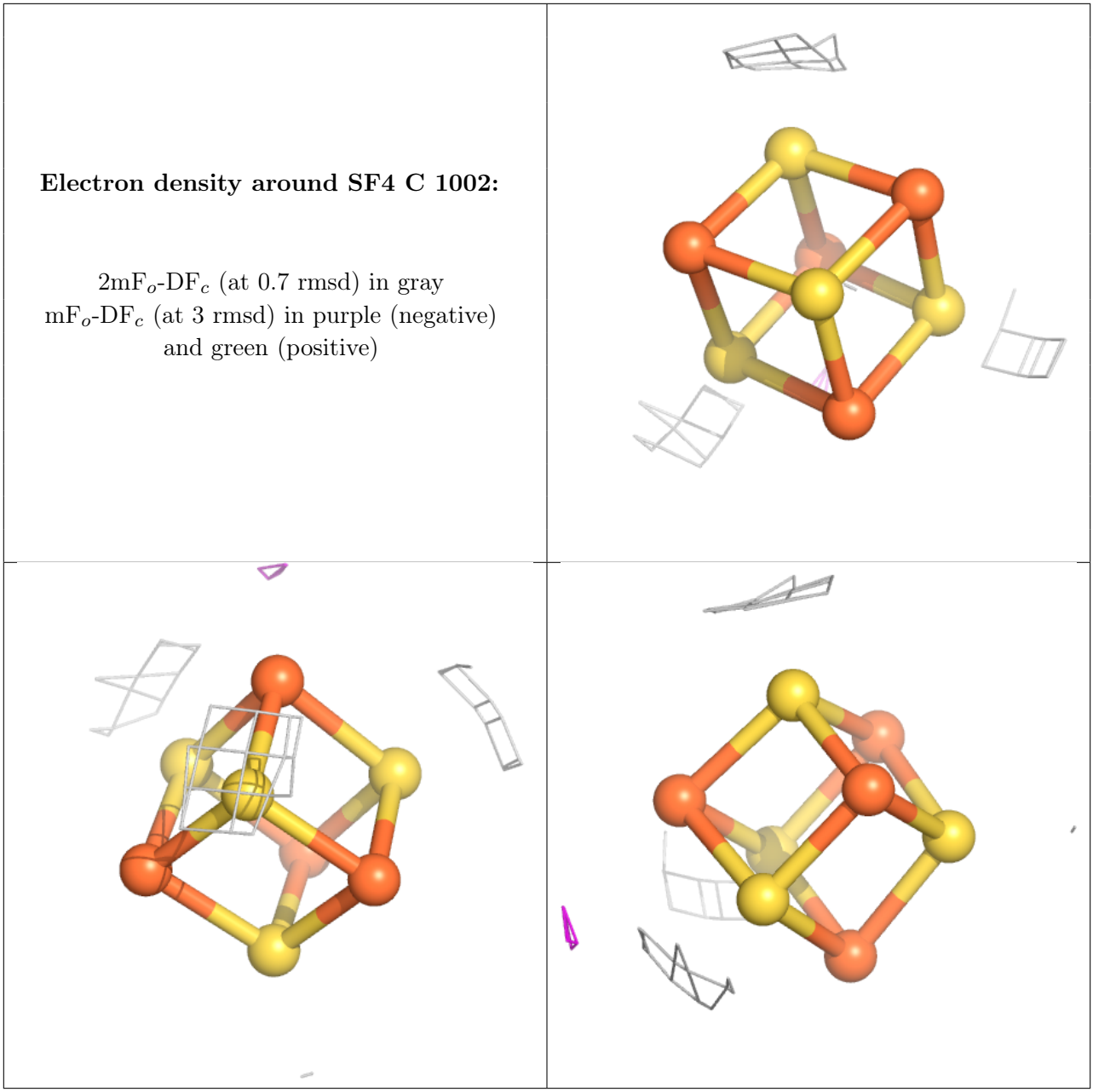
Electron density around SF4 C 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SF4 C 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.