



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:43 PM UTC

PDB ID : 6FOS / pdb_00006fos
Title : Cyanidioschyzon merolae photosystem I
Authors : Nelson, N.; Hippler, M.; Antoshvili, M.; Caspy, I.
Deposited on : 2018-02-08
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

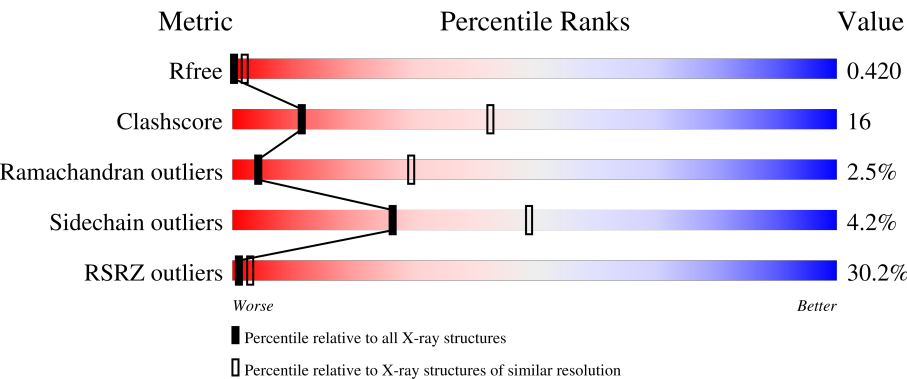
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 $\leq 5\%$. 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	2	222	23% 45% 19% . 35%
1	3	222	20% 32% 28% 7% . 32%
2	4	214	19% 36% 14% . 46%
3	A	740	26% 64% 35% .
4	B	725	34% 66% 33% .

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Mol	Chain	Length	Quality of chain
5	C	80	
6	D	124	
7	E	69	
8	F	155	
9	I	32	
10	J	38	
11	K	47	
12	L	140	
13	M	29	
14	O	98	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	2	601	X	-	-	-
15	CLA	2	602	X	-	-	-
15	CLA	2	603	X	-	-	-
15	CLA	2	604	X	-	-	-
15	CLA	2	605	X	-	-	-
15	CLA	2	606	X	-	-	-
15	CLA	2	607	X	-	-	-
15	CLA	2	608	X	-	-	-
15	CLA	2	610	X	-	-	-
15	CLA	2	611	X	-	-	-
15	CLA	2	612	X	-	-	-
15	CLA	2	613	X	-	-	-
15	CLA	2	614	X	-	-	-
15	CLA	2	615	X	-	-	-
15	CLA	2	616	X	-	-	-
15	CLA	3	601	X	-	-	-
15	CLA	3	602	X	-	-	-
15	CLA	3	603	X	-	-	-
15	CLA	3	604	X	-	-	-
15	CLA	3	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	3	607	X	-	-	-
15	CLA	3	608	X	-	-	-
15	CLA	3	610	X	-	-	-
15	CLA	3	611	X	-	-	-
15	CLA	3	612	X	-	-	-
15	CLA	3	614	X	-	-	-
15	CLA	4	601	X	-	-	-
15	CLA	4	602	X	-	-	-
15	CLA	4	603	X	-	-	-
15	CLA	4	604	X	-	-	-
15	CLA	4	605	X	-	-	-
15	CLA	4	606	X	-	-	-
15	CLA	4	608	X	-	-	-
15	CLA	4	609	X	-	-	-
15	CLA	4	610	X	-	-	-
15	CLA	4	611	X	-	-	-
15	CLA	4	612	X	-	-	-
15	CLA	4	615	X	-	-	-
15	CLA	4	616	X	-	-	-
15	CLA	A	1011	X	-	-	-
15	CLA	A	1012	X	-	-	-
15	CLA	A	1013	X	-	-	-
15	CLA	A	1101	X	-	-	-
15	CLA	A	1102	X	-	-	-
15	CLA	A	1103	X	-	-	-
15	CLA	A	1104	X	-	-	-
15	CLA	A	1105	X	-	-	-
15	CLA	A	1106	X	-	-	-
15	CLA	A	1107	X	-	-	-
15	CLA	A	1108	X	-	-	-
15	CLA	A	1109	X	-	-	-
15	CLA	A	1110	X	-	-	-
15	CLA	A	1111	X	-	-	-
15	CLA	A	1112	X	-	-	-
15	CLA	A	1113	X	-	-	-
15	CLA	A	1114	X	-	-	-
15	CLA	A	1115	X	-	-	-
15	CLA	A	1116	X	-	-	-
15	CLA	A	1117	X	-	-	-
15	CLA	A	1118	X	-	-	-
15	CLA	A	1119	X	-	-	-
15	CLA	A	1120	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	1121	X	-	-	-
15	CLA	A	1122	X	-	-	-
15	CLA	A	1123	X	-	-	-
15	CLA	A	1124	X	-	-	-
15	CLA	A	1125	X	-	-	-
15	CLA	A	1126	X	-	-	-
15	CLA	A	1127	X	-	-	-
15	CLA	A	1128	X	-	-	-
15	CLA	A	1129	X	-	-	-
15	CLA	A	1130	X	-	-	-
15	CLA	A	1131	X	-	-	-
15	CLA	A	1132	X	-	-	-
15	CLA	A	1133	X	-	-	-
15	CLA	A	1134	X	-	-	-
15	CLA	A	1135	X	-	-	-
15	CLA	A	1136	X	-	-	-
15	CLA	A	1137	X	-	-	-
15	CLA	A	1138	X	-	-	-
15	CLA	A	1139	X	-	-	-
15	CLA	A	1140	X	-	-	-
15	CLA	A	1141	X	-	-	-
15	CLA	B	1021	X	-	-	-
15	CLA	B	1022	X	-	-	-
15	CLA	B	1023	X	-	-	-
15	CLA	B	1201	X	-	-	-
15	CLA	B	1202	X	-	-	-
15	CLA	B	1203	X	-	-	-
15	CLA	B	1204	X	-	-	-
15	CLA	B	1205	X	-	-	-
15	CLA	B	1206	X	-	-	-
15	CLA	B	1207	X	-	-	-
15	CLA	B	1208	X	-	-	-
15	CLA	B	1209	X	-	-	-
15	CLA	B	1210	X	-	-	-
15	CLA	B	1211	X	-	-	-
15	CLA	B	1212	X	-	-	-
15	CLA	B	1214	X	-	-	-
15	CLA	B	1215	X	-	-	-
15	CLA	B	1216	X	-	-	-
15	CLA	B	1217	X	-	-	-
15	CLA	B	1218	X	-	-	-
15	CLA	B	1219	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	1220	X	-	-	-
15	CLA	B	1221	X	-	-	-
15	CLA	B	1222	X	-	-	-
15	CLA	B	1223	X	-	-	-
15	CLA	B	1224	X	-	-	-
15	CLA	B	1225	X	-	-	-
15	CLA	B	1226	X	-	-	-
15	CLA	B	1227	X	-	-	-
15	CLA	B	1228	X	-	-	-
15	CLA	B	1229	X	-	-	-
15	CLA	B	1230	X	-	-	-
15	CLA	B	1231	X	-	-	-
15	CLA	B	1232	X	-	-	-
15	CLA	B	1234	X	-	-	-
15	CLA	B	1235	X	-	-	-
15	CLA	B	1236	X	-	-	-
15	CLA	B	1237	X	-	-	-
15	CLA	B	1238	X	-	-	-
15	CLA	B	1239	X	-	-	-
15	CLA	F	1301	X	-	-	-
15	CLA	F	1302	X	-	-	-
15	CLA	J	1302	X	-	-	-
15	CLA	K	1401	X	-	-	-
15	CLA	K	1402	X	-	-	-
15	CLA	L	1501	X	-	-	-
15	CLA	L	1502	X	-	-	-
15	CLA	L	1503	X	-	-	-
15	CLA	O	1601	X	-	-	-
15	CLA	O	1602	X	-	-	-
15	CLA	O	1603	X	-	-	-
17	SF4	C	3002	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 25611 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 Similar to chlorophyll a/b-binding protein, CP24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	144	Total	C	N	O	S	0	0	0
			1116	726	193	192	5			
1	3	150	Total	C	N	O	S	0	0	0
			1181	769	200	206	6			

- Molecule 2 is a protein called Similar to light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	4	116	Total	C	N	O	S	0	0	0
			935	618	157	153	7			

- Molecule 3 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	740	Total	C	N	O	S	0	0	0
			5790	3787	994	982	27			

- Molecule 4 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	725	Total	C	N	O	S	0	0	1
			5766	3791	974	982	19			

- Molecule 5 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	80	Total	C	N	O	S	0	0	0
			597	367	104	114	12			

- Molecule 6 is a protein called Photosystem I p700 chlorophyll A apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	124	Total	C	N	O	S	0	0	0
			976	618	171	182	5			

- Molecule 7 is a protein called Photosystem I iron-sulfur center subunit VII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	69	Total	C	N	O	S	0	0	0
			555	360	88	106	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	153	Total	C	N	O	S	0	0	0
			1256	806	213	233	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	32	Total	C	N	O	S	0	0	0
			238	163	33	40	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	38	Total	C	N	O	S	0	0	0
			312	214	46	51	1			

- Molecule 11 is a protein called Photosystem I reaction center subunit X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	47	Total	C	N	O	S	0	0	0
			331	211	58	58	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	14	MET	-	initiating methionine	UNP Q85G51

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	140	Total	C	N	O	S	0	0	0
			1071	703	174	191	3			

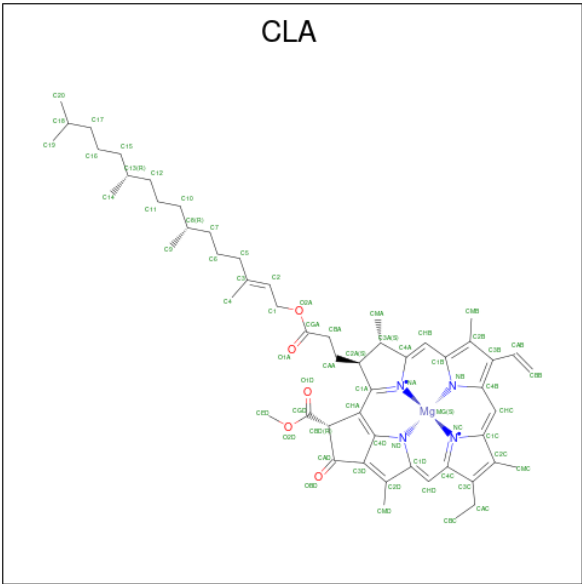
- Molecule 13 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	29	Total	C	N	O	S	0	0	0
			214	142	34	36	2			

- Molecule 14 is a protein called PsaM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	O	98	Total	C	N	O	S	0	0	0
			755	509	116	129	1			

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	2	1	Total 25	C 20	Mg 1	N 4	0	0
15	2	1	Total 25	C 20	Mg 1	N 4	0	0
15	2	1	Total 25	C 20	Mg 1	N 4	0	0
15	2	1	Total 25	C 20	Mg 1	N 4	0	0
15	2	1	Total 25	C 20	Mg 1	N 4	0	0
15	2	1	Total 25	C 20	Mg 1	N 4	0	0
15	2	1	Total 25	C 20	Mg 1	N 4	0	0
15	2	1	Total 25	C 20	Mg 1	N 4	0	0
15	2	1	Total 25	C 20	Mg 1	N 4	0	0
15	2	1	Total 25	C 20	Mg 1	N 4	0	0
15	2	1	Total 25	C 20	Mg 1	N 4	0	0
15	3	1	Total 25	C 20	Mg 1	N 4	0	0
15	3	1	Total 25	C 20	Mg 1	N 4	0	0
15	3	1	Total 25	C 20	Mg 1	N 4	0	0
15	3	1	Total 25	C 20	Mg 1	N 4	0	0
15	3	1	Total 25	C 20	Mg 1	N 4	0	0
15	3	1	Total 25	C 20	Mg 1	N 4	0	0
15	3	1	Total 25	C 20	Mg 1	N 4	0	0
15	3	1	Total 25	C 20	Mg 1	N 4	0	0
15	3	1	Total 25	C 20	Mg 1	N 4	0	0
15	3	1	Total 25	C 20	Mg 1	N 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	3	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	4	1	Total 25	C 20	Mg 1	N 4	0	0
15	A	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
15	A	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
15	A	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
15	A	1	Total 45	C 35	Mg 1	N 4 O 5	0	0
15	A	1	Total 25	C 20	Mg 1	N 4	0	0
15	A	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
15	A	1	Total 55	C 45	Mg 1	N 4 O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	A	1	Total 25	C 20	Mg 1	N 4		0	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	B	1	Total 25	C 20	Mg 1	N 4		0	0
15	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
15	B	1	Total 25	C 20	Mg 1	N 4		0	0
15	B	1	Total 25	C 20	Mg 1	N 4		0	0

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

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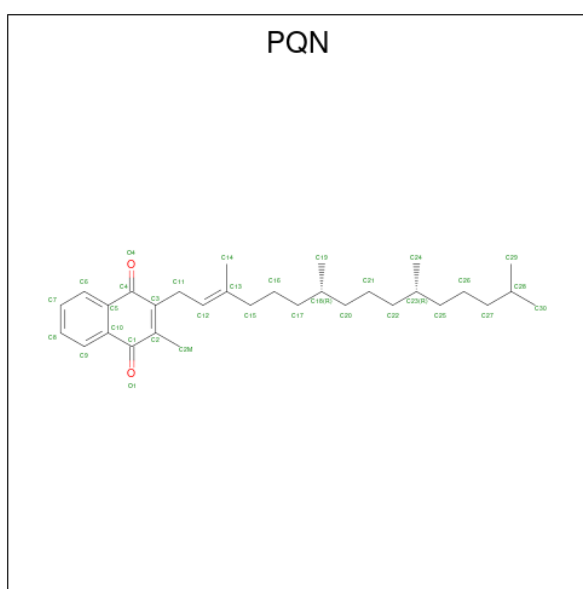
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	F	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	K	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	K	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	L	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	L	1	Total	C	Mg	N		0	0
			25	20	1	4			

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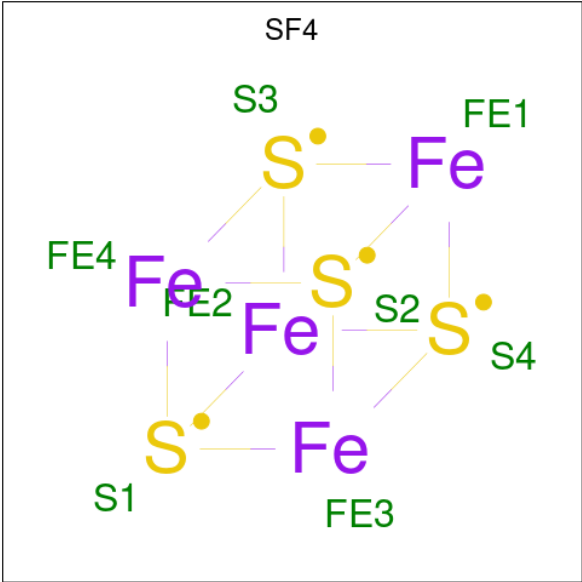
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	O	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	O	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	O	1	Total	C	Mg	N	0	0
			25	20	1	4		

- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



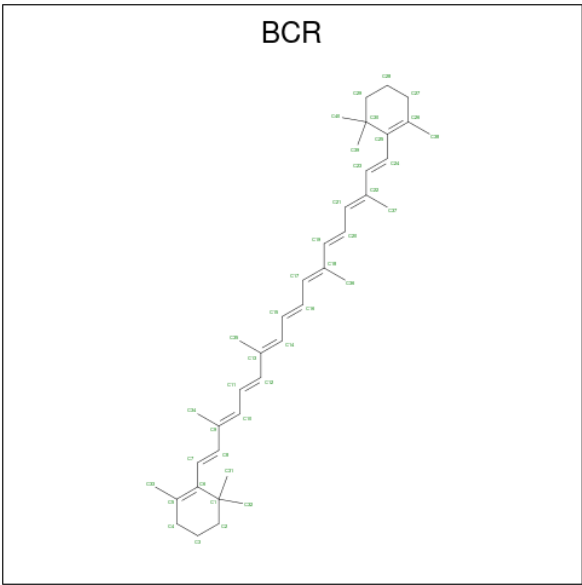
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	C	O	0	0
			33	31	2		
16	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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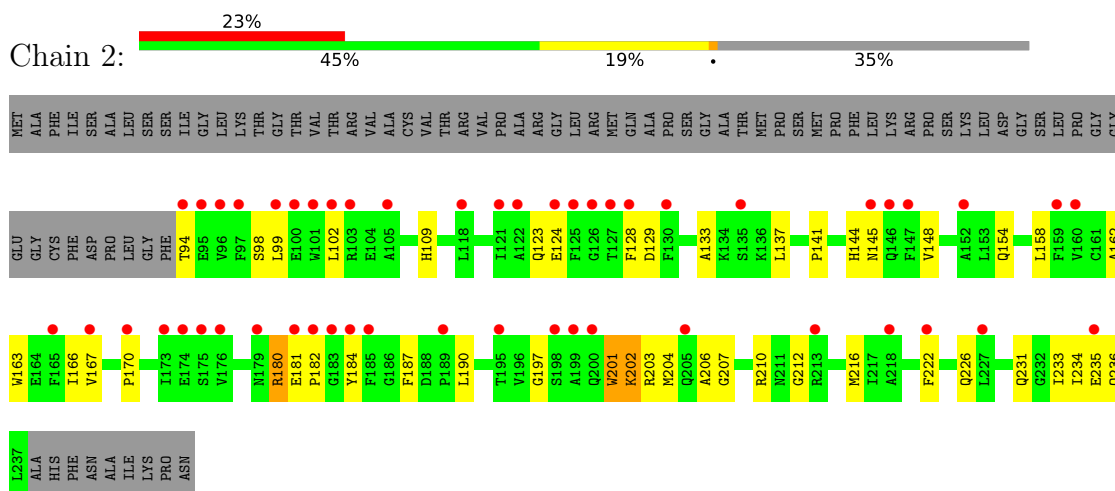
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C 40 40	0	0
18	A	1	Total C 40 40	0	0
18	A	1	Total C 40 40	0	0
18	A	1	Total C 40 40	0	0
18	B	1	Total C 40 40	0	0
18	B	1	Total C 40 40	0	0
18	I	1	Total C 40 40	0	0

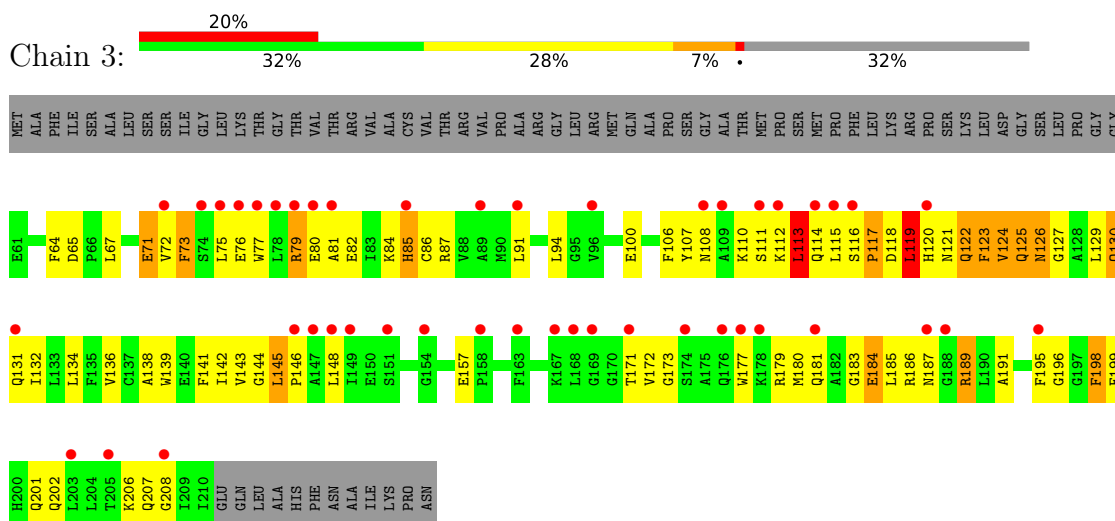
3 Residue-property plots

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

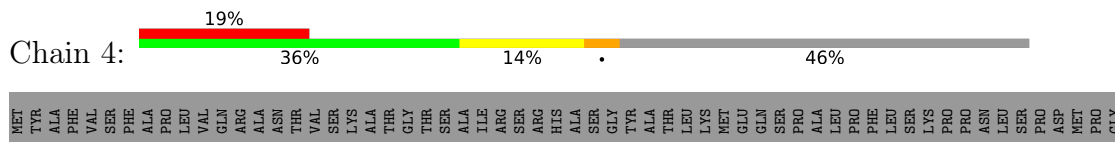
- Molecule 1: Similar to chlorophyll a/b-binding protein, CP24

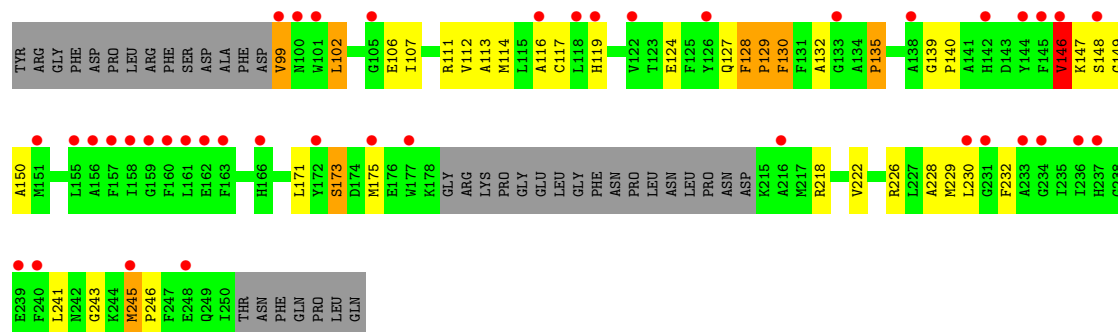


- Molecule 1: Similar to chlorophyll a/b-binding protein, CP24

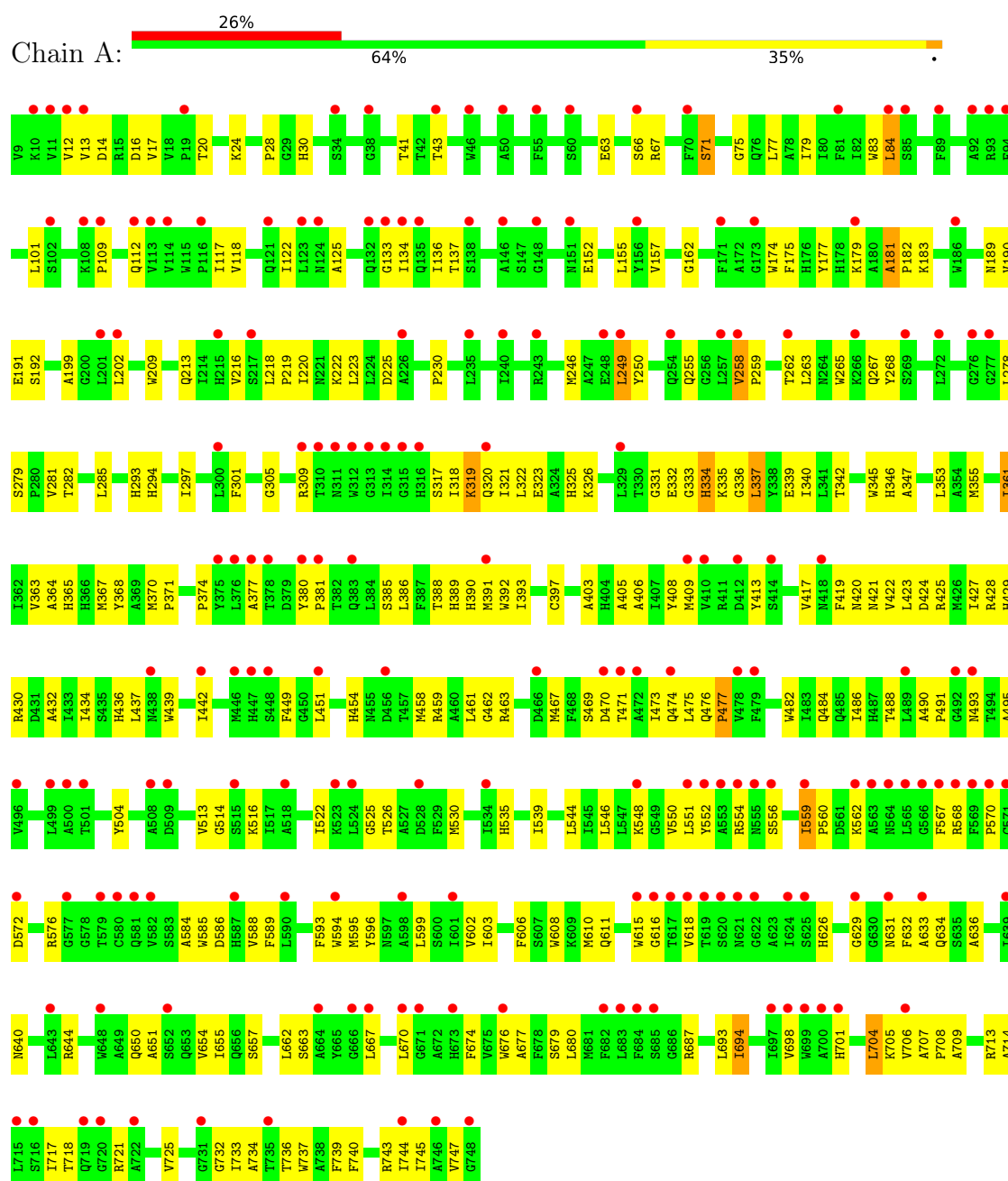


- Molecule 2: Similar to light harvesting protein

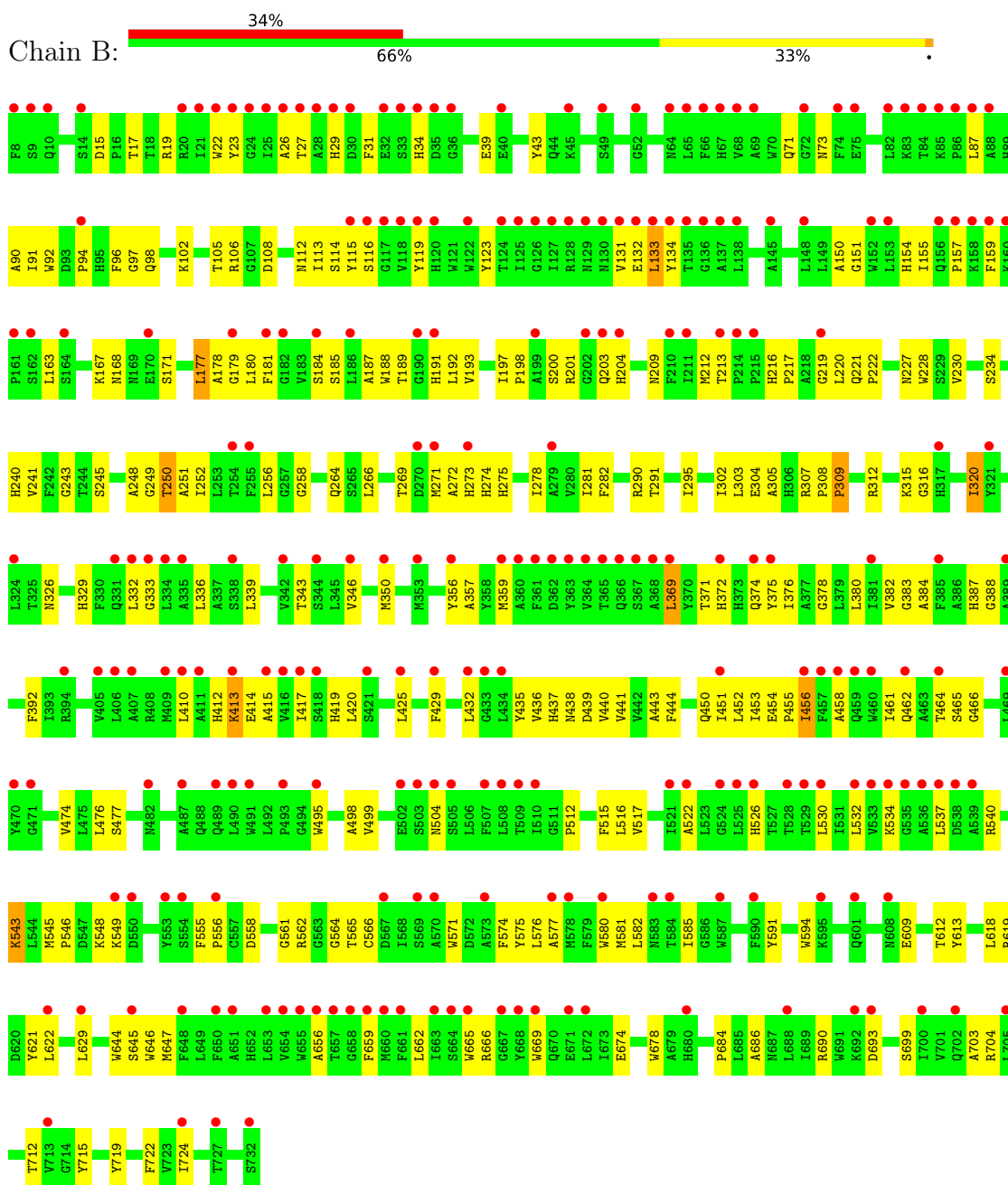




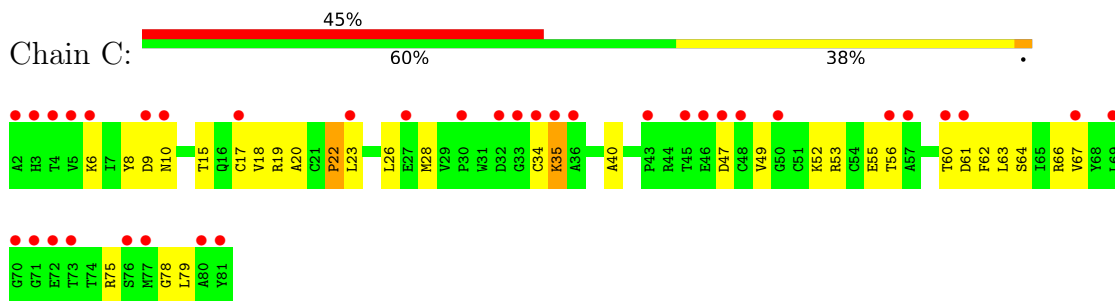
- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A1



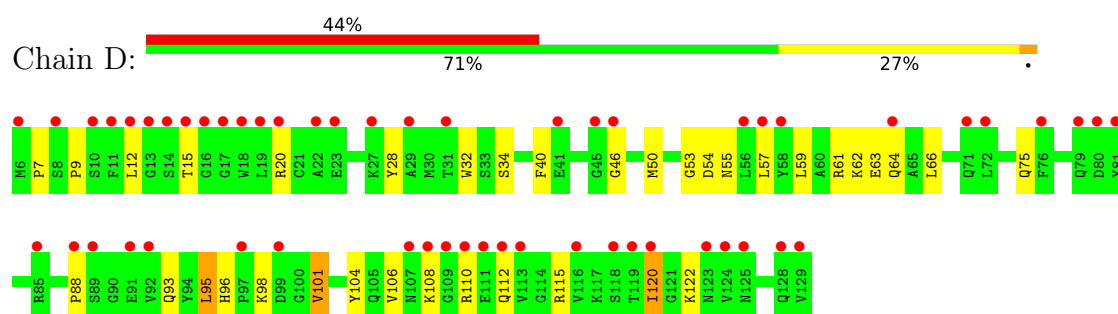
- Molecule 4: Photosystem I P700 chlorophyll a apoprotein A2



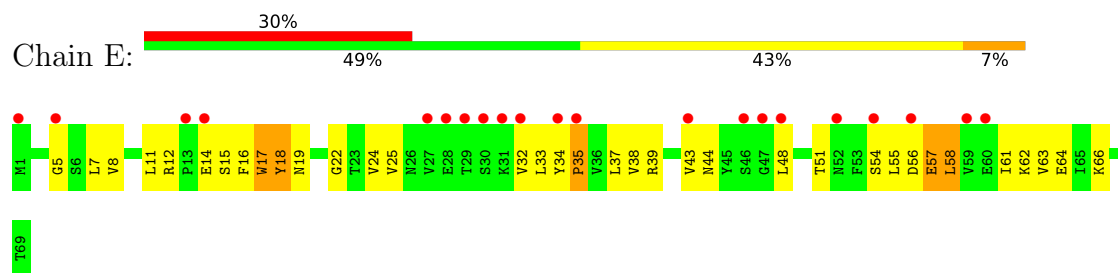
- Molecule 5: Photosystem I iron-sulfur center



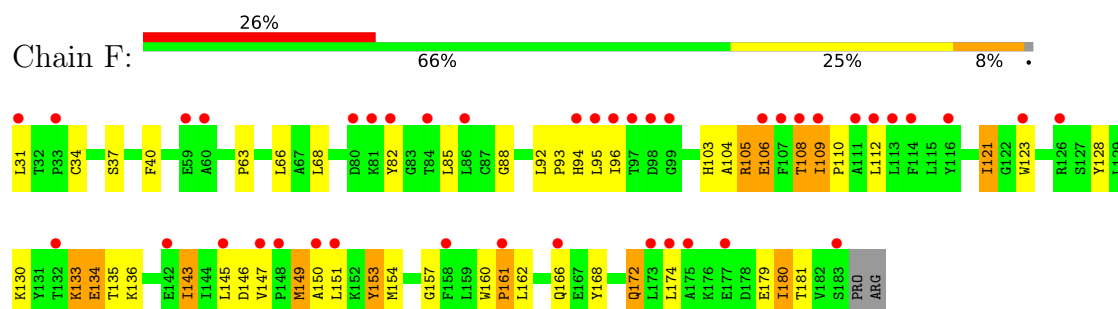
- Molecule 6: Photosystem I p700 chlorophyll A apoprotein A2



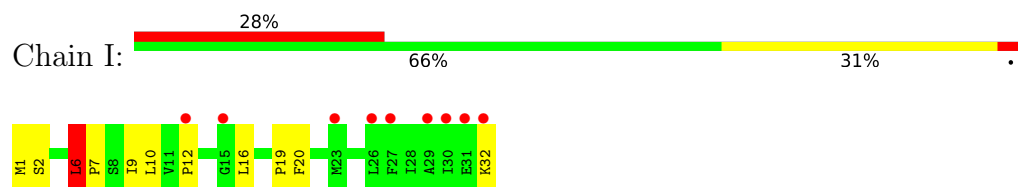
• Molecule 7: Photosystem I iron-sulfur center subunit VII



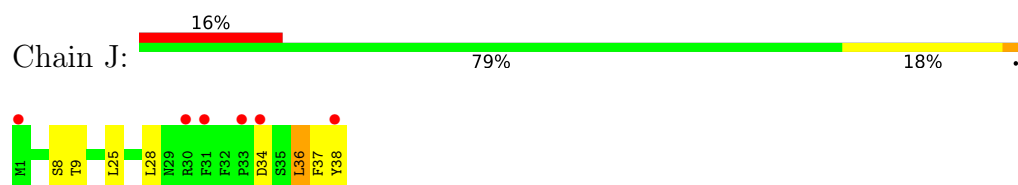
• Molecule 8: Photosystem I reaction center subunit II



• Molecule 9: Photosystem I reaction center subunit VIII

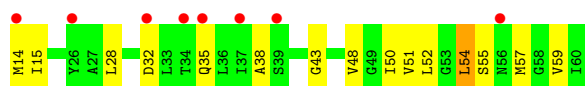


• Molecule 10: Photosystem I reaction center subunit IX

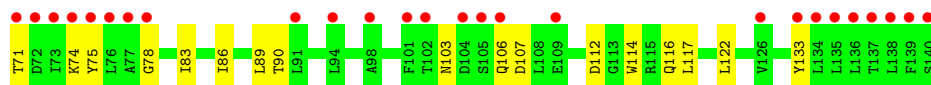
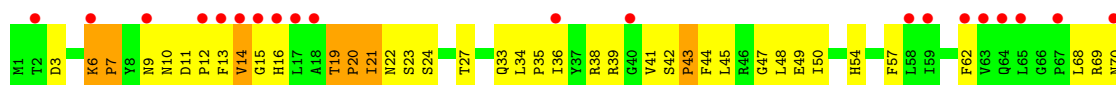


• Molecule 11: Photosystem I reaction center subunit X

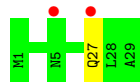




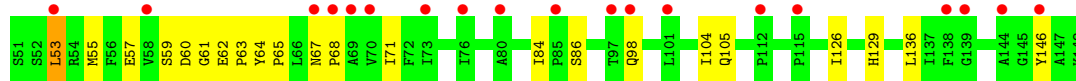
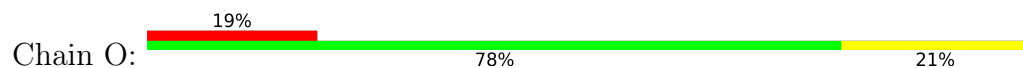
• Molecule 12: Photosystem I reaction center subunit XI



• Molecule 13: Photosystem I reaction center subunit XII



• Molecule 14: PsaM



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	163.13Å 213.52Å 349.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.53 – 4.00 48.53 – 4.00	Depositor EDS
% Data completeness (in resolution range)	80.9 (48.53-4.00) 80.9 (48.53-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.40Å)	Xtriage
Refinement program	PHENIX (dev_3042: ???)	Depositor
R, R_{free}	0.378 , 0.430 0.380 , 0.420	Depositor DCC
R_{free} test set	912 reflections (0.91%)	wwPDB-VP
Wilson B-factor (Å ²)	137.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 85.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	25611	wwPDB-VP
Average B, all atoms (Å ²)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PQN, SF4, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2	0.11	0/1142	0.35	0/1544
1	3	0.18	0/1210	0.60	0/1633
2	4	0.12	0/961	0.33	0/1289
3	A	0.10	0/5977	0.28	0/8146
4	B	0.10	0/5973	0.28	0/8163
5	C	0.11	0/607	0.35	0/822
6	D	0.10	0/998	0.29	0/1349
7	E	0.10	0/564	0.35	0/763
8	F	0.14	0/1289	0.37	0/1750
9	I	0.18	0/243	0.42	0/331
10	J	0.11	0/321	0.37	0/437
11	K	0.08	0/333	0.32	0/448
12	L	0.16	0/1097	0.42	0/1492
13	M	0.08	0/215	0.23	0/291
14	O	0.12	0/780	0.36	0/1068
All	All	0.12	0/21710	0.34	0/29526

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1116	0	1088	40	0
1	3	1181	0	1169	75	0
2	4	935	0	926	28	0
3	A	5790	0	5719	231	0
4	B	5766	0	5589	193	0
5	C	597	0	584	36	0
6	D	976	0	967	31	0
7	E	555	0	576	25	0
8	F	1256	0	1227	60	0
9	I	238	0	265	9	0
10	J	312	0	327	11	0
11	K	331	0	349	9	0
12	L	1071	0	1090	41	0
13	M	214	0	236	0	0
14	O	755	0	760	13	0
15	2	375	0	45	2	0
15	3	275	0	33	5	0
15	4	325	0	39	3	0
15	A	1546	0	801	55	0
15	B	1267	0	522	52	0
15	F	70	0	35	0	0
15	J	50	0	38	1	0
15	K	50	0	6	0	0
15	L	75	0	9	2	0
15	O	75	0	9	0	0
16	A	33	0	46	3	0
16	B	33	0	46	1	0
17	A	8	0	0	0	0
17	C	16	0	0	4	0
18	A	200	0	260	25	0
18	B	80	0	105	8	0
18	I	40	0	53	4	0
All	All	25611	0	22919	779	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (779) 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)
15:A:1012:CLA:H51	4:B:436:VAL:HG13	1.54	0.87
4:B:185:SER:HA	4:B:275:HIS:HD1	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:10:ASN:HB3	5:C:60:THR:HG21	1.63	0.79
3:A:391:MET:HE2	3:A:602:VAL:HG11	1.65	0.79
15:B:1230:CLA:HBA1	18:B:4005:BCR:H281	1.65	0.79
3:A:157:VAL:HG21	15:A:1114:CLA:HAA2	1.66	0.78
3:A:391:MET:HG3	3:A:599:LEU:HD12	1.65	0.77
8:F:34:CYS:HA	8:F:37:SER:HB3	1.67	0.76
3:A:346:HIS:HB3	3:A:408:TYR:HE1	1.51	0.76
14:O:84:ILE:HG22	14:O:86:SER:H	1.51	0.75
1:3:196:GLY:HA2	1:3:199:PHE:HB2	1.69	0.74
3:A:670:LEU:HD12	4:B:618:LEU:HD22	1.69	0.74
4:B:517:VAL:HG11	4:B:591:TYR:HB2	1.68	0.74
4:B:203:GLN:HE22	4:B:213:THR:HB	1.50	0.73
4:B:571:TRP:HH2	4:B:704:ARG:HB2	1.52	0.73
12:L:19:THR:HG23	12:L:24:SER:HA	1.71	0.73
4:B:200:SER:O	4:B:240:HIS:NE2	2.22	0.73
3:A:459:ARG:NH2	3:A:634:GLN:O	2.16	0.72
4:B:437:HIS:CD2	4:B:451:ILE:HG22	2.24	0.72
1:3:179:ARG:HD3	1:3:186:ARG:HH12	1.55	0.72
4:B:180:LEU:HD13	15:B:1210:CLA:HHD	1.71	0.71
3:A:346:HIS:HB3	3:A:408:TYR:CE1	2.24	0.71
5:C:10:ASN:OD1	7:E:12:ARG:NH1	2.23	0.71
3:A:430:ARG:HB2	3:A:551:LEU:HD13	1.73	0.71
8:F:130:LYS:HZ1	8:F:133:LYS:HD3	1.56	0.71
7:E:7:LEU:HB3	7:E:61:ILE:HG21	1.71	0.71
4:B:91:ILE:HD11	4:B:114:SER:HB3	1.72	0.70
1:2:187:PHE:HA	1:2:190:LEU:HB2	1.72	0.70
1:2:234:ILE:HG13	1:3:123:PHE:H	1.55	0.70
4:B:498:ALA:O	4:B:504:ASN:ND2	2.25	0.69
3:A:403:ALA:HA	3:A:588:VAL:HG21	1.74	0.69
3:A:285:LEU:HD21	3:A:370:MET:HB2	1.74	0.69
4:B:719:TYR:HB2	15:B:1021:CLA:HED3	1.74	0.69
2:4:99:VAL:HG22	8:F:149:MET:HG3	1.73	0.69
2:4:245:MET:H	2:4:246:PRO:HD3	1.57	0.69
5:C:15:THR:HA	5:C:28:MET:HE3	1.73	0.69
1:3:79:ARG:HB2	1:3:145:LEU:HD13	1.74	0.69
15:A:1105:CLA:HHB	15:A:1106:CLA:HMB3	1.75	0.69
3:A:392:TRP:HE1	3:A:603:ILE:HD13	1.56	0.68
5:C:6:LYS:HB3	6:D:115:ARG:HE	1.58	0.68
5:C:79:LEU:HA	6:D:61:ARG:HH11	1.58	0.68
3:A:476:GLN:HB3	3:A:477:PRO:HD2	1.75	0.67
8:F:105:ARG:HD2	10:J:36:LEU:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:356:TYR:HB2	4:B:359:MET:HG2	1.76	0.66
12:L:35:PRO:HA	12:L:38:ARG:HB2	1.76	0.66
3:A:477:PRO:HD2	3:A:525:GLY:HA2	1.77	0.66
12:L:19:THR:H	12:L:20:PRO:HD2	1.60	0.66
4:B:90:ALA:HA	4:B:113:ILE:HG12	1.78	0.66
12:L:19:THR:O	12:L:21:ILE:N	2.29	0.66
12:L:47:GLY:O	12:L:49:GLU:N	2.29	0.66
3:A:125:ALA:N	3:A:133:GLY:O	2.29	0.66
3:A:432:ALA:O	3:A:436:HIS:ND1	2.29	0.66
4:B:264:GLN:HB2	4:B:357:ALA:HB2	1.78	0.65
12:L:71:THR:OG1	12:L:74:LYS:NZ	2.25	0.65
2:4:106:GLU:HG2	2:4:229:MET:HE1	1.78	0.65
3:A:655:ILE:HG21	4:B:619:ARG:HB3	1.78	0.65
12:L:6:LYS:HE2	12:L:10:ASN:HB2	1.78	0.65
4:B:222:PRO:HB3	4:B:230:VAL:HB	1.79	0.64
3:A:323:GLU:HA	3:A:335:LYS:HG2	1.80	0.64
2:4:226:ARG:HH11	2:4:230:LEU:HD12	1.61	0.64
3:A:463:ARG:H	4:B:97:GLY:HA3	1.63	0.64
4:B:228:TRP:CD1	4:B:230:VAL:H	2.15	0.64
4:B:336:LEU:HD22	4:B:380:LEU:HD22	1.79	0.64
8:F:146:ASP:O	10:J:8:SER:OG	2.16	0.64
9:I:20:PHE:HE1	18:I:4018:BCR:H363	1.62	0.64
6:D:7:PRO:O	6:D:55:ASN:ND2	2.27	0.63
12:L:107:ASP:HB3	12:L:112:ASP:HB3	1.80	0.63
1:3:142:ILE:HA	1:3:145:LEU:HD12	1.79	0.63
1:3:183:GLY:HA2	1:3:186:ARG:HD2	1.80	0.63
1:3:122:GLN:HA	1:3:125:GLN:OE1	1.98	0.63
3:A:594:TRP:HE1	15:B:1023:CLA:C1D	2.12	0.63
3:A:677:ALA:O	15:A:1013:CLA:HAB	1.98	0.63
4:B:466:GLY:HA2	4:B:476:LEU:HB3	1.81	0.63
7:E:48:LEU:HD11	7:E:51:THR:HG22	1.79	0.63
1:3:145:LEU:H	1:3:146:PRO:HD2	1.64	0.62
3:A:409:MET:HB3	3:A:554:ARG:HB2	1.80	0.62
6:D:9:PRO:HD2	6:D:57:LEU:HD21	1.80	0.62
12:L:75:TYR:OH	12:L:133:TYR:O	2.17	0.62
1:2:99:LEU:HD23	1:2:102:LEU:HD12	1.81	0.62
1:3:115:LEU:HA	1:3:118:ASP:HB2	1.81	0.62
4:B:522:ALA:O	4:B:526:HIS:ND1	2.23	0.62
3:A:213:GLN:HA	3:A:216:VAL:HG12	1.81	0.61
3:A:526:THR:HG21	3:A:633:ALA:HA	1.82	0.61
12:L:103:ASN:HB3	12:L:106:GLN:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:171:THR:O	1:3:173:GLY:N	2.33	0.61
12:L:16:HIS:HB3	12:L:19:THR:HB	1.83	0.61
3:A:319:LYS:NZ	3:A:339:GLU:OE2	2.33	0.61
15:A:1131:CLA:HMB3	18:I:4018:BCR:H291	1.83	0.61
4:B:39:GLU:OE2	4:B:167:LYS:NZ	2.34	0.61
5:C:17:CYS:SG	5:C:18:VAL:N	2.74	0.61
2:4:245:MET:N	2:4:246:PRO:HD3	2.16	0.60
12:L:44:PHE:N	12:L:116:GLN:O	2.21	0.60
3:A:676:TRP:O	3:A:679:SER:OG	2.18	0.60
3:A:736:THR:H	15:A:1011:CLA:HED2	1.66	0.60
12:L:70:ASN:H	12:L:74:LYS:HE2	1.64	0.60
1:3:91:LEU:HA	1:3:94:LEU:HG	1.84	0.60
1:3:94:LEU:HD13	15:3:606:CLA:HHC	1.82	0.60
4:B:561:GLY:HA3	5:C:56:THR:HG22	1.84	0.60
3:A:66:SER:OG	3:A:345:TRP:NE1	2.31	0.60
3:A:199:ALA:HB2	3:A:305:GLY:HA3	1.83	0.60
3:A:219:PRO:HA	3:A:223:LEU:HD12	1.83	0.60
4:B:23:TYR:HA	4:B:26:ALA:HB3	1.82	0.60
4:B:415:ALA:O	4:B:419:HIS:ND1	2.33	0.60
4:B:436:VAL:HB	15:B:1230:CLA:HMC2	1.83	0.60
3:A:41:THR:HG22	3:A:43:THR:H	1.65	0.60
4:B:278:ILE:HD13	4:B:281:ILE:HD12	1.84	0.60
12:L:90:THR:HG21	12:L:122:LEU:HD12	1.82	0.60
3:A:718:THR:HG22	3:A:721:ARG:HH21	1.67	0.59
1:3:129:LEU:HA	1:3:132:ILE:HB	1.85	0.59
4:B:558:ASP:OD1	5:C:66:ARG:NH2	2.36	0.59
1:2:222:PHE:O	1:2:226:GLN:NE2	2.35	0.59
3:A:322:LEU:HD13	3:A:337:LEU:HB3	1.84	0.59
4:B:256:LEU:H	4:B:266:LEU:HD23	1.68	0.59
5:C:47:ASP:OD1	5:C:75:ARG:NH1	2.35	0.59
12:L:22:ASN:OD1	12:L:23:SER:N	2.36	0.59
3:A:333:GLY:HA2	3:A:422:VAL:HG23	1.85	0.58
4:B:571:TRP:CH2	4:B:704:ARG:HB2	2.35	0.58
8:F:105:ARG:HE	10:J:37:PHE:C	2.10	0.58
3:A:674:PHE:CG	18:A:4011:BCR:H363	2.38	0.58
4:B:545:MET:HE2	4:B:548:LYS:HA	1.84	0.58
1:2:184:TYR:HA	1:2:187:PHE:HB2	1.85	0.58
3:A:572:ASP:OD2	3:A:576:ARG:NH2	2.37	0.58
4:B:43:TYR:OH	4:B:326:ASN:O	2.21	0.58
3:A:513:VAL:HG21	3:A:618:VAL:HG21	1.86	0.58
3:A:626:HIS:HB2	3:A:629:GLY:HA2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:193:VAL:HG11	4:B:272:ALA:HB2	1.86	0.58
14:O:62:GLU:HG3	14:O:63:PRO:HD3	1.85	0.58
4:B:382:VAL:HG21	4:B:581:MET:HG3	1.83	0.58
4:B:376:ILE:HG21	15:B:1225:CLA:HAB	1.86	0.58
4:B:574:PHE:HE1	15:B:1226:CLA:HAC2	1.68	0.58
3:A:421:ASN:HA	3:A:424:ASP:HB2	1.86	0.58
4:B:217:PRO:HD3	4:B:250:THR:HG23	1.85	0.58
8:F:31:LEU:HD12	8:F:88:GLY:HA2	1.84	0.57
3:A:361:ILE:HG21	15:A:1124:CLA:C2A	2.34	0.57
3:A:346:HIS:O	3:A:408:TYR:OH	2.17	0.57
8:F:121:ILE:HA	8:F:160:TRP:CD1	2.39	0.57
3:A:677:ALA:HA	3:A:680:LEU:HG	1.85	0.57
4:B:150:ALA:O	4:B:154:HIS:ND1	2.36	0.57
4:B:241:VAL:HG12	4:B:243:GLY:H	1.69	0.57
3:A:14:ASP:HB2	3:A:183:LYS:HD2	1.86	0.57
18:A:4002:BCR:H343	18:A:4002:BCR:HC31	1.85	0.57
15:B:1227:CLA:C3C	15:B:1228:CLA:C2A	2.82	0.57
3:A:657:SER:HB2	3:A:662:LEU:HB2	1.87	0.57
1:3:84:LYS:HG2	1:3:87:ARG:HE	1.69	0.57
3:A:474:GLN:O	3:A:476:GLN:N	2.37	0.56
4:B:339:LEU:O	4:B:343:THR:OG1	2.16	0.56
1:3:84:LYS:HD2	1:3:142:ILE:HD11	1.88	0.56
3:A:28:PRO:HD3	8:F:145:LEU:HD11	1.87	0.56
8:F:150:ALA:HA	8:F:153:TYR:HD1	1.69	0.56
1:2:197:GLY:HA3	1:2:201:TRP:HB2	1.87	0.56
1:3:119:LEU:HD12	1:3:125:GLN:HE21	1.71	0.56
8:F:130:LYS:NZ	8:F:133:LYS:HD3	2.20	0.56
4:B:613:TYR:HE2	4:B:619:ARG:HH12	1.54	0.56
3:A:572:ASP:OD2	5:C:53:ARG:NH2	2.38	0.56
3:A:708:PRO:HA	8:F:130:LYS:NZ	2.20	0.56
3:A:708:PRO:HA	8:F:130:LYS:HZ2	1.71	0.56
4:B:419:HIS:CD2	15:B:1228:CLA:C4A	2.83	0.56
8:F:121:ILE:HA	8:F:160:TRP:NE1	2.20	0.56
4:B:198:PRO:HG3	4:B:204:HIS:HA	1.88	0.56
5:C:8:TYR:CE2	5:C:66:ARG:HB2	2.41	0.56
12:L:43:PRO:HA	12:L:116:GLN:HB3	1.86	0.56
1:3:112:LYS:HB3	1:3:117:PRO:HD3	1.88	0.55
7:E:8:VAL:HB	7:E:58:LEU:HD22	1.87	0.55
3:A:461:LEU:HD13	4:B:96:PHE:HD1	1.70	0.55
16:A:2001:PQN:H142	18:B:4005:BCR:H312	1.86	0.55
1:3:157:GLU:H	1:3:157:GLU:CD	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:111:ARG:NH1	2:4:114:MET:SD	2.79	0.55
4:B:674:GLU:OE2	6:D:61:ARG:NH1	2.38	0.55
1:3:186:ARG:HA	1:3:189:ARG:HE	1.70	0.55
4:B:436:VAL:HG12	15:B:1230:CLA:HAC1	1.88	0.55
5:C:26:LEU:HD12	5:C:40:ALA:HB1	1.89	0.55
7:E:12:ARG:NH2	7:E:14:GLU:OE2	2.40	0.55
4:B:656:ALA:O	15:B:1023:CLA:HAB	2.07	0.55
7:E:24:VAL:HA	7:E:38:VAL:HG12	1.89	0.55
3:A:101:LEU:HD12	3:A:230:PRO:HB3	1.88	0.55
3:A:550:VAL:HG21	18:A:4008:BCR:H282	1.88	0.55
4:B:417:ILE:HD11	4:B:537:LEU:HD12	1.88	0.55
6:D:101:VAL:HG23	6:D:104:TYR:HB2	1.87	0.55
3:A:122:ILE:HG21	4:B:444:PHE:HA	1.88	0.55
3:A:556:SER:OG	3:A:559:ILE:O	2.25	0.55
6:D:34:SER:OG	6:D:53:GLY:O	2.25	0.55
1:2:233:ILE:HG22	1:2:234:ILE:HD13	1.88	0.55
5:C:78:GLY:O	6:D:61:ARG:NE	2.38	0.55
15:A:1104:CLA:H12	15:A:1104:CLA:H2A	1.89	0.54
5:C:22:PRO:HD3	5:C:53:ARG:HE	1.71	0.54
1:3:71:GLU:HB2	15:3:604:CLA:CHD	2.36	0.54
1:3:186:ARG:HA	1:3:189:ARG:NE	2.22	0.54
3:A:255:GLN:HE22	3:A:267:GLN:HB3	1.73	0.54
8:F:105:ARG:HG3	10:J:38:TYR:CD1	2.43	0.54
12:L:6:LYS:O	12:L:9:ASN:N	2.40	0.54
1:2:94:THR:OG1	3:A:179:LYS:O	2.25	0.54
2:4:127:GLN:HA	2:4:132:ALA:HB1	1.89	0.54
4:B:258:GLY:HA2	4:B:498:ALA:HB2	1.90	0.54
15:B:1229:CLA:HHC	15:B:1230:CLA:HMB2	1.90	0.54
3:A:403:ALA:HB2	3:A:588:VAL:HG11	1.88	0.54
3:A:677:ALA:HB3	15:A:1013:CLA:HBB2	1.90	0.54
4:B:187:ALA:O	4:B:191:HIS:ND1	2.41	0.54
4:B:629:LEU:HD22	4:B:722:PHE:HD1	1.73	0.54
3:A:109:PRO:HB2	3:A:136:ILE:HG13	1.89	0.54
3:A:332:GLU:HB2	3:A:421:ASN:HB2	1.88	0.53
3:A:632:PHE:CD2	3:A:636:ALA:HB2	2.43	0.53
3:A:190:VAL:HG21	3:A:342:THR:HG22	1.90	0.53
4:B:167:LYS:HE2	4:B:326:ASN:HA	1.91	0.53
7:E:66:LYS:H	7:E:66:LYS:HD3	1.73	0.53
3:A:705:LYS:NZ	8:F:174:LEU:HB2	2.24	0.53
12:L:42:SER:HB2	12:L:43:PRO:HD2	1.90	0.53
14:O:57:GLU:HG3	14:O:59:SER:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:82:TYR:CE1	8:F:93:PRO:HB2	2.43	0.53
3:A:687:ARG:H	4:B:566:CYS:HB2	1.73	0.53
1:3:202:GLN:HA	1:3:206:LYS:HE3	1.91	0.53
4:B:618:LEU:HD12	4:B:622:LEU:HD12	1.91	0.53
11:K:54:LEU:HD13	11:K:57:MET:H	1.73	0.53
3:A:385:SER:HB3	15:A:1126:CLA:HMA3	1.91	0.53
3:A:606:PHE:O	3:A:610:MET:HG2	2.09	0.53
15:A:1012:CLA:HAB	4:B:580:TRP:CZ3	2.44	0.53
15:A:1013:CLA:HAA2	4:B:425:LEU:HD23	1.91	0.53
4:B:452:LEU:HG	8:F:92:LEU:HG	1.91	0.53
6:D:32:TRP:HD1	6:D:34:SER:HB3	1.73	0.53
3:A:346:HIS:CG	15:A:1103:CLA:HBC1	2.43	0.53
4:B:290:ARG:HH22	4:B:295:ILE:HG13	1.72	0.53
6:D:110:ARG:HG3	6:D:112:GLN:HE22	1.73	0.52
7:E:8:VAL:N	7:E:22:GLY:O	2.33	0.52
1:3:136:VAL:HA	1:3:139:TRP:CE3	2.44	0.52
5:C:9:ASP:HB2	7:E:33:LEU:HD11	1.91	0.52
1:3:67:LEU:HD23	1:3:67:LEU:H	1.74	0.52
3:A:117:ILE:HG22	3:A:118:VAL:HG13	1.90	0.52
3:A:209:TRP:HD1	3:A:294:HIS:HD1	1.58	0.52
3:A:340:ILE:HG21	18:A:4007:BCR:HC22	1.89	0.52
3:A:654:VAL:HG13	3:A:655:ILE:HG13	1.92	0.52
3:A:736:THR:HA	3:A:739:PHE:HB3	1.91	0.52
5:C:23:LEU:HD13	6:D:62:LYS:HD3	1.91	0.52
8:F:104:ALA:HB1	8:F:109:ILE:HG13	1.90	0.52
4:B:98:GLN:HG3	4:B:102:LYS:HE3	1.92	0.52
15:B:1232:CLA:H122	15:B:1232:CLA:H52	1.91	0.52
1:2:181:GLU:HA	1:2:184:TYR:CZ	2.45	0.52
3:A:24:LYS:HB3	3:A:30:HIS:CG	2.44	0.52
18:A:4011:BCR:H292	15:B:1229:CLA:HMB1	1.92	0.52
4:B:333:GLY:HA2	4:B:384:ALA:HA	1.92	0.52
4:B:582:LEU:HD21	4:B:712:THR:HA	1.92	0.52
3:A:347:ALA:HA	3:A:408:TYR:CZ	2.46	0.51
3:A:491:PRO:HA	3:A:495:ALA:HB3	1.92	0.51
3:A:705:LYS:HZ1	8:F:174:LEU:HB2	1.75	0.51
12:L:68:LEU:HB3	12:L:74:LYS:HD2	1.93	0.51
1:2:235:GLU:HG2	1:3:125:GLN:HB3	1.91	0.51
3:A:451:LEU:HB2	3:A:530:MET:HE1	1.93	0.51
3:A:546:LEU:O	3:A:550:VAL:HG23	2.11	0.51
8:F:157:GLY:HA3	8:F:160:TRP:CE2	2.45	0.51
12:L:36:ILE:HD12	12:L:50:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:63:GLU:O	3:A:67:ARG:NE	2.42	0.51
3:A:282:THR:HB	3:A:374:PRO:HB3	1.91	0.51
3:A:363:VAL:HG22	3:A:367:MET:HE2	1.93	0.51
5:C:15:THR:HG22	5:C:28:MET:HG3	1.91	0.51
11:K:14:MET:HG3	11:K:15:ILE:H	1.76	0.51
12:L:39:ARG:H	12:L:39:ARG:HD3	1.75	0.51
1:3:75:LEU:HB3	1:3:77:TRP:CE3	2.45	0.51
3:A:737:TRP:NE1	15:A:1126:CLA:O1A	2.38	0.51
4:B:245:SER:HB2	4:B:248:ALA:HB3	1.91	0.51
12:L:11:ASP:O	12:L:13:PHE:N	2.44	0.51
3:A:709:ALA:H	8:F:143:ILE:HD11	1.75	0.51
4:B:201:ARG:HA	4:B:240:HIS:CE1	2.46	0.51
4:B:454:GLU:HB2	8:F:94:HIS:HB3	1.92	0.51
4:B:456:ILE:HD11	8:F:96:ILE:HA	1.93	0.51
4:B:543:LYS:HE2	8:F:180:ILE:HG22	1.91	0.51
1:3:132:ILE:O	1:3:136:VAL:HG23	2.11	0.51
3:A:258:VAL:H	3:A:259:PRO:HD2	1.76	0.51
4:B:543:LYS:NZ	8:F:181:THR:OG1	2.43	0.51
3:A:162:GLY:HA2	18:A:4002:BCR:H322	1.92	0.51
3:A:736:THR:OG1	15:A:1011:CLA:OBD	2.28	0.51
4:B:132:GLU:OE1	4:B:132:GLU:N	2.44	0.51
8:F:85:LEU:HD12	8:F:106:GLU:OE2	2.11	0.51
4:B:92:TRP:CH2	9:I:12:PRO:HG3	2.46	0.51
7:E:32:VAL:HG22	7:E:35:PRO:HB3	1.93	0.51
11:K:51:VAL:O	11:K:55:SER:N	2.42	0.51
1:2:231:GLN:HG2	1:2:233:ILE:HG13	1.93	0.50
3:A:353:LEU:HB3	3:A:397:CYS:O	2.11	0.50
3:A:409:MET:HE1	3:A:423:LEU:HD11	1.93	0.50
3:A:548:LYS:HG3	3:A:552:TYR:CD2	2.46	0.50
8:F:121:ILE:HA	8:F:160:TRP:HE1	1.75	0.50
3:A:321:ILE:O	3:A:325:HIS:ND1	2.42	0.50
15:B:1203:CLA:C3C	15:B:1226:CLA:HAB	2.41	0.50
3:A:14:ASP:N	3:A:181:ALA:O	2.36	0.50
4:B:546:PRO:HG2	5:C:62:PHE:CE2	2.47	0.50
15:B:1225:CLA:H2	15:B:1225:CLA:HAA1	1.93	0.50
9:I:1:MET:HG3	9:I:2:SER:H	1.76	0.50
12:L:19:THR:H	12:L:20:PRO:CD	2.23	0.50
3:A:662:LEU:HD21	3:A:745:ILE:HG21	1.93	0.50
4:B:180:LEU:O	4:B:184:SER:OG	2.25	0.50
8:F:147:VAL:HG12	8:F:149:MET:H	1.76	0.50
3:A:434:ILE:HD13	3:A:551:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:659:PHE:HB3	15:B:1023:CLA:HMC2	1.94	0.50
18:B:4005:BCR:H391	10:J:25:LEU:HD11	1.93	0.50
2:4:128:PHE:HB2	2:4:129:PRO:HD3	1.94	0.50
3:A:449:PHE:CE1	15:B:1022:CLA:HHD	2.46	0.50
7:E:34:TYR:CE1	7:E:54:SER:HB2	2.47	0.50
12:L:47:GLY:HA3	12:L:117:LEU:O	2.12	0.50
1:3:130:GLN:HE21	1:3:131:GLN:HG3	1.76	0.50
3:A:405:ALA:HA	3:A:408:TYR:CD2	2.47	0.50
3:A:476:GLN:HB3	3:A:525:GLY:HA2	1.92	0.50
3:A:663:SER:HB2	4:B:443:ALA:HB1	1.94	0.50
4:B:376:ILE:HG21	15:B:1225:CLA:HHC	1.93	0.50
4:B:388:GLY:HA3	18:B:4008:BCR:H271	1.94	0.50
7:E:5:GLY:H	7:E:24:VAL:HB	1.77	0.50
7:E:12:ARG:HG2	7:E:14:GLU:HG3	1.94	0.50
2:4:107:ILE:HD11	2:4:222:VAL:HA	1.94	0.49
15:A:1117:CLA:HMB1	15:A:1117:CLA:HBB1	1.94	0.49
5:C:34:CYS:SG	5:C:35:LYS:N	2.85	0.49
5:C:52:LYS:HE3	5:C:67:VAL:HB	1.93	0.49
8:F:82:TYR:CZ	8:F:93:PRO:HB2	2.47	0.49
1:3:179:ARG:HD3	1:3:186:ARG:NH1	2.26	0.49
4:B:438:ASN:HB3	4:B:613:TYR:HB3	1.94	0.49
4:B:684:PRO:O	4:B:686:ALA:N	2.43	0.49
1:3:123:PHE:CD2	1:3:124:VAL:HG22	2.47	0.49
3:A:611:GLN:HA	3:A:615:TRP:HB2	1.94	0.49
4:B:316:GLY:O	4:B:320:ILE:HG13	2.13	0.49
1:3:87:ARG:HH22	1:3:141:PHE:HD1	1.61	0.49
2:4:148:SER:O	2:4:150:ALA:N	2.45	0.49
3:A:189:ASN:HB3	3:A:192:SER:HB3	1.94	0.49
3:A:363:VAL:O	3:A:367:MET:HG2	2.13	0.49
4:B:105:THR:OG1	4:B:112:ASN:OD1	2.31	0.49
5:C:67:VAL:HG21	17:C:3002:SF4:S1	2.53	0.49
7:E:11:LEU:H	7:E:57:GLU:HA	1.78	0.49
8:F:105:ARG:HH21	10:J:38:TYR:H	1.61	0.49
4:B:227:ASN:OD1	4:B:228:TRP:N	2.46	0.49
4:B:329:HIS:HB3	4:B:387:HIS:O	2.12	0.49
4:B:437:HIS:HB2	15:B:1230:CLA:C1C	2.42	0.49
1:2:202:LYS:H	1:2:202:LYS:HD2	1.77	0.49
1:3:81:ALA:HB1	1:3:85:HIS:CE1	2.47	0.49
3:A:576:ARG:NH1	6:D:63:GLU:OE1	2.46	0.49
15:A:1126:CLA:H61	18:A:4011:BCR:H331	1.95	0.49
4:B:574:PHE:CE1	15:B:1226:CLA:HHD	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:715:TYR:CZ	15:B:1021:CLA:HED1	2.48	0.49
15:B:1201:CLA:HHC	15:B:1203:CLA:C2A	2.43	0.49
5:C:55:GLU:HB2	5:C:63:LEU:HD22	1.95	0.49
3:A:320:GLN:HA	3:A:323:GLU:HB2	1.94	0.48
11:K:28:LEU:HD22	11:K:43:GLY:HA2	1.93	0.48
3:A:222:LYS:HB3	3:A:249:LEU:HD12	1.95	0.48
4:B:87:LEU:HB3	4:B:113:ILE:HG21	1.95	0.48
4:B:558:ASP:CG	4:B:562:ARG:HH22	2.22	0.48
3:A:278:LEU:H	3:A:504:TYR:HE2	1.59	0.48
15:B:1205:CLA:C3A	15:B:1224:CLA:HBA1	2.43	0.48
7:E:33:LEU:HD23	7:E:33:LEU:H	1.77	0.48
1:3:86:CYS:HB2	1:3:184:GLU:HG3	1.95	0.48
1:3:121:ASN:O	1:3:125:GLN:NE2	2.44	0.48
3:A:701:HIS:CD2	3:A:706:VAL:HG13	2.48	0.48
4:B:209:ASN:HB2	4:B:212:MET:HB3	1.95	0.48
4:B:266:LEU:O	4:B:269:THR:OG1	2.19	0.48
14:O:68:PRO:HA	14:O:71:ILE:HB	1.95	0.48
1:2:234:ILE:HG12	1:3:123:PHE:CD1	2.49	0.48
15:A:1012:CLA:H52	18:A:4011:BCR:H362	1.95	0.48
4:B:371:THR:HB	15:B:1224:CLA:HMB2	1.94	0.48
1:2:180:ARG:HD3	1:2:181:GLU:HG3	1.95	0.48
1:2:234:ILE:HD12	1:3:121:ASN:HA	1.96	0.48
3:A:391:MET:HG3	3:A:599:LEU:CD1	2.40	0.48
3:A:586:ASP:HA	3:A:589:PHE:HB3	1.96	0.48
4:B:15:ASP:OD2	4:B:17:THR:OG1	2.31	0.48
1:3:112:LYS:O	1:3:114:GLN:N	2.47	0.48
4:B:594:TRP:HE1	4:B:621:TYR:HB2	1.78	0.48
7:E:16:PHE:HB3	8:F:181:THR:HB	1.94	0.48
3:A:175:PHE:HD1	3:A:179:LYS:HD2	1.79	0.48
3:A:437:LEU:HB3	3:A:544:LEU:HD12	1.95	0.48
6:D:54:ASP:N	6:D:54:ASP:OD1	2.43	0.48
12:L:19:THR:N	12:L:20:PRO:HD2	2.28	0.48
3:A:651:ALA:HB2	15:A:1011:CLA:HBC1	1.95	0.48
4:B:73:ASN:ND2	4:B:108:ASP:OD2	2.47	0.48
7:E:54:SER:OG	7:E:55:LEU:N	2.46	0.48
8:F:157:GLY:HA3	8:F:160:TRP:CZ2	2.49	0.48
1:3:119:LEU:HB2	1:3:122:GLN:HG3	1.96	0.48
15:B:1224:CLA:HBA2	15:B:1224:CLA:H3A	1.37	0.48
3:A:175:PHE:CD1	3:A:179:LYS:HD2	2.50	0.47
1:2:210:ARG:HD3	15:2:607:CLA:C2A	2.44	0.47
1:2:234:ILE:HG12	1:3:123:PHE:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1224:CLA:H61	15:B:1224:CLA:H41	1.45	0.47
1:2:123:GLN:HG3	1:2:124:GLU:HG3	1.97	0.47
3:A:309:ARG:NH1	3:A:317:SER:OG	2.47	0.47
4:B:558:ASP:HB3	4:B:565:THR:HG21	1.96	0.47
4:B:629:LEU:O	4:B:645:SER:HB3	2.14	0.47
3:A:71:SER:N	3:A:177:TYR:OH	2.48	0.47
4:B:315:LYS:N	4:B:315:LYS:HD2	2.29	0.47
3:A:364:ALA:HB2	3:A:390:HIS:HB2	1.96	0.47
11:K:35:GLN:HG3	11:K:38:ALA:HB3	1.96	0.47
1:2:234:ILE:O	1:2:236:GLN:NE2	2.47	0.47
1:3:115:LEU:HD11	15:3:610:CLA:C3B	2.45	0.47
3:A:425:ARG:HB3	3:A:429:HIS:CE1	2.49	0.47
4:B:332:LEU:HD13	15:B:1202:CLA:C4A	2.45	0.47
12:L:36:ILE:HG21	15:L:1502:CLA:C2A	2.45	0.47
1:2:158:LEU:HD22	15:2:612:CLA:HHC	1.97	0.47
1:2:202:LYS:H	1:2:202:LYS:CD	2.27	0.47
2:4:113:ALA:O	2:4:116:ALA:N	2.46	0.47
3:A:326:LYS:HZ3	3:A:332:GLU:HA	1.80	0.47
15:A:1122:CLA:HHB	18:A:4007:BCR:H321	1.96	0.47
4:B:410:LEU:HA	4:B:413:LYS:HG2	1.95	0.47
4:B:474:VAL:HG23	4:B:477:SER:HB2	1.96	0.47
4:B:540:ARG:O	4:B:549:LYS:N	2.48	0.47
5:C:15:THR:N	17:C:3003:SF4:S3	2.88	0.47
8:F:103:HIS:HB3	8:F:106:GLU:CD	2.40	0.47
8:F:121:ILE:HG12	8:F:160:TRP:CD1	2.50	0.47
1:3:73:PHE:HD2	1:3:76:GLU:HA	1.80	0.47
3:A:616:GLY:HA3	3:A:626:HIS:HA	1.96	0.47
4:B:31:PHE:HA	4:B:34:HIS:ND1	2.30	0.47
4:B:571:TRP:HZ3	4:B:704:ARG:HD2	1.80	0.47
3:A:421:ASN:OD1	3:A:428:ARG:NH2	2.48	0.47
1:2:162:ALA:O	1:2:166:ILE:HG13	2.14	0.46
1:2:181:GLU:HB2	1:2:182:PRO:HD3	1.97	0.46
1:2:236:GLN:HE21	1:3:124:VAL:HG21	1.80	0.46
3:A:667:LEU:HD13	4:B:440:VAL:HG22	1.97	0.46
15:A:1013:CLA:CHD	4:B:580:TRP:HE1	2.28	0.46
8:F:105:ARG:HH11	10:J:36:LEU:HD12	1.80	0.46
8:F:108:THR:OG1	8:F:109:ILE:N	2.48	0.46
3:A:191:GLU:HG3	3:A:318:ILE:HD12	1.97	0.46
3:A:408:TYR:HD2	18:A:4007:BCR:HC42	1.81	0.46
3:A:701:HIS:NE2	15:A:1139:CLA:HHB	2.30	0.46
3:A:734:ALA:HA	3:A:737:TRP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:92:TRP:CZ3	4:B:94:PRO:HD3	2.50	0.46
3:A:218:LEU:HD23	3:A:218:LEU:H	1.81	0.46
4:B:201:ARG:HA	4:B:240:HIS:HE1	1.80	0.46
7:E:25:VAL:HG22	7:E:39:ARG:HG3	1.97	0.46
3:A:137:THR:HG22	3:A:381:PRO:HB2	1.97	0.46
3:A:514:GLY:C	3:A:516:LYS:H	2.23	0.46
15:A:1106:CLA:C3D	15:A:1126:CLA:HBA1	2.45	0.46
4:B:307:ARG:O	4:B:309:PRO:HD3	2.15	0.46
7:E:62:LYS:C	7:E:64:GLU:H	2.22	0.46
8:F:63:PRO:HA	8:F:66:LEU:HD12	1.96	0.46
1:3:108:ASN:CG	1:3:113:LEU:HA	2.40	0.46
1:3:122:GLN:NE2	1:3:126:ASN:OD1	2.48	0.46
3:A:333:GLY:O	3:A:335:LYS:N	2.44	0.46
3:A:568:ARG:HG2	3:A:585:TRP:CG	2.50	0.46
3:A:650:GLN:NE2	15:A:1011:CLA:HHD	2.31	0.46
4:B:29:HIS:HB2	15:B:1226:CLA:HBA1	1.97	0.46
15:B:1226:CLA:H51	15:B:1226:CLA:H8	1.43	0.46
14:O:67:ASN:HB2	14:O:68:PRO:HD3	1.98	0.46
1:3:81:ALA:O	1:3:85:HIS:ND1	2.48	0.46
3:A:218:LEU:HB3	3:A:250:TYR:HE2	1.81	0.46
15:A:1106:CLA:H3A	15:A:1106:CLA:HBA2	1.44	0.46
12:L:3:ASP:OD2	12:L:7:PRO:HD3	2.16	0.46
14:O:61:GLY:HA2	14:O:64:TYR:CD2	2.50	0.46
3:A:439:TRP:CE2	15:A:1130:CLA:HAB	2.51	0.46
3:A:596:TYR:HE1	3:A:732:GLY:O	1.99	0.46
3:A:694:ILE:HD11	3:A:714:ALA:HB2	1.96	0.46
3:A:704:LEU:HD21	8:F:168:TYR:CD1	2.51	0.46
4:B:19:ARG:HA	4:B:22:TRP:HD1	1.80	0.46
4:B:383:GLY:O	4:B:387:HIS:ND1	2.41	0.46
4:B:690:ARG:HD2	6:D:20:ARG:HH11	1.80	0.46
2:4:106:GLU:HG2	2:4:229:MET:CE	2.45	0.46
15:A:1107:CLA:H52	15:A:1107:CLA:H8	1.67	0.46
15:A:1126:CLA:H62	18:A:4011:BCR:H343	1.97	0.46
16:A:2001:PQN:H292	16:A:2001:PQN:H262	1.76	0.46
4:B:346:VAL:O	4:B:350:MET:HG2	2.16	0.46
1:2:145:ASN:O	1:2:148:VAL:HG23	2.16	0.46
1:3:73:PHE:HB2	1:3:76:GLU:HA	1.98	0.46
3:A:595:MET:HG2	3:A:599:LEU:HD23	1.97	0.46
8:F:150:ALA:HA	8:F:153:TYR:CD1	2.51	0.46
3:A:392:TRP:CD1	15:A:1126:CLA:HAB	2.51	0.45
8:F:88:GLY:H	8:F:93:PRO:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:SER:HB2	9:I:6:LEU:HB2	1.97	0.45
2:4:218:ARG:HD2	15:4:615:CLA:C3B	2.46	0.45
3:A:365:HIS:HA	3:A:368:TYR:CE1	2.51	0.45
6:D:28:TYR:HB2	6:D:59:LEU:HB2	1.97	0.45
6:D:98:LYS:HD2	6:D:106:VAL:HG21	1.97	0.45
1:3:119:LEU:HB2	1:3:122:GLN:CG	2.45	0.45
3:A:442:ILE:HA	15:B:1023:CLA:CGA	2.45	0.45
15:A:1126:CLA:O1D	15:A:1127:CLA:HHD	2.16	0.45
4:B:119:TYR:HE1	4:B:369:LEU:HB2	1.81	0.45
3:A:650:GLN:HE21	15:A:1011:CLA:HAC1	1.80	0.45
15:B:1224:CLA:O1D	15:B:1225:CLA:HMA1	2.17	0.45
5:C:52:LYS:HE2	5:C:52:LYS:HA	1.98	0.45
7:E:16:PHE:O	7:E:18:TYR:N	2.49	0.45
8:F:34:CYS:HB3	8:F:40:PHE:CD2	2.51	0.45
3:A:83:TRP:HE3	3:A:84:LEU:HD12	1.81	0.45
3:A:428:ARG:HD2	6:D:12:LEU:O	2.16	0.45
15:A:1013:CLA:H93	18:A:4011:BCR:H373	1.98	0.45
4:B:185:SER:HA	4:B:275:HIS:ND1	2.23	0.45
6:D:96:HIS:HE2	6:D:101:VAL:HA	1.81	0.45
8:F:130:LYS:HA	8:F:130:LYS:HE2	1.99	0.45
2:4:173:SER:C	2:4:175:MET:H	2.25	0.45
3:A:265:TRP:CD1	11:K:52:LEU:HD21	2.52	0.45
3:A:459:ARG:NH2	3:A:634:GLN:OE1	2.49	0.45
15:A:1126:CLA:H3A	15:A:1126:CLA:HBA2	1.49	0.45
3:A:425:ARG:HG3	3:A:428:ARG:HH21	1.81	0.45
3:A:490:ALA:HB3	3:A:491:PRO:HD3	1.99	0.45
3:A:559:ILE:HG22	3:A:576:ARG:HH12	1.82	0.45
3:A:713:ARG:NH2	7:E:43:VAL:O	2.50	0.45
1:3:191:ALA:HB1	1:3:195:PHE:CE2	2.52	0.45
3:A:12:VAL:HG12	3:A:183:LYS:HD3	1.99	0.45
3:A:334:HIS:N	3:A:420:ASN:HD21	2.14	0.45
3:A:484:GLN:O	3:A:488:THR:HG23	2.16	0.45
3:A:677:ALA:C	15:A:1013:CLA:HAB	2.42	0.45
15:A:1012:CLA:HAB	4:B:580:TRP:HZ3	1.82	0.45
18:A:4007:BCR:H16C	18:A:4007:BCR:H19C	1.81	0.45
4:B:181:PHE:HB2	4:B:282:PHE:CZ	2.52	0.45
4:B:453:ILE:HG12	4:B:515:PHE:CE2	2.52	0.45
8:F:162:LEU:O	8:F:166:GLN:HG3	2.16	0.45
1:2:133:ALA:O	1:2:137:LEU:N	2.50	0.45
15:B:1229:CLA:H2	8:F:123:TRP:NE1	2.32	0.45
3:A:608:TRP:HA	3:A:611:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:303:LEU:HD12	4:B:304:GLU:HB2	1.98	0.45
4:B:372:HIS:O	4:B:376:ILE:HG12	2.17	0.45
4:B:378:GLY:O	4:B:382:VAL:HG23	2.17	0.45
1:3:110:LYS:HG2	1:3:111:SER:H	1.81	0.44
1:3:201:GLN:OE1	1:3:201:GLN:N	2.38	0.44
3:A:293:HIS:O	3:A:297:ILE:HG12	2.17	0.44
3:A:333:GLY:C	3:A:335:LYS:H	2.24	0.44
3:A:389:HIS:CE1	3:A:393:ILE:HD11	2.52	0.44
3:A:427:ILE:HA	3:A:430:ARG:HB3	2.00	0.44
4:B:116:SER:HA	15:B:1207:CLA:C3A	2.47	0.44
4:B:151:GLY:O	4:B:155:ILE:HG12	2.16	0.44
15:B:1232:CLA:H51	15:B:1232:CLA:H11	1.77	0.44
5:C:23:LEU:HA	6:D:66:LEU:HG	1.99	0.44
1:2:234:ILE:HD12	1:3:121:ASN:CB	2.48	0.44
3:A:331:GLY:HA3	3:A:425:ARG:HH21	1.82	0.44
4:B:178:ALA:HA	4:B:282:PHE:CD2	2.51	0.44
6:D:93:GLN:NE2	6:D:95:LEU:O	2.35	0.44
1:3:119:LEU:HD12	1:3:125:GLN:NE2	2.32	0.44
3:A:454:HIS:O	3:A:458:MET:HG3	2.17	0.44
15:A:1130:CLA:CGA	12:L:22:ASN:HA	2.47	0.44
4:B:234:SER:OG	4:B:249:GLY:O	2.35	0.44
5:C:66:ARG:HA	5:C:66:ARG:HD2	1.82	0.44
2:4:146:VAL:HG12	2:4:147:LYS:H	1.82	0.44
3:A:406:ALA:HB1	3:A:584:ALA:HB1	2.00	0.44
3:A:593:PHE:CE1	3:A:725:VAL:HG23	2.52	0.44
3:A:651:ALA:HA	3:A:654:VAL:HG12	1.99	0.44
18:A:4017:BCR:H14C	15:B:1239:CLA:C3C	2.48	0.44
4:B:305:ALA:O	4:B:308:PRO:HD2	2.18	0.44
15:B:1021:CLA:HBA2	15:B:1021:CLA:H3A	1.67	0.44
15:B:1237:CLA:H61	15:B:1237:CLA:H41	1.66	0.44
5:C:26:LEU:HD23	17:C:3002:SF4:S3	2.57	0.44
5:C:53:ARG:HG2	17:C:3002:SF4:S4	2.58	0.44
15:J:1302:CLA:HBD	15:J:1302:CLA:HBA1	1.99	0.44
12:L:6:LYS:O	12:L:7:PRO:C	2.59	0.44
1:3:94:LEU:HD22	15:3:606:CLA:HHC	2.00	0.44
1:3:139:TRP:HA	1:3:143:VAL:HG23	2.00	0.44
3:A:371:PRO:HG2	3:A:377:ALA:HB2	1.99	0.44
4:B:106:ARG:NE	4:B:115:TYR:OH	2.49	0.44
12:L:24:SER:N	12:L:27:THR:HB	2.31	0.44
1:3:138:ALA:HB1	1:3:142:ILE:HD12	1.99	0.44
3:A:461:LEU:O	4:B:97:GLY:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:698:VAL:HA	3:A:701:HIS:HB2	1.99	0.44
15:B:1229:CLA:CMB	18:B:4005:BCR:H21C	2.48	0.44
1:3:198:PHE:N	1:3:198:PHE:CD2	2.86	0.44
2:4:228:ALA:O	2:4:232:PHE:HD2	2.01	0.44
3:A:701:HIS:HB3	3:A:707:ALA:HA	1.99	0.44
15:A:1112:CLA:HHD	18:A:4002:BCR:H332	1.99	0.44
4:B:420:LEU:HD13	4:B:530:LEU:HA	2.00	0.44
4:B:441:VAL:HG11	4:B:450:GLN:HA	2.00	0.44
8:F:134:GLU:HB2	8:F:135:THR:H	1.57	0.44
1:3:100:GLU:HB2	1:3:106:PHE:HD1	1.82	0.44
2:4:113:ALA:HB1	2:4:232:PHE:CD2	2.53	0.44
3:A:355:MET:HG3	15:A:1123:CLA:HHD	1.99	0.44
18:A:4011:BCR:H372	4:B:436:VAL:HG21	2.00	0.44
4:B:71:GLN:HG2	4:B:90:ALA:HB2	2.00	0.44
4:B:678:TRP:HE1	6:D:15:THR:HA	1.83	0.44
6:D:32:TRP:O	6:D:54:ASP:HA	2.18	0.44
12:L:41:VAL:HG21	12:L:45:LEU:HD22	1.98	0.44
3:A:17:VAL:HG21	3:A:67:ARG:NH1	2.32	0.44
3:A:112:GLN:O	3:A:134:ILE:N	2.50	0.44
3:A:693:LEU:HA	4:B:534:LYS:NZ	2.32	0.44
3:A:704:LEU:HD23	8:F:172:GLN:OE1	2.17	0.44
4:B:197:ILE:HG22	4:B:198:PRO:HD3	2.00	0.44
4:B:622:LEU:HA	15:B:1021:CLA:HMD2	2.00	0.44
18:B:4005:BCR:H351	18:B:4005:BCR:H15C	1.55	0.44
10:J:34:ASP:N	10:J:34:ASP:OD1	2.50	0.44
12:L:114:TRP:O	12:L:117:LEU:HG	2.18	0.44
3:A:218:LEU:HG	3:A:219:PRO:HD3	2.00	0.43
4:B:73:ASN:HD22	4:B:108:ASP:HB2	1.83	0.43
4:B:375:TYR:CE1	4:B:585:ILE:HG23	2.53	0.43
7:E:15:SER:HB2	7:E:17:TRP:CD1	2.53	0.43
1:3:122:GLN:HG2	1:3:125:GLN:HE22	1.83	0.43
3:A:470:ASP:OD1	3:A:471:THR:N	2.50	0.43
4:B:458:ALA:O	4:B:462:GLN:NE2	2.51	0.43
12:L:62:PHE:HB2	12:L:78:GLY:HA2	2.00	0.43
3:A:386:LEU:O	3:A:390:HIS:ND1	2.50	0.43
3:A:388:THR:HG21	3:A:740:PHE:CE2	2.52	0.43
15:A:1105:CLA:HBA2	15:A:1105:CLA:H3A	1.40	0.43
3:A:413:TYR:OH	3:A:424:ASP:OD1	2.35	0.43
3:A:694:ILE:H	3:A:694:ILE:HG12	1.32	0.43
4:B:612:THR:HG21	8:F:92:LEU:HD21	2.00	0.43
1:3:144:GLY:HA2	1:3:148:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:198:PHE:N	1:3:198:PHE:HD2	2.16	0.43
4:B:163:LEU:HD11	4:B:167:LYS:HE3	1.99	0.43
4:B:181:PHE:O	4:B:185:SER:OG	2.18	0.43
5:C:22:PRO:HB2	6:D:63:GLU:HG3	2.01	0.43
9:I:16:LEU:C	9:I:19:PRO:HD2	2.43	0.43
3:A:259:PRO:HG2	3:A:268:TYR:CE2	2.53	0.43
3:A:263:LEU:HD21	11:K:48:VAL:HG22	2.00	0.43
3:A:422:VAL:HG13	15:A:1129:CLA:C3A	2.49	0.43
3:A:709:ALA:HB2	8:F:133:LYS:HD2	1.99	0.43
4:B:439:ASP:OD1	4:B:613:TYR:HB2	2.19	0.43
4:B:609:GLU:HA	8:F:92:LEU:HD22	2.00	0.43
14:O:60:ASP:C	14:O:63:PRO:HD2	2.43	0.43
1:3:145:LEU:H	1:3:146:PRO:CD	2.29	0.43
3:A:322:LEU:HB3	3:A:334:HIS:O	2.19	0.43
3:A:439:TRP:CZ2	15:A:1130:CLA:HAB	2.54	0.43
15:A:1105:CLA:HBB1	15:A:1105:CLA:H92	2.00	0.43
15:A:1106:CLA:H42	18:A:4011:BCR:H321	2.00	0.43
5:C:8:TYR:HB2	5:C:64:SER:HA	2.01	0.43
8:F:160:TRP:O	8:F:161:PRO:C	2.62	0.43
12:L:42:SER:CB	12:L:43:PRO:HD2	2.48	0.43
4:B:577:ALA:O	4:B:581:MET:HG2	2.18	0.43
15:B:1212:CLA:C2B	18:I:4018:BCR:H21C	2.48	0.43
15:B:1230:CLA:C2	18:B:4005:BCR:H291	2.48	0.43
3:A:535:HIS:O	3:A:539:ILE:HG12	2.19	0.43
3:A:462:GLY:HA3	4:B:97:GLY:HA3	2.00	0.43
3:A:482:TRP:CH2	3:A:486:ILE:HD11	2.54	0.43
3:A:701:HIS:HB3	3:A:707:ALA:CA	2.48	0.43
18:A:4017:BCR:HC21	4:B:646:TRP:CZ3	2.54	0.43
4:B:123:TYR:CE2	4:B:357:ALA:HB3	2.54	0.43
4:B:438:ASN:HA	4:B:450:GLN:HG3	2.01	0.43
15:B:1232:CLA:H152	15:B:1232:CLA:H112	1.50	0.43
15:B:1236:CLA:HHC	15:B:1236:CLA:HBB1	2.00	0.43
14:O:67:ASN:O	14:O:71:ILE:HG12	2.19	0.43
3:A:209:TRP:HD1	3:A:294:HIS:ND1	2.16	0.42
3:A:278:LEU:HD21	3:A:371:PRO:HD2	2.01	0.42
3:A:279:SER:OG	3:A:282:THR:OG1	2.32	0.42
3:A:602:VAL:HG13	15:A:1135:CLA:HHC	2.01	0.42
4:B:188:TRP:CH2	4:B:192:LEU:HD22	2.54	0.42
4:B:307:ARG:HB3	4:B:308:PRO:HD3	2.01	0.42
4:B:495:TRP:O	4:B:499:VAL:HG23	2.18	0.42
8:F:82:TYR:O	8:F:82:TYR:HD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:203:ARG:HD2	1:2:206:ALA:HB3	2.01	0.42
1:2:235:GLU:OE1	1:2:235:GLU:N	2.39	0.42
1:3:110:LYS:NZ	1:3:208:GLY:O	2.52	0.42
1:3:141:PHE:N	1:3:141:PHE:CD2	2.85	0.42
3:A:380:TYR:HB3	3:A:744:ILE:HD11	1.99	0.42
4:B:29:HIS:C	15:B:1226:CLA:HAA2	2.44	0.42
4:B:219:GLY:O	4:B:221:GLN:N	2.47	0.42
4:B:420:LEU:HB3	4:B:530:LEU:HB2	2.01	0.42
4:B:644:TRP:CH2	4:B:724:ILE:HG13	2.54	0.42
8:F:145:LEU:HD21	10:J:9:THR:HG22	2.01	0.42
14:O:53:LEU:HD12	14:O:55:MET:HB2	2.00	0.42
1:2:98:SER:OG	3:A:179:LYS:NZ	2.45	0.42
3:A:469:SER:O	3:A:473:ILE:HG12	2.20	0.42
3:A:734:ALA:HA	18:A:4011:BCR:HC42	2.01	0.42
6:D:32:TRP:CD1	6:D:34:SER:HB3	2.52	0.42
1:2:234:ILE:HG21	1:3:123:PHE:N	2.35	0.42
2:4:112:VAL:HG21	15:4:612:CLA:C3A	2.49	0.42
3:A:216:VAL:C	3:A:219:PRO:HD2	2.45	0.42
3:A:336:GLY:HA3	3:A:419:PHE:O	2.19	0.42
3:A:576:ARG:HD3	5:C:49:VAL:HB	2.00	0.42
4:B:465:SER:HA	4:B:495:TRP:HE1	1.84	0.42
8:F:96:ILE:HB	8:F:103:HIS:CB	2.49	0.42
8:F:108:THR:O	8:F:112:LEU:HB3	2.19	0.42
1:2:141:PRO:HA	1:2:144:HIS:ND1	2.35	0.42
1:3:75:LEU:HD23	1:3:75:LEU:HA	1.85	0.42
1:3:139:TRP:O	1:3:143:VAL:HB	2.20	0.42
2:4:229:MET:HE2	2:4:229:MET:HB2	1.89	0.42
3:A:175:PHE:C	3:A:177:TYR:H	2.27	0.42
3:A:560:PRO:HG3	6:D:64:GLN:HA	2.00	0.42
15:A:1012:CLA:H52	15:A:1012:CLA:H12	1.80	0.42
4:B:414:GLU:H	4:B:414:GLU:CD	2.27	0.42
4:B:432:LEU:O	4:B:436:VAL:HG23	2.20	0.42
4:B:575:TYR:CE1	4:B:704:ARG:HB3	2.54	0.42
15:B:1225:CLA:HBA2	15:B:1225:CLA:H3A	1.52	0.42
14:O:98:GLN:OE1	14:O:105:GLN:NE2	2.52	0.42
2:4:241:LEU:O	2:4:243:GLY:N	2.50	0.42
3:A:717:ILE:HD11	4:B:564:GLY:HA3	2.01	0.42
4:B:656:ALA:HB3	15:B:1023:CLA:HBB2	2.02	0.42
1:3:179:ARG:HE	1:3:179:ARG:HB2	1.69	0.42
3:A:225:ASP:HB3	3:A:281:VAL:HG11	2.01	0.42
3:A:439:TRP:CH2	15:A:1130:CLA:HAB	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:640:ASN:O	3:A:644:ARG:N	2.52	0.42
4:B:375:TYR:HB3	15:B:1224:CLA:HMC2	2.01	0.42
6:D:9:PRO:HD3	6:D:55:ASN:HB3	2.00	0.42
9:I:6:LEU:O	9:I:9:ILE:HG12	2.19	0.42
15:A:1131:CLA:HHB	18:I:4018:BCR:H292	2.02	0.42
4:B:189:THR:O	4:B:193:VAL:HG22	2.20	0.42
4:B:271:MET:HA	4:B:274:HIS:CD2	2.55	0.42
4:B:674:GLU:CD	6:D:61:ARG:HH12	2.27	0.42
5:C:61:ASP:HA	7:E:44:ASN:ND2	2.35	0.42
14:O:64:TYR:O	14:O:68:PRO:HD2	2.19	0.42
1:2:163:TRP:HA	1:2:166:ILE:HB	2.01	0.42
3:A:595:MET:HE3	3:A:595:MET:HB3	1.96	0.42
15:A:1126:CLA:H62	15:A:1126:CLA:H41	1.73	0.42
4:B:699:SER:O	4:B:703:ALA:N	2.44	0.42
5:C:15:THR:O	5:C:19:ARG:HG2	2.20	0.42
12:L:14:VAL:HG23	12:L:15:GLY:H	1.84	0.42
1:3:181:GLN:HG2	15:3:601:CLA:C3A	2.50	0.42
2:4:124:GLU:CD	2:4:127:GLN:HE21	2.28	0.42
3:A:632:PHE:CG	3:A:636:ALA:HB2	2.55	0.42
4:B:157:PRO:C	4:B:159:PHE:H	2.27	0.42
5:C:20:ALA:O	5:C:53:ARG:HD2	2.19	0.42
7:E:17:TRP:O	7:E:19:ASN:N	2.53	0.42
12:L:33:GLN:HA	12:L:39:ARG:NH1	2.35	0.42
1:3:127:GLY:HA3	1:3:130:GLN:HB3	2.01	0.41
2:4:102:LEU:HB3	8:F:149:MET:HE3	2.02	0.41
3:A:202:LEU:HB3	3:A:301:PHE:CD2	2.55	0.41
15:A:1013:CLA:H51	4:B:429:PHE:CE1	2.55	0.41
4:B:274:HIS:O	4:B:278:ILE:HG12	2.20	0.41
1:2:109:HIS:ND1	1:2:216:MET:SD	2.89	0.41
2:4:245:MET:N	2:4:246:PRO:CD	2.81	0.41
15:A:1117:CLA:C4A	15:A:1117:CLA:H12	2.50	0.41
9:I:32:LYS:HB3	9:I:32:LYS:HE3	1.88	0.41
1:2:235:GLU:O	1:3:125:GLN:HB3	2.21	0.41
1:3:118:ASP:O	1:3:122:GLN:HG3	2.20	0.41
3:A:567:PHE:CE2	3:A:585:TRP:HB2	2.56	0.41
3:A:610:MET:HB3	3:A:615:TRP:CE2	2.55	0.41
4:B:216:HIS:CE1	4:B:251:ALA:HA	2.55	0.41
4:B:332:LEU:HD23	4:B:387:HIS:CD2	2.55	0.41
15:B:1229:CLA:HMB1	18:B:4005:BCR:H21C	2.02	0.41
14:O:64:TYR:HB2	14:O:65:PRO:HD3	2.03	0.41
1:2:203:ARG:HD2	1:2:203:ARG:HA	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:13:VAL:HA	3:A:182:PRO:HA	2.03	0.41
3:A:439:TRP:CD2	15:A:1130:CLA:HAB	2.55	0.41
4:B:302:ILE:HA	4:B:308:PRO:HG2	2.02	0.41
4:B:392:PHE:CZ	4:B:410:LEU:HD22	2.55	0.41
4:B:461:ILE:O	4:B:464:THR:OG1	2.33	0.41
8:F:153:TYR:CD2	8:F:153:TYR:C	2.98	0.41
12:L:54:HIS:HA	12:L:57:PHE:CE1	2.55	0.41
1:2:167:VAL:C	1:2:170:PRO:HD2	2.46	0.41
2:4:117:CYS:HB3	2:4:232:PHE:CE1	2.55	0.41
15:A:1117:CLA:H12	15:A:1117:CLA:CHB	2.51	0.41
18:A:4017:BCR:H322	15:B:1206:CLA:C4B	2.50	0.41
2:4:124:GLU:HA	2:4:127:GLN:HG2	2.01	0.41
3:A:420:ASN:ND2	3:A:422:VAL:H	2.18	0.41
3:A:576:ARG:HG3	5:C:78:GLY:HA3	2.03	0.41
3:A:608:TRP:HZ3	3:A:743:ARG:CZ	2.33	0.41
6:D:108:LYS:O	6:D:110:ARG:NH1	2.54	0.41
11:K:32:ASP:OD1	11:K:32:ASP:N	2.54	0.41
3:A:246:MET:HE3	3:A:246:MET:HB3	1.89	0.41
3:A:674:PHE:HB2	15:A:1012:CLA:O1A	2.21	0.41
3:A:693:LEU:HA	4:B:534:LYS:HZ1	1.84	0.41
15:A:1106:CLA:H43	15:A:1126:CLA:C2D	2.51	0.41
4:B:23:TYR:O	4:B:27:THR:N	2.46	0.41
4:B:168:ASN:HB2	4:B:171:SER:HB3	2.03	0.41
4:B:548:LYS:HG3	4:B:555:PHE:HZ	1.85	0.41
1:3:180:MET:HB3	1:3:180:MET:HE2	1.80	0.41
3:A:409:MET:O	3:A:554:ARG:HD3	2.21	0.41
4:B:455:PRO:HB3	4:B:515:PHE:HB2	2.03	0.41
6:D:40:PHE:CD1	6:D:50:MET:HB2	2.55	0.41
3:A:75:GLY:O	3:A:79:ILE:HG12	2.21	0.41
3:A:152:GLU:HA	3:A:155:LEU:HD23	2.03	0.41
3:A:332:GLU:H	3:A:421:ASN:HD22	1.67	0.41
18:A:4017:BCR:H281	4:B:669:TRP:CZ3	2.56	0.41
4:B:558:ASP:CG	5:C:66:ARG:HH22	2.28	0.41
7:E:37:LEU:H	7:E:37:LEU:HD23	1.86	0.41
12:L:83:ILE:HD13	12:L:86:ILE:HD12	2.03	0.41
14:O:126:ILE:HA	14:O:129:HIS:ND1	2.35	0.41
1:2:234:ILE:HD12	1:3:121:ASN:CA	2.50	0.41
1:3:141:PHE:N	1:3:141:PHE:HD2	2.18	0.41
3:A:392:TRP:NE1	3:A:603:ILE:HD13	2.28	0.41
18:A:4011:BCR:H292	15:B:1229:CLA:CMB	2.51	0.41
18:A:4017:BCR:H333	15:B:1224:CLA:H62	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:374:GLN:HG3	4:B:585:ILE:HD11	2.01	0.41
6:D:120:ILE:HD11	6:D:122:LYS:NZ	2.35	0.41
8:F:105:ARG:HH21	10:J:38:TYR:N	2.19	0.41
3:A:733:ILE:HG22	18:A:4011:BCR:HC31	2.02	0.40
18:A:4017:BCR:HC42	4:B:647:MET:HE2	2.03	0.40
4:B:665:TRP:HB3	4:B:666:ARG:H	1.67	0.40
16:B:2002:PQN:H262	16:B:2002:PQN:H292	1.81	0.40
8:F:133:LYS:HE3	8:F:133:LYS:HB3	1.58	0.40
1:2:154:GLN:O	1:2:158:LEU:HG	2.21	0.40
2:4:119:HIS:NE2	15:4:606:CLA:HHC	2.36	0.40
3:A:259:PRO:HG2	3:A:268:TYR:CZ	2.56	0.40
3:A:318:ILE:HD12	3:A:318:ILE:H	1.85	0.40
3:A:467:MET:HG3	12:L:69:ARG:NH2	2.37	0.40
3:A:650:GLN:HB3	3:A:743:ARG:HH22	1.87	0.40
3:A:743:ARG:O	3:A:747:VAL:HG22	2.22	0.40
3:A:744:ILE:HA	3:A:744:ILE:HD12	1.88	0.40
15:A:1107:CLA:HBA1	15:A:1107:CLA:H12	1.85	0.40
4:B:92:TRP:CZ3	9:I:12:PRO:HG3	2.56	0.40
4:B:575:TYR:OH	4:B:662:LEU:HG	2.21	0.40
8:F:105:ARG:CD	10:J:36:LEU:HB2	2.51	0.40
9:I:6:LEU:CB	9:I:7:PRO:HD3	2.50	0.40
2:4:135:PRO:HD2	2:4:140:PRO:HG3	2.02	0.40
3:A:20:THR:HG21	3:A:174:TRP:HZ2	1.86	0.40
3:A:334:HIS:H	3:A:420:ASN:HD21	1.70	0.40
4:B:17:THR:C	4:B:693:ASP:HB3	2.46	0.40
4:B:23:TYR:O	4:B:27:THR:OG1	2.35	0.40
4:B:188:TRP:CZ2	4:B:192:LEU:HD13	2.56	0.40
4:B:690:ARG:NH1	6:D:20:ARG:HG3	2.36	0.40
12:L:20:PRO:C	12:L:22:ASN:H	2.30	0.40
2:4:129:PRO:HB2	2:4:130:PHE:CD2	2.56	0.40
3:A:454:HIS:NE2	3:A:458:MET:SD	2.95	0.40
4:B:131:VAL:HG13	4:B:134:TYR:OH	2.21	0.40
4:B:132:GLU:HG2	4:B:133:LEU:N	2.36	0.40
11:K:50:ILE:O	11:K:54:LEU:N	2.49	0.40
12:L:33:GLN:HB3	15:L:1501:CLA:C2B	2.51	0.40
1:2:212:GLY:O	1:2:216:MET:HG2	2.21	0.40
1:3:77:TRP:HA	1:3:79:ARG:NE	2.36	0.40
3:A:552:TYR:O	3:A:562:LYS:NZ	2.36	0.40
16:A:2001:PQN:H162	16:A:2001:PQN:H141	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	2	142/222 (64%)	122 (86%)	17 (12%)	3 (2%)	5	32
1	3	148/222 (67%)	124 (84%)	18 (12%)	6 (4%)	2	21
2	4	112/214 (52%)	96 (86%)	7 (6%)	9 (8%)	1	12
3	A	738/740 (100%)	645 (87%)	82 (11%)	11 (2%)	8	38
4	B	723/725 (100%)	630 (87%)	86 (12%)	7 (1%)	12	45
5	C	78/80 (98%)	69 (88%)	8 (10%)	1 (1%)	9	41
6	D	122/124 (98%)	107 (88%)	12 (10%)	3 (2%)	4	29
7	E	67/69 (97%)	52 (78%)	9 (13%)	6 (9%)	0	10
8	F	151/155 (97%)	132 (87%)	14 (9%)	5 (3%)	3	24
9	I	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	24
10	J	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	27
11	K	45/47 (96%)	36 (80%)	8 (18%)	1 (2%)	5	31
12	L	138/140 (99%)	110 (80%)	20 (14%)	8 (6%)	1	16
13	M	27/29 (93%)	25 (93%)	1 (4%)	1 (4%)	2	22
14	O	96/98 (98%)	84 (88%)	10 (10%)	2 (2%)	5	32
All	All	2653/2935 (90%)	2293 (86%)	295 (11%)	65 (2%)	4	29

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	113	LEU
1	3	145	LEU
1	3	172	VAL
3	A	477	PRO
7	E	56	ASP
7	E	63	VAL
8	F	161	PRO
9	I	6	LEU

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Mol	Chain	Res	Type
10	J	36	LEU
12	L	7	PRO
12	L	12	PRO
12	L	21	ILE
12	L	43	PRO
1	3	72	VAL
2	4	135	PRO
2	4	146	VAL
2	4	149	GLY
3	A	522	ILE
3	A	570	PRO
4	B	556	PRO
6	D	75	GLN
6	D	88	PRO
7	E	17	TRP
7	E	18	TYR
8	F	110	PRO
11	K	59	VAL
12	L	20	PRO
12	L	48	LEU
1	3	119	LEU
3	A	475	LEU
4	B	309	PRO
4	B	312	ARG
7	E	35	PRO
7	E	57	GLU
8	F	154	MET
13	M	27	GLN
14	O	146	TYR
1	2	129	ASP
1	2	201	TRP
1	2	207	GLY
1	3	117	PRO
3	A	16	ASP
3	A	319	LYS
8	F	108	THR
12	L	19	THR
2	4	128	PHE
2	4	129	PRO
2	4	245	MET
3	A	258	VAL
3	A	334	HIS

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Mol	Chain	Res	Type
3	A	493	ASN
4	B	177	LEU
4	B	320	ILE
14	O	104	ILE
2	4	130	PHE
2	4	173	SER
5	C	22	PRO
3	A	181	ALA
4	B	512	PRO
12	L	6	LYS
4	B	179	GLY
8	F	109	ILE
2	4	139	GLY
6	D	46	GLY
3	A	417	VAL

5.3.2 Protein sidechains ⓘ

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	2	109/178 (61%)	105 (96%)	4 (4%)	30	52
1	3	121/178 (68%)	94 (78%)	27 (22%)	1	6
2	4	93/175 (53%)	89 (96%)	4 (4%)	26	48
3	A	597/597 (100%)	585 (98%)	12 (2%)	48	66
4	B	592/593 (100%)	576 (97%)	16 (3%)	39	60
5	C	66/66 (100%)	65 (98%)	1 (2%)	57	70
6	D	104/104 (100%)	101 (97%)	3 (3%)	37	58
7	E	66/66 (100%)	65 (98%)	1 (2%)	57	70
8	F	135/137 (98%)	119 (88%)	16 (12%)	5	21
9	I	27/27 (100%)	25 (93%)	2 (7%)	13	36
10	J	34/34 (100%)	33 (97%)	1 (3%)	37	58
11	K	35/36 (97%)	34 (97%)	1 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	113/113 (100%)	110 (97%)	3 (3%)	39	60
13	M	22/23 (96%)	22 (100%)	0	100	100
14	O	77/77 (100%)	75 (97%)	2 (3%)	40	61
All	All	2191/2404 (91%)	2098 (96%)	93 (4%)	26	49

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	128	PHE
1	2	180	ARG
1	2	202	LYS
1	2	204	MET
1	3	64	PHE
1	3	65	ASP
1	3	71	GLU
1	3	73	PHE
1	3	79	ARG
1	3	80	GLU
1	3	82	GLU
1	3	85	HIS
1	3	107	TYR
1	3	113	LEU
1	3	116	SER
1	3	119	LEU
1	3	120	HIS
1	3	122	GLN
1	3	123	PHE
1	3	124	VAL
1	3	125	GLN
1	3	126	ASN
1	3	130	GLN
1	3	134	LEU
1	3	177	TRP
1	3	184	GLU
1	3	185	LEU
1	3	187	ASN
1	3	189	ARG
1	3	198	PHE
1	3	207	GLN
2	4	99	VAL
2	4	102	LEU

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Mol	Chain	Res	Type
2	4	146	VAL
2	4	171	LEU
3	A	71	SER
3	A	77	LEU
3	A	84	LEU
3	A	220	ILE
3	A	249	LEU
3	A	262	THR
3	A	337	LEU
3	A	361	ILE
3	A	559	ILE
3	A	631	ASN
3	A	694	ILE
3	A	704	LEU
4	B	133	LEU
4	B	177	LEU
4	B	220	LEU
4	B	250	THR
4	B	252	ILE
4	B	273	HIS
4	B	291	THR
4	B	369	LEU
4	B	412	HIS
4	B	413	LYS
4	B	435	TYR
4	B	456	ILE
4	B	516	LEU
4	B	532	LEU
4	B	543	LYS
4	B	576	LEU
5	C	35	LYS
6	D	95	LEU
6	D	101	VAL
6	D	120	ILE
7	E	58	LEU
8	F	68	LEU
8	F	95	LEU
8	F	105	ARG
8	F	106	GLU
8	F	121	ILE
8	F	128	TYR
8	F	133	LYS

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Mol	Chain	Res	Type
8	F	134	GLU
8	F	136	LYS
8	F	143	ILE
8	F	149	MET
8	F	151	LEU
8	F	153	TYR
8	F	172	GLN
8	F	179	GLU
8	F	180	ILE
9	I	6	LEU
9	I	10	LEU
10	J	28	LEU
11	K	54	LEU
12	L	14	VAL
12	L	34	LEU
12	L	89	LEU
14	O	53	LEU
14	O	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	179	ASN
1	2	236	GLN
1	3	122	GLN
1	3	126	ASN
1	3	130	GLN
3	A	213	GLN
3	A	215	HIS
3	A	255	GLN
3	A	383	GLN
3	A	420	ASN
3	A	485	GLN
4	B	44	GLN
4	B	175	HIS
4	B	203	GLN
4	B	450	GLN
4	B	462	GLN
4	B	603	ASN
6	D	71	GLN
6	D	75	GLN
6	D	123	ASN

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Mol	Chain	Res	Type
12	L	116	GLN
14	O	67	ASN
14	O	105	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

147 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	$\# Z > 2$
15	CLA	B	1205	-	24,32,73	3.28	11 (45%)	31,54,113	2.52	11 (35%)
15	CLA	B	1225	-	54,58,73	1.52	6 (11%)	64,95,113	2.04	19 (29%)
15	CLA	O	1603	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	4	604	-	24,32,73	3.32	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	4	615	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	A	1117	-	59,63,73	1.46	7 (11%)	70,101,113	2.01	17 (24%)
15	CLA	B	1201	-	24,32,73	3.32	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	B	1228	-	24,32,73	3.33	10 (41%)	31,54,113	2.53	11 (35%)
15	CLA	B	1224	-	59,63,73	1.46	7 (11%)	70,101,113	2.02	19 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	4	612	-	24,32,73	3.32	11 (45%)	31,54,113	2.49	11 (35%)
16	PQN	A	2001	-	34,34,34	0.44	0	43,45,45	1.09	3 (6%)
15	CLA	2	610	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	A	1127	-	24,32,73	3.34	11 (45%)	31,54,113	2.48	12 (38%)
17	SF4	A	3001	-	0,12,12	-	-	-	-	-
15	CLA	A	1012	-	59,63,73	1.47	8 (13%)	70,101,113	1.94	17 (24%)
15	CLA	B	1215	-	24,32,73	3.33	11 (45%)	31,54,113	2.48	12 (38%)
15	CLA	B	1216	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	K	1401	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	A	1128	-	24,32,73	3.33	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	B	1021	-	49,53,73	1.60	7 (14%)	58,89,113	1.97	15 (25%)
15	CLA	L	1502	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	12 (38%)
15	CLA	3	601	-	24,32,73	3.32	11 (45%)	31,54,113	2.51	11 (35%)
15	CLA	3	606	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	12 (38%)
15	CLA	B	1231	-	24,32,73	3.32	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	A	1104	-	59,63,73	1.47	8 (13%)	70,101,113	1.99	18 (25%)
15	CLA	2	608	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	3	610	-	24,32,73	3.33	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	B	1023	-	54,58,73	1.52	7 (12%)	64,95,113	2.04	18 (28%)
15	CLA	B	1206	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	A	1113	-	24,32,73	3.33	11 (45%)	31,54,113	2.49	12 (38%)
15	CLA	A	1112	-	24,32,73	3.33	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	B	1211	-	24,32,73	3.31	11 (45%)	31,54,113	2.48	12 (38%)
15	CLA	2	603	-	24,32,73	3.30	11 (45%)	31,54,113	2.47	10 (32%)
15	CLA	B	1212	-	24,32,73	3.32	11 (45%)	31,54,113	2.46	11 (35%)
15	CLA	2	601	-	24,32,73	3.31	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	B	1203	-	24,32,73	3.33	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	B	1223	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	3	612	-	24,32,73	3.28	11 (45%)	31,54,113	2.49	10 (32%)
15	CLA	2	605	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	2	607	-	24,32,73	3.30	11 (45%)	31,54,113	2.42	10 (32%)
15	CLA	L	1501	-	24,32,73	3.30	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	B	1237	-	59,63,73	1.48	8 (13%)	70,101,113	1.95	18 (25%)
15	CLA	3	604	-	24,32,73	3.32	11 (45%)	31,54,113	2.50	11 (35%)
15	CLA	A	1110	-	24,32,73	3.31	11 (45%)	31,54,113	2.48	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	SF4	C	3002	-	0,12,12	-	-	-		
15	CLA	A	1116	-	59,63,73	1.47	7 (11%)	70,101,113	1.96	19 (27%)
15	CLA	A	1125	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	10 (32%)
15	CLA	3	603	-	24,32,73	3.33	11 (45%)	31,54,113	2.53	11 (35%)
18	BCR	A	4017	-	41,41,41	1.62	4 (9%)	56,56,56	4.68	13 (23%)
15	CLA	B	1227	-	24,32,73	3.33	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	2	604	-	24,32,73	3.33	11 (45%)	31,54,113	2.49	12 (38%)
15	CLA	A	1107	3	59,63,73	1.47	7 (11%)	70,101,113	2.00	18 (25%)
15	CLA	B	1238	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	B	1229	-	54,58,73	1.54	7 (12%)	64,95,113	2.14	19 (29%)
15	CLA	F	1301	-	49,53,73	1.60	8 (16%)	58,89,113	2.05	15 (25%)
15	CLA	4	605	-	24,32,73	3.32	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	A	1121	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	A	1132	-	24,32,73	3.30	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	A	1119	-	24,32,73	3.31	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	A	1118	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	J	1302	-	54,58,73	1.54	8 (14%)	64,95,113	2.16	19 (29%)
15	CLA	O	1601	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
18	BCR	B	4005	-	41,41,41	1.61	4 (9%)	56,56,56	4.53	18 (32%)
15	CLA	A	1138	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	3	608	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	12 (38%)
15	CLA	A	1106	-	59,63,73	1.46	7 (11%)	70,101,113	2.00	20 (28%)
15	CLA	B	1202	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	4	616	-	24,32,73	3.31	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	2	611	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	12 (38%)
15	CLA	A	1124	-	24,32,73	3.33	11 (45%)	31,54,113	2.49	12 (38%)
18	BCR	A	4008	-	41,41,41	1.60	4 (9%)	56,56,56	4.53	16 (28%)
15	CLA	B	1217	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	A	1129	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	12 (38%)
15	CLA	A	1120	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	A	1108	-	24,32,73	3.33	11 (45%)	31,54,113	2.47	12 (38%)
15	CLA	4	610	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	A	1101	-	49,53,73	1.60	7 (14%)	58,89,113	2.04	16 (27%)
15	CLA	A	1122	-	24,32,73	3.31	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	A	1140	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	O	1602	-	24,32,73	3.31	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	B	1235	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	A	1133	-	24,32,73	3.31	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	A	1141	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	B	1210	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	A	1139	-	24,32,73	3.31	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	3	602	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	12 (38%)
15	CLA	2	615	-	24,32,73	3.31	11 (45%)	31,54,113	2.47	11 (35%)
18	BCR	A	4007	-	41,41,41	1.61	5 (12%)	56,56,56	4.76	18 (32%)
15	CLA	A	1137	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	4	609	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
18	BCR	A	4011	-	41,41,41	1.60	4 (9%)	56,56,56	4.51	17 (30%)
15	CLA	4	603	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	L	1503	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	2	616	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
18	BCR	A	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.62	18 (32%)
15	CLA	A	1105	-	59,63,73	1.46	7 (11%)	70,101,113	2.03	18 (25%)
15	CLA	B	1219	-	24,32,73	3.31	11 (45%)	31,54,113	2.47	11 (35%)
17	SF4	C	3003	-	0,12,12	-	-	-	-	-
15	CLA	A	1134	-	24,32,73	3.33	11 (45%)	31,54,113	2.48	12 (38%)
15	CLA	4	606	-	24,32,73	3.31	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	A	1111	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	B	1204	-	24,32,73	3.31	11 (45%)	31,54,113	2.47	12 (38%)
15	CLA	A	1013	-	59,63,73	1.47	7 (11%)	70,101,113	1.96	16 (22%)
15	CLA	B	1232	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	19 (23%)
15	CLA	A	1135	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
18	BCR	I	4018	-	41,41,41	1.60	4 (9%)	56,56,56	4.49	18 (32%)
15	CLA	2	612	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	B	1220	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
18	BCR	B	4008	-	41,41,41	1.60	4 (9%)	56,56,56	4.71	15 (26%)
15	CLA	B	1234	-	24,32,73	3.32	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	K	1402	-	24,32,73	3.28	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	2	602	-	24,32,73	3.33	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	4	602	-	24,32,73	3.32	11 (45%)	31,54,113	2.49	11 (35%)
16	PQN	B	2002	-	34,34,34	0.40	0	43,45,45	1.18	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1236	-	49,53,73	1.59	7 (14%)	58,89,113	2.09	16 (27%)
15	CLA	2	613	-	24,32,73	3.31	11 (45%)	31,54,113	2.46	11 (35%)
15	CLA	A	1011	-	54,58,73	1.53	7 (12%)	64,95,113	2.11	19 (29%)
15	CLA	3	611	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	3	614	-	24,32,73	3.33	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	A	1109	-	24,32,73	3.31	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	A	1126	-	59,63,73	1.47	7 (11%)	70,101,113	1.97	18 (25%)
15	CLA	B	1222	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	12 (38%)
15	CLA	B	1239	-	24,32,73	3.33	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	B	1230	-	51,55,73	1.57	7 (13%)	60,91,113	2.21	16 (26%)
15	CLA	B	1209	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	A	1115	-	59,63,73	1.48	7 (11%)	70,101,113	2.00	20 (28%)
15	CLA	A	1131	-	49,53,73	1.61	7 (14%)	58,89,113	2.01	14 (24%)
15	CLA	A	1136	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	B	1226	-	59,63,73	1.47	8 (13%)	70,101,113	2.03	15 (21%)
15	CLA	2	606	-	24,32,73	3.31	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	A	1114	-	50,54,73	1.59	8 (16%)	59,90,113	2.01	14 (23%)
15	CLA	A	1123	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	B	1214	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	A	1130	-	59,63,73	1.47	7 (11%)	70,101,113	2.01	20 (28%)
15	CLA	F	1302	-	24,32,73	3.31	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	4	601	-	24,32,73	3.32	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	B	1022	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	12 (38%)
15	CLA	B	1207	-	24,32,73	3.32	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	3	607	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	12 (38%)
15	CLA	A	1102	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	B	1221	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	2	614	-	24,32,73	3.31	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	B	1218	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	11 (35%)
15	CLA	B	1208	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)
15	CLA	4	608	-	24,32,73	3.32	11 (45%)	31,54,113	2.49	11 (35%)
15	CLA	A	1103	-	59,63,73	1.45	7 (11%)	70,101,113	1.98	20 (28%)
15	CLA	4	611	-	24,32,73	3.32	11 (45%)	31,54,113	2.48	11 (35%)

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
15	CLA	B	1205	-	1/1/4/20	-	-
15	CLA	B	1225	-	1/1/12/20	8/21/97/115	-
15	CLA	O	1603	-	1/1/4/20	-	-
15	CLA	4	604	-	1/1/4/20	-	-
15	CLA	4	615	-	1/1/4/20	-	-
15	CLA	A	1117	-	1/1/13/20	10/27/103/115	-
15	CLA	B	1201	-	1/1/4/20	-	-
15	CLA	B	1228	-	1/1/4/20	-	-
15	CLA	B	1224	-	1/1/13/20	16/27/103/115	-
15	CLA	4	612	-	1/1/4/20	-	-
16	PQN	A	2001	-	-	10/23/43/43	0/2/2/2
15	CLA	2	610	-	1/1/4/20	-	-
15	CLA	A	1127	-	1/1/4/20	-	-
17	SF4	A	3001	-	-	-	0/6/5/5
15	CLA	A	1012	-	1/1/13/20	14/27/103/115	-
15	CLA	B	1215	-	1/1/4/20	-	-
15	CLA	B	1216	-	1/1/4/20	-	-
15	CLA	K	1401	-	1/1/4/20	-	-
15	CLA	A	1128	-	1/1/4/20	-	-
15	CLA	B	1021	-	1/1/11/20	4/15/91/115	-
15	CLA	L	1502	-	1/1/4/20	-	-
15	CLA	3	601	-	1/1/4/20	-	-
15	CLA	3	606	-	1/1/4/20	-	-
15	CLA	B	1231	-	1/1/4/20	-	-
15	CLA	A	1104	-	1/1/13/20	12/27/103/115	-
15	CLA	2	608	-	1/1/4/20	-	-
15	CLA	3	610	-	1/1/4/20	-	-
15	CLA	B	1023	-	1/1/12/20	7/21/97/115	-
15	CLA	B	1206	-	1/1/4/20	-	-
15	CLA	A	1113	-	1/1/4/20	-	-
15	CLA	A	1112	-	1/1/4/20	-	-
15	CLA	B	1211	-	1/1/4/20	-	-
15	CLA	2	603	-	1/1/4/20	-	-
15	CLA	B	1212	-	1/1/4/20	-	-
15	CLA	2	601	-	1/1/4/20	-	-
15	CLA	B	1203	-	1/1/4/20	-	-
15	CLA	B	1223	-	1/1/4/20	-	-
15	CLA	3	612	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	2	605	-	1/1/4/20	-	-
15	CLA	2	607	-	1/1/4/20	-	-
15	CLA	L	1501	-	1/1/4/20	-	-
15	CLA	B	1237	-	1/1/13/20	9/27/103/115	-
15	CLA	3	604	-	1/1/4/20	-	-
15	CLA	A	1110	-	1/1/4/20	-	-
17	SF4	C	3002	-	-	-	0/6/5/5
15	CLA	A	1116	-	1/1/13/20	16/27/103/115	-
15	CLA	A	1125	-	1/1/4/20	-	-
15	CLA	3	603	-	1/1/4/20	-	-
18	BCR	A	4017	-	-	12/29/63/63	0/2/2/2
15	CLA	B	1227	-	1/1/4/20	-	-
15	CLA	2	604	-	1/1/4/20	-	-
15	CLA	A	1107	3	1/1/13/20	10/27/103/115	-
15	CLA	B	1238	-	1/1/4/20	-	-
15	CLA	B	1229	-	1/1/12/20	6/21/97/115	-
15	CLA	F	1301	-	1/1/11/20	7/15/91/115	-
15	CLA	4	605	-	1/1/4/20	-	-
15	CLA	A	1121	-	1/1/4/20	-	-
15	CLA	A	1132	-	1/1/4/20	-	-
15	CLA	A	1119	-	1/1/4/20	-	-
15	CLA	A	1118	-	1/1/4/20	-	-
15	CLA	J	1302	-	1/1/12/20	13/21/97/115	-
15	CLA	O	1601	-	1/1/4/20	-	-
18	BCR	B	4005	-	-	15/29/63/63	0/2/2/2
15	CLA	A	1138	-	1/1/4/20	-	-
15	CLA	3	608	-	1/1/4/20	-	-
15	CLA	A	1106	-	1/1/13/20	12/27/103/115	-
15	CLA	B	1202	-	1/1/4/20	-	-
15	CLA	4	616	-	1/1/4/20	-	-
15	CLA	2	611	-	1/1/4/20	-	-
15	CLA	A	1124	-	1/1/4/20	-	-
18	BCR	A	4008	-	-	14/29/63/63	0/2/2/2
15	CLA	B	1217	-	1/1/4/20	-	-
15	CLA	A	1129	-	1/1/4/20	-	-
15	CLA	A	1120	-	1/1/4/20	-	-
15	CLA	A	1108	-	1/1/4/20	-	-
15	CLA	4	610	-	1/1/4/20	-	-
15	CLA	A	1101	-	1/1/11/20	9/15/91/115	-
15	CLA	A	1122	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1140	-	1/1/4/20	-	-
15	CLA	O	1602	-	1/1/4/20	-	-
15	CLA	B	1235	-	1/1/4/20	-	-
15	CLA	A	1133	-	1/1/4/20	-	-
15	CLA	A	1141	-	1/1/4/20	-	-
15	CLA	B	1210	-	1/1/4/20	-	-
15	CLA	A	1139	-	1/1/4/20	-	-
15	CLA	3	602	-	1/1/4/20	-	-
15	CLA	2	615	-	1/1/4/20	-	-
18	BCR	A	4007	-	-	18/29/63/63	0/2/2/2
15	CLA	A	1137	-	1/1/4/20	-	-
15	CLA	4	609	-	1/1/4/20	-	-
18	BCR	A	4011	-	-	11/29/63/63	0/2/2/2
15	CLA	4	603	-	1/1/4/20	-	-
15	CLA	L	1503	-	1/1/4/20	-	-
15	CLA	2	616	-	1/1/4/20	-	-
18	BCR	A	4002	-	-	8/29/63/63	0/2/2/2
15	CLA	A	1105	-	1/1/13/20	9/27/103/115	-
15	CLA	B	1219	-	1/1/4/20	-	-
17	SF4	C	3003	-	-	-	0/6/5/5
15	CLA	A	1134	-	1/1/4/20	-	-
15	CLA	4	606	-	1/1/4/20	-	-
15	CLA	A	1111	-	1/1/4/20	-	-
15	CLA	B	1204	-	1/1/4/20	-	-
15	CLA	A	1013	-	1/1/13/20	13/27/103/115	-
15	CLA	B	1232	-	1/1/15/20	20/39/115/115	-
15	CLA	A	1135	-	1/1/4/20	-	-
18	BCR	I	4018	-	-	17/29/63/63	0/2/2/2
15	CLA	2	612	-	1/1/4/20	-	-
15	CLA	B	1220	-	1/1/4/20	-	-
18	BCR	B	4008	-	-	14/29/63/63	0/2/2/2
15	CLA	B	1234	-	1/1/4/20	-	-
15	CLA	K	1402	-	1/1/4/20	-	-
15	CLA	2	602	-	1/1/4/20	-	-
15	CLA	4	602	-	1/1/4/20	-	-
16	PQN	B	2002	-	-	7/23/43/43	0/2/2/2
15	CLA	B	1236	-	1/1/11/20	6/15/91/115	-
15	CLA	2	613	-	1/1/4/20	-	-
15	CLA	A	1011	-	1/1/12/20	6/21/97/115	-
15	CLA	3	611	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	3	614	-	1/1/4/20	-	-
15	CLA	A	1109	-	1/1/4/20	-	-
15	CLA	A	1126	-	1/1/13/20	11/27/103/115	-
15	CLA	B	1222	-	1/1/4/20	-	-
15	CLA	B	1239	-	1/1/4/20	-	-
15	CLA	B	1230	-	1/1/11/20	9/18/94/115	-
15	CLA	B	1209	-	1/1/4/20	-	-
15	CLA	A	1115	-	1/1/13/20	12/27/103/115	-
15	CLA	A	1131	-	1/1/11/20	4/15/91/115	-
15	CLA	A	1136	-	1/1/4/20	-	-
15	CLA	B	1226	-	1/1/13/20	12/27/103/115	-
15	CLA	2	606	-	1/1/4/20	-	-
15	CLA	A	1114	-	1/1/11/20	7/17/93/115	-
15	CLA	A	1123	-	1/1/4/20	-	-
15	CLA	B	1214	-	1/1/4/20	-	-
15	CLA	A	1130	-	1/1/13/20	12/27/103/115	-
15	CLA	F	1302	-	1/1/4/20	-	-
15	CLA	4	601	-	1/1/4/20	-	-
15	CLA	B	1022	-	1/1/4/20	-	-
15	CLA	B	1207	-	1/1/4/20	-	-
15	CLA	3	607	-	1/1/4/20	-	-
15	CLA	A	1102	-	1/1/4/20	-	-
15	CLA	B	1221	-	1/1/4/20	-	-
15	CLA	2	614	-	1/1/4/20	-	-
15	CLA	B	1218	-	1/1/4/20	-	-
15	CLA	B	1208	-	1/1/4/20	-	-
15	CLA	4	608	-	1/1/4/20	-	-
15	CLA	A	1103	-	1/1/13/20	11/27/103/115	-
15	CLA	4	611	-	1/1/4/20	-	-

All (1400) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1128	CLA	C3D-C2D	8.69	1.54	1.35
15	A	1127	CLA	C3D-C2D	8.69	1.54	1.35
15	B	1239	CLA	C3D-C2D	8.68	1.54	1.35
15	A	1108	CLA	C3D-C2D	8.68	1.54	1.35
15	A	1124	CLA	C3D-C2D	8.68	1.54	1.35
15	2	602	CLA	C3D-C2D	8.68	1.54	1.35
15	A	1134	CLA	C3D-C2D	8.68	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1227	CLA	C3D-C2D	8.67	1.54	1.35
15	A	1129	CLA	C3D-C2D	8.67	1.54	1.35
15	B	1221	CLA	C3D-C2D	8.67	1.54	1.35
15	L	1503	CLA	C3D-C2D	8.67	1.54	1.35
15	B	1215	CLA	C3D-C2D	8.67	1.54	1.35
15	2	604	CLA	C3D-C2D	8.67	1.54	1.35
15	B	1218	CLA	C3D-C2D	8.67	1.54	1.35
15	B	1203	CLA	C3D-C2D	8.67	1.54	1.35
15	O	1601	CLA	C3D-C2D	8.67	1.54	1.35
15	3	602	CLA	C3D-C2D	8.67	1.54	1.35
15	3	606	CLA	C3D-C2D	8.67	1.54	1.35
15	B	1234	CLA	C3D-C2D	8.66	1.54	1.35
15	4	606	CLA	C3D-C2D	8.66	1.54	1.35
15	A	1125	CLA	C3D-C2D	8.66	1.54	1.35
15	B	1206	CLA	C3D-C2D	8.66	1.54	1.35
15	B	1220	CLA	C3D-C2D	8.66	1.54	1.35
15	B	1231	CLA	C3D-C2D	8.66	1.54	1.35
15	B	1222	CLA	C3D-C2D	8.66	1.54	1.35
15	2	616	CLA	C3D-C2D	8.66	1.54	1.35
15	4	603	CLA	C3D-C2D	8.66	1.54	1.35
15	A	1113	CLA	C3D-C2D	8.66	1.54	1.35
15	3	603	CLA	C3D-C2D	8.66	1.54	1.35
15	3	608	CLA	C3D-C2D	8.66	1.54	1.35
15	2	612	CLA	C3D-C2D	8.65	1.54	1.35
15	2	601	CLA	C3D-C2D	8.65	1.54	1.35
15	4	615	CLA	C3D-C2D	8.65	1.54	1.35
15	3	610	CLA	C3D-C2D	8.65	1.54	1.35
15	A	1139	CLA	C3D-C2D	8.65	1.54	1.35
15	A	1118	CLA	C3D-C2D	8.65	1.54	1.35
15	4	605	CLA	C3D-C2D	8.65	1.54	1.35
15	A	1102	CLA	C3D-C2D	8.65	1.54	1.35
15	B	1207	CLA	C3D-C2D	8.65	1.54	1.35
15	L	1501	CLA	C3D-C2D	8.65	1.54	1.35
15	A	1120	CLA	C3D-C2D	8.65	1.54	1.35
15	B	1209	CLA	C3D-C2D	8.65	1.54	1.35
15	A	1133	CLA	C3D-C2D	8.65	1.54	1.35
15	B	1201	CLA	C3D-C2D	8.65	1.54	1.35
15	B	1210	CLA	C3D-C2D	8.65	1.54	1.35
15	A	1141	CLA	C3D-C2D	8.65	1.54	1.35
15	O	1603	CLA	C3D-C2D	8.65	1.54	1.35
15	B	1235	CLA	C3D-C2D	8.64	1.54	1.35
15	2	610	CLA	C3D-C2D	8.64	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	604	CLA	C3D-C2D	8.64	1.54	1.35
15	A	1112	CLA	C3D-C2D	8.64	1.54	1.35
15	A	1140	CLA	C3D-C2D	8.64	1.54	1.35
15	4	608	CLA	C3D-C2D	8.64	1.54	1.35
15	2	608	CLA	C3D-C2D	8.64	1.54	1.35
15	4	601	CLA	C3D-C2D	8.64	1.54	1.35
15	2	605	CLA	C3D-C2D	8.64	1.54	1.35
15	4	602	CLA	C3D-C2D	8.64	1.54	1.35
15	A	1137	CLA	C3D-C2D	8.64	1.54	1.35
15	3	611	CLA	C3D-C2D	8.64	1.54	1.35
15	F	1302	CLA	C3D-C2D	8.64	1.54	1.35
15	A	1121	CLA	C3D-C2D	8.64	1.54	1.35
15	B	1211	CLA	C3D-C2D	8.64	1.54	1.35
15	A	1123	CLA	C3D-C2D	8.64	1.54	1.35
15	B	1022	CLA	C3D-C2D	8.64	1.54	1.35
15	B	1238	CLA	C3D-C2D	8.64	1.54	1.35
15	3	607	CLA	C3D-C2D	8.63	1.54	1.35
15	A	1136	CLA	C3D-C2D	8.63	1.54	1.35
15	B	1214	CLA	C3D-C2D	8.63	1.54	1.35
15	L	1502	CLA	C3D-C2D	8.63	1.54	1.35
15	4	611	CLA	C3D-C2D	8.63	1.54	1.35
15	A	1111	CLA	C3D-C2D	8.63	1.54	1.35
15	3	601	CLA	C3D-C2D	8.63	1.54	1.35
15	B	1223	CLA	C3D-C2D	8.63	1.54	1.35
15	3	604	CLA	C3D-C2D	8.63	1.54	1.35
15	A	1110	CLA	C3D-C2D	8.63	1.54	1.35
15	B	1212	CLA	C3D-C2D	8.63	1.54	1.35
15	B	1216	CLA	C3D-C2D	8.63	1.54	1.35
15	2	614	CLA	C3D-C2D	8.63	1.54	1.35
15	3	612	CLA	C3D-C2D	8.63	1.54	1.35
15	A	1122	CLA	C3D-C2D	8.63	1.54	1.35
15	B	1219	CLA	C3D-C2D	8.63	1.54	1.35
15	2	611	CLA	C3D-C2D	8.63	1.54	1.35
15	2	613	CLA	C3D-C2D	8.63	1.54	1.35
15	A	1109	CLA	C3D-C2D	8.63	1.54	1.35
15	K	1401	CLA	C3D-C2D	8.63	1.54	1.35
15	B	1202	CLA	C3D-C2D	8.62	1.54	1.35
15	3	614	CLA	C3D-C2D	8.62	1.54	1.35
15	A	1132	CLA	C3D-C2D	8.62	1.54	1.35
15	4	609	CLA	C3D-C2D	8.62	1.54	1.35
15	B	1217	CLA	C3D-C2D	8.62	1.54	1.35
15	4	612	CLA	C3D-C2D	8.62	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1135	CLA	C3D-C2D	8.62	1.54	1.35
15	4	616	CLA	C3D-C2D	8.62	1.54	1.35
15	4	610	CLA	C3D-C2D	8.62	1.54	1.35
15	B	1208	CLA	C3D-C2D	8.61	1.54	1.35
15	O	1602	CLA	C3D-C2D	8.61	1.54	1.35
15	A	1138	CLA	C3D-C2D	8.61	1.54	1.35
15	2	615	CLA	C3D-C2D	8.61	1.54	1.35
15	2	606	CLA	C3D-C2D	8.60	1.54	1.35
15	B	1204	CLA	C3D-C2D	8.60	1.54	1.35
15	A	1119	CLA	C3D-C2D	8.59	1.54	1.35
15	B	1228	CLA	C3D-C2D	8.59	1.54	1.35
15	B	1205	CLA	C3D-C2D	8.59	1.54	1.35
15	K	1402	CLA	C3D-C2D	8.58	1.54	1.35
15	2	603	CLA	C3D-C2D	8.55	1.54	1.35
15	2	607	CLA	C3D-C2D	8.50	1.54	1.35
15	B	1228	CLA	MG-ND	8.08	2.21	2.05
15	B	1227	CLA	MG-ND	7.99	2.21	2.05
15	A	1127	CLA	MG-ND	7.96	2.21	2.05
15	A	1125	CLA	MG-ND	7.93	2.21	2.05
15	3	604	CLA	MG-ND	7.92	2.21	2.05
15	A	1135	CLA	MG-ND	7.92	2.21	2.05
15	B	1212	CLA	MG-ND	7.92	2.21	2.05
15	B	1022	CLA	MG-ND	7.92	2.21	2.05
15	4	611	CLA	MG-ND	7.92	2.21	2.05
15	B	1203	CLA	MG-ND	7.91	2.21	2.05
15	A	1137	CLA	MG-ND	7.91	2.21	2.05
15	A	1129	CLA	MG-ND	7.91	2.21	2.05
15	3	614	CLA	MG-ND	7.91	2.21	2.05
15	4	609	CLA	MG-ND	7.90	2.21	2.05
15	A	1113	CLA	MG-ND	7.90	2.21	2.05
15	B	1202	CLA	MG-ND	7.90	2.21	2.05
15	B	1239	CLA	MG-ND	7.90	2.21	2.05
15	B	1209	CLA	MG-ND	7.89	2.21	2.05
15	2	604	CLA	MG-ND	7.89	2.21	2.05
15	A	1102	CLA	MG-ND	7.89	2.21	2.05
15	A	1141	CLA	MG-ND	7.89	2.21	2.05
15	A	1121	CLA	MG-ND	7.89	2.21	2.05
15	B	1206	CLA	MG-ND	7.89	2.21	2.05
15	A	1108	CLA	MG-ND	7.89	2.21	2.05
15	A	1128	CLA	MG-ND	7.89	2.21	2.05
15	2	611	CLA	MG-ND	7.89	2.21	2.05
15	A	1120	CLA	MG-ND	7.89	2.21	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	610	CLA	MG-ND	7.89	2.21	2.05
15	A	1134	CLA	MG-ND	7.89	2.21	2.05
15	A	1140	CLA	MG-ND	7.89	2.21	2.05
15	B	1208	CLA	MG-ND	7.89	2.21	2.05
15	B	1234	CLA	MG-ND	7.89	2.21	2.05
15	A	1112	CLA	MG-ND	7.88	2.21	2.05
15	A	1122	CLA	MG-ND	7.88	2.21	2.05
15	B	1215	CLA	MG-ND	7.88	2.21	2.05
15	4	612	CLA	MG-ND	7.88	2.21	2.05
15	4	605	CLA	MG-ND	7.88	2.21	2.05
15	2	602	CLA	MG-ND	7.88	2.21	2.05
15	2	610	CLA	MG-ND	7.88	2.21	2.05
15	3	602	CLA	MG-ND	7.88	2.21	2.05
15	B	1222	CLA	MG-ND	7.88	2.21	2.05
15	4	608	CLA	MG-ND	7.88	2.21	2.05
15	4	616	CLA	MG-ND	7.88	2.21	2.05
15	2	616	CLA	MG-ND	7.87	2.21	2.05
15	3	610	CLA	MG-ND	7.87	2.21	2.05
15	A	1124	CLA	MG-ND	7.87	2.21	2.05
15	B	1231	CLA	MG-ND	7.87	2.21	2.05
15	4	604	CLA	MG-ND	7.87	2.21	2.05
15	B	1214	CLA	MG-ND	7.87	2.21	2.05
15	A	1111	CLA	MG-ND	7.87	2.21	2.05
15	A	1133	CLA	MG-ND	7.87	2.21	2.05
15	3	601	CLA	MG-ND	7.87	2.21	2.05
15	B	1218	CLA	MG-ND	7.87	2.21	2.05
15	4	603	CLA	MG-ND	7.87	2.21	2.05
15	A	1123	CLA	MG-ND	7.86	2.21	2.05
15	3	603	CLA	MG-ND	7.86	2.21	2.05
15	3	611	CLA	MG-ND	7.86	2.21	2.05
15	B	1219	CLA	MG-ND	7.86	2.21	2.05
15	A	1136	CLA	MG-ND	7.86	2.21	2.05
15	B	1238	CLA	MG-ND	7.86	2.21	2.05
15	4	601	CLA	MG-ND	7.86	2.21	2.05
15	F	1302	CLA	MG-ND	7.86	2.21	2.05
15	K	1401	CLA	MG-ND	7.86	2.21	2.05
15	B	1217	CLA	MG-ND	7.85	2.21	2.05
15	2	606	CLA	MG-ND	7.85	2.21	2.05
15	B	1211	CLA	MG-ND	7.85	2.21	2.05
15	3	607	CLA	MG-ND	7.85	2.21	2.05
15	B	1223	CLA	MG-ND	7.85	2.21	2.05
15	3	608	CLA	MG-ND	7.85	2.21	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	602	CLA	MG-ND	7.85	2.21	2.05
15	O	1603	CLA	MG-ND	7.85	2.21	2.05
15	B	1221	CLA	MG-ND	7.85	2.21	2.05
15	B	1220	CLA	MG-ND	7.85	2.21	2.05
15	B	1235	CLA	MG-ND	7.85	2.21	2.05
15	L	1502	CLA	MG-ND	7.85	2.21	2.05
15	2	605	CLA	MG-ND	7.85	2.21	2.05
15	2	608	CLA	MG-ND	7.84	2.21	2.05
15	A	1139	CLA	MG-ND	7.84	2.21	2.05
15	2	614	CLA	MG-ND	7.84	2.21	2.05
15	B	1210	CLA	MG-ND	7.84	2.21	2.05
15	2	615	CLA	MG-ND	7.84	2.21	2.05
15	A	1138	CLA	MG-ND	7.84	2.21	2.05
15	4	606	CLA	MG-ND	7.84	2.21	2.05
15	A	1119	CLA	MG-ND	7.84	2.21	2.05
15	O	1601	CLA	MG-ND	7.84	2.21	2.05
15	2	613	CLA	MG-ND	7.84	2.21	2.05
15	B	1216	CLA	MG-ND	7.83	2.21	2.05
15	2	612	CLA	MG-ND	7.83	2.21	2.05
15	A	1110	CLA	MG-ND	7.83	2.21	2.05
15	B	1204	CLA	MG-ND	7.83	2.21	2.05
15	L	1503	CLA	MG-ND	7.83	2.21	2.05
15	3	606	CLA	MG-ND	7.82	2.21	2.05
15	B	1201	CLA	MG-ND	7.82	2.21	2.05
15	2	601	CLA	MG-ND	7.82	2.21	2.05
15	A	1118	CLA	MG-ND	7.81	2.21	2.05
15	A	1109	CLA	MG-ND	7.81	2.21	2.05
15	B	1207	CLA	MG-ND	7.81	2.21	2.05
15	4	615	CLA	MG-ND	7.81	2.21	2.05
15	L	1501	CLA	MG-ND	7.79	2.21	2.05
15	O	1602	CLA	MG-ND	7.79	2.21	2.05
15	A	1132	CLA	MG-ND	7.79	2.21	2.05
15	2	603	CLA	MG-ND	7.78	2.21	2.05
15	2	607	CLA	MG-ND	7.78	2.21	2.05
15	B	1205	CLA	MG-ND	7.77	2.21	2.05
15	K	1402	CLA	MG-ND	7.72	2.21	2.05
15	3	612	CLA	MG-ND	7.70	2.21	2.05
15	B	1232	CLA	MG-NA	6.46	2.21	2.06
15	A	1101	CLA	MG-NA	6.44	2.21	2.06
15	A	1107	CLA	MG-NA	6.43	2.21	2.06
15	J	1302	CLA	MG-NA	6.42	2.21	2.06
15	A	1126	CLA	MG-NA	6.41	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	1301	CLA	MG-NA	6.40	2.21	2.06
15	B	1237	CLA	MG-NA	6.40	2.21	2.06
15	A	1116	CLA	MG-NA	6.40	2.21	2.06
15	A	1013	CLA	MG-NA	6.39	2.21	2.06
15	B	1236	CLA	MG-NA	6.38	2.21	2.06
15	A	1115	CLA	MG-NA	6.38	2.21	2.06
15	A	1130	CLA	MG-NA	6.38	2.21	2.06
15	A	1105	CLA	MG-NA	6.37	2.21	2.06
15	A	1104	CLA	MG-NA	6.37	2.21	2.06
15	A	1131	CLA	MG-NA	6.36	2.21	2.06
15	A	1114	CLA	MG-NA	6.35	2.21	2.06
15	B	1023	CLA	MG-NA	6.34	2.21	2.06
15	A	1106	CLA	MG-NA	6.34	2.21	2.06
15	A	1012	CLA	MG-NA	6.33	2.21	2.06
15	B	1021	CLA	MG-NA	6.33	2.21	2.06
15	A	1117	CLA	MG-NA	6.33	2.21	2.06
15	A	1103	CLA	MG-NA	6.32	2.21	2.06
15	B	1224	CLA	MG-NA	6.28	2.21	2.06
15	B	1225	CLA	MG-NA	6.28	2.21	2.06
15	A	1011	CLA	MG-NA	6.26	2.21	2.06
15	B	1229	CLA	MG-NA	6.25	2.21	2.06
15	B	1226	CLA	MG-NA	6.24	2.21	2.06
15	B	1230	CLA	MG-NA	6.20	2.21	2.06
18	B	4008	BCR	C24-C23	5.91	1.50	1.33
18	B	4005	BCR	C24-C23	5.89	1.50	1.33
18	A	4002	BCR	C24-C23	5.84	1.50	1.33
18	A	4011	BCR	C24-C23	5.84	1.50	1.33
18	A	4007	BCR	C24-C23	5.79	1.50	1.33
18	A	4017	BCR	C24-C23	5.78	1.50	1.33
18	A	4008	BCR	C24-C23	5.70	1.50	1.33
18	I	4018	BCR	C24-C23	5.63	1.49	1.33
15	2	607	CLA	CHA-C4D	5.52	1.51	1.38
15	3	614	CLA	CHA-C4D	5.40	1.51	1.38
15	B	1207	CLA	C3A-C2A	-5.40	1.39	1.52
15	A	1112	CLA	CHA-C4D	5.39	1.51	1.38
15	A	1127	CLA	CHA-C4D	5.39	1.51	1.38
15	3	604	CLA	C3A-C2A	-5.39	1.39	1.52
15	4	605	CLA	CHA-C4D	5.38	1.51	1.38
15	2	603	CLA	CHA-C4D	5.38	1.51	1.38
15	A	1128	CLA	CHA-C4D	5.38	1.51	1.38
15	4	604	CLA	CHA-C4D	5.38	1.51	1.38
15	A	1111	CLA	CHA-C4D	5.37	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1218	CLA	CHA-C4D	5.37	1.51	1.38
15	B	1227	CLA	CHA-C4D	5.37	1.51	1.38
15	B	1222	CLA	CHA-C4D	5.37	1.51	1.38
15	A	1135	CLA	CHA-C4D	5.37	1.51	1.38
15	2	610	CLA	CHA-C4D	5.36	1.51	1.38
15	4	601	CLA	CHA-C4D	5.36	1.51	1.38
15	B	1203	CLA	C3A-C2A	-5.36	1.39	1.52
15	3	606	CLA	CHA-C4D	5.36	1.51	1.38
15	4	610	CLA	CHA-C4D	5.36	1.51	1.38
15	A	1123	CLA	CHA-C4D	5.36	1.51	1.38
15	4	608	CLA	CHA-C4D	5.36	1.51	1.38
15	O	1603	CLA	CHA-C4D	5.36	1.51	1.38
15	3	607	CLA	CHA-C4D	5.36	1.51	1.38
15	B	1239	CLA	CHA-C4D	5.36	1.51	1.38
15	B	1235	CLA	CHA-C4D	5.36	1.51	1.38
15	A	1124	CLA	CHA-C4D	5.36	1.51	1.38
15	2	611	CLA	CHA-C4D	5.36	1.51	1.38
15	B	1201	CLA	CHA-C4D	5.36	1.51	1.38
15	A	1133	CLA	CHA-C4D	5.36	1.51	1.38
15	3	603	CLA	C3A-C2A	-5.36	1.39	1.52
15	2	604	CLA	CHA-C4D	5.36	1.51	1.38
15	K	1401	CLA	CHA-C4D	5.36	1.51	1.38
15	3	602	CLA	CHA-C4D	5.35	1.51	1.38
15	4	603	CLA	CHA-C4D	5.35	1.51	1.38
15	4	615	CLA	CHA-C4D	5.35	1.51	1.38
15	3	612	CLA	C3A-C2A	-5.35	1.39	1.52
15	A	1134	CLA	CHA-C4D	5.35	1.51	1.38
15	B	1208	CLA	CHA-C4D	5.35	1.51	1.38
15	B	1210	CLA	CHA-C4D	5.35	1.51	1.38
15	A	1125	CLA	C3A-C2A	-5.35	1.39	1.52
15	B	1022	CLA	C3A-C2A	-5.35	1.39	1.52
15	B	1228	CLA	C3A-C2A	-5.35	1.39	1.52
15	A	1140	CLA	CHA-C4D	5.35	1.51	1.38
15	B	1212	CLA	CHA-C4D	5.35	1.51	1.38
15	B	1206	CLA	CHA-C4D	5.35	1.51	1.38
15	B	1238	CLA	CHA-C4D	5.35	1.51	1.38
15	A	1108	CLA	CHA-C4D	5.35	1.51	1.38
15	B	1217	CLA	CHA-C4D	5.35	1.51	1.38
15	4	602	CLA	C3A-C2A	-5.35	1.39	1.52
15	B	1223	CLA	CHA-C4D	5.35	1.51	1.38
15	A	1109	CLA	CHA-C4D	5.35	1.51	1.38
15	2	612	CLA	CHA-C4D	5.34	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1216	CLA	CHA-C4D	5.34	1.51	1.38
15	B	1204	CLA	CHA-C4D	5.34	1.51	1.38
15	3	601	CLA	CHA-C4D	5.34	1.51	1.38
15	3	611	CLA	CHA-C4D	5.34	1.51	1.38
15	A	1132	CLA	CHA-C4D	5.34	1.51	1.38
15	A	1132	CLA	C3A-C2A	-5.34	1.39	1.52
15	A	1121	CLA	CHA-C4D	5.34	1.51	1.38
15	L	1503	CLA	CHA-C4D	5.34	1.51	1.38
15	B	1223	CLA	C3A-C2A	-5.34	1.39	1.52
15	A	1125	CLA	CHA-C4D	5.34	1.51	1.38
15	B	1211	CLA	C3A-C2A	-5.34	1.39	1.52
15	B	1214	CLA	C3A-C2A	-5.34	1.39	1.52
15	A	1137	CLA	CHA-C4D	5.34	1.51	1.38
15	L	1502	CLA	CHA-C4D	5.34	1.51	1.38
15	3	602	CLA	C3A-C2A	-5.34	1.39	1.52
18	A	4007	BCR	C11-C12	-5.34	1.20	1.34
15	A	1122	CLA	CHA-C4D	5.34	1.51	1.38
15	3	603	CLA	CHA-C4D	5.34	1.51	1.38
15	4	602	CLA	CHA-C4D	5.34	1.51	1.38
15	F	1302	CLA	CHA-C4D	5.34	1.51	1.38
15	4	603	CLA	C3A-C2A	-5.34	1.39	1.52
15	4	609	CLA	CHA-C4D	5.34	1.51	1.38
15	2	602	CLA	CHA-C4D	5.34	1.51	1.38
15	2	606	CLA	CHA-C4D	5.34	1.51	1.38
15	B	1219	CLA	CHA-C4D	5.34	1.51	1.38
15	2	611	CLA	C3A-C2A	-5.34	1.39	1.52
15	4	608	CLA	C3A-C2A	-5.34	1.39	1.52
15	4	611	CLA	CHA-C4D	5.33	1.51	1.38
15	A	1102	CLA	CHA-C4D	5.33	1.51	1.38
15	A	1136	CLA	CHA-C4D	5.33	1.51	1.38
15	K	1401	CLA	C3A-C2A	-5.33	1.39	1.52
15	A	1119	CLA	CHA-C4D	5.33	1.51	1.38
15	A	1124	CLA	C3A-C2A	-5.33	1.39	1.52
15	B	1220	CLA	CHA-C4D	5.33	1.51	1.38
15	2	605	CLA	CHA-C4D	5.33	1.51	1.38
15	2	608	CLA	CHA-C4D	5.33	1.51	1.38
15	2	601	CLA	CHA-C4D	5.33	1.51	1.38
15	A	1113	CLA	CHA-C4D	5.33	1.51	1.38
15	A	1118	CLA	CHA-C4D	5.33	1.51	1.38
15	A	1112	CLA	C3A-C2A	-5.33	1.39	1.52
15	B	1234	CLA	C3A-C2A	-5.33	1.39	1.52
15	B	1210	CLA	C3A-C2A	-5.33	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1239	CLA	C3A-C2A	-5.33	1.39	1.52
15	B	1202	CLA	CHA-C4D	5.33	1.51	1.38
15	B	1212	CLA	C3A-C2A	-5.33	1.39	1.52
15	B	1214	CLA	CHA-C4D	5.33	1.51	1.38
15	A	1138	CLA	CHA-C4D	5.33	1.51	1.38
15	B	1231	CLA	CHA-C4D	5.33	1.51	1.38
15	3	607	CLA	C3A-C2A	-5.33	1.39	1.52
15	2	604	CLA	C3A-C2A	-5.33	1.39	1.52
15	2	614	CLA	C3A-C2A	-5.33	1.39	1.52
15	2	615	CLA	CHA-C4D	5.33	1.51	1.38
15	2	616	CLA	C3A-C2A	-5.33	1.39	1.52
15	2	608	CLA	C3A-C2A	-5.33	1.39	1.52
15	3	611	CLA	C3A-C2A	-5.33	1.39	1.52
15	A	1113	CLA	C3A-C2A	-5.33	1.39	1.52
15	B	1222	CLA	C3A-C2A	-5.33	1.39	1.52
15	3	610	CLA	CHA-C4D	5.33	1.51	1.38
15	B	1022	CLA	CHA-C4D	5.33	1.51	1.38
15	B	1203	CLA	CHA-C4D	5.33	1.51	1.38
15	2	603	CLA	C3A-C2A	-5.33	1.39	1.52
15	4	612	CLA	C3A-C2A	-5.33	1.39	1.52
15	B	1217	CLA	C3A-C2A	-5.33	1.39	1.52
15	L	1501	CLA	C3A-C2A	-5.33	1.39	1.52
15	2	614	CLA	CHA-C4D	5.33	1.51	1.38
15	B	1208	CLA	C3A-C2A	-5.33	1.39	1.52
15	A	1119	CLA	C3A-C2A	-5.33	1.39	1.52
15	A	1134	CLA	C3A-C2A	-5.33	1.39	1.52
15	A	1141	CLA	CHA-C4D	5.32	1.51	1.38
15	4	605	CLA	C3A-C2A	-5.32	1.39	1.52
15	A	1102	CLA	C3A-C2A	-5.32	1.39	1.52
15	B	1209	CLA	CHA-C4D	5.32	1.51	1.38
15	B	1238	CLA	C3A-C2A	-5.32	1.39	1.52
15	4	616	CLA	C3A-C2A	-5.32	1.39	1.52
15	L	1501	CLA	CHA-C4D	5.32	1.51	1.38
15	O	1601	CLA	CHA-C4D	5.32	1.51	1.38
15	3	608	CLA	CHA-C4D	5.32	1.51	1.38
15	B	1221	CLA	CHA-C4D	5.32	1.51	1.38
15	A	1139	CLA	CHA-C4D	5.32	1.51	1.38
15	A	1129	CLA	CHA-C4D	5.32	1.51	1.38
15	2	613	CLA	CHA-C4D	5.32	1.51	1.38
15	A	1118	CLA	C3A-C2A	-5.32	1.39	1.52
15	A	1129	CLA	C3A-C2A	-5.32	1.39	1.52
15	A	1133	CLA	C3A-C2A	-5.32	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	607	CLA	C3A-C2A	-5.32	1.39	1.52
15	B	1227	CLA	C3A-C2A	-5.32	1.39	1.52
15	3	606	CLA	C3A-C2A	-5.32	1.39	1.52
15	4	604	CLA	C3A-C2A	-5.32	1.39	1.52
15	3	614	CLA	C3A-C2A	-5.32	1.39	1.52
15	A	1108	CLA	C3A-C2A	-5.32	1.39	1.52
15	A	1141	CLA	C3A-C2A	-5.32	1.39	1.52
15	4	606	CLA	CHA-C4D	5.32	1.51	1.38
15	2	602	CLA	C3A-C2A	-5.32	1.39	1.52
15	2	613	CLA	C3A-C2A	-5.32	1.39	1.52
15	B	1202	CLA	C3A-C2A	-5.32	1.39	1.52
15	4	611	CLA	C3A-C2A	-5.32	1.39	1.52
15	O	1603	CLA	C3A-C2A	-5.32	1.39	1.52
15	2	606	CLA	C3A-C2A	-5.31	1.39	1.52
15	O	1601	CLA	C3A-C2A	-5.31	1.39	1.52
15	3	610	CLA	C3A-C2A	-5.31	1.39	1.52
15	A	1139	CLA	C3A-C2A	-5.31	1.39	1.52
15	K	1402	CLA	C3A-C2A	-5.31	1.39	1.52
15	2	610	CLA	C3A-C2A	-5.31	1.39	1.52
15	2	616	CLA	CHA-C4D	5.31	1.51	1.38
15	B	1234	CLA	CHA-C4D	5.31	1.51	1.38
15	A	1109	CLA	C3A-C2A	-5.31	1.39	1.52
15	K	1402	CLA	CHA-C4D	5.31	1.51	1.38
15	O	1602	CLA	CHA-C4D	5.31	1.51	1.38
15	4	612	CLA	CHA-C4D	5.31	1.51	1.38
15	A	1110	CLA	CHA-C4D	5.31	1.51	1.38
15	B	1207	CLA	CHA-C4D	5.31	1.51	1.38
15	2	601	CLA	C3A-C2A	-5.31	1.39	1.52
15	B	1215	CLA	C3A-C2A	-5.31	1.39	1.52
15	A	1120	CLA	CHA-C4D	5.31	1.51	1.38
15	B	1221	CLA	C3A-C2A	-5.31	1.39	1.52
15	L	1502	CLA	C3A-C2A	-5.31	1.39	1.52
15	A	1135	CLA	C3A-C2A	-5.31	1.39	1.52
15	2	615	CLA	C3A-C2A	-5.31	1.39	1.52
15	F	1302	CLA	C3A-C2A	-5.31	1.39	1.52
15	B	1231	CLA	C3A-C2A	-5.31	1.39	1.52
15	4	615	CLA	C3A-C2A	-5.31	1.39	1.52
15	L	1503	CLA	C3A-C2A	-5.31	1.39	1.52
15	A	1122	CLA	C3A-C2A	-5.31	1.39	1.52
15	A	1138	CLA	C3A-C2A	-5.31	1.39	1.52
15	B	1204	CLA	C3A-C2A	-5.30	1.39	1.52
15	3	601	CLA	C3A-C2A	-5.30	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1111	CLA	C3A-C2A	-5.30	1.39	1.52
15	B	1216	CLA	C3A-C2A	-5.30	1.39	1.52
15	4	601	CLA	C3A-C2A	-5.30	1.39	1.52
15	3	608	CLA	C3A-C2A	-5.30	1.39	1.52
15	A	1123	CLA	C3A-C2A	-5.30	1.39	1.52
15	O	1602	CLA	C3A-C2A	-5.30	1.39	1.52
15	B	1205	CLA	C3A-C2A	-5.30	1.39	1.52
15	B	1215	CLA	CHA-C4D	5.30	1.51	1.38
15	B	1206	CLA	C3A-C2A	-5.30	1.39	1.52
15	4	610	CLA	C3A-C2A	-5.30	1.39	1.52
15	A	1121	CLA	C3A-C2A	-5.30	1.39	1.52
15	B	1218	CLA	C3A-C2A	-5.30	1.39	1.52
15	B	1220	CLA	C3A-C2A	-5.30	1.39	1.52
15	A	1128	CLA	C3A-C2A	-5.30	1.39	1.52
15	2	605	CLA	C3A-C2A	-5.30	1.39	1.52
15	2	612	CLA	C3A-C2A	-5.30	1.39	1.52
15	B	1209	CLA	C3A-C2A	-5.30	1.39	1.52
15	4	609	CLA	C3A-C2A	-5.30	1.39	1.52
15	A	1120	CLA	C3A-C2A	-5.29	1.39	1.52
15	4	606	CLA	C3A-C2A	-5.29	1.39	1.52
15	A	1137	CLA	C3A-C2A	-5.29	1.39	1.52
15	4	616	CLA	CHA-C4D	5.29	1.51	1.38
15	B	1219	CLA	C3A-C2A	-5.29	1.39	1.52
15	A	1136	CLA	C3A-C2A	-5.29	1.39	1.52
15	A	1110	CLA	C3A-C2A	-5.29	1.39	1.52
15	3	604	CLA	CHA-C4D	5.29	1.51	1.38
15	B	1235	CLA	C3A-C2A	-5.28	1.39	1.52
15	B	1201	CLA	C3A-C2A	-5.28	1.39	1.52
15	A	1140	CLA	C3A-C2A	-5.28	1.39	1.52
15	B	1211	CLA	CHA-C4D	5.28	1.51	1.38
15	A	1127	CLA	C3A-C2A	-5.27	1.39	1.52
15	3	612	CLA	CHA-C4D	5.25	1.51	1.38
18	A	4017	BCR	C11-C12	-5.22	1.21	1.34
15	B	1205	CLA	CHA-C4D	5.19	1.51	1.38
18	A	4008	BCR	C11-C12	-5.19	1.21	1.34
18	B	4005	BCR	C11-C12	-5.08	1.21	1.34
18	A	4002	BCR	C11-C12	-5.06	1.21	1.34
18	A	4011	BCR	C11-C12	-5.05	1.21	1.34
18	I	4018	BCR	C11-C12	-5.05	1.21	1.34
18	B	4008	BCR	C11-C12	-5.03	1.21	1.34
15	B	1228	CLA	CHA-C4D	4.99	1.50	1.38
15	B	1229	CLA	CBB-CAB	4.44	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1103	CLA	CBB-CAB	4.43	1.51	1.30
15	A	1115	CLA	CBB-CAB	4.43	1.51	1.30
15	A	1104	CLA	CBB-CAB	4.43	1.51	1.30
15	A	1012	CLA	CBB-CAB	4.42	1.51	1.30
15	B	1236	CLA	CBB-CAB	4.42	1.51	1.30
15	B	1237	CLA	CBB-CAB	4.41	1.51	1.30
15	A	1011	CLA	CBB-CAB	4.41	1.51	1.30
15	F	1301	CLA	CBB-CAB	4.41	1.51	1.30
15	A	1130	CLA	CBB-CAB	4.41	1.51	1.30
15	A	1106	CLA	CBB-CAB	4.41	1.51	1.30
15	B	1225	CLA	CBB-CAB	4.41	1.51	1.30
15	J	1302	CLA	CBB-CAB	4.41	1.51	1.30
15	A	1117	CLA	CBB-CAB	4.41	1.51	1.30
15	B	1232	CLA	CBB-CAB	4.41	1.51	1.30
15	A	1116	CLA	CBB-CAB	4.40	1.51	1.30
15	B	1230	CLA	CBB-CAB	4.40	1.51	1.30
15	A	1126	CLA	CBB-CAB	4.40	1.51	1.30
15	B	1021	CLA	CBB-CAB	4.40	1.51	1.30
15	A	1131	CLA	CBB-CAB	4.40	1.51	1.30
15	B	1226	CLA	CBB-CAB	4.40	1.51	1.30
15	A	1101	CLA	CBB-CAB	4.39	1.51	1.30
15	A	1114	CLA	CBB-CAB	4.39	1.51	1.30
15	A	1107	CLA	CBB-CAB	4.39	1.51	1.30
15	A	1105	CLA	CBB-CAB	4.39	1.51	1.30
15	B	1023	CLA	CBB-CAB	4.39	1.51	1.30
15	B	1224	CLA	CBB-CAB	4.38	1.51	1.30
15	A	1013	CLA	CBB-CAB	4.38	1.51	1.30
18	A	4008	BCR	C16-C17	-4.28	1.29	1.43
18	I	4018	BCR	C16-C17	-4.26	1.30	1.43
18	I	4018	BCR	C10-C9	4.26	1.45	1.35
18	A	4011	BCR	C16-C17	-4.20	1.30	1.43
18	B	4008	BCR	C10-C9	4.18	1.45	1.35
18	A	4017	BCR	C16-C17	-4.18	1.30	1.43
15	A	1109	CLA	C3B-C4B	4.17	1.49	1.40
15	A	1127	CLA	C3B-C4B	4.16	1.49	1.40
15	A	1108	CLA	C3B-C4B	4.16	1.49	1.40
15	A	1134	CLA	C3B-C4B	4.15	1.49	1.40
15	A	1121	CLA	C3B-C4B	4.15	1.49	1.40
15	K	1401	CLA	C3B-C4B	4.15	1.49	1.40
18	B	4005	BCR	C10-C9	4.15	1.45	1.35
15	A	1111	CLA	C3B-C4B	4.15	1.49	1.40
15	B	1207	CLA	C3B-C4B	4.14	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1135	CLA	C3B-C4B	4.14	1.49	1.40
15	B	1231	CLA	C3B-C4B	4.14	1.49	1.40
15	2	612	CLA	C3B-C4B	4.14	1.49	1.40
15	2	605	CLA	C3B-C4B	4.14	1.49	1.40
15	A	1129	CLA	C3B-C4B	4.14	1.49	1.40
15	3	614	CLA	C3B-C4B	4.14	1.49	1.40
15	A	1137	CLA	C3B-C4B	4.14	1.49	1.40
15	2	610	CLA	C3B-C4B	4.13	1.49	1.40
15	2	615	CLA	C3B-C4B	4.13	1.49	1.40
15	B	1221	CLA	C3B-C4B	4.13	1.49	1.40
15	B	1204	CLA	C3B-C4B	4.13	1.49	1.40
15	A	1132	CLA	C3B-C4B	4.13	1.49	1.40
15	3	611	CLA	C3B-C4B	4.13	1.49	1.40
18	A	4011	BCR	C10-C9	4.13	1.45	1.35
15	B	1201	CLA	C3B-C4B	4.13	1.49	1.40
15	2	601	CLA	C3B-C4B	4.12	1.49	1.40
15	2	604	CLA	C3B-C4B	4.12	1.49	1.40
15	3	608	CLA	C3B-C4B	4.12	1.49	1.40
15	2	607	CLA	C3B-C4B	4.12	1.49	1.40
15	A	1118	CLA	C3B-C4B	4.12	1.49	1.40
15	A	1112	CLA	C3B-C4B	4.12	1.49	1.40
15	2	606	CLA	C3B-C4B	4.12	1.49	1.40
15	F	1302	CLA	C3B-C4B	4.12	1.49	1.40
15	B	1215	CLA	C3B-C4B	4.12	1.49	1.40
15	B	1216	CLA	C3B-C4B	4.12	1.49	1.40
15	2	608	CLA	C3B-C4B	4.12	1.49	1.40
15	4	615	CLA	C3B-C4B	4.12	1.49	1.40
15	2	603	CLA	C3B-C4B	4.12	1.49	1.40
15	4	602	CLA	C3B-C4B	4.12	1.49	1.40
15	A	1141	CLA	C3B-C4B	4.12	1.49	1.40
15	2	602	CLA	C3B-C4B	4.12	1.49	1.40
15	O	1602	CLA	C3B-C4B	4.12	1.49	1.40
15	A	1113	CLA	C3B-C4B	4.11	1.49	1.40
15	B	1209	CLA	C3B-C4B	4.11	1.49	1.40
15	3	601	CLA	C3B-C4B	4.11	1.49	1.40
15	A	1140	CLA	C3B-C4B	4.11	1.49	1.40
15	B	1202	CLA	C3B-C4B	4.11	1.49	1.40
15	B	1238	CLA	C3B-C4B	4.11	1.49	1.40
15	4	601	CLA	C3B-C4B	4.11	1.49	1.40
15	4	603	CLA	C3B-C4B	4.11	1.49	1.40
15	A	1128	CLA	C3B-C4B	4.11	1.49	1.40
15	B	1022	CLA	C3B-C4B	4.11	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	610	CLA	C3B-C4B	4.11	1.49	1.40
15	A	1138	CLA	C3B-C4B	4.11	1.49	1.40
15	B	1203	CLA	C3B-C4B	4.11	1.49	1.40
15	4	604	CLA	C3B-C4B	4.11	1.49	1.40
15	A	1124	CLA	C3B-C4B	4.11	1.49	1.40
18	B	4005	BCR	C16-C17	-4.11	1.30	1.43
15	A	1102	CLA	C3B-C4B	4.11	1.49	1.40
15	O	1601	CLA	C3B-C4B	4.11	1.49	1.40
15	4	612	CLA	C3B-C4B	4.11	1.49	1.40
15	B	1211	CLA	C3B-C4B	4.11	1.49	1.40
15	2	613	CLA	C3B-C4B	4.11	1.49	1.40
18	A	4007	BCR	C16-C17	-4.10	1.30	1.43
15	3	602	CLA	C3B-C4B	4.10	1.49	1.40
15	3	603	CLA	C3B-C4B	4.10	1.49	1.40
15	4	611	CLA	C3B-C4B	4.10	1.49	1.40
15	O	1603	CLA	C3B-C4B	4.10	1.49	1.40
15	A	1123	CLA	C3B-C4B	4.10	1.49	1.40
15	4	616	CLA	C3B-C4B	4.10	1.49	1.40
15	B	1217	CLA	C3B-C4B	4.10	1.49	1.40
18	B	4008	BCR	C16-C17	-4.10	1.30	1.43
15	A	1136	CLA	C3B-C4B	4.10	1.49	1.40
15	B	1220	CLA	C3B-C4B	4.10	1.49	1.40
15	B	1228	CLA	C3B-C4B	4.10	1.49	1.40
15	B	1206	CLA	C3B-C4B	4.10	1.49	1.40
15	B	1219	CLA	C3B-C4B	4.10	1.49	1.40
15	4	606	CLA	C3B-C4B	4.10	1.49	1.40
15	L	1502	CLA	C3B-C4B	4.10	1.49	1.40
15	B	1214	CLA	C3B-C4B	4.09	1.48	1.40
15	B	1208	CLA	C3B-C4B	4.09	1.48	1.40
15	3	604	CLA	C3B-C4B	4.09	1.48	1.40
15	L	1503	CLA	C3B-C4B	4.09	1.48	1.40
15	B	1239	CLA	C3B-C4B	4.09	1.48	1.40
15	A	1110	CLA	C3B-C4B	4.09	1.48	1.40
15	4	610	CLA	C3B-C4B	4.09	1.48	1.40
15	3	607	CLA	C3B-C4B	4.09	1.48	1.40
15	2	611	CLA	C3B-C4B	4.09	1.48	1.40
15	2	614	CLA	C3B-C4B	4.09	1.48	1.40
15	B	1218	CLA	C3B-C4B	4.09	1.48	1.40
15	A	1120	CLA	C3B-C4B	4.09	1.48	1.40
15	A	1133	CLA	C3B-C4B	4.09	1.48	1.40
15	A	1139	CLA	C3B-C4B	4.09	1.48	1.40
15	4	605	CLA	C3B-C4B	4.09	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1223	CLA	C3B-C4B	4.09	1.48	1.40
15	B	1222	CLA	C3B-C4B	4.08	1.48	1.40
15	B	1235	CLA	C3B-C4B	4.08	1.48	1.40
15	B	1210	CLA	C3B-C4B	4.08	1.48	1.40
15	K	1402	CLA	C3B-C4B	4.08	1.48	1.40
18	A	4002	BCR	C10-C9	4.08	1.45	1.35
18	A	4002	BCR	C16-C17	-4.08	1.30	1.43
15	B	1234	CLA	C3B-C4B	4.08	1.48	1.40
15	A	1119	CLA	C3B-C4B	4.07	1.48	1.40
15	2	616	CLA	C3B-C4B	4.07	1.48	1.40
15	3	606	CLA	C3B-C4B	4.07	1.48	1.40
15	B	1205	CLA	C3B-C4B	4.07	1.48	1.40
15	4	609	CLA	C3B-C4B	4.07	1.48	1.40
15	4	608	CLA	C3B-C4B	4.06	1.48	1.40
15	3	612	CLA	C3B-C4B	4.06	1.48	1.40
15	B	1212	CLA	C3B-C4B	4.05	1.48	1.40
18	A	4017	BCR	C10-C9	4.05	1.45	1.35
15	A	1122	CLA	C3B-C4B	4.04	1.48	1.40
15	L	1501	CLA	C3B-C4B	4.04	1.48	1.40
15	B	1227	CLA	C3B-C4B	4.01	1.48	1.40
18	A	4008	BCR	C10-C9	4.00	1.45	1.35
15	A	1125	CLA	C3B-C4B	3.93	1.48	1.40
15	B	1226	CLA	MG-ND	-3.84	1.98	2.05
15	B	1237	CLA	MG-ND	-3.84	1.98	2.05
15	A	1114	CLA	MG-ND	-3.83	1.98	2.05
15	B	1224	CLA	MG-ND	-3.82	1.98	2.05
15	A	1013	CLA	MG-ND	-3.80	1.98	2.05
15	A	1131	CLA	MG-ND	-3.79	1.98	2.05
15	B	1021	CLA	MG-ND	-3.78	1.98	2.05
15	F	1301	CLA	MG-ND	-3.78	1.98	2.05
18	A	4007	BCR	C10-C9	3.77	1.44	1.35
15	A	1107	CLA	MG-ND	-3.75	1.98	2.05
15	A	1012	CLA	MG-ND	-3.75	1.98	2.05
15	A	1116	CLA	MG-ND	-3.72	1.98	2.05
15	A	1011	CLA	MG-ND	-3.71	1.98	2.05
15	J	1302	CLA	MG-ND	-3.71	1.98	2.05
15	B	1230	CLA	MG-ND	-3.71	1.98	2.05
15	A	1115	CLA	MG-ND	-3.71	1.98	2.05
15	A	1105	CLA	MG-ND	-3.71	1.98	2.05
15	A	1101	CLA	MG-ND	-3.70	1.98	2.05
15	B	1023	CLA	MG-ND	-3.70	1.98	2.05
15	B	1232	CLA	MG-ND	-3.70	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1106	CLA	MG-ND	-3.69	1.98	2.05
15	A	1130	CLA	MG-ND	-3.69	1.98	2.05
15	A	1126	CLA	MG-ND	-3.68	1.98	2.05
15	B	1229	CLA	MG-ND	-3.68	1.98	2.05
15	B	1236	CLA	MG-ND	-3.67	1.98	2.05
15	B	1225	CLA	MG-ND	-3.66	1.98	2.05
15	A	1104	CLA	MG-ND	-3.65	1.98	2.05
15	A	1103	CLA	MG-ND	-3.64	1.98	2.05
15	B	1228	CLA	MG-NA	-3.63	1.97	2.06
15	A	1117	CLA	MG-ND	-3.62	1.98	2.05
15	B	1230	CLA	C1C-NC	-3.52	1.32	1.37
15	B	1227	CLA	MG-NA	-3.36	1.98	2.06
15	B	1203	CLA	MG-NA	-3.33	1.98	2.06
15	B	1226	CLA	C1C-NC	-3.32	1.32	1.37
15	3	603	CLA	MG-NA	-3.32	1.98	2.06
15	B	1207	CLA	MG-NA	-3.31	1.98	2.06
15	B	1205	CLA	MG-NA	-3.30	1.98	2.06
15	B	1022	CLA	MG-NA	-3.29	1.98	2.06
15	4	602	CLA	MG-NA	-3.29	1.98	2.06
15	B	1211	CLA	MG-NA	-3.29	1.98	2.06
15	B	1216	CLA	MG-NA	-3.28	1.98	2.06
15	2	614	CLA	MG-NA	-3.28	1.98	2.06
15	3	607	CLA	MG-NA	-3.28	1.98	2.06
15	B	1220	CLA	MG-NA	-3.28	1.98	2.06
15	3	610	CLA	MG-NA	-3.28	1.98	2.06
15	O	1602	CLA	MG-NA	-3.28	1.98	2.06
15	B	1214	CLA	MG-NA	-3.27	1.98	2.06
15	L	1502	CLA	MG-NA	-3.27	1.98	2.06
15	3	601	CLA	MG-NA	-3.27	1.98	2.06
15	2	616	CLA	MG-NA	-3.27	1.98	2.06
15	4	604	CLA	MG-NA	-3.27	1.98	2.06
15	B	1218	CLA	MG-NA	-3.27	1.98	2.06
15	B	1221	CLA	MG-NA	-3.27	1.98	2.06
15	2	612	CLA	MG-NA	-3.27	1.98	2.06
15	O	1601	CLA	MG-NA	-3.27	1.98	2.06
15	4	616	CLA	MG-NA	-3.27	1.98	2.06
15	3	611	CLA	MG-NA	-3.27	1.98	2.06
15	O	1603	CLA	MG-NA	-3.26	1.98	2.06
15	L	1503	CLA	MG-NA	-3.26	1.98	2.06
15	4	612	CLA	MG-NA	-3.26	1.98	2.06
15	4	606	CLA	MG-NA	-3.26	1.98	2.06
15	B	1212	CLA	MG-NA	-3.26	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	608	CLA	MG-NA	-3.26	1.98	2.06
15	A	1108	CLA	MG-NA	-3.26	1.98	2.06
15	B	1215	CLA	MG-NA	-3.26	1.98	2.06
15	A	1113	CLA	MG-NA	-3.26	1.98	2.06
15	B	1208	CLA	MG-NA	-3.26	1.98	2.06
15	B	1234	CLA	MG-NA	-3.26	1.98	2.06
15	4	610	CLA	MG-NA	-3.26	1.98	2.06
15	4	608	CLA	MG-NA	-3.25	1.98	2.06
15	4	609	CLA	MG-NA	-3.25	1.98	2.06
15	A	1138	CLA	MG-NA	-3.25	1.98	2.06
15	B	1201	CLA	MG-NA	-3.25	1.98	2.06
15	B	1238	CLA	MG-NA	-3.25	1.98	2.06
15	2	605	CLA	MG-NA	-3.25	1.98	2.06
15	A	1120	CLA	MG-NA	-3.25	1.98	2.06
15	4	601	CLA	MG-NA	-3.25	1.98	2.06
15	2	602	CLA	MG-NA	-3.25	1.98	2.06
15	A	1140	CLA	MG-NA	-3.25	1.98	2.06
15	B	1209	CLA	MG-NA	-3.25	1.98	2.06
15	3	608	CLA	MG-NA	-3.25	1.98	2.06
15	3	614	CLA	MG-NA	-3.25	1.98	2.06
15	B	1206	CLA	MG-NA	-3.25	1.98	2.06
15	3	606	CLA	MG-NA	-3.25	1.98	2.06
15	3	602	CLA	MG-NA	-3.25	1.98	2.06
15	4	605	CLA	MG-NA	-3.24	1.98	2.06
15	2	603	CLA	MG-NA	-3.24	1.98	2.06
15	2	613	CLA	MG-NA	-3.24	1.98	2.06
15	L	1501	CLA	MG-NA	-3.24	1.98	2.06
15	A	1123	CLA	MG-NA	-3.24	1.98	2.06
15	B	1202	CLA	MG-NA	-3.24	1.98	2.06
15	4	615	CLA	MG-NA	-3.24	1.98	2.06
15	4	611	CLA	MG-NA	-3.24	1.98	2.06
15	A	1141	CLA	MG-NA	-3.24	1.98	2.06
15	2	611	CLA	MG-NA	-3.24	1.98	2.06
15	B	1204	CLA	MG-NA	-3.24	1.98	2.06
15	2	610	CLA	MG-NA	-3.24	1.98	2.06
15	A	1118	CLA	MG-NA	-3.24	1.98	2.06
15	K	1402	CLA	MG-NA	-3.24	1.98	2.06
15	A	1119	CLA	MG-NA	-3.24	1.98	2.06
15	A	1136	CLA	MG-NA	-3.24	1.98	2.06
15	B	1235	CLA	MG-NA	-3.24	1.98	2.06
15	F	1302	CLA	MG-NA	-3.23	1.98	2.06
15	B	1217	CLA	MG-NA	-3.23	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1229	CLA	C1C-NC	-3.23	1.32	1.37
15	2	604	CLA	MG-NA	-3.23	1.98	2.06
15	B	1219	CLA	MG-NA	-3.23	1.98	2.06
15	B	1222	CLA	MG-NA	-3.23	1.98	2.06
15	2	607	CLA	MG-NA	-3.23	1.98	2.06
15	2	615	CLA	MG-NA	-3.23	1.98	2.06
15	A	1132	CLA	MG-NA	-3.23	1.98	2.06
15	B	1231	CLA	MG-NA	-3.22	1.98	2.06
15	A	1134	CLA	MG-NA	-3.22	1.98	2.06
15	A	1129	CLA	MG-NA	-3.22	1.98	2.06
15	B	1223	CLA	MG-NA	-3.22	1.98	2.06
15	2	606	CLA	MG-NA	-3.22	1.98	2.06
15	B	1210	CLA	MG-NA	-3.22	1.98	2.06
15	A	1137	CLA	MG-NA	-3.22	1.98	2.06
15	4	603	CLA	MG-NA	-3.22	1.98	2.06
15	B	1239	CLA	MG-NA	-3.22	1.98	2.06
15	A	1125	CLA	MG-NA	-3.21	1.98	2.06
15	A	1139	CLA	MG-NA	-3.21	1.98	2.06
15	A	1122	CLA	MG-NA	-3.21	1.98	2.06
15	A	1124	CLA	MG-NA	-3.21	1.98	2.06
15	A	1110	CLA	MG-NA	-3.21	1.98	2.06
15	A	1133	CLA	MG-NA	-3.21	1.98	2.06
15	A	1109	CLA	MG-NA	-3.21	1.98	2.06
15	3	612	CLA	MG-NA	-3.21	1.98	2.06
15	2	601	CLA	MG-NA	-3.20	1.98	2.06
15	A	1112	CLA	MG-NA	-3.20	1.98	2.06
15	A	1128	CLA	MG-NA	-3.20	1.98	2.06
15	K	1401	CLA	MG-NA	-3.19	1.98	2.06
15	A	1111	CLA	MG-NA	-3.19	1.98	2.06
15	A	1121	CLA	MG-NA	-3.19	1.98	2.06
15	3	604	CLA	MG-NA	-3.18	1.98	2.06
15	A	1127	CLA	MG-NA	-3.15	1.98	2.06
15	A	1135	CLA	MG-NA	-3.14	1.98	2.06
15	A	1102	CLA	MG-NA	-3.14	1.98	2.06
15	A	1011	CLA	C1C-NC	-3.13	1.33	1.37
15	J	1302	CLA	C1C-NC	-3.08	1.33	1.37
15	B	1236	CLA	C1C-NC	-3.08	1.33	1.37
15	A	1116	CLA	C1C-NC	-3.07	1.33	1.37
15	A	1101	CLA	C1C-NC	-3.07	1.33	1.37
15	A	1107	CLA	C1C-NC	-3.05	1.33	1.37
15	A	1131	CLA	C1C-NC	-3.05	1.33	1.37
15	A	1126	CLA	C1C-NC	-3.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1115	CLA	C1C-NC	-3.04	1.33	1.37
15	A	1117	CLA	C1C-NC	-3.03	1.33	1.37
15	A	1114	CLA	C1C-NC	-3.03	1.33	1.37
15	A	1106	CLA	C1C-NC	-3.03	1.33	1.37
15	A	1105	CLA	C1C-NC	-3.03	1.33	1.37
15	B	1237	CLA	C1C-NC	-3.02	1.33	1.37
15	A	1130	CLA	C1C-NC	-3.02	1.33	1.37
15	B	1021	CLA	C1C-NC	-3.02	1.33	1.37
15	A	1013	CLA	C1C-NC	-3.01	1.33	1.37
15	B	1225	CLA	C1C-NC	-3.01	1.33	1.37
15	B	1023	CLA	C1C-NC	-2.99	1.33	1.37
15	B	1224	CLA	C1C-NC	-2.99	1.33	1.37
15	A	1104	CLA	C1C-NC	-2.98	1.33	1.37
15	A	1012	CLA	C1C-NC	-2.97	1.33	1.37
15	B	1232	CLA	C1C-NC	-2.97	1.33	1.37
15	A	1135	CLA	C2B-C1B	2.95	1.46	1.40
15	O	1603	CLA	C2B-C1B	2.94	1.46	1.40
15	A	1108	CLA	C2B-C1B	2.94	1.46	1.40
15	A	1111	CLA	C2B-C1B	2.93	1.46	1.40
15	3	607	CLA	C2B-C1B	2.93	1.46	1.40
15	3	601	CLA	C2B-C1B	2.93	1.46	1.40
15	A	1123	CLA	C2B-C1B	2.93	1.46	1.40
15	A	1140	CLA	C2B-C1B	2.93	1.46	1.40
15	B	1215	CLA	C2B-C1B	2.93	1.46	1.40
15	B	1235	CLA	C2B-C1B	2.93	1.46	1.40
15	A	1109	CLA	C2B-C1B	2.92	1.46	1.40
15	B	1204	CLA	C2B-C1B	2.92	1.46	1.40
15	F	1301	CLA	C1C-NC	-2.92	1.33	1.37
15	O	1602	CLA	C2B-C1B	2.92	1.46	1.40
15	A	1112	CLA	C2B-C1B	2.92	1.46	1.40
15	A	1137	CLA	C2B-C1B	2.92	1.46	1.40
15	B	1216	CLA	C2B-C1B	2.92	1.46	1.40
15	B	1221	CLA	C2B-C1B	2.92	1.46	1.40
15	A	1113	CLA	C2B-C1B	2.92	1.46	1.40
15	B	1219	CLA	C2B-C1B	2.92	1.46	1.40
15	2	603	CLA	C2B-C1B	2.92	1.46	1.40
15	A	1121	CLA	C2B-C1B	2.92	1.46	1.40
15	B	1238	CLA	C2B-C1B	2.92	1.46	1.40
15	2	613	CLA	C2B-C1B	2.92	1.46	1.40
15	A	1128	CLA	C2B-C1B	2.91	1.46	1.40
15	4	603	CLA	C2B-C1B	2.91	1.46	1.40
15	K	1401	CLA	C2B-C1B	2.91	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	603	CLA	C2B-C1B	2.91	1.46	1.40
15	B	1208	CLA	C2B-C1B	2.91	1.46	1.40
15	2	611	CLA	C2B-C1B	2.91	1.46	1.40
15	B	1227	CLA	C2B-C1B	2.91	1.46	1.40
15	4	616	CLA	C2B-C1B	2.91	1.46	1.40
15	4	606	CLA	C2B-C1B	2.91	1.46	1.40
15	4	610	CLA	C2B-C1B	2.91	1.46	1.40
15	A	1119	CLA	C2B-C1B	2.91	1.46	1.40
15	A	1138	CLA	C2B-C1B	2.90	1.46	1.40
15	A	1120	CLA	C2B-C1B	2.90	1.46	1.40
15	B	1220	CLA	C2B-C1B	2.90	1.46	1.40
15	B	1223	CLA	C2B-C1B	2.90	1.46	1.40
15	B	1234	CLA	C2B-C1B	2.90	1.46	1.40
15	B	1222	CLA	C2B-C1B	2.90	1.46	1.40
15	4	602	CLA	C2B-C1B	2.90	1.46	1.40
15	B	1201	CLA	C2B-C1B	2.90	1.46	1.40
15	3	610	CLA	C2B-C1B	2.90	1.46	1.40
15	B	1214	CLA	C2B-C1B	2.90	1.46	1.40
15	A	1103	CLA	C1C-NC	-2.90	1.33	1.37
15	A	1110	CLA	C2B-C1B	2.90	1.46	1.40
15	B	1211	CLA	C2B-C1B	2.90	1.46	1.40
15	B	1231	CLA	C2B-C1B	2.90	1.46	1.40
15	3	614	CLA	C2B-C1B	2.90	1.46	1.40
15	B	1206	CLA	C2B-C1B	2.90	1.46	1.40
15	L	1503	CLA	C2B-C1B	2.90	1.46	1.40
15	2	616	CLA	C2B-C1B	2.90	1.46	1.40
15	A	1134	CLA	C2B-C1B	2.90	1.46	1.40
15	B	1203	CLA	C2B-C1B	2.90	1.46	1.40
15	3	612	CLA	C2B-C1B	2.90	1.46	1.40
15	2	605	CLA	C2B-C1B	2.90	1.46	1.40
15	A	1133	CLA	C2B-C1B	2.90	1.46	1.40
15	A	1102	CLA	C2B-C1B	2.89	1.46	1.40
15	4	615	CLA	C2B-C1B	2.89	1.46	1.40
15	O	1601	CLA	C2B-C1B	2.89	1.46	1.40
15	4	611	CLA	C2B-C1B	2.89	1.46	1.40
15	4	605	CLA	C2B-C1B	2.89	1.46	1.40
15	2	608	CLA	C2B-C1B	2.89	1.46	1.40
15	3	604	CLA	C2B-C1B	2.89	1.46	1.40
15	2	604	CLA	C2B-C1B	2.89	1.46	1.40
15	3	608	CLA	C2B-C1B	2.89	1.46	1.40
15	4	601	CLA	C2B-C1B	2.89	1.46	1.40
15	4	608	CLA	C2B-C1B	2.89	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	612	CLA	C2B-C1B	2.89	1.46	1.40
15	4	609	CLA	C2B-C1B	2.89	1.46	1.40
15	B	1209	CLA	C2B-C1B	2.89	1.46	1.40
15	2	610	CLA	C2B-C1B	2.88	1.46	1.40
15	A	1129	CLA	C2B-C1B	2.88	1.46	1.40
15	B	1218	CLA	C2B-C1B	2.88	1.46	1.40
15	4	612	CLA	C2B-C1B	2.88	1.46	1.40
15	A	1122	CLA	C2B-C1B	2.88	1.46	1.40
15	B	1205	CLA	C2B-C1B	2.88	1.46	1.40
15	A	1139	CLA	C2B-C1B	2.88	1.46	1.40
15	B	1202	CLA	C2B-C1B	2.88	1.46	1.40
15	A	1141	CLA	C2B-C1B	2.88	1.46	1.40
15	2	602	CLA	C2B-C1B	2.87	1.46	1.40
15	B	1210	CLA	C2B-C1B	2.87	1.46	1.40
15	B	1239	CLA	C2B-C1B	2.87	1.46	1.40
15	2	607	CLA	C2B-C1B	2.87	1.46	1.40
15	A	1127	CLA	C2B-C1B	2.87	1.46	1.40
15	2	615	CLA	C2B-C1B	2.87	1.46	1.40
15	2	614	CLA	C2B-C1B	2.87	1.46	1.40
15	4	604	CLA	C2B-C1B	2.87	1.46	1.40
15	A	1118	CLA	C2B-C1B	2.87	1.46	1.40
15	B	1022	CLA	C2B-C1B	2.87	1.46	1.40
15	2	606	CLA	C2B-C1B	2.87	1.46	1.40
15	A	1132	CLA	C2B-C1B	2.87	1.46	1.40
15	3	602	CLA	C2B-C1B	2.86	1.46	1.40
15	F	1302	CLA	C2B-C1B	2.86	1.46	1.40
15	A	1124	CLA	C2B-C1B	2.86	1.46	1.40
15	A	1136	CLA	C2B-C1B	2.86	1.46	1.40
15	B	1207	CLA	C2B-C1B	2.86	1.46	1.40
15	3	611	CLA	C2B-C1B	2.86	1.46	1.40
15	L	1502	CLA	C2B-C1B	2.86	1.46	1.40
15	3	606	CLA	C2B-C1B	2.86	1.46	1.40
15	B	1217	CLA	C2B-C1B	2.86	1.46	1.40
15	K	1402	CLA	C2B-C1B	2.85	1.46	1.40
15	B	1212	CLA	C2B-C1B	2.85	1.46	1.40
15	B	1230	CLA	C4B-NB	-2.85	1.34	1.37
15	2	601	CLA	C2B-C1B	2.84	1.46	1.40
15	B	1228	CLA	C2B-C1B	2.83	1.46	1.40
15	L	1501	CLA	C2B-C1B	2.82	1.46	1.40
15	B	1229	CLA	C4B-NB	-2.81	1.34	1.37
15	A	1125	CLA	C2B-C1B	2.79	1.46	1.40
15	B	1215	CLA	C2D-C1D	2.76	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1127	CLA	MG-NB	2.75	2.11	2.05
15	A	1125	CLA	C2D-C1D	2.75	1.51	1.44
15	B	1228	CLA	MG-NB	2.75	2.11	2.05
15	A	1128	CLA	C2D-C1D	2.74	1.51	1.44
15	B	1227	CLA	C2D-C1D	2.74	1.51	1.44
15	A	1127	CLA	C2D-C1D	2.74	1.51	1.44
15	B	1228	CLA	C2D-C1D	2.74	1.51	1.44
15	A	1111	CLA	MG-NB	2.74	2.11	2.05
15	A	1124	CLA	MG-NB	2.74	2.11	2.05
15	3	607	CLA	C2D-C1D	2.74	1.51	1.44
15	A	1122	CLA	C2D-C1D	2.74	1.51	1.44
15	A	1113	CLA	C2D-C1D	2.73	1.51	1.44
15	3	608	CLA	C2D-C1D	2.73	1.51	1.44
15	2	602	CLA	MG-NB	2.73	2.11	2.05
15	B	1207	CLA	MG-NB	2.73	2.11	2.05
15	B	1216	CLA	C2D-C1D	2.73	1.51	1.44
15	A	1118	CLA	MG-NB	2.73	2.11	2.05
15	2	616	CLA	C2D-C1D	2.73	1.51	1.44
15	4	604	CLA	C2D-C1D	2.73	1.51	1.44
15	4	610	CLA	C2D-C1D	2.73	1.51	1.44
15	4	603	CLA	C2D-C1D	2.72	1.51	1.44
15	B	1207	CLA	C2D-C1D	2.72	1.51	1.44
15	3	603	CLA	C2D-C1D	2.72	1.51	1.44
15	O	1601	CLA	C2D-C1D	2.72	1.51	1.44
15	A	1118	CLA	C2D-C1D	2.72	1.51	1.44
15	A	1108	CLA	MG-NB	2.72	2.11	2.05
15	A	1119	CLA	MG-NB	2.72	2.11	2.05
15	B	1234	CLA	C2D-C1D	2.72	1.51	1.44
15	3	610	CLA	C2D-C1D	2.72	1.51	1.44
15	A	1137	CLA	C2D-C1D	2.72	1.51	1.44
15	A	1102	CLA	MG-NB	2.72	2.11	2.05
15	A	1136	CLA	C2D-C1D	2.72	1.51	1.44
15	B	1222	CLA	C2D-C1D	2.72	1.51	1.44
15	B	1238	CLA	MG-NB	2.72	2.11	2.05
15	B	1206	CLA	C2D-C1D	2.72	1.51	1.44
15	L	1501	CLA	C2D-C1D	2.72	1.51	1.44
15	B	1226	CLA	C4B-NB	-2.72	1.34	1.37
15	3	604	CLA	C2D-C1D	2.72	1.51	1.44
15	4	609	CLA	C2D-C1D	2.72	1.51	1.44
15	A	1139	CLA	C2D-C1D	2.72	1.51	1.44
15	B	1210	CLA	C2D-C1D	2.71	1.51	1.44
15	A	1121	CLA	C2D-C1D	2.71	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1204	CLA	C2D-C1D	2.71	1.51	1.44
15	4	615	CLA	C2D-C1D	2.71	1.51	1.44
15	B	1219	CLA	C2D-C1D	2.71	1.51	1.44
15	2	615	CLA	MG-NB	2.71	2.11	2.05
15	2	602	CLA	C2D-C1D	2.71	1.51	1.44
15	2	613	CLA	MG-NB	2.71	2.11	2.05
15	4	612	CLA	C2D-C1D	2.71	1.51	1.44
15	A	1138	CLA	C2D-C1D	2.71	1.51	1.44
15	B	1224	CLA	C4B-NB	-2.71	1.34	1.37
15	A	1135	CLA	MG-NB	2.71	2.11	2.05
15	2	601	CLA	MG-NB	2.71	2.11	2.05
15	A	1140	CLA	MG-NB	2.71	2.11	2.05
15	B	1211	CLA	C2D-C1D	2.71	1.50	1.44
15	4	602	CLA	C2D-C1D	2.71	1.50	1.44
15	A	1112	CLA	C2D-C1D	2.71	1.50	1.44
15	B	1217	CLA	C2D-C1D	2.71	1.50	1.44
15	2	611	CLA	C2D-C1D	2.71	1.50	1.44
15	3	602	CLA	C2D-C1D	2.71	1.50	1.44
15	B	1238	CLA	C2D-C1D	2.71	1.50	1.44
15	L	1502	CLA	C2D-C1D	2.71	1.50	1.44
15	B	1235	CLA	C2D-C1D	2.71	1.50	1.44
15	4	615	CLA	MG-NB	2.71	2.11	2.05
15	B	1201	CLA	MG-NB	2.71	2.11	2.05
15	A	1011	CLA	C4B-NB	-2.70	1.34	1.37
15	A	1134	CLA	MG-NB	2.70	2.11	2.05
15	B	1022	CLA	C2D-C1D	2.70	1.50	1.44
15	B	1220	CLA	C2D-C1D	2.70	1.50	1.44
15	B	1221	CLA	MG-NB	2.70	2.11	2.05
15	L	1502	CLA	MG-NB	2.70	2.11	2.05
15	B	1203	CLA	C2D-C1D	2.70	1.50	1.44
15	F	1302	CLA	C2D-C1D	2.70	1.50	1.44
15	A	1129	CLA	C2D-C1D	2.70	1.50	1.44
15	B	1209	CLA	C2D-C1D	2.70	1.50	1.44
15	A	1121	CLA	MG-NB	2.70	2.11	2.05
15	4	605	CLA	C2D-C1D	2.70	1.50	1.44
15	A	1013	CLA	C4B-NB	-2.70	1.34	1.37
15	B	1239	CLA	C2D-C1D	2.70	1.50	1.44
15	B	1218	CLA	MG-NB	2.70	2.11	2.05
15	B	1221	CLA	C2D-C1D	2.70	1.50	1.44
15	2	606	CLA	C2D-C1D	2.70	1.50	1.44
15	3	606	CLA	C2D-C1D	2.70	1.50	1.44
15	3	607	CLA	MG-NB	2.70	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1138	CLA	MG-NB	2.70	2.11	2.05
15	A	1102	CLA	C2D-C1D	2.70	1.50	1.44
15	B	1212	CLA	C2D-C1D	2.70	1.50	1.44
15	2	607	CLA	MG-NB	2.70	2.11	2.05
15	3	608	CLA	MG-NB	2.70	2.11	2.05
15	B	1208	CLA	MG-NB	2.70	2.11	2.05
15	3	603	CLA	MG-NB	2.70	2.11	2.05
15	B	1239	CLA	MG-NB	2.70	2.11	2.05
15	2	606	CLA	MG-NB	2.70	2.11	2.05
15	A	1134	CLA	C2D-C1D	2.70	1.50	1.44
15	2	614	CLA	C2D-C1D	2.70	1.50	1.44
15	2	611	CLA	MG-NB	2.70	2.11	2.05
15	B	1223	CLA	C2D-C1D	2.70	1.50	1.44
15	B	1222	CLA	MG-NB	2.69	2.11	2.05
15	2	615	CLA	C2D-C1D	2.69	1.50	1.44
15	3	601	CLA	C2D-C1D	2.69	1.50	1.44
15	4	616	CLA	C2D-C1D	2.69	1.50	1.44
15	B	1217	CLA	MG-NB	2.69	2.11	2.05
15	4	608	CLA	C2D-C1D	2.69	1.50	1.44
15	A	1123	CLA	C2D-C1D	2.69	1.50	1.44
15	A	1141	CLA	C2D-C1D	2.69	1.50	1.44
15	A	1110	CLA	MG-NB	2.69	2.11	2.05
15	3	611	CLA	C2D-C1D	2.69	1.50	1.44
15	O	1603	CLA	C2D-C1D	2.69	1.50	1.44
15	2	605	CLA	C2D-C1D	2.69	1.50	1.44
15	3	601	CLA	MG-NB	2.69	2.11	2.05
15	2	613	CLA	C2D-C1D	2.69	1.50	1.44
15	A	1108	CLA	C2D-C1D	2.69	1.50	1.44
15	A	1110	CLA	C2D-C1D	2.69	1.50	1.44
15	B	1208	CLA	C2D-C1D	2.69	1.50	1.44
15	A	1120	CLA	C2D-C1D	2.69	1.50	1.44
15	A	1124	CLA	C2D-C1D	2.69	1.50	1.44
15	2	608	CLA	C2D-C1D	2.69	1.50	1.44
15	4	611	CLA	C2D-C1D	2.69	1.50	1.44
15	4	601	CLA	C2D-C1D	2.69	1.50	1.44
15	4	612	CLA	MG-NB	2.69	2.11	2.05
15	A	1125	CLA	MG-NB	2.69	2.11	2.05
15	A	1139	CLA	MG-NB	2.69	2.11	2.05
15	B	1223	CLA	MG-NB	2.69	2.11	2.05
15	3	610	CLA	C3D-C4D	2.69	1.50	1.44
15	A	1140	CLA	C2D-C1D	2.69	1.50	1.44
15	K	1401	CLA	C2D-C1D	2.69	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	602	CLA	MG-NB	2.69	2.11	2.05
15	2	601	CLA	C2D-C1D	2.68	1.50	1.44
15	A	1141	CLA	MG-NB	2.68	2.11	2.05
15	B	1203	CLA	MG-NB	2.68	2.11	2.05
15	2	604	CLA	MG-NB	2.68	2.11	2.05
15	A	1136	CLA	MG-NB	2.68	2.11	2.05
15	3	610	CLA	MG-NB	2.68	2.11	2.05
15	4	610	CLA	MG-NB	2.68	2.11	2.05
15	B	1206	CLA	MG-NB	2.68	2.11	2.05
15	2	612	CLA	C2D-C1D	2.68	1.50	1.44
15	B	1202	CLA	C2D-C1D	2.68	1.50	1.44
15	A	1129	CLA	MG-NB	2.68	2.11	2.05
15	B	1235	CLA	MG-NB	2.68	2.11	2.05
15	2	610	CLA	C2D-C1D	2.68	1.50	1.44
15	B	1210	CLA	MG-NB	2.68	2.11	2.05
15	B	1215	CLA	MG-NB	2.68	2.11	2.05
15	3	614	CLA	C2D-C1D	2.68	1.50	1.44
15	A	1119	CLA	C2D-C1D	2.68	1.50	1.44
15	B	1218	CLA	C2D-C1D	2.68	1.50	1.44
15	2	605	CLA	MG-NB	2.68	2.11	2.05
15	B	1231	CLA	C2D-C1D	2.68	1.50	1.44
15	A	1137	CLA	C3D-C4D	2.68	1.50	1.44
15	A	1112	CLA	MG-NB	2.68	2.11	2.05
15	A	1113	CLA	MG-NB	2.68	2.11	2.05
15	4	606	CLA	C2D-C1D	2.67	1.50	1.44
15	O	1602	CLA	C2D-C1D	2.67	1.50	1.44
15	A	1133	CLA	C2D-C1D	2.67	1.50	1.44
15	L	1503	CLA	C2D-C1D	2.67	1.50	1.44
15	A	1109	CLA	C2D-C1D	2.67	1.50	1.44
15	B	1214	CLA	C2D-C1D	2.67	1.50	1.44
15	3	611	CLA	MG-NB	2.67	2.11	2.05
15	A	1137	CLA	MG-NB	2.67	2.11	2.05
15	A	1123	CLA	MG-NB	2.67	2.11	2.05
15	B	1211	CLA	MG-NB	2.67	2.11	2.05
15	A	1135	CLA	C2D-C1D	2.67	1.50	1.44
15	3	606	CLA	MG-NB	2.67	2.11	2.05
15	2	616	CLA	MG-NB	2.67	2.11	2.05
15	4	604	CLA	MG-NB	2.67	2.11	2.05
15	2	612	CLA	MG-NB	2.67	2.11	2.05
15	2	608	CLA	C3D-C4D	2.67	1.50	1.44
15	B	1207	CLA	C3D-C4D	2.67	1.50	1.44
15	B	1205	CLA	C2D-C1D	2.67	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	614	CLA	MG-NB	2.67	2.11	2.05
15	4	601	CLA	MG-NB	2.67	2.11	2.05
15	2	604	CLA	C2D-C1D	2.67	1.50	1.44
15	4	602	CLA	MG-NB	2.67	2.11	2.05
15	O	1602	CLA	MG-NB	2.67	2.11	2.05
15	A	1127	CLA	C3D-C4D	2.67	1.50	1.44
15	B	1214	CLA	MG-NB	2.67	2.11	2.05
15	B	1204	CLA	MG-NB	2.67	2.11	2.05
15	K	1401	CLA	MG-NB	2.67	2.11	2.05
15	B	1201	CLA	C2D-C1D	2.66	1.50	1.44
15	B	1022	CLA	MG-NB	2.66	2.11	2.05
15	L	1503	CLA	MG-NB	2.66	2.11	2.05
15	A	1136	CLA	C3D-C4D	2.66	1.50	1.44
15	B	1208	CLA	C3D-C4D	2.66	1.50	1.44
15	A	1111	CLA	C2D-C1D	2.66	1.50	1.44
15	A	1132	CLA	C2D-C1D	2.66	1.50	1.44
15	A	1128	CLA	MG-NB	2.66	2.11	2.05
15	O	1601	CLA	C3D-C4D	2.66	1.50	1.44
15	4	605	CLA	MG-NB	2.66	2.11	2.05
15	4	611	CLA	MG-NB	2.66	2.11	2.05
15	4	616	CLA	MG-NB	2.66	2.11	2.05
15	4	601	CLA	C3D-C4D	2.66	1.50	1.44
15	A	1135	CLA	C3D-C4D	2.66	1.50	1.44
15	B	1234	CLA	MG-NB	2.66	2.11	2.05
15	2	601	CLA	C3D-C4D	2.66	1.50	1.44
15	A	1122	CLA	C3D-C4D	2.66	1.50	1.44
15	4	610	CLA	C3D-C4D	2.66	1.50	1.44
15	B	1231	CLA	MG-NB	2.66	2.11	2.05
15	2	607	CLA	C3D-C4D	2.66	1.50	1.44
15	O	1601	CLA	MG-NB	2.66	2.11	2.05
15	A	1113	CLA	C3D-C4D	2.65	1.50	1.44
15	2	610	CLA	MG-NB	2.65	2.11	2.05
15	A	1124	CLA	C3D-C4D	2.65	1.50	1.44
15	B	1201	CLA	C3D-C4D	2.65	1.50	1.44
15	A	1130	CLA	C4B-NB	-2.65	1.34	1.37
15	2	608	CLA	MG-NB	2.65	2.11	2.05
15	A	1128	CLA	C3D-C4D	2.65	1.50	1.44
15	B	1216	CLA	MG-NB	2.65	2.11	2.05
15	B	1227	CLA	MG-NB	2.65	2.11	2.05
15	O	1603	CLA	MG-NB	2.65	2.11	2.05
15	2	603	CLA	C2D-C1D	2.65	1.50	1.44
15	A	1120	CLA	MG-NB	2.65	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1215	CLA	C3D-C4D	2.65	1.50	1.44
15	B	1219	CLA	C3D-C4D	2.65	1.50	1.44
15	B	1235	CLA	C3D-C4D	2.65	1.50	1.44
15	2	615	CLA	C3D-C4D	2.65	1.50	1.44
15	B	1209	CLA	C3D-C4D	2.65	1.50	1.44
15	B	1238	CLA	C3D-C4D	2.65	1.50	1.44
15	2	616	CLA	C3D-C4D	2.65	1.50	1.44
15	3	606	CLA	C3D-C4D	2.65	1.50	1.44
15	4	606	CLA	MG-NB	2.64	2.11	2.05
15	B	1220	CLA	MG-NB	2.64	2.11	2.05
15	B	1223	CLA	C3D-C4D	2.64	1.50	1.44
15	O	1603	CLA	C3D-C4D	2.64	1.50	1.44
15	3	614	CLA	C3D-C4D	2.64	1.50	1.44
15	2	614	CLA	MG-NB	2.64	2.11	2.05
15	B	1209	CLA	MG-NB	2.64	2.11	2.05
15	B	1231	CLA	C3D-C4D	2.64	1.50	1.44
15	B	1212	CLA	MG-NB	2.64	2.11	2.05
15	3	602	CLA	C3D-C4D	2.64	1.50	1.44
15	4	605	CLA	C3D-C4D	2.64	1.50	1.44
15	A	1120	CLA	C3D-C4D	2.64	1.50	1.44
15	A	1125	CLA	C3D-C4D	2.64	1.50	1.44
15	2	611	CLA	C3D-C4D	2.64	1.50	1.44
15	A	1138	CLA	C3D-C4D	2.64	1.50	1.44
15	4	608	CLA	C3D-C4D	2.64	1.50	1.44
15	4	609	CLA	MG-NB	2.64	2.11	2.05
15	A	1122	CLA	MG-NB	2.64	2.11	2.05
15	B	1221	CLA	C3D-C4D	2.64	1.50	1.44
15	F	1302	CLA	MG-NB	2.64	2.11	2.05
15	4	612	CLA	C3D-C4D	2.64	1.50	1.44
15	A	1133	CLA	MG-NB	2.64	2.11	2.05
15	A	1140	CLA	C3D-C4D	2.64	1.50	1.44
15	3	607	CLA	C3D-C4D	2.64	1.50	1.44
15	B	1239	CLA	C3D-C4D	2.64	1.50	1.44
15	4	616	CLA	C3D-C4D	2.64	1.50	1.44
15	L	1501	CLA	C3D-C4D	2.64	1.50	1.44
15	A	1112	CLA	C3D-C4D	2.63	1.50	1.44
15	3	604	CLA	C3D-C4D	2.63	1.50	1.44
15	4	609	CLA	C3D-C4D	2.63	1.50	1.44
15	B	1217	CLA	C3D-C4D	2.63	1.50	1.44
15	B	1220	CLA	C3D-C4D	2.63	1.50	1.44
15	4	606	CLA	C3D-C4D	2.63	1.50	1.44
15	A	1117	CLA	C4B-NB	-2.63	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1202	CLA	C3D-C4D	2.63	1.50	1.44
15	2	603	CLA	MG-NB	2.63	2.11	2.05
15	B	1227	CLA	C3D-C4D	2.63	1.50	1.44
15	3	603	CLA	C3D-C4D	2.63	1.50	1.44
15	4	611	CLA	C3D-C4D	2.63	1.50	1.44
15	A	1109	CLA	MG-NB	2.63	2.11	2.05
15	B	1214	CLA	C3D-C4D	2.63	1.50	1.44
15	A	1134	CLA	C3D-C4D	2.62	1.50	1.44
15	A	1139	CLA	C3D-C4D	2.62	1.50	1.44
15	2	606	CLA	C3D-C4D	2.62	1.50	1.44
15	4	603	CLA	MG-NB	2.62	2.11	2.05
15	2	604	CLA	C3D-C4D	2.62	1.50	1.44
15	B	1212	CLA	C3D-C4D	2.62	1.50	1.44
15	K	1401	CLA	C3D-C4D	2.62	1.50	1.44
15	2	605	CLA	C3D-C4D	2.62	1.50	1.44
15	A	1121	CLA	C3D-C4D	2.62	1.50	1.44
15	B	1216	CLA	C3D-C4D	2.62	1.50	1.44
15	B	1210	CLA	C3D-C4D	2.62	1.50	1.44
15	A	1102	CLA	C3D-C4D	2.62	1.50	1.44
15	B	1219	CLA	MG-NB	2.62	2.11	2.05
15	B	1202	CLA	MG-NB	2.62	2.11	2.05
15	A	1110	CLA	C3D-C4D	2.62	1.50	1.44
15	A	1123	CLA	C3D-C4D	2.62	1.50	1.44
15	B	1228	CLA	C3D-C4D	2.62	1.50	1.44
15	L	1502	CLA	C3D-C4D	2.62	1.50	1.44
15	4	602	CLA	C3D-C4D	2.62	1.50	1.44
15	A	1108	CLA	C3D-C4D	2.62	1.50	1.44
15	4	615	CLA	C3D-C4D	2.62	1.50	1.44
15	F	1301	CLA	C4B-NB	-2.62	1.34	1.37
15	A	1119	CLA	C3D-C4D	2.62	1.50	1.44
15	B	1234	CLA	C3D-C4D	2.62	1.50	1.44
15	2	602	CLA	C3D-C4D	2.62	1.50	1.44
15	A	1118	CLA	C3D-C4D	2.62	1.50	1.44
15	2	614	CLA	C3D-C4D	2.62	1.50	1.44
15	B	1218	CLA	C3D-C4D	2.62	1.50	1.44
15	L	1501	CLA	MG-NB	2.62	2.11	2.05
15	2	607	CLA	C2D-C1D	2.62	1.50	1.44
15	2	612	CLA	C3D-C4D	2.61	1.50	1.44
15	3	611	CLA	C3D-C4D	2.61	1.50	1.44
15	B	1204	CLA	C3D-C4D	2.61	1.50	1.44
15	4	603	CLA	C3D-C4D	2.61	1.50	1.44
15	4	608	CLA	MG-NB	2.61	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1129	CLA	C3D-C4D	2.61	1.50	1.44
15	2	613	CLA	C3D-C4D	2.61	1.50	1.44
15	2	610	CLA	C3D-C4D	2.61	1.50	1.44
15	3	601	CLA	C3D-C4D	2.61	1.50	1.44
15	3	612	CLA	C2D-C1D	2.61	1.50	1.44
15	A	1141	CLA	C3D-C4D	2.61	1.50	1.44
15	B	1022	CLA	C3D-C4D	2.61	1.50	1.44
15	A	1111	CLA	C3D-C4D	2.61	1.50	1.44
15	F	1302	CLA	C3D-C4D	2.61	1.50	1.44
15	B	1203	CLA	C3D-C4D	2.60	1.50	1.44
15	L	1503	CLA	C3D-C4D	2.60	1.50	1.44
15	3	608	CLA	C3D-C4D	2.60	1.50	1.44
15	B	1211	CLA	C3D-C4D	2.60	1.50	1.44
15	A	1126	CLA	C4B-NB	-2.60	1.34	1.37
15	B	1222	CLA	C3D-C4D	2.60	1.50	1.44
15	K	1402	CLA	MG-NB	2.60	2.10	2.05
15	O	1602	CLA	C3D-C4D	2.60	1.50	1.44
15	B	1206	CLA	C3D-C4D	2.59	1.50	1.44
15	B	1021	CLA	C4B-NB	-2.59	1.34	1.37
15	A	1132	CLA	MG-NB	2.59	2.10	2.05
15	B	1237	CLA	C4B-NB	-2.59	1.34	1.37
15	B	1205	CLA	MG-NB	2.58	2.10	2.05
15	4	604	CLA	C3D-C4D	2.58	1.50	1.44
15	A	1103	CLA	C4B-NB	-2.58	1.34	1.37
15	A	1109	CLA	C3D-C4D	2.58	1.50	1.44
15	A	1012	CLA	C4B-NB	-2.58	1.34	1.37
15	2	603	CLA	C3D-C4D	2.58	1.50	1.44
15	J	1302	CLA	C4B-NB	-2.57	1.34	1.37
15	A	1131	CLA	C4B-NB	-2.56	1.34	1.37
15	3	604	CLA	MG-NB	2.56	2.10	2.05
15	A	1133	CLA	C3D-C4D	2.56	1.50	1.44
15	B	1225	CLA	C4B-NB	-2.56	1.34	1.37
15	A	1104	CLA	C4B-NB	-2.55	1.34	1.37
15	K	1402	CLA	C2D-C1D	2.55	1.50	1.44
15	3	612	CLA	MG-NB	2.54	2.10	2.05
15	B	1023	CLA	C4B-NB	-2.54	1.34	1.37
15	A	1106	CLA	C4B-NB	-2.54	1.34	1.37
15	A	1115	CLA	C4B-NB	-2.53	1.34	1.37
15	K	1402	CLA	C3D-C4D	2.53	1.50	1.44
15	A	1114	CLA	C4B-NB	-2.53	1.34	1.37
15	A	1105	CLA	C4B-NB	-2.53	1.34	1.37
15	A	1132	CLA	C3D-C4D	2.52	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1205	CLA	C3D-C4D	2.52	1.50	1.44
15	B	1232	CLA	C4B-NB	-2.44	1.34	1.37
15	A	1101	CLA	C4B-NB	-2.43	1.34	1.37
15	A	1107	CLA	C4B-NB	-2.43	1.34	1.37
15	3	612	CLA	C3D-C4D	2.40	1.50	1.44
15	A	1116	CLA	C4B-NB	-2.38	1.34	1.37
15	B	1236	CLA	C4B-NB	-2.31	1.34	1.37
15	B	1230	CLA	C1A-CHA	2.26	1.52	1.43
15	A	1115	CLA	C1C-C2C	2.21	1.49	1.44
15	J	1302	CLA	C1A-CHA	2.20	1.52	1.43
15	A	1105	CLA	C1A-CHA	2.19	1.52	1.43
15	A	1012	CLA	C1A-CHA	2.18	1.52	1.43
15	A	1101	CLA	C1A-CHA	2.18	1.52	1.43
15	F	1301	CLA	C1A-CHA	2.18	1.52	1.43
15	A	1104	CLA	C1C-C2C	2.17	1.48	1.44
15	A	1111	CLA	CHB-C4A	2.17	1.42	1.36
15	B	1236	CLA	C1A-CHA	2.17	1.52	1.43
15	A	1013	CLA	C1A-CHA	2.17	1.52	1.43
15	A	1116	CLA	C1C-C2C	2.17	1.48	1.44
15	A	1110	CLA	CHB-C4A	2.17	1.42	1.36
15	2	607	CLA	CHB-C4A	2.17	1.42	1.36
15	B	1023	CLA	C1A-CHA	2.17	1.52	1.43
15	B	1225	CLA	C1C-C2C	2.17	1.48	1.44
15	A	1130	CLA	C1A-CHA	2.16	1.52	1.43
15	A	1134	CLA	CHB-C4A	2.16	1.42	1.36
15	2	604	CLA	CHB-C4A	2.16	1.42	1.36
15	A	1112	CLA	CHB-C4A	2.16	1.42	1.36
15	A	1118	CLA	CHB-C4A	2.16	1.42	1.36
15	A	1126	CLA	C1C-C2C	2.15	1.48	1.44
15	2	603	CLA	CHB-C4A	2.15	1.42	1.36
15	A	1113	CLA	CHB-C4A	2.15	1.42	1.36
15	O	1603	CLA	CHB-C4A	2.15	1.42	1.36
15	A	1127	CLA	CHB-C4A	2.15	1.42	1.36
15	B	1209	CLA	CHB-C4A	2.15	1.42	1.36
15	A	1123	CLA	CHB-C4A	2.15	1.42	1.36
15	A	1128	CLA	CHB-C4A	2.15	1.42	1.36
15	4	603	CLA	CHB-C4A	2.15	1.42	1.36
15	B	1204	CLA	CHB-C4A	2.15	1.42	1.36
15	A	1012	CLA	C1C-C2C	2.15	1.48	1.44
15	A	1138	CLA	CHB-C4A	2.15	1.42	1.36
15	A	1109	CLA	CHB-C4A	2.15	1.42	1.36
15	A	1135	CLA	CHB-C4A	2.15	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	610	CLA	CHB-C4A	2.14	1.42	1.36
15	A	1108	CLA	CHB-C4A	2.14	1.42	1.36
15	B	1232	CLA	C1A-CHA	2.14	1.51	1.43
15	O	1602	CLA	CHB-C4A	2.14	1.42	1.36
15	B	1229	CLA	C1C-C2C	2.14	1.48	1.44
15	2	605	CLA	CHB-C4A	2.14	1.42	1.36
15	L	1502	CLA	CHB-C4A	2.14	1.42	1.36
15	A	1115	CLA	C1A-CHA	2.14	1.51	1.43
15	4	610	CLA	CHB-C4A	2.14	1.42	1.36
15	3	607	CLA	CHB-C4A	2.14	1.42	1.36
15	B	1227	CLA	CHB-C4A	2.14	1.42	1.36
15	B	1211	CLA	CHB-C4A	2.14	1.42	1.36
15	2	602	CLA	CHB-C4A	2.14	1.42	1.36
15	2	614	CLA	CHB-C4A	2.14	1.42	1.36
15	B	1234	CLA	CHB-C4A	2.14	1.42	1.36
15	3	608	CLA	CHB-C4A	2.14	1.42	1.36
15	A	1141	CLA	CHB-C4A	2.14	1.42	1.36
15	A	1102	CLA	CHB-C4A	2.14	1.42	1.36
15	A	1125	CLA	CHB-C4A	2.14	1.42	1.36
15	B	1239	CLA	CHB-C4A	2.14	1.42	1.36
15	4	604	CLA	CHB-C4A	2.14	1.42	1.36
15	A	1137	CLA	CHB-C4A	2.13	1.42	1.36
15	L	1503	CLA	CHB-C4A	2.13	1.42	1.36
15	2	601	CLA	CHB-C4A	2.13	1.42	1.36
15	B	1219	CLA	CHB-C4A	2.13	1.42	1.36
15	4	601	CLA	CHB-C4A	2.13	1.42	1.36
15	2	615	CLA	CHB-C4A	2.13	1.42	1.36
15	B	1216	CLA	CHB-C4A	2.13	1.42	1.36
15	A	1116	CLA	C1A-CHA	2.13	1.51	1.43
15	A	1124	CLA	CHB-C4A	2.13	1.42	1.36
15	B	1201	CLA	CHB-C4A	2.13	1.42	1.36
15	B	1237	CLA	C1C-C2C	2.13	1.48	1.44
15	2	606	CLA	CHB-C4A	2.13	1.42	1.36
15	A	1129	CLA	CHB-C4A	2.13	1.42	1.36
15	2	608	CLA	CHB-C4A	2.13	1.42	1.36
15	B	1217	CLA	CHB-C4A	2.13	1.42	1.36
15	4	602	CLA	CHB-C4A	2.13	1.42	1.36
15	4	612	CLA	CHB-C4A	2.13	1.42	1.36
15	B	1238	CLA	CHB-C4A	2.12	1.42	1.36
15	B	1208	CLA	CHB-C4A	2.12	1.42	1.36
15	B	1231	CLA	CHB-C4A	2.12	1.42	1.36
15	3	611	CLA	CHB-C4A	2.12	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1132	CLA	CHB-C4A	2.12	1.42	1.36
15	2	616	CLA	CHB-C4A	2.12	1.42	1.36
15	B	1210	CLA	CHB-C4A	2.12	1.42	1.36
15	O	1601	CLA	CHB-C4A	2.12	1.42	1.36
15	B	1236	CLA	C1C-C2C	2.12	1.48	1.44
15	K	1401	CLA	CHB-C4A	2.12	1.42	1.36
15	A	1120	CLA	CHB-C4A	2.12	1.42	1.36
15	B	1235	CLA	CHB-C4A	2.12	1.42	1.36
15	4	605	CLA	CHB-C4A	2.12	1.42	1.36
15	A	1119	CLA	CHB-C4A	2.12	1.42	1.36
15	A	1140	CLA	CHB-C4A	2.12	1.42	1.36
15	B	1237	CLA	C1A-CHA	2.12	1.51	1.43
15	B	1220	CLA	CHB-C4A	2.12	1.42	1.36
15	A	1133	CLA	CHB-C4A	2.12	1.42	1.36
15	4	609	CLA	CHB-C4A	2.12	1.42	1.36
15	B	1222	CLA	CHB-C4A	2.12	1.42	1.36
15	B	1214	CLA	CHB-C4A	2.12	1.42	1.36
15	B	1223	CLA	CHB-C4A	2.12	1.42	1.36
15	4	616	CLA	CHB-C4A	2.12	1.42	1.36
15	B	1206	CLA	CHB-C4A	2.12	1.42	1.36
15	B	1202	CLA	CHB-C4A	2.11	1.42	1.36
15	A	1139	CLA	CHB-C4A	2.11	1.42	1.36
15	2	612	CLA	CHB-C4A	2.11	1.42	1.36
15	3	604	CLA	CHB-C4A	2.11	1.42	1.36
15	B	1212	CLA	CHB-C4A	2.11	1.42	1.36
15	3	614	CLA	CHB-C4A	2.11	1.42	1.36
15	3	602	CLA	CHB-C4A	2.11	1.42	1.36
15	4	608	CLA	CHB-C4A	2.11	1.42	1.36
15	A	1107	CLA	C1C-C2C	2.11	1.48	1.44
15	4	606	CLA	CHB-C4A	2.11	1.41	1.36
15	B	1218	CLA	CHB-C4A	2.11	1.41	1.36
15	A	1126	CLA	C1A-CHA	2.11	1.51	1.43
15	A	1117	CLA	C1A-CHA	2.11	1.51	1.43
15	A	1131	CLA	C1A-CHA	2.11	1.51	1.43
15	2	613	CLA	CHB-C4A	2.11	1.41	1.36
15	A	1105	CLA	C1C-C2C	2.11	1.48	1.44
15	A	1130	CLA	C1C-C2C	2.11	1.48	1.44
15	B	1023	CLA	C1C-C2C	2.11	1.48	1.44
15	A	1122	CLA	CHB-C4A	2.10	1.41	1.36
15	4	611	CLA	CHB-C4A	2.10	1.41	1.36
15	B	1022	CLA	CHB-C4A	2.10	1.41	1.36
15	2	611	CLA	CHB-C4A	2.10	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	610	CLA	CHB-C4A	2.10	1.41	1.36
15	A	1114	CLA	C1C-C2C	2.10	1.48	1.44
15	4	615	CLA	CHB-C4A	2.10	1.41	1.36
15	A	1121	CLA	CHB-C4A	2.10	1.41	1.36
15	A	1136	CLA	CHB-C4A	2.10	1.41	1.36
15	B	1215	CLA	CHB-C4A	2.10	1.41	1.36
15	A	1131	CLA	C1C-C2C	2.10	1.48	1.44
15	B	1224	CLA	C1C-C2C	2.10	1.48	1.44
15	K	1402	CLA	CHB-C4A	2.10	1.41	1.36
15	B	1221	CLA	CHB-C4A	2.10	1.41	1.36
15	B	1203	CLA	CHB-C4A	2.10	1.41	1.36
15	F	1302	CLA	CHB-C4A	2.09	1.41	1.36
15	B	1021	CLA	C1A-CHA	2.09	1.51	1.43
15	A	1106	CLA	C1C-C2C	2.09	1.48	1.44
15	L	1501	CLA	CHB-C4A	2.09	1.41	1.36
15	A	1107	CLA	C1A-CHA	2.09	1.51	1.43
15	A	1103	CLA	C1A-CHA	2.09	1.51	1.43
15	B	1226	CLA	C1A-CHA	2.09	1.51	1.43
15	A	1117	CLA	C1C-C2C	2.09	1.48	1.44
15	3	612	CLA	CHB-C4A	2.08	1.41	1.36
15	A	1106	CLA	C1A-CHA	2.08	1.51	1.43
15	B	1021	CLA	C1C-C2C	2.08	1.48	1.44
15	3	606	CLA	CHB-C4A	2.08	1.41	1.36
15	3	603	CLA	CHB-C4A	2.08	1.41	1.36
15	J	1302	CLA	C1C-C2C	2.08	1.48	1.44
15	A	1104	CLA	C1A-CHA	2.07	1.51	1.43
15	A	1101	CLA	C1C-C2C	2.07	1.48	1.44
15	B	1232	CLA	C1C-C2C	2.07	1.48	1.44
15	B	1226	CLA	CHD-C1D	2.07	1.42	1.38
15	F	1301	CLA	C1C-C2C	2.07	1.48	1.44
15	B	1226	CLA	C3D-C4D	-2.07	1.39	1.44
15	A	1011	CLA	C1A-CHA	2.06	1.51	1.43
18	A	4007	BCR	C12-C13	-2.06	1.41	1.46
15	A	1103	CLA	C1C-C2C	2.06	1.48	1.44
15	B	1207	CLA	CHB-C4A	2.05	1.41	1.36
15	B	1230	CLA	CHD-C1D	2.05	1.42	1.38
15	B	1224	CLA	C1A-CHA	2.05	1.51	1.43
15	B	1205	CLA	CHB-C4A	2.05	1.41	1.36
15	3	601	CLA	CHB-C4A	2.04	1.41	1.36
15	A	1114	CLA	C1A-CHA	2.04	1.51	1.43
15	A	1012	CLA	MG-NC	2.04	2.11	2.06
15	A	1114	CLA	C3D-C4D	-2.03	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1237	CLA	MG-NC	2.02	2.11	2.06
15	F	1301	CLA	MG-NC	2.01	2.11	2.06
15	J	1302	CLA	MG-NC	2.01	2.11	2.06
15	B	1229	CLA	C1A-CHA	2.01	1.51	1.43
15	A	1011	CLA	C1C-C2C	2.01	1.48	1.44
15	A	1104	CLA	MG-NC	2.01	2.11	2.06
15	A	1013	CLA	CHD-C1D	2.00	1.42	1.38

All (1811) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	4007	BCR	C10-C11-C12	19.60	179.99	123.20
18	A	4008	BCR	C10-C11-C12	19.29	179.09	123.20
18	A	4017	BCR	C10-C11-C12	19.09	178.52	123.20
18	B	4008	BCR	C10-C11-C12	18.97	178.17	123.20
18	B	4005	BCR	C10-C11-C12	18.87	177.87	123.20
18	A	4002	BCR	C10-C11-C12	18.83	177.75	123.20
18	I	4018	BCR	C10-C11-C12	18.32	176.30	123.20
18	A	4011	BCR	C10-C11-C12	18.20	175.93	123.20
18	A	4007	BCR	C16-C15-C14	16.55	157.39	123.52
18	A	4008	BCR	C16-C15-C14	16.19	156.65	123.52
18	B	4008	BCR	C16-C15-C14	15.79	155.83	123.52
18	A	4017	BCR	C16-C15-C14	15.75	155.74	123.52
18	A	4002	BCR	C16-C15-C14	14.91	154.04	123.52
18	B	4005	BCR	C16-C15-C14	14.51	153.22	123.52
18	I	4018	BCR	C11-C10-C9	14.15	147.12	127.28
18	A	4017	BCR	C21-C20-C19	13.66	162.79	123.20
18	B	4008	BCR	C11-C10-C9	13.40	146.07	127.28
18	A	4011	BCR	C11-C10-C9	13.38	146.04	127.28
18	B	4008	BCR	C21-C20-C19	13.33	161.82	123.20
18	A	4002	BCR	C21-C20-C19	13.15	161.29	123.20
18	A	4007	BCR	C21-C20-C19	13.05	161.01	123.20
18	B	4005	BCR	C21-C20-C19	13.01	160.89	123.20
18	I	4018	BCR	C16-C15-C14	12.70	149.51	123.52
18	A	4011	BCR	C16-C15-C14	12.31	148.71	123.52
18	I	4018	BCR	C21-C20-C19	12.11	158.28	123.20
18	A	4002	BCR	C11-C10-C9	11.99	144.09	127.28
18	A	4011	BCR	C21-C20-C19	11.77	157.30	123.20
18	A	4011	BCR	C11-C12-C13	11.72	158.49	126.36
18	A	4008	BCR	C21-C20-C19	11.49	156.49	123.20
18	A	4017	BCR	C11-C10-C9	11.43	143.30	127.28
18	A	4002	BCR	C11-C12-C13	11.10	156.79	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	4005	BCR	C11-C10-C9	10.92	142.59	127.28
18	B	4005	BCR	C11-C12-C13	10.42	154.92	126.36
18	I	4018	BCR	C11-C12-C13	9.92	153.57	126.36
18	A	4017	BCR	C11-C12-C13	9.79	153.21	126.36
18	A	4008	BCR	C20-C19-C18	9.71	152.98	126.36
18	B	4008	BCR	C11-C12-C13	9.54	152.51	126.36
18	A	4007	BCR	C11-C10-C9	9.38	140.43	127.28
18	A	4008	BCR	C11-C10-C9	9.37	140.41	127.28
15	B	1230	CLA	C4A-NA-C1A	9.35	110.94	106.68
18	A	4011	BCR	C20-C19-C18	9.33	151.96	126.36
15	A	1105	CLA	C4A-NA-C1A	9.13	110.84	106.68
18	A	4007	BCR	C11-C12-C13	9.04	151.14	126.36
18	A	4007	BCR	C20-C19-C18	9.02	151.11	126.36
15	F	1301	CLA	C4A-NA-C1A	9.02	110.79	106.68
15	J	1302	CLA	C4A-NA-C1A	8.97	110.77	106.68
18	I	4018	BCR	C20-C19-C18	8.96	150.92	126.36
18	A	4008	BCR	C11-C12-C13	8.94	150.89	126.36
15	A	1103	CLA	C4A-NA-C1A	8.93	110.75	106.68
15	A	1130	CLA	C4A-NA-C1A	8.88	110.73	106.68
15	A	1106	CLA	C4A-NA-C1A	8.84	110.71	106.68
15	B	1236	CLA	C4A-NA-C1A	8.83	110.71	106.68
15	B	1232	CLA	C4A-NA-C1A	8.77	110.68	106.68
15	A	1101	CLA	C4A-NA-C1A	8.74	110.67	106.68
15	A	1131	CLA	C4A-NA-C1A	8.73	110.66	106.68
15	B	1226	CLA	C4A-NA-C1A	8.72	110.66	106.68
15	A	1117	CLA	C4A-NA-C1A	8.71	110.65	106.68
15	B	1229	CLA	C4A-NA-C1A	8.71	110.65	106.68
15	A	1116	CLA	C4A-NA-C1A	8.69	110.64	106.68
15	A	1126	CLA	C4A-NA-C1A	8.68	110.64	106.68
15	B	1023	CLA	C4A-NA-C1A	8.67	110.63	106.68
15	A	1012	CLA	C4A-NA-C1A	8.66	110.63	106.68
15	A	1115	CLA	C4A-NA-C1A	8.65	110.62	106.68
15	A	1104	CLA	C4A-NA-C1A	8.63	110.62	106.68
15	B	1224	CLA	C4A-NA-C1A	8.44	110.53	106.68
18	A	4007	BCR	C15-C14-C13	-8.44	115.45	127.28
15	B	1021	CLA	C4A-NA-C1A	8.43	110.52	106.68
15	B	1225	CLA	C4A-NA-C1A	8.41	110.52	106.68
15	B	1237	CLA	C4A-NA-C1A	8.37	110.50	106.68
15	A	1013	CLA	C4A-NA-C1A	8.26	110.45	106.68
15	A	1011	CLA	C4A-NA-C1A	8.24	110.44	106.68
15	A	1114	CLA	C4A-NA-C1A	8.21	110.42	106.68
18	B	4005	BCR	C20-C19-C18	8.18	148.81	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1107	CLA	C4A-NA-C1A	8.10	110.37	106.68
18	A	4002	BCR	C20-C19-C18	8.02	148.35	126.36
18	A	4017	BCR	C20-C19-C18	8.01	148.32	126.36
18	B	4008	BCR	C20-C19-C18	7.93	148.12	126.36
15	B	1228	CLA	C2A-C1A-CHA	-7.42	109.98	122.63
15	3	604	CLA	C2A-C1A-CHA	-6.84	110.97	122.63
15	B	1205	CLA	C2A-C1A-CHA	-6.79	111.06	122.63
15	L	1502	CLA	C2A-C1A-CHA	-6.77	111.08	122.63
15	A	1119	CLA	C2A-C1A-CHA	-6.77	111.09	122.63
15	3	612	CLA	C2A-C1A-CHA	-6.77	111.09	122.63
15	B	1222	CLA	C2A-C1A-CHA	-6.76	111.10	122.63
15	3	601	CLA	C2A-C1A-CHA	-6.76	111.11	122.63
15	O	1602	CLA	C2A-C1A-CHA	-6.75	111.11	122.63
15	B	1022	CLA	C2A-C1A-CHA	-6.75	111.12	122.63
15	4	612	CLA	C2A-C1A-CHA	-6.75	111.12	122.63
15	A	1140	CLA	C2A-C1A-CHA	-6.75	111.12	122.63
15	2	605	CLA	C2A-C1A-CHA	-6.75	111.12	122.63
15	A	1132	CLA	C2A-C1A-CHA	-6.75	111.12	122.63
15	4	610	CLA	C2A-C1A-CHA	-6.75	111.13	122.63
15	B	1202	CLA	C2A-C1A-CHA	-6.74	111.13	122.63
15	L	1503	CLA	C2A-C1A-CHA	-6.74	111.13	122.63
15	2	612	CLA	C2A-C1A-CHA	-6.74	111.13	122.63
15	K	1402	CLA	C2A-C1A-CHA	-6.74	111.13	122.63
15	3	610	CLA	C2A-C1A-CHA	-6.74	111.13	122.63
15	B	1208	CLA	C2A-C1A-CHA	-6.74	111.14	122.63
15	B	1217	CLA	C2A-C1A-CHA	-6.74	111.14	122.63
15	B	1219	CLA	C2A-C1A-CHA	-6.74	111.14	122.63
15	F	1302	CLA	C2A-C1A-CHA	-6.74	111.14	122.63
15	3	607	CLA	C2A-C1A-CHA	-6.74	111.14	122.63
15	A	1138	CLA	C2A-C1A-CHA	-6.74	111.15	122.63
15	A	1129	CLA	C2A-C1A-CHA	-6.73	111.15	122.63
15	4	606	CLA	C2A-C1A-CHA	-6.73	111.15	122.63
15	4	608	CLA	C2A-C1A-CHA	-6.73	111.15	122.63
15	B	1206	CLA	C2A-C1A-CHA	-6.73	111.15	122.63
15	B	1211	CLA	C2A-C1A-CHA	-6.73	111.15	122.63
15	B	1214	CLA	C2A-C1A-CHA	-6.73	111.15	122.63
15	2	601	CLA	C2A-C1A-CHA	-6.73	111.15	122.63
15	B	1231	CLA	C2A-C1A-CHA	-6.73	111.15	122.63
15	4	611	CLA	C2A-C1A-CHA	-6.73	111.15	122.63
15	4	601	CLA	C2A-C1A-CHA	-6.73	111.16	122.63
15	A	1102	CLA	C2A-C1A-CHA	-6.73	111.16	122.63
15	B	1234	CLA	C2A-C1A-CHA	-6.73	111.16	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1125	CLA	C2A-C1A-CHA	-6.73	111.16	122.63
15	3	611	CLA	C2A-C1A-CHA	-6.73	111.16	122.63
15	A	1121	CLA	C2A-C1A-CHA	-6.73	111.16	122.63
15	B	1209	CLA	C2A-C1A-CHA	-6.73	111.16	122.63
15	B	1216	CLA	C2A-C1A-CHA	-6.73	111.16	122.63
15	A	1141	CLA	C2A-C1A-CHA	-6.72	111.16	122.63
15	B	1235	CLA	C2A-C1A-CHA	-6.72	111.17	122.63
15	2	604	CLA	C2A-C1A-CHA	-6.72	111.17	122.63
15	2	602	CLA	C2A-C1A-CHA	-6.72	111.17	122.63
15	B	1204	CLA	C2A-C1A-CHA	-6.72	111.17	122.63
15	2	615	CLA	C2A-C1A-CHA	-6.72	111.17	122.63
15	B	1201	CLA	C2A-C1A-CHA	-6.72	111.17	122.63
15	B	1239	CLA	C2A-C1A-CHA	-6.72	111.17	122.63
15	O	1603	CLA	C2A-C1A-CHA	-6.72	111.17	122.63
15	A	1120	CLA	C2A-C1A-CHA	-6.72	111.18	122.63
15	A	1133	CLA	C2A-C1A-CHA	-6.72	111.18	122.63
15	A	1108	CLA	C2A-C1A-CHA	-6.72	111.18	122.63
15	4	609	CLA	C2A-C1A-CHA	-6.72	111.18	122.63
15	A	1134	CLA	C2A-C1A-CHA	-6.72	111.18	122.63
15	4	602	CLA	C2A-C1A-CHA	-6.71	111.18	122.63
15	B	1218	CLA	C2A-C1A-CHA	-6.71	111.18	122.63
15	L	1501	CLA	C2A-C1A-CHA	-6.71	111.18	122.63
15	3	608	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	A	1112	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	A	1139	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	B	1220	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	2	608	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	2	614	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	A	1110	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	4	604	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	2	611	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	2	606	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	4	603	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	4	605	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	B	1210	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	B	1215	CLA	C2A-C1A-CHA	-6.71	111.19	122.63
15	2	616	CLA	C2A-C1A-CHA	-6.71	111.20	122.63
15	B	1221	CLA	C2A-C1A-CHA	-6.71	111.20	122.63
15	3	606	CLA	C2A-C1A-CHA	-6.70	111.20	122.63
15	A	1109	CLA	C2A-C1A-CHA	-6.70	111.20	122.63
15	3	603	CLA	C2A-C1A-CHA	-6.70	111.20	122.63
15	A	1118	CLA	C2A-C1A-CHA	-6.70	111.20	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1212	CLA	C2A-C1A-CHA	-6.70	111.20	122.63
15	A	1135	CLA	C2A-C1A-CHA	-6.70	111.21	122.63
15	B	1238	CLA	C2A-C1A-CHA	-6.70	111.21	122.63
15	A	1123	CLA	C2A-C1A-CHA	-6.70	111.21	122.63
15	A	1122	CLA	C2A-C1A-CHA	-6.69	111.22	122.63
15	2	610	CLA	C2A-C1A-CHA	-6.69	111.22	122.63
15	2	613	CLA	C2A-C1A-CHA	-6.69	111.22	122.63
15	A	1127	CLA	C2A-C1A-CHA	-6.69	111.22	122.63
15	B	1207	CLA	C2A-C1A-CHA	-6.69	111.22	122.63
15	3	614	CLA	C2A-C1A-CHA	-6.69	111.22	122.63
15	4	616	CLA	C2A-C1A-CHA	-6.69	111.22	122.63
15	O	1601	CLA	C2A-C1A-CHA	-6.69	111.22	122.63
15	A	1136	CLA	C2A-C1A-CHA	-6.69	111.22	122.63
15	B	1203	CLA	C2A-C1A-CHA	-6.69	111.23	122.63
15	A	1111	CLA	C2A-C1A-CHA	-6.69	111.23	122.63
15	K	1401	CLA	C2A-C1A-CHA	-6.68	111.23	122.63
15	4	615	CLA	C2A-C1A-CHA	-6.68	111.23	122.63
15	B	1223	CLA	C2A-C1A-CHA	-6.68	111.24	122.63
15	2	603	CLA	C2A-C1A-CHA	-6.68	111.24	122.63
15	3	602	CLA	C2A-C1A-CHA	-6.67	111.25	122.63
15	A	1137	CLA	C2A-C1A-CHA	-6.67	111.26	122.63
15	B	1227	CLA	C2A-C1A-CHA	-6.66	111.28	122.63
15	A	1128	CLA	C2A-C1A-CHA	-6.66	111.28	122.63
15	A	1113	CLA	C2A-C1A-CHA	-6.65	111.29	122.63
18	A	4017	BCR	C15-C14-C13	-6.65	117.95	127.28
15	A	1124	CLA	C2A-C1A-CHA	-6.65	111.30	122.63
15	2	607	CLA	C2A-C1A-CHA	-6.61	111.36	122.63
15	A	1011	CLA	O2D-CGD-CBD	6.43	122.47	111.23
15	B	1230	CLA	O2D-CGD-CBD	6.36	122.35	111.23
18	B	4008	BCR	C15-C14-C13	-6.33	118.40	127.28
15	3	612	CLA	C4D-ND-C1D	6.27	110.71	106.31
15	2	607	CLA	C4D-ND-C1D	6.17	110.64	106.31
15	B	1227	CLA	C4D-ND-C1D	6.16	110.63	106.31
15	A	1122	CLA	C4D-ND-C1D	6.14	110.62	106.31
15	K	1402	CLA	C4D-ND-C1D	6.13	110.62	106.31
15	A	1125	CLA	C4D-ND-C1D	6.12	110.61	106.31
15	A	1124	CLA	C4D-ND-C1D	6.10	110.59	106.31
15	A	1102	CLA	C4D-ND-C1D	6.09	110.58	106.31
15	A	1139	CLA	C4D-ND-C1D	6.07	110.57	106.31
15	4	606	CLA	C4D-ND-C1D	6.07	110.57	106.31
15	A	1128	CLA	C4D-ND-C1D	6.07	110.57	106.31
15	2	603	CLA	C4D-ND-C1D	6.06	110.57	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1110	CLA	C4D-ND-C1D	6.06	110.57	106.31
15	4	609	CLA	C4D-ND-C1D	6.06	110.56	106.31
15	O	1602	CLA	C4D-ND-C1D	6.06	110.56	106.31
15	B	1231	CLA	C4D-ND-C1D	6.06	110.56	106.31
15	A	1132	CLA	C4D-ND-C1D	6.04	110.55	106.31
15	B	1234	CLA	C4D-ND-C1D	6.04	110.55	106.31
15	4	616	CLA	C4D-ND-C1D	6.04	110.55	106.31
15	4	612	CLA	C4D-ND-C1D	6.04	110.55	106.31
15	2	608	CLA	C4D-ND-C1D	6.04	110.55	106.31
15	A	1123	CLA	C4D-ND-C1D	6.03	110.55	106.31
15	A	1136	CLA	C4D-ND-C1D	6.03	110.54	106.31
15	A	1140	CLA	C4D-ND-C1D	6.03	110.54	106.31
15	2	616	CLA	C4D-ND-C1D	6.03	110.54	106.31
15	4	605	CLA	C4D-ND-C1D	6.03	110.54	106.31
15	4	608	CLA	C4D-ND-C1D	6.03	110.54	106.31
15	O	1601	CLA	C4D-ND-C1D	6.02	110.53	106.31
15	4	601	CLA	C4D-ND-C1D	6.01	110.53	106.31
15	B	1207	CLA	C4D-ND-C1D	6.01	110.53	106.31
15	B	1208	CLA	C4D-ND-C1D	6.01	110.53	106.31
15	A	1119	CLA	C4D-ND-C1D	6.01	110.53	106.31
15	A	1133	CLA	C4D-ND-C1D	6.01	110.53	106.31
15	4	615	CLA	C4D-ND-C1D	6.01	110.53	106.31
15	4	602	CLA	C4D-ND-C1D	6.00	110.53	106.31
15	4	604	CLA	C4D-ND-C1D	6.00	110.53	106.31
15	A	1112	CLA	C4D-ND-C1D	6.00	110.53	106.31
15	4	610	CLA	C4D-ND-C1D	6.00	110.52	106.31
15	A	1137	CLA	C4D-ND-C1D	6.00	110.52	106.31
15	B	1238	CLA	C4D-ND-C1D	6.00	110.52	106.31
15	2	610	CLA	C4D-ND-C1D	6.00	110.52	106.31
15	A	1121	CLA	C4D-ND-C1D	6.00	110.52	106.31
15	B	1223	CLA	C4D-ND-C1D	6.00	110.52	106.31
15	L	1501	CLA	C4D-ND-C1D	6.00	110.52	106.31
15	3	603	CLA	C4D-ND-C1D	6.00	110.52	106.31
15	A	1111	CLA	C4D-ND-C1D	6.00	110.52	106.31
15	A	1141	CLA	C4D-ND-C1D	6.00	110.52	106.31
15	2	602	CLA	C4D-ND-C1D	5.99	110.52	106.31
15	A	1135	CLA	C4D-ND-C1D	5.99	110.52	106.31
15	B	1206	CLA	C4D-ND-C1D	5.99	110.52	106.31
15	B	1214	CLA	C4D-ND-C1D	5.99	110.52	106.31
15	A	1113	CLA	C4D-ND-C1D	5.99	110.51	106.31
15	4	611	CLA	C4D-ND-C1D	5.99	110.51	106.31
15	B	1218	CLA	C4D-ND-C1D	5.99	110.51	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	606	CLA	C4D-ND-C1D	5.98	110.51	106.31
15	A	1138	CLA	C4D-ND-C1D	5.98	110.51	106.31
15	2	615	CLA	C4D-ND-C1D	5.98	110.51	106.31
15	A	1120	CLA	C4D-ND-C1D	5.98	110.51	106.31
15	B	1216	CLA	C4D-ND-C1D	5.98	110.51	106.31
15	B	1222	CLA	C4D-ND-C1D	5.98	110.51	106.31
15	K	1401	CLA	C4D-ND-C1D	5.98	110.51	106.31
15	F	1302	CLA	C4D-ND-C1D	5.98	110.50	106.31
15	A	1109	CLA	C4D-ND-C1D	5.97	110.50	106.31
15	3	601	CLA	C4D-ND-C1D	5.97	110.50	106.31
15	B	1239	CLA	C4D-ND-C1D	5.97	110.50	106.31
15	3	602	CLA	C4D-ND-C1D	5.97	110.50	106.31
15	B	1212	CLA	C4D-ND-C1D	5.97	110.50	106.31
15	3	607	CLA	C4D-ND-C1D	5.97	110.50	106.31
15	B	1209	CLA	C4D-ND-C1D	5.97	110.50	106.31
15	B	1221	CLA	C4D-ND-C1D	5.97	110.50	106.31
15	B	1210	CLA	C4D-ND-C1D	5.96	110.50	106.31
15	B	1226	CLA	CMD-C2D-C1D	5.96	135.23	124.73
15	4	603	CLA	C4D-ND-C1D	5.96	110.50	106.31
15	B	1201	CLA	C4D-ND-C1D	5.96	110.50	106.31
15	B	1219	CLA	C4D-ND-C1D	5.96	110.49	106.31
15	2	613	CLA	C4D-ND-C1D	5.96	110.49	106.31
15	B	1220	CLA	C4D-ND-C1D	5.96	110.49	106.31
15	2	601	CLA	C4D-ND-C1D	5.96	110.49	106.31
15	L	1503	CLA	C4D-ND-C1D	5.96	110.49	106.31
15	3	608	CLA	C4D-ND-C1D	5.95	110.49	106.31
15	B	1203	CLA	C4D-ND-C1D	5.95	110.49	106.31
15	3	610	CLA	C4D-ND-C1D	5.95	110.49	106.31
15	2	612	CLA	C4D-ND-C1D	5.95	110.49	106.31
15	2	606	CLA	C4D-ND-C1D	5.95	110.49	106.31
15	A	1127	CLA	C4D-ND-C1D	5.95	110.49	106.31
15	B	1205	CLA	C4D-ND-C1D	5.95	110.49	106.31
15	B	1215	CLA	C4D-ND-C1D	5.95	110.49	106.31
15	A	1118	CLA	C4D-ND-C1D	5.95	110.48	106.31
15	O	1603	CLA	C4D-ND-C1D	5.94	110.48	106.31
15	A	1129	CLA	C4D-ND-C1D	5.94	110.48	106.31
15	B	1211	CLA	C4D-ND-C1D	5.93	110.47	106.31
15	2	614	CLA	C4D-ND-C1D	5.92	110.46	106.31
15	B	1202	CLA	C4D-ND-C1D	5.91	110.46	106.31
15	2	604	CLA	C4D-ND-C1D	5.91	110.46	106.31
15	B	1235	CLA	C4D-ND-C1D	5.91	110.46	106.31
15	2	611	CLA	C4D-ND-C1D	5.91	110.46	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1134	CLA	C4D-ND-C1D	5.90	110.45	106.31
15	B	1217	CLA	C4D-ND-C1D	5.90	110.45	106.31
15	B	1204	CLA	C4D-ND-C1D	5.89	110.45	106.31
15	3	614	CLA	C4D-ND-C1D	5.89	110.44	106.31
15	L	1502	CLA	C4D-ND-C1D	5.87	110.43	106.31
15	A	1108	CLA	C4D-ND-C1D	5.86	110.43	106.31
15	3	611	CLA	C4D-ND-C1D	5.86	110.42	106.31
15	2	605	CLA	C4D-ND-C1D	5.86	110.42	106.31
15	B	1022	CLA	C4D-ND-C1D	5.82	110.40	106.31
15	3	604	CLA	C4D-ND-C1D	5.80	110.38	106.31
15	B	1236	CLA	O2D-CGD-CBD	5.79	121.35	111.23
15	B	1229	CLA	O2D-CGD-CBD	5.68	121.16	111.23
15	A	1106	CLA	CMD-C2D-C1D	5.63	134.64	124.73
15	B	1229	CLA	CMD-C2D-C1D	5.60	134.59	124.73
15	B	1224	CLA	CMD-C2D-C1D	5.58	134.55	124.73
15	A	1013	CLA	CMD-C2D-C1D	5.57	134.54	124.73
15	A	1114	CLA	CMD-C2D-C1D	5.56	134.53	124.73
15	A	1115	CLA	CMD-C2D-C1D	5.55	134.49	124.73
15	B	1023	CLA	CMD-C2D-C1D	5.52	134.46	124.73
15	B	1232	CLA	CMD-C2D-C1D	5.52	134.46	124.73
15	A	1105	CLA	CMD-C2D-C1D	5.52	134.45	124.73
15	A	1117	CLA	CMD-C2D-C1D	5.52	134.45	124.73
15	A	1106	CLA	O2D-CGD-CBD	5.51	120.86	111.23
15	B	1225	CLA	CMD-C2D-C1D	5.49	134.40	124.73
15	A	1116	CLA	O2D-CGD-CBD	5.49	120.82	111.23
15	A	1101	CLA	CMD-C2D-C1D	5.48	134.38	124.73
15	J	1302	CLA	CMD-C2D-C1D	5.48	134.38	124.73
15	F	1301	CLA	CMD-C2D-C1D	5.48	134.38	124.73
15	A	1011	CLA	CMD-C2D-C1D	5.47	134.37	124.73
15	A	1126	CLA	CMD-C2D-C1D	5.45	134.32	124.73
15	B	1021	CLA	CMD-C2D-C1D	5.44	134.31	124.73
15	B	1230	CLA	CMD-C2D-C1D	5.44	134.30	124.73
15	A	1130	CLA	CMD-C2D-C1D	5.42	134.28	124.73
15	B	1236	CLA	CMD-C2D-C1D	5.42	134.27	124.73
15	A	1116	CLA	CMD-C2D-C1D	5.41	134.26	124.73
15	A	1104	CLA	CMD-C2D-C1D	5.40	134.25	124.73
15	A	1107	CLA	CMD-C2D-C1D	5.38	134.21	124.73
15	A	1115	CLA	O2D-CGD-CBD	5.36	120.60	111.23
15	A	1103	CLA	CMD-C2D-C1D	5.31	134.08	124.73
15	A	1107	CLA	O2D-CGD-CBD	5.30	120.49	111.23
15	A	1117	CLA	O2D-CGD-CBD	5.24	120.39	111.23
15	A	1012	CLA	O2D-CGD-CBD	5.22	120.35	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1225	CLA	O2D-CGD-CBD	5.21	120.34	111.23
15	J	1302	CLA	O2D-CGD-CBD	5.21	120.34	111.23
15	B	1232	CLA	O2D-CGD-CBD	5.19	120.30	111.23
15	A	1130	CLA	O2D-CGD-CBD	5.10	120.15	111.23
15	B	1237	CLA	O2D-CGD-CBD	5.10	120.15	111.23
15	A	1104	CLA	O2D-CGD-CBD	5.08	120.11	111.23
15	A	1131	CLA	CMD-C2D-C1D	5.07	133.66	124.73
15	A	1103	CLA	O2D-CGD-CBD	5.06	120.07	111.23
15	B	1228	CLA	C4D-ND-C1D	5.05	109.86	106.31
15	B	1226	CLA	O2D-CGD-CBD	5.03	120.03	111.23
15	A	1012	CLA	CMD-C2D-C1D	5.00	133.53	124.73
15	A	1131	CLA	O2D-CGD-CBD	4.98	119.94	111.23
15	A	1101	CLA	O2D-CGD-CBD	4.98	119.93	111.23
15	F	1301	CLA	O2D-CGD-CBD	4.96	119.90	111.23
15	A	1013	CLA	O2D-CGD-CBD	4.94	119.86	111.23
15	B	1224	CLA	O2D-CGD-CBD	4.93	119.84	111.23
15	A	1114	CLA	O2D-CGD-CBD	4.92	119.83	111.23
15	B	1228	CLA	C1C-NC-C4C	4.91	108.92	106.68
15	B	1021	CLA	O2D-CGD-CBD	4.88	119.77	111.23
15	A	1105	CLA	O2D-CGD-CBD	4.84	119.70	111.23
15	B	1237	CLA	CMD-C2D-C1D	4.83	133.23	124.73
15	A	1126	CLA	O2D-CGD-CBD	4.78	119.59	111.23
15	B	1232	CLA	C1-C2-C3	-4.62	118.63	126.20
15	B	1203	CLA	C1C-NC-C4C	4.62	108.78	106.68
15	B	1227	CLA	C1C-NC-C4C	4.56	108.76	106.68
15	B	1207	CLA	C1C-NC-C4C	4.56	108.76	106.68
15	3	603	CLA	C1C-NC-C4C	4.53	108.75	106.68
18	B	4005	BCR	C15-C14-C13	-4.50	120.96	127.28
15	3	610	CLA	C1C-NC-C4C	4.47	108.72	106.68
15	B	1205	CLA	C1C-NC-C4C	4.46	108.71	106.68
15	L	1502	CLA	C1C-NC-C4C	4.45	108.71	106.68
15	3	601	CLA	C1C-NC-C4C	4.45	108.71	106.68
15	4	612	CLA	C1C-NC-C4C	4.45	108.71	106.68
15	B	1224	CLA	C1-C2-C3	-4.44	118.92	126.20
15	2	604	CLA	C1C-NC-C4C	4.42	108.70	106.68
15	3	604	CLA	C1C-NC-C4C	4.42	108.70	106.68
15	4	604	CLA	C1C-NC-C4C	4.42	108.70	106.68
15	B	1228	CLA	C2D-C3D-C4D	-4.42	101.98	107.35
15	4	602	CLA	C1C-NC-C4C	4.41	108.69	106.68
15	3	614	CLA	C1C-NC-C4C	4.41	108.69	106.68
18	A	4008	BCR	C33-C5-C6	-4.39	119.70	124.48
15	A	1133	CLA	C1C-NC-C4C	4.37	108.67	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1202	CLA	C1C-NC-C4C	4.37	108.67	106.68
15	L	1501	CLA	C1C-NC-C4C	4.37	108.67	106.68
15	3	607	CLA	C1C-NC-C4C	4.37	108.67	106.68
15	B	1022	CLA	C1C-NC-C4C	4.36	108.67	106.68
15	4	605	CLA	C1C-NC-C4C	4.36	108.67	106.68
15	2	601	CLA	C1C-NC-C4C	4.36	108.67	106.68
15	B	1231	CLA	C1C-NC-C4C	4.36	108.67	106.68
15	K	1401	CLA	C1C-NC-C4C	4.36	108.67	106.68
15	B	1208	CLA	C1C-NC-C4C	4.35	108.67	106.68
15	A	1137	CLA	C1C-NC-C4C	4.35	108.66	106.68
15	B	1235	CLA	C1C-NC-C4C	4.35	108.66	106.68
15	A	1111	CLA	C1C-NC-C4C	4.35	108.66	106.68
15	A	1113	CLA	C1C-NC-C4C	4.35	108.66	106.68
15	A	1135	CLA	C1C-NC-C4C	4.34	108.66	106.68
15	3	608	CLA	C1C-NC-C4C	4.34	108.66	106.68
15	B	1220	CLA	C1C-NC-C4C	4.34	108.66	106.68
15	3	611	CLA	C1C-NC-C4C	4.34	108.66	106.68
15	B	1234	CLA	C1C-NC-C4C	4.34	108.66	106.68
15	B	1222	CLA	C1C-NC-C4C	4.33	108.66	106.68
15	4	601	CLA	C1C-NC-C4C	4.33	108.66	106.68
15	A	1141	CLA	C1C-NC-C4C	4.33	108.66	106.68
15	B	1211	CLA	C1C-NC-C4C	4.33	108.66	106.68
15	B	1217	CLA	C1C-NC-C4C	4.33	108.66	106.68
15	2	612	CLA	C1C-NC-C4C	4.33	108.65	106.68
15	A	1125	CLA	C1C-NC-C4C	4.33	108.65	106.68
15	2	605	CLA	C1C-NC-C4C	4.33	108.65	106.68
15	A	1139	CLA	C1C-NC-C4C	4.33	108.65	106.68
15	B	1216	CLA	C1C-NC-C4C	4.33	108.65	106.68
15	B	1238	CLA	C1C-NC-C4C	4.32	108.65	106.68
15	B	1209	CLA	C1C-NC-C4C	4.32	108.65	106.68
15	2	615	CLA	C1C-NC-C4C	4.32	108.65	106.68
15	4	615	CLA	C1C-NC-C4C	4.32	108.65	106.68
15	2	608	CLA	C1C-NC-C4C	4.31	108.65	106.68
15	A	1140	CLA	C1C-NC-C4C	4.31	108.65	106.68
15	4	606	CLA	C1C-NC-C4C	4.31	108.64	106.68
15	B	1215	CLA	C1C-NC-C4C	4.31	108.64	106.68
15	2	602	CLA	C1C-NC-C4C	4.31	108.64	106.68
15	A	1129	CLA	C1C-NC-C4C	4.30	108.64	106.68
15	4	603	CLA	C1C-NC-C4C	4.30	108.64	106.68
15	4	609	CLA	C1C-NC-C4C	4.30	108.64	106.68
15	A	1124	CLA	C1C-NC-C4C	4.30	108.64	106.68
15	B	1239	CLA	C1C-NC-C4C	4.30	108.64	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	616	CLA	C1C-NC-C4C	4.30	108.64	106.68
15	A	1121	CLA	C1C-NC-C4C	4.30	108.64	106.68
15	A	1112	CLA	C1C-NC-C4C	4.30	108.64	106.68
15	B	1201	CLA	C1C-NC-C4C	4.29	108.64	106.68
15	2	606	CLA	C1C-NC-C4C	4.29	108.64	106.68
15	2	611	CLA	C1C-NC-C4C	4.29	108.64	106.68
15	B	1214	CLA	C1C-NC-C4C	4.29	108.64	106.68
15	4	611	CLA	C1C-NC-C4C	4.28	108.63	106.68
15	A	1118	CLA	C1C-NC-C4C	4.28	108.63	106.68
15	A	1123	CLA	C1C-NC-C4C	4.28	108.63	106.68
15	B	1210	CLA	C1C-NC-C4C	4.28	108.63	106.68
15	B	1223	CLA	C1C-NC-C4C	4.28	108.63	106.68
15	4	616	CLA	C1C-NC-C4C	4.28	108.63	106.68
15	2	614	CLA	C1C-NC-C4C	4.27	108.63	106.68
15	A	1109	CLA	C1C-NC-C4C	4.27	108.63	106.68
15	A	1134	CLA	C1C-NC-C4C	4.26	108.62	106.68
15	A	1136	CLA	C1C-NC-C4C	4.26	108.62	106.68
15	A	1127	CLA	C1C-NC-C4C	4.26	108.62	106.68
15	3	602	CLA	C1C-NC-C4C	4.25	108.62	106.68
15	A	1120	CLA	C1C-NC-C4C	4.25	108.62	106.68
15	O	1602	CLA	C1C-NC-C4C	4.25	108.62	106.68
15	4	608	CLA	C1C-NC-C4C	4.25	108.62	106.68
15	3	606	CLA	C1C-NC-C4C	4.25	108.62	106.68
15	A	1119	CLA	C1C-NC-C4C	4.25	108.62	106.68
15	A	1102	CLA	C1C-NC-C4C	4.24	108.61	106.68
15	O	1601	CLA	C1C-NC-C4C	4.24	108.61	106.68
15	L	1503	CLA	C1C-NC-C4C	4.24	108.61	106.68
15	B	1204	CLA	C1C-NC-C4C	4.24	108.61	106.68
15	4	610	CLA	C1C-NC-C4C	4.23	108.61	106.68
15	A	1108	CLA	C1C-NC-C4C	4.23	108.61	106.68
15	A	1122	CLA	C1C-NC-C4C	4.23	108.61	106.68
15	A	1138	CLA	C1C-NC-C4C	4.23	108.61	106.68
15	B	1218	CLA	C1C-NC-C4C	4.23	108.61	106.68
15	2	613	CLA	C1C-NC-C4C	4.23	108.61	106.68
15	A	1110	CLA	C1C-NC-C4C	4.23	108.61	106.68
15	B	1221	CLA	C1C-NC-C4C	4.23	108.61	106.68
15	2	610	CLA	C1C-NC-C4C	4.22	108.61	106.68
15	F	1302	CLA	C1C-NC-C4C	4.22	108.61	106.68
15	J	1302	CLA	O2A-C1-C2	4.22	124.34	108.11
15	O	1603	CLA	C1C-NC-C4C	4.20	108.60	106.68
15	B	1219	CLA	C1C-NC-C4C	4.20	108.59	106.68
15	A	1128	CLA	C1C-NC-C4C	4.19	108.59	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	1402	CLA	C1C-NC-C4C	4.18	108.58	106.68
15	B	1206	CLA	C1C-NC-C4C	4.16	108.58	106.68
15	B	1212	CLA	C1C-NC-C4C	4.13	108.56	106.68
15	A	1119	CLA	C2D-C3D-C4D	-4.13	102.34	107.35
15	3	612	CLA	C1C-NC-C4C	4.13	108.56	106.68
15	K	1402	CLA	C2D-C3D-C4D	-4.09	102.38	107.35
15	A	1107	CLA	C1-C2-C3	-4.08	119.50	126.20
15	2	603	CLA	C1C-NC-C4C	4.08	108.54	106.68
15	2	607	CLA	C1C-NC-C4C	4.07	108.54	106.68
15	B	1023	CLA	O2D-CGD-CBD	4.07	118.35	111.23
15	A	1132	CLA	C1C-NC-C4C	4.06	108.53	106.68
15	A	1125	CLA	C2D-C3D-C4D	-4.06	102.42	107.35
15	3	604	CLA	C2D-C3D-C4D	-4.06	102.42	107.35
18	A	4008	BCR	C23-C24-C25	-4.06	116.16	127.00
15	A	1124	CLA	C2D-C3D-C4D	-4.05	102.43	107.35
15	O	1602	CLA	C2D-C3D-C4D	-4.05	102.43	107.35
15	A	1129	CLA	C2D-C3D-C4D	-4.05	102.43	107.35
15	B	1207	CLA	C2D-C3D-C4D	-4.04	102.44	107.35
15	3	610	CLA	C2D-C3D-C4D	-4.03	102.45	107.35
15	B	1205	CLA	C4A-NA-C1A	-4.03	104.84	106.68
15	2	604	CLA	C2D-C3D-C4D	-4.01	102.48	107.35
15	B	1203	CLA	C2D-C3D-C4D	-4.00	102.48	107.35
15	B	1227	CLA	C2D-C3D-C4D	-4.00	102.49	107.35
15	3	607	CLA	C2D-C3D-C4D	-4.00	102.49	107.35
15	A	1104	CLA	C1-C2-C3	-4.00	119.64	126.20
15	2	601	CLA	C2D-C3D-C4D	-3.99	102.50	107.35
15	4	608	CLA	C2D-C3D-C4D	-3.99	102.50	107.35
15	O	1603	CLA	C2D-C3D-C4D	-3.99	102.50	107.35
15	B	1214	CLA	C2D-C3D-C4D	-3.99	102.50	107.35
15	2	608	CLA	C2D-C3D-C4D	-3.99	102.50	107.35
15	4	601	CLA	C2D-C3D-C4D	-3.99	102.50	107.35
15	4	611	CLA	C2D-C3D-C4D	-3.99	102.50	107.35
15	A	1120	CLA	C2D-C3D-C4D	-3.99	102.50	107.35
15	B	1211	CLA	C2D-C3D-C4D	-3.99	102.50	107.35
15	L	1502	CLA	C2D-C3D-C4D	-3.99	102.50	107.35
15	3	601	CLA	C2D-C3D-C4D	-3.98	102.51	107.35
15	B	1202	CLA	C2D-C3D-C4D	-3.98	102.51	107.35
15	A	1134	CLA	C2D-C3D-C4D	-3.98	102.51	107.35
15	B	1215	CLA	C2D-C3D-C4D	-3.98	102.51	107.35
15	B	1231	CLA	C2D-C3D-C4D	-3.98	102.51	107.35
15	B	1238	CLA	C2D-C3D-C4D	-3.98	102.51	107.35
15	2	605	CLA	C2D-C3D-C4D	-3.98	102.52	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1022	CLA	C2D-C3D-C4D	-3.98	102.52	107.35
15	4	606	CLA	C2D-C3D-C4D	-3.98	102.52	107.35
15	2	602	CLA	C2D-C3D-C4D	-3.97	102.52	107.35
15	B	1235	CLA	C2D-C3D-C4D	-3.97	102.52	107.35
15	B	1239	CLA	C2D-C3D-C4D	-3.97	102.52	107.35
15	2	606	CLA	C2D-C3D-C4D	-3.97	102.53	107.35
15	2	615	CLA	C2D-C3D-C4D	-3.97	102.53	107.35
15	B	1210	CLA	C2D-C3D-C4D	-3.97	102.53	107.35
15	B	1223	CLA	C2D-C3D-C4D	-3.97	102.53	107.35
15	B	1208	CLA	C2D-C3D-C4D	-3.97	102.53	107.35
15	3	603	CLA	C2D-C3D-C4D	-3.97	102.53	107.35
15	2	611	CLA	C2D-C3D-C4D	-3.97	102.53	107.35
15	B	1216	CLA	C2D-C3D-C4D	-3.97	102.53	107.35
15	B	1220	CLA	C2D-C3D-C4D	-3.97	102.53	107.35
15	2	616	CLA	C2D-C3D-C4D	-3.97	102.53	107.35
15	A	1122	CLA	C2D-C3D-C4D	-3.97	102.53	107.35
15	4	604	CLA	C2D-C3D-C4D	-3.96	102.53	107.35
15	4	610	CLA	C2D-C3D-C4D	-3.96	102.53	107.35
15	O	1601	CLA	C2D-C3D-C4D	-3.96	102.54	107.35
15	B	1201	CLA	C2D-C3D-C4D	-3.96	102.54	107.35
15	B	1218	CLA	C2D-C3D-C4D	-3.96	102.54	107.35
15	3	602	CLA	C2D-C3D-C4D	-3.96	102.54	107.35
15	B	1222	CLA	C2D-C3D-C4D	-3.96	102.54	107.35
15	A	1137	CLA	C2D-C3D-C4D	-3.96	102.54	107.35
15	B	1212	CLA	C2D-C3D-C4D	-3.96	102.54	107.35
15	L	1503	CLA	C2D-C3D-C4D	-3.96	102.54	107.35
15	3	611	CLA	C2D-C3D-C4D	-3.96	102.54	107.35
15	A	1121	CLA	C2D-C3D-C4D	-3.96	102.54	107.35
15	B	1217	CLA	C2D-C3D-C4D	-3.96	102.54	107.35
15	4	605	CLA	C2D-C3D-C4D	-3.95	102.55	107.35
15	3	614	CLA	C2D-C3D-C4D	-3.95	102.55	107.35
15	4	612	CLA	C2D-C3D-C4D	-3.95	102.55	107.35
15	A	1113	CLA	C2D-C3D-C4D	-3.95	102.55	107.35
15	A	1141	CLA	C2D-C3D-C4D	-3.95	102.55	107.35
15	2	610	CLA	C2D-C3D-C4D	-3.95	102.55	107.35
15	2	612	CLA	C2D-C3D-C4D	-3.95	102.55	107.35
15	B	1221	CLA	C2D-C3D-C4D	-3.95	102.55	107.35
15	A	1108	CLA	C2D-C3D-C4D	-3.95	102.56	107.35
15	A	1102	CLA	C2D-C3D-C4D	-3.95	102.56	107.35
15	B	1237	CLA	C1-C2-C3	-3.94	119.73	126.20
15	4	603	CLA	C2D-C3D-C4D	-3.94	102.56	107.35
15	4	609	CLA	C2D-C3D-C4D	-3.94	102.56	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	616	CLA	C2D-C3D-C4D	-3.94	102.56	107.35
15	A	1109	CLA	C2D-C3D-C4D	-3.94	102.56	107.35
15	A	1135	CLA	C2D-C3D-C4D	-3.94	102.56	107.35
15	B	1219	CLA	C2D-C3D-C4D	-3.94	102.56	107.35
15	A	1136	CLA	C2D-C3D-C4D	-3.94	102.56	107.35
15	F	1302	CLA	C2D-C3D-C4D	-3.94	102.56	107.35
15	K	1401	CLA	C2D-C3D-C4D	-3.94	102.56	107.35
15	B	1209	CLA	C2D-C3D-C4D	-3.94	102.56	107.35
15	A	1118	CLA	C2D-C3D-C4D	-3.94	102.57	107.35
15	3	606	CLA	C2D-C3D-C4D	-3.93	102.57	107.35
15	B	1204	CLA	C2D-C3D-C4D	-3.93	102.57	107.35
15	4	602	CLA	C2D-C3D-C4D	-3.93	102.57	107.35
15	L	1501	CLA	C2D-C3D-C4D	-3.93	102.57	107.35
15	2	607	CLA	C3D-C2D-C1D	-3.93	102.57	107.35
15	3	608	CLA	C2D-C3D-C4D	-3.93	102.58	107.35
15	A	1139	CLA	C2D-C3D-C4D	-3.93	102.58	107.35
15	B	1234	CLA	C2D-C3D-C4D	-3.93	102.58	107.35
15	B	1206	CLA	C2D-C3D-C4D	-3.93	102.58	107.35
15	A	1133	CLA	C2D-C3D-C4D	-3.92	102.58	107.35
15	3	612	CLA	C4A-NA-C1A	-3.92	104.89	106.68
15	4	615	CLA	C2D-C3D-C4D	-3.92	102.58	107.35
15	2	613	CLA	C2D-C3D-C4D	-3.92	102.58	107.35
15	A	1138	CLA	C2D-C3D-C4D	-3.91	102.59	107.35
15	3	604	CLA	C4A-NA-C1A	-3.91	104.89	106.68
15	2	614	CLA	C2D-C3D-C4D	-3.91	102.60	107.35
15	A	1110	CLA	C2D-C3D-C4D	-3.91	102.60	107.35
15	A	1128	CLA	C2D-C3D-C4D	-3.90	102.61	107.35
15	B	1023	CLA	C1-C2-C3	-3.90	120.45	126.76
15	A	1112	CLA	C2D-C3D-C4D	-3.90	102.62	107.35
15	A	1111	CLA	C2D-C3D-C4D	-3.89	102.62	107.35
15	A	1140	CLA	C2D-C3D-C4D	-3.88	102.63	107.35
15	A	1123	CLA	C2D-C3D-C4D	-3.88	102.63	107.35
15	A	1105	CLA	C1-C2-C3	-3.86	119.87	126.20
15	A	1011	CLA	C1-C2-C3	-3.85	120.53	126.76
15	A	1130	CLA	O2A-C1-C2	3.84	122.90	108.11
15	B	1205	CLA	C2D-C3D-C4D	-3.84	102.68	107.35
15	2	603	CLA	C3D-C2D-C1D	-3.84	102.68	107.35
15	A	1127	CLA	C2D-C3D-C4D	-3.82	102.71	107.35
15	A	1132	CLA	C2D-C3D-C4D	-3.81	102.72	107.35
15	3	612	CLA	C3D-C2D-C1D	-3.79	102.75	107.35
15	3	601	CLA	C4A-NA-C1A	-3.79	104.95	106.68
18	A	4002	BCR	C33-C5-C6	-3.74	120.40	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1226	CLA	C1-C2-C3	-3.74	120.08	126.20
15	A	1112	CLA	C4A-NA-C1A	-3.73	104.98	106.68
15	K	1402	CLA	C4A-NA-C1A	-3.72	104.98	106.68
15	A	1132	CLA	C4A-NA-C1A	-3.72	104.98	106.68
15	O	1602	CLA	C4A-NA-C1A	-3.72	104.98	106.68
18	B	4008	BCR	C33-C5-C6	-3.72	120.43	124.48
15	B	1229	CLA	C1-C2-C3	-3.71	120.76	126.76
15	A	1013	CLA	O2A-C1-C2	3.70	122.36	108.11
15	A	1127	CLA	C3D-C2D-C1D	-3.70	102.86	107.35
15	A	1125	CLA	C4A-NA-C1A	-3.69	105.00	106.68
15	4	602	CLA	C4A-NA-C1A	-3.69	105.00	106.68
15	A	1119	CLA	C4A-NA-C1A	-3.68	105.00	106.68
15	A	1132	CLA	C3D-C2D-C1D	-3.68	102.88	107.35
15	A	1105	CLA	O2A-C1-C2	3.67	122.22	108.11
15	A	1115	CLA	O2A-C1-C2	3.66	122.21	108.11
15	A	1113	CLA	C4A-NA-C1A	-3.66	105.01	106.68
15	A	1117	CLA	C1-C2-C3	-3.66	120.20	126.20
15	B	1237	CLA	O2A-C1-C2	3.66	122.20	108.11
15	B	1023	CLA	O2A-C1-C2	3.65	122.16	108.11
15	4	608	CLA	C4A-NA-C1A	-3.65	105.01	106.68
15	A	1135	CLA	C4A-NA-C1A	-3.65	105.01	106.68
15	A	1140	CLA	C4A-NA-C1A	-3.65	105.01	106.68
15	B	1205	CLA	C3D-C2D-C1D	-3.65	102.92	107.35
15	A	1133	CLA	C4A-NA-C1A	-3.64	105.02	106.68
15	A	1139	CLA	C4A-NA-C1A	-3.63	105.02	106.68
15	3	612	CLA	C2D-C3D-C4D	-3.63	102.94	107.35
15	B	1215	CLA	C3D-C2D-C1D	-3.63	102.94	107.35
15	O	1603	CLA	C4A-NA-C1A	-3.63	105.02	106.68
15	A	1107	CLA	O2A-C1-C2	3.62	122.05	108.11
15	4	609	CLA	C4A-NA-C1A	-3.62	105.03	106.68
15	B	1202	CLA	C4A-NA-C1A	-3.62	105.03	106.68
15	A	1112	CLA	C3D-C2D-C1D	-3.62	102.96	107.35
15	A	1104	CLA	O2A-C1-C2	3.62	122.02	108.11
15	B	1231	CLA	C4A-NA-C1A	-3.61	105.03	106.68
15	3	603	CLA	C4A-NA-C1A	-3.61	105.03	106.68
15	2	603	CLA	C4A-NA-C1A	-3.61	105.03	106.68
15	A	1138	CLA	C4A-NA-C1A	-3.61	105.03	106.68
15	F	1302	CLA	C4A-NA-C1A	-3.61	105.03	106.68
15	B	1209	CLA	C3D-C2D-C1D	-3.61	102.96	107.35
15	B	1206	CLA	C4A-NA-C1A	-3.61	105.03	106.68
15	A	1123	CLA	C3D-C2D-C1D	-3.61	102.97	107.35
18	A	4017	BCR	C33-C5-C6	-3.60	120.55	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1221	CLA	C3D-C2D-C1D	-3.60	102.97	107.35
15	L	1503	CLA	C4A-NA-C1A	-3.60	105.04	106.68
15	2	614	CLA	C4A-NA-C1A	-3.60	105.04	106.68
15	A	1118	CLA	C4A-NA-C1A	-3.60	105.04	106.68
15	B	1234	CLA	C4A-NA-C1A	-3.60	105.04	106.68
15	4	604	CLA	C4A-NA-C1A	-3.60	105.04	106.68
15	A	1127	CLA	C4A-NA-C1A	-3.60	105.04	106.68
15	4	615	CLA	C3D-C2D-C1D	-3.60	102.98	107.35
15	B	1220	CLA	C4A-NA-C1A	-3.59	105.04	106.68
15	2	603	CLA	C2D-C3D-C4D	-3.59	102.98	107.35
15	2	610	CLA	C4A-NA-C1A	-3.59	105.04	106.68
15	A	1122	CLA	C4A-NA-C1A	-3.59	105.04	106.68
15	A	1128	CLA	C3D-C2D-C1D	-3.59	102.98	107.35
15	A	1111	CLA	C3D-C2D-C1D	-3.59	102.99	107.35
15	B	1206	CLA	C3D-C2D-C1D	-3.59	102.99	107.35
15	B	1210	CLA	C4A-NA-C1A	-3.59	105.04	106.68
15	3	606	CLA	C3D-C2D-C1D	-3.59	102.99	107.35
15	2	614	CLA	C3D-C2D-C1D	-3.59	102.99	107.35
15	3	602	CLA	C3D-C2D-C1D	-3.58	102.99	107.35
15	B	1219	CLA	C4A-NA-C1A	-3.58	105.04	106.68
15	L	1501	CLA	C3D-C2D-C1D	-3.58	103.00	107.35
15	4	602	CLA	C3D-C2D-C1D	-3.58	103.00	107.35
15	B	1234	CLA	C3D-C2D-C1D	-3.58	103.00	107.35
15	L	1503	CLA	C3D-C2D-C1D	-3.58	103.00	107.35
15	B	1216	CLA	C4A-NA-C1A	-3.58	105.05	106.68
15	3	611	CLA	C3D-C2D-C1D	-3.58	103.00	107.35
15	4	601	CLA	C4A-NA-C1A	-3.58	105.05	106.68
15	B	1208	CLA	C4A-NA-C1A	-3.58	105.05	106.68
15	3	608	CLA	C3D-C2D-C1D	-3.58	103.00	107.35
15	2	616	CLA	C3D-C2D-C1D	-3.58	103.00	107.35
15	2	611	CLA	C3D-C2D-C1D	-3.57	103.01	107.35
15	B	1235	CLA	C3D-C2D-C1D	-3.57	103.01	107.35
15	B	1217	CLA	C3D-C2D-C1D	-3.57	103.01	107.35
15	3	603	CLA	C3D-C2D-C1D	-3.57	103.01	107.35
15	2	612	CLA	C3D-C2D-C1D	-3.57	103.01	107.35
15	2	612	CLA	C4A-NA-C1A	-3.57	105.05	106.68
15	A	1110	CLA	C4A-NA-C1A	-3.57	105.05	106.68
15	4	609	CLA	C3D-C2D-C1D	-3.57	103.01	107.35
15	A	1108	CLA	C3D-C2D-C1D	-3.57	103.01	107.35
15	F	1302	CLA	C3D-C2D-C1D	-3.57	103.01	107.35
15	3	610	CLA	C4A-NA-C1A	-3.57	105.05	106.68
15	A	1113	CLA	C3D-C2D-C1D	-3.57	103.02	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	601	CLA	C4A-NA-C1A	-3.57	105.05	106.68
15	4	603	CLA	C3D-C2D-C1D	-3.57	103.02	107.35
15	2	613	CLA	C3D-C2D-C1D	-3.56	103.02	107.35
15	O	1601	CLA	C3D-C2D-C1D	-3.56	103.02	107.35
15	2	605	CLA	C3D-C2D-C1D	-3.56	103.02	107.35
15	A	1118	CLA	C3D-C2D-C1D	-3.56	103.02	107.35
15	B	1222	CLA	C3D-C2D-C1D	-3.56	103.02	107.35
15	B	1221	CLA	C4A-NA-C1A	-3.56	105.05	106.68
15	A	1133	CLA	C3D-C2D-C1D	-3.56	103.02	107.35
15	L	1502	CLA	C3D-C2D-C1D	-3.56	103.02	107.35
15	B	1218	CLA	C3D-C2D-C1D	-3.56	103.02	107.35
15	B	1022	CLA	C3D-C2D-C1D	-3.56	103.02	107.35
15	B	1212	CLA	C3D-C2D-C1D	-3.56	103.02	107.35
15	B	1239	CLA	C4A-NA-C1A	-3.56	105.06	106.68
15	A	1139	CLA	C3D-C2D-C1D	-3.56	103.03	107.35
15	K	1401	CLA	C3D-C2D-C1D	-3.56	103.03	107.35
15	4	604	CLA	C3D-C2D-C1D	-3.56	103.03	107.35
15	B	1204	CLA	C3D-C2D-C1D	-3.56	103.03	107.35
15	2	602	CLA	C3D-C2D-C1D	-3.56	103.03	107.35
15	B	1239	CLA	C3D-C2D-C1D	-3.56	103.03	107.35
15	A	1110	CLA	C3D-C2D-C1D	-3.56	103.03	107.35
15	B	1219	CLA	C3D-C2D-C1D	-3.56	103.03	107.35
15	4	605	CLA	C3D-C2D-C1D	-3.55	103.03	107.35
15	3	614	CLA	C3D-C2D-C1D	-3.55	103.03	107.35
15	2	604	CLA	C3D-C2D-C1D	-3.55	103.03	107.35
15	2	611	CLA	C4A-NA-C1A	-3.55	105.06	106.68
15	A	1123	CLA	C4A-NA-C1A	-3.55	105.06	106.68
15	L	1501	CLA	C4A-NA-C1A	-3.55	105.06	106.68
15	A	1140	CLA	C3D-C2D-C1D	-3.55	103.03	107.35
18	A	4011	BCR	C28-C27-C26	-3.55	107.72	114.06
15	2	610	CLA	C3D-C2D-C1D	-3.55	103.04	107.35
15	A	1109	CLA	C3D-C2D-C1D	-3.55	103.04	107.35
15	A	1141	CLA	C3D-C2D-C1D	-3.55	103.04	107.35
15	B	1214	CLA	C3D-C2D-C1D	-3.55	103.04	107.35
15	4	616	CLA	C3D-C2D-C1D	-3.55	103.04	107.35
15	B	1201	CLA	C3D-C2D-C1D	-3.55	103.04	107.35
15	B	1216	CLA	C3D-C2D-C1D	-3.55	103.04	107.35
15	A	1136	CLA	C3D-C2D-C1D	-3.55	103.04	107.35
15	B	1214	CLA	C4A-NA-C1A	-3.54	105.06	106.68
15	A	1135	CLA	C3D-C2D-C1D	-3.54	103.04	107.35
15	B	1220	CLA	C3D-C2D-C1D	-3.54	103.05	107.35
15	4	606	CLA	C3D-C2D-C1D	-3.54	103.05	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1210	CLA	C3D-C2D-C1D	-3.54	103.05	107.35
15	4	616	CLA	C4A-NA-C1A	-3.54	105.06	106.68
15	A	1109	CLA	C4A-NA-C1A	-3.54	105.06	106.68
15	O	1601	CLA	C4A-NA-C1A	-3.54	105.06	106.68
15	4	601	CLA	C3D-C2D-C1D	-3.54	103.05	107.35
15	4	608	CLA	C3D-C2D-C1D	-3.54	103.05	107.35
15	4	610	CLA	C3D-C2D-C1D	-3.54	103.05	107.35
15	B	1203	CLA	C3D-C2D-C1D	-3.54	103.05	107.35
15	B	1208	CLA	C3D-C2D-C1D	-3.54	103.05	107.35
15	3	604	CLA	C3D-C2D-C1D	-3.54	103.05	107.35
15	2	602	CLA	C4A-NA-C1A	-3.53	105.07	106.68
15	B	1222	CLA	C4A-NA-C1A	-3.53	105.07	106.68
15	B	1231	CLA	C3D-C2D-C1D	-3.53	103.06	107.35
15	A	1136	CLA	C4A-NA-C1A	-3.53	105.07	106.68
15	A	1138	CLA	C3D-C2D-C1D	-3.53	103.06	107.35
15	O	1603	CLA	C3D-C2D-C1D	-3.53	103.06	107.35
15	A	1137	CLA	C3D-C2D-C1D	-3.53	103.06	107.35
15	B	1223	CLA	C3D-C2D-C1D	-3.53	103.06	107.35
15	B	1201	CLA	C4A-NA-C1A	-3.53	105.07	106.68
15	A	1102	CLA	C3D-C2D-C1D	-3.53	103.06	107.35
15	B	1238	CLA	C3D-C2D-C1D	-3.53	103.06	107.35
15	A	1102	CLA	C4A-NA-C1A	-3.53	105.07	106.68
15	A	1134	CLA	C3D-C2D-C1D	-3.53	103.06	107.35
15	B	1211	CLA	C3D-C2D-C1D	-3.53	103.06	107.35
15	4	612	CLA	C3D-C2D-C1D	-3.53	103.07	107.35
15	4	605	CLA	C4A-NA-C1A	-3.52	105.07	106.68
15	A	1120	CLA	C4A-NA-C1A	-3.52	105.07	106.68
15	B	1204	CLA	C4A-NA-C1A	-3.52	105.07	106.68
15	B	1211	CLA	C4A-NA-C1A	-3.52	105.07	106.68
15	2	615	CLA	C3D-C2D-C1D	-3.52	103.07	107.35
15	3	607	CLA	C3D-C2D-C1D	-3.52	103.07	107.35
15	A	1121	CLA	C3D-C2D-C1D	-3.52	103.07	107.35
15	B	1202	CLA	C3D-C2D-C1D	-3.52	103.07	107.35
15	B	1217	CLA	C4A-NA-C1A	-3.52	105.07	106.68
15	2	616	CLA	C4A-NA-C1A	-3.52	105.07	106.68
15	4	606	CLA	C4A-NA-C1A	-3.52	105.07	106.68
15	2	606	CLA	C3D-C2D-C1D	-3.52	103.08	107.35
15	3	601	CLA	C3D-C2D-C1D	-3.52	103.08	107.35
15	A	1117	CLA	O2A-C1-C2	3.52	121.64	108.11
15	2	608	CLA	C4A-NA-C1A	-3.52	105.08	106.68
15	A	1129	CLA	C3D-C2D-C1D	-3.52	103.08	107.35
15	2	608	CLA	C3D-C2D-C1D	-3.51	103.08	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	601	CLA	C3D-C2D-C1D	-3.51	103.08	107.35
15	4	611	CLA	C3D-C2D-C1D	-3.51	103.08	107.35
15	A	1120	CLA	C3D-C2D-C1D	-3.51	103.08	107.35
15	B	1230	CLA	O2A-C1-C2	3.51	120.99	108.40
15	3	610	CLA	C3D-C2D-C1D	-3.51	103.09	107.35
15	3	602	CLA	C4A-NA-C1A	-3.50	105.08	106.68
15	A	1141	CLA	C4A-NA-C1A	-3.50	105.08	106.68
15	B	1228	CLA	C3D-C2D-C1D	-3.50	103.10	107.35
15	4	611	CLA	C4A-NA-C1A	-3.50	105.08	106.68
15	2	606	CLA	C4A-NA-C1A	-3.50	105.08	106.68
15	A	1134	CLA	C4A-NA-C1A	-3.50	105.08	106.68
15	3	608	CLA	C4A-NA-C1A	-3.49	105.08	106.68
15	B	1209	CLA	C4A-NA-C1A	-3.49	105.08	106.68
15	4	603	CLA	C4A-NA-C1A	-3.49	105.09	106.68
15	A	1124	CLA	C3D-C2D-C1D	-3.49	103.11	107.35
15	B	1212	CLA	C4A-NA-C1A	-3.49	105.09	106.68
15	B	1227	CLA	C3D-C2D-C1D	-3.48	103.11	107.35
15	A	1128	CLA	C4A-NA-C1A	-3.48	105.09	106.68
15	A	1122	CLA	C3D-C2D-C1D	-3.48	103.12	107.35
15	3	614	CLA	C4A-NA-C1A	-3.48	105.09	106.68
15	2	604	CLA	C4A-NA-C1A	-3.48	105.09	106.68
15	B	1235	CLA	C4A-NA-C1A	-3.48	105.09	106.68
15	K	1401	CLA	C4A-NA-C1A	-3.48	105.09	106.68
15	B	1207	CLA	C3D-C2D-C1D	-3.48	103.12	107.35
15	B	1238	CLA	C4A-NA-C1A	-3.47	105.09	106.68
15	2	613	CLA	C4A-NA-C1A	-3.47	105.09	106.68
15	B	1223	CLA	C4A-NA-C1A	-3.47	105.10	106.68
15	A	1137	CLA	C4A-NA-C1A	-3.47	105.10	106.68
15	B	1226	CLA	O2A-C1-C2	3.46	121.43	108.11
15	A	1111	CLA	C4A-NA-C1A	-3.46	105.10	106.68
15	A	1129	CLA	C4A-NA-C1A	-3.45	105.10	106.68
15	B	1207	CLA	C4A-NA-C1A	-3.45	105.10	106.68
15	4	610	CLA	C4A-NA-C1A	-3.45	105.11	106.68
15	4	612	CLA	C4A-NA-C1A	-3.45	105.11	106.68
15	A	1106	CLA	O2A-C1-C2	3.45	121.37	108.11
15	2	615	CLA	C4A-NA-C1A	-3.44	105.11	106.68
15	O	1602	CLA	C3D-C2D-C1D	-3.43	103.18	107.35
15	2	605	CLA	C4A-NA-C1A	-3.43	105.11	106.68
15	3	607	CLA	C4A-NA-C1A	-3.42	105.12	106.68
15	A	1108	CLA	C4A-NA-C1A	-3.41	105.12	106.68
15	A	1125	CLA	C3D-C2D-C1D	-3.41	103.21	107.35
15	B	1022	CLA	C4A-NA-C1A	-3.41	105.12	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	1502	CLA	C4A-NA-C1A	-3.41	105.12	106.68
15	B	1225	CLA	C1-C2-C3	-3.40	121.26	126.76
15	B	1215	CLA	C4A-NA-C1A	-3.40	105.13	106.68
18	I	4018	BCR	C23-C24-C25	-3.39	117.94	127.00
15	A	1115	CLA	C1-C2-C3	-3.39	120.65	126.20
15	B	1218	CLA	C4A-NA-C1A	-3.38	105.14	106.68
15	B	1224	CLA	O2A-C1-C2	3.38	121.11	108.11
15	A	1121	CLA	C4A-NA-C1A	-3.38	105.14	106.68
15	4	615	CLA	C4A-NA-C1A	-3.37	105.14	106.68
15	B	1225	CLA	O2A-C1-C2	3.37	121.06	108.11
15	A	1119	CLA	C3D-C2D-C1D	-3.36	103.26	107.35
15	3	611	CLA	C4A-NA-C1A	-3.35	105.15	106.68
15	B	1230	CLA	C2C-C1C-NC	3.35	113.50	109.98
15	2	607	CLA	C2D-C3D-C4D	-3.34	103.30	107.35
15	B	1203	CLA	C4A-NA-C1A	-3.32	105.16	106.68
15	B	1227	CLA	C2B-C3B-C4B	-3.32	103.12	106.81
18	A	4007	BCR	C33-C5-C6	-3.32	120.86	124.48
16	B	2002	PQN	C11-C12-C13	-3.32	121.12	126.83
15	B	1227	CLA	C4A-NA-C1A	-3.31	105.17	106.68
15	B	1232	CLA	O2A-C1-C2	3.31	120.85	108.11
15	K	1402	CLA	C3D-C2D-C1D	-3.29	103.35	107.35
15	B	1229	CLA	O2A-C1-C2	3.27	120.70	108.11
15	3	606	CLA	C4A-NA-C1A	-3.27	105.19	106.68
15	A	1126	CLA	C1-C2-C3	-3.26	120.86	126.20
18	I	4018	BCR	C15-C14-C13	-3.25	122.72	127.28
15	A	1124	CLA	C4A-NA-C1A	-3.25	105.20	106.68
15	B	1226	CLA	C2C-C1C-NC	3.24	113.38	109.98
18	A	4011	BCR	C33-C5-C6	-3.21	120.98	124.48
15	A	1126	CLA	O2A-C1-C2	3.21	120.46	108.11
15	A	1126	CLA	CMA-C3A-C4A	3.18	120.33	111.77
15	A	1130	CLA	C1-C2-C3	-3.17	121.00	126.20
15	A	1011	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
15	B	1201	CLA	C2B-C3B-C4B	-3.17	103.28	106.81
15	A	1122	CLA	C2B-C3B-C4B	-3.15	103.30	106.81
15	3	603	CLA	C2B-C3B-C4B	-3.13	103.32	106.81
15	A	1124	CLA	C2B-C3B-C4B	-3.12	103.34	106.81
15	B	1228	CLA	C3A-C4A-CHB	3.12	127.73	123.91
15	A	1134	CLA	C2B-C3B-C4B	-3.11	103.34	106.81
15	3	601	CLA	C2B-C3B-C4B	-3.09	103.37	106.81
15	A	1103	CLA	C1-C2-C3	-3.09	121.14	126.20
15	B	1239	CLA	C2B-C3B-C4B	-3.09	103.37	106.81
15	B	1226	CLA	CMA-C3A-C4A	3.08	120.06	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J	1302	CLA	CMA-C3A-C4A	3.08	120.06	111.77
15	A	1117	CLA	CMA-C3A-C4A	3.08	120.05	111.77
15	B	1205	CLA	C2B-C3B-C4B	-3.08	103.38	106.81
15	2	604	CLA	C2B-C3B-C4B	-3.08	103.39	106.81
15	A	1130	CLA	CMA-C3A-C4A	3.07	120.03	111.77
15	4	601	CLA	C2B-C3B-C4B	-3.07	103.39	106.81
15	A	1111	CLA	C2B-C3B-C4B	-3.07	103.39	106.81
15	A	1131	CLA	CMA-C3A-C4A	3.07	120.03	111.77
15	F	1302	CLA	C2B-C3B-C4B	-3.07	103.39	106.81
15	3	611	CLA	C2B-C3B-C4B	-3.07	103.39	106.81
15	4	602	CLA	C2B-C3B-C4B	-3.07	103.40	106.81
15	3	608	CLA	C2B-C3B-C4B	-3.06	103.40	106.81
15	A	1116	CLA	O2A-C1-C2	3.06	119.90	108.11
15	A	1101	CLA	CMA-C3A-C4A	3.06	120.00	111.77
15	A	1141	CLA	C2B-C3B-C4B	-3.06	103.41	106.81
15	B	1224	CLA	CMA-C3A-C4A	3.06	119.99	111.77
15	2	603	CLA	C2B-C3B-C4B	-3.06	103.41	106.81
15	3	602	CLA	C2B-C3B-C4B	-3.06	103.41	106.81
15	B	1203	CLA	C2B-C3B-C4B	-3.06	103.41	106.81
15	L	1503	CLA	C2B-C3B-C4B	-3.06	103.41	106.81
15	A	1114	CLA	CMA-C3A-C4A	3.05	119.98	111.77
15	4	612	CLA	C2B-C3B-C4B	-3.05	103.41	106.81
15	2	605	CLA	C2B-C3B-C4B	-3.05	103.42	106.81
15	4	616	CLA	C2B-C3B-C4B	-3.05	103.42	106.81
15	2	602	CLA	C2B-C3B-C4B	-3.05	103.42	106.81
15	A	1137	CLA	C2B-C3B-C4B	-3.05	103.42	106.81
15	B	1218	CLA	C2B-C3B-C4B	-3.04	103.42	106.81
15	2	615	CLA	C2B-C3B-C4B	-3.04	103.43	106.81
15	4	611	CLA	C2B-C3B-C4B	-3.04	103.43	106.81
15	B	1210	CLA	C2B-C3B-C4B	-3.04	103.43	106.81
15	2	601	CLA	C2B-C3B-C4B	-3.03	103.43	106.81
15	B	1215	CLA	C2B-C3B-C4B	-3.03	103.43	106.81
15	4	603	CLA	C2B-C3B-C4B	-3.03	103.43	106.81
18	A	4007	BCR	C33-C5-C4	3.03	120.06	113.60
15	A	1112	CLA	C2B-C3B-C4B	-3.03	103.43	106.81
16	A	2001	PQN	C14-C13-C15	3.03	120.49	115.23
15	A	1011	CLA	O2A-C1-C2	3.03	119.78	108.11
15	A	1138	CLA	C2B-C3B-C4B	-3.03	103.44	106.81
15	L	1502	CLA	C2B-C3B-C4B	-3.03	103.44	106.81
15	B	1230	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
15	A	1129	CLA	C2B-C3B-C4B	-3.03	103.44	106.81
15	2	607	CLA	C2B-C3B-C4B	-3.03	103.44	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1231	CLA	C2B-C3B-C4B	-3.03	103.44	106.81
15	L	1501	CLA	C2B-C3B-C4B	-3.03	103.44	106.81
15	2	614	CLA	C2B-C3B-C4B	-3.03	103.44	106.81
15	B	1220	CLA	C2B-C3B-C4B	-3.03	103.44	106.81
15	4	605	CLA	C2B-C3B-C4B	-3.03	103.44	106.81
15	B	1204	CLA	C2B-C3B-C4B	-3.02	103.44	106.81
15	O	1601	CLA	C2B-C3B-C4B	-3.02	103.44	106.81
15	4	610	CLA	C2B-C3B-C4B	-3.02	103.44	106.81
15	A	1102	CLA	C2B-C3B-C4B	-3.02	103.44	106.81
15	B	1223	CLA	C2B-C3B-C4B	-3.02	103.44	106.81
15	B	1209	CLA	C2B-C3B-C4B	-3.02	103.45	106.81
15	B	1237	CLA	CMA-C3A-C4A	3.02	119.89	111.77
15	A	1113	CLA	C2B-C3B-C4B	-3.02	103.45	106.81
15	A	1133	CLA	C2B-C3B-C4B	-3.02	103.45	106.81
15	O	1602	CLA	C2B-C3B-C4B	-3.02	103.45	106.81
15	2	610	CLA	C2B-C3B-C4B	-3.02	103.45	106.81
15	A	1118	CLA	C2B-C3B-C4B	-3.01	103.45	106.81
15	A	1012	CLA	O2A-C1-C2	3.01	119.71	108.11
15	B	1222	CLA	C2B-C3B-C4B	-3.01	103.45	106.81
15	2	612	CLA	C2B-C3B-C4B	-3.01	103.46	106.81
15	3	606	CLA	C2B-C3B-C4B	-3.01	103.46	106.81
18	A	4002	BCR	C33-C5-C4	3.01	120.02	113.60
15	A	1110	CLA	C2B-C3B-C4B	-3.01	103.46	106.81
15	3	614	CLA	C2B-C3B-C4B	-3.01	103.46	106.81
15	A	1132	CLA	C2B-C3B-C4B	-3.01	103.46	106.81
15	A	1139	CLA	C2B-C3B-C4B	-3.01	103.46	106.81
15	B	1214	CLA	C2B-C3B-C4B	-3.01	103.46	106.81
15	K	1402	CLA	C2B-C3B-C4B	-3.01	103.46	106.81
15	B	1217	CLA	C2B-C3B-C4B	-3.01	103.46	106.81
15	B	1221	CLA	C2B-C3B-C4B	-3.01	103.46	106.81
15	2	606	CLA	C2B-C3B-C4B	-3.00	103.47	106.81
15	B	1208	CLA	C2B-C3B-C4B	-3.00	103.47	106.81
15	B	1216	CLA	C2B-C3B-C4B	-3.00	103.47	106.81
15	A	1121	CLA	C2B-C3B-C4B	-3.00	103.47	106.81
15	B	1207	CLA	C2B-C3B-C4B	-3.00	103.47	106.81
15	B	1212	CLA	C2B-C3B-C4B	-3.00	103.47	106.81
15	A	1103	CLA	C1C-C2C-C3C	-3.00	103.83	106.98
15	4	608	CLA	C2B-C3B-C4B	-3.00	103.47	106.81
15	A	1136	CLA	C2B-C3B-C4B	-3.00	103.47	106.81
15	2	613	CLA	C2B-C3B-C4B	-2.99	103.48	106.81
15	3	607	CLA	C2B-C3B-C4B	-2.99	103.48	106.81
15	4	604	CLA	C2B-C3B-C4B	-2.99	103.48	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	606	CLA	C2B-C3B-C4B	-2.99	103.48	106.81
15	A	1127	CLA	C2B-C3B-C4B	-2.99	103.48	106.81
15	B	1234	CLA	C2B-C3B-C4B	-2.99	103.48	106.81
15	A	1013	CLA	C1-C2-C3	-2.99	121.30	126.20
15	A	1119	CLA	C2B-C3B-C4B	-2.99	103.49	106.81
15	B	1219	CLA	C2B-C3B-C4B	-2.99	103.49	106.81
15	O	1603	CLA	C2B-C3B-C4B	-2.99	103.49	106.81
15	2	608	CLA	C2B-C3B-C4B	-2.99	103.49	106.81
15	K	1401	CLA	C2B-C3B-C4B	-2.98	103.49	106.81
15	J	1302	CLA	C2C-C1C-NC	2.98	113.12	109.98
15	4	609	CLA	C2B-C3B-C4B	-2.98	103.49	106.81
15	B	1238	CLA	C2B-C3B-C4B	-2.98	103.49	106.81
15	2	611	CLA	C2B-C3B-C4B	-2.98	103.50	106.81
15	B	1232	CLA	CMA-C3A-C4A	2.97	119.77	111.77
15	2	616	CLA	C2B-C3B-C4B	-2.97	103.50	106.81
15	B	1206	CLA	C2B-C3B-C4B	-2.97	103.50	106.81
15	3	610	CLA	C2B-C3B-C4B	-2.97	103.51	106.81
15	2	607	CLA	C4A-NA-C1A	-2.97	105.33	106.68
15	B	1211	CLA	C2B-C3B-C4B	-2.97	103.51	106.81
15	B	1022	CLA	C2B-C3B-C4B	-2.96	103.51	106.81
15	A	1125	CLA	C2B-C3B-C4B	-2.96	103.51	106.81
15	A	1128	CLA	C2B-C3B-C4B	-2.96	103.51	106.81
15	A	1108	CLA	C2B-C3B-C4B	-2.96	103.52	106.81
15	A	1109	CLA	C2B-C3B-C4B	-2.95	103.52	106.81
15	A	1120	CLA	C2B-C3B-C4B	-2.95	103.52	106.81
18	A	4008	BCR	C27-C26-C25	-2.95	118.72	122.70
15	3	604	CLA	C2B-C3B-C4B	-2.95	103.53	106.81
15	B	1235	CLA	C2B-C3B-C4B	-2.95	103.53	106.81
15	A	1135	CLA	C2B-C3B-C4B	-2.94	103.53	106.81
15	J	1302	CLA	C1-O2A-CGA	2.94	123.77	116.65
15	B	1230	CLA	CMA-C3A-C4A	2.94	119.67	111.77
15	A	1105	CLA	CMA-C3A-C4A	2.94	119.67	111.77
15	F	1301	CLA	CMA-C3A-C4A	2.93	119.65	111.77
15	A	1123	CLA	C2B-C3B-C4B	-2.92	103.56	106.81
15	A	1107	CLA	CMA-C3A-C4A	2.92	119.62	111.77
15	3	612	CLA	C2B-C3B-C4B	-2.92	103.56	106.81
15	4	615	CLA	C2B-C3B-C4B	-2.92	103.56	106.81
15	A	1103	CLA	O2A-C1-C2	2.91	119.31	108.11
15	A	1140	CLA	C2B-C3B-C4B	-2.91	103.58	106.81
15	A	1115	CLA	CMA-C3A-C4A	2.90	119.58	111.77
15	F	1301	CLA	C2C-C1C-NC	2.90	113.03	109.98
15	B	1202	CLA	C2B-C3B-C4B	-2.90	103.59	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1105	CLA	C2C-C1C-NC	2.89	113.02	109.98
15	B	1236	CLA	C2C-C1C-NC	2.89	113.02	109.98
16	B	2002	PQN	C14-C13-C15	2.88	120.23	115.23
15	B	1228	CLA	C2B-C3B-C4B	-2.88	103.60	106.81
15	A	1131	CLA	C2C-C1C-NC	2.88	113.00	109.98
15	3	603	CLA	C3A-C4A-CHB	2.88	127.44	123.91
15	A	1122	CLA	C3A-C4A-CHB	2.87	127.43	123.91
18	A	4011	BCR	C33-C5-C4	2.87	119.70	113.60
15	B	1229	CLA	C2C-C1C-NC	2.86	112.99	109.98
15	A	1116	CLA	CMA-C3A-C4A	2.86	119.46	111.77
15	J	1302	CLA	CAA-C2A-C3A	-2.86	105.28	113.00
15	K	1402	CLA	C3A-C4A-CHB	2.85	127.41	123.91
15	A	1123	CLA	C3A-C4A-CHB	2.85	127.40	123.91
15	A	1106	CLA	CMA-C3A-C4A	2.85	119.43	111.77
15	B	1226	CLA	CMD-C2D-C3D	-2.85	121.16	127.69
15	B	1232	CLA	C2C-C1C-NC	2.84	112.97	109.98
15	F	1301	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
15	B	1229	CLA	CMA-C3A-C4A	2.84	119.40	111.77
15	3	602	CLA	C3A-C4A-CHB	2.84	127.39	123.91
15	B	1205	CLA	C3A-C4A-CHB	2.83	127.38	123.91
15	B	1212	CLA	C3A-C4A-CHB	2.83	127.38	123.91
15	3	607	CLA	C3A-C4A-CHB	2.83	127.38	123.91
15	B	1224	CLA	C3B-C4B-NB	-2.83	108.01	110.53
15	A	1140	CLA	C3A-C4A-CHB	2.82	127.37	123.91
15	B	1229	CLA	C4B-CHC-C1C	2.82	132.88	126.25
15	A	1112	CLA	C3A-C4A-CHB	2.82	127.36	123.91
18	B	4005	BCR	C30-C25-C26	-2.82	118.79	122.64
15	A	1102	CLA	C3A-C4A-CHB	2.82	127.36	123.91
15	B	1239	CLA	C3A-C4A-CHB	2.82	127.36	123.91
15	A	1124	CLA	C3A-C4A-CHB	2.81	127.36	123.91
15	O	1601	CLA	C3A-C4A-CHB	2.81	127.36	123.91
15	A	1108	CLA	C3A-C4A-CHB	2.81	127.36	123.91
15	A	1128	CLA	C3A-C4A-CHB	2.81	127.36	123.91
15	B	1218	CLA	C3A-C4A-CHB	2.81	127.36	123.91
15	A	1013	CLA	C2C-C1C-NC	2.81	112.94	109.98
15	A	1119	CLA	C3A-C4A-CHB	2.81	127.35	123.91
15	A	1012	CLA	C2C-C1C-NC	2.81	112.93	109.98
15	3	601	CLA	C3A-C4A-CHB	2.80	127.35	123.91
15	A	1134	CLA	C3A-C4A-CHB	2.80	127.34	123.91
15	B	1229	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
15	2	611	CLA	C3A-C4A-CHB	2.80	127.34	123.91
15	B	1204	CLA	C3A-C4A-CHB	2.80	127.34	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	612	CLA	C3A-C4A-CHB	2.80	127.34	123.91
15	4	604	CLA	C3A-C4A-CHB	2.80	127.34	123.91
15	A	1106	CLA	C1-C2-C3	-2.79	121.62	126.20
15	J	1302	CLA	C1C-C2C-C3C	-2.79	104.04	106.98
15	A	1139	CLA	C3A-C4A-CHB	2.79	127.33	123.91
15	A	1116	CLA	O2A-CGA-CBA	2.79	120.34	111.83
15	B	1225	CLA	CMA-C3A-C4A	2.79	119.27	111.77
15	4	610	CLA	C3A-C4A-CHB	2.79	127.33	123.91
15	A	1110	CLA	C3A-C4A-CHB	2.79	127.33	123.91
15	A	1138	CLA	C3A-C4A-CHB	2.78	127.32	123.91
15	B	1222	CLA	C3A-C4A-CHB	2.78	127.32	123.91
15	F	1302	CLA	C3A-C4A-CHB	2.78	127.32	123.91
15	B	1221	CLA	C3A-C4A-CHB	2.78	127.32	123.91
15	B	1231	CLA	C3A-C4A-CHB	2.78	127.32	123.91
15	2	603	CLA	C3A-C4A-CHB	2.78	127.32	123.91
15	A	1141	CLA	C3A-C4A-CHB	2.78	127.32	123.91
15	A	1125	CLA	C3A-C4A-CHB	2.78	127.32	123.91
15	4	601	CLA	C3A-C4A-CHB	2.78	127.32	123.91
15	B	1228	CLA	C3D-C4D-ND	2.78	113.30	109.50
15	B	1214	CLA	C3A-C4A-CHB	2.78	127.31	123.91
15	K	1401	CLA	C3A-C4A-CHB	2.78	127.31	123.91
15	L	1502	CLA	C3A-C4A-CHB	2.78	127.31	123.91
15	O	1603	CLA	C3A-C4A-CHB	2.78	127.31	123.91
15	2	604	CLA	C3A-C4A-CHB	2.78	127.31	123.91
15	A	1109	CLA	C3A-C4A-CHB	2.77	127.31	123.91
15	4	611	CLA	C3A-C4A-CHB	2.77	127.31	123.91
15	4	608	CLA	C3A-C4A-CHB	2.77	127.31	123.91
15	2	601	CLA	C3A-C4A-CHB	2.77	127.31	123.91
15	2	608	CLA	C3A-C4A-CHB	2.77	127.31	123.91
15	2	614	CLA	C3A-C4A-CHB	2.77	127.31	123.91
15	B	1223	CLA	C3A-C4A-CHB	2.77	127.30	123.91
15	B	1235	CLA	C3A-C4A-CHB	2.77	127.30	123.91
15	B	1227	CLA	C3A-C4A-CHB	2.77	127.30	123.91
15	4	603	CLA	C3A-C4A-CHB	2.77	127.30	123.91
15	A	1133	CLA	C3A-C4A-CHB	2.77	127.30	123.91
15	J	1302	CLA	C1-C2-C3	-2.77	122.29	126.76
15	2	602	CLA	C3A-C4A-CHB	2.77	127.30	123.91
15	A	1137	CLA	C3A-C4A-CHB	2.77	127.30	123.91
15	A	1132	CLA	C3A-C4A-CHB	2.76	127.30	123.91
15	A	1013	CLA	O2A-CGA-CBA	2.76	120.26	111.83
15	A	1107	CLA	C2C-C1C-NC	2.76	112.88	109.98
15	3	608	CLA	C3A-C4A-CHB	2.76	127.30	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1209	CLA	C3A-C4A-CHB	2.76	127.29	123.91
15	O	1602	CLA	C3A-C4A-CHB	2.76	127.29	123.91
15	A	1121	CLA	C3A-C4A-CHB	2.76	127.29	123.91
15	L	1501	CLA	C3A-C4A-CHB	2.76	127.29	123.91
15	B	1236	CLA	CMA-C3A-C4A	2.76	119.18	111.77
15	A	1101	CLA	C2C-C1C-NC	2.76	112.88	109.98
15	2	616	CLA	C3A-C4A-CHB	2.76	127.29	123.91
15	A	1111	CLA	C3A-C4A-CHB	2.75	127.29	123.91
15	B	1234	CLA	C3A-C4A-CHB	2.75	127.29	123.91
15	2	605	CLA	C3A-C4A-CHB	2.75	127.28	123.91
15	A	1129	CLA	C3A-C4A-CHB	2.75	127.28	123.91
15	4	616	CLA	C3A-C4A-CHB	2.75	127.28	123.91
15	B	1210	CLA	C3A-C4A-CHB	2.75	127.28	123.91
15	A	1118	CLA	C3A-C4A-CHB	2.75	127.28	123.91
15	B	1237	CLA	C2C-C1C-NC	2.75	112.87	109.98
15	B	1238	CLA	C3A-C4A-CHB	2.74	127.27	123.91
15	3	610	CLA	C3A-C4A-CHB	2.74	127.27	123.91
15	2	606	CLA	C3A-C4A-CHB	2.74	127.27	123.91
15	2	615	CLA	C3A-C4A-CHB	2.74	127.27	123.91
15	4	609	CLA	C3A-C4A-CHB	2.74	127.27	123.91
15	A	1135	CLA	C3A-C4A-CHB	2.74	127.27	123.91
15	B	1208	CLA	C3A-C4A-CHB	2.74	127.27	123.91
15	L	1503	CLA	C3A-C4A-CHB	2.74	127.27	123.91
15	4	606	CLA	C3A-C4A-CHB	2.74	127.27	123.91
15	4	602	CLA	C3A-C4A-CHB	2.74	127.27	123.91
15	F	1301	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
15	3	612	CLA	C3A-C4A-CHB	2.73	127.26	123.91
15	A	1106	CLA	C2C-C1C-NC	2.73	112.85	109.98
15	A	1130	CLA	C2C-C1C-NC	2.73	112.85	109.98
15	A	1103	CLA	C2C-C1C-NC	2.73	112.85	109.98
18	A	4007	BCR	C23-C24-C25	-2.73	119.70	127.00
15	A	1136	CLA	C3A-C4A-CHB	2.73	127.26	123.91
15	B	1215	CLA	C3A-C4A-CHB	2.73	127.26	123.91
15	B	1219	CLA	C3A-C4A-CHB	2.73	127.26	123.91
15	B	1216	CLA	C3A-C4A-CHB	2.73	127.25	123.91
18	I	4018	BCR	C4-C5-C6	-2.73	119.02	122.70
15	A	1107	CLA	C3B-C4B-NB	-2.73	108.09	110.53
15	A	1127	CLA	C3A-C4A-CHB	2.73	127.25	123.91
15	B	1236	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
15	2	613	CLA	C3A-C4A-CHB	2.72	127.25	123.91
15	3	606	CLA	C3A-C4A-CHB	2.72	127.25	123.91
15	A	1116	CLA	C3B-C4B-NB	-2.72	108.10	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1220	CLA	C3A-C4A-CHB	2.72	127.25	123.91
15	A	1131	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
15	B	1232	CLA	O2A-CGA-CBA	2.72	120.12	111.83
15	A	1113	CLA	C3A-C4A-CHB	2.72	127.24	123.91
15	B	1207	CLA	C3A-C4A-CHB	2.72	127.24	123.91
15	A	1012	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
15	B	1236	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
15	A	1104	CLA	CMA-C3A-C4A	2.71	119.07	111.77
15	3	614	CLA	C3A-C4A-CHB	2.71	127.24	123.91
18	A	4011	BCR	C35-C13-C12	2.71	122.23	118.09
15	2	612	CLA	C3A-C4A-CHB	2.71	127.23	123.91
15	4	615	CLA	C3A-C4A-CHB	2.71	127.23	123.91
15	B	1217	CLA	C3A-C4A-CHB	2.71	127.23	123.91
15	A	1105	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
15	A	1103	CLA	CMA-C3A-C4A	2.71	119.05	111.77
15	A	1104	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
15	3	611	CLA	C3A-C4A-CHB	2.71	127.23	123.91
15	A	1120	CLA	C3A-C4A-CHB	2.70	127.22	123.91
15	A	1126	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
15	B	1206	CLA	C3A-C4A-CHB	2.70	127.22	123.91
15	A	1126	CLA	C2C-C1C-NC	2.70	112.82	109.98
15	2	610	CLA	C3A-C4A-CHB	2.70	127.22	123.91
15	B	1202	CLA	C3A-C4A-CHB	2.70	127.22	123.91
15	B	1226	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
15	4	605	CLA	C3A-C4A-CHB	2.69	127.21	123.91
15	A	1012	CLA	CMA-C3A-C4A	2.69	119.01	111.77
15	B	1236	CLA	C4B-CHC-C1C	2.69	132.58	126.25
15	A	1013	CLA	C3B-C4B-NB	-2.69	108.13	110.53
15	B	1211	CLA	C3A-C4A-CHB	2.69	127.20	123.91
18	A	4007	BCR	C4-C5-C6	-2.69	119.07	122.70
15	A	1114	CLA	C2C-C1C-NC	2.69	112.80	109.98
18	A	4007	BCR	C27-C26-C25	-2.68	119.08	122.70
15	A	1114	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
18	A	4007	BCR	C34-C9-C10	-2.68	118.47	122.82
15	B	1201	CLA	C3A-C4A-CHB	2.68	127.19	123.91
15	A	1107	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
16	A	2001	PQN	C11-C12-C13	-2.67	122.23	126.83
15	B	1228	CLA	CHA-C4D-ND	-2.67	121.08	124.84
15	B	1022	CLA	C3A-C4A-CHB	2.67	127.18	123.91
15	2	607	CLA	C3A-C4A-CHB	2.66	127.17	123.91
18	A	4008	BCR	C33-C5-C4	2.66	119.27	113.60
15	A	1104	CLA	C2C-C1C-NC	2.66	112.78	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1101	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
15	3	604	CLA	C3A-C4A-CHB	2.66	127.17	123.91
15	A	1130	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
15	B	1225	CLA	C1D-ND-C4D	-2.65	104.45	106.31
15	A	1106	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
15	B	1203	CLA	C3A-C4A-CHB	2.65	127.16	123.91
18	I	4018	BCR	C34-C9-C10	-2.64	118.54	122.82
15	A	1115	CLA	C2C-C1C-NC	2.63	112.75	109.98
15	B	1023	CLA	O2A-CGA-CBA	2.63	119.86	111.83
18	A	4002	BCR	C27-C26-C25	-2.63	119.15	122.70
18	A	4017	BCR	C33-C5-C4	2.63	119.20	113.60
15	A	1105	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
15	B	1023	CLA	C3B-C4B-NB	-2.62	108.19	110.53
15	A	1105	CLA	O2A-CGA-CBA	2.62	119.82	111.83
18	A	4011	BCR	C8-C7-C6	-2.61	120.03	127.00
15	A	1011	CLA	CMA-C3A-C4A	2.61	118.78	111.77
18	B	4005	BCR	C27-C26-C25	-2.60	119.19	122.70
15	A	1101	CLA	C3B-C4B-NB	-2.60	108.21	110.53
15	A	1012	CLA	O2A-CGA-CBA	2.60	119.76	111.83
15	A	1115	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
15	B	1021	CLA	C2C-C1C-NC	2.60	112.71	109.98
15	B	1232	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
15	B	1232	CLA	C3B-C4B-NB	-2.59	108.22	110.53
18	A	4011	BCR	C27-C26-C25	-2.59	119.21	122.70
15	B	1237	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
15	A	1114	CLA	C3B-C4B-NB	-2.58	108.22	110.53
15	A	1013	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
15	B	1229	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
15	A	1117	CLA	O2A-CGA-CBA	2.57	119.68	111.83
15	A	1117	CLA	C2C-C1C-NC	2.57	112.68	109.98
15	A	1106	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
15	J	1302	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
15	A	1012	CLA	C3B-C4B-NB	-2.56	108.25	110.53
15	A	1126	CLA	C4B-CHC-C1C	2.55	132.25	126.25
15	B	1225	CLA	C3B-C4B-NB	-2.55	108.26	110.53
15	B	1236	CLA	C3B-C4B-NB	-2.54	108.26	110.53
15	B	1224	CLA	C2C-C1C-NC	2.54	112.65	109.98
18	B	4005	BCR	C4-C5-C6	-2.54	119.28	122.70
15	A	1013	CLA	CHA-C4D-ND	2.53	137.78	132.55
18	A	4008	BCR	C15-C14-C13	-2.53	123.72	127.28
15	A	1107	CLA	C4B-CHC-C1C	2.53	132.20	126.25
15	A	1117	CLA	O2D-CGD-O1D	-2.53	118.92	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1116	CLA	C2C-C1C-NC	2.53	112.64	109.98
15	B	1225	CLA	CHD-C1D-ND	-2.53	121.25	124.80
15	B	1021	CLA	CMA-C3A-C4A	2.52	118.56	111.77
15	A	1114	CLA	CMD-C2D-C3D	-2.52	121.91	127.69
15	A	1013	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
15	A	1011	CLA	C2C-C1C-NC	2.52	112.63	109.98
18	A	4011	BCR	C4-C5-C6	-2.51	119.31	122.70
18	A	4007	BCR	C12-C13-C14	2.51	122.96	119.01
15	3	606	CLA	C1C-CHC-C4B	2.51	132.67	126.04
15	A	1117	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
18	B	4005	BCR	C28-C27-C26	-2.50	109.59	114.06
15	A	1126	CLA	O2A-CGA-CBA	2.50	119.45	111.83
18	I	4018	BCR	C33-C5-C4	2.50	118.92	113.60
15	A	1011	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
15	B	1237	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
15	A	1116	CLA	C4B-CHC-C1C	2.48	132.09	126.25
15	A	1115	CLA	C3B-C4B-NB	-2.48	108.31	110.53
15	A	1012	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
15	B	1225	CLA	C1C-C2C-C3C	-2.48	104.37	106.98
15	A	1011	CLA	CHD-C1D-ND	-2.48	121.31	124.80
15	A	1105	CLA	CHA-C4D-ND	2.48	137.66	132.55
15	A	1115	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
15	A	1114	CLA	CHA-C4D-ND	2.47	137.65	132.55
15	B	1232	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
15	F	1301	CLA	CHA-C4D-ND	2.47	137.65	132.55
15	B	1232	CLA	CHA-C4D-ND	2.47	137.65	132.55
15	B	1236	CLA	CHA-C4D-ND	2.47	137.64	132.55
15	A	1013	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
15	A	1101	CLA	C4B-CHC-C1C	2.46	132.04	126.25
15	B	1237	CLA	C4B-CHC-C1C	2.46	132.03	126.25
15	A	1130	CLA	C3B-C4B-NB	-2.46	108.33	110.53
15	A	1115	CLA	CHA-C4D-ND	2.46	137.62	132.55
15	B	1226	CLA	CHA-C4D-ND	2.46	137.62	132.55
15	B	1021	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
15	A	1101	CLA	CHA-C4D-ND	2.45	137.61	132.55
15	B	1230	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
15	B	1201	CLA	C1C-CHC-C4B	2.45	132.49	126.04
15	B	1021	CLA	CHA-C4D-ND	2.45	137.59	132.55
15	A	1124	CLA	C1C-CHC-C4B	2.44	132.47	126.04
18	B	4005	BCR	C34-C9-C10	-2.44	118.87	122.82
15	A	1104	CLA	CHA-C4D-ND	2.43	137.57	132.55
15	A	1117	CLA	CHD-C1D-ND	-2.43	121.38	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1232	CLA	C4B-CHC-C1C	2.43	131.96	126.25
15	J	1302	CLA	CHA-C4D-ND	2.43	137.56	132.55
15	J	1302	CLA	O2A-CGA-CBA	2.43	119.25	111.83
15	A	1116	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
15	A	1012	CLA	CHA-C4D-ND	2.43	137.56	132.55
15	B	1224	CLA	CHD-C1D-ND	-2.43	121.39	124.80
15	B	1224	CLA	C1C-C2C-C3C	-2.43	104.43	106.98
15	A	1106	CLA	CHD-C1D-ND	-2.42	121.39	124.80
15	A	1103	CLA	CHA-C4D-ND	2.42	137.55	132.55
15	B	1229	CLA	C1D-ND-C4D	-2.42	104.61	106.31
15	A	1107	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
15	B	1225	CLA	C4B-CHC-C1C	2.42	131.94	126.25
18	A	4011	BCR	C29-C30-C25	2.42	113.95	110.44
18	B	4008	BCR	C27-C26-C25	-2.42	119.44	122.70
15	A	1115	CLA	CHD-C1D-ND	-2.42	121.40	124.80
15	B	1226	CLA	CHD-C1D-ND	-2.42	121.40	124.80
15	A	1116	CLA	C1C-C2C-C3C	-2.42	104.44	106.98
15	B	1230	CLA	CHA-C4D-ND	2.41	137.53	132.55
18	A	4002	BCR	C35-C13-C12	2.41	121.77	118.09
15	A	1131	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
15	B	1023	CLA	C2C-C1C-NC	2.41	112.51	109.98
15	A	1106	CLA	CHA-C4D-ND	2.41	137.51	132.55
15	A	1116	CLA	CHA-C4D-ND	2.41	137.51	132.55
15	A	1130	CLA	C1-O2A-CGA	2.40	122.47	116.65
15	B	1023	CLA	C1C-C2C-C3C	-2.40	104.45	106.98
15	A	1107	CLA	CHA-C4D-ND	2.40	137.51	132.55
15	B	1023	CLA	CHA-C4D-ND	2.40	137.50	132.55
15	B	1225	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
15	3	603	CLA	C1C-CHC-C4B	2.40	132.37	126.04
15	A	1117	CLA	C4B-CHC-C1C	2.40	131.89	126.25
15	A	1106	CLA	C4B-CHC-C1C	2.40	131.89	126.25
15	A	1013	CLA	CHD-C1D-ND	-2.40	121.43	124.80
15	A	1104	CLA	O2D-CGD-O1D	-2.40	119.19	123.85
15	B	1224	CLA	C4B-CHC-C1C	2.39	131.88	126.25
15	B	1023	CLA	CHD-C1D-ND	-2.39	121.44	124.80
15	A	1105	CLA	C4B-CHC-C1C	2.39	131.86	126.25
15	A	1126	CLA	CHA-C4D-ND	2.38	137.47	132.55
15	B	1230	CLA	CAC-C3C-C4C	2.37	127.88	124.79
15	A	1130	CLA	C4B-CHC-C1C	2.37	131.83	126.25
15	B	1230	CLA	C1C-C2C-C3C	-2.37	104.48	106.98
15	A	1103	CLA	CBC-CAC-C3C	-2.37	105.99	112.42
15	J	1302	CLA	C4B-CHC-C1C	2.37	131.82	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1117	CLA	CHA-C4D-ND	2.37	137.44	132.55
15	A	1131	CLA	CHA-C4D-ND	2.37	137.44	132.55
15	B	1224	CLA	CHA-C4D-ND	2.37	137.43	132.55
15	B	1225	CLA	O2A-CGA-CBA	2.37	119.05	111.83
15	B	1225	CLA	C2C-C1C-NC	2.37	112.47	109.98
15	A	1011	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
15	A	1126	CLA	C3B-C4B-NB	-2.36	108.42	110.53
18	I	4018	BCR	C8-C9-C10	2.36	122.73	119.01
18	A	4002	BCR	C36-C18-C17	-2.36	118.99	122.82
15	A	1115	CLA	C4B-CHC-C1C	2.36	131.79	126.25
15	A	1011	CLA	C4B-CHC-C1C	2.36	131.79	126.25
15	A	1130	CLA	CHA-C4D-ND	2.36	137.41	132.55
15	A	1114	CLA	C4B-CHC-C1C	2.36	131.78	126.25
15	B	1023	CLA	C4B-CHC-C1C	2.36	131.78	126.25
15	B	1237	CLA	CHA-C4D-ND	2.35	137.41	132.55
15	B	1232	CLA	CHD-C1D-ND	-2.35	121.49	124.80
15	A	1104	CLA	CHD-C1D-ND	-2.35	121.49	124.80
15	A	1012	CLA	C4B-CHC-C1C	2.35	131.77	126.25
16	B	2002	PQN	C2M-C2-C3	-2.35	120.59	124.45
15	B	1021	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
15	B	1226	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
15	A	1013	CLA	C4B-CHC-C1C	2.34	131.76	126.25
18	B	4005	BCR	C33-C5-C4	2.34	118.59	113.60
15	A	1106	CLA	C1D-ND-C4D	-2.34	104.67	106.31
15	F	1301	CLA	C4B-CHC-C1C	2.34	131.74	126.25
15	A	1105	CLA	CHD-C1D-ND	-2.34	121.52	124.80
15	A	1115	CLA	O2A-CGA-CBA	2.33	118.95	111.83
15	A	1011	CLA	C1D-ND-C4D	-2.33	104.68	106.31
15	A	1131	CLA	C3B-C4B-NB	-2.33	108.45	110.53
15	B	1229	CLA	O2A-CGA-CBA	2.33	118.94	111.83
15	B	1021	CLA	C4B-CHC-C1C	2.33	131.72	126.25
15	A	1011	CLA	CHA-C4D-ND	2.33	137.35	132.55
15	B	1229	CLA	CMD-C2D-C3D	-2.33	122.36	127.69
15	2	610	CLA	C1C-CHC-C4B	2.32	132.18	126.04
15	B	1228	CLA	C1C-CHC-C4B	2.32	132.16	126.04
15	A	1132	CLA	C1C-CHC-C4B	2.32	132.16	126.04
15	A	1011	CLA	O2A-CGA-CBA	2.32	118.91	111.83
15	A	1103	CLA	CHD-C1D-ND	-2.32	121.54	124.80
15	A	1012	CLA	C1-C2-C3	-2.32	122.40	126.20
15	2	612	CLA	C1C-CHC-C4B	2.32	132.16	126.04
15	A	1130	CLA	CHD-C1D-ND	-2.31	121.55	124.80
18	B	4005	BCR	C38-C26-C27	2.31	118.53	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	4002	BCR	C4-C5-C6	-2.31	119.58	122.70
15	A	1106	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
15	B	1225	CLA	CHA-C4D-ND	2.31	137.31	132.55
15	B	1229	CLA	CHA-C4D-ND	2.31	137.31	132.55
15	B	1021	CLA	CHD-C1D-ND	-2.30	121.56	124.80
15	B	1237	CLA	C3B-C4B-NB	-2.30	108.47	110.53
15	A	1104	CLA	C4B-CHC-C1C	2.30	131.66	126.25
15	A	1103	CLA	O2A-CGA-CBA	2.30	118.85	111.83
15	A	1131	CLA	C4B-CHC-C1C	2.30	131.66	126.25
15	A	1117	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
15	B	1232	CLA	CHA-C1A-NA	-2.30	121.19	126.39
18	A	4017	BCR	C38-C26-C25	-2.29	121.98	124.48
15	A	1126	CLA	CHD-C1D-ND	-2.29	121.58	124.80
15	B	1229	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
15	A	1013	CLA	CHA-C1A-NA	-2.29	121.20	126.39
15	B	1021	CLA	C3B-C4B-NB	-2.29	108.48	110.53
15	J	1302	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
15	A	1117	CLA	C1D-ND-C4D	-2.29	104.70	106.31
15	B	1230	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
15	A	1116	CLA	CHD-C1D-ND	-2.29	121.58	124.80
15	A	1114	CLA	CHD-C1D-ND	-2.28	121.59	124.80
18	A	4007	BCR	C38-C26-C27	2.28	118.47	113.60
15	B	1237	CLA	O2A-CGA-CBA	2.28	118.80	111.83
15	F	1301	CLA	CHD-C1D-ND	-2.28	121.59	124.80
15	A	1104	CLA	C3B-C4B-NB	-2.28	108.49	110.53
15	B	1224	CLA	O2A-CGA-CBA	2.28	118.79	111.83
15	B	1230	CLA	O2A-CGA-CBA	2.28	118.79	111.83
15	A	1011	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
15	B	1224	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
15	J	1302	CLA	CHD-C1D-ND	-2.28	121.60	124.80
15	A	1116	CLA	C1D-ND-C4D	-2.28	104.72	106.31
15	B	1238	CLA	C1C-CHC-C4B	2.27	132.04	126.04
15	A	1101	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
15	A	1103	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
15	4	606	CLA	C1C-CHC-C4B	2.27	132.03	126.04
15	3	604	CLA	C3D-C4D-ND	2.27	112.60	109.50
15	A	1105	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
15	A	1130	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
15	A	1115	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
15	A	1107	CLA	CHD-C1D-ND	-2.26	121.62	124.80
15	A	1116	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
15	B	1229	CLA	CHD-C1D-ND	-2.26	121.62	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1103	CLA	C4B-CHC-C1C	2.26	131.56	126.25
15	A	1109	CLA	C1C-CHC-C4B	2.26	132.00	126.04
15	B	1225	CLA	C2D-C1D-ND	2.26	112.36	110.13
15	A	1141	CLA	C1C-CHC-C4B	2.25	131.99	126.04
15	4	615	CLA	C1C-CHC-C4B	2.25	131.98	126.04
18	B	4008	BCR	C33-C5-C4	2.25	118.39	113.60
15	3	604	CLA	C1C-CHC-C4B	2.25	131.97	126.04
15	3	612	CLA	C1C-CHC-C4B	2.25	131.97	126.04
15	B	1226	CLA	CAC-C3C-C4C	2.25	127.71	124.79
15	B	1021	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
15	K	1401	CLA	C1C-CHC-C4B	2.25	131.97	126.04
15	A	1137	CLA	C2C-C3C-C4C	-2.25	104.40	107.24
15	A	1111	CLA	C1C-CHC-C4B	2.25	131.97	126.04
15	B	1236	CLA	CHD-C1D-ND	-2.25	121.64	124.80
18	A	4002	BCR	C34-C9-C10	-2.24	119.18	122.82
15	A	1126	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
15	B	1023	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
15	B	1232	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
18	A	4008	BCR	C38-C26-C27	2.24	118.37	113.60
15	2	603	CLA	C1C-CHC-C4B	2.24	131.95	126.04
15	3	606	CLA	C2C-C3C-C4C	-2.24	104.40	107.24
15	B	1211	CLA	C1C-CHC-C4B	2.24	131.95	126.04
15	A	1011	CLA	C3B-C4B-NB	-2.24	108.53	110.53
15	B	1021	CLA	C1D-ND-C4D	-2.24	104.74	106.31
15	B	1206	CLA	C1C-CHC-C4B	2.24	131.95	126.04
15	J	1302	CLA	C3B-C4B-NB	-2.24	108.53	110.53
15	A	1114	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
15	A	1101	CLA	O2D-CGD-O1D	-2.24	119.50	123.85
15	B	1023	CLA	CHA-C1A-NA	-2.23	121.33	126.39
15	A	1119	CLA	C3D-C4D-ND	2.23	112.56	109.50
15	F	1301	CLA	CMD-C2D-C3D	-2.23	122.56	127.69
15	B	1210	CLA	C1C-CHC-C4B	2.23	131.94	126.04
15	B	1236	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
15	A	1103	CLA	C1D-ND-C4D	-2.23	104.75	106.31
15	3	608	CLA	C1C-CHC-C4B	2.23	131.93	126.04
15	A	1113	CLA	C1C-CHC-C4B	2.23	131.93	126.04
15	A	1128	CLA	C1C-CHC-C4B	2.23	131.93	126.04
15	4	609	CLA	C1C-CHC-C4B	2.23	131.93	126.04
15	A	1107	CLA	O2A-CGA-CBA	2.23	118.63	111.83
15	A	1118	CLA	C1C-CHC-C4B	2.23	131.92	126.04
15	4	616	CLA	C1C-CHC-C4B	2.23	131.92	126.04
15	A	1127	CLA	C1C-CHC-C4B	2.23	131.92	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1104	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
18	A	4008	BCR	C34-C9-C10	-2.23	119.21	122.82
15	B	1239	CLA	C1C-CHC-C4B	2.22	131.91	126.04
15	A	1134	CLA	C1C-CHC-C4B	2.22	131.91	126.04
15	2	611	CLA	C1C-CHC-C4B	2.22	131.91	126.04
15	K	1402	CLA	C1C-CHC-C4B	2.22	131.91	126.04
15	J	1302	CLA	CHA-C1A-NA	-2.22	121.36	126.39
15	A	1138	CLA	C1C-CHC-C4B	2.22	131.91	126.04
15	B	1217	CLA	C1C-CHC-C4B	2.22	131.91	126.04
15	O	1603	CLA	C1C-CHC-C4B	2.22	131.91	126.04
15	3	607	CLA	C1C-CHC-C4B	2.22	131.91	126.04
15	A	1129	CLA	C3D-C4D-ND	2.22	112.54	109.50
15	3	614	CLA	C1C-CHC-C4B	2.22	131.91	126.04
18	A	4007	BCR	C1-C6-C7	2.22	121.68	115.65
15	A	1132	CLA	C2C-C3C-C4C	-2.22	104.43	107.24
15	B	1230	CLA	C4B-CHC-C1C	2.22	131.47	126.25
15	B	1225	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
15	A	1120	CLA	C1C-CHC-C4B	2.22	131.90	126.04
15	B	1022	CLA	C1C-CHC-C4B	2.22	131.90	126.04
15	A	1112	CLA	C1C-CHC-C4B	2.22	131.90	126.04
15	2	604	CLA	C1C-CHC-C4B	2.22	131.90	126.04
15	A	1108	CLA	C1C-CHC-C4B	2.22	131.90	126.04
15	2	613	CLA	C1C-CHC-C4B	2.22	131.90	126.04
15	A	1133	CLA	C1C-CHC-C4B	2.22	131.90	126.04
15	A	1136	CLA	C1C-CHC-C4B	2.22	131.90	126.04
15	B	1220	CLA	C1C-CHC-C4B	2.22	131.90	126.04
15	A	1140	CLA	C1C-CHC-C4B	2.22	131.89	126.04
18	I	4018	BCR	C33-C5-C6	-2.22	122.06	124.48
15	2	616	CLA	C1C-CHC-C4B	2.22	131.89	126.04
15	B	1204	CLA	C1C-CHC-C4B	2.22	131.89	126.04
15	A	1107	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
15	A	1129	CLA	C1C-CHC-C4B	2.22	131.89	126.04
15	L	1502	CLA	C3D-C4D-ND	2.22	112.53	109.50
15	2	607	CLA	C2C-C3C-C4C	-2.21	104.44	107.24
15	4	611	CLA	C1C-CHC-C4B	2.21	131.88	126.04
15	4	608	CLA	C1C-CHC-C4B	2.21	131.88	126.04
15	B	1236	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
15	A	1110	CLA	C1C-CHC-C4B	2.21	131.88	126.04
15	L	1503	CLA	C1C-CHC-C4B	2.21	131.88	126.04
15	4	605	CLA	C1C-CHC-C4B	2.21	131.88	126.04
15	O	1601	CLA	C1C-CHC-C4B	2.21	131.87	126.04
15	A	1135	CLA	C1C-CHC-C4B	2.21	131.87	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1137	CLA	C1C-CHC-C4B	2.21	131.87	126.04
15	B	1234	CLA	C1C-CHC-C4B	2.21	131.87	126.04
15	A	1121	CLA	C1C-CHC-C4B	2.21	131.87	126.04
15	B	1205	CLA	C1C-CHC-C4B	2.21	131.87	126.04
15	A	1101	CLA	CHD-C1D-ND	-2.21	121.69	124.80
15	A	1106	CLA	C3B-C4B-NB	-2.21	108.56	110.53
15	A	1119	CLA	C1C-CHC-C4B	2.21	131.87	126.04
15	B	1219	CLA	C1C-CHC-C4B	2.21	131.87	126.04
15	B	1022	CLA	C3D-C4D-ND	2.21	112.52	109.50
15	2	608	CLA	C1C-CHC-C4B	2.21	131.87	126.04
15	A	1013	CLA	CMA-C3A-C4A	2.21	117.70	111.77
15	B	1224	CLA	C1D-ND-C4D	-2.20	104.77	106.31
18	A	4002	BCR	C38-C26-C27	2.20	118.30	113.60
15	A	1111	CLA	C2C-C3C-C4C	-2.20	104.45	107.24
15	2	615	CLA	C1C-CHC-C4B	2.20	131.86	126.04
15	4	610	CLA	C1C-CHC-C4B	2.20	131.86	126.04
15	B	1235	CLA	C1C-CHC-C4B	2.20	131.86	126.04
15	B	1023	CLA	C1D-ND-C4D	-2.20	104.77	106.31
15	2	606	CLA	C1C-CHC-C4B	2.20	131.85	126.04
15	B	1202	CLA	C1C-CHC-C4B	2.20	131.85	126.04
15	3	611	CLA	C1C-CHC-C4B	2.20	131.85	126.04
15	K	1402	CLA	C2C-C3C-C4C	-2.20	104.45	107.24
15	B	1224	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
15	B	1215	CLA	C3D-C4D-ND	2.20	112.51	109.50
15	B	1201	CLA	C2C-C3C-C4C	-2.20	104.45	107.24
18	A	4002	BCR	C23-C24-C25	-2.20	121.12	127.00
15	2	614	CLA	C1C-CHC-C4B	2.20	131.85	126.04
15	B	1216	CLA	C1C-CHC-C4B	2.20	131.84	126.04
15	B	1222	CLA	C1C-CHC-C4B	2.20	131.84	126.04
15	B	1202	CLA	C2C-C3C-C4C	-2.20	104.46	107.24
15	2	604	CLA	C3D-C4D-ND	2.20	112.50	109.50
15	3	612	CLA	C2C-C3C-C4C	-2.20	104.46	107.24
15	A	1124	CLA	C2C-C3C-C4C	-2.20	104.46	107.24
15	O	1602	CLA	C1C-CHC-C4B	2.20	131.84	126.04
15	B	1211	CLA	C3D-C4D-ND	2.20	112.50	109.50
15	4	603	CLA	C1C-CHC-C4B	2.20	131.84	126.04
15	3	602	CLA	C1C-CHC-C4B	2.20	131.84	126.04
15	A	1117	CLA	C3B-C4B-NB	-2.20	108.57	110.53
15	A	1106	CLA	C2D-C1D-ND	2.20	112.30	110.13
15	B	1218	CLA	C1C-CHC-C4B	2.20	131.83	126.04
15	B	1214	CLA	C1C-CHC-C4B	2.19	131.83	126.04
15	A	1139	CLA	C1C-CHC-C4B	2.19	131.83	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1223	CLA	C1C-CHC-C4B	2.19	131.83	126.04
15	A	1122	CLA	C1C-CHC-C4B	2.19	131.83	126.04
15	B	1212	CLA	C1C-CHC-C4B	2.19	131.82	126.04
15	B	1023	CLA	C2D-C1D-ND	2.19	112.30	110.13
15	B	1209	CLA	C1C-CHC-C4B	2.19	131.82	126.04
15	L	1502	CLA	C1C-CHC-C4B	2.19	131.82	126.04
15	3	607	CLA	C3D-C4D-ND	2.19	112.50	109.50
15	2	602	CLA	C1C-CHC-C4B	2.19	131.82	126.04
15	B	1221	CLA	C1C-CHC-C4B	2.19	131.82	126.04
15	A	1131	CLA	C1D-ND-C4D	-2.19	104.78	106.31
15	4	601	CLA	C1C-CHC-C4B	2.19	131.82	126.04
15	A	1104	CLA	C1D-ND-C4D	-2.19	104.78	106.31
15	2	601	CLA	C1C-CHC-C4B	2.19	131.82	126.04
15	B	1208	CLA	C1C-CHC-C4B	2.19	131.82	126.04
18	A	4002	BCR	C37-C22-C21	-2.19	119.27	122.82
15	B	1231	CLA	C1C-CHC-C4B	2.19	131.81	126.04
15	2	603	CLA	C2C-C3C-C4C	-2.19	104.47	107.24
15	A	1107	CLA	C1D-ND-C4D	-2.19	104.78	106.31
15	4	602	CLA	C1C-CHC-C4B	2.19	131.81	126.04
15	A	1126	CLA	C1D-ND-C4D	-2.18	104.78	106.31
15	A	1130	CLA	C1D-ND-C4D	-2.18	104.78	106.31
15	B	1203	CLA	C3D-C4D-ND	2.18	112.48	109.50
15	B	1215	CLA	C1C-CHC-C4B	2.18	131.80	126.04
15	2	605	CLA	C1C-CHC-C4B	2.18	131.80	126.04
15	A	1130	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
15	4	604	CLA	C1C-CHC-C4B	2.18	131.79	126.04
15	A	1103	CLA	C3B-C4B-NB	-2.18	108.58	110.53
15	3	610	CLA	C3D-C4D-ND	2.18	112.48	109.50
15	A	1134	CLA	C3D-C4D-ND	2.18	112.48	109.50
15	4	605	CLA	C2C-C3C-C4C	-2.18	104.48	107.24
15	A	1123	CLA	C1C-CHC-C4B	2.18	131.79	126.04
15	A	1108	CLA	C2C-C3C-C4C	-2.18	104.48	107.24
15	B	1203	CLA	C1C-CHC-C4B	2.18	131.79	126.04
15	2	611	CLA	C3D-C4D-ND	2.18	112.48	109.50
15	3	604	CLA	C2C-C3C-C4C	-2.18	104.48	107.24
15	A	1105	CLA	C3B-C4B-NB	-2.18	108.59	110.53
15	O	1603	CLA	C3D-C4D-ND	2.18	112.47	109.50
15	B	1226	CLA	C4B-CHC-C1C	2.18	131.36	126.25
15	3	611	CLA	C3D-C4D-ND	2.18	112.47	109.50
15	B	1216	CLA	C3D-C4D-ND	2.17	112.47	109.50
15	B	1235	CLA	C3D-C4D-ND	2.17	112.47	109.50
15	2	605	CLA	C3D-C4D-ND	2.17	112.47	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1108	CLA	C3D-C4D-ND	2.17	112.47	109.50
15	B	1221	CLA	C2C-C3C-C4C	-2.17	104.49	107.24
15	F	1302	CLA	C1C-CHC-C4B	2.17	131.77	126.04
15	4	611	CLA	C3D-C4D-ND	2.17	112.47	109.50
15	B	1214	CLA	C2C-C3C-C4C	-2.17	104.49	107.24
15	A	1104	CLA	O2A-CGA-CBA	2.17	118.45	111.83
15	2	606	CLA	C3D-C4D-ND	2.17	112.47	109.50
15	4	604	CLA	C3D-C4D-ND	2.17	112.47	109.50
15	B	1222	CLA	C3D-C4D-ND	2.17	112.47	109.50
15	L	1501	CLA	C1C-CHC-C4B	2.17	131.76	126.04
15	4	604	CLA	C2C-C3C-C4C	-2.17	104.50	107.24
15	4	615	CLA	C2C-C3C-C4C	-2.17	104.50	107.24
15	A	1116	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
15	B	1207	CLA	C1C-CHC-C4B	2.17	131.75	126.04
15	L	1501	CLA	C2C-C3C-C4C	-2.16	104.50	107.24
15	B	1212	CLA	C3D-C4D-ND	2.16	112.46	109.50
15	B	1214	CLA	C3D-C4D-ND	2.16	112.46	109.50
15	O	1602	CLA	C3D-C4D-ND	2.16	112.46	109.50
15	2	602	CLA	C3D-C4D-ND	2.16	112.46	109.50
15	3	608	CLA	C3D-C4D-ND	2.16	112.46	109.50
15	B	1207	CLA	C3D-C4D-ND	2.16	112.46	109.50
15	A	1103	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
15	3	603	CLA	C3D-C4D-ND	2.16	112.45	109.50
15	B	1202	CLA	C3D-C4D-ND	2.16	112.45	109.50
15	A	1127	CLA	C2C-C3C-C4C	-2.16	104.50	107.24
15	A	1125	CLA	C3D-C4D-ND	2.16	112.45	109.50
15	B	1206	CLA	C2C-C3C-C4C	-2.16	104.50	107.24
15	2	610	CLA	C2C-C3C-C4C	-2.16	104.51	107.24
15	4	610	CLA	C2C-C3C-C4C	-2.16	104.51	107.24
15	A	1113	CLA	C2C-C3C-C4C	-2.16	104.51	107.24
15	4	612	CLA	C1C-CHC-C4B	2.16	131.74	126.04
15	A	1124	CLA	C3D-C4D-ND	2.16	112.45	109.50
15	B	1220	CLA	C3D-C4D-ND	2.16	112.45	109.50
15	A	1102	CLA	C1C-CHC-C4B	2.16	131.74	126.04
15	3	603	CLA	C2C-C3C-C4C	-2.16	104.51	107.24
15	A	1120	CLA	C3D-C4D-ND	2.16	112.45	109.50
15	B	1217	CLA	C3D-C4D-ND	2.16	112.45	109.50
15	L	1503	CLA	C3D-C4D-ND	2.16	112.45	109.50
15	2	606	CLA	C2C-C3C-C4C	-2.16	104.51	107.24
15	3	601	CLA	C3D-C4D-ND	2.16	112.45	109.50
15	3	602	CLA	C3D-C4D-ND	2.16	112.45	109.50
15	3	614	CLA	C3D-C4D-ND	2.16	112.45	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1204	CLA	C3D-C4D-ND	2.16	112.45	109.50
15	B	1210	CLA	C3D-C4D-ND	2.16	112.45	109.50
18	A	4011	BCR	C32-C1-C6	-2.16	106.86	110.24
15	2	607	CLA	C1C-CHC-C4B	2.16	131.73	126.04
15	B	1239	CLA	C3D-C4D-ND	2.16	112.45	109.50
15	A	1128	CLA	C2C-C3C-C4C	-2.15	104.51	107.24
15	2	615	CLA	C3D-C4D-ND	2.15	112.44	109.50
15	4	603	CLA	C3D-C4D-ND	2.15	112.44	109.50
15	B	1221	CLA	C3D-C4D-ND	2.15	112.44	109.50
15	A	1012	CLA	CHA-C1A-NA	-2.15	121.52	126.39
15	A	1118	CLA	C3D-C4D-ND	2.15	112.44	109.50
18	B	4005	BCR	C33-C5-C6	-2.15	122.14	124.48
15	A	1131	CLA	CHD-C1D-ND	-2.15	121.77	124.80
15	A	1133	CLA	C2C-C3C-C4C	-2.15	104.52	107.24
15	2	601	CLA	C3D-C4D-ND	2.15	112.44	109.50
15	4	601	CLA	C3D-C4D-ND	2.15	112.44	109.50
15	4	608	CLA	C3D-C4D-ND	2.15	112.44	109.50
15	2	601	CLA	C2C-C3C-C4C	-2.15	104.52	107.24
15	A	1112	CLA	C2C-C3C-C4C	-2.15	104.52	107.24
15	B	1216	CLA	C2C-C3C-C4C	-2.15	104.52	107.24
15	2	616	CLA	C3D-C4D-ND	2.15	112.44	109.50
15	A	1113	CLA	C3D-C4D-ND	2.15	112.44	109.50
15	A	1141	CLA	C2C-C3C-C4C	-2.15	104.52	107.24
15	B	1227	CLA	C3D-C4D-ND	2.15	112.44	109.50
15	A	1130	CLA	O2A-CGA-CBA	2.15	118.38	111.83
15	B	1218	CLA	C3D-C4D-ND	2.15	112.44	109.50
15	2	612	CLA	C3D-C4D-ND	2.15	112.43	109.50
15	A	1109	CLA	C3D-C4D-ND	2.15	112.43	109.50
18	A	4017	BCR	C29-C28-C27	2.15	116.00	111.28
15	A	1106	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
15	4	608	CLA	C2C-C3C-C4C	-2.15	104.52	107.24
15	B	1238	CLA	C2C-C3C-C4C	-2.15	104.52	107.24
15	B	1238	CLA	C3D-C4D-ND	2.14	112.43	109.50
15	O	1601	CLA	C3D-C4D-ND	2.14	112.43	109.50
18	I	4018	BCR	C27-C26-C25	-2.14	119.81	122.70
15	3	610	CLA	C1C-CHC-C4B	2.14	131.70	126.04
15	B	1219	CLA	C2C-C3C-C4C	-2.14	104.53	107.24
15	B	1228	CLA	C2C-C3C-C4C	-2.14	104.53	107.24
15	A	1126	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
15	A	1121	CLA	C3D-C4D-ND	2.14	112.43	109.50
15	2	610	CLA	C3D-C4D-ND	2.14	112.43	109.50
15	K	1401	CLA	C3D-C4D-ND	2.14	112.43	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1206	CLA	C3D-C4D-ND	2.14	112.43	109.50
15	A	1131	CLA	C2D-C1D-ND	2.14	112.25	110.13
15	3	606	CLA	C3D-C4D-ND	2.14	112.43	109.50
15	4	602	CLA	C3D-C4D-ND	2.14	112.43	109.50
15	B	1201	CLA	C3D-C4D-ND	2.14	112.43	109.50
15	F	1302	CLA	C3D-C4D-ND	2.14	112.42	109.50
15	2	608	CLA	C2C-C3C-C4C	-2.14	104.53	107.24
15	3	602	CLA	C2C-C3C-C4C	-2.14	104.53	107.24
15	A	1116	CLA	C2D-C1D-ND	2.14	112.24	110.13
15	3	601	CLA	C1C-CHC-C4B	2.14	131.68	126.04
15	B	1211	CLA	C2C-C3C-C4C	-2.14	104.53	107.24
15	B	1219	CLA	C3D-C4D-ND	2.14	112.42	109.50
15	B	1236	CLA	C1D-ND-C4D	-2.14	104.81	106.31
15	A	1109	CLA	C2C-C3C-C4C	-2.14	104.54	107.24
15	B	1223	CLA	C2C-C3C-C4C	-2.14	104.54	107.24
15	O	1601	CLA	C2C-C3C-C4C	-2.14	104.54	107.24
15	4	605	CLA	C3D-C4D-ND	2.14	112.42	109.50
15	B	1223	CLA	C3D-C4D-ND	2.14	112.42	109.50
15	2	615	CLA	C2C-C3C-C4C	-2.14	104.54	107.24
15	2	616	CLA	C2C-C3C-C4C	-2.13	104.54	107.24
15	4	610	CLA	C3D-C4D-ND	2.13	112.42	109.50
15	A	1125	CLA	C1C-CHC-C4B	2.13	131.67	126.04
15	A	1135	CLA	C2C-C3C-C4C	-2.13	104.54	107.24
15	A	1141	CLA	C3D-C4D-ND	2.13	112.42	109.50
15	B	1209	CLA	C2C-C3C-C4C	-2.13	104.54	107.24
15	B	1218	CLA	C2C-C3C-C4C	-2.13	104.54	107.24
15	B	1208	CLA	C2C-C3C-C4C	-2.13	104.54	107.24
15	A	1139	CLA	C2C-C3C-C4C	-2.13	104.54	107.24
15	2	614	CLA	C3D-C4D-ND	2.13	112.41	109.50
15	A	1137	CLA	C3D-C4D-ND	2.13	112.41	109.50
15	A	1101	CLA	C1D-ND-C4D	-2.13	104.82	106.31
16	A	2001	PQN	C2M-C2-C3	-2.13	120.95	124.45
18	A	4007	BCR	C35-C13-C14	-2.13	119.37	122.82
15	2	608	CLA	C3D-C4D-ND	2.13	112.41	109.50
15	4	609	CLA	C3D-C4D-ND	2.13	112.41	109.50
15	A	1011	CLA	CHA-C1A-NA	-2.13	121.57	126.39
15	K	1402	CLA	C3D-C4D-ND	2.13	112.41	109.50
15	A	1012	CLA	C2D-C1D-ND	2.13	112.23	110.13
15	4	616	CLA	C2C-C3C-C4C	-2.13	104.55	107.24
15	A	1136	CLA	C2C-C3C-C4C	-2.13	104.55	107.24
15	B	1231	CLA	C3D-C4D-ND	2.13	112.41	109.50
15	B	1021	CLA	CHA-C1A-NA	-2.13	121.57	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1138	CLA	C2C-C3C-C4C	-2.13	104.55	107.24
15	B	1209	CLA	C3D-C4D-ND	2.13	112.41	109.50
15	4	601	CLA	C2C-C3C-C4C	-2.13	104.55	107.24
15	A	1110	CLA	C2C-C3C-C4C	-2.13	104.55	107.24
15	L	1501	CLA	C3D-C4D-ND	2.13	112.41	109.50
18	B	4008	BCR	C37-C22-C21	-2.13	119.37	122.82
15	O	1603	CLA	C2C-C3C-C4C	-2.13	104.55	107.24
15	2	602	CLA	C2C-C3C-C4C	-2.12	104.55	107.24
15	B	1022	CLA	C2C-C3C-C4C	-2.12	104.55	107.24
15	2	613	CLA	C3D-C4D-ND	2.12	112.40	109.50
15	4	615	CLA	C3D-C4D-ND	2.12	112.40	109.50
15	B	1208	CLA	C3D-C4D-ND	2.12	112.40	109.50
15	4	602	CLA	C2C-C3C-C4C	-2.12	104.55	107.24
15	B	1226	CLA	O2A-CGA-CBA	2.12	118.31	111.83
15	4	612	CLA	C3D-C4D-ND	2.12	112.40	109.50
15	A	1107	CLA	CHA-C1A-NA	-2.12	121.58	126.39
15	A	1133	CLA	C3D-C4D-ND	2.12	112.40	109.50
15	A	1121	CLA	C2C-C3C-C4C	-2.12	104.55	107.24
15	B	1205	CLA	C2C-C3C-C4C	-2.12	104.55	107.24
15	B	1215	CLA	C2C-C3C-C4C	-2.12	104.55	107.24
15	4	606	CLA	C3D-C4D-ND	2.12	112.40	109.50
15	A	1136	CLA	C3D-C4D-ND	2.12	112.40	109.50
15	2	604	CLA	C2C-C3C-C4C	-2.12	104.56	107.24
15	4	609	CLA	C2C-C3C-C4C	-2.12	104.56	107.24
15	A	1101	CLA	CHA-C1A-NA	-2.12	121.59	126.39
15	B	1205	CLA	C3D-C4D-ND	2.12	112.40	109.50
15	B	1210	CLA	C2C-C3C-C4C	-2.12	104.56	107.24
15	L	1503	CLA	C2C-C3C-C4C	-2.12	104.56	107.24
15	O	1602	CLA	C2C-C3C-C4C	-2.12	104.56	107.24
15	B	1224	CLA	C2D-C1D-ND	2.12	112.22	110.13
15	B	1234	CLA	C3D-C4D-ND	2.12	112.40	109.50
15	A	1104	CLA	CHA-C1A-NA	-2.12	121.59	126.39
15	2	613	CLA	C2C-C3C-C4C	-2.12	104.56	107.24
15	B	1231	CLA	C2C-C3C-C4C	-2.12	104.56	107.24
15	K	1401	CLA	C2C-C3C-C4C	-2.12	104.56	107.24
15	B	1237	CLA	CHD-C1D-ND	-2.12	121.82	124.80
18	A	4007	BCR	C8-C9-C10	2.12	122.34	119.01
15	4	616	CLA	C3D-C4D-ND	2.12	112.39	109.50
18	I	4018	BCR	C38-C26-C25	-2.12	122.17	124.48
15	B	1204	CLA	C2C-C3C-C4C	-2.12	104.56	107.24
15	A	1105	CLA	C1D-ND-C4D	-2.12	104.83	106.31
18	B	4008	BCR	C30-C25-C26	-2.11	119.75	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1235	CLA	C2C-C3C-C4C	-2.11	104.56	107.24
18	B	4008	BCR	C34-C9-C10	-2.11	119.39	122.82
15	B	1021	CLA	C2D-C1D-ND	2.11	112.22	110.13
15	A	1122	CLA	C3D-C4D-ND	2.11	112.39	109.50
15	B	1217	CLA	C2C-C3C-C4C	-2.11	104.57	107.24
15	B	1239	CLA	C2C-C3C-C4C	-2.11	104.57	107.24
15	3	611	CLA	C2C-C3C-C4C	-2.11	104.57	107.24
15	A	1138	CLA	C3D-C4D-ND	2.11	112.38	109.50
15	B	1230	CLA	CHD-C1D-ND	-2.11	121.84	124.80
15	2	611	CLA	C2C-C3C-C4C	-2.11	104.57	107.24
15	2	612	CLA	C2C-C3C-C4C	-2.11	104.57	107.24
15	B	1207	CLA	C2C-C3C-C4C	-2.11	104.57	107.24
18	A	4008	BCR	C1-C6-C7	2.11	121.36	115.65
15	B	1232	CLA	C1D-ND-C4D	-2.11	104.83	106.31
15	B	1220	CLA	C2C-C3C-C4C	-2.11	104.58	107.24
15	A	1128	CLA	C3D-C4D-ND	2.10	112.38	109.50
15	A	1112	CLA	C3D-C4D-ND	2.10	112.38	109.50
15	A	1135	CLA	C3D-C4D-ND	2.10	112.38	109.50
15	A	1115	CLA	C1D-ND-C4D	-2.10	104.84	106.31
15	A	1115	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
15	F	1302	CLA	C2C-C3C-C4C	-2.10	104.58	107.24
15	A	1106	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
15	3	610	CLA	C2C-C3C-C4C	-2.10	104.58	107.24
15	A	1107	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
15	A	1102	CLA	C3D-C4D-ND	2.10	112.37	109.50
18	A	4011	BCR	C3-C4-C5	-2.10	110.31	114.06
15	3	601	CLA	C2C-C3C-C4C	-2.10	104.58	107.24
15	A	1122	CLA	C2C-C3C-C4C	-2.10	104.58	107.24
15	A	1129	CLA	C2C-C3C-C4C	-2.10	104.58	107.24
15	A	1134	CLA	C2C-C3C-C4C	-2.10	104.58	107.24
15	A	1116	CLA	CHA-C1A-NA	-2.10	121.64	126.39
15	A	1105	CLA	C2D-C1D-ND	2.10	112.20	110.13
15	B	1236	CLA	CHA-C1A-NA	-2.09	121.65	126.39
15	A	1139	CLA	C3D-C4D-ND	2.09	112.36	109.50
15	2	614	CLA	C2C-C3C-C4C	-2.09	104.59	107.24
15	4	606	CLA	C2C-C3C-C4C	-2.09	104.59	107.24
15	A	1118	CLA	C2C-C3C-C4C	-2.09	104.59	107.24
15	B	1237	CLA	C1D-ND-C4D	-2.09	104.84	106.31
15	A	1111	CLA	C3D-C4D-ND	2.09	112.36	109.50
15	4	611	CLA	C2C-C3C-C4C	-2.09	104.59	107.24
15	A	1114	CLA	C1D-ND-C4D	-2.09	104.84	106.31
15	4	603	CLA	C2C-C3C-C4C	-2.09	104.60	107.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1110	CLA	C3D-C4D-ND	2.09	112.36	109.50
15	3	607	CLA	C2C-C3C-C4C	-2.09	104.60	107.24
15	A	1123	CLA	C3D-C4D-ND	2.09	112.35	109.50
15	A	1130	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
15	F	1301	CLA	CHA-C1A-NA	-2.09	121.67	126.39
15	3	608	CLA	C2C-C3C-C4C	-2.08	104.60	107.24
15	A	1012	CLA	CHD-C1D-ND	-2.08	121.87	124.80
15	B	1236	CLA	C2D-C1D-ND	2.08	112.19	110.13
15	2	605	CLA	C2C-C3C-C4C	-2.08	104.61	107.24
15	B	1237	CLA	CHA-C1A-NA	-2.08	121.68	126.39
15	B	1224	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
18	I	4018	BCR	C1-C6-C5	-2.08	119.80	122.64
15	B	1234	CLA	C2C-C3C-C4C	-2.08	104.61	107.24
15	B	1023	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
15	B	1232	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
15	B	1212	CLA	C2C-C3C-C4C	-2.08	104.61	107.24
15	B	1222	CLA	C2C-C3C-C4C	-2.08	104.61	107.24
18	I	4018	BCR	C38-C26-C27	2.07	118.02	113.60
15	B	1232	CLA	C2D-C1D-ND	2.07	112.18	110.13
15	A	1127	CLA	C3D-C4D-ND	2.07	112.33	109.50
15	A	1132	CLA	C3D-C4D-ND	2.07	112.33	109.50
15	A	1115	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
15	A	1115	CLA	C2D-C1D-ND	2.07	112.18	110.13
15	L	1502	CLA	C2C-C3C-C4C	-2.07	104.62	107.24
15	B	1225	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
15	A	1140	CLA	C2C-C3C-C4C	-2.07	104.63	107.24
15	B	1237	CLA	C1-O2A-CGA	2.06	121.65	116.65
15	A	1116	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
15	3	614	CLA	C2C-C3C-C4C	-2.06	104.63	107.24
18	A	4017	BCR	C37-C22-C21	-2.06	119.47	122.82
15	A	1103	CLA	C2D-C1D-ND	2.06	112.17	110.13
15	A	1114	CLA	CHA-C1A-NA	-2.06	121.73	126.39
15	A	1106	CLA	O2A-CGA-CBA	2.06	118.10	111.83
18	B	4008	BCR	C35-C13-C14	-2.06	119.49	122.82
15	A	1102	CLA	C2C-C3C-C4C	-2.05	104.64	107.24
15	A	1126	CLA	CHA-C1A-NA	-2.05	121.74	126.39
15	A	1117	CLA	C2D-C1D-ND	2.05	112.16	110.13
15	A	1140	CLA	C3D-C4D-ND	2.05	112.31	109.50
15	B	1225	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
18	B	4005	BCR	C37-C22-C21	-2.05	119.49	122.82
15	B	1022	CLA	CHA-C4D-ND	-2.05	121.95	124.84
18	A	4011	BCR	C12-C13-C14	-2.05	115.78	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1123	CLA	C2C-C3C-C4C	-2.05	104.64	107.24
15	A	1101	CLA	C2D-C1D-ND	2.05	112.16	110.13
15	B	1229	CLA	C2D-C1D-ND	2.05	112.16	110.13
18	I	4018	BCR	C37-C22-C23	2.05	121.22	118.09
15	A	1127	CLA	CHA-C4D-ND	-2.05	121.95	124.84
18	A	4017	BCR	C8-C7-C6	-2.05	121.53	127.00
15	A	1120	CLA	C2C-C3C-C4C	-2.05	104.65	107.24
18	A	4002	BCR	C34-C9-C8	2.05	121.22	118.09
15	A	1130	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
15	B	1230	CLA	CMC-C2C-C3C	2.04	131.68	126.15
15	A	1104	CLA	C2D-C1D-ND	2.04	112.15	110.13
15	A	1130	CLA	C2D-C1D-ND	2.04	112.15	110.13
15	F	1301	CLA	C1D-ND-C4D	-2.04	104.88	106.31
18	B	4005	BCR	C8-C9-C10	2.04	122.22	119.01
15	A	1126	CLA	C2D-C1D-ND	2.04	112.15	110.13
15	A	1103	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
15	A	1011	CLA	C2D-C1D-ND	2.04	112.14	110.13
15	B	1227	CLA	CHA-C4D-ND	-2.04	121.97	124.84
15	F	1301	CLA	C2D-C1D-ND	2.04	112.14	110.13
15	B	1215	CLA	CHA-C4D-ND	-2.04	121.97	124.84
15	B	1023	CLA	CMA-C3A-C4A	2.04	117.24	111.77
15	B	1229	CLA	C3D-C2D-C1D	-2.03	103.05	105.83
15	4	612	CLA	C2C-C3C-C4C	-2.03	104.67	107.24
15	A	1119	CLA	C2C-C3C-C4C	-2.03	104.67	107.24
18	B	4008	BCR	C8-C7-C6	-2.03	121.56	127.00
15	3	602	CLA	CHA-C4D-ND	-2.03	121.98	124.84
15	A	1134	CLA	CHA-C4D-ND	-2.03	121.98	124.84
15	A	1105	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
15	F	1301	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
15	B	1237	CLA	C2D-C1D-ND	2.03	112.14	110.13
15	A	1106	CLA	C1-O2A-CGA	2.03	121.56	116.65
15	B	1229	CLA	CHA-C1A-NA	-2.03	121.80	126.39
15	3	606	CLA	CHA-C4D-ND	-2.03	121.98	124.84
15	A	1103	CLA	CHA-C1A-NA	-2.03	121.80	126.39
18	A	4002	BCR	C19-C18-C17	2.03	122.20	119.01
15	B	1203	CLA	CHA-C4D-ND	-2.03	121.99	124.84
15	2	604	CLA	CHA-C4D-ND	-2.02	121.99	124.84
15	L	1502	CLA	CHA-C4D-ND	-2.02	121.99	124.84
15	A	1115	CLA	CHA-C1A-NA	-2.02	121.81	126.39
15	B	1224	CLA	CHA-C1A-NA	-2.02	121.82	126.39
18	B	4005	BCR	C38-C26-C25	-2.02	122.28	124.48
15	A	1113	CLA	CHA-C4D-ND	-2.02	122.00	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1129	CLA	CHA-C4D-ND	-2.02	122.00	124.84
15	J	1302	CLA	CBA-CAA-C2A	2.02	119.79	113.79
15	3	608	CLA	CHA-C4D-ND	-2.02	122.00	124.84
15	B	1204	CLA	CHA-C4D-ND	-2.01	122.00	124.84
15	A	1012	CLA	C1D-ND-C4D	-2.01	104.90	106.31
15	A	1131	CLA	CHA-C1A-NA	-2.01	121.83	126.39
15	B	1211	CLA	CHA-C4D-ND	-2.01	122.00	124.84
15	3	607	CLA	CHA-C4D-ND	-2.01	122.01	124.84
15	A	1108	CLA	CHA-C4D-ND	-2.01	122.01	124.84
15	2	611	CLA	CHA-C4D-ND	-2.01	122.01	124.84
18	A	4008	BCR	C37-C22-C23	2.01	121.15	118.09
15	A	1124	CLA	CHA-C4D-ND	-2.01	122.01	124.84
15	B	1222	CLA	CHA-C4D-ND	-2.01	122.01	124.84
15	B	1227	CLA	C1C-CHC-C4B	2.00	131.33	126.04
18	A	4008	BCR	C36-C18-C19	2.00	121.15	118.09
15	A	1101	CLA	O1D-CGD-CBD	-2.00	120.57	124.52

All (134) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	2	601	CLA	ND
15	2	602	CLA	ND
15	2	603	CLA	ND
15	2	604	CLA	ND
15	2	605	CLA	ND
15	2	606	CLA	ND
15	2	607	CLA	ND
15	2	608	CLA	ND
15	2	610	CLA	ND
15	2	611	CLA	ND
15	2	612	CLA	ND
15	2	613	CLA	ND
15	2	614	CLA	ND
15	2	615	CLA	ND
15	2	616	CLA	ND
15	3	601	CLA	ND
15	3	602	CLA	ND
15	3	603	CLA	ND
15	3	604	CLA	ND
15	3	606	CLA	ND
15	3	607	CLA	ND
15	3	608	CLA	ND

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Mol	Chain	Res	Type	Atom
15	3	610	CLA	ND
15	3	611	CLA	ND
15	3	612	CLA	ND
15	3	614	CLA	ND
15	4	601	CLA	ND
15	4	602	CLA	ND
15	4	603	CLA	ND
15	4	604	CLA	ND
15	4	605	CLA	ND
15	4	606	CLA	ND
15	4	608	CLA	ND
15	4	609	CLA	ND
15	4	610	CLA	ND
15	4	611	CLA	ND
15	4	612	CLA	ND
15	4	615	CLA	ND
15	4	616	CLA	ND
15	A	1011	CLA	ND
15	A	1012	CLA	ND
15	A	1013	CLA	ND
15	A	1101	CLA	ND
15	A	1102	CLA	ND
15	A	1103	CLA	ND
15	A	1104	CLA	ND
15	A	1105	CLA	ND
15	A	1106	CLA	ND
15	A	1107	CLA	ND
15	A	1108	CLA	ND
15	A	1109	CLA	ND
15	A	1110	CLA	ND
15	A	1111	CLA	ND
15	A	1112	CLA	ND
15	A	1113	CLA	ND
15	A	1114	CLA	ND
15	A	1115	CLA	ND
15	A	1116	CLA	ND
15	A	1117	CLA	ND
15	A	1118	CLA	ND
15	A	1119	CLA	ND
15	A	1120	CLA	ND
15	A	1121	CLA	ND
15	A	1122	CLA	ND

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Mol	Chain	Res	Type	Atom
15	A	1123	CLA	ND
15	A	1124	CLA	ND
15	A	1125	CLA	ND
15	A	1126	CLA	ND
15	A	1127	CLA	ND
15	A	1128	CLA	ND
15	A	1129	CLA	ND
15	A	1130	CLA	ND
15	A	1131	CLA	ND
15	A	1132	CLA	ND
15	A	1133	CLA	ND
15	A	1134	CLA	ND
15	A	1135	CLA	ND
15	A	1136	CLA	ND
15	A	1137	CLA	ND
15	A	1138	CLA	ND
15	A	1139	CLA	ND
15	A	1140	CLA	ND
15	A	1141	CLA	ND
15	B	1021	CLA	ND
15	B	1022	CLA	ND
15	B	1023	CLA	ND
15	B	1201	CLA	ND
15	B	1202	CLA	ND
15	B	1203	CLA	ND
15	B	1204	CLA	ND
15	B	1205	CLA	ND
15	B	1206	CLA	ND
15	B	1207	CLA	ND
15	B	1208	CLA	ND
15	B	1209	CLA	ND
15	B	1210	CLA	ND
15	B	1211	CLA	ND
15	B	1212	CLA	ND
15	B	1214	CLA	ND
15	B	1215	CLA	ND
15	B	1216	CLA	ND
15	B	1217	CLA	ND
15	B	1218	CLA	ND
15	B	1219	CLA	ND
15	B	1220	CLA	ND
15	B	1221	CLA	ND

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Mol	Chain	Res	Type	Atom
15	B	1222	CLA	ND
15	B	1223	CLA	ND
15	B	1224	CLA	ND
15	B	1225	CLA	ND
15	B	1226	CLA	ND
15	B	1227	CLA	ND
15	B	1228	CLA	ND
15	B	1229	CLA	ND
15	B	1230	CLA	ND
15	B	1231	CLA	ND
15	B	1232	CLA	ND
15	B	1234	CLA	ND
15	B	1235	CLA	ND
15	B	1236	CLA	ND
15	B	1237	CLA	ND
15	B	1238	CLA	ND
15	B	1239	CLA	ND
15	F	1301	CLA	ND
15	F	1302	CLA	ND
15	J	1302	CLA	ND
15	K	1401	CLA	ND
15	K	1402	CLA	ND
15	L	1501	CLA	ND
15	L	1502	CLA	ND
15	L	1503	CLA	ND
15	O	1601	CLA	ND
15	O	1602	CLA	ND
15	O	1603	CLA	ND

All (411) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	1011	CLA	C1A-C2A-CAA-CBA
15	A	1012	CLA	CAD-CBD-CGD-O1D
15	A	1012	CLA	CAD-CBD-CGD-O2D
15	A	1012	CLA	CBD-CGD-O2D-CED
15	A	1101	CLA	C1A-C2A-CAA-CBA
15	A	1103	CLA	C1A-C2A-CAA-CBA
15	A	1103	CLA	C3A-C2A-CAA-CBA
15	A	1103	CLA	C2-C1-O2A-CGA
15	A	1103	CLA	CBD-CGD-O2D-CED
15	A	1105	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	1105	CLA	C3A-C2A-CAA-CBA
15	A	1105	CLA	CBD-CGD-O2D-CED
15	A	1106	CLA	C3A-C2A-CAA-CBA
15	A	1106	CLA	CHA-CBD-CGD-O1D
15	A	1106	CLA	CHA-CBD-CGD-O2D
15	A	1107	CLA	CBD-CGD-O2D-CED
15	A	1114	CLA	CBD-CGD-O2D-CED
15	A	1115	CLA	CBD-CGD-O2D-CED
15	A	1115	CLA	C4-C3-C5-C6
15	A	1116	CLA	C3A-C2A-CAA-CBA
15	A	1116	CLA	C2-C1-O2A-CGA
15	A	1116	CLA	CBD-CGD-O2D-CED
15	A	1117	CLA	CBD-CGD-O2D-CED
15	A	1126	CLA	C1A-C2A-CAA-CBA
15	A	1126	CLA	C3A-C2A-CAA-CBA
15	A	1126	CLA	C2-C1-O2A-CGA
15	A	1130	CLA	C1A-C2A-CAA-CBA
15	A	1130	CLA	C3A-C2A-CAA-CBA
15	B	1021	CLA	C1A-C2A-CAA-CBA
15	B	1021	CLA	C3A-C2A-CAA-CBA
15	B	1023	CLA	CBD-CGD-O2D-CED
15	B	1224	CLA	C1A-C2A-CAA-CBA
15	B	1224	CLA	C3A-C2A-CAA-CBA
15	B	1224	CLA	CBD-CGD-O2D-CED
15	B	1225	CLA	C1A-C2A-CAA-CBA
15	B	1225	CLA	C3A-C2A-CAA-CBA
15	B	1226	CLA	CBD-CGD-O2D-CED
15	B	1229	CLA	C2-C1-O2A-CGA
15	B	1230	CLA	CHA-CBD-CGD-O1D
15	B	1230	CLA	CHA-CBD-CGD-O2D
15	B	1232	CLA	C1A-C2A-CAA-CBA
15	B	1232	CLA	C3A-C2A-CAA-CBA
15	B	1232	CLA	CHA-CBD-CGD-O1D
15	B	1232	CLA	CHA-CBD-CGD-O2D
15	B	1236	CLA	C1A-C2A-CAA-CBA
15	B	1236	CLA	C3A-C2A-CAA-CBA
15	B	1236	CLA	CHA-CBD-CGD-O1D
15	B	1236	CLA	CHA-CBD-CGD-O2D
15	B	1237	CLA	CBD-CGD-O2D-CED
15	F	1301	CLA	CAD-CBD-CGD-O1D
15	F	1301	CLA	CAD-CBD-CGD-O2D
15	J	1302	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	J	1302	CLA	C3A-C2A-CAA-CBA
15	J	1302	CLA	C2-C1-O2A-CGA
15	J	1302	CLA	CAD-CBD-CGD-O1D
15	J	1302	CLA	CAD-CBD-CGD-O2D
15	J	1302	CLA	CBD-CGD-O2D-CED
18	A	4002	BCR	C11-C10-C9-C8
18	A	4002	BCR	C11-C10-C9-C34
18	A	4007	BCR	C5-C6-C7-C8
18	A	4007	BCR	C7-C8-C9-C10
18	A	4007	BCR	C11-C10-C9-C8
18	A	4007	BCR	C11-C10-C9-C34
18	A	4008	BCR	C1-C6-C7-C8
18	A	4008	BCR	C5-C6-C7-C8
18	A	4008	BCR	C11-C12-C13-C14
18	A	4008	BCR	C11-C12-C13-C35
18	A	4008	BCR	C13-C14-C15-C16
18	A	4011	BCR	C11-C10-C9-C8
18	A	4011	BCR	C11-C10-C9-C34
18	A	4011	BCR	C11-C12-C13-C14
18	A	4011	BCR	C11-C12-C13-C35
18	A	4011	BCR	C19-C20-C21-C22
18	A	4011	BCR	C21-C22-C23-C24
18	A	4011	BCR	C37-C22-C23-C24
18	A	4017	BCR	C11-C10-C9-C8
18	A	4017	BCR	C11-C10-C9-C34
18	A	4017	BCR	C21-C22-C23-C24
18	B	4005	BCR	C7-C8-C9-C10
18	B	4005	BCR	C7-C8-C9-C34
18	B	4005	BCR	C11-C10-C9-C8
18	B	4005	BCR	C11-C10-C9-C34
18	B	4005	BCR	C11-C12-C13-C14
18	B	4005	BCR	C11-C12-C13-C35
18	B	4005	BCR	C17-C18-C19-C20
18	B	4005	BCR	C36-C18-C19-C20
18	B	4008	BCR	C11-C10-C9-C8
18	B	4008	BCR	C11-C10-C9-C34
18	B	4008	BCR	C10-C11-C12-C13
18	I	4018	BCR	C7-C8-C9-C10
18	I	4018	BCR	C7-C8-C9-C34
18	I	4018	BCR	C10-C11-C12-C13
15	B	1021	CLA	O1D-CGD-O2D-CED
15	B	1023	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1224	CLA	O1D-CGD-O2D-CED
15	A	1101	CLA	O1D-CGD-O2D-CED
15	A	1013	CLA	CBD-CGD-O2D-CED
15	A	1101	CLA	CBD-CGD-O2D-CED
15	A	1104	CLA	CBD-CGD-O2D-CED
15	A	1130	CLA	CBD-CGD-O2D-CED
15	A	1131	CLA	CBD-CGD-O2D-CED
15	B	1021	CLA	CBD-CGD-O2D-CED
15	B	1229	CLA	CBD-CGD-O2D-CED
15	B	1230	CLA	CBD-CGD-O2D-CED
15	B	1236	CLA	CBD-CGD-O2D-CED
15	F	1301	CLA	CBD-CGD-O2D-CED
15	A	1107	CLA	O1A-CGA-O2A-C1
15	A	1114	CLA	O1A-CGA-O2A-C1
15	A	1114	CLA	CBA-CGA-O2A-C1
15	A	1130	CLA	O1D-CGD-O2D-CED
15	A	1131	CLA	O1D-CGD-O2D-CED
15	B	1229	CLA	O1D-CGD-O2D-CED
15	A	1107	CLA	CBA-CGA-O2A-C1
15	A	1106	CLA	CBD-CGD-O2D-CED
15	A	1105	CLA	O1A-CGA-O2A-C1
15	B	1226	CLA	O1A-CGA-O2A-C1
15	A	1013	CLA	O1D-CGD-O2D-CED
15	A	1103	CLA	O1D-CGD-O2D-CED
15	A	1104	CLA	O1D-CGD-O2D-CED
15	A	1105	CLA	O1D-CGD-O2D-CED
15	A	1012	CLA	O1D-CGD-O2D-CED
15	A	1114	CLA	O1D-CGD-O2D-CED
15	A	1115	CLA	O1D-CGD-O2D-CED
15	A	1116	CLA	O1D-CGD-O2D-CED
15	A	1117	CLA	O1D-CGD-O2D-CED
15	B	1237	CLA	O1D-CGD-O2D-CED
15	J	1302	CLA	O1D-CGD-O2D-CED
15	A	1012	CLA	C3-C5-C6-C7
15	A	1107	CLA	O1D-CGD-O2D-CED
15	B	1226	CLA	O1D-CGD-O2D-CED
15	A	1105	CLA	CBA-CGA-O2A-C1
15	A	1126	CLA	CBA-CGA-O2A-C1
15	B	1226	CLA	CBA-CGA-O2A-C1
15	B	1230	CLA	C2-C1-O2A-CGA
15	A	1126	CLA	CBD-CGD-O2D-CED
15	A	1115	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	A	1013	CLA	C3-C5-C6-C7
15	A	1117	CLA	C3-C5-C6-C7
15	A	1116	CLA	CBA-CGA-O2A-C1
15	A	1117	CLA	CBA-CGA-O2A-C1
15	B	1225	CLA	CBA-CGA-O2A-C1
18	A	4007	BCR	C9-C10-C11-C12
18	A	4017	BCR	C19-C20-C21-C22
18	B	4008	BCR	C9-C10-C11-C12
18	I	4018	BCR	C13-C14-C15-C16
15	A	1126	CLA	O1A-CGA-O2A-C1
15	B	1229	CLA	O1A-CGA-O2A-C1
15	B	1230	CLA	O1A-CGA-O2A-C1
15	B	1236	CLA	O1D-CGD-O2D-CED
15	F	1301	CLA	O1D-CGD-O2D-CED
15	A	1107	CLA	C3-C5-C6-C7
15	B	1237	CLA	C3-C5-C6-C7
15	A	1013	CLA	CBA-CGA-O2A-C1
15	A	1103	CLA	CBA-CGA-O2A-C1
15	B	1229	CLA	CBA-CGA-O2A-C1
15	B	1230	CLA	CBA-CGA-O2A-C1
15	B	1230	CLA	O1D-CGD-O2D-CED
15	B	1232	CLA	CBA-CGA-O2A-C1
15	A	1013	CLA	C4-C3-C5-C6
15	B	1224	CLA	C4-C3-C5-C6
15	B	1224	CLA	C2-C3-C5-C6
15	A	1116	CLA	O1A-CGA-O2A-C1
15	A	1117	CLA	O1A-CGA-O2A-C1
15	B	1225	CLA	O1A-CGA-O2A-C1
15	B	1226	CLA	C5-C6-C7-C8
15	A	1106	CLA	O1D-CGD-O2D-CED
15	A	1013	CLA	O1A-CGA-O2A-C1
15	B	1232	CLA	O1A-CGA-O2A-C1
15	B	1232	CLA	CBD-CGD-O2D-CED
15	A	1103	CLA	O1A-CGA-O2A-C1
15	A	1106	CLA	C3-C5-C6-C7
18	I	4018	BCR	C9-C10-C11-C12
15	A	1011	CLA	CBA-CGA-O2A-C1
15	A	1104	CLA	CBA-CGA-O2A-C1
15	B	1224	CLA	CBA-CGA-O2A-C1
15	A	1126	CLA	O1D-CGD-O2D-CED
15	A	1104	CLA	O1A-CGA-O2A-C1
18	A	4002	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
18	A	4007	BCR	C7-C8-C9-C34
18	A	4008	BCR	C7-C8-C9-C34
18	A	4008	BCR	C36-C18-C19-C20
18	A	4011	BCR	C36-C18-C19-C20
18	A	4017	BCR	C37-C22-C23-C24
18	B	4008	BCR	C36-C18-C19-C20
18	I	4018	BCR	C37-C22-C23-C24
18	A	4002	BCR	C11-C12-C13-C14
18	B	4008	BCR	C17-C18-C19-C20
15	A	1012	CLA	C2A-CAA-CBA-CGA
15	A	1011	CLA	O1A-CGA-O2A-C1
15	B	1224	CLA	O1A-CGA-O2A-C1
15	B	1224	CLA	C3-C5-C6-C7
15	A	1011	CLA	C2-C1-O2A-CGA
15	A	1012	CLA	C2-C1-O2A-CGA
15	A	1013	CLA	C2-C1-O2A-CGA
15	B	1225	CLA	C2-C1-O2A-CGA
15	B	1232	CLA	C5-C6-C7-C8
15	B	1232	CLA	C8-C10-C11-C12
18	A	4002	BCR	C13-C14-C15-C16
15	B	1224	CLA	C5-C6-C7-C8
15	B	1225	CLA	C2A-CAA-CBA-CGA
15	B	1232	CLA	C15-C16-C17-C18
15	A	1105	CLA	C5-C6-C7-C8
15	A	1126	CLA	C5-C6-C7-C8
16	B	2002	PQN	C23-C25-C26-C27
15	A	1115	CLA	CBA-CGA-O2A-C1
15	B	1232	CLA	C10-C11-C12-C13
16	A	2001	PQN	C14-C13-C15-C16
15	A	1115	CLA	C6-C7-C8-C9
18	A	4002	BCR	C7-C8-C9-C34
18	A	4007	BCR	C37-C22-C23-C24
18	A	4017	BCR	C7-C8-C9-C34
18	B	4008	BCR	C11-C12-C13-C35
18	A	4002	BCR	C7-C8-C9-C10
18	A	4008	BCR	C7-C8-C9-C10
18	A	4011	BCR	C17-C18-C19-C20
15	A	1115	CLA	O1A-CGA-O2A-C1
15	A	1013	CLA	C2A-CAA-CBA-CGA
15	A	1103	CLA	C3-C5-C6-C7
15	A	1013	CLA	C2-C3-C5-C6
15	A	1130	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
15	B	1224	CLA	C2-C1-O2A-CGA
16	B	2002	PQN	C20-C21-C22-C23
15	A	1011	CLA	C3A-C2A-CAA-CBA
15	A	1101	CLA	C3A-C2A-CAA-CBA
15	A	1104	CLA	C3A-C2A-CAA-CBA
15	B	1232	CLA	O1D-CGD-O2D-CED
18	A	4008	BCR	C19-C20-C21-C22
18	I	4018	BCR	C19-C20-C21-C22
15	B	1226	CLA	C3-C5-C6-C7
16	B	2002	PQN	C25-C26-C27-C28
15	A	1107	CLA	C6-C7-C8-C9
18	A	4007	BCR	C1-C6-C7-C8
18	B	4008	BCR	C1-C6-C7-C8
18	B	4008	BCR	C5-C6-C7-C8
15	A	1105	CLA	C2A-CAA-CBA-CGA
15	A	1116	CLA	C2A-CAA-CBA-CGA
18	A	4017	BCR	C10-C11-C12-C13
16	A	2001	PQN	C12-C13-C15-C16
15	A	1012	CLA	CBA-CGA-O2A-C1
15	A	1115	CLA	C6-C7-C8-C10
18	I	4018	BCR	C36-C18-C19-C20
15	A	1130	CLA	C3-C5-C6-C7
15	A	1104	CLA	C6-C7-C8-C9
15	A	1104	CLA	C6-C7-C8-C10
15	A	1107	CLA	C6-C7-C8-C10
16	A	2001	PQN	C20-C21-C22-C23
15	A	1117	CLA	C6-C7-C8-C10
15	B	1232	CLA	C13-C15-C16-C17
15	B	1226	CLA	C2-C1-O2A-CGA
15	A	1126	CLA	C4-C3-C5-C6
15	A	1114	CLA	C2A-CAA-CBA-CGA
15	B	1023	CLA	C2A-CAA-CBA-CGA
15	A	1104	CLA	C1A-C2A-CAA-CBA
15	A	1106	CLA	C1A-C2A-CAA-CBA
15	A	1116	CLA	C1A-C2A-CAA-CBA
15	A	1117	CLA	C1A-C2A-CAA-CBA
15	B	1230	CLA	C1A-C2A-CAA-CBA
16	A	2001	PQN	C18-C20-C21-C22
15	B	1232	CLA	C6-C7-C8-C10
15	A	1116	CLA	C6-C7-C8-C9
15	B	1237	CLA	C4-C3-C5-C6
15	A	1106	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
15	A	1117	CLA	C6-C7-C8-C9
18	A	4008	BCR	C37-C22-C23-C24
18	A	4008	BCR	C17-C18-C19-C20
18	I	4018	BCR	C21-C22-C23-C24
15	A	1012	CLA	O1A-CGA-O2A-C1
15	A	1106	CLA	C2A-CAA-CBA-CGA
15	A	1106	CLA	C2-C1-O2A-CGA
15	B	1232	CLA	C6-C7-C8-C9
16	B	2002	PQN	C21-C22-C23-C24
15	A	1114	CLA	C4B-C3B-CAB-CBB
15	B	1224	CLA	C4B-C3B-CAB-CBB
15	A	1106	CLA	C5-C6-C7-C8
15	B	1226	CLA	C6-C7-C8-C10
15	A	1013	CLA	CAA-CBA-CGA-O2A
15	A	1130	CLA	CBA-CGA-O2A-C1
18	A	4002	BCR	C15-C16-C17-C18
15	A	1104	CLA	C2A-CAA-CBA-CGA
15	A	1104	CLA	C5-C6-C7-C8
18	A	4007	BCR	C23-C24-C25-C30
18	I	4018	BCR	C23-C24-C25-C30
16	A	2001	PQN	C15-C16-C17-C18
15	B	1226	CLA	C6-C7-C8-C9
16	B	2002	PQN	C16-C17-C18-C20
16	B	2002	PQN	C21-C22-C23-C25
18	A	4007	BCR	C21-C22-C23-C24
18	A	4017	BCR	C7-C8-C9-C10
18	I	4018	BCR	C17-C18-C19-C20
15	A	1116	CLA	C6-C7-C8-C10
15	B	1224	CLA	CAA-CBA-CGA-O2A
15	A	1130	CLA	O1A-CGA-O2A-C1
15	A	1106	CLA	C6-C7-C8-C9
15	A	1116	CLA	C5-C6-C7-C8
15	A	1107	CLA	C5-C6-C7-C8
15	A	1115	CLA	C2-C1-O2A-CGA
15	A	1101	CLA	C4B-C3B-CAB-CBB
15	A	1107	CLA	C1A-C2A-CAA-CBA
15	A	1116	CLA	C4B-C3B-CAB-CBB
15	B	1232	CLA	C4B-C3B-CAB-CBB
18	B	4008	BCR	C11-C12-C13-C14
15	A	1115	CLA	C2A-CAA-CBA-CGA
15	A	1115	CLA	C3A-C2A-CAA-CBA
15	A	1126	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	B	2002	PQN	C16-C17-C18-C19
18	I	4018	BCR	C15-C16-C17-C18
15	A	1126	CLA	CAA-CBA-CGA-O2A
15	B	1237	CLA	C2-C3-C5-C6
15	A	1103	CLA	CAD-CBD-CGD-O1D
18	B	4005	BCR	C19-C20-C21-C22
18	A	4008	BCR	C23-C24-C25-C30
15	B	1023	CLA	CBA-CGA-O2A-C1
15	B	1023	CLA	O1A-CGA-O2A-C1
18	A	4007	BCR	C10-C11-C12-C13
18	A	4007	BCR	C18-C19-C20-C21
18	A	4007	BCR	C19-C20-C21-C22
15	A	1117	CLA	C5-C6-C7-C8
18	A	4007	BCR	C36-C18-C19-C20
15	B	1230	CLA	CAA-CBA-CGA-O2A
15	B	1224	CLA	C2A-CAA-CBA-CGA
15	B	1237	CLA	C2A-CAA-CBA-CGA
15	A	1107	CLA	C4B-C3B-CAB-CBB
15	J	1302	CLA	C4B-C3B-CAB-CBB
15	A	1012	CLA	C6-C7-C8-C10
15	B	1232	CLA	C11-C12-C13-C15
15	A	1013	CLA	C3A-C2A-CAA-CBA
18	A	4007	BCR	C16-C17-C18-C36
18	A	4011	BCR	C16-C17-C18-C36
18	A	4017	BCR	C16-C17-C18-C36
18	B	4005	BCR	C16-C17-C18-C36
18	I	4018	BCR	C11-C10-C9-C34
15	A	1115	CLA	C3-C5-C6-C7
15	A	1130	CLA	C6-C7-C8-C10
15	A	1117	CLA	C2A-CAA-CBA-CGA
15	B	1237	CLA	C5-C6-C7-C8
18	A	4007	BCR	C16-C17-C18-C19
18	A	4011	BCR	C16-C17-C18-C19
18	A	4017	BCR	C16-C17-C18-C19
18	B	4005	BCR	C16-C17-C18-C19
15	A	1101	CLA	C2B-C3B-CAB-CBB
15	A	1114	CLA	C2B-C3B-CAB-CBB
15	A	1116	CLA	C2B-C3B-CAB-CBB
15	B	1232	CLA	C2B-C3B-CAB-CBB
15	J	1302	CLA	C2B-C3B-CAB-CBB
18	A	4007	BCR	C23-C24-C25-C26
18	A	4017	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
18	B	4005	BCR	C1-C6-C7-C8
18	B	4008	BCR	C23-C24-C25-C30
18	I	4018	BCR	C1-C6-C7-C8
18	I	4018	BCR	C23-C24-C25-C26
16	A	2001	PQN	C17-C18-C20-C21
16	A	2001	PQN	C21-C22-C23-C25
15	A	1011	CLA	C2A-CAA-CBA-CGA
15	A	1131	CLA	CAA-CBA-CGA-O2A
15	A	1131	CLA	CAA-CBA-CGA-O1A
18	B	4008	BCR	C7-C8-C9-C34
15	A	1103	CLA	C4-C3-C5-C6
15	A	1105	CLA	C4-C3-C5-C6
15	A	1116	CLA	C4-C3-C5-C6
15	J	1302	CLA	C2C-C3C-CAC-CBC
15	A	1013	CLA	CAA-CBA-CGA-O1A
15	A	1012	CLA	C4-C3-C5-C6
15	B	1226	CLA	C4B-C3B-CAB-CBB
15	A	1101	CLA	CAA-CBA-CGA-O2A
15	A	1130	CLA	C4-C3-C5-C6
15	B	1232	CLA	C2A-CAA-CBA-CGA
15	A	1012	CLA	C6-C7-C8-C9
15	A	1101	CLA	CAA-CBA-CGA-O1A
15	A	1130	CLA	C5-C6-C7-C8
18	I	4018	BCR	C11-C10-C9-C8
15	F	1301	CLA	CAA-CBA-CGA-O1A
15	A	1130	CLA	C6-C7-C8-C9
15	F	1301	CLA	CAA-CBA-CGA-O2A
15	B	1224	CLA	C2B-C3B-CAB-CBB
15	B	1226	CLA	C2B-C3B-CAB-CBB
18	A	4008	BCR	C23-C24-C25-C26
18	A	4017	BCR	C23-C24-C25-C26
18	B	4005	BCR	C5-C6-C7-C8
18	B	4005	BCR	C23-C24-C25-C26
18	B	4005	BCR	C23-C24-C25-C30
18	B	4008	BCR	C23-C24-C25-C26
18	I	4018	BCR	C5-C6-C7-C8
15	B	1237	CLA	CAA-CBA-CGA-O2A
15	J	1302	CLA	C4C-C3C-CAC-CBC
15	A	1012	CLA	CAA-CBA-CGA-O2A
15	J	1302	CLA	CAA-CBA-CGA-O2A
15	A	1104	CLA	C3-C5-C6-C7
16	A	2001	PQN	C19-C18-C20-C21

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Mol	Chain	Res	Type	Atoms
16	A	2001	PQN	C21-C22-C23-C24
15	A	1013	CLA	C1A-C2A-CAA-CBA
15	F	1301	CLA	C1A-C2A-CAA-CBA
18	A	4008	BCR	C21-C22-C23-C24
18	B	4008	BCR	C7-C8-C9-C10
15	A	1116	CLA	CAA-CBA-CGA-O2A
15	B	1023	CLA	CAA-CBA-CGA-O2A
15	B	1229	CLA	C2A-CAA-CBA-CGA
15	B	1225	CLA	CAA-CBA-CGA-O2A
16	A	2001	PQN	C26-C27-C28-C29
15	B	1224	CLA	CAA-CBA-CGA-O1A
15	J	1302	CLA	CAA-CBA-CGA-O1A
15	A	1012	CLA	CAA-CBA-CGA-O1A
15	B	1237	CLA	CAA-CBA-CGA-O1A
18	A	4007	BCR	C17-C18-C19-C20
15	B	1225	CLA	CAA-CBA-CGA-O1A
15	B	1023	CLA	CAA-CBA-CGA-O1A
15	A	1101	CLA	CAD-CBD-CGD-O2D
15	A	1103	CLA	CAD-CBD-CGD-O2D
15	B	1226	CLA	CAD-CBD-CGD-O2D
15	A	1116	CLA	CAA-CBA-CGA-O1A
15	A	1104	CLA	CAA-CBA-CGA-O2A
15	B	1232	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

67 monomers are involved in 145 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1205	CLA	1	0
15	B	1225	CLA	5	0
15	4	615	CLA	1	0
15	A	1117	CLA	3	0
15	B	1201	CLA	1	0
15	B	1228	CLA	2	0
15	B	1224	CLA	7	0
15	4	612	CLA	1	0
16	A	2001	PQN	3	0
15	A	1127	CLA	1	0
15	A	1012	CLA	6	0
15	B	1021	CLA	4	0
15	L	1502	CLA	1	0
15	3	601	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	606	CLA	2	0
15	A	1104	CLA	1	0
15	3	610	CLA	1	0
15	B	1023	CLA	5	0
15	B	1206	CLA	1	0
15	A	1112	CLA	1	0
15	B	1212	CLA	1	0
15	B	1203	CLA	2	0
15	2	607	CLA	1	0
15	L	1501	CLA	1	0
15	B	1237	CLA	1	0
15	3	604	CLA	1	0
17	C	3002	SF4	3	0
18	A	4017	BCR	6	0
15	B	1227	CLA	1	0
15	A	1107	CLA	2	0
15	B	1229	CLA	6	0
15	J	1302	CLA	1	0
18	B	4005	BCR	7	0
15	A	1106	CLA	5	0
15	B	1202	CLA	1	0
15	A	1124	CLA	1	0
18	A	4008	BCR	1	0
15	A	1129	CLA	1	0
15	A	1122	CLA	1	0
15	B	1210	CLA	1	0
15	A	1139	CLA	1	0
18	A	4007	BCR	4	0
18	A	4011	BCR	11	0
18	A	4002	BCR	3	0
15	A	1105	CLA	3	0
17	C	3003	SF4	1	0
15	4	606	CLA	1	0
15	A	1013	CLA	7	0
15	B	1232	CLA	3	0
15	A	1135	CLA	1	0
18	I	4018	BCR	4	0
15	2	612	CLA	1	0
18	B	4008	BCR	1	0
16	B	2002	PQN	1	0
15	B	1236	CLA	1	0
15	A	1011	CLA	5	0

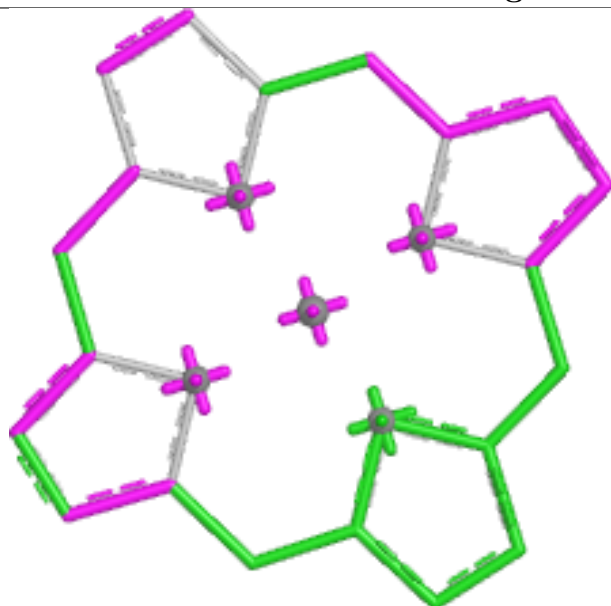
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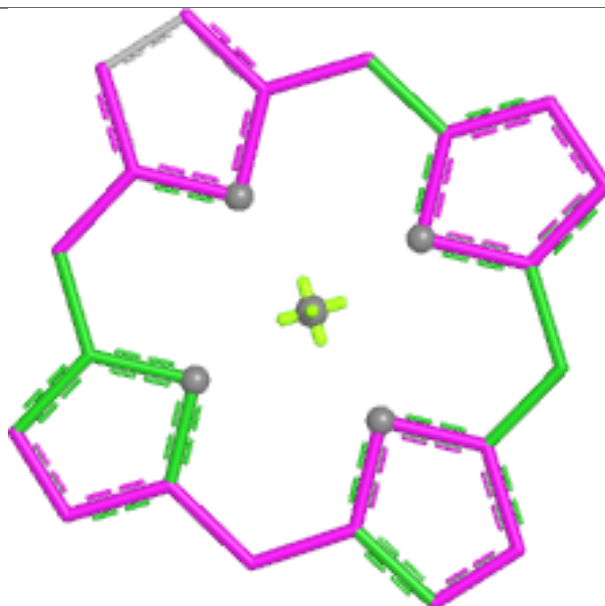
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1126	CLA	10	0
15	B	1239	CLA	1	0
15	B	1230	CLA	6	0
15	A	1131	CLA	2	0
15	B	1226	CLA	6	0
15	A	1114	CLA	1	0
15	A	1123	CLA	1	0
15	A	1130	CLA	5	0
15	B	1022	CLA	1	0
15	B	1207	CLA	1	0
15	A	1103	CLA	1	0

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 than 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.

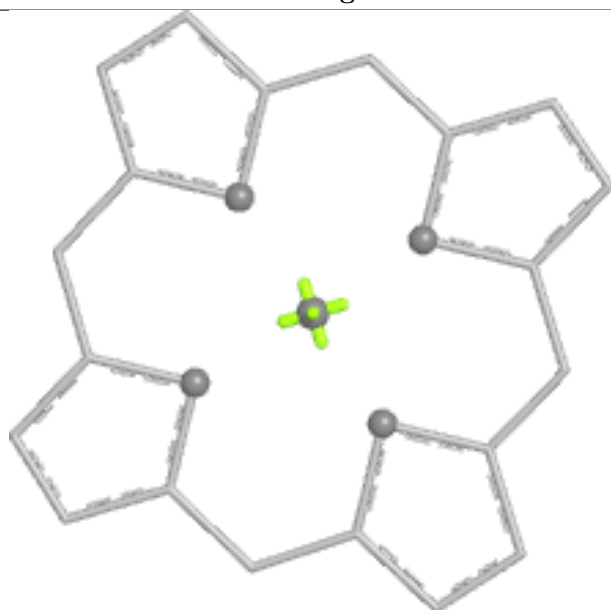
Ligand CLA B 1205



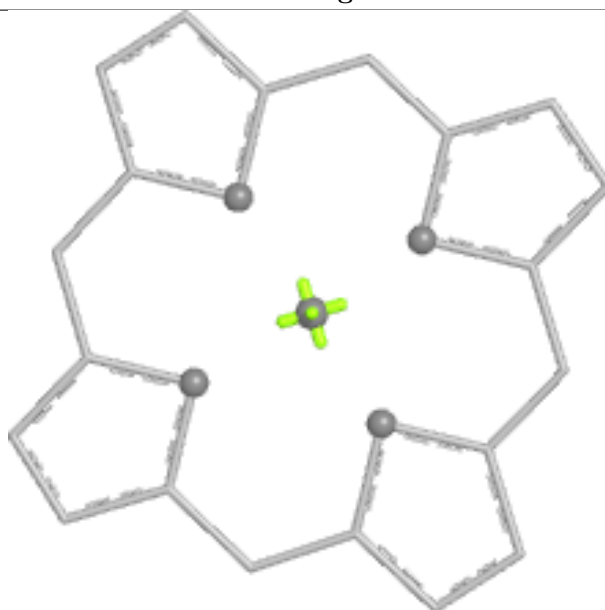
Bond lengths



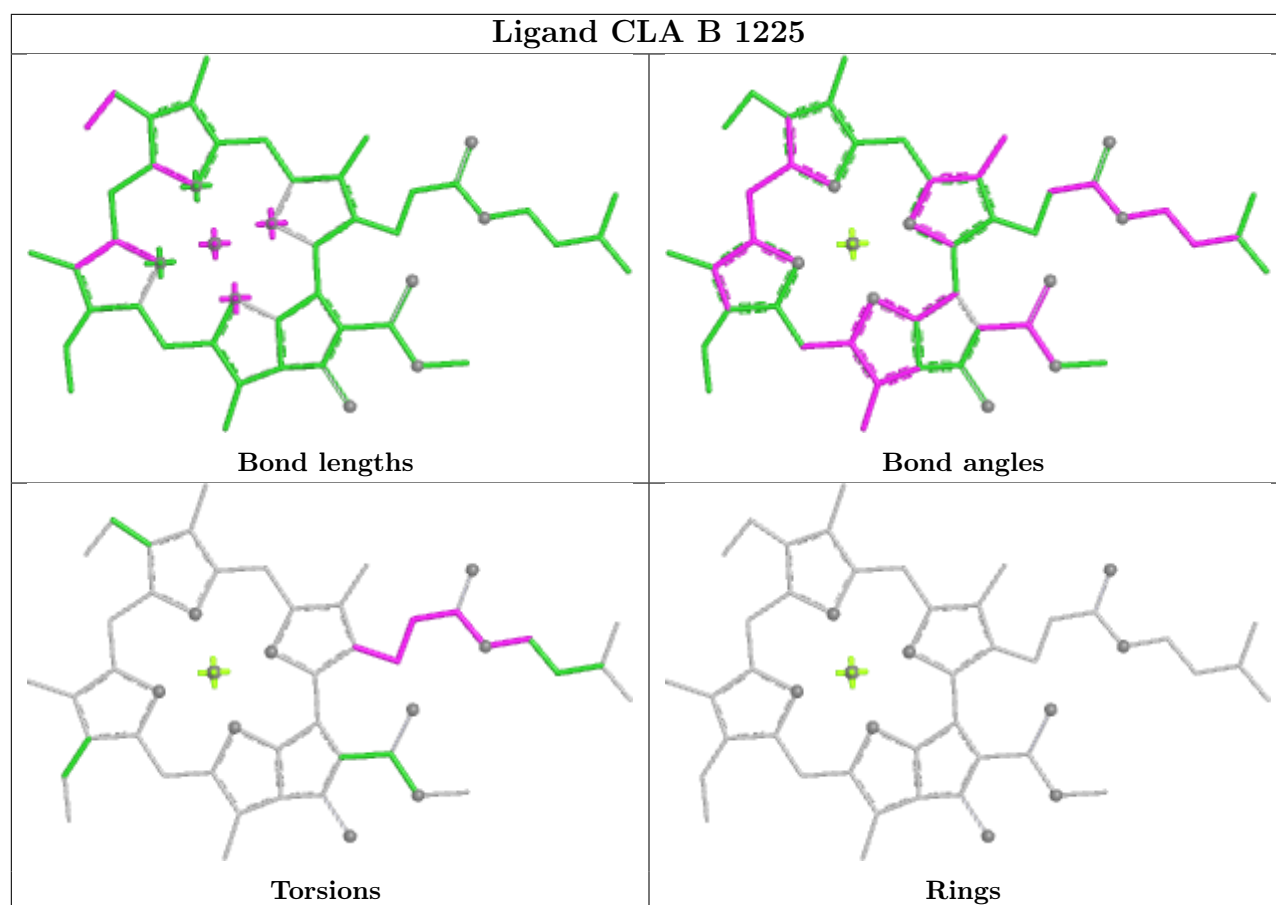
Bond angles



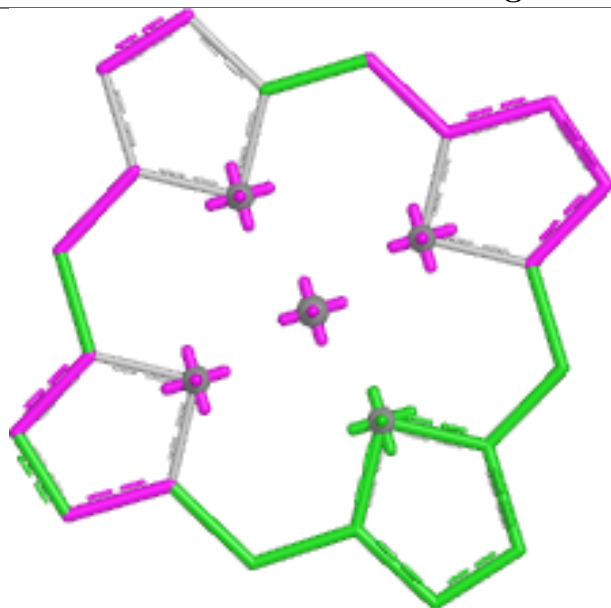
Torsions



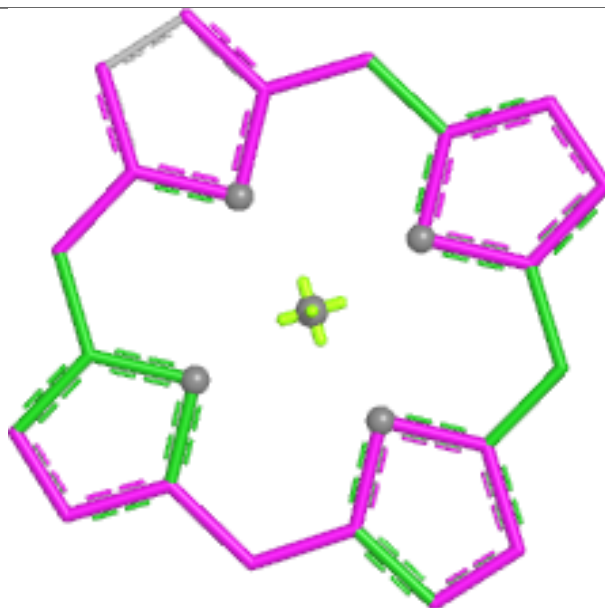
Rings



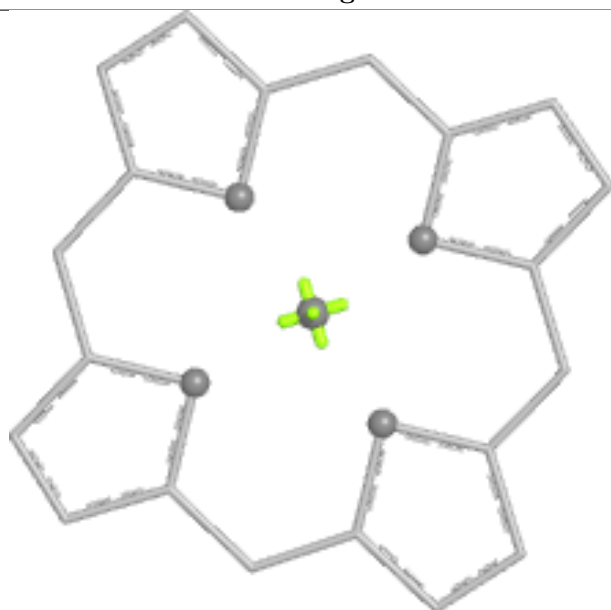
Ligand CLA O 1603



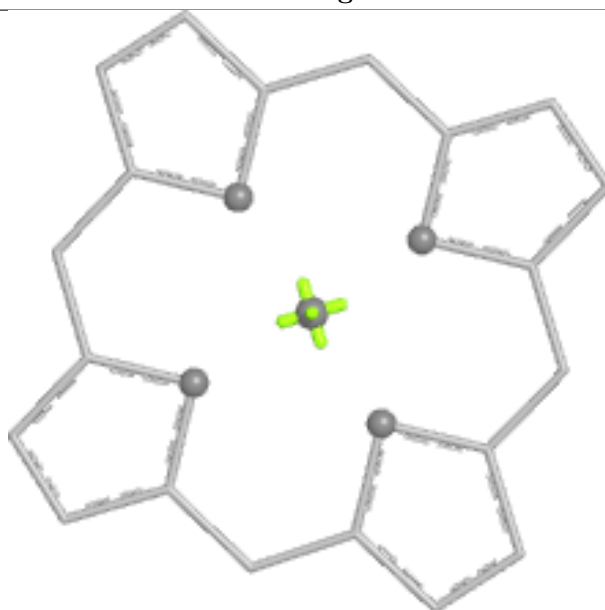
Bond lengths



Bond angles

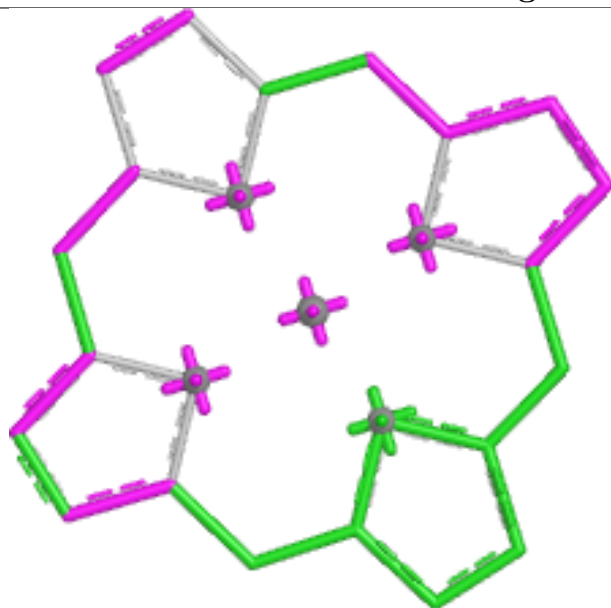


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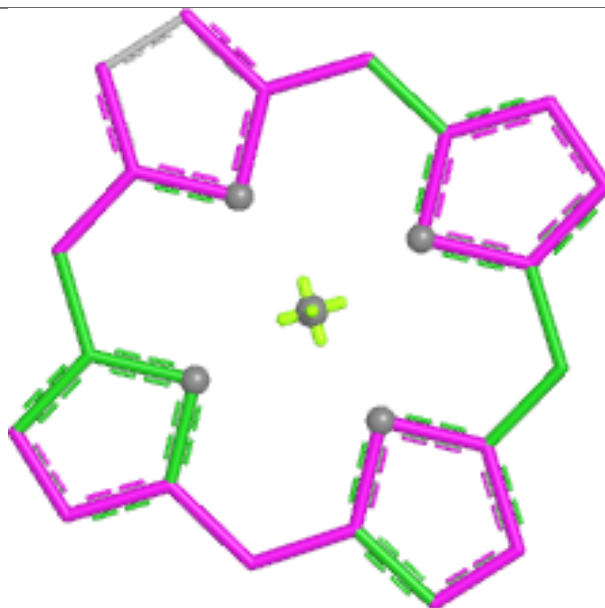


Rings

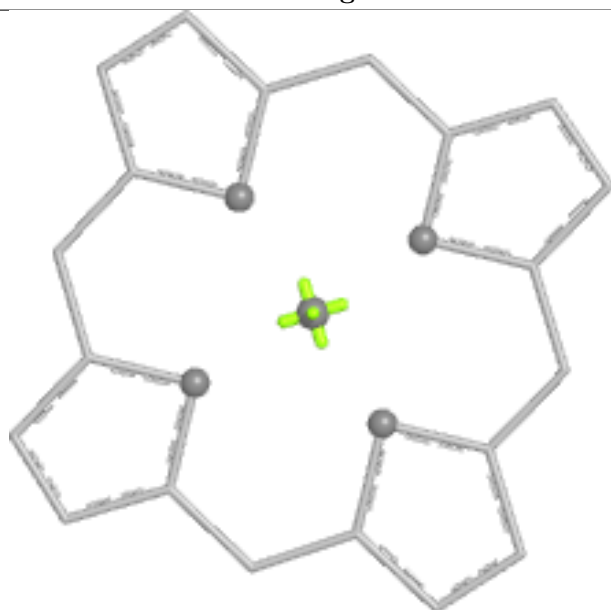
Ligand CLA 4 604



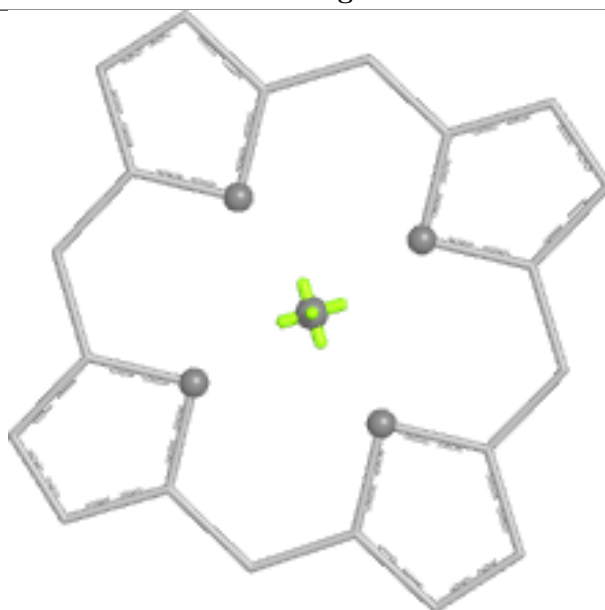
Bond lengths



Bond angles

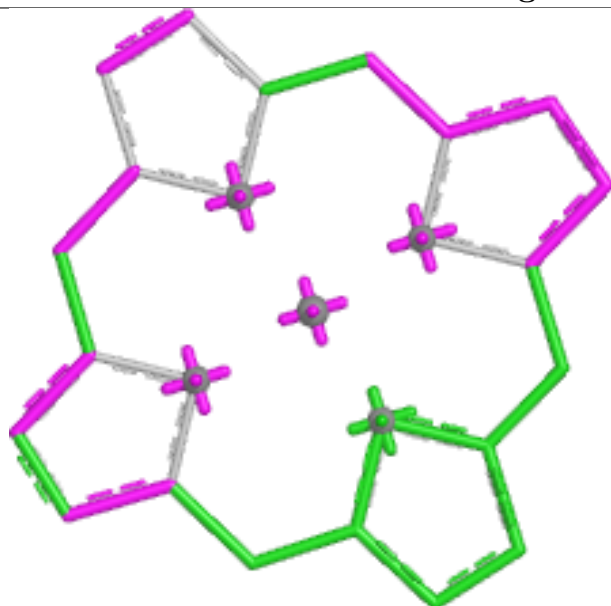


Torsions

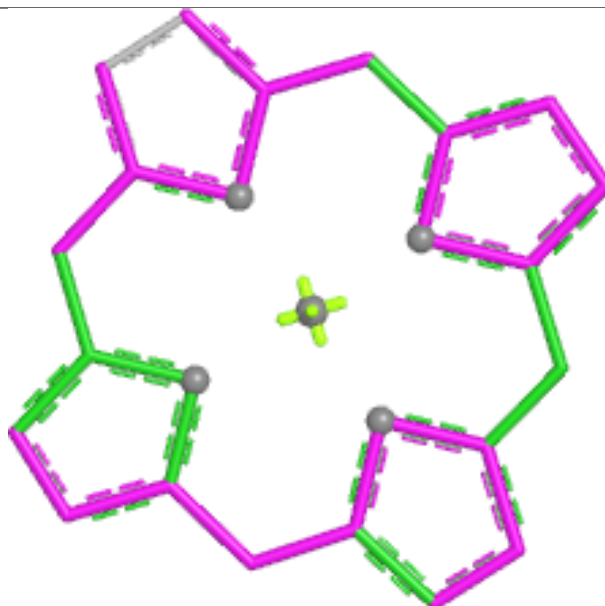


Rings

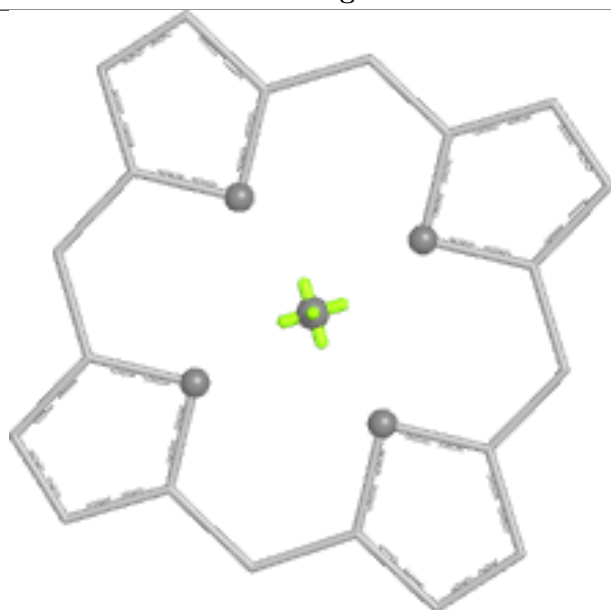
Ligand CLA 4 615



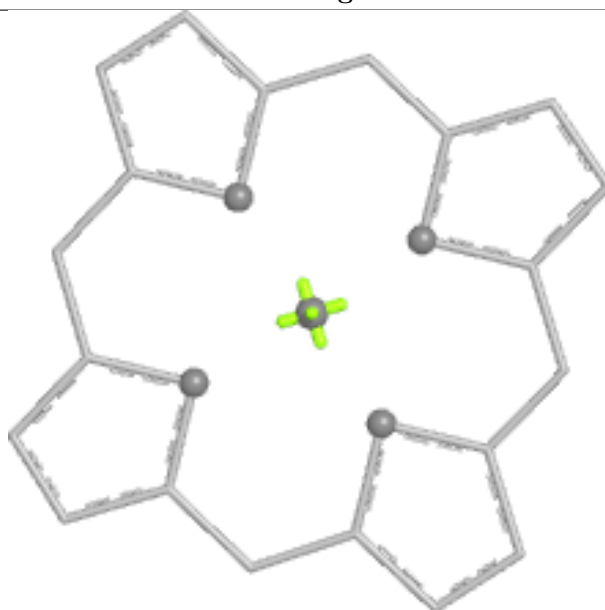
Bond lengths



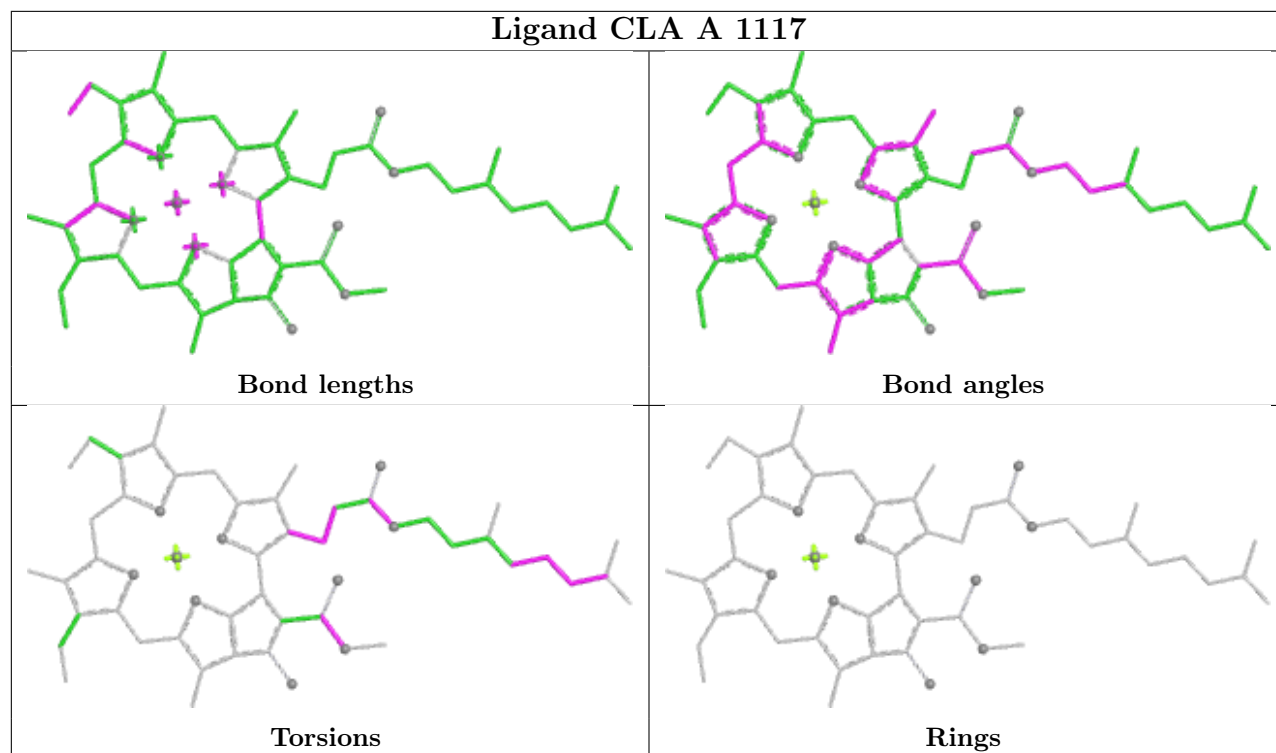
Bond angles



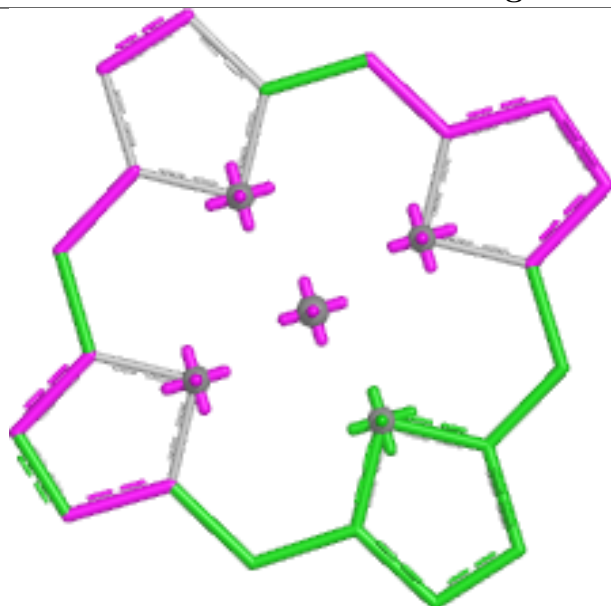
Torsions



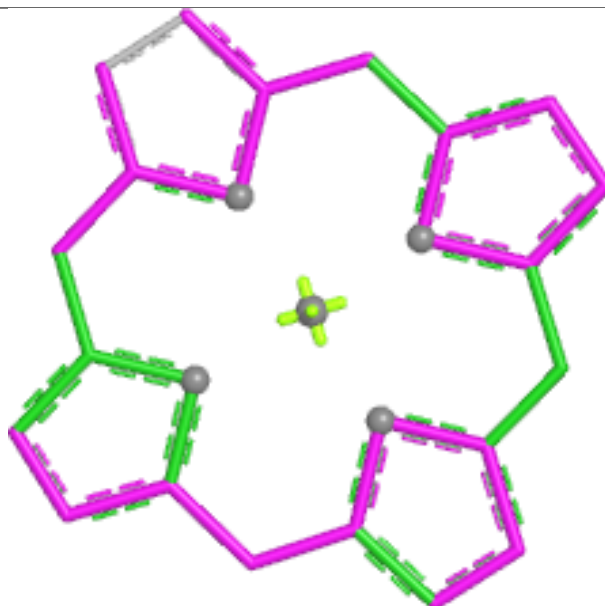
Rings



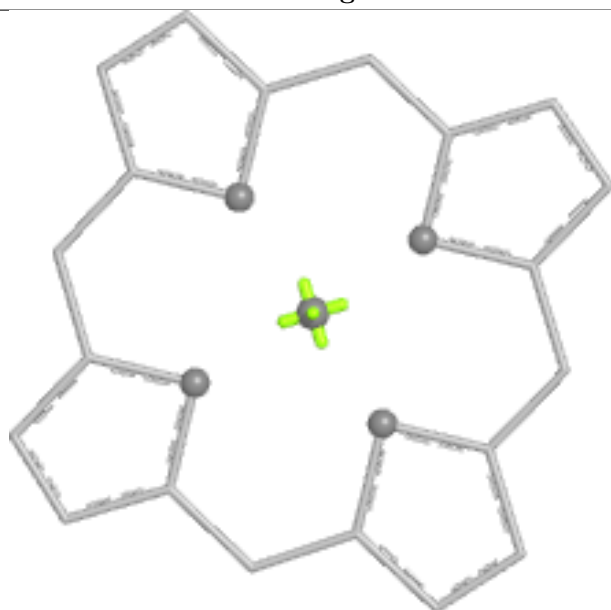
Ligand CLA B 1201



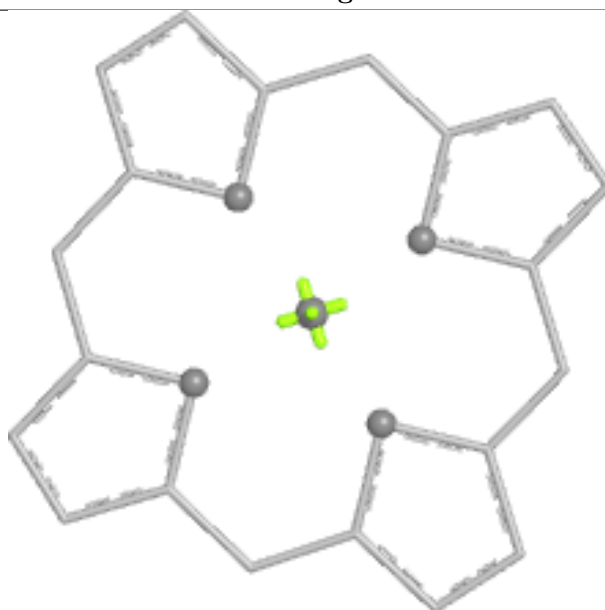
Bond lengths



Bond angles

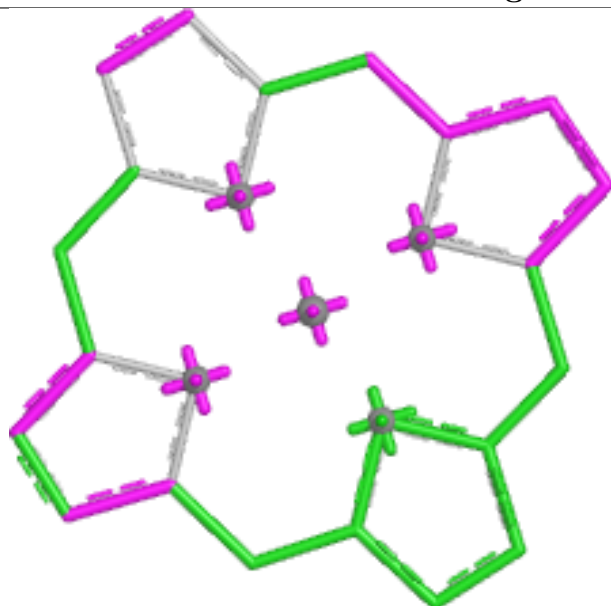


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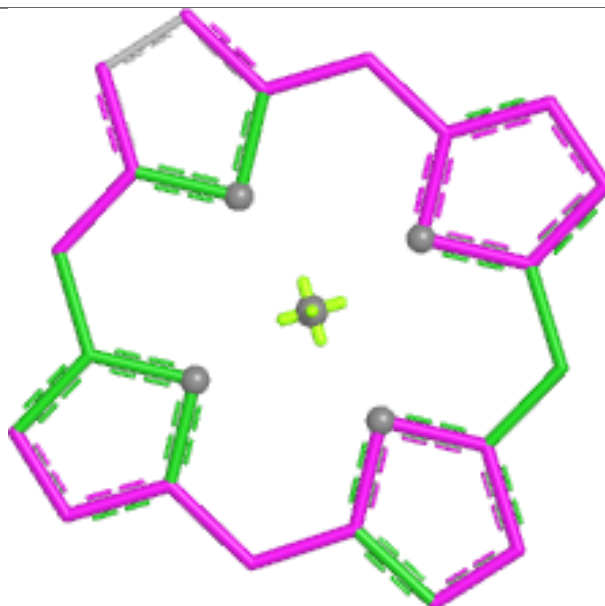


Rings

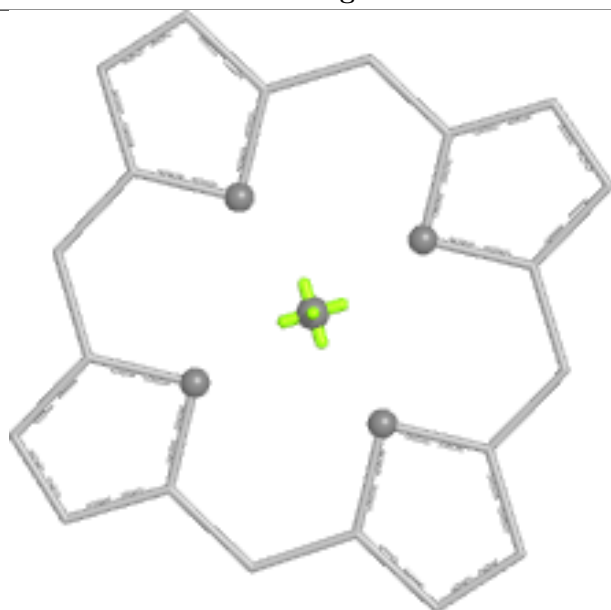
Ligand CLA B 1228



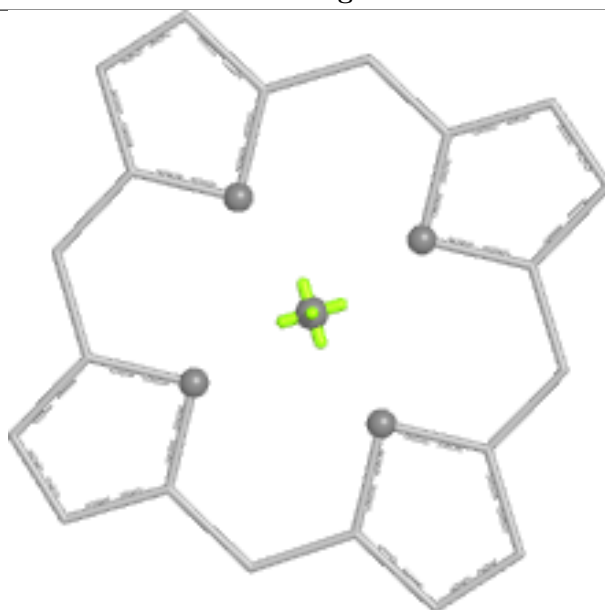
Bond lengths



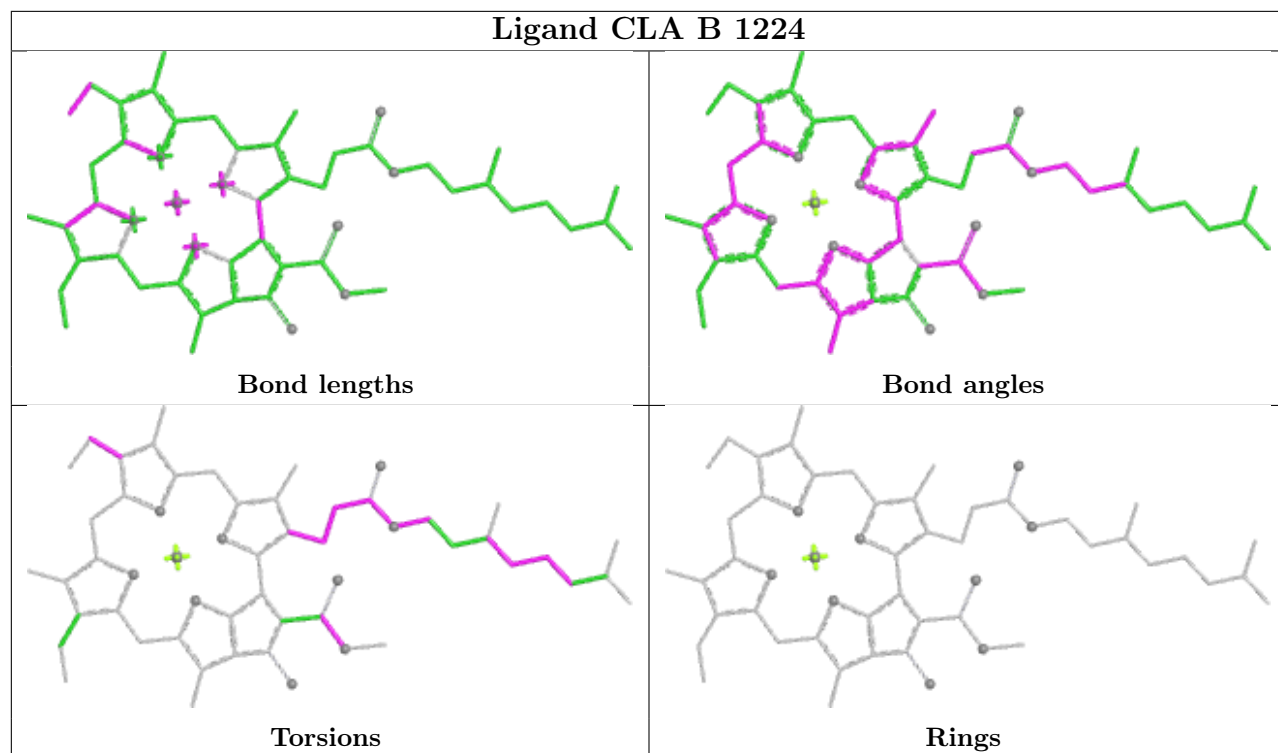
Bond angles



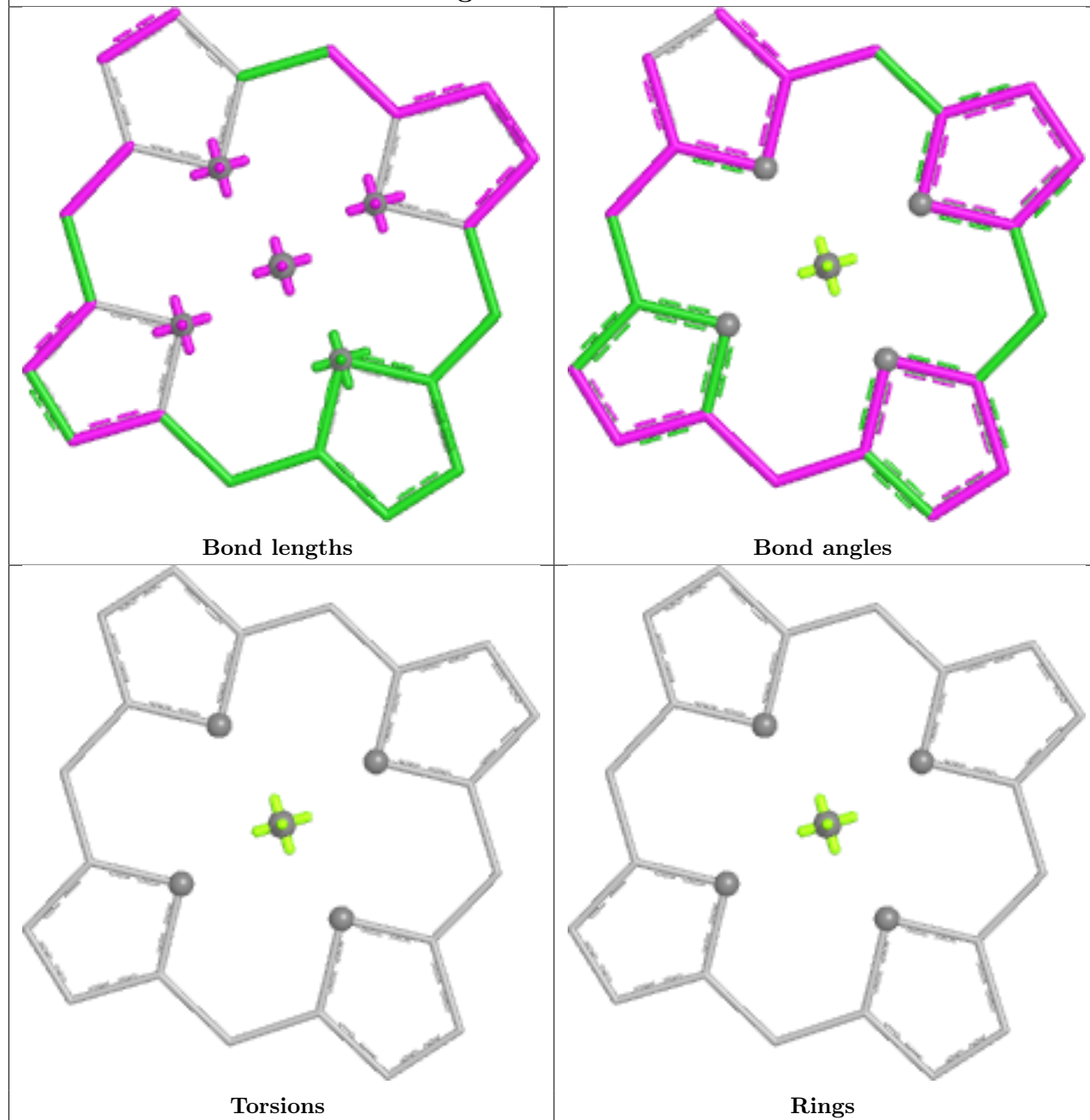
Torsions



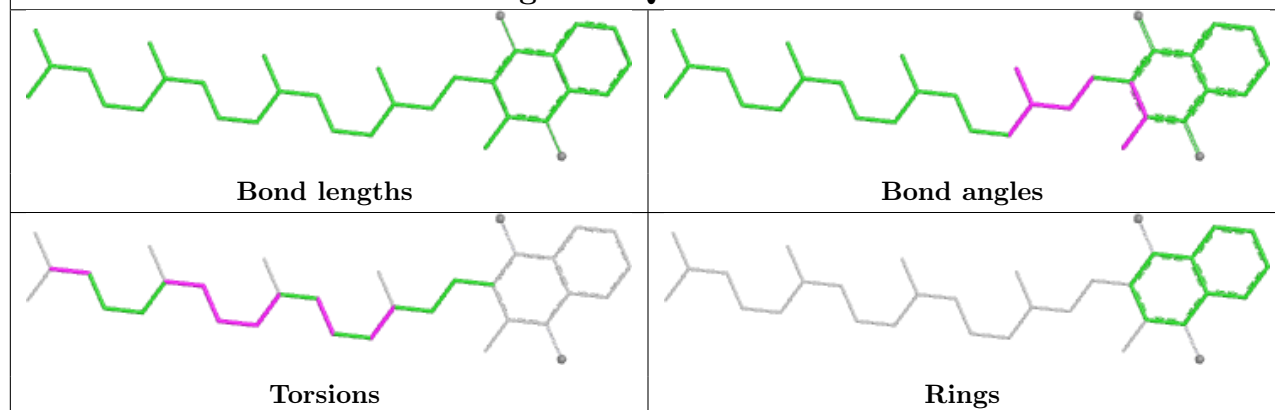
Rings



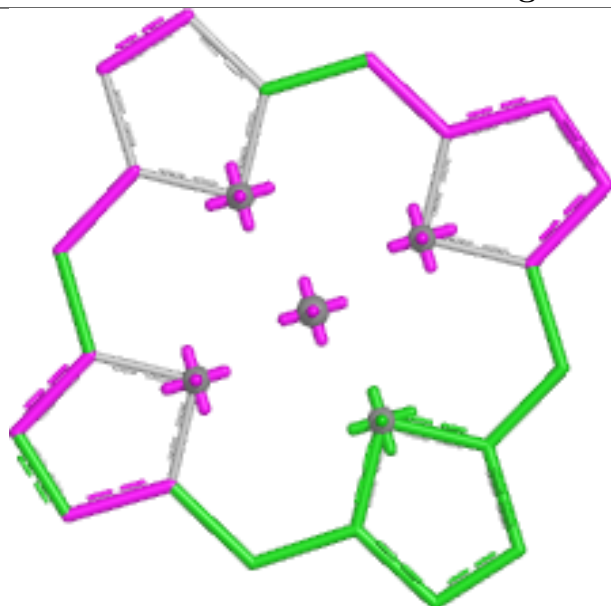
Ligand CLA 4 612



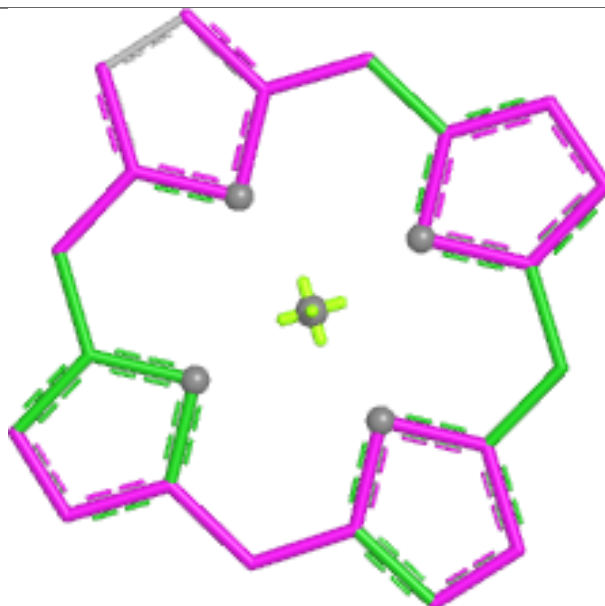
Ligand PQN A 2001



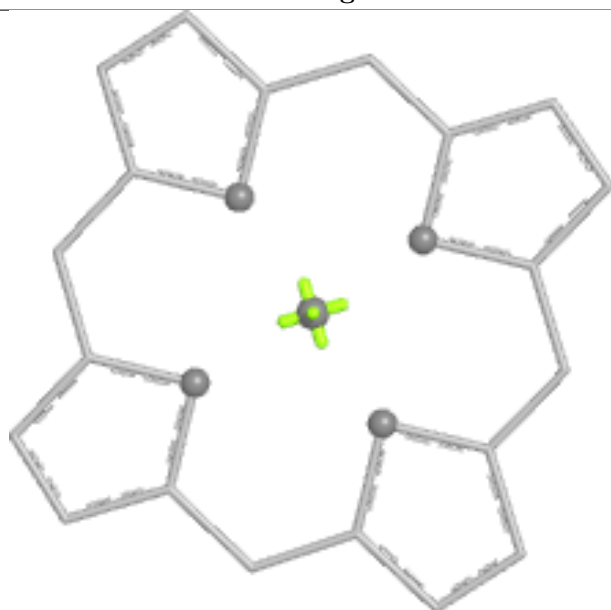
Ligand CLA 2 610



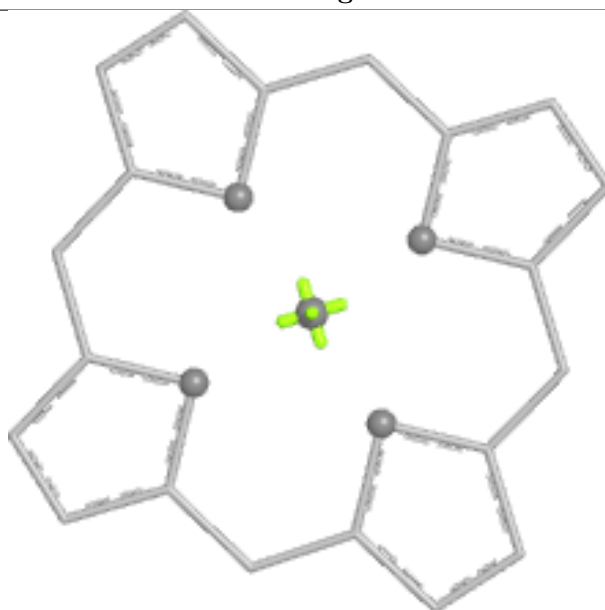
Bond lengths



Bond angles

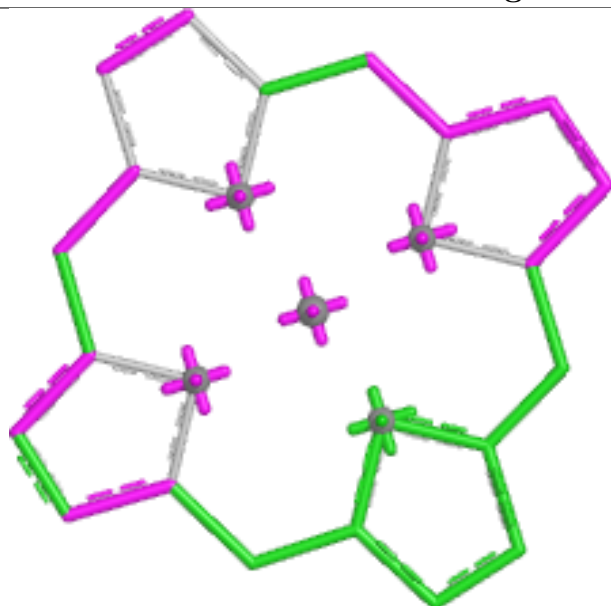


Torsions

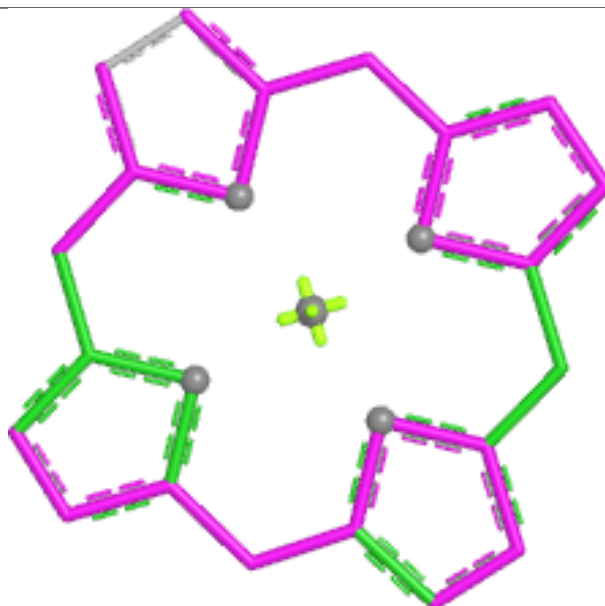


Rings

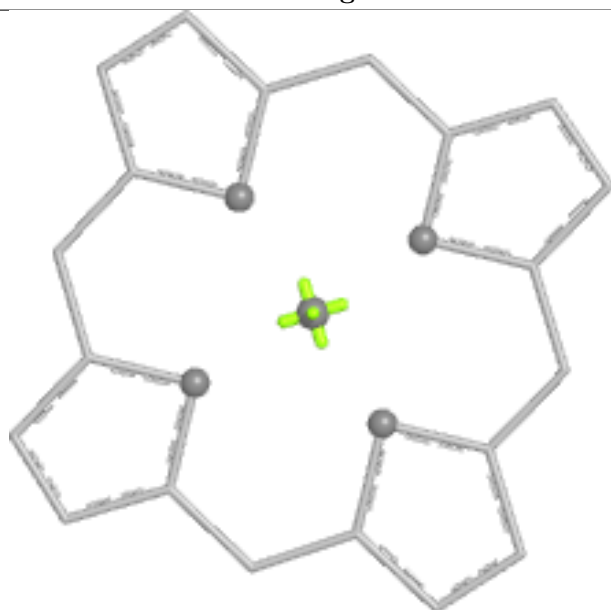
Ligand CLA A 1127



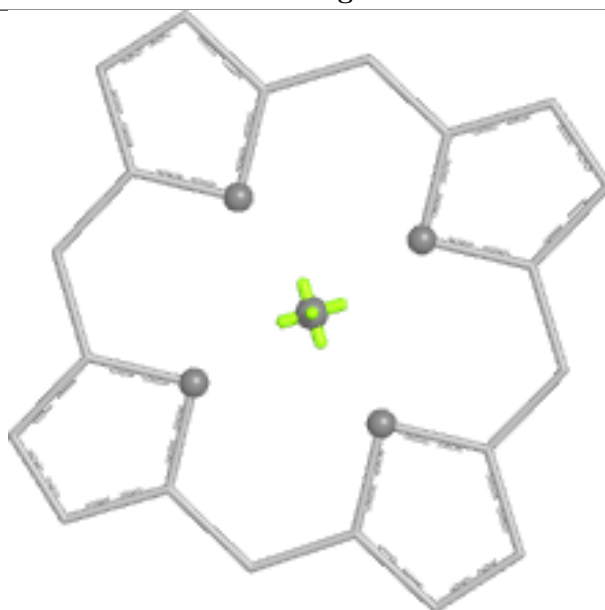
Bond lengths



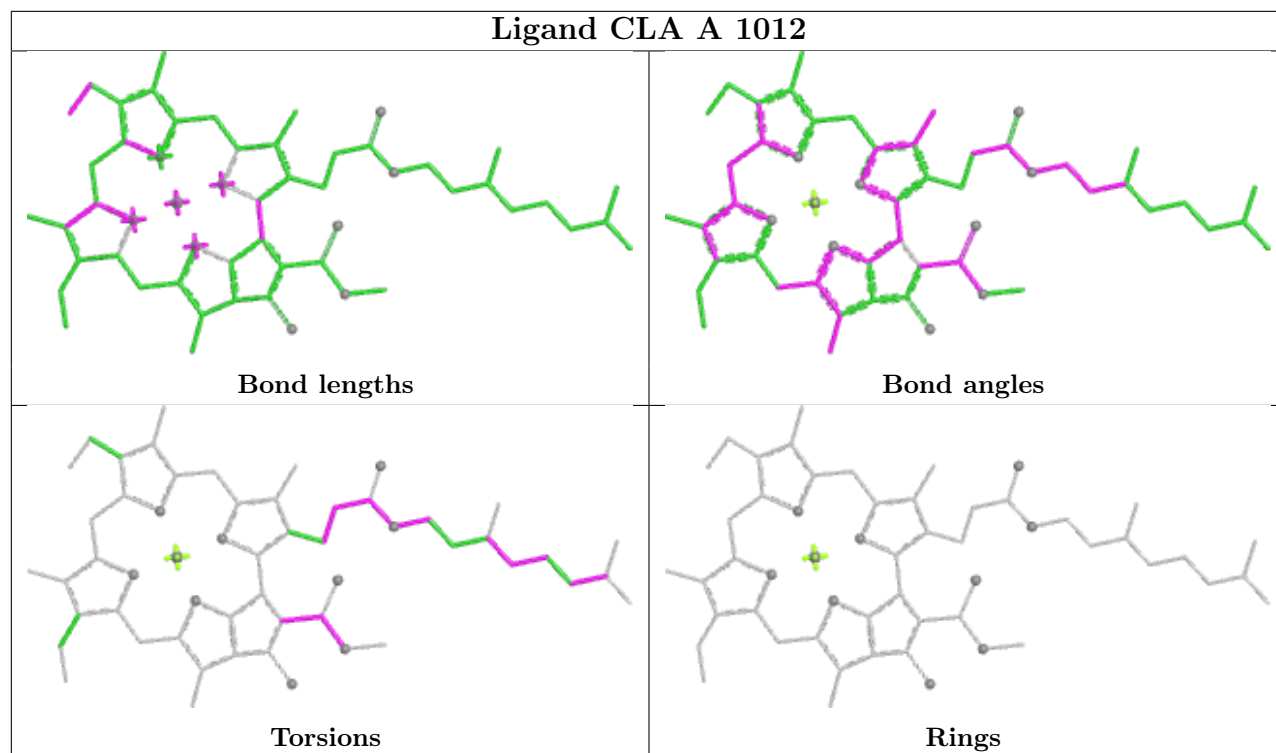
Bond angles



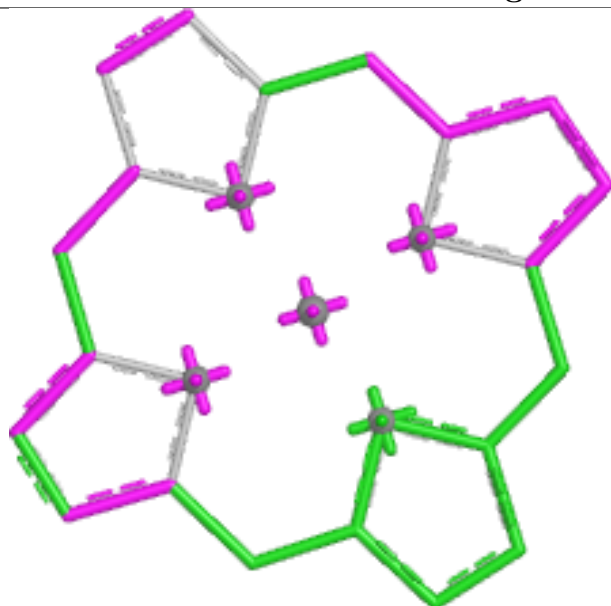
Torsions



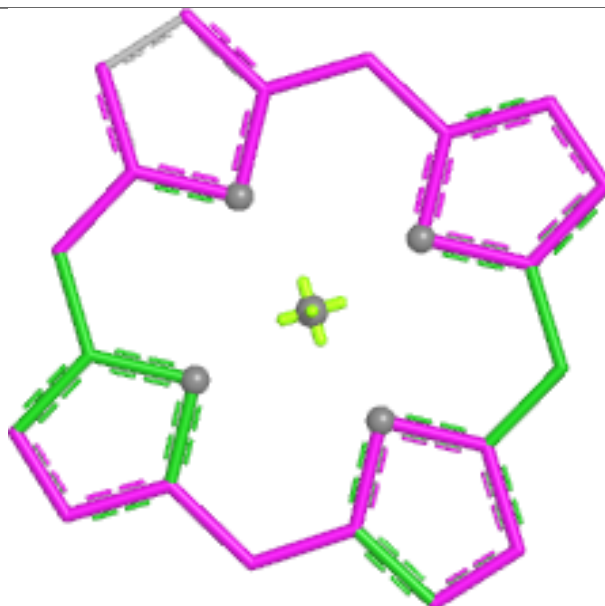
Rings



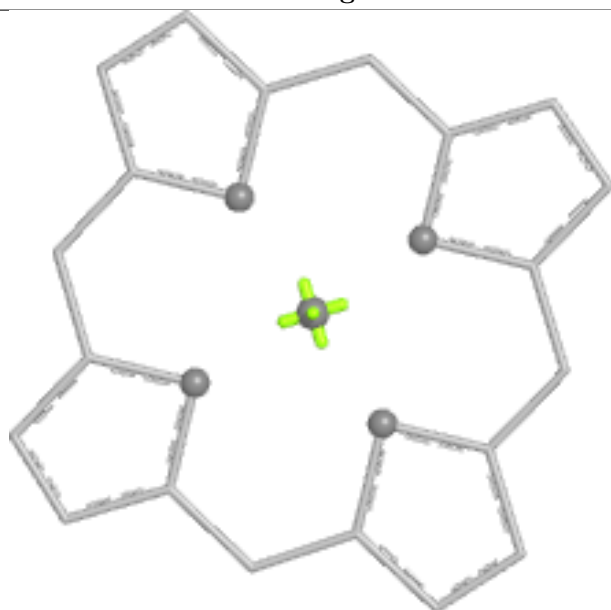
Ligand CLA B 1215



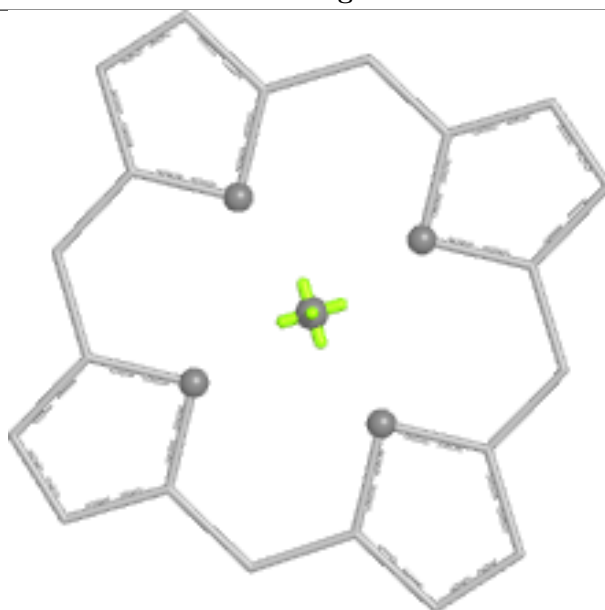
Bond lengths



Bond angles

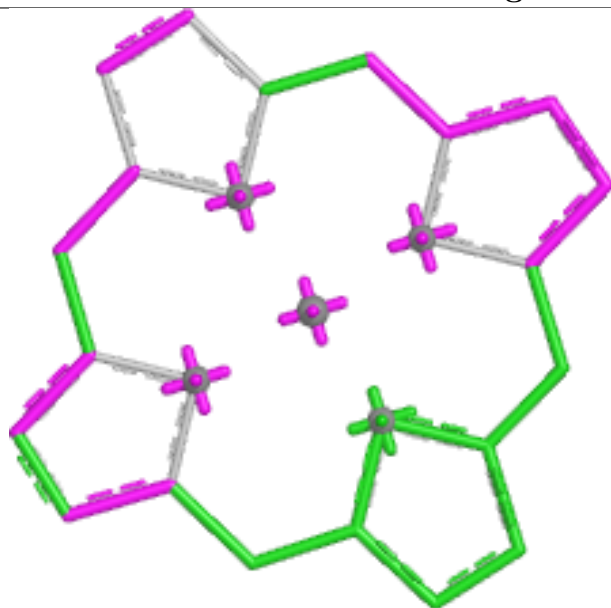


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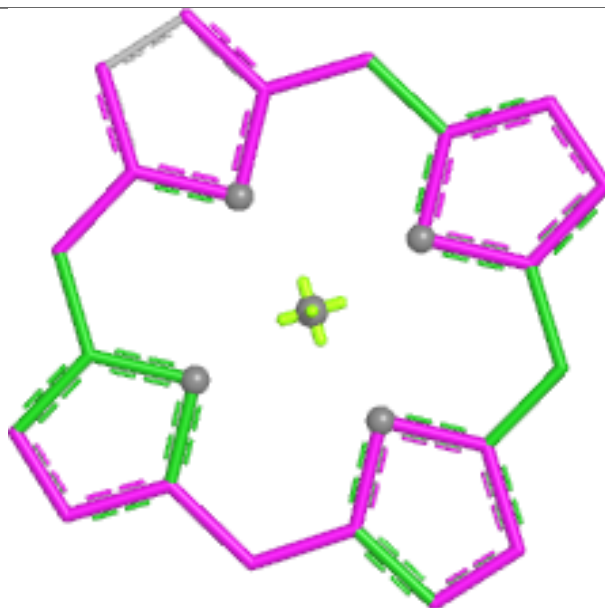


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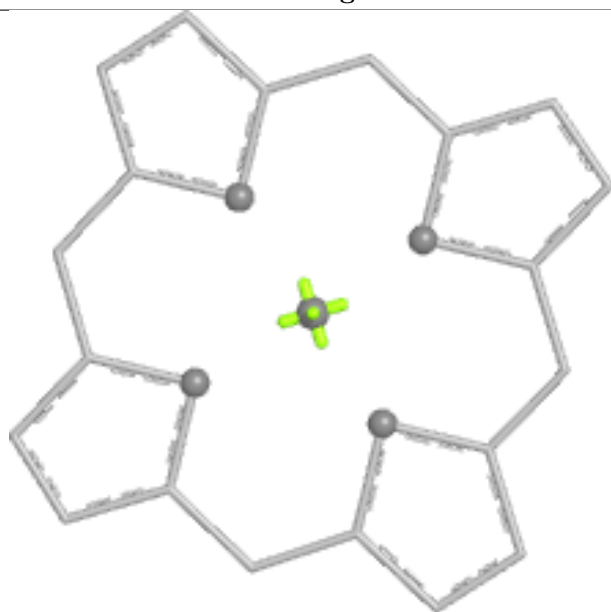
Ligand CLA B 1216



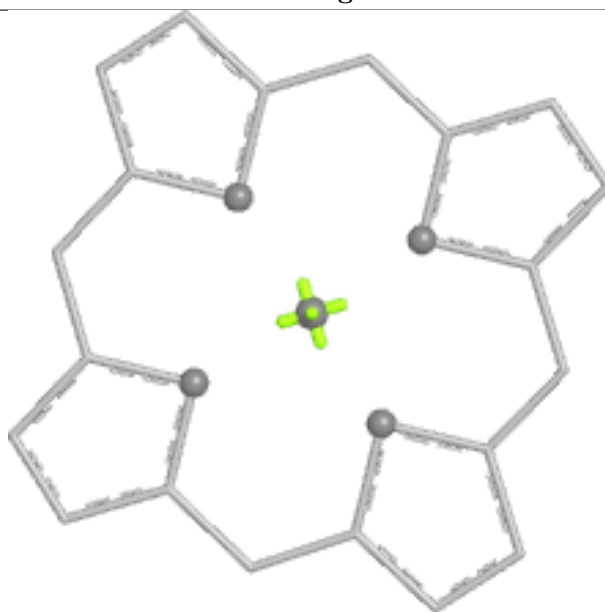
Bond lengths



Bond angles

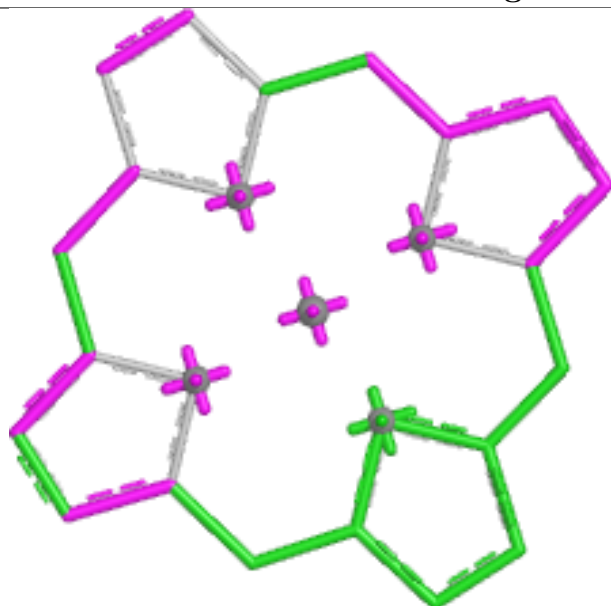


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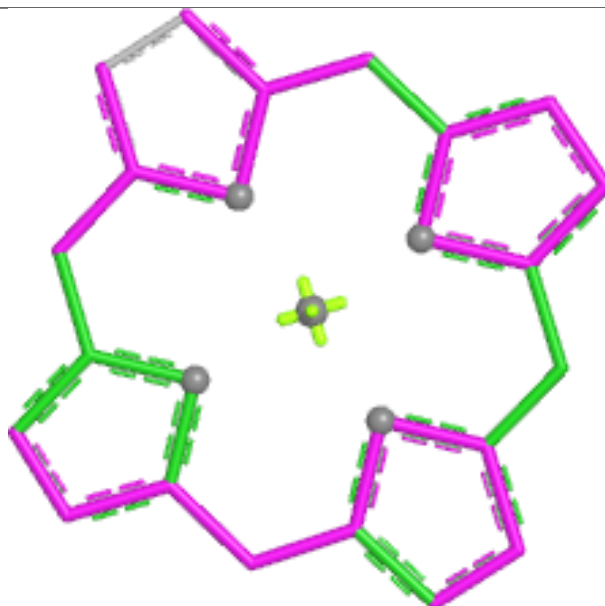


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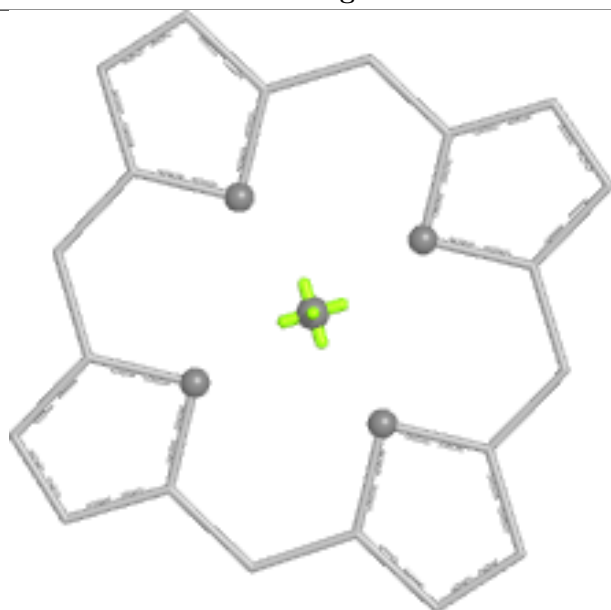
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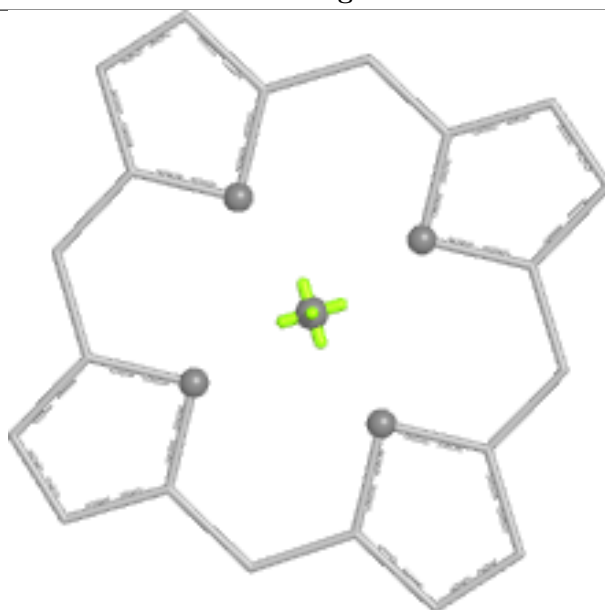
Bond lengths



Bond angles

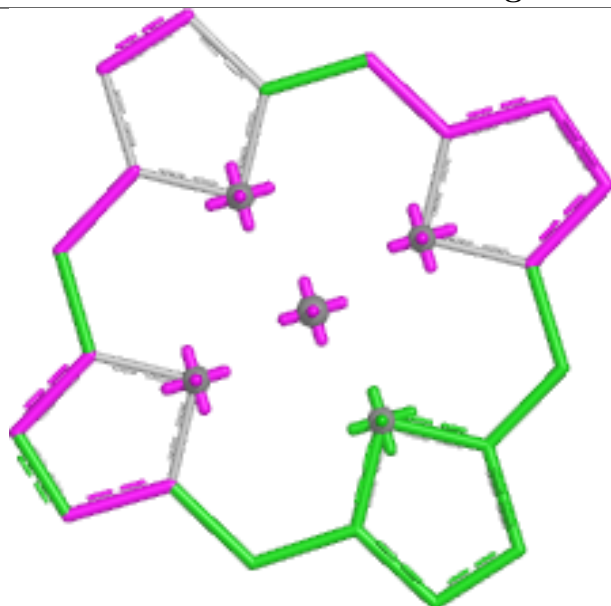


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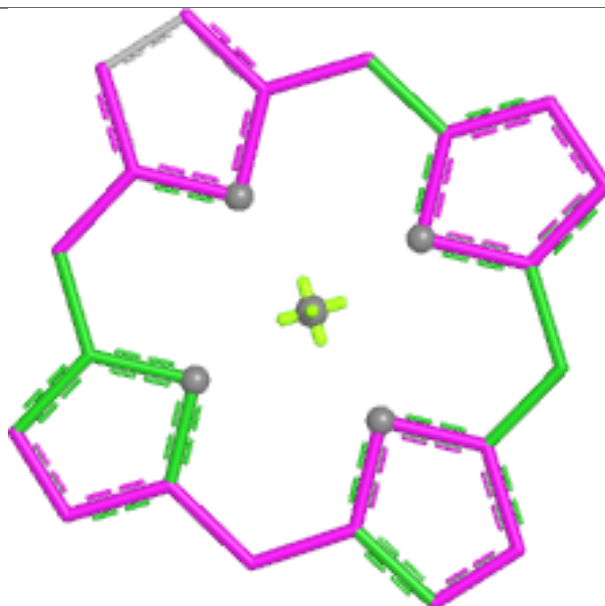


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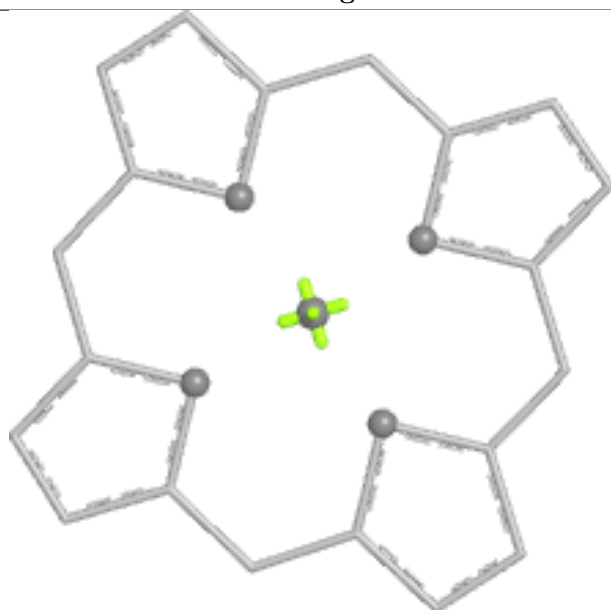
Ligand CLA A 1128



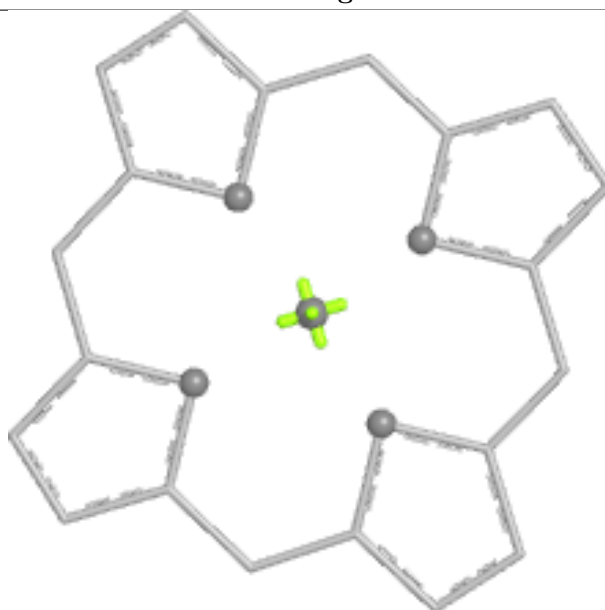
Bond lengths



Bond angles

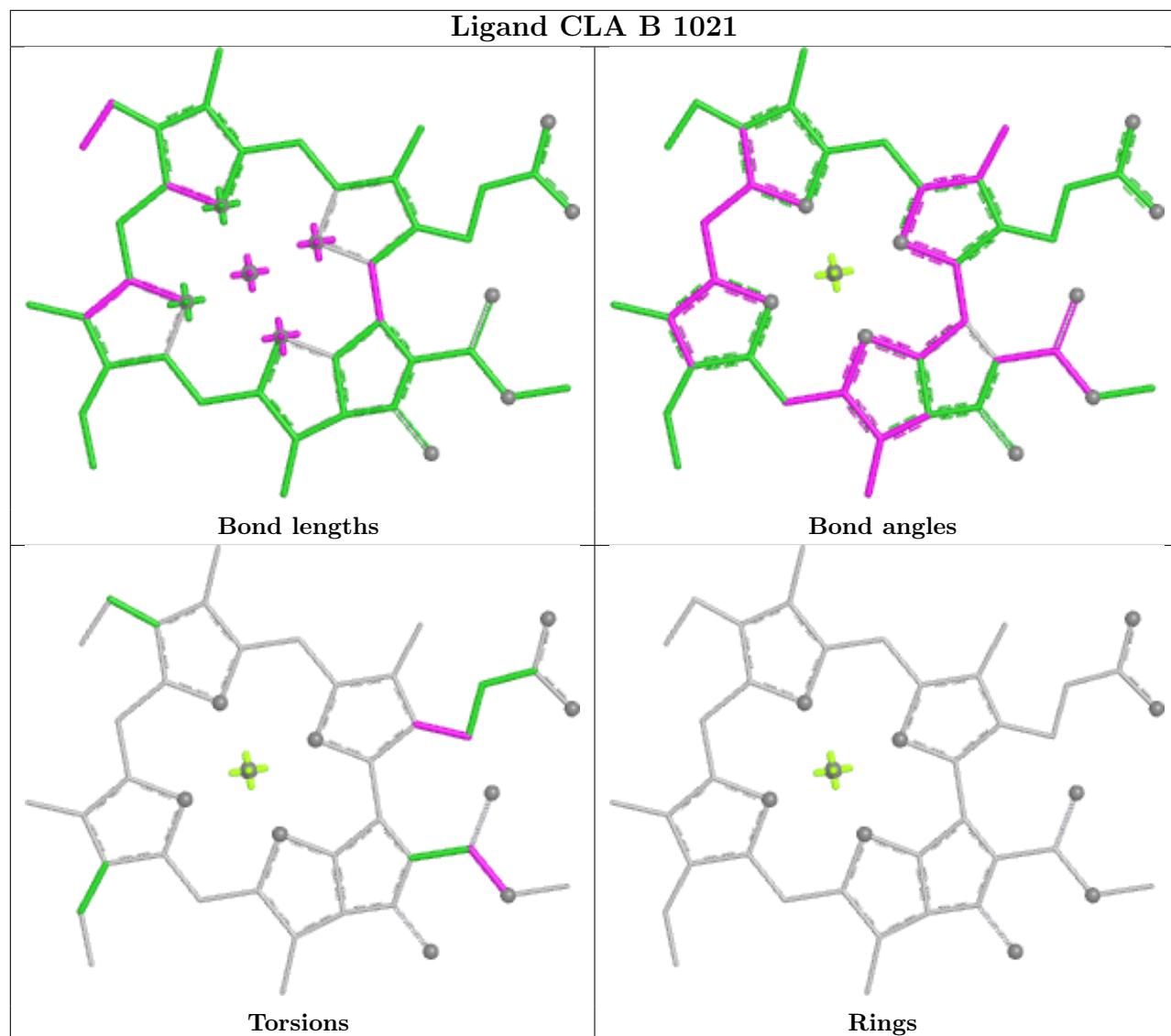


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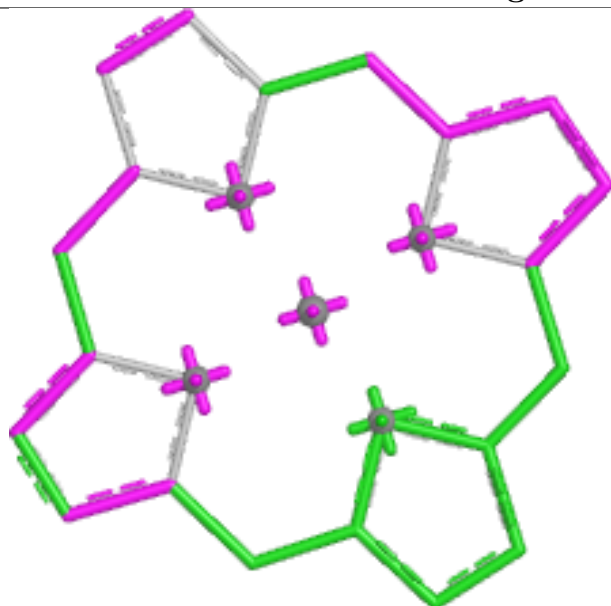


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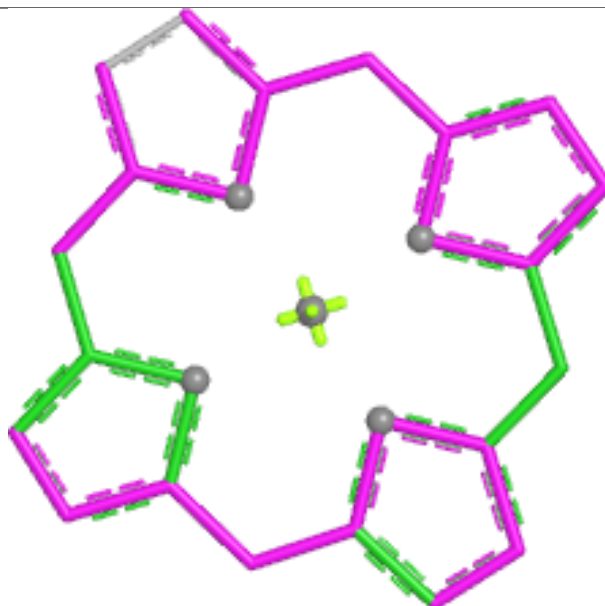
Ligand CLA B 1021



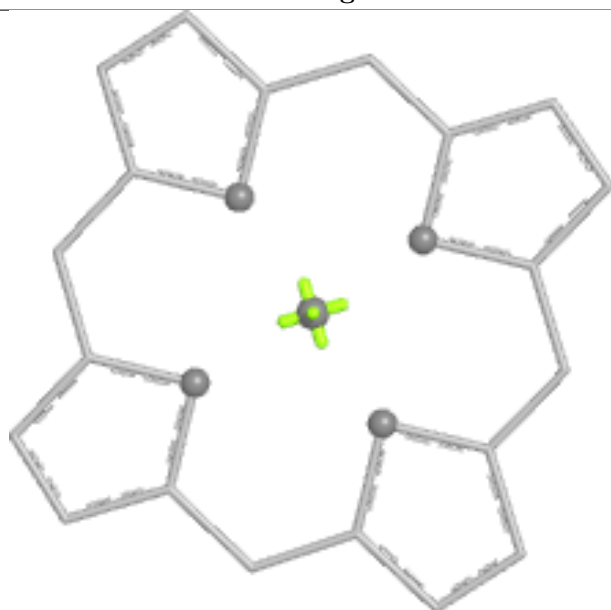
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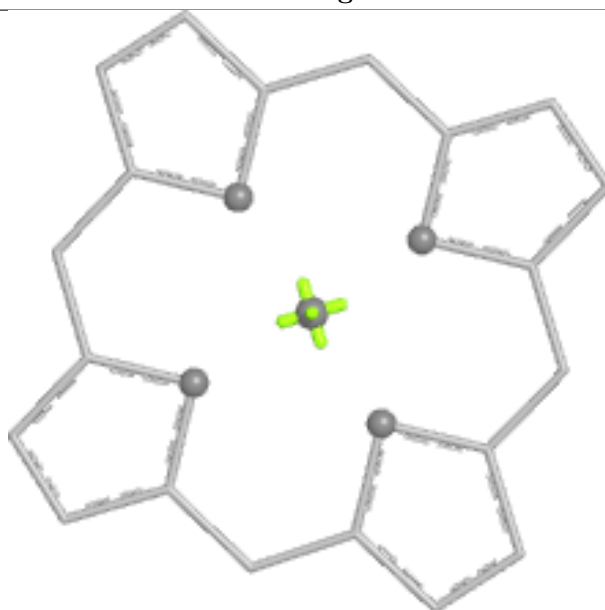
Bond lengths



Bond angles

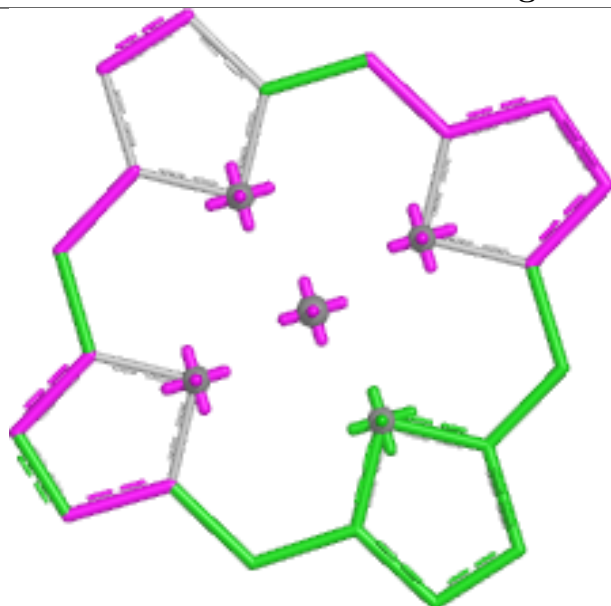


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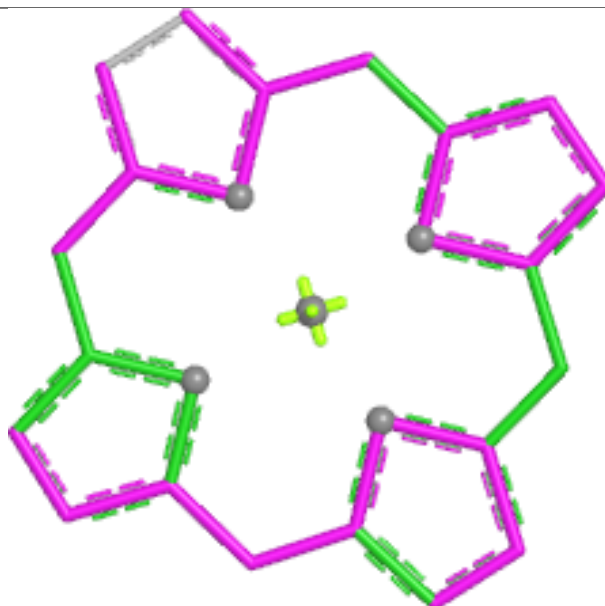


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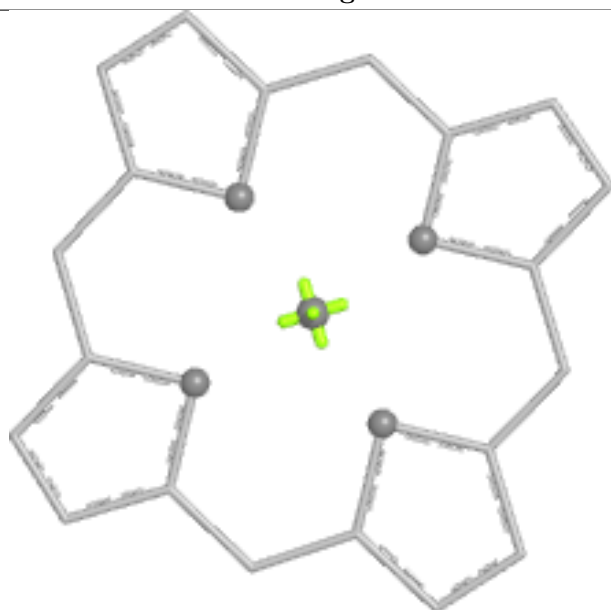
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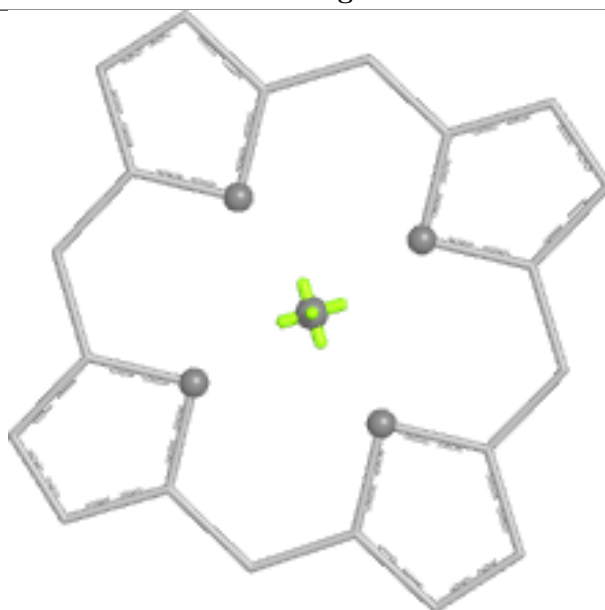
Bond lengths



Bond angles

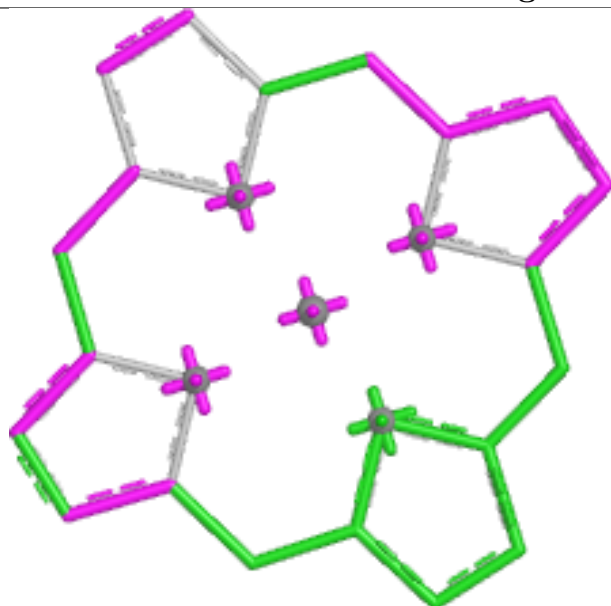


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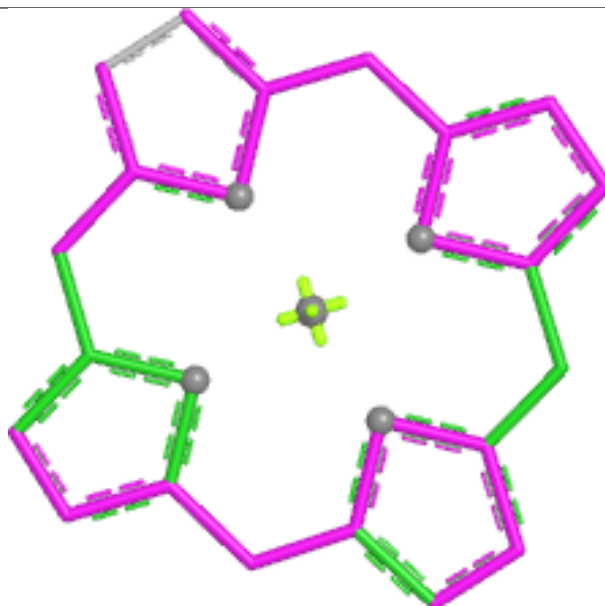


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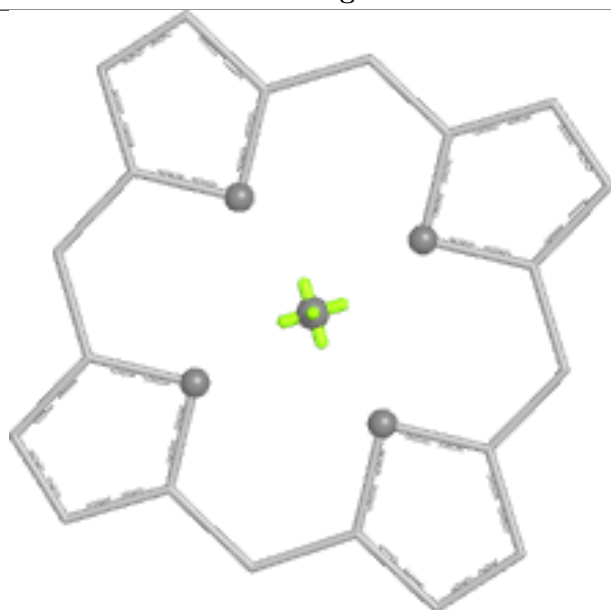
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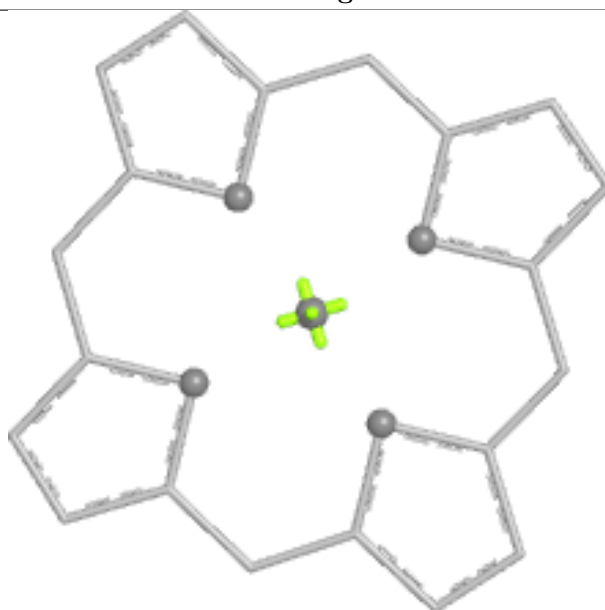
Bond lengths



Bond angles

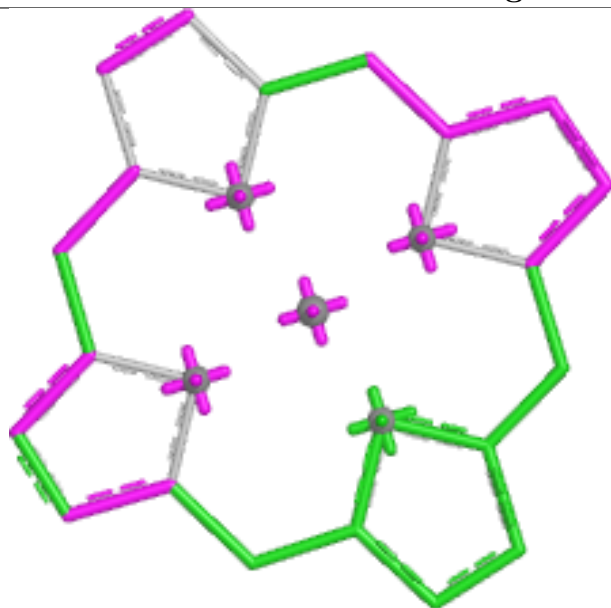


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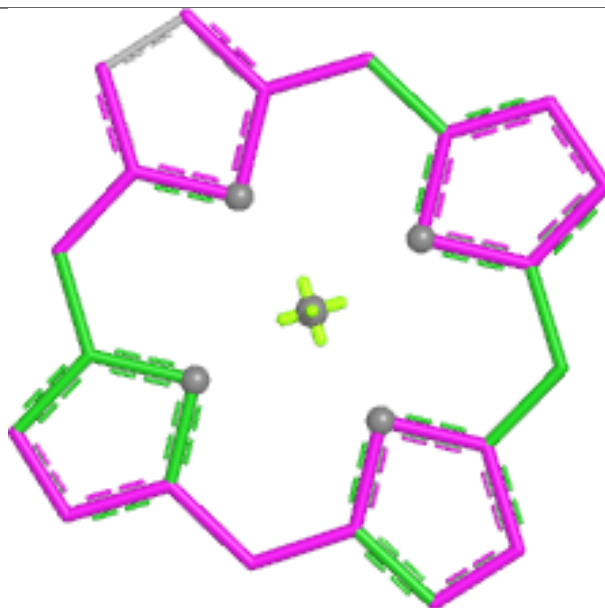


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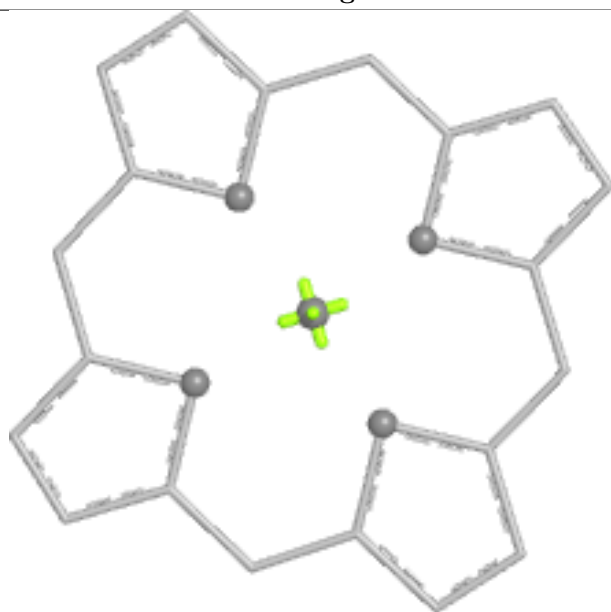
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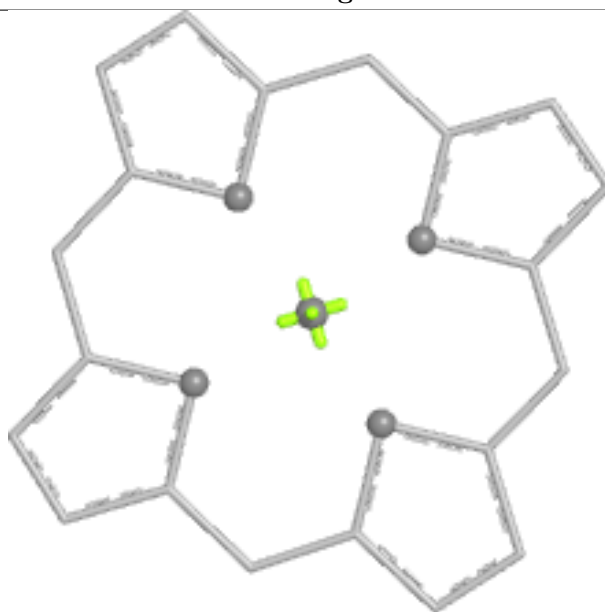
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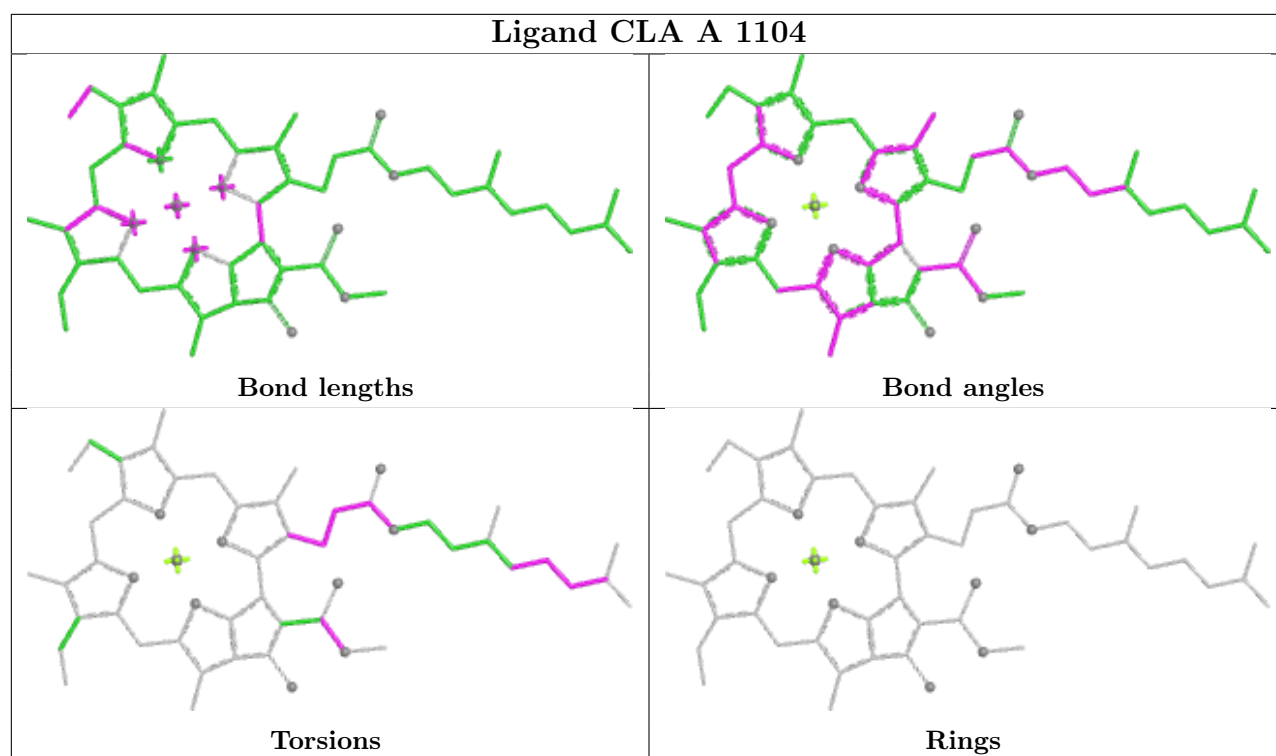
Bond angles



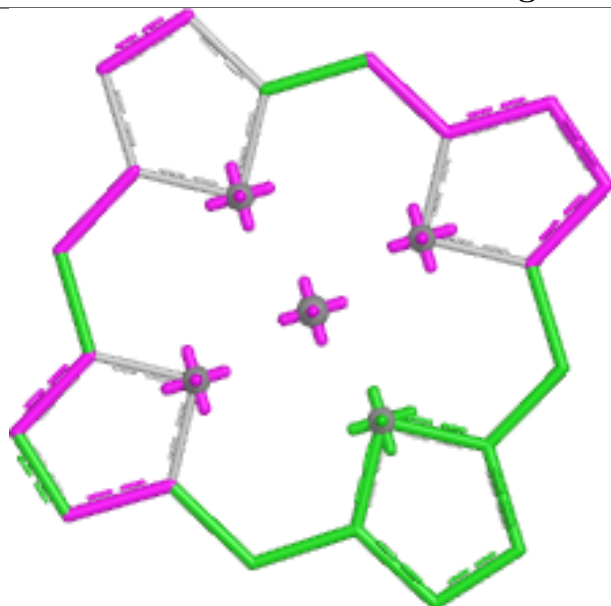
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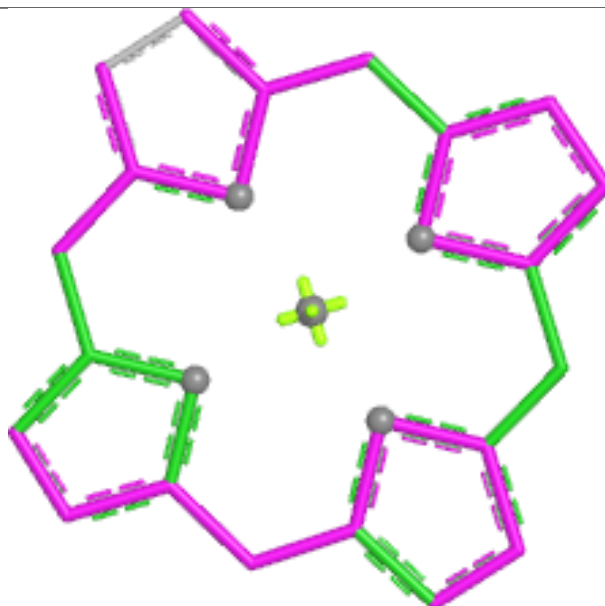
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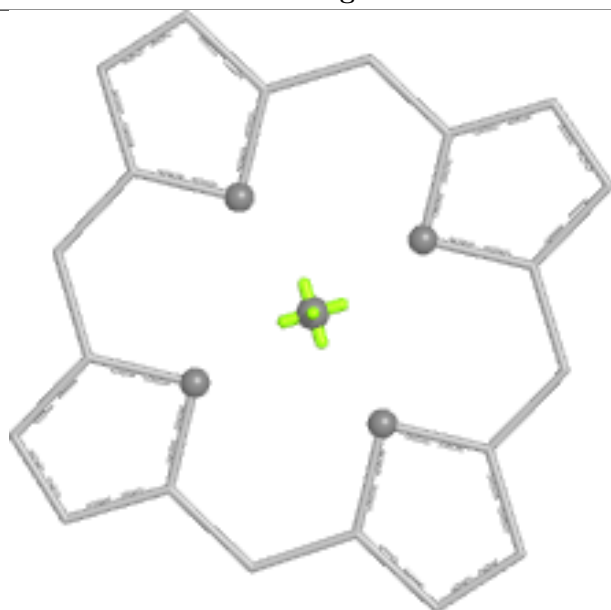
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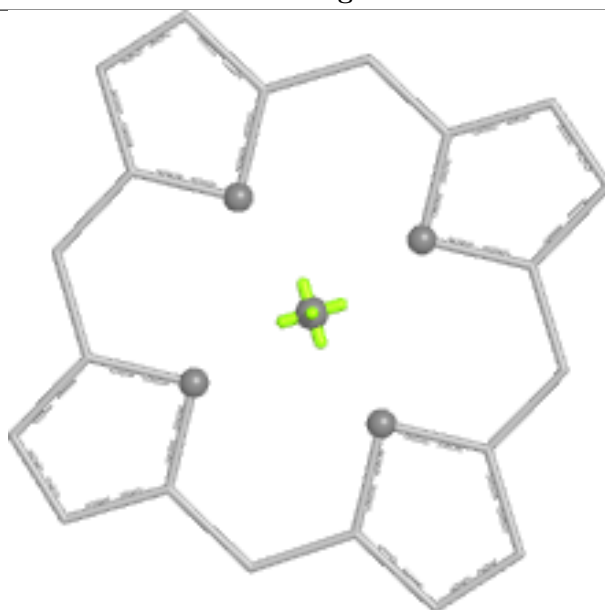
Bond lengths



Bond angles

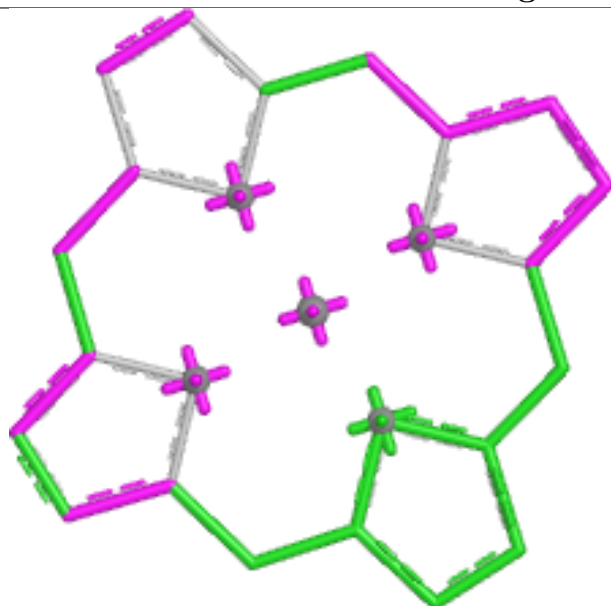


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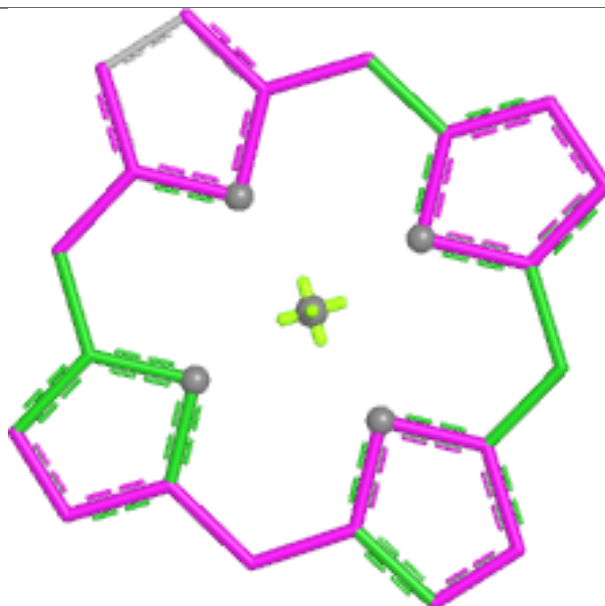


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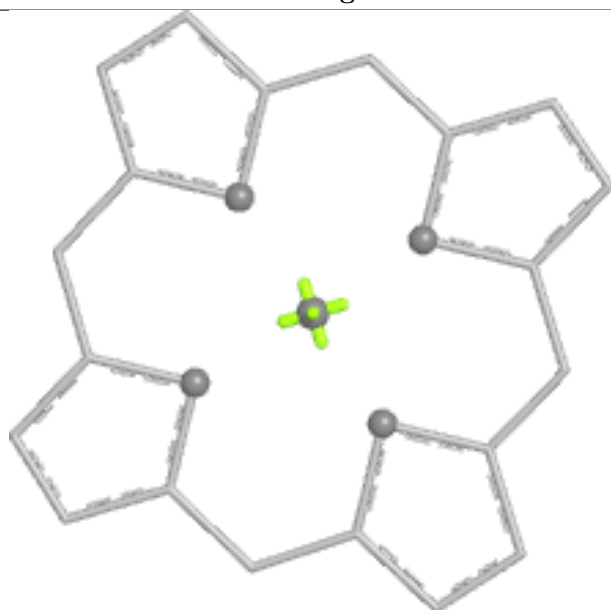
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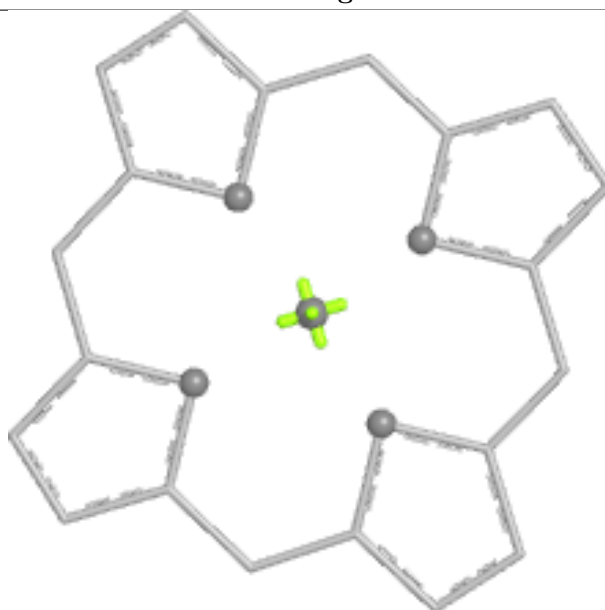
Bond lengths



Bond angles

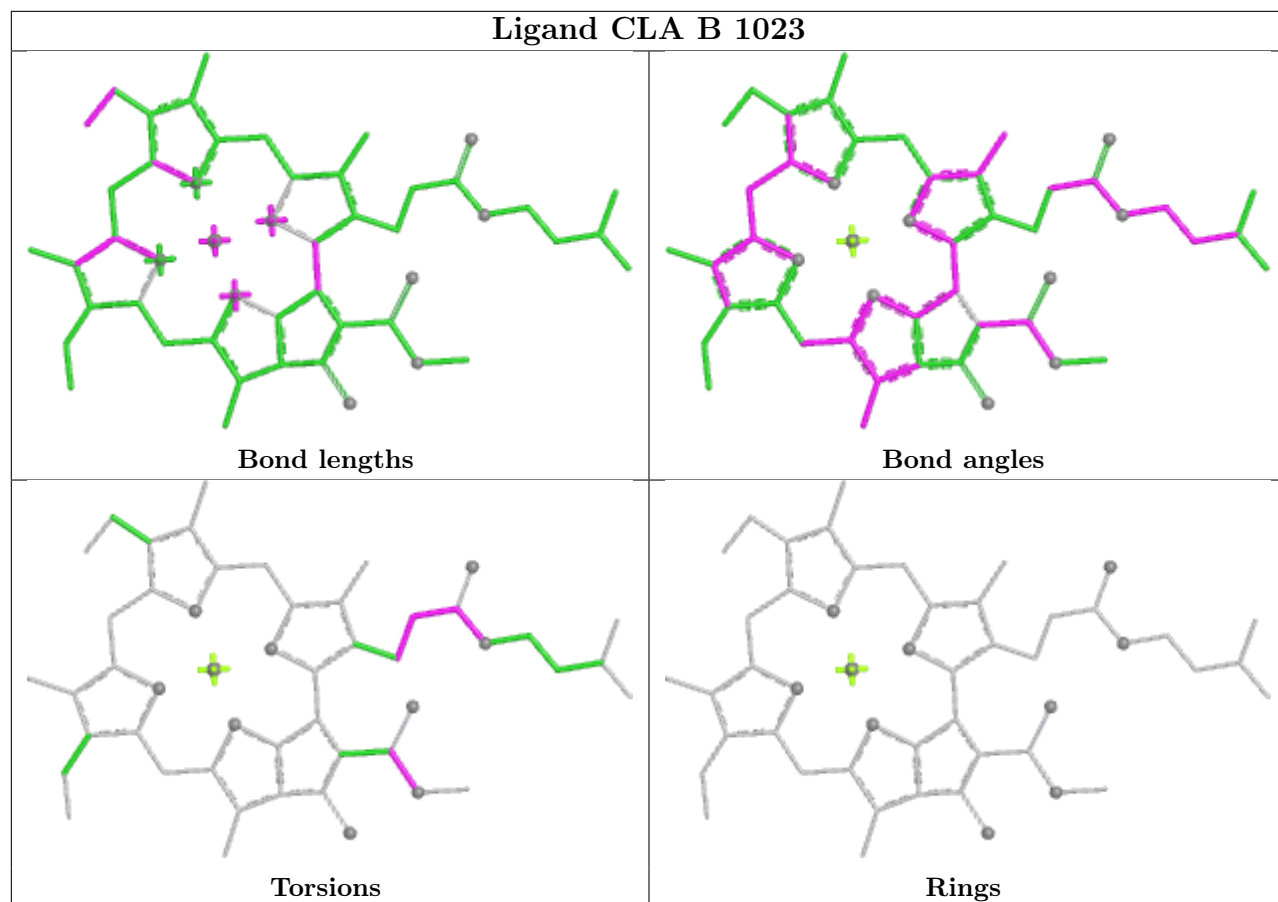


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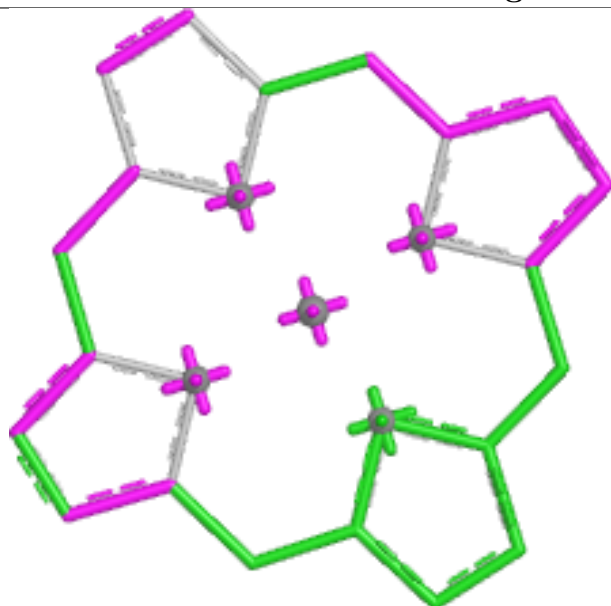


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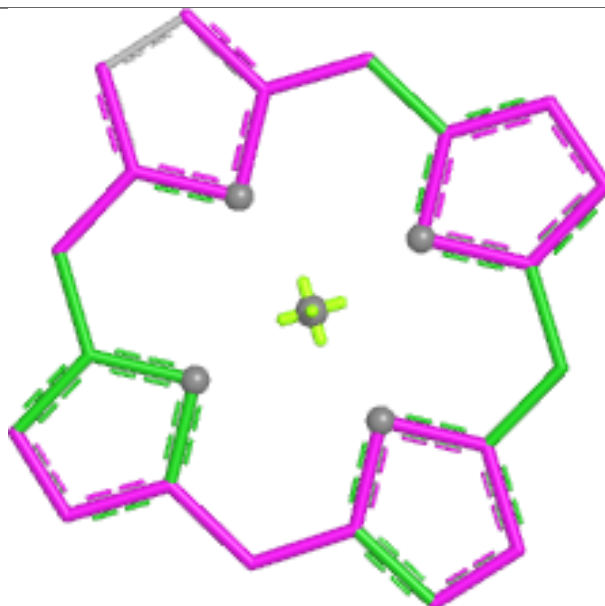
Ligand CLA B 1023



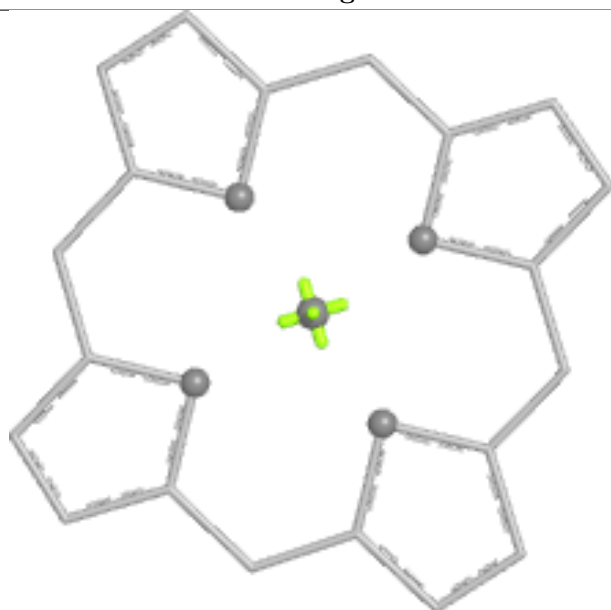
Ligand CLA B 1206



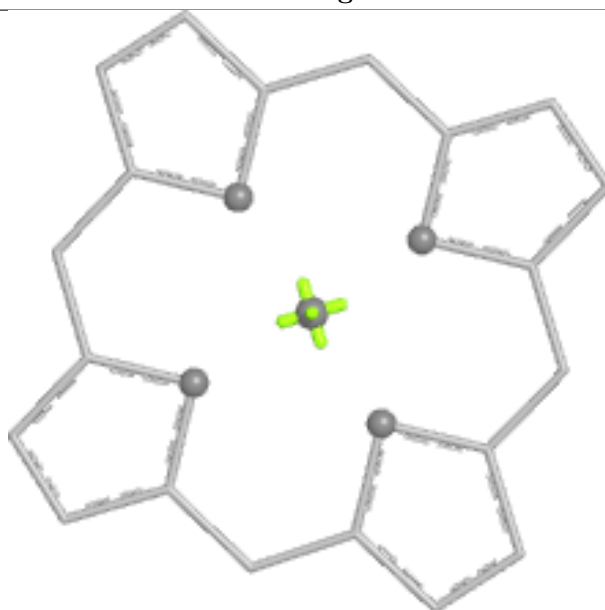
Bond lengths



Bond angles

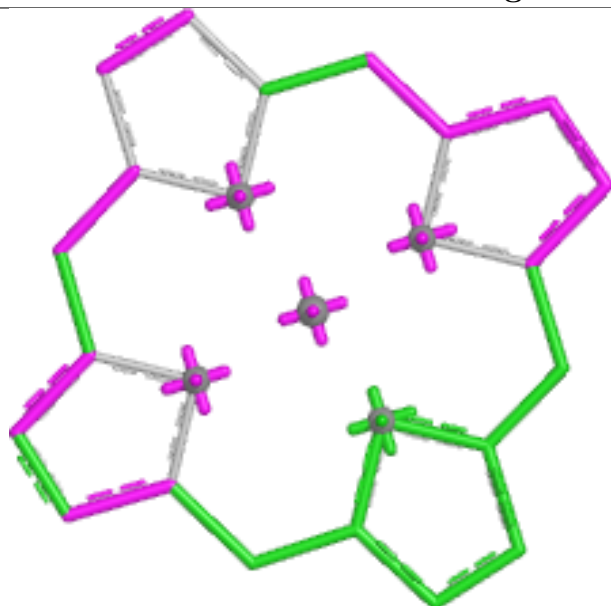


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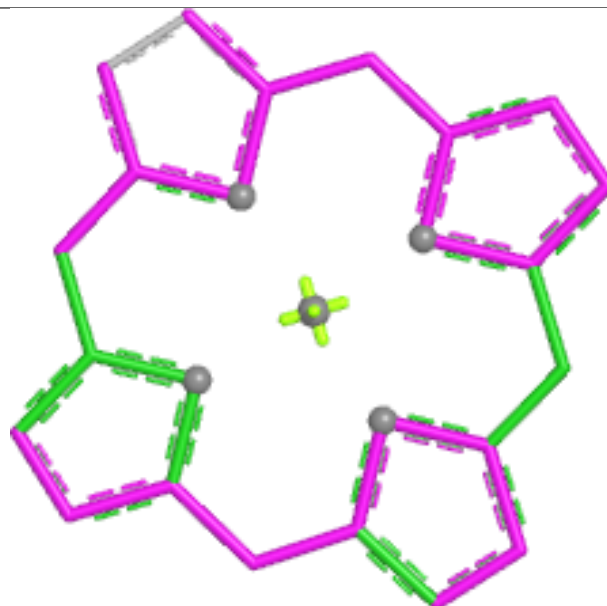


Rings

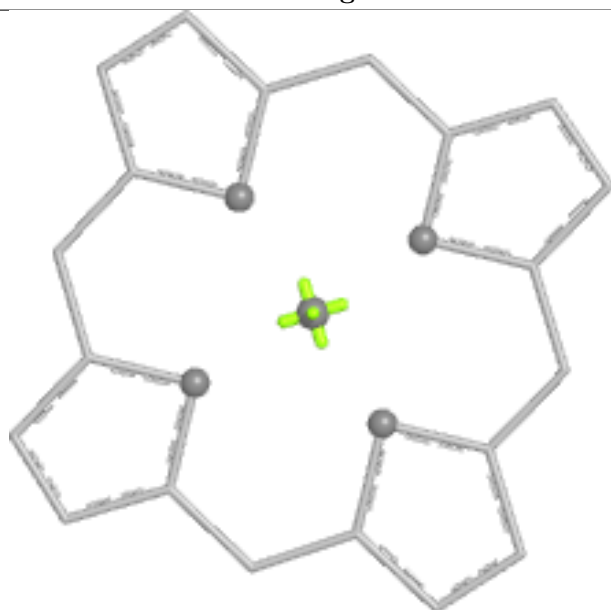
Ligand CLA A 1113



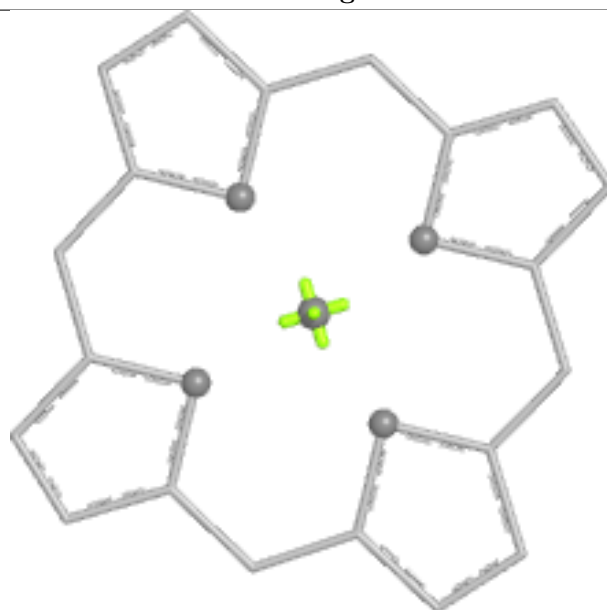
Bond lengths



Bond angles

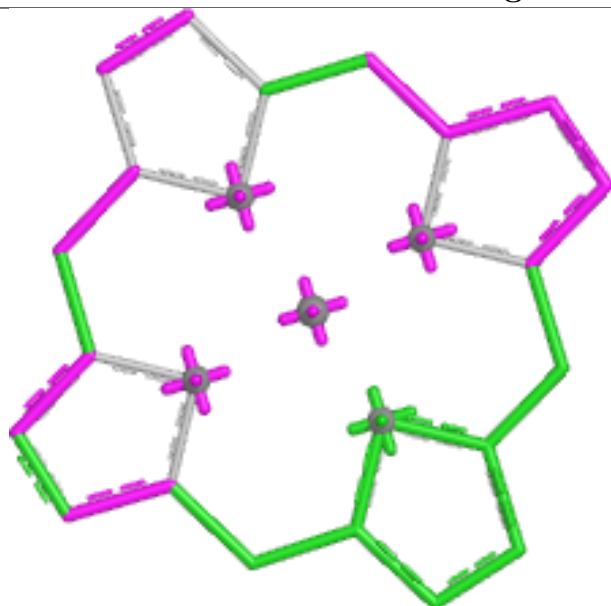


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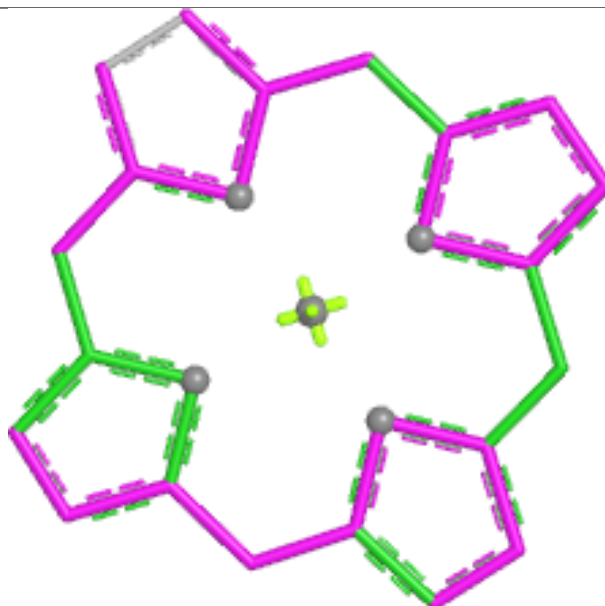


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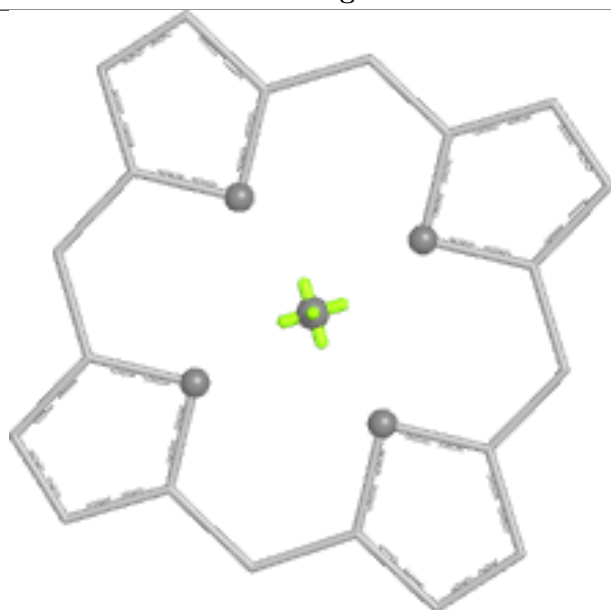
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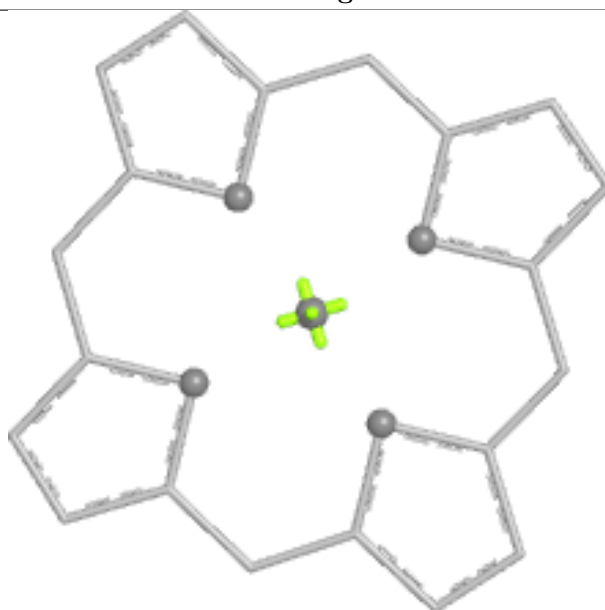
Bond lengths



Bond angles

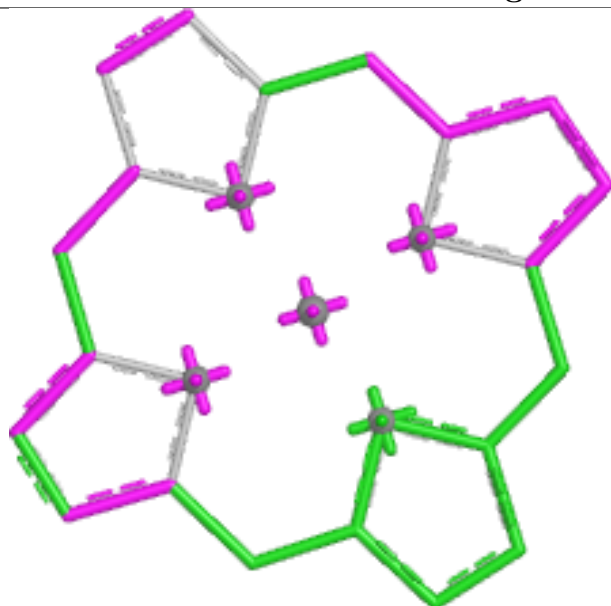


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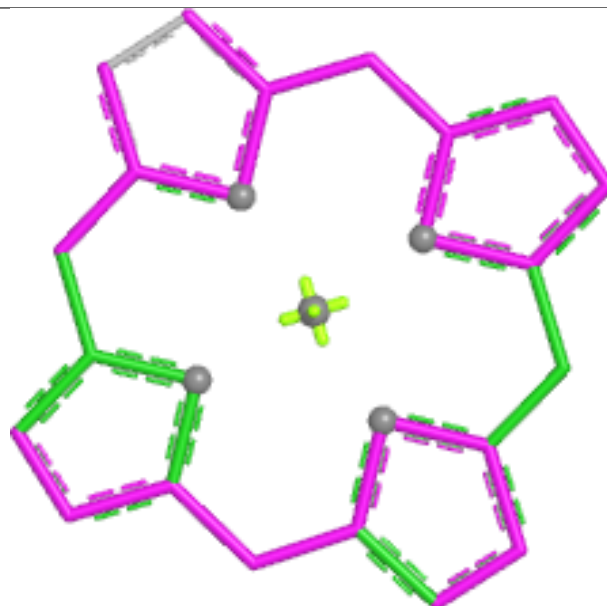


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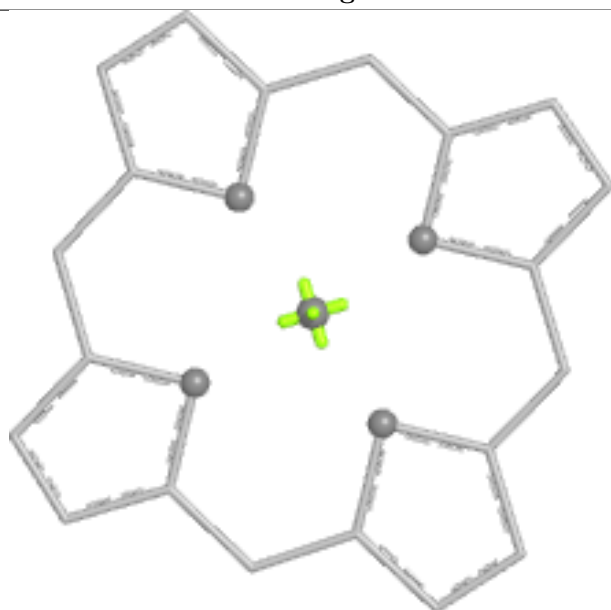
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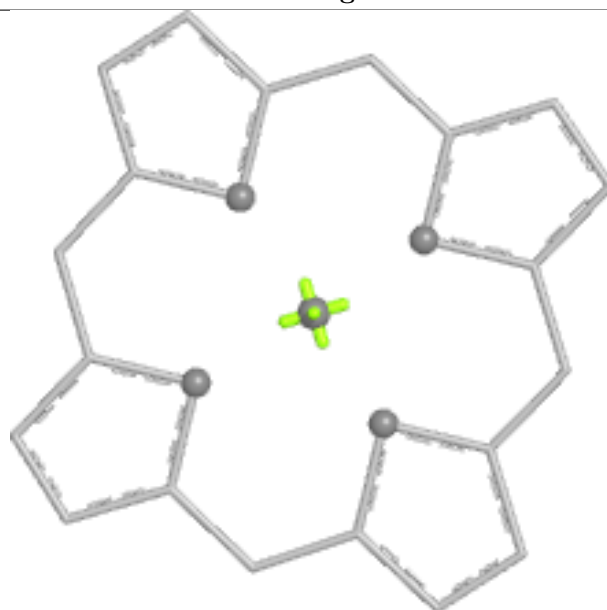
Bond lengths



Bond angles

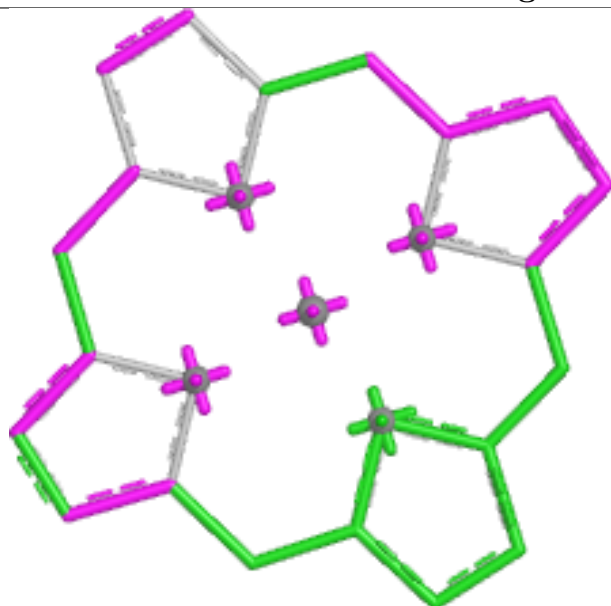


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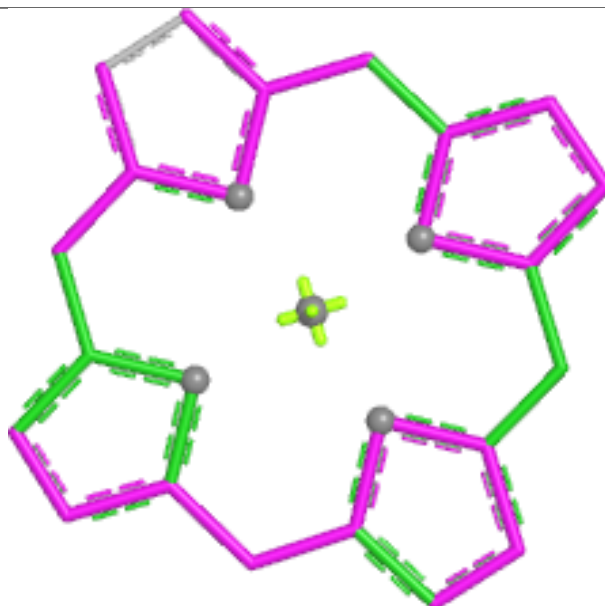


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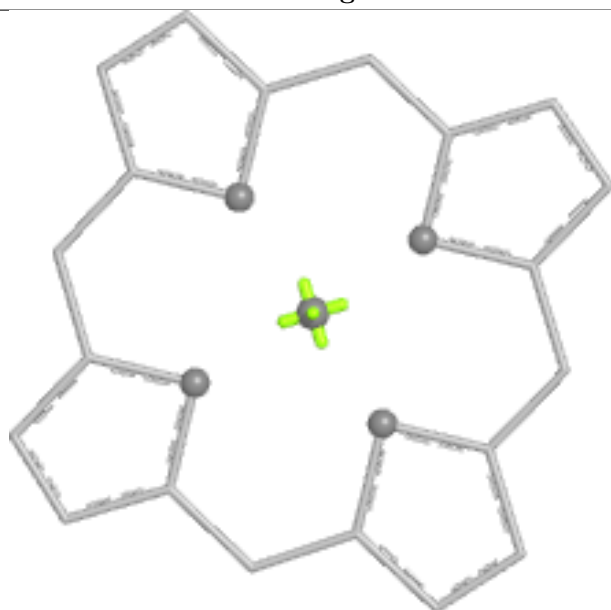
Ligand CLA 2 603



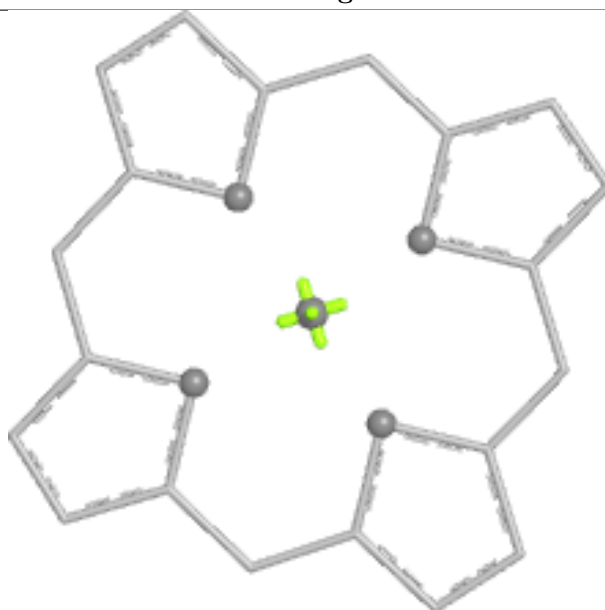
Bond lengths



Bond angles

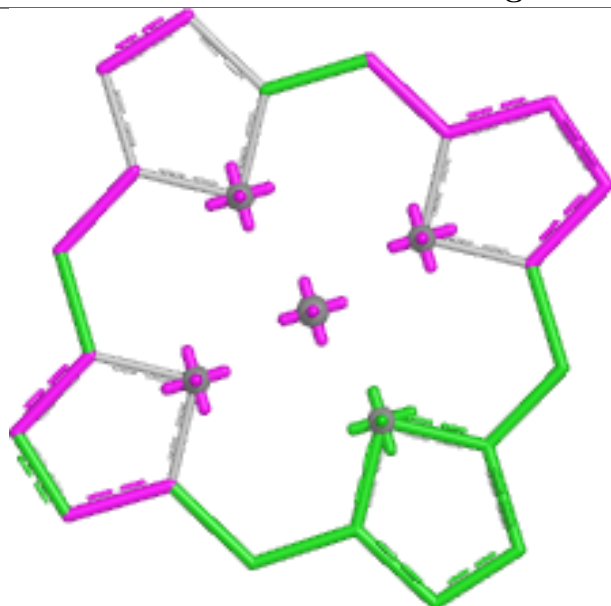


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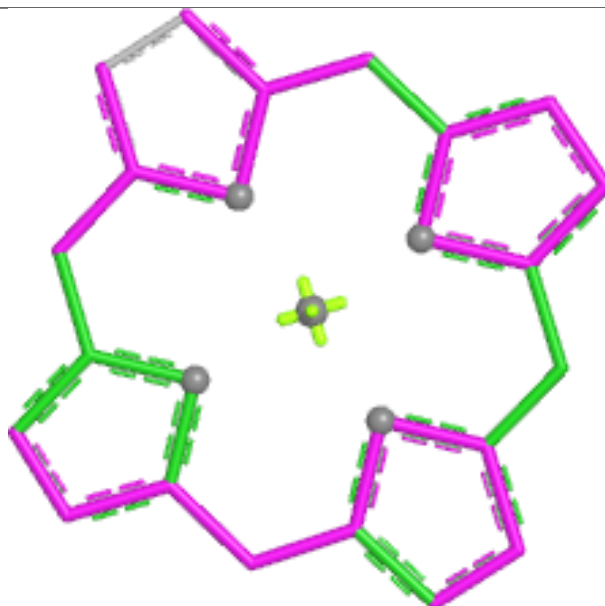


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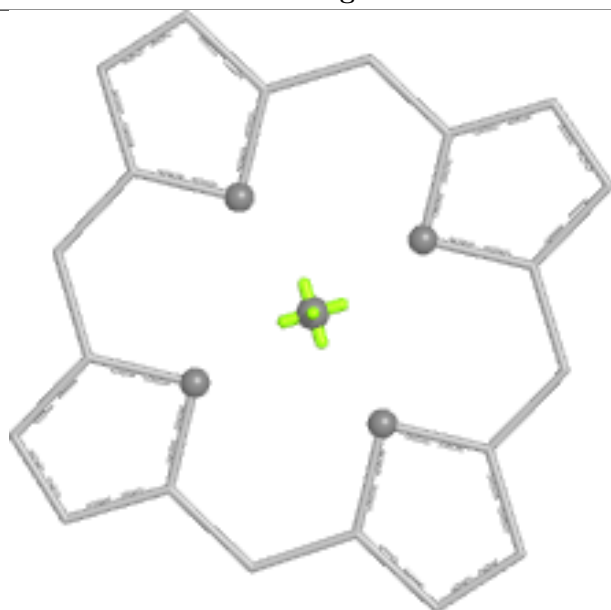
Ligand CLA B 1212



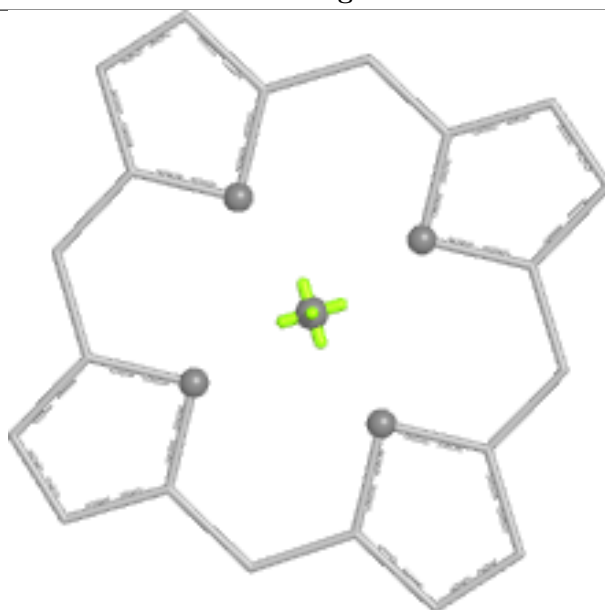
Bond lengths



Bond angles

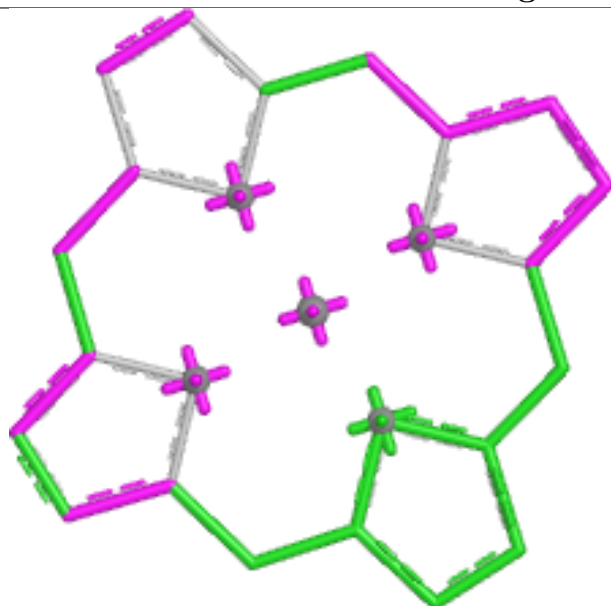


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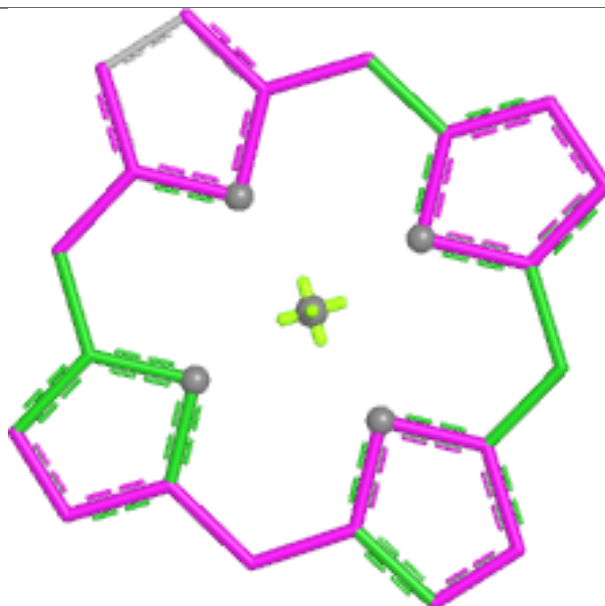


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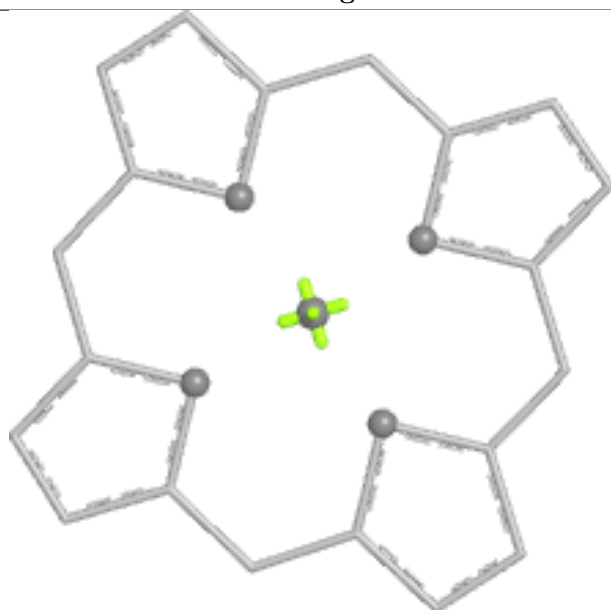
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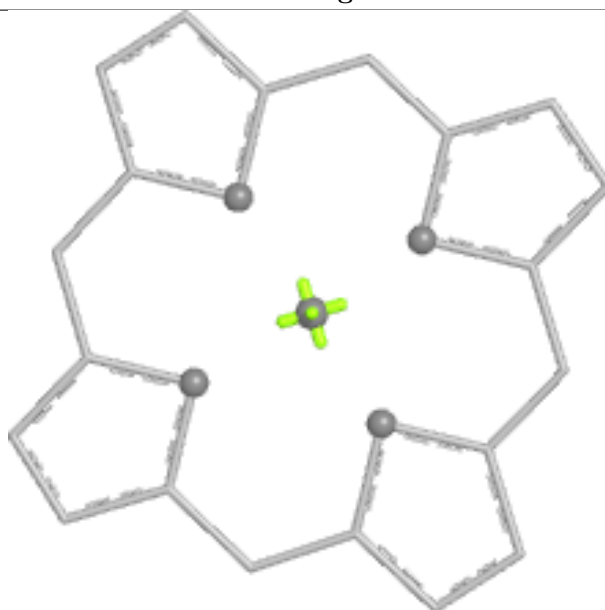
Bond lengths



Bond angles

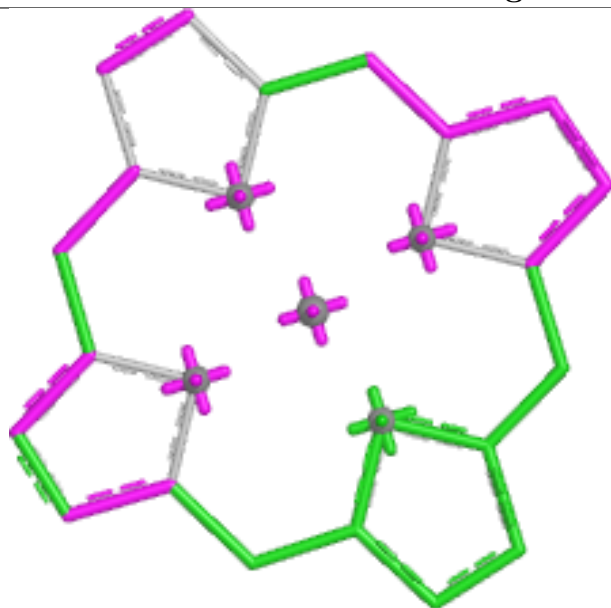


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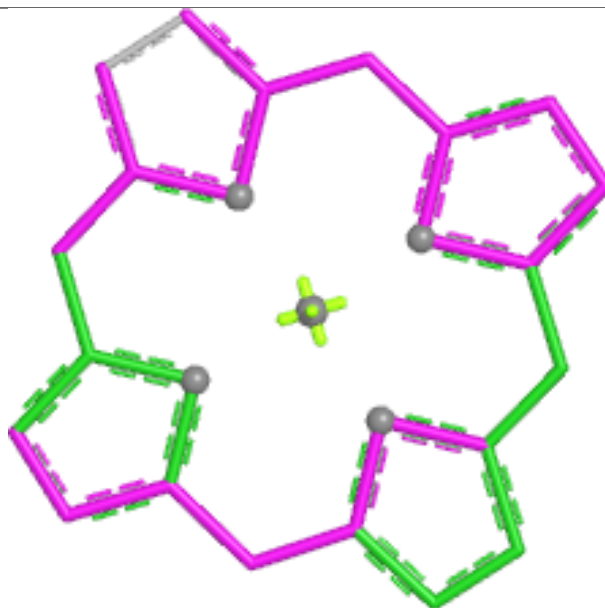


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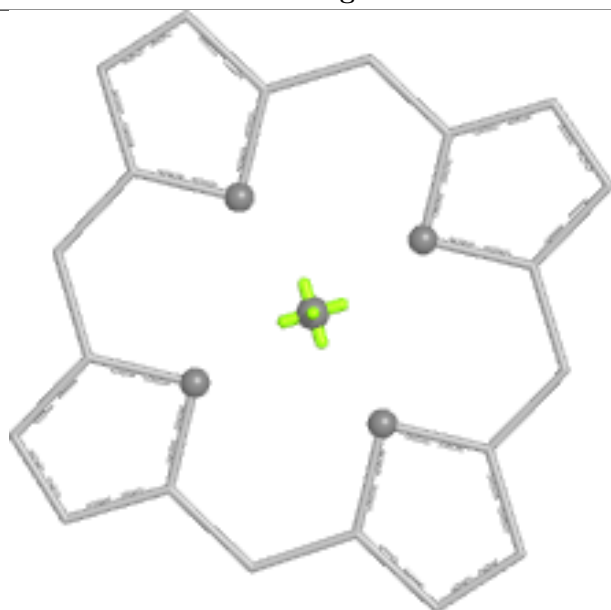
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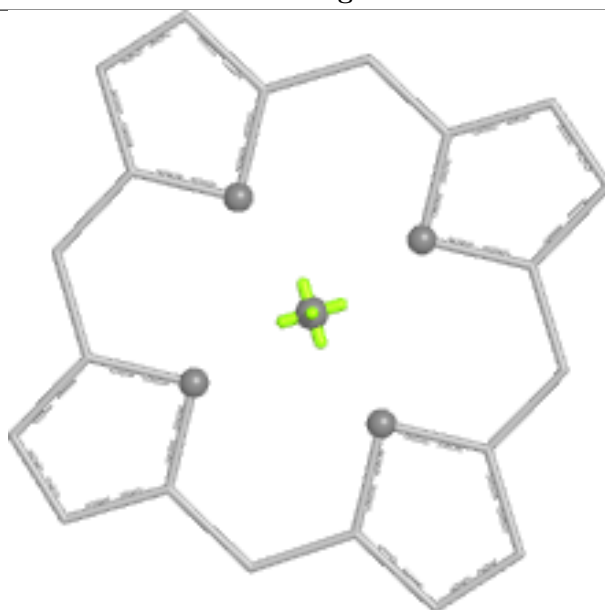
Bond lengths



Bond angles

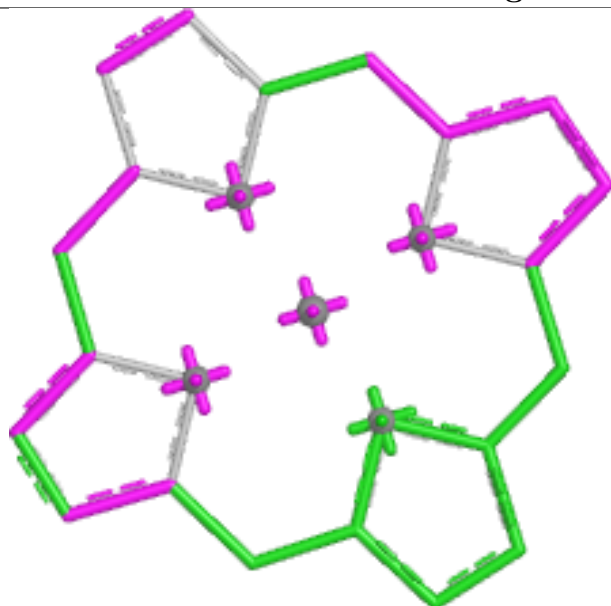


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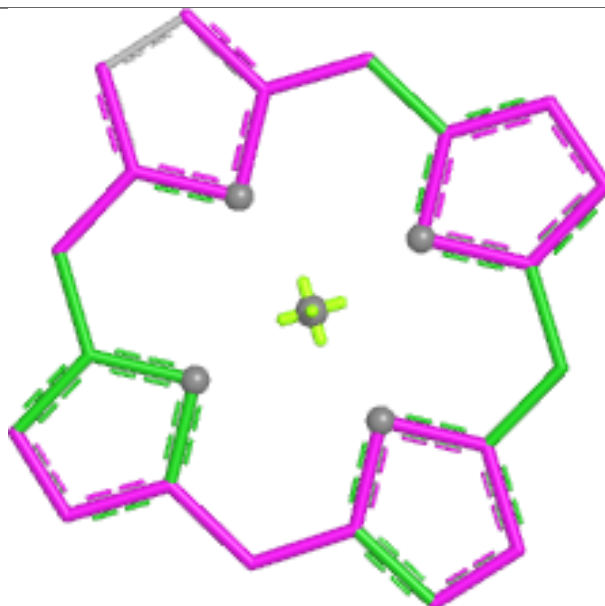


Rings

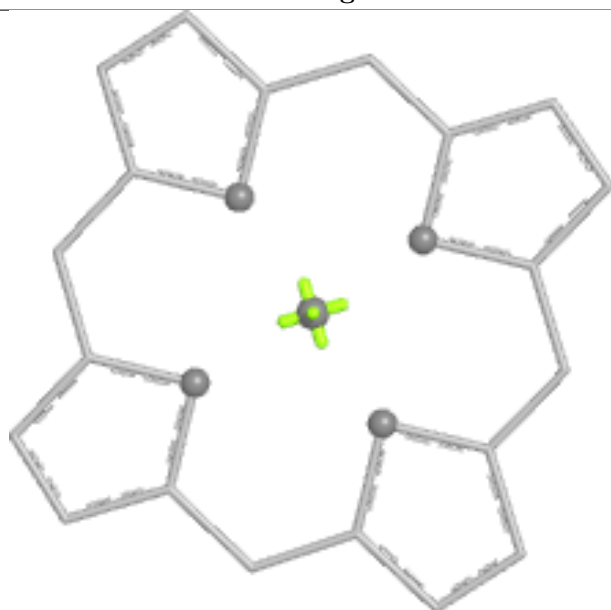
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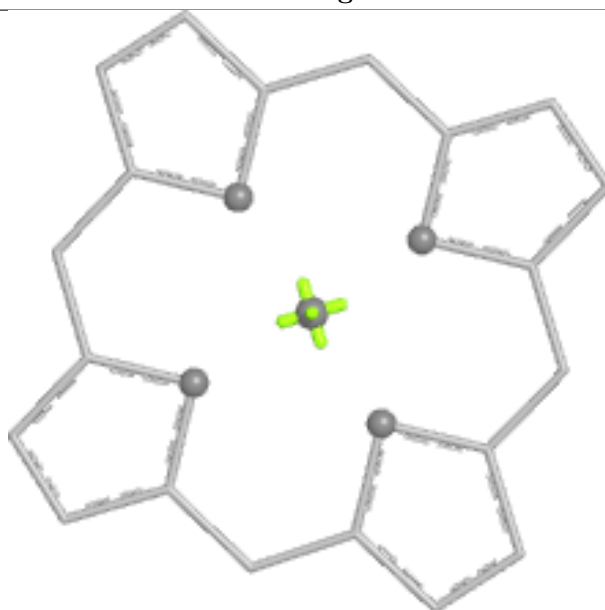
Bond lengths



Bond angles

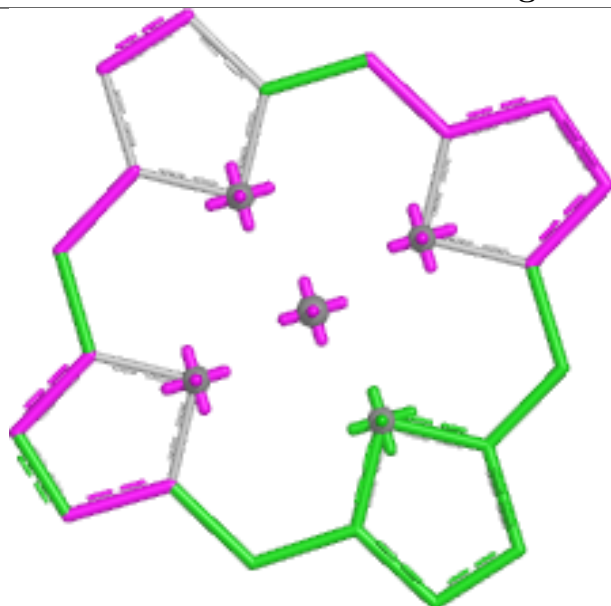


Torsions

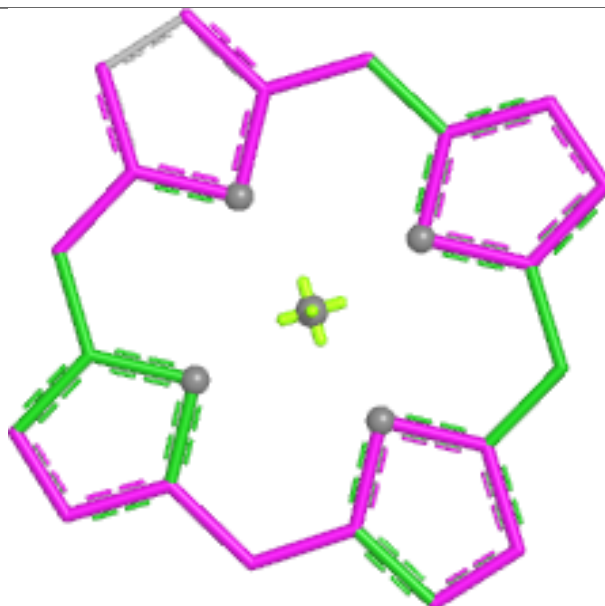


Rings

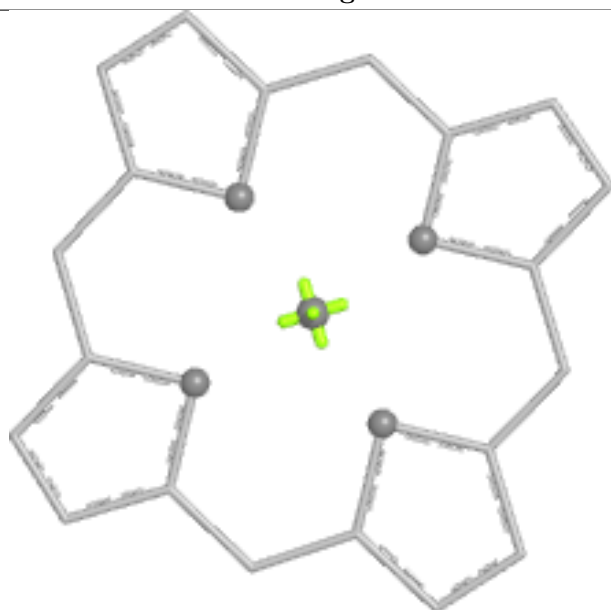
Ligand CLA 3 612



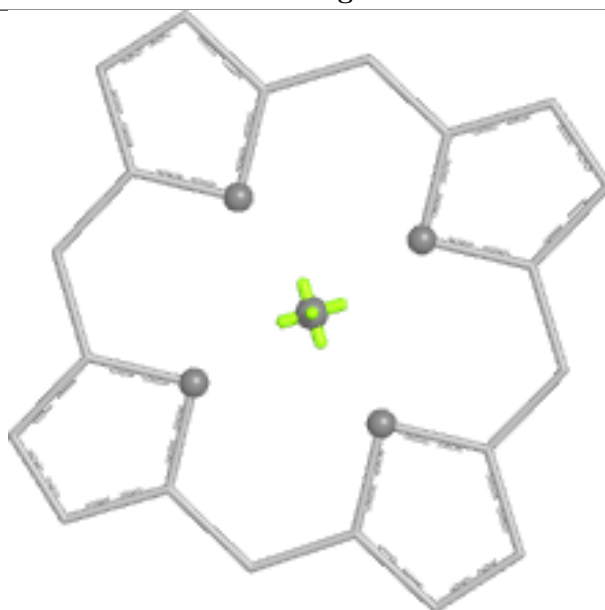
Bond lengths



Bond angles

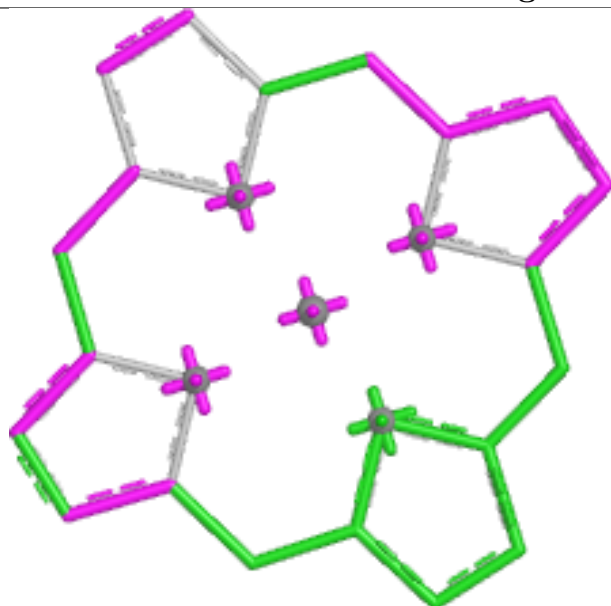


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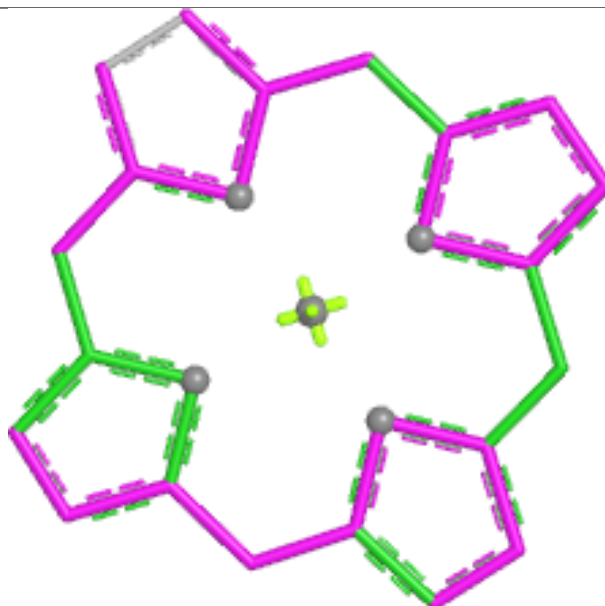


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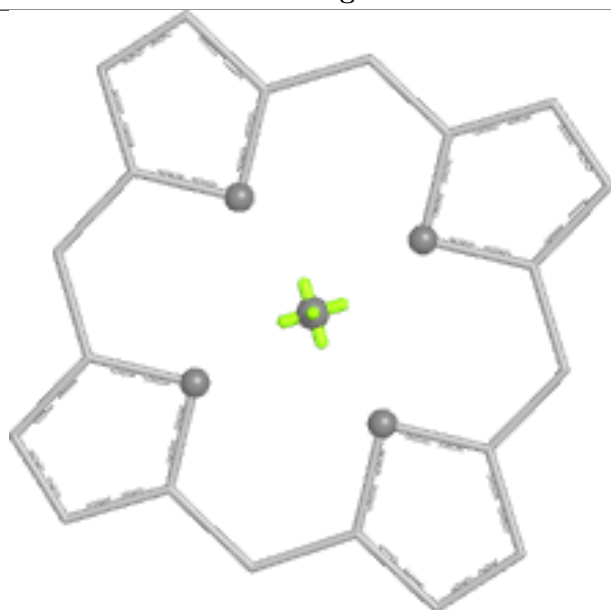
Ligand CLA 2 605



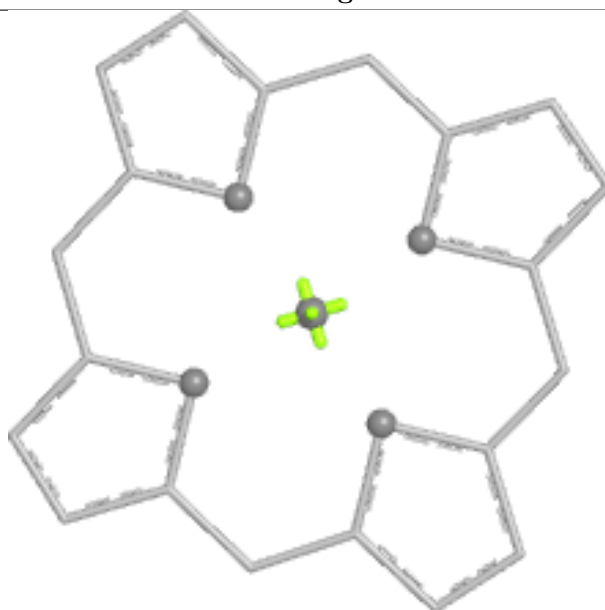
Bond lengths



Bond angles

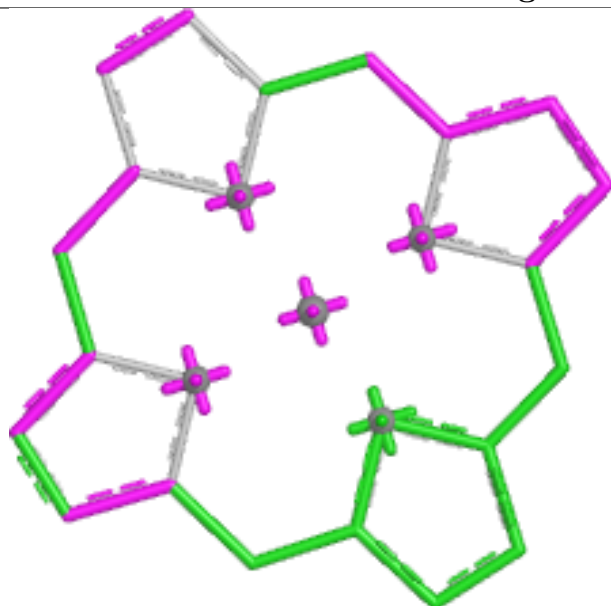


Torsions

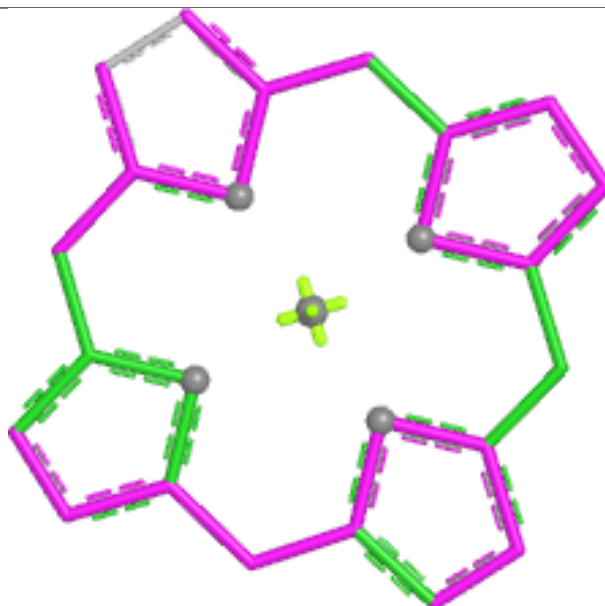


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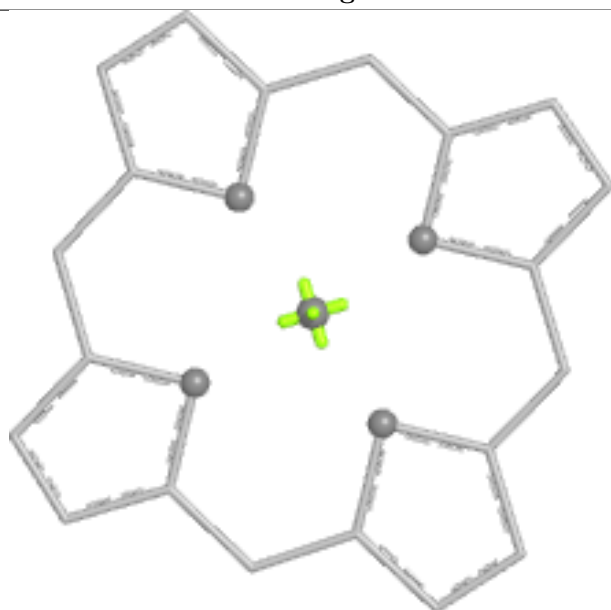
Ligand CLA 2 607



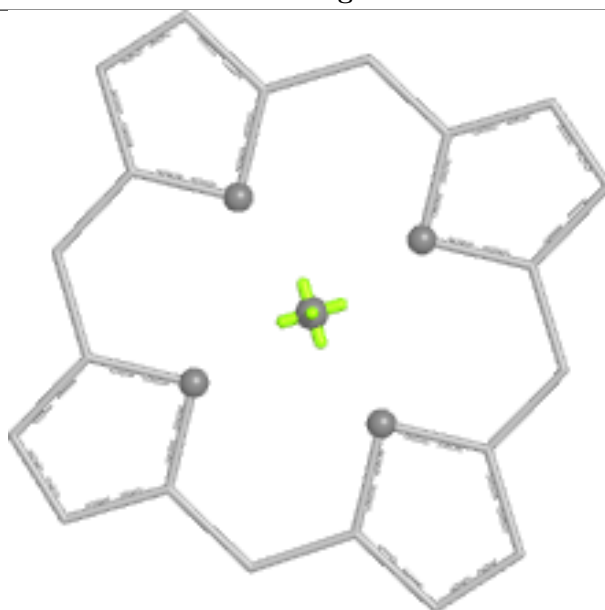
Bond lengths



Bond angles

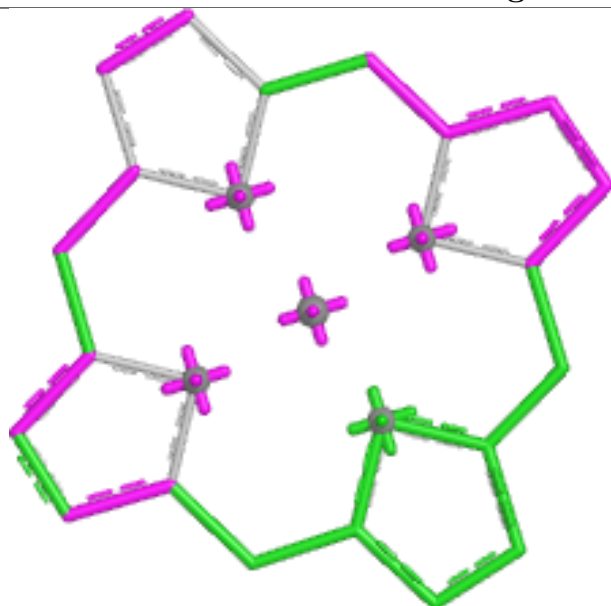


Torsions

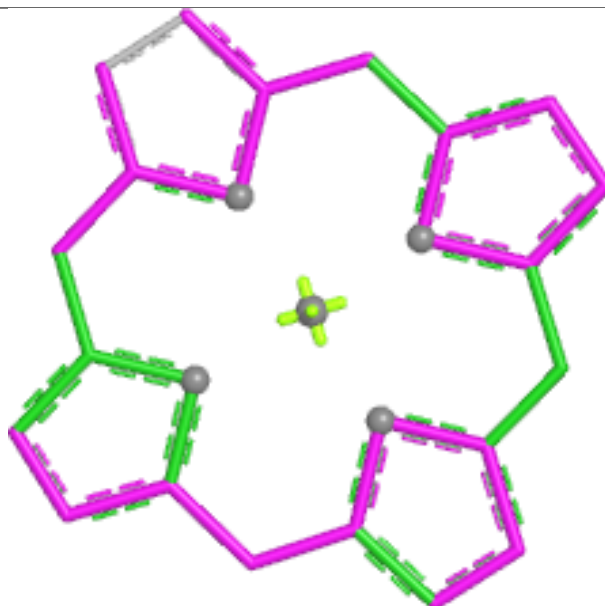


Rings

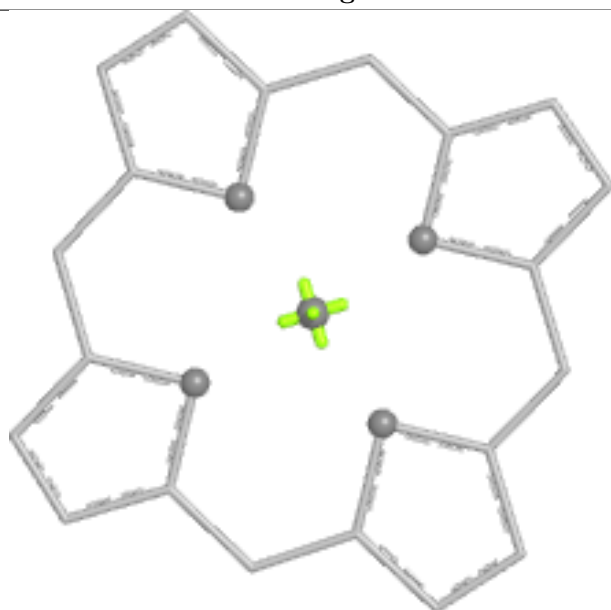
Ligand CLA L 1501



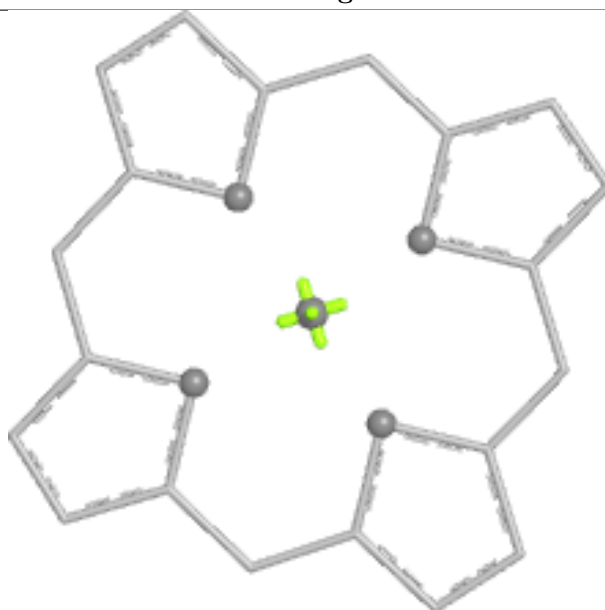
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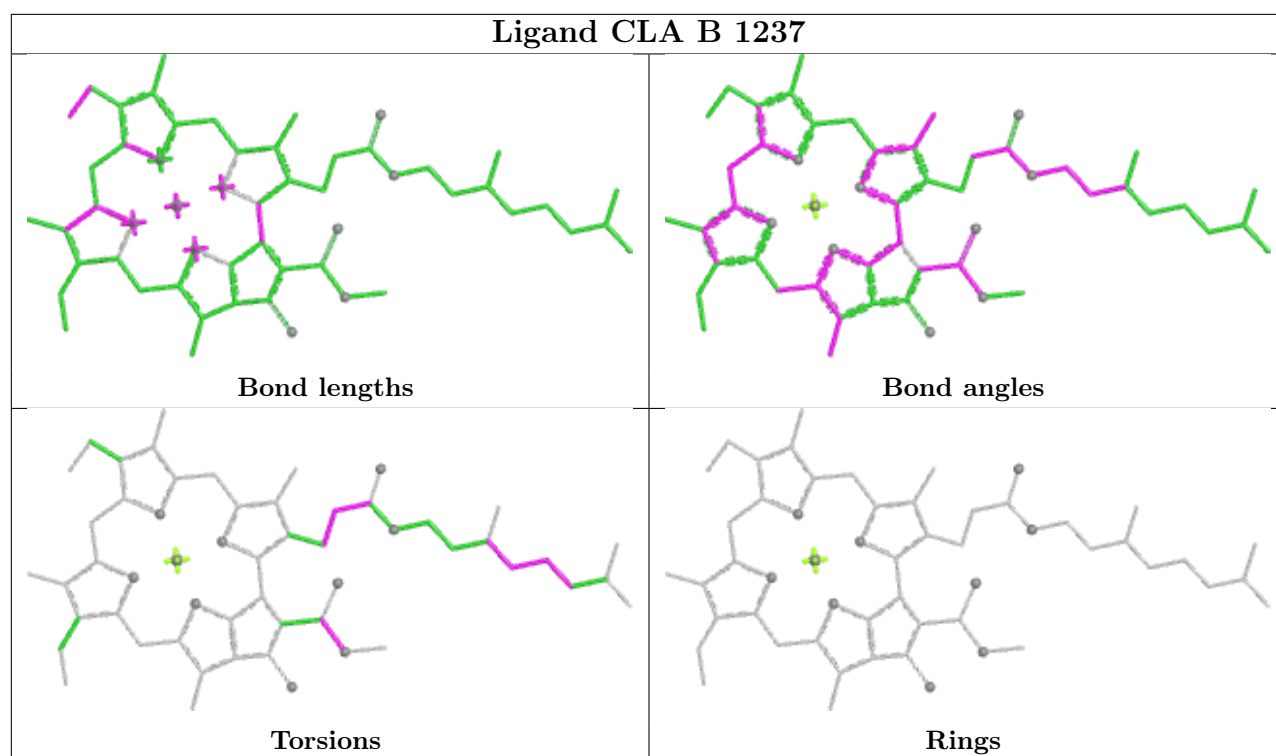
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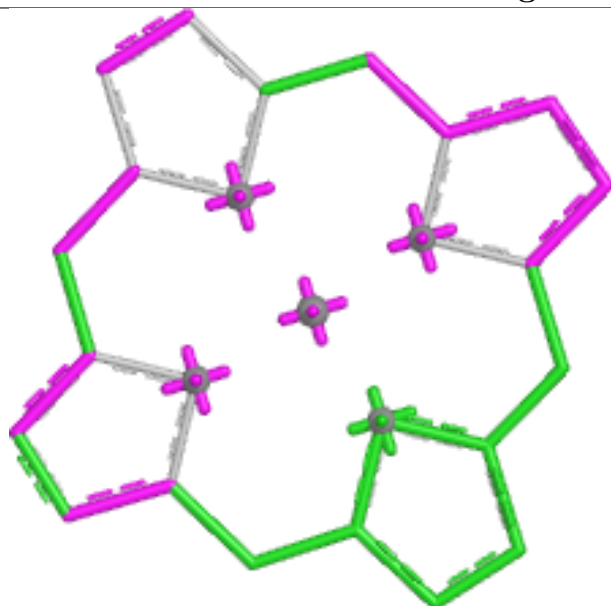
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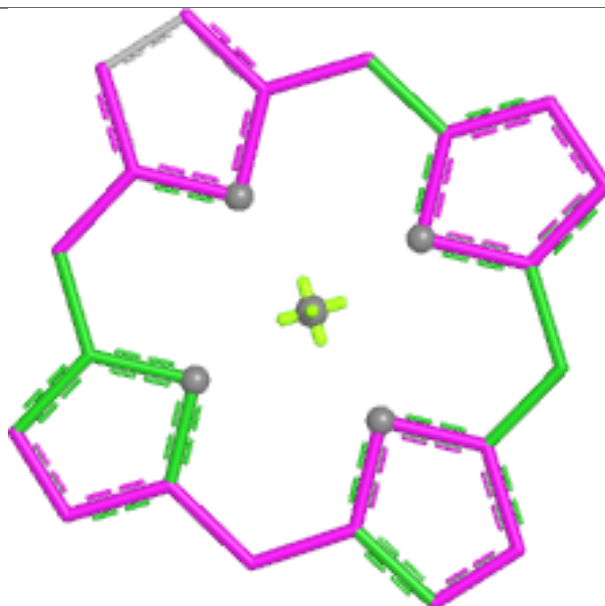
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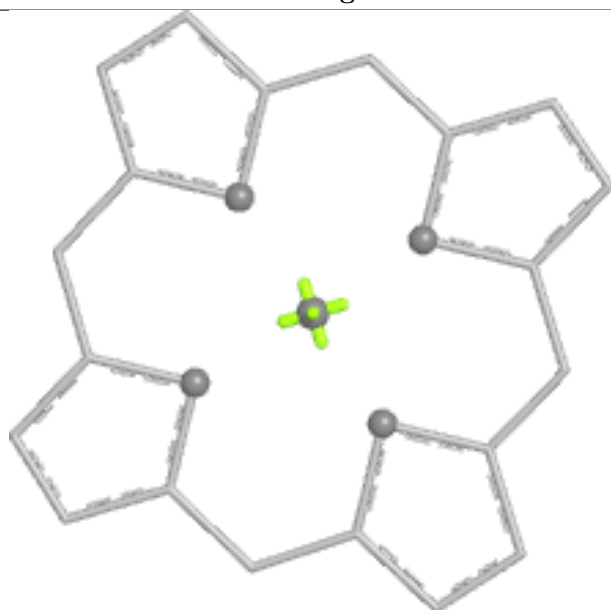
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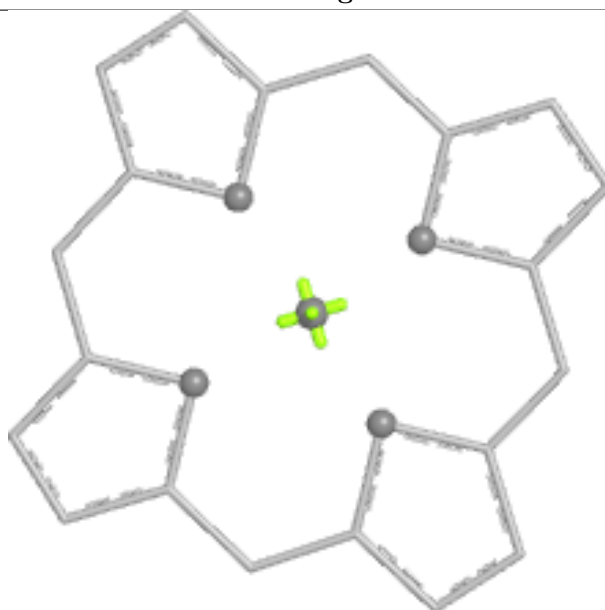
Bond lengths



Bond angles

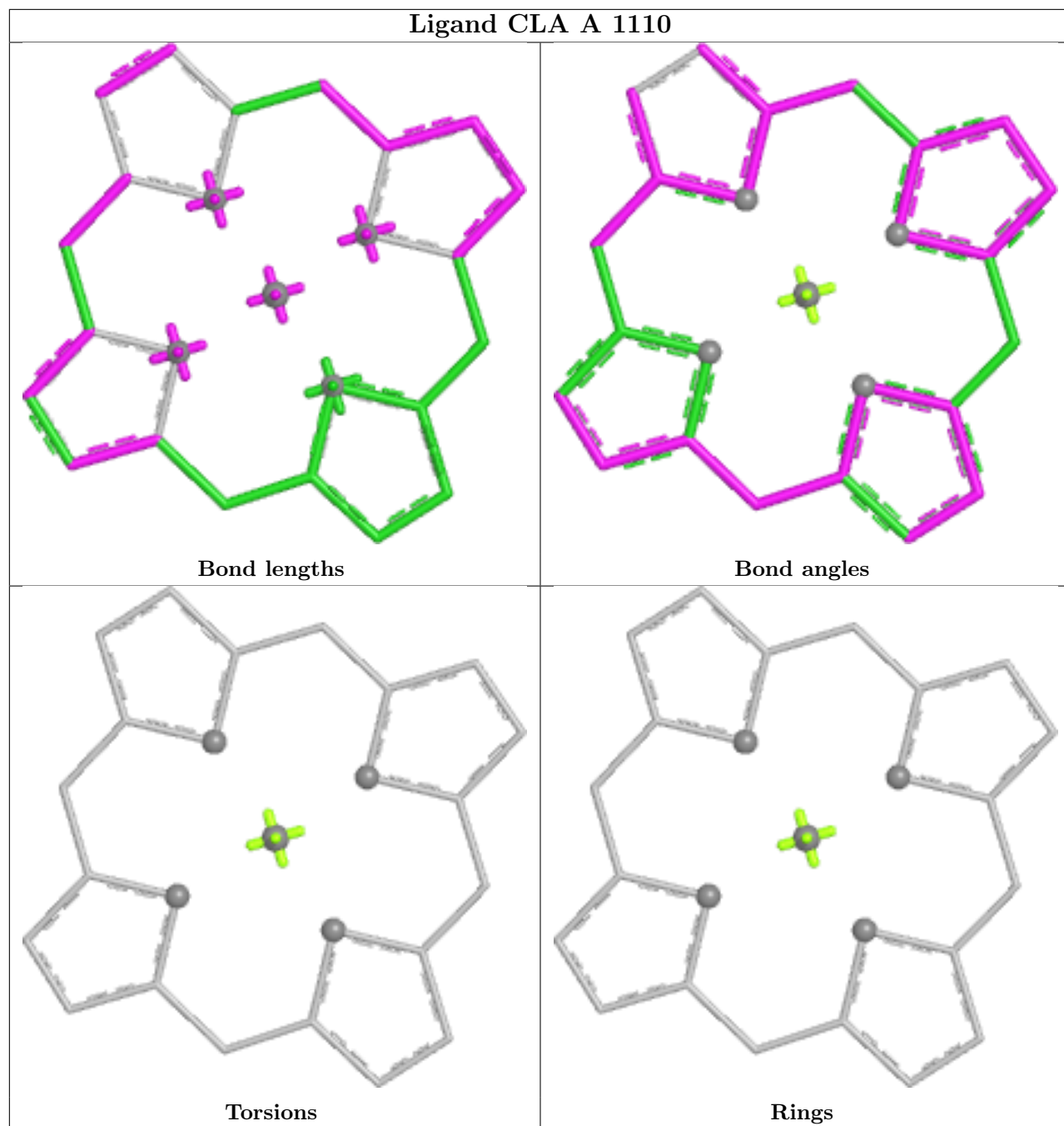


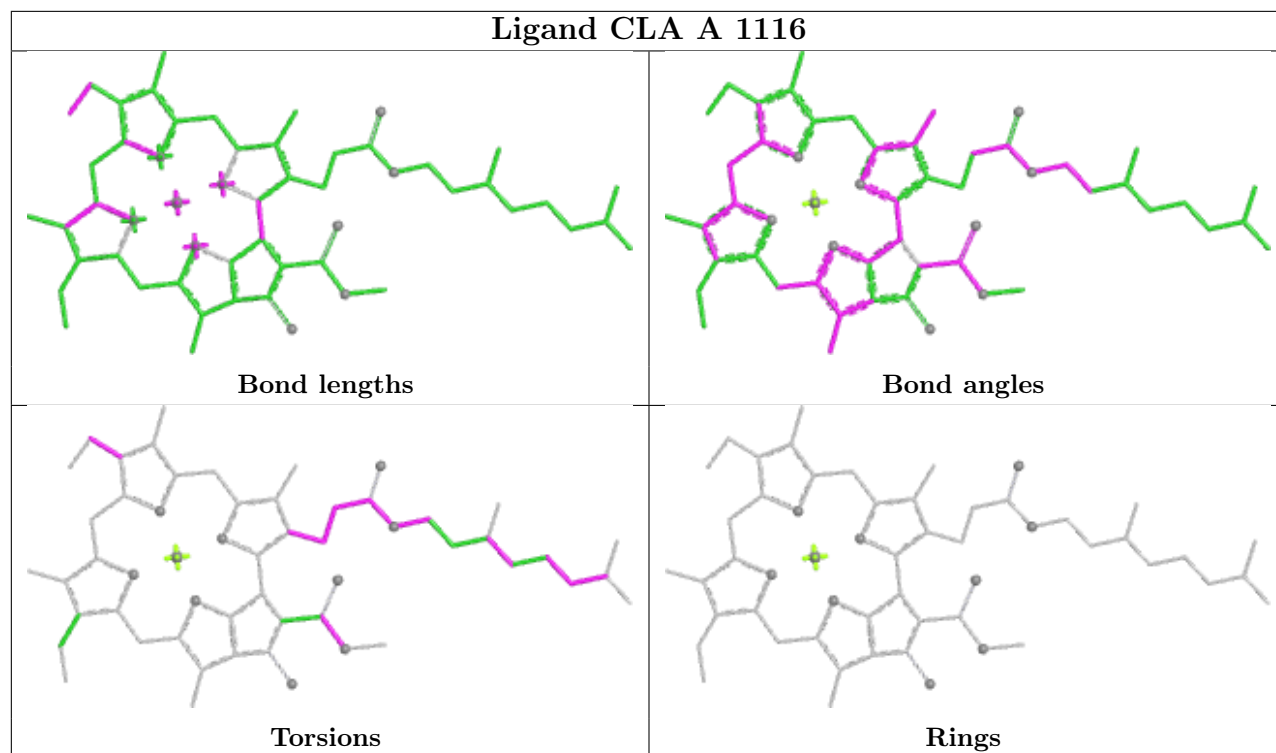
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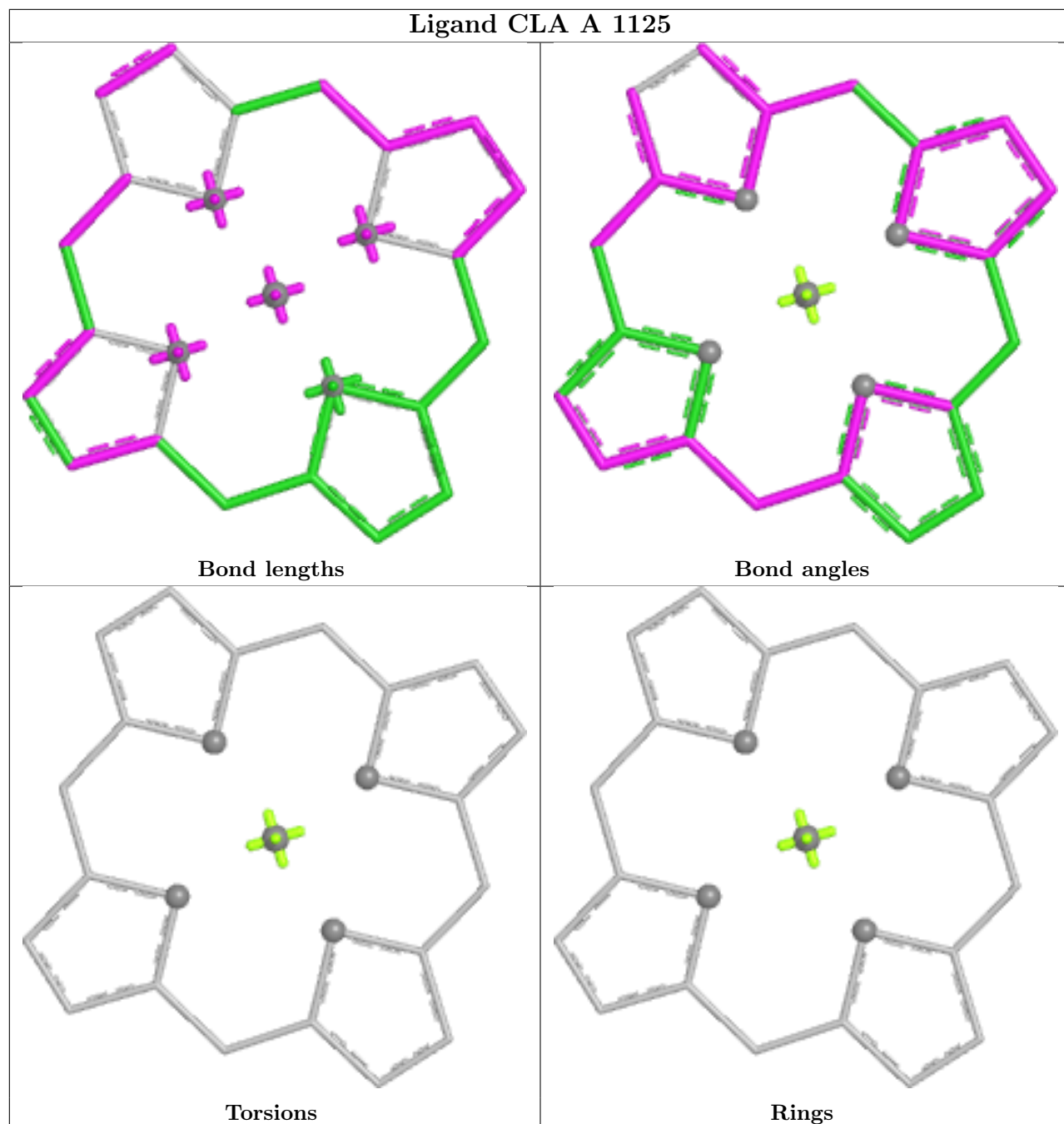
Rings

Ligand CLA A 1110

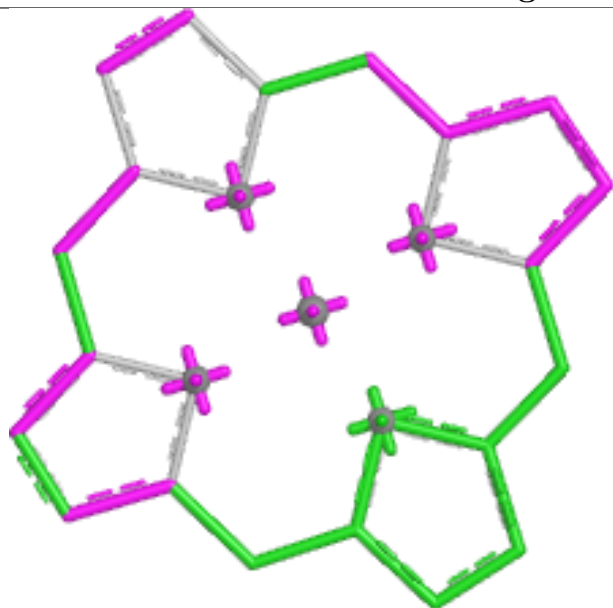




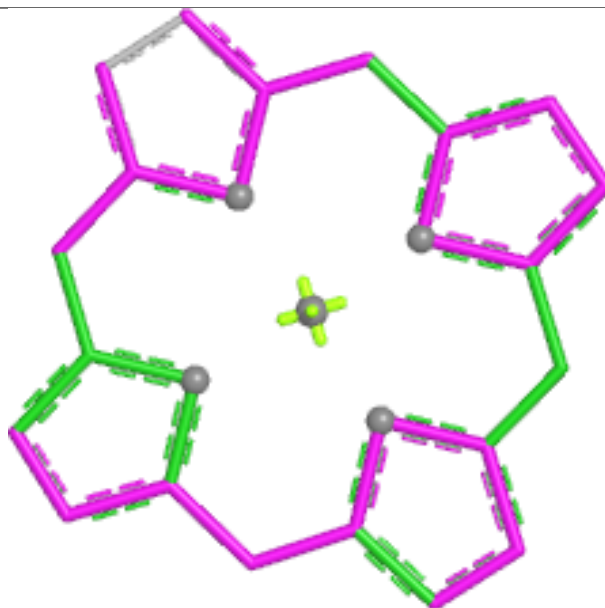
Ligand CLA A 1125



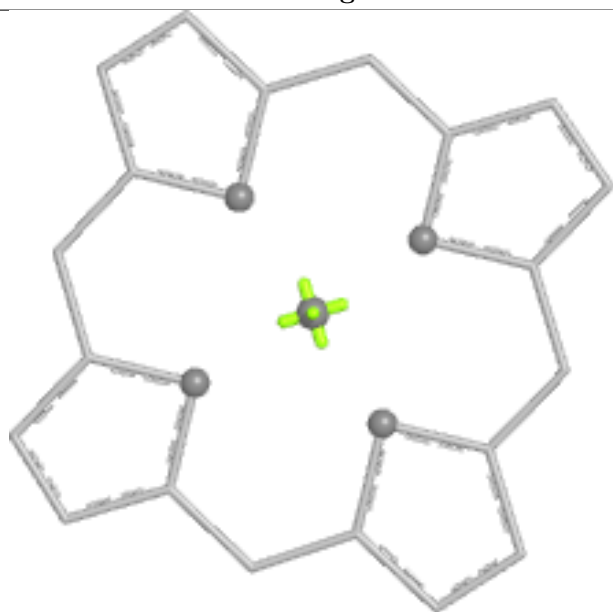
Ligand CLA 3 603



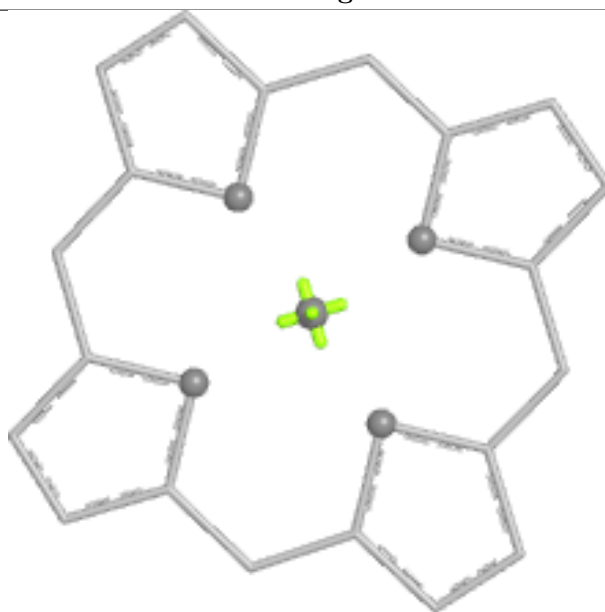
Bond lengths



Bond angles

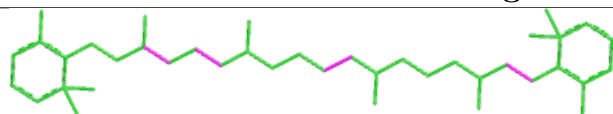


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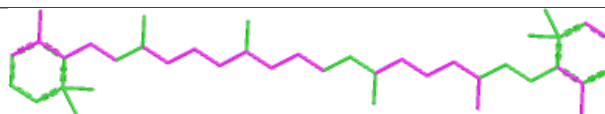


Rings

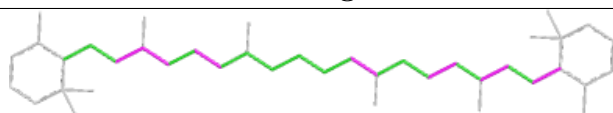
Ligand BCR A 4017



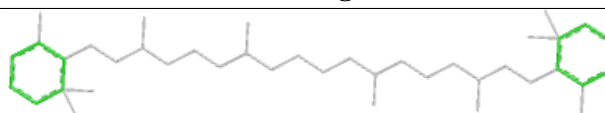
Bond lengths



Bond angles

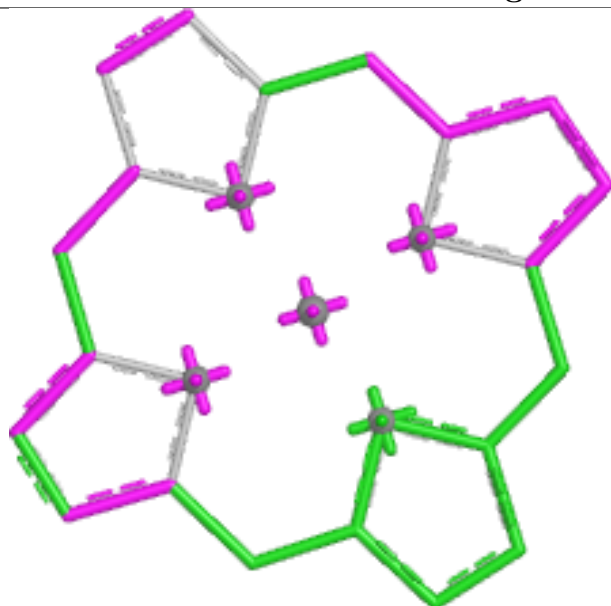


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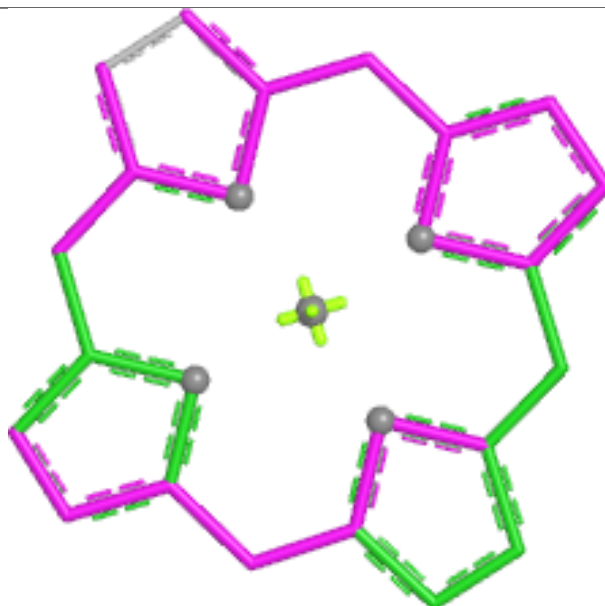


Rings

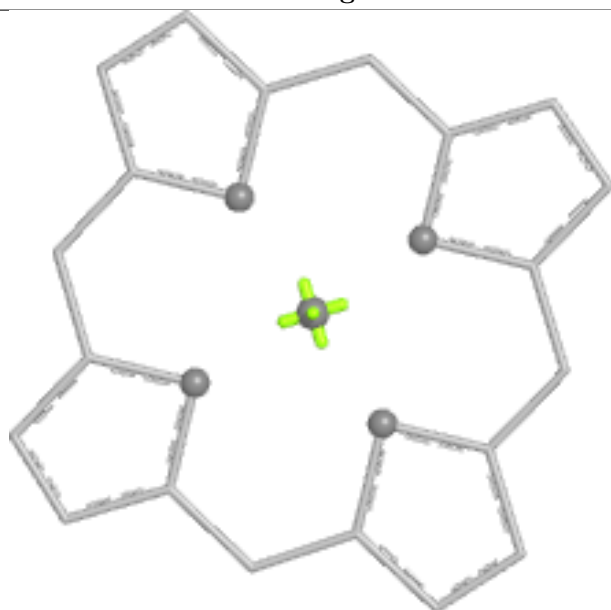
Ligand CLA B 1227



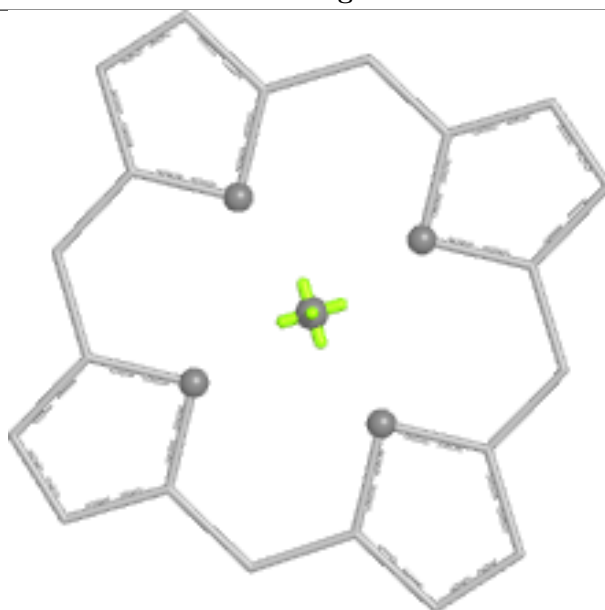
Bond lengths



Bond angles

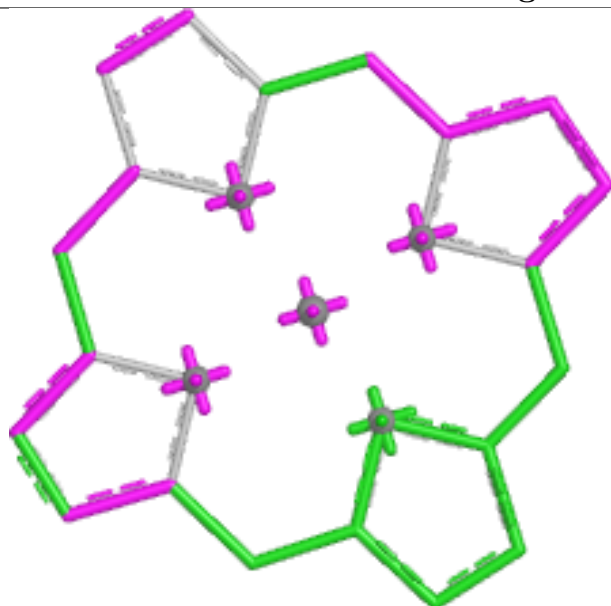


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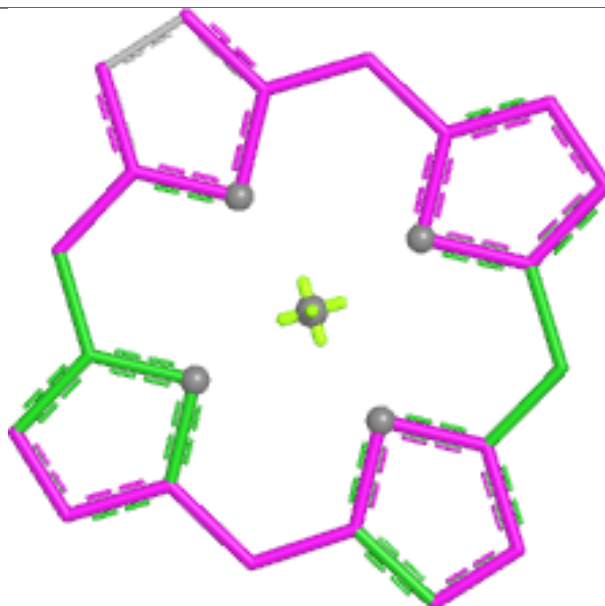


Rings

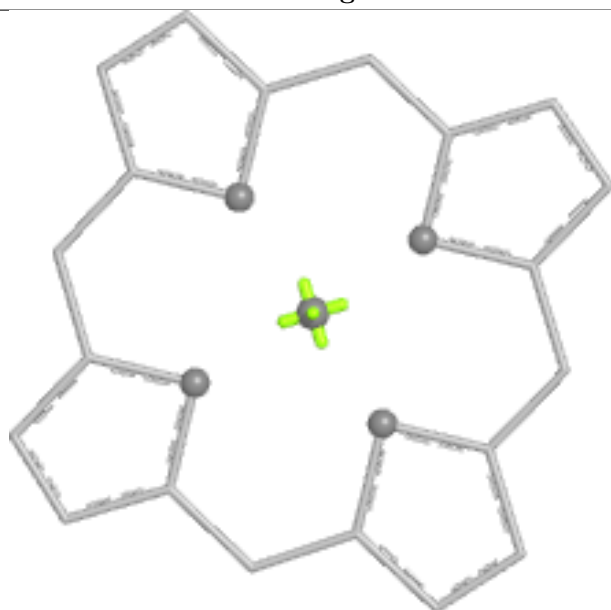
Ligand CLA 2 604



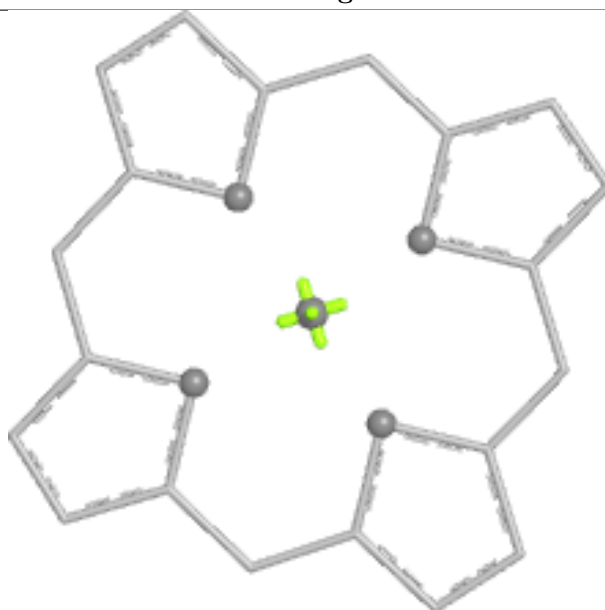
Bond lengths



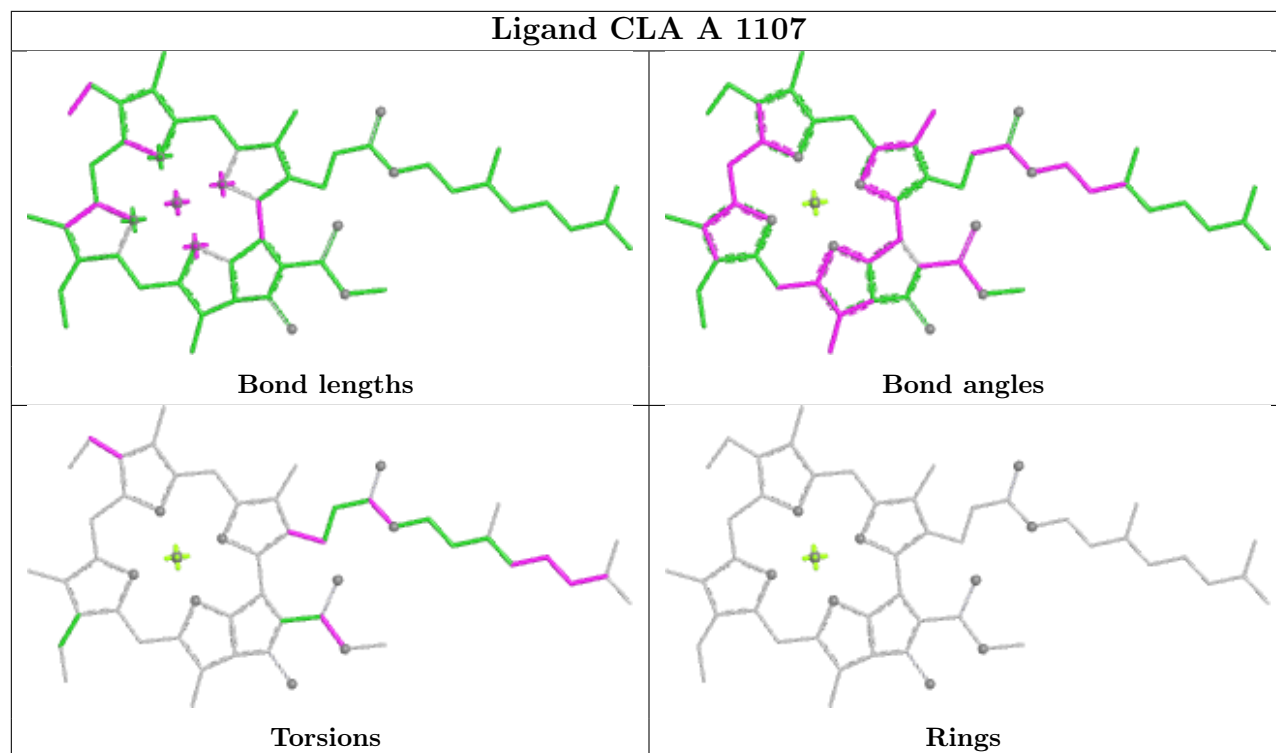
Bond angles



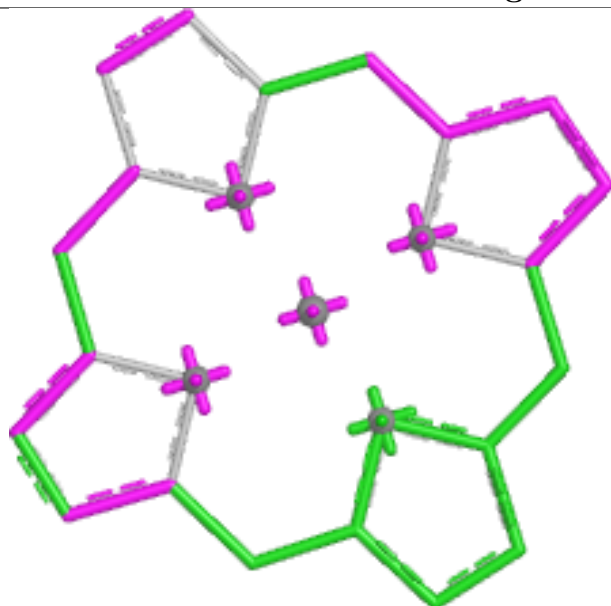
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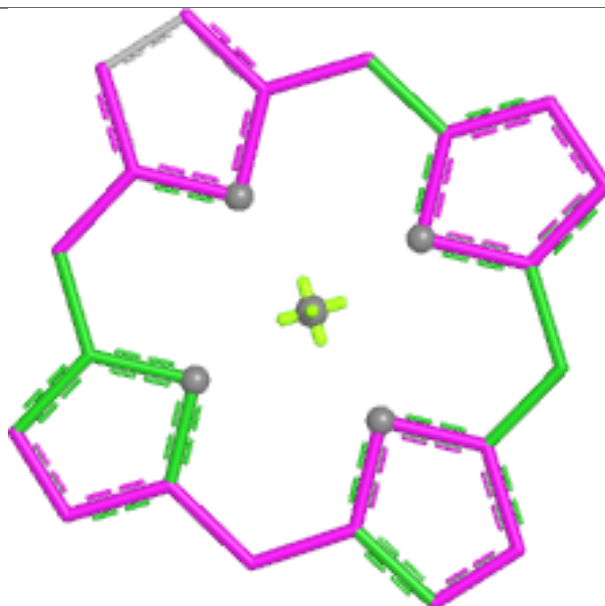
Rings



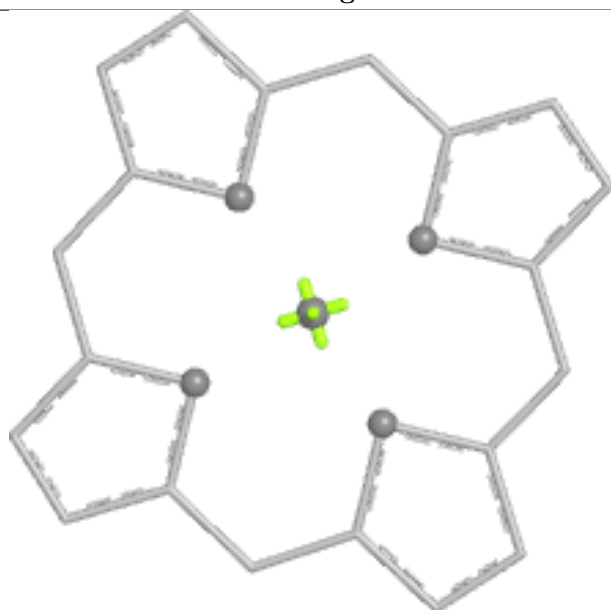
Ligand CLA B 1238



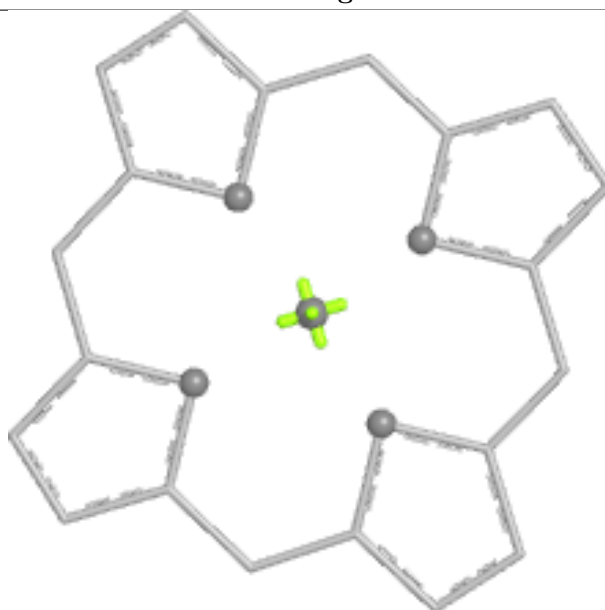
Bond lengths



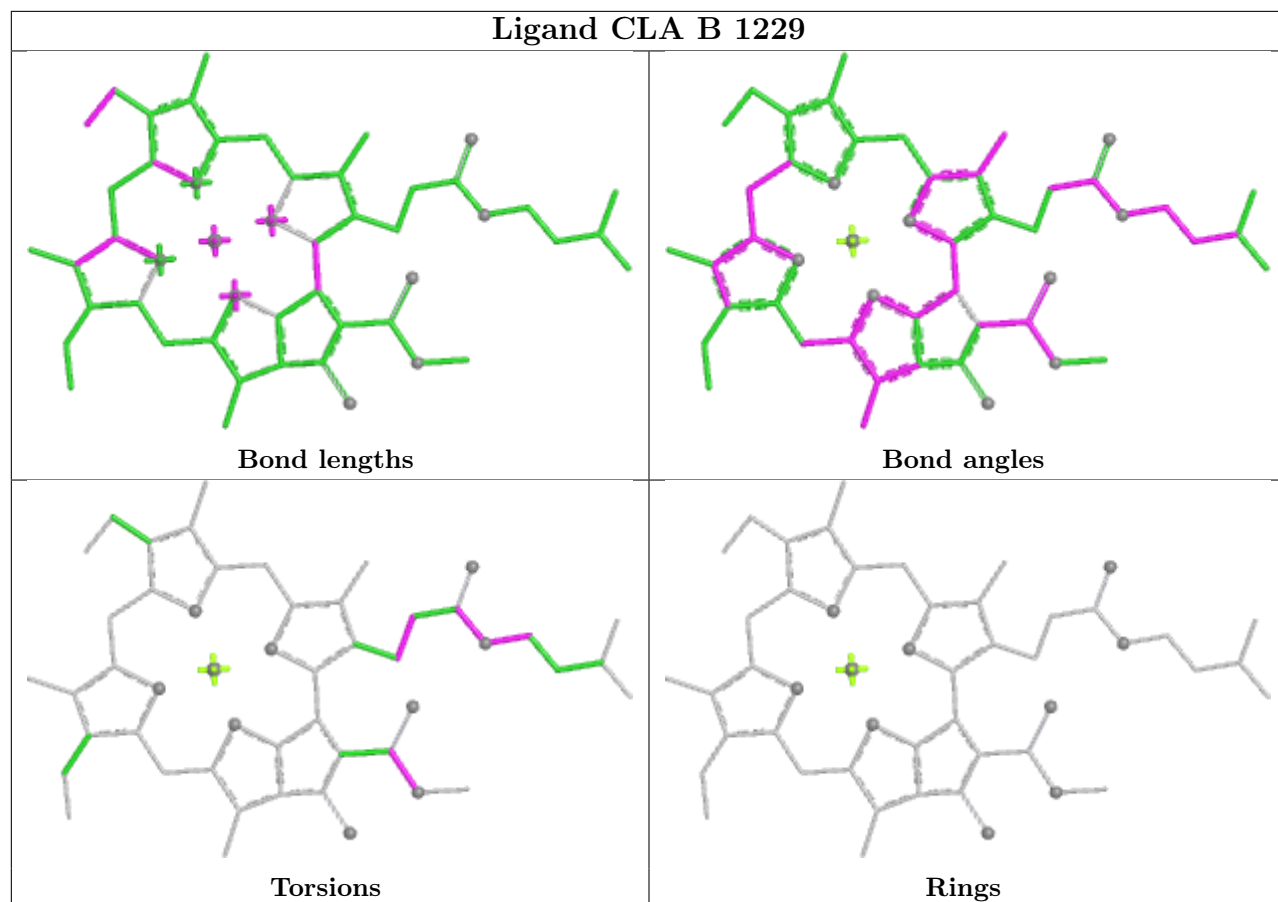
Bond angles

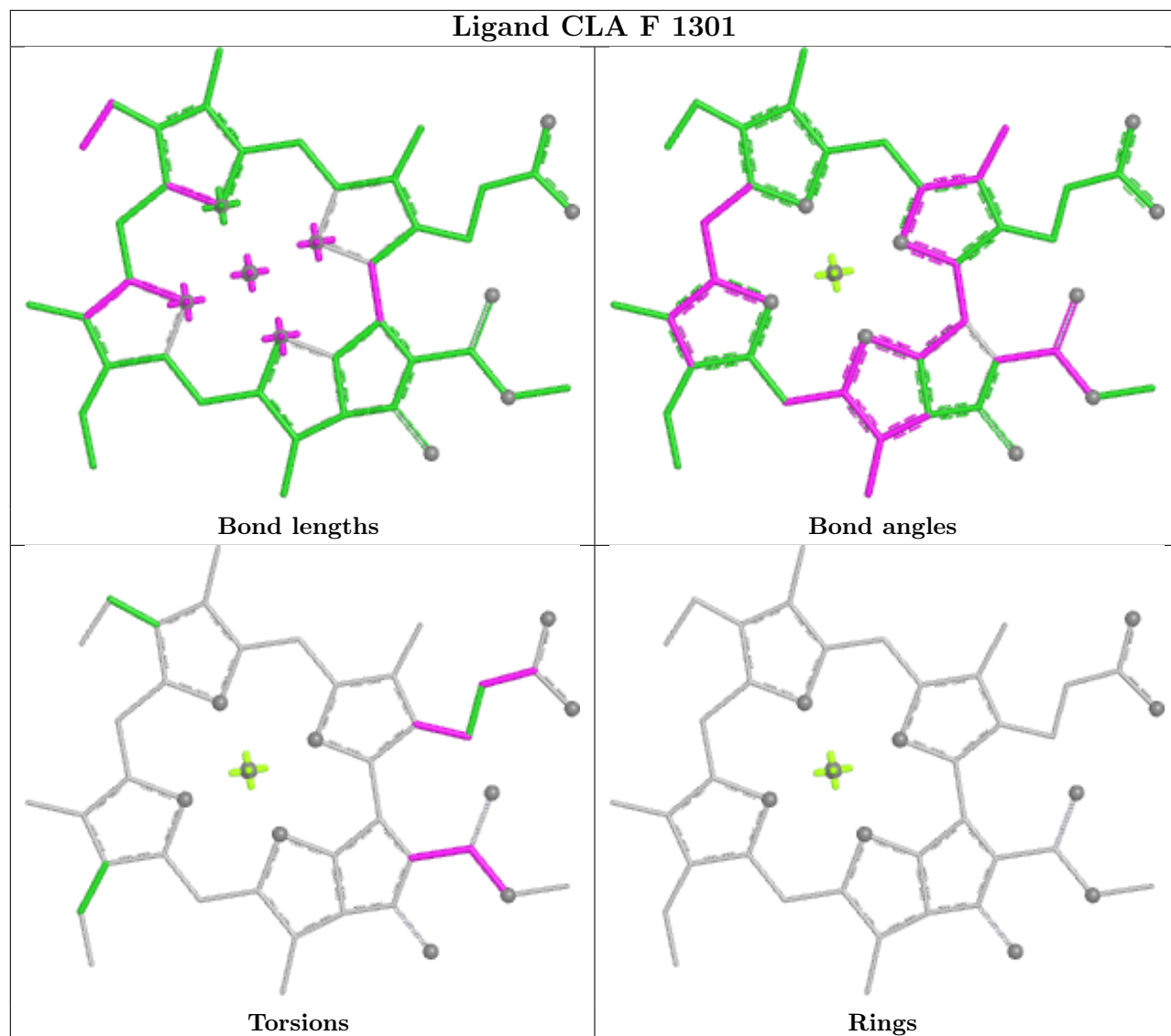


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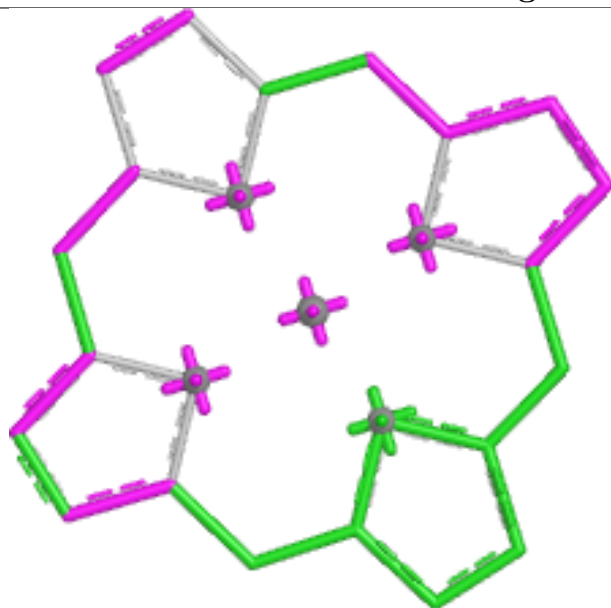


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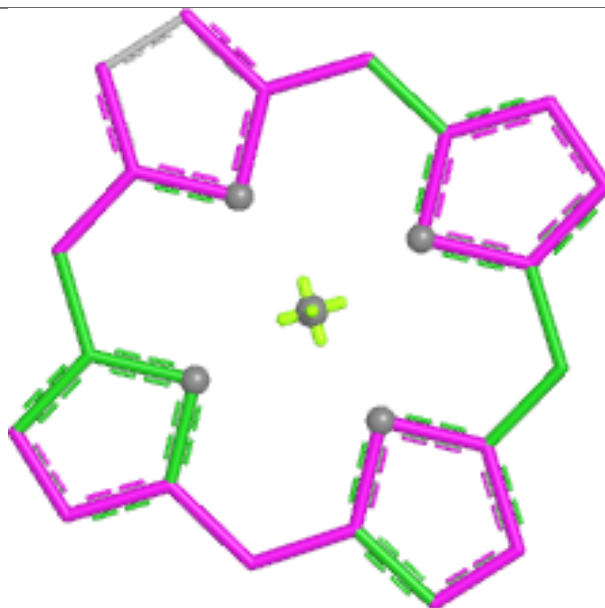




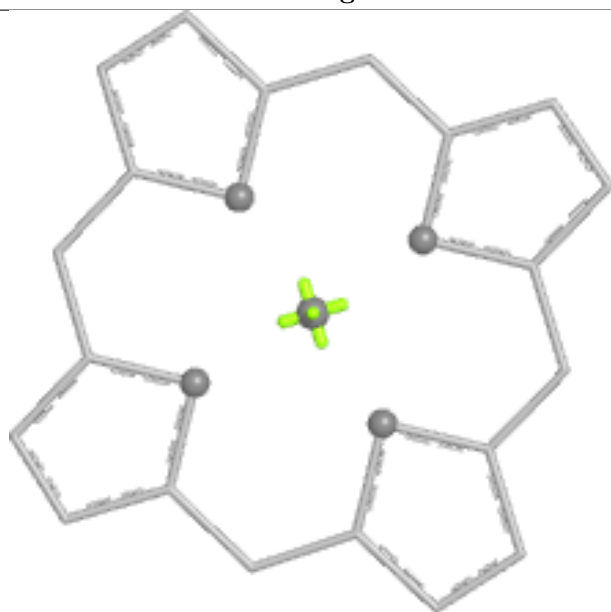
Ligand CLA 4 605



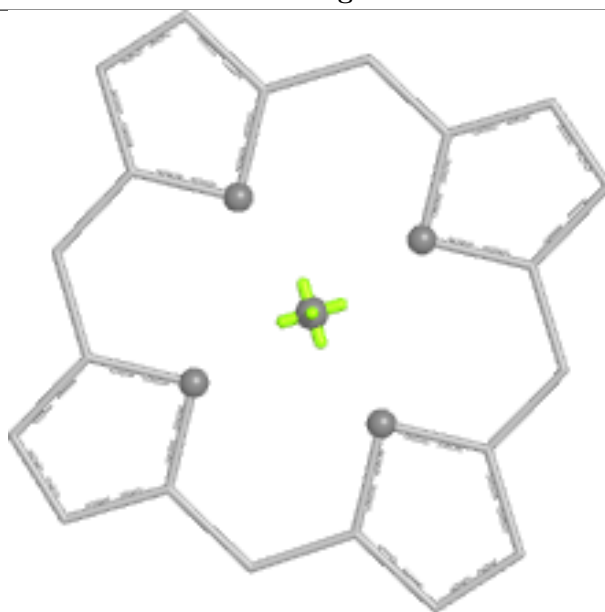
Bond lengths



Bond angles

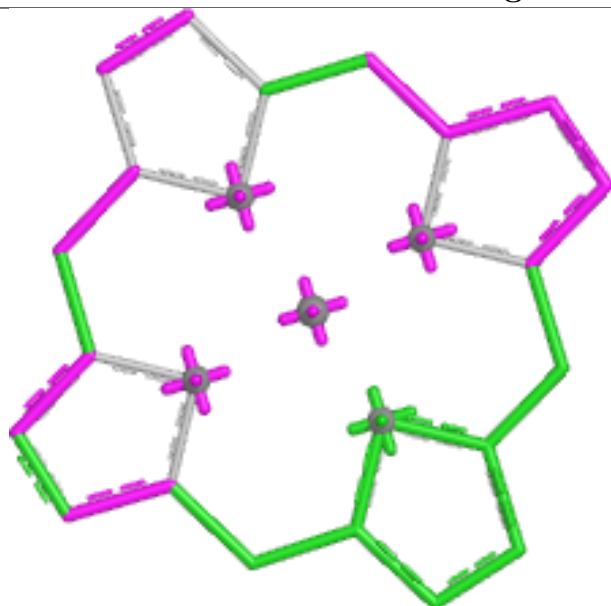


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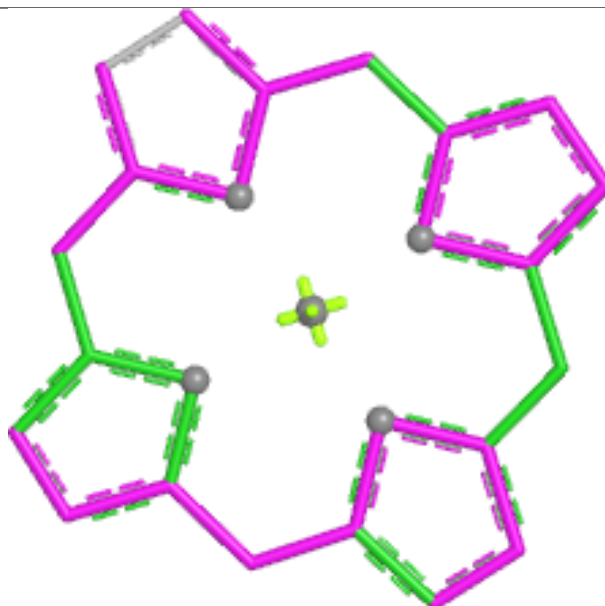


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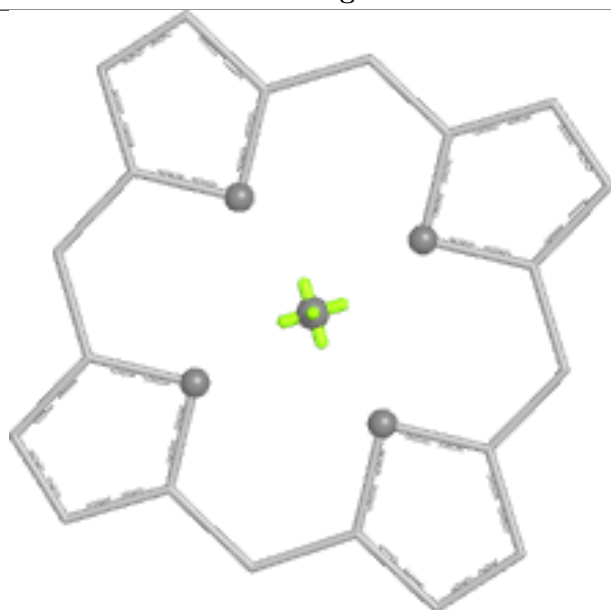
Ligand CLA A 1121



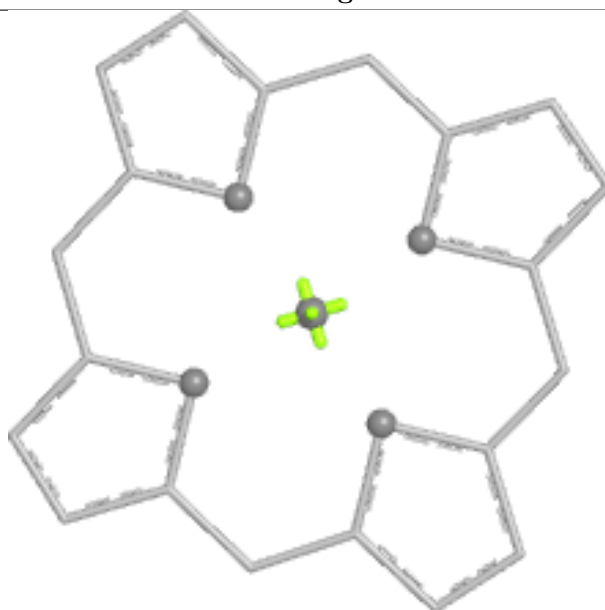
Bond lengths



Bond angles

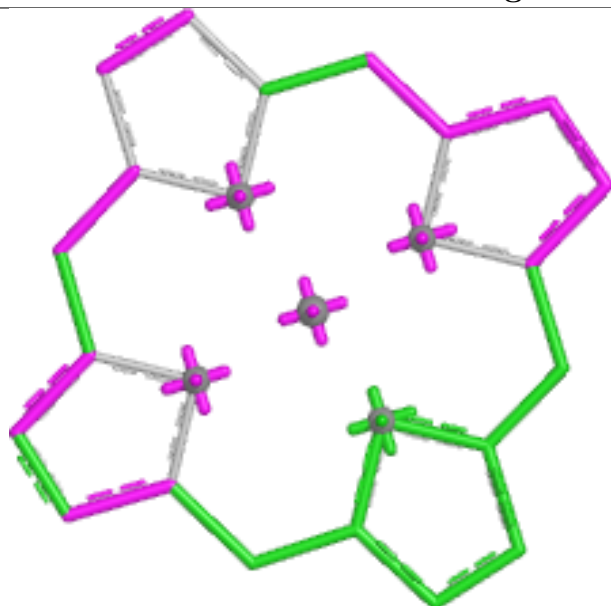


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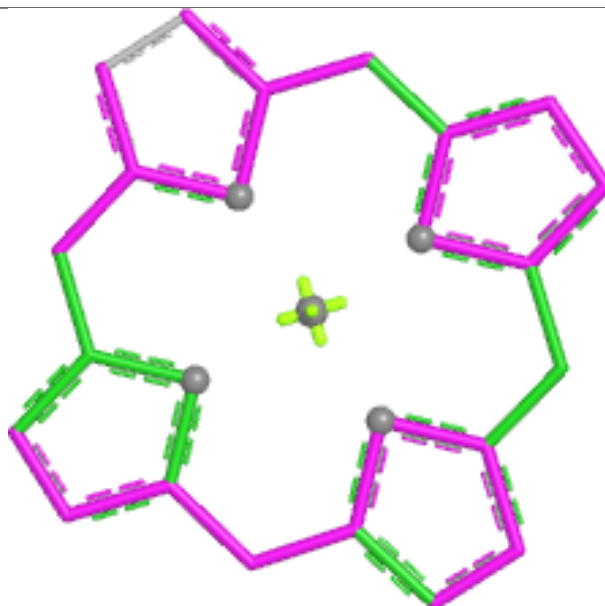


Rings

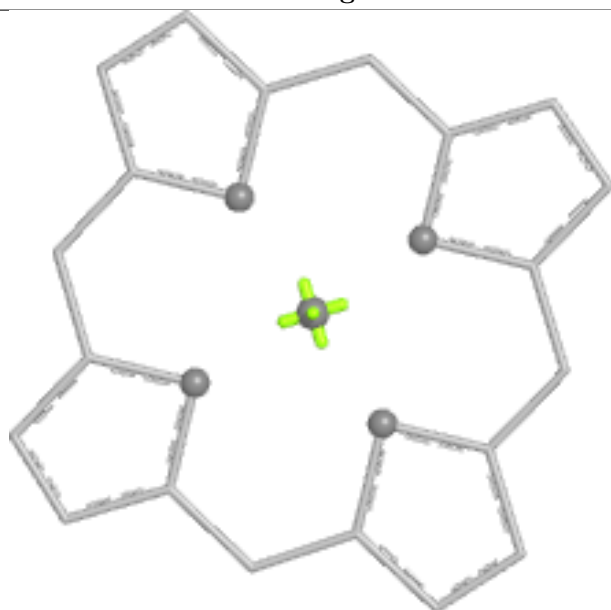
Ligand CLA A 1132



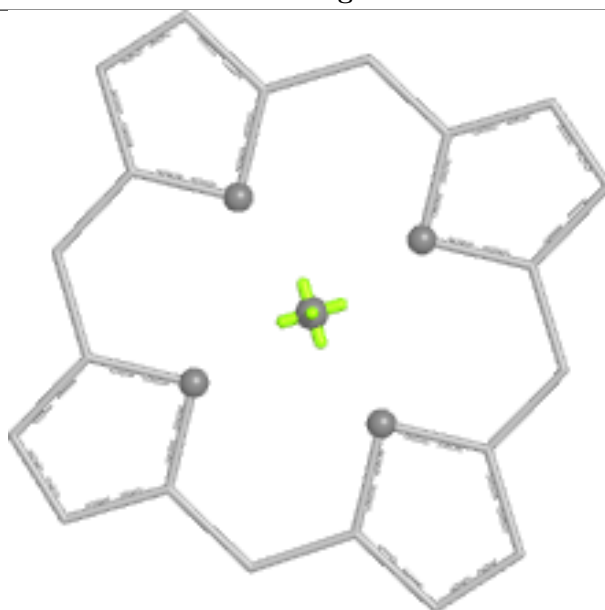
Bond lengths



Bond angles

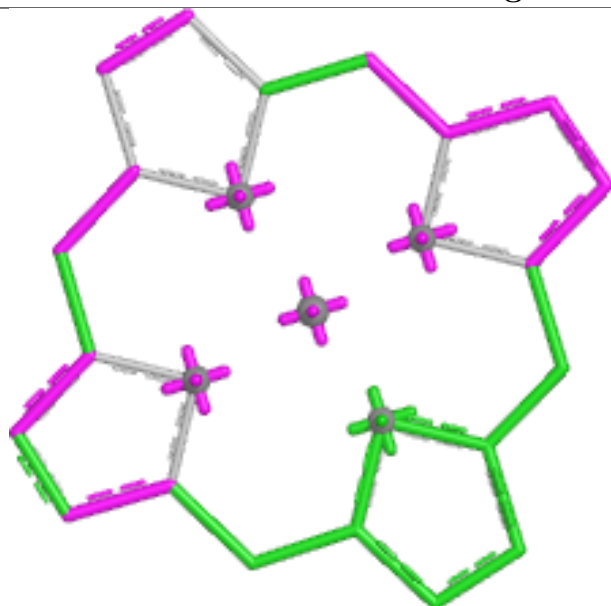


Torsions

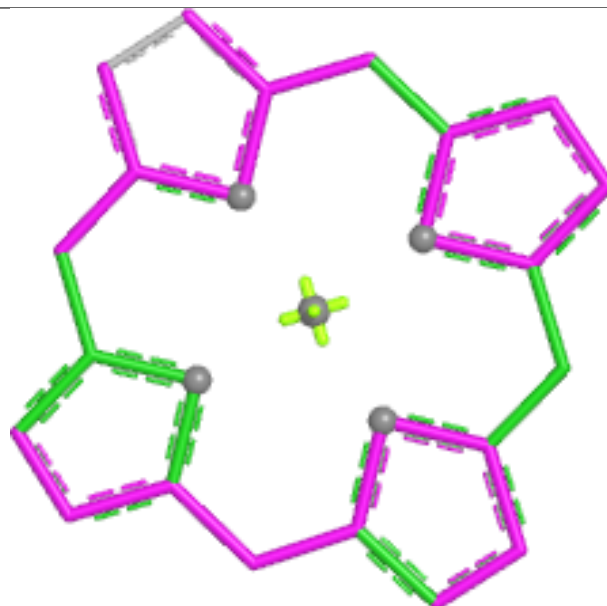


Rings

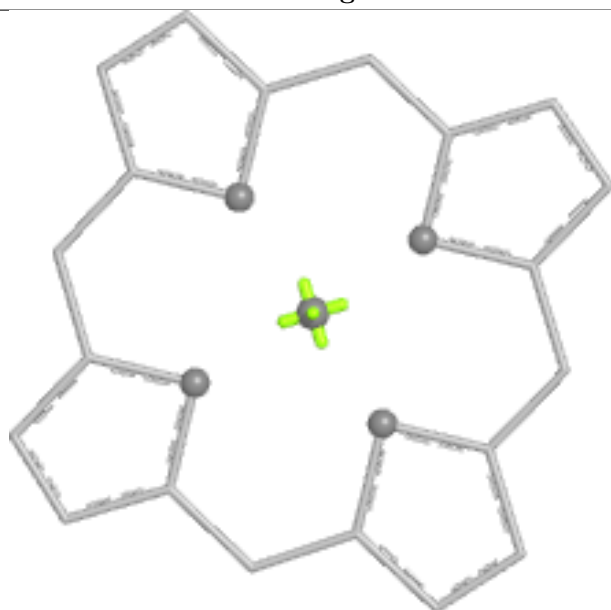
Ligand CLA A 1119



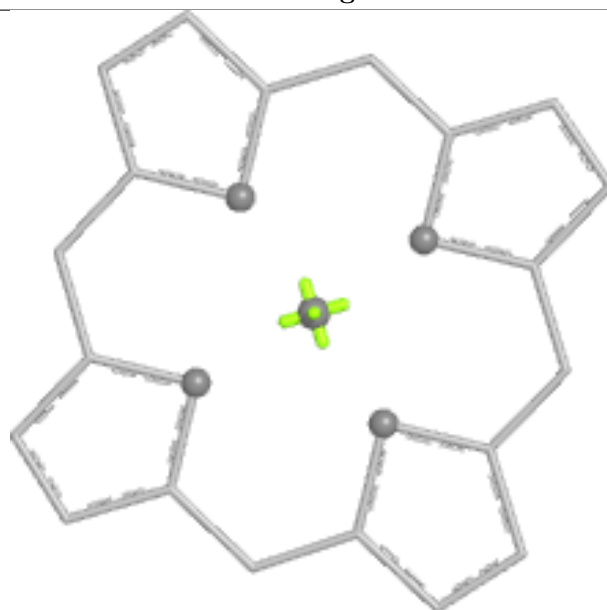
Bond lengths



Bond angles

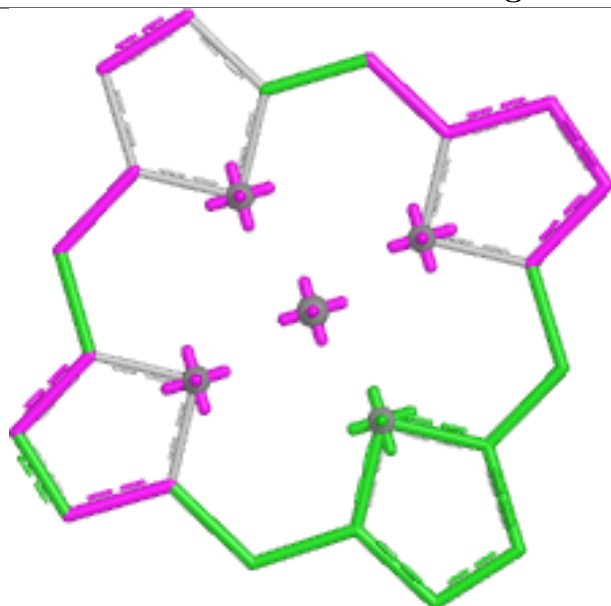


Torsions

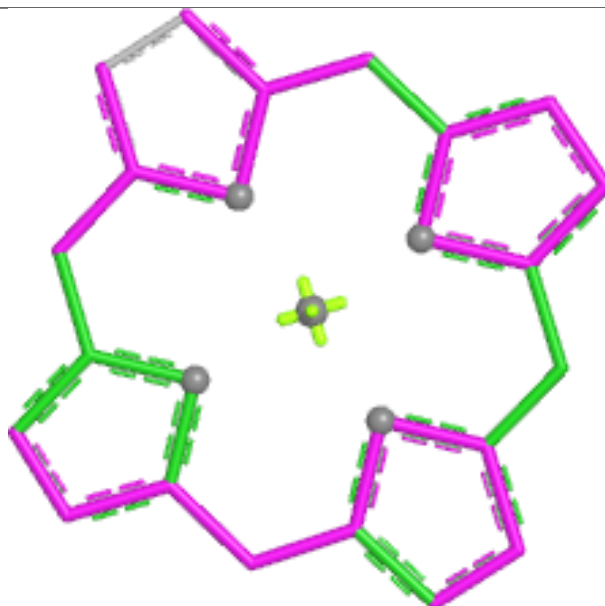


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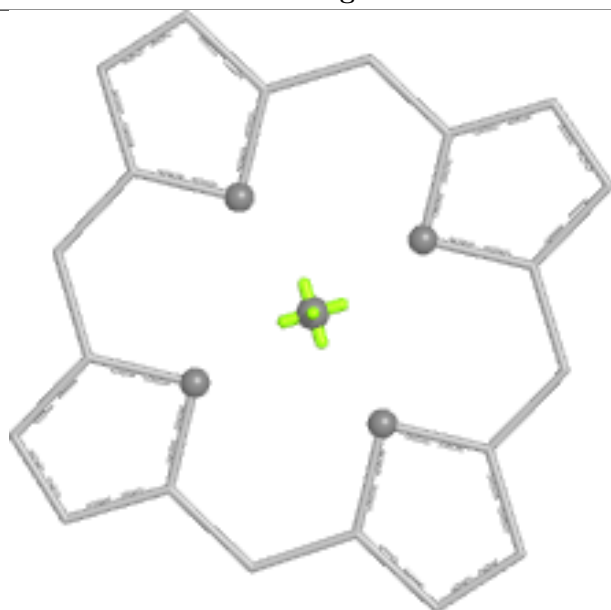
Ligand CLA A 1118



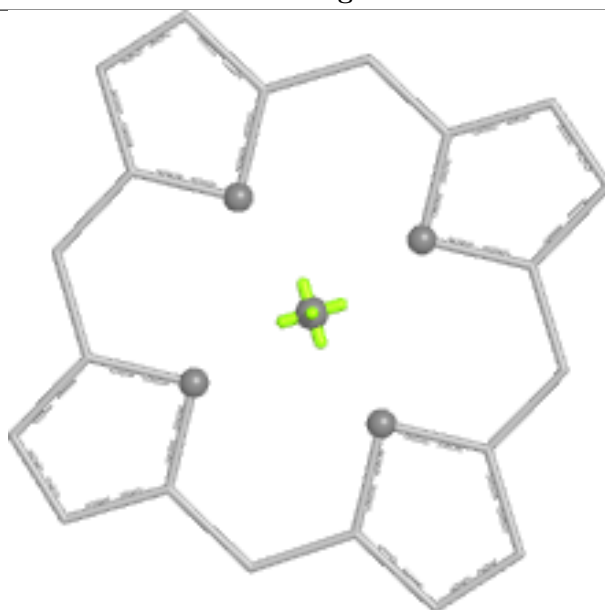
Bond lengths



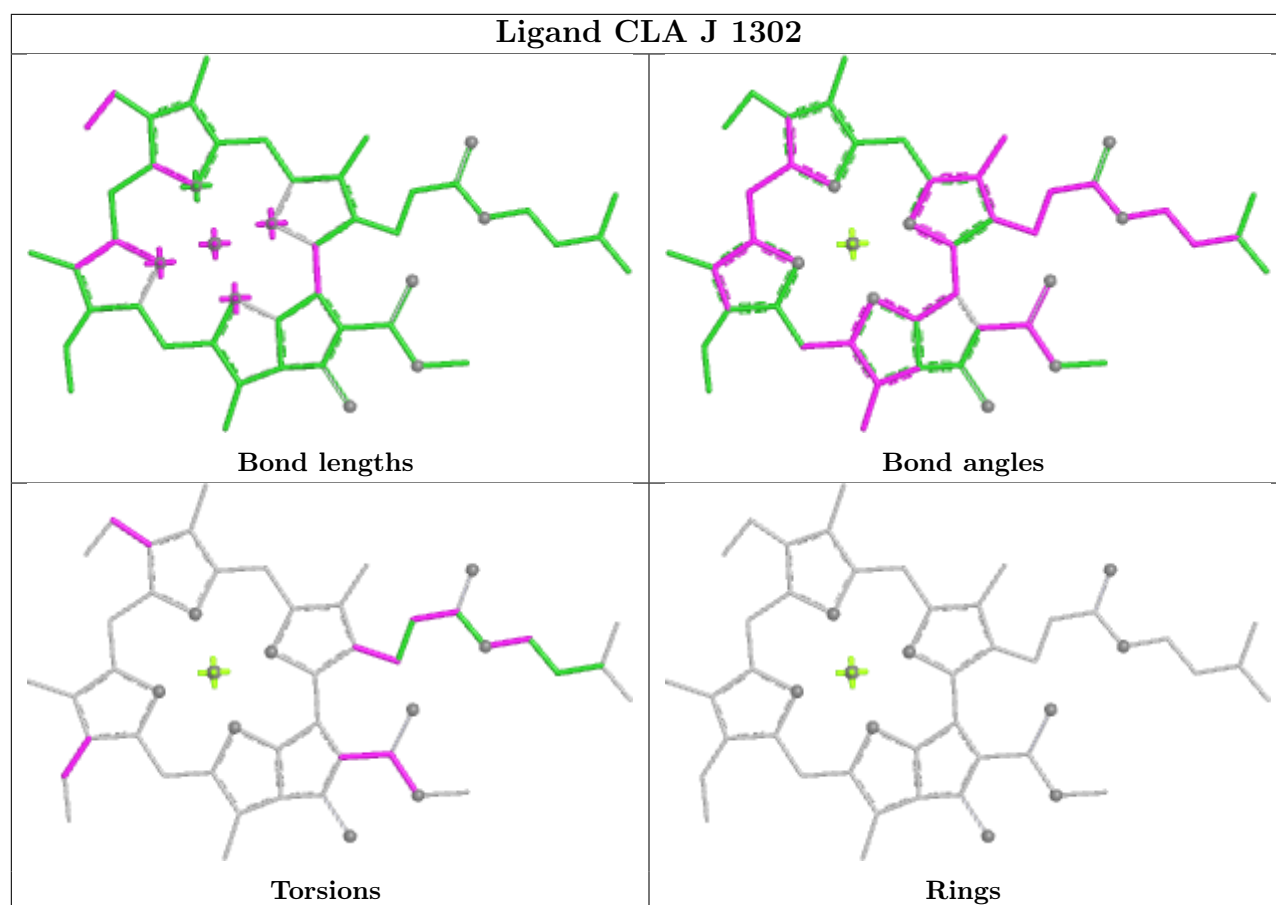
Bond angles



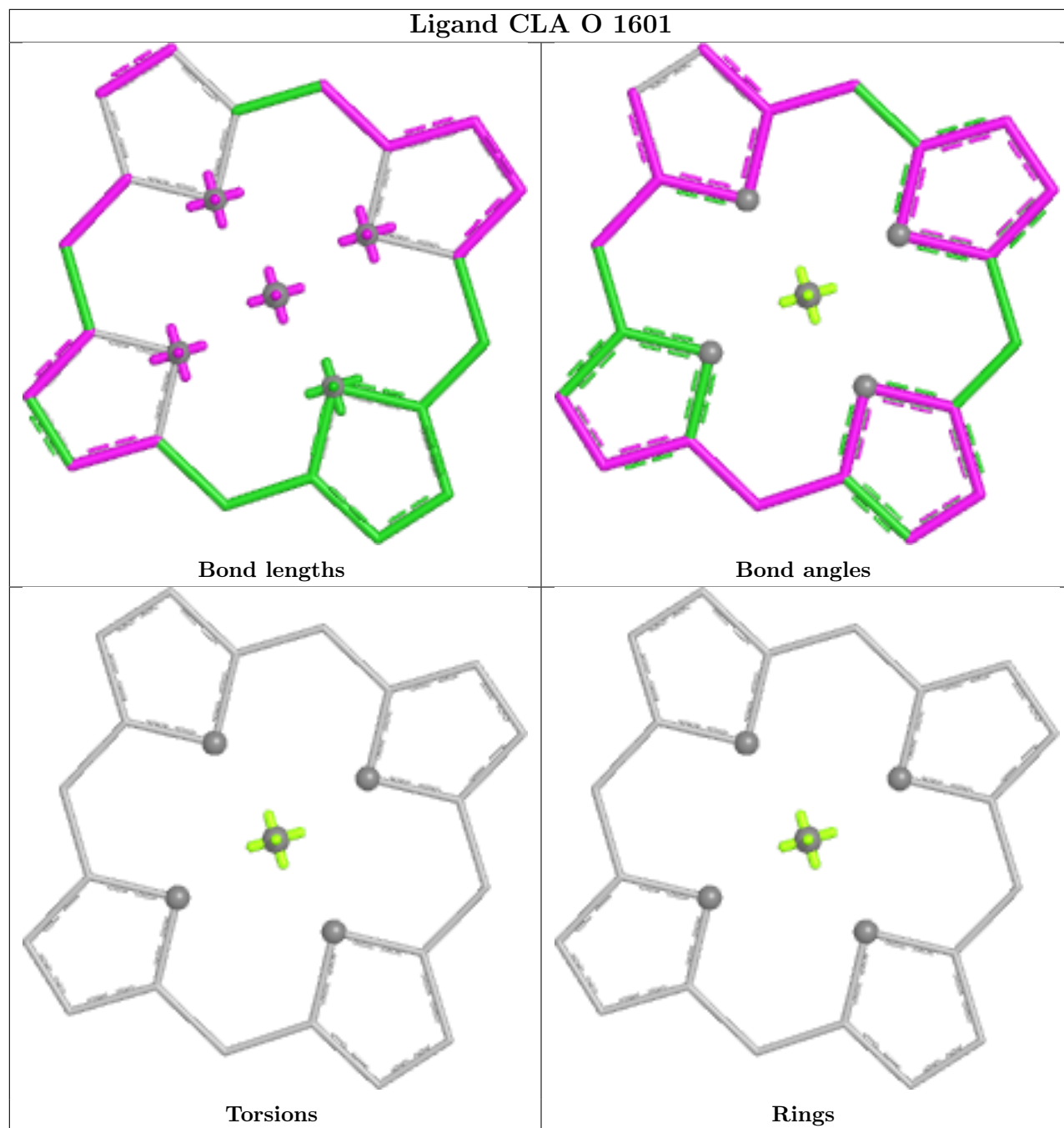
Torsions



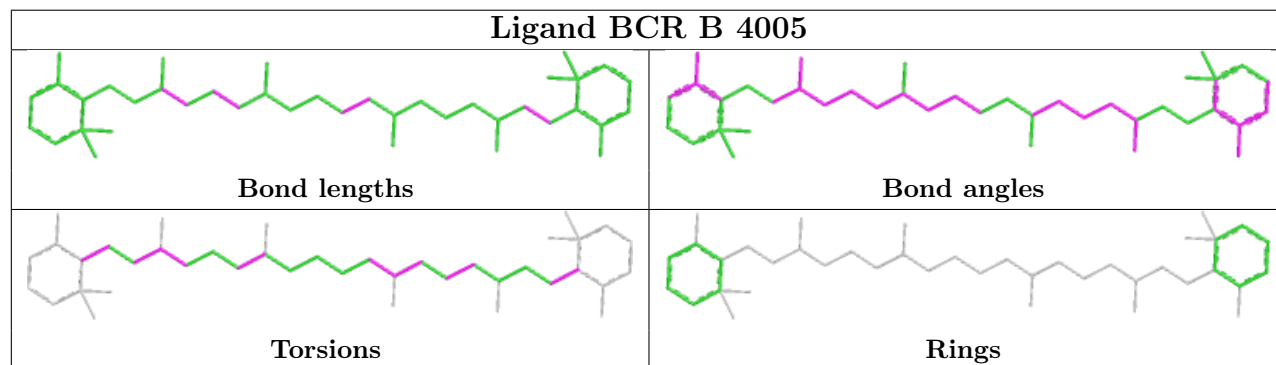
Rings



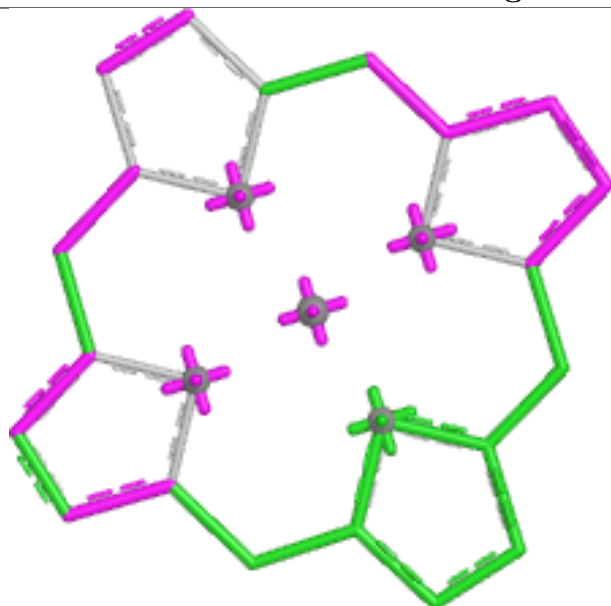
Ligand CLA O 1601



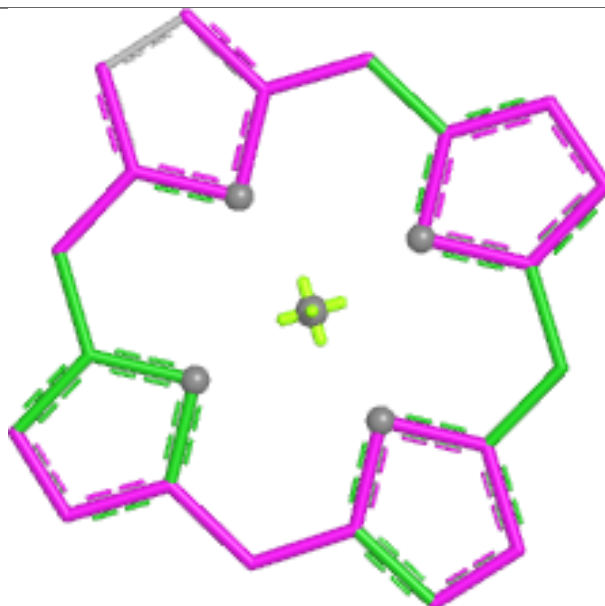
Ligand BCR B 4005



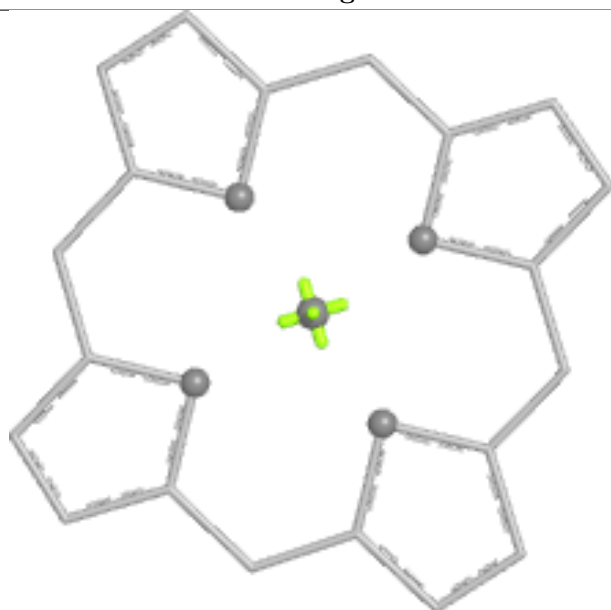
Ligand CLA A 1138



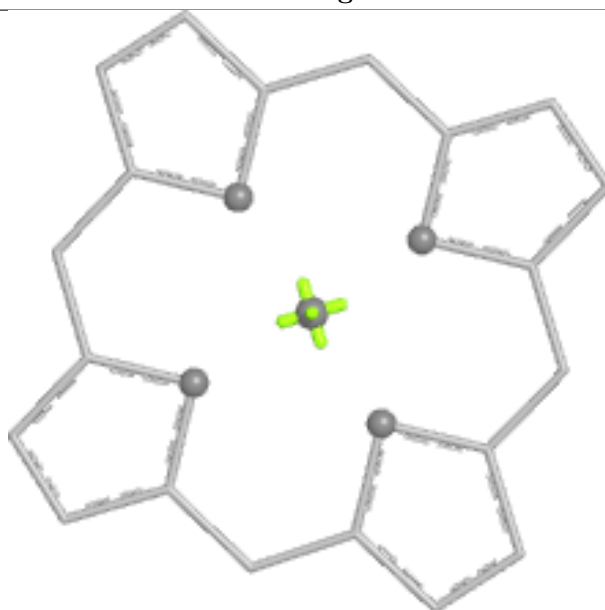
Bond lengths



Bond angles

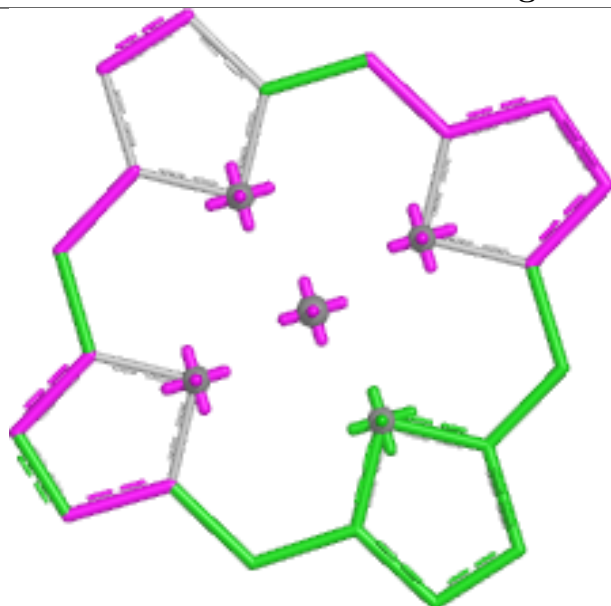


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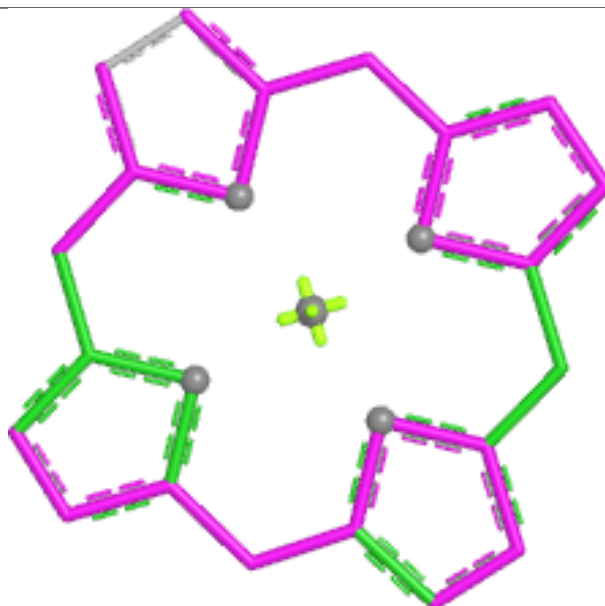


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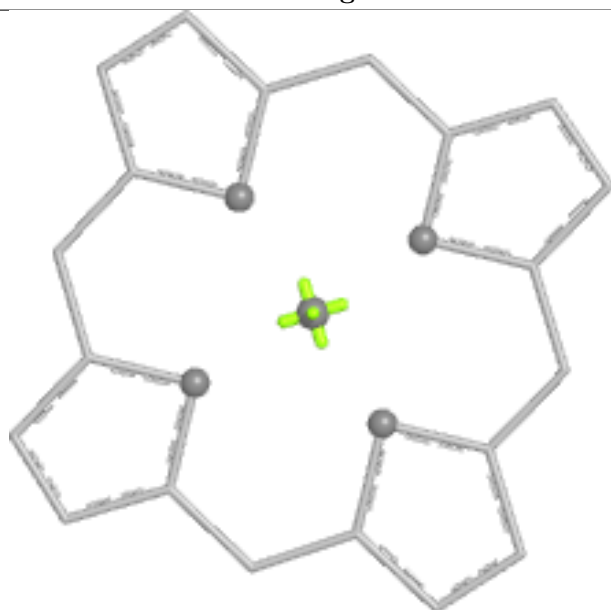
Ligand CLA 3 608



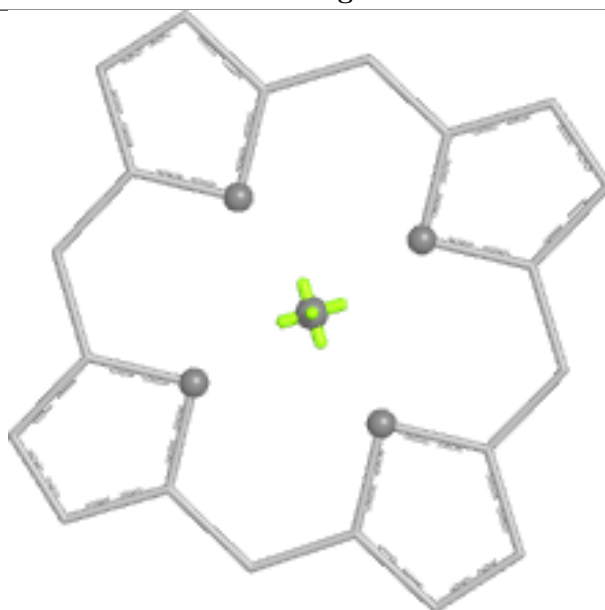
Bond lengths



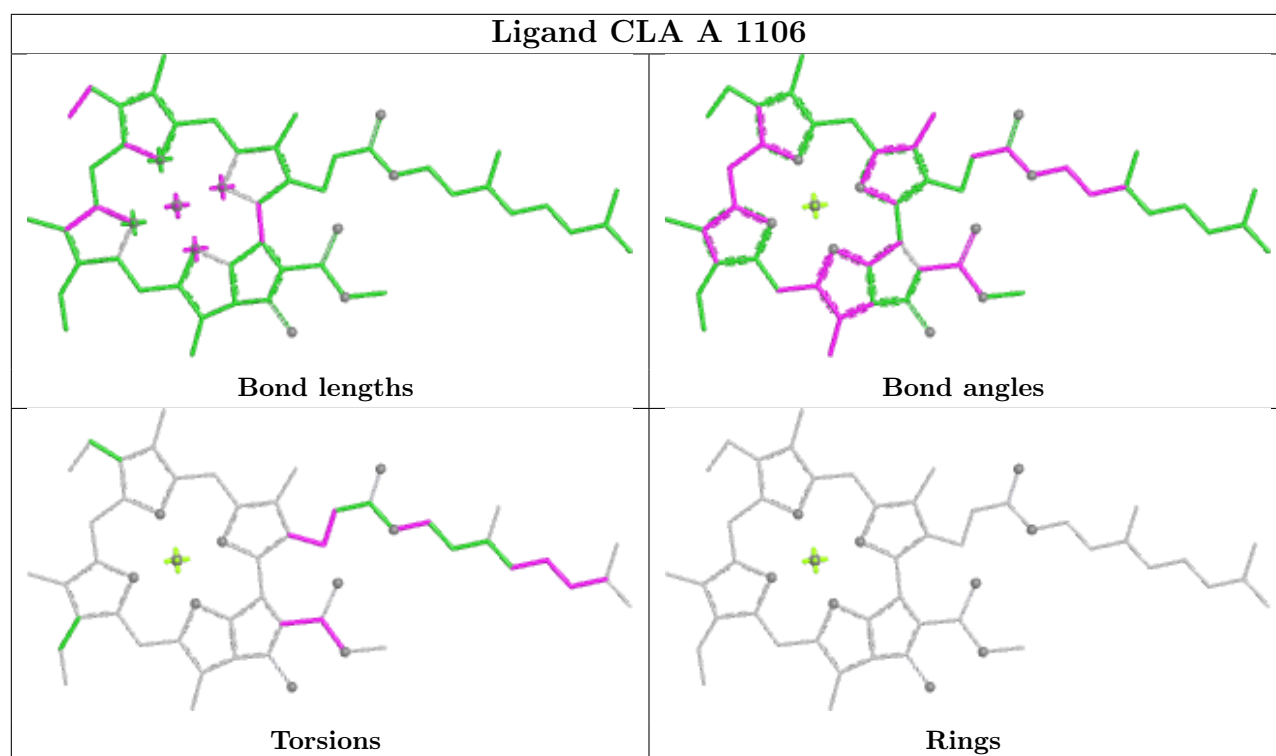
Bond angles



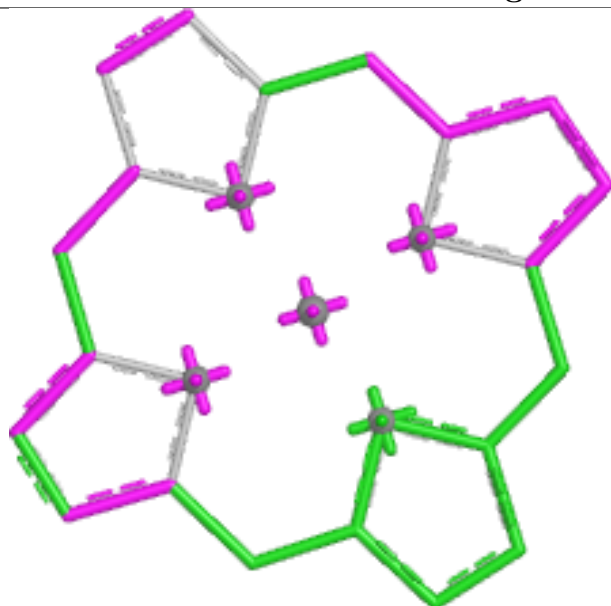
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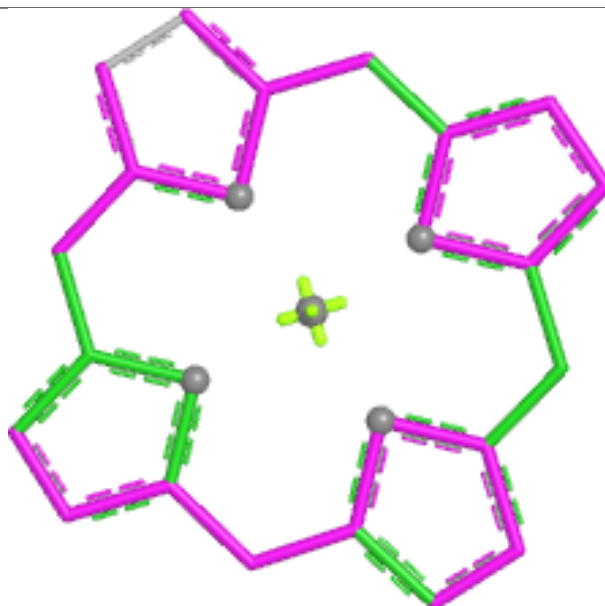
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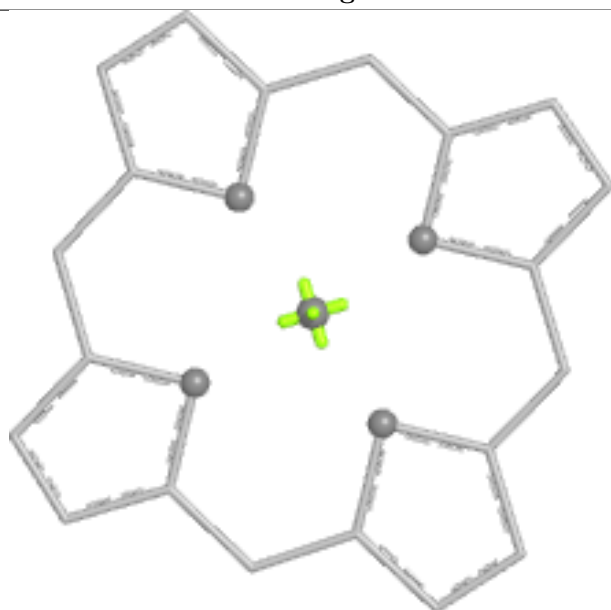
Ligand CLA B 1202



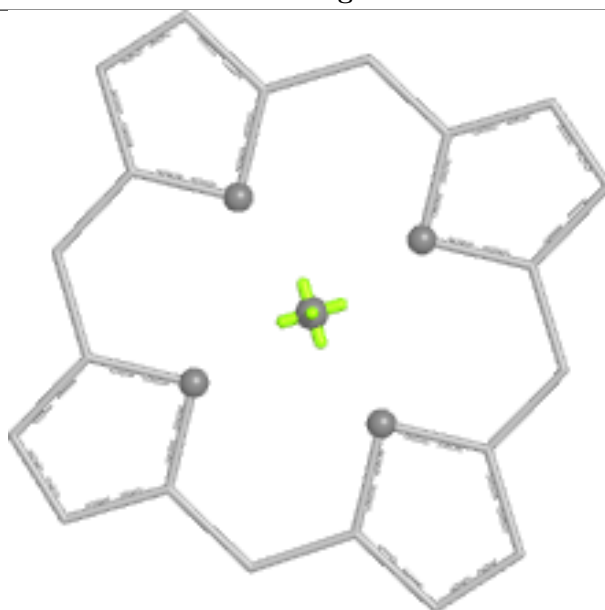
Bond lengths



Bond angles

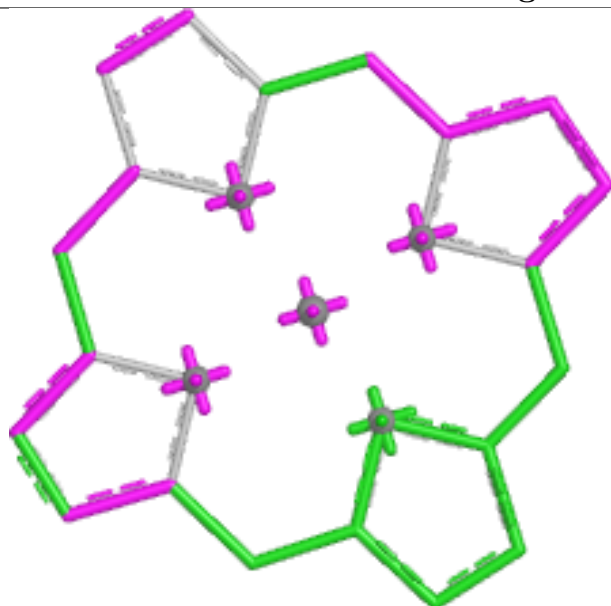


Torsions

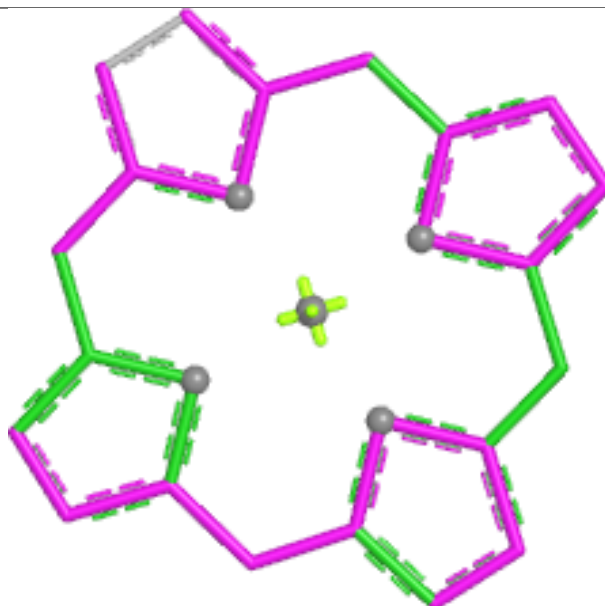


Rings

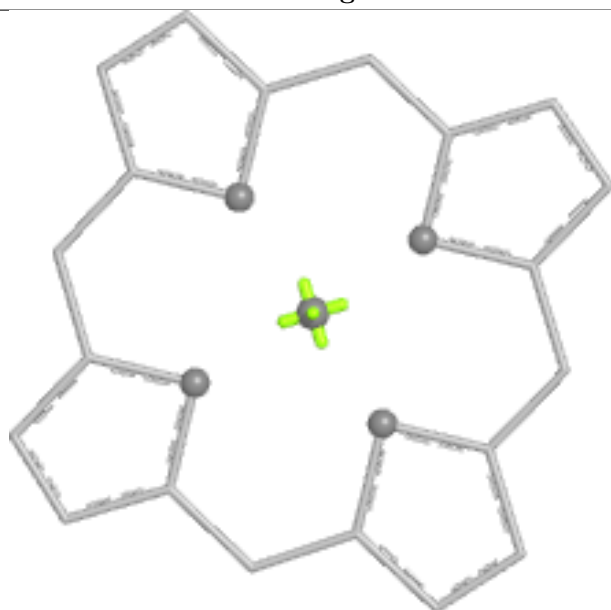
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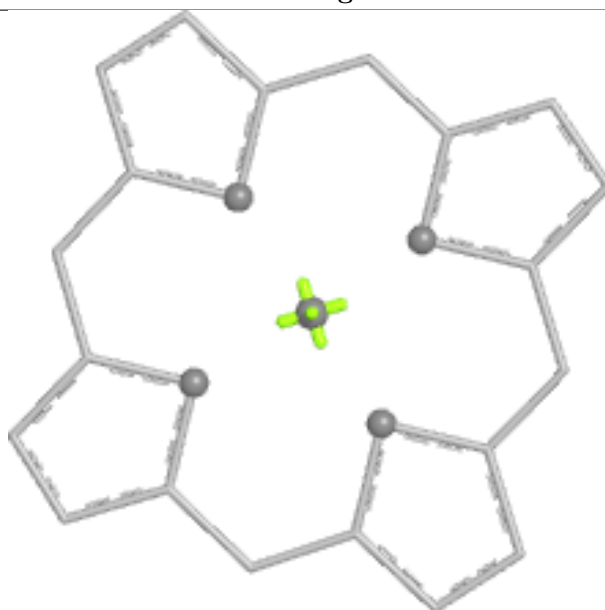
Bond lengths



Bond angles

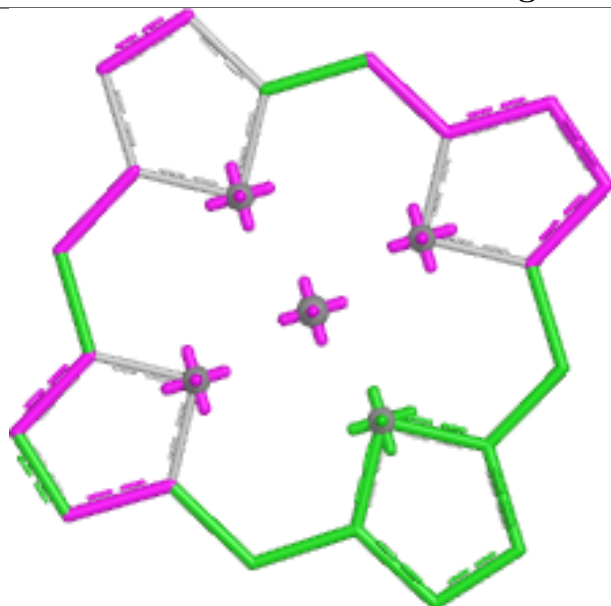


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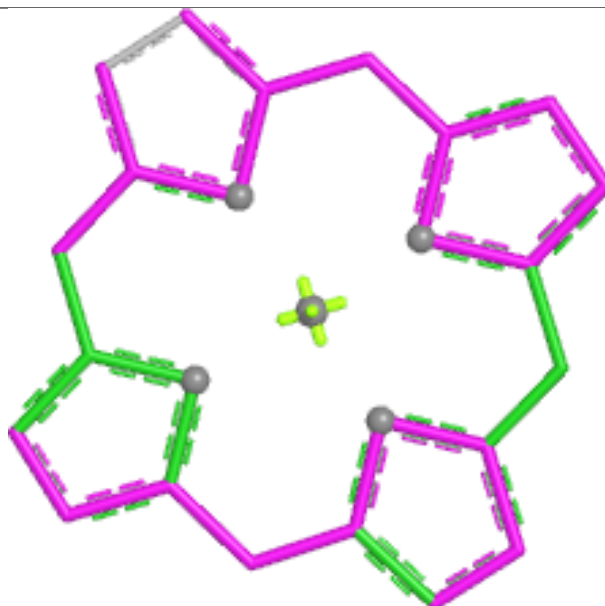


Rings

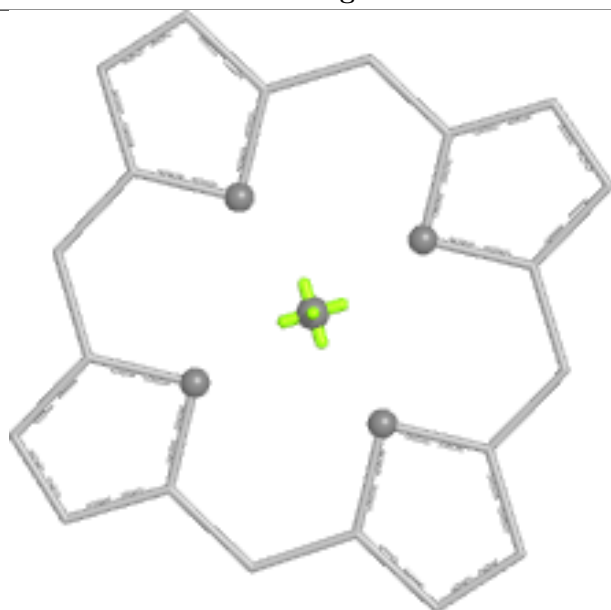
Ligand CLA 2 611



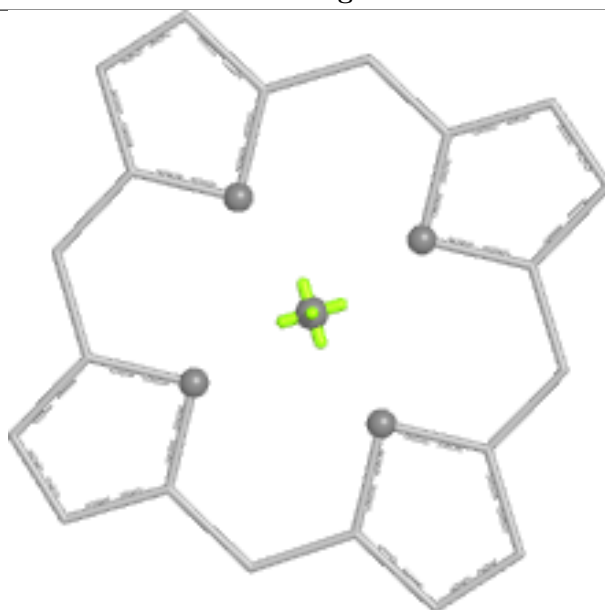
Bond lengths



Bond angles

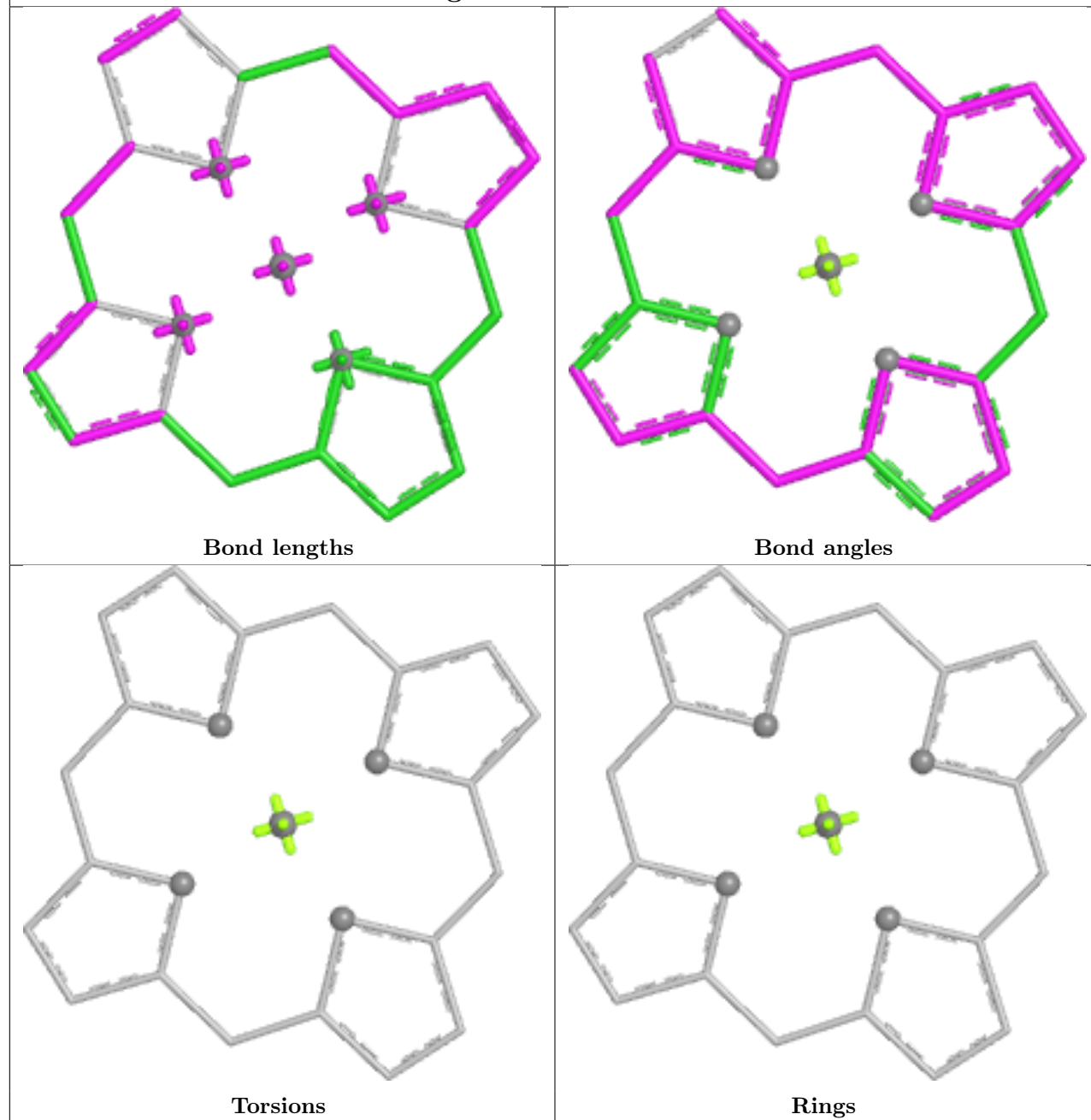


Torsions

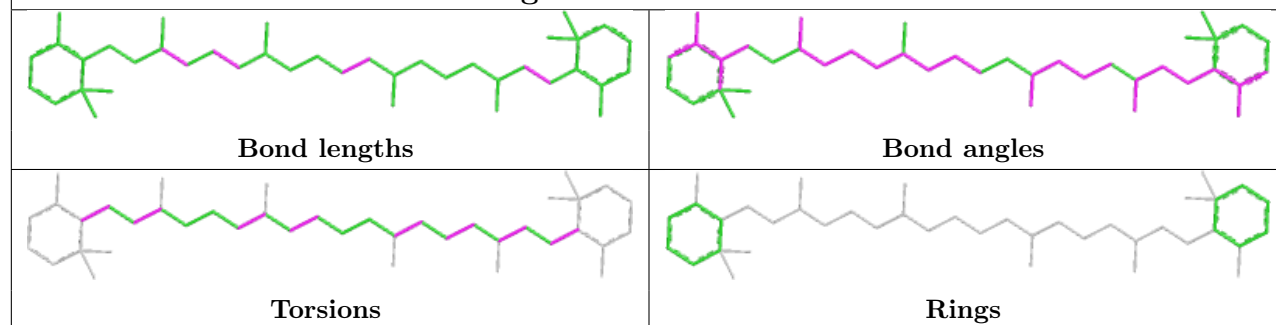


Rings

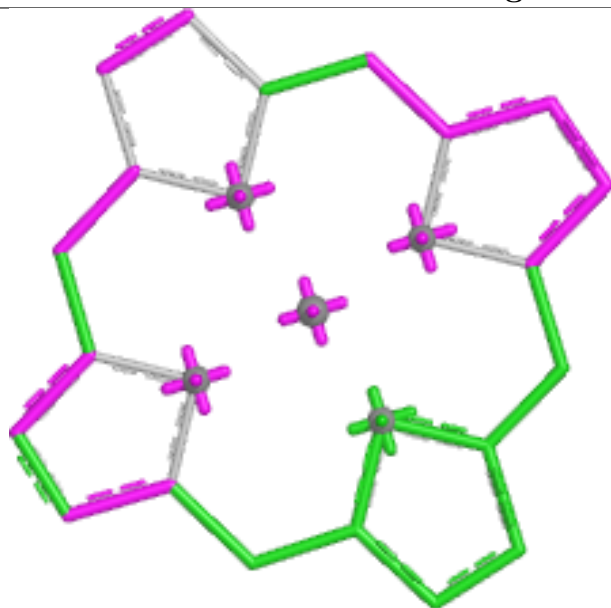
Ligand CLA A 1124



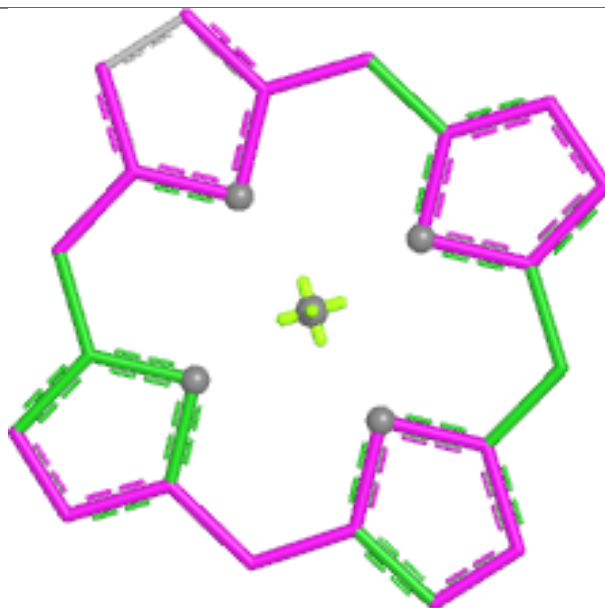
Ligand BCR A 4008



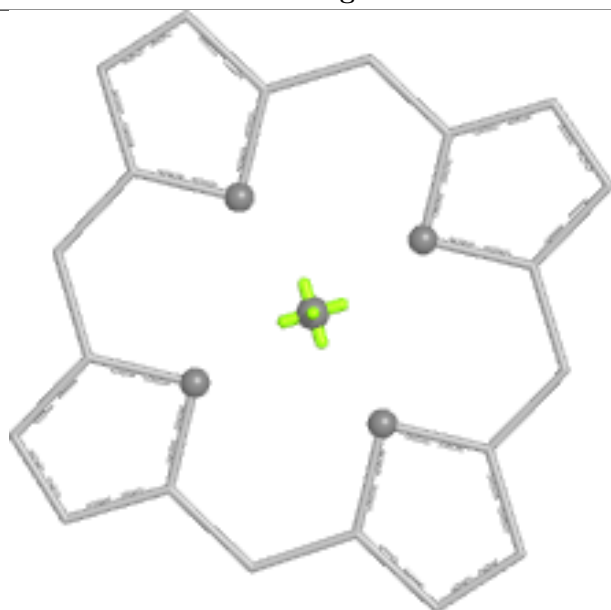
Ligand CLA B 1217



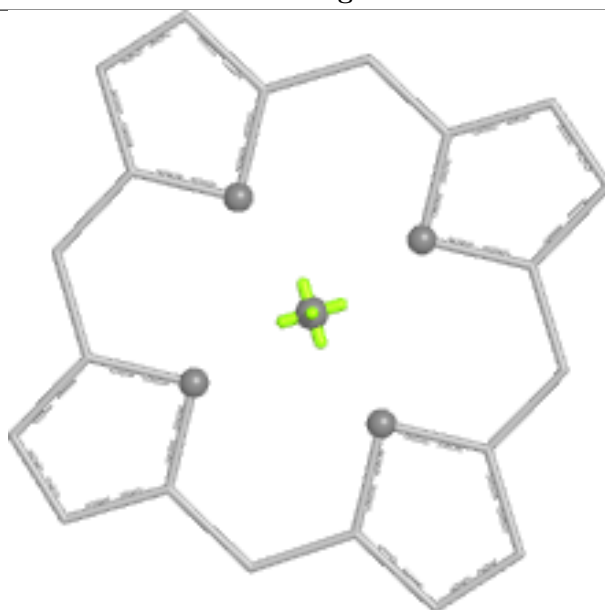
Bond lengths



Bond angles

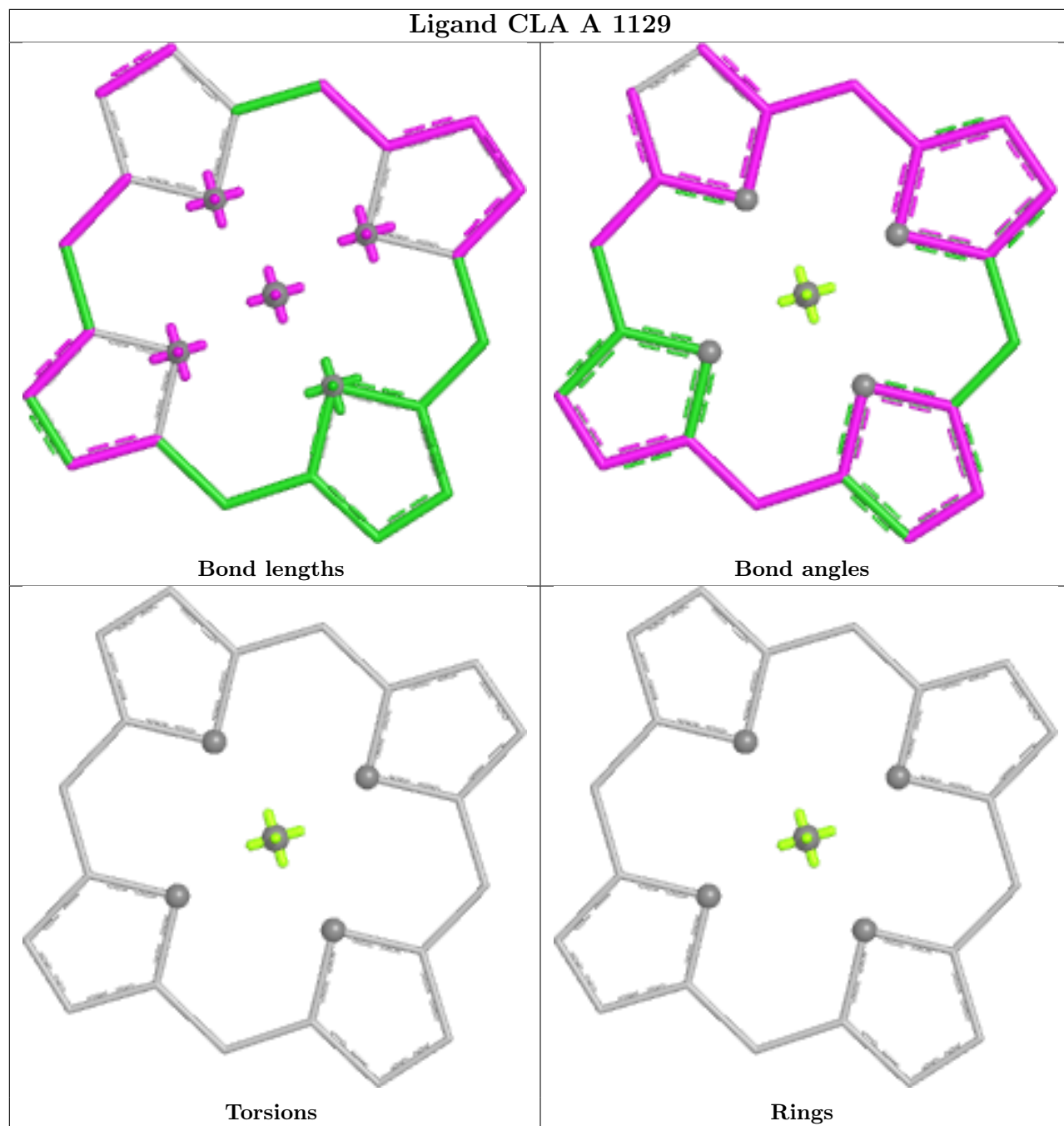


Torsions

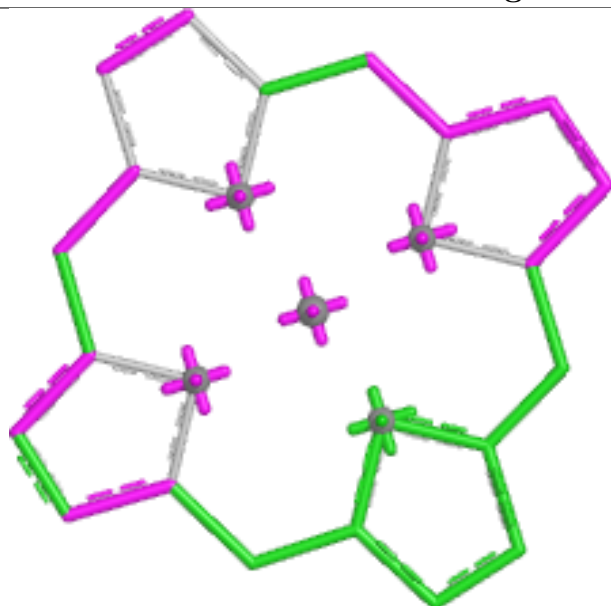


Rings

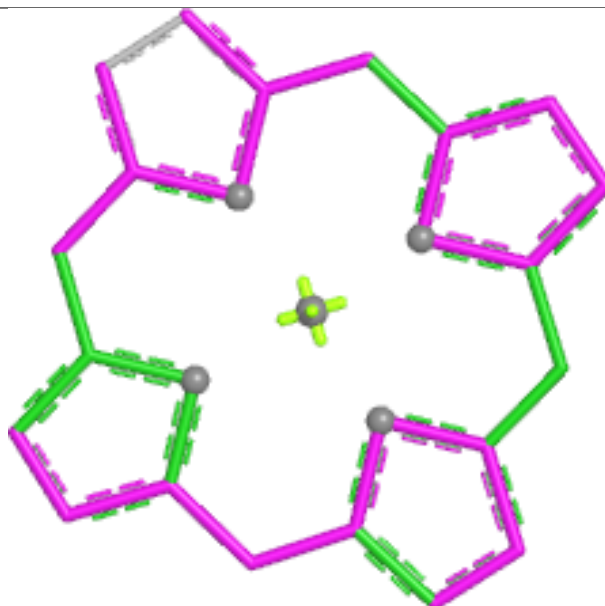
Ligand CLA A 1129



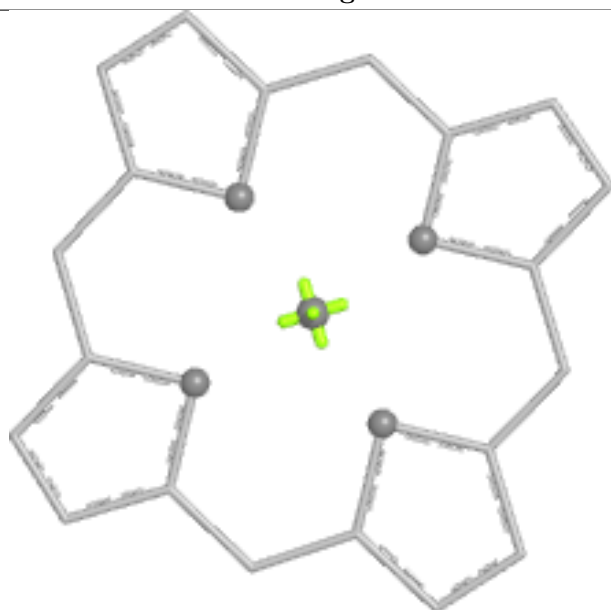
Ligand CLA A 1120



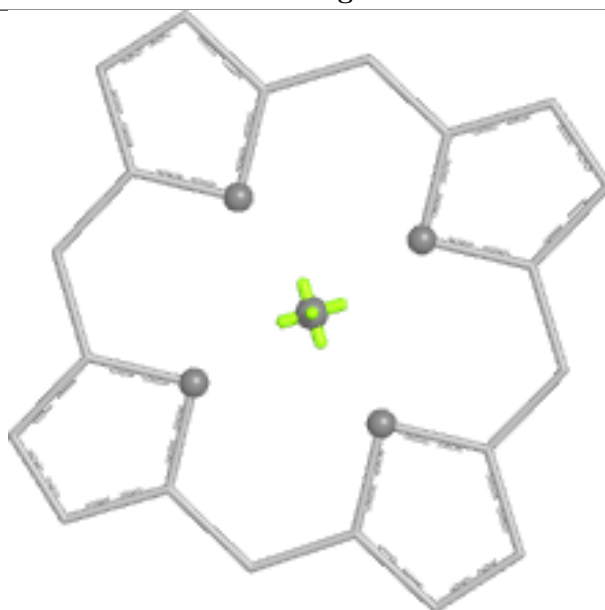
Bond lengths



Bond angles

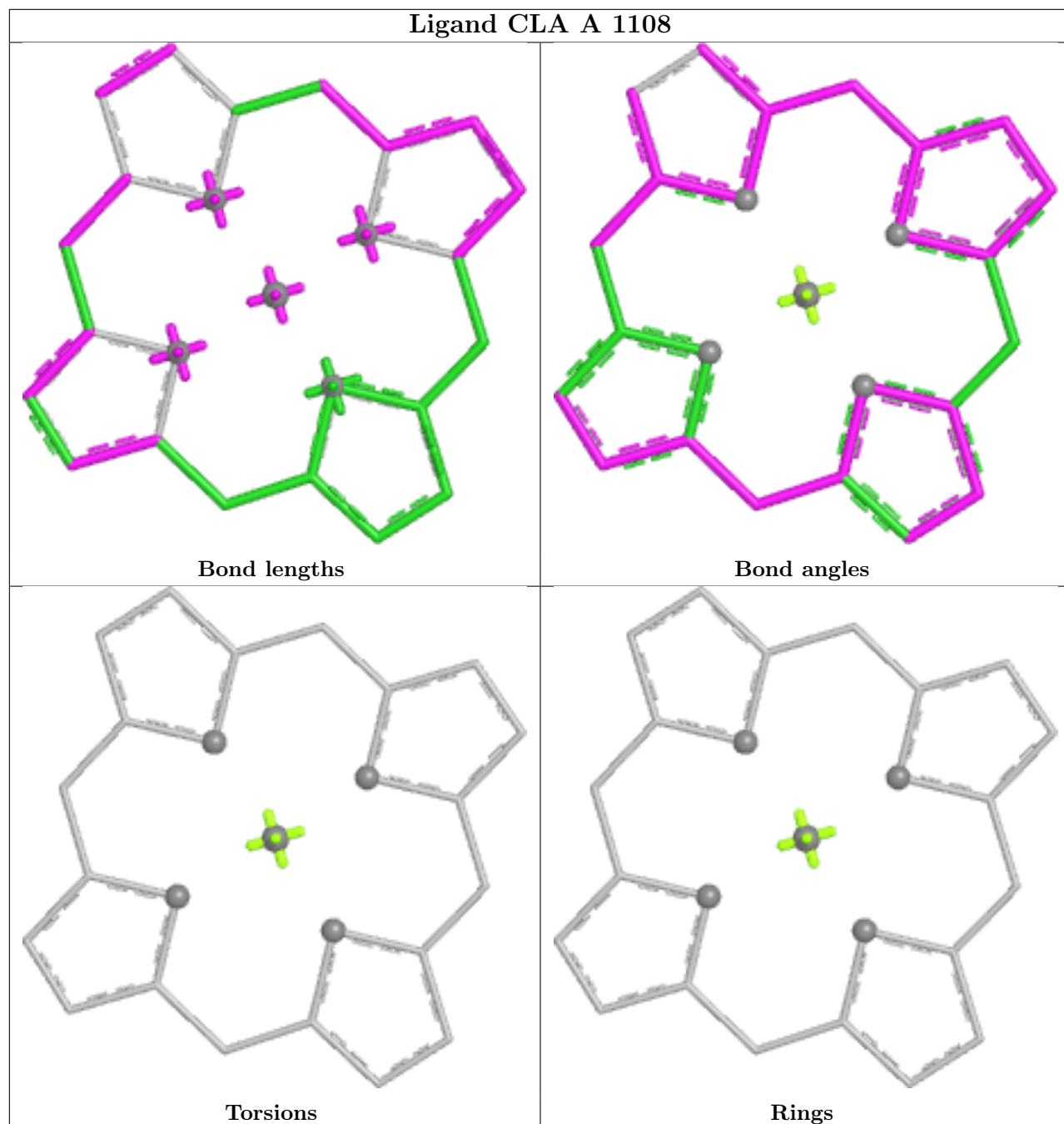


Torsions

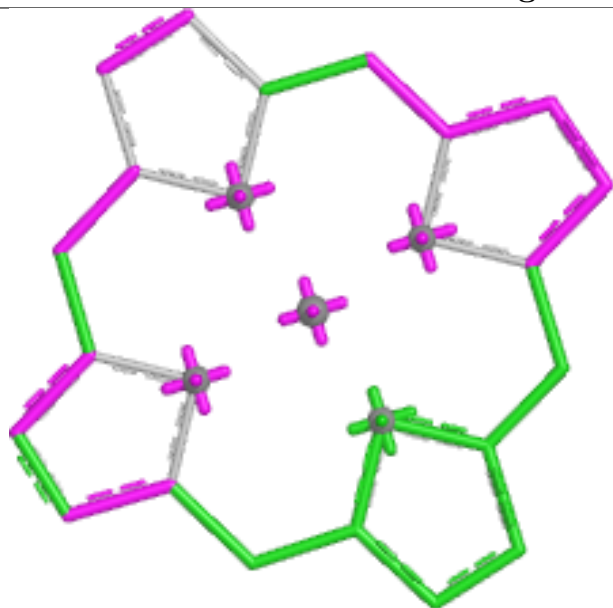


Rings

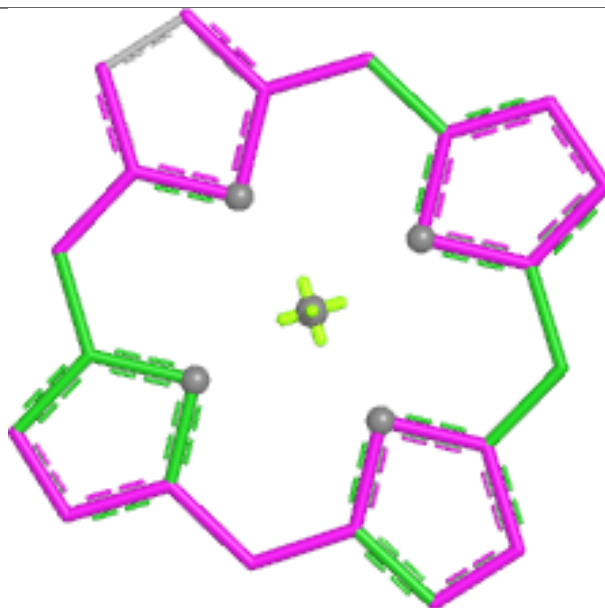
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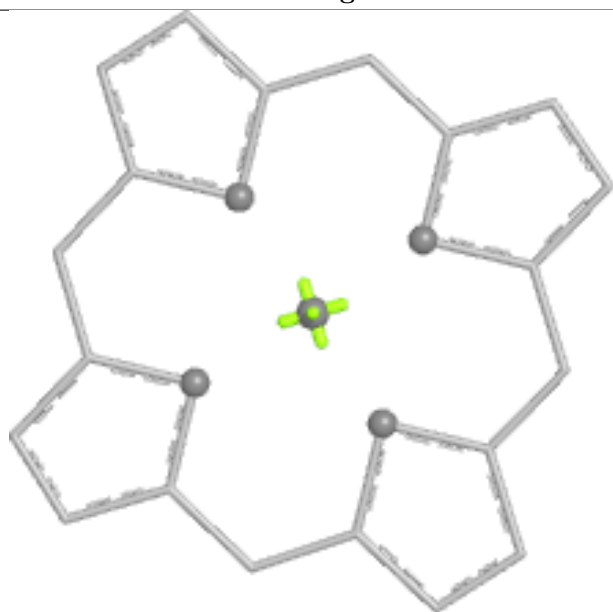
Ligand CLA 4 610



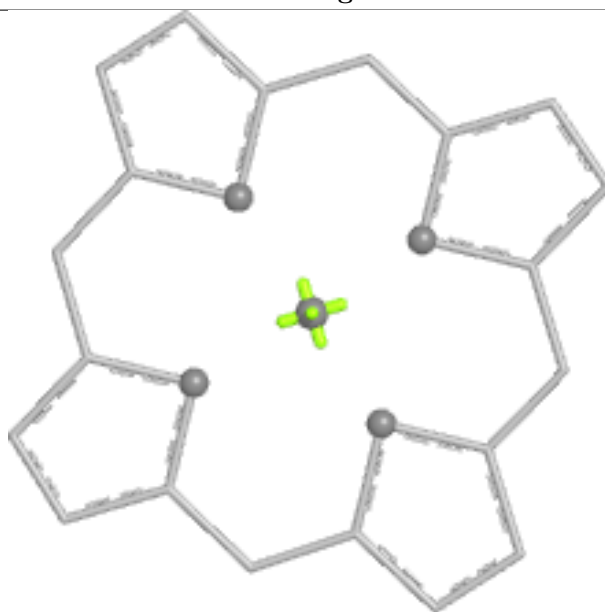
Bond lengths



Bond angles

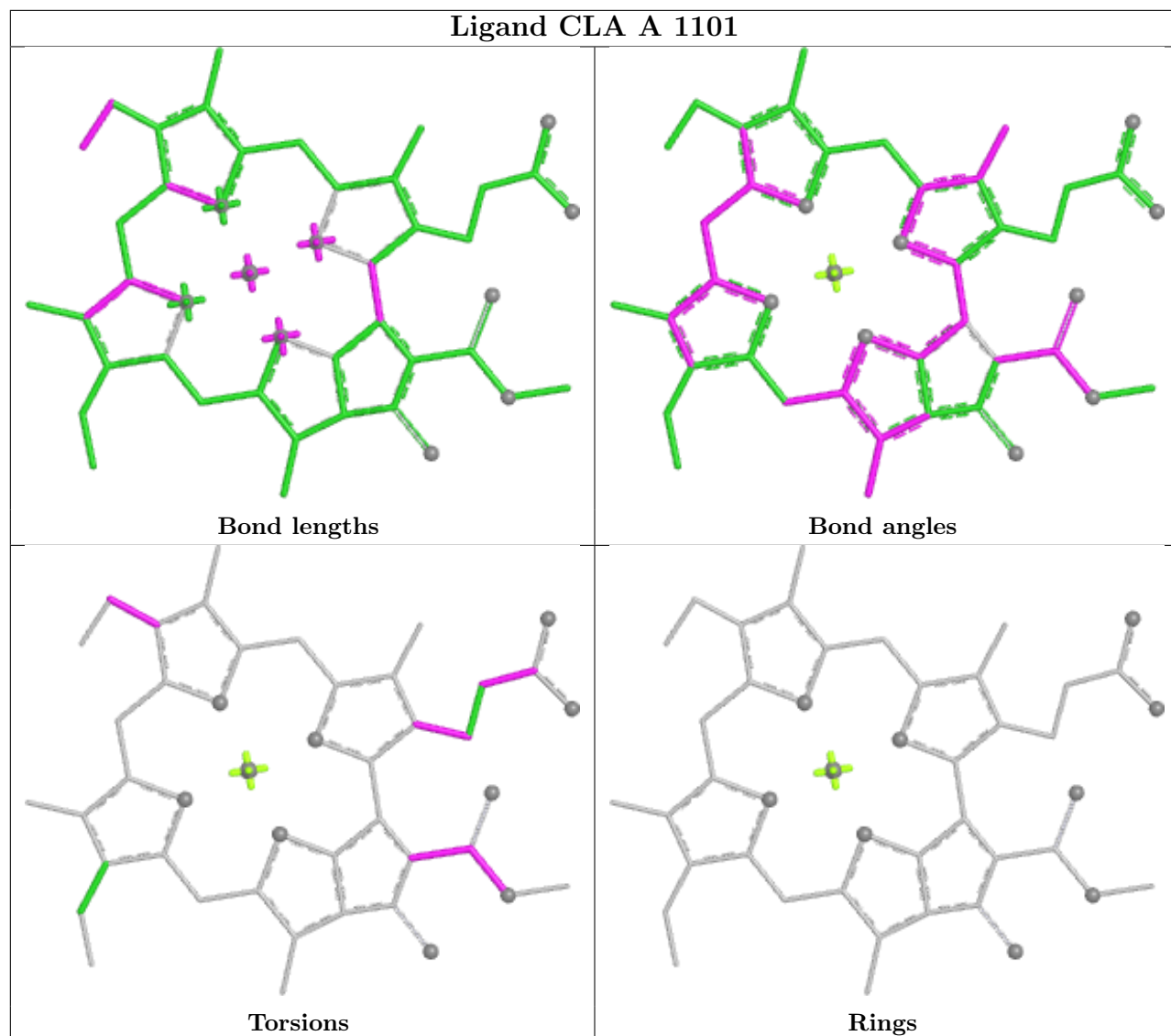


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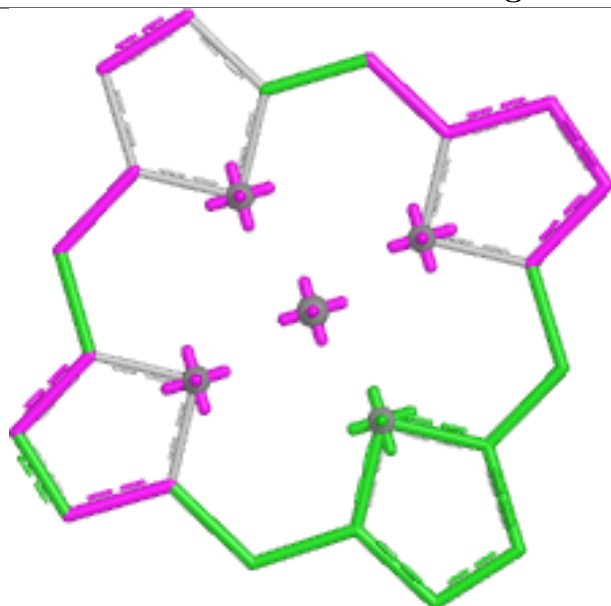


Rings

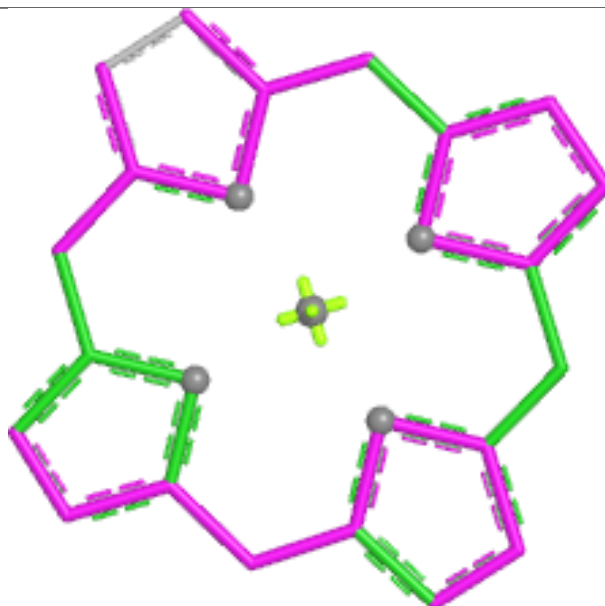
Ligand CLA A 1101



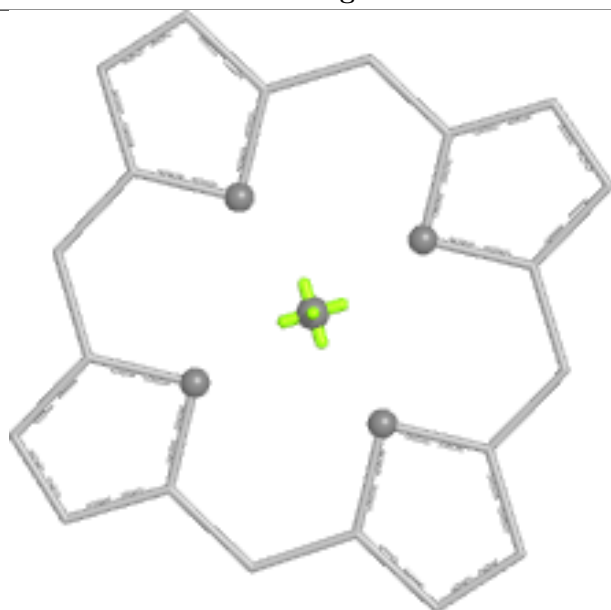
Ligand CLA A 1122



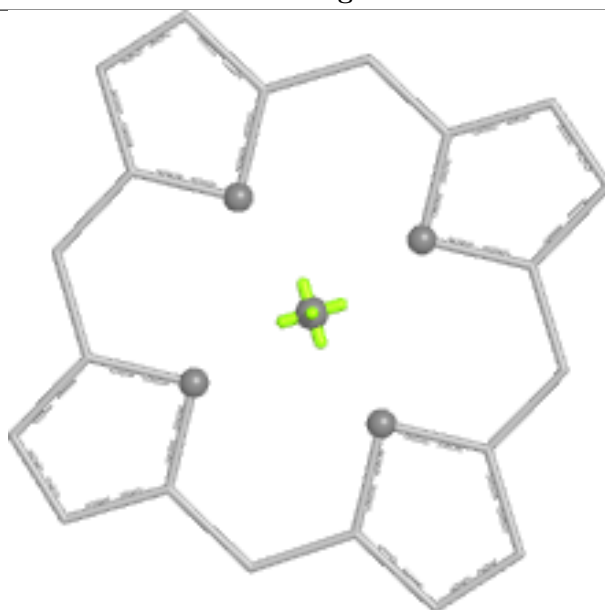
Bond lengths



Bond angles

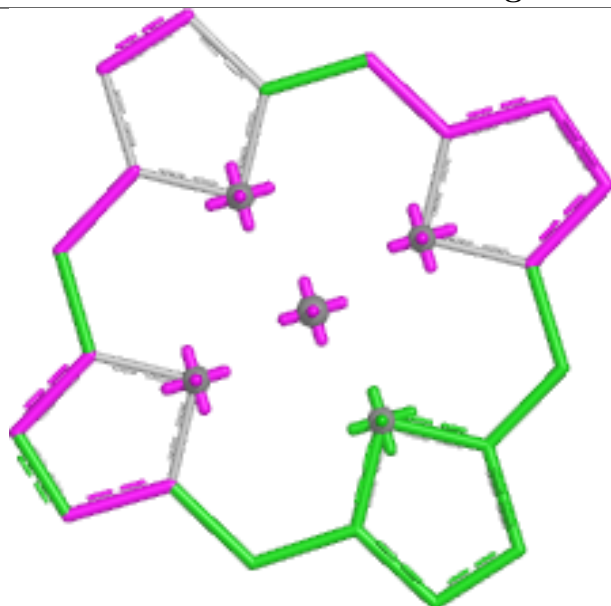


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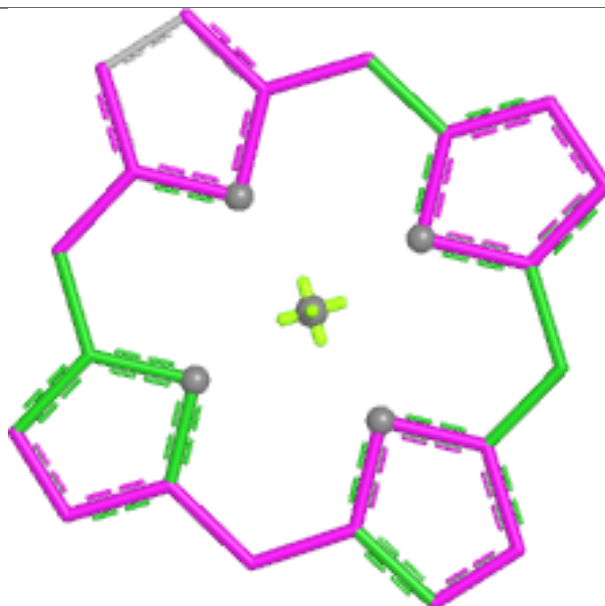


Rings

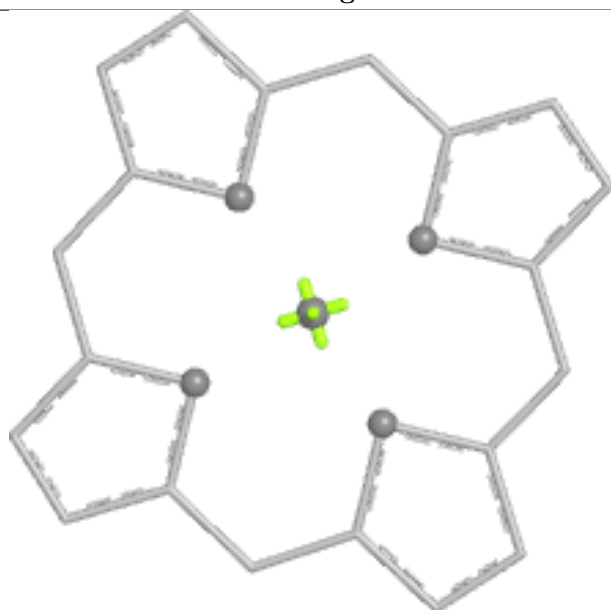
Ligand CLA A 1140



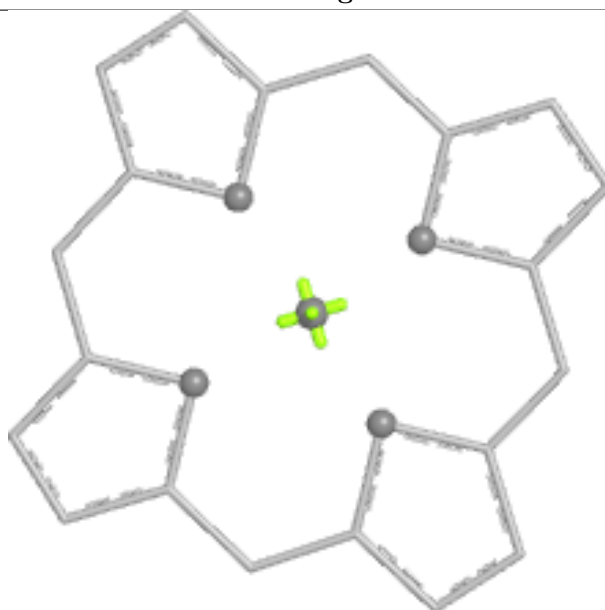
Bond lengths



Bond angles

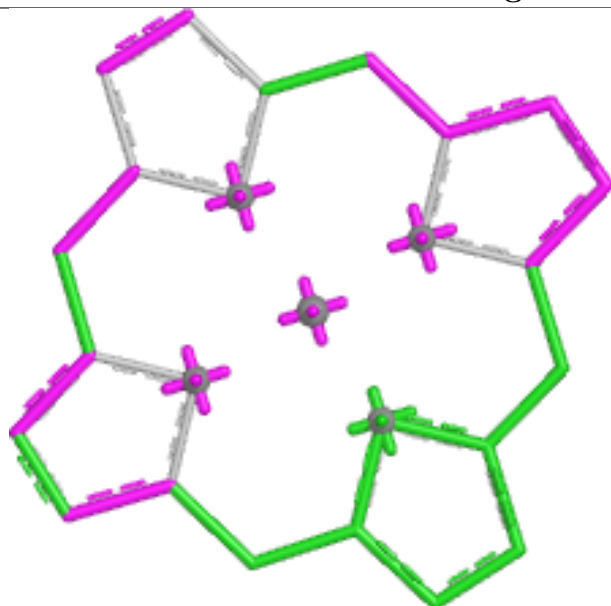


Torsions

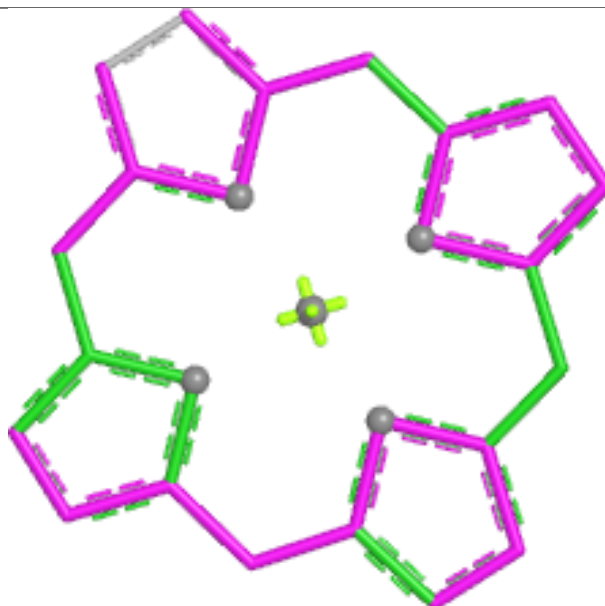


Rings

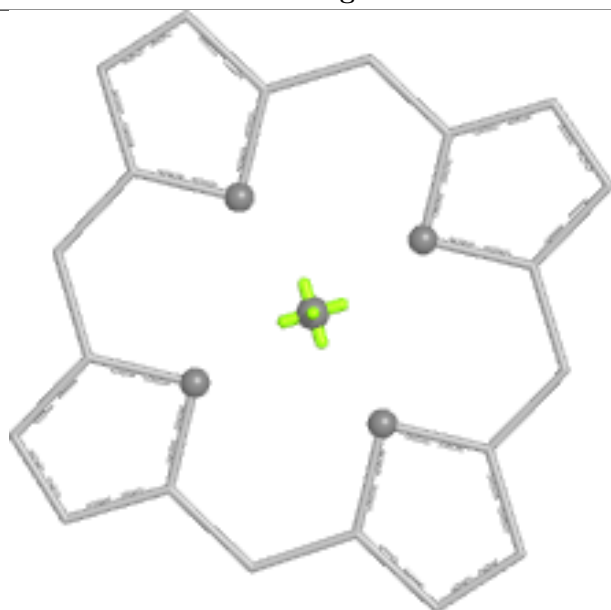
Ligand CLA O 1602



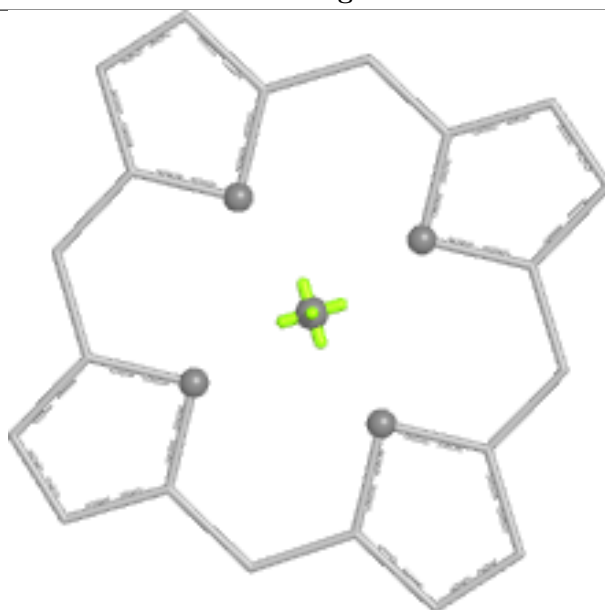
Bond lengths



Bond angles

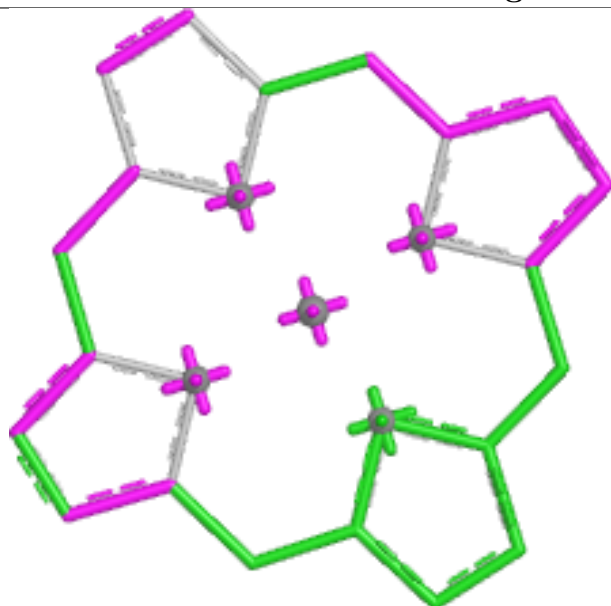


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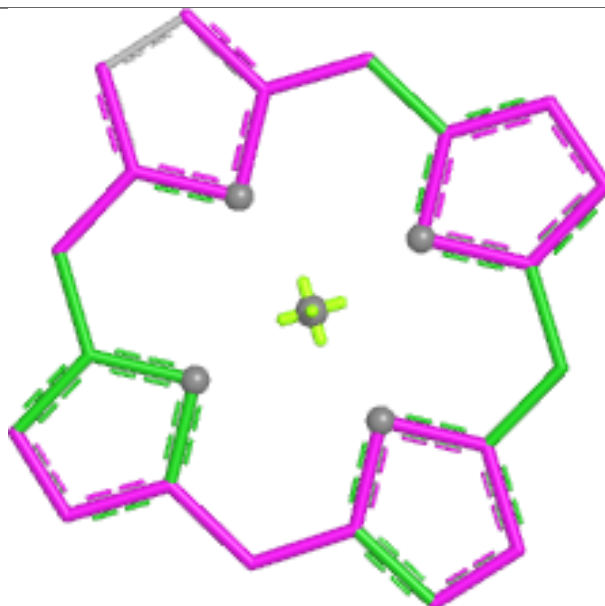


Rings

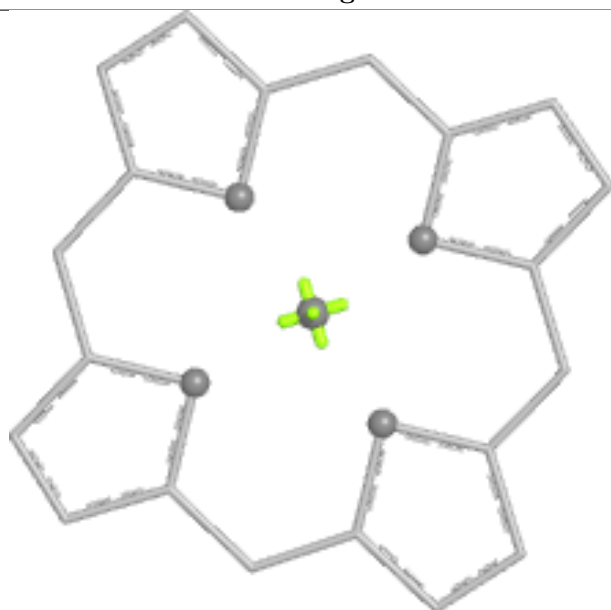
Ligand CLA B 1235



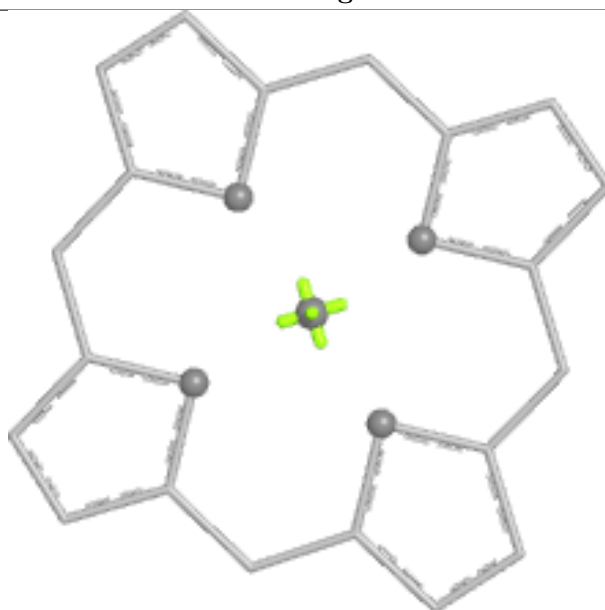
Bond lengths



Bond angles

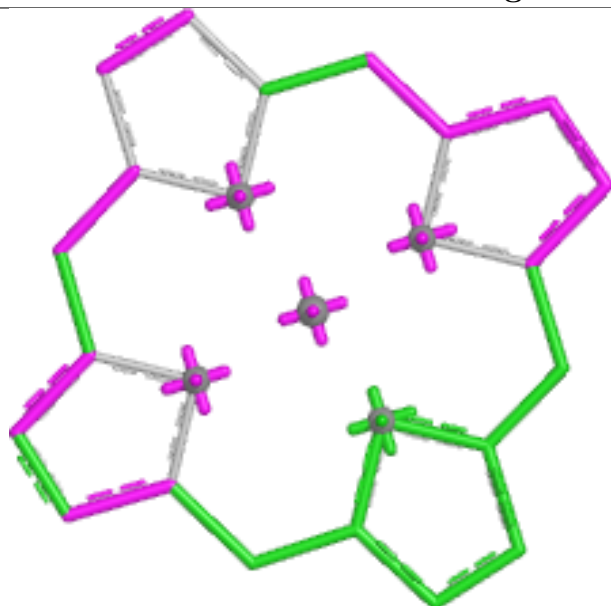


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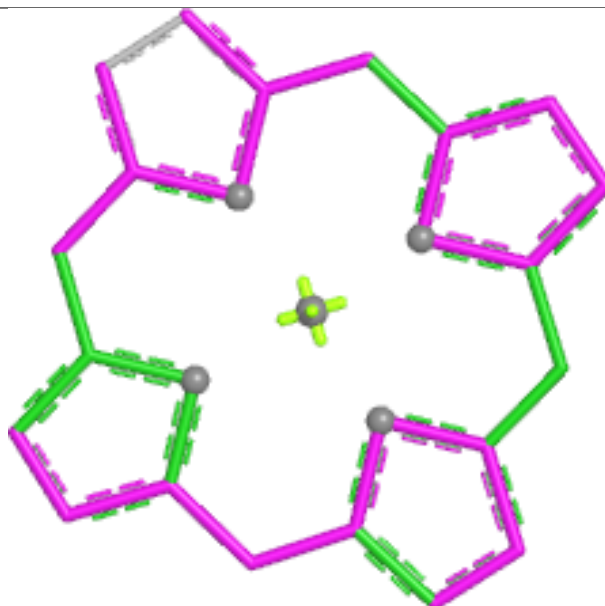


Rings

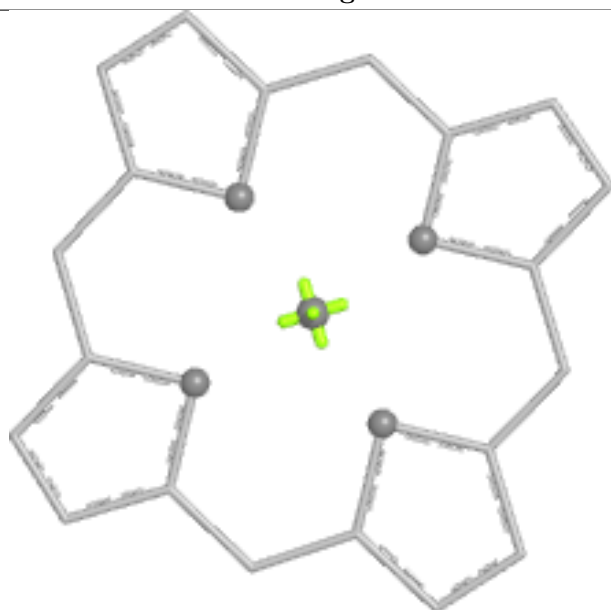
Ligand CLA A 1133



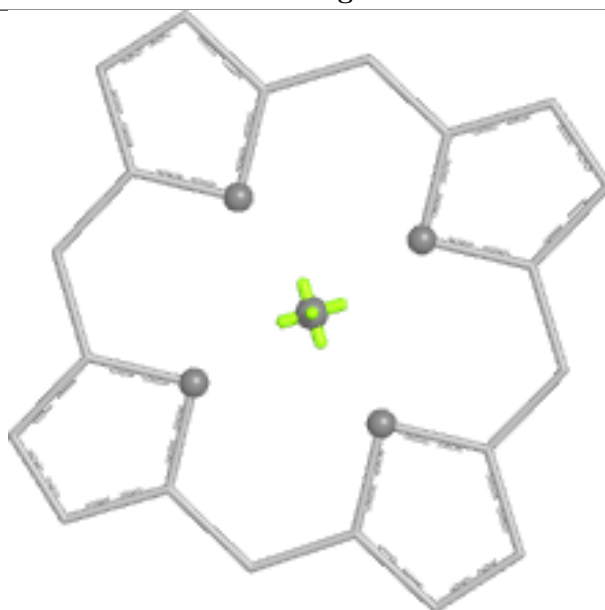
Bond lengths



Bond angles

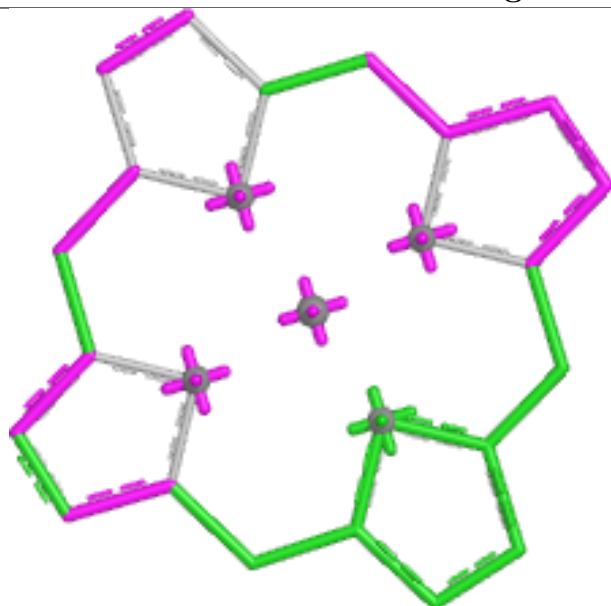


Torsions

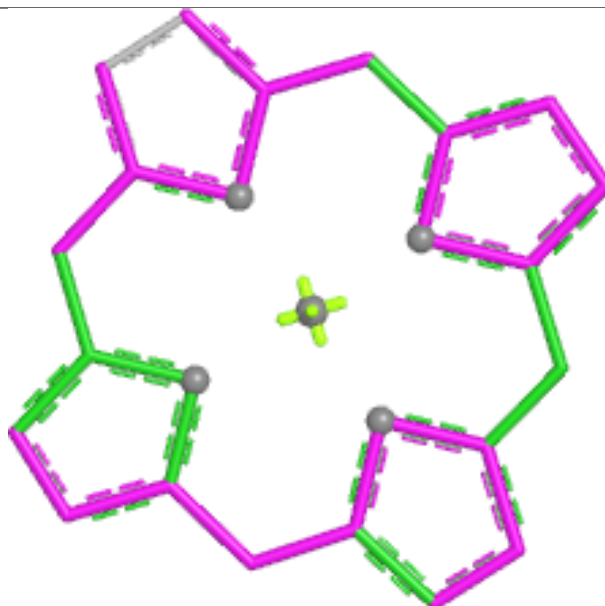


Rings

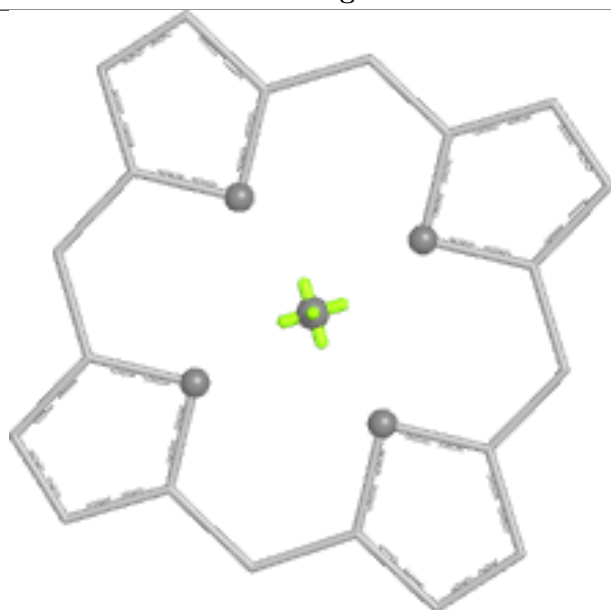
Ligand CLA A 1141



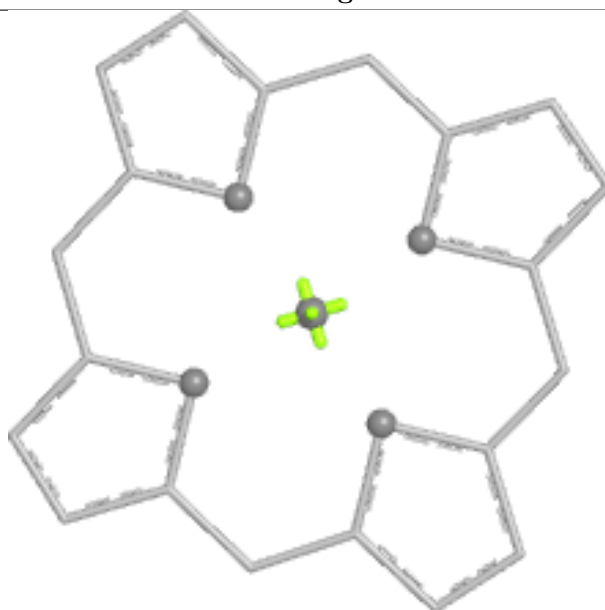
Bond lengths



Bond angles

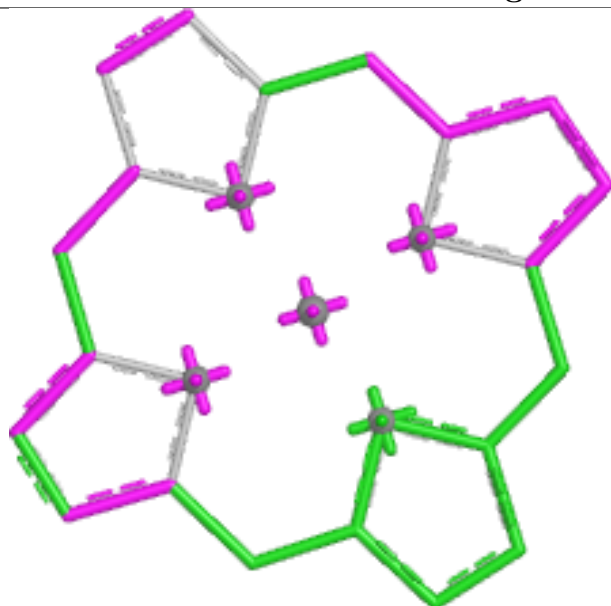


Torsions

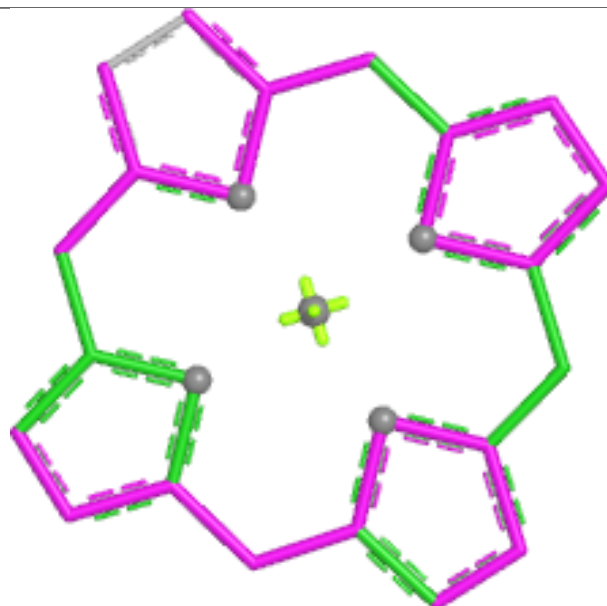


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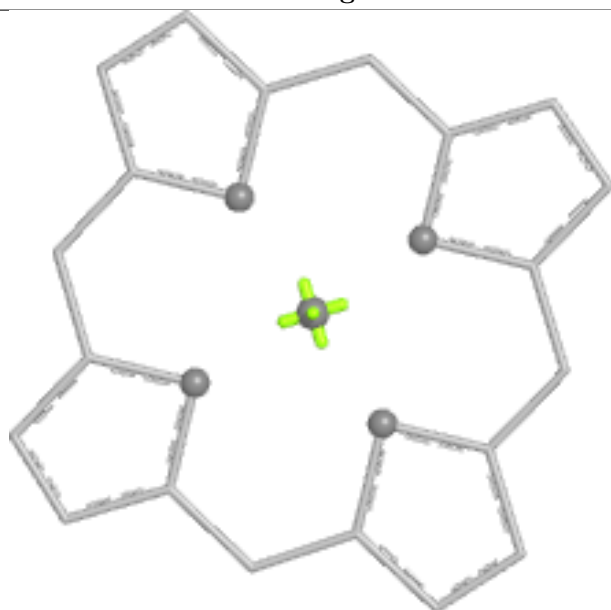
Ligand CLA B 1210



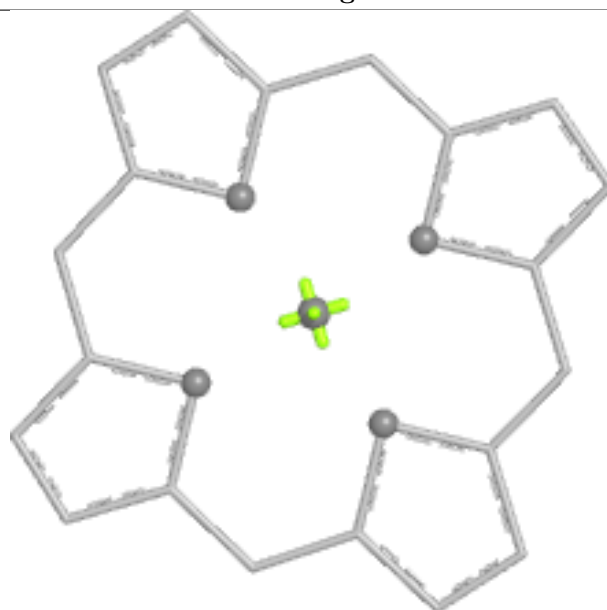
Bond lengths



Bond angles

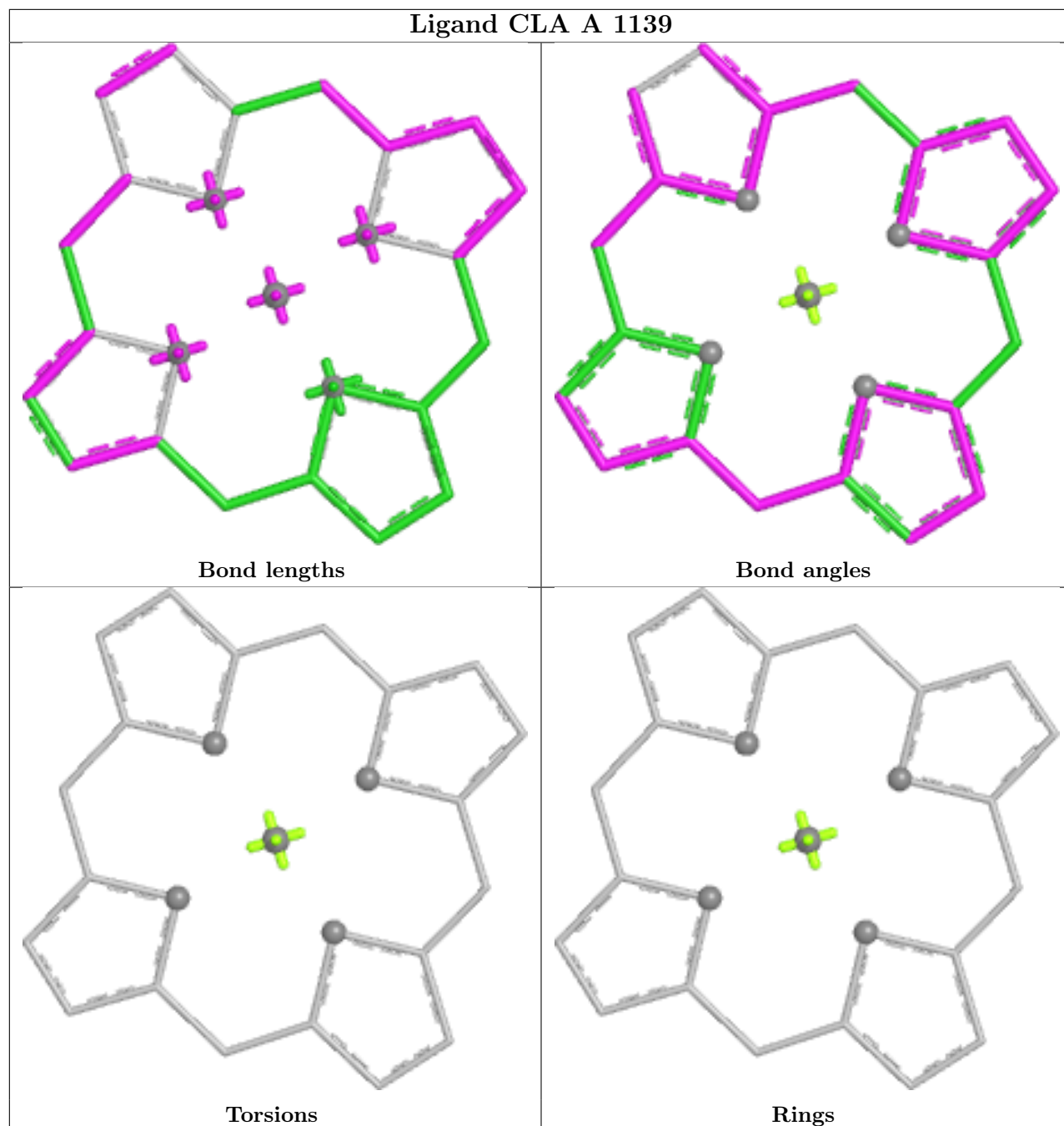


Torsions

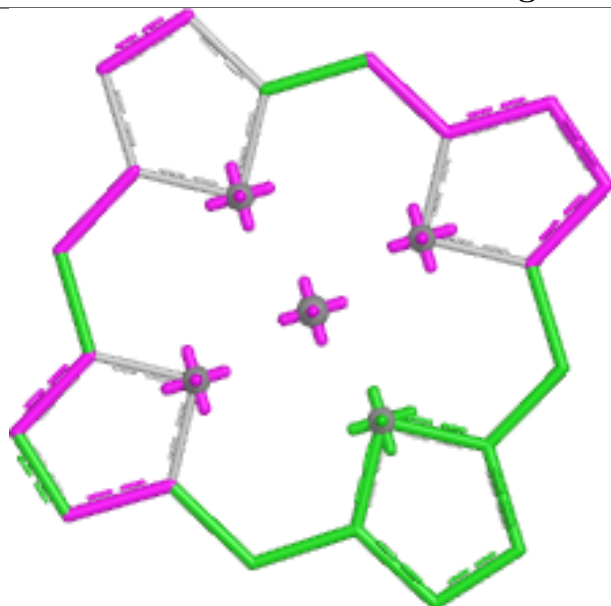


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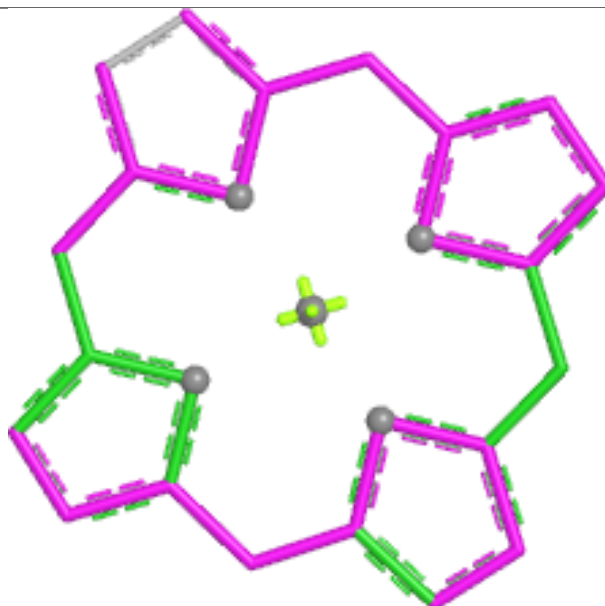
Ligand CLA A 1139



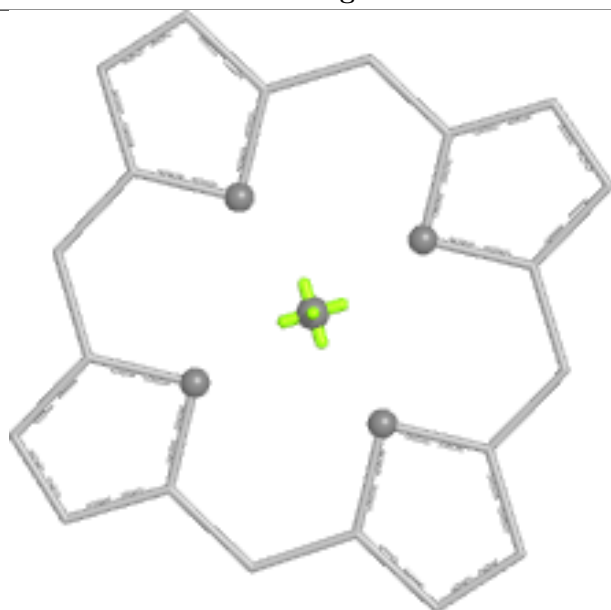
Ligand CLA 3 602



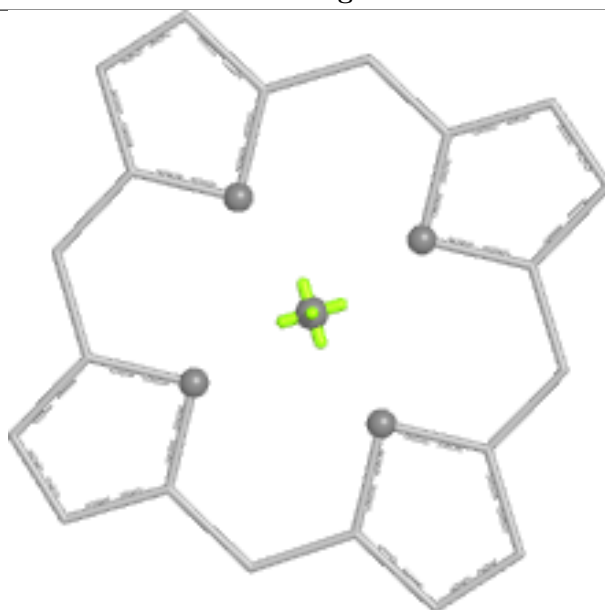
Bond lengths



Bond angles

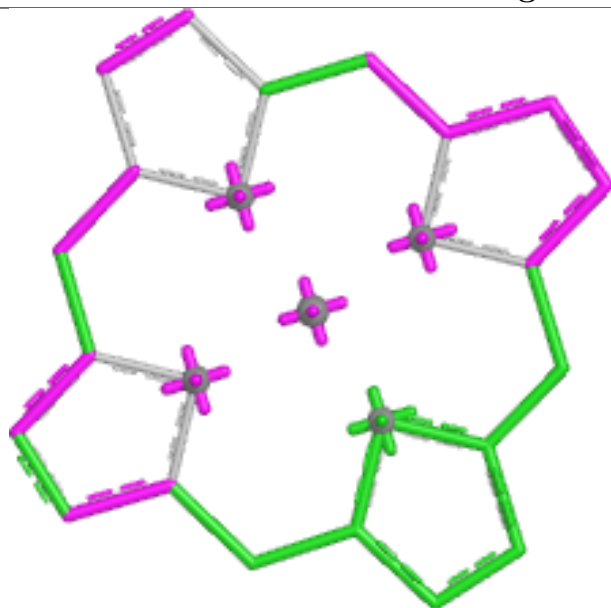


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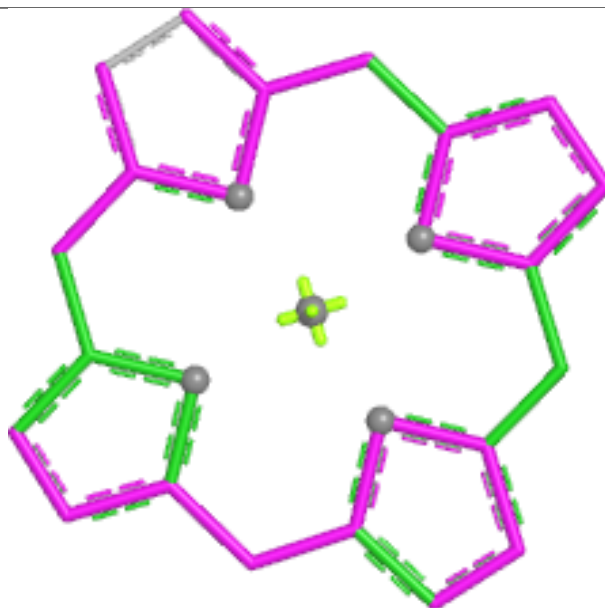


Rings

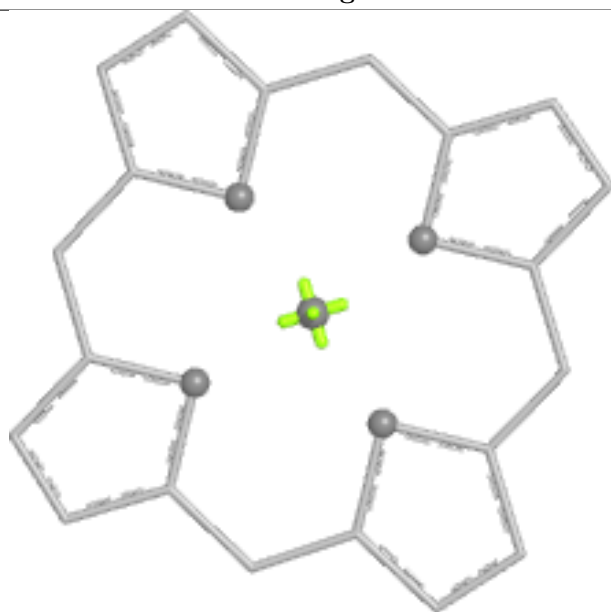
Ligand CLA 2 615



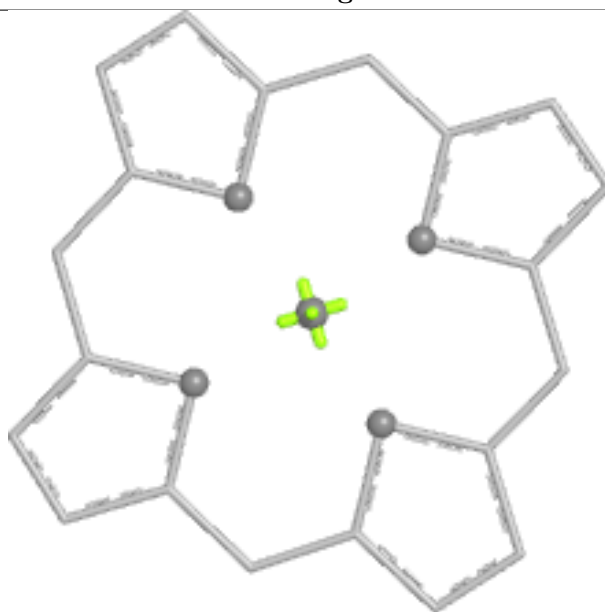
Bond lengths



Bond angles

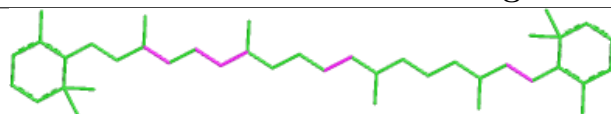


Torsions

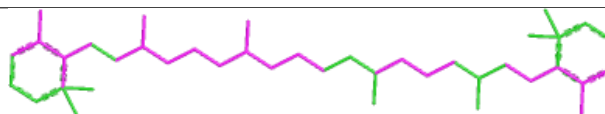


Rings

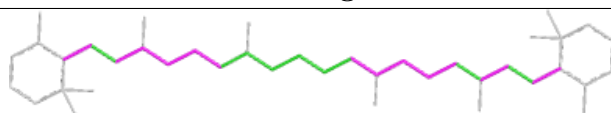
Ligand BCR A 4007



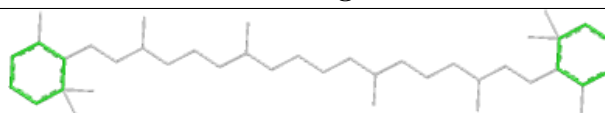
Bond lengths



Bond angles

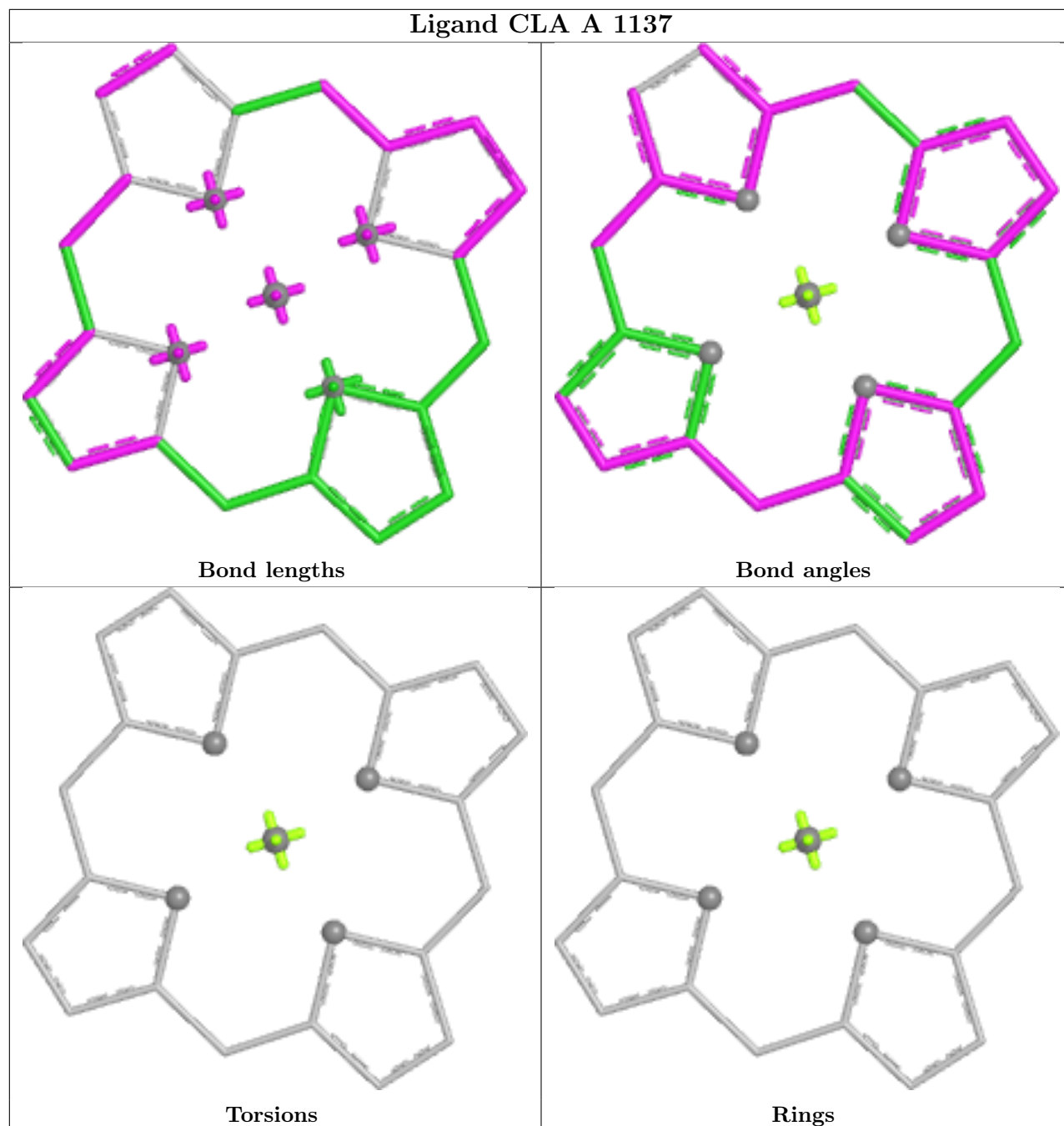


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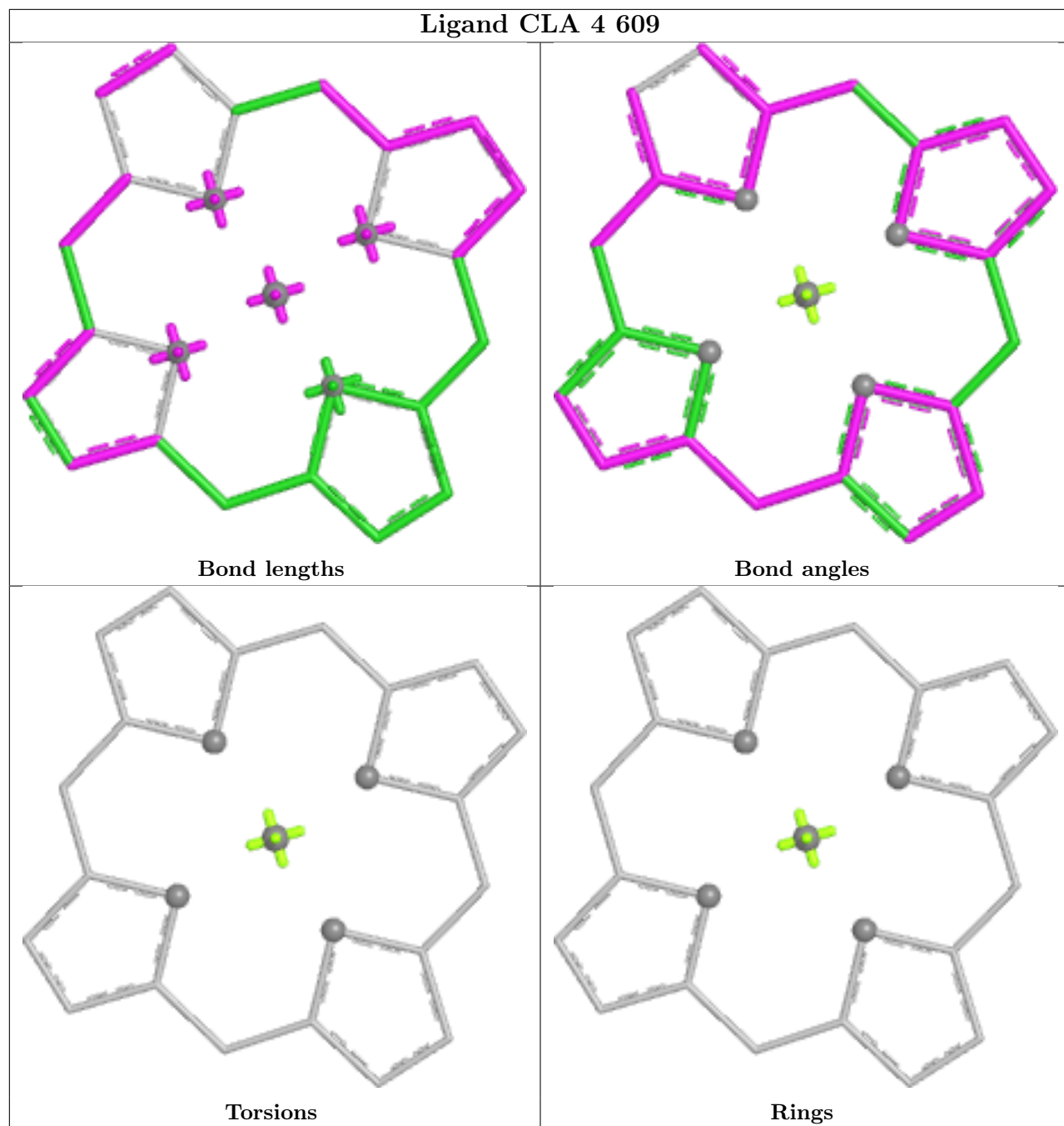


Rings

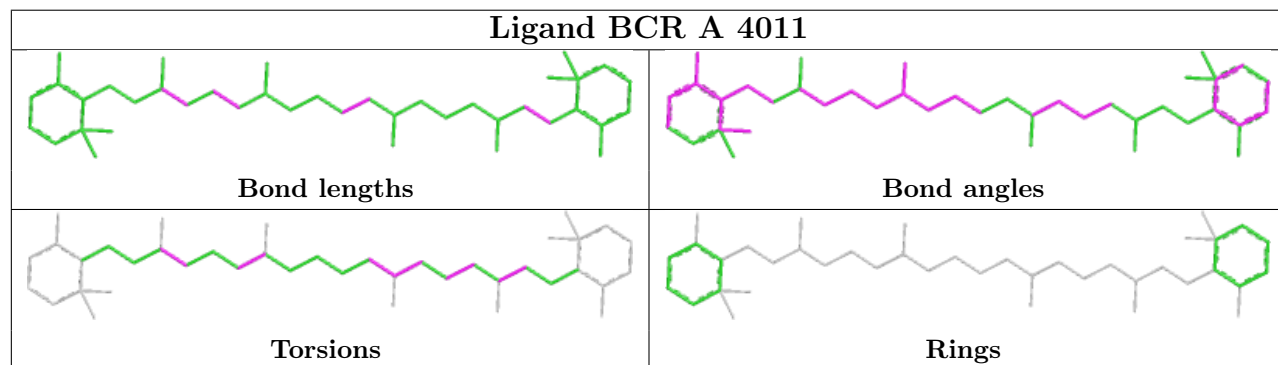
Ligand CLA A 1137



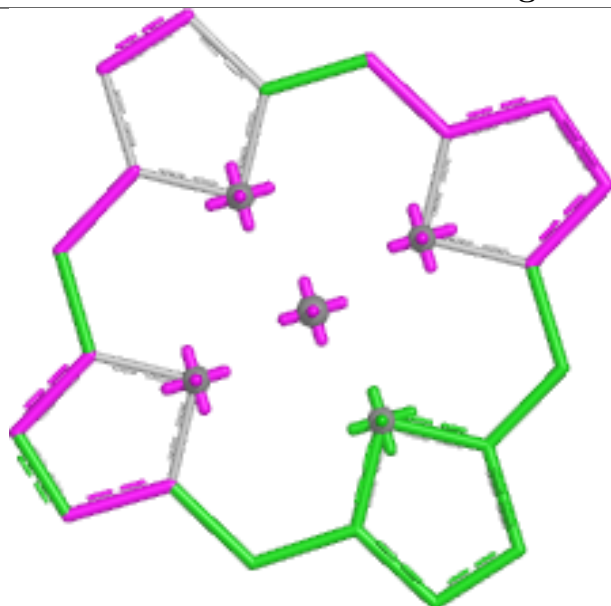
Ligand CLA 4 609



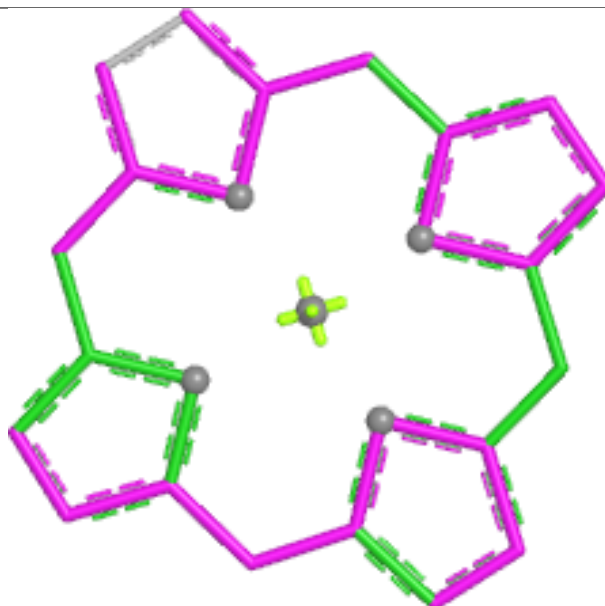
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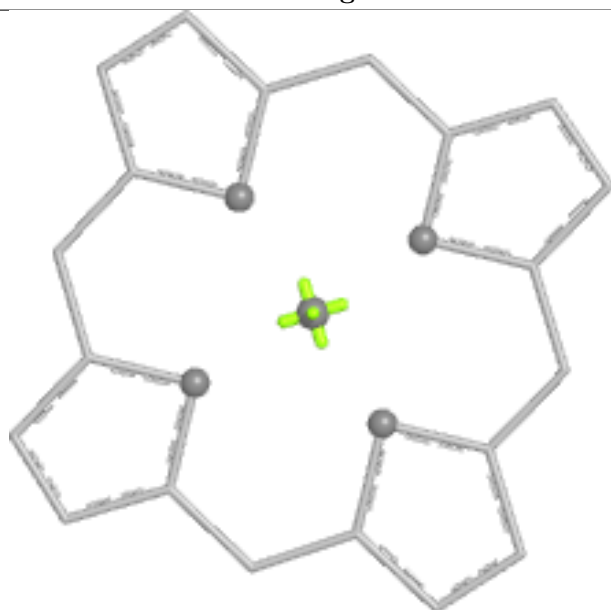
Ligand CLA 4 603



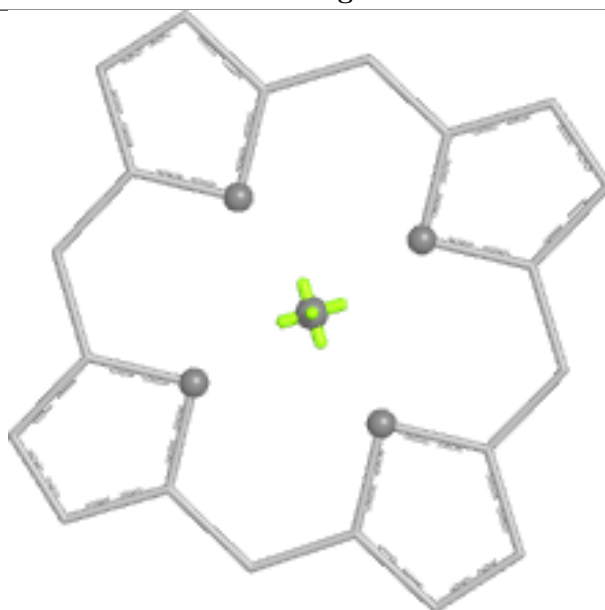
Bond lengths



Bond angles

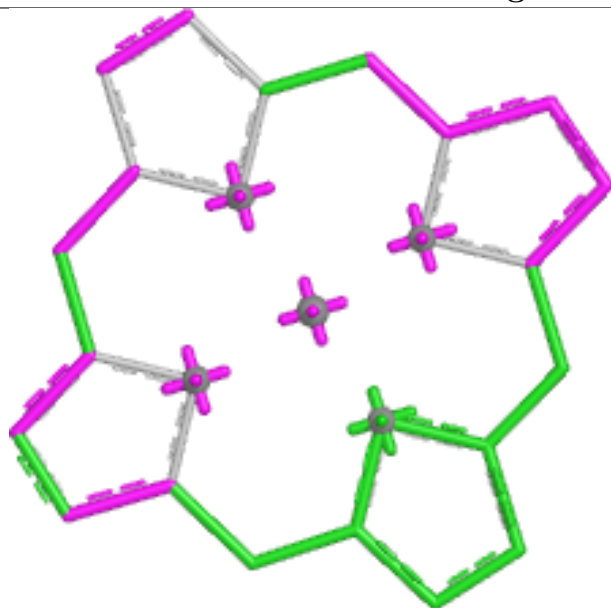


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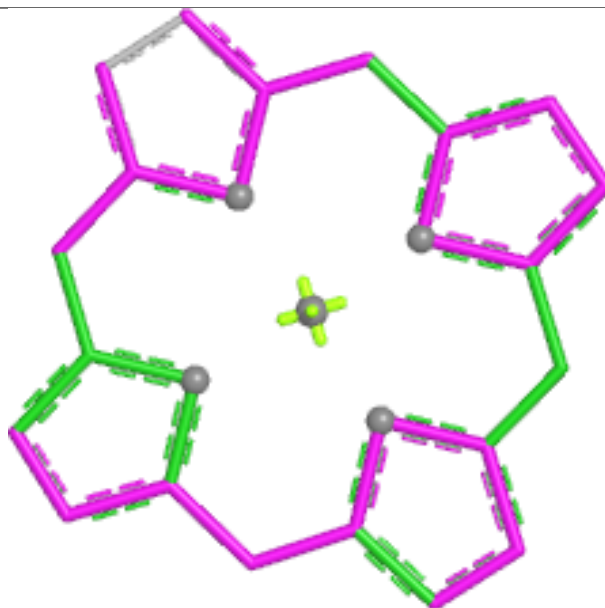


Rings

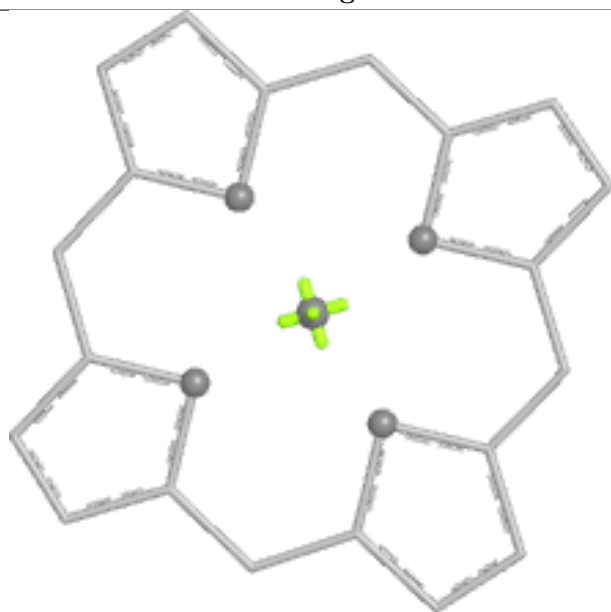
Ligand CLA L 1503



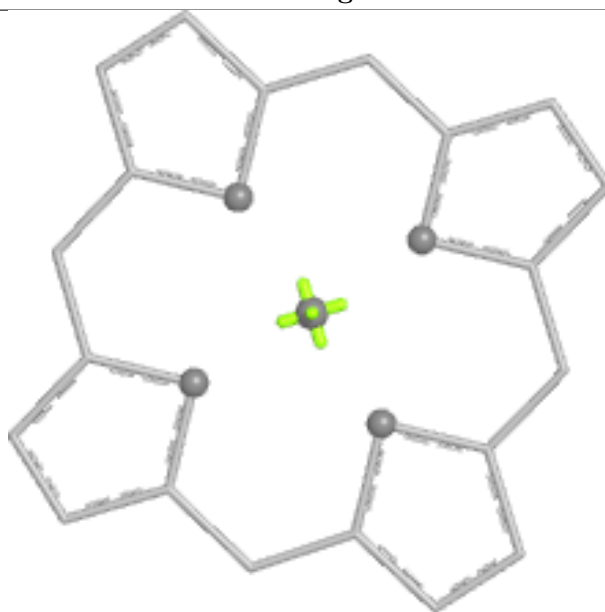
Bond lengths



Bond angles

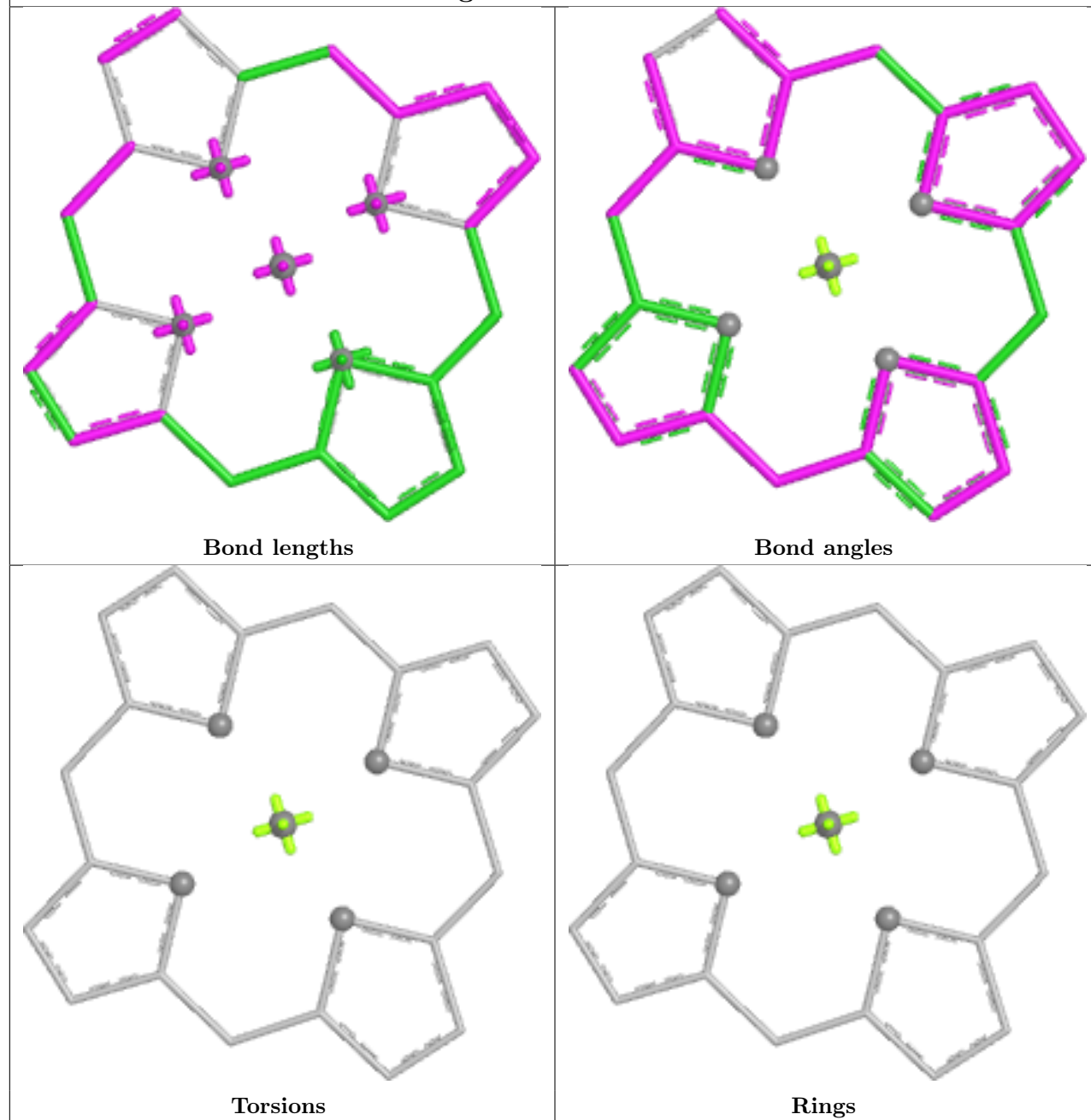


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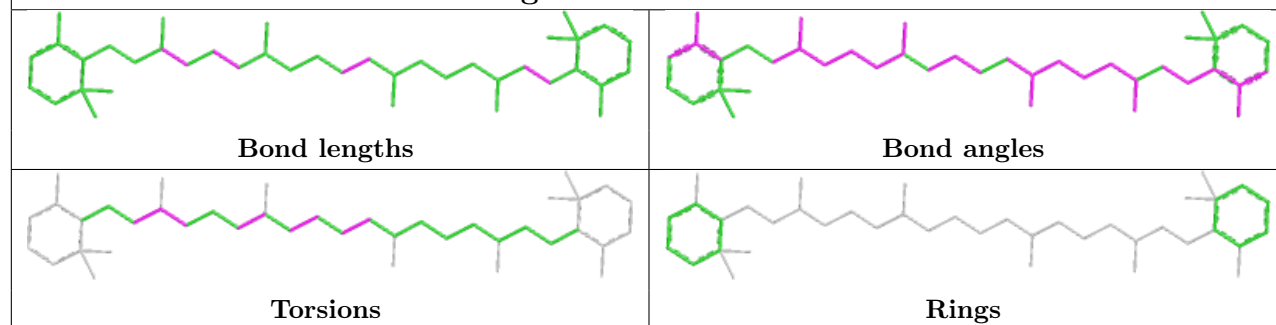


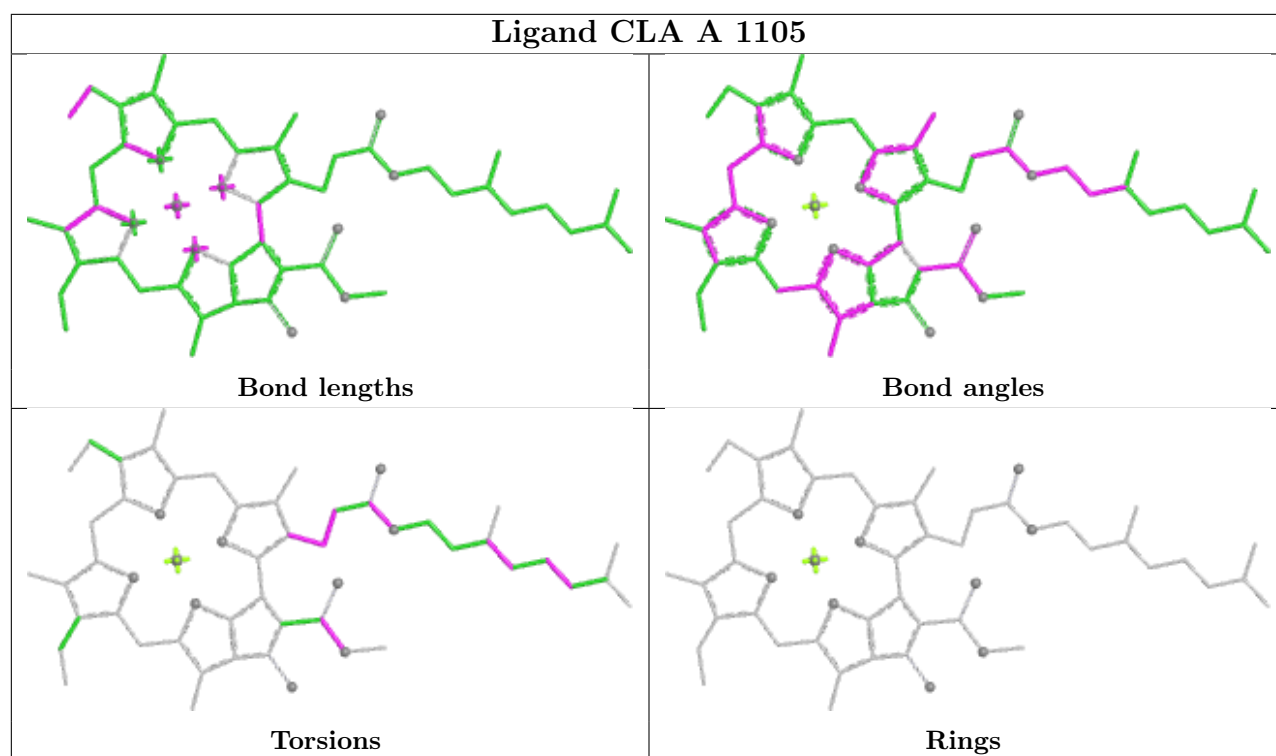
Rings

Ligand CLA 2 616

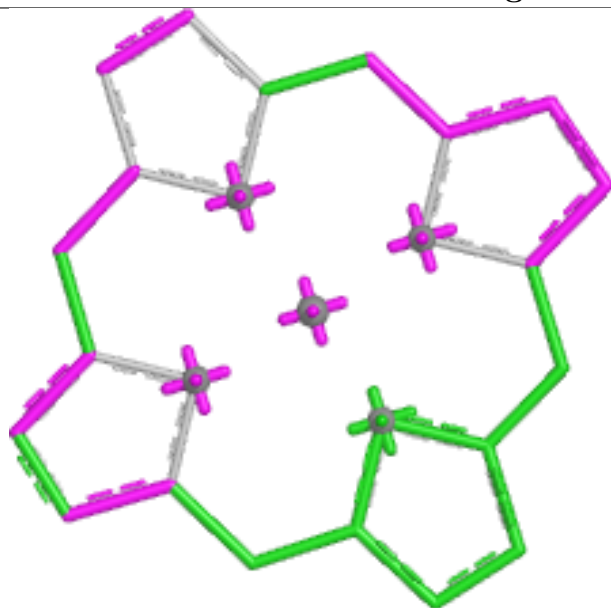


Ligand BCR A 4002

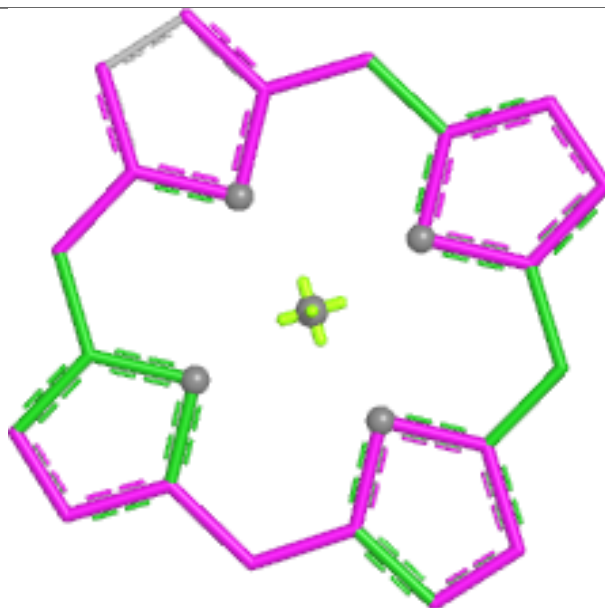




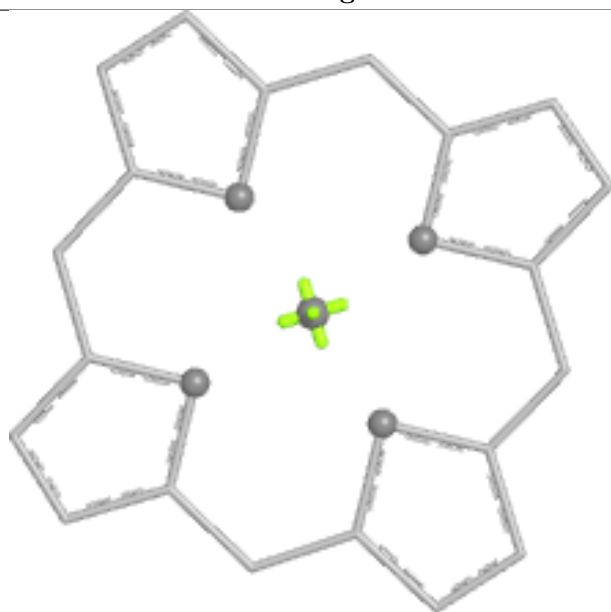
Ligand CLA B 1219



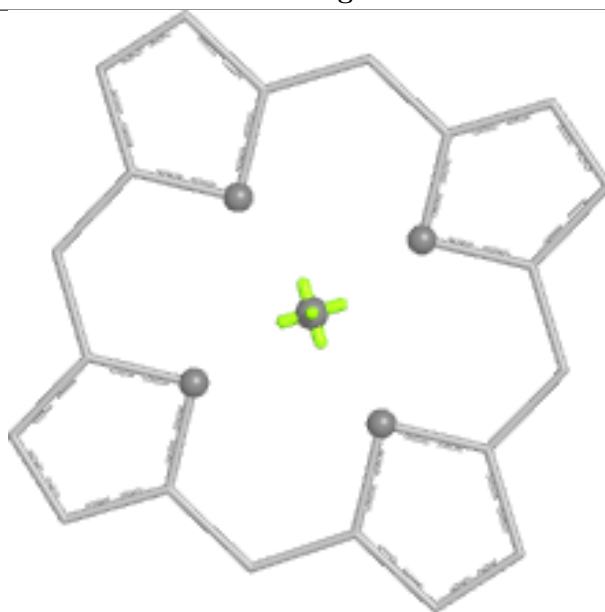
Bond lengths



Bond angles

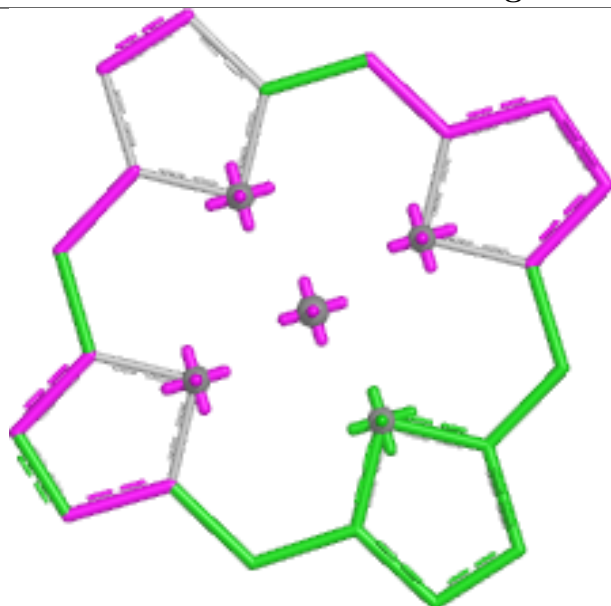


Torsions

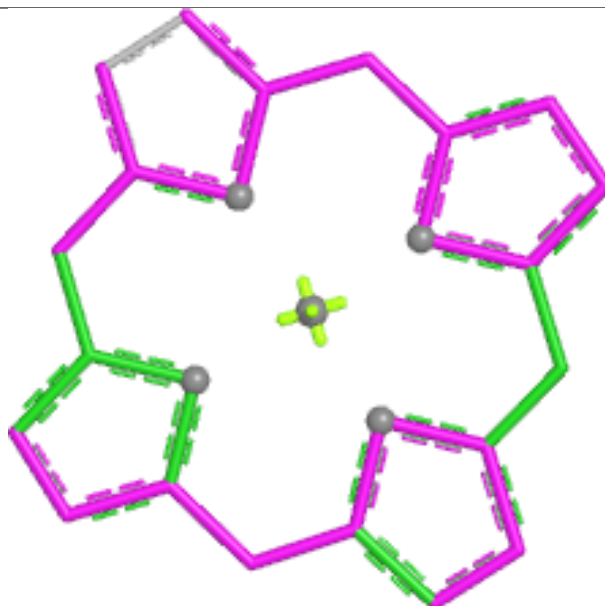


Rings

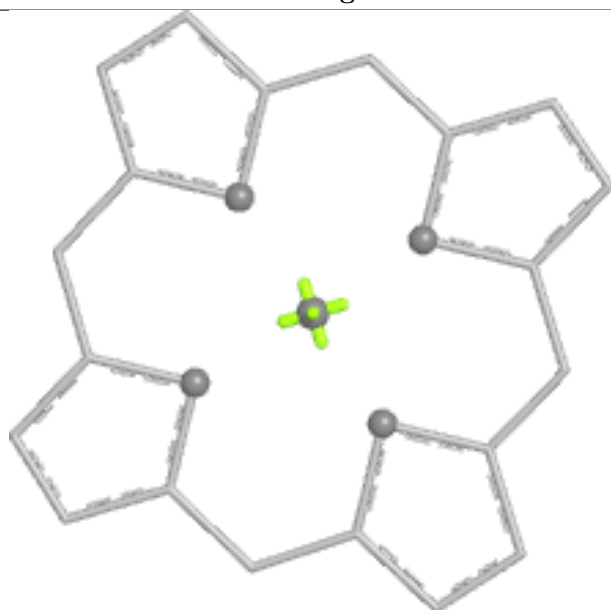
Ligand CLA A 1134



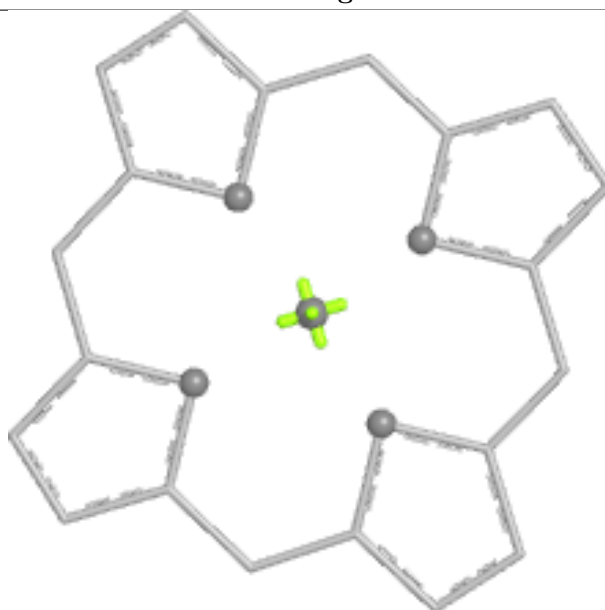
Bond lengths



Bond angles

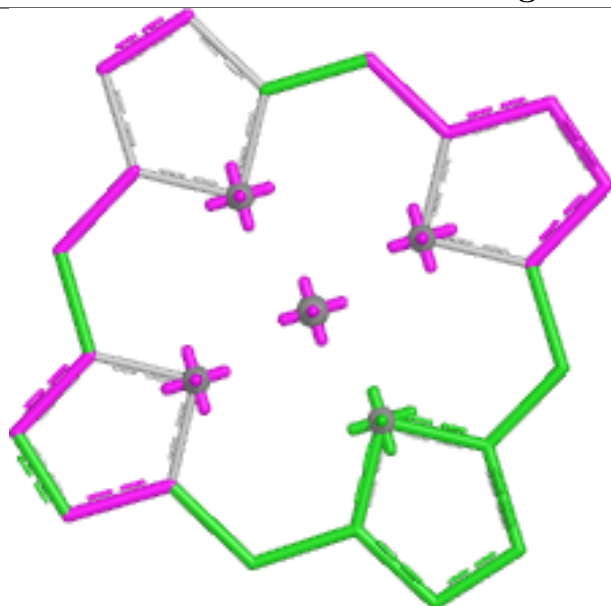


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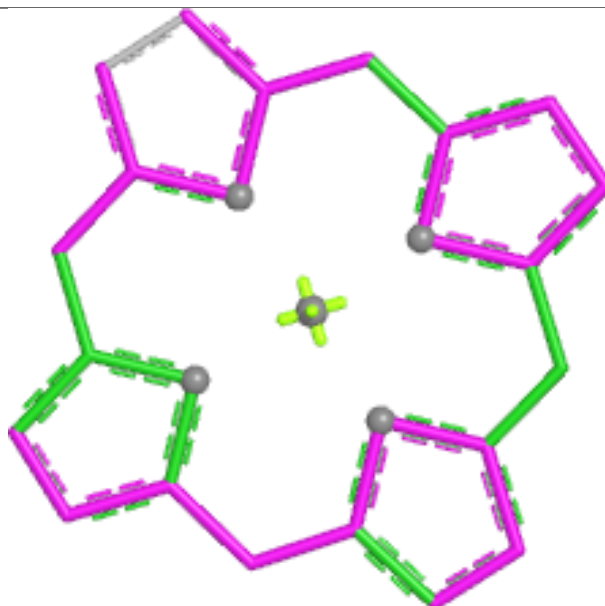


Rings

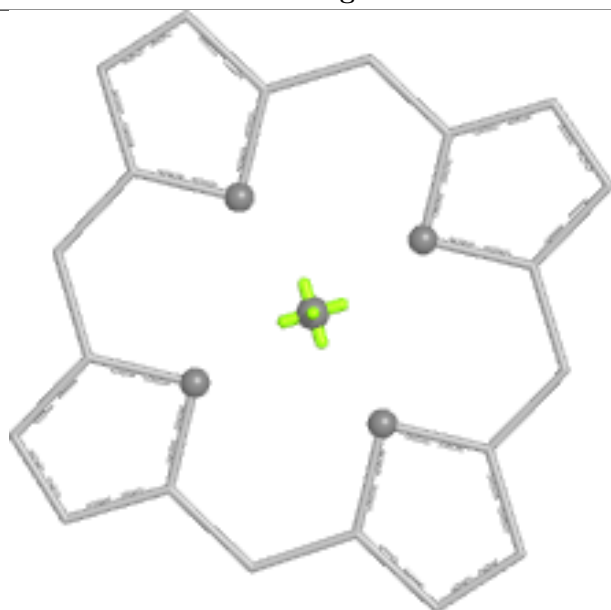
Ligand CLA 4 606



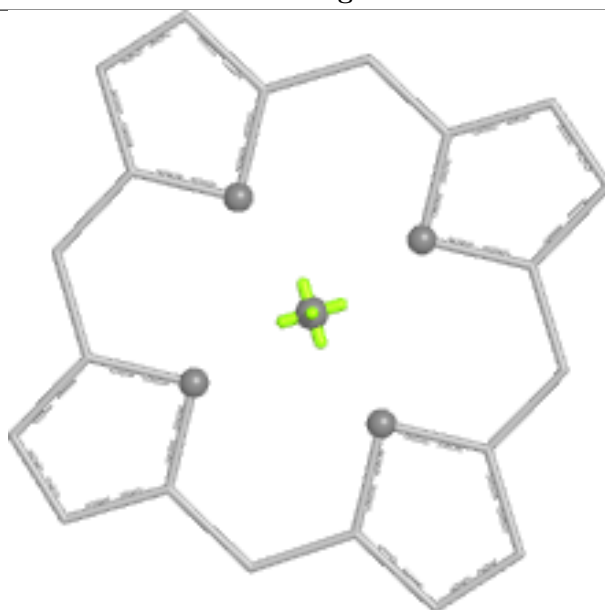
Bond lengths



Bond angles

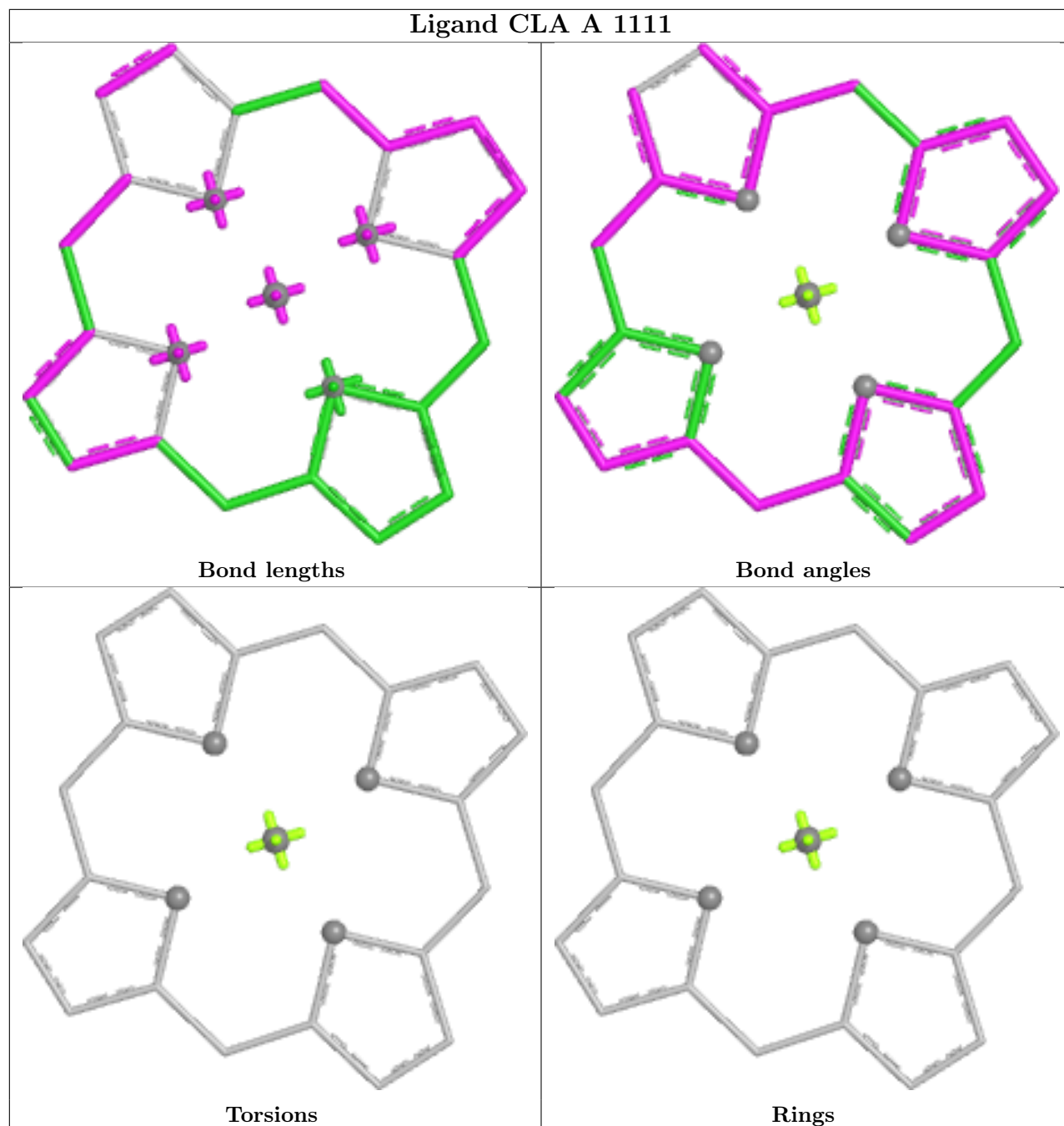


Torsions

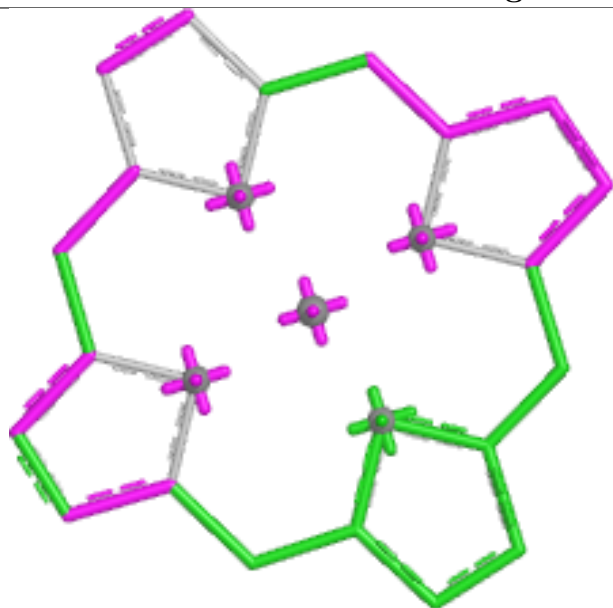


Rings

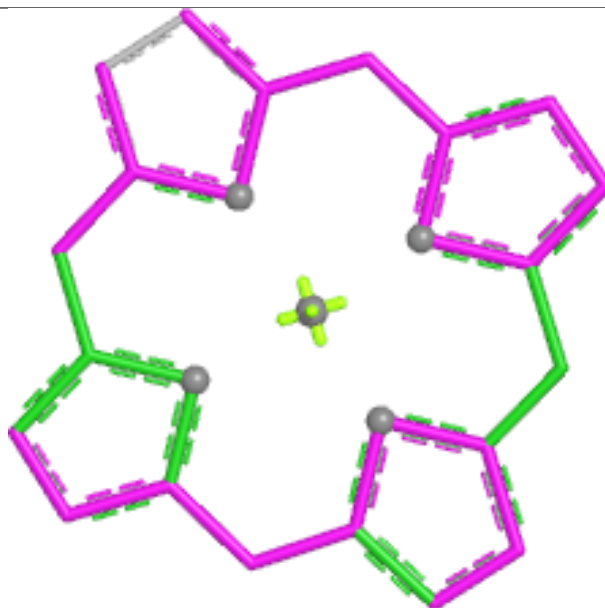
Ligand CLA A 1111



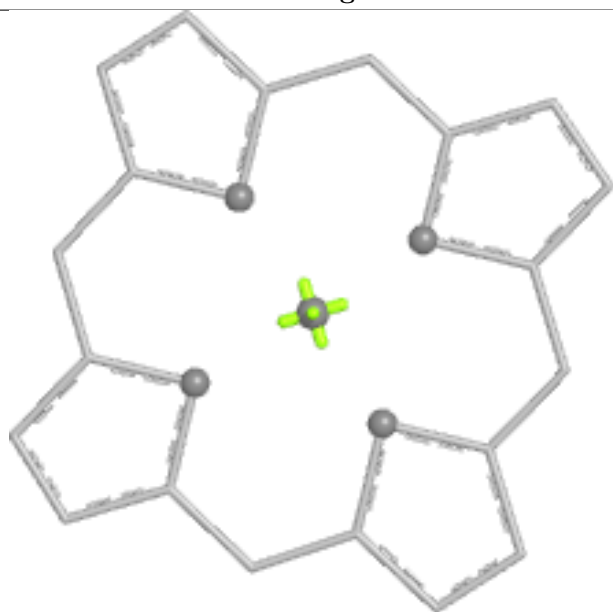
Ligand CLA B 1204



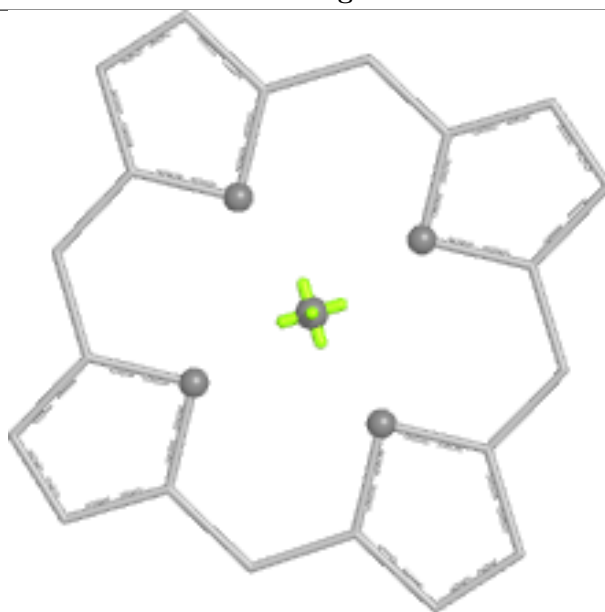
Bond lengths



Bond angles

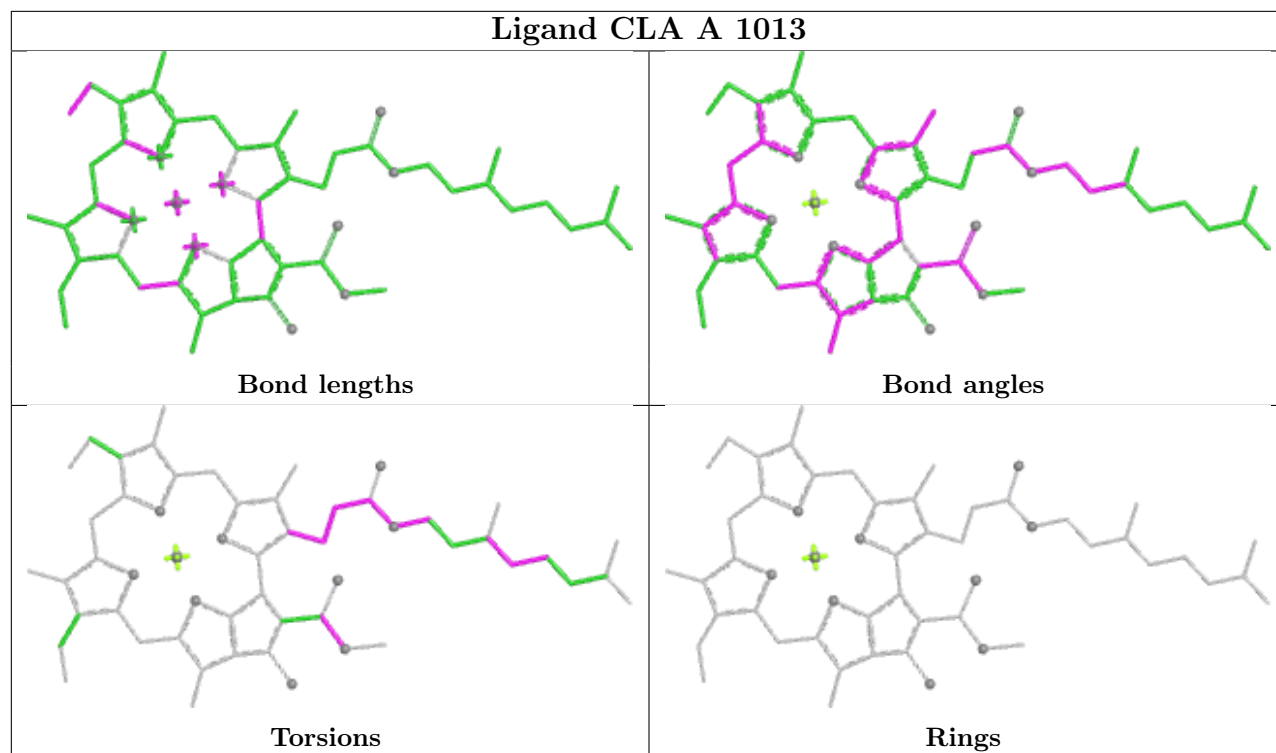


Torsions

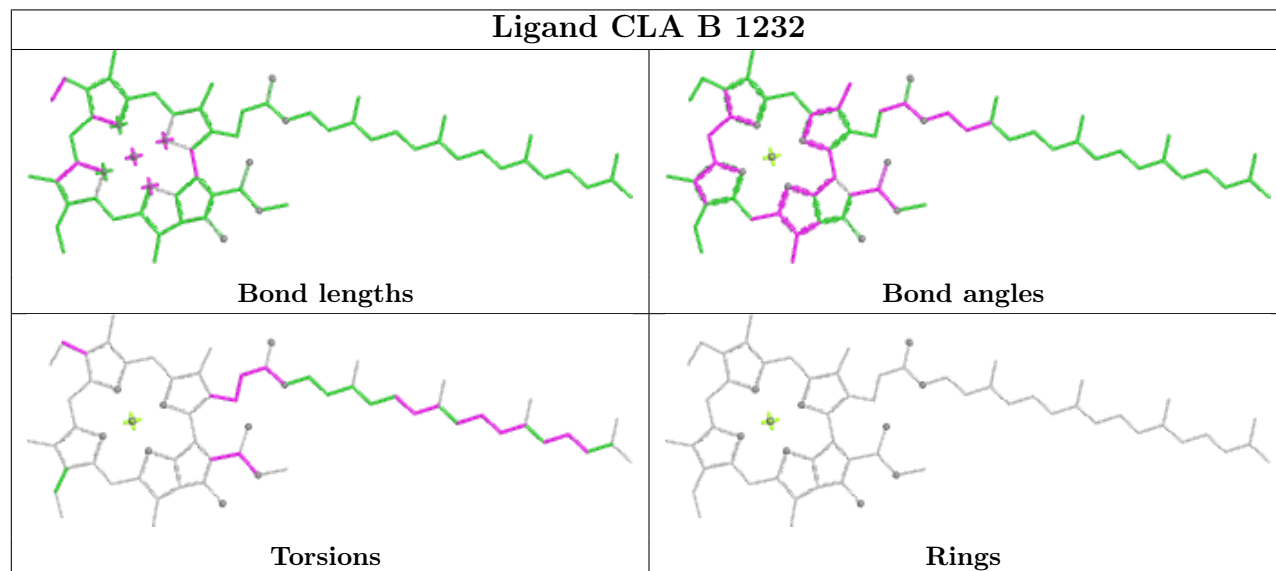


Rings

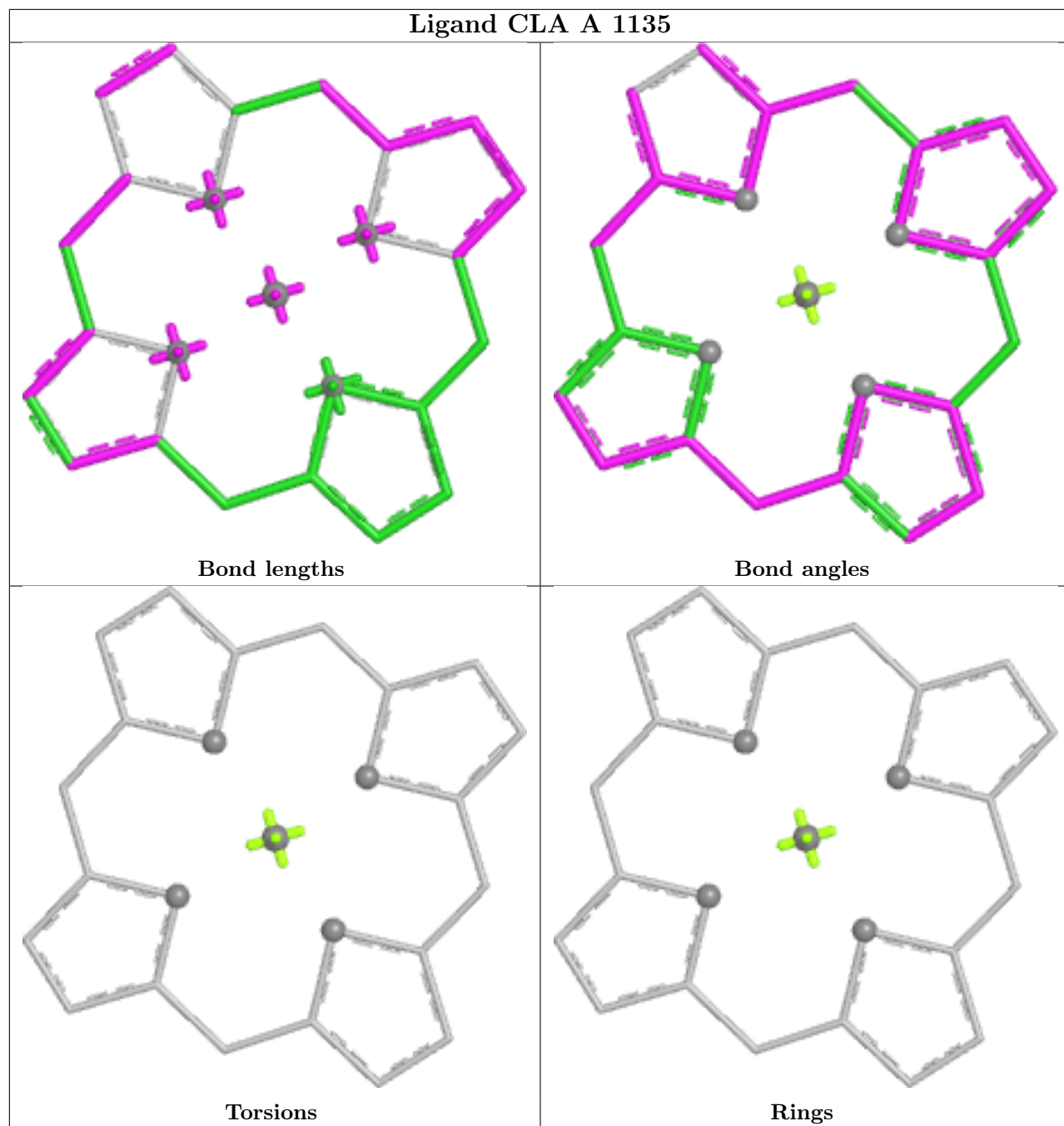
Ligand CLA A 1013



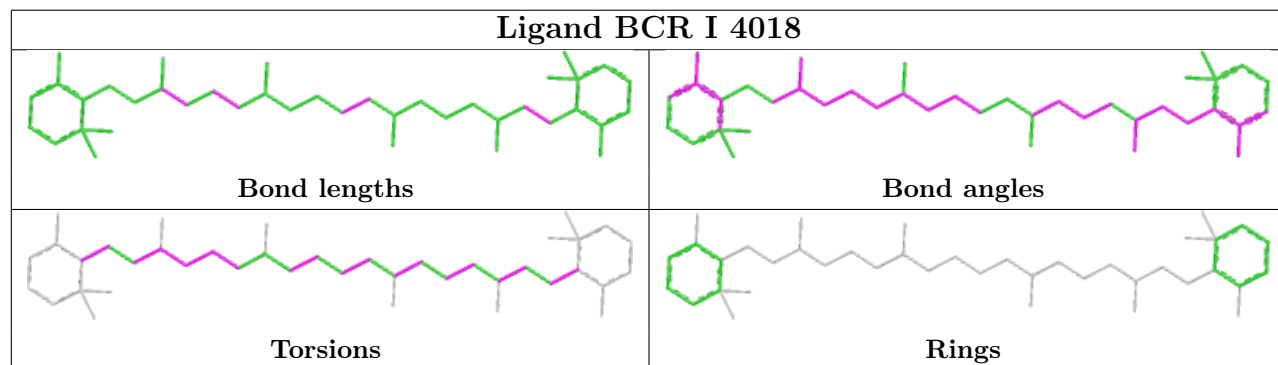
Ligand CLA B 1232



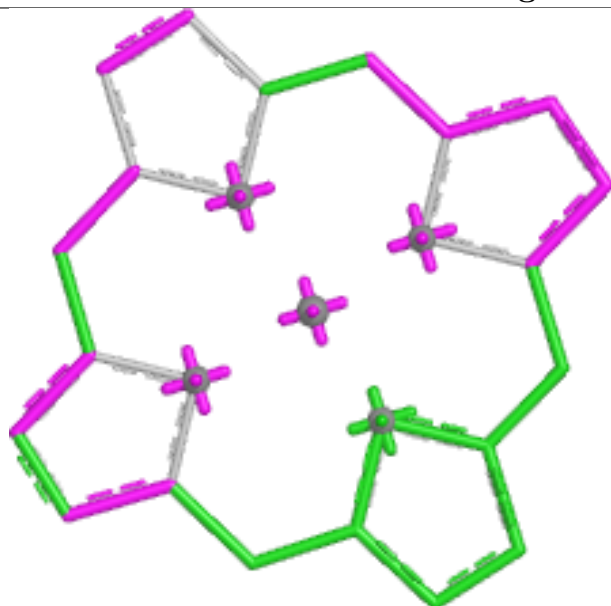
Ligand CLA A 1135



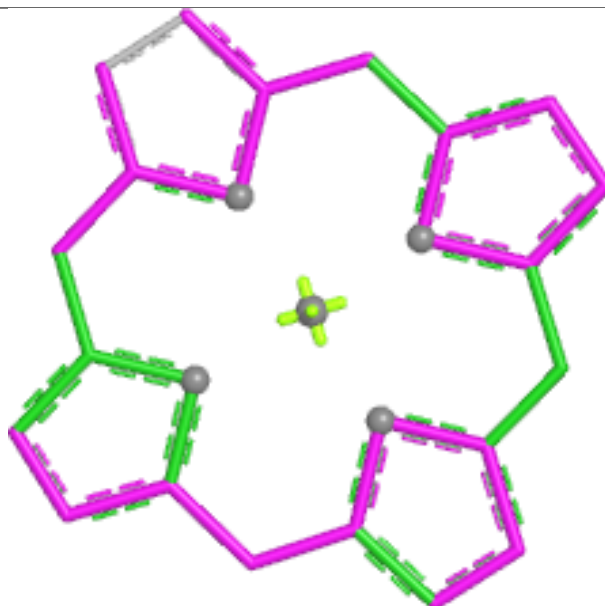
Ligand BCR I 4018



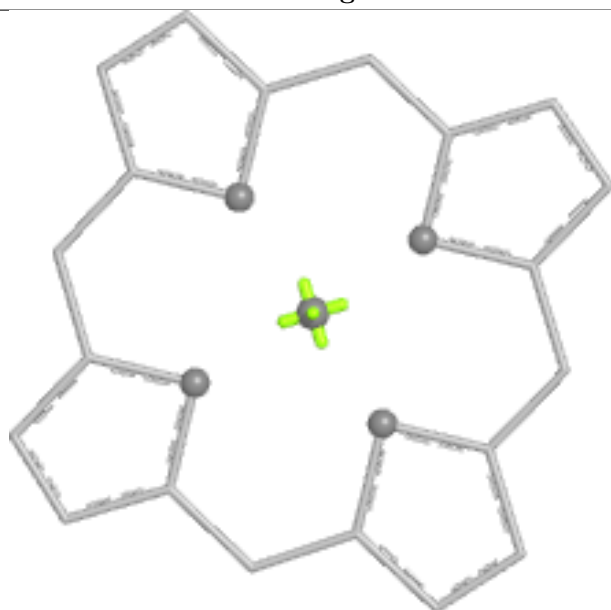
Ligand CLA 2 612



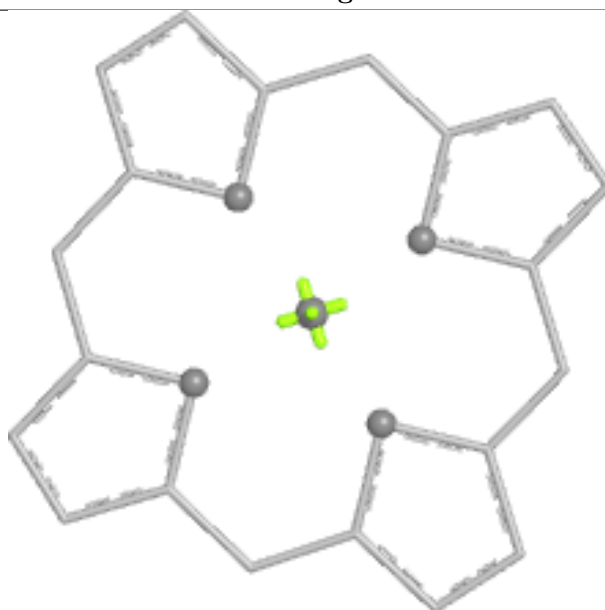
Bond lengths



Bond angles

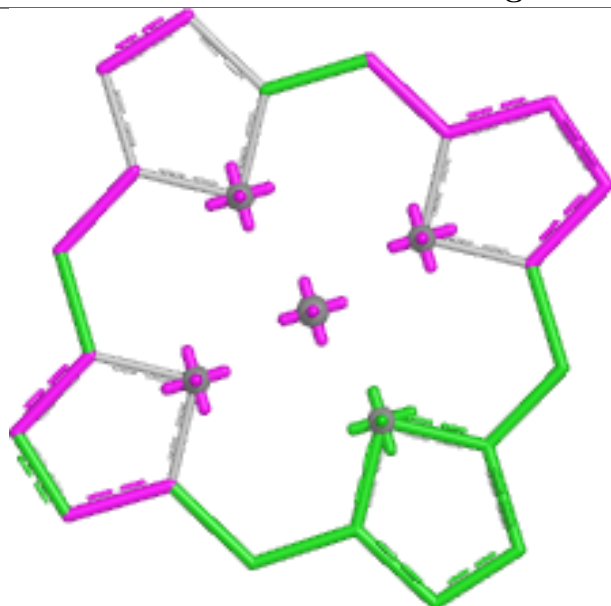


Torsions

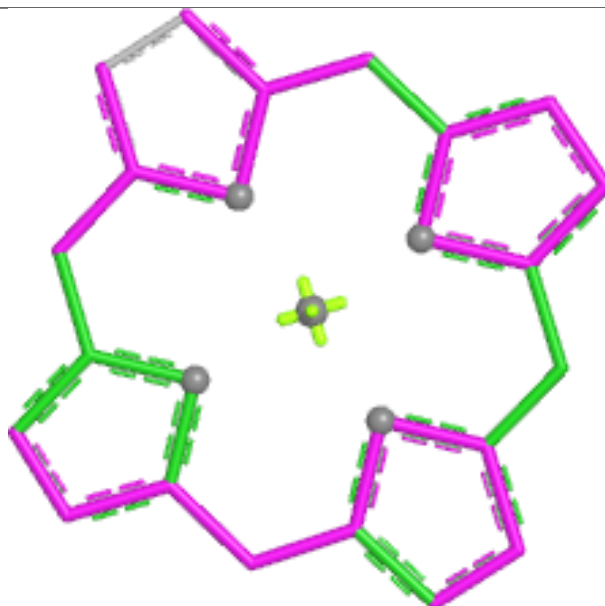


Rings

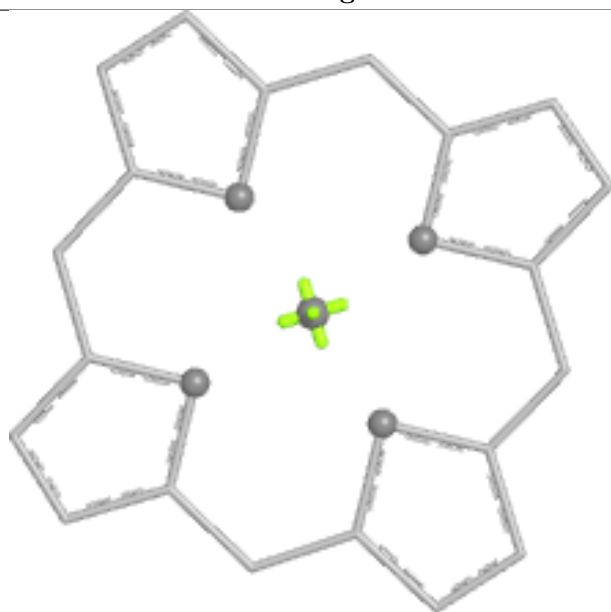
Ligand CLA B 1220



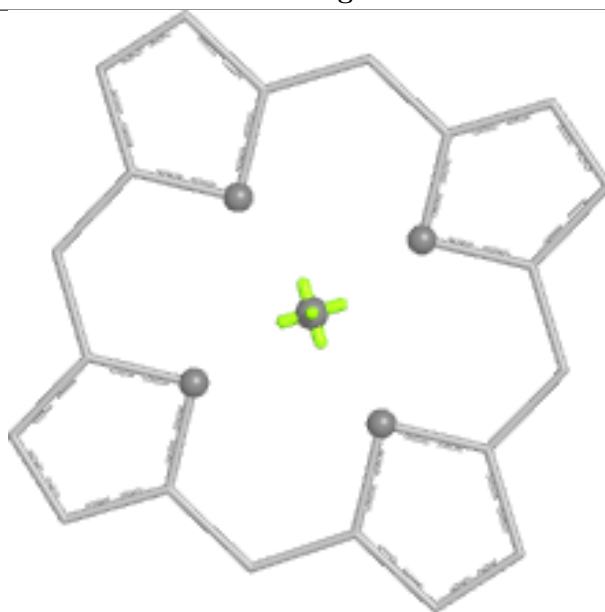
Bond lengths



Bond angles

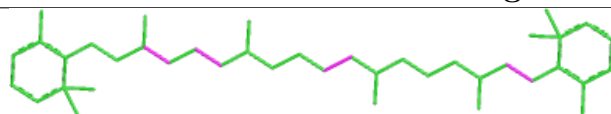


Torsions

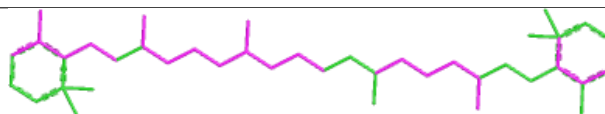


Rings

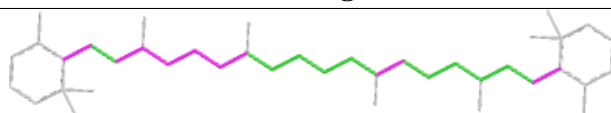
Ligand BCR B 4008



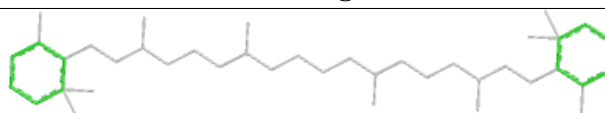
Bond lengths



Bond angles

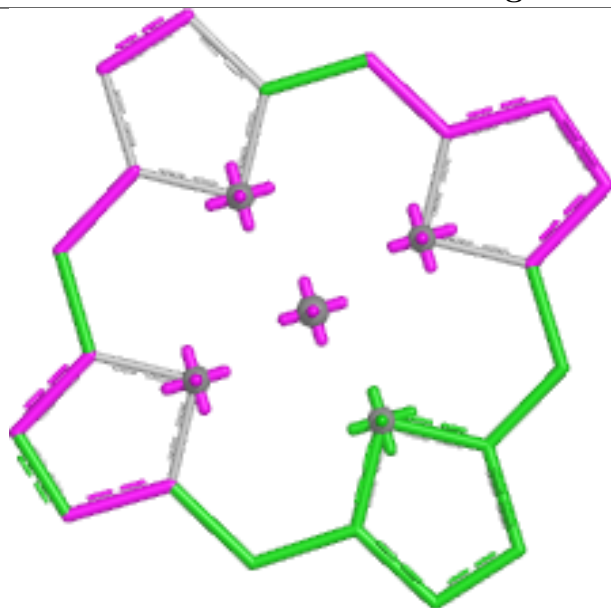


Torsions

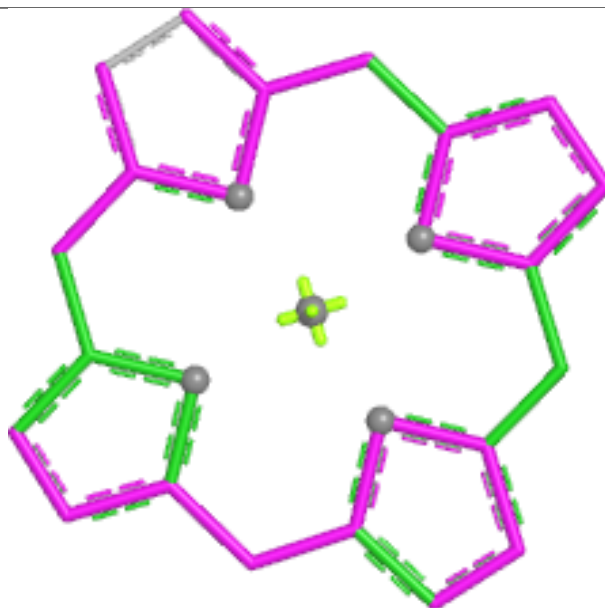


Rings

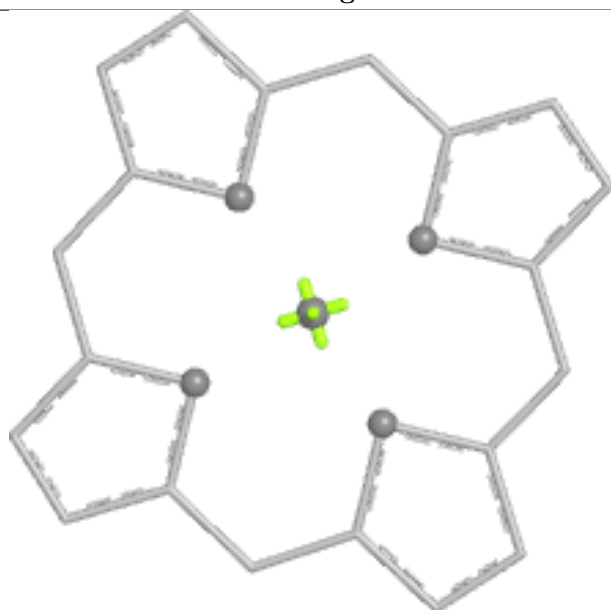
Ligand CLA B 1234



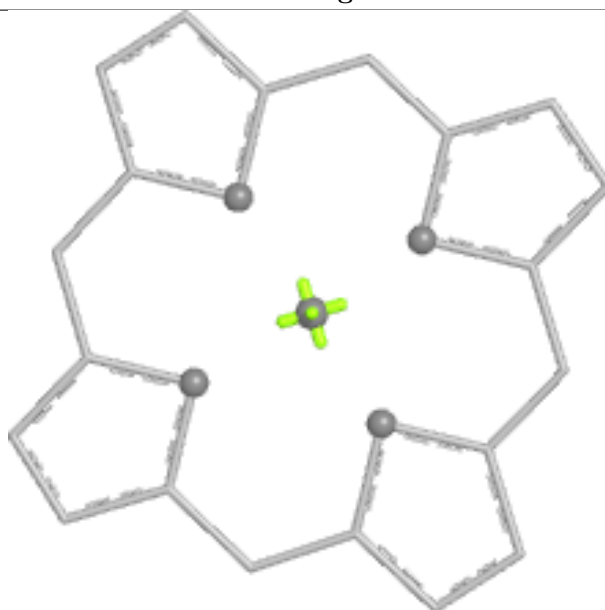
Bond lengths



Bond angles

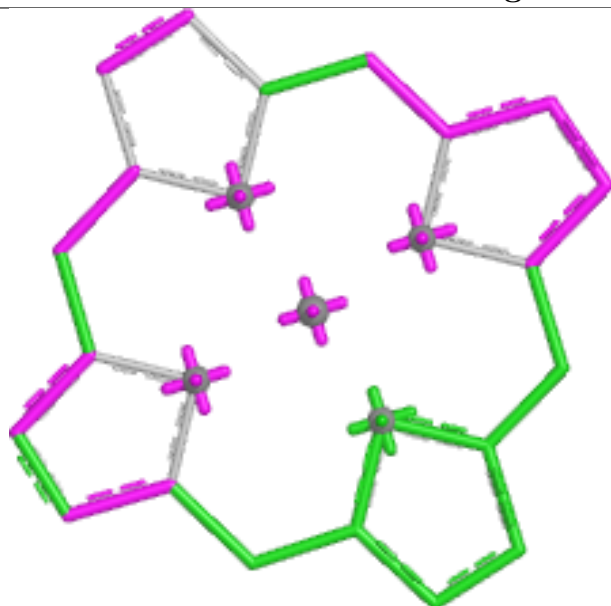


Torsions

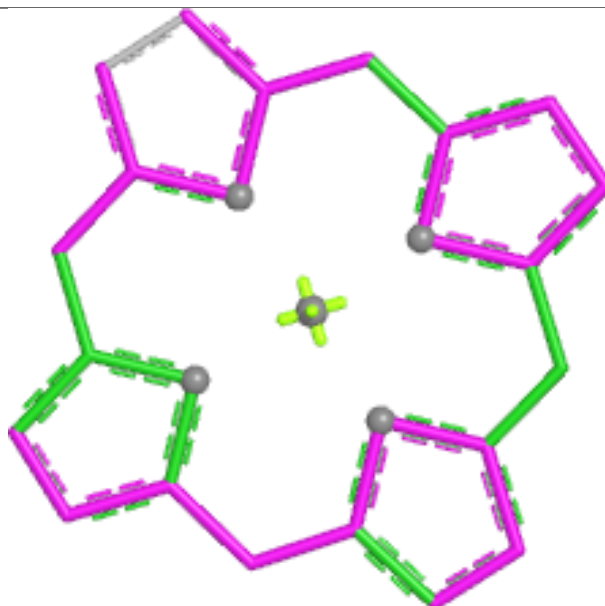


Rings

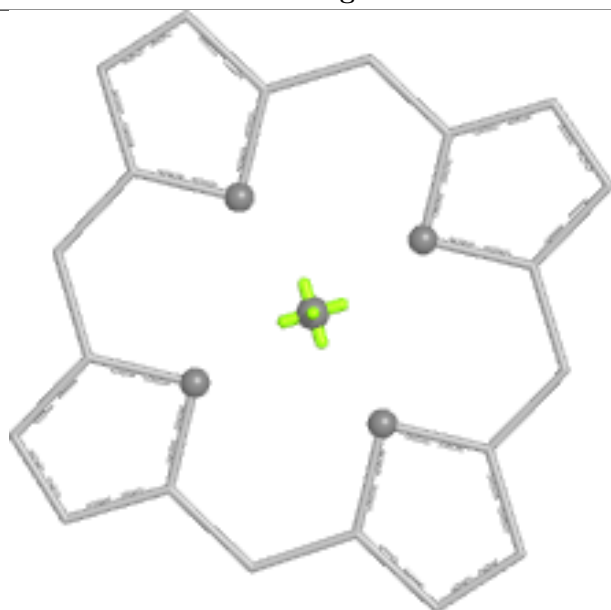
Ligand CLA K 1402



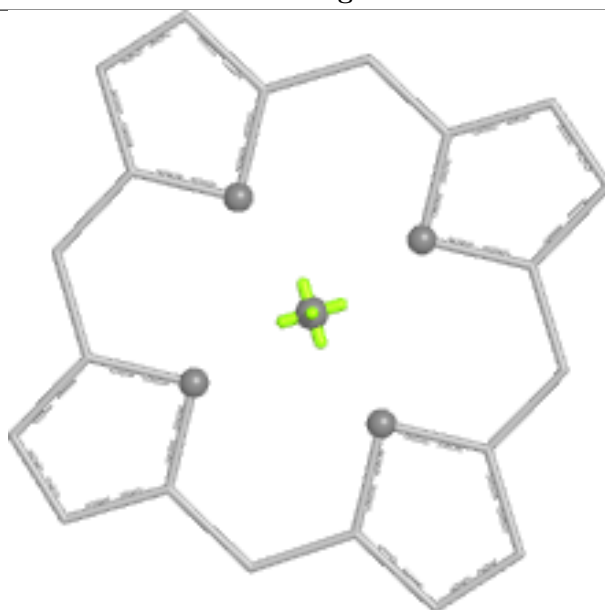
Bond lengths



Bond angles

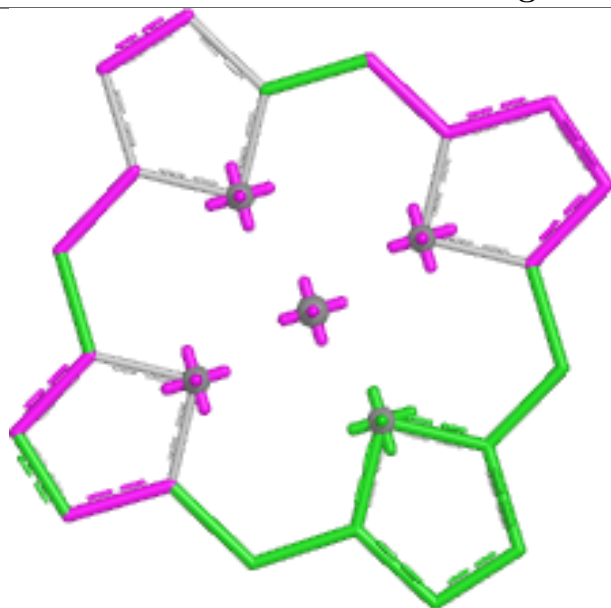


Torsions

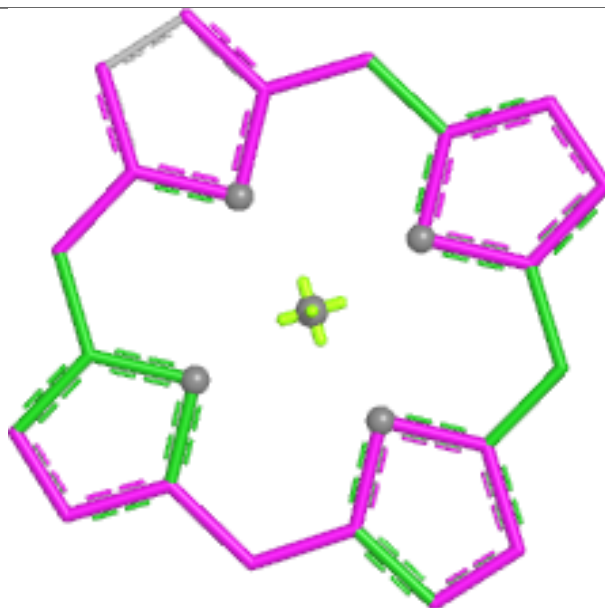


Rings

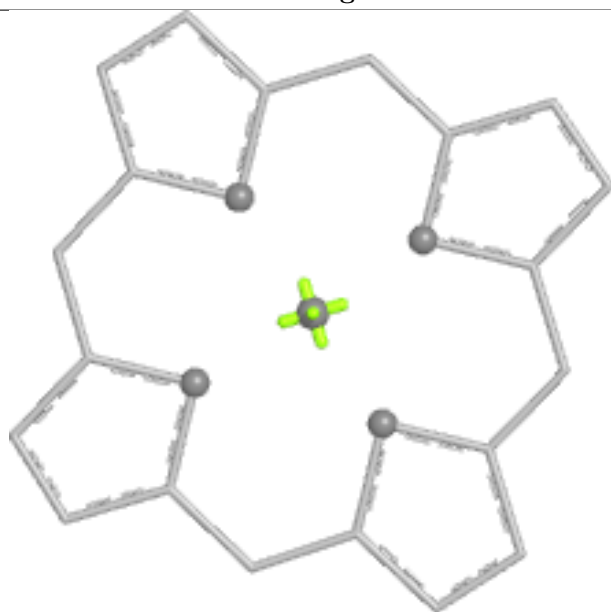
Ligand CLA 2 602



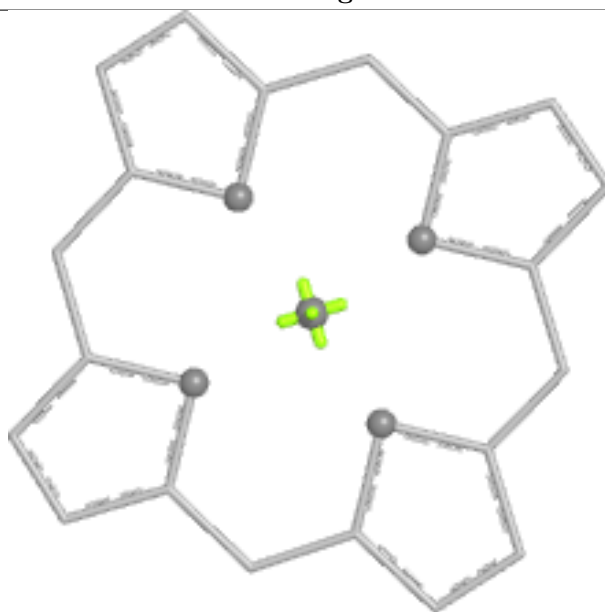
Bond lengths



Bond angles

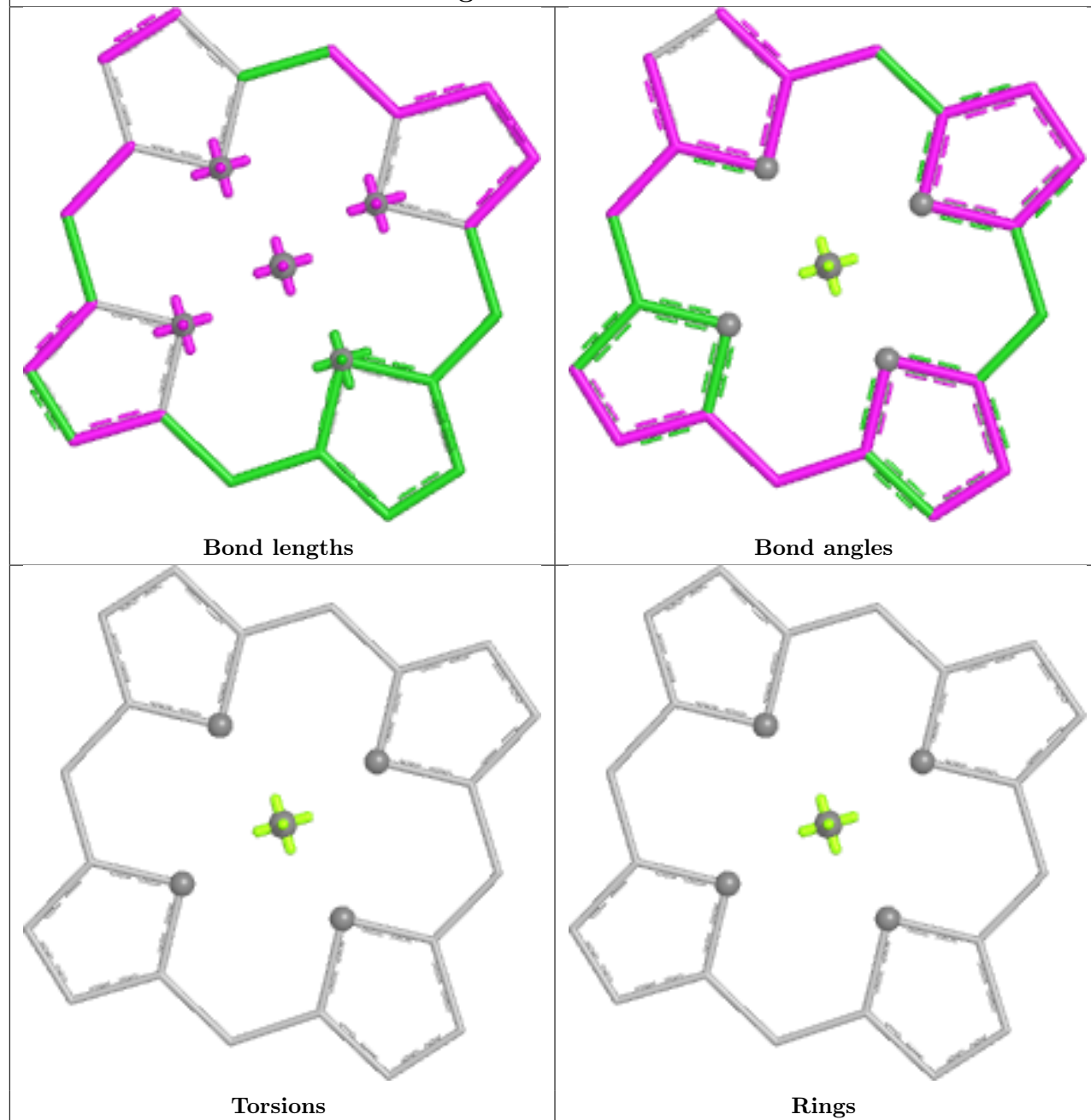


Torsions

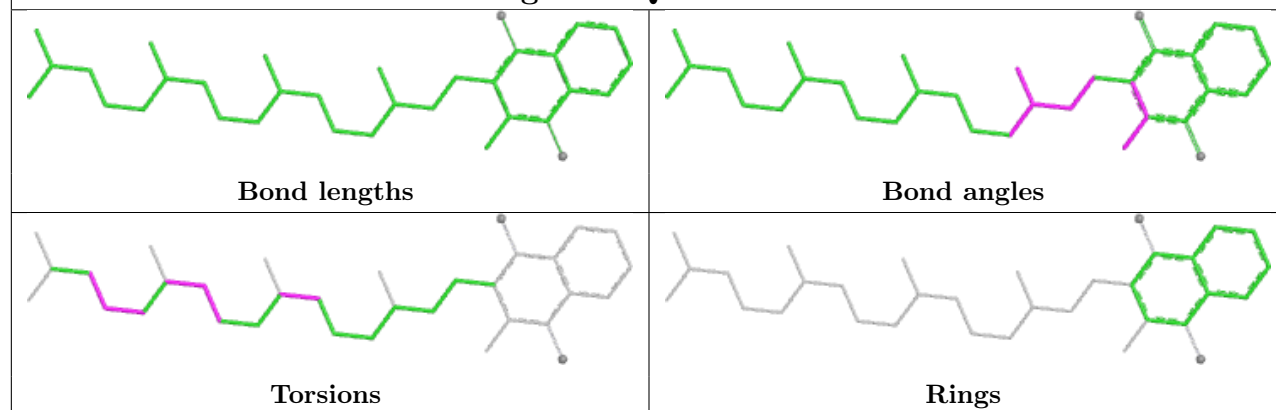


Rings

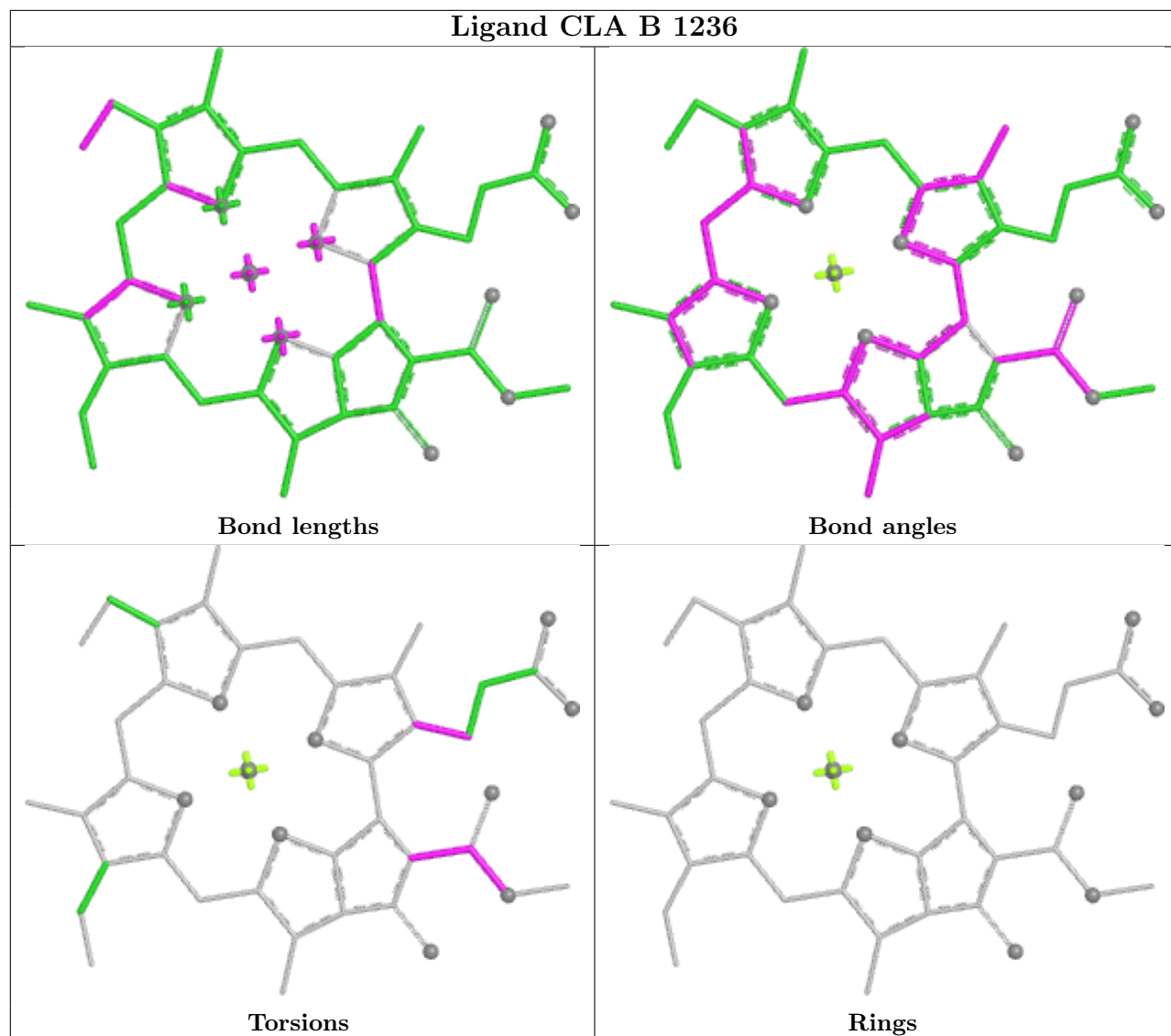
Ligand CLA 4 602



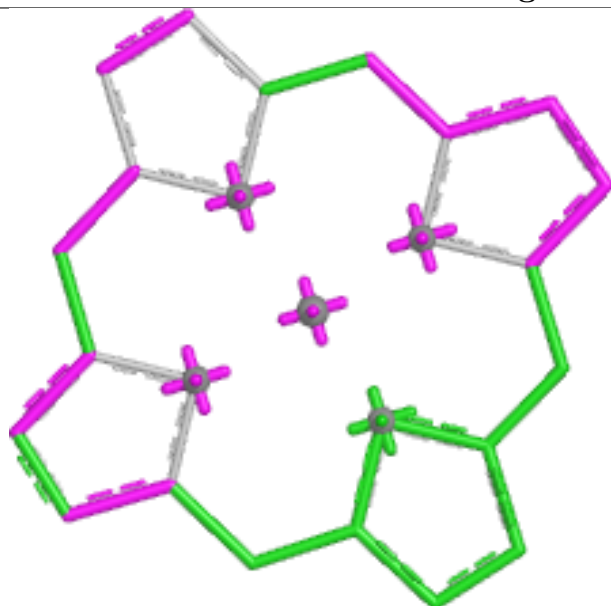
Ligand PQN B 2002



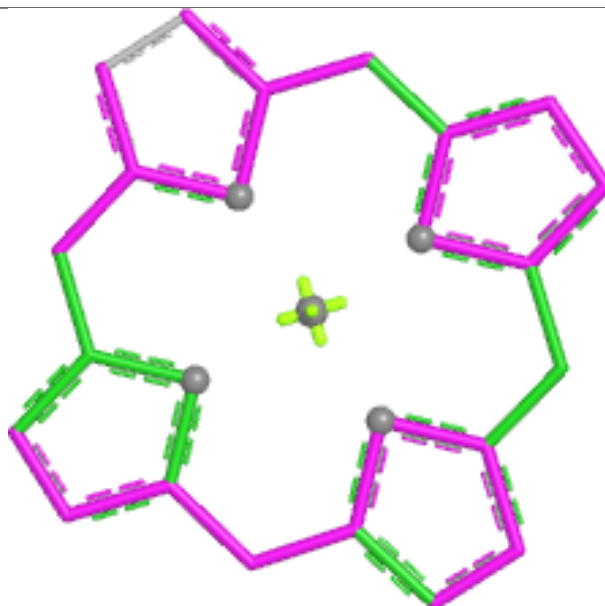
Ligand CLA B 1236



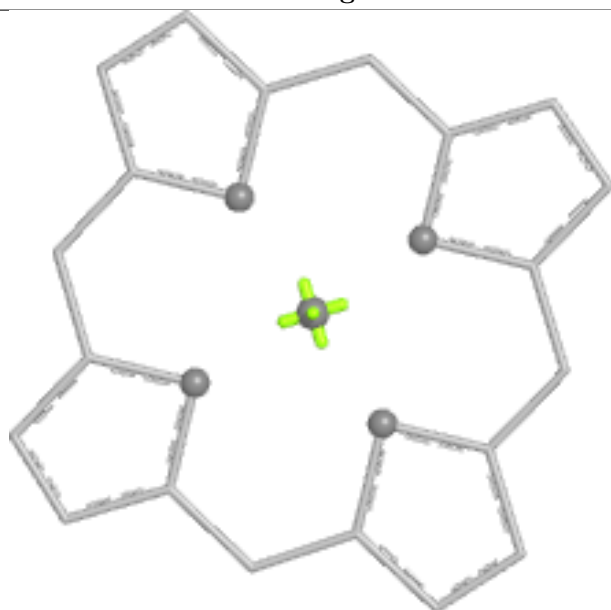
Ligand CLA 2 613



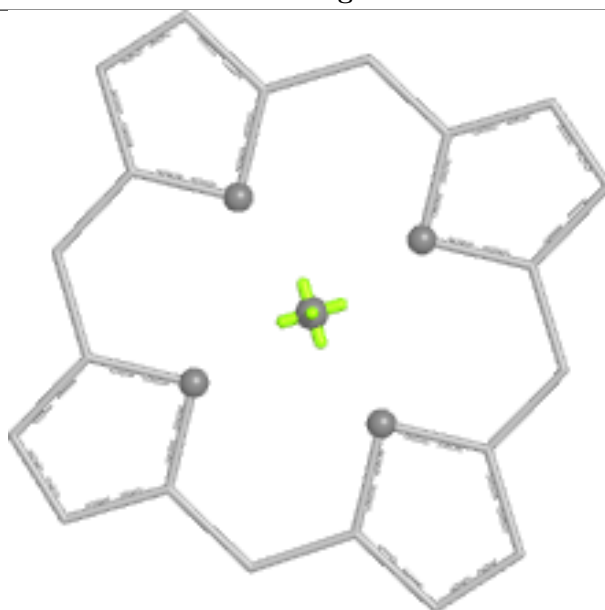
Bond lengths



Bond angles

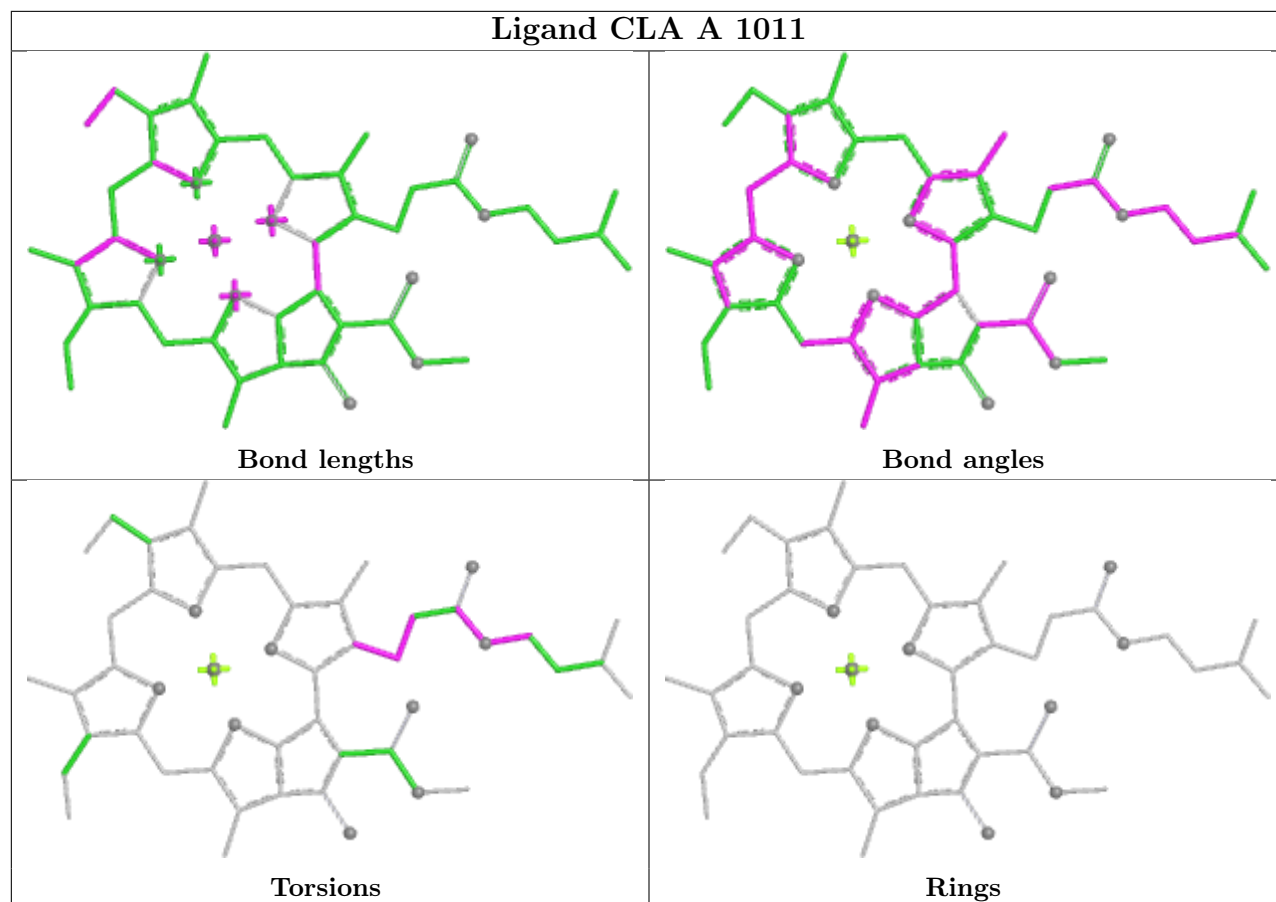


Torsions

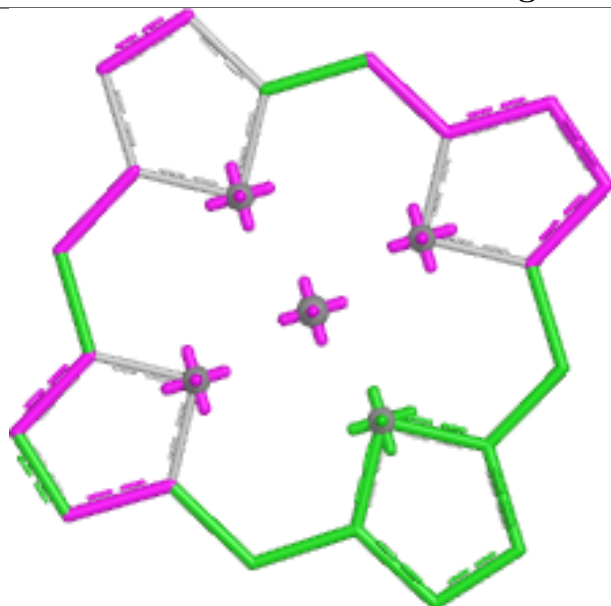


Rings

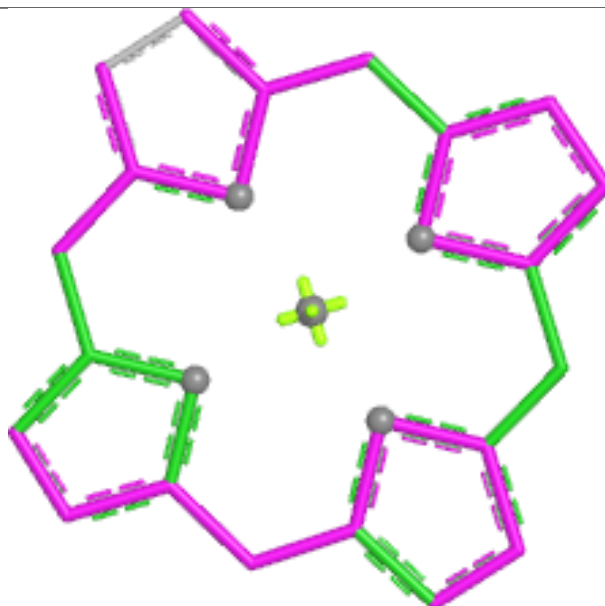
Ligand CLA A 1011



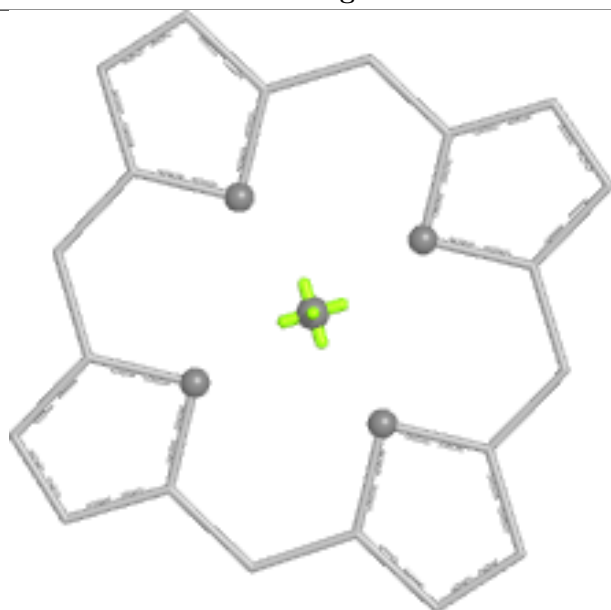
Ligand CLA 3 611



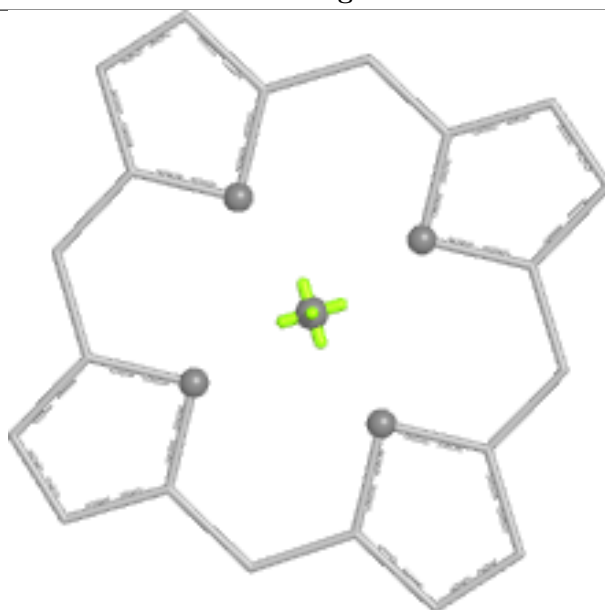
Bond lengths



Bond angles

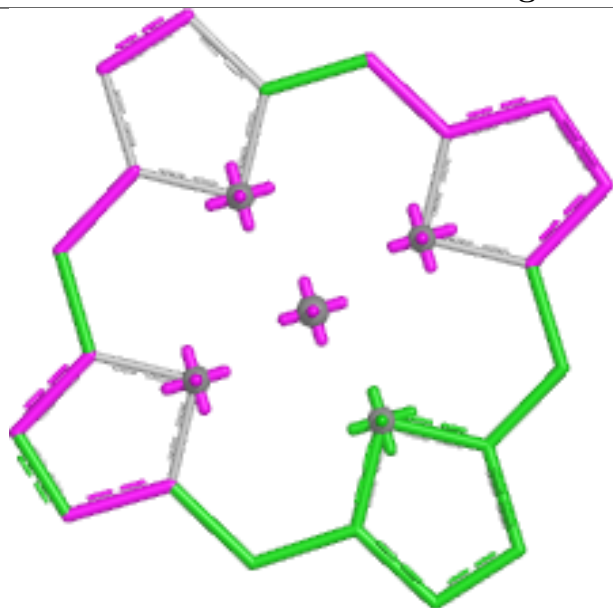


Torsions

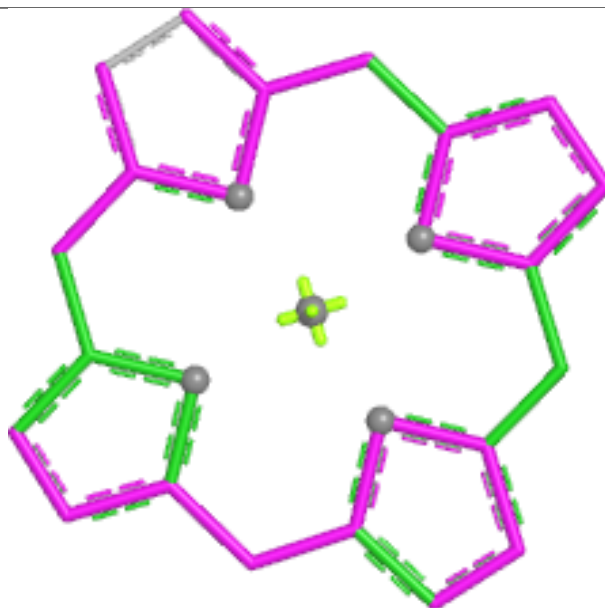


Rings

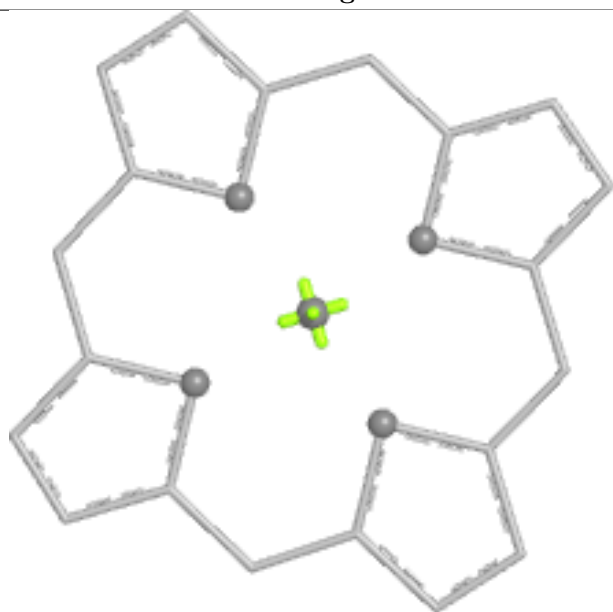
Ligand CLA 3 614



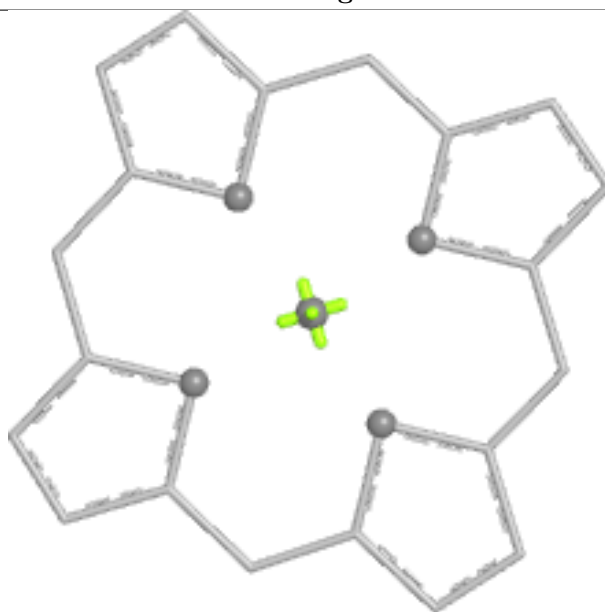
Bond lengths



Bond angles

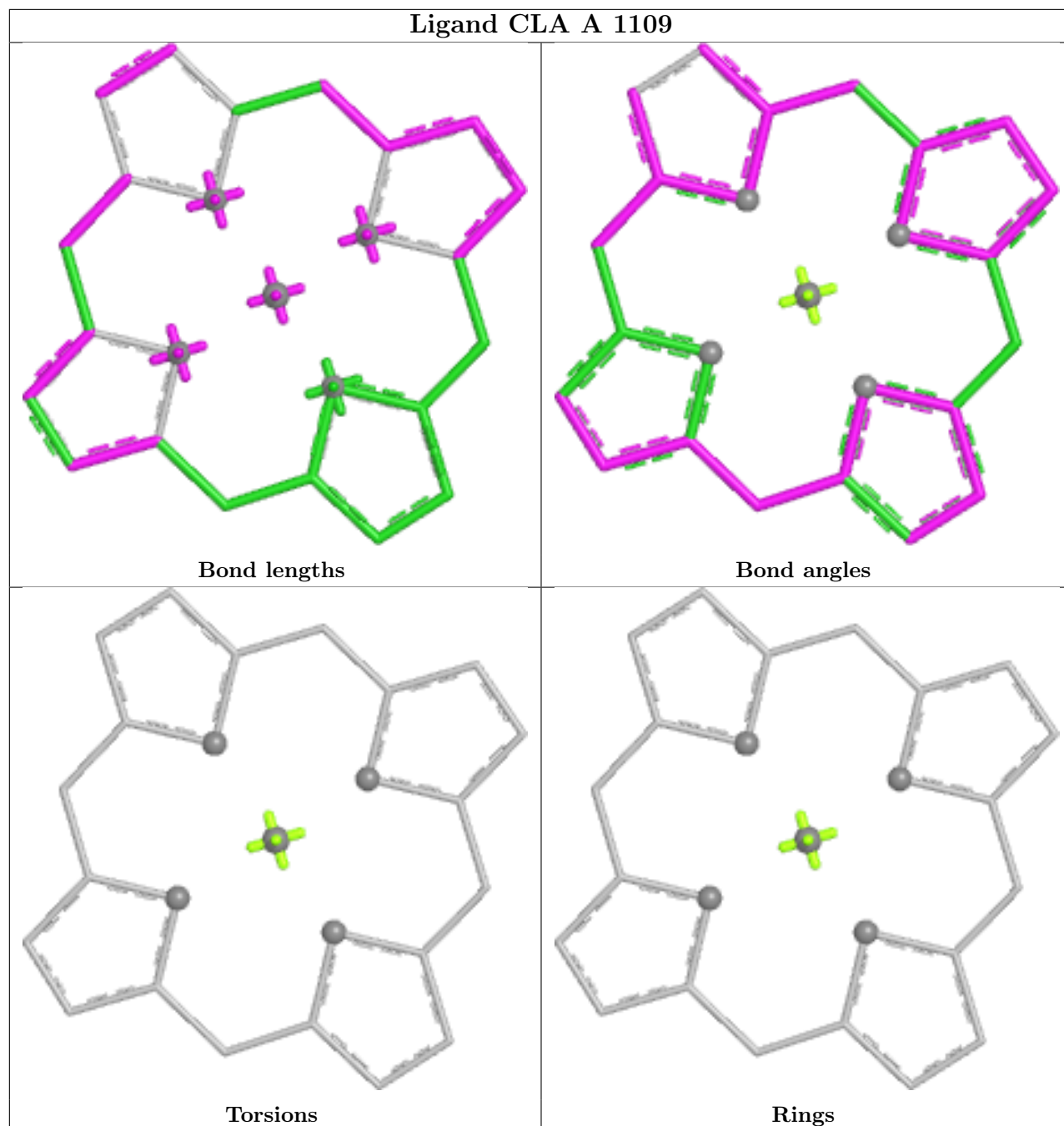


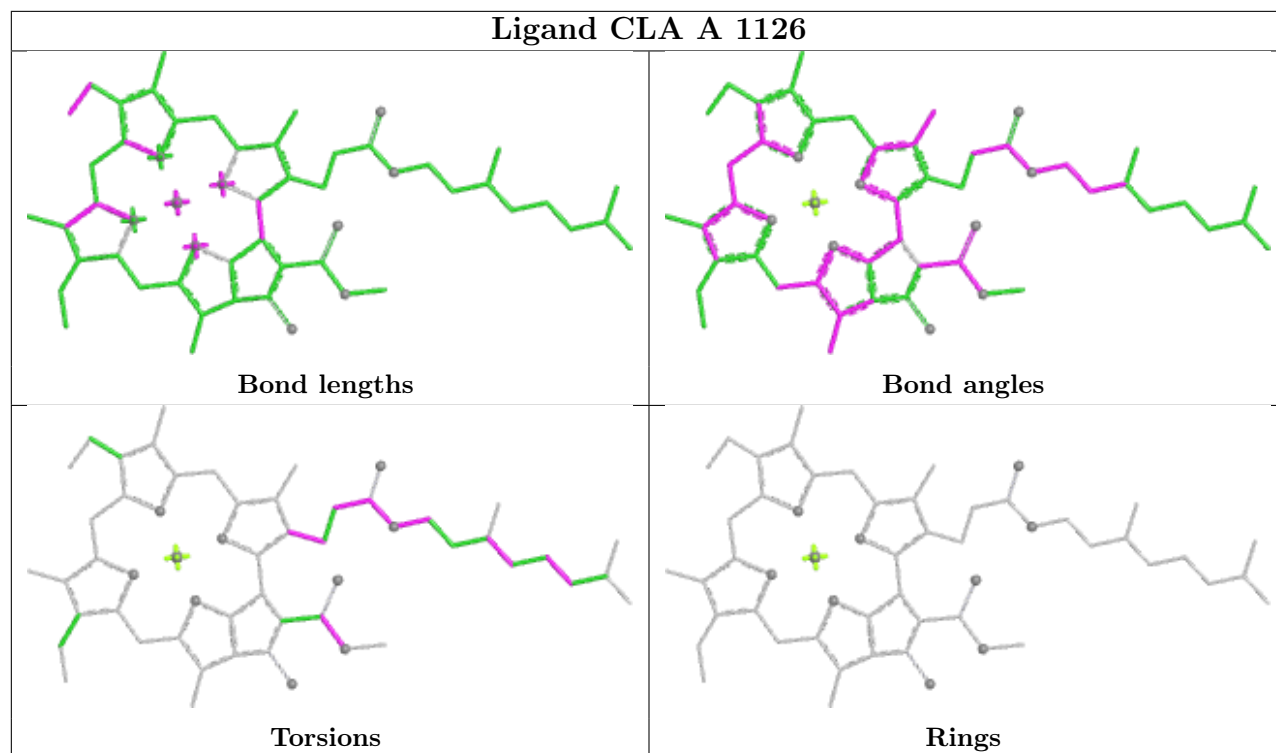
Torsions



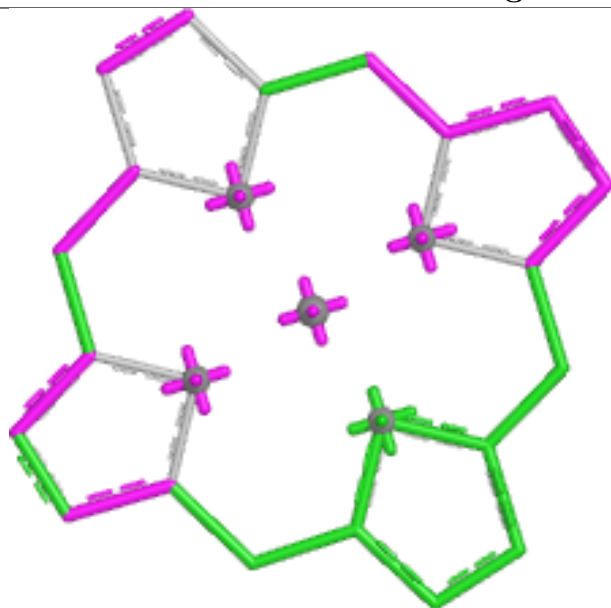
Rings

Ligand CLA A 1109

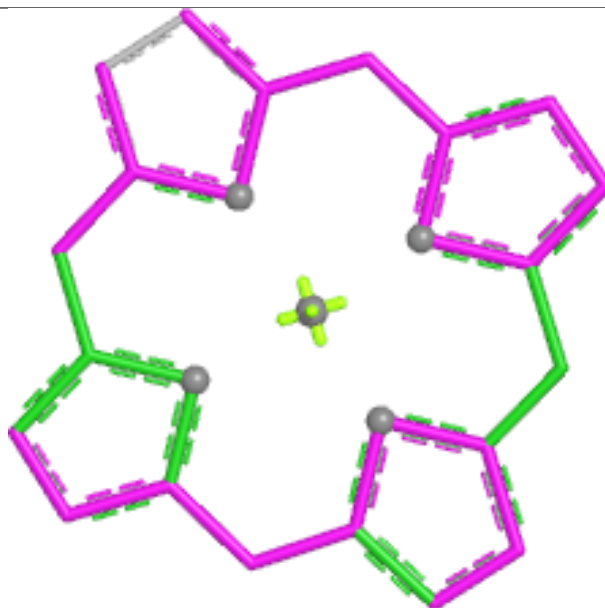




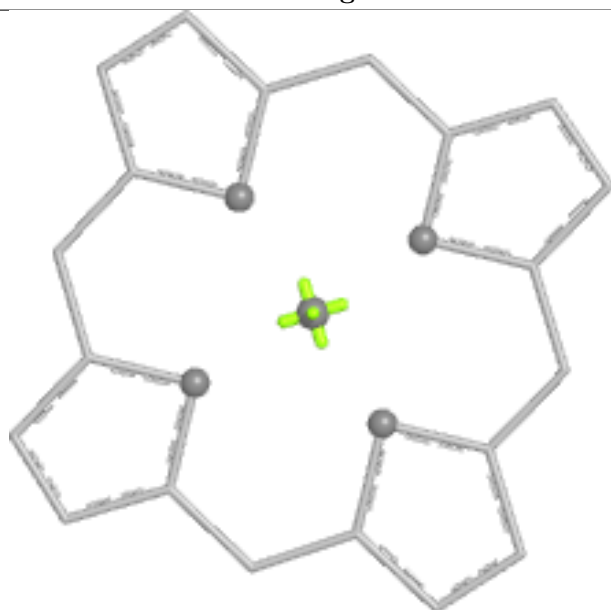
Ligand CLA B 1222



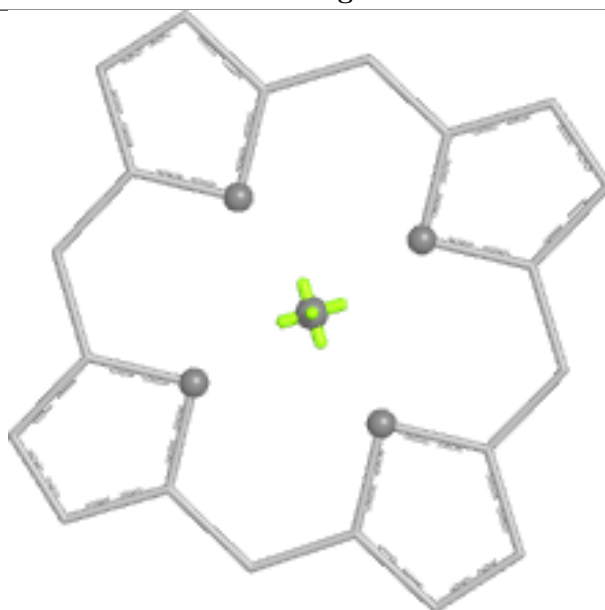
Bond lengths



Bond angles

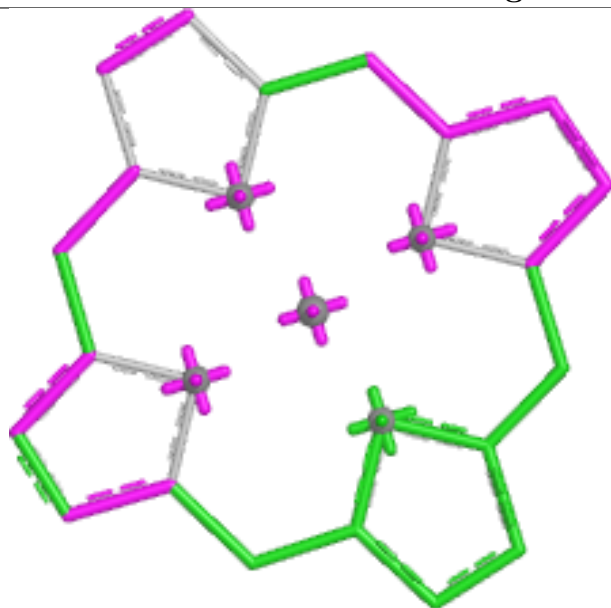


Torsions

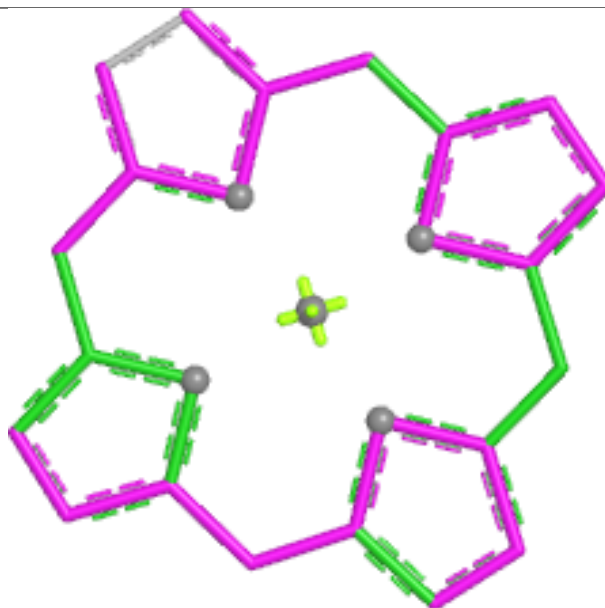


Rings

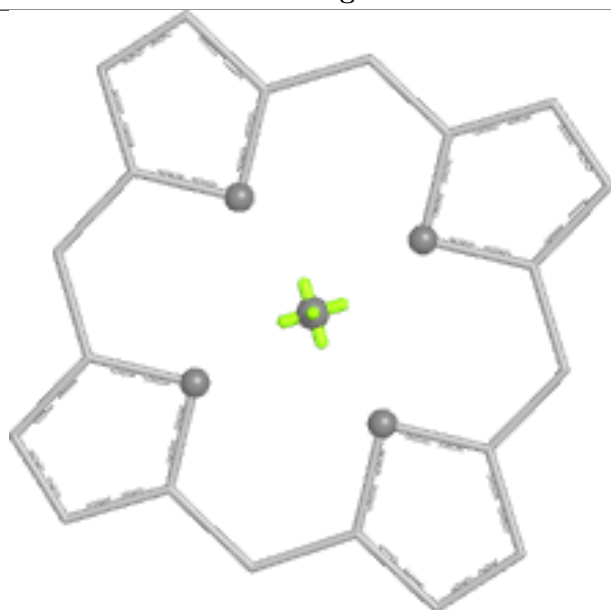
Ligand CLA B 1239



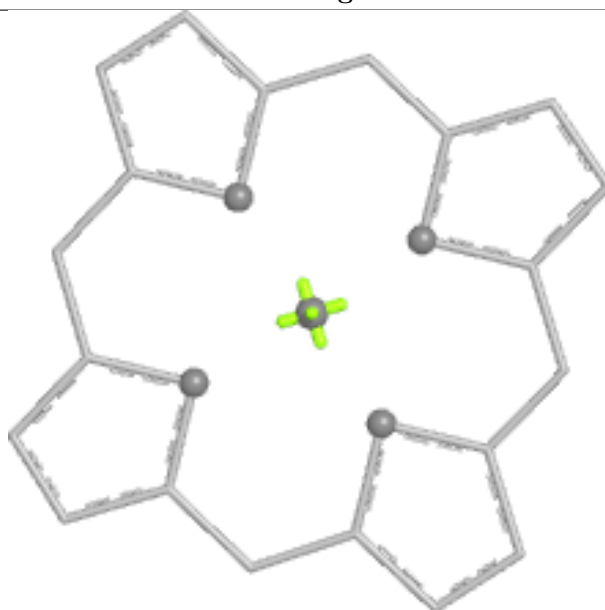
Bond lengths



Bond angles

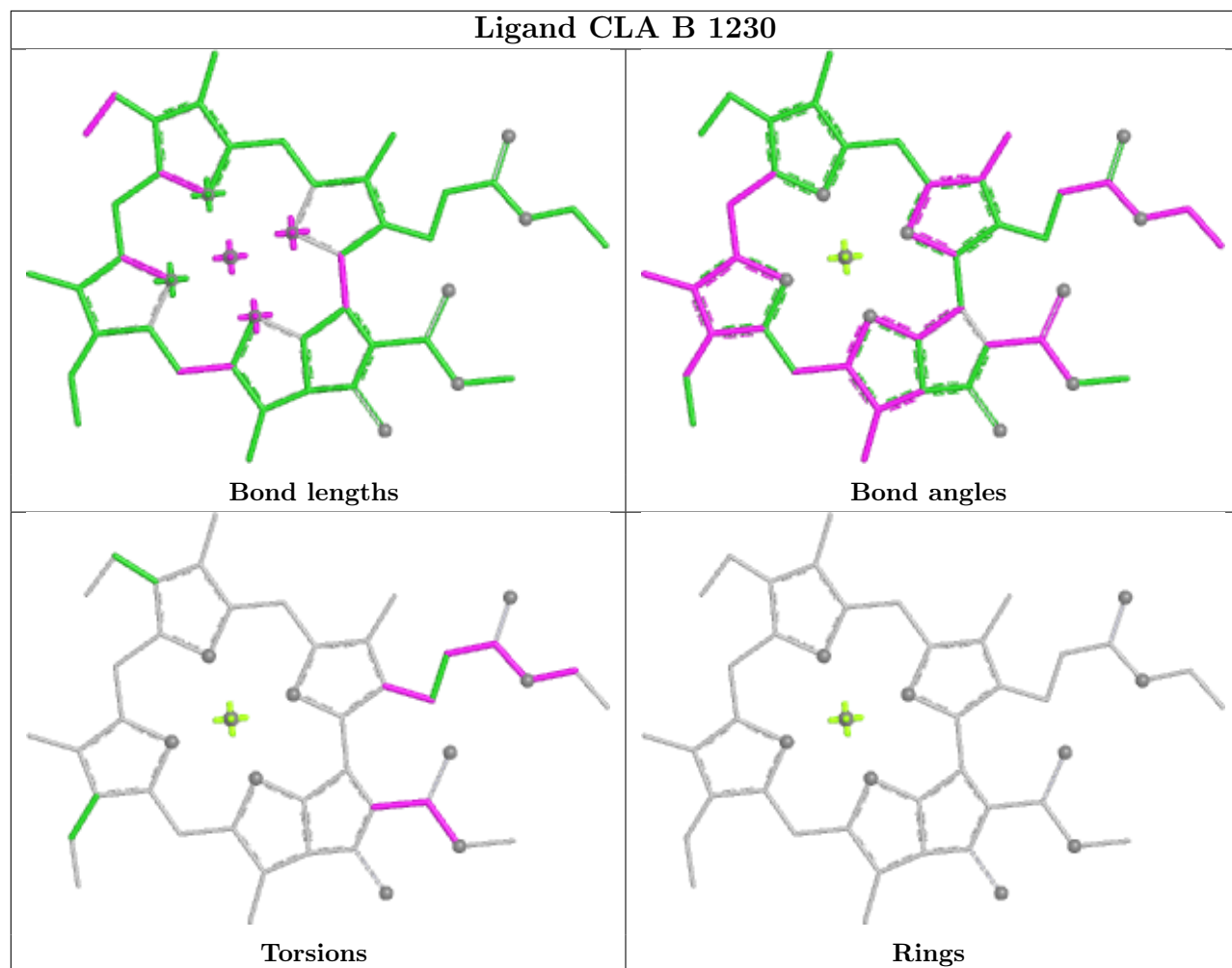


Torsions

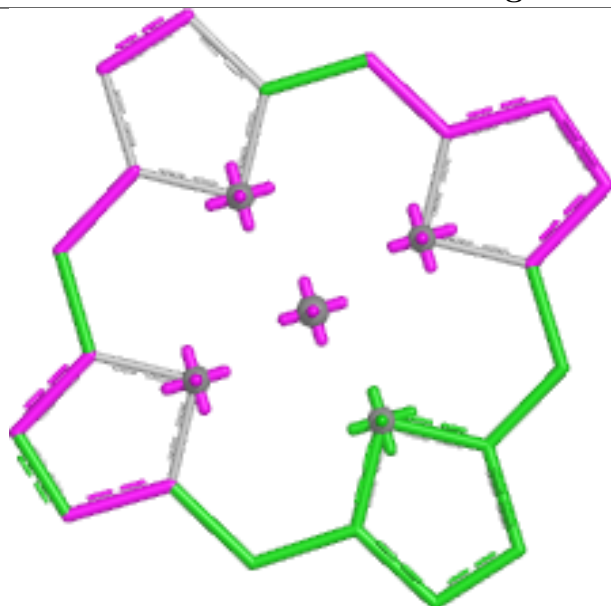


Rings

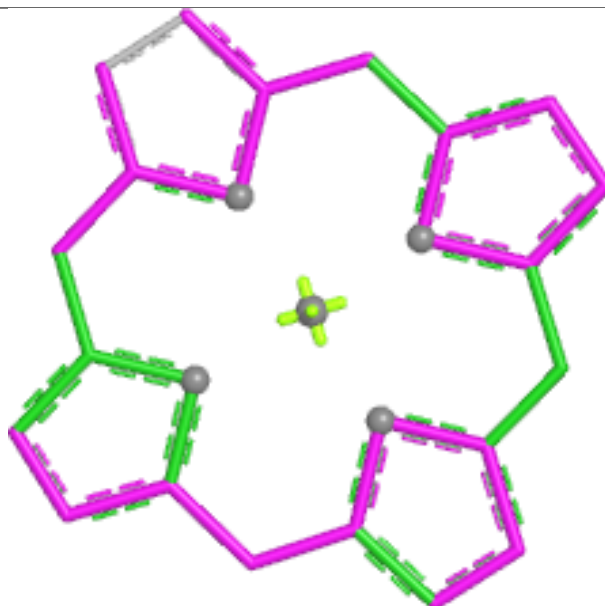
Ligand CLA B 1230



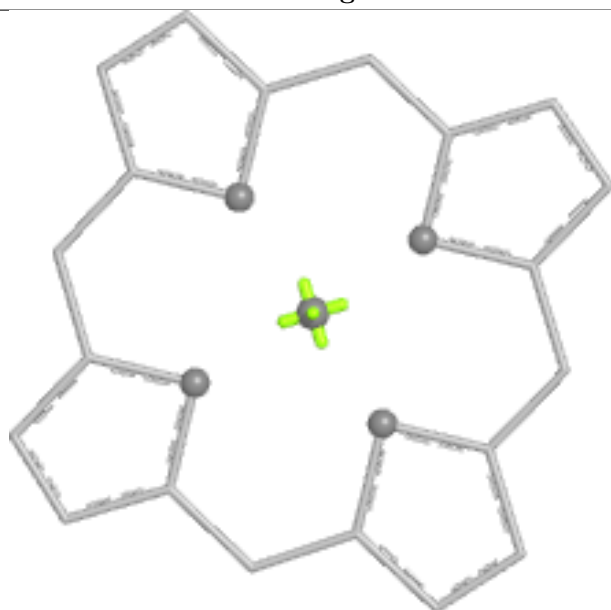
Ligand CLA B 1209



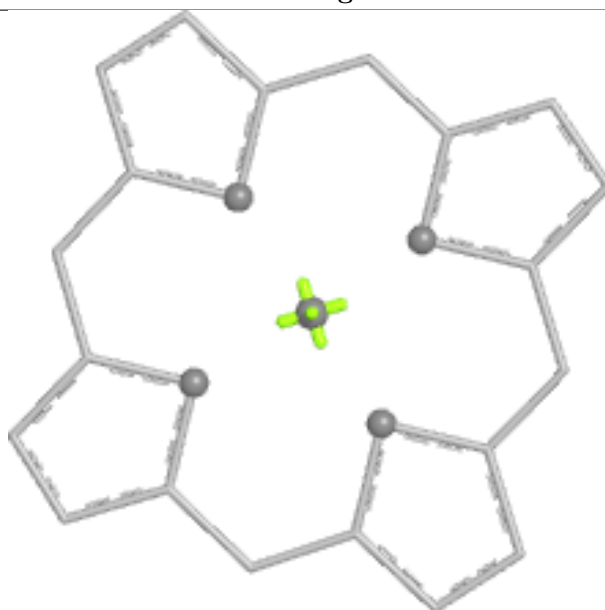
Bond lengths



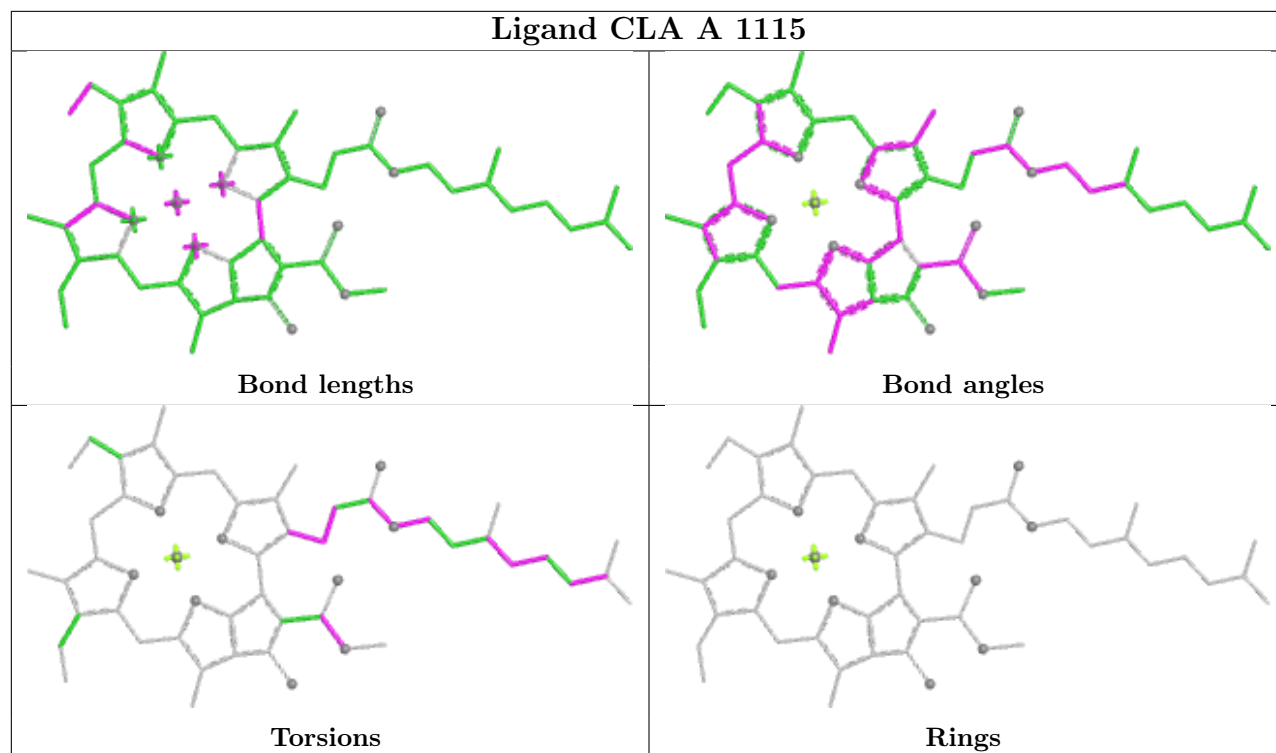
Bond angles



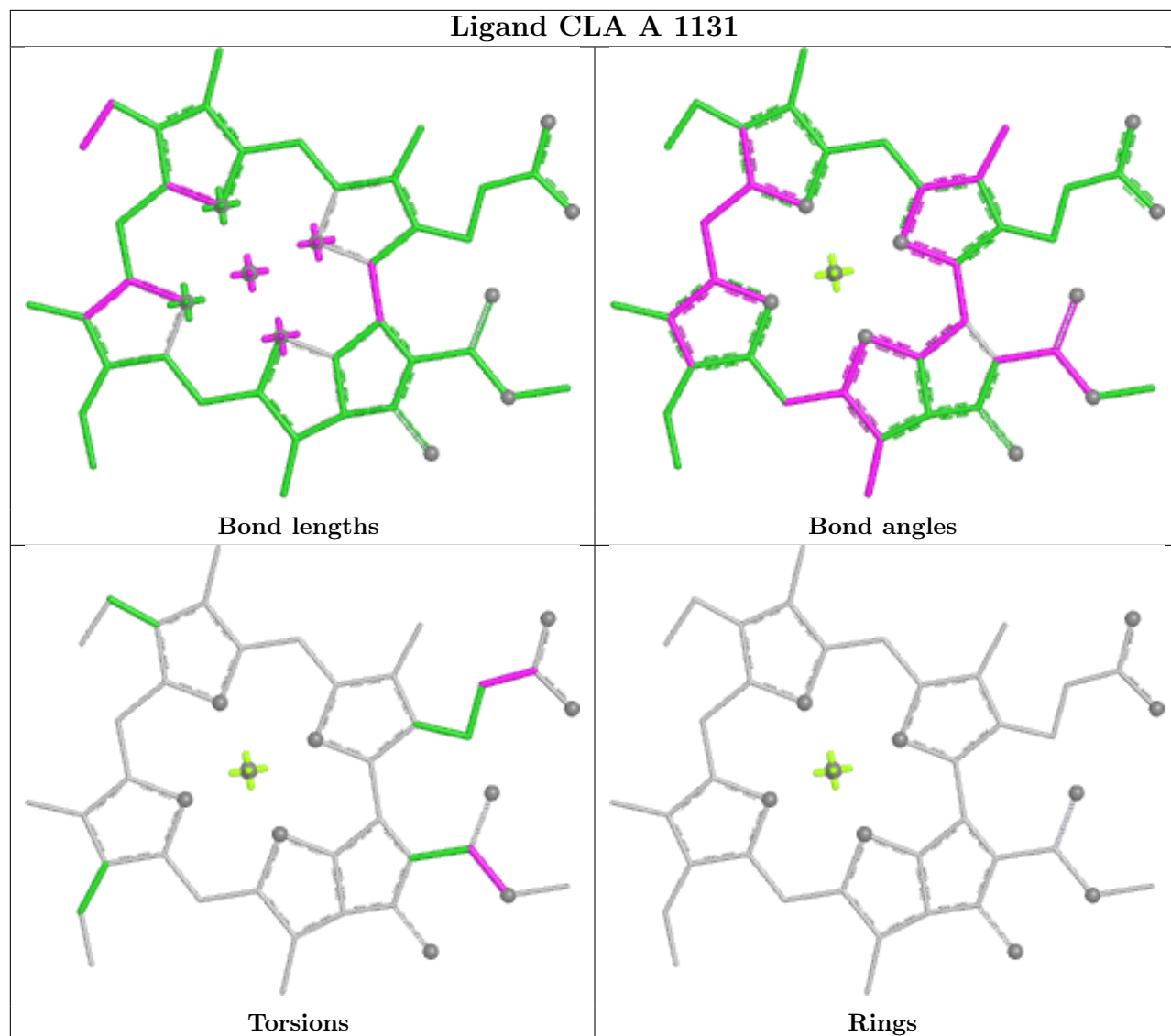
Torsions



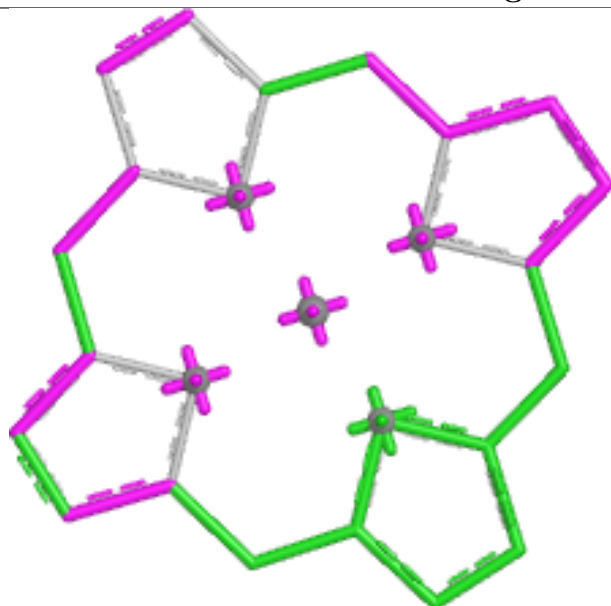
Rings



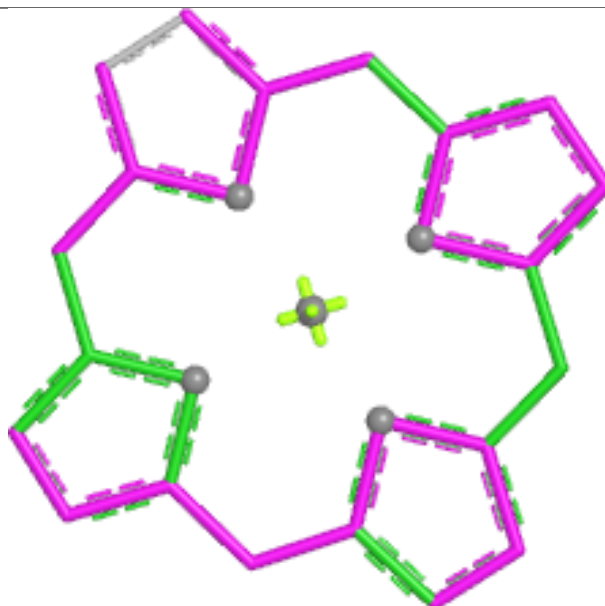
Ligand CLA A 1131



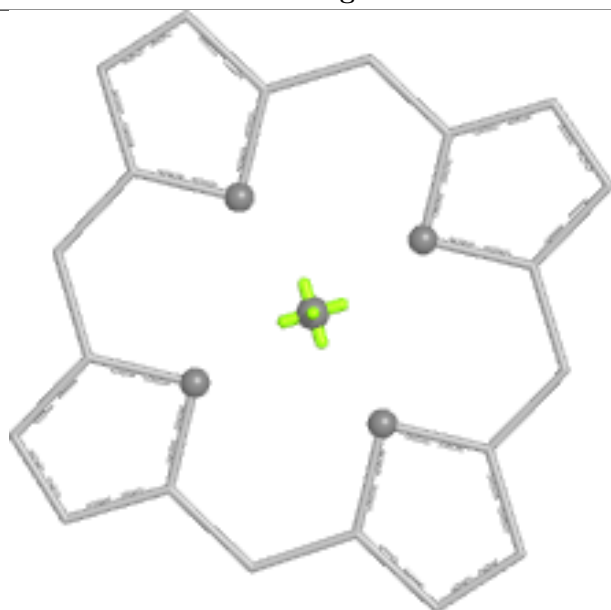
Ligand CLA A 1136



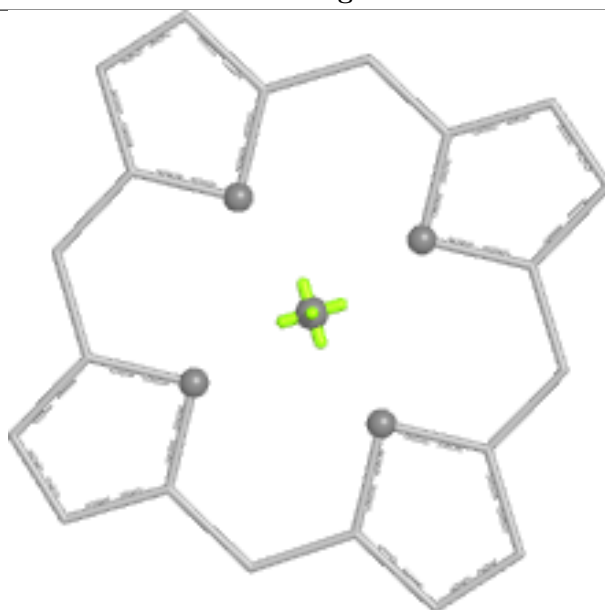
Bond lengths



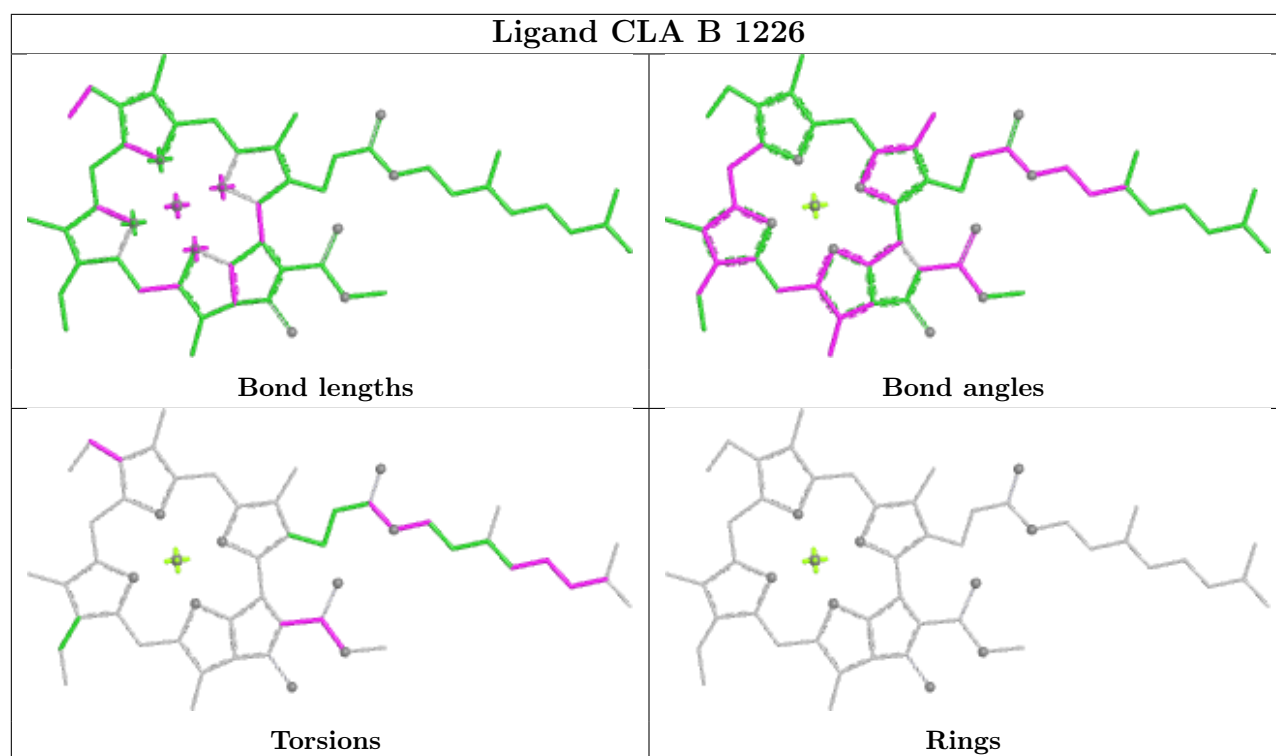
Bond angles



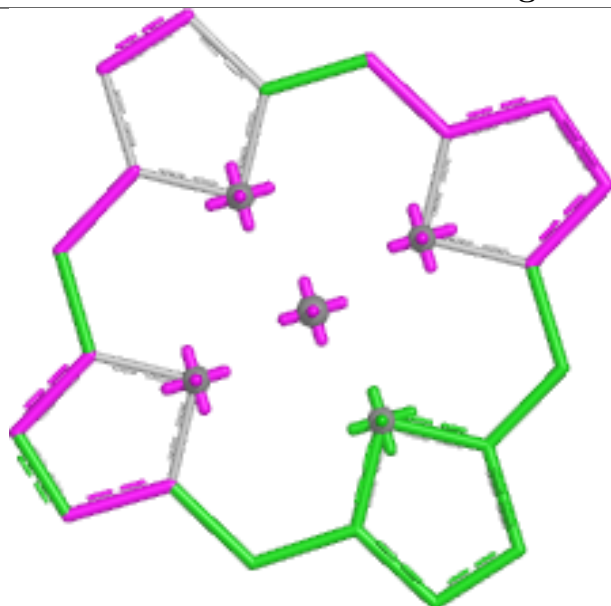
Torsions



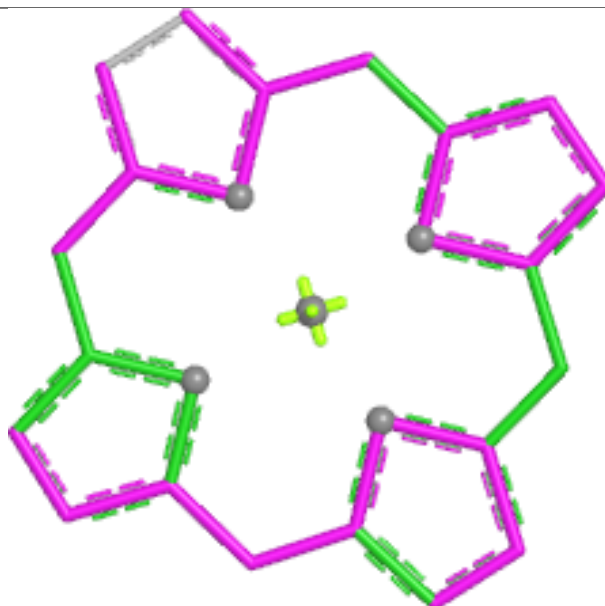
Rings



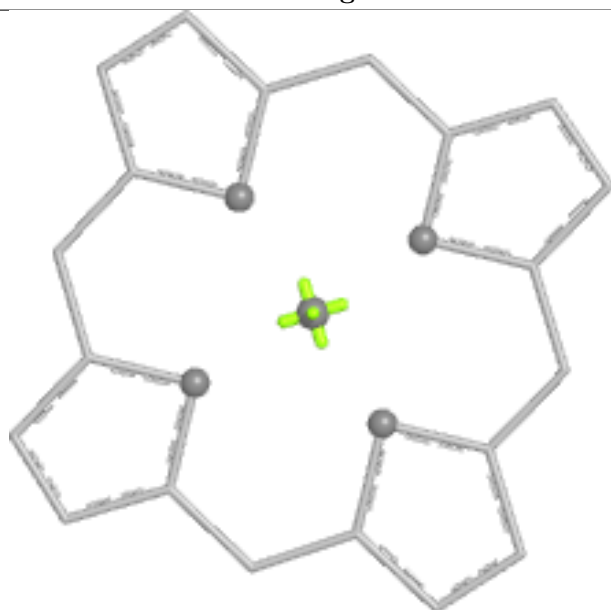
Ligand CLA 2 606



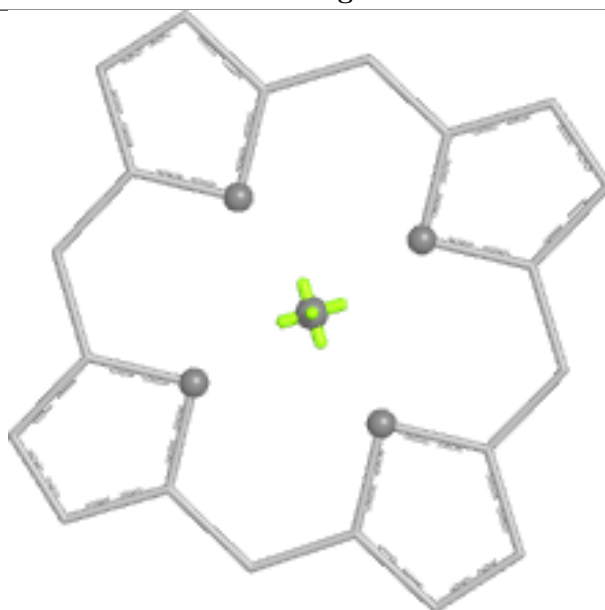
Bond lengths



Bond angles

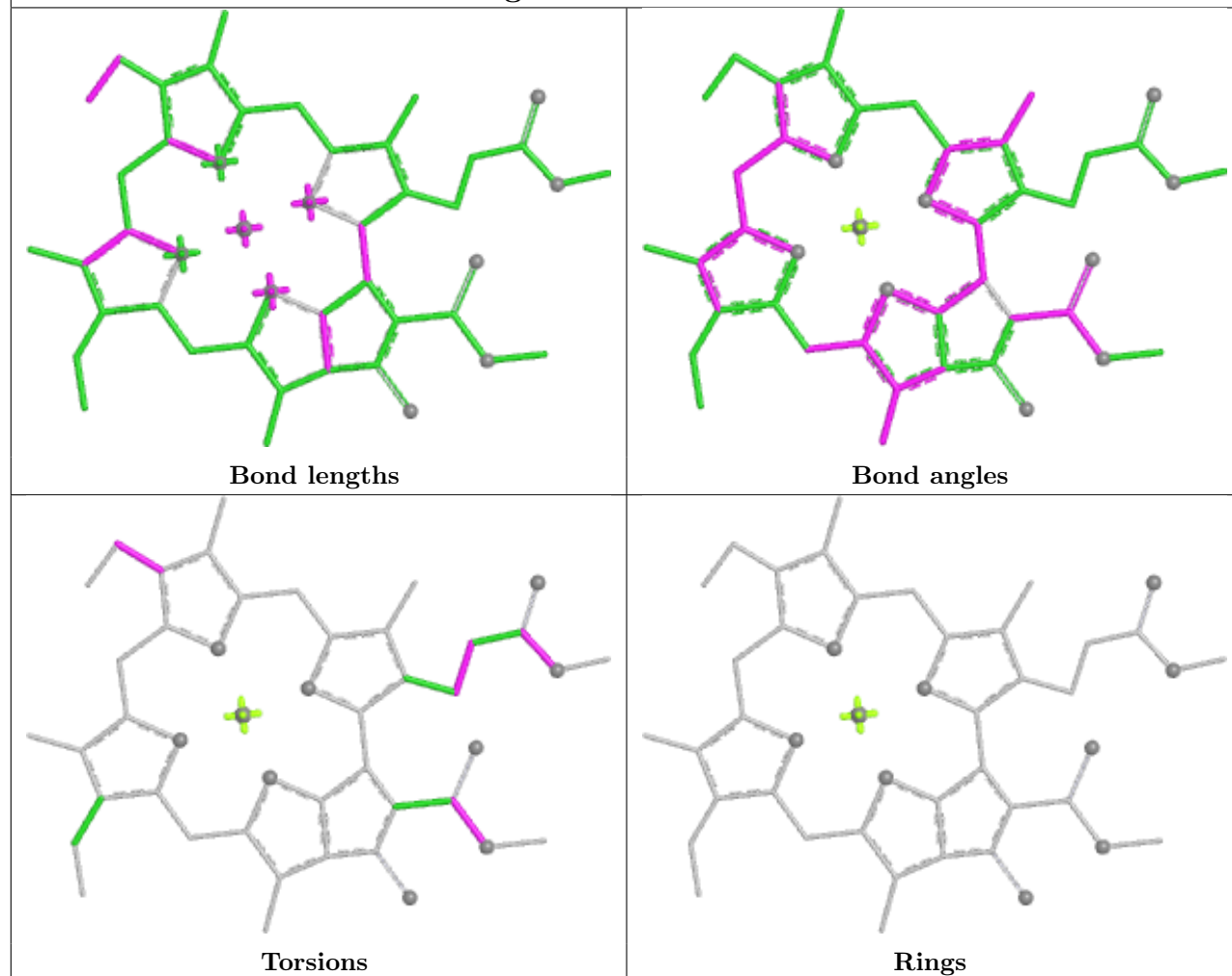


Torsions

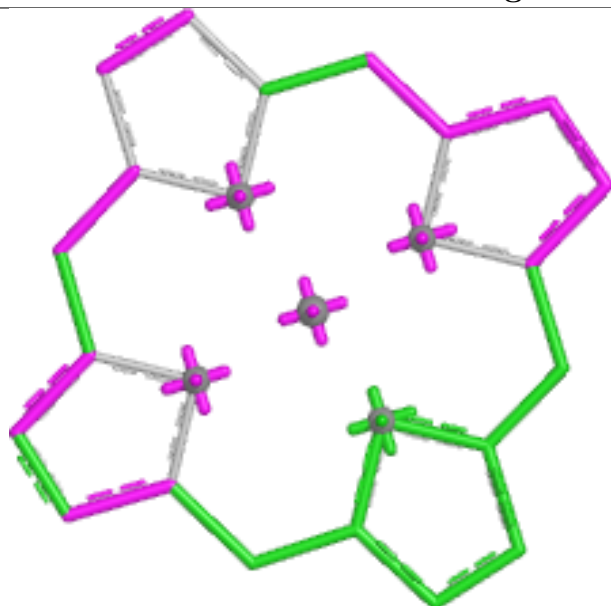


Rings

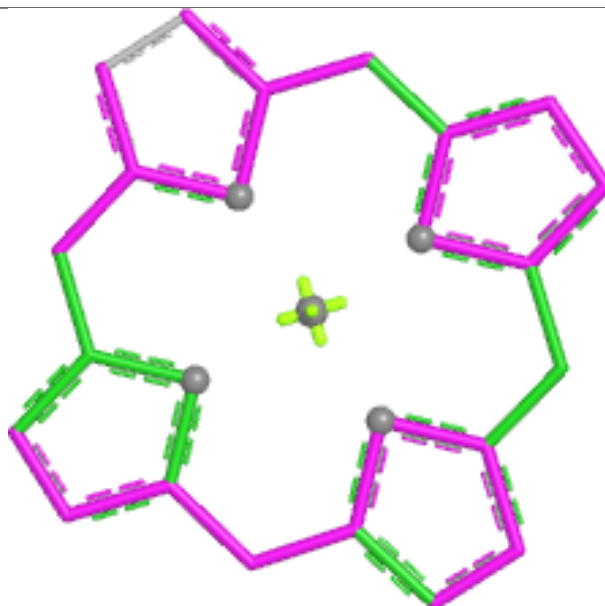
Ligand CLA A 1114



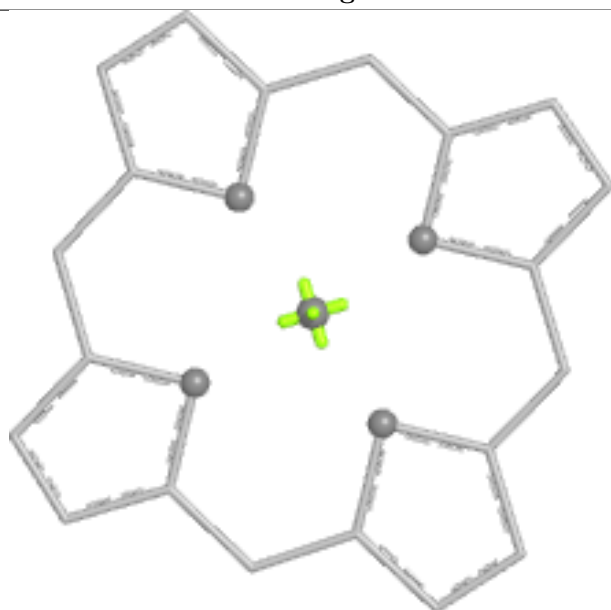
Ligand CLA A 1123



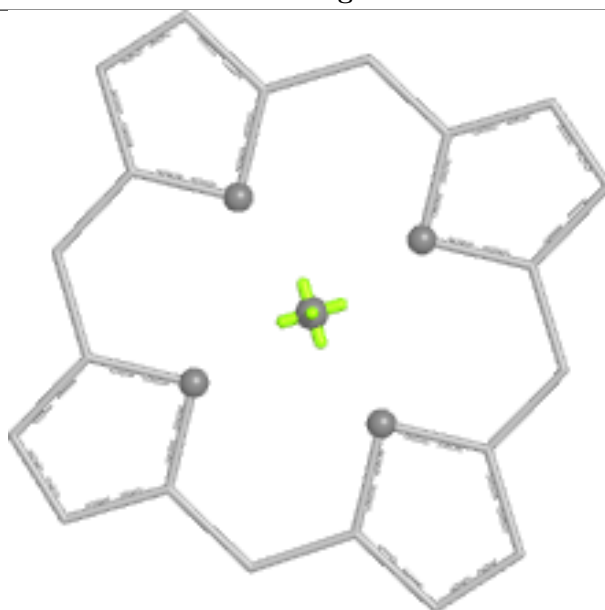
Bond lengths



Bond angles

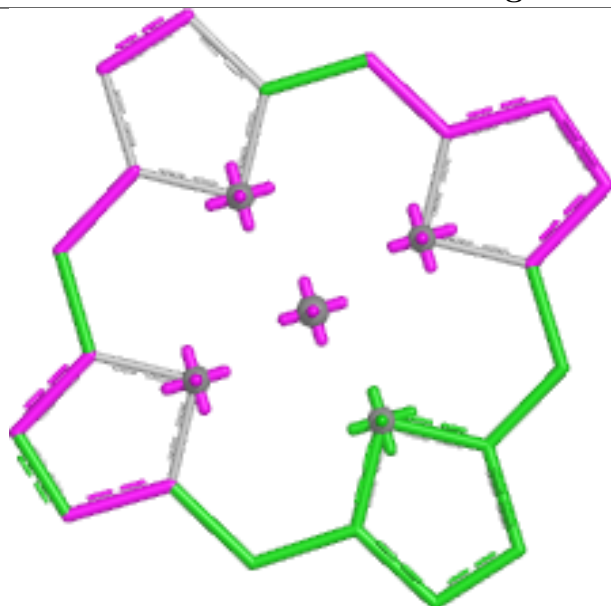


Torsions

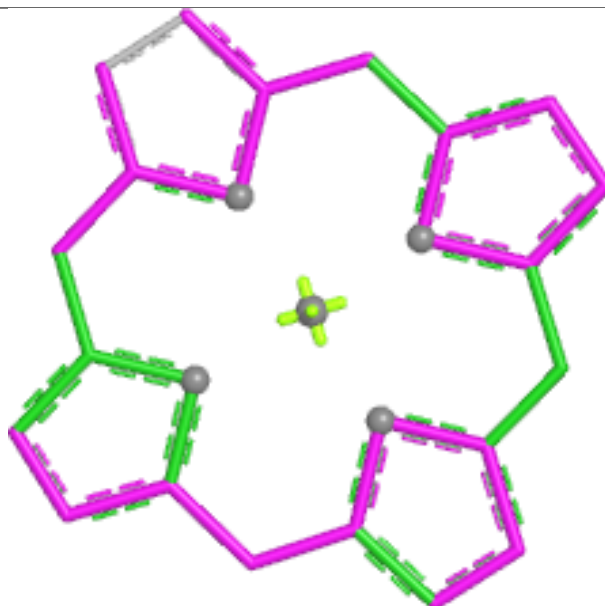


Rings

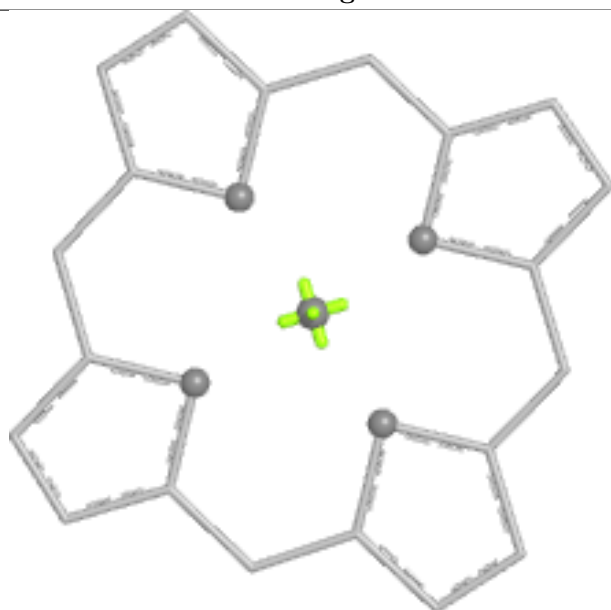
Ligand CLA B 1214



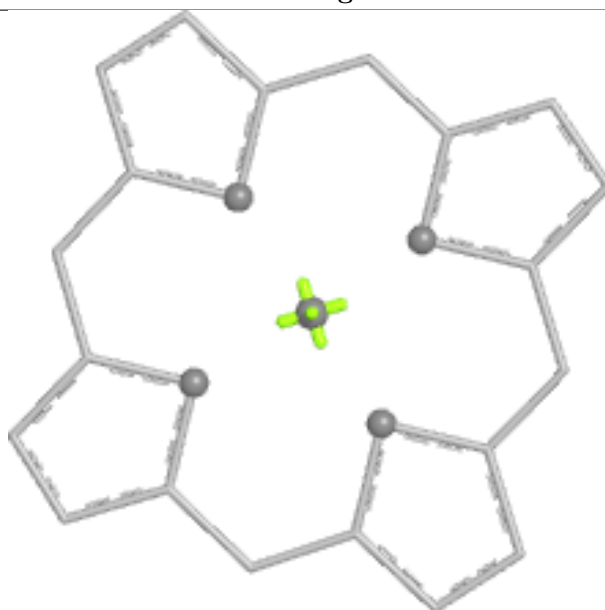
Bond lengths



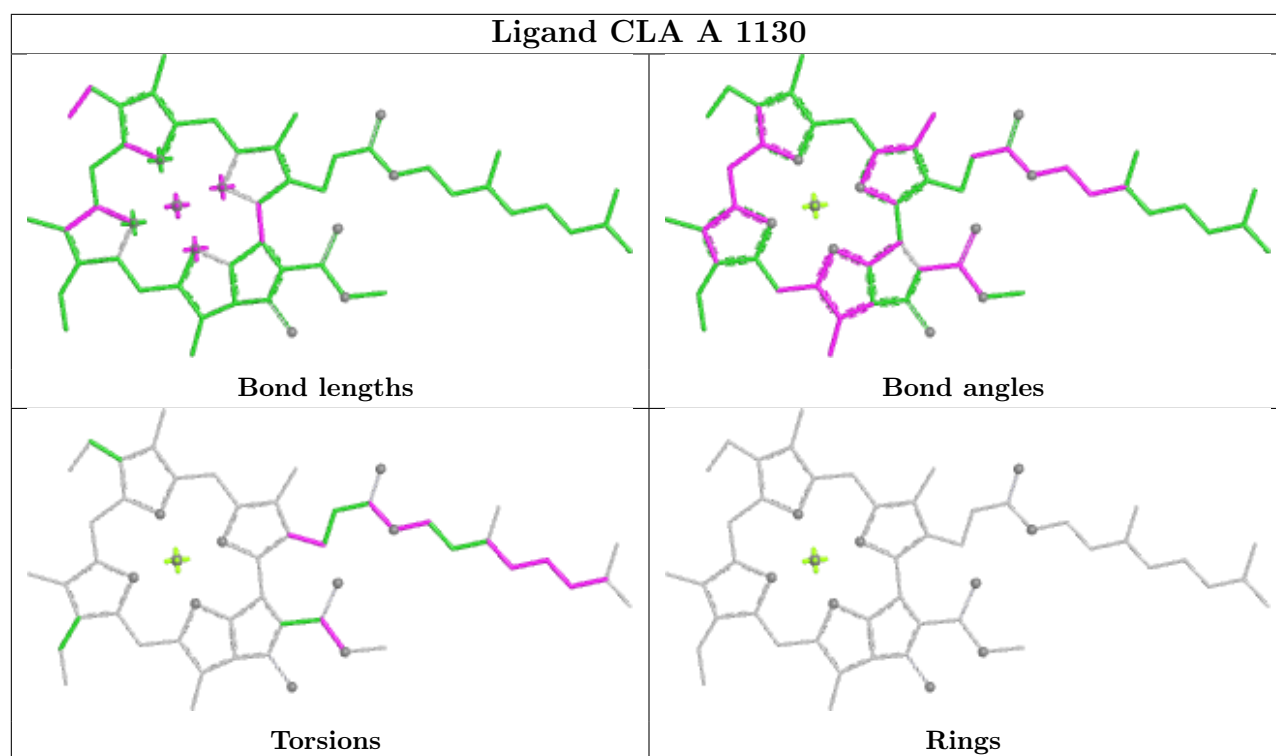
Bond angles



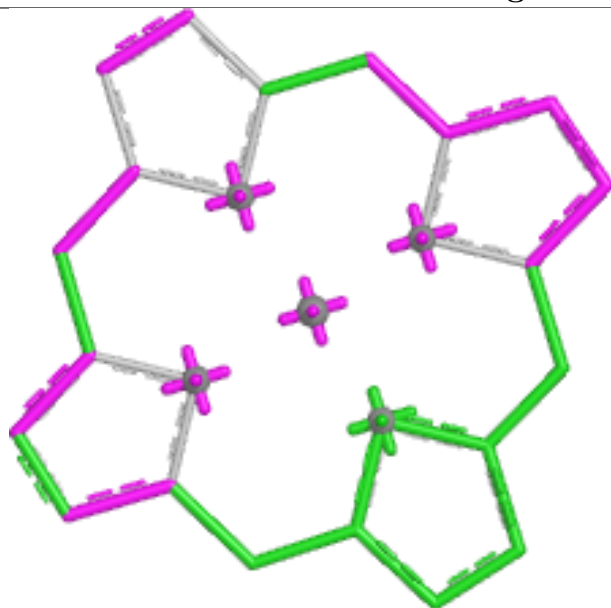
Torsions



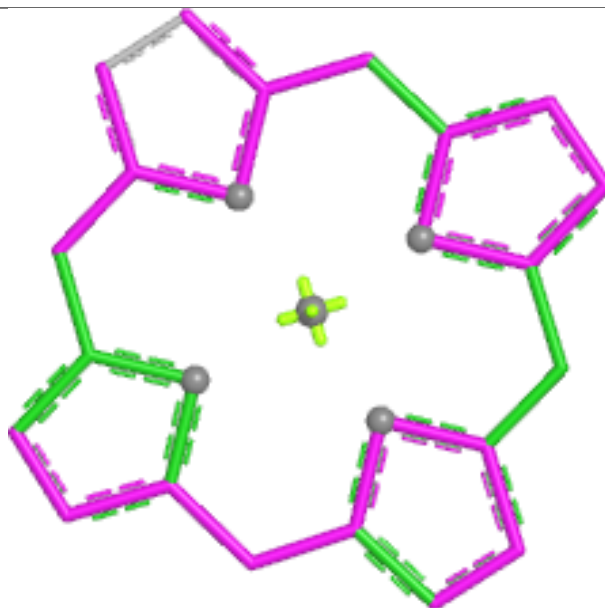
Rings



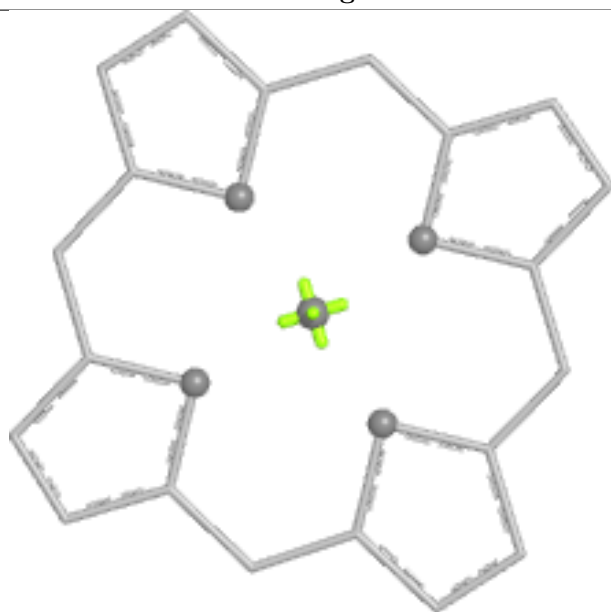
Ligand CLA F 1302



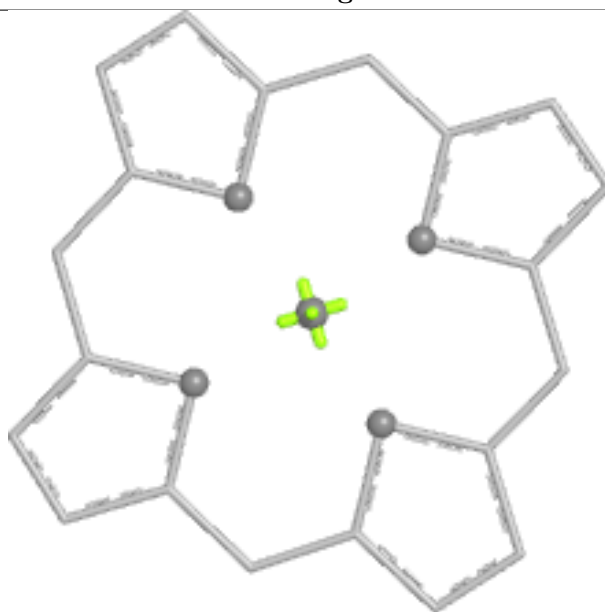
Bond lengths



Bond angles

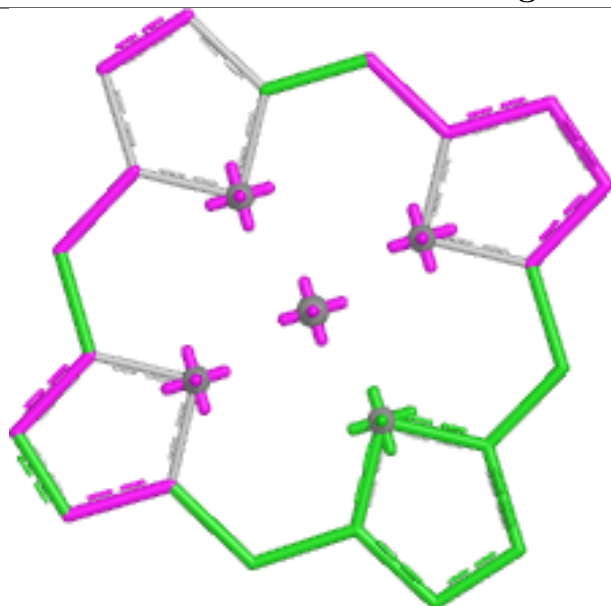


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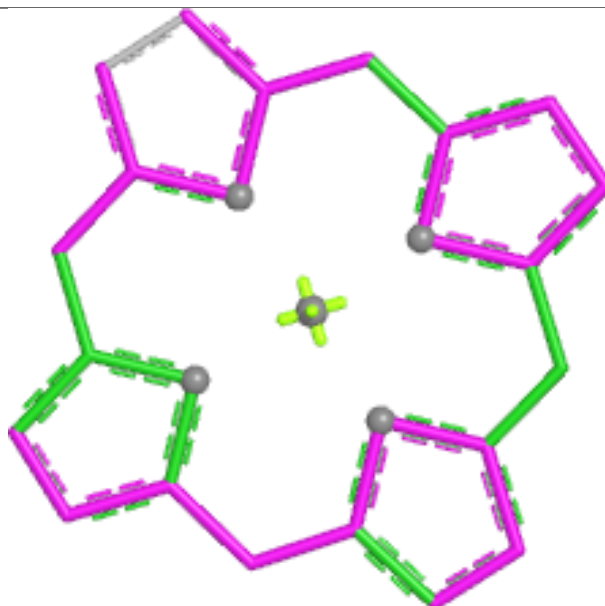


Rings

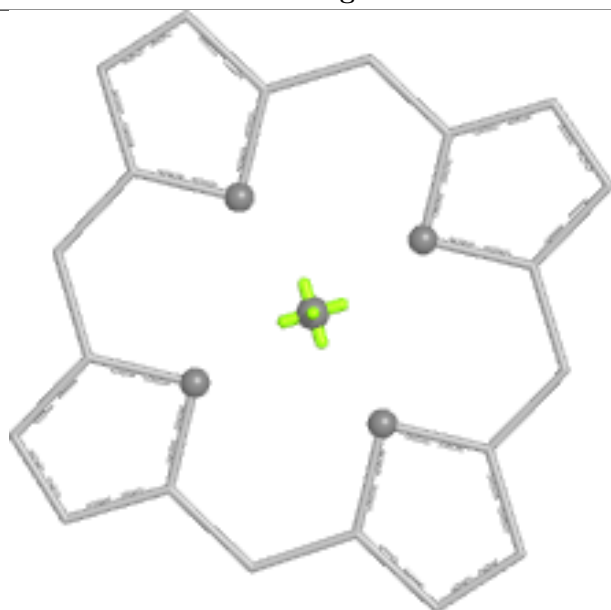
Ligand CLA 4 601



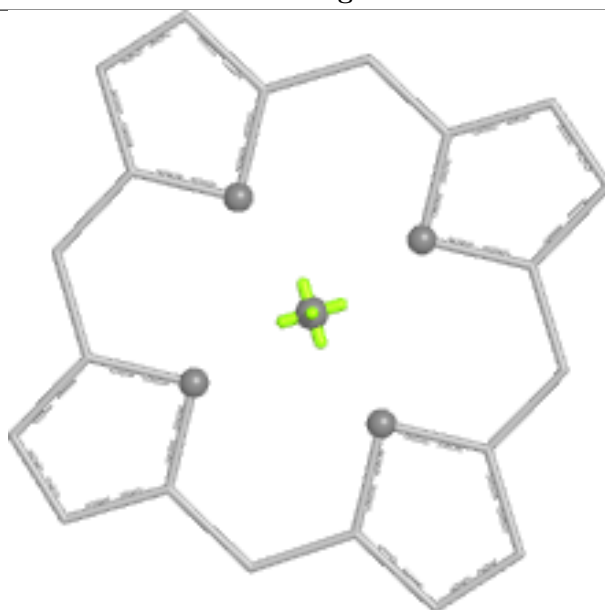
Bond lengths



Bond angles

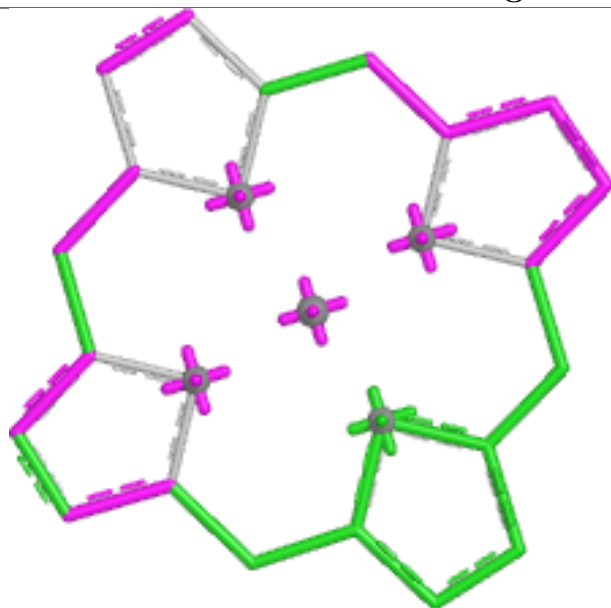


Torsions

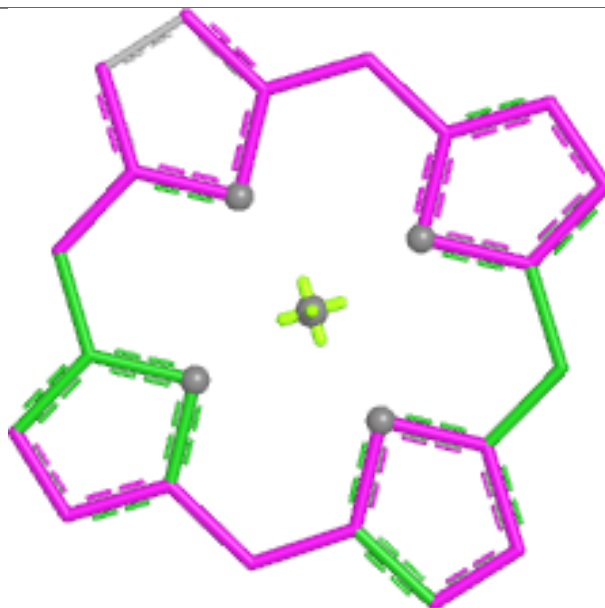


Rings

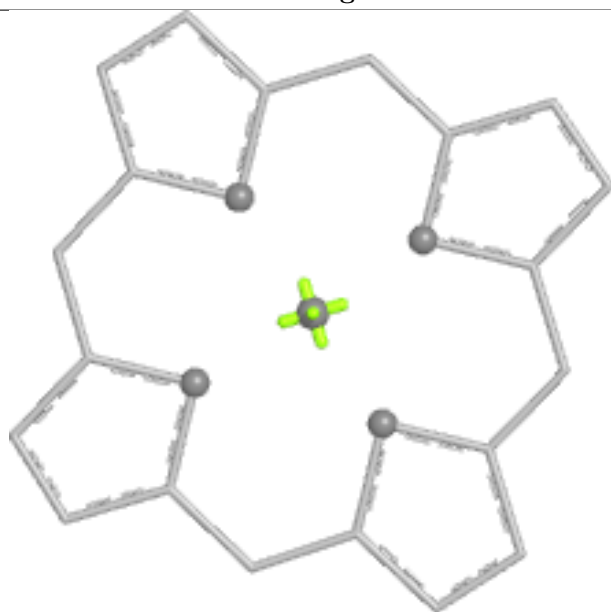
Ligand CLA B 1022



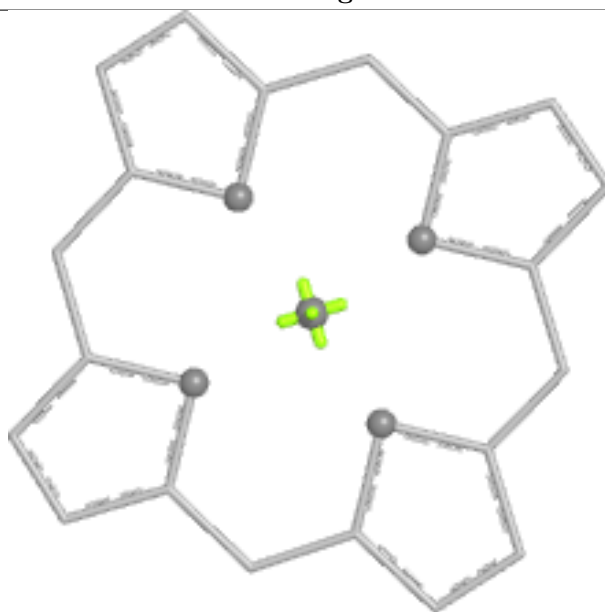
Bond lengths



Bond angles

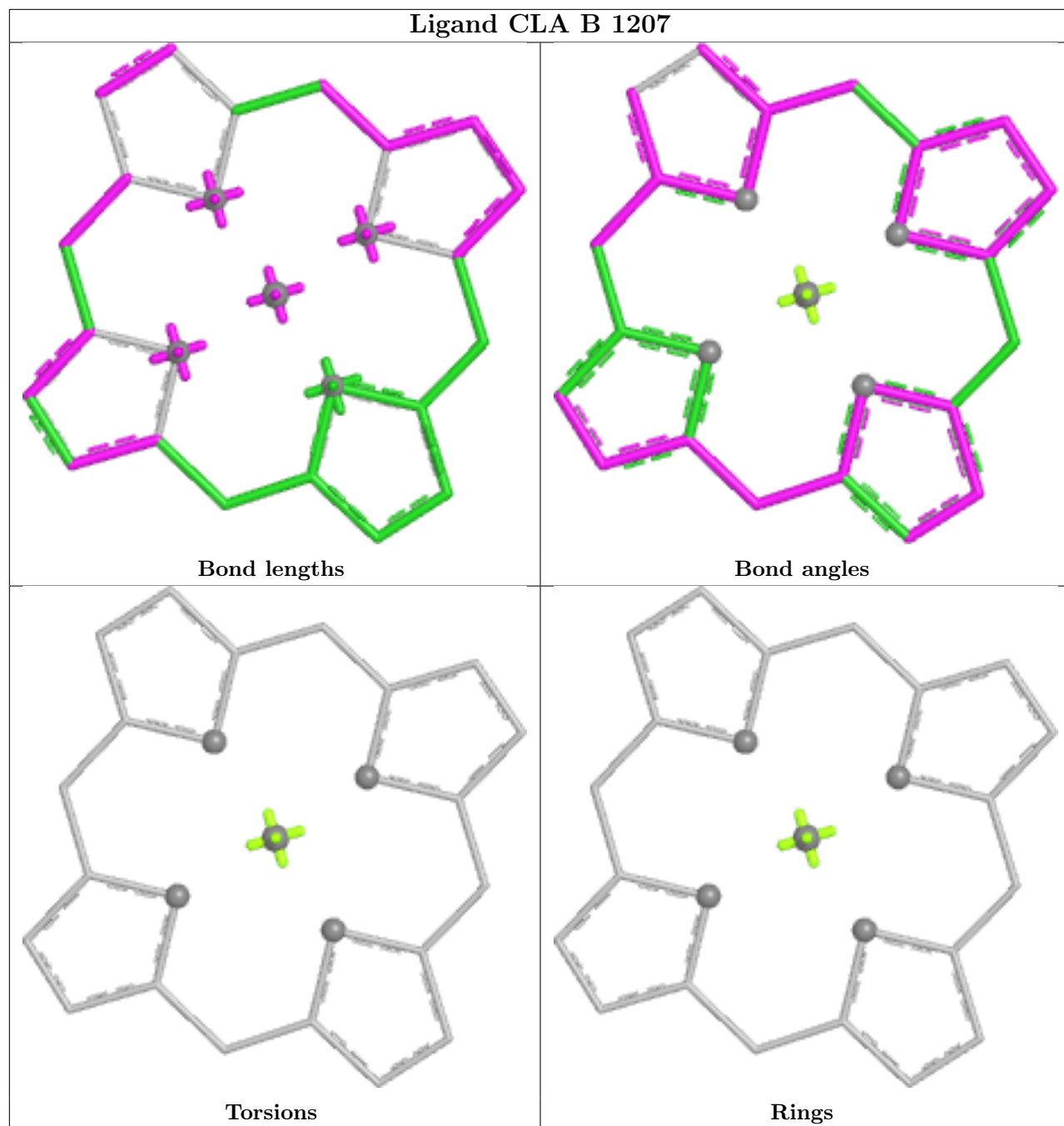


Torsions

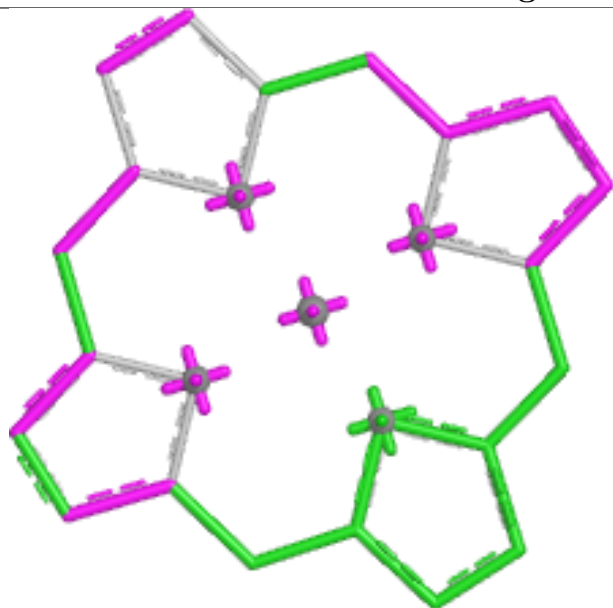


Rings

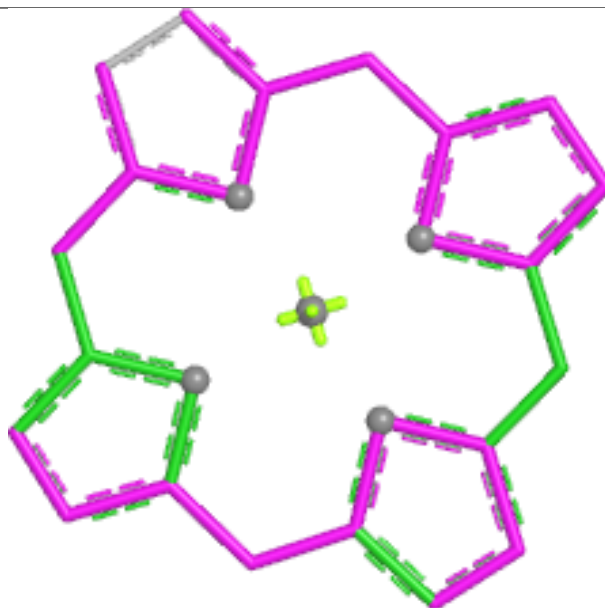
Ligand CLA B 1207



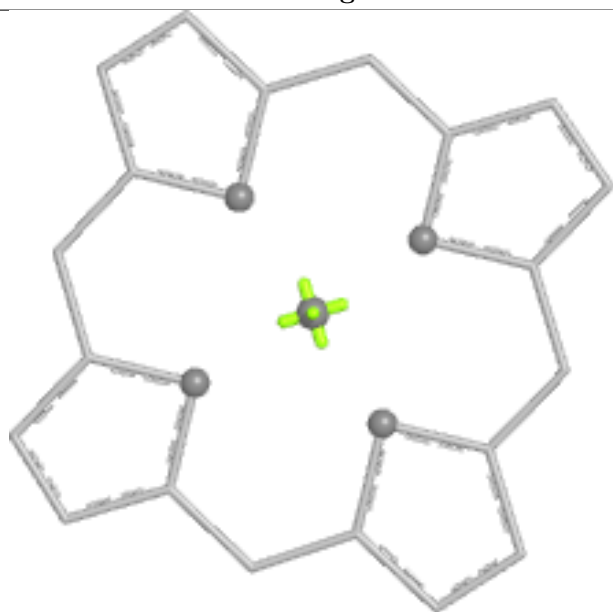
Ligand CLA 3 607



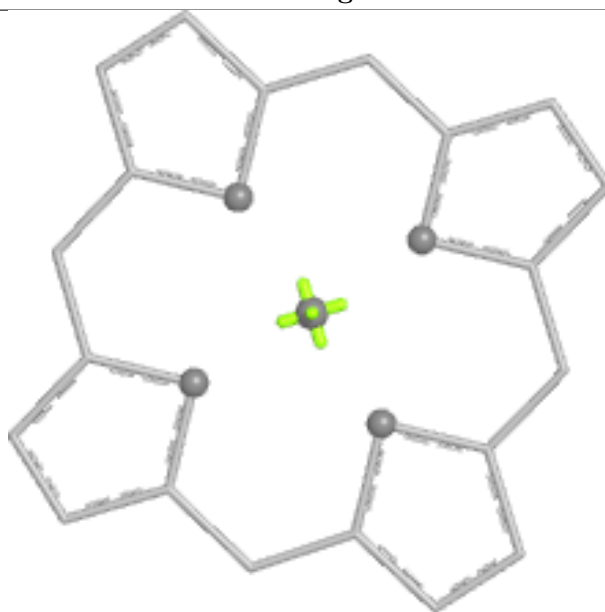
Bond lengths



Bond angles

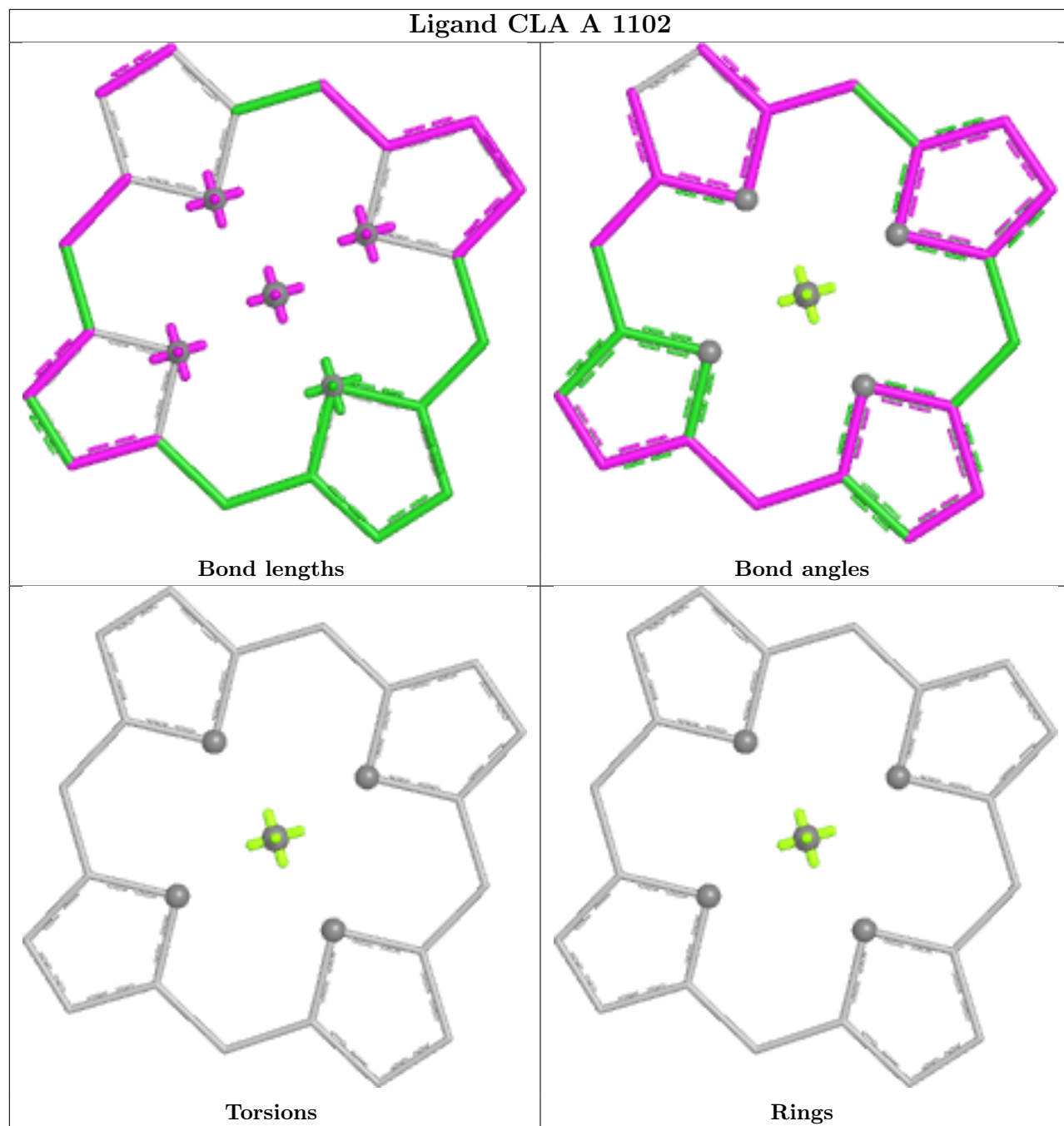


Torsions

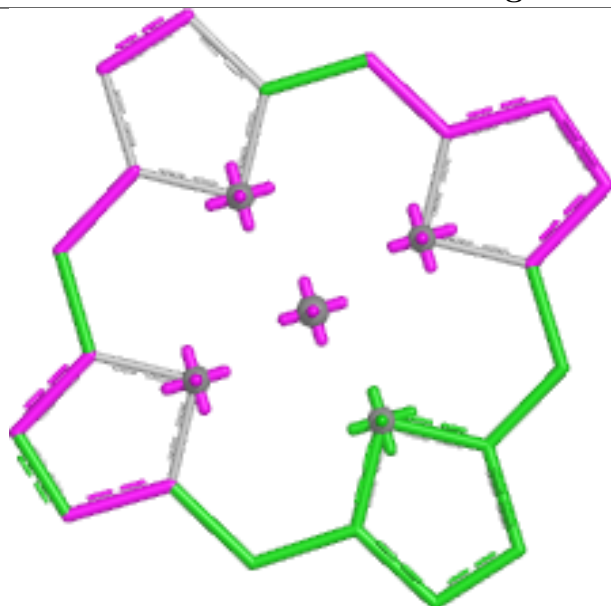


Rings

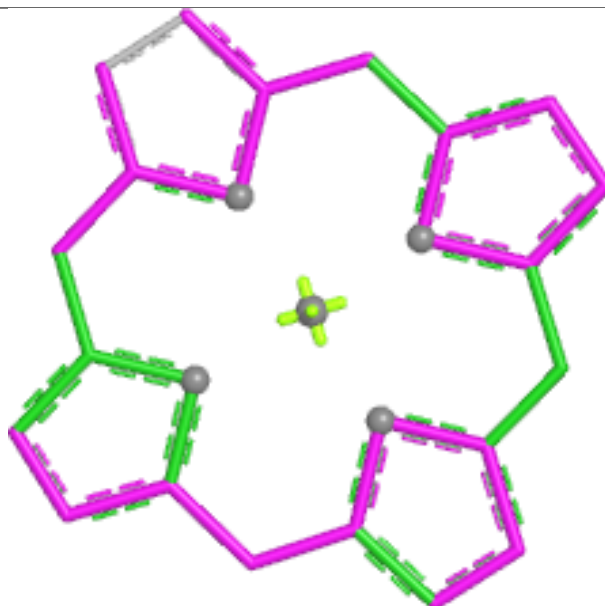
Ligand CLA A 1102



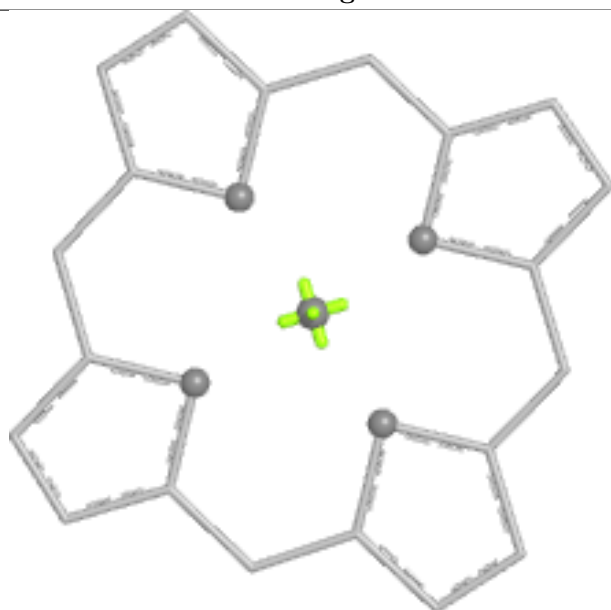
Ligand CLA B 1221



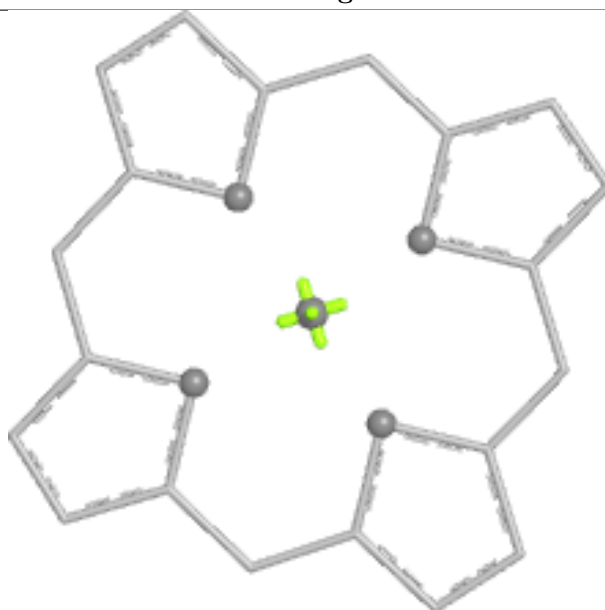
Bond lengths



Bond angles

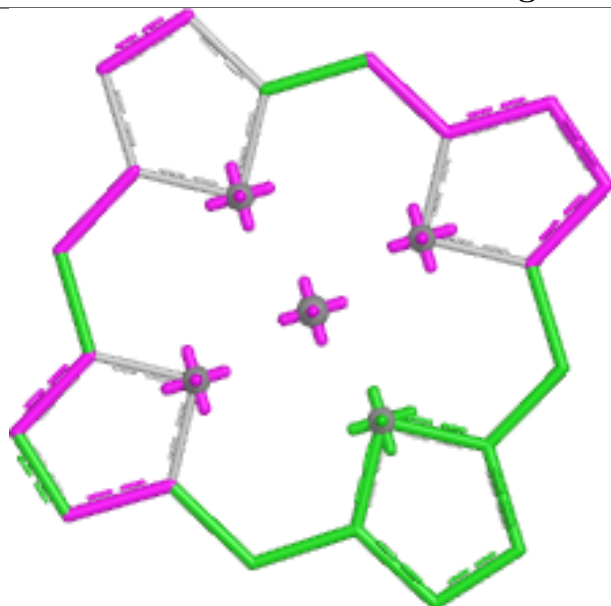


Torsions

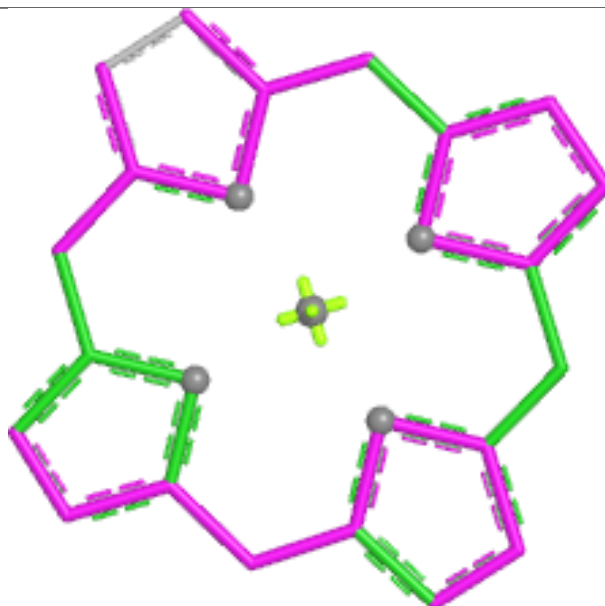


Rings

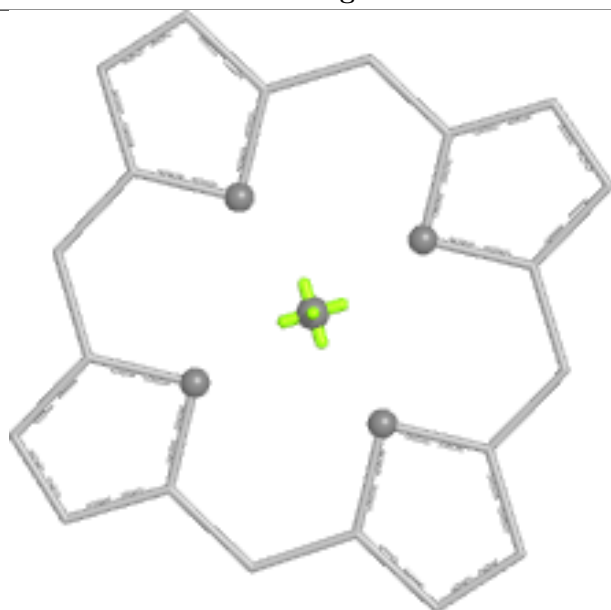
Ligand CLA 2 614



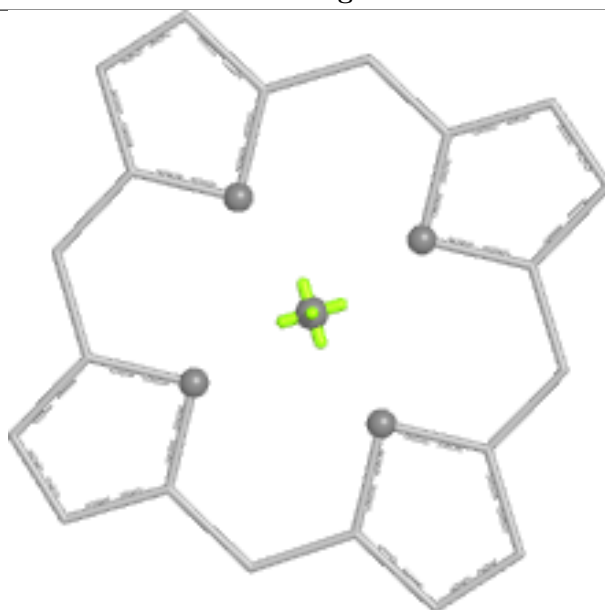
Bond lengths



Bond angles

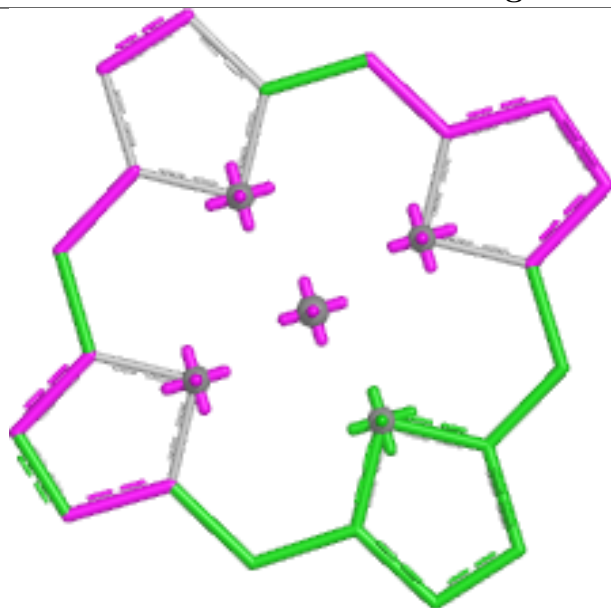


Torsions

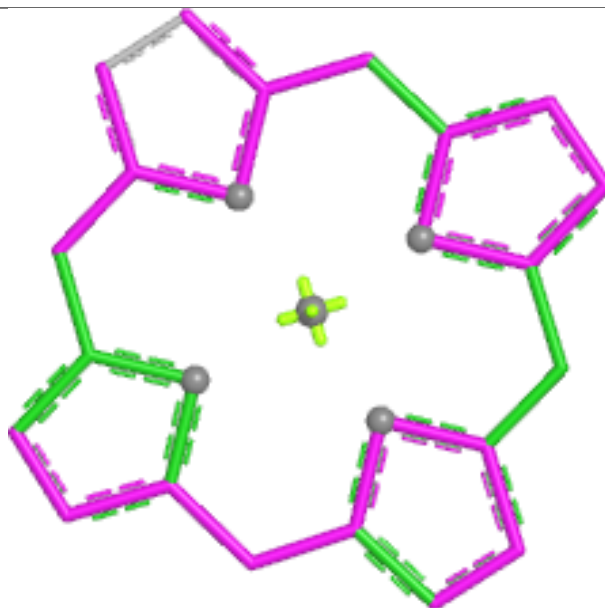


Rings

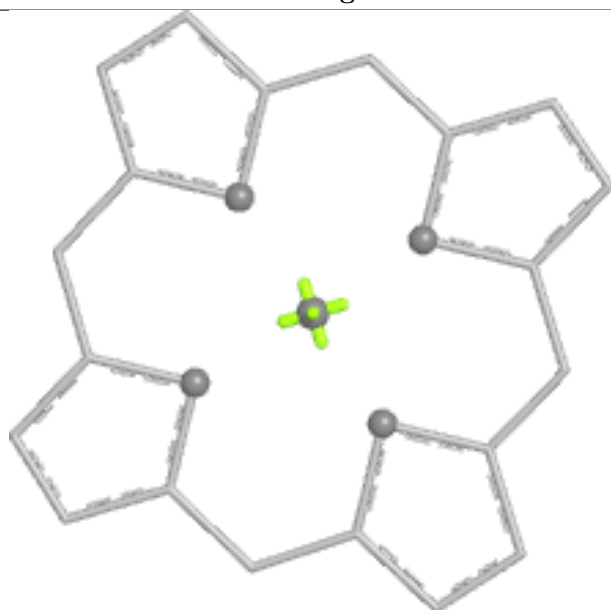
Ligand CLA B 1218



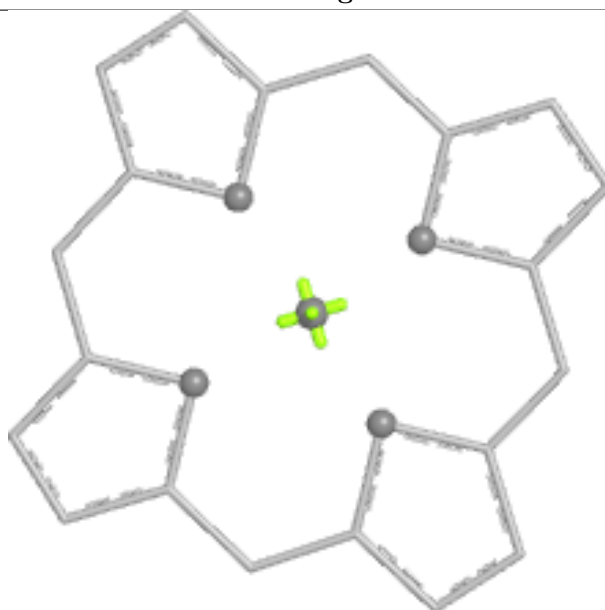
Bond lengths



Bond angles

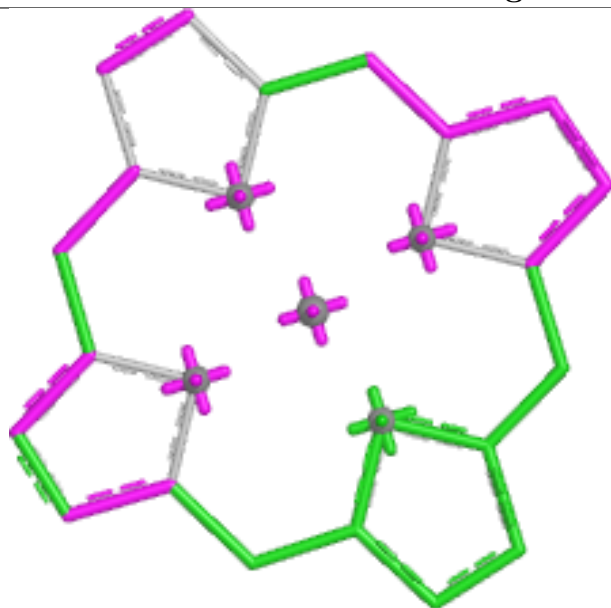


Torsions

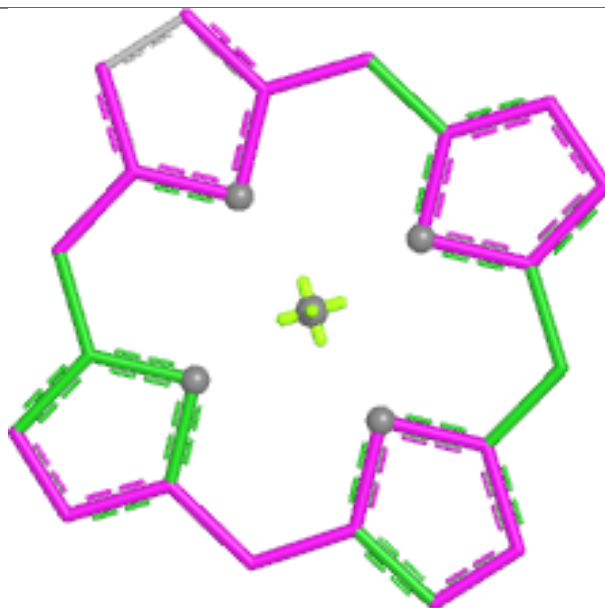


Rings

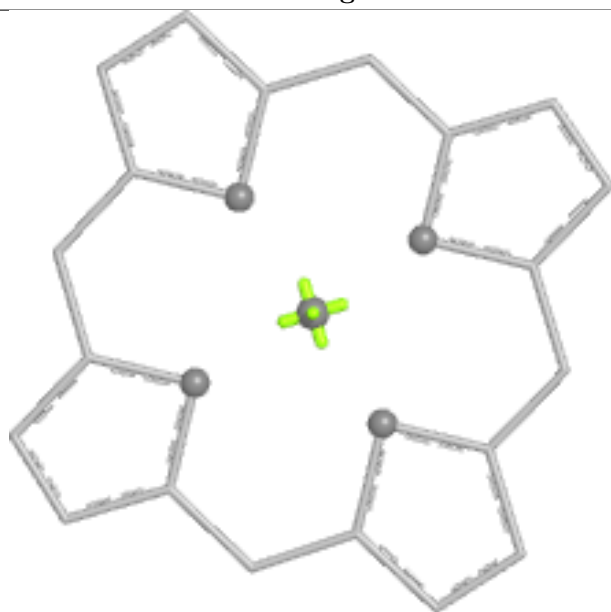
Ligand CLA B 1208



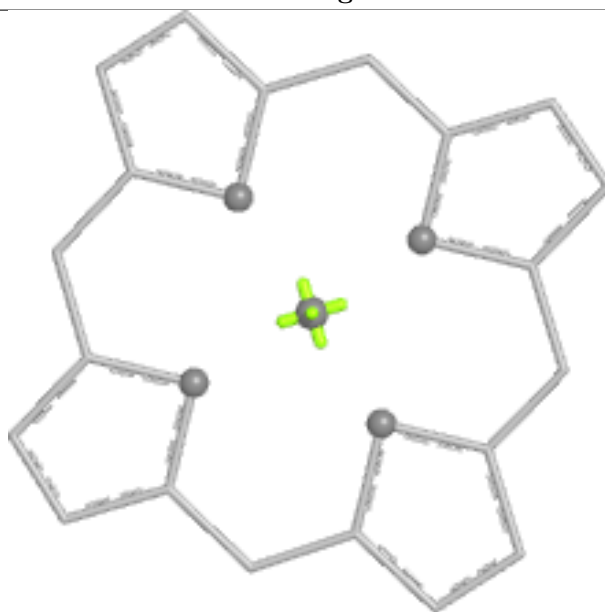
Bond lengths



Bond angles

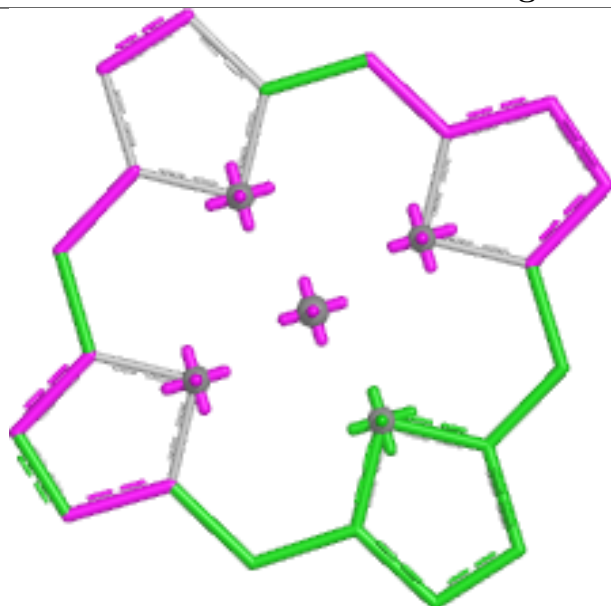


Torsions

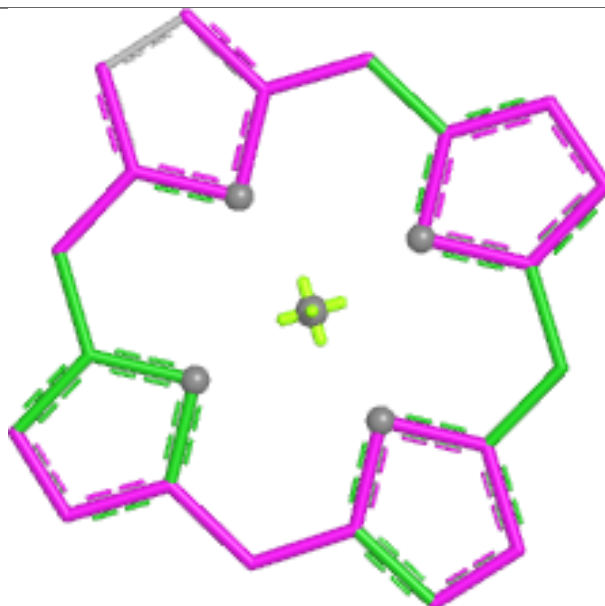


Rings

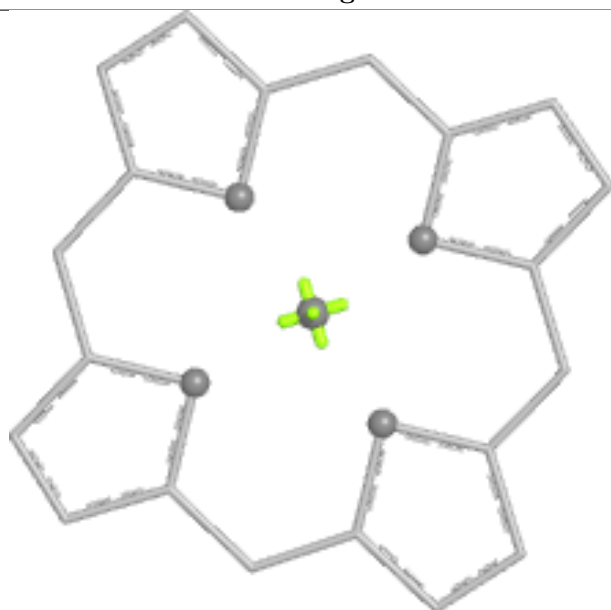
Ligand CLA 4 608



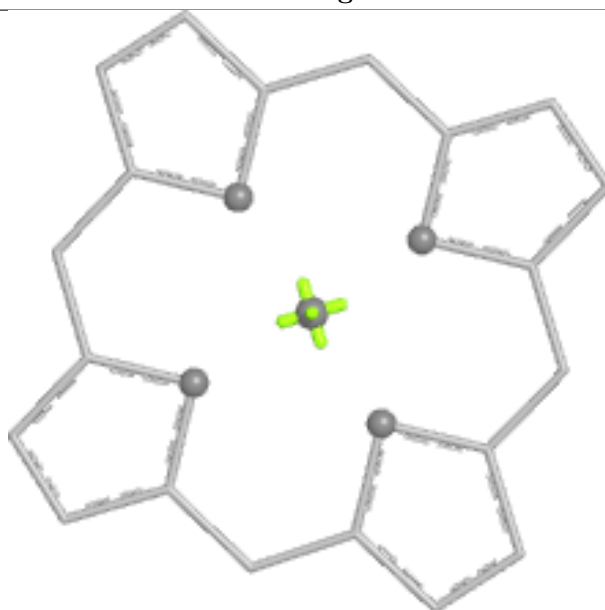
Bond lengths



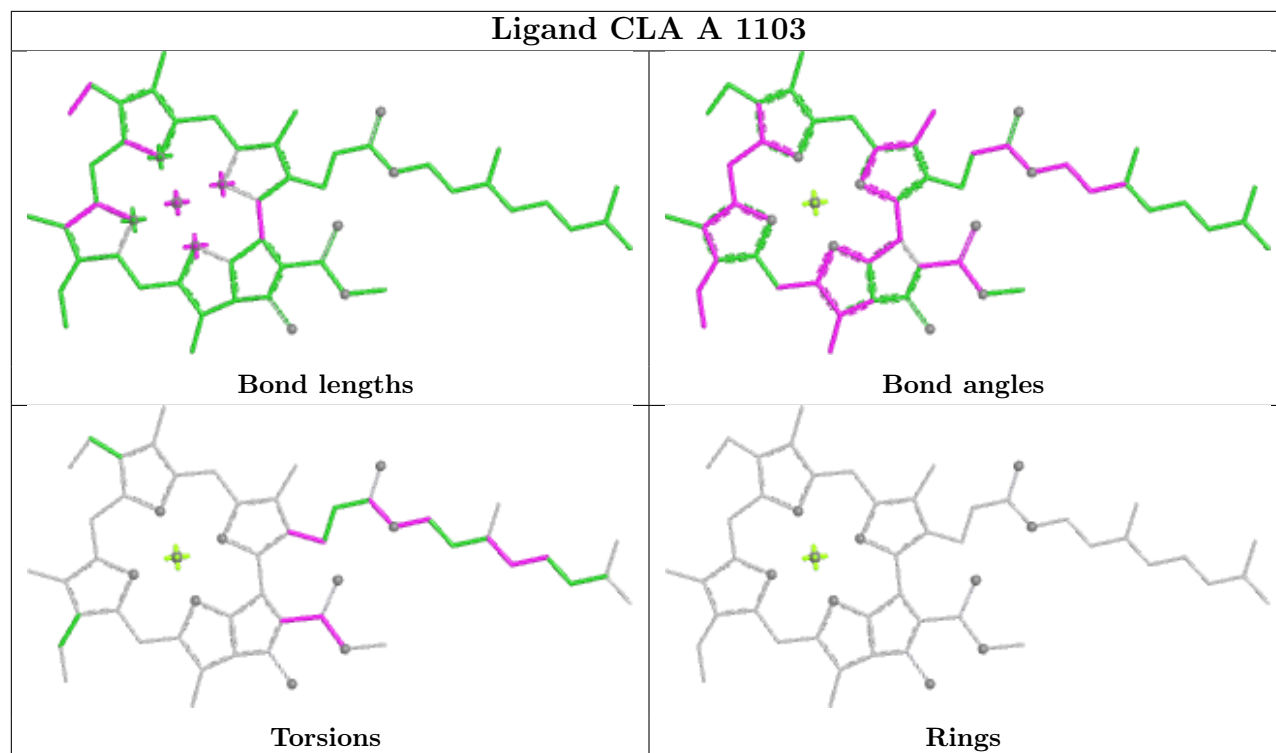
Bond angles

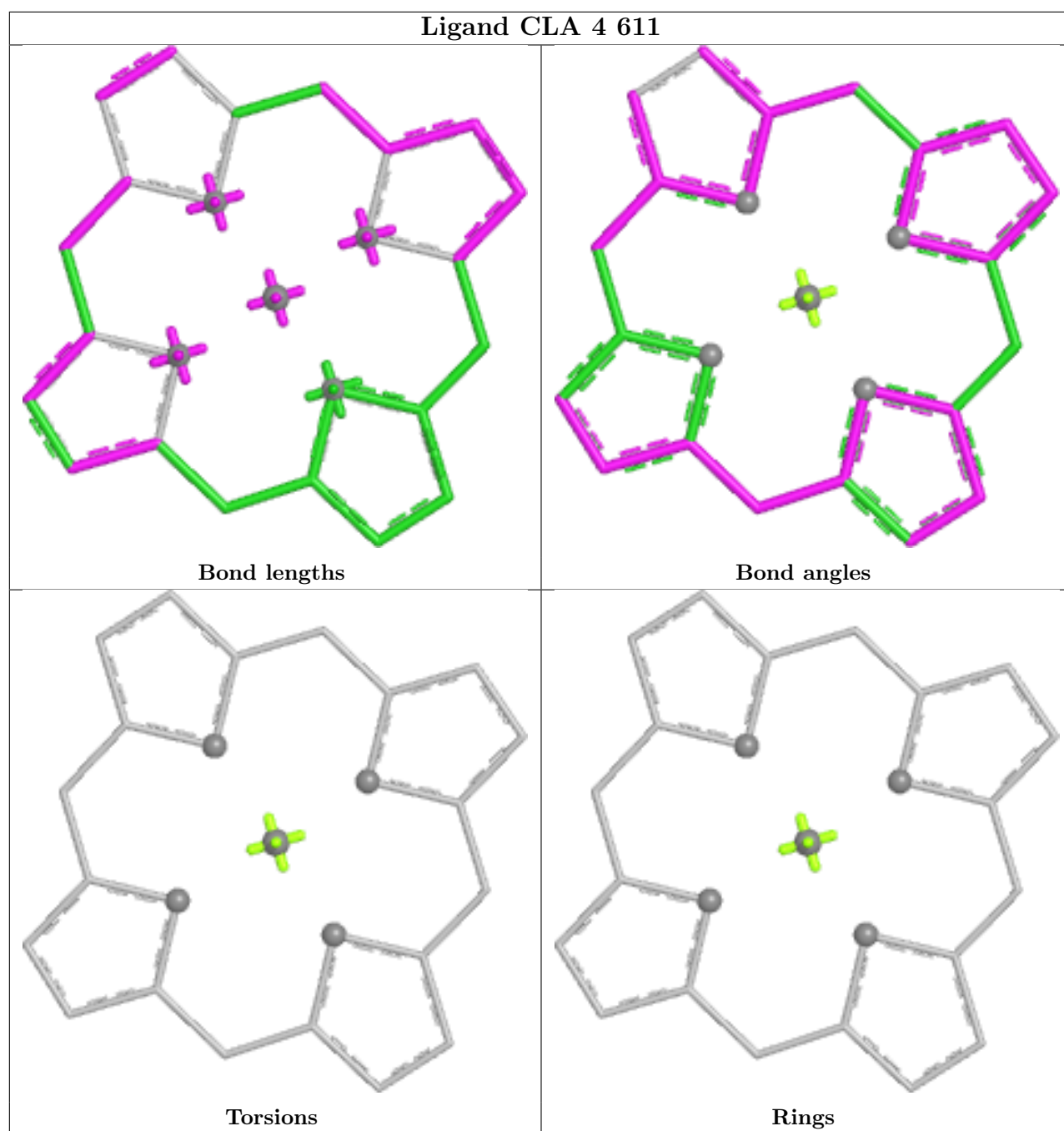


Torsions



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, 95th 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	2	144/222 (64%)	2.10	50 (34%) 1 2	118, 215, 376, 389	0
1	3	150/222 (67%)	1.77	45 (30%) 1 3	117, 198, 289, 310	0
2	4	116/214 (54%)	1.89	41 (35%) 1 2	169, 252, 362, 412	0
3	A	740/740 (100%)	1.62	189 (25%) 1 4	40, 129, 195, 255	0
4	B	725/725 (100%)	2.05	244 (33%) 1 2	101, 201, 318, 438	0
5	C	80/80 (100%)	2.67	36 (45%) 0 1	113, 162, 221, 292	0
6	D	124/124 (100%)	2.95	54 (43%) 0 1	132, 186, 251, 415	0
7	E	69/69 (100%)	3.20	21 (30%) 1 3	138, 189, 265, 445	0
8	F	153/155 (98%)	1.42	41 (26%) 1 3	117, 180, 248, 265	0
9	I	32/32 (100%)	1.52	9 (28%) 1 3	184, 254, 380, 425	0
10	J	38/38 (100%)	1.04	6 (15%) 5 9	88, 121, 212, 234	0
11	K	47/47 (100%)	1.01	8 (17%) 4 7	132, 172, 260, 291	0
12	L	140/140 (100%)	1.93	46 (32%) 1 2	156, 233, 383, 404	0
13	M	29/29 (100%)	0.87	2 (6%) 23 21	177, 247, 271, 276	0
14	O	98/98 (100%)	1.45	19 (19%) 3 6	212, 278, 405, 427	0
All	All	2685/2935 (91%)	1.89	811 (30%) 1 3	40, 183, 328, 445	0

All (811) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	E	30	SER	45.8
7	E	29	THR	38.4
6	D	107	ASN	33.8
7	E	31	LYS	31.9
4	B	130	ASN	26.2
4	B	128	ARG	18.4
5	C	2	ALA	18.0

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Mol	Chain	Res	Type	RSRZ
3	A	566	GLY	17.4
1	2	174	GLU	17.0
4	B	157	PRO	16.4
4	B	126	GLY	16.3
4	B	664	SER	15.0
5	C	32	ASP	14.8
6	D	109	GLY	14.6
4	B	75	GLU	14.3
4	B	127	ILE	14.3
4	B	129	ASN	14.2
6	D	125	ASN	14.2
1	3	74	SER	13.4
3	A	564	ASN	12.9
3	A	553	ALA	12.3
4	B	661	PHE	12.1
1	2	125	PHE	12.0
4	B	459	GLN	11.9
6	D	99	ASP	11.9
3	A	565	LEU	11.8
4	B	125	ILE	11.8
4	B	491	TRP	11.6
3	A	569	PHE	11.6
4	B	657	THR	11.3
3	A	313	GLY	11.2
6	D	18	TRP	11.1
14	O	70	VAL	11.0
5	C	3	HIS	10.9
4	B	470	TYR	10.9
1	2	94	THR	10.8
3	A	581	GLN	10.8
4	B	456	ILE	10.7
4	B	367	SER	10.6
4	B	660	MET	10.5
4	B	331	GLN	10.5
4	B	665	TRP	10.4
6	D	124	VAL	10.4
1	3	168	LEU	10.3
6	D	14	SER	9.9
4	B	119	TYR	9.8
3	A	410	VAL	9.7
6	D	112	GLN	9.5
12	L	13	PHE	9.5

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Mol	Chain	Res	Type	RSRZ
7	E	32	VAL	9.5
14	O	73	ILE	9.4
1	2	96	VAL	9.3
12	L	15	GLY	9.3
2	4	159	GLY	9.3
1	2	100	GLU	9.2
3	A	572	ASP	9.2
8	F	108	THR	9.2
3	A	554	ARG	9.1
4	B	74	PHE	9.1
3	A	571	CYS	8.9
6	D	108	LYS	8.9
4	B	658	GLY	8.9
3	A	570	PRO	8.9
12	L	76	LEU	8.8
1	3	76	GLU	8.8
11	K	35	GLN	8.7
6	D	113	VAL	8.7
3	A	151	ASN	8.6
4	B	68	VAL	8.4
12	L	17	LEU	8.4
6	D	81	TYR	8.3
4	B	160	LYS	8.3
4	B	118	VAL	8.3
3	A	563	ALA	8.3
3	A	311	ASN	8.2
12	L	75	TYR	8.2
1	2	173	ILE	8.2
4	B	133	LEU	8.2
2	4	233	ALA	8.1
4	B	509	THR	8.0
6	D	19	LEU	8.0
1	3	148	LEU	7.9
12	L	64	GLN	7.8
3	A	11	VAL	7.8
3	A	617	THR	7.7
4	B	537	LEU	7.6
4	B	131	VAL	7.6
1	3	77	TRP	7.5
2	4	156	ALA	7.5
3	A	625	SER	7.4
4	B	433	GLY	7.4

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Mol	Chain	Res	Type	RSRZ
4	B	409	MET	7.4
2	4	99	VAL	7.2
4	B	668	TYR	7.2
5	C	71	GLY	7.2
7	E	47	GLY	7.1
3	A	556	SER	7.1
4	B	124	THR	7.0
3	A	113	VAL	6.9
5	C	5	VAL	6.9
4	B	334	LEU	6.9
4	B	416	VAL	6.9
8	F	97	THR	6.8
3	A	562	LYS	6.8
7	E	28	GLU	6.7
1	2	95	GLU	6.7
4	B	671	GLU	6.7
4	B	417	ILE	6.7
4	B	554	SER	6.7
4	B	656	ALA	6.7
3	A	616	GLY	6.6
5	C	73	THR	6.6
2	4	162	GLU	6.6
5	C	4	THR	6.6
6	D	110	ARG	6.6
6	D	41	GLU	6.6
4	B	88	ALA	6.5
3	A	555	ASN	6.5
14	O	98	GLN	6.5
4	B	364	VAL	6.5
8	F	173	LEU	6.4
1	2	122	ALA	6.4
1	2	121	ILE	6.3
1	3	169	GLY	6.3
12	L	9	ASN	6.3
6	D	46	GLY	6.2
1	3	171	THR	6.1
6	D	123	ASN	6.1
3	A	552	TYR	6.0
4	B	69	ALA	6.0
8	F	86	LEU	6.0
3	A	109	PRO	6.0
1	3	147	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
5	C	35	LYS	5.9
4	B	122	TRP	5.9
6	D	97	PRO	5.9
1	3	181	GLN	5.9
3	A	722	ALA	5.9
2	4	234	GLY	5.8
12	L	136	LEU	5.8
5	C	33	GLY	5.8
8	F	96	ILE	5.8
3	A	94	PHE	5.8
6	D	12	LEU	5.8
6	D	11	PHE	5.7
1	2	175	SER	5.7
6	D	15	THR	5.7
12	L	70	ASN	5.7
4	B	669	TRP	5.7
3	A	10	LYS	5.7
3	A	582	VAL	5.7
4	B	503	SER	5.6
6	D	16	GLY	5.6
4	B	663	ILE	5.6
6	D	17	GLY	5.6
4	B	359	MET	5.6
4	B	158	LYS	5.6
2	4	163	PHE	5.6
4	B	692	LYS	5.6
2	4	230	LEU	5.5
3	A	186	TRP	5.5
4	B	270	ASP	5.5
12	L	65	LEU	5.4
4	B	366	GLN	5.4
6	D	58	TYR	5.4
4	B	86	PRO	5.4
3	A	479	PHE	5.3
6	D	128	GLN	5.3
4	B	410	LEU	5.3
4	B	429	PHE	5.3
4	B	273	HIS	5.2
9	I	27	PHE	5.2
11	K	56	ASN	5.2
2	4	100	ASN	5.2
4	B	156	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
3	A	567	PHE	5.1
4	B	732	SER	5.1
5	C	56	THR	5.1
4	B	83	LYS	5.1
3	A	508	ALA	5.1
5	C	50	GLY	5.1
1	2	103	ARG	5.1
3	A	524	LEU	5.0
3	A	746	ALA	5.0
3	A	579	THR	5.0
4	B	162	SER	5.0
4	B	115	TYR	5.0
4	B	116	SER	5.0
1	3	146	PRO	4.9
4	B	24	GLY	4.9
4	B	87	LEU	4.9
1	2	101	TRP	4.9
3	A	266	LYS	4.9
8	F	81	LYS	4.9
8	F	111	ALA	4.9
4	B	667	GLY	4.9
3	A	697	ILE	4.9
4	B	14	SER	4.9
4	B	202	GLY	4.9
3	A	269	SER	4.8
8	F	177	GLU	4.8
4	B	353	MET	4.8
12	L	139	PHE	4.8
3	A	84	LEU	4.8
2	4	158	ILE	4.8
3	A	664	ALA	4.8
4	B	132	GLU	4.8
3	A	619	THR	4.8
4	B	584	THR	4.8
4	B	587	TRP	4.8
8	F	123	TRP	4.8
4	B	493	PRO	4.7
3	A	568	ARG	4.7
4	B	469	LEU	4.7
9	I	26	LEU	4.7
1	3	78	LEU	4.7
1	3	177	TRP	4.6

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Mol	Chain	Res	Type	RSRZ
5	C	48	CYS	4.6
8	F	95	LEU	4.6
6	D	129	VAL	4.6
4	B	159	PHE	4.6
4	B	65	LEU	4.5
4	B	536	ALA	4.5
6	D	56	LEU	4.5
4	B	255	PHE	4.5
9	I	30	ILE	4.5
8	F	183	SER	4.5
2	4	119	HIS	4.5
3	A	300	LEU	4.5
4	B	533	VAL	4.5
4	B	659	PHE	4.4
4	B	134	TYR	4.4
4	B	595	LYS	4.4
14	O	67	ASN	4.4
3	A	548	LYS	4.4
4	B	672	LEU	4.4
3	A	60	SER	4.4
1	3	81	ALA	4.4
8	F	84	THR	4.4
14	O	97	THR	4.4
3	A	309	ARG	4.4
4	B	413	LYS	4.4
12	L	74	LYS	4.3
3	A	133	GLY	4.3
3	A	108	LYS	4.3
2	4	231	GLY	4.3
3	A	179	LYS	4.3
12	L	6	LYS	4.3
8	F	98	ASP	4.3
3	A	577	GLY	4.3
4	B	451	ILE	4.3
8	F	106	GLU	4.3
3	A	666	GLY	4.3
3	A	34	SER	4.2
3	A	633	ALA	4.2
7	E	59	VAL	4.2
3	A	215	HIS	4.2
1	2	185	PHE	4.2
4	B	650	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
12	L	73	ILE	4.2
8	F	126	ARG	4.1
10	J	30	ARG	4.1
4	B	338	SER	4.1
3	A	621	ASN	4.1
10	J	33	PRO	4.1
4	B	27	THR	4.1
4	B	490	LEU	4.1
6	D	23	GLU	4.0
3	A	156	TYR	4.0
8	F	116	TYR	4.0
3	A	19	PRO	4.0
1	3	75	LEU	4.0
6	D	92	VAL	4.0
4	B	502	GLU	3.9
3	A	719	GLN	3.9
4	B	335	ALA	3.9
3	A	380	TYR	3.9
4	B	152	TRP	3.9
3	A	132	GLN	3.8
2	4	160	PHE	3.8
12	L	137	THR	3.8
3	A	509	ASP	3.8
4	B	425	LEU	3.8
4	B	549	LYS	3.8
4	B	535	GLY	3.8
6	D	10	SER	3.8
4	B	36	GLY	3.8
3	A	13	VAL	3.8
3	A	89	PHE	3.8
1	3	178	LYS	3.8
9	I	32	LYS	3.8
6	D	45	GLY	3.7
4	B	405	VAL	3.7
3	A	243	ARG	3.7
2	4	157	PHE	3.7
3	A	618	VAL	3.7
4	B	136	GLY	3.7
5	C	70	GLY	3.7
3	A	383	GLN	3.7
5	C	81	TYR	3.7
3	A	643	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	2	176	VAL	3.7
5	C	76	SER	3.7
4	B	385	PHE	3.7
1	2	189	PRO	3.7
3	A	631	ASN	3.7
4	B	539	ALA	3.7
12	L	67	PRO	3.7
12	L	16	HIS	3.7
4	B	64	ASN	3.7
5	C	46	GLU	3.7
4	B	434	LEU	3.6
6	D	91	GLU	3.6
1	2	235	GLU	3.6
4	B	487	ALA	3.6
5	C	77	MET	3.6
7	E	52	ASN	3.6
7	E	14	GLU	3.6
1	2	128	PHE	3.6
4	B	356	TYR	3.6
3	A	478	VAL	3.6
3	A	123	LEU	3.6
14	O	144	ALA	3.5
4	B	407	ALA	3.5
1	2	135	SER	3.5
4	B	418	SER	3.5
3	A	254	GLN	3.5
12	L	91	LEU	3.5
4	B	28	ALA	3.5
3	A	587	HIS	3.5
12	L	40	GLY	3.5
3	A	217	SER	3.5
3	A	652	SER	3.5
4	B	365	THR	3.5
4	B	374	GLN	3.5
9	I	23	MET	3.5
4	B	601	GLN	3.5
3	A	381	PRO	3.5
3	A	320	GLN	3.4
1	2	182	PRO	3.4
4	B	33	SER	3.4
1	2	102	LEU	3.4
1	2	195	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	3	174	SER	3.4
12	L	14	VAL	3.4
4	B	117	GLY	3.4
4	B	164	SER	3.4
4	B	254	THR	3.4
3	A	226	ALA	3.4
1	2	130	PHE	3.4
1	3	188	GLY	3.4
9	I	29	ALA	3.4
9	I	31	GLU	3.4
5	C	61	ASP	3.4
7	E	43	VAL	3.4
3	A	624	ILE	3.4
2	4	118	LEU	3.4
4	B	556	PRO	3.3
12	L	133	TYR	3.3
3	A	580	CYS	3.3
8	F	80	ASP	3.3
3	A	667	LEU	3.3
7	E	48	LEU	3.3
12	L	71	THR	3.3
3	A	124	ASN	3.3
1	3	120	HIS	3.3
1	3	80	GLU	3.3
3	A	528	ASP	3.3
4	B	534	LYS	3.3
4	B	148	LEU	3.3
4	B	526	HIS	3.3
6	D	6	MET	3.3
3	A	314	ILE	3.3
8	F	112	LEU	3.3
12	L	106	GLN	3.3
3	A	412	ASP	3.3
4	B	344	SER	3.3
12	L	12	PRO	3.3
4	B	700	ILE	3.3
12	L	59	ILE	3.3
1	2	183	GLY	3.3
2	4	122	VAL	3.3
8	F	132	THR	3.3
3	A	447	HIS	3.3
4	B	510	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
4	B	580	TRP	3.3
1	3	205	THR	3.3
3	A	471	THR	3.3
12	L	36	ILE	3.3
1	2	97	PHE	3.2
4	B	137	ALA	3.2
3	A	201	LEU	3.2
4	B	411	ALA	3.2
4	B	654	VAL	3.2
3	A	534	ILE	3.2
3	A	701	HIS	3.2
12	L	2	THR	3.2
4	B	138	LEU	3.2
8	F	107	PHE	3.2
4	B	214	PRO	3.2
4	B	406	LEU	3.2
4	B	135	THR	3.2
4	B	26	ALA	3.2
4	B	82	LEU	3.1
4	B	363	TYR	3.1
3	A	700	ALA	3.1
3	A	735	THR	3.1
4	B	629	LEU	3.1
4	B	346	VAL	3.1
8	F	99	GLY	3.1
4	B	271	MET	3.1
2	4	175	MET	3.1
4	B	40	GLU	3.1
6	D	118	SER	3.1
13	M	27	GLN	3.1
2	4	105	GLY	3.1
3	A	315	GLY	3.1
3	A	744	ILE	3.1
10	J	31	PHE	3.1
11	K	34	THR	3.1
5	C	57	ALA	3.1
6	D	85	ARG	3.1
3	A	112	GLN	3.1
1	2	99	LEU	3.1
4	B	507	PHE	3.0
4	B	120	HIS	3.0
3	A	622	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
3	A	272	LEU	3.0
3	A	594	TRP	3.0
4	B	23	TYR	3.0
6	D	79	GLN	3.0
1	2	147	PHE	3.0
3	A	446	MET	3.0
3	A	135	GLN	3.0
3	A	138	SER	3.0
3	A	620	SER	3.0
4	B	505	SER	3.0
4	B	713	VAL	3.0
5	C	9	ASP	3.0
12	L	140	SER	3.0
4	B	350	MET	3.0
4	B	622	LEU	3.0
2	4	133	GLY	3.0
4	B	182	GLY	3.0
4	B	170	GLU	3.0
6	D	27	LYS	3.0
6	D	120	ILE	3.0
11	K	32	ASP	3.0
8	F	94	HIS	3.0
3	A	474	GLN	3.0
6	D	71	GLN	3.0
4	B	645	SER	3.0
1	3	85	HIS	3.0
12	L	18	ALA	3.0
3	A	114	VAL	3.0
3	A	329	LEU	2.9
6	D	88	PRO	2.9
3	A	673	HIS	2.9
1	2	181	GLU	2.9
3	A	66	SER	2.9
6	D	119	THR	2.9
4	B	653	LEU	2.9
5	C	23	LEU	2.9
1	3	167	LYS	2.9
6	D	8	SER	2.9
2	4	142	HIS	2.9
5	C	6	LYS	2.9
4	B	52	GLY	2.9
4	B	648	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
5	C	43	PRO	2.9
2	4	146	VAL	2.9
3	A	146	ALA	2.9
7	E	54	SER	2.9
3	A	615	TRP	2.9
3	A	683	LEU	2.9
1	2	167	VAL	2.9
3	A	706	VAL	2.9
12	L	104	ASP	2.9
5	C	10	ASN	2.9
3	A	248	GLU	2.9
4	B	10	GLN	2.9
9	I	15	GLY	2.9
4	B	724	ILE	2.8
2	4	161	LEU	2.8
4	B	72	GLY	2.8
1	2	184	TYR	2.8
3	A	409	MET	2.8
1	3	89	ALA	2.8
4	B	368	ALA	2.8
5	C	17	CYS	2.8
7	E	27	VAL	2.8
1	2	170	PRO	2.8
3	A	472	ALA	2.8
2	4	145	PHE	2.8
3	A	499	LEU	2.8
6	D	13	GLY	2.8
8	F	109	ILE	2.8
14	O	58	VAL	2.8
3	A	50	ALA	2.8
3	A	748	GLY	2.8
4	B	360	ALA	2.8
3	A	671	GLY	2.8
1	3	111	SER	2.8
4	B	570	ALA	2.8
1	3	158	PRO	2.8
3	A	670	LEU	2.8
4	B	508	LEU	2.8
1	2	222	PHE	2.8
4	B	482	ASN	2.8
4	B	521	ILE	2.8
12	L	63	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
14	O	76	ILE	2.8
4	B	219	GLY	2.8
3	A	414	SER	2.8
3	A	500	ALA	2.8
4	B	199	ALA	2.8
12	L	98	ALA	2.8
4	B	525	LEU	2.8
12	L	101	PHE	2.8
1	2	126	GLY	2.7
7	E	5	GLY	2.7
1	3	109	ALA	2.7
4	B	458	ALA	2.7
4	B	49	SER	2.7
4	B	550	ASP	2.7
3	A	375	TYR	2.7
4	B	693	ASP	2.7
4	B	705	LEU	2.7
3	A	598	ALA	2.7
4	B	590	PHE	2.7
5	C	67	VAL	2.7
4	B	153	LEU	2.7
4	B	432	LEU	2.7
4	B	524	GLY	2.7
12	L	138	LEU	2.7
1	3	79	ARG	2.7
5	C	45	THR	2.7
4	B	35	ASP	2.7
10	J	34	ASP	2.7
4	B	145	ALA	2.7
4	B	181	PHE	2.7
6	D	57	LEU	2.7
3	A	515	SER	2.7
4	B	421	SER	2.7
6	D	22	ALA	2.7
3	A	134	ILE	2.7
3	A	316	HIS	2.7
4	B	583	ASN	2.7
12	L	126	VAL	2.7
4	B	688	LEU	2.7
1	2	198	SER	2.7
3	A	629	GLY	2.7
3	A	716	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	3	203	LEU	2.6
1	3	176	GLN	2.6
4	B	462	GLN	2.6
3	A	378	THR	2.6
3	A	715	LEU	2.6
1	2	146	GLN	2.6
2	4	248	GLU	2.6
4	B	528	THR	2.6
14	O	69	ALA	2.6
8	F	147	VAL	2.6
4	B	204	HIS	2.6
3	A	310	THR	2.6
4	B	186	LEU	2.6
6	D	20	ARG	2.6
7	E	13	PRO	2.6
8	F	33	PRO	2.6
8	F	148	PRO	2.6
3	A	121	GLN	2.6
4	B	8	PHE	2.6
4	B	361	PHE	2.6
3	A	466	ASP	2.6
1	2	118	LEU	2.6
1	3	151	SER	2.6
14	O	115	PRO	2.6
1	3	149	ILE	2.6
3	A	92	ALA	2.6
4	B	460	TRP	2.5
4	B	569	SER	2.5
4	B	25	ILE	2.5
4	B	332	LEU	2.5
2	4	245	MET	2.5
14	O	85	PRO	2.5
12	L	102	THR	2.5
3	A	639	ILE	2.5
4	B	67	HIS	2.5
3	A	720	GLY	2.5
2	4	144	TYR	2.5
3	A	685	SER	2.5
6	D	89	SER	2.5
3	A	377	ALA	2.5
4	B	30	ASP	2.5
3	A	171	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	684	PHE	2.5
4	B	66	PHE	2.5
3	A	202	LEU	2.5
3	A	257	LEU	2.5
4	B	573	ALA	2.5
11	K	37	ILE	2.5
5	C	60	THR	2.5
3	A	448	SER	2.5
1	3	112	LYS	2.5
4	B	489	GLN	2.5
3	A	55	PHE	2.5
11	K	14	MET	2.5
1	2	200	GLN	2.5
8	F	59	GLU	2.5
4	B	211	ILE	2.5
7	E	1	MET	2.5
3	A	493	ASN	2.5
3	A	699	TRP	2.4
1	2	159	PHE	2.4
3	A	81	PHE	2.4
4	B	34	HIS	2.4
12	L	134	LEU	2.4
3	A	376	LEU	2.4
4	B	369	LEU	2.4
8	F	113	LEU	2.4
1	2	127	THR	2.4
8	F	166	GLN	2.4
5	C	34	CYS	2.4
3	A	676	TRP	2.4
1	3	195	PHE	2.4
12	L	62	PHE	2.4
4	B	680	HIS	2.4
1	2	205	GLN	2.4
4	B	32	GLU	2.4
4	B	529	THR	2.4
4	B	161	PRO	2.4
4	B	702	GLN	2.4
3	A	235	LEU	2.4
4	B	333	GLY	2.4
4	B	394	ARG	2.4
1	3	208	GLY	2.4
3	A	492	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
8	F	158	PHE	2.4
12	L	77	ALA	2.4
14	O	138	PHE	2.4
3	A	46	TRP	2.4
4	B	21	ILE	2.4
7	E	35	PRO	2.4
14	O	139	GLY	2.4
12	L	105	SER	2.4
2	4	151	MET	2.4
4	B	317	HIS	2.4
13	M	5	ASN	2.4
1	3	154	GLY	2.3
3	A	85	SER	2.3
3	A	258	VAL	2.3
3	A	470	ASP	2.3
3	A	451	LEU	2.3
3	A	682	PHE	2.3
4	B	213	THR	2.3
4	B	321	TYR	2.3
12	L	94	LEU	2.3
4	B	191	HIS	2.3
3	A	148	GLY	2.3
8	F	60	ALA	2.3
10	J	38	TYR	2.3
4	B	567	ASP	2.3
4	B	522	ALA	2.3
8	F	175	ALA	2.3
3	A	698	VAL	2.3
3	A	93	ARG	2.3
4	B	22	TRP	2.3
3	A	102	SER	2.3
1	2	199	ALA	2.3
1	2	145	ASN	2.3
3	A	551	LEU	2.3
3	A	590	LEU	2.3
4	B	608	ASN	2.3
4	B	184	SER	2.3
4	B	190	GLY	2.3
1	2	152	ALA	2.3
4	B	372	HIS	2.3
1	3	131	GLN	2.3
6	D	111	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	3	187	ASN	2.3
3	A	262	THR	2.3
6	D	31	THR	2.3
4	B	415	ALA	2.3
6	D	116	VAL	2.3
4	B	362	ASP	2.3
12	L	72	ASP	2.3
7	E	60	GLU	2.2
3	A	240	ILE	2.2
4	B	727	THR	2.2
4	B	94	PRO	2.2
4	B	530	LEU	2.2
4	B	532	LEU	2.2
8	F	150	ALA	2.2
8	F	174	LEU	2.2
14	O	112	PRO	2.2
4	B	203	GLN	2.2
4	B	538	ASP	2.2
8	F	142	GLU	2.2
2	4	240	PHE	2.2
4	B	553	TYR	2.2
5	C	69	LEU	2.2
1	2	105	ALA	2.2
1	3	72	VAL	2.2
7	E	46	SER	2.2
14	O	80	ALA	2.2
4	B	457	PHE	2.2
6	D	76	PHE	2.2
4	B	45	LYS	2.2
4	B	495	TRP	2.2
14	O	53	LEU	2.2
4	B	578	MET	2.2
1	3	116	SER	2.2
1	3	91	LEU	2.2
8	F	145	LEU	2.2
12	L	135	LEU	2.2
1	2	218	ALA	2.2
4	B	20	ARG	2.2
4	B	471	GLY	2.2
5	C	30	PRO	2.2
10	J	1	MET	2.2
2	4	239	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	12	VAL	2.2
4	B	342	VAL	2.2
5	C	36	ALA	2.2
3	A	501	THR	2.2
4	B	84	THR	2.2
4	B	210	PHE	2.2
2	4	172	TYR	2.2
12	L	109	GLU	2.2
1	3	163	PHE	2.2
1	2	227	LEU	2.2
3	A	523	LYS	2.2
6	D	64	GLN	2.2
2	4	177	TRP	2.2
3	A	391	MET	2.2
3	A	456	ASP	2.1
3	A	731	GLY	2.1
4	B	279	ALA	2.1
12	L	78	GLY	2.1
1	3	108	ASN	2.1
4	B	381	ILE	2.1
11	K	26	TYR	2.1
3	A	38	GLY	2.1
14	O	68	PRO	2.1
1	2	179	ASN	2.1
3	A	418	ASN	2.1
4	B	464	THR	2.1
2	4	116	ALA	2.1
5	C	72	GLU	2.1
4	B	85	LYS	2.1
9	I	12	PRO	2.1
1	3	96	VAL	2.1
2	4	126	TYR	2.1
14	O	146	TYR	2.1
11	K	39	SER	2.1
4	B	577	ALA	2.1
4	B	651	ALA	2.1
5	C	27	GLU	2.1
1	2	165	PHE	2.1
3	A	496	VAL	2.1
4	B	29	HIS	2.1
4	B	504	ASN	2.1
1	3	114	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	277	GLY	2.1
3	A	312	TRP	2.1
3	A	559	ILE	2.1
1	2	160	VAL	2.1
4	B	375	TYR	2.1
2	4	155	LEU	2.1
3	A	438	ASN	2.1
12	L	58	LEU	2.1
1	2	124	GLU	2.1
5	C	47	ASP	2.1
7	E	56	ASP	2.1
3	A	249	LEU	2.1
3	A	489	LEU	2.1
8	F	151	LEU	2.1
3	A	518	ALA	2.1
8	F	114	PHE	2.1
4	B	655	TRP	2.1
7	E	34	TYR	2.0
2	4	216	ALA	2.0
3	A	442	ILE	2.0
4	B	389	ALA	2.0
5	C	80	ALA	2.0
6	D	29	ALA	2.0
2	4	101	TRP	2.0
3	A	43	THR	2.0
3	A	116	PRO	2.0
4	B	9	SER	2.0
4	B	324	LEU	2.0
6	D	72	LEU	2.0
8	F	31	LEU	2.0
14	O	101	LEU	2.0
2	4	236	ILE	2.0
3	A	601	ILE	2.0
8	F	82	TYR	2.0
2	4	138	ALA	2.0
3	A	173	GLY	2.0
4	B	179	GLY	2.0
6	D	80	ASP	2.0
3	A	648	TRP	2.0
8	F	161	PRO	2.0
1	2	213	ARG	2.0
1	3	115	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	4	148	SER	2.0
3	A	70	PHE	2.0
3	A	276	GLY	2.0
2	4	166	HIS	2.0
2	4	237	HIS	2.0
4	B	215	PRO	2.0

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, 95th 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($\text{\AA}^2$)	Q<0.9
15	CLA	3	603	25/65	-0.32	0.21	246,261,286,294	0
15	CLA	3	608	25/65	-0.16	0.26	298,335,354,361	0
15	CLA	B	1218	25/65	-0.03	0.18	300,335,347,356	0
15	CLA	B	1227	25/65	0.09	0.28	211,262,292,303	0
15	CLA	3	607	25/65	0.28	0.17	213,230,253,258	0
15	CLA	O	1603	25/65	0.33	0.15	179,204,218,223	0
15	CLA	2	606	25/65	0.34	0.20	191,219,239,244	0
15	CLA	B	1217	25/65	0.36	0.20	231,256,273,279	0
15	CLA	3	611	25/65	0.39	0.24	118,182,201,208	0
15	CLA	2	601	25/65	0.41	0.21	164,206,231,233	0
15	CLA	4	611	25/65	0.41	0.14	216,237,248,253	0
15	CLA	4	601	25/65	0.42	0.18	182,213,243,269	0
15	CLA	4	602	25/65	0.45	0.34	496,534,558,558	0
15	CLA	B	1209	25/65	0.45	0.24	235,264,283,284	0
15	CLA	O	1602	25/65	0.46	0.26	303,330,344,350	0
15	CLA	2	611	25/65	0.48	0.24	183,236,260,270	0
15	CLA	4	604	25/65	0.49	0.26	156,208,225,230	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CLA	2	613	25/65	0.49	0.20	182,222,233,242	0
15	CLA	2	616	25/65	0.53	0.26	150,192,224,226	0
15	CLA	2	608	25/65	0.53	0.16	188,210,232,242	0
15	CLA	2	615	25/65	0.53	0.16	232,276,300,304	0
15	CLA	B	1232	65/65	0.55	0.13	128,185,220,230	0
15	CLA	B	1208	25/65	0.58	0.17	203,267,283,288	0
15	CLA	4	608	25/65	0.58	0.29	343,352,370,376	0
15	CLA	O	1601	25/65	0.59	0.24	333,342,346,354	0
15	CLA	4	616	25/65	0.60	0.16	189,214,233,237	0
15	CLA	4	610	25/65	0.60	0.24	157,182,206,213	0
15	CLA	2	602	25/65	0.61	0.14	132,169,184,193	0
15	CLA	3	602	25/65	0.62	0.15	135,182,210,216	0
15	CLA	B	1219	25/65	0.63	0.14	159,177,201,218	0
15	CLA	4	615	25/65	0.63	0.28	236,276,298,305	0
15	CLA	3	614	25/65	0.63	0.20	104,155,182,201	0
15	CLA	B	1212	25/65	0.64	0.27	184,204,223,230	0
16	PQN	B	2002	33/33	0.64	0.29	126,151,167,174	0
15	CLA	B	1223	25/65	0.65	0.28	233,265,282,284	0
15	CLA	B	1216	25/65	0.65	0.24	337,368,376,377	0
15	CLA	B	1210	25/65	0.65	0.16	227,262,274,291	0
15	CLA	L	1501	25/65	0.65	0.15	151,182,196,207	0
15	CLA	2	614	25/65	0.66	0.23	181,245,252,253	0
18	BCR	A	4008	40/40	0.66	0.40	48,114,172,181	0
18	BCR	A	4007	40/40	0.67	0.31	60,129,164,195	0
15	CLA	L	1502	25/65	0.67	0.24	146,181,197,213	0
15	CLA	2	603	25/65	0.68	0.18	157,184,202,206	0
15	CLA	B	1221	25/65	0.68	0.30	178,214,233,234	0
15	CLA	B	1231	25/65	0.68	0.27	247,265,279,286	0
15	CLA	3	601	25/65	0.69	0.15	144,196,210,234	0
18	BCR	I	4018	40/40	0.69	0.28	82,148,219,223	0
15	CLA	4	609	25/65	0.70	0.25	252,286,299,301	0
15	CLA	B	1204	25/65	0.70	0.26	259,286,298,310	0
15	CLA	2	607	25/65	0.70	0.18	159,202,220,235	0
15	CLA	4	603	25/65	0.71	0.15	103,149,175,192	0
15	CLA	B	1236	45/65	0.71	0.29	123,190,211,222	0
15	CLA	K	1402	25/65	0.71	0.21	139,167,192,202	0
15	CLA	3	604	25/65	0.73	0.18	189,234,254,266	0
15	CLA	A	1109	25/65	0.73	0.16	55,102,136,154	0
18	BCR	A	4017	40/40	0.73	0.33	86,164,194,202	0
15	CLA	2	610	25/65	0.73	0.17	164,216,237,243	0
15	CLA	K	1401	25/65	0.74	0.16	151,187,207,218	0
15	CLA	3	606	25/65	0.76	0.15	172,210,242,250	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CLA	3	612	25/65	0.76	0.20	163,188,205,220	0
15	CLA	A	1120	25/65	0.76	0.22	109,183,229,234	0
15	CLA	B	1214	25/65	0.77	0.36	274,296,313,326	0
15	CLA	L	1503	25/65	0.78	0.21	237,249,262,268	0
15	CLA	A	1112	25/65	0.78	0.20	97,124,135,141	0
15	CLA	B	1021	45/65	0.78	0.28	114,149,172,191	0
15	CLA	2	604	25/65	0.79	0.21	139,163,200,206	0
15	CLA	A	1137	25/65	0.79	0.24	71,135,157,165	0
15	CLA	4	606	25/65	0.79	0.17	161,216,236,250	0
15	CLA	B	1238	25/65	0.79	0.16	103,134,162,167	0
15	CLA	F	1302	25/65	0.79	0.17	186,229,263,264	0
15	CLA	B	1203	25/65	0.79	0.27	100,156,175,184	0
15	CLA	A	1119	25/65	0.79	0.22	110,152,178,187	0
18	BCR	A	4011	40/40	0.79	0.33	51,112,139,162	0
15	CLA	B	1207	25/65	0.79	0.17	262,286,303,307	0
18	BCR	B	4008	40/40	0.79	0.38	172,230,254,261	0
15	CLA	B	1228	25/65	0.79	0.16	132,186,206,213	0
15	CLA	A	1121	25/65	0.80	0.20	105,146,174,178	0
15	CLA	4	612	25/65	0.80	0.17	87,127,149,161	0
15	CLA	A	1138	25/65	0.80	0.21	107,137,164,202	0
15	CLA	A	1116	55/65	0.80	0.26	42,90,116,124	0
16	PQN	A	2001	33/33	0.81	0.24	36,100,136,159	0
15	CLA	B	1235	25/65	0.81	0.17	105,137,154,160	0
18	BCR	A	4002	40/40	0.82	0.24	29,93,126,132	0
15	CLA	F	1301	45/65	0.82	0.23	96,146,168,177	0
15	CLA	B	1220	25/65	0.82	0.17	197,228,243,255	0
15	CLA	A	1123	25/65	0.82	0.23	90,121,141,147	0
15	CLA	A	1103	55/65	0.82	0.25	48,92,121,124	0
18	BCR	B	4005	40/40	0.82	0.29	90,132,165,170	0
15	CLA	A	1114	46/65	0.82	0.18	44,120,152,168	0
15	CLA	A	1101	45/65	0.82	0.24	62,120,151,173	0
15	CLA	A	1105	55/65	0.83	0.21	39,125,150,190	0
15	CLA	B	1023	50/65	0.83	0.23	88,147,172,183	0
15	CLA	J	1302	50/65	0.83	0.18	88,178,204,225	0
15	CLA	A	1131	45/65	0.84	0.20	57,87,101,121	0
15	CLA	B	1226	55/65	0.84	0.29	72,163,196,199	0
15	CLA	A	1111	25/65	0.84	0.17	62,104,123,138	0
15	CLA	A	1012	55/65	0.84	0.25	67,145,178,191	0
15	CLA	A	1141	25/65	0.84	0.15	145,178,193,196	0
15	CLA	A	1125	25/65	0.84	0.20	14,51,82,84	0
15	CLA	B	1230	47/65	0.85	0.18	84,129,151,175	0
15	CLA	A	1115	55/65	0.85	0.14	77,115,144,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CLA	A	1128	25/65	0.85	0.16	46,72,86,89	0
15	CLA	2	605	25/65	0.85	0.13	88,123,137,147	0
15	CLA	B	1225	50/65	0.85	0.26	89,228,243,267	0
15	CLA	A	1134	25/65	0.85	0.16	96,146,167,169	0
15	CLA	A	1135	25/65	0.85	0.20	101,119,157,168	0
15	CLA	B	1201	25/65	0.85	0.18	139,156,172,175	0
15	CLA	B	1229	50/65	0.85	0.17	105,140,167,180	0
15	CLA	A	1130	55/65	0.86	0.23	121,209,233,235	0
15	CLA	2	612	25/65	0.86	0.22	142,175,184,189	0
15	CLA	B	1234	25/65	0.86	0.26	228,248,256,260	0
15	CLA	A	1133	25/65	0.86	0.18	127,167,194,209	0
15	CLA	B	1202	25/65	0.86	0.21	128,158,167,172	0
15	CLA	B	1237	55/65	0.86	0.19	82,150,181,203	0
15	CLA	A	1118	25/65	0.86	0.28	155,183,211,214	0
15	CLA	A	1011	50/65	0.87	0.28	98,141,159,202	0
15	CLA	B	1022	25/65	0.87	0.20	106,141,159,178	0
15	CLA	A	1107	55/65	0.87	0.20	55,115,172,216	0
15	CLA	A	1129	25/65	0.87	0.24	142,179,197,200	0
15	CLA	A	1108	25/65	0.87	0.19	45,123,143,151	0
15	CLA	B	1215	25/65	0.87	0.17	134,189,204,215	0
15	CLA	A	1113	25/65	0.87	0.14	86,119,141,149	0
15	CLA	A	1139	25/65	0.87	0.20	91,143,148,161	0
15	CLA	B	1239	25/65	0.87	0.17	131,149,167,170	0
15	CLA	A	1132	25/65	0.87	0.17	69,121,152,153	0
15	CLA	A	1122	25/65	0.88	0.13	52,112,129,135	0
15	CLA	A	1102	25/65	0.88	0.19	58,103,120,128	0
15	CLA	A	1110	25/65	0.88	0.19	139,192,211,225	0
15	CLA	A	1127	25/65	0.88	0.15	0,57,91,97	0
15	CLA	A	1013	55/65	0.88	0.23	45,141,172,184	0
15	CLA	A	1104	55/65	0.88	0.20	41,85,120,133	0
15	CLA	4	605	25/65	0.89	0.15	105,126,145,154	0
15	CLA	A	1117	55/65	0.89	0.27	12,113,142,154	0
15	CLA	B	1222	25/65	0.89	0.25	204,224,242,243	0
15	CLA	A	1124	25/65	0.89	0.16	50,82,106,122	0
15	CLA	B	1224	55/65	0.89	0.34	174,218,261,270	0
15	CLA	3	610	25/65	0.89	0.13	144,167,182,195	0
15	CLA	B	1211	25/65	0.89	0.14	166,183,201,217	0
15	CLA	B	1206	25/65	0.89	0.19	148,173,194,203	0
15	CLA	A	1106	55/65	0.91	0.23	61,117,147,168	0
15	CLA	B	1205	25/65	0.92	0.17	260,280,296,302	0
15	CLA	A	1136	25/65	0.92	0.24	87,161,186,206	0
15	CLA	A	1126	55/65	0.92	0.23	26,91,120,129	0

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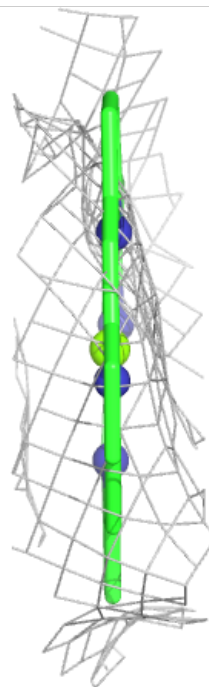
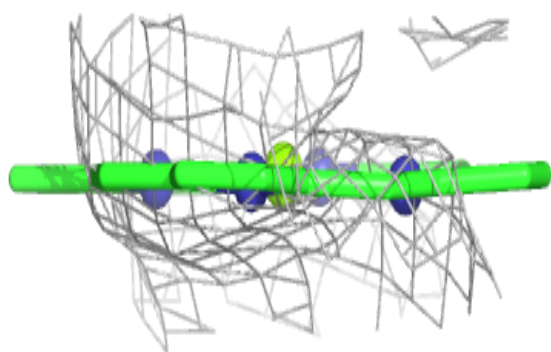
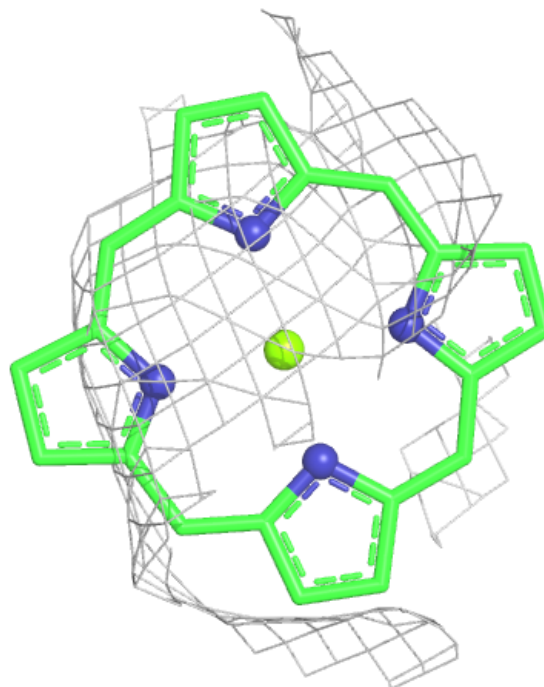
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CLA	A	1140	25/65	0.93	0.17	68,92,127,132	0
17	SF4	C	3003	8/8	0.94	0.21	117,158,186,198	0
17	SF4	C	3002	8/8	0.95	0.15	137,166,186,216	0
17	SF4	A	3001	8/8	0.95	0.14	145,192,216,219	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.

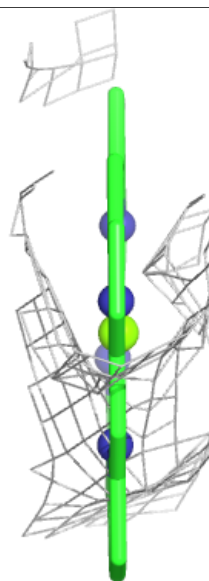
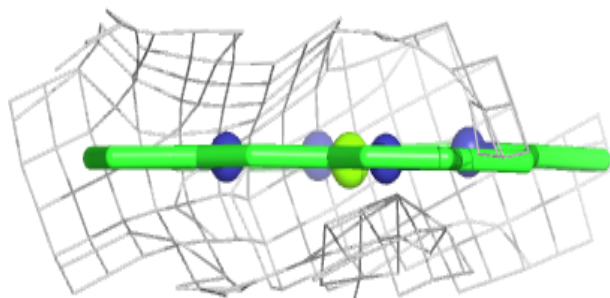
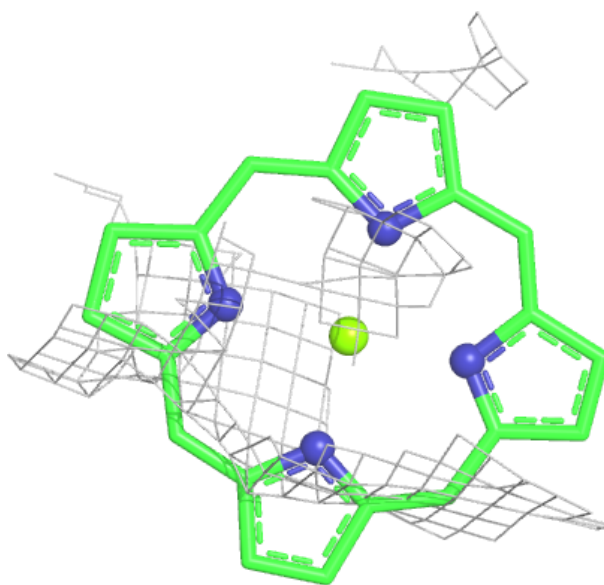
Electron density around CLA 3 603:

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



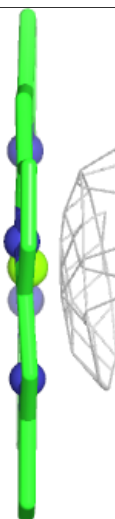
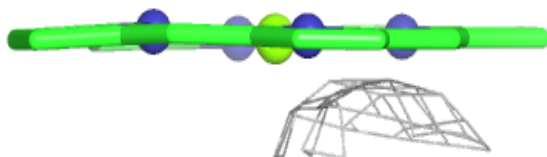
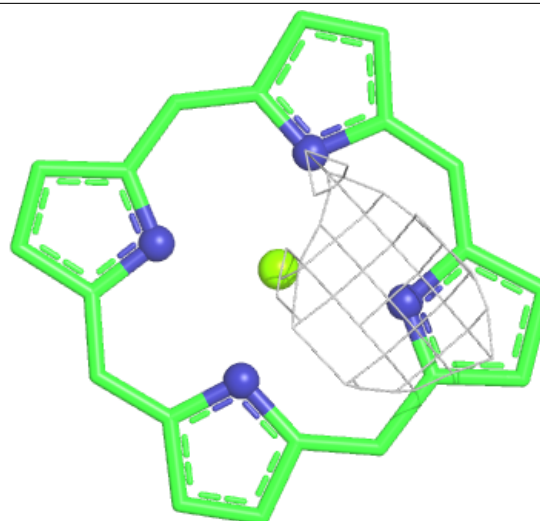
Electron density around CLA 3 608:

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



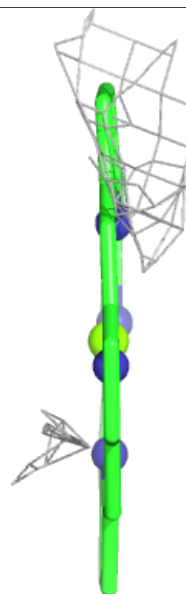
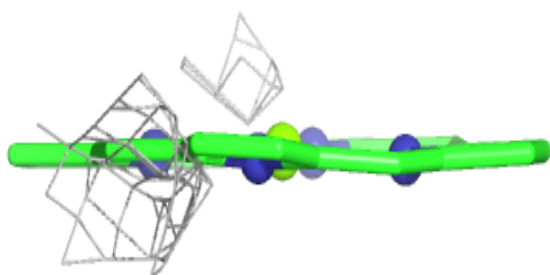
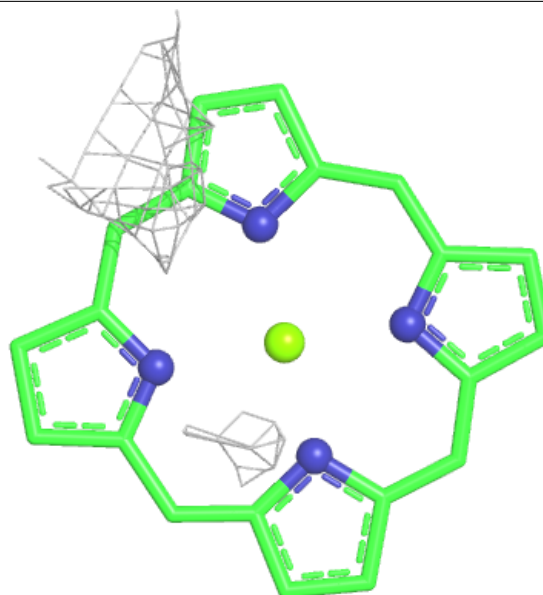
Electron density around CLA B 1218:

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



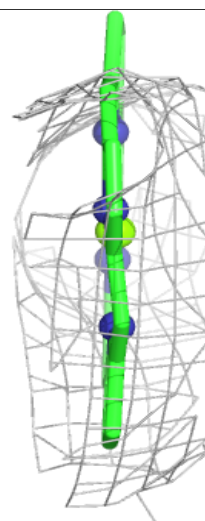
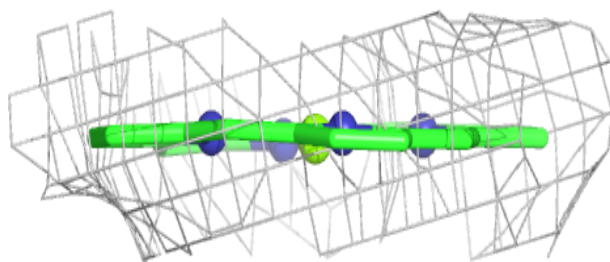
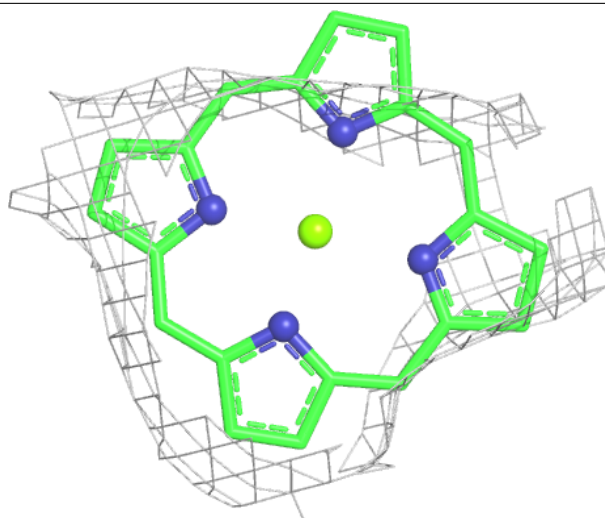
Electron density around CLA B 1227:

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and green (positive)



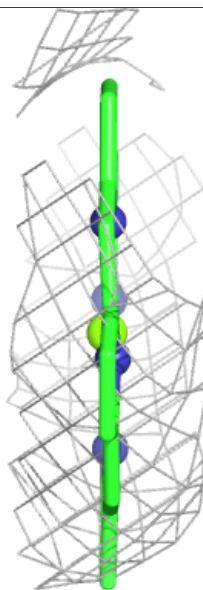
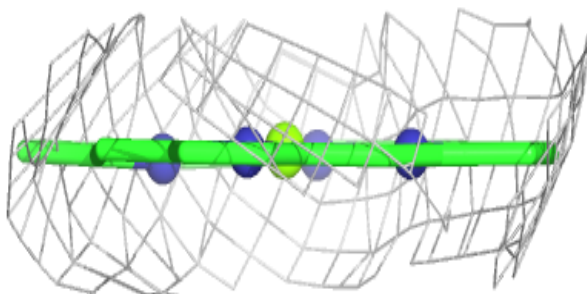
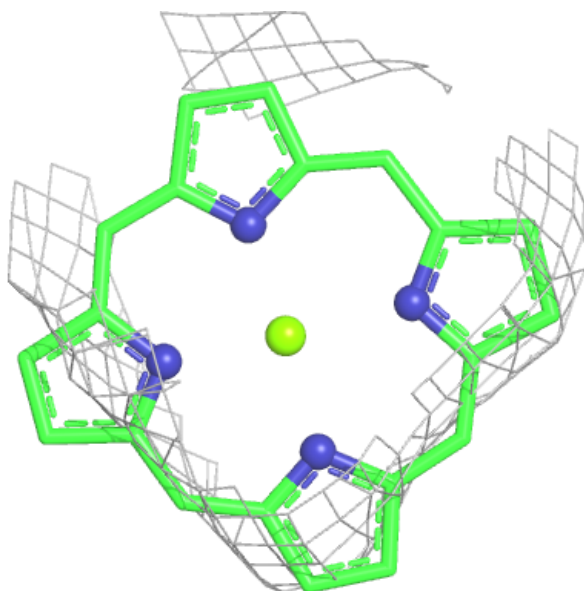
Electron density around CLA 3 607:

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and green (positive)



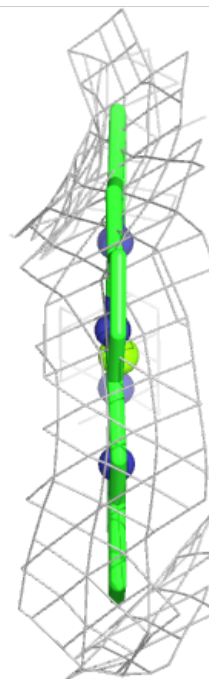
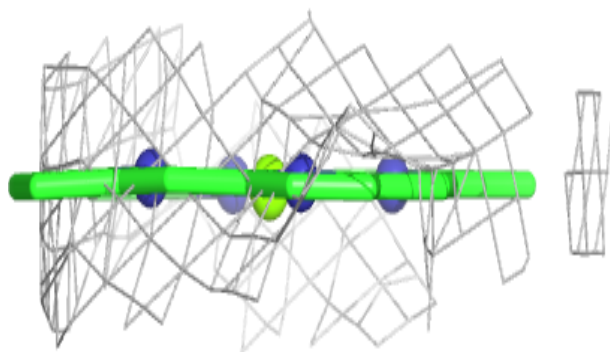
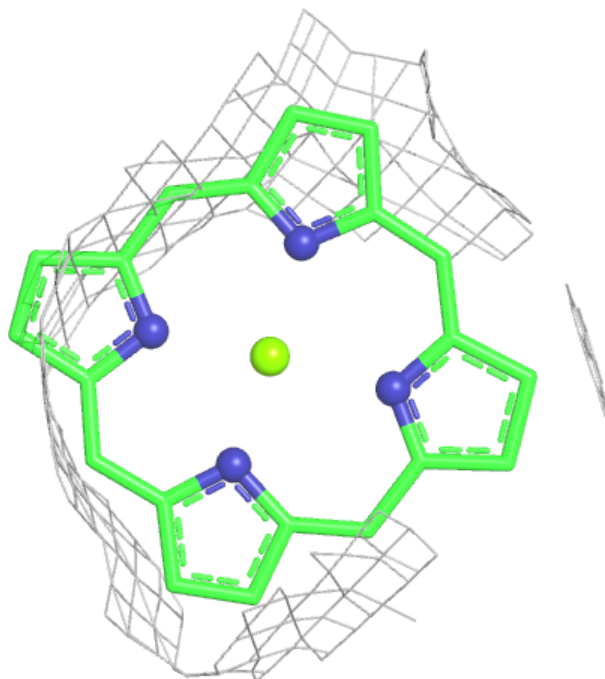
Electron density around CLA O 1603:

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



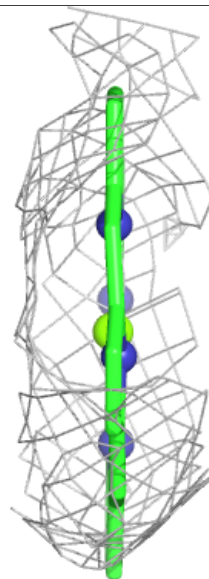
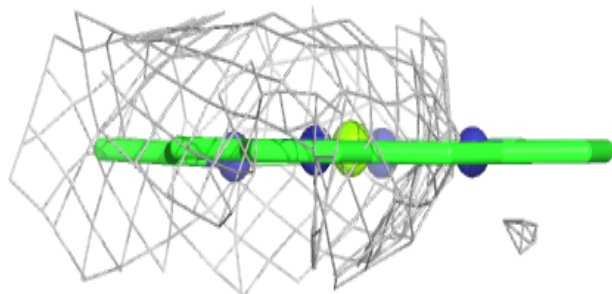
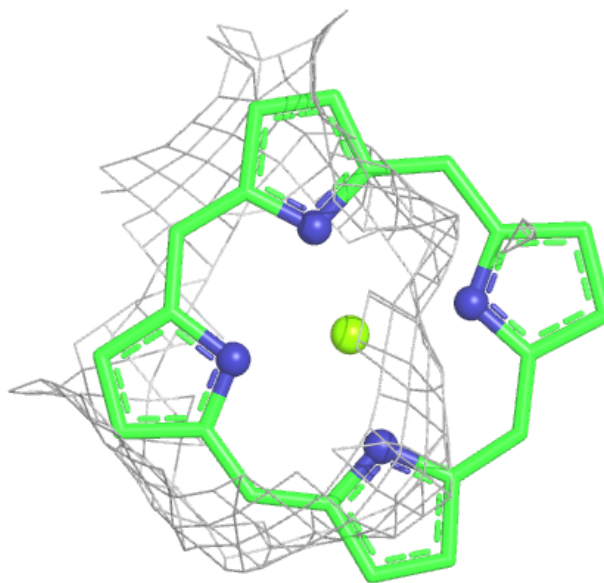
Electron density around CLA 2 606:

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



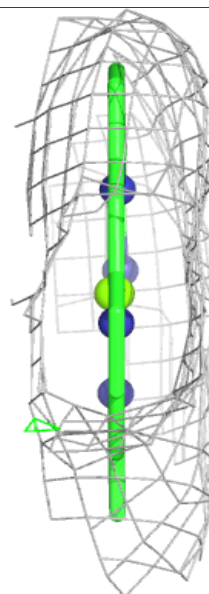
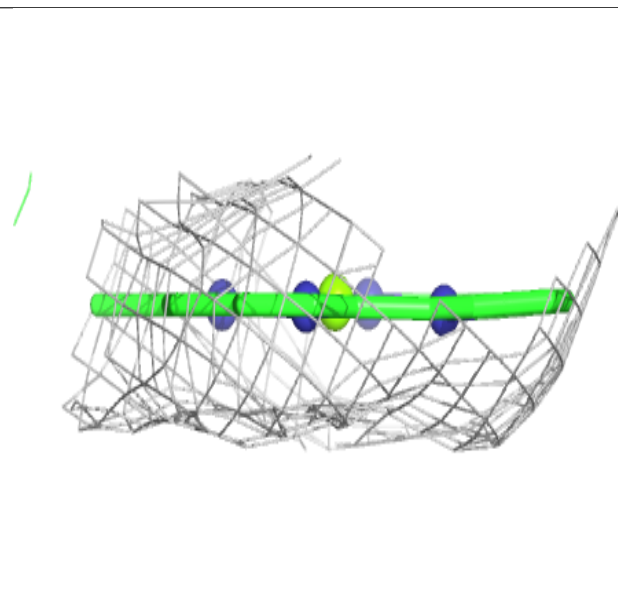
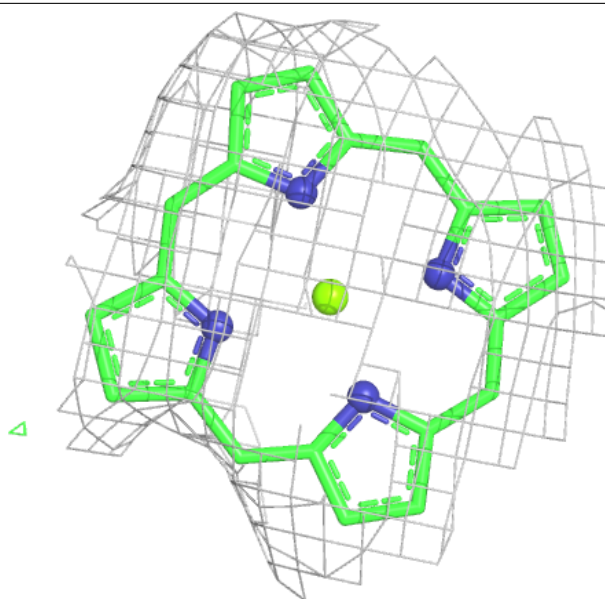
Electron density around CLA B 1217:

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



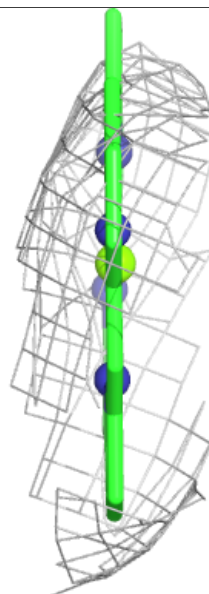
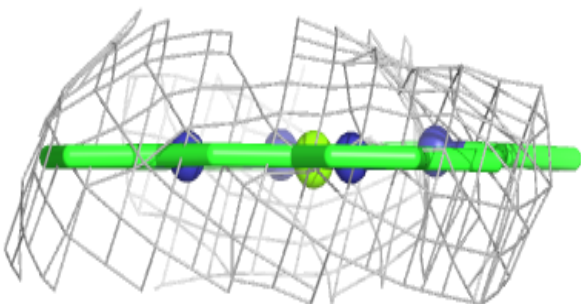
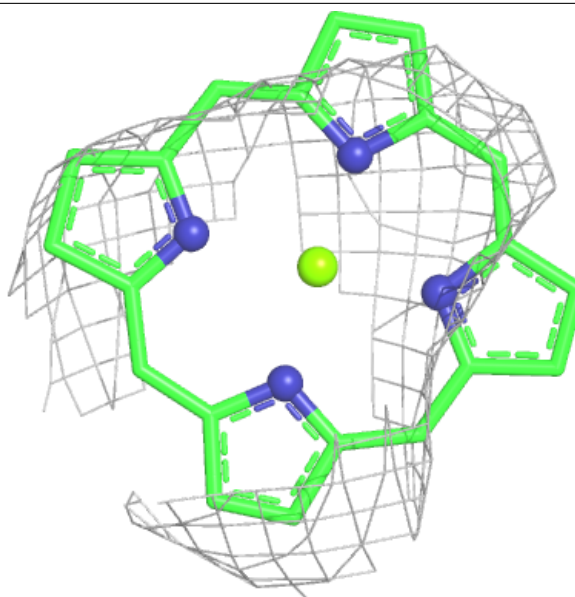
Electron density around CLA 3 611:

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and green (positive)



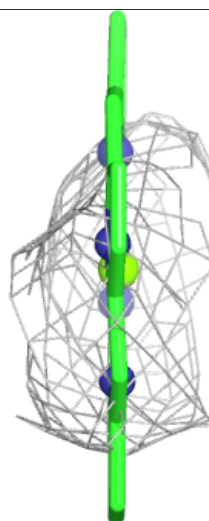
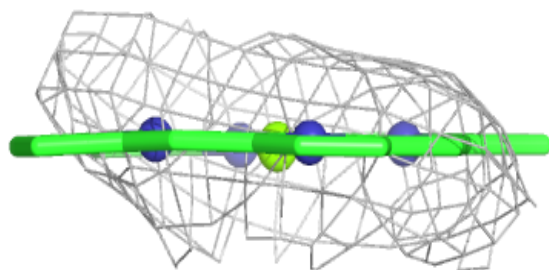
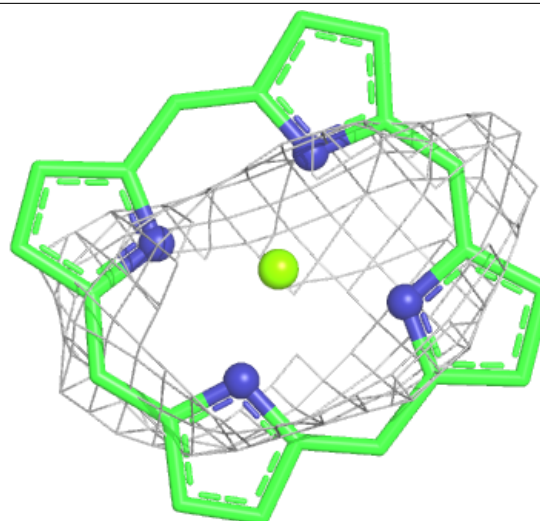
Electron density around CLA 2 601:

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and green (positive)



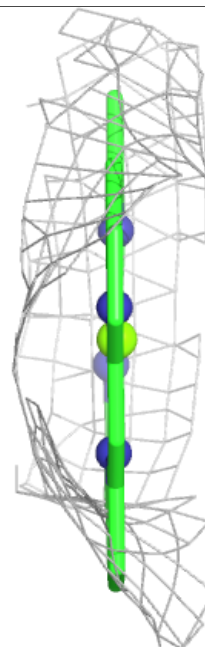
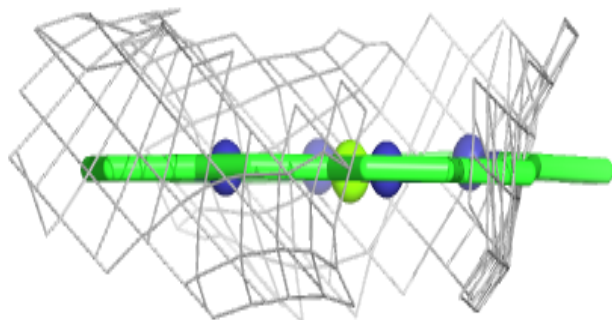
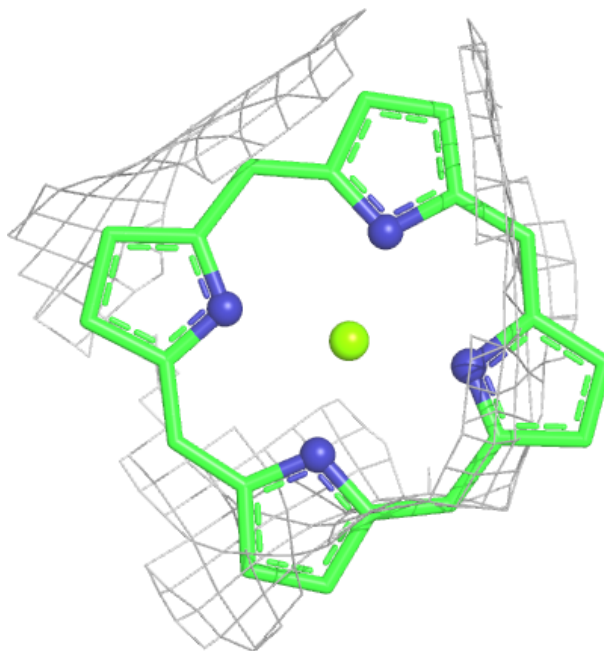
Electron density around CLA 4 611:

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and green (positive)



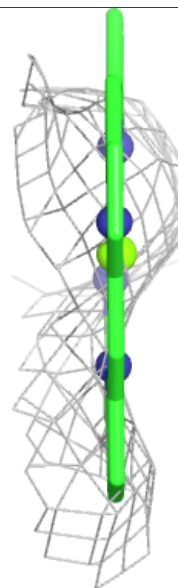
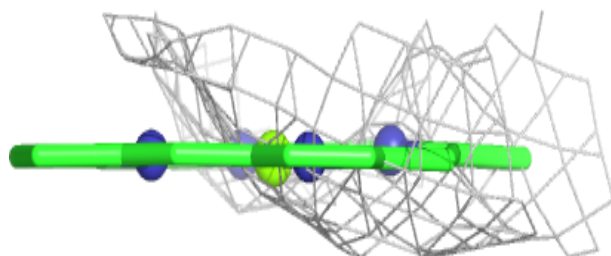
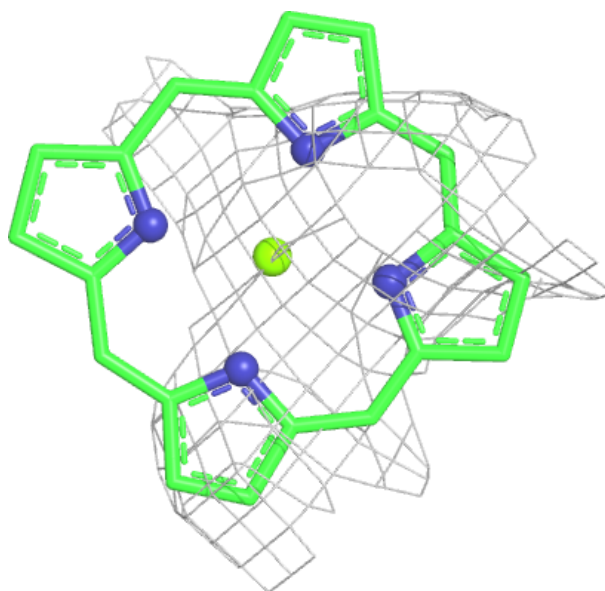
Electron density around CLA 4 601:

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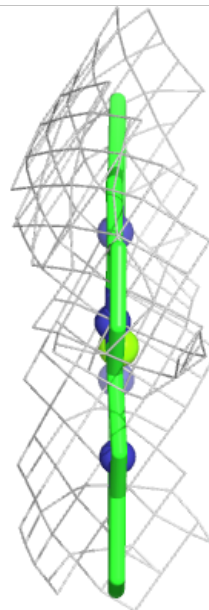
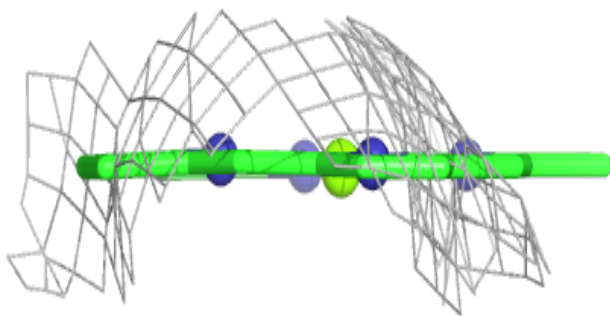
Electron density around CLA 4 602:

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



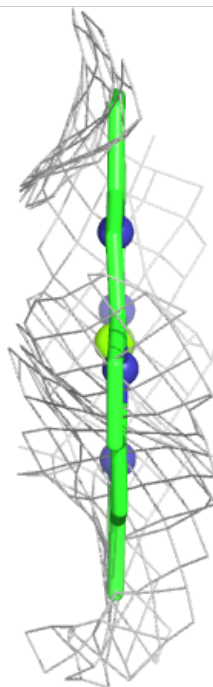
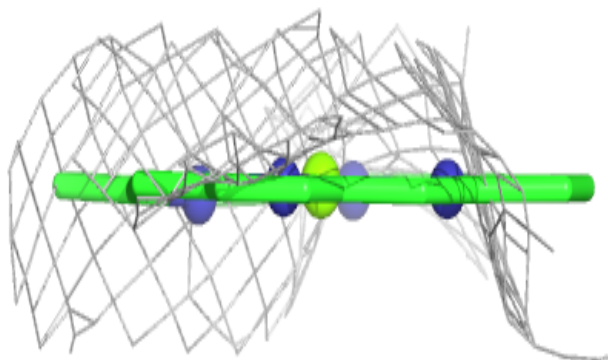
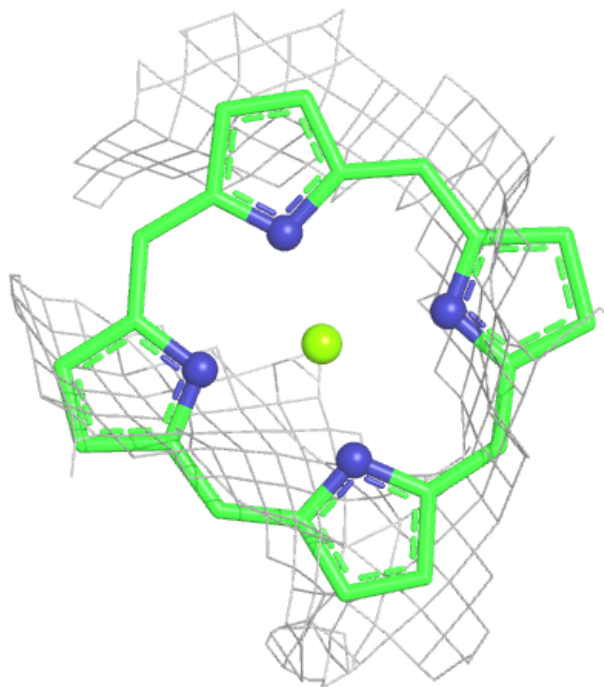
Electron density around CLA B 1209:

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



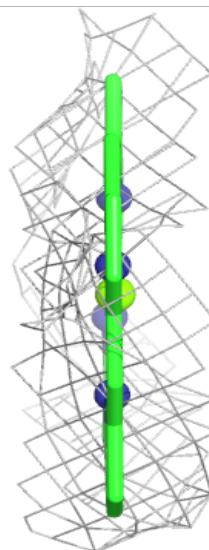
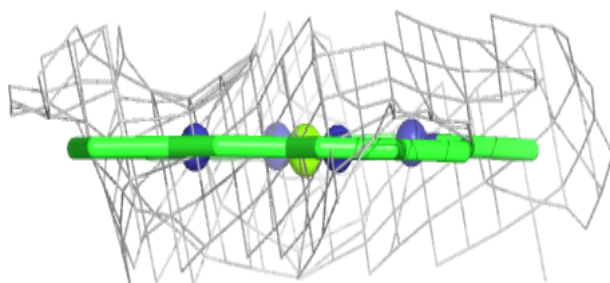
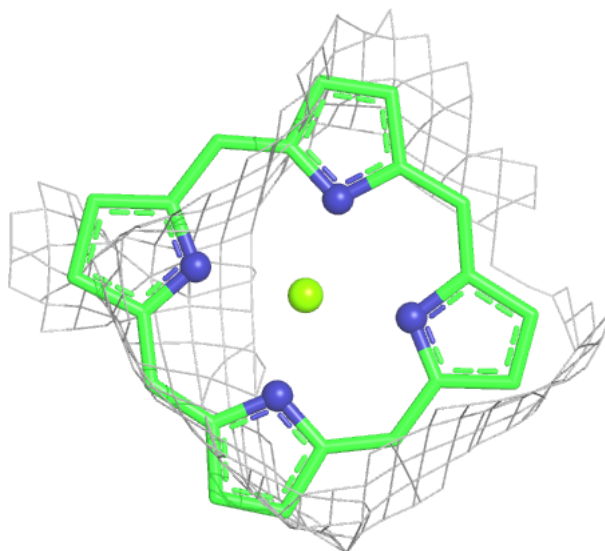
Electron density around CLA O 1602:

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



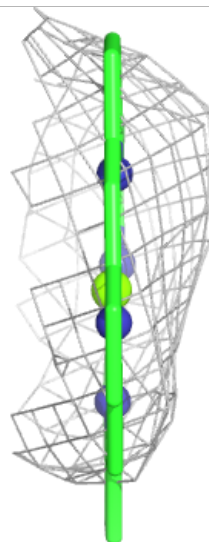
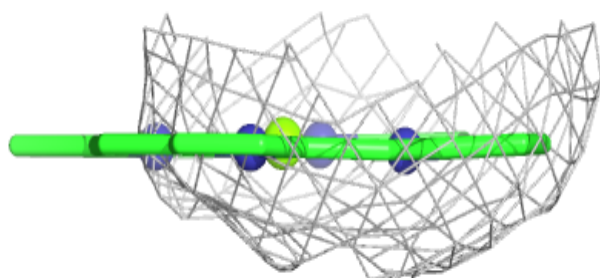
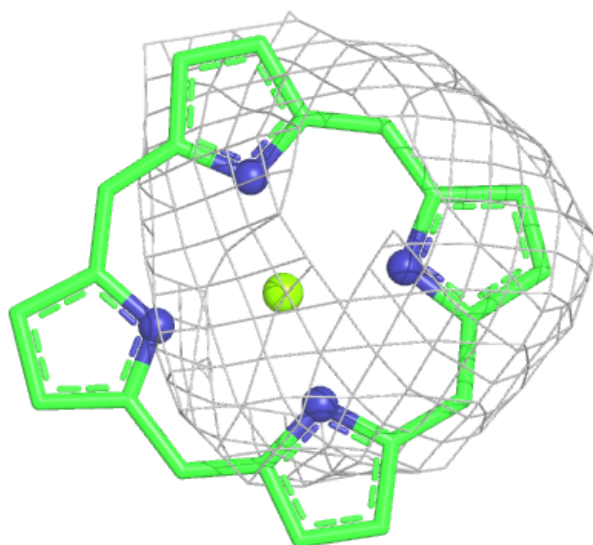
Electron density around CLA 2 611:

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



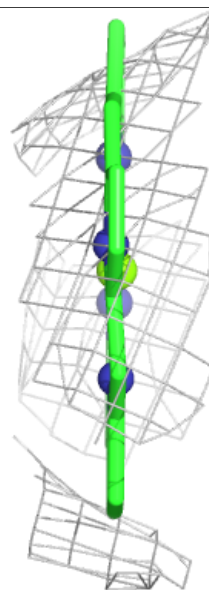
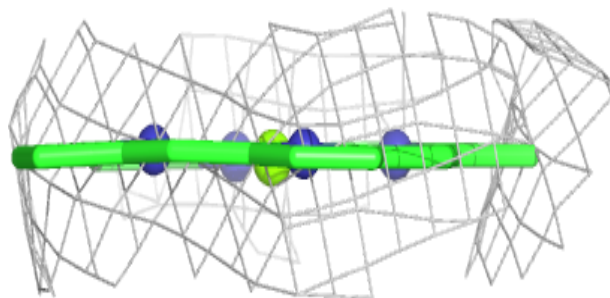
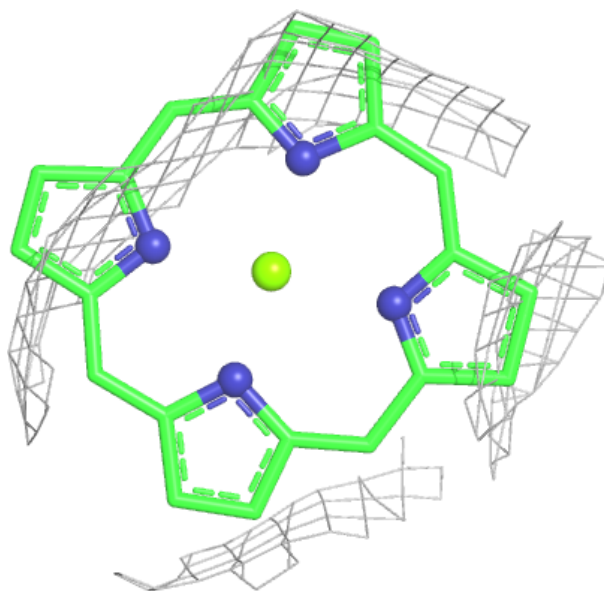
Electron density around CLA 4 604:

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



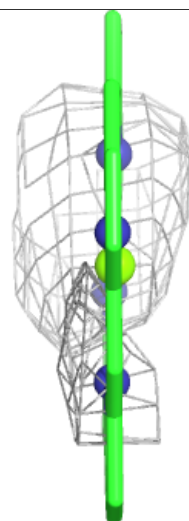
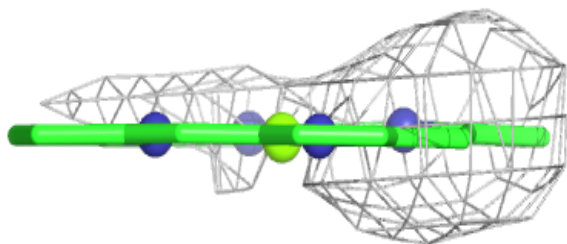
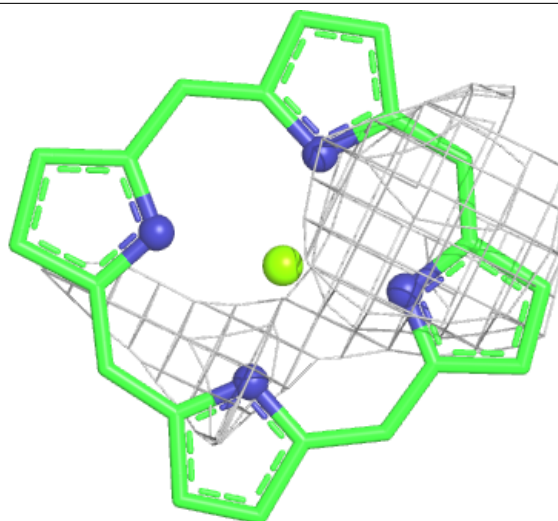
Electron density around CLA 2 613:

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



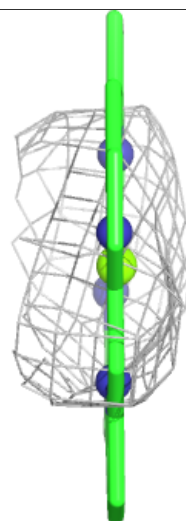
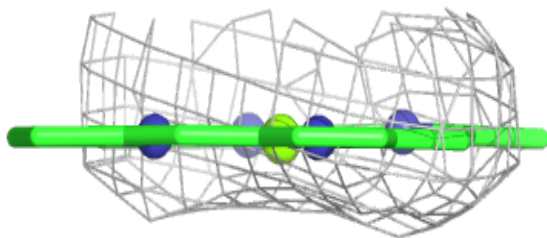
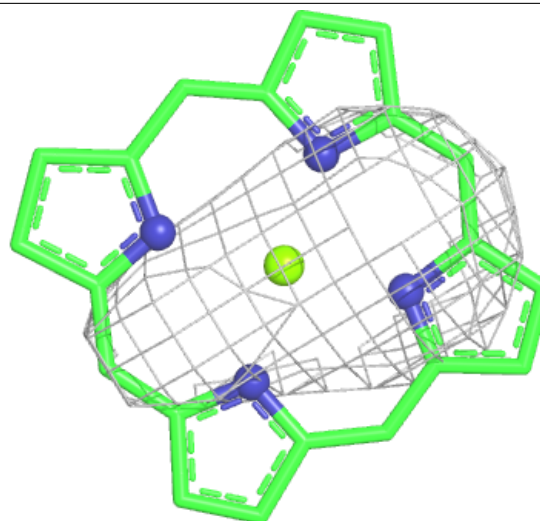
Electron density around CLA 2 616:

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



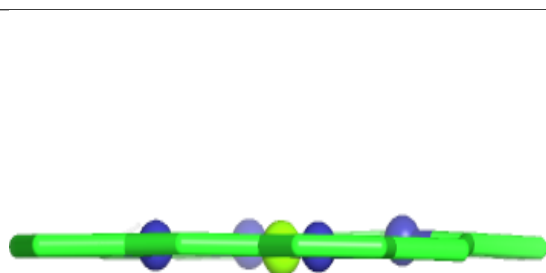
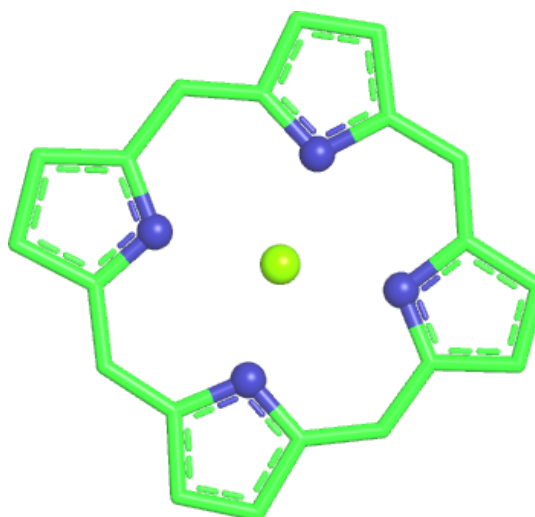
Electron density around CLA 2 608:

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



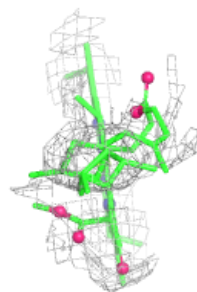
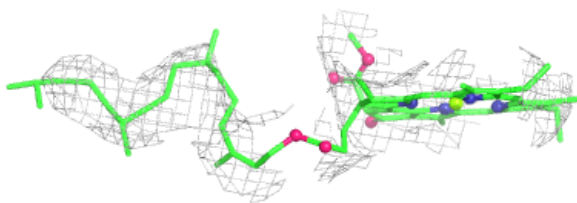
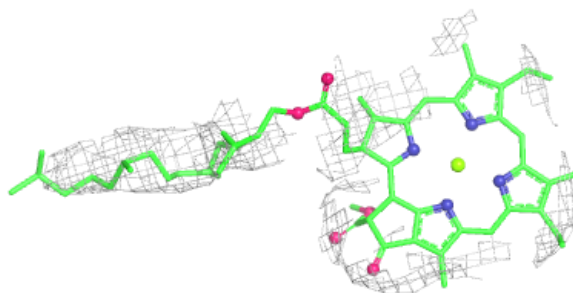
Electron density around CLA 2 615:

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



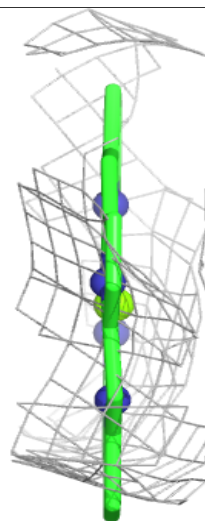
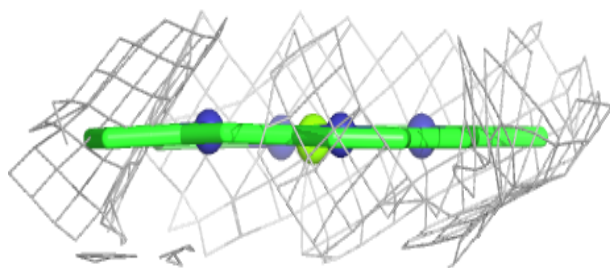
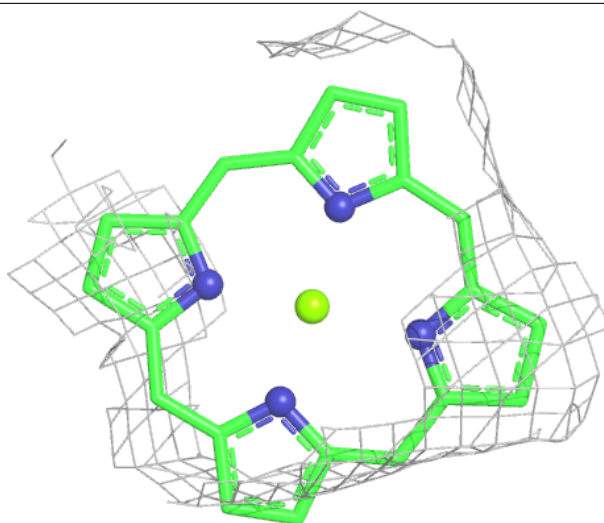
Electron density around CLA B 1232:

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



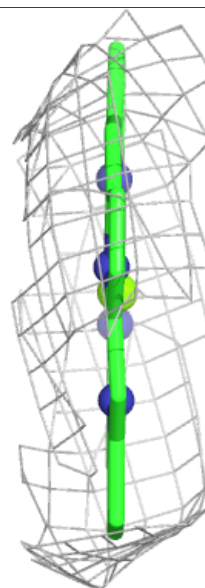
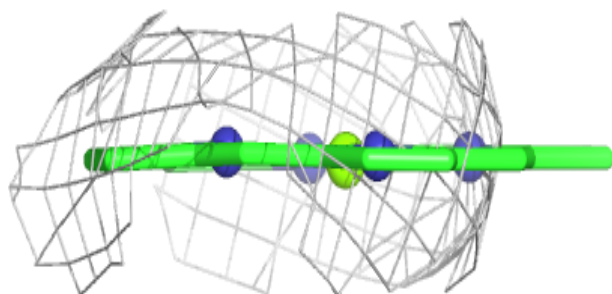
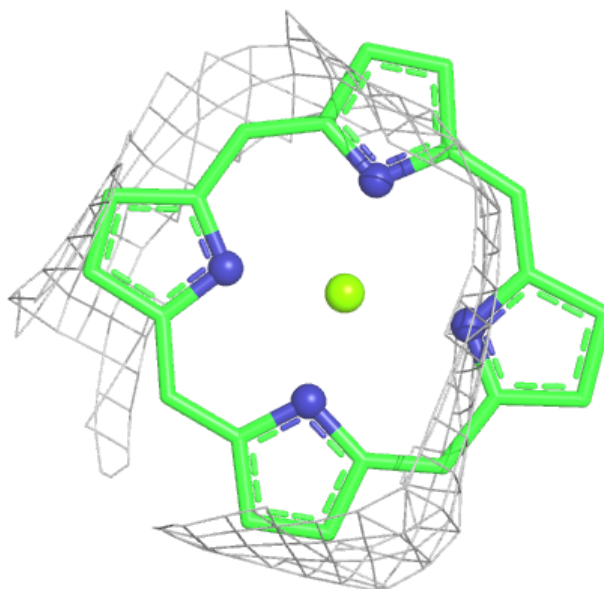
Electron density around CLA B 1208:

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



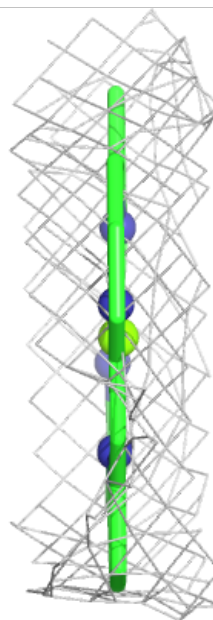
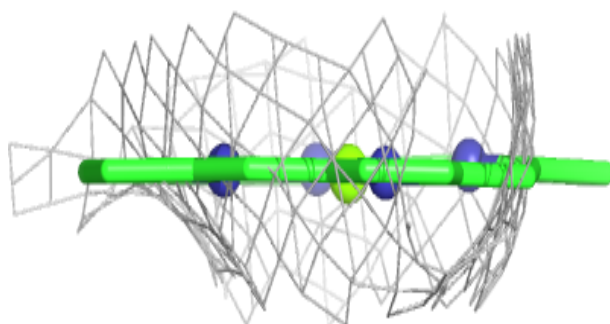
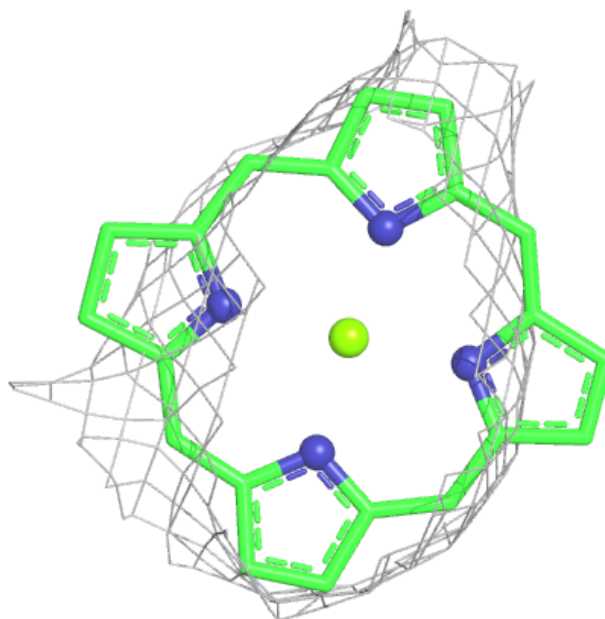
Electron density around CLA 4 608:

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



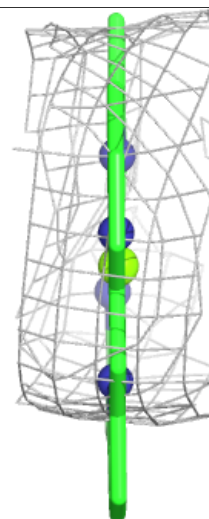
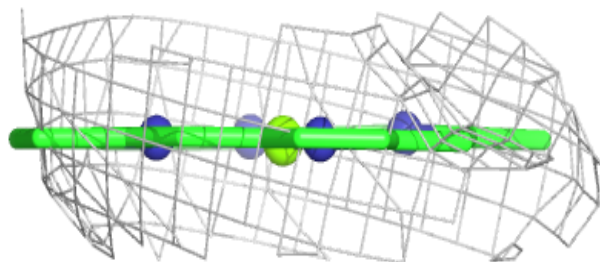
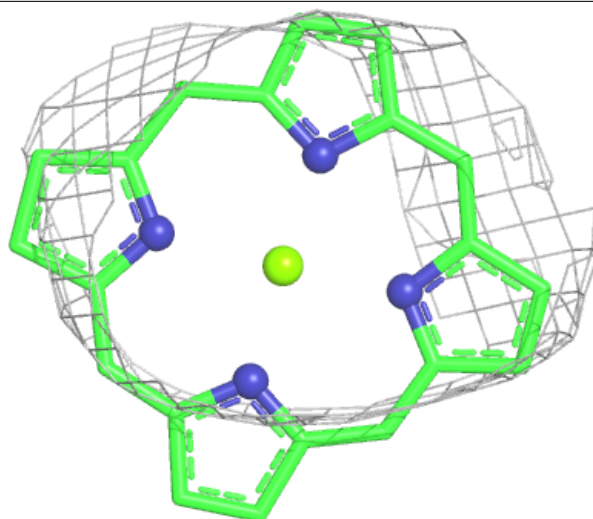
Electron density around CLA O 1601:

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



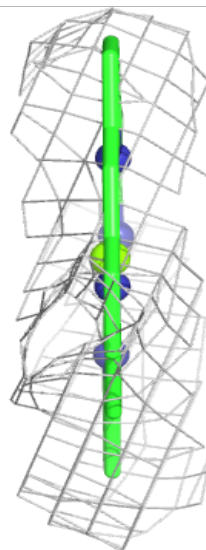
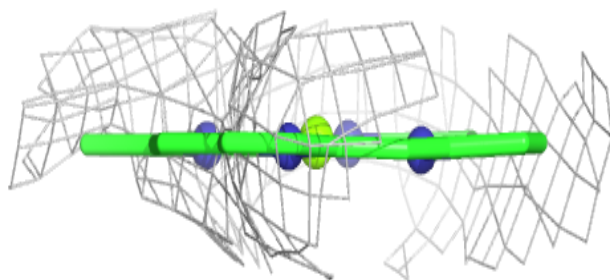
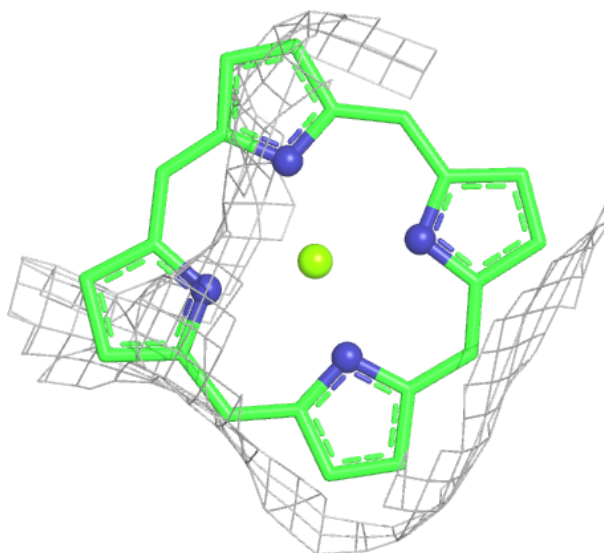
Electron density around CLA 4 616:

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



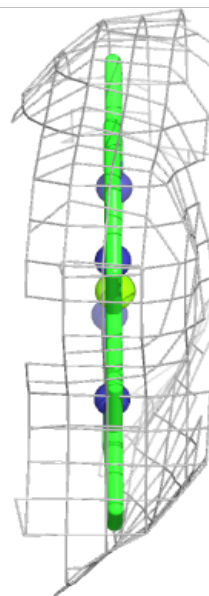
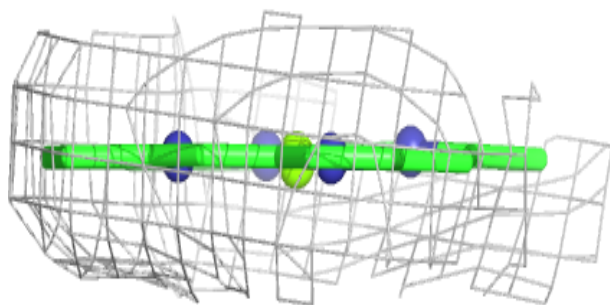
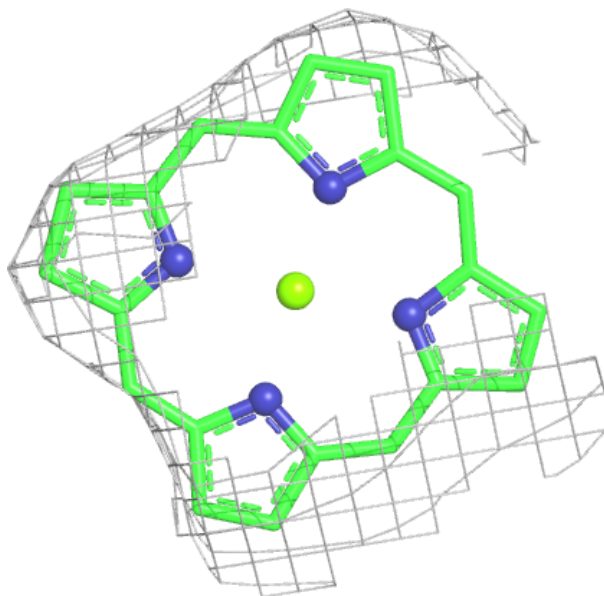
Electron density around CLA 4 610:

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



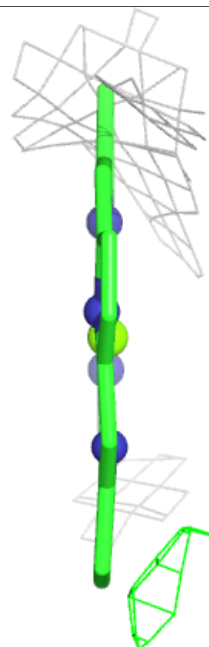
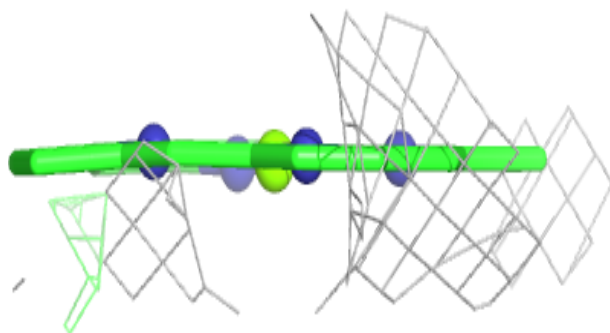
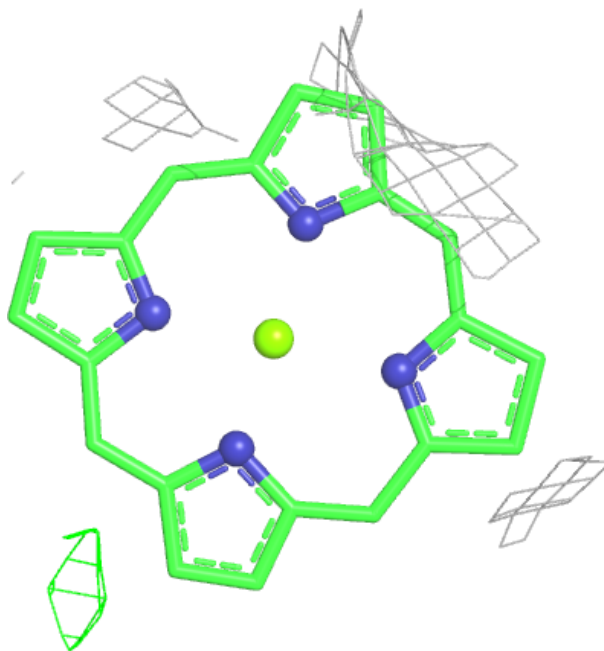
Electron density around CLA 2 602:

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



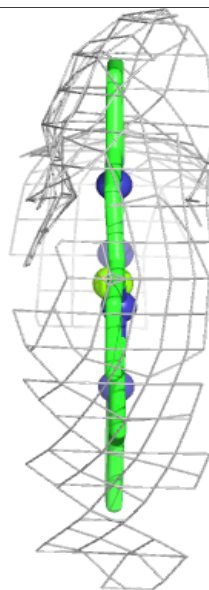
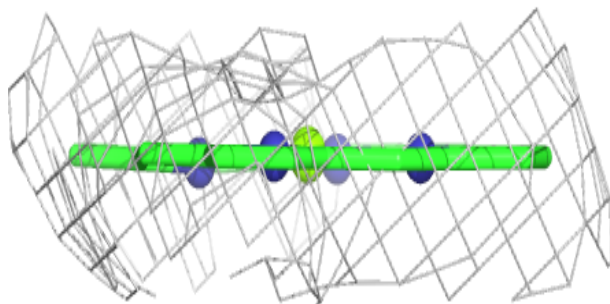
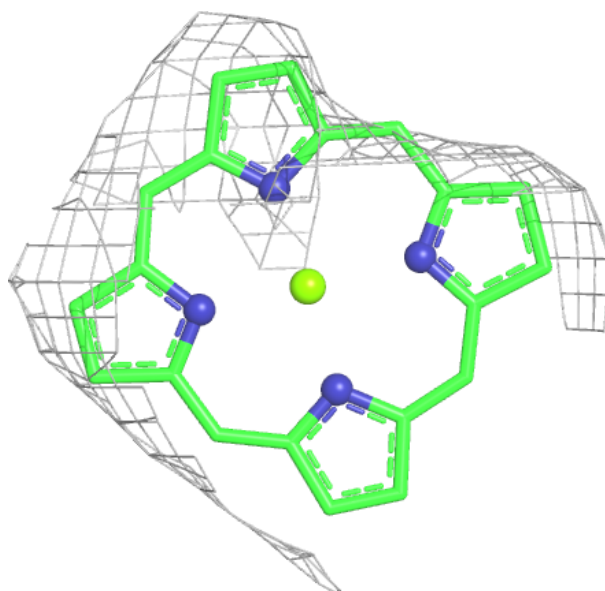
Electron density around CLA 3 602:

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



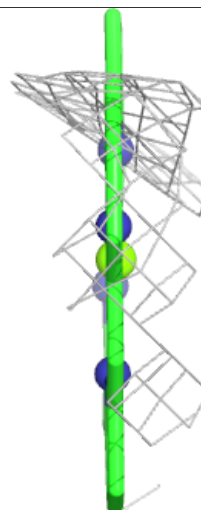
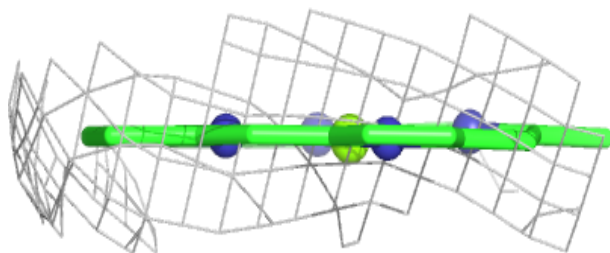
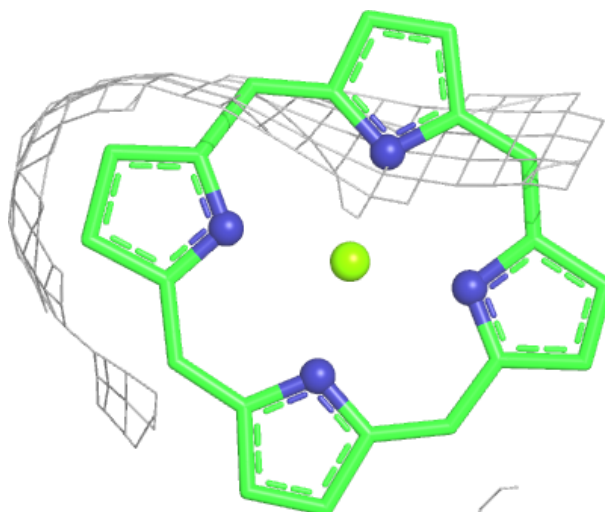
Electron density around CLA B 1219:

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



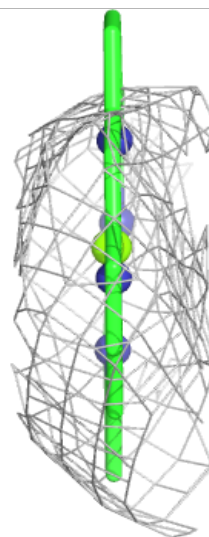
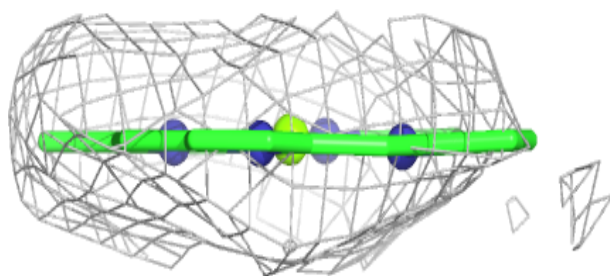
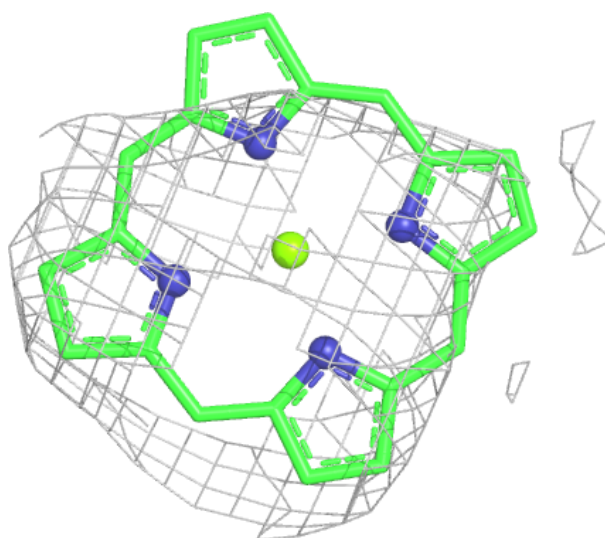
Electron density around CLA 4 615:

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



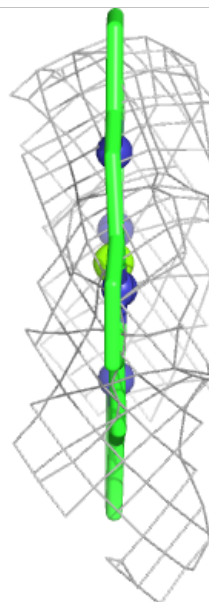
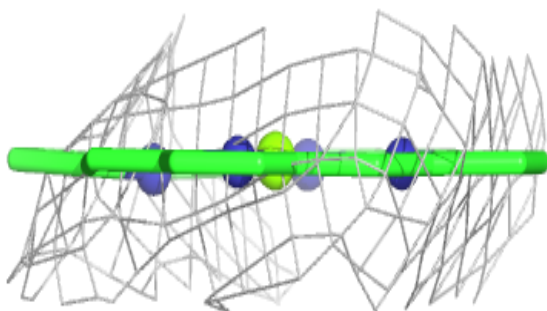
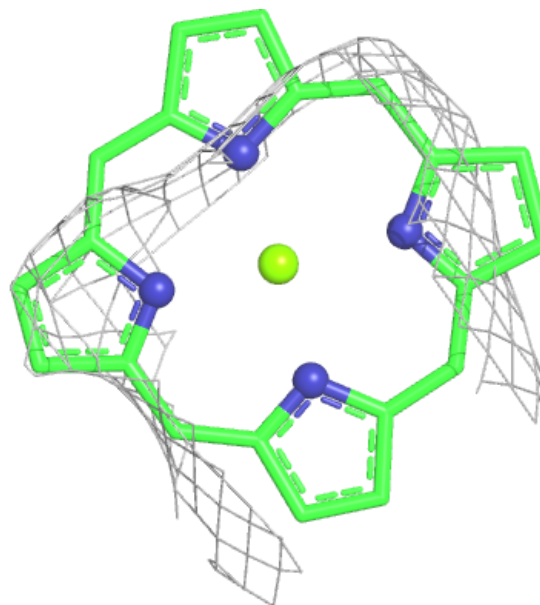
Electron density around CLA 3 614:

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



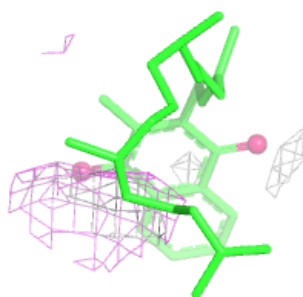
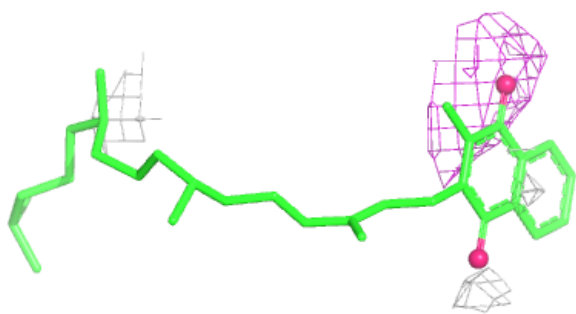
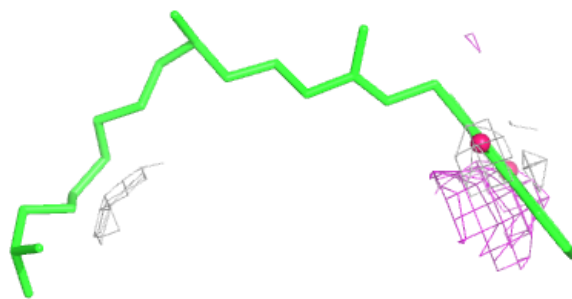
Electron density around CLA B 1212:

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



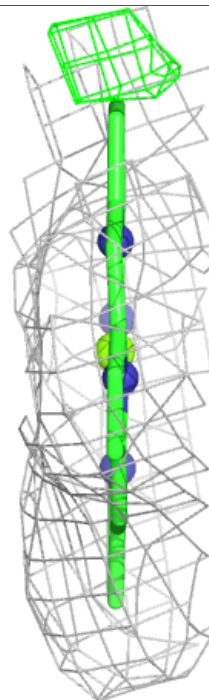
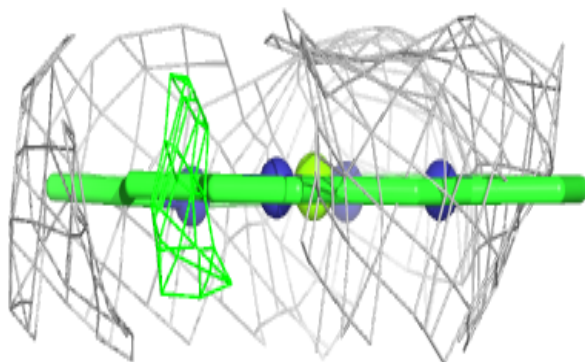
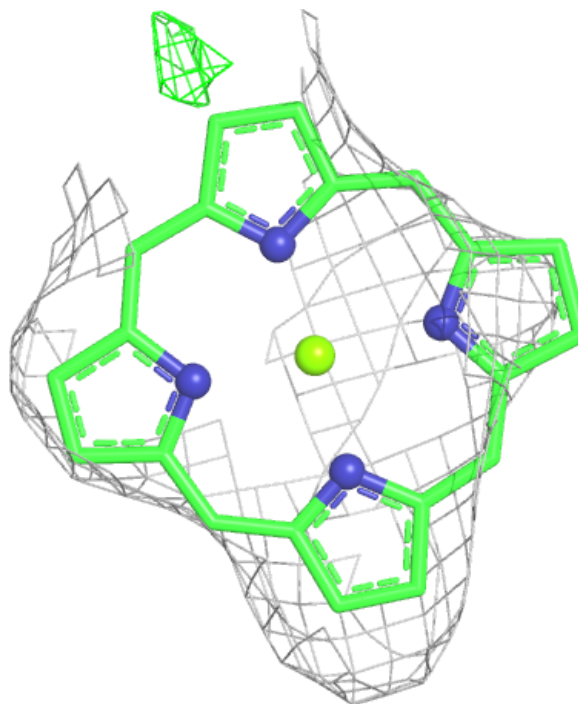
Electron density around PQN B 2002:

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



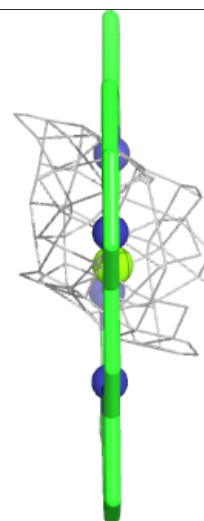
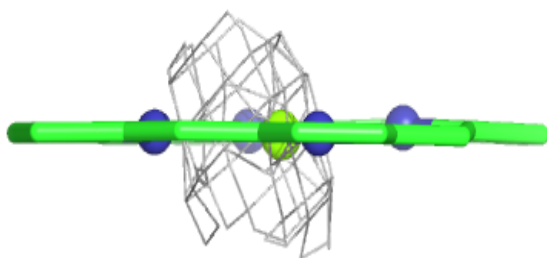
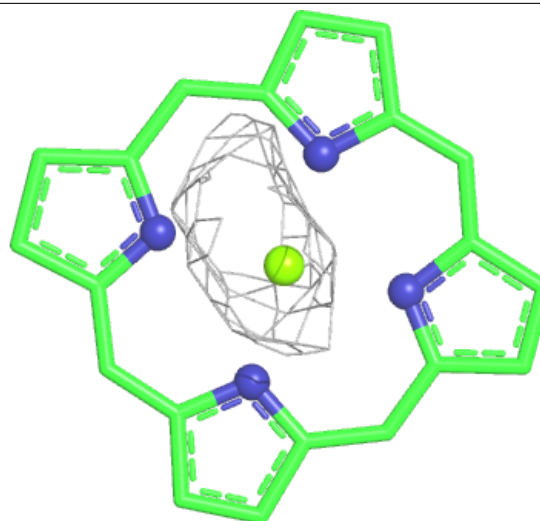
Electron density around CLA B 1223:

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



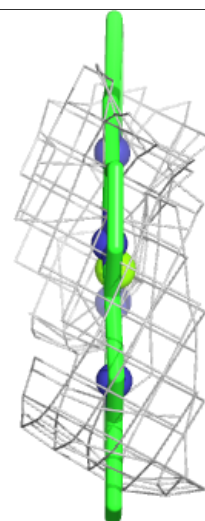
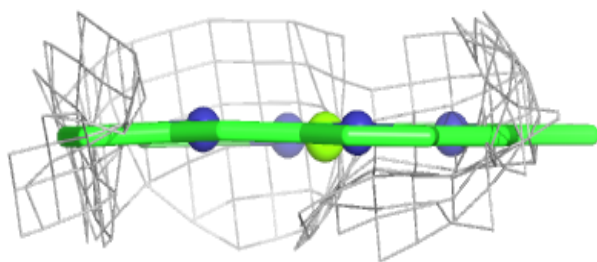
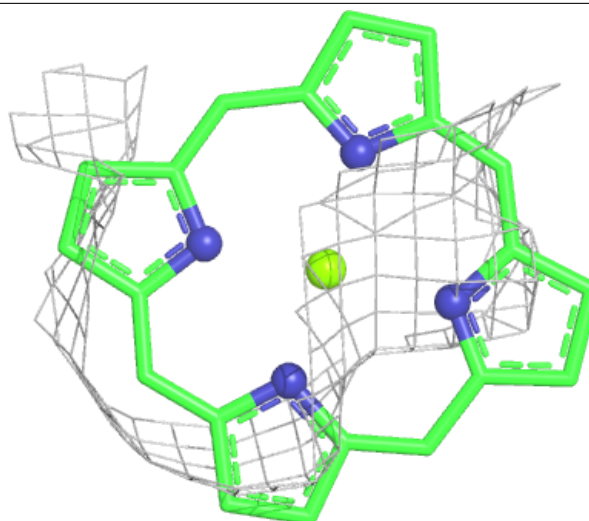
Electron density around CLA B 1216:

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



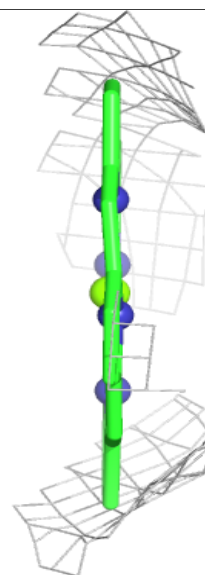
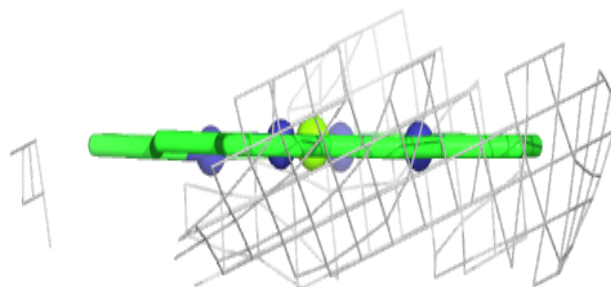
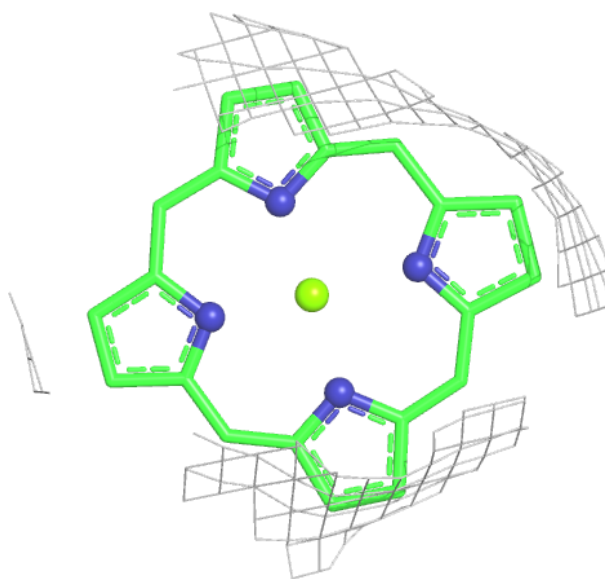
Electron density around CLA B 1210:

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



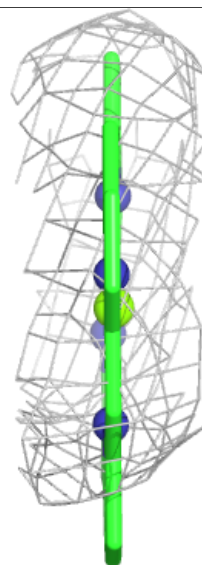
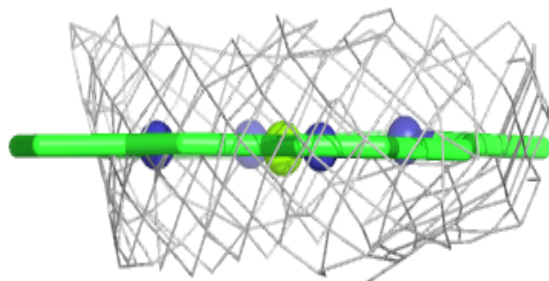
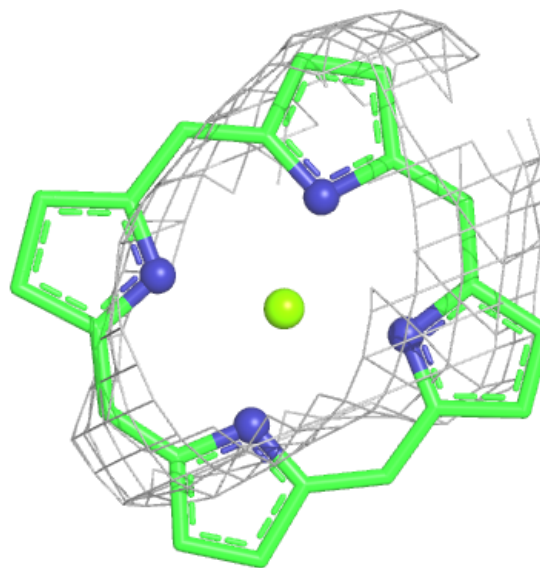
Electron density around CLA L 1501:

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



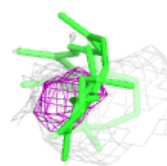
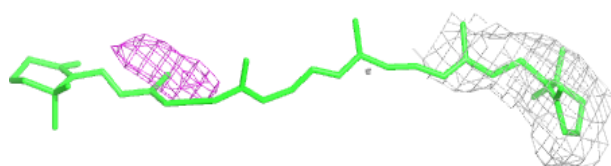
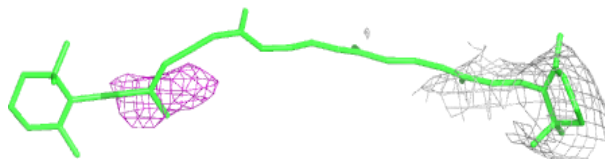
Electron density around CLA 2 614:

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

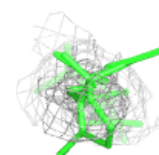
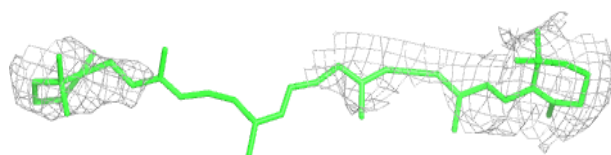
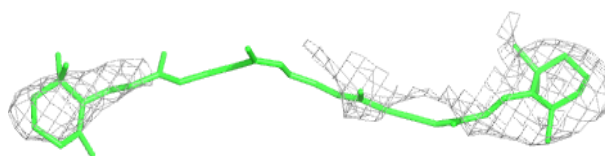


Electron density around BCR A 4008:

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

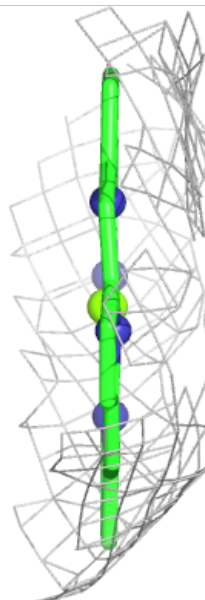
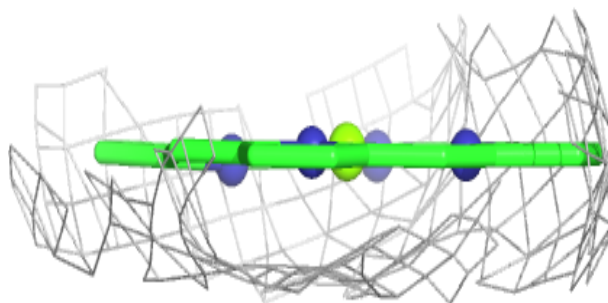
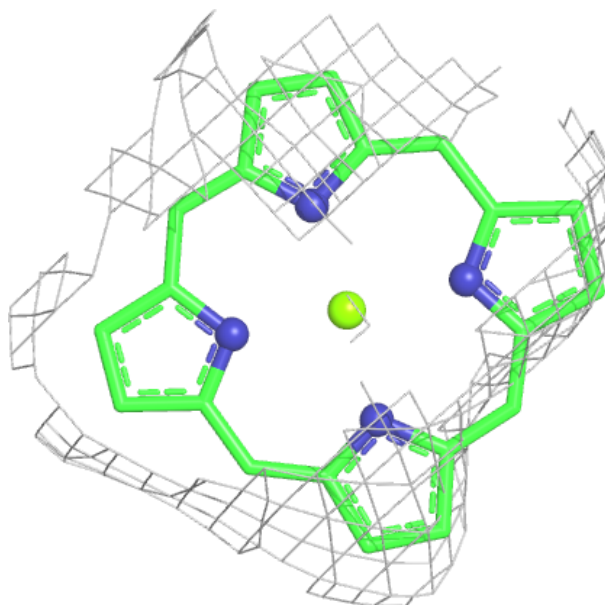
**Electron density around BCR A 4007:**

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



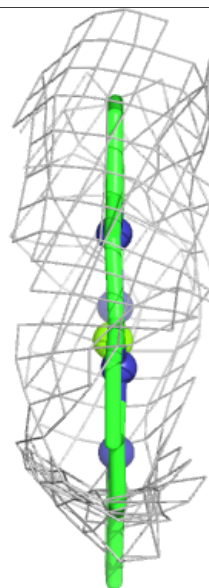
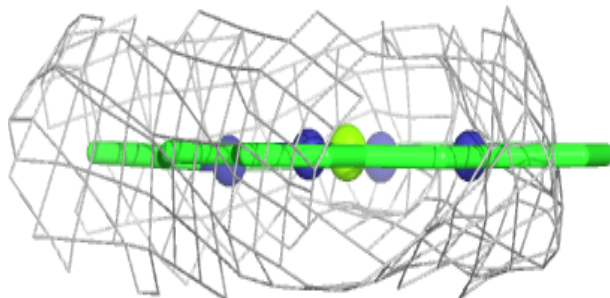
Electron density around CLA L 1502:

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



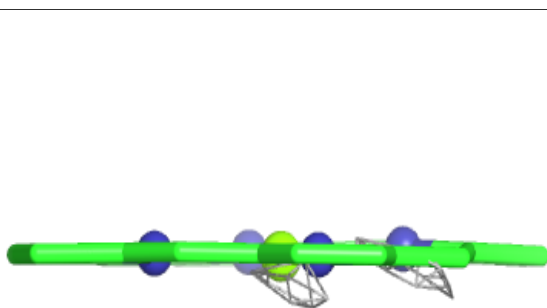
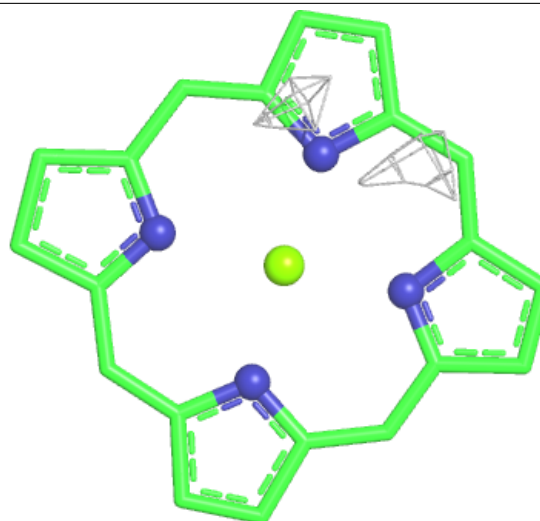
Electron density around CLA 2 603:

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



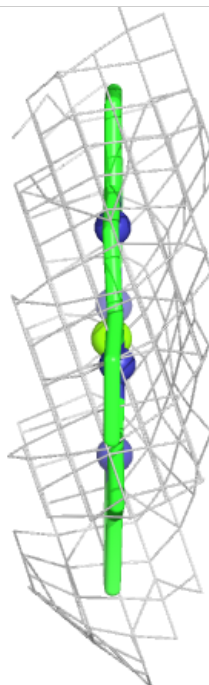
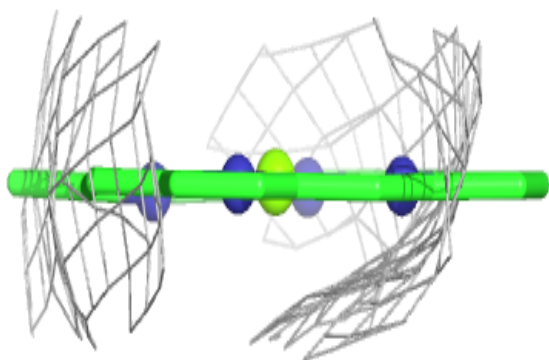
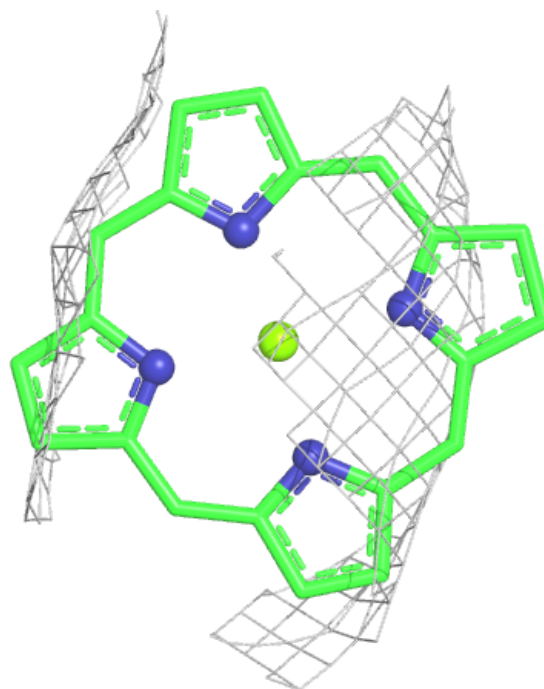
Electron density around CLA B 1221:

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



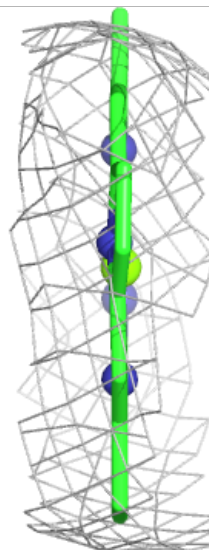
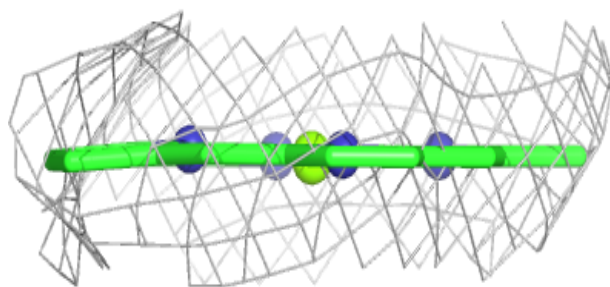
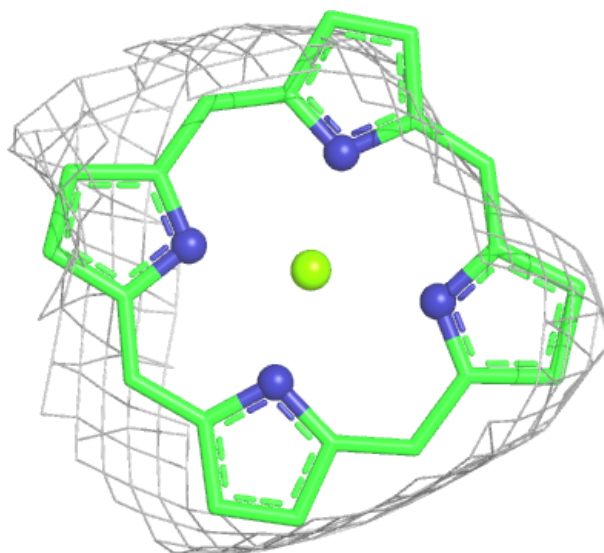
Electron density around CLA B 1231:

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



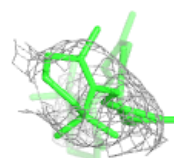
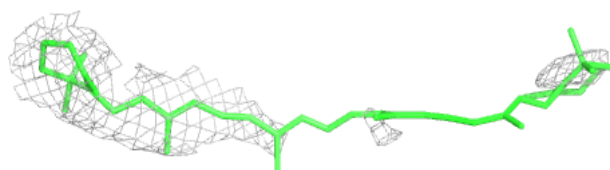
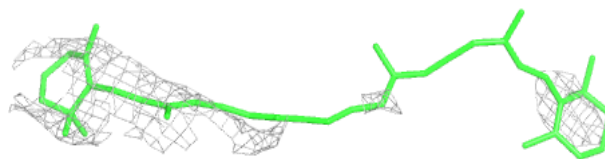
Electron density around CLA 3 601:

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



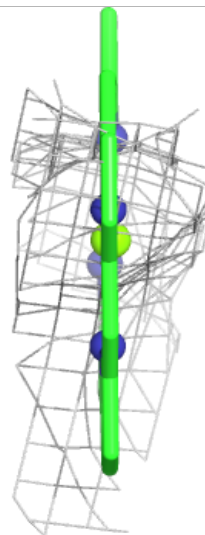
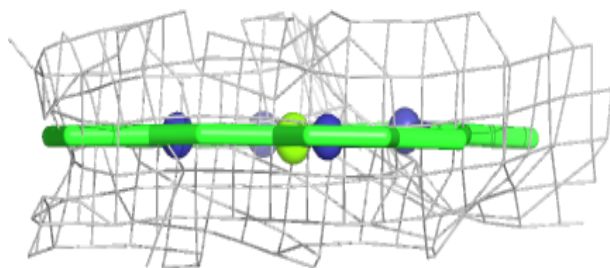
Electron density around BCR I 4018:

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



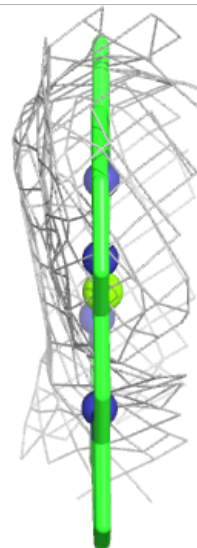
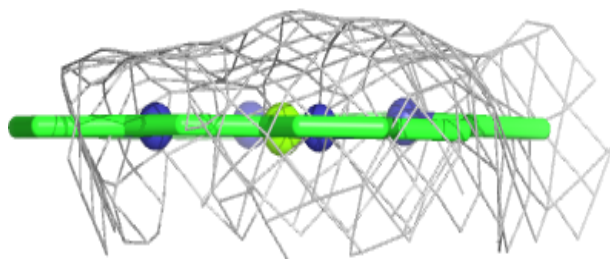
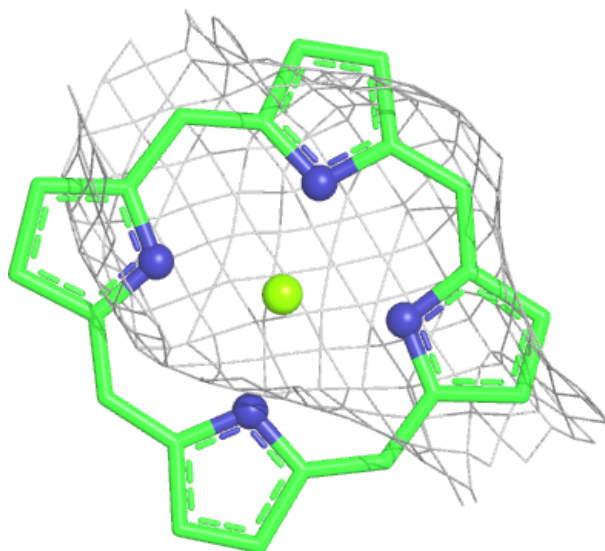
Electron density around CLA 4 609:

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



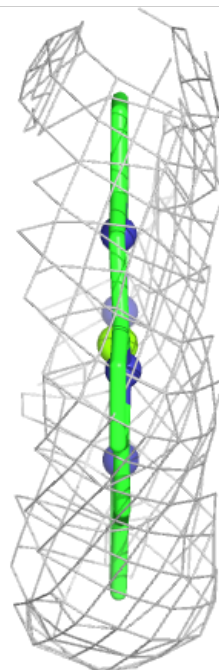
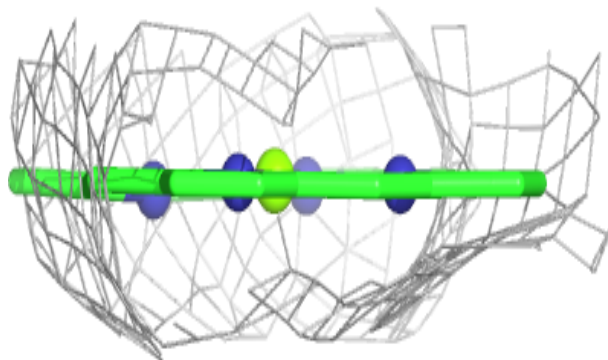
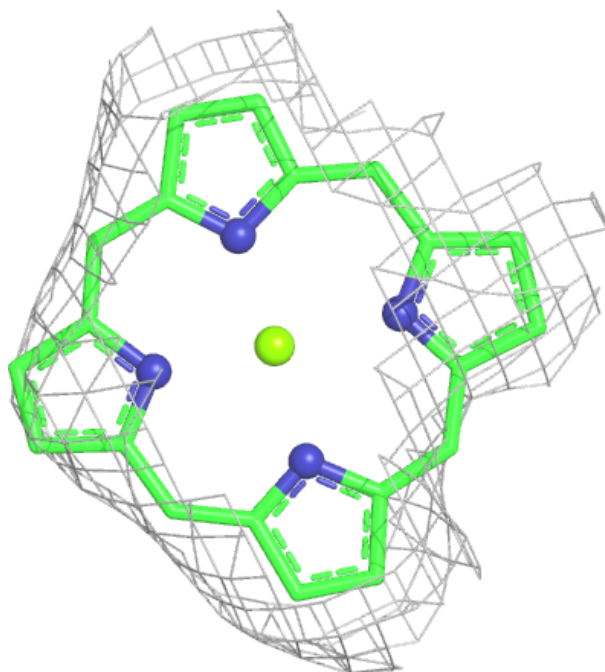
Electron density around CLA B 1204:

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



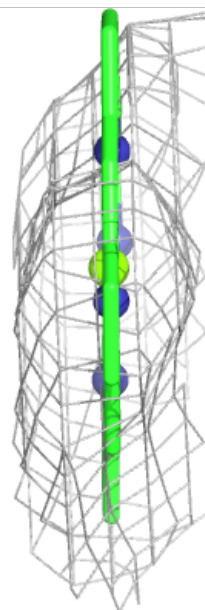
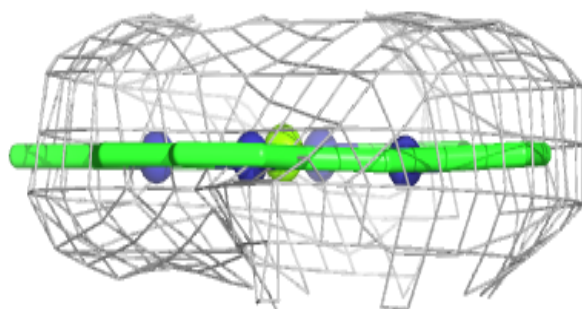
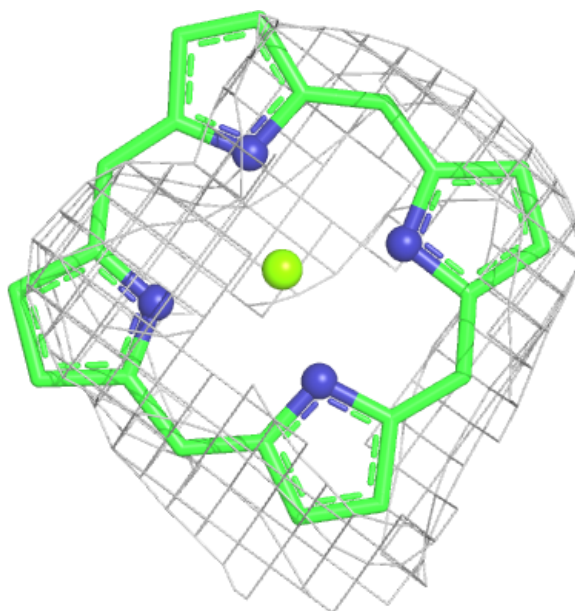
Electron density around CLA 2 607:

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



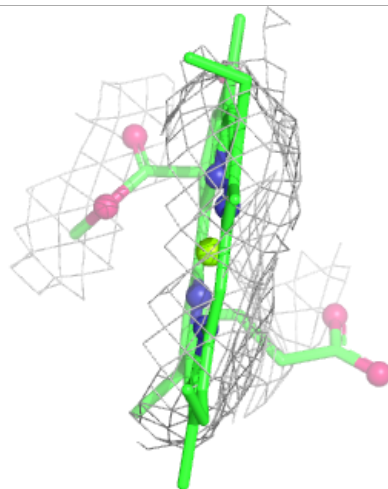
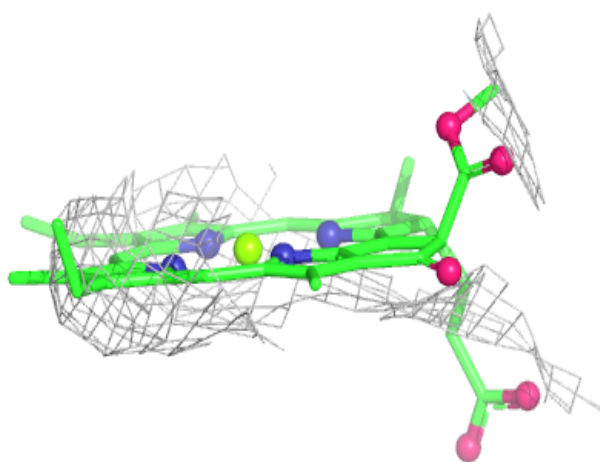
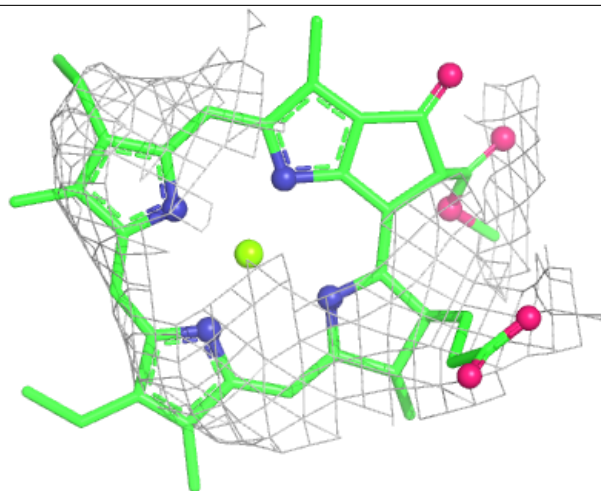
Electron density around CLA 4 603:

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



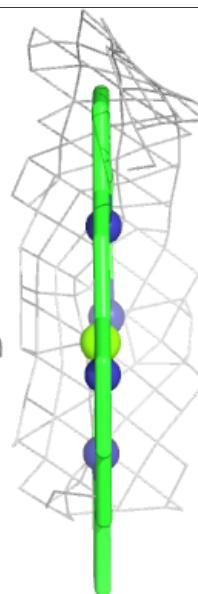
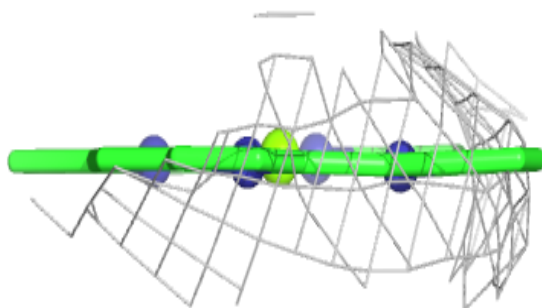
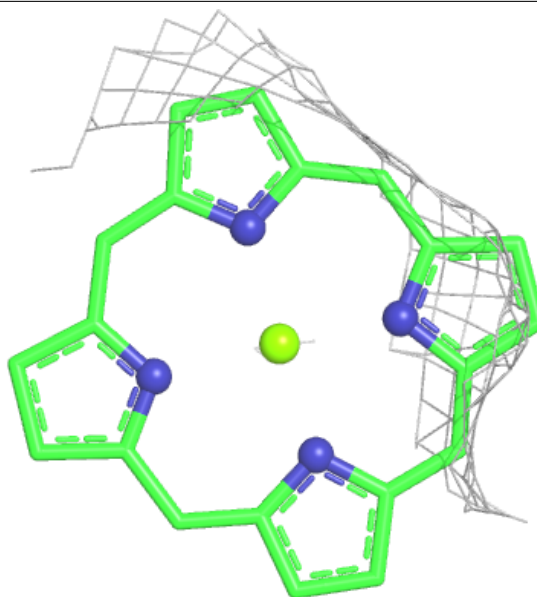
Electron density around CLA B 1236:

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



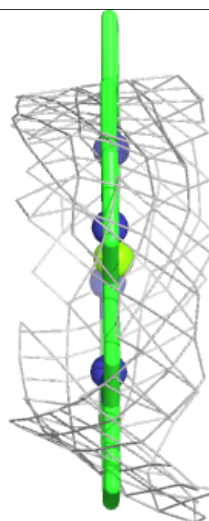
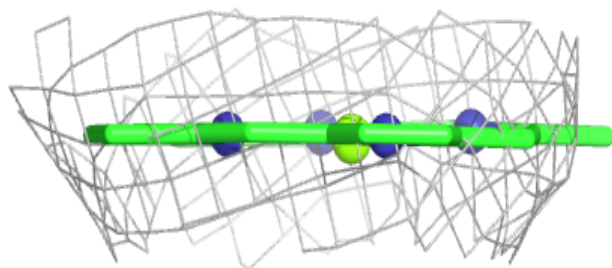
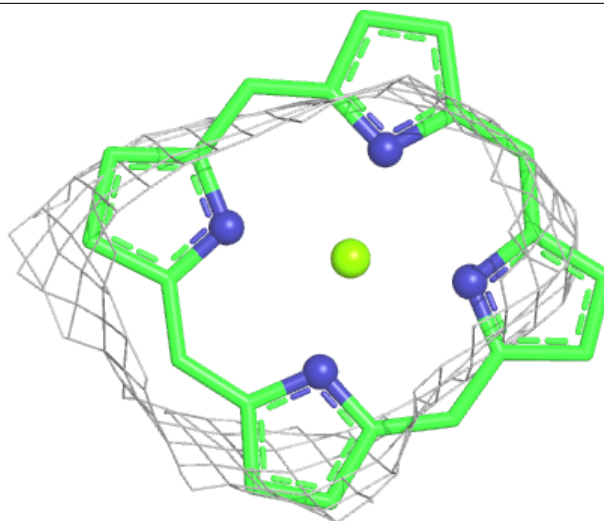
Electron density around CLA K 1402:

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



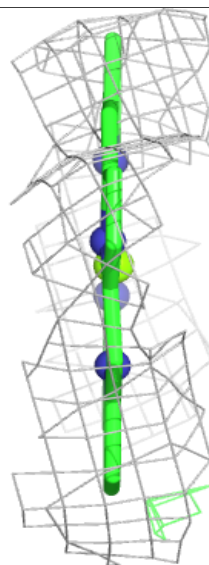
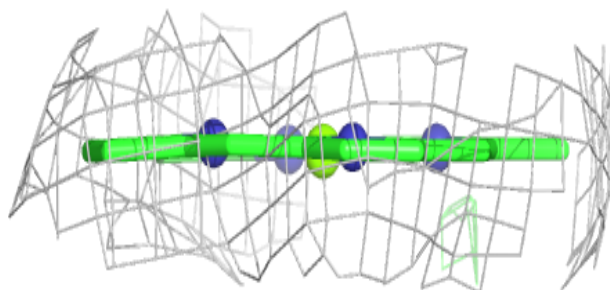
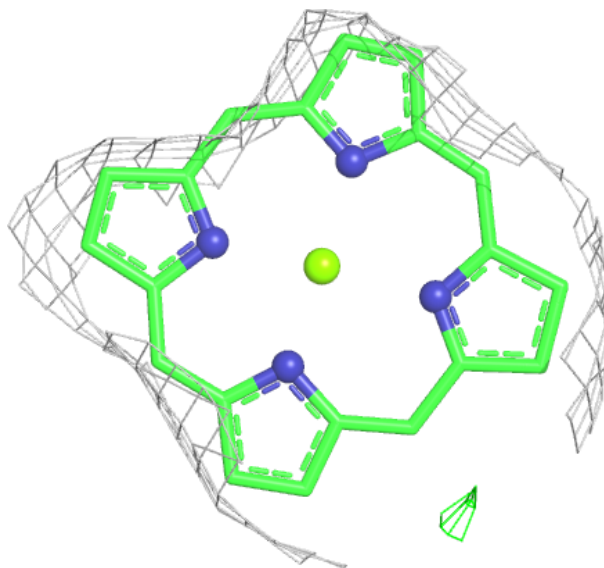
Electron density around CLA 3 604:

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



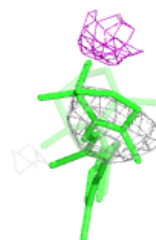
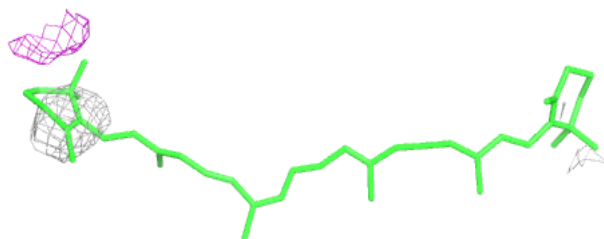
Electron density around CLA A 1109:

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



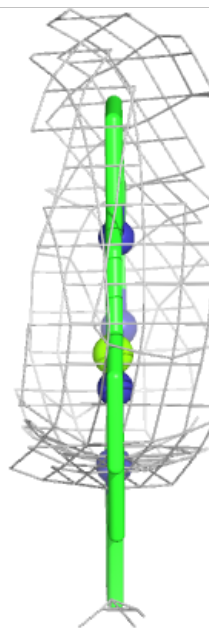
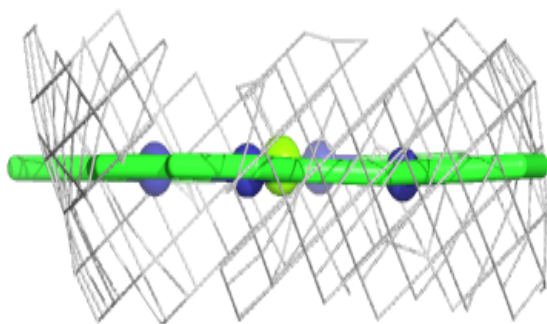
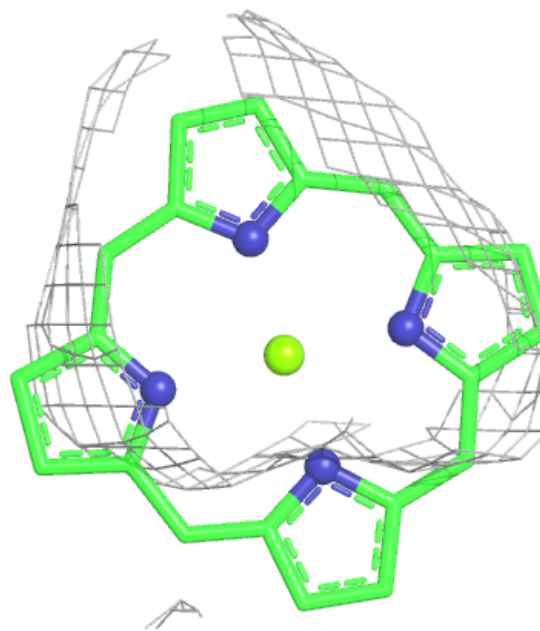
Electron density around BCR A 4017:

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



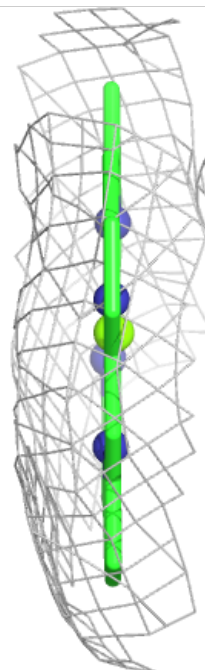
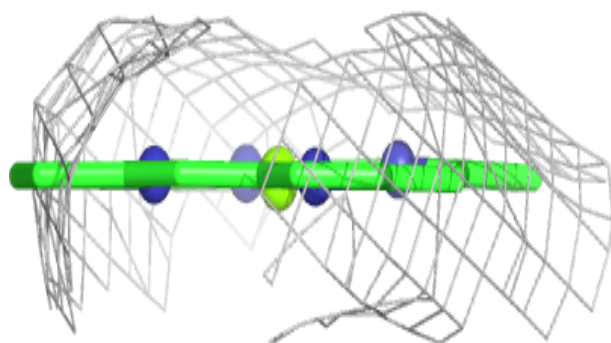
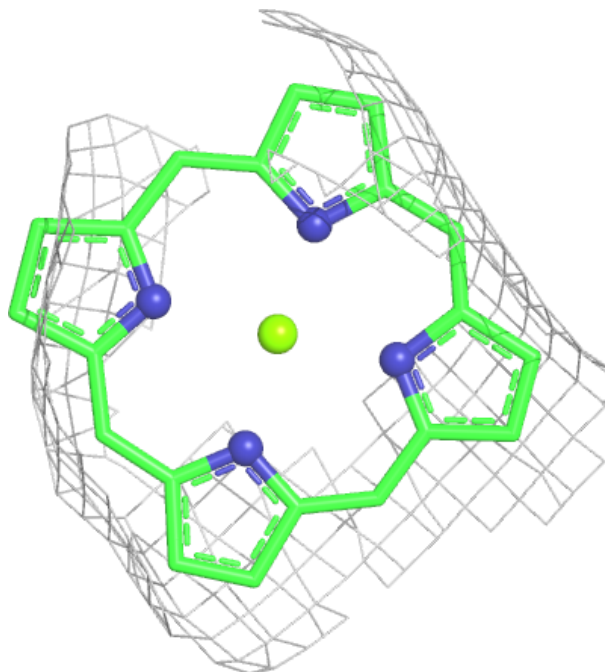
Electron density around CLA 2 610:

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



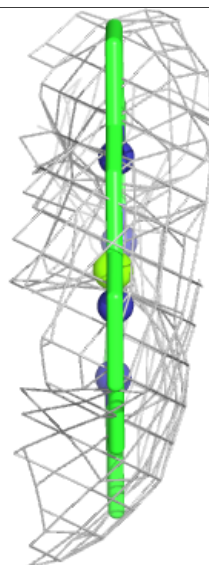
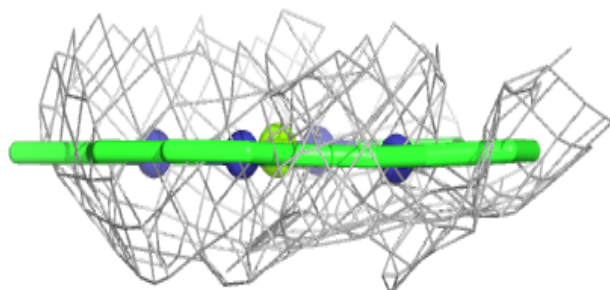
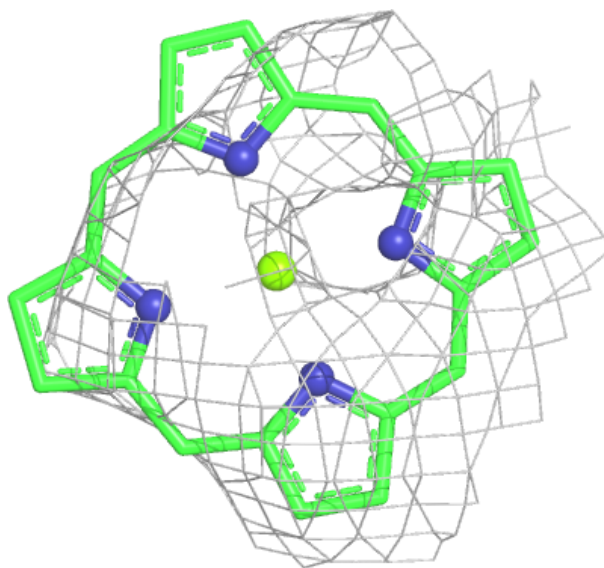
Electron density around CLA K 1401:

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



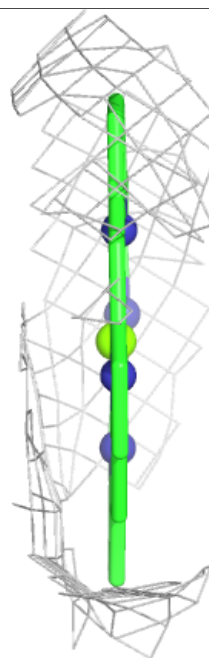
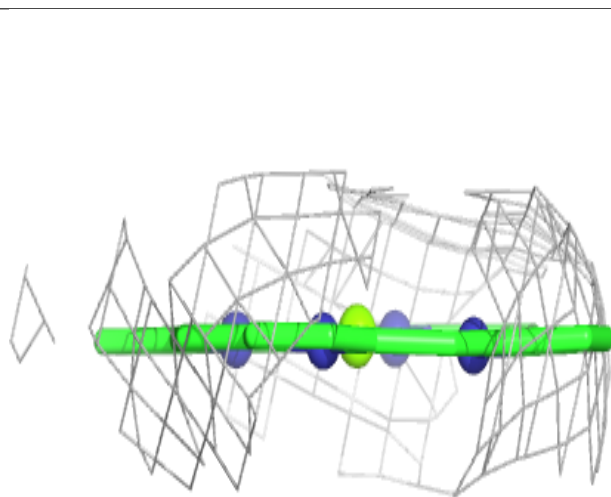
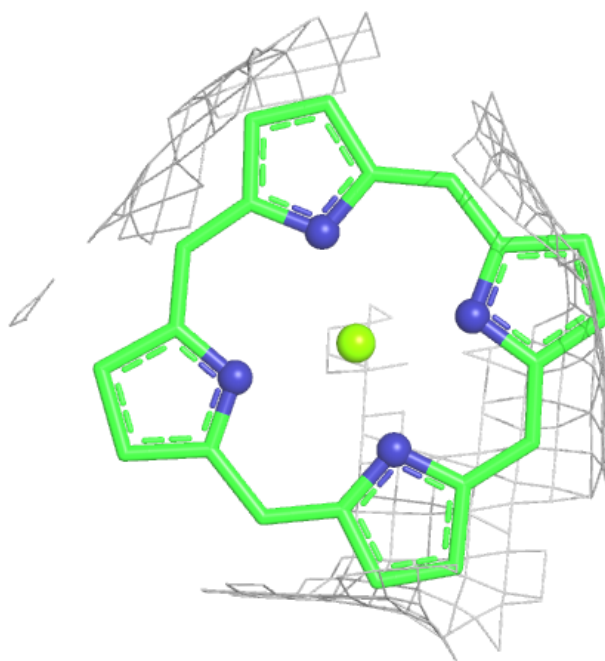
Electron density around CLA 3 606:

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



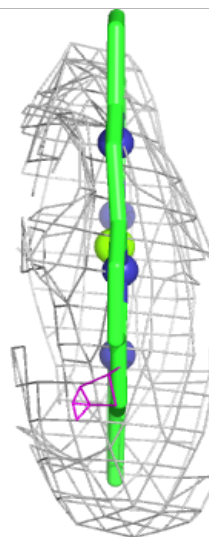
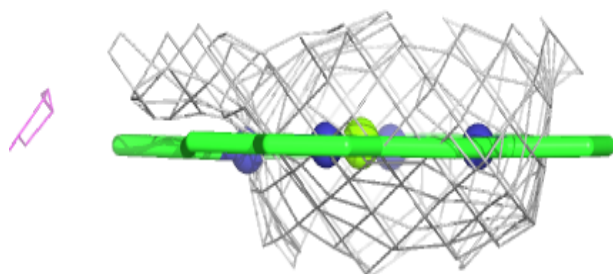
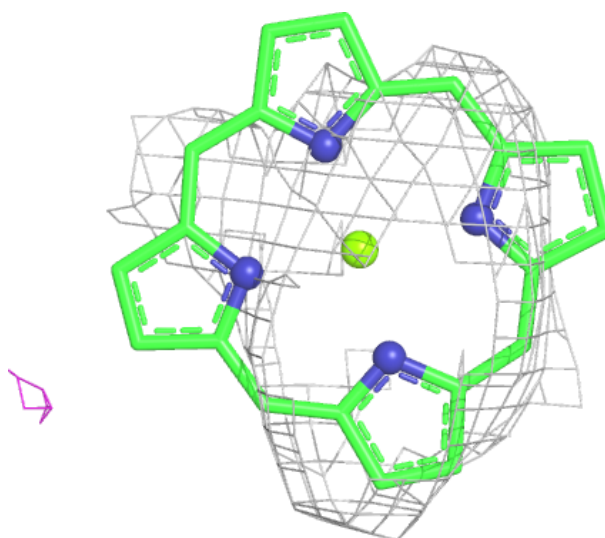
Electron density around CLA 3 612:

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



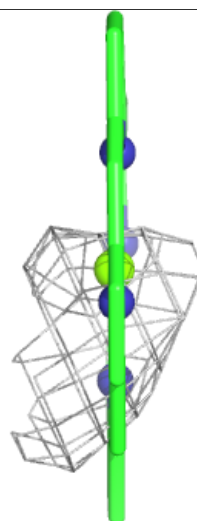
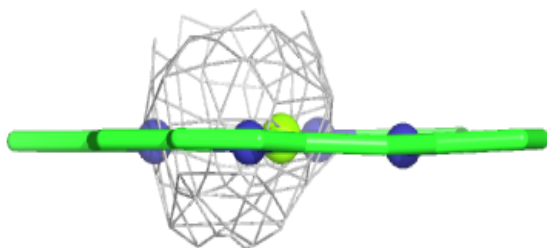
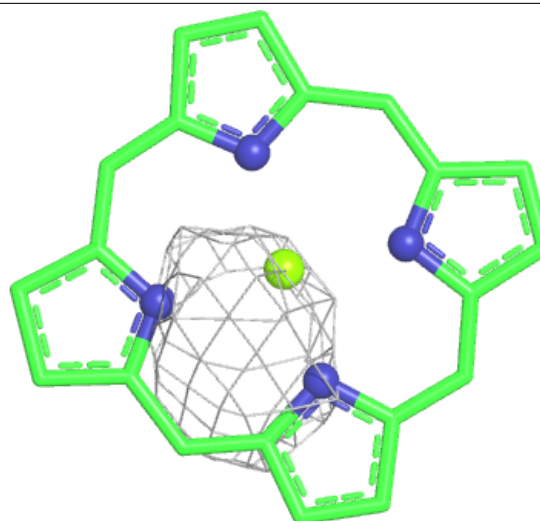
Electron density around CLA A 1120:

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



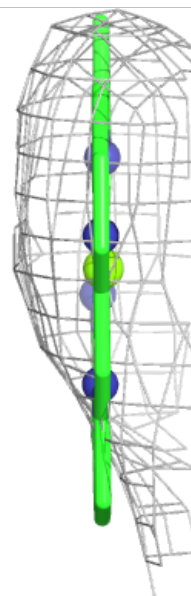
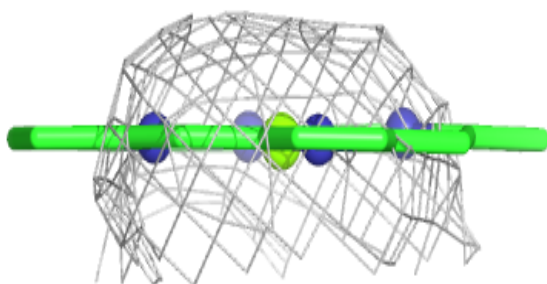
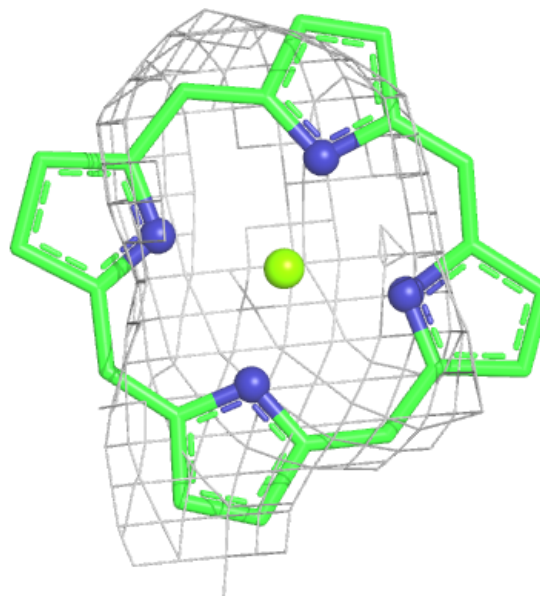
Electron density around CLA B 1214:

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



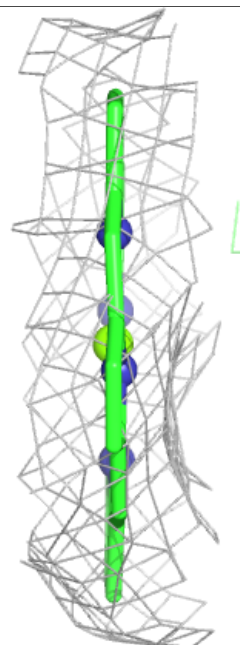
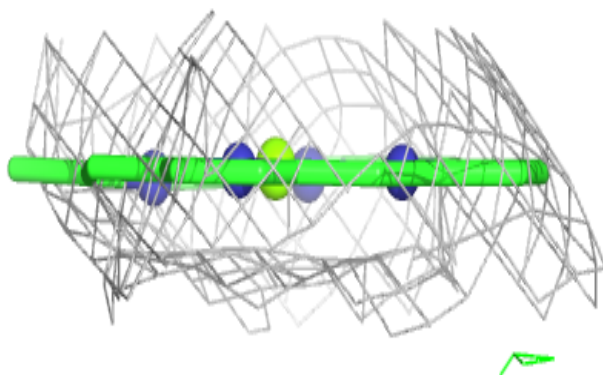
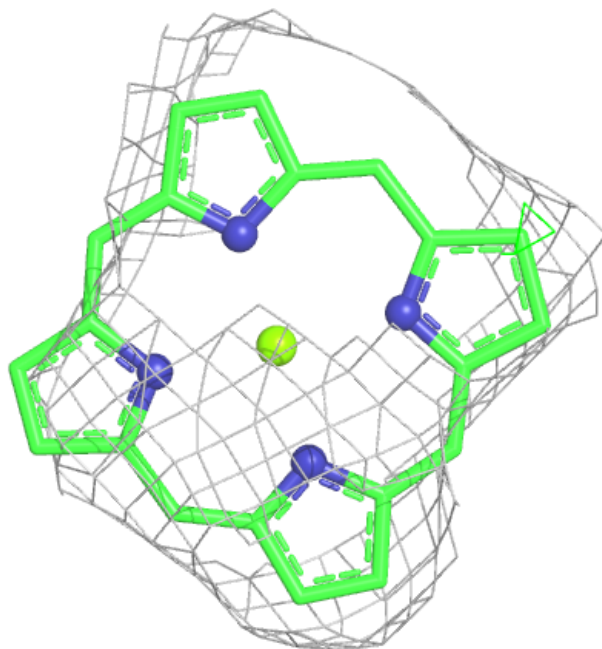
Electron density around CLA L 1503:

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



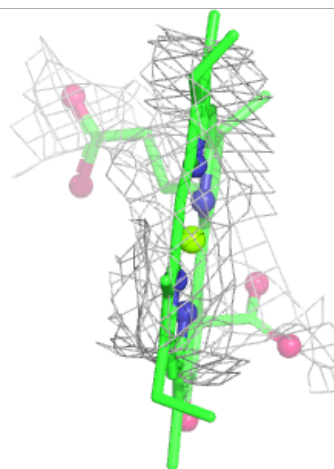
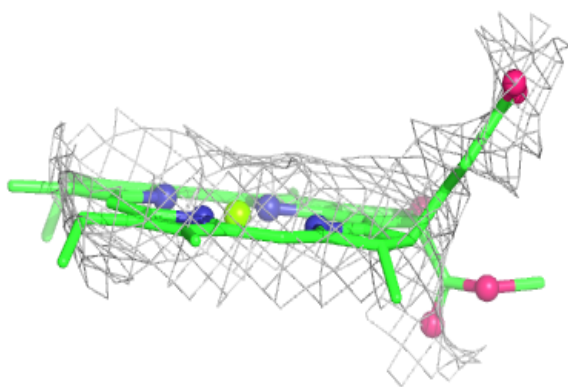
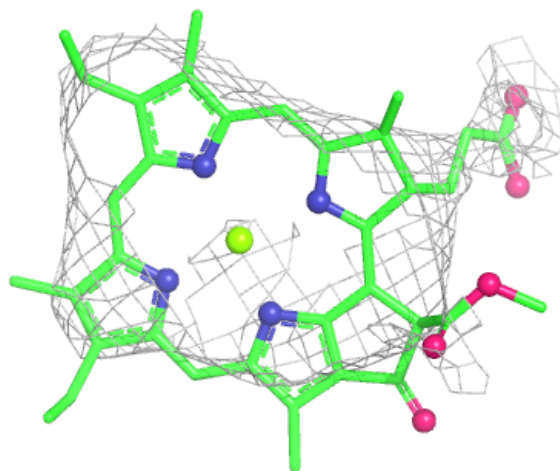
Electron density around CLA A 1112:

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



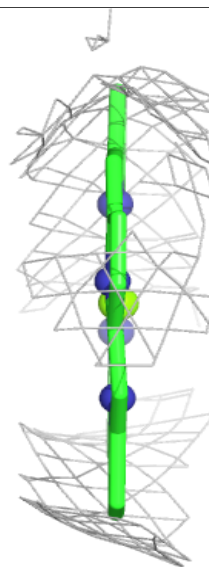
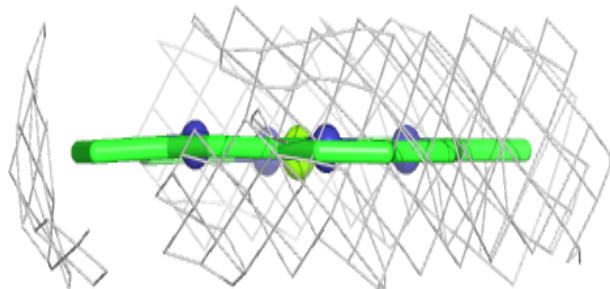
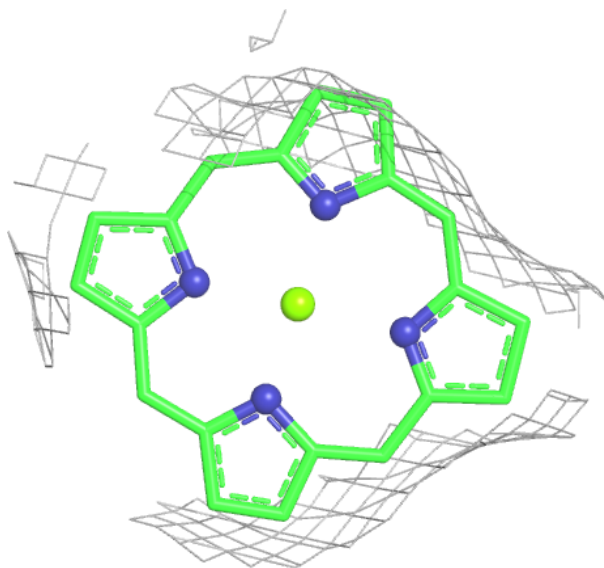
Electron density around CLA B 1021:

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



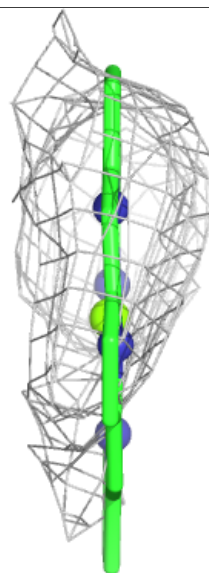
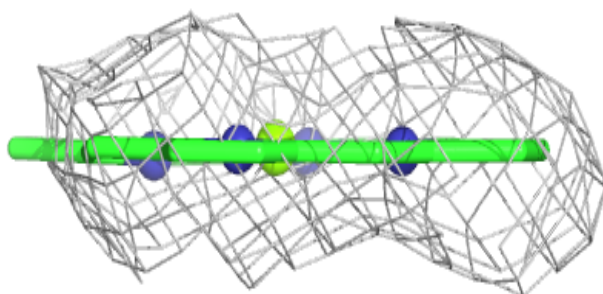
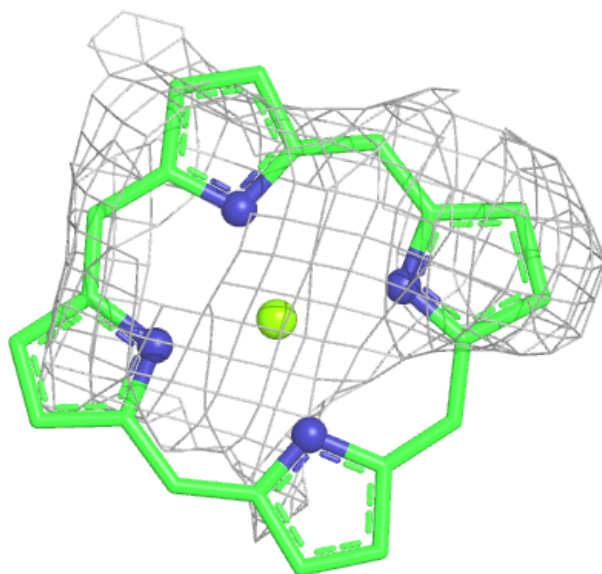
Electron density around CLA 2 604:

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



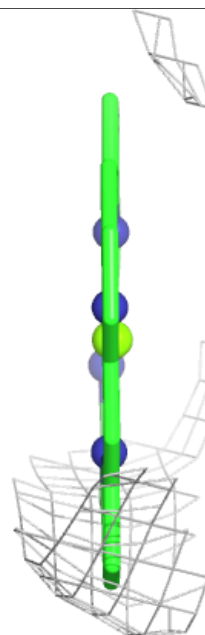
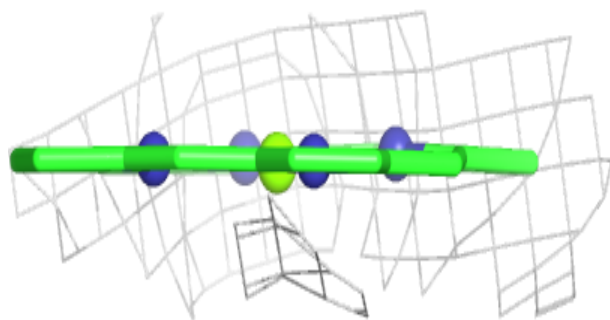
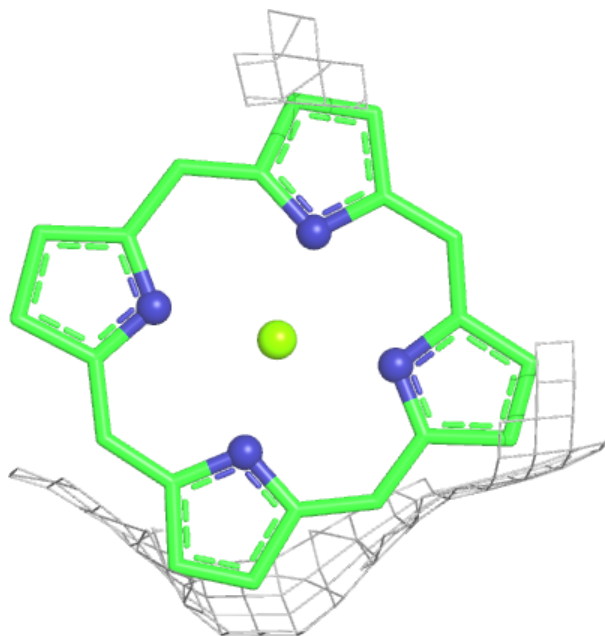
Electron density around CLA A 1137:

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



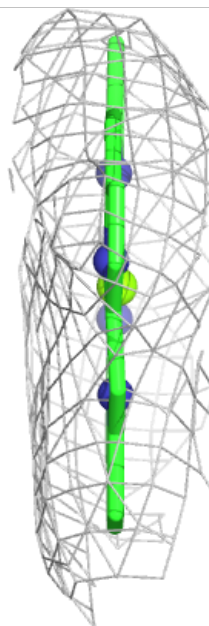
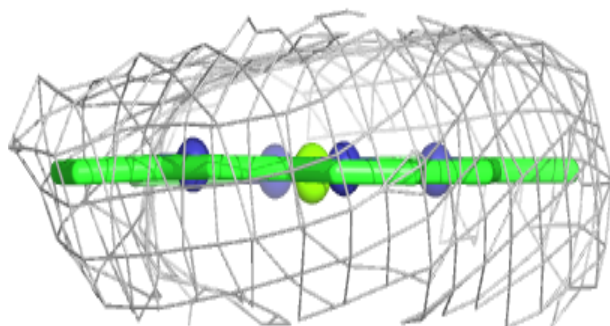
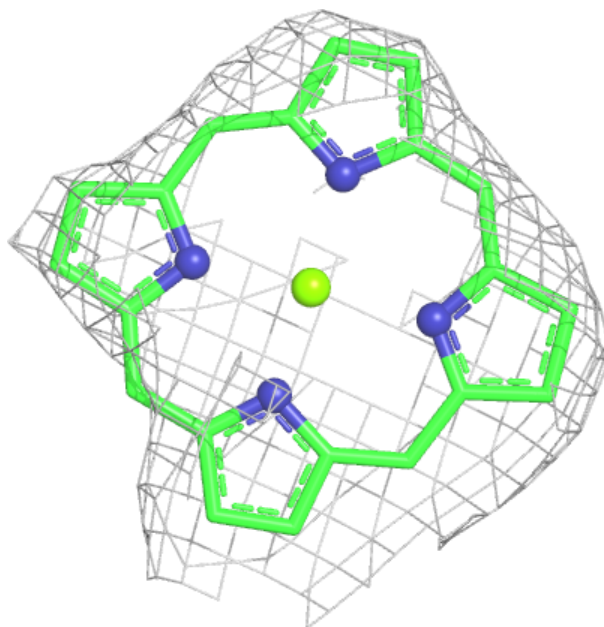
Electron density around CLA 4 606:

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



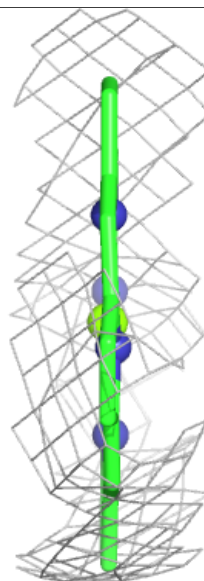
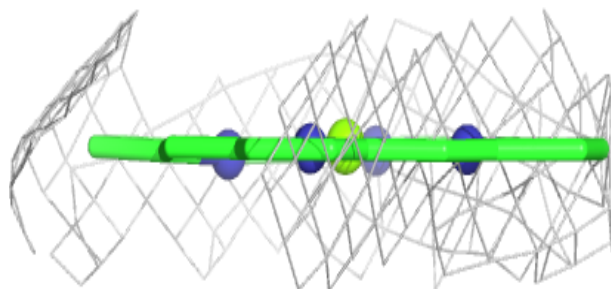
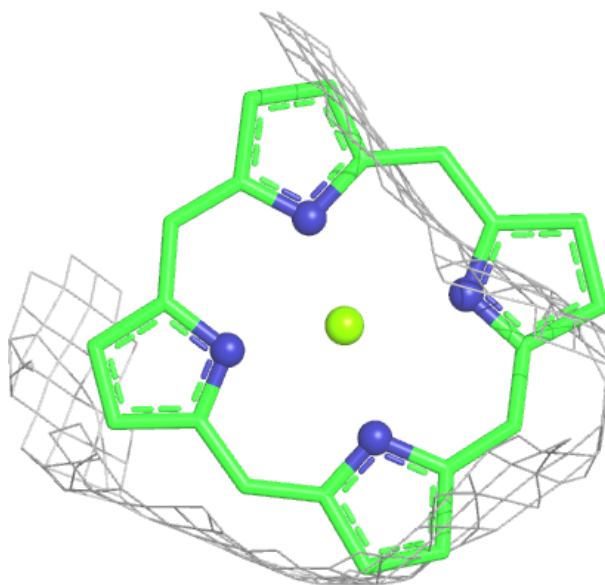
Electron density around CLA B 1238:

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



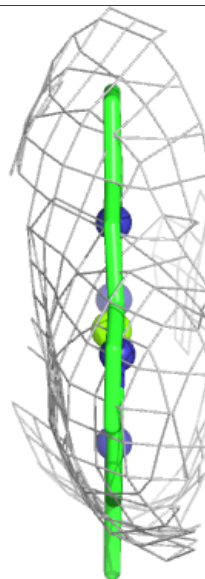
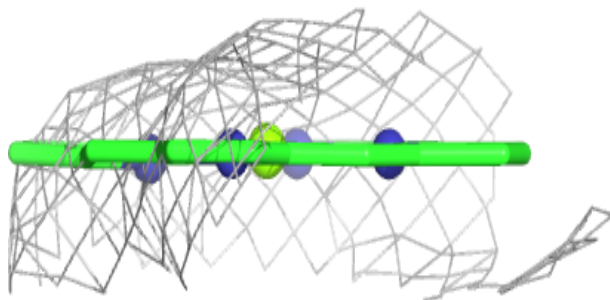
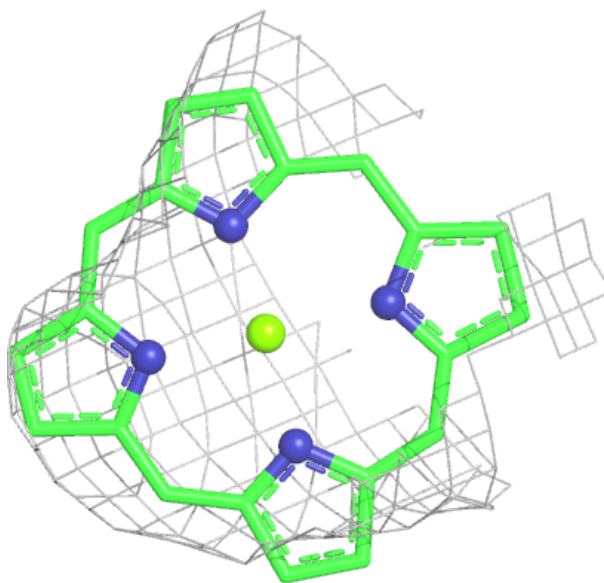
Electron density around CLA F 1302:

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



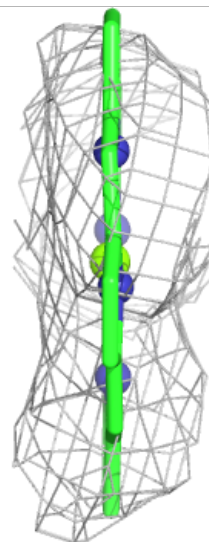
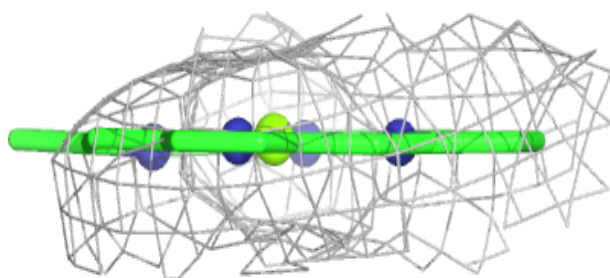
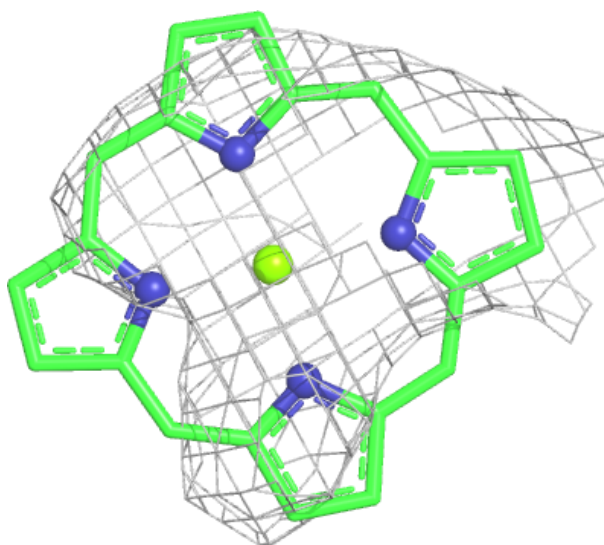
Electron density around CLA B 1203:

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



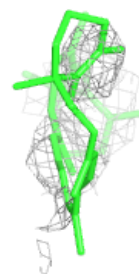
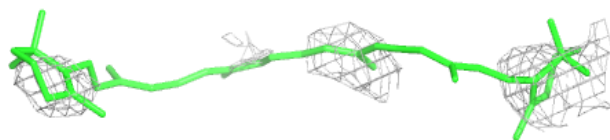
Electron density around CLA A 1119:

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



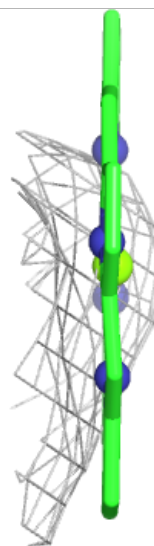
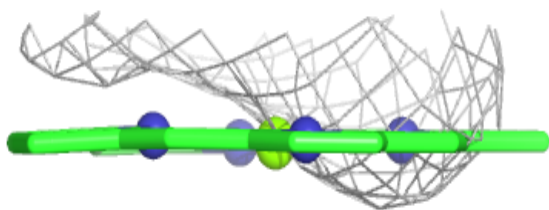
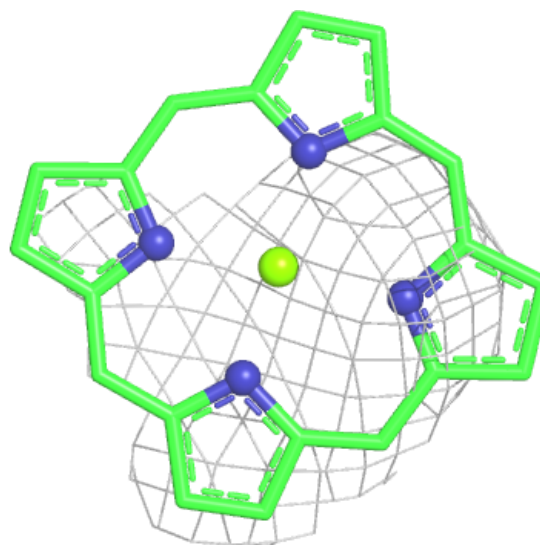
Electron density around BCR A 4011:

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



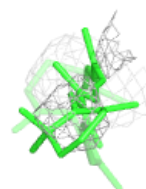
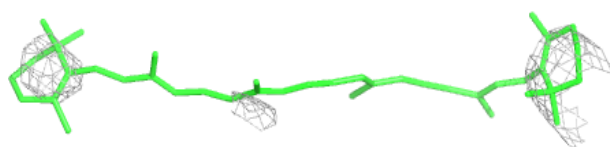
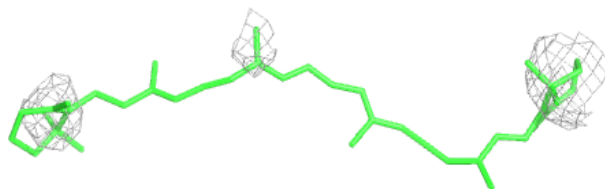
Electron density around CLA B 1207:

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



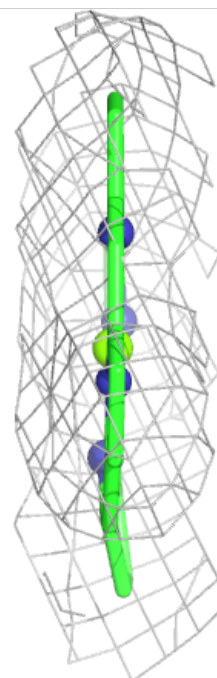
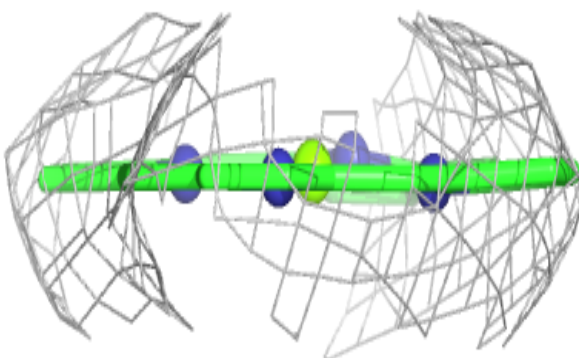
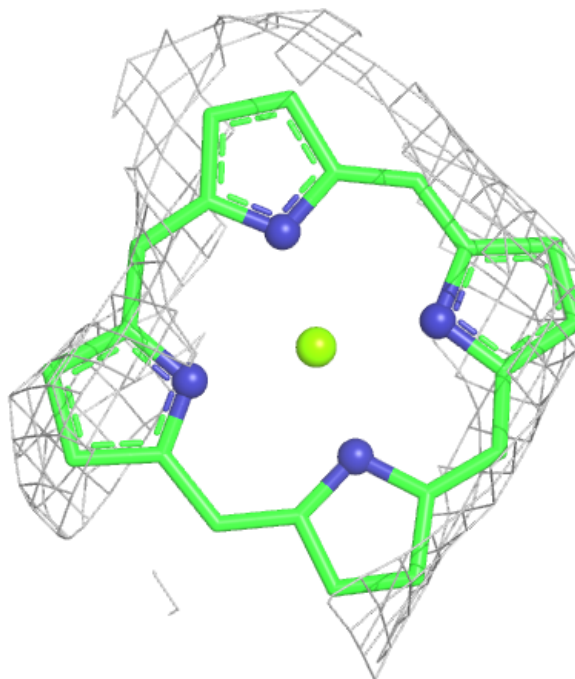
Electron density around BCR B 4008:

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



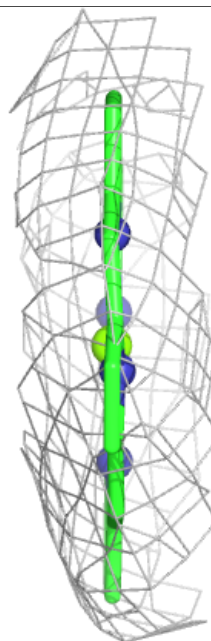
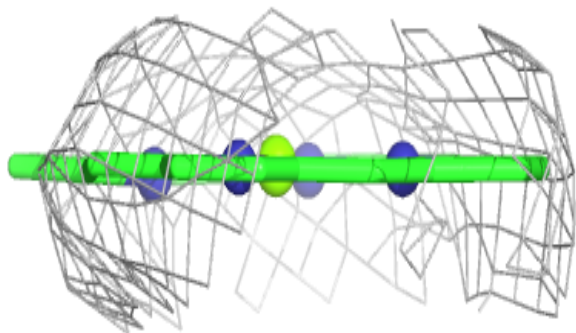
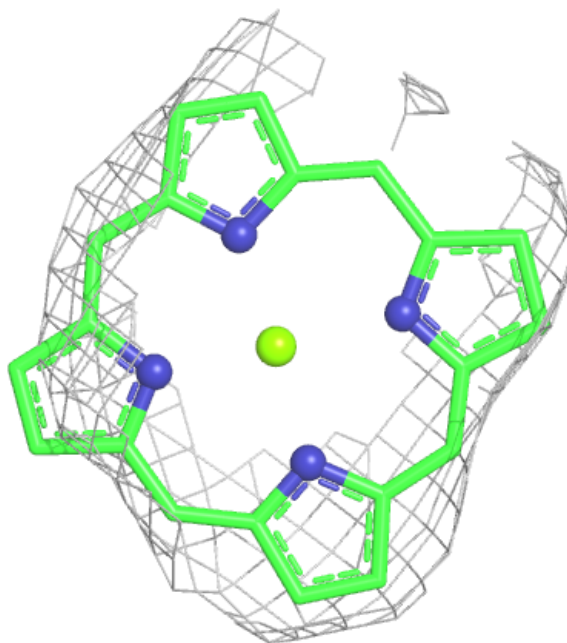
Electron density around CLA B 1228:

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



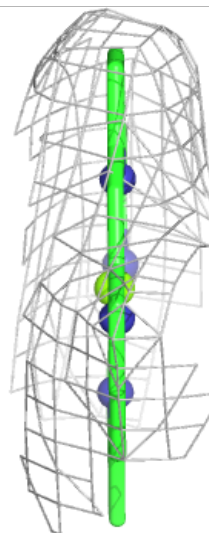
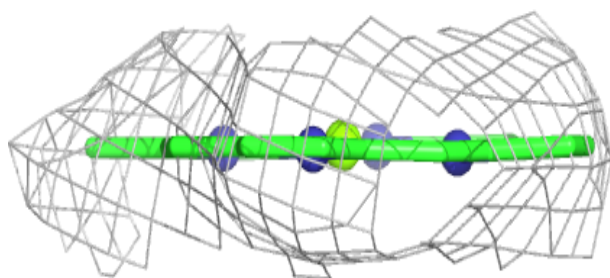
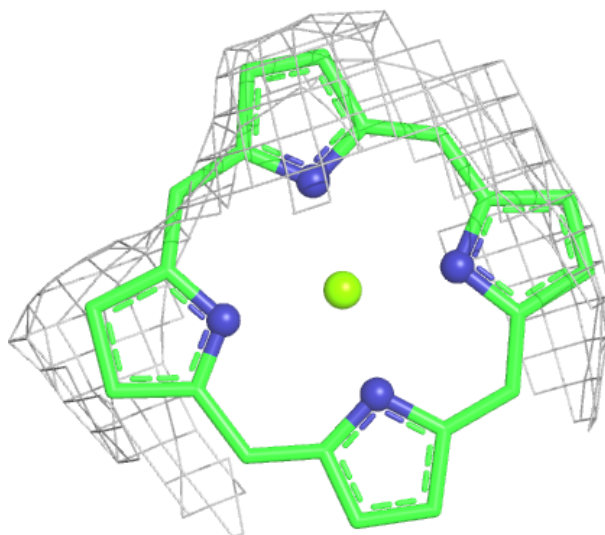
Electron density around CLA A 1121:

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



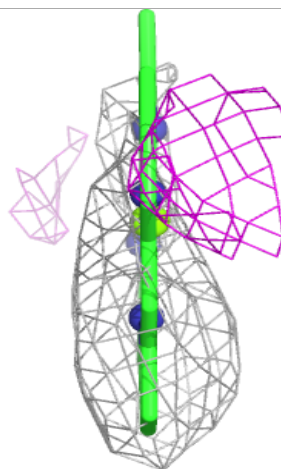
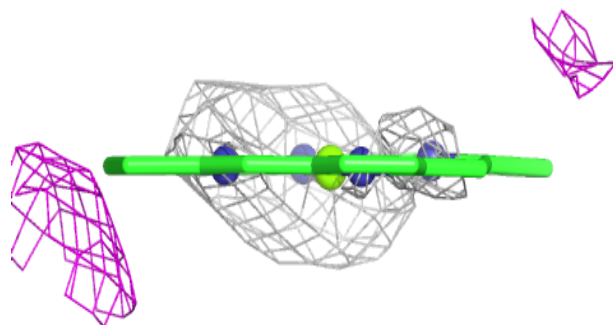
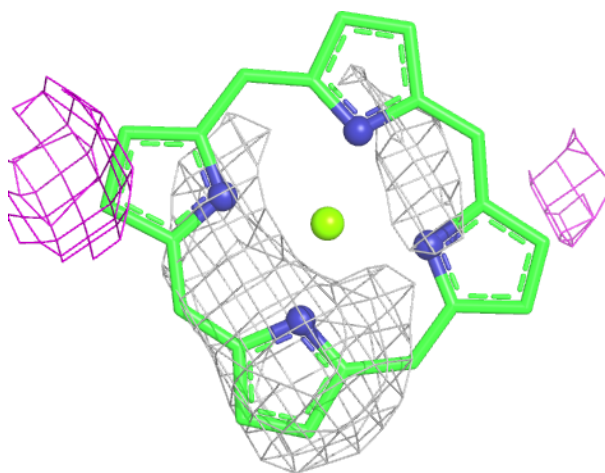
Electron density around CLA 4 612:

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



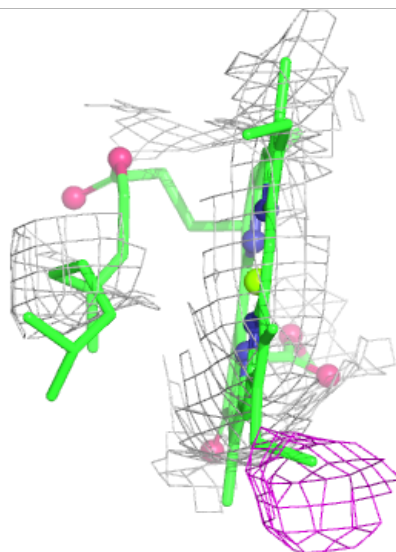
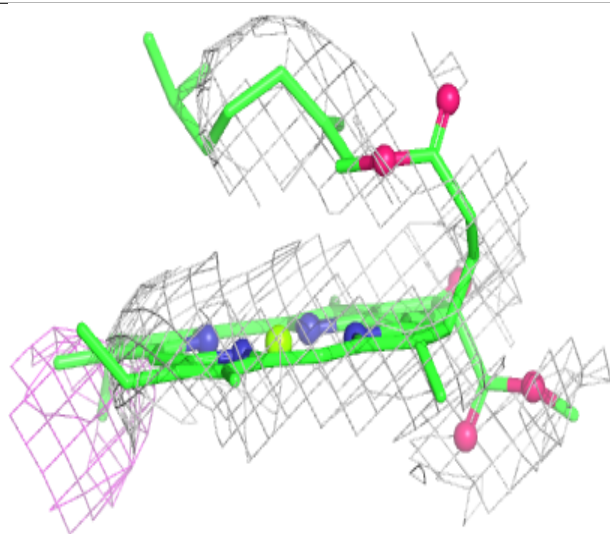
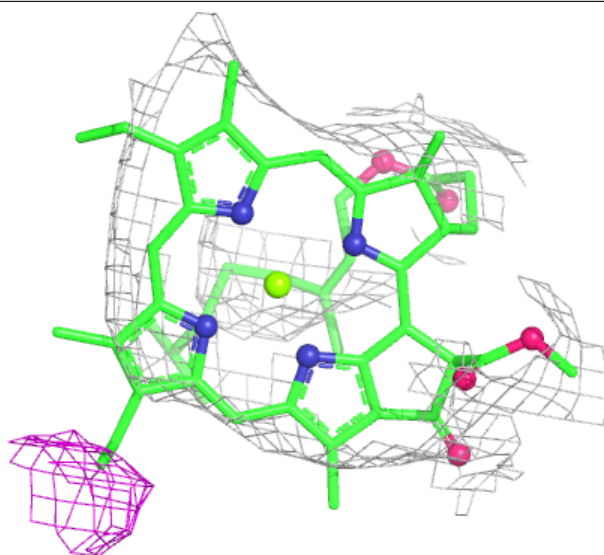
Electron density around CLA A 1138:

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



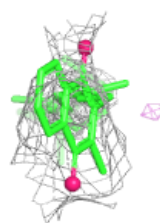
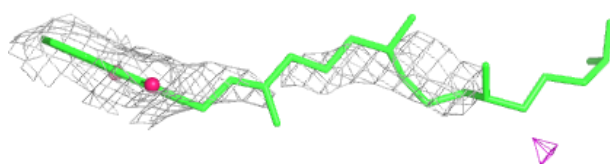
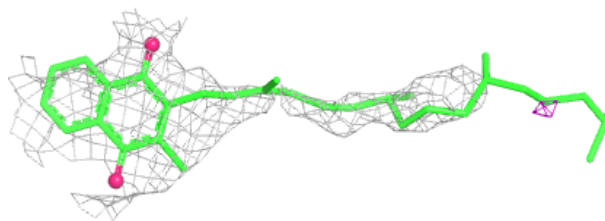
Electron density around CLA A 1116:

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



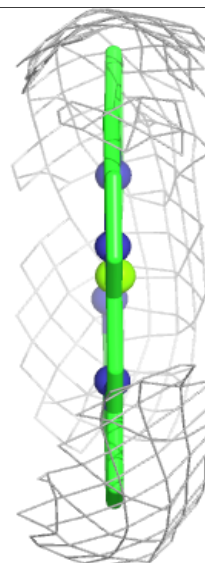
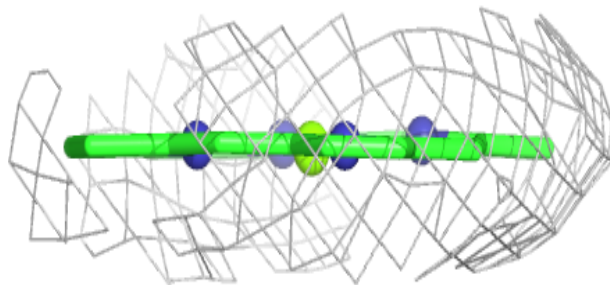
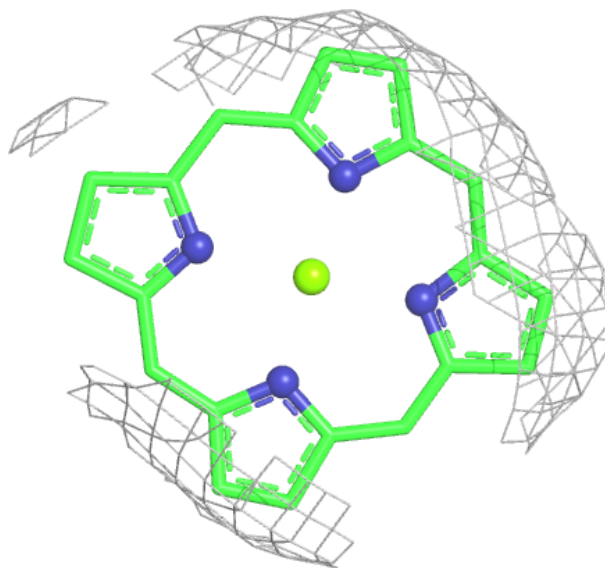
Electron density around PQN A 2001:

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



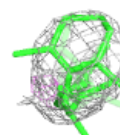
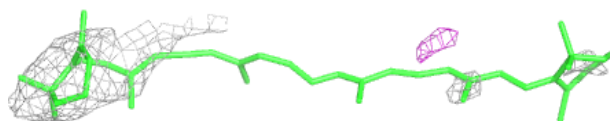
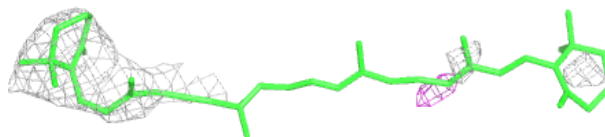
Electron density around CLA B 1235:

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

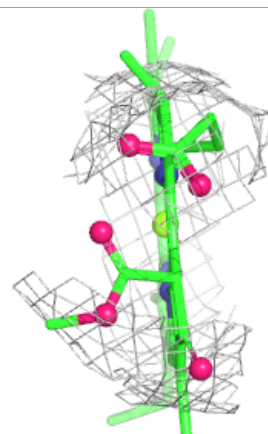
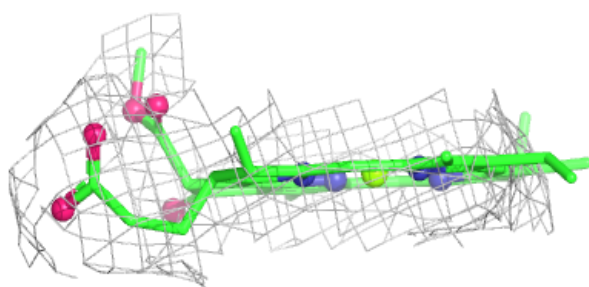
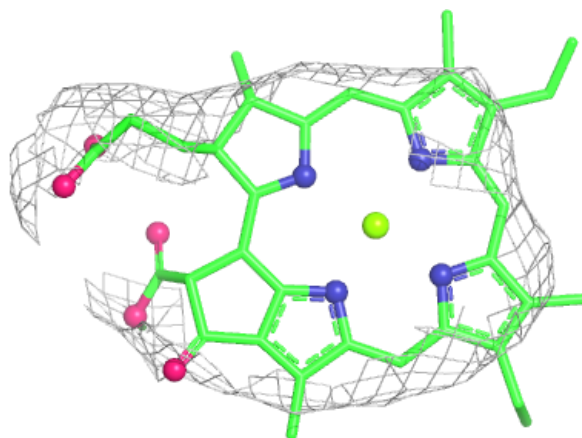


Electron density around BCR A 4002:

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

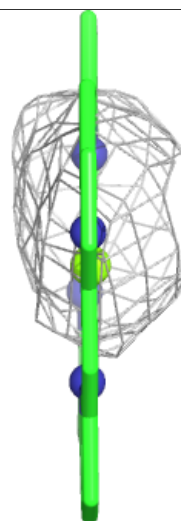
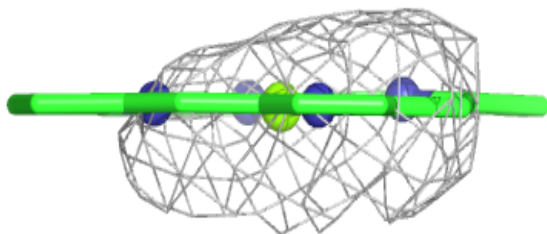
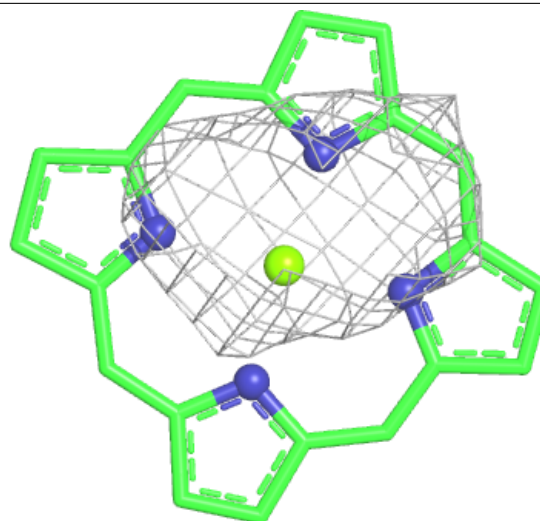
**Electron density around CLA F 1301:**

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



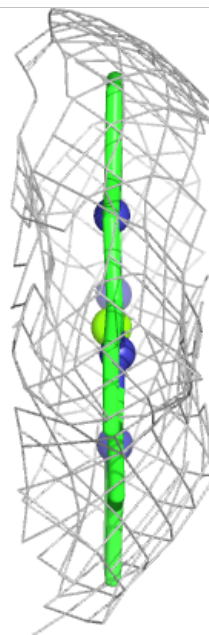
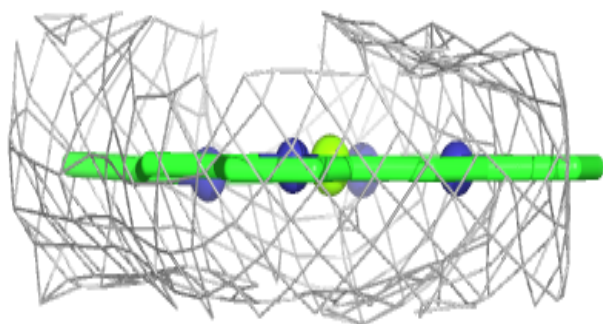
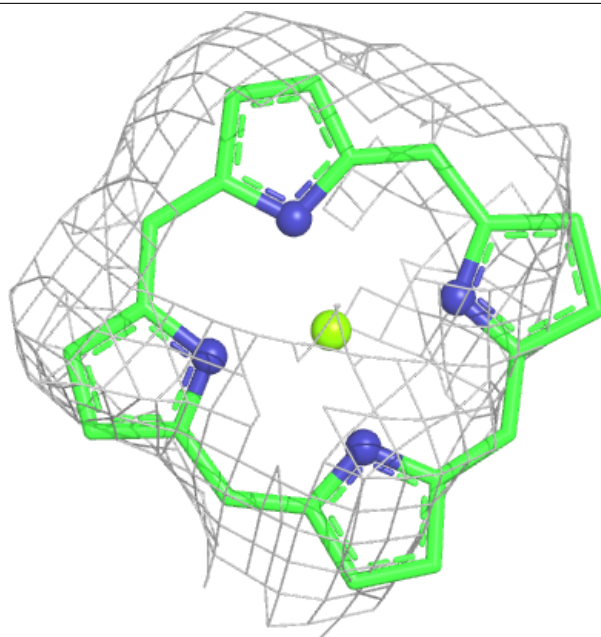
Electron density around CLA B 1220:

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



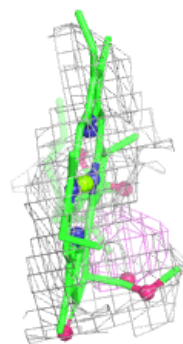
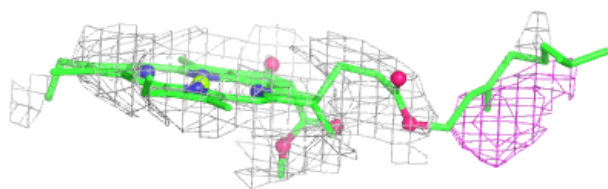
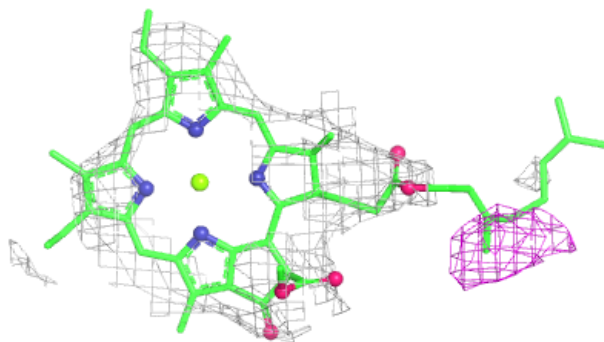
Electron density around CLA A 1123:

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

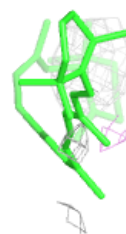
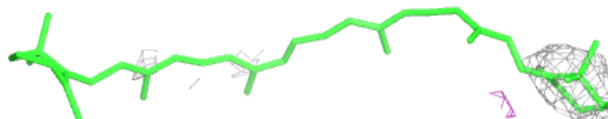
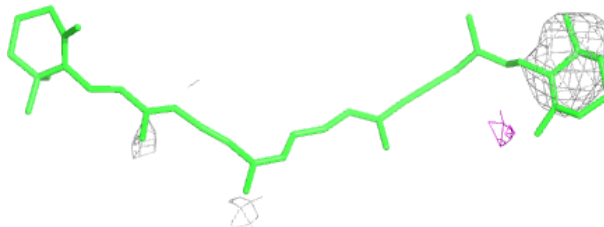


Electron density around CLA A 1103:

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

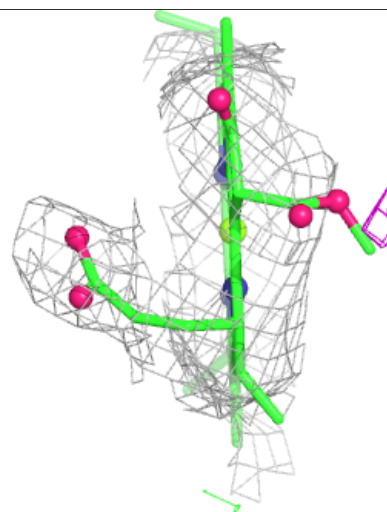
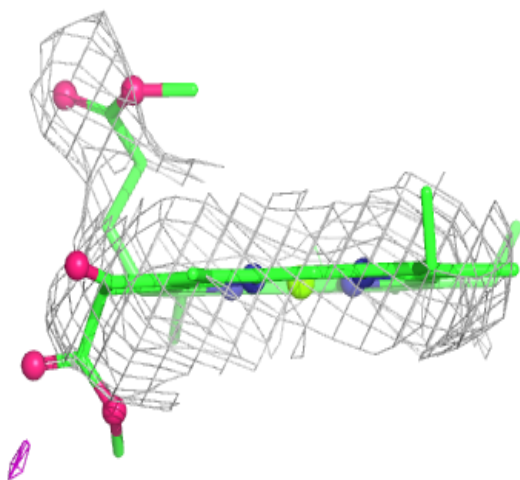
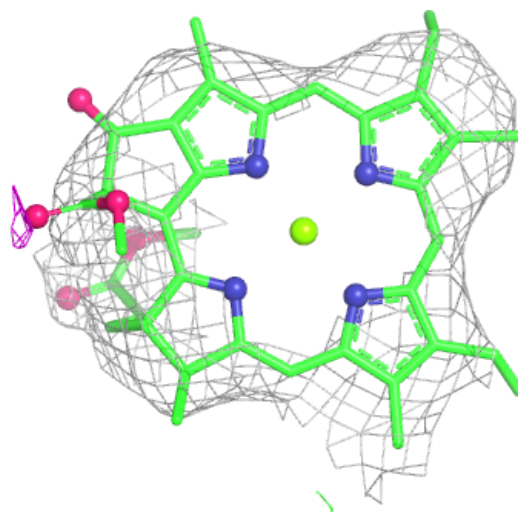
**Electron density around BCR B 4005:**

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



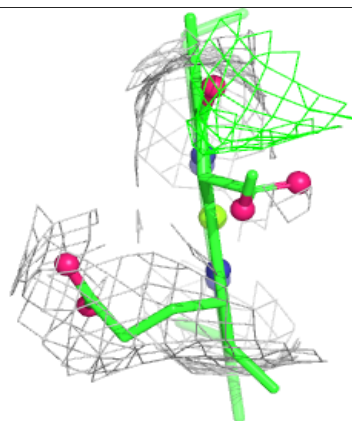
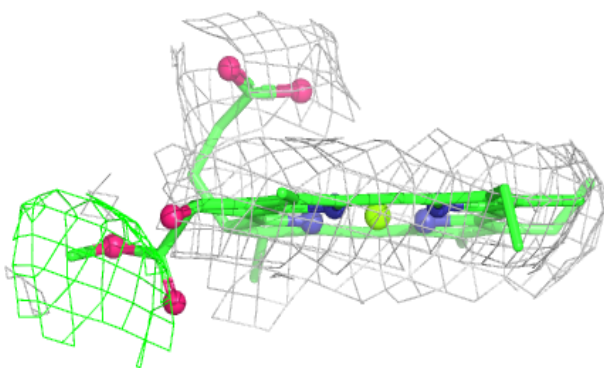
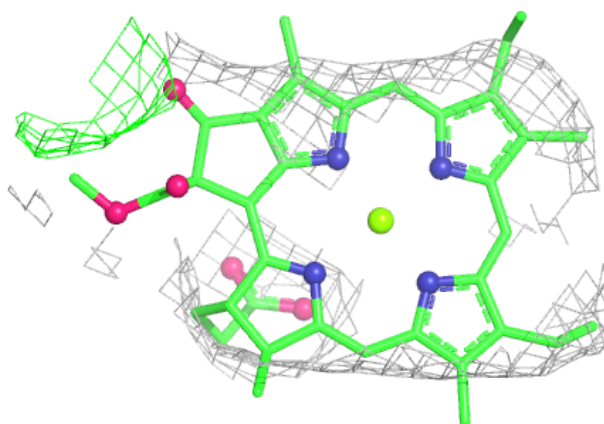
Electron density around CLA A 1114:

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



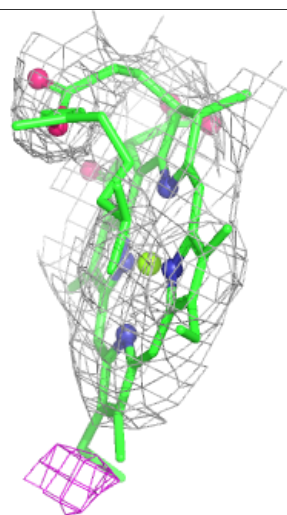
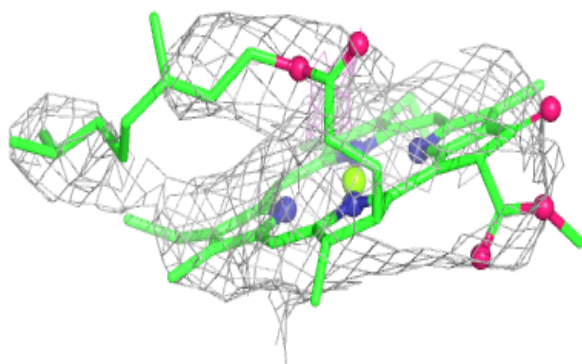
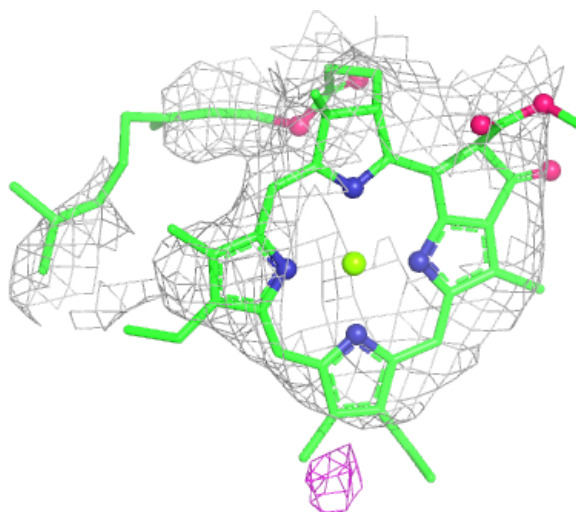
Electron density around CLA A 1101:

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



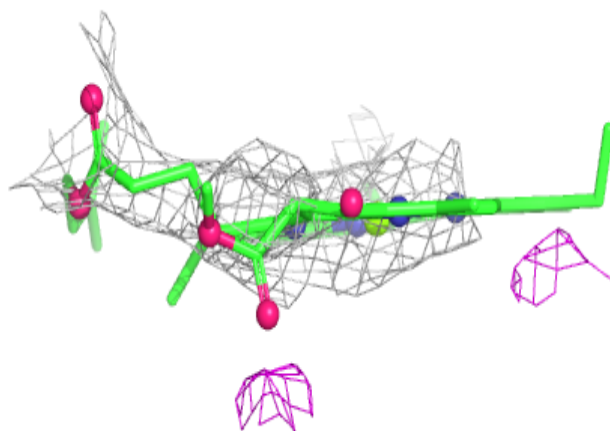
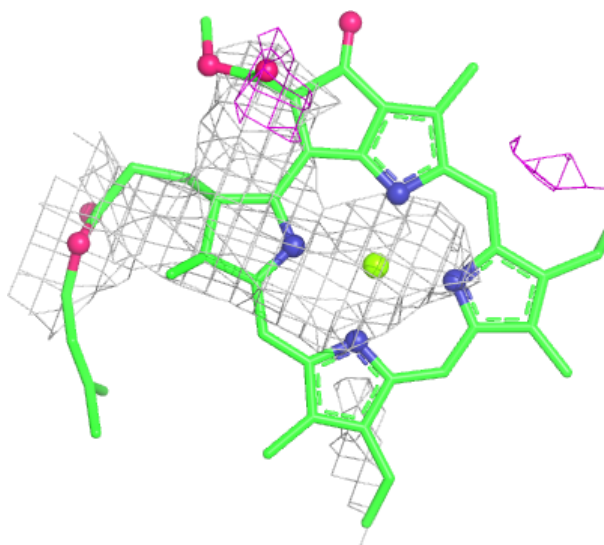
Electron density around CLA A 1105:

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



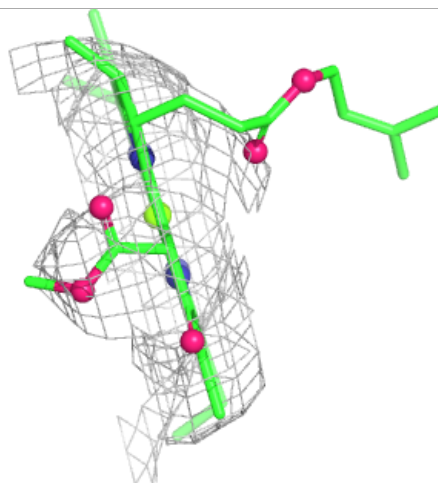
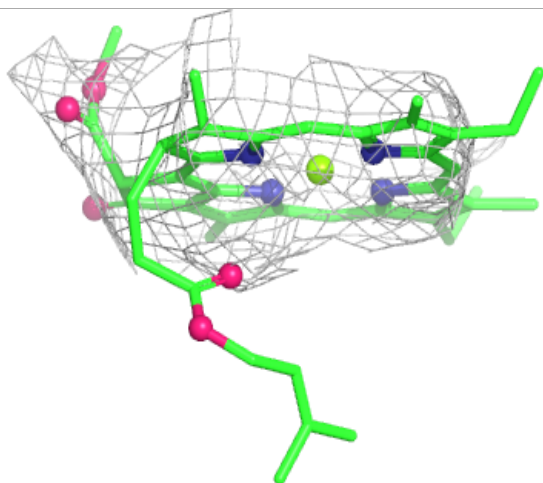
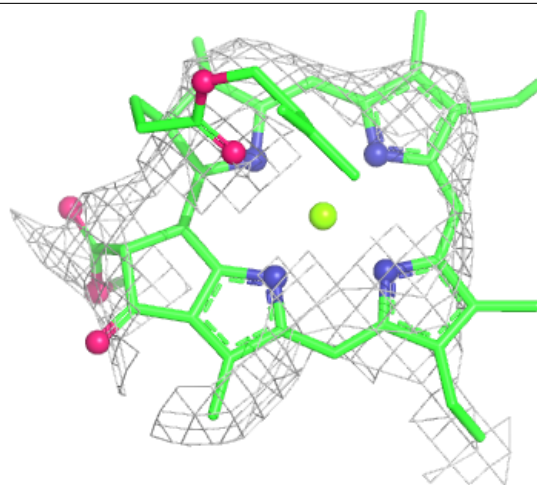
Electron density around CLA B 1023:

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



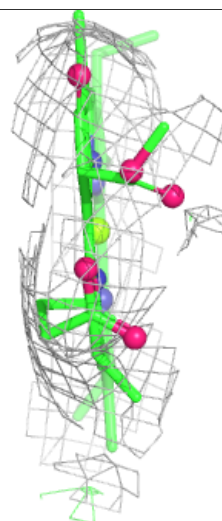
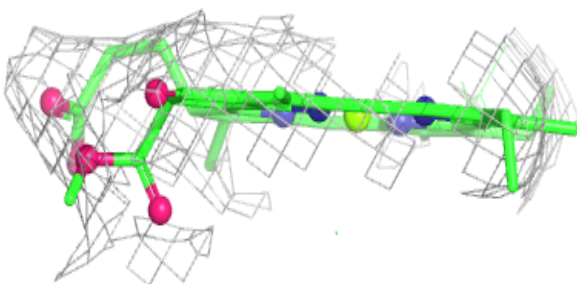
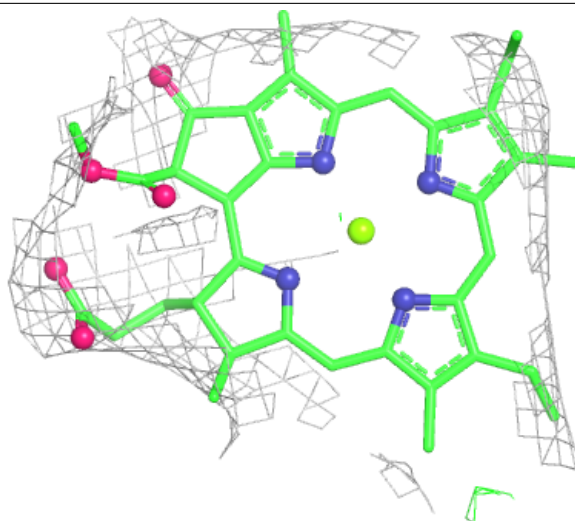
Electron density around CLA J 1302:

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



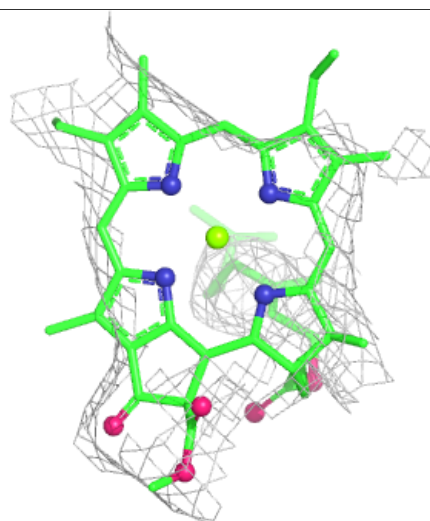
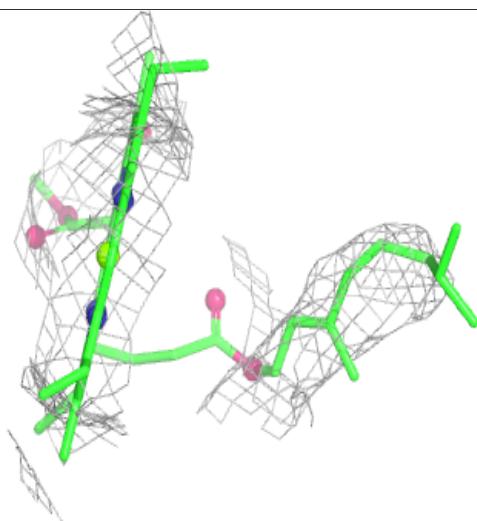
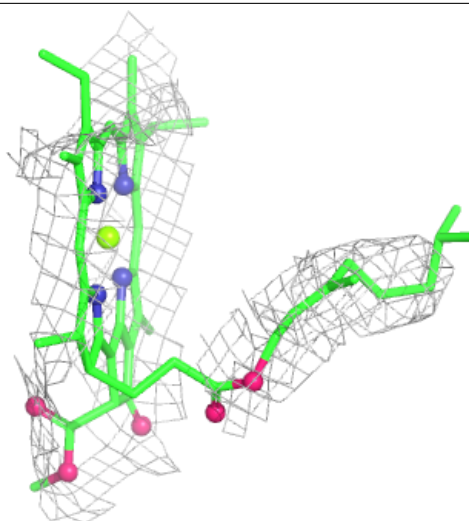
Electron density around CLA A 1131:

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



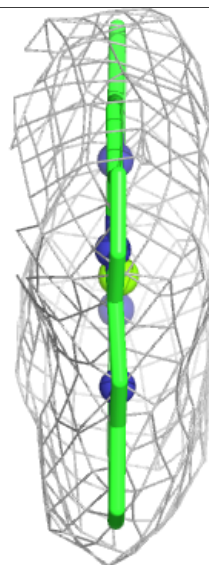
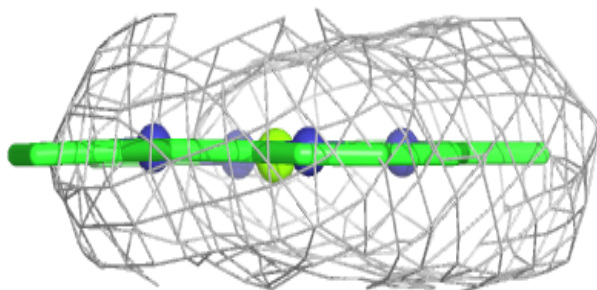
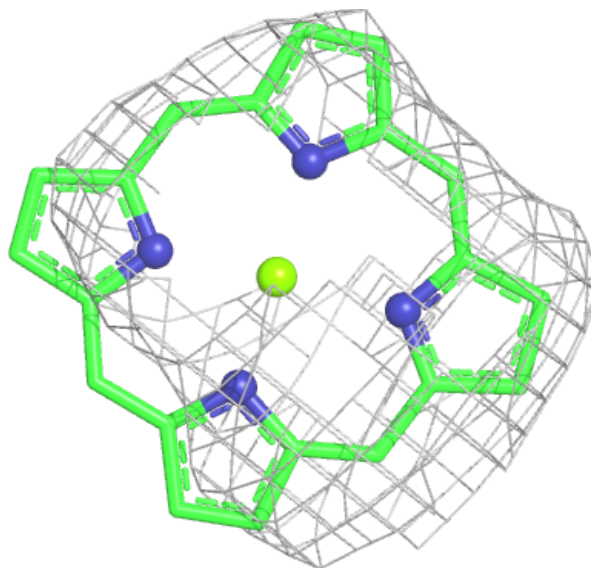
Electron density around CLA B 1226:

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



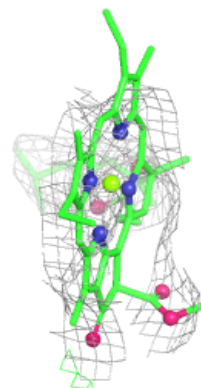
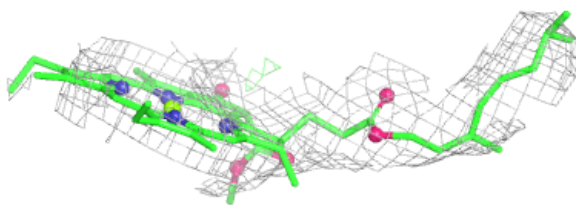
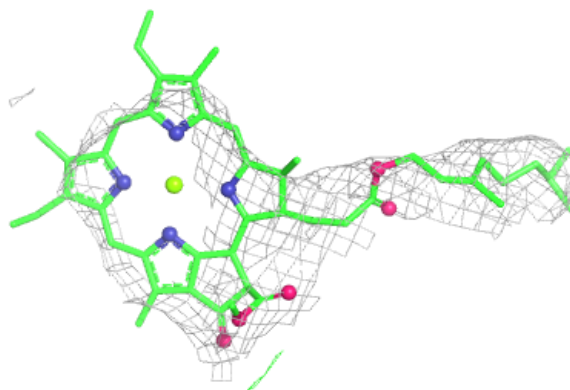
Electron density around CLA A 1111:

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



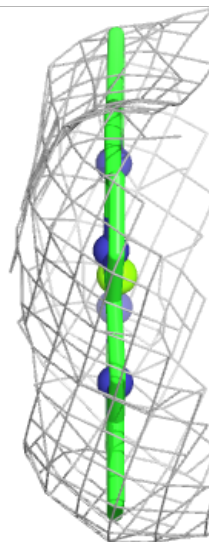
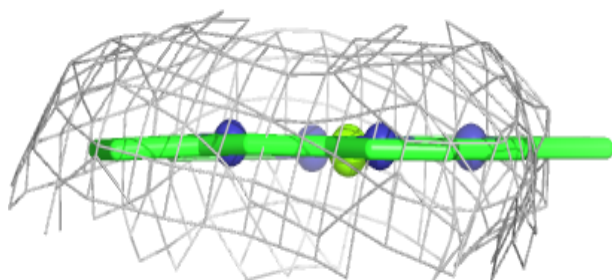
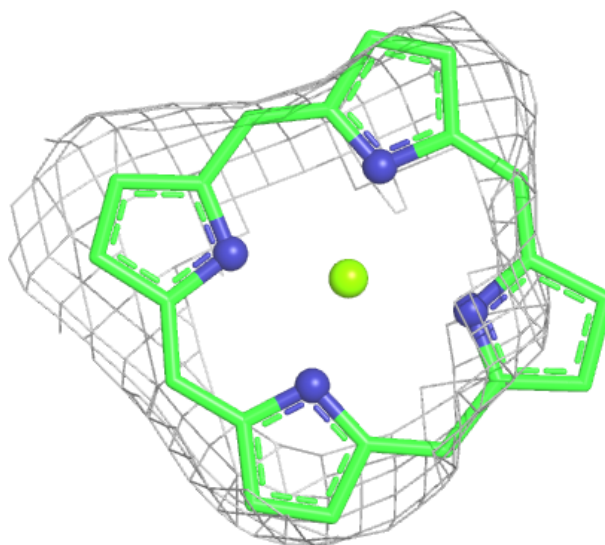
Electron density around CLA A 1012:

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



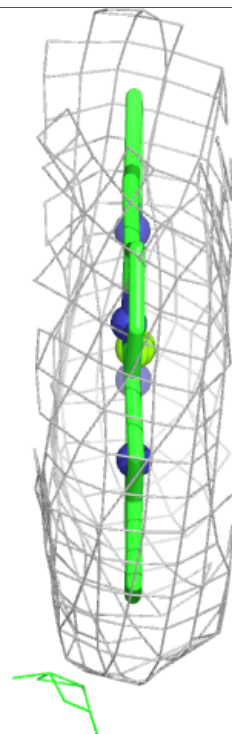
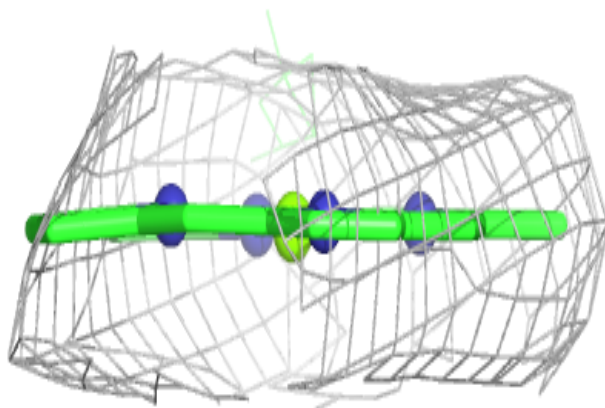
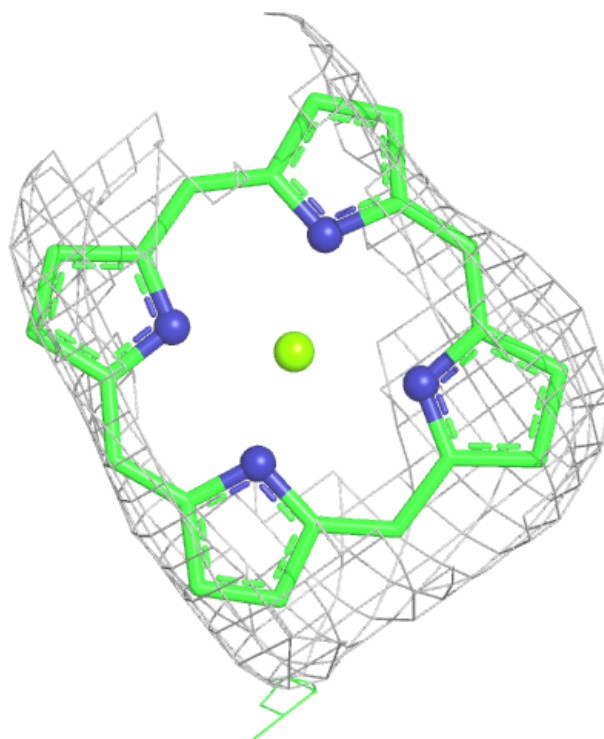
Electron density around CLA A 1141:

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



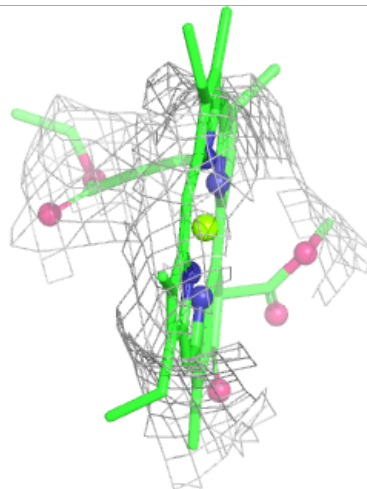
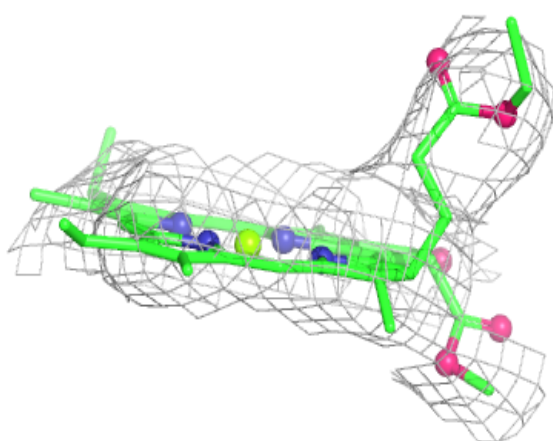
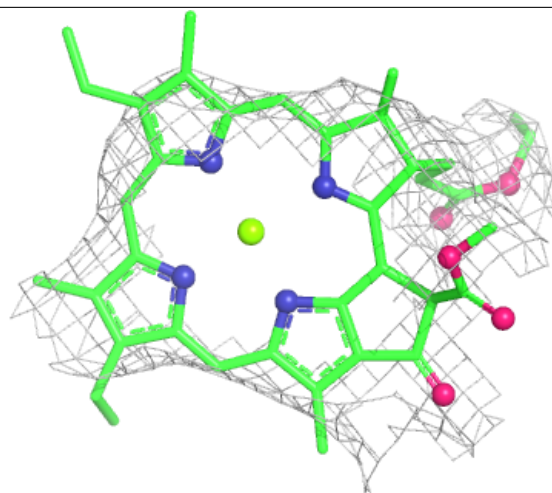
Electron density around CLA A 1125:

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



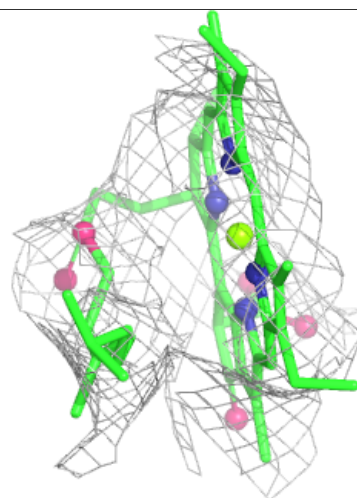
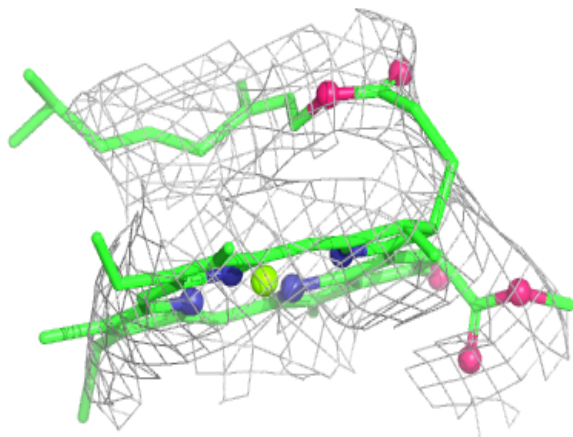
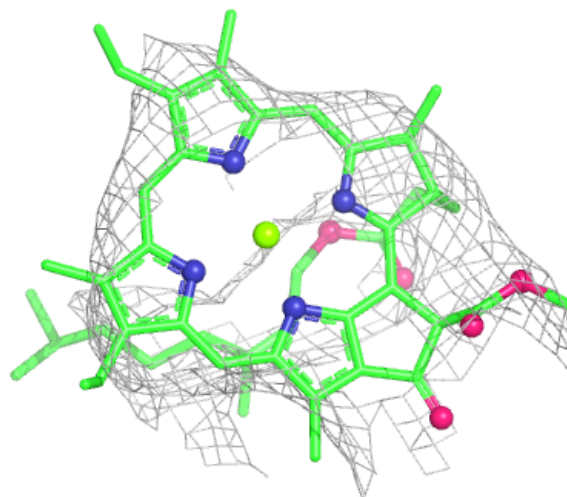
Electron density around CLA B 1230:

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



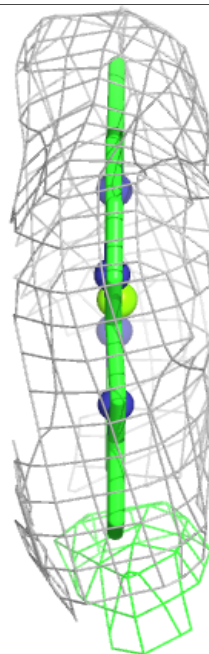
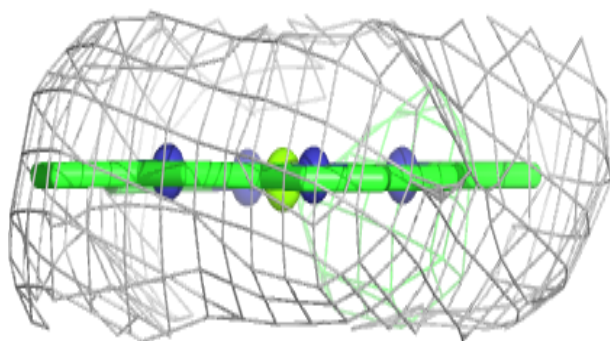
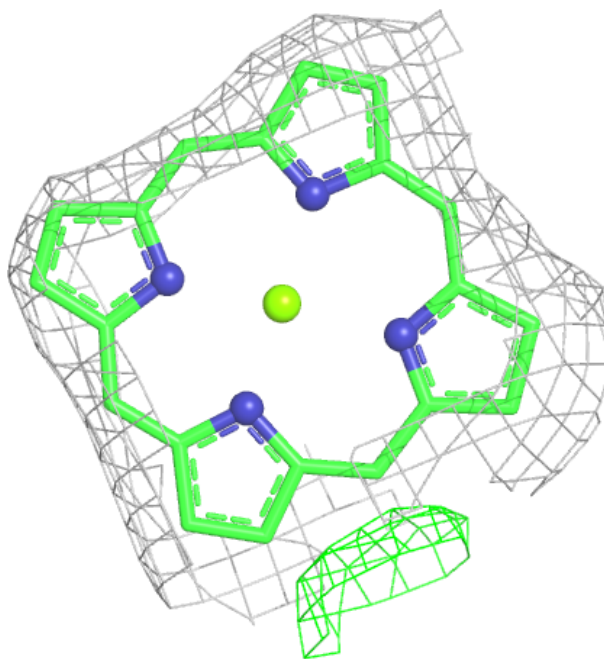
Electron density around CLA A 1115:

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



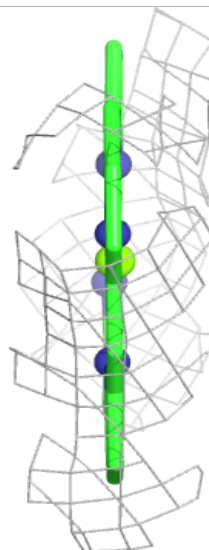
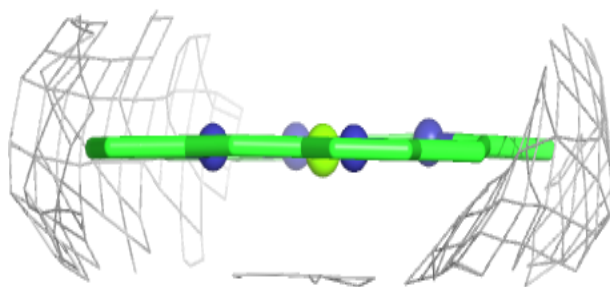
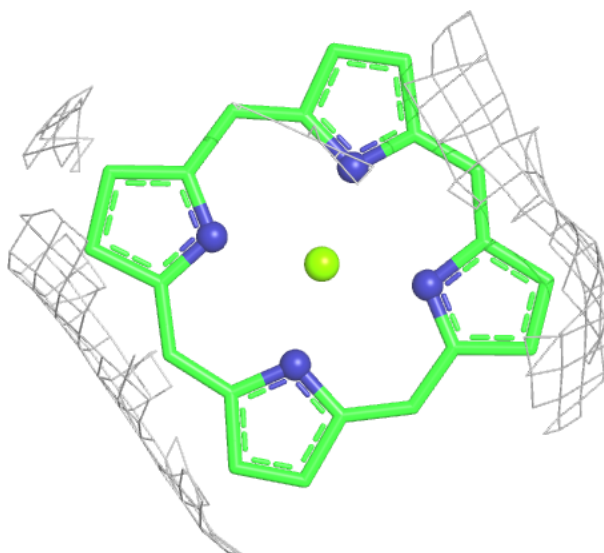
Electron density around CLA A 1128:

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



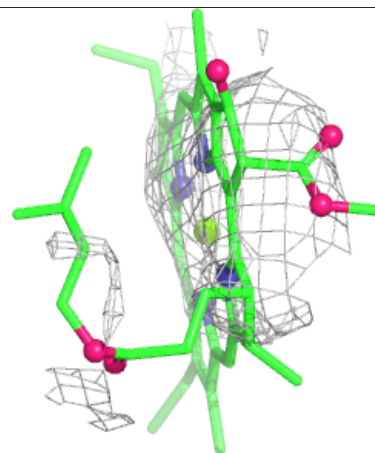
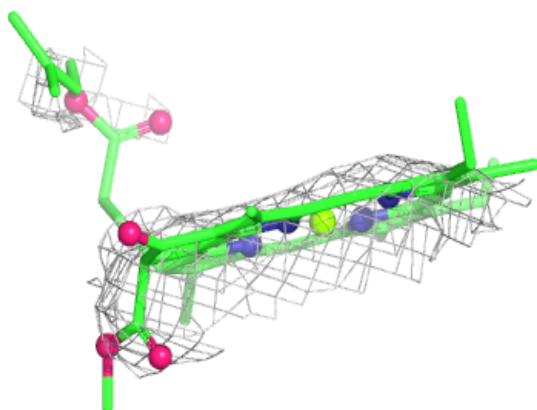
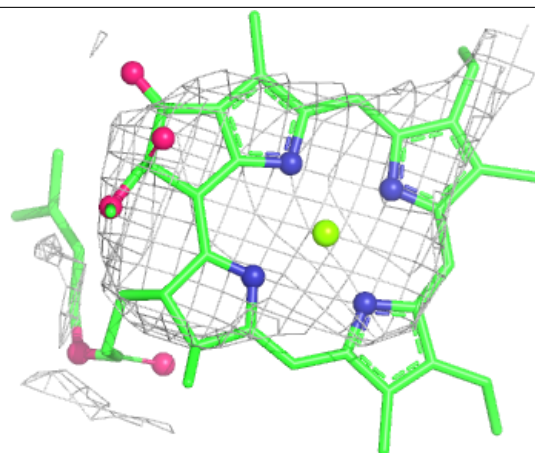
Electron density around CLA 2 605:

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



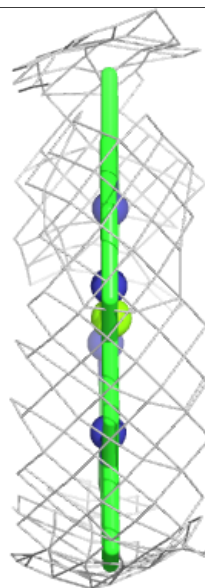
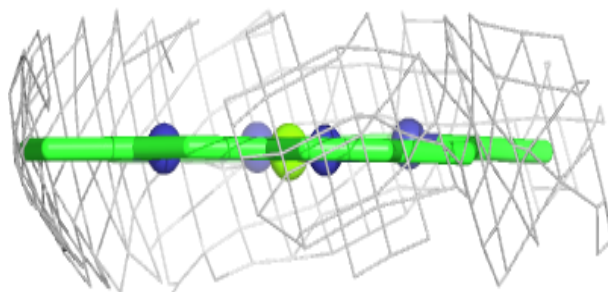
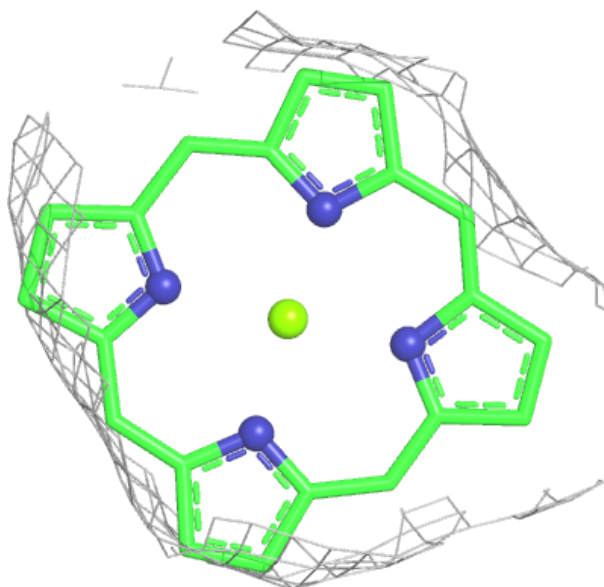
Electron density around CLA B 1225:

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



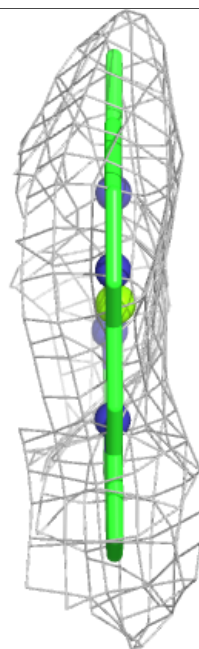
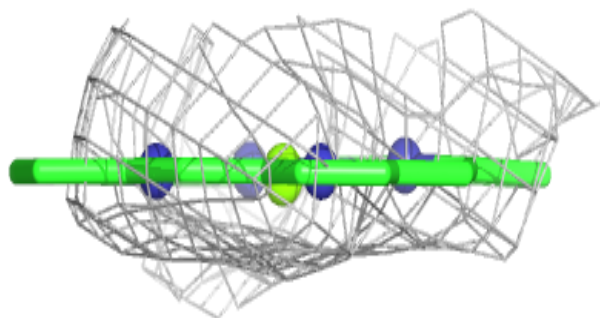
Electron density around CLA A 1134:

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



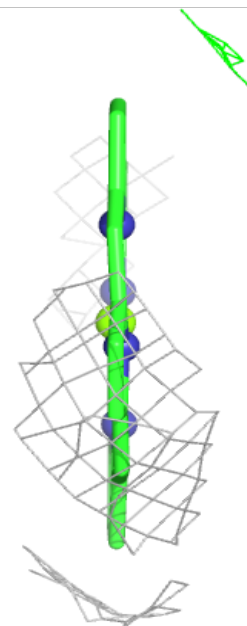
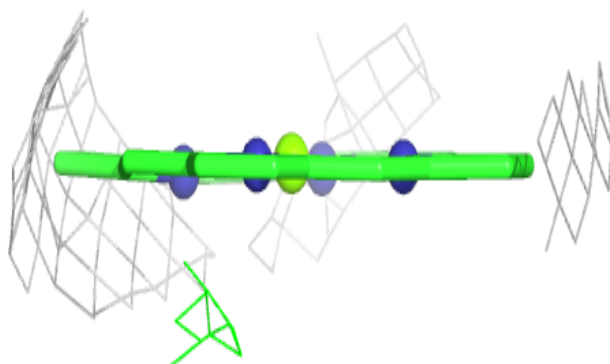
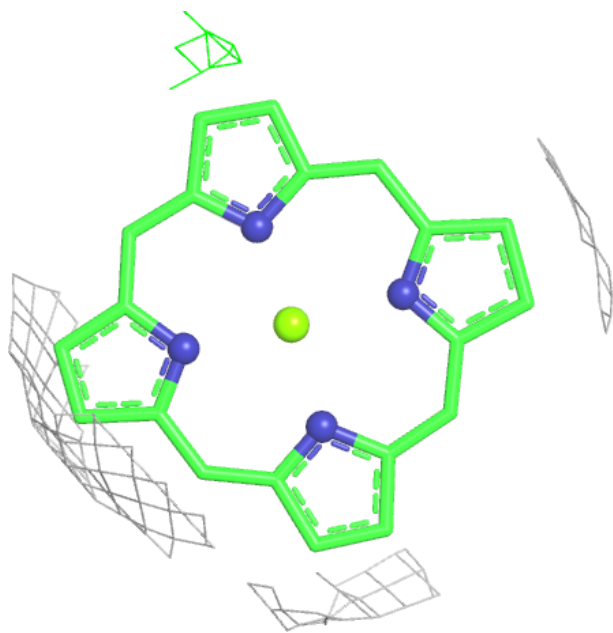
Electron density around CLA A 1135:

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



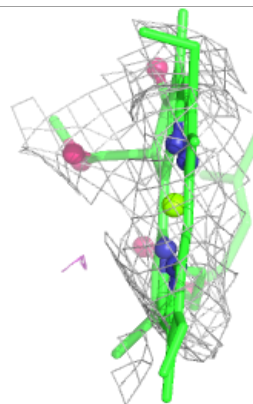
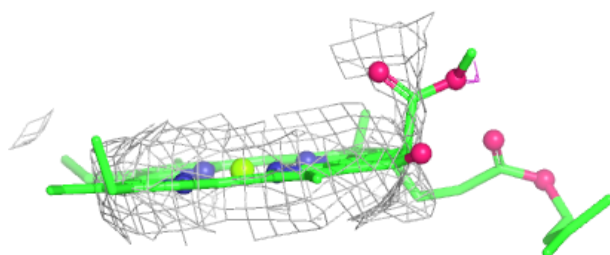
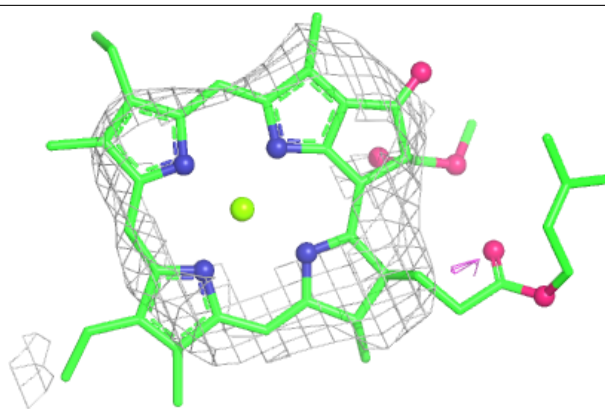
Electron density around CLA B 1201:

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

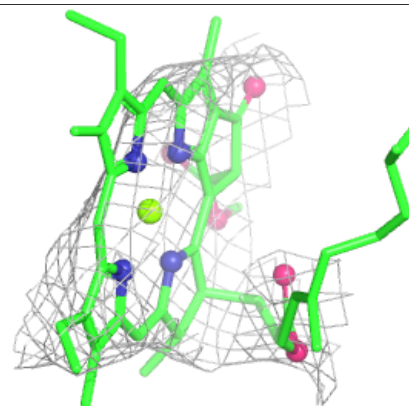
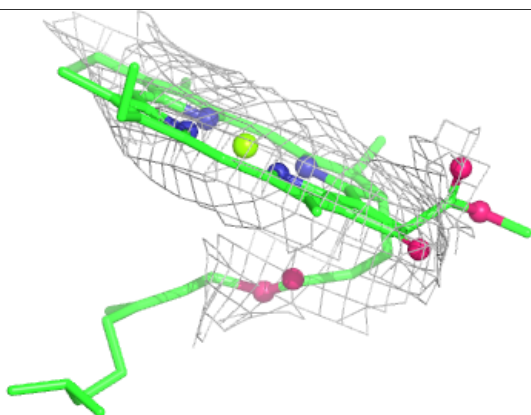
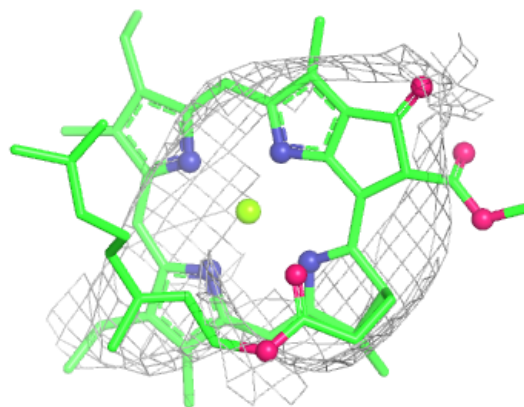


Electron density around CLA B 1229:

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

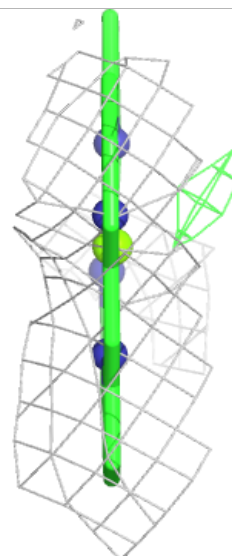
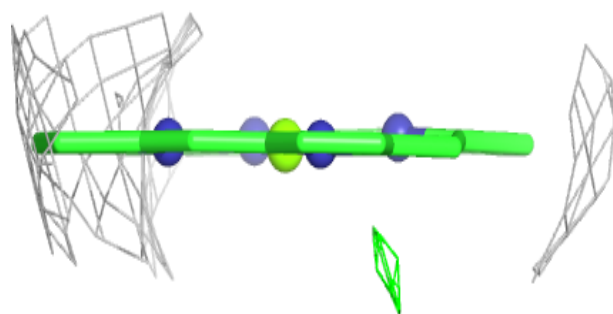
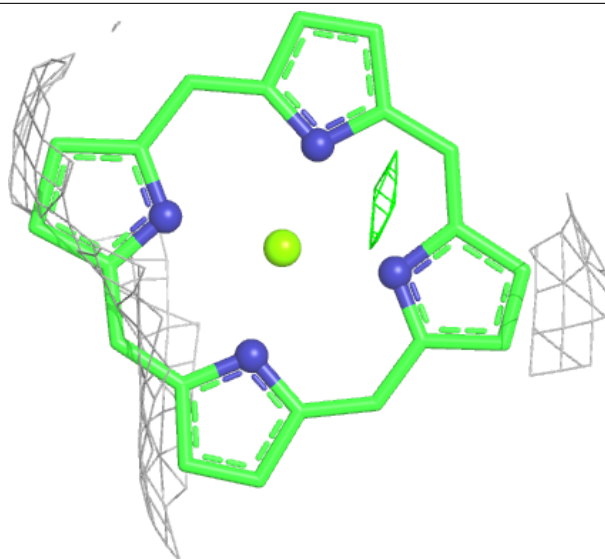
**Electron density around CLA A 1130:**

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



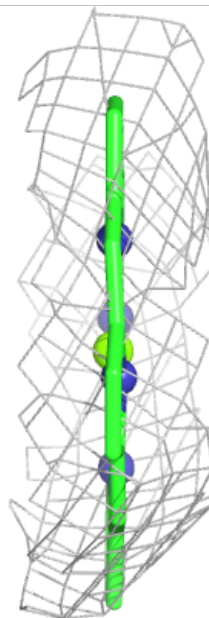
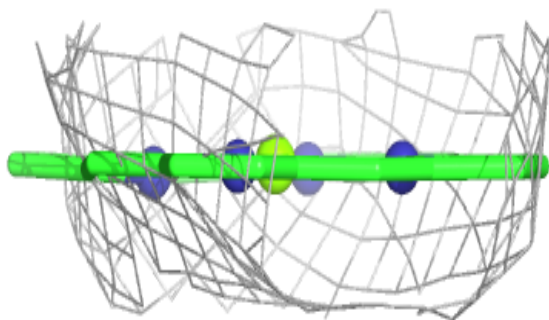
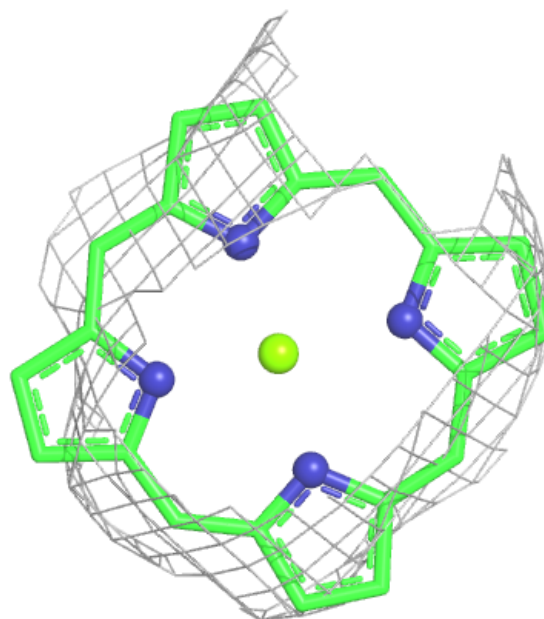
Electron density around CLA 2 612:

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



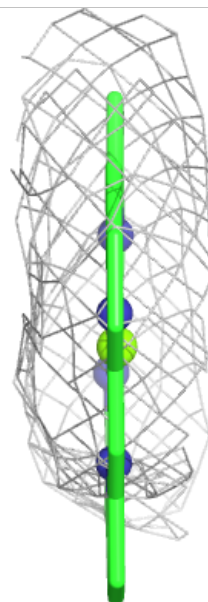
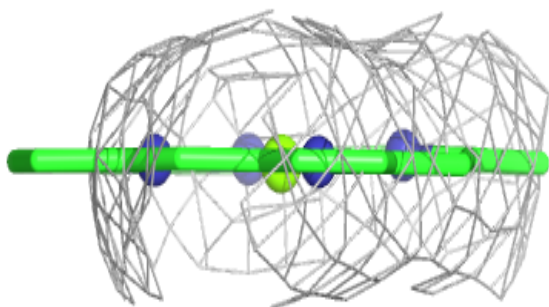
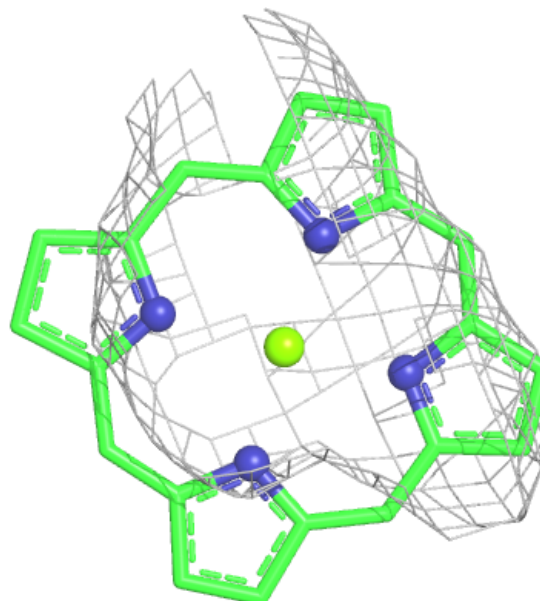
Electron density around CLA B 1234:

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



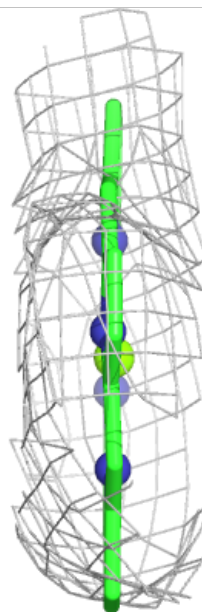
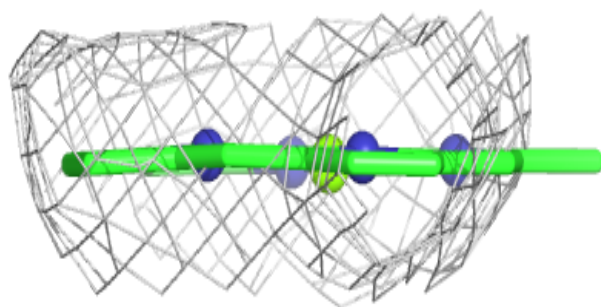
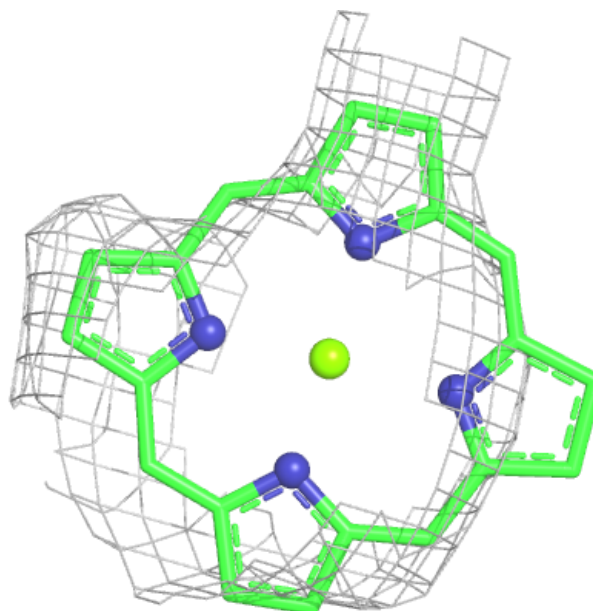
Electron density around CLA A 1133:

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



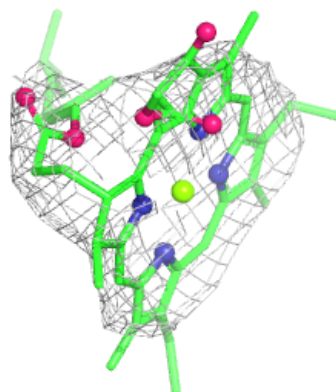
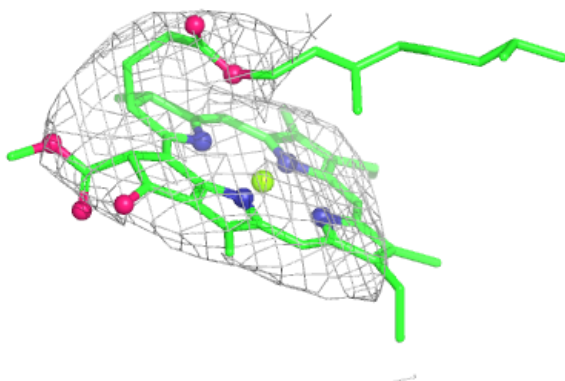
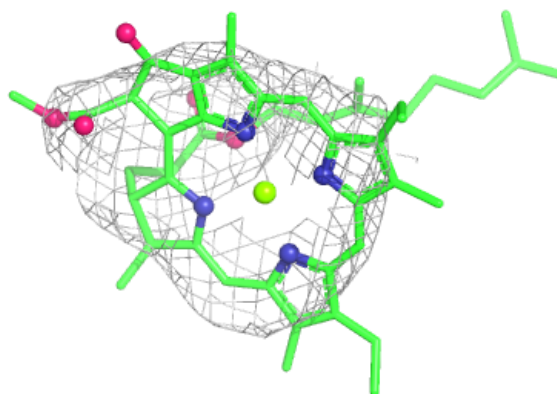
Electron density around CLA B 1202:

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



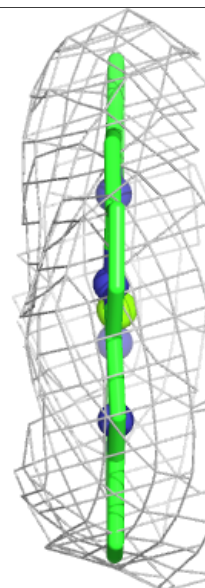
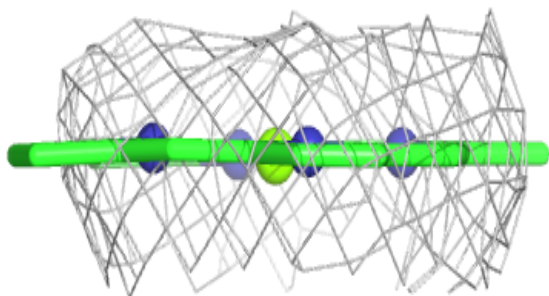
Electron density around CLA B 1237:

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



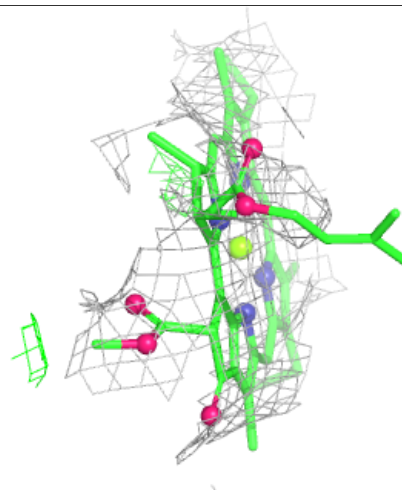
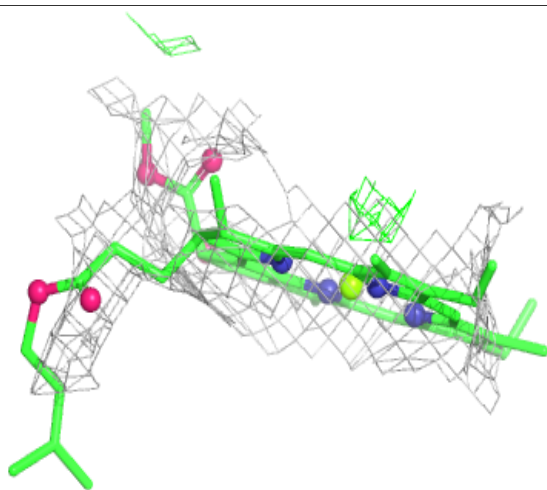
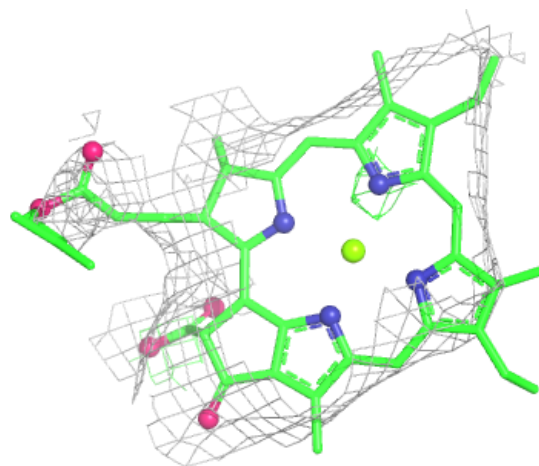
Electron density around CLA A 1118:

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



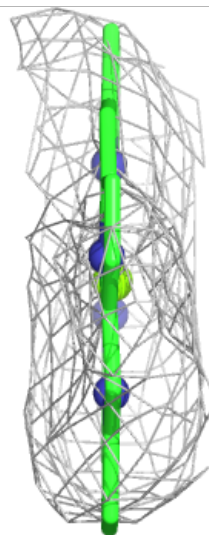
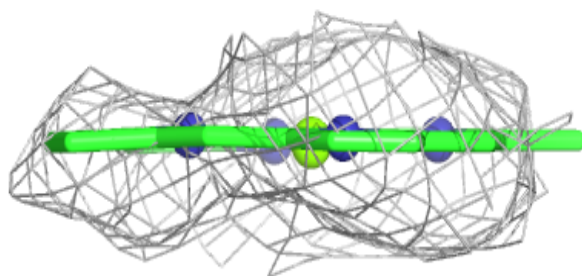
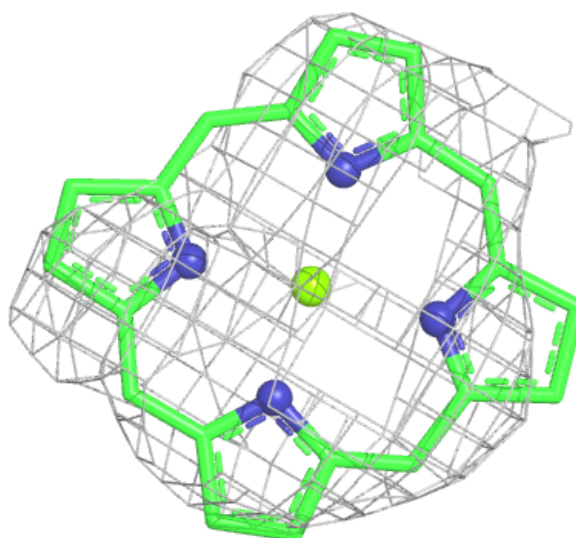
Electron density around CLA A 1011:

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



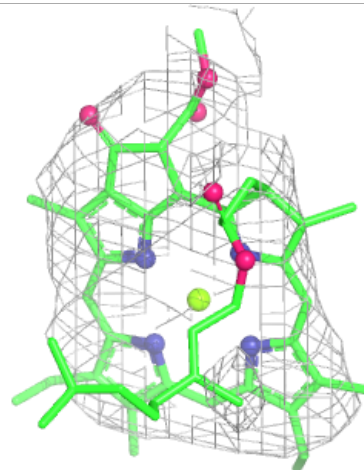
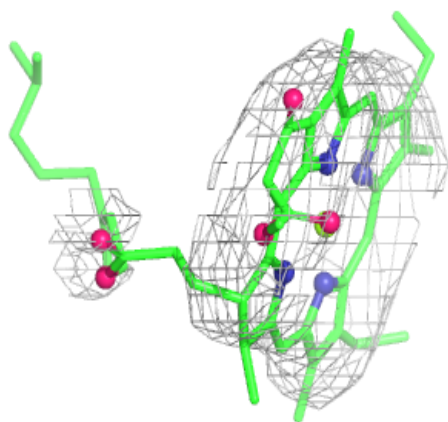
Electron density around CLA B 1022:

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



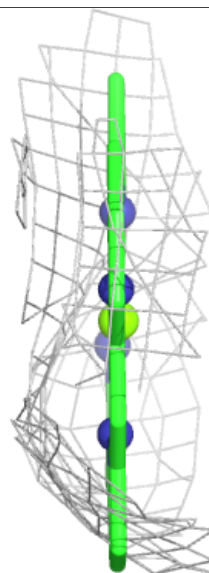
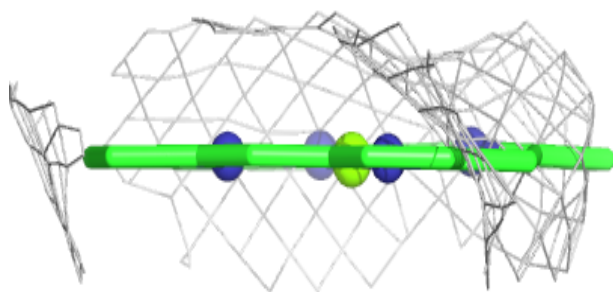
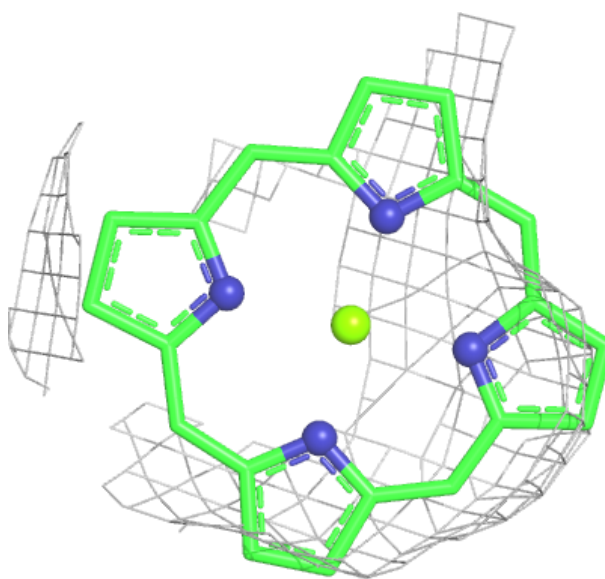
Electron density around CLA A 1107:

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



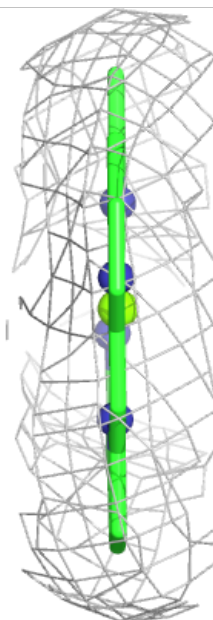
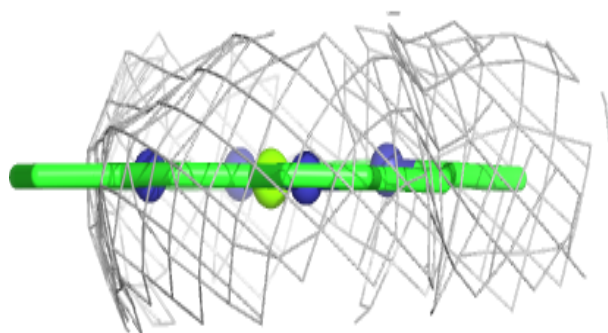
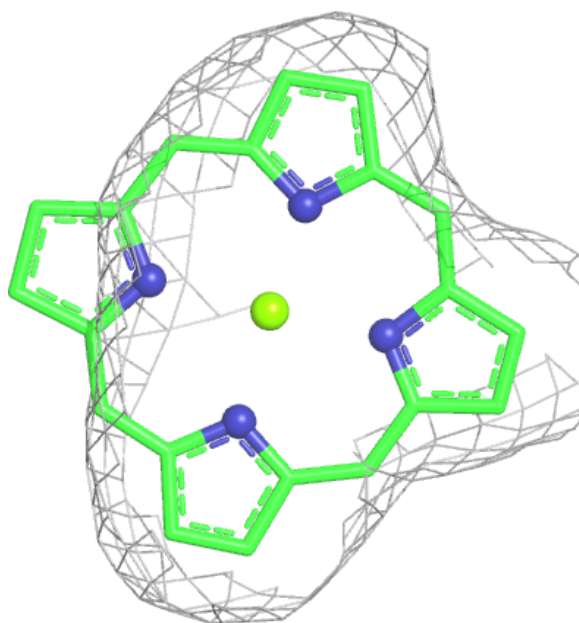
Electron density around CLA A 1129:

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



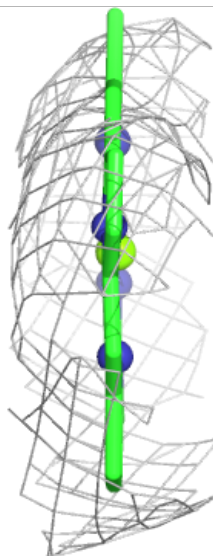
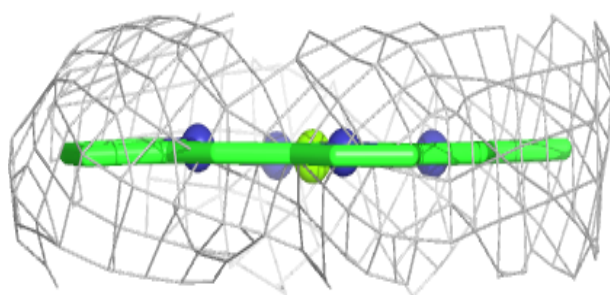
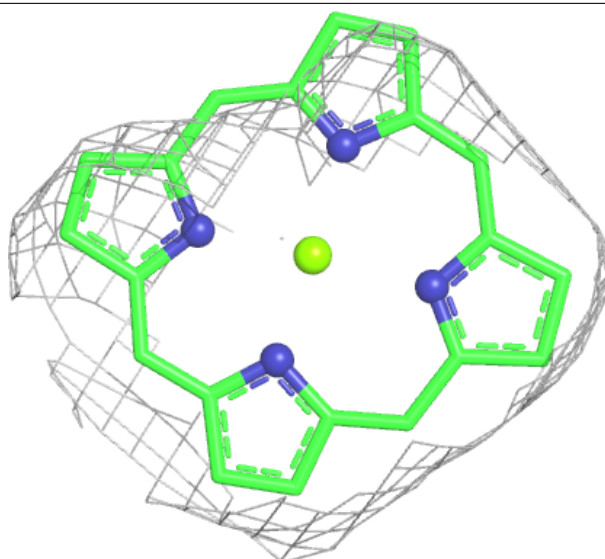
Electron density around CLA A 1108:

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



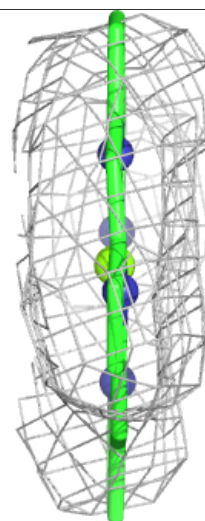
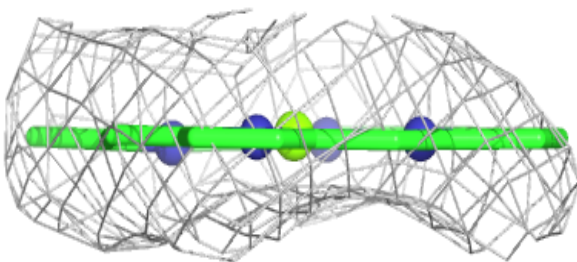
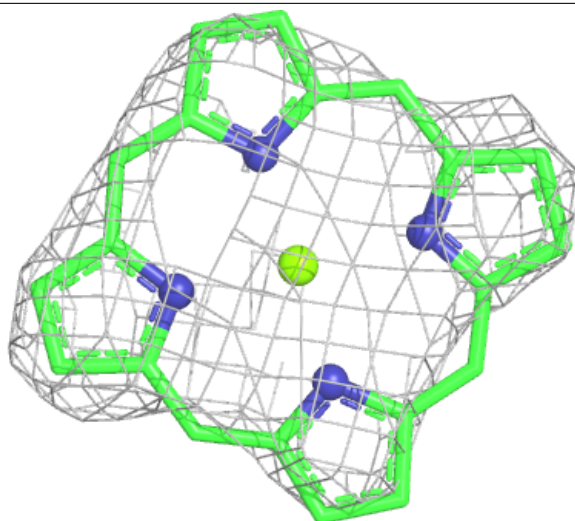
Electron density around CLA B 1215:

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



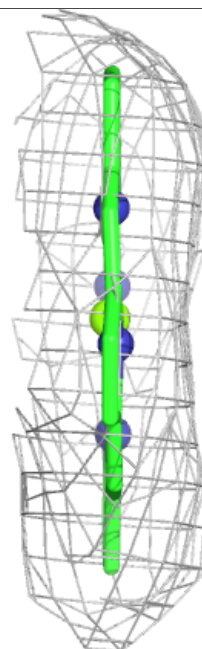
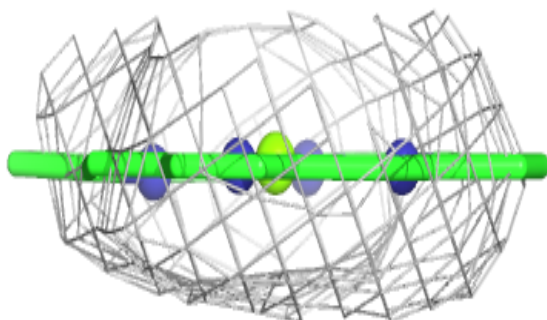
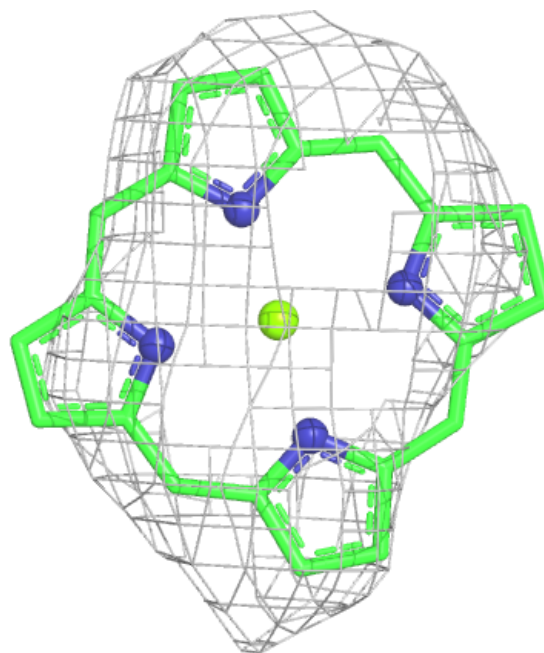
Electron density around CLA A 1113:

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



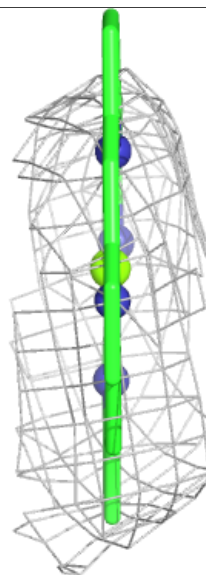
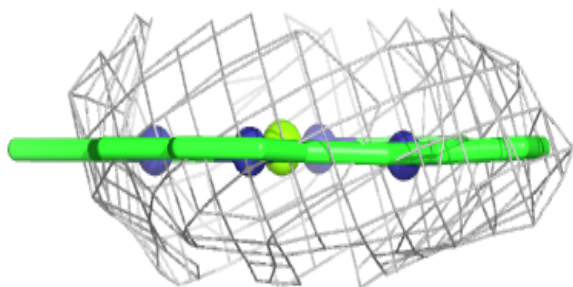
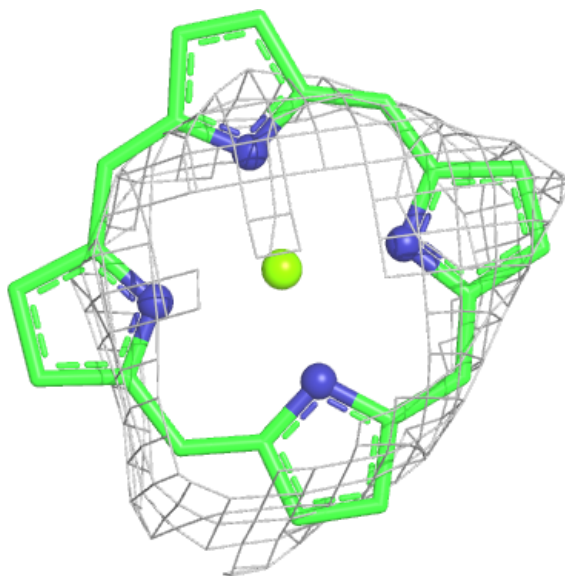
Electron density around CLA A 1139:

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



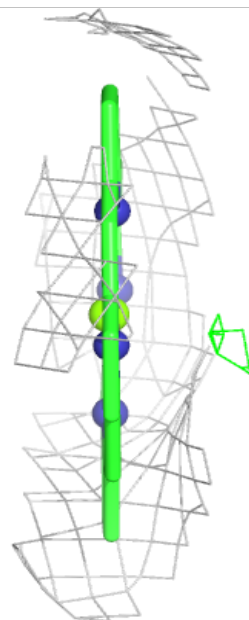
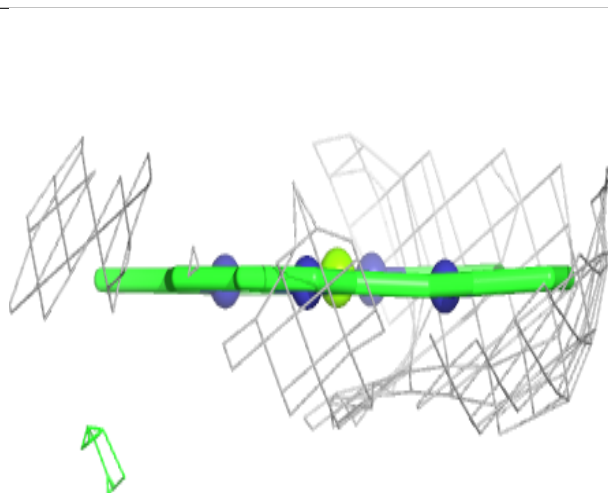
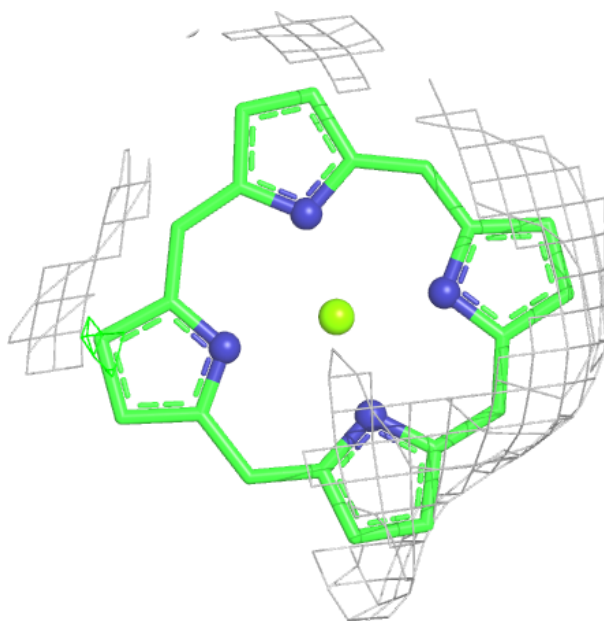
Electron density around CLA B 1239:

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



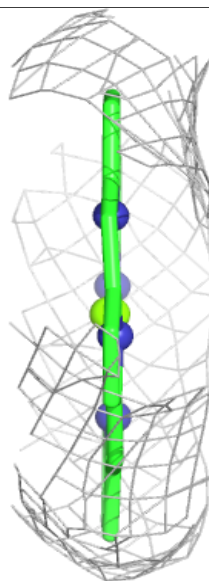
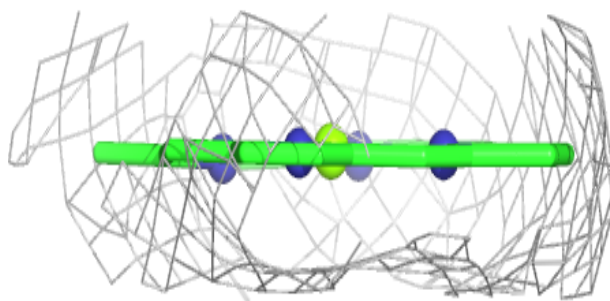
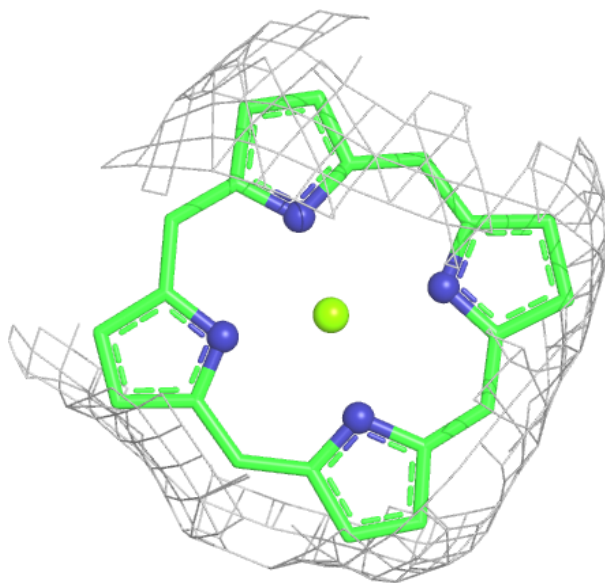
Electron density around CLA A 1132:

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



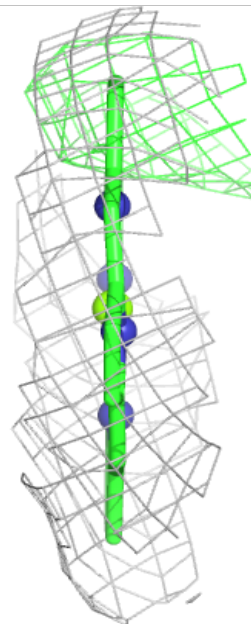
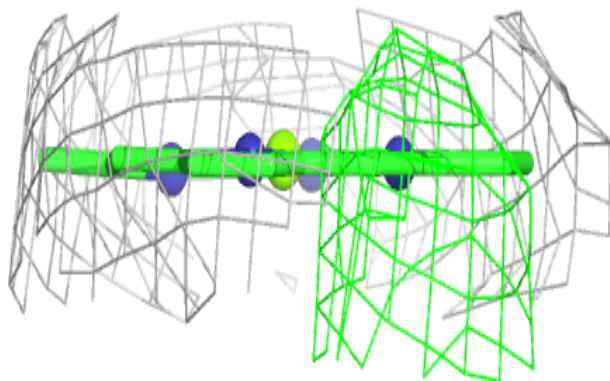
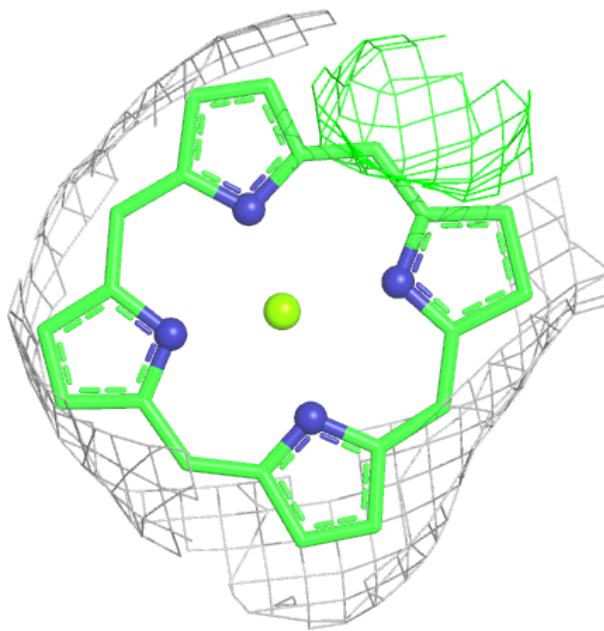
Electron density around CLA A 1122:

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



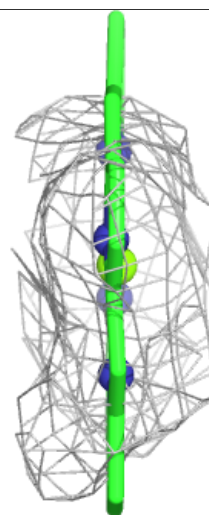
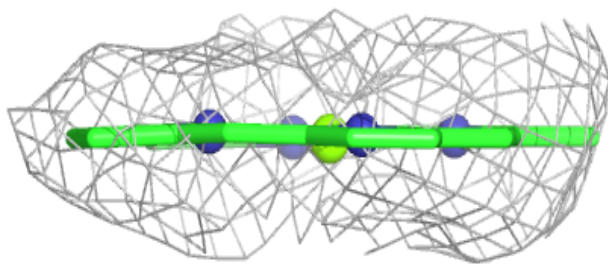
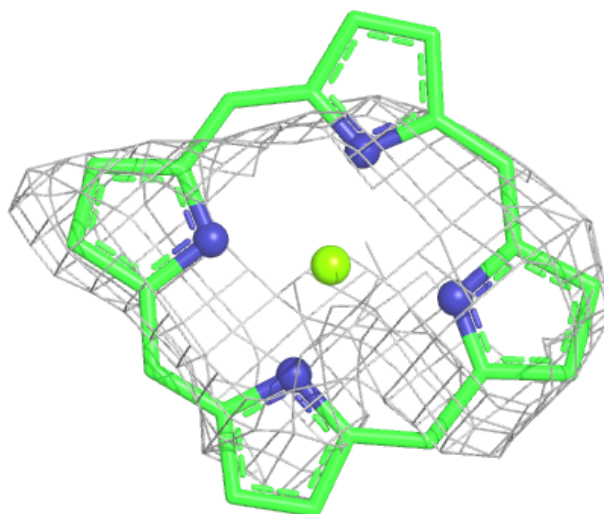
Electron density around CLA A 1102:

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



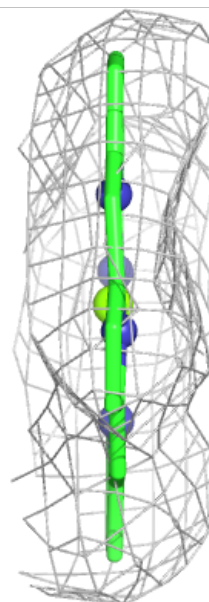
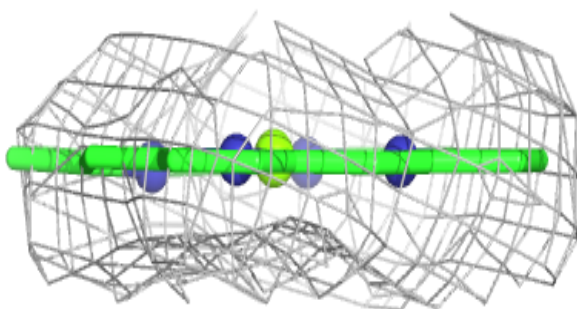
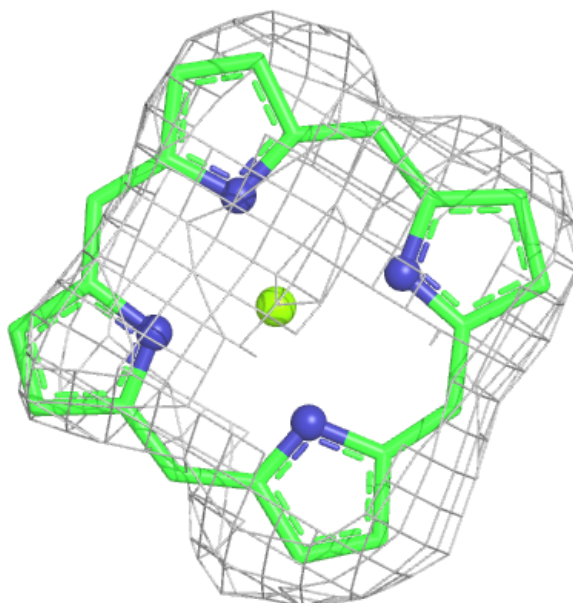
Electron density around CLA A 1110:

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



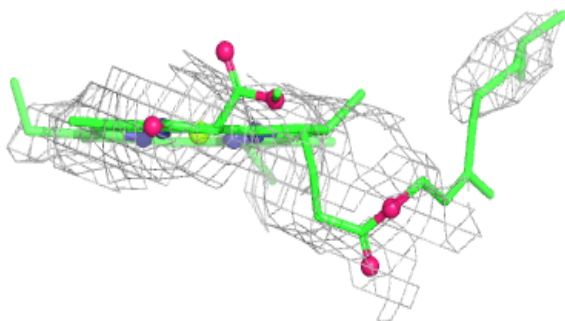
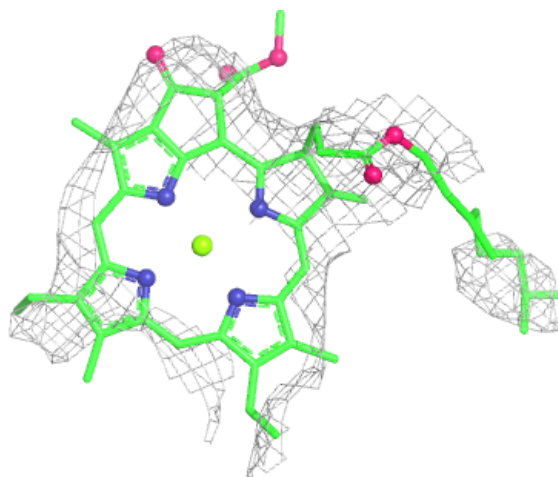
Electron density around CLA A 1127:

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



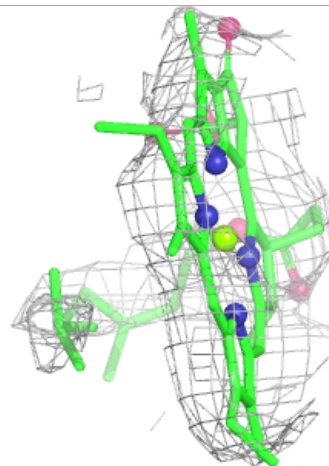
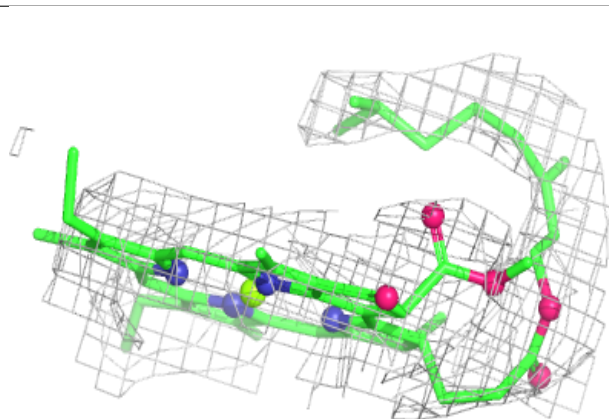
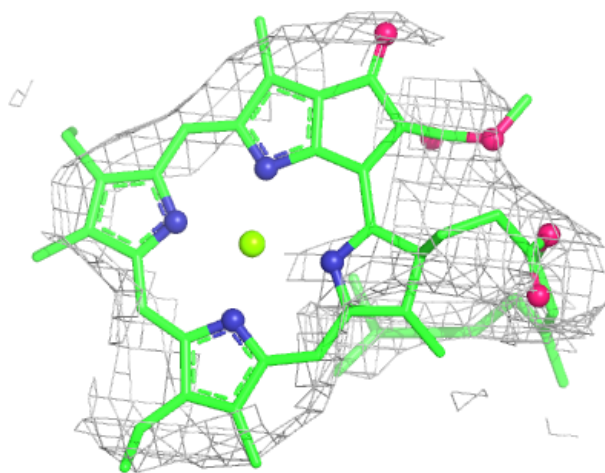
Electron density around CLA A 1013:

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



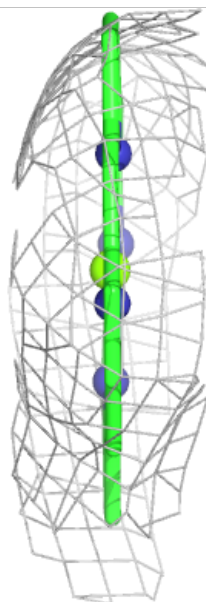
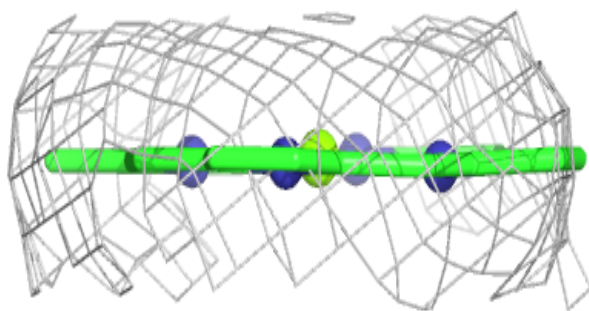
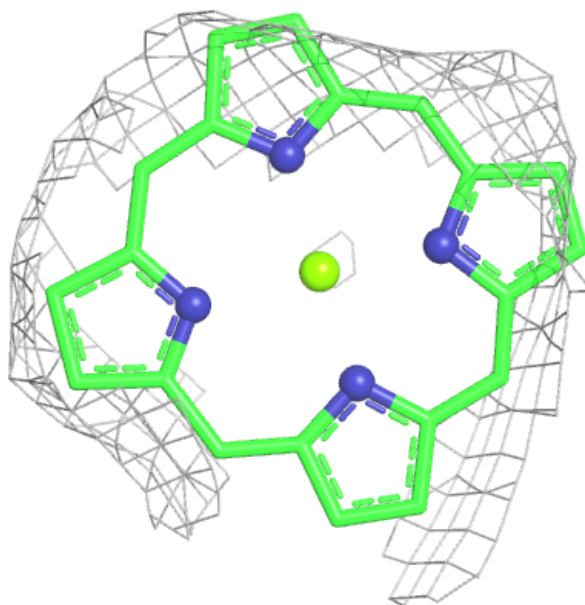
Electron density around CLA A 1104:

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



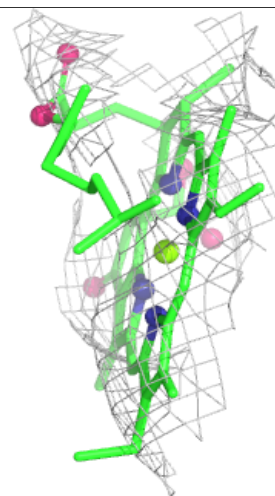
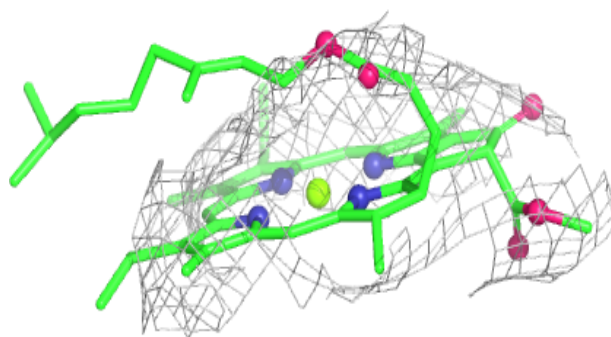
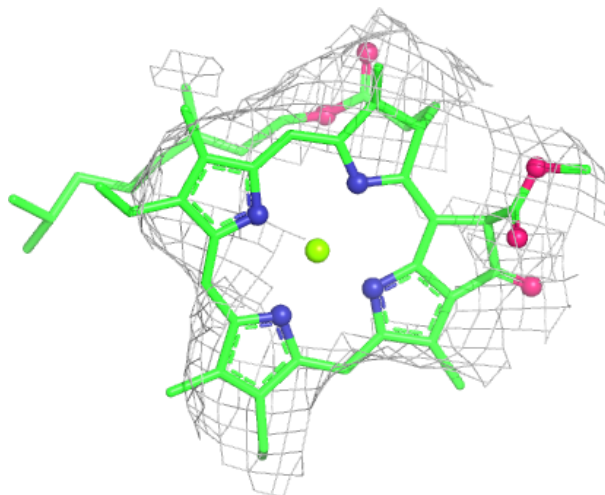
Electron density around CLA 4 605:

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



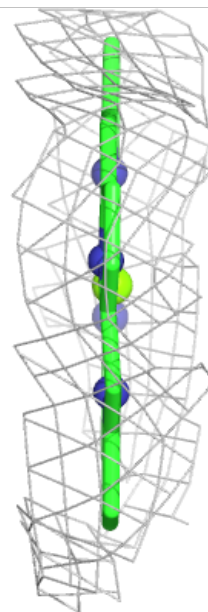
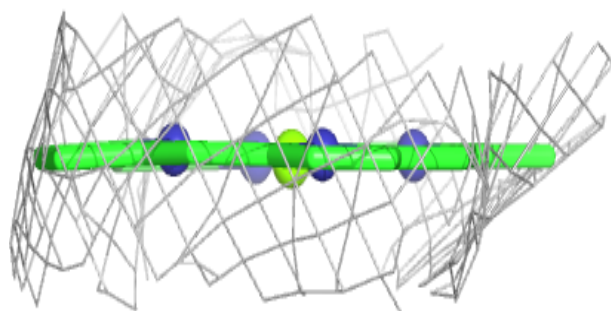
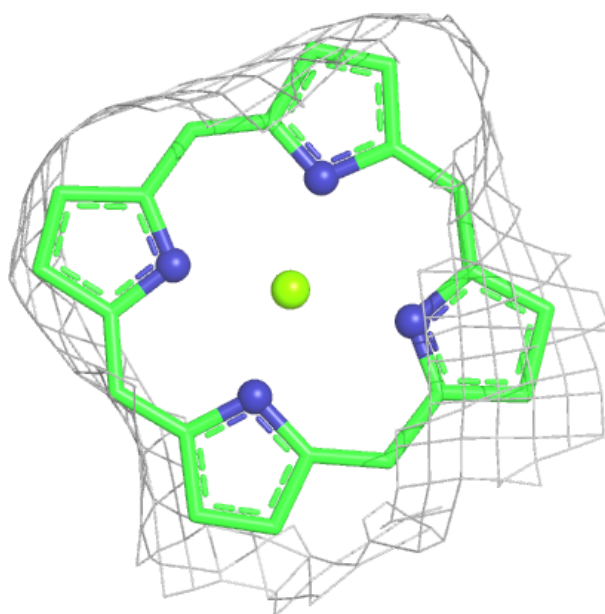
Electron density around CLA A 1117:

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



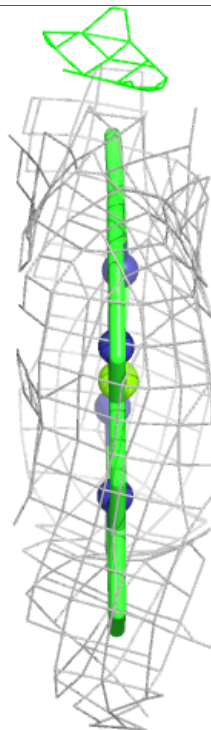
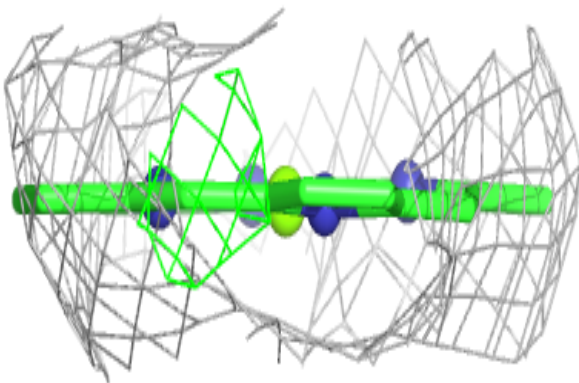
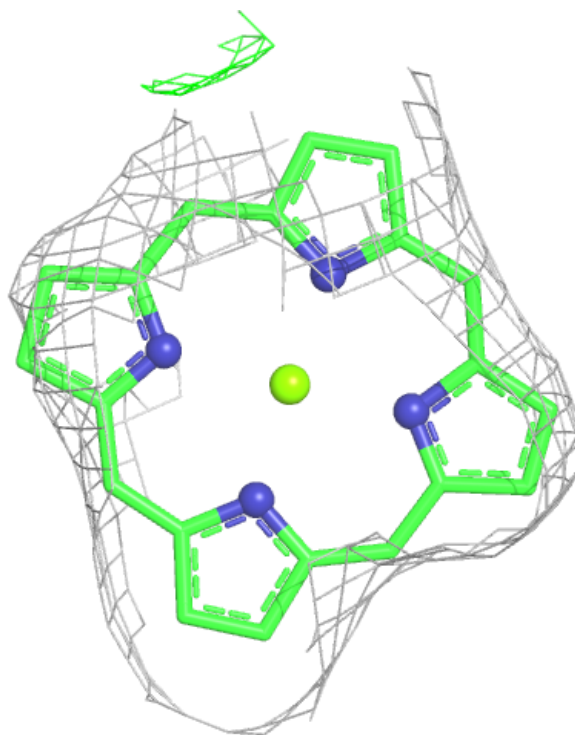
Electron density around CLA B 1222:

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



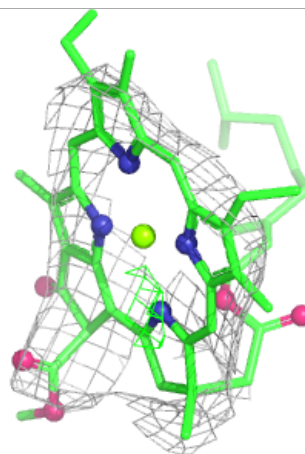
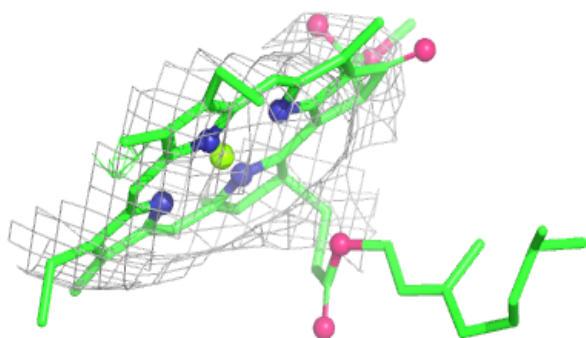
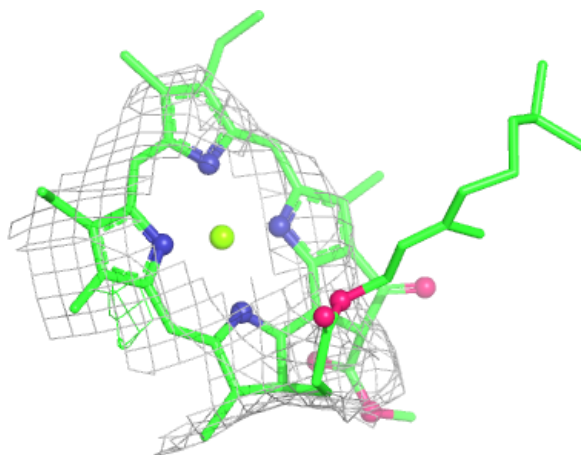
Electron density around CLA A 1124:

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



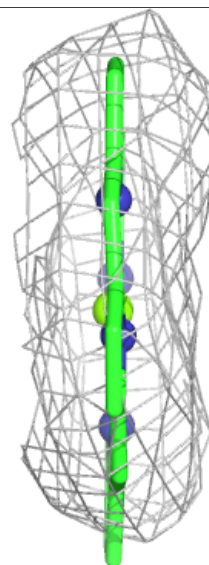
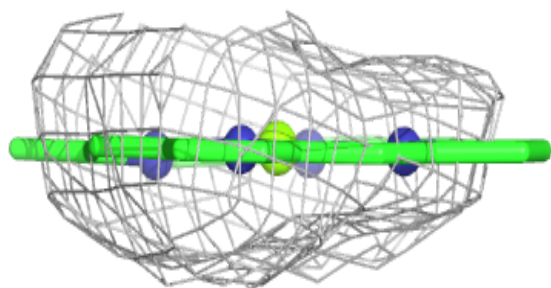
Electron density around CLA B 1224:

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



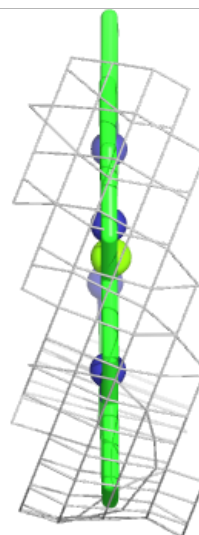
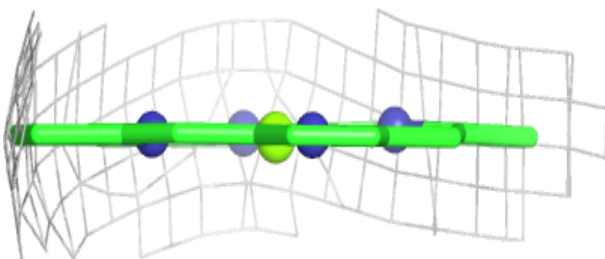
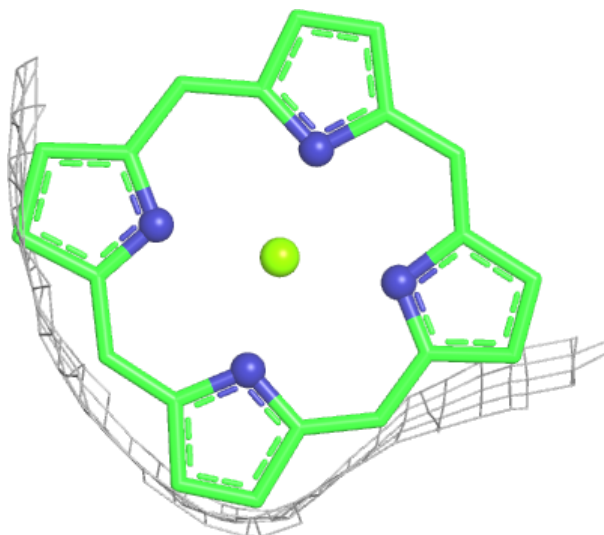
Electron density around CLA 3 610:

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



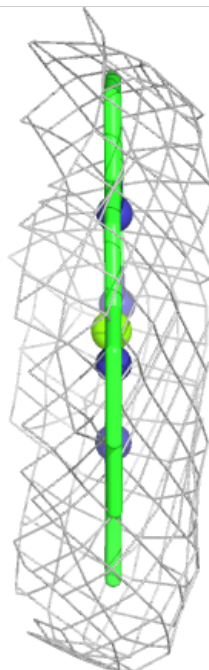
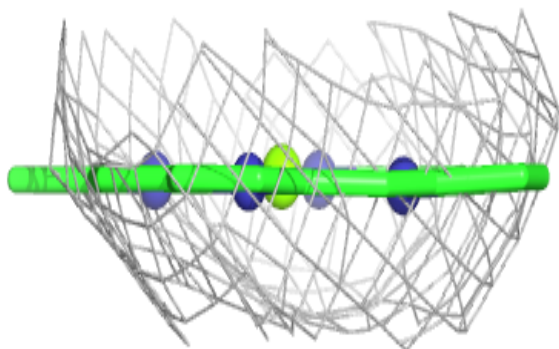
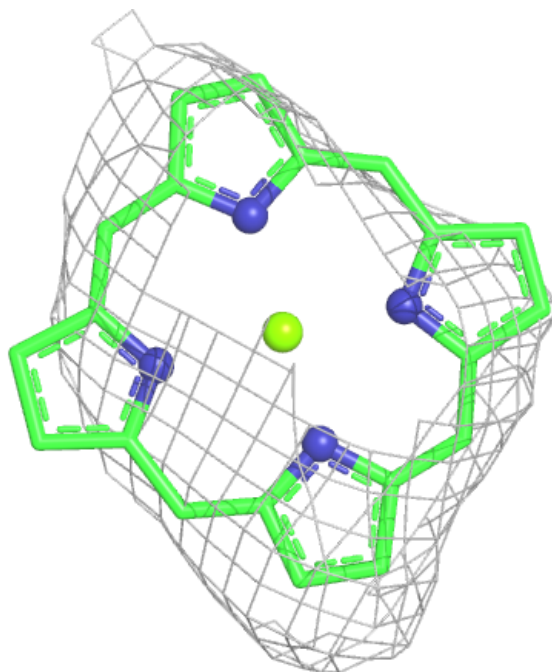
Electron density around CLA B 1211:

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



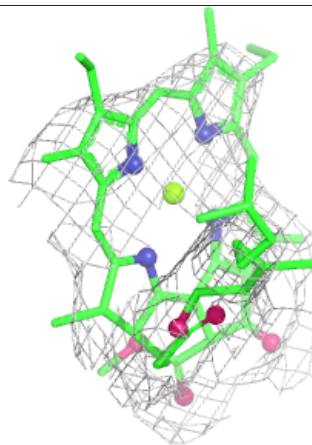
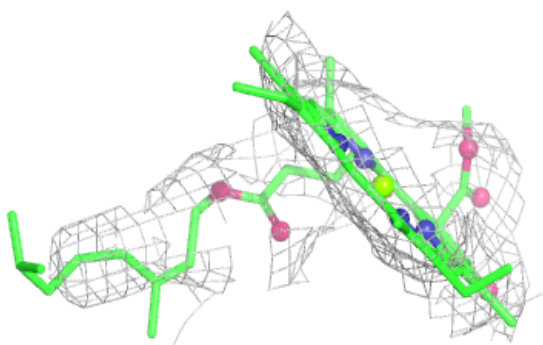
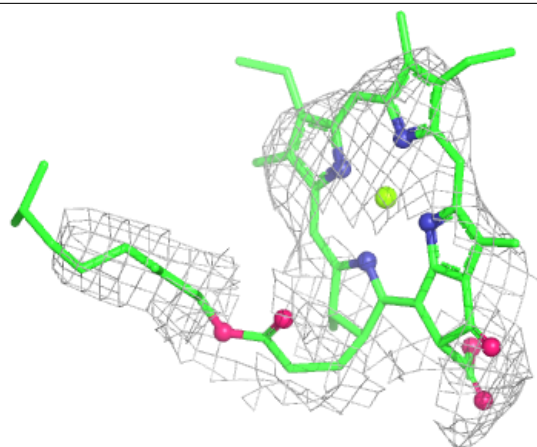
Electron density around CLA B 1206:

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



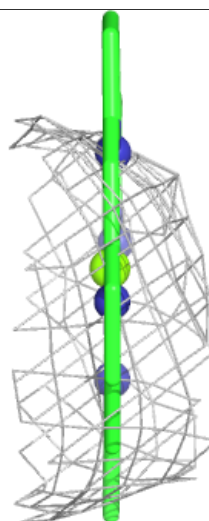
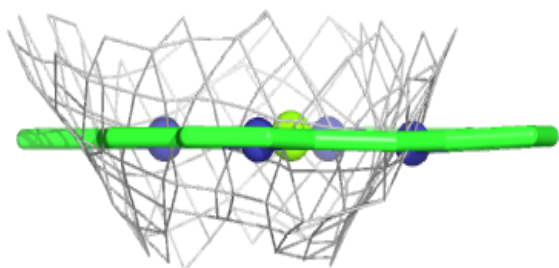
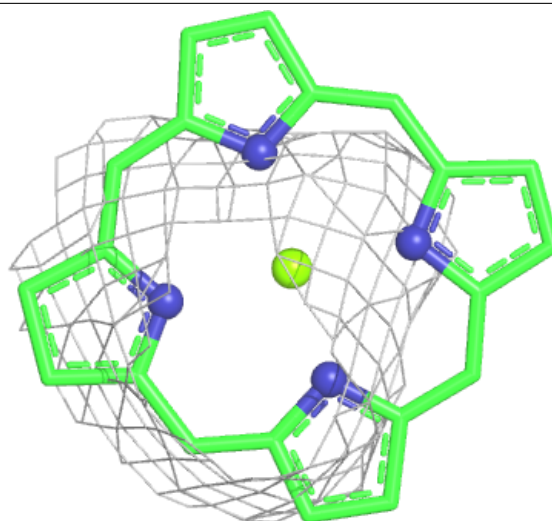
Electron density around CLA A 1106:

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



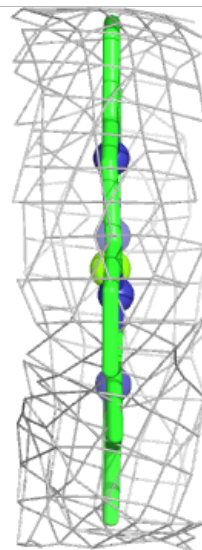
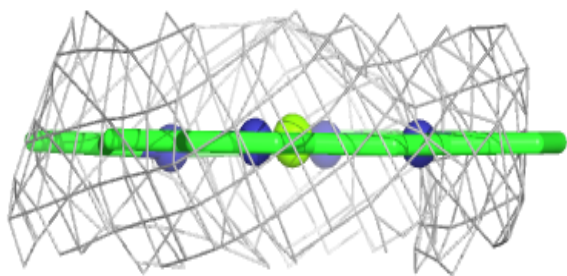
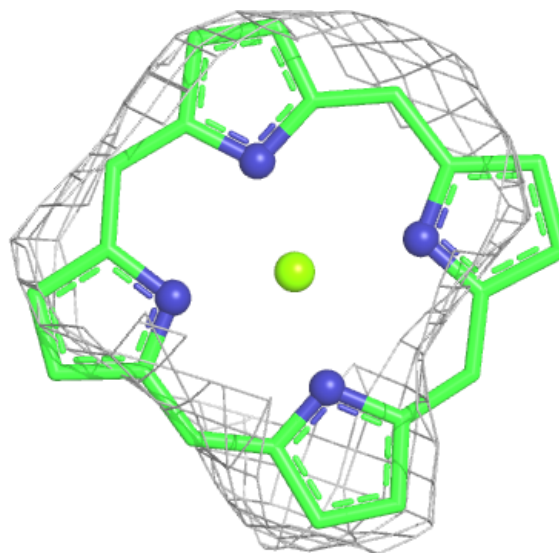
Electron density around CLA B 1205:

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



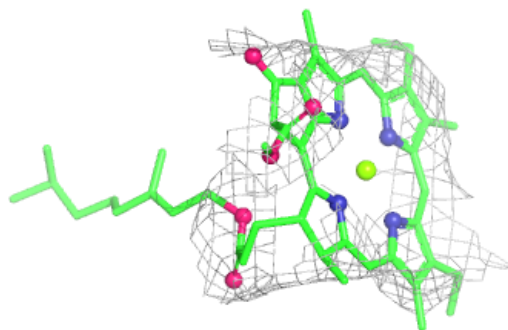
Electron density around CLA A 1136:

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



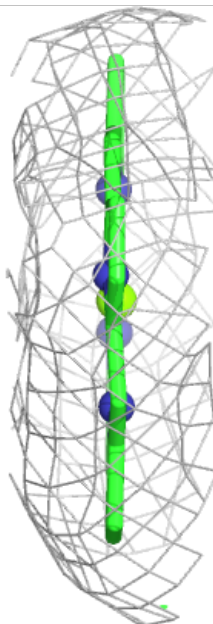
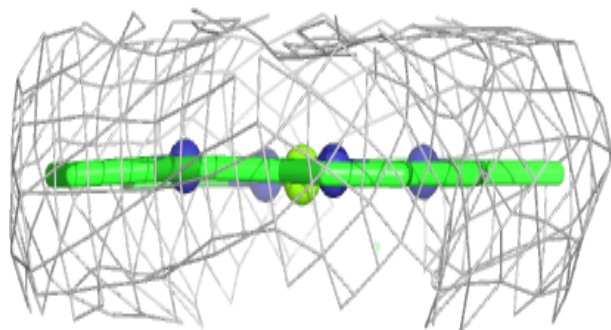
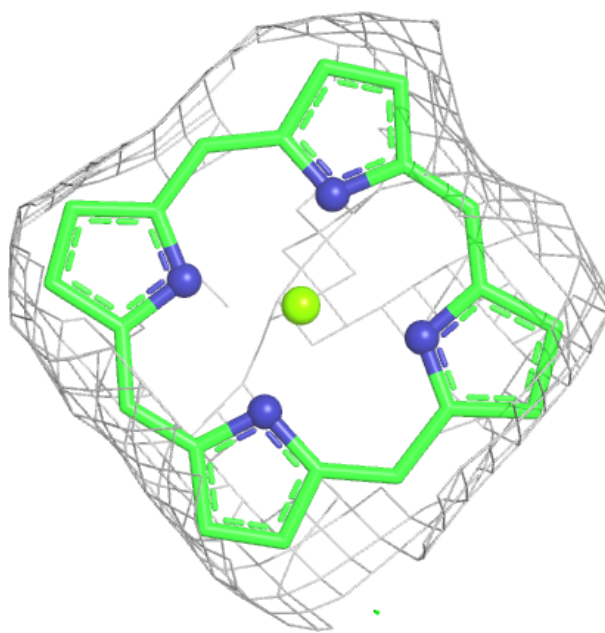
Electron density around CLA A 1126:

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



Electron density around CLA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.