Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:01 pm BST

PDB ID	:	1FE1
Title	:	CRYSTAL STRUCTURE PHOTOSYSTEM II
Authors	:	Zouni, A.; Witt, H.-T.; Kern, J.; Fromme, P.; Krauss, N.; Saenger, W.; Orth, P.
Deposited on	:	2000-07-20
Resolution	:	3.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

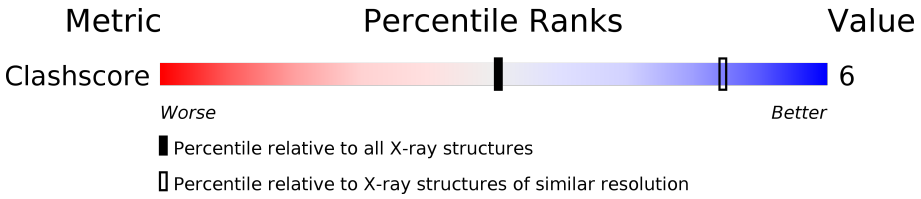
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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))
Clashscore	141614	1288 (4.00-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	169	97% .
1	J	169	97% .
2	B	174	97% .
2	K	174	97% .
3	C	156	99% .
3	L	156	99% .
4	D	155	100%
4	M	155	100%
5	E	40	100%
5	N	40	100%

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Mol	Chain	Length	Quality of chain
6	F	30	100%
6	O	30	100%
7	G	312	100%
7	P	312	100%
8	H	115	100%
8	Q	115	100%
9	I	87	100%
9	R	87	100%

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
12	CLA	A	175	X	-	-	-
12	CLA	A	176	X	-	-	-
12	CLA	A	177	X	-	-	-
12	CLA	A	179	X	-	-	-
12	CLA	B	177	X	-	-	-
12	CLA	B	179	X	-	-	-
12	CLA	C	157	X	-	-	-
12	CLA	C	158	X	-	-	-
12	CLA	C	159	X	-	-	-
12	CLA	C	160	X	-	-	-
12	CLA	C	161	X	-	-	-
12	CLA	C	162	X	-	-	-
12	CLA	C	163	X	-	-	-
12	CLA	C	164	X	-	-	-
12	CLA	C	165	X	-	-	-
12	CLA	C	166	X	-	-	-
12	CLA	C	167	X	-	-	-
12	CLA	C	168	X	-	-	-
12	CLA	D	156	X	-	-	-
12	CLA	D	157	X	-	-	-
12	CLA	D	158	X	-	-	-
12	CLA	D	159	X	-	-	-
12	CLA	D	160	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	D	161	X	-	-	-
12	CLA	D	162	X	-	-	-
12	CLA	D	163	X	-	-	-
12	CLA	D	164	X	-	-	-
12	CLA	D	165	X	-	-	-
12	CLA	D	166	X	-	-	-
12	CLA	D	167	X	-	-	-
12	CLA	D	168	X	-	-	-
12	CLA	G	313	X	-	-	-
12	CLA	J	175	X	-	-	-
12	CLA	J	176	X	-	-	-
12	CLA	J	177	X	-	-	-
12	CLA	J	179	X	-	-	-
12	CLA	K	177	X	-	-	-
12	CLA	K	179	X	-	-	-
12	CLA	L	157	X	-	-	-
12	CLA	L	158	X	-	-	-
12	CLA	L	159	X	-	-	-
12	CLA	L	160	X	-	-	-
12	CLA	L	161	X	-	-	-
12	CLA	L	162	X	-	-	-
12	CLA	L	163	X	-	-	-
12	CLA	L	164	X	-	-	-
12	CLA	L	165	X	-	-	-
12	CLA	L	166	X	-	-	-
12	CLA	L	167	X	-	-	-
12	CLA	L	168	X	-	-	-
12	CLA	M	156	X	-	-	-
12	CLA	M	157	X	-	-	-
12	CLA	M	158	X	-	-	-
12	CLA	M	159	X	-	-	-
12	CLA	M	160	X	-	-	-
12	CLA	M	161	X	-	-	-
12	CLA	M	162	X	-	-	-
12	CLA	M	163	X	-	-	-
12	CLA	M	164	X	-	-	-
12	CLA	M	165	X	-	-	-
12	CLA	M	166	X	-	-	-
12	CLA	M	167	X	-	-	-
12	CLA	M	168	X	-	-	-
12	CLA	P	313	X	-	-	-
15	PLA	B	180	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	PLA	K	180	-	X	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 4328 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 PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBA).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	169	Total C 169 169	0	0	169
1	J	169	Total C 169 169	0	0	169

- Molecule 2 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBD).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	174	Total C 174 174	0	0	174
2	K	174	Total C 174 174	0	0	174

- Molecule 3 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBC).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	156	Total C 156 156	0	0	156
3	L	156	Total C 156 156	0	0	156

- Molecule 4 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBB).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	D	155	Total C 155 155	0	0	155
4	M	155	Total C 155 155	0	0	155

- Molecule 5 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBE).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	40	Total C 40 40	0	0	40
5	N	40	Total C 40 40	0	0	40

- Molecule 6 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBF).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	30	Total C 30 30	0	0	30
6	O	30	Total C 30 30	0	0	30

- Molecule 7 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT UNKNOWN).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	312	Total C 312 312	0	0	312
7	P	312	Total C 312 312	0	0	312

- Molecule 8 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBO).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	115	Total C 115 115	0	0	115
8	Q	115	Total C 115 115	0	0	115

- Molecule 9 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBV).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	I	87	Total C 87 87	0	0	87
9	R	87	Total C 87 87	0	0	87

- Molecule 10 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	J	4	Total Mn 4 4	0	0

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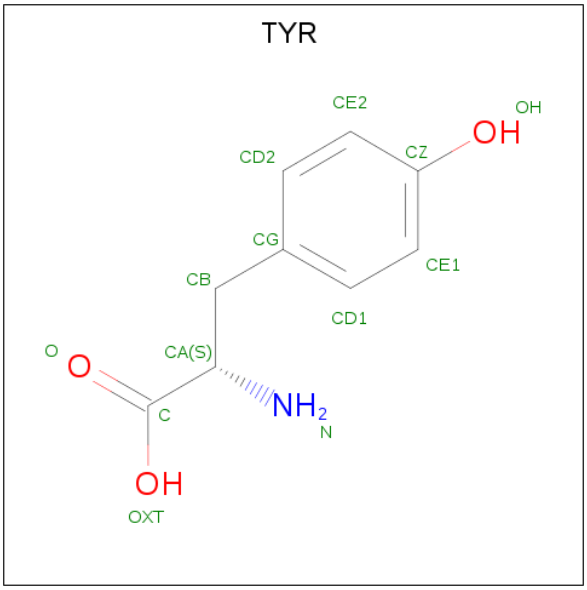
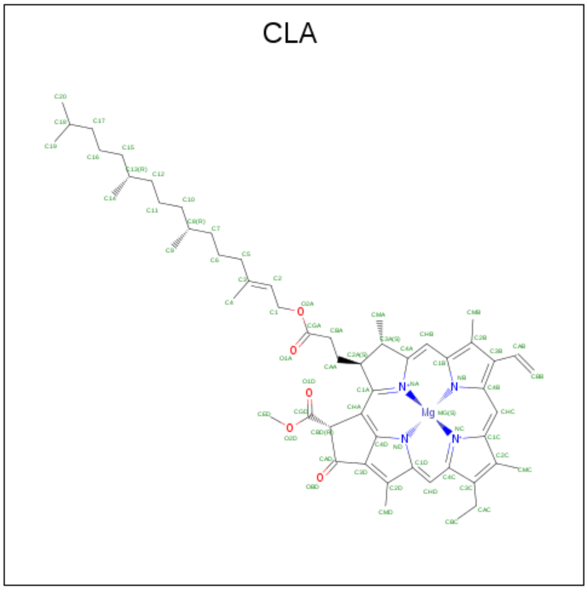
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	4	Total Mn 4 4	0	0

- Molecule 11 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 8 7 1	0	0
11	B	1	Total C O 8 7 1	0	0
11	J	1	Total C O 8 7 1	0	0
11	K	1	Total C O 8 7 1	0	0

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total 25	C 20	Mg 1	N 4	0	0
12	A	1	Total 25	C 20	Mg 1	N 4	0	0
12	A	1	Total 25	C 20	Mg 1	N 4	0	0
12	A	1	Total 25	C 20	Mg 1	N 4	0	0
12	B	1	Total 25	C 20	Mg 1	N 4	0	0
12	B	1	Total 25	C 20	Mg 1	N 4	0	0
12	C	1	Total 25	C 20	Mg 1	N 4	0	0
12	C	1	Total 25	C 20	Mg 1	N 4	0	0
12	C	1	Total 25	C 20	Mg 1	N 4	0	0
12	C	1	Total 25	C 20	Mg 1	N 4	0	0
12	C	1	Total 25	C 20	Mg 1	N 4	0	0
12	C	1	Total 25	C 20	Mg 1	N 4	0	0
12	C	1	Total 25	C 20	Mg 1	N 4	0	0
12	C	1	Total 25	C 20	Mg 1	N 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C Mg N 25 20 1 4	0	0
12	C	1	Total C Mg N 25 20 1 4	0	0
12	C	1	Total C Mg N 25 20 1 4	0	0
12	C	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	D	1	Total C Mg N 25 20 1 4	0	0
12	G	1	Total C Mg N 25 20 1 4	0	0
12	J	1	Total C Mg N 25 20 1 4	0	0
12	J	1	Total C Mg N 25 20 1 4	0	0
12	J	1	Total C Mg N 25 20 1 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	J	1	Total C Mg N 25 20 1 4	0	0
12	K	1	Total C Mg N 25 20 1 4	0	0
12	K	1	Total C Mg N 25 20 1 4	0	0
12	L	1	Total C Mg N 25 20 1 4	0	0
12	L	1	Total C Mg N 25 20 1 4	0	0
12	L	1	Total C Mg N 25 20 1 4	0	0
12	L	1	Total C Mg N 25 20 1 4	0	0
12	L	1	Total C Mg N 25 20 1 4	0	0
12	L	1	Total C Mg N 25 20 1 4	0	0
12	L	1	Total C Mg N 25 20 1 4	0	0
12	L	1	Total C Mg N 25 20 1 4	0	0
12	L	1	Total C Mg N 25 20 1 4	0	0
12	L	1	Total C Mg N 25 20 1 4	0	0
12	L	1	Total C Mg N 25 20 1 4	0	0
12	L	1	Total C Mg N 25 20 1 4	0	0
12	M	1	Total C Mg N 25 20 1 4	0	0
12	M	1	Total C Mg N 25 20 1 4	0	0
12	M	1	Total C Mg N 25 20 1 4	0	0
12	M	1	Total C Mg N 25 20 1 4	0	0
12	M	1	Total C Mg N 25 20 1 4	0	0
12	M	1	Total C Mg N 25 20 1 4	0	0

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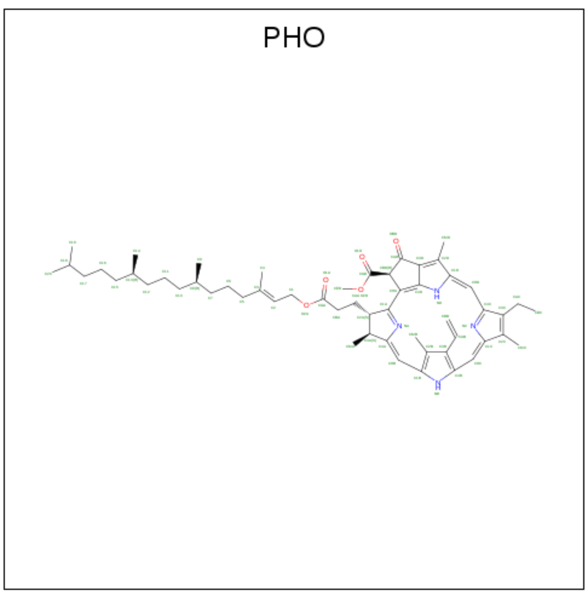
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	M	1	Total 25	C 20	Mg 1	N 4	0	0
12	M	1	Total 25	C 20	Mg 1	N 4	0	0
12	M	1	Total 25	C 20	Mg 1	N 4	0	0
12	M	1	Total 25	C 20	Mg 1	N 4	0	0
12	M	1	Total 25	C 20	Mg 1	N 4	0	0
12	M	1	Total 25	C 20	Mg 1	N 4	0	0
12	M	1	Total 25	C 20	Mg 1	N 4	0	0
12	P	1	Total 25	C 20	Mg 1	N 4	0	0

- Molecule 13 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total 24	C 20	N 4	0	0
13	B	1	Total 24	C 20	N 4	0	0
13	J	1	Total 24	C 20	N 4	0	0

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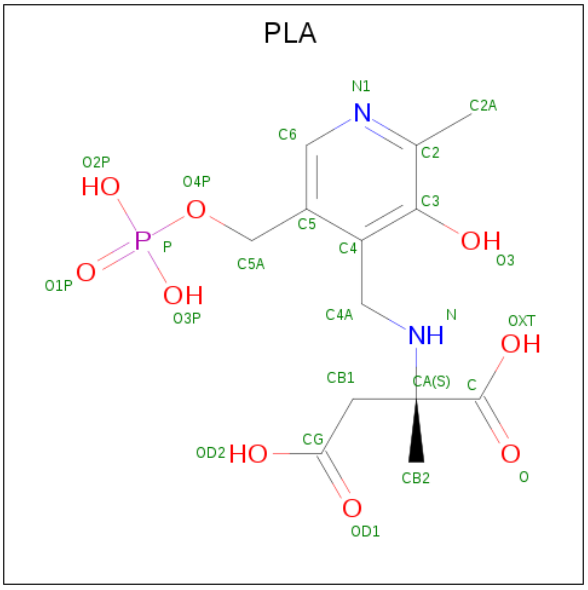
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	K	1	Total C N 24 20 4	0	0

- Molecule 14 is FE (III) ION (three-letter code: FE) (formula: Fe).

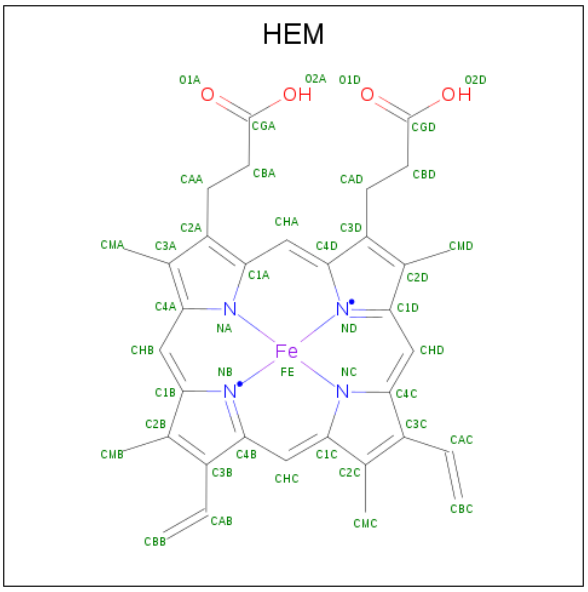
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total Fe 1 1	0	0
14	K	1	Total Fe 1 1	0	0

- Molecule 15 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-2-METHYL-SUCCINIC ACID (three-letter code: PLA) (formula: $C_{13}H_{19}N_2O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C N 6 5 1	0	0
15	K	1	Total C N 6 5 1	0	0

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	F	1	Total	C	Fe	N	0	0
			25	20	1	4		
16	I	1	Total	C	Fe	N	0	0
			25	20	1	4		
16	O	1	Total	C	Fe	N	0	0
			25	20	1	4		
16	R	1	Total	C	Fe	N	0	0
			25	20	1	4		

- Molecule 17 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	1	Total	Cd	0	0
			1	1		
17	Q	1	Total	Cd	0	0
			1	1		

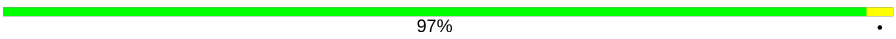
3 Residue-property plots (i)

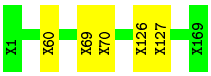
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBA)

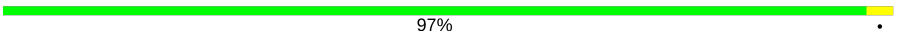
Chain A:

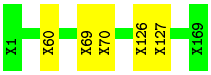




- Molecule 1: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBA)

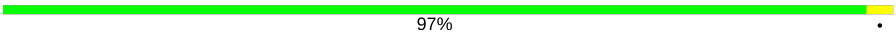
Chain J:

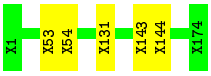




- Molecule 2: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBD)

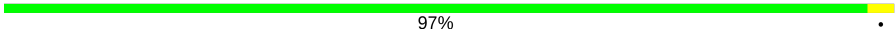
Chain B:





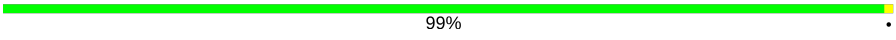
- Molecule 2: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBD)

Chain K:

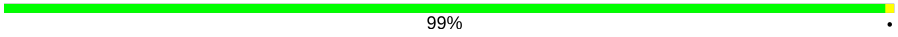


- Molecule 3: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBC)

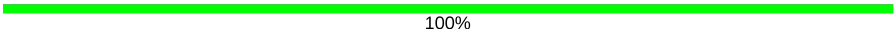
Chain C:



- Molecule 3: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBC)

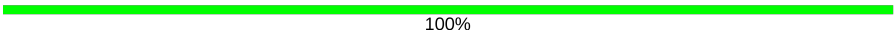
Chain L: 

• Molecule 4: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBB)

Chain D: 

There are no outlier residues recorded for this chain.

• Molecule 4: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBB)

Chain M: 

There are no outlier residues recorded for this chain.

• Molecule 5: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBE)

Chain E: 

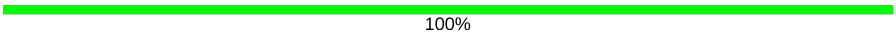
There are no outlier residues recorded for this chain.

• Molecule 5: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBE)

Chain N: 

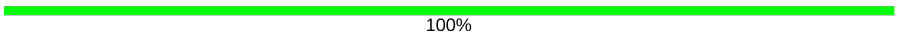
There are no outlier residues recorded for this chain.

• Molecule 6: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBF)

Chain F: 

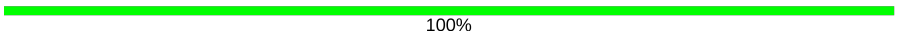
There are no outlier residues recorded for this chain.

• Molecule 6: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBF)

Chain O: 

There are no outlier residues recorded for this chain.

• Molecule 7: PROTEIN (PHOTOSYSTEM II: SUBUNIT UNKNOWN)

Chain G: 

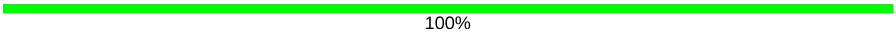
There are no outlier residues recorded for this chain.

• Molecule 7: PROTEIN (PHOTOSYSTEM II: SUBUNIT UNKNOWN)

Chain P: 

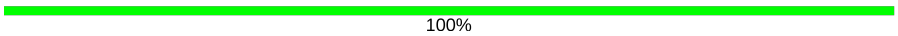
There are no outlier residues recorded for this chain.

• Molecule 8: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBO)

Chain H: 

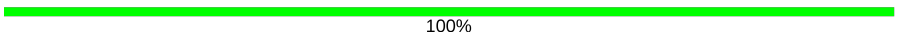
There are no outlier residues recorded for this chain.

• Molecule 8: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBO)

Chain Q: 

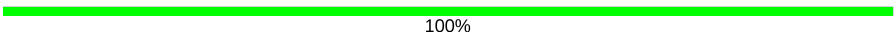
There are no outlier residues recorded for this chain.

• Molecule 9: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBV)

Chain I: 

There are no outlier residues recorded for this chain.

• Molecule 9: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBV)

Chain R: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	130.01Å 226.72Å 308.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4328	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PHO, MN, CLA, CD, FE, PLA, HEM

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	A	169	0	0	4	0
1	J	169	0	0	4	0
2	B	174	0	0	4	0
2	K	174	0	0	4	0
3	C	156	0	0	2	0
3	L	156	0	0	2	0
4	D	155	0	0	0	0
4	M	155	0	0	0	0
5	E	40	0	0	0	0
5	N	40	0	0	0	0
6	F	30	0	0	0	0
6	O	30	0	0	0	0
7	G	312	0	0	0	0
7	P	312	0	0	0	0
8	H	115	0	0	0	0
8	Q	115	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	87	0	0	0	0
9	R	87	0	0	0	0
10	A	4	0	0	0	0
10	J	4	0	0	0	0
11	A	8	0	5	0	0
11	B	8	0	5	0	0
11	J	8	0	5	0	0
11	K	8	0	5	0	0
12	A	100	0	12	0	0
12	B	50	0	6	0	0
12	C	300	0	36	2	0
12	D	325	0	39	6	0
12	G	25	0	3	0	0
12	J	100	0	12	0	0
12	K	50	0	6	0	0
12	L	300	0	36	2	0
12	M	325	0	39	6	0
12	P	25	0	3	0	0
13	A	24	0	5	0	0
13	B	24	0	5	0	0
13	J	24	0	5	0	0
13	K	24	0	5	0	0
14	B	1	0	0	0	0
14	K	1	0	0	0	0
15	B	6	0	1	0	0
15	K	6	0	1	0	0
16	F	25	0	4	0	0
16	I	25	0	4	0	0
16	O	25	0	4	0	0
16	R	25	0	4	0	0
17	H	1	0	0	0	0
17	Q	1	0	0	0	0
All	All	4328	0	250	26	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 6.

All (26) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:127:UNK:CA	2:K:53:UNK:CA	1.88	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:UNK:CA	2:B:53:UNK:CA	1.88	1.49
1:A:60:UNK:CA	2:B:131:UNK:CA	1.95	1.45
1:J:60:UNK:CA	2:K:131:UNK:CA	1.95	1.44
3:L:149:UNK:CA	12:L:166:CLA:C2A	2.23	1.17
3:C:149:UNK:CA	12:C:166:CLA:C2A	2.23	1.15
12:D:159:CLA:HHB	12:D:162:CLA:CHD	1.81	1.10
12:M:159:CLA:HHB	12:M:162:CLA:CHD	1.81	1.08
12:M:159:CLA:HHB	12:M:162:CLA:HHD	1.01	1.01
12:M:159:CLA:CHB	12:M:162:CLA:HHD	1.92	1.00
12:D:159:CLA:CHB	12:D:162:CLA:HHD	1.92	0.98
12:D:159:CLA:HHB	12:D:162:CLA:HHD	1.02	0.97
1:J:126:UNK:CA	2:K:54:UNK:CA	2.66	0.74
1:A:126:UNK:CA	2:B:54:UNK:CA	2.66	0.73
3:C:149:UNK:CA	12:C:166:CLA:C3A	2.69	0.70
3:L:149:UNK:CA	12:L:166:CLA:C3A	2.69	0.70
1:A:69:UNK:CA	1:A:70:UNK:CA	2.76	0.64
1:J:69:UNK:CA	1:J:70:UNK:CA	2.76	0.63
12:M:159:CLA:HHB	12:M:162:CLA:C1D	2.35	0.56
12:D:159:CLA:HHB	12:D:162:CLA:C1D	2.35	0.53
12:D:159:CLA:HHB	12:D:162:CLA:C2D	2.42	0.50
12:M:159:CLA:HHB	12:M:162:CLA:C2D	2.42	0.49
2:B:143:UNK:CA	2:B:144:UNK:CA	2.91	0.48
2:K:143:UNK:CA	2:K:144:UNK:CA	2.91	0.48
12:D:159:CLA:CHB	12:D:162:CLA:C2D	2.97	0.43
12:M:159:CLA:CHB	12:M:162:CLA:C2D	2.97	0.43

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 90 ligands modelled in this entry, 12 are monoatomic - leaving 78 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	CLA	M	163	-	22,32,73	2.66	6 (27%)	26,54,113	2.95	8 (30%)
16	HEM	I	88	-	12,32,50	3.17	2 (16%)	23,54,82	3.69	11 (47%)
12	CLA	L	160	-	22,32,73	2.65	6 (27%)	26,54,113	2.99	8 (30%)
12	CLA	C	162	-	22,32,73	2.69	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	K	177	-	22,32,73	2.68	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	C	163	-	22,32,73	2.66	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	D	161	-	22,32,73	2.68	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	J	177	-	22,32,73	2.64	6 (27%)	26,54,113	3.01	8 (30%)
12	CLA	D	160	-	22,32,73	2.65	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	D	165	-	22,32,73	2.66	6 (27%)	26,54,113	2.96	8 (30%)
13	PHO	A	178	-	18,28,69	1.15	0	7,40,99	1.83	3 (42%)
12	CLA	D	164	-	22,32,73	2.65	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	B	177	-	22,32,73	2.67	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	J	175	-	22,32,73	2.66	6 (27%)	26,54,113	2.99	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	M	161	-	22,32,73	2.66	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	C	165	-	22,32,73	2.67	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	C	168	-	22,32,73	2.66	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	C	157	-	22,32,73	2.69	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	C	161	-	22,32,73	2.65	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	C	159	-	22,32,73	2.66	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	G	313	-	22,32,73	2.65	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	L	165	-	22,32,73	2.66	6 (27%)	26,54,113	2.97	8 (30%)
13	PHO	B	178	-	18,28,69	1.15	0	7,40,99	1.83	3 (42%)
12	CLA	L	164	-	22,32,73	2.66	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	D	157	-	22,32,73	2.68	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	A	179	-	22,32,73	2.67	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	C	164	-	22,32,73	2.66	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	L	157	-	22,32,73	2.68	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	M	162	-	22,32,73	2.66	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	B	179	-	22,32,73	2.67	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	P	313	-	22,32,73	2.66	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	L	162	-	22,32,73	2.69	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	M	166	-	22,32,73	2.69	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	M	159	-	22,32,73	2.67	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	L	166	-	22,32,73	2.67	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	M	157	-	22,32,73	2.69	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	M	158	-	22,32,73	2.68	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	C	166	-	22,32,73	2.67	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	D	162	-	22,32,73	2.65	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	D	168	-	22,32,73	2.66	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	M	160	-	22,32,73	2.67	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	C	158	-	22,32,73	2.67	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	L	168	-	22,32,73	2.64	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	M	164	-	22,32,73	2.66	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	L	163	-	22,32,73	2.67	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	M	165	-	22,32,73	2.67	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	A	177	-	22,32,73	2.65	6 (27%)	26,54,113	3.00	8 (30%)
12	CLA	C	160	-	22,32,73	2.64	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	L	158	-	22,32,73	2.66	6 (27%)	26,54,113	2.98	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	PHO	K	178	-	18,28,69	1.15	0	7,40,99	1.81	3 (42%)
12	CLA	L	159	-	22,32,73	2.64	6 (27%)	26,54,113	2.99	8 (30%)
15	PLA	B	180	-	6,6,25	2.92	6 (100%)	6,6,37	0.89	0
16	HEM	R	88	-	12,32,50	3.17	2 (16%)	23,54,82	3.69	11 (47%)
12	CLA	J	176	-	22,32,73	2.69	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	J	179	-	22,32,73	2.67	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	M	168	-	22,32,73	2.66	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	C	167	-	22,32,73	2.65	6 (27%)	26,54,113	2.95	8 (30%)
16	HEM	F	31	-	12,32,50	3.16	2 (16%)	23,54,82	3.66	11 (47%)
12	CLA	D	166	-	22,32,73	2.69	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	M	156	-	22,32,73	2.69	6 (27%)	26,54,113	2.96	8 (30%)
16	HEM	O	58	-	12,32,50	3.17	2 (16%)	23,54,82	3.65	11 (47%)
12	CLA	L	161	-	22,32,73	2.66	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	L	167	-	22,32,73	2.65	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	A	176	-	22,32,73	2.69	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	K	179	-	22,32,73	2.67	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	A	175	-	22,32,73	2.64	6 (27%)	26,54,113	2.99	8 (30%)
12	CLA	D	163	-	22,32,73	2.66	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	M	167	-	22,32,73	2.68	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	D	167	-	22,32,73	2.68	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	D	159	-	22,32,73	2.66	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	D	158	-	22,32,73	2.68	6 (27%)	26,54,113	2.98	8 (30%)
13	PHO	J	178	-	18,28,69	1.15	0	7,40,99	1.82	3 (42%)
12	CLA	D	156	-	22,32,73	2.69	6 (27%)	26,54,113	2.95	8 (30%)
15	PLA	K	180	-	6,6,25	2.92	6 (100%)	6,6,37	0.89	0

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
12	CLA	M	163	-	3/3/7/25	-	-
12	CLA	M	161	-	3/3/7/25	-	-
12	CLA	L	160	-	3/3/7/25	-	-
12	CLA	C	162	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	K	177	-	3/3/7/25	-	-
12	CLA	C	163	-	3/3/7/25	-	-
12	CLA	D	161	-	3/3/7/25	-	-
12	CLA	J	177	-	3/3/7/25	-	-
12	CLA	P	313	-	3/3/7/25	-	-
12	CLA	D	165	-	3/3/7/25	-	-
12	CLA	D	164	-	3/3/7/25	-	-
12	CLA	B	177	-	3/3/7/25	-	-
12	CLA	J	175	-	3/3/7/25	-	-
12	CLA	D	160	-	3/3/7/25	-	-
12	CLA	C	165	-	3/3/7/25	-	-
12	CLA	C	168	-	3/3/7/25	-	-
12	CLA	C	157	-	3/3/7/25	-	-
12	CLA	C	161	-	3/3/7/25	-	-
12	CLA	C	159	-	3/3/7/25	-	-
12	CLA	G	313	-	3/3/7/25	-	-
12	CLA	L	165	-	3/3/7/25	-	-
12	CLA	M	167	-	3/3/7/25	-	-
12	CLA	L	164	-	3/3/7/25	-	-
12	CLA	D	157	-	3/3/7/25	-	-
12	CLA	A	179	-	3/3/7/25	-	-
12	CLA	C	164	-	3/3/7/25	-	-
12	CLA	L	157	-	3/3/7/25	-	-
12	CLA	M	162	-	3/3/7/25	-	-
12	CLA	B	179	-	3/3/7/25	-	-
12	CLA	L	162	-	3/3/7/25	-	-
12	CLA	M	166	-	3/3/7/25	-	-
12	CLA	M	159	-	3/3/7/25	-	-
12	CLA	L	166	-	3/3/7/25	-	-
12	CLA	M	157	-	3/3/7/25	-	-
12	CLA	M	158	-	3/3/7/25	-	-
12	CLA	C	166	-	3/3/7/25	-	-
12	CLA	D	162	-	3/3/7/25	-	-
12	CLA	D	168	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PHO	B	178	-	-	0/8/34/103	0/4/5/6
12	CLA	M	160	-	3/3/7/25	-	-
12	CLA	C	158	-	3/3/7/25	-	-
12	CLA	L	168	-	3/3/7/25	-	-
12	CLA	M	164	-	3/3/7/25	-	-
12	CLA	L	163	-	3/3/7/25	-	-
12	CLA	M	165	-	3/3/7/25	-	-
12	CLA	A	177	-	3/3/7/25	-	-
12	CLA	C	160	-	3/3/7/25	-	-
12	CLA	L	158	-	3/3/7/25	-	-
13	PHO	K	178	-	-	0/8/34/103	0/4/5/6
12	CLA	L	159	-	3/3/7/25	-	-
15	PLA	B	180	-	-	-	0/1/1/1
12	CLA	J	176	-	3/3/7/25	-	-
12	CLA	J	179	-	3/3/7/25	-	-
12	CLA	M	168	-	3/3/7/25	-	-
12	CLA	C	167	-	3/3/7/25	-	-
13	PHO	A	178	-	-	0/8/34/103	0/4/5/6
12	CLA	D	166	-	3/3/7/25	-	-
12	CLA	M	156	-	3/3/7/25	-	-
12	CLA	L	161	-	3/3/7/25	-	-
12	CLA	L	167	-	3/3/7/25	-	-
12	CLA	A	176	-	3/3/7/25	-	-
12	CLA	K	179	-	3/3/7/25	-	-
12	CLA	A	175	-	3/3/7/25	-	-
12	CLA	D	163	-	3/3/7/25	-	-
12	CLA	D	167	-	3/3/7/25	-	-
15	PLA	K	180	-	-	-	0/1/1/1
12	CLA	D	158	-	3/3/7/25	-	-
13	PHO	J	178	-	-	0/8/34/103	0/4/5/6
12	CLA	D	156	-	3/3/7/25	-	-
12	CLA	D	159	-	3/3/7/25	-	-

All (404) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	162	CLA	CHB-C4A	7.71	1.40	1.34
12	L	162	CLA	CHB-C4A	7.70	1.40	1.34
12	M	156	CLA	CHB-C4A	7.66	1.40	1.34
12	M	160	CLA	CHB-C4A	7.65	1.40	1.34
12	D	156	CLA	CHB-C4A	7.63	1.40	1.34
12	A	176	CLA	CHB-C4A	7.63	1.40	1.34
12	J	176	CLA	CHB-C4A	7.62	1.40	1.34
12	K	177	CLA	CHB-C4A	7.62	1.40	1.34
12	M	157	CLA	CHB-C4A	7.58	1.40	1.34
12	D	167	CLA	CHB-C4A	7.58	1.40	1.34
12	D	161	CLA	CHB-C4A	7.57	1.40	1.34
12	D	166	CLA	CHB-C4A	7.57	1.40	1.34
12	B	177	CLA	CHB-C4A	7.56	1.40	1.34
12	D	157	CLA	CHB-C4A	7.56	1.40	1.34
12	D	160	CLA	CHB-C4A	7.56	1.40	1.34
12	C	157	CLA	CHB-C4A	7.56	1.40	1.34
12	M	158	CLA	CHB-C4A	7.56	1.40	1.34
12	M	166	CLA	CHB-C4A	7.55	1.40	1.34
12	M	167	CLA	CHB-C4A	7.55	1.40	1.34
12	D	158	CLA	CHB-C4A	7.54	1.40	1.34
12	C	166	CLA	CHB-C4A	7.53	1.40	1.34
12	L	161	CLA	CHB-C4A	7.53	1.40	1.34
12	C	164	CLA	CHB-C4A	7.52	1.40	1.34
12	M	159	CLA	CHB-C4A	7.51	1.40	1.34
12	M	165	CLA	CHB-C4A	7.50	1.40	1.34
12	L	166	CLA	CHB-C4A	7.50	1.40	1.34
12	C	158	CLA	CHB-C4A	7.49	1.40	1.34
12	P	313	CLA	CHB-C4A	7.49	1.40	1.34
12	M	164	CLA	CHB-C4A	7.49	1.40	1.34
12	A	179	CLA	CHB-C4A	7.49	1.40	1.34
12	L	164	CLA	CHB-C4A	7.48	1.40	1.34
12	C	168	CLA	CHB-C4A	7.47	1.40	1.34
12	D	165	CLA	CHB-C4A	7.47	1.40	1.34
12	L	158	CLA	CHB-C4A	7.47	1.40	1.34
12	D	168	CLA	CHB-C4A	7.46	1.40	1.34
12	K	179	CLA	CHB-C4A	7.45	1.40	1.34
12	M	161	CLA	CHB-C4A	7.45	1.40	1.34
12	L	163	CLA	CHB-C4A	7.45	1.40	1.34
12	B	179	CLA	CHB-C4A	7.44	1.40	1.34
12	J	179	CLA	CHB-C4A	7.43	1.40	1.34
12	D	159	CLA	CHB-C4A	7.43	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	165	CLA	CHB-C4A	7.43	1.40	1.34
12	C	161	CLA	CHB-C4A	7.42	1.40	1.34
12	L	157	CLA	CHB-C4A	7.42	1.40	1.34
12	C	163	CLA	CHB-C4A	7.41	1.40	1.34
12	C	159	CLA	CHB-C4A	7.40	1.40	1.34
12	M	168	CLA	CHB-C4A	7.40	1.40	1.34
12	G	313	CLA	CHB-C4A	7.40	1.40	1.34
12	M	163	CLA	CHB-C4A	7.39	1.40	1.34
16	R	88	HEM	C2A-C1A	7.38	1.52	1.39
12	D	164	CLA	CHB-C4A	7.38	1.40	1.34
12	L	167	CLA	CHB-C4A	7.37	1.40	1.34
12	L	165	CLA	CHB-C4A	7.37	1.40	1.34
12	D	163	CLA	CHB-C4A	7.36	1.40	1.34
16	I	88	HEM	C2A-C1A	7.36	1.52	1.39
12	C	167	CLA	CHB-C4A	7.36	1.40	1.34
12	L	168	CLA	CHB-C4A	7.36	1.40	1.34
12	J	175	CLA	CHB-C4A	7.35	1.40	1.34
16	O	58	HEM	C2A-C1A	7.35	1.52	1.39
16	F	31	HEM	C2A-C1A	7.35	1.52	1.39
12	L	160	CLA	CHB-C4A	7.33	1.40	1.34
12	A	177	CLA	CHB-C4A	7.33	1.40	1.34
12	A	175	CLA	CHB-C4A	7.31	1.40	1.34
12	M	162	CLA	CHB-C4A	7.29	1.40	1.34
12	C	160	CLA	CHB-C4A	7.29	1.40	1.34
12	L	159	CLA	CHB-C4A	7.28	1.40	1.34
12	D	162	CLA	CHB-C4A	7.24	1.40	1.34
12	J	177	CLA	CHB-C4A	7.23	1.40	1.34
16	O	58	HEM	C3A-C4A	6.85	1.52	1.39
16	R	88	HEM	C3A-C4A	6.82	1.51	1.39
16	I	88	HEM	C3A-C4A	6.82	1.51	1.39
16	F	31	HEM	C3A-C4A	6.81	1.51	1.39
12	M	163	CLA	C3C-C2C	6.17	1.49	1.35
12	J	177	CLA	C3C-C2C	6.16	1.49	1.35
12	A	175	CLA	C3C-C2C	6.16	1.49	1.35
12	M	162	CLA	C3C-C2C	6.16	1.49	1.35
12	D	163	CLA	C3C-C2C	6.15	1.49	1.35
12	J	175	CLA	C3C-C2C	6.15	1.48	1.35
12	A	177	CLA	C3C-C2C	6.15	1.48	1.35
12	L	163	CLA	C3C-C2C	6.13	1.48	1.35
12	C	165	CLA	C3C-C2C	6.13	1.48	1.35
12	L	165	CLA	C3C-C2C	6.13	1.48	1.35
12	L	157	CLA	C3C-C2C	6.12	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	162	CLA	C3C-C2C	6.12	1.48	1.35
12	D	164	CLA	C3C-C2C	6.12	1.48	1.35
12	D	161	CLA	C3C-C2C	6.12	1.48	1.35
12	M	161	CLA	C3C-C2C	6.11	1.48	1.35
12	M	157	CLA	C3C-C2C	6.11	1.48	1.35
12	D	166	CLA	C3C-C2C	6.11	1.48	1.35
12	C	163	CLA	C3C-C2C	6.11	1.48	1.35
12	C	166	CLA	C3C-C2C	6.11	1.48	1.35
12	D	157	CLA	C3C-C2C	6.11	1.48	1.35
12	L	166	CLA	C3C-C2C	6.10	1.48	1.35
12	D	156	CLA	C3C-C2C	6.10	1.48	1.35
12	M	166	CLA	C3C-C2C	6.10	1.48	1.35
12	C	157	CLA	C3C-C2C	6.10	1.48	1.35
12	M	156	CLA	C3C-C2C	6.10	1.48	1.35
12	P	313	CLA	C3C-C2C	6.09	1.48	1.35
12	J	176	CLA	C3C-C2C	6.09	1.48	1.35
12	M	164	CLA	C3C-C2C	6.09	1.48	1.35
12	K	177	CLA	C3C-C2C	6.09	1.48	1.35
12	L	159	CLA	C3C-C2C	6.09	1.48	1.35
12	A	176	CLA	C3C-C2C	6.09	1.48	1.35
12	G	313	CLA	C3C-C2C	6.09	1.48	1.35
12	C	158	CLA	C3C-C2C	6.09	1.48	1.35
12	B	177	CLA	C3C-C2C	6.09	1.48	1.35
12	L	162	CLA	C3C-C2C	6.09	1.48	1.35
12	M	165	CLA	C3C-C2C	6.09	1.48	1.35
12	C	168	CLA	C3C-C2C	6.08	1.48	1.35
12	D	158	CLA	C3C-C2C	6.08	1.48	1.35
12	M	158	CLA	C3C-C2C	6.08	1.48	1.35
12	C	161	CLA	C3C-C2C	6.08	1.48	1.35
12	D	168	CLA	C3C-C2C	6.08	1.48	1.35
12	C	159	CLA	C3C-C2C	6.08	1.48	1.35
12	L	168	CLA	C3C-C2C	6.08	1.48	1.35
12	J	179	CLA	C3C-C2C	6.08	1.48	1.35
12	D	165	CLA	C3C-C2C	6.08	1.48	1.35
12	D	159	CLA	C3C-C2C	6.07	1.48	1.35
12	C	162	CLA	C3C-C2C	6.07	1.48	1.35
12	M	168	CLA	C3C-C2C	6.07	1.48	1.35
12	L	160	CLA	C3C-C2C	6.07	1.48	1.35
12	C	160	CLA	C3C-C2C	6.06	1.48	1.35
12	L	158	CLA	C3C-C2C	6.06	1.48	1.35
12	D	167	CLA	C3C-C2C	6.06	1.48	1.35
12	M	159	CLA	C3C-C2C	6.06	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	161	CLA	C3C-C2C	6.06	1.48	1.35
12	A	179	CLA	C3C-C2C	6.05	1.48	1.35
12	K	179	CLA	C3C-C2C	6.05	1.48	1.35
12	M	167	CLA	C3C-C2C	6.05	1.48	1.35
12	B	179	CLA	C3C-C2C	6.05	1.48	1.35
12	C	167	CLA	C3C-C2C	6.04	1.48	1.35
12	C	164	CLA	C3C-C2C	6.04	1.48	1.35
12	L	167	CLA	C3C-C2C	6.04	1.48	1.35
12	L	164	CLA	C3C-C2C	6.03	1.48	1.35
12	M	160	CLA	C3C-C2C	6.02	1.48	1.35
12	D	160	CLA	C3C-C2C	6.01	1.48	1.35
12	K	177	CLA	C3C-C4C	4.34	1.53	1.43
12	L	158	CLA	C3C-C4C	4.33	1.53	1.43
12	D	166	CLA	C3C-C4C	4.33	1.53	1.43
12	M	162	CLA	C3C-C4C	4.32	1.53	1.43
12	C	158	CLA	C3C-C4C	4.32	1.53	1.43
12	B	177	CLA	C3C-C4C	4.31	1.53	1.43
12	J	176	CLA	C3C-C4C	4.31	1.53	1.43
12	M	157	CLA	C3C-C4C	4.31	1.53	1.43
12	D	157	CLA	C3C-C4C	4.31	1.53	1.43
12	J	175	CLA	C3C-C4C	4.31	1.53	1.43
12	A	175	CLA	C3C-C4C	4.30	1.53	1.43
12	C	162	CLA	C3C-C4C	4.30	1.53	1.43
12	M	166	CLA	C3C-C4C	4.30	1.53	1.43
12	D	162	CLA	C3C-C4C	4.30	1.53	1.43
12	D	158	CLA	C3C-C4C	4.30	1.53	1.43
12	C	159	CLA	C3C-C4C	4.30	1.53	1.43
12	L	159	CLA	C3C-C4C	4.29	1.53	1.43
12	A	179	CLA	C3C-C4C	4.29	1.53	1.43
12	C	165	CLA	C3C-C4C	4.29	1.53	1.43
12	J	179	CLA	C3C-C4C	4.29	1.53	1.43
12	C	157	CLA	C3C-C4C	4.28	1.53	1.43
12	M	158	CLA	C3C-C4C	4.28	1.53	1.43
12	L	164	CLA	C3C-C4C	4.28	1.53	1.43
12	M	156	CLA	C3C-C4C	4.28	1.53	1.43
12	C	167	CLA	C3C-C4C	4.28	1.53	1.43
12	A	176	CLA	C3C-C4C	4.28	1.53	1.43
12	D	165	CLA	C3C-C4C	4.28	1.53	1.43
12	C	168	CLA	C3C-C4C	4.27	1.53	1.43
12	M	163	CLA	C3C-C4C	4.27	1.53	1.43
12	L	165	CLA	C3C-C4C	4.27	1.53	1.43
12	D	163	CLA	C3C-C4C	4.27	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	160	CLA	C3C-C4C	4.27	1.53	1.43
12	D	156	CLA	C3C-C4C	4.27	1.53	1.43
12	C	164	CLA	C3C-C4C	4.27	1.53	1.43
12	L	162	CLA	C3C-C4C	4.27	1.53	1.43
12	B	179	CLA	C3C-C4C	4.27	1.53	1.43
12	K	179	CLA	C3C-C4C	4.27	1.53	1.43
12	G	313	CLA	C3C-C4C	4.26	1.53	1.43
12	M	165	CLA	C3C-C4C	4.26	1.53	1.43
12	D	159	CLA	C3C-C4C	4.26	1.53	1.43
12	C	161	CLA	C3C-C4C	4.26	1.53	1.43
12	M	164	CLA	C3C-C4C	4.26	1.53	1.43
12	D	167	CLA	C3C-C4C	4.26	1.53	1.43
12	D	168	CLA	C3C-C4C	4.26	1.53	1.43
12	L	168	CLA	C3C-C4C	4.26	1.53	1.43
12	L	157	CLA	C3C-C4C	4.25	1.53	1.43
12	M	159	CLA	C3C-C4C	4.25	1.53	1.43
12	C	166	CLA	C3C-C4C	4.25	1.53	1.43
12	L	163	CLA	C3C-C4C	4.25	1.53	1.43
12	L	160	CLA	C3C-C4C	4.25	1.53	1.43
12	L	166	CLA	C3C-C4C	4.25	1.53	1.43
12	M	168	CLA	C3C-C4C	4.25	1.53	1.43
12	M	167	CLA	C3C-C4C	4.25	1.53	1.43
12	D	164	CLA	C3C-C4C	4.25	1.53	1.43
12	P	313	CLA	C3C-C4C	4.25	1.53	1.43
12	L	161	CLA	C3C-C4C	4.25	1.53	1.43
12	D	161	CLA	C3C-C4C	4.25	1.53	1.43
12	C	163	CLA	C3C-C4C	4.25	1.53	1.43
12	C	160	CLA	C3C-C4C	4.24	1.53	1.43
12	L	167	CLA	C3C-C4C	4.24	1.53	1.43
12	D	160	CLA	C3C-C4C	4.24	1.53	1.43
12	J	177	CLA	C3C-C4C	4.24	1.53	1.43
12	A	177	CLA	C3C-C4C	4.22	1.53	1.43
12	M	161	CLA	C3C-C4C	4.21	1.53	1.43
12	L	160	CLA	C2C-C1C	4.00	1.52	1.43
12	A	179	CLA	C2C-C1C	3.99	1.52	1.43
12	L	165	CLA	C2C-C1C	3.99	1.52	1.43
12	C	165	CLA	C2C-C1C	3.98	1.52	1.43
12	J	179	CLA	C2C-C1C	3.98	1.52	1.43
12	M	167	CLA	C2C-C1C	3.98	1.52	1.43
12	L	168	CLA	C2C-C1C	3.98	1.52	1.43
12	C	163	CLA	C2C-C1C	3.98	1.52	1.43
12	K	179	CLA	C2C-C1C	3.98	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	160	CLA	C2C-C1C	3.97	1.52	1.43
12	D	162	CLA	C2C-C1C	3.97	1.52	1.43
12	C	168	CLA	C2C-C1C	3.97	1.52	1.43
12	J	175	CLA	C2C-C1C	3.97	1.52	1.43
12	A	176	CLA	C2C-C1C	3.97	1.52	1.43
12	L	167	CLA	C2C-C1C	3.96	1.52	1.43
12	D	167	CLA	C2C-C1C	3.96	1.52	1.43
12	D	168	CLA	C2C-C1C	3.96	1.52	1.43
12	A	175	CLA	C2C-C1C	3.96	1.52	1.43
12	D	165	CLA	C2C-C1C	3.96	1.52	1.43
12	L	164	CLA	C2C-C1C	3.96	1.52	1.43
12	B	179	CLA	C2C-C1C	3.96	1.52	1.43
12	C	162	CLA	C2C-C1C	3.96	1.52	1.43
12	L	162	CLA	C2C-C1C	3.96	1.52	1.43
12	L	161	CLA	C2C-C1C	3.95	1.52	1.43
12	M	164	CLA	C2C-C1C	3.95	1.52	1.43
12	L	163	CLA	C2C-C1C	3.95	1.52	1.43
12	C	159	CLA	C2C-C1C	3.95	1.52	1.43
12	C	158	CLA	C2C-C1C	3.95	1.52	1.43
12	M	166	CLA	C2C-C1C	3.95	1.52	1.43
12	C	167	CLA	C2C-C1C	3.94	1.52	1.43
12	D	166	CLA	C2C-C1C	3.94	1.52	1.43
12	C	164	CLA	C2C-C1C	3.94	1.52	1.43
12	M	165	CLA	C2C-C1C	3.94	1.52	1.43
12	C	161	CLA	C2C-C1C	3.94	1.52	1.43
12	L	159	CLA	C2C-C1C	3.94	1.52	1.43
12	M	160	CLA	C2C-C1C	3.93	1.52	1.43
12	A	177	CLA	C2C-C1C	3.93	1.52	1.43
12	L	158	CLA	C2C-C1C	3.93	1.52	1.43
12	J	176	CLA	C2C-C1C	3.93	1.52	1.43
12	M	162	CLA	C2C-C1C	3.93	1.52	1.43
12	M	159	CLA	C2C-C1C	3.93	1.52	1.43
12	C	166	CLA	C2C-C1C	3.93	1.52	1.43
12	M	168	CLA	C2C-C1C	3.93	1.52	1.43
12	D	158	CLA	C2C-C1C	3.92	1.52	1.43
12	D	157	CLA	C2C-C1C	3.92	1.52	1.43
12	J	177	CLA	C2C-C1C	3.92	1.52	1.43
12	D	164	CLA	C2C-C1C	3.92	1.52	1.43
12	M	158	CLA	C2C-C1C	3.92	1.52	1.43
12	M	161	CLA	C2C-C1C	3.92	1.52	1.43
12	L	166	CLA	C2C-C1C	3.92	1.52	1.43
12	D	161	CLA	C2C-C1C	3.91	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	157	CLA	C2C-C1C	3.91	1.52	1.43
12	M	156	CLA	C2C-C1C	3.91	1.52	1.43
12	D	163	CLA	C2C-C1C	3.91	1.52	1.43
12	D	156	CLA	C2C-C1C	3.91	1.52	1.43
12	D	160	CLA	C2C-C1C	3.91	1.52	1.43
12	M	163	CLA	C2C-C1C	3.91	1.52	1.43
12	P	313	CLA	C2C-C1C	3.90	1.52	1.43
12	D	159	CLA	C2C-C1C	3.90	1.52	1.43
12	C	157	CLA	C2C-C1C	3.90	1.52	1.43
12	G	313	CLA	C2C-C1C	3.90	1.52	1.43
12	B	177	CLA	C2C-C1C	3.90	1.52	1.43
12	L	157	CLA	C2C-C1C	3.89	1.52	1.43
12	K	177	CLA	C2C-C1C	3.87	1.52	1.43
12	L	157	CLA	C4B-NB	3.77	1.38	1.35
15	K	180	PLA	C6-N1	3.70	1.44	1.33
15	B	180	PLA	C6-N1	3.70	1.44	1.33
12	C	157	CLA	C4B-NB	3.68	1.38	1.35
12	M	167	CLA	C4B-NB	3.63	1.38	1.35
12	C	163	CLA	C4B-NB	3.61	1.38	1.35
12	L	167	CLA	C4B-NB	3.58	1.38	1.35
12	L	163	CLA	C4B-NB	3.57	1.38	1.35
12	D	167	CLA	C4B-NB	3.57	1.38	1.35
12	B	179	CLA	C4B-NB	3.55	1.38	1.35
12	M	166	CLA	C4B-NB	3.54	1.38	1.35
12	M	157	CLA	C4B-NB	3.54	1.38	1.35
12	G	313	CLA	C4B-NB	3.53	1.38	1.35
12	L	161	CLA	C4B-NB	3.53	1.38	1.35
12	D	166	CLA	C4B-NB	3.53	1.38	1.35
12	D	156	CLA	C4B-NB	3.52	1.38	1.35
12	K	179	CLA	C4B-NB	3.52	1.38	1.35
12	M	156	CLA	C4B-NB	3.51	1.38	1.35
12	D	161	CLA	C4B-NB	3.51	1.38	1.35
12	D	162	CLA	C4B-NB	3.51	1.38	1.35
12	D	159	CLA	C4B-NB	3.50	1.38	1.35
12	D	157	CLA	C4B-NB	3.50	1.38	1.35
12	M	158	CLA	C4B-NB	3.50	1.38	1.35
12	L	160	CLA	C4B-NB	3.50	1.38	1.35
15	B	180	PLA	C2-N1	3.49	1.44	1.33
12	P	313	CLA	C4B-NB	3.49	1.38	1.35
12	M	159	CLA	C4B-NB	3.49	1.38	1.35
12	C	166	CLA	C4B-NB	3.49	1.38	1.35
12	C	167	CLA	C4B-NB	3.49	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	161	CLA	C4B-NB	3.48	1.38	1.35
15	K	180	PLA	C2-N1	3.48	1.44	1.33
12	M	162	CLA	C4B-NB	3.48	1.38	1.35
12	M	165	CLA	C4B-NB	3.48	1.38	1.35
12	K	177	CLA	C4B-NB	3.47	1.38	1.35
12	L	166	CLA	C4B-NB	3.47	1.38	1.35
12	C	165	CLA	C4B-NB	3.46	1.38	1.35
12	M	163	CLA	C4B-NB	3.46	1.38	1.35
12	D	158	CLA	C4B-NB	3.46	1.38	1.35
12	L	165	CLA	C4B-NB	3.46	1.38	1.35
12	C	160	CLA	C4B-NB	3.46	1.38	1.35
12	D	163	CLA	C4B-NB	3.46	1.38	1.35
12	B	177	CLA	C4B-NB	3.46	1.38	1.35
12	A	177	CLA	C4B-NB	3.45	1.38	1.35
12	J	177	CLA	C4B-NB	3.45	1.38	1.35
12	C	159	CLA	C4B-NB	3.44	1.38	1.35
12	M	161	CLA	C4B-NB	3.44	1.38	1.35
12	C	158	CLA	C4B-NB	3.44	1.38	1.35
12	M	168	CLA	C4B-NB	3.44	1.38	1.35
12	D	168	CLA	C4B-NB	3.44	1.38	1.35
12	L	158	CLA	C4B-NB	3.43	1.38	1.35
12	D	164	CLA	C4B-NB	3.43	1.38	1.35
12	C	164	CLA	C4B-NB	3.43	1.38	1.35
12	A	179	CLA	C4B-NB	3.42	1.38	1.35
12	A	176	CLA	C4B-NB	3.42	1.38	1.35
12	D	165	CLA	C4B-NB	3.42	1.38	1.35
12	J	176	CLA	C4B-NB	3.41	1.38	1.35
12	C	168	CLA	C4B-NB	3.41	1.38	1.35
12	L	159	CLA	C4B-NB	3.39	1.38	1.35
12	M	164	CLA	C4B-NB	3.38	1.38	1.35
12	L	164	CLA	C4B-NB	3.38	1.38	1.35
12	L	168	CLA	C4B-NB	3.35	1.38	1.35
12	J	179	CLA	C4B-NB	3.35	1.38	1.35
12	C	162	CLA	C4B-NB	3.34	1.38	1.35
12	J	175	CLA	C4B-NB	3.34	1.38	1.35
12	A	175	CLA	C4B-NB	3.31	1.38	1.35
12	M	160	CLA	C4B-NB	3.30	1.38	1.35
12	L	162	CLA	C4B-NB	3.29	1.38	1.35
12	D	160	CLA	C4B-NB	3.26	1.38	1.35
15	B	180	PLA	C5-C6	2.93	1.46	1.37
15	K	180	PLA	C5-C6	2.92	1.46	1.37
15	B	180	PLA	C5-C4	2.70	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	180	PLA	C5-C4	2.70	1.45	1.38
12	K	179	CLA	C1B-NB	2.58	1.37	1.35
12	M	168	CLA	C1B-NB	2.57	1.37	1.35
12	D	158	CLA	C1B-NB	2.57	1.37	1.35
12	B	179	CLA	C1B-NB	2.57	1.37	1.35
12	D	162	CLA	C1B-NB	2.55	1.37	1.35
12	J	179	CLA	C1B-NB	2.54	1.37	1.35
12	M	158	CLA	C1B-NB	2.54	1.37	1.35
12	D	161	CLA	C1B-NB	2.53	1.37	1.35
12	A	177	CLA	C1B-NB	2.53	1.37	1.35
12	M	161	CLA	C1B-NB	2.53	1.37	1.35
12	J	177	CLA	C1B-NB	2.52	1.37	1.35
12	A	179	CLA	C1B-NB	2.52	1.37	1.35
12	C	162	CLA	C1B-NB	2.49	1.37	1.35
12	M	162	CLA	C1B-NB	2.49	1.37	1.35
12	L	162	CLA	C1B-NB	2.49	1.37	1.35
12	J	175	CLA	C1B-NB	2.49	1.37	1.35
12	C	160	CLA	C1B-NB	2.48	1.37	1.35
12	D	168	CLA	C1B-NB	2.48	1.37	1.35
12	L	160	CLA	C1B-NB	2.48	1.37	1.35
12	C	165	CLA	C1B-NB	2.47	1.37	1.35
12	M	157	CLA	C1B-NB	2.47	1.37	1.35
12	C	168	CLA	C1B-NB	2.47	1.37	1.35
12	D	157	CLA	C1B-NB	2.46	1.37	1.35
12	L	164	CLA	C1B-NB	2.45	1.37	1.35
12	M	159	CLA	C1B-NB	2.44	1.37	1.35
12	C	157	CLA	C1B-NB	2.44	1.37	1.35
12	D	163	CLA	C1B-NB	2.44	1.37	1.35
12	L	168	CLA	C1B-NB	2.44	1.37	1.35
12	D	164	CLA	C1B-NB	2.44	1.37	1.35
12	D	160	CLA	C1B-NB	2.44	1.37	1.35
12	A	176	CLA	C1B-NB	2.44	1.37	1.35
12	A	175	CLA	C1B-NB	2.43	1.37	1.35
12	L	157	CLA	C1B-NB	2.43	1.37	1.35
12	C	167	CLA	C1B-NB	2.43	1.37	1.35
12	M	156	CLA	C1B-NB	2.42	1.37	1.35
12	J	176	CLA	C1B-NB	2.42	1.37	1.35
12	L	165	CLA	C1B-NB	2.42	1.37	1.35
12	C	164	CLA	C1B-NB	2.41	1.37	1.35
12	M	160	CLA	C1B-NB	2.40	1.37	1.35
12	M	164	CLA	C1B-NB	2.40	1.37	1.35
12	D	156	CLA	C1B-NB	2.40	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	159	CLA	C1B-NB	2.40	1.37	1.35
12	L	166	CLA	C1B-NB	2.39	1.37	1.35
12	M	163	CLA	C1B-NB	2.39	1.37	1.35
12	D	166	CLA	C1B-NB	2.38	1.37	1.35
12	L	159	CLA	C1B-NB	2.38	1.37	1.35
12	D	167	CLA	C1B-NB	2.38	1.37	1.35
12	M	166	CLA	C1B-NB	2.37	1.37	1.35
12	L	158	CLA	C1B-NB	2.37	1.37	1.35
12	M	165	CLA	C1B-NB	2.37	1.37	1.35
12	L	167	CLA	C1B-NB	2.37	1.37	1.35
12	C	158	CLA	C1B-NB	2.36	1.37	1.35
12	C	159	CLA	C1B-NB	2.36	1.37	1.35
12	D	165	CLA	C1B-NB	2.35	1.37	1.35
12	C	163	CLA	C1B-NB	2.34	1.37	1.35
12	K	177	CLA	C1B-NB	2.34	1.37	1.35
12	G	313	CLA	C1B-NB	2.34	1.37	1.35
12	C	166	CLA	C1B-NB	2.34	1.37	1.35
12	B	177	CLA	C1B-NB	2.33	1.37	1.35
12	C	161	CLA	C1B-NB	2.33	1.37	1.35
15	B	180	PLA	C4-C3	2.32	1.44	1.38
12	L	163	CLA	C1B-NB	2.31	1.37	1.35
12	M	167	CLA	C1B-NB	2.31	1.37	1.35
15	K	180	PLA	C4-C3	2.30	1.44	1.38
12	L	161	CLA	C1B-NB	2.28	1.37	1.35
12	P	313	CLA	C1B-NB	2.22	1.37	1.35
15	K	180	PLA	C3-C2	2.00	1.43	1.37
15	B	180	PLA	C3-C2	2.00	1.43	1.37

All (568) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	R	88	HEM	C3D-C4D-ND	10.20	116.33	108.27
16	I	88	HEM	C3D-C4D-ND	10.17	116.30	108.27
16	F	31	HEM	C3D-C4D-ND	10.07	116.23	108.27
16	O	58	HEM	C3D-C4D-ND	10.04	116.20	108.27
12	J	177	CLA	C2D-C3D-C4D	-8.84	98.68	106.30
12	A	177	CLA	C2D-C3D-C4D	-8.80	98.72	106.30
12	L	160	CLA	C2D-C3D-C4D	-8.78	98.73	106.30
12	K	179	CLA	C2D-C3D-C4D	-8.77	98.75	106.30
12	M	160	CLA	C2D-C3D-C4D	-8.76	98.75	106.30
12	M	166	CLA	C2D-C3D-C4D	-8.76	98.75	106.30
12	A	179	CLA	C2D-C3D-C4D	-8.76	98.75	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	160	CLA	C2D-C3D-C4D	-8.76	98.76	106.30
12	D	158	CLA	C2D-C3D-C4D	-8.75	98.76	106.30
12	D	160	CLA	C2D-C3D-C4D	-8.74	98.77	106.30
12	L	159	CLA	C2D-C3D-C4D	-8.74	98.77	106.30
12	C	158	CLA	C2D-C3D-C4D	-8.74	98.77	106.30
12	D	166	CLA	C2D-C3D-C4D	-8.74	98.77	106.30
12	A	175	CLA	C2D-C3D-C4D	-8.74	98.77	106.30
12	C	159	CLA	C2D-C3D-C4D	-8.73	98.78	106.30
12	B	179	CLA	C2D-C3D-C4D	-8.73	98.78	106.30
12	L	158	CLA	C2D-C3D-C4D	-8.73	98.78	106.30
12	M	161	CLA	C2D-C3D-C4D	-8.73	98.78	106.30
16	I	88	HEM	C2D-C3D-C4D	-8.73	98.78	106.30
12	C	168	CLA	C2D-C3D-C4D	-8.72	98.79	106.30
12	J	176	CLA	C2D-C3D-C4D	-8.72	98.79	106.30
12	C	165	CLA	C2D-C3D-C4D	-8.72	98.79	106.30
16	R	88	HEM	C2D-C3D-C4D	-8.72	98.79	106.30
12	J	179	CLA	C2D-C3D-C4D	-8.71	98.79	106.30
12	J	175	CLA	C2D-C3D-C4D	-8.71	98.80	106.30
12	A	176	CLA	C2D-C3D-C4D	-8.71	98.80	106.30
12	D	161	CLA	C2D-C3D-C4D	-8.71	98.80	106.30
12	M	158	CLA	C2D-C3D-C4D	-8.71	98.80	106.30
12	L	165	CLA	C2D-C3D-C4D	-8.71	98.80	106.30
12	D	163	CLA	C2D-C3D-C4D	-8.70	98.80	106.30
12	L	162	CLA	C2D-C3D-C4D	-8.70	98.81	106.30
12	M	168	CLA	C2D-C3D-C4D	-8.70	98.81	106.30
12	L	168	CLA	C2D-C3D-C4D	-8.70	98.81	106.30
12	M	167	CLA	C2D-C3D-C4D	-8.70	98.81	106.30
12	L	161	CLA	C2D-C3D-C4D	-8.69	98.81	106.30
12	L	166	CLA	C2D-C3D-C4D	-8.69	98.81	106.30
12	M	163	CLA	C2D-C3D-C4D	-8.69	98.82	106.30
12	C	161	CLA	C2D-C3D-C4D	-8.69	98.82	106.30
12	C	167	CLA	C2D-C3D-C4D	-8.68	98.82	106.30
12	D	164	CLA	C2D-C3D-C4D	-8.68	98.82	106.30
12	C	162	CLA	C2D-C3D-C4D	-8.68	98.82	106.30
12	L	167	CLA	C2D-C3D-C4D	-8.68	98.82	106.30
12	M	164	CLA	C2D-C3D-C4D	-8.68	98.82	106.30
12	D	162	CLA	C2D-C3D-C4D	-8.68	98.82	106.30
12	C	166	CLA	C2D-C3D-C4D	-8.68	98.82	106.30
12	D	165	CLA	C2D-C3D-C4D	-8.68	98.82	106.30
12	C	164	CLA	C2D-C3D-C4D	-8.68	98.82	106.30
12	L	163	CLA	C2D-C3D-C4D	-8.67	98.83	106.30
12	G	313	CLA	C2D-C3D-C4D	-8.67	98.83	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	168	CLA	C2D-C3D-C4D	-8.67	98.83	106.30
12	M	162	CLA	C2D-C3D-C4D	-8.67	98.83	106.30
12	D	167	CLA	C2D-C3D-C4D	-8.67	98.83	106.30
12	C	157	CLA	C2D-C3D-C4D	-8.67	98.83	106.30
12	P	313	CLA	C2D-C3D-C4D	-8.67	98.84	106.30
12	L	164	CLA	C2D-C3D-C4D	-8.67	98.84	106.30
12	M	165	CLA	C2D-C3D-C4D	-8.66	98.84	106.30
12	K	177	CLA	C2D-C3D-C4D	-8.66	98.85	106.30
12	C	163	CLA	C2D-C3D-C4D	-8.65	98.85	106.30
12	D	157	CLA	C2D-C3D-C4D	-8.65	98.85	106.30
12	M	157	CLA	C2D-C3D-C4D	-8.65	98.85	106.30
12	B	177	CLA	C2D-C3D-C4D	-8.65	98.85	106.30
12	M	156	CLA	C2D-C3D-C4D	-8.64	98.85	106.30
12	L	157	CLA	C2D-C3D-C4D	-8.64	98.86	106.30
16	F	31	HEM	C2D-C3D-C4D	-8.62	98.87	106.30
12	D	156	CLA	C2D-C3D-C4D	-8.62	98.88	106.30
12	D	159	CLA	C2D-C3D-C4D	-8.61	98.88	106.30
12	M	159	CLA	C2D-C3D-C4D	-8.61	98.88	106.30
16	O	58	HEM	C2D-C3D-C4D	-8.58	98.91	106.30
12	M	160	CLA	C3D-C4D-ND	7.17	116.38	110.14
12	P	313	CLA	C3D-C4D-ND	7.17	116.37	110.14
12	D	164	CLA	C3D-C4D-ND	7.17	116.37	110.14
12	J	175	CLA	C3D-C4D-ND	7.16	116.37	110.14
12	M	158	CLA	C3D-C4D-ND	7.16	116.36	110.14
12	D	158	CLA	C3D-C4D-ND	7.16	116.36	110.14
12	J	177	CLA	C3D-C4D-ND	7.15	116.36	110.14
12	M	164	CLA	C3D-C4D-ND	7.15	116.36	110.14
12	L	158	CLA	C3D-C4D-ND	7.15	116.35	110.14
12	A	179	CLA	C3D-C4D-ND	7.14	116.35	110.14
12	A	176	CLA	C3D-C4D-ND	7.14	116.35	110.14
12	A	175	CLA	C3D-C4D-ND	7.14	116.34	110.14
12	L	160	CLA	C3D-C4D-ND	7.13	116.34	110.14
12	C	159	CLA	C3D-C4D-ND	7.13	116.34	110.14
12	D	160	CLA	C3D-C4D-ND	7.13	116.34	110.14
12	C	160	CLA	C3D-C4D-ND	7.13	116.34	110.14
12	M	166	CLA	C3D-C4D-ND	7.12	116.33	110.14
12	A	177	CLA	C3D-C4D-ND	7.12	116.33	110.14
12	C	158	CLA	C3D-C4D-ND	7.12	116.33	110.14
12	J	176	CLA	C3D-C4D-ND	7.12	116.33	110.14
12	M	161	CLA	C3D-C4D-ND	7.12	116.33	110.14
12	L	159	CLA	C3D-C4D-ND	7.12	116.33	110.14
12	G	313	CLA	C3D-C4D-ND	7.12	116.33	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	168	CLA	C3D-C4D-ND	7.11	116.32	110.14
12	C	165	CLA	C3D-C4D-ND	7.11	116.32	110.14
12	L	163	CLA	C3D-C4D-ND	7.10	116.31	110.14
12	L	165	CLA	C3D-C4D-ND	7.10	116.31	110.14
12	M	167	CLA	C3D-C4D-ND	7.10	116.31	110.14
12	C	168	CLA	C3D-C4D-ND	7.10	116.31	110.14
12	D	161	CLA	C3D-C4D-ND	7.09	116.31	110.14
12	M	157	CLA	C3D-C4D-ND	7.09	116.31	110.14
12	D	168	CLA	C3D-C4D-ND	7.09	116.31	110.14
12	C	157	CLA	C3D-C4D-ND	7.09	116.30	110.14
12	B	179	CLA	C3D-C4D-ND	7.09	116.30	110.14
12	D	167	CLA	C3D-C4D-ND	7.09	116.30	110.14
12	J	179	CLA	C3D-C4D-ND	7.08	116.30	110.14
12	M	156	CLA	C3D-C4D-ND	7.08	116.30	110.14
12	D	166	CLA	C3D-C4D-ND	7.08	116.29	110.14
12	L	166	CLA	C3D-C4D-ND	7.08	116.29	110.14
12	C	163	CLA	C3D-C4D-ND	7.08	116.29	110.14
12	L	162	CLA	C3D-C4D-ND	7.08	116.29	110.14
12	L	161	CLA	C3D-C4D-ND	7.07	116.28	110.14
12	C	166	CLA	C3D-C4D-ND	7.07	116.28	110.14
12	D	156	CLA	C3D-C4D-ND	7.06	116.28	110.14
12	L	168	CLA	C3D-C4D-ND	7.06	116.28	110.14
12	C	164	CLA	C3D-C4D-ND	7.06	116.28	110.14
12	D	163	CLA	C3D-C4D-ND	7.05	116.27	110.14
12	C	162	CLA	C3D-C4D-ND	7.05	116.27	110.14
12	K	179	CLA	C3D-C4D-ND	7.05	116.27	110.14
12	D	162	CLA	C3D-C4D-ND	7.05	116.27	110.14
12	L	157	CLA	C3D-C4D-ND	7.05	116.27	110.14
12	M	163	CLA	C3D-C4D-ND	7.05	116.27	110.14
12	D	157	CLA	C3D-C4D-ND	7.05	116.26	110.14
12	C	161	CLA	C3D-C4D-ND	7.04	116.26	110.14
12	D	165	CLA	C3D-C4D-ND	7.02	116.24	110.14
12	L	164	CLA	C3D-C4D-ND	7.02	116.24	110.14
12	L	167	CLA	C3D-C4D-ND	7.01	116.23	110.14
12	M	162	CLA	C3D-C4D-ND	7.01	116.23	110.14
12	C	167	CLA	C3D-C4D-ND	6.99	116.22	110.14
12	B	177	CLA	C3D-C4D-ND	6.99	116.22	110.14
12	M	165	CLA	C3D-C4D-ND	6.99	116.21	110.14
12	M	159	CLA	C3D-C4D-ND	6.97	116.20	110.14
12	D	159	CLA	C3D-C4D-ND	6.97	116.20	110.14
12	K	177	CLA	C3D-C4D-ND	6.96	116.19	110.14
12	L	159	CLA	C3D-C2D-C1D	6.01	111.48	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	160	CLA	C3D-C2D-C1D	6.00	111.47	106.30
16	R	88	HEM	C3D-C2D-C1D	5.98	111.41	106.29
12	J	177	CLA	C3D-C2D-C1D	5.98	111.45	106.30
12	C	159	CLA	C3D-C2D-C1D	5.98	111.45	106.30
16	I	88	HEM	C3D-C2D-C1D	5.97	111.40	106.29
12	C	160	CLA	C3D-C2D-C1D	5.96	111.44	106.30
12	K	179	CLA	C3D-C2D-C1D	5.96	111.43	106.30
12	A	175	CLA	C3D-C2D-C1D	5.95	111.42	106.30
12	A	177	CLA	C3D-C2D-C1D	5.94	111.42	106.30
12	J	175	CLA	C3D-C2D-C1D	5.94	111.42	106.30
12	D	166	CLA	C3D-C2D-C1D	5.93	111.42	106.30
12	M	156	CLA	C3D-C2D-C1D	5.92	111.41	106.30
12	C	158	CLA	C3D-C2D-C1D	5.92	111.40	106.30
12	C	168	CLA	C3D-C2D-C1D	5.91	111.39	106.30
12	L	168	CLA	C3D-C2D-C1D	5.91	111.39	106.30
12	B	179	CLA	C3D-C2D-C1D	5.90	111.39	106.30
12	M	162	CLA	C3D-C2D-C1D	5.90	111.38	106.30
12	C	161	CLA	C3D-C2D-C1D	5.89	111.38	106.30
12	L	158	CLA	C3D-C2D-C1D	5.89	111.38	106.30
12	M	166	CLA	C3D-C2D-C1D	5.89	111.37	106.30
12	D	158	CLA	C3D-C2D-C1D	5.88	111.37	106.30
12	D	162	CLA	C3D-C2D-C1D	5.88	111.37	106.30
12	D	163	CLA	C3D-C2D-C1D	5.88	111.37	106.30
12	C	165	CLA	C3D-C2D-C1D	5.88	111.37	106.30
12	M	161	CLA	C3D-C2D-C1D	5.88	111.37	106.30
12	M	160	CLA	C3D-C2D-C1D	5.88	111.37	106.30
12	M	165	CLA	C3D-C2D-C1D	5.88	111.37	106.30
12	J	176	CLA	C3D-C2D-C1D	5.88	111.37	106.30
12	D	156	CLA	C3D-C2D-C1D	5.87	111.36	106.30
12	D	160	CLA	C3D-C2D-C1D	5.87	111.36	106.30
12	L	161	CLA	C3D-C2D-C1D	5.87	111.36	106.30
12	M	163	CLA	C3D-C2D-C1D	5.87	111.36	106.30
12	D	159	CLA	C3D-C2D-C1D	5.87	111.36	106.30
12	C	157	CLA	C3D-C2D-C1D	5.87	111.36	106.30
12	D	161	CLA	C3D-C2D-C1D	5.86	111.35	106.30
12	L	162	CLA	C3D-C2D-C1D	5.86	111.35	106.30
12	M	159	CLA	C3D-C2D-C1D	5.86	111.35	106.30
12	M	164	CLA	C3D-C2D-C1D	5.86	111.35	106.30
12	A	176	CLA	C3D-C2D-C1D	5.86	111.35	106.30
12	D	165	CLA	C3D-C2D-C1D	5.86	111.35	106.30
12	C	162	CLA	C3D-C2D-C1D	5.86	111.35	106.30
12	A	179	CLA	C3D-C2D-C1D	5.86	111.35	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	157	CLA	C3D-C2D-C1D	5.86	111.35	106.30
12	L	166	CLA	C3D-C2D-C1D	5.85	111.35	106.30
12	C	166	CLA	C3D-C2D-C1D	5.85	111.34	106.30
12	M	157	CLA	C3D-C2D-C1D	5.85	111.34	106.30
12	M	167	CLA	C3D-C2D-C1D	5.85	111.34	106.30
12	L	164	CLA	C3D-C2D-C1D	5.85	111.34	106.30
12	L	165	CLA	C3D-C2D-C1D	5.85	111.34	106.30
12	D	164	CLA	C3D-C2D-C1D	5.85	111.34	106.30
12	C	163	CLA	C3D-C2D-C1D	5.84	111.34	106.30
12	M	168	CLA	C3D-C2D-C1D	5.84	111.34	106.30
12	D	167	CLA	C3D-C2D-C1D	5.84	111.34	106.30
12	B	177	CLA	C3D-C2D-C1D	5.84	111.33	106.30
12	L	157	CLA	C3D-C2D-C1D	5.84	111.33	106.30
12	K	177	CLA	C3D-C2D-C1D	5.84	111.33	106.30
12	J	179	CLA	C3D-C2D-C1D	5.84	111.33	106.30
12	L	167	CLA	C3D-C2D-C1D	5.84	111.33	106.30
12	G	313	CLA	C3D-C2D-C1D	5.83	111.33	106.30
12	M	158	CLA	C3D-C2D-C1D	5.83	111.33	106.30
12	P	313	CLA	C3D-C2D-C1D	5.83	111.33	106.30
12	C	167	CLA	C3D-C2D-C1D	5.83	111.33	106.30
12	D	168	CLA	C3D-C2D-C1D	5.83	111.33	106.30
12	C	164	CLA	C3D-C2D-C1D	5.83	111.33	106.30
16	F	31	HEM	C3D-C2D-C1D	5.81	111.26	106.29
12	L	163	CLA	C3D-C2D-C1D	5.80	111.30	106.30
16	O	58	HEM	C3D-C2D-C1D	5.77	111.23	106.29
16	F	31	HEM	C2C-C1C-NC	4.67	111.96	108.27
16	O	58	HEM	C2C-C1C-NC	4.66	111.95	108.27
16	I	88	HEM	C2C-C1C-NC	4.63	111.92	108.27
16	R	88	HEM	C2C-C1C-NC	4.63	111.92	108.27
12	J	177	CLA	C4A-NA-C1A	4.17	108.58	106.71
12	J	179	CLA	C4A-NA-C1A	4.15	108.57	106.71
12	L	160	CLA	C4A-NA-C1A	4.14	108.57	106.71
12	A	179	CLA	C4A-NA-C1A	4.13	108.56	106.71
12	C	160	CLA	C4A-NA-C1A	4.12	108.56	106.71
12	A	177	CLA	C4A-NA-C1A	4.12	108.56	106.71
12	G	313	CLA	C4A-NA-C1A	4.11	108.56	106.71
12	D	158	CLA	C4A-NA-C1A	4.10	108.55	106.71
12	M	159	CLA	C4A-NA-C1A	4.10	108.55	106.71
12	M	161	CLA	C4A-NA-C1A	4.10	108.55	106.71
12	L	165	CLA	C4A-NA-C1A	4.09	108.54	106.71
12	J	175	CLA	C4A-NA-C1A	4.09	108.54	106.71
12	C	162	CLA	C4A-NA-C1A	4.08	108.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	158	CLA	C4A-NA-C1A	4.08	108.54	106.71
12	J	176	CLA	C4A-NA-C1A	4.08	108.54	106.71
12	A	175	CLA	C4A-NA-C1A	4.07	108.54	106.71
12	L	159	CLA	C4A-NA-C1A	4.07	108.54	106.71
12	C	167	CLA	C4A-NA-C1A	4.07	108.54	106.71
12	L	157	CLA	C4A-NA-C1A	4.07	108.54	106.71
12	A	176	CLA	C4A-NA-C1A	4.07	108.54	106.71
12	M	165	CLA	C4A-NA-C1A	4.06	108.53	106.71
12	L	162	CLA	C4A-NA-C1A	4.06	108.53	106.71
12	L	168	CLA	C4A-NA-C1A	4.06	108.53	106.71
12	C	159	CLA	C4A-NA-C1A	4.06	108.53	106.71
12	D	159	CLA	C4A-NA-C1A	4.05	108.53	106.71
12	M	157	CLA	C4A-NA-C1A	4.04	108.52	106.71
12	D	165	CLA	C4A-NA-C1A	4.04	108.52	106.71
12	D	157	CLA	C4A-NA-C1A	4.03	108.52	106.71
12	P	313	CLA	C4A-NA-C1A	4.03	108.52	106.71
12	M	158	CLA	C4A-NA-C1A	4.02	108.52	106.71
12	C	168	CLA	C4A-NA-C1A	4.02	108.51	106.71
12	L	167	CLA	C4A-NA-C1A	4.02	108.51	106.71
12	C	163	CLA	C4A-NA-C1A	4.01	108.51	106.71
12	B	179	CLA	C4A-NA-C1A	4.00	108.50	106.71
12	C	158	CLA	C4A-NA-C1A	3.99	108.50	106.71
12	L	163	CLA	C4A-NA-C1A	3.99	108.50	106.71
12	D	161	CLA	C4A-NA-C1A	3.99	108.50	106.71
12	M	156	CLA	C4A-NA-C1A	3.99	108.50	106.71
12	D	168	CLA	C4A-NA-C1A	3.98	108.50	106.71
12	K	177	CLA	C4A-NA-C1A	3.98	108.50	106.71
12	B	177	CLA	C4A-NA-C1A	3.98	108.50	106.71
12	C	161	CLA	C4A-NA-C1A	3.96	108.49	106.71
12	D	164	CLA	C4A-NA-C1A	3.96	108.48	106.71
12	D	156	CLA	C4A-NA-C1A	3.95	108.48	106.71
12	C	165	CLA	C4A-NA-C1A	3.95	108.48	106.71
12	C	157	CLA	C4A-NA-C1A	3.95	108.48	106.71
12	D	166	CLA	C4A-NA-C1A	3.94	108.48	106.71
12	K	179	CLA	C4A-NA-C1A	3.93	108.47	106.71
12	M	164	CLA	C4A-NA-C1A	3.92	108.47	106.71
12	M	162	CLA	C4A-NA-C1A	3.91	108.46	106.71
12	L	166	CLA	C4A-NA-C1A	3.90	108.46	106.71
16	F	31	HEM	C2B-C1B-NB	3.90	111.35	108.27
12	M	168	CLA	C4A-NA-C1A	3.90	108.46	106.71
12	D	167	CLA	C4A-NA-C1A	3.89	108.46	106.71
12	L	164	CLA	C4A-NA-C1A	3.89	108.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	166	CLA	C4A-NA-C1A	3.89	108.45	106.71
12	M	167	CLA	C4A-NA-C1A	3.89	108.45	106.71
12	D	160	CLA	C4A-NA-C1A	3.88	108.45	106.71
16	I	88	HEM	C2B-C1B-NB	3.88	111.33	108.27
16	R	88	HEM	C2B-C1B-NB	3.87	111.33	108.27
16	O	58	HEM	C2B-C1B-NB	3.87	111.33	108.27
12	M	167	CLA	C1C-NC-C4C	3.87	108.44	106.71
12	A	176	CLA	C1C-NC-C4C	3.86	108.44	106.71
12	M	166	CLA	C4A-NA-C1A	3.86	108.44	106.71
12	D	162	CLA	C4A-NA-C1A	3.86	108.44	106.71
12	L	161	CLA	C4A-NA-C1A	3.85	108.44	106.71
12	M	162	CLA	C1C-NC-C4C	3.85	108.44	106.71
12	C	164	CLA	C4A-NA-C1A	3.85	108.44	106.71
12	M	160	CLA	C4A-NA-C1A	3.84	108.43	106.71
12	L	161	CLA	C1C-NC-C4C	3.84	108.43	106.71
12	M	163	CLA	C4A-NA-C1A	3.83	108.43	106.71
12	J	176	CLA	C1C-NC-C4C	3.80	108.42	106.71
12	C	162	CLA	C1C-NC-C4C	3.80	108.41	106.71
12	D	163	CLA	C4A-NA-C1A	3.79	108.41	106.71
12	D	162	CLA	C1C-NC-C4C	3.78	108.41	106.71
12	K	177	CLA	C1C-NC-C4C	3.78	108.41	106.71
12	C	158	CLA	C1C-NC-C4C	3.78	108.41	106.71
12	M	166	CLA	C1C-NC-C4C	3.78	108.40	106.71
12	L	162	CLA	C1C-NC-C4C	3.75	108.39	106.71
12	B	177	CLA	C1C-NC-C4C	3.75	108.39	106.71
12	C	168	CLA	C1C-NC-C4C	3.74	108.39	106.71
12	D	166	CLA	C1C-NC-C4C	3.74	108.39	106.71
12	L	158	CLA	C1C-NC-C4C	3.73	108.39	106.71
12	C	161	CLA	C1C-NC-C4C	3.73	108.38	106.71
12	C	157	CLA	C1C-NC-C4C	3.73	108.38	106.71
12	J	175	CLA	C1C-NC-C4C	3.73	108.38	106.71
12	D	167	CLA	C1C-NC-C4C	3.73	108.38	106.71
12	L	157	CLA	C1C-NC-C4C	3.72	108.38	106.71
12	C	163	CLA	C1C-NC-C4C	3.71	108.37	106.71
12	A	175	CLA	C1C-NC-C4C	3.70	108.37	106.71
12	L	168	CLA	C1C-NC-C4C	3.69	108.36	106.71
12	L	163	CLA	C1C-NC-C4C	3.69	108.36	106.71
12	D	163	CLA	C1C-NC-C4C	3.69	108.36	106.71
16	R	88	HEM	C3C-C4C-NC	3.68	111.18	108.27
12	M	163	CLA	C1C-NC-C4C	3.66	108.35	106.71
12	D	164	CLA	C1C-NC-C4C	3.65	108.35	106.71
12	C	166	CLA	C1C-NC-C4C	3.65	108.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	160	CLA	C1C-NC-C4C	3.63	108.34	106.71
12	K	179	CLA	C1C-NC-C4C	3.63	108.34	106.71
12	B	179	CLA	C1C-NC-C4C	3.63	108.34	106.71
12	L	164	CLA	C1C-NC-C4C	3.63	108.34	106.71
12	M	164	CLA	C1C-NC-C4C	3.63	108.34	106.71
16	I	88	HEM	C3C-C4C-NC	3.63	111.13	108.27
16	F	31	HEM	C3C-C4C-NC	3.62	111.13	108.27
16	O	58	HEM	C3C-C4C-NC	3.61	111.13	108.27
12	L	166	CLA	C1C-NC-C4C	3.61	108.33	106.71
12	D	168	CLA	C1C-NC-C4C	3.61	108.33	106.71
12	C	165	CLA	C1C-NC-C4C	3.60	108.33	106.71
12	D	160	CLA	C1C-NC-C4C	3.60	108.32	106.71
12	D	165	CLA	C1C-NC-C4C	3.59	108.32	106.71
12	L	159	CLA	C1C-NC-C4C	3.58	108.32	106.71
12	C	164	CLA	C1C-NC-C4C	3.58	108.32	106.71
12	G	313	CLA	C1C-NC-C4C	3.58	108.31	106.71
12	P	313	CLA	C1C-NC-C4C	3.57	108.31	106.71
12	M	156	CLA	C1C-NC-C4C	3.57	108.31	106.71
12	D	156	CLA	C1C-NC-C4C	3.57	108.31	106.71
12	C	159	CLA	C1C-NC-C4C	3.57	108.31	106.71
12	M	168	CLA	C1C-NC-C4C	3.57	108.31	106.71
12	M	165	CLA	C1C-NC-C4C	3.57	108.31	106.71
12	C	167	CLA	C1C-NC-C4C	3.55	108.30	106.71
12	A	177	CLA	C1C-NC-C4C	3.55	108.30	106.71
12	D	158	CLA	C1C-NC-C4C	3.55	108.30	106.71
12	M	158	CLA	C1C-NC-C4C	3.54	108.30	106.71
12	L	167	CLA	C1C-NC-C4C	3.53	108.29	106.71
12	L	165	CLA	C1C-NC-C4C	3.53	108.29	106.71
12	D	157	CLA	C1C-NC-C4C	3.52	108.29	106.71
12	M	159	CLA	C1C-NC-C4C	3.52	108.29	106.71
12	C	160	CLA	C1C-NC-C4C	3.51	108.28	106.71
12	A	179	CLA	C1C-NC-C4C	3.51	108.28	106.71
12	J	179	CLA	C1C-NC-C4C	3.51	108.28	106.71
12	J	177	CLA	C1C-NC-C4C	3.49	108.28	106.71
12	L	160	CLA	C1C-NC-C4C	3.48	108.27	106.71
12	D	159	CLA	C1C-NC-C4C	3.47	108.27	106.71
16	F	31	HEM	C4C-NC-C1C	3.47	108.40	105.79
12	M	157	CLA	C1C-NC-C4C	3.46	108.26	106.71
16	I	88	HEM	C4C-NC-C1C	3.45	108.39	105.79
16	O	58	HEM	C4C-NC-C1C	3.45	108.39	105.79
12	M	161	CLA	C1C-NC-C4C	3.43	108.25	106.71
12	D	161	CLA	C1C-NC-C4C	3.43	108.25	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	R	88	HEM	C4C-NC-C1C	3.42	108.36	105.79
12	M	158	CLA	C2A-C1A-CHA	2.79	127.40	122.63
12	C	166	CLA	C2A-C1A-CHA	2.79	127.40	122.63
12	L	162	CLA	C2A-C1A-CHA	2.79	127.39	122.63
12	D	162	CLA	C2A-C1A-CHA	2.79	127.39	122.63
12	M	156	CLA	C2A-C1A-CHA	2.79	127.39	122.63
12	M	167	CLA	C2A-C1A-CHA	2.79	127.39	122.63
12	C	162	CLA	C2A-C1A-CHA	2.79	127.39	122.63
12	D	158	CLA	C2A-C1A-CHA	2.79	127.39	122.63
12	M	160	CLA	C2A-C1A-CHA	2.79	127.39	122.63
12	D	160	CLA	C2A-C1A-CHA	2.79	127.39	122.63
12	M	162	CLA	C2A-C1A-CHA	2.79	127.39	122.63
12	C	157	CLA	C2A-C1A-CHA	2.78	127.38	122.63
12	D	167	CLA	C2A-C1A-CHA	2.78	127.38	122.63
12	L	157	CLA	C2A-C1A-CHA	2.78	127.38	122.63
12	D	156	CLA	C2A-C1A-CHA	2.78	127.38	122.63
12	L	166	CLA	C2A-C1A-CHA	2.78	127.37	122.63
12	L	159	CLA	C2A-C1A-CHA	2.78	127.37	122.63
12	M	157	CLA	C2A-C1A-CHA	2.77	127.37	122.63
12	P	313	CLA	C2A-C1A-CHA	2.77	127.36	122.63
12	D	157	CLA	C2A-C1A-CHA	2.77	127.36	122.63
12	D	166	CLA	C2A-C1A-CHA	2.77	127.36	122.63
12	C	158	CLA	C2A-C1A-CHA	2.76	127.35	122.63
12	M	163	CLA	C2A-C1A-CHA	2.76	127.34	122.63
12	J	177	CLA	C2A-C1A-CHA	2.76	127.34	122.63
12	G	313	CLA	C2A-C1A-CHA	2.76	127.34	122.63
12	L	158	CLA	C2A-C1A-CHA	2.76	127.34	122.63
12	L	160	CLA	C2A-C1A-CHA	2.76	127.33	122.63
12	L	164	CLA	C2A-C1A-CHA	2.76	127.33	122.63
12	A	177	CLA	C2A-C1A-CHA	2.76	127.33	122.63
12	C	167	CLA	C2A-C1A-CHA	2.75	127.33	122.63
12	M	166	CLA	C2A-C1A-CHA	2.75	127.33	122.63
12	C	160	CLA	C2A-C1A-CHA	2.75	127.33	122.63
12	C	165	CLA	C2A-C1A-CHA	2.75	127.32	122.63
12	D	163	CLA	C2A-C1A-CHA	2.75	127.32	122.63
12	D	159	CLA	C2A-C1A-CHA	2.75	127.32	122.63
12	K	177	CLA	C2A-C1A-CHA	2.75	127.32	122.63
12	C	159	CLA	C2A-C1A-CHA	2.74	127.31	122.63
12	L	167	CLA	C2A-C1A-CHA	2.74	127.31	122.63
12	D	161	CLA	C2A-C1A-CHA	2.74	127.31	122.63
12	C	164	CLA	C2A-C1A-CHA	2.74	127.31	122.63
12	C	168	CLA	C2A-C1A-CHA	2.74	127.31	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	163	CLA	C2A-C1A-CHA	2.74	127.31	122.63
12	D	164	CLA	C2A-C1A-CHA	2.74	127.30	122.63
12	B	179	CLA	C2A-C1A-CHA	2.74	127.30	122.63
12	D	168	CLA	C2A-C1A-CHA	2.74	127.30	122.63
12	L	165	CLA	C2A-C1A-CHA	2.74	127.30	122.63
12	B	177	CLA	C2A-C1A-CHA	2.73	127.30	122.63
12	M	159	CLA	C2A-C1A-CHA	2.73	127.30	122.63
12	M	168	CLA	C2A-C1A-CHA	2.73	127.30	122.63
12	A	175	CLA	C2A-C1A-CHA	2.73	127.30	122.63
12	D	165	CLA	C2A-C1A-CHA	2.73	127.30	122.63
12	L	163	CLA	C2A-C1A-CHA	2.73	127.30	122.63
12	A	179	CLA	C2A-C1A-CHA	2.73	127.29	122.63
12	M	161	CLA	C2A-C1A-CHA	2.73	127.29	122.63
12	M	164	CLA	C2A-C1A-CHA	2.73	127.29	122.63
12	L	168	CLA	C2A-C1A-CHA	2.72	127.28	122.63
12	A	176	CLA	C2A-C1A-CHA	2.72	127.28	122.63
12	J	179	CLA	C2A-C1A-CHA	2.72	127.27	122.63
12	M	165	CLA	C2A-C1A-CHA	2.72	127.27	122.63
12	K	179	CLA	C2A-C1A-CHA	2.71	127.26	122.63
12	J	175	CLA	C2A-C1A-CHA	2.71	127.25	122.63
12	J	176	CLA	C2A-C1A-CHA	2.70	127.23	122.63
12	C	161	CLA	C2A-C1A-CHA	2.70	127.23	122.63
12	L	161	CLA	C2A-C1A-CHA	2.69	127.23	122.63
13	A	178	PHO	CHA-C1A-NA	-2.69	121.79	125.36
13	J	178	PHO	CHA-C1A-NA	-2.67	121.82	125.36
13	B	178	PHO	CHA-C1A-NA	-2.67	121.82	125.36
13	K	178	PHO	CHA-C1A-NA	-2.65	121.84	125.36
12	J	179	CLA	C3C-C2C-C1C	-2.65	104.04	107.21
12	A	179	CLA	C3C-C2C-C1C	-2.65	104.04	107.21
12	M	163	CLA	C3C-C2C-C1C	-2.64	104.05	107.21
12	D	163	CLA	C3C-C2C-C1C	-2.61	104.08	107.21
12	J	177	CLA	C3C-C2C-C1C	-2.61	104.08	107.21
12	C	168	CLA	C3C-C2C-C1C	-2.61	104.08	107.21
12	D	168	CLA	C3C-C2C-C1C	-2.61	104.09	107.21
12	L	165	CLA	C3C-C2C-C1C	-2.61	104.09	107.21
12	L	168	CLA	C3C-C2C-C1C	-2.61	104.09	107.21
12	K	179	CLA	C3C-C2C-C1C	-2.60	104.09	107.21
12	D	157	CLA	C3C-C2C-C1C	-2.60	104.09	107.21
12	D	162	CLA	C3C-C2C-C1C	-2.60	104.10	107.21
12	D	167	CLA	C3C-C2C-C1C	-2.60	104.10	107.21
12	M	164	CLA	C3C-C2C-C1C	-2.60	104.10	107.21
12	M	167	CLA	C3C-C2C-C1C	-2.60	104.10	107.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	168	CLA	C3C-C2C-C1C	-2.60	104.10	107.21
12	D	166	CLA	C3C-C2C-C1C	-2.60	104.10	107.21
12	M	162	CLA	C3C-C2C-C1C	-2.59	104.10	107.21
12	A	177	CLA	C3C-C2C-C1C	-2.59	104.11	107.21
12	L	166	CLA	C3C-C2C-C1C	-2.59	104.11	107.21
12	L	159	CLA	C3C-C2C-C1C	-2.59	104.11	107.21
12	B	179	CLA	C3C-C2C-C1C	-2.59	104.11	107.21
13	B	178	PHO	C3C-C2C-C1C	-2.58	104.08	106.30
12	D	164	CLA	C3C-C2C-C1C	-2.58	104.12	107.21
12	M	166	CLA	C3C-C2C-C1C	-2.58	104.12	107.21
12	M	157	CLA	C3C-C2C-C1C	-2.58	104.12	107.21
12	C	165	CLA	C3C-C2C-C1C	-2.58	104.12	107.21
12	C	159	CLA	C3C-C2C-C1C	-2.58	104.12	107.21
12	D	161	CLA	C3C-C2C-C1C	-2.58	104.12	107.21
12	C	158	CLA	C3C-C2C-C1C	-2.57	104.13	107.21
12	D	165	CLA	C3C-C2C-C1C	-2.57	104.13	107.21
12	M	161	CLA	C3C-C2C-C1C	-2.57	104.13	107.21
12	C	166	CLA	C3C-C2C-C1C	-2.57	104.13	107.21
12	D	158	CLA	C3C-C2C-C1C	-2.57	104.13	107.21
12	C	157	CLA	C3C-C2C-C1C	-2.57	104.14	107.21
12	M	159	CLA	C3C-C2C-C1C	-2.57	104.14	107.21
12	D	159	CLA	C3C-C2C-C1C	-2.57	104.14	107.21
12	D	156	CLA	C3C-C2C-C1C	-2.56	104.14	107.21
12	C	160	CLA	C3C-C2C-C1C	-2.56	104.14	107.21
12	M	165	CLA	C3C-C2C-C1C	-2.56	104.14	107.21
12	L	162	CLA	C3C-C2C-C1C	-2.56	104.14	107.21
12	L	163	CLA	C3C-C2C-C1C	-2.56	104.14	107.21
16	F	31	HEM	C3C-C2C-C1C	-2.56	104.10	106.30
12	C	161	CLA	C3C-C2C-C1C	-2.56	104.15	107.21
12	C	163	CLA	C3C-C2C-C1C	-2.56	104.15	107.21
12	G	313	CLA	C3C-C2C-C1C	-2.56	104.15	107.21
13	K	178	PHO	C3C-C2C-C1C	-2.56	104.10	106.30
12	P	313	CLA	C3C-C2C-C1C	-2.56	104.15	107.21
12	M	158	CLA	C3C-C2C-C1C	-2.56	104.15	107.21
12	L	157	CLA	C3C-C2C-C1C	-2.55	104.15	107.21
12	L	167	CLA	C3C-C2C-C1C	-2.55	104.15	107.21
12	L	160	CLA	C3C-C2C-C1C	-2.55	104.15	107.21
12	M	156	CLA	C3C-C2C-C1C	-2.55	104.16	107.21
12	B	177	CLA	C3C-C2C-C1C	-2.55	104.16	107.21
12	A	176	CLA	C3C-C2C-C1C	-2.54	104.16	107.21
12	C	162	CLA	C3C-C2C-C1C	-2.54	104.16	107.21
12	D	160	CLA	C3C-C2C-C1C	-2.54	104.17	107.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	R	88	HEM	C3C-C2C-C1C	-2.54	104.11	106.30
12	C	167	CLA	C3C-C2C-C1C	-2.54	104.17	107.21
12	C	164	CLA	C3C-C2C-C1C	-2.54	104.17	107.21
12	L	161	CLA	C3C-C2C-C1C	-2.54	104.17	107.21
16	O	58	HEM	C3C-C2C-C1C	-2.54	104.12	106.30
12	L	158	CLA	C3C-C2C-C1C	-2.53	104.17	107.21
12	M	160	CLA	C3C-C2C-C1C	-2.53	104.18	107.21
12	J	176	CLA	C3C-C2C-C1C	-2.52	104.19	107.21
16	I	88	HEM	C3C-C2C-C1C	-2.52	104.13	106.30
12	L	164	CLA	C3C-C2C-C1C	-2.52	104.19	107.21
12	K	177	CLA	C3C-C2C-C1C	-2.52	104.19	107.21
12	A	175	CLA	C3C-C2C-C1C	-2.51	104.21	107.21
12	J	175	CLA	C3C-C2C-C1C	-2.50	104.22	107.21
13	J	178	PHO	C3C-C2C-C1C	-2.50	104.15	106.30
13	A	178	PHO	C3C-C2C-C1C	-2.46	104.18	106.30
12	A	175	CLA	C2C-C3C-C4C	-2.46	104.27	107.21
12	J	175	CLA	C2C-C3C-C4C	-2.45	104.28	107.21
12	L	163	CLA	C2C-C3C-C4C	-2.44	104.29	107.21
12	J	176	CLA	C2C-C3C-C4C	-2.40	104.33	107.21
12	C	163	CLA	C2C-C3C-C4C	-2.40	104.34	107.21
12	J	177	CLA	C2C-C3C-C4C	-2.39	104.35	107.21
12	A	177	CLA	C2C-C3C-C4C	-2.39	104.35	107.21
12	K	177	CLA	C2C-C3C-C4C	-2.38	104.36	107.21
12	C	165	CLA	C2C-C3C-C4C	-2.38	104.36	107.21
12	D	164	CLA	C2C-C3C-C4C	-2.37	104.38	107.21
12	L	165	CLA	C2C-C3C-C4C	-2.37	104.38	107.21
12	D	161	CLA	C2C-C3C-C4C	-2.36	104.38	107.21
12	D	159	CLA	C2C-C3C-C4C	-2.36	104.38	107.21
12	M	157	CLA	C2C-C3C-C4C	-2.36	104.38	107.21
12	P	313	CLA	C2C-C3C-C4C	-2.36	104.38	107.21
12	C	167	CLA	C2C-C3C-C4C	-2.36	104.38	107.21
12	L	164	CLA	C2C-C3C-C4C	-2.36	104.39	107.21
12	M	162	CLA	C2C-C3C-C4C	-2.36	104.39	107.21
12	M	163	CLA	C2C-C3C-C4C	-2.36	104.39	107.21
12	G	313	CLA	C2C-C3C-C4C	-2.36	104.39	107.21
12	M	161	CLA	C2C-C3C-C4C	-2.36	104.39	107.21
12	B	177	CLA	C2C-C3C-C4C	-2.36	104.39	107.21
12	L	157	CLA	C2C-C3C-C4C	-2.36	104.39	107.21
12	A	176	CLA	C2C-C3C-C4C	-2.35	104.39	107.21
12	M	164	CLA	C2C-C3C-C4C	-2.35	104.39	107.21
12	M	156	CLA	C2C-C3C-C4C	-2.35	104.39	107.21
12	M	159	CLA	C2C-C3C-C4C	-2.35	104.40	107.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	157	CLA	C2C-C3C-C4C	-2.35	104.40	107.21
12	L	167	CLA	C2C-C3C-C4C	-2.35	104.40	107.21
12	C	159	CLA	C2C-C3C-C4C	-2.34	104.40	107.21
12	C	166	CLA	C2C-C3C-C4C	-2.34	104.41	107.21
12	C	164	CLA	C2C-C3C-C4C	-2.34	104.41	107.21
12	D	163	CLA	C2C-C3C-C4C	-2.34	104.41	107.21
12	L	160	CLA	C2C-C3C-C4C	-2.34	104.41	107.21
12	D	158	CLA	C2C-C3C-C4C	-2.34	104.41	107.21
12	M	158	CLA	C2C-C3C-C4C	-2.34	104.41	107.21
12	C	157	CLA	C2C-C3C-C4C	-2.34	104.41	107.21
12	L	159	CLA	C2C-C3C-C4C	-2.34	104.41	107.21
12	M	165	CLA	C2C-C3C-C4C	-2.34	104.41	107.21
12	C	162	CLA	C2C-C3C-C4C	-2.34	104.41	107.21
12	D	156	CLA	C2C-C3C-C4C	-2.34	104.41	107.21
12	D	162	CLA	C2C-C3C-C4C	-2.34	104.41	107.21
12	C	161	CLA	C2C-C3C-C4C	-2.33	104.42	107.21
12	L	162	CLA	C2C-C3C-C4C	-2.33	104.42	107.21
12	L	166	CLA	C2C-C3C-C4C	-2.33	104.42	107.21
12	C	160	CLA	C2C-C3C-C4C	-2.33	104.42	107.21
12	D	165	CLA	C2C-C3C-C4C	-2.33	104.42	107.21
12	L	158	CLA	C2C-C3C-C4C	-2.33	104.42	107.21
12	C	168	CLA	C2C-C3C-C4C	-2.32	104.43	107.21
12	L	168	CLA	C2C-C3C-C4C	-2.32	104.43	107.21
12	L	161	CLA	C2C-C3C-C4C	-2.32	104.44	107.21
12	C	158	CLA	C2C-C3C-C4C	-2.31	104.44	107.21
12	D	166	CLA	C2C-C3C-C4C	-2.31	104.44	107.21
12	B	179	CLA	C2C-C3C-C4C	-2.31	104.44	107.21
12	M	160	CLA	C2C-C3C-C4C	-2.31	104.45	107.21
12	M	166	CLA	C2C-C3C-C4C	-2.31	104.45	107.21
12	D	168	CLA	C2C-C3C-C4C	-2.30	104.45	107.21
12	D	167	CLA	C2C-C3C-C4C	-2.30	104.45	107.21
12	M	168	CLA	C2C-C3C-C4C	-2.30	104.46	107.21
12	A	179	CLA	C2C-C3C-C4C	-2.30	104.46	107.21
12	K	179	CLA	C2C-C3C-C4C	-2.29	104.46	107.21
12	D	160	CLA	C2C-C3C-C4C	-2.29	104.47	107.21
12	J	179	CLA	C2C-C3C-C4C	-2.29	104.47	107.21
12	M	167	CLA	C2C-C3C-C4C	-2.28	104.48	107.21
16	F	31	HEM	C3A-C2A-C1A	-2.24	104.37	106.29
13	A	178	PHO	C2C-C3C-C4C	-2.24	104.38	106.30
16	R	88	HEM	C3A-C2A-C1A	-2.23	104.38	106.29
13	J	178	PHO	C2C-C3C-C4C	-2.22	104.39	106.30
16	I	88	HEM	C3A-C2A-C1A	-2.22	104.39	106.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	O	58	HEM	C3A-C2A-C1A	-2.21	104.39	106.29
16	F	31	HEM	C2C-C3C-C4C	-2.20	104.41	106.30
16	O	58	HEM	C2C-C3C-C4C	-2.19	104.41	106.30
16	R	88	HEM	C2C-C3C-C4C	-2.19	104.41	106.30
16	I	88	HEM	C2C-C3C-C4C	-2.19	104.42	106.30
13	B	178	PHO	C2C-C3C-C4C	-2.16	104.44	106.30
13	K	178	PHO	C2C-C3C-C4C	-2.15	104.45	106.30
16	F	31	HEM	C4D-CHA-C1A	-2.06	126.47	129.64
16	I	88	HEM	C4D-CHA-C1A	-2.05	126.48	129.64
16	R	88	HEM	C4D-CHA-C1A	-2.03	126.51	129.64
16	O	58	HEM	C4D-CHA-C1A	-2.03	126.52	129.64

All (192) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	L	160	CLA	NC
12	L	160	CLA	ND
12	L	160	CLA	NA
12	D	161	CLA	NC
12	D	161	CLA	ND
12	D	161	CLA	NA
12	J	177	CLA	NC
12	J	177	CLA	ND
12	J	177	CLA	NA
12	D	164	CLA	NC
12	D	164	CLA	ND
12	D	164	CLA	NA
12	C	168	CLA	NC
12	C	168	CLA	ND
12	C	168	CLA	NA
12	C	157	CLA	NC
12	C	157	CLA	ND
12	C	157	CLA	NA
12	L	164	CLA	NC
12	L	164	CLA	ND
12	L	164	CLA	NA
12	B	179	CLA	NC
12	B	179	CLA	ND
12	B	179	CLA	NA
12	M	166	CLA	NC
12	M	166	CLA	ND
12	M	166	CLA	NA

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Mol	Chain	Res	Type	Atom
12	M	157	CLA	NC
12	M	157	CLA	ND
12	M	157	CLA	NA
12	D	162	CLA	NC
12	D	162	CLA	ND
12	D	162	CLA	NA
12	P	313	CLA	NC
12	P	313	CLA	ND
12	P	313	CLA	NA
12	M	161	CLA	NC
12	M	161	CLA	ND
12	M	161	CLA	NA
12	D	166	CLA	NC
12	D	166	CLA	ND
12	D	166	CLA	NA
12	M	156	CLA	NC
12	M	156	CLA	ND
12	M	156	CLA	NA
12	D	156	CLA	NC
12	D	156	CLA	ND
12	D	156	CLA	NA
12	C	163	CLA	NC
12	C	163	CLA	ND
12	C	163	CLA	NA
12	B	177	CLA	NC
12	B	177	CLA	ND
12	B	177	CLA	NA
12	M	162	CLA	NC
12	M	162	CLA	ND
12	M	162	CLA	NA
12	L	166	CLA	NC
12	L	166	CLA	ND
12	L	166	CLA	NA
12	C	158	CLA	NC
12	C	158	CLA	ND
12	C	158	CLA	NA
12	L	168	CLA	NC
12	L	168	CLA	ND
12	L	168	CLA	NA
12	J	176	CLA	NC
12	J	176	CLA	ND
12	J	176	CLA	NA

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Mol	Chain	Res	Type	Atom
12	J	179	CLA	NC
12	J	179	CLA	ND
12	J	179	CLA	NA
12	M	168	CLA	NC
12	M	168	CLA	ND
12	M	168	CLA	NA
12	A	177	CLA	NC
12	A	177	CLA	ND
12	A	177	CLA	NA
12	D	168	CLA	NC
12	D	168	CLA	ND
12	D	168	CLA	NA
12	D	159	CLA	NC
12	D	159	CLA	ND
12	D	159	CLA	NA
12	D	158	CLA	NC
12	D	158	CLA	ND
12	D	158	CLA	NA
12	D	160	CLA	NC
12	D	160	CLA	ND
12	D	160	CLA	NA
12	G	313	CLA	NC
12	G	313	CLA	ND
12	G	313	CLA	NA
12	L	165	CLA	NC
12	L	165	CLA	ND
12	L	165	CLA	NA
12	C	164	CLA	NC
12	C	164	CLA	ND
12	C	164	CLA	NA
12	L	157	CLA	NC
12	L	157	CLA	ND
12	L	157	CLA	NA
12	A	175	CLA	NC
12	A	175	CLA	ND
12	A	175	CLA	NA
12	M	158	CLA	NC
12	M	158	CLA	ND
12	M	158	CLA	NA
12	C	166	CLA	NC
12	C	166	CLA	ND
12	C	166	CLA	NA

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Mol	Chain	Res	Type	Atom
12	M	160	CLA	NC
12	M	160	CLA	ND
12	M	160	CLA	NA
12	M	165	CLA	NC
12	M	165	CLA	ND
12	M	165	CLA	NA
12	C	160	CLA	NC
12	C	160	CLA	ND
12	C	160	CLA	NA
12	L	159	CLA	NC
12	L	159	CLA	ND
12	L	159	CLA	NA
12	L	161	CLA	NC
12	L	161	CLA	ND
12	L	161	CLA	NA
12	L	167	CLA	NC
12	L	167	CLA	ND
12	L	167	CLA	NA
12	A	176	CLA	NC
12	A	176	CLA	ND
12	A	176	CLA	NA
12	K	179	CLA	NC
12	K	179	CLA	ND
12	K	179	CLA	NA
12	D	163	CLA	NC
12	D	163	CLA	ND
12	D	163	CLA	NA
12	M	163	CLA	NC
12	M	163	CLA	ND
12	M	163	CLA	NA
12	C	162	CLA	NC
12	C	162	CLA	ND
12	C	162	CLA	NA
12	K	177	CLA	NC
12	K	177	CLA	ND
12	K	177	CLA	NA
12	D	165	CLA	NC
12	D	165	CLA	ND
12	D	165	CLA	NA
12	J	175	CLA	NC
12	J	175	CLA	ND
12	J	175	CLA	NA

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Mol	Chain	Res	Type	Atom
12	C	165	CLA	NC
12	C	165	CLA	ND
12	C	165	CLA	NA
12	C	161	CLA	NC
12	C	161	CLA	ND
12	C	161	CLA	NA
12	C	159	CLA	NC
12	C	159	CLA	ND
12	C	159	CLA	NA
12	D	157	CLA	NC
12	D	157	CLA	ND
12	D	157	CLA	NA
12	A	179	CLA	NC
12	A	179	CLA	ND
12	A	179	CLA	NA
12	L	162	CLA	NC
12	L	162	CLA	ND
12	L	162	CLA	NA
12	M	159	CLA	NC
12	M	159	CLA	ND
12	M	159	CLA	NA
12	M	164	CLA	NC
12	M	164	CLA	ND
12	M	164	CLA	NA
12	L	163	CLA	NC
12	L	163	CLA	ND
12	L	163	CLA	NA
12	L	158	CLA	NC
12	L	158	CLA	ND
12	L	158	CLA	NA
12	M	167	CLA	NC
12	M	167	CLA	ND
12	M	167	CLA	NA
12	C	167	CLA	NC
12	C	167	CLA	ND
12	C	167	CLA	NA
12	D	167	CLA	NC
12	D	167	CLA	ND
12	D	167	CLA	NA

There are no torsion outliers.

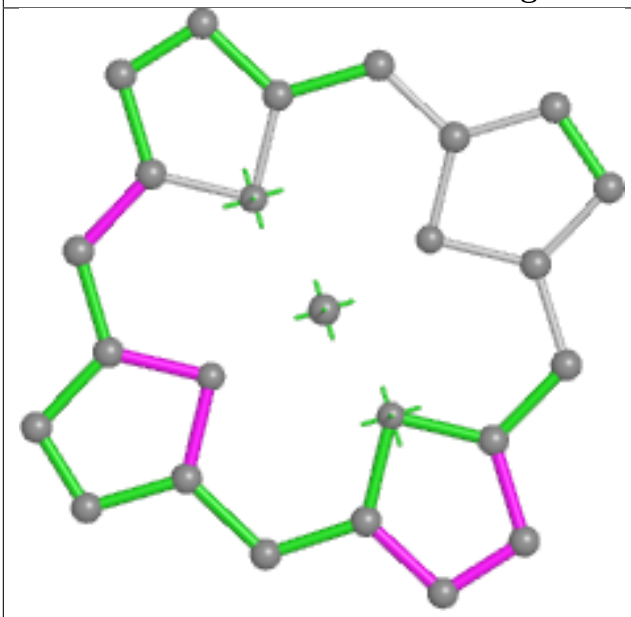
There are no ring outliers.

6 monomers are involved in 16 short contacts:

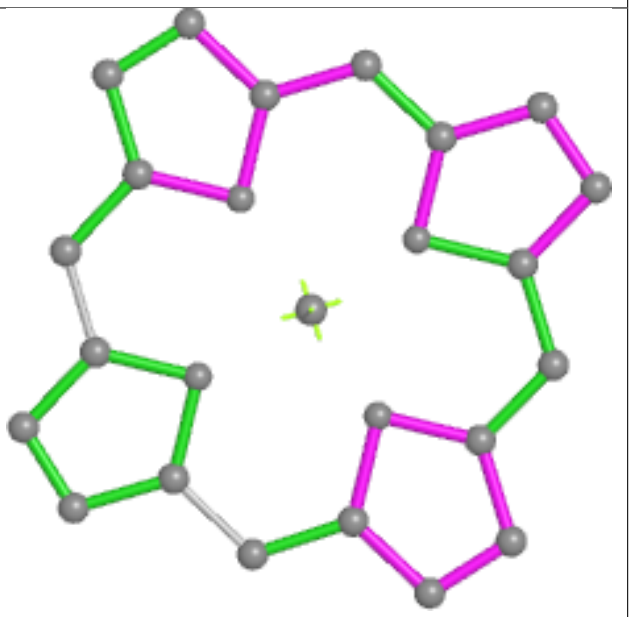
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	162	CLA	6	0
12	M	159	CLA	6	0
12	L	166	CLA	2	0
12	C	166	CLA	2	0
12	D	162	CLA	6	0
12	D	159	CLA	6	0

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

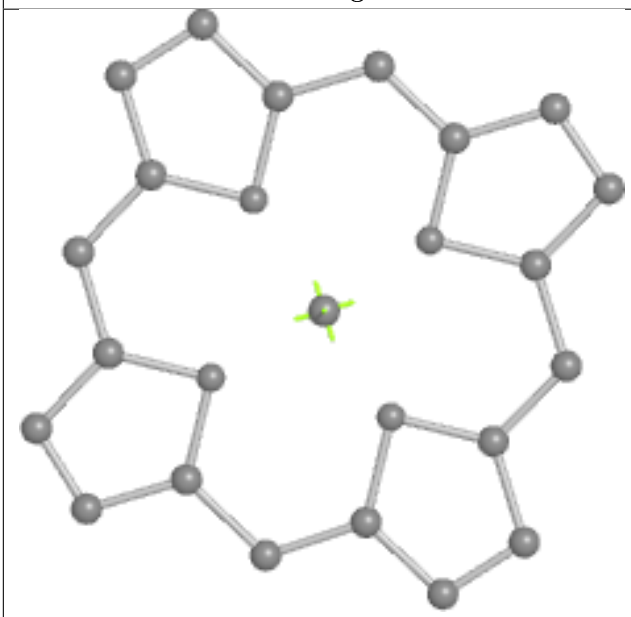
Ligand CLA M 163



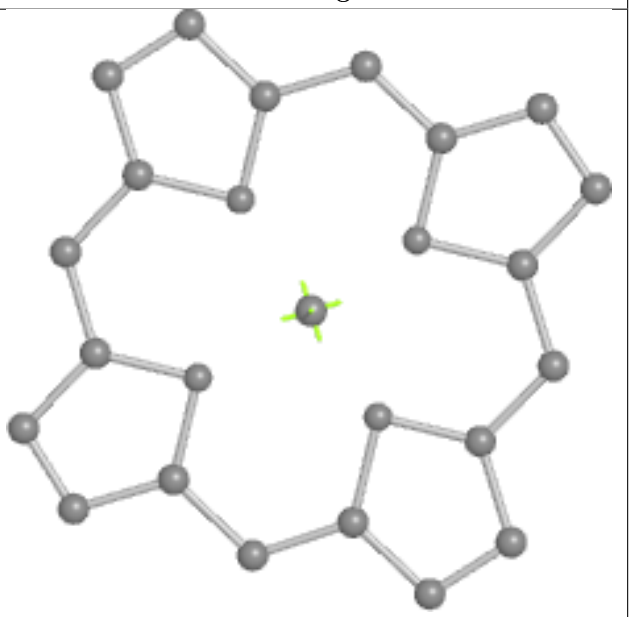
Bond lengths



Bond angles

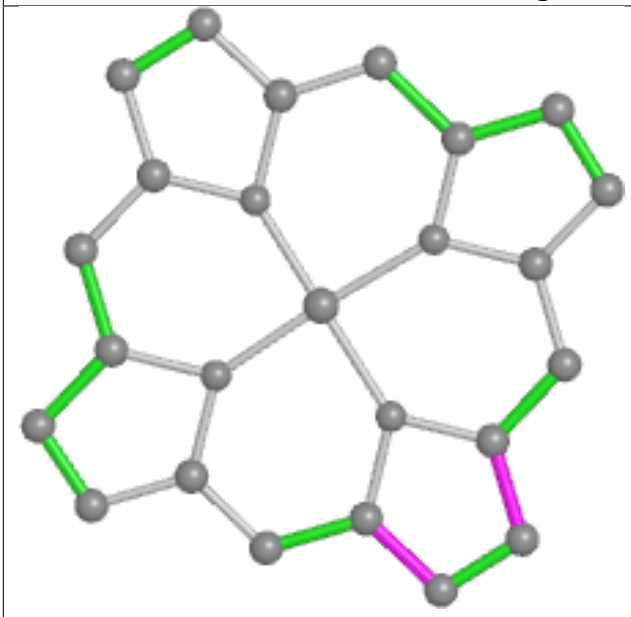


Torsions

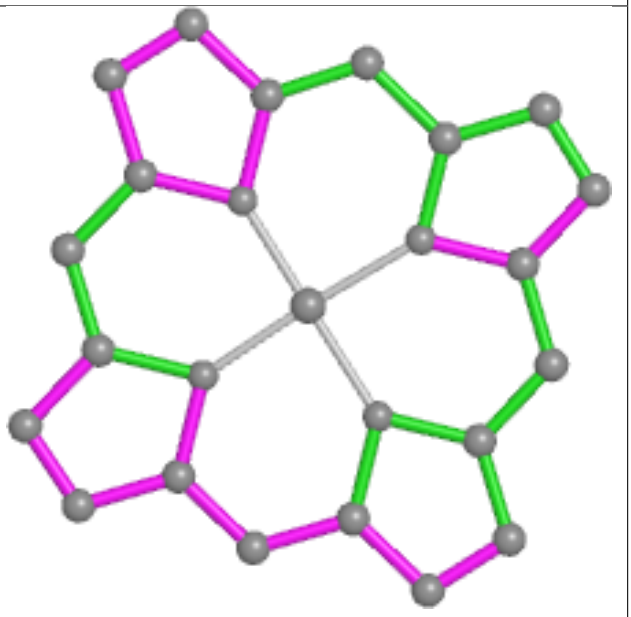


Rings

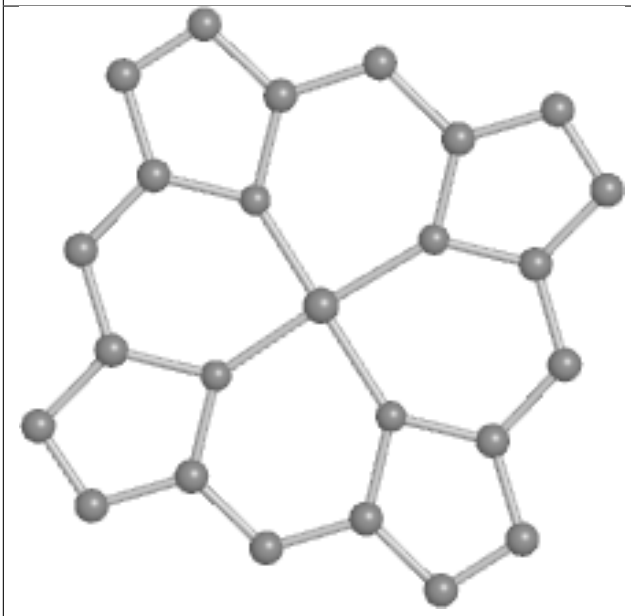
Ligand HEM I 88



Bond lengths



Bond angles



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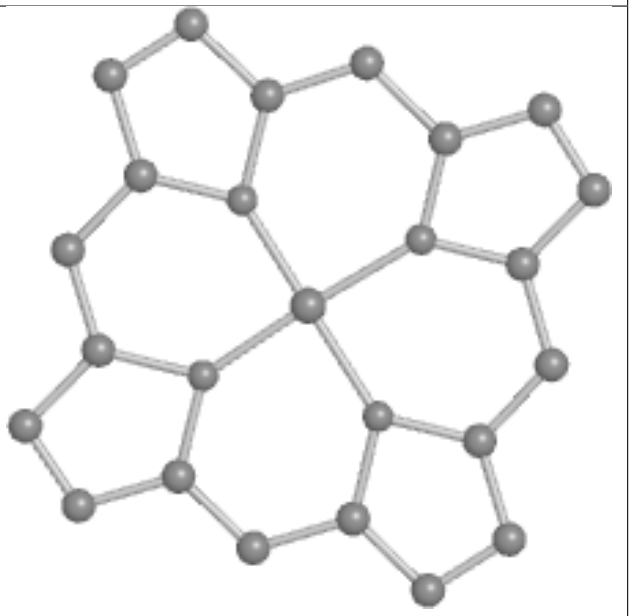
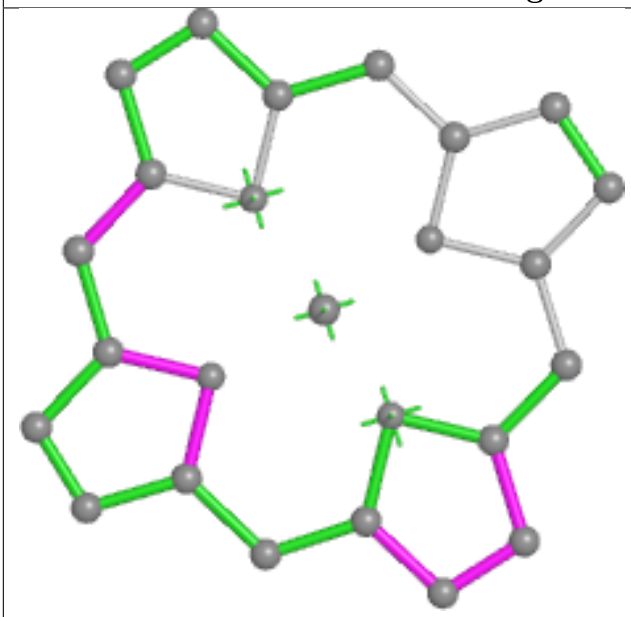
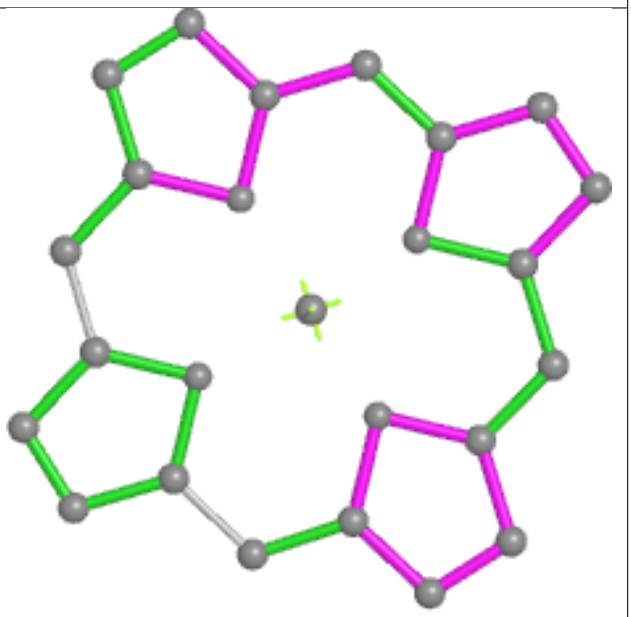


Rings

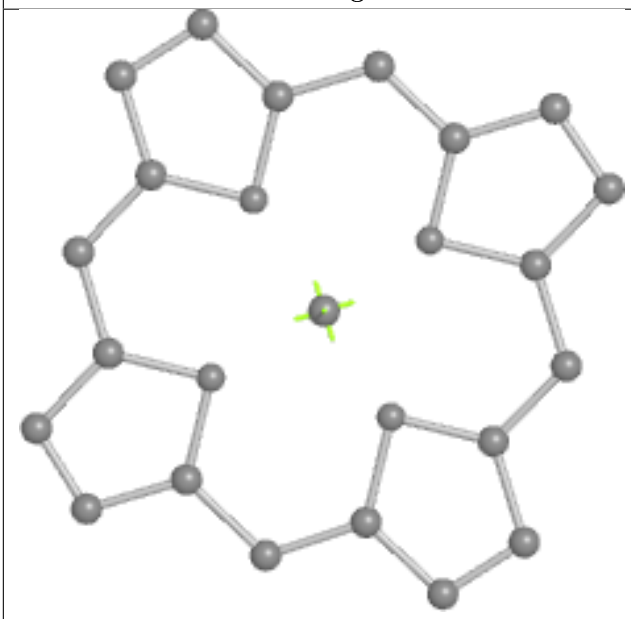
Ligand CLA L 160



Bond lengths



Bond angles



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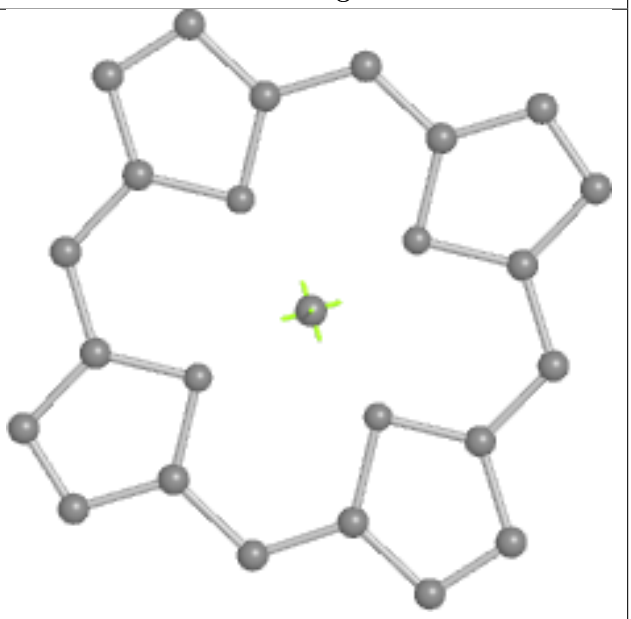
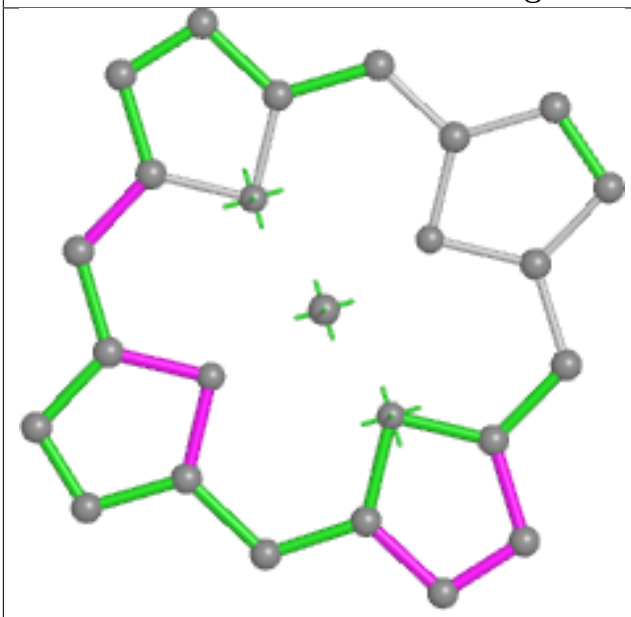
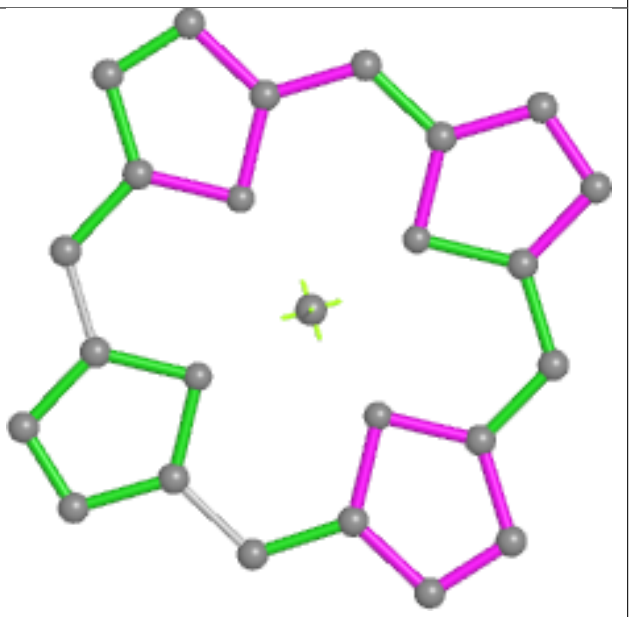


Rings

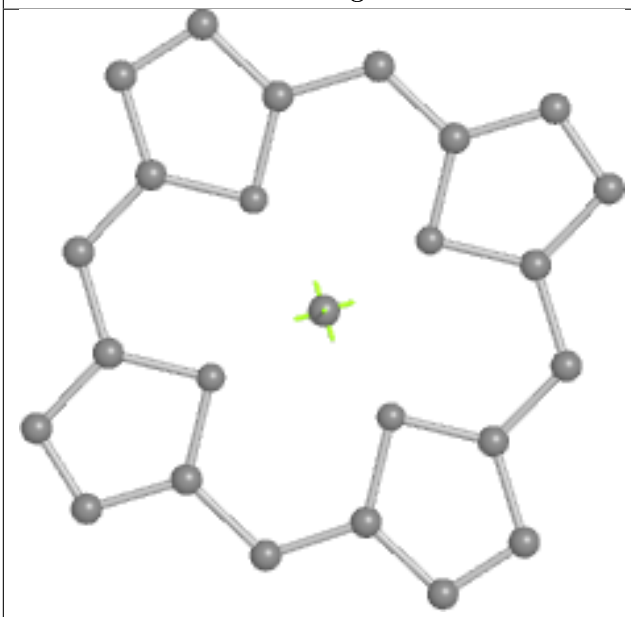
Ligand CLA C 162



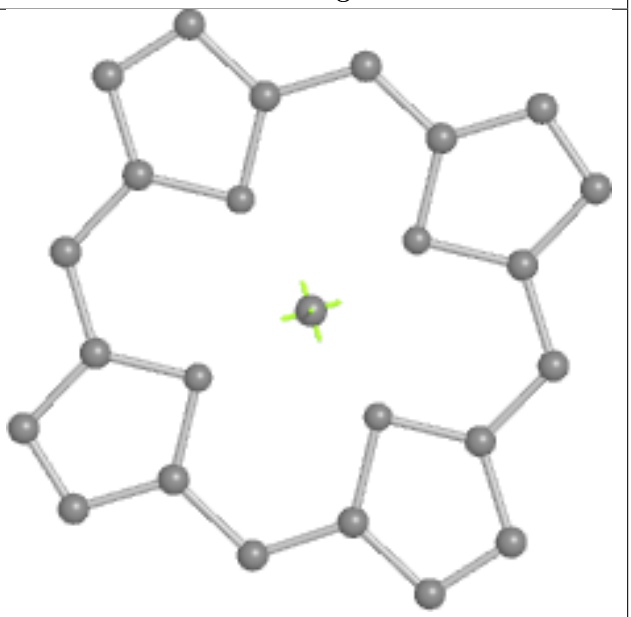
Bond lengths



Bond angles

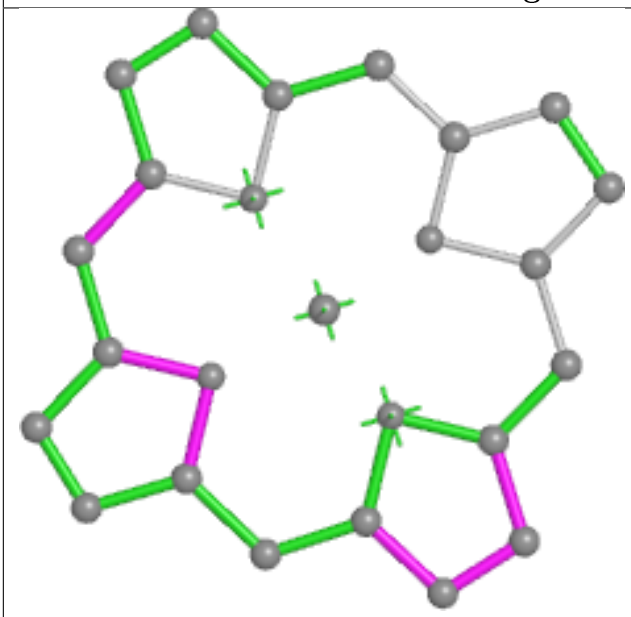


Torsions

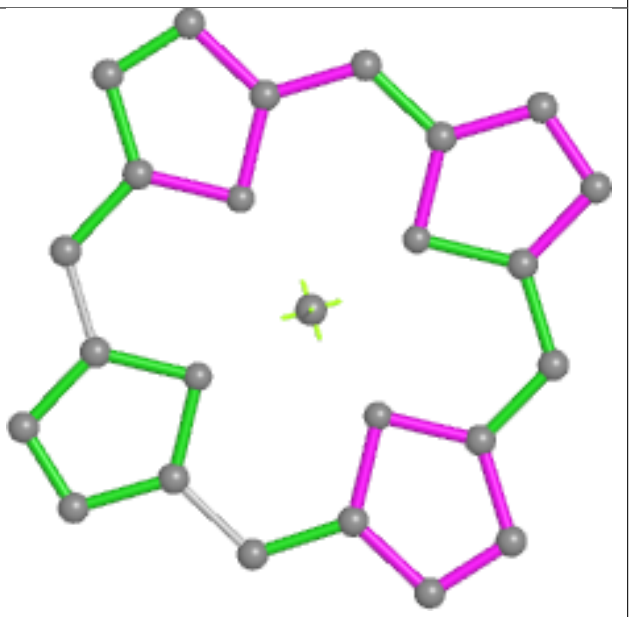


Rings

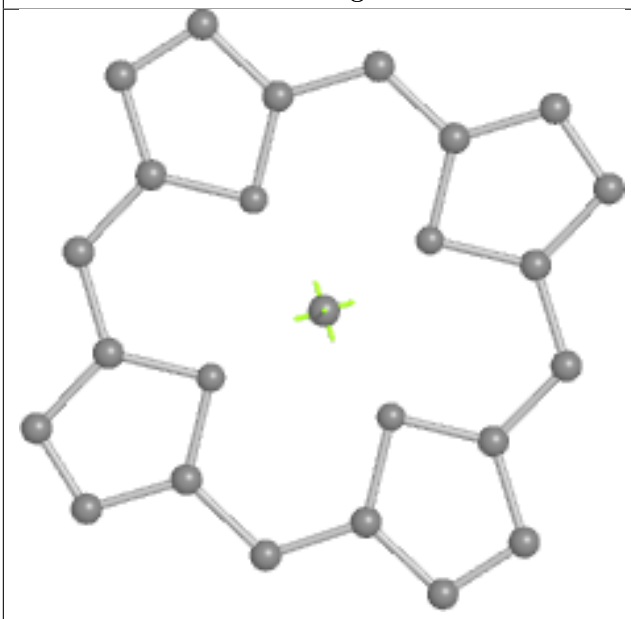
Ligand CLA K 177



Bond lengths



Bond angles



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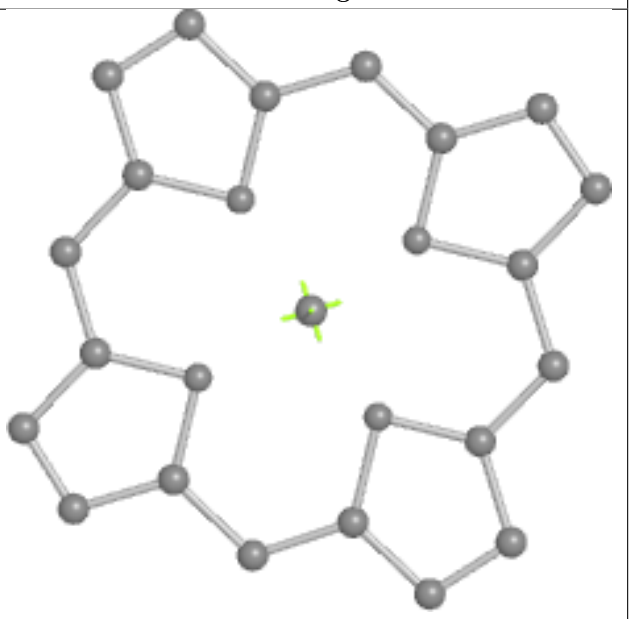
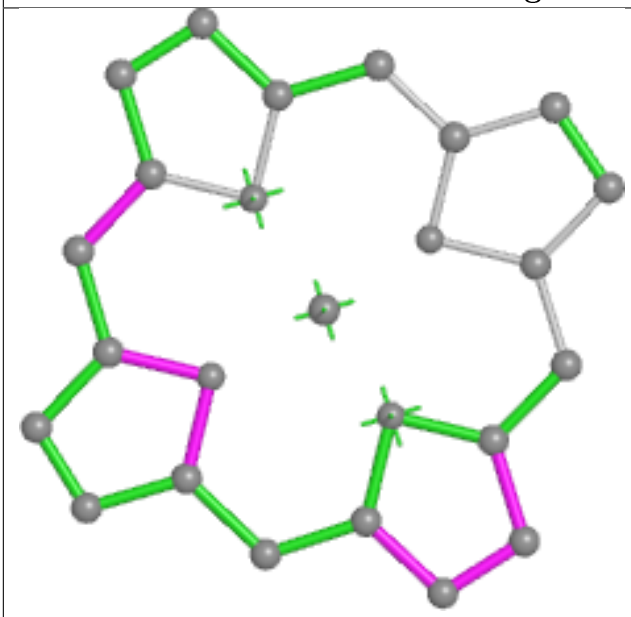


Rings

Ligand CLA C 163



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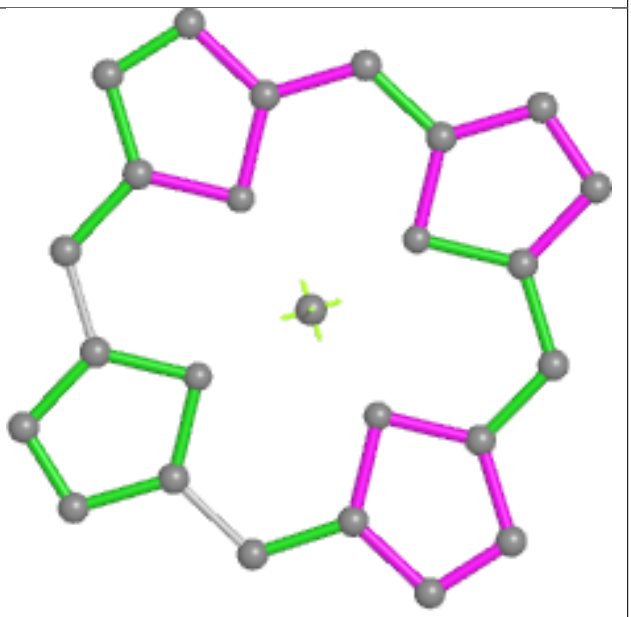
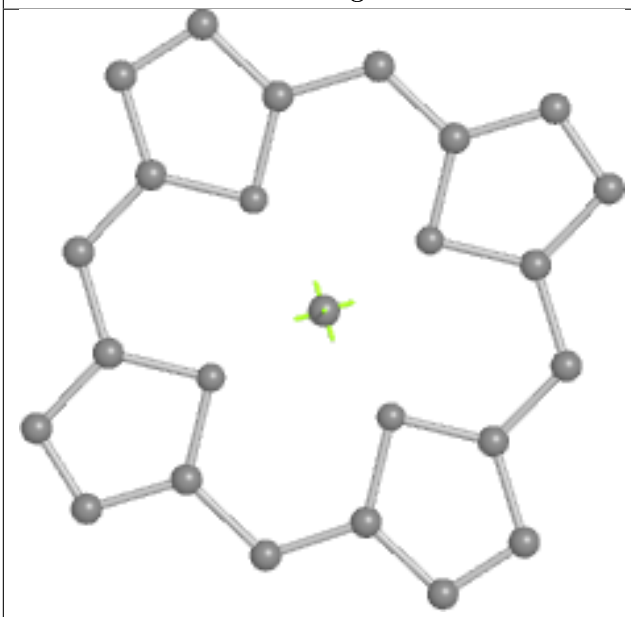


Bond angles



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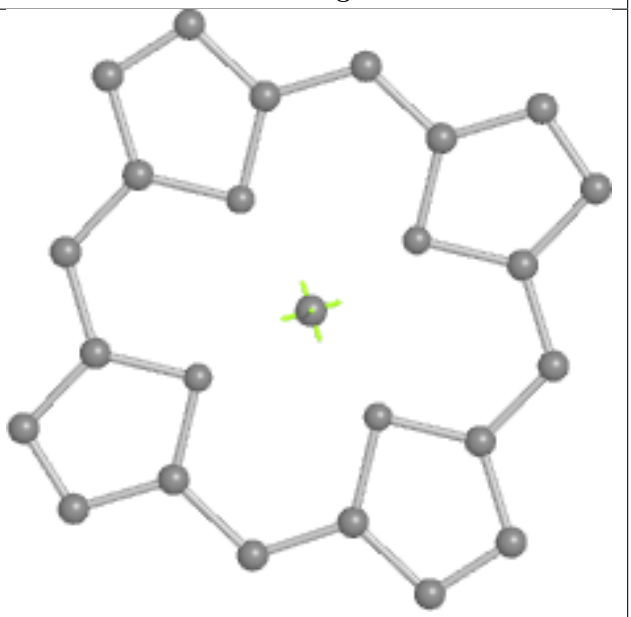
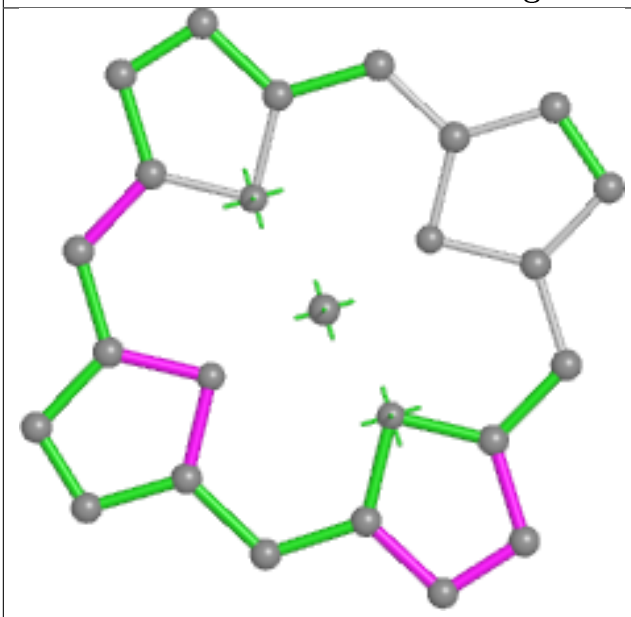


Rings

Ligand CLA D 161



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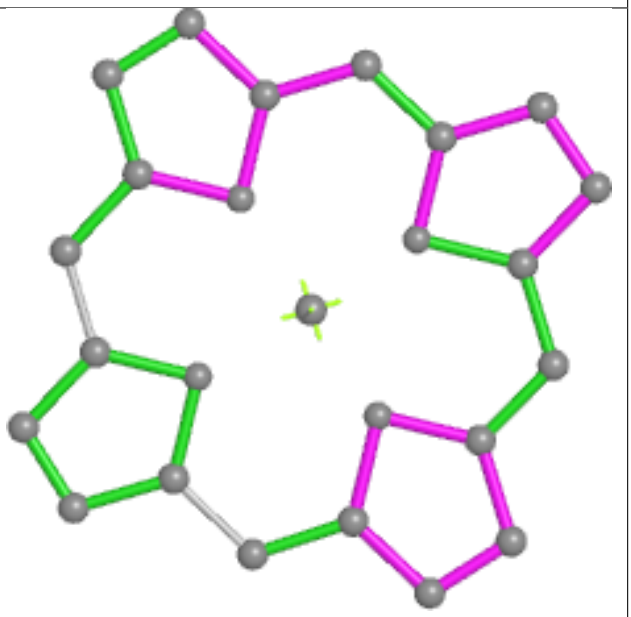
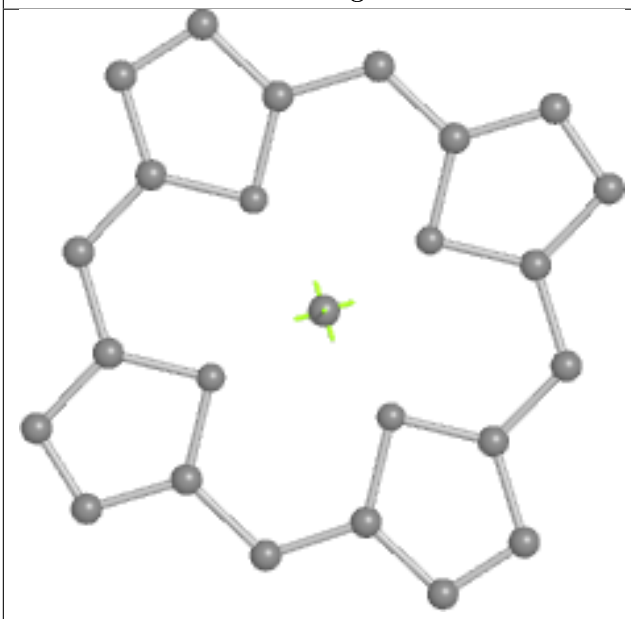


Bond angles



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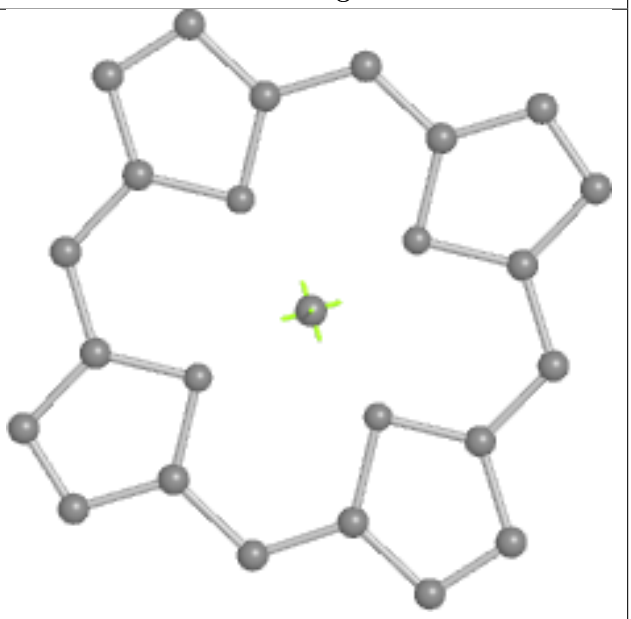
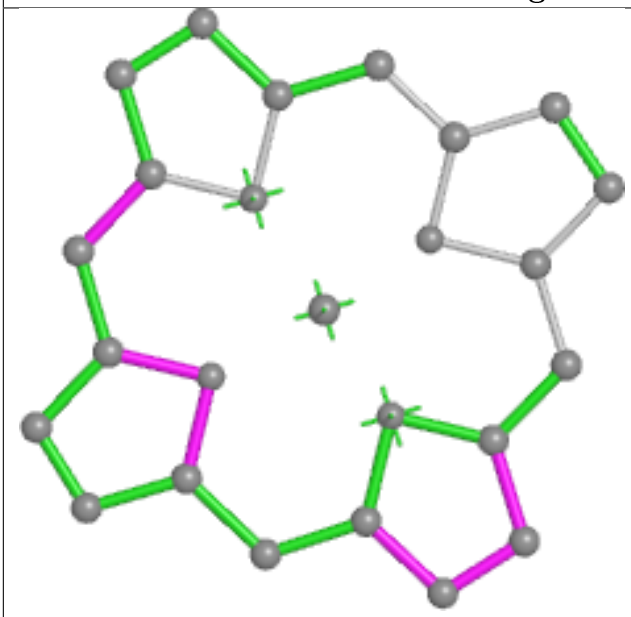
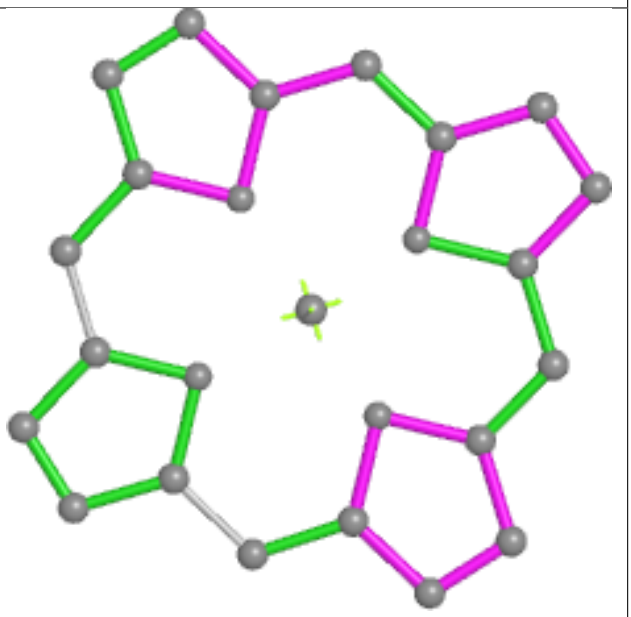


Rings

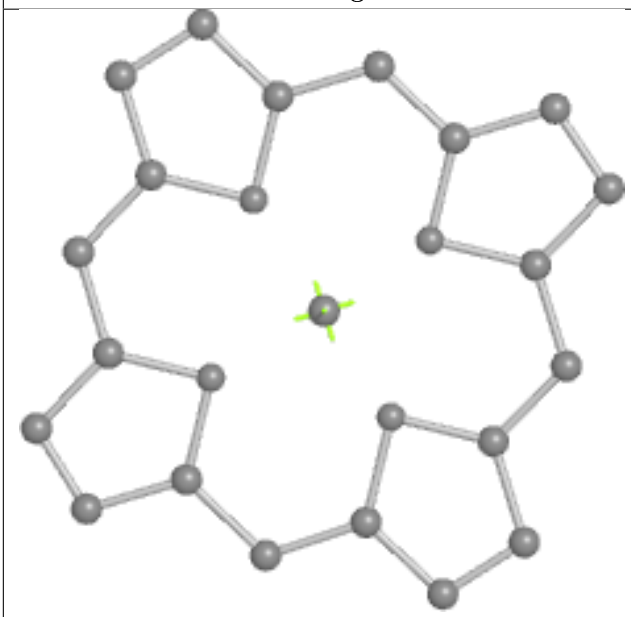
Ligand CLA J 177



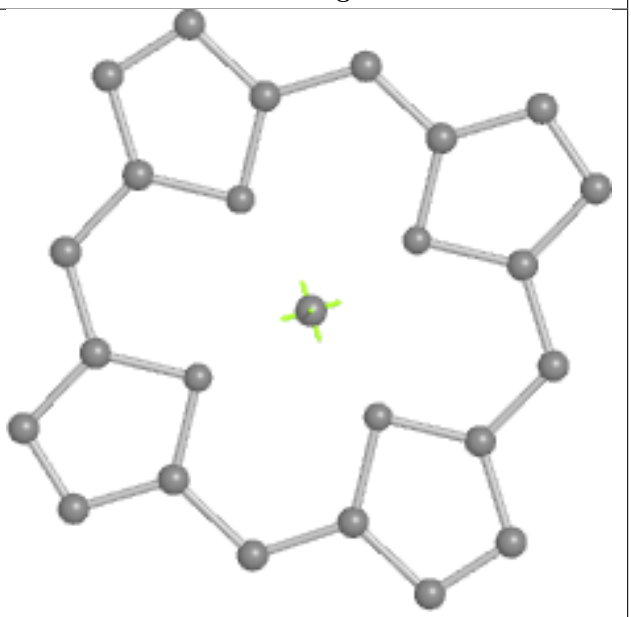
Bond lengths



Bond angles

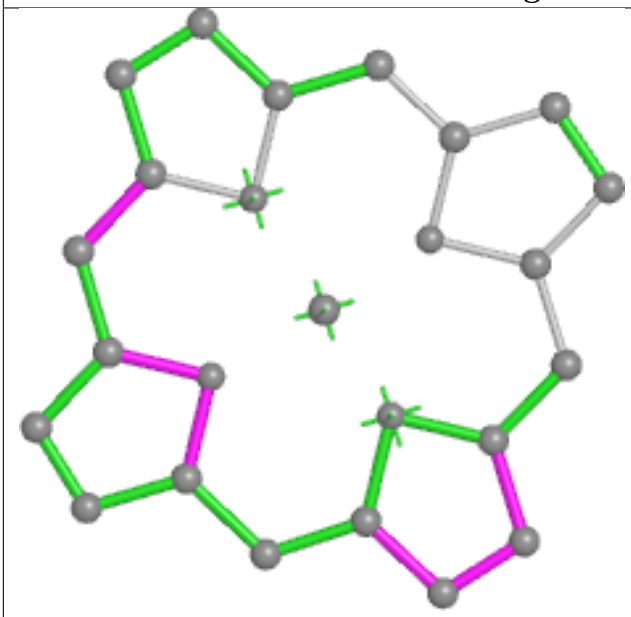


Torsions



Rings

Ligand CLA D 160



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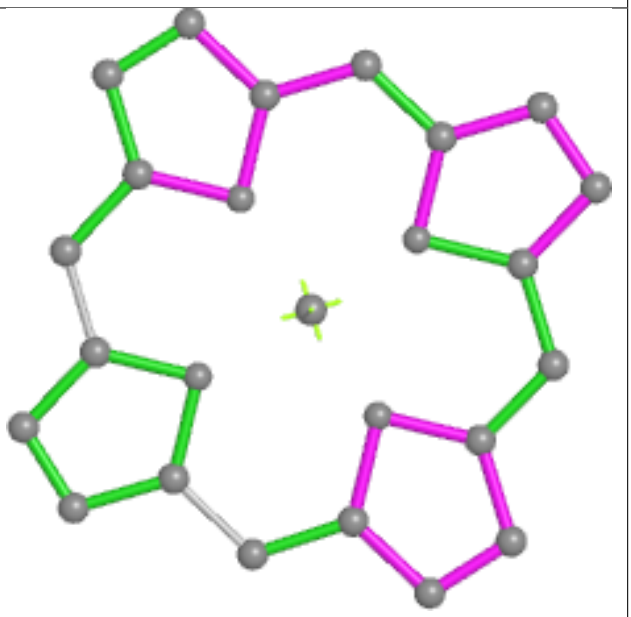
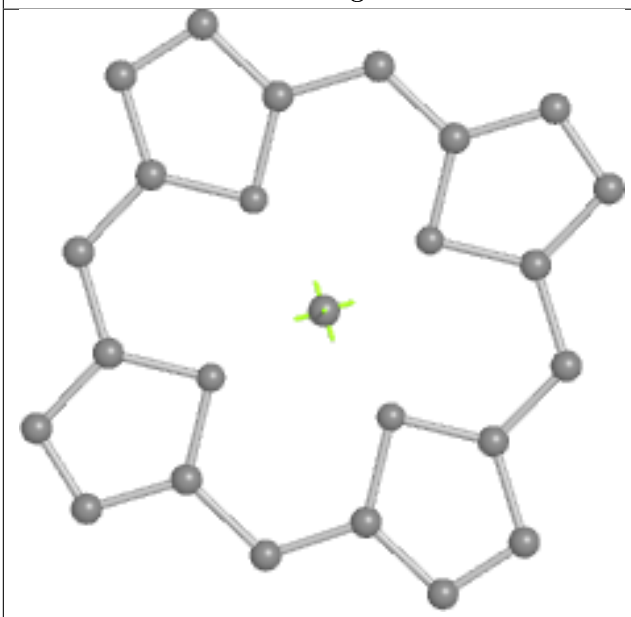


Bond angles



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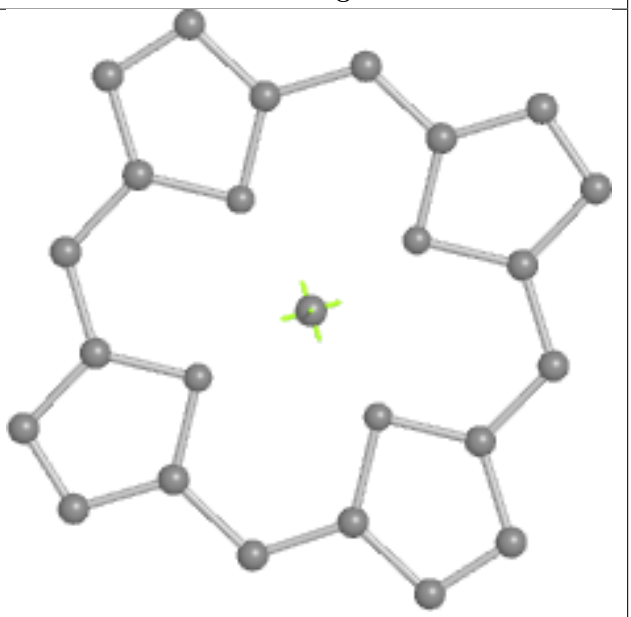
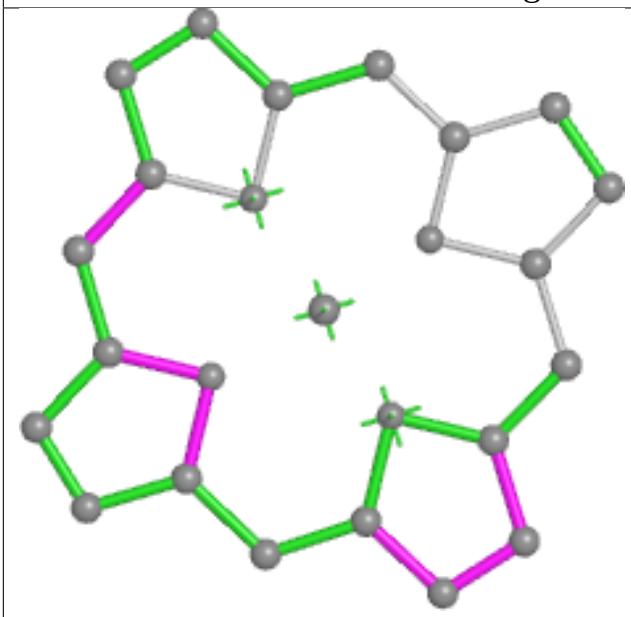


Rings

Ligand CLA D 165



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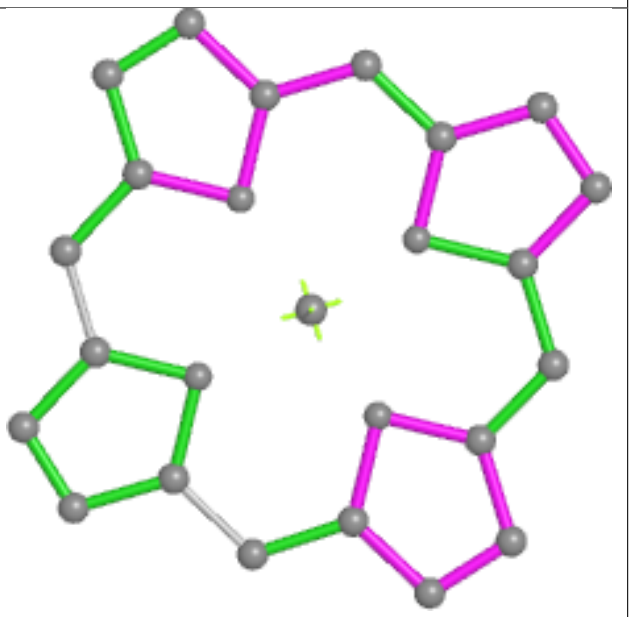
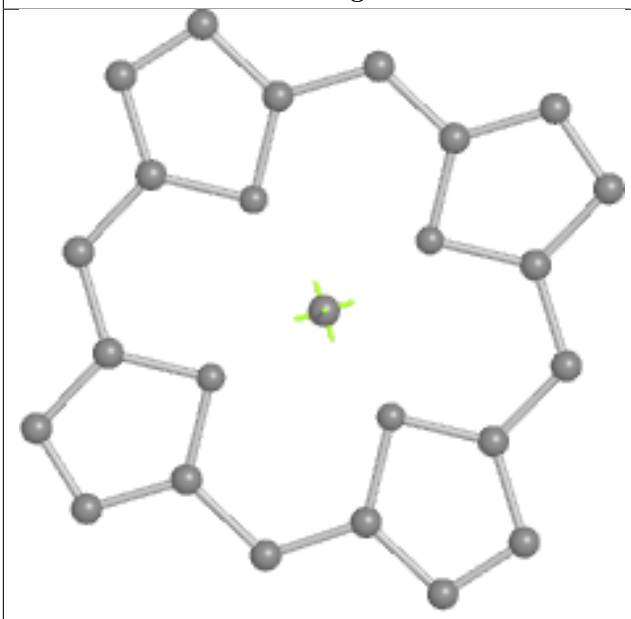


Bond angles



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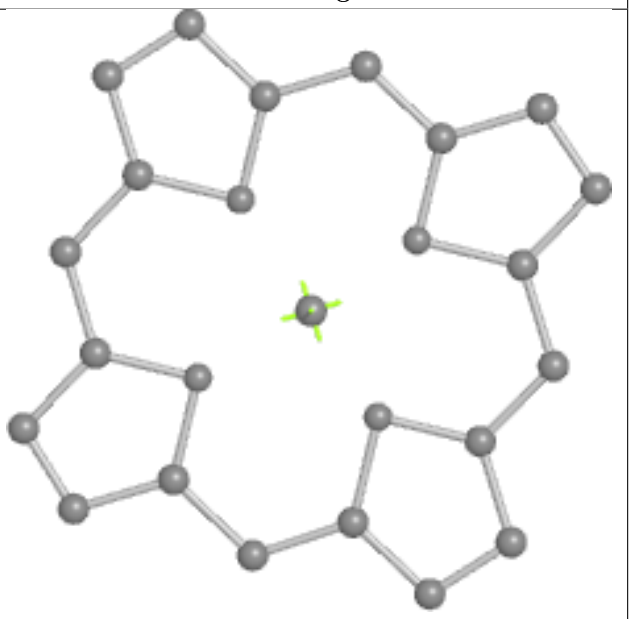
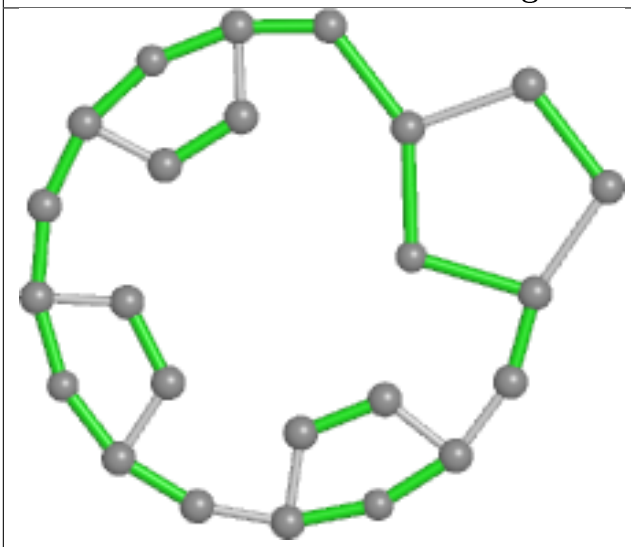
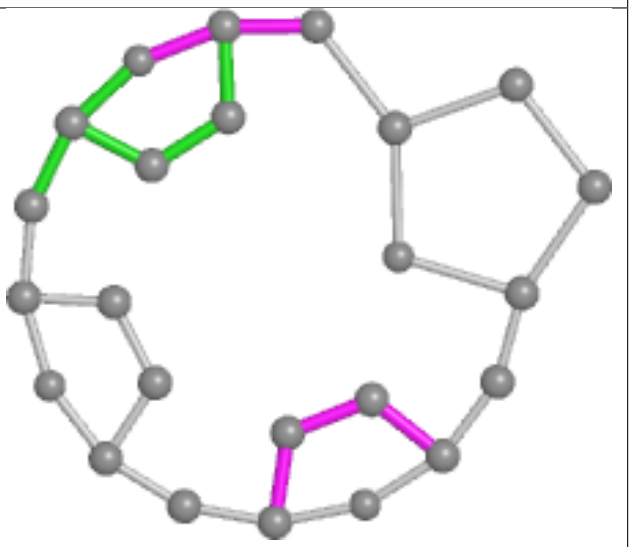


Rings

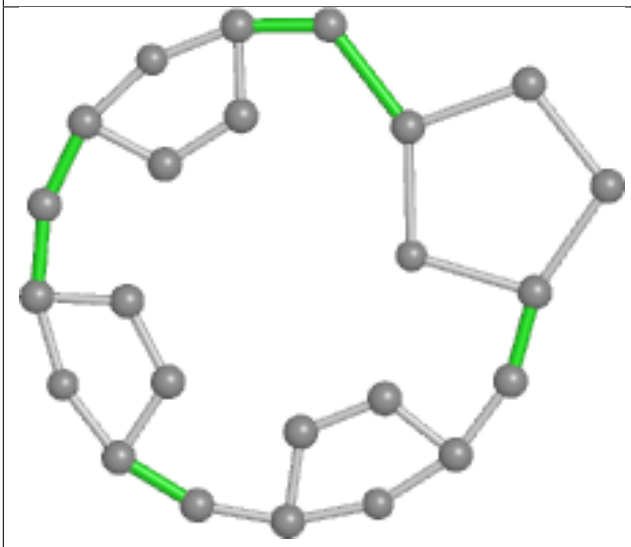
Ligand PHO A 178



Bond lengths



Bond angles



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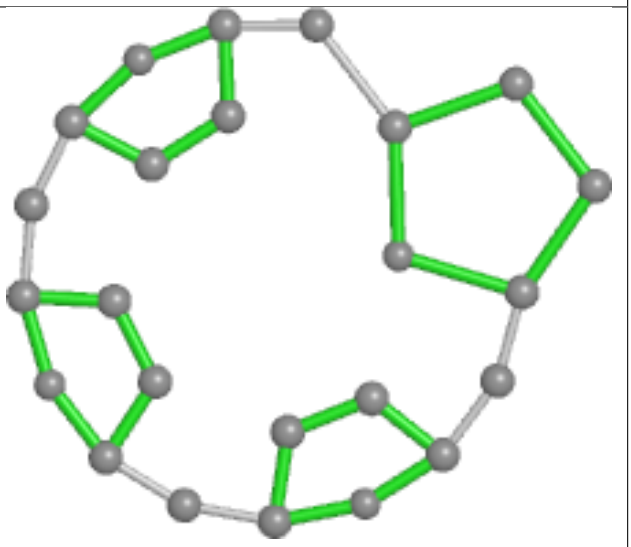
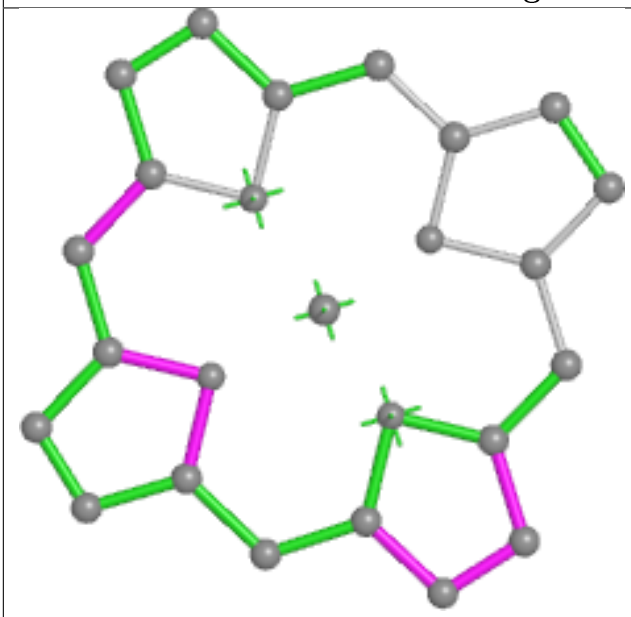
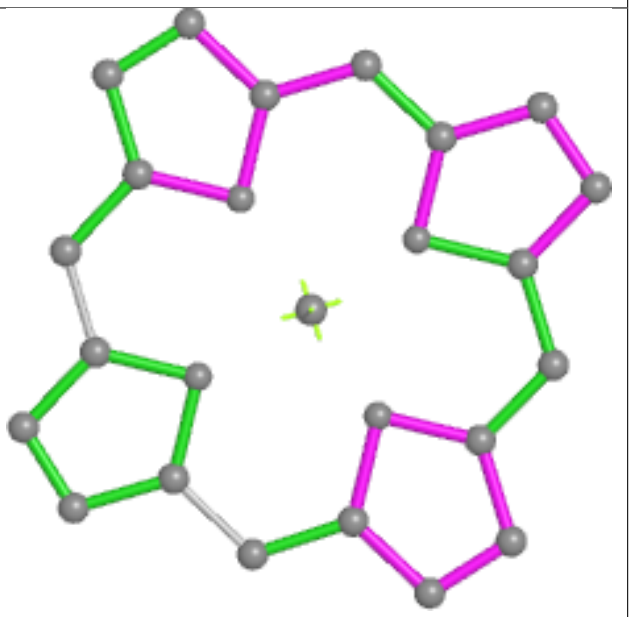


Rings

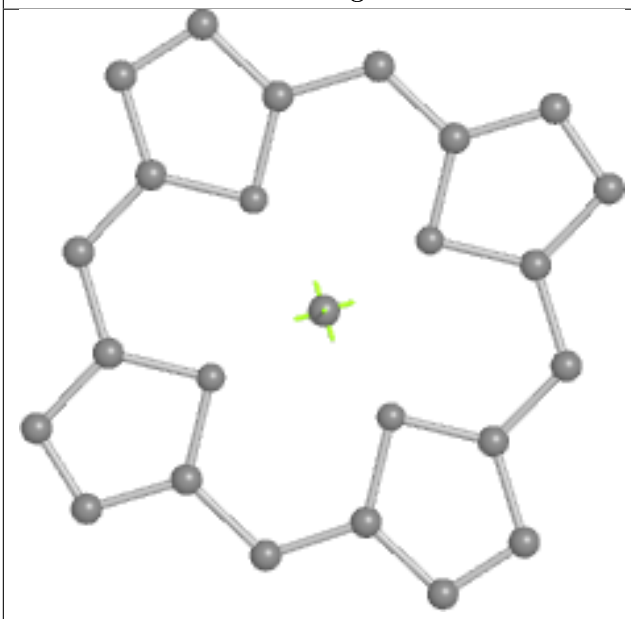
Ligand CLA D 164



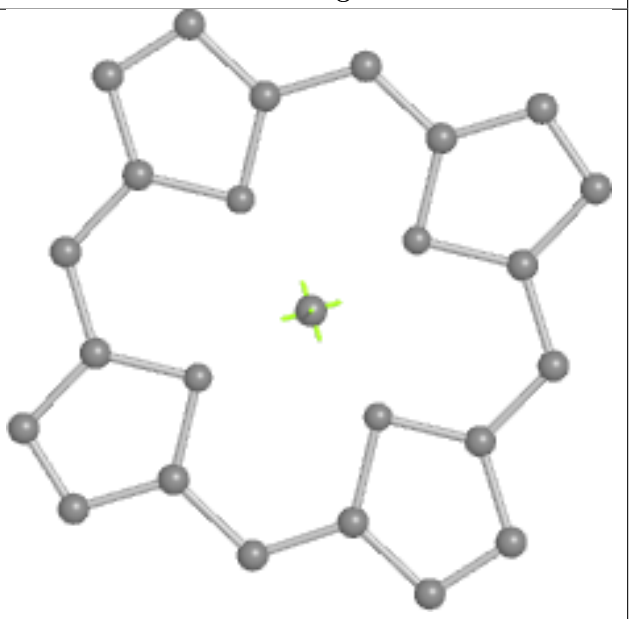
Bond lengths



Bond angles

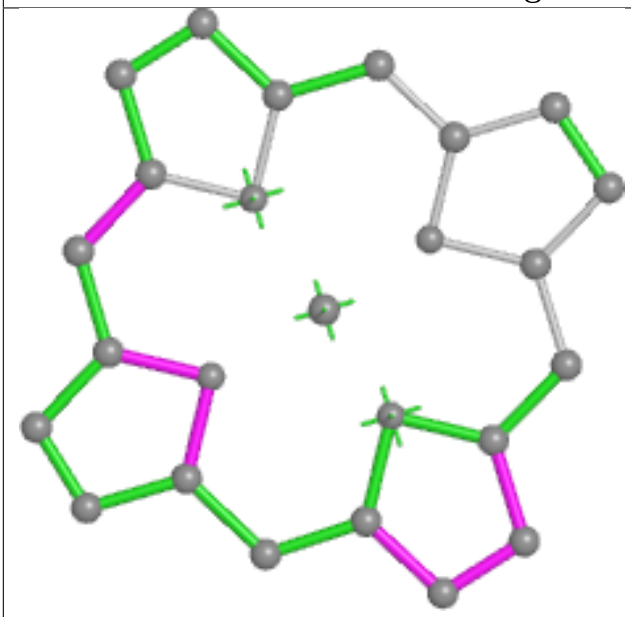


Torsions

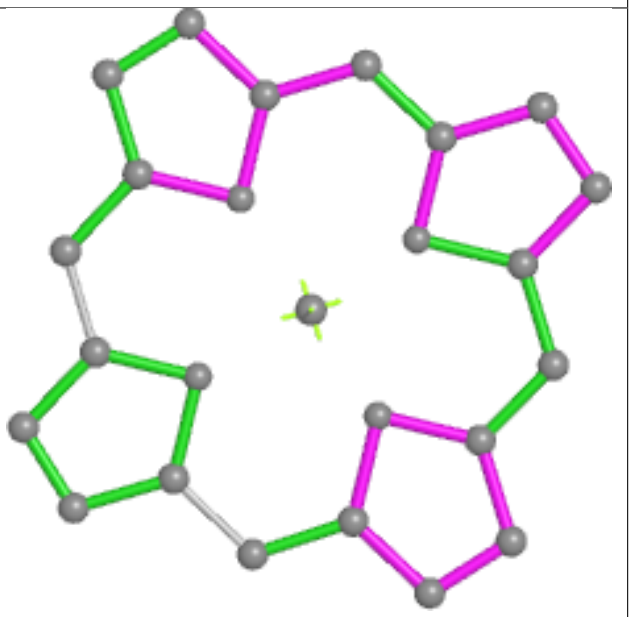


Rings

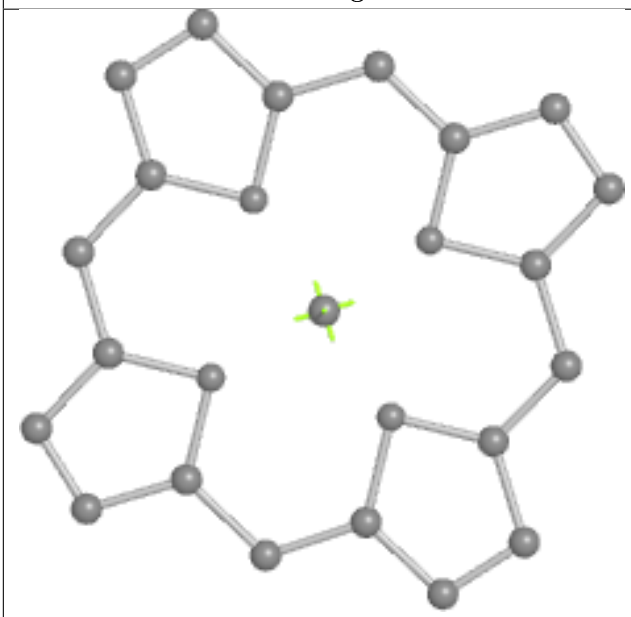
Ligand CLA B 177



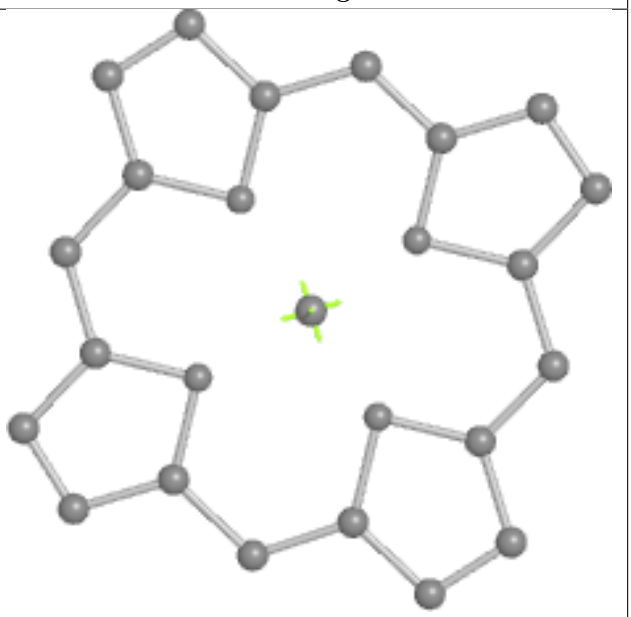
Bond lengths



Bond angles

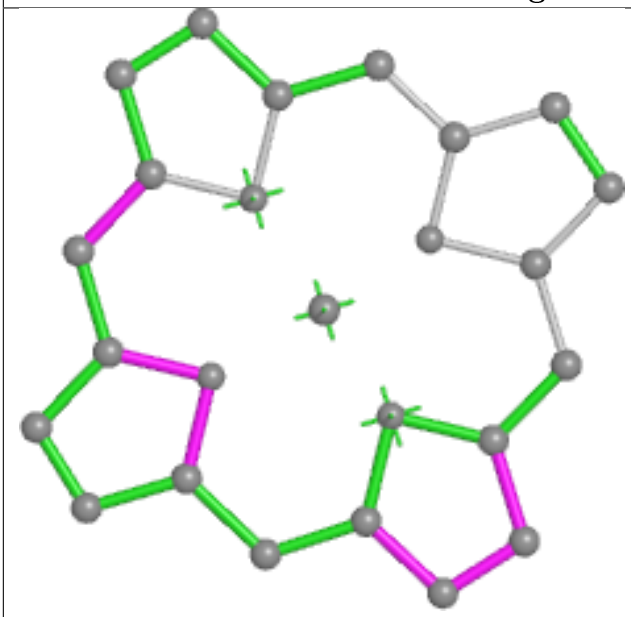


Torsions



Rings

Ligand CLA J 175



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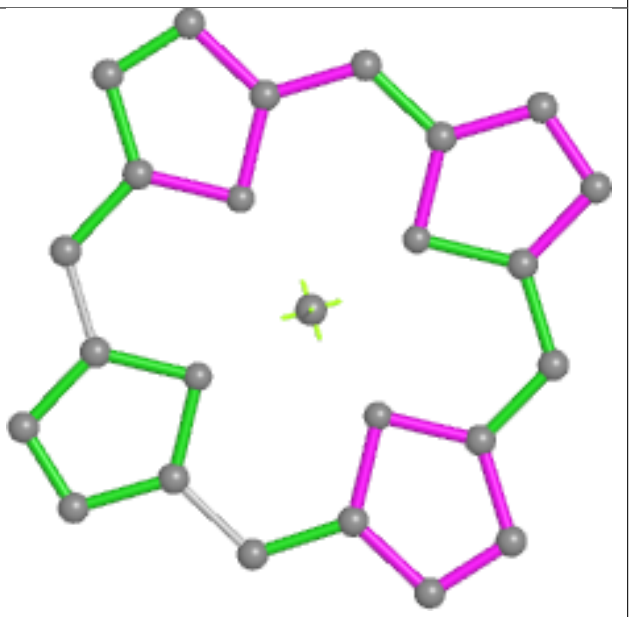
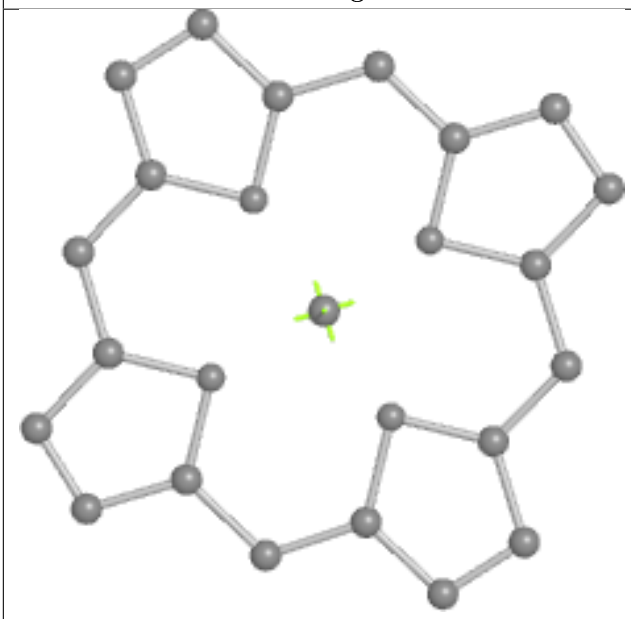


Bond angles



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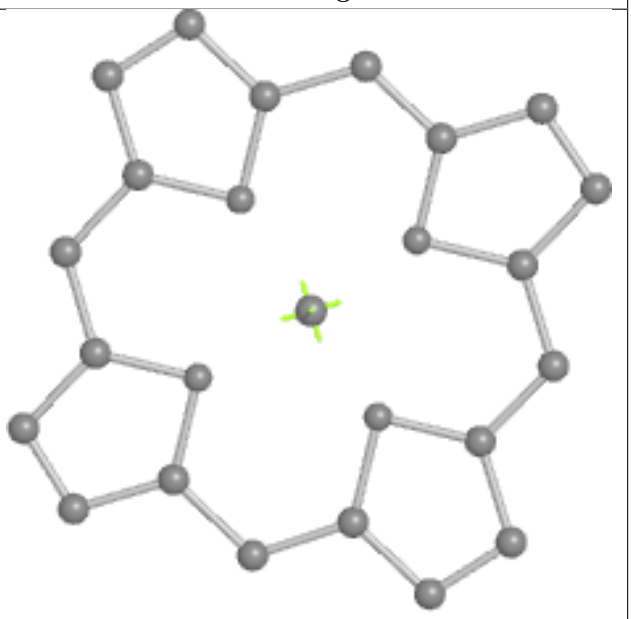
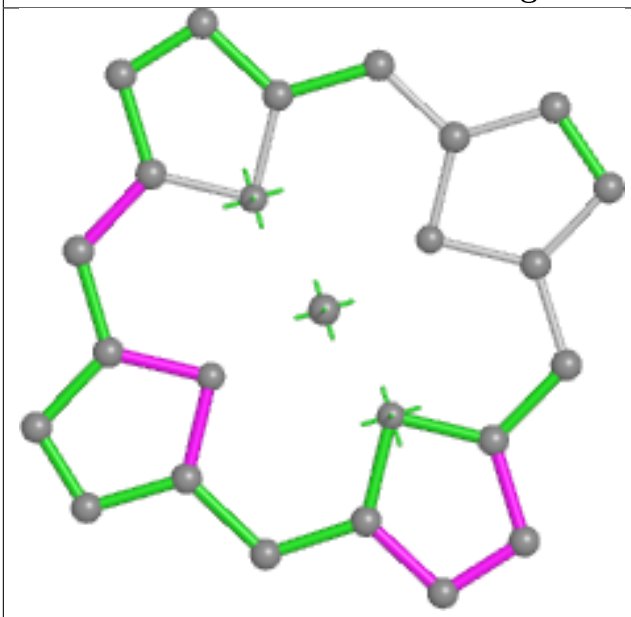


Rings

Ligand CLA M 161



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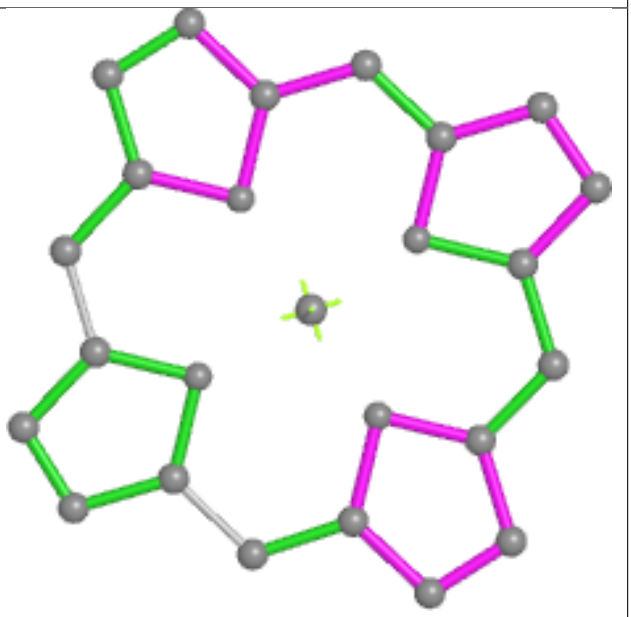
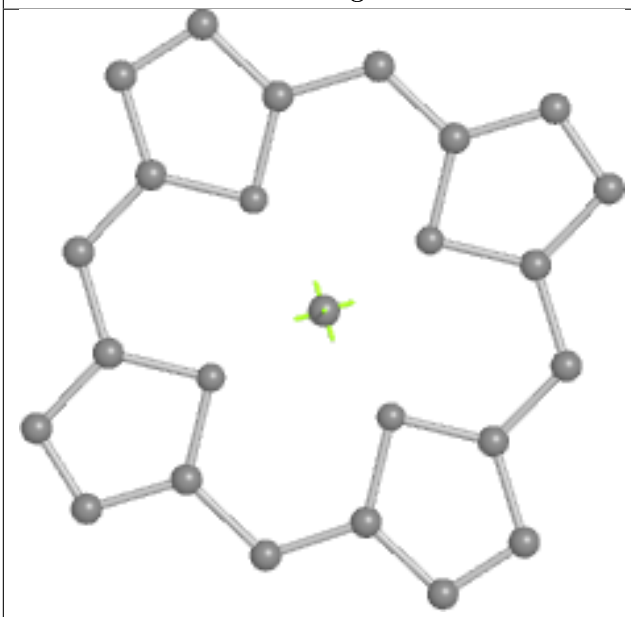


Bond angles



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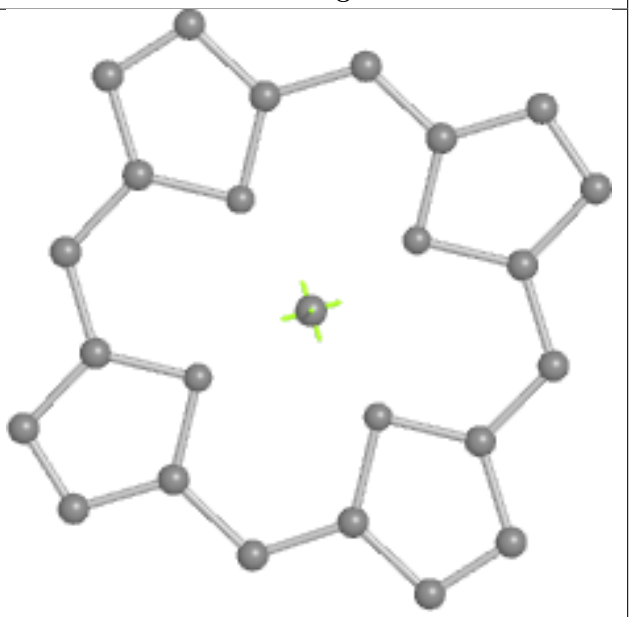
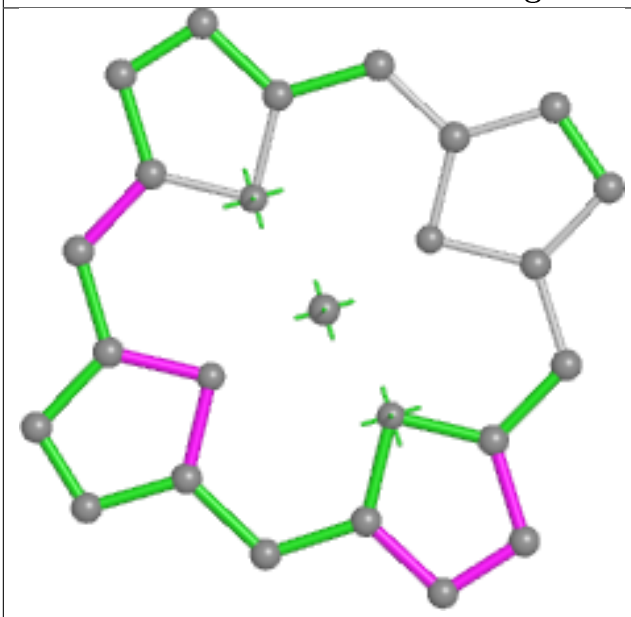


Rings

Ligand CLA C 165



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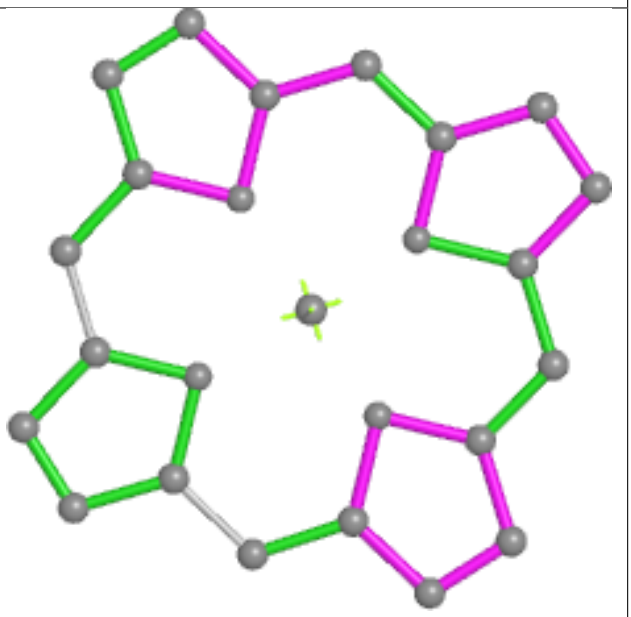
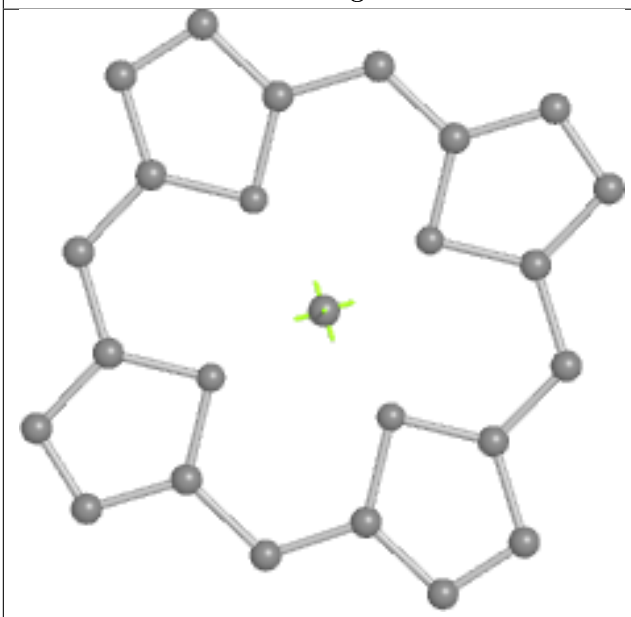


Bond angles



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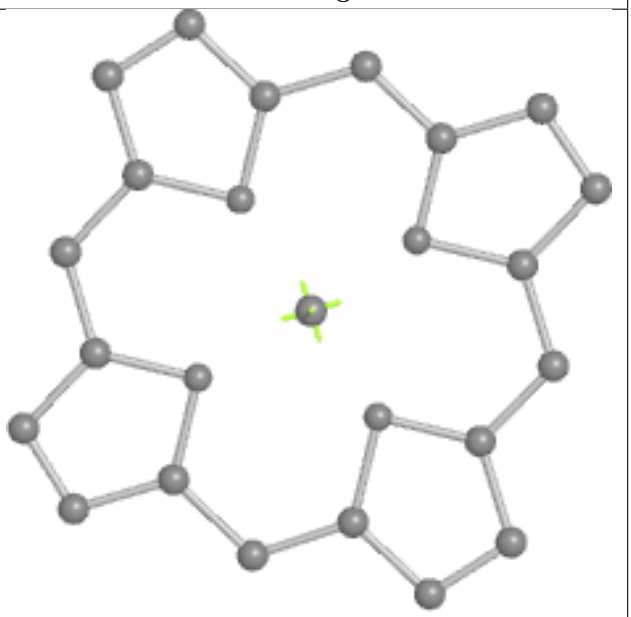
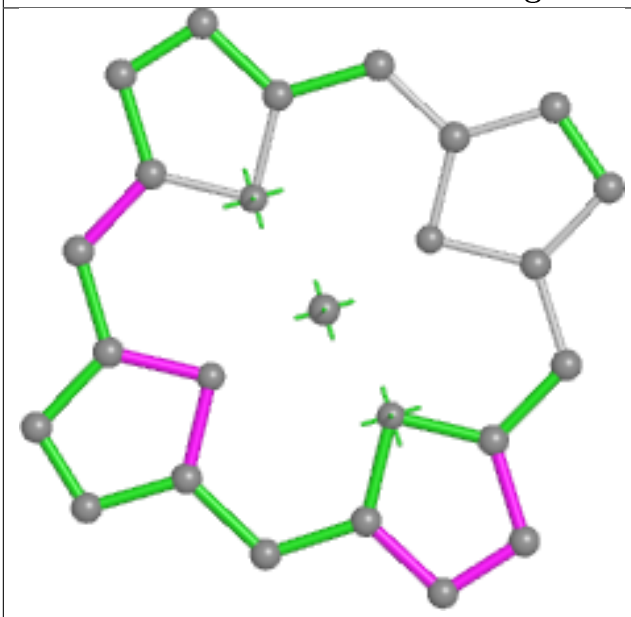


Rings

Ligand CLA C 168



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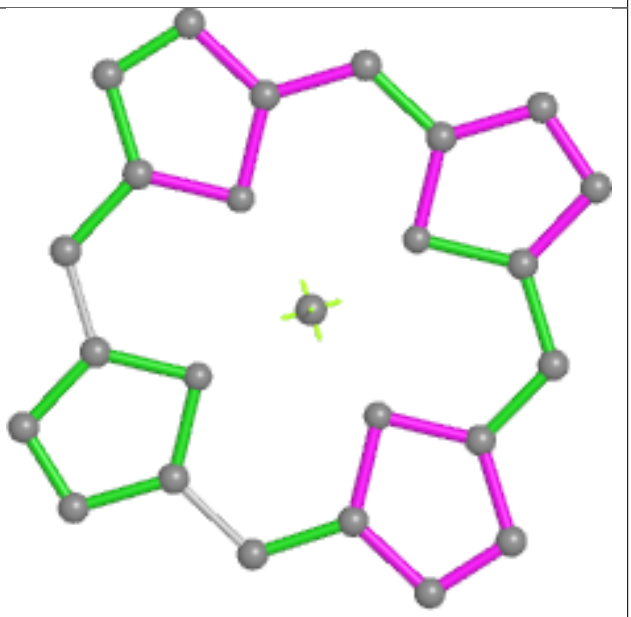
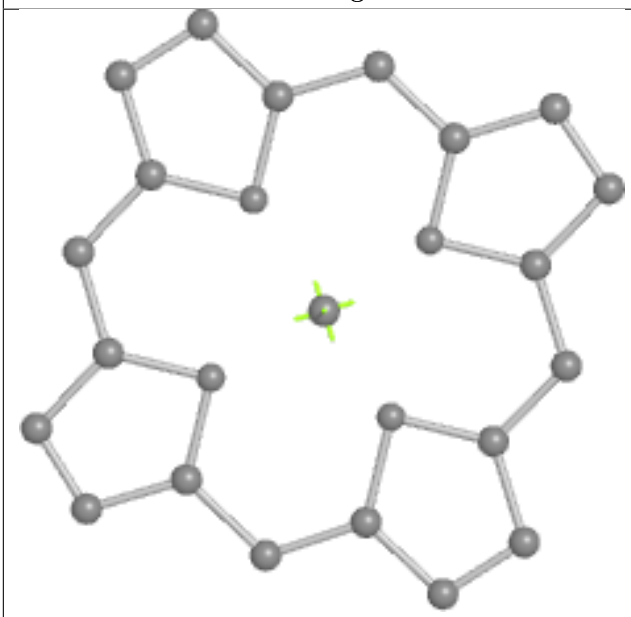


Bond angles



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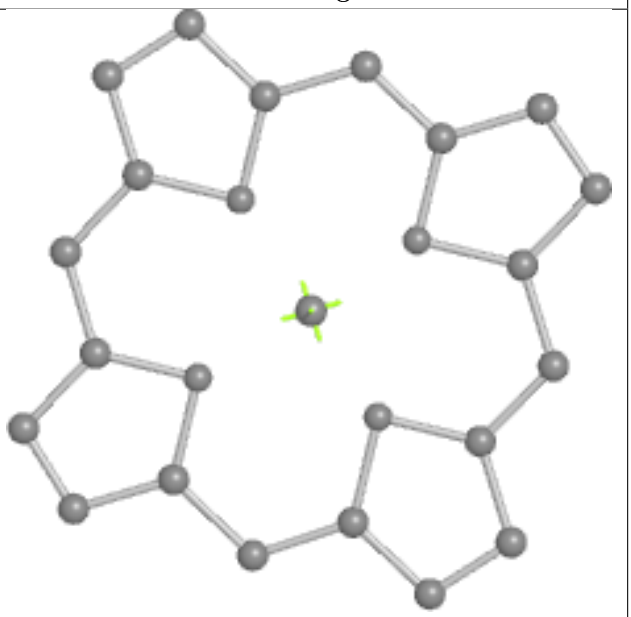
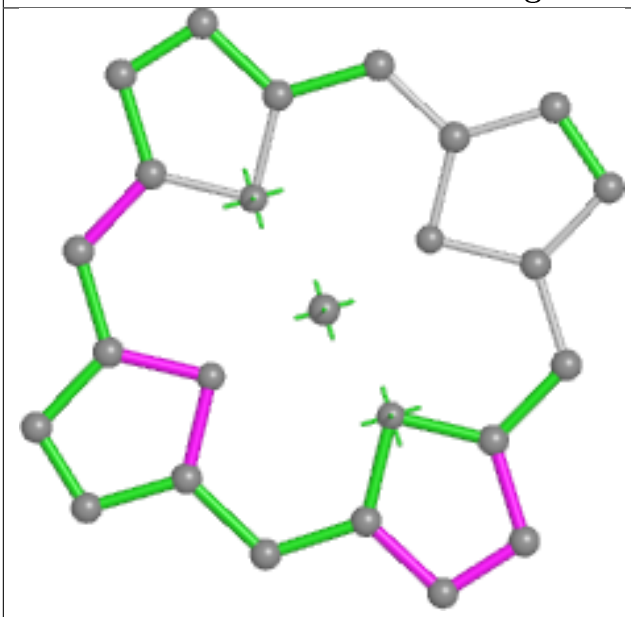


Rings

Ligand CLA C 157



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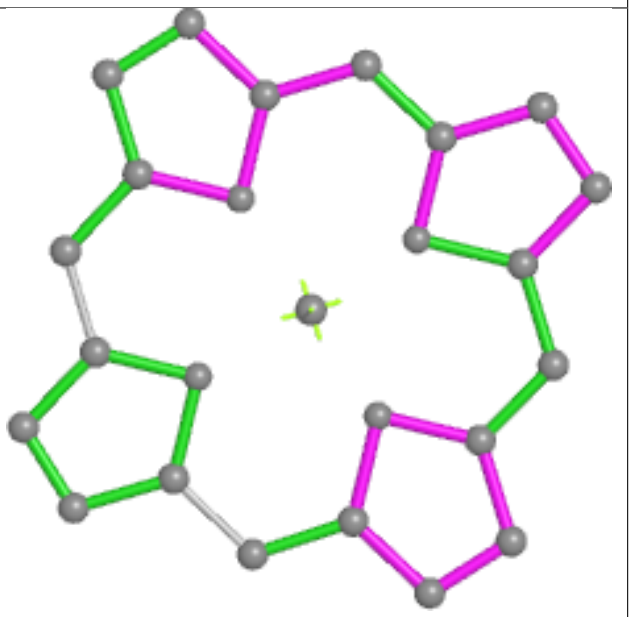
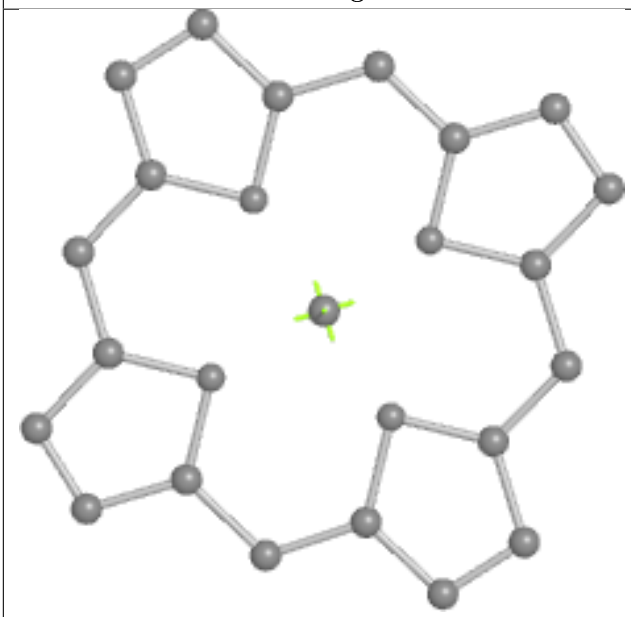


Bond angles



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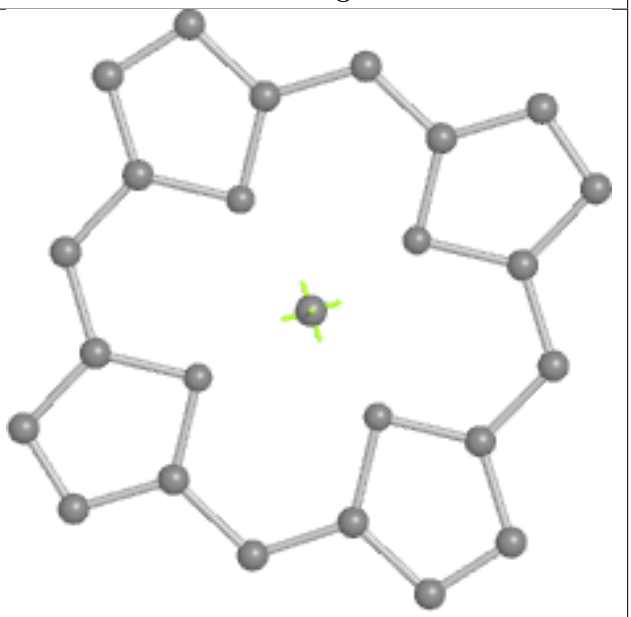
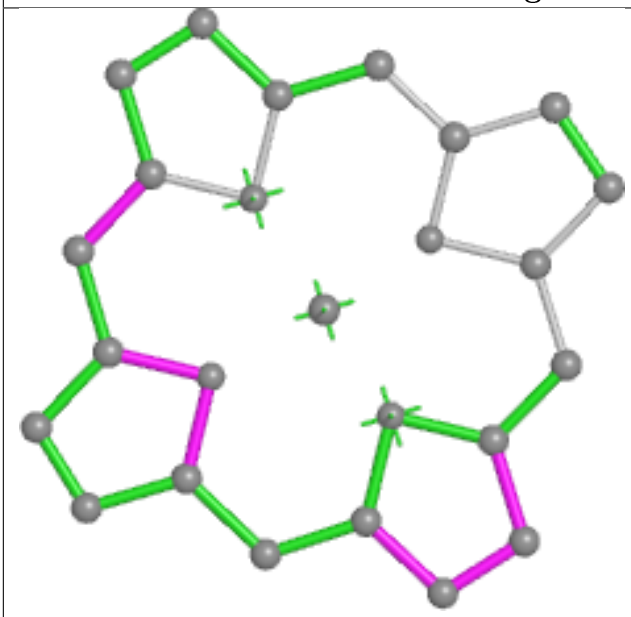
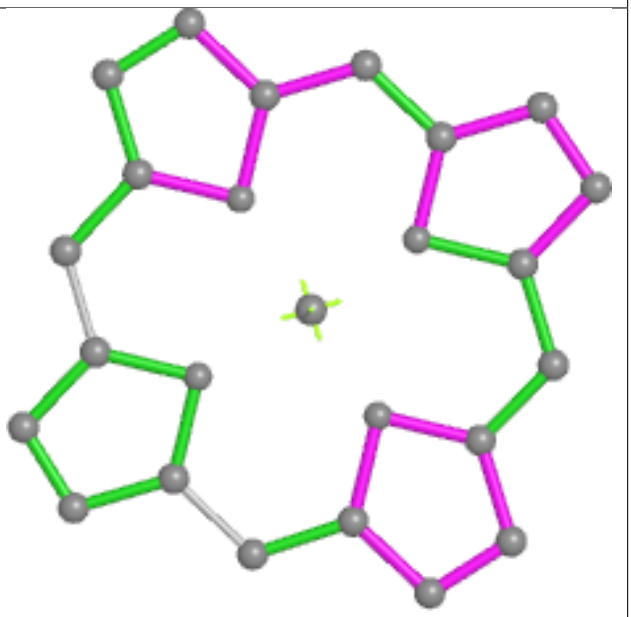


Rings

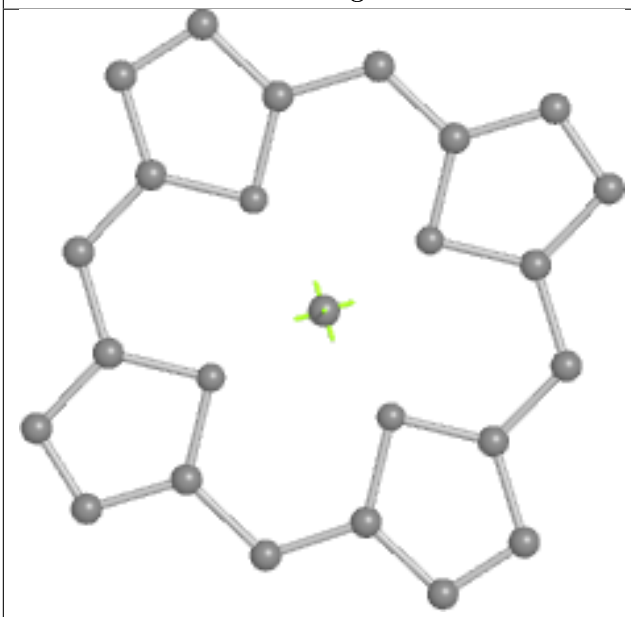
Ligand CLA C 161



Bond lengths



Bond angles



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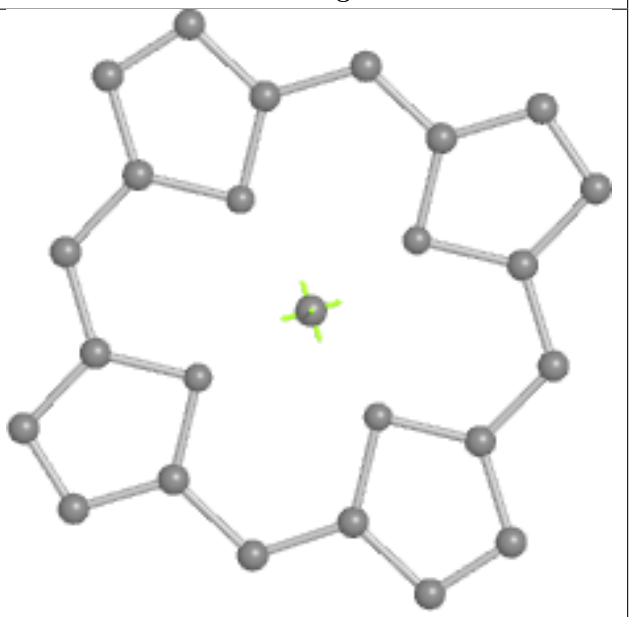
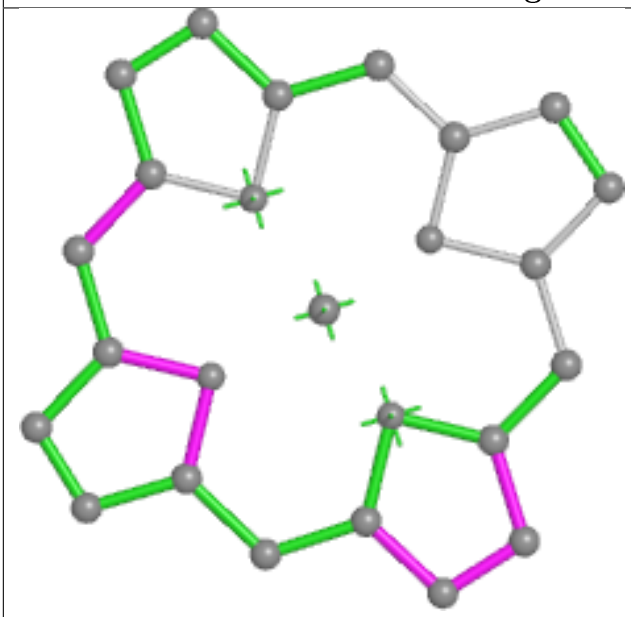
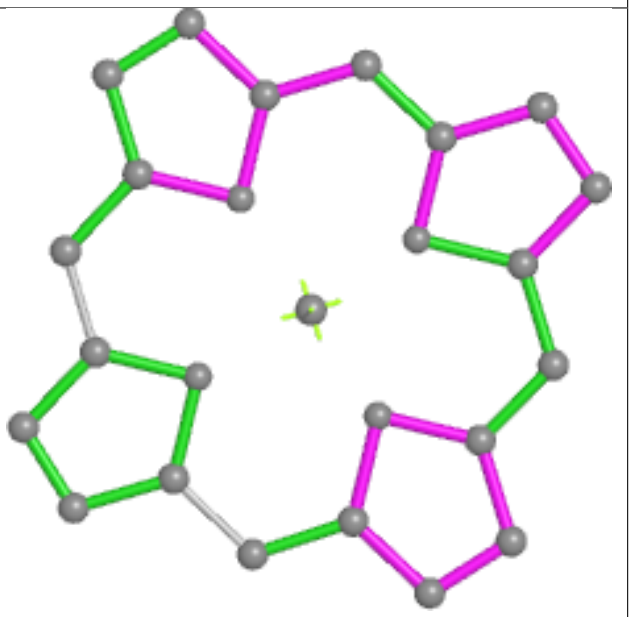


Rings

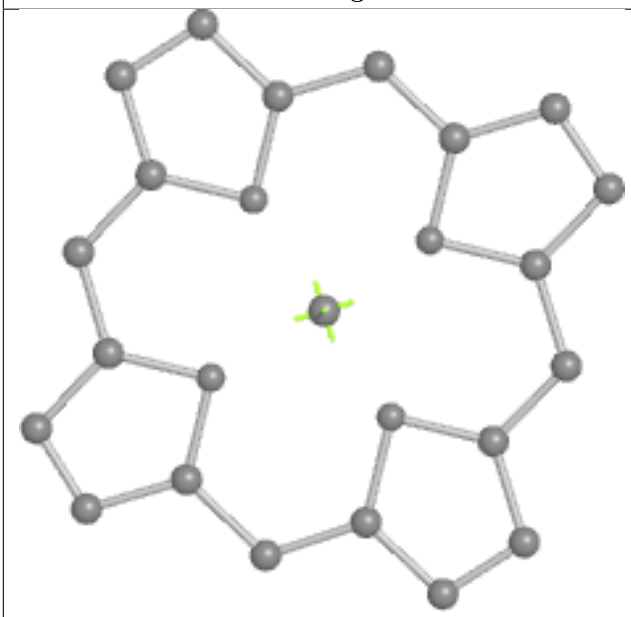
Ligand CLA C 159



Bond lengths



Bond angles



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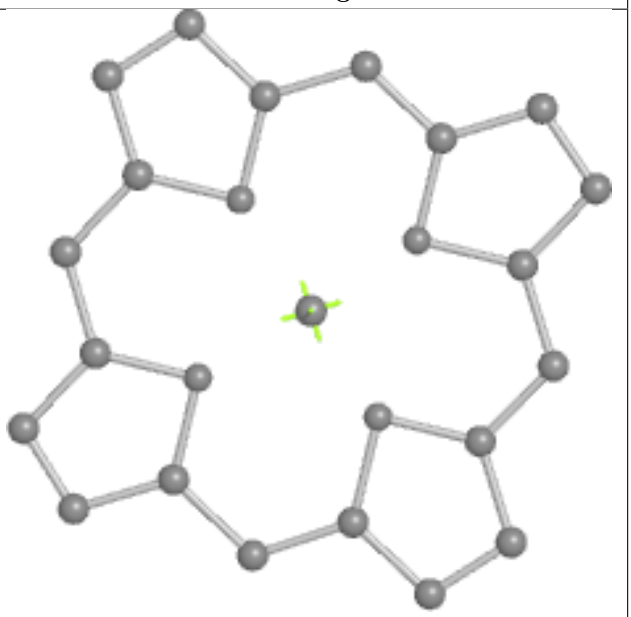
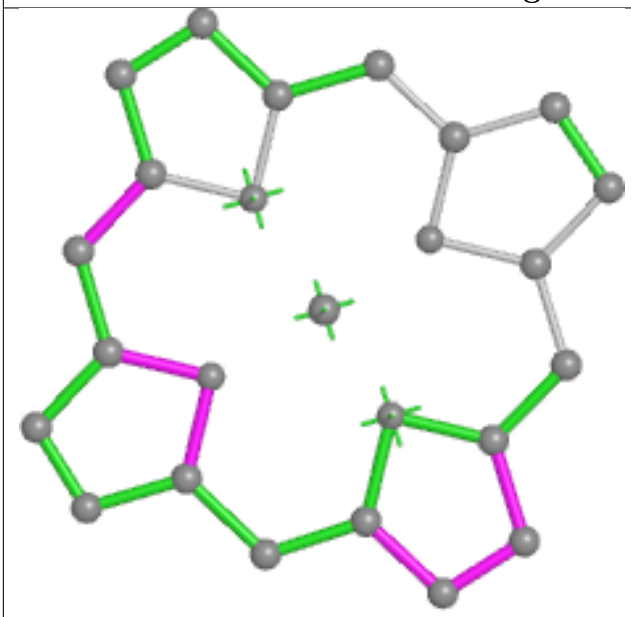


Rings

Ligand CLA G 313



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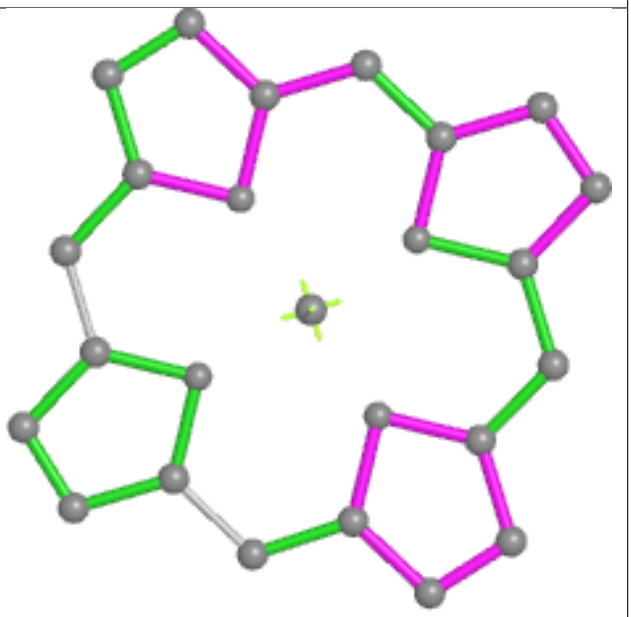
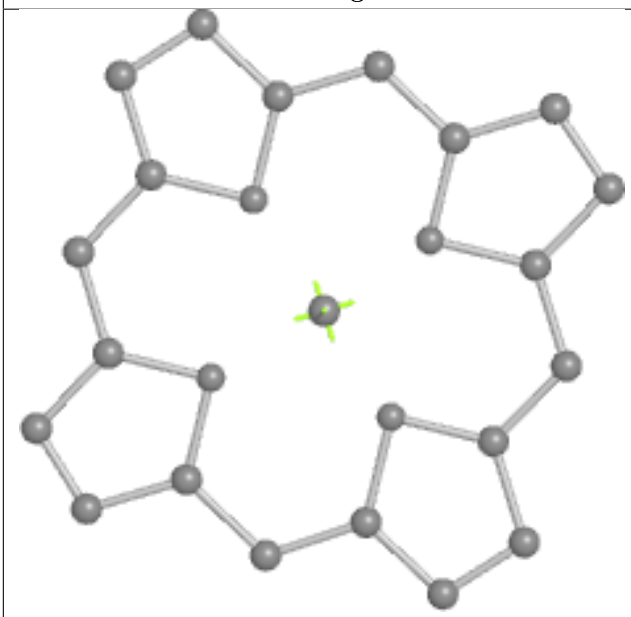


Bond angles



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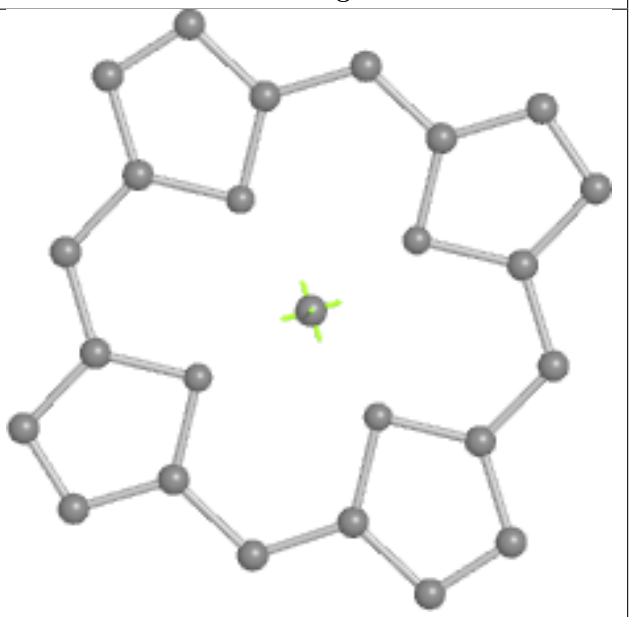
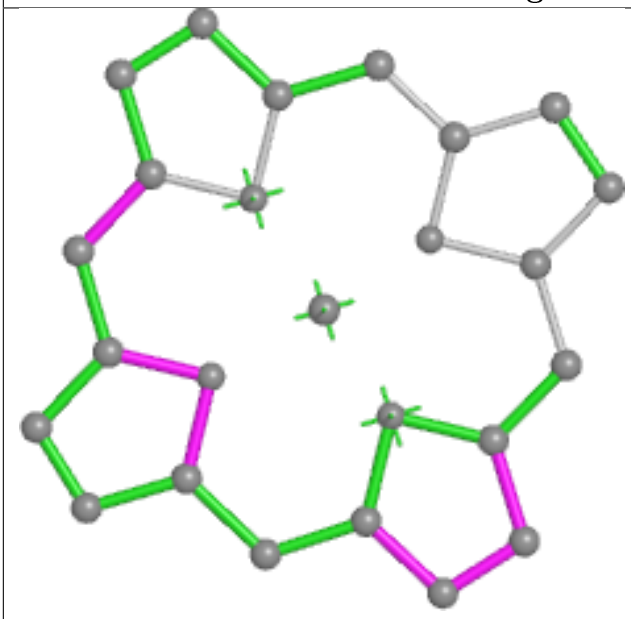


Rings

Ligand CLA L 165



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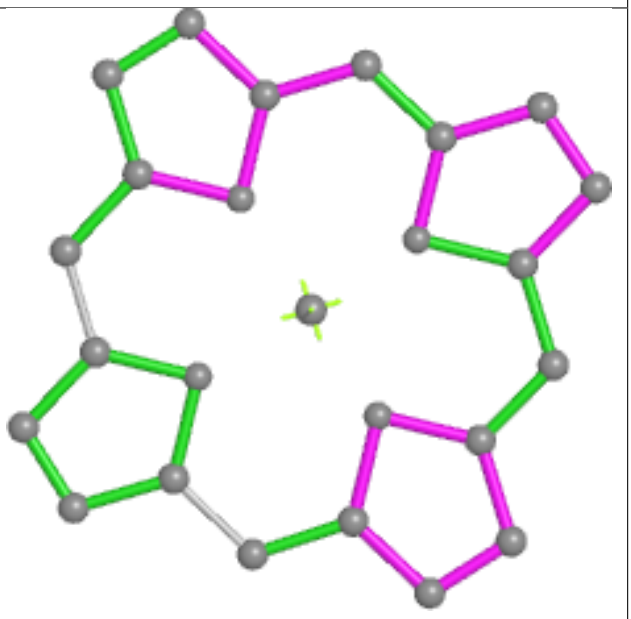
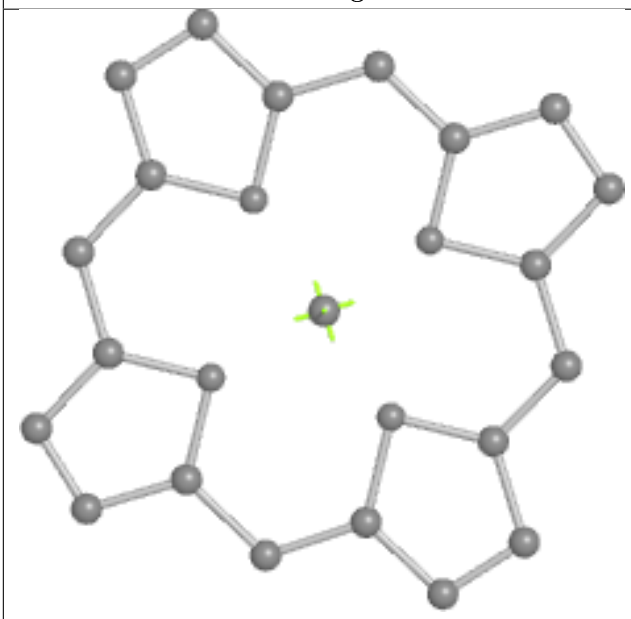


Bond angles



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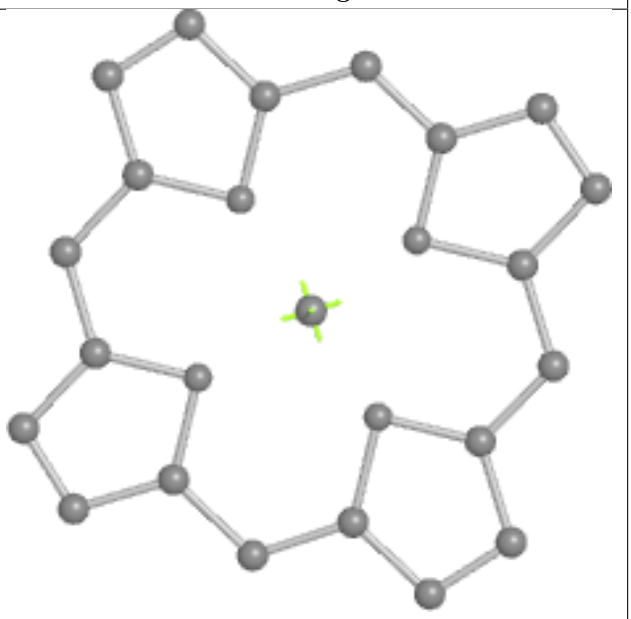
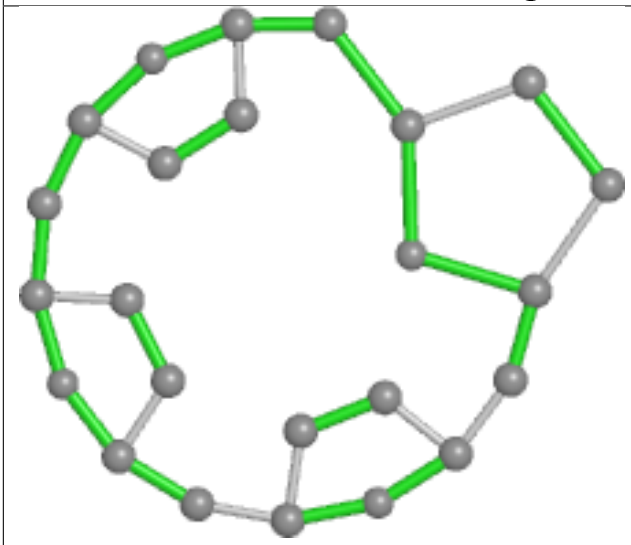


Rings

Ligand PHO B 178



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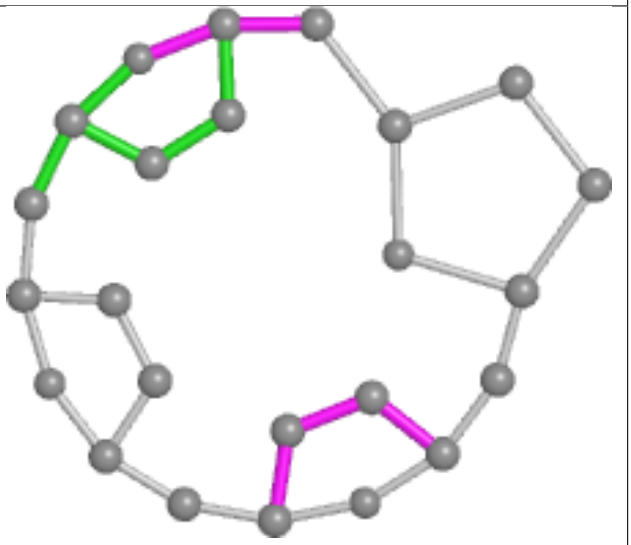
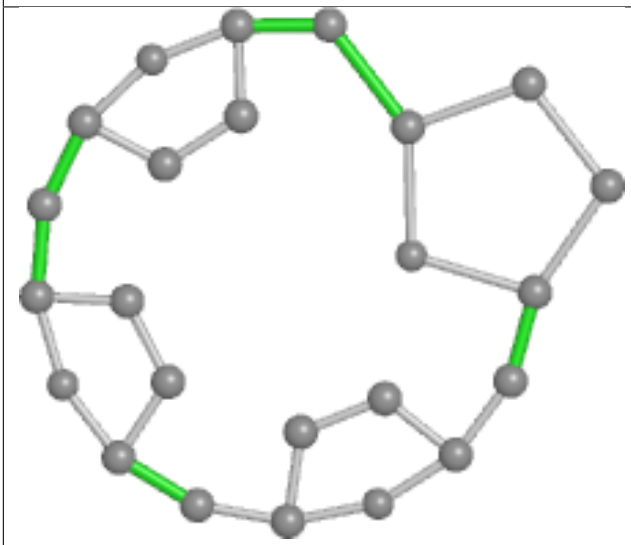


Bond angles



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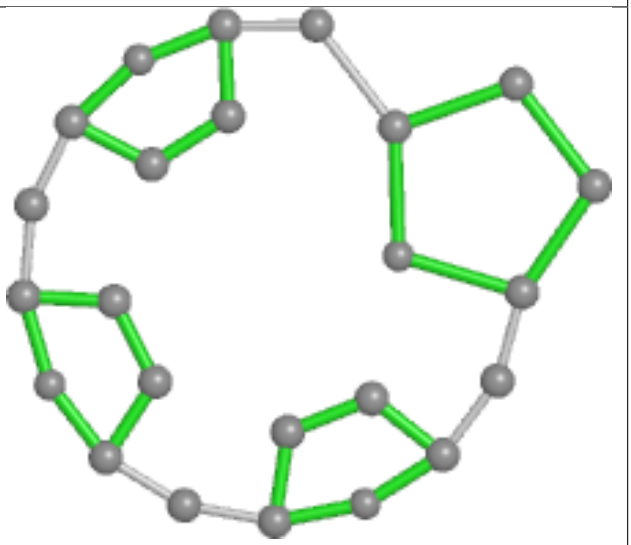
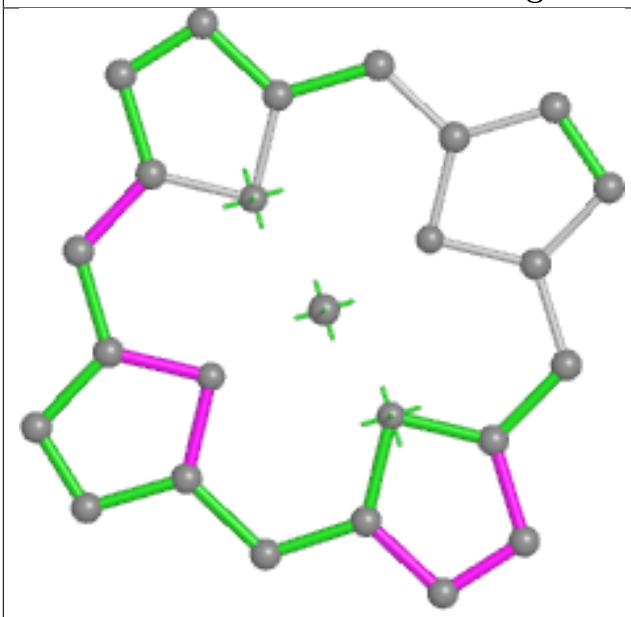


Rings

Ligand CLA L 164



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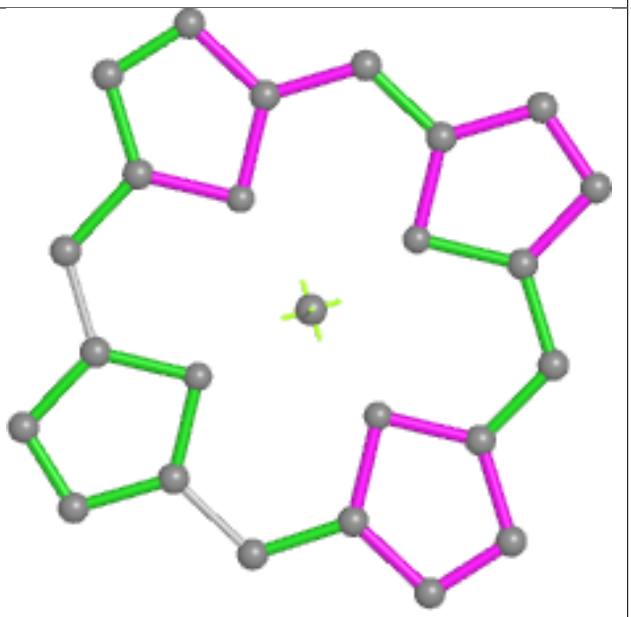
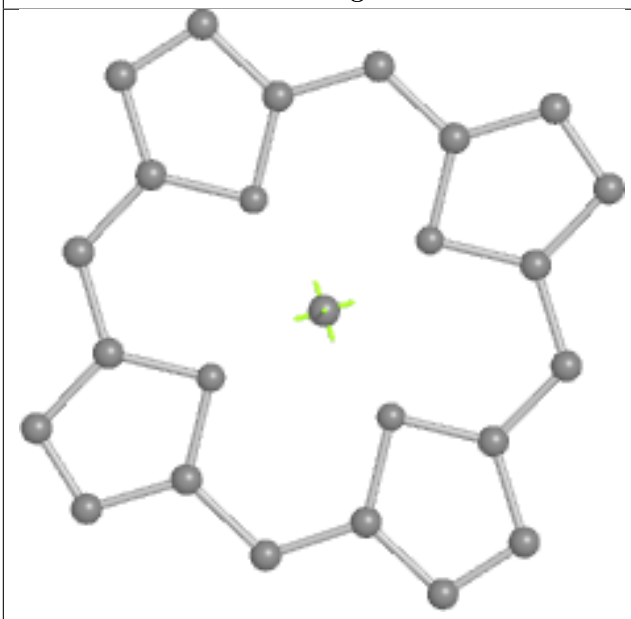


Bond angles



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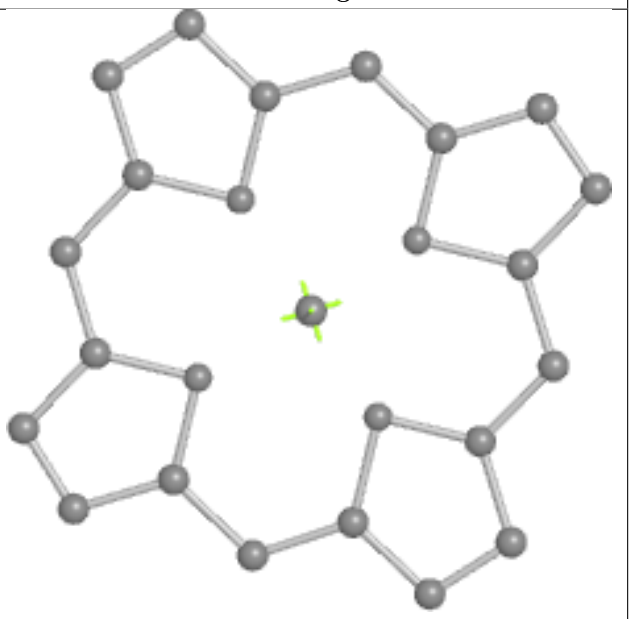
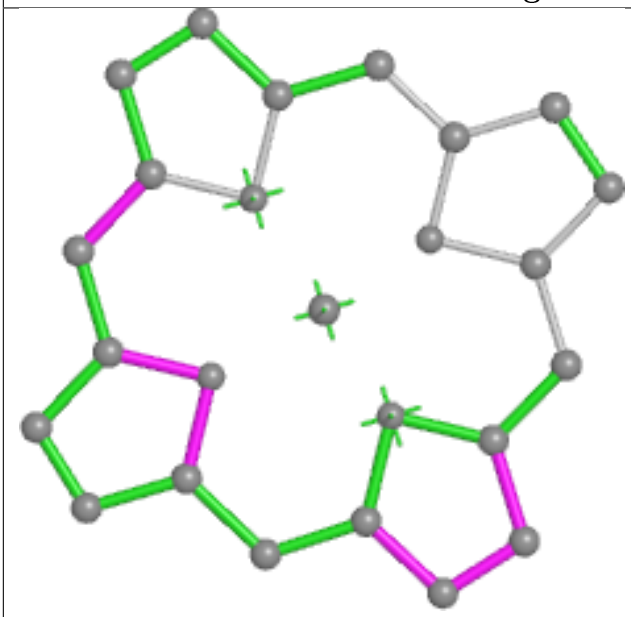
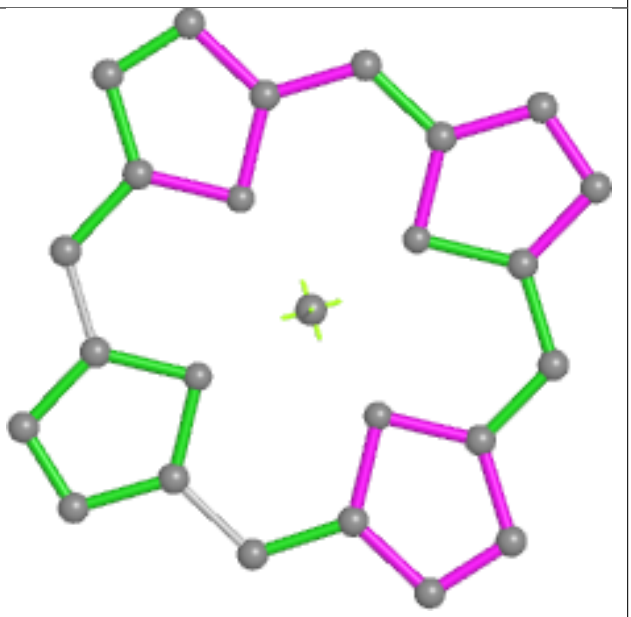


Rings

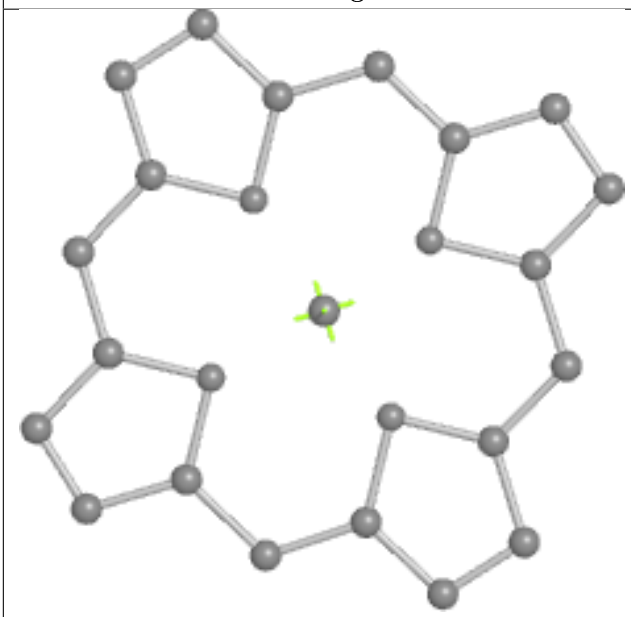
Ligand CLA D 157



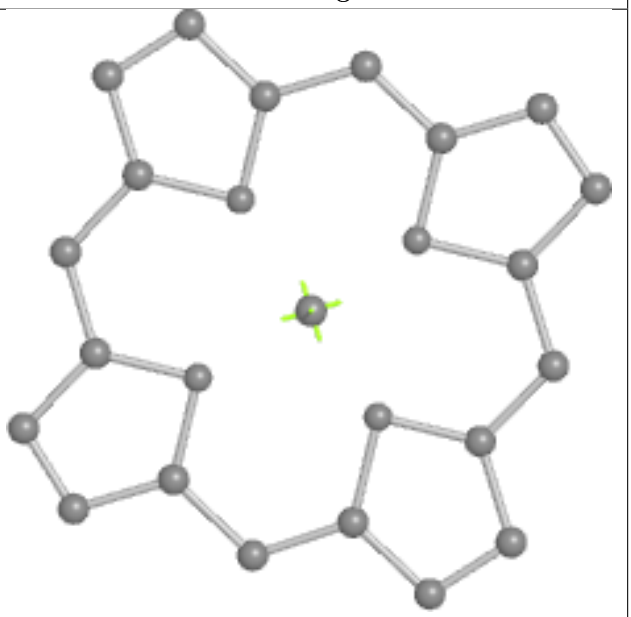
Bond lengths



Bond angles

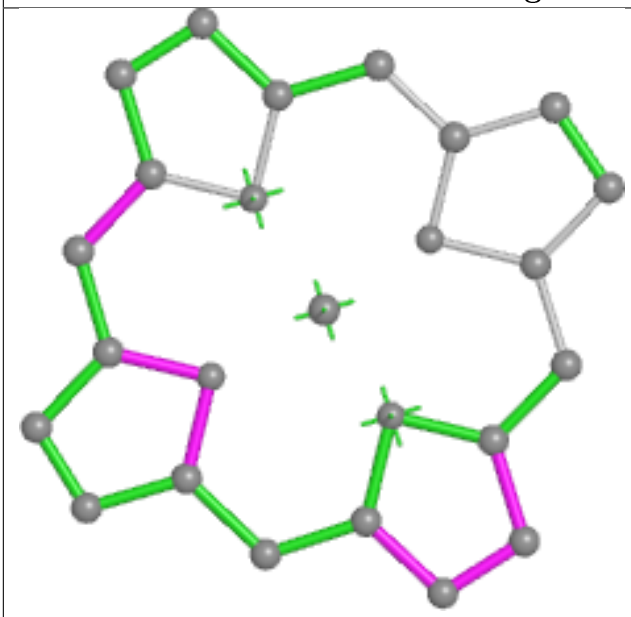


Torsions

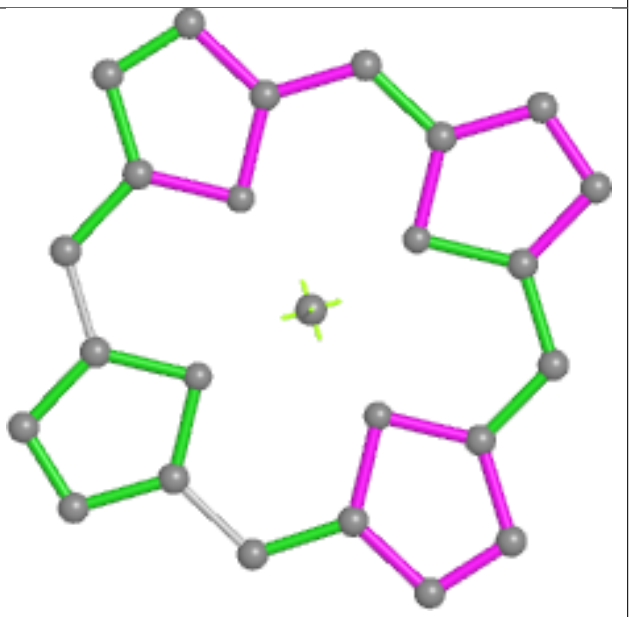


Rings

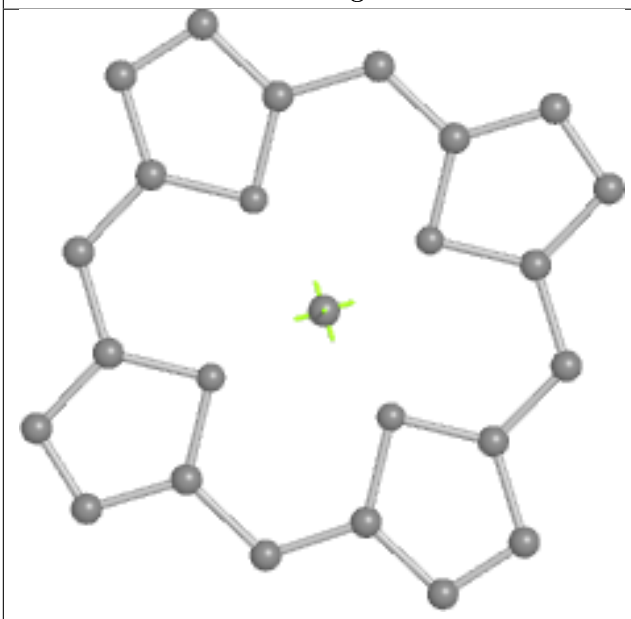
Ligand CLA A 179



Bond lengths



Bond angles



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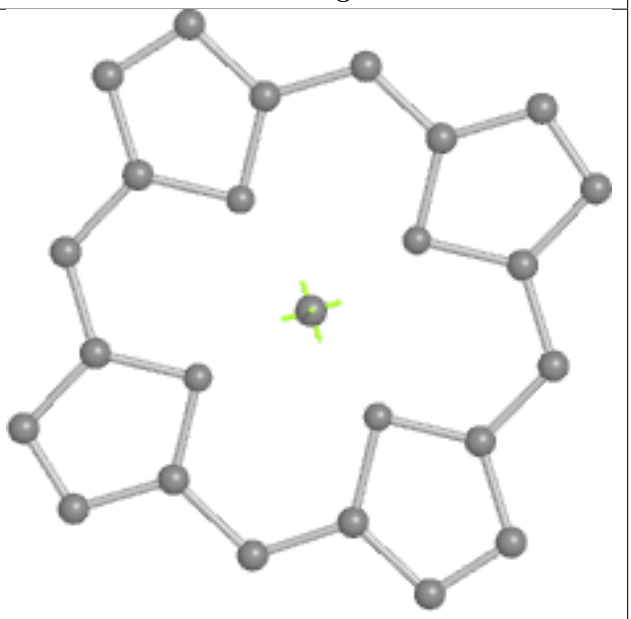
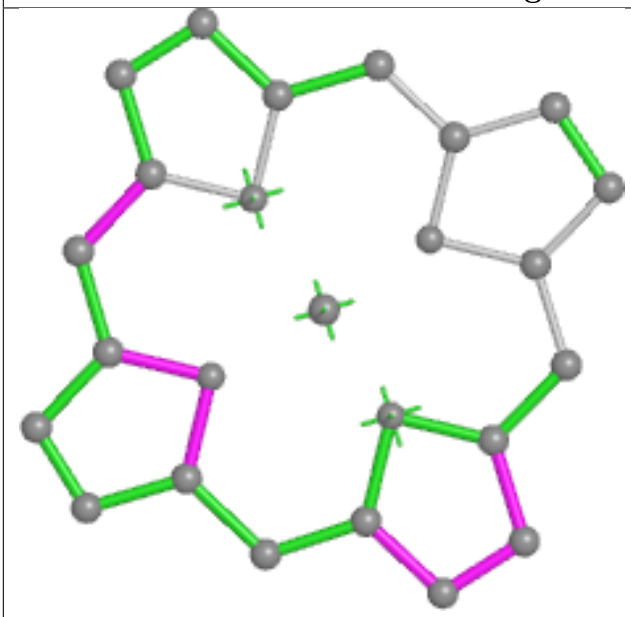
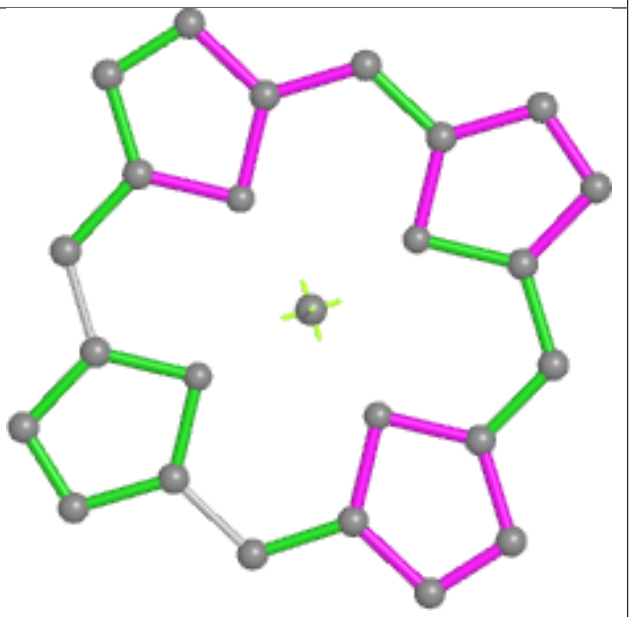


Rings

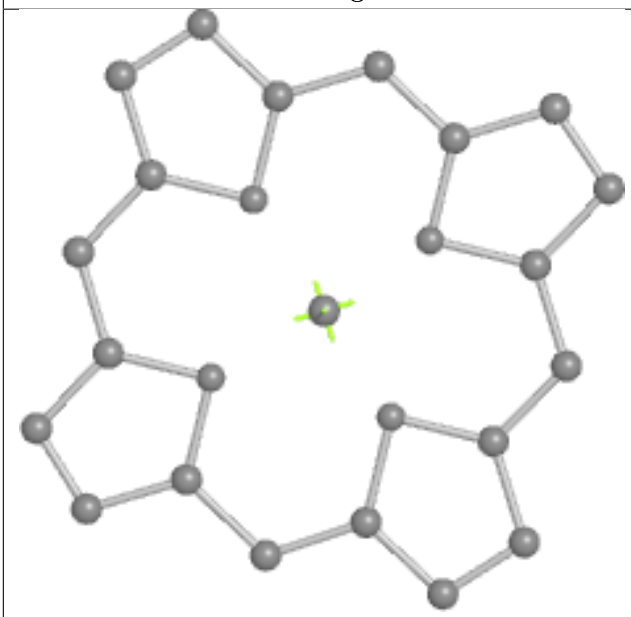
Ligand CLA C 164



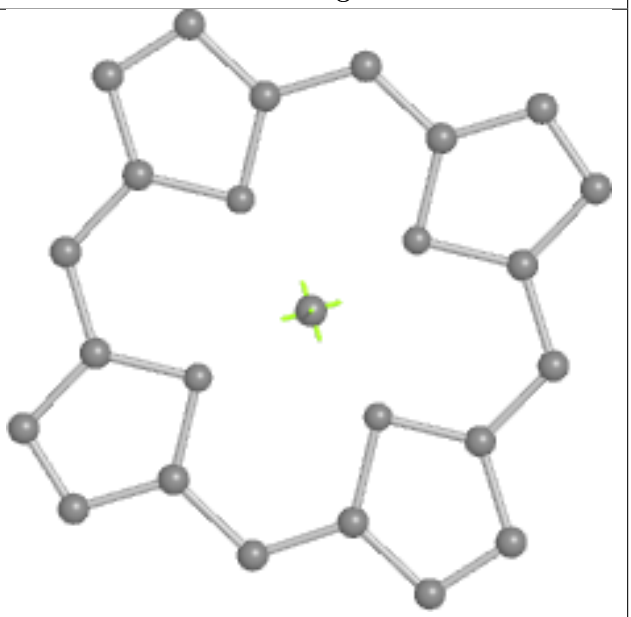
Bond lengths



Bond angles

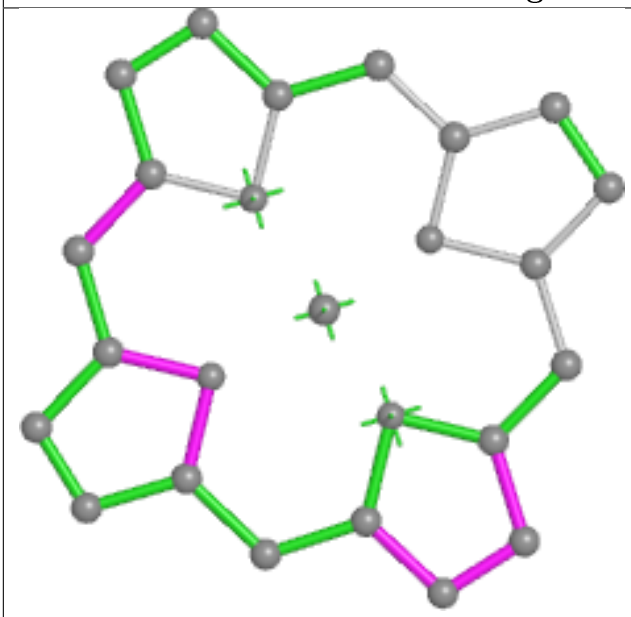


Torsions



Rings

Ligand CLA L 157



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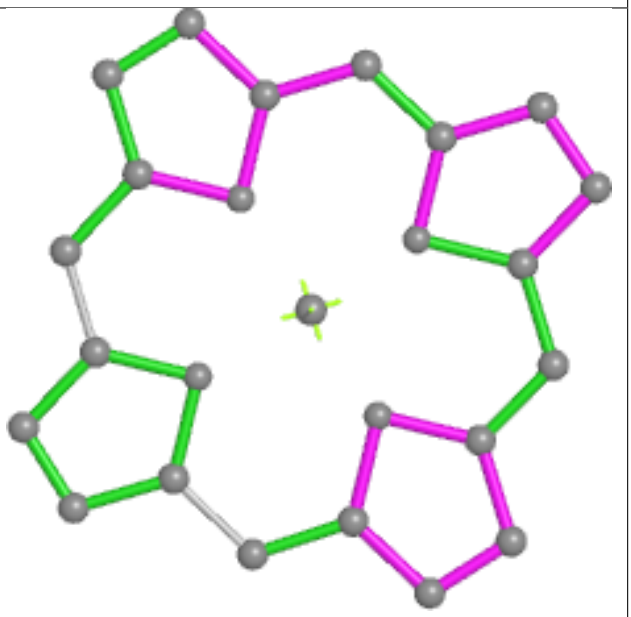
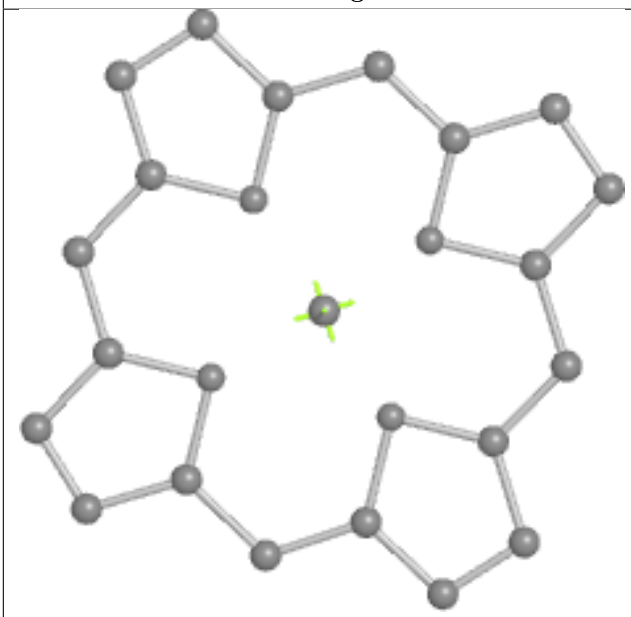


Bond angles



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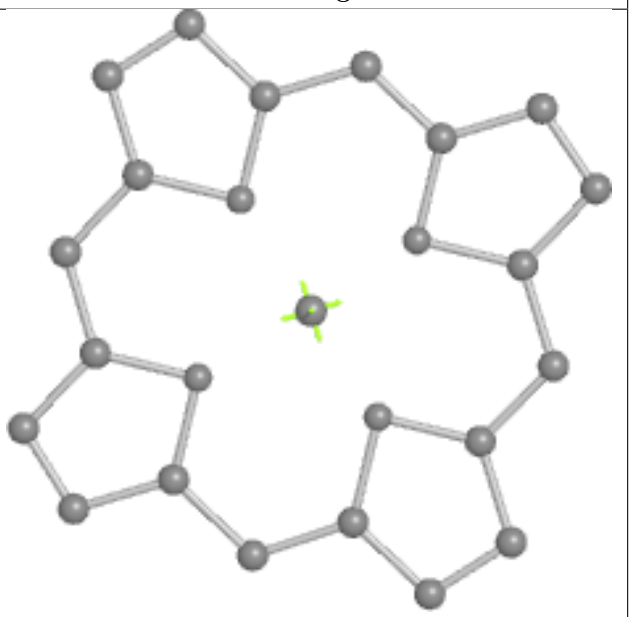
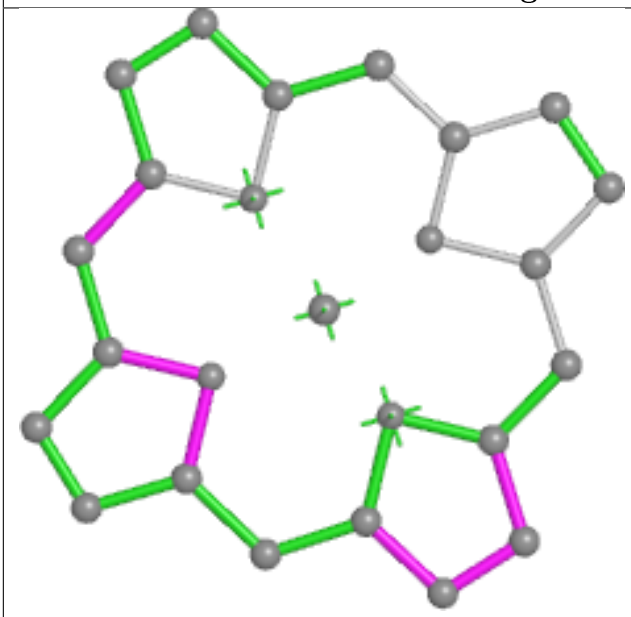


Rings

Ligand CLA M 162



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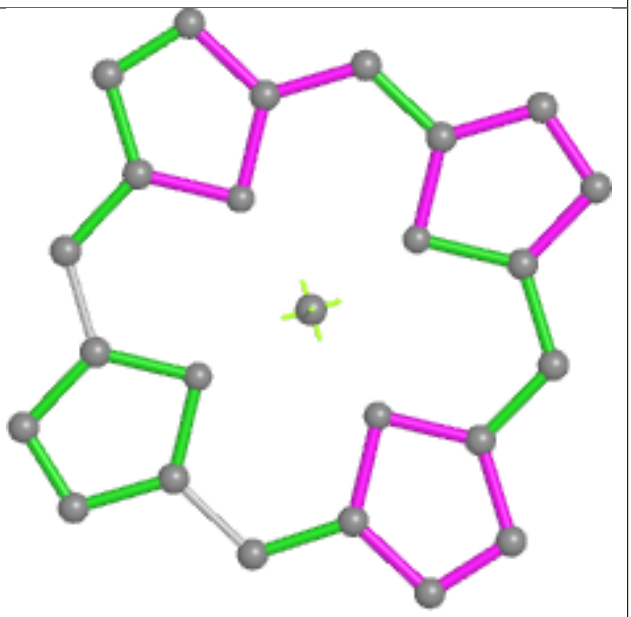
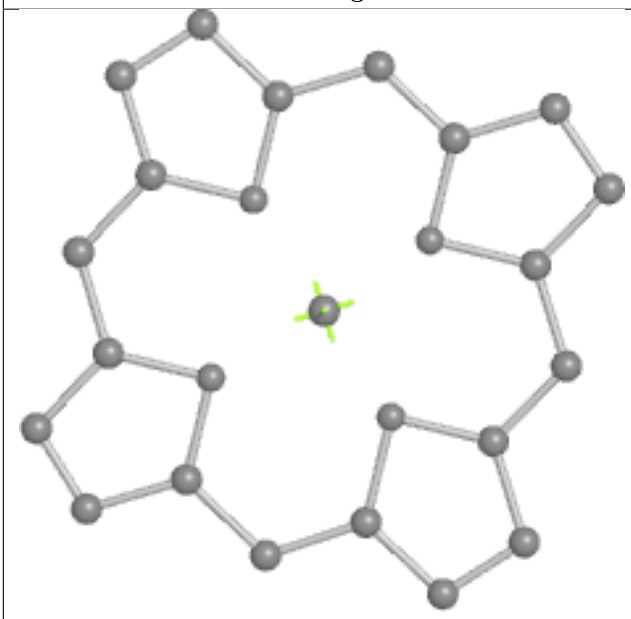


Bond angles



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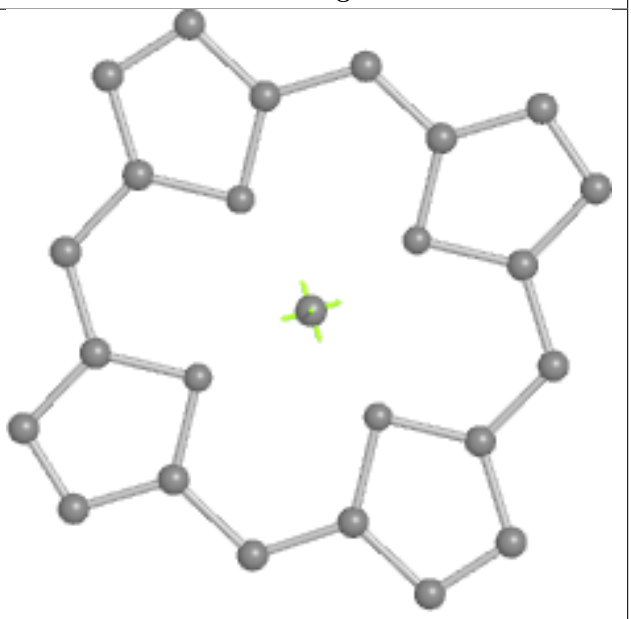
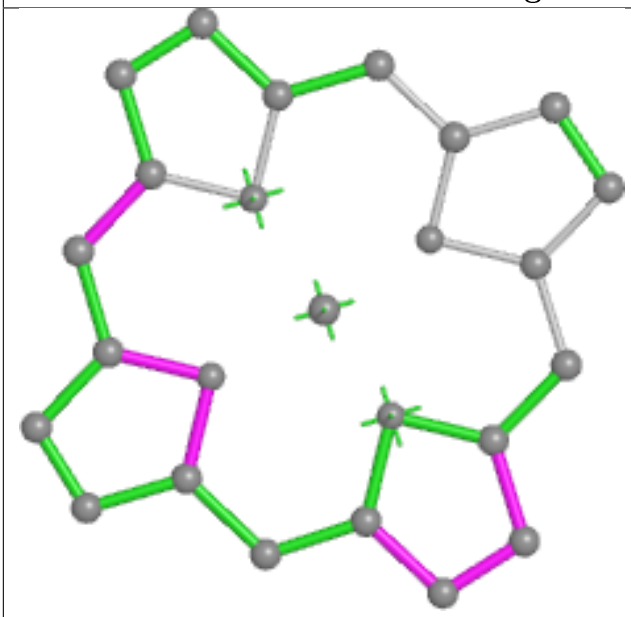


Rings

Ligand CLA B 179



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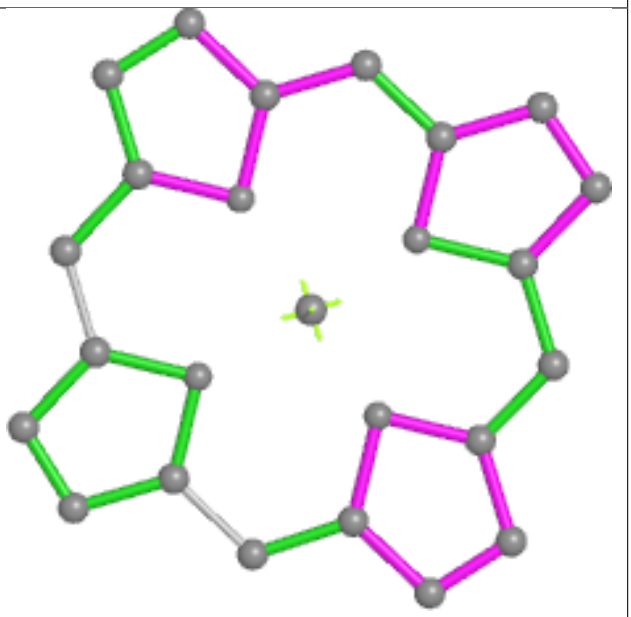
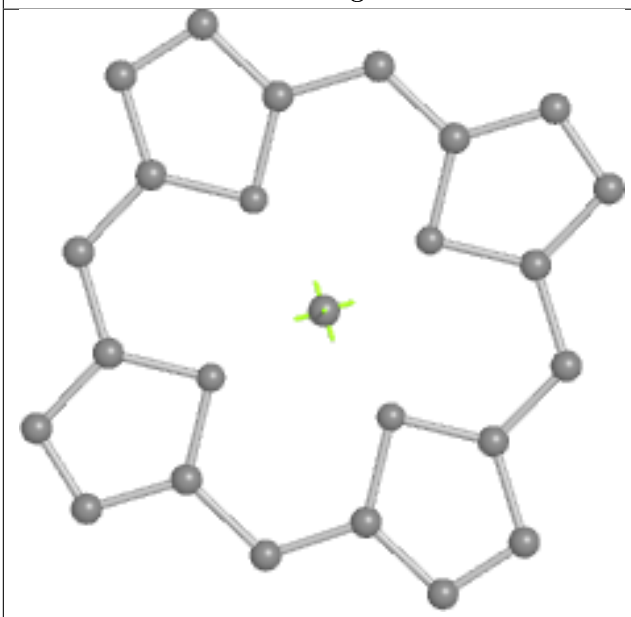


Bond angles



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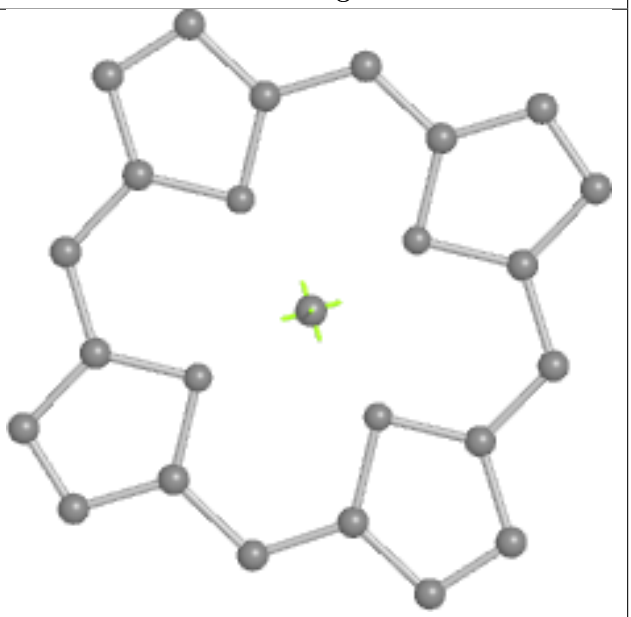
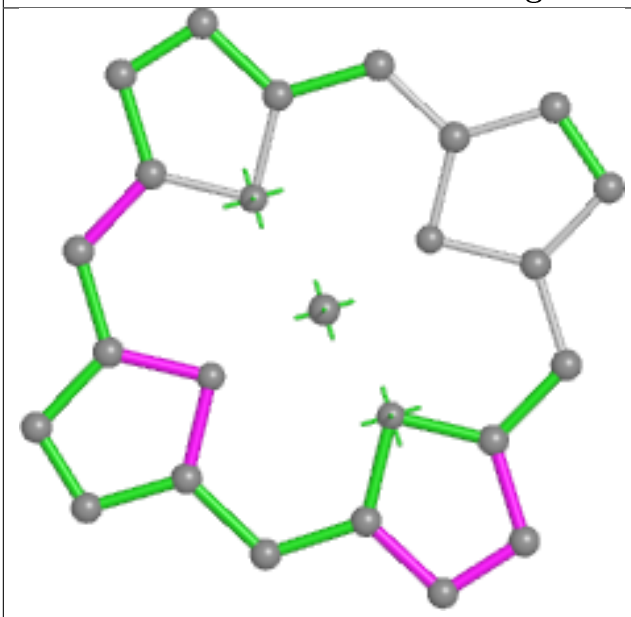


Rings

Ligand CLA P 313



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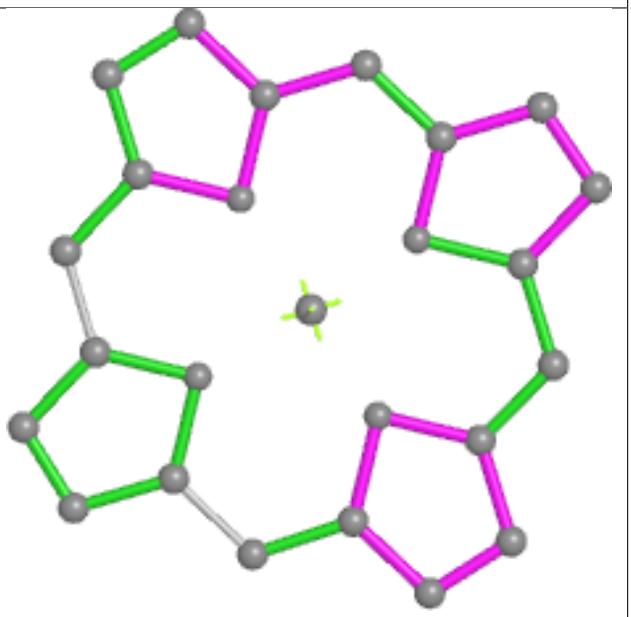

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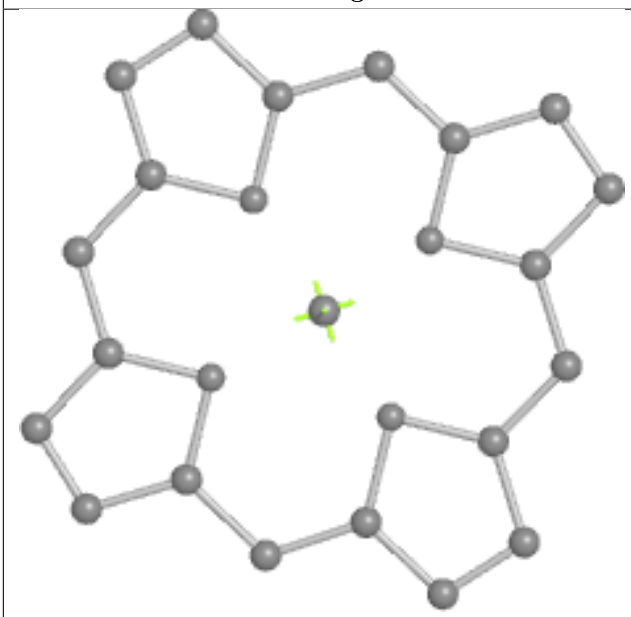

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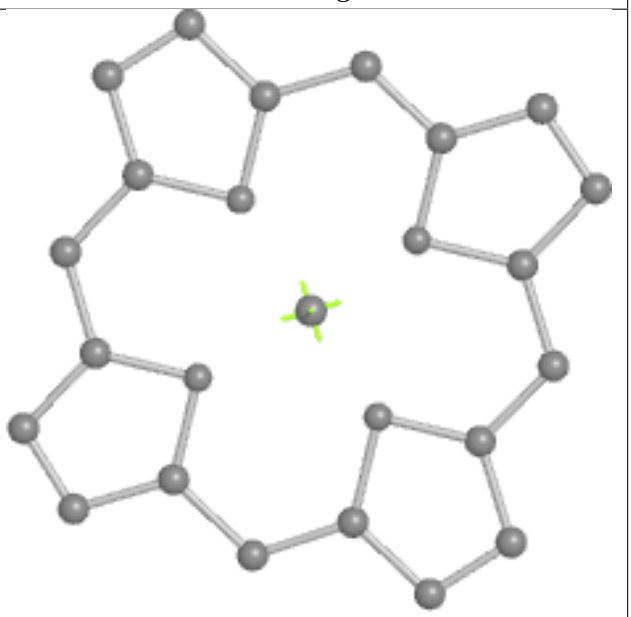
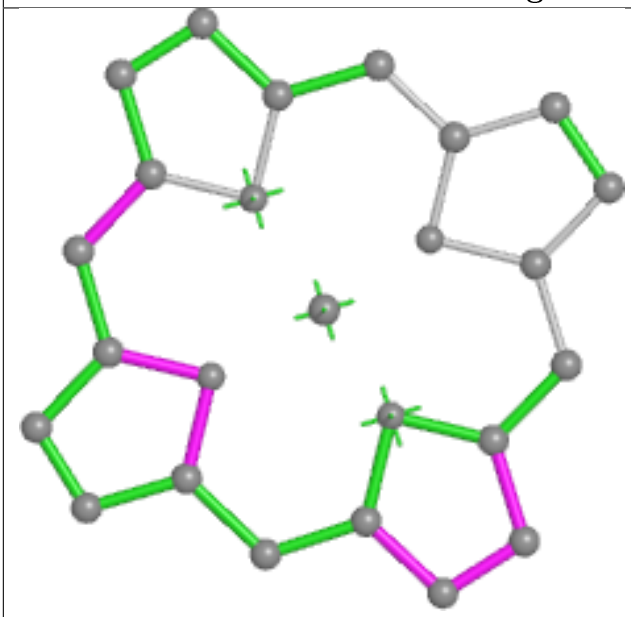


Rings

Ligand CLA L 162



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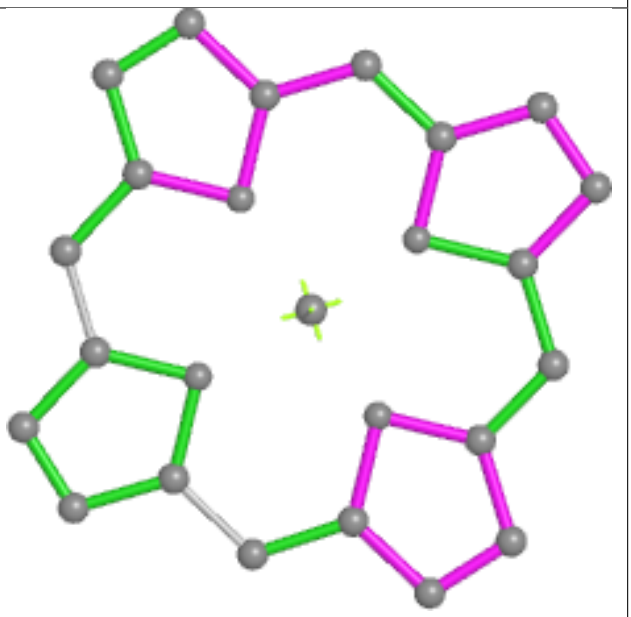
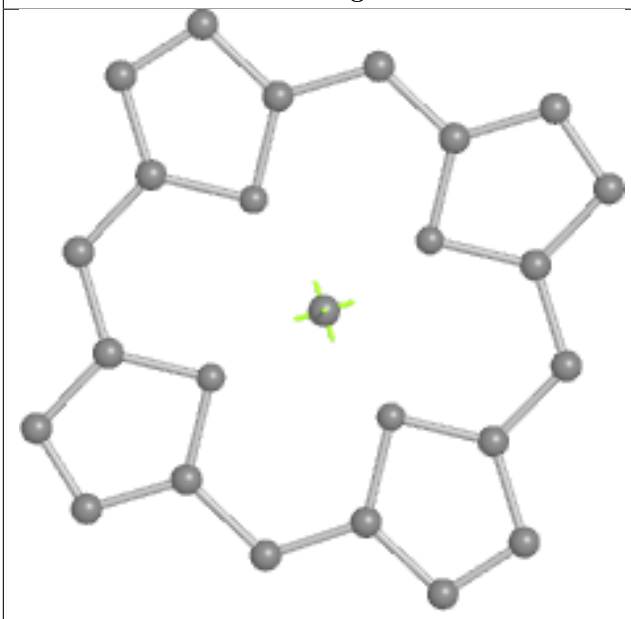


Bond angles



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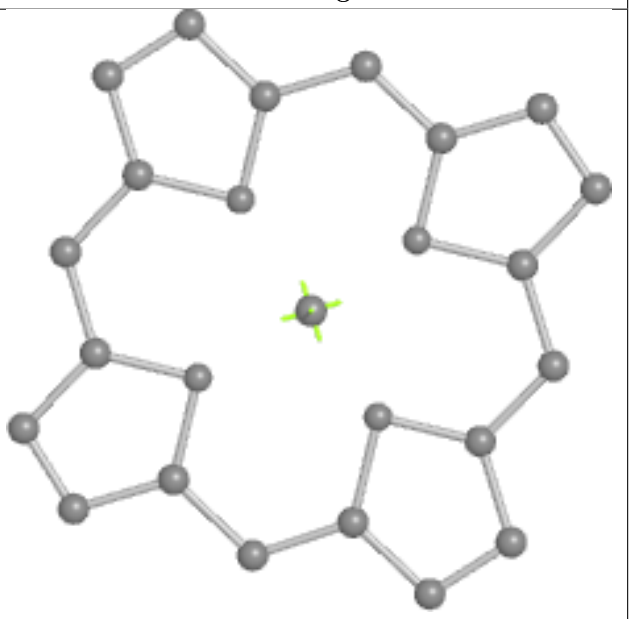
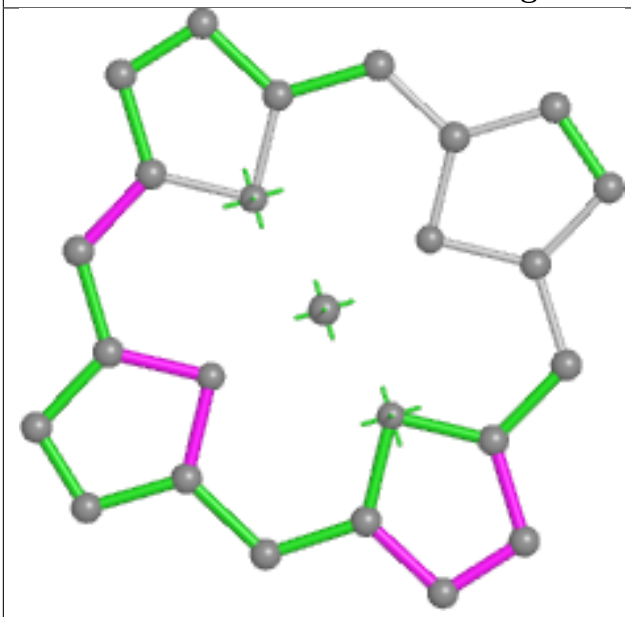


Rings

Ligand CLA M 166



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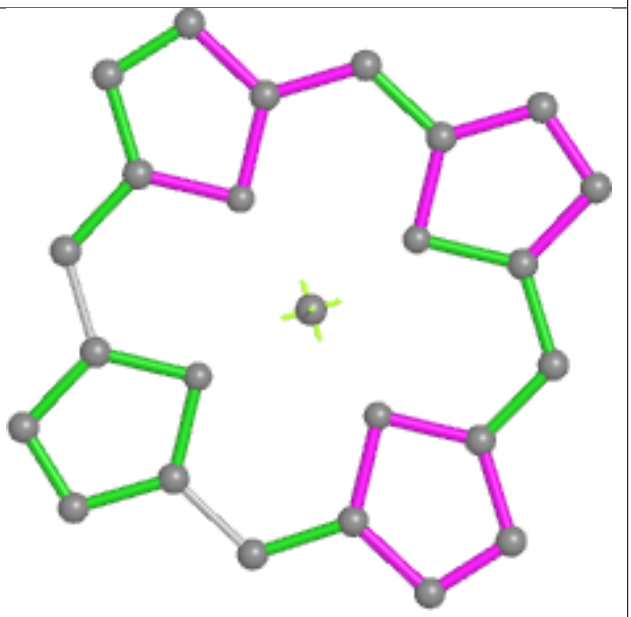
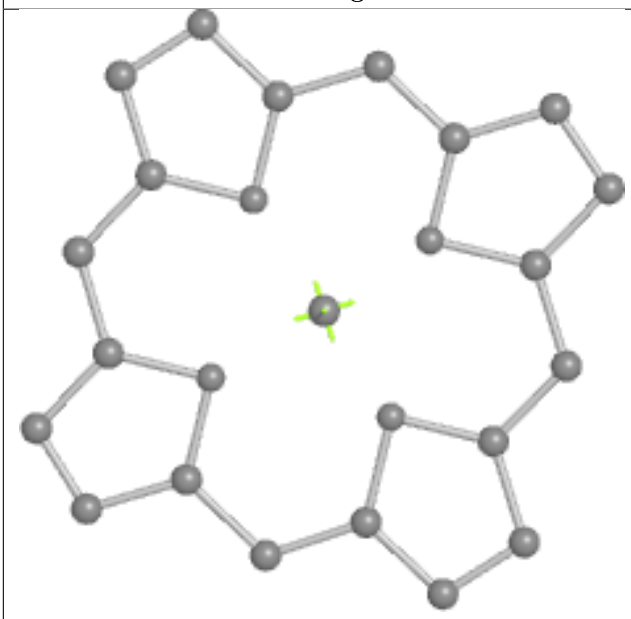


Bond angles



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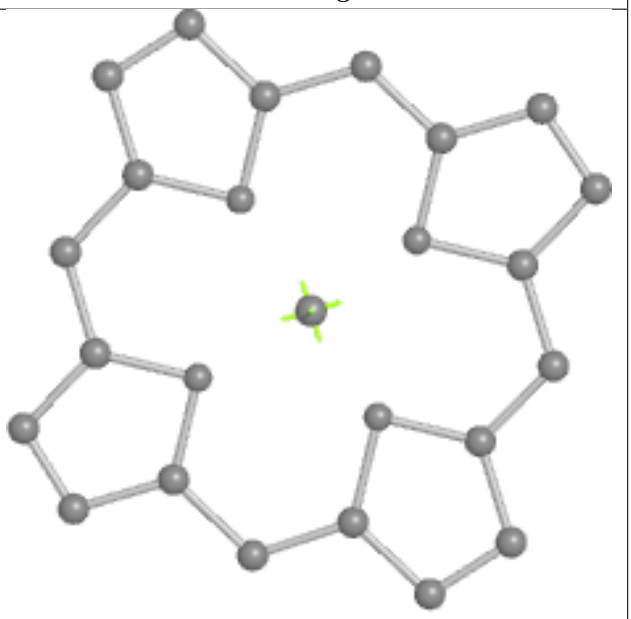
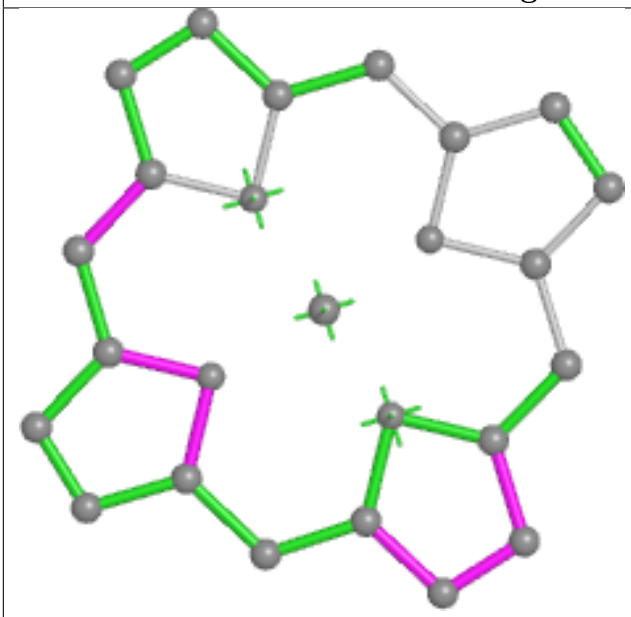


Rings

Ligand CLA M 159



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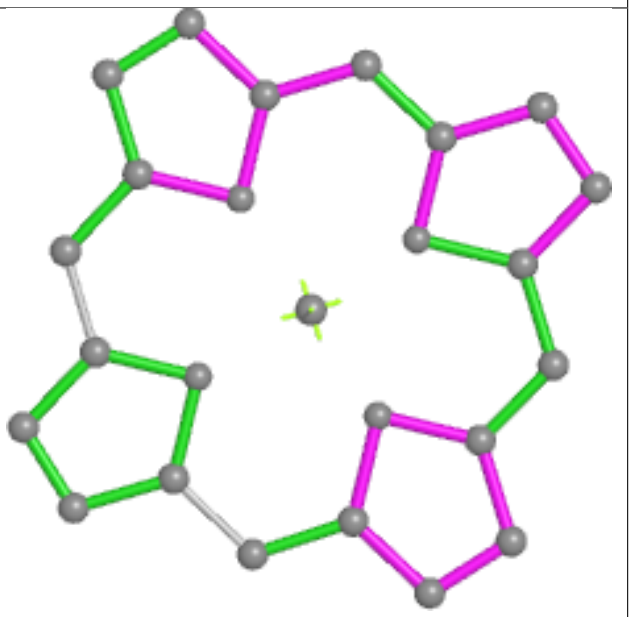
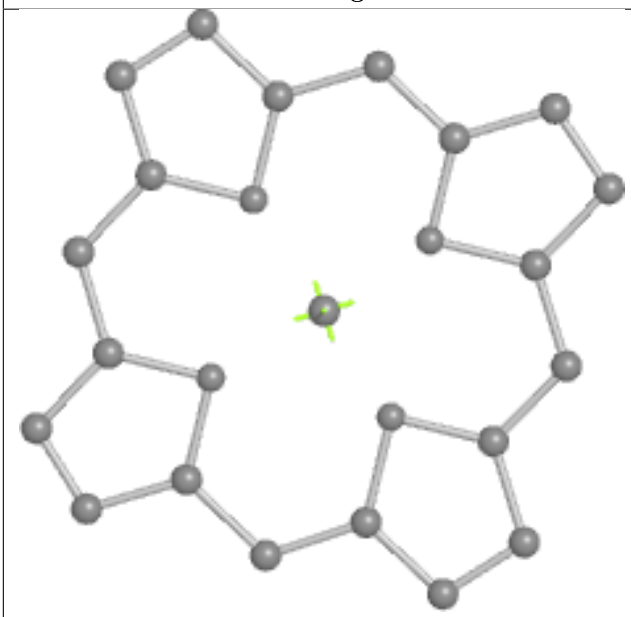


Bond angles



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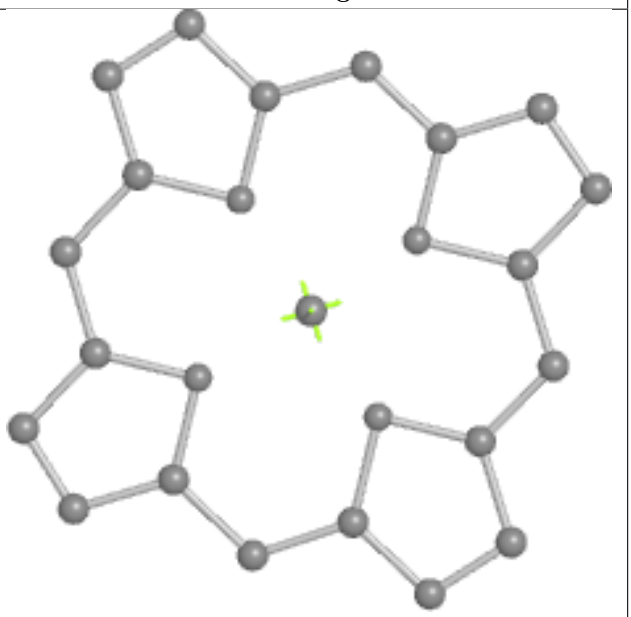
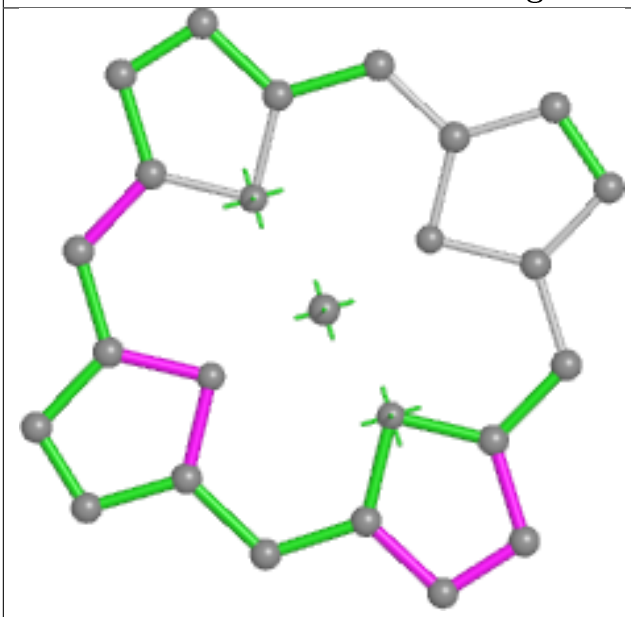
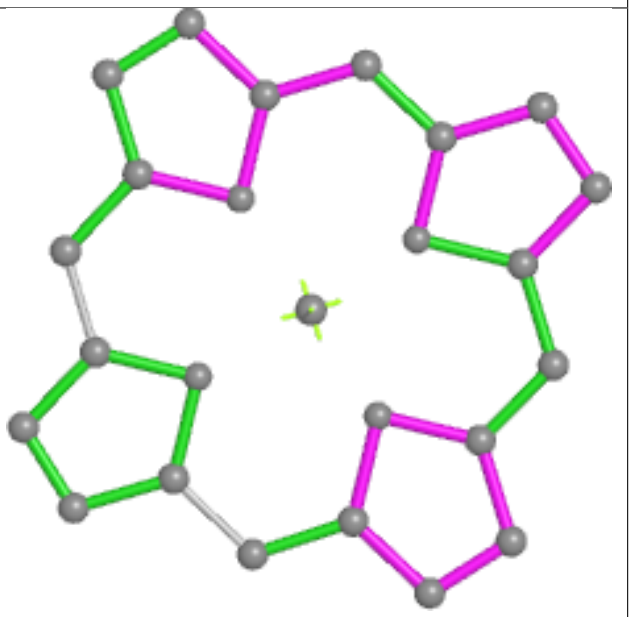


Rings

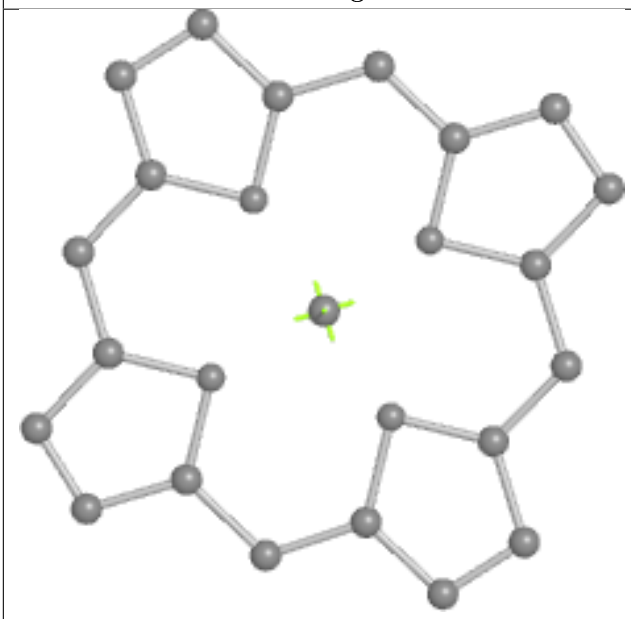
Ligand CLA L 166



Bond lengths



Bond angles



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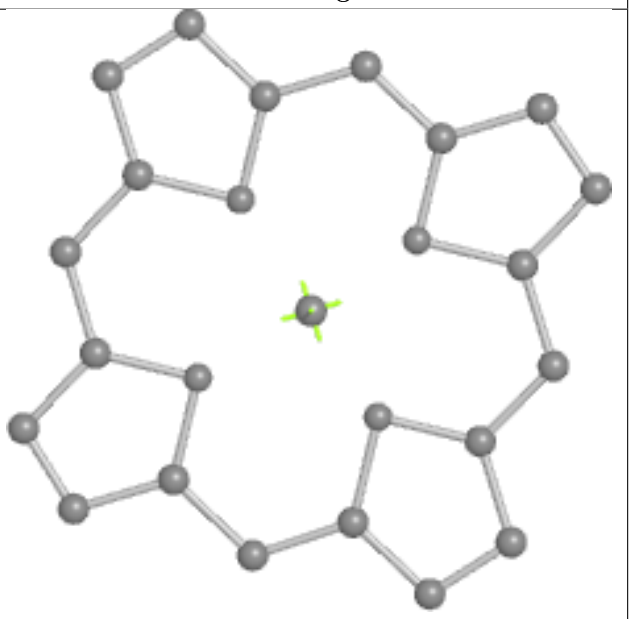
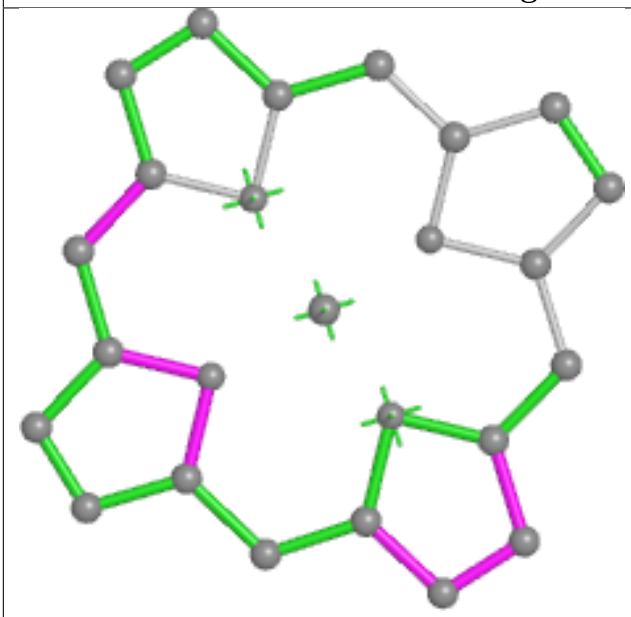


Rings

Ligand CLA M 157



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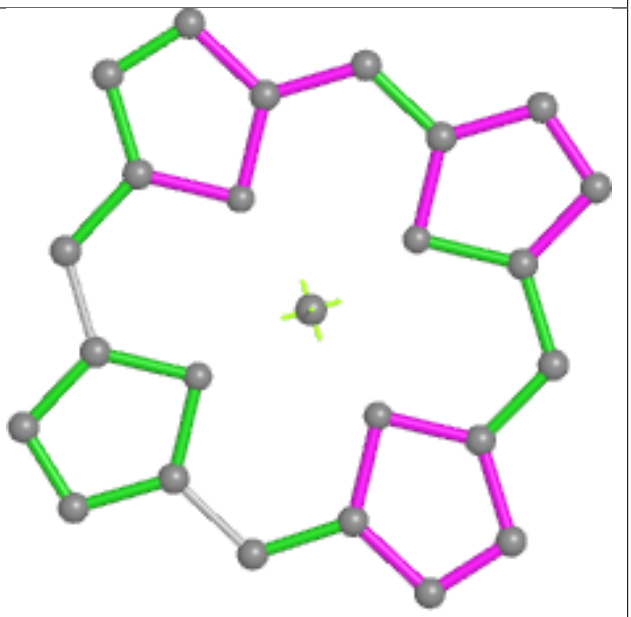

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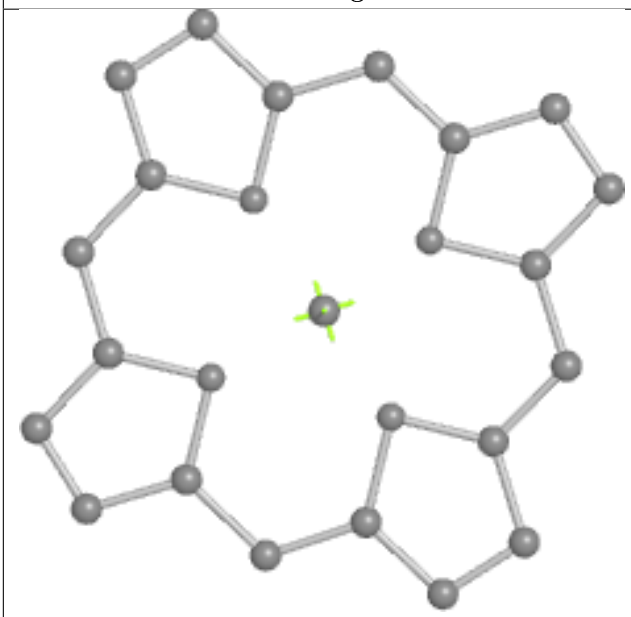

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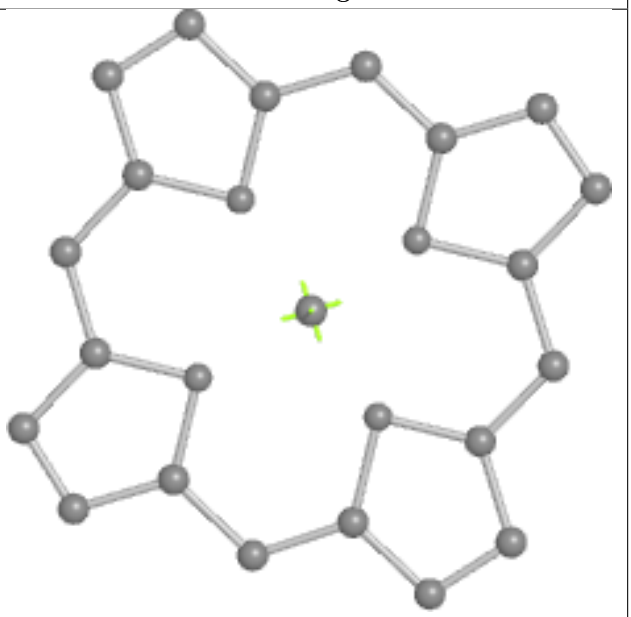
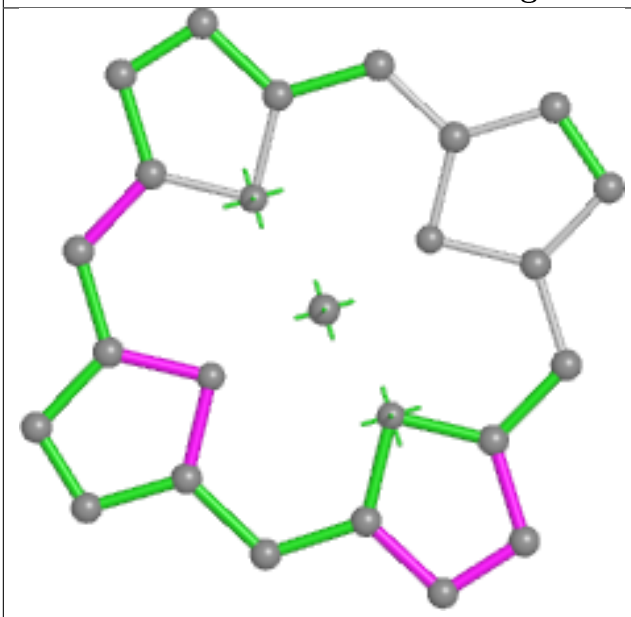


Rings

Ligand CLA M 158



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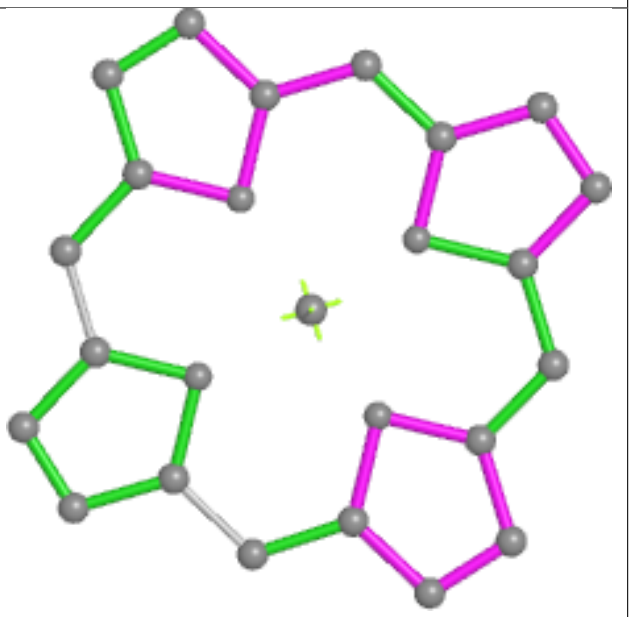
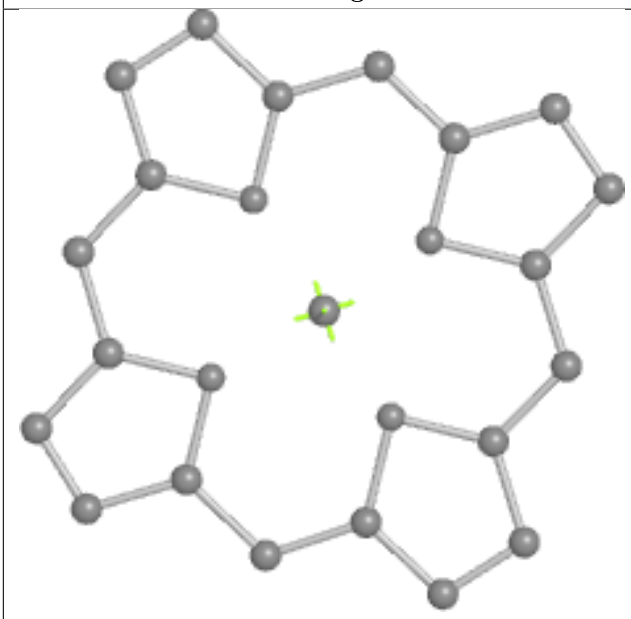


Bond angles



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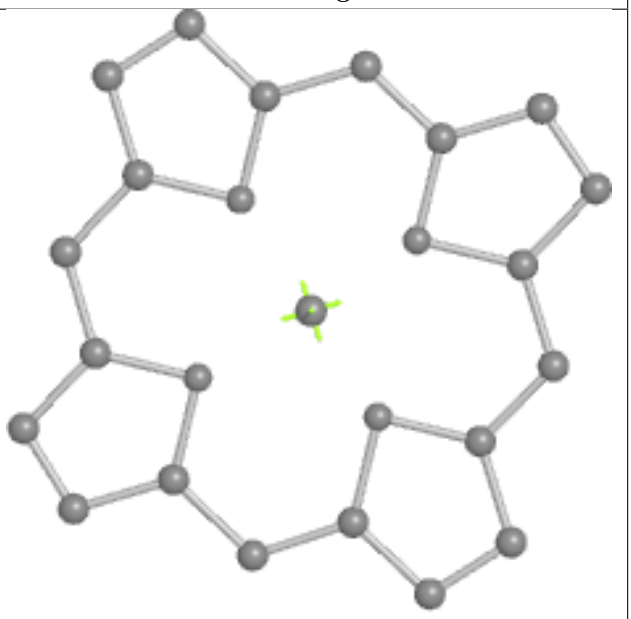
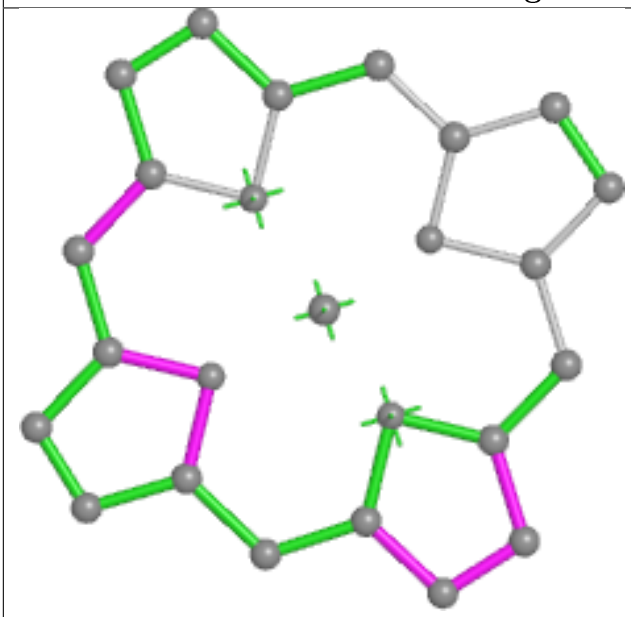


Rings

Ligand CLA C 166



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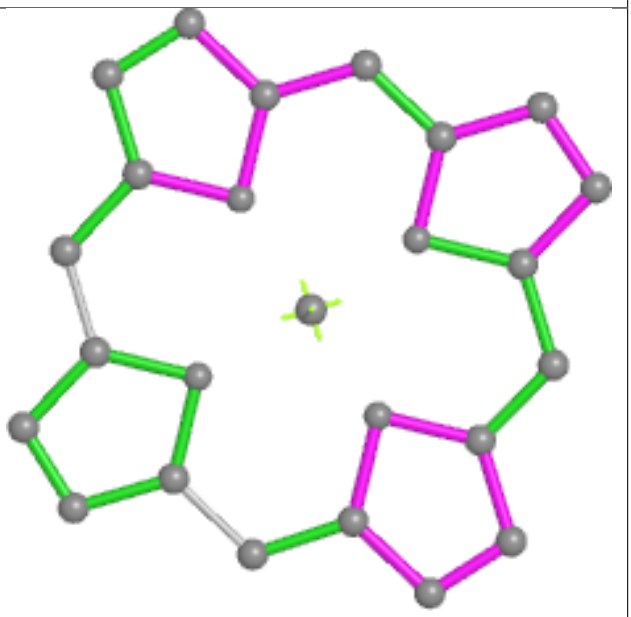
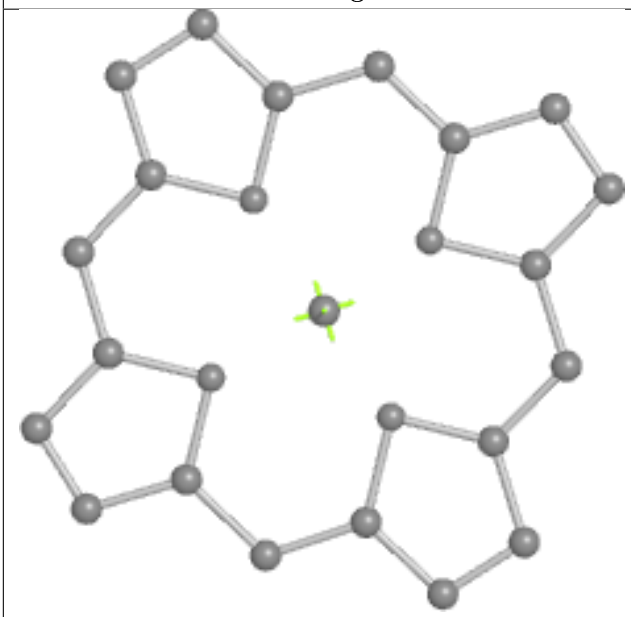


Bond angles



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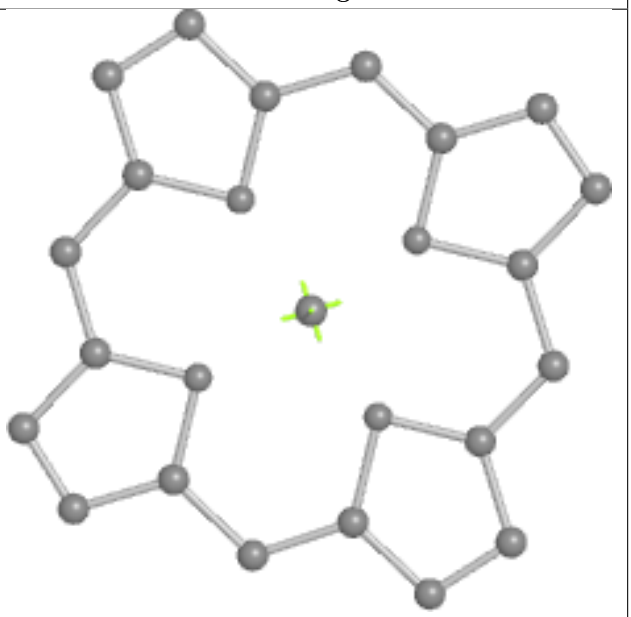
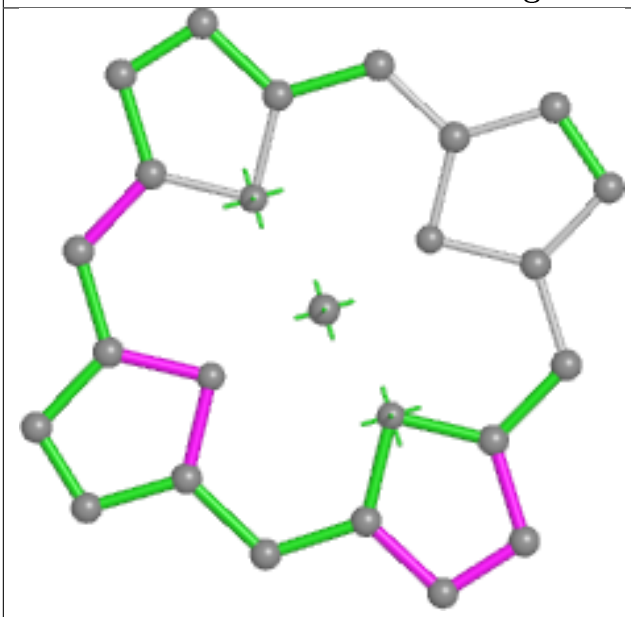


Rings

Ligand CLA D 162



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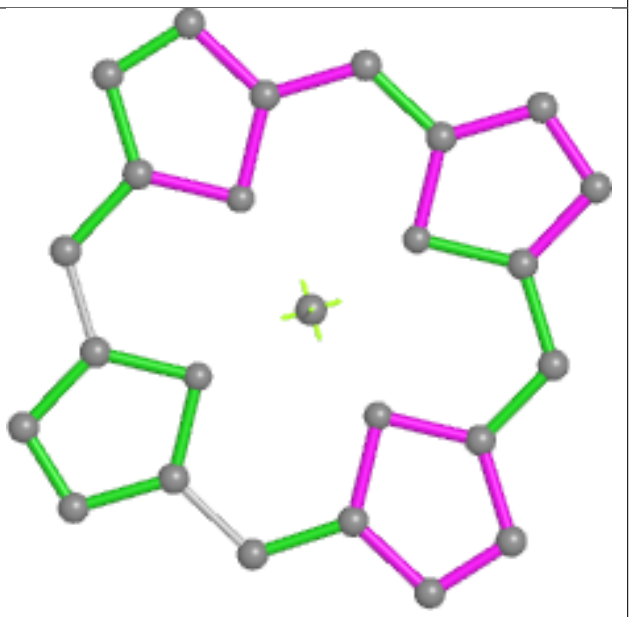
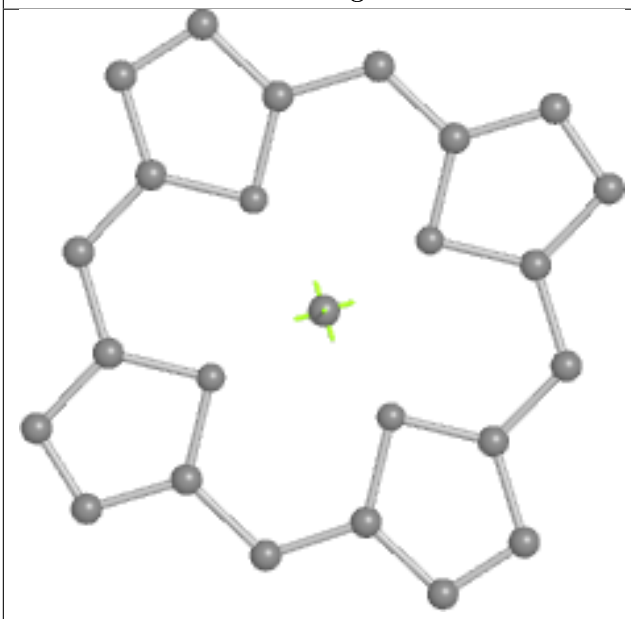
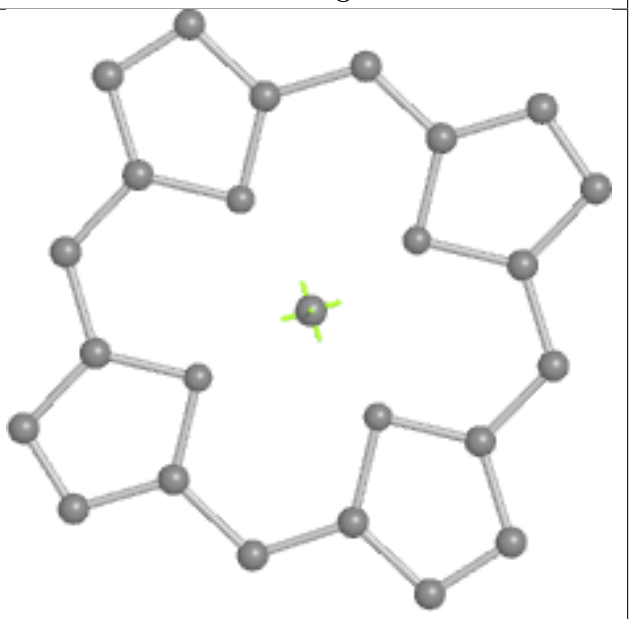


Bond angles

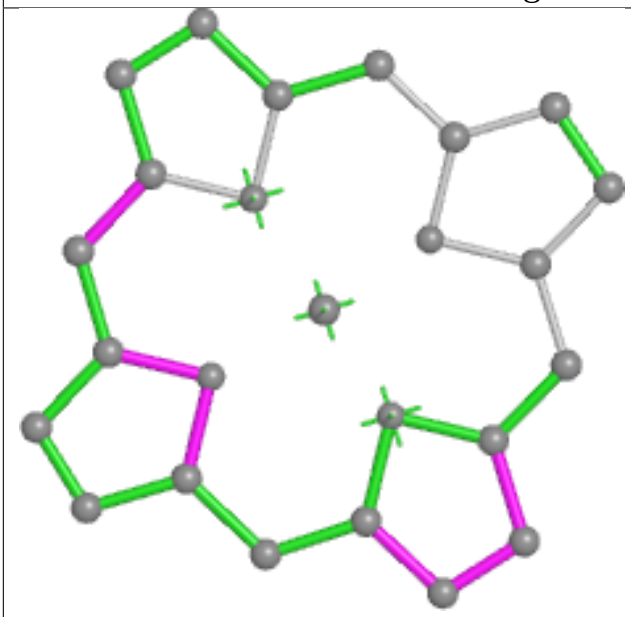


Torsions

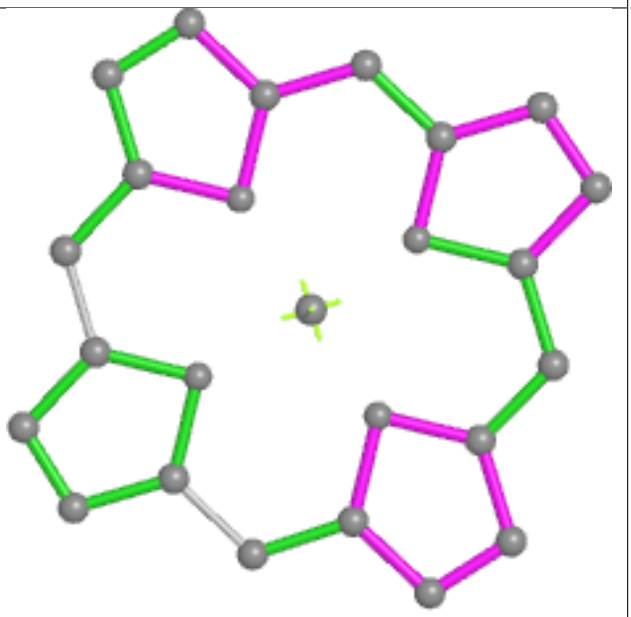


Rings

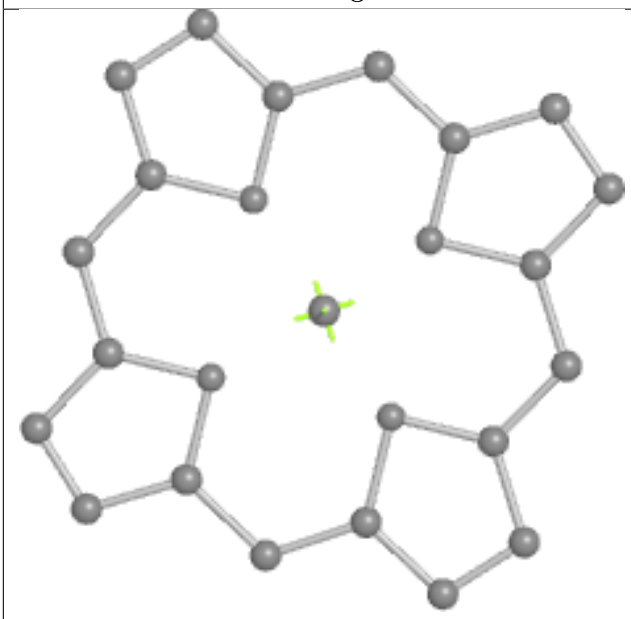
Ligand CLA D 168



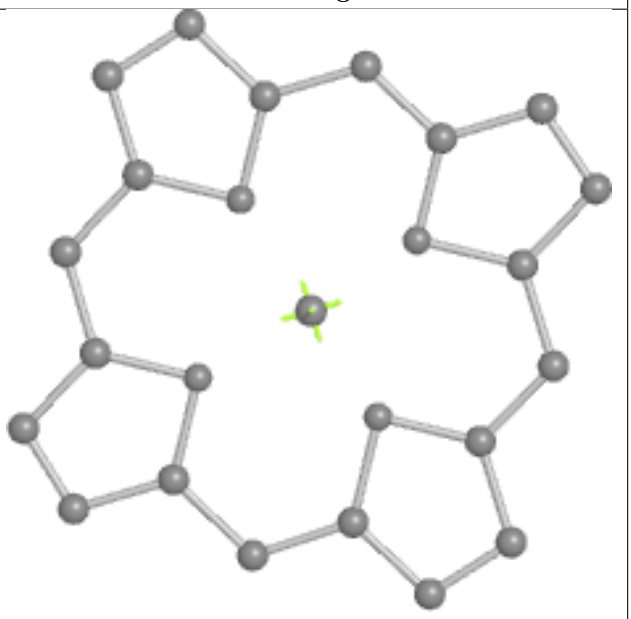
Bond lengths



Bond angles

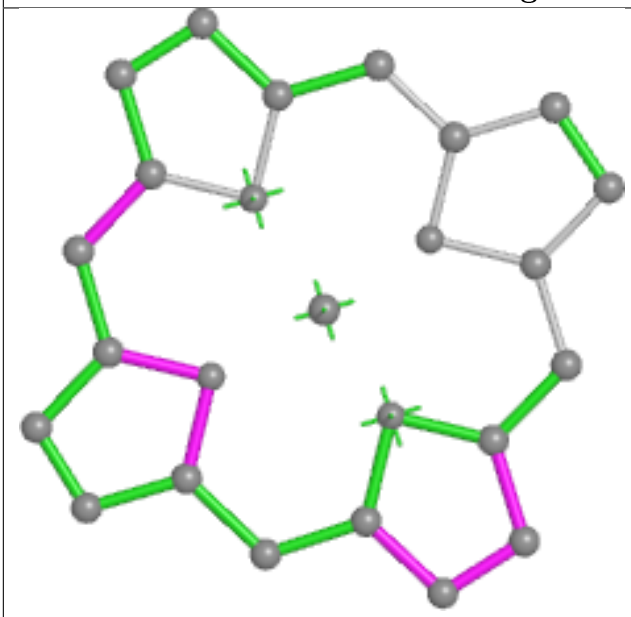


Torsions

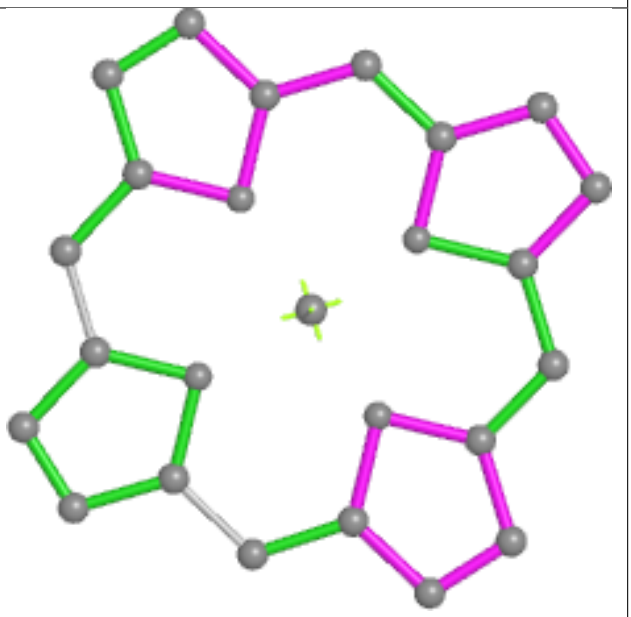


Rings

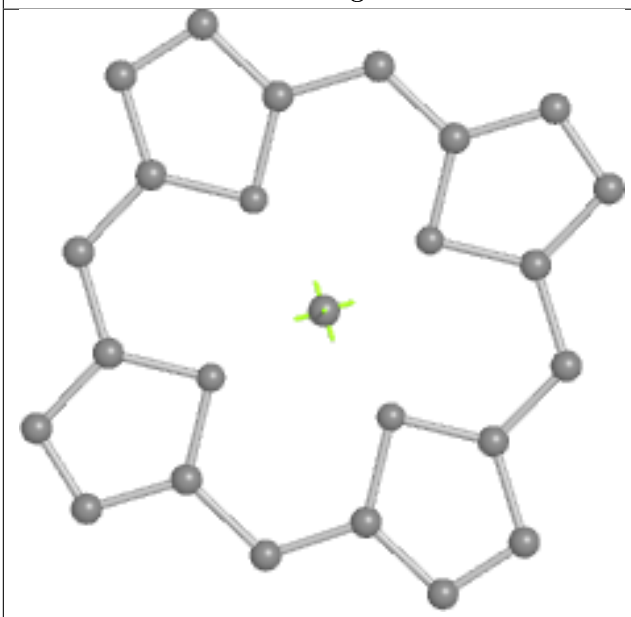
Ligand CLA M 160



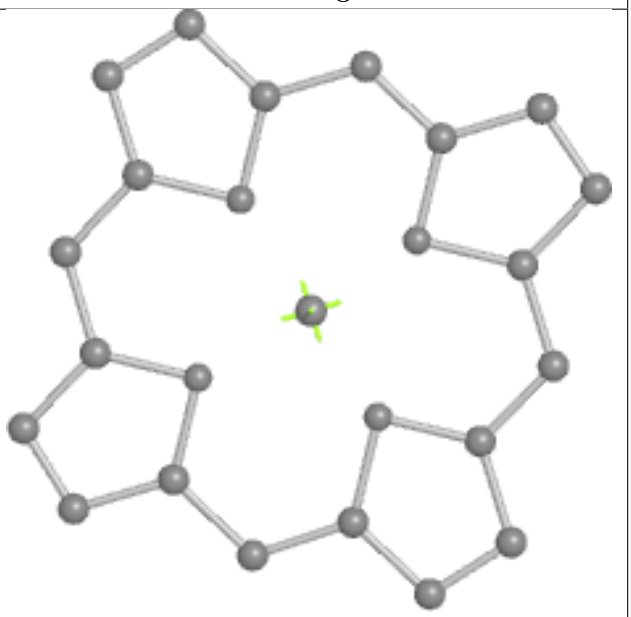
Bond lengths



Bond angles

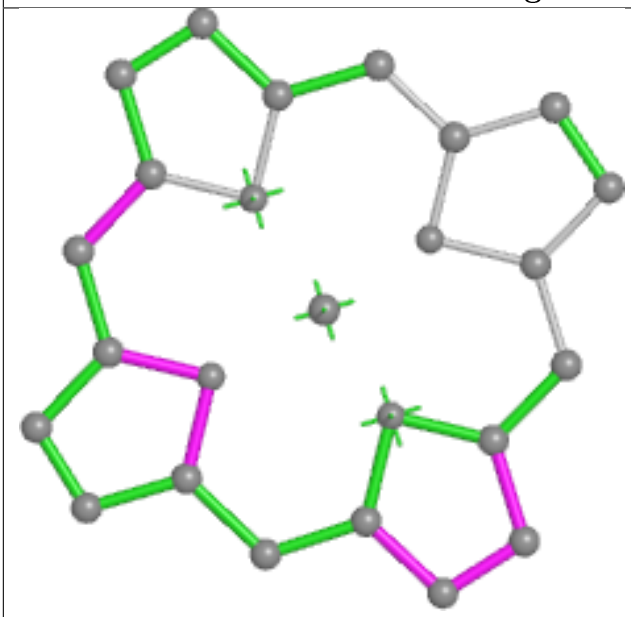


Torsions

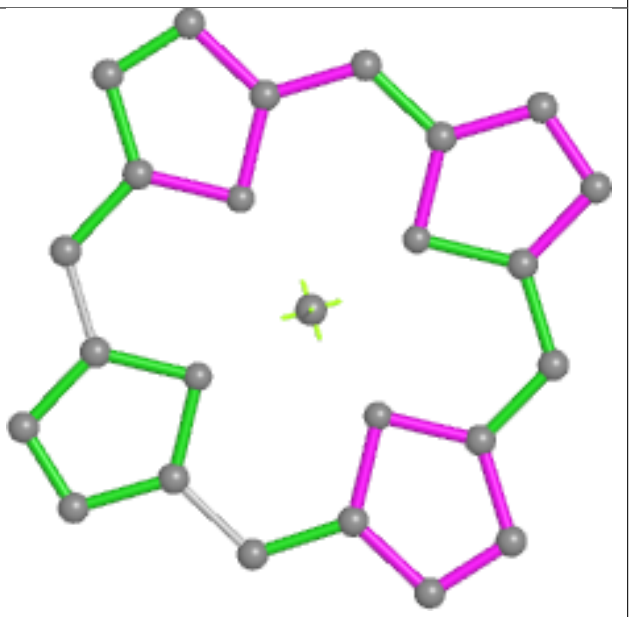


Rings

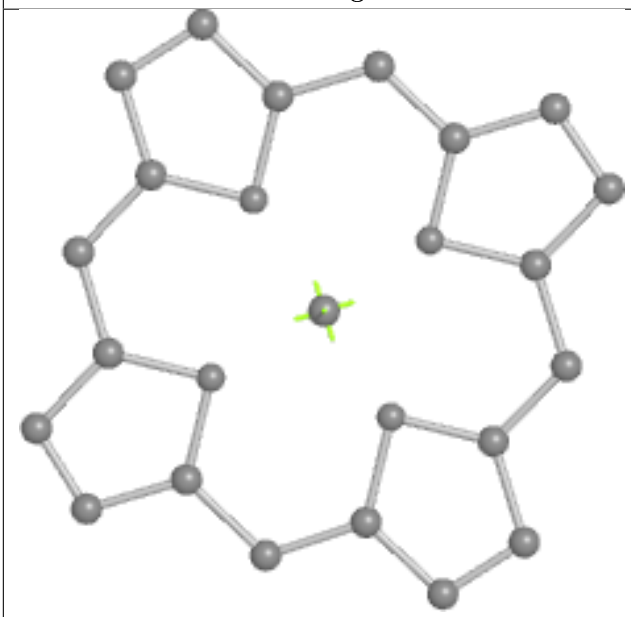
Ligand CLA C 158



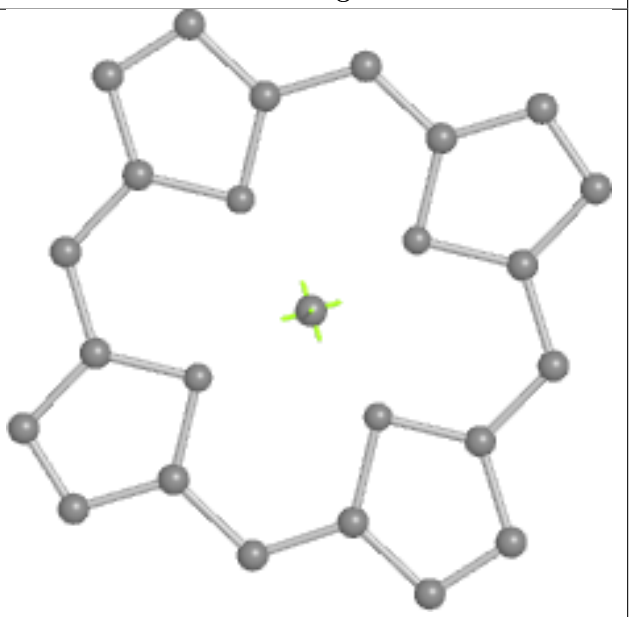
Bond lengths



Bond angles

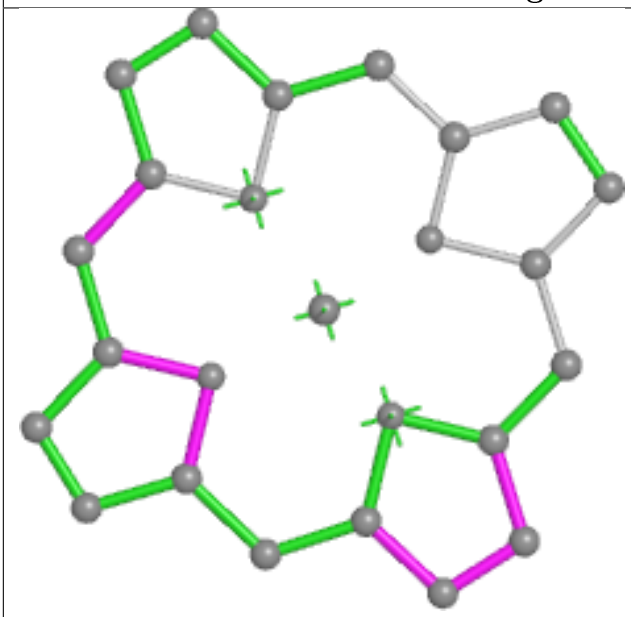


Torsions

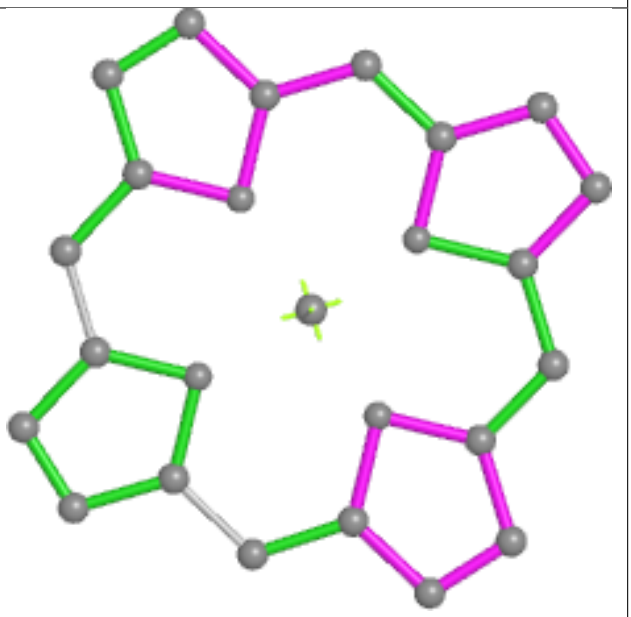


Rings

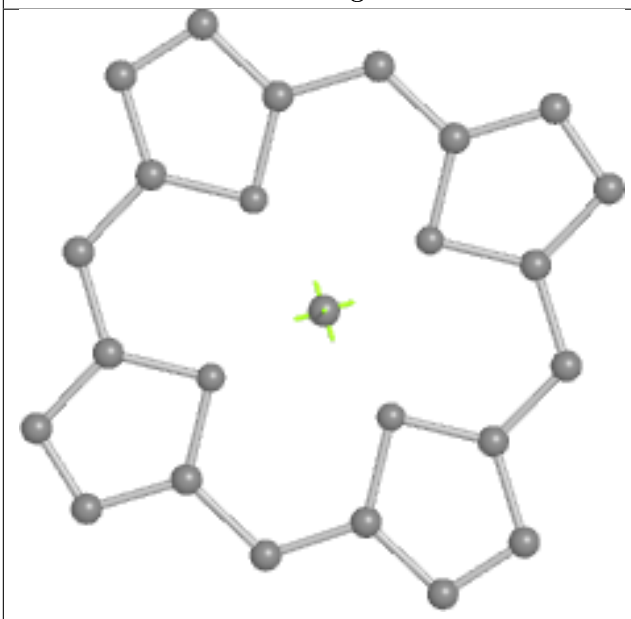
Ligand CLA L 168



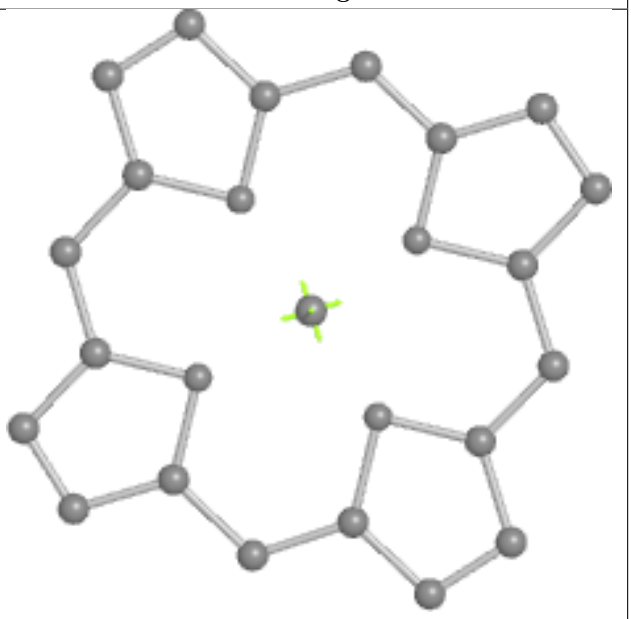
Bond lengths



Bond angles

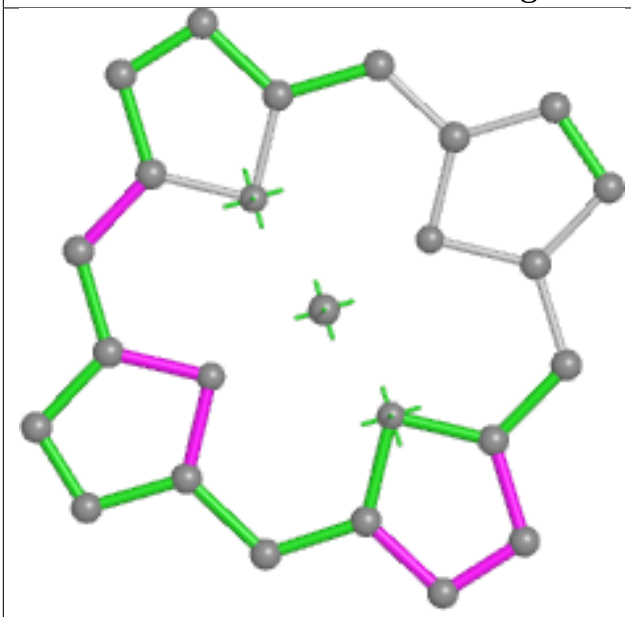


Torsions



Rings

Ligand CLA M 164



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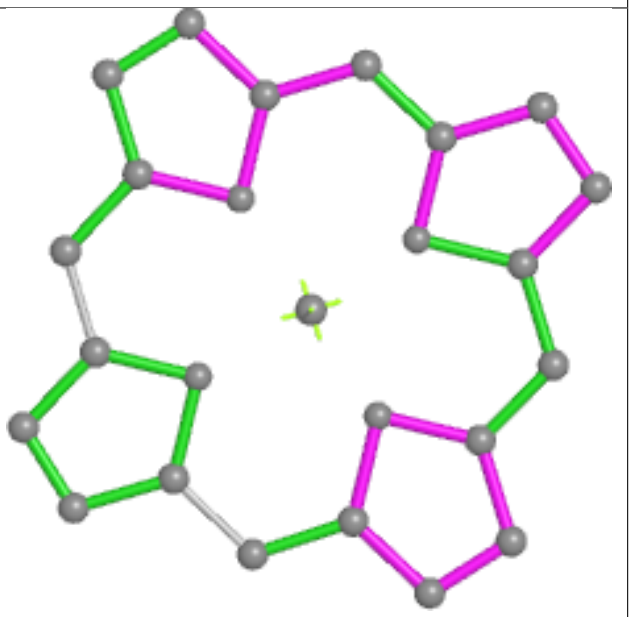

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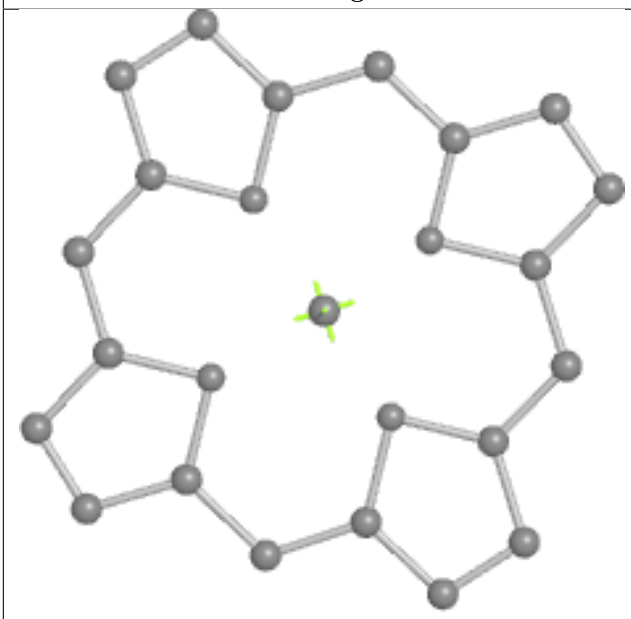
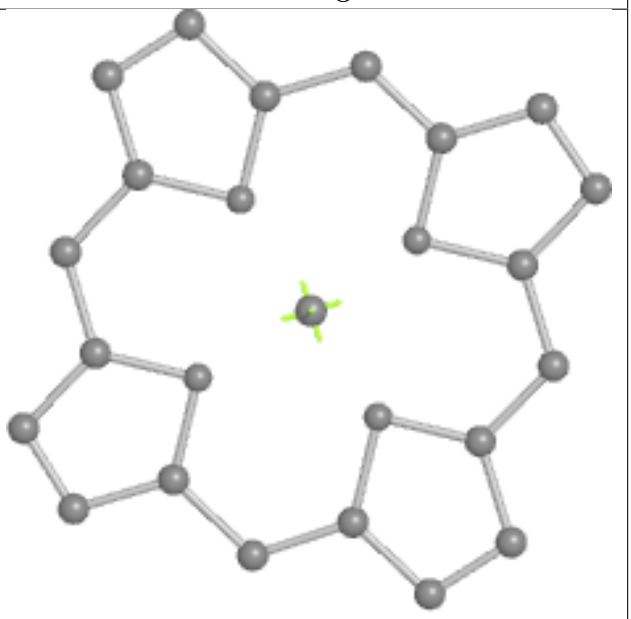
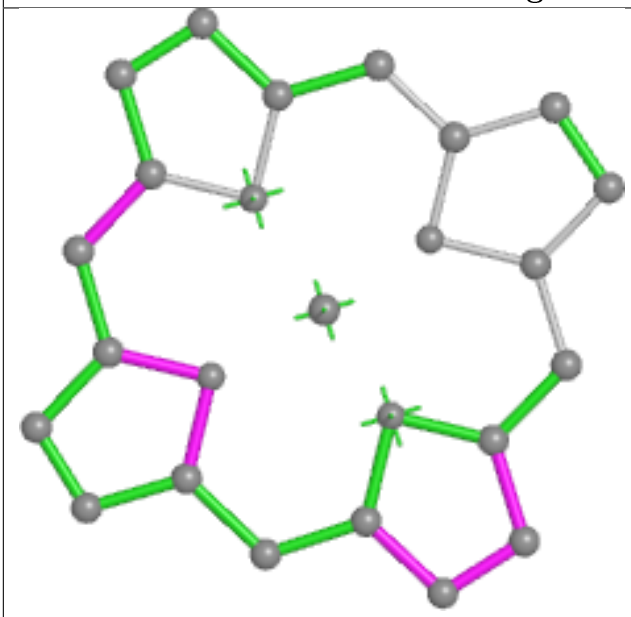


Torsions

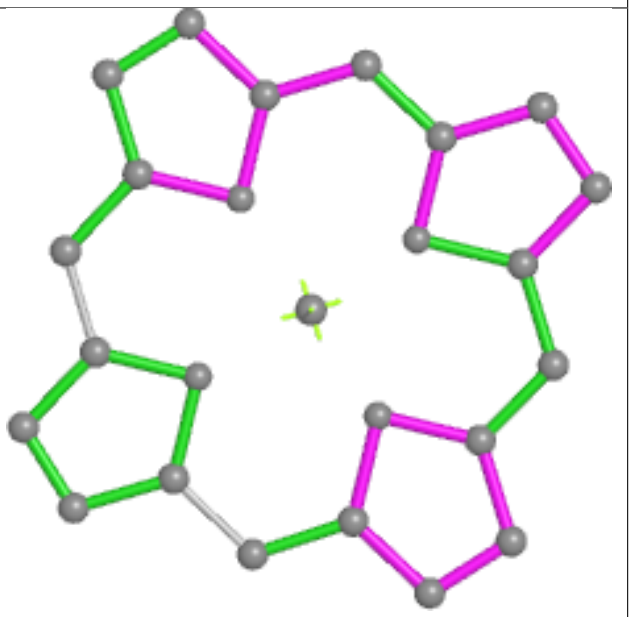


Rings

Ligand CLA L 163



Bond lengths



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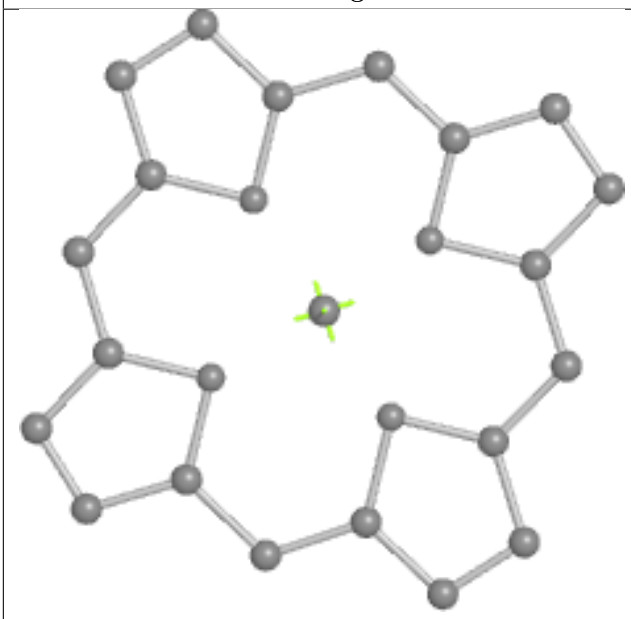

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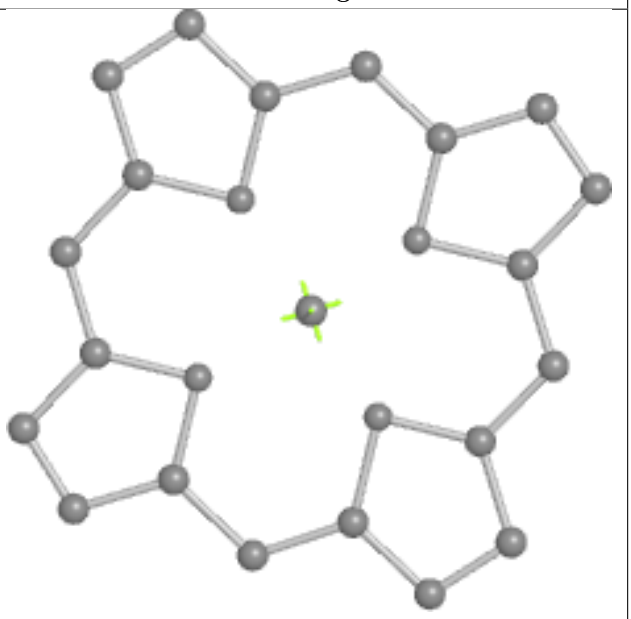
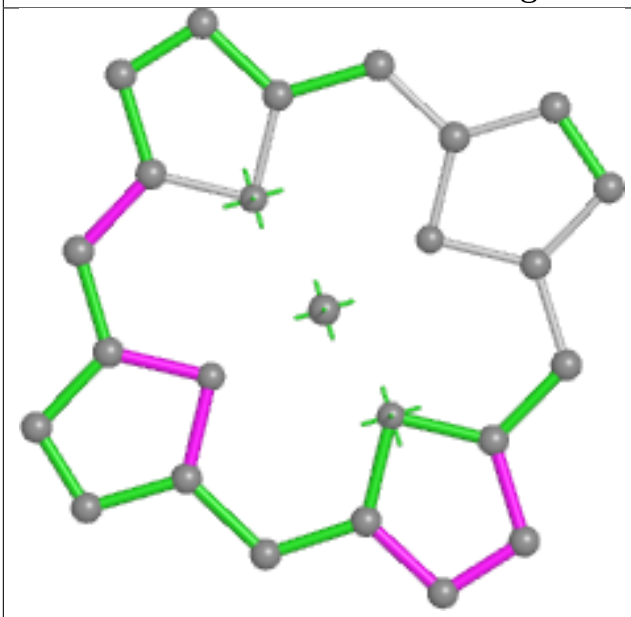
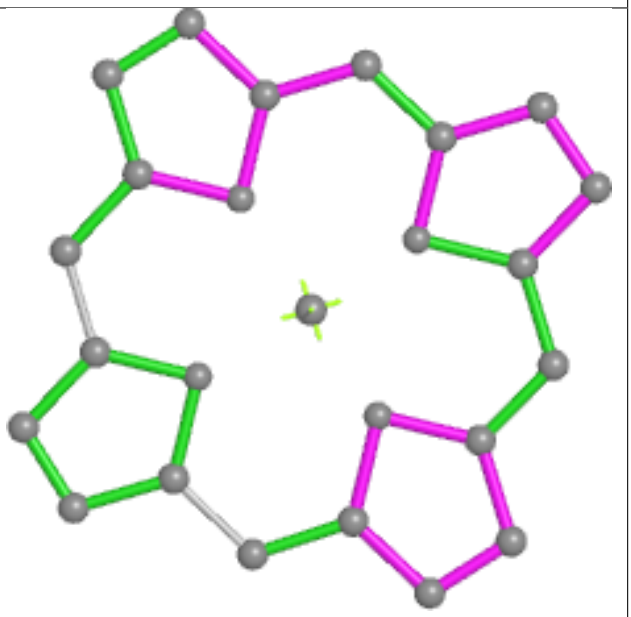


Rings

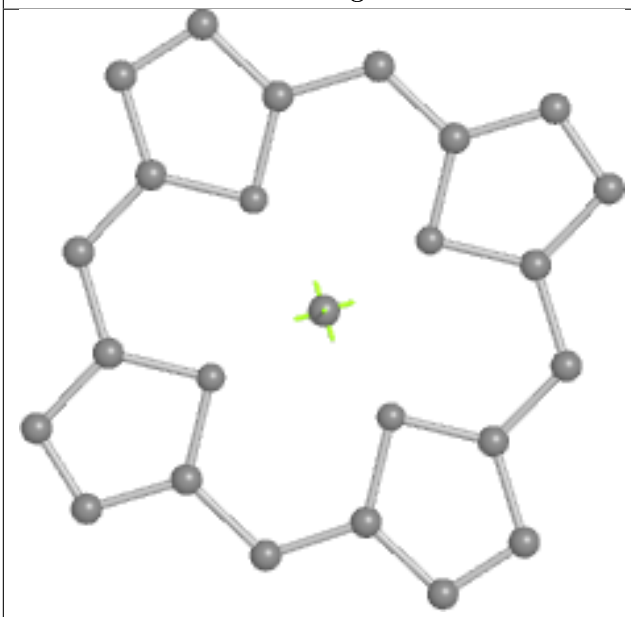
Ligand CLA M 165



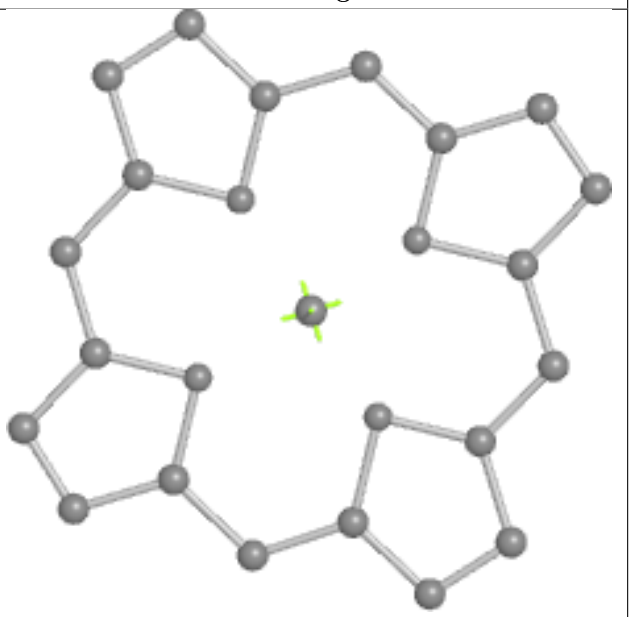
Bond lengths



Bond angles

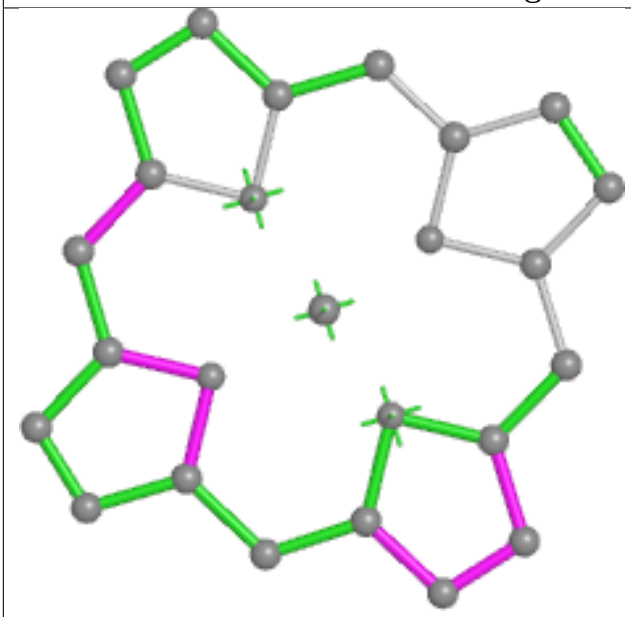


Torsions

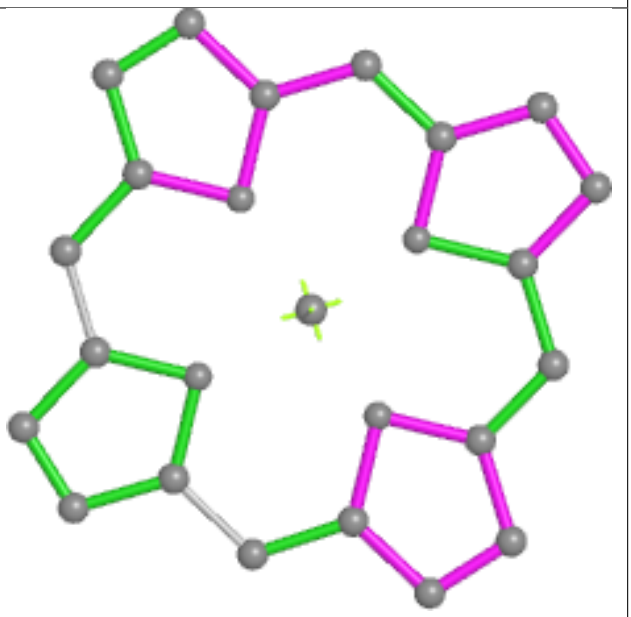


Rings

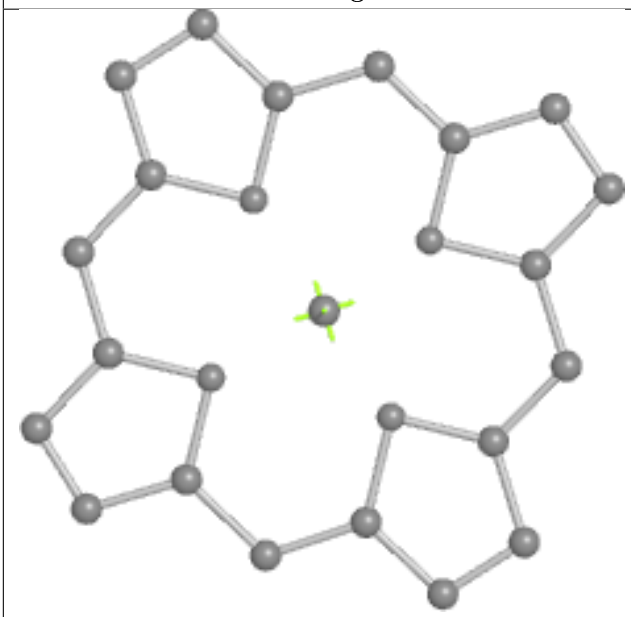
Ligand CLA A 177



Bond lengths



Bond angles



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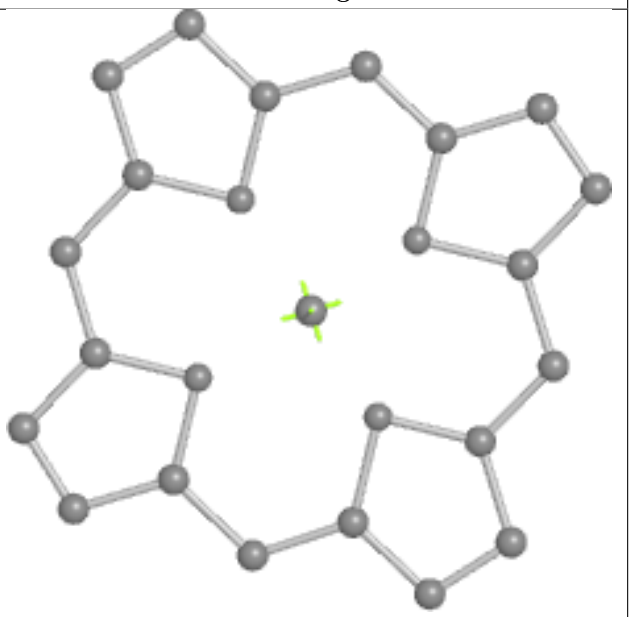
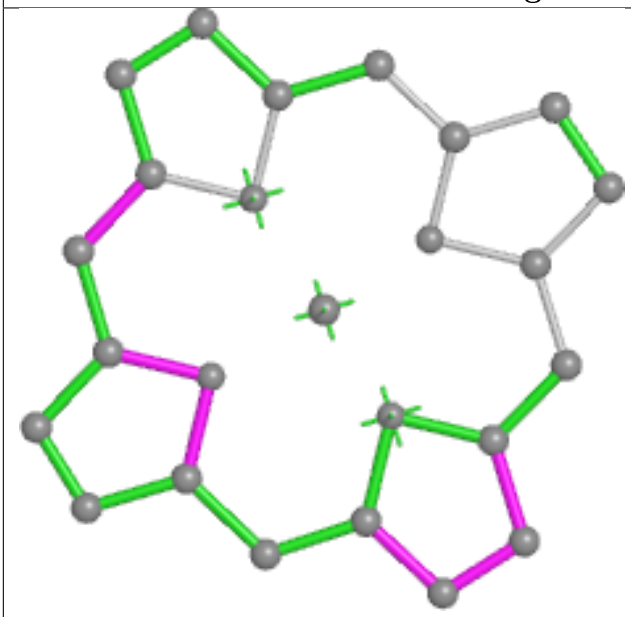


Rings

Ligand CLA C 160



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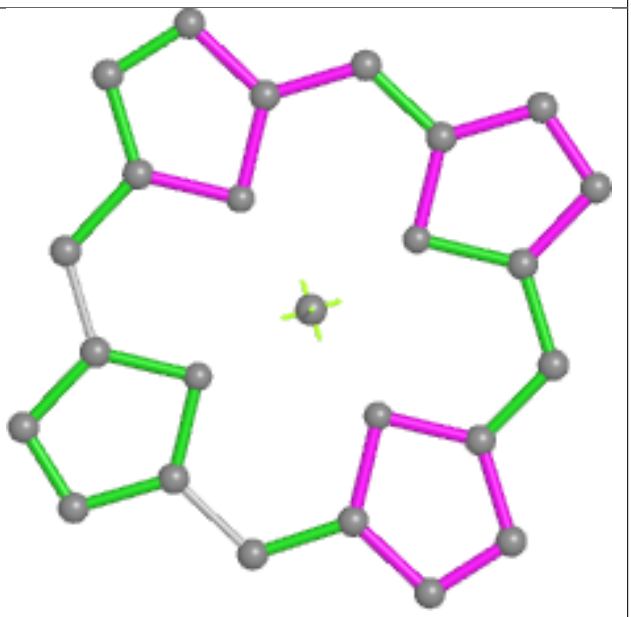
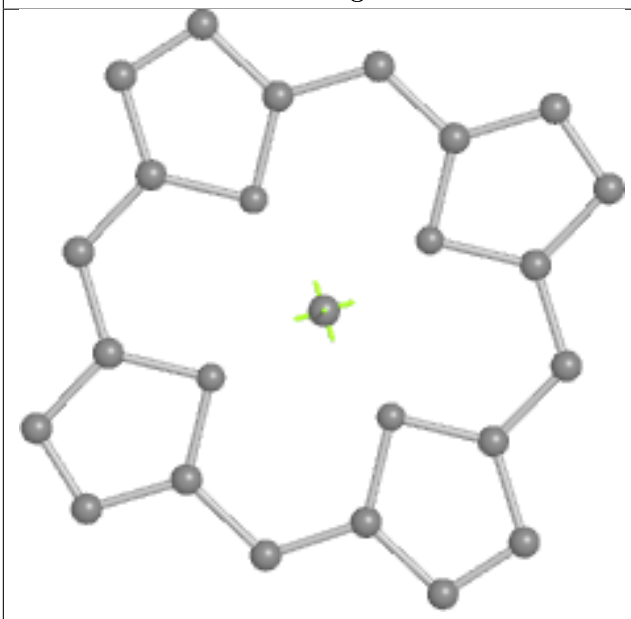
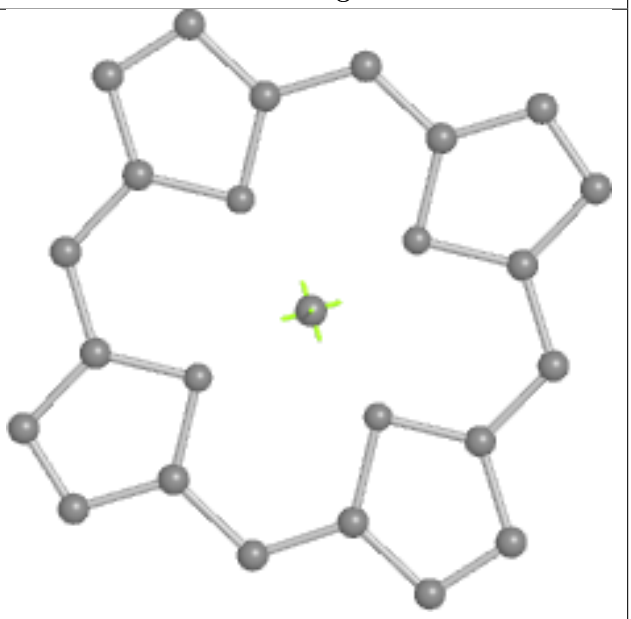


Bond angles

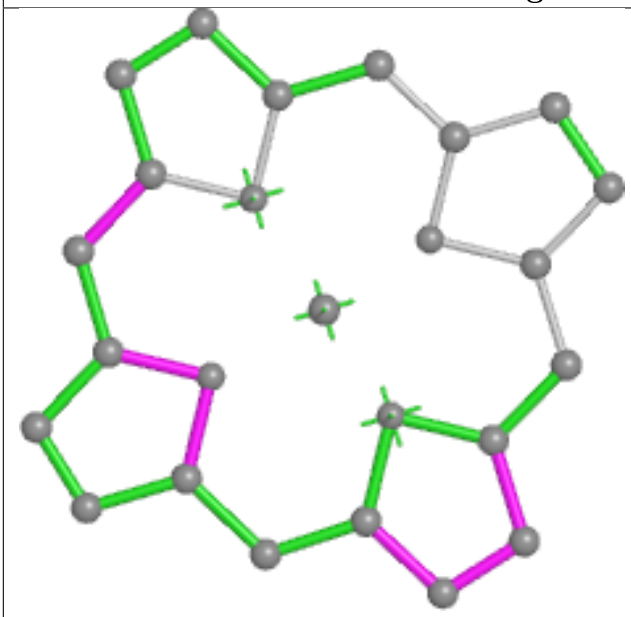


Torsions



Rings

Ligand CLA L 158



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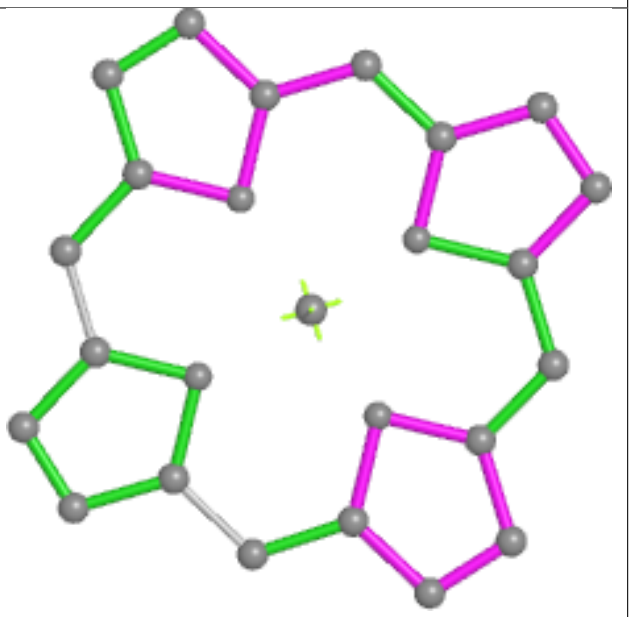
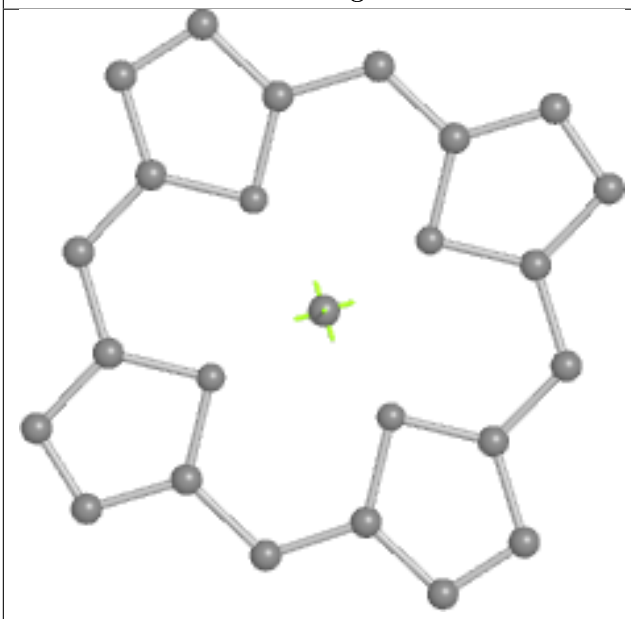


Bond angles



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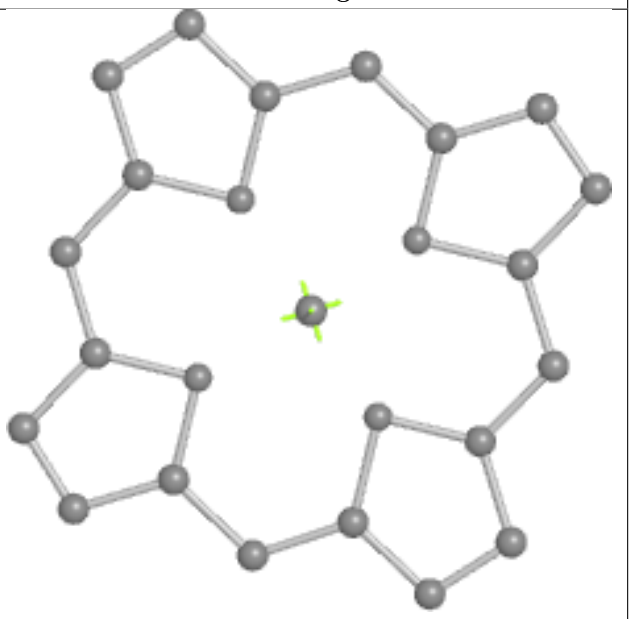
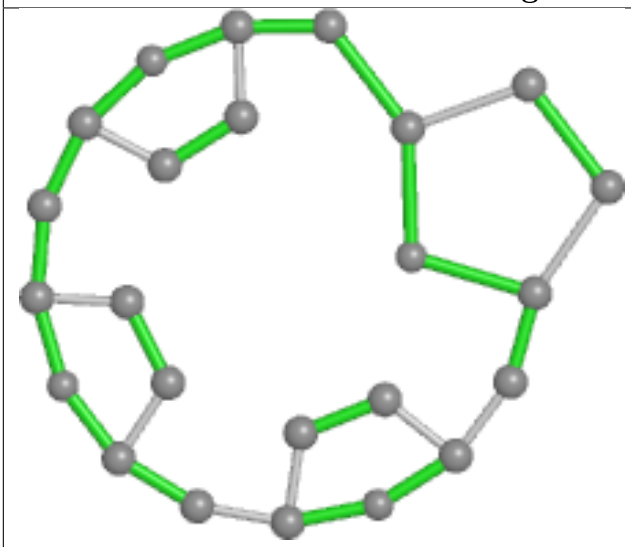
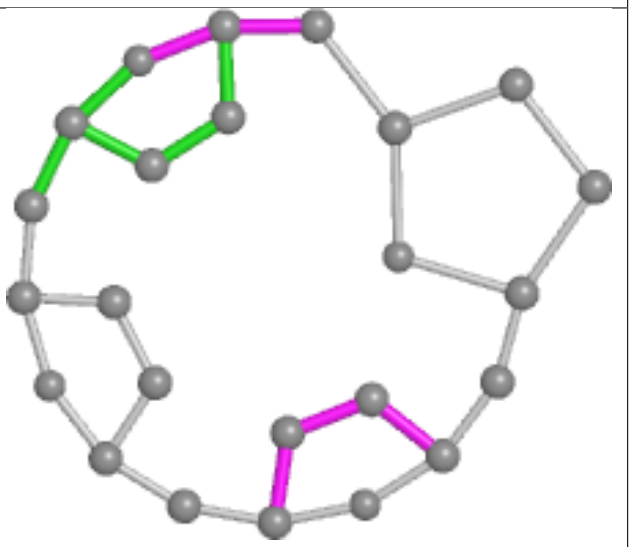


Rings

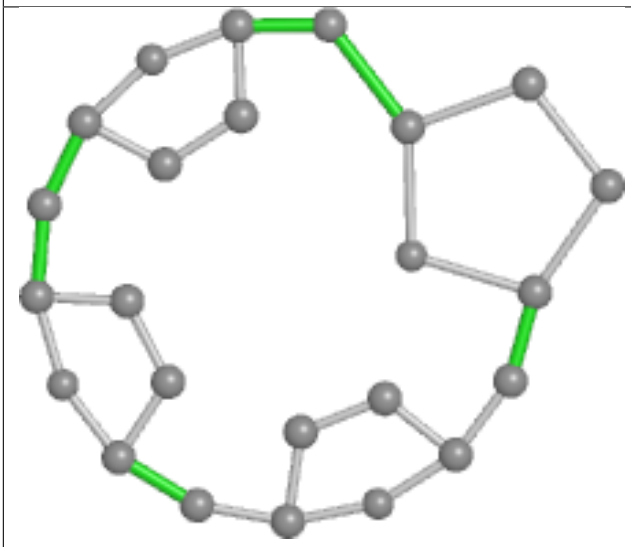
Ligand PHO K 178



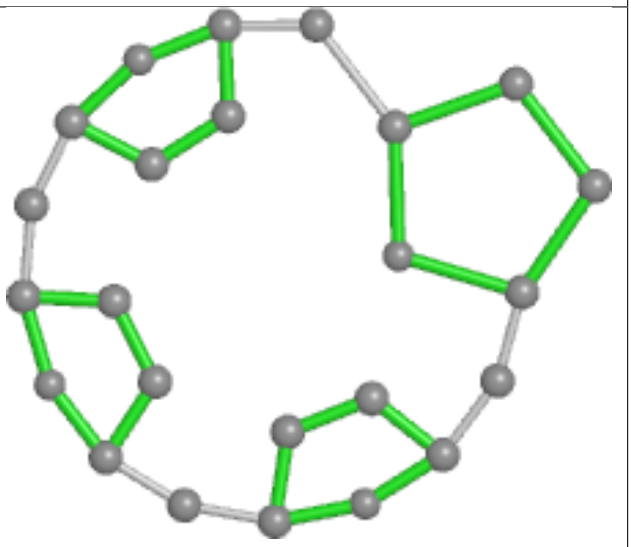
Bond lengths



Bond angles

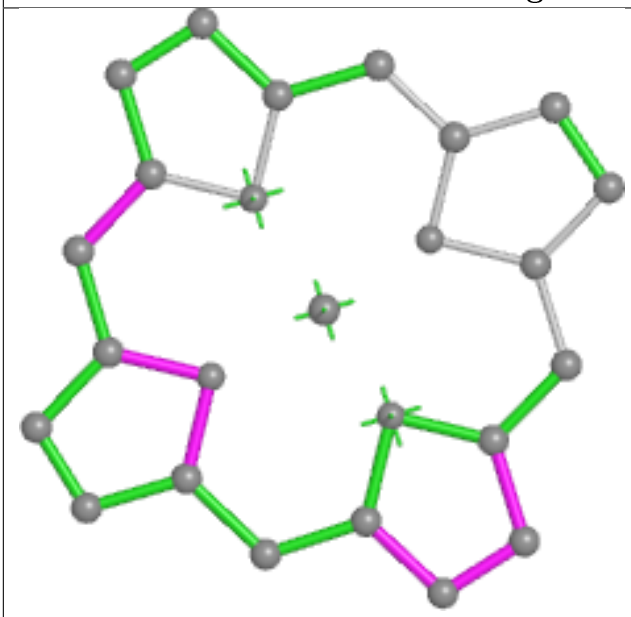


Torsions



Rings

Ligand CLA L 159



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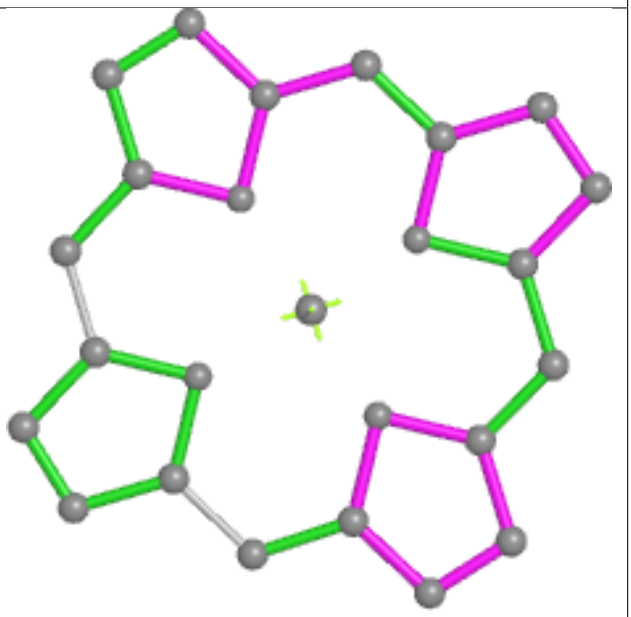
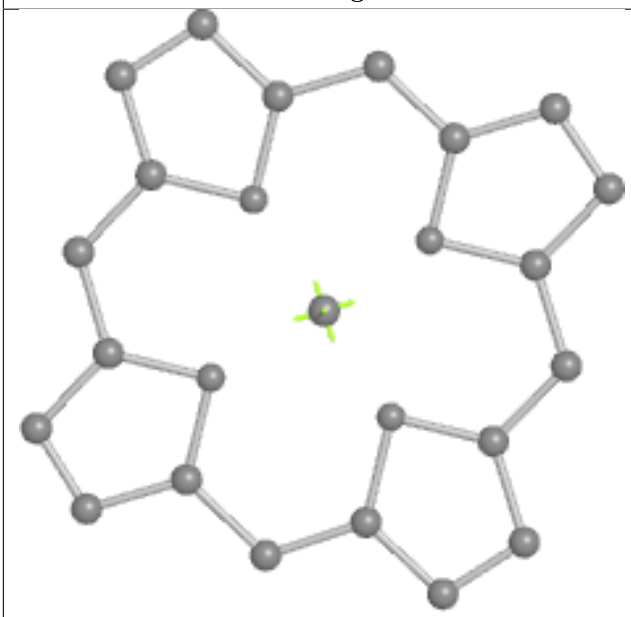


Bond angles



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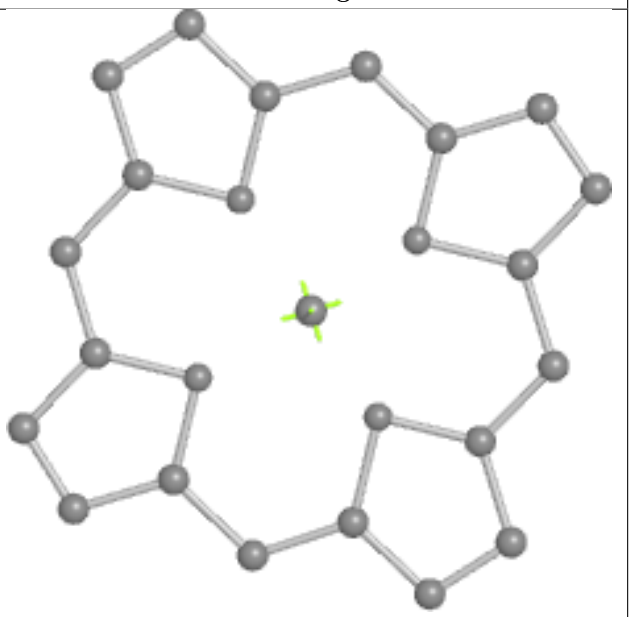
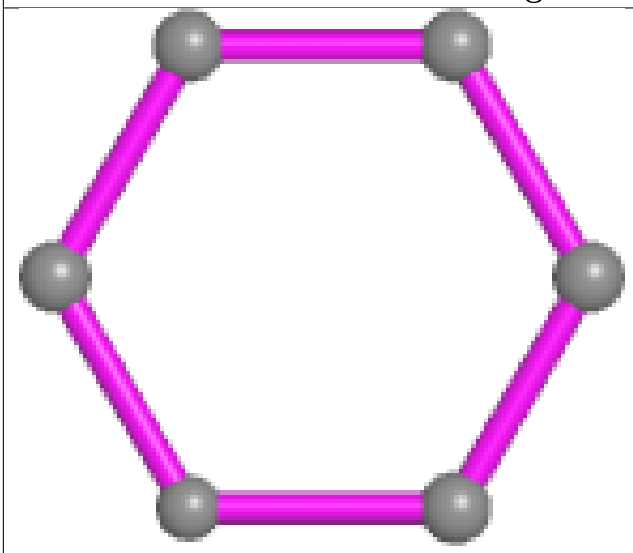


Rings

Ligand PLA B 180



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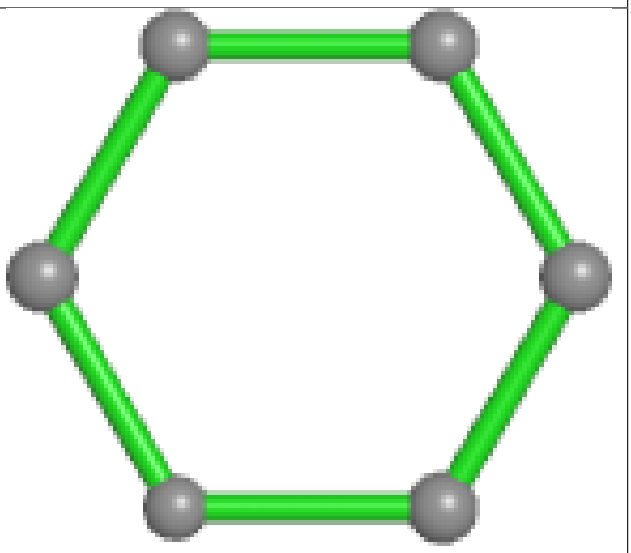
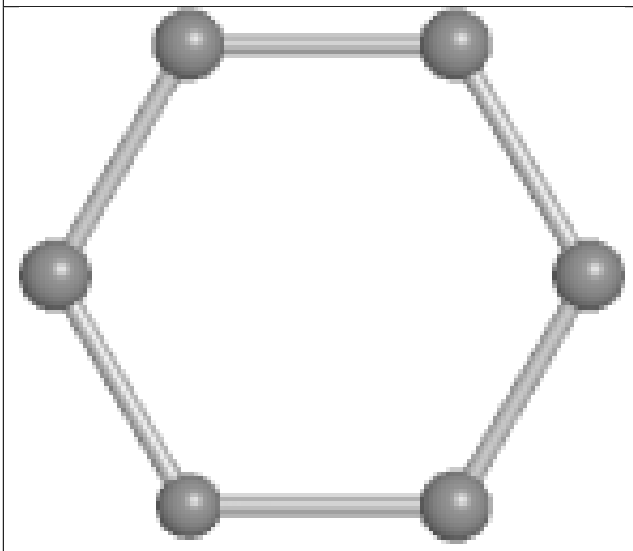


Bond angles



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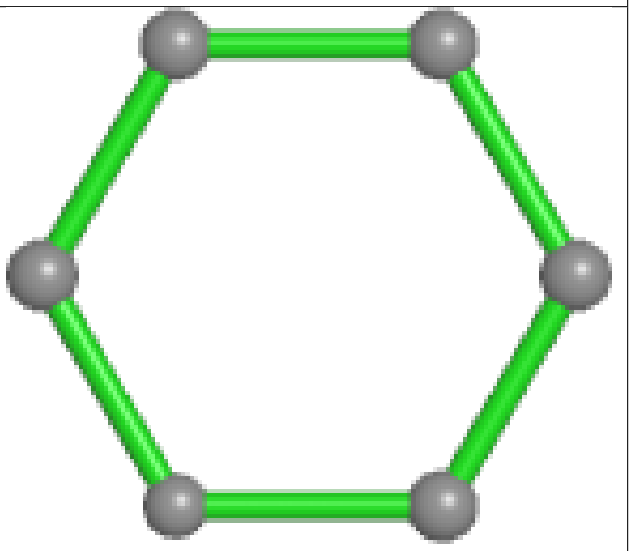
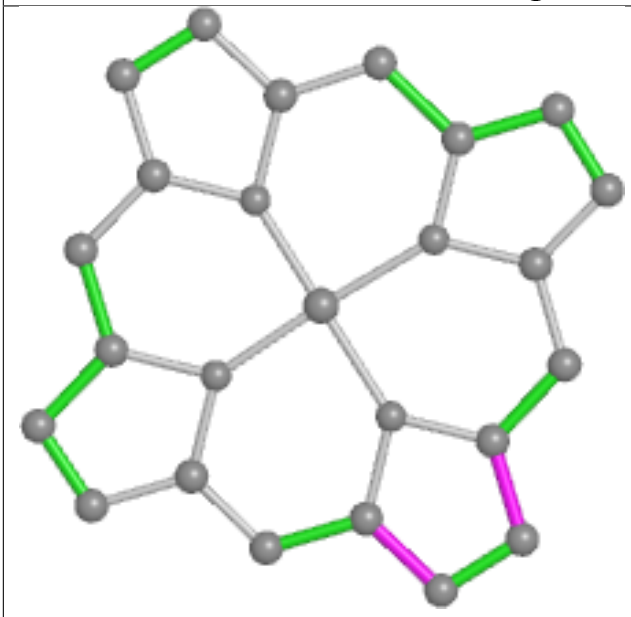


Rings

Ligand HEM R 88



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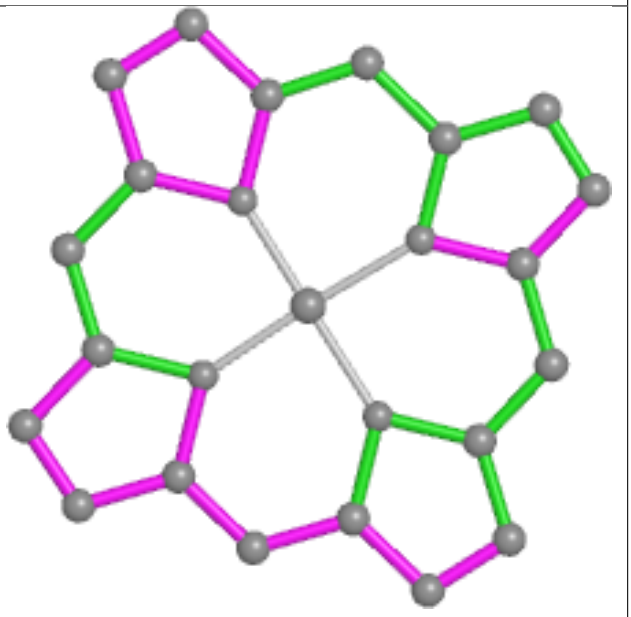
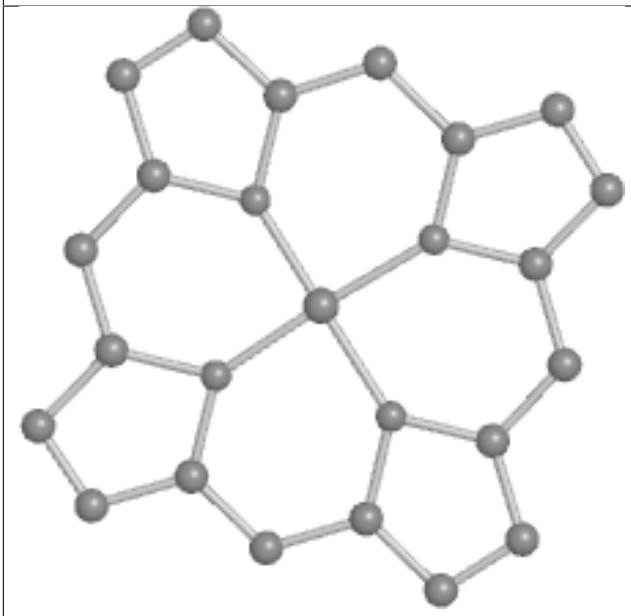
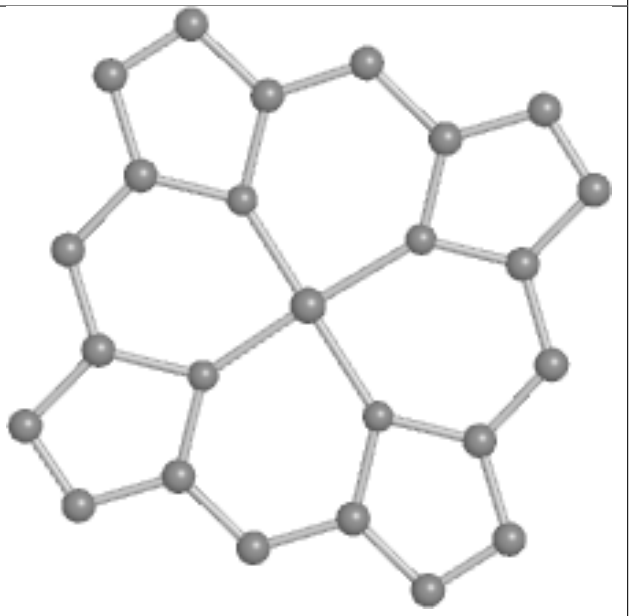


Bond angles

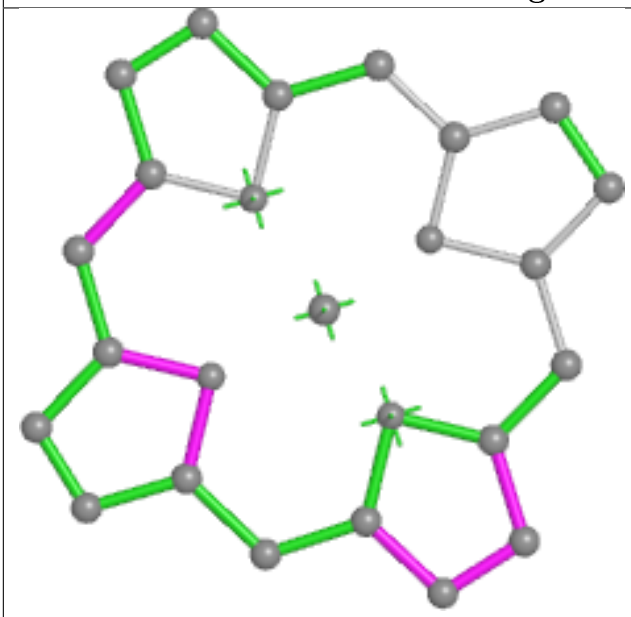


Torsions



Rings

Ligand CLA J 176



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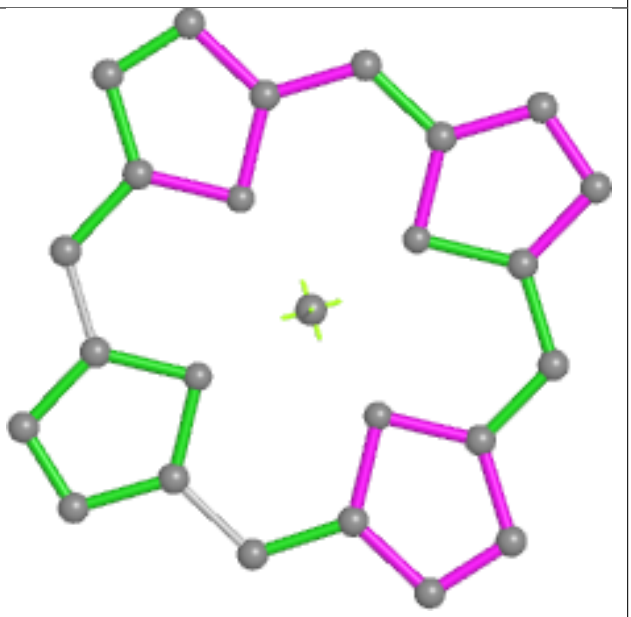
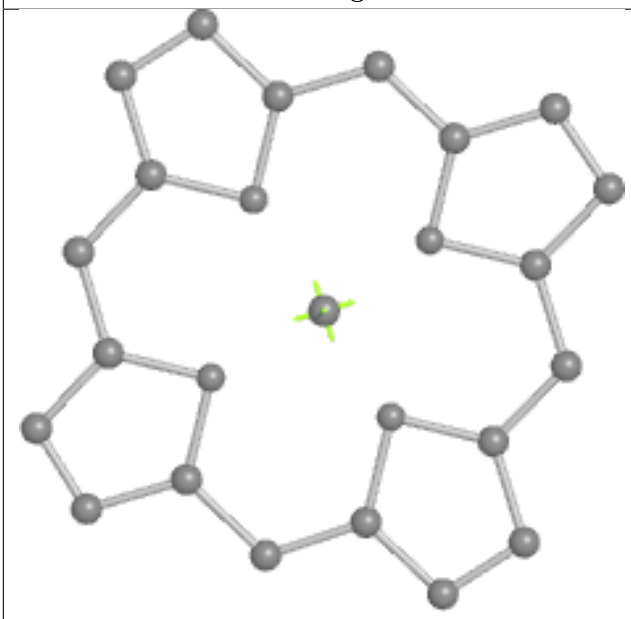
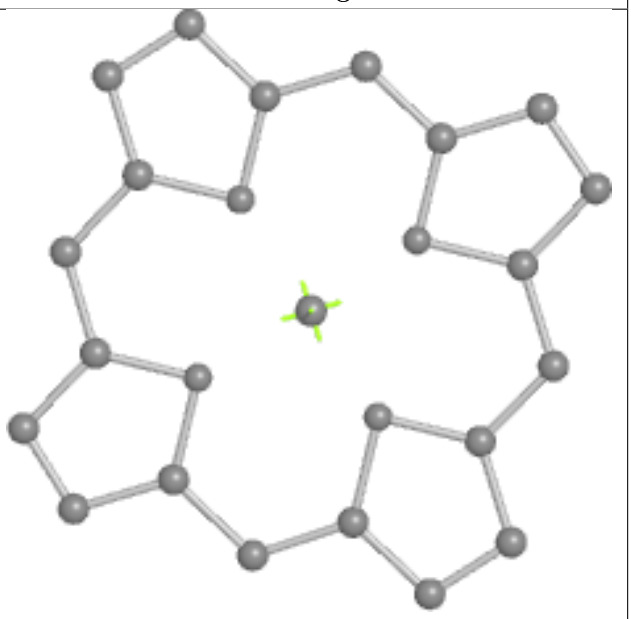


Bond angles

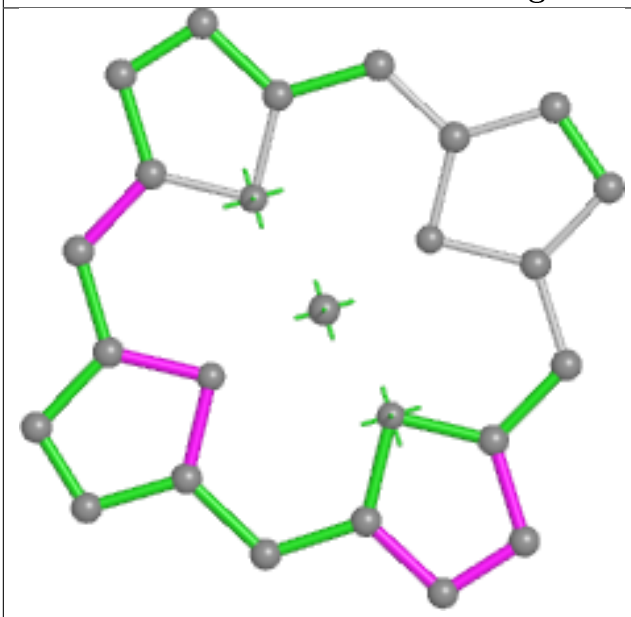


Torsions

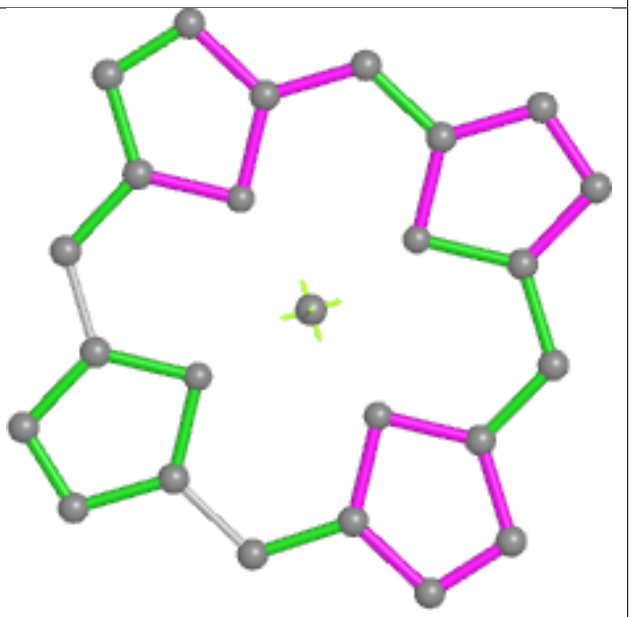


Rings

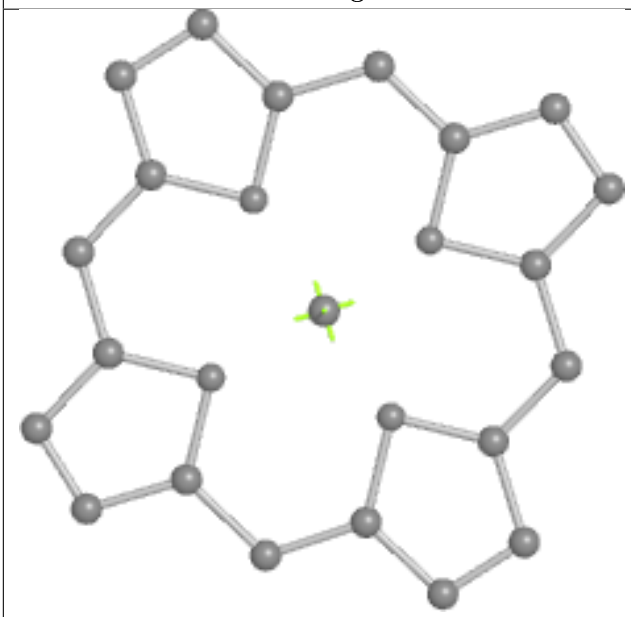
Ligand CLA J 179



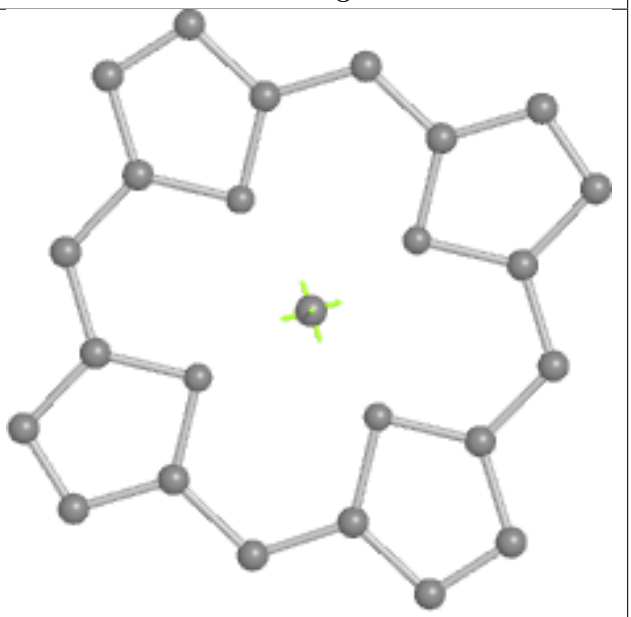
Bond lengths



Bond angles

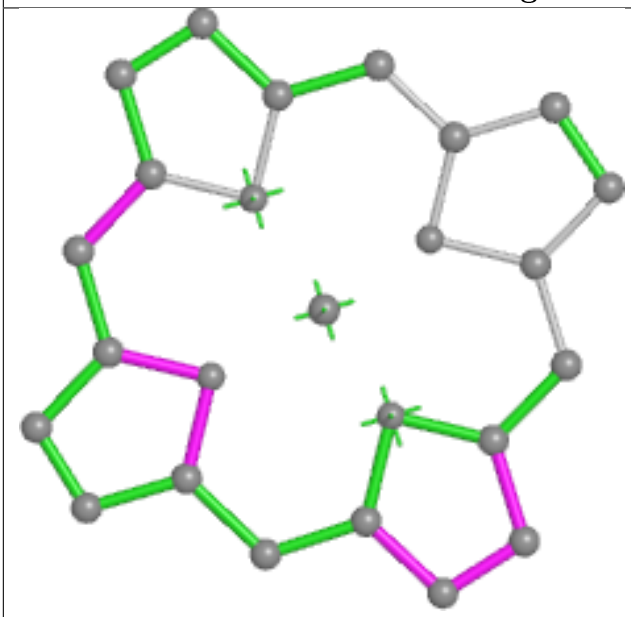


Torsions

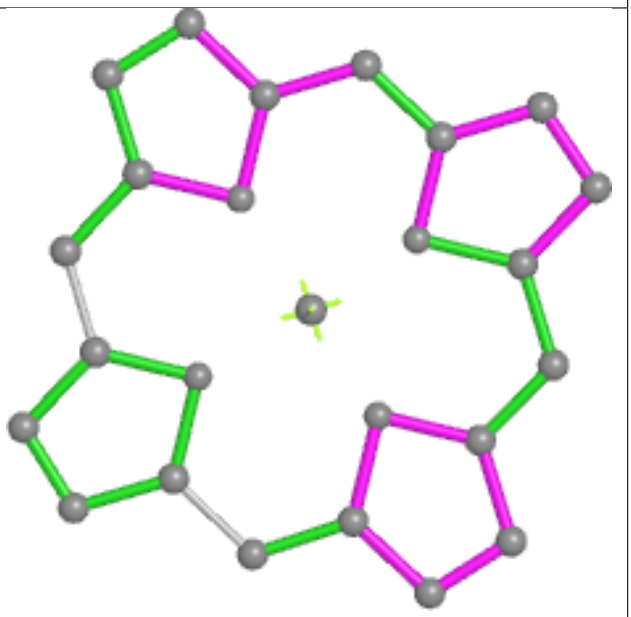


Rings

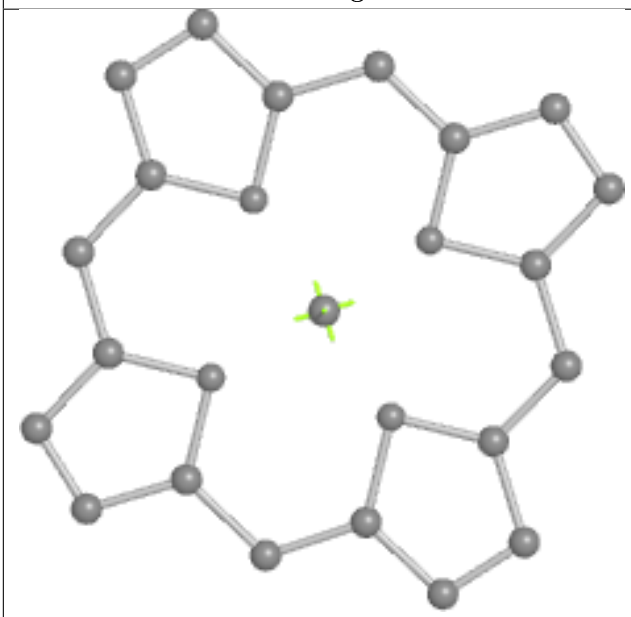
Ligand CLA M 168



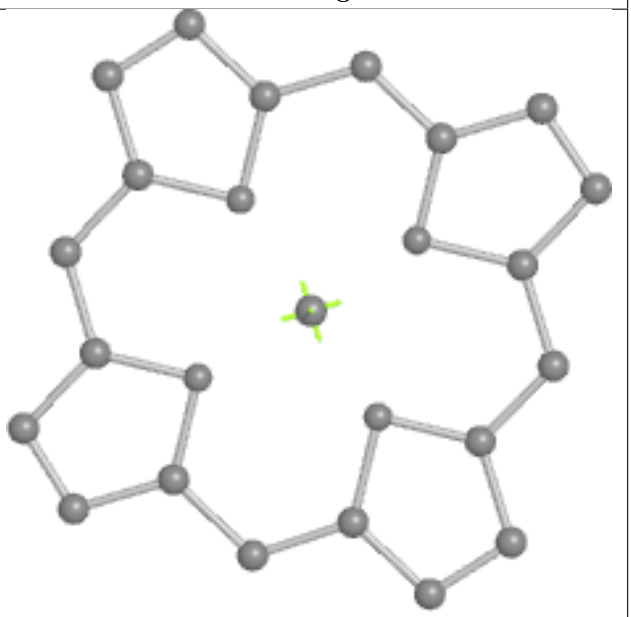
Bond lengths



Bond angles

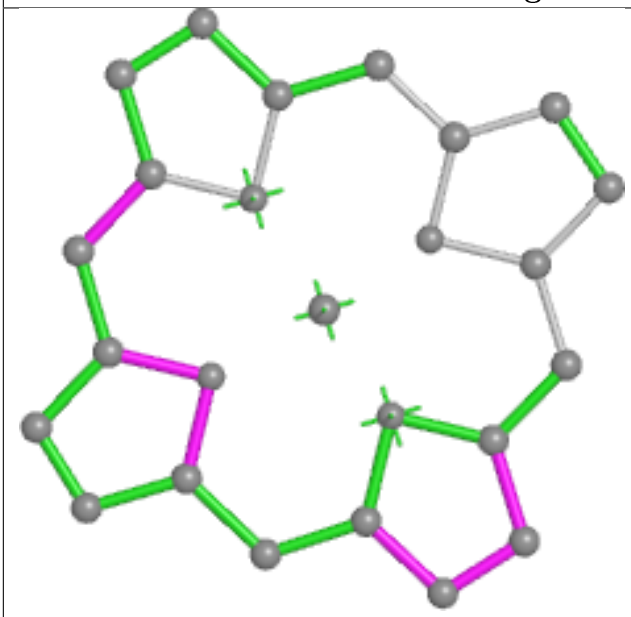


Torsions



Rings

Ligand CLA C 167



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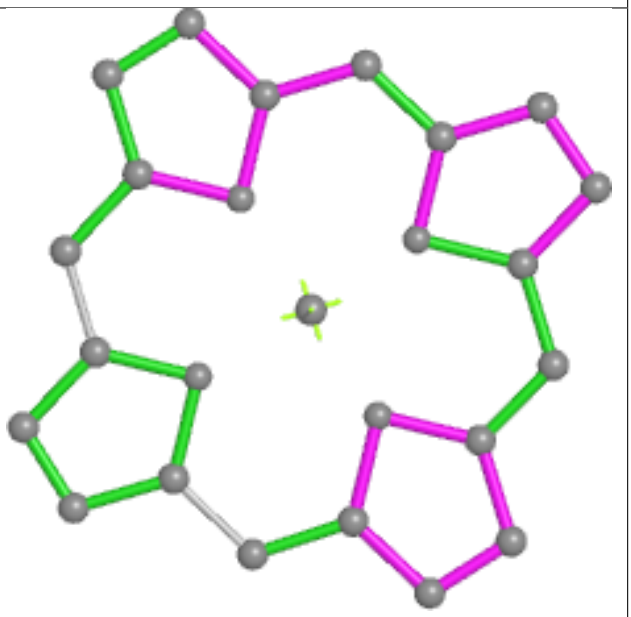

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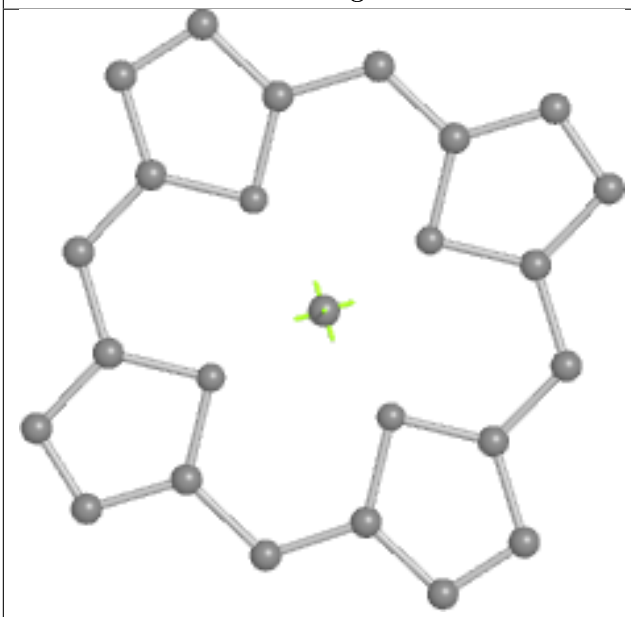

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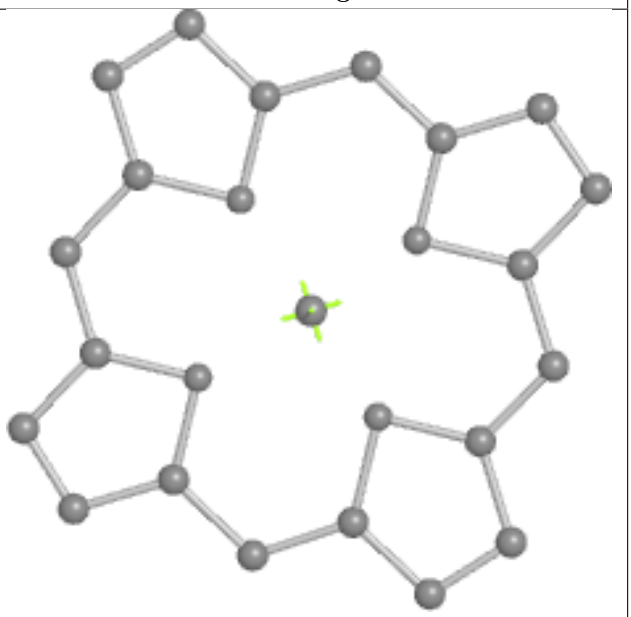
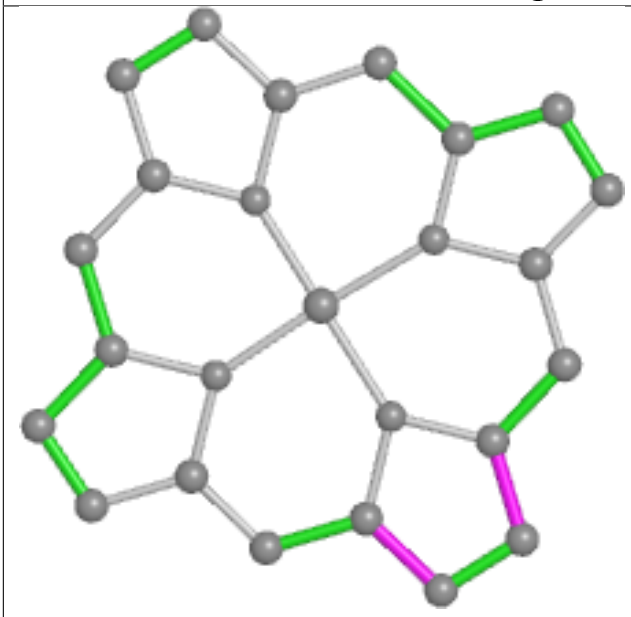


Rings

Ligand HEM F 31



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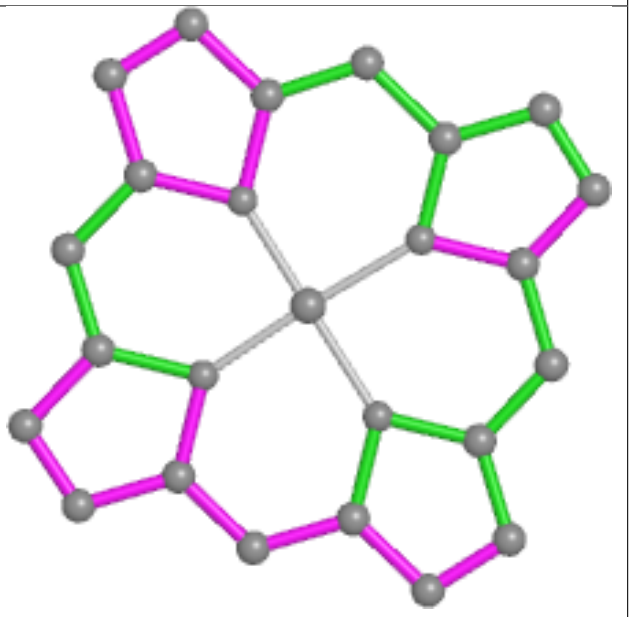

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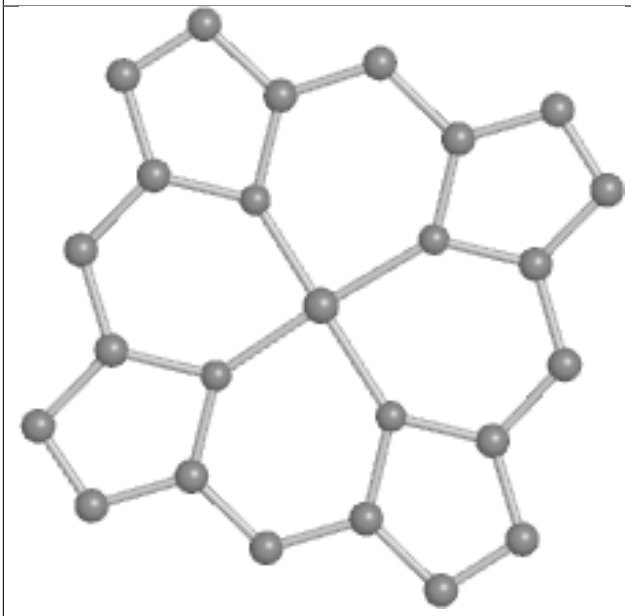

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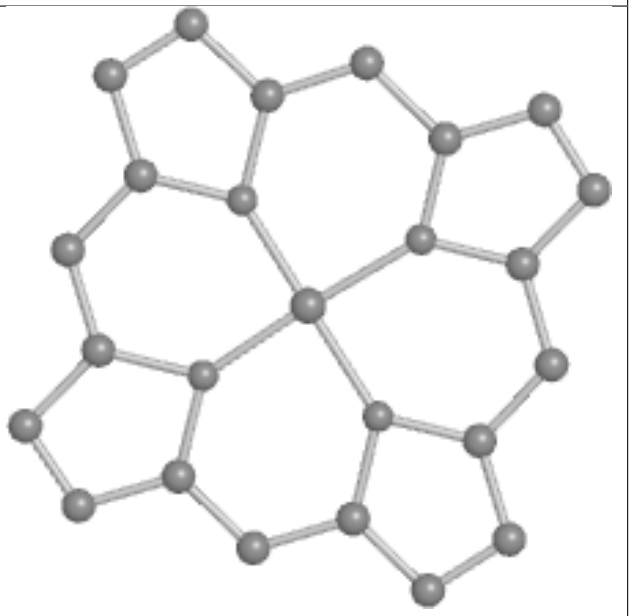
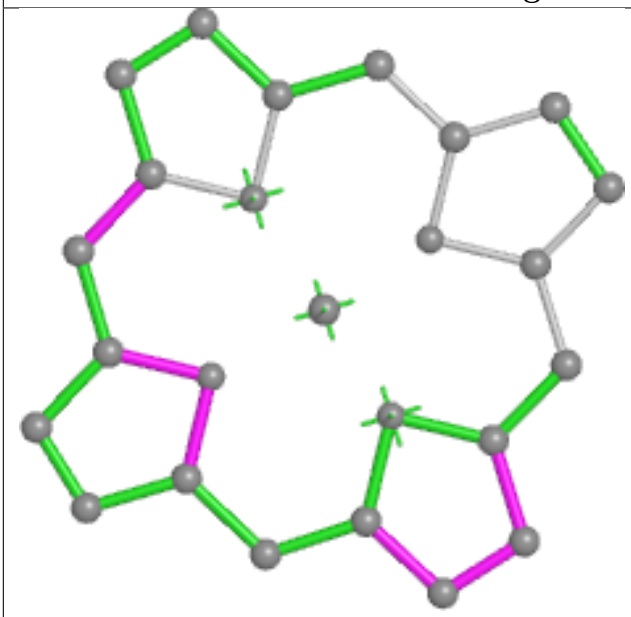


Rings

Ligand CLA D 166



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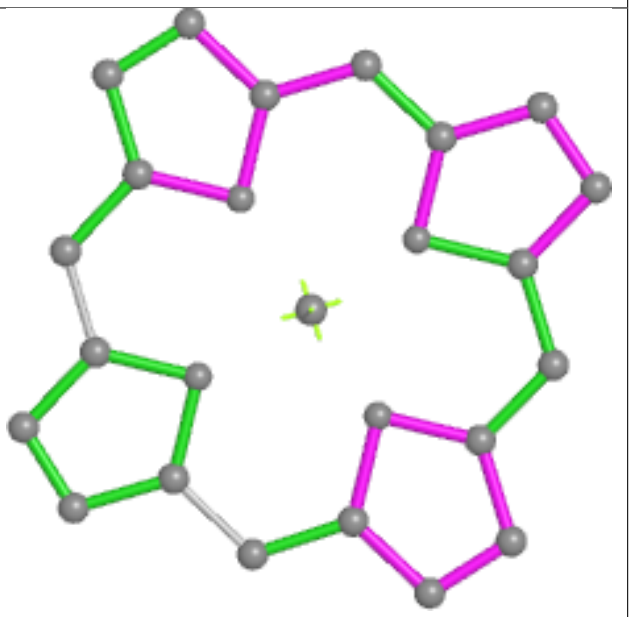
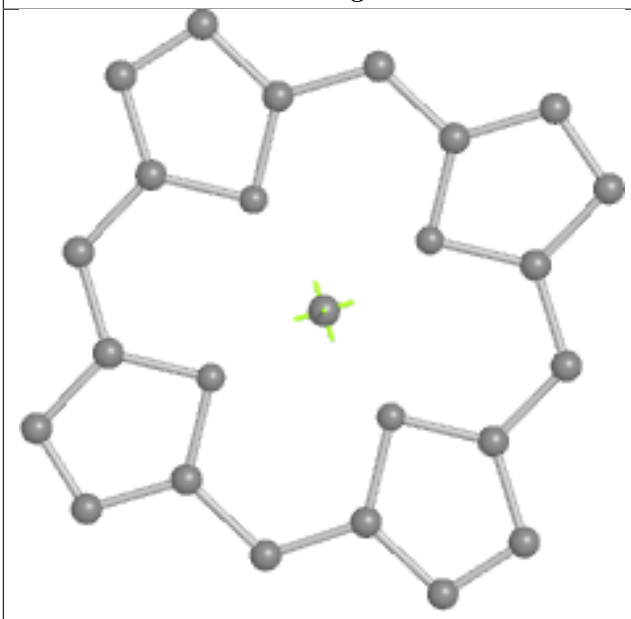


Bond angles



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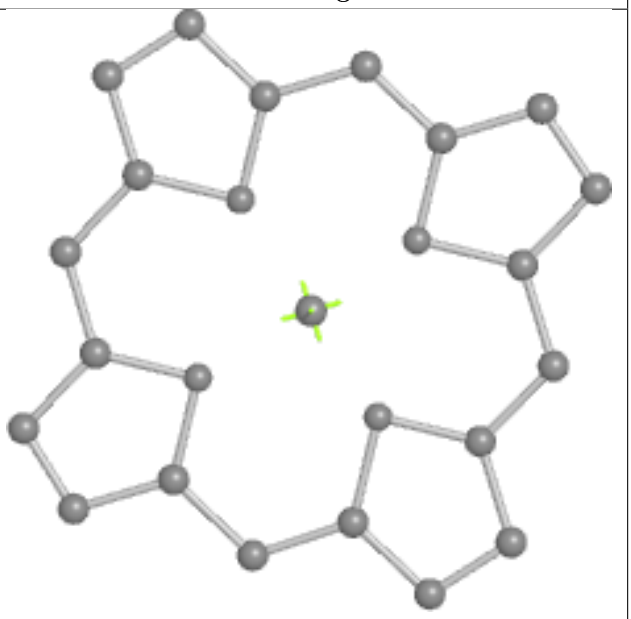
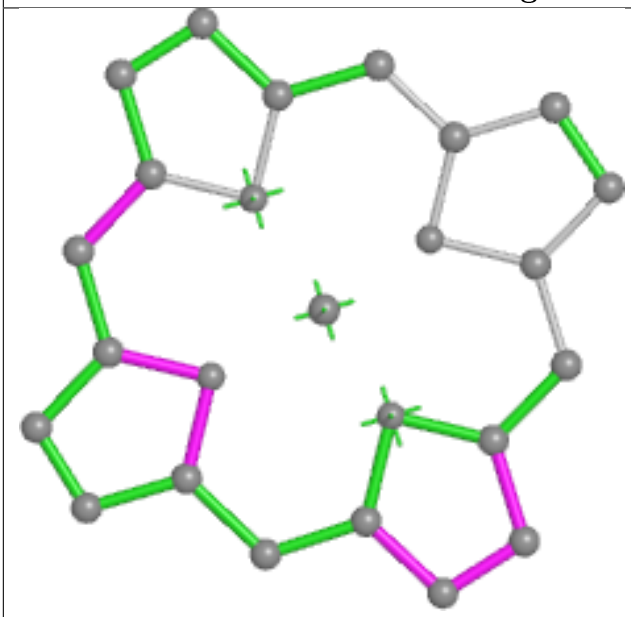


Rings

Ligand CLA M 156



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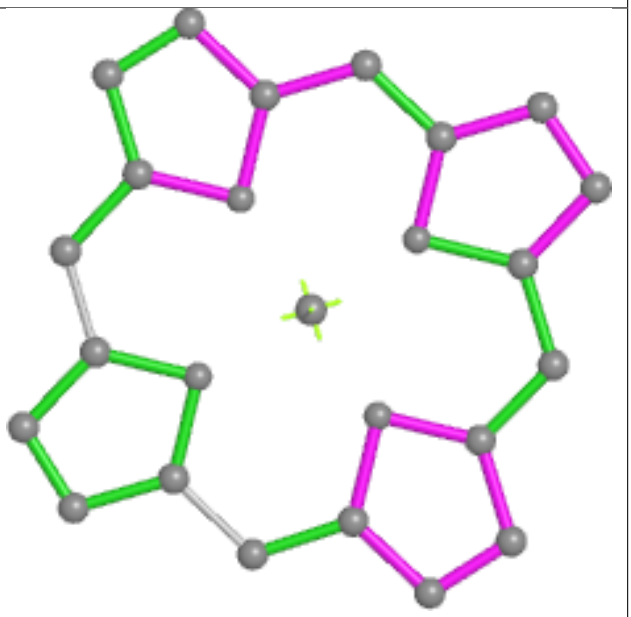

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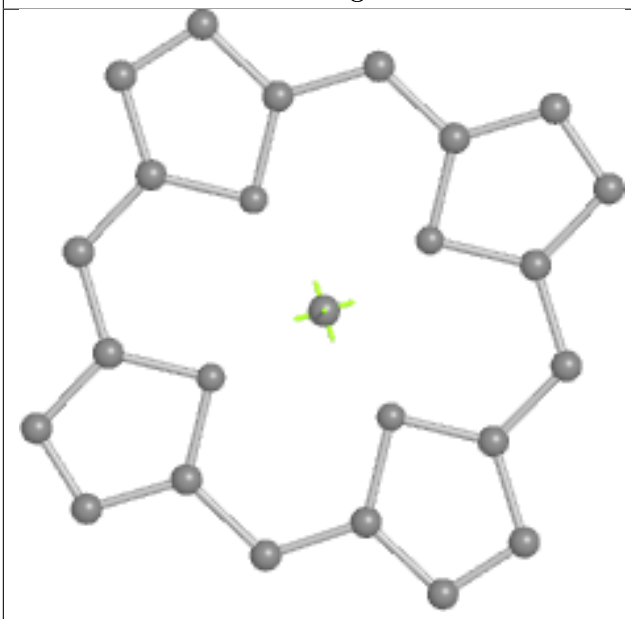

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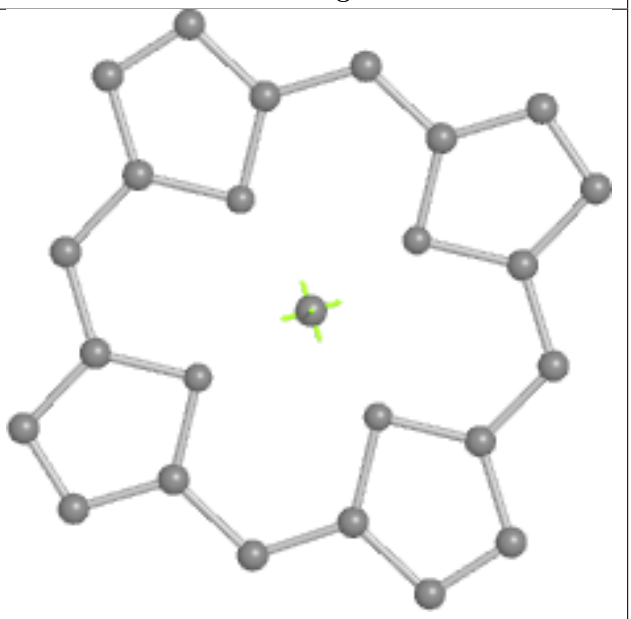
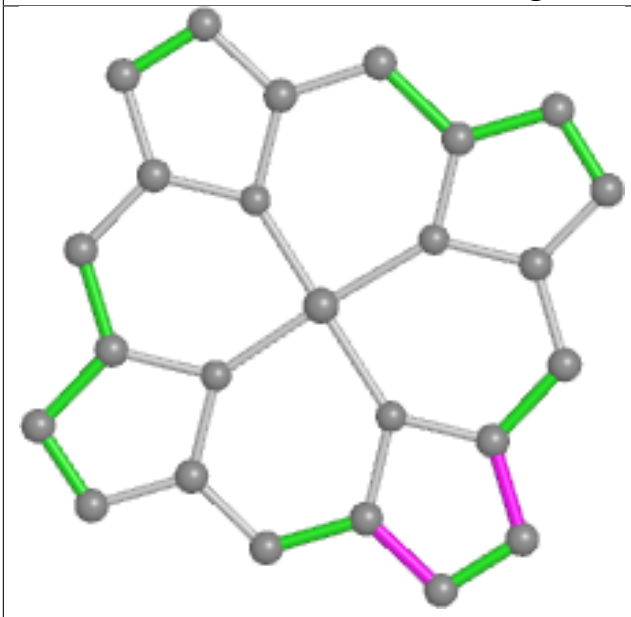


Rings

Ligand HEM O 58



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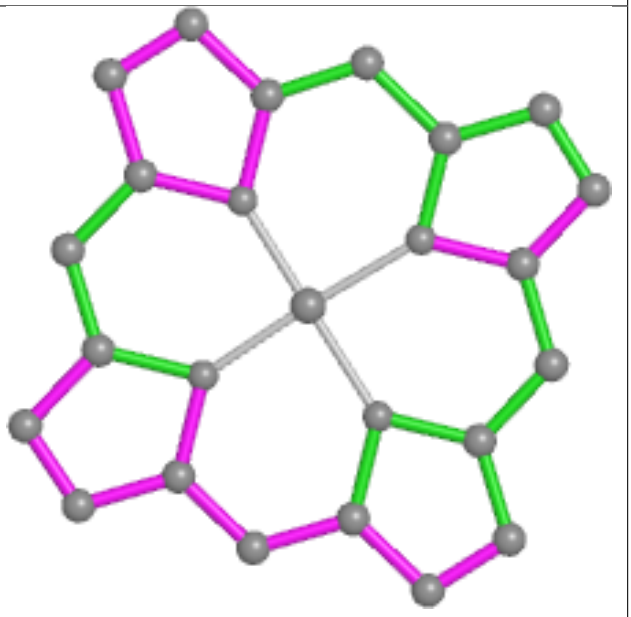
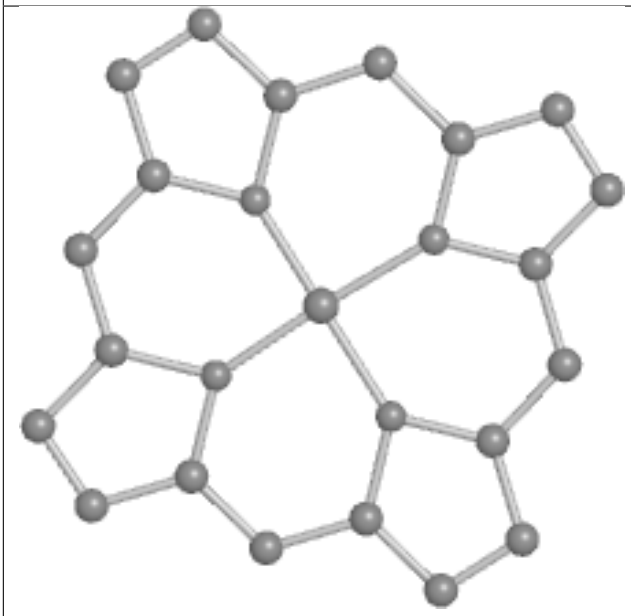


Bond angles



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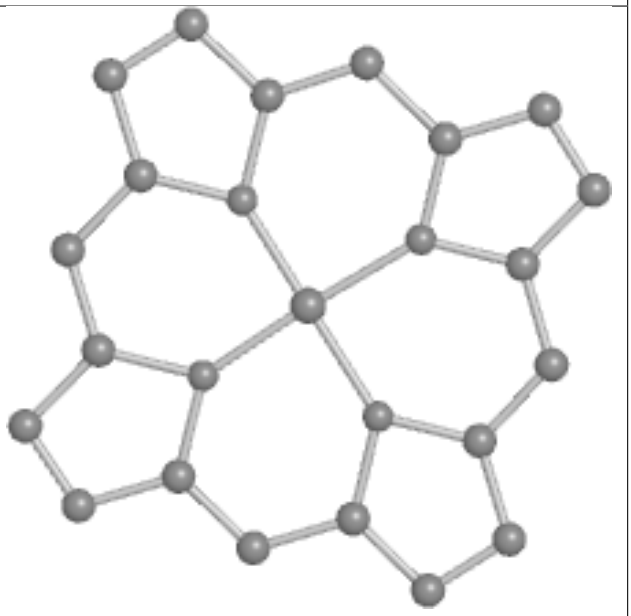
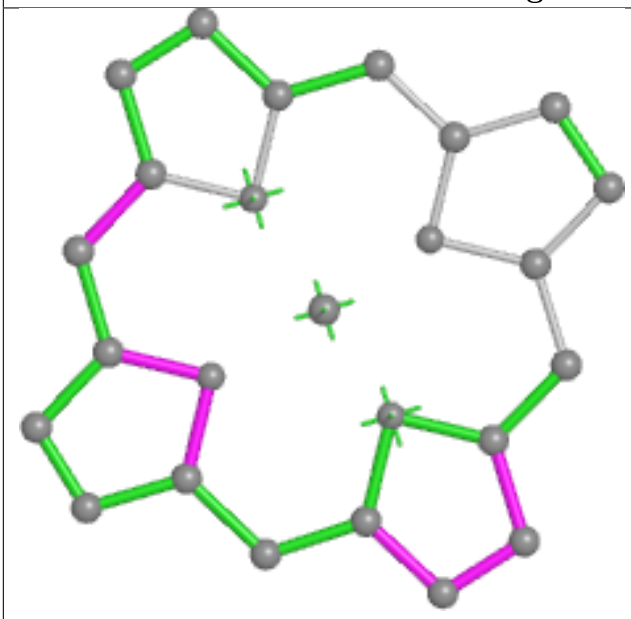


Rings

Ligand CLA L 161



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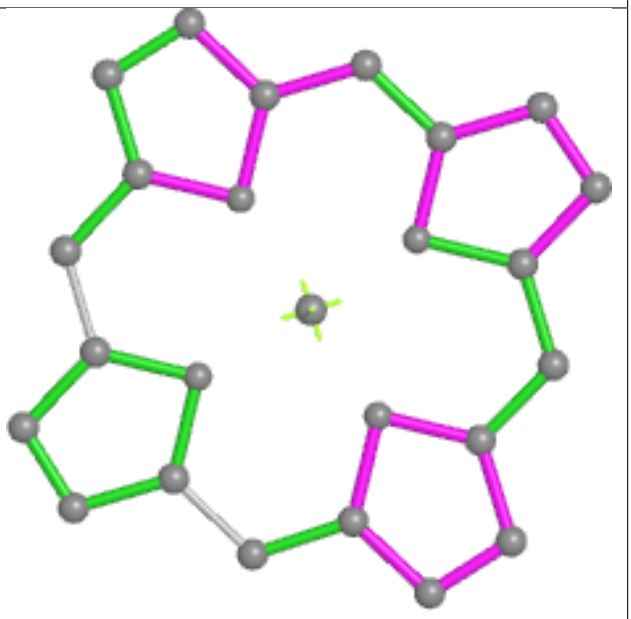

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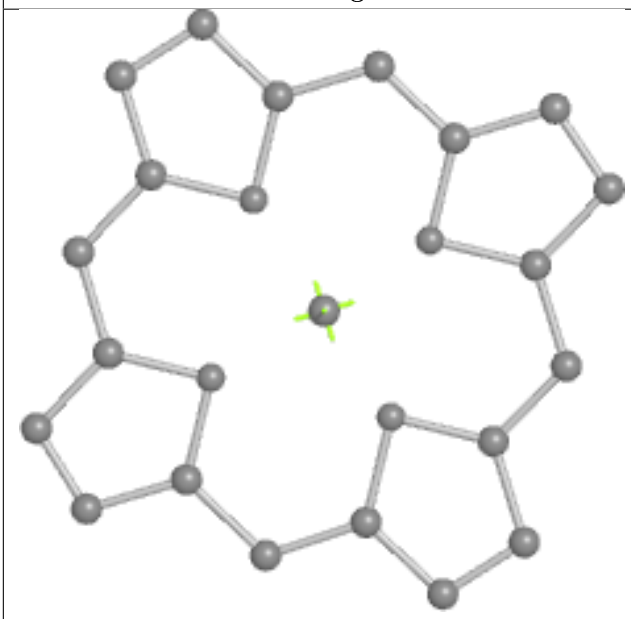

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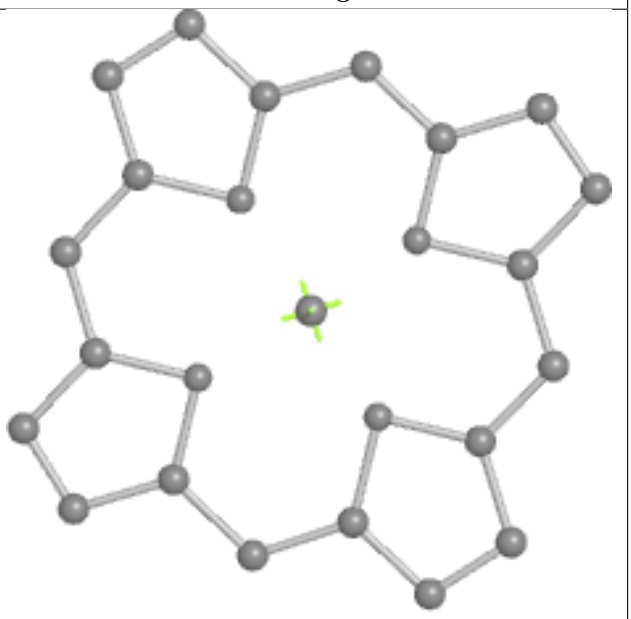
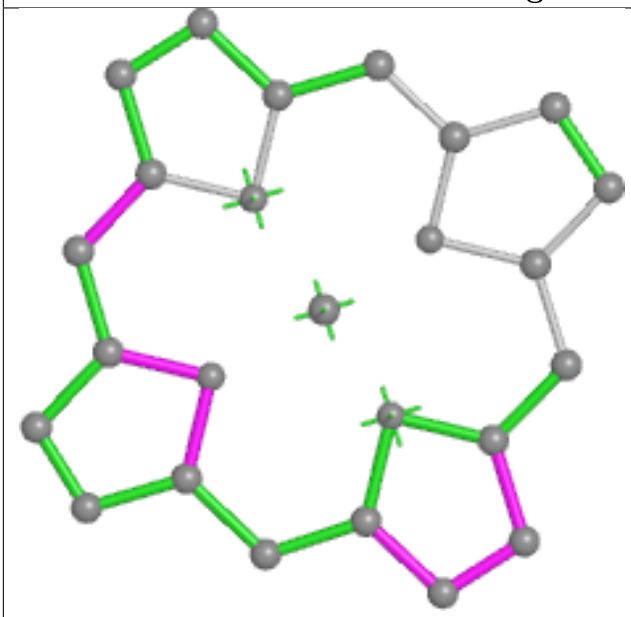


Rings

Ligand CLA L 167



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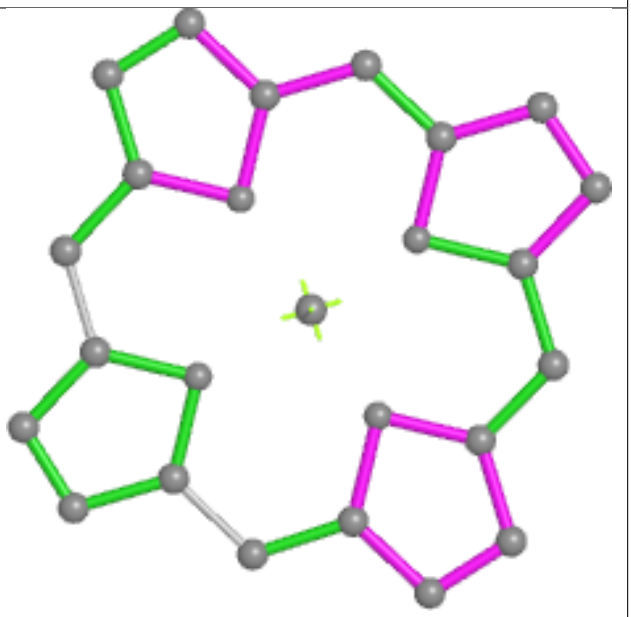
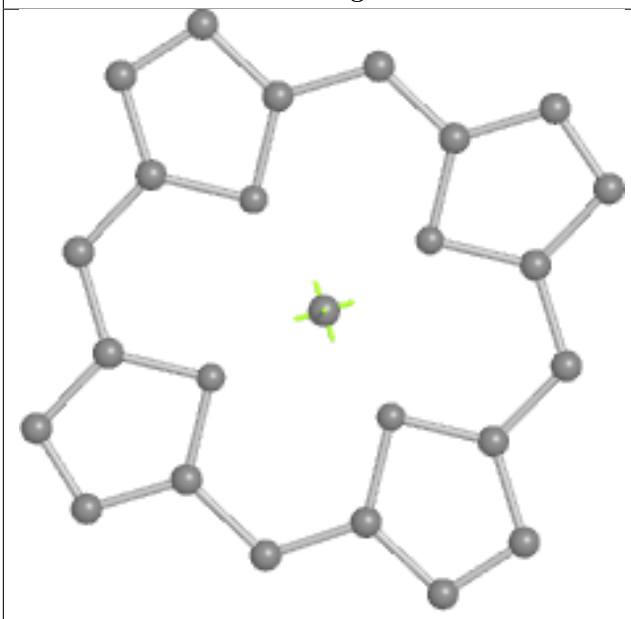


Bond angles



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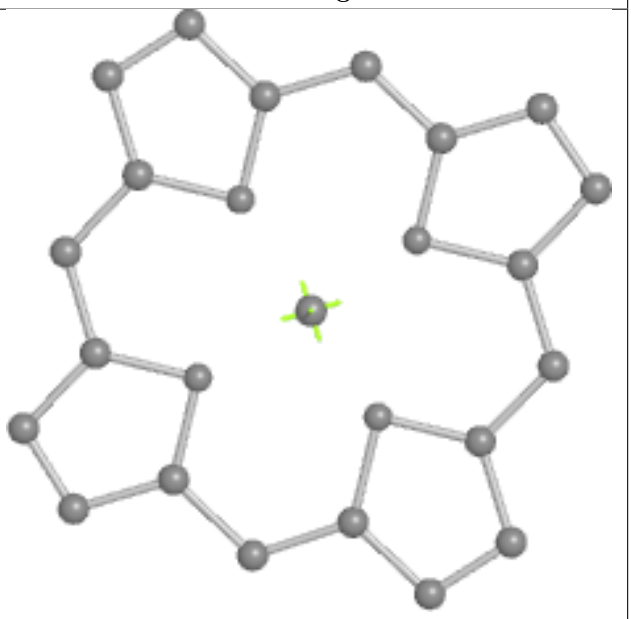
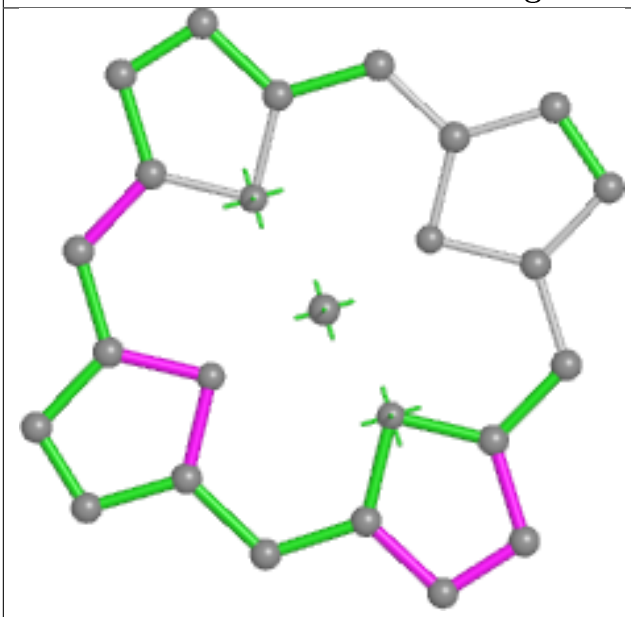


Rings

Ligand CLA A 176



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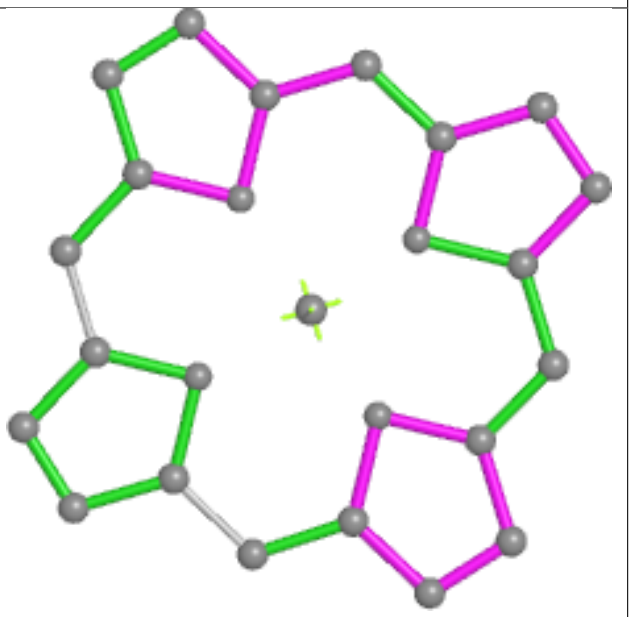
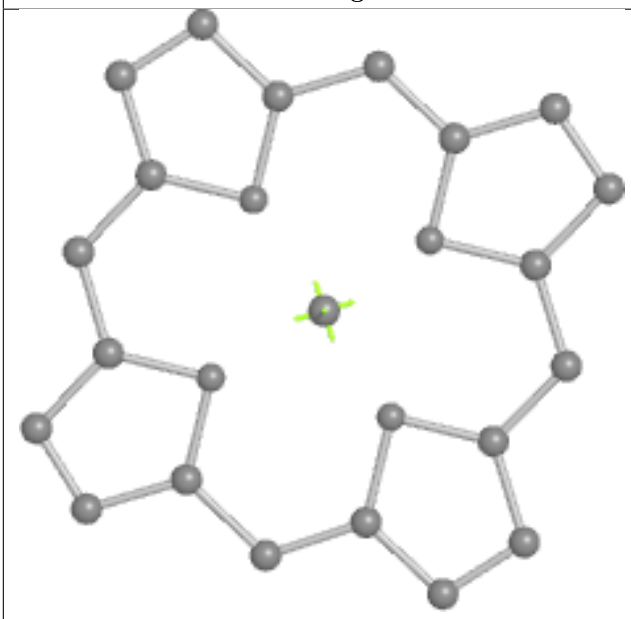


Bond angles



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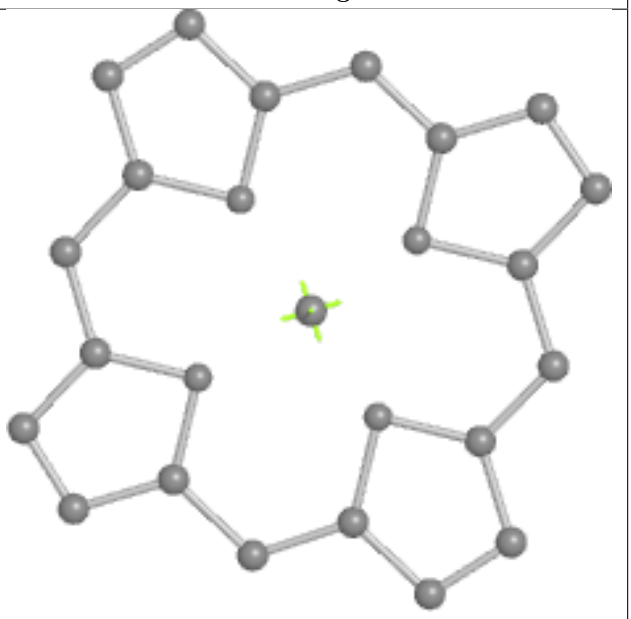
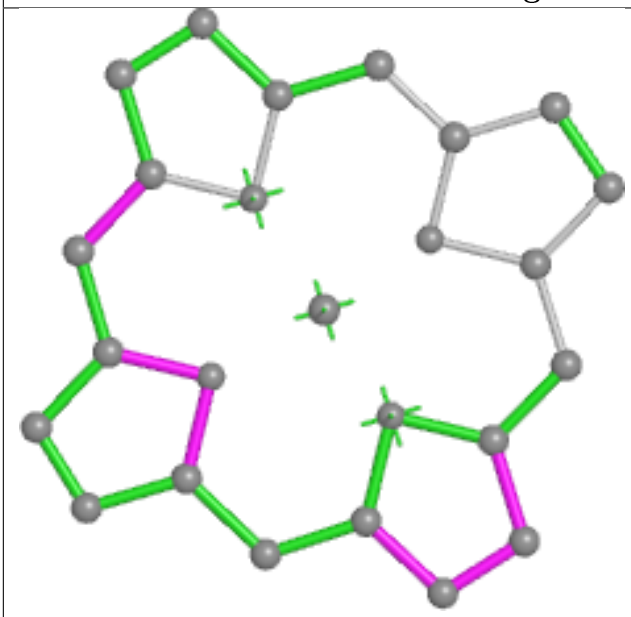


Rings

Ligand CLA K 179



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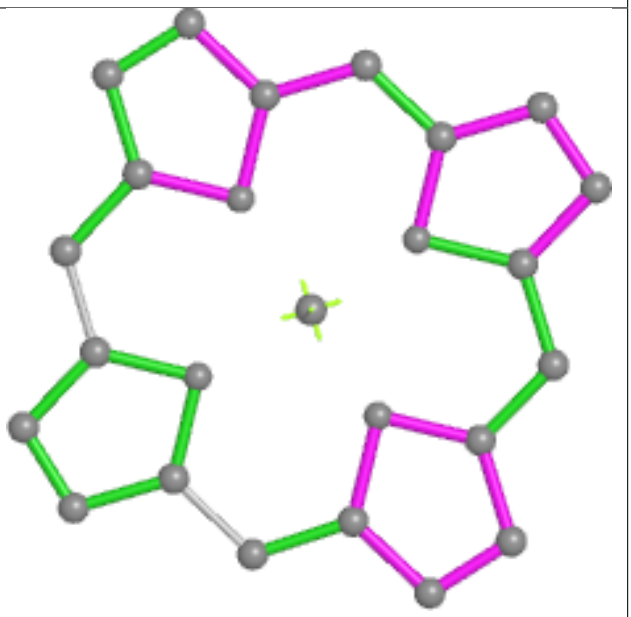
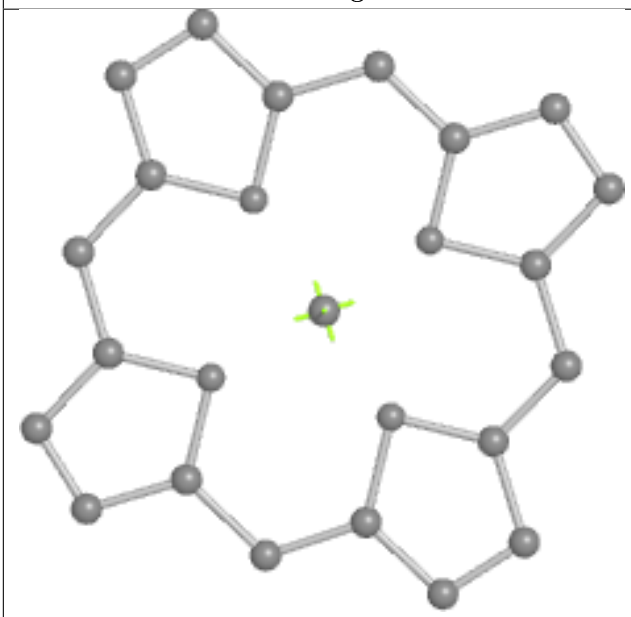


Bond angles



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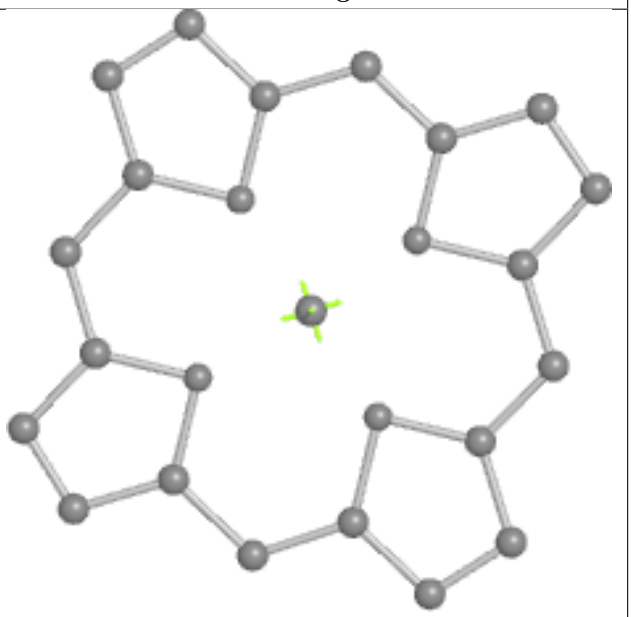
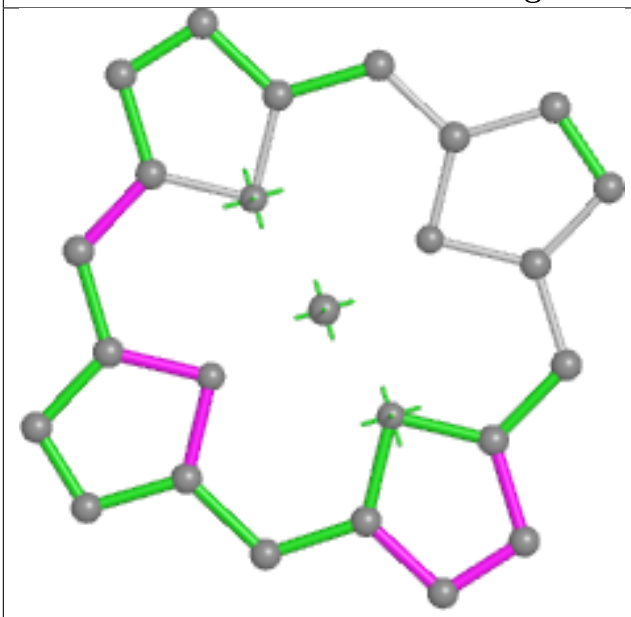


Rings

Ligand CLA A 175



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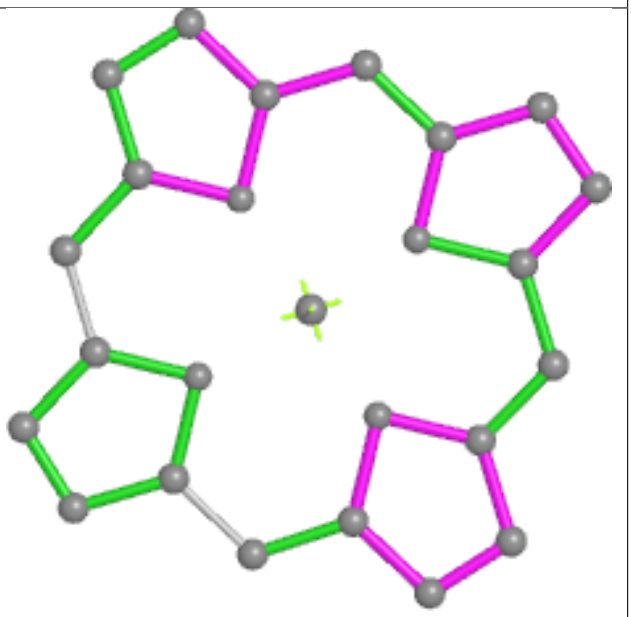
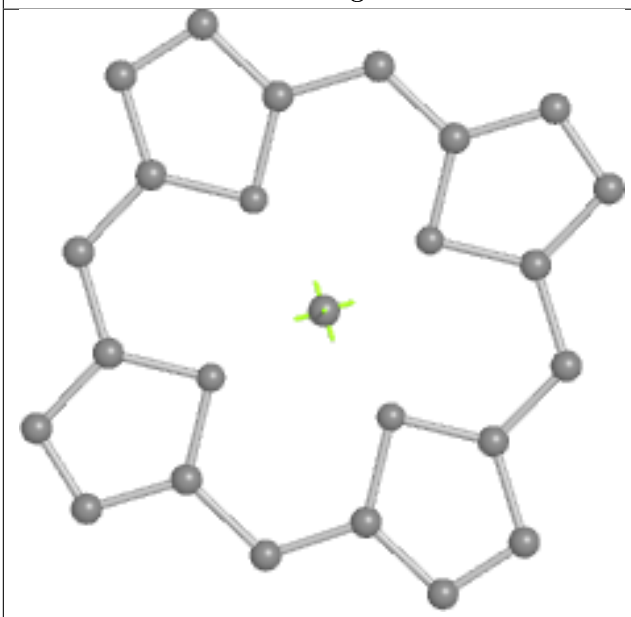


Bond angles



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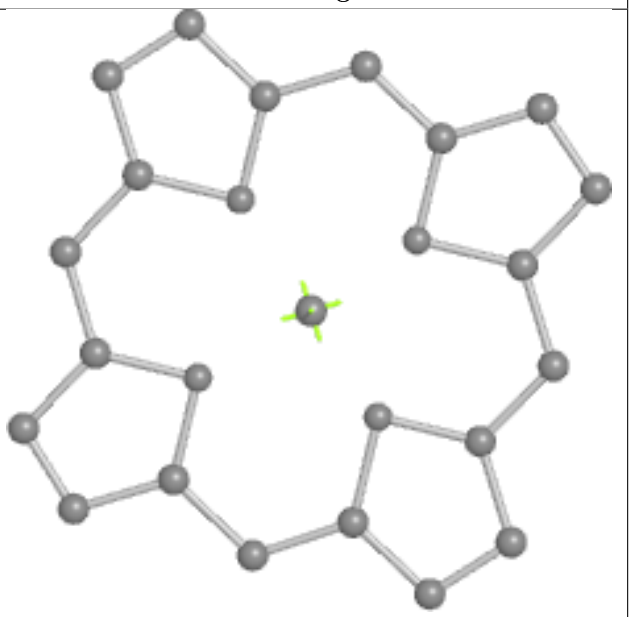
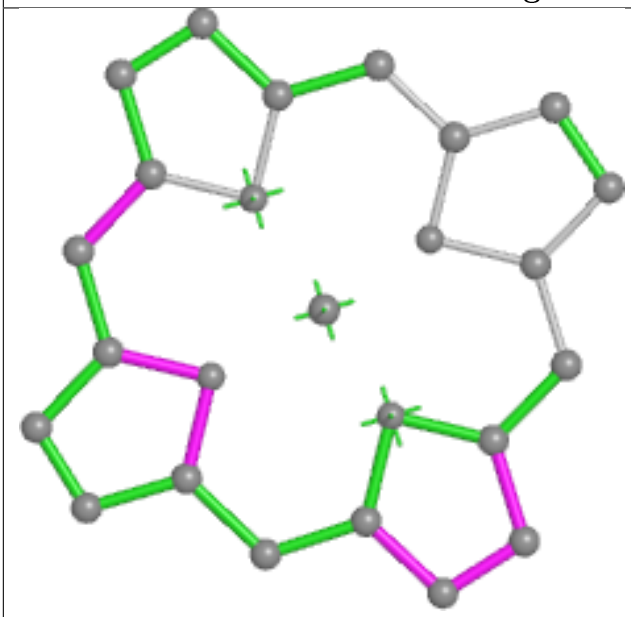


Rings

Ligand CLA D 163



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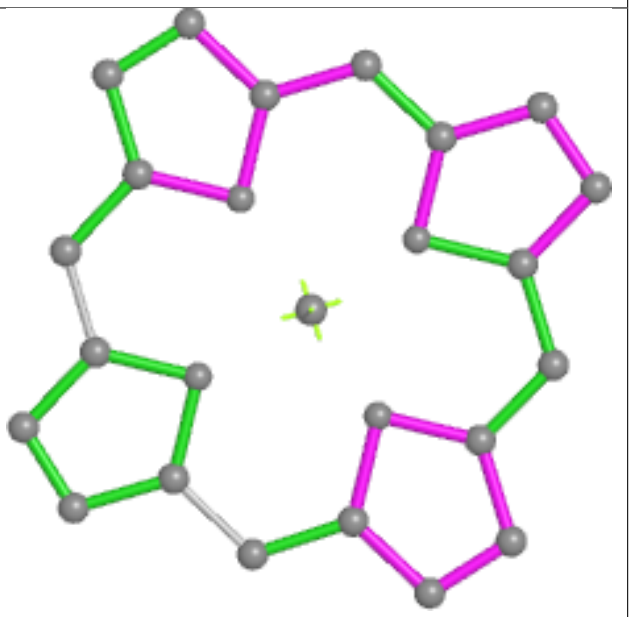
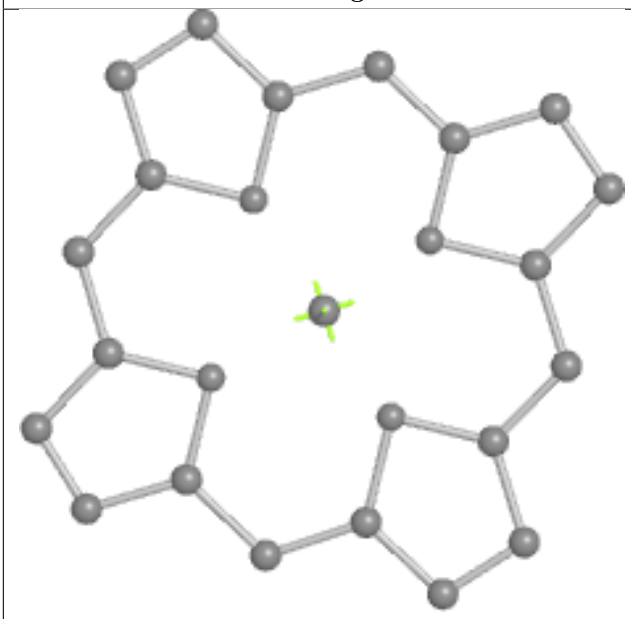


Bond angles



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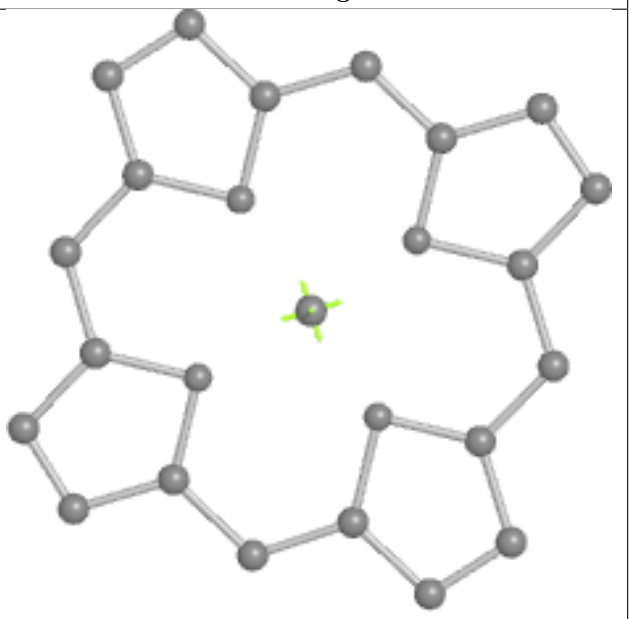
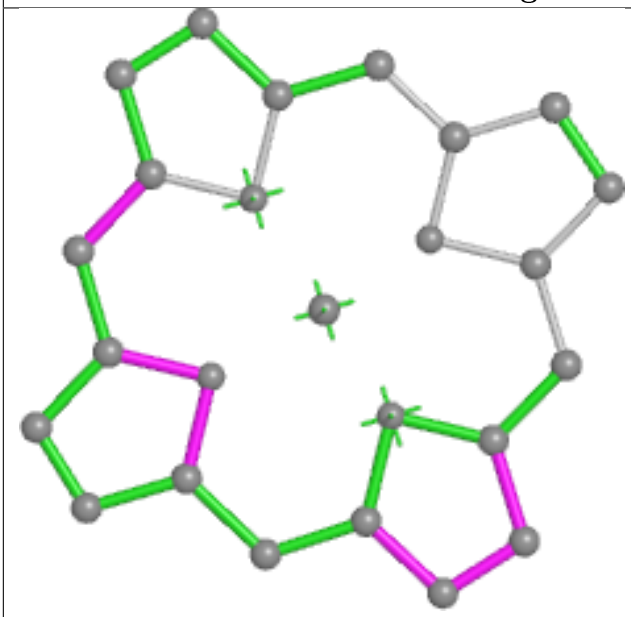


Rings

Ligand CLA M 167



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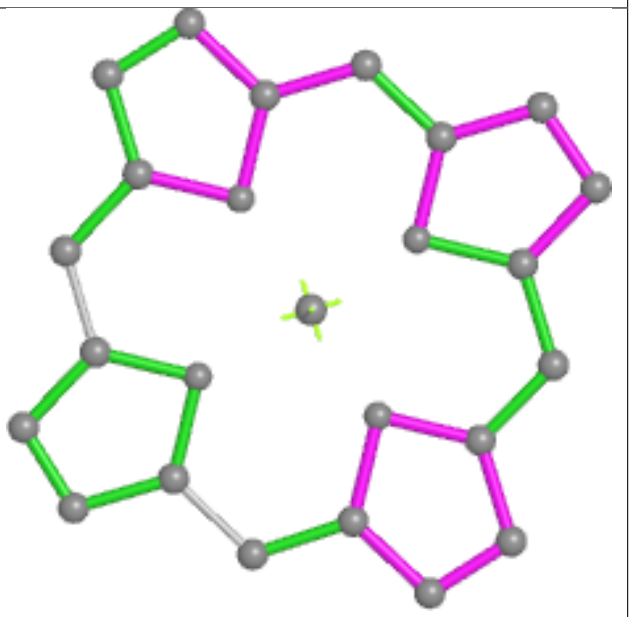

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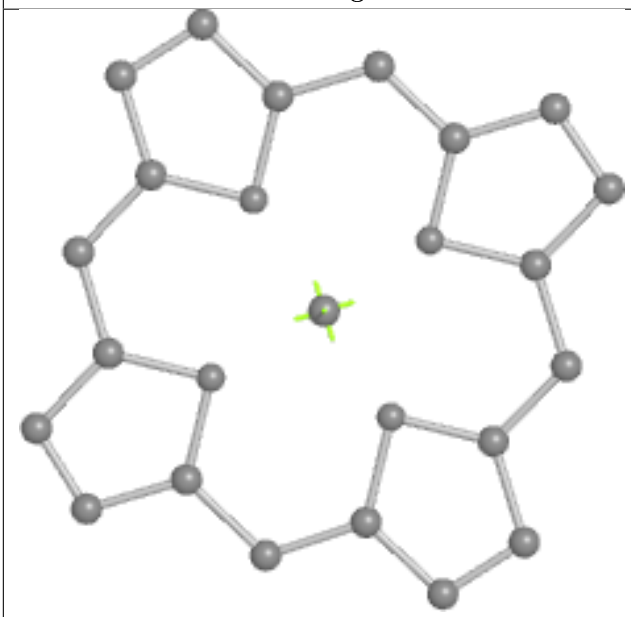

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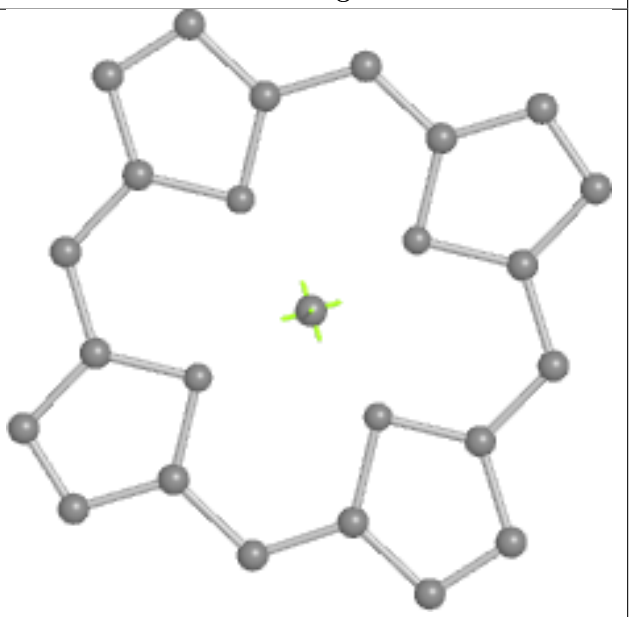
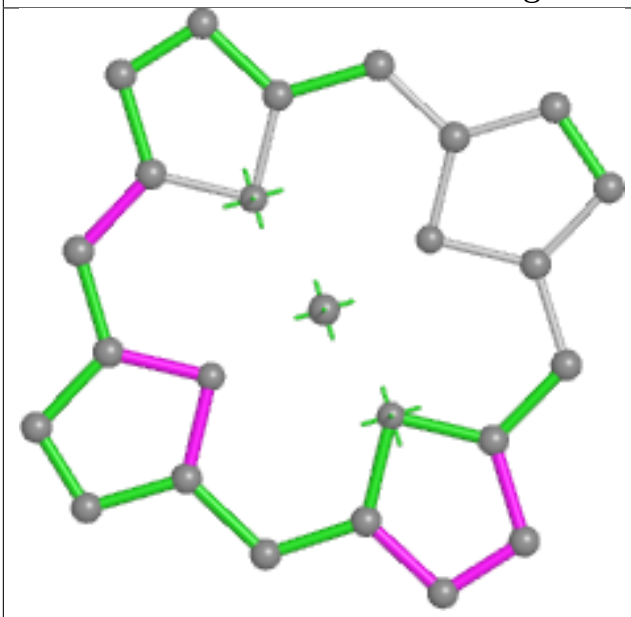


Rings

Ligand CLA D 167



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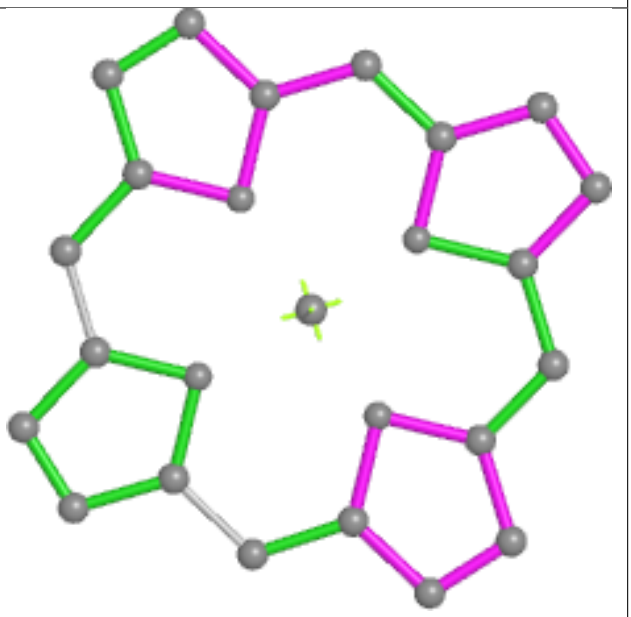
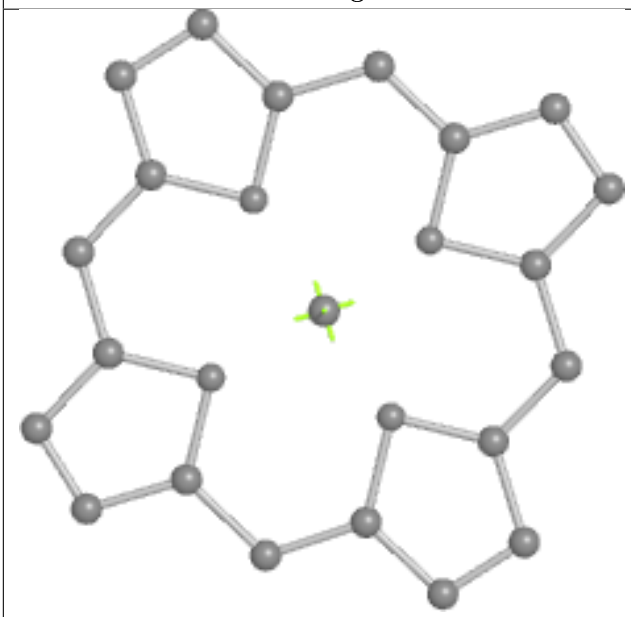
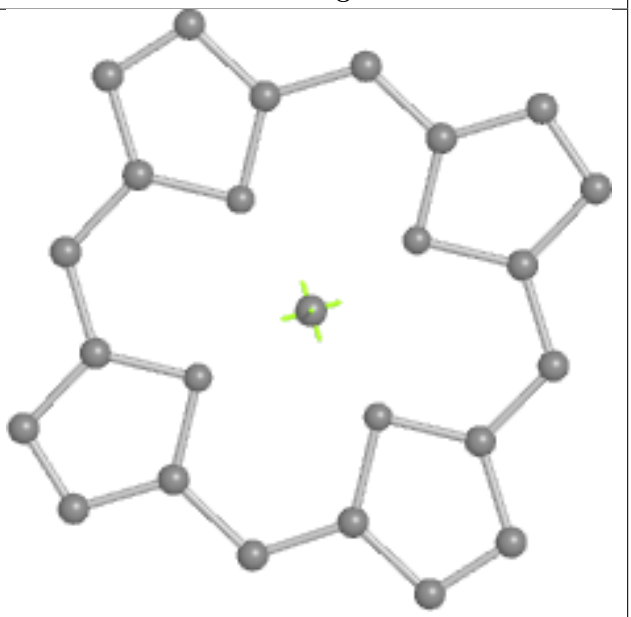


Bond angles

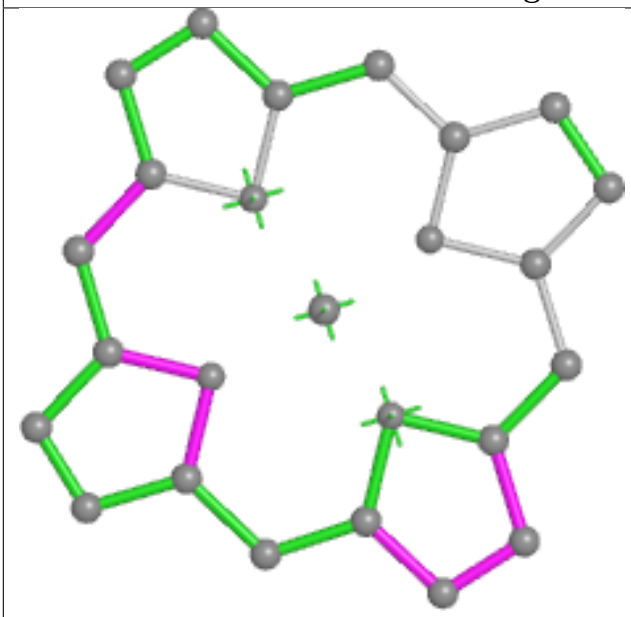


Torsions



Rings

Ligand CLA D 159



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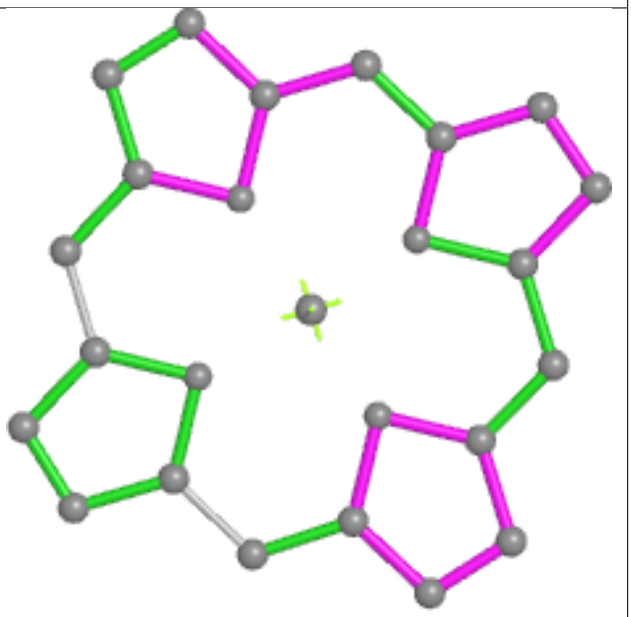
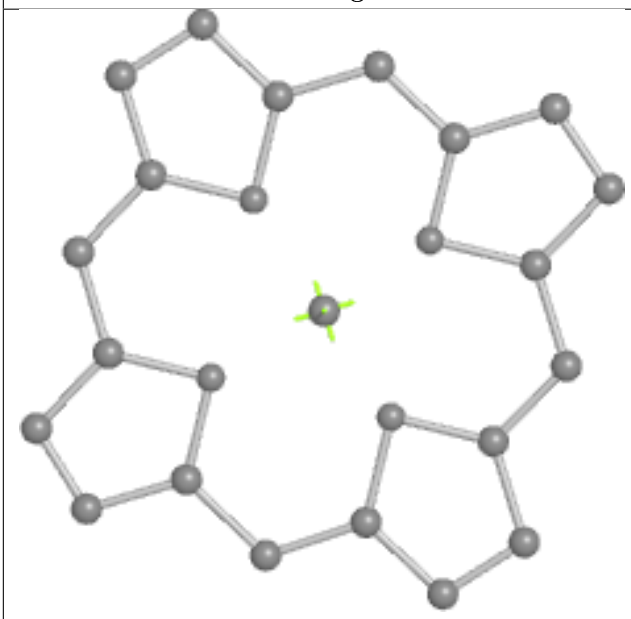
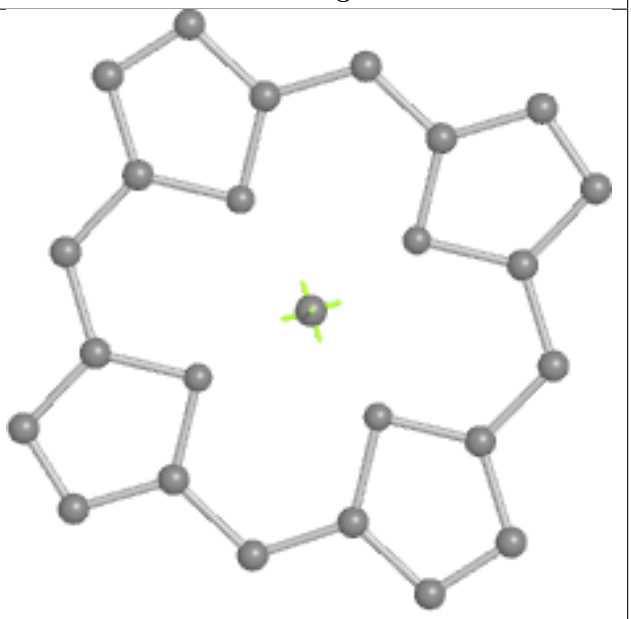


Bond angles

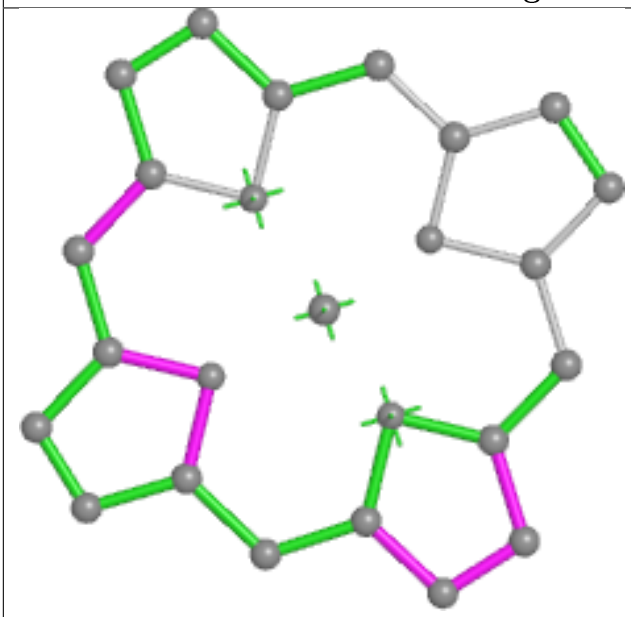


Torsions

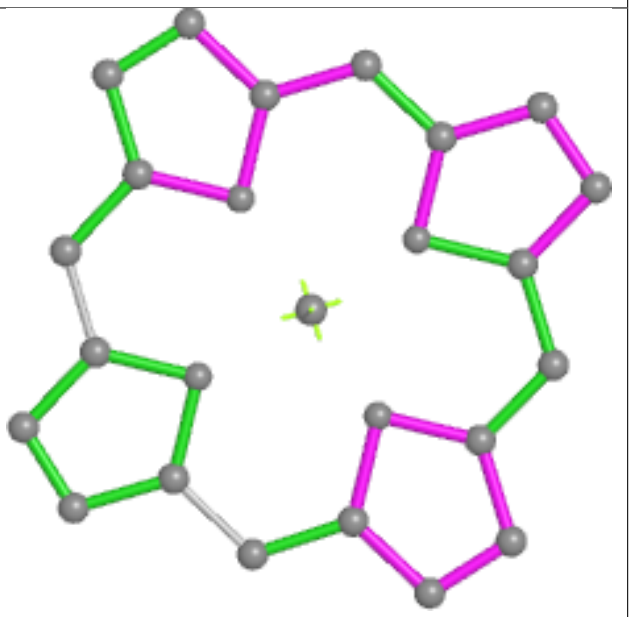


Rings

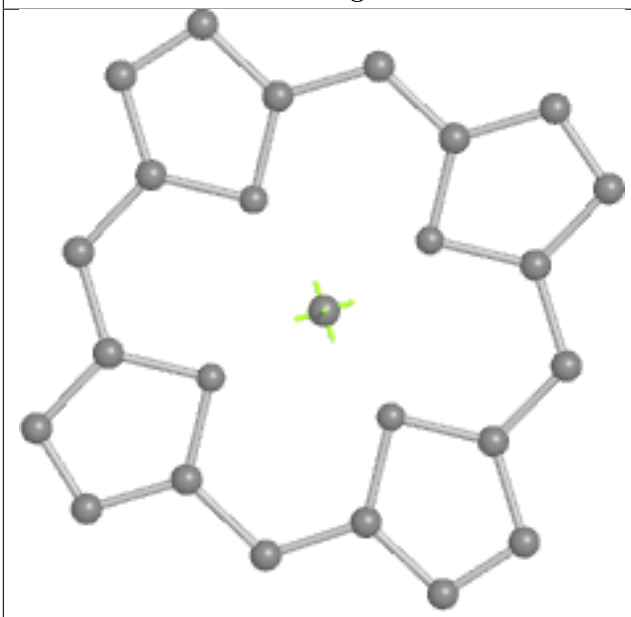
Ligand CLA D 158



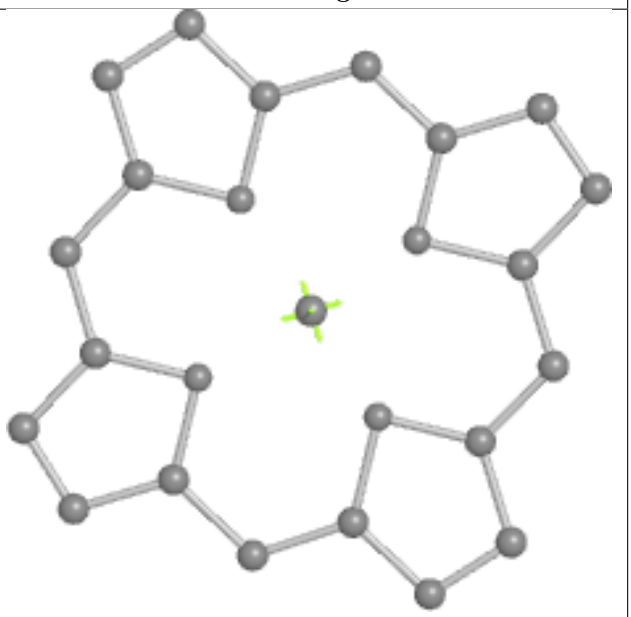
Bond lengths



Bond angles

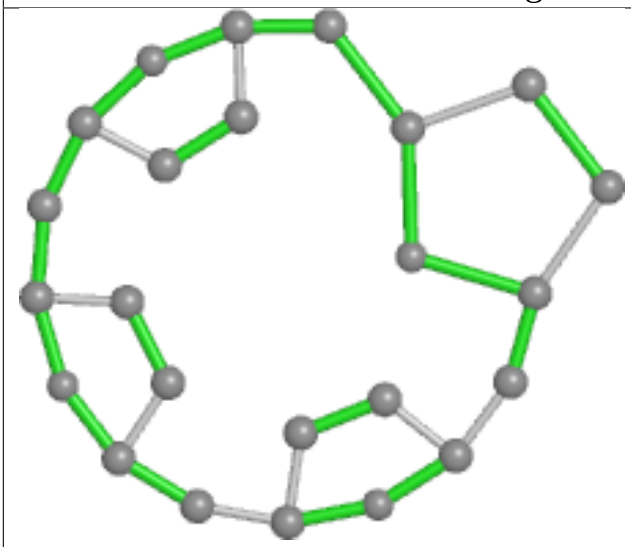


Torsions

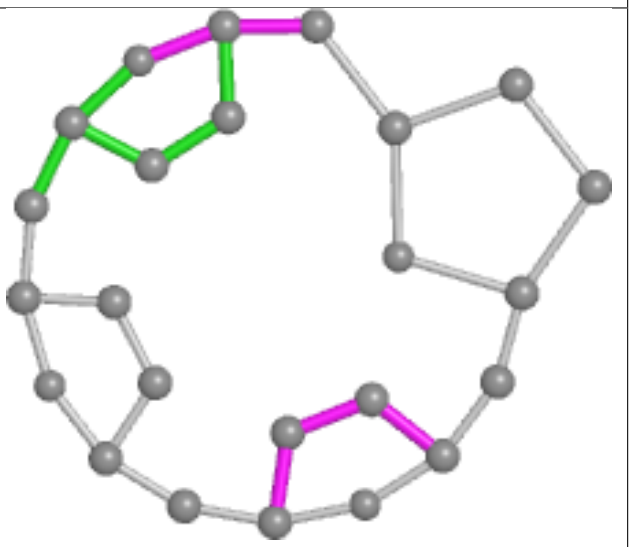


Rings

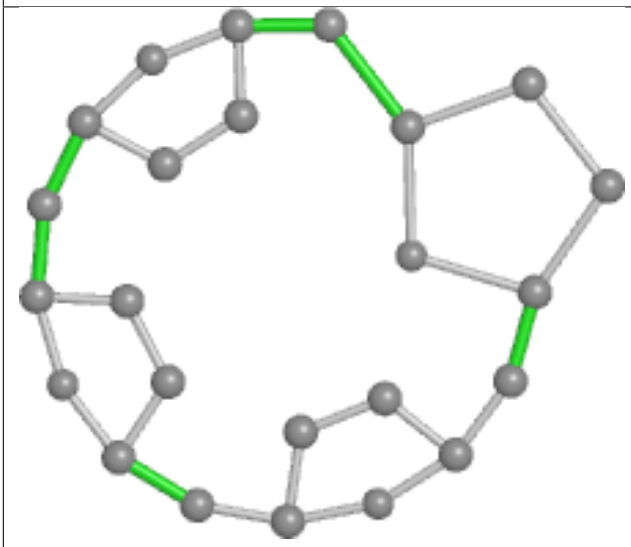
Ligand PHO J 178



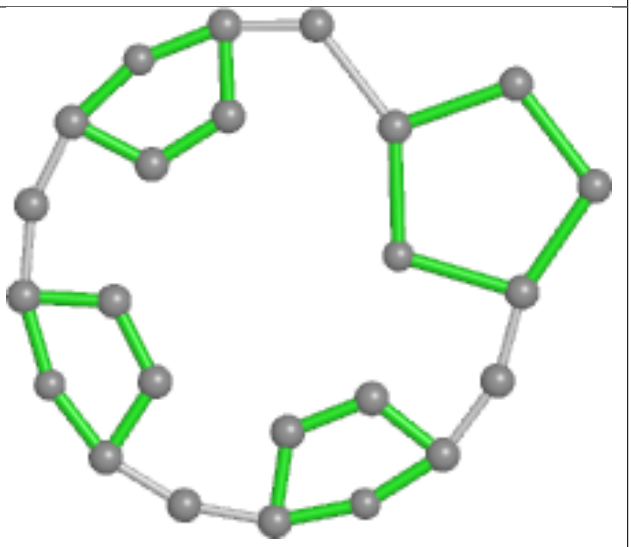
Bond lengths



Bond angles

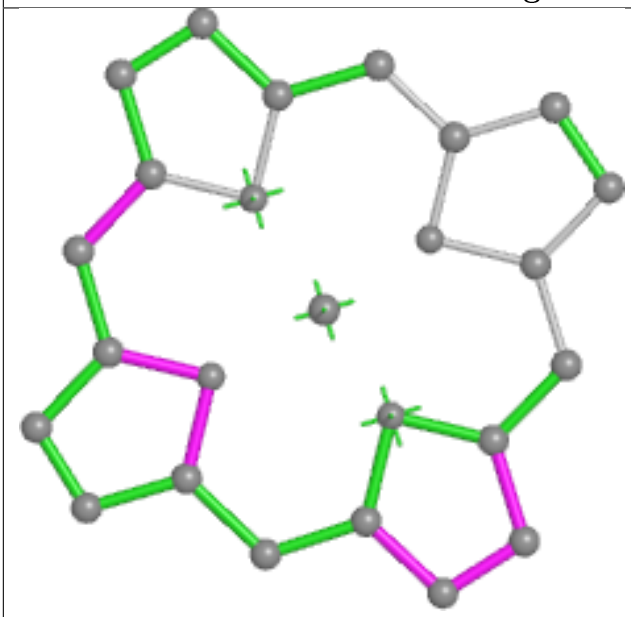


Torsions

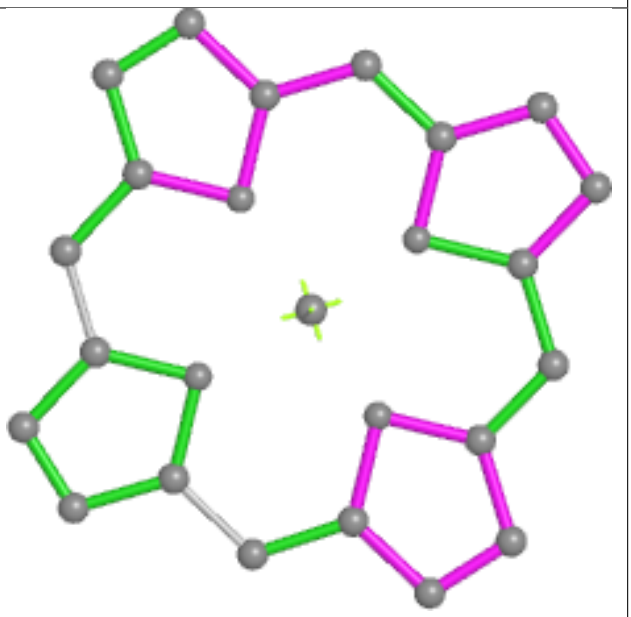


Rings

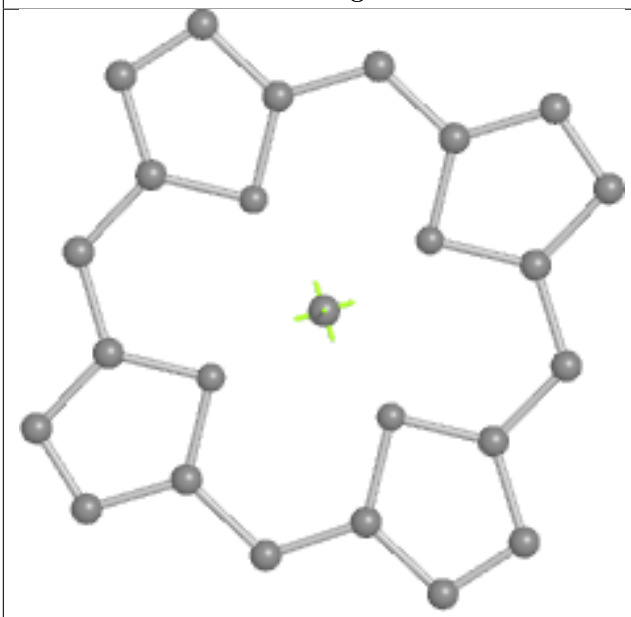
Ligand CLA D 156



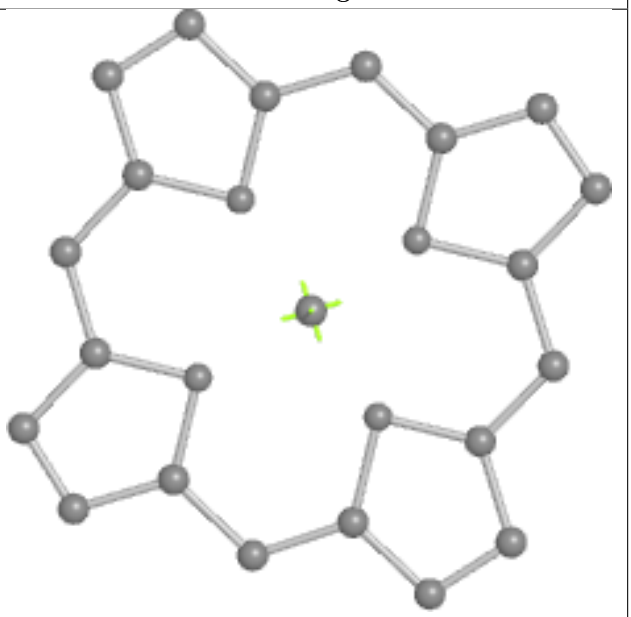
Bond lengths



Bond angles

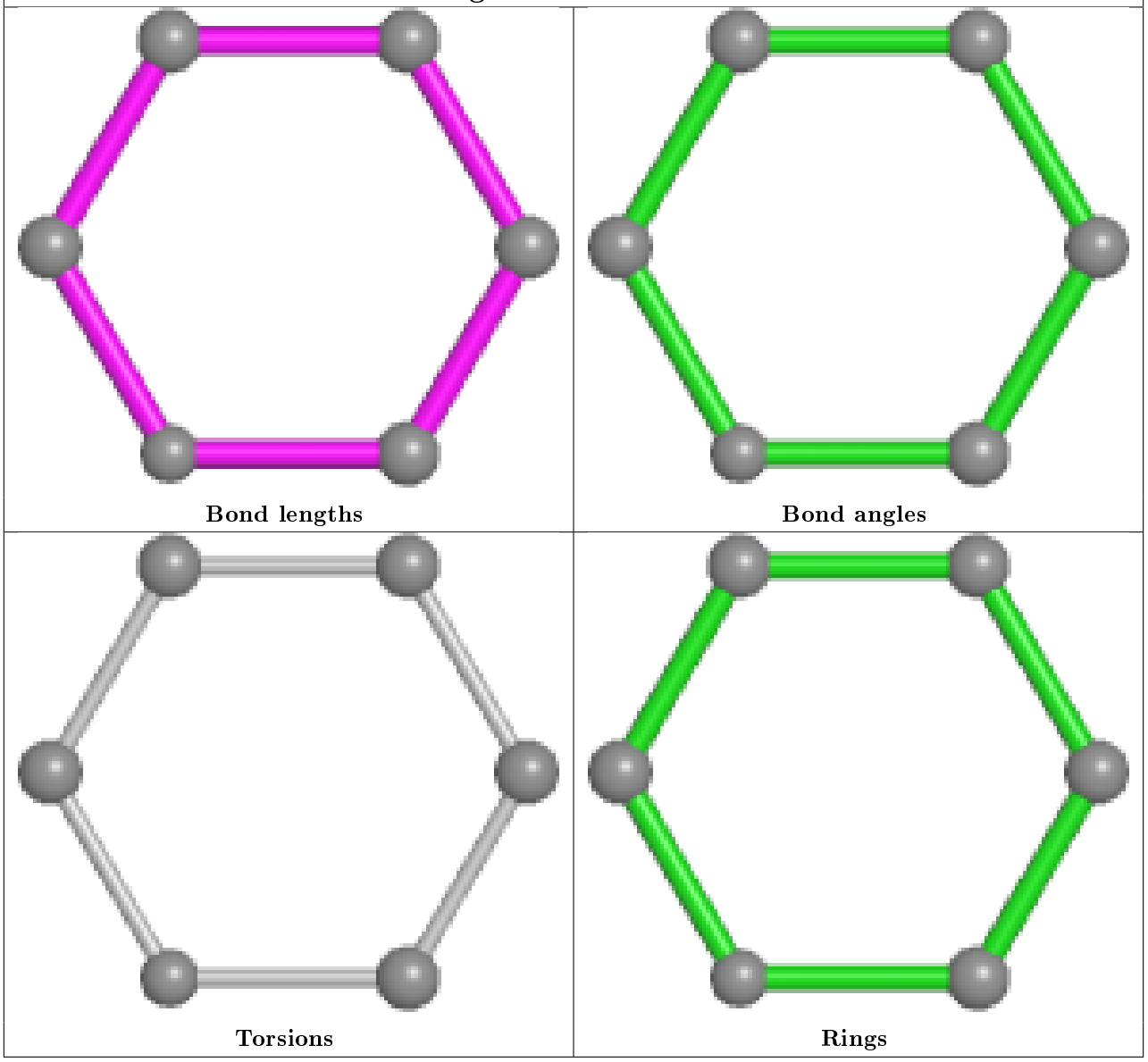


Torsions



Rings

Ligand PLA K 180



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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.