wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 11:57 AM EDT

PDB ID	:	2O01 / pdb_00002o01
Title	:	The Structure of a plant photosystem I supercomplex at 3.4 Angstrom resolution
Authors	:	Amunts, A.; Drory, O.; Nelson, N.
Deposited on	:	2006-11-27
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:

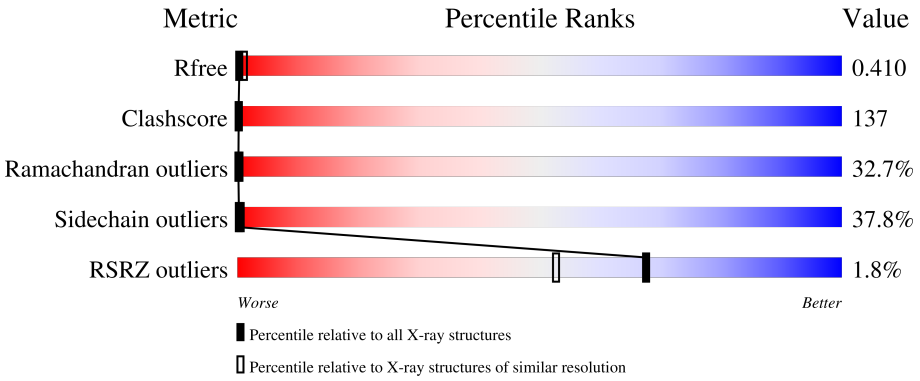
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	754	2% 5% 34% 41% 16%
2	B	732	% 5% 40% 40% 15%
3	C	80	31% 40% 28%
4	D	138	2% 5% 31% 41% 23%
5	E	62	2% 6% 40% 34% 19%

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Mol	Chain	Length	Quality of chain
6	F	154	40% 38% 19%
7	G	95	2% 6% 33% 44% 17%
8	H	75	5% 37% 39% 19%
9	I	30	3% 43% 50% 7%
10	J	42	10% 48% 31% 12%
11	K	38	53% 45%
12	L	164	2% 6% 36% 40% 18%
13	N	85	44% 32% 24%
14	1	187	3% 14% 42% 31% 7% 6%
15	2	186	% 13% 37% 25% 15% 11%
16	3	165	% 8% 28% 27% 7% 30%
17	4	165	4% 12% 44% 32% 13%

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
18	CLA	4	1304	X	-	-	-
18	CLA	A	1103	-	-	X	-
18	CLA	A	1107	X	-	-	-
18	CLA	A	1119	X	-	-	-
18	CLA	A	1122	X	-	-	-
18	CLA	A	1123	X	-	X	-
18	CLA	A	1126	X	-	X	-
18	CLA	A	1128	X	-	-	-
18	CLA	A	1129	X	-	-	-
18	CLA	A	1136	X	-	X	-
18	CLA	A	1137	X	-	-	-
18	CLA	A	1140	X	-	X	-
18	CLA	A	9011	X	-	X	-
18	CLA	B	1138	X	-	X	-
18	CLA	B	1202	-	-	X	-
18	CLA	B	1205	X	-	-	-
18	CLA	B	1207	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	1208	X	-	-	-
18	CLA	B	1209	X	-	X	-
18	CLA	B	1212	X	-	-	-
18	CLA	B	1214	-	-	X	-
18	CLA	B	1215	-	-	X	-
18	CLA	B	1216	X	-	X	-
18	CLA	B	1218	-	-	X	-
18	CLA	B	1220	X	-	X	-
18	CLA	B	1222	X	-	-	-
18	CLA	B	1225	-	-	X	-
18	CLA	B	1228	X	-	X	-
18	CLA	B	1232	X	-	-	-
18	CLA	B	1234	-	-	X	-
18	CLA	B	1235	X	-	-	-
18	CLA	B	1238	-	-	X	-
18	CLA	B	1239	X	-	X	-
18	CLA	B	9010	-	-	X	-
18	CLA	B	9012	X	-	-	-
18	CLA	F	1302	X	-	-	-
18	CLA	H	1501	X	-	-	-
18	CLA	I	1204	X	-	-	-
18	CLA	J	2107	X	-	-	-
18	CLA	L	1503	-	-	X	-
18	CLA	L	1504	X	-	-	-
19	PQN	A	5001	X	-	X	-
19	PQN	B	5002	X	-	-	-
21	SF4	B	3101	-	-	X	-
21	SF4	C	3102	-	-	X	-
21	SF4	C	3103	-	-	X	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 29846 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	728	Total	C	N	O	S	0	0	0
			5732	3758	975	981	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLY	ARG	conflict	UNP P05310

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	732	Total	C	N	O	S	0	0	0
			5844	3841	996	994	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	147	ALA	PHE	conflict	UNP P05311

- 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
			611	379	107	114	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1095	704	189	198	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	62	Total	C	N	O	0	0	0
			503	321	90	92			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	S	0	0	0
			744	484	121	137	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	0	0	0
			577	379	96	102			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	42	Total	C	N	O	S	0	0	0
			344	236	51	56	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	37	Total	C	N	O	0	0	0
			185	111	37	37			

- Molecule 12 is a protein called Photosystem I reaction center subunit XI, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	164	Total	C	N	O	S	0	0	0
			1235	815	197	218	5			

- Molecule 13 is a protein called Photosystem I-N subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 14 is a protein called AT3g54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1	175	Total	C	N	O	S	0	0	0
			1187	755	211	217	4			

- Molecule 15 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2	166	Total	C	N	O	S	0	0	0
			1268	828	207	230	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	17	GLU	PRO	conflict	UNP Q41038
2	35	SER	GLY	conflict	UNP Q41038

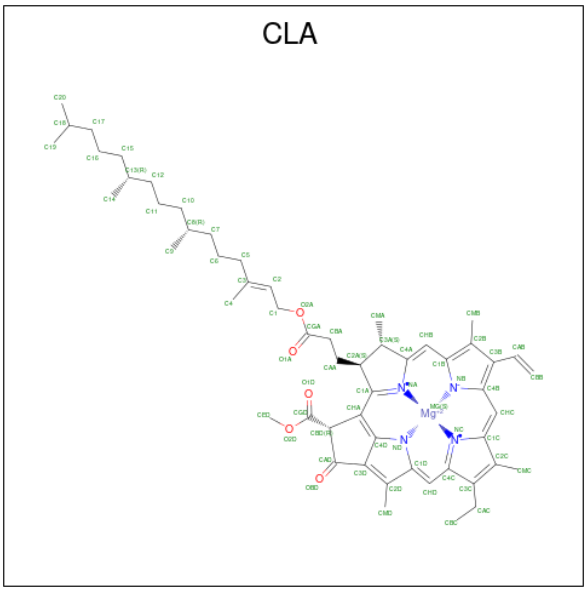
- Molecule 16 is a protein called PSI type III chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3	115	Total	C	N	O	S	0	0	0
			857	559	141	153	4			

- Molecule 17 is a protein called PSI light-harvesting antenna chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4	165	Total	C	N	O	S	0	0	0
			1282	839	214	226	3			

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N O 47 37 1 4 5	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N O 41 33 1 4 3	0	0
18	A	1	Total C Mg N O 57 47 1 4 5	0	0
18	A	1	Total C Mg N O 50 40 1 4 5	0	0
18	A	1	Total C Mg N 24 19 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N O 50 40 1 4 5	0	0
18	A	1	Total C Mg N O 47 37 1 4 5	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N O 55 45 1 4 5	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N O 55 45 1 4 5	0	0
18	A	1	Total C Mg N O 55 45 1 4 5	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N O 55 45 1 4 5	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N O 55 45 1 4 5	0	0
18	A	1	Total C Mg N O 55 45 1 4 5	0	0
18	A	1	Total C Mg N O 44 34 1 4 5	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N O 45 35 1 4 5	0	0
18	A	1	Total C Mg N O 55 45 1 4 5	0	0
18	A	1	Total C Mg N O 55 45 1 4 5	0	0
18	A	1	Total C Mg N O 55 45 1 4 5	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	A	1	Total C Mg N O 55 45 1 4 5	0	0
18	A	1	Total C Mg N O 46 36 1 4 5	0	0
18	A	1	Total C Mg N 25 20 1 4	0	0
18	B	1	Total C Mg N O 56 46 1 4 5	0	0
18	B	1	Total C Mg N O 47 37 1 4 5	0	0
18	B	1	Total C Mg N O 55 45 1 4 5	0	0
18	B	1	Total C Mg N O 54 44 1 4 5	0	0
18	B	1	Total C Mg N O 47 37 1 4 5	0	0
18	B	1	Total C Mg N 25 20 1 4	0	0
18	B	1	Total C Mg N O 50 40 1 4 5	0	0
18	B	1	Total C Mg N O 48 38 1 4 5	0	0
18	B	1	Total C Mg N O 55 45 1 4 5	0	0
18	B	1	Total C Mg N 25 20 1 4	0	0
18	B	1	Total C Mg N O 55 45 1 4 5	0	0
18	B	1	Total C Mg N O 55 45 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	B	1	Total C Mg N O 55 45 1 4 5	0	0
18	B	1	Total C Mg N 25 20 1 4	0	0
18	B	1	Total C Mg N 25 20 1 4	0	0
18	B	1	Total C Mg N O 60 50 1 4 5	0	0
18	B	1	Total C Mg N 25 20 1 4	0	0
18	B	1	Total C Mg N O 49 39 1 4 5	0	0
18	B	1	Total C Mg N O 52 42 1 4 5	0	0
18	B	1	Total C Mg N O 56 46 1 4 5	0	0
18	B	1	Total C Mg N O 50 40 1 4 5	0	0
18	B	1	Total C Mg N O 51 41 1 4 5	0	0
18	B	1	Total C Mg N O 51 41 1 4 5	0	0
18	B	1	Total C Mg N O 60 50 1 4 5	0	0
18	B	1	Total C Mg N O 48 38 1 4 5	0	0
18	B	1	Total C Mg N O 65 55 1 4 5	0	0
18	B	1	Total C Mg N 25 20 1 4	0	0
18	B	1	Total C Mg N O 51 41 1 4 5	0	0
18	B	1	Total C Mg N O 45 35 1 4 5	0	0
18	B	1	Total C Mg N 25 20 1 4	0	0
18	B	1	Total C Mg N O 50 40 1 4 5	0	0
18	B	1	Total C Mg N O 55 45 1 4 5	0	0
18	B	1	Total C Mg N O 49 39 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	B	1	Total C Mg N 25 20 1 4	0	0
18	B	1	Total C Mg N O 46 36 1 4 5	0	0
18	B	1	Total C Mg N O 55 45 1 4 5	0	0
18	B	1	Total C Mg N O 50 40 1 4 5	0	0
18	B	1	Total C Mg N O 55 45 1 4 5	0	0
18	B	1	Total C Mg N O 46 36 1 4 5	0	0
18	B	1	Total C Mg N O 51 41 1 4 5	0	0
18	B	1	Total C Mg N O 54 44 1 4 5	0	0
18	B	1	Total C Mg N O 55 45 1 4 5	0	0
18	B	1	Total C Mg N 25 20 1 4	0	0
18	B	1	Total C Mg N O 47 37 1 4 5	0	0
18	B	1	Total C Mg N 25 20 1 4	0	0
18	F	1	Total C Mg N O 44 35 1 4 4	0	0
18	F	1	Total C Mg N 25 20 1 4	0	0
18	F	1	Total C Mg N O 55 45 1 4 5	0	0
18	F	1	Total C Mg N 25 20 1 4	0	0
18	F	1	Total C Mg N 25 20 1 4	0	0
18	F	1	Total C Mg N 25 20 1 4	0	0
18	F	1	Total C Mg N 25 20 1 4	0	0
18	G	1	Total C Mg N O 51 41 1 4 5	0	0
18	G	1	Total C Mg N 25 20 1 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	H	1	Total C Mg N O 55 45 1 4 5	0	0
18	H	1	Total C Mg N 25 20 1 4	0	0
18	I	1	Total C Mg N O 55 45 1 4 5	0	0
18	J	1	Total C Mg N 25 20 1 4	0	0
18	J	1	Total C Mg N 25 20 1 4	0	0
18	J	1	Total C Mg N O 61 51 1 4 5	0	0
18	K	1	Total C Mg N 25 20 1 4	0	0
18	K	1	Total C Mg N 25 20 1 4	0	0
18	K	1	Total C Mg N 25 20 1 4	0	0
18	L	1	Total C Mg N 25 20 1 4	0	0
18	L	1	Total C Mg N O 50 40 1 4 5	0	0
18	L	1	Total C Mg N O 51 41 1 4 5	0	0
18	L	1	Total C Mg N O 46 36 1 4 5	0	0
18	L	1	Total C Mg N O 55 45 1 4 5	0	0
18	1	1	Total C Mg N 25 20 1 4	0	0
18	1	1	Total C Mg N 25 20 1 4	0	0
18	1	1	Total C Mg N 25 20 1 4	0	0
18	1	1	Total C Mg N 25 20 1 4	0	0
18	1	1	Total C Mg N 25 20 1 4	0	0
18	1	1	Total C Mg N 25 20 1 4	0	0
18	1	1	Total C Mg N 25 20 1 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	3	1	Total	C	Mg	N	0	0
			25	20	1	4		

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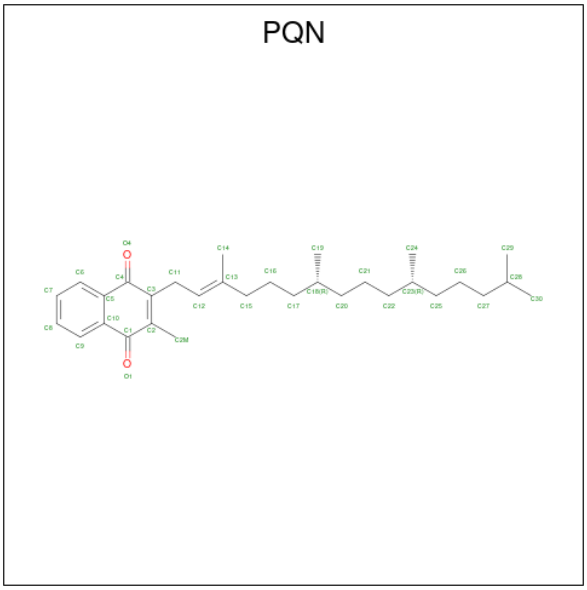
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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18	3	1	Total C Mg N 25 20 1 4	0	0
18	3	1	Total C Mg N 25 20 1 4	0	0
18	3	1	Total C Mg N 25 20 1 4	0	0
18	3	1	Total C Mg N 25 20 1 4	0	0
18	3	1	Total C Mg N 25 20 1 4	0	0
18	3	1	Total C Mg N 25 20 1 4	0	0
18	3	1	Total C Mg N 25 20 1 4	0	0
18	3	1	Total C Mg N 25 20 1 4	0	0
18	3	1	Total C Mg N 25 20 1 4	0	0
18	3	1	Total C Mg N 25 20 1 4	0	0
18	3	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N O 55 45 1 4 5	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0

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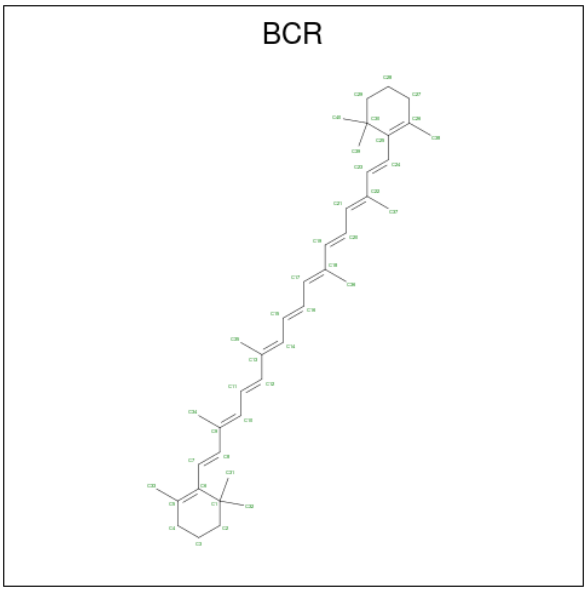
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	4	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0
18	4	1	Total C Mg N 25 20 1 4	0	0

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



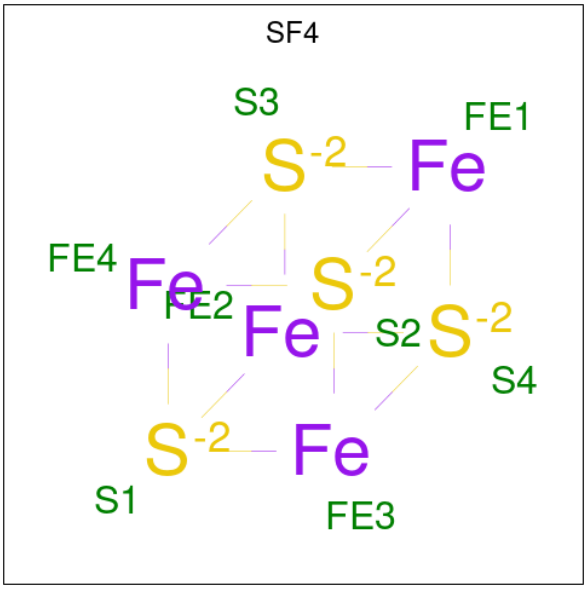
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 33 31 2	0	0
19	B	1	Total C O 33 31 2	0	0

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	F	1	Total C 40 40	0	0
20	I	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

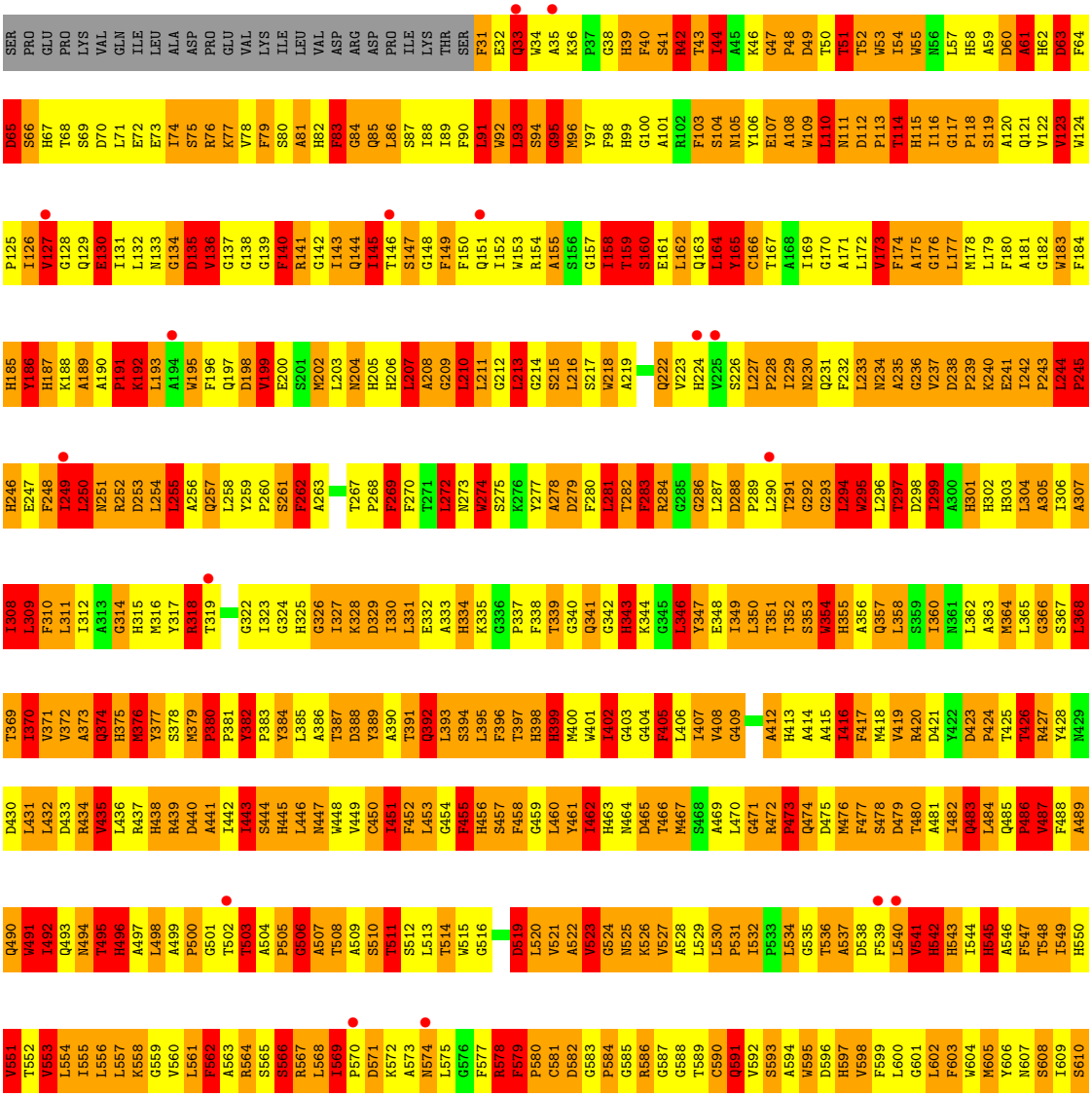
3 Residue-property plots (i)

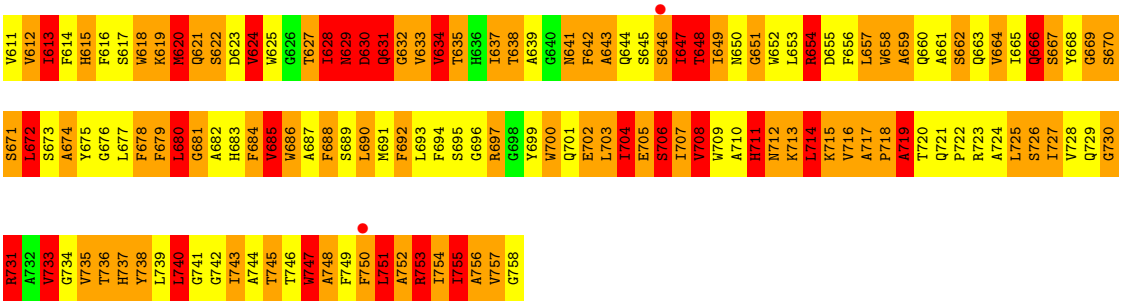
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

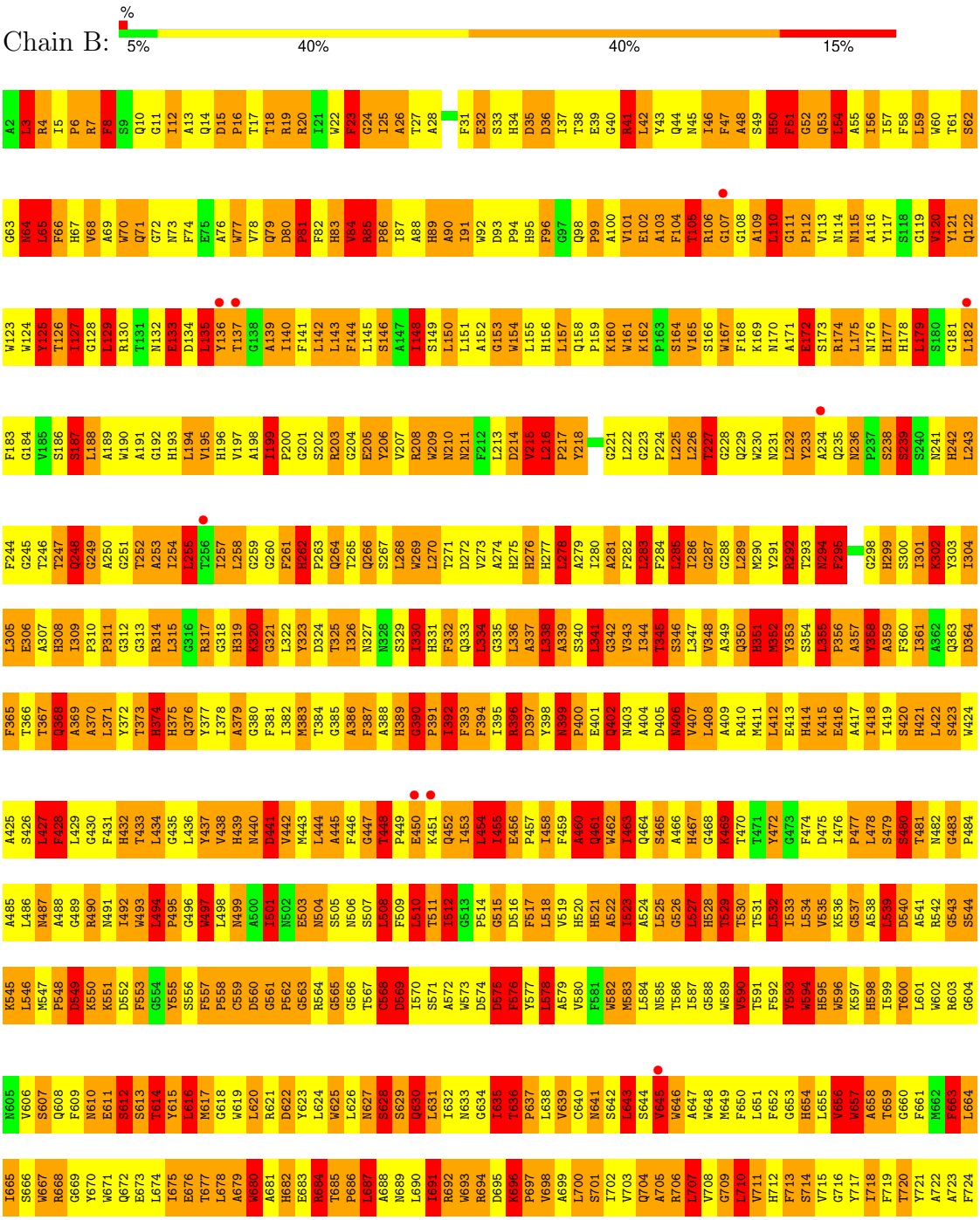
Chain A:

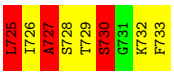






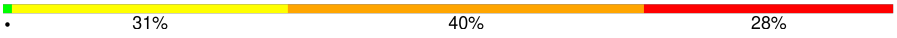
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





• Molecule 3: Photosystem I iron-sulfur center

Chain C:

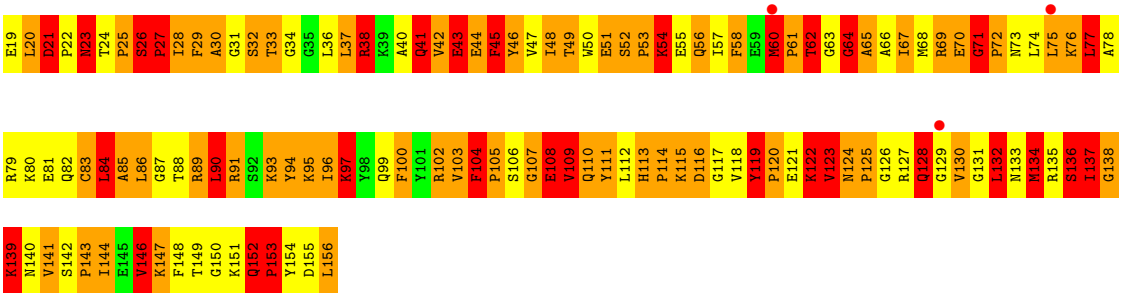




• Molecule 4: Photosystem I reaction center subunit II, chloroplast

Chain D:

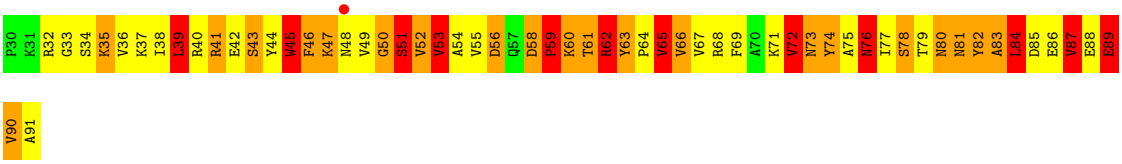




• Molecule 5: Photosystem I reaction center subunit IV A, chloroplast

Chain E:

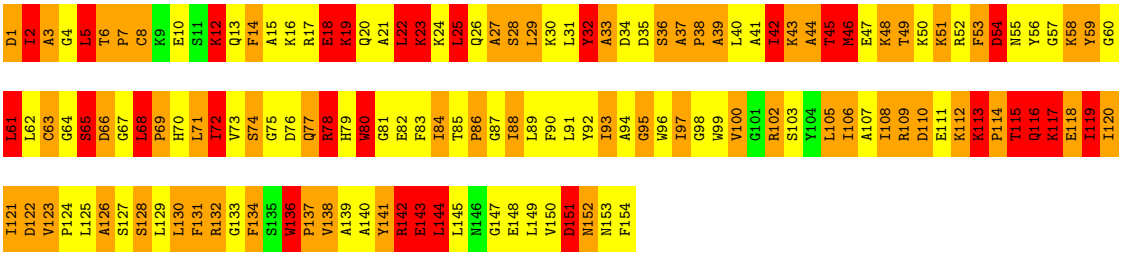




• Molecule 6: Photosystem I reaction center subunit III, chloroplast

Chain F:

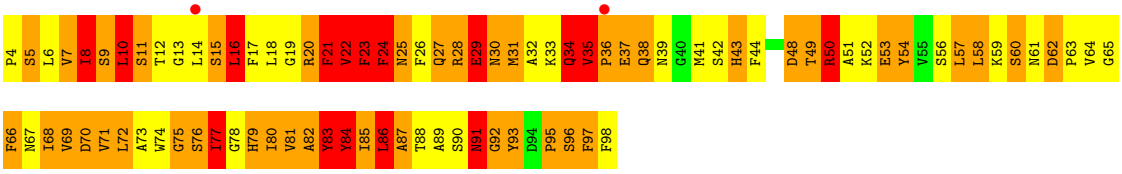




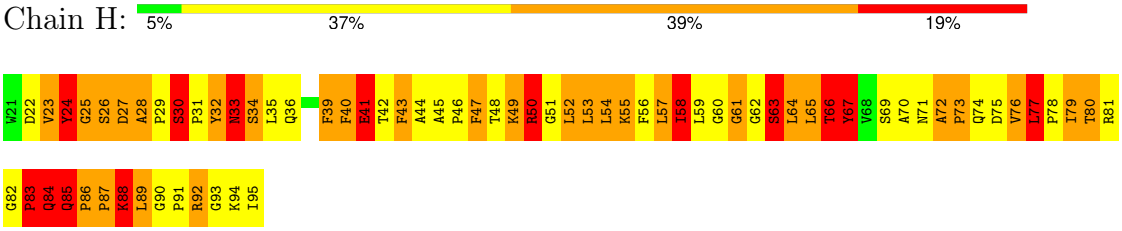
• Molecule 7: Photosystem I reaction center subunit V, chloroplast

Chain G:

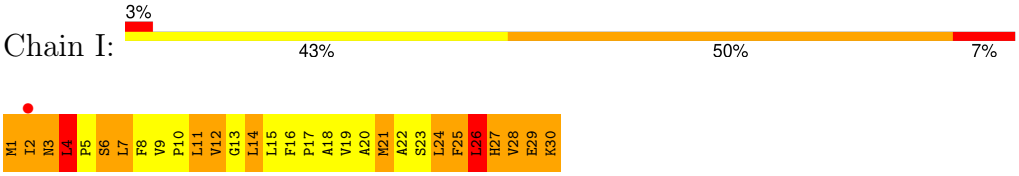




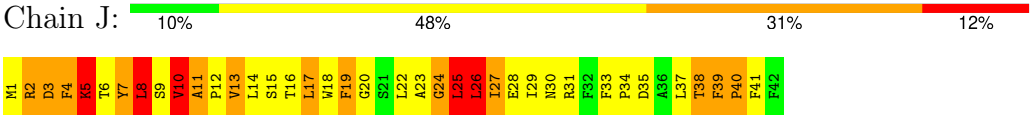
• Molecule 8: Photosystem I reaction center subunit VI, chloroplast



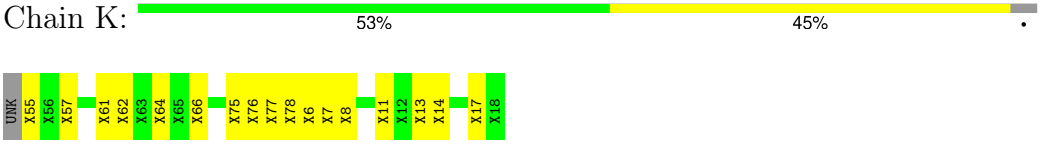
• Molecule 9: Photosystem I reaction center subunit VIII



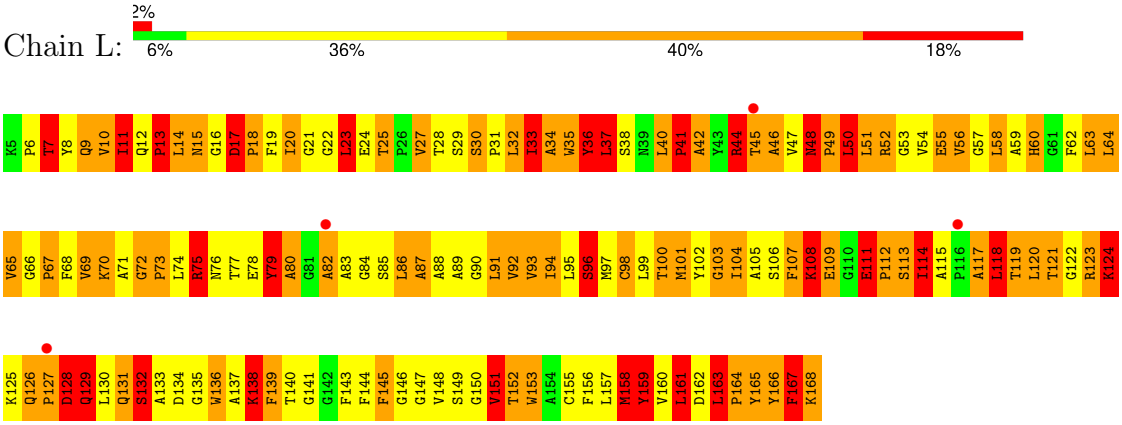
• Molecule 10: Photosystem I reaction center subunit IX



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

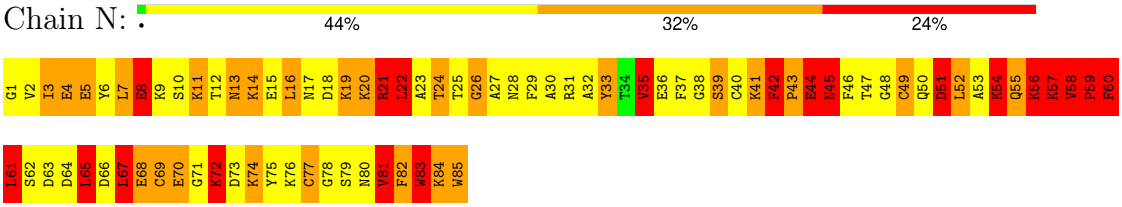


• Molecule 12: Photosystem I reaction center subunit XI, chloroplast



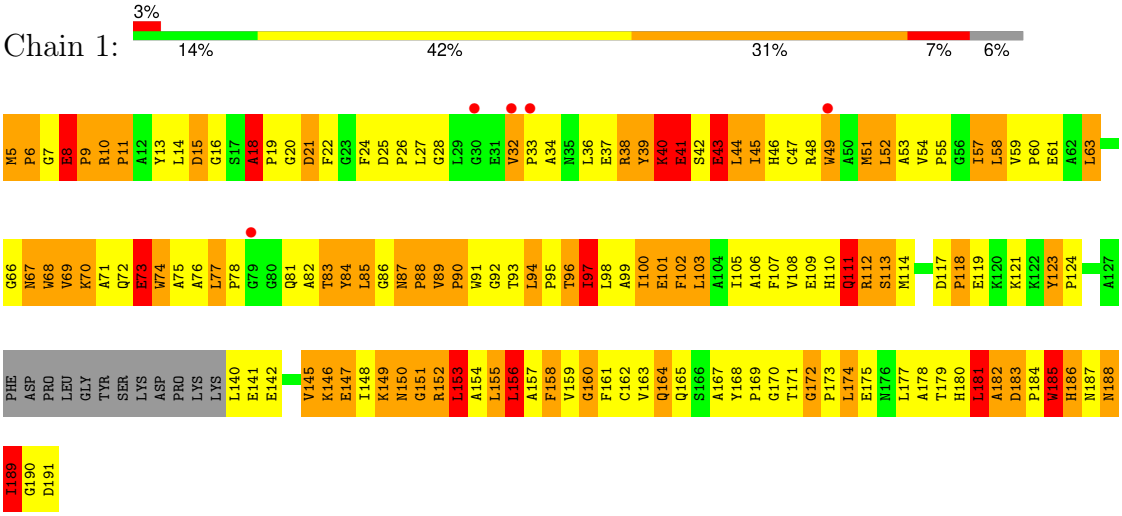
• Molecule 13: Photosystem I-N subunit

Chain N:



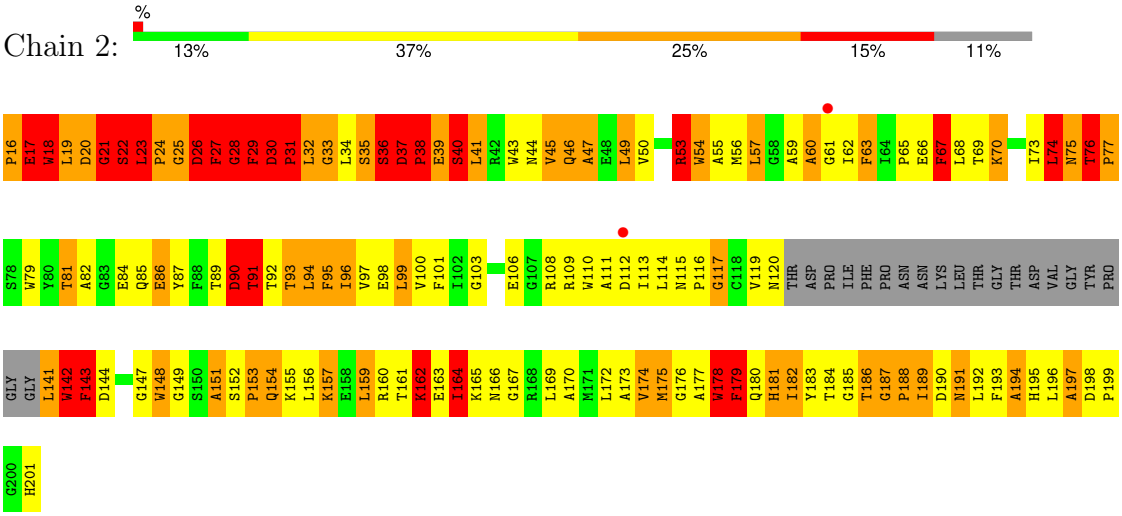
• Molecule 14: AT3g54890

Chain 1:



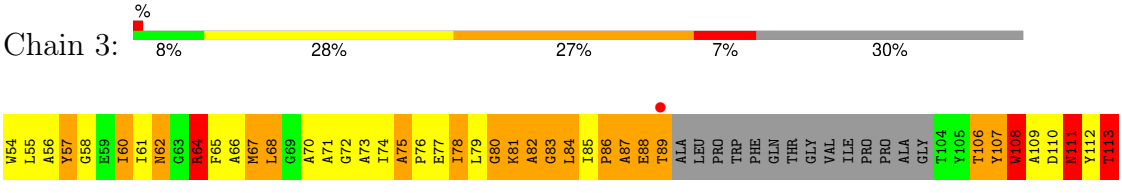
• Molecule 15: Type II chlorophyll a/b binding protein from photosystem I

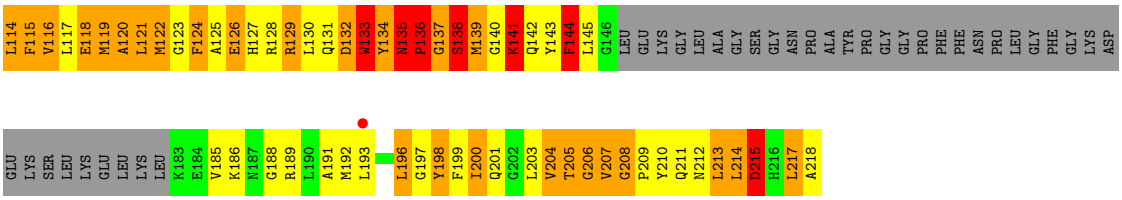
Chain 2:



• Molecule 16: PSI type III chlorophyll a/b-binding protein

Chain 3:

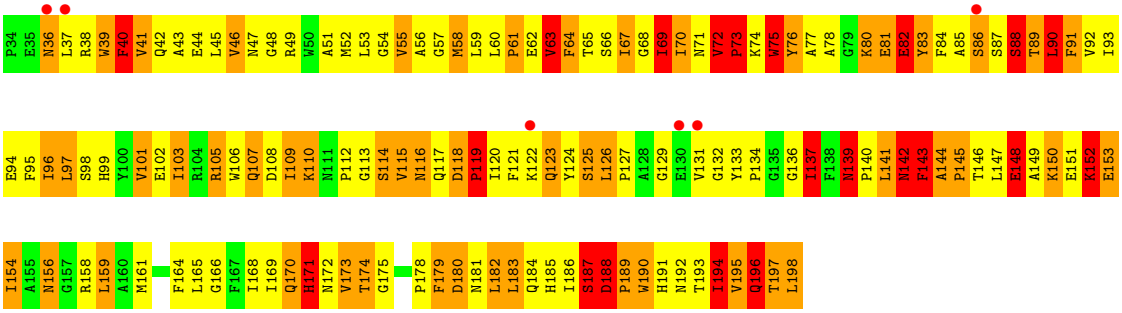




• Molecule 17: PSI light-harvesting antenna chlorophyll a/b-binding protein

Chain 4:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.05Å 188.78Å 127.52Å 90.00° 95.19° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 40.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	90.8 (40.00-3.40) 76.1 (40.00-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.348 , 0.409 0.353 , 0.410	Depositor DCC
R_{free} test set	3517 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å^2)	96.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 976.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	29846	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, CLA, BCR, 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	0.98	6/5928 (0.1%)	1.46	90/8092 (1.1%)
2	B	0.98	7/6054 (0.1%)	1.45	98/8273 (1.2%)
3	C	1.26	5/624 (0.8%)	1.65	18/846 (2.1%)
4	D	1.10	3/1122 (0.3%)	1.59	24/1514 (1.6%)
5	E	0.90	0/513	1.46	14/694 (2.0%)
6	F	0.99	0/1250	1.50	25/1687 (1.5%)
7	G	0.93	1/764 (0.1%)	1.54	15/1035 (1.4%)
8	H	1.01	0/595	1.59	16/810 (2.0%)
9	I	1.04	0/235	1.44	2/320 (0.6%)
10	J	1.01	0/356	1.44	8/484 (1.7%)
12	L	0.99	1/1272 (0.1%)	1.56	39/1736 (2.2%)
13	N	0.74	0/699	1.43	9/936 (1.0%)
14	1	0.80	0/1215	1.28	16/1666 (1.0%)
15	2	0.93	3/1309 (0.2%)	1.60	21/1787 (1.2%)
16	3	0.76	0/879	1.25	9/1194 (0.8%)
17	4	0.87	1/1319 (0.1%)	1.21	11/1797 (0.6%)
All	All	0.96	27/24134 (0.1%)	1.46	415/32871 (1.3%)

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	32
2	B	0	32
3	C	0	4
4	D	0	14
5	E	0	3
6	F	0	9
7	G	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	4
9	I	0	2
12	L	0	4
13	N	3	11
14	1	0	5
15	2	3	21
16	3	1	14
17	4	0	13
All	All	7	174

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	40	SER	C-N	-8.54	1.21	1.33
2	B	455	ILE	CA-CB	7.01	1.61	1.53
3	C	9	ASP	N-CA	6.86	1.55	1.45
2	B	89	HIS	CA-C	6.52	1.58	1.52
4	D	48	ILE	CA-CB	6.30	1.62	1.54

The worst 5 of 415 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	2	37	ASP	CA-C-N	22.23	147.63	119.84
15	2	37	ASP	C-N-CA	22.23	147.63	119.84
4	D	26	SER	C-N-CD	-17.32	82.50	120.60
15	2	40	SER	CA-C-N	-16.24	90.53	121.54
15	2	40	SER	C-N-CA	-16.24	90.53	121.54

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	N	59	PRO	CA
13	N	61	LEU	CA
13	N	83	TRP	CA
15	2	20	ASP	CA
15	2	23	LEU	CA

5 of 174 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	SER	Peptide
1	A	117	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	33	GLN	Peptide
1	A	47	GLY	Peptide
1	A	65	ASP	Peptide

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	5732	0	5577	1916	0
2	B	5844	0	5659	2029	0
3	C	611	0	594	268	0
4	D	1095	0	1112	371	0
5	E	503	0	510	136	0
6	F	1221	0	1250	383	0
7	G	744	0	721	218	0
8	H	577	0	587	142	0
9	I	229	0	252	108	0
10	J	344	0	347	106	0
11	K	185	0	40	12	0
12	L	1235	0	1244	376	1
13	N	685	0	672	273	0
14	1	1187	0	1019	246	1
15	2	1268	0	1177	511	1
16	3	857	0	789	236	0
17	4	1282	0	1241	283	1
18	1	325	0	39	12	0
18	2	325	0	39	15	0
18	3	375	0	45	12	0
18	4	405	0	90	15	0
18	A	1601	0	870	342	0
18	B	2078	0	1535	681	0
18	F	224	0	94	41	0
18	G	76	0	43	12	0
18	H	80	0	51	12	0
18	I	55	0	48	9	0
18	J	111	0	66	8	0
18	K	75	0	9	5	0
18	L	227	0	162	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	33	0	46	30	0
19	B	33	0	46	20	0
20	A	40	0	54	17	0
20	B	40	0	54	17	0
20	F	40	0	54	13	0
20	I	40	0	54	13	0
20	L	40	0	54	17	0
21	B	8	0	0	4	0
21	C	16	0	0	15	0
All	All	29846	0	26244	7693	2

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 137.

The worst 5 of 7693 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)
3:C:22:PRO:HG2	3:C:51:CYS:SG	1.33	1.68
2:B:289:LEU:C	18:B:1218:CLA:HBC1	1.22	1.59
15:2:192:LEU:HA	15:2:195:HIS:CE1	1.34	1.58
2:B:290:MET:CA	18:B:1218:CLA:HBC2	1.12	1.57
15:2:26:ASP:HB3	15:2:27:PHE:CB	1.34	1.56

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:161:LEU:O	17:4:141:LEU:O[1_655]	1.55	0.65
14:1:71:ALA:CB	15:2:30:ASP:OD1[1_556]	1.96	0.24

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	726/754 (96%)	290 (40%)	201 (28%)	235 (32%)	0	0
2	B	730/732 (100%)	290 (40%)	209 (29%)	231 (32%)	0	0
3	C	78/80 (98%)	20 (26%)	23 (30%)	35 (45%)	0	0
4	D	136/138 (99%)	50 (37%)	28 (21%)	58 (43%)	0	0
5	E	60/62 (97%)	28 (47%)	13 (22%)	19 (32%)	0	0
6	F	152/154 (99%)	59 (39%)	40 (26%)	53 (35%)	0	0
7	G	93/95 (98%)	40 (43%)	22 (24%)	31 (33%)	0	0
8	H	73/75 (97%)	21 (29%)	18 (25%)	34 (47%)	0	0
9	I	28/30 (93%)	9 (32%)	11 (39%)	8 (29%)	0	0
10	J	40/42 (95%)	16 (40%)	14 (35%)	10 (25%)	0	0
12	L	162/164 (99%)	64 (40%)	40 (25%)	58 (36%)	0	0
13	N	83/85 (98%)	26 (31%)	26 (31%)	31 (37%)	0	0
14	1	171/187 (91%)	74 (43%)	43 (25%)	54 (32%)	0	0
15	2	162/186 (87%)	72 (44%)	46 (28%)	44 (27%)	0	0
16	3	109/165 (66%)	49 (45%)	36 (33%)	24 (22%)	0	0
17	4	163/165 (99%)	69 (42%)	48 (29%)	46 (28%)	0	0
All	All	2966/3114 (95%)	1177 (40%)	818 (28%)	971 (33%)	0	0

5 of 971 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	48	PRO
1	A	51	THR
1	A	52	THR
1	A	61	ALA

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	588/613 (96%)	341 (58%)	247 (42%)	0	0
2	B	598/598 (100%)	387 (65%)	211 (35%)	0	0
3	C	69/69 (100%)	39 (56%)	30 (44%)	0	0
4	D	118/118 (100%)	79 (67%)	39 (33%)	0	0
5	E	55/55 (100%)	38 (69%)	17 (31%)	0	0
6	F	127/127 (100%)	83 (65%)	44 (35%)	0	0
7	G	80/80 (100%)	44 (55%)	36 (45%)	0	0
8	H	62/62 (100%)	37 (60%)	25 (40%)	0	0
9	I	26/26 (100%)	17 (65%)	9 (35%)	0	0
10	J	37/37 (100%)	28 (76%)	9 (24%)	1	2
12	L	127/127 (100%)	77 (61%)	50 (39%)	0	0
13	N	74/74 (100%)	45 (61%)	29 (39%)	0	0
14	1	92/147 (63%)	58 (63%)	34 (37%)	0	0
15	2	122/151 (81%)	80 (66%)	42 (34%)	0	0
16	3	74/123 (60%)	44 (60%)	30 (40%)	0	0
17	4	130/139 (94%)	83 (64%)	47 (36%)	0	0
All	All	2379/2546 (93%)	1480 (62%)	899 (38%)	0	0

5 of 899 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	17	CYS
17	4	168	ILE
6	F	102	ARG
17	4	143	PHE
15	2	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	439	HIS
4	D	128	GLN
17	4	196	GLN
16	3	127	HIS
2	B	504	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

178 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	$\#\|Z\| > 2$
18	CLA	2	2015	-	24,32,73	2.34	8 (33%)	31,54,113	2.76	17 (54%)
18	CLA	K	1153	-	24,32,73	2.27	8 (33%)	31,54,113	2.72	19 (61%)
18	CLA	2	2003	-	24,32,73	2.33	10 (41%)	31,54,113	2.99	19 (61%)
18	CLA	A	1101	1	24,32,73	2.35	8 (33%)	31,54,113	2.96	19 (61%)
18	CLA	3	3009	-	24,32,73	2.40	9 (37%)	31,54,113	2.80	19 (61%)
18	CLA	A	1113	-	54,58,73	2.44	15 (27%)	64,95,113	3.14	28 (43%)
18	CLA	2	2002	-	24,32,73	2.34	8 (33%)	31,54,113	2.77	18 (58%)
18	CLA	A	1309	-	24,32,73	2.31	8 (33%)	31,54,113	2.77	17 (54%)
18	CLA	4	4001	-	24,32,73	2.37	8 (33%)	31,54,113	2.82	18 (58%)
18	CLA	B	1238	-	58,62,73	2.42	15 (25%)	68,99,113	2.96	30 (44%)
18	CLA	4	4007	-	24,32,73	2.40	8 (33%)	31,54,113	2.83	18 (58%)
18	CLA	A	1123	-	59,63,73	2.42	17 (28%)	70,101,113	2.81	25 (35%)
18	CLA	B	1223	2	24,32,73	2.39	9 (37%)	31,54,113	2.83	17 (54%)
18	CLA	A	1103	1	51,55,73	2.51	15 (29%)	60,91,113	3.10	23 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	B	1222	-	69,73,73	2.12	13 (18%)	82,113,113	2.49	29 (35%)
18	CLA	1	1001	-	24,32,73	2.40	8 (33%)	31,54,113	2.73	18 (58%)
18	CLA	4	4011	-	24,32,73	2.32	8 (33%)	31,54,113	2.75	17 (54%)
18	CLA	B	1226	18	24,32,73	2.37	8 (33%)	31,54,113	2.78	19 (61%)
18	CLA	I	1204	-	59,63,73	2.36	16 (27%)	70,101,113	2.67	26 (37%)
20	BCR	L	6020	-	41,41,41	1.66	3 (7%)	56,56,56	4.94	25 (44%)
18	CLA	A	1122	-	59,63,73	2.41	17 (28%)	70,101,113	2.82	27 (38%)
18	CLA	A	9013	-	50,54,73	2.51	16 (32%)	59,90,113	2.80	25 (42%)
18	CLA	A	1105	1	24,32,73	2.30	8 (33%)	31,54,113	2.81	18 (58%)
18	CLA	A	1106	-	45,49,73	2.46	14 (31%)	54,84,113	3.47	26 (48%)
18	CLA	A	1140	1	59,63,73	2.39	15 (25%)	70,101,113	2.91	27 (38%)
18	CLA	3	3006	16	24,32,73	2.33	8 (33%)	31,54,113	2.79	19 (61%)
18	CLA	1	1013	-	24,32,73	2.37	8 (33%)	31,54,113	2.77	18 (58%)
18	CLA	F	1139	-	47,52,73	2.49	12 (25%)	55,87,113	3.02	24 (43%)
18	CLA	1	1006	-	24,32,73	2.33	8 (33%)	31,54,113	2.80	17 (54%)
18	CLA	4	4013	-	24,32,73	2.36	8 (33%)	31,54,113	2.85	18 (58%)
18	CLA	B	1205	2	59,63,73	2.31	15 (25%)	70,101,113	3.00	26 (37%)
18	CLA	4	1009	-	24,32,73	2.40	7 (29%)	31,54,113	2.73	17 (54%)
18	CLA	B	1230	-	24,32,73	2.34	8 (33%)	31,54,113	2.71	17 (54%)
18	CLA	A	1115	-	51,55,73	2.50	17 (33%)	60,91,113	3.00	26 (43%)
18	CLA	4	1304	-	59,63,73	2.32	14 (23%)	70,101,113	2.69	27 (38%)
18	CLA	2	2001	-	24,32,73	2.36	8 (33%)	31,54,113	2.77	17 (54%)
18	CLA	B	1235	-	59,63,73	2.38	16 (27%)	70,101,113	2.78	23 (32%)
18	CLA	B	1212	-	64,68,73	2.25	15 (23%)	76,107,113	2.69	26 (34%)
18	CLA	F	1305	-	24,32,73	2.31	8 (33%)	31,54,113	2.81	18 (58%)
18	CLA	B	1242	-	51,55,73	2.57	17 (33%)	60,91,113	3.03	21 (35%)
18	CLA	3	3004	-	24,32,73	2.37	9 (37%)	31,54,113	2.84	19 (61%)
18	CLA	A	1144	-	24,32,73	2.30	8 (33%)	31,54,113	2.87	18 (58%)
18	CLA	F	4015	-	24,32,73	2.33	8 (33%)	31,54,113	2.89	19 (61%)
18	CLA	A	1152	-	24,32,73	2.33	8 (33%)	31,54,113	2.76	17 (54%)
18	CLA	1	1010	-	24,32,73	2.36	8 (33%)	31,54,113	2.79	19 (61%)
18	CLA	A	1135	-	49,53,73	2.52	16 (32%)	58,89,113	3.02	21 (36%)
18	CLA	A	9011	1	59,63,73	2.28	16 (27%)	70,101,113	2.91	29 (41%)
18	CLA	K	1141	-	24,32,73	2.33	8 (33%)	31,54,113	2.71	17 (54%)
18	CLA	4	4002	-	24,32,73	2.29	8 (33%)	31,54,113	2.83	19 (61%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	B	9022	-	58,62,73	2.41	16 (27%)	68,99,113	3.39	30 (44%)
18	CLA	2	2006	-	24,32,73	2.32	8 (33%)	31,54,113	2.79	18 (58%)
18	CLA	3	3001	-	24,32,73	2.40	8 (33%)	31,54,113	2.85	18 (58%)
18	CLA	A	1127	1	24,32,73	2.35	10 (41%)	31,54,113	2.78	19 (61%)
18	CLA	A	1102	-	24,32,73	2.37	8 (33%)	31,54,113	2.79	18 (58%)
18	CLA	A	1108	1	54,58,73	2.40	15 (27%)	64,95,113	3.01	25 (39%)
18	CLA	B	1221	-	52,56,73	2.45	14 (26%)	61,92,113	2.90	27 (44%)
20	BCR	I	6018	-	41,41,41	1.56	4 (9%)	56,56,56	4.92	32 (57%)
18	CLA	A	1128	-	59,63,73	2.36	17 (28%)	70,101,113	2.61	26 (37%)
21	SF4	C	3103	3	0,12,12	-	-	-		
18	CLA	B	1203	18	50,56,73	2.32	12 (24%)	58,92,113	2.76	26 (44%)
18	CLA	A	1142	-	24,32,73	2.35	8 (33%)	31,54,113	2.76	18 (58%)
18	CLA	F	1303	-	24,32,73	2.37	8 (33%)	31,54,113	2.81	17 (54%)
18	CLA	A	1137	-	59,63,73	2.37	16 (27%)	70,101,113	2.75	27 (38%)
18	CLA	1	1011	14	24,32,73	2.36	8 (33%)	31,54,113	2.82	18 (58%)
20	BCR	B	6017	-	41,41,41	1.38	4 (9%)	56,56,56	4.38	25 (44%)
18	CLA	B	1217	-	54,58,73	2.49	18 (33%)	64,95,113	3.00	24 (37%)
18	CLA	B	1301	-	24,32,73	2.44	8 (33%)	31,54,113	2.76	19 (61%)
18	CLA	A	1117	-	24,32,73	2.32	8 (33%)	31,54,113	2.77	18 (58%)
18	CLA	A	1124	-	24,32,73	2.39	7 (29%)	31,54,113	2.93	18 (58%)
18	CLA	4	4003	-	24,32,73	2.36	8 (33%)	31,54,113	2.73	19 (61%)
18	CLA	J	2107	10	65,69,73	2.24	15 (23%)	77,108,113	2.67	25 (32%)
18	CLA	1	1012	14	24,32,73	2.32	8 (33%)	31,54,113	2.97	19 (61%)
18	CLA	4	4012	-	24,32,73	2.49	9 (37%)	31,54,113	2.94	19 (61%)
18	CLA	B	1210	-	24,32,73	2.36	8 (33%)	31,54,113	2.77	19 (61%)
18	CLA	A	1111	-	24,32,73	2.43	8 (33%)	31,54,113	2.78	18 (58%)
18	CLA	4	4004	-	24,32,73	2.36	10 (41%)	31,54,113	2.76	17 (54%)
18	CLA	A	1134	1	24,32,73	2.31	8 (33%)	31,54,113	2.89	20 (64%)
18	CLA	B	1241	-	24,32,73	2.40	8 (33%)	31,54,113	2.76	18 (58%)
18	CLA	G	1248	-	24,32,73	2.33	10 (41%)	31,54,113	2.98	19 (61%)
20	BCR	F	6016	-	41,41,41	1.28	2 (4%)	56,56,56	4.95	32 (57%)
18	CLA	A	1119	-	59,63,73	2.39	14 (23%)	70,101,113	2.73	25 (35%)
18	CLA	A	1118	-	24,32,73	2.38	9 (37%)	31,54,113	2.88	19 (61%)
19	PQN	A	5001	-	34,34,34	1.78	2 (5%)	43,45,45	1.43	5 (11%)
18	CLA	2	2010	-	24,32,73	2.35	8 (33%)	31,54,113	2.86	18 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	A	1133	-	24,32,73	2.41	9 (37%)	31,54,113	2.73	18 (58%)
18	CLA	B	1225	2	49,53,73	2.60	16 (32%)	58,89,113	3.50	30 (51%)
18	CLA	A	1126	1	59,63,73	2.41	18 (30%)	70,101,113	3.05	32 (45%)
18	CLA	B	1227	2	54,58,73	2.42	16 (29%)	64,95,113	2.98	27 (42%)
18	CLA	B	1228	2	59,63,73	2.37	18 (30%)	70,101,113	3.15	28 (40%)
18	CLA	1	1007	-	24,32,73	2.37	8 (33%)	31,54,113	2.75	19 (61%)
18	CLA	3	3012	-	24,32,73	2.34	10 (41%)	31,54,113	2.72	18 (58%)
18	CLA	4	4009	-	24,32,73	2.33	8 (33%)	31,54,113	2.84	17 (54%)
18	CLA	A	1147	1	24,32,73	2.35	9 (37%)	31,54,113	2.80	18 (58%)
18	CLA	F	1302	-	59,63,73	2.29	14 (23%)	70,101,113	2.74	26 (37%)
18	CLA	B	9012	-	59,63,73	2.44	16 (27%)	70,101,113	2.87	33 (47%)
18	CLA	A	1129	-	59,63,73	2.40	16 (27%)	70,101,113	2.88	29 (41%)
18	CLA	B	1239	2	59,63,73	2.35	15 (25%)	70,101,113	2.75	26 (37%)
18	CLA	A	1131	-	48,52,73	2.71	14 (29%)	59,88,113	2.83	26 (44%)
18	CLA	B	1236	-	50,54,73	2.54	15 (30%)	59,90,113	3.21	23 (38%)
18	CLA	2	2004	-	24,32,73	2.39	8 (33%)	31,54,113	2.84	20 (64%)
18	CLA	L	1130	-	54,58,73	2.46	16 (29%)	64,95,113	2.74	27 (42%)
18	CLA	B	1206	2	24,32,73	2.36	9 (37%)	31,54,113	2.86	20 (64%)
18	CLA	B	1224	-	55,59,73	2.35	17 (30%)	64,96,113	2.63	27 (42%)
18	CLA	L	1125	-	24,32,73	2.37	8 (33%)	31,54,113	2.75	17 (54%)
18	CLA	B	1209	-	59,63,73	2.35	16 (27%)	70,101,113	2.80	26 (37%)
18	CLA	A	1132	-	24,32,73	2.37	9 (37%)	31,54,113	2.80	19 (61%)
18	CLA	H	1505	8	24,32,73	2.32	9 (37%)	31,54,113	2.84	18 (58%)
18	CLA	A	1107	1	61,65,73	2.42	17 (27%)	72,103,113	3.03	31 (43%)
18	CLA	1	1008	14	24,32,73	2.37	8 (33%)	31,54,113	2.80	18 (58%)
18	CLA	3	2009	-	24,32,73	2.34	8 (33%)	31,54,113	2.83	18 (58%)
18	CLA	L	1504	-	59,63,73	2.29	15 (25%)	70,101,113	2.78	23 (32%)
18	CLA	3	3003	16	24,32,73	2.37	8 (33%)	31,54,113	2.70	17 (54%)
18	CLA	A	1104	1	24,32,73	2.30	8 (33%)	31,54,113	2.62	16 (51%)
18	CLA	B	1201	-	24,32,73	2.42	8 (33%)	31,54,113	2.91	19 (61%)
18	CLA	B	1232	-	59,63,73	2.34	14 (23%)	70,101,113	2.78	22 (31%)
18	CLA	3	3010	-	24,32,73	2.32	8 (33%)	31,54,113	2.74	17 (54%)
18	CLA	J	1307	-	24,32,73	2.40	8 (33%)	31,54,113	2.77	19 (61%)
18	CLA	3	3015	-	24,32,73	2.33	8 (33%)	31,54,113	2.75	19 (61%)
18	CLA	L	1502	12	55,59,73	2.46	15 (27%)	64,96,113	2.77	25 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	4	4010	-	24,32,73	2.36	8 (33%)	31,54,113	2.78	18 (58%)
21	SF4	C	3102	3	0,12,12	-	-	-		
18	CLA	2	2008	-	24,32,73	2.32	8 (33%)	31,54,113	2.86	19 (61%)
21	SF4	B	3101	2,1	0,12,12	-	-	-		
18	CLA	B	9023	-	51,55,73	2.47	18 (35%)	60,91,113	3.00	26 (43%)
20	BCR	A	6011	-	41,41,41	1.42	3 (7%)	56,56,56	4.59	17 (30%)
18	CLA	B	1219	2	55,59,73	2.44	13 (23%)	64,96,113	2.90	25 (39%)
18	CLA	B	1213	2	24,32,73	2.32	8 (33%)	31,54,113	2.79	18 (58%)
18	CLA	4	4008	-	24,32,73	2.35	8 (33%)	31,54,113	2.78	18 (58%)
18	CLA	L	1503	-	50,54,73	2.95	24 (48%)	61,90,113	3.74	31 (50%)
18	CLA	2	2011	-	24,32,73	2.35	8 (33%)	31,54,113	2.81	19 (61%)
18	CLA	3	3013	-	24,32,73	2.35	8 (33%)	31,54,113	2.80	19 (61%)
18	CLA	1	1003	-	24,32,73	2.31	8 (33%)	31,54,113	2.75	17 (54%)
18	CLA	2	2005	-	24,32,73	2.42	8 (33%)	31,54,113	2.77	18 (58%)
18	CLA	A	1110	-	24,32,73	2.34	8 (33%)	31,54,113	2.93	19 (61%)
18	CLA	K	1150	-	24,32,73	2.34	8 (33%)	31,54,113	2.83	19 (61%)
18	CLA	A	1136	1	59,63,73	2.31	15 (25%)	70,101,113	3.04	29 (41%)
18	CLA	G	1233	-	55,59,73	2.49	16 (29%)	64,96,113	2.81	21 (32%)
18	CLA	3	3005	-	24,32,73	2.33	9 (37%)	31,54,113	2.94	19 (61%)
18	CLA	3	3008	-	24,32,73	2.36	8 (33%)	31,54,113	2.91	17 (54%)
18	CLA	1	1004	-	24,32,73	2.38	8 (33%)	31,54,113	2.74	19 (61%)
18	CLA	F	1240	-	24,32,73	2.38	8 (33%)	31,54,113	2.98	20 (64%)
18	CLA	B	1215	2	56,60,73	2.40	16 (28%)	65,97,113	2.95	34 (52%)
18	CLA	3	3002	-	24,32,73	2.36	8 (33%)	31,54,113	2.81	18 (58%)
18	CLA	A	1146	-	24,32,73	2.41	8 (33%)	31,54,113	2.72	18 (58%)
18	CLA	1	1002	-	24,32,73	2.34	8 (33%)	31,54,113	2.81	17 (54%)
18	CLA	4	4006	-	24,32,73	2.45	8 (33%)	31,54,113	2.85	19 (61%)
18	CLA	B	9010	2	51,55,73	2.52	17 (33%)	60,91,113	3.13	30 (50%)
18	CLA	A	1148	-	24,32,73	2.34	8 (33%)	31,54,113	2.89	18 (58%)
18	CLA	B	1216	-	60,64,73	2.37	14 (23%)	71,102,113	2.72	26 (36%)
18	CLA	B	1218	-	55,59,73	2.77	23 (41%)	64,96,113	3.03	27 (42%)
18	CLA	B	1220	-	64,68,73	2.19	16 (25%)	76,107,113	2.99	28 (36%)
18	CLA	2	2012	-	24,32,73	2.39	10 (41%)	31,54,113	2.79	19 (61%)
18	CLA	2	2007	-	24,32,73	2.31	8 (33%)	31,54,113	2.89	19 (61%)
18	CLA	1	1005	-	24,32,73	2.41	8 (33%)	31,54,113	2.82	18 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	A	1116	-	24,32,73	2.36	9 (37%)	31,54,113	2.85	18 (58%)
18	CLA	A	1151	-	24,32,73	2.36	8 (33%)	31,54,113	2.76	18 (58%)
18	CLA	B	1138	-	60,64,73	2.38	17 (28%)	71,102,113	2.63	29 (40%)
18	CLA	H	1501	-	59,63,73	2.35	15 (25%)	70,101,113	2.83	30 (42%)
18	CLA	3	3007	-	24,32,73	2.28	8 (33%)	31,54,113	2.94	17 (54%)
18	CLA	B	1211	2	24,32,73	2.30	8 (33%)	31,54,113	2.91	19 (61%)
18	CLA	F	1306	-	24,32,73	2.42	8 (33%)	31,54,113	2.81	19 (61%)
18	CLA	A	1120	-	24,32,73	2.38	8 (33%)	31,54,113	2.90	18 (58%)
18	CLA	J	1308	-	24,32,73	2.36	8 (33%)	31,54,113	2.90	17 (54%)
18	CLA	A	1143	-	24,32,73	2.38	8 (33%)	31,54,113	2.78	19 (61%)
18	CLA	B	1202	-	54,58,73	2.52	16 (29%)	64,95,113	3.40	28 (43%)
18	CLA	B	1208	-	59,63,73	2.40	17 (28%)	70,101,113	3.10	35 (50%)
18	CLA	B	1214	-	53,57,73	2.52	17 (32%)	61,93,113	2.85	27 (44%)
18	CLA	B	1231	2	50,54,73	2.59	15 (30%)	59,90,113	2.99	22 (37%)
18	CLA	B	1234	2	54,58,73	2.45	15 (27%)	64,95,113	2.83	25 (39%)
18	CLA	B	1229	-	53,57,73	2.67	17 (32%)	65,94,113	3.19	24 (36%)
18	CLA	4	4005	-	24,32,73	2.39	8 (33%)	31,54,113	2.96	20 (64%)
19	PQN	B	5002	-	34,34,34	1.81	2 (5%)	43,45,45	1.62	8 (18%)
18	CLA	3	3011	-	24,32,73	2.36	8 (33%)	31,54,113	2.72	17 (54%)
18	CLA	B	1237	-	55,59,73	2.42	14 (25%)	64,96,113	3.26	28 (43%)
18	CLA	1	1014	-	24,32,73	2.34	8 (33%)	31,54,113	2.86	19 (61%)
18	CLA	A	1109	-	24,30,73	2.98	10 (41%)	28,49,113	2.94	14 (50%)
18	CLA	2	2013	-	24,32,73	2.37	8 (33%)	31,54,113	2.77	18 (58%)
18	CLA	B	1207	2	59,63,73	2.28	17 (28%)	70,101,113	3.12	30 (42%)

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
18	CLA	B	1219	2	-	13/23/99/115	-
18	CLA	B	1212	-	1/1/14/20	20/33/109/115	-
18	CLA	L	1503	-	-	6/16/92/115	-
18	CLA	B	1236	-	-	5/17/93/115	-
18	CLA	B	1242	-	-	12/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1135	-	-	8/15/91/115	-
20	BCR	F	6016	-	-	13/29/63/63	0/2/2/2
18	CLA	A	1113	-	-	6/21/97/115	-
18	CLA	A	1119	-	1/1/13/20	14/27/103/115	-
18	CLA	A	9011	1	1/1/13/20	12/27/103/115	-
18	CLA	A	1136	1	1/1/13/20	12/27/103/115	-
19	PQN	A	5001	-	1/1/8/9	11/23/43/43	0/2/2/2
18	CLA	G	1233	-	-	10/23/99/115	-
18	CLA	B	1225	2	-	6/15/91/115	-
18	CLA	B	9022	-	-	13/26/102/115	-
18	CLA	A	1126	1	1/1/13/20	13/27/103/115	-
18	CLA	B	1227	2	-	10/21/97/115	-
18	CLA	B	1228	2	1/1/13/20	10/27/103/115	-
18	CLA	A	1108	1	-	6/21/97/115	-
18	CLA	B	1215	2	-	13/24/100/115	-
18	CLA	B	1221	-	-	13/19/95/115	-
18	CLA	A	1128	-	1/1/13/20	10/27/103/115	-
21	SF4	C	3103	3	-	-	0/6/5/5
18	CLA	F	1302	-	1/1/13/20	7/27/103/115	-
18	CLA	B	1203	18	-	11/19/95/115	-
18	CLA	B	1238	-	-	11/26/102/115	-
18	CLA	B	9012	-	1/1/13/20	16/27/103/115	-
18	CLA	A	1129	-	1/1/13/20	10/27/103/115	-
18	CLA	B	1239	2	1/1/13/20	6/27/103/115	-
18	CLA	B	9010	2	-	7/18/94/115	-
18	CLA	A	1123	-	1/1/13/20	15/27/103/115	-
18	CLA	A	1131	-	-	6/13/89/115	-
18	CLA	B	1216	-	1/1/13/20	11/29/105/115	-
18	CLA	B	1222	-	1/1/15/20	19/39/115/115	-
18	CLA	A	1103	1	-	11/18/94/115	-
18	CLA	B	1218	-	-	11/23/99/115	-
18	CLA	B	1224	-	-	5/23/99/115	-
18	CLA	A	1137	-	1/1/13/20	14/27/103/115	-
18	CLA	B	1220	-	1/1/14/20	18/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	1209	-	1/1/13/20	13/27/103/115	-
18	CLA	L	1130	-	-	4/21/97/115	-
20	BCR	B	6017	-	-	19/29/63/63	0/2/2/2
18	CLA	B	1217	-	-	7/21/97/115	-
18	CLA	I	1204	-	1/1/13/20	17/27/103/115	-
20	BCR	L	6020	-	-	16/29/63/63	0/2/2/2
18	CLA	A	1107	1	1/1/13/20	19/30/106/115	-
18	CLA	B	1138	-	1/1/13/20	13/29/105/115	-
18	CLA	A	1122	-	1/1/13/20	8/27/103/115	-
18	CLA	H	1501	-	1/1/13/20	10/27/103/115	-
18	CLA	A	9013	-	-	4/17/93/115	-
18	CLA	L	1504	-	1/1/13/20	10/27/103/115	-
18	CLA	A	1140	1	1/1/13/20	13/27/103/115	-
18	CLA	A	1106	-	-	3/10/86/115	-
18	CLA	B	1232	-	1/1/13/20	11/27/103/115	-
18	CLA	F	1139	-	-	8/14/90/115	-
18	CLA	B	1205	2	1/1/13/20	13/27/103/115	-
18	CLA	B	1202	-	-	7/21/97/115	-
18	CLA	B	1208	-	1/1/13/20	13/27/103/115	-
18	CLA	J	2107	10	1/1/14/20	14/35/111/115	-
18	CLA	B	1214	-	-	7/20/96/115	-
18	CLA	L	1502	12	-	9/23/99/115	-
18	CLA	B	1231	2	-	9/17/93/115	-
21	SF4	B	3101	2,1	-	-	0/6/5/5
18	CLA	B	1234	2	-	9/21/97/115	-
18	CLA	B	1229	-	-	8/19/95/115	-
21	SF4	C	3102	3	-	-	0/6/5/5
19	PQN	B	5002	-	1/1/8/9	9/23/43/43	0/2/2/2
20	BCR	A	6011	-	-	15/29/63/63	0/2/2/2
18	CLA	4	1304	-	1/1/13/20	10/27/103/115	-
18	CLA	A	1115	-	-	8/18/94/115	-
18	CLA	B	1237	-	-	10/23/99/115	-
20	BCR	I	6018	-	-	11/29/63/63	0/2/2/2
18	CLA	B	9023	-	-	6/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	1207	2	1/1/13/20	12/27/103/115	-
18	CLA	B	1235	-	1/1/13/20	11/27/103/115	-

The worst 5 of 1896 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	5002	PQN	C3-C2	8.64	1.50	1.35
19	A	5001	PQN	C3-C2	8.33	1.50	1.35
18	B	1229	CLA	CAB-C3B	-7.87	1.34	1.50
18	A	1131	CLA	CAB-C3B	-7.79	1.34	1.50
20	L	6020	BCR	C11-C10	-7.61	1.19	1.43

The worst 5 of 3757 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	6011	BCR	C11-C10-C9	29.52	168.68	127.28
20	L	6020	BCR	C11-C10-C9	27.37	165.66	127.28
20	F	6016	BCR	C11-C10-C9	27.31	165.58	127.28
20	B	6017	BCR	C11-C10-C9	24.78	162.03	127.28
20	I	6018	BCR	C11-C10-C9	20.82	156.47	127.28

5 of 33 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	1107	CLA	C8
18	A	1119	CLA	C8
18	A	1122	CLA	C8
18	A	1123	CLA	C8
18	A	1126	CLA	C8

5 of 770 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	1103	CLA	C1A-C2A-CAA-CBA
18	A	1106	CLA	CHA-CBD-CGD-O1D
18	A	1106	CLA	CHA-CBD-CGD-O2D
18	A	1107	CLA	C2-C1-O2A-CGA
18	A	1107	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

131 monomers are involved in 1317 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	2003	CLA	1	0
18	A	1101	CLA	4	0
18	A	1113	CLA	6	0
18	2	2002	CLA	2	0
18	4	4001	CLA	3	0
18	B	1238	CLA	21	0
18	A	1123	CLA	25	0
18	B	1223	CLA	5	0
18	A	1103	CLA	21	0
18	B	1222	CLA	12	0
18	4	4011	CLA	1	0
18	B	1226	CLA	5	0
18	I	1204	CLA	9	0
20	L	6020	BCR	17	0
18	A	1122	CLA	4	0
18	A	9013	CLA	19	0
18	A	1105	CLA	3	0
18	A	1106	CLA	13	0
18	A	1140	CLA	23	0
18	3	3006	CLA	1	0
18	1	1013	CLA	3	0
18	F	1139	CLA	18	0
18	1	1006	CLA	2	0
18	4	4013	CLA	1	0
18	B	1205	CLA	15	0
18	B	1230	CLA	6	0
18	A	1115	CLA	8	0
18	4	1304	CLA	9	0
18	B	1235	CLA	18	0
18	B	1212	CLA	13	0
18	B	1242	CLA	20	0
18	3	3004	CLA	2	0
18	F	4015	CLA	2	0
18	A	1135	CLA	6	0
18	A	9011	CLA	22	0
18	K	1141	CLA	5	0
18	B	9022	CLA	19	0
18	2	2006	CLA	2	0
18	A	1127	CLA	6	0
18	A	1108	CLA	11	0
18	B	1221	CLA	19	0
20	I	6018	BCR	13	0
18	A	1128	CLA	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	C	3103	SF4	7	0
18	B	1203	CLA	15	0
18	F	1303	CLA	2	0
18	A	1137	CLA	18	0
20	B	6017	BCR	17	0
18	B	1217	CLA	14	0
18	B	1301	CLA	3	0
18	A	1124	CLA	14	0
18	J	2107	CLA	8	0
18	1	1012	CLA	3	0
18	4	4012	CLA	1	0
18	B	1210	CLA	15	0
18	A	1111	CLA	2	0
18	A	1134	CLA	7	0
18	B	1241	CLA	6	0
18	G	1248	CLA	4	0
20	F	6016	BCR	13	0
18	A	1119	CLA	8	0
18	A	1118	CLA	7	0
19	A	5001	PQN	30	0
18	A	1133	CLA	2	0
18	B	1225	CLA	41	0
18	A	1126	CLA	23	0
18	B	1227	CLA	20	0
18	B	1228	CLA	22	0
18	A	1147	CLA	6	0
18	F	1302	CLA	17	0
18	B	9012	CLA	18	0
18	A	1129	CLA	17	0
18	B	1239	CLA	29	0
18	A	1131	CLA	10	0
18	B	1236	CLA	11	0
18	2	2004	CLA	3	0
18	L	1130	CLA	20	0
18	B	1206	CLA	5	0
18	B	1224	CLA	14	0
18	B	1209	CLA	39	0
18	A	1132	CLA	11	0
18	H	1505	CLA	2	0
18	A	1107	CLA	18	0
18	1	1008	CLA	1	0
18	L	1504	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	1232	CLA	7	0
18	3	3010	CLA	2	0
18	L	1502	CLA	19	0
18	4	4010	CLA	1	0
21	C	3102	SF4	8	0
21	B	3101	SF4	4	0
18	B	9023	CLA	14	0
20	A	6011	BCR	17	0
18	B	1219	CLA	11	0
18	B	1213	CLA	1	0
18	L	1503	CLA	56	0
18	2	2011	CLA	1	0
18	1	1003	CLA	3	0
18	2	2005	CLA	1	0
18	A	1110	CLA	3	0
18	A	1136	CLA	22	0
18	G	1233	CLA	8	0
18	3	3005	CLA	5	0
18	F	1240	CLA	2	0
18	B	1215	CLA	21	0
18	3	3002	CLA	2	0
18	A	1146	CLA	1	0
18	B	9010	CLA	26	0
18	A	1148	CLA	4	0
18	B	1216	CLA	23	0
18	B	1218	CLA	46	0
18	B	1220	CLA	26	0
18	2	2012	CLA	5	0
18	2	2007	CLA	2	0
18	A	1116	CLA	5	0
18	B	1138	CLA	24	0
18	H	1501	CLA	12	0
18	3	3007	CLA	1	0
18	B	1211	CLA	8	0
18	A	1120	CLA	1	0
18	B	1202	CLA	42	0
18	B	1208	CLA	11	0
18	B	1214	CLA	31	0
18	B	1231	CLA	2	0
18	B	1234	CLA	26	0
18	B	1229	CLA	14	0
18	4	4005	CLA	1	0

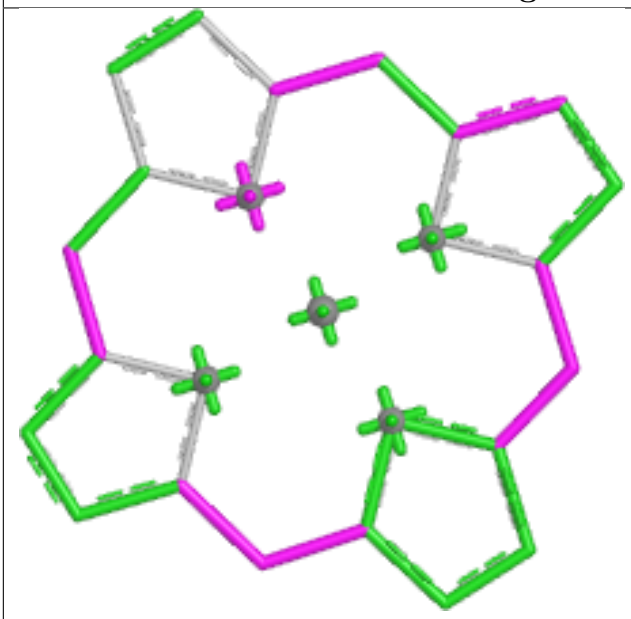
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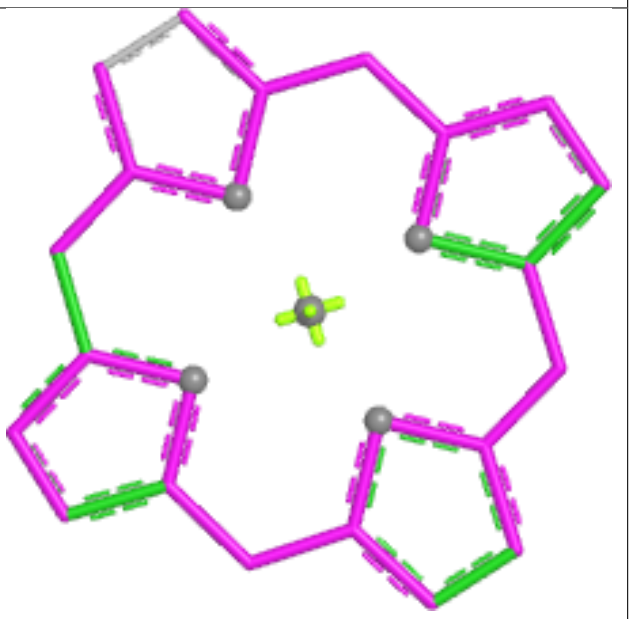
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	5002	PQN	20	0
18	B	1237	CLA	11	0
18	A	1109	CLA	12	0
18	B	1207	CLA	16	0

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.

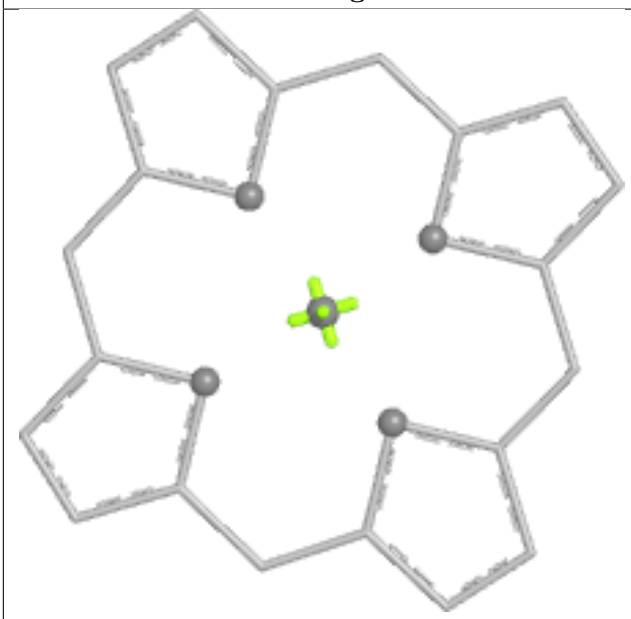
Ligand CLA 2 2015



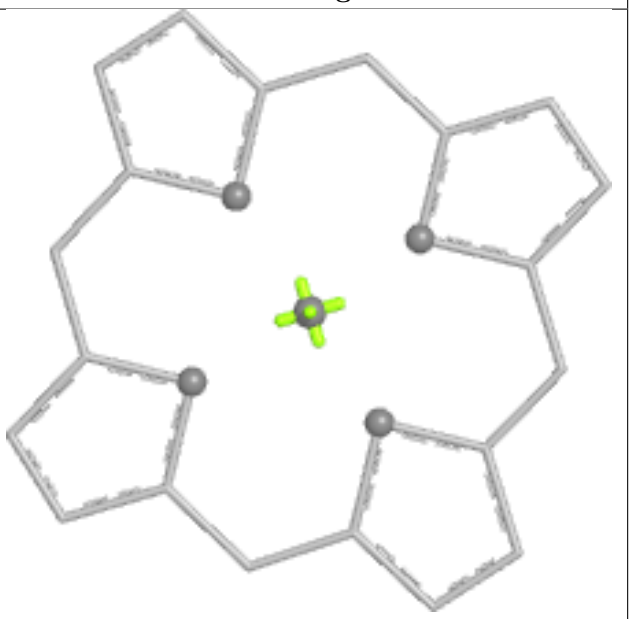
Bond lengths



Bond angles

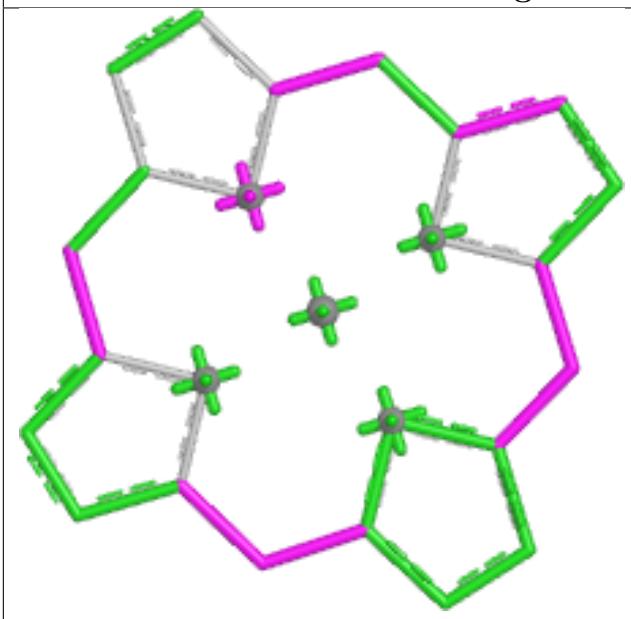


Torsions

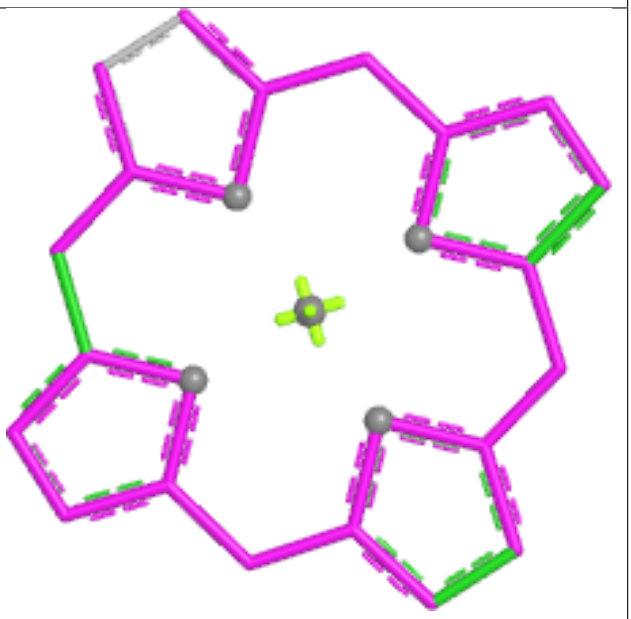


Rings

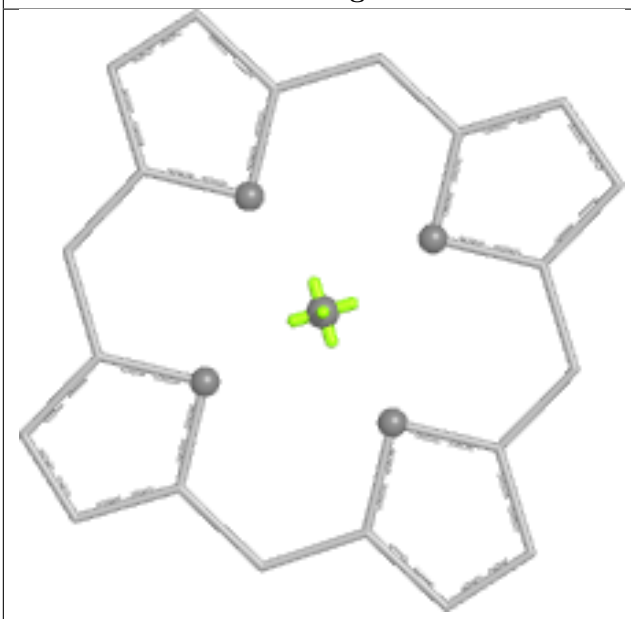
Ligand CLA K 1153



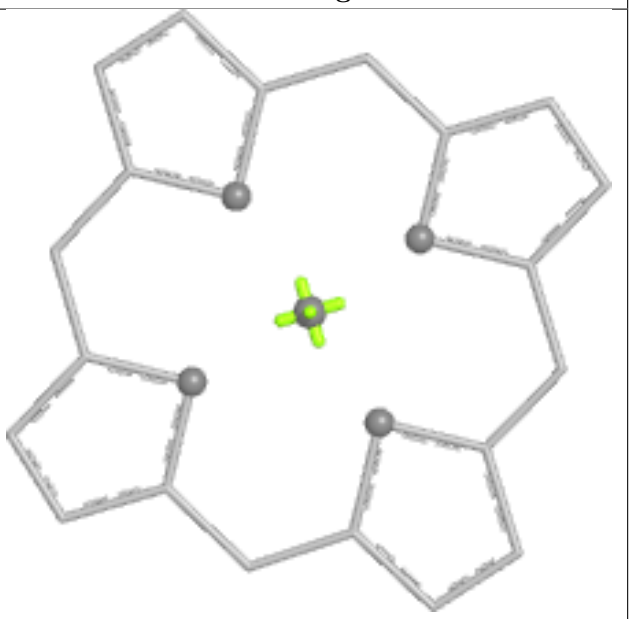
Bond lengths



Bond angles

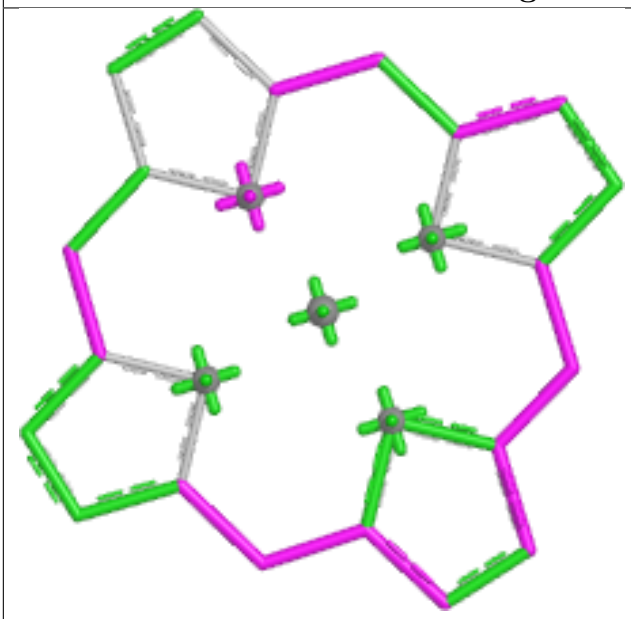


Torsions

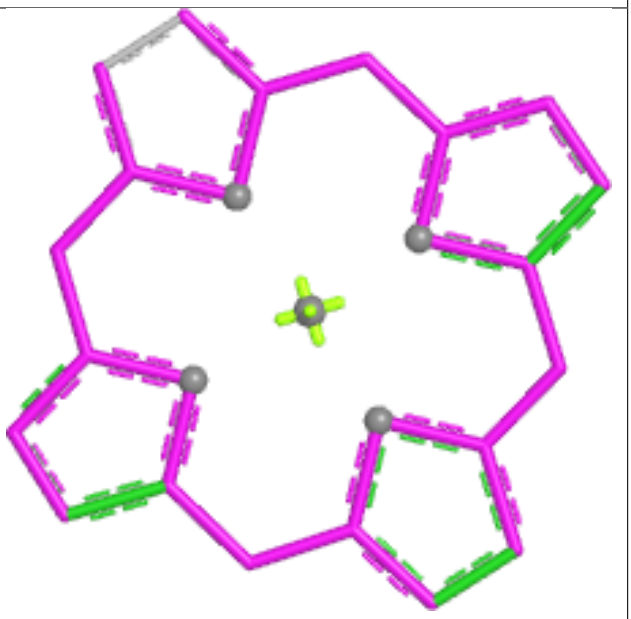


Rings

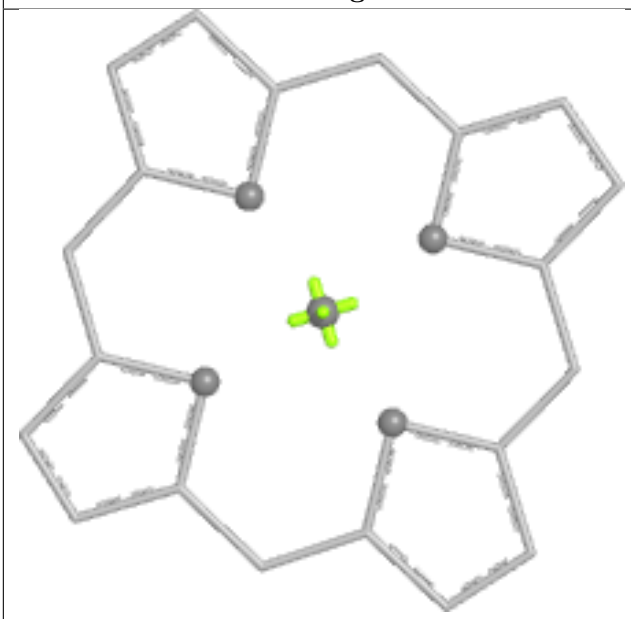
Ligand CLA 2 2003



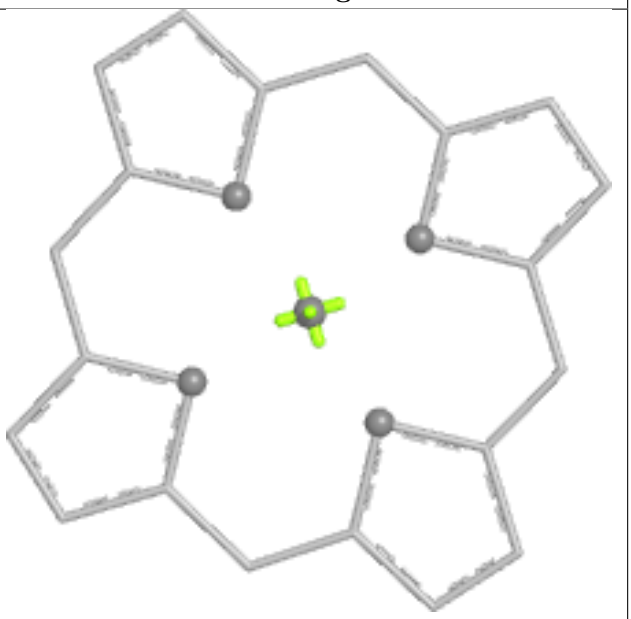
Bond lengths



Bond angles

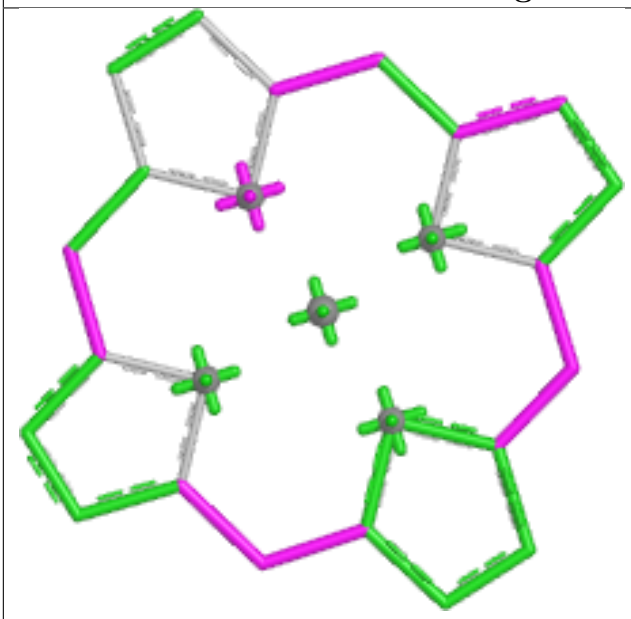


Torsions

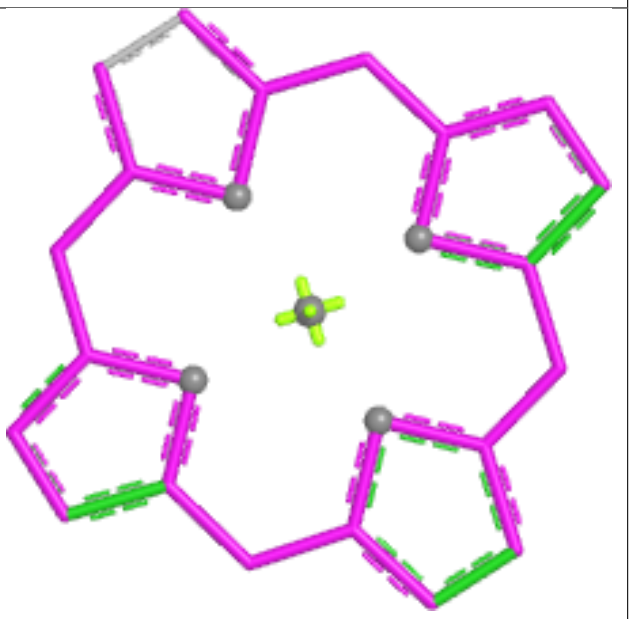


Rings

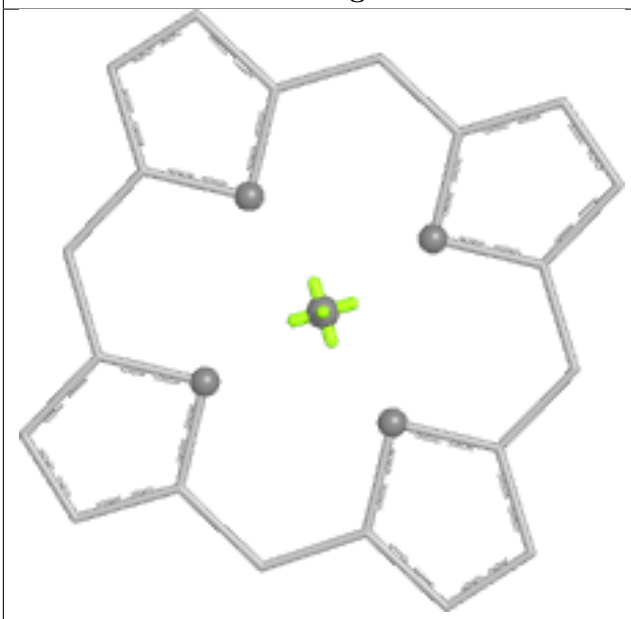
Ligand CLA A 1101



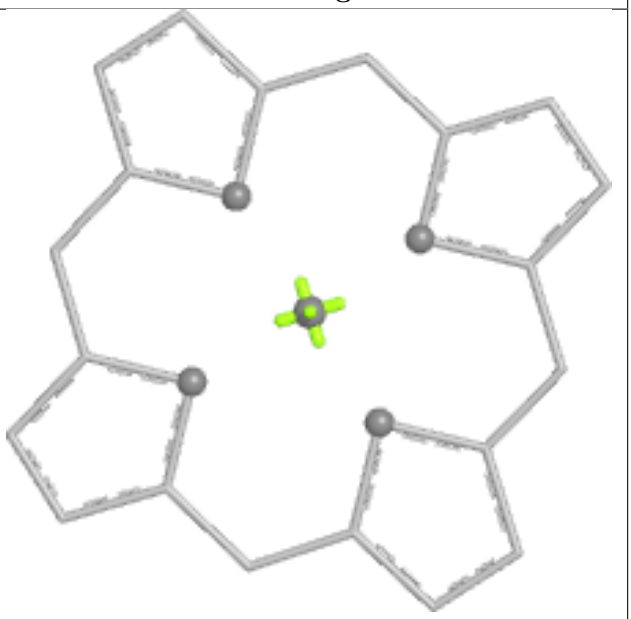
Bond lengths



Bond angles

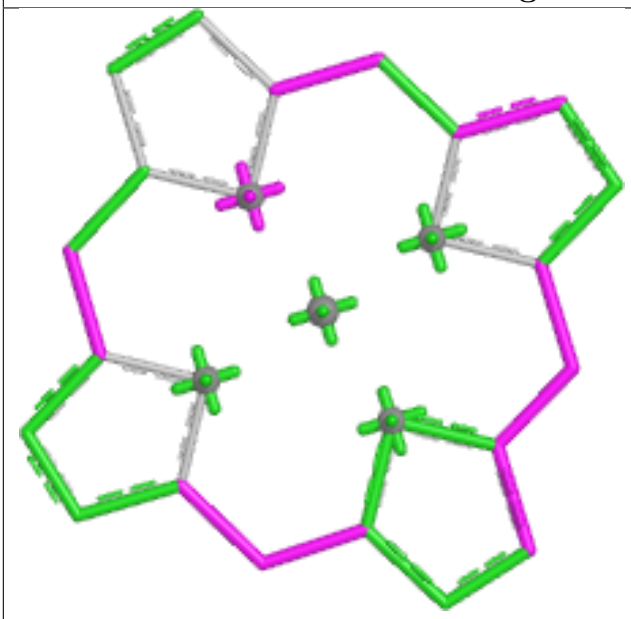


Torsions

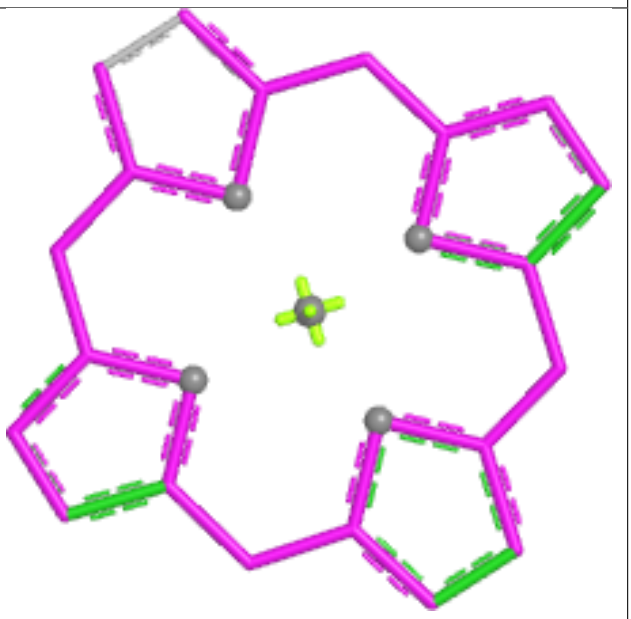


Rings

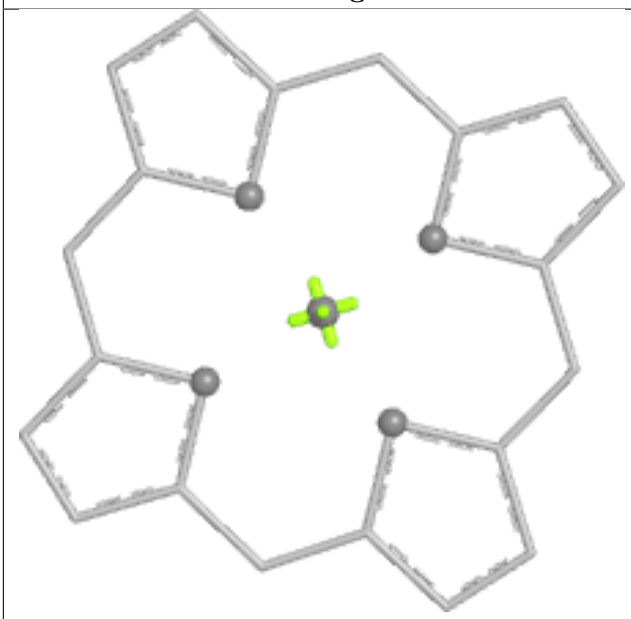
Ligand CLA 3 3009



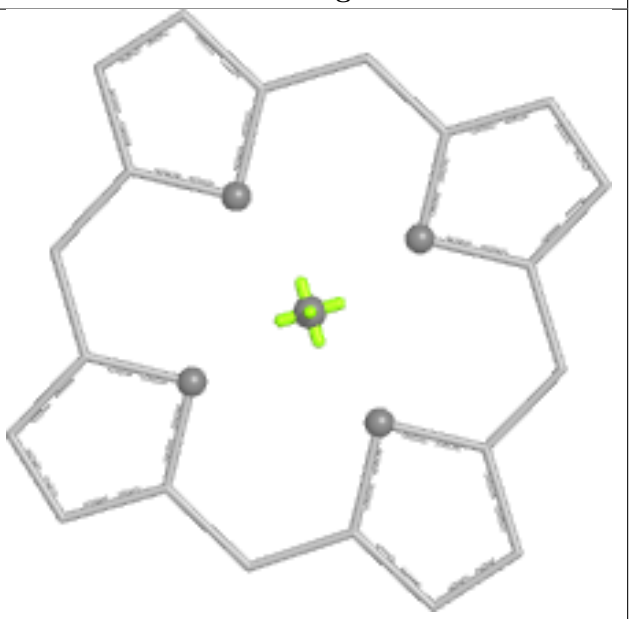
Bond lengths



Bond angles

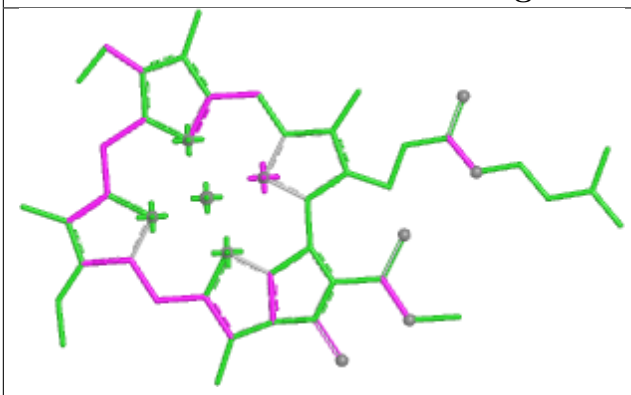


Torsions

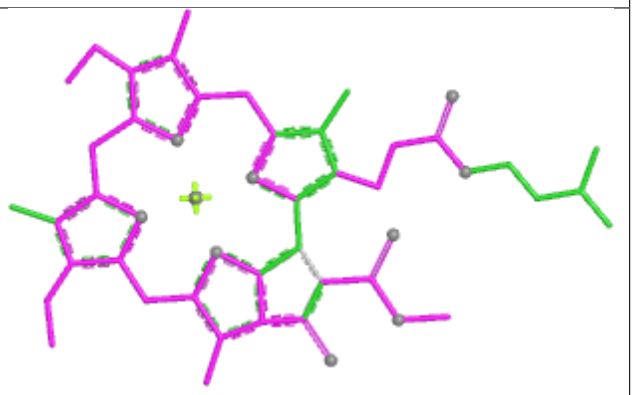


Rings

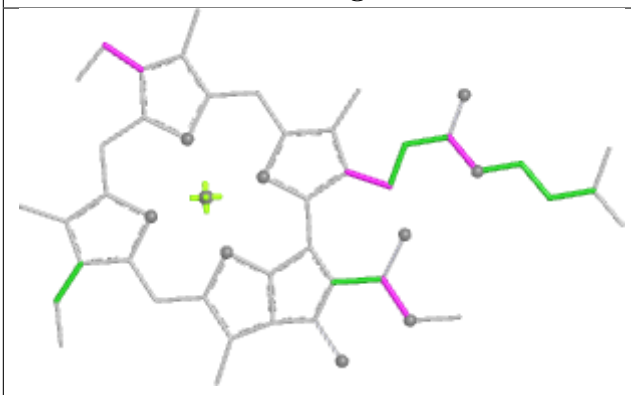
Ligand CLA A 1113



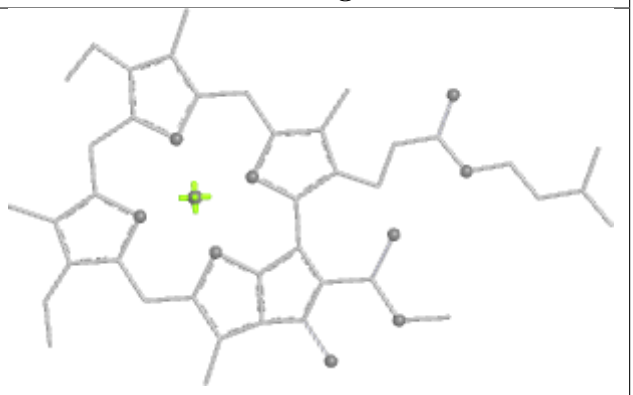
Bond lengths



Bond angles

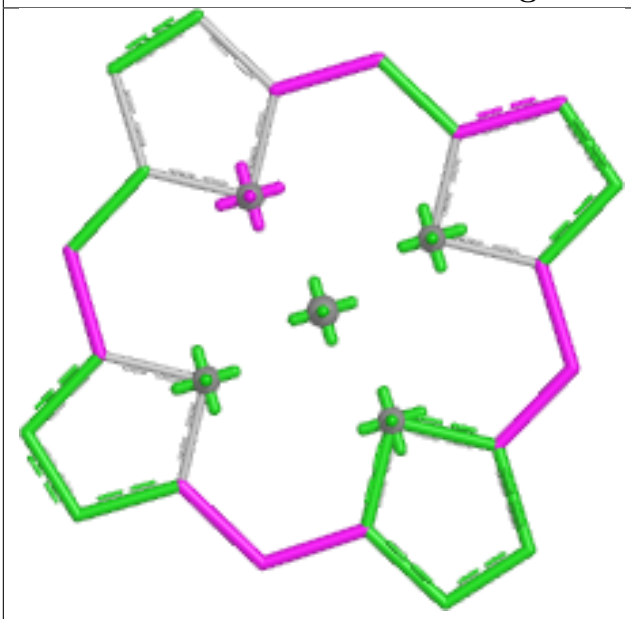


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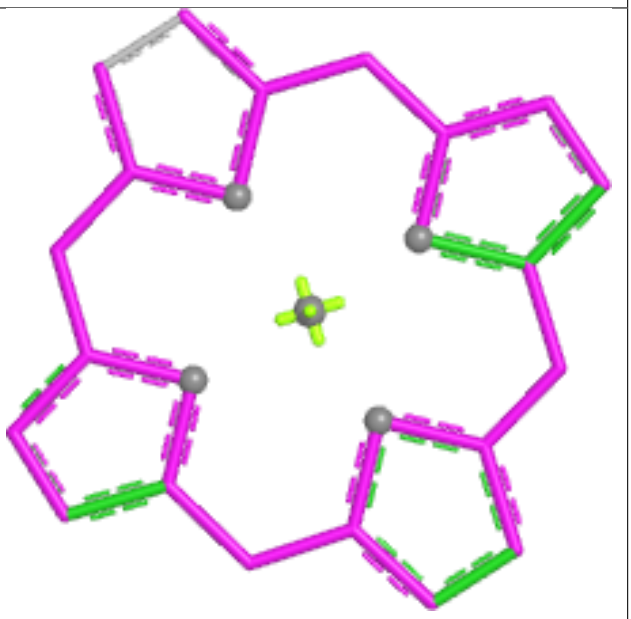


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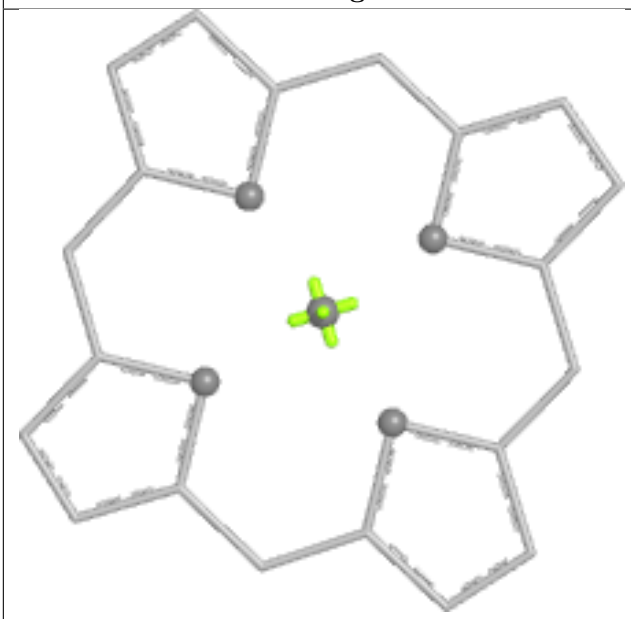
Ligand CLA 2 2002



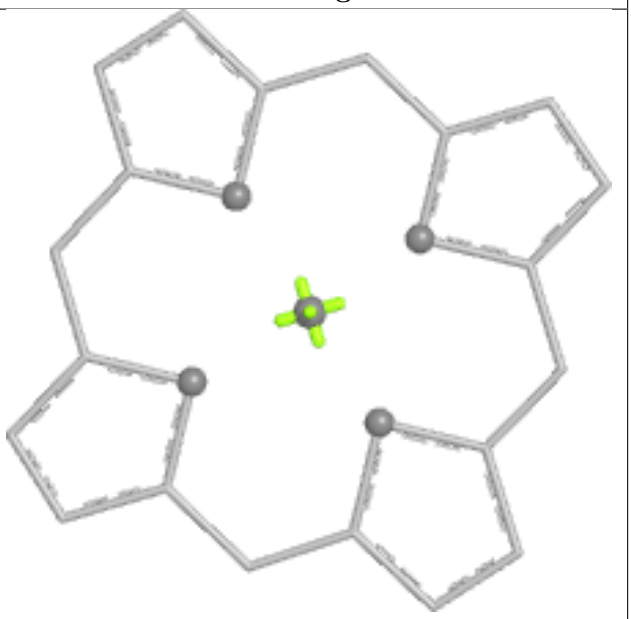
Bond lengths



Bond angles

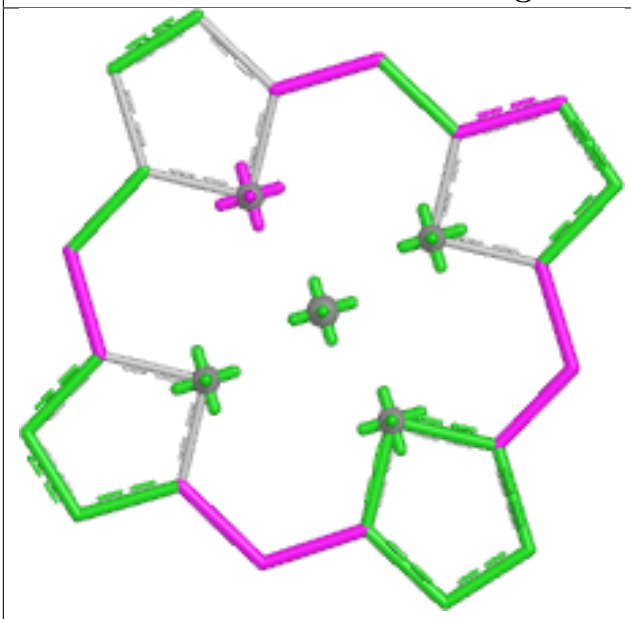


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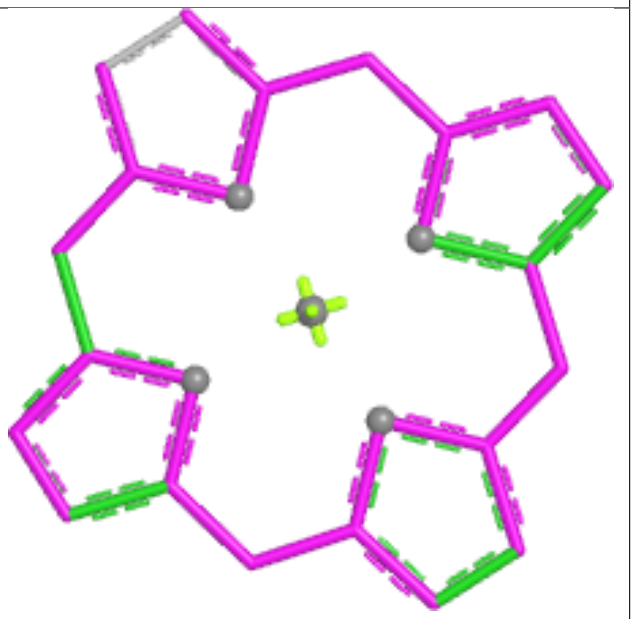


Rings

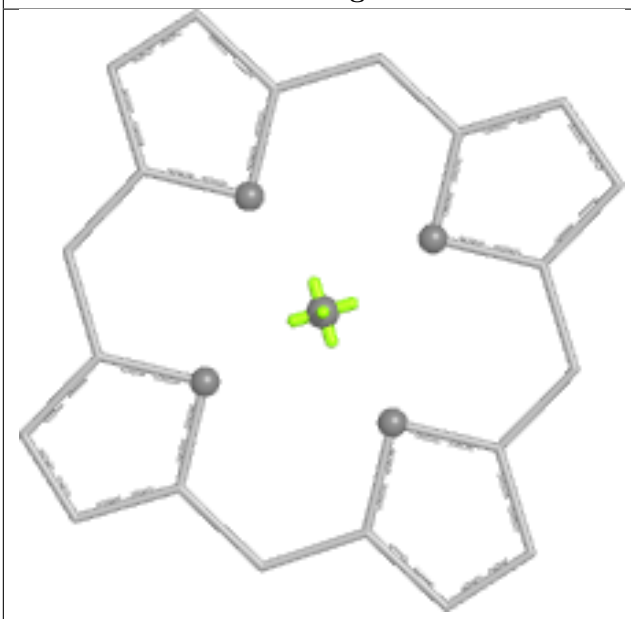
Ligand CLA A 1309



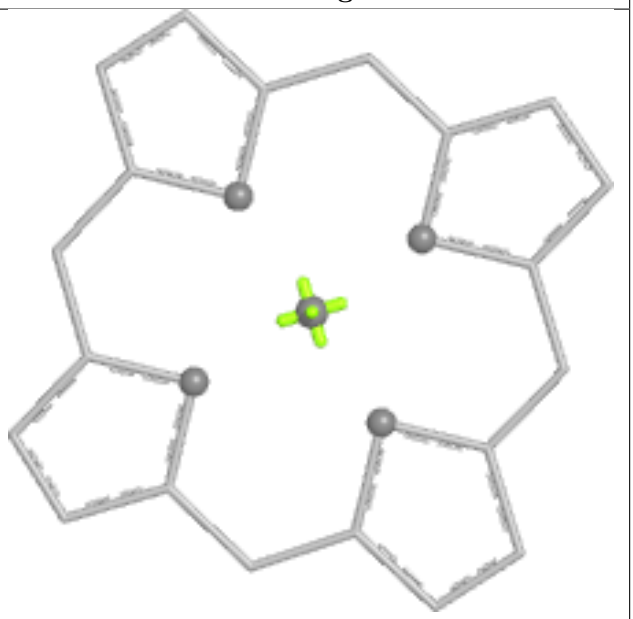
Bond lengths



Bond angles

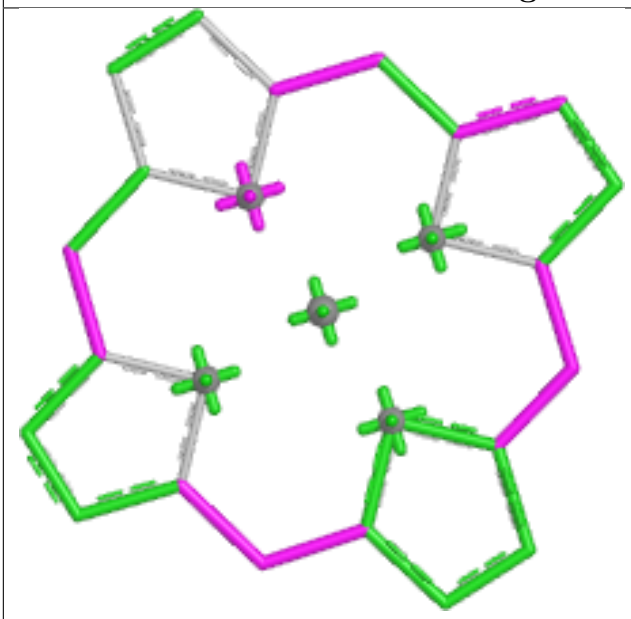


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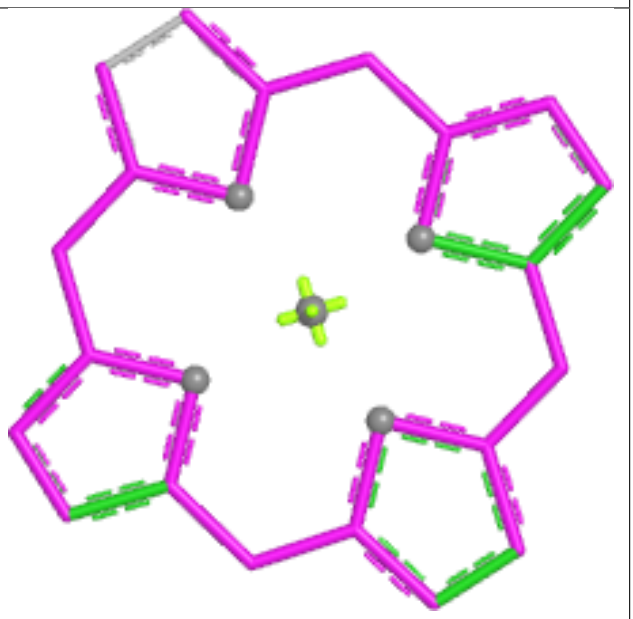


Rings

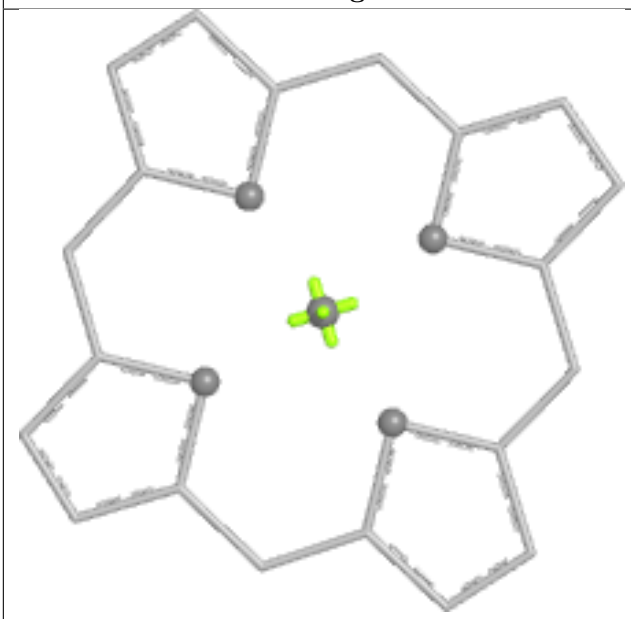
Ligand CLA 4 4001



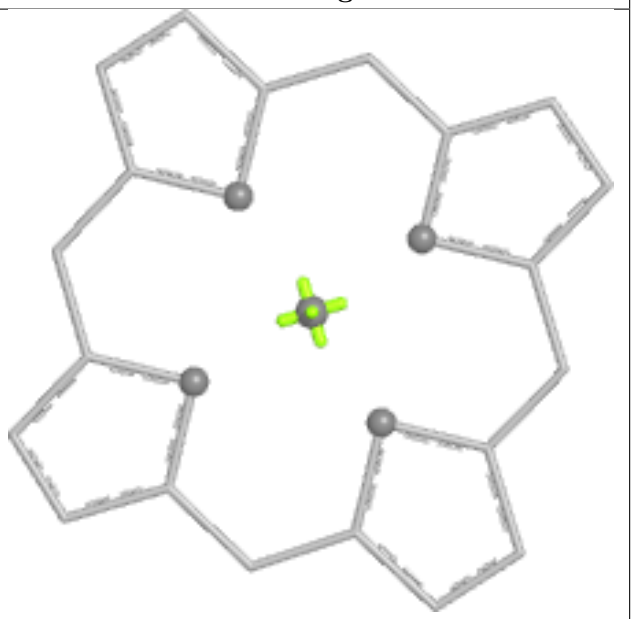
Bond lengths



Bond angles

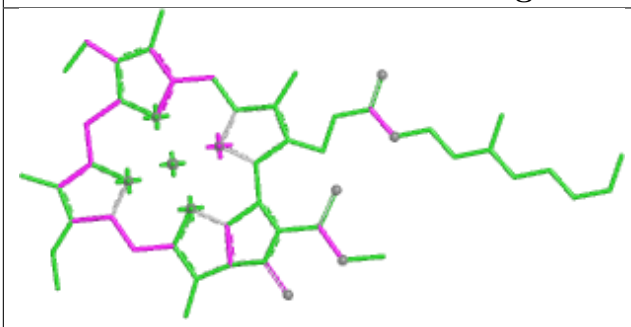


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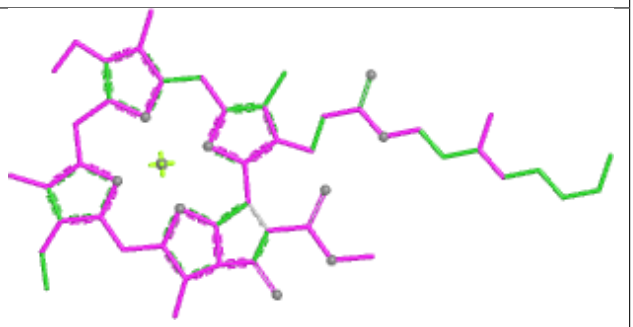


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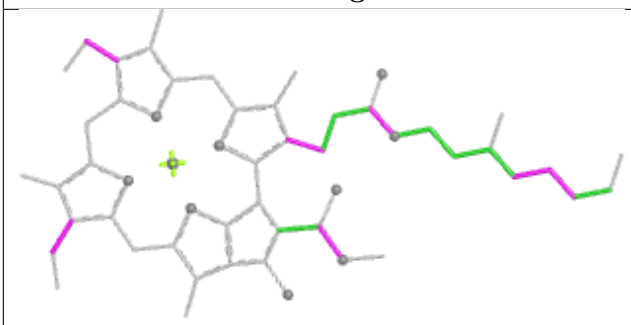
Ligand CLA B 1238



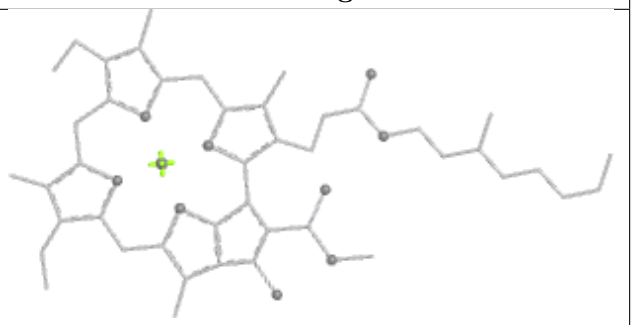
Bond lengths



Bond angles

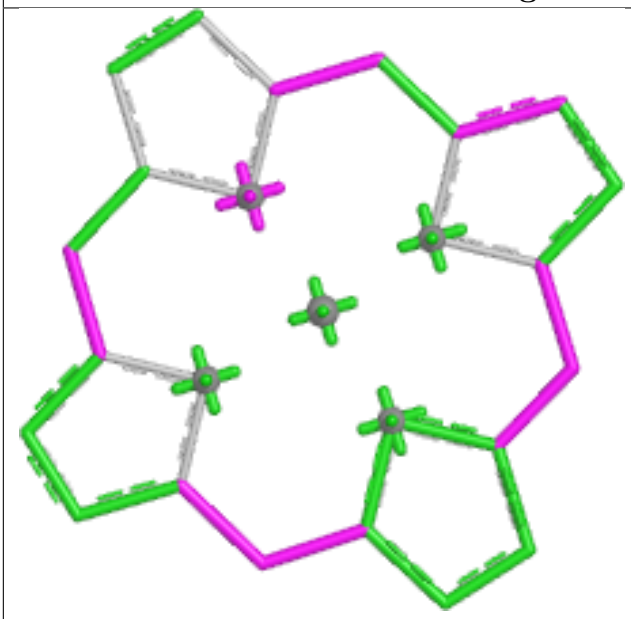


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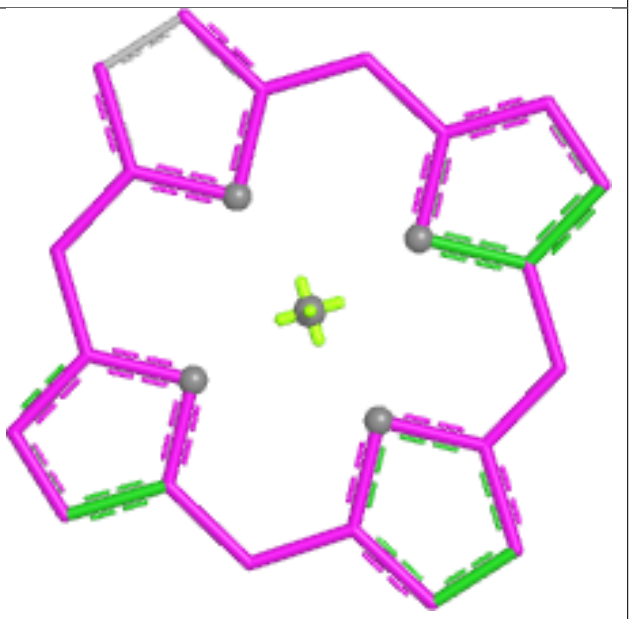


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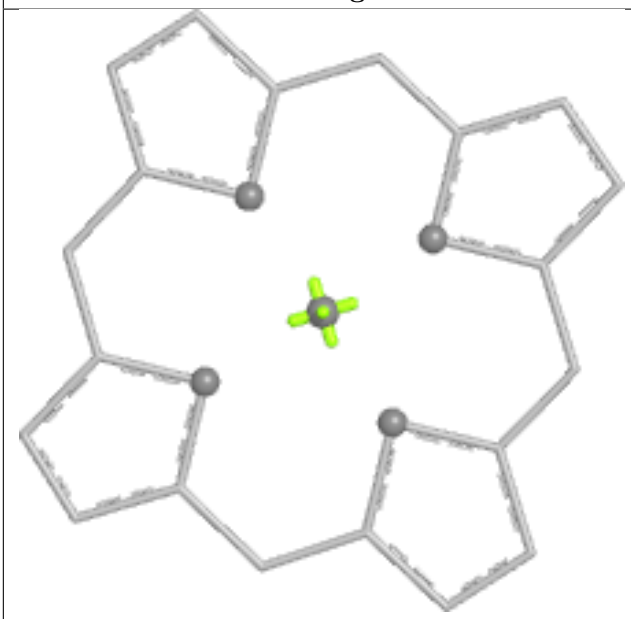
Ligand CLA 4 4007



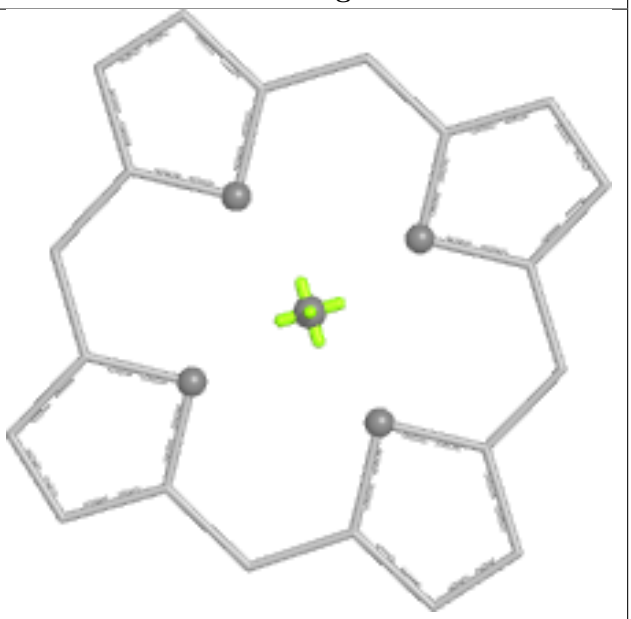
Bond lengths



Bond angles

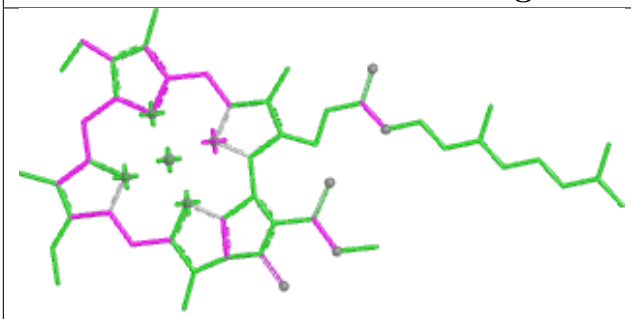


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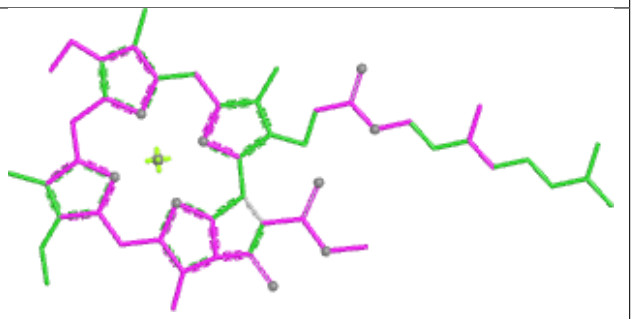


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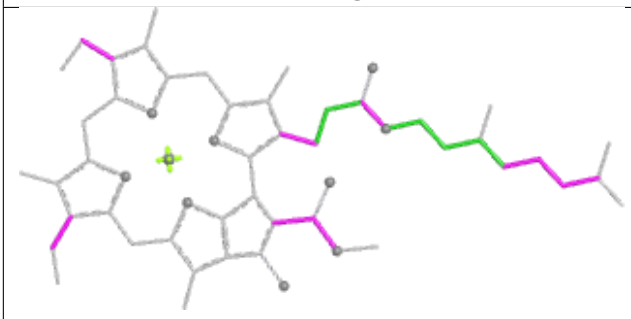
Ligand CLA A 1123



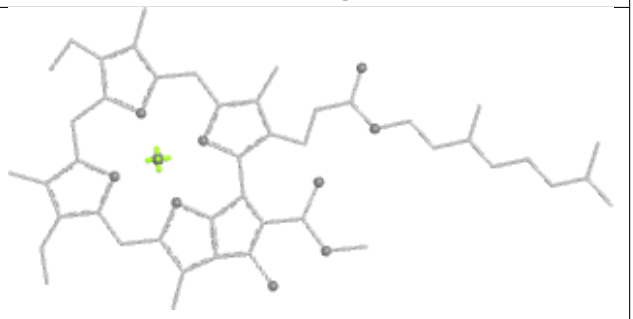
Bond lengths



Bond angles

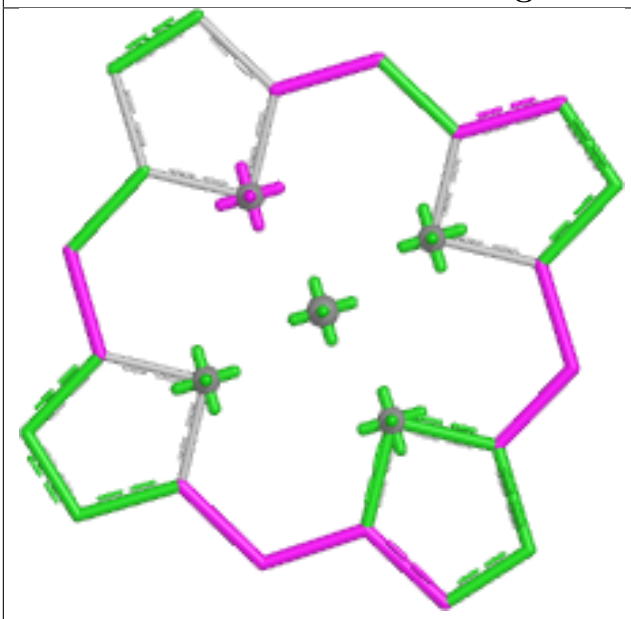


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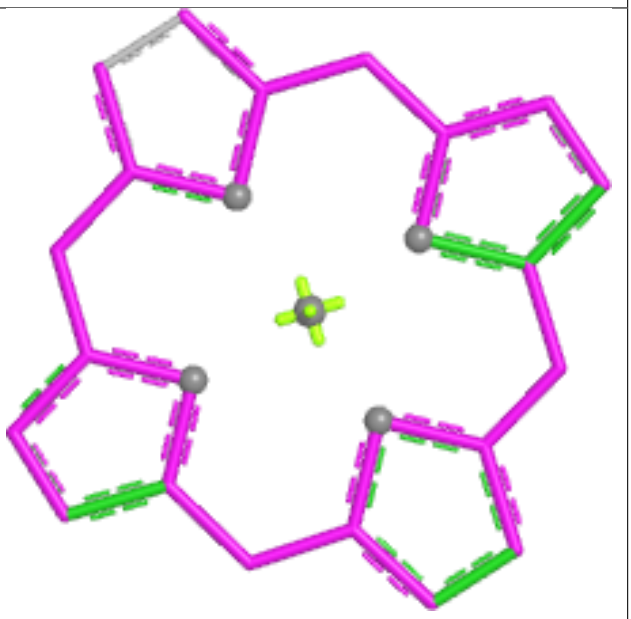


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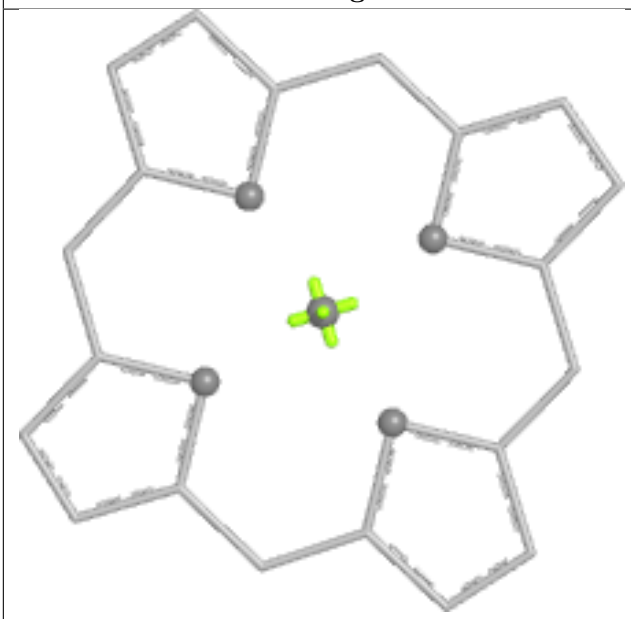
Ligand CLA B 1223



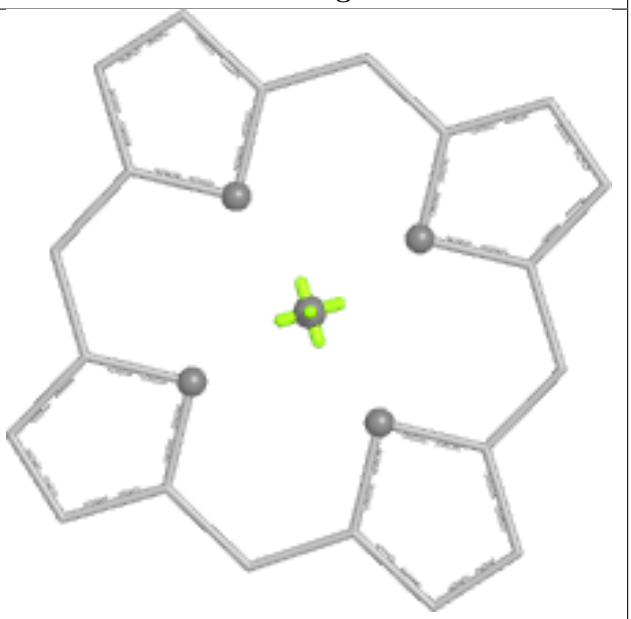
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Bond angles

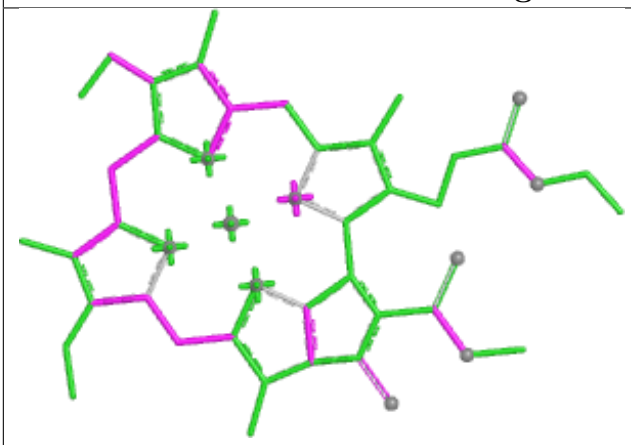


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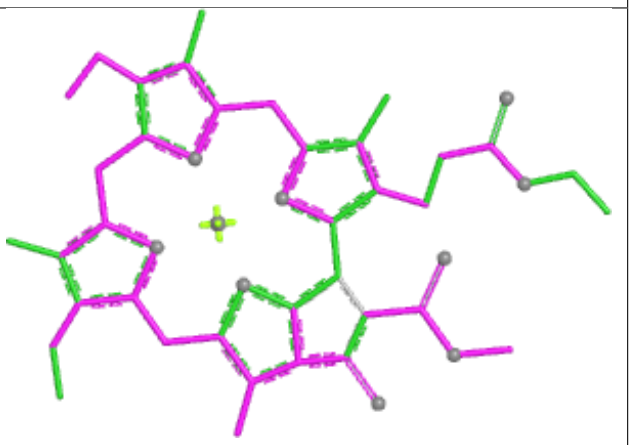


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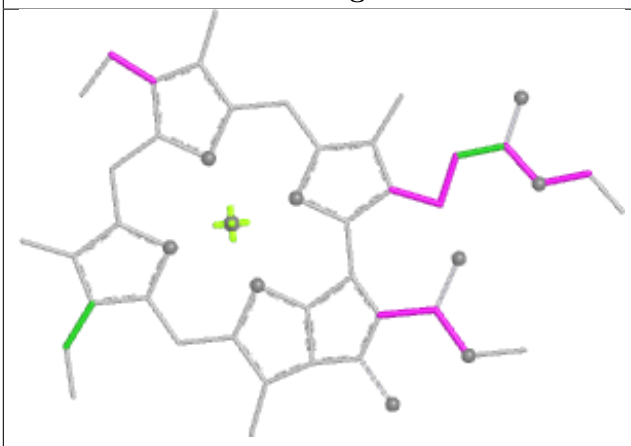
Ligand CLA A 1103



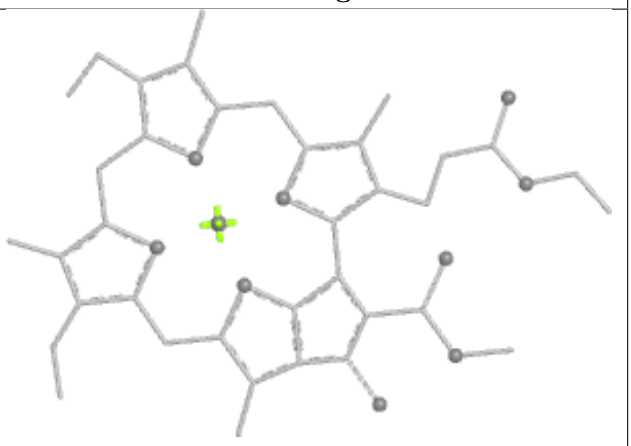
Bond lengths



Bond angles

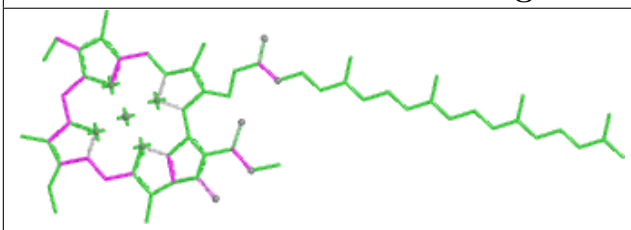


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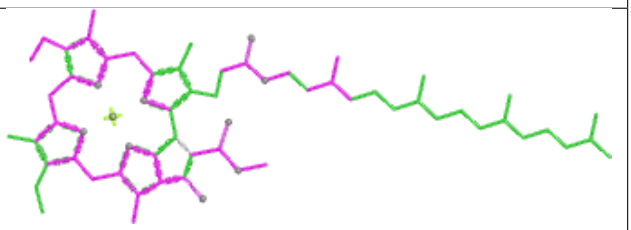


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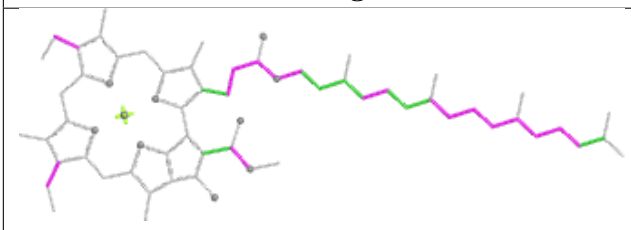
Ligand CLA B 1222



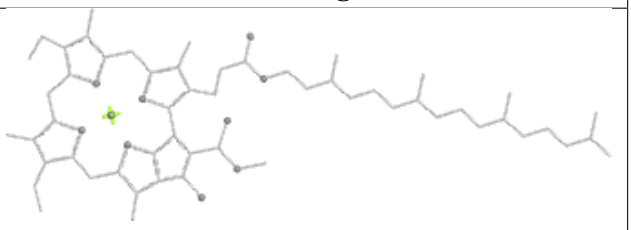
Bond lengths



Bond angles

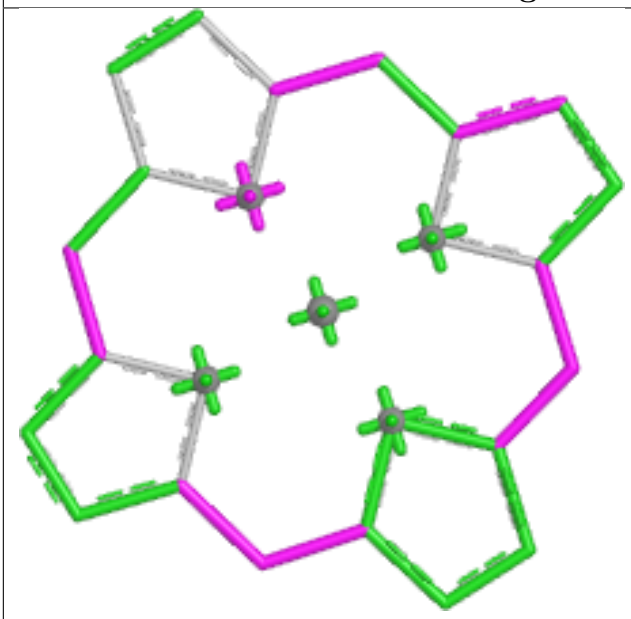


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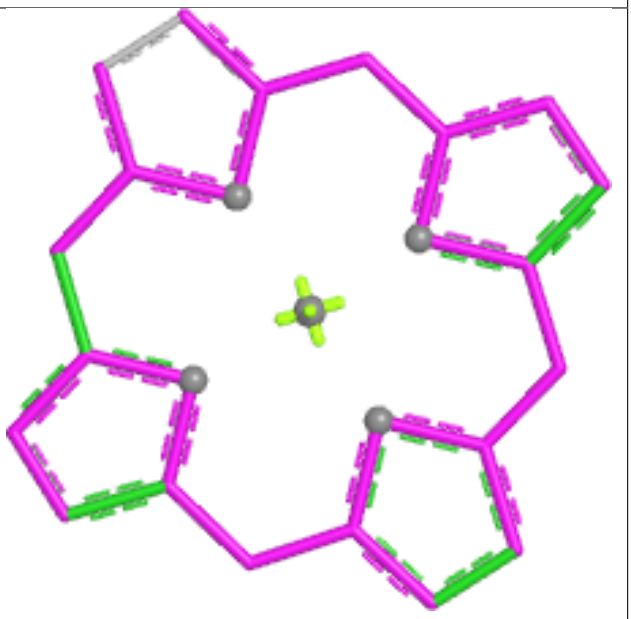


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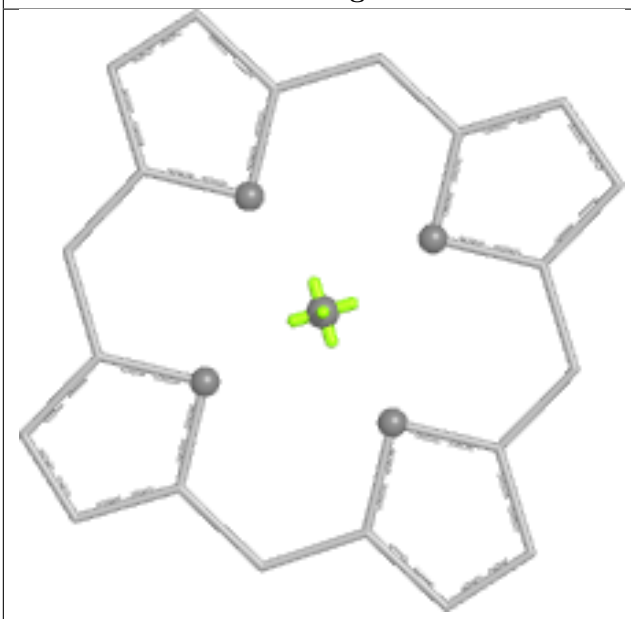
Ligand CLA 1 1001



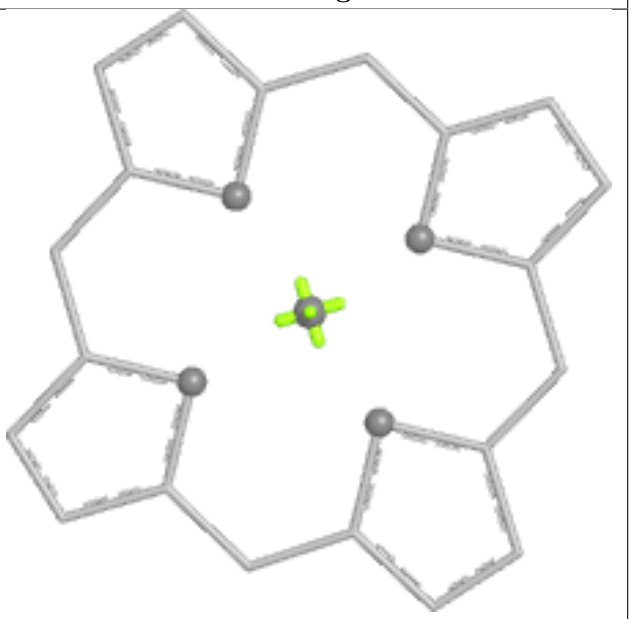
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Bond angles

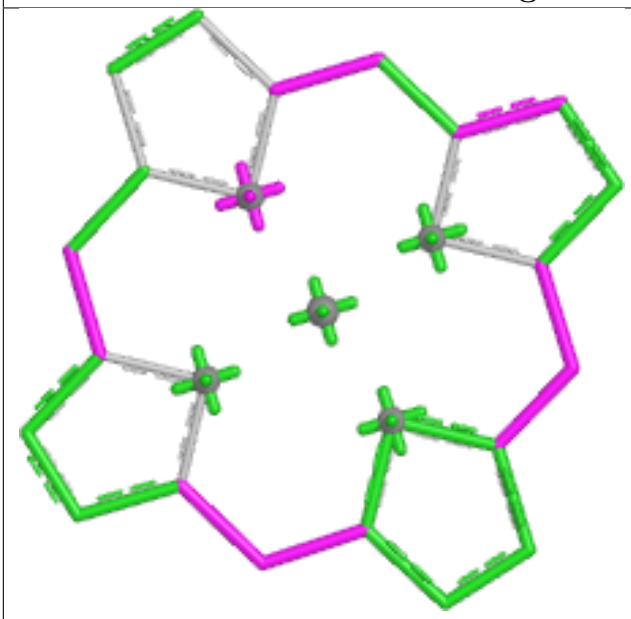


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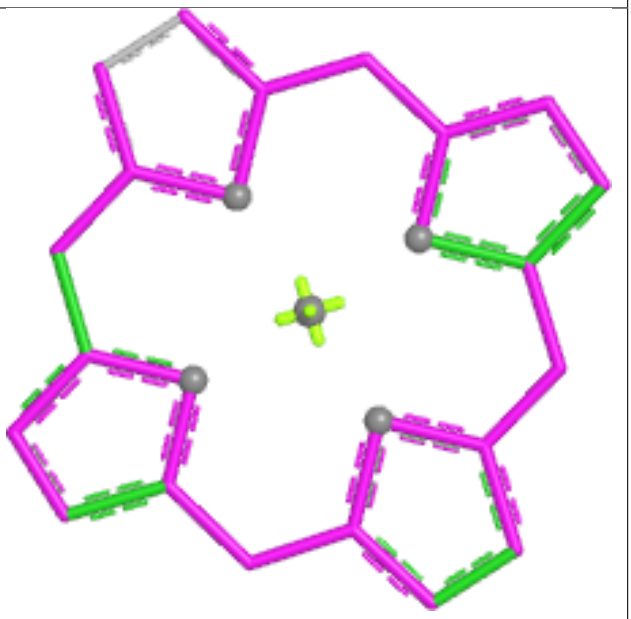


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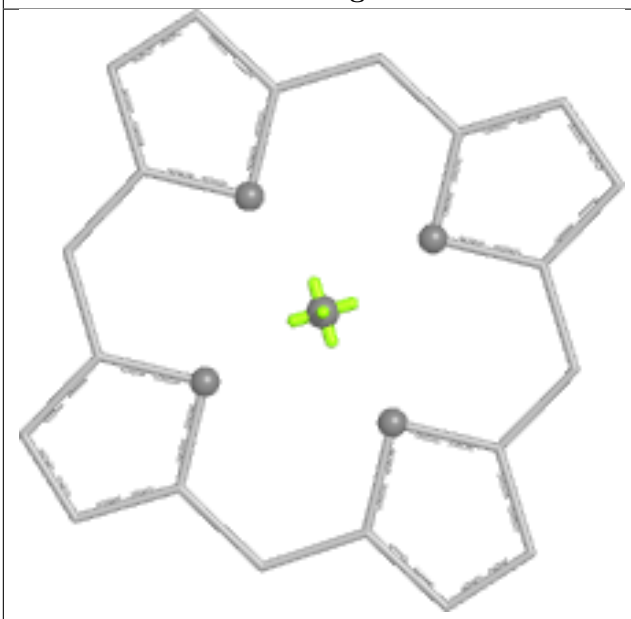
Ligand CLA 4 4011



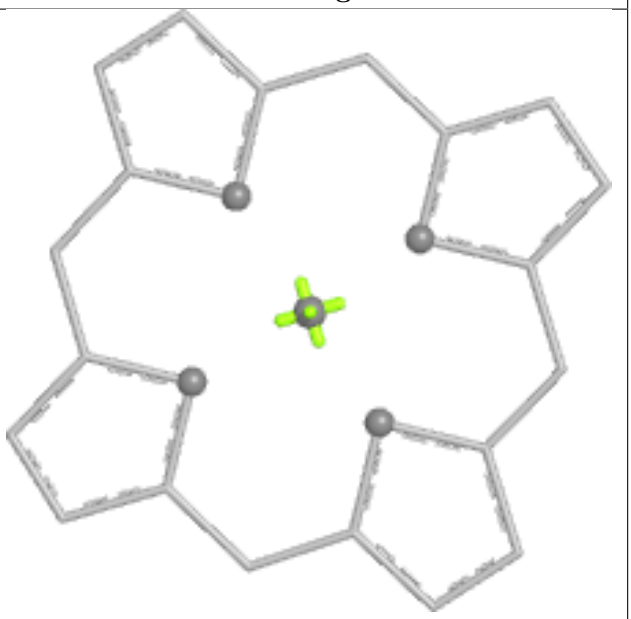
Bond lengths



Bond angles

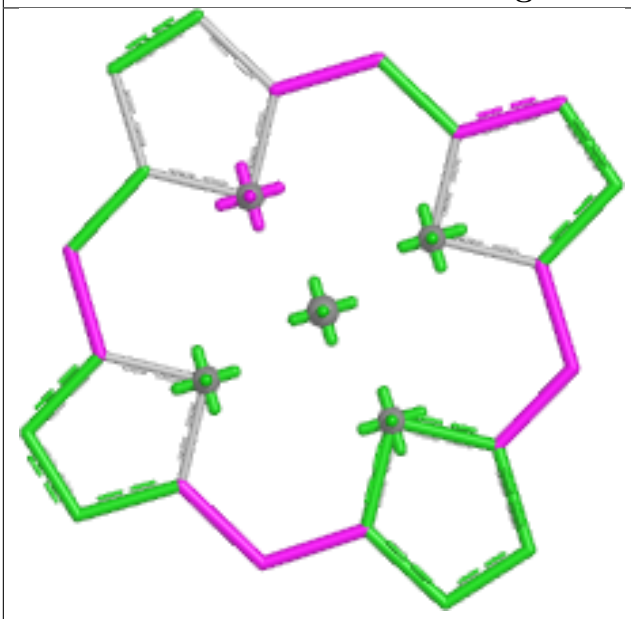


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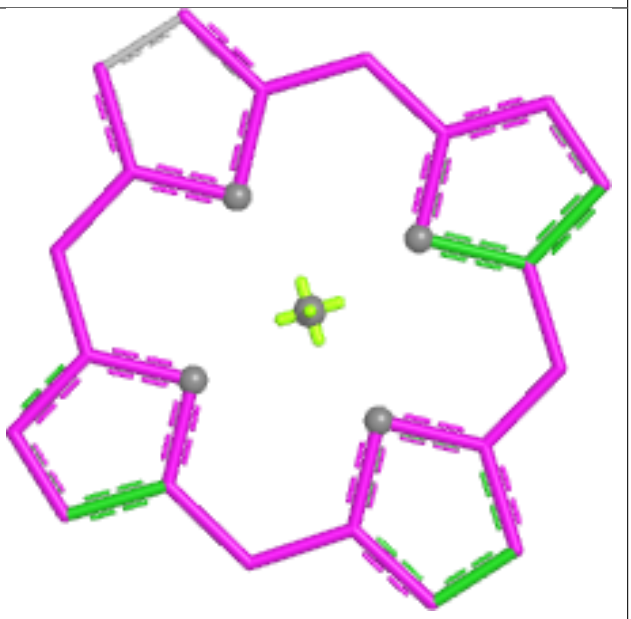


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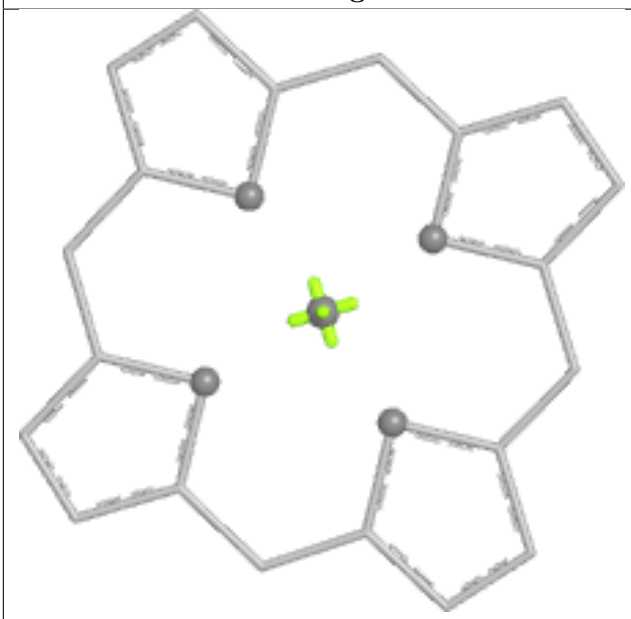
Ligand CLA B 1226



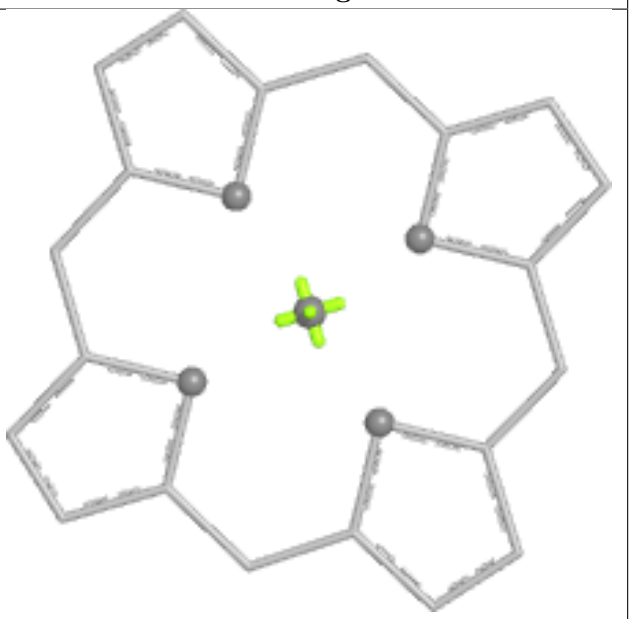
Bond lengths



Bond angles

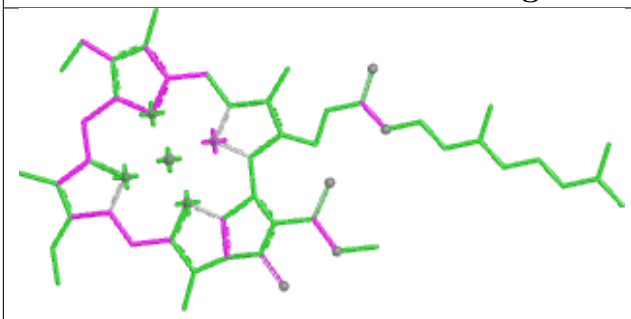


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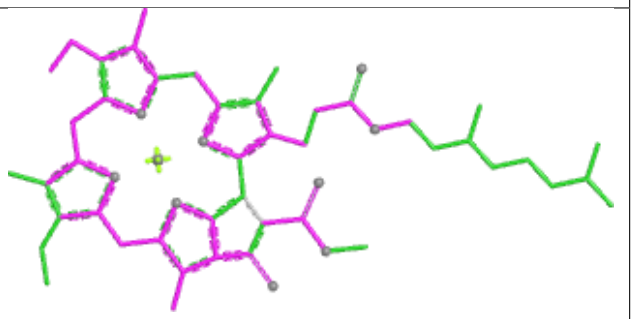


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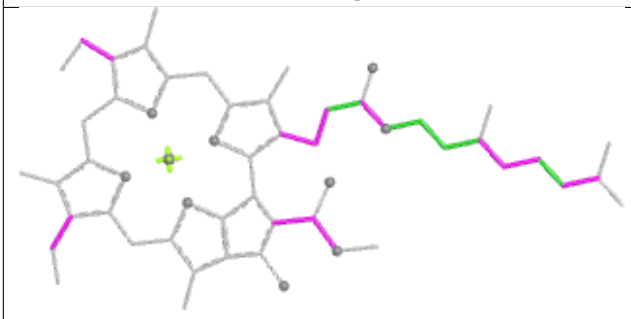
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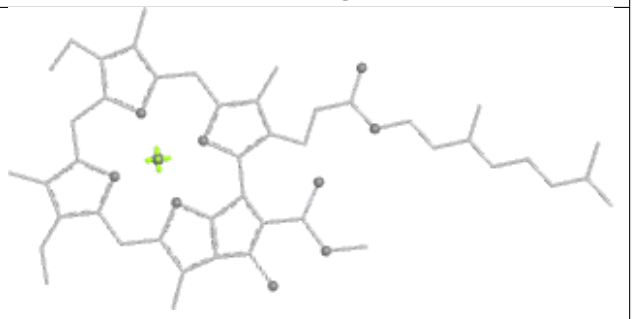
Bond lengths



Bond angles

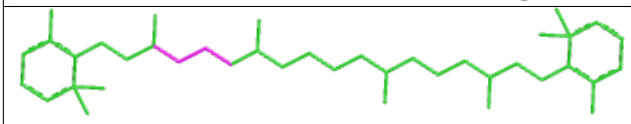


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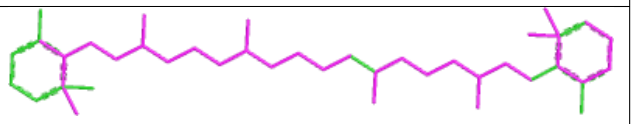


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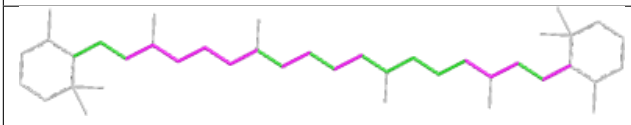
Ligand BCR L 6020



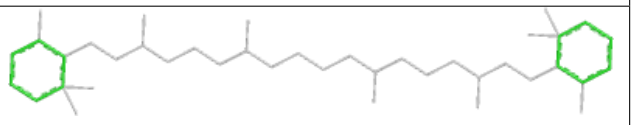
Bond lengths



Bond angles

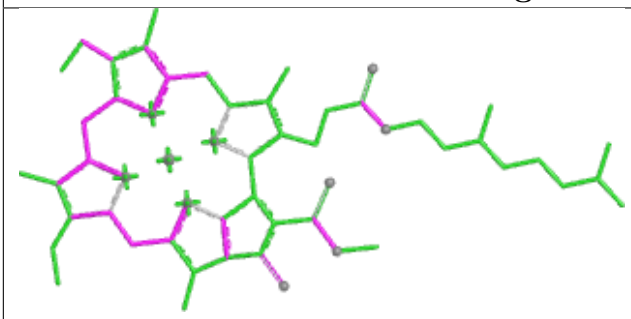


Torsions

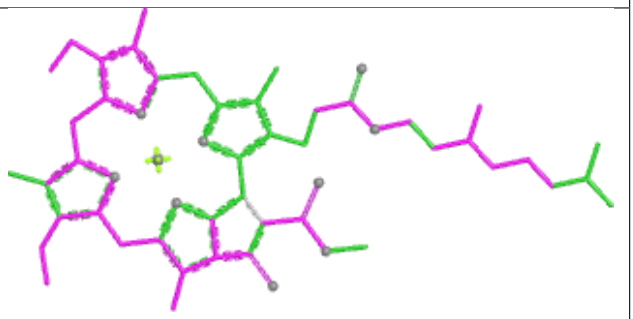


Rings

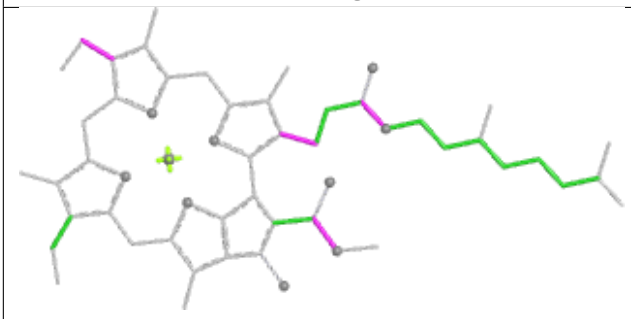
Ligand CLA A 1122



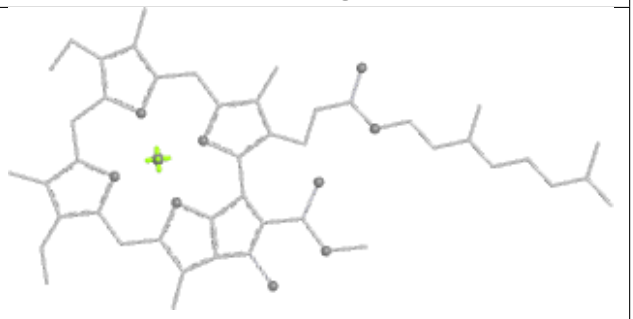
Bond lengths



Bond angles

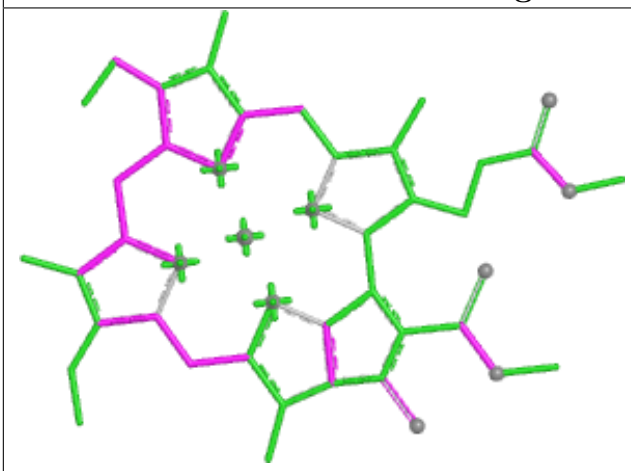


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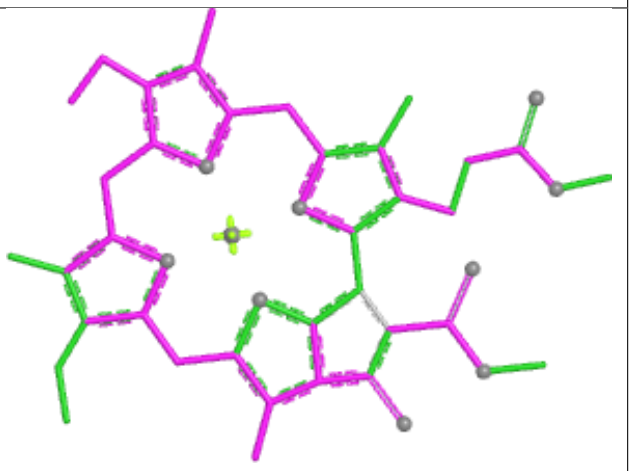


Rings

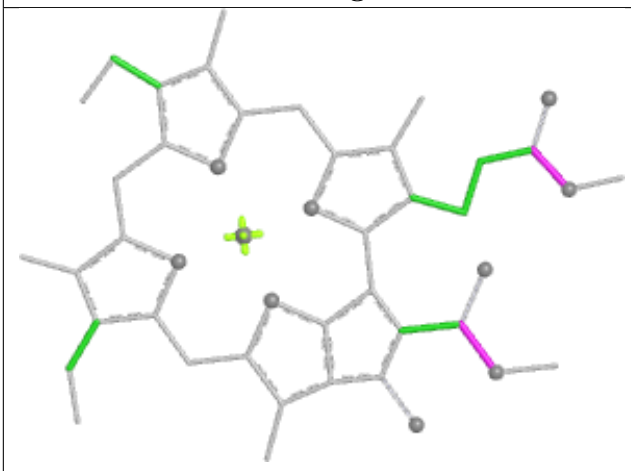
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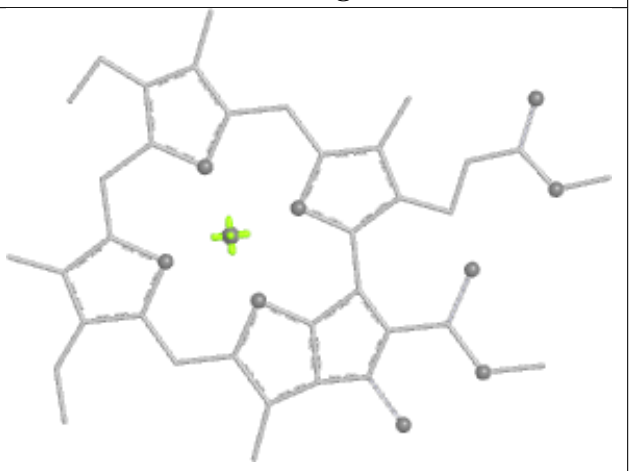
Bond lengths



Bond angles

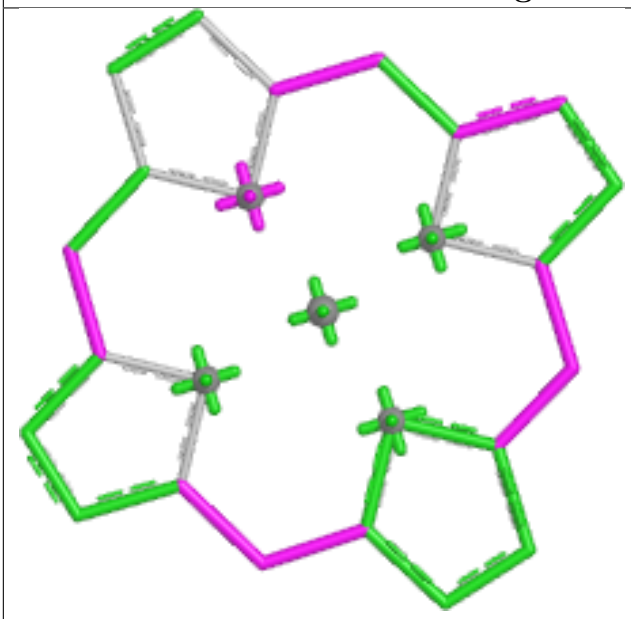


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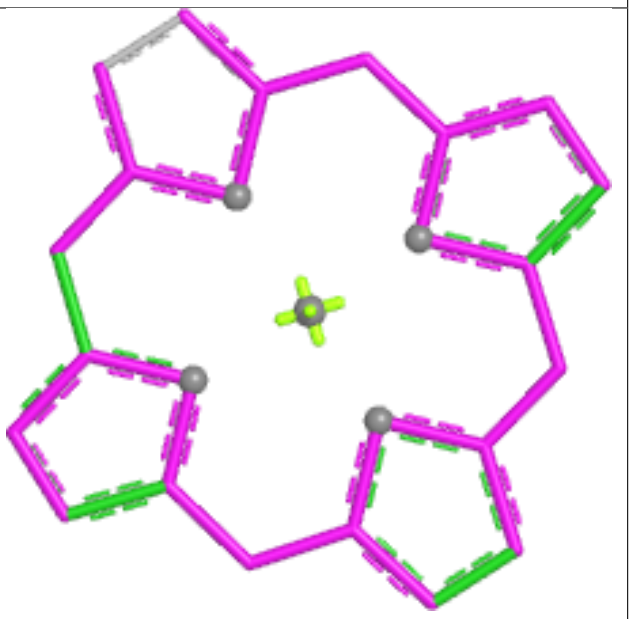


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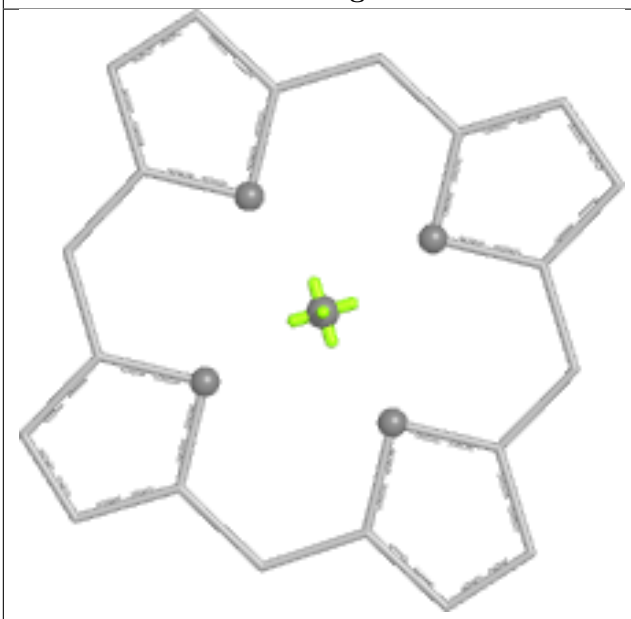
Ligand CLA A 1105



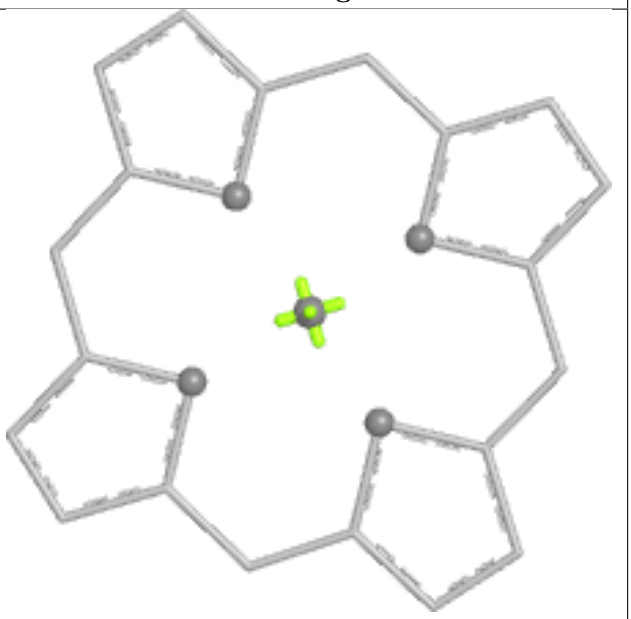
Bond lengths



Bond angles

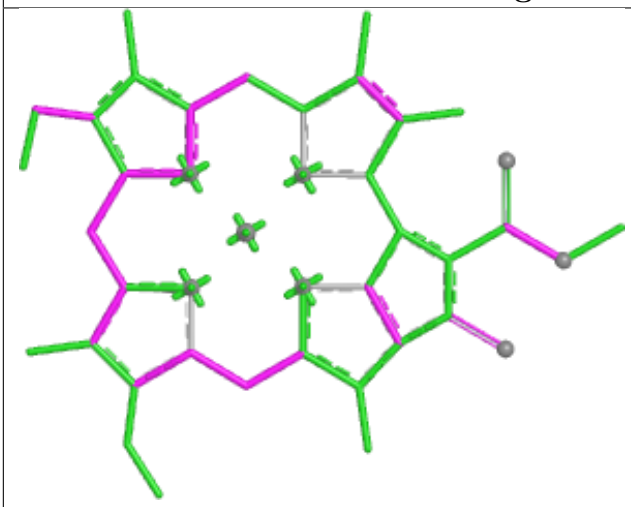


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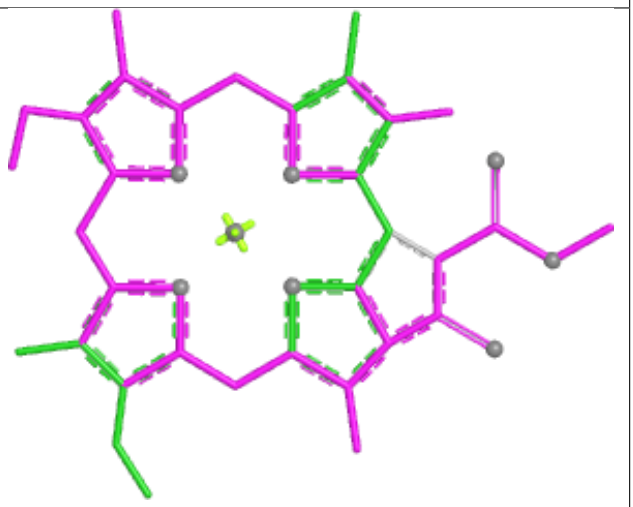


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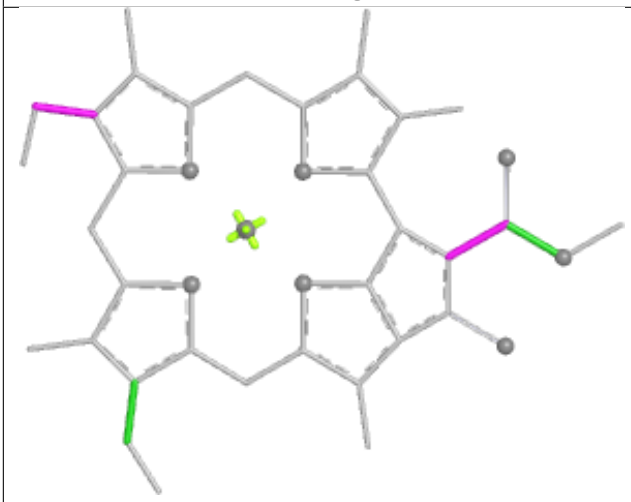
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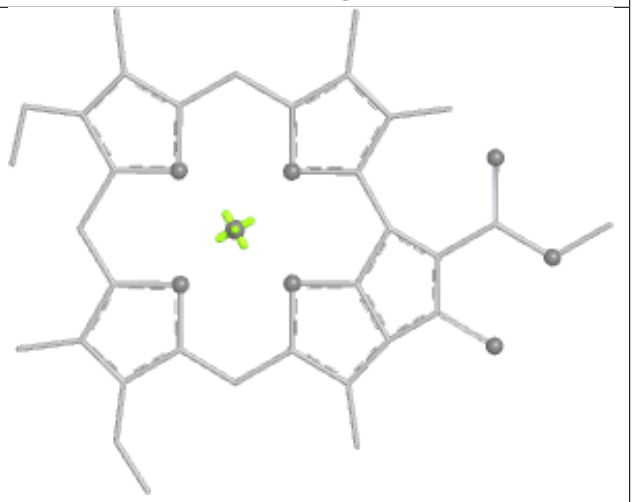
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Bond angles

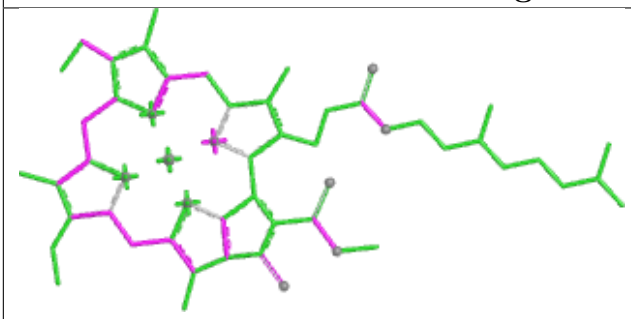


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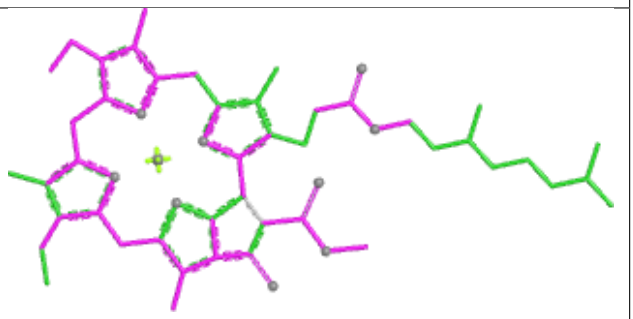


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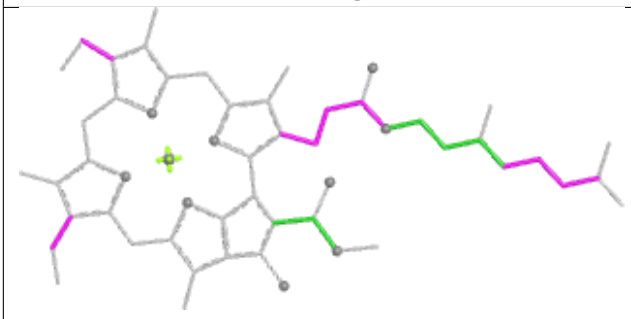
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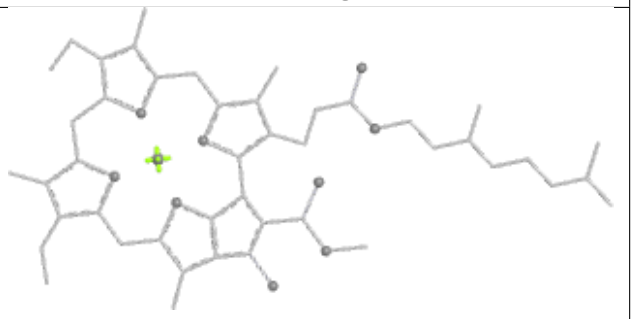
Bond lengths



Bond angles

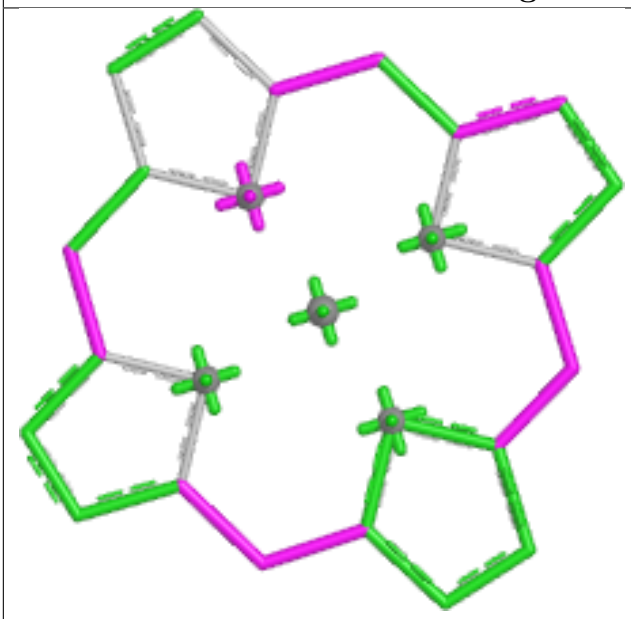


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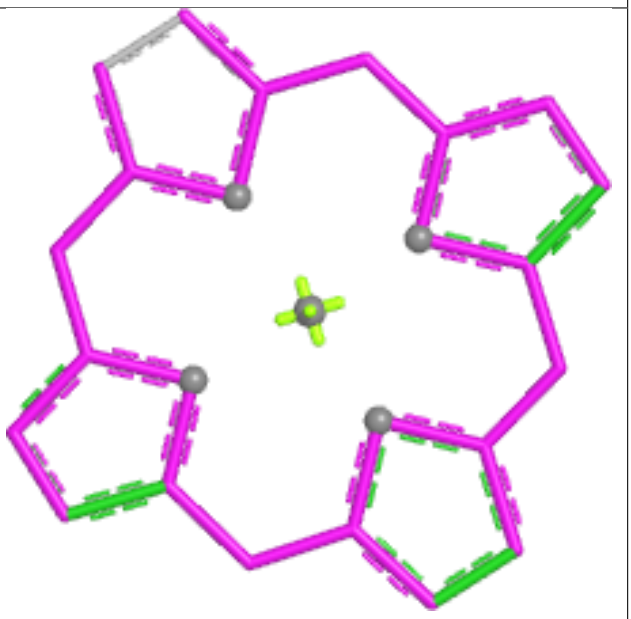


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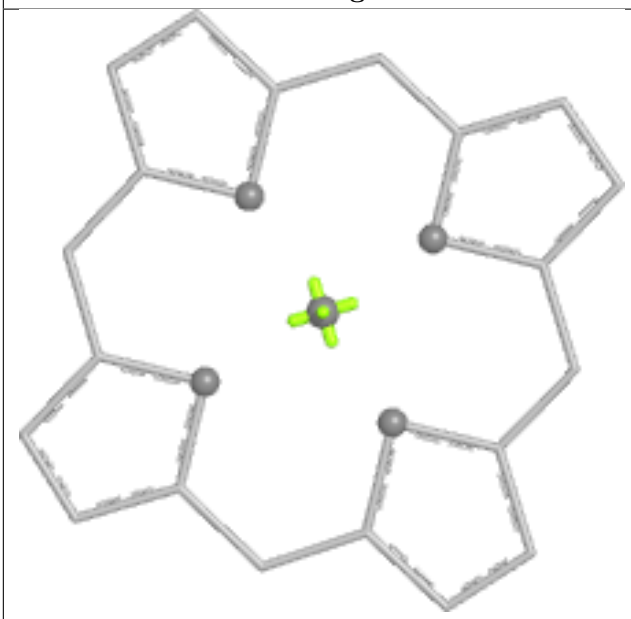
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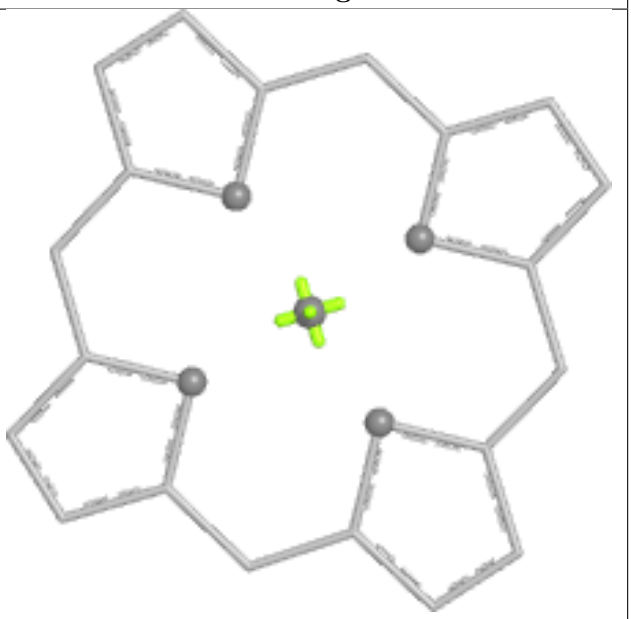
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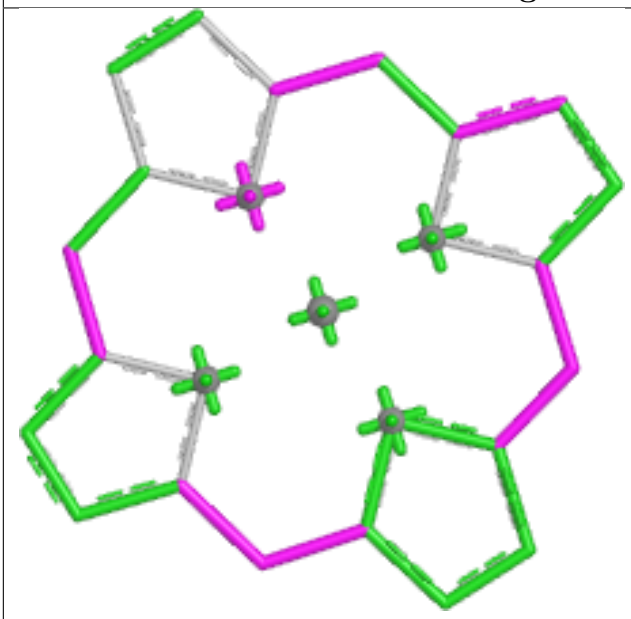


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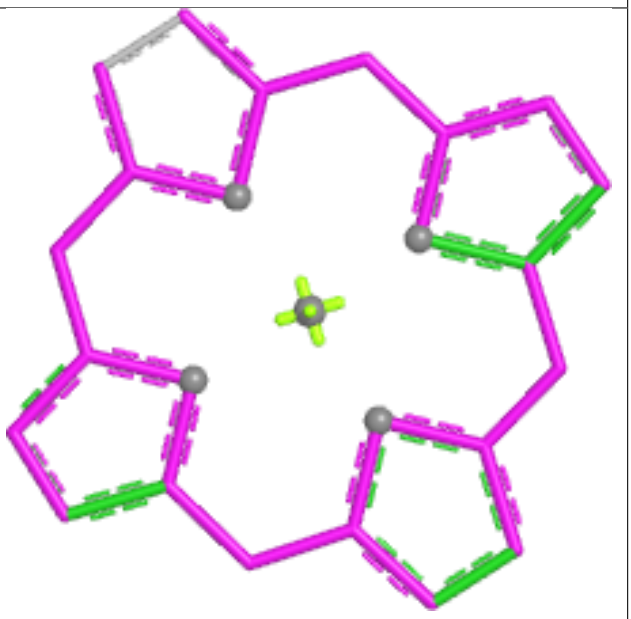


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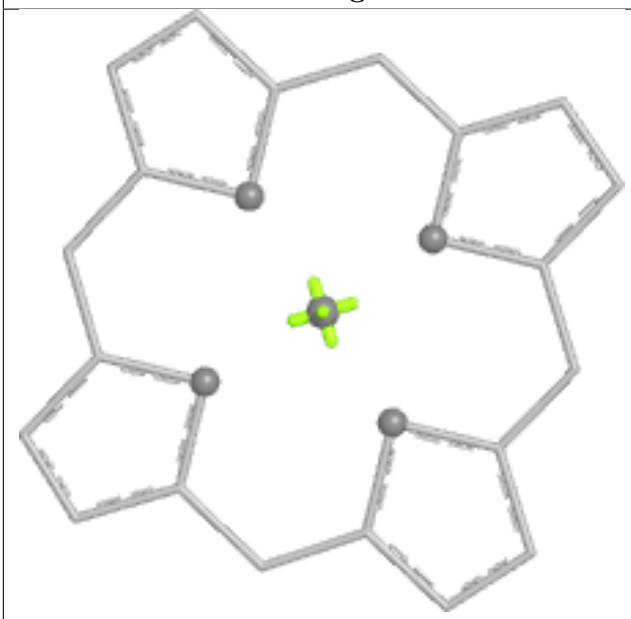
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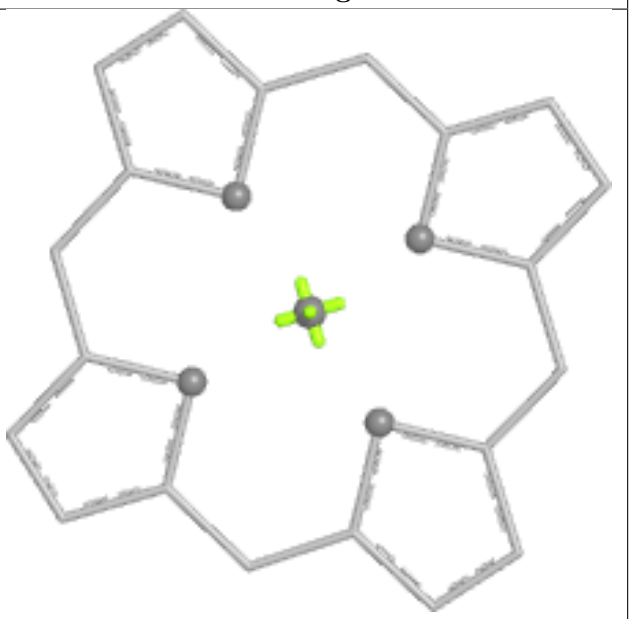
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Bond angles

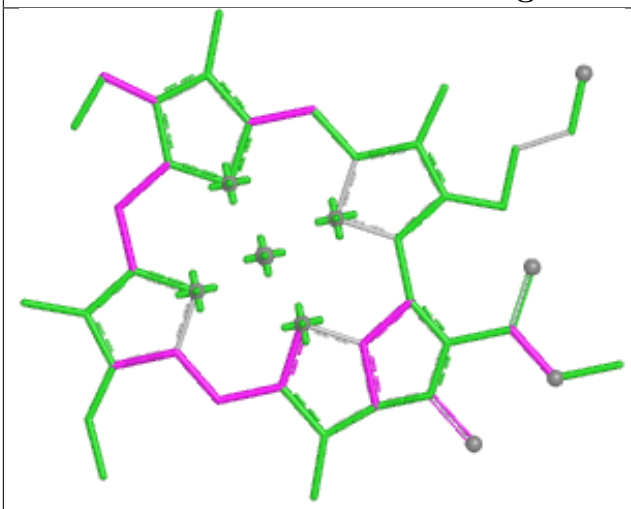


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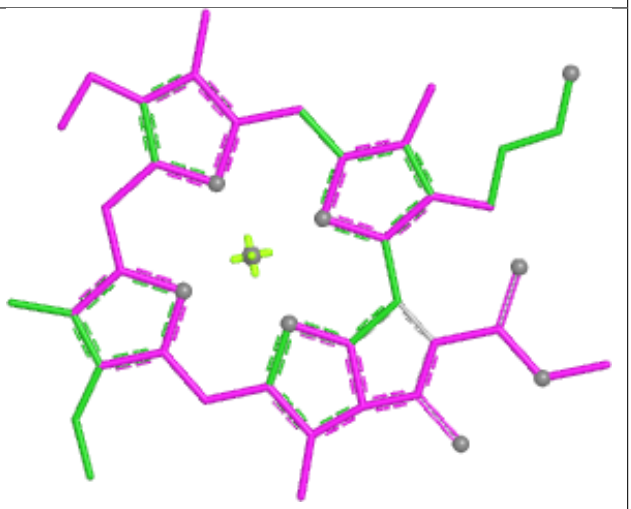


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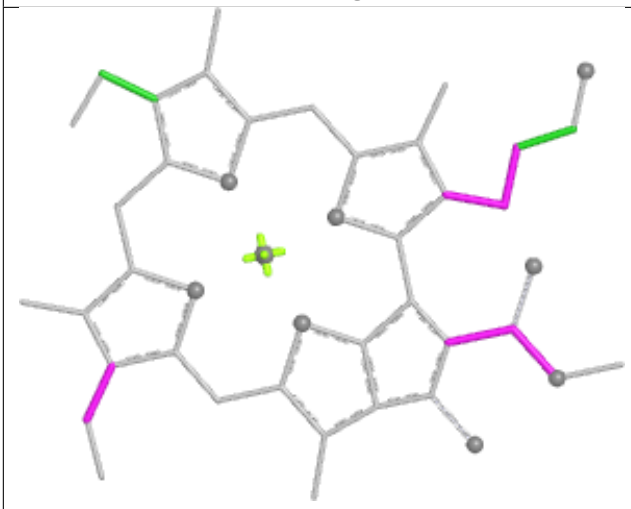
Ligand CLA F 1139



Bond lengths



Bond angles

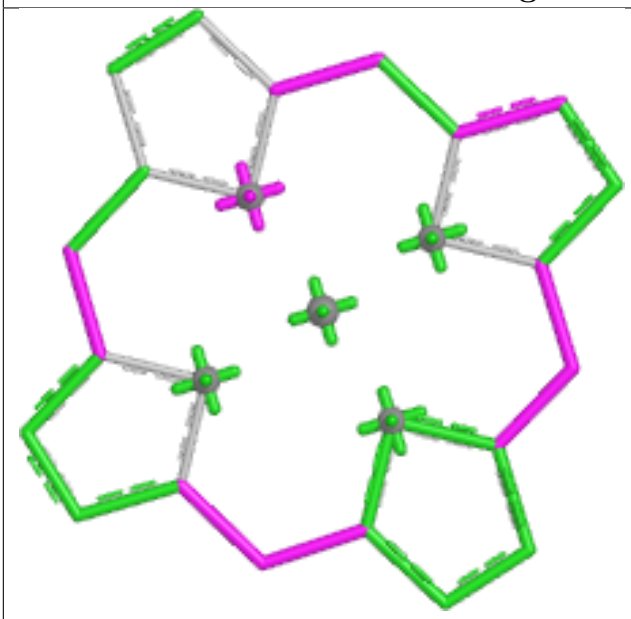


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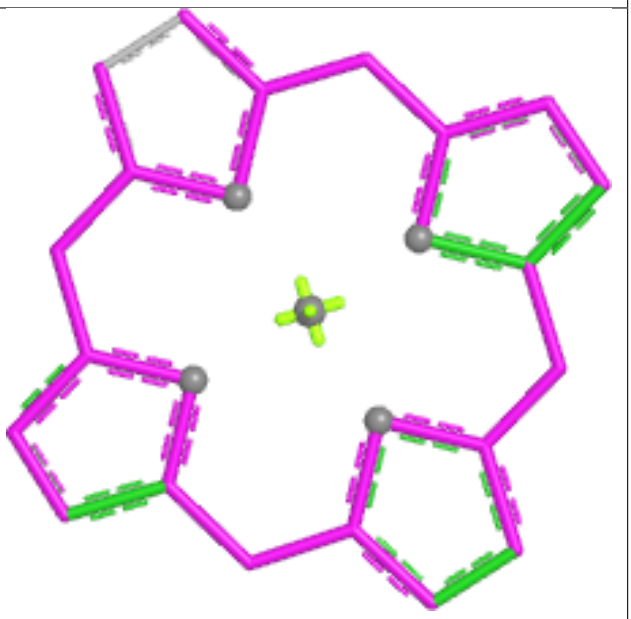


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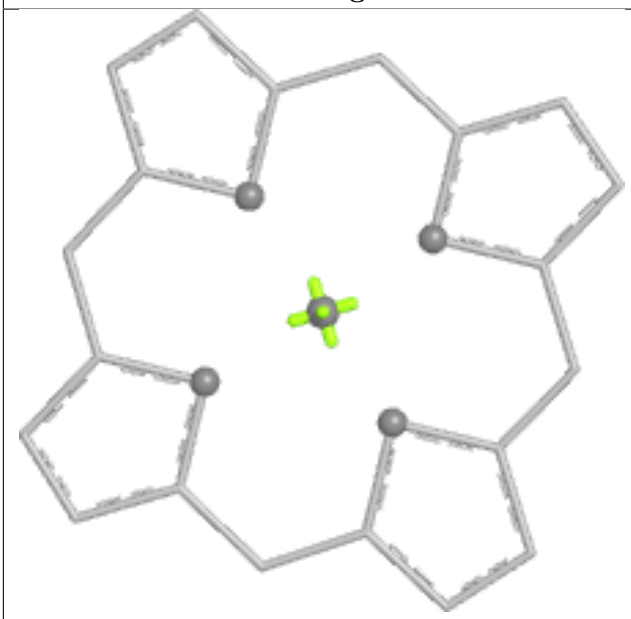
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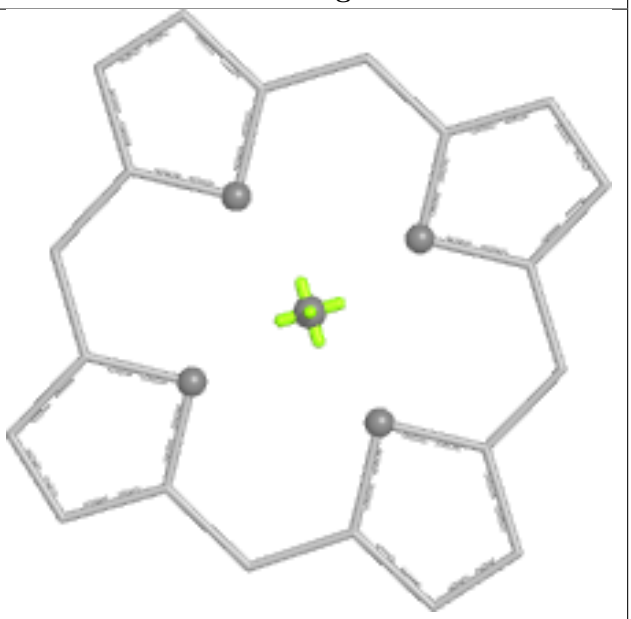
Bond lengths



Bond angles

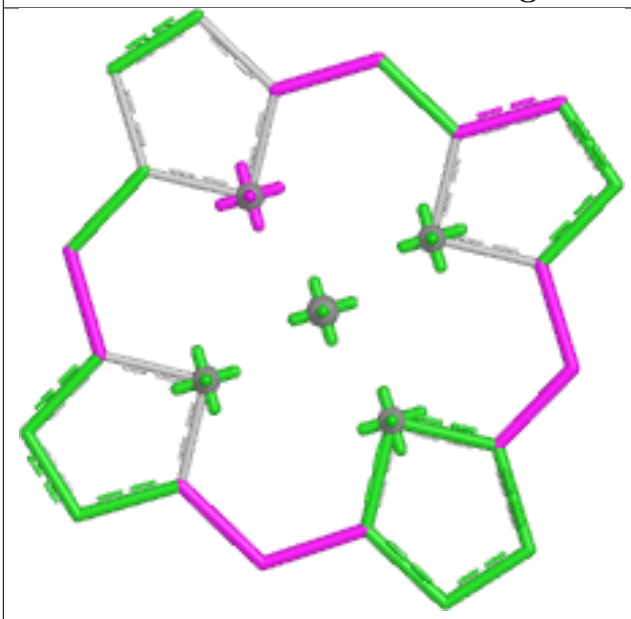


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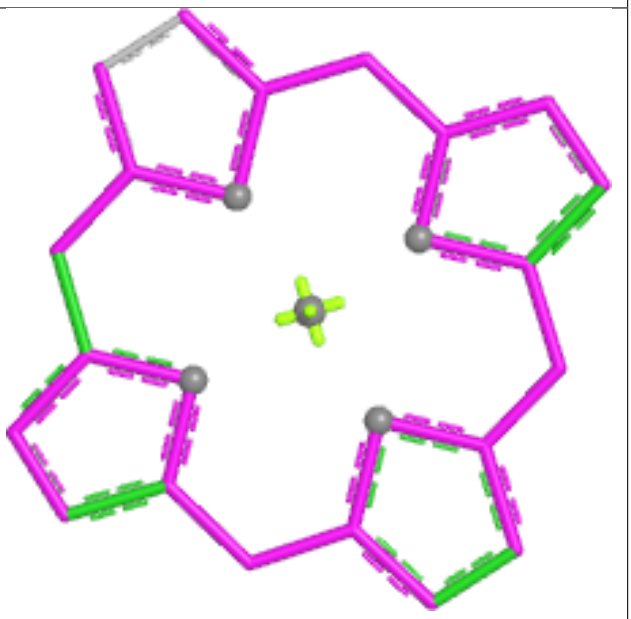


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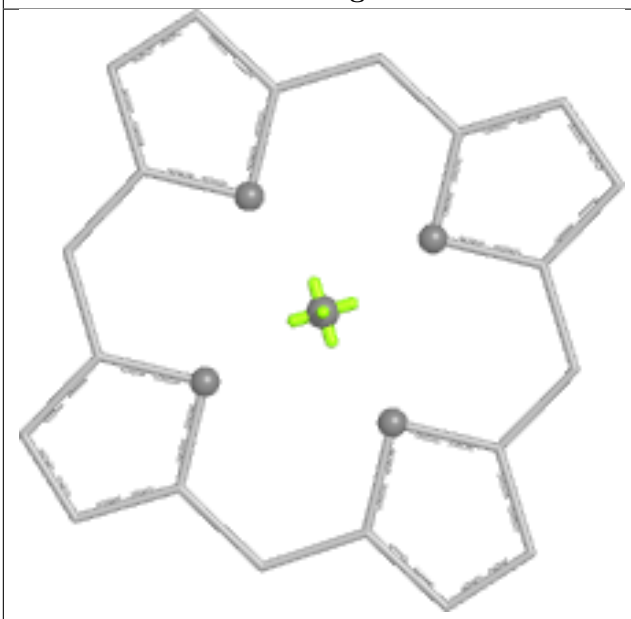
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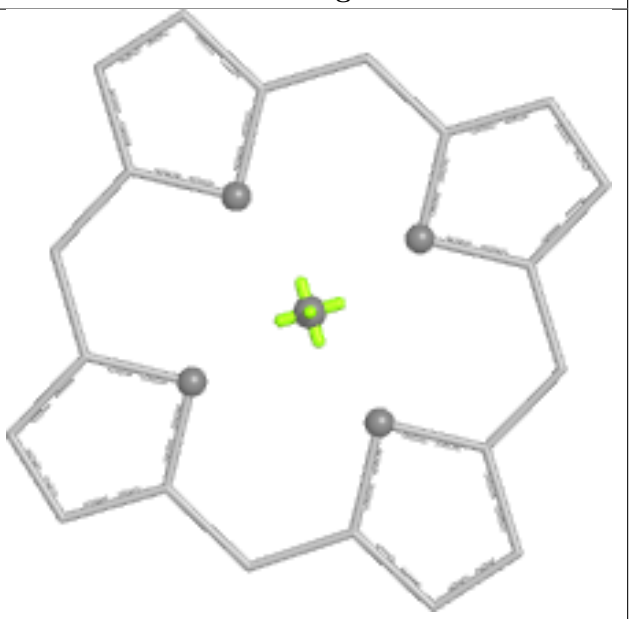
Bond lengths



Bond angles

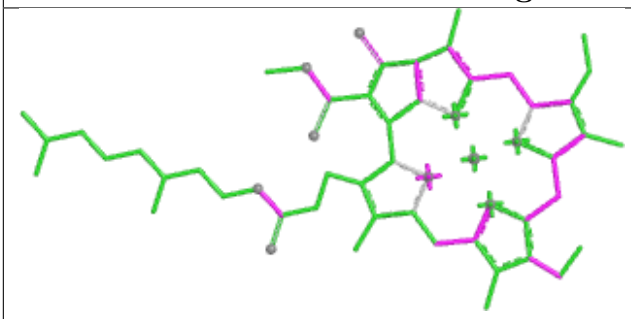


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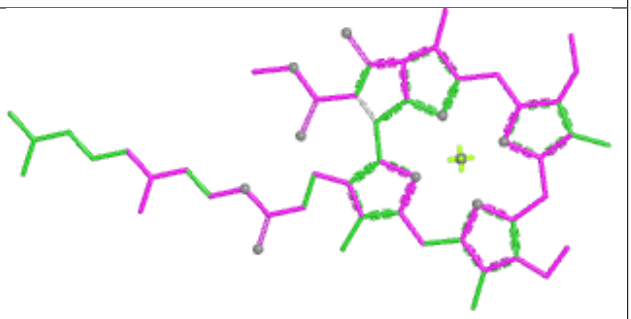


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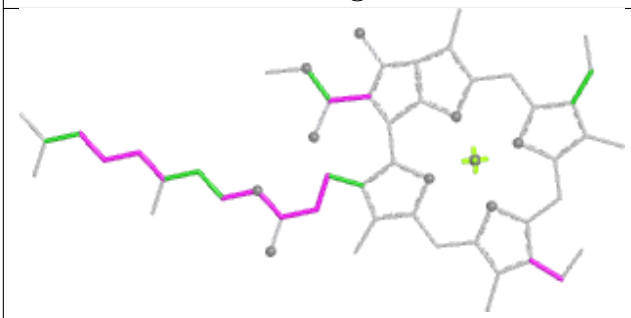
Ligand CLA B 1205



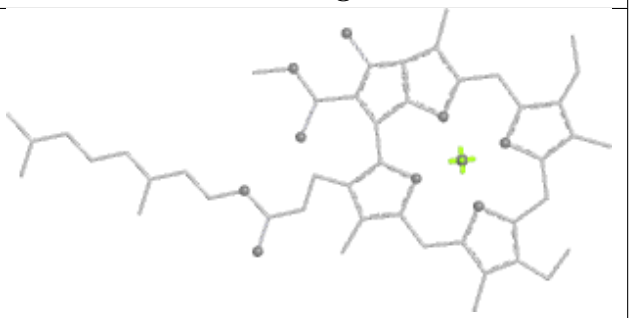
Bond lengths



Bond angles

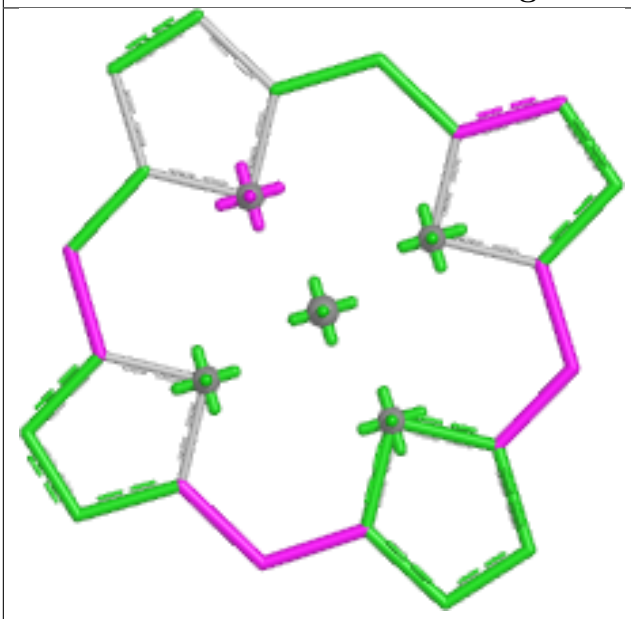


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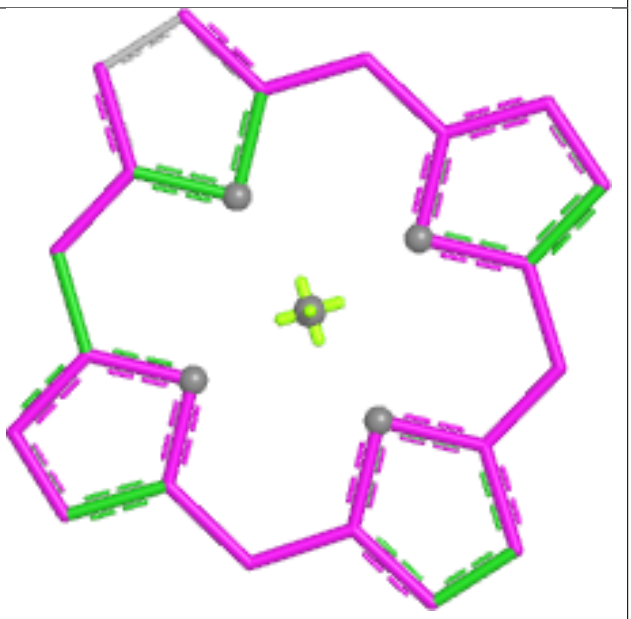


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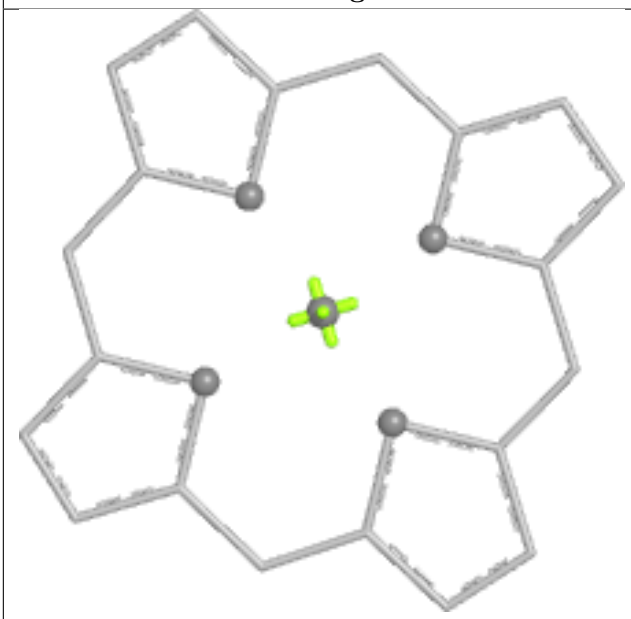
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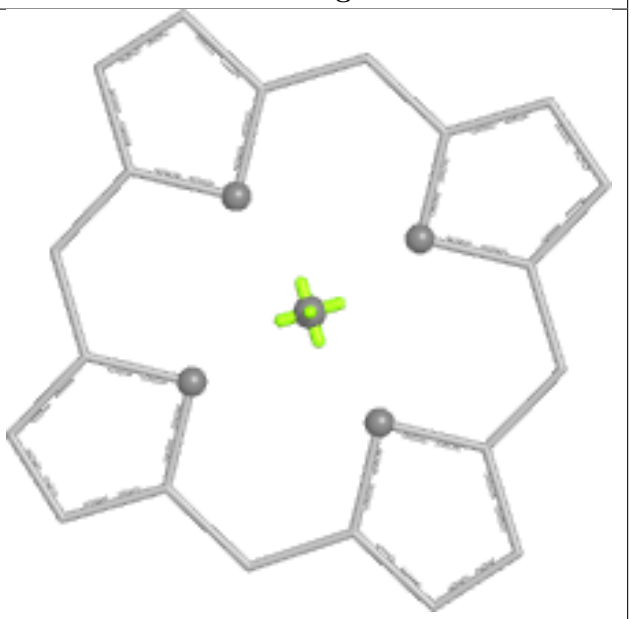
Bond lengths



Bond angles

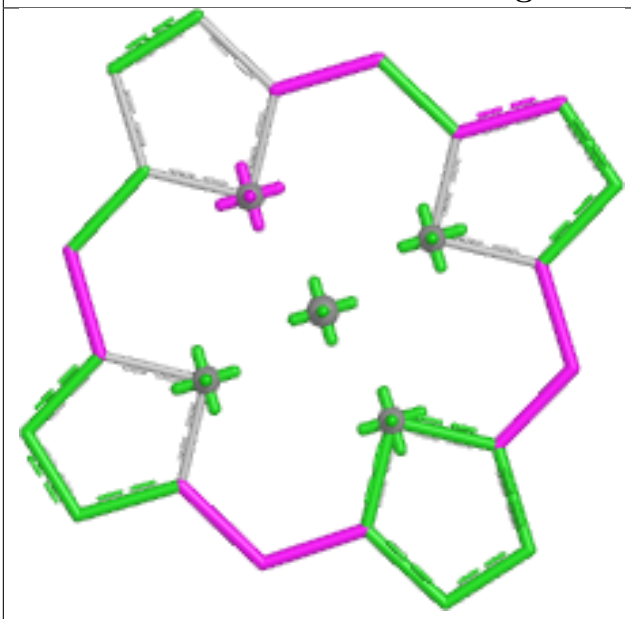


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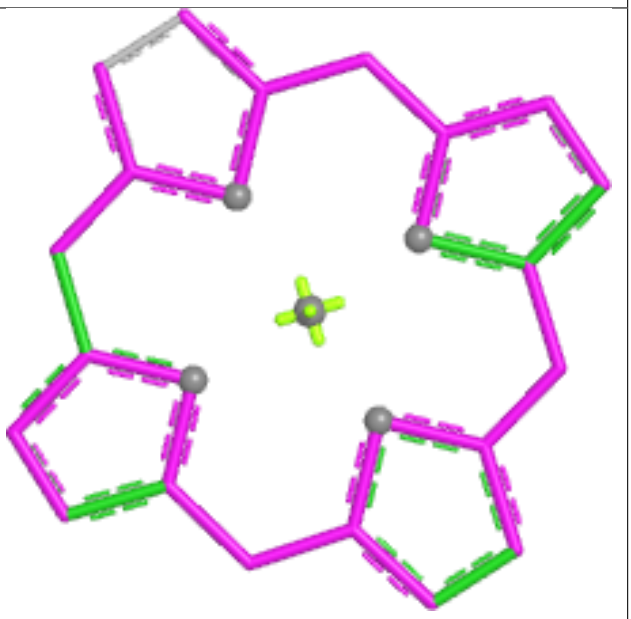


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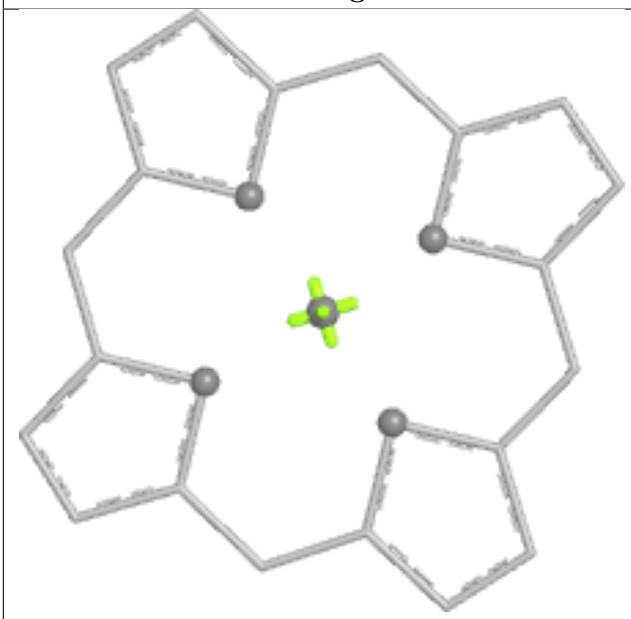
Ligand CLA B 1230



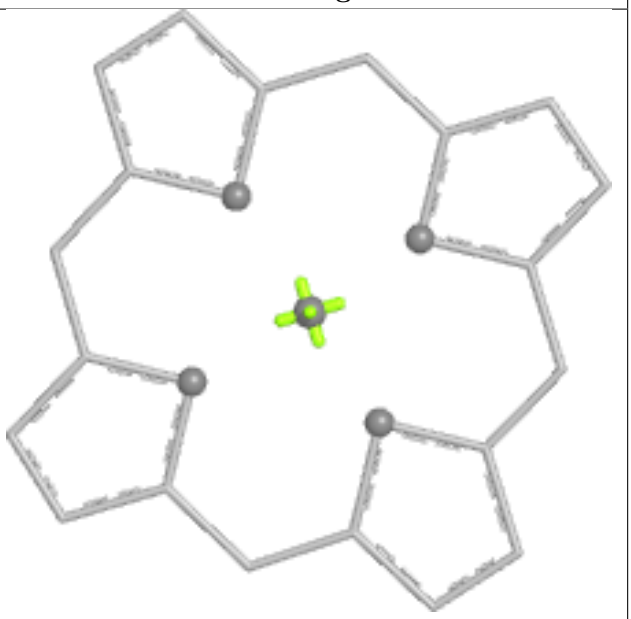
Bond lengths



Bond angles

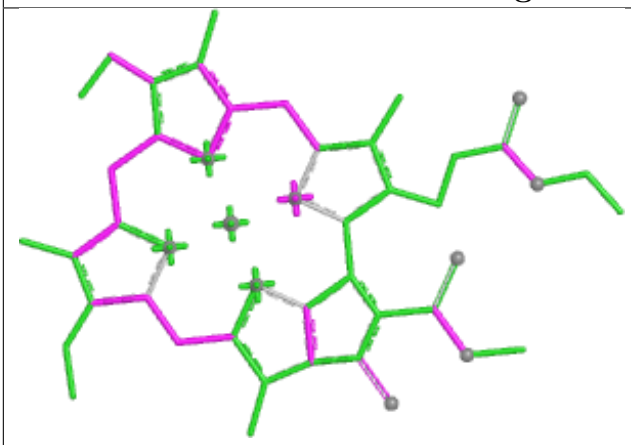


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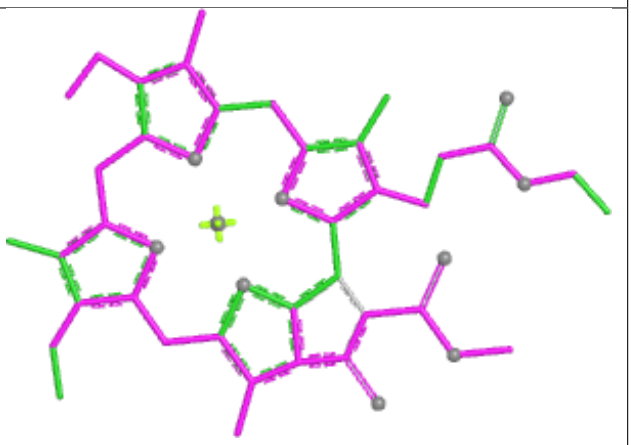


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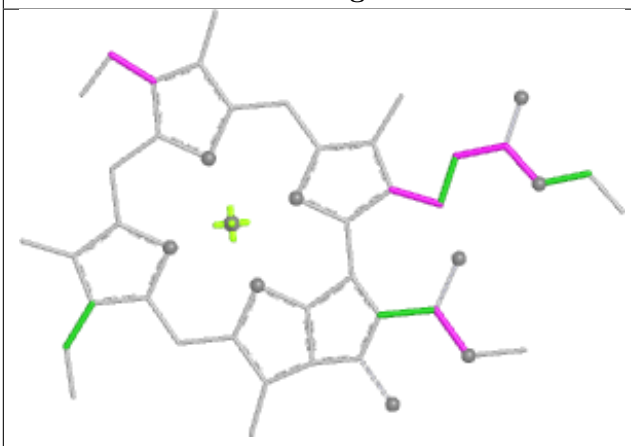
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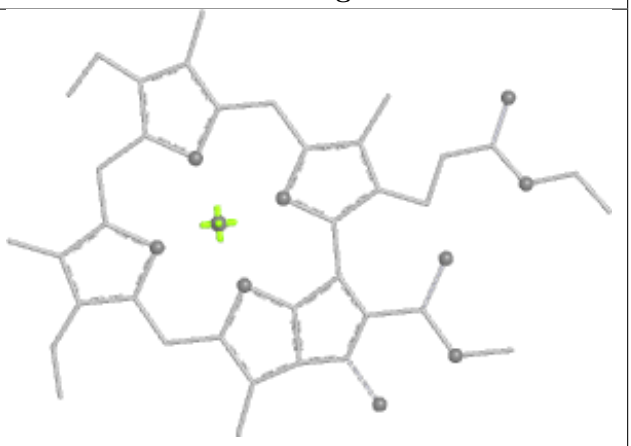
Bond lengths



Bond angles

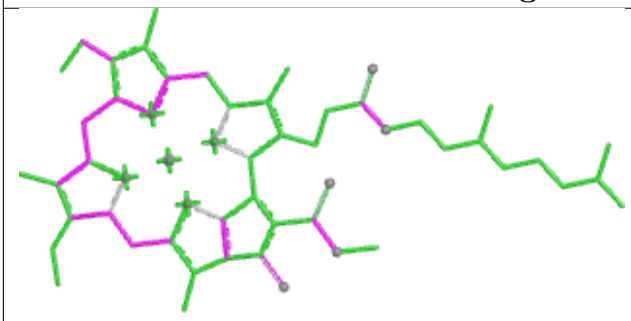


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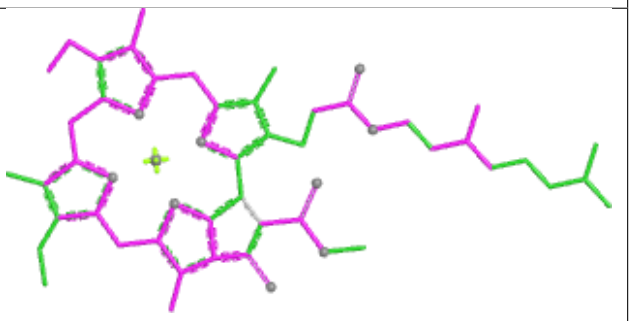


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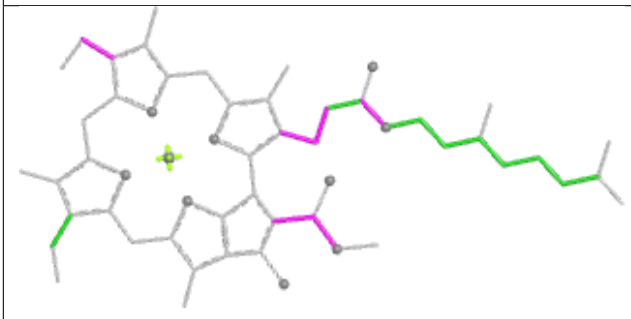
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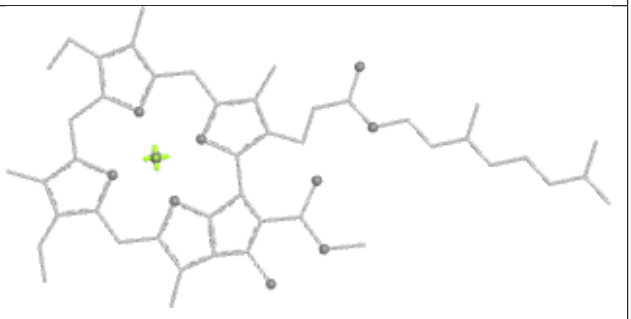
Bond lengths



Bond angles

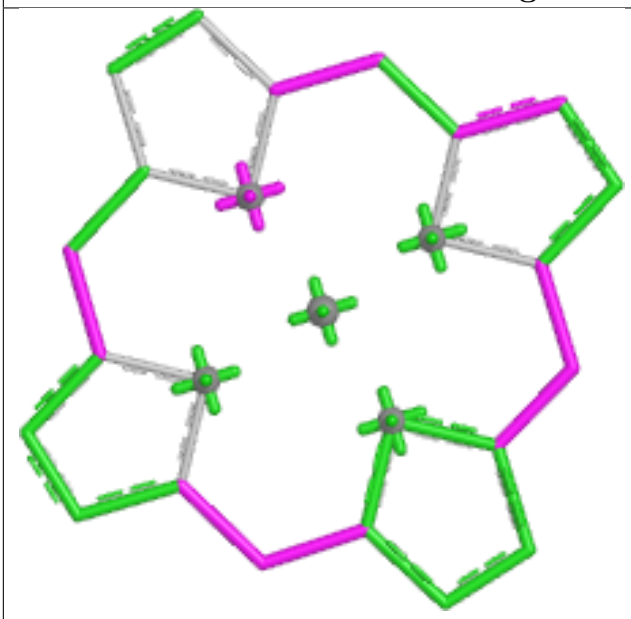


Torsions

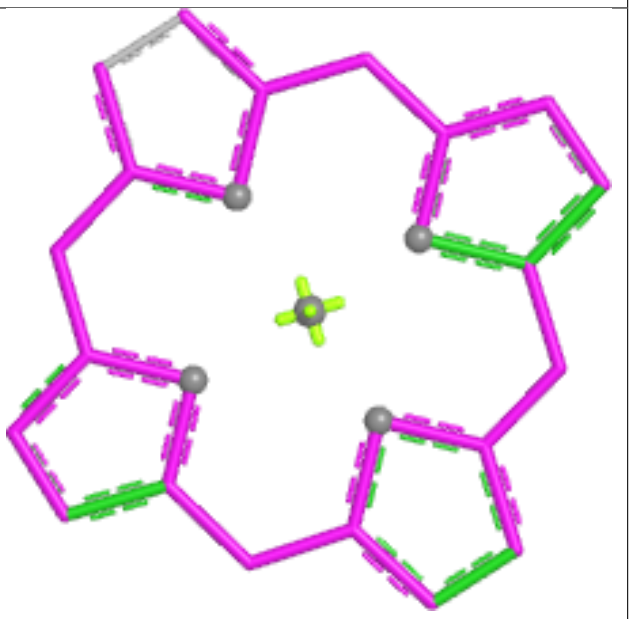


Rings

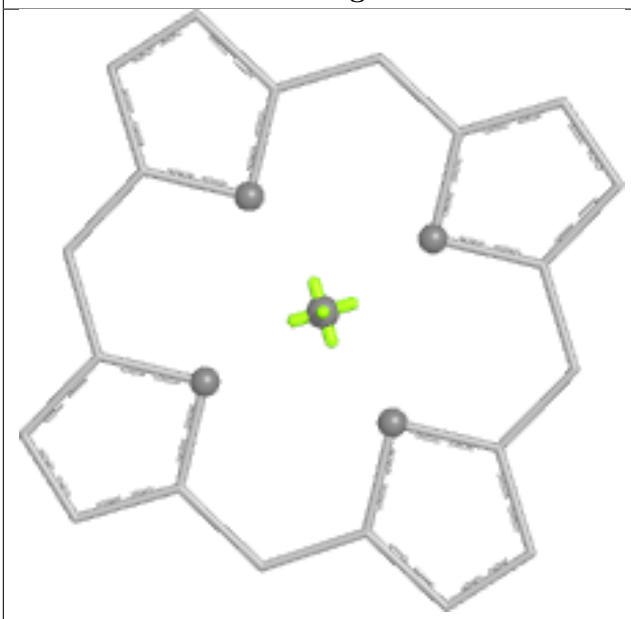
Ligand CLA 2 2001



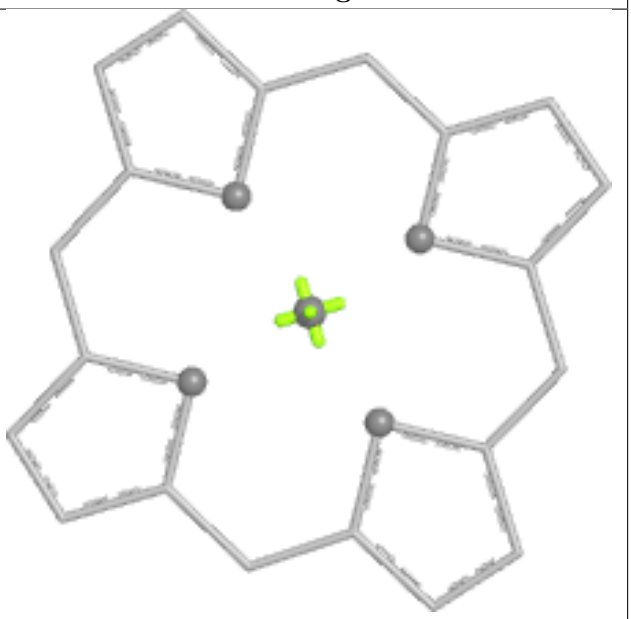
Bond lengths



Bond angles

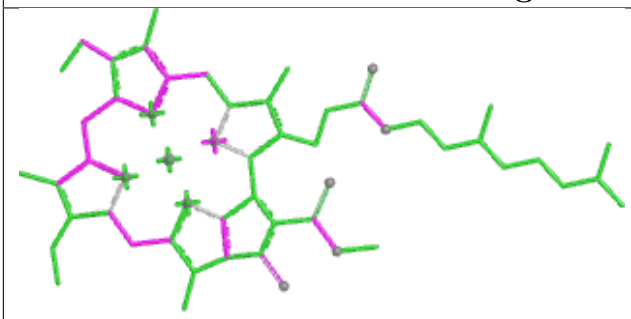


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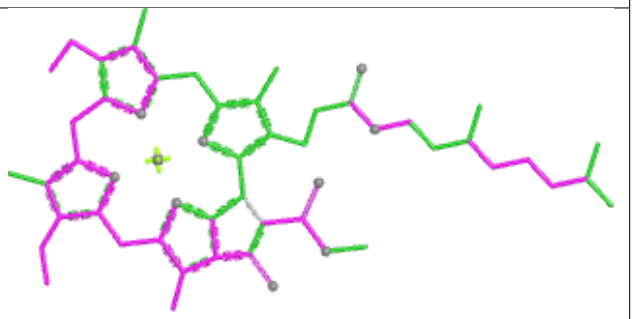


Rings

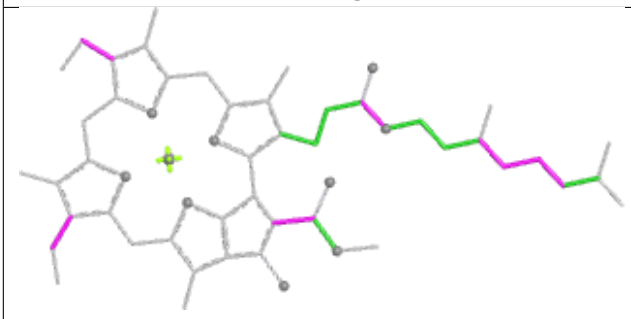
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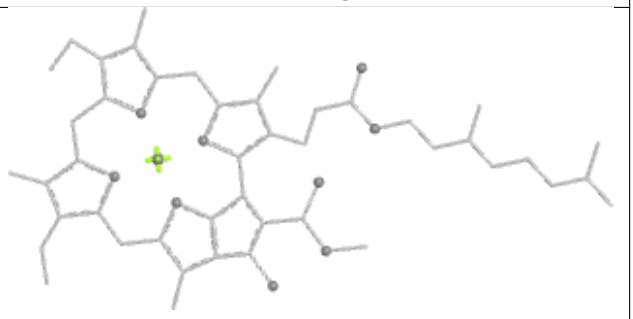
Bond lengths



Bond angles

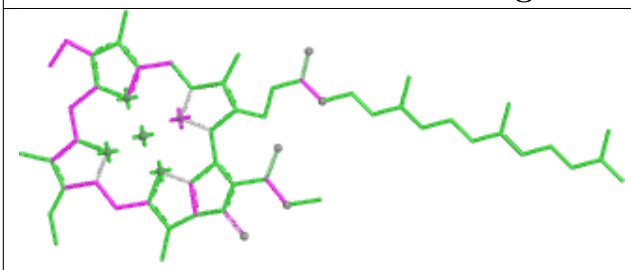


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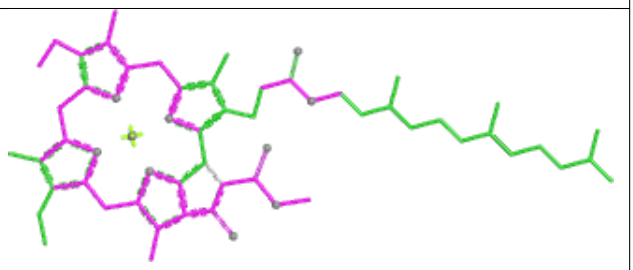


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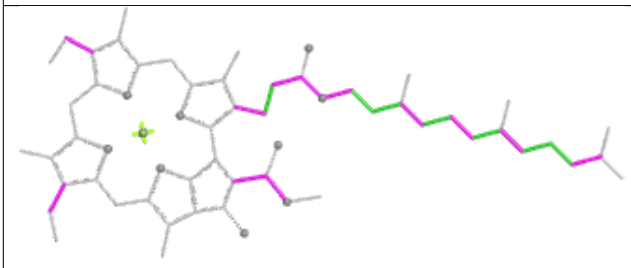
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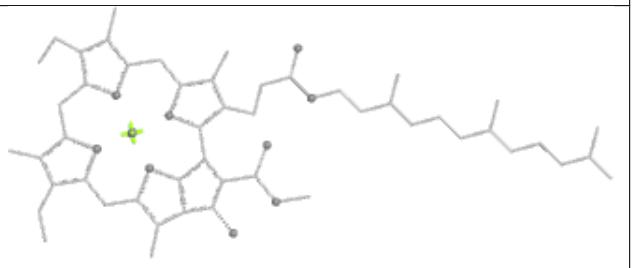
Bond lengths



Bond angles

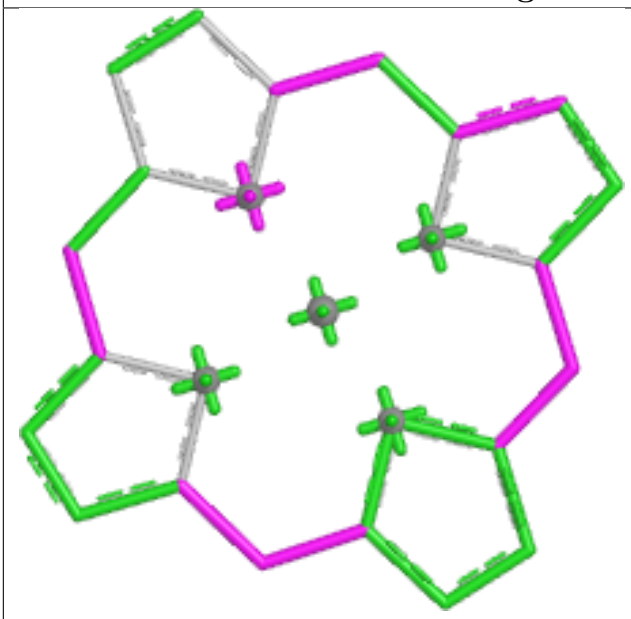


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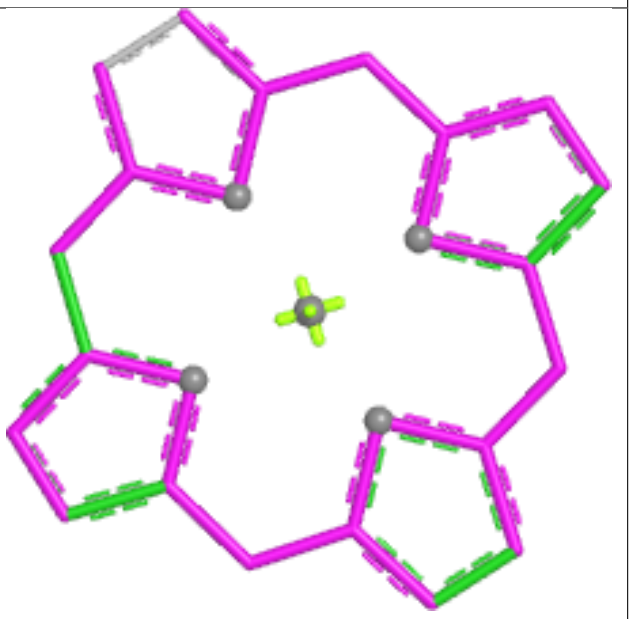


Rings

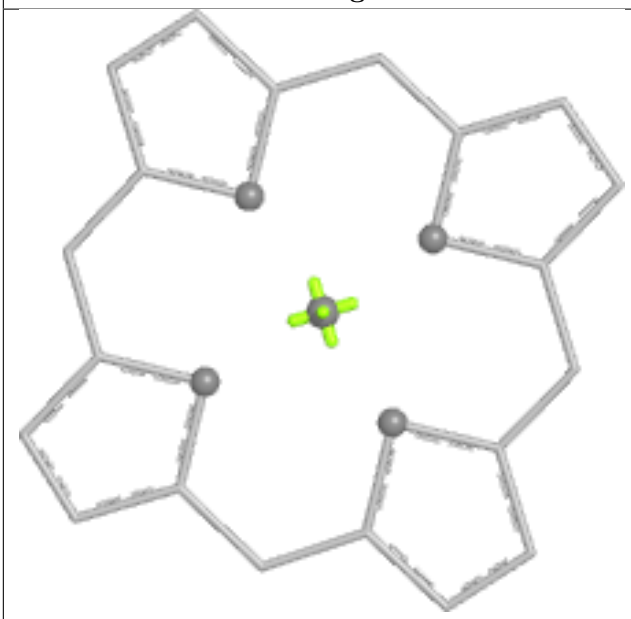
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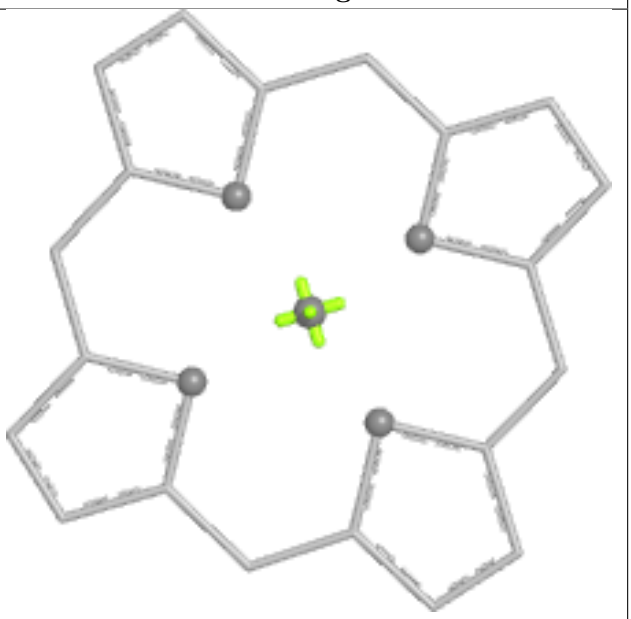
Bond lengths



Bond angles

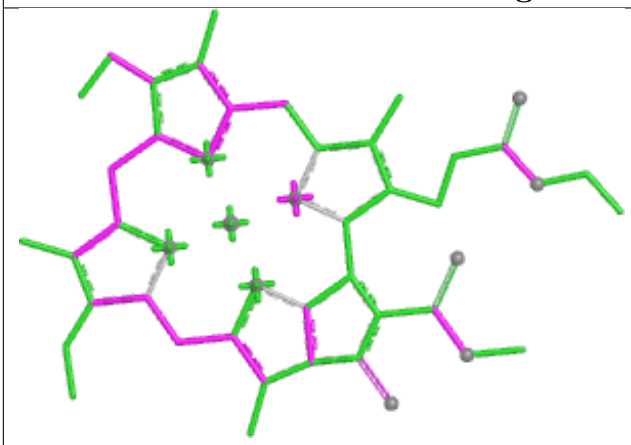


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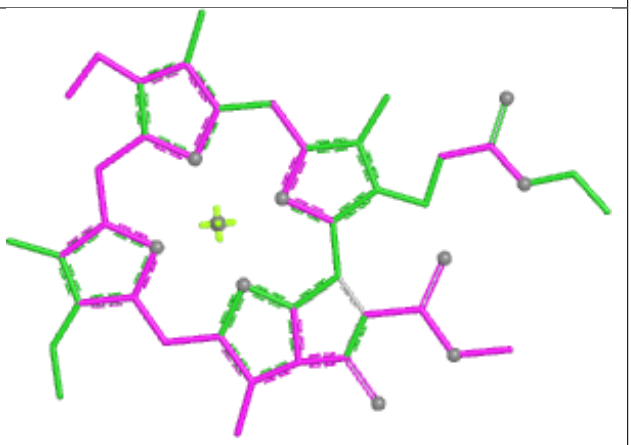


Rings

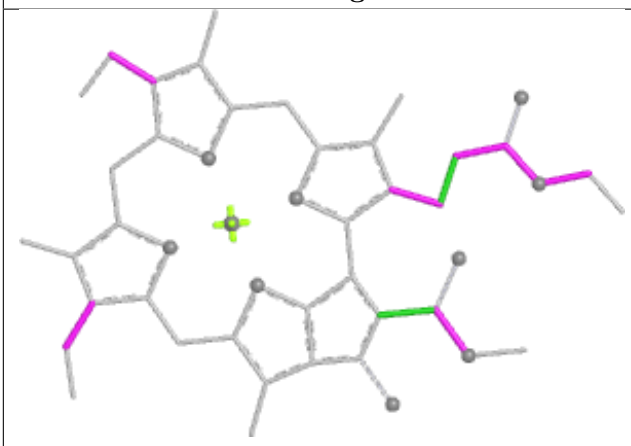
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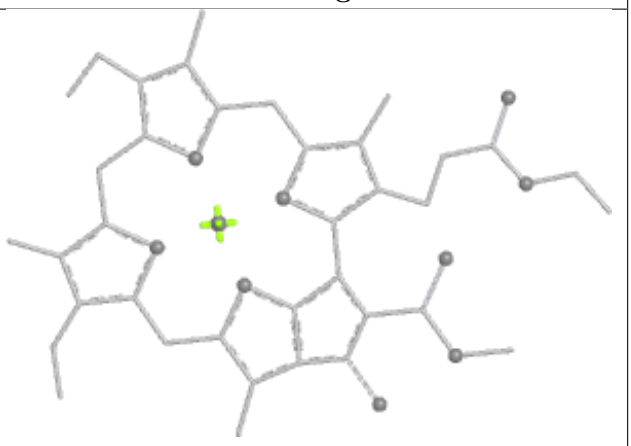
Bond lengths



Bond angles

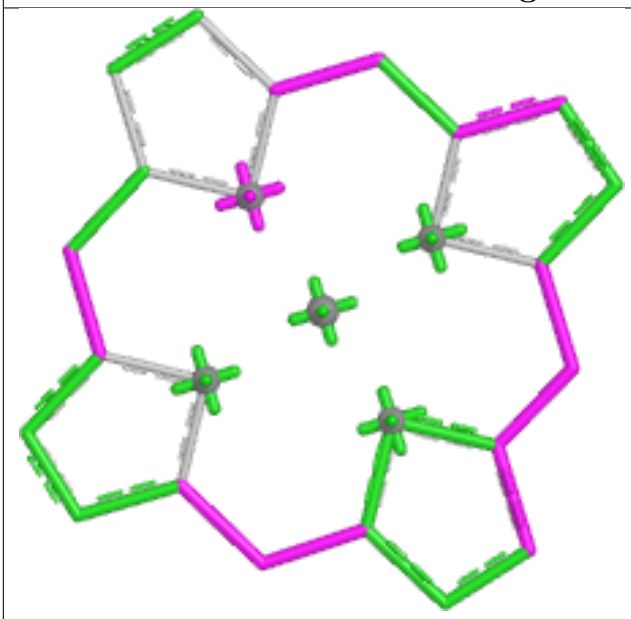


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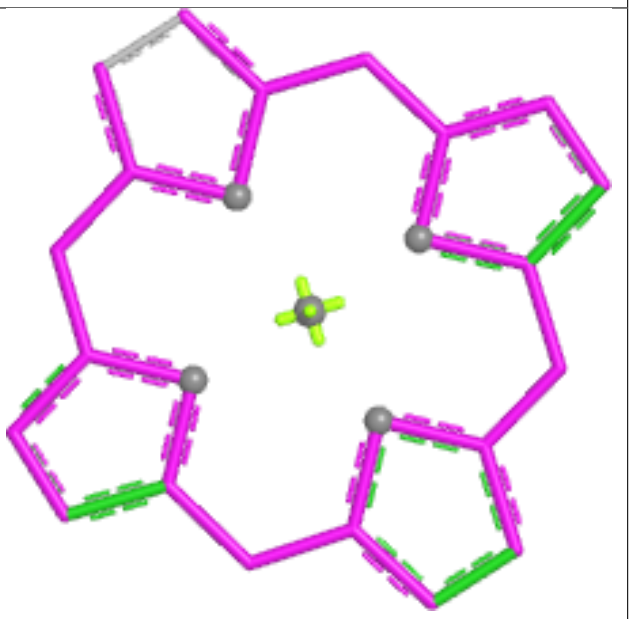


Rings

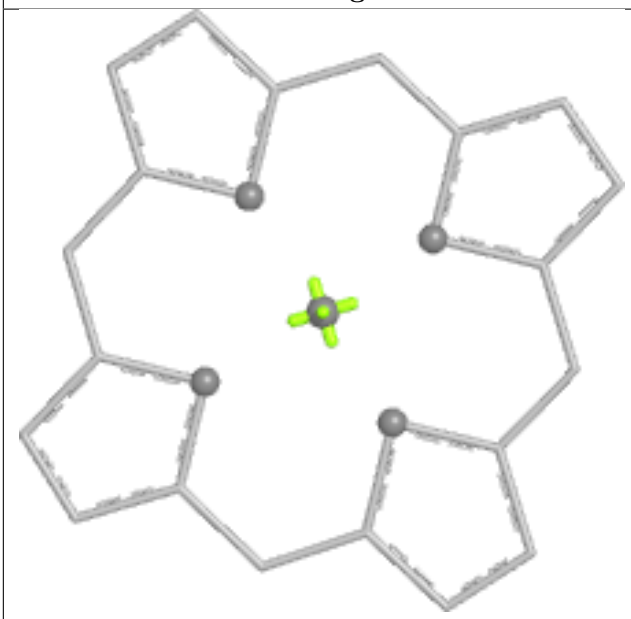
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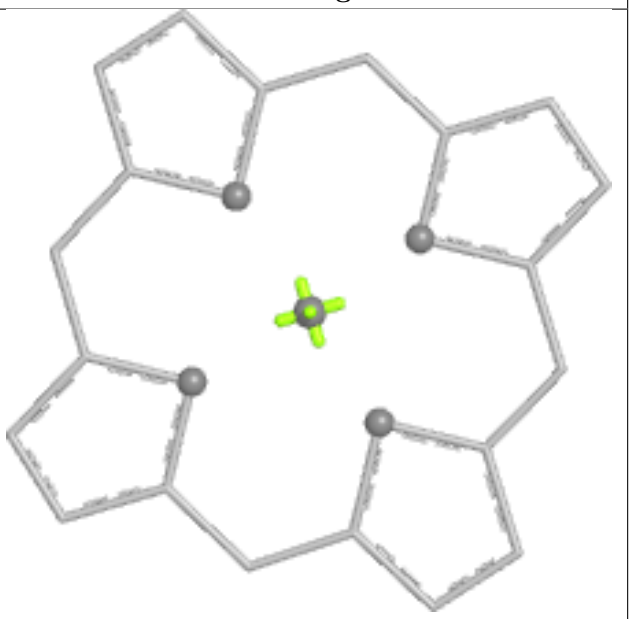
Bond lengths



Bond angles

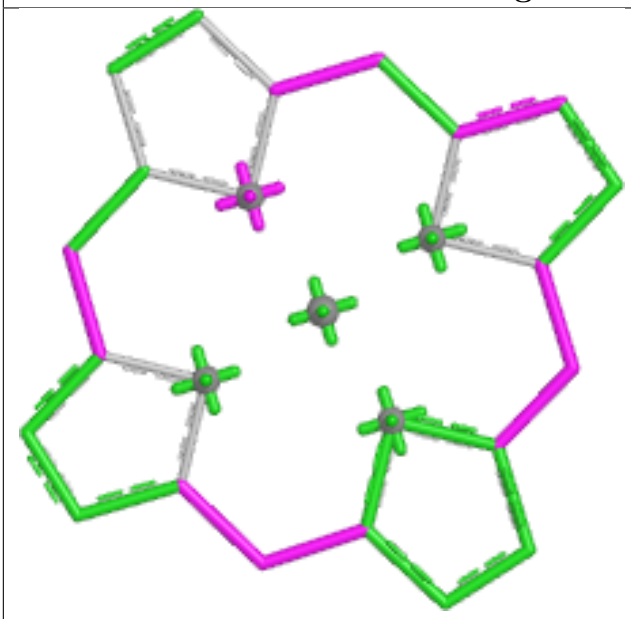


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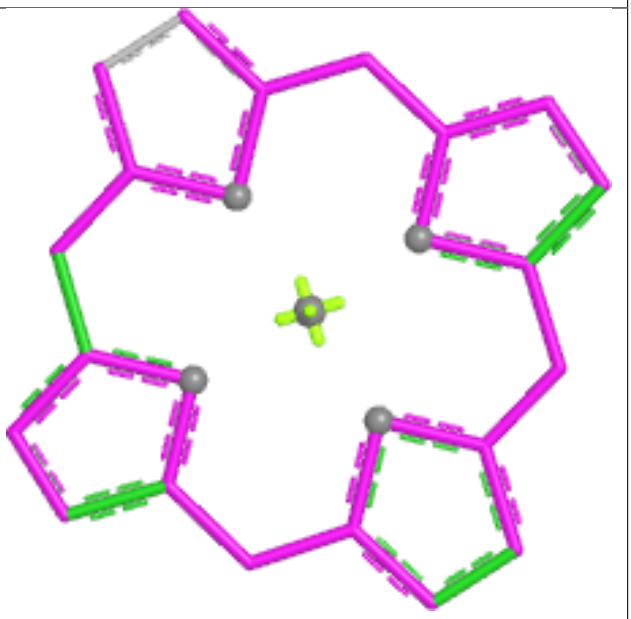


Rings

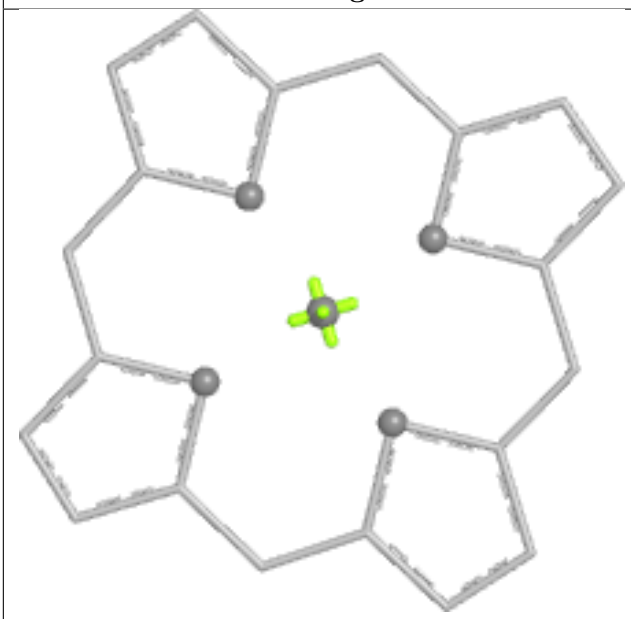
Ligand CLA A 1144



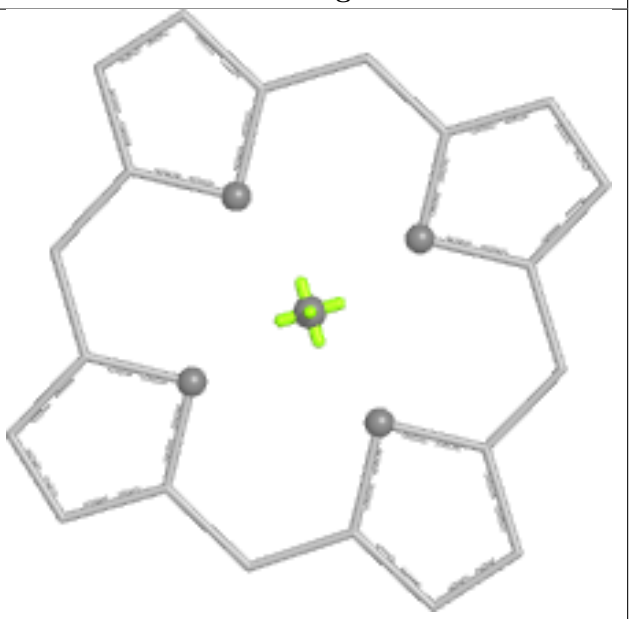
Bond lengths



Bond angles

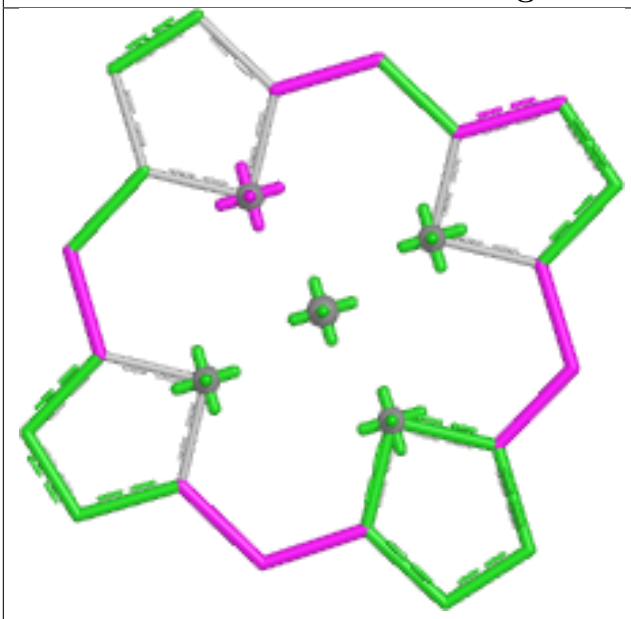


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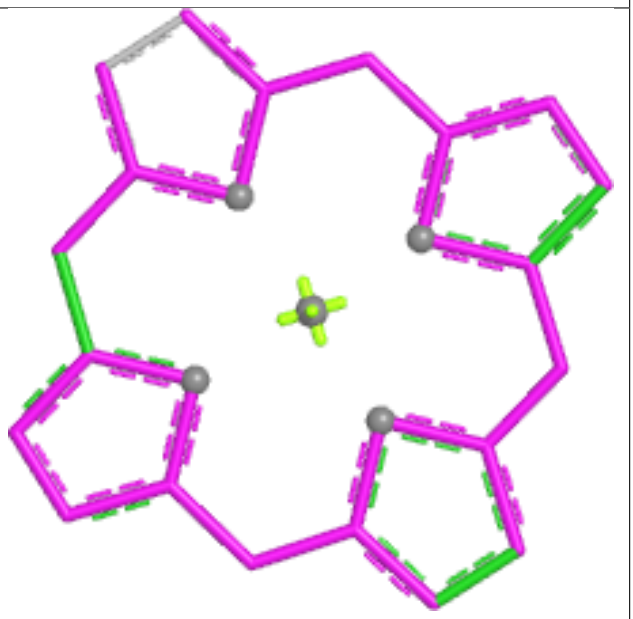


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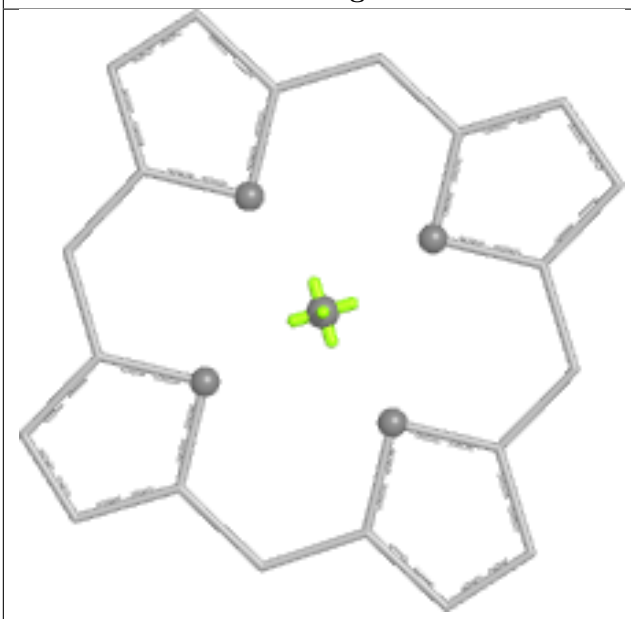
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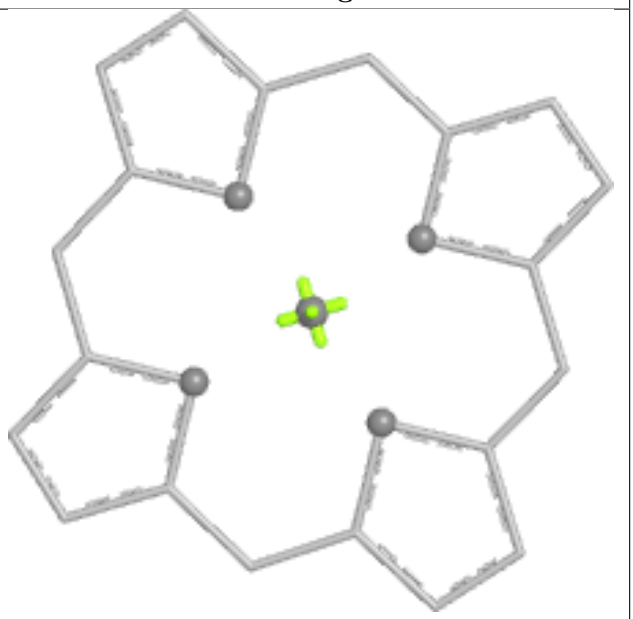
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Bond angles

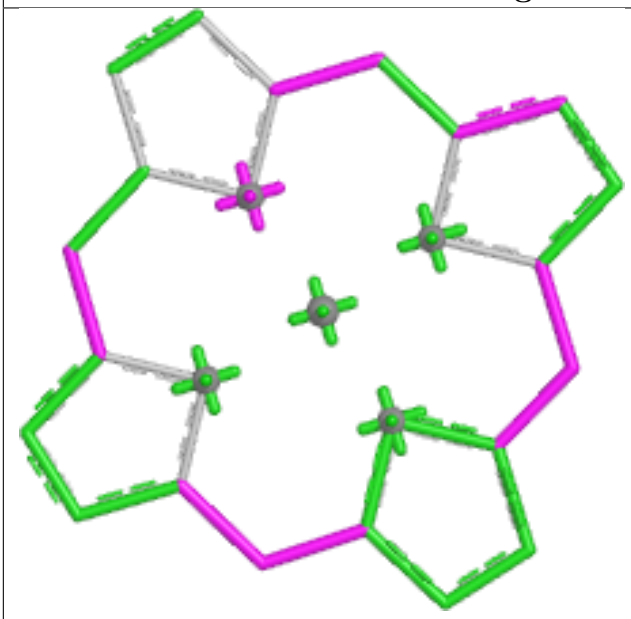


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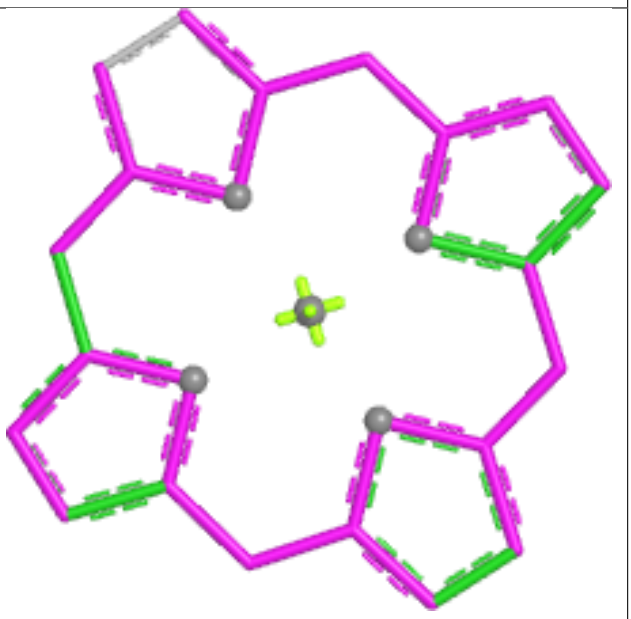


Rings

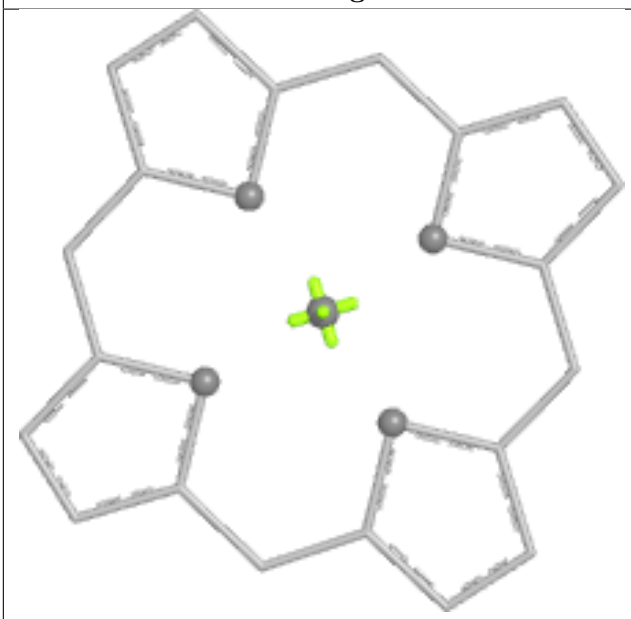
Ligand CLA A 1152



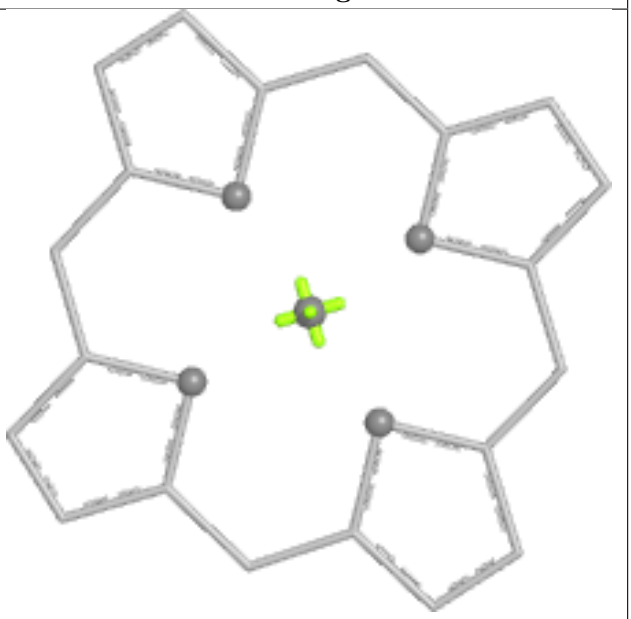
Bond lengths



Bond angles

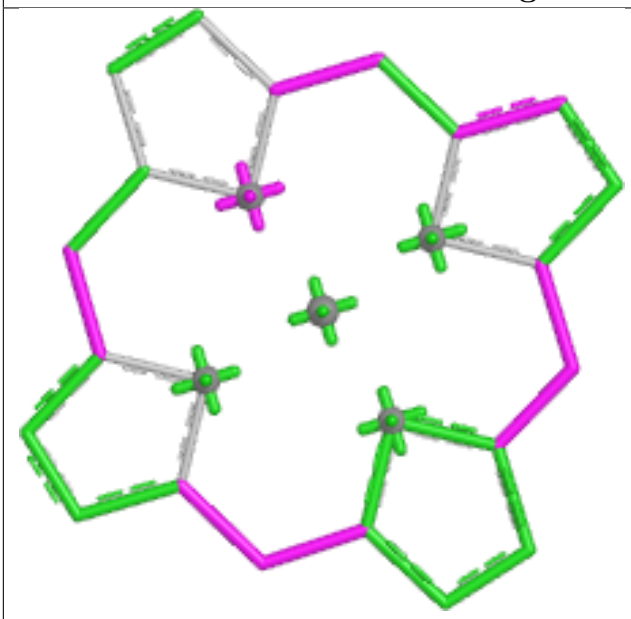


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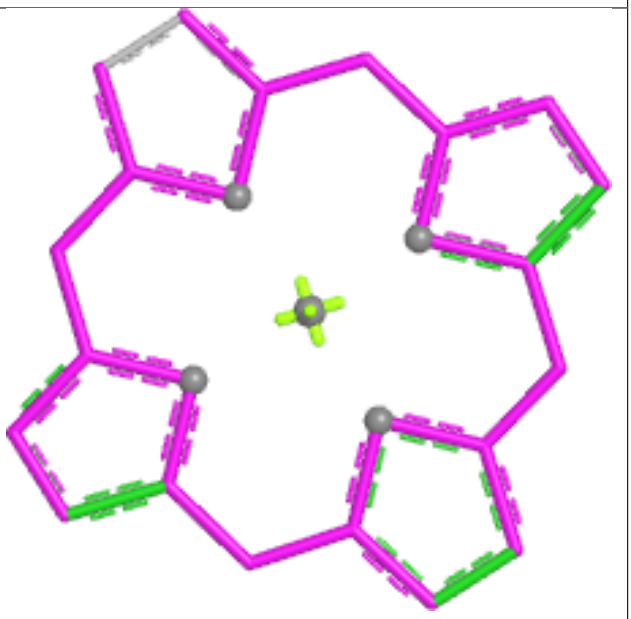


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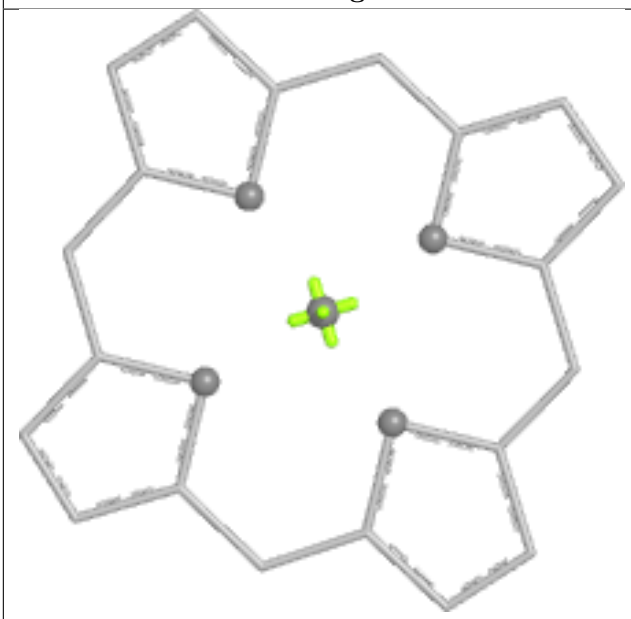
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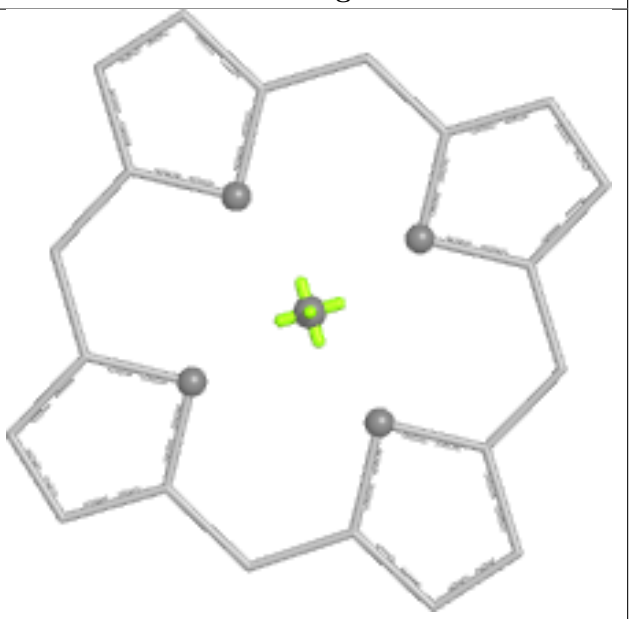
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Bond angles

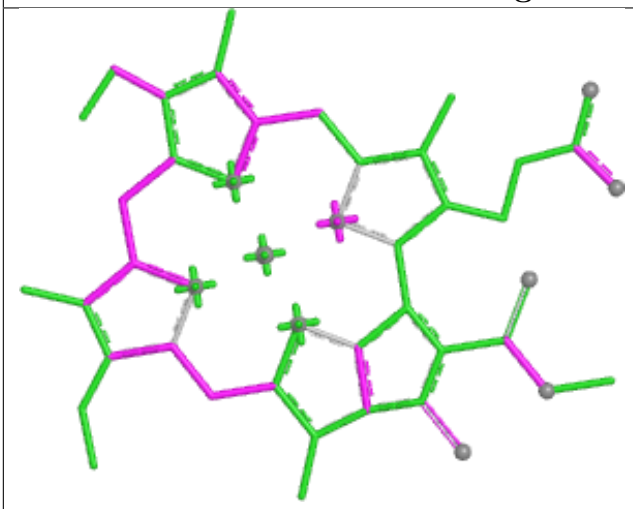


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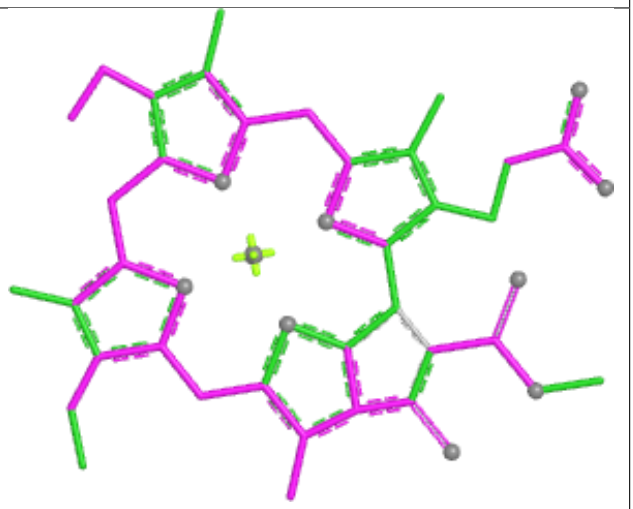


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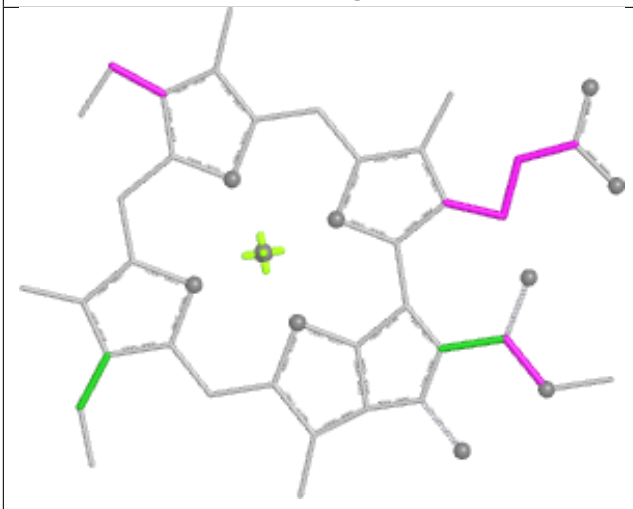
Ligand CLA A 1135



Bond lengths



Bond angles

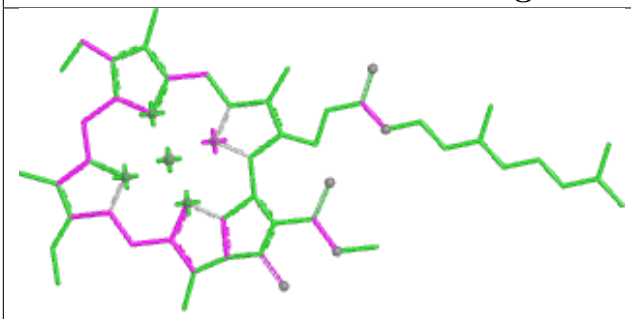


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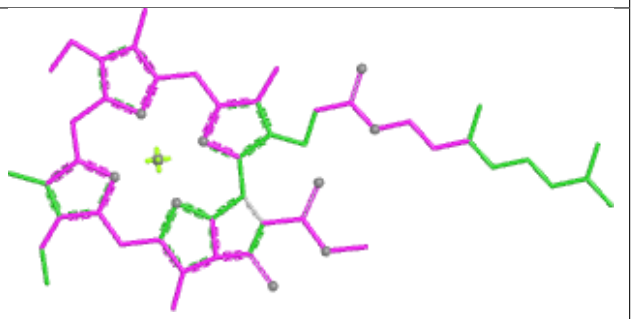


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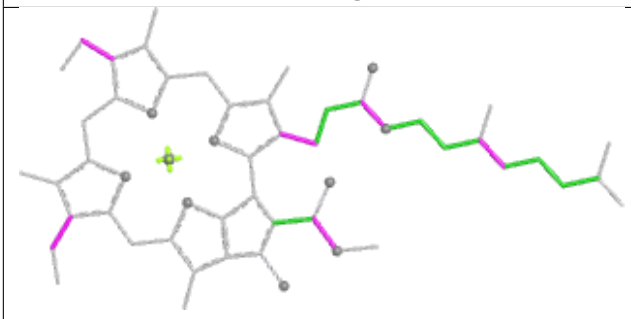
Ligand CLA A 9011



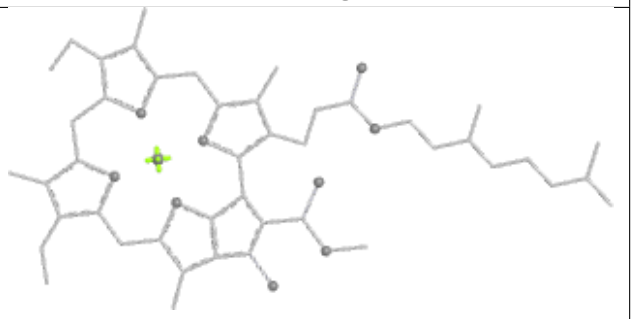
Bond lengths



Bond angles

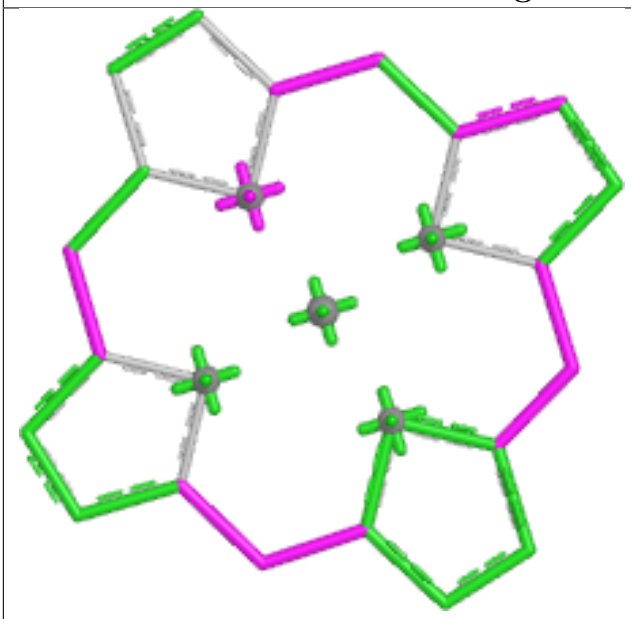


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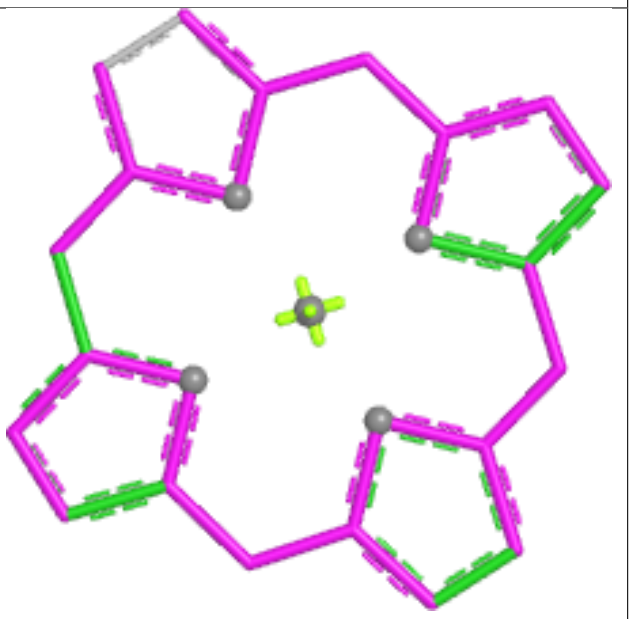


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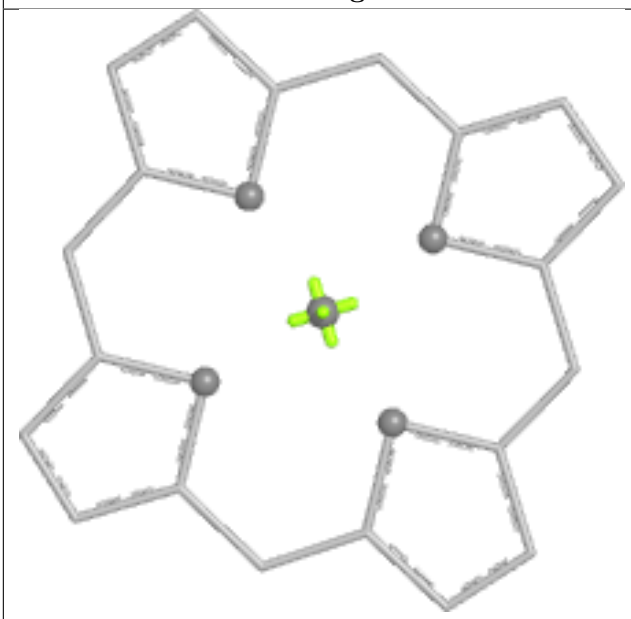
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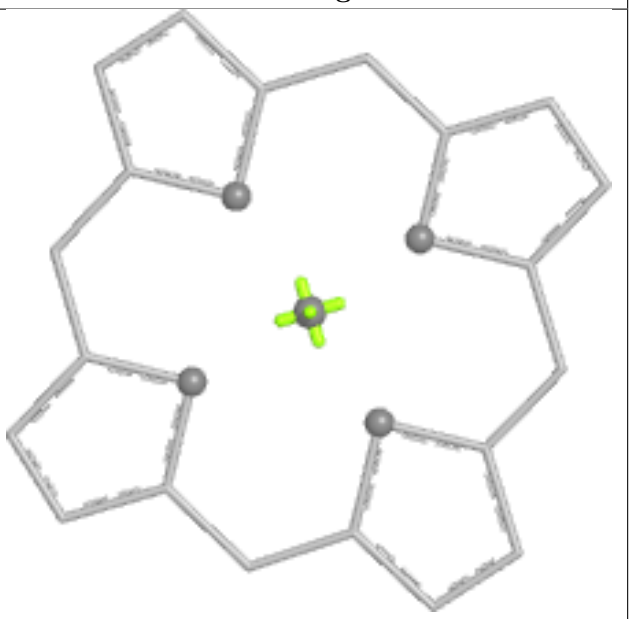
Bond lengths



Bond angles

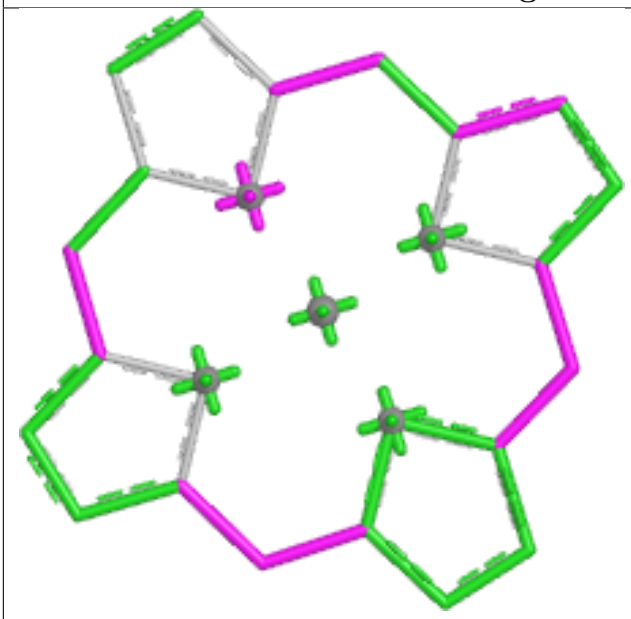


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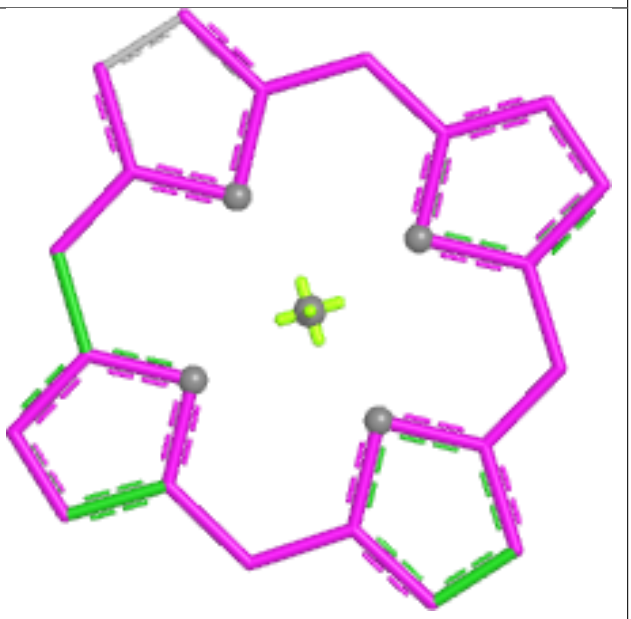


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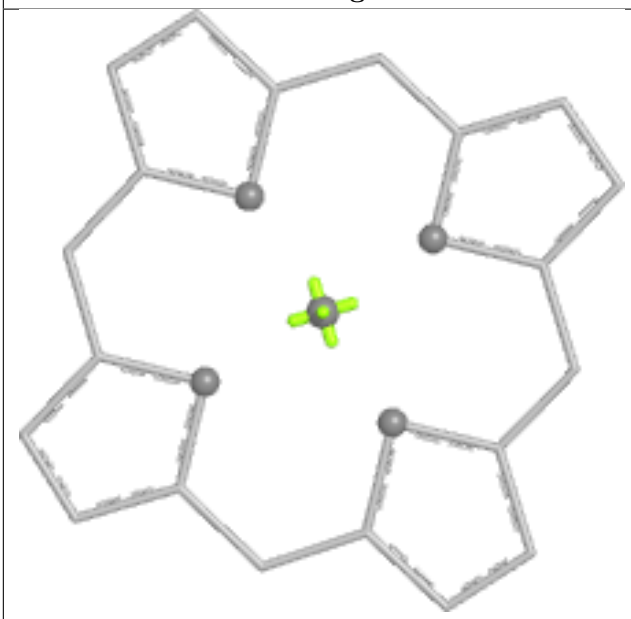
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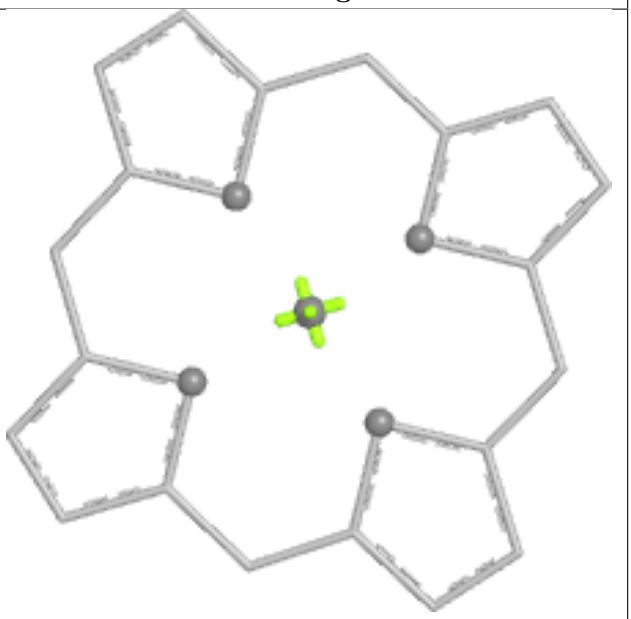
Bond lengths



Bond angles

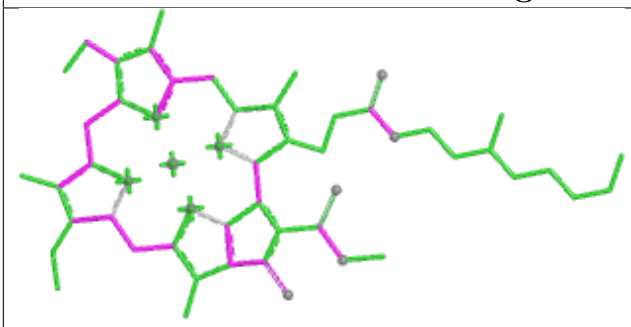


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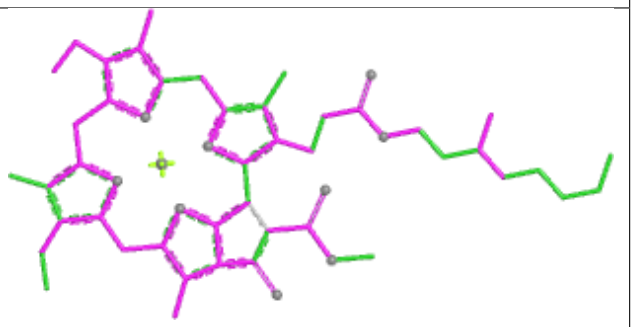


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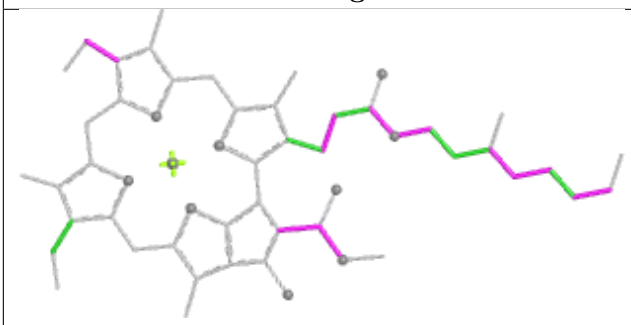
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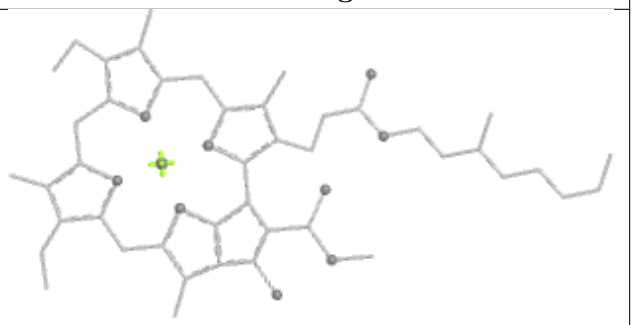
Bond lengths



Bond angles

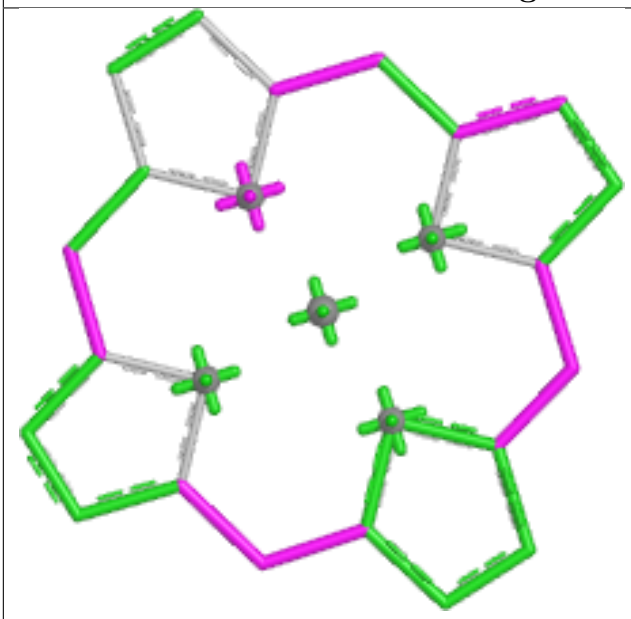


Torsions

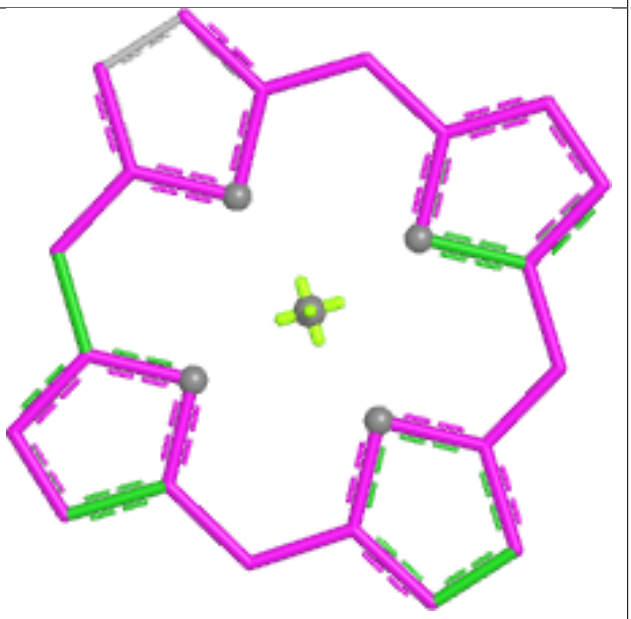


Rings

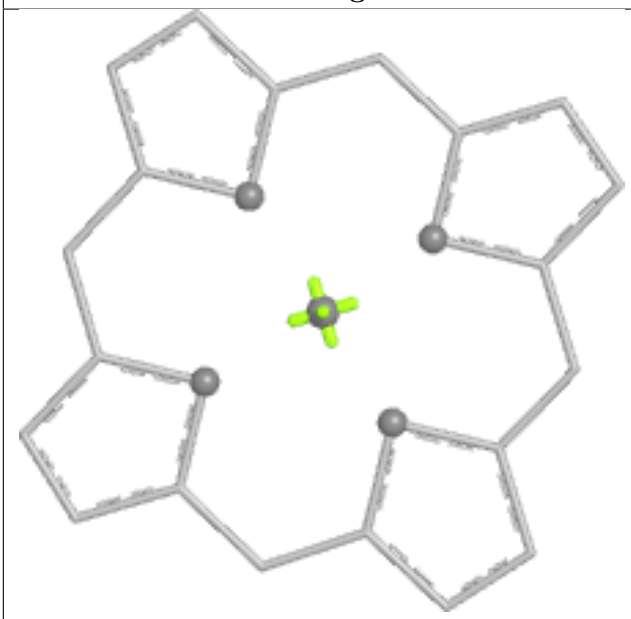
Ligand CLA 2 2006



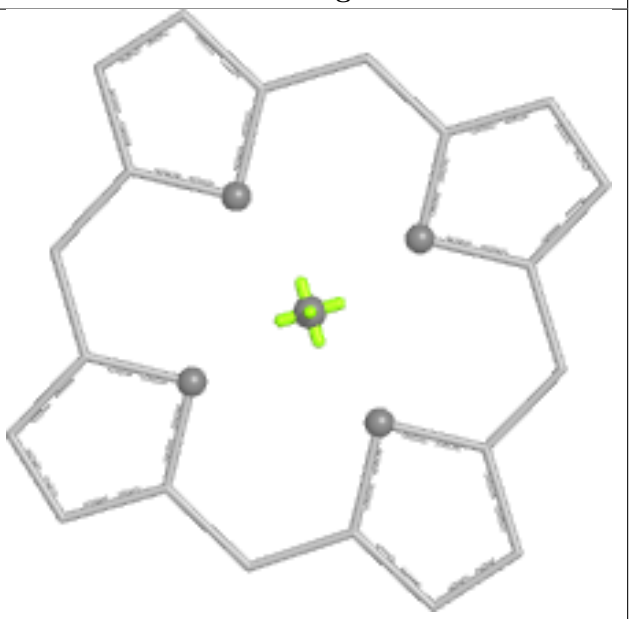
Bond lengths



Bond angles

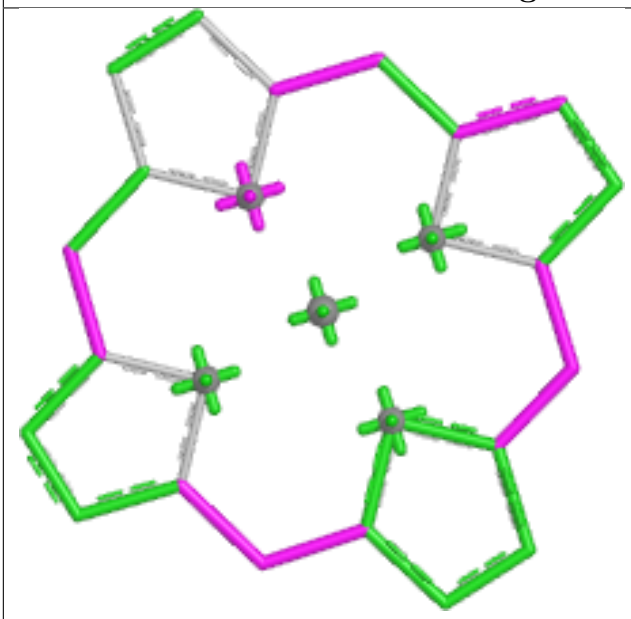


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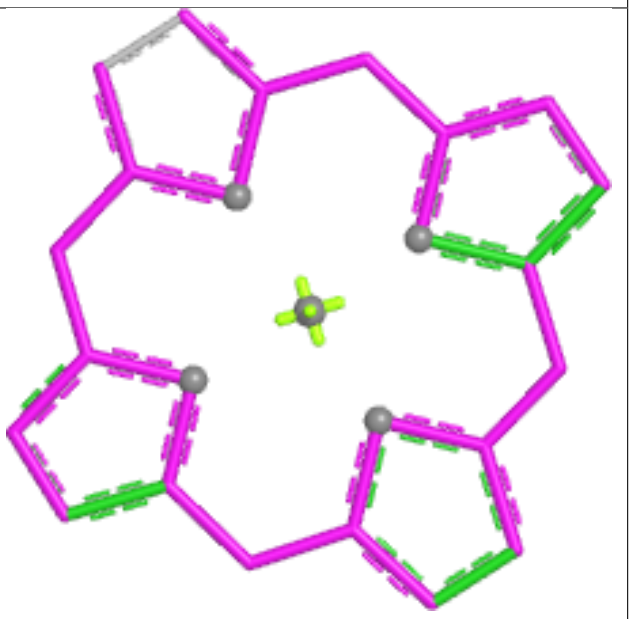


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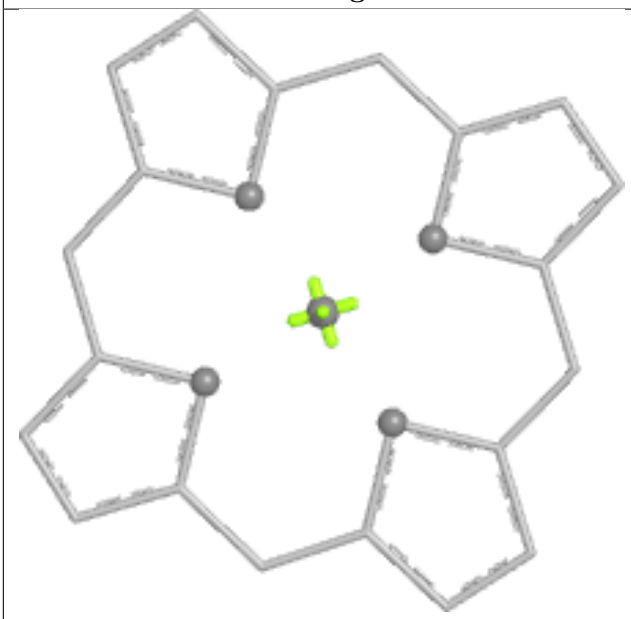
Ligand CLA 3 3001



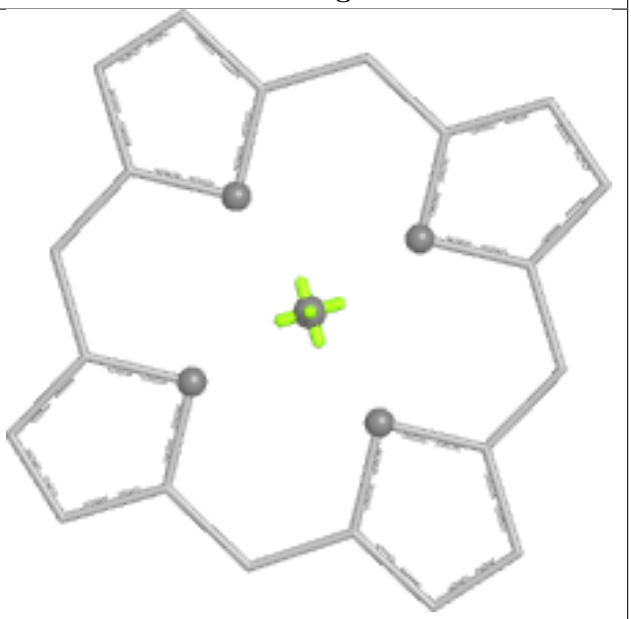
Bond lengths



Bond angles

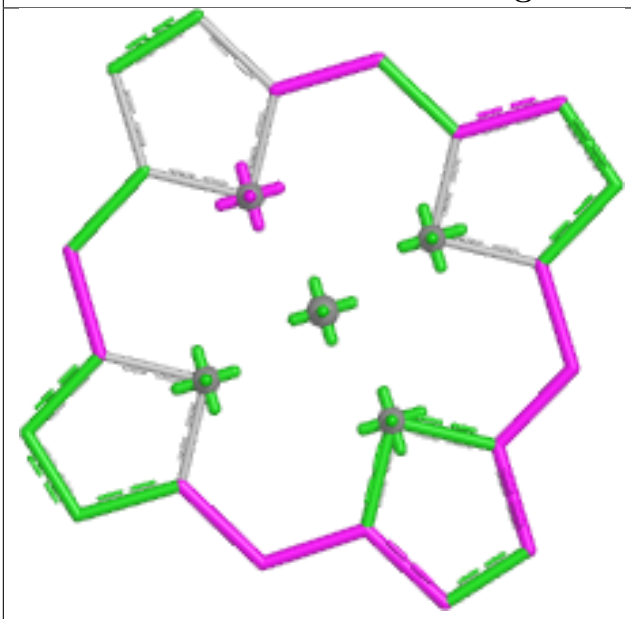


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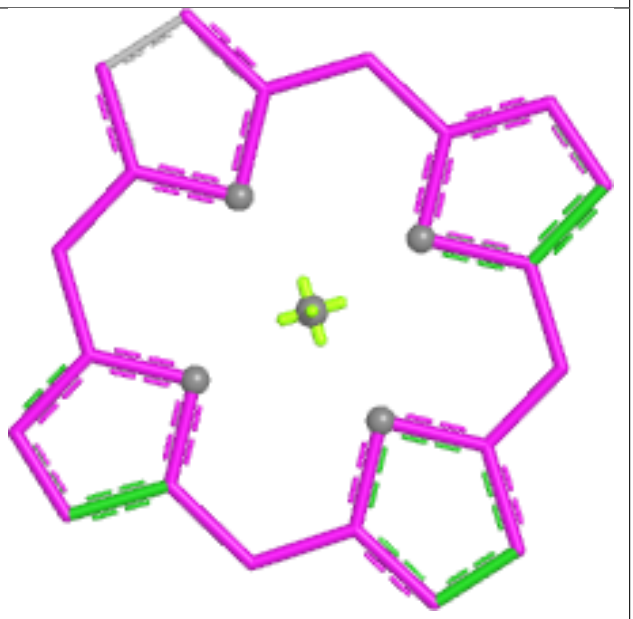


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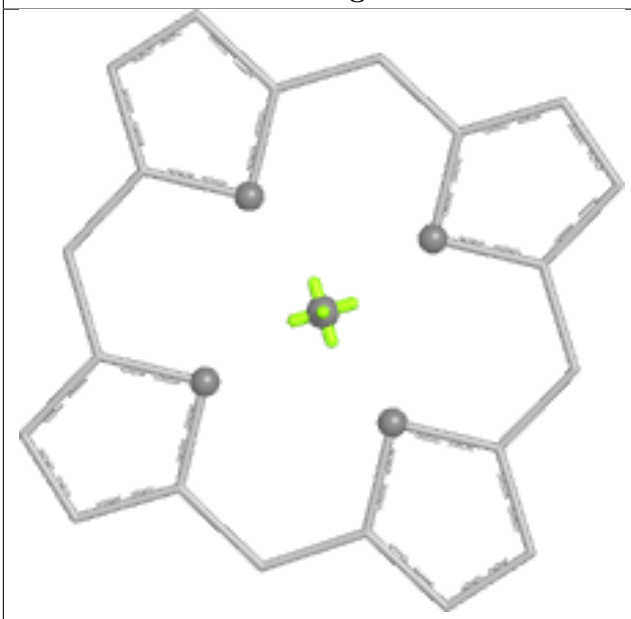
Ligand CLA A 1127



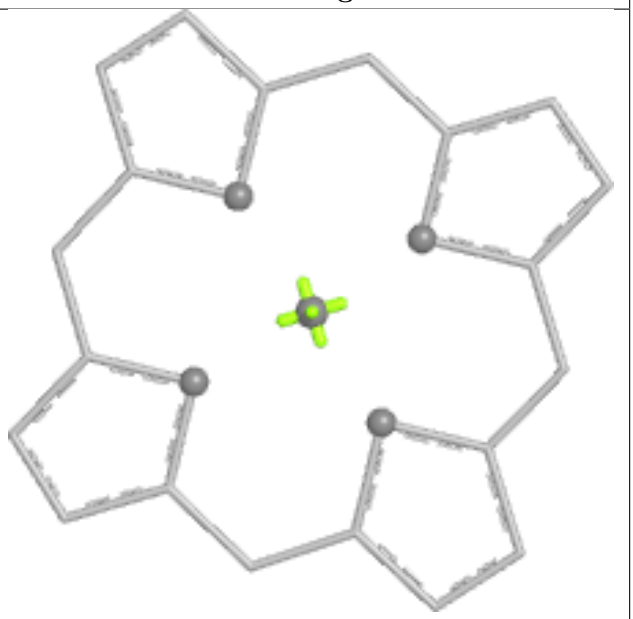
Bond lengths



Bond angles

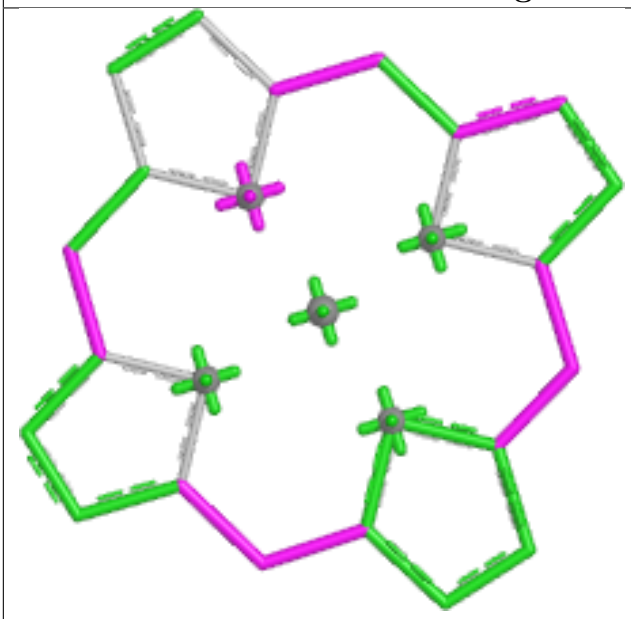


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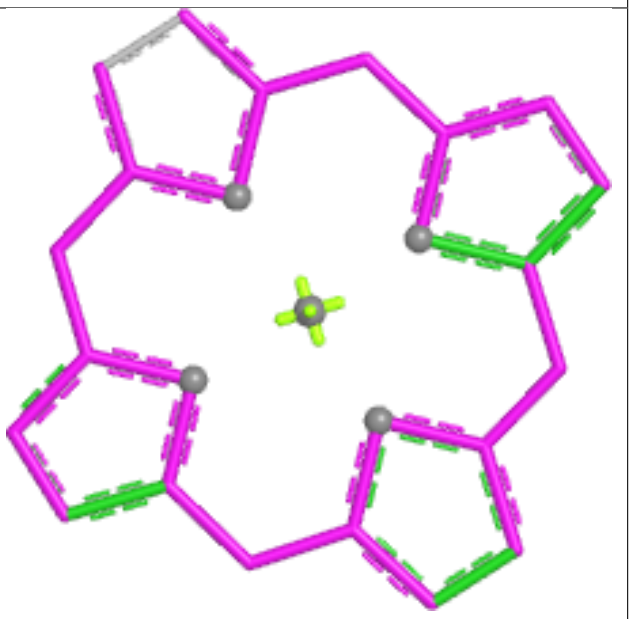


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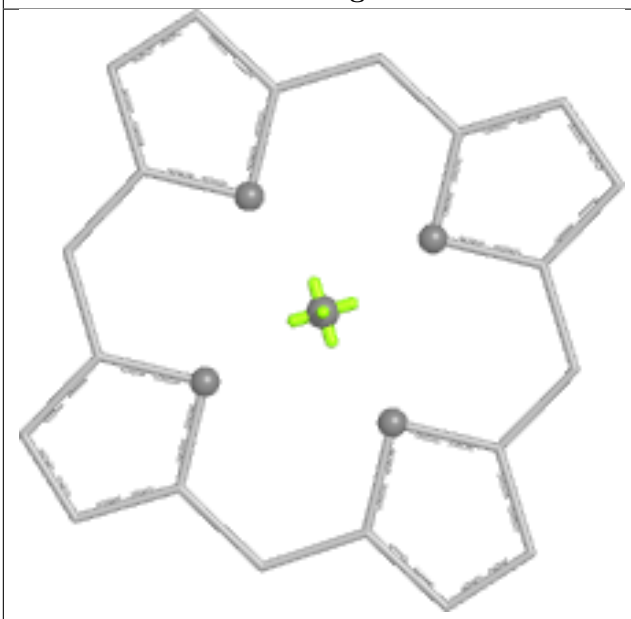
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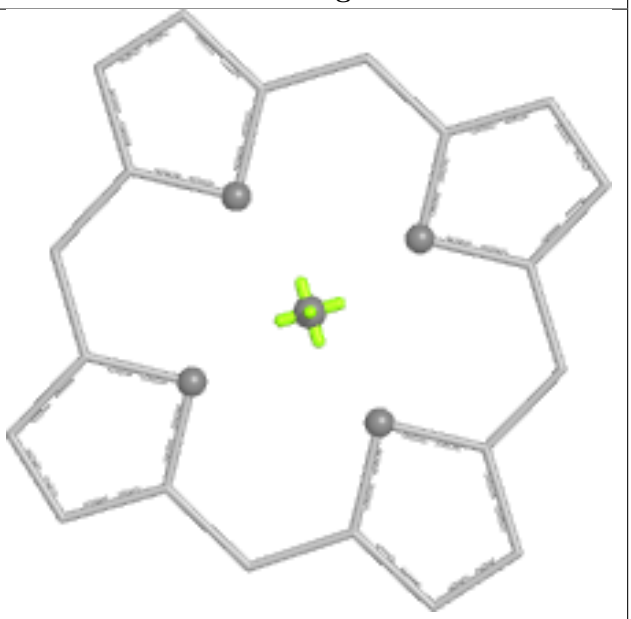
Bond lengths



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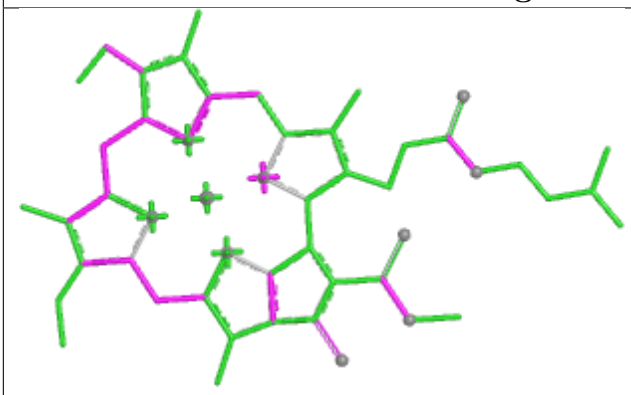


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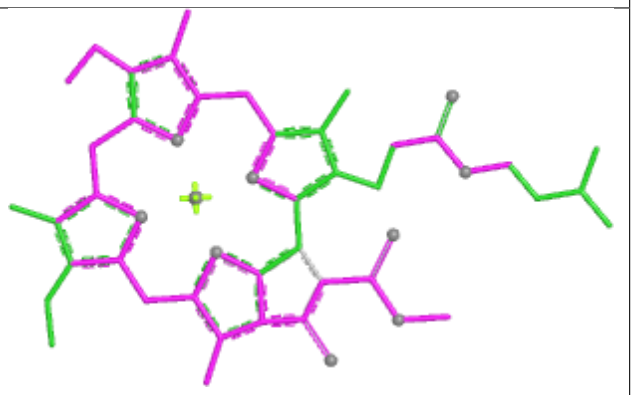


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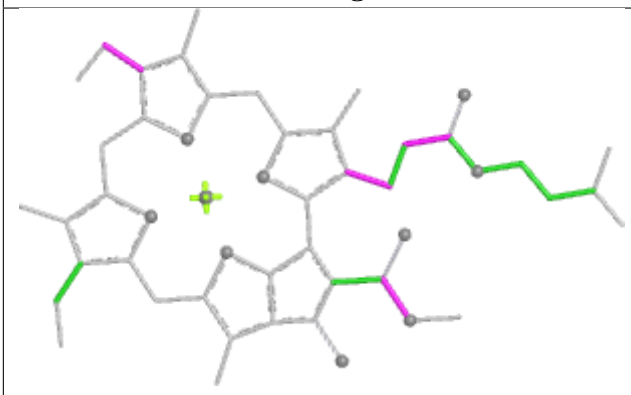
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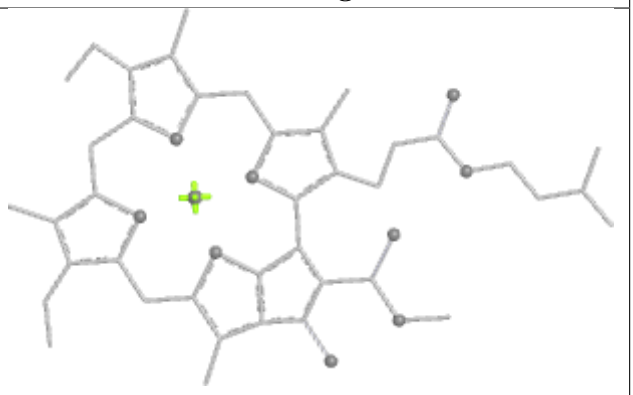
Bond lengths



Bond angles

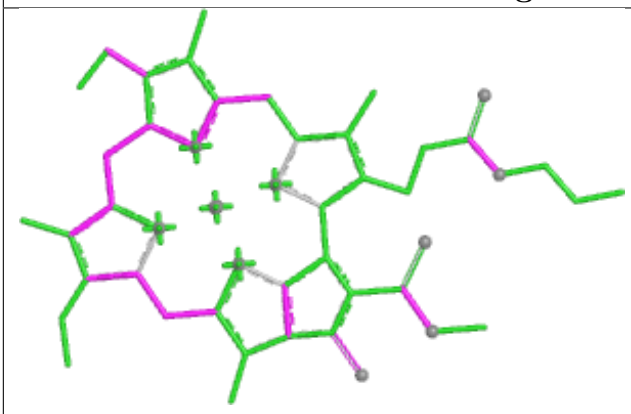


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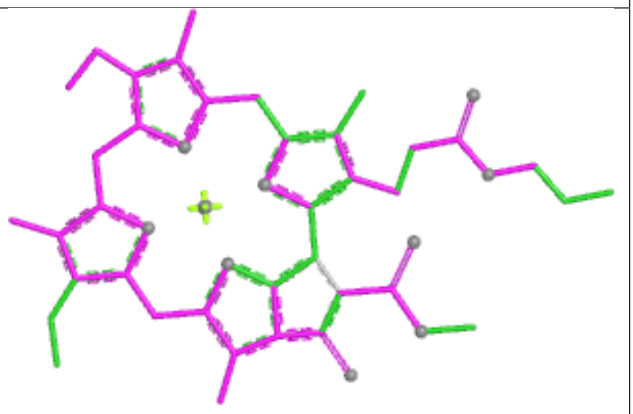


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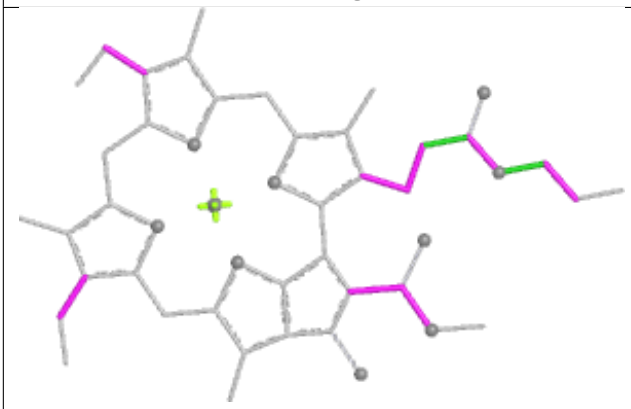
Ligand CLA B 1221



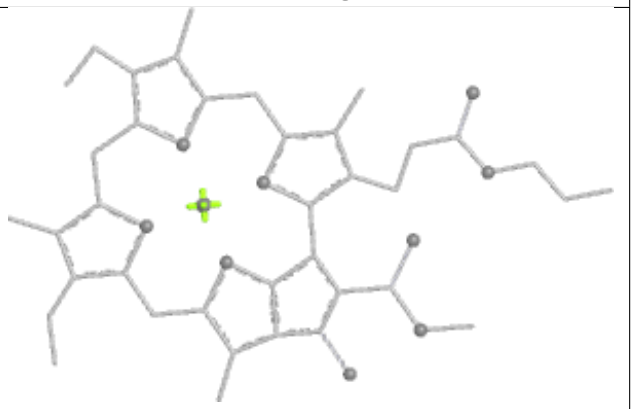
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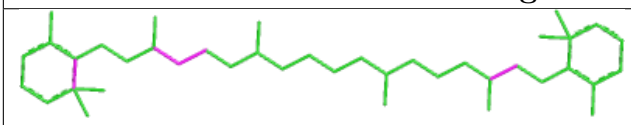


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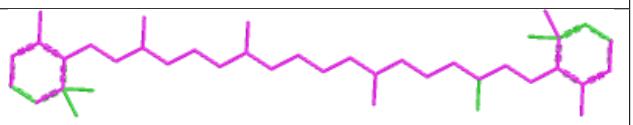


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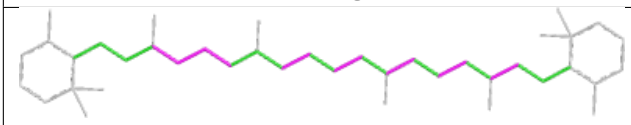
Ligand BCR I 6018



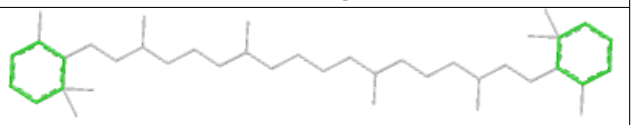
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Bond angles

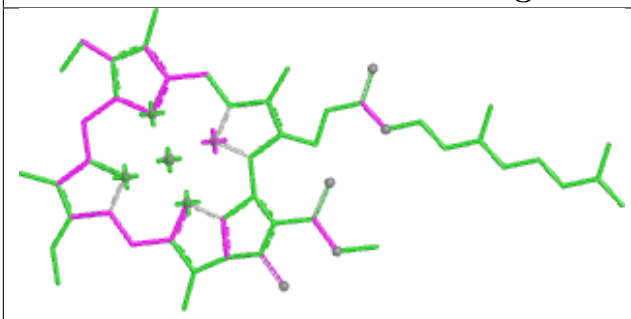


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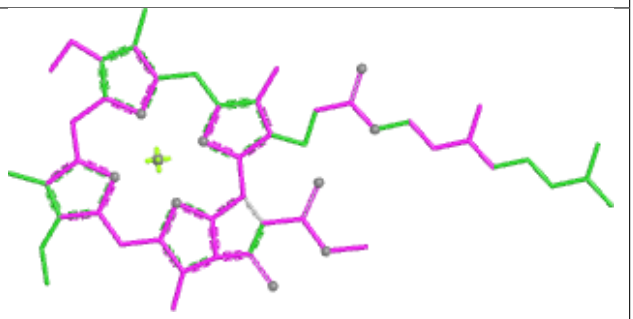


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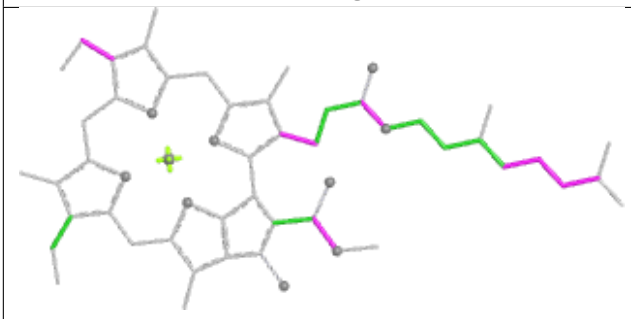
Ligand CLA A 1128



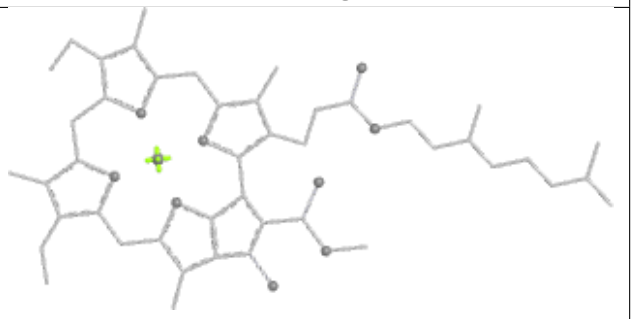
Bond lengths



Bond angles

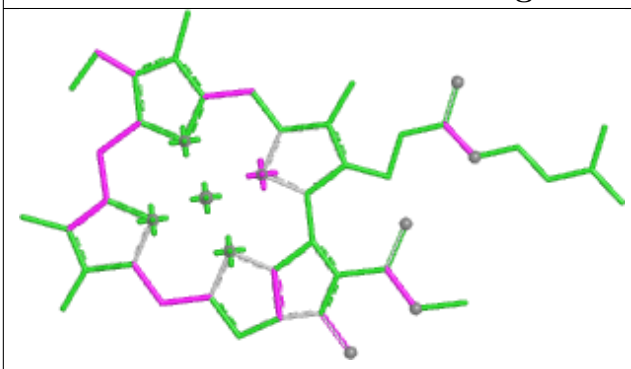


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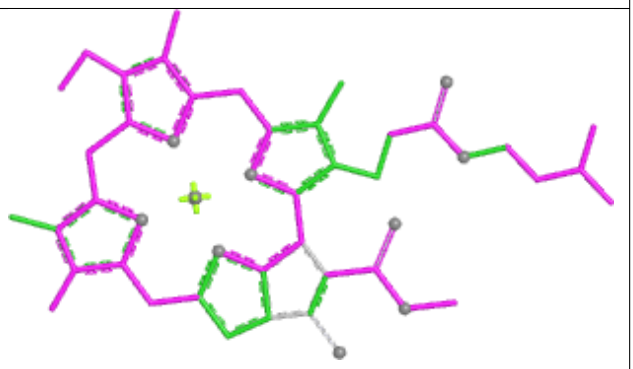


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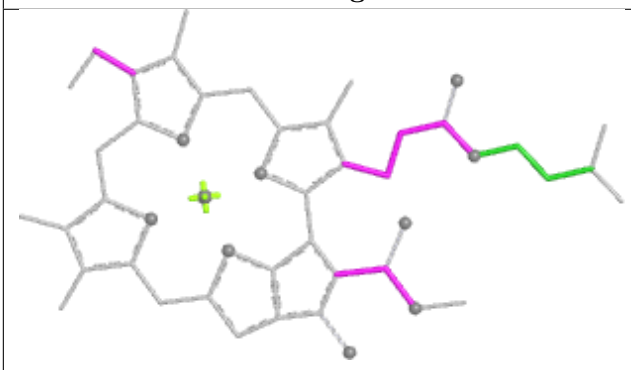
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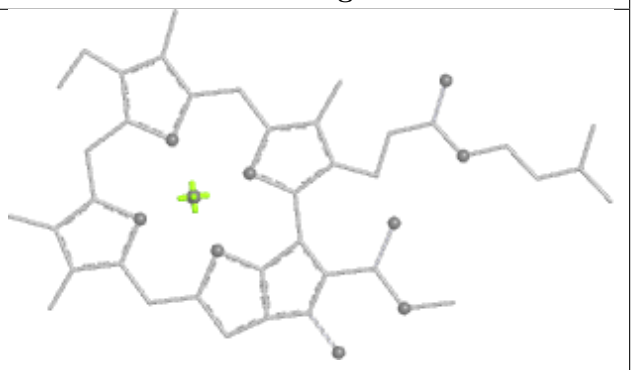
Bond lengths



Bond angles

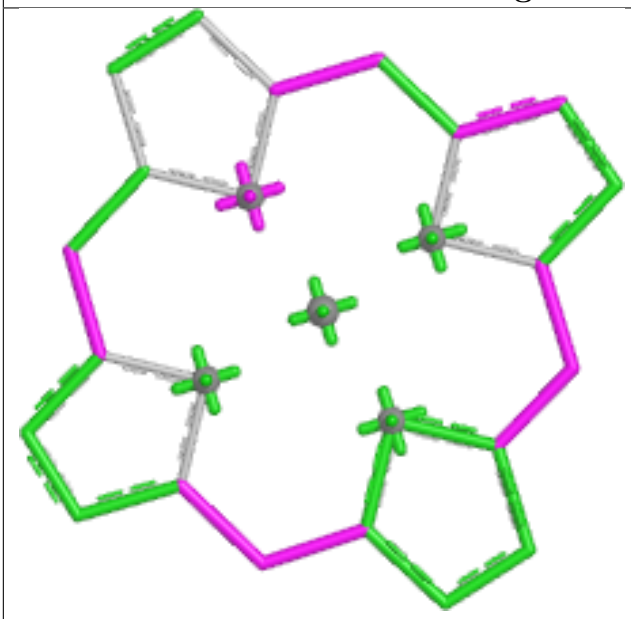


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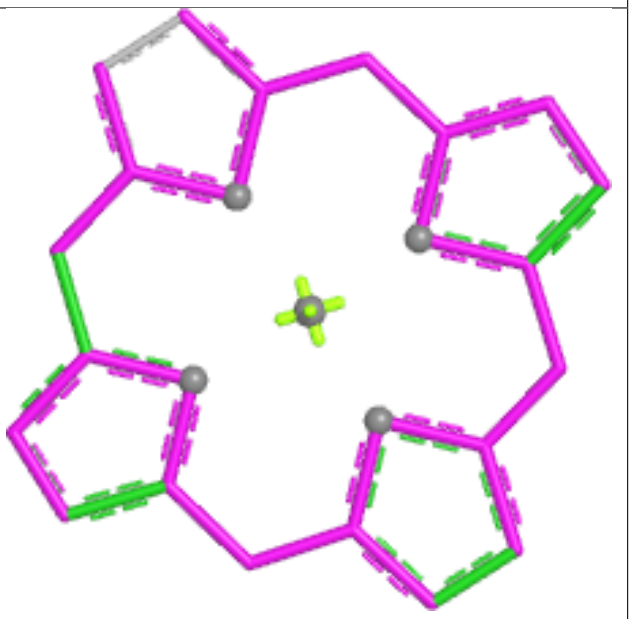


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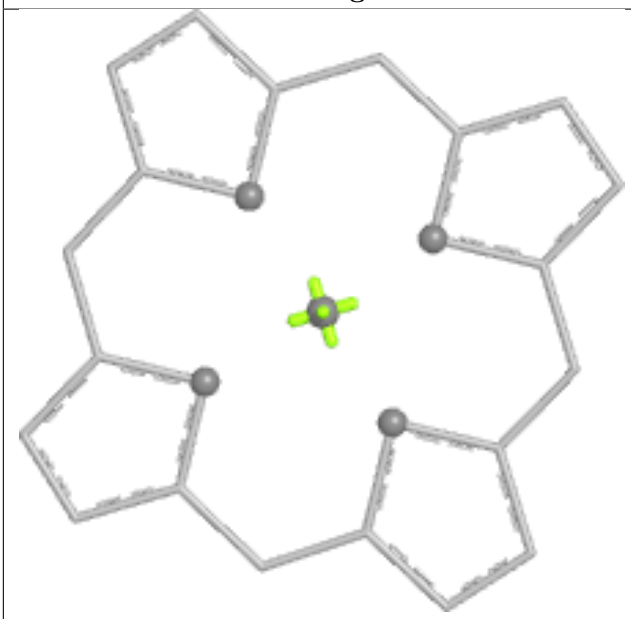
Ligand CLA A 1142



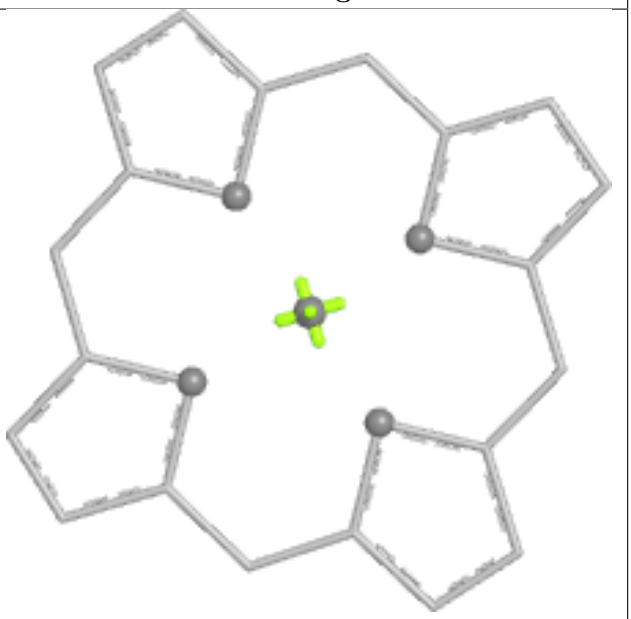
Bond lengths



Bond angles

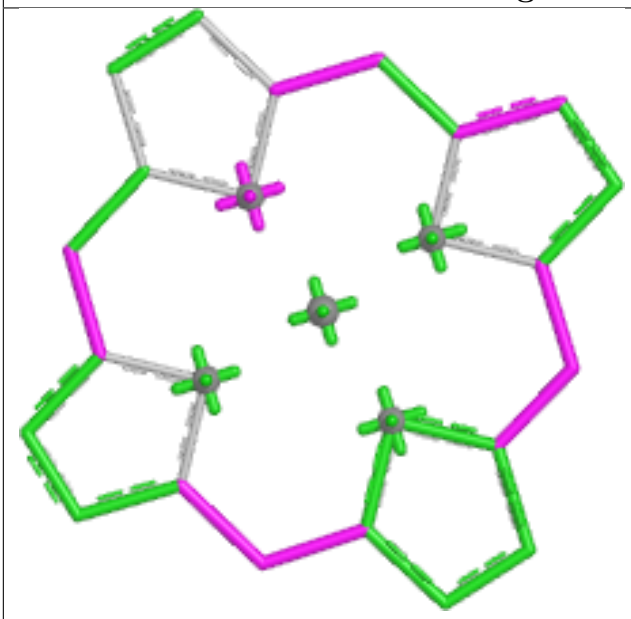


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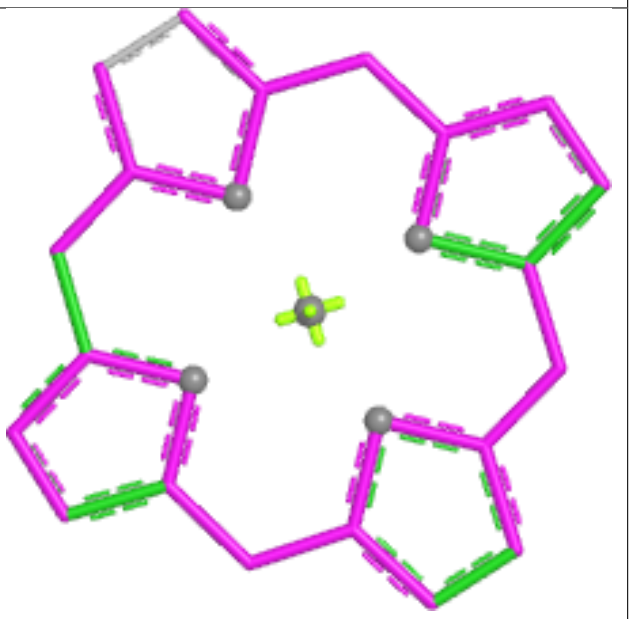


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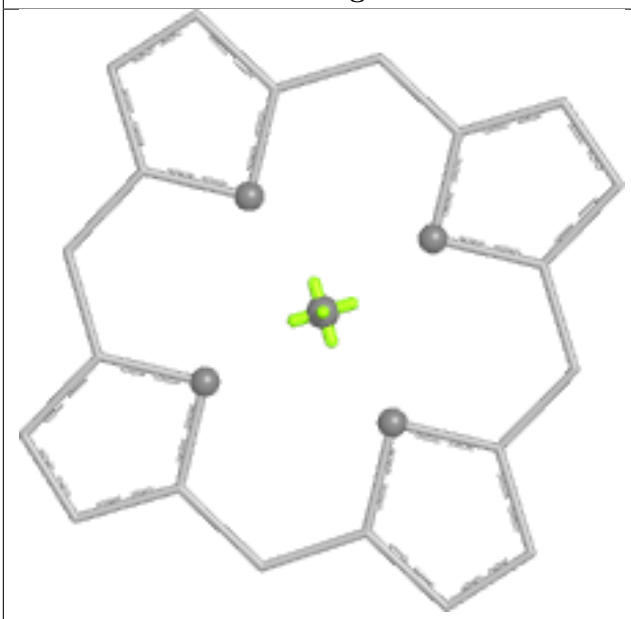
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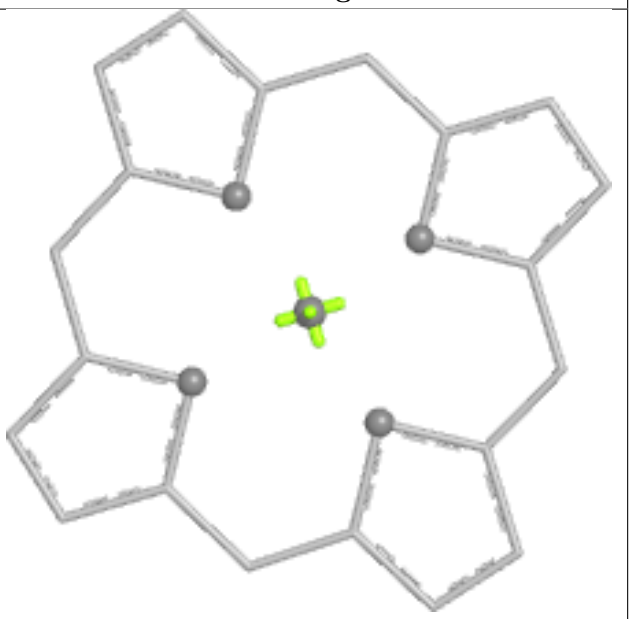
Bond lengths



Bond angles

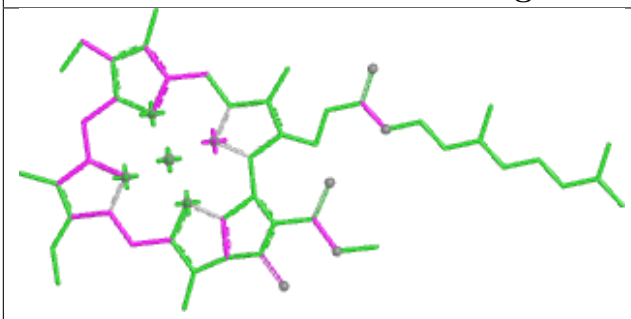


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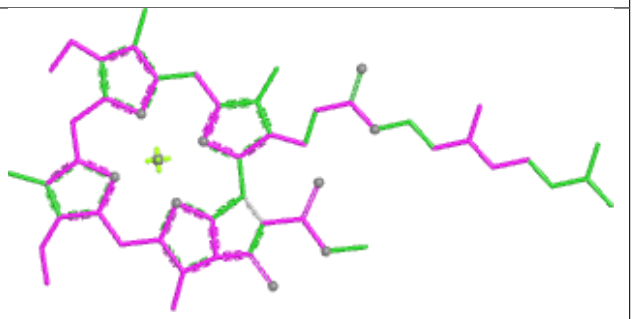


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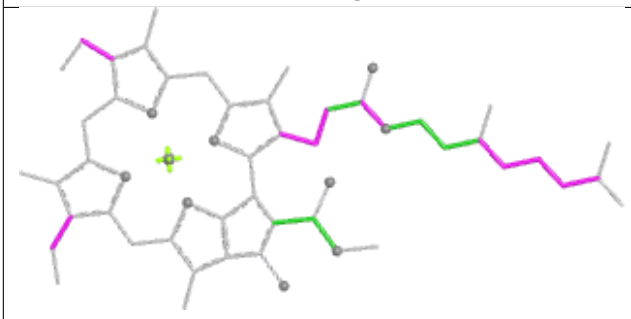
Ligand CLA A 1137



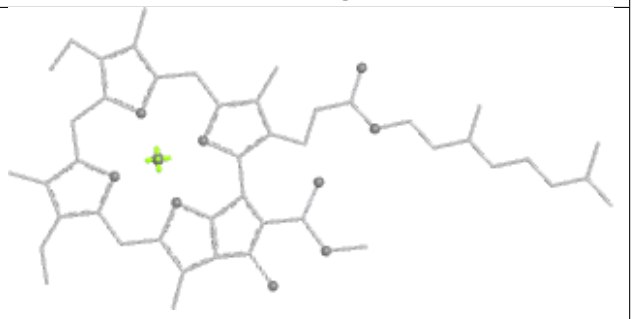
Bond lengths



Bond angles

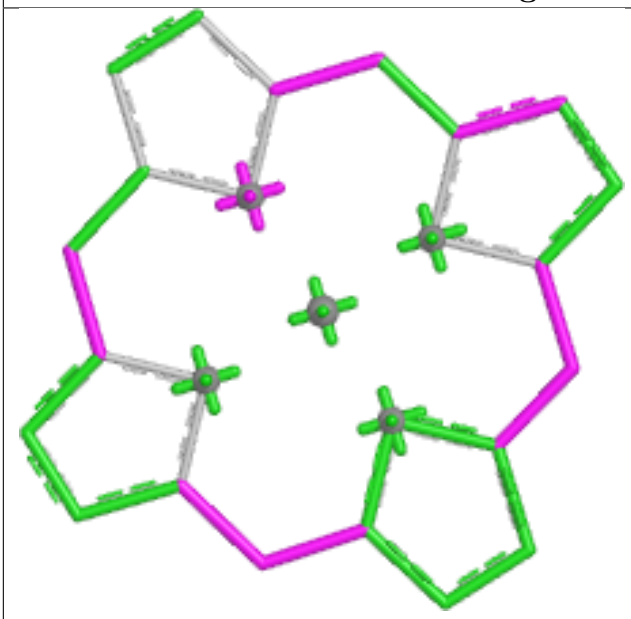


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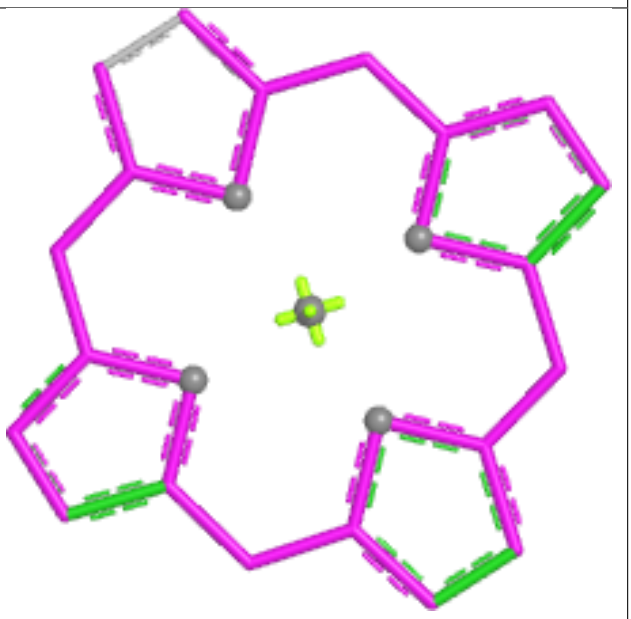


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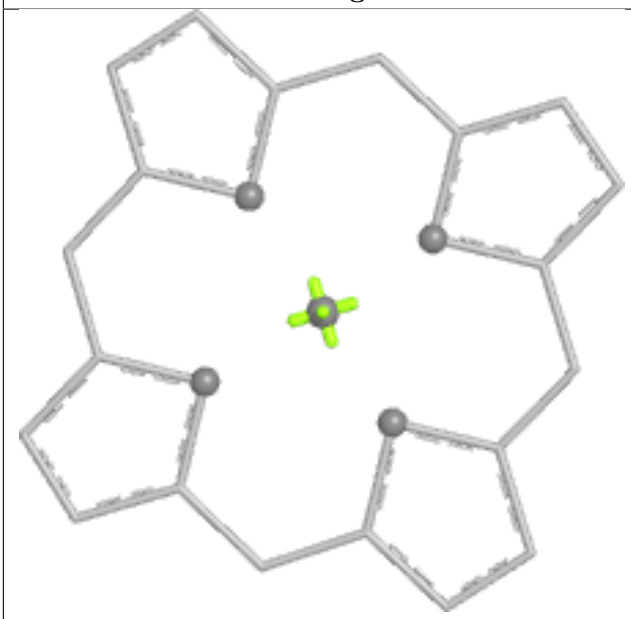
Ligand CLA 1 1011



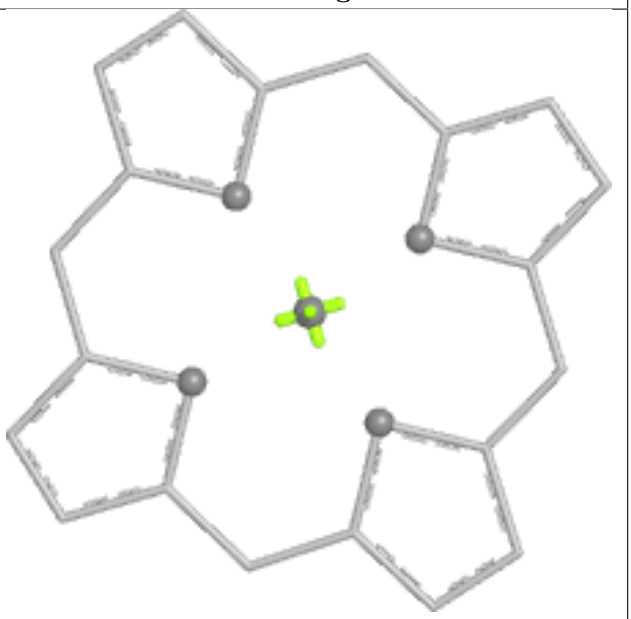
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Bond angles

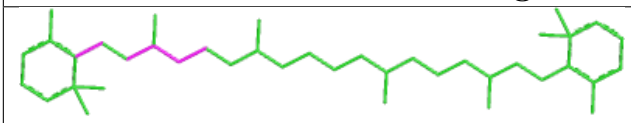


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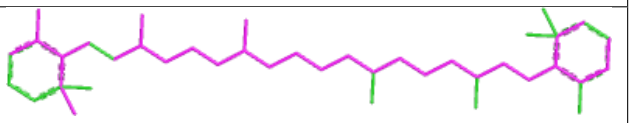


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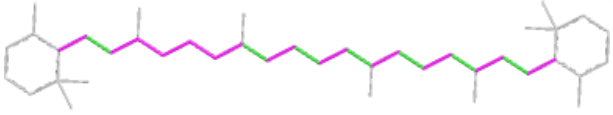
Ligand BCR B 6017



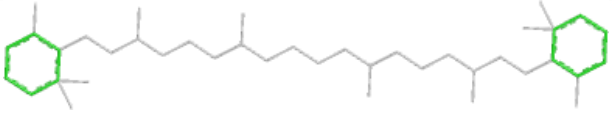
Bond lengths



Bond angles

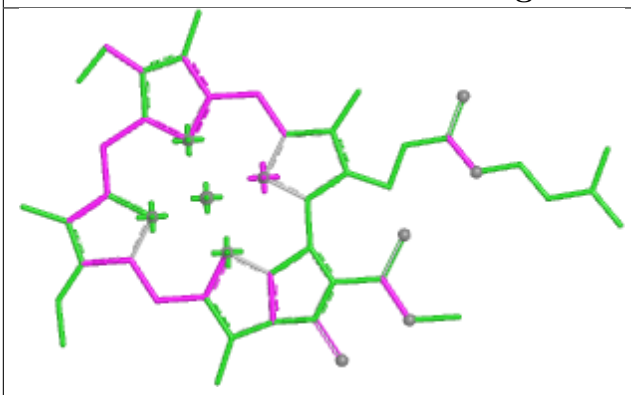


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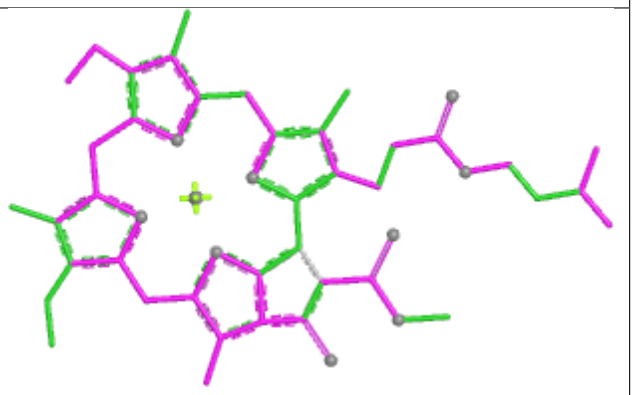


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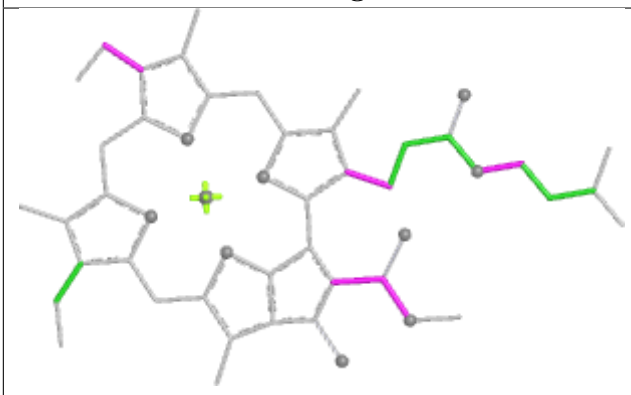
Ligand CLA B 1217



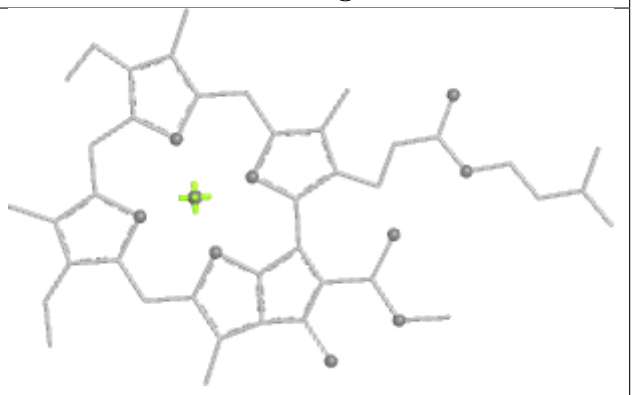
Bond lengths



Bond angles

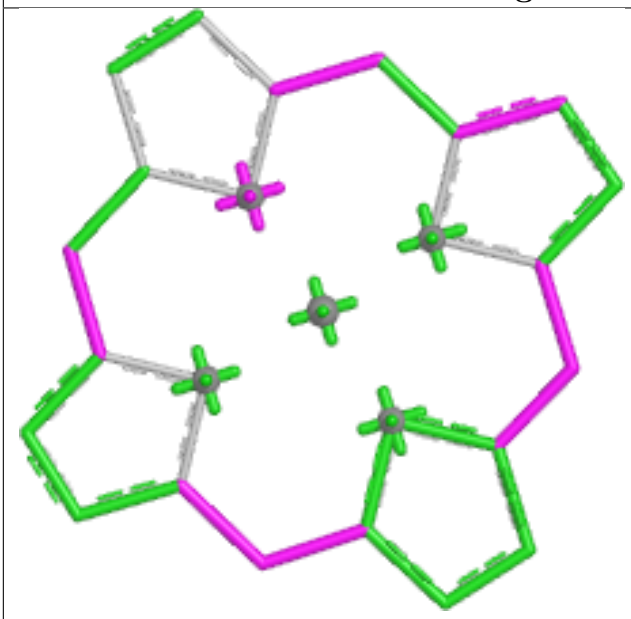


Torsions

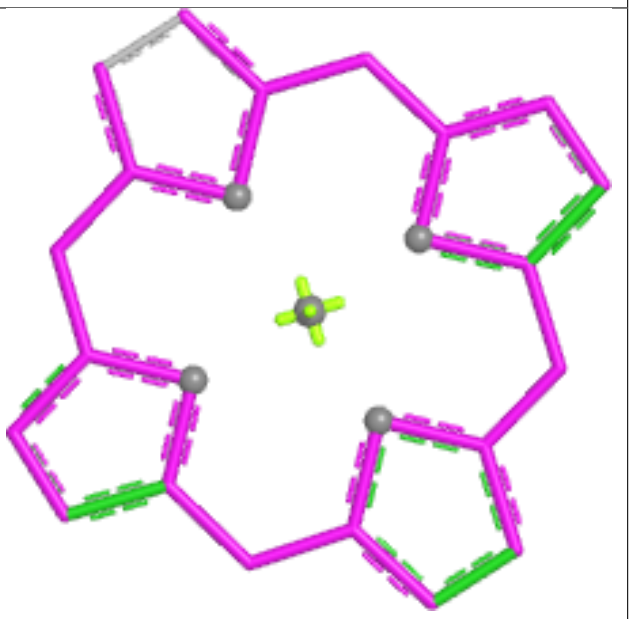


Rings

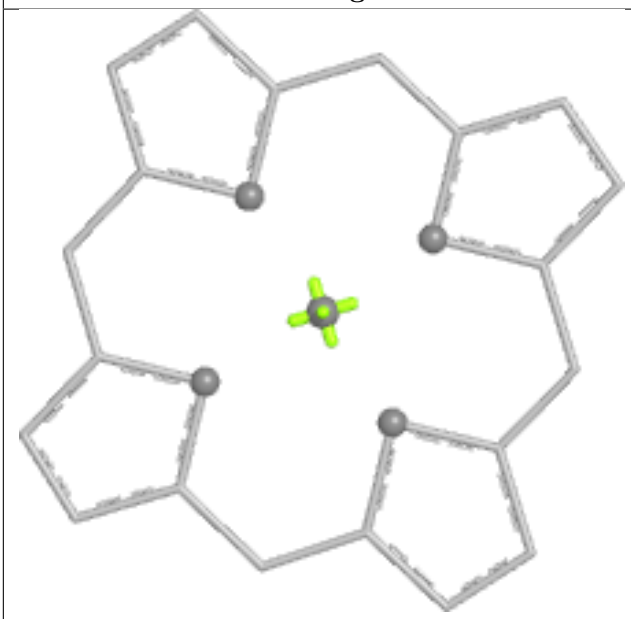
Ligand CLA B 1301



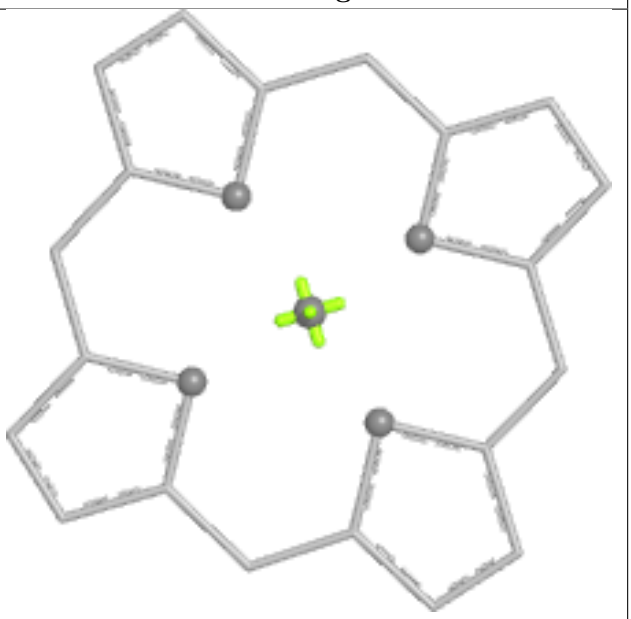
Bond lengths



Bond angles

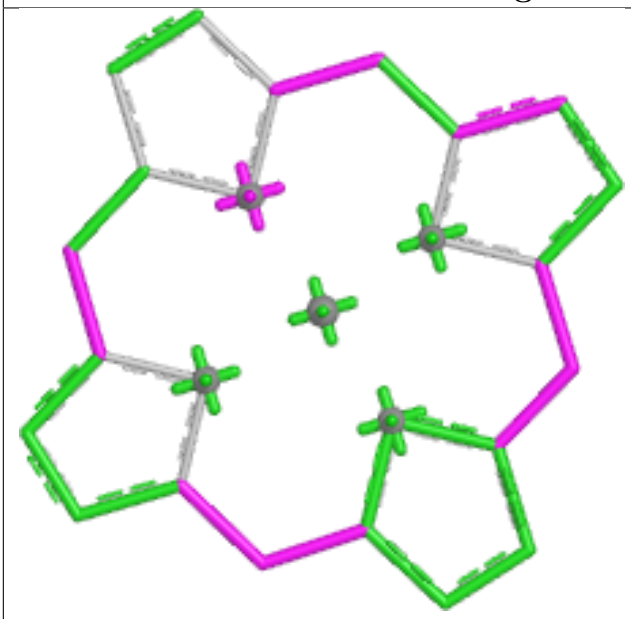


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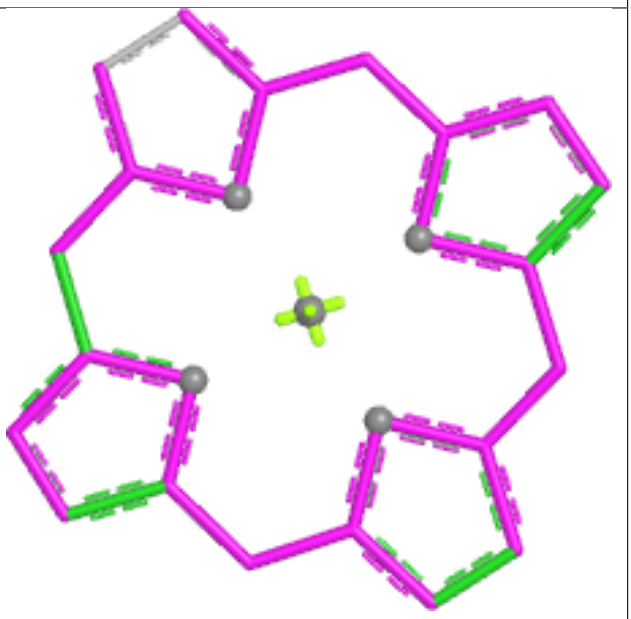


Rings

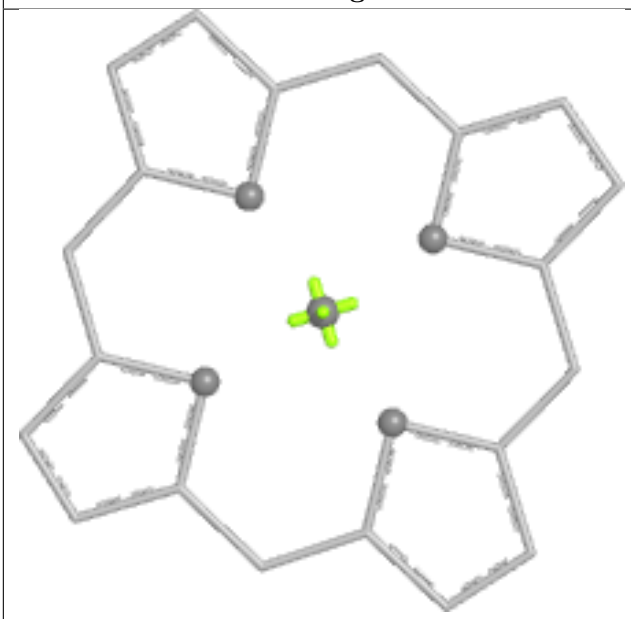
Ligand CLA A 1117



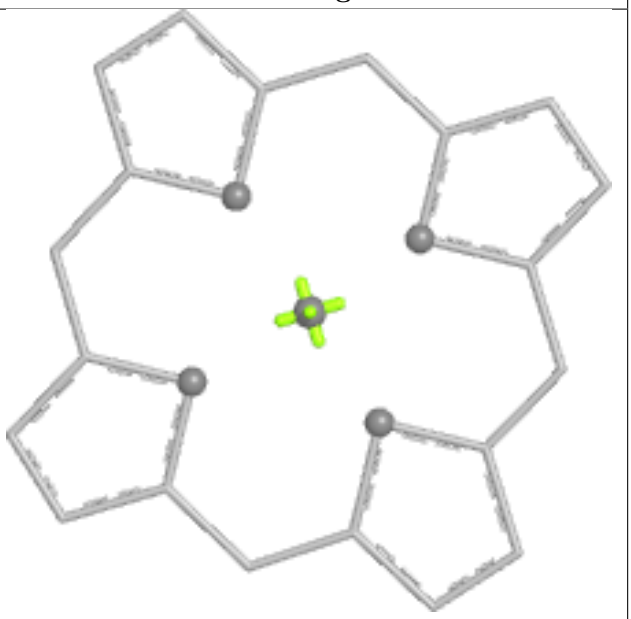
Bond lengths



Bond angles

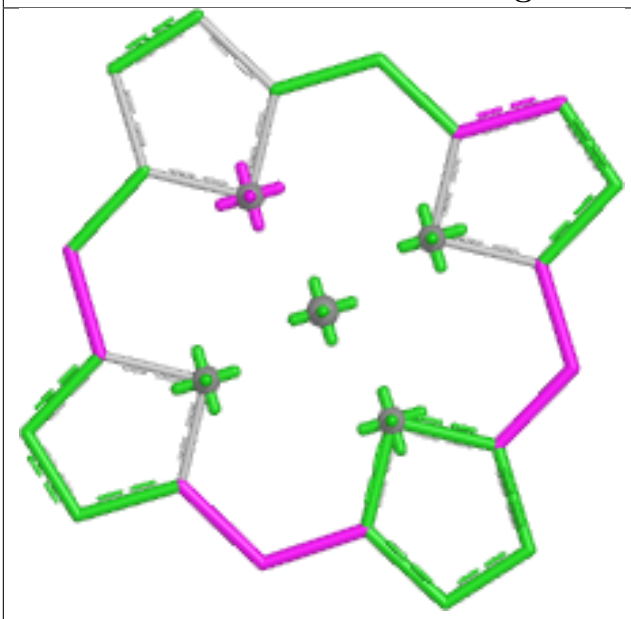


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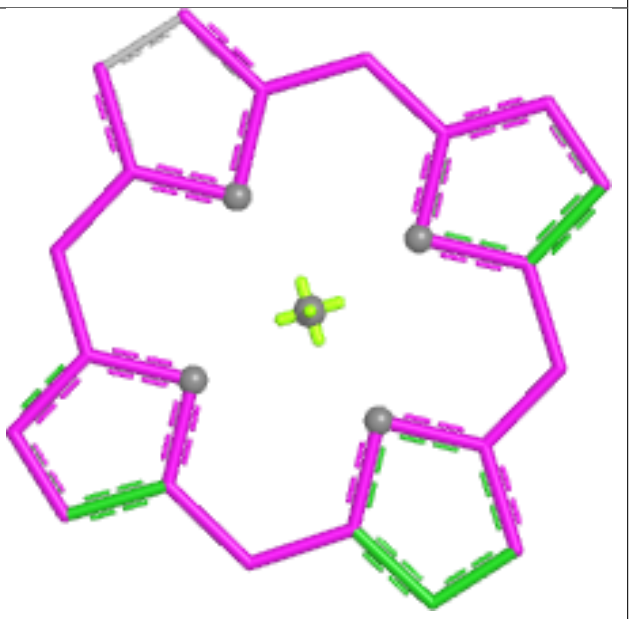


Rings

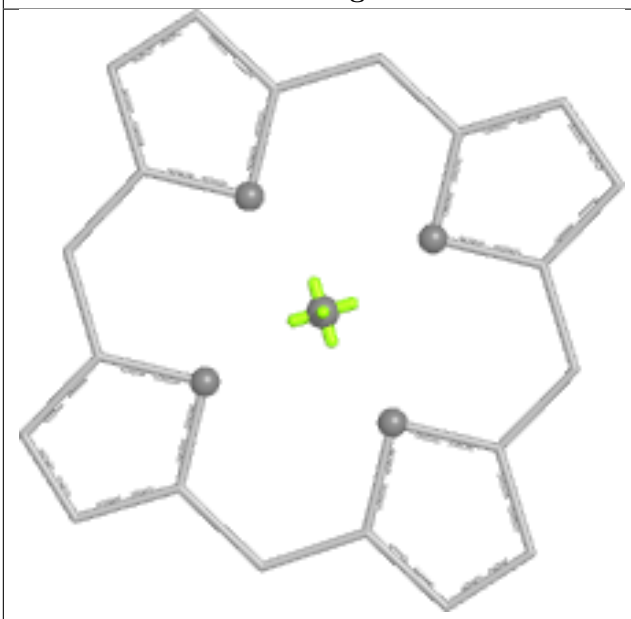
Ligand CLA A 1124



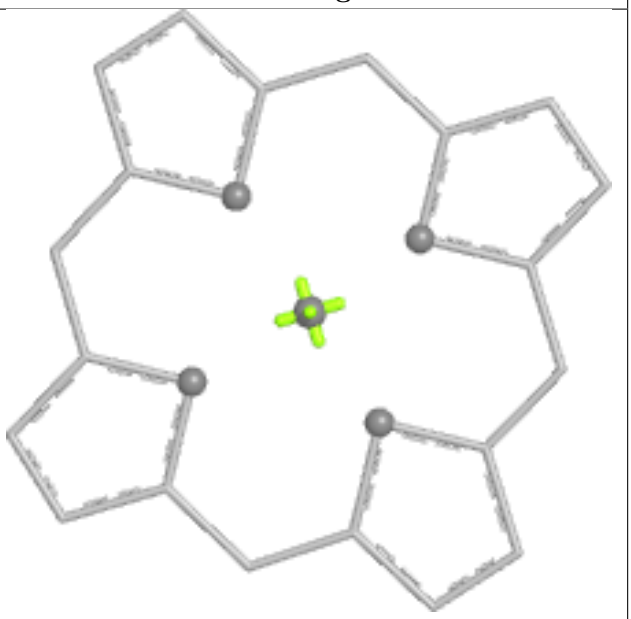
Bond lengths



Bond angles

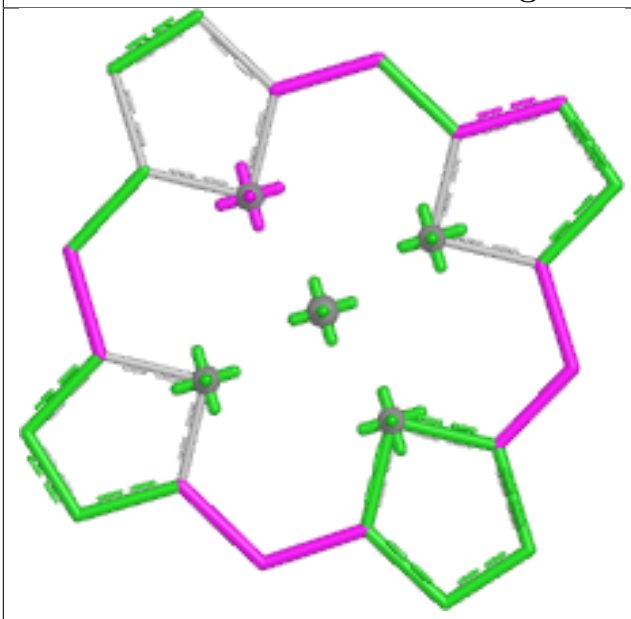


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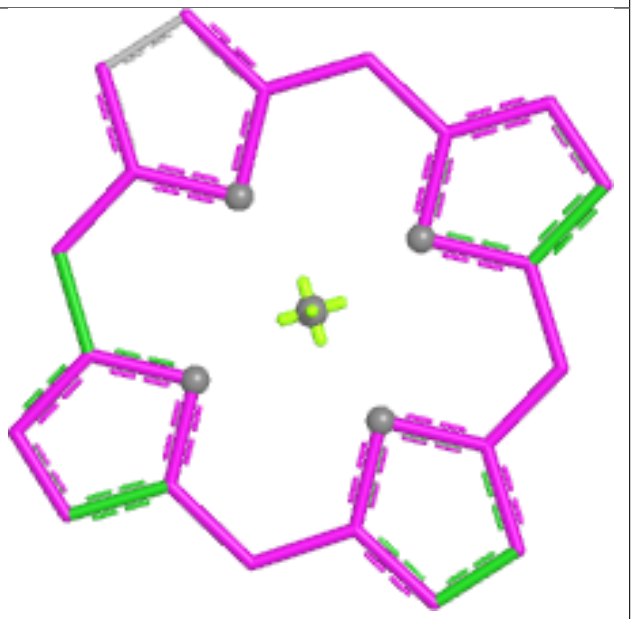


Rings

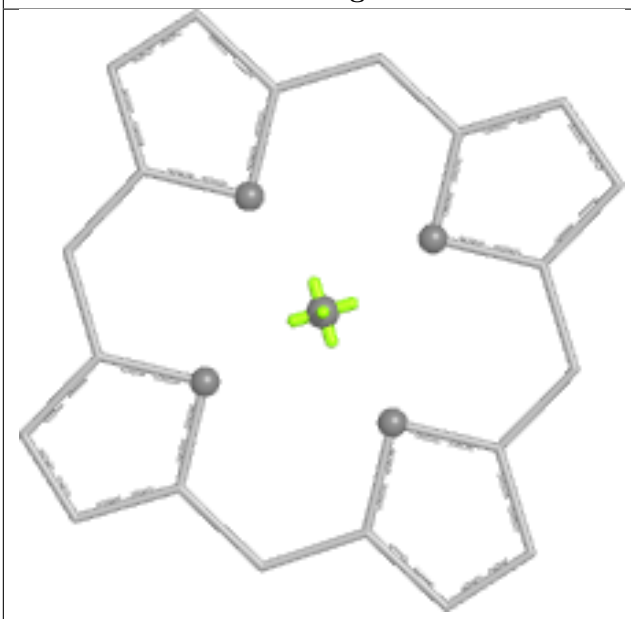
Ligand CLA 4 4003



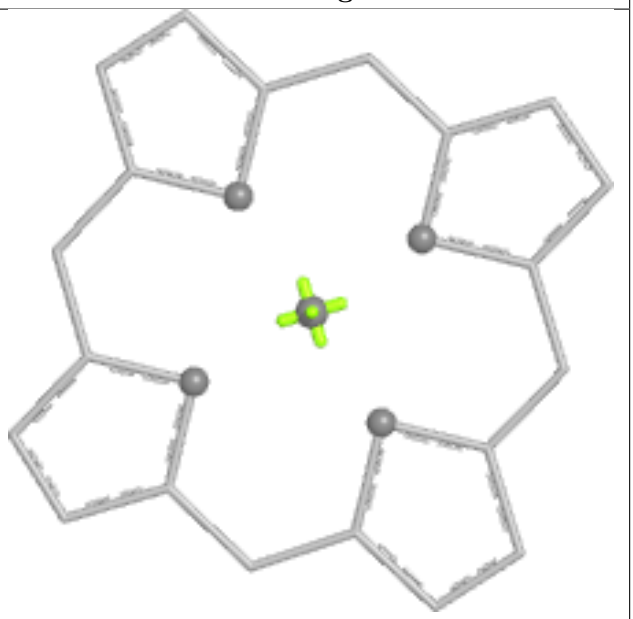
Bond lengths



Bond angles

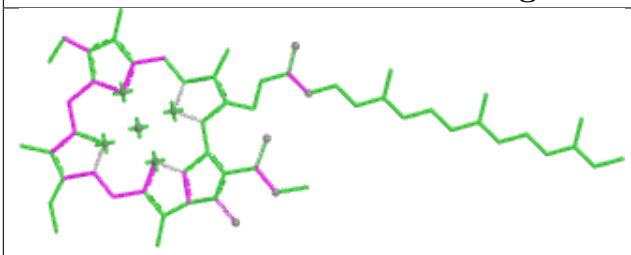


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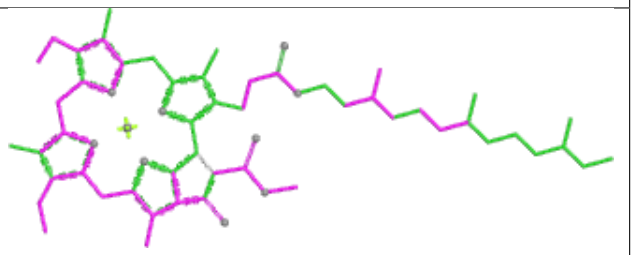


Rings

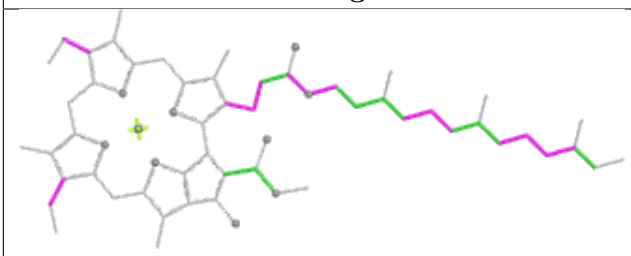
Ligand CLA J 2107



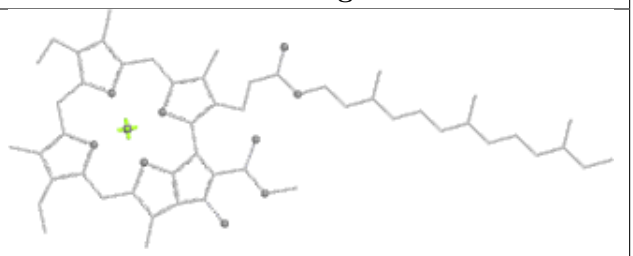
Bond lengths



Bond angles

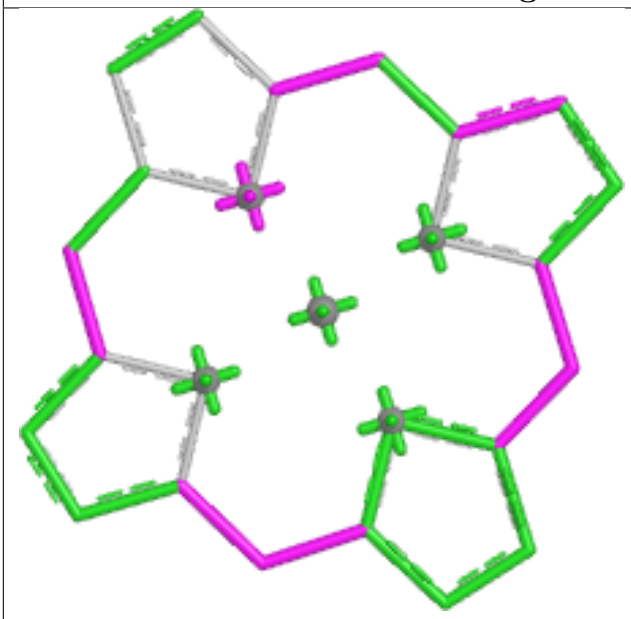


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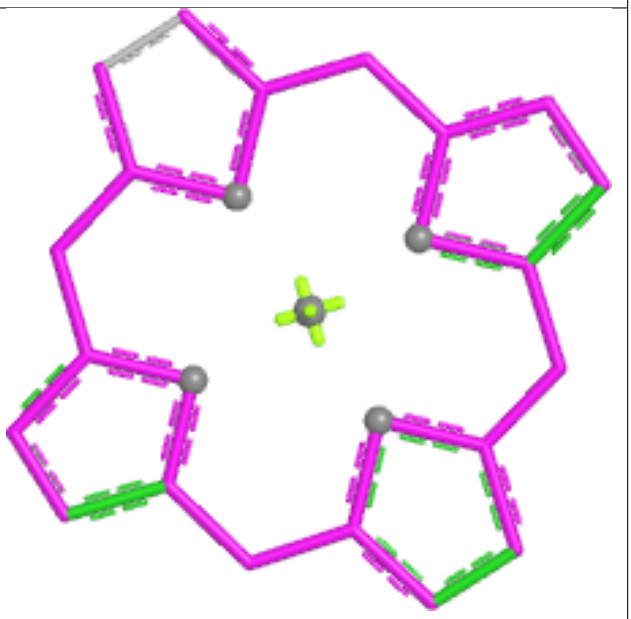


Rings

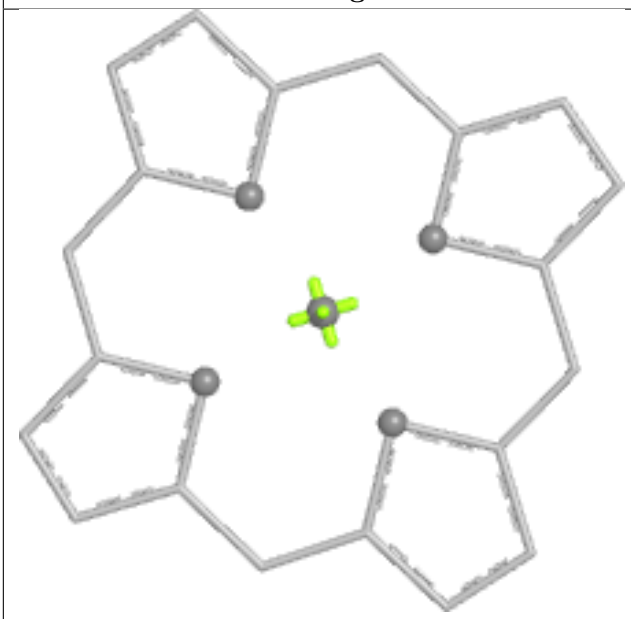
Ligand CLA 1 1012



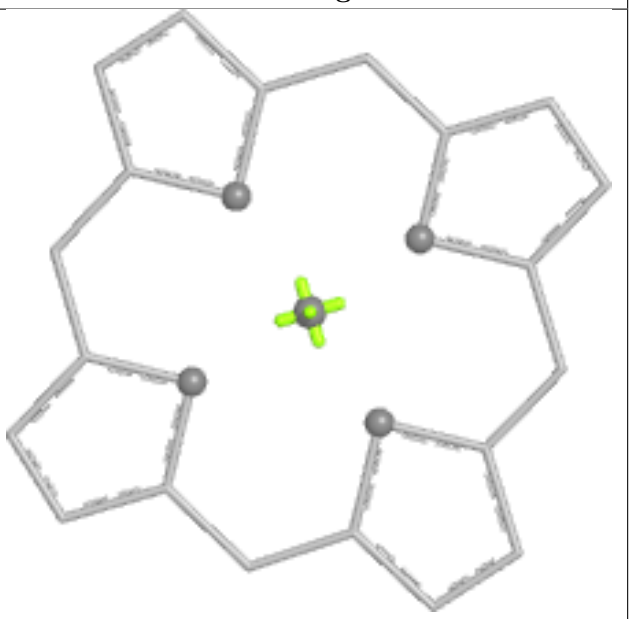
Bond lengths



Bond angles

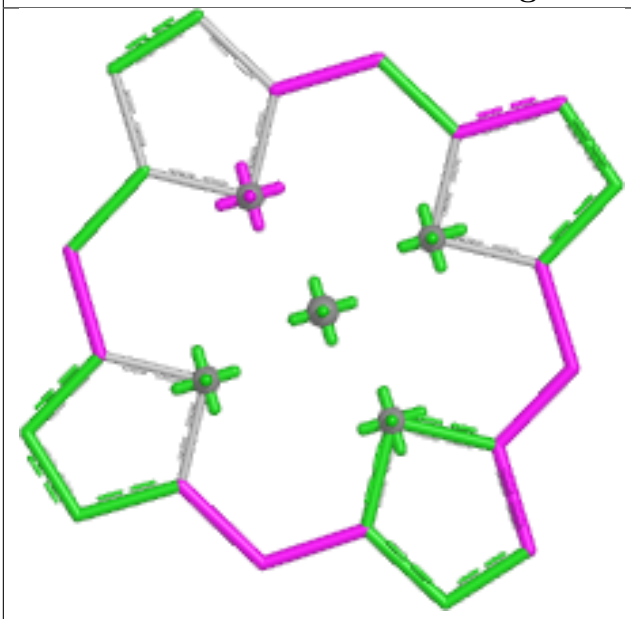


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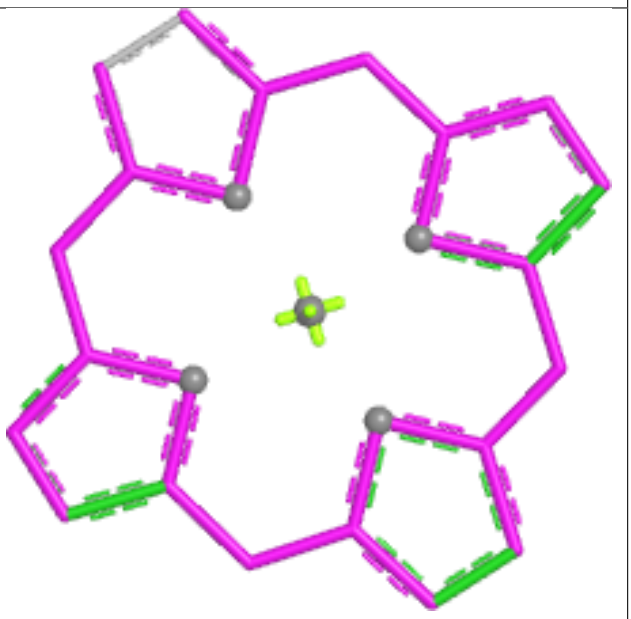


Rings

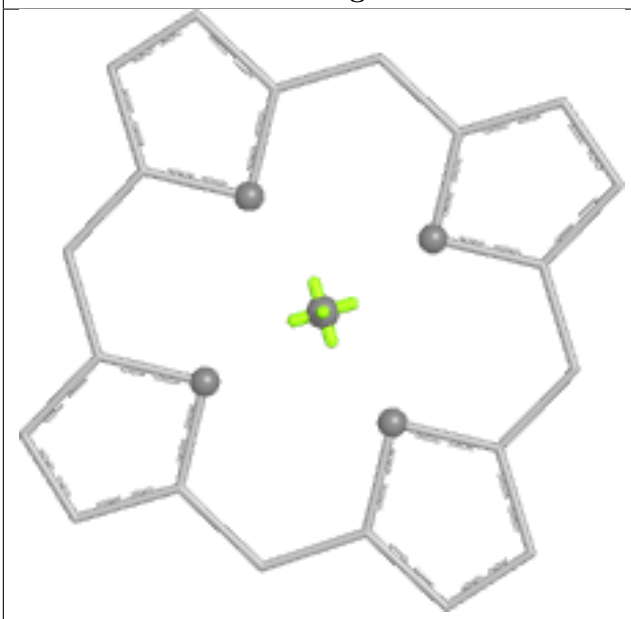
Ligand CLA 4 4012



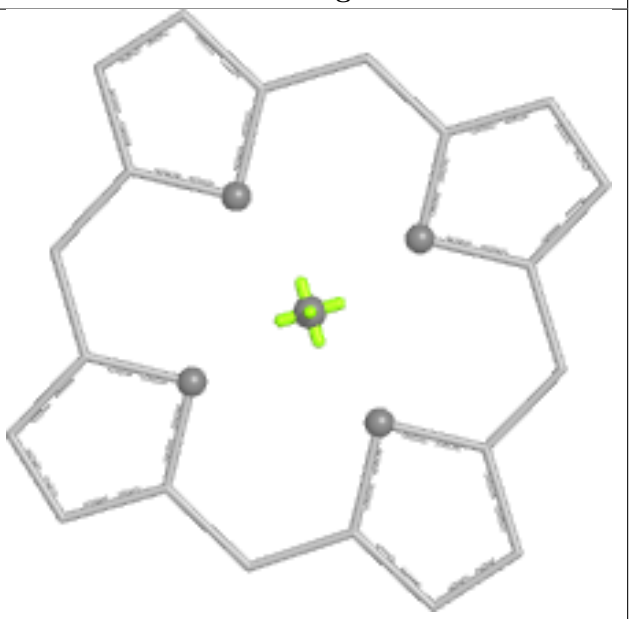
Bond lengths



Bond angles

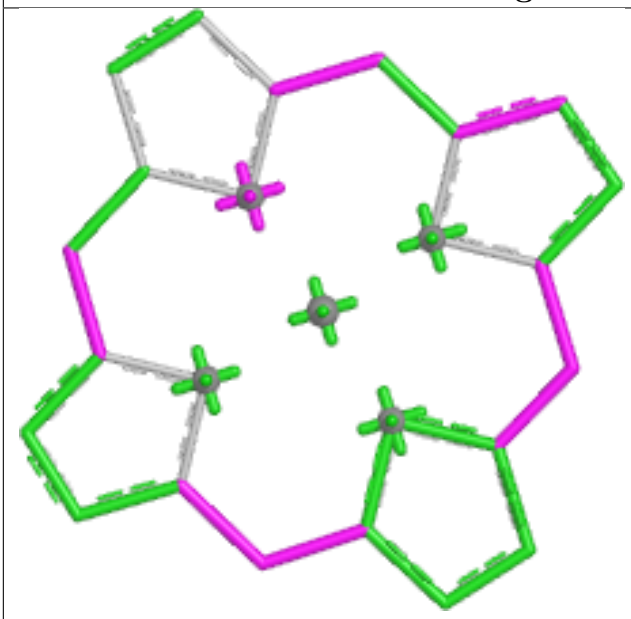


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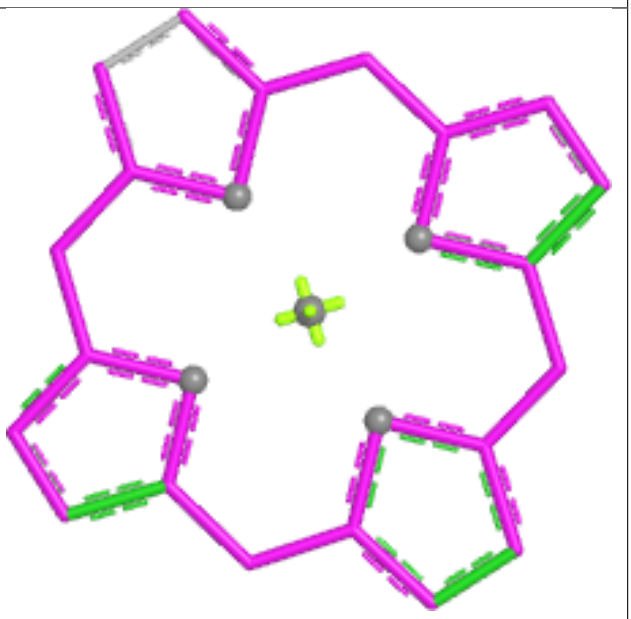


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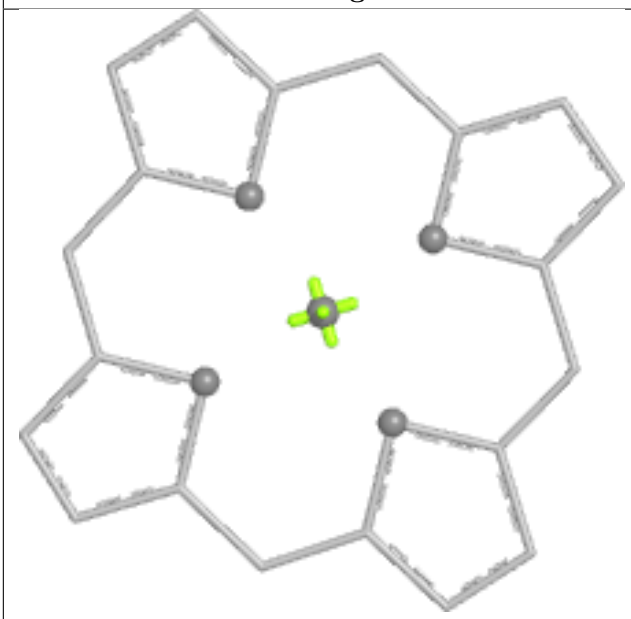
Ligand CLA B 1210



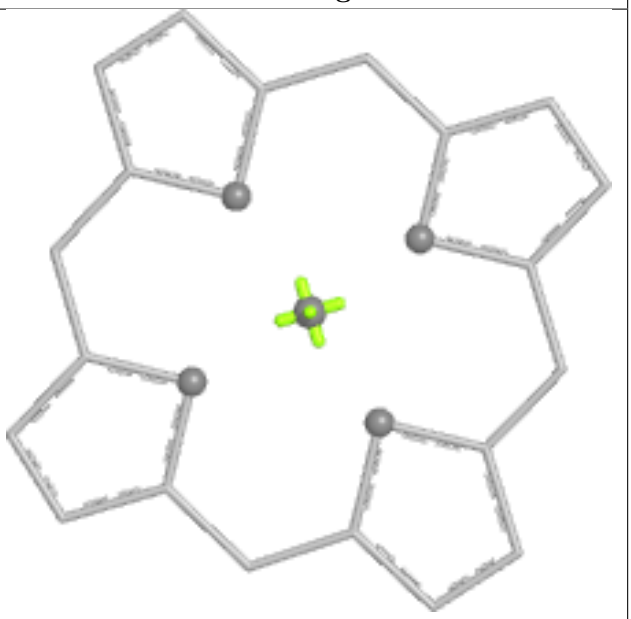
Bond lengths



Bond angles

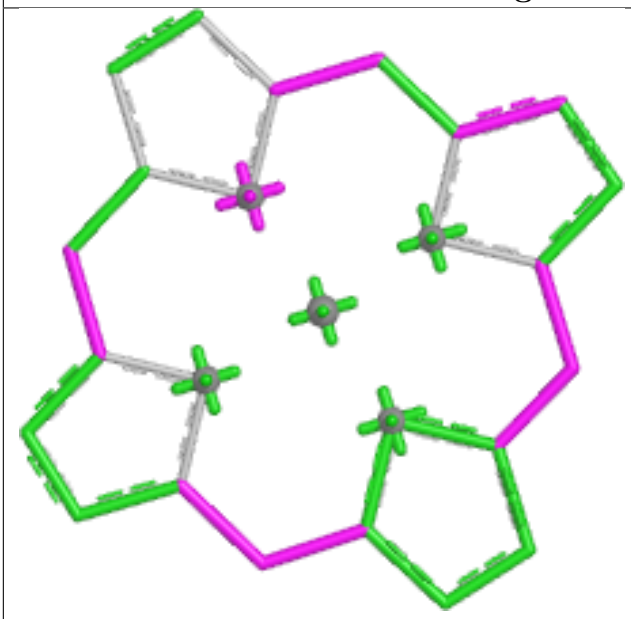


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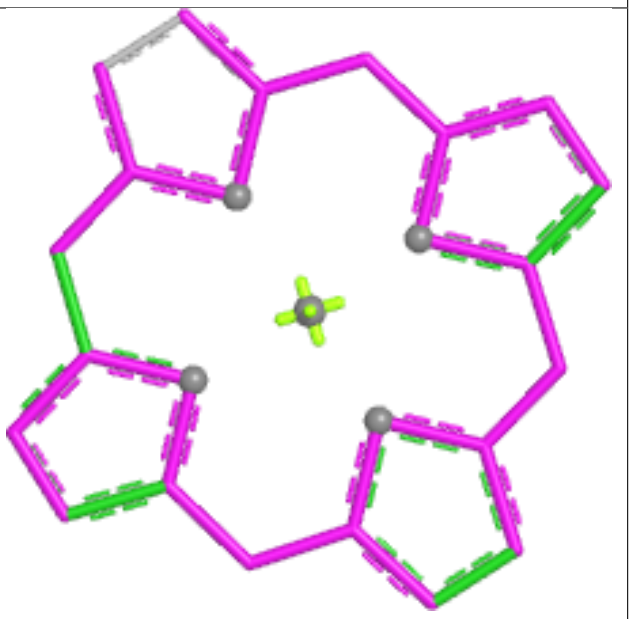


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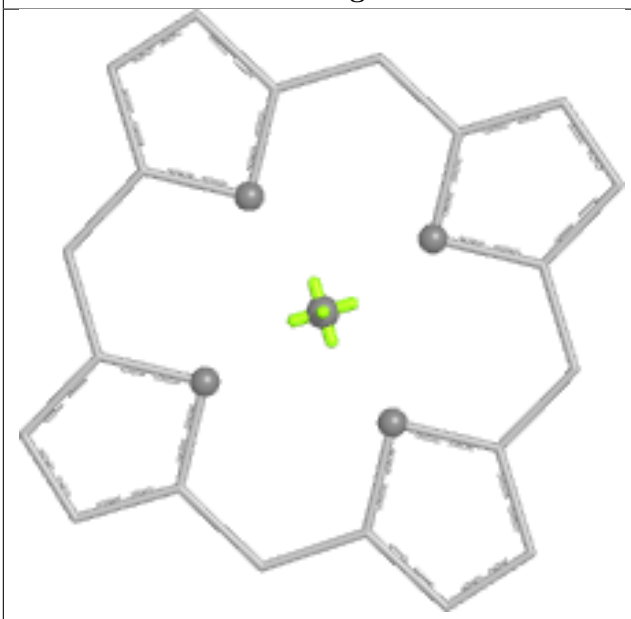
Ligand CLA A 1111



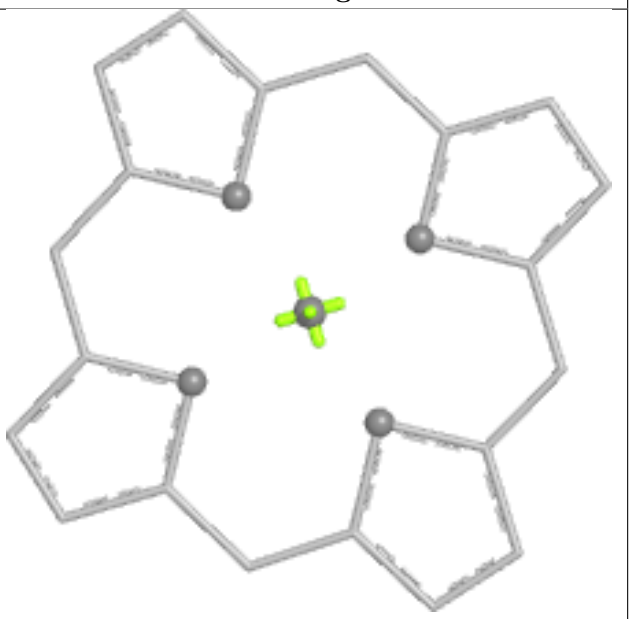
Bond lengths



Bond angles

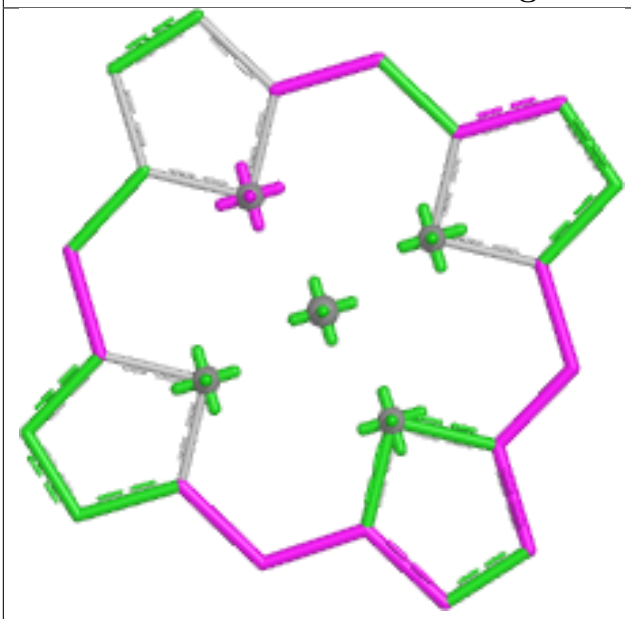


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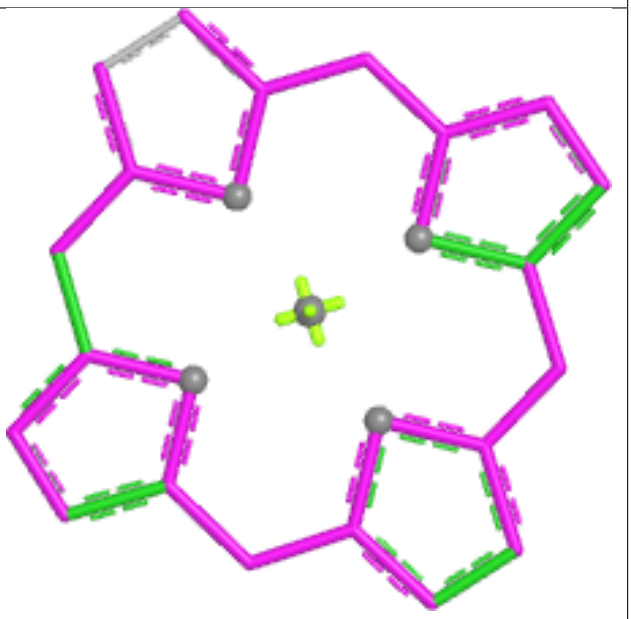


Rings

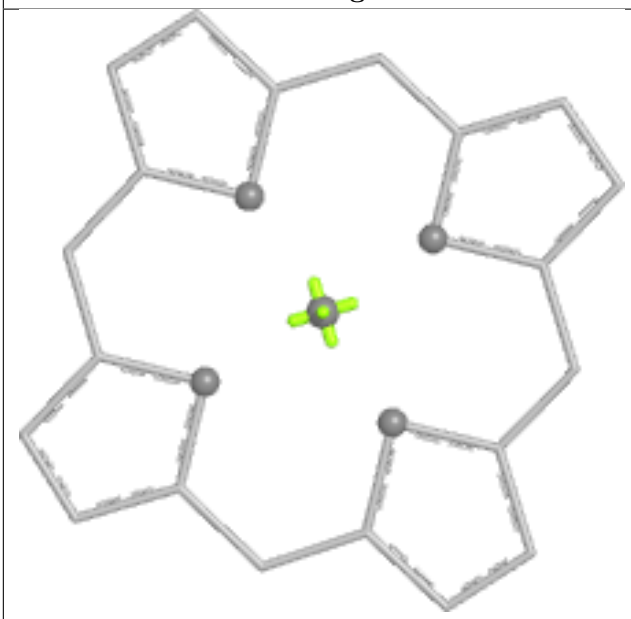
Ligand CLA 4 4004



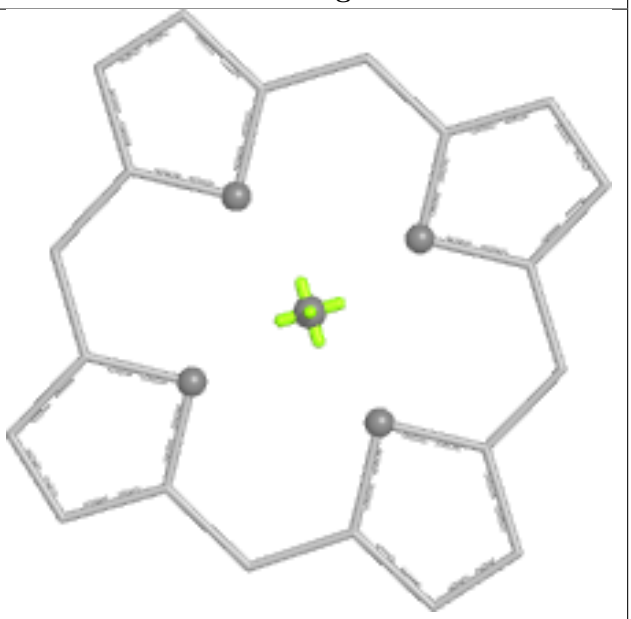
Bond lengths



Bond angles

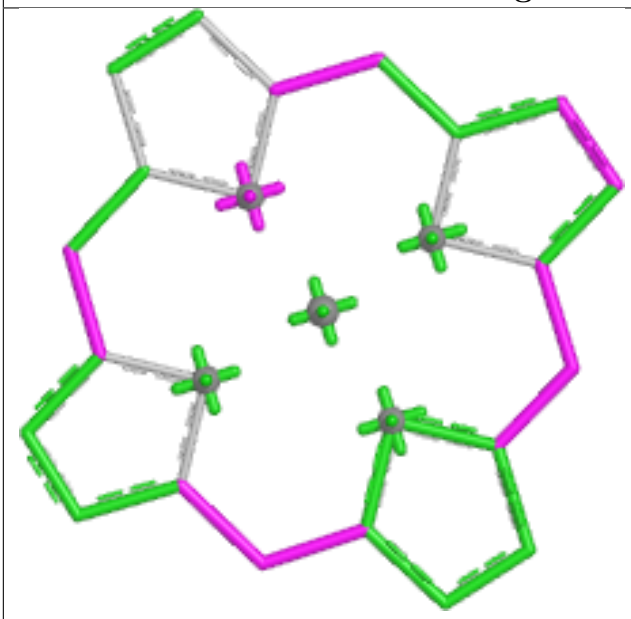


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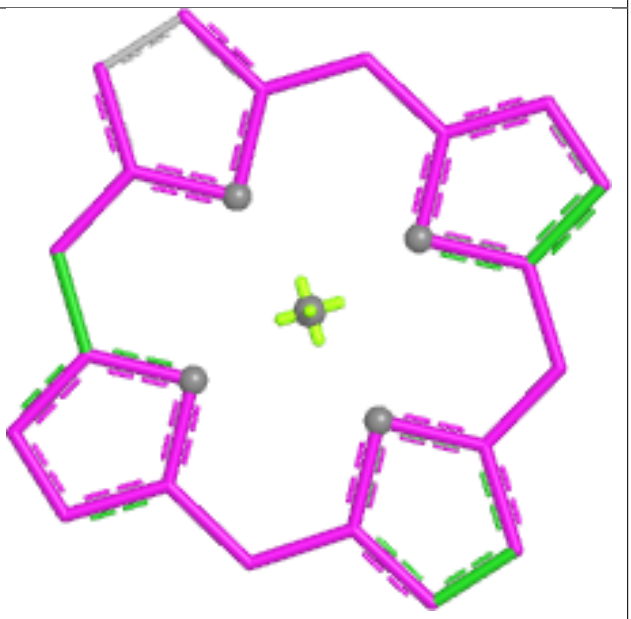


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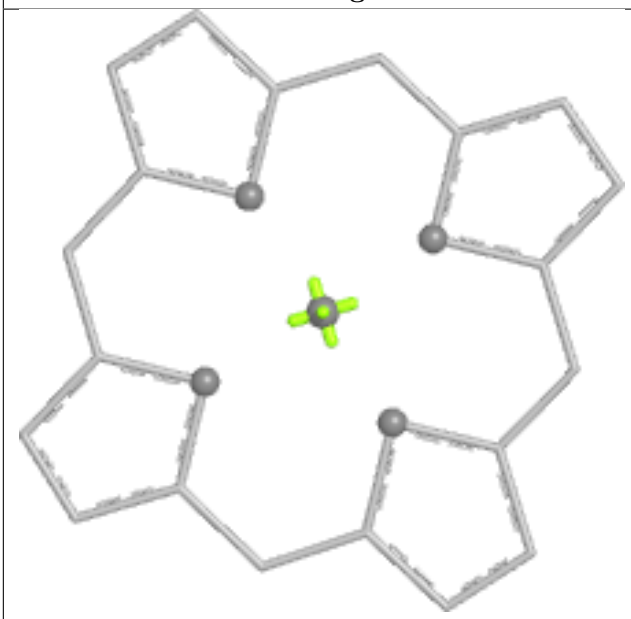
Ligand CLA A 1134



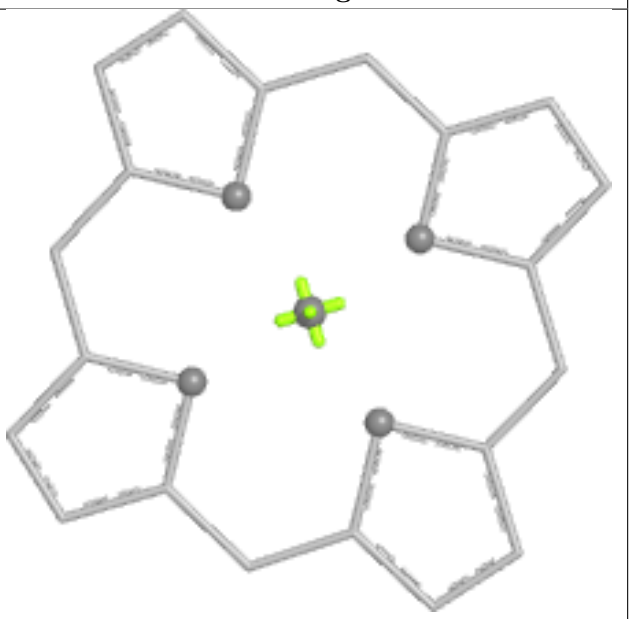
Bond lengths



Bond angles

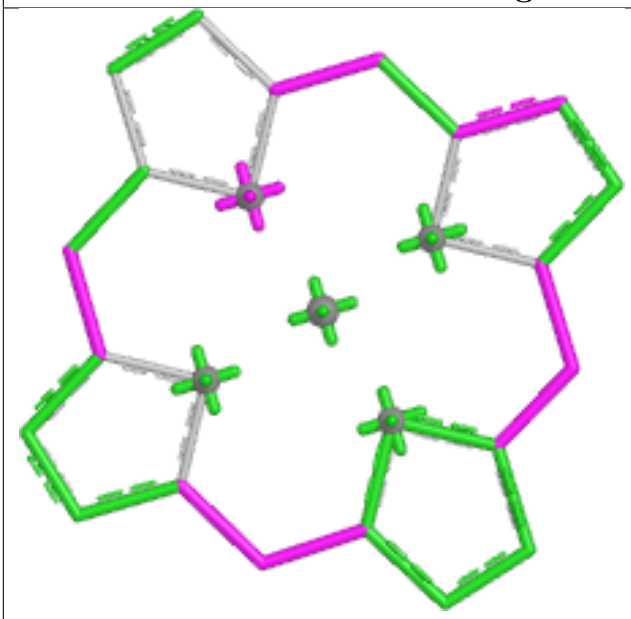


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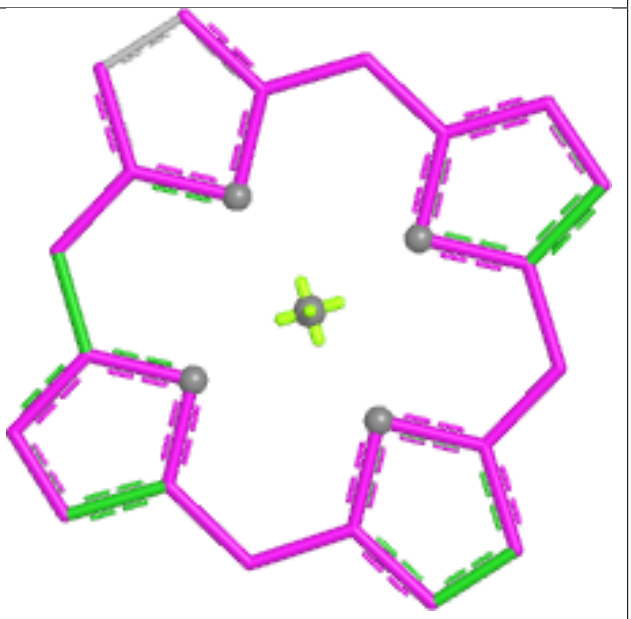


Rings

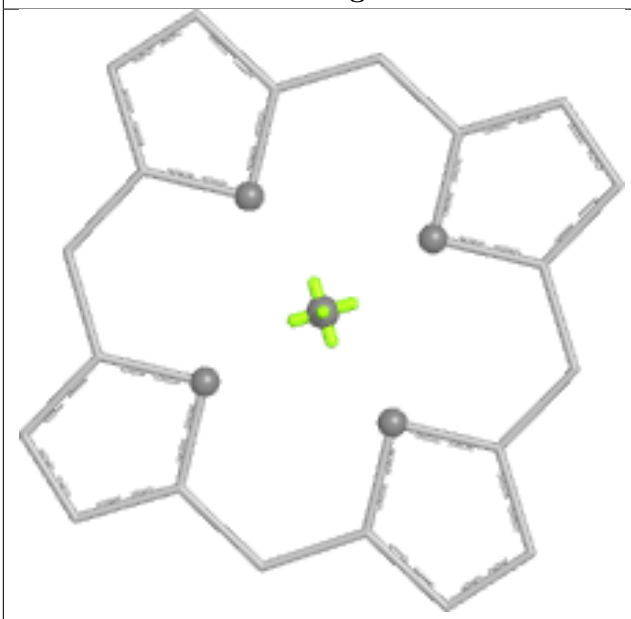
Ligand CLA B 1241



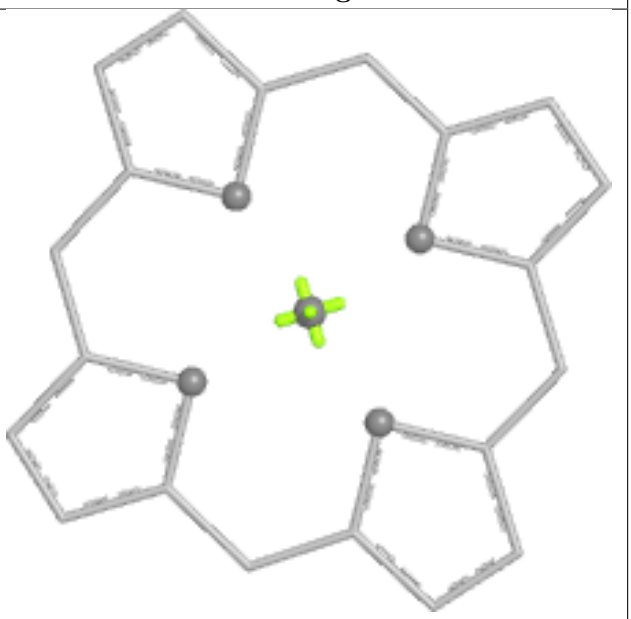
Bond lengths



Bond angles

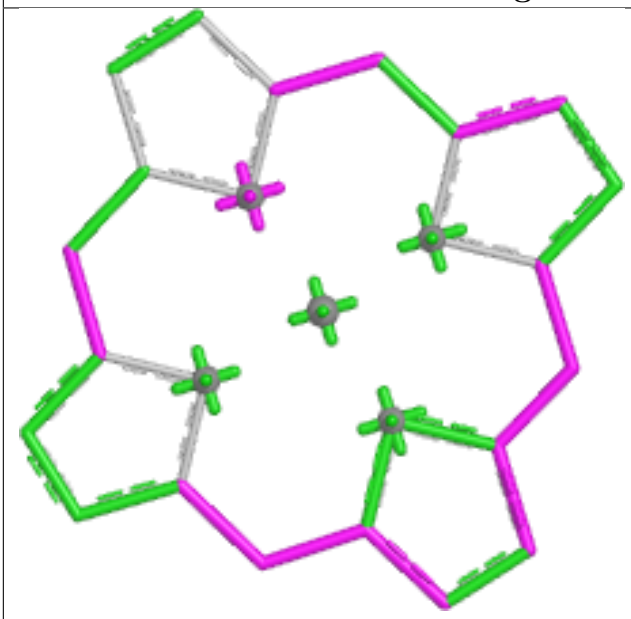


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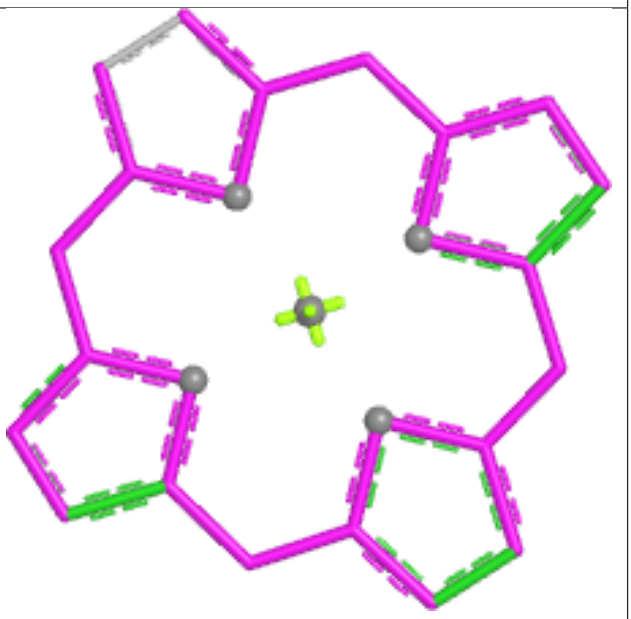


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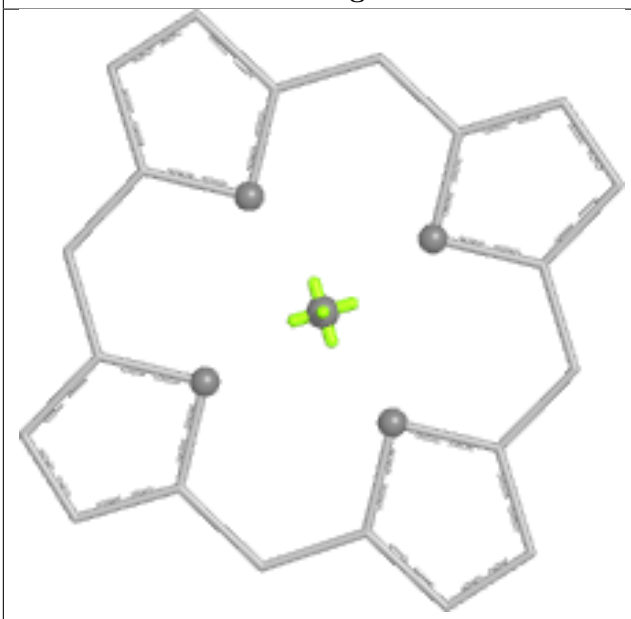
Ligand CLA G 1248



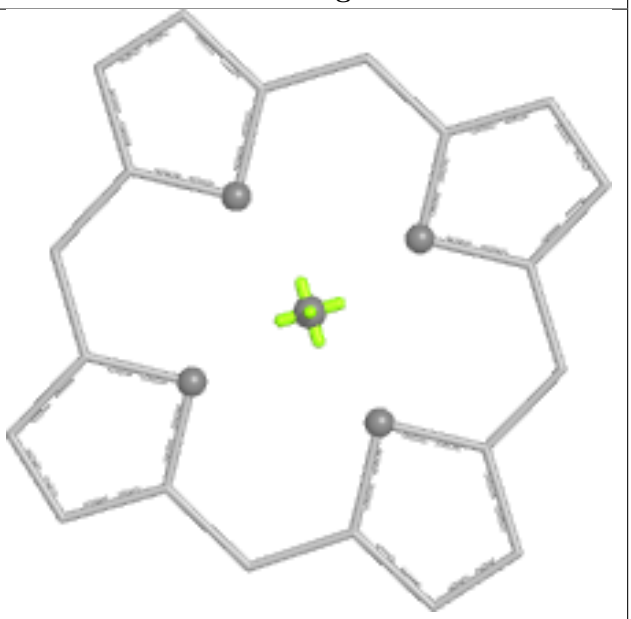
Bond lengths



Bond angles

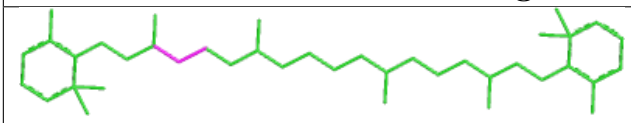


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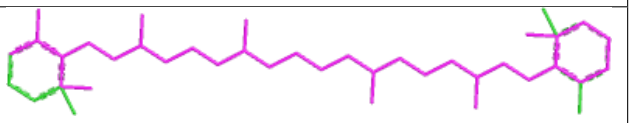


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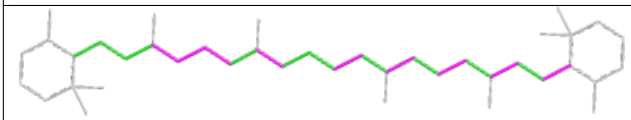
Ligand BCR F 6016



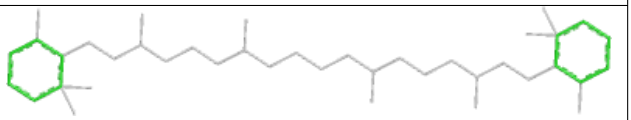
Bond lengths



Bond angles

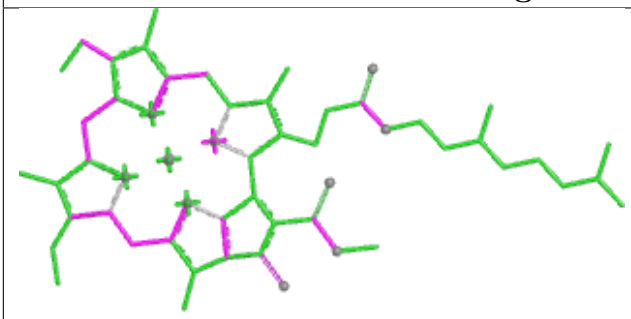


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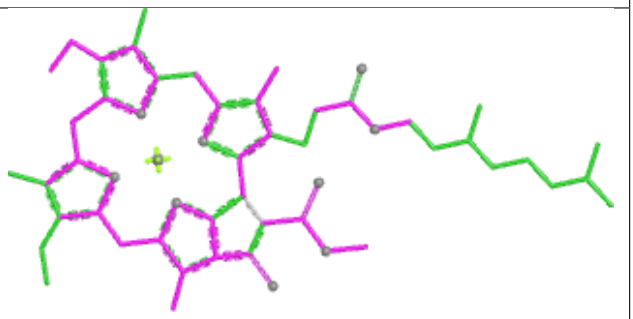


Rings

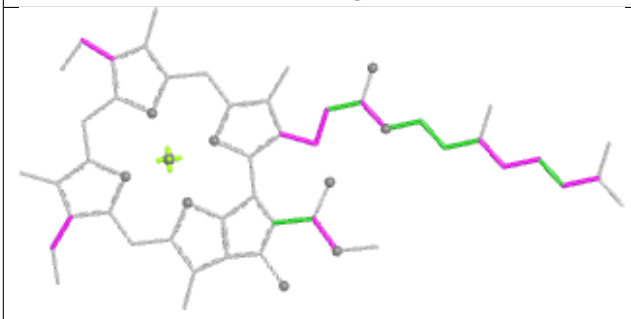
Ligand CLA A 1119



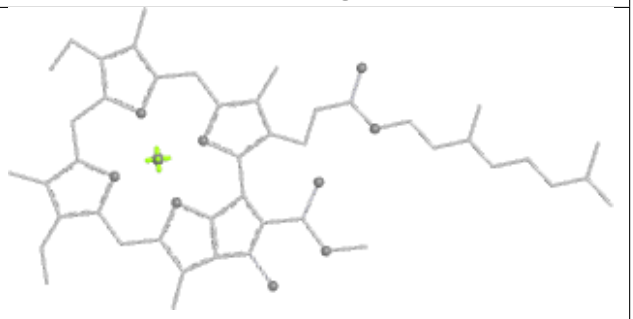
Bond lengths



Bond angles

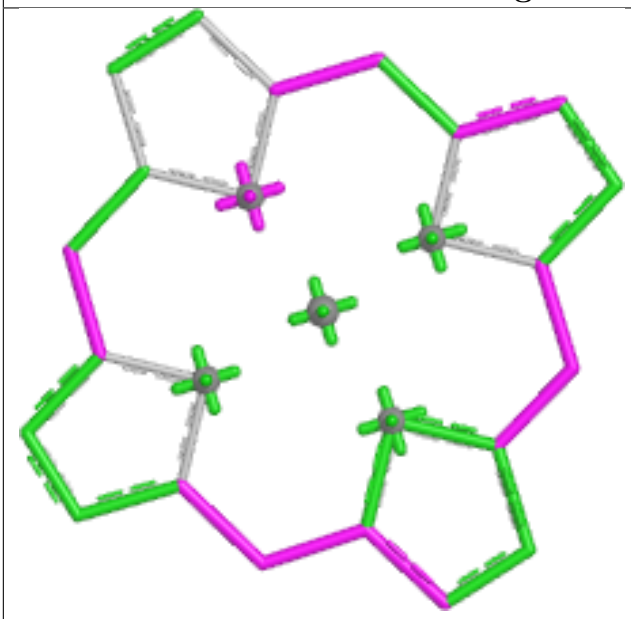


Torsions

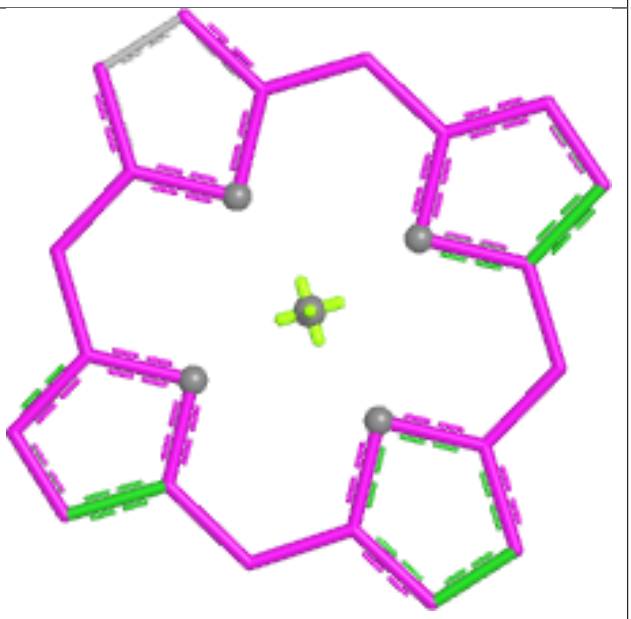


Rings

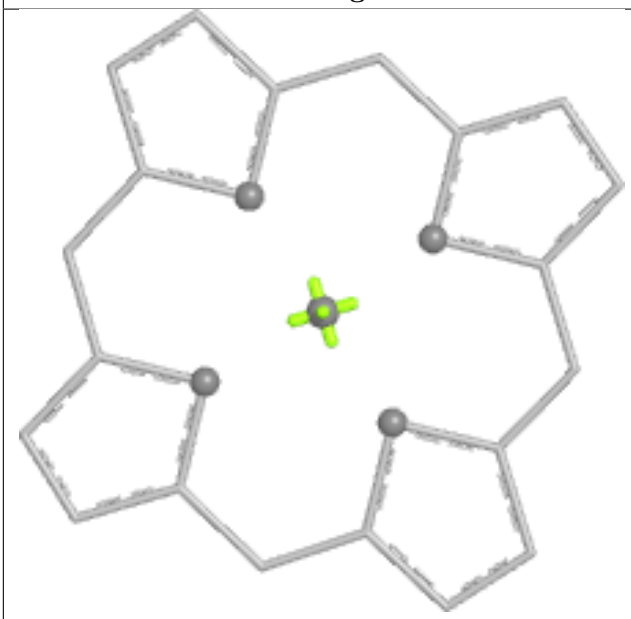
Ligand CLA A 1118



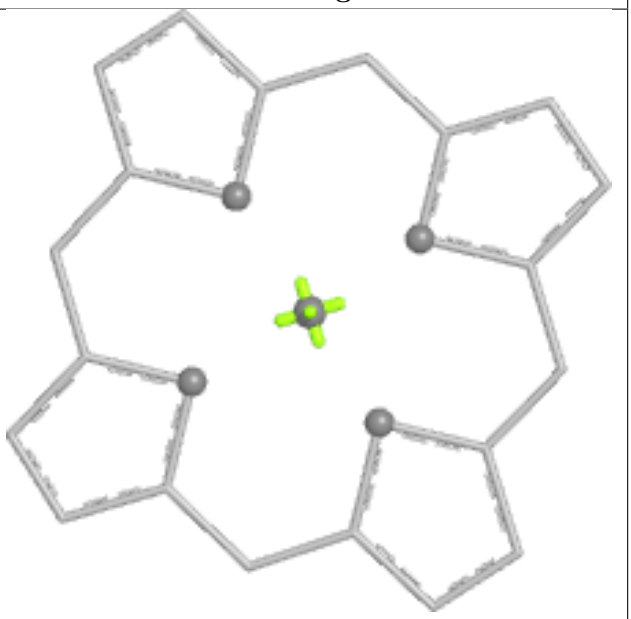
Bond lengths



Bond angles

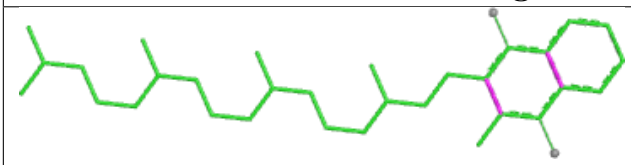


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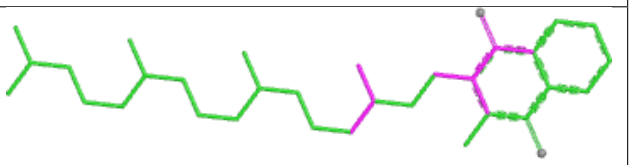


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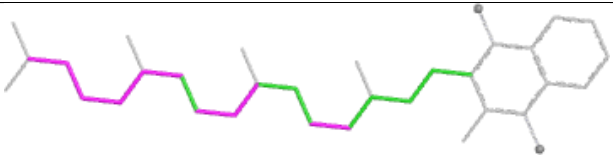
Ligand PQN A 5001



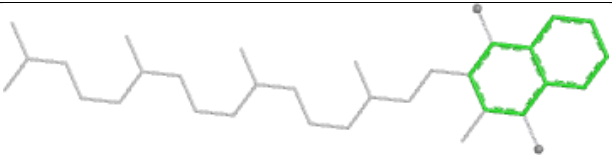
Bond lengths



Bond angles

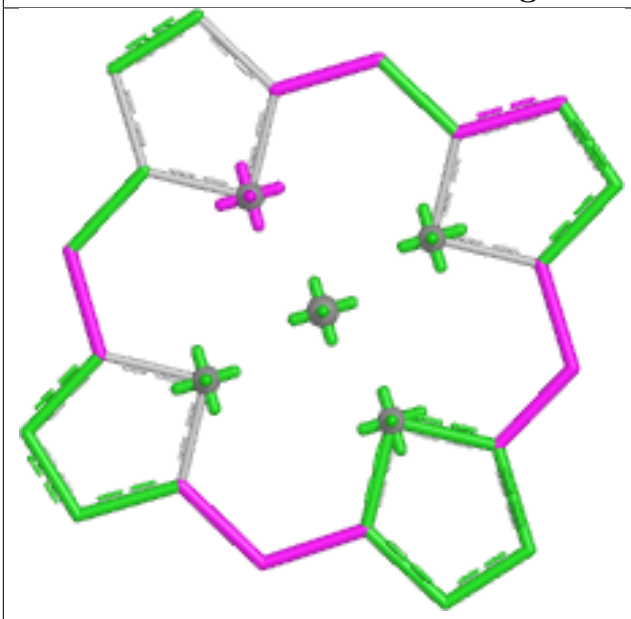


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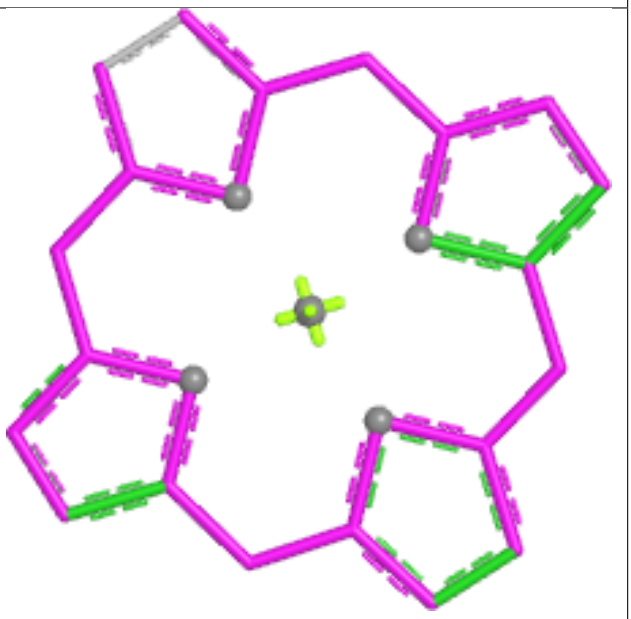


Rings

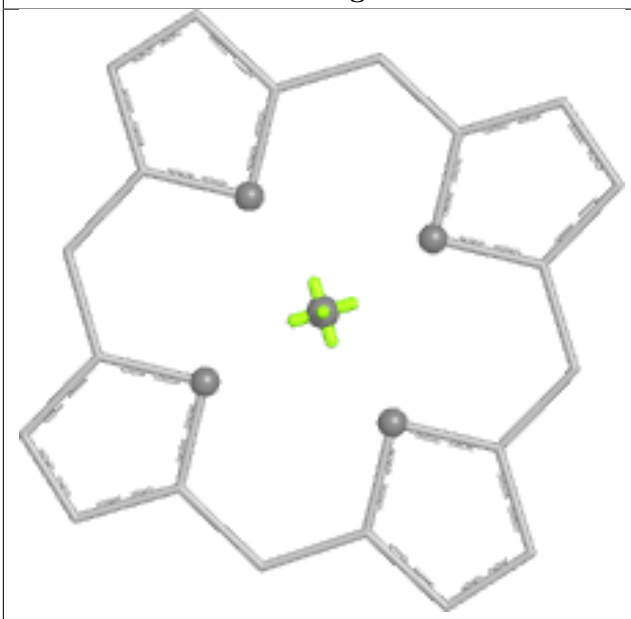
Ligand CLA 2 2010



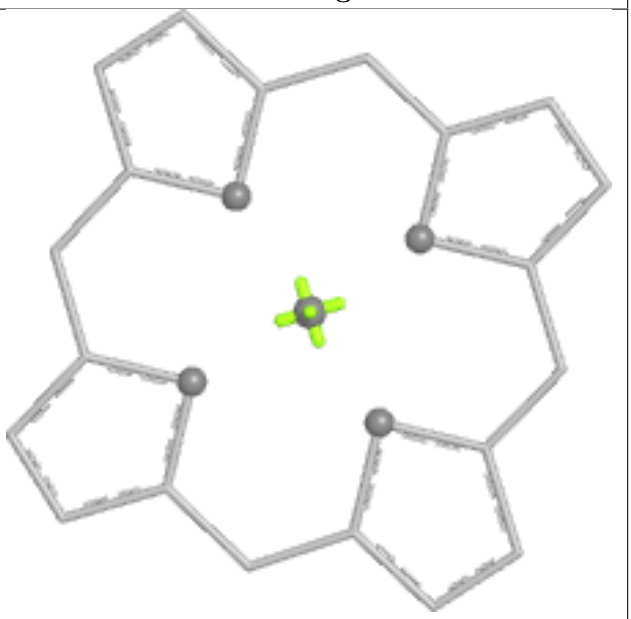
Bond lengths



Bond angles

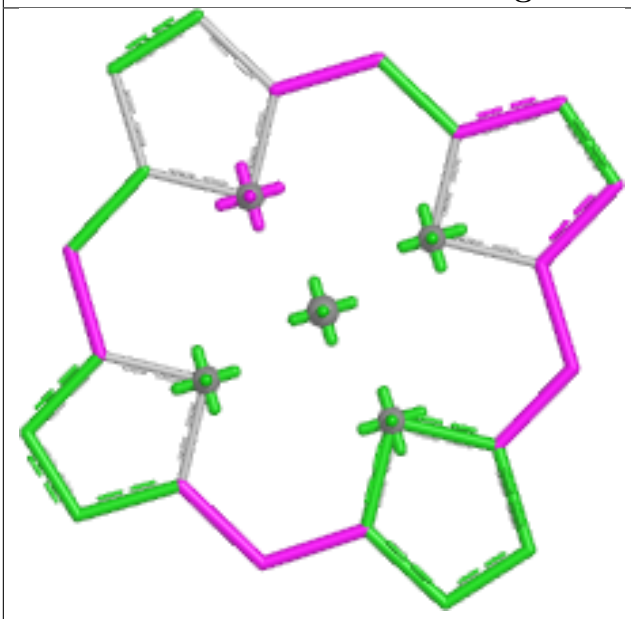


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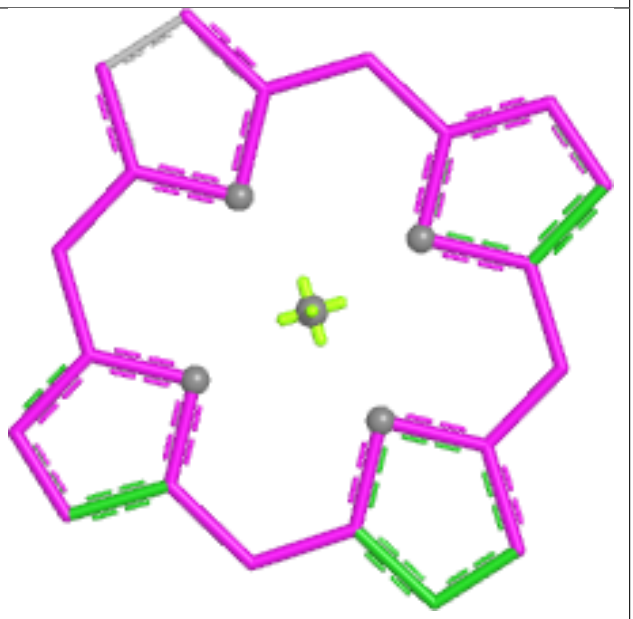


Rings

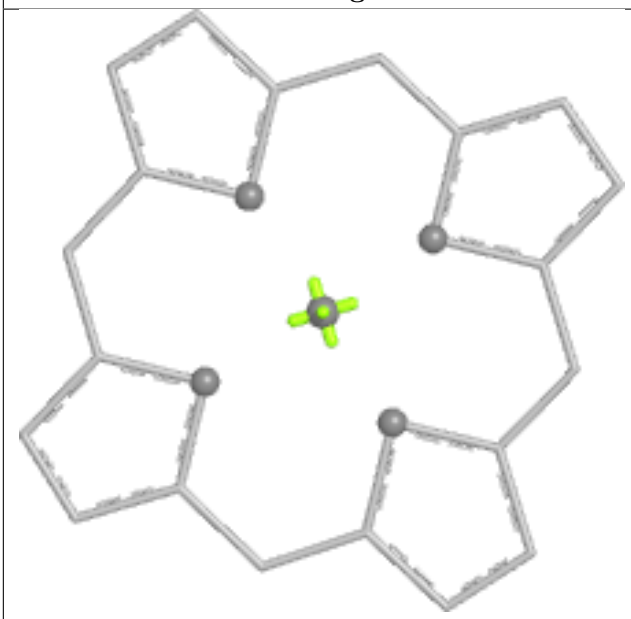
Ligand CLA A 1133



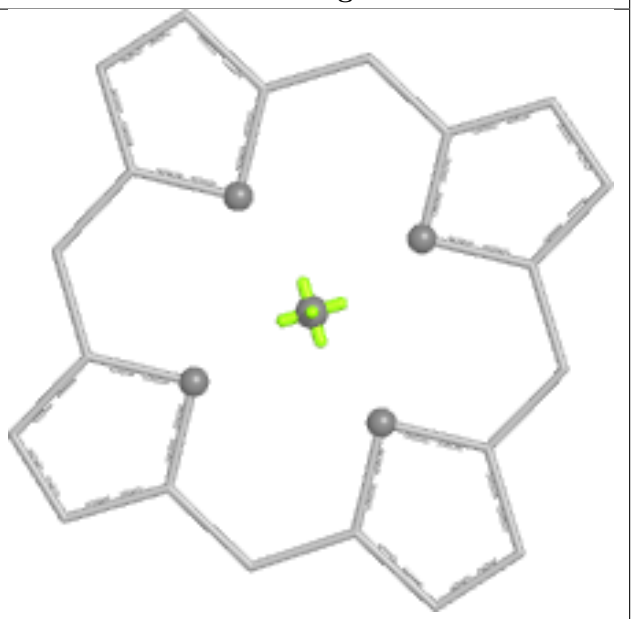
Bond lengths



Bond angles

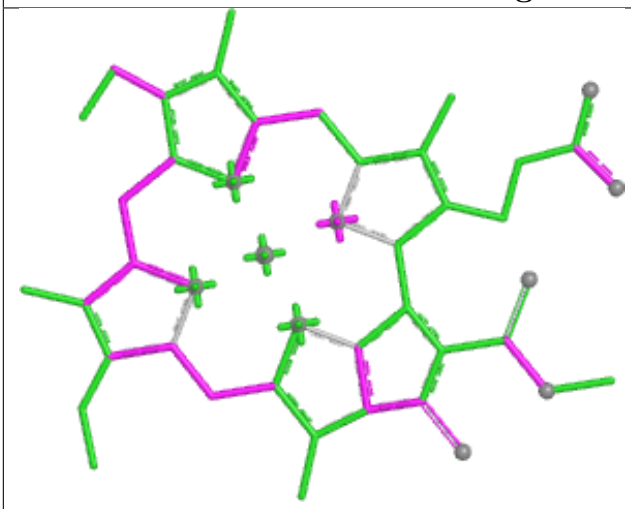


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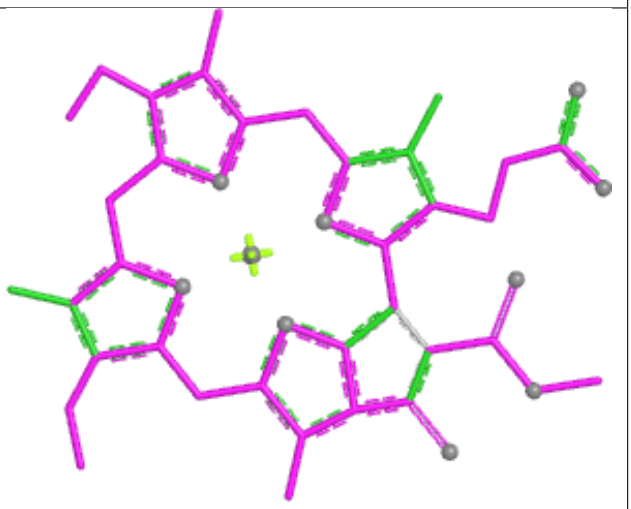


Rings

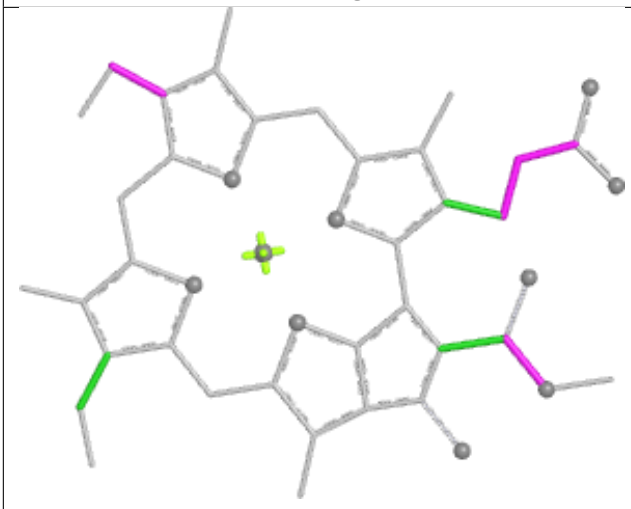
Ligand CLA B 1225



Bond lengths



Bond angles

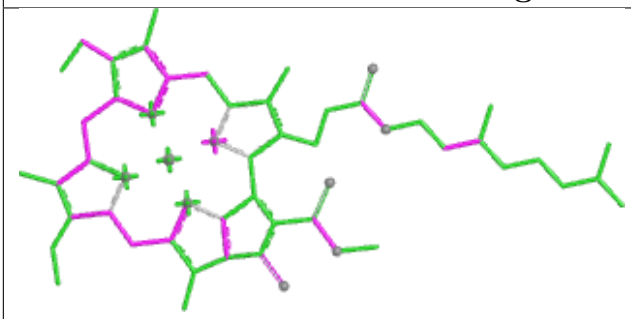


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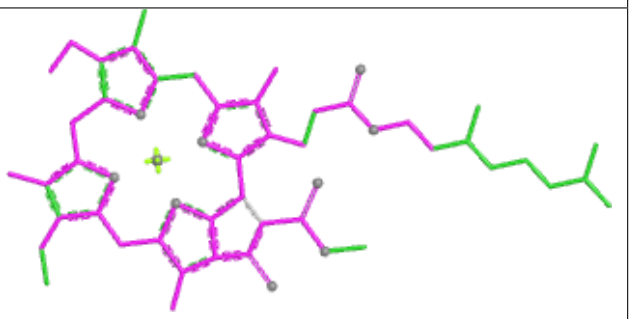


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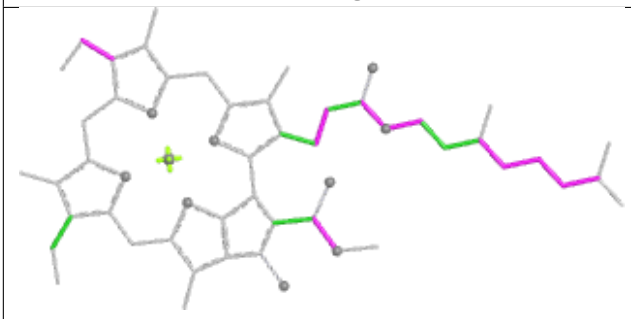
Ligand CLA A 1126



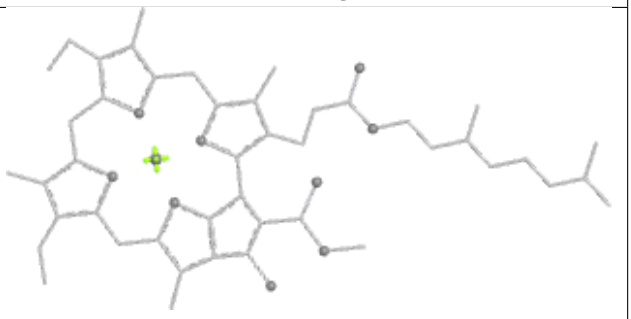
Bond lengths



Bond angles

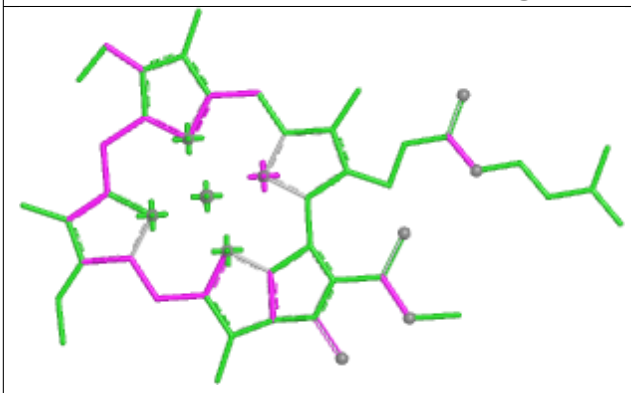


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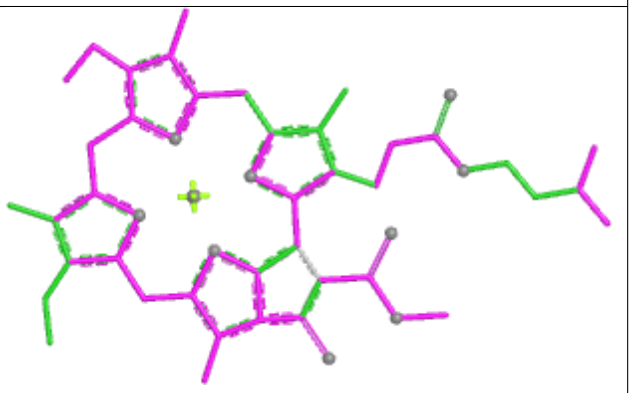


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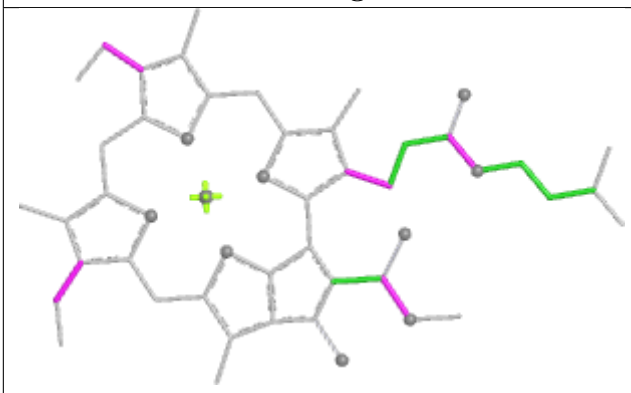
Ligand CLA B 1227



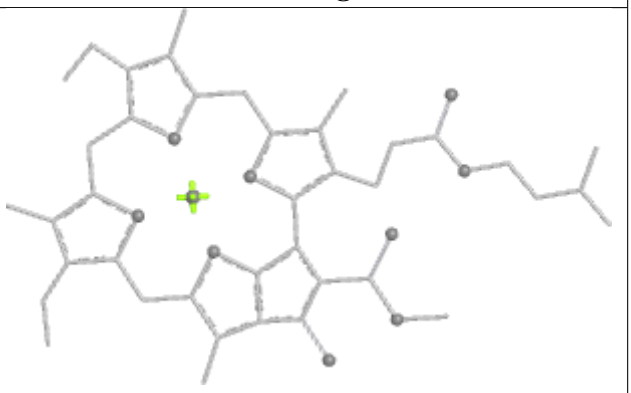
Bond lengths



Bond angles

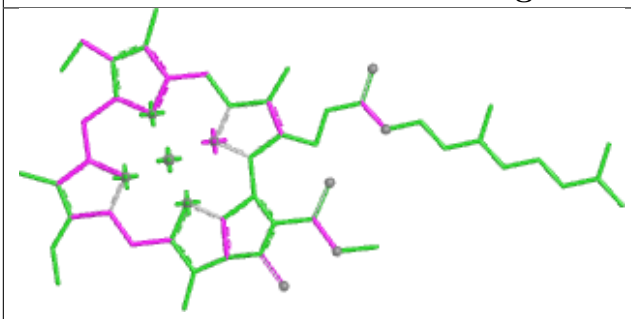


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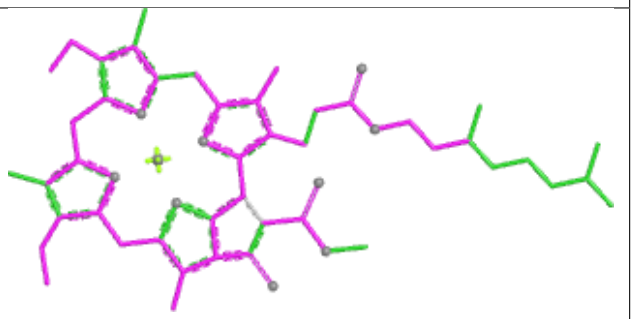


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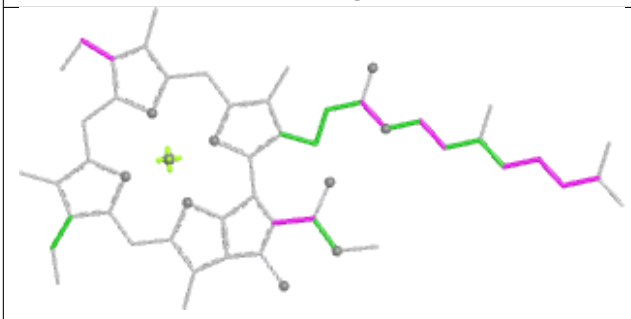
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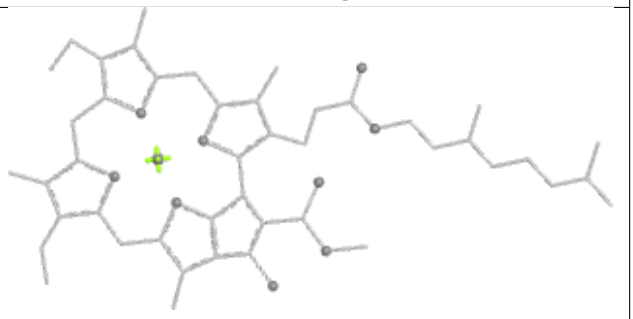
Bond lengths



Bond angles

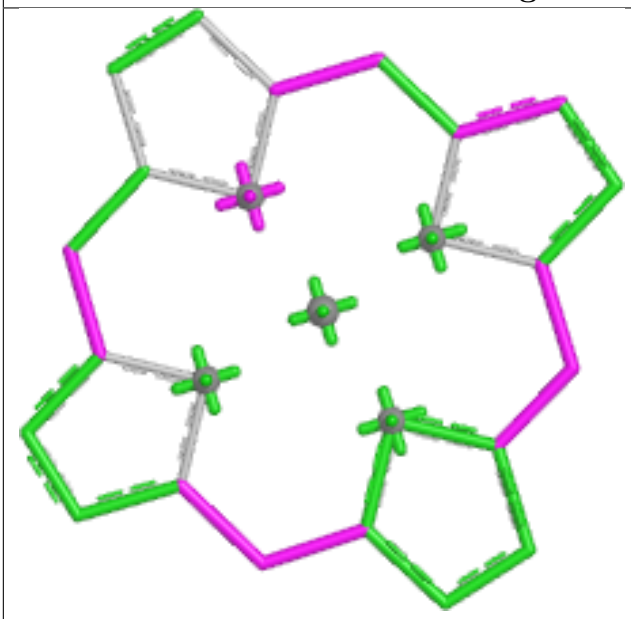


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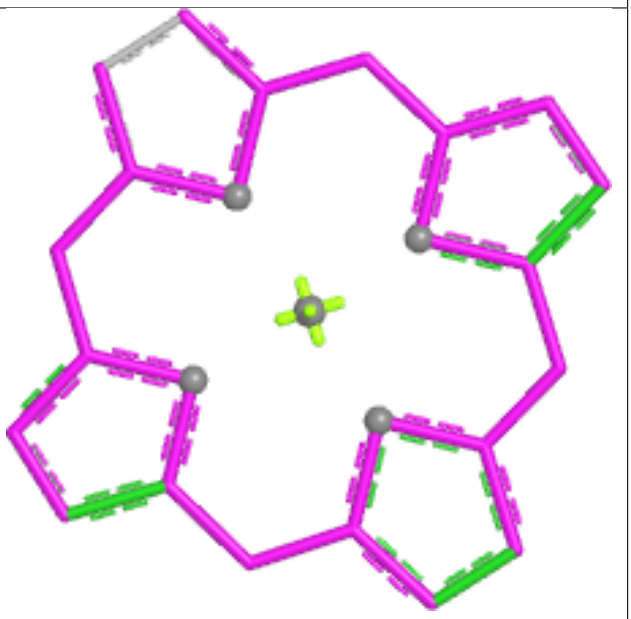


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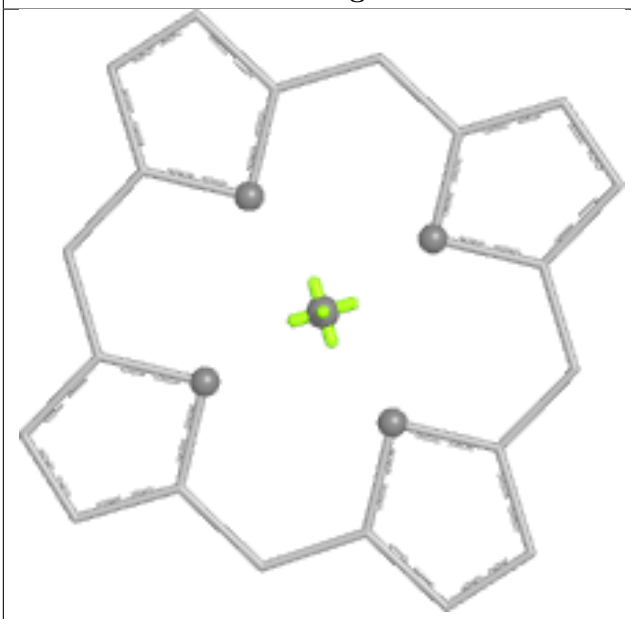
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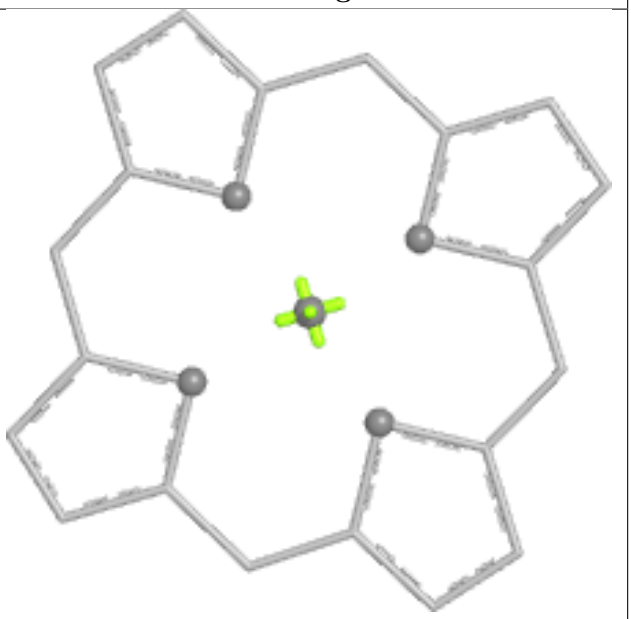
Bond lengths



Bond angles

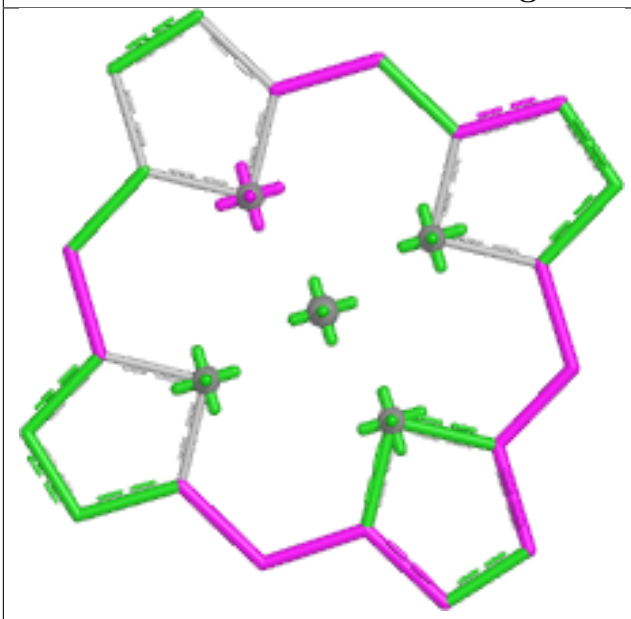


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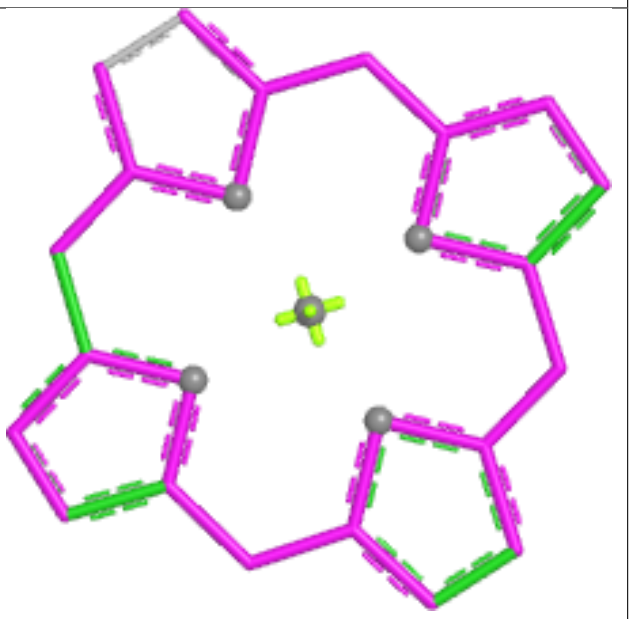


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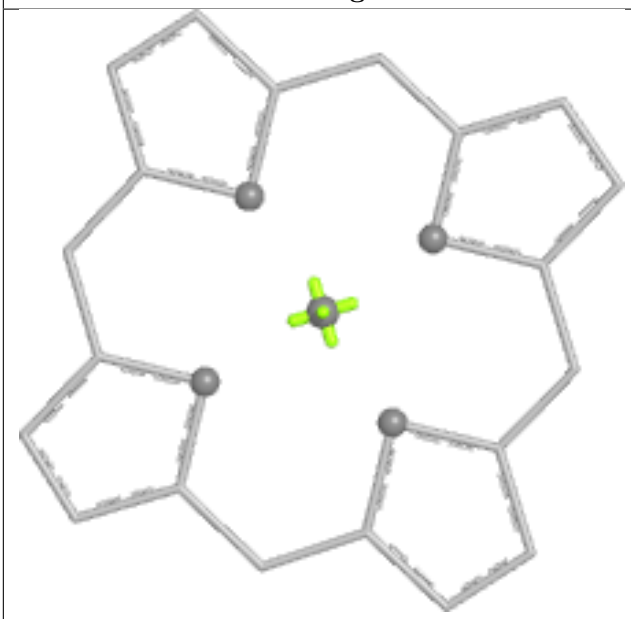
Ligand CLA 3 3012



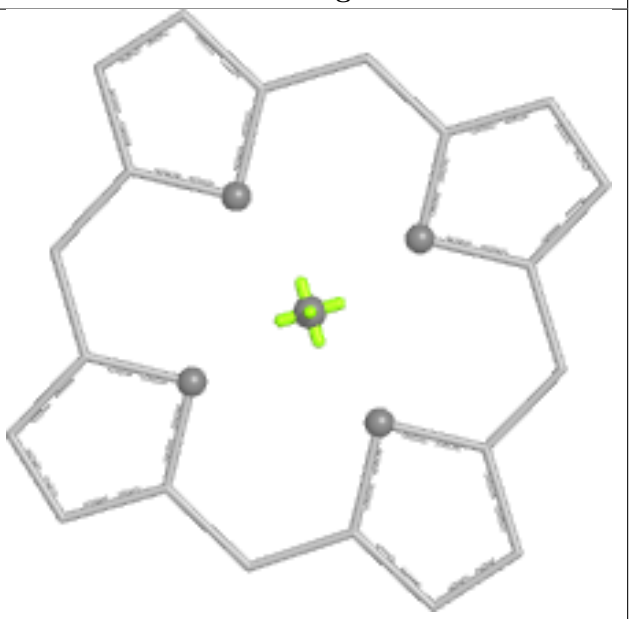
Bond lengths



Bond angles

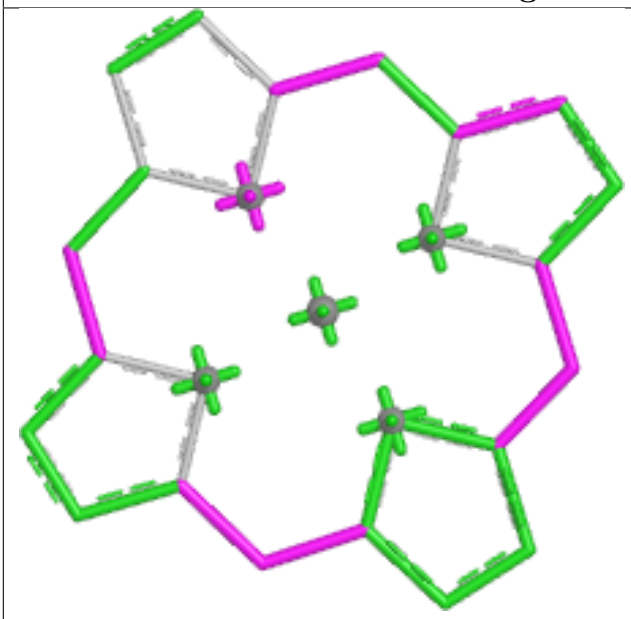


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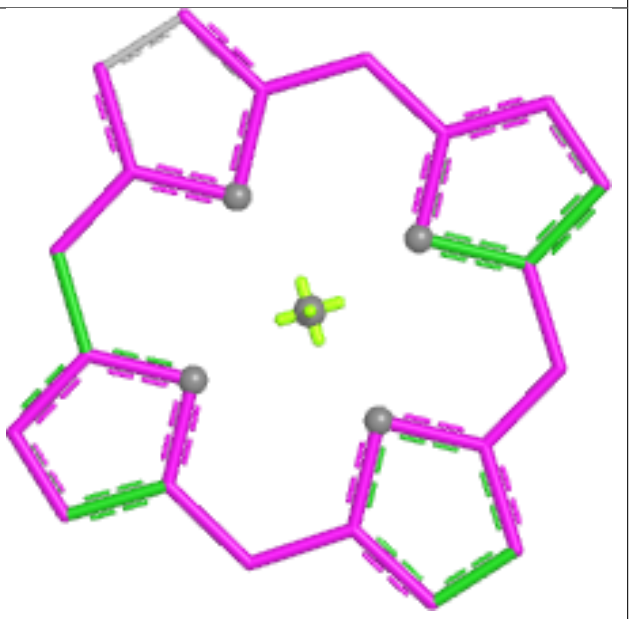


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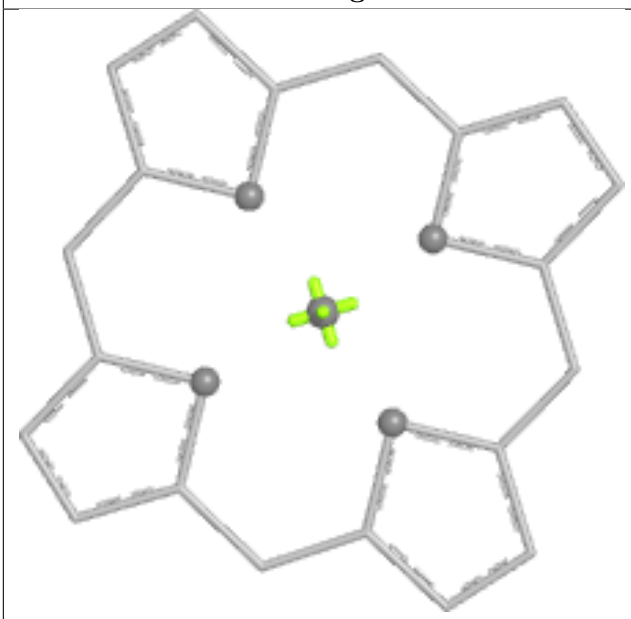
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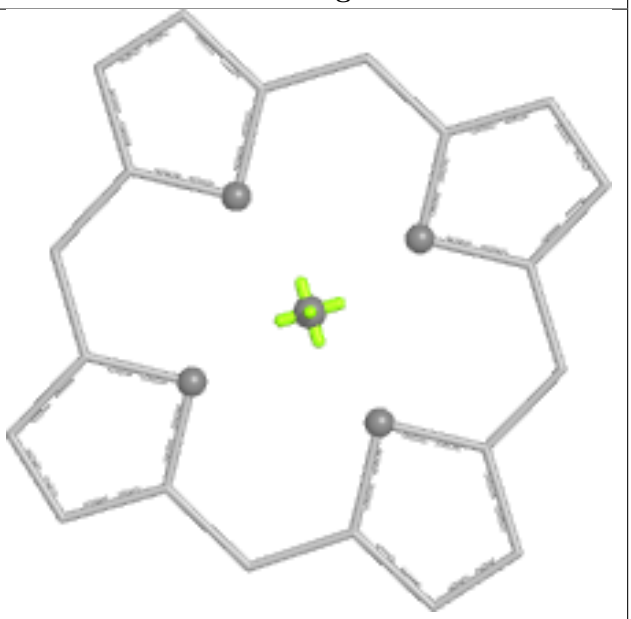
Bond lengths



Bond angles

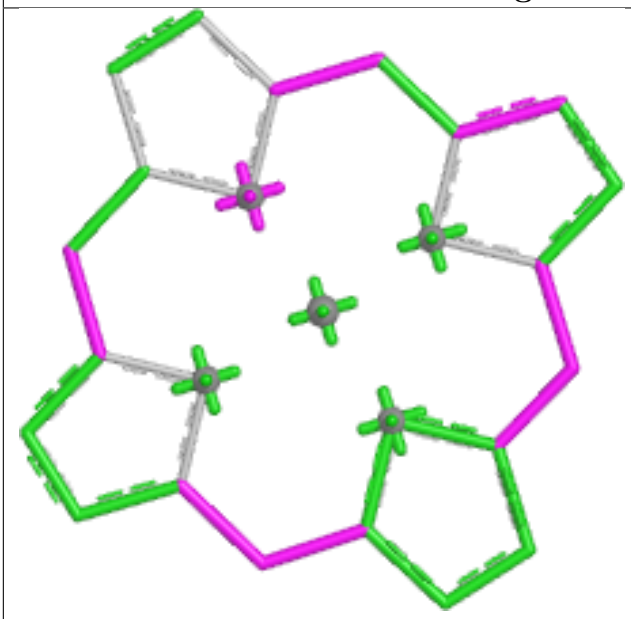


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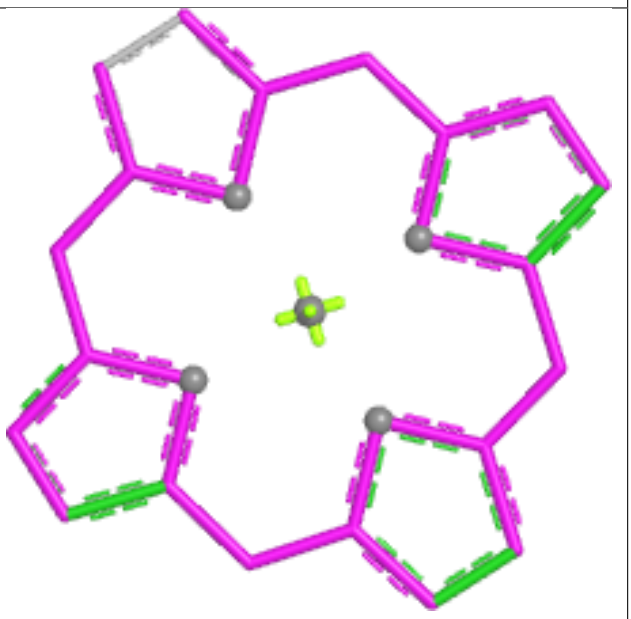


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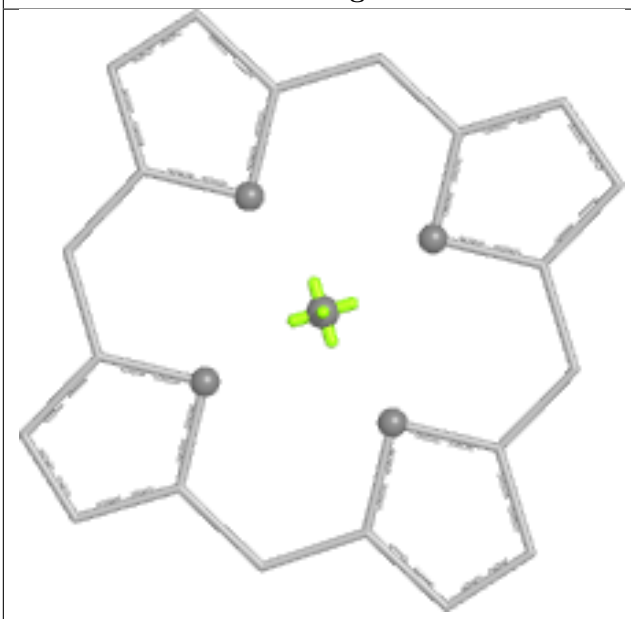
Ligand CLA A 1147



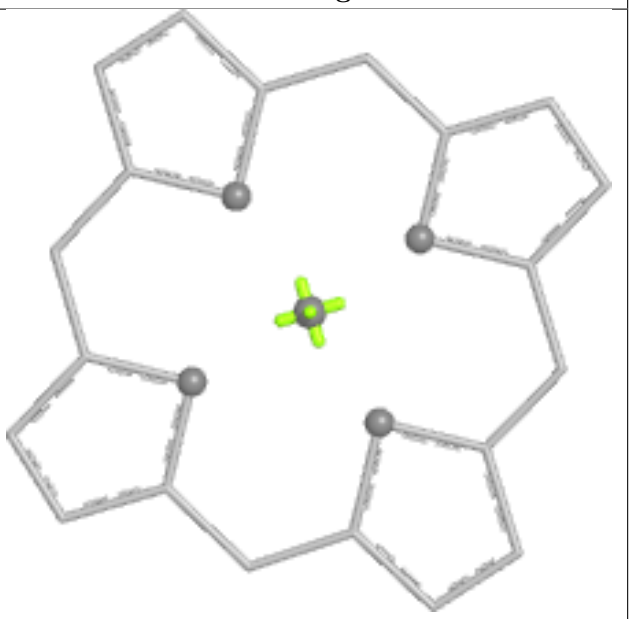
Bond lengths



Bond angles

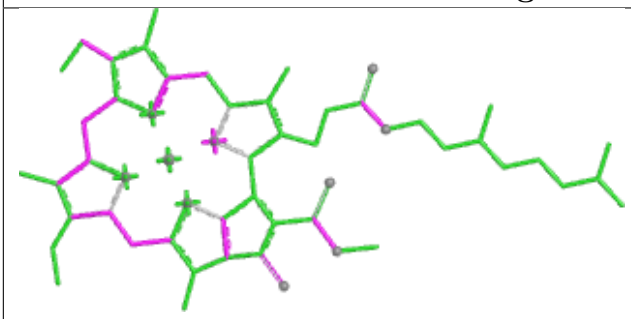


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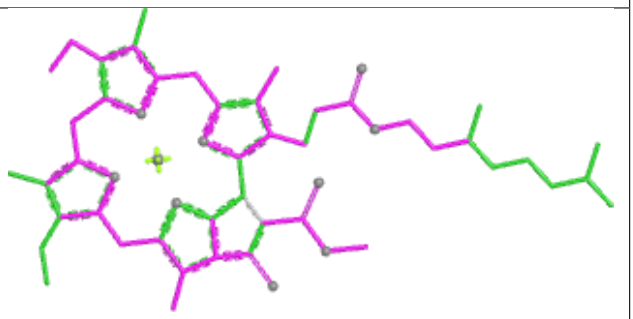


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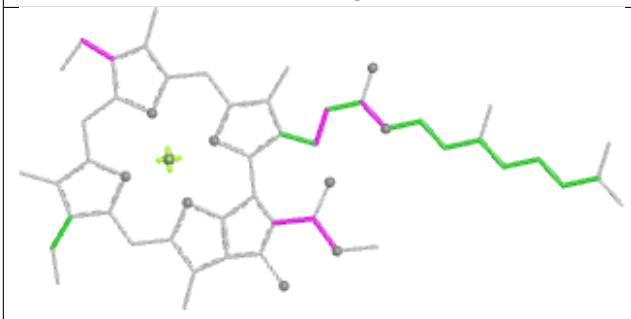
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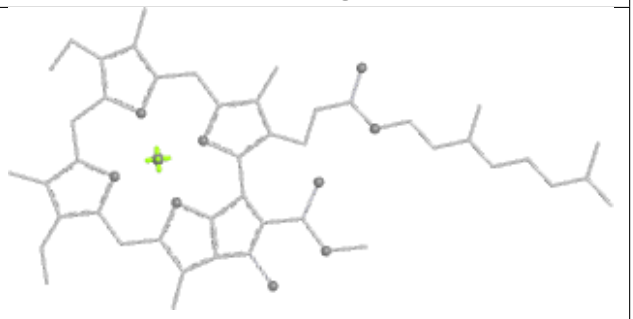
Bond lengths



Bond angles

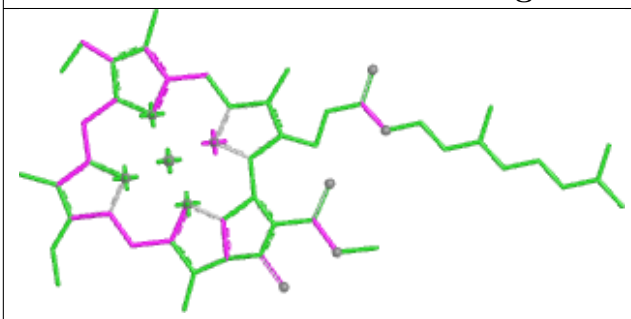


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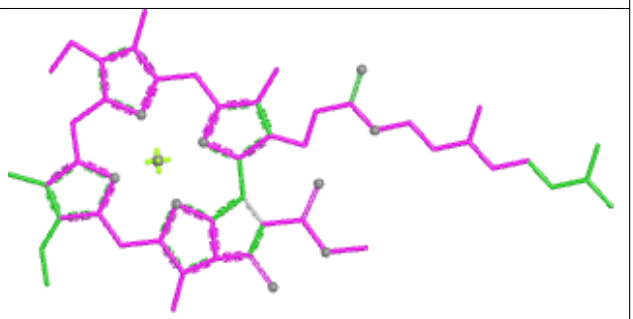


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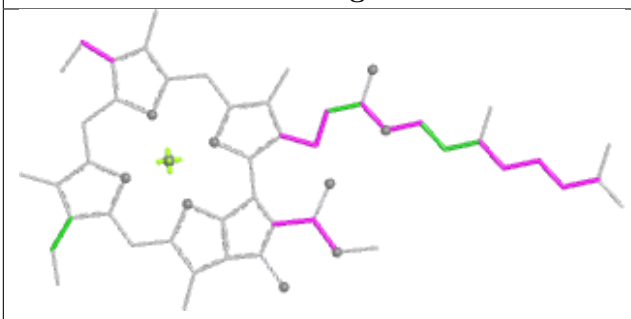
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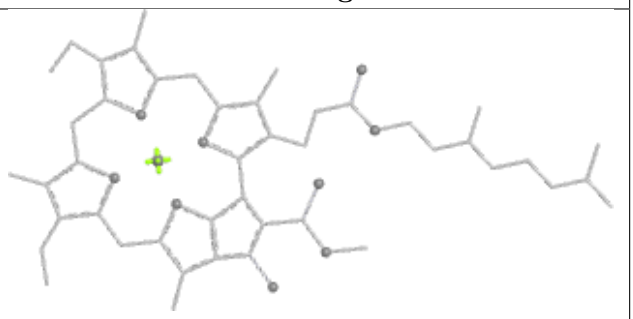
Bond lengths



Bond angles

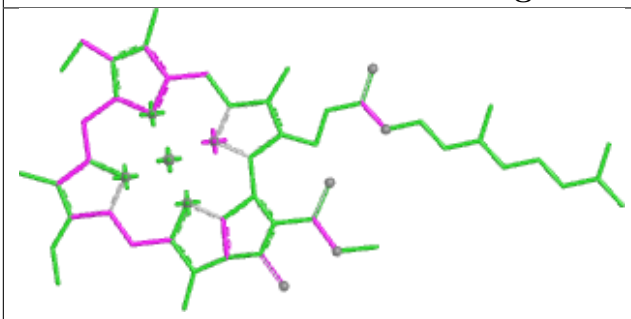


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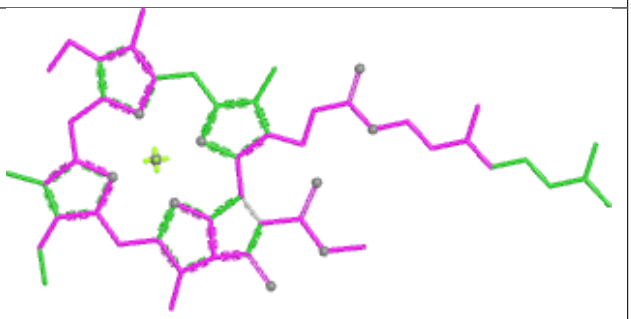


Rings

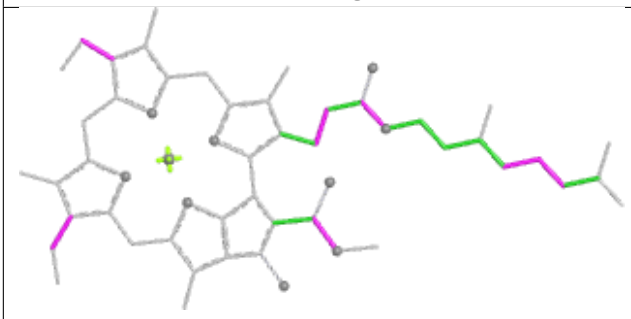
Ligand CLA A 1129



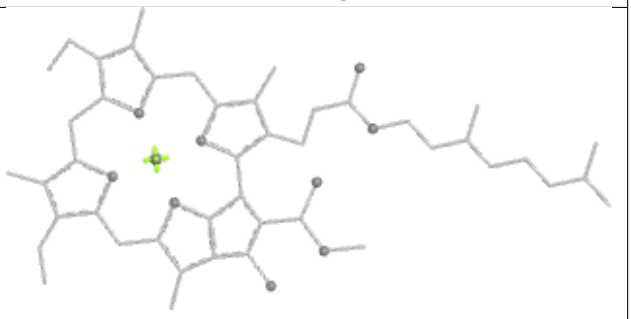
Bond lengths



Bond angles

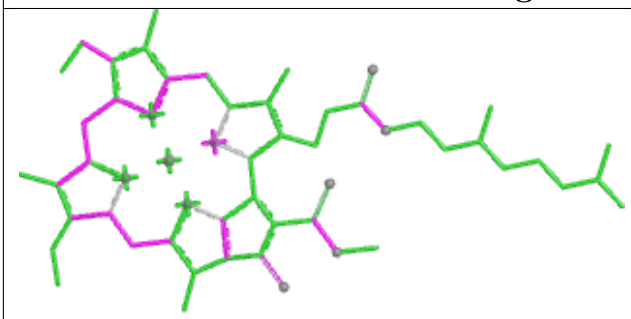


Torsions

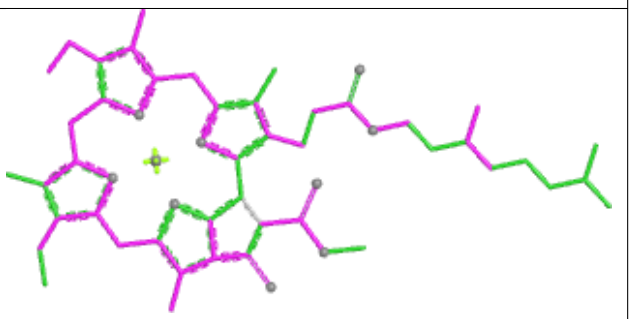


Rings

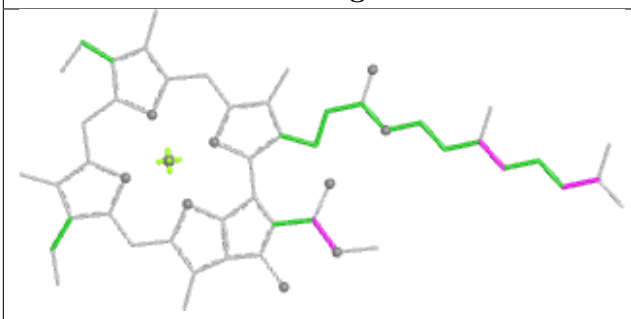
Ligand CLA B 1239



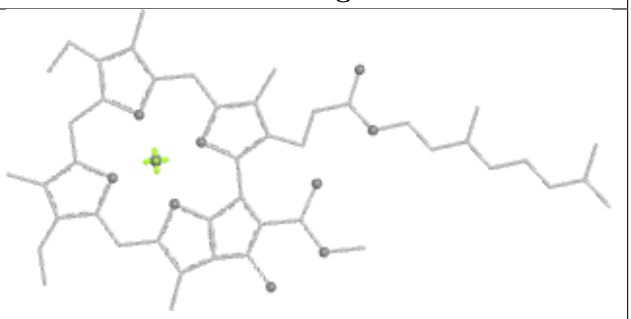
Bond lengths



Bond angles

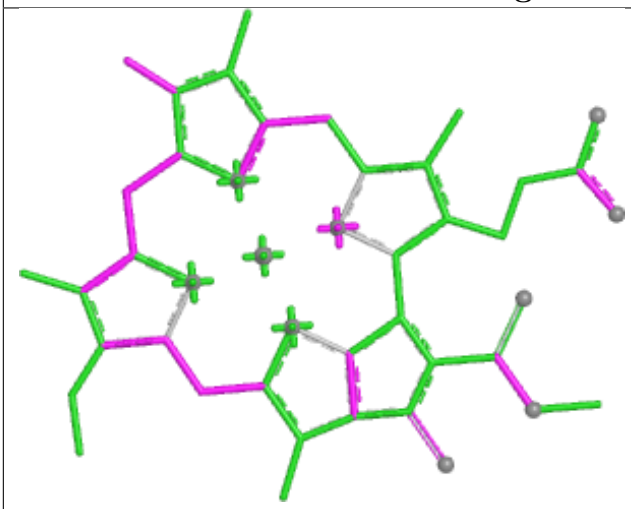


Torsions

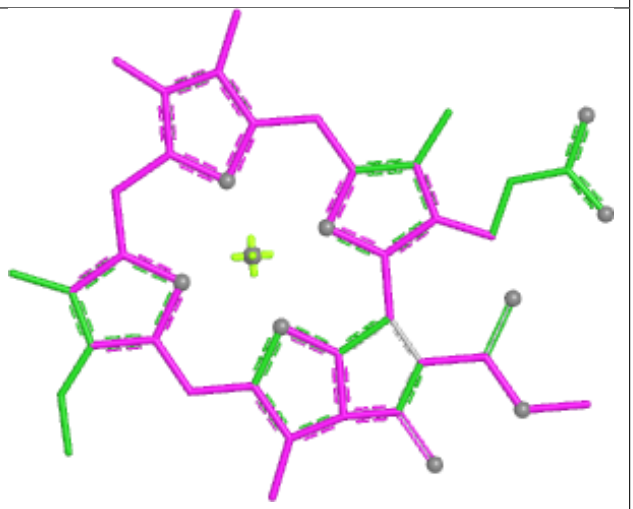


Rings

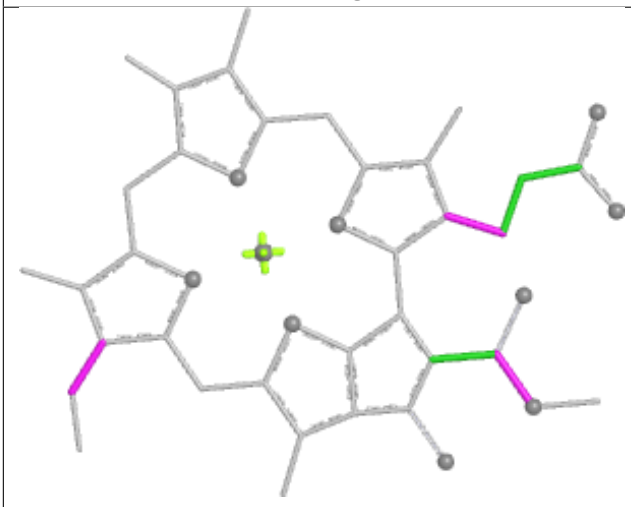
Ligand CLA A 1131



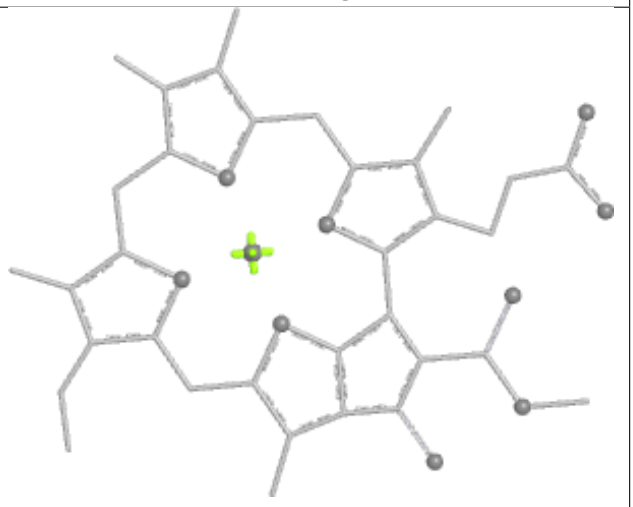
Bond lengths



Bond angles

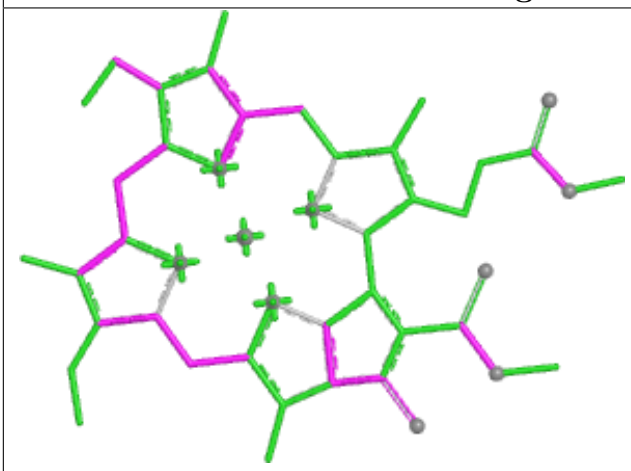


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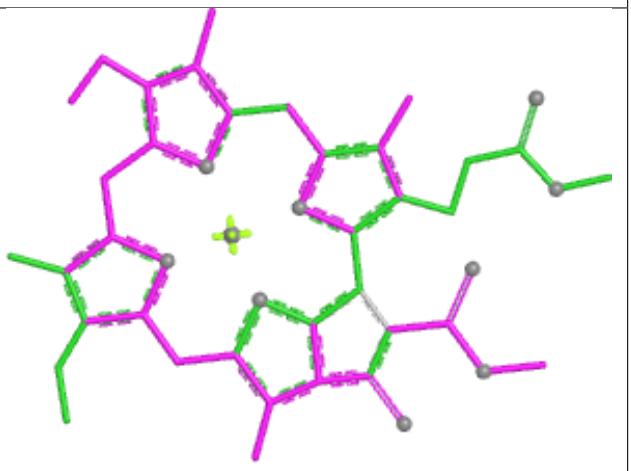


Rings

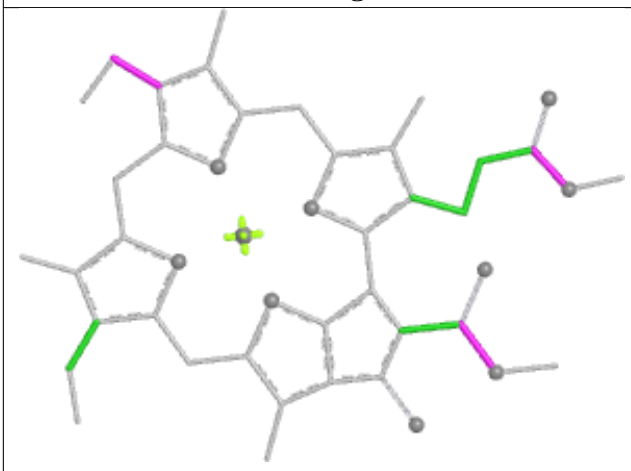
Ligand CLA B 1236



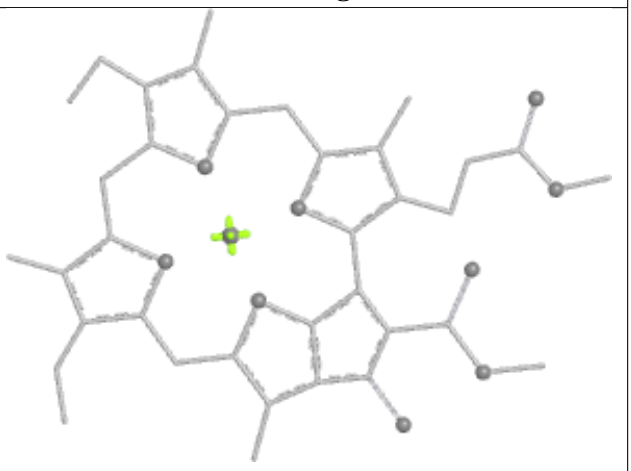
Bond lengths



Bond angles

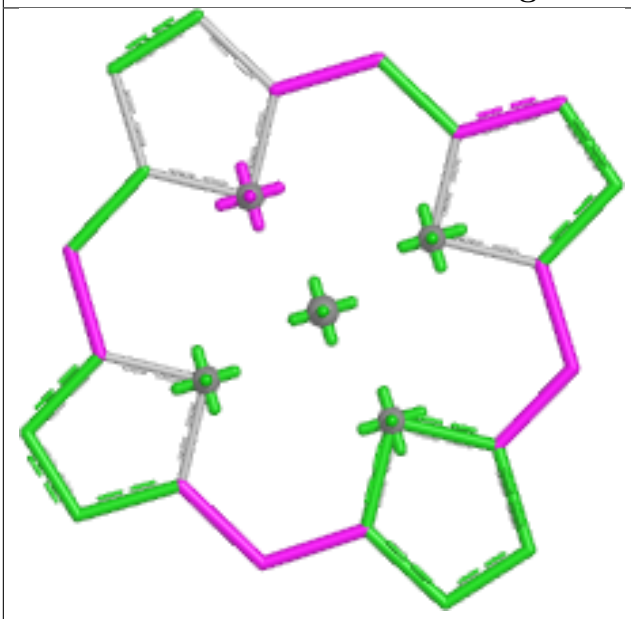


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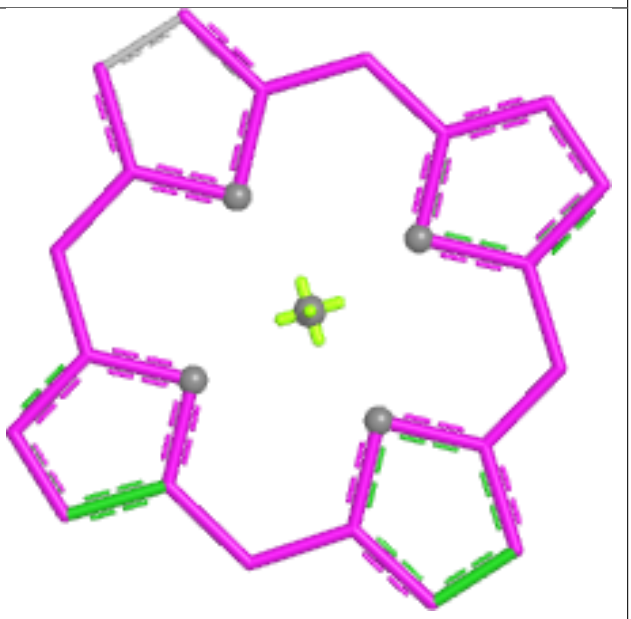


Rings

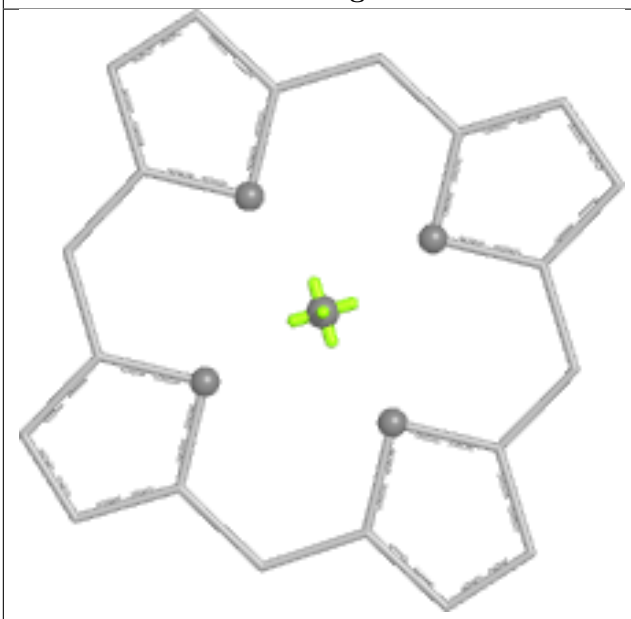
Ligand CLA 2 2004



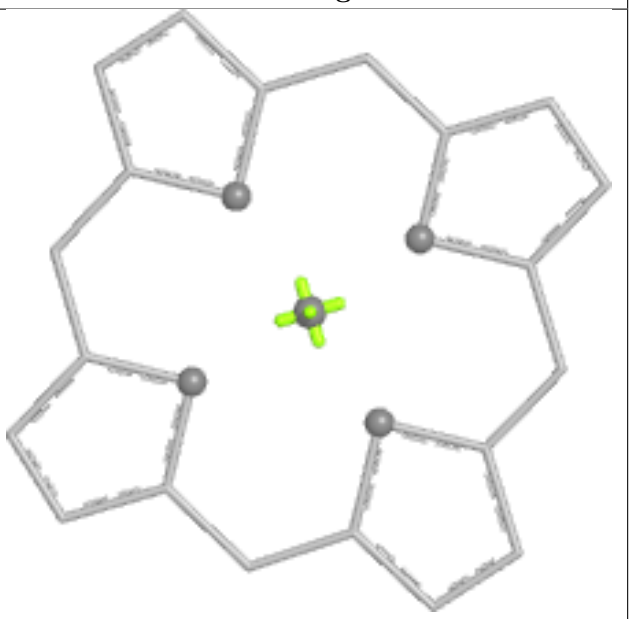
Bond lengths



Bond angles

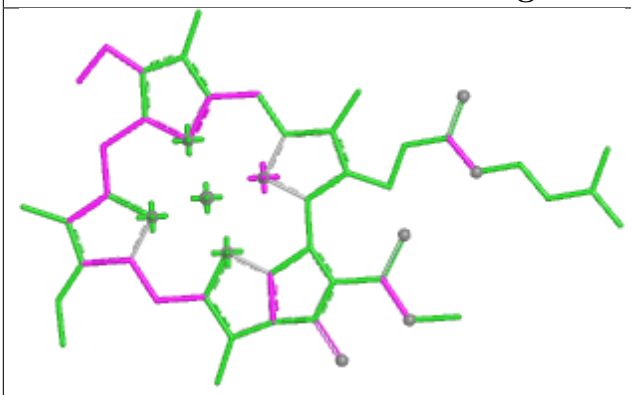


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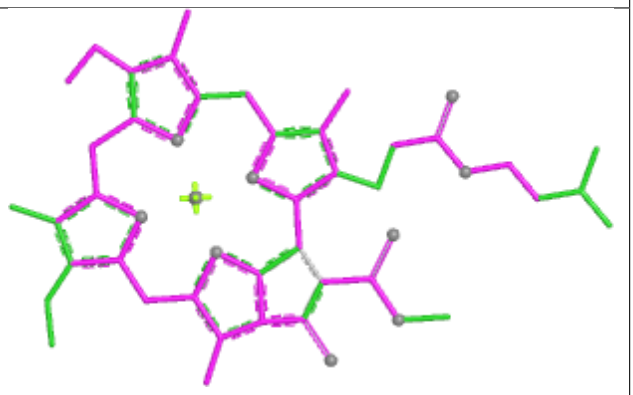


Rings

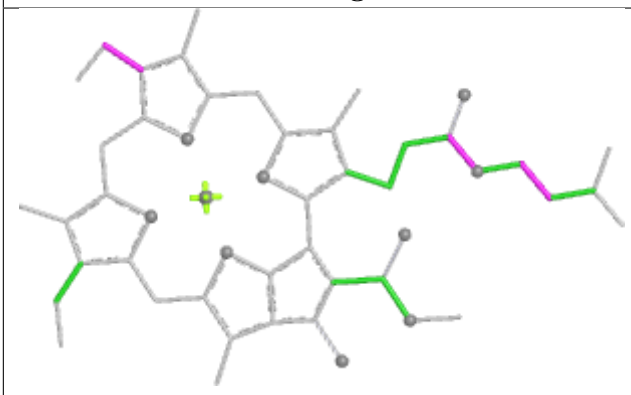
Ligand CLA L 1130



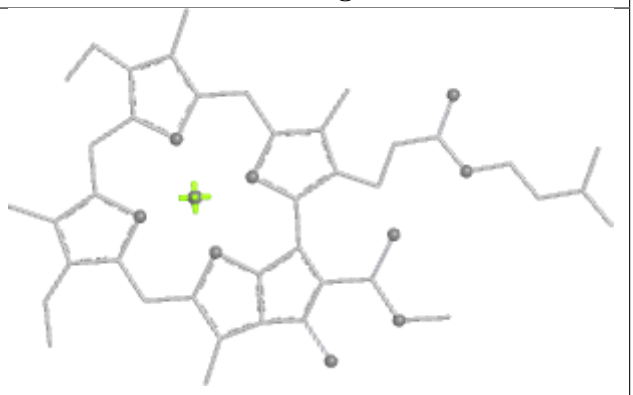
Bond lengths



Bond angles

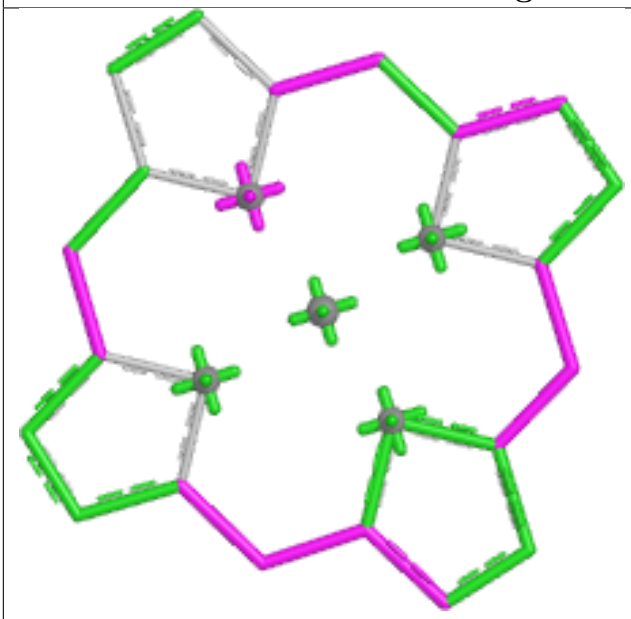


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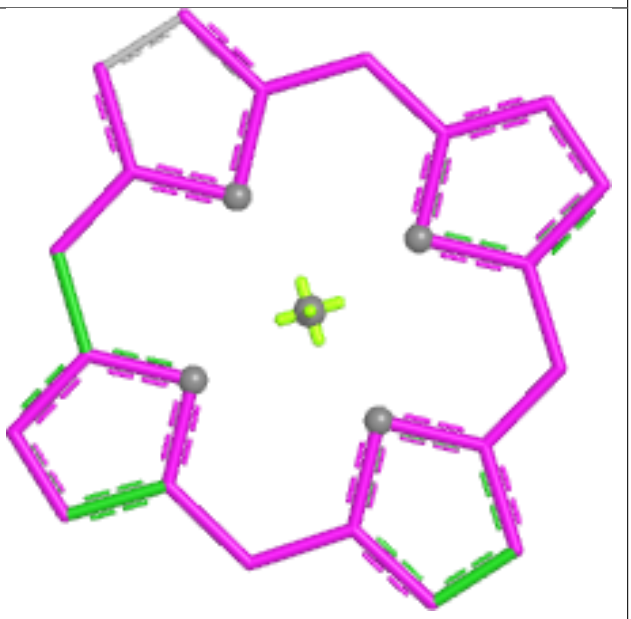


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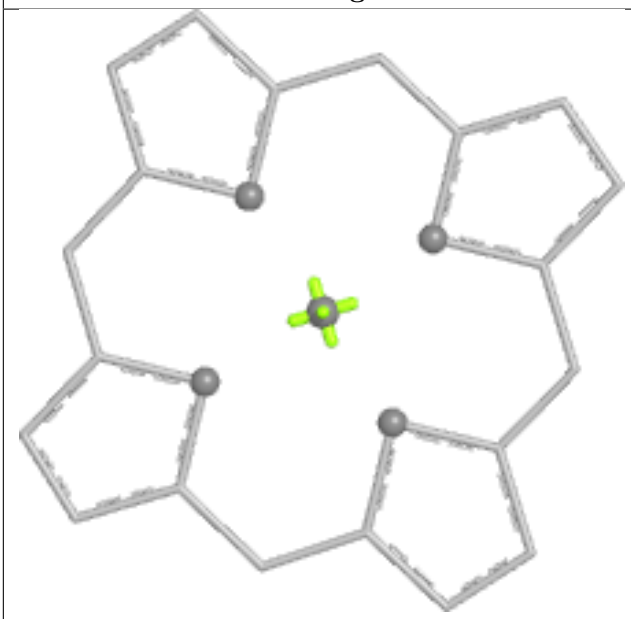
Ligand CLA B 1206



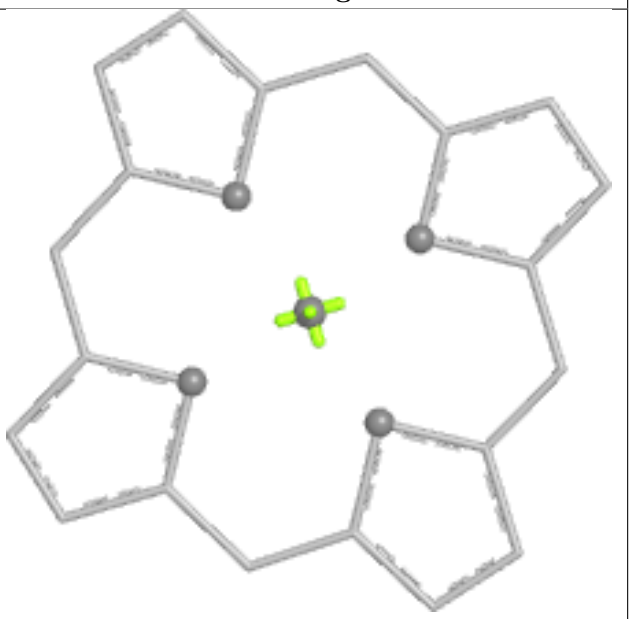
Bond lengths



Bond angles

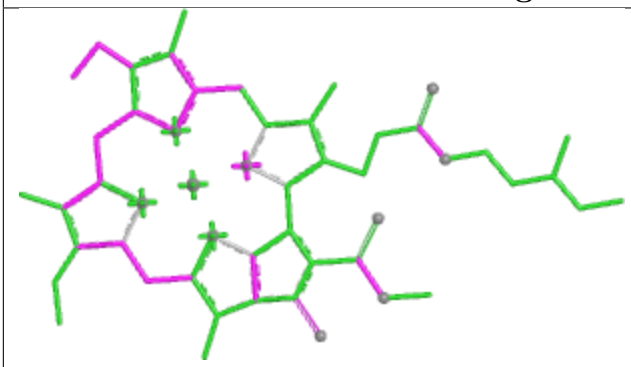


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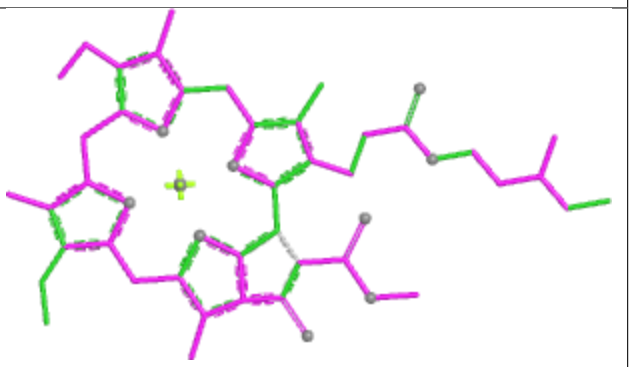


Rings

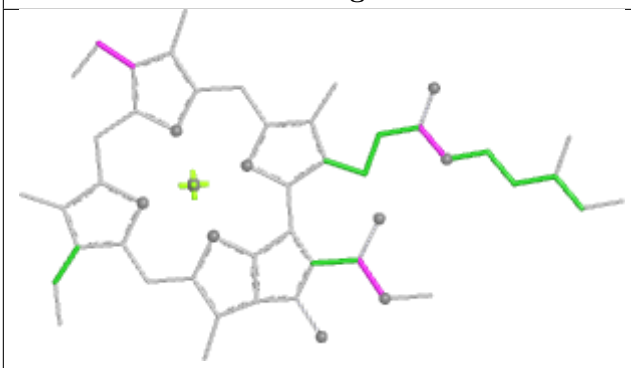
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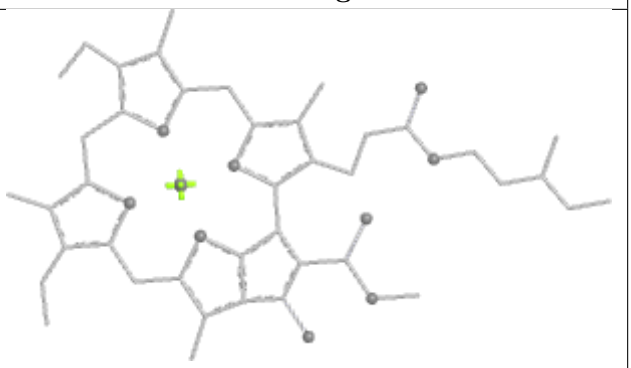
Bond lengths



Bond angles

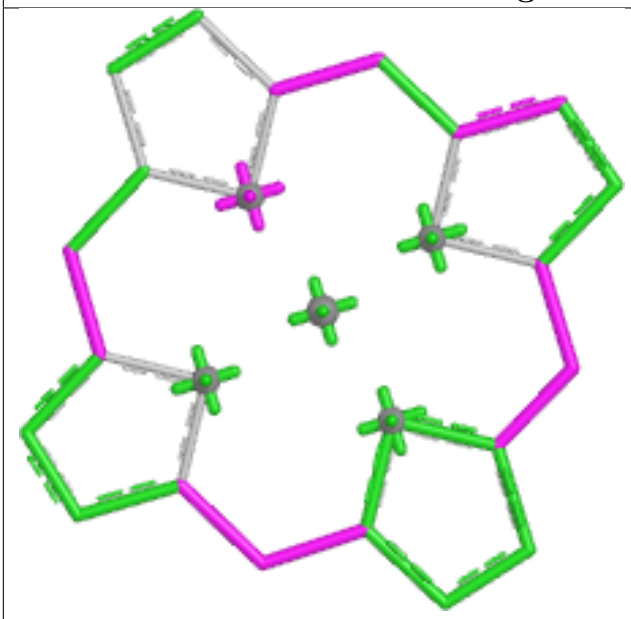


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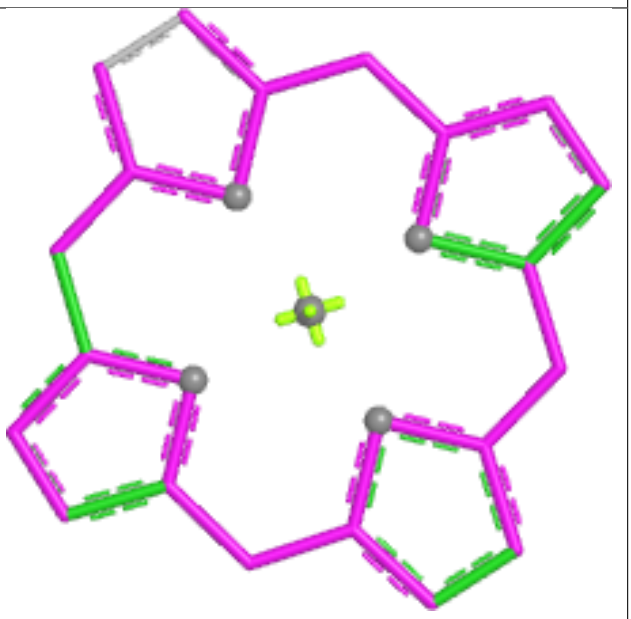


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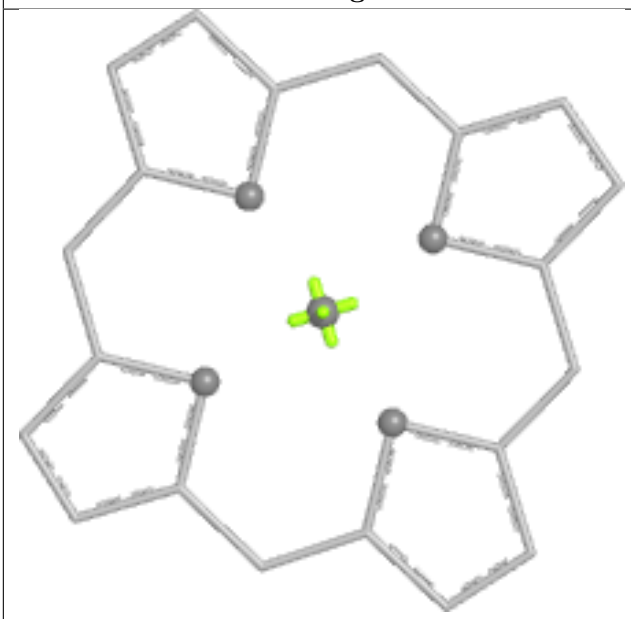
Ligand CLA L 1125



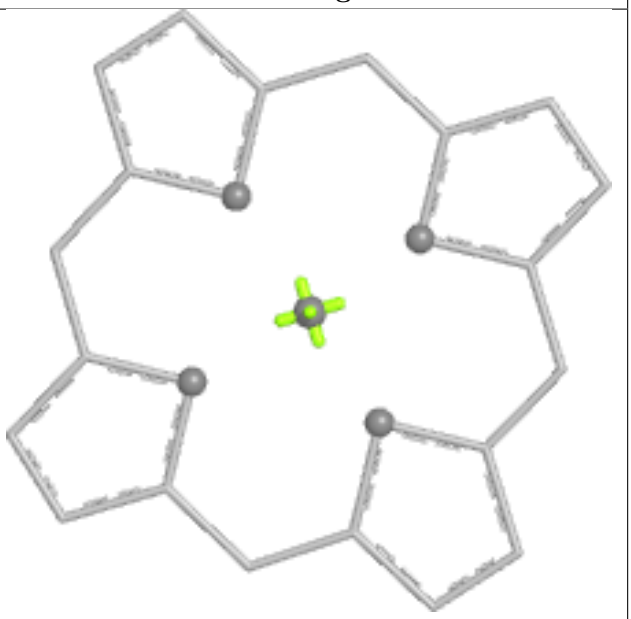
Bond lengths



Bond angles

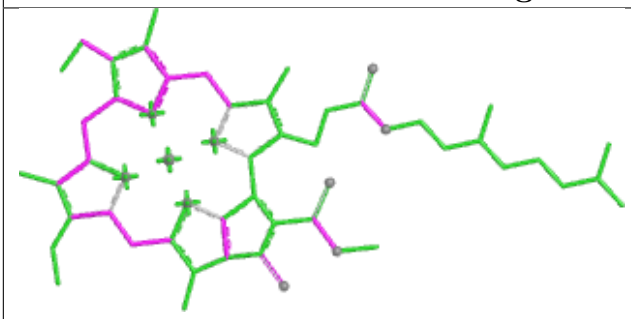


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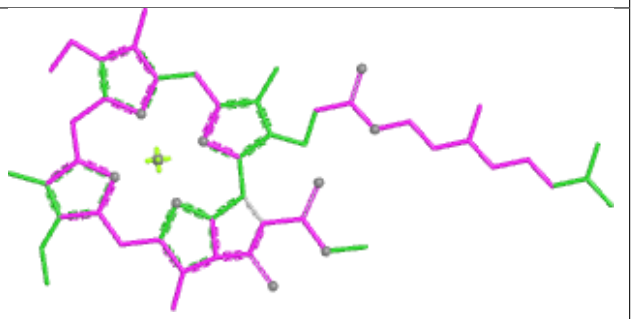


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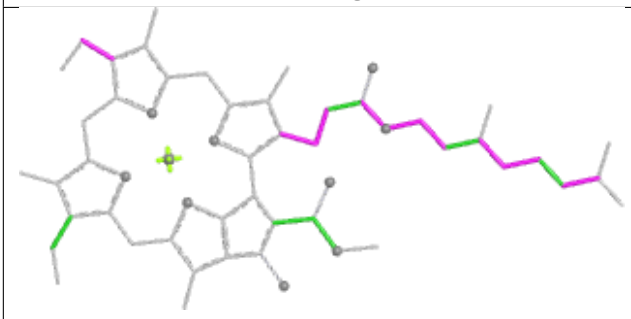
Ligand CLA B 1209



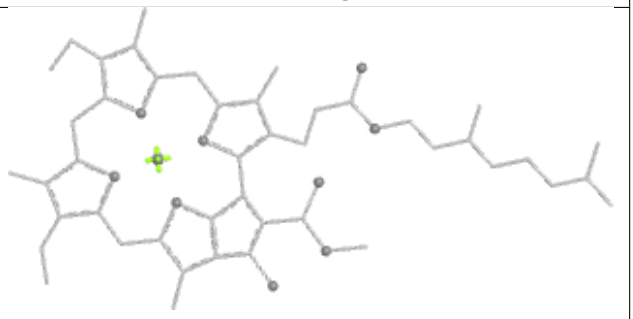
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Bond angles

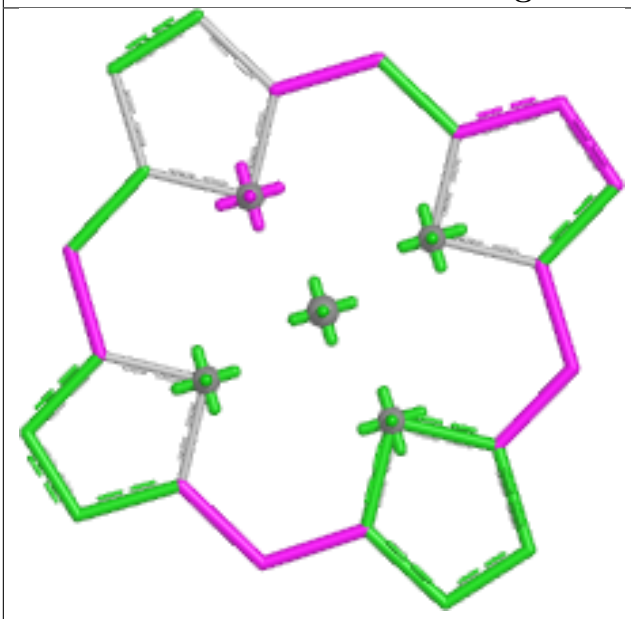


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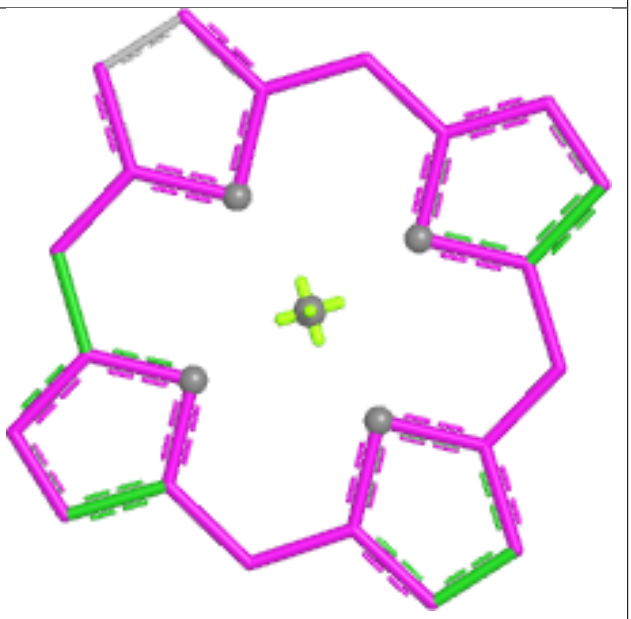


Rings

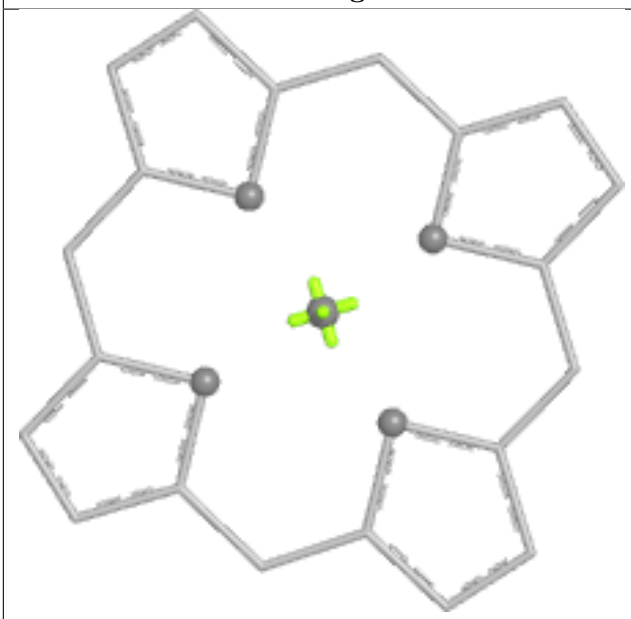
Ligand CLA A 1132



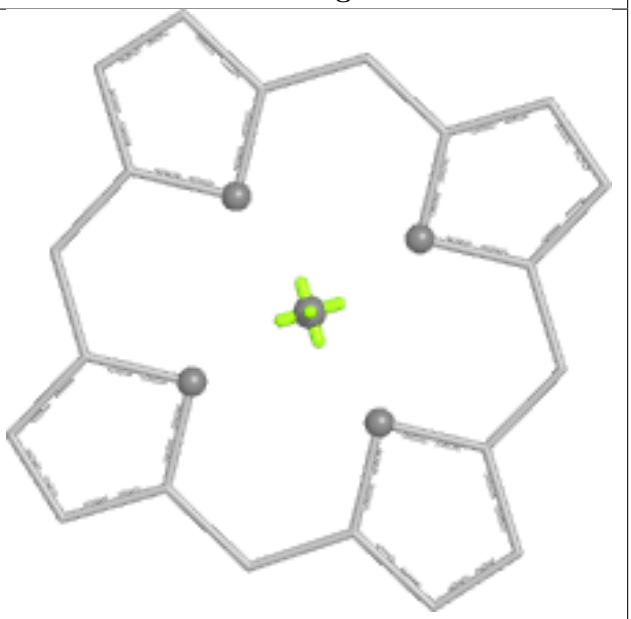
Bond lengths



Bond angles

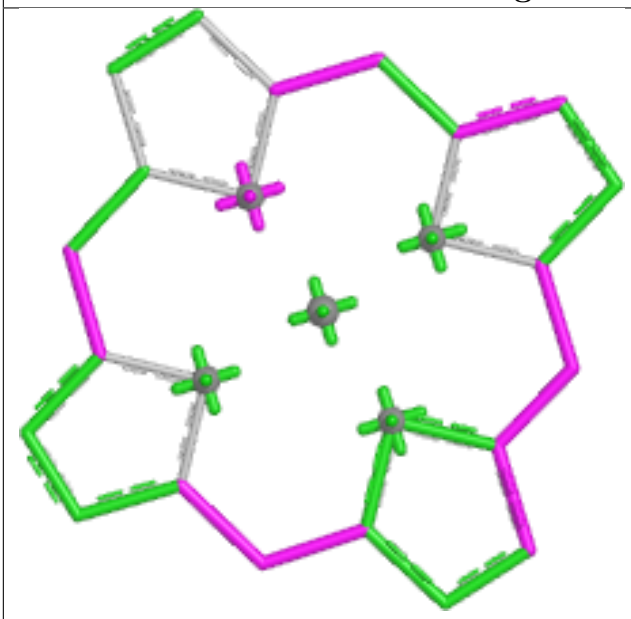


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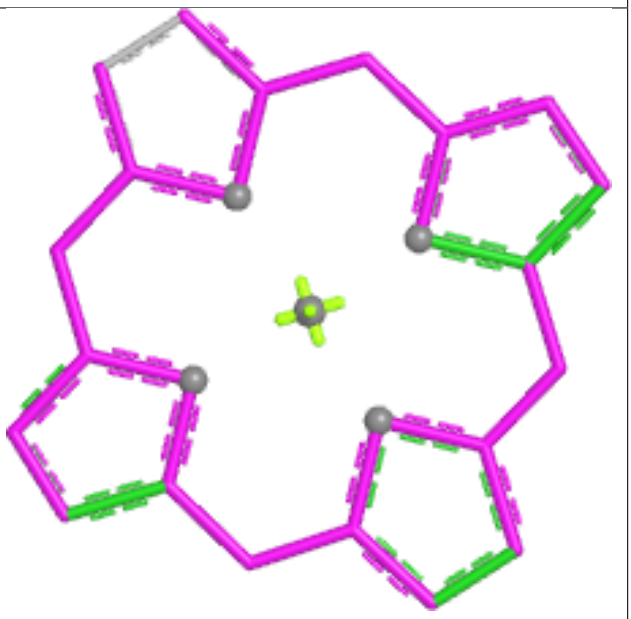


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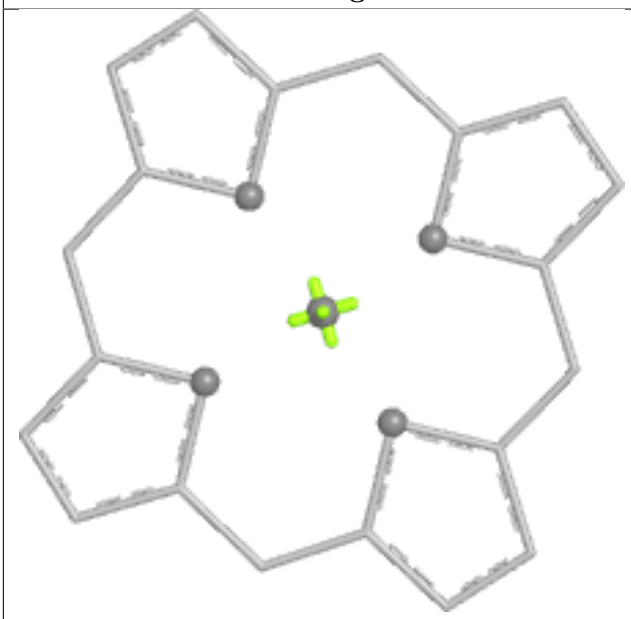
Ligand CLA H 1505



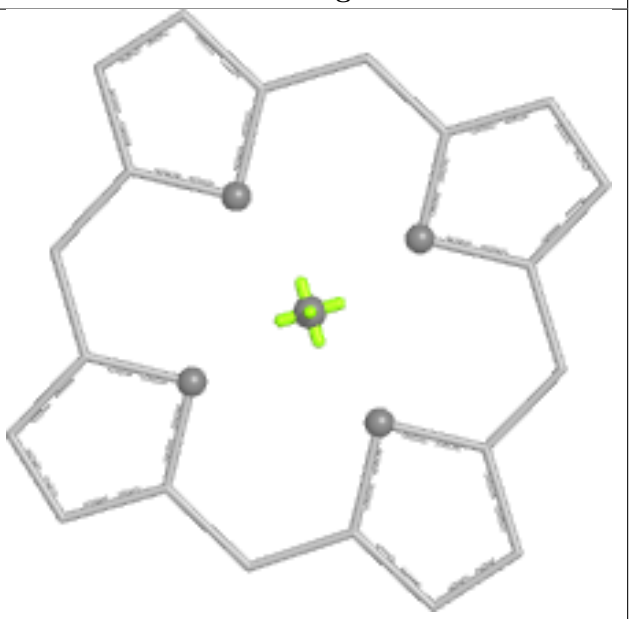
Bond lengths



Bond angles

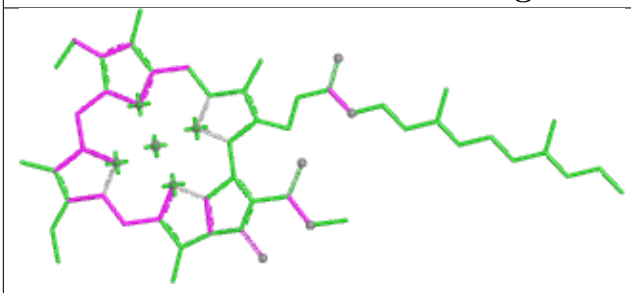


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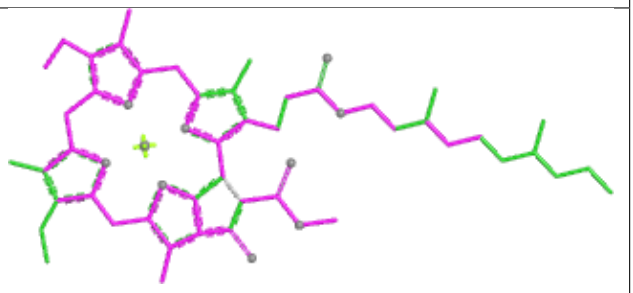


Rings

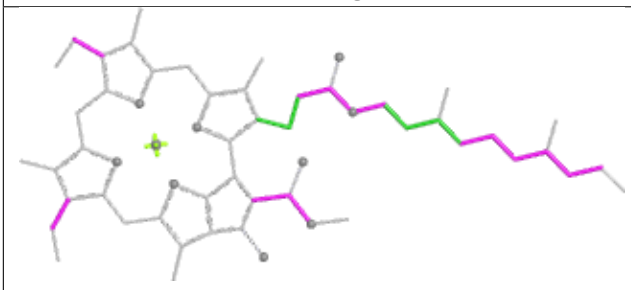
Ligand CLA A 1107



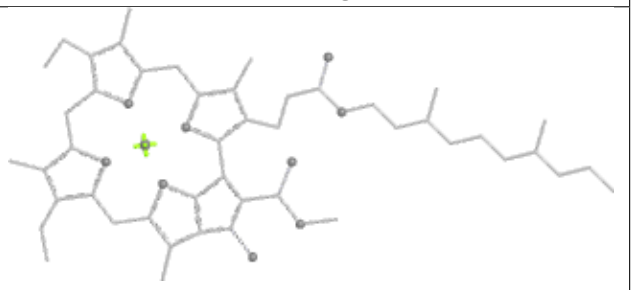
Bond lengths



Bond angles

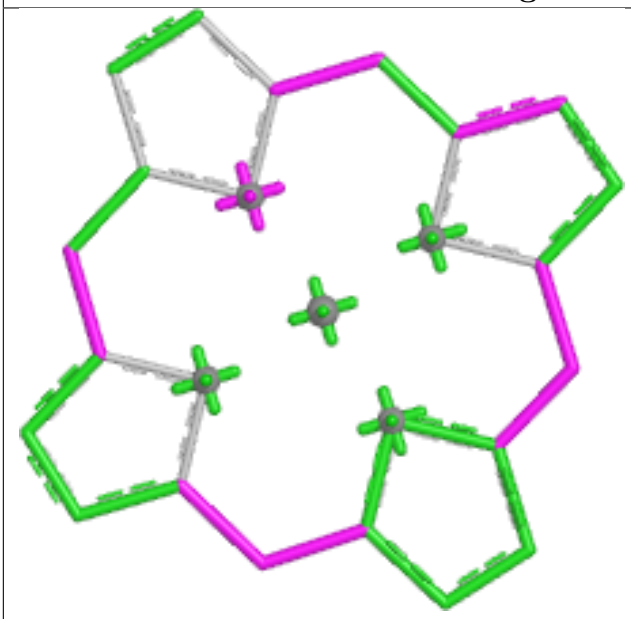


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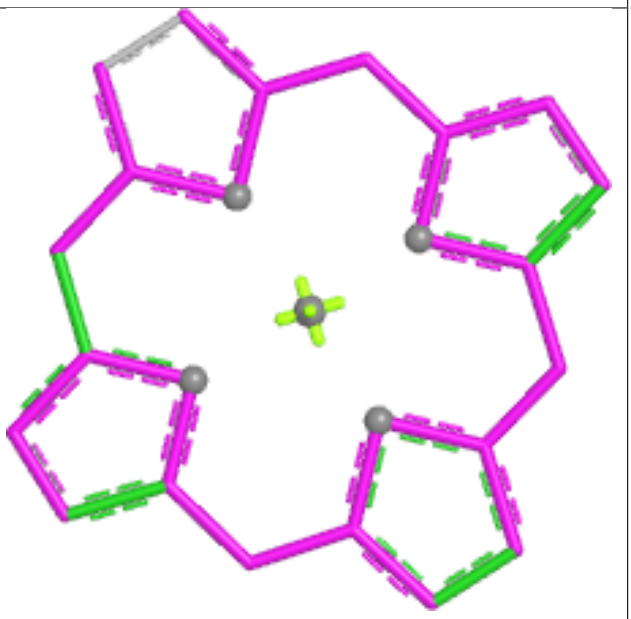


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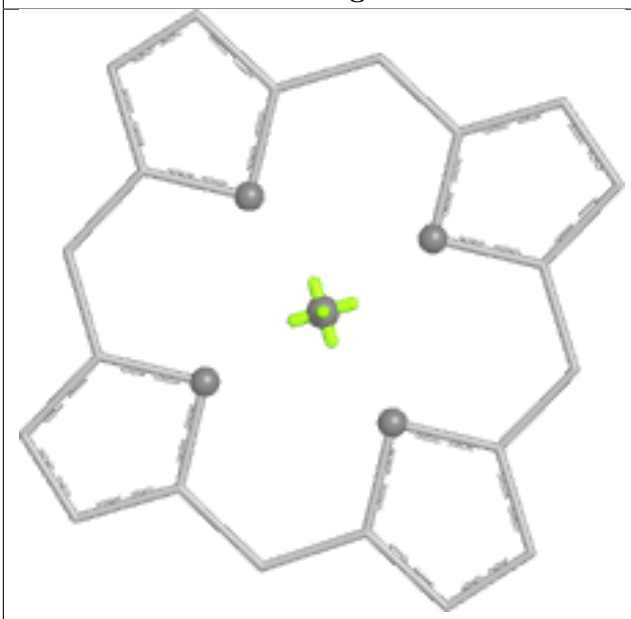
Ligand CLA 1 1008



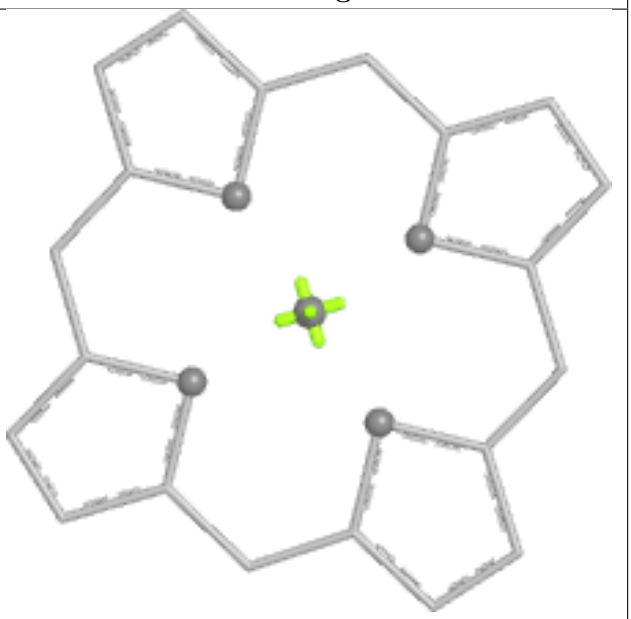
Bond lengths



Bond angles

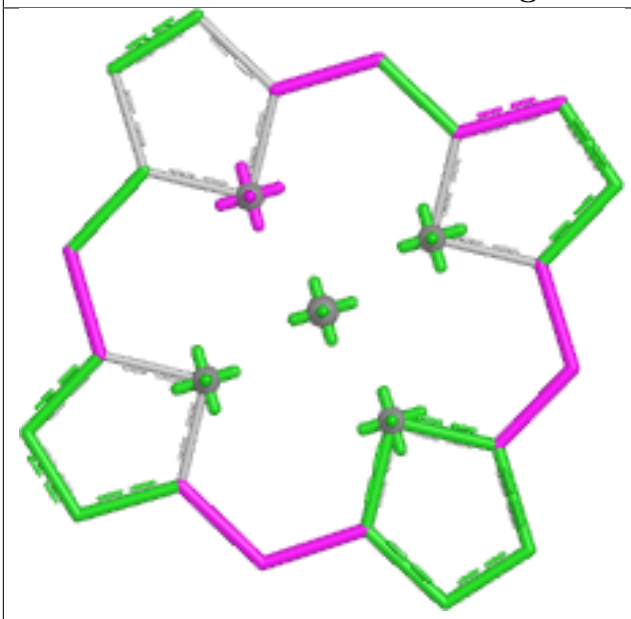


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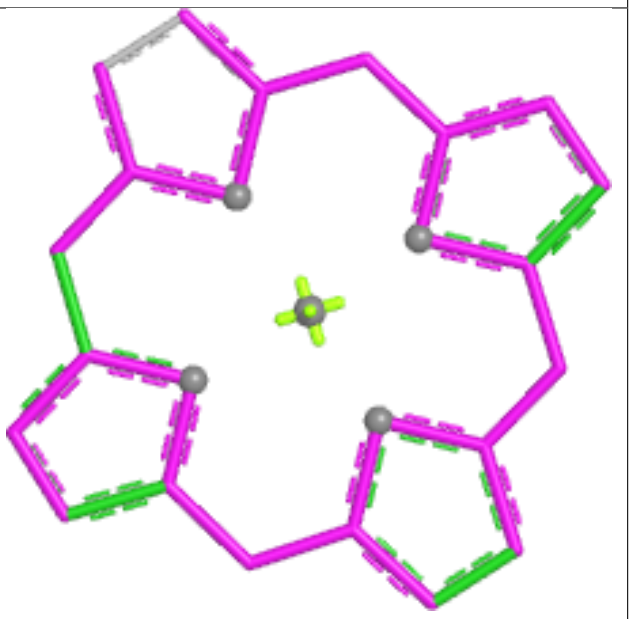


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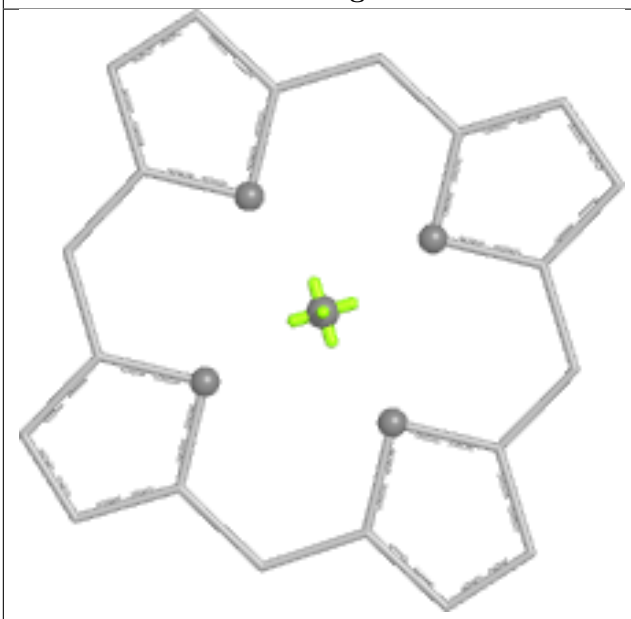
Ligand CLA 3 2009



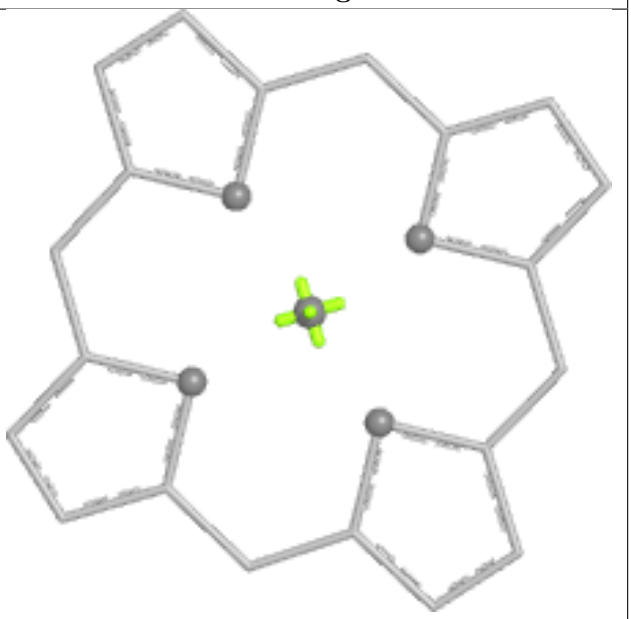
Bond lengths



Bond angles

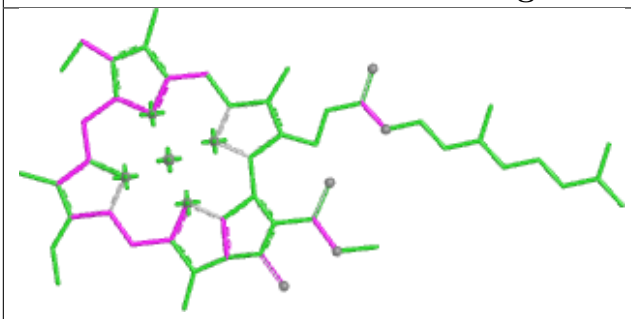


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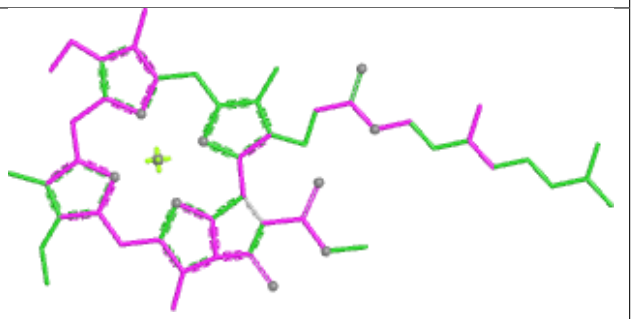


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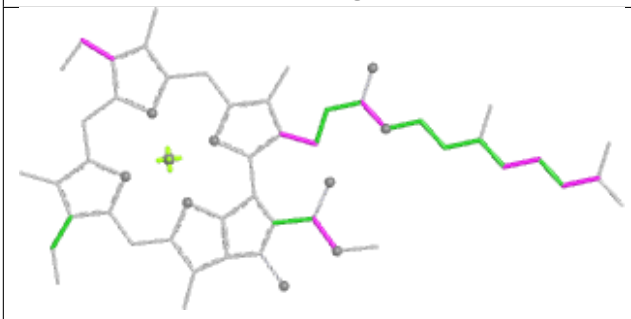
Ligand CLA L 1504



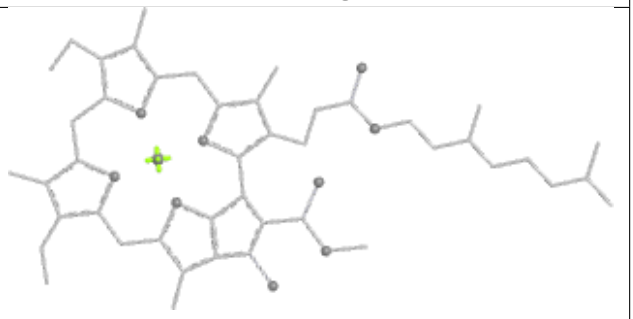
Bond lengths



Bond angles

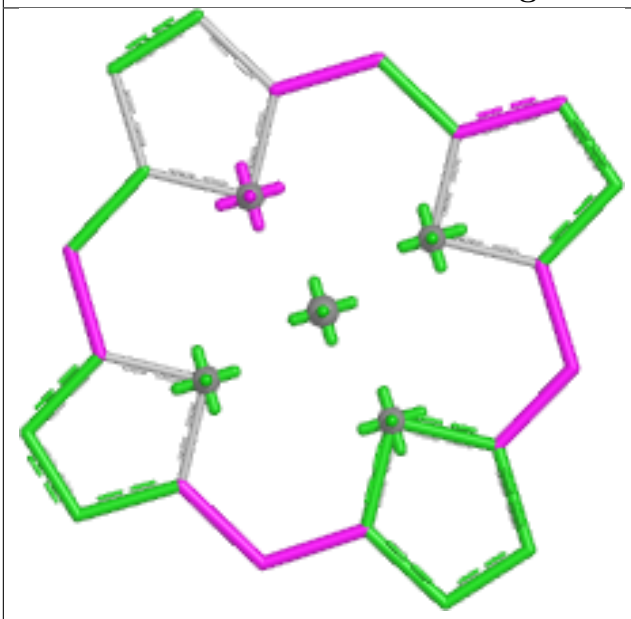


Torsions

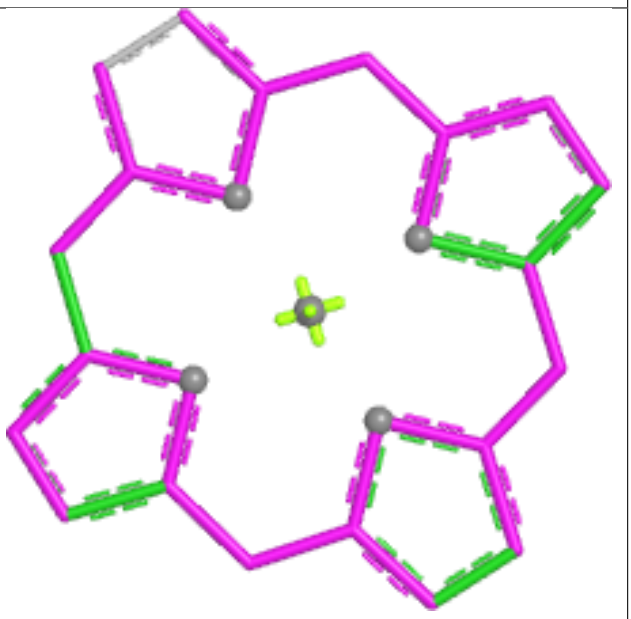


Rings

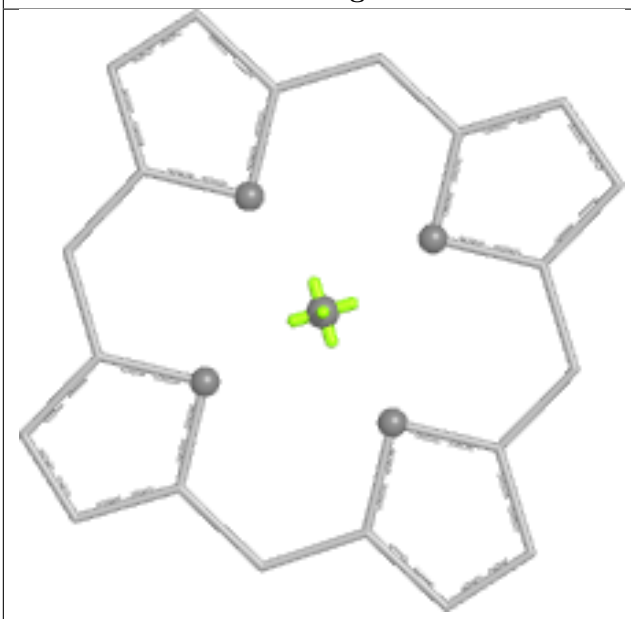
Ligand CLA 3 3003



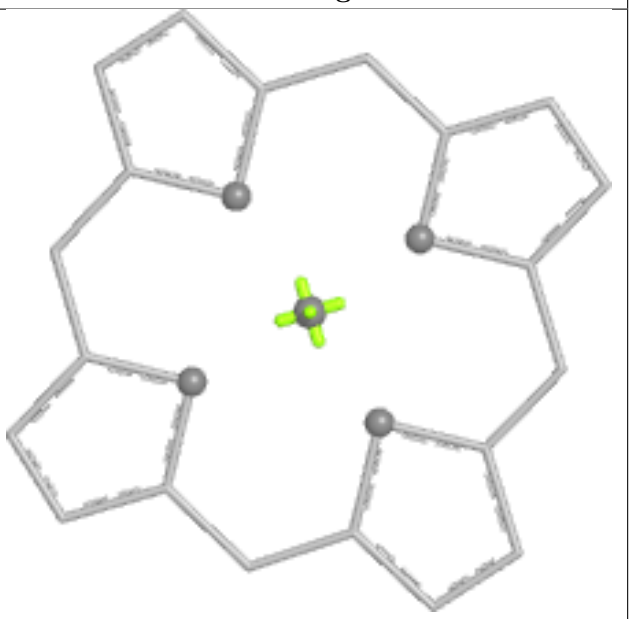
Bond lengths



Bond angles

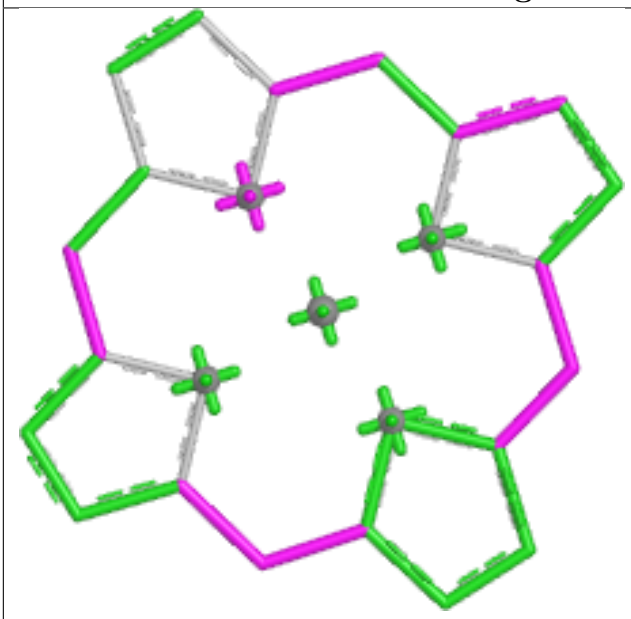


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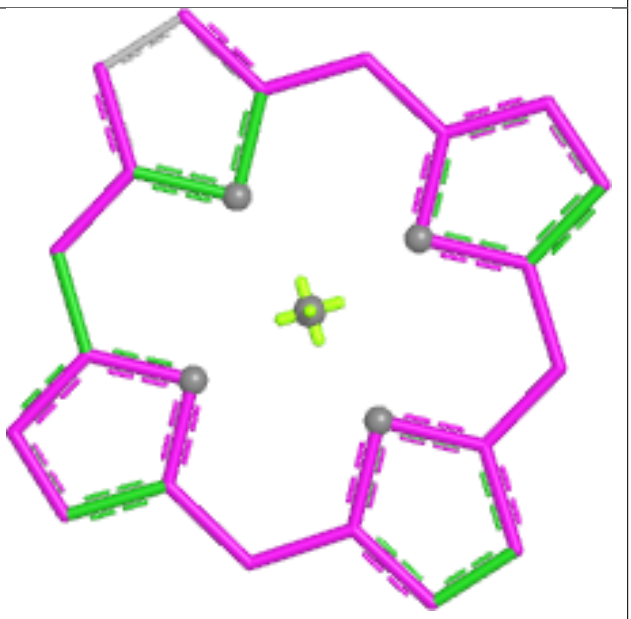


Rings

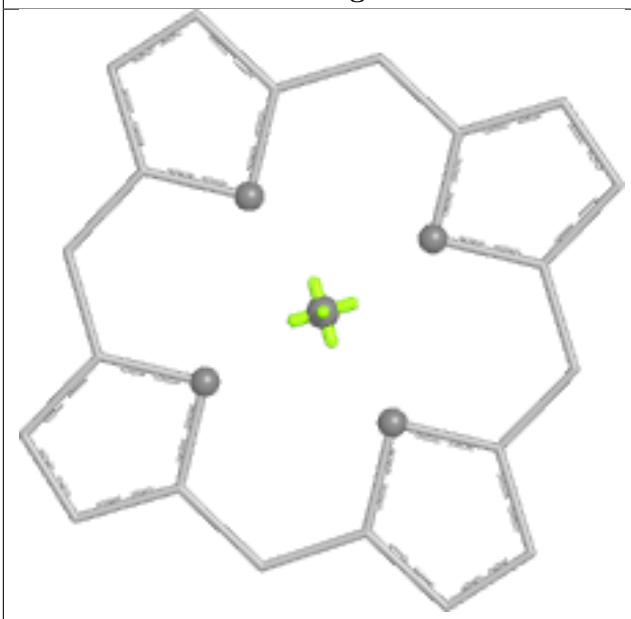
Ligand CLA A 1104



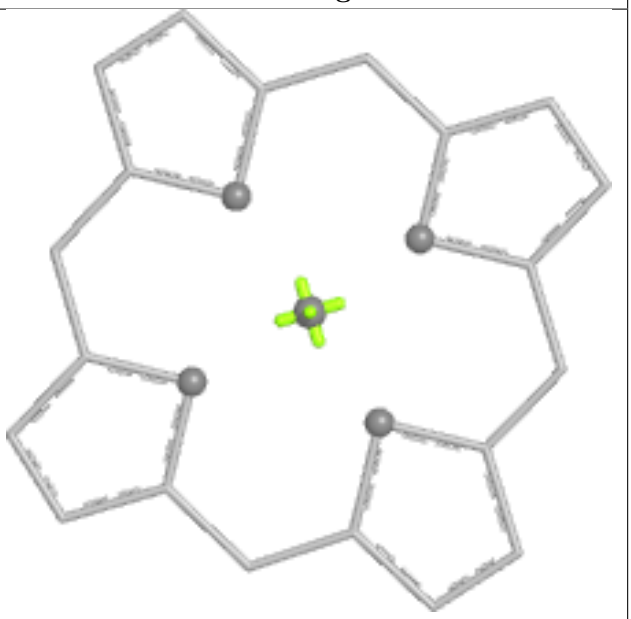
Bond lengths



Bond angles

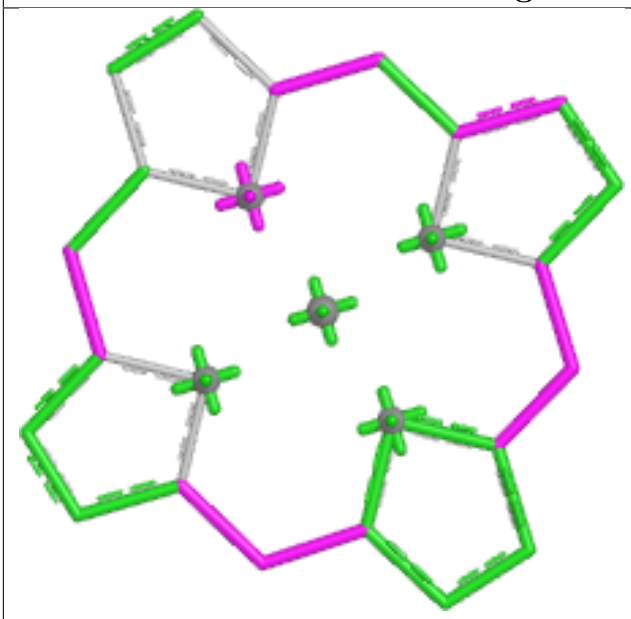


Torsions

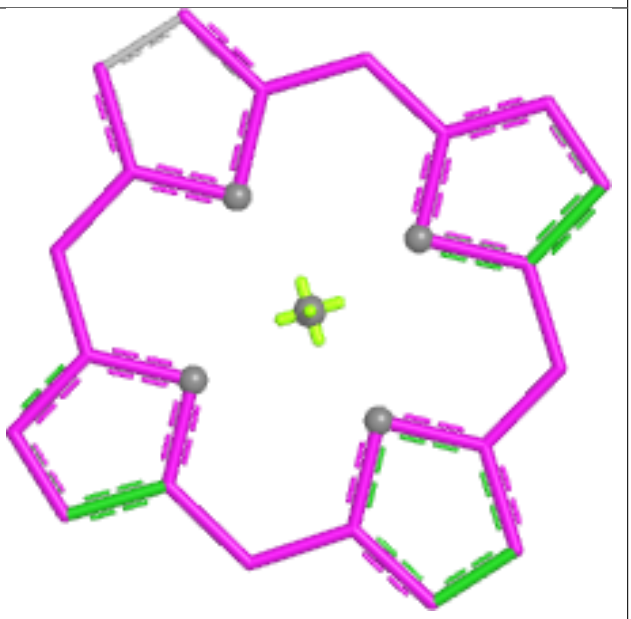


Rings

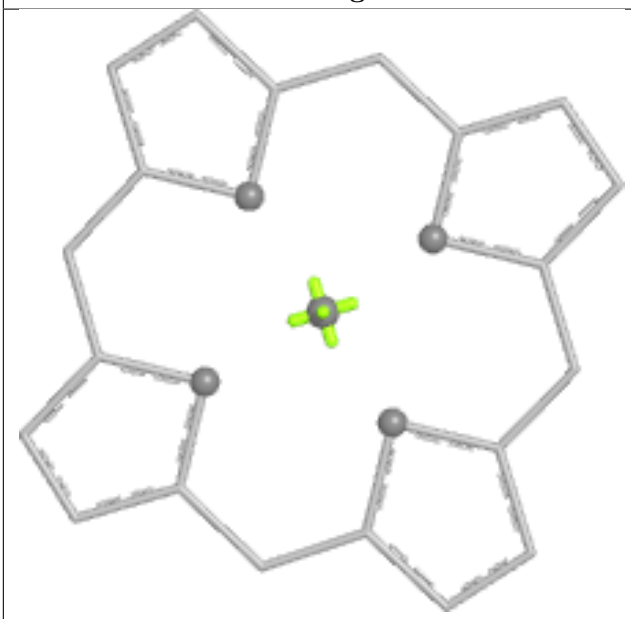
Ligand CLA B 1201



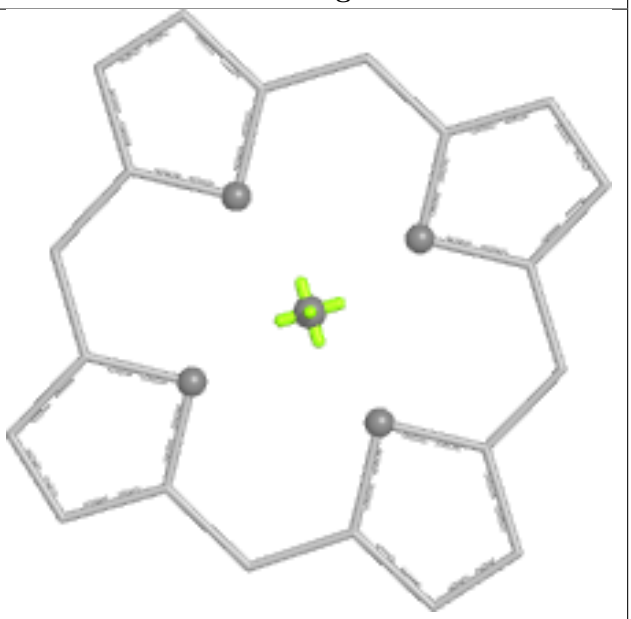
Bond lengths



Bond angles

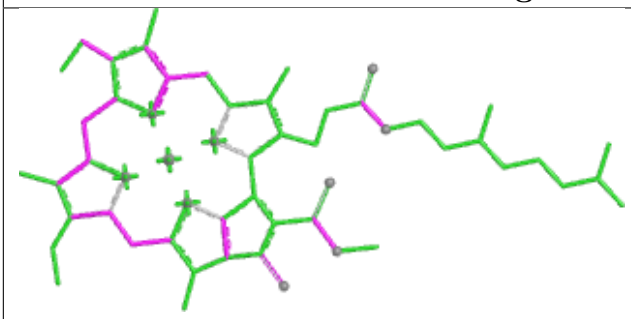


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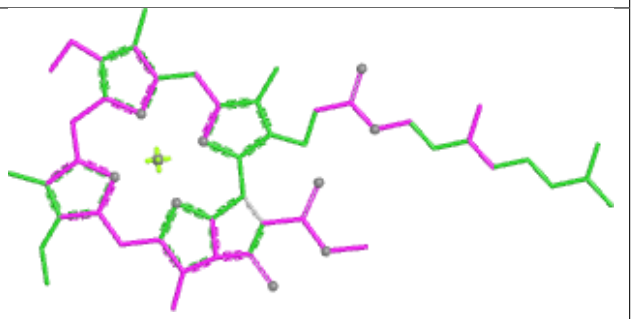


Rings

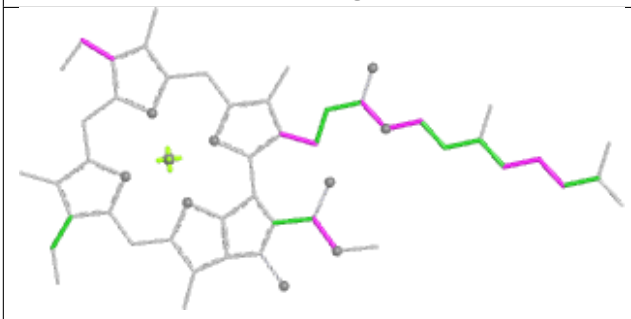
Ligand CLA B 1232



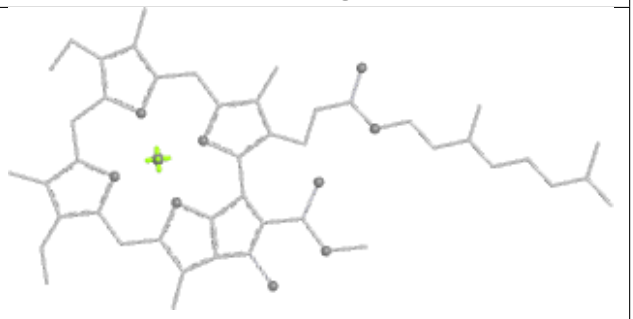
Bond lengths



Bond angles

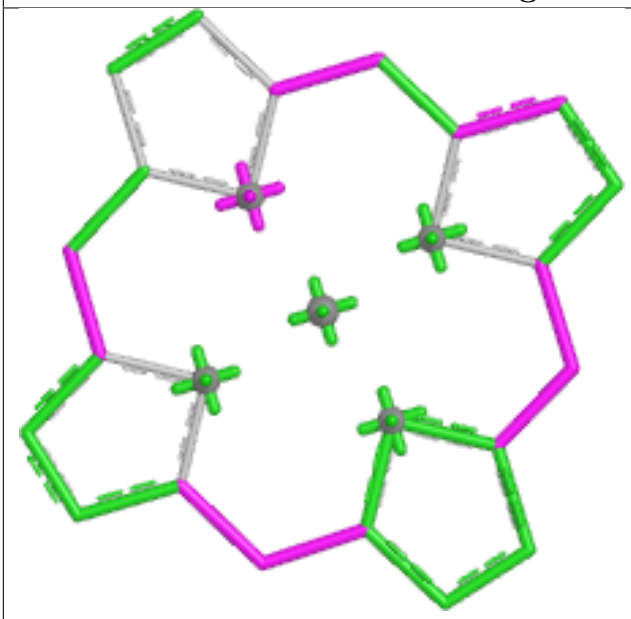


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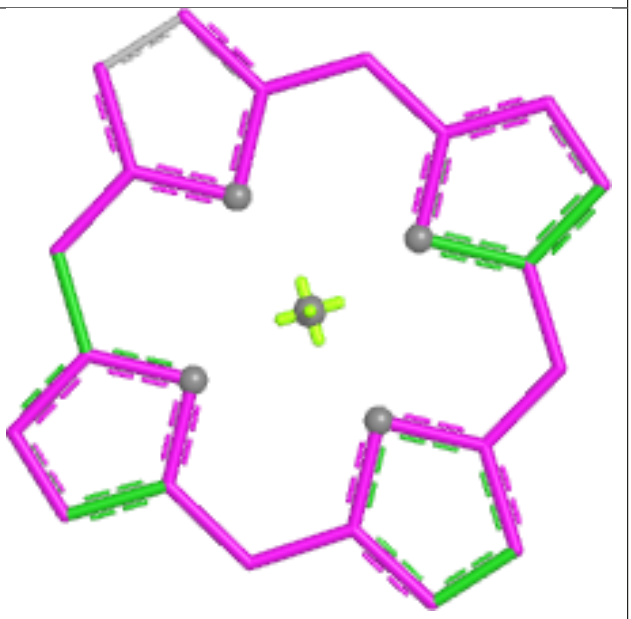


Rings

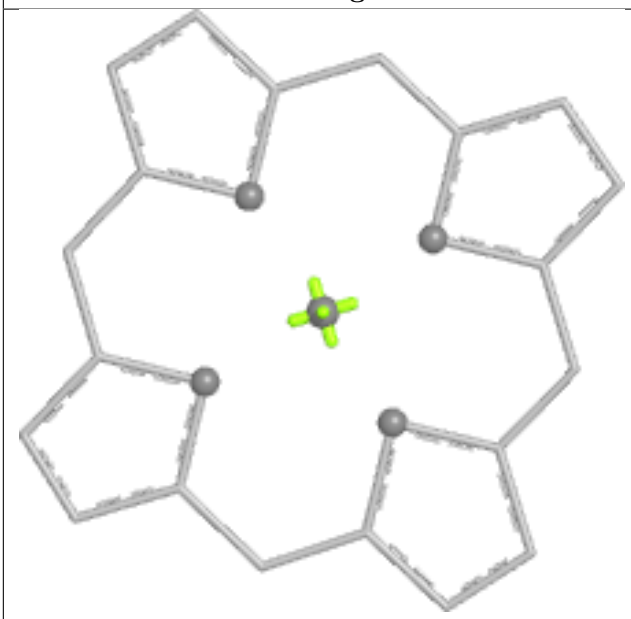
Ligand CLA 3 3010



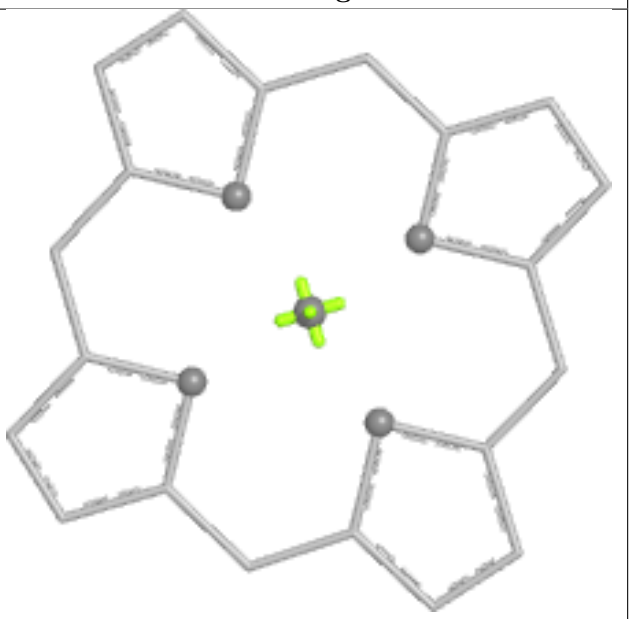
Bond lengths



Bond angles

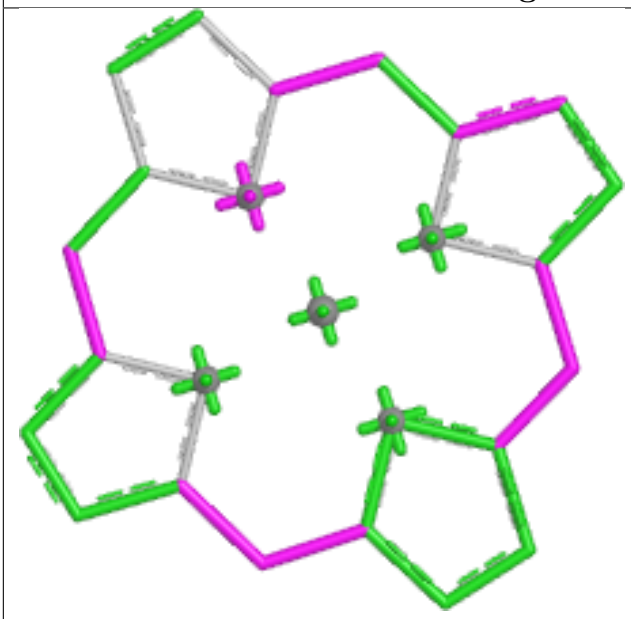


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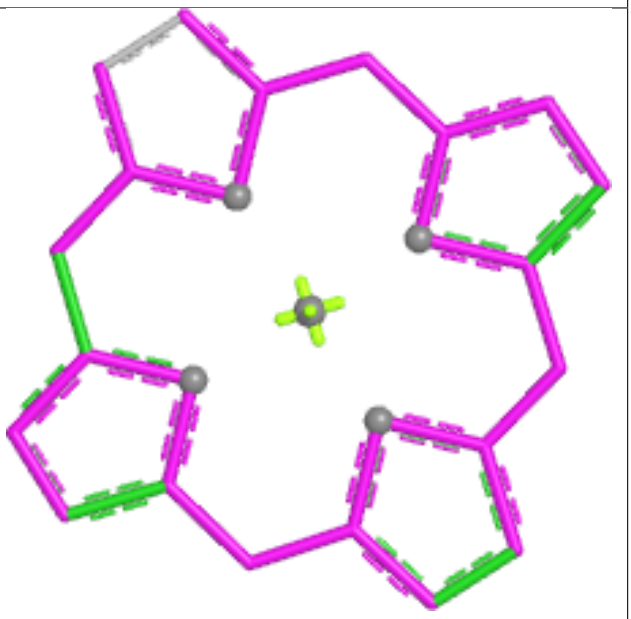


Rings

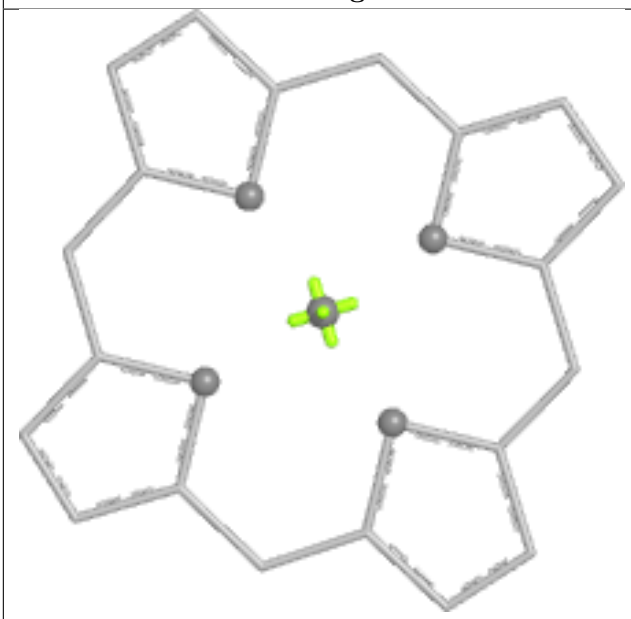
Ligand CLA J 1307



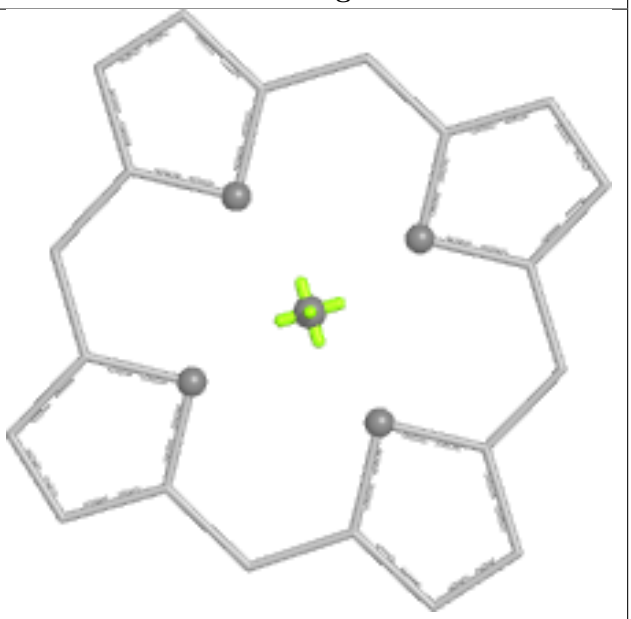
Bond lengths



Bond angles

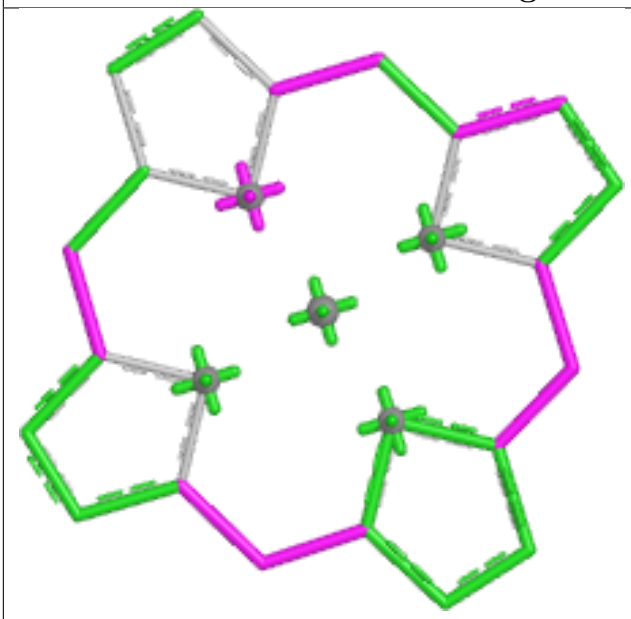


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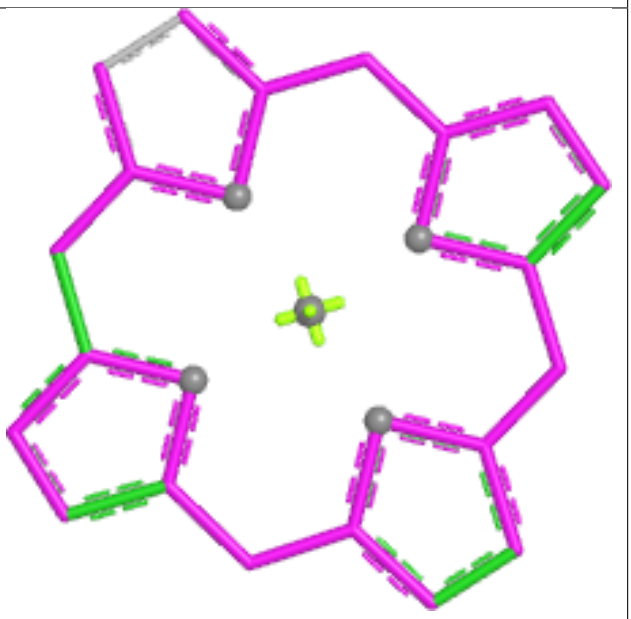


Rings

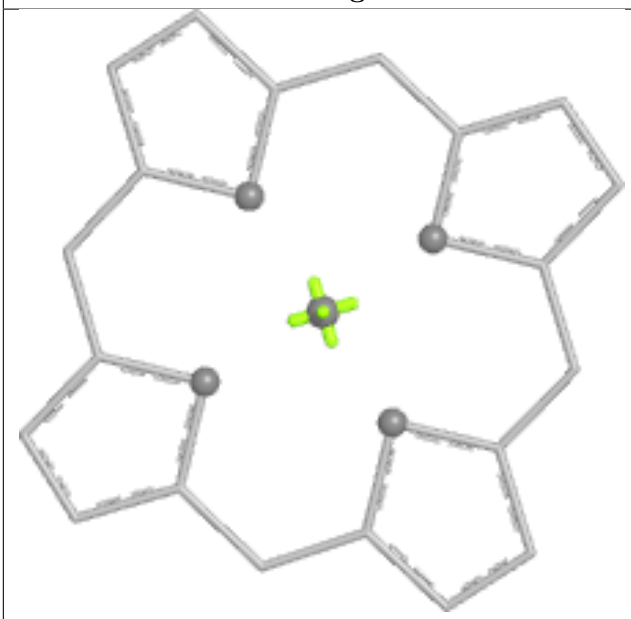
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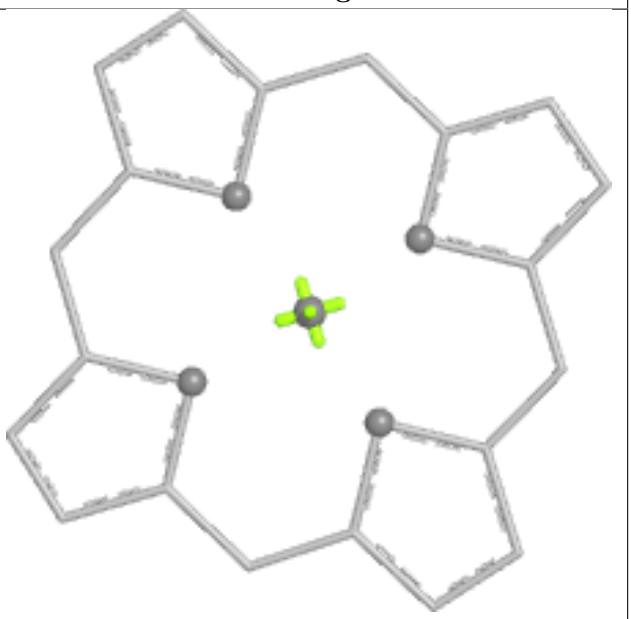
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Bond angles

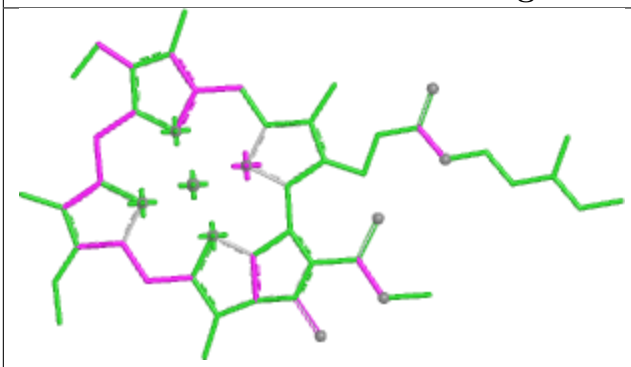


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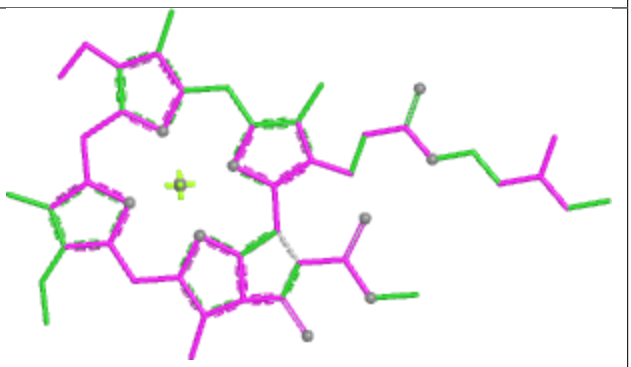


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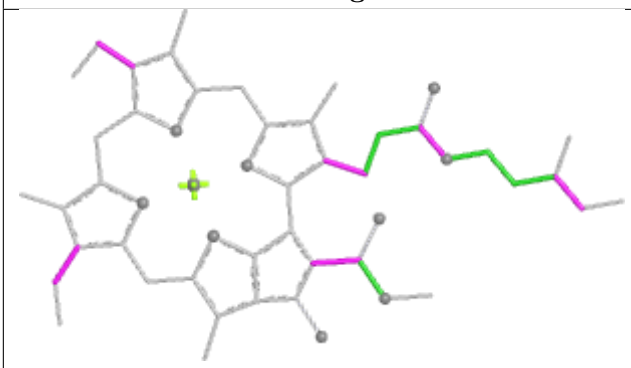
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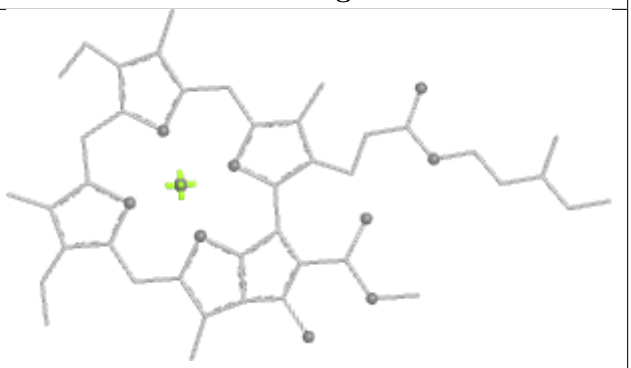
Bond lengths



Bond angles

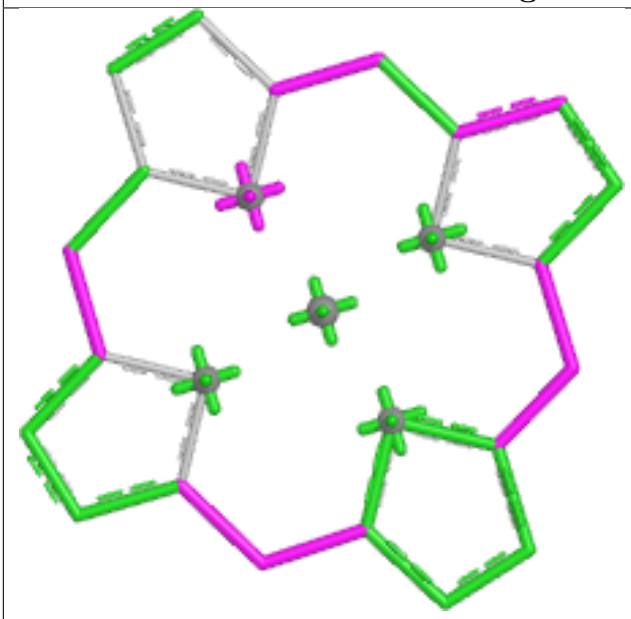


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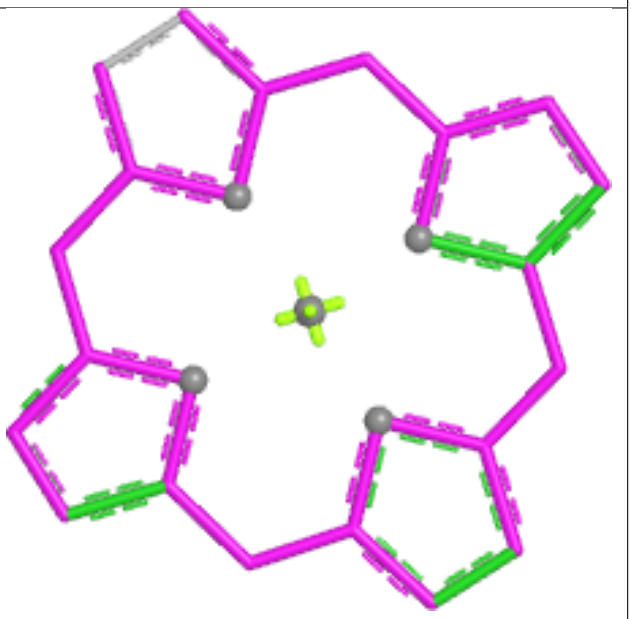


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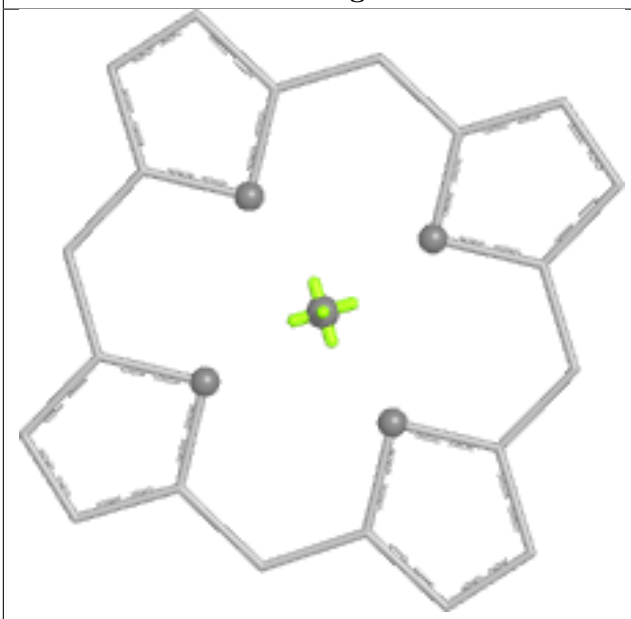
Ligand CLA 4 4010



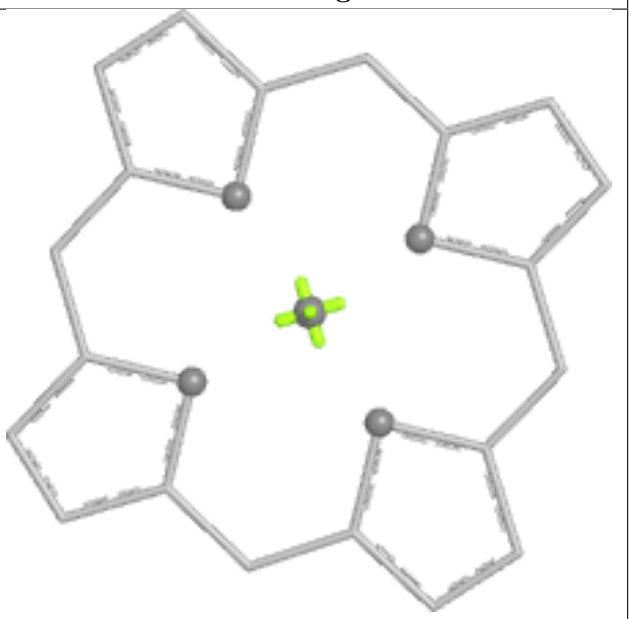
Bond lengths



Bond angles

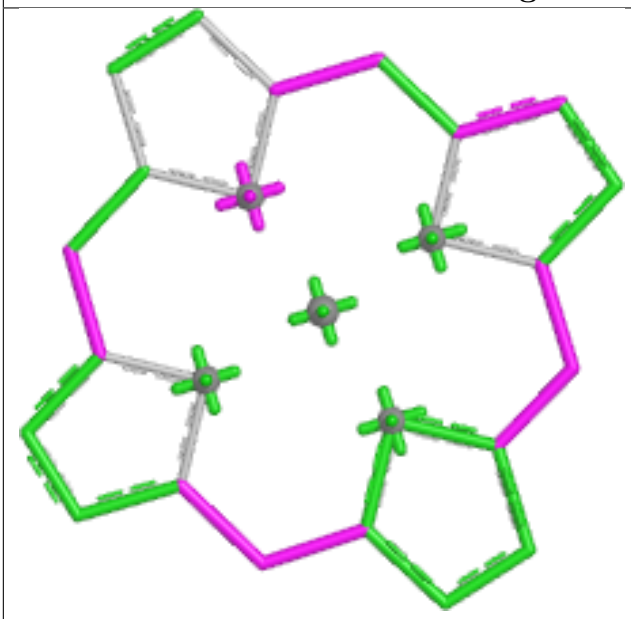


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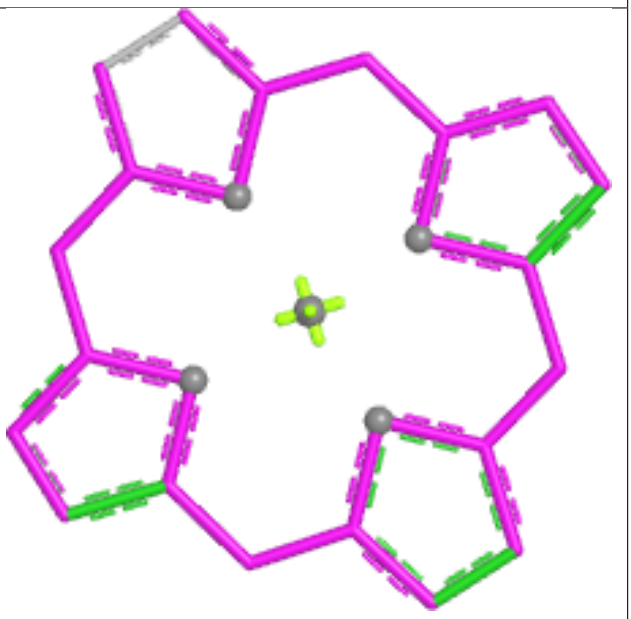


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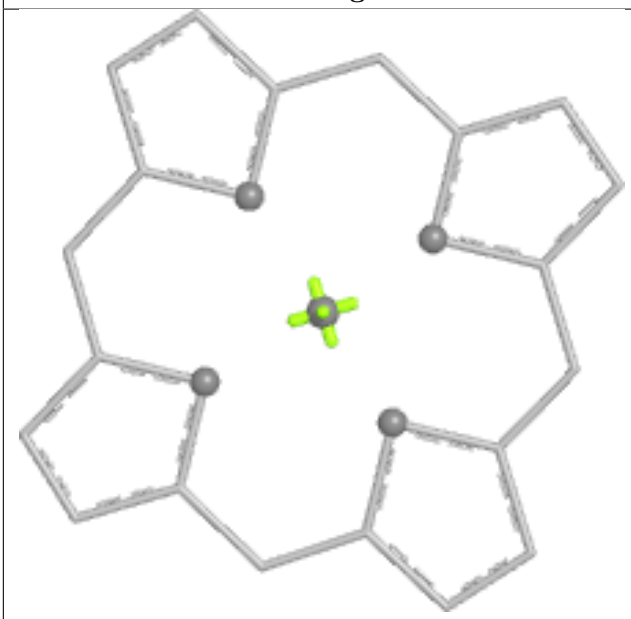
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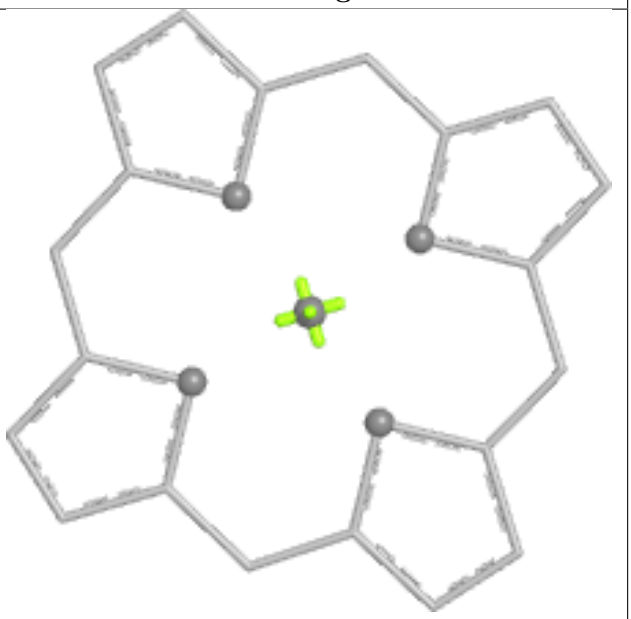
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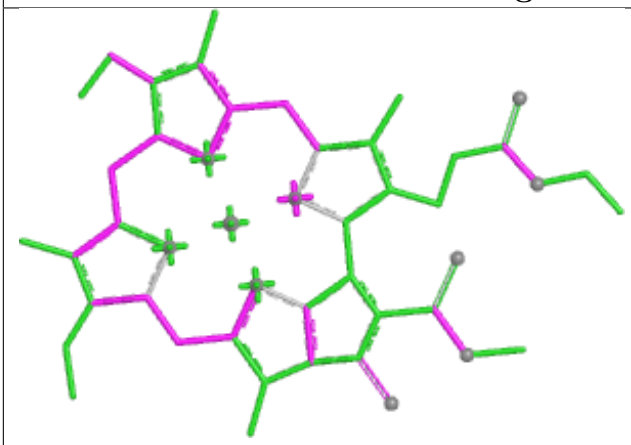


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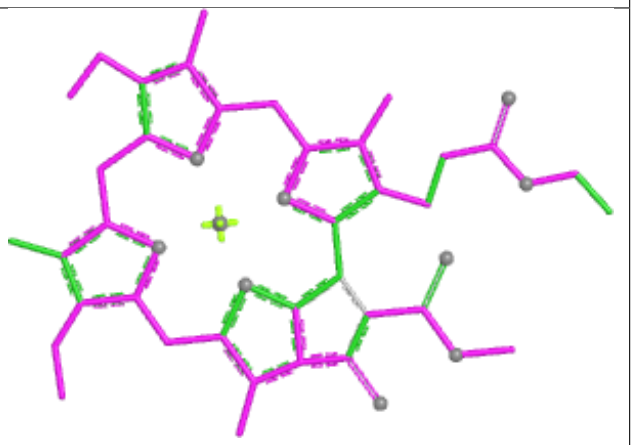


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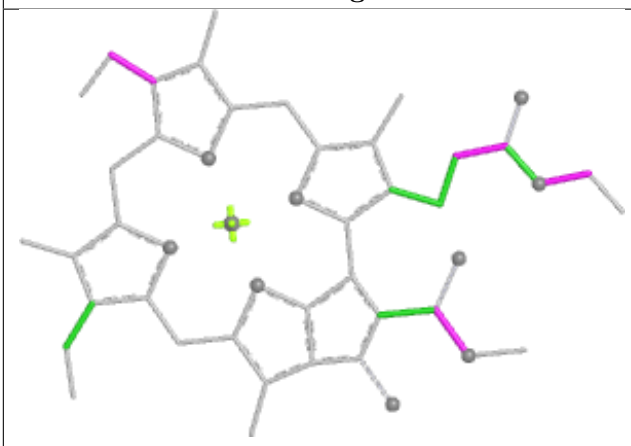
Ligand CLA B 9023



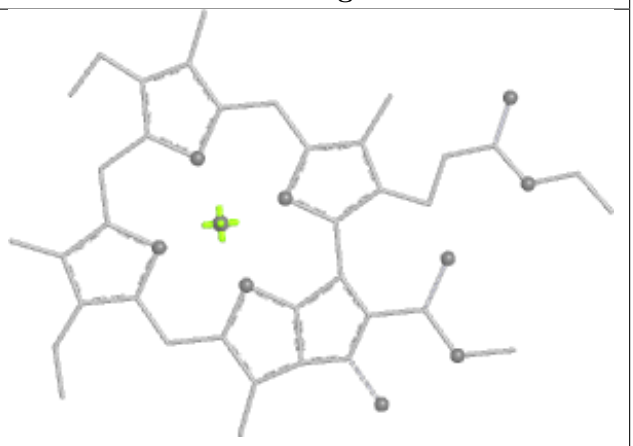
Bond lengths



Bond angles



Torsions

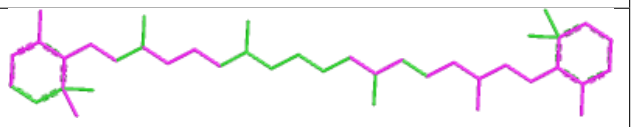


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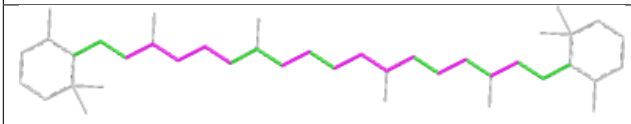
Ligand BCR A 6011



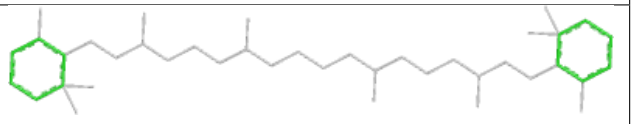
Bond lengths



Bond angles

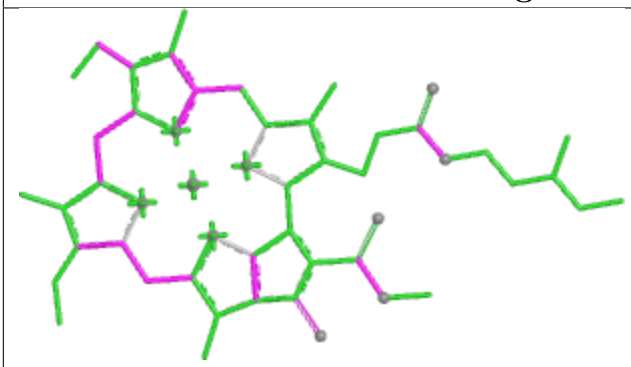


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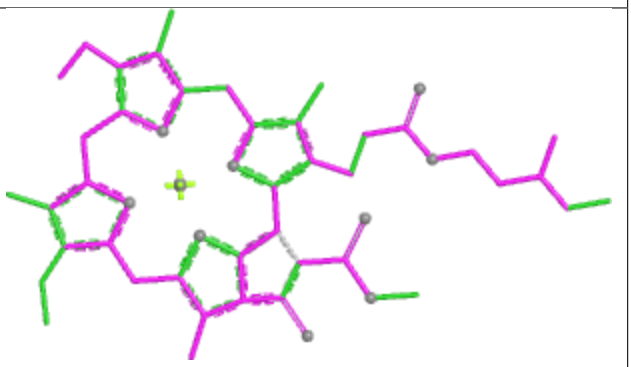


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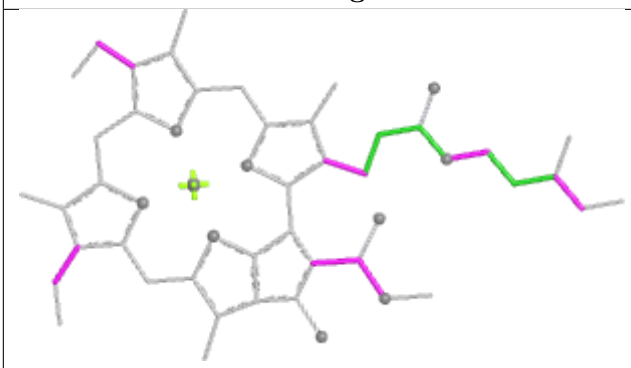
Ligand CLA B 1219



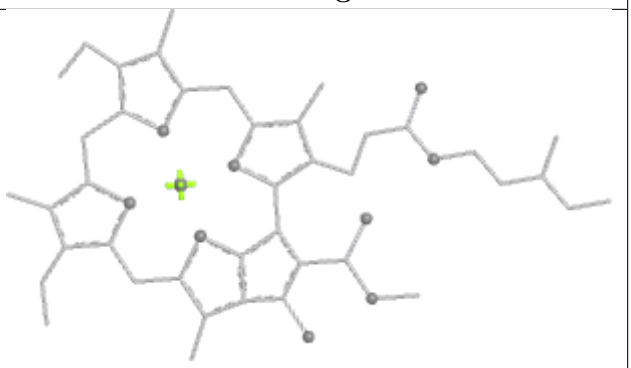
Bond lengths



Bond angles

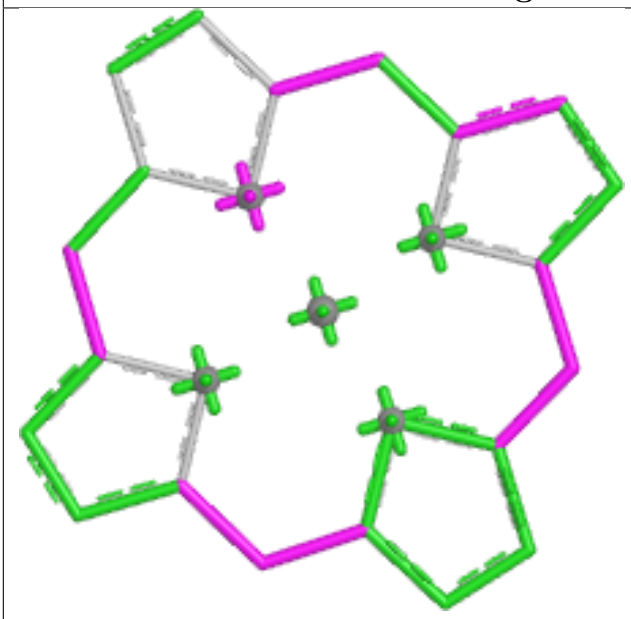


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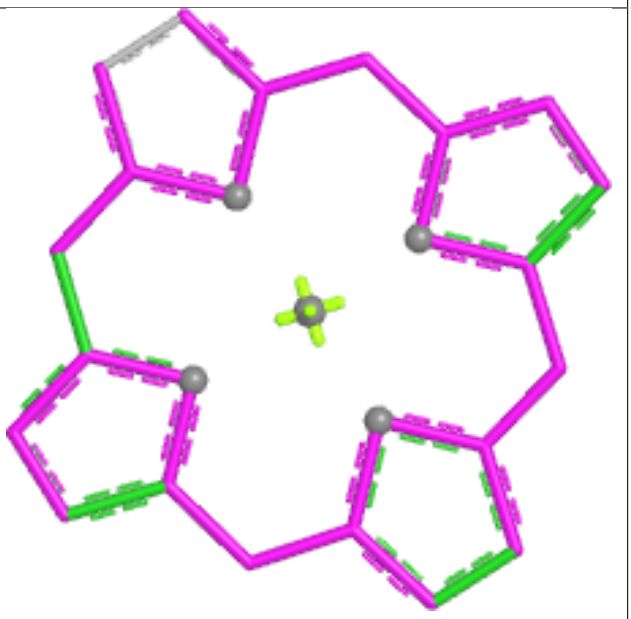


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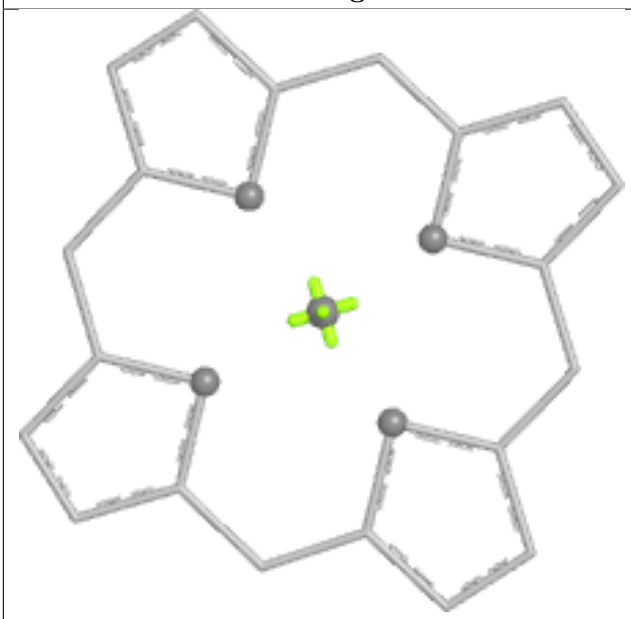
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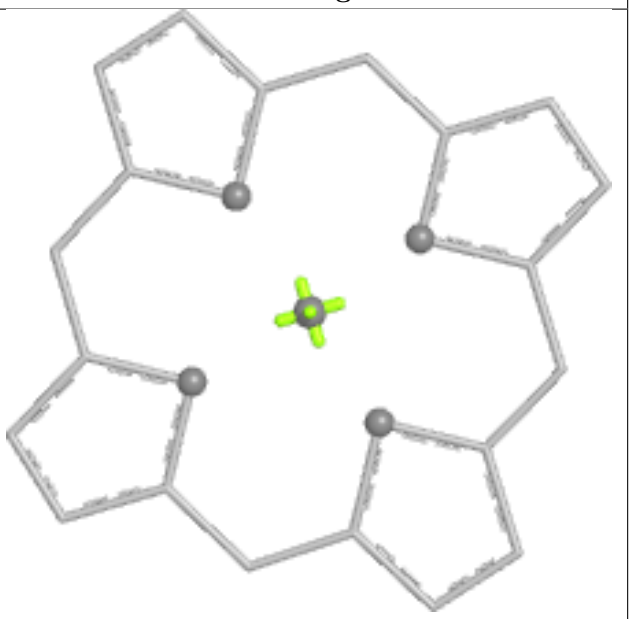
Bond lengths



Bond angles

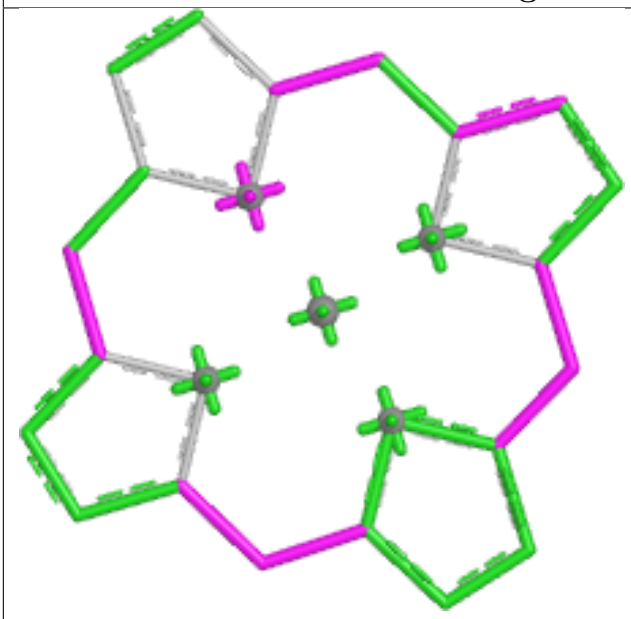


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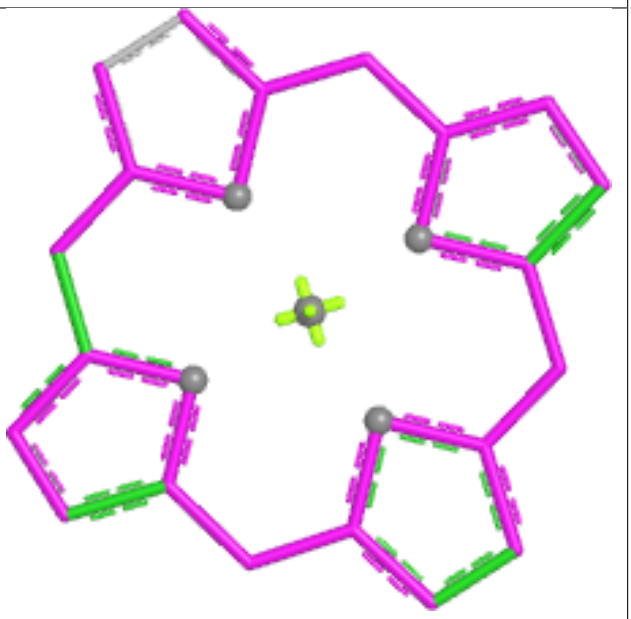


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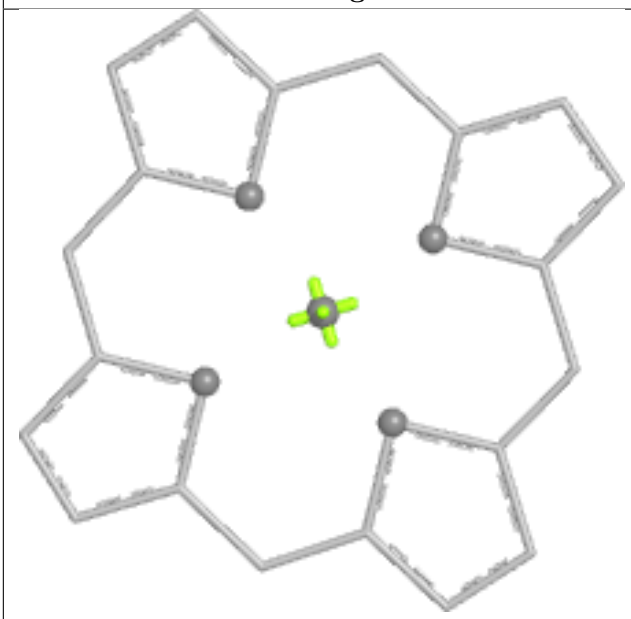
Ligand CLA 4 4008



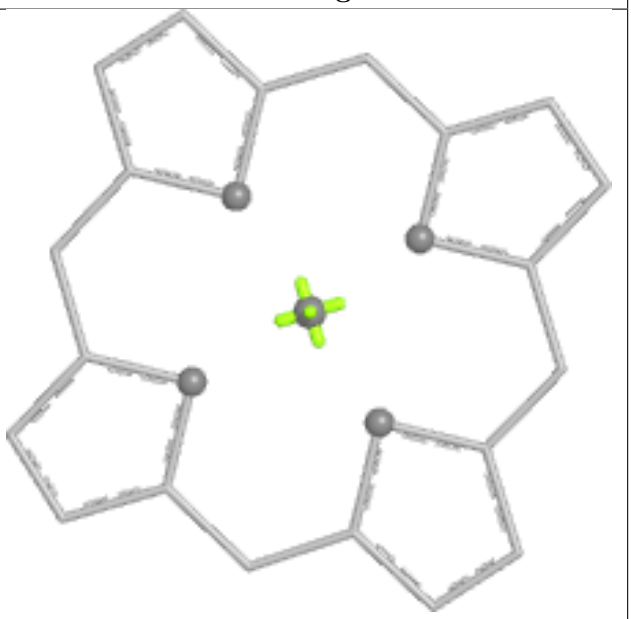
Bond lengths



Bond angles

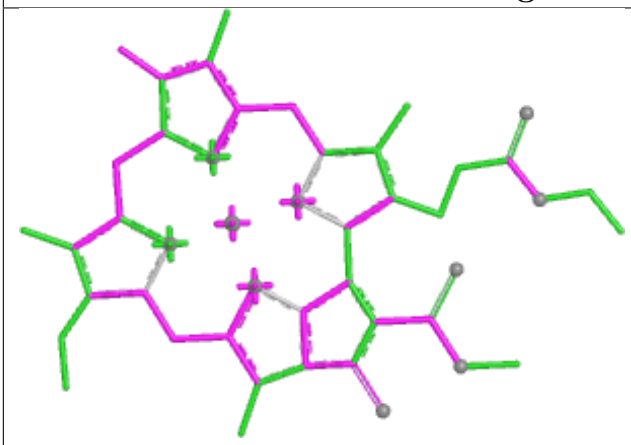


Torsions

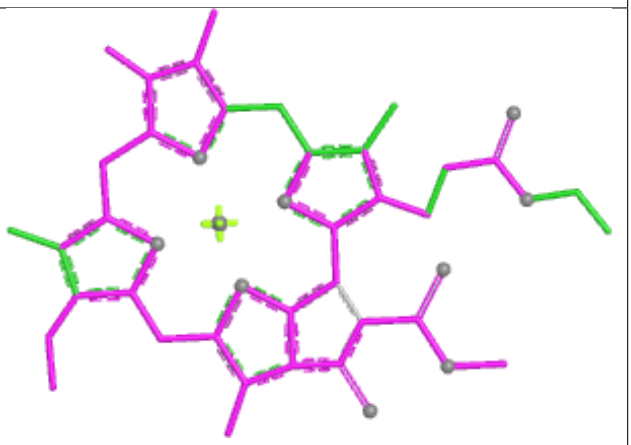


Rings

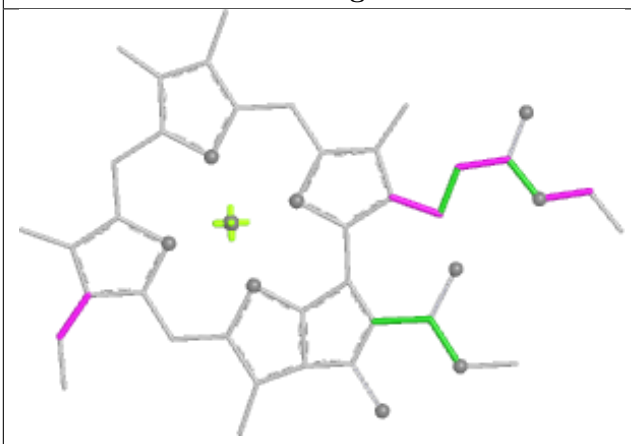
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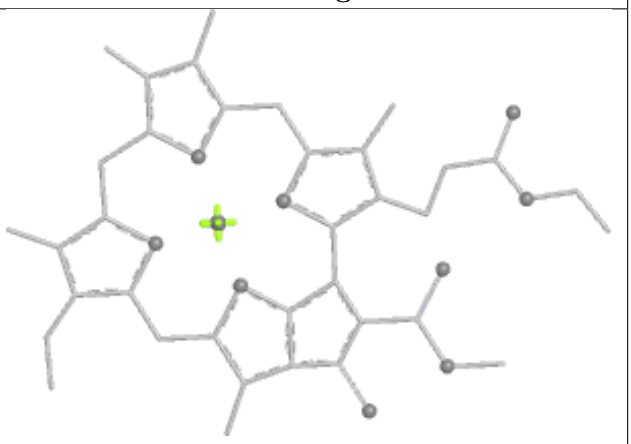
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Bond angles

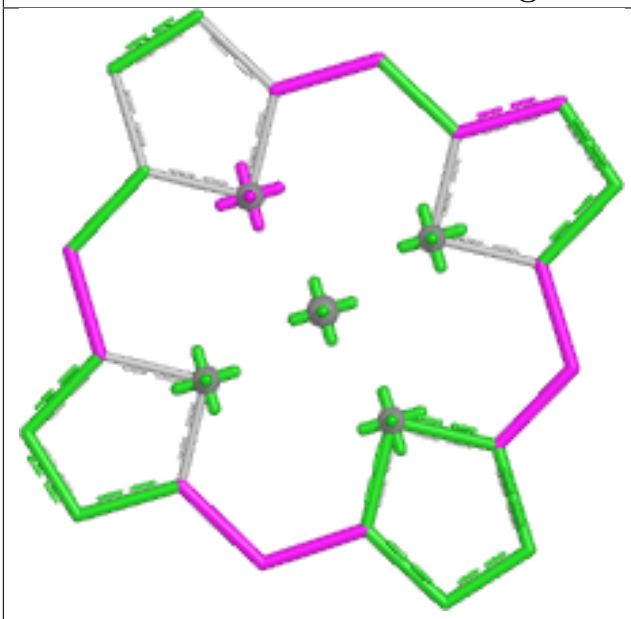


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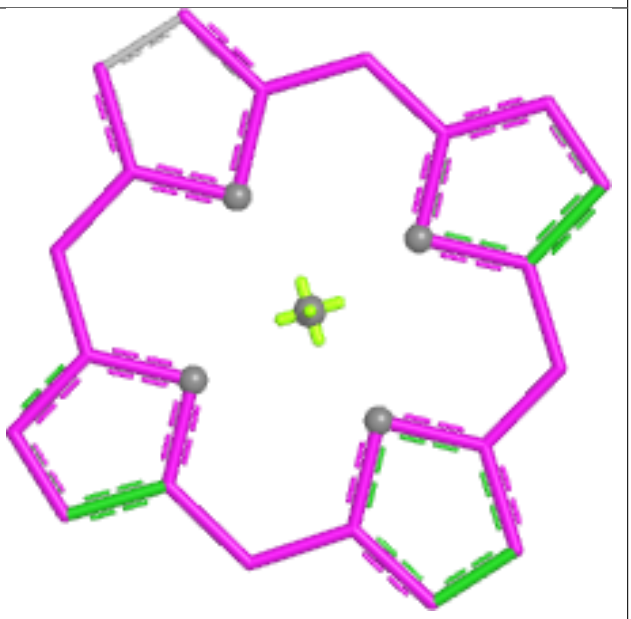


Rings

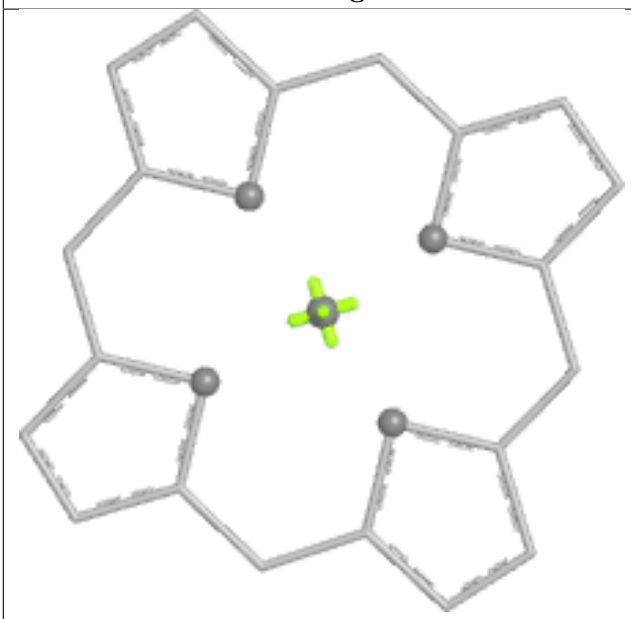
Ligand CLA 2 2011



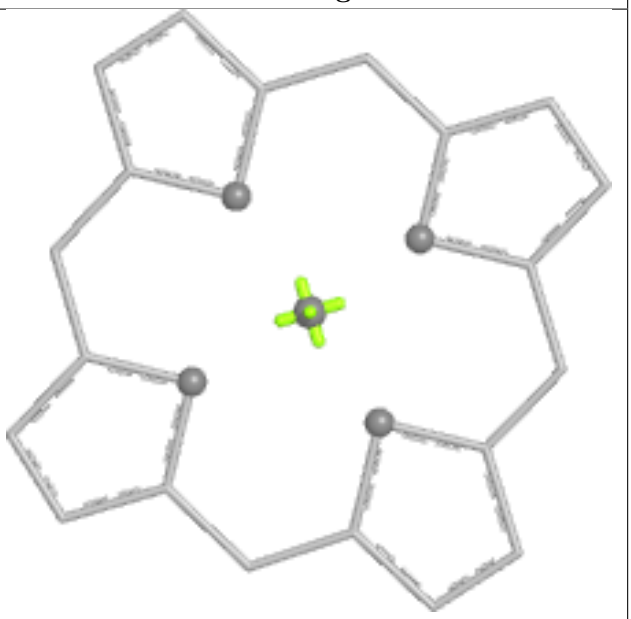
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Bond angles

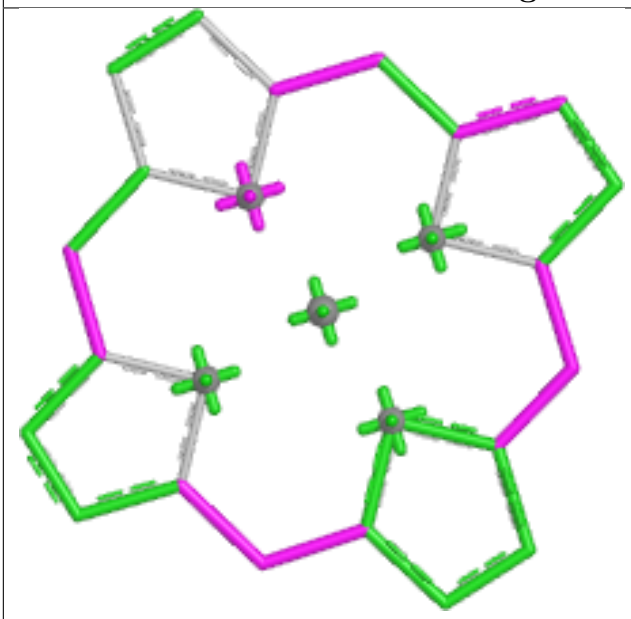


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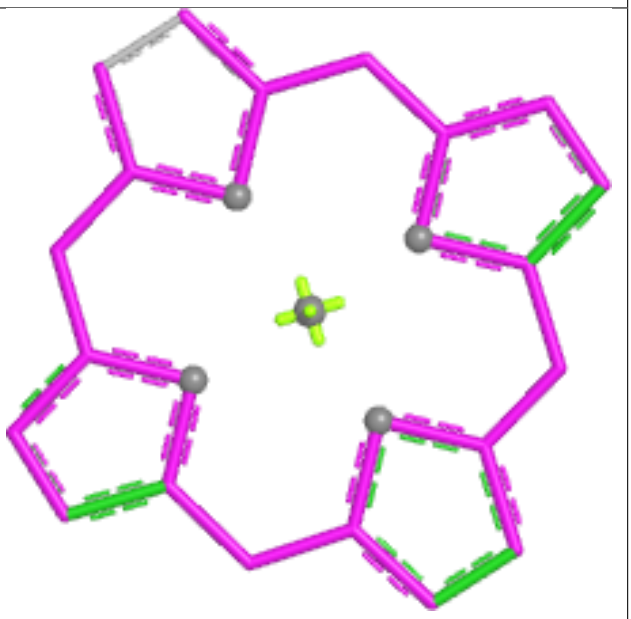


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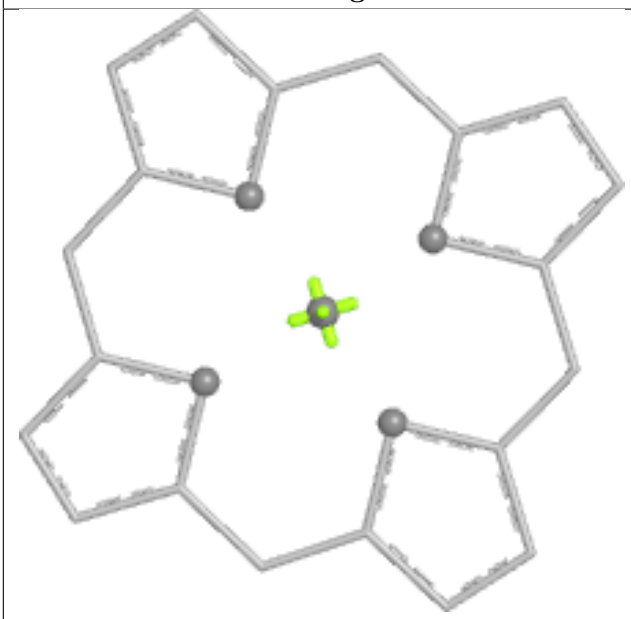
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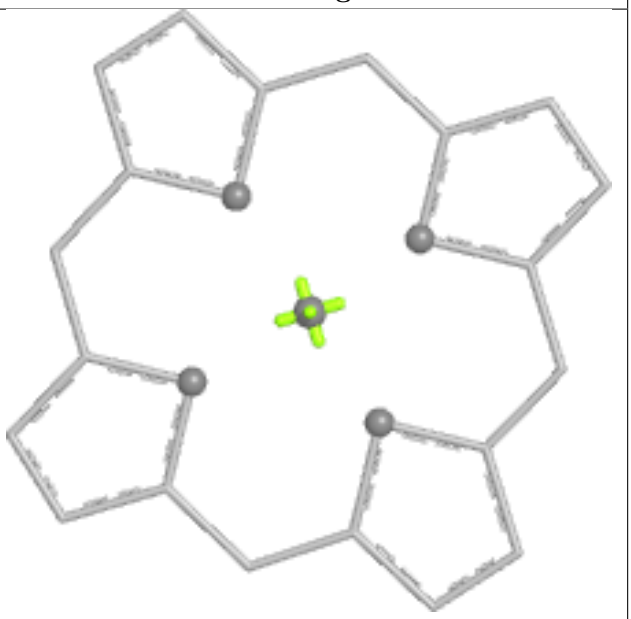
Bond lengths



Bond angles

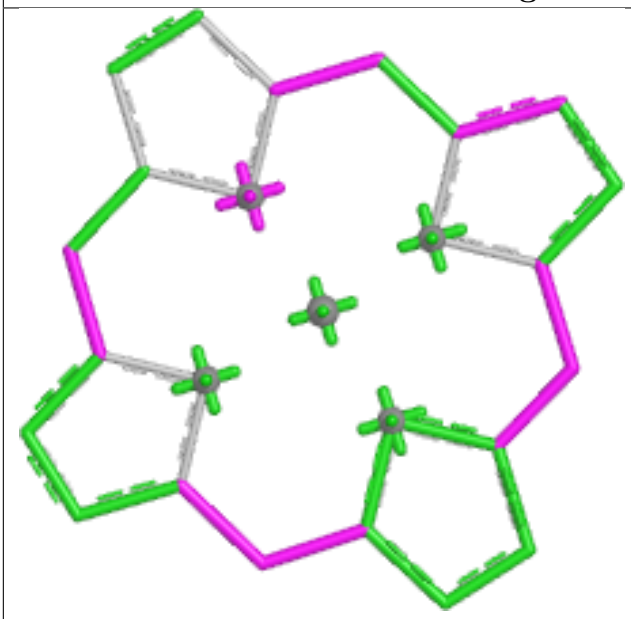


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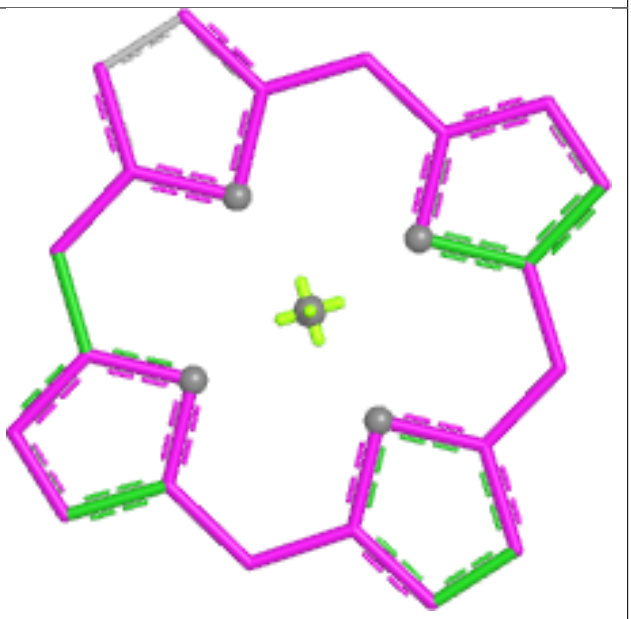


Rings

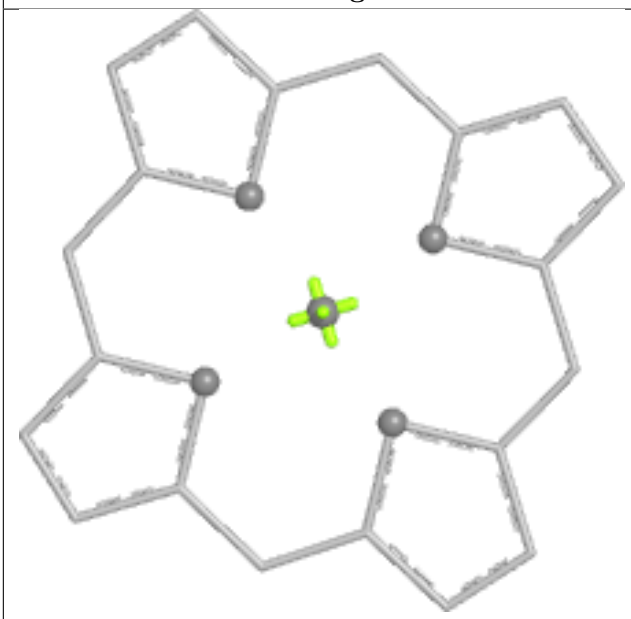
Ligand CLA 1 1003



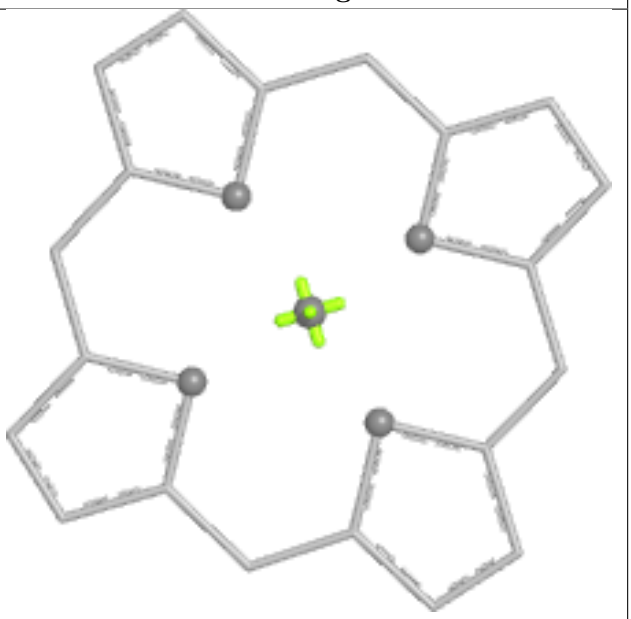
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Bond angles

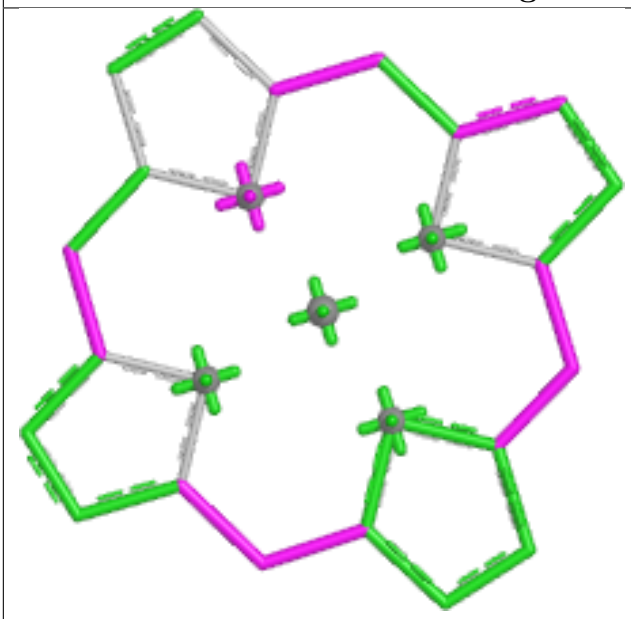


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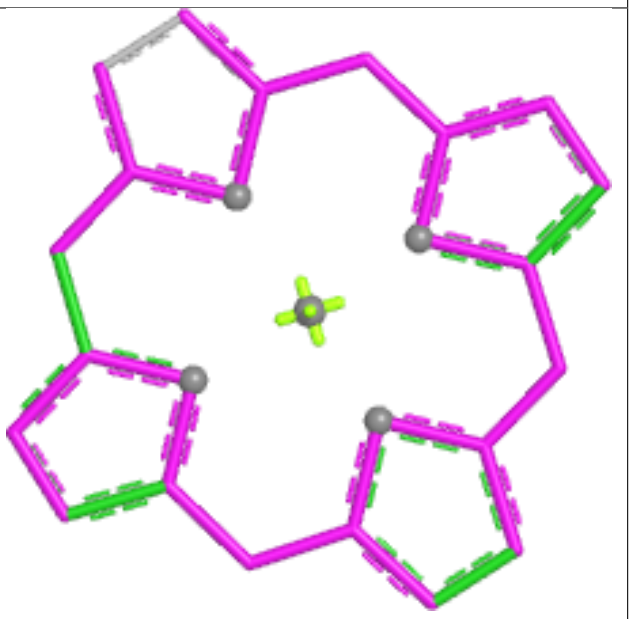


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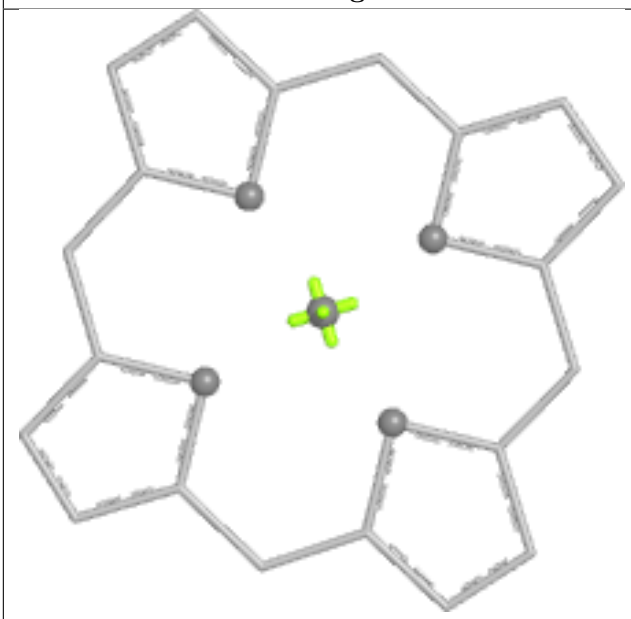
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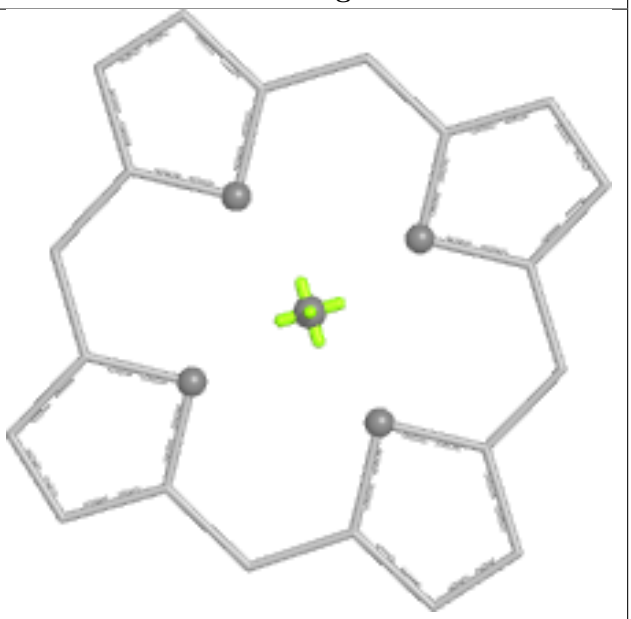
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Bond angles

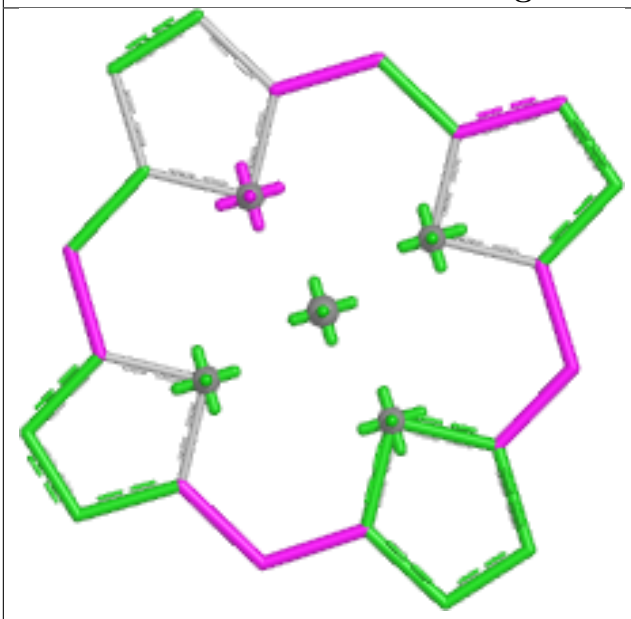


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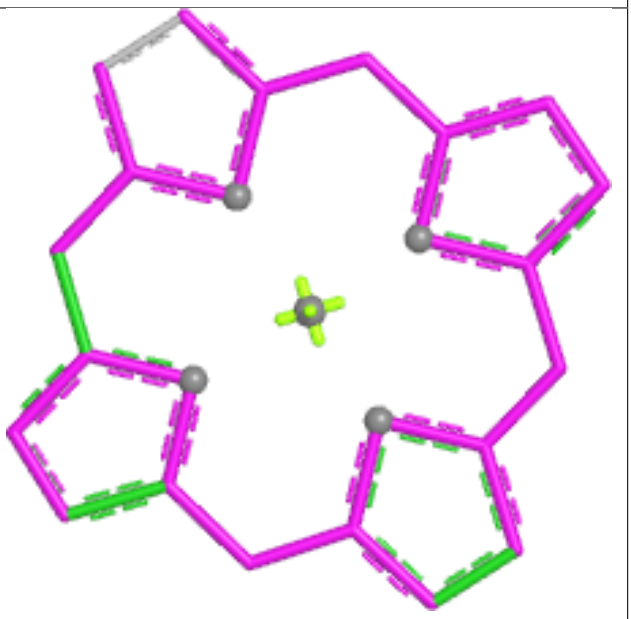


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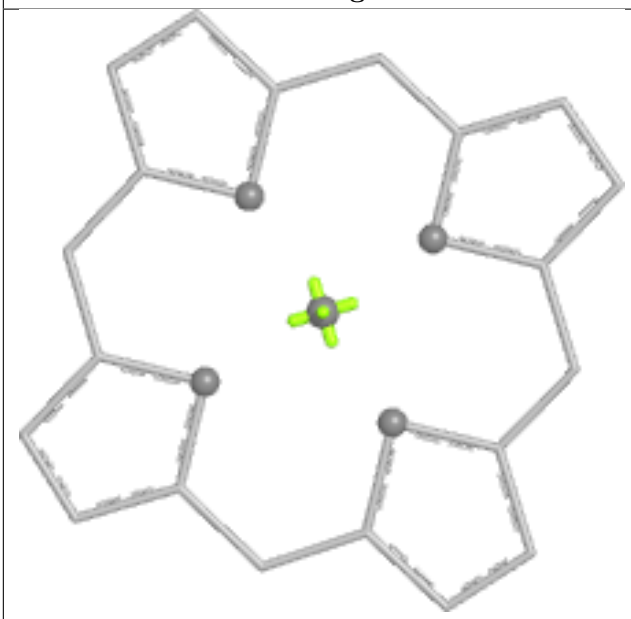
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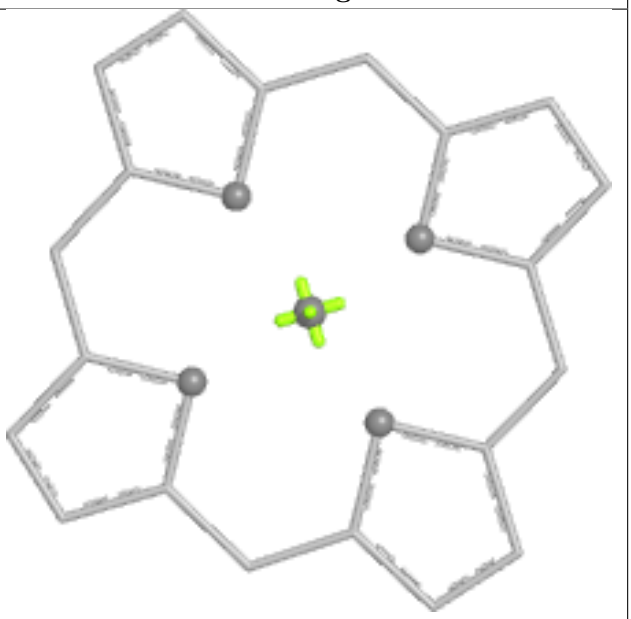
Bond lengths



Bond angles

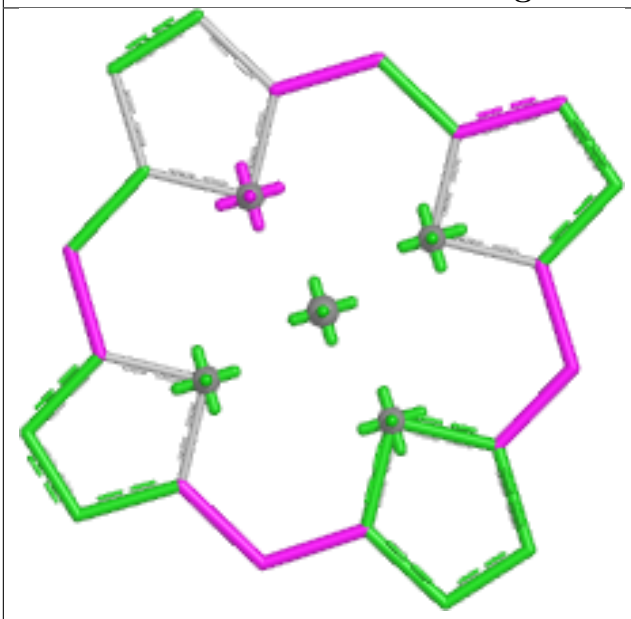


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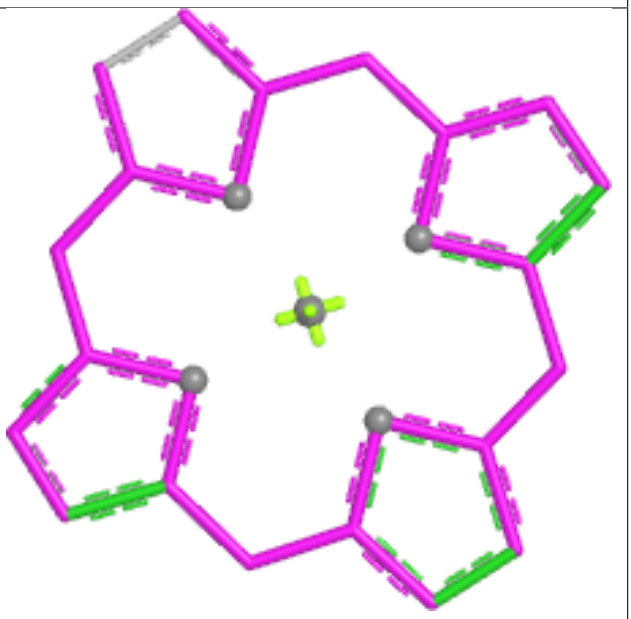


Rings

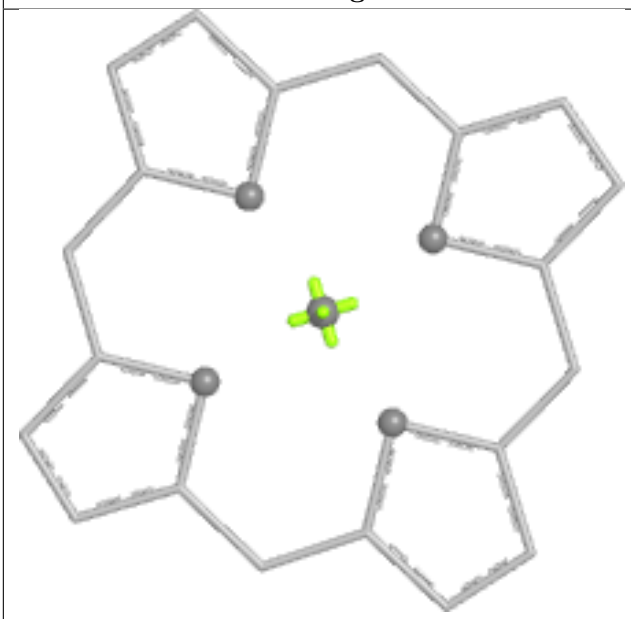
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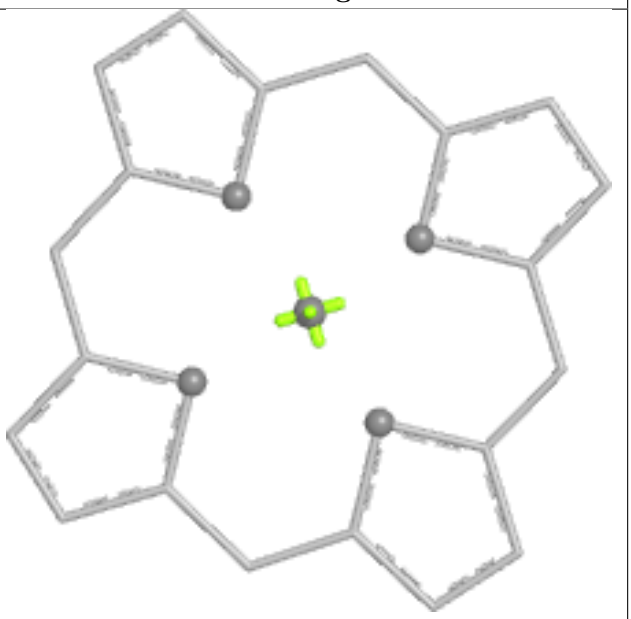
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Bond angles

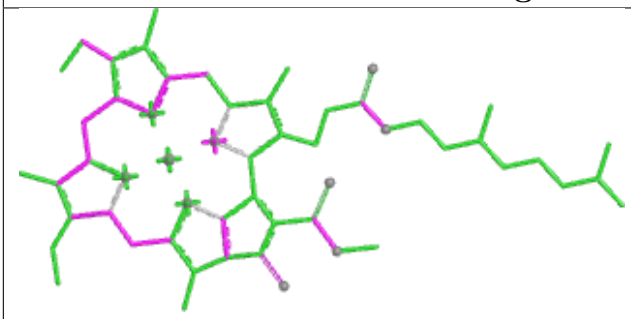


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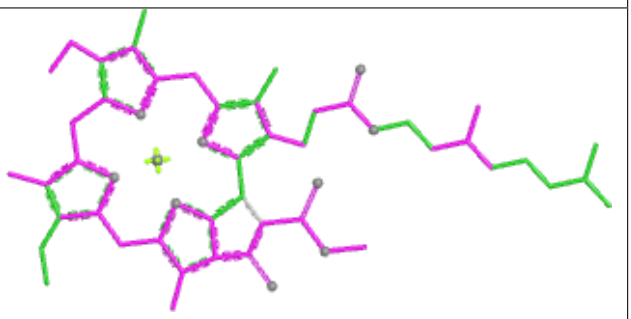


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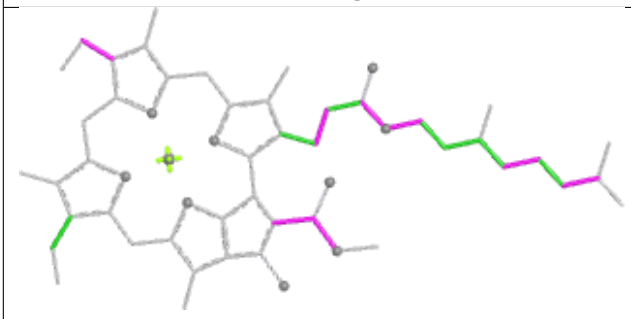
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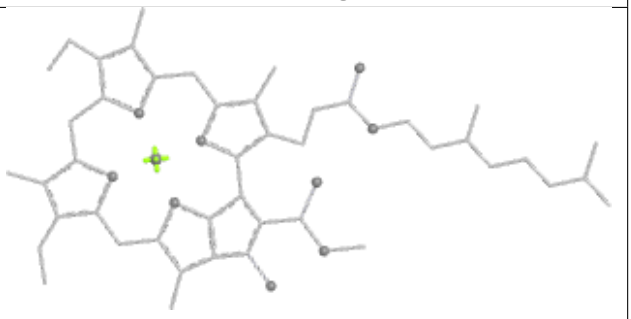
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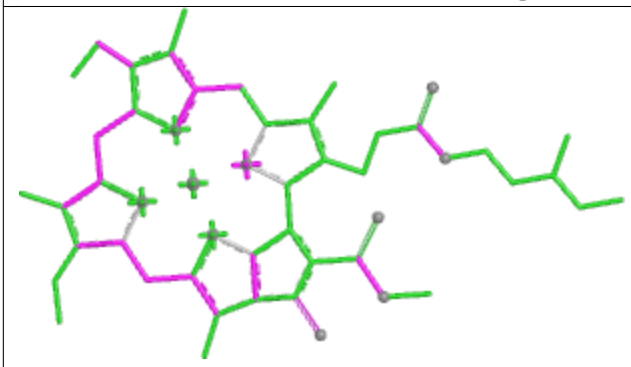


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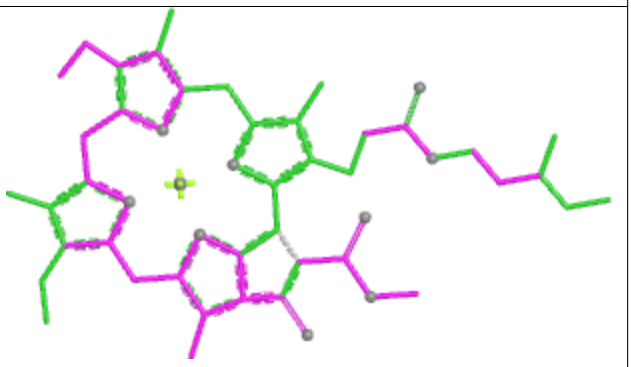


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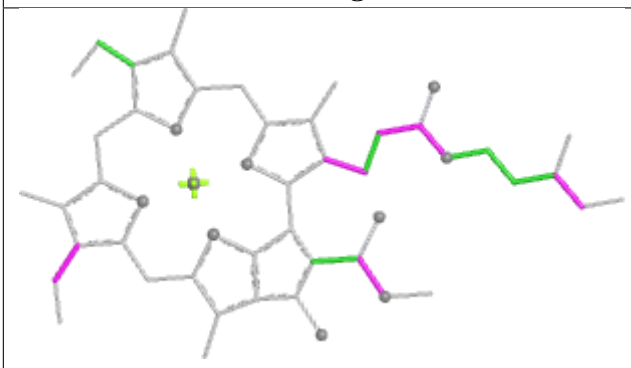
Ligand CLA G 1233



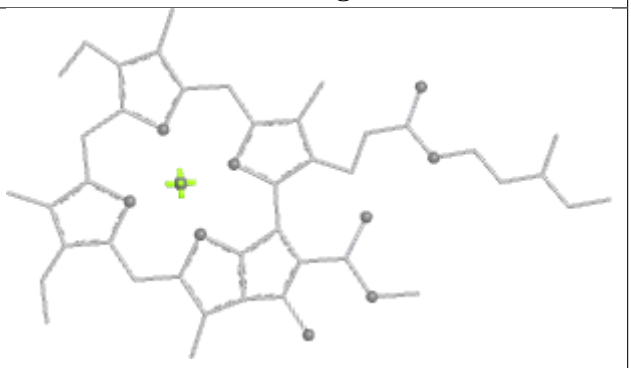
Bond lengths



Bond angles

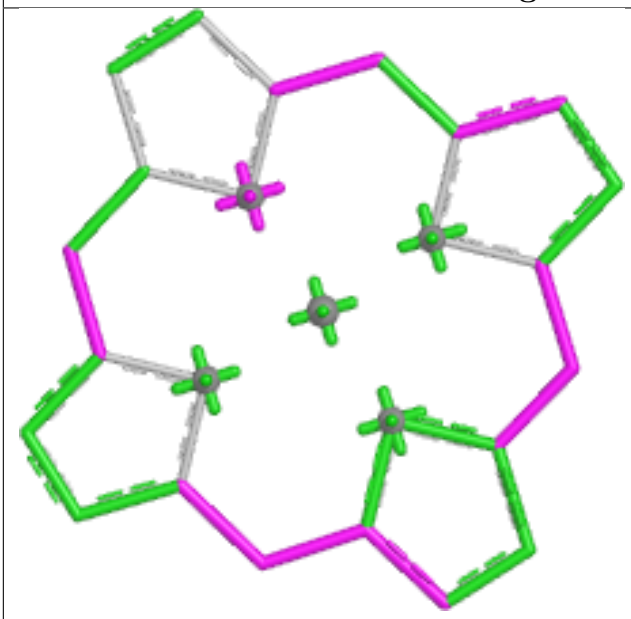


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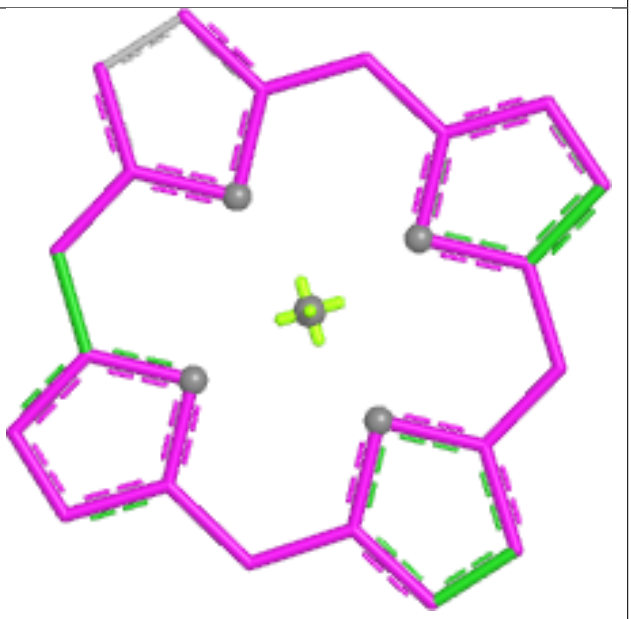


Rings

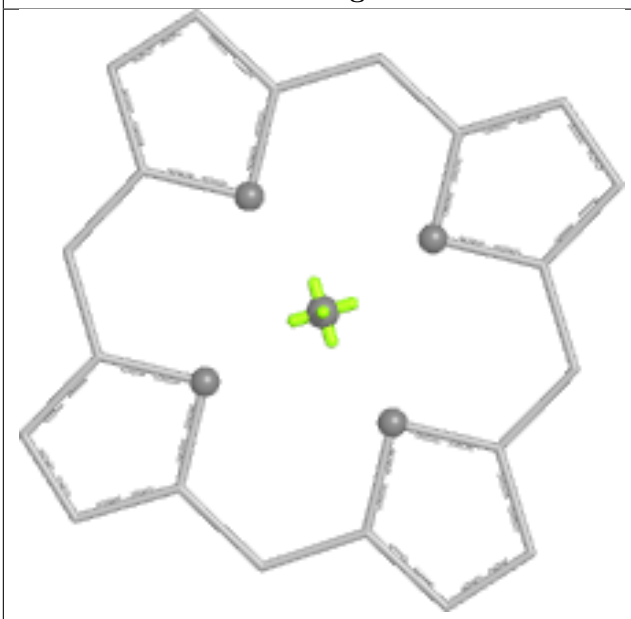
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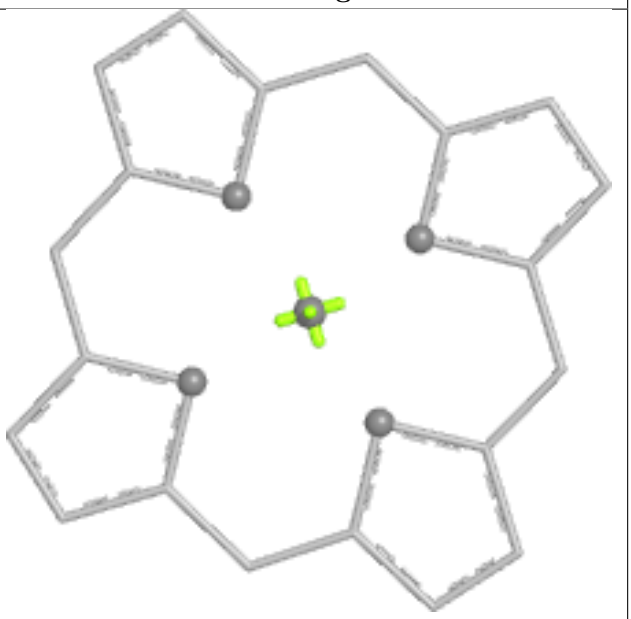
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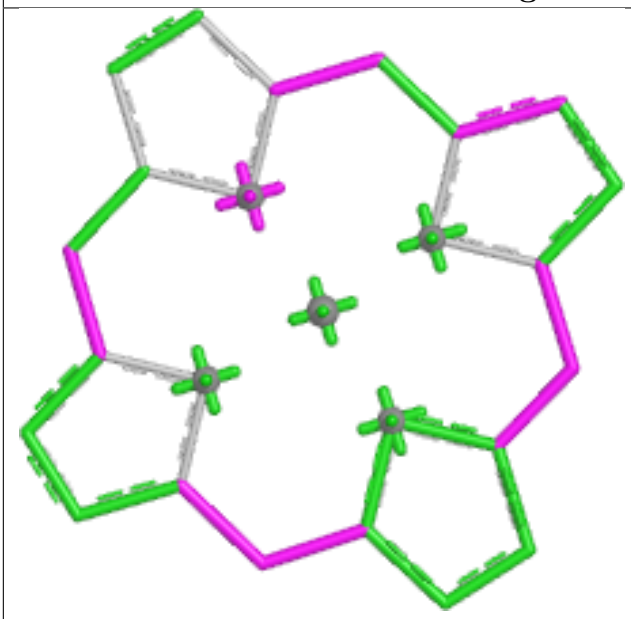


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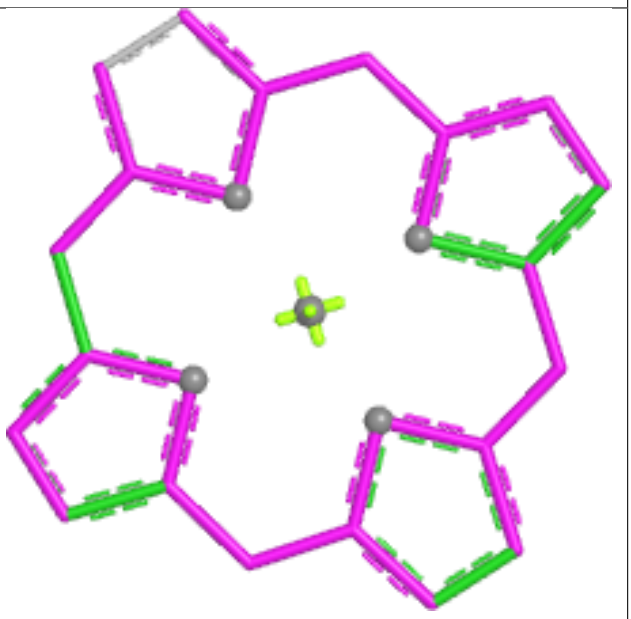


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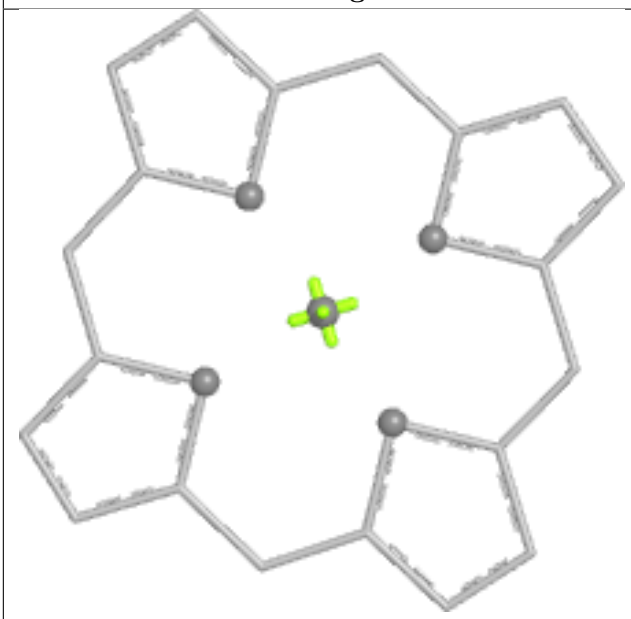
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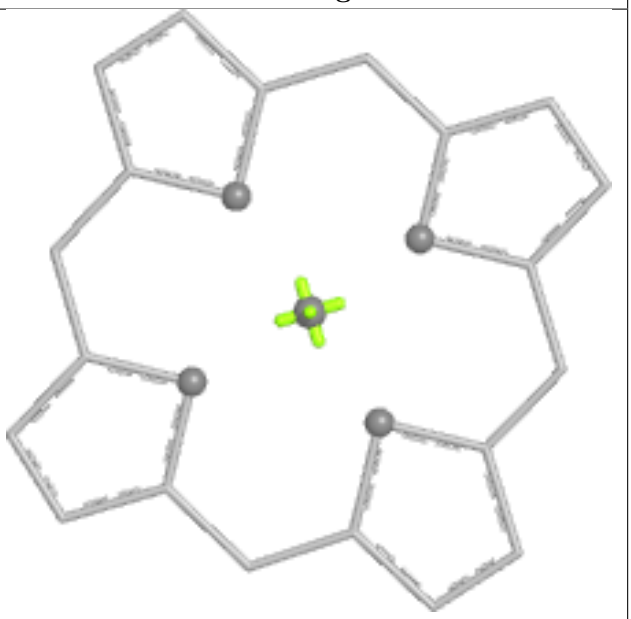
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Bond angles

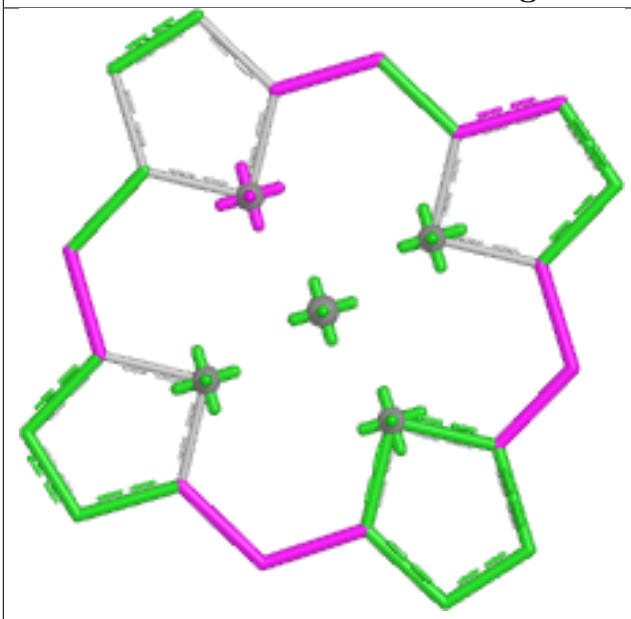


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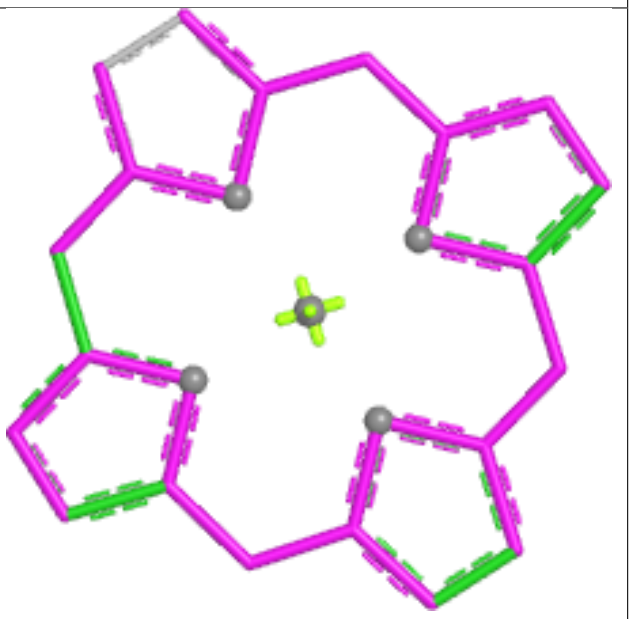


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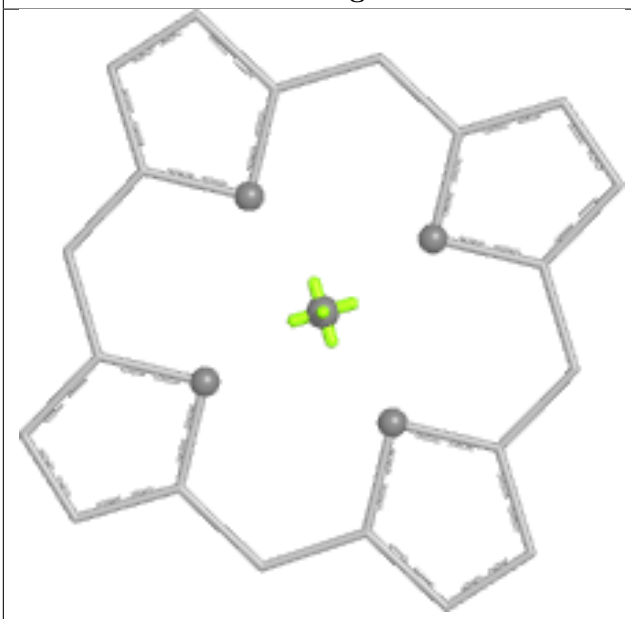
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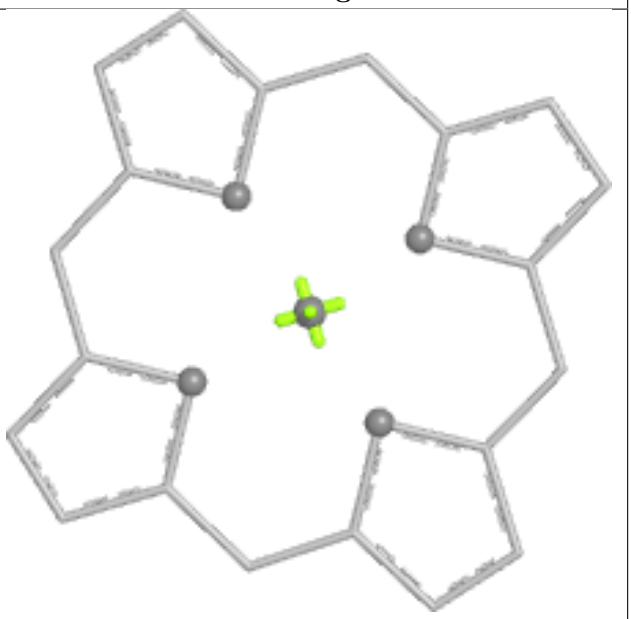
Bond lengths



Bond angles

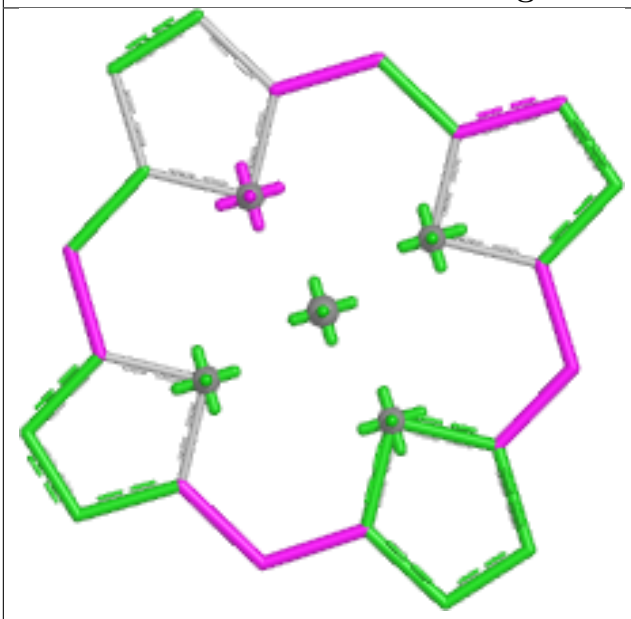


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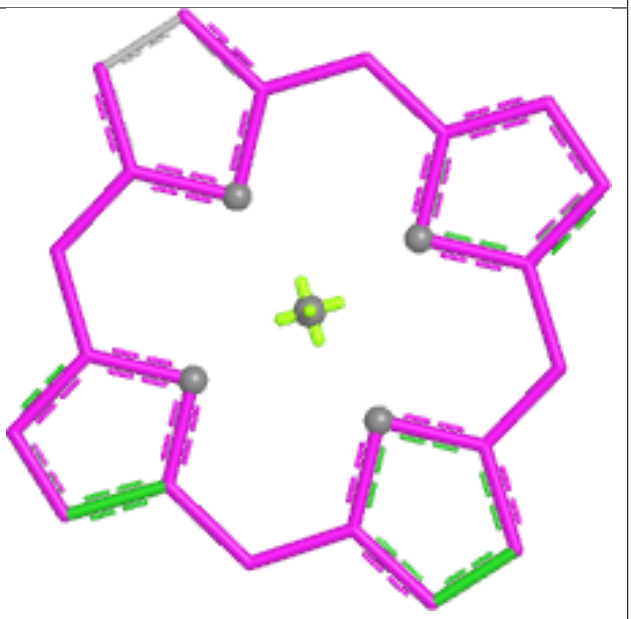


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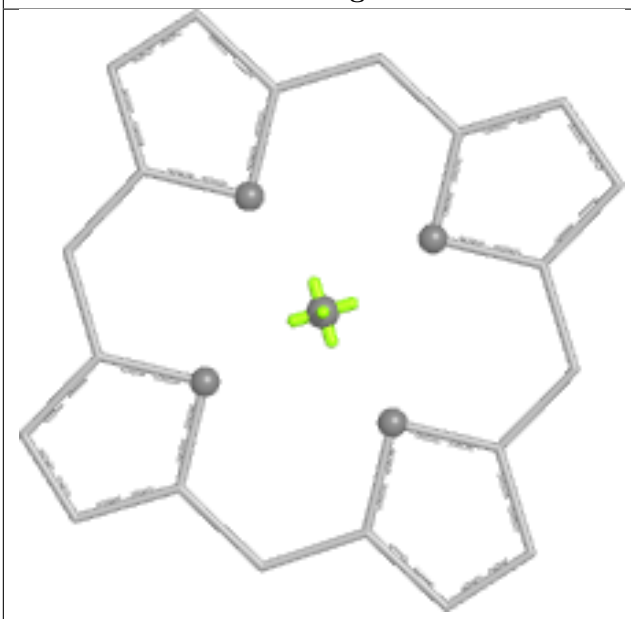
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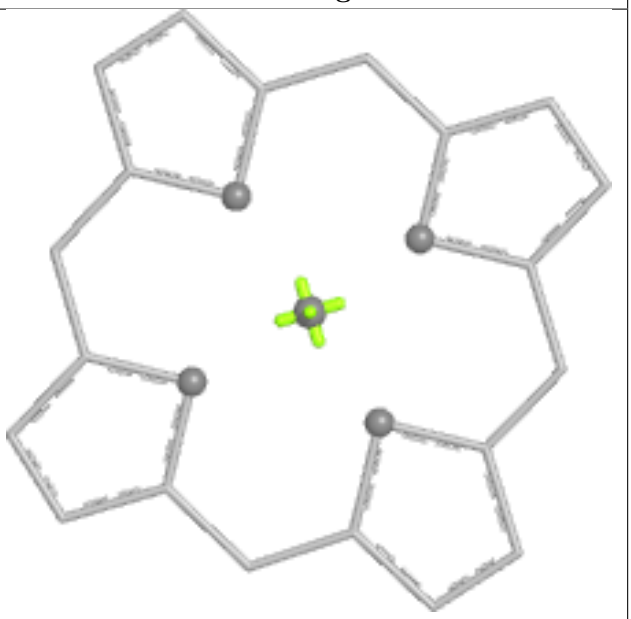
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Bond angles

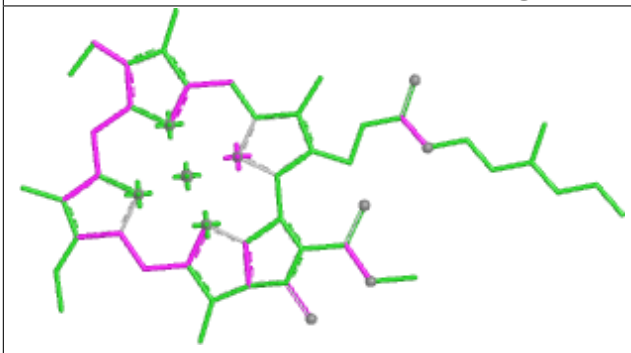


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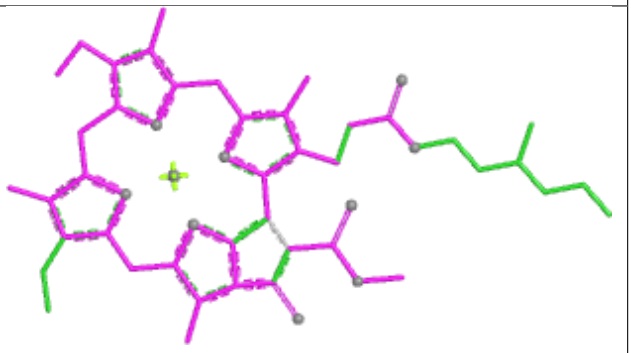


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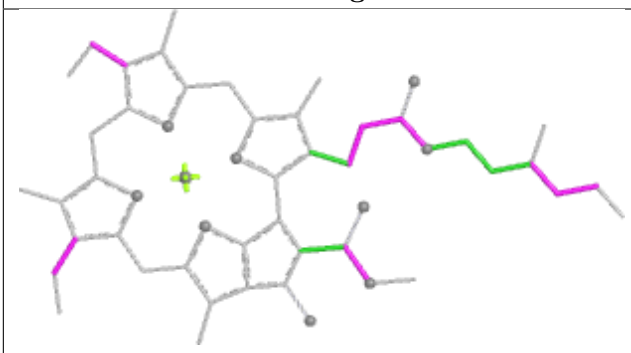
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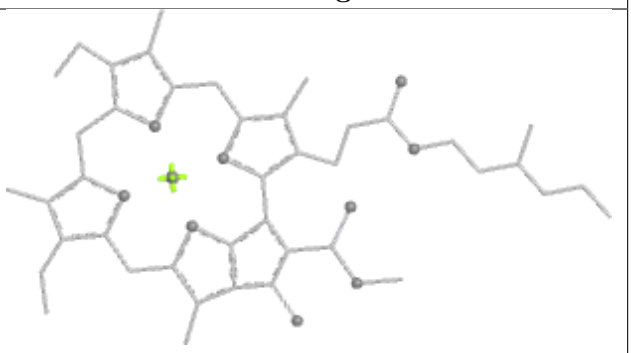
Bond lengths



Bond angles

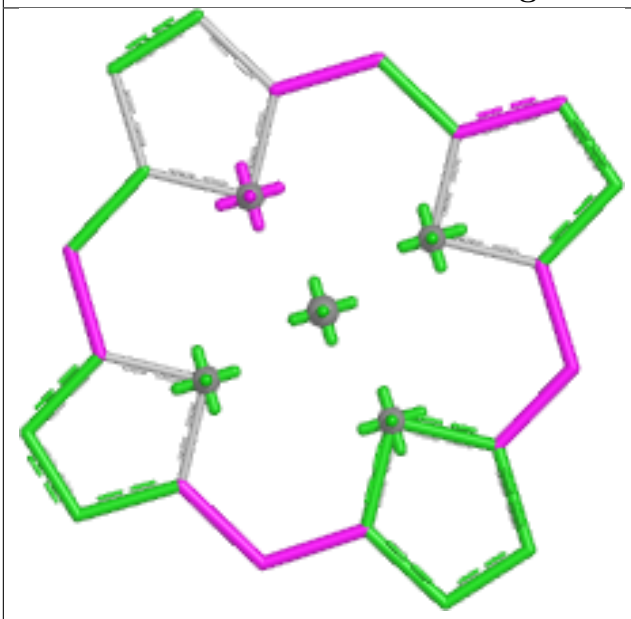


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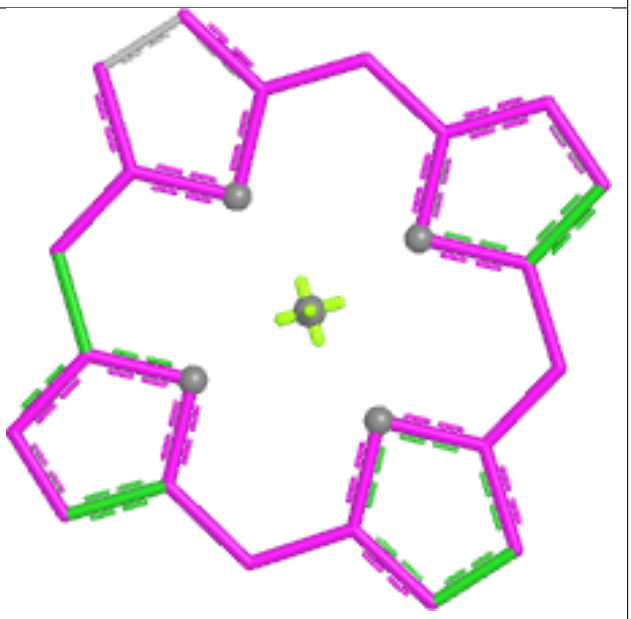


Rings

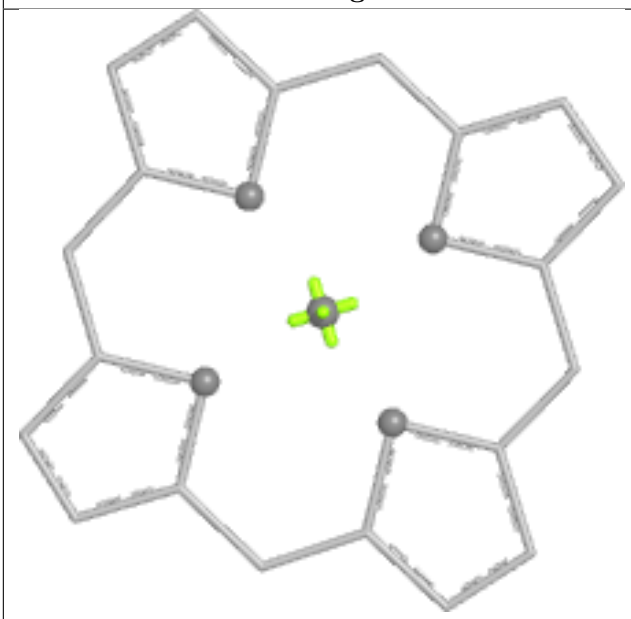
Ligand CLA 3 3002



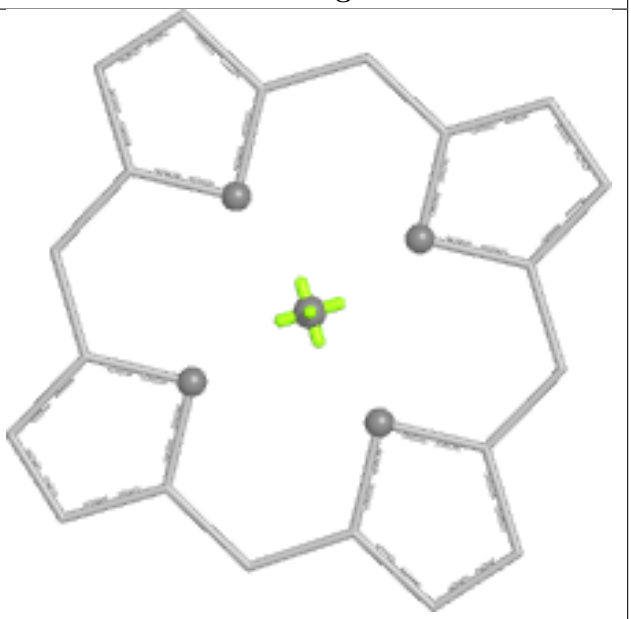
Bond lengths



Bond angles

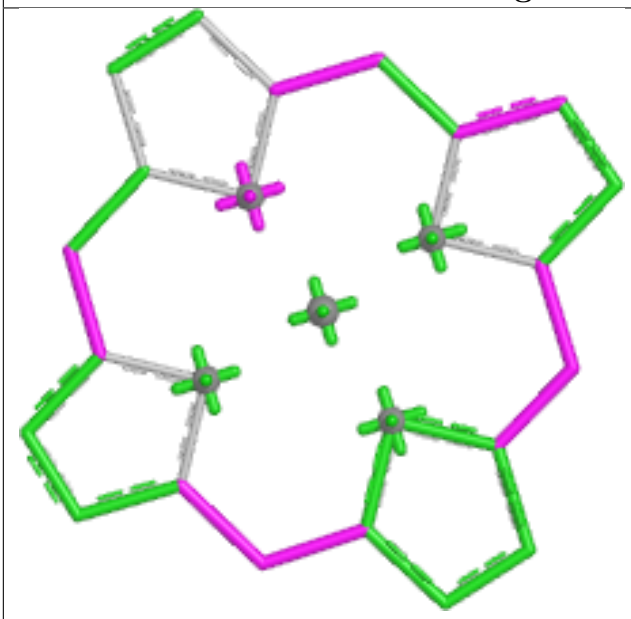


Torsions

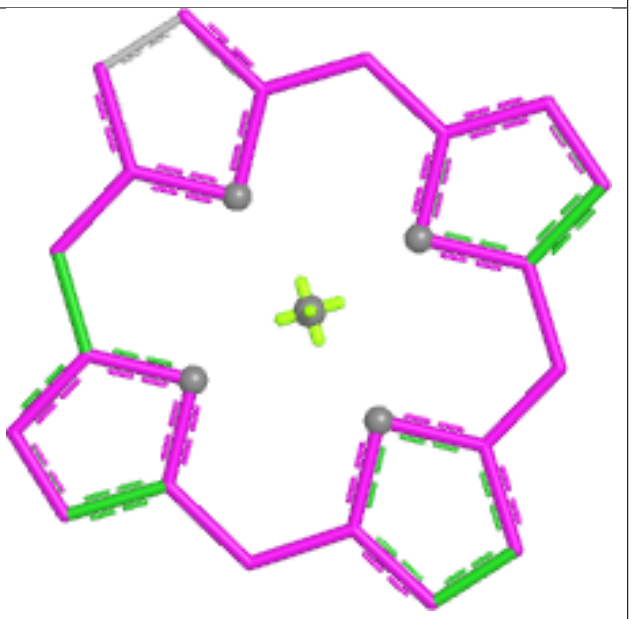


Rings

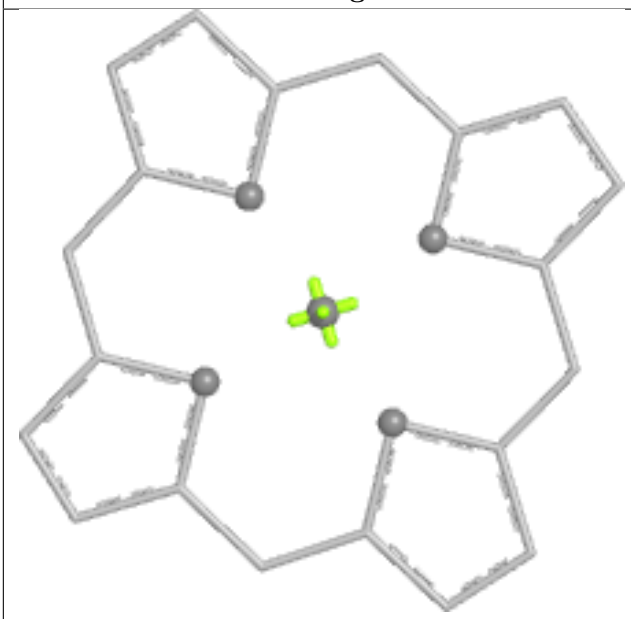
Ligand CLA A 1146



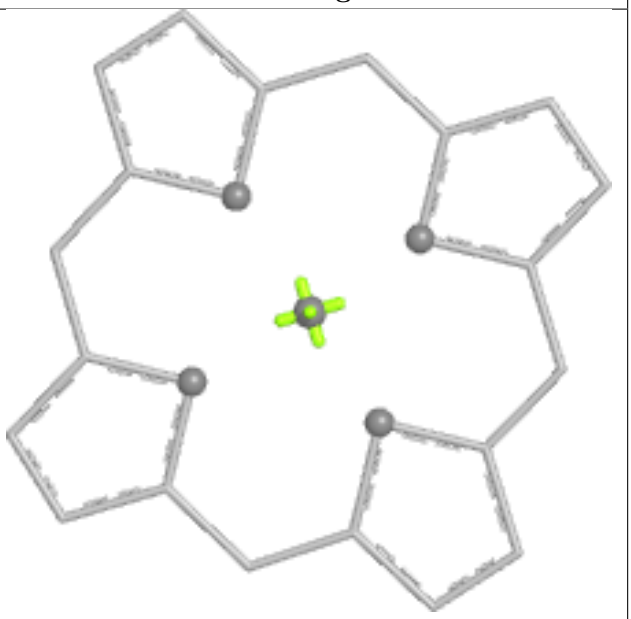
Bond lengths



Bond angles

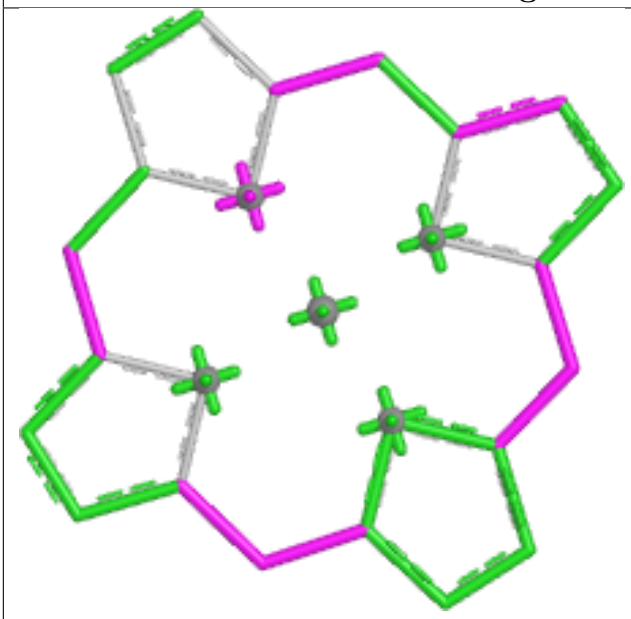


Torsions

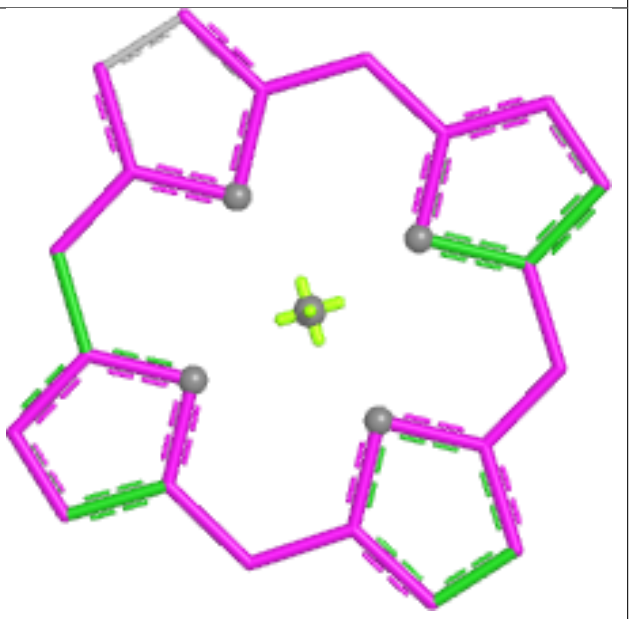


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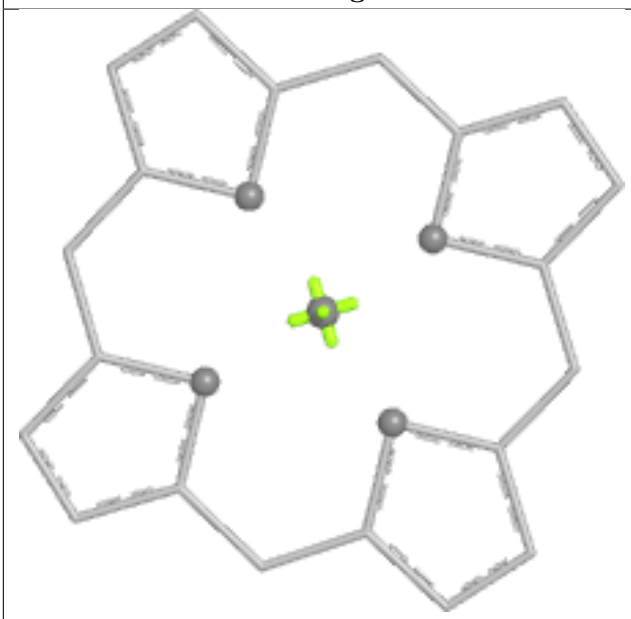
Ligand CLA 1 1002



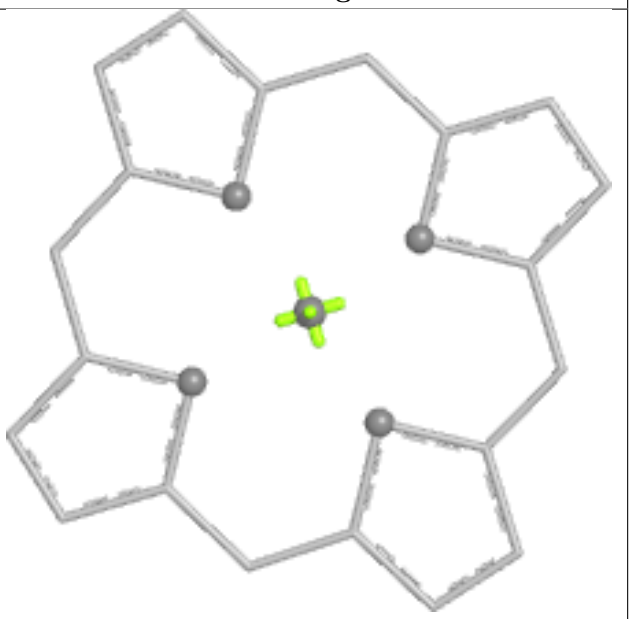
Bond lengths



Bond angles

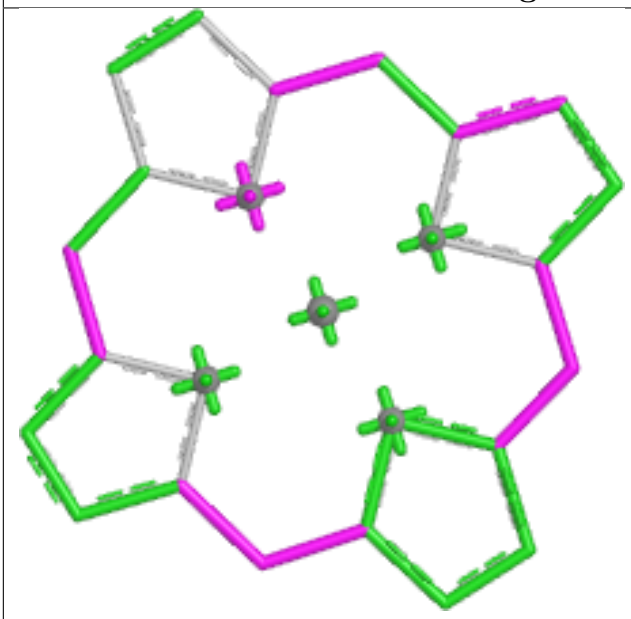


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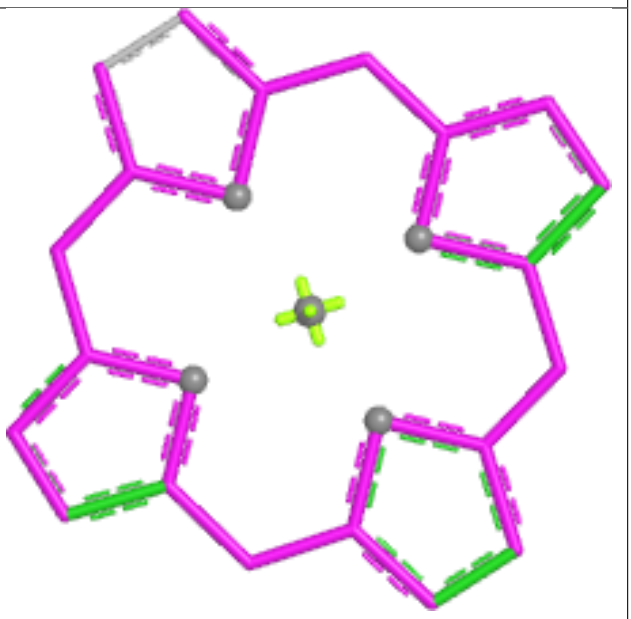


Rings

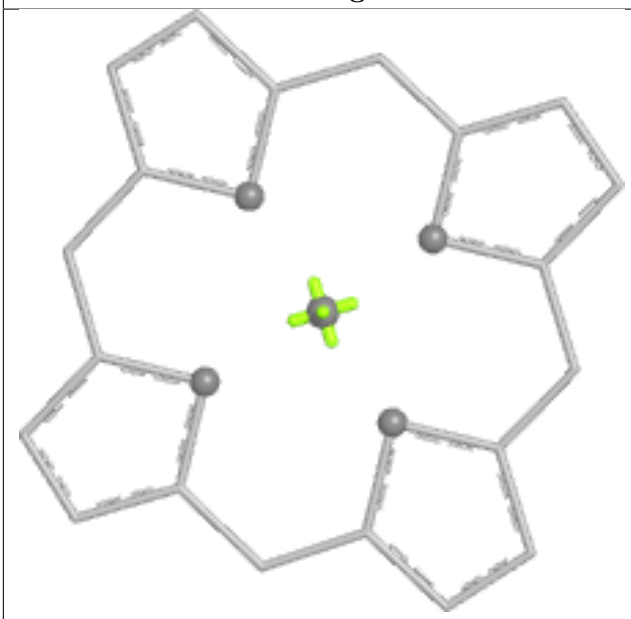
Ligand CLA 4 4006



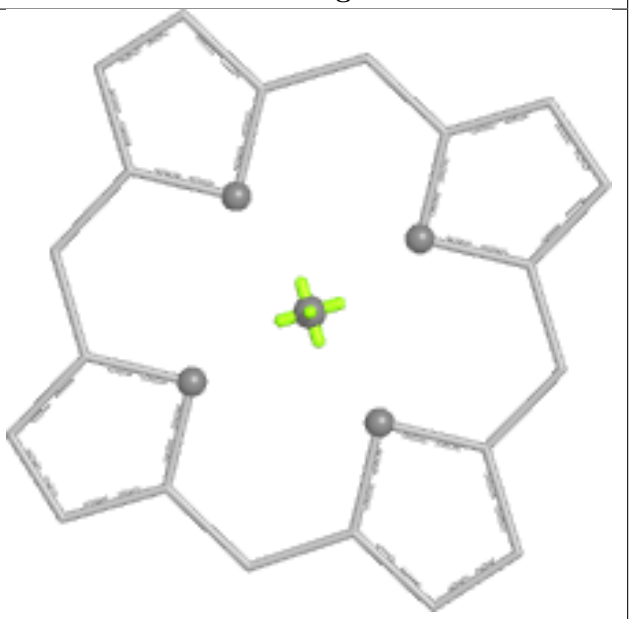
Bond lengths



Bond angles

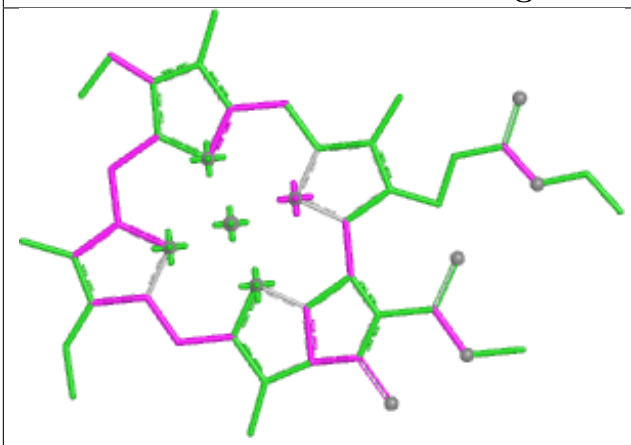


Torsions

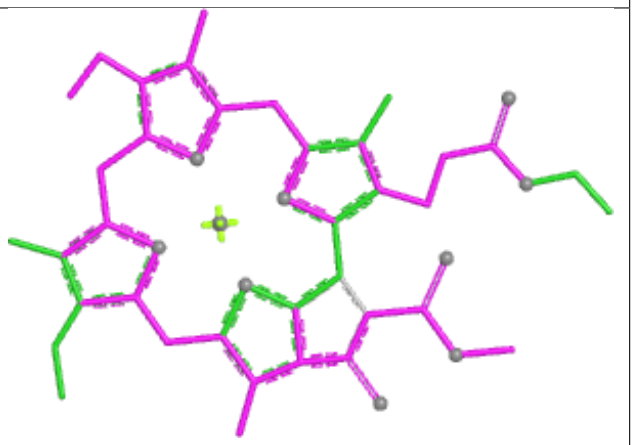


Rings

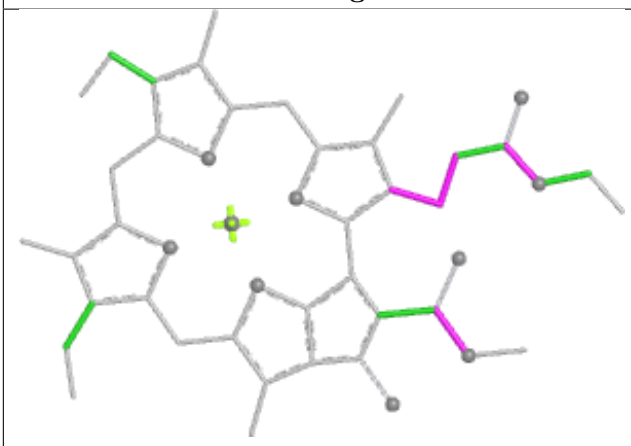
Ligand CLA B 9010



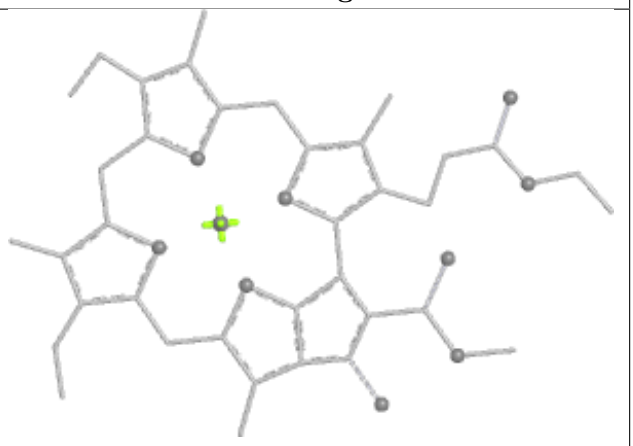
Bond lengths



Bond angles

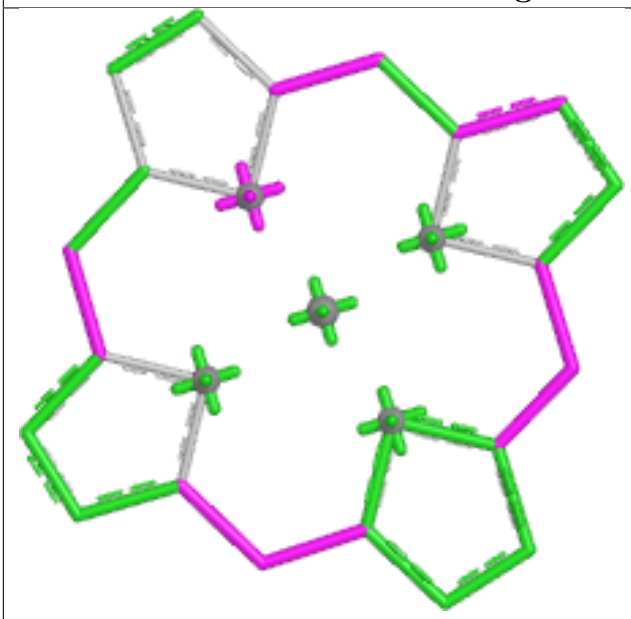


Torsions

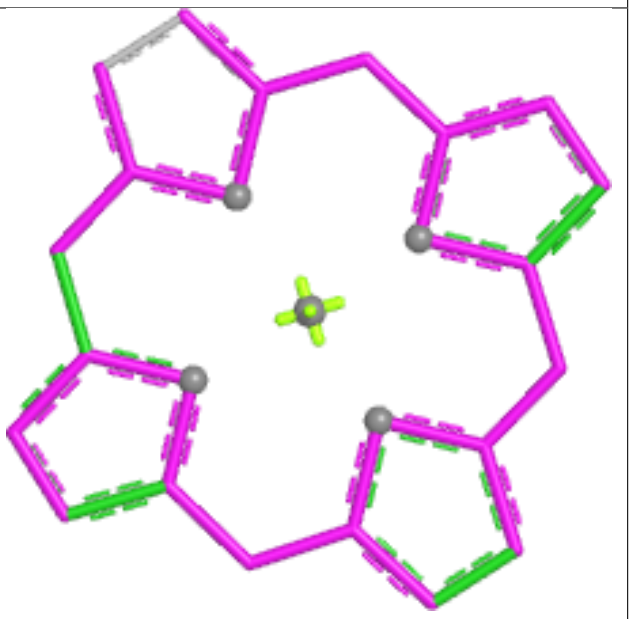


Rings

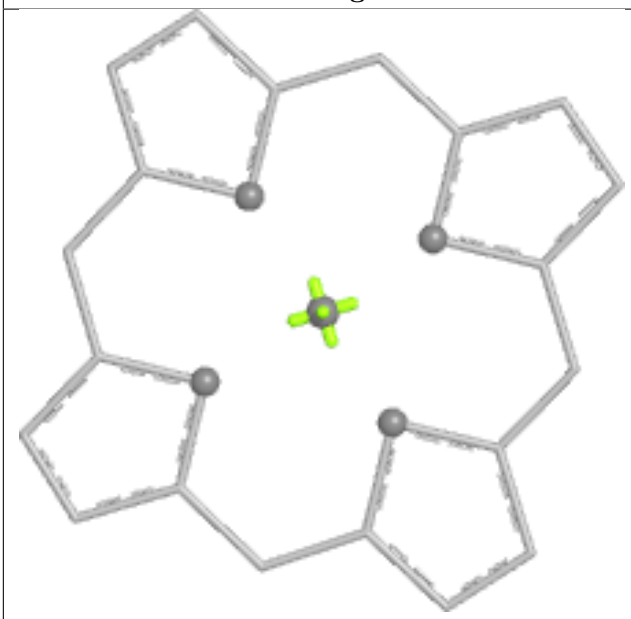
Ligand CLA A 1148



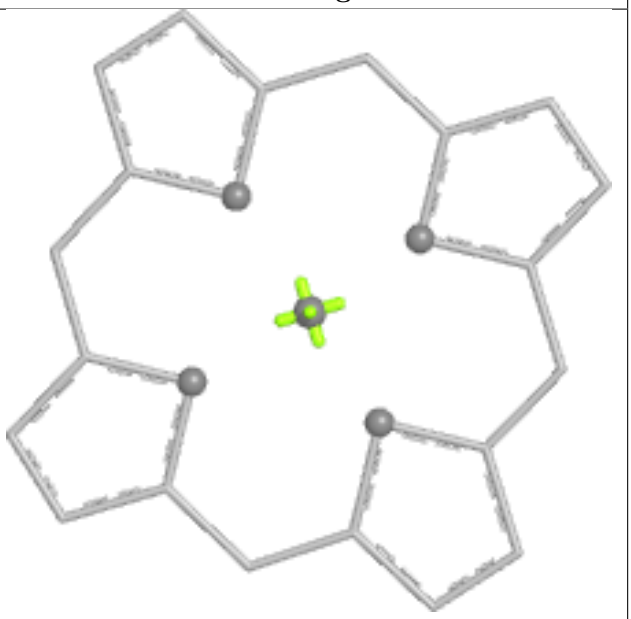
Bond lengths



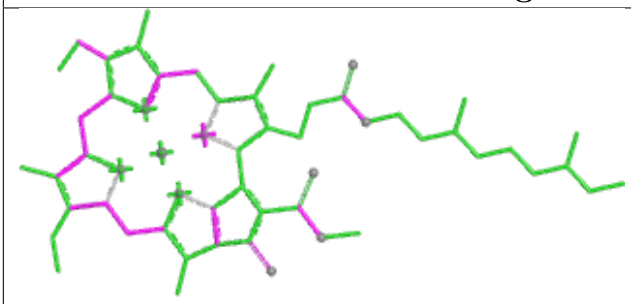
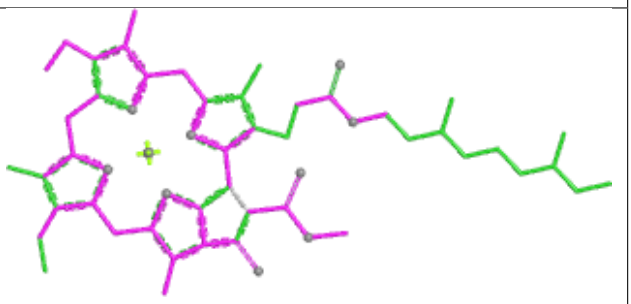
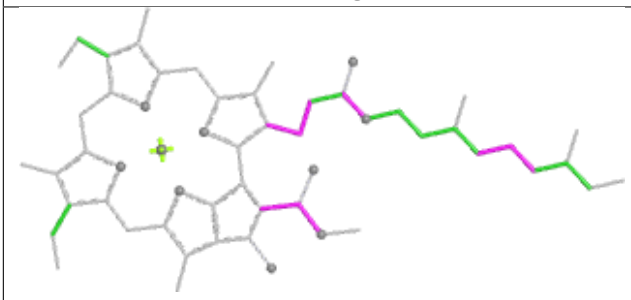
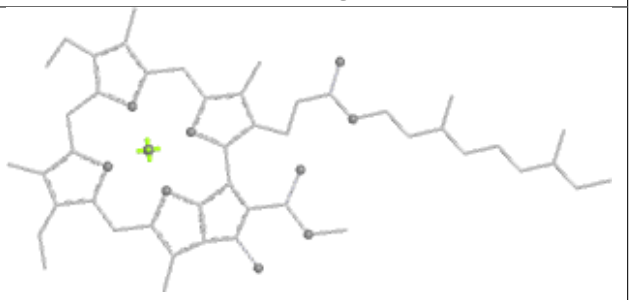
Bond angles

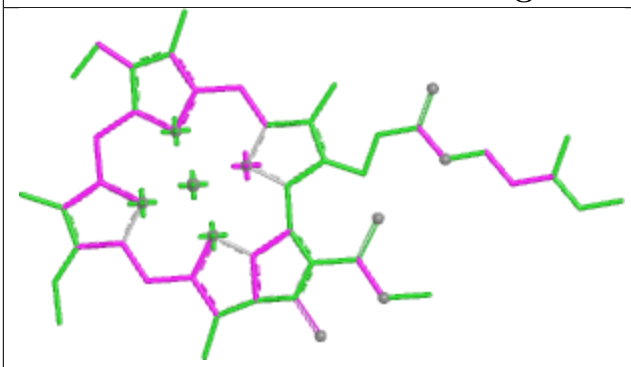
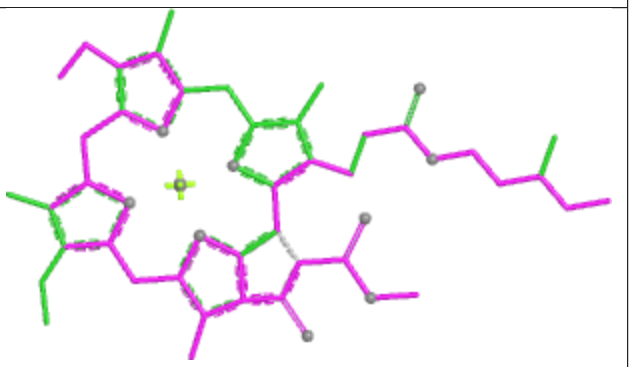
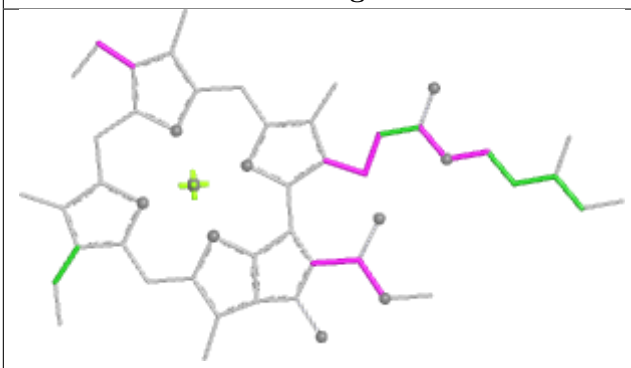
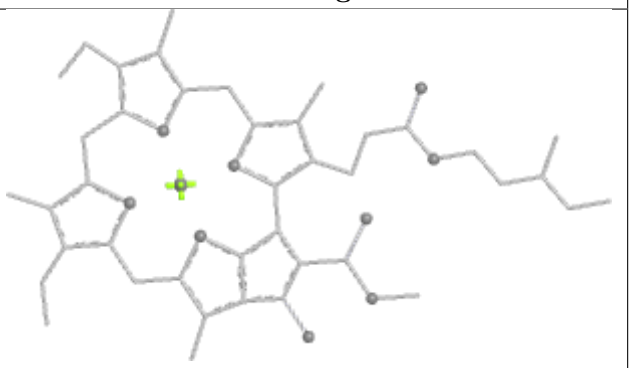


Torsions

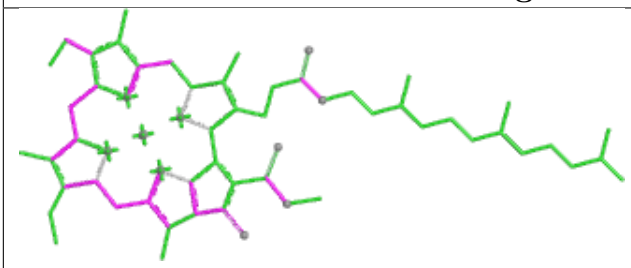


Rings

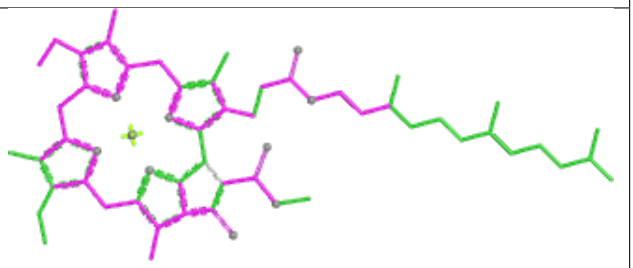
Ligand CLA B 1216	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1218	
	
Bond lengths	Bond angles
	
Torsions	Rings

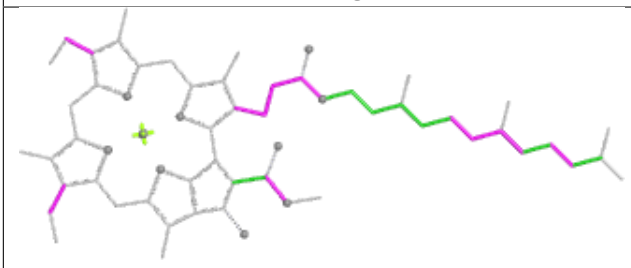
Ligand CLA B 1220



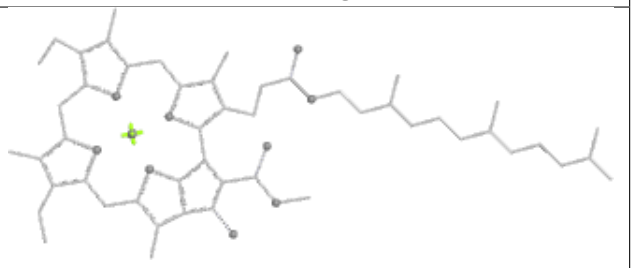
Bond lengths



Bond angles

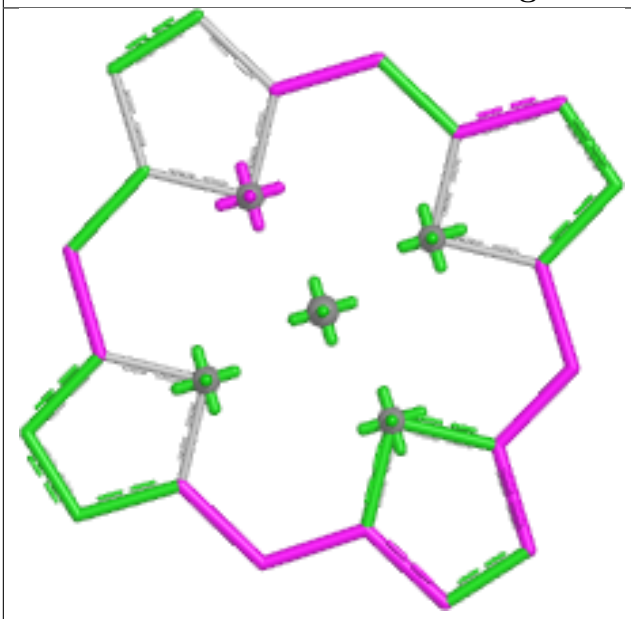


Torsions

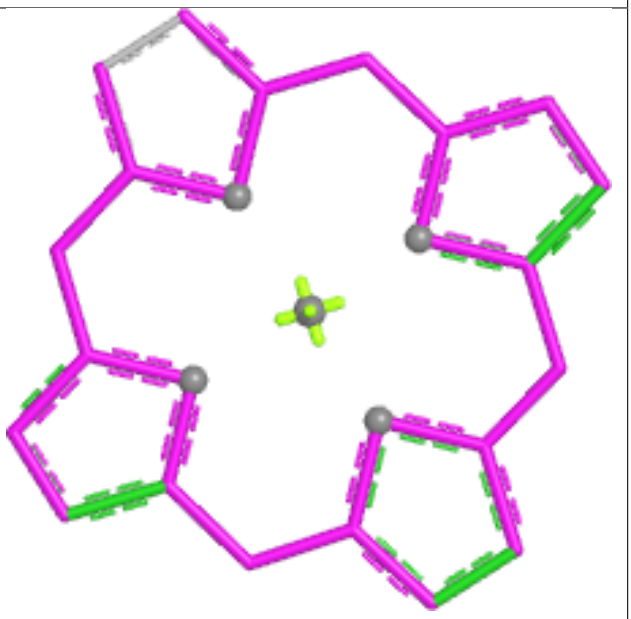


Rings

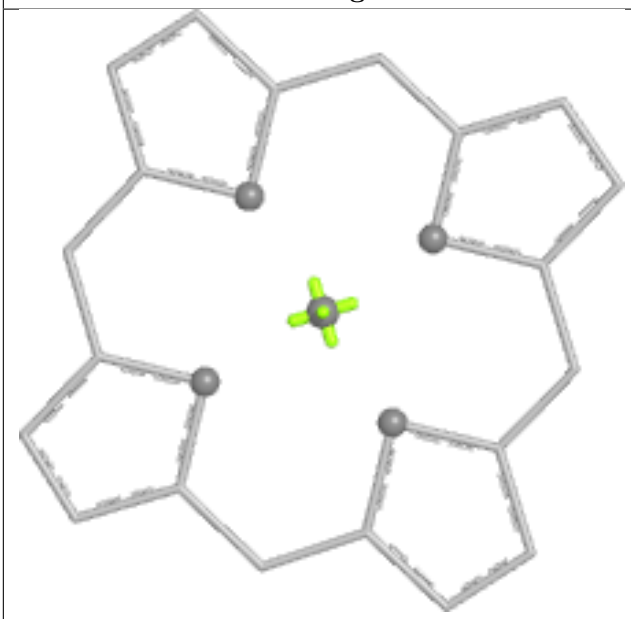
Ligand CLA 2 2012



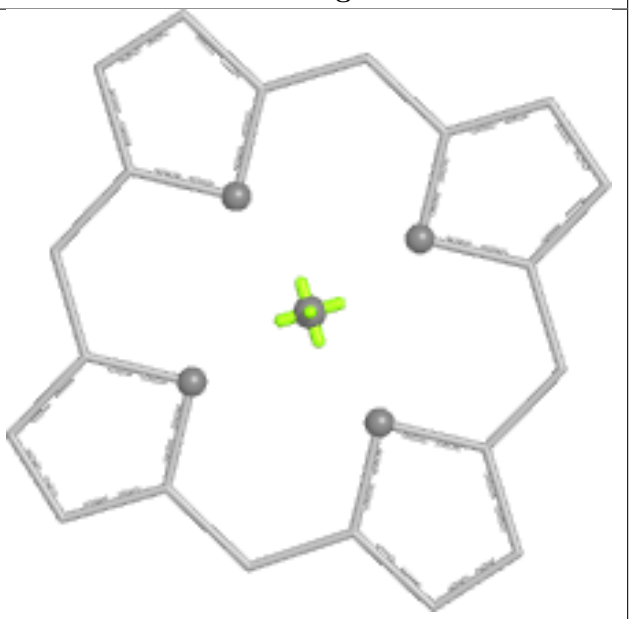
Bond lengths



Bond angles

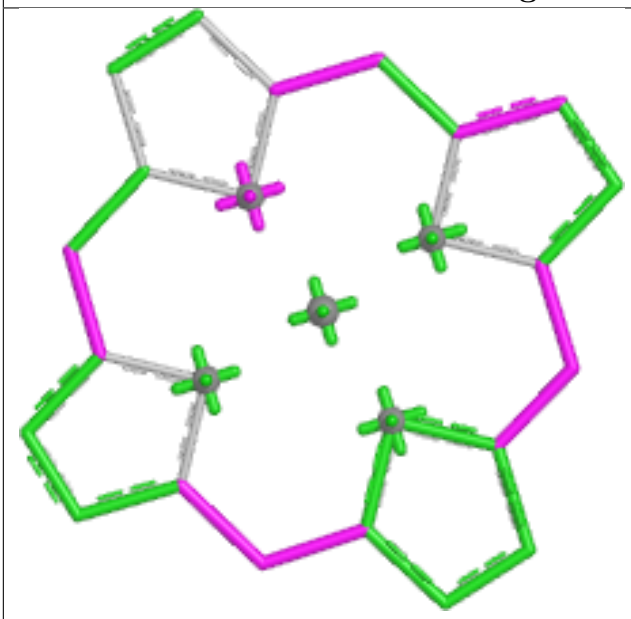


Torsions

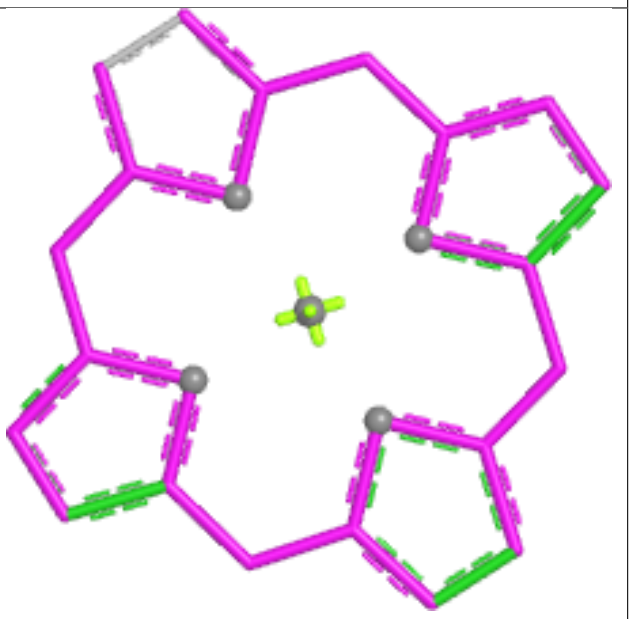


Rings

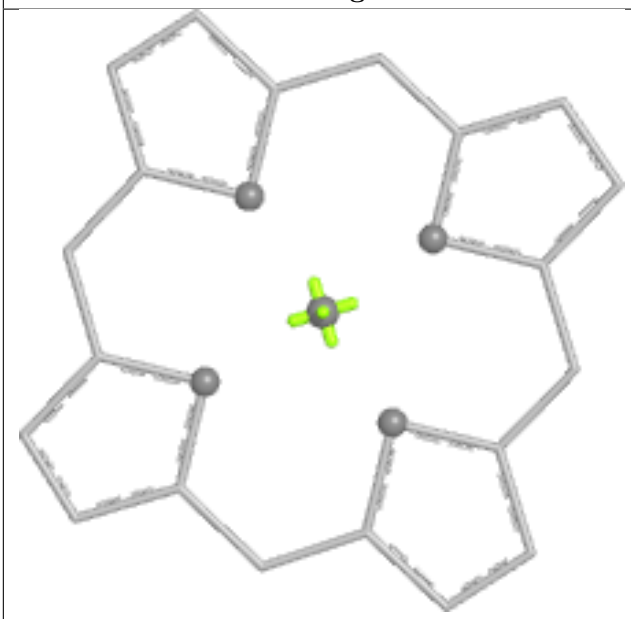
Ligand CLA 2 2007



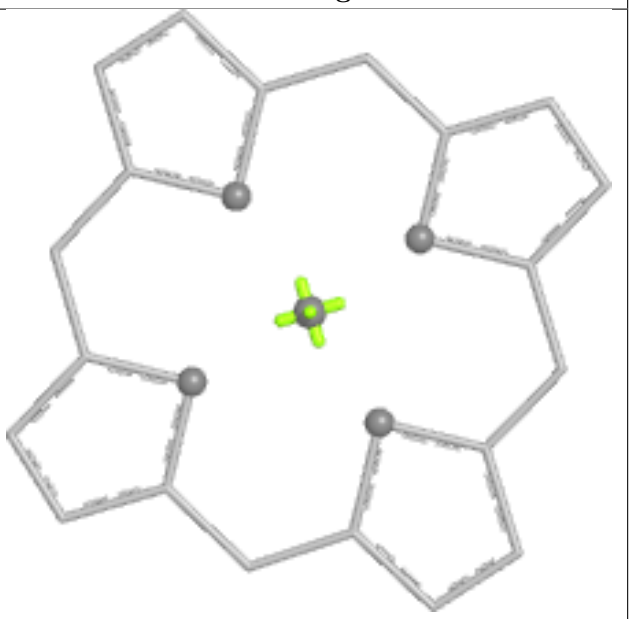
Bond lengths



Bond angles

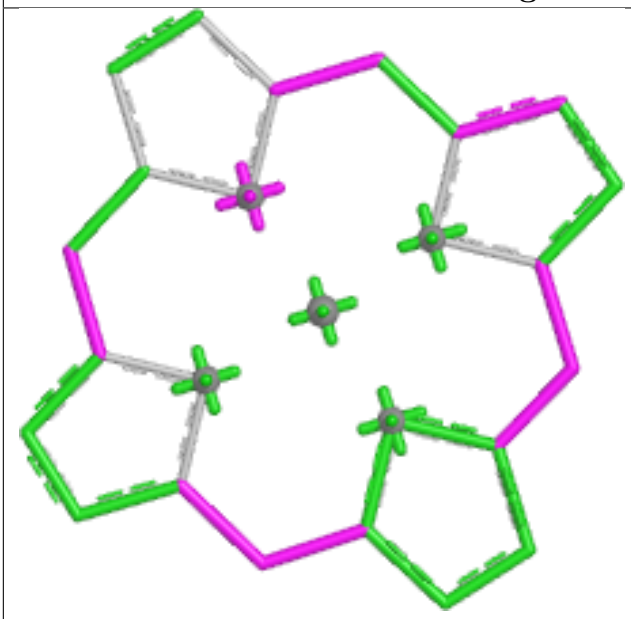


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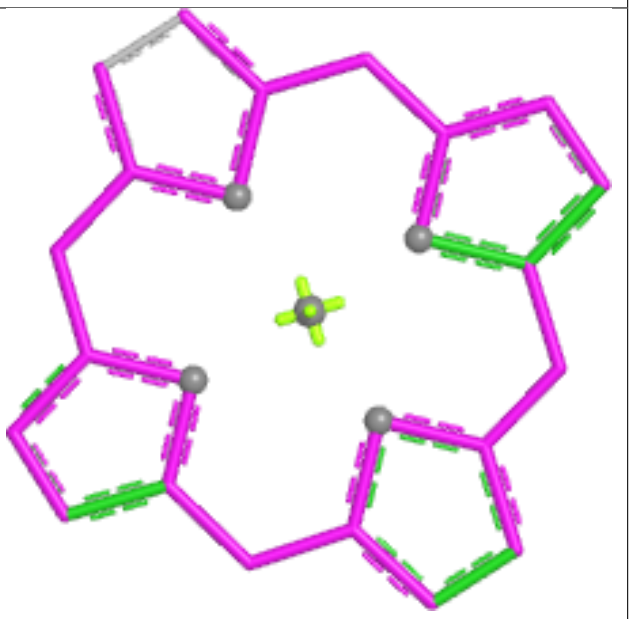


Rings

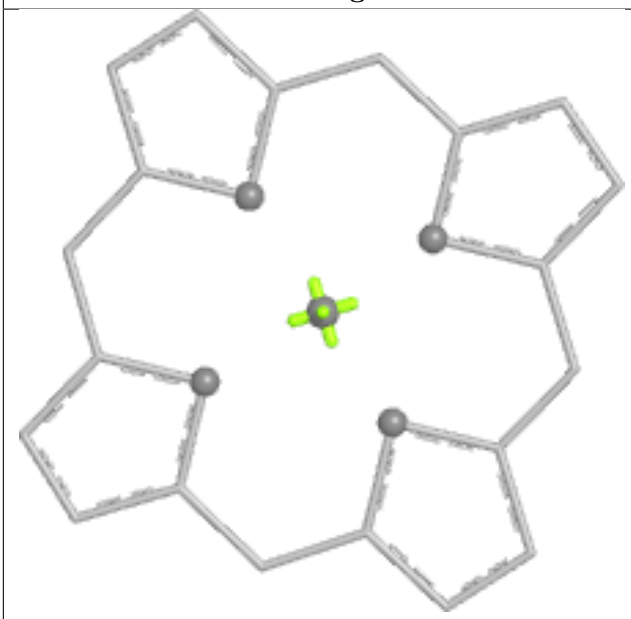
Ligand CLA 1 1005



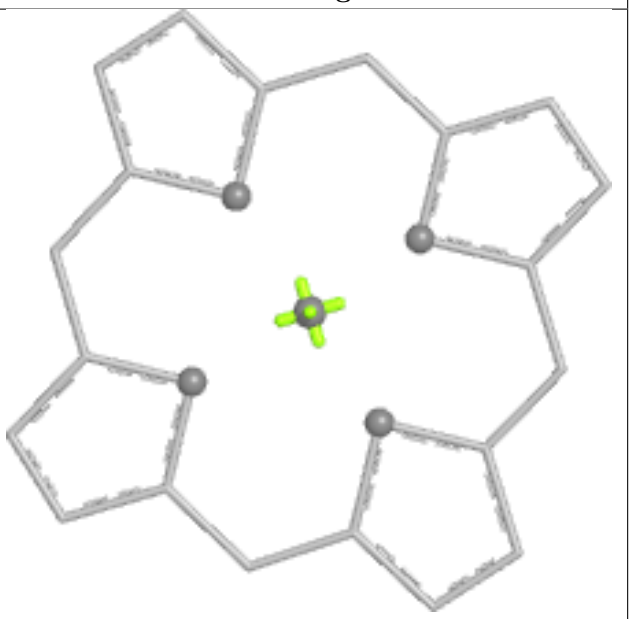
Bond lengths



Bond angles

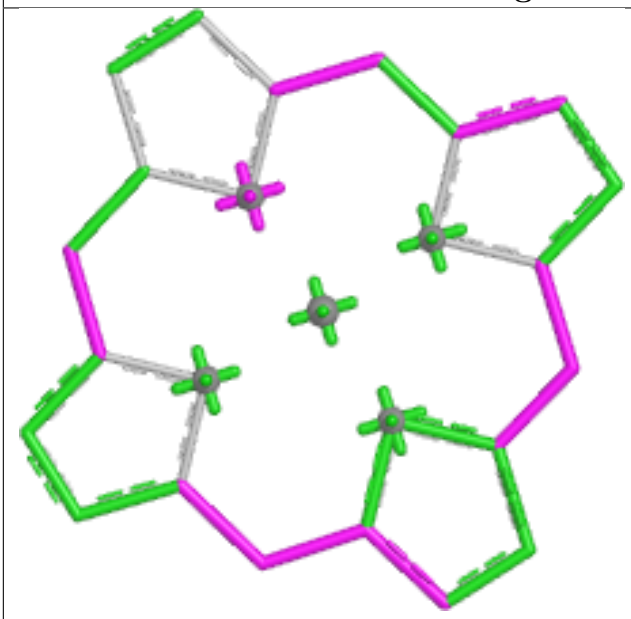


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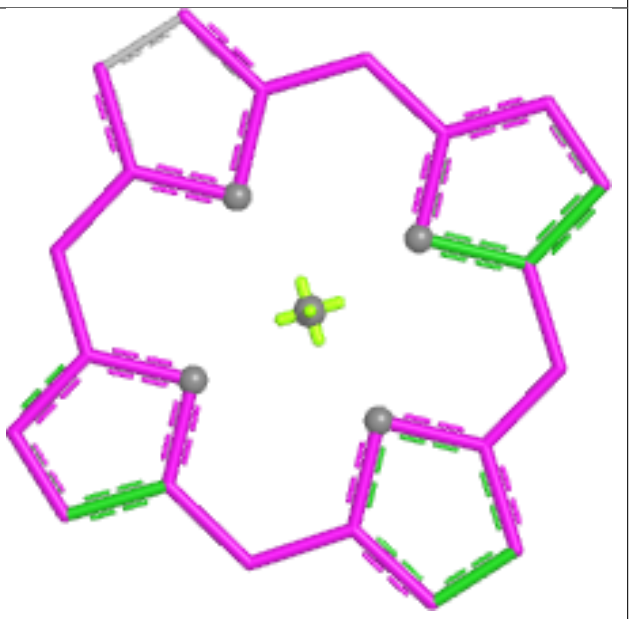


Rings

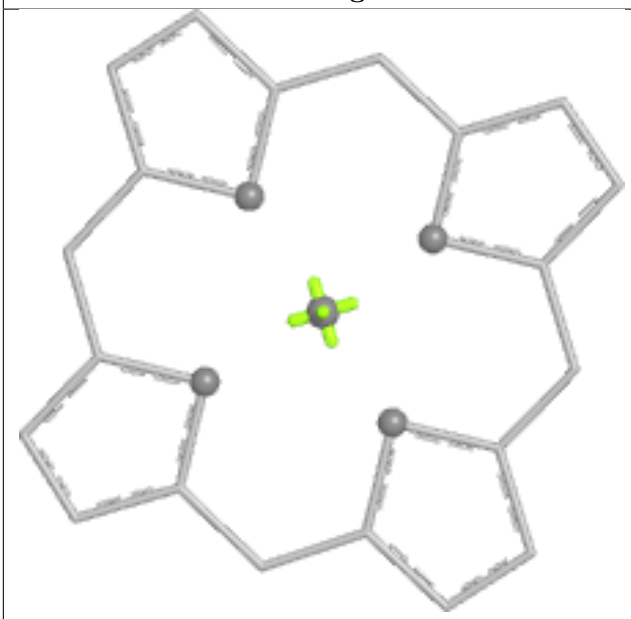
Ligand CLA A 1116



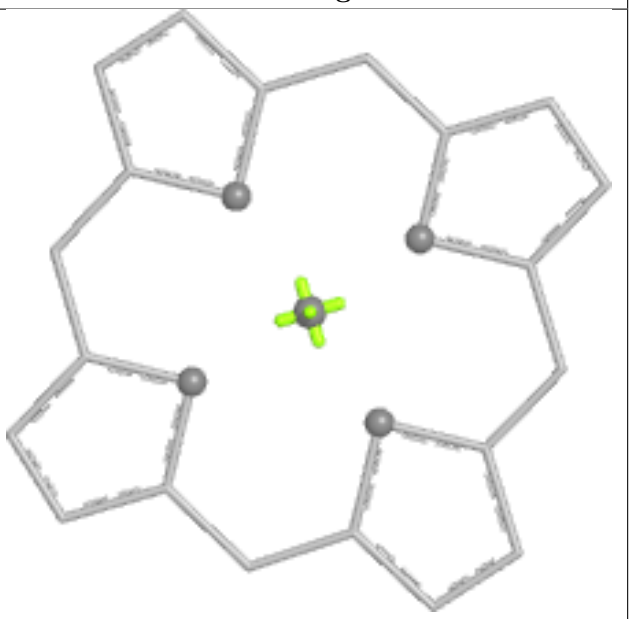
Bond lengths



Bond angles

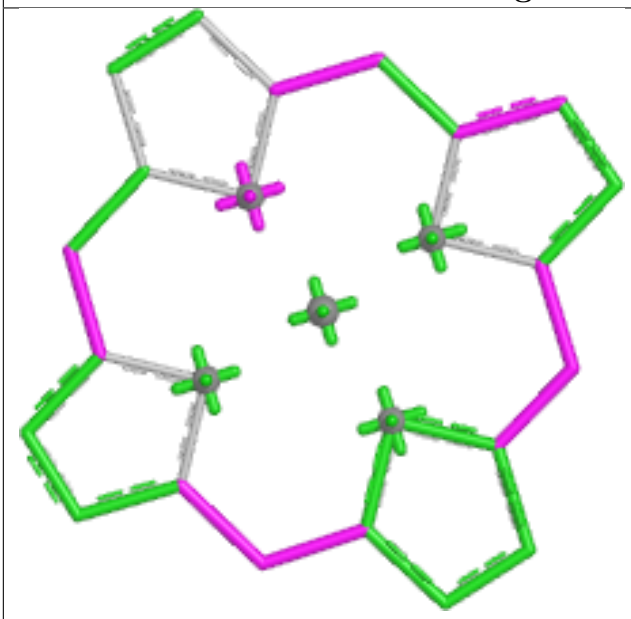


Torsions

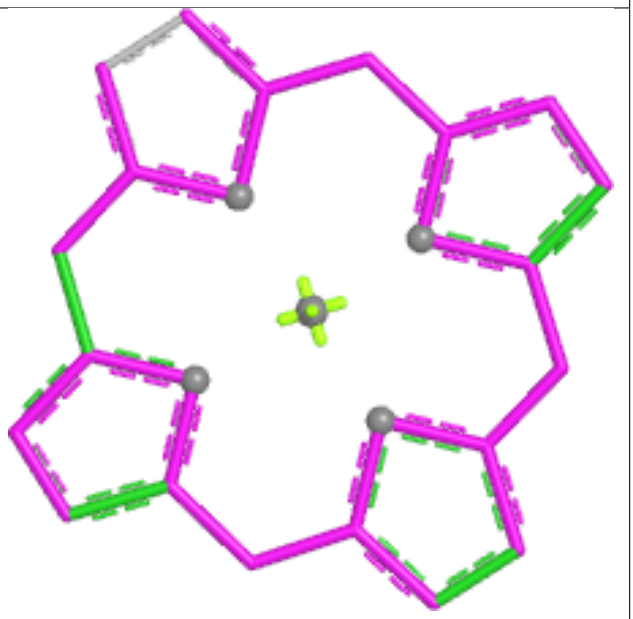


Rings

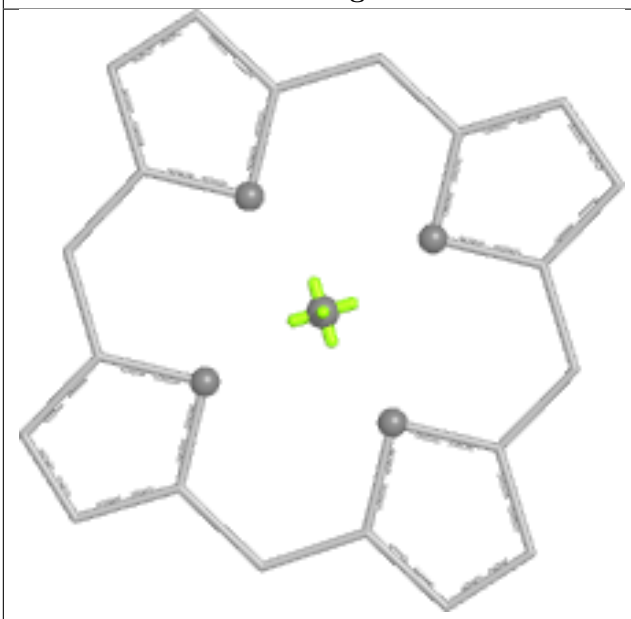
Ligand CLA A 1151



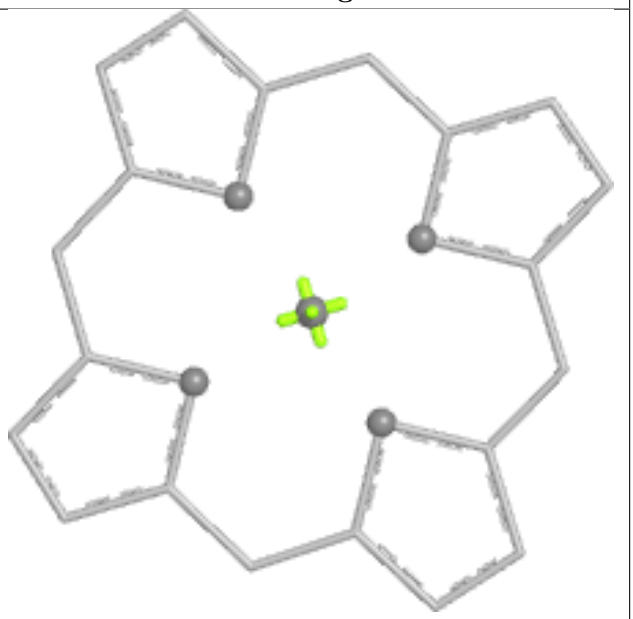
Bond lengths



Bond angles

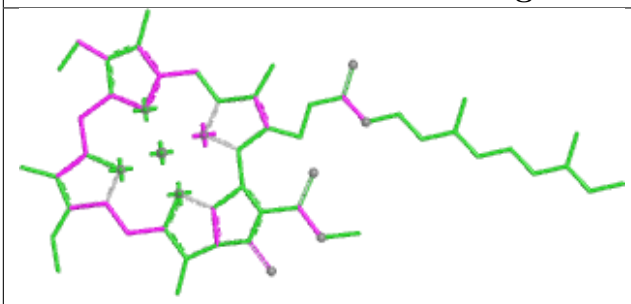


Torsions

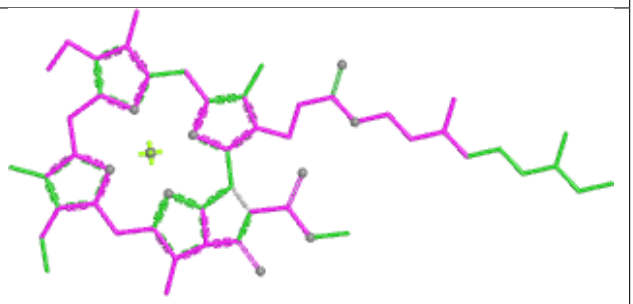


Rings

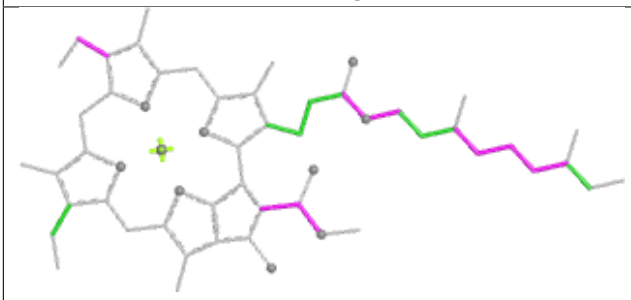
Ligand CLA B 1138



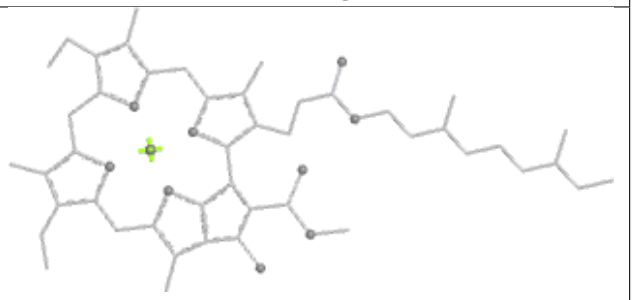
Bond lengths



Bond angles

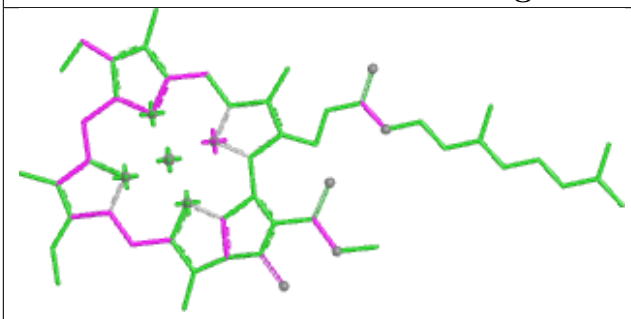


Torsions

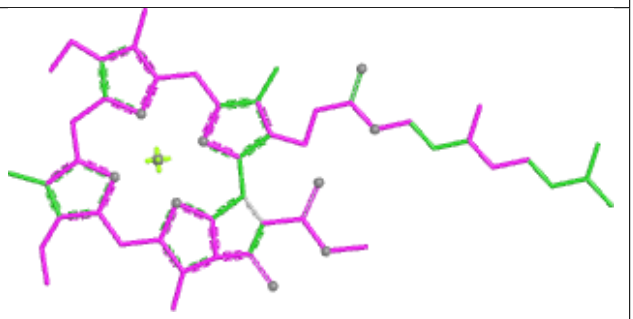


Rings

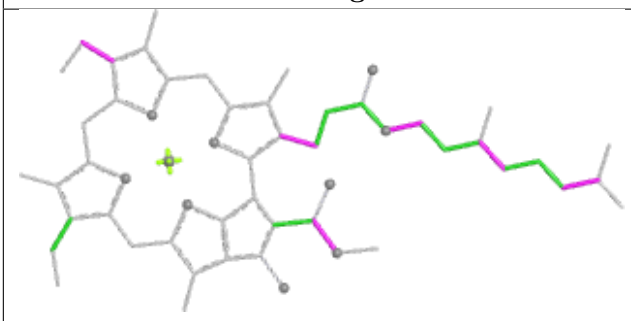
Ligand CLA H 1501



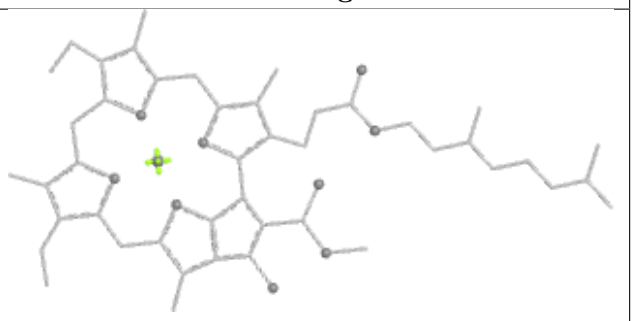
Bond lengths



Bond angles

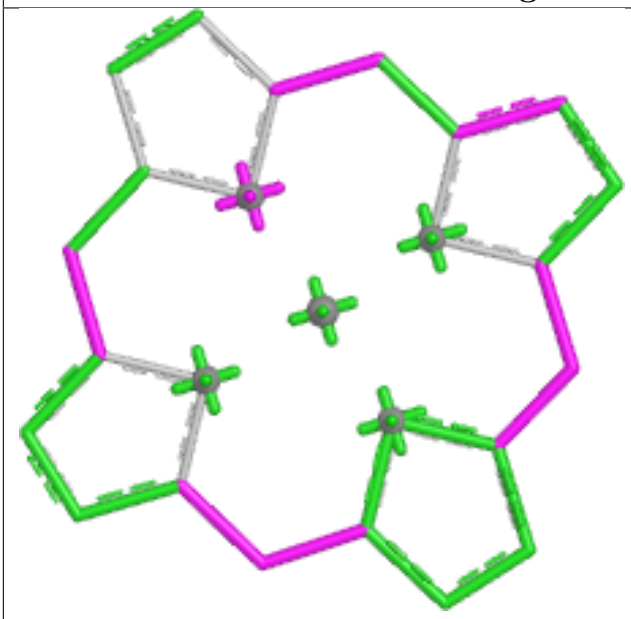


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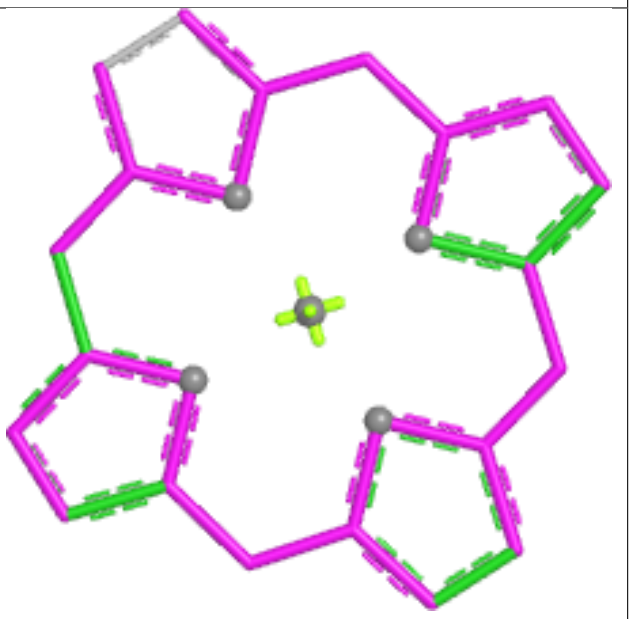


Rings

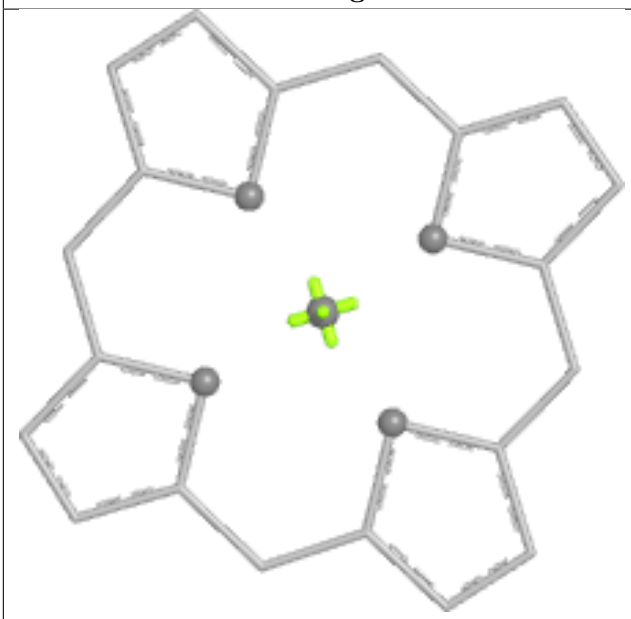
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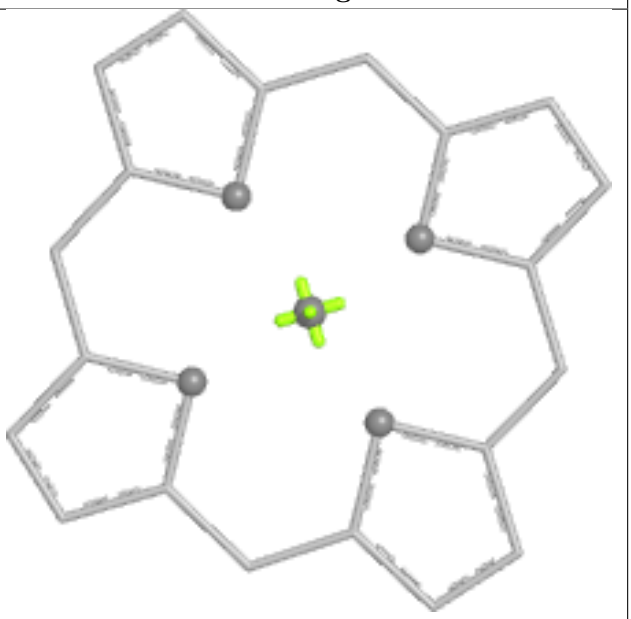
Bond lengths



Bond angles

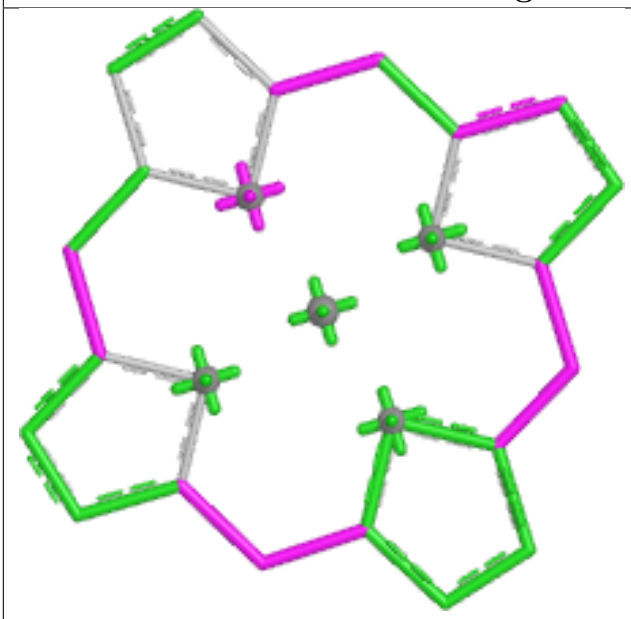


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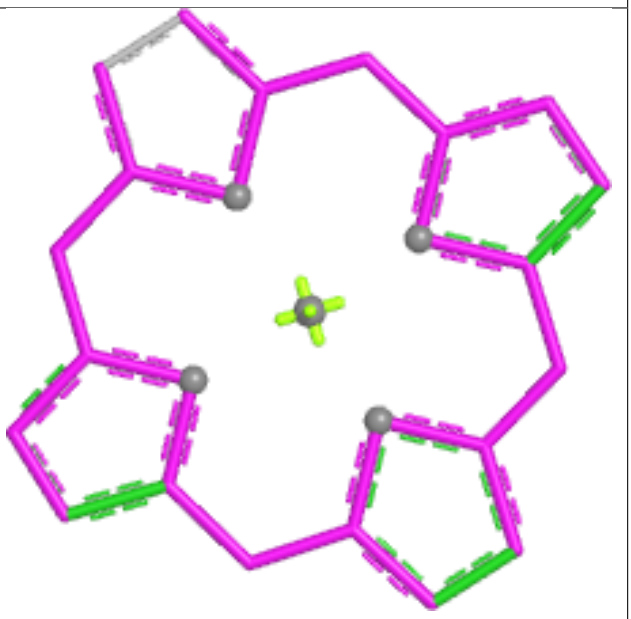


Rings

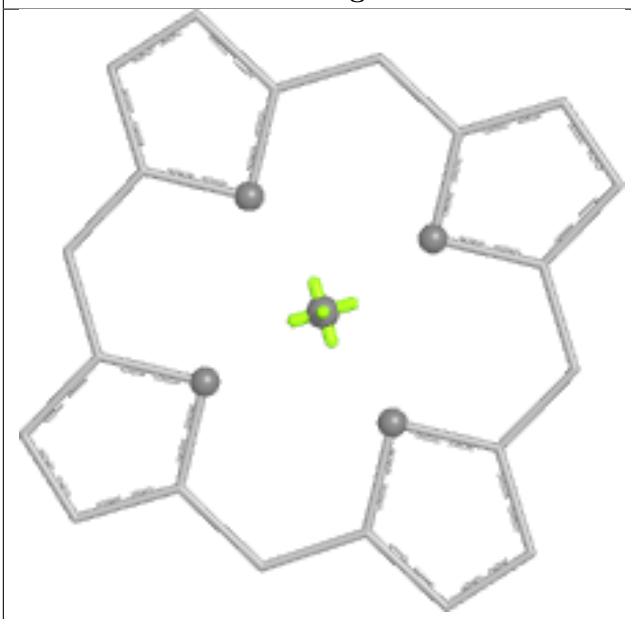
Ligand CLA B 1211



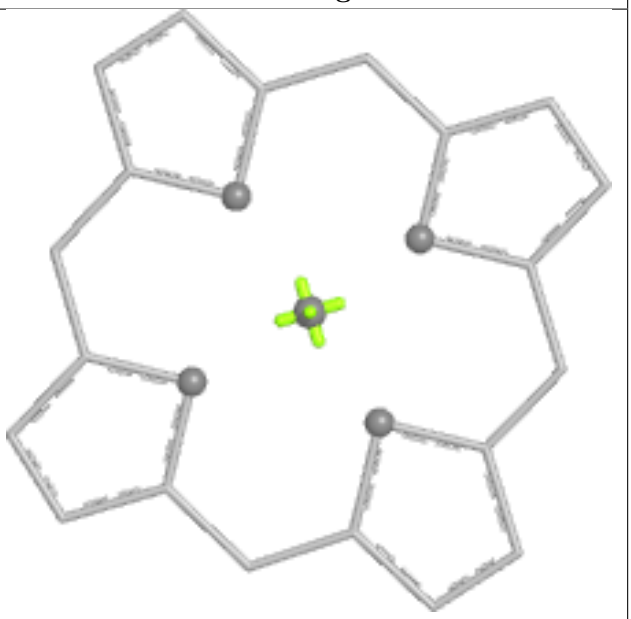
Bond lengths



Bond angles

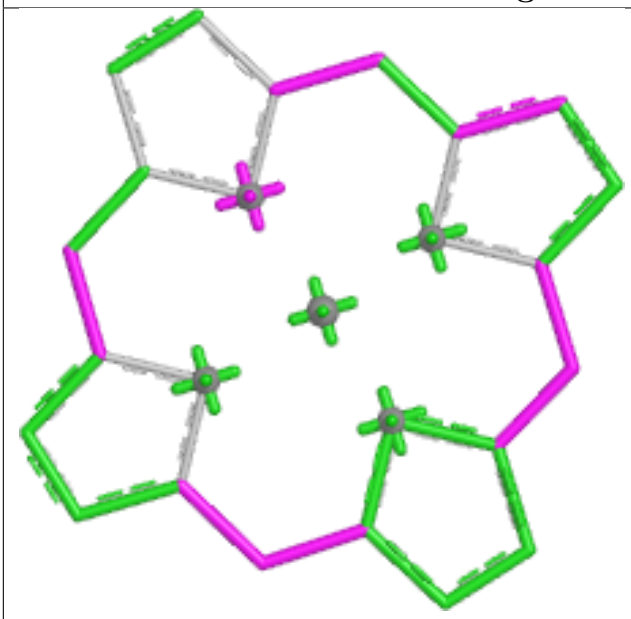


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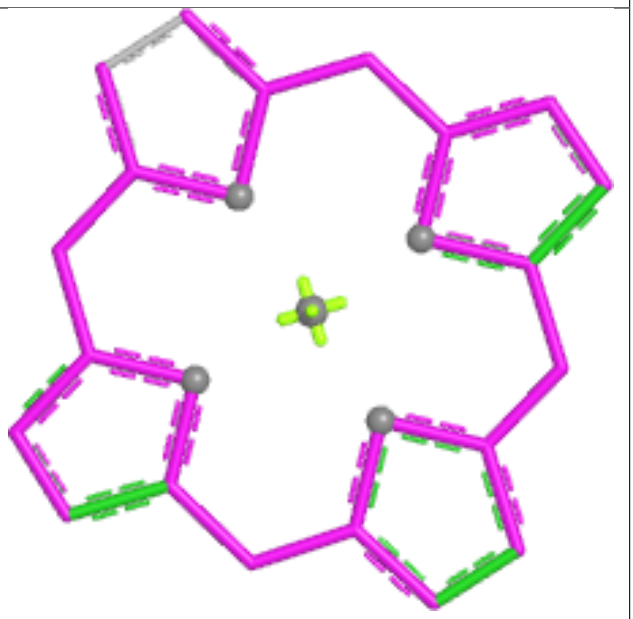


Rings

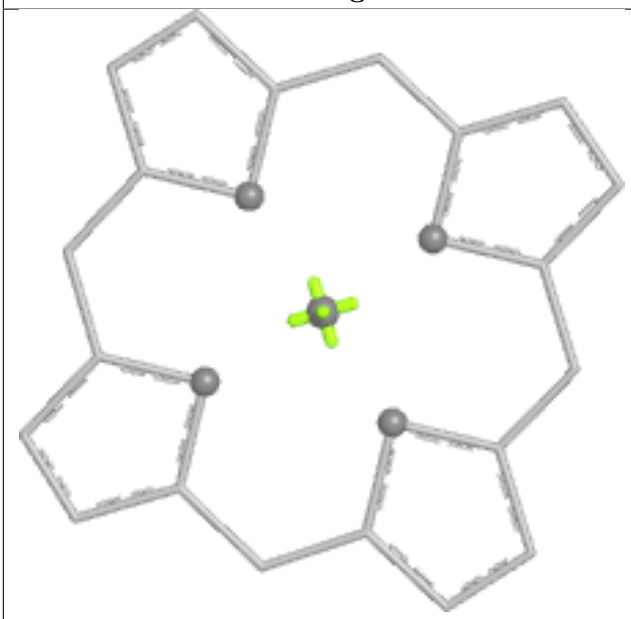
Ligand CLA F 1306



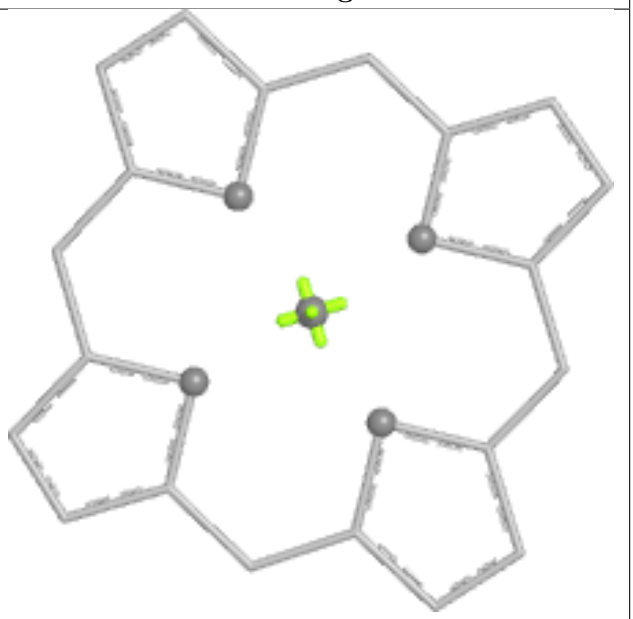
Bond lengths



Bond angles

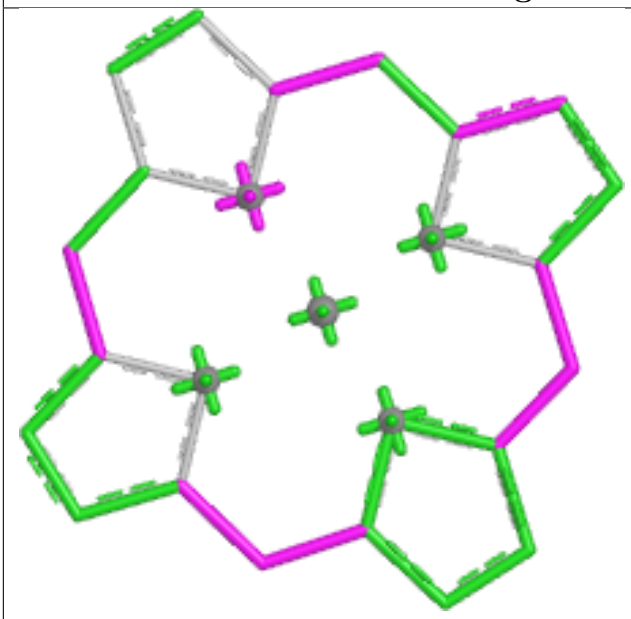


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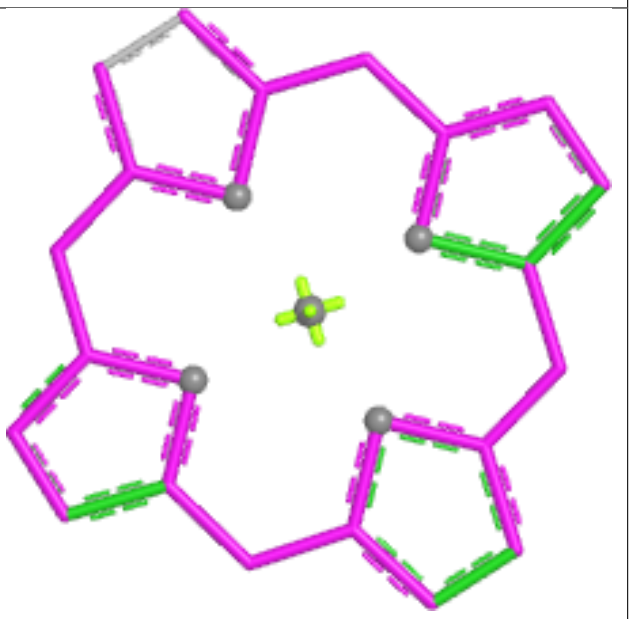


Rings

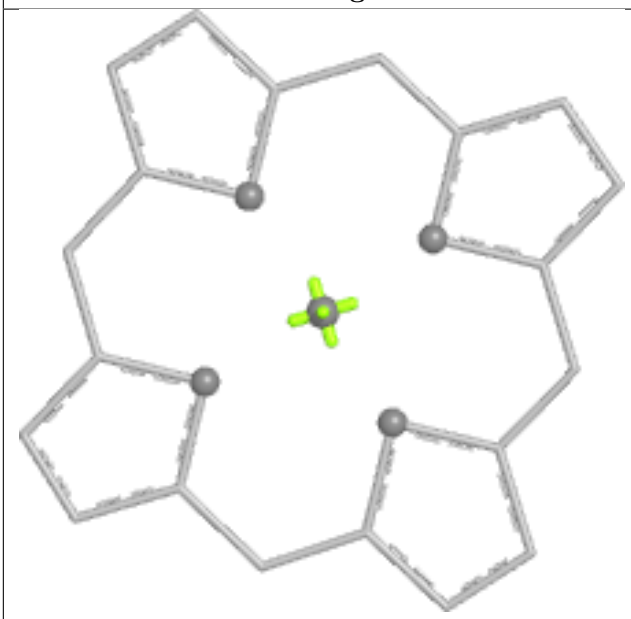
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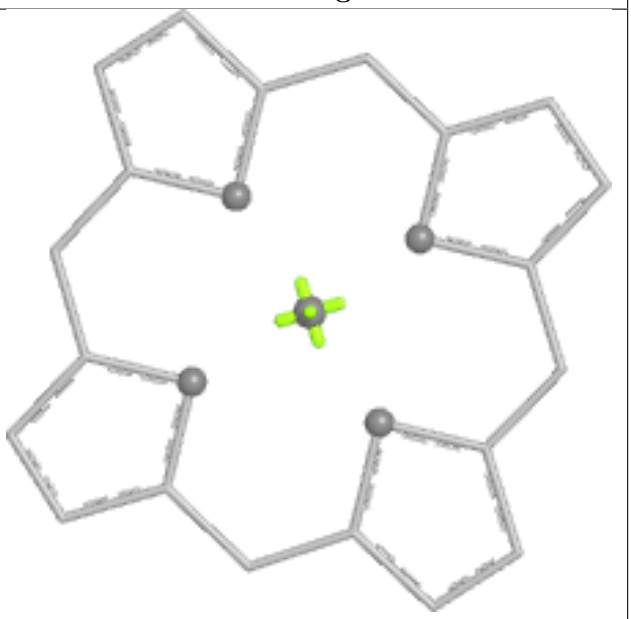
Bond lengths



Bond angles

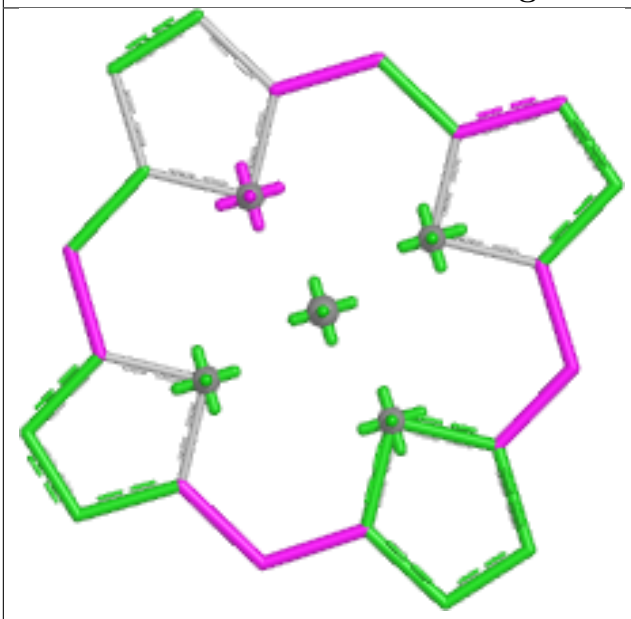


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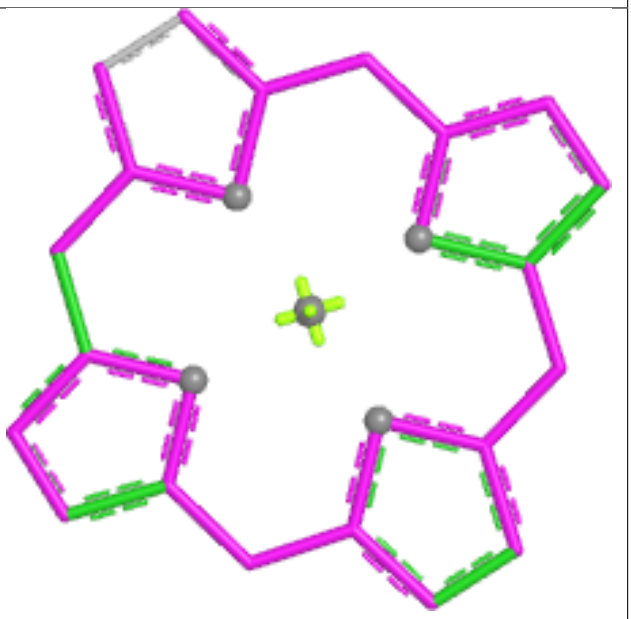


Rings

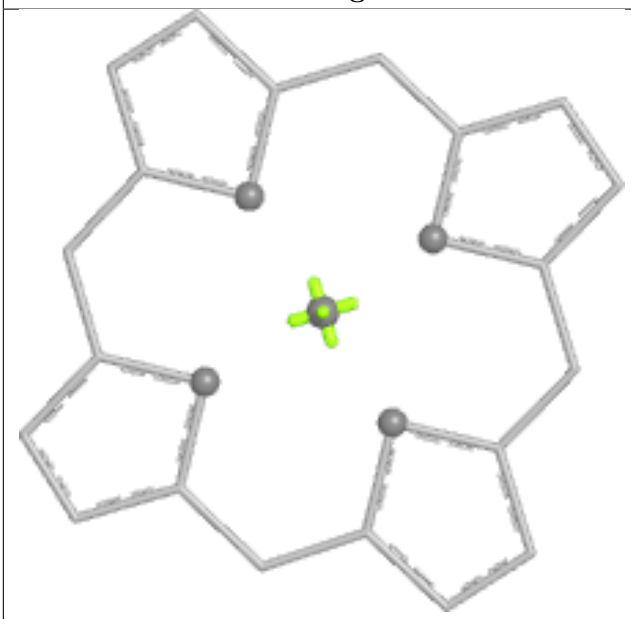
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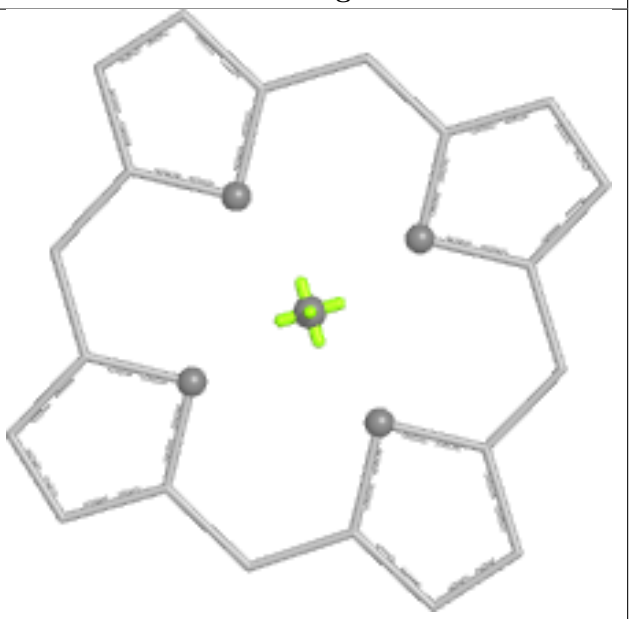
Bond lengths



Bond angles

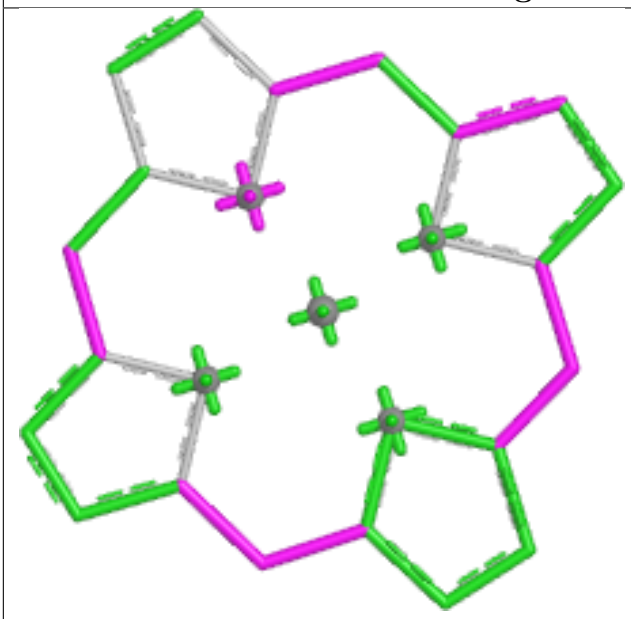


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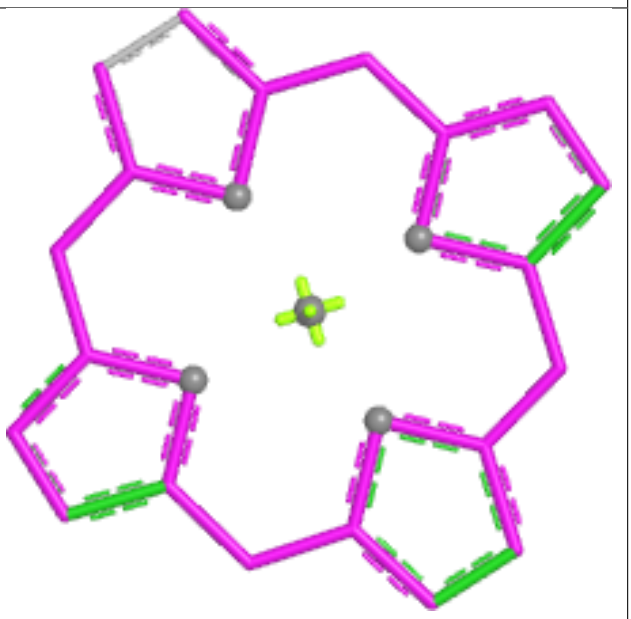


Rings

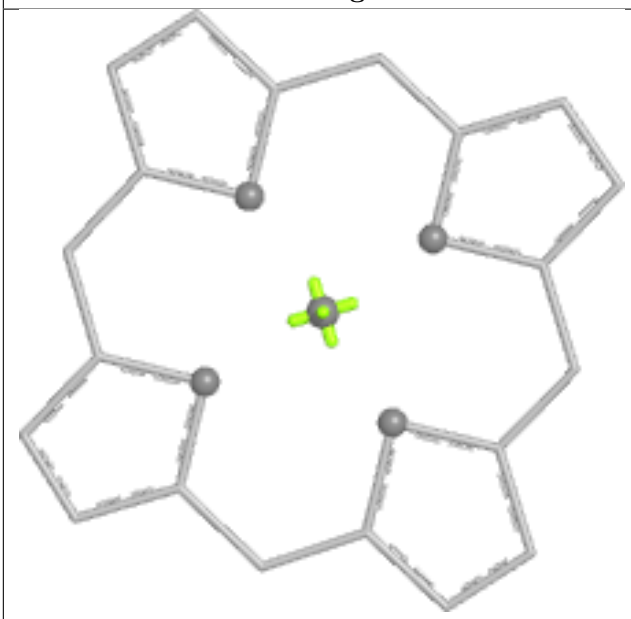
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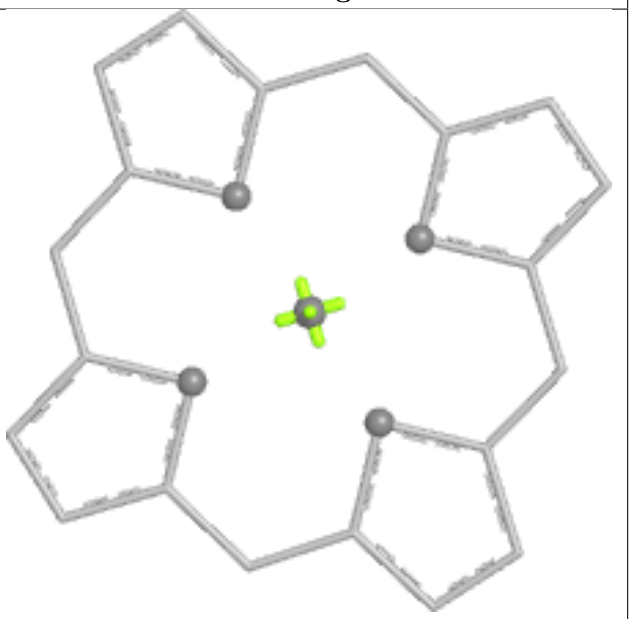
Bond lengths



Bond angles

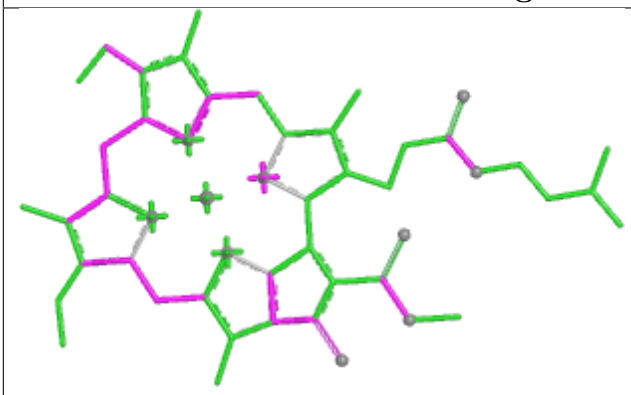


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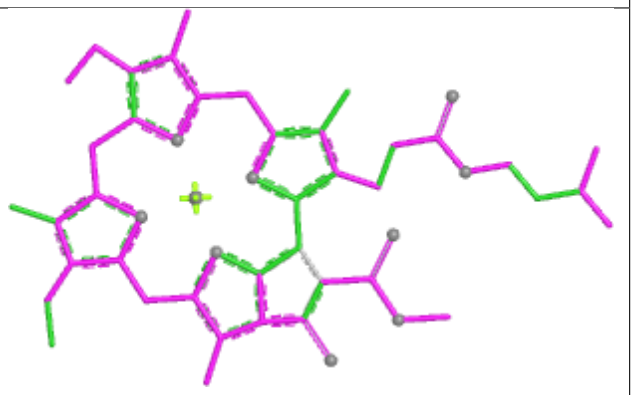


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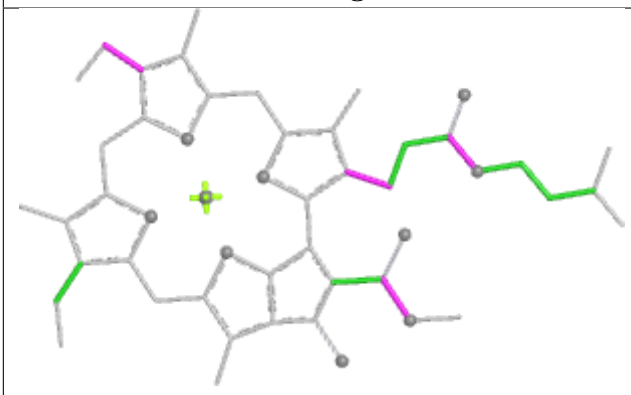
Ligand CLA B 1202



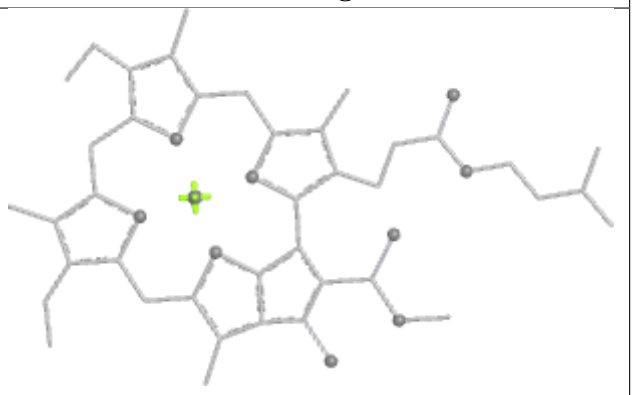
Bond lengths



Bond angles

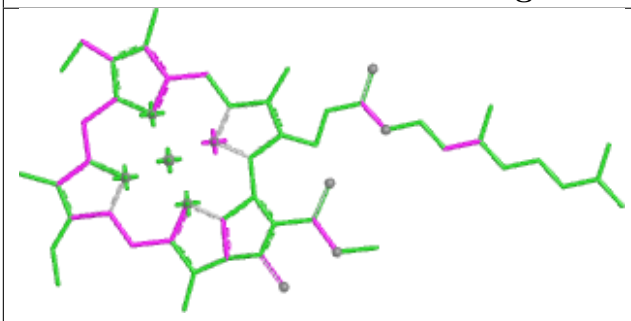


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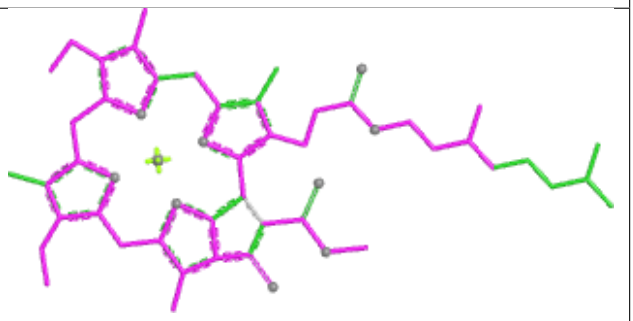


Rings

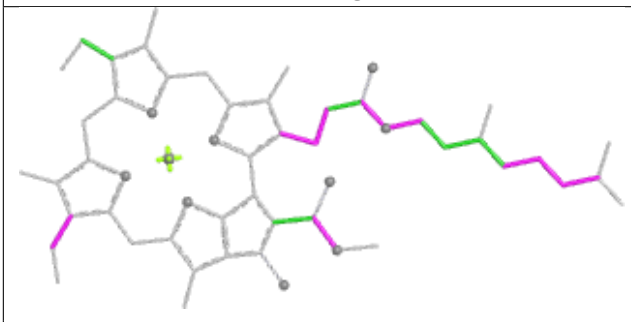
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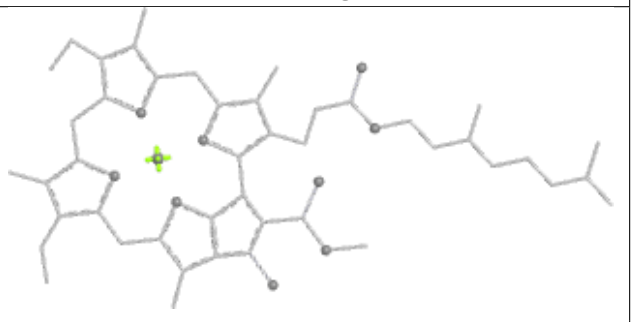
Bond lengths



Bond angles

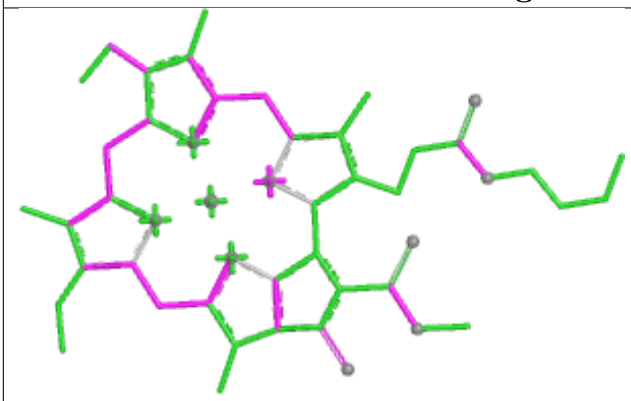


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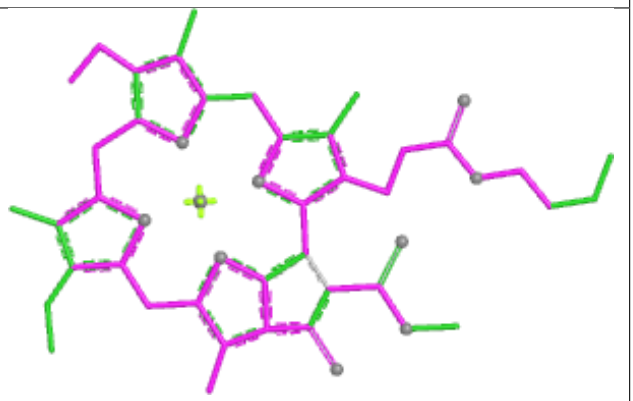


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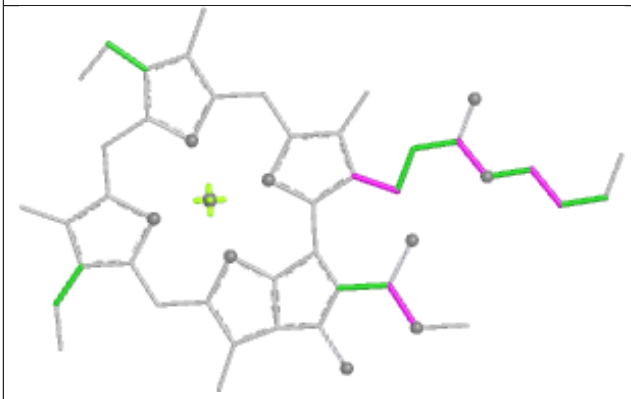
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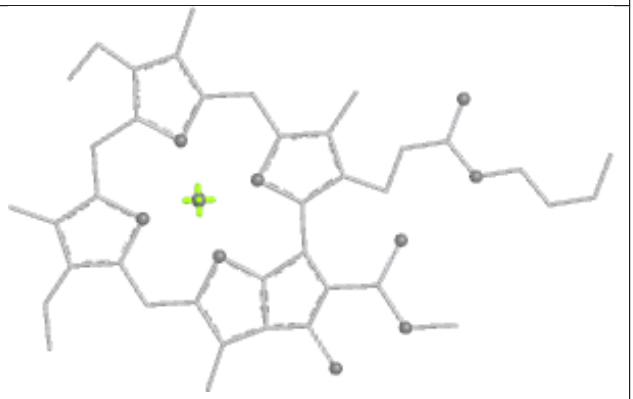
Bond lengths



Bond angles

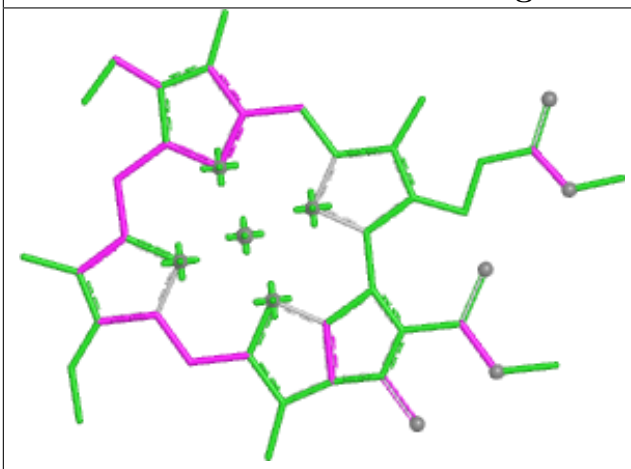


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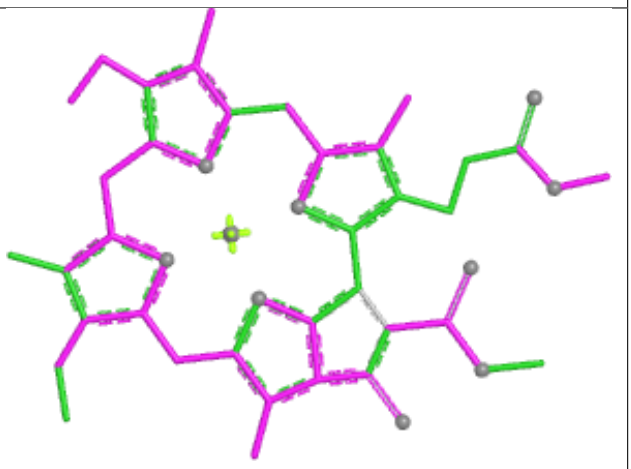


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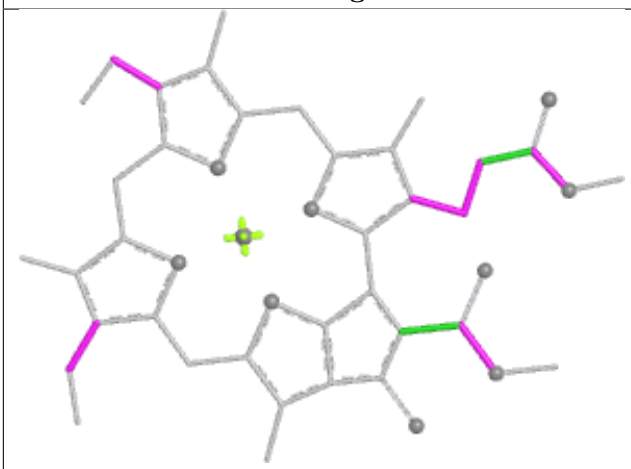
Ligand CLA B 1231



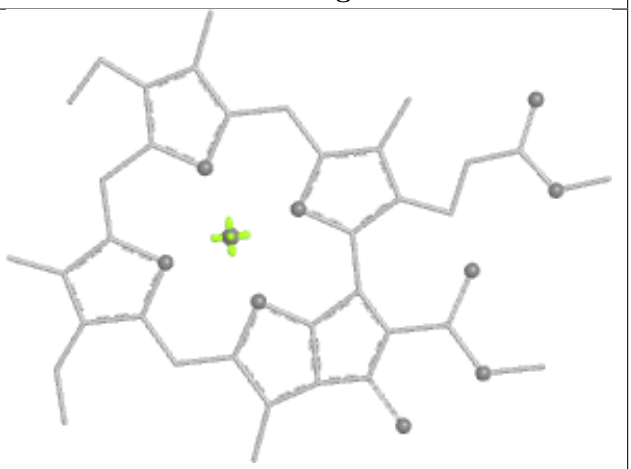
Bond lengths



Bond angles

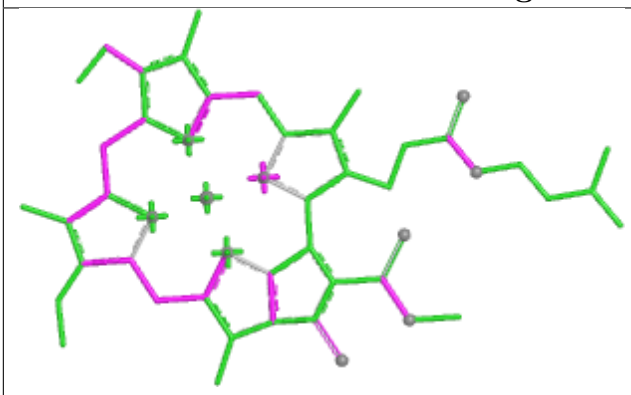


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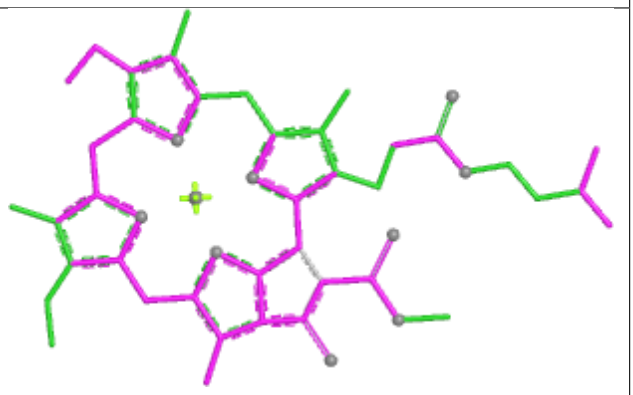


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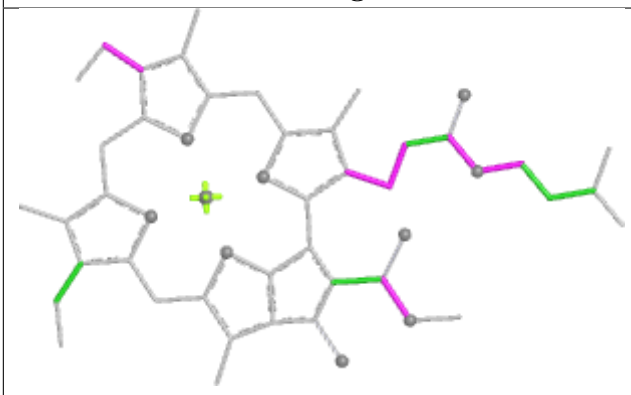
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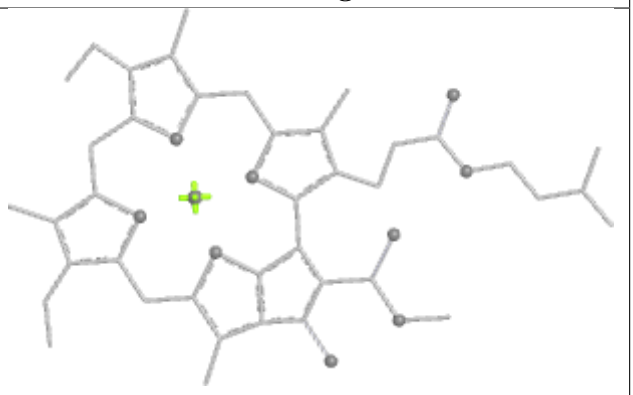
Bond lengths



Bond angles

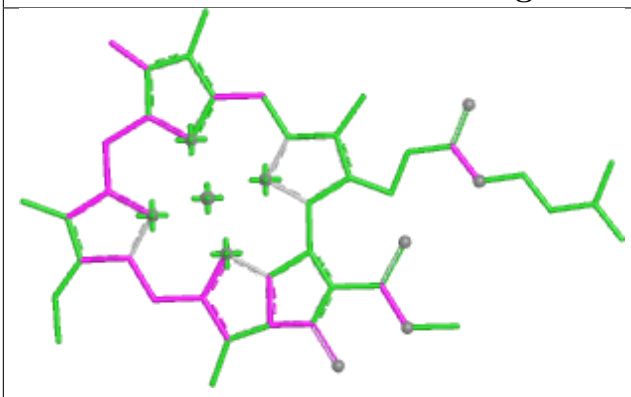


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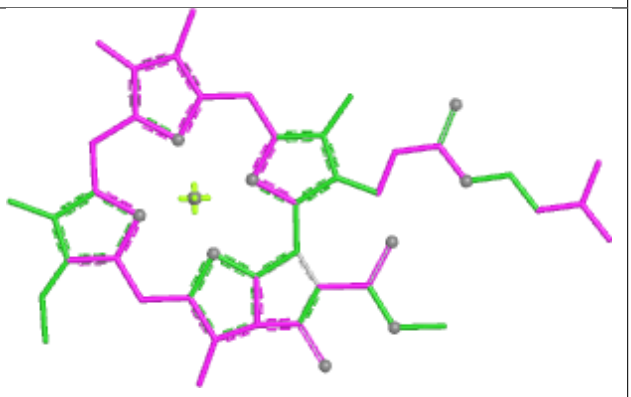


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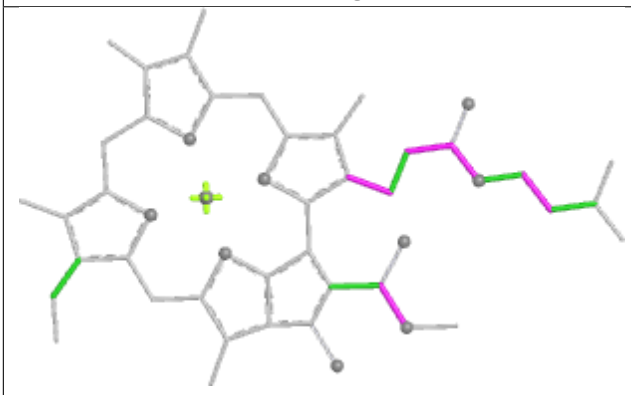
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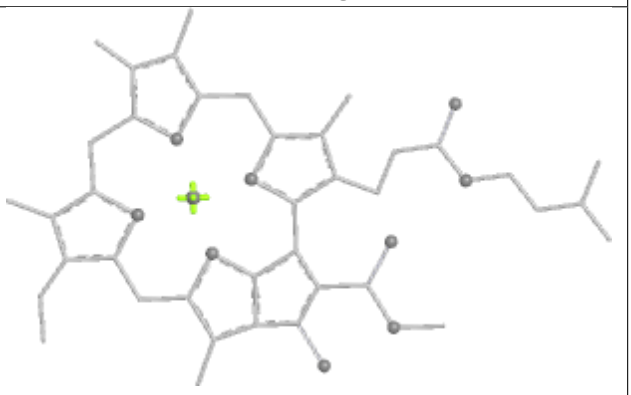
Bond lengths



Bond angles

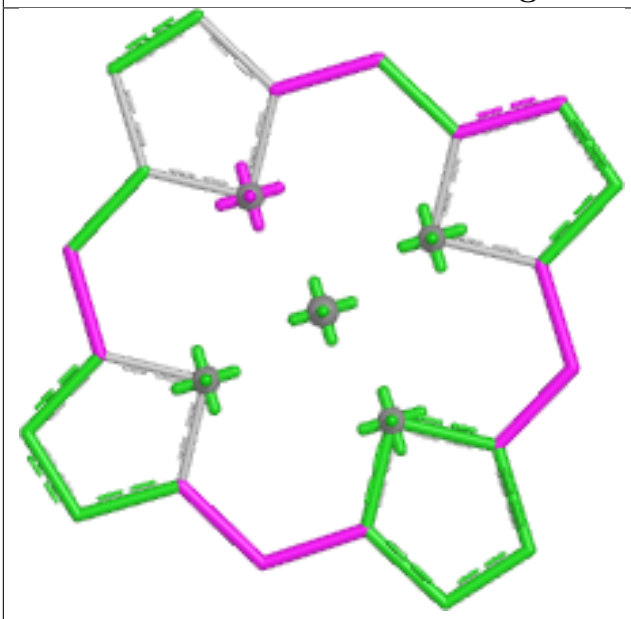


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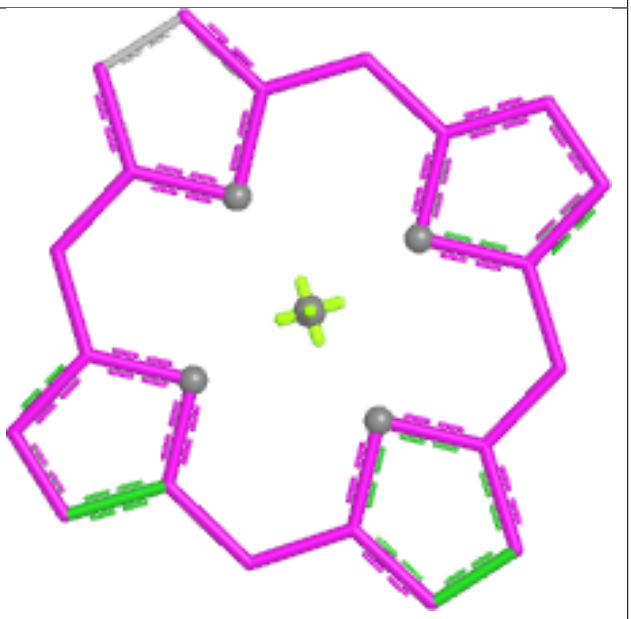


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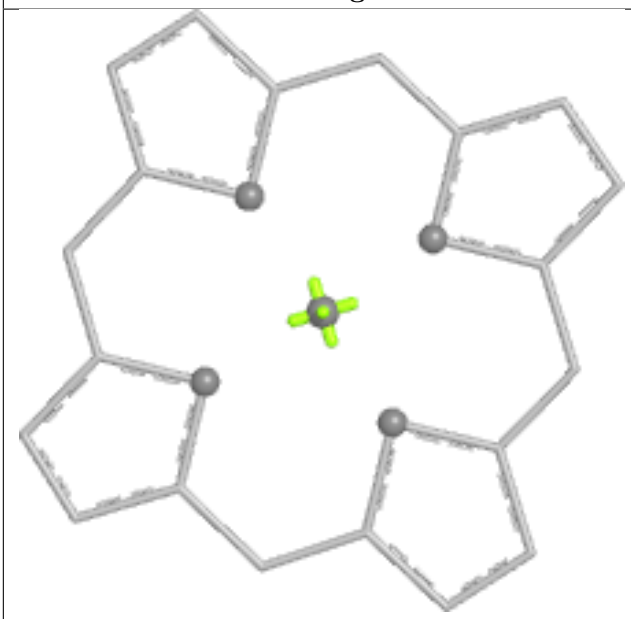
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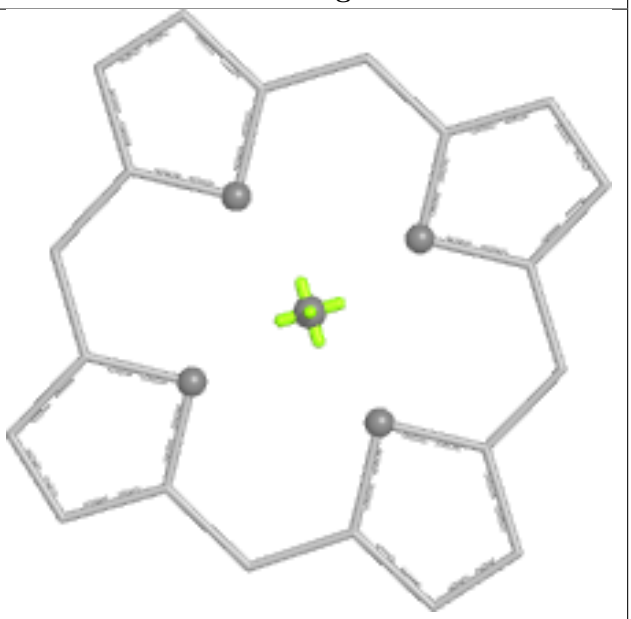
Bond lengths



Bond angles

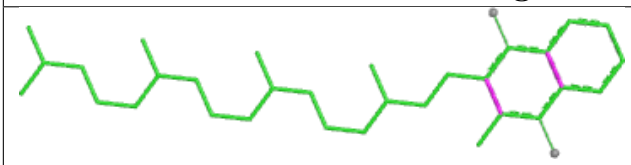


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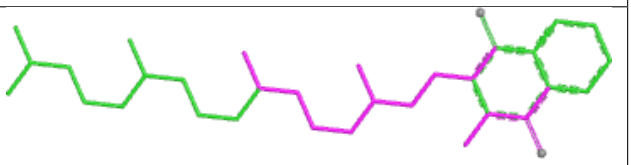


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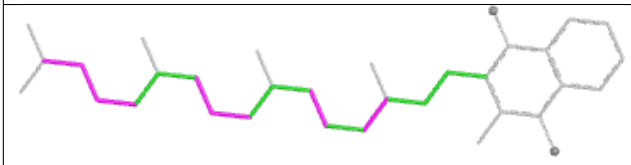
Ligand PQN B 5002



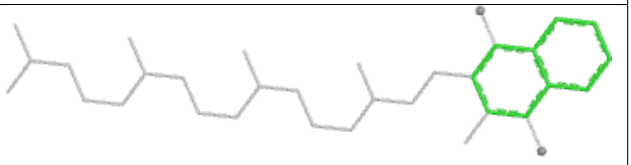
Bond lengths



Bond angles

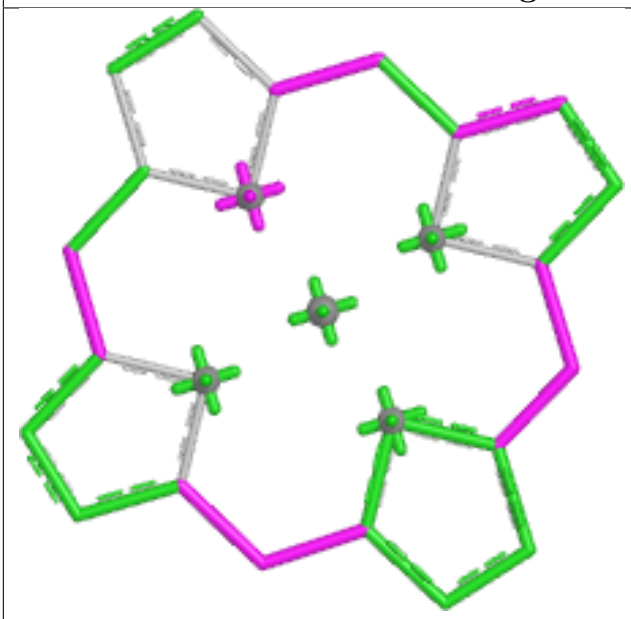


Torsions

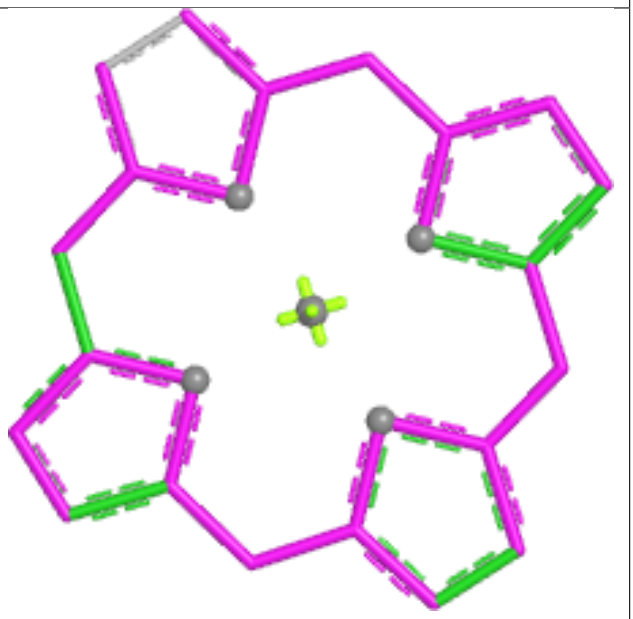


Rings

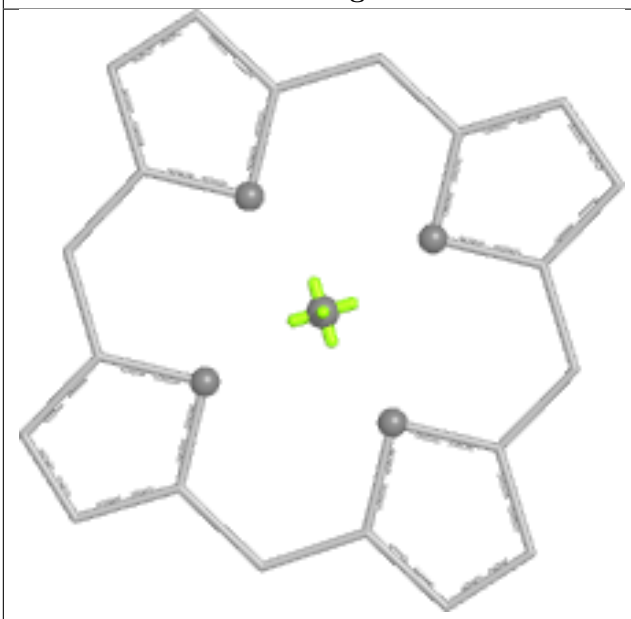
Ligand CLA 3 3011



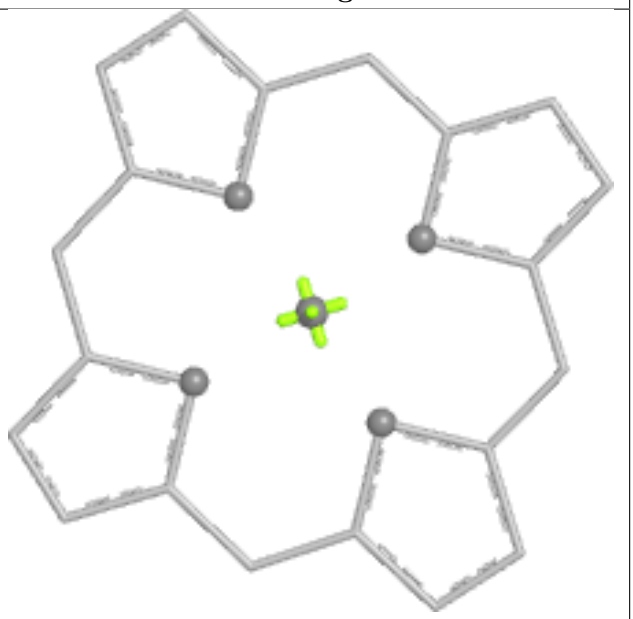
Bond lengths



Bond angles

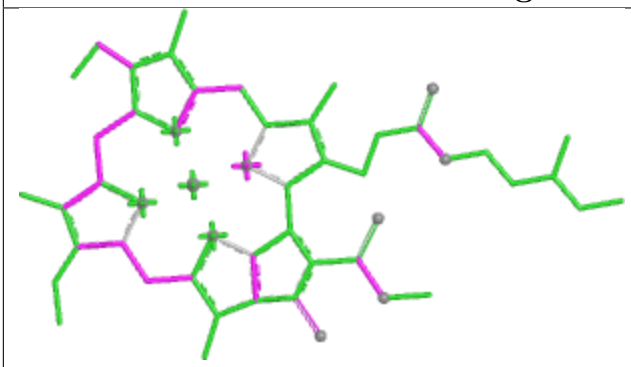


Torsions

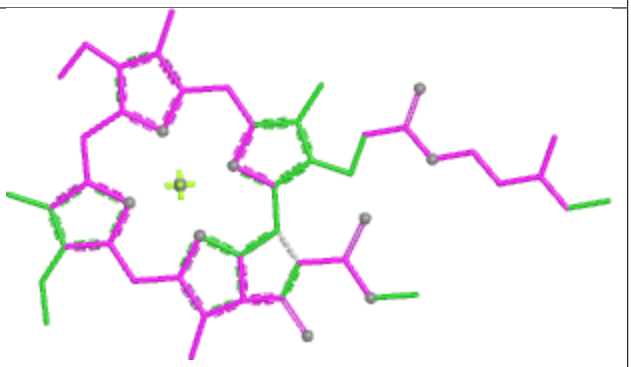


Rings

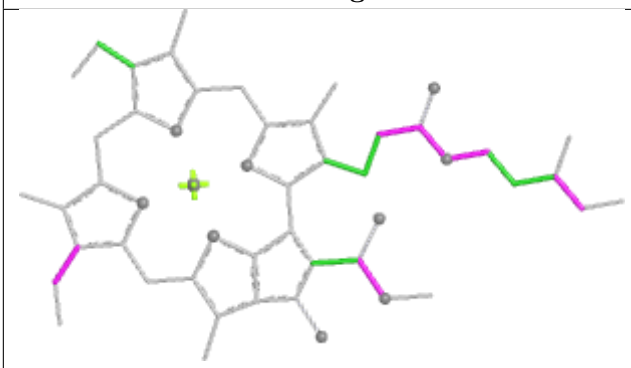
Ligand CLA B 1237



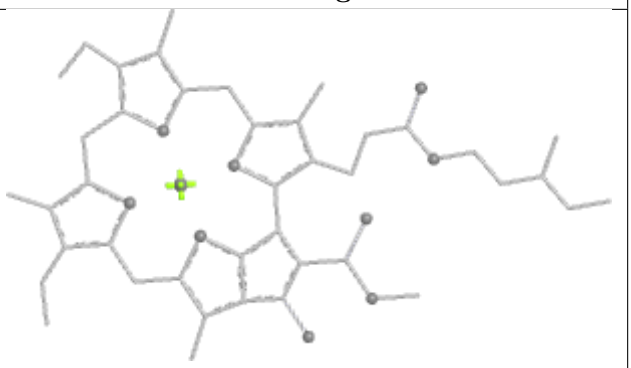
Bond lengths



Bond angles

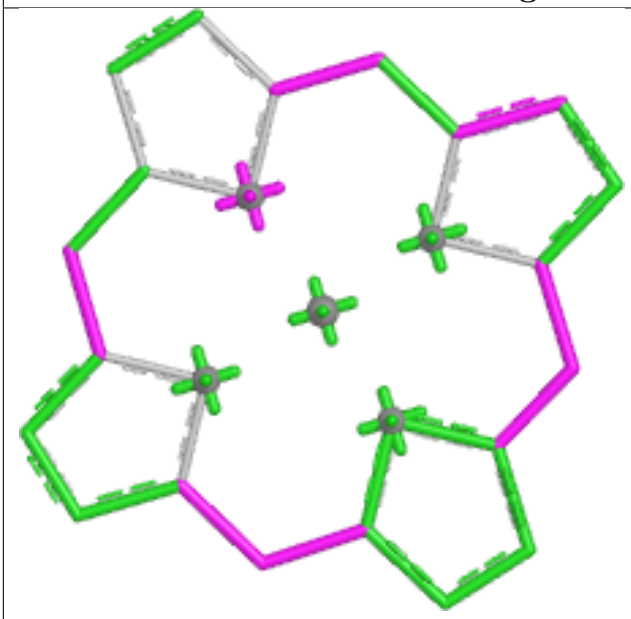


Torsions

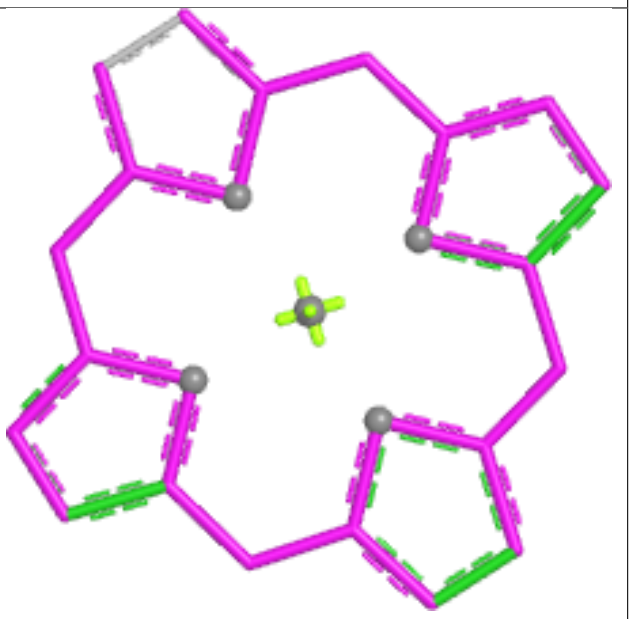


Rings

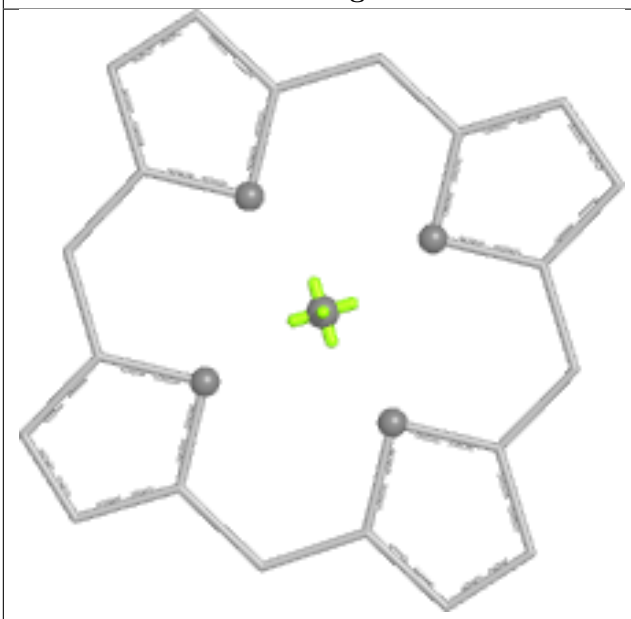
Ligand CLA 1 1014



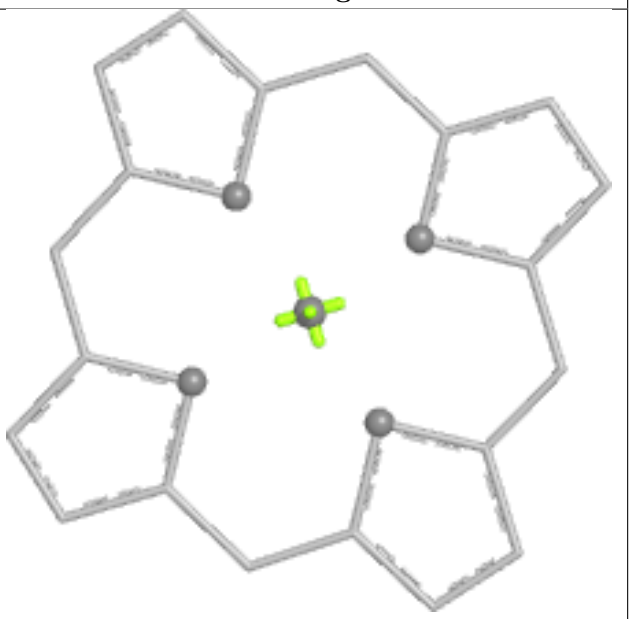
Bond lengths



Bond angles

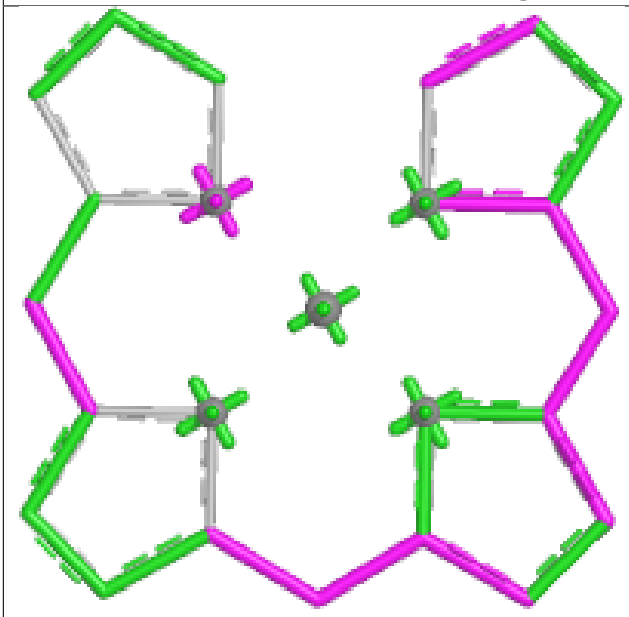


Torsions

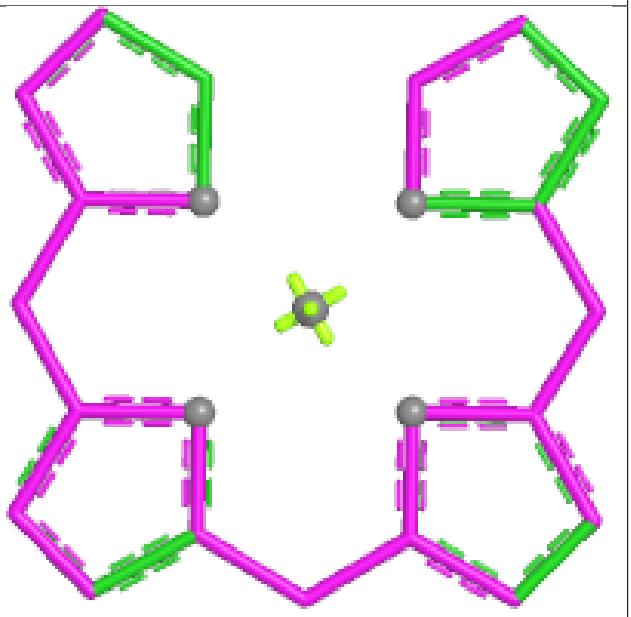


Rings

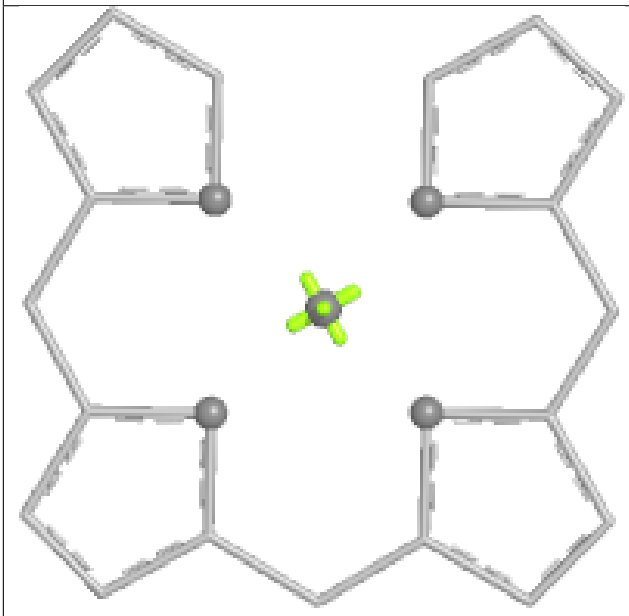
Ligand CLA A 1109



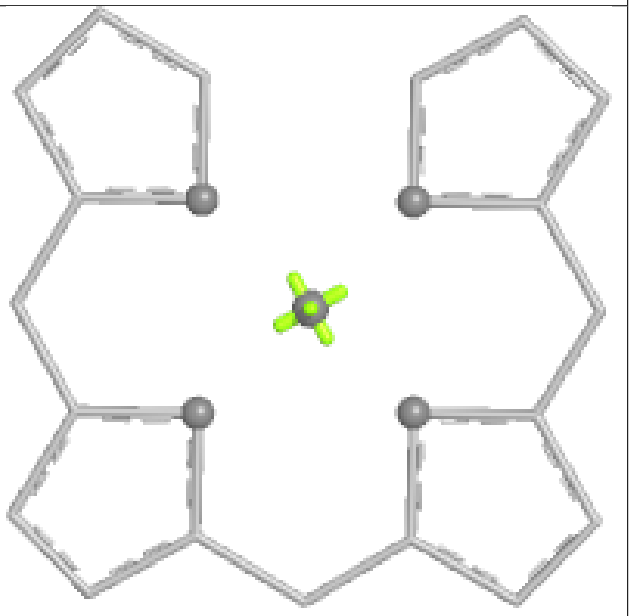
Bond lengths



Bond angles

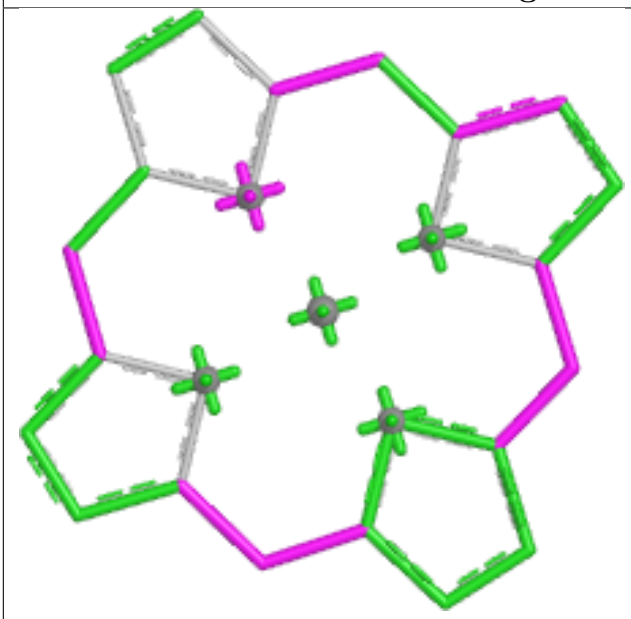


Torsions

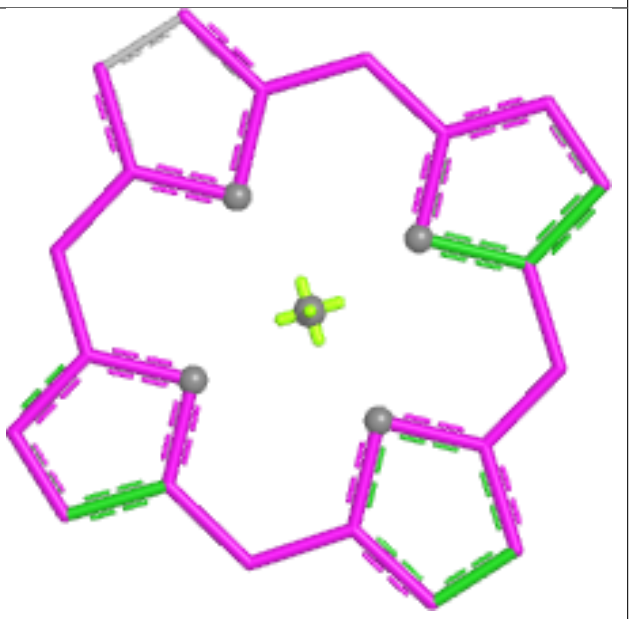


Rings

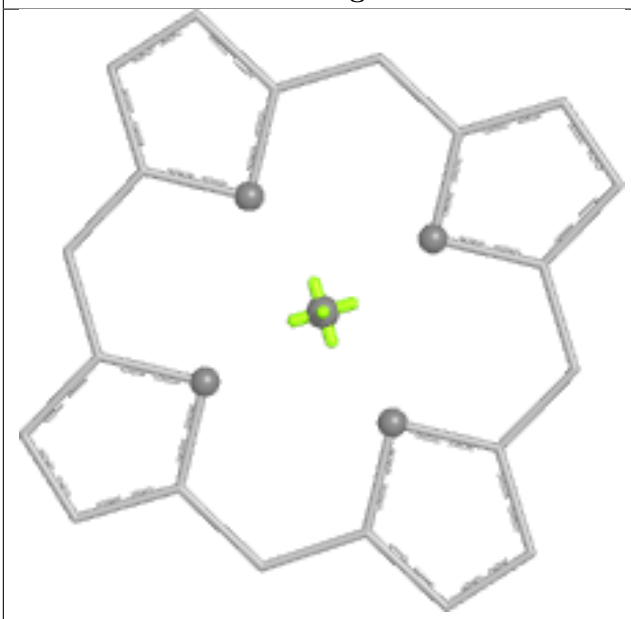
Ligand CLA 2 2013



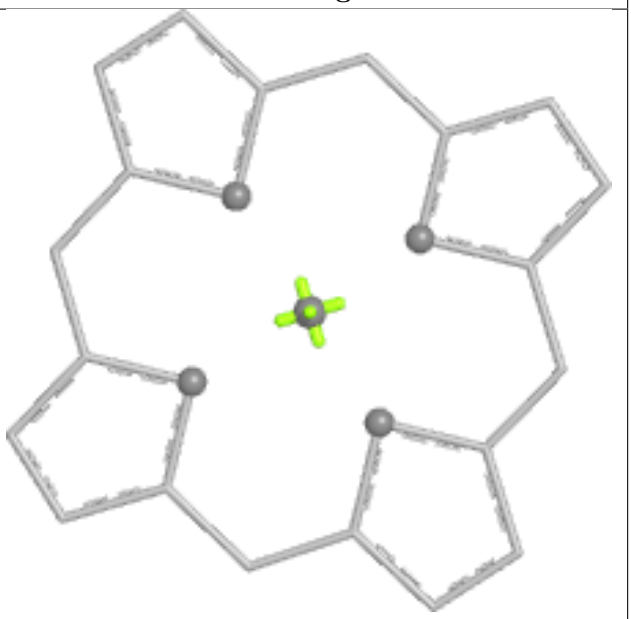
Bond lengths



Bond angles

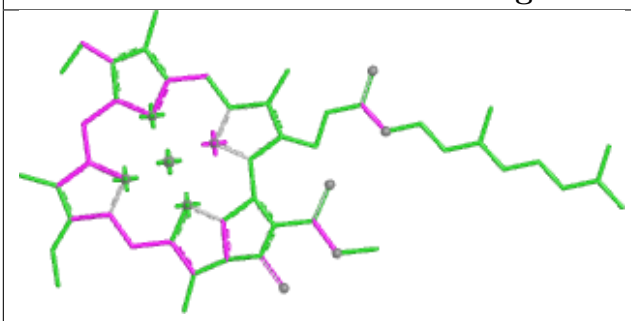


Torsions

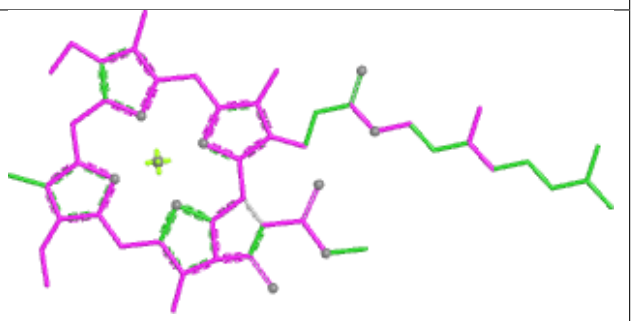


Rings

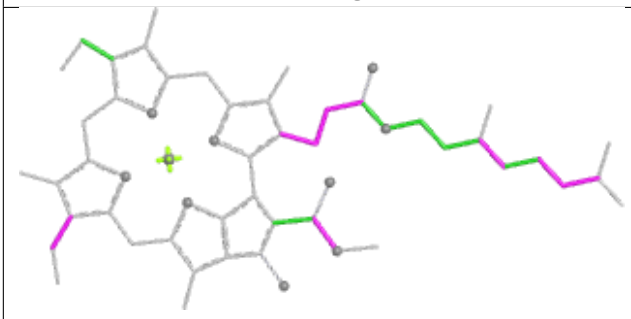
Ligand CLA B 1207



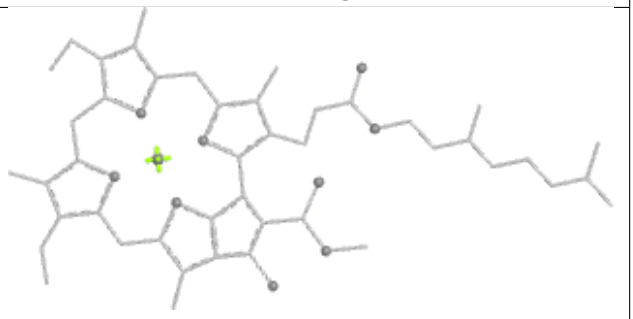
Bond lengths



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	728/754 (96%)	-0.45	18 (2%) 58 43	12, 39, 59, 72	0
2	B	732/732 (100%)	-0.53	9 (1%) 76 63	13, 39, 58, 64	0
3	C	80/80 (100%)	-0.49	0 100 100	32, 38, 46, 48	0
4	D	138/138 (100%)	-0.55	3 (2%) 62 47	25, 45, 53, 55	0
5	E	62/62 (100%)	-0.67	1 (1%) 70 56	41, 52, 59, 59	0
6	F	154/154 (100%)	-0.62	0 100 100	25, 47, 60, 62	0
7	G	95/95 (100%)	-0.41	2 (2%) 63 48	50, 61, 68, 73	0
8	H	75/75 (100%)	-0.73	0 100 100	43, 56, 75, 83	0
9	I	30/30 (100%)	-0.61	1 (3%) 49 36	39, 46, 55, 58	0
10	J	42/42 (100%)	-0.73	0 100 100	28, 55, 65, 67	0
11	K	0/38	-	-	-	-
12	L	164/164 (100%)	-0.45	4 (2%) 59 45	24, 49, 62, 69	0
13	N	85/85 (100%)	-0.64	0 100 100	25, 70, 87, 90	0
14	1	175/187 (93%)	-0.48	5 (2%) 53 39	28, 71, 84, 87	0
15	2	166/186 (89%)	-0.66	2 (1%) 76 63	25, 71, 86, 91	0
16	3	115/165 (69%)	-0.50	2 (1%) 69 54	57, 79, 88, 89	0
17	4	165/165 (100%)	-0.39	6 (3%) 46 33	23, 65, 72, 75	0
All	All	3006/3152 (95%)	-0.52	53 (1%) 67 53	12, 47, 78, 91	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	1	32	VAL	6.5
4	D	60	MET	5.8
1	A	502	THR	5.6
15	2	61	GLY	4.9
1	A	35	ALA	4.6

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 oligosaccharides 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
18	CLA	F	1303	25/65	0.94	0.08	76,77,77,77	0
18	CLA	1	1007	25/65	0.94	0.09	68,68,69,69	0
18	CLA	2	2001	25/65	0.94	0.08	61,63,65,65	0
18	CLA	2	2015	25/65	0.94	0.07	92,93,93,93	0
18	CLA	3	3009	25/65	0.94	0.10	94,94,94,95	0
18	CLA	3	3012	25/65	0.94	0.07	77,79,81,81	0
20	BCR	F	6016	40/40	0.94	0.09	28,33,39,40	0
18	CLA	1	1005	25/65	0.95	0.10	77,78,78,78	0
18	CLA	A	1309	25/65	0.95	0.10	112,112,112,112	0
18	CLA	1	1008	25/65	0.95	0.07	79,79,79,80	0
18	CLA	2	2005	25/65	0.95	0.07	64,65,66,66	0
18	CLA	F	1305	25/65	0.95	0.07	78,79,79,79	0
18	CLA	2	2011	25/65	0.95	0.08	93,94,94,94	0
18	CLA	F	1306	25/65	0.95	0.07	87,88,89,89	0
18	CLA	G	1233	51/65	0.95	0.06	61,66,67,67	0
18	CLA	J	1307	25/65	0.95	0.07	77,78,78,79	0
18	CLA	4	4005	25/65	0.95	0.09	60,62,63,63	0
18	CLA	4	4001	25/65	0.95	0.11	82,83,83,84	0
18	CLA	L	1504	55/65	0.95	0.11	32,67,68,71	0
18	CLA	K	1141	25/65	0.96	0.06	78,79,79,80	0
18	CLA	K	1150	25/65	0.96	0.07	88,90,90,90	0
18	CLA	L	1125	25/65	0.96	0.07	80,80,82,82	0
18	CLA	A	1151	25/65	0.96	0.06	73,76,77,77	0
18	CLA	A	1118	25/65	0.96	0.07	89,90,91,91	0
18	CLA	1	1013	25/65	0.96	0.07	86,87,88,88	0
18	CLA	1	1011	25/65	0.96	0.06	94,95,95,96	0
18	CLA	1	1001	25/65	0.96	0.08	63,64,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	B	1201	25/65	0.96	0.09	50,51,53,53	0
18	CLA	1	1002	25/65	0.96	0.08	86,86,87,88	0
18	CLA	B	1232	55/65	0.96	0.08	74,91,93,93	0
18	CLA	B	1301	25/65	0.96	0.06	73,74,75,75	0
18	CLA	2	2006	25/65	0.96	0.08	81,82,82,83	0
18	CLA	2	2010	25/65	0.96	0.07	90,90,91,91	0
18	CLA	A	1119	55/65	0.96	0.11	60,66,68,69	0
18	CLA	A	1127	25/65	0.96	0.10	58,59,60,60	0
18	CLA	2	2012	25/65	0.96	0.09	99,100,100,100	0
18	CLA	A	1144	25/65	0.96	0.08	101,101,101,102	0
18	CLA	F	4015	25/65	0.96	0.09	132,133,133,133	0
18	CLA	A	1147	25/65	0.96	0.07	66,67,68,69	0
18	CLA	3	3001	25/65	0.96	0.11	137,137,138,138	0
18	CLA	3	3002	25/65	0.96	0.05	68,70,70,70	0
18	CLA	3	3015	25/65	0.96	0.06	72,73,74,75	0
18	CLA	4	1009	25/65	0.96	0.08	78,79,79,79	0
18	CLA	4	4009	25/65	0.96	0.07	80,81,82,82	0
18	CLA	4	4004	25/65	0.96	0.07	71,72,74,74	0
18	CLA	H	1505	25/65	0.96	0.09	84,85,86,86	0
18	CLA	4	4006	25/65	0.96	0.09	82,83,84,85	0
18	CLA	A	1148	25/65	0.96	0.09	93,94,95,95	0
18	CLA	4	4007	25/65	0.96	0.08	89,91,91,91	0
18	CLA	4	4002	25/65	0.96	0.06	65,66,67,67	0
18	CLA	4	4003	25/65	0.96	0.07	80,81,81,81	0
20	BCR	A	6011	40/40	0.96	0.08	9,12,19,21	0
18	CLA	J	1308	25/65	0.96	0.07	106,107,107,108	0
20	BCR	I	6018	40/40	0.96	0.09	6,19,26,28	0
18	CLA	B	1236	46/65	0.97	0.08	34,44,46,47	0
18	CLA	B	1239	55/65	0.97	0.08	27,52,53,55	0
18	CLA	B	1242	47/65	0.97	0.10	85,91,92,94	0
18	CLA	A	1102	25/65	0.97	0.08	72,73,75,75	0
18	CLA	F	1139	44/65	0.97	0.08	36,40,42,43	0
18	CLA	F	1302	55/65	0.97	0.10	19,75,77,79	0
18	CLA	A	1104	25/65	0.97	0.06	40,42,43,44	0
18	CLA	A	1120	25/65	0.97	0.07	76,78,79,80	0
18	CLA	A	1122	55/65	0.97	0.07	18,39,41,43	0
18	CLA	A	1123	55/65	0.97	0.08	37,46,49,50	0
18	CLA	A	1124	25/65	0.97	0.06	48,51,52,53	0
18	CLA	G	1248	25/65	0.97	0.07	109,110,111,111	0
18	CLA	H	1501	55/65	0.97	0.08	49,68,70,73	0
18	CLA	A	1126	55/65	0.97	0.08	15,40,42,44	0
18	CLA	I	1204	55/65	0.97	0.08	40,44,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	A	1106	41/65	0.97	0.09	16,20,22,24	0
18	CLA	A	1128	55/65	0.97	0.07	20,37,39,40	0
18	CLA	J	2107	61/65	0.97	0.07	40,62,63,63	0
18	CLA	A	1129	55/65	0.97	0.08	35,58,60,61	0
18	CLA	A	1131	44/65	0.97	0.08	35,39,42,44	0
18	CLA	K	1153	25/65	0.97	0.06	54,55,56,56	0
18	CLA	A	1133	25/65	0.97	0.06	44,46,47,48	0
18	CLA	L	1130	50/65	0.97	0.09	57,66,69,70	0
18	CLA	L	1502	51/65	0.97	0.08	36,63,65,65	0
18	CLA	A	1134	25/65	0.97	0.07	49,51,52,52	0
18	CLA	A	1135	45/65	0.97	0.09	39,54,55,56	0
18	CLA	1	1006	25/65	0.97	0.05	60,62,63,63	0
18	CLA	A	1137	55/65	0.97	0.08	20,28,30,32	0
18	CLA	1	1010	25/65	0.97	0.08	81,81,82,82	0
18	CLA	A	1140	55/65	0.97	0.10	12,39,41,43	0
18	CLA	A	1142	25/65	0.97	0.07	88,89,90,91	0
18	CLA	A	1143	25/65	0.97	0.09	116,118,118,118	0
18	CLA	A	1108	50/65	0.97	0.06	52,74,76,76	0
18	CLA	1	1003	25/65	0.97	0.07	84,85,86,86	0
18	CLA	A	1146	25/65	0.97	0.06	70,72,73,73	0
18	CLA	1	1014	25/65	0.97	0.05	67,68,70,70	0
18	CLA	A	1110	25/65	0.97	0.05	70,71,72,72	0
18	CLA	A	1111	25/65	0.97	0.08	65,66,68,68	0
18	CLA	A	1113	50/65	0.97	0.08	41,60,62,63	0
18	CLA	A	1152	25/65	0.97	0.08	68,69,70,71	0
18	CLA	A	9011	55/65	0.97	0.09	2,26,28,29	0
18	CLA	A	9013	46/65	0.97	0.10	11,17,21,24	0
18	CLA	A	1115	47/65	0.97	0.07	40,44,48,50	0
18	CLA	2	2007	25/65	0.97	0.05	79,80,81,81	0
18	CLA	2	2002	25/65	0.97	0.08	103,103,104,104	0
18	CLA	2	2003	25/65	0.97	0.06	114,114,115,115	0
18	CLA	3	2009	25/65	0.97	0.06	94,94,95,95	0
18	CLA	B	9010	47/65	0.97	0.09	23,37,40,41	0
18	CLA	3	3004	25/65	0.97	0.07	76,77,78,78	0
18	CLA	3	3005	25/65	0.97	0.06	95,96,97,97	0
18	CLA	B	9012	55/65	0.97	0.11	16,47,50,52	0
18	CLA	3	3006	25/65	0.97	0.07	112,113,113,114	0
18	CLA	3	3013	25/65	0.97	0.07	77,78,78,78	0
18	CLA	3	3010	25/65	0.97	0.07	92,93,93,93	0
18	CLA	A	1116	25/65	0.97	0.09	81,82,83,83	0
18	CLA	3	3011	25/65	0.97	0.07	107,107,108,108	0
18	CLA	B	1205	55/65	0.97	0.08	17,41,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	B	1208	55/65	0.97	0.07	36,39,41,42	0
18	CLA	3	3003	25/65	0.97	0.04	67,68,70,70	0
18	CLA	3	3008	25/65	0.97	0.07	90,90,91,91	0
18	CLA	4	1304	55/65	0.97	0.08	40,77,78,79	0
18	CLA	B	1210	25/65	0.97	0.10	75,76,76,77	0
18	CLA	B	1212	60/65	0.97	0.10	59,73,75,77	0
18	CLA	B	1216	56/65	0.97	0.10	66,72,73,73	0
18	CLA	B	1217	50/65	0.97	0.08	60,66,68,68	0
18	CLA	B	1219	51/65	0.97	0.07	27,47,48,49	0
18	CLA	4	4013	25/65	0.97	0.06	86,86,87,87	0
18	CLA	4	4010	25/65	0.97	0.10	99,99,99,99	0
18	CLA	4	4011	25/65	0.97	0.07	51,52,53,54	0
18	CLA	4	4012	25/65	0.97	0.08	63,65,66,67	0
18	CLA	B	1220	60/65	0.97	0.08	31,39,50,53	0
18	CLA	B	1221	48/65	0.97	0.08	20,31,38,42	0
18	CLA	B	1222	65/65	0.97	0.09	46,69,70,73	0
18	CLA	B	1228	55/65	0.97	0.08	42,46,47,49	0
18	CLA	4	4008	25/65	0.97	0.09	72,74,74,74	0
19	PQN	A	5001	33/33	0.97	0.08	15,23,34,36	0
19	PQN	B	5002	33/33	0.97	0.08	8,18,21,21	0
18	CLA	B	1229	49/65	0.97	0.09	35,48,50,51	0
20	BCR	B	6017	40/40	0.97	0.09	27,33,46,47	0
18	CLA	A	1117	25/65	0.97	0.06	47,48,49,49	0
18	CLA	B	1235	55/65	0.97	0.09	31,40,42,44	0
20	BCR	L	6020	40/40	0.97	0.08	11,24,35,38	0
18	CLA	B	9022	54/65	0.98	0.08	28,31,41,41	0
18	CLA	2	2008	25/65	0.98	0.05	60,61,62,63	0
18	CLA	B	9023	47/65	0.98	0.08	36,40,41,43	0
18	CLA	A	1103	47/65	0.98	0.09	67,77,78,79	0
18	CLA	B	1223	25/65	0.98	0.06	46,48,49,50	0
18	CLA	B	1224	51/65	0.98	0.09	47,55,56,57	0
18	CLA	B	1225	45/65	0.98	0.07	34,50,52,52	0
18	CLA	B	1226	25/65	0.98	0.07	50,53,54,54	0
18	CLA	B	1227	50/65	0.98	0.06	34,41,44,45	0
18	CLA	B	1202	50/65	0.98	0.08	23,37,39,42	0
18	CLA	B	1203	48/65	0.98	0.06	2,23,24,26	0
18	CLA	B	1230	25/65	0.98	0.09	73,75,76,76	0
18	CLA	L	1503	46/65	0.98	0.06	19,22,25,28	0
18	CLA	3	3007	25/65	0.98	0.05	80,81,82,83	0
18	CLA	B	1231	46/65	0.98	0.07	36,46,49,51	0
18	CLA	1	1004	25/65	0.98	0.09	88,89,89,90	0
18	CLA	A	1132	25/65	0.98	0.06	27,29,31,32	0

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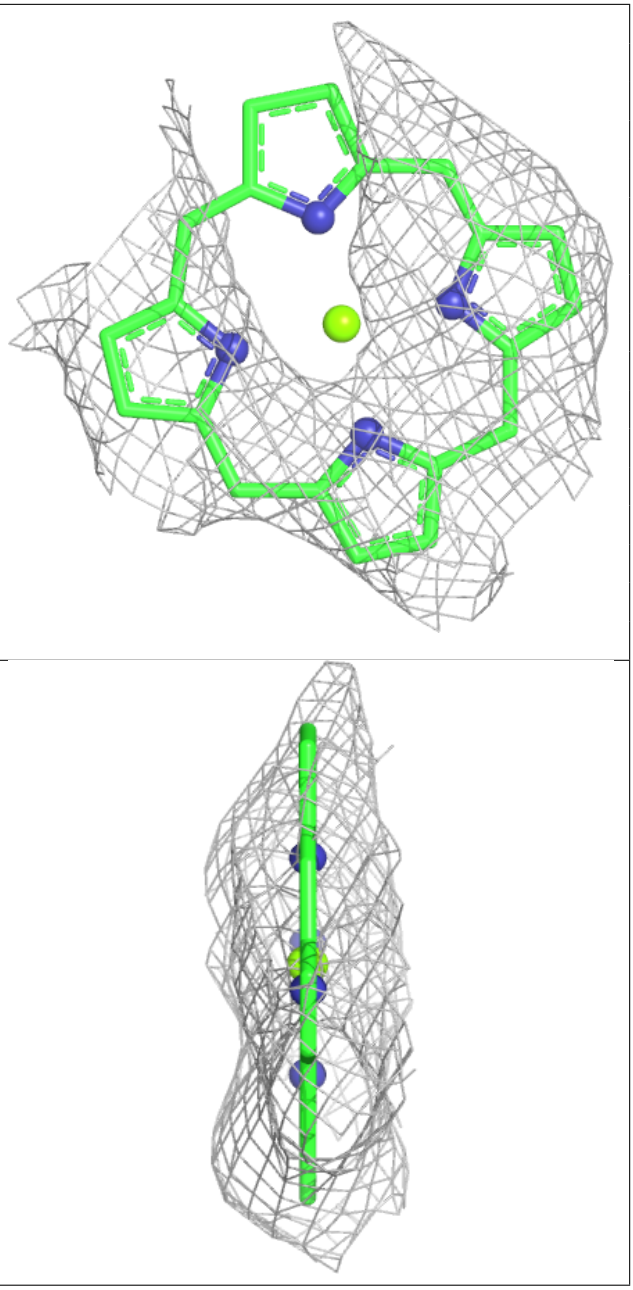
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	B	1234	50/65	0.98	0.08	35,53,55,56	0
18	CLA	B	1206	25/65	0.98	0.08	50,54,55,56	0
18	CLA	B	1207	55/65	0.98	0.07	19,30,35,37	0
18	CLA	B	1237	51/65	0.98	0.08	29,59,62,62	0
18	CLA	1	1012	25/65	0.98	0.06	76,77,77,77	0
18	CLA	B	1238	54/65	0.98	0.08	13,27,32,33	0
18	CLA	A	1107	57/65	0.98	0.06	21,26,30,33	0
18	CLA	B	1241	25/65	0.98	0.09	103,104,104,104	0
18	CLA	B	1209	55/65	0.98	0.06	32,50,53,54	0
18	CLA	A	1101	25/65	0.98	0.07	61,63,64,64	0
18	CLA	B	1211	25/65	0.98	0.07	52,54,55,55	0
18	CLA	2	2004	25/65	0.98	0.07	83,84,84,85	0
18	CLA	F	1240	25/65	0.98	0.04	43,44,45,46	0
18	CLA	A	1109	24/65	0.98	0.07	48,49,50,51	0
18	CLA	B	1213	25/65	0.98	0.08	79,81,82,82	0
18	CLA	2	2013	25/65	0.98	0.07	81,82,84,84	0
18	CLA	B	1214	49/65	0.98	0.07	51,69,70,71	0
18	CLA	B	1215	52/65	0.98	0.06	11,16,27,30	0
18	CLA	B	1138	56/65	0.98	0.06	18,47,50,53	0
18	CLA	A	1136	55/65	0.98	0.06	40,45,57,58	0
18	CLA	B	1218	51/65	0.98	0.05	20,47,50,51	0
18	CLA	A	1105	25/65	0.98	0.08	83,83,84,84	0
21	SF4	B	3101	8/8	1.00	0.02	14,21,22,25	0
21	SF4	C	3102	8/8	1.00	0.03	19,21,24,26	0
21	SF4	C	3103	8/8	1.00	0.03	10,12,15,15	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.

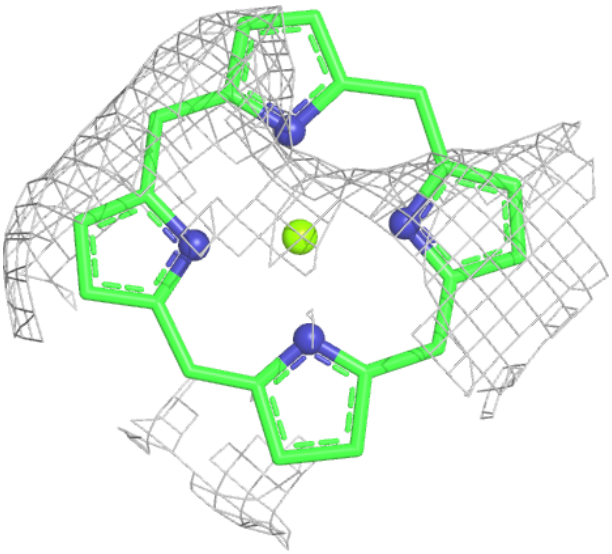
Electron density around CLA F 1303:

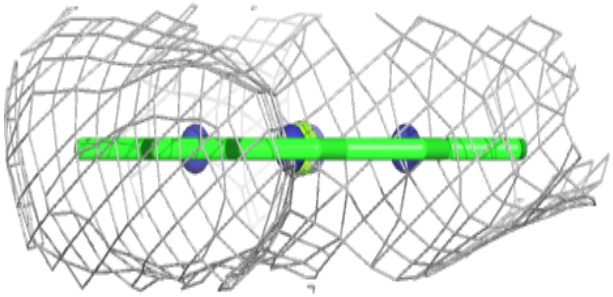
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

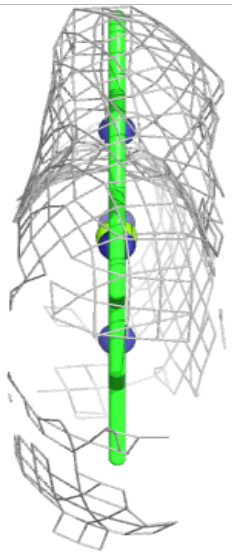


Electron density around CLA 1 1007:

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

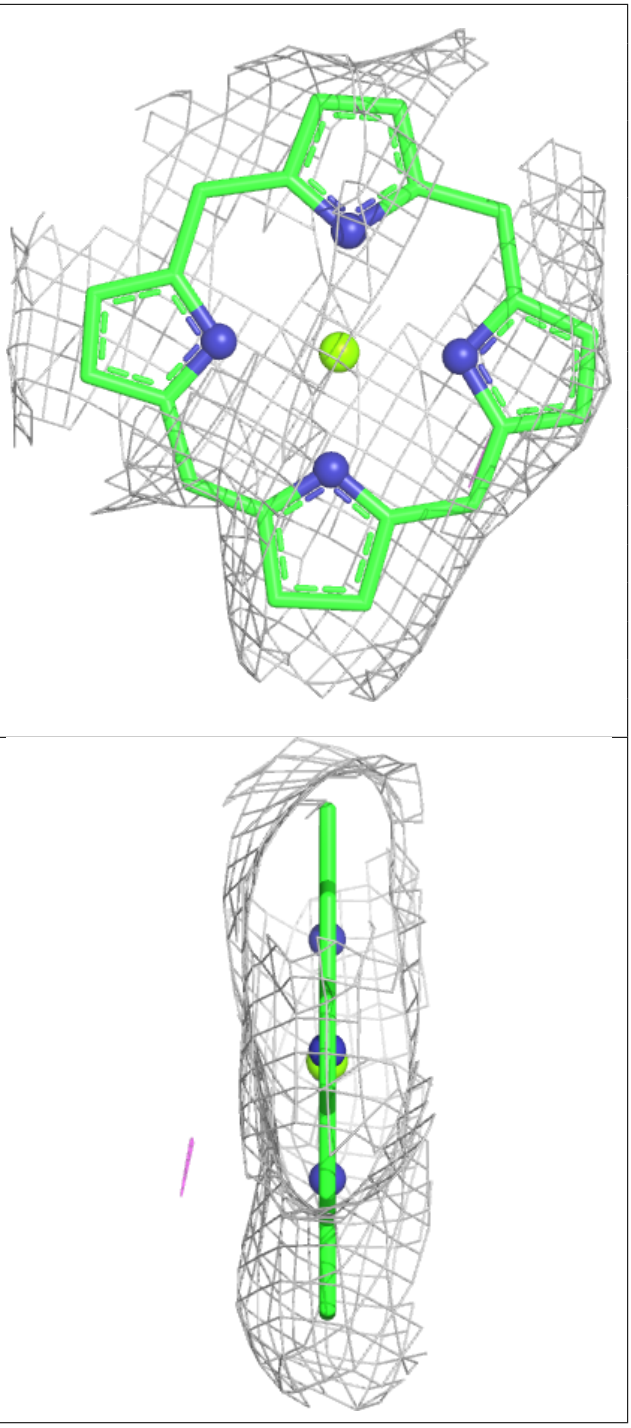






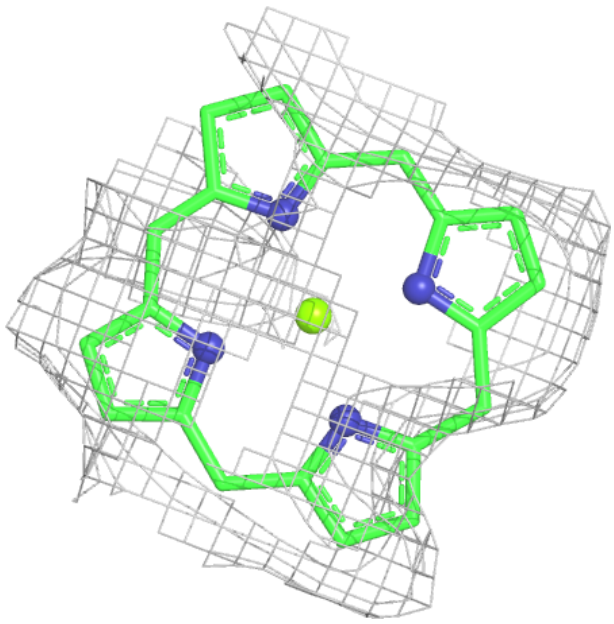
Electron density around CLA 2 2001:

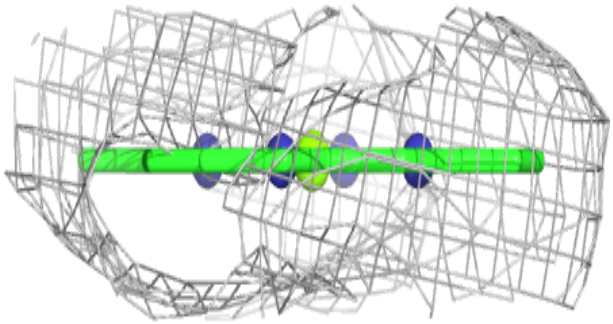
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

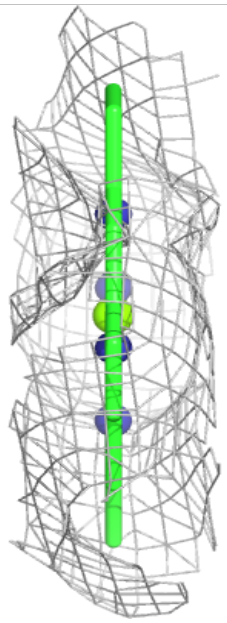


Electron density around CLA 2 2015:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

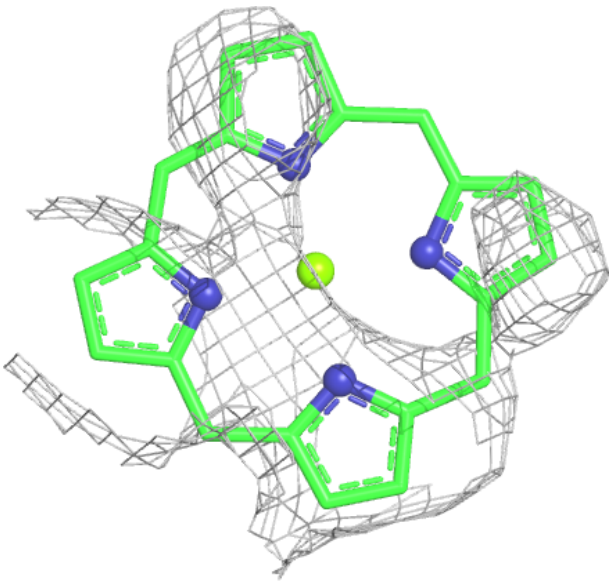


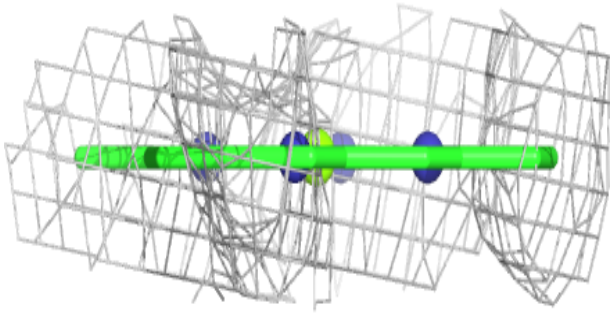


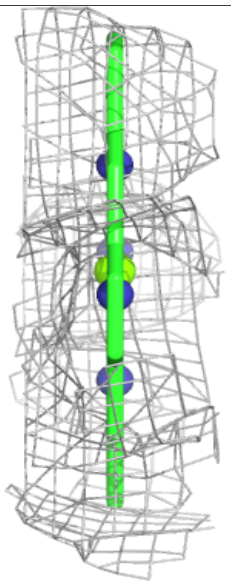


Electron density around CLA 3 3009:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

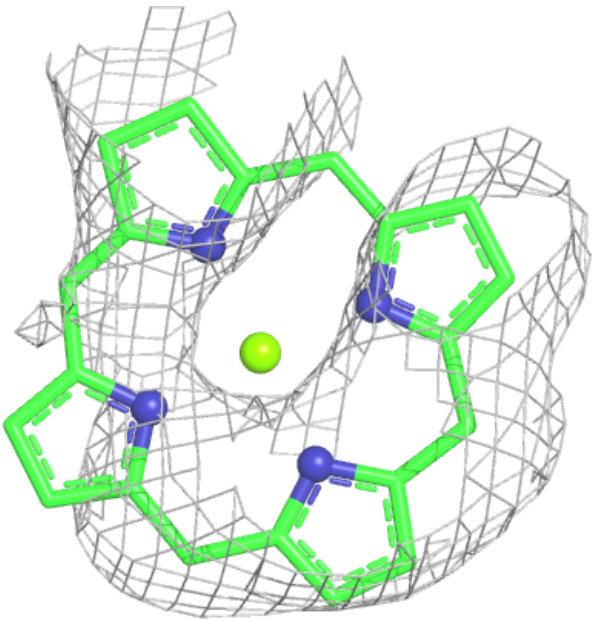


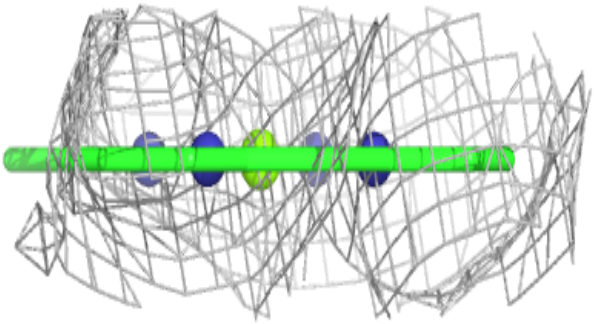


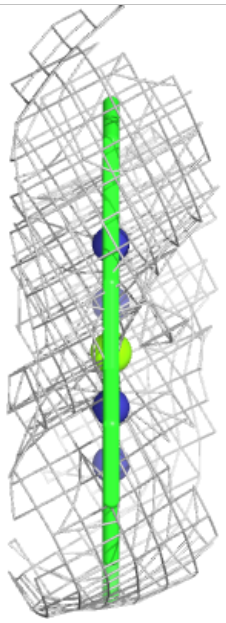


Electron density around CLA 3 3012:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

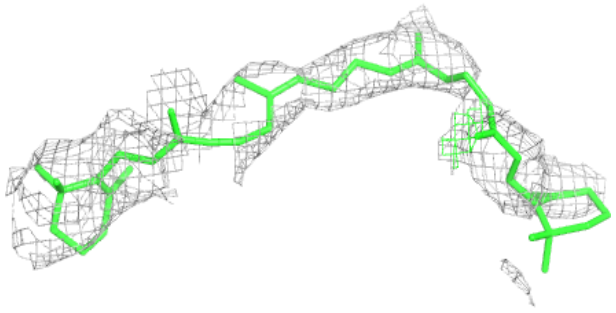




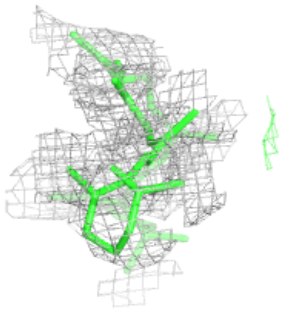


Electron density around BCR F 6016:

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

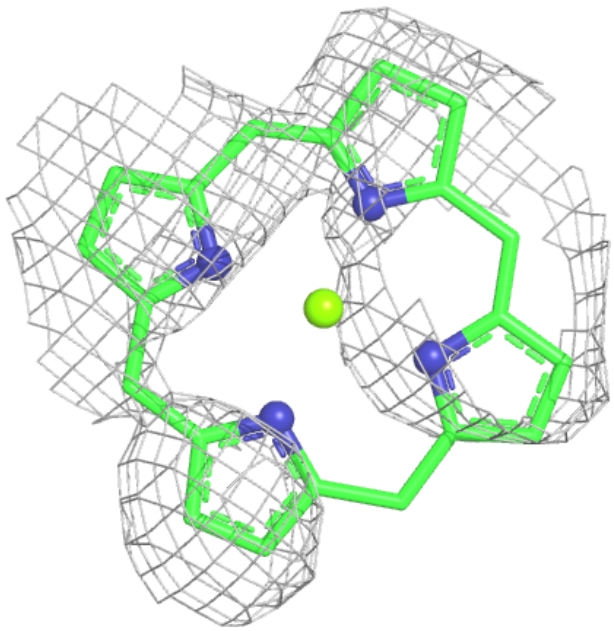


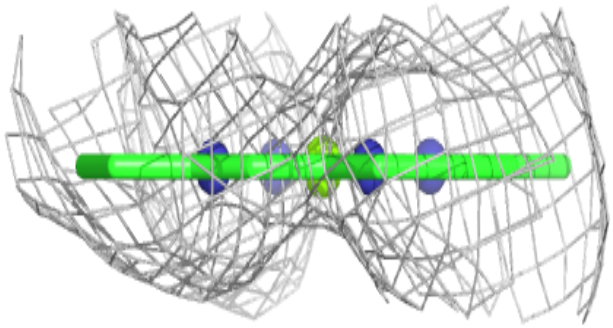


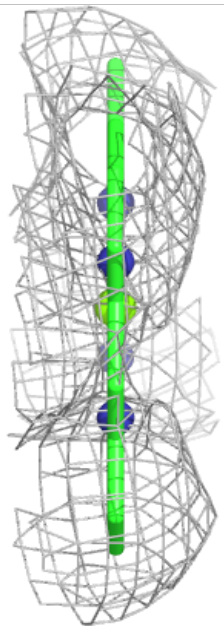


Electron density around CLA 1 1005:

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

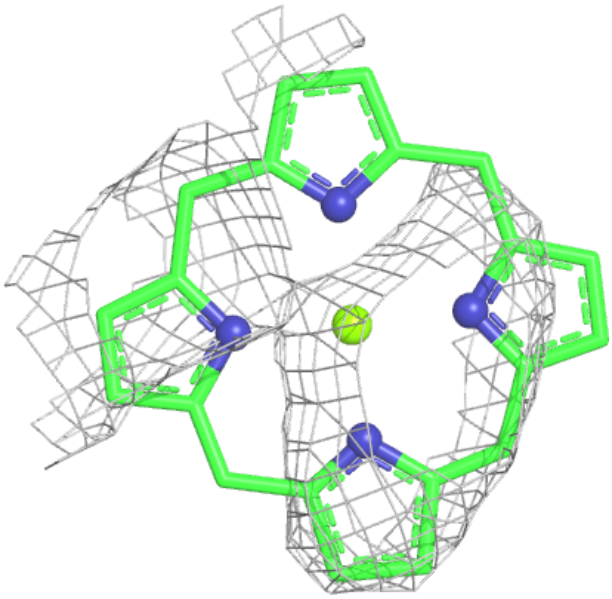


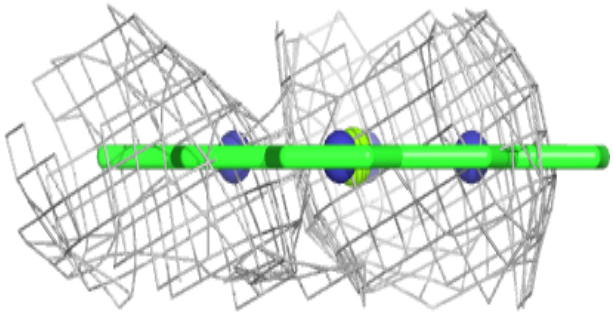


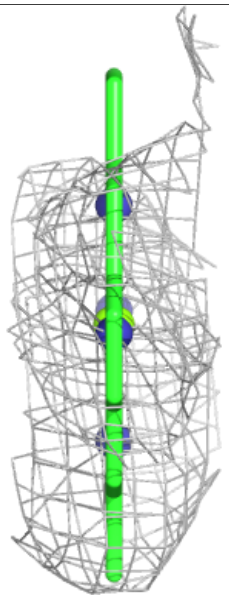


Electron density around CLA A 1309:

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

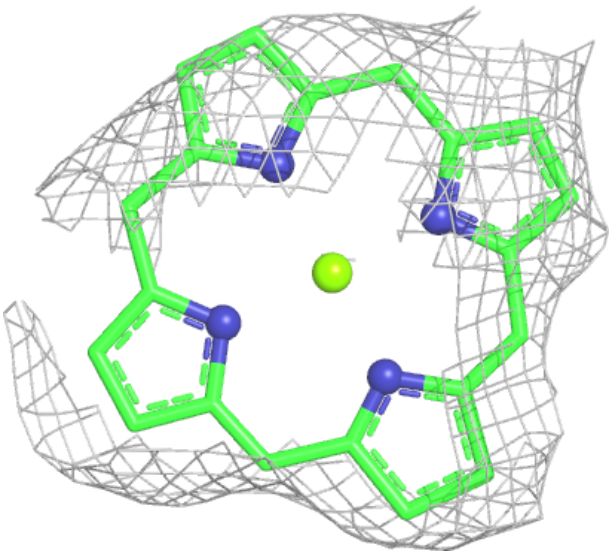


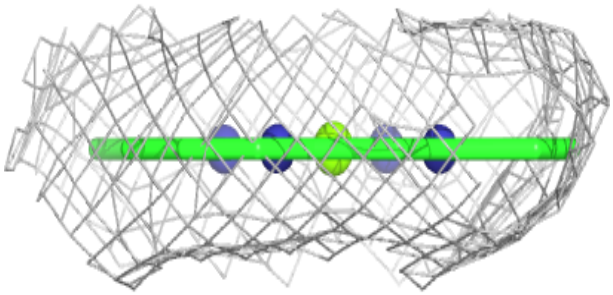


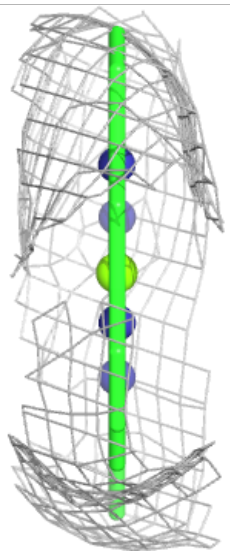


Electron density around CLA 1 1008:

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

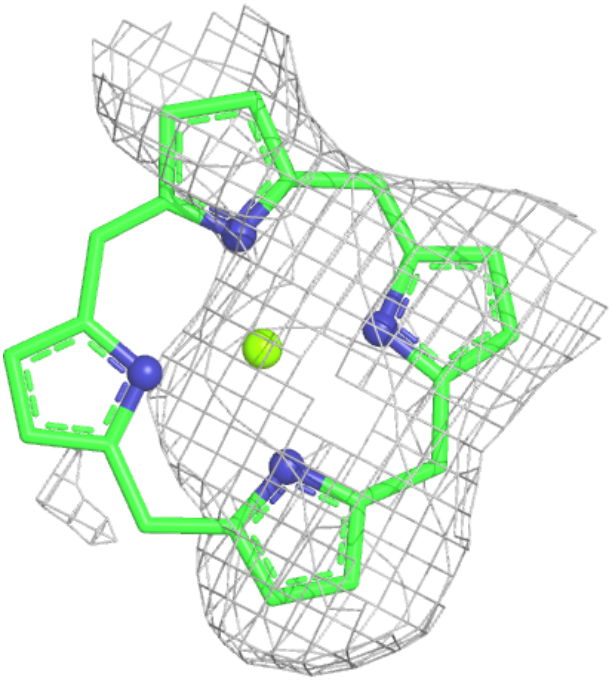


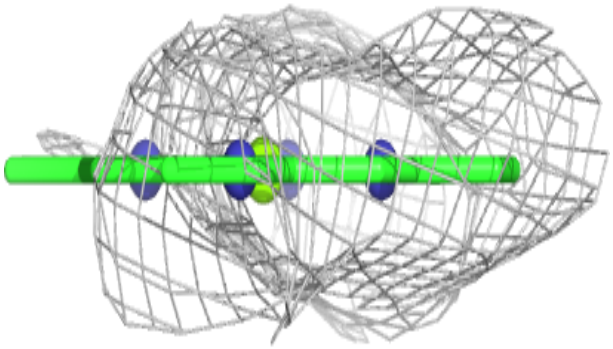


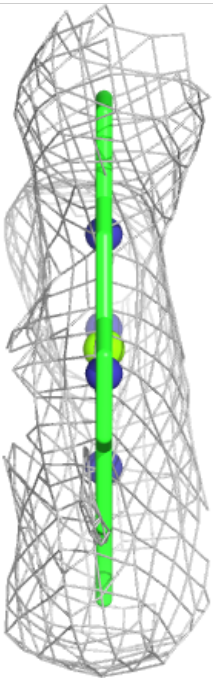


Electron density around CLA 2 2005:

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

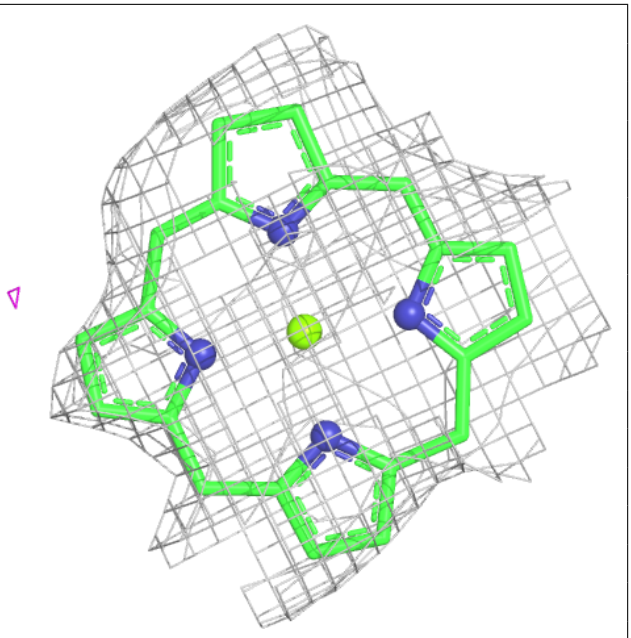


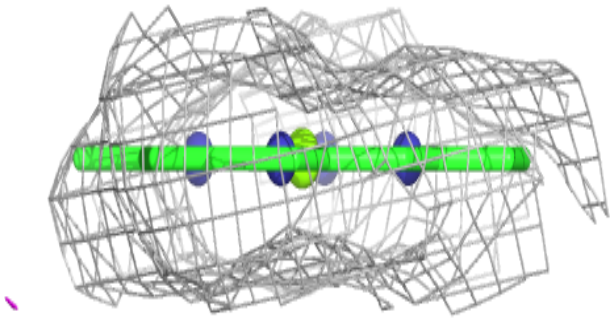


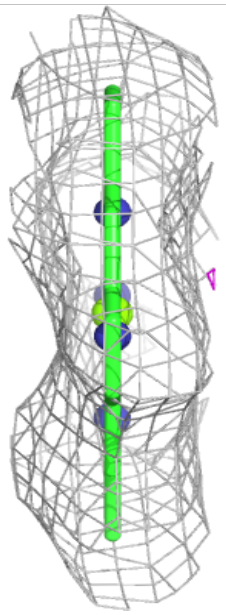


Electron density around CLA F 1305:

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

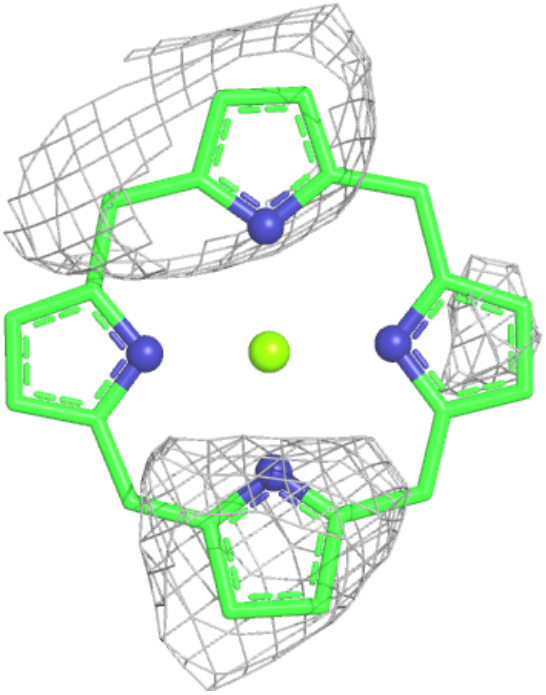


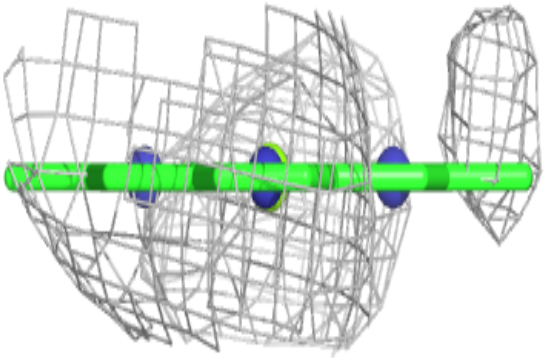


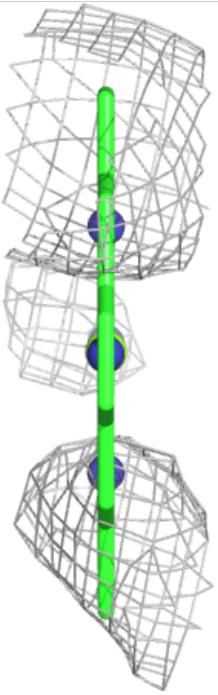


Electron density around CLA 2 2011:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

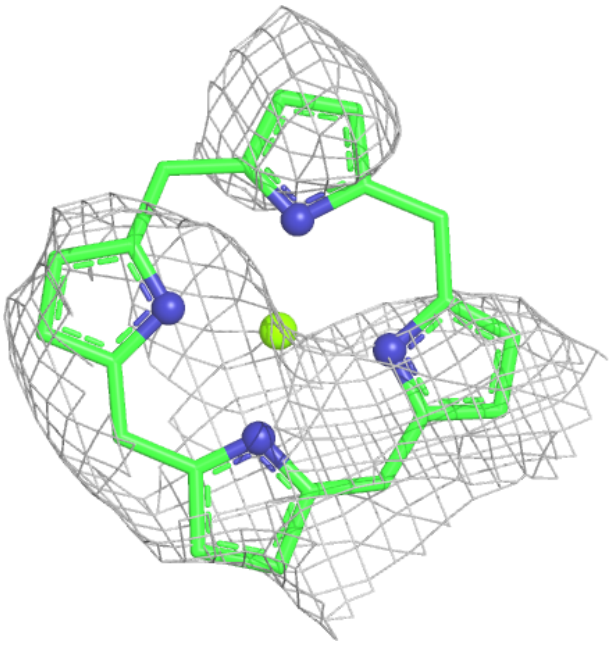


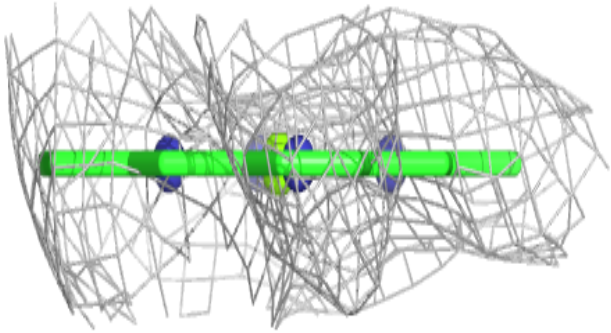


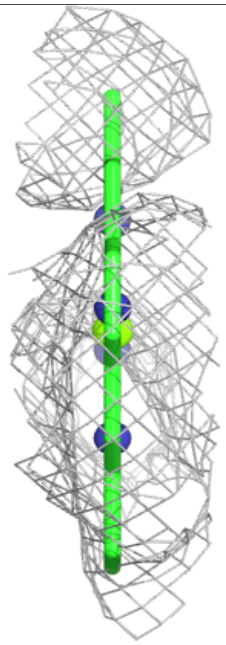


Electron density around CLA F 1306:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

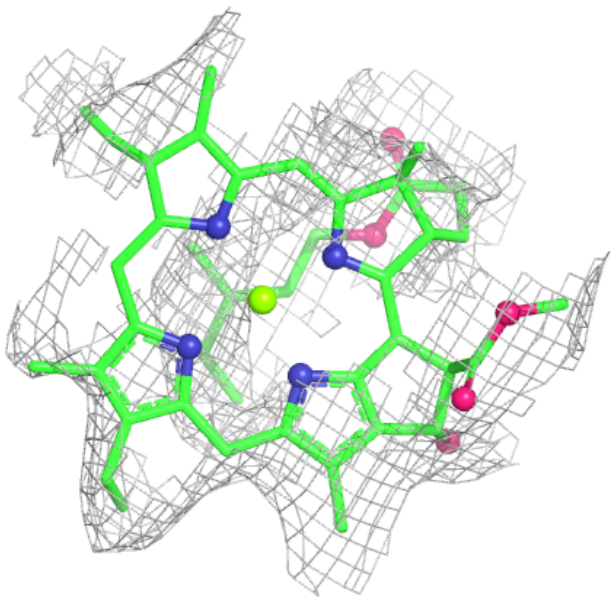


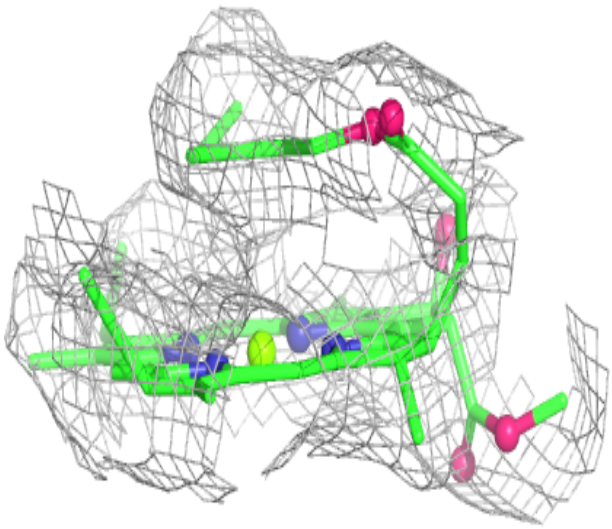


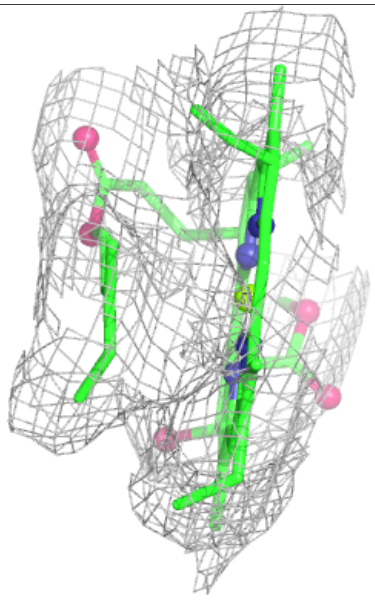


Electron density around CLA G 1233:

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

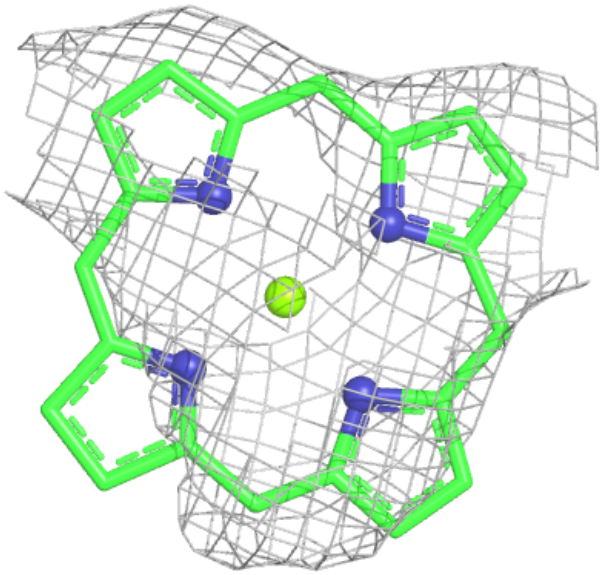


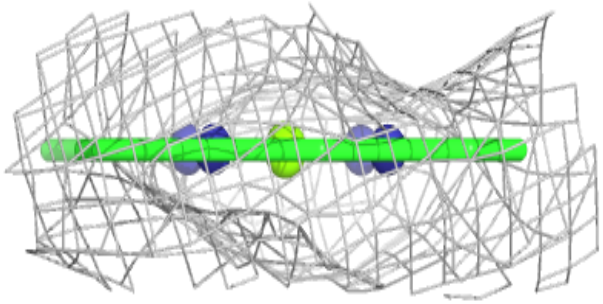


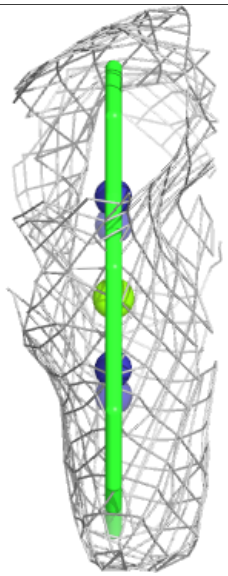


Electron density around CLA J 1307:

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

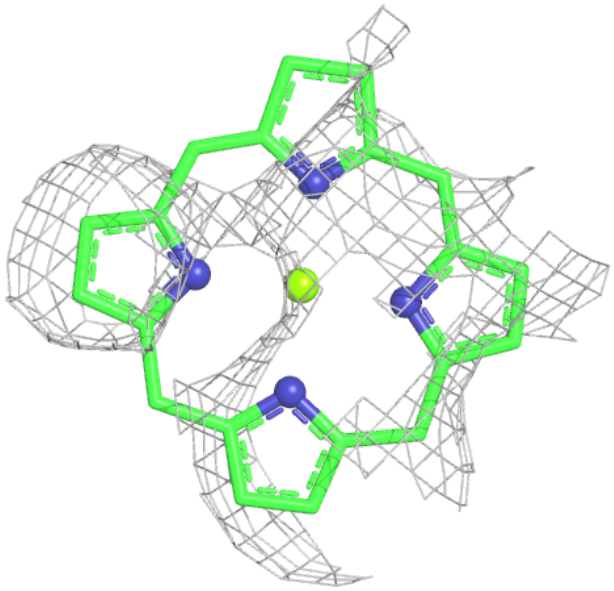


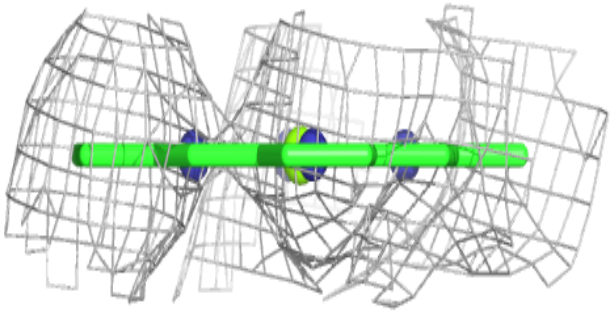


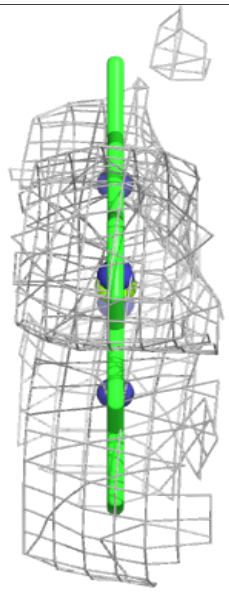


Electron density around CLA 4 4005:

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

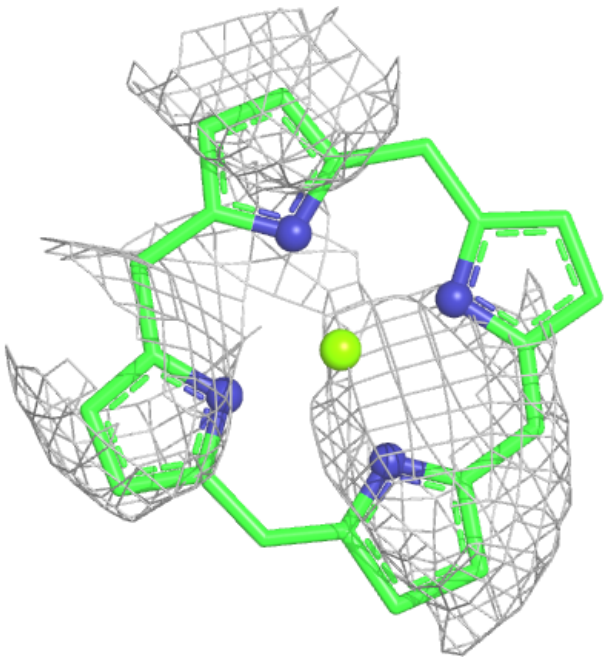


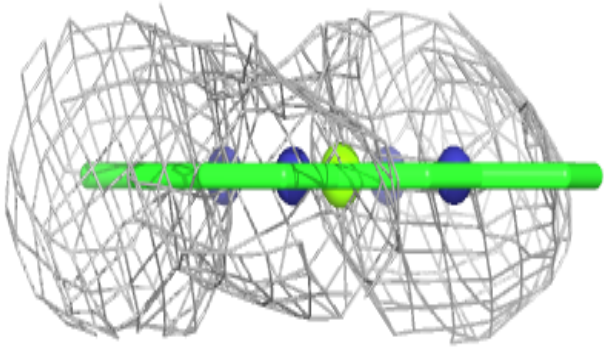


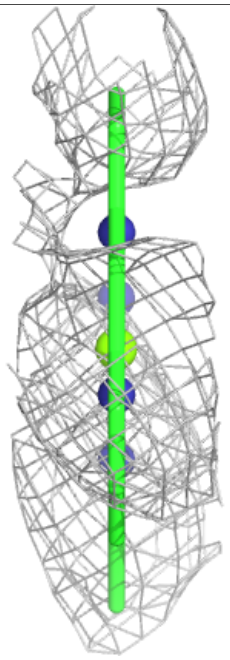


Electron density around CLA 4 4001:

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

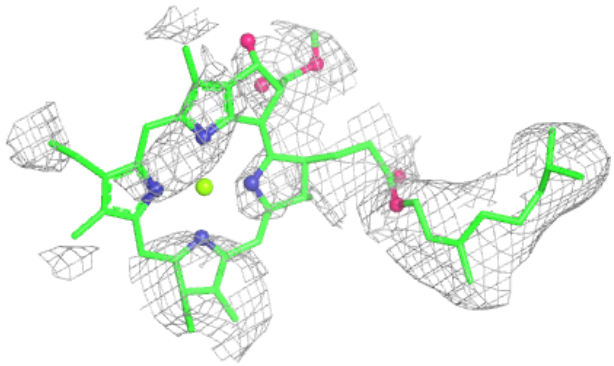


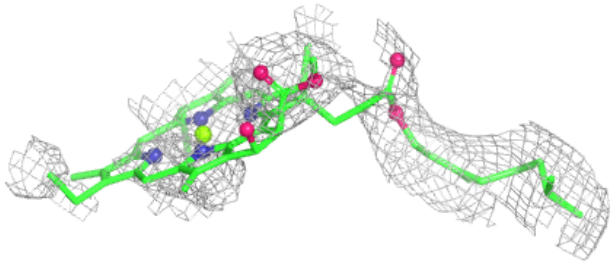


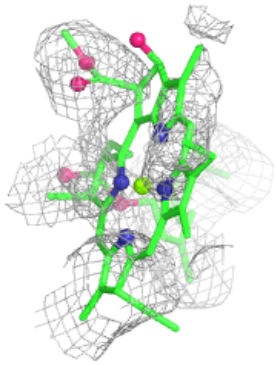


Electron density around CLA L 1504:

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

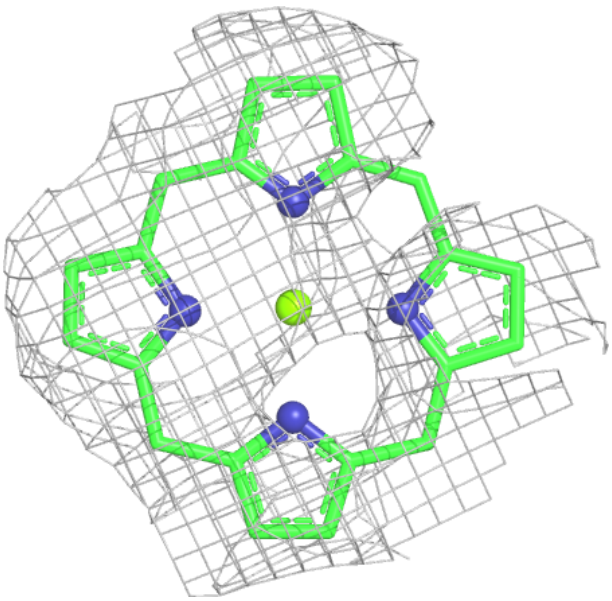


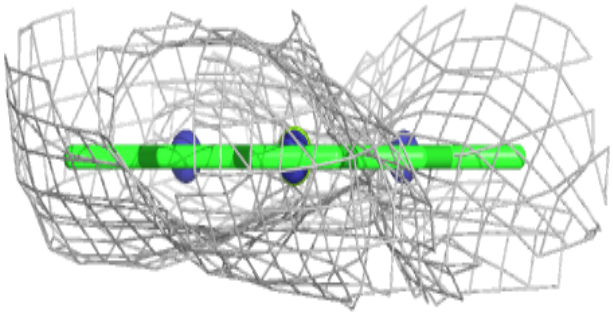


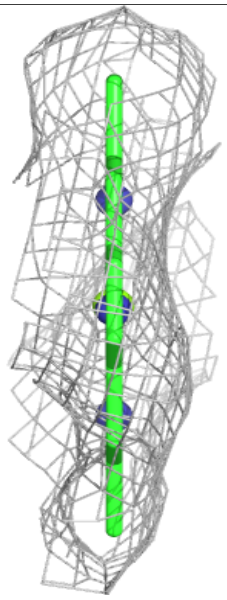


Electron density around CLA K 1141:

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

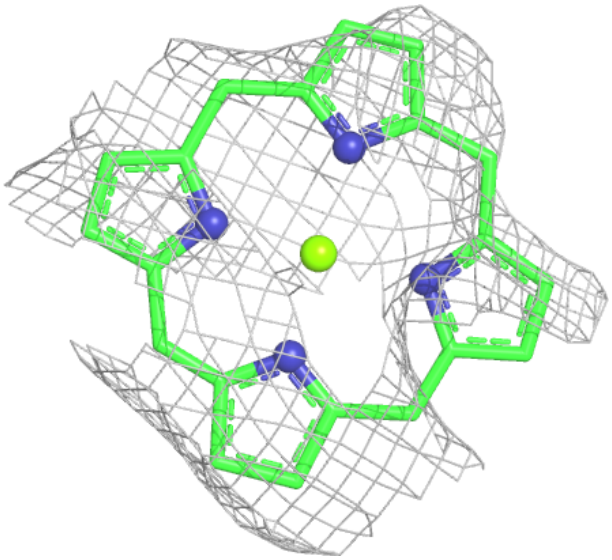


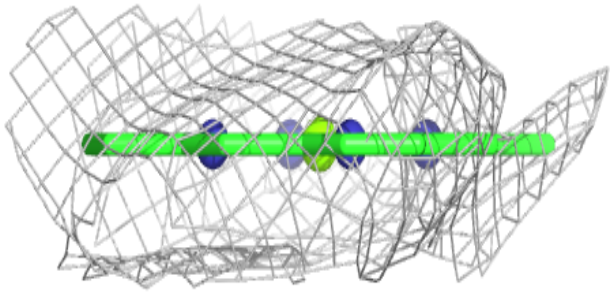


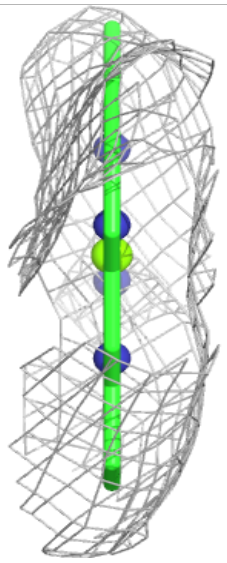


Electron density around CLA K 1150:

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

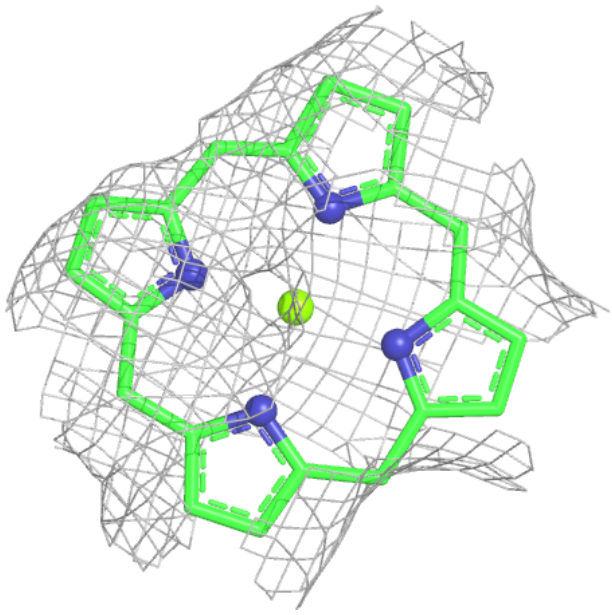


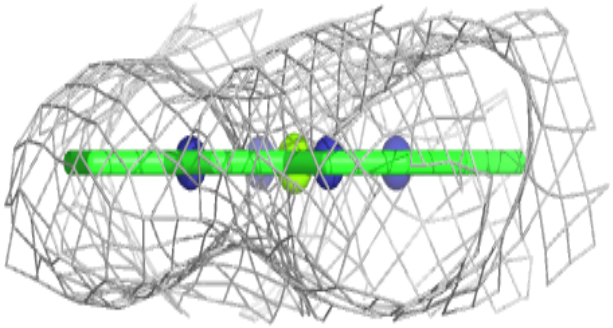


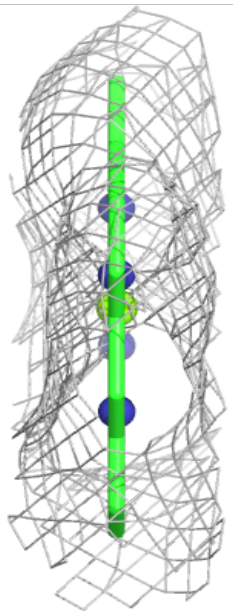


Electron density around CLA L 1125:

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

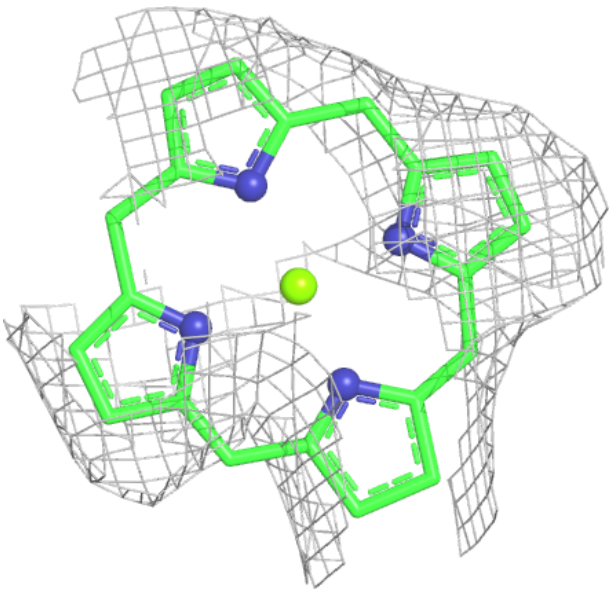


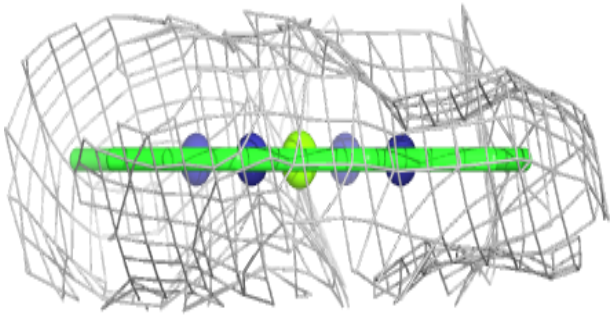


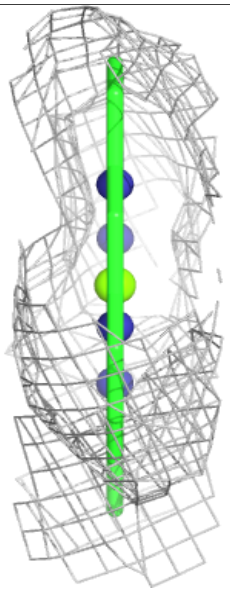


Electron density around CLA A 1151:

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

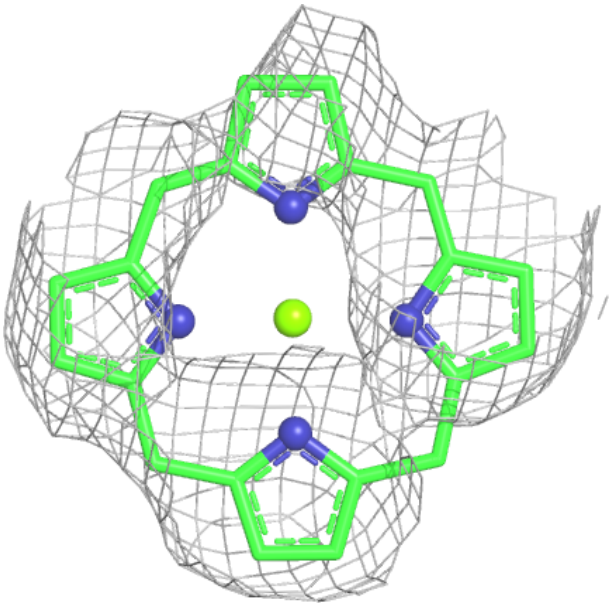


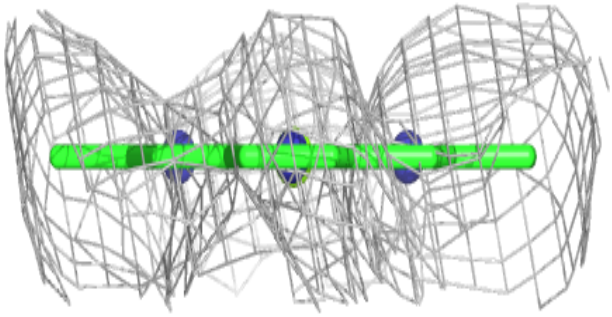


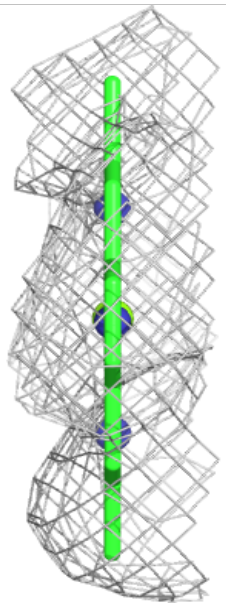


Electron density around CLA A 1118:

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

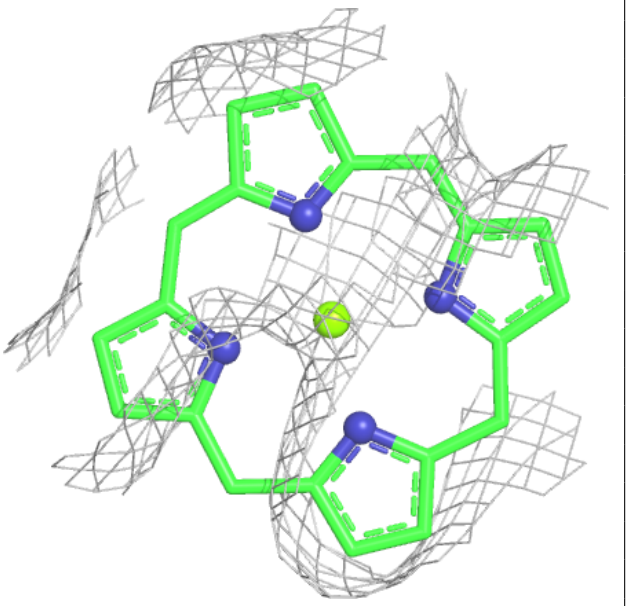


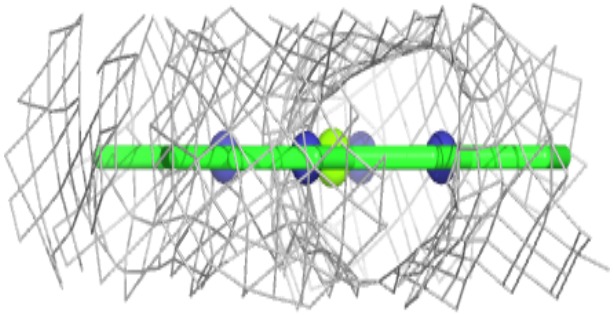


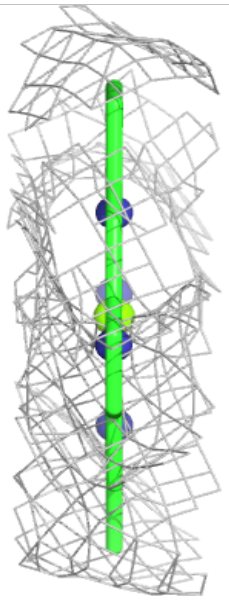


Electron density around CLA 1 1013:

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

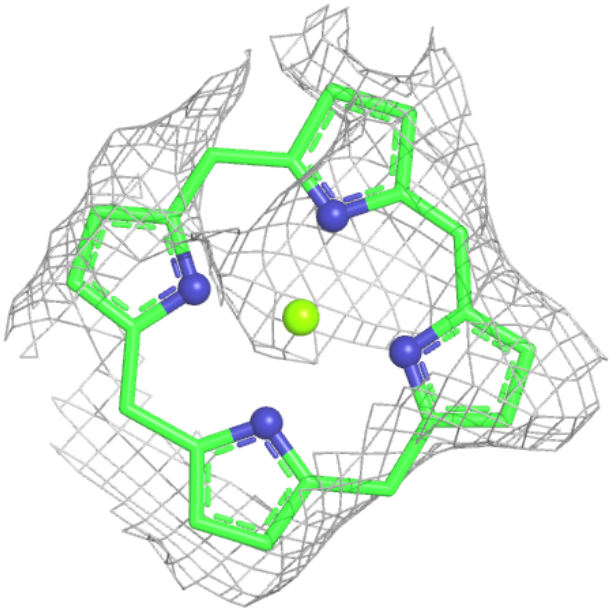


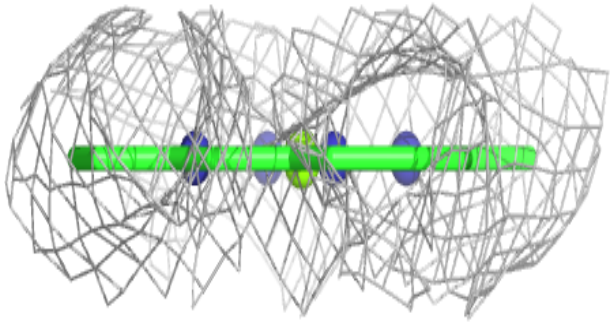


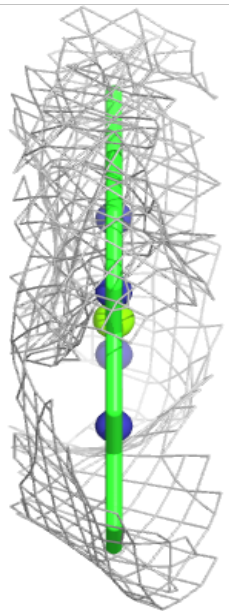


Electron density around CLA 1 1011:

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

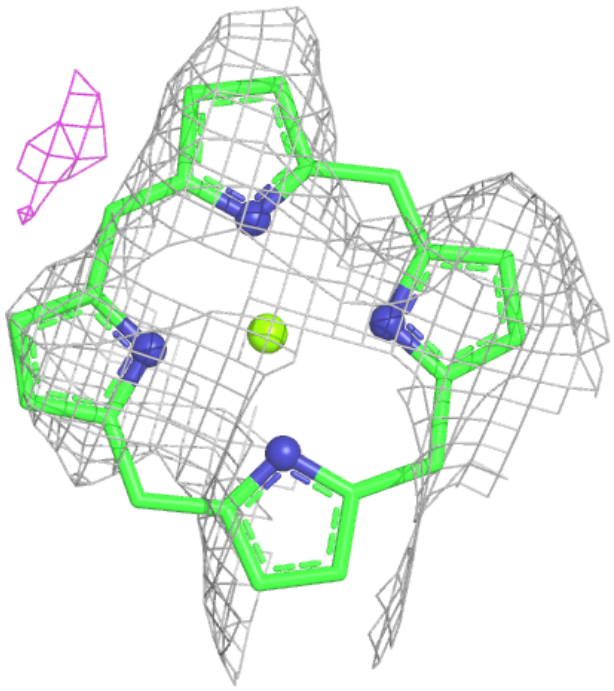


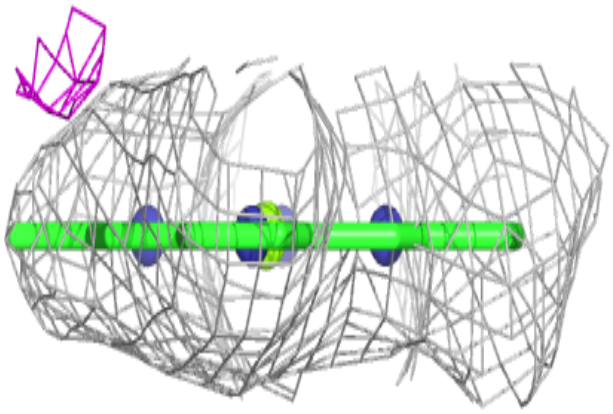


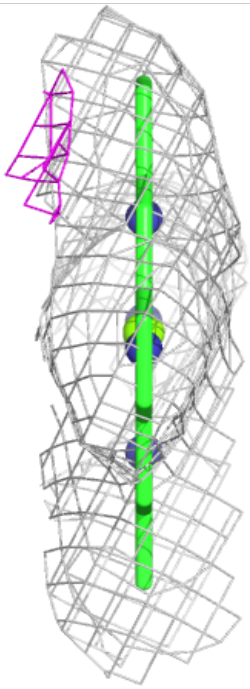


Electron density around CLA 1 1001:

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

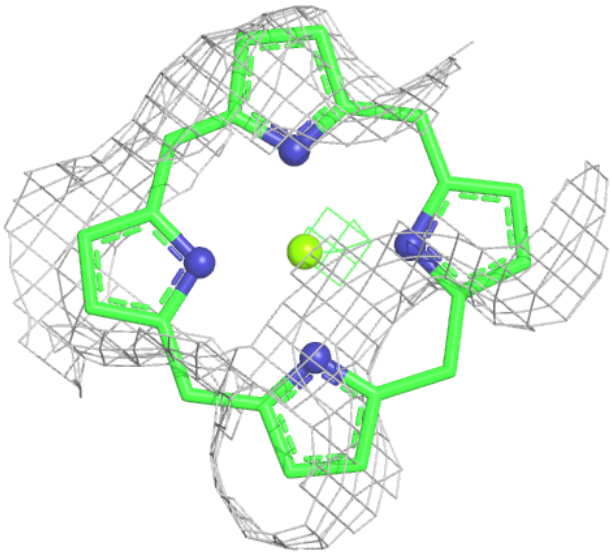


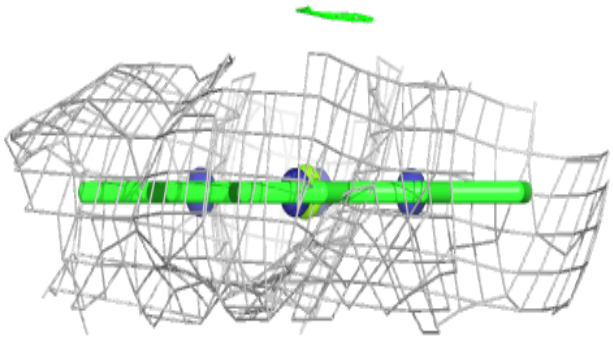


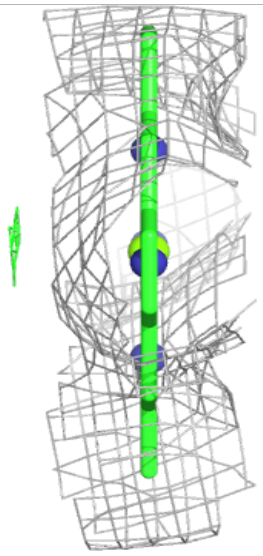


Electron density around CLA B 1201:

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

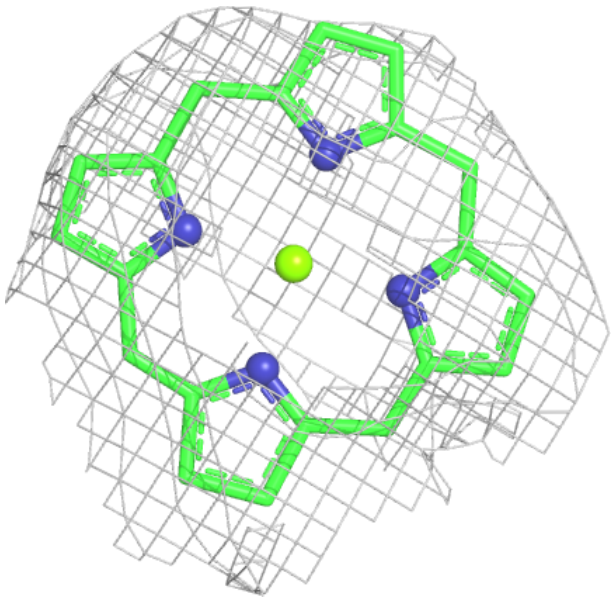


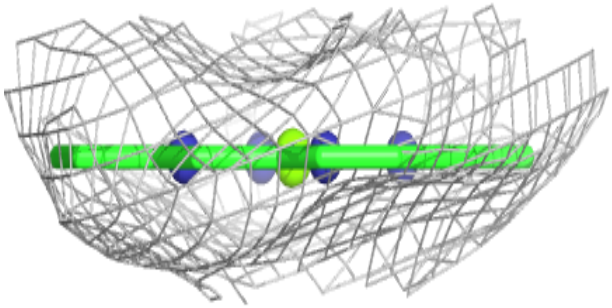


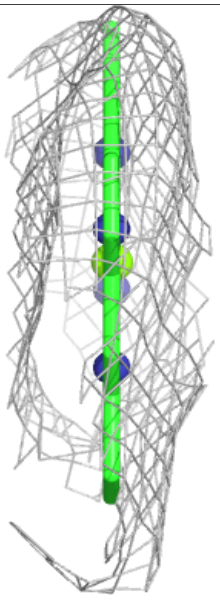


Electron density around CLA 1 1002:

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

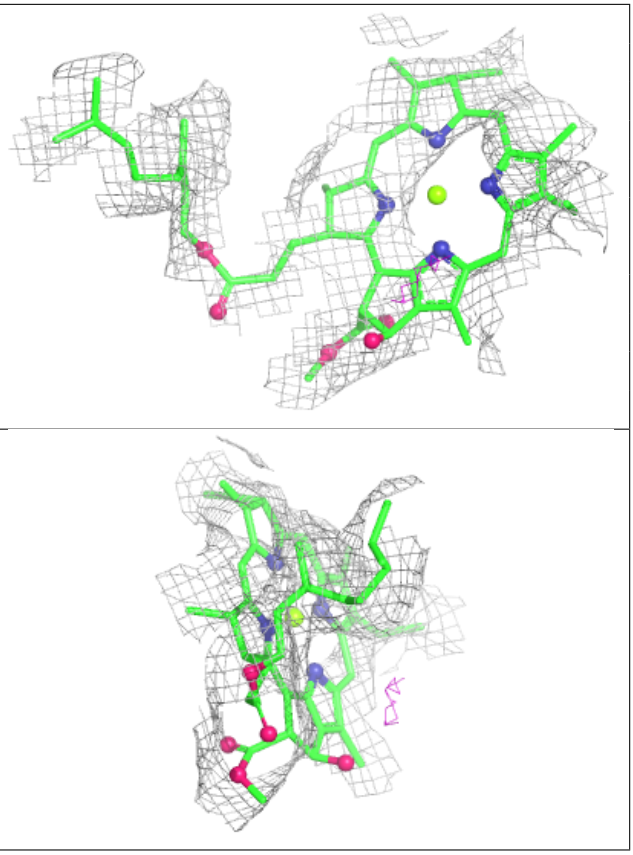






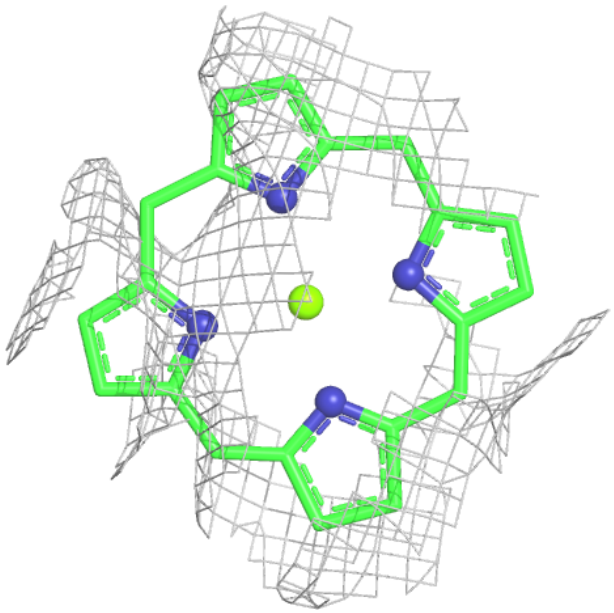
Electron density around CLA B 1232:

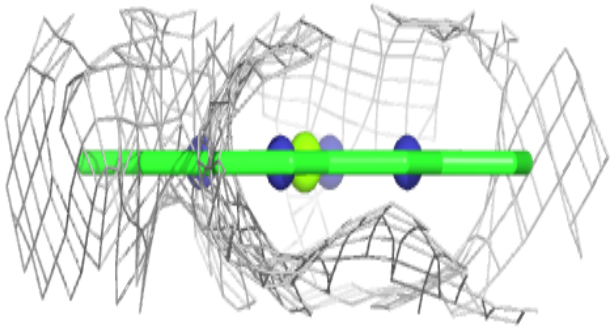
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

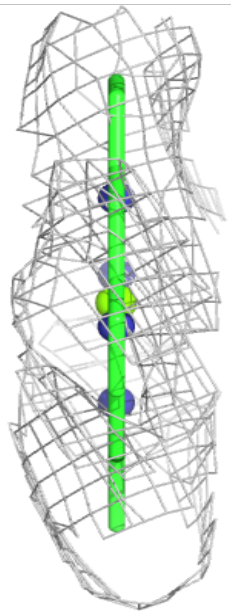


Electron density around CLA B 1301:

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

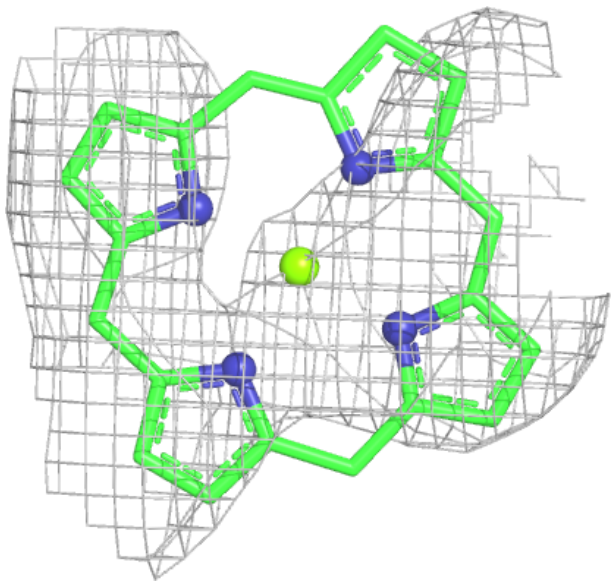


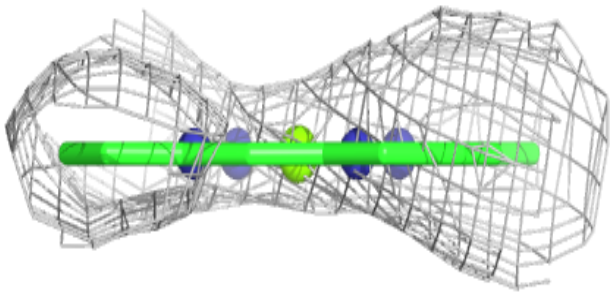


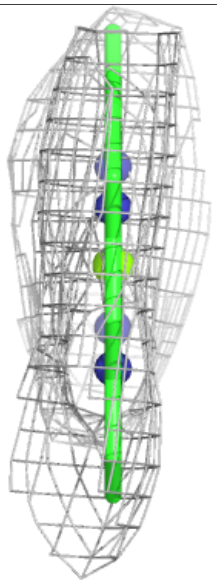


Electron density around CLA 2 2006:

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

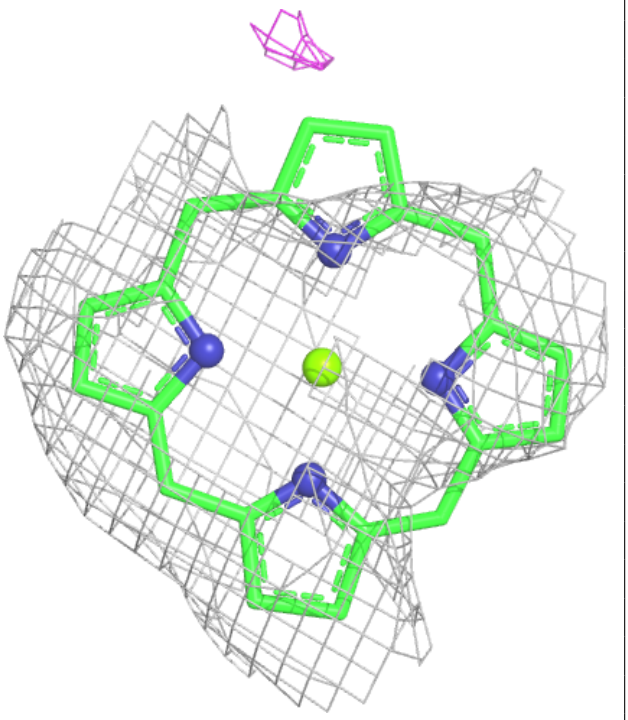


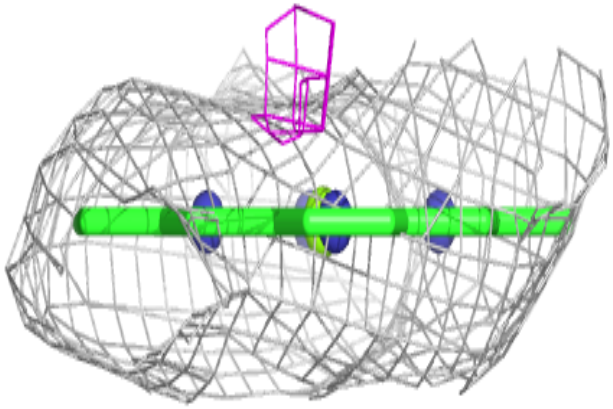


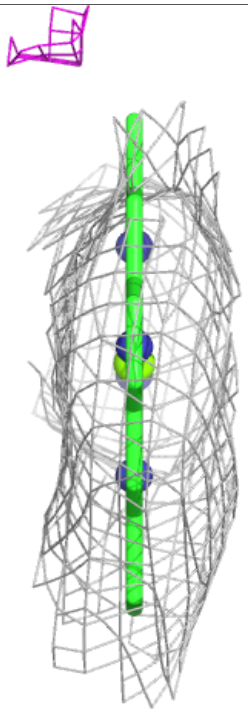


Electron density around CLA 2 2010:

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

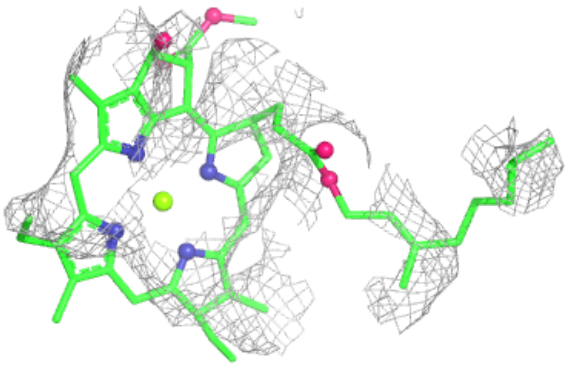


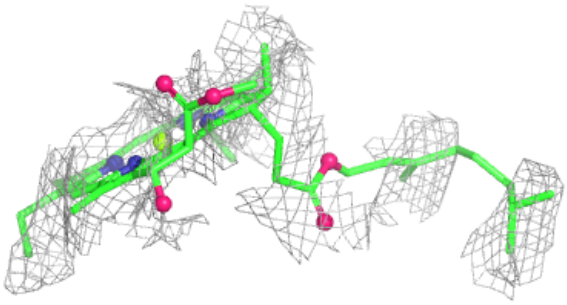


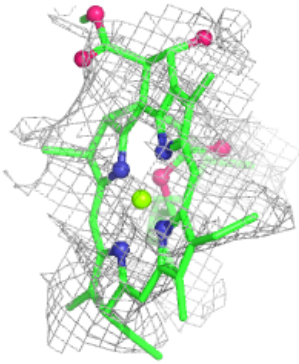


Electron density around CLA A 1119:

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

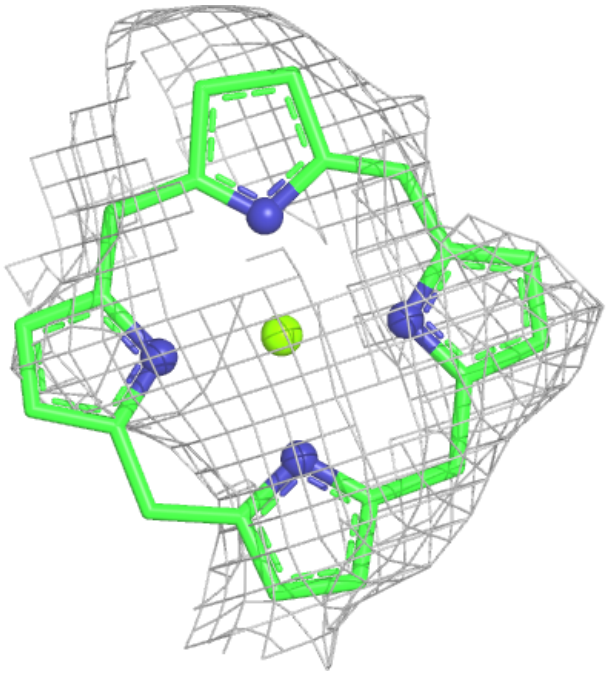


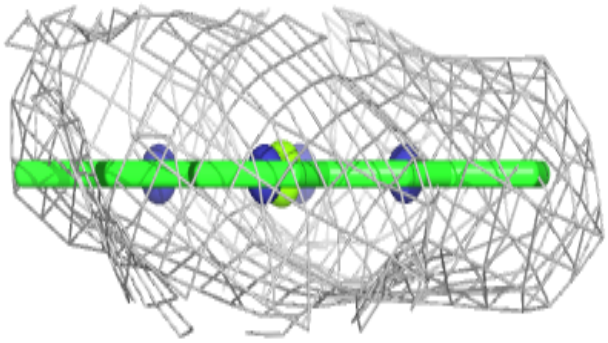


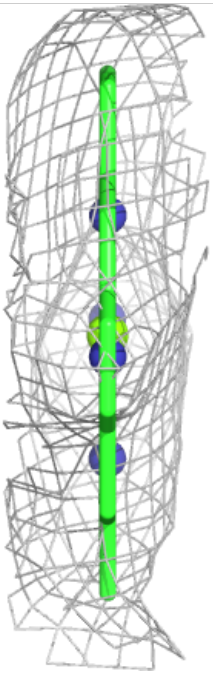


Electron density around CLA A 1127:

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

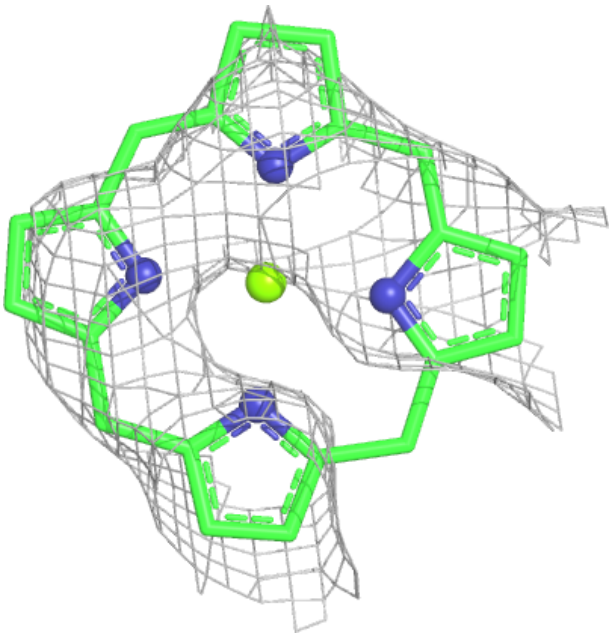


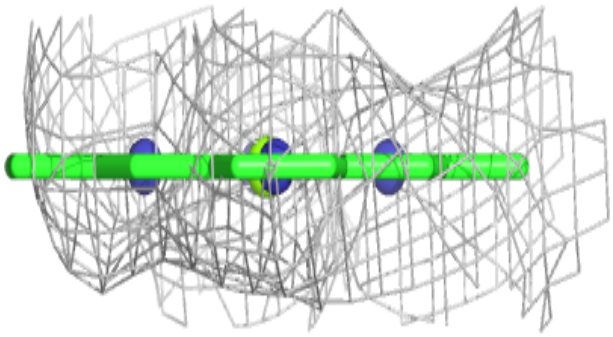


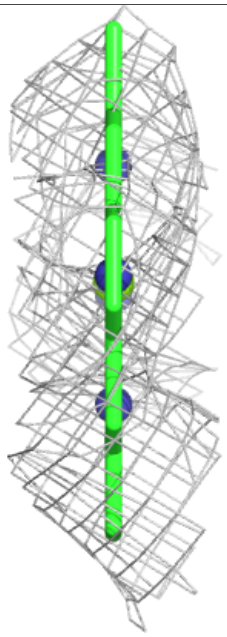


Electron density around CLA 2 2012:

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

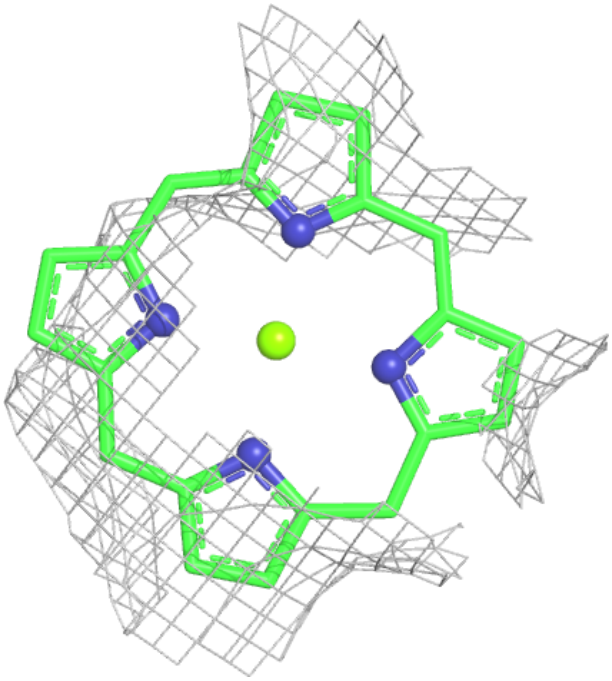


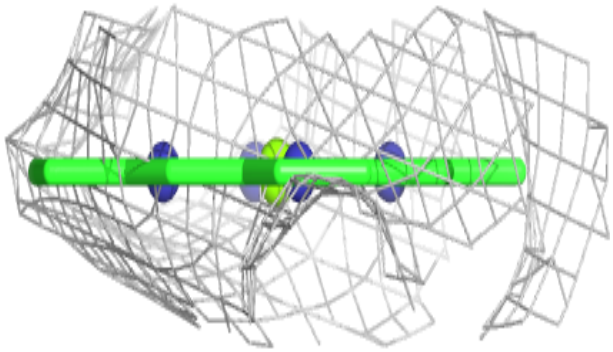


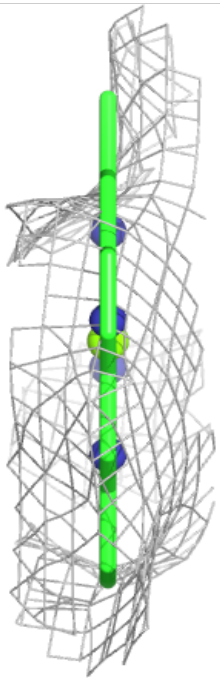


Electron density around CLA A 1144:

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

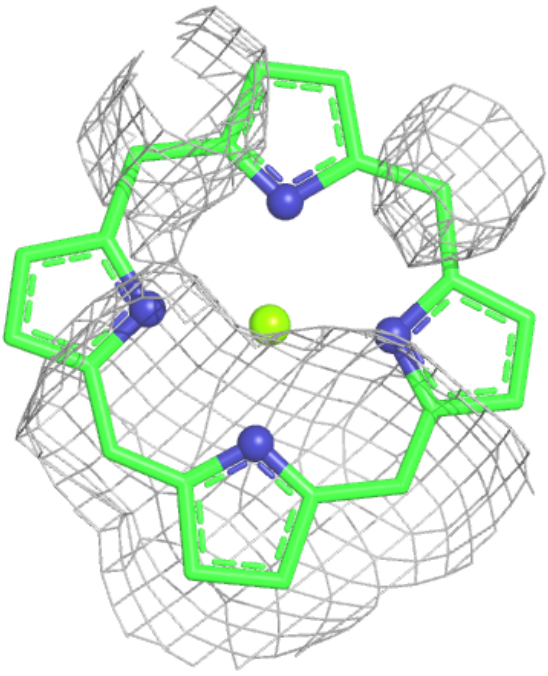


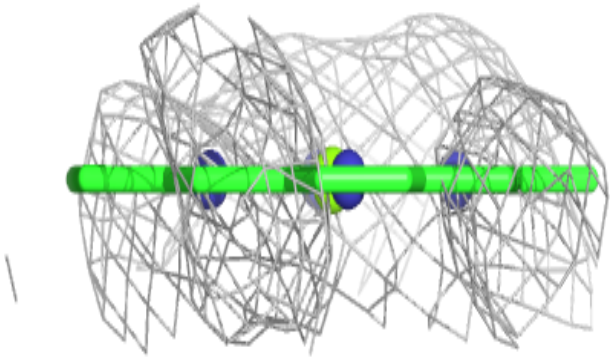


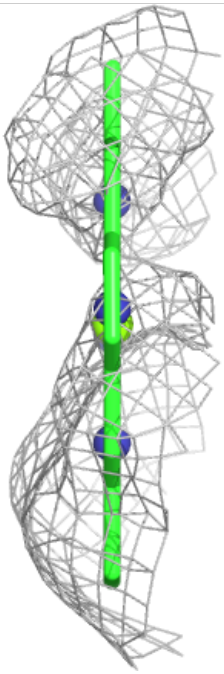


Electron density around CLA F 4015:

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

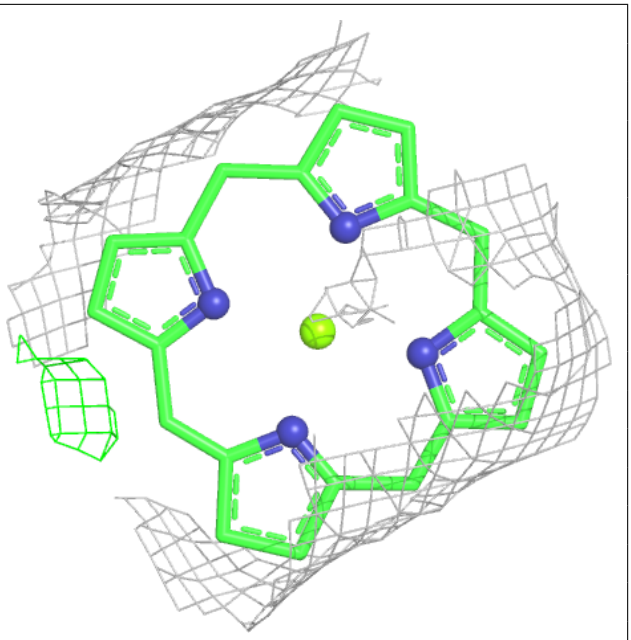


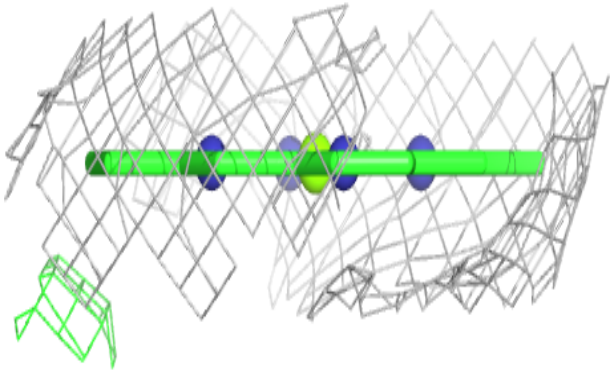


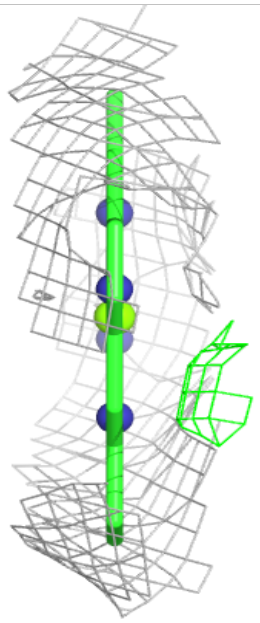


Electron density around CLA A 1147:

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

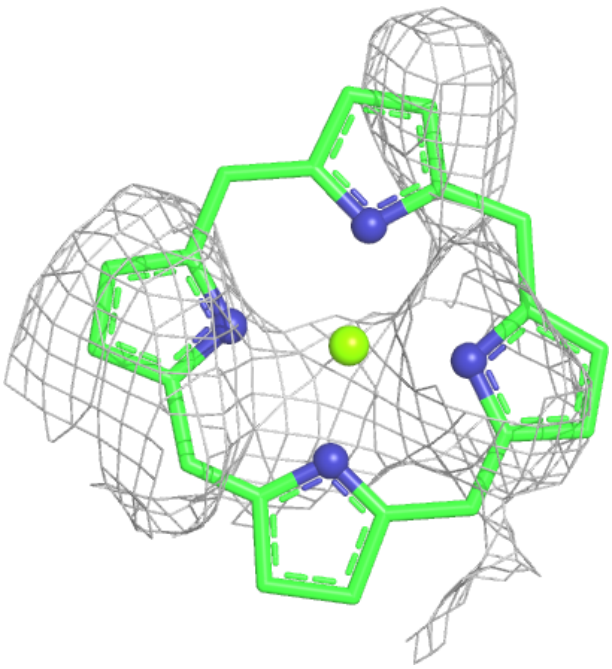


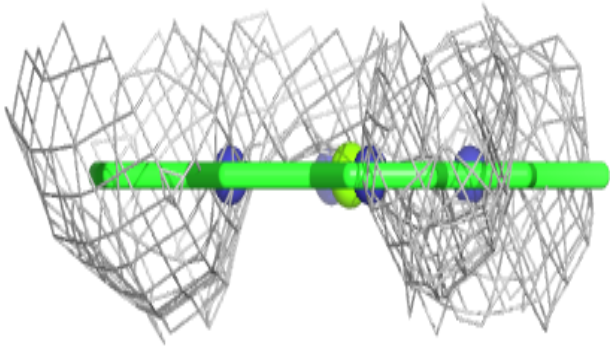


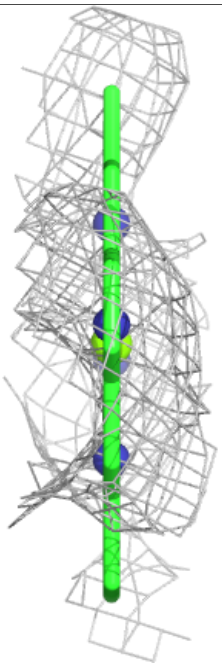


Electron density around CLA 3 3001:

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

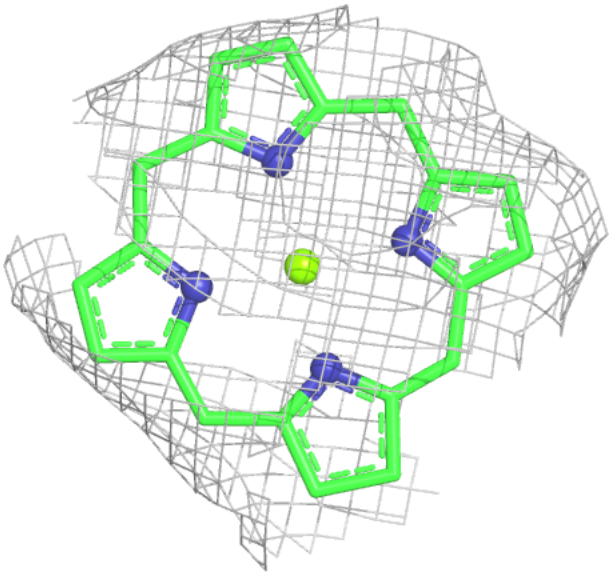


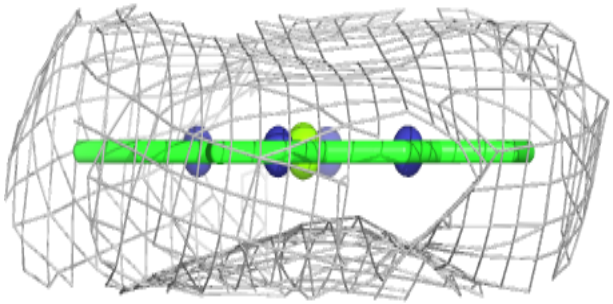


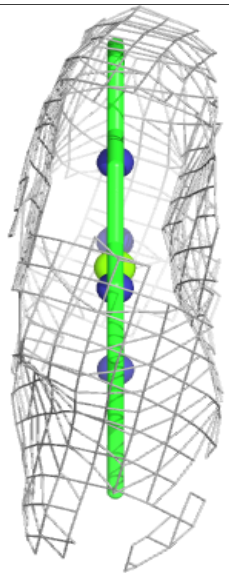


Electron density around CLA 3 3002:

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

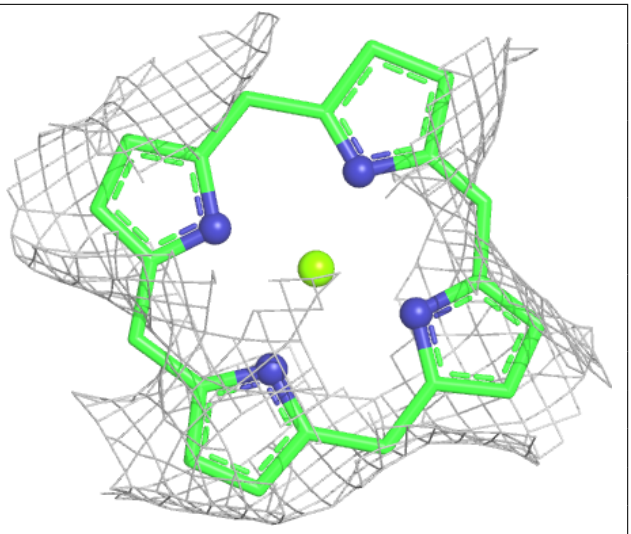


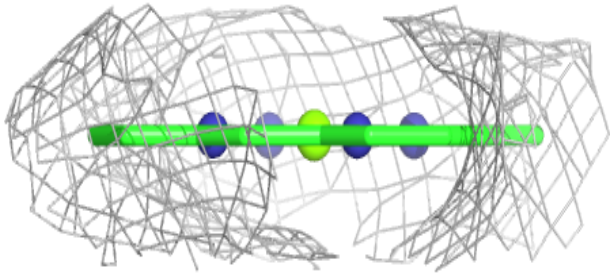


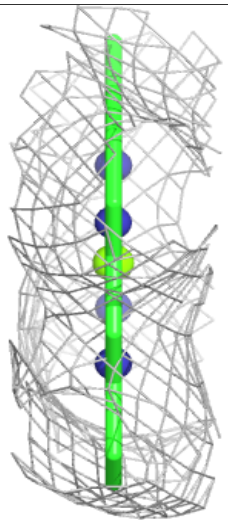


Electron density around CLA 3 3015:

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

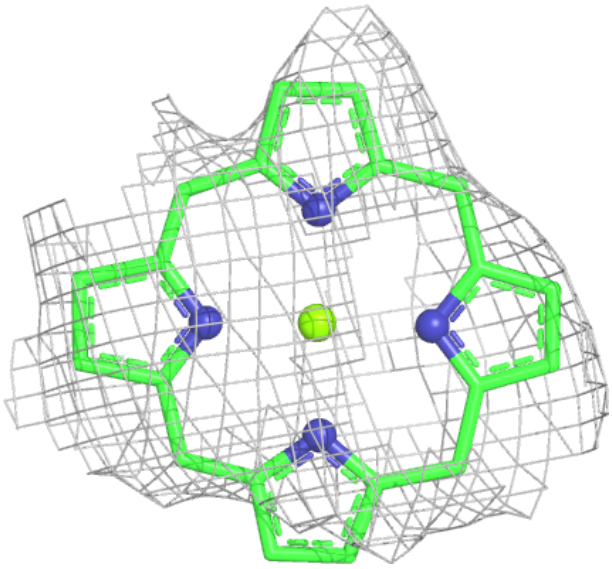


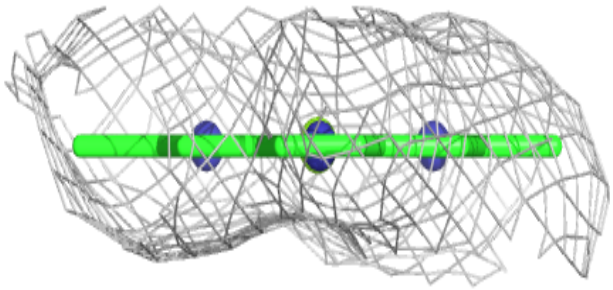


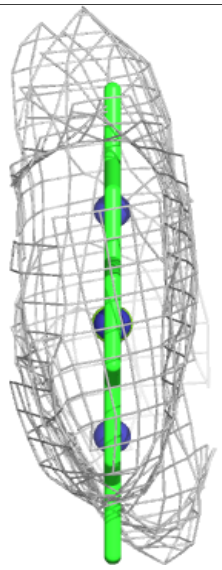


Electron density around CLA 4 1009:

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

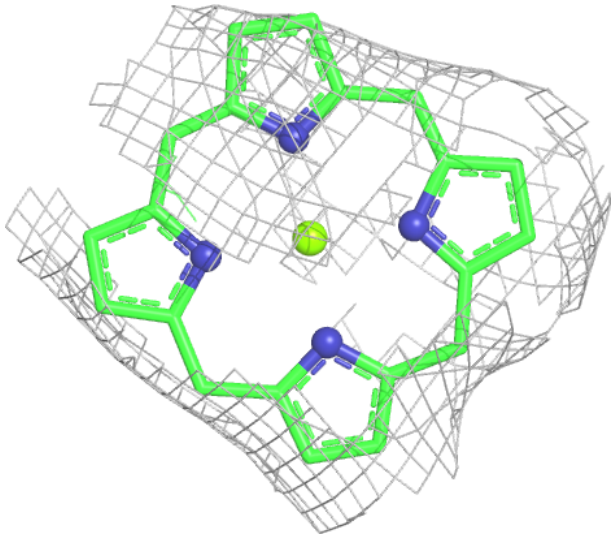


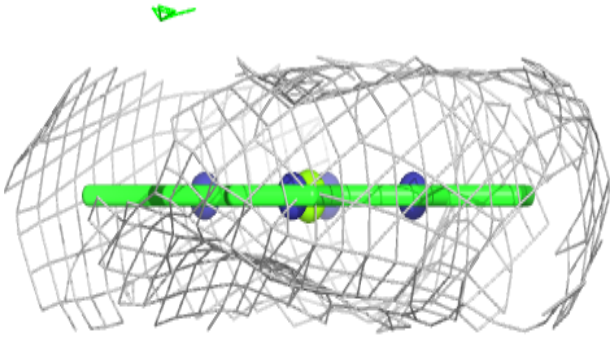


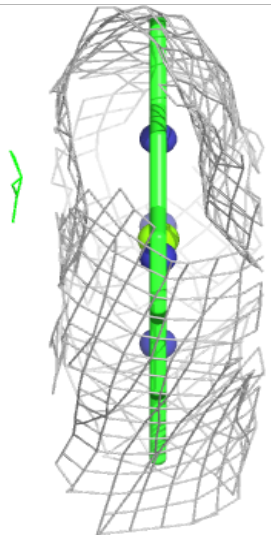


Electron density around CLA 4 4009:

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

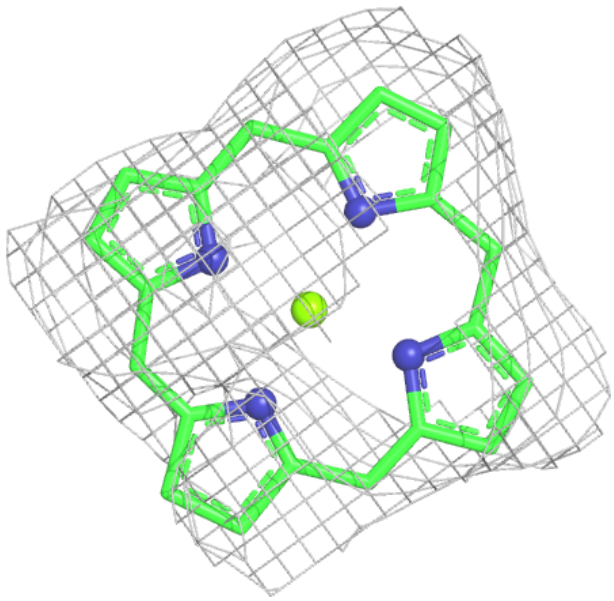


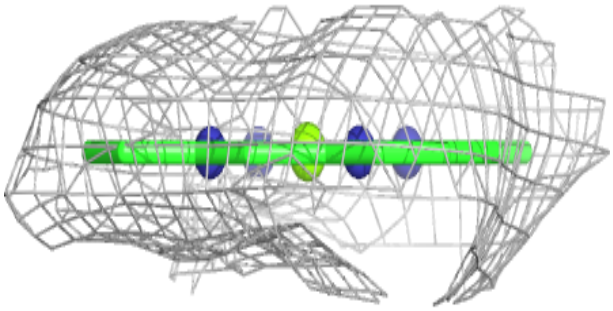


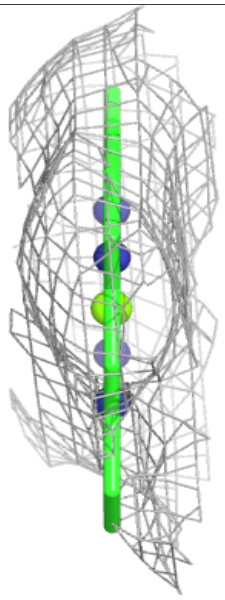


Electron density around CLA 4 4004:

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

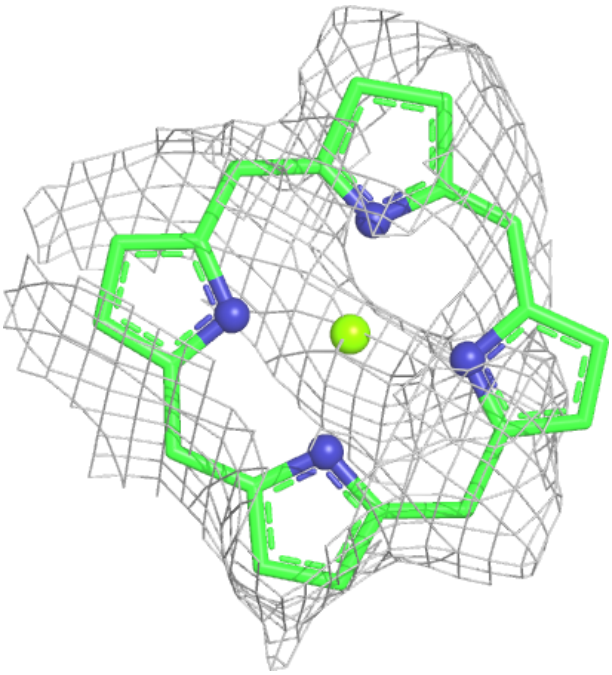


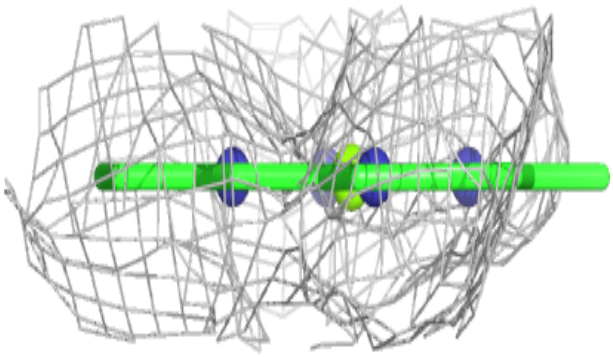


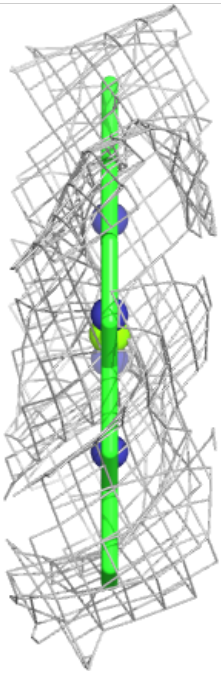


Electron density around CLA H 1505:

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

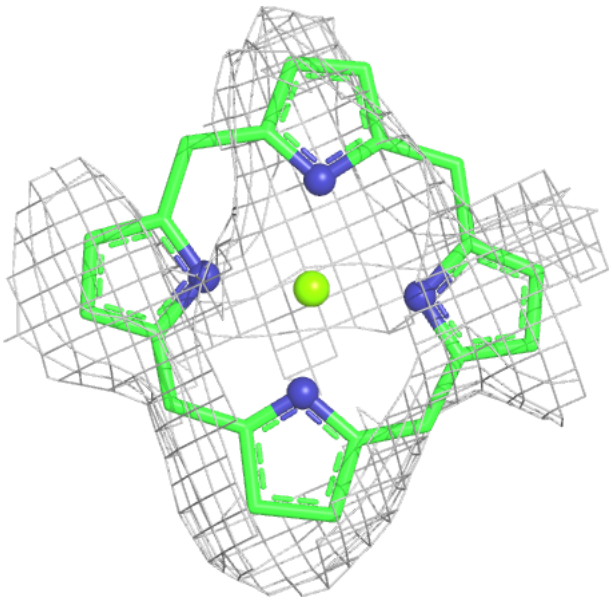


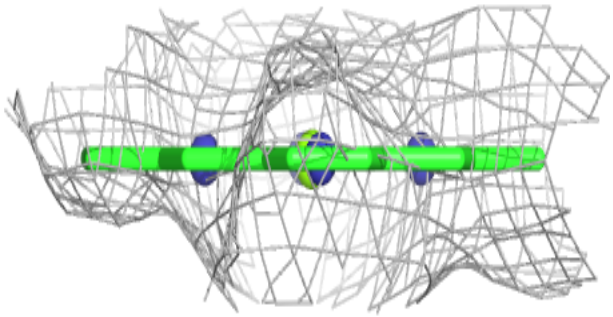


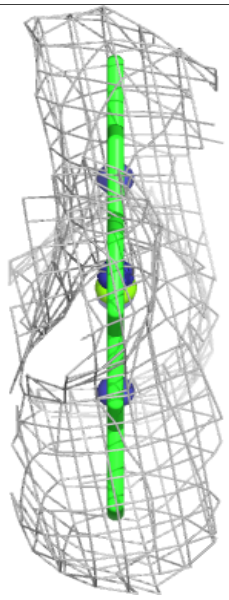


Electron density around CLA 4 4006:

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

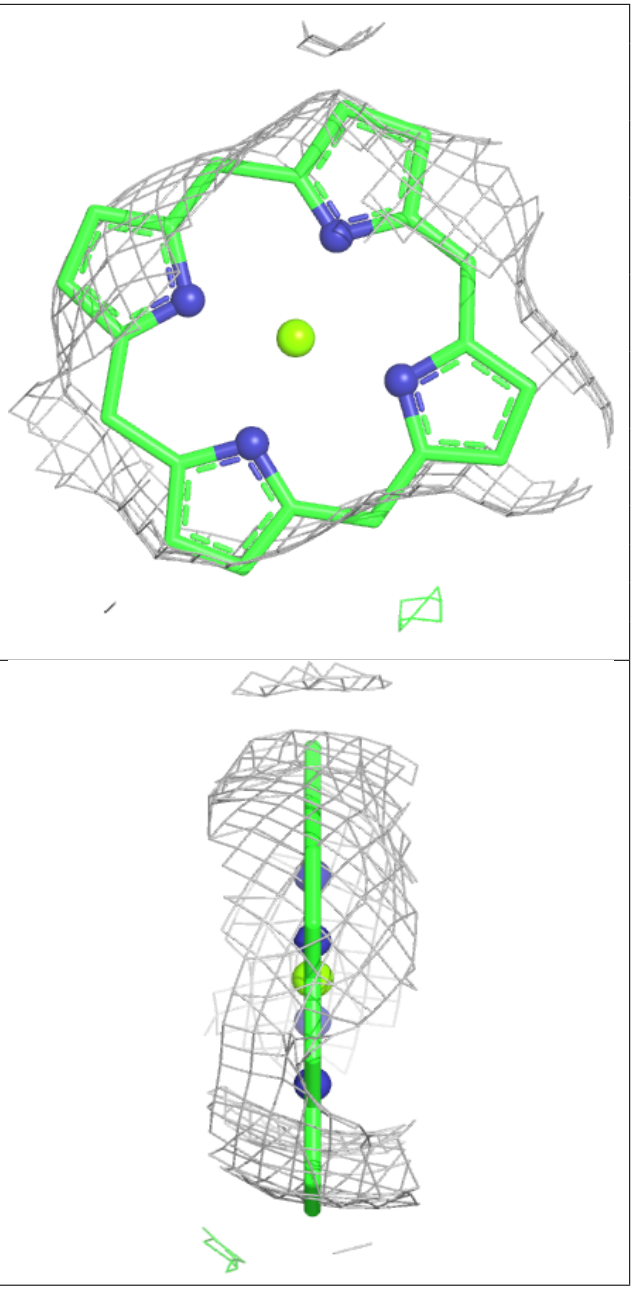






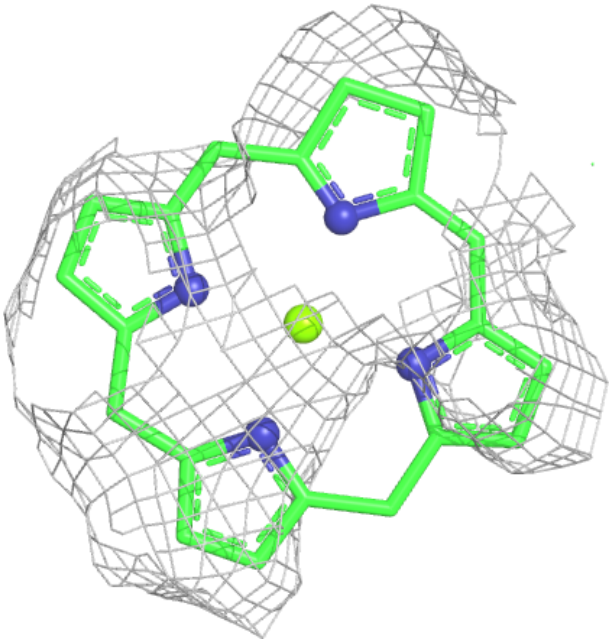
Electron density around CLA A 1148:

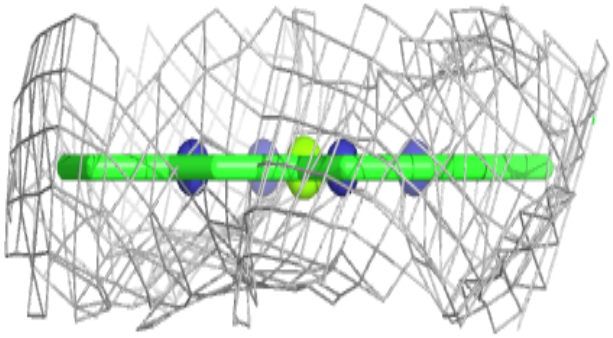
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

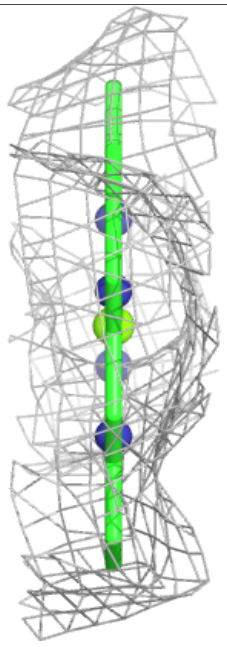


Electron density around CLA 4 4007:

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

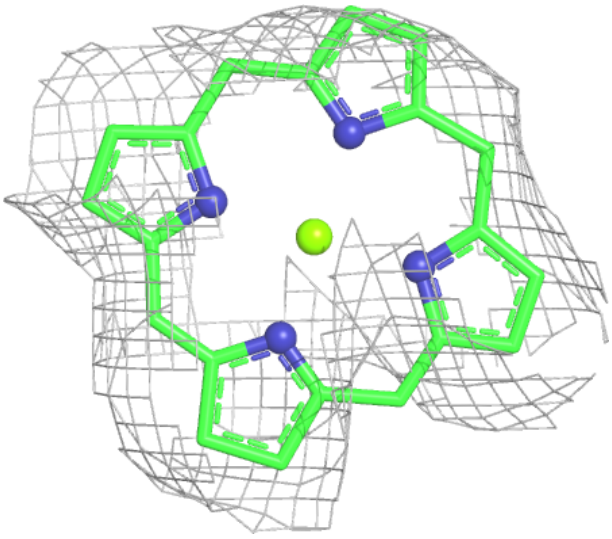


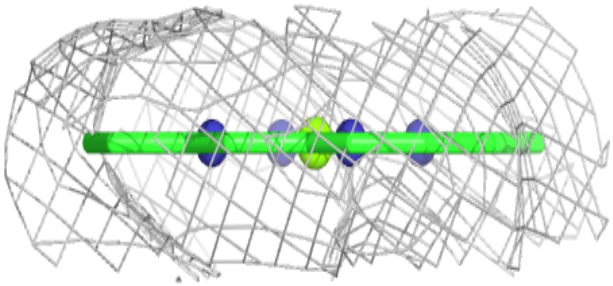


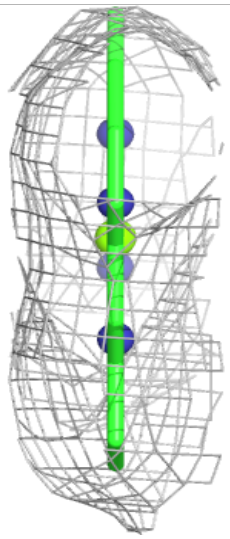


Electron density around CLA 4 4002:

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

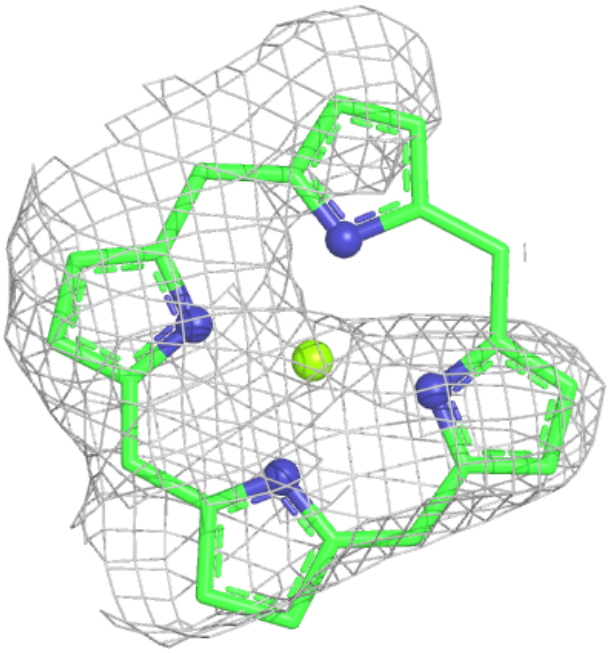


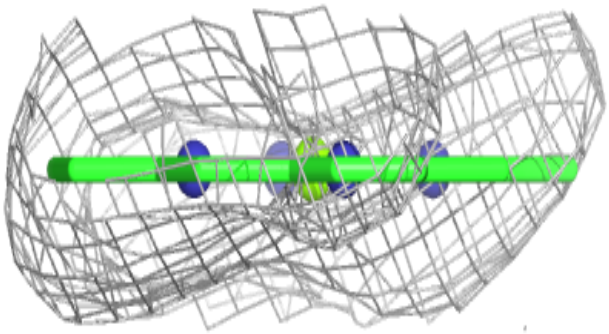


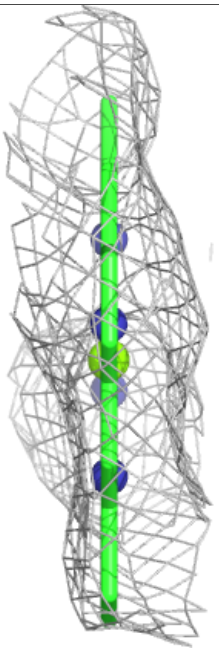


Electron density around CLA 4 4003:

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



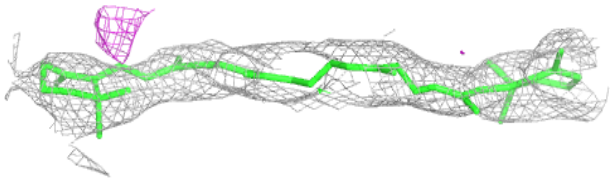


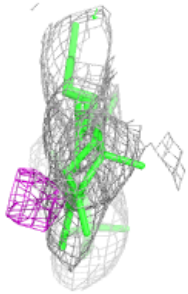


Electron density around BCR A 6011:

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

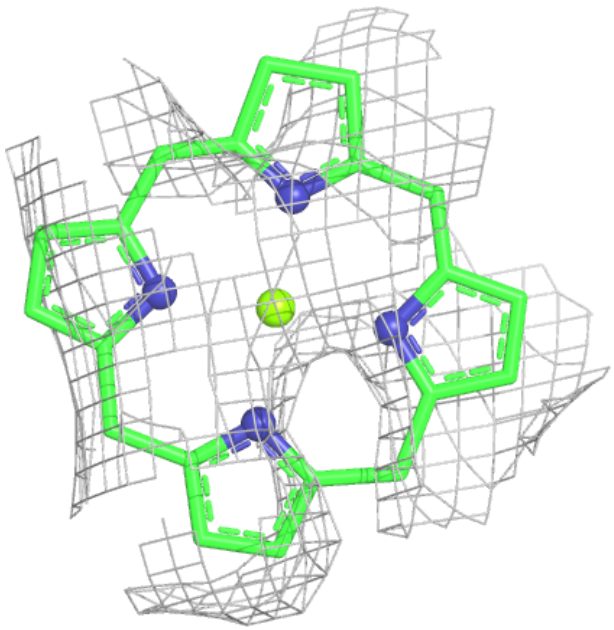


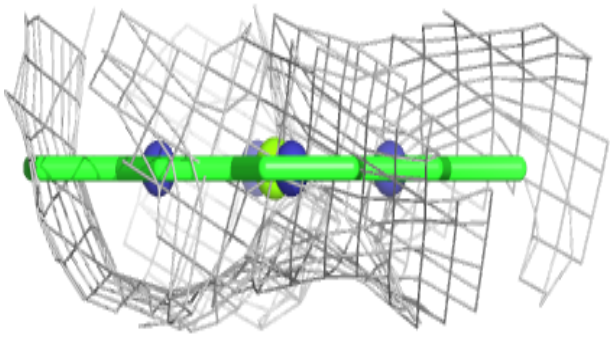


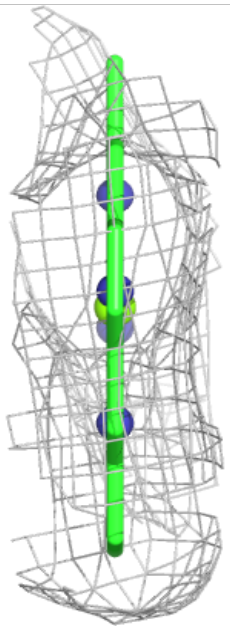


Electron density around CLA J 1308:

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

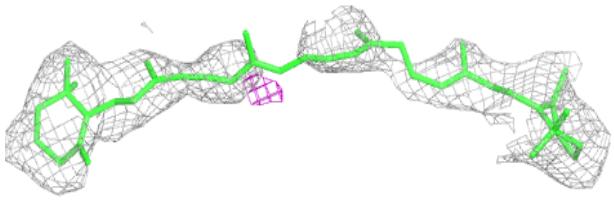


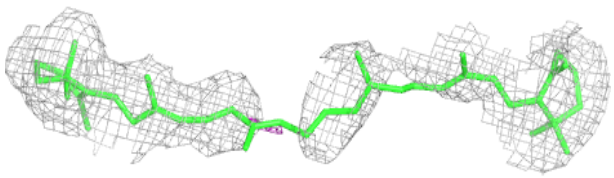


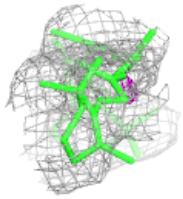


Electron density around BCR I 6018:

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

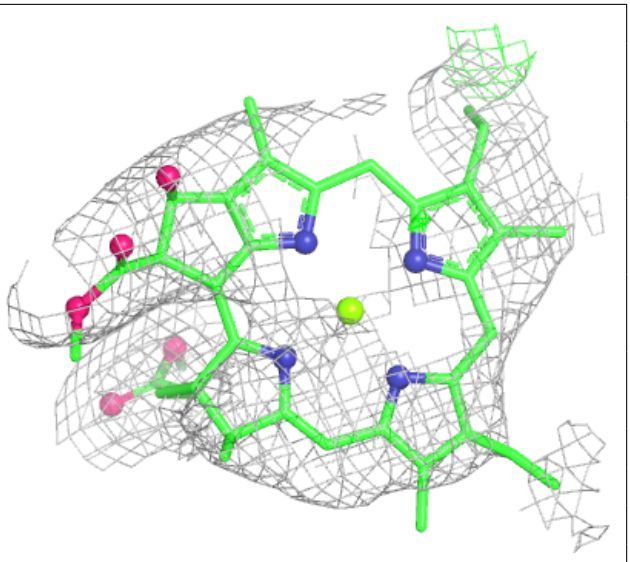


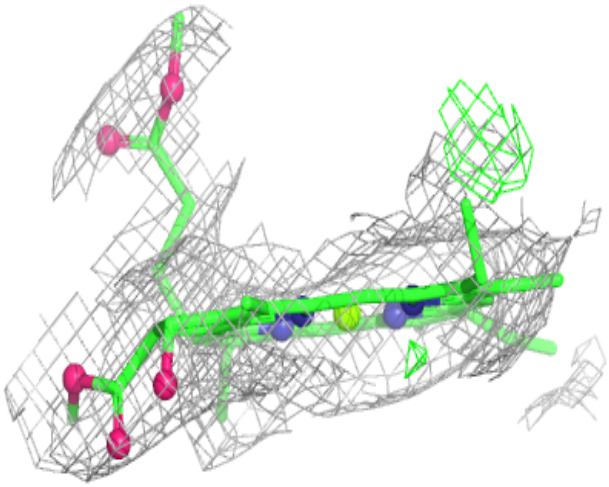


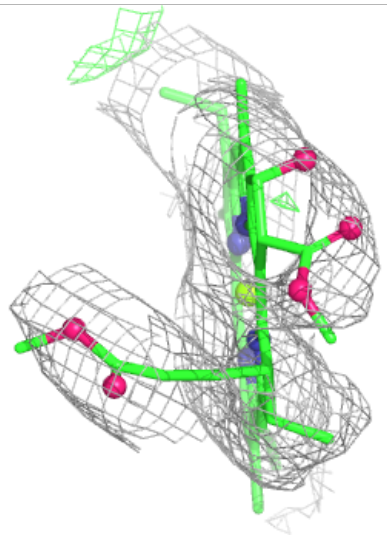


Electron density around CLA B 1236:

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

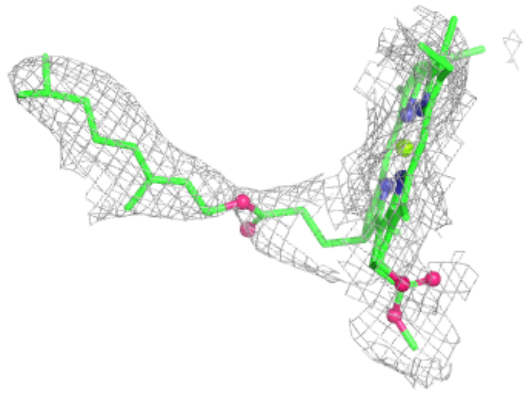


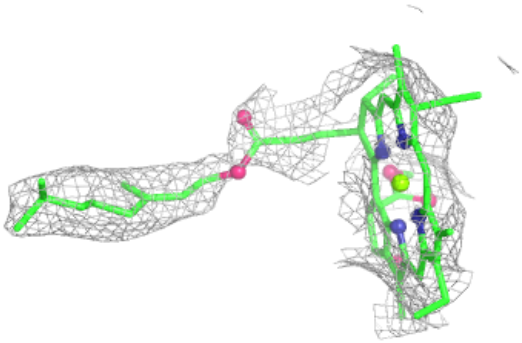


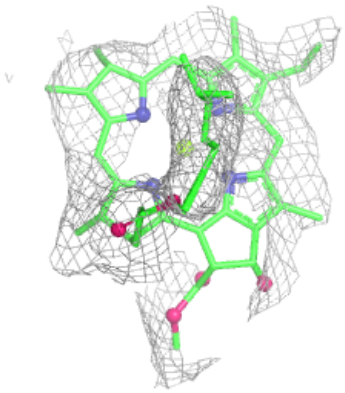


Electron density around CLA B 1239:

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

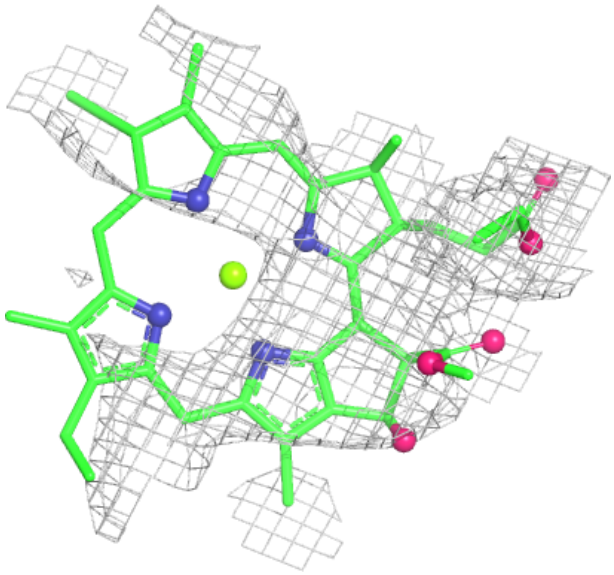


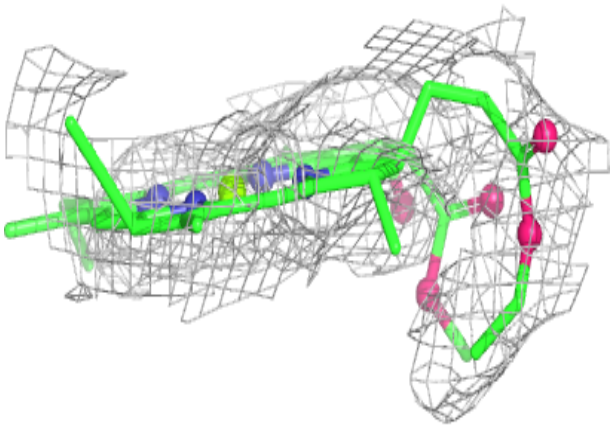


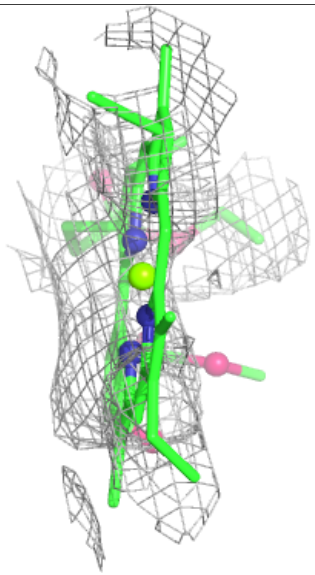


Electron density around CLA B 1242:

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

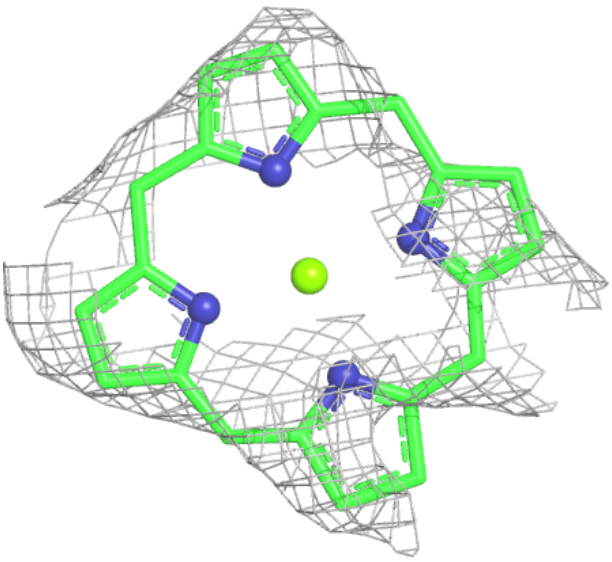


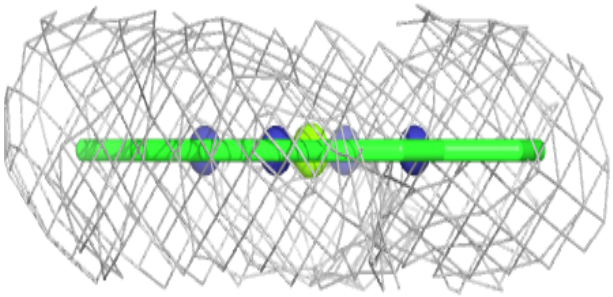


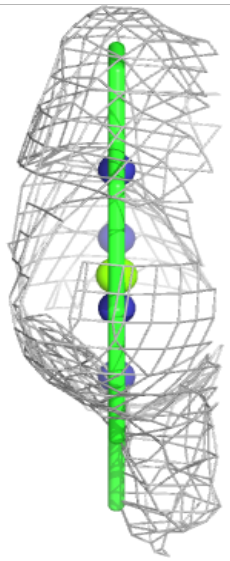


Electron density around CLA A 1102:

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

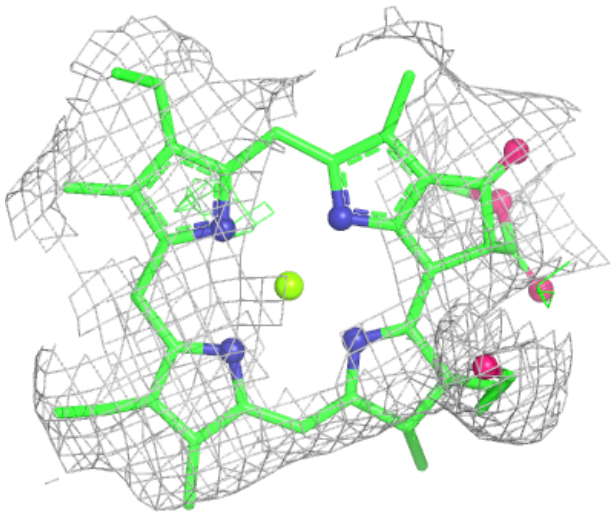


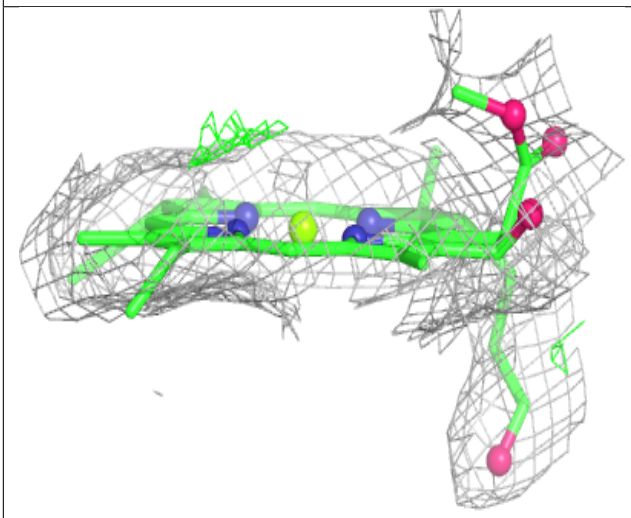


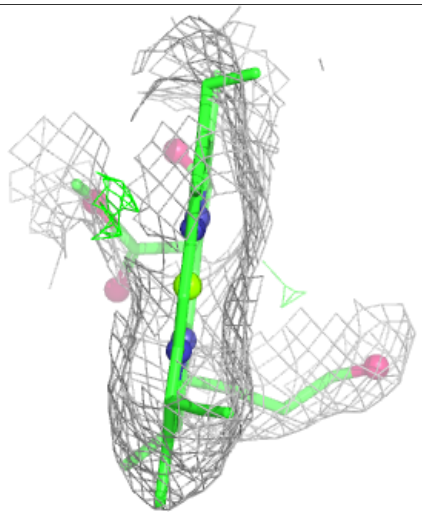


Electron density around CLA F 1139:

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

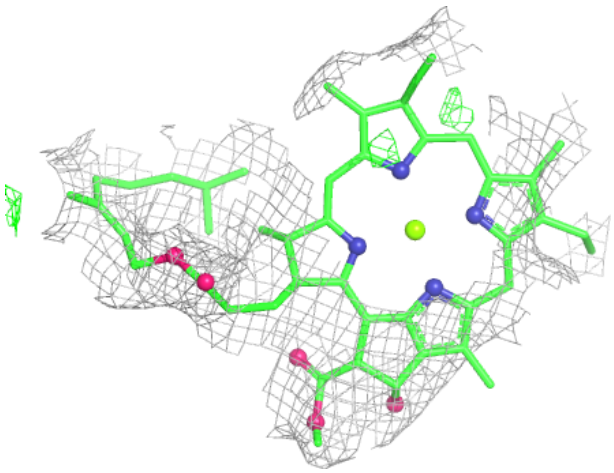


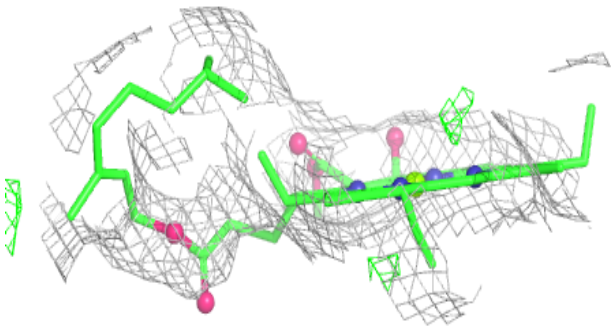


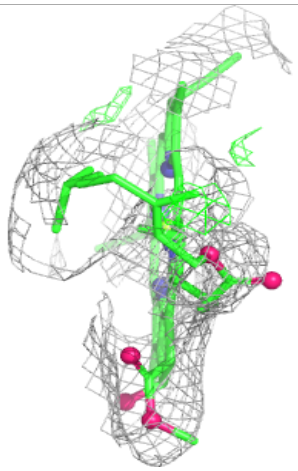


Electron density around CLA F 1302:

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

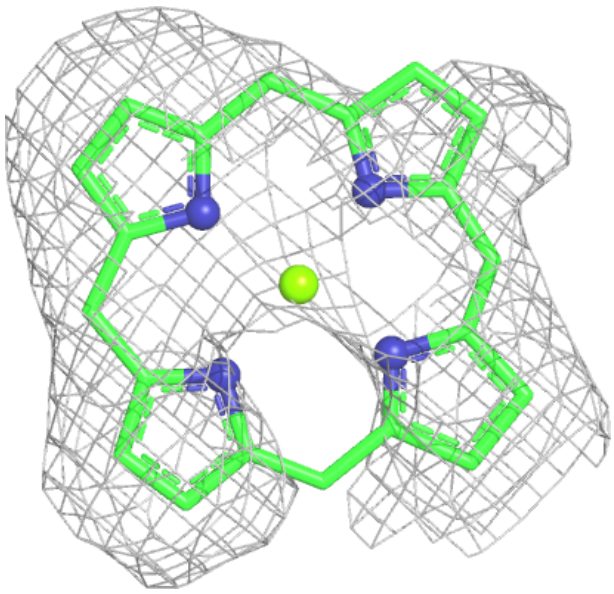


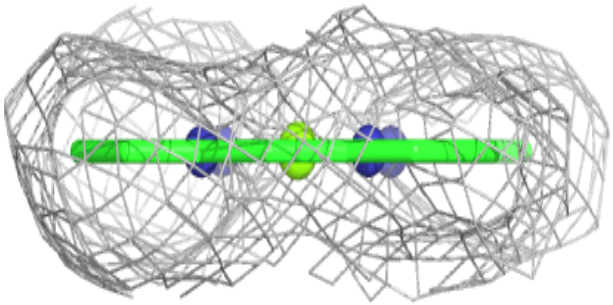


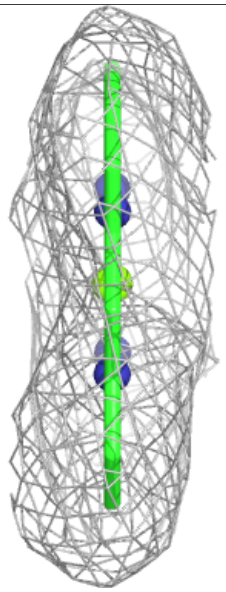


Electron density around CLA A 1104:

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

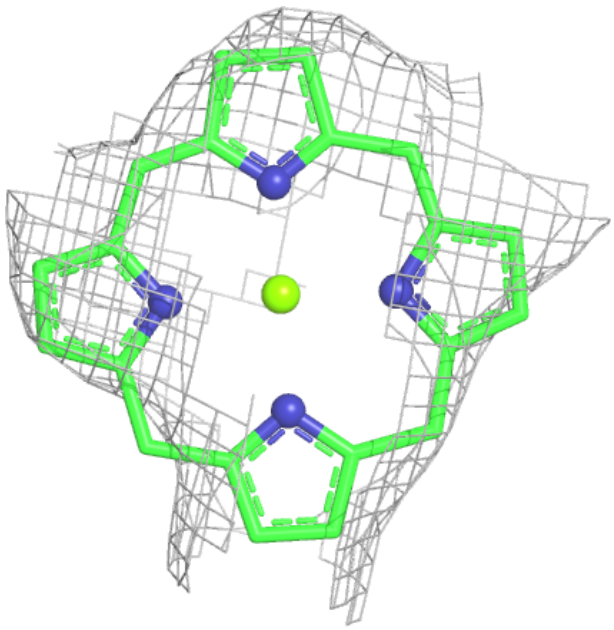


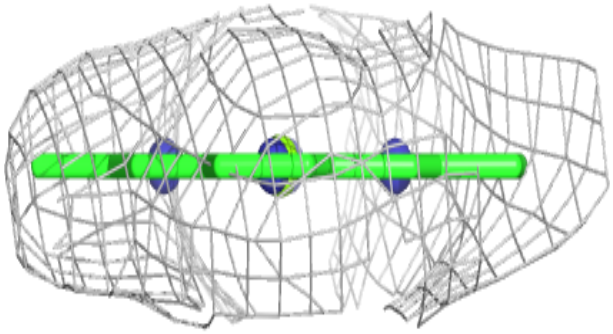


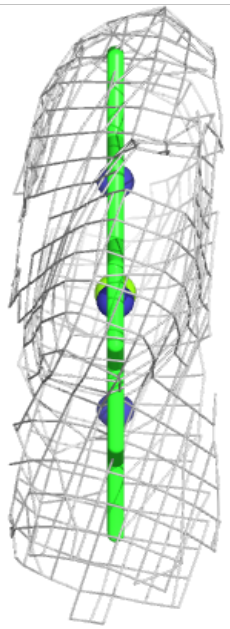


Electron density around CLA A 1120:

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

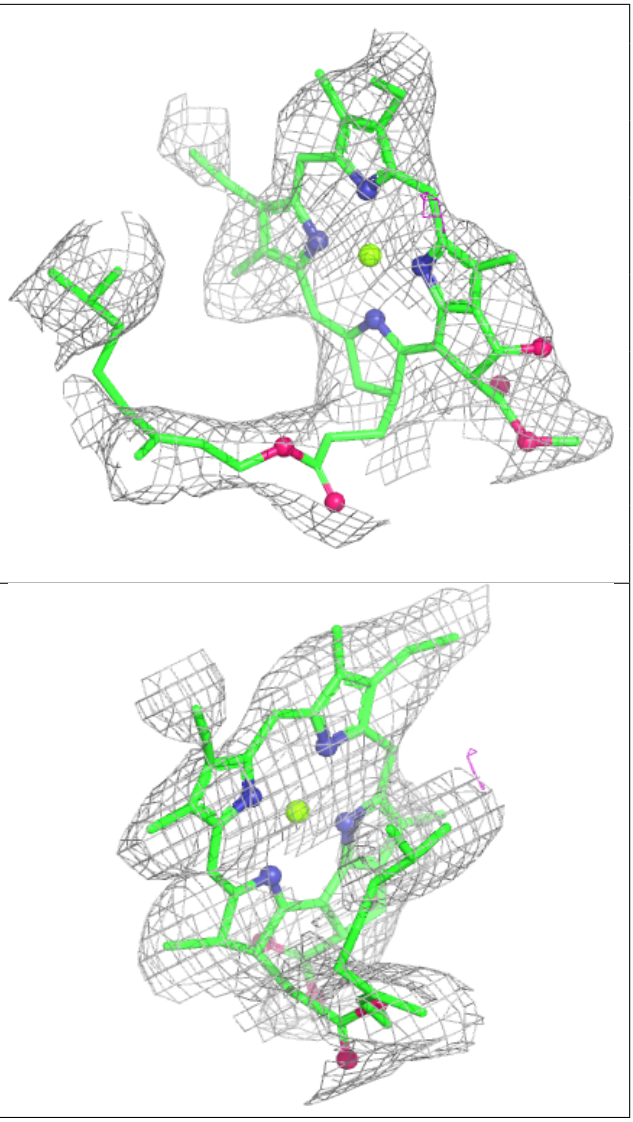






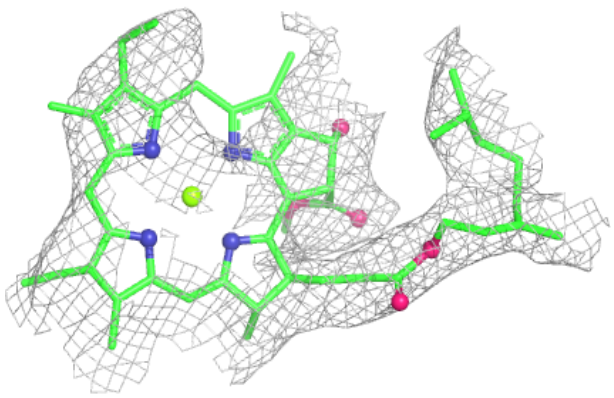
Electron density around CLA A 1122:

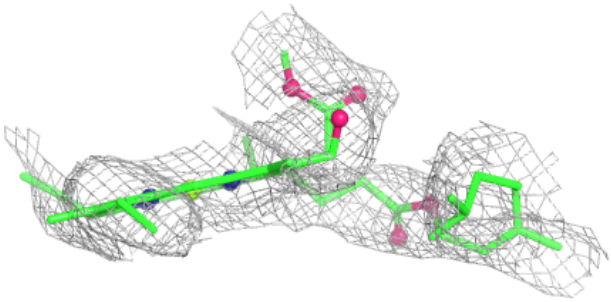
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

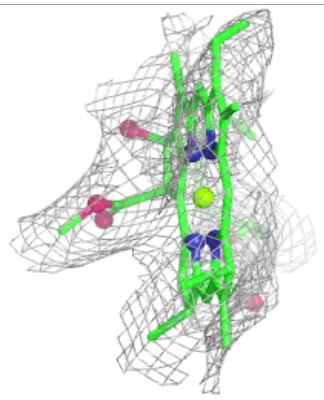


Electron density around CLA A 1123:

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

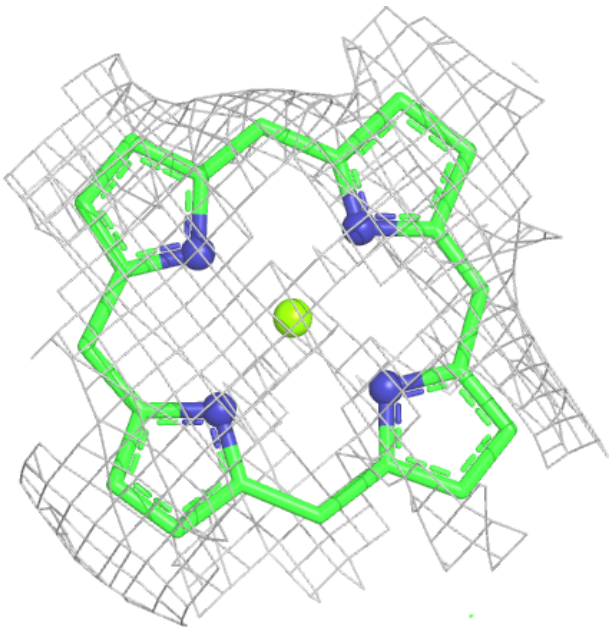


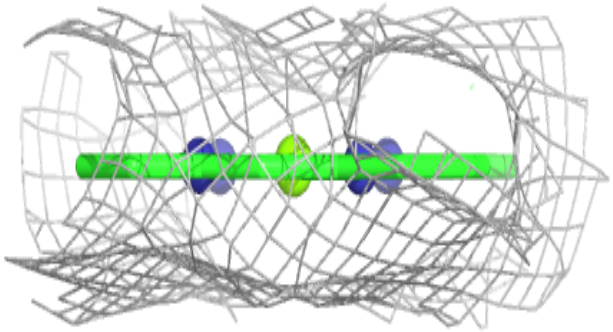


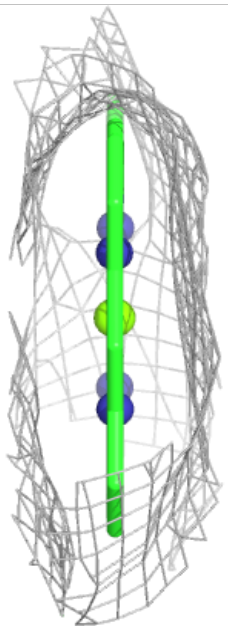


Electron density around CLA A 1124:

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

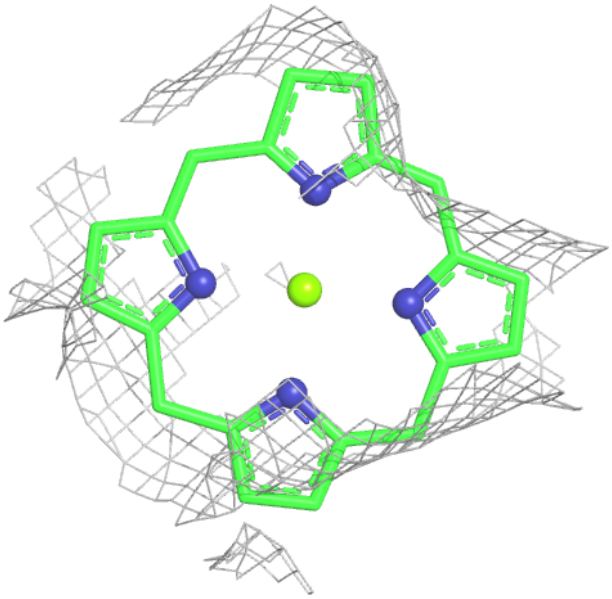


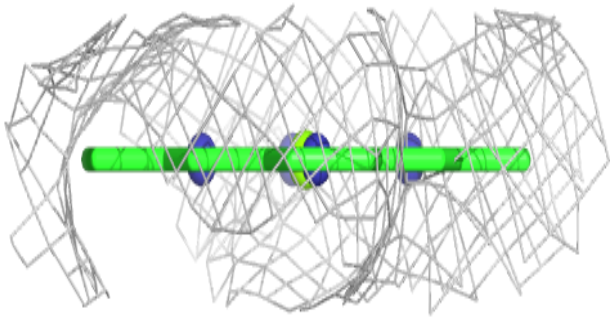


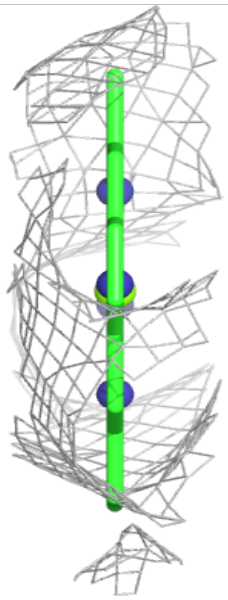


Electron density around CLA G 1248:

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

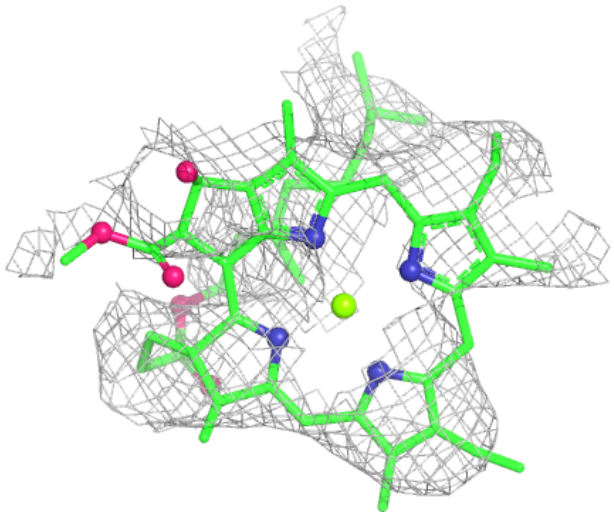


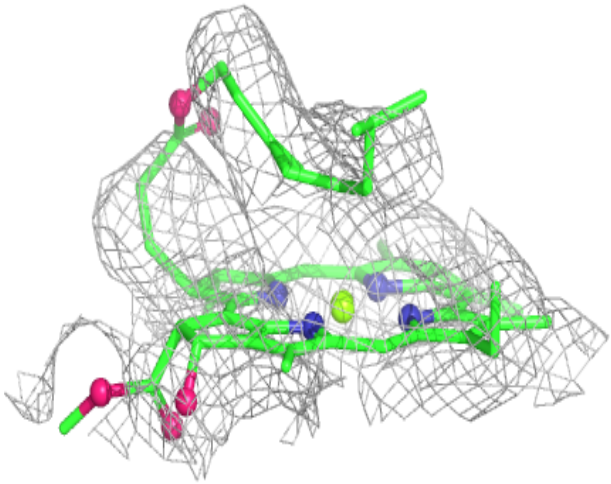


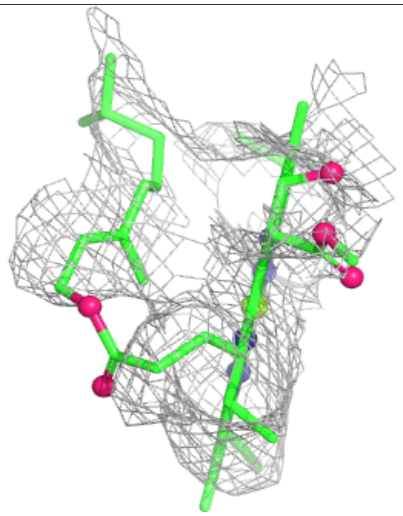


Electron density around CLA H 1501:

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

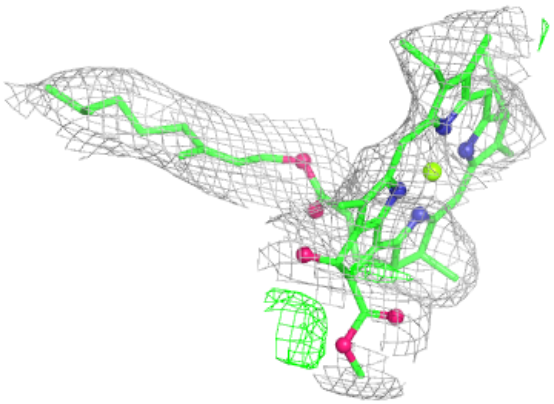


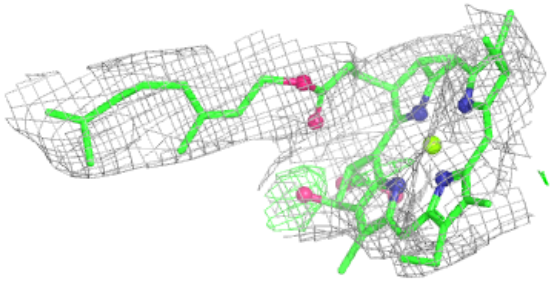


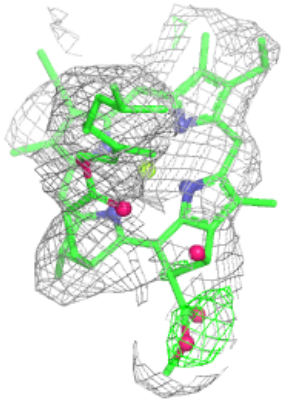


Electron density around CLA A 1126:

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

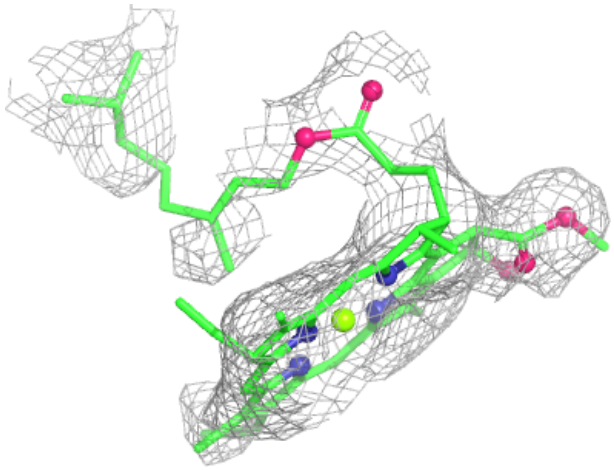


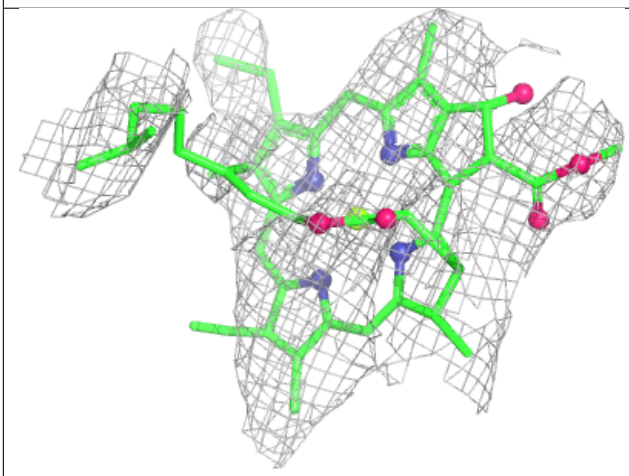


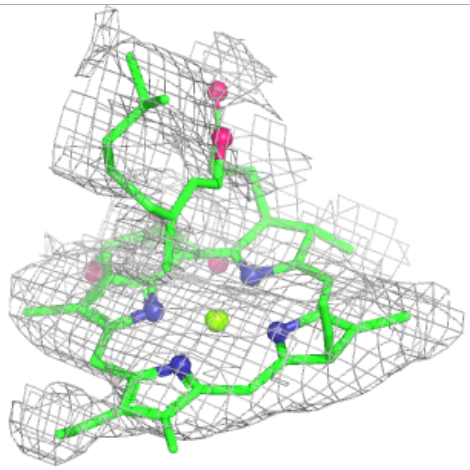


Electron density around CLA I 1204:

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

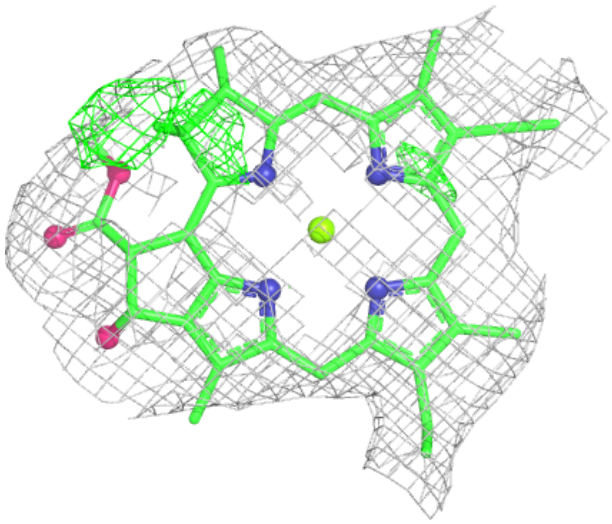


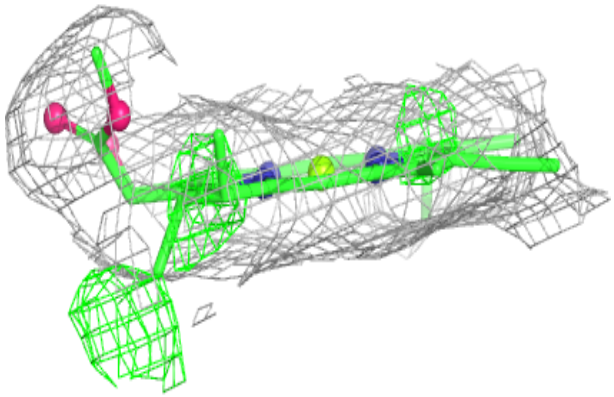


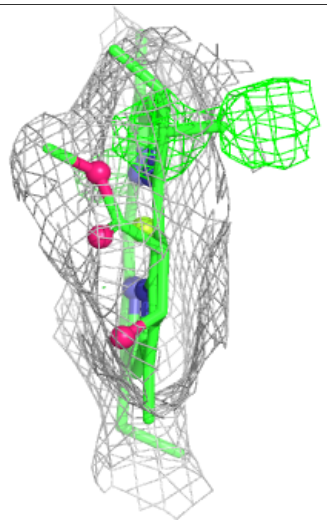


Electron density around CLA A 1106:

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

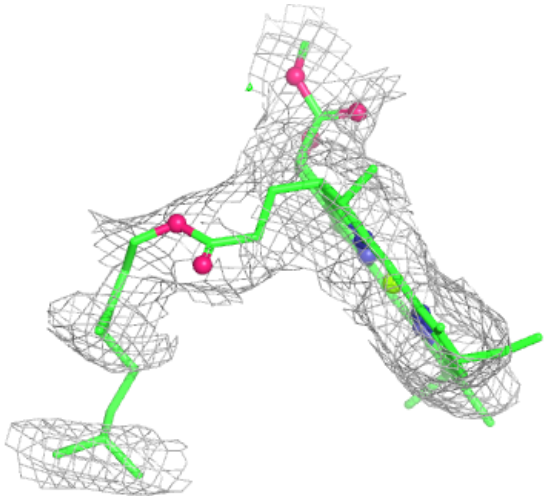


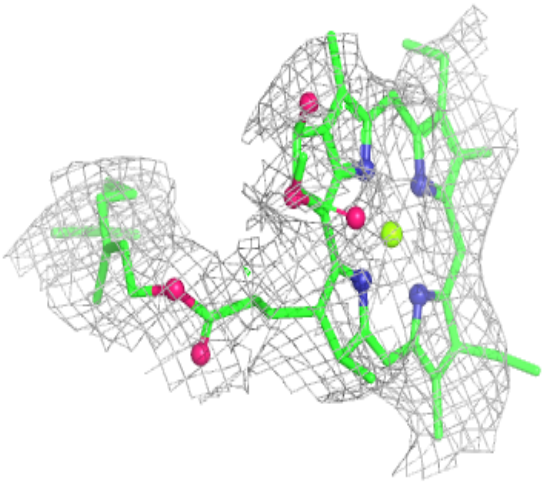


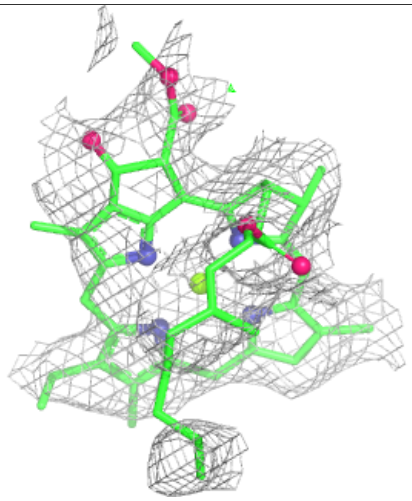


Electron density around CLA A 1128:

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

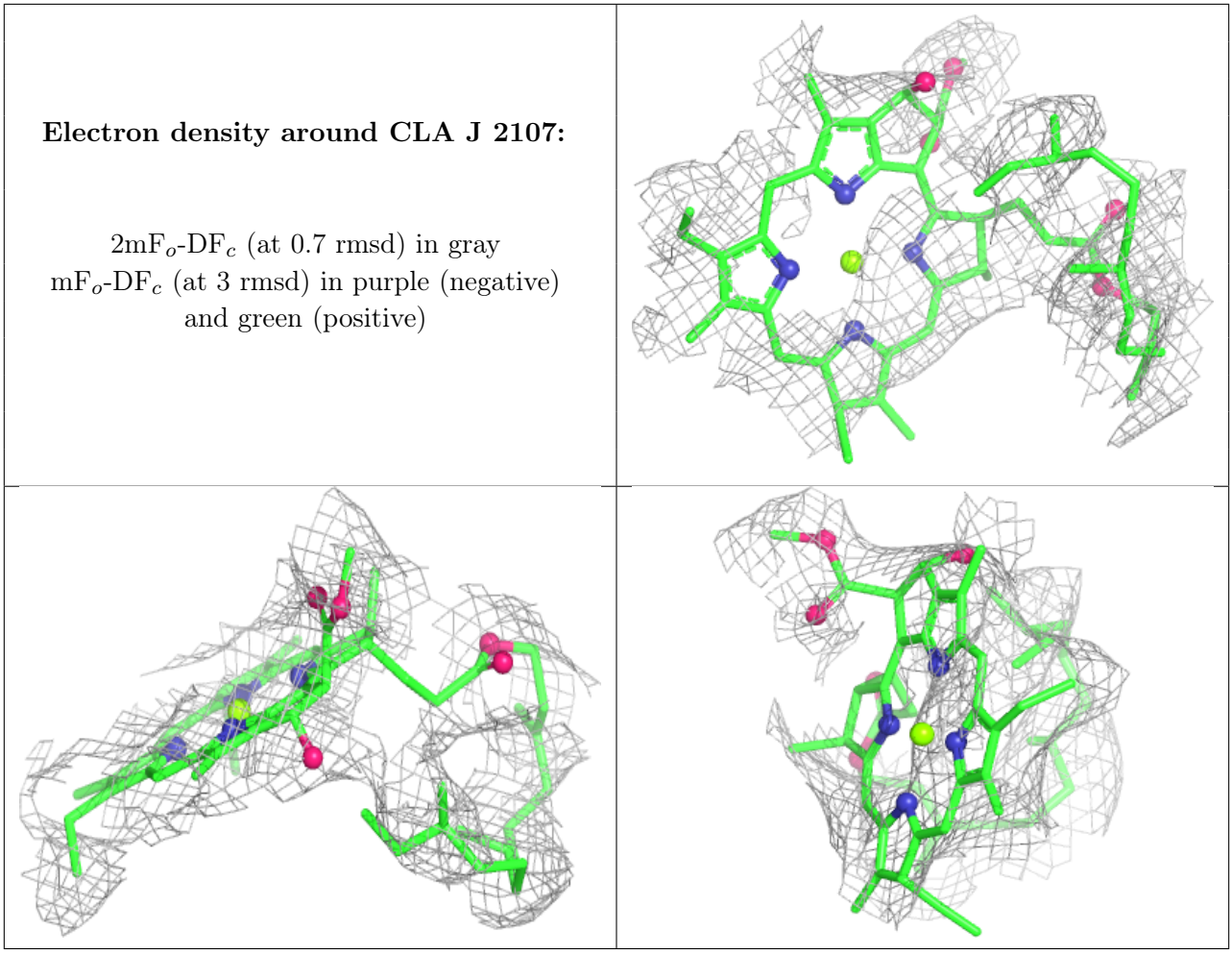






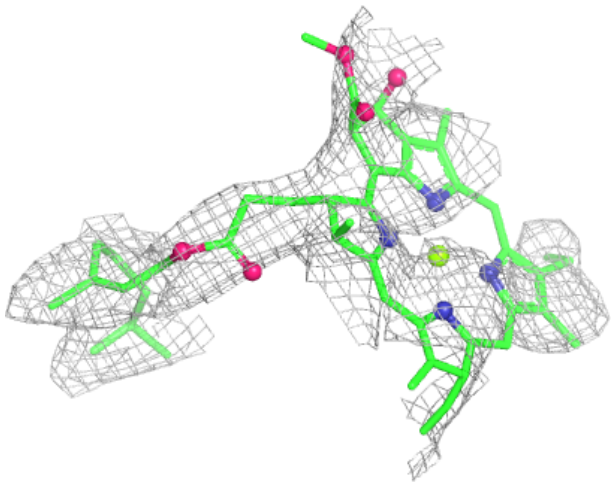
Electron density around CLA J 2107:

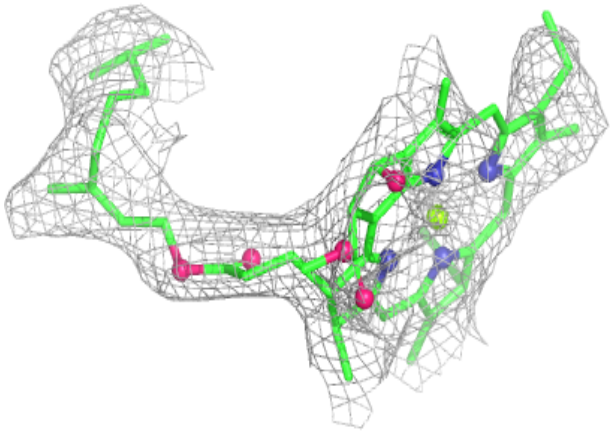
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

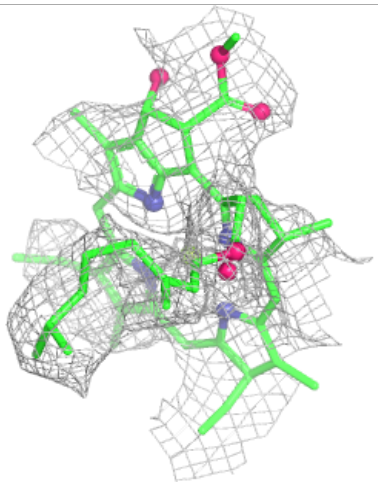


Electron density around CLA A 1129:

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

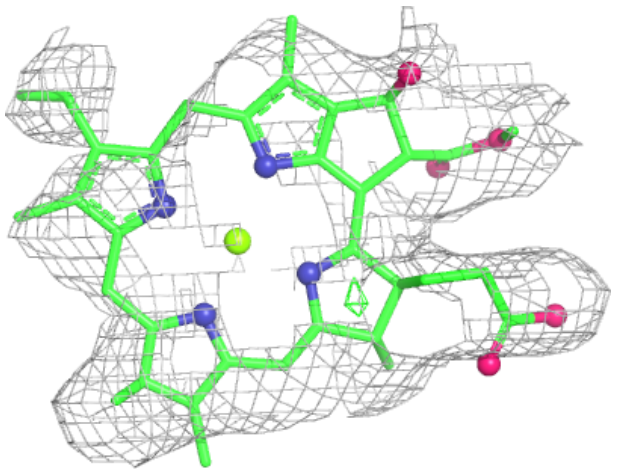


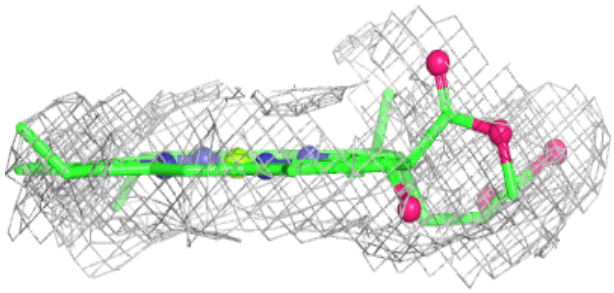


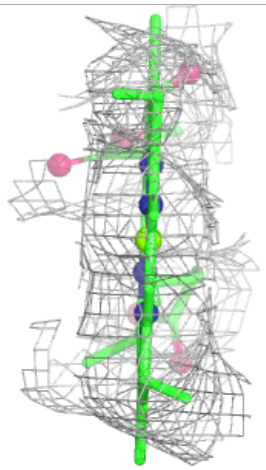


Electron density around CLA A 1131:

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

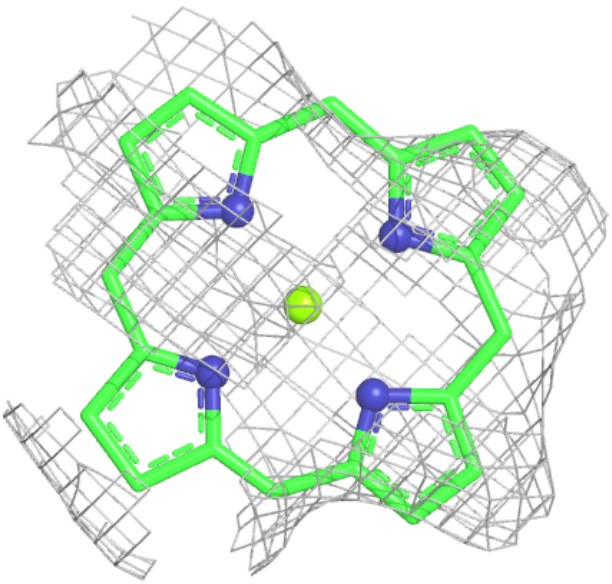


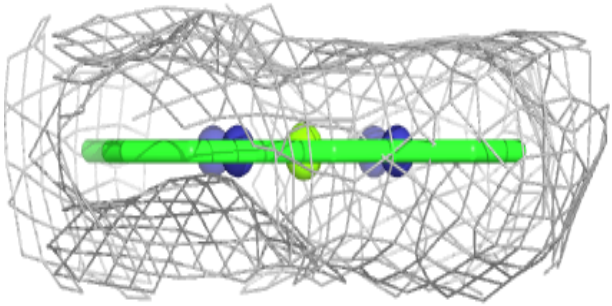


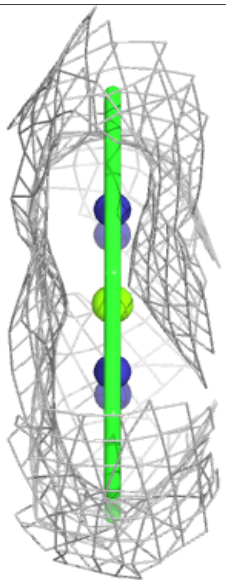


Electron density around CLA K 1153:

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

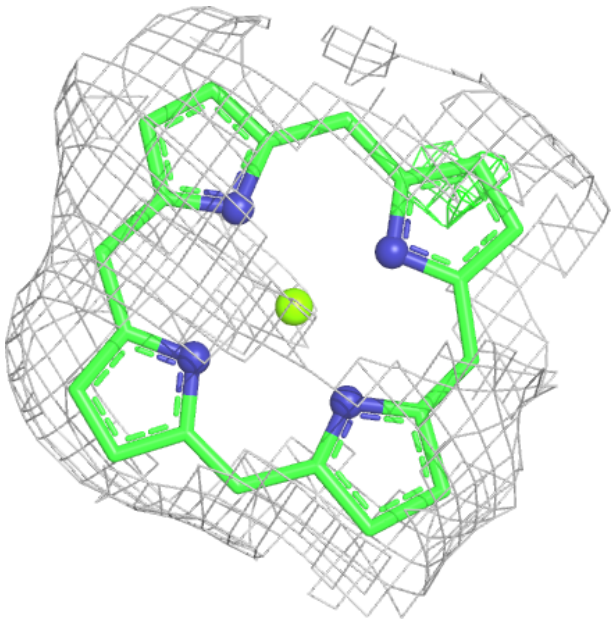


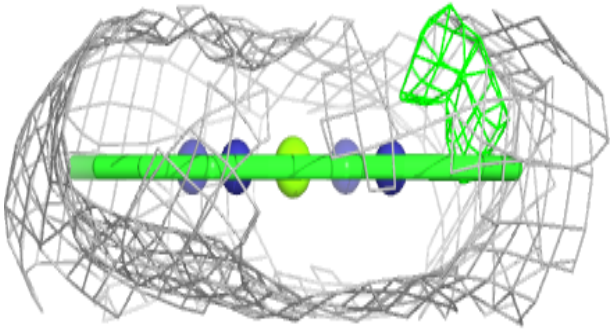


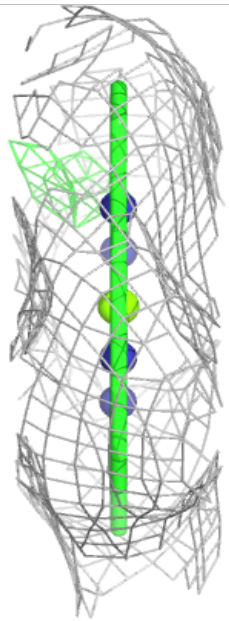


Electron density around CLA A 1133:

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

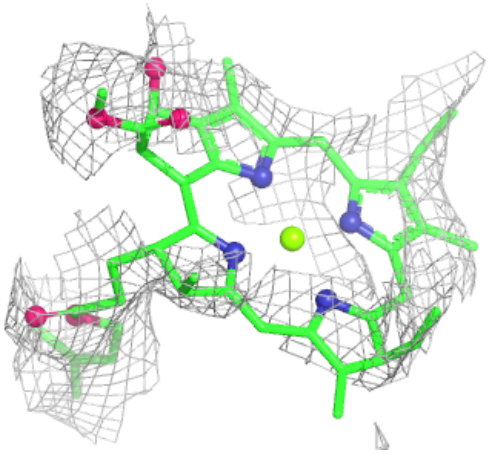


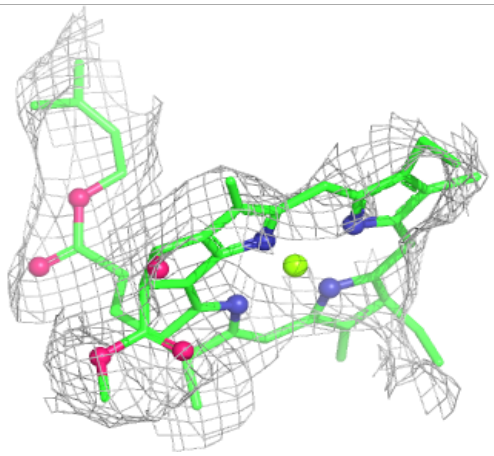


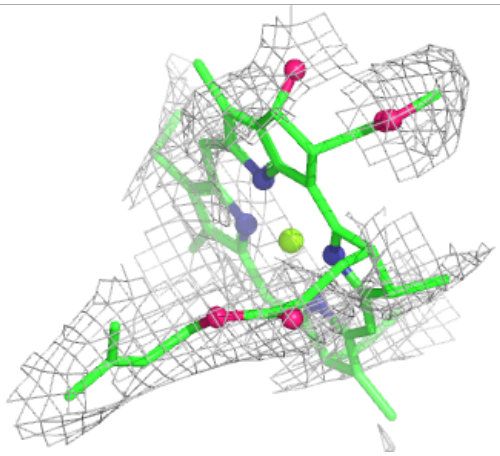


Electron density around CLA L 1130:

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

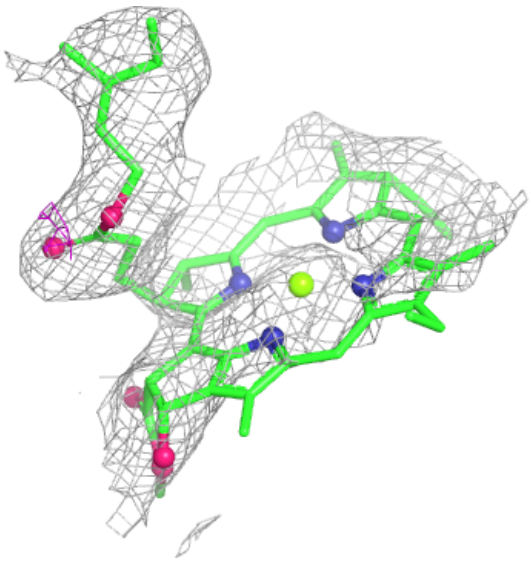


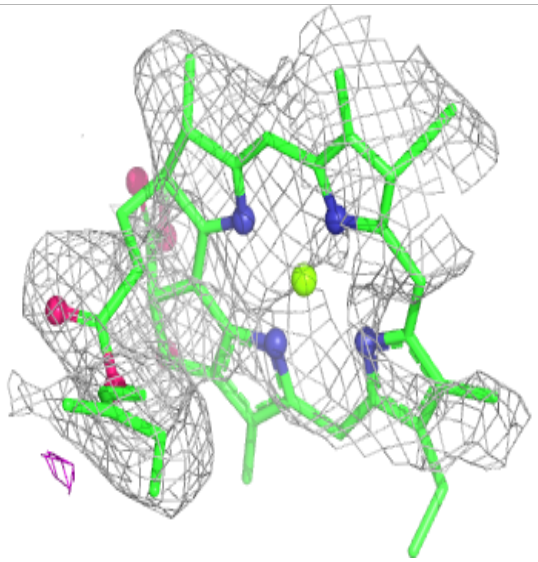


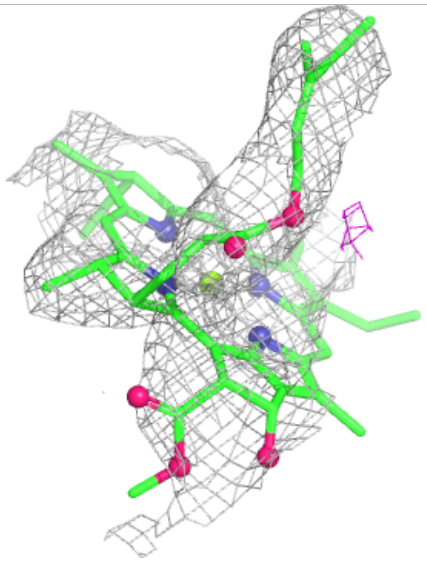


Electron density around CLA L 1502:

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

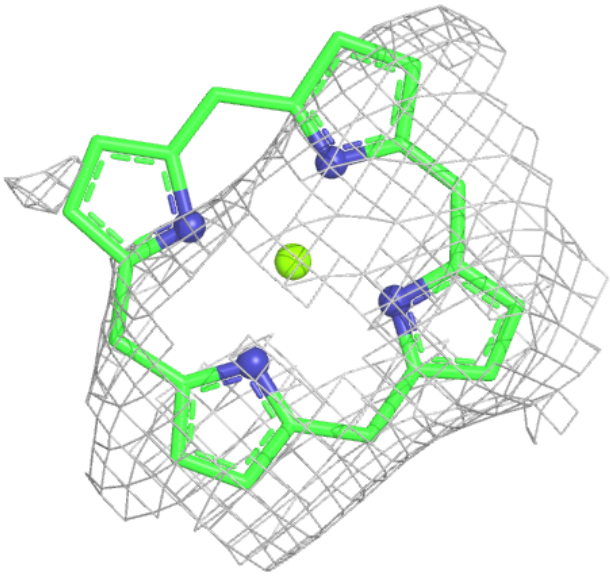


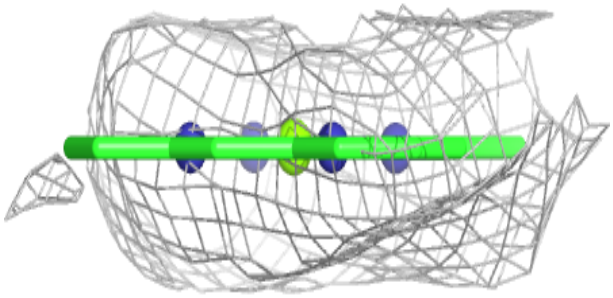


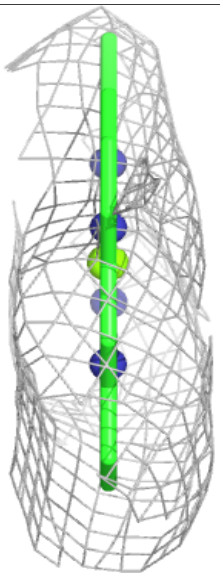


Electron density around CLA A 1134:

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

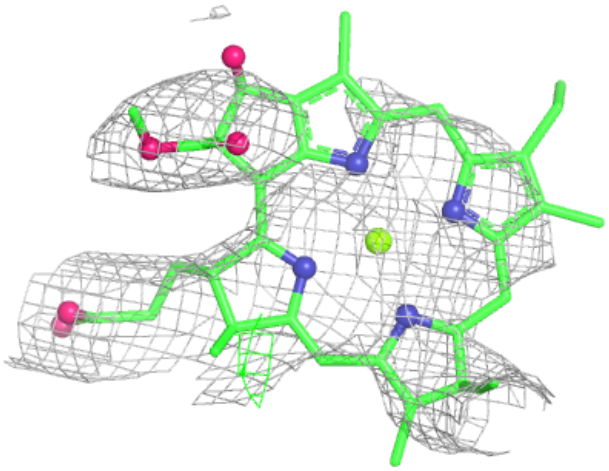


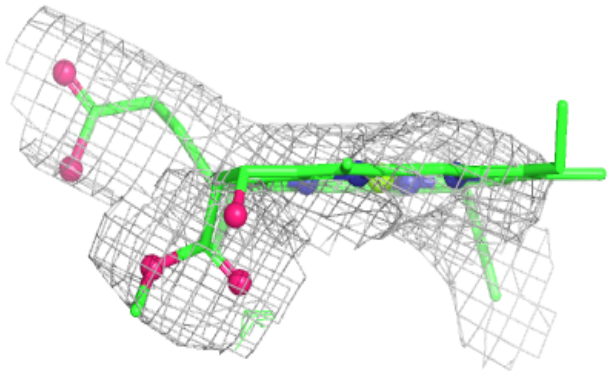


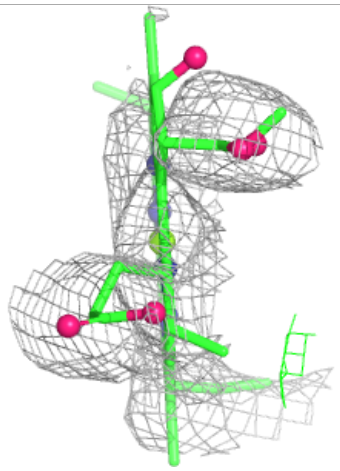


Electron density around CLA A 1135:

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

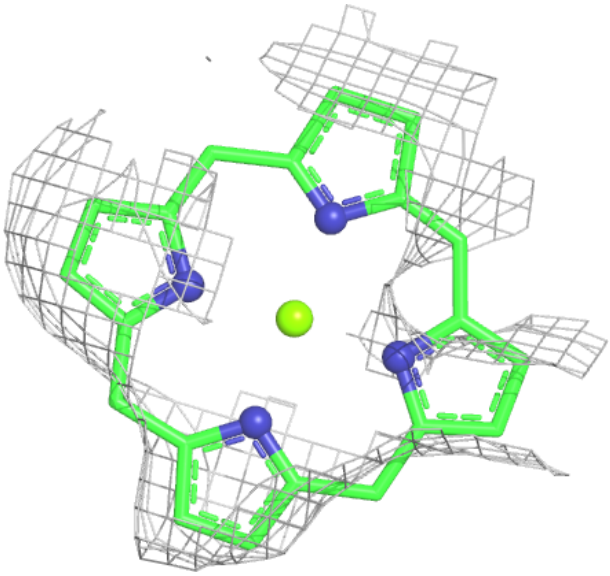


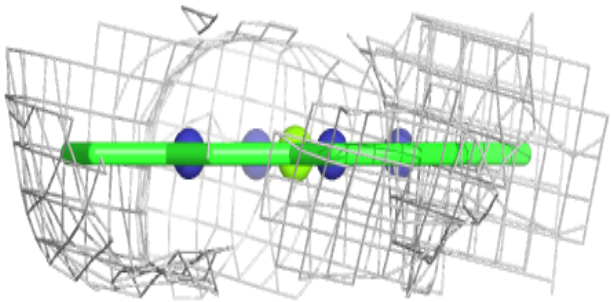


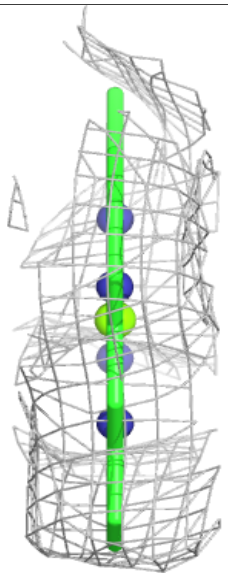


Electron density around CLA 1 1006:

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

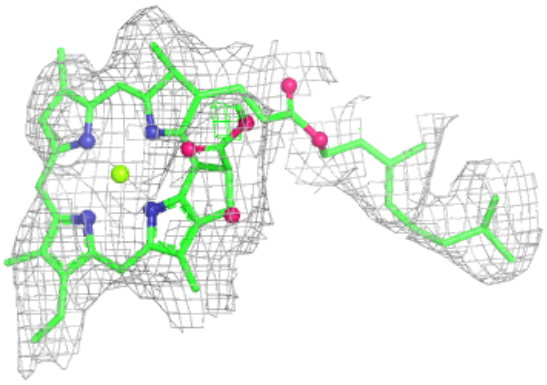


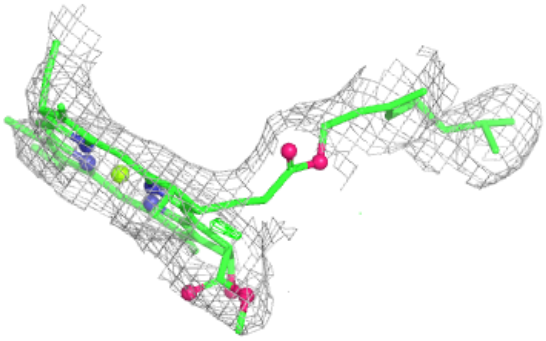


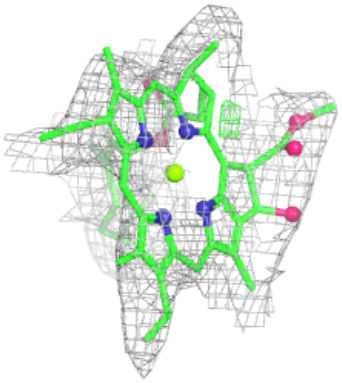


Electron density around CLA A 1137:

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

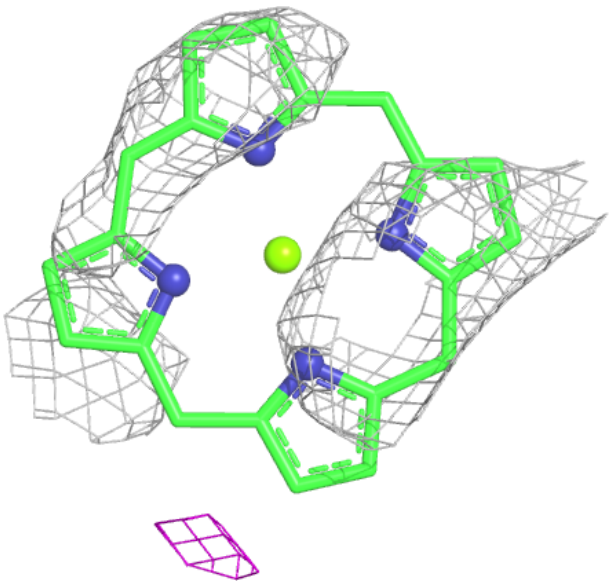


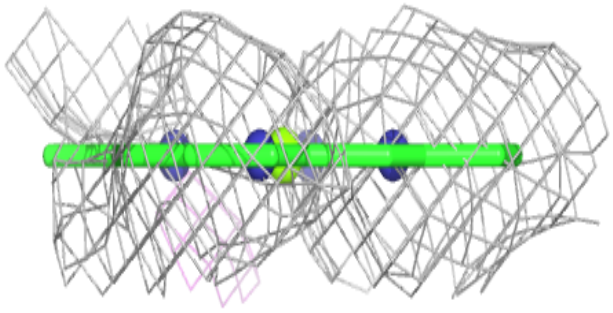


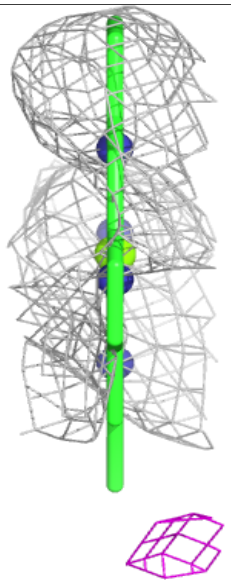


Electron density around CLA 1 1010:

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

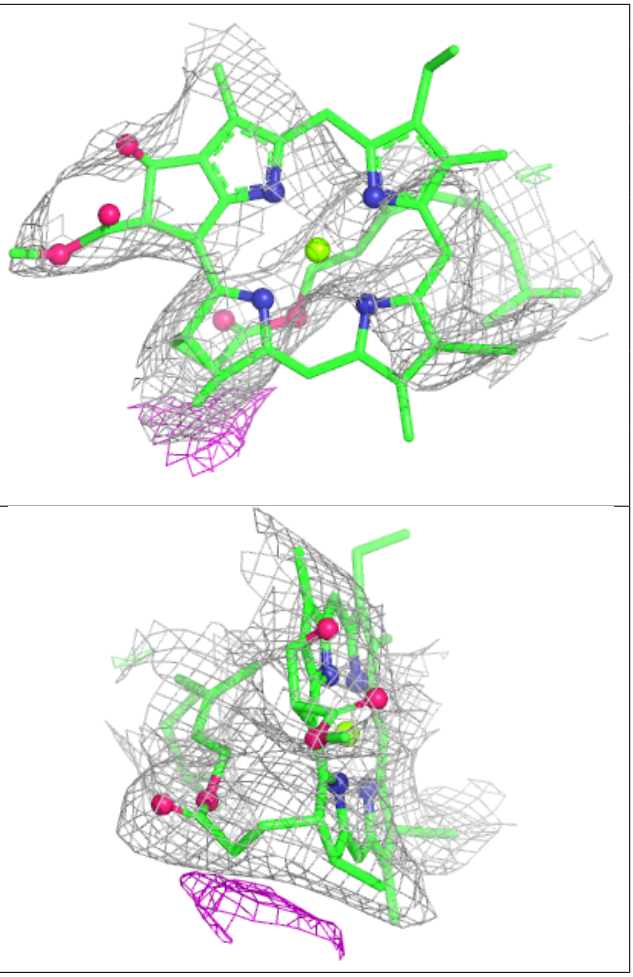






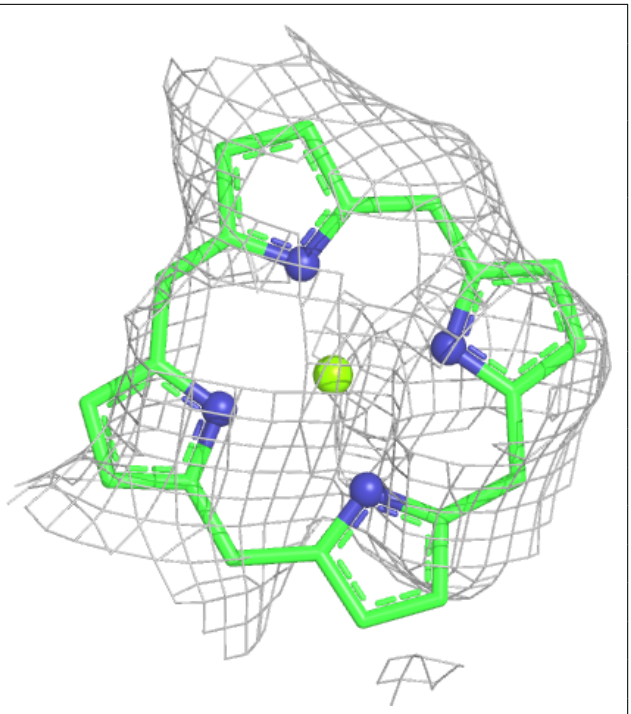
Electron density around CLA A 1140:

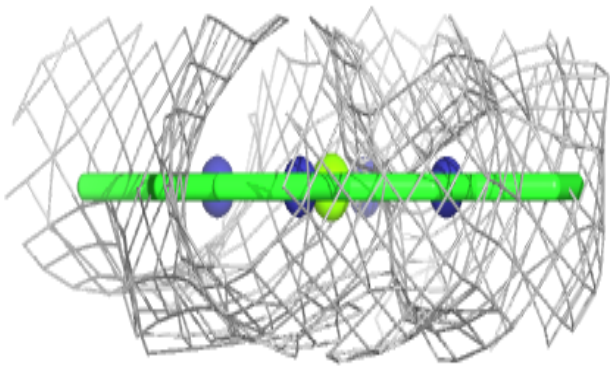
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

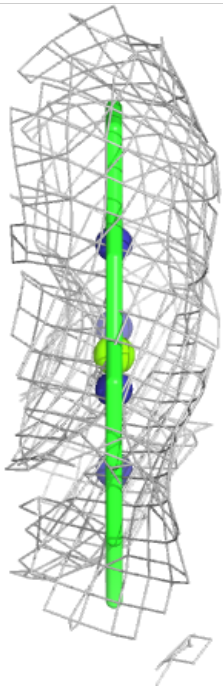


Electron density around CLA A 1142:

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

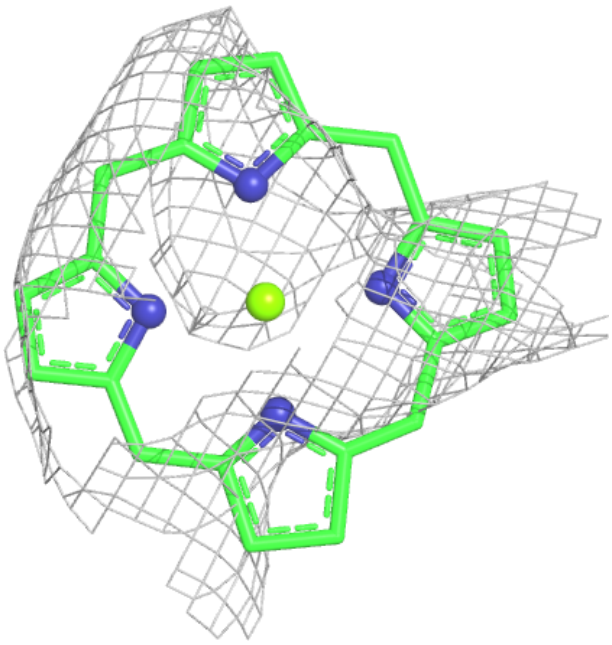


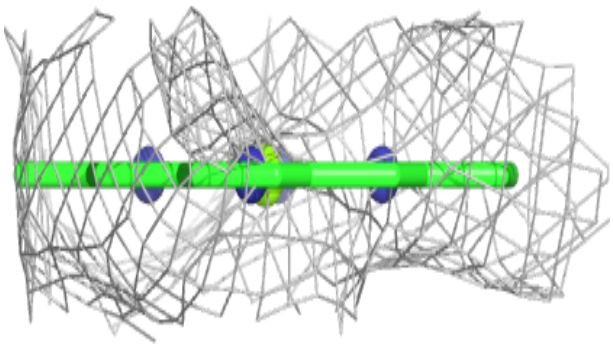


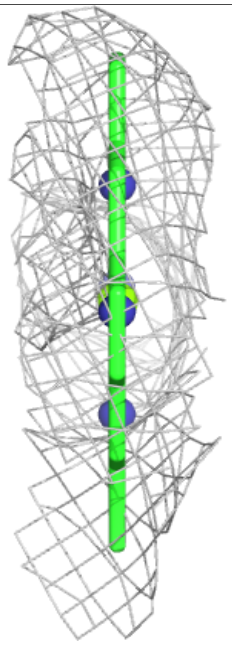


Electron density around CLA A 1143:

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

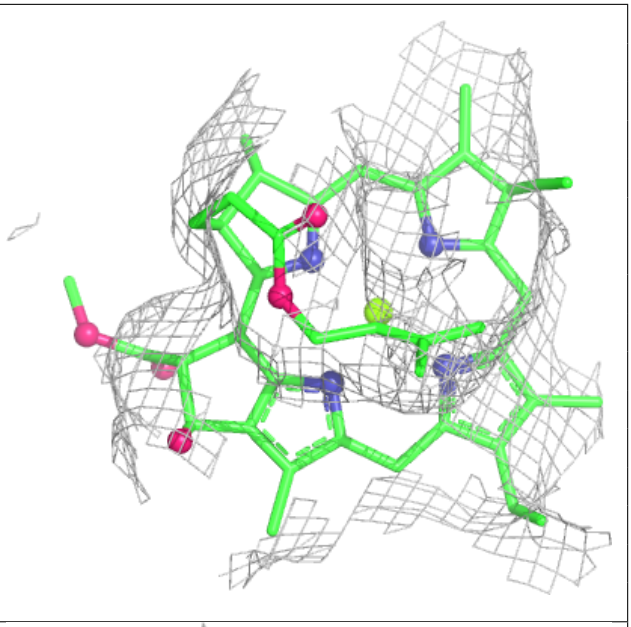


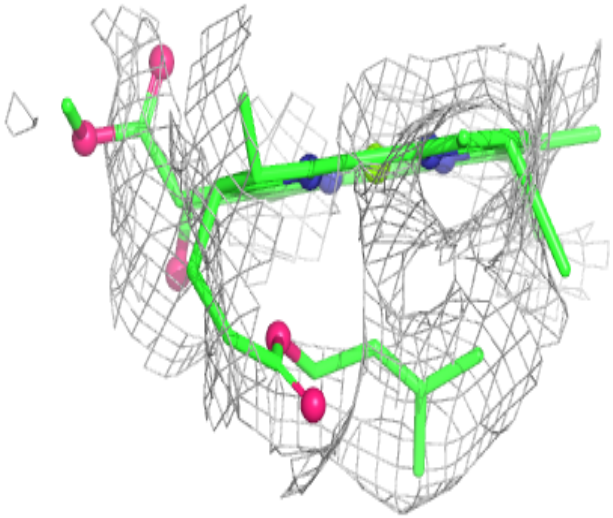


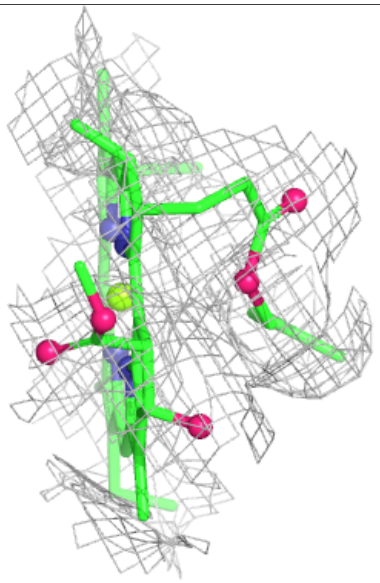


Electron density around CLA A 1108:

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

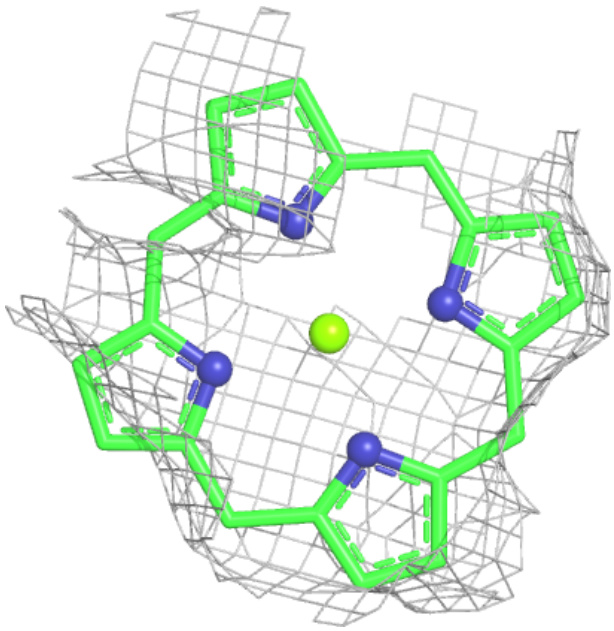


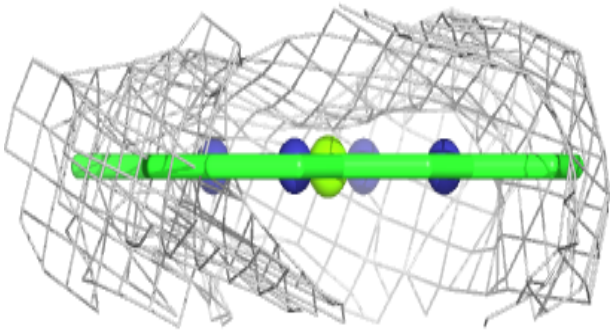


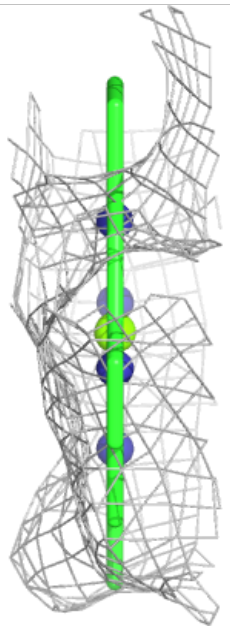


Electron density around CLA 1 1003:

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

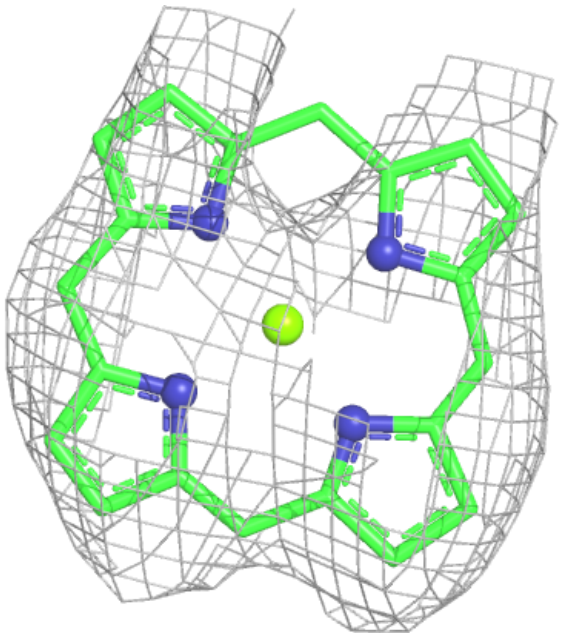


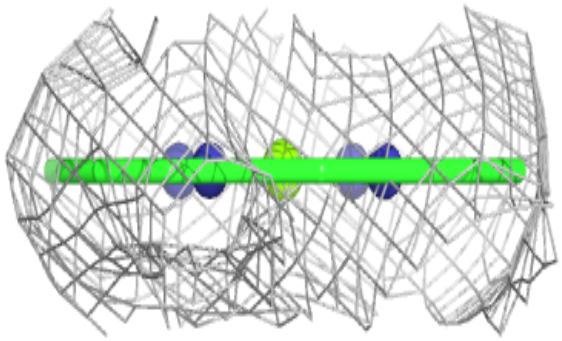


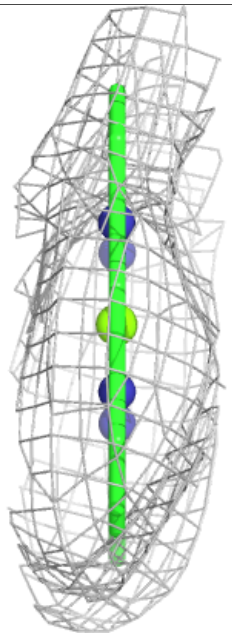


Electron density around CLA A 1146:

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

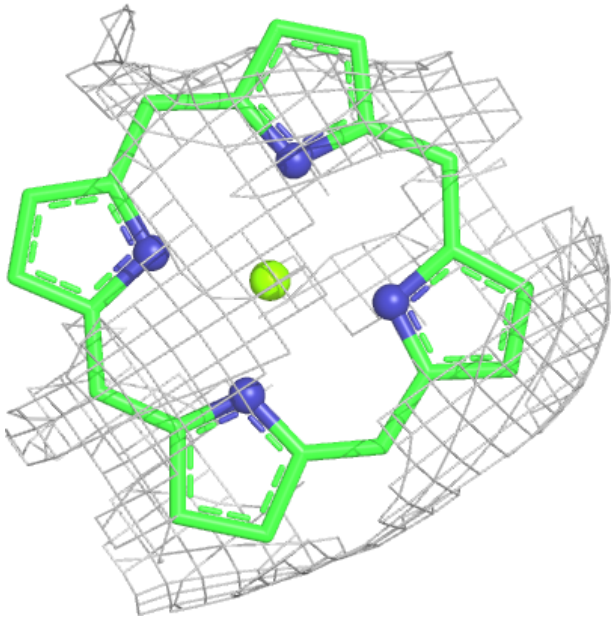


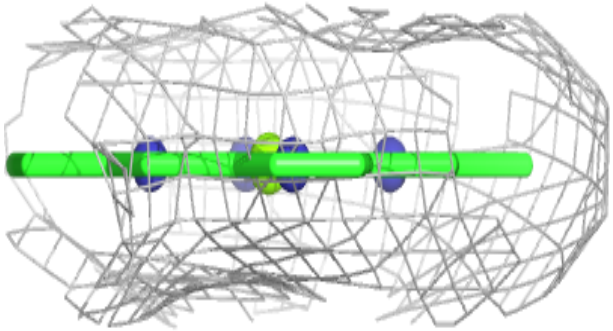


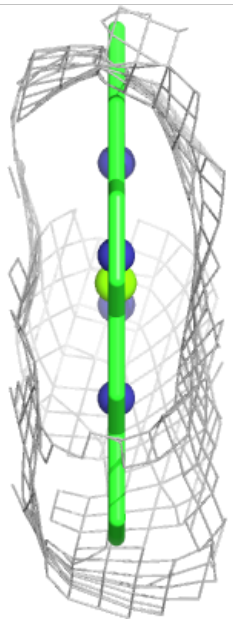


Electron density around CLA 1 1014:

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

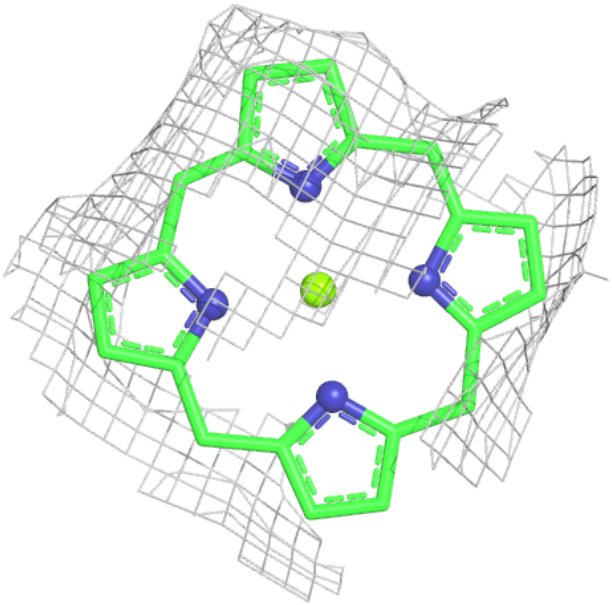


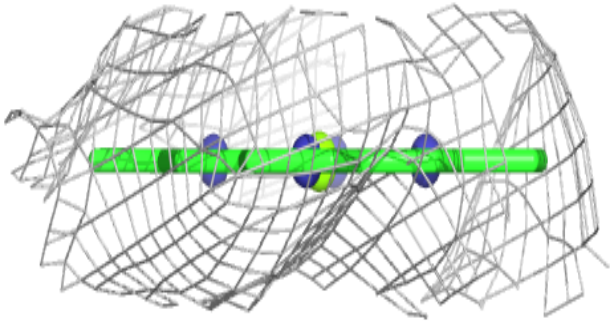


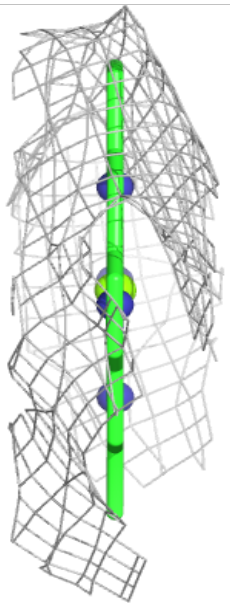


Electron density around CLA A 1110:

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

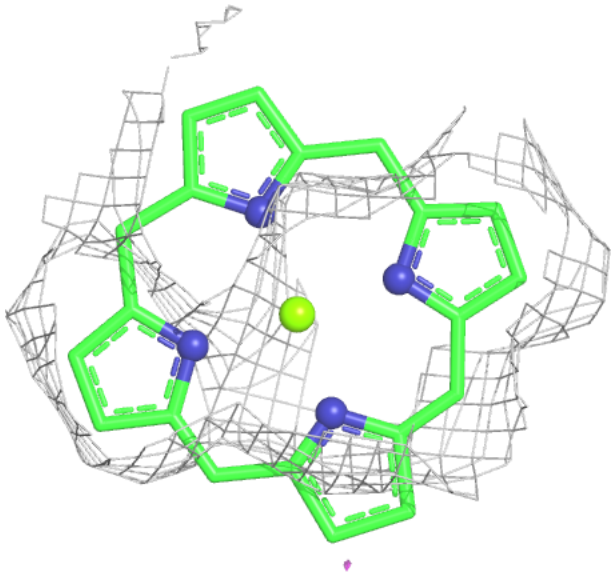


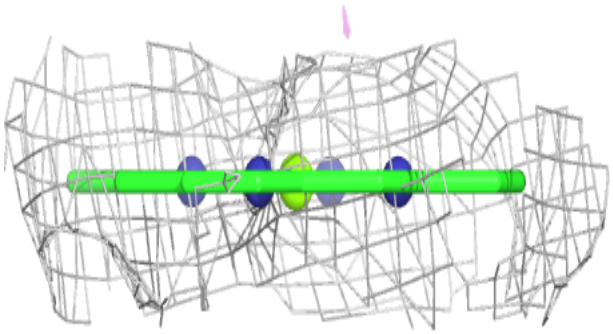


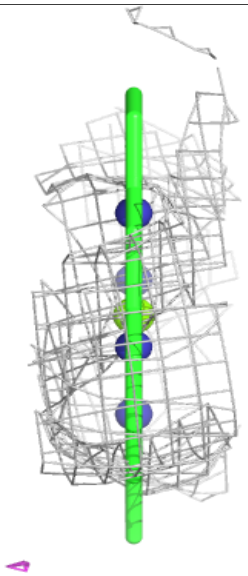


Electron density around CLA A 1111:

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

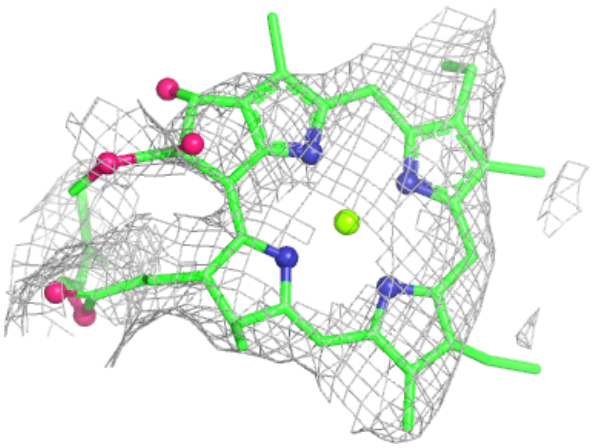


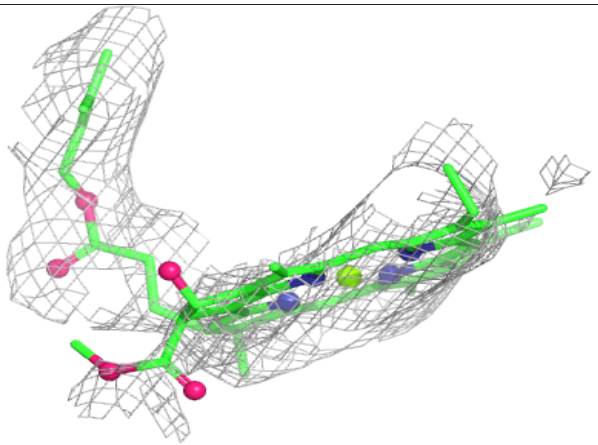


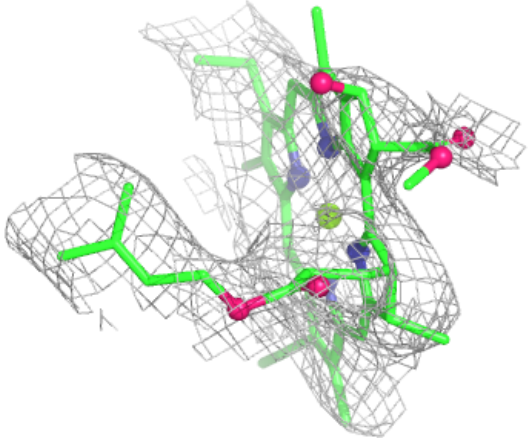


Electron density around CLA A 1113:

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

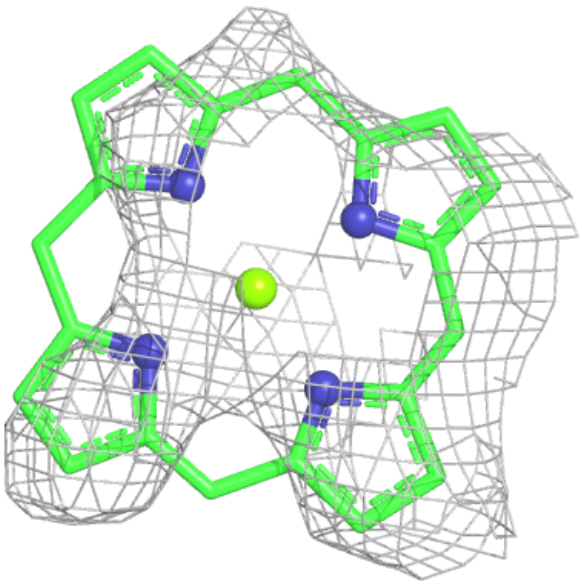


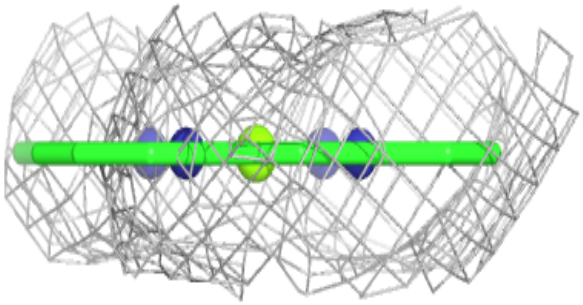


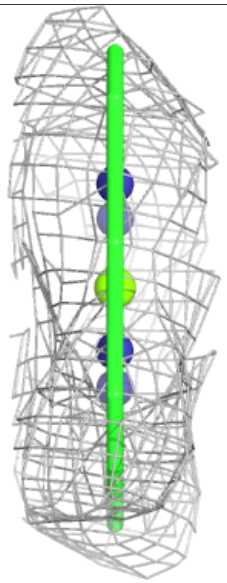


Electron density around CLA A 1152:

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

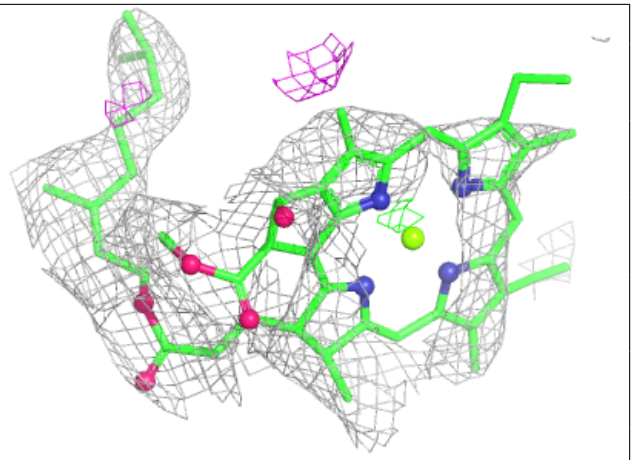


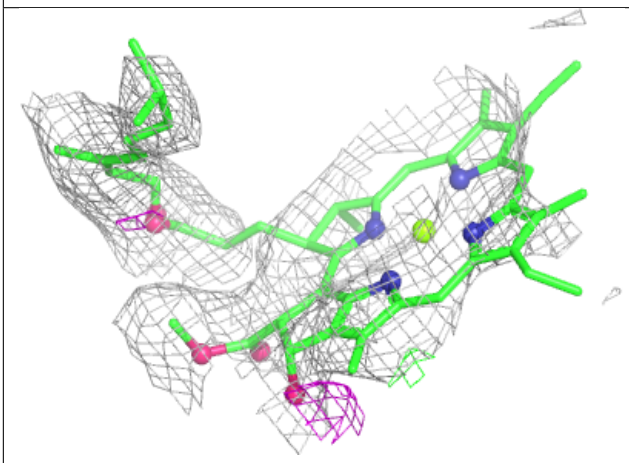


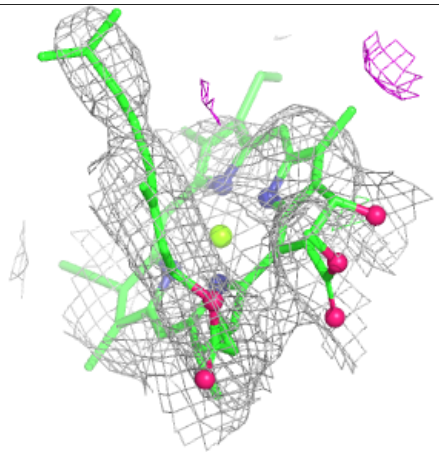


Electron density around CLA A 9011:

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

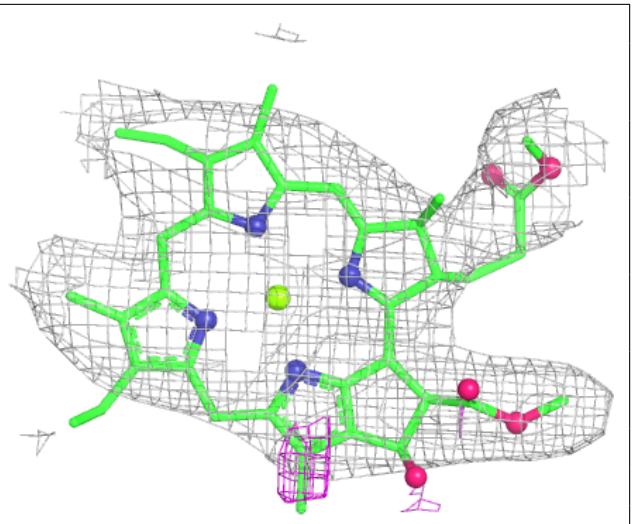


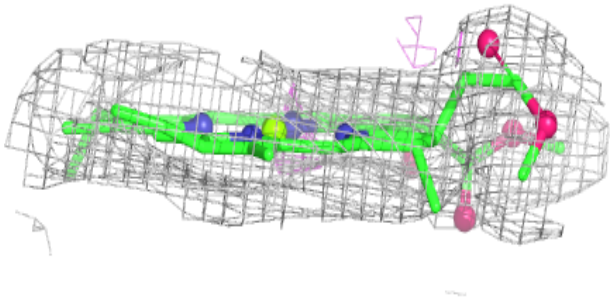




Electron density around CLA A 9013:

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

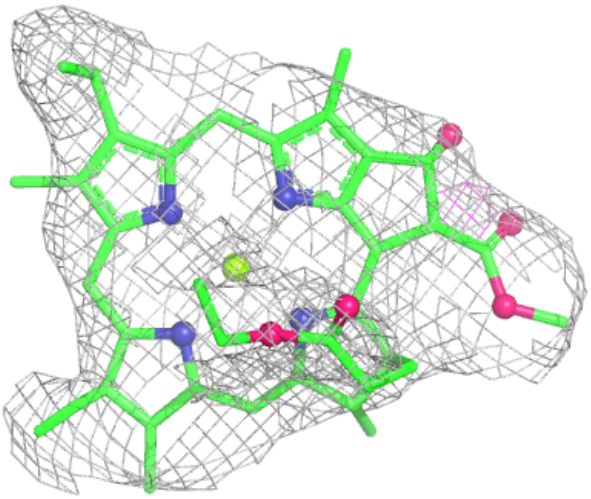


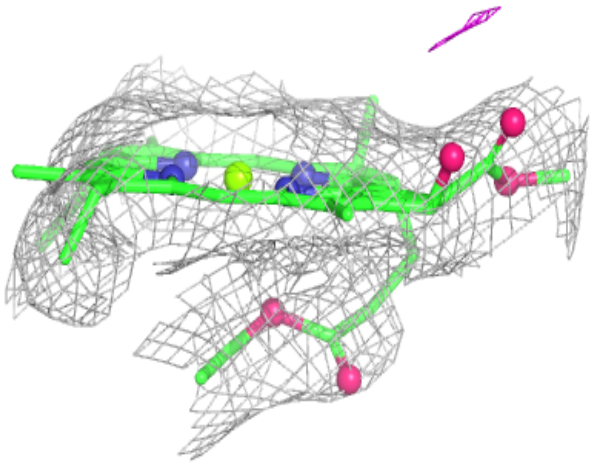


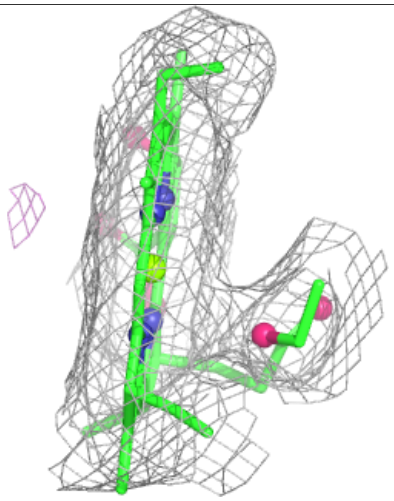


Electron density around CLA A 1115:

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

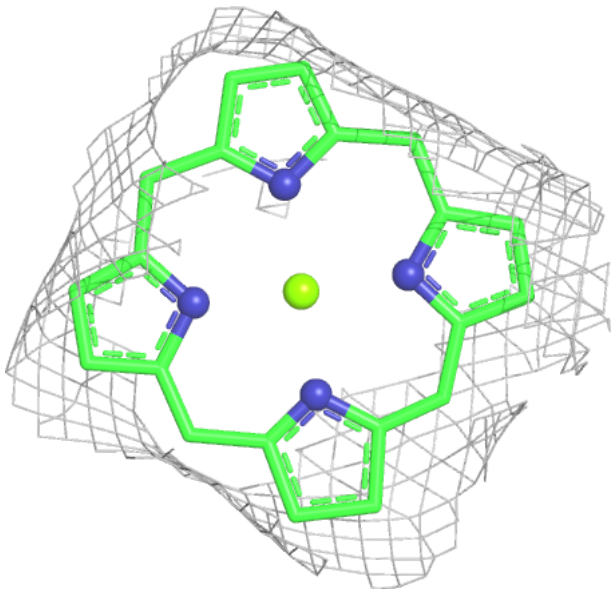


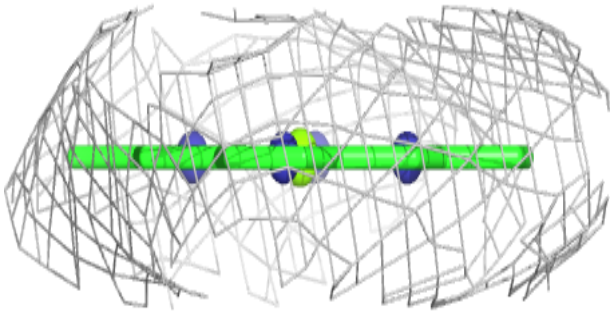


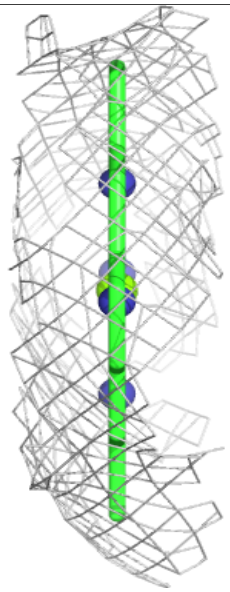


Electron density around CLA 2 2007:

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

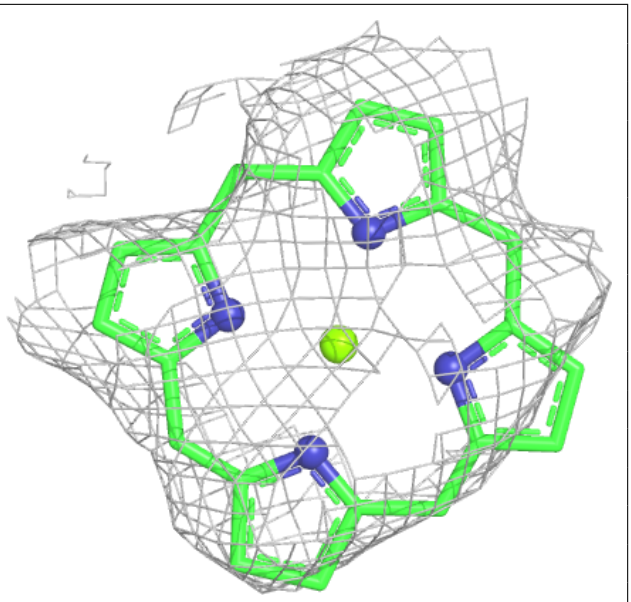


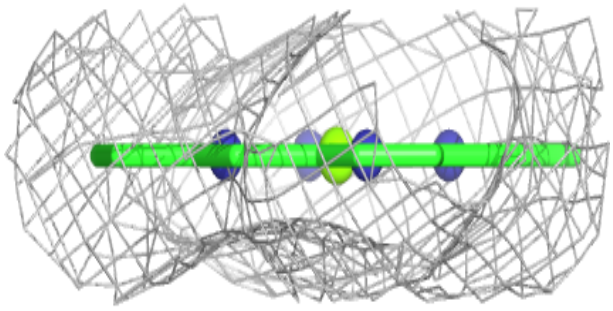


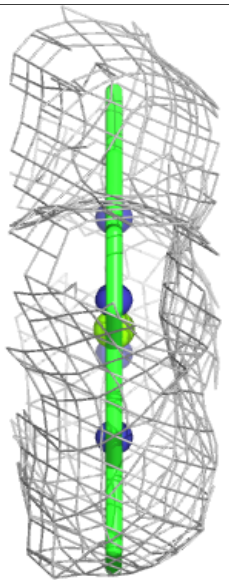


Electron density around CLA 2 2002:

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

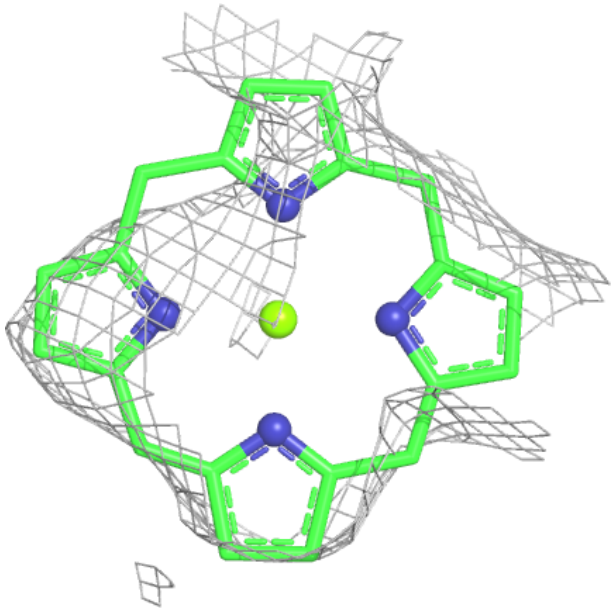


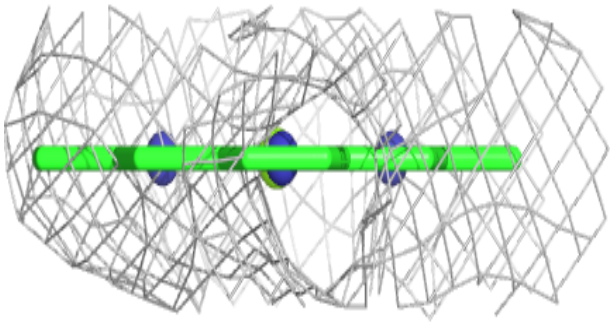


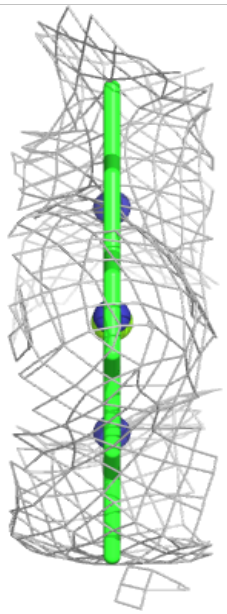


Electron density around CLA 2 2003:

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

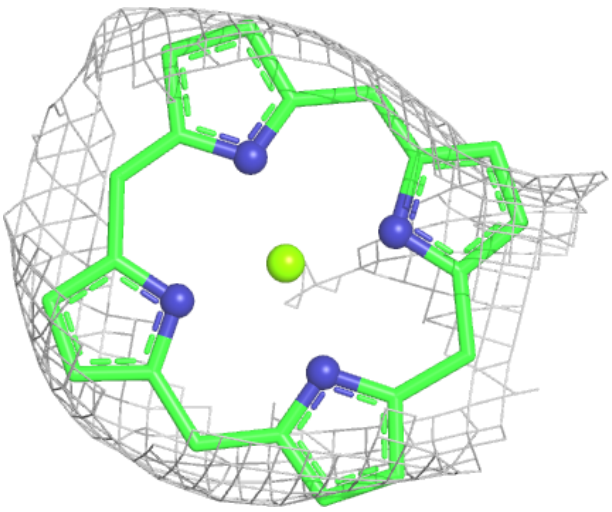


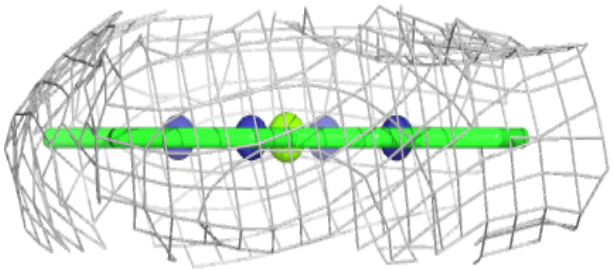


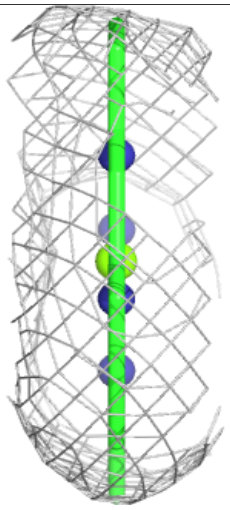


Electron density around CLA 3 2009:

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

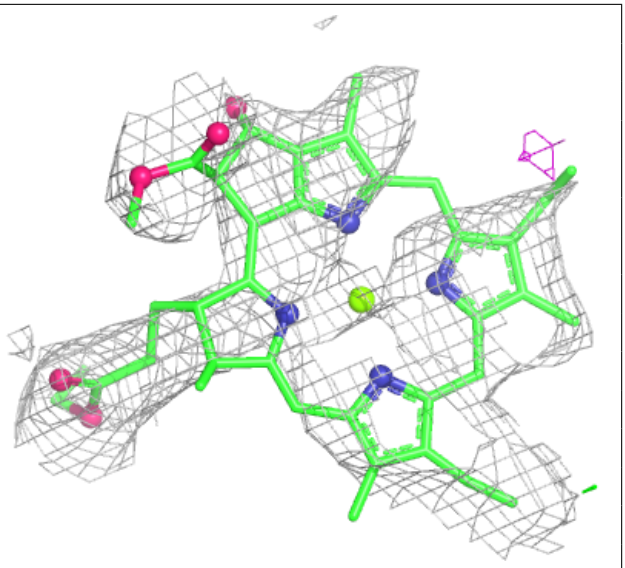


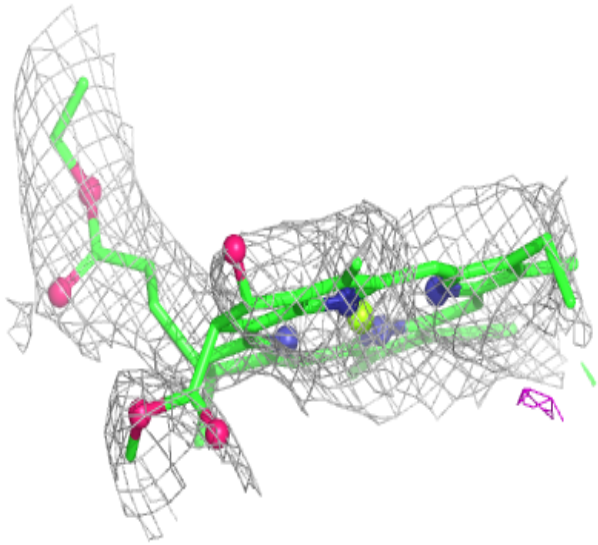


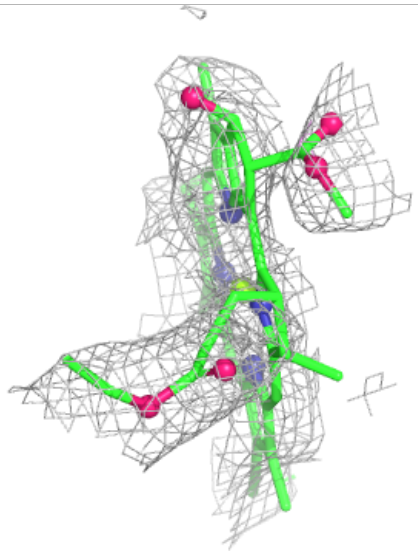


Electron density around CLA B 9010:

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

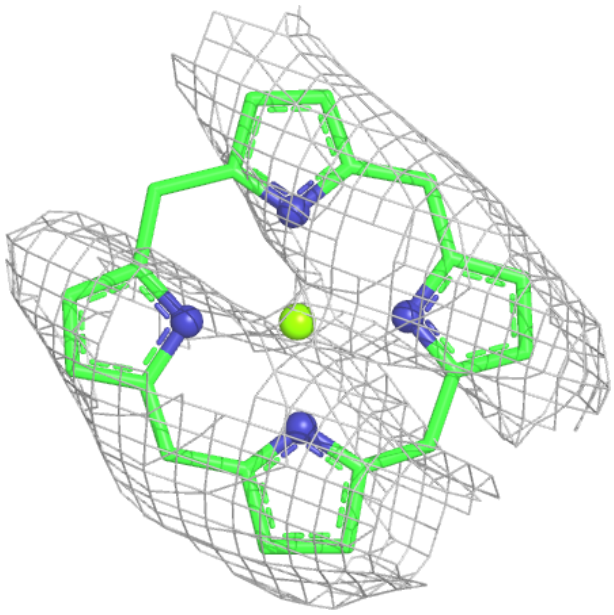


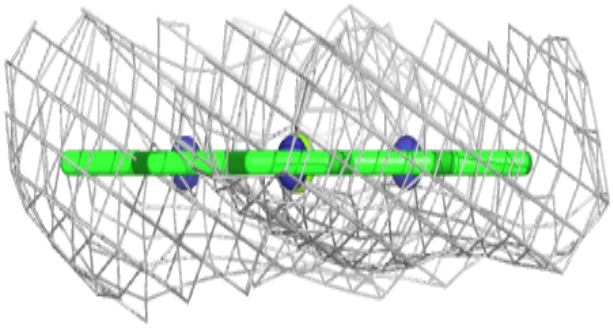


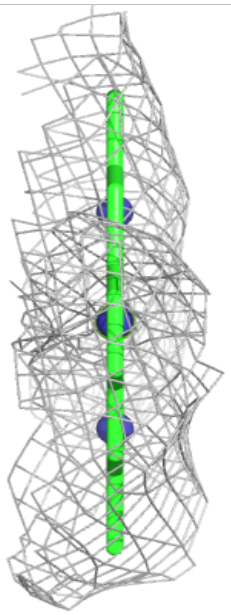


Electron density around CLA 3 3004:

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

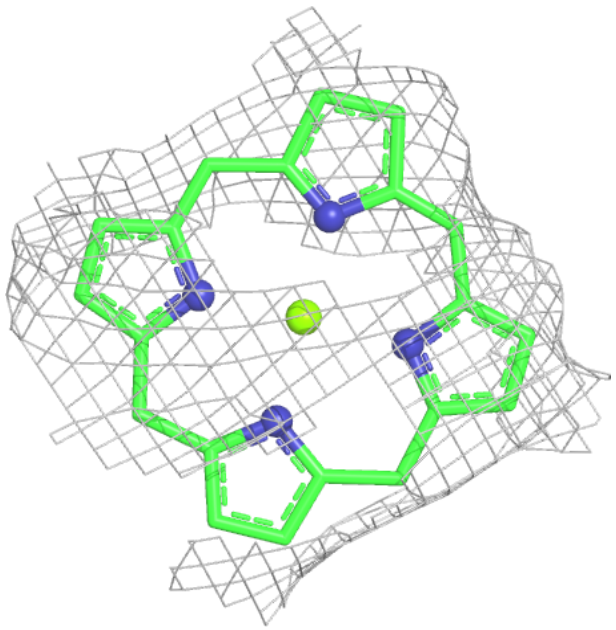


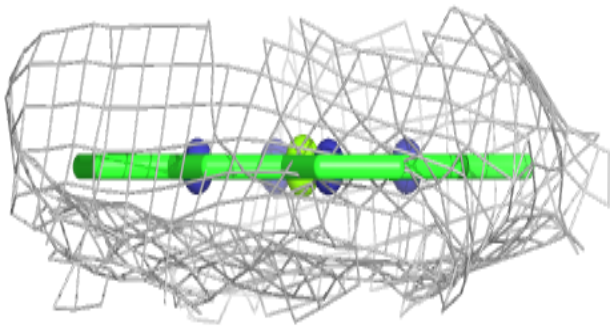


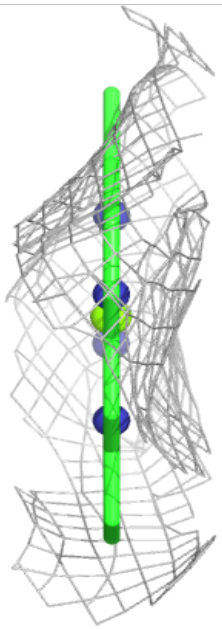


Electron density around CLA 3 3005:

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

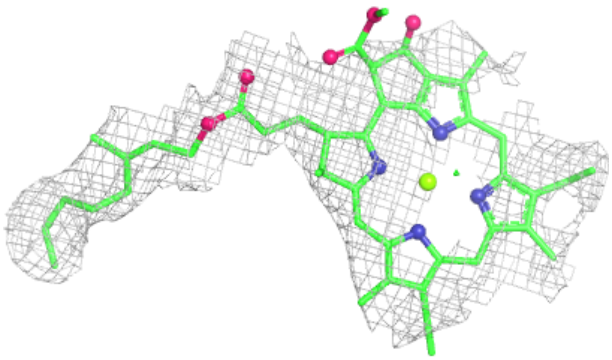


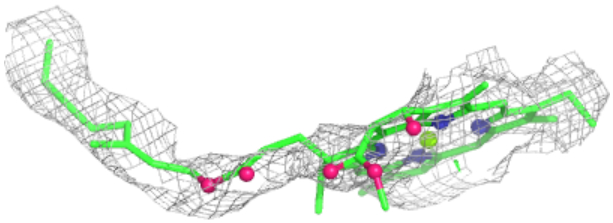


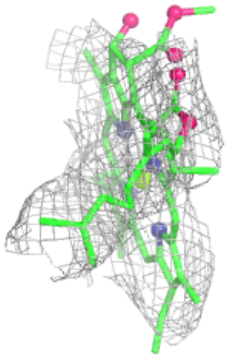


Electron density around CLA B 9012:

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

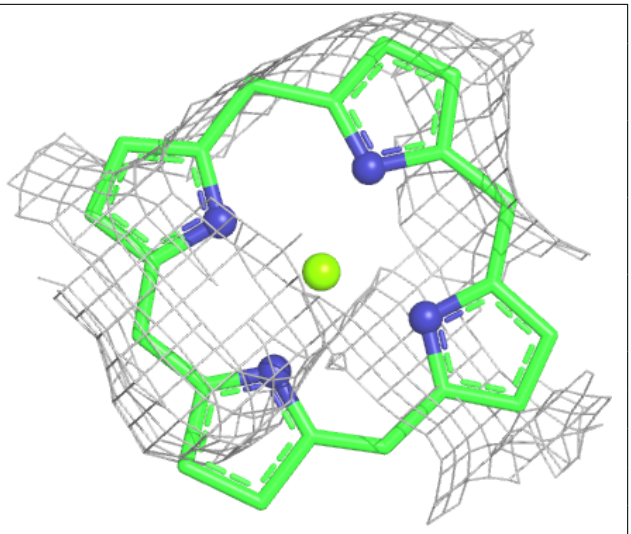


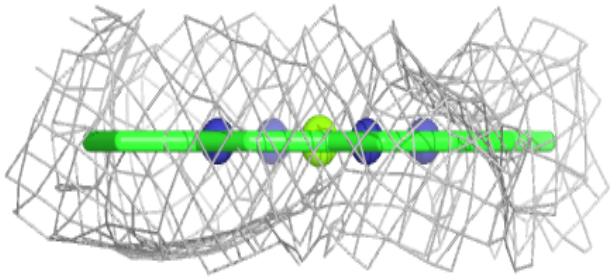


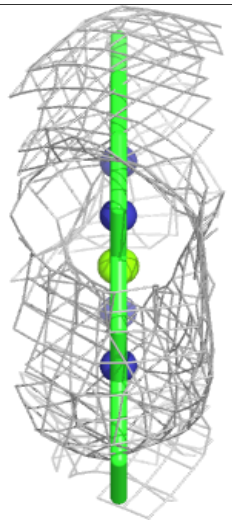


Electron density around CLA 3 3006:

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

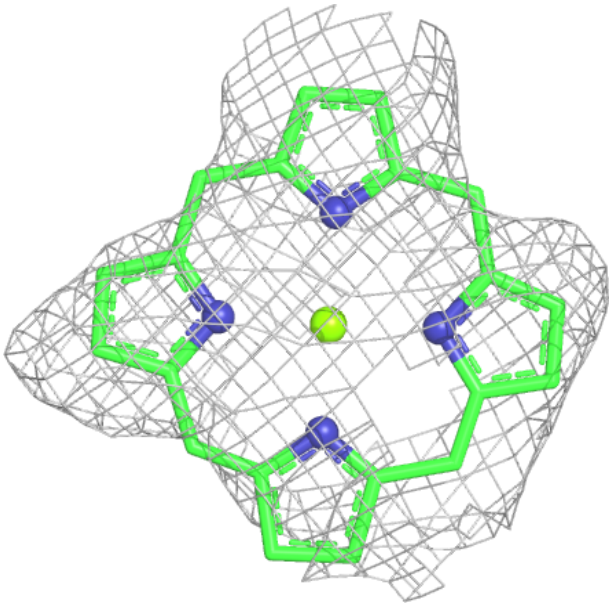


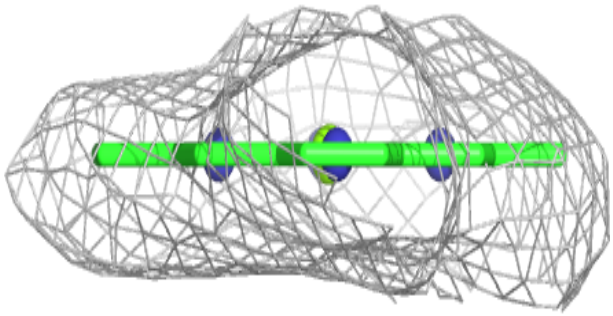


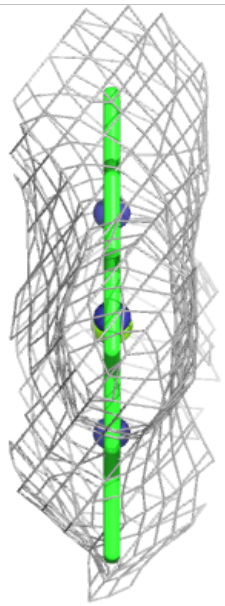


Electron density around CLA 3 3013:

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

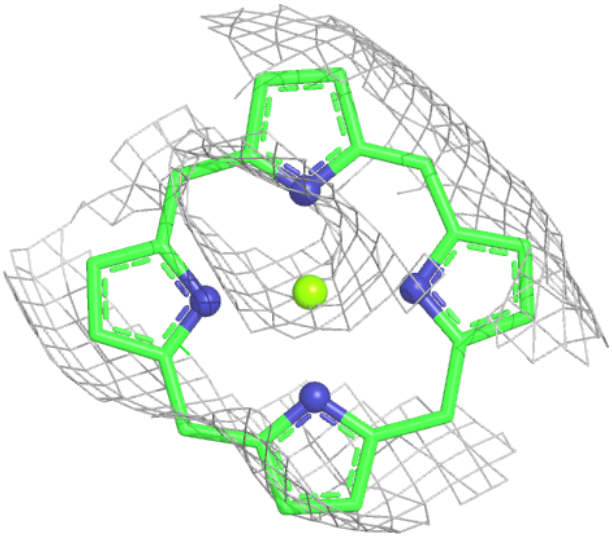


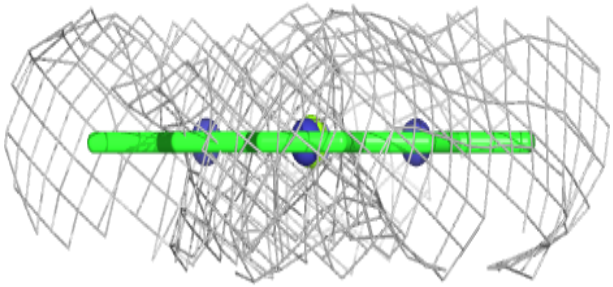


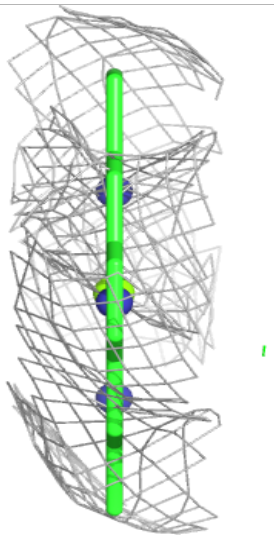


Electron density around CLA 3 3010:

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

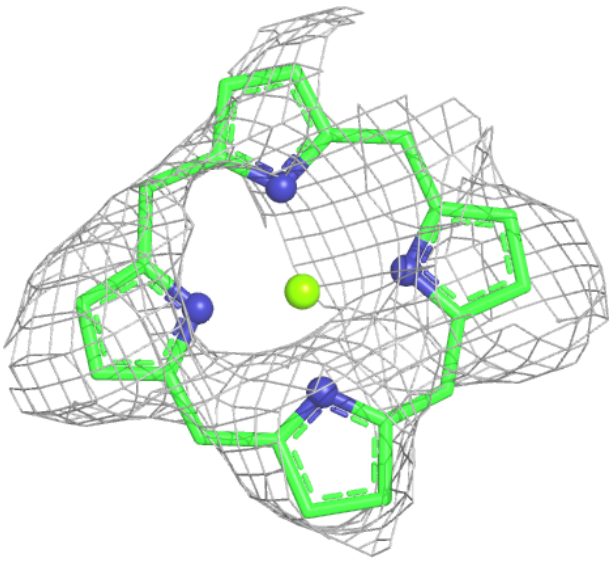


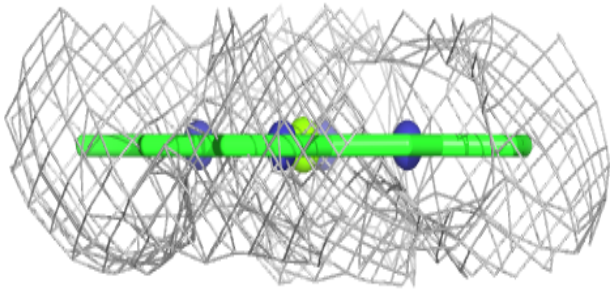


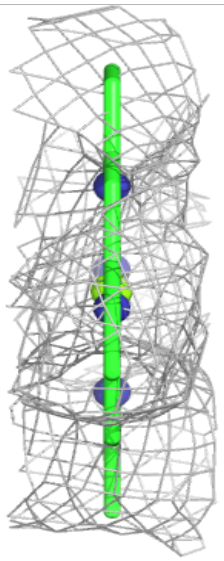


Electron density around CLA A 1116:

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

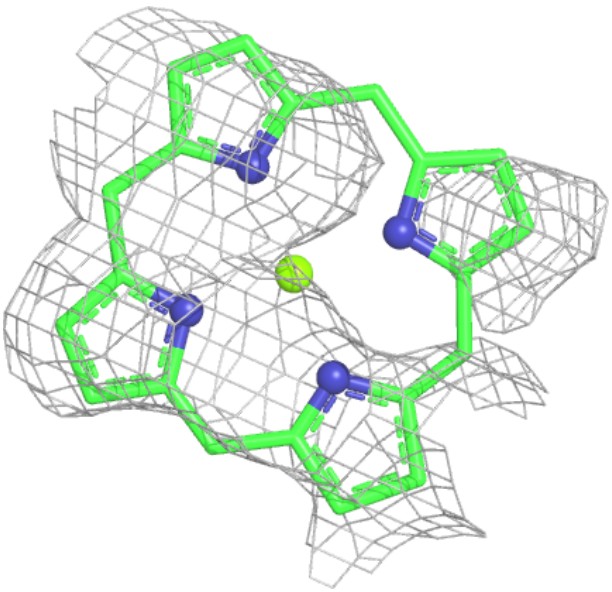


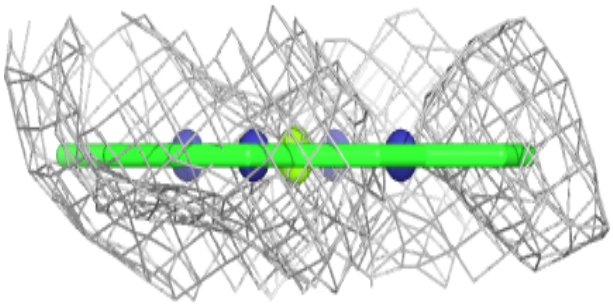


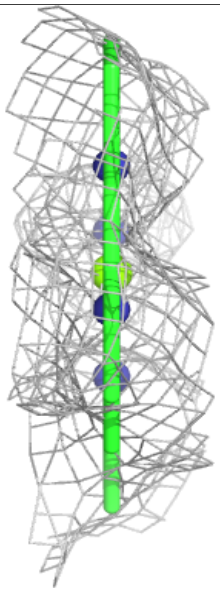


Electron density around CLA 3 3011:

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

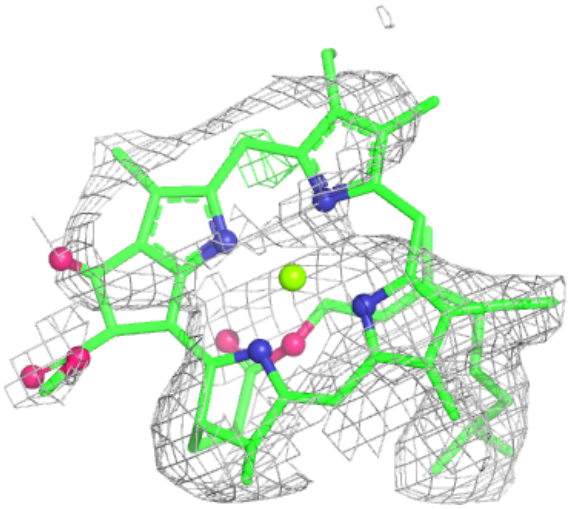


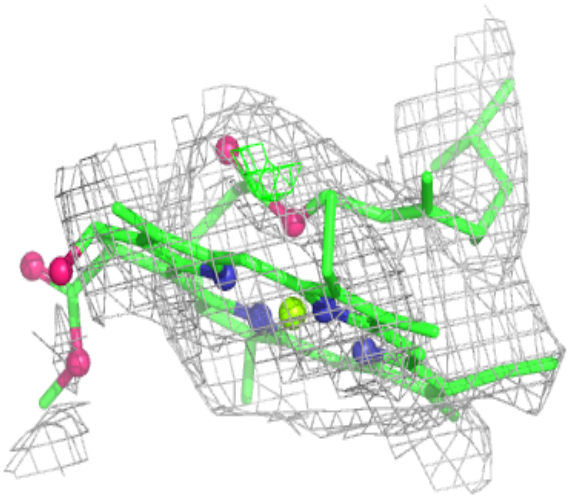


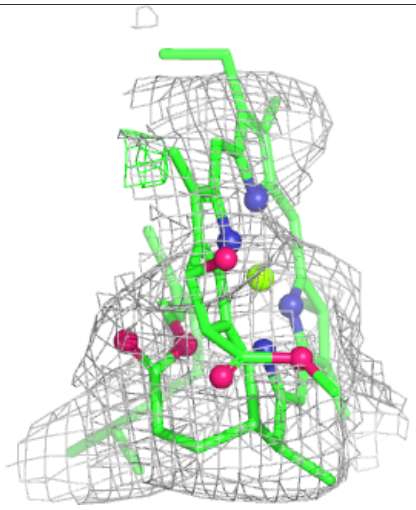


Electron density around CLA B 1205:

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

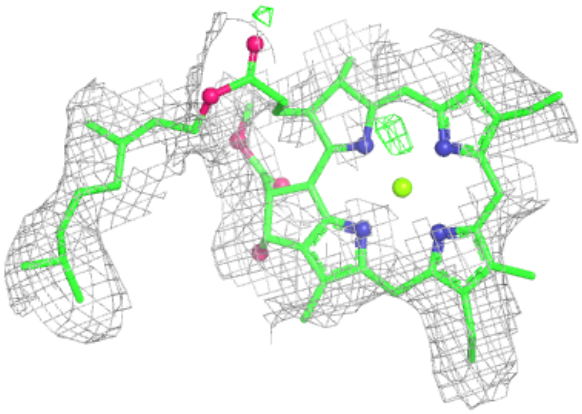


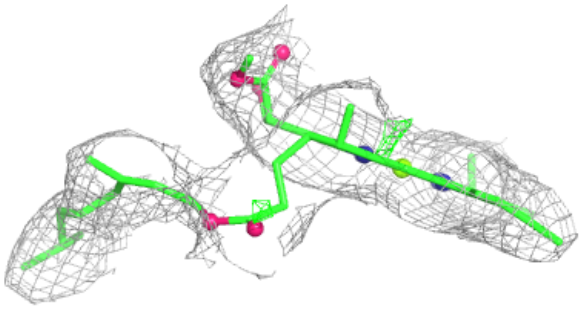




Electron density around CLA B 1208:

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



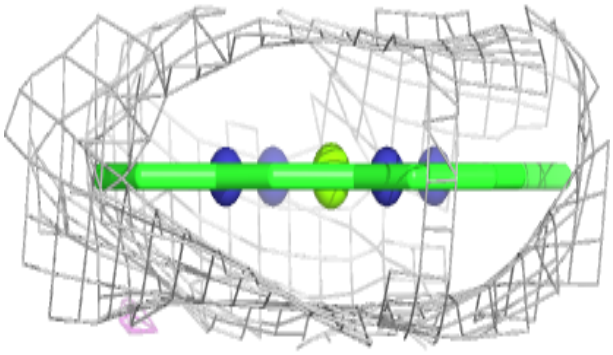


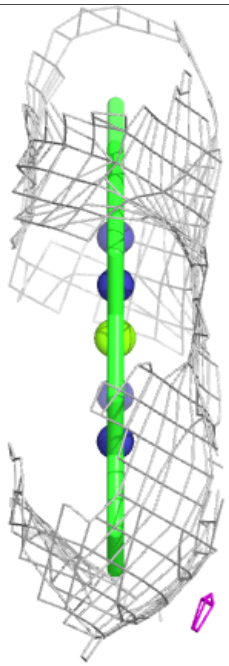


Electron density around CLA 3 3003:

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

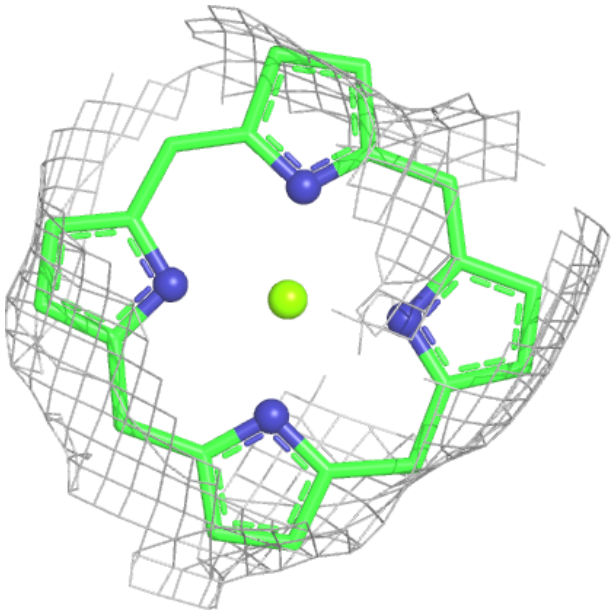


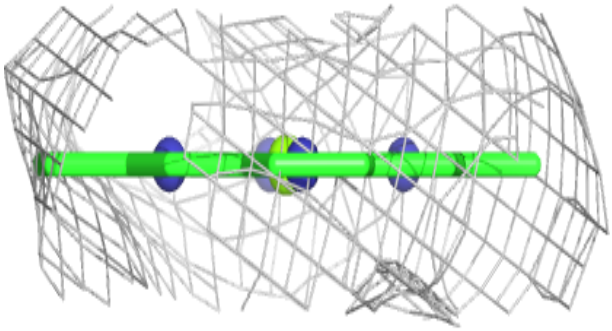


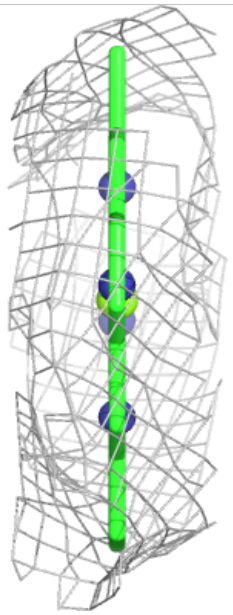


Electron density around CLA 3 3008:

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

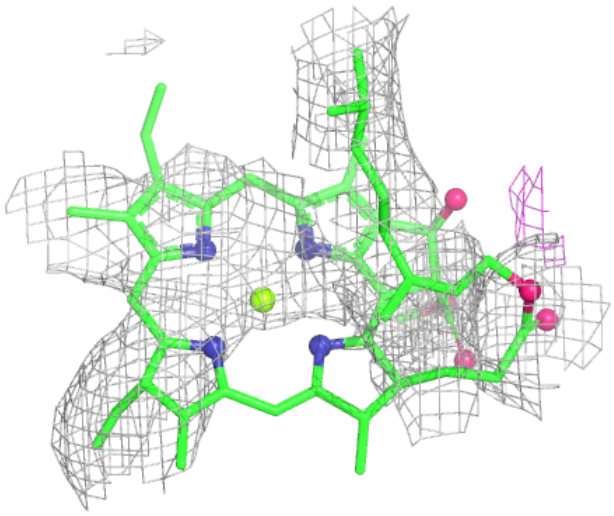


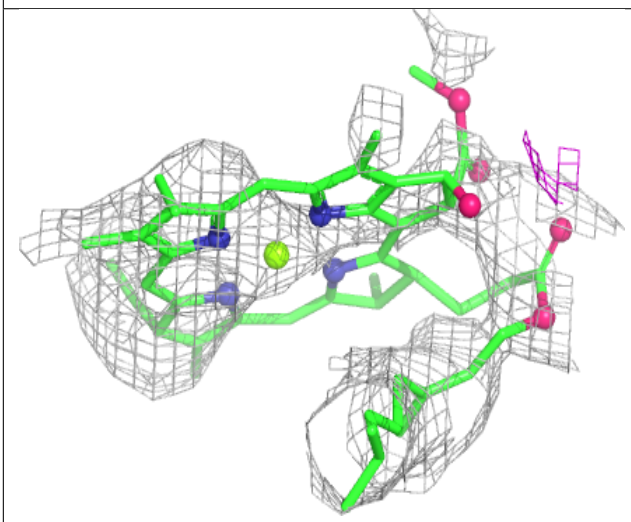


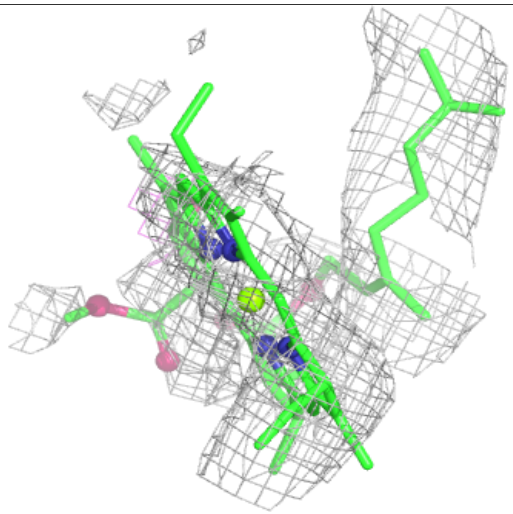


Electron density around CLA 4 1304:

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

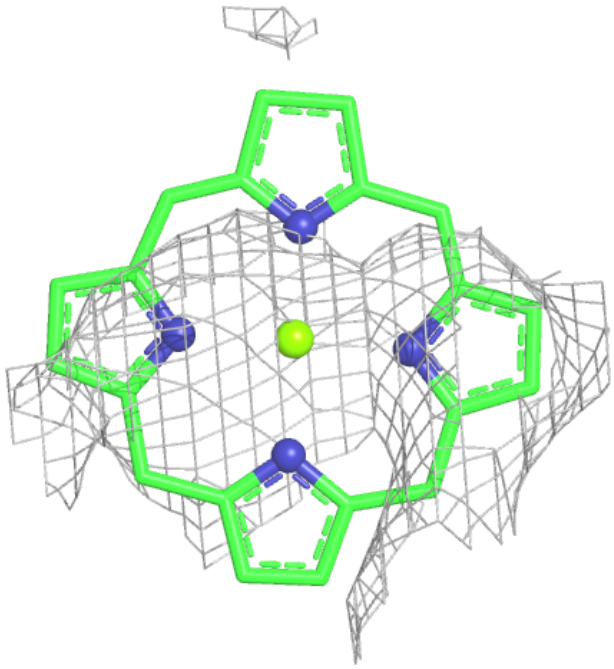


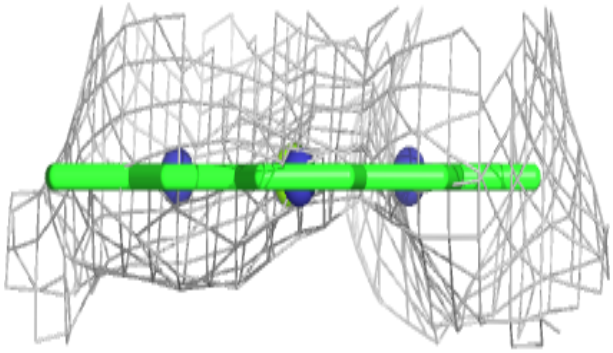


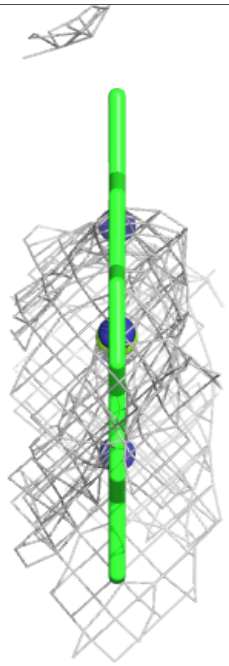


Electron density around CLA B 1210:

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

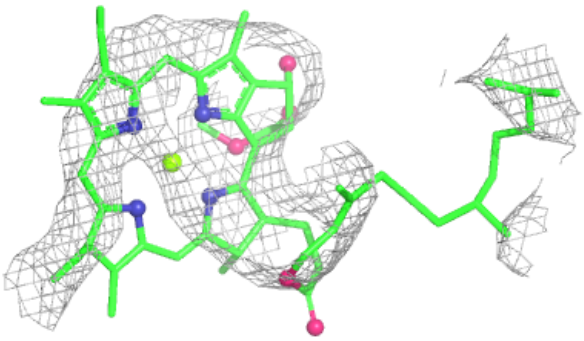


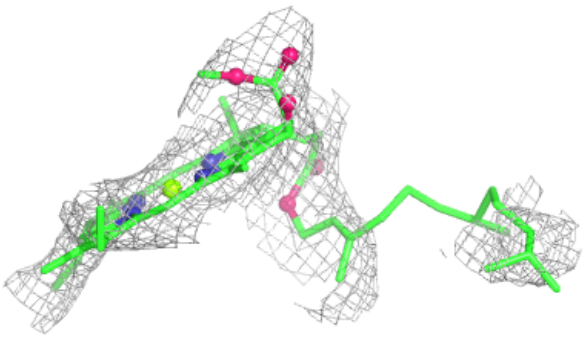


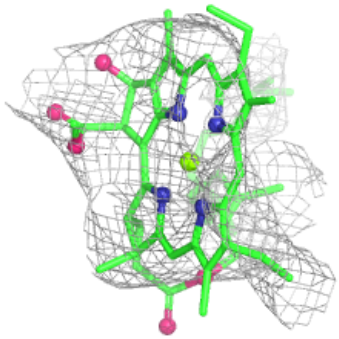


Electron density around CLA B 1212:

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

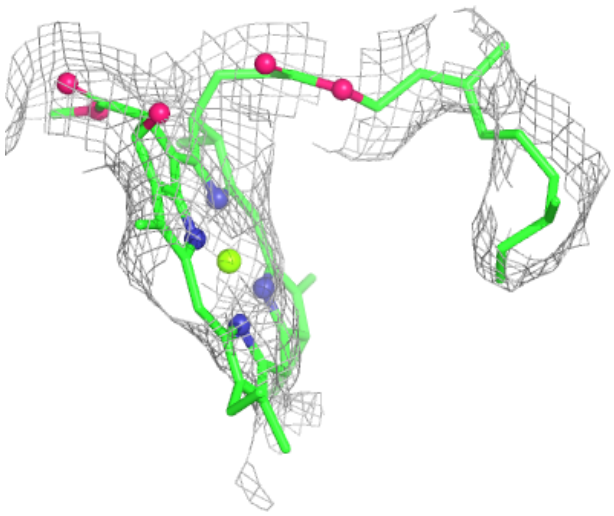


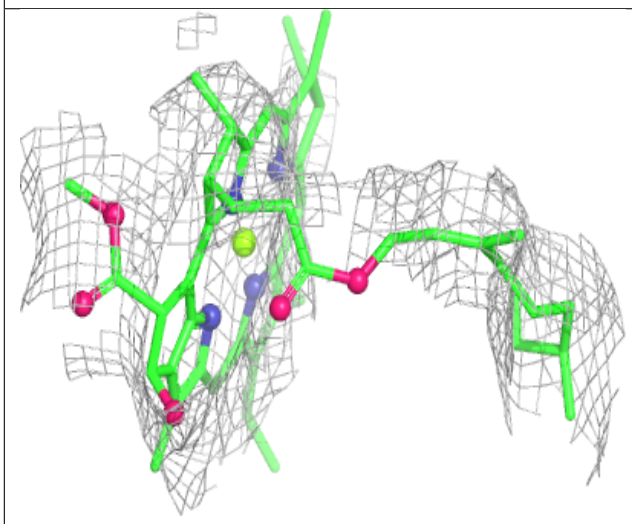


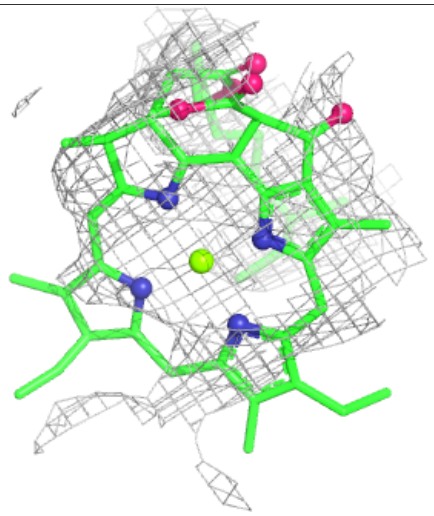


Electron density around CLA B 1216:

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

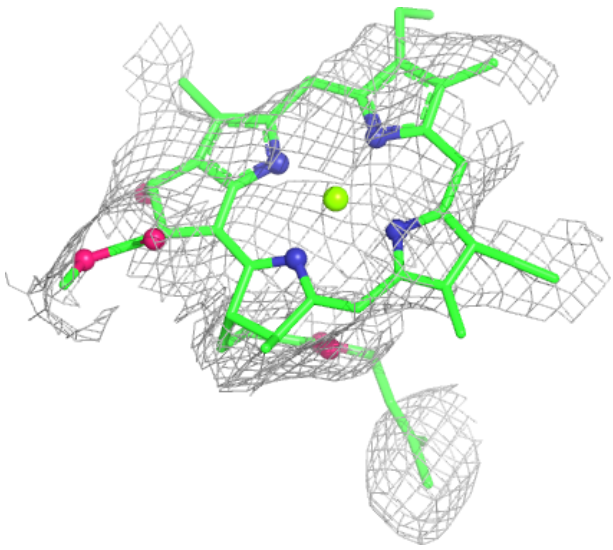


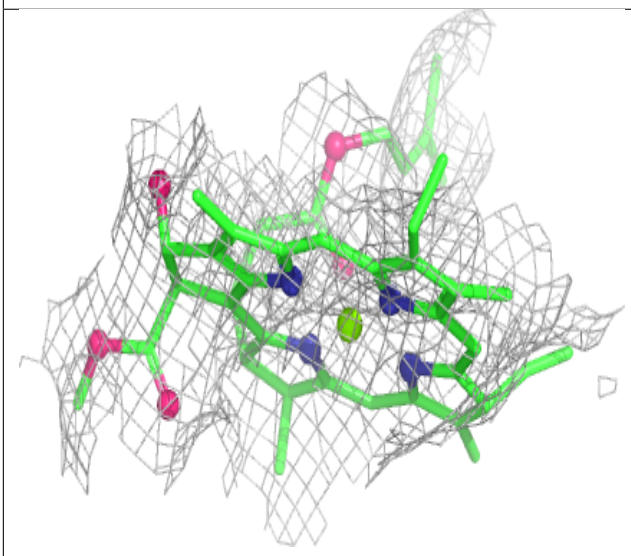


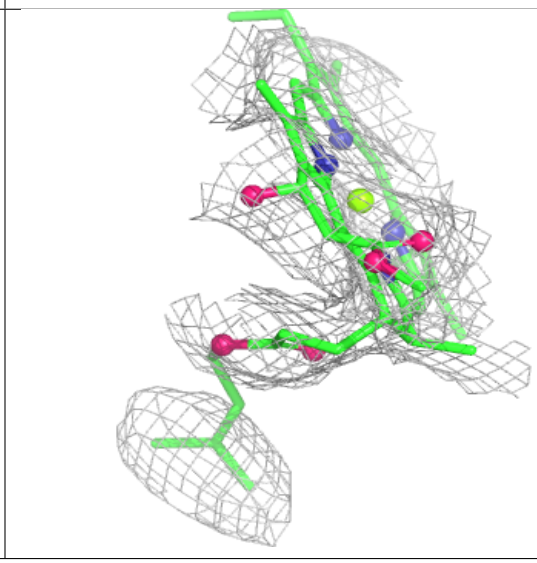


Electron density around CLA B 1217:

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

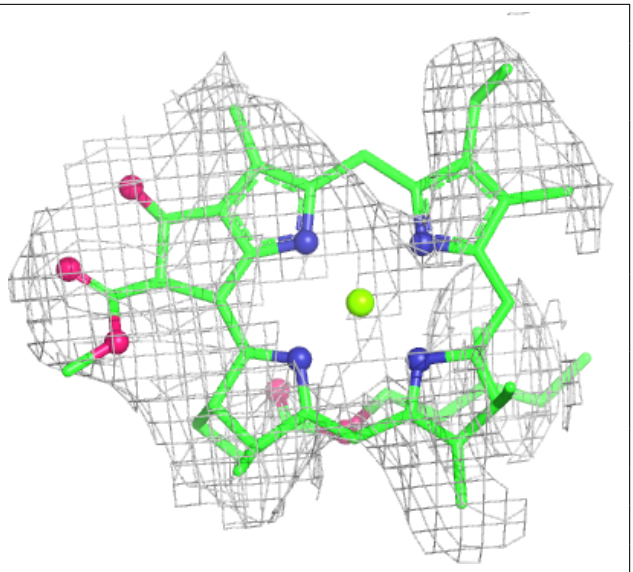


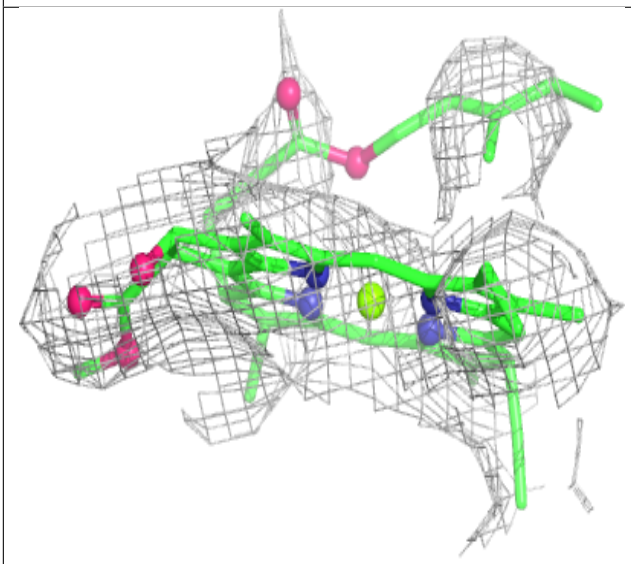




Electron density around CLA B 1219:

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

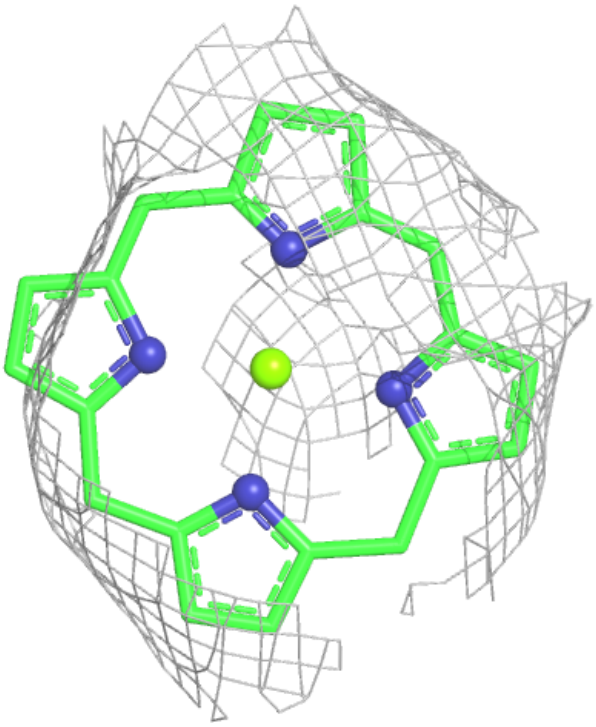


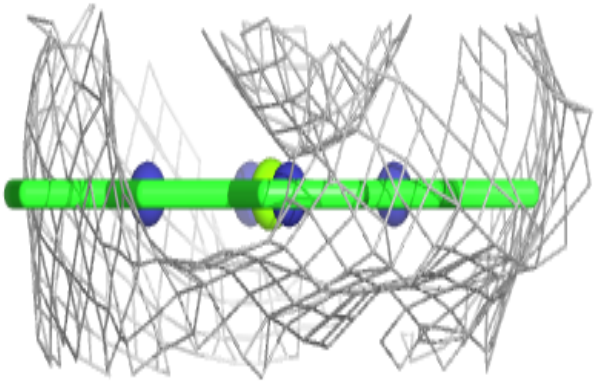


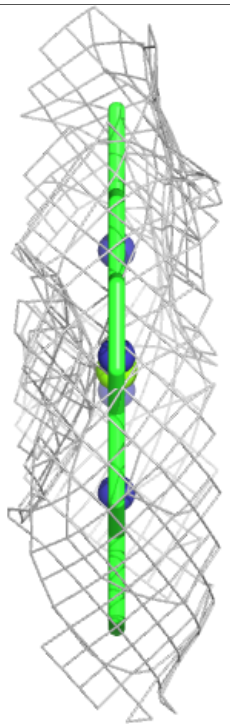


Electron density around CLA 4 4013:

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

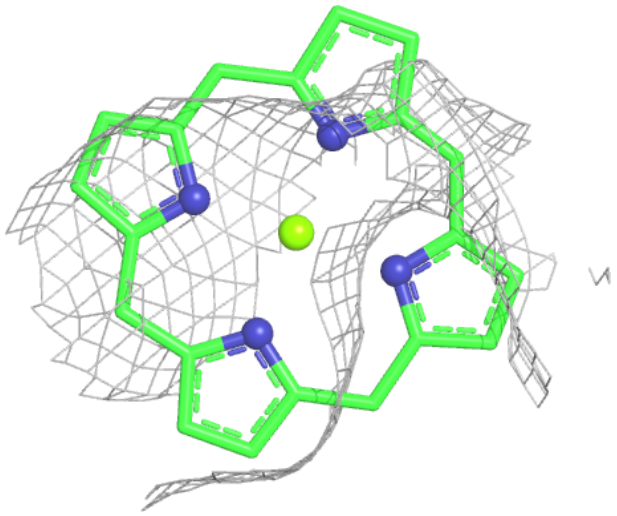


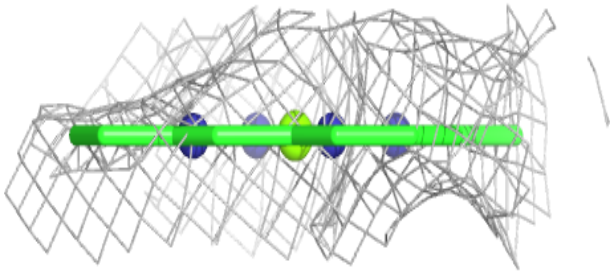


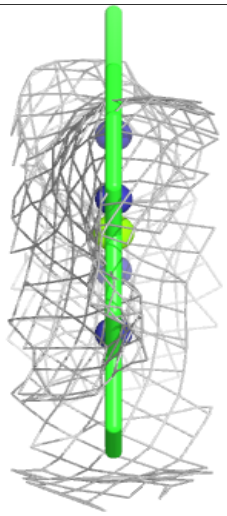


Electron density around CLA 4 4010:

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

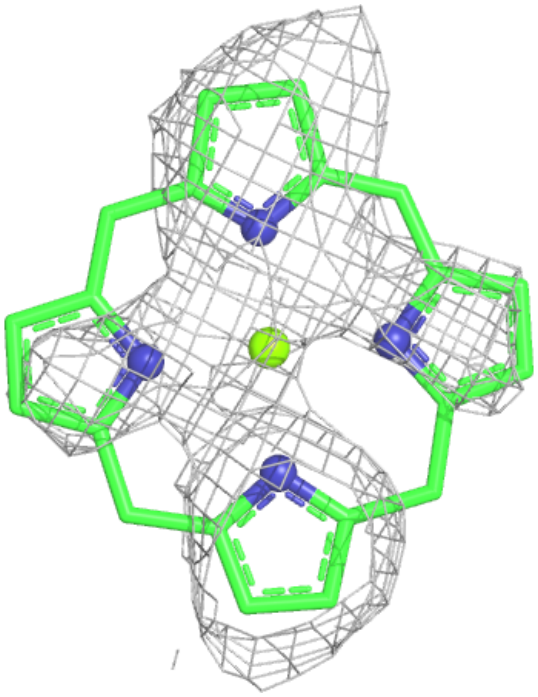


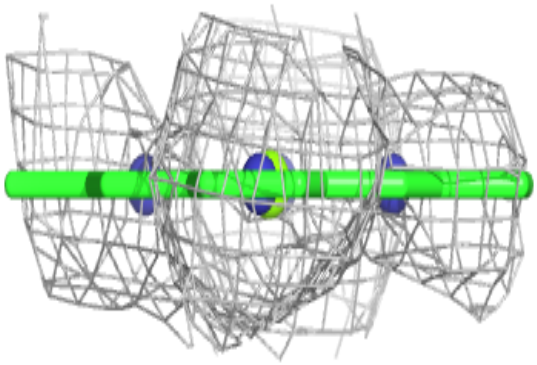


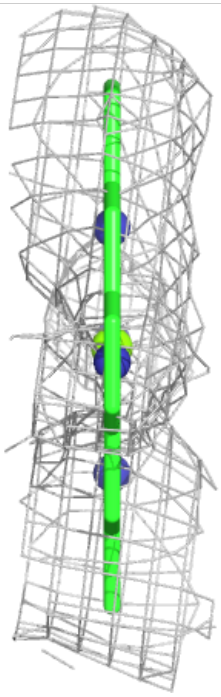


Electron density around CLA 4 4011:

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

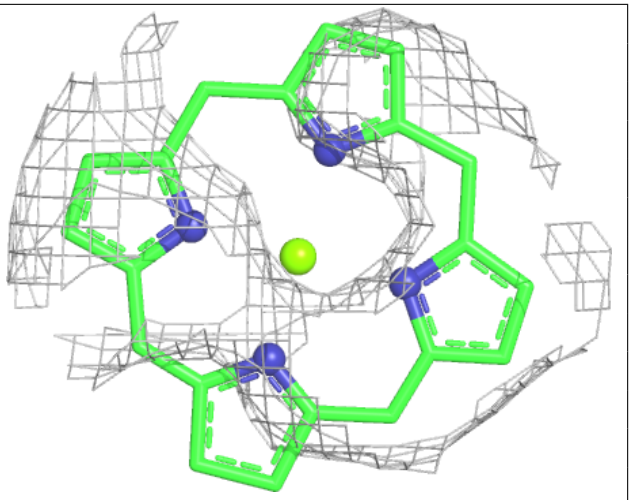


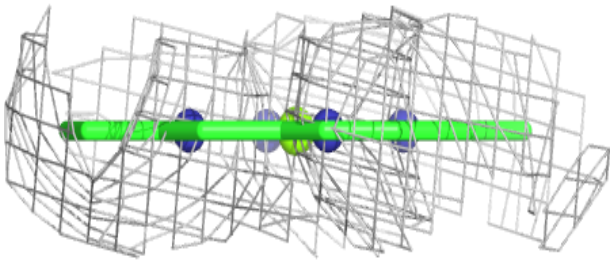


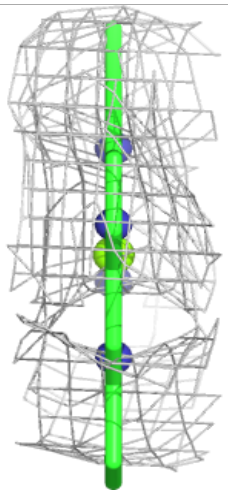


Electron density around CLA 4 4012:

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

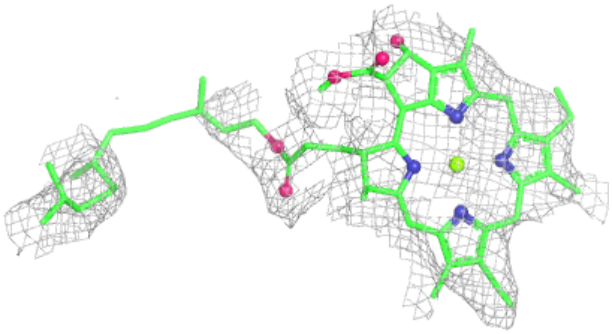


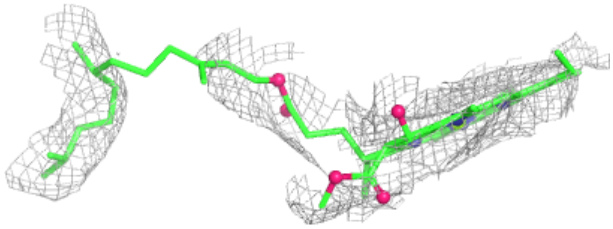




Electron density around CLA B 1220:

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

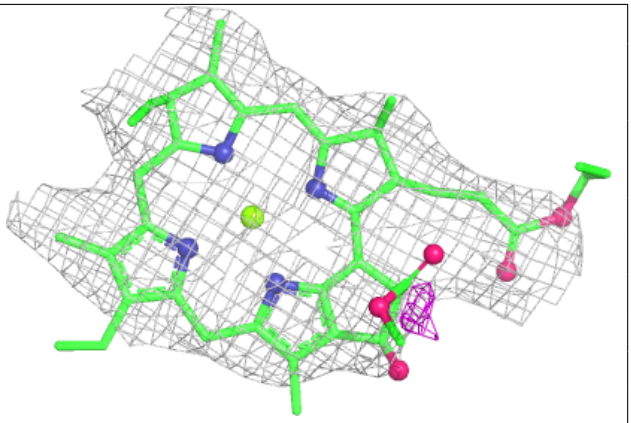


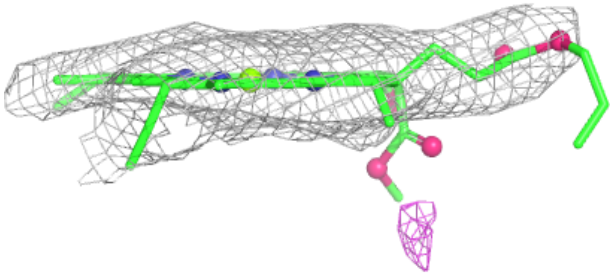


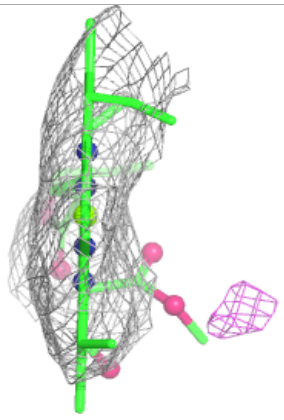


Electron density around CLA B 1221:

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

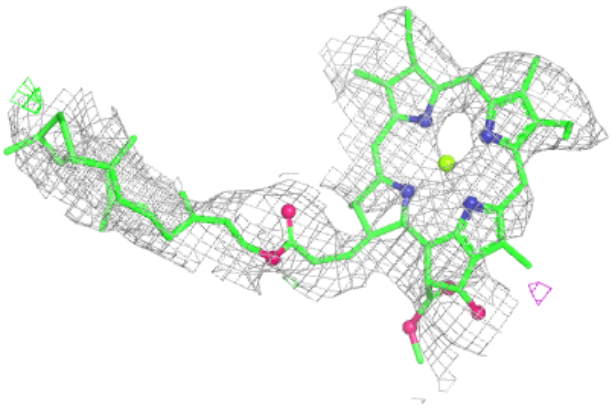


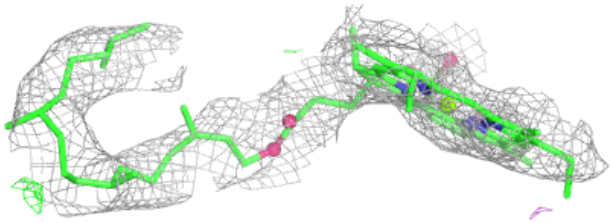




Electron density around CLA B 1222:

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

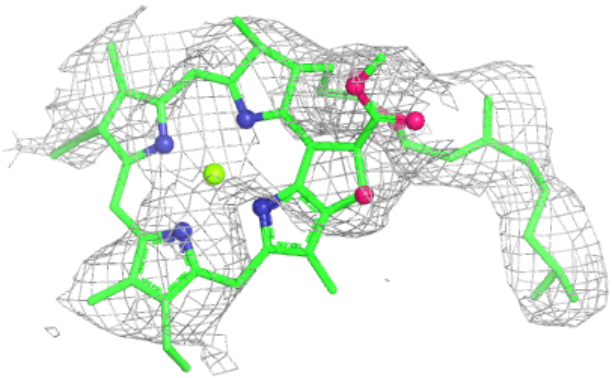


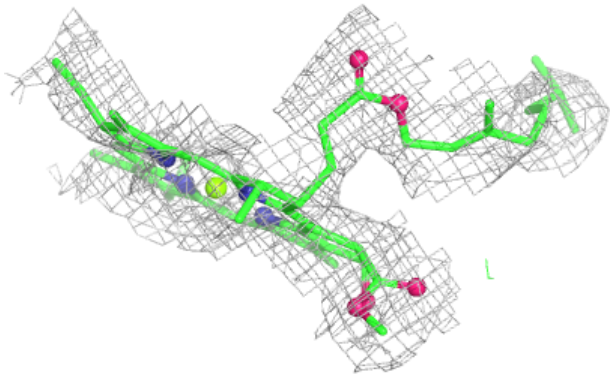


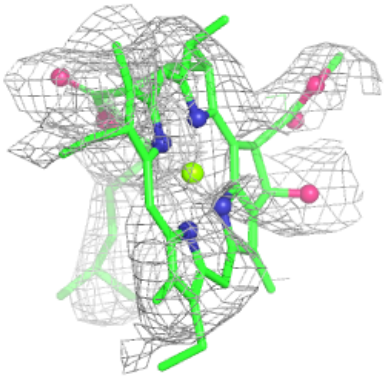


Electron density around CLA B 1228:

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



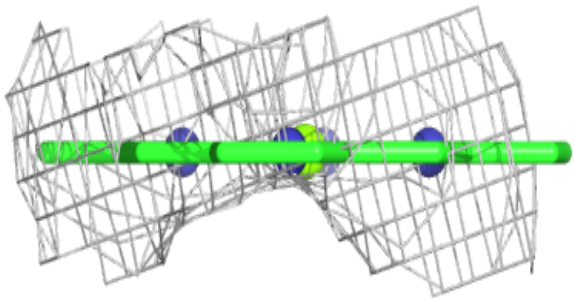


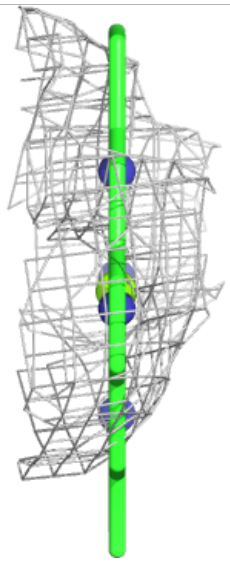


Electron density around CLA 4 4008:

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

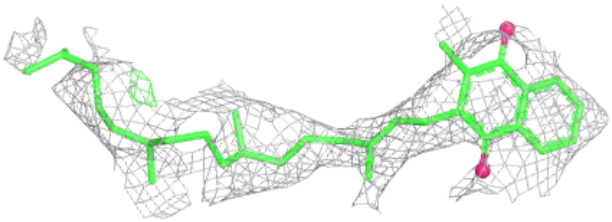


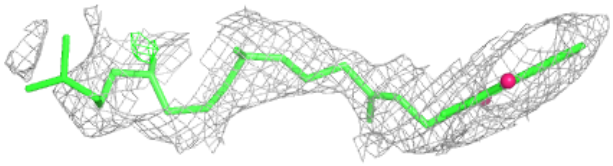


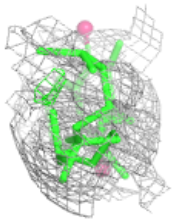


Electron density around PQN A 5001:

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

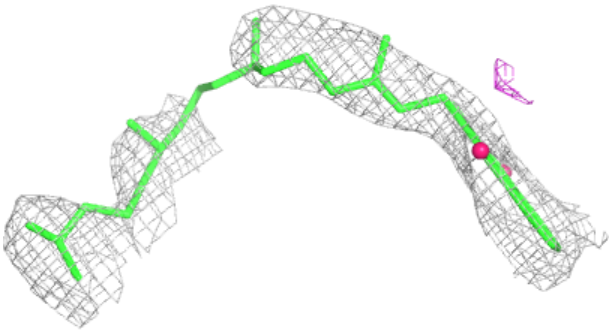


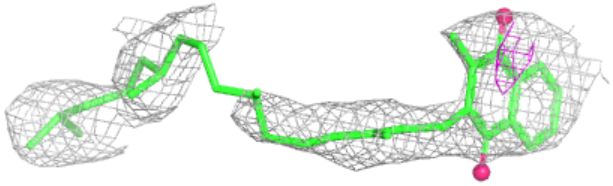




Electron density around PQN B 5002:

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

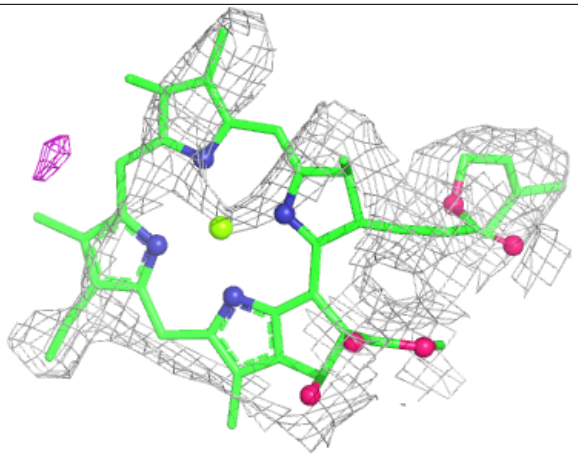


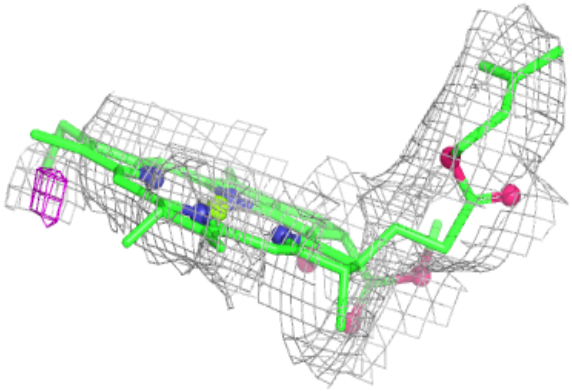


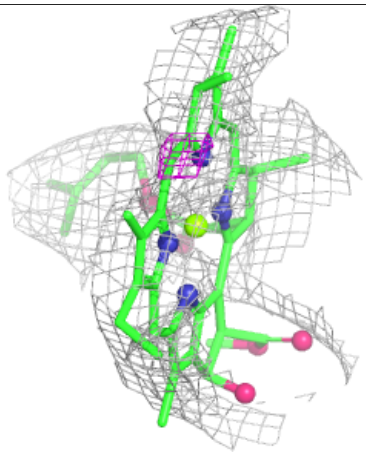


Electron density around CLA B 1229:

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

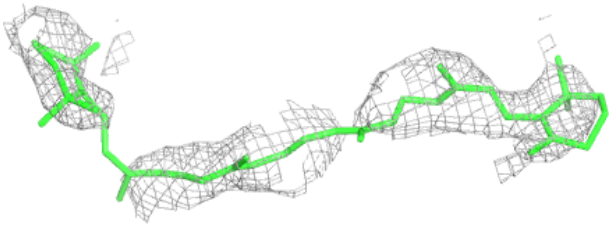


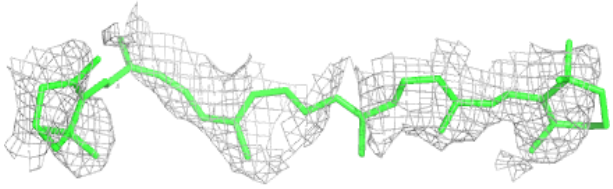


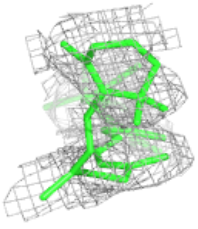


Electron density around BCR B 6017:

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

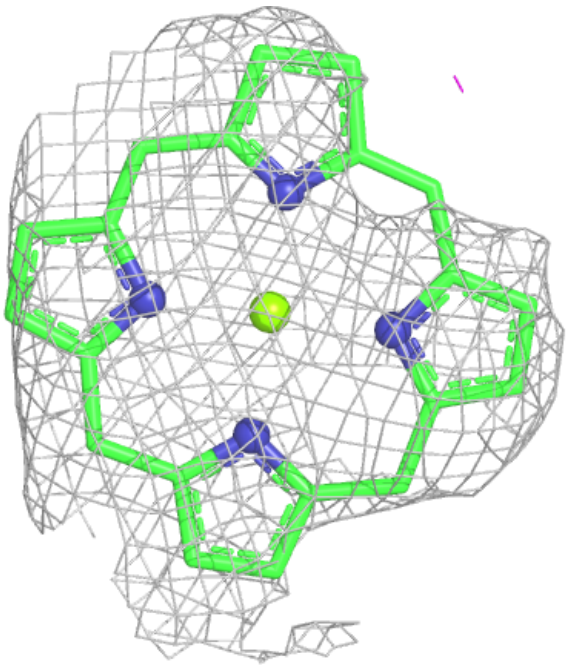


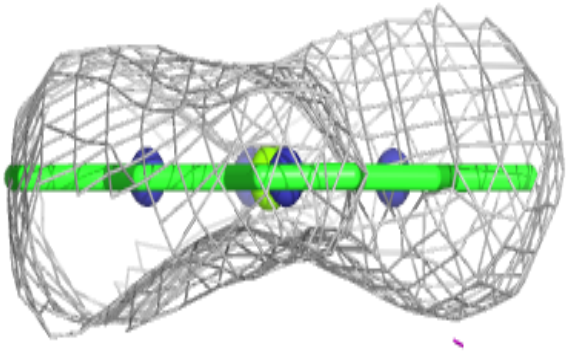


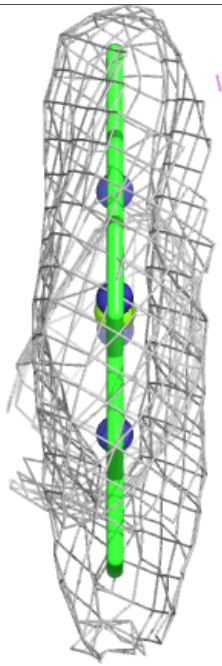


Electron density around CLA A 1117:

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

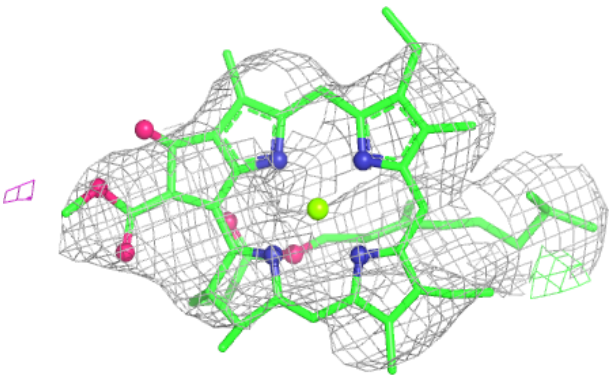


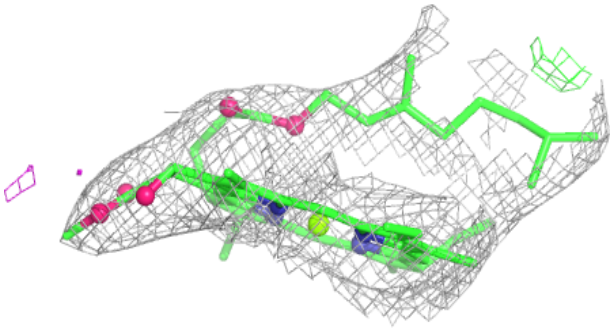


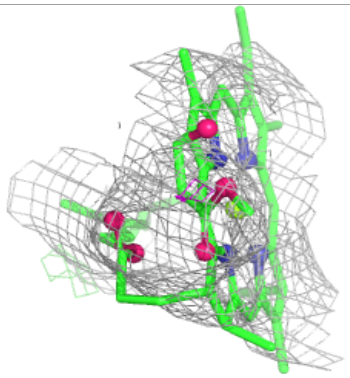


Electron density around CLA B 1235:

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

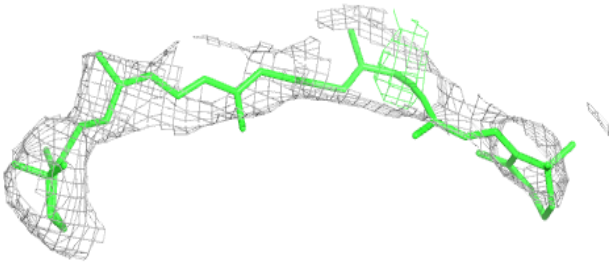






Electron density around BCR L 6020:

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

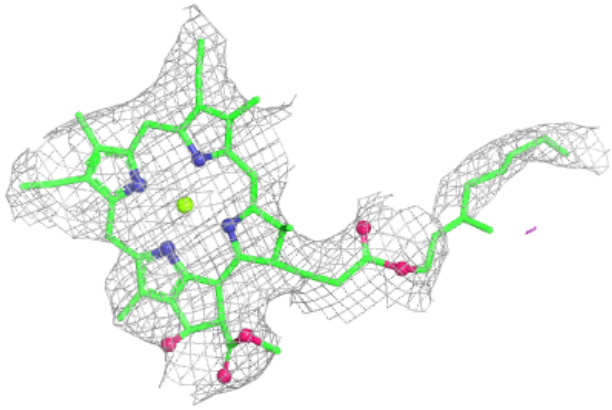


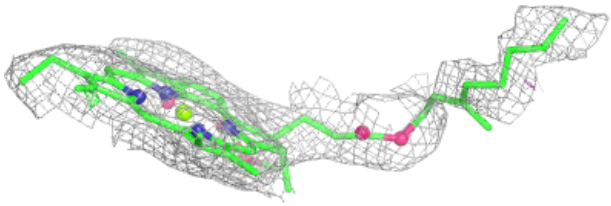


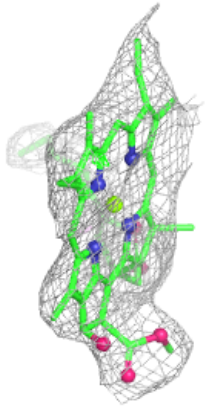


Electron density around CLA B 9022:

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

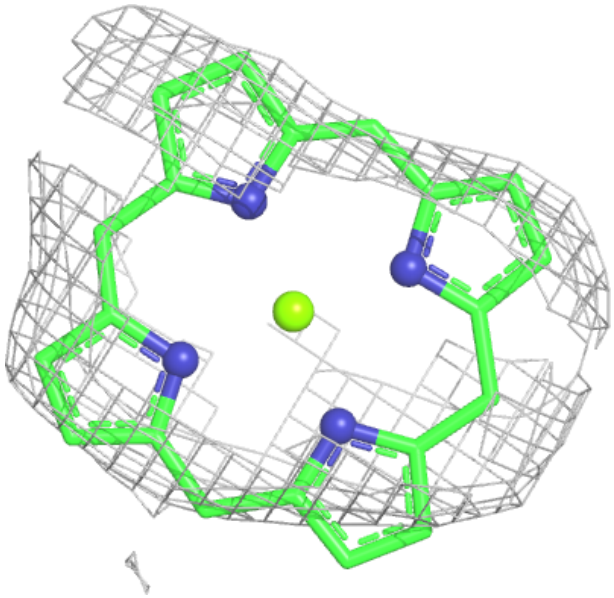


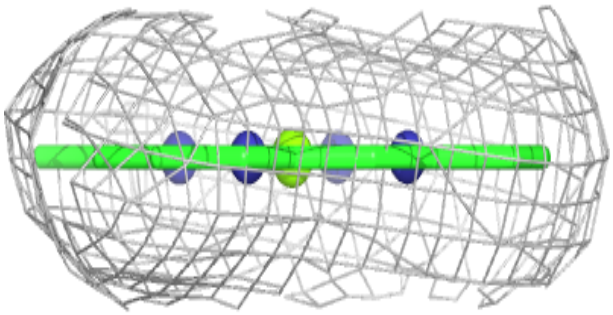


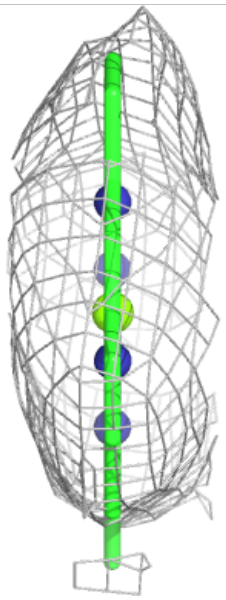


Electron density around CLA 2 2008:

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

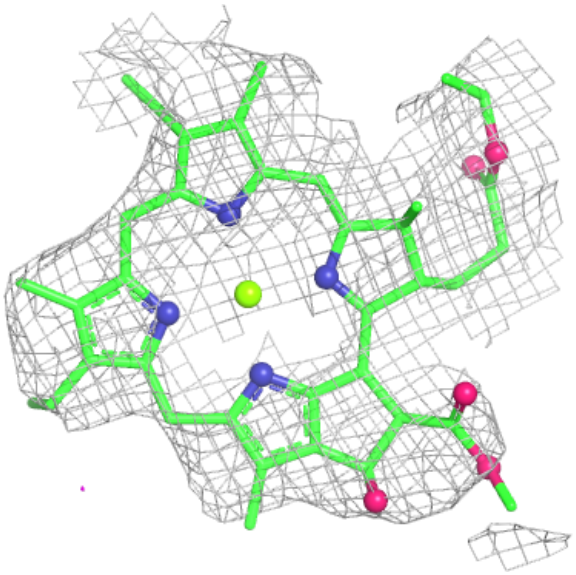


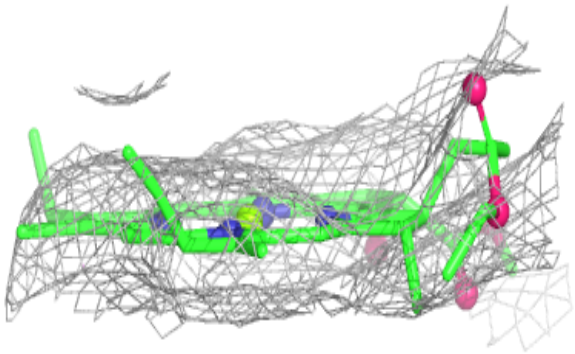


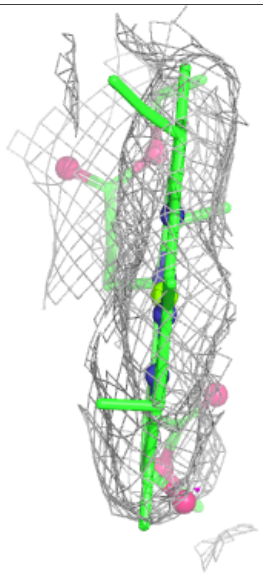


Electron density around CLA B 9023:

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

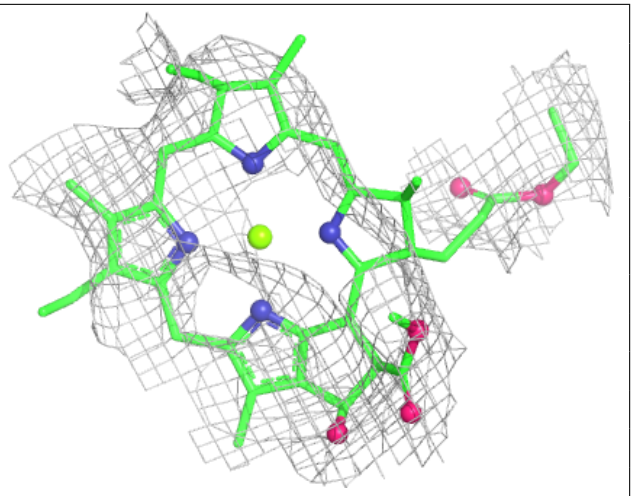


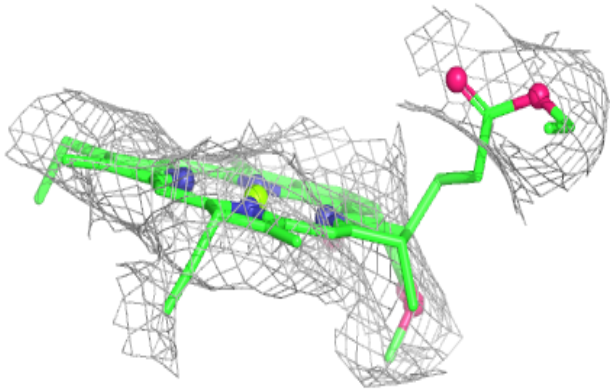


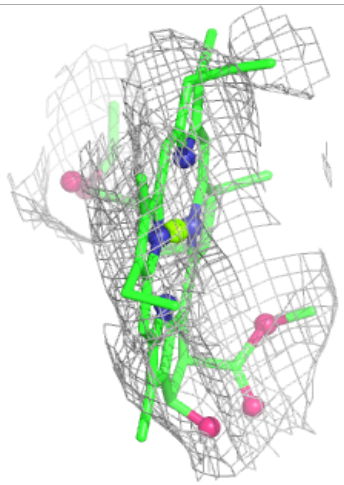


Electron density around CLA A 1103:

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

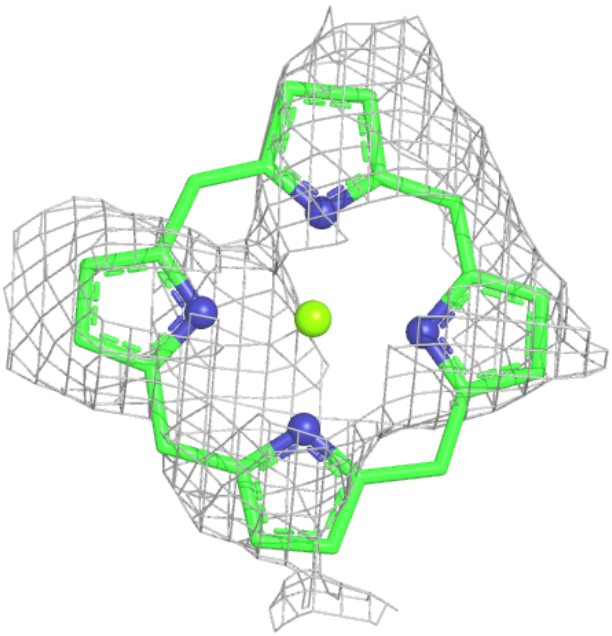


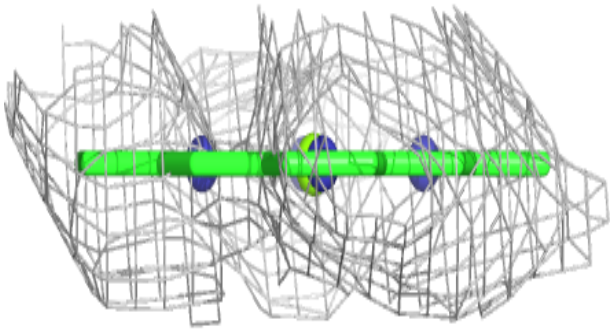


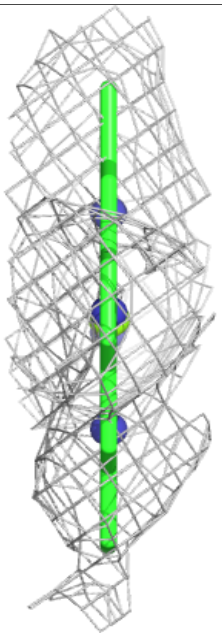


Electron density around CLA B 1223:

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

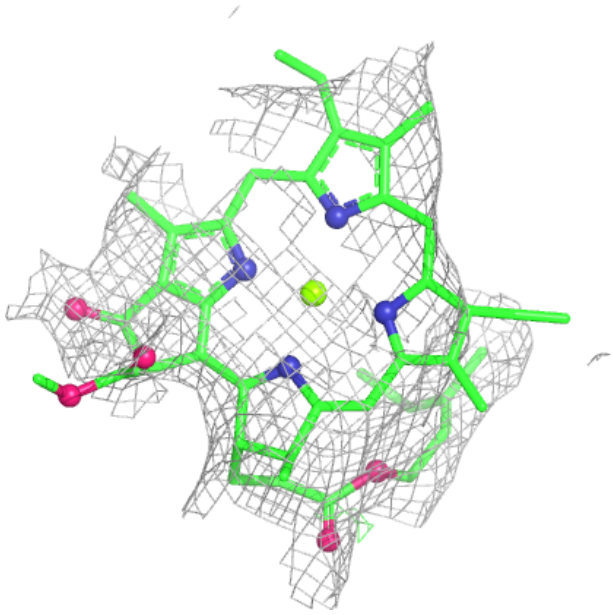


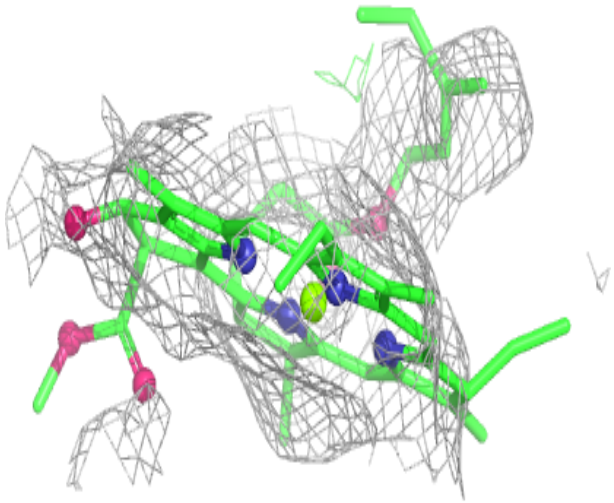


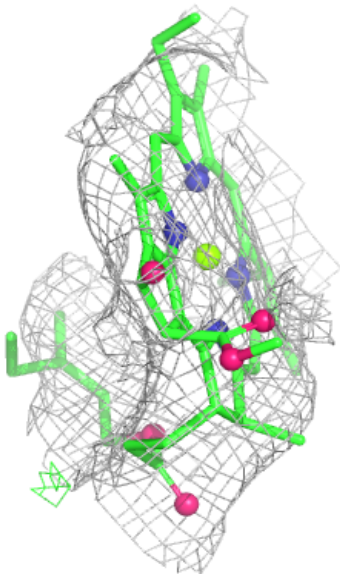


Electron density around CLA B 1224:

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

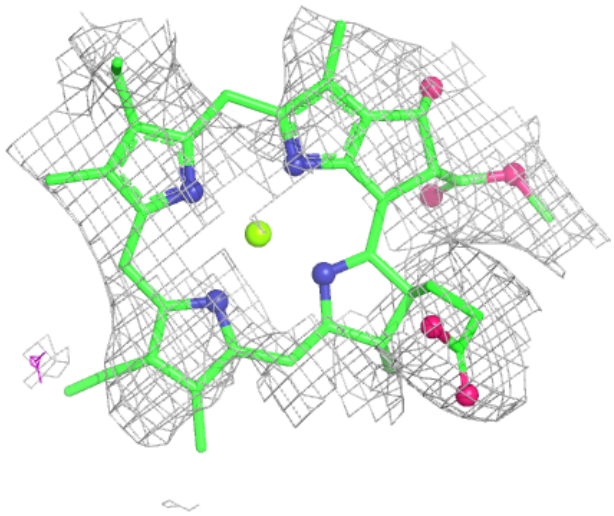


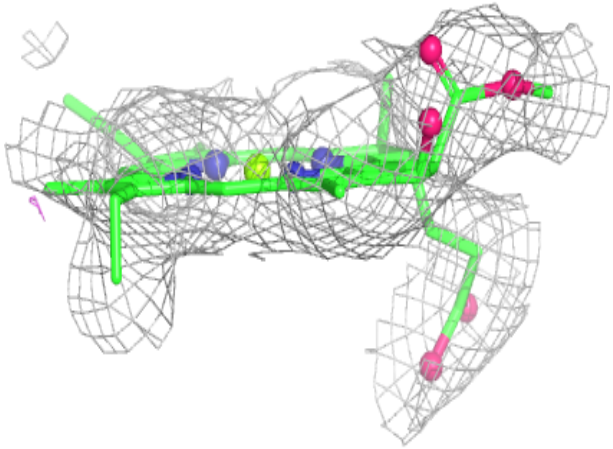


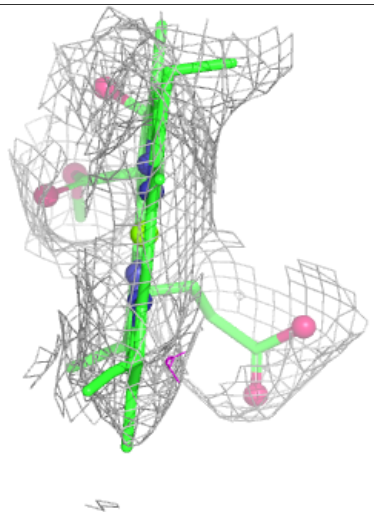


Electron density around CLA B 1225:

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

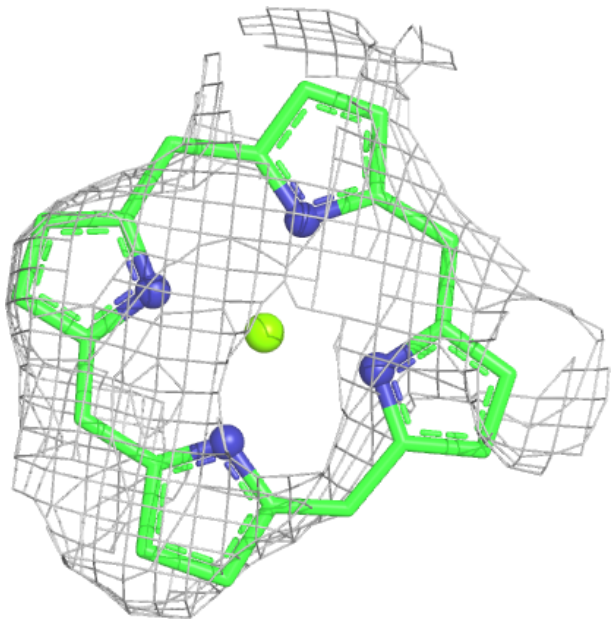


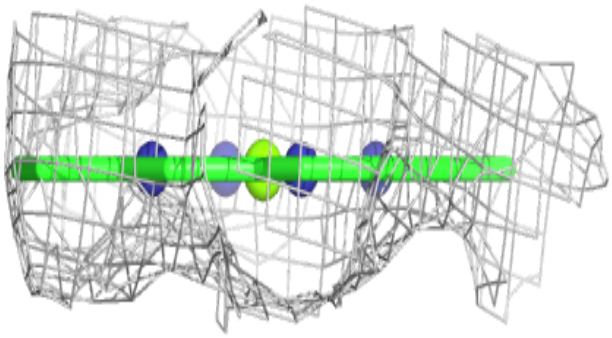


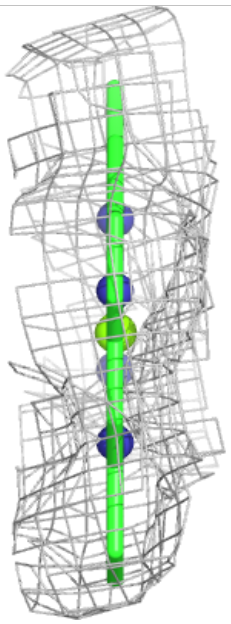


Electron density around CLA B 1226:

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

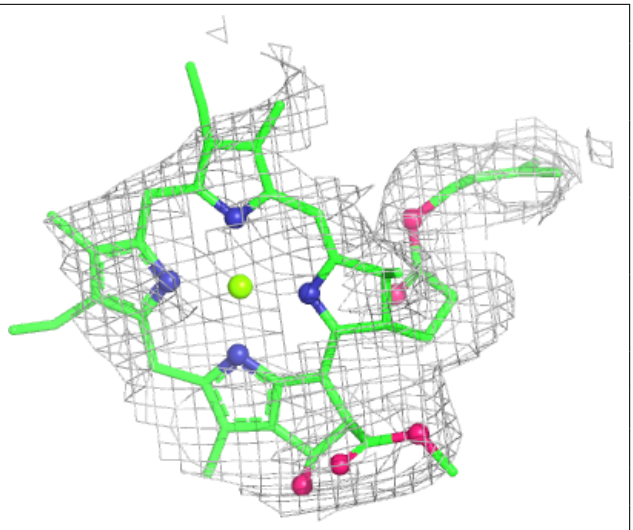


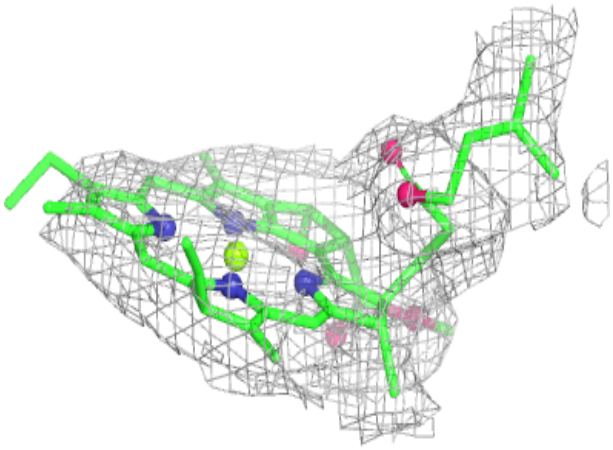


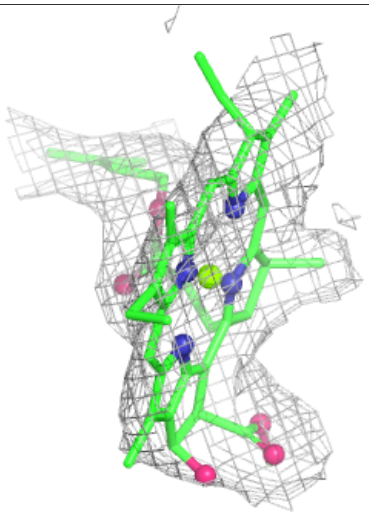


Electron density around CLA B 1227:

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

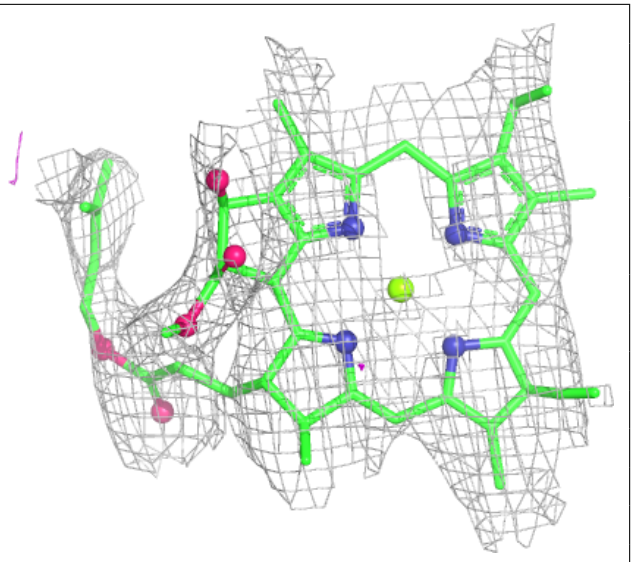


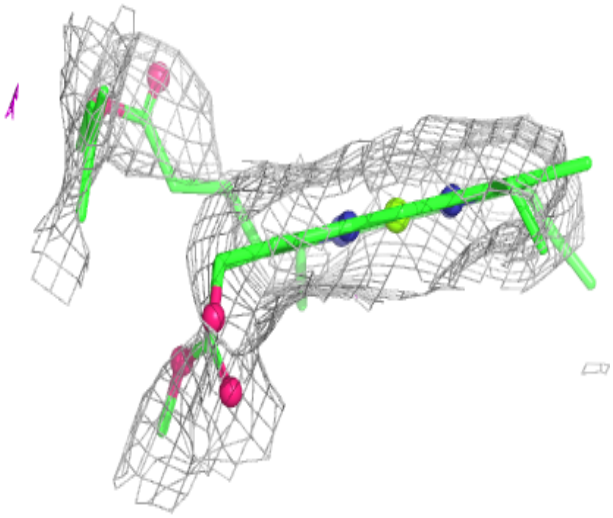


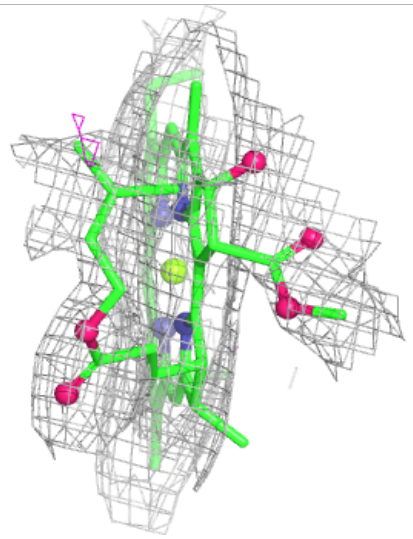


Electron density around CLA B 1202:

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

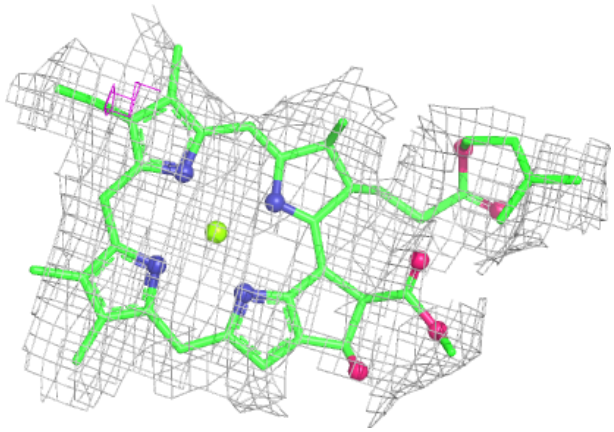


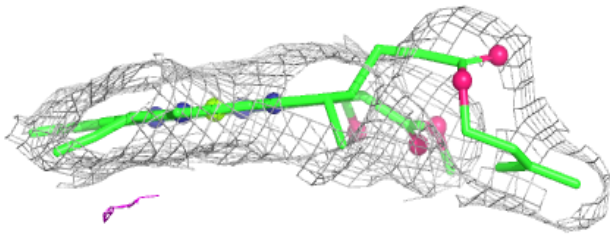


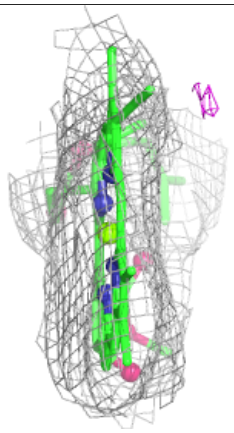


Electron density around CLA B 1203:

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

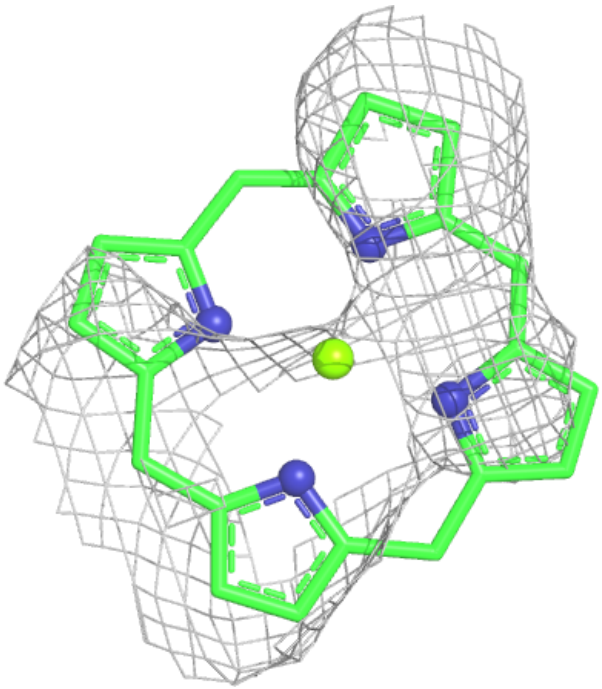


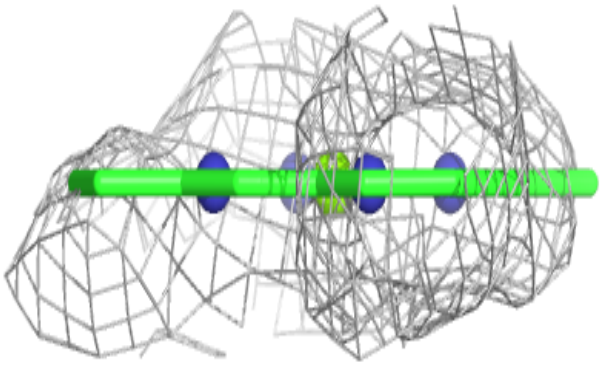


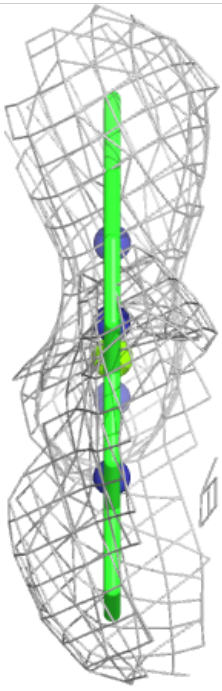


Electron density around CLA B 1230:

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

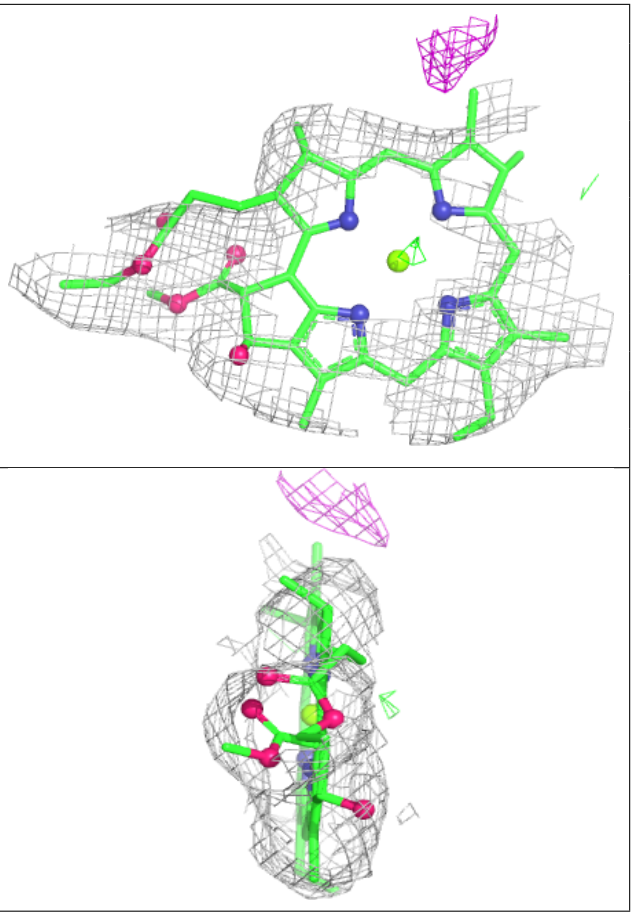






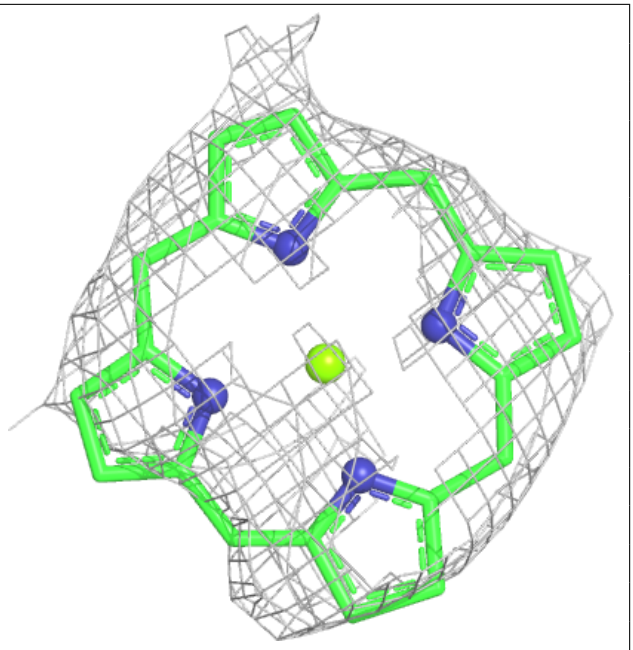
Electron density around CLA L 1503:

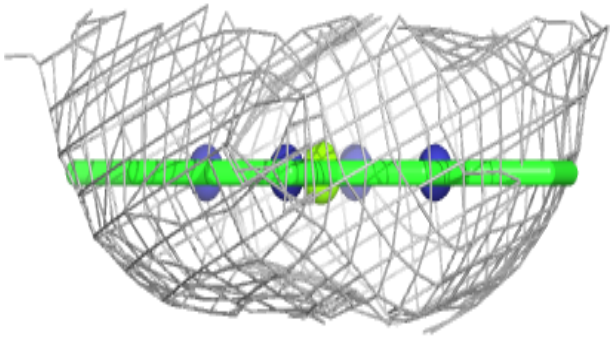
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

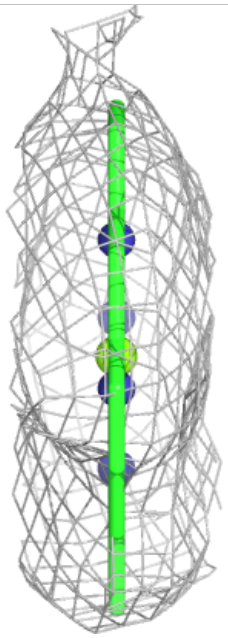


Electron density around CLA 3 3007:

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

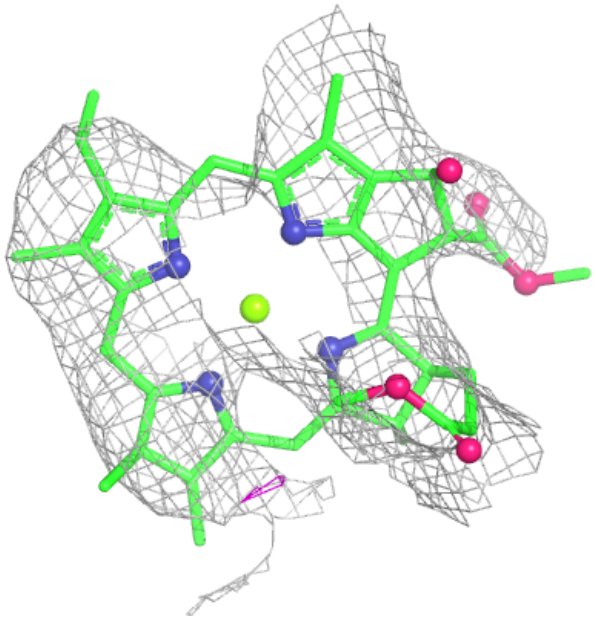


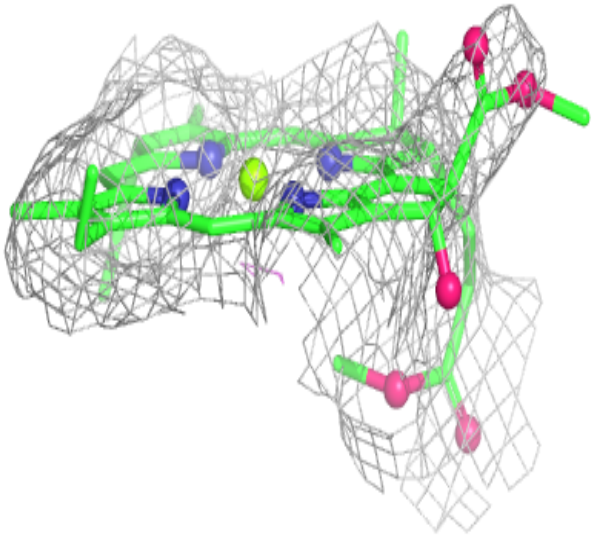


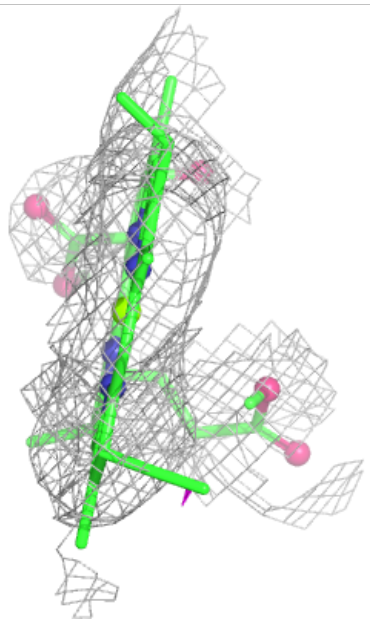


Electron density around CLA B 1231:

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

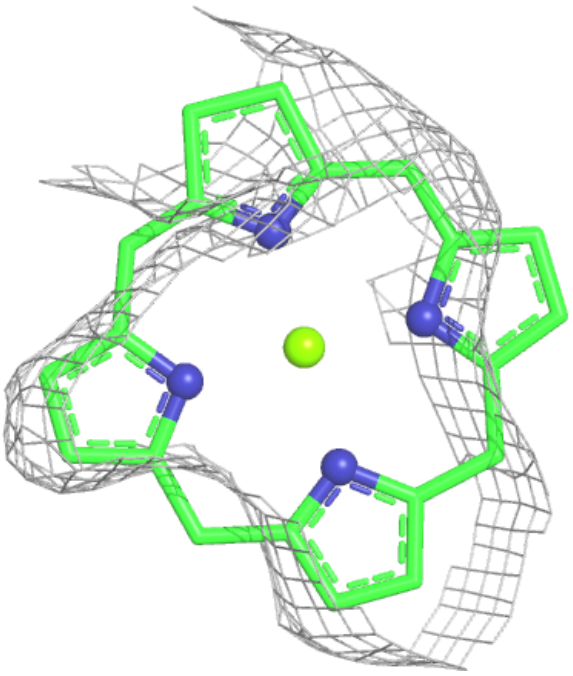


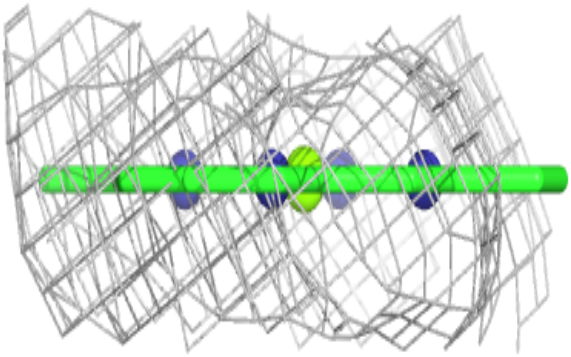


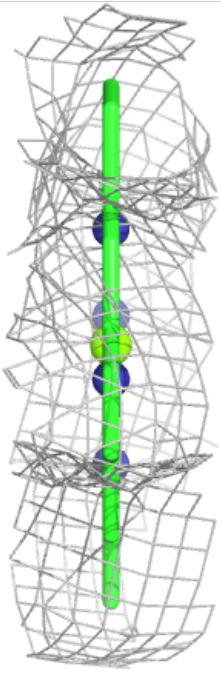


Electron density around CLA 1 1004:

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

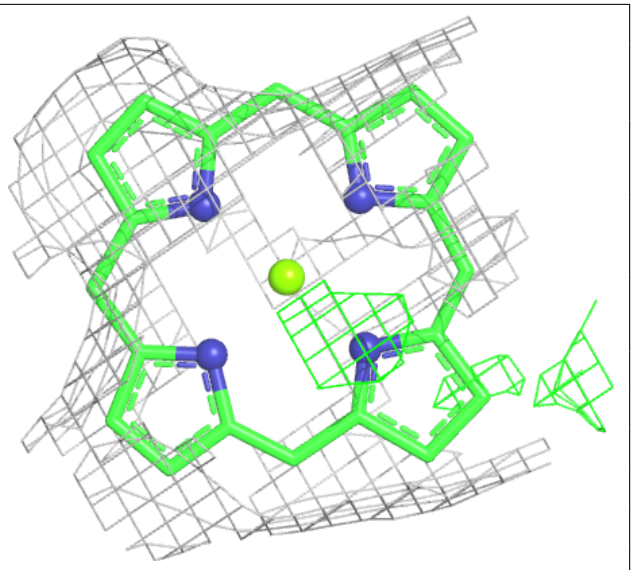


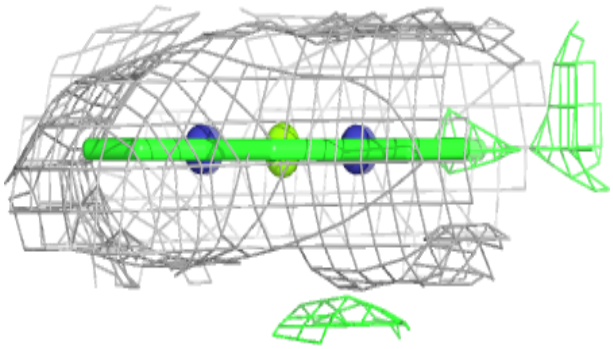


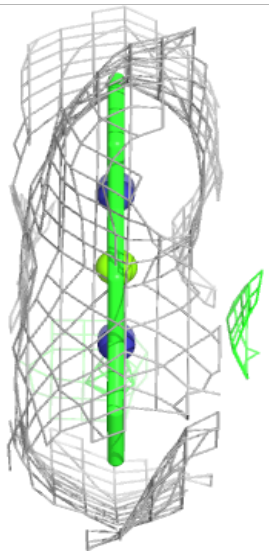


Electron density around CLA A 1132:

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

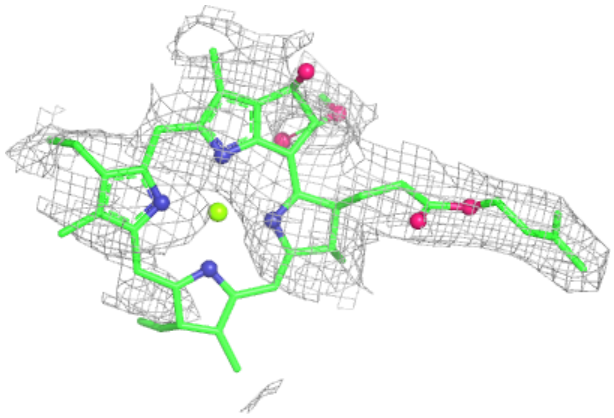


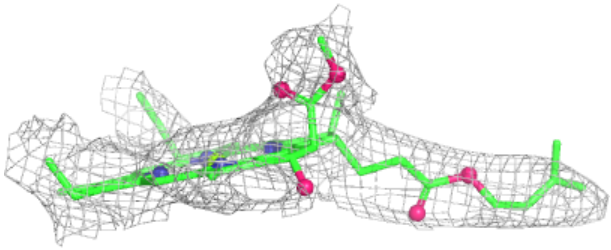


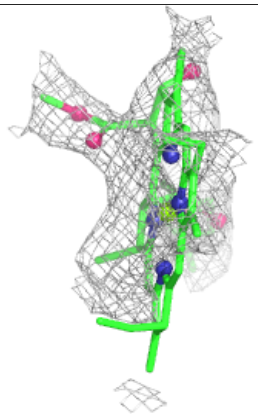


Electron density around CLA B 1234:

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

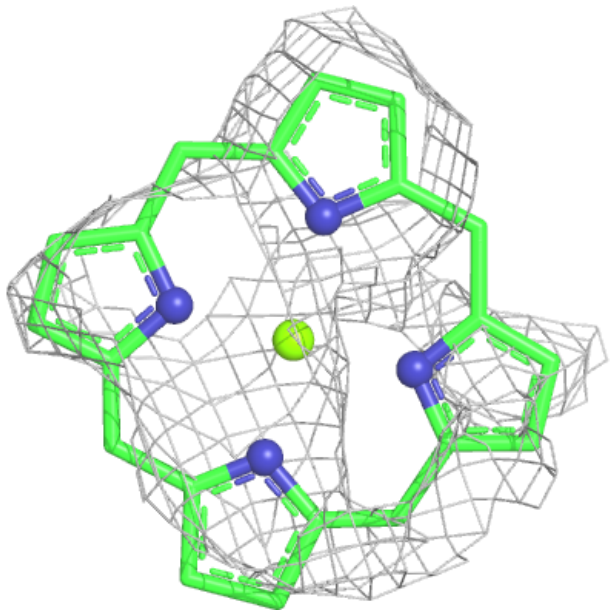


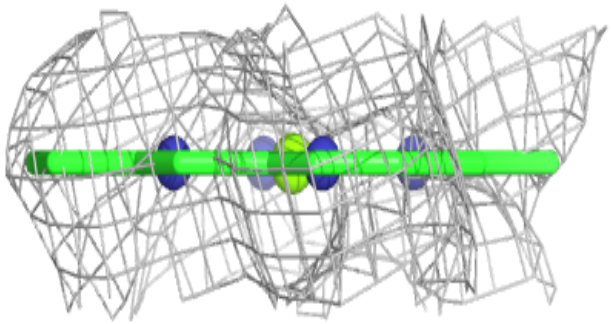


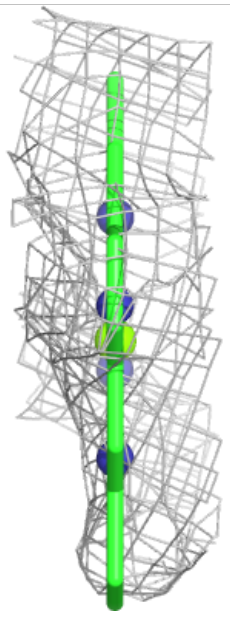


Electron density around CLA B 1206:

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

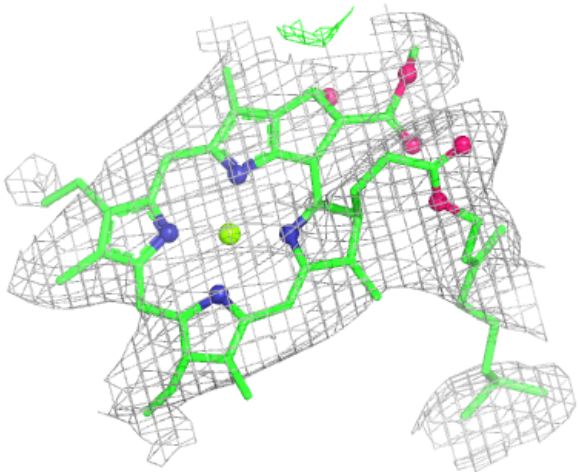


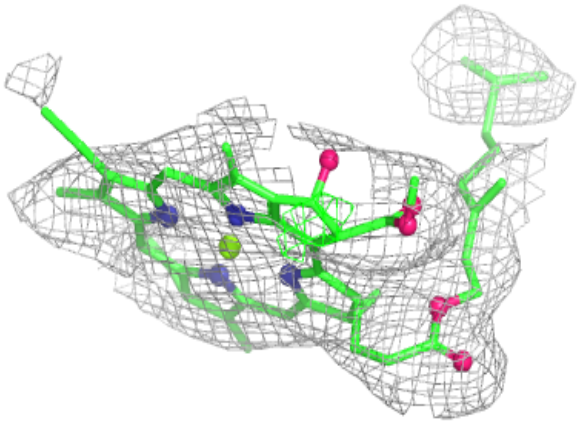


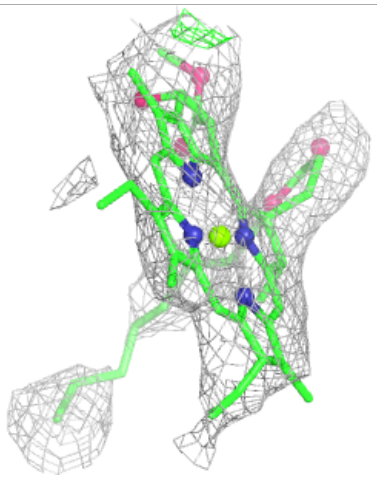


Electron density around CLA B 1207:

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

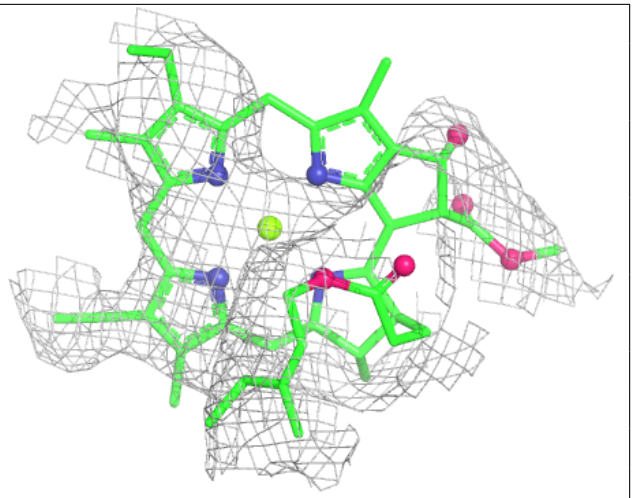


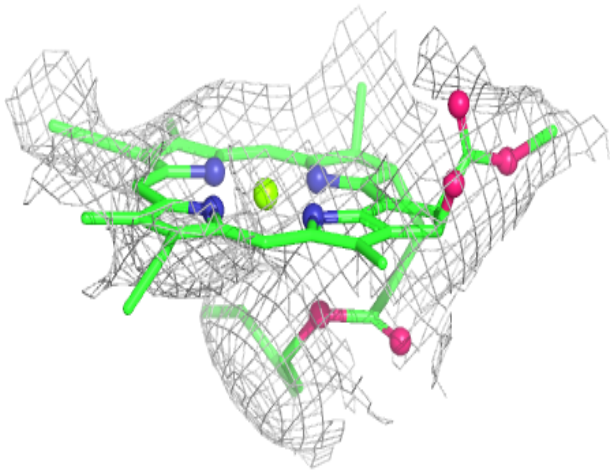


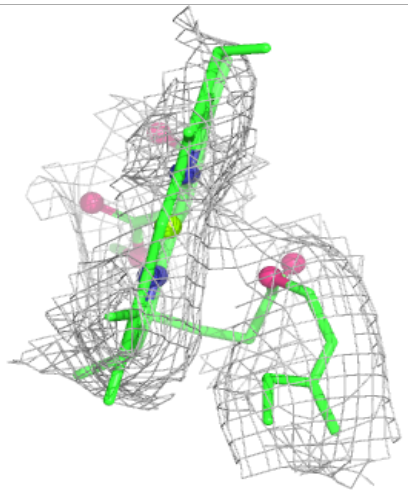


Electron density around CLA B 1237:

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

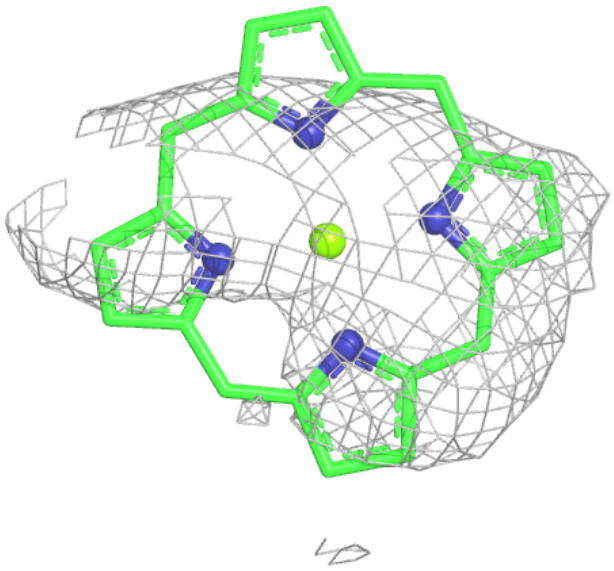


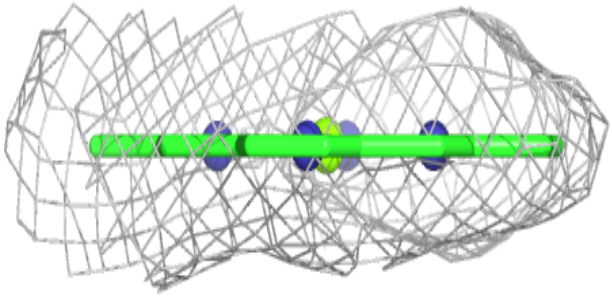


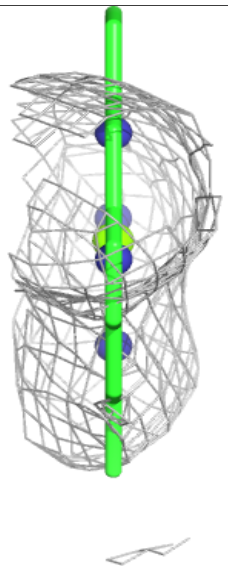


Electron density around CLA 1 1012:

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

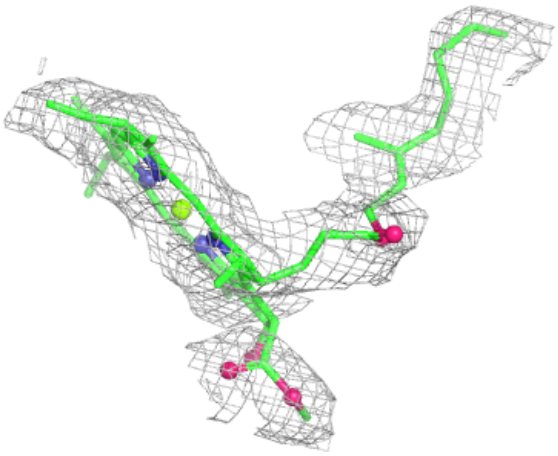


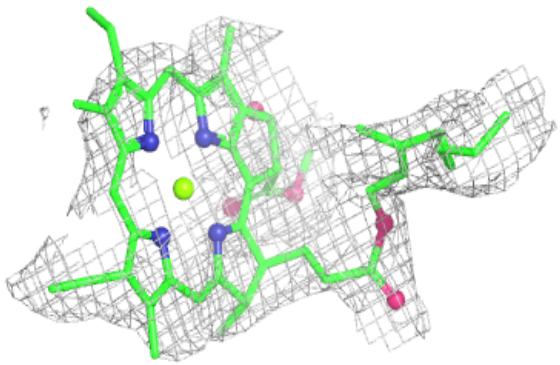


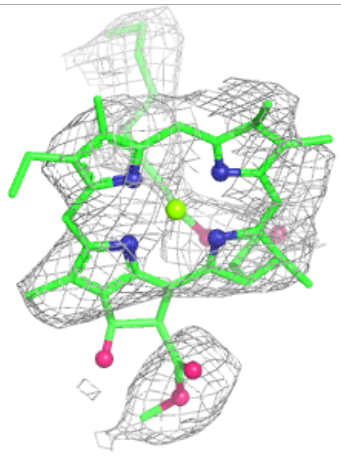


Electron density around CLA B 1238:

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

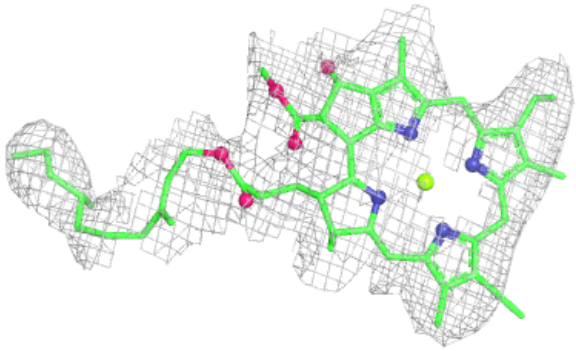


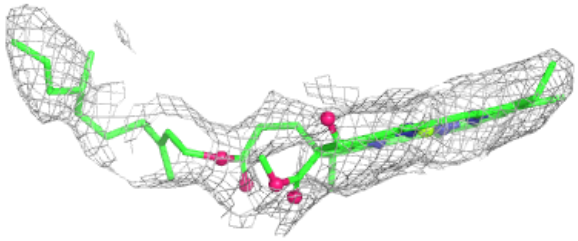


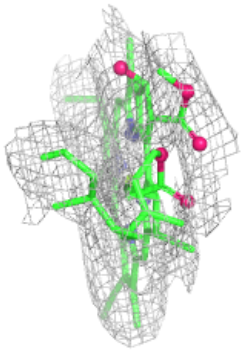


Electron density around CLA A 1107:

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

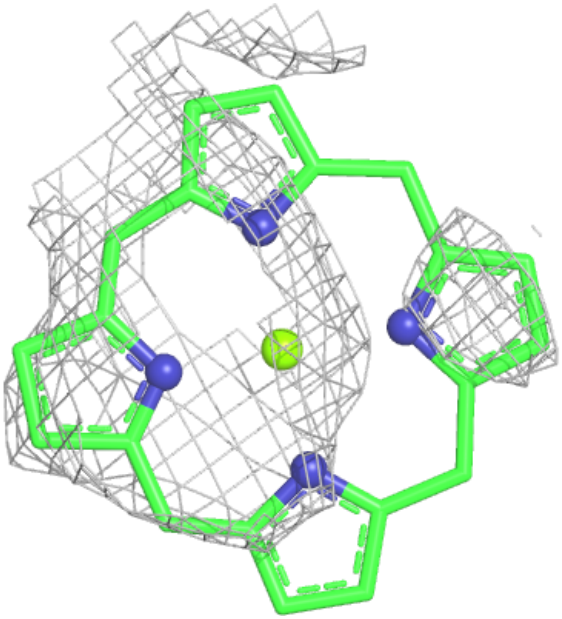


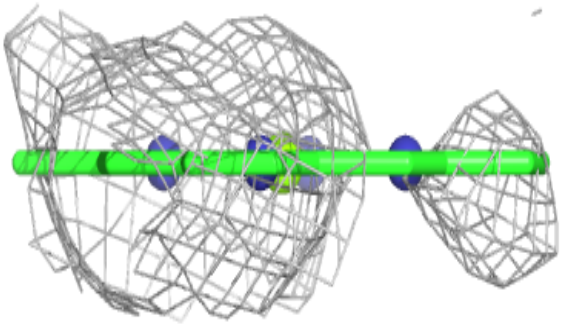


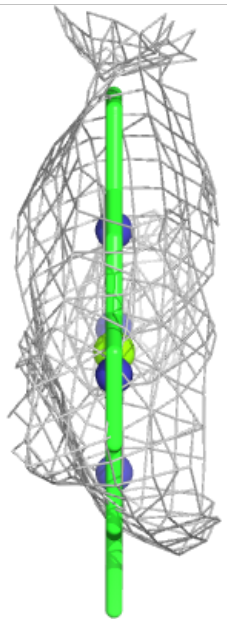


Electron density around CLA B 1241:

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

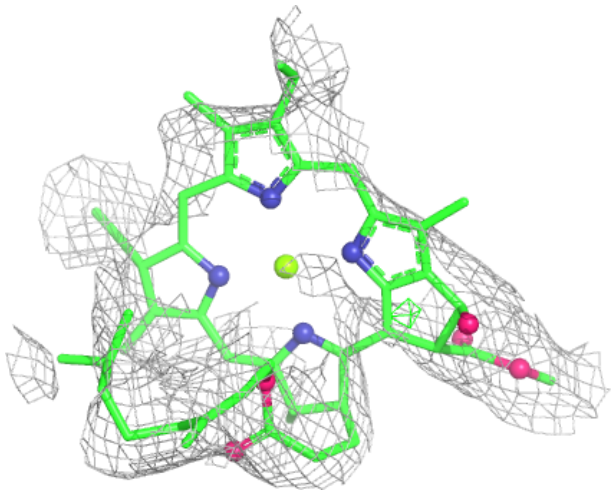


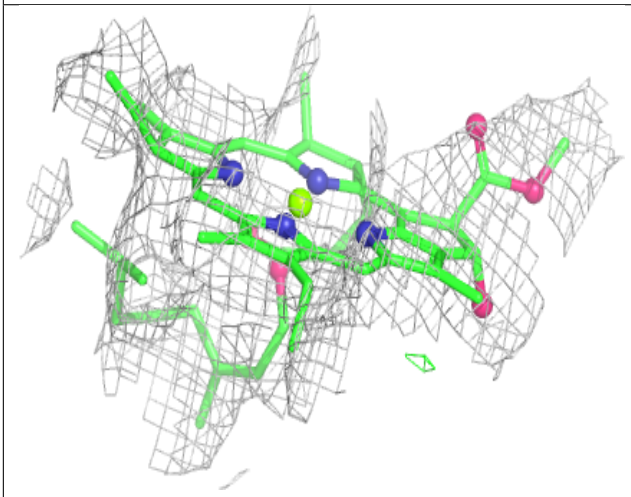


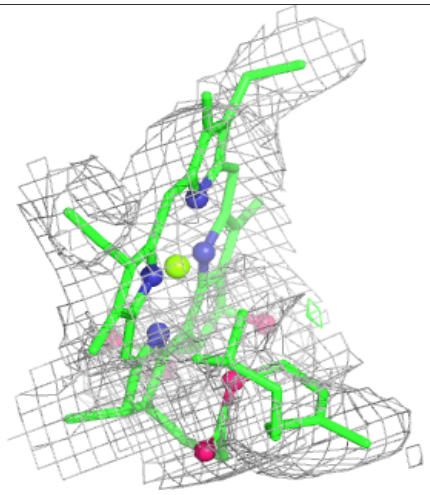


Electron density around CLA B 1209:

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

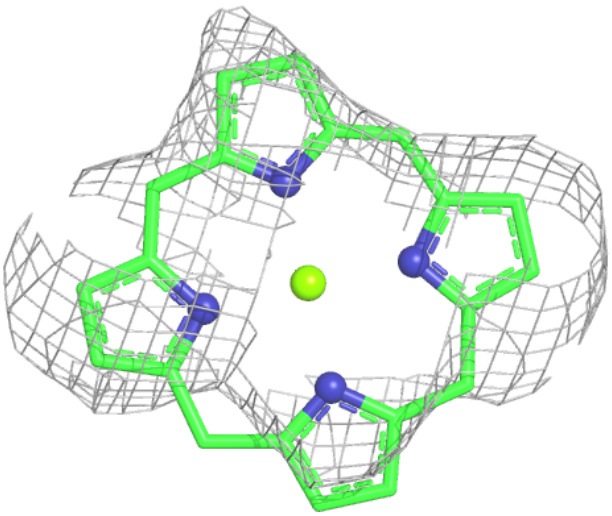


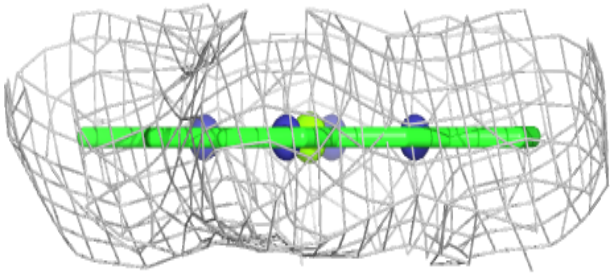


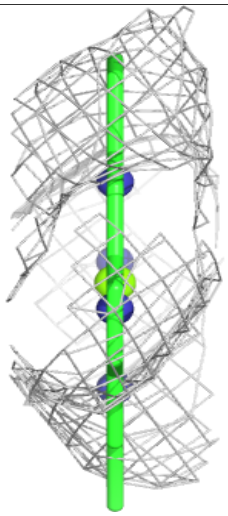


Electron density around CLA A 1101:

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

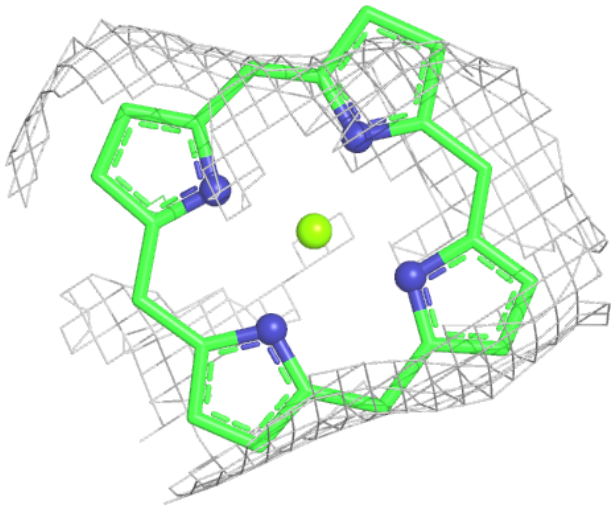


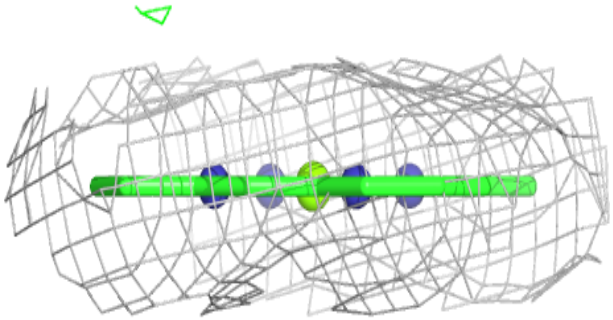


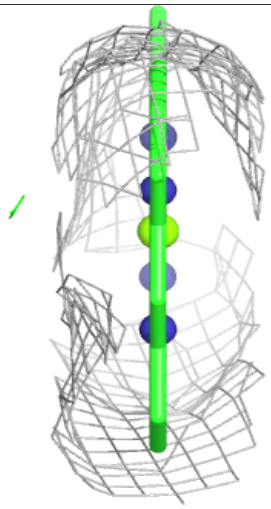


Electron density around CLA B 1211:

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

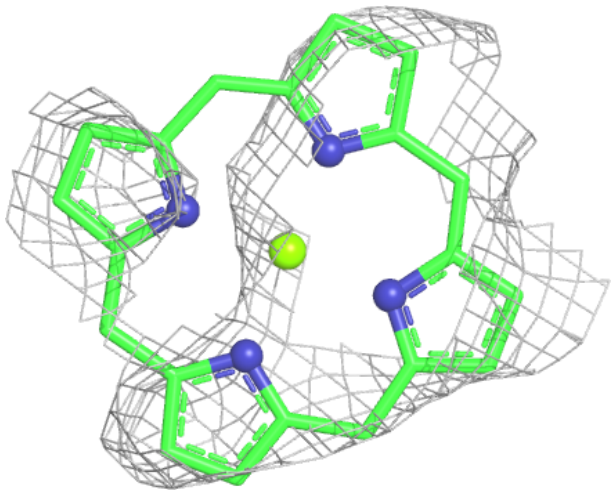


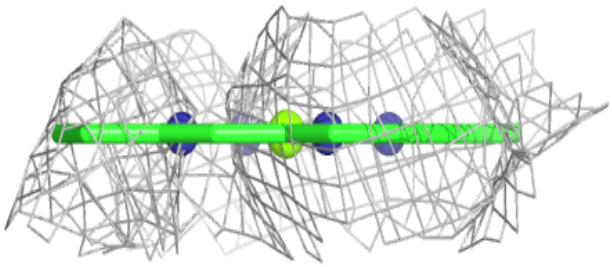


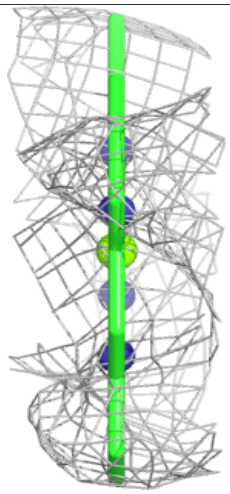


Electron density around CLA 2 2004:

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

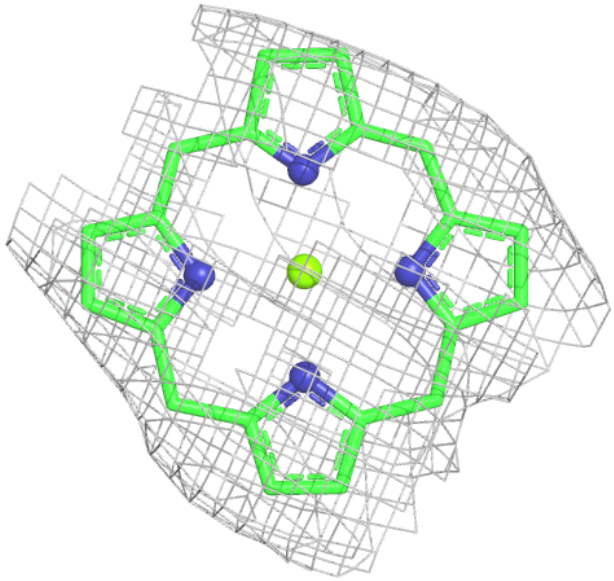


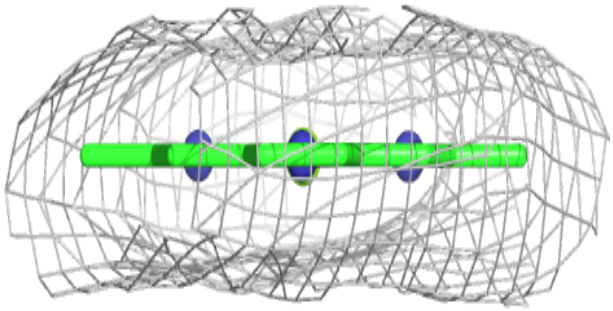


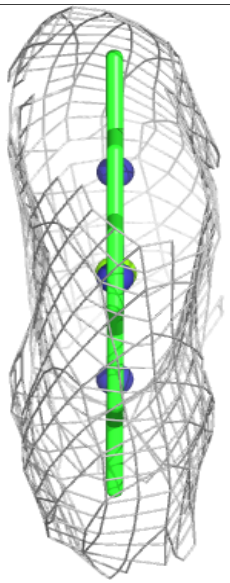


Electron density around CLA F 1240:

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

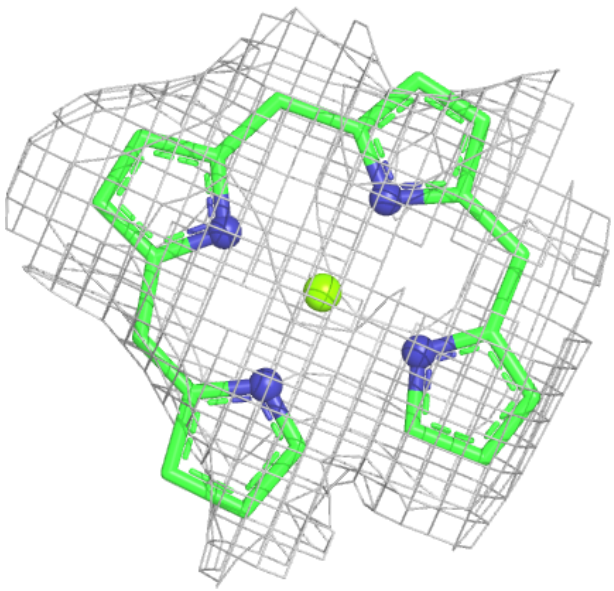


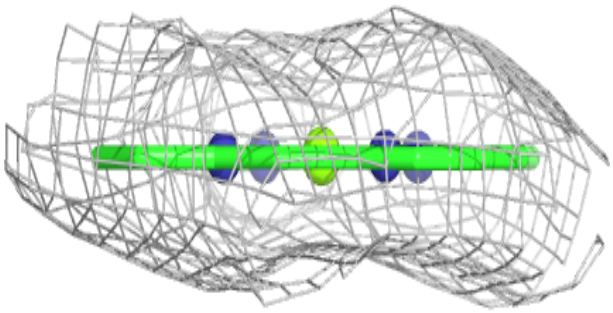


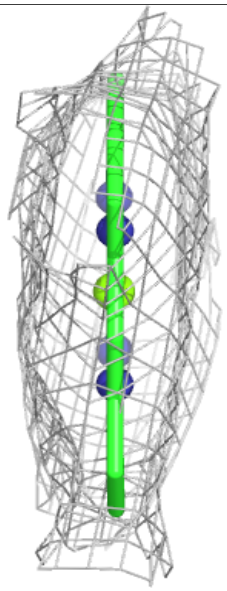


Electron density around CLA A 1109:

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

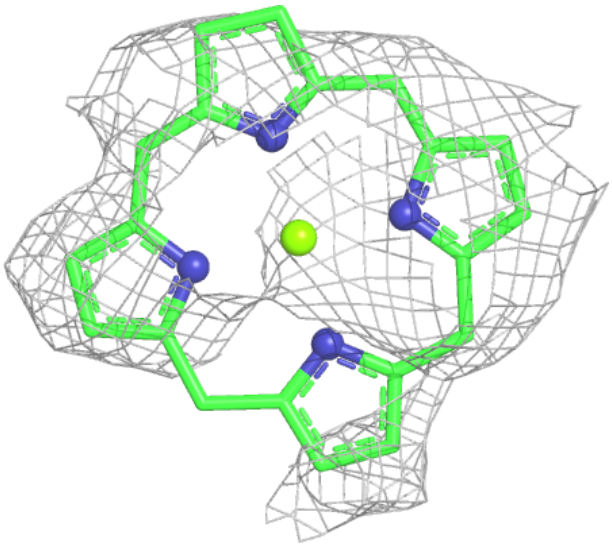


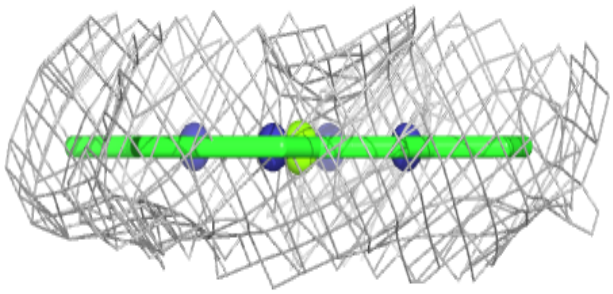


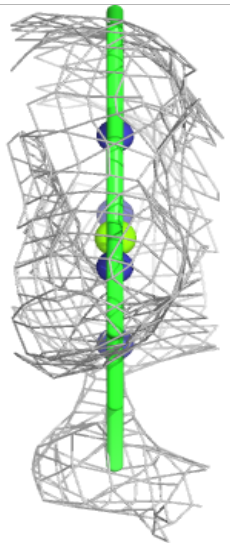


Electron density around CLA B 1213:

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

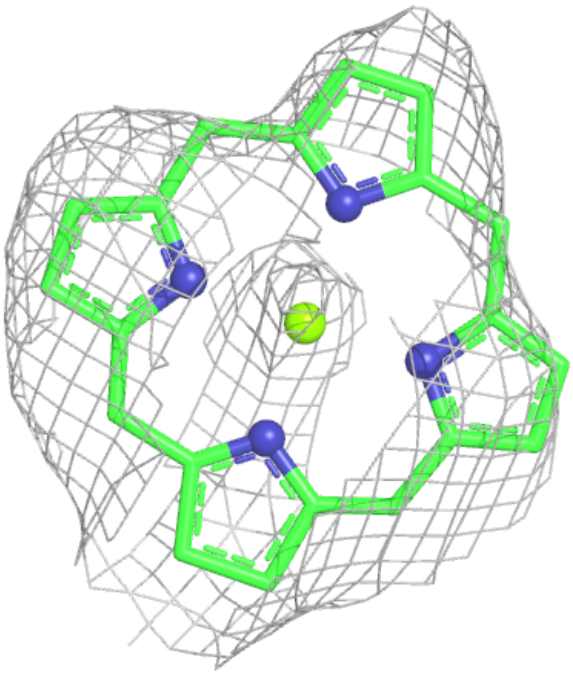


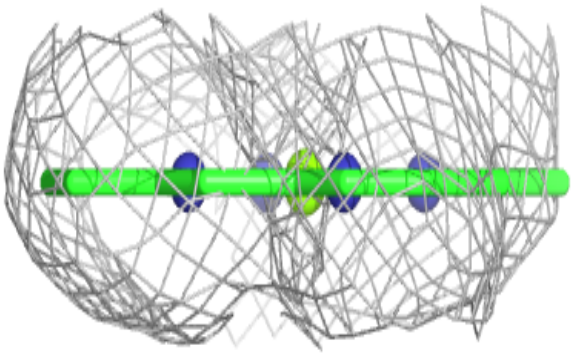


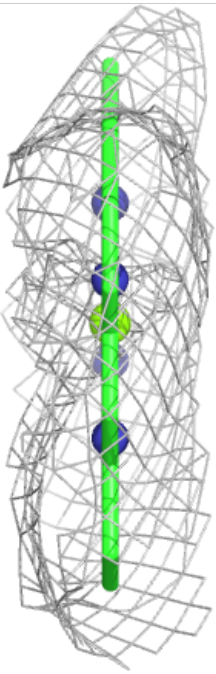


Electron density around CLA 2 2013:

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

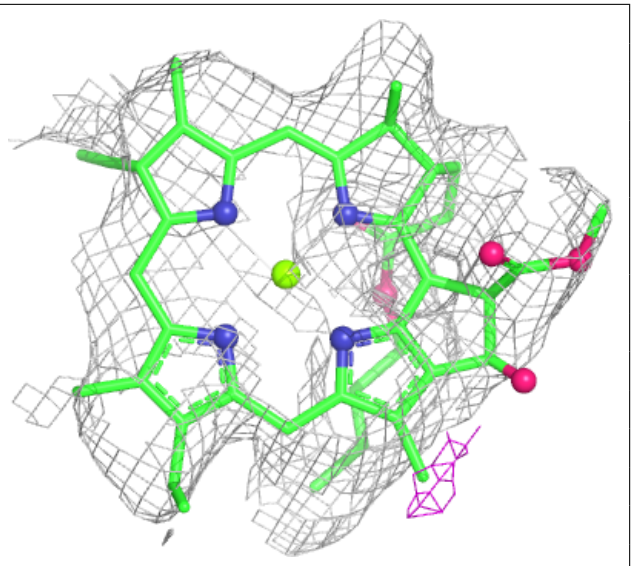


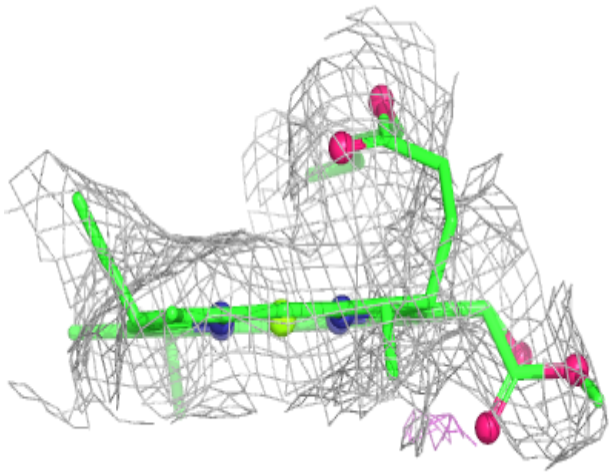


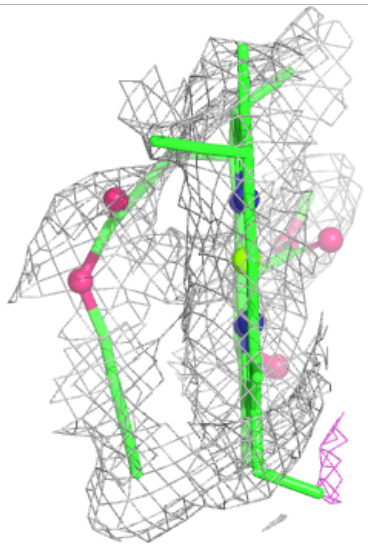


Electron density around CLA B 1214:

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

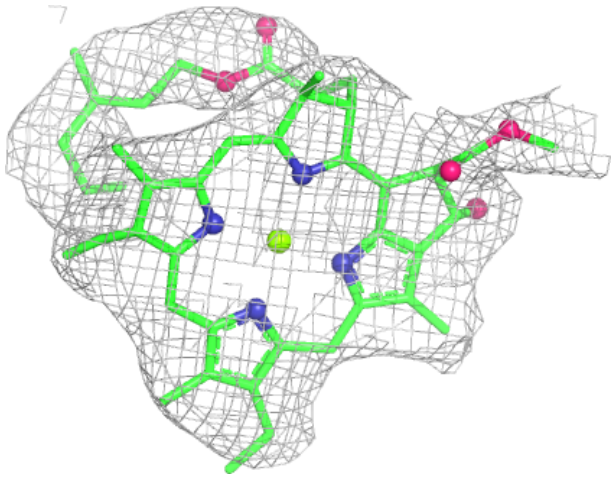


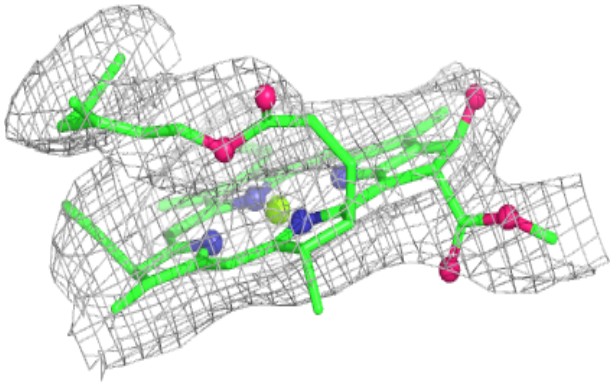


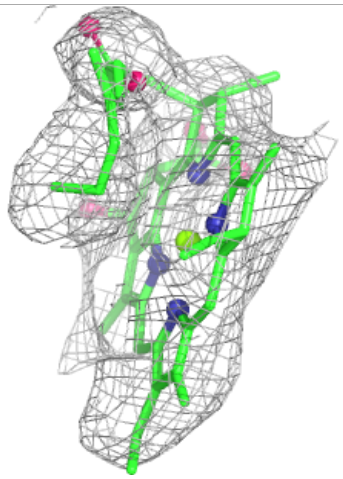


Electron density around CLA B 1215:

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

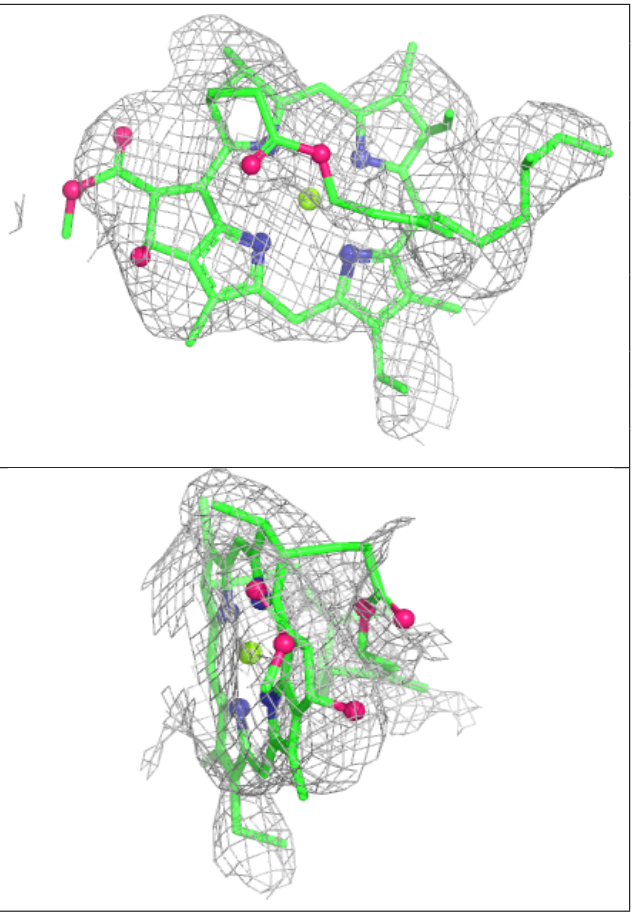


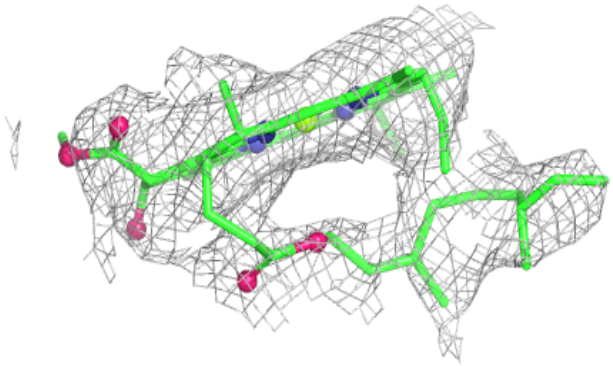




Electron density around CLA B 1138:

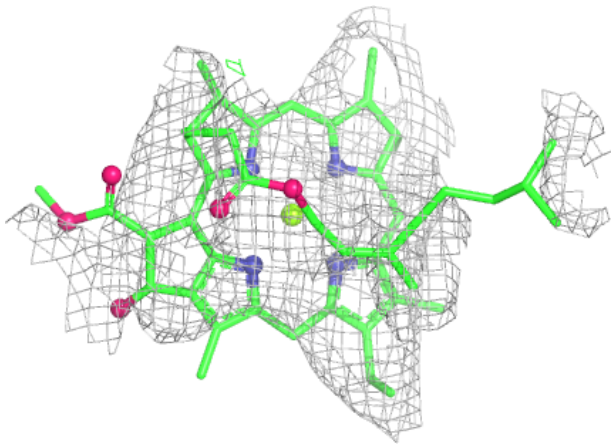
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

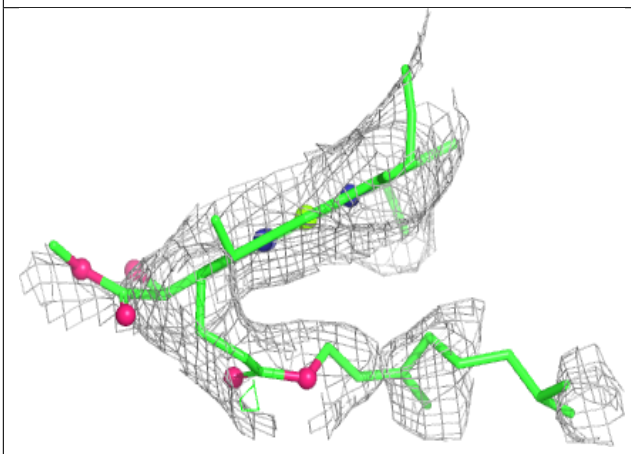


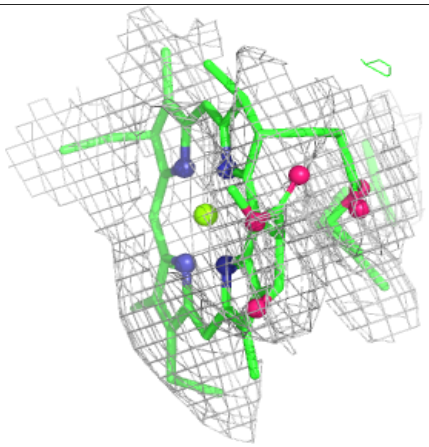


Electron density around CLA A 1136:

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

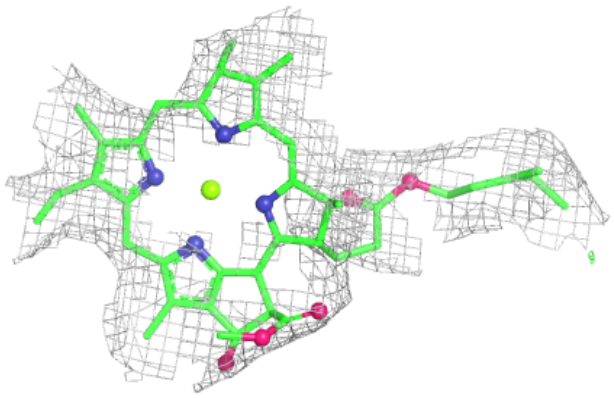


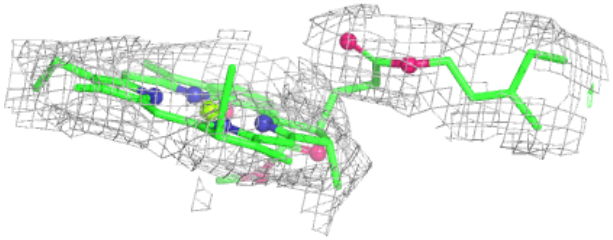


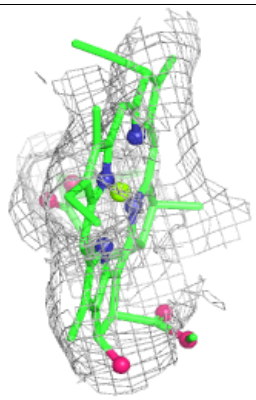


Electron density around CLA B 1218:

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

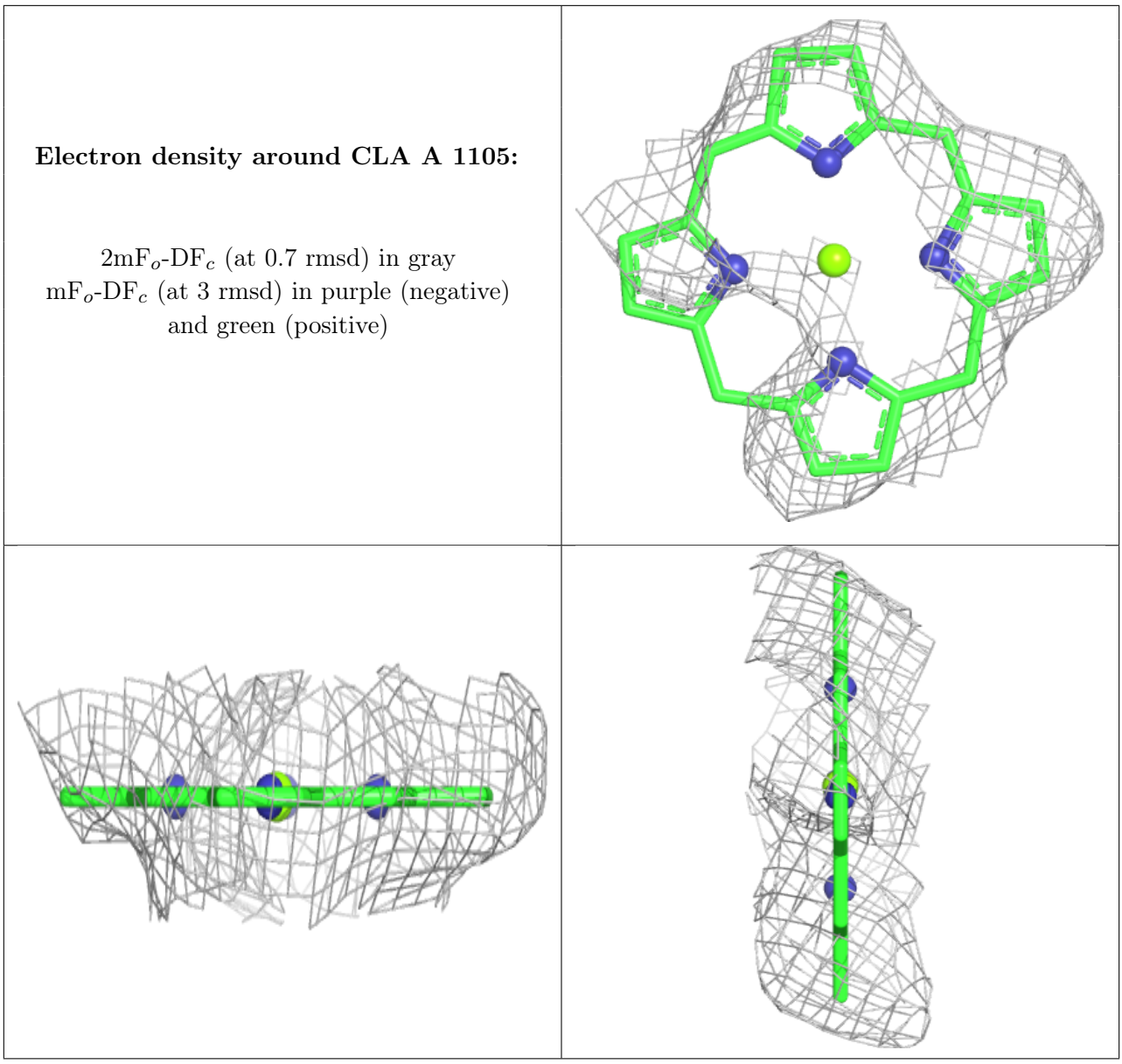






Electron density around CLA A 1105:

$2mF_o$-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.