Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:10 AM EDT

PDB ID	:	1ILX / pdb_00001ilx
Title	:	Excited State Dynamics in Photosystem II Revised. New Insights from the X-ray Structure.
Authors	:	Vasilev, S.; Orth, P.; Zouni, A.; Owens, T.G.; Bruce, D.
Deposited on	:	2001-05-09
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

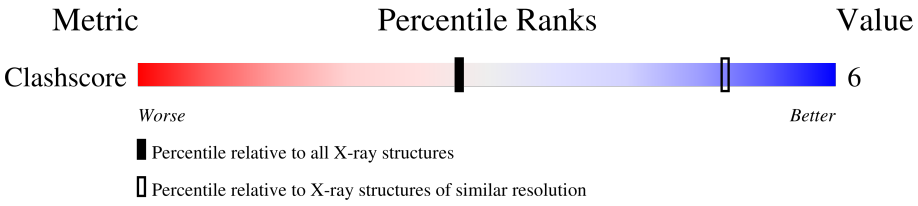
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	190562	1012 (3.94-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

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	99%
4	M	155	99%
5	E	40	100%
5	N	40	100%

Continued on next page...

Continued from previous page...

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%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 4594 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOTOSYSTEM 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 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 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 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 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 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 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 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 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 (CCD ID: MN) (formula: Mn).

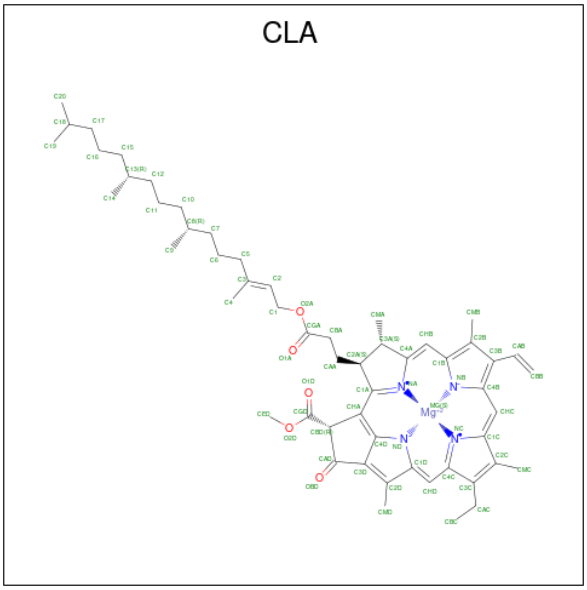
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	4	Total Mn 4 4	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C Mg N 27 22 1 4	0	0
11	A	1	Total C Mg N 27 22 1 4	0	0
11	A	1	Total C Mg N 27 22 1 4	0	0
11	A	1	Total C Mg N 27 22 1 4	0	0
11	A	1	Total C Mg N 27 22 1 4	0	0
11	B	1	Total C Mg N 27 22 1 4	0	0
11	B	1	Total C Mg N 27 22 1 4	0	0
11	C	1	Total C Mg N 27 22 1 4	0	0
11	C	1	Total C Mg N 27 22 1 4	0	0
11	C	1	Total C Mg N 27 22 1 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	C	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	C	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	C	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	C	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	C	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	C	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	C	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	C	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		

Continued on next page...

Continued from previous page...

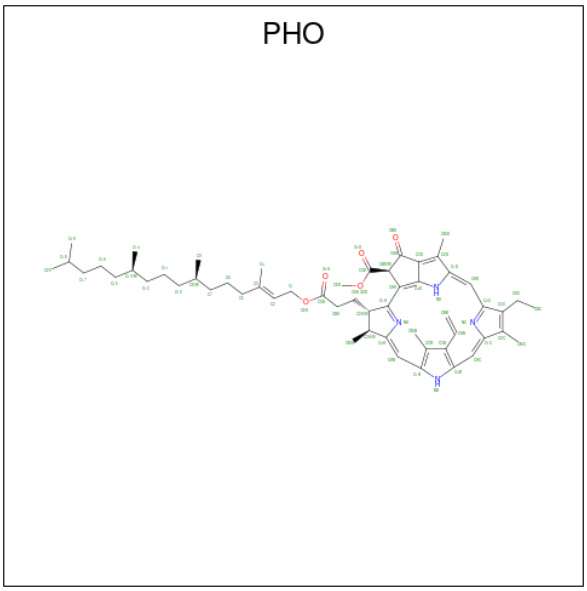
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	G	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	J	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	J	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	J	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	J	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	J	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	K	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	K	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	L	1	Total	C	Mg	N	0	0
			27	22	1	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	L	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	M	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	P	1	Total	C	Mg	N	0	0
			27	22	1	4		

- Molecule 12 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).

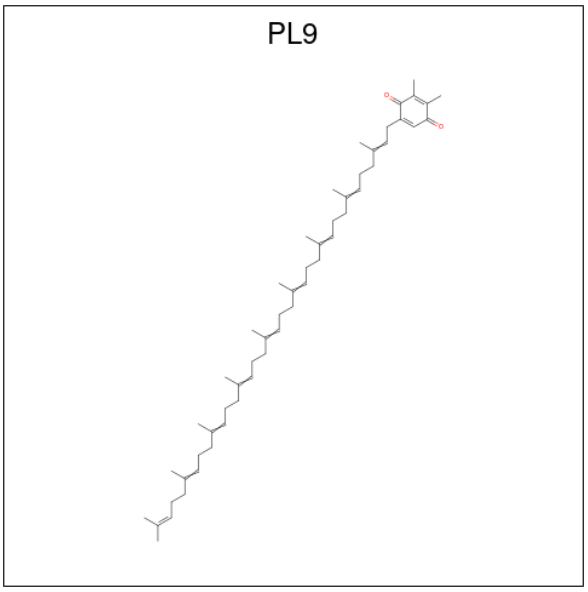


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C N 26 22 4	0	0
12	B	1	Total C N 26 22 4	0	0
12	J	1	Total C N 26 22 4	0	0
12	K	1	Total C N 26 22 4	0	0

- Molecule 13 is FE (III) ION (CCD ID: FE) (formula: Fe).

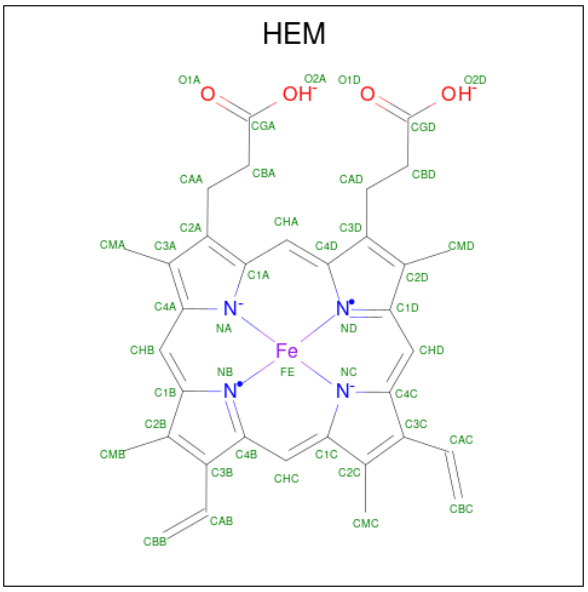
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total Fe 1 1	0	0
13	K	1	Total Fe 1 1	0	0

- Molecule 14 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total C 6 6	0	0
14	K	1	Total C 6 6	0	0

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	F	1	Total C Fe N 25 20 1 4	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 16 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

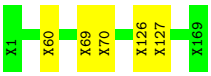
3 Residue-property plots (i)

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

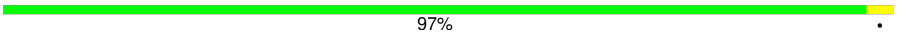
• Molecule 1: PHOTOSYSTEM II: SUBUNIT PSBA

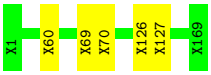
Chain A:



• Molecule 1: PHOTOSYSTEM II: SUBUNIT PSBA

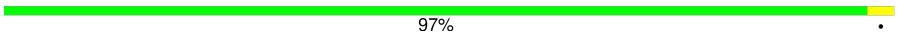
Chain J:





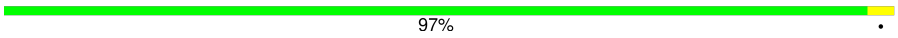
• Molecule 2: PHOTOSYSTEM II: SUBUNIT PSBD

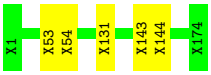
Chain B:



• Molecule 2: PHOTOSYSTEM II: SUBUNIT PSBD

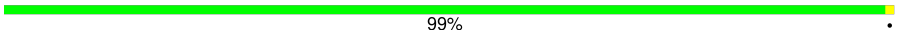
Chain K:

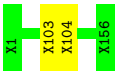




• Molecule 3: PHOTOSYSTEM II: SUBUNIT PSBC

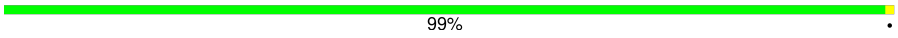
Chain C:

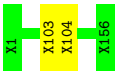




• Molecule 3: PHOTOSYSTEM II: SUBUNIT PSBC

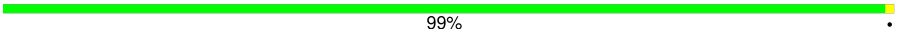
Chain L:





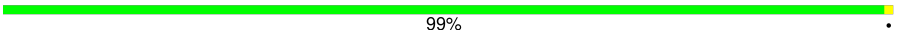
• Molecule 4: PHOTOSYSTEM II: SUBUNIT PSBB

Chain D:



• Molecule 4: PHOTOSYSTEM II: SUBUNIT PSBB

Chain M:



• Molecule 5: PHOTOSYSTEM II: SUBUNIT PSBE

Chain E:

There are no outlier residues recorded for this chain.

• Molecule 5: PHOTOSYSTEM II: SUBUNIT PSBE

Chain N:

There are no outlier residues recorded for this chain.

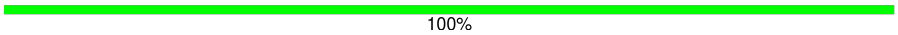
• Molecule 6: PHOTOSYSTEM II: SUBUNIT PSBF

Chain F:

There are no outlier residues recorded for this chain.

• Molecule 6: PHOTOSYSTEM II: SUBUNIT PSBF

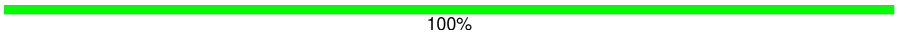
Chain O:



There are no outlier residues recorded for this chain.

• Molecule 7: PHOTOSYSTEM II: SUBUNIT UNKNOWN

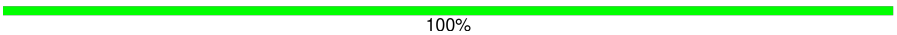
Chain G:



There are no outlier residues recorded for this chain.

• Molecule 7: PHOTOSYSTEM II: SUBUNIT UNKNOWN

Chain P:



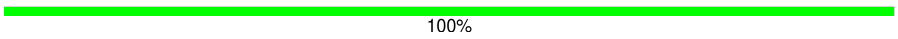
There are no outlier residues recorded for this chain.

• Molecule 8: PHOTOSYSTEM II: SUBUNIT PSBO

Chain H:

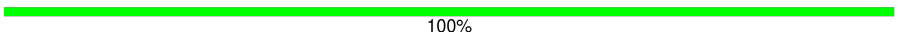
There are no outlier residues recorded for this chain.

• Molecule 8: PHOTOSYSTEM II: SUBUNIT PSBO

Chain Q: 

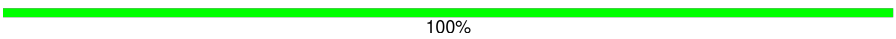
There are no outlier residues recorded for this chain.

• Molecule 9: PHOTOSYSTEM II: SUBUNIT PSBV

Chain I: 

There are no outlier residues recorded for this chain.

• Molecule 9: 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	4594	wwPDB-VP
Average B, all atoms (Å^2)	1.0	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: MN, PL9, CLA, FE, PHO, HEM, CD

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	3	0
4	M	155	0	0	3	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

Continued on next page...

Continued from previous page...

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	135	0	15	0	0
11	B	54	0	6	0	0
11	C	324	0	36	2	0
11	D	405	0	45	7	0
11	G	27	0	3	4	0
11	J	135	0	15	0	0
11	K	54	0	6	0	0
11	L	324	0	36	2	0
11	M	405	0	45	7	0
11	P	27	0	3	4	0
12	A	26	0	5	0	0
12	B	26	0	5	0	0
12	J	26	0	5	0	0
12	K	26	0	5	0	0
13	B	1	0	0	0	0
13	K	1	0	0	0	0
14	B	6	0	1	0	0
14	K	6	0	1	0	0
15	F	25	0	4	0	0
15	I	25	0	4	0	0
15	O	25	0	4	0	0
15	R	25	0	4	0	0
16	H	1	0	0	0	0
16	Q	1	0	0	0	0
All	All	4594	0	248	28	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 (28) 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
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:103:UNK:CA	11:L:168:CLA:C2A	2.41	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:UNK:CA	11:C:168:CLA:C2A	2.41	0.98
11:M:168:CLA:CAD	11:P:313:CLA:CAD	2.54	0.85
11:D:168:CLA:CAD	11:G:313:CLA:CAD	2.54	0.85
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
11:M:168:CLA:CBD	11:P:313:CLA:CAD	2.68	0.72
11:D:168:CLA:CBD	11:G:313:CLA:CAD	2.68	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
4:D:22:UNK:CA	11:D:165:CLA:CHC	2.77	0.62
4:M:22:UNK:CA	11:M:165:CLA:CHC	2.77	0.62
4:D:22:UNK:CA	11:D:165:CLA:C4B	2.80	0.60
4:M:22:UNK:CA	11:M:165:CLA:C3B	2.81	0.59
4:M:22:UNK:CA	11:M:165:CLA:C4B	2.80	0.59
4:D:22:UNK:CA	11:D:165:CLA:C3B	2.81	0.58
11:M:168:CLA:CHA	11:P:313:CLA:CBD	2.90	0.50
11:D:168:CLA:CHA	11:G:313:CLA:CBD	2.90	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
3:L:104:UNK:CA	11:L:168:CLA:CBD	2.94	0.45
3:C:104:UNK:CA	11:C:168:CLA:CBD	2.94	0.45
11:D:168:CLA:C3D	11:G:313:CLA:CAD	2.98	0.41
11:M:168:CLA:C3D	11:P:313:CLA:CAD	2.98	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

5.3.2 Protein sidechains

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 (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 92 ligands modelled in this entry, 12 are monoatomic - leaving 80 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	$\#\|Z\| > 2$
11	CLA	C	165	-	27,35,73	2.20	8 (29%)	32,60,113	2.17	4 (12%)
11	CLA	M	159	-	27,35,73	2.20	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	L	159	-	27,35,73	2.20	8 (29%)	32,60,113	2.17	4 (12%)
11	CLA	A	175	-	27,35,73	2.21	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	L	164	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
15	HEM	O	90	-	32,32,50	2.67	13 (40%)	30,54,82	2.79	12 (40%)
11	CLA	J	179	-	27,35,73	2.21	8 (29%)	32,60,113	2.14	4 (12%)
11	CLA	L	163	-	27,35,73	2.19	8 (29%)	32,60,113	2.17	4 (12%)
11	CLA	L	168	-	27,35,73	2.20	8 (29%)	32,60,113	2.19	4 (12%)
11	CLA	M	164	-	27,35,73	2.20	8 (29%)	32,60,113	2.20	4 (12%)
11	CLA	J	174	-	27,35,73	2.21	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	C	168	-	27,35,73	2.21	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	D	159	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	D	166	-	27,35,73	2.20	8 (29%)	32,60,113	2.17	4 (12%)
11	CLA	G	313	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
15	HEM	R	91	-	32,32,50	2.66	14 (43%)	30,54,82	2.82	12 (40%)
11	CLA	B	176	-	27,35,73	2.19	8 (29%)	32,60,113	2.15	4 (12%)
11	CLA	D	168	-	27,35,73	2.20	8 (29%)	32,60,113	2.18	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	A	174	-	27,35,73	2.21	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	M	160	-	27,35,73	2.21	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	C	164	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	D	169	-	27,35,73	2.20	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	M	157	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	L	160	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	C	162	-	27,35,73	2.19	8 (29%)	32,60,113	2.15	4 (12%)
11	CLA	L	166	-	27,35,73	2.20	8 (29%)	32,60,113	2.14	4 (12%)
11	CLA	J	175	-	27,35,73	2.21	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	C	161	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	C	166	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	B	178	-	27,35,73	2.20	8 (29%)	32,60,113	2.15	4 (12%)
11	CLA	D	158	-	27,35,73	2.21	8 (29%)	32,60,113	2.19	4 (12%)
12	PHO	A	177	-	19,31,69	3.45	7 (36%)	12,46,99	3.20	6 (50%)
11	CLA	C	159	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
12	PHO	K	177	-	19,31,69	3.45	7 (36%)	12,46,99	3.19	6 (50%)
11	CLA	A	179	-	27,35,73	2.20	8 (29%)	32,60,113	2.14	4 (12%)
11	CLA	D	170	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
15	HEM	I	88	-	32,32,50	2.66	14 (43%)	30,54,82	2.82	12 (40%)
11	CLA	M	158	-	27,35,73	2.21	8 (29%)	32,60,113	2.15	4 (12%)
11	CLA	D	162	-	27,35,73	2.21	8 (29%)	32,60,113	2.15	4 (12%)
11	CLA	J	176	-	27,35,73	2.20	8 (29%)	32,60,113	2.15	4 (12%)
11	CLA	M	167	-	27,35,73	2.20	8 (29%)	32,60,113	2.14	4 (12%)
11	CLA	A	178	-	27,35,73	2.20	8 (29%)	32,60,113	2.17	4 (12%)
11	CLA	J	178	-	27,35,73	2.21	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	K	178	-	27,35,73	2.20	8 (29%)	32,60,113	2.14	4 (12%)
11	CLA	M	156	-	27,35,73	2.20	8 (29%)	32,60,113	2.19	4 (12%)
11	CLA	C	160	-	27,35,73	2.19	8 (29%)	32,60,113	2.15	4 (12%)
11	CLA	C	157	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	P	313	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
15	HEM	F	50	-	32,32,50	2.67	14 (43%)	30,54,82	2.80	12 (40%)
11	CLA	D	156	-	27,35,73	2.20	8 (29%)	32,60,113	2.17	4 (12%)
11	CLA	A	176	-	27,35,73	2.19	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	D	165	-	27,35,73	2.20	8 (29%)	32,60,113	2.17	4 (12%)
11	CLA	L	167	-	27,35,73	2.20	8 (29%)	32,60,113	2.15	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	D	163	-	27,35,73	2.20	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	L	165	-	27,35,73	2.20	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	K	176	-	27,35,73	2.19	8 (29%)	32,60,113	2.15	4 (12%)
11	CLA	M	161	-	27,35,73	2.20	8 (29%)	32,60,113	2.15	4 (12%)
12	PHO	J	177	-	19,31,69	3.47	7 (36%)	12,46,99	3.20	6 (50%)
12	PHO	B	177	-	19,31,69	3.45	7 (36%)	12,46,99	3.19	6 (50%)
11	CLA	L	158	-	27,35,73	2.19	8 (29%)	32,60,113	2.17	4 (12%)
11	CLA	C	158	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	M	165	-	27,35,73	2.20	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	D	160	-	27,35,73	2.21	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	D	157	-	27,35,73	2.19	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	C	163	-	27,35,73	2.20	8 (29%)	32,60,113	2.18	4 (12%)
14	PL9	B	179	-	6,6,55	2.32	2 (33%)	6,6,69	1.09	0
11	CLA	M	162	-	27,35,73	2.21	8 (29%)	32,60,113	2.15	4 (12%)
11	CLA	M	163	-	27,35,73	2.20	8 (29%)	32,60,113	2.17	4 (12%)
11	CLA	L	161	-	27,35,73	2.19	8 (29%)	32,60,113	2.16	4 (12%)
11	CLA	L	162	-	27,35,73	2.20	8 (29%)	32,60,113	2.17	4 (12%)
11	CLA	D	164	-	27,35,73	2.20	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	M	166	-	27,35,73	2.21	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	M	168	-	27,35,73	2.21	8 (29%)	32,60,113	2.20	4 (12%)
11	CLA	D	167	-	27,35,73	2.20	8 (29%)	32,60,113	2.14	4 (12%)
11	CLA	M	170	-	27,35,73	2.20	8 (29%)	32,60,113	2.15	4 (12%)
11	CLA	D	161	-	27,35,73	2.20	8 (29%)	32,60,113	2.17	4 (12%)
11	CLA	L	157	-	27,35,73	2.20	8 (29%)	32,60,113	2.17	4 (12%)
11	CLA	M	169	-	27,35,73	2.20	8 (29%)	32,60,113	2.18	4 (12%)
11	CLA	C	167	-	27,35,73	2.21	8 (29%)	32,60,113	2.17	4 (12%)
14	PL9	K	179	-	6,6,55	2.32	2 (33%)	6,6,69	1.09	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	PHO	K	177	-	-	0/0/43/103	0/5/6/6
12	PHO	A	177	-	-	0/0/43/103	0/5/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PHO	J	177	-	-	0/0/43/103	0/5/6/6
14	PL9	B	179	-	-	-	0/1/1/1
12	PHO	B	177	-	-	0/0/43/103	0/5/6/6
14	PL9	K	179	-	-	-	0/1/1/1

All (647) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	J	177	PHO	C3B-C4B	10.11	1.48	1.39
12	B	177	PHO	C3B-C4B	10.09	1.48	1.39
12	K	177	PHO	C3B-C4B	10.05	1.48	1.39
12	A	177	PHO	C3B-C4B	10.05	1.48	1.39
12	A	177	PHO	C2B-C1B	7.60	1.46	1.39
12	J	177	PHO	C2B-C1B	7.59	1.46	1.39
12	K	177	PHO	C2B-C1B	7.58	1.46	1.39
12	B	177	PHO	C2B-C1B	7.57	1.46	1.39
15	R	91	HEM	C3C-C2C	6.04	1.48	1.35
15	I	88	HEM	C3C-C2C	6.03	1.48	1.35
15	F	50	HEM	C3C-C2C	6.02	1.48	1.35
15	O	90	HEM	C3C-C2C	6.00	1.48	1.35
15	R	91	HEM	C2A-C1A	5.98	1.52	1.40
15	I	88	HEM	C2A-C1A	5.96	1.52	1.40
15	O	90	HEM	C2A-C1A	5.95	1.52	1.40
15	F	50	HEM	C2A-C1A	5.95	1.52	1.40
12	K	177	PHO	CAD-C3D	-5.55	1.42	1.51
12	J	177	PHO	CAD-C3D	-5.55	1.42	1.51
12	A	177	PHO	CAD-C3D	-5.54	1.42	1.51
12	B	177	PHO	CAD-C3D	-5.54	1.42	1.51
15	O	90	HEM	C3A-C4A	5.53	1.52	1.40
15	R	91	HEM	C3A-C4A	5.51	1.51	1.40
15	I	88	HEM	C3A-C4A	5.51	1.51	1.40
15	F	50	HEM	C3A-C4A	5.50	1.51	1.40
11	M	169	CLA	MG-NA	4.84	2.17	2.06
11	D	168	CLA	MG-NA	4.83	2.17	2.06
11	M	168	CLA	MG-NA	4.83	2.17	2.06
11	L	168	CLA	MG-NA	4.83	2.17	2.06
11	M	164	CLA	MG-NA	4.83	2.17	2.06
11	J	178	CLA	MG-NA	4.82	2.17	2.06
11	D	169	CLA	MG-NA	4.82	2.17	2.06
11	C	168	CLA	MG-NA	4.82	2.17	2.06
11	D	164	CLA	MG-NA	4.81	2.17	2.06
11	M	157	CLA	MG-NA	4.81	2.17	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	160	CLA	MG-NA	4.81	2.17	2.06
11	D	160	CLA	MG-NA	4.81	2.17	2.06
11	A	178	CLA	MG-NA	4.81	2.17	2.06
11	L	163	CLA	MG-NA	4.80	2.17	2.06
11	D	167	CLA	MG-NA	4.80	2.17	2.06
11	D	157	CLA	MG-NA	4.80	2.17	2.06
11	C	163	CLA	MG-NA	4.80	2.17	2.06
11	M	159	CLA	MG-NA	4.80	2.17	2.06
11	J	174	CLA	MG-NA	4.80	2.17	2.06
11	D	163	CLA	MG-NA	4.80	2.17	2.06
11	M	158	CLA	MG-NA	4.80	2.17	2.06
11	M	167	CLA	MG-NA	4.80	2.17	2.06
11	C	157	CLA	MG-NA	4.80	2.17	2.06
11	J	175	CLA	MG-NA	4.80	2.17	2.06
11	D	166	CLA	MG-NA	4.80	2.17	2.06
11	D	162	CLA	MG-ND	-4.80	1.96	2.05
11	D	158	CLA	MG-NA	4.79	2.17	2.06
11	D	165	CLA	MG-NA	4.79	2.17	2.06
11	L	165	CLA	MG-NA	4.79	2.17	2.06
11	M	166	CLA	MG-NA	4.79	2.17	2.06
11	C	167	CLA	MG-NA	4.79	2.17	2.06
11	L	157	CLA	MG-NA	4.79	2.17	2.06
11	A	174	CLA	MG-NA	4.79	2.17	2.06
11	M	165	CLA	MG-NA	4.79	2.17	2.06
11	D	159	CLA	MG-NA	4.79	2.17	2.06
11	C	159	CLA	MG-NA	4.79	2.17	2.06
11	M	163	CLA	MG-NA	4.79	2.17	2.06
11	M	162	CLA	MG-ND	-4.79	1.96	2.05
11	L	162	CLA	MG-NA	4.78	2.17	2.06
11	C	165	CLA	MG-NA	4.78	2.17	2.06
11	C	166	CLA	MG-NA	4.78	2.17	2.06
11	M	156	CLA	MG-NA	4.78	2.17	2.06
11	P	313	CLA	MG-ND	-4.78	1.96	2.05
11	L	159	CLA	MG-NA	4.78	2.17	2.06
11	D	156	CLA	MG-NA	4.78	2.17	2.06
11	B	178	CLA	MG-ND	-4.77	1.96	2.05
11	C	158	CLA	MG-NA	4.77	2.17	2.06
11	C	161	CLA	MG-NA	4.77	2.17	2.06
11	G	313	CLA	MG-ND	-4.77	1.96	2.05
11	J	176	CLA	MG-ND	-4.77	1.96	2.05
11	A	175	CLA	MG-NA	4.77	2.17	2.06
11	L	158	CLA	MG-NA	4.77	2.17	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	160	CLA	MG-NA	4.77	2.17	2.06
11	L	164	CLA	MG-NA	4.77	2.17	2.06
11	D	161	CLA	MG-NA	4.77	2.17	2.06
11	C	164	CLA	MG-NA	4.77	2.17	2.06
11	L	161	CLA	MG-NA	4.77	2.17	2.06
11	C	166	CLA	MG-ND	-4.77	1.96	2.05
11	D	170	CLA	MG-NA	4.77	2.17	2.06
11	J	179	CLA	MG-NA	4.76	2.17	2.06
11	D	162	CLA	MG-NA	4.76	2.17	2.06
11	G	313	CLA	MG-NA	4.76	2.17	2.06
11	A	176	CLA	MG-ND	-4.76	1.96	2.05
11	A	179	CLA	MG-NA	4.76	2.17	2.06
11	M	170	CLA	MG-NA	4.76	2.17	2.06
11	C	162	CLA	MG-NA	4.76	2.17	2.06
11	J	175	CLA	MG-ND	-4.76	1.96	2.05
11	L	166	CLA	MG-ND	-4.76	1.96	2.05
11	L	167	CLA	MG-NA	4.76	2.17	2.06
11	M	161	CLA	MG-NA	4.76	2.17	2.06
11	M	158	CLA	MG-ND	-4.75	1.96	2.05
11	L	166	CLA	MG-NA	4.75	2.17	2.06
11	A	174	CLA	MG-ND	-4.75	1.96	2.05
11	P	313	CLA	MG-NA	4.75	2.17	2.06
11	B	176	CLA	MG-NA	4.75	2.17	2.06
11	D	158	CLA	MG-ND	-4.75	1.96	2.05
11	J	176	CLA	MG-NA	4.75	2.17	2.06
11	K	176	CLA	MG-NA	4.75	2.17	2.06
11	L	159	CLA	MG-ND	-4.75	1.96	2.05
11	M	162	CLA	MG-NA	4.75	2.17	2.06
11	L	160	CLA	MG-ND	-4.75	1.96	2.05
11	J	174	CLA	MG-ND	-4.74	1.96	2.05
11	B	176	CLA	MG-ND	-4.74	1.96	2.05
11	A	176	CLA	MG-NA	4.74	2.17	2.06
11	A	175	CLA	MG-ND	-4.74	1.96	2.05
11	K	178	CLA	MG-ND	-4.74	1.96	2.05
11	C	160	CLA	MG-NA	4.74	2.17	2.06
11	D	161	CLA	MG-ND	-4.74	1.96	2.05
11	C	160	CLA	MG-ND	-4.74	1.96	2.05
11	D	163	CLA	MG-ND	-4.74	1.96	2.05
11	J	179	CLA	MG-ND	-4.73	1.96	2.05
11	C	159	CLA	MG-ND	-4.73	1.96	2.05
11	J	178	CLA	MG-ND	-4.73	1.96	2.05
11	L	163	CLA	MG-ND	-4.73	1.96	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	161	CLA	MG-ND	-4.73	1.96	2.05
11	C	163	CLA	MG-ND	-4.73	1.96	2.05
11	C	168	CLA	MG-ND	-4.73	1.96	2.05
11	A	179	CLA	MG-ND	-4.73	1.96	2.05
11	M	163	CLA	MG-ND	-4.73	1.96	2.05
11	L	157	CLA	MG-ND	-4.72	1.96	2.05
11	C	165	CLA	MG-ND	-4.72	1.96	2.05
11	D	160	CLA	MG-ND	-4.72	1.96	2.05
11	L	165	CLA	MG-ND	-4.72	1.96	2.05
11	M	157	CLA	MG-ND	-4.72	1.96	2.05
11	M	166	CLA	MG-ND	-4.72	1.96	2.05
11	D	156	CLA	MG-ND	-4.72	1.96	2.05
11	C	164	CLA	MG-ND	-4.72	1.96	2.05
11	M	167	CLA	MG-ND	-4.72	1.96	2.05
11	B	178	CLA	MG-NA	4.72	2.17	2.06
11	A	178	CLA	MG-ND	-4.71	1.96	2.05
11	C	161	CLA	MG-ND	-4.71	1.96	2.05
11	C	162	CLA	MG-ND	-4.71	1.96	2.05
11	D	166	CLA	MG-ND	-4.71	1.96	2.05
11	L	162	CLA	MG-ND	-4.71	1.96	2.05
11	M	160	CLA	MG-ND	-4.71	1.96	2.05
11	D	157	CLA	MG-ND	-4.71	1.96	2.05
11	C	167	CLA	MG-ND	-4.71	1.96	2.05
11	K	176	CLA	MG-ND	-4.71	1.96	2.05
11	D	165	CLA	MG-ND	-4.71	1.96	2.05
11	M	170	CLA	MG-ND	-4.71	1.96	2.05
11	D	159	CLA	MG-ND	-4.71	1.96	2.05
11	D	167	CLA	MG-ND	-4.70	1.96	2.05
11	M	165	CLA	MG-ND	-4.70	1.96	2.05
11	M	164	CLA	MG-ND	-4.70	1.96	2.05
11	C	157	CLA	MG-ND	-4.70	1.96	2.05
11	L	167	CLA	MG-ND	-4.70	1.96	2.05
11	K	178	CLA	MG-NA	4.70	2.17	2.06
11	D	169	CLA	MG-ND	-4.70	1.96	2.05
11	D	170	CLA	MG-ND	-4.70	1.96	2.05
11	L	164	CLA	MG-ND	-4.70	1.96	2.05
11	D	164	CLA	MG-ND	-4.70	1.96	2.05
11	D	168	CLA	MG-ND	-4.69	1.96	2.05
11	L	158	CLA	MG-ND	-4.69	1.96	2.05
11	L	168	CLA	MG-ND	-4.69	1.96	2.05
11	M	159	CLA	MG-ND	-4.69	1.96	2.05
11	C	158	CLA	MG-ND	-4.69	1.96	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	156	CLA	MG-ND	-4.69	1.96	2.05
11	L	161	CLA	MG-ND	-4.68	1.96	2.05
11	M	169	CLA	MG-ND	-4.68	1.96	2.05
11	M	168	CLA	MG-ND	-4.66	1.96	2.05
15	O	90	HEM	FE-NB	4.60	2.09	1.94
15	F	50	HEM	FE-NB	4.59	2.09	1.94
15	I	88	HEM	FE-NB	4.57	2.09	1.94
15	R	91	HEM	FE-NB	4.56	2.08	1.94
11	J	179	CLA	CAD-C3D	-4.55	1.42	1.50
11	A	174	CLA	CAD-C3D	-4.50	1.42	1.50
11	L	157	CLA	CAD-C3D	-4.50	1.42	1.50
11	C	167	CLA	CAD-C3D	-4.49	1.42	1.50
11	A	179	CLA	CAD-C3D	-4.49	1.42	1.50
11	C	168	CLA	CAD-C3D	-4.47	1.42	1.50
11	J	174	CLA	CAD-C3D	-4.47	1.42	1.50
11	L	167	CLA	CAD-C3D	-4.47	1.42	1.50
11	J	178	CLA	CAD-C3D	-4.47	1.42	1.50
11	D	170	CLA	CAD-C3D	-4.47	1.42	1.50
11	M	163	CLA	CAD-C3D	-4.47	1.42	1.50
11	L	168	CLA	CAD-C3D	-4.47	1.42	1.50
11	G	313	CLA	CAD-C3D	-4.46	1.42	1.50
11	B	178	CLA	CAD-C3D	-4.46	1.42	1.50
11	M	170	CLA	CAD-C3D	-4.46	1.42	1.50
11	C	157	CLA	CAD-C3D	-4.46	1.42	1.50
11	C	165	CLA	CAD-C3D	-4.46	1.42	1.50
11	M	162	CLA	CAD-C3D	-4.46	1.42	1.50
11	D	159	CLA	CAD-C3D	-4.46	1.42	1.50
11	M	165	CLA	CAD-C3D	-4.46	1.42	1.50
11	D	167	CLA	CAD-C3D	-4.45	1.42	1.50
11	M	159	CLA	CAD-C3D	-4.45	1.42	1.50
11	P	313	CLA	CAD-C3D	-4.45	1.42	1.50
11	A	178	CLA	CAD-C3D	-4.45	1.42	1.50
11	D	165	CLA	CAD-C3D	-4.45	1.42	1.50
11	L	166	CLA	CAD-C3D	-4.45	1.42	1.50
11	M	167	CLA	CAD-C3D	-4.45	1.42	1.50
11	D	163	CLA	CAD-C3D	-4.45	1.42	1.50
11	L	160	CLA	CAD-C3D	-4.45	1.42	1.50
11	J	175	CLA	CAD-C3D	-4.45	1.42	1.50
11	M	166	CLA	CAD-C3D	-4.45	1.42	1.50
11	L	165	CLA	CAD-C3D	-4.44	1.42	1.50
11	D	168	CLA	CAD-C3D	-4.44	1.42	1.50
11	C	158	CLA	CAD-C3D	-4.44	1.42	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	158	CLA	CAD-C3D	-4.44	1.42	1.50
11	D	166	CLA	CAD-C3D	-4.44	1.42	1.50
11	D	158	CLA	CAD-C3D	-4.44	1.42	1.50
11	K	178	CLA	CAD-C3D	-4.44	1.42	1.50
11	J	176	CLA	CAD-C3D	-4.44	1.42	1.50
11	M	156	CLA	CAD-C3D	-4.44	1.42	1.50
11	D	156	CLA	CAD-C3D	-4.43	1.42	1.50
11	M	168	CLA	CAD-C3D	-4.43	1.42	1.50
11	A	175	CLA	CAD-C3D	-4.43	1.42	1.50
11	C	164	CLA	CAD-C3D	-4.43	1.42	1.50
11	C	160	CLA	CAD-C3D	-4.43	1.42	1.50
11	L	158	CLA	CAD-C3D	-4.42	1.42	1.50
11	C	161	CLA	CAD-C3D	-4.42	1.42	1.50
11	L	159	CLA	CAD-C3D	-4.42	1.42	1.50
11	D	161	CLA	CAD-C3D	-4.42	1.42	1.50
11	D	162	CLA	CAD-C3D	-4.42	1.42	1.50
11	D	160	CLA	CAD-C3D	-4.42	1.42	1.50
11	D	169	CLA	CAD-C3D	-4.42	1.42	1.50
11	M	161	CLA	CAD-C3D	-4.41	1.42	1.50
11	C	166	CLA	CAD-C3D	-4.41	1.42	1.50
11	M	160	CLA	CAD-C3D	-4.41	1.42	1.50
11	A	176	CLA	CAD-C3D	-4.41	1.42	1.50
11	C	159	CLA	CAD-C3D	-4.41	1.42	1.50
11	L	164	CLA	CAD-C3D	-4.40	1.42	1.50
11	C	162	CLA	CAD-C3D	-4.40	1.42	1.50
11	L	161	CLA	CAD-C3D	-4.40	1.42	1.50
11	B	176	CLA	CAD-C3D	-4.40	1.42	1.50
11	C	163	CLA	CAD-C3D	-4.40	1.42	1.50
11	M	169	CLA	CAD-C3D	-4.38	1.42	1.50
11	D	164	CLA	CAD-C3D	-4.38	1.42	1.50
11	L	162	CLA	CAD-C3D	-4.38	1.42	1.50
11	L	163	CLA	CAD-C3D	-4.38	1.42	1.50
11	M	164	CLA	CAD-C3D	-4.38	1.42	1.50
11	K	176	CLA	CAD-C3D	-4.37	1.42	1.50
11	M	157	CLA	CAD-C3D	-4.35	1.42	1.50
11	D	157	CLA	CAD-C3D	-4.35	1.42	1.50
14	B	179	PL9	C6-C5	4.31	1.46	1.32
14	K	179	PL9	C6-C5	4.30	1.46	1.32
11	L	167	CLA	C3B-C4B	3.94	1.48	1.40
11	M	163	CLA	C3B-C4B	3.93	1.48	1.40
11	M	160	CLA	C3B-C4B	3.93	1.48	1.40
11	D	160	CLA	C3B-C4B	3.93	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	165	CLA	C3B-C4B	3.93	1.48	1.40
11	M	165	CLA	C3B-C4B	3.92	1.48	1.40
11	A	175	CLA	C3B-C4B	3.92	1.48	1.40
11	D	170	CLA	C3B-C4B	3.92	1.48	1.40
11	C	167	CLA	C3B-C4B	3.91	1.48	1.40
11	D	163	CLA	C3B-C4B	3.91	1.48	1.40
11	L	159	CLA	C3B-C4B	3.91	1.48	1.40
11	M	156	CLA	C3B-C4B	3.91	1.48	1.40
11	J	175	CLA	C3B-C4B	3.91	1.48	1.40
11	C	159	CLA	C3B-C4B	3.90	1.48	1.40
11	D	164	CLA	C3B-C4B	3.90	1.48	1.40
11	C	166	CLA	C3B-C4B	3.90	1.48	1.40
11	M	170	CLA	C3B-C4B	3.90	1.48	1.40
11	L	166	CLA	C3B-C4B	3.90	1.48	1.40
11	M	164	CLA	C3B-C4B	3.90	1.48	1.40
11	K	178	CLA	C3B-C4B	3.89	1.48	1.40
11	L	157	CLA	C3B-C4B	3.89	1.48	1.40
11	A	179	CLA	C3B-C4B	3.89	1.48	1.40
11	B	178	CLA	C3B-C4B	3.89	1.48	1.40
11	L	162	CLA	C3B-C4B	3.89	1.48	1.40
11	M	166	CLA	C3B-C4B	3.89	1.48	1.40
11	M	169	CLA	C3B-C4B	3.89	1.48	1.40
11	M	159	CLA	C3B-C4B	3.89	1.48	1.40
11	C	157	CLA	C3B-C4B	3.88	1.48	1.40
11	D	161	CLA	C3B-C4B	3.88	1.48	1.40
11	D	158	CLA	C3B-C4B	3.88	1.48	1.40
11	J	179	CLA	C3B-C4B	3.88	1.48	1.40
11	M	161	CLA	C3B-C4B	3.88	1.48	1.40
11	M	162	CLA	C3B-C4B	3.88	1.48	1.40
11	A	174	CLA	C3B-C4B	3.88	1.48	1.40
11	D	162	CLA	C3B-C4B	3.88	1.48	1.40
11	D	166	CLA	C3B-C4B	3.88	1.48	1.40
11	D	167	CLA	C3B-C4B	3.88	1.48	1.40
11	D	156	CLA	C3B-C4B	3.87	1.48	1.40
11	C	158	CLA	C3B-C4B	3.87	1.48	1.40
11	C	163	CLA	C3B-C4B	3.87	1.48	1.40
11	L	168	CLA	C3B-C4B	3.87	1.48	1.40
11	C	161	CLA	C3B-C4B	3.87	1.48	1.40
11	L	164	CLA	C3B-C4B	3.87	1.48	1.40
11	C	162	CLA	C3B-C4B	3.87	1.48	1.40
11	J	176	CLA	C3B-C4B	3.87	1.48	1.40
11	L	161	CLA	C3B-C4B	3.87	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	157	CLA	C3B-C4B	3.87	1.48	1.40
11	C	168	CLA	C3B-C4B	3.87	1.48	1.40
11	P	313	CLA	C3B-C4B	3.87	1.48	1.40
11	C	165	CLA	C3B-C4B	3.86	1.48	1.40
11	M	167	CLA	C3B-C4B	3.86	1.48	1.40
11	A	176	CLA	C3B-C4B	3.86	1.48	1.40
11	G	313	CLA	C3B-C4B	3.86	1.48	1.40
11	D	169	CLA	C3B-C4B	3.86	1.48	1.40
11	M	158	CLA	C3B-C4B	3.86	1.48	1.40
11	D	157	CLA	C3B-C4B	3.86	1.48	1.40
11	D	159	CLA	C3B-C4B	3.86	1.48	1.40
11	J	174	CLA	C3B-C4B	3.86	1.48	1.40
11	L	163	CLA	C3B-C4B	3.86	1.48	1.40
11	C	164	CLA	C3B-C4B	3.85	1.48	1.40
11	L	158	CLA	C3B-C4B	3.85	1.48	1.40
11	J	178	CLA	C3B-C4B	3.85	1.48	1.40
11	A	178	CLA	C3B-C4B	3.84	1.48	1.40
11	M	168	CLA	C3B-C4B	3.84	1.48	1.40
11	L	165	CLA	C3B-C4B	3.84	1.48	1.40
11	D	168	CLA	C3B-C4B	3.83	1.48	1.40
11	B	176	CLA	C3B-C4B	3.83	1.48	1.40
11	C	160	CLA	C3B-C4B	3.81	1.48	1.40
11	L	160	CLA	C3B-C4B	3.80	1.48	1.40
11	K	176	CLA	C3B-C4B	3.78	1.48	1.40
15	F	50	HEM	FE-NC	3.75	2.07	1.95
15	I	88	HEM	FE-NC	3.74	2.07	1.95
15	O	90	HEM	FE-NC	3.74	2.07	1.95
15	R	91	HEM	FE-NC	3.73	2.07	1.95
15	O	90	HEM	C3C-C4C	3.66	1.53	1.44
15	F	50	HEM	C3C-C4C	3.64	1.53	1.44
15	I	88	HEM	C3C-C4C	3.62	1.53	1.44
15	R	91	HEM	C3C-C4C	3.62	1.53	1.44
14	B	179	PL9	C3-C2	3.46	1.43	1.32
14	K	179	PL9	C3-C2	3.46	1.43	1.32
15	R	91	HEM	C2C-C1C	3.32	1.52	1.44
15	I	88	HEM	C2C-C1C	3.31	1.52	1.44
15	O	90	HEM	C2C-C1C	3.31	1.52	1.44
15	F	50	HEM	C2C-C1C	3.30	1.52	1.44
15	R	91	HEM	FE-NA	3.29	2.06	1.95
15	I	88	HEM	FE-NA	3.28	2.06	1.95
15	O	90	HEM	FE-NA	3.28	2.06	1.95
15	F	50	HEM	FE-NA	3.27	2.06	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	169	CLA	C4D-C3D	-3.25	1.39	1.46
11	D	169	CLA	C4D-C3D	-3.24	1.39	1.46
11	L	162	CLA	C4D-C3D	-3.24	1.39	1.46
11	M	157	CLA	C4D-C3D	-3.24	1.39	1.46
11	D	157	CLA	C4D-C3D	-3.23	1.39	1.46
11	K	176	CLA	C4D-C3D	-3.22	1.39	1.46
11	D	164	CLA	C4D-C3D	-3.22	1.39	1.46
11	D	162	CLA	C4D-C3D	-3.21	1.39	1.46
11	J	174	CLA	C4D-C3D	-3.21	1.39	1.46
11	D	166	CLA	C4D-C3D	-3.21	1.39	1.46
11	A	175	CLA	C4D-C3D	-3.21	1.39	1.46
11	J	175	CLA	C4D-C3D	-3.20	1.39	1.46
11	M	166	CLA	C4D-C3D	-3.20	1.39	1.46
11	M	164	CLA	C4D-C3D	-3.20	1.39	1.46
11	D	158	CLA	C4D-C3D	-3.20	1.39	1.46
11	L	164	CLA	C4D-C3D	-3.20	1.39	1.46
11	A	174	CLA	C4D-C3D	-3.20	1.39	1.46
11	M	161	CLA	C4D-C3D	-3.20	1.39	1.46
11	B	176	CLA	C4D-C3D	-3.20	1.39	1.46
11	M	158	CLA	C4D-C3D	-3.20	1.39	1.46
11	D	161	CLA	C4D-C3D	-3.19	1.39	1.46
11	M	160	CLA	C4D-C3D	-3.19	1.39	1.46
11	M	167	CLA	C4D-C3D	-3.19	1.39	1.46
11	D	160	CLA	C4D-C3D	-3.19	1.39	1.46
11	C	162	CLA	C4D-C3D	-3.19	1.39	1.46
11	C	160	CLA	C4D-C3D	-3.19	1.39	1.46
11	D	167	CLA	C4D-C3D	-3.19	1.39	1.46
11	A	178	CLA	C4D-C3D	-3.19	1.39	1.46
11	J	176	CLA	C4D-C3D	-3.19	1.39	1.46
11	C	164	CLA	C4D-C3D	-3.19	1.39	1.46
11	C	159	CLA	C4D-C3D	-3.19	1.39	1.46
11	M	156	CLA	C4D-C3D	-3.19	1.39	1.46
11	A	176	CLA	C4D-C3D	-3.18	1.39	1.46
11	L	168	CLA	C4D-C3D	-3.18	1.39	1.46
11	L	158	CLA	C4D-C3D	-3.18	1.39	1.46
11	M	162	CLA	C4D-C3D	-3.18	1.39	1.46
11	M	168	CLA	C4D-C3D	-3.18	1.39	1.46
11	K	178	CLA	C4D-C3D	-3.18	1.39	1.46
11	A	179	CLA	C4D-C3D	-3.18	1.39	1.46
11	C	157	CLA	C4D-C3D	-3.17	1.39	1.46
11	L	160	CLA	C4D-C3D	-3.17	1.39	1.46
11	C	158	CLA	C4D-C3D	-3.17	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	179	CLA	C4D-C3D	-3.17	1.39	1.46
11	D	159	CLA	C4D-C3D	-3.17	1.39	1.46
11	M	159	CLA	C4D-C3D	-3.17	1.39	1.46
11	M	170	CLA	C4D-C3D	-3.17	1.39	1.46
11	L	166	CLA	C4D-C3D	-3.17	1.39	1.46
11	C	168	CLA	C4D-C3D	-3.17	1.39	1.46
11	D	156	CLA	C4D-C3D	-3.17	1.39	1.46
11	C	161	CLA	C4D-C3D	-3.17	1.39	1.46
11	B	178	CLA	C4D-C3D	-3.16	1.39	1.46
11	L	157	CLA	C4D-C3D	-3.16	1.39	1.46
11	J	178	CLA	C4D-C3D	-3.16	1.39	1.46
11	L	159	CLA	C4D-C3D	-3.16	1.39	1.46
11	D	168	CLA	C4D-C3D	-3.16	1.39	1.46
11	C	165	CLA	C4D-C3D	-3.16	1.39	1.46
11	L	167	CLA	C4D-C3D	-3.16	1.39	1.46
11	G	313	CLA	C4D-C3D	-3.15	1.39	1.46
11	C	166	CLA	C4D-C3D	-3.15	1.39	1.46
11	C	167	CLA	C4D-C3D	-3.15	1.39	1.46
11	D	165	CLA	C4D-C3D	-3.15	1.40	1.46
11	D	170	CLA	C4D-C3D	-3.15	1.40	1.46
11	P	313	CLA	C4D-C3D	-3.15	1.40	1.46
12	K	177	PHO	C2D-C1D	3.14	1.42	1.39
11	L	165	CLA	C4D-C3D	-3.14	1.40	1.46
11	M	165	CLA	C4D-C3D	-3.14	1.40	1.46
11	C	163	CLA	C4D-C3D	-3.14	1.40	1.46
11	D	163	CLA	C4D-C3D	-3.13	1.40	1.46
11	L	161	CLA	C4D-C3D	-3.13	1.40	1.46
12	B	177	PHO	C2D-C1D	3.12	1.42	1.39
11	M	163	CLA	C4D-C3D	-3.12	1.40	1.46
11	L	163	CLA	C4D-C3D	-3.11	1.40	1.46
12	J	177	PHO	C2D-C1D	3.05	1.42	1.39
15	F	50	HEM	C3B-C2B	3.00	1.42	1.35
12	A	177	PHO	C2D-C1D	2.99	1.42	1.39
15	O	90	HEM	C3B-C2B	2.98	1.42	1.35
15	I	88	HEM	C3B-C2B	2.97	1.42	1.35
15	R	91	HEM	C3B-C2B	2.96	1.42	1.35
11	M	160	CLA	C2B-C1B	2.86	1.46	1.40
11	J	178	CLA	C2B-C1B	2.86	1.46	1.40
11	L	164	CLA	C2B-C1B	2.85	1.46	1.40
11	L	167	CLA	C2B-C1B	2.85	1.46	1.40
11	M	166	CLA	C2B-C1B	2.85	1.46	1.40
11	C	164	CLA	C2B-C1B	2.84	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	156	CLA	C2B-C1B	2.84	1.46	1.40
11	M	164	CLA	C2B-C1B	2.84	1.46	1.40
11	B	176	CLA	C2B-C1B	2.84	1.46	1.40
11	D	160	CLA	C2B-C1B	2.84	1.46	1.40
11	L	165	CLA	C2B-C1B	2.84	1.46	1.40
11	K	176	CLA	C2B-C1B	2.84	1.46	1.40
11	D	158	CLA	C2B-C1B	2.83	1.46	1.40
11	K	178	CLA	C2B-C1B	2.83	1.46	1.40
11	L	166	CLA	C2B-C1B	2.83	1.46	1.40
11	C	165	CLA	C2B-C1B	2.83	1.46	1.40
11	M	161	CLA	C2B-C1B	2.83	1.46	1.40
11	C	167	CLA	C2B-C1B	2.83	1.46	1.40
11	L	161	CLA	C2B-C1B	2.83	1.46	1.40
11	C	161	CLA	C2B-C1B	2.83	1.46	1.40
15	O	90	HEM	FE-ND	2.83	2.03	1.94
11	M	162	CLA	C2B-C1B	2.83	1.46	1.40
11	D	156	CLA	C2B-C1B	2.83	1.46	1.40
11	A	178	CLA	C2B-C1B	2.82	1.46	1.40
11	D	159	CLA	C2B-C1B	2.82	1.46	1.40
11	G	313	CLA	C2B-C1B	2.82	1.46	1.40
11	B	178	CLA	C2B-C1B	2.82	1.46	1.40
11	M	158	CLA	C2B-C1B	2.82	1.46	1.40
11	L	168	CLA	C2B-C1B	2.82	1.46	1.40
11	L	162	CLA	C2B-C1B	2.82	1.46	1.40
15	F	50	HEM	FE-ND	2.82	2.03	1.94
11	D	161	CLA	C2B-C1B	2.82	1.46	1.40
11	D	164	CLA	C2B-C1B	2.82	1.46	1.40
11	P	313	CLA	C2B-C1B	2.82	1.46	1.40
11	C	163	CLA	C2B-C1B	2.82	1.46	1.40
11	M	170	CLA	C2B-C1B	2.82	1.46	1.40
11	M	157	CLA	C2B-C1B	2.82	1.46	1.40
11	C	166	CLA	C2B-C1B	2.82	1.46	1.40
11	D	169	CLA	C2B-C1B	2.82	1.46	1.40
11	D	165	CLA	C2B-C1B	2.81	1.46	1.40
11	D	166	CLA	C2B-C1B	2.81	1.46	1.40
11	M	169	CLA	C2B-C1B	2.81	1.46	1.40
11	C	162	CLA	C2B-C1B	2.81	1.46	1.40
11	D	163	CLA	C2B-C1B	2.81	1.46	1.40
11	D	162	CLA	C2B-C1B	2.81	1.46	1.40
11	L	159	CLA	C2B-C1B	2.81	1.46	1.40
11	M	159	CLA	C2B-C1B	2.81	1.46	1.40
11	M	167	CLA	C2B-C1B	2.81	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	158	CLA	C2B-C1B	2.80	1.46	1.40
11	D	157	CLA	C2B-C1B	2.80	1.46	1.40
11	C	160	CLA	C2B-C1B	2.80	1.46	1.40
11	J	175	CLA	C2B-C1B	2.80	1.46	1.40
15	R	91	HEM	FE-ND	2.80	2.03	1.94
11	M	165	CLA	C2B-C1B	2.80	1.46	1.40
15	I	88	HEM	C3D-C2D	2.80	1.41	1.35
11	D	167	CLA	C2B-C1B	2.80	1.46	1.40
11	C	168	CLA	C2B-C1B	2.80	1.46	1.40
11	L	160	CLA	C2B-C1B	2.80	1.46	1.40
15	I	88	HEM	FE-ND	2.79	2.03	1.94
11	L	163	CLA	C2B-C1B	2.79	1.46	1.40
11	C	159	CLA	C2B-C1B	2.79	1.46	1.40
11	L	158	CLA	C2B-C1B	2.79	1.46	1.40
11	J	179	CLA	C2B-C1B	2.79	1.46	1.40
11	A	175	CLA	C2B-C1B	2.79	1.46	1.40
11	M	163	CLA	C2B-C1B	2.79	1.46	1.40
11	J	176	CLA	C2B-C1B	2.79	1.46	1.40
11	A	174	CLA	C2B-C1B	2.79	1.46	1.40
11	D	170	CLA	C2B-C1B	2.79	1.46	1.40
15	F	50	HEM	C3D-C2D	2.78	1.41	1.35
15	O	90	HEM	C3D-C2D	2.78	1.41	1.35
11	D	168	CLA	C2B-C1B	2.78	1.46	1.40
15	R	91	HEM	C3D-C2D	2.78	1.41	1.35
11	A	179	CLA	C2B-C1B	2.78	1.46	1.40
11	A	176	CLA	C2B-C1B	2.77	1.46	1.40
12	J	177	PHO	C2A-C1A	2.76	1.52	1.50
11	M	168	CLA	C2B-C1B	2.76	1.46	1.40
11	J	174	CLA	C2B-C1B	2.76	1.46	1.40
11	C	157	CLA	C2B-C1B	2.76	1.46	1.40
11	L	157	CLA	C2B-C1B	2.75	1.46	1.40
12	A	177	PHO	C2A-C1A	2.69	1.52	1.50
12	K	177	PHO	C2A-C1A	2.69	1.52	1.50
15	I	88	HEM	C3A-C2A	2.65	1.48	1.39
12	B	177	PHO	C2A-C1A	2.65	1.52	1.50
15	F	50	HEM	C3A-C2A	2.64	1.48	1.39
15	O	90	HEM	C3A-C2A	2.63	1.48	1.39
15	R	91	HEM	C3A-C2A	2.63	1.48	1.39
15	F	50	HEM	C4D-ND	-2.62	1.34	1.40
15	I	88	HEM	C4D-ND	-2.61	1.34	1.40
15	R	91	HEM	C4D-ND	-2.61	1.34	1.40
15	O	90	HEM	C4D-ND	-2.60	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	170	CLA	CHC-C1C	2.58	1.43	1.38
11	K	178	CLA	CHC-C1C	2.55	1.43	1.38
11	J	174	CLA	CHC-C1C	2.55	1.43	1.38
11	D	170	CLA	CHC-C1C	2.55	1.43	1.38
11	L	167	CLA	CHC-C1C	2.53	1.43	1.38
11	C	166	CLA	CHC-C1C	2.53	1.43	1.38
11	A	174	CLA	CHC-C1C	2.53	1.43	1.38
11	L	163	CLA	CHC-C1C	2.53	1.43	1.38
11	B	178	CLA	CHC-C1C	2.53	1.43	1.38
11	J	179	CLA	CHC-C1C	2.52	1.43	1.38
11	M	156	CLA	CHC-C1C	2.52	1.43	1.38
11	C	163	CLA	CHC-C1C	2.52	1.43	1.38
11	D	156	CLA	CHC-C1C	2.52	1.43	1.38
11	C	167	CLA	CHC-C1C	2.52	1.43	1.38
11	L	166	CLA	CHC-C1C	2.52	1.43	1.38
11	L	162	CLA	CHC-C1C	2.51	1.43	1.38
11	A	179	CLA	CHC-C1C	2.51	1.43	1.38
11	M	157	CLA	CHC-C1C	2.51	1.43	1.38
11	D	157	CLA	CHC-C1C	2.51	1.43	1.38
11	D	165	CLA	CHC-C1C	2.51	1.43	1.38
11	D	159	CLA	CHC-C1C	2.51	1.43	1.38
11	L	161	CLA	CHC-C1C	2.51	1.43	1.38
11	C	161	CLA	CHC-C1C	2.50	1.43	1.38
11	A	176	CLA	CHC-C1C	2.50	1.43	1.38
11	D	158	CLA	CHC-C1C	2.50	1.43	1.38
11	G	313	CLA	CHC-C1C	2.50	1.43	1.38
11	C	162	CLA	CHC-C1C	2.50	1.43	1.38
11	M	168	CLA	CHC-C1C	2.50	1.43	1.38
11	A	175	CLA	CHC-C1C	2.50	1.43	1.38
11	M	160	CLA	CHC-C1C	2.50	1.43	1.38
11	M	158	CLA	CHC-C1C	2.49	1.43	1.38
11	D	167	CLA	CHC-C1C	2.49	1.43	1.38
11	D	160	CLA	CHC-C1C	2.49	1.43	1.38
11	A	178	CLA	CHC-C1C	2.49	1.43	1.38
11	M	165	CLA	CHC-C1C	2.49	1.43	1.38
11	M	161	CLA	CHC-C1C	2.49	1.43	1.38
11	C	158	CLA	CHC-C1C	2.49	1.43	1.38
11	M	159	CLA	CHC-C1C	2.49	1.43	1.38
11	L	165	CLA	CHC-C1C	2.49	1.43	1.38
11	D	168	CLA	CHC-C1C	2.49	1.43	1.38
11	M	164	CLA	CHC-C1C	2.49	1.43	1.38
11	D	164	CLA	CHC-C1C	2.48	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	166	CLA	CHC-C1C	2.48	1.43	1.38
11	D	163	CLA	CHC-C1C	2.48	1.43	1.38
11	J	176	CLA	CHC-C1C	2.48	1.43	1.38
11	D	162	CLA	CHC-C1C	2.47	1.43	1.38
11	P	313	CLA	CHC-C1C	2.47	1.43	1.38
11	C	165	CLA	CHC-C1C	2.47	1.43	1.38
11	L	158	CLA	CHC-C1C	2.47	1.43	1.38
11	J	178	CLA	CHC-C1C	2.47	1.43	1.38
11	J	175	CLA	CHC-C1C	2.47	1.43	1.38
11	C	160	CLA	CHC-C1C	2.47	1.43	1.38
11	D	161	CLA	CHC-C1C	2.47	1.43	1.38
11	L	164	CLA	CHC-C1C	2.47	1.43	1.38
11	M	167	CLA	CHC-C1C	2.46	1.43	1.38
11	L	159	CLA	CHC-C1C	2.46	1.43	1.38
11	C	157	CLA	CHC-C1C	2.46	1.43	1.38
11	C	168	CLA	CHC-C1C	2.46	1.43	1.38
11	B	176	CLA	CHC-C1C	2.46	1.43	1.38
11	K	176	CLA	CHC-C1C	2.46	1.43	1.38
11	M	163	CLA	CHC-C1C	2.46	1.43	1.38
11	D	166	CLA	CHC-C1C	2.46	1.43	1.38
11	L	160	CLA	CHC-C1C	2.46	1.43	1.38
11	M	169	CLA	CHC-C1C	2.46	1.43	1.38
11	C	164	CLA	CHC-C1C	2.45	1.43	1.38
11	L	168	CLA	CHC-C1C	2.45	1.43	1.38
11	M	162	CLA	CHC-C1C	2.45	1.43	1.38
11	L	157	CLA	CHC-C1C	2.45	1.43	1.38
11	C	159	CLA	CHC-C1C	2.44	1.43	1.38
11	D	169	CLA	CHC-C1C	2.44	1.43	1.38
11	J	175	CLA	MG-NB	2.35	2.10	2.05
11	K	178	CLA	MG-NB	2.35	2.10	2.05
11	M	162	CLA	MG-NB	2.34	2.10	2.05
11	D	162	CLA	MG-NB	2.34	2.10	2.05
11	B	178	CLA	MG-NB	2.34	2.10	2.05
11	A	175	CLA	MG-NB	2.33	2.10	2.05
11	D	161	CLA	MG-NB	2.33	2.10	2.05
11	D	160	CLA	MG-NB	2.33	2.10	2.05
11	D	168	CLA	MG-NB	2.33	2.10	2.05
11	M	160	CLA	MG-NB	2.32	2.10	2.05
11	M	164	CLA	MG-NB	2.32	2.10	2.05
11	M	161	CLA	MG-NB	2.32	2.10	2.05
11	M	168	CLA	MG-NB	2.32	2.10	2.05
11	J	176	CLA	MG-NB	2.32	2.10	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	176	CLA	MG-NB	2.32	2.10	2.05
11	L	157	CLA	MG-NB	2.32	2.10	2.05
11	M	170	CLA	MG-NB	2.31	2.10	2.05
11	P	313	CLA	MG-NB	2.31	2.10	2.05
11	C	166	CLA	MG-NB	2.31	2.10	2.05
11	A	174	CLA	MG-NB	2.31	2.10	2.05
11	D	164	CLA	MG-NB	2.31	2.10	2.05
11	M	166	CLA	MG-NB	2.31	2.10	2.05
11	D	158	CLA	MG-NB	2.31	2.10	2.05
11	C	161	CLA	MG-NB	2.31	2.10	2.05
11	C	167	CLA	MG-NB	2.31	2.10	2.05
11	D	166	CLA	MG-NB	2.31	2.10	2.05
11	C	164	CLA	MG-NB	2.30	2.10	2.05
11	D	170	CLA	MG-NB	2.30	2.10	2.05
11	G	313	CLA	MG-NB	2.30	2.10	2.05
11	L	158	CLA	MG-NB	2.30	2.10	2.05
11	M	158	CLA	MG-NB	2.30	2.10	2.05
11	B	176	CLA	MG-NB	2.30	2.10	2.05
11	M	167	CLA	MG-NB	2.30	2.10	2.05
11	D	165	CLA	MG-NB	2.30	2.10	2.05
11	D	159	CLA	MG-NB	2.30	2.10	2.05
11	J	174	CLA	MG-NB	2.30	2.10	2.05
11	M	159	CLA	MG-NB	2.30	2.10	2.05
11	L	161	CLA	MG-NB	2.29	2.10	2.05
11	D	157	CLA	MG-NB	2.29	2.10	2.05
11	L	163	CLA	MG-NB	2.29	2.10	2.05
11	C	162	CLA	MG-NB	2.29	2.10	2.05
11	C	168	CLA	MG-NB	2.29	2.10	2.05
11	J	178	CLA	MG-NB	2.29	2.10	2.05
11	A	179	CLA	MG-NB	2.29	2.10	2.05
11	D	156	CLA	MG-NB	2.29	2.10	2.05
11	C	160	CLA	MG-NB	2.29	2.10	2.05
11	J	179	CLA	MG-NB	2.29	2.10	2.05
11	L	164	CLA	MG-NB	2.29	2.10	2.05
11	C	157	CLA	MG-NB	2.29	2.10	2.05
11	L	167	CLA	MG-NB	2.28	2.10	2.05
11	C	158	CLA	MG-NB	2.28	2.10	2.05
11	A	178	CLA	MG-NB	2.28	2.10	2.05
11	D	163	CLA	MG-NB	2.28	2.10	2.05
11	C	163	CLA	MG-NB	2.28	2.10	2.05
11	M	157	CLA	MG-NB	2.28	2.10	2.05
11	L	165	CLA	MG-NB	2.28	2.10	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	160	CLA	MG-NB	2.28	2.10	2.05
11	D	169	CLA	MG-NB	2.27	2.10	2.05
11	D	167	CLA	MG-NB	2.27	2.10	2.05
11	L	166	CLA	MG-NB	2.27	2.10	2.05
11	C	165	CLA	MG-NB	2.27	2.10	2.05
11	M	169	CLA	MG-NB	2.27	2.10	2.05
11	L	168	CLA	MG-NB	2.27	2.10	2.05
11	M	156	CLA	MG-NB	2.26	2.10	2.05
11	M	165	CLA	MG-NB	2.26	2.10	2.05
11	L	159	CLA	MG-NB	2.26	2.10	2.05
11	C	159	CLA	MG-NB	2.26	2.10	2.05
11	L	162	CLA	MG-NB	2.26	2.10	2.05
11	K	176	CLA	MG-NB	2.24	2.10	2.05
11	M	163	CLA	MG-NB	2.23	2.10	2.05
12	J	177	PHO	C1C-C2C	2.22	1.46	1.42
12	A	177	PHO	C1C-C2C	2.21	1.46	1.42
12	K	177	PHO	C1C-C2C	2.15	1.46	1.42
12	B	177	PHO	C1C-C2C	2.13	1.46	1.42
12	J	177	PHO	C4C-C3C	2.11	1.46	1.42
12	B	177	PHO	C4C-C3C	2.08	1.46	1.42
12	A	177	PHO	C4C-C3C	2.07	1.46	1.42
15	I	88	HEM	C2D-C1D	-2.07	1.38	1.43
15	R	91	HEM	C2D-C1D	-2.06	1.38	1.43
12	K	177	PHO	C4C-C3C	2.05	1.46	1.42
15	F	50	HEM	C2D-C1D	-2.02	1.38	1.43

All (352) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	168	CLA	C4A-NA-C1A	10.40	111.42	106.68
11	M	164	CLA	C4A-NA-C1A	10.39	111.42	106.68
11	M	168	CLA	C4A-NA-C1A	10.38	111.42	106.68
11	M	169	CLA	C4A-NA-C1A	10.36	111.40	106.68
11	D	163	CLA	C4A-NA-C1A	10.35	111.40	106.68
11	C	168	CLA	C4A-NA-C1A	10.34	111.40	106.68
11	M	156	CLA	C4A-NA-C1A	10.34	111.40	106.68
11	M	159	CLA	C4A-NA-C1A	10.34	111.40	106.68
11	D	168	CLA	C4A-NA-C1A	10.33	111.39	106.68
11	D	169	CLA	C4A-NA-C1A	10.33	111.39	106.68
11	M	166	CLA	C4A-NA-C1A	10.33	111.39	106.68
11	D	158	CLA	C4A-NA-C1A	10.32	111.39	106.68
11	D	166	CLA	C4A-NA-C1A	10.32	111.39	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	163	CLA	C4A-NA-C1A	10.31	111.38	106.68
11	L	165	CLA	C4A-NA-C1A	10.31	111.38	106.68
11	J	178	CLA	C4A-NA-C1A	10.30	111.38	106.68
11	M	163	CLA	C4A-NA-C1A	10.30	111.38	106.68
11	D	164	CLA	C4A-NA-C1A	10.30	111.38	106.68
11	D	160	CLA	C4A-NA-C1A	10.28	111.37	106.68
11	D	156	CLA	C4A-NA-C1A	10.28	111.37	106.68
11	A	175	CLA	C4A-NA-C1A	10.28	111.37	106.68
11	J	175	CLA	C4A-NA-C1A	10.28	111.37	106.68
11	D	161	CLA	C4A-NA-C1A	10.27	111.37	106.68
11	L	163	CLA	C4A-NA-C1A	10.26	111.36	106.68
11	M	160	CLA	C4A-NA-C1A	10.26	111.36	106.68
11	A	174	CLA	C4A-NA-C1A	10.26	111.36	106.68
11	L	161	CLA	C4A-NA-C1A	10.26	111.36	106.68
11	M	157	CLA	C4A-NA-C1A	10.26	111.36	106.68
11	J	174	CLA	C4A-NA-C1A	10.26	111.36	106.68
11	L	162	CLA	C4A-NA-C1A	10.26	111.36	106.68
11	M	170	CLA	C4A-NA-C1A	10.25	111.36	106.68
11	C	165	CLA	C4A-NA-C1A	10.24	111.35	106.68
11	C	161	CLA	C4A-NA-C1A	10.24	111.35	106.68
11	L	157	CLA	C4A-NA-C1A	10.24	111.35	106.68
11	A	178	CLA	C4A-NA-C1A	10.24	111.35	106.68
11	D	170	CLA	C4A-NA-C1A	10.23	111.35	106.68
11	L	159	CLA	C4A-NA-C1A	10.23	111.35	106.68
11	D	157	CLA	C4A-NA-C1A	10.23	111.34	106.68
11	C	157	CLA	C4A-NA-C1A	10.22	111.34	106.68
11	D	159	CLA	C4A-NA-C1A	10.22	111.34	106.68
11	P	313	CLA	C4A-NA-C1A	10.21	111.34	106.68
11	L	158	CLA	C4A-NA-C1A	10.21	111.34	106.68
11	C	158	CLA	C4A-NA-C1A	10.21	111.34	106.68
11	C	167	CLA	C4A-NA-C1A	10.21	111.34	106.68
11	M	161	CLA	C4A-NA-C1A	10.21	111.34	106.68
11	C	159	CLA	C4A-NA-C1A	10.20	111.33	106.68
11	M	165	CLA	C4A-NA-C1A	10.20	111.33	106.68
11	G	313	CLA	C4A-NA-C1A	10.19	111.33	106.68
11	D	165	CLA	C4A-NA-C1A	10.19	111.33	106.68
11	C	166	CLA	C4A-NA-C1A	10.18	111.33	106.68
11	C	162	CLA	C4A-NA-C1A	10.17	111.32	106.68
11	M	167	CLA	C4A-NA-C1A	10.17	111.32	106.68
11	D	167	CLA	C4A-NA-C1A	10.16	111.31	106.68
11	M	158	CLA	C4A-NA-C1A	10.16	111.31	106.68
11	D	162	CLA	C4A-NA-C1A	10.16	111.31	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	160	CLA	C4A-NA-C1A	10.15	111.31	106.68
11	L	164	CLA	C4A-NA-C1A	10.15	111.31	106.68
11	C	160	CLA	C4A-NA-C1A	10.15	111.31	106.68
11	L	167	CLA	C4A-NA-C1A	10.14	111.30	106.68
11	A	176	CLA	C4A-NA-C1A	10.13	111.30	106.68
11	C	164	CLA	C4A-NA-C1A	10.13	111.30	106.68
11	K	176	CLA	C4A-NA-C1A	10.12	111.29	106.68
11	M	162	CLA	C4A-NA-C1A	10.11	111.29	106.68
11	B	176	CLA	C4A-NA-C1A	10.11	111.29	106.68
11	J	176	CLA	C4A-NA-C1A	10.10	111.29	106.68
11	B	178	CLA	C4A-NA-C1A	10.07	111.27	106.68
11	A	179	CLA	C4A-NA-C1A	10.05	111.27	106.68
11	L	166	CLA	C4A-NA-C1A	10.05	111.27	106.68
11	K	178	CLA	C4A-NA-C1A	10.02	111.25	106.68
11	J	179	CLA	C4A-NA-C1A	10.01	111.25	106.68
15	R	91	HEM	C3D-C4D-ND	9.79	116.33	109.42
15	I	88	HEM	C3D-C4D-ND	9.76	116.30	109.42
15	F	50	HEM	C3D-C4D-ND	9.65	116.23	109.42
15	O	90	HEM	C3D-C4D-ND	9.61	116.20	109.42
15	I	88	HEM	C2D-C3D-C4D	-6.69	98.78	107.24
15	R	91	HEM	C2D-C3D-C4D	-6.68	98.79	107.24
12	B	177	PHO	C1D-C2D-C3D	-6.67	104.76	110.99
12	K	177	PHO	C1D-C2D-C3D	-6.66	104.77	110.99
15	F	50	HEM	C2D-C3D-C4D	-6.62	98.87	107.24
12	J	177	PHO	C1D-C2D-C3D	-6.60	104.82	110.99
15	O	90	HEM	C2D-C3D-C4D	-6.59	98.91	107.24
12	A	177	PHO	C1D-C2D-C3D	-6.59	104.83	110.99
12	A	177	PHO	CAD-C3D-C2D	4.94	144.89	132.89
12	J	177	PHO	CAD-C3D-C2D	4.93	144.85	132.89
12	K	177	PHO	CAD-C3D-C2D	4.90	144.79	132.89
12	B	177	PHO	CAD-C3D-C2D	4.90	144.79	132.89
12	J	177	PHO	C4D-ND-C1D	-4.85	105.90	108.99
12	A	177	PHO	C4D-ND-C1D	-4.85	105.90	108.99
12	B	177	PHO	C4D-ND-C1D	-4.80	105.93	108.99
12	K	177	PHO	C4D-ND-C1D	-4.78	105.95	108.99
15	I	88	HEM	CHC-C4B-NB	-3.68	120.36	124.78
15	R	91	HEM	CHC-C4B-NB	-3.67	120.37	124.78
15	O	90	HEM	CHC-C4B-NB	-3.63	120.42	124.78
15	F	50	HEM	CHC-C4B-NB	-3.62	120.43	124.78
11	M	164	CLA	C1B-NB-C4B	3.53	108.79	106.31
11	M	160	CLA	C1B-NB-C4B	3.52	108.78	106.31
11	M	168	CLA	C1B-NB-C4B	3.50	108.77	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	160	CLA	C1B-NB-C4B	3.50	108.77	106.31
11	J	175	CLA	C1B-NB-C4B	3.49	108.76	106.31
11	L	167	CLA	C1B-NB-C4B	3.48	108.76	106.31
11	D	165	CLA	C1B-NB-C4B	3.48	108.75	106.31
11	C	167	CLA	C1B-NB-C4B	3.47	108.75	106.31
11	A	175	CLA	C1B-NB-C4B	3.46	108.74	106.31
11	C	164	CLA	C1B-NB-C4B	3.45	108.73	106.31
11	D	164	CLA	C1B-NB-C4B	3.45	108.73	106.31
11	M	159	CLA	C1B-NB-C4B	3.45	108.73	106.31
11	K	178	CLA	C1B-NB-C4B	3.45	108.73	106.31
11	D	168	CLA	C1B-NB-C4B	3.44	108.73	106.31
11	D	157	CLA	C1B-NB-C4B	3.44	108.72	106.31
15	I	88	HEM	C3D-C4D-CHA	-3.43	116.84	125.84
11	D	158	CLA	C1B-NB-C4B	3.43	108.72	106.31
11	L	164	CLA	C1B-NB-C4B	3.43	108.72	106.31
11	M	166	CLA	C1B-NB-C4B	3.43	108.72	106.31
11	D	159	CLA	C1B-NB-C4B	3.42	108.71	106.31
11	C	163	CLA	C1B-NB-C4B	3.42	108.71	106.31
11	M	156	CLA	C1B-NB-C4B	3.42	108.71	106.31
11	M	162	CLA	C1B-NB-C4B	3.42	108.71	106.31
11	D	161	CLA	C1B-NB-C4B	3.42	108.71	106.31
15	R	91	HEM	C3D-C4D-CHA	-3.42	116.89	125.84
11	C	166	CLA	C1B-NB-C4B	3.41	108.71	106.31
11	L	158	CLA	C1B-NB-C4B	3.41	108.71	106.31
11	L	162	CLA	C1B-NB-C4B	3.41	108.71	106.31
11	B	176	CLA	C1B-NB-C4B	3.41	108.71	106.31
11	J	179	CLA	C1B-NB-C4B	3.41	108.71	106.31
11	L	157	CLA	C1B-NB-C4B	3.41	108.71	106.31
11	A	176	CLA	C1B-NB-C4B	3.41	108.71	106.31
11	M	169	CLA	C1B-NB-C4B	3.41	108.71	106.31
11	B	178	CLA	C1B-NB-C4B	3.41	108.70	106.31
11	D	156	CLA	C1B-NB-C4B	3.41	108.70	106.31
11	C	157	CLA	C1B-NB-C4B	3.40	108.70	106.31
11	D	166	CLA	C1B-NB-C4B	3.40	108.70	106.31
11	C	162	CLA	C1B-NB-C4B	3.40	108.70	106.31
11	J	176	CLA	C1B-NB-C4B	3.40	108.70	106.31
11	L	161	CLA	C1B-NB-C4B	3.40	108.70	106.31
11	C	160	CLA	C1B-NB-C4B	3.40	108.70	106.31
11	M	165	CLA	C1B-NB-C4B	3.40	108.70	106.31
11	C	158	CLA	C1B-NB-C4B	3.40	108.70	106.31
11	M	157	CLA	C1B-NB-C4B	3.40	108.70	106.31
11	M	161	CLA	C1B-NB-C4B	3.40	108.69	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	179	CLA	C1B-NB-C4B	3.39	108.69	106.31
11	D	170	CLA	C1B-NB-C4B	3.39	108.69	106.31
15	F	50	HEM	C3D-C4D-CHA	-3.39	116.95	125.84
11	D	162	CLA	C1B-NB-C4B	3.39	108.69	106.31
11	C	161	CLA	C1B-NB-C4B	3.39	108.69	106.31
11	D	163	CLA	C1B-NB-C4B	3.39	108.69	106.31
11	M	158	CLA	C1B-NB-C4B	3.39	108.69	106.31
11	L	166	CLA	C1B-NB-C4B	3.38	108.69	106.31
11	J	178	CLA	C1B-NB-C4B	3.37	108.68	106.31
11	D	169	CLA	C1B-NB-C4B	3.37	108.68	106.31
15	O	90	HEM	C3D-C4D-CHA	-3.37	117.01	125.84
11	M	170	CLA	C1B-NB-C4B	3.37	108.68	106.31
11	A	174	CLA	C1B-NB-C4B	3.37	108.67	106.31
11	G	313	CLA	C1B-NB-C4B	3.36	108.67	106.31
11	A	178	CLA	C1B-NB-C4B	3.36	108.67	106.31
11	L	163	CLA	C1B-NB-C4B	3.36	108.67	106.31
11	C	165	CLA	C1B-NB-C4B	3.36	108.67	106.31
11	L	160	CLA	C1B-NB-C4B	3.35	108.67	106.31
11	C	168	CLA	C1B-NB-C4B	3.35	108.66	106.31
11	P	313	CLA	C1B-NB-C4B	3.35	108.66	106.31
11	L	159	CLA	C1B-NB-C4B	3.34	108.66	106.31
11	M	163	CLA	C1B-NB-C4B	3.34	108.66	106.31
11	J	174	CLA	C1B-NB-C4B	3.34	108.65	106.31
11	C	159	CLA	C1B-NB-C4B	3.33	108.65	106.31
11	L	165	CLA	C1B-NB-C4B	3.33	108.65	106.31
11	K	176	CLA	C1B-NB-C4B	3.33	108.65	106.31
11	L	168	CLA	C1B-NB-C4B	3.32	108.64	106.31
11	M	167	CLA	C1B-NB-C4B	3.32	108.64	106.31
11	C	159	CLA	C1C-NC-C4C	3.31	108.19	106.68
12	K	177	PHO	CBD-CHA-C4D	-3.31	105.42	110.32
11	D	167	CLA	C1B-NB-C4B	3.31	108.63	106.31
12	B	177	PHO	CBD-CHA-C4D	-3.30	105.43	110.32
15	R	91	HEM	C3D-C2D-C1D	3.30	111.41	107.24
12	A	177	PHO	CBD-CHA-C4D	-3.30	105.44	110.32
15	I	88	HEM	C3D-C2D-C1D	3.29	111.40	107.24
11	A	178	CLA	C1C-NC-C4C	3.29	108.18	106.68
11	B	178	CLA	C1C-NC-C4C	3.29	108.18	106.68
11	A	179	CLA	C1C-NC-C4C	3.28	108.18	106.68
11	J	178	CLA	C1C-NC-C4C	3.28	108.18	106.68
12	J	177	PHO	CBD-CHA-C4D	-3.28	105.47	110.32
11	J	179	CLA	C1C-NC-C4C	3.27	108.17	106.68
11	J	176	CLA	C1C-NC-C4C	3.27	108.17	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	167	CLA	C1C-NC-C4C	3.27	108.17	106.68
11	L	157	CLA	C1C-NC-C4C	3.26	108.17	106.68
11	L	168	CLA	C1C-NC-C4C	3.26	108.17	106.68
11	C	165	CLA	C1C-NC-C4C	3.25	108.16	106.68
11	C	168	CLA	C1C-NC-C4C	3.25	108.16	106.68
11	L	163	CLA	C1C-NC-C4C	3.25	108.16	106.68
11	A	176	CLA	C1C-NC-C4C	3.25	108.16	106.68
11	K	176	CLA	C1C-NC-C4C	3.25	108.16	106.68
11	L	158	CLA	C1C-NC-C4C	3.25	108.16	106.68
11	L	159	CLA	C1C-NC-C4C	3.25	108.16	106.68
11	L	160	CLA	C1C-NC-C4C	3.25	108.16	106.68
11	C	163	CLA	C1C-NC-C4C	3.24	108.16	106.68
11	C	164	CLA	C1C-NC-C4C	3.24	108.16	106.68
11	D	158	CLA	C1C-NC-C4C	3.24	108.16	106.68
12	A	177	PHO	C2D-C1D-ND	3.23	111.86	109.48
11	B	176	CLA	C1C-NC-C4C	3.23	108.15	106.68
11	M	168	CLA	C1C-NC-C4C	3.23	108.15	106.68
11	A	175	CLA	C1C-NC-C4C	3.23	108.15	106.68
12	B	177	PHO	C2D-C1D-ND	3.22	111.85	109.48
11	L	164	CLA	C1C-NC-C4C	3.22	108.15	106.68
11	C	157	CLA	C1C-NC-C4C	3.21	108.14	106.68
11	D	162	CLA	C1C-NC-C4C	3.21	108.14	106.68
11	K	178	CLA	C1C-NC-C4C	3.21	108.14	106.68
11	L	165	CLA	C1C-NC-C4C	3.21	108.14	106.68
11	D	164	CLA	C1C-NC-C4C	3.21	108.14	106.68
11	P	313	CLA	C1C-NC-C4C	3.21	108.14	106.68
12	J	177	PHO	C2D-C1D-ND	3.21	111.84	109.48
11	D	165	CLA	C1C-NC-C4C	3.20	108.14	106.68
12	K	177	PHO	C2D-C1D-ND	3.20	111.83	109.48
11	J	175	CLA	C1C-NC-C4C	3.20	108.14	106.68
11	M	162	CLA	C1C-NC-C4C	3.19	108.14	106.68
15	F	50	HEM	C3D-C2D-C1D	3.19	111.26	107.24
11	D	163	CLA	C1C-NC-C4C	3.18	108.13	106.68
11	D	160	CLA	C1C-NC-C4C	3.17	108.13	106.68
11	C	158	CLA	C1C-NC-C4C	3.17	108.12	106.68
11	L	161	CLA	C1C-NC-C4C	3.17	108.12	106.68
11	M	159	CLA	C1C-NC-C4C	3.17	108.12	106.68
11	M	160	CLA	C1C-NC-C4C	3.17	108.12	106.68
11	L	162	CLA	C1C-NC-C4C	3.17	108.12	106.68
11	M	165	CLA	C1C-NC-C4C	3.16	108.12	106.68
11	M	156	CLA	C1C-NC-C4C	3.16	108.12	106.68
11	D	168	CLA	C1C-NC-C4C	3.16	108.12	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	90	HEM	C3D-C2D-C1D	3.16	111.23	107.24
11	C	161	CLA	C1C-NC-C4C	3.15	108.11	106.68
11	D	156	CLA	C1C-NC-C4C	3.15	108.11	106.68
11	D	159	CLA	C1C-NC-C4C	3.15	108.11	106.68
11	D	169	CLA	C1C-NC-C4C	3.15	108.11	106.68
11	M	164	CLA	C1C-NC-C4C	3.15	108.11	106.68
11	G	313	CLA	C1C-NC-C4C	3.14	108.11	106.68
11	D	161	CLA	C1C-NC-C4C	3.14	108.11	106.68
11	L	167	CLA	C1C-NC-C4C	3.14	108.11	106.68
11	M	163	CLA	C1C-NC-C4C	3.12	108.10	106.68
11	D	166	CLA	C1C-NC-C4C	3.12	108.10	106.68
11	L	166	CLA	C1C-NC-C4C	3.12	108.10	106.68
11	M	169	CLA	C1C-NC-C4C	3.12	108.10	106.68
11	C	162	CLA	C1C-NC-C4C	3.10	108.09	106.68
11	C	166	CLA	C1C-NC-C4C	3.10	108.09	106.68
11	C	160	CLA	C1C-NC-C4C	3.09	108.09	106.68
11	J	174	CLA	C1C-NC-C4C	3.09	108.09	106.68
11	M	158	CLA	C1C-NC-C4C	3.09	108.09	106.68
11	D	167	CLA	C1C-NC-C4C	3.08	108.09	106.68
11	A	174	CLA	C1C-NC-C4C	3.06	108.08	106.68
11	M	161	CLA	C1C-NC-C4C	3.06	108.08	106.68
11	M	166	CLA	C1C-NC-C4C	3.06	108.08	106.68
11	D	170	CLA	C1C-NC-C4C	3.06	108.08	106.68
11	M	167	CLA	C1C-NC-C4C	3.05	108.07	106.68
12	A	177	PHO	CBD-CAD-C3D	3.04	107.22	105.02
11	D	157	CLA	C1C-NC-C4C	3.01	108.05	106.68
12	J	177	PHO	CBD-CAD-C3D	3.00	107.19	105.02
11	M	157	CLA	C1C-NC-C4C	2.99	108.04	106.68
11	M	170	CLA	C1C-NC-C4C	2.96	108.03	106.68
12	B	177	PHO	CBD-CAD-C3D	2.92	107.13	105.02
12	K	177	PHO	CBD-CAD-C3D	2.88	107.11	105.02
15	O	90	HEM	C4A-NA-C1A	2.84	108.55	106.25
15	F	50	HEM	C4A-NA-C1A	2.82	108.52	106.25
15	R	91	HEM	C4A-NA-C1A	2.80	108.51	106.25
15	I	88	HEM	C4A-NA-C1A	2.79	108.50	106.25
15	F	50	HEM	C2B-C1B-NB	2.75	111.35	109.42
15	I	88	HEM	C2B-C1B-NB	2.72	111.33	109.42
15	R	91	HEM	C2B-C1B-NB	2.71	111.33	109.42
15	O	90	HEM	C2B-C1B-NB	2.71	111.33	109.42
15	F	50	HEM	C3C-C2C-C1C	-2.68	104.10	107.35
15	R	91	HEM	C3C-C2C-C1C	-2.66	104.11	107.35
15	F	50	HEM	C4C-NC-C1C	2.66	108.40	106.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	90	HEM	C3C-C2C-C1C	-2.66	104.12	107.35
15	I	88	HEM	C3C-C2C-C1C	-2.65	104.13	107.35
15	I	88	HEM	C4C-NC-C1C	2.65	108.39	106.25
15	O	90	HEM	C4C-NC-C1C	2.64	108.39	106.25
15	R	91	HEM	C4C-NC-C1C	2.62	108.36	106.25
11	L	166	CLA	C2A-C1A-CHA	2.51	126.60	122.71
11	L	165	CLA	C2A-C1A-CHA	2.50	126.59	122.71
11	J	174	CLA	C2A-C1A-CHA	2.50	126.59	122.71
11	A	174	CLA	C2A-C1A-CHA	2.49	126.58	122.71
11	M	159	CLA	C2A-C1A-CHA	2.49	126.58	122.71
11	C	164	CLA	C2A-C1A-CHA	2.49	126.57	122.71
11	M	156	CLA	C2A-C1A-CHA	2.48	126.56	122.71
11	G	313	CLA	C2A-C1A-CHA	2.48	126.56	122.71
11	C	166	CLA	C2A-C1A-CHA	2.48	126.55	122.71
11	D	159	CLA	C2A-C1A-CHA	2.48	126.55	122.71
11	D	156	CLA	C2A-C1A-CHA	2.47	126.55	122.71
11	K	178	CLA	C2A-C1A-CHA	2.47	126.54	122.71
11	D	161	CLA	C2A-C1A-CHA	2.47	126.54	122.71
11	L	157	CLA	C2A-C1A-CHA	2.47	126.54	122.71
11	D	162	CLA	C2A-C1A-CHA	2.47	126.54	122.71
11	C	157	CLA	C2A-C1A-CHA	2.47	126.54	122.71
11	D	169	CLA	C2A-C1A-CHA	2.47	126.54	122.71
11	M	161	CLA	C2A-C1A-CHA	2.47	126.54	122.71
11	A	176	CLA	C2A-C1A-CHA	2.47	126.53	122.71
11	D	167	CLA	C2A-C1A-CHA	2.47	126.53	122.71
11	B	178	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	L	164	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	M	162	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	D	170	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	P	313	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	M	164	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	M	168	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	M	157	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	D	165	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	J	175	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	C	158	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	C	161	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	M	166	CLA	C2A-C1A-CHA	2.46	126.52	122.71
11	M	169	CLA	C2A-C1A-CHA	2.46	126.52	122.71
11	A	175	CLA	C2A-C1A-CHA	2.46	126.52	122.71
11	D	157	CLA	C2A-C1A-CHA	2.46	126.52	122.71
11	D	163	CLA	C2A-C1A-CHA	2.46	126.52	122.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	J	176	CLA	C2A-C1A-CHA	2.46	126.52	122.71
11	A	179	CLA	C2A-C1A-CHA	2.45	126.52	122.71
11	D	166	CLA	C2A-C1A-CHA	2.45	126.52	122.71
11	M	165	CLA	C2A-C1A-CHA	2.45	126.51	122.71
11	L	162	CLA	C2A-C1A-CHA	2.45	126.51	122.71
11	L	163	CLA	C2A-C1A-CHA	2.45	126.51	122.71
11	B	176	CLA	C2A-C1A-CHA	2.45	126.51	122.71
11	A	178	CLA	C2A-C1A-CHA	2.45	126.51	122.71
11	C	165	CLA	C2A-C1A-CHA	2.45	126.51	122.71
11	D	164	CLA	C2A-C1A-CHA	2.45	126.51	122.71
11	L	168	CLA	C2A-C1A-CHA	2.45	126.51	122.71
11	M	167	CLA	C2A-C1A-CHA	2.45	126.51	122.71
11	C	167	CLA	C2A-C1A-CHA	2.45	126.50	122.71
11	D	158	CLA	C2A-C1A-CHA	2.45	126.50	122.71
11	M	163	CLA	C2A-C1A-CHA	2.45	126.50	122.71
11	C	162	CLA	C2A-C1A-CHA	2.45	126.50	122.71
11	C	160	CLA	C2A-C1A-CHA	2.44	126.50	122.71
11	M	158	CLA	C2A-C1A-CHA	2.44	126.50	122.71
11	C	163	CLA	C2A-C1A-CHA	2.44	126.49	122.71
11	C	168	CLA	C2A-C1A-CHA	2.44	126.49	122.71
11	D	160	CLA	C2A-C1A-CHA	2.44	126.49	122.71
11	M	170	CLA	C2A-C1A-CHA	2.44	126.49	122.71
11	M	160	CLA	C2A-C1A-CHA	2.44	126.49	122.71
11	J	178	CLA	C2A-C1A-CHA	2.43	126.48	122.71
11	D	168	CLA	C2A-C1A-CHA	2.43	126.48	122.71
11	J	179	CLA	C2A-C1A-CHA	2.43	126.48	122.71
11	K	176	CLA	C2A-C1A-CHA	2.43	126.48	122.71
11	L	159	CLA	C2A-C1A-CHA	2.43	126.48	122.71
11	L	158	CLA	C2A-C1A-CHA	2.42	126.47	122.71
11	L	161	CLA	C2A-C1A-CHA	2.42	126.47	122.71
11	C	159	CLA	C2A-C1A-CHA	2.42	126.46	122.71
11	L	167	CLA	C2A-C1A-CHA	2.42	126.46	122.71
15	F	50	HEM	C2C-C3C-C4C	-2.42	104.41	107.35
15	O	90	HEM	C2C-C3C-C4C	-2.42	104.41	107.35
15	R	91	HEM	C2C-C3C-C4C	-2.42	104.41	107.35
15	I	88	HEM	C2C-C3C-C4C	-2.41	104.42	107.35
11	L	160	CLA	C2A-C1A-CHA	2.41	126.44	122.71
15	F	50	HEM	C3A-C2A-C1A	-2.19	104.37	106.81
15	R	91	HEM	C3A-C2A-C1A	-2.18	104.38	106.81
15	I	88	HEM	C3A-C2A-C1A	-2.17	104.39	106.81
15	O	90	HEM	C3A-C2A-C1A	-2.17	104.39	106.81
15	R	91	HEM	C4B-CHC-C1C	2.08	131.90	125.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	I	88	HEM	C4B-CHC-C1C	2.07	131.89	125.98
15	O	90	HEM	C4B-CHC-C1C	2.04	131.78	125.98
15	F	50	HEM	C4B-CHC-C1C	2.03	131.75	125.98

There are no chirality outliers.

There are no torsion outliers.

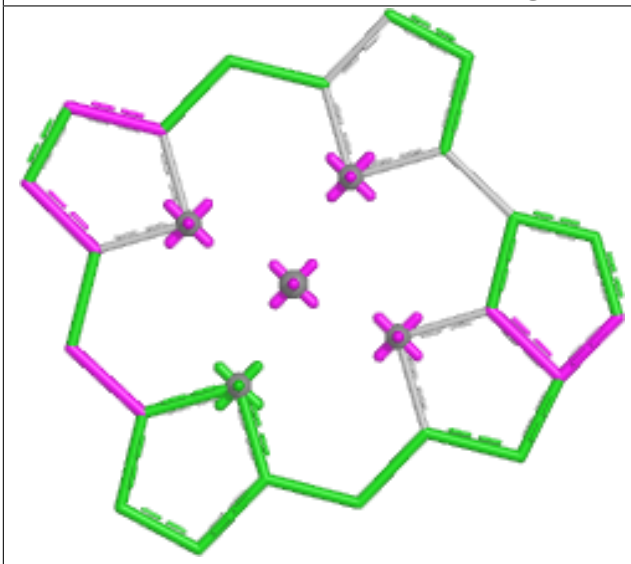
There are no ring outliers.

8 monomers are involved in 18 short contacts:

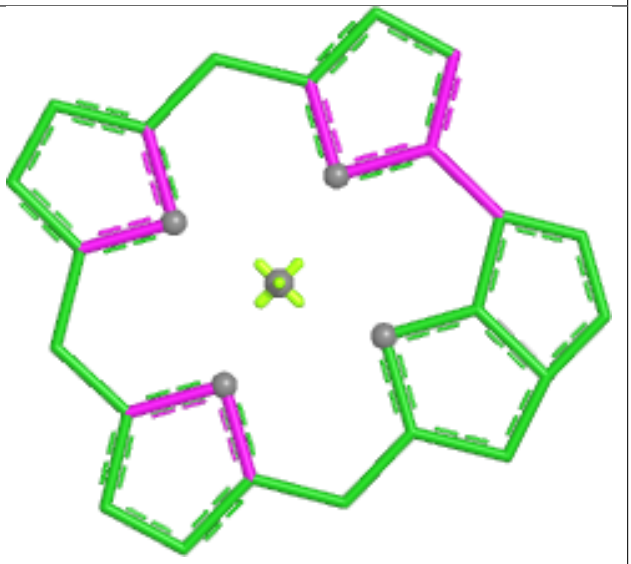
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	168	CLA	2	0
11	C	168	CLA	2	0
11	G	313	CLA	4	0
11	D	168	CLA	4	0
11	P	313	CLA	4	0
11	D	165	CLA	3	0
11	M	165	CLA	3	0
11	M	168	CLA	4	0

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.

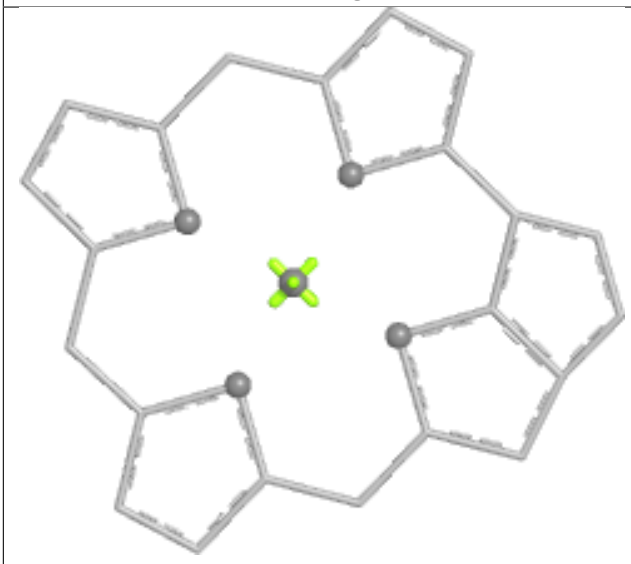
Ligand CLA C 165



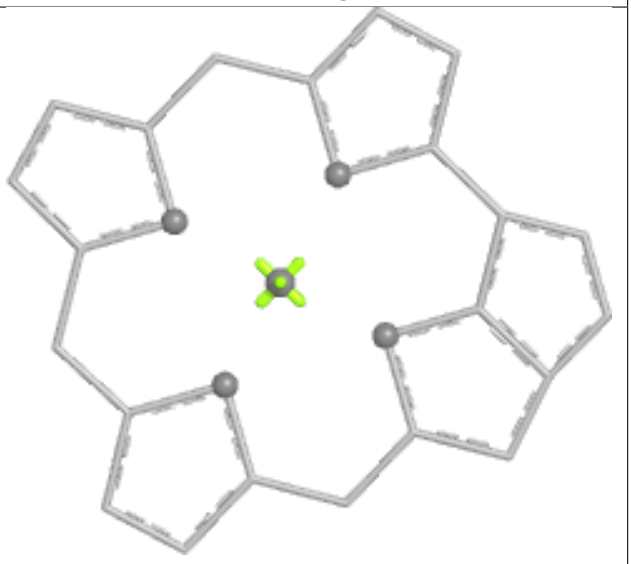
Bond lengths



Bond angles

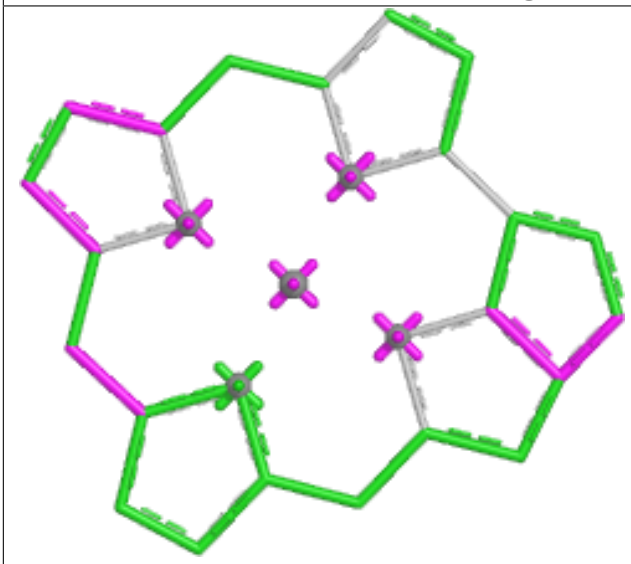


Torsions

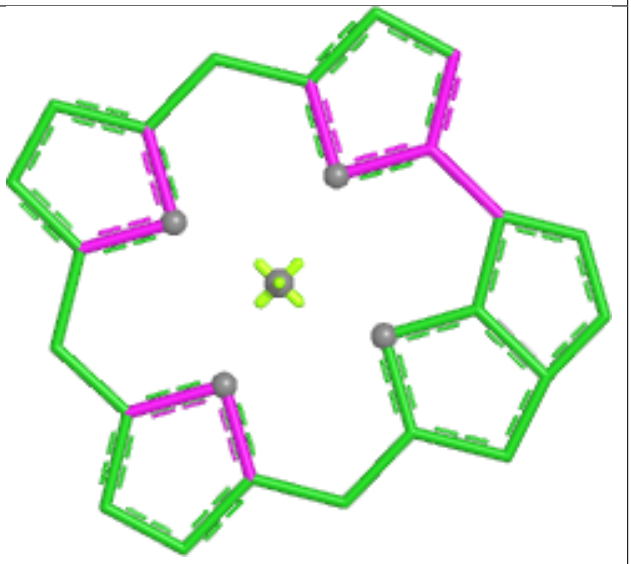


Rings

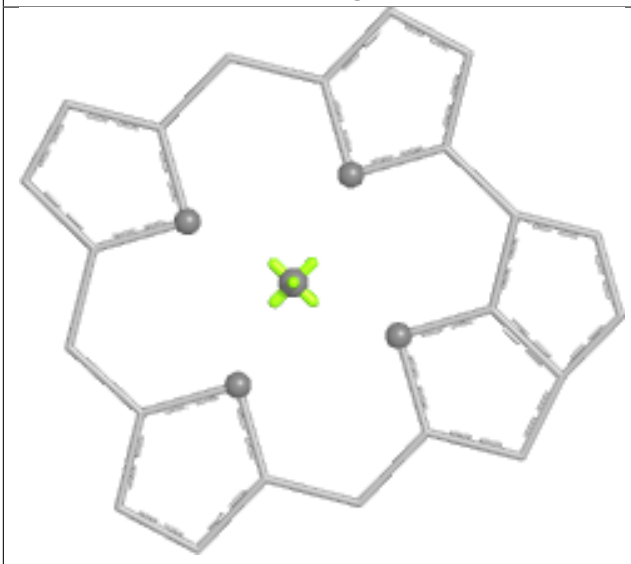
Ligand CLA M 159



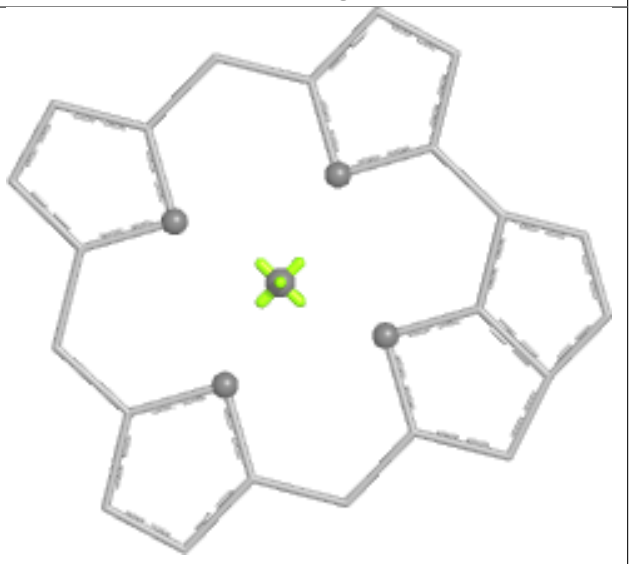
Bond lengths



Bond angles

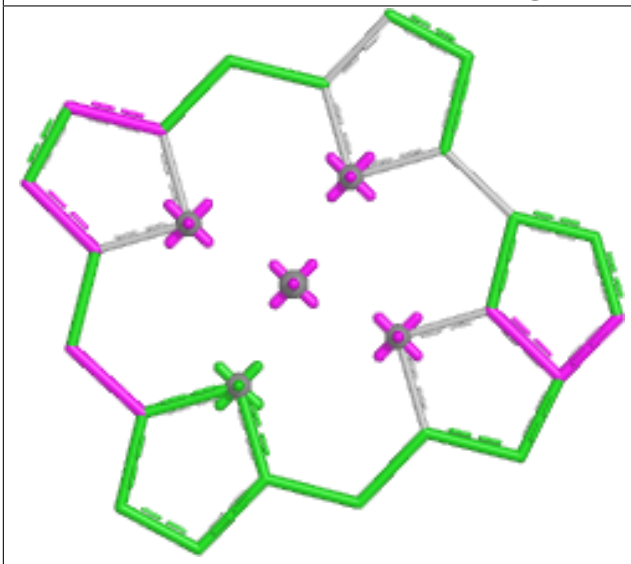


Torsions

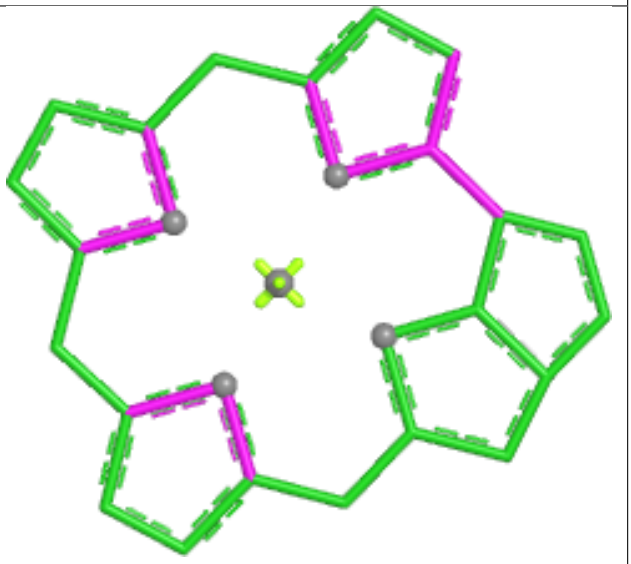


Rings

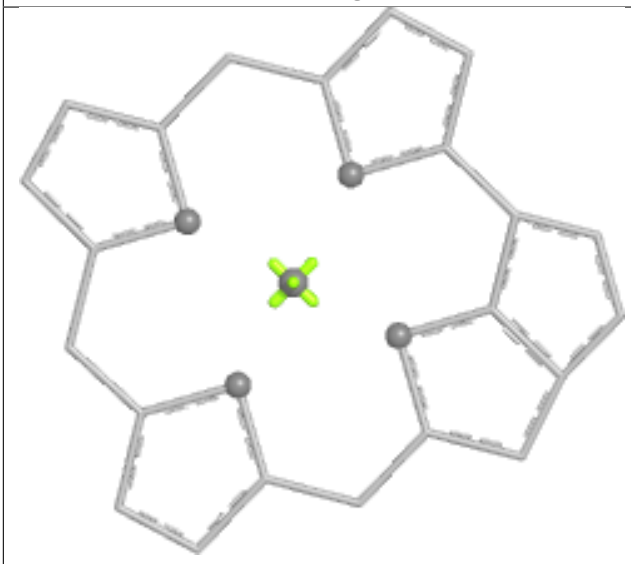
Ligand CLA L 159



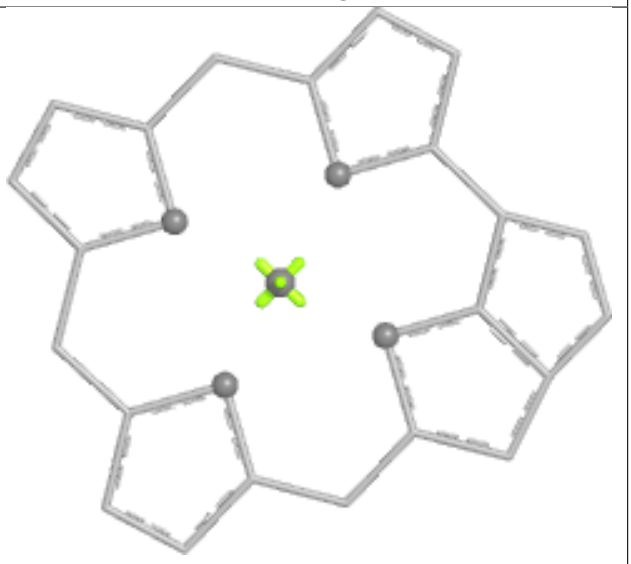
Bond lengths



Bond angles

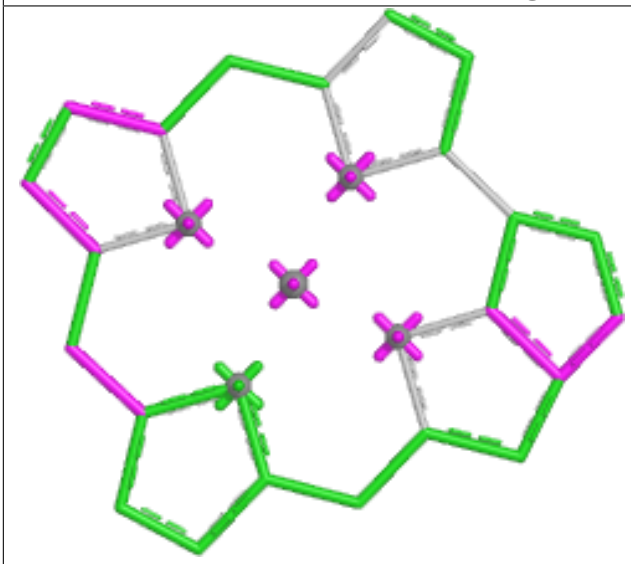


Torsions

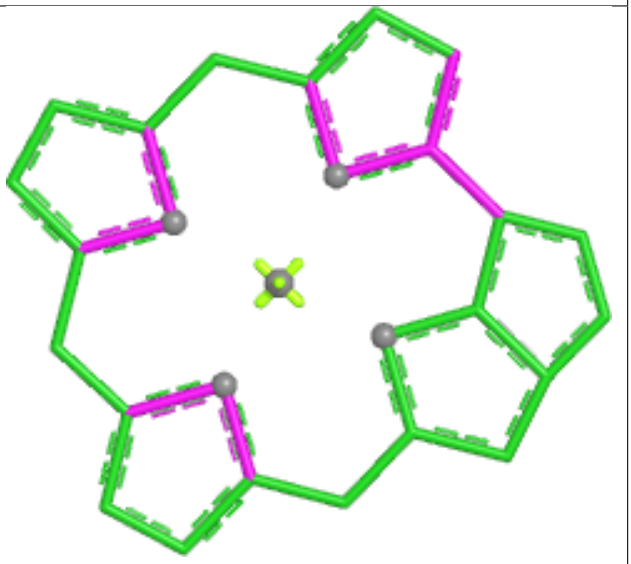


Rings

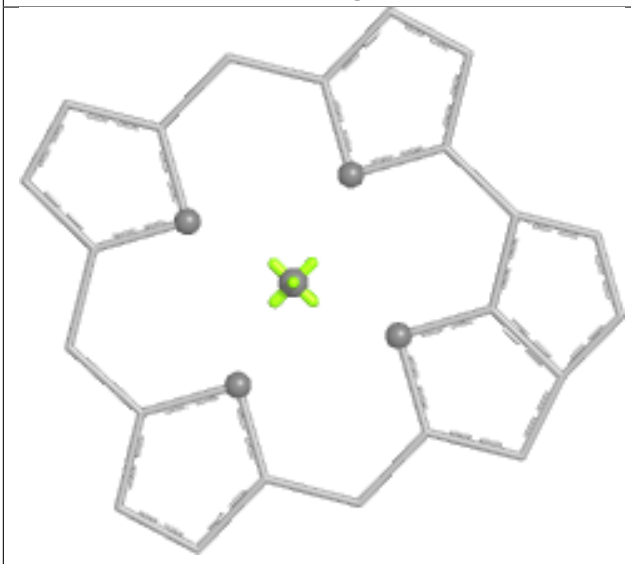
Ligand CLA A 175



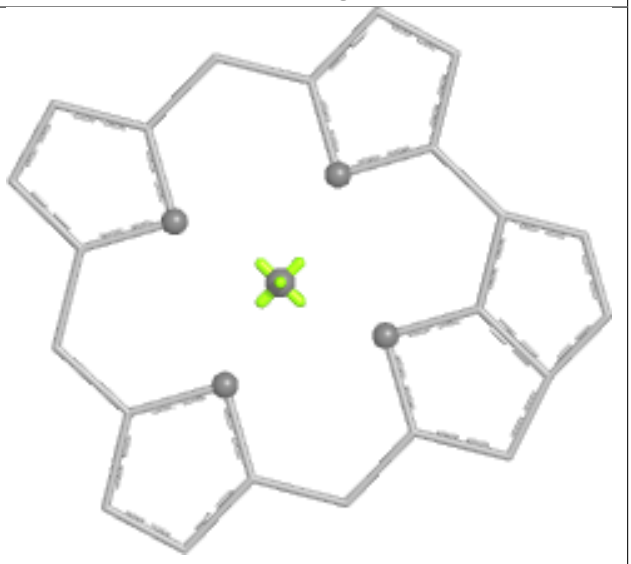
Bond lengths



Bond angles

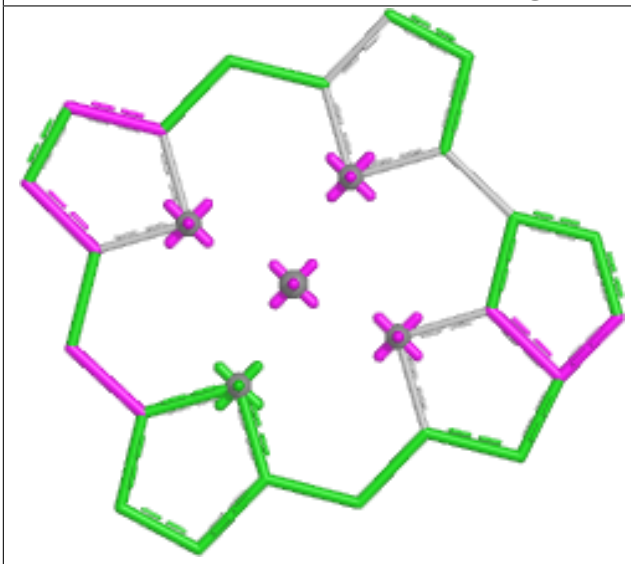


Torsions

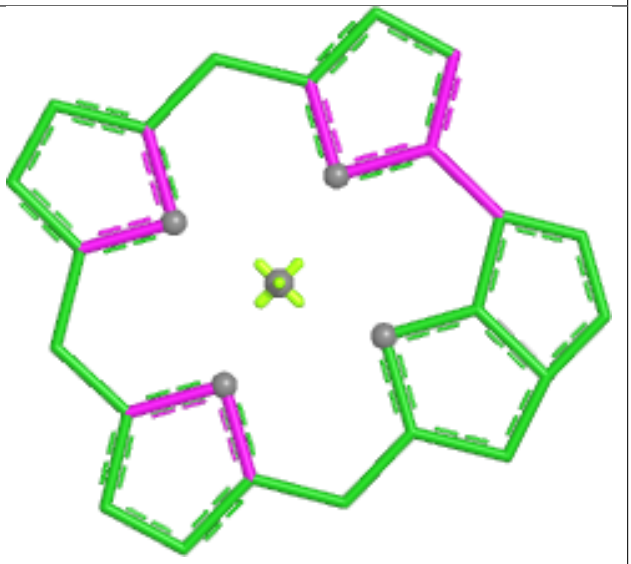


Rings

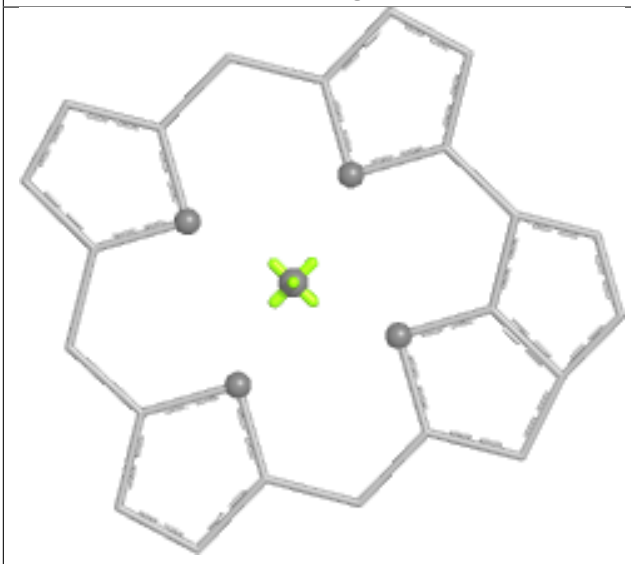
Ligand CLA L 164



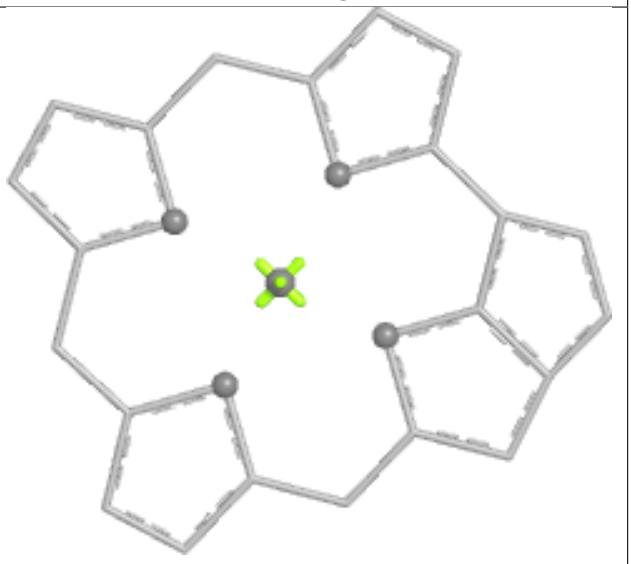
Bond lengths



Bond angles

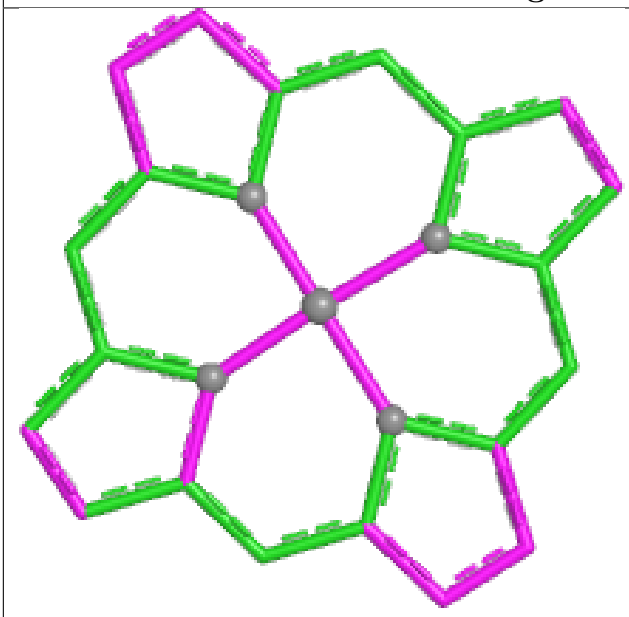


Torsions

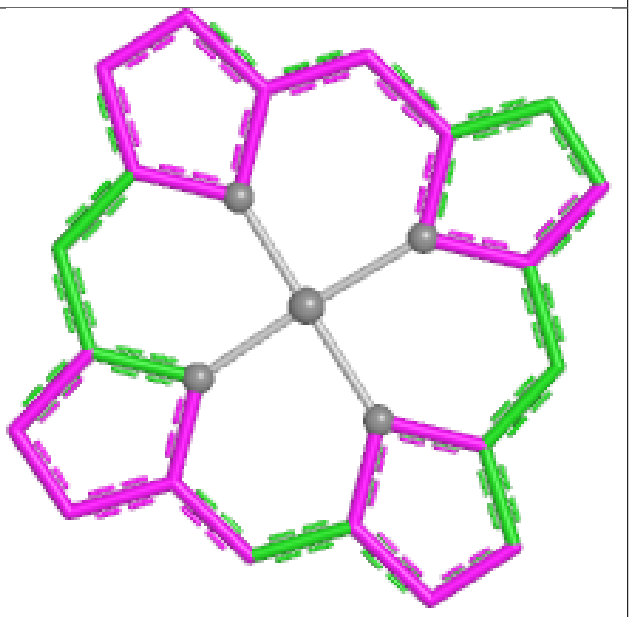


Rings

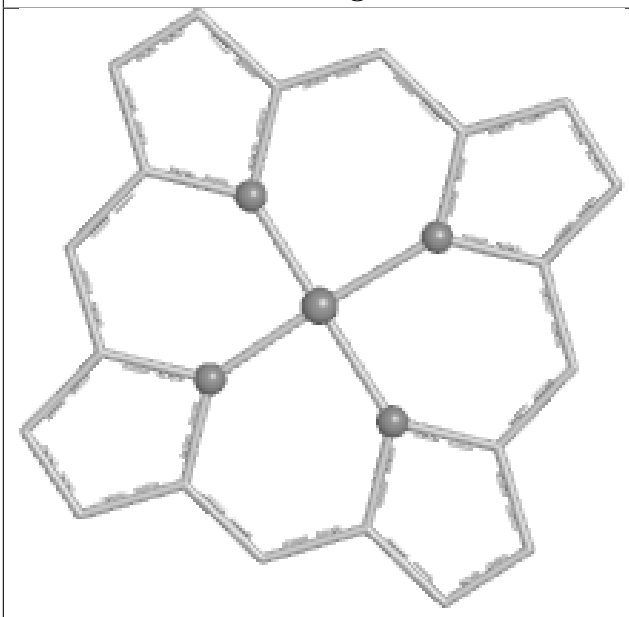
Ligand HEM O 90



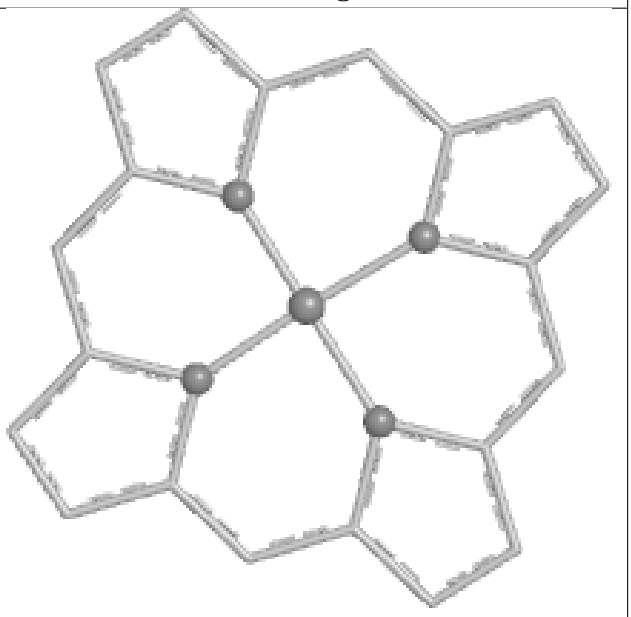
Bond lengths



Bond angles

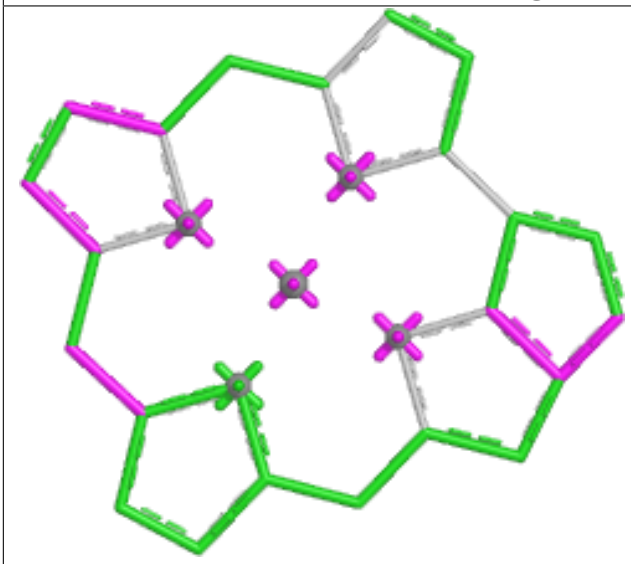


Torsions

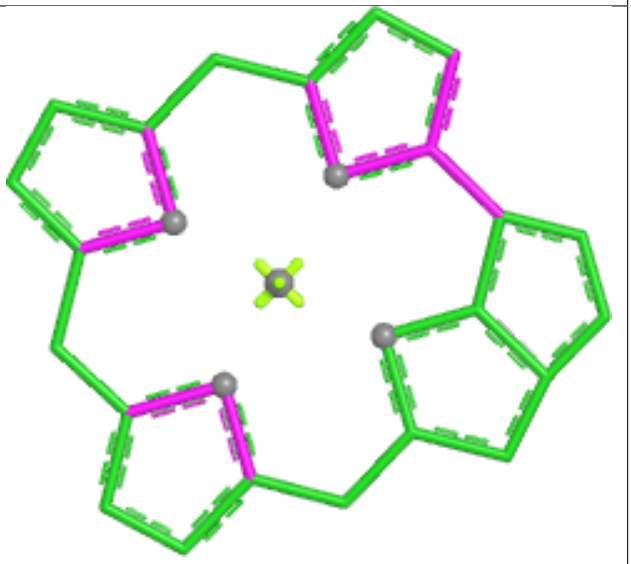


Rings

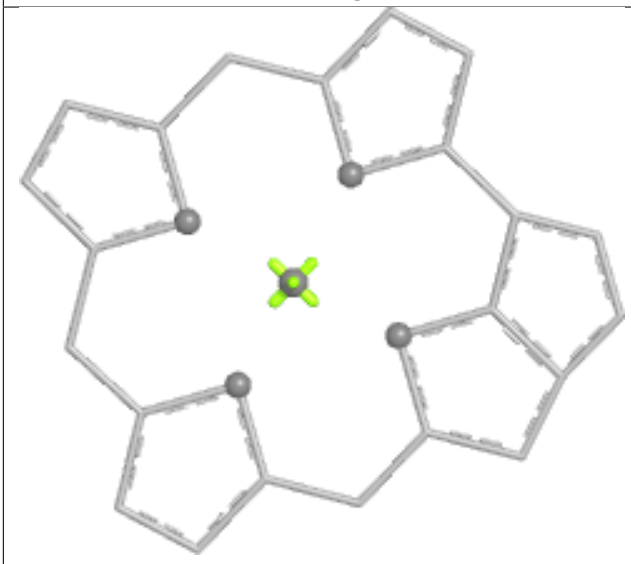
Ligand CLA J 179



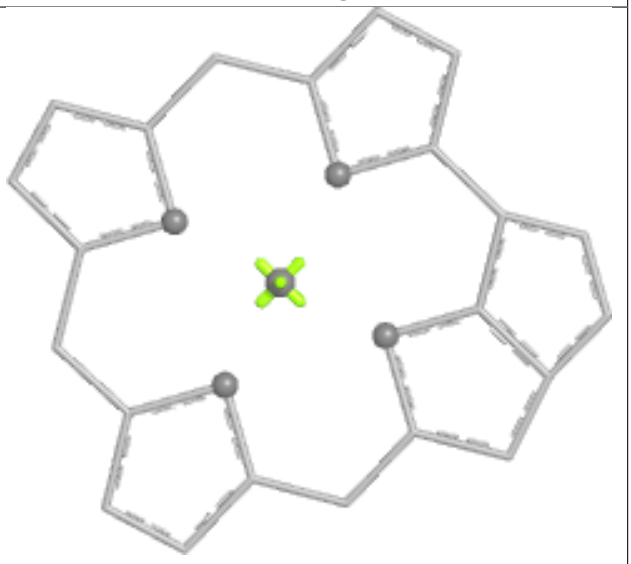
Bond lengths



Bond angles

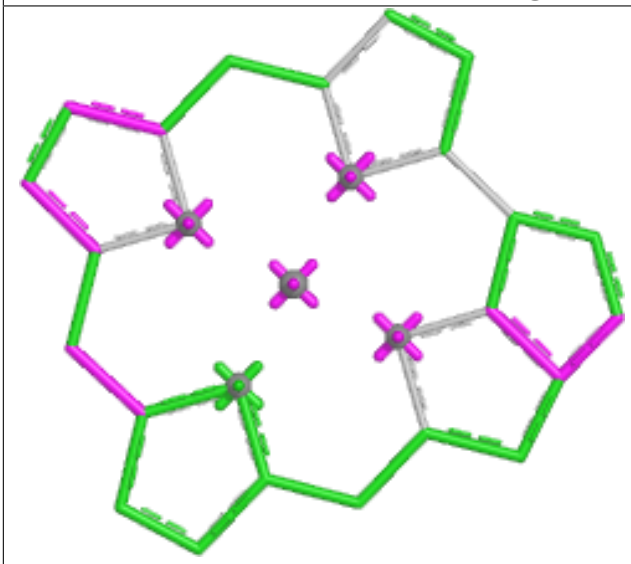


Torsions

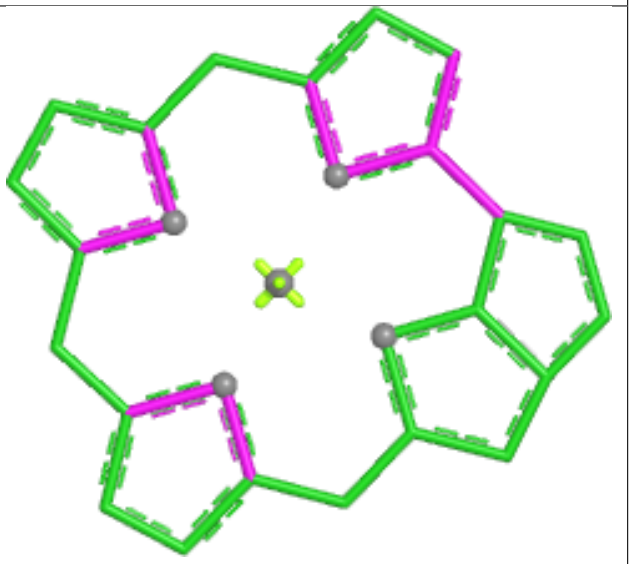


Rings

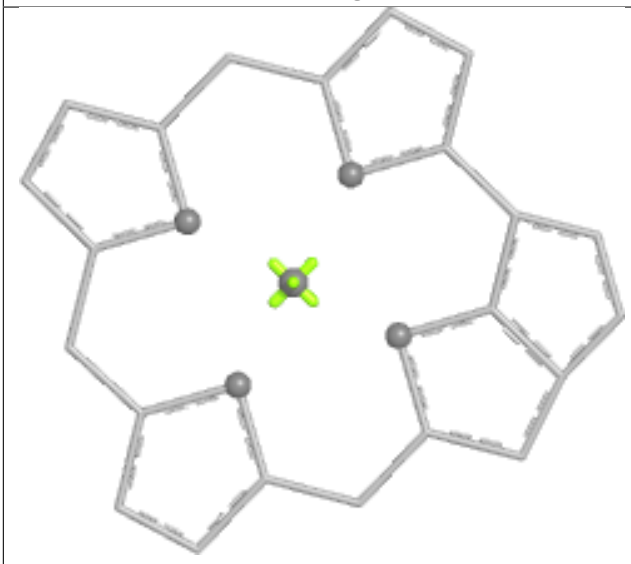
Ligand CLA L 163



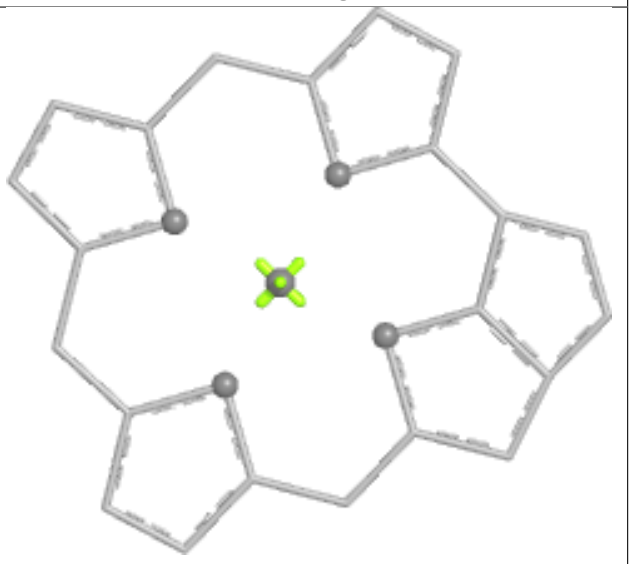
Bond lengths



Bond angles

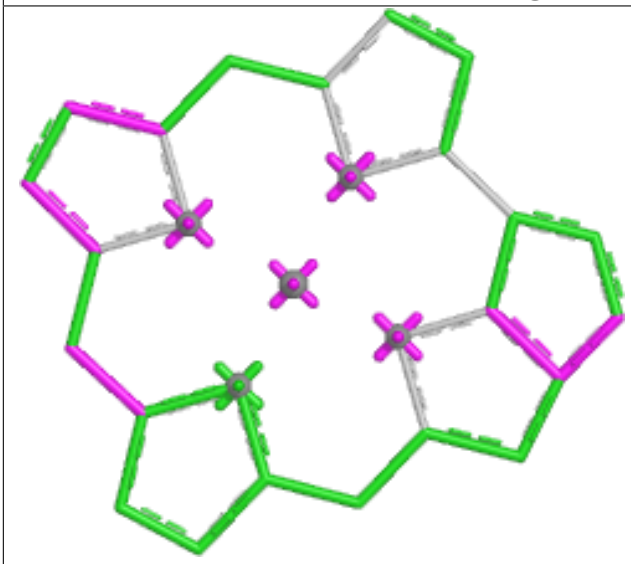


Torsions

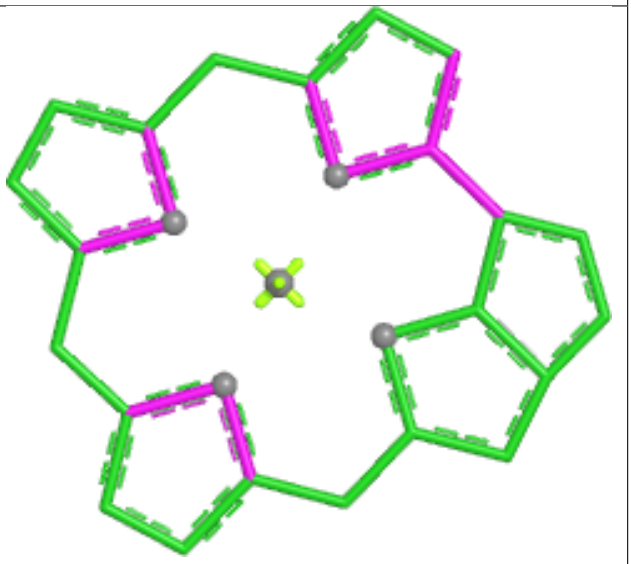


Rings

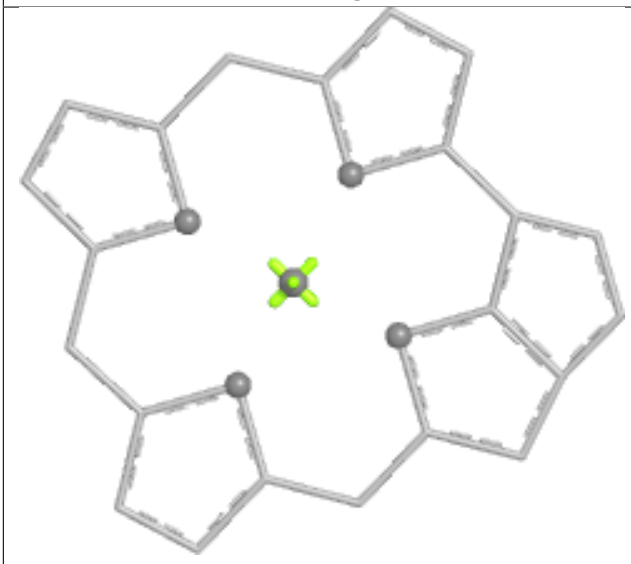
Ligand CLA L 168



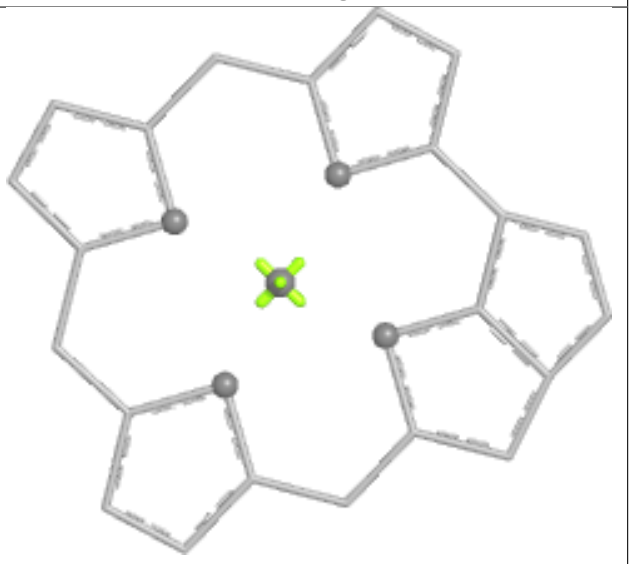
Bond lengths



Bond angles

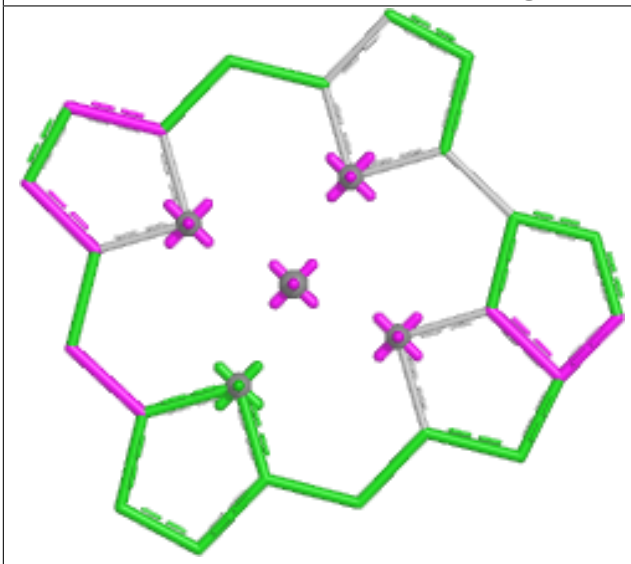


Torsions

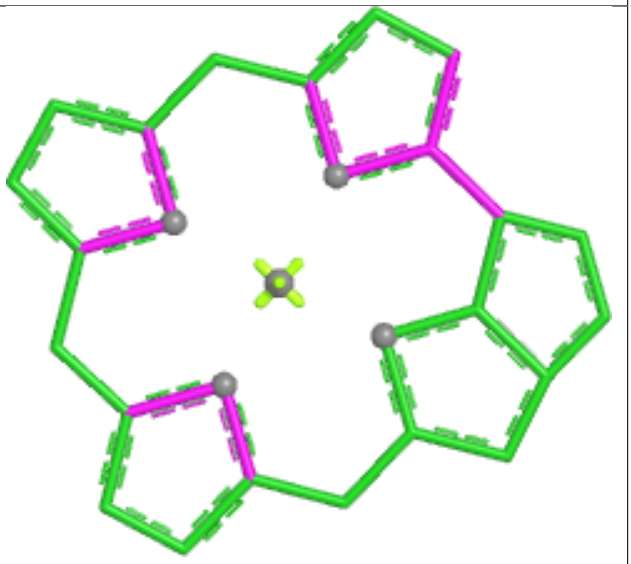


Rings

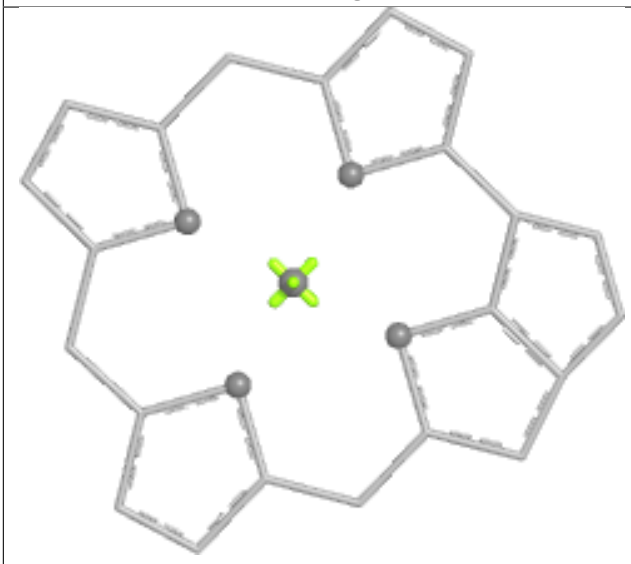
Ligand CLA M 164



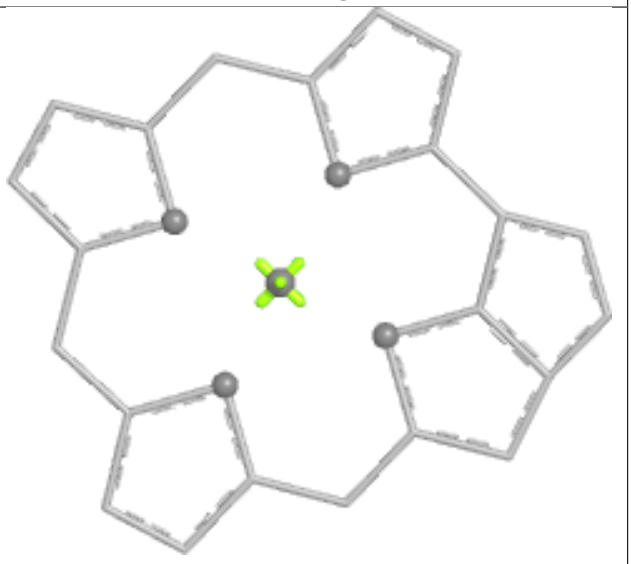
Bond lengths



Bond angles

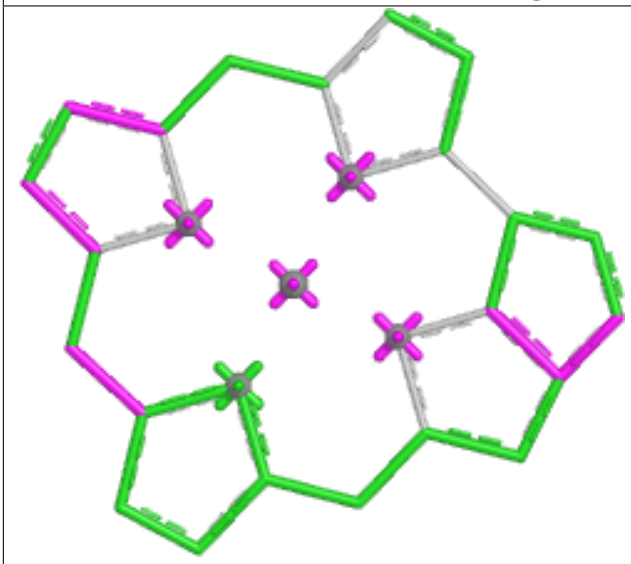


Torsions

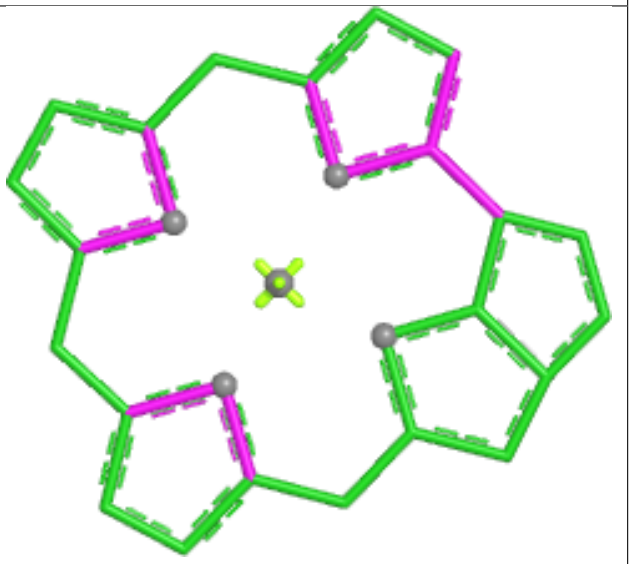


Rings

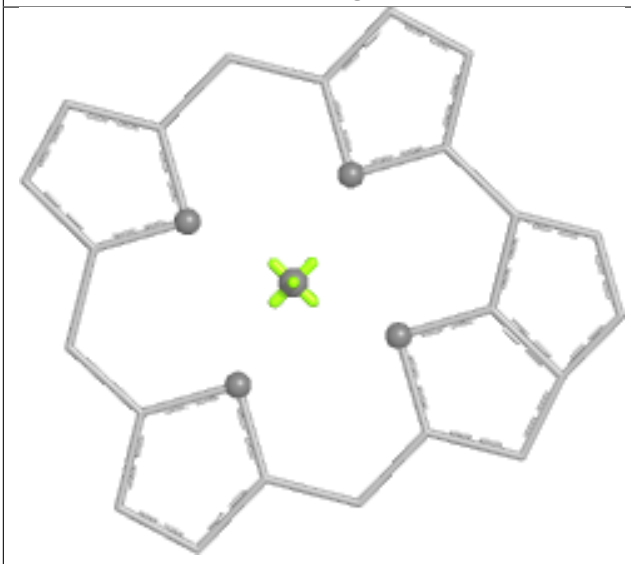
Ligand CLA J 174



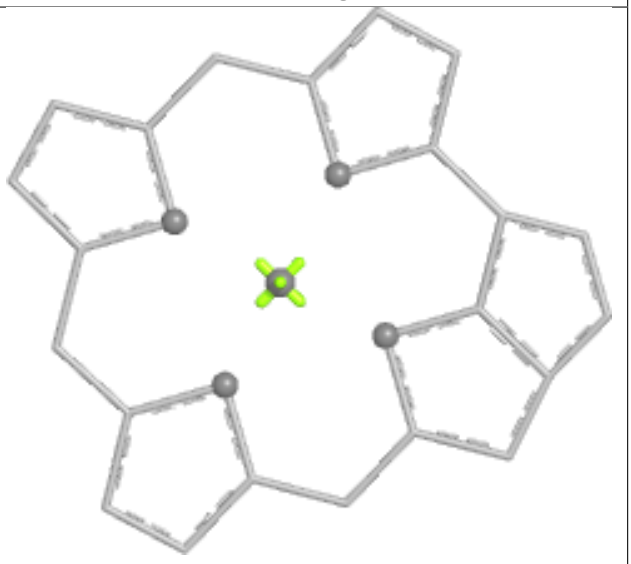
Bond lengths



Bond angles

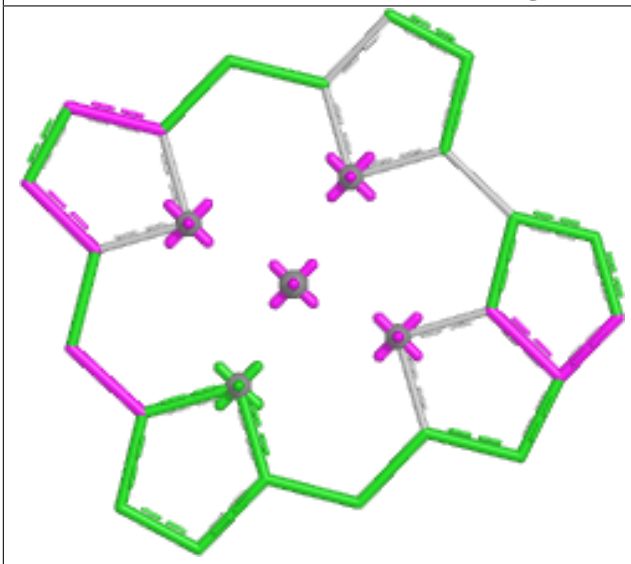


Torsions

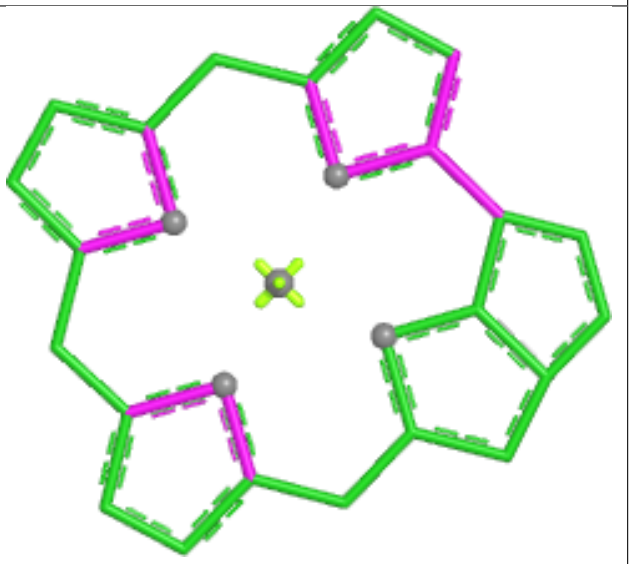


Rings

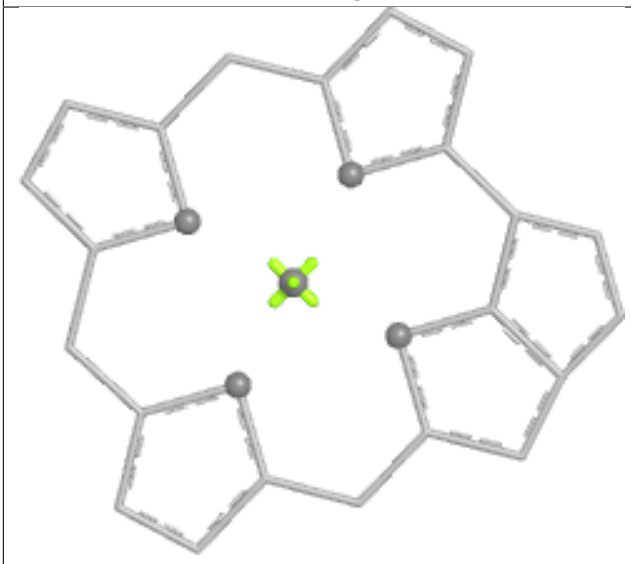
Ligand CLA C 168



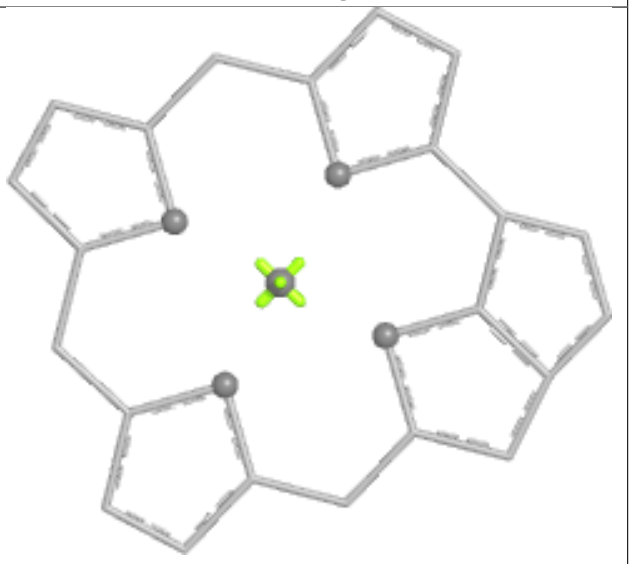
Bond lengths



Bond angles

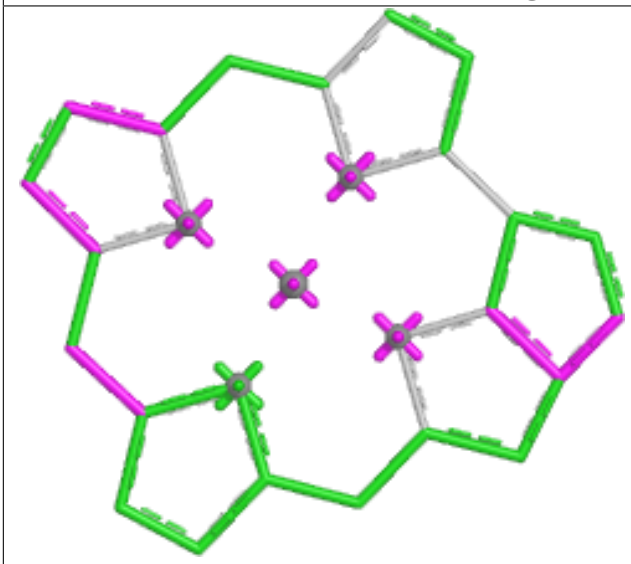


Torsions

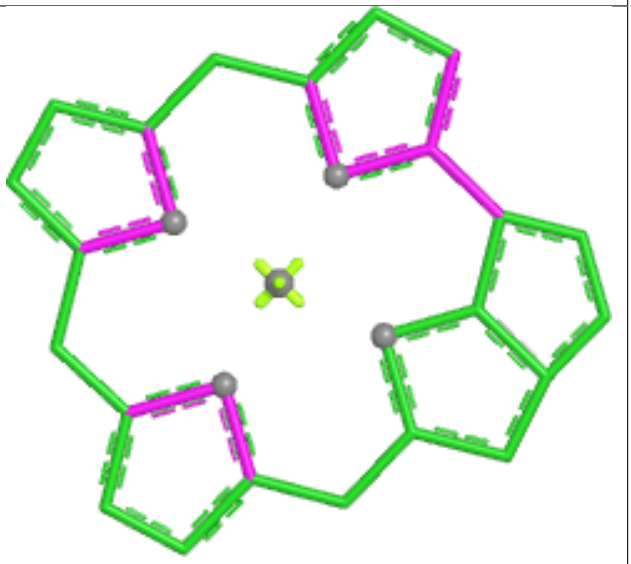


Rings

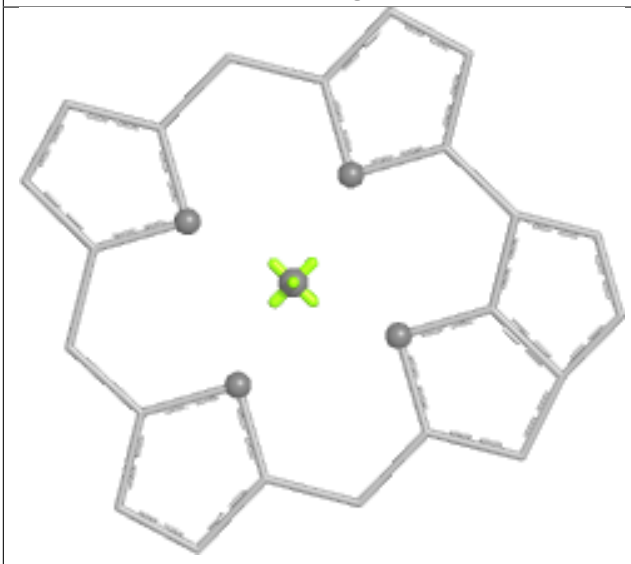
Ligand CLA D 159



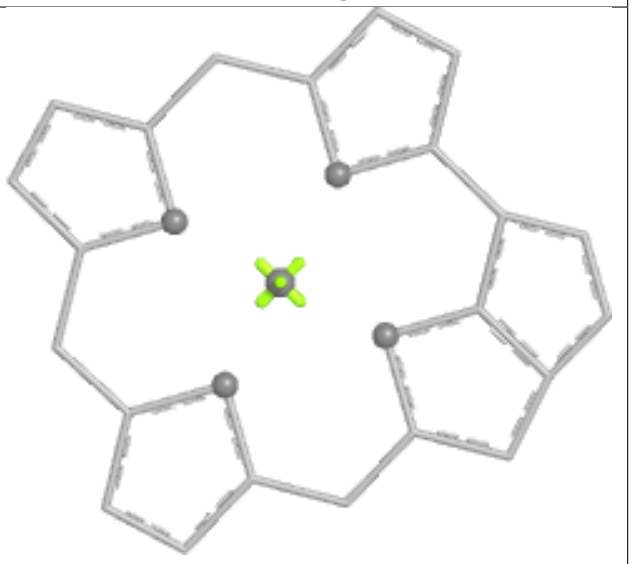
Bond lengths



Bond angles

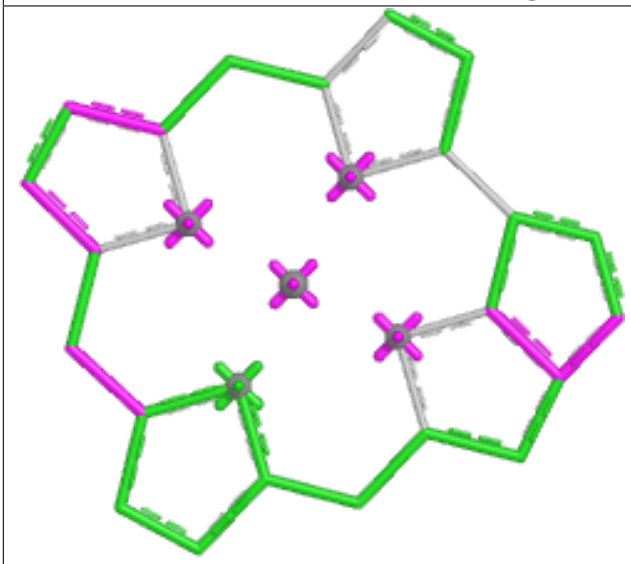


Torsions

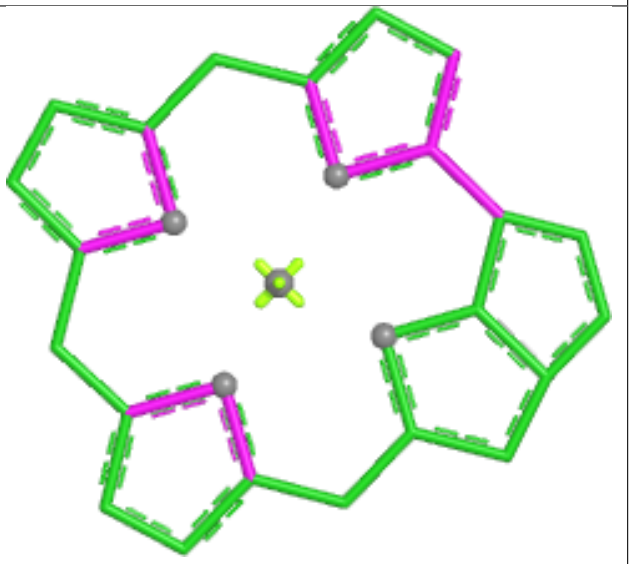


Rings

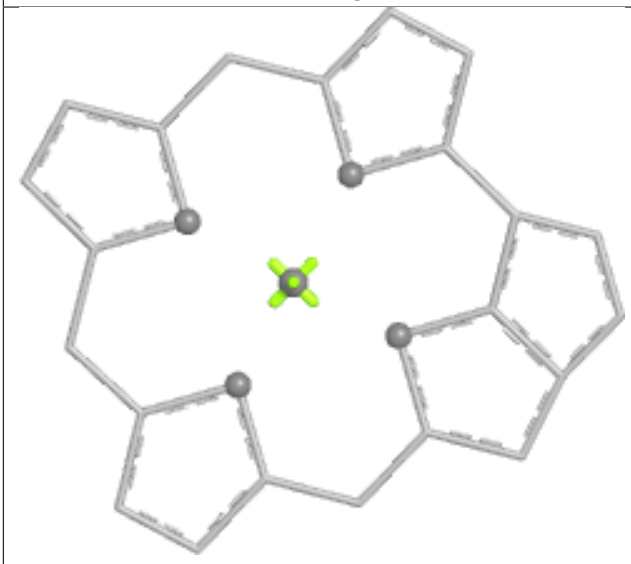
Ligand CLA D 166



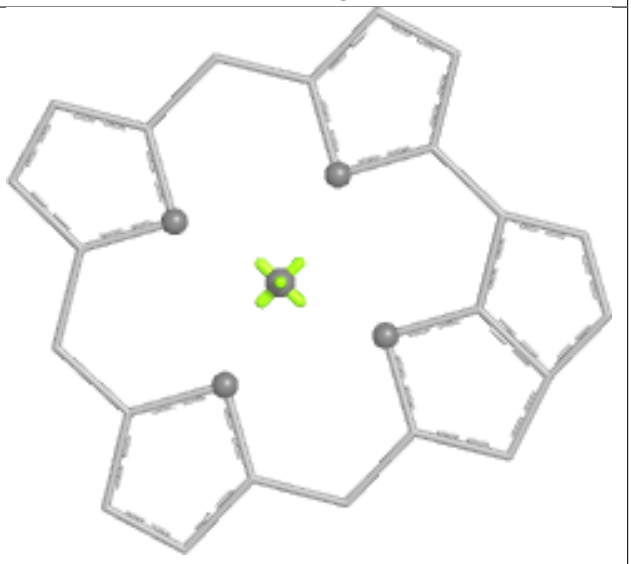
Bond lengths



Bond angles

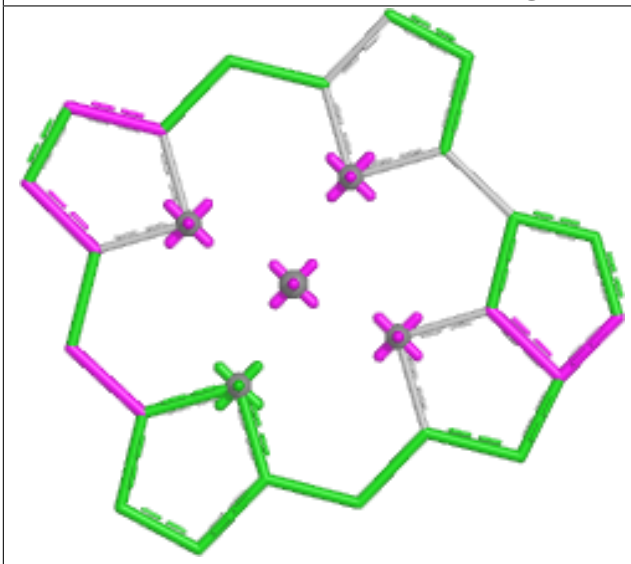


Torsions

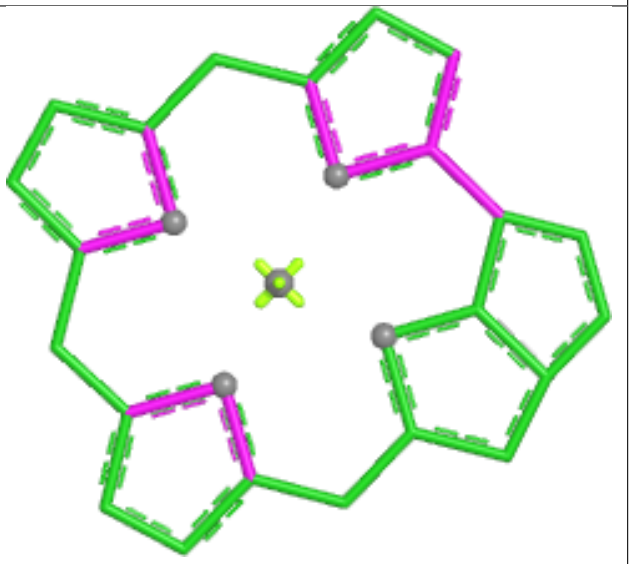


Rings

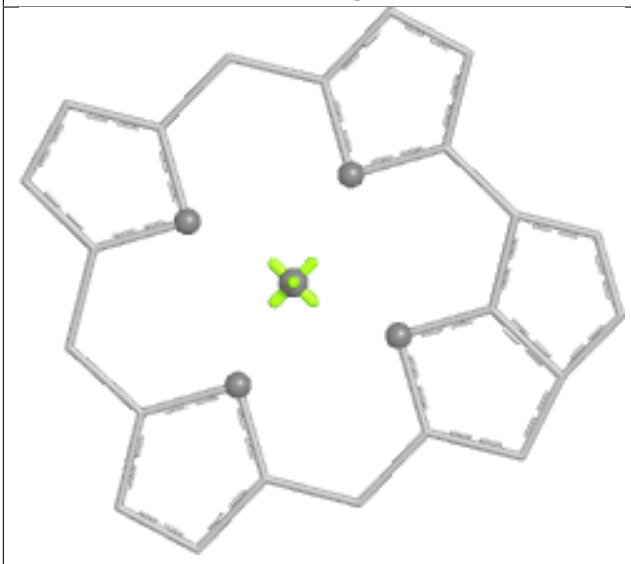
Ligand CLA G 313



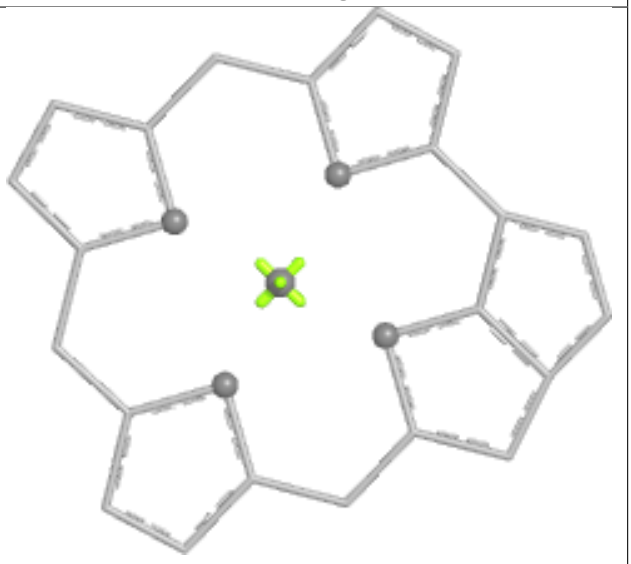
Bond lengths



Bond angles

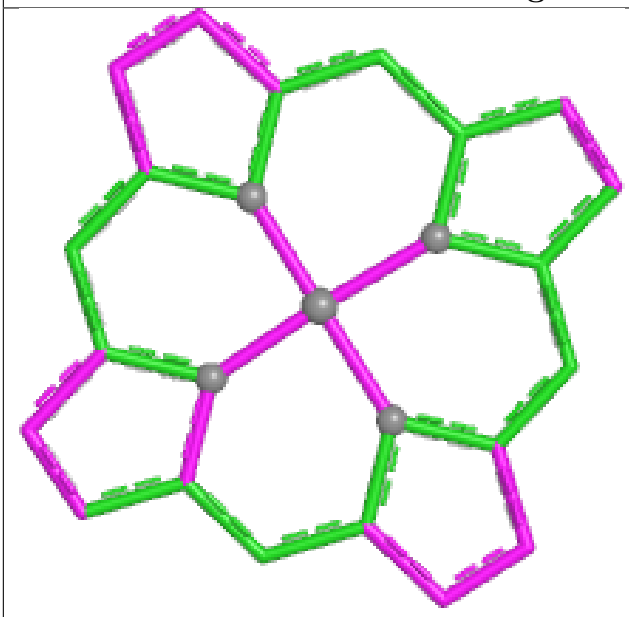


Torsions

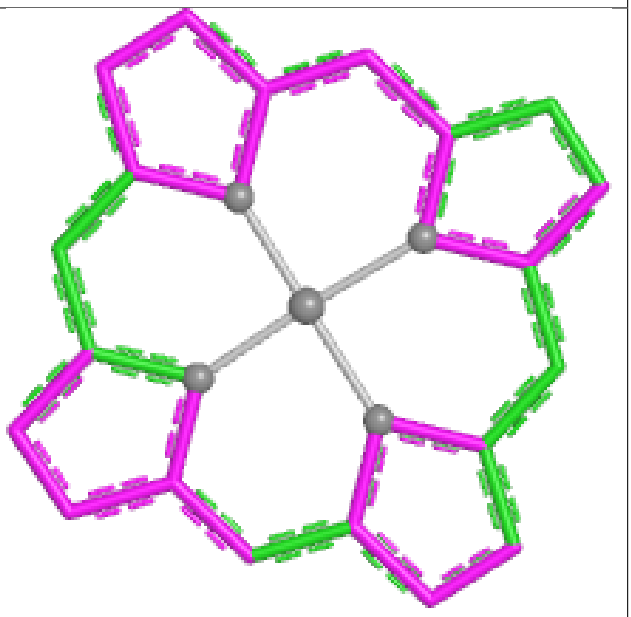


Rings

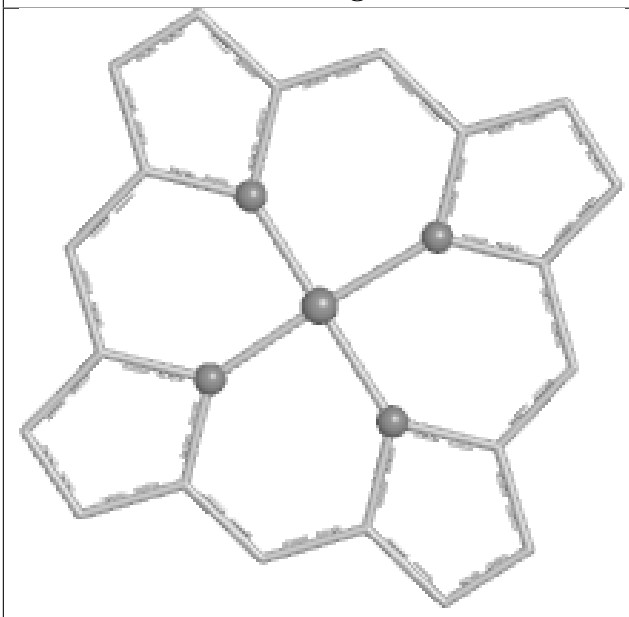
Ligand HEM R 91



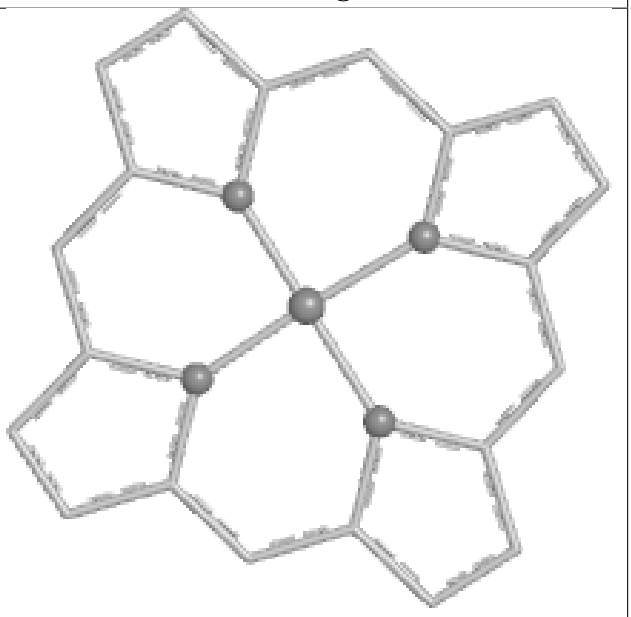
Bond lengths



Bond angles

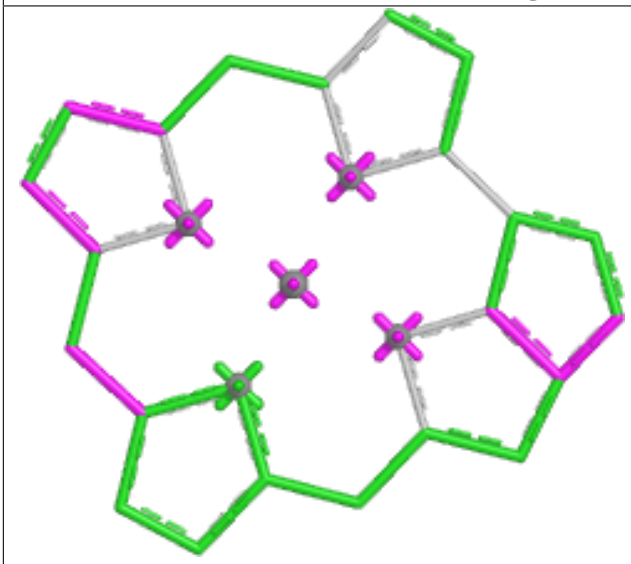


Torsions

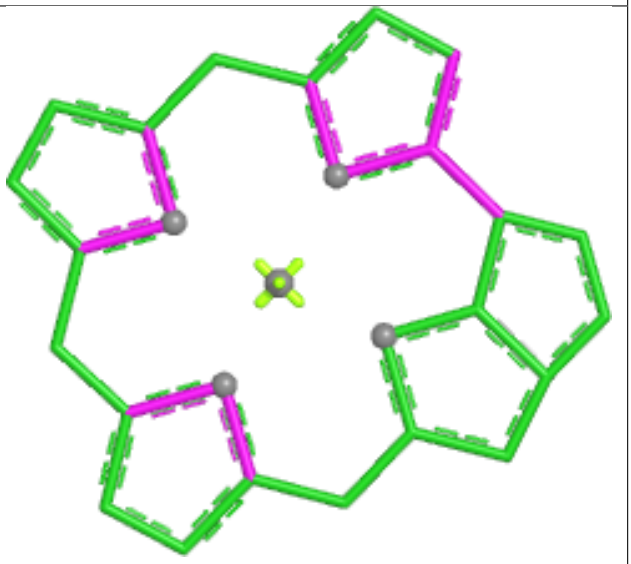


Rings

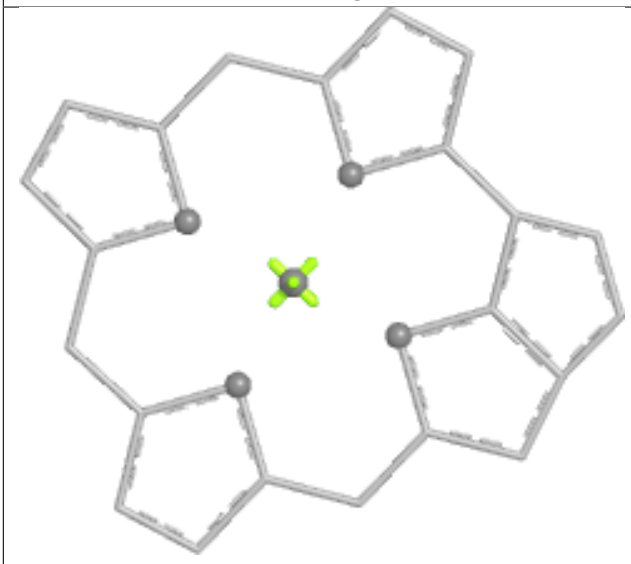
Ligand CLA B 176



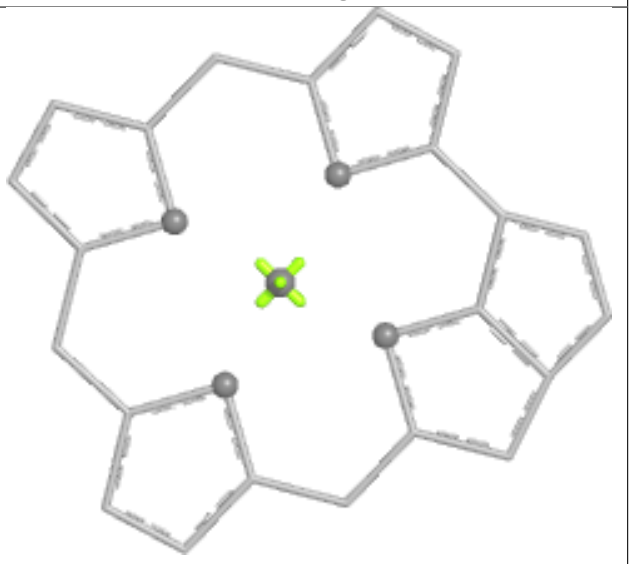
Bond lengths



Bond angles

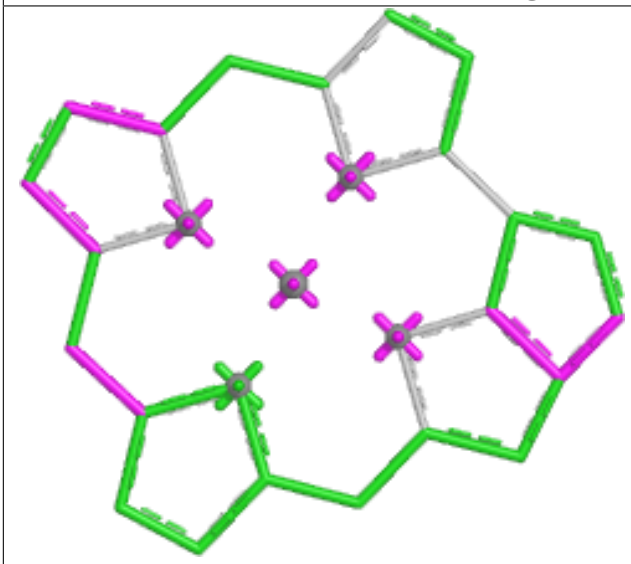


Torsions

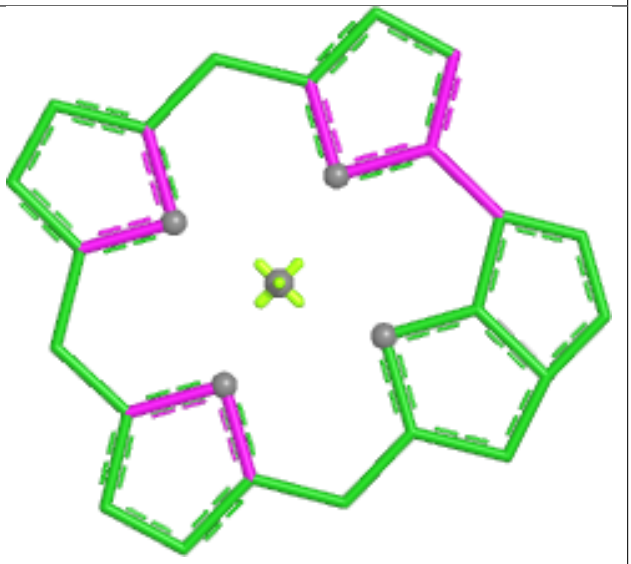


Rings

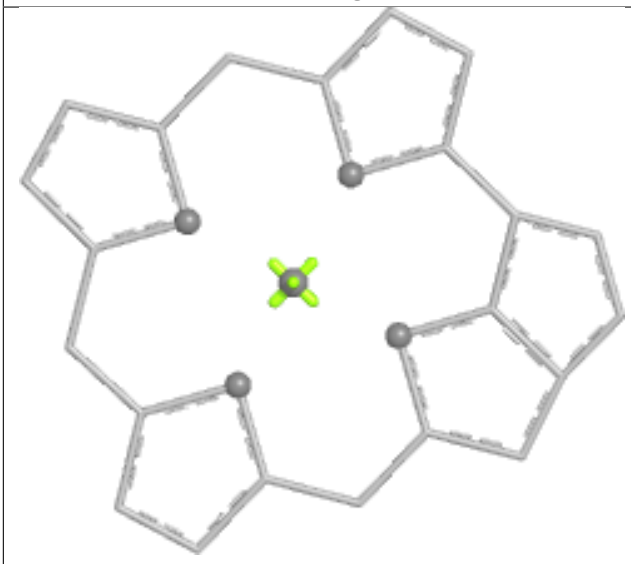
Ligand CLA D 168



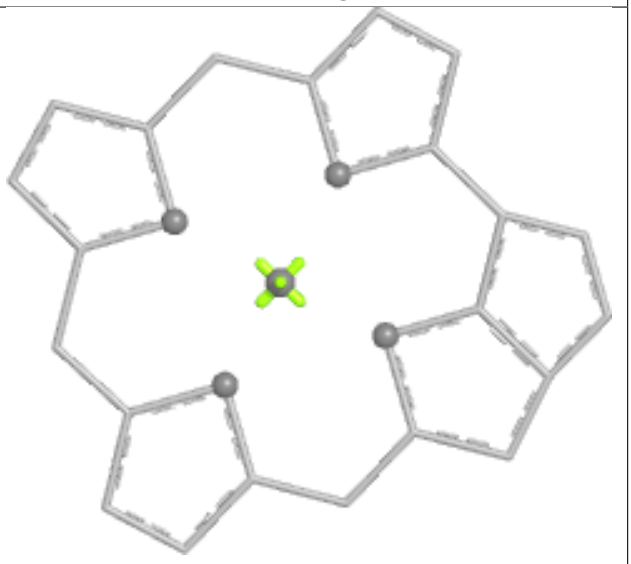
Bond lengths



Bond angles

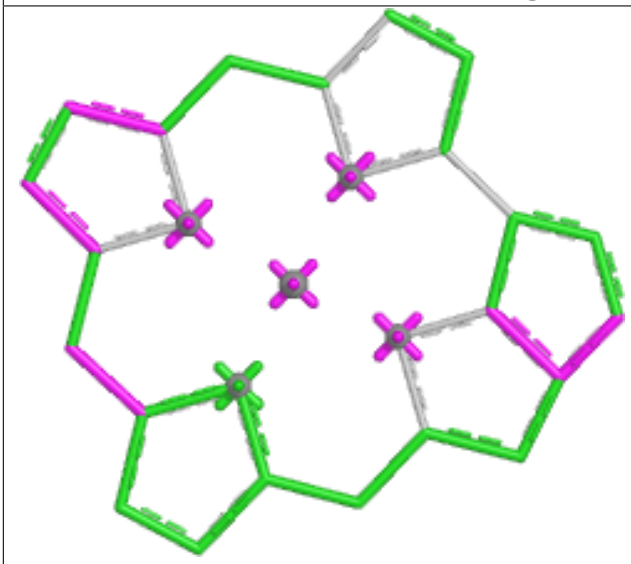


Torsions

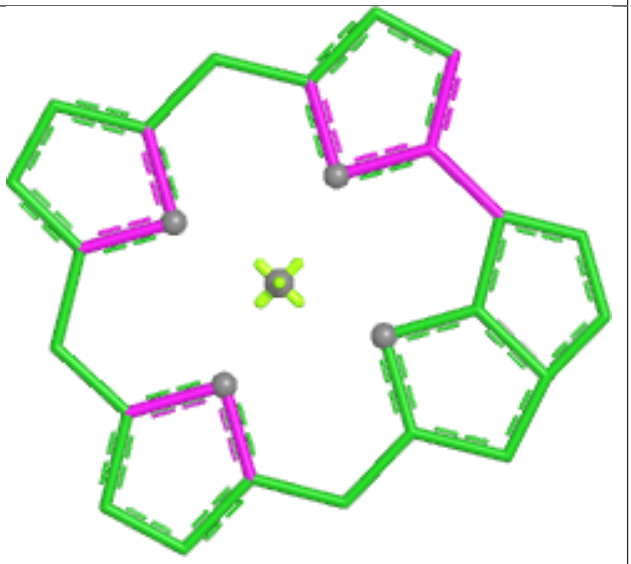


Rings

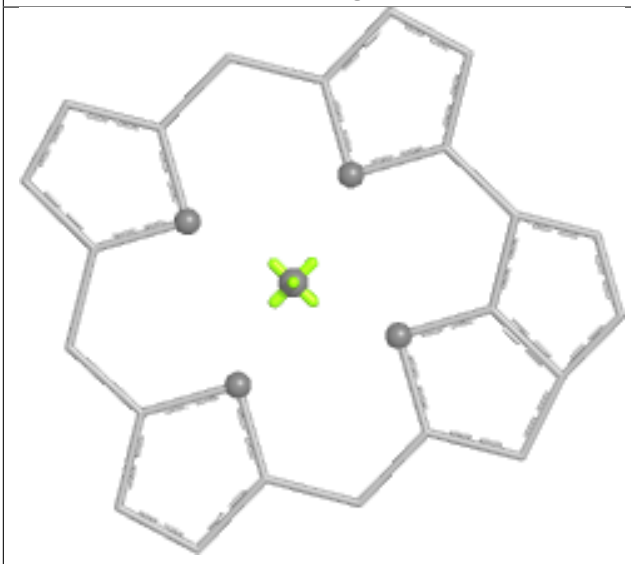
Ligand CLA A 174



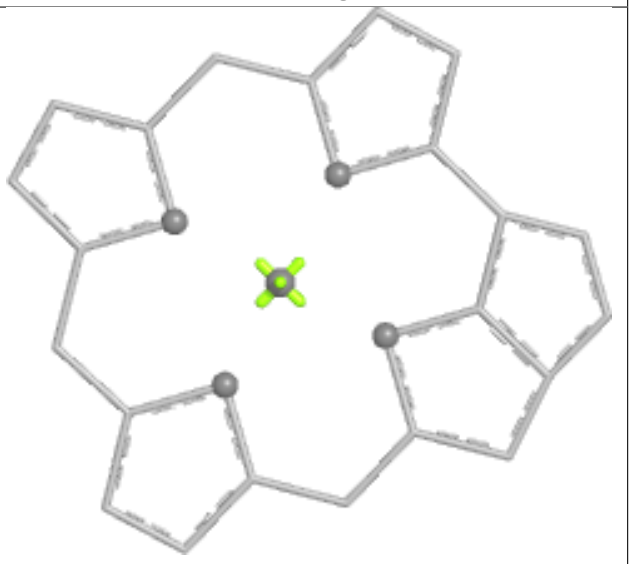
Bond lengths



Bond angles

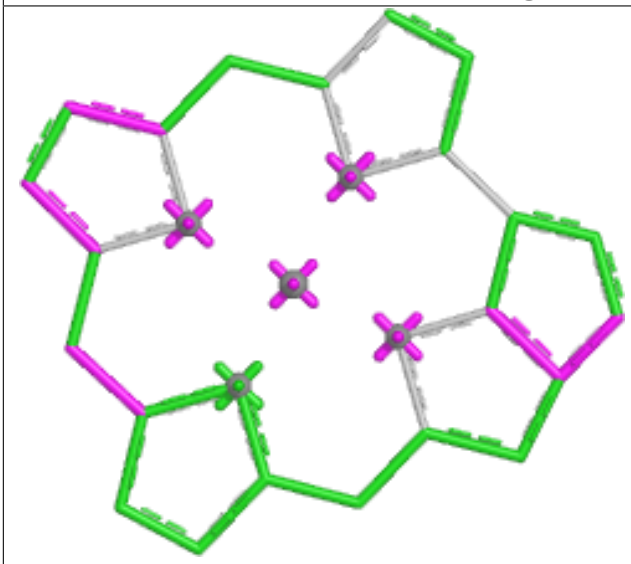


Torsions

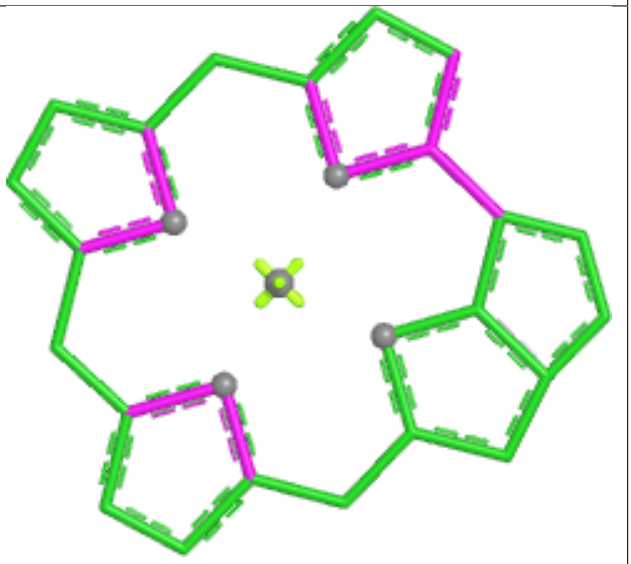


Rings

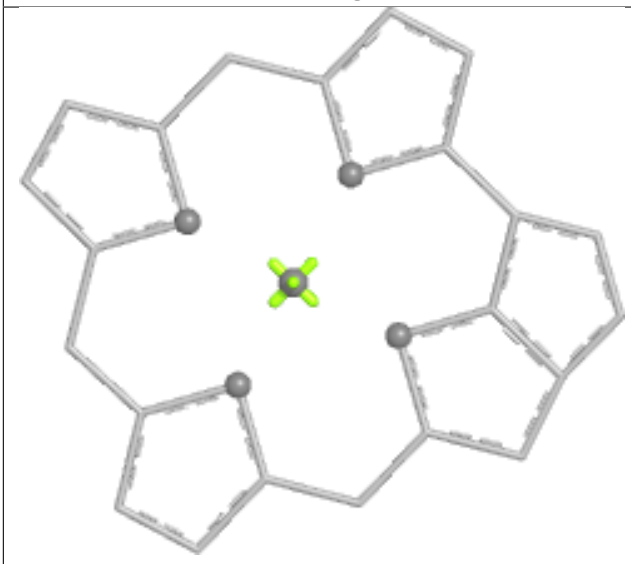
Ligand CLA M 160



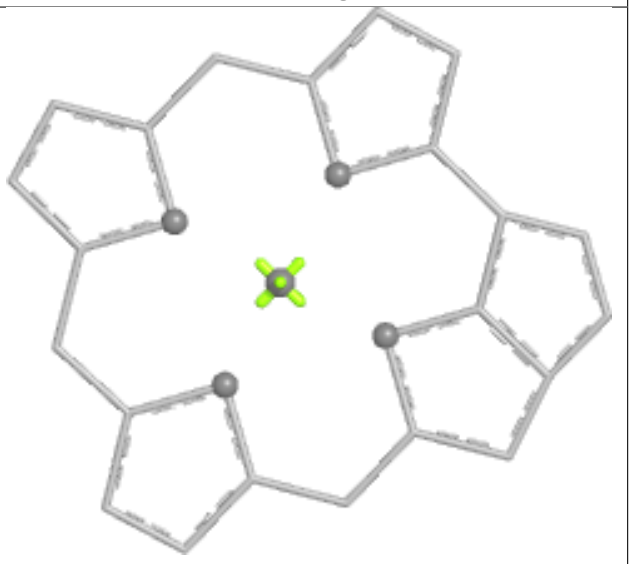
Bond lengths



Bond angles

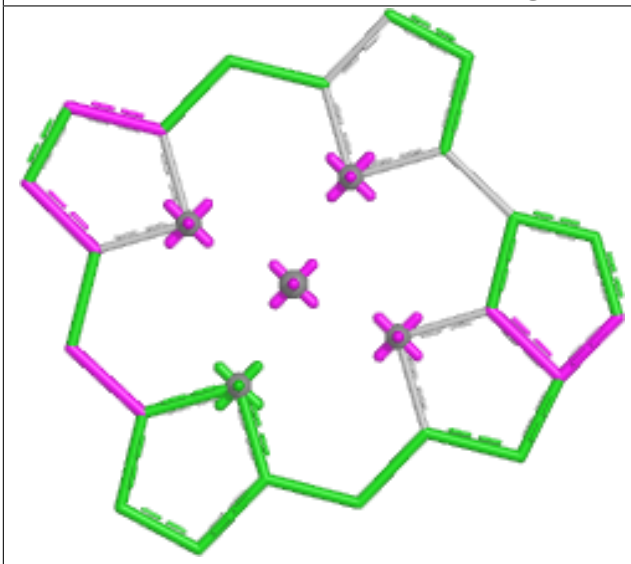


Torsions

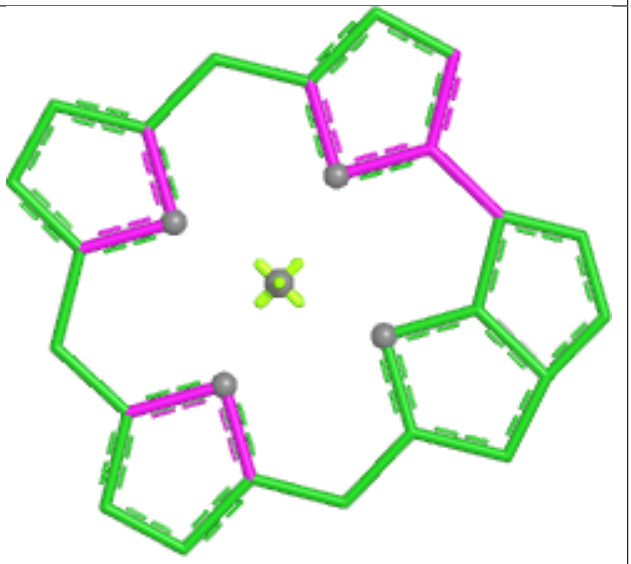


Rings

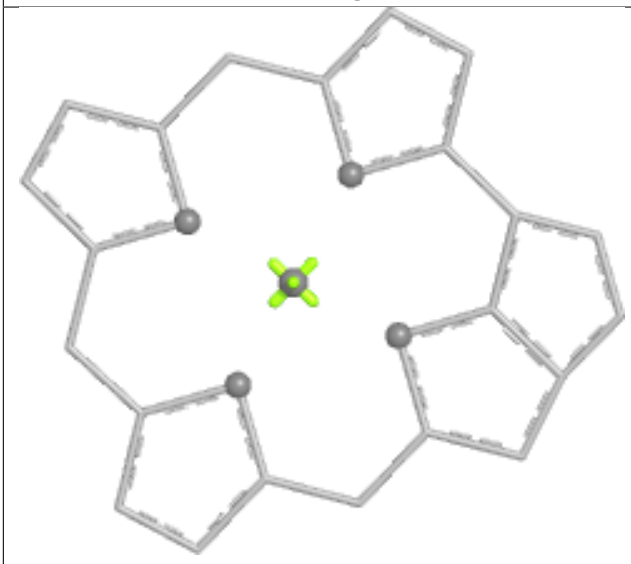
Ligand CLA C 164



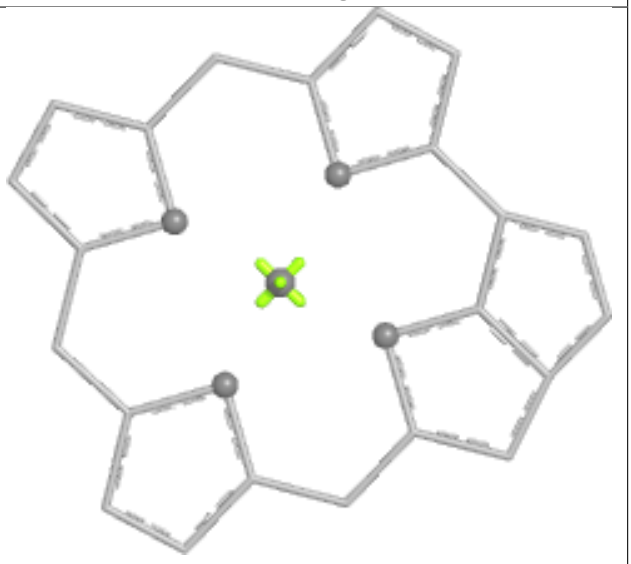
Bond lengths



Bond angles

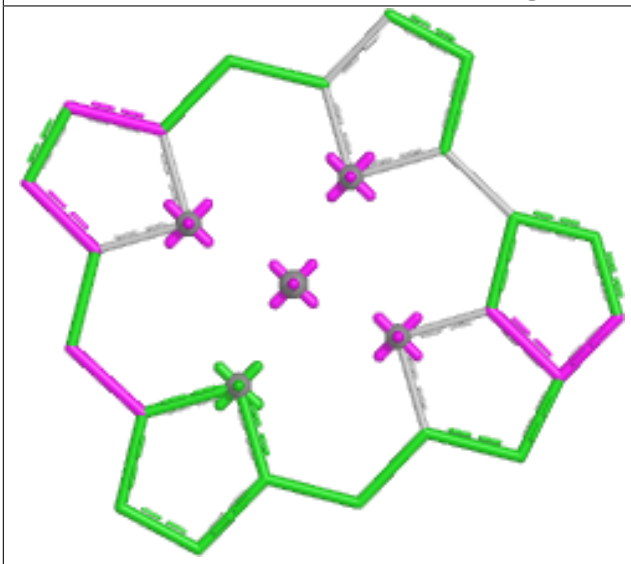


Torsions

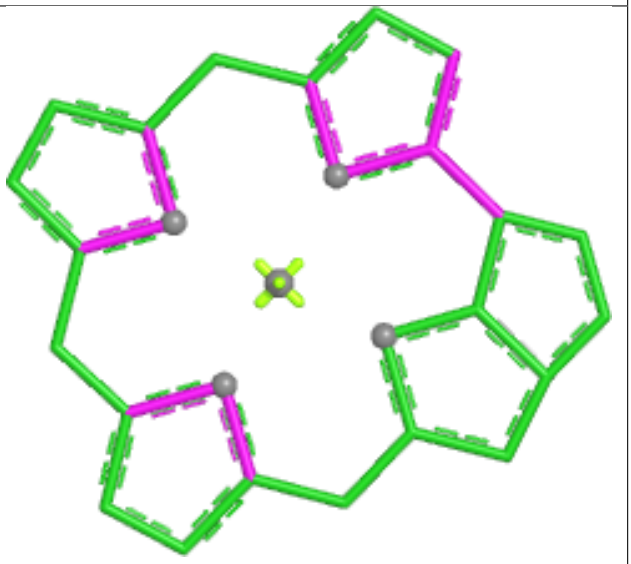


Rings

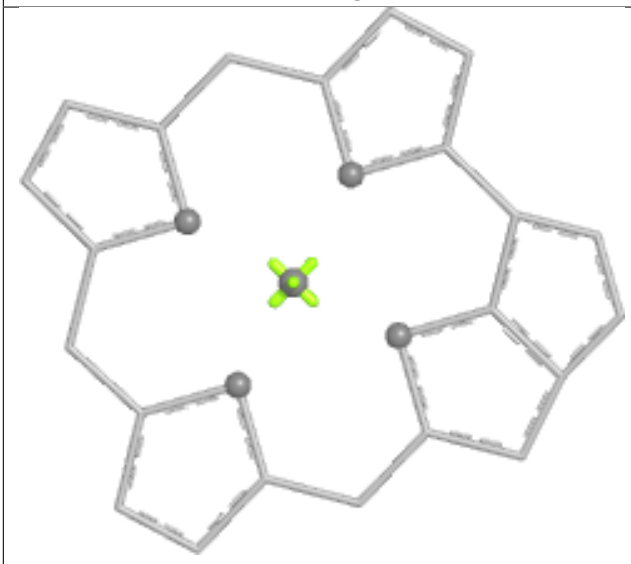
Ligand CLA D 169



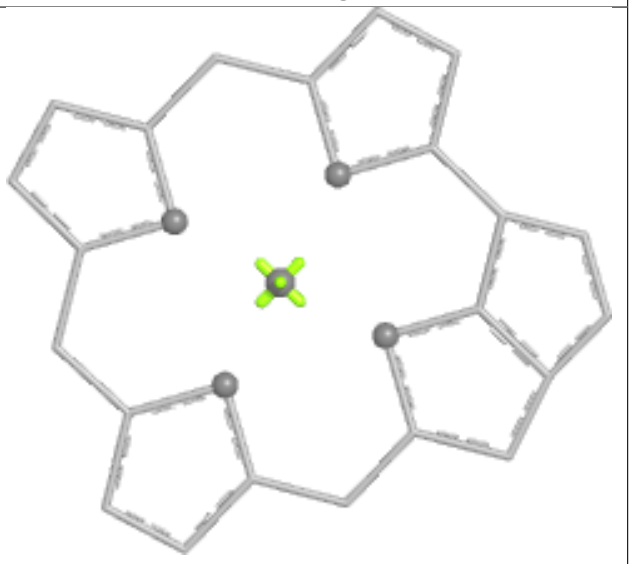
Bond lengths



Bond angles

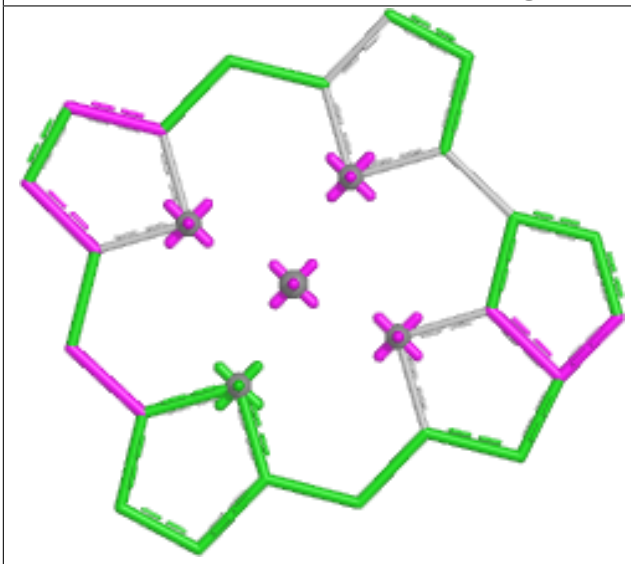


Torsions

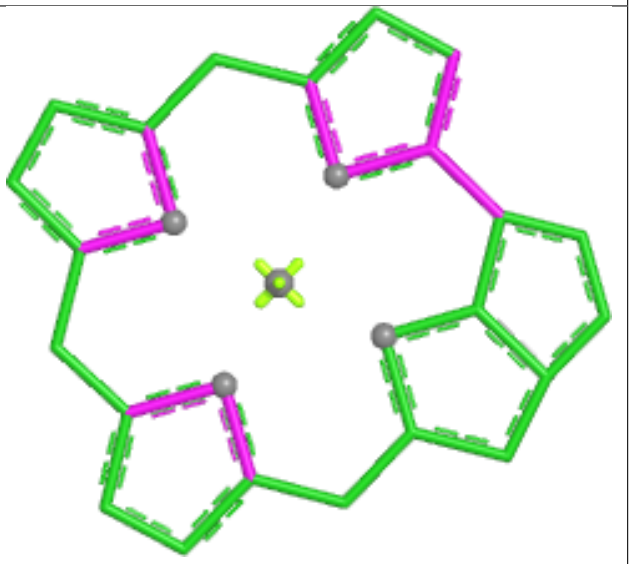


Rings

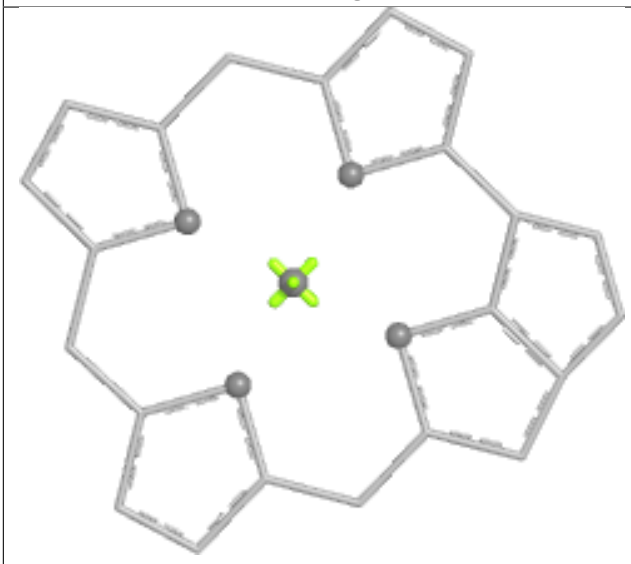
Ligand CLA M 157



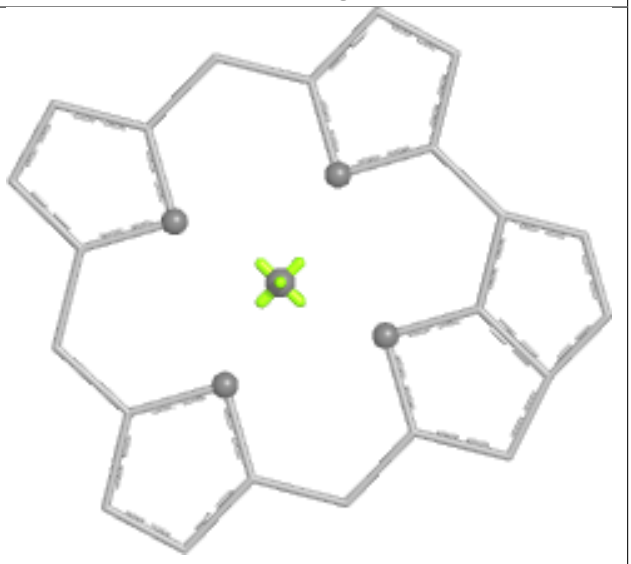
Bond lengths



Bond angles

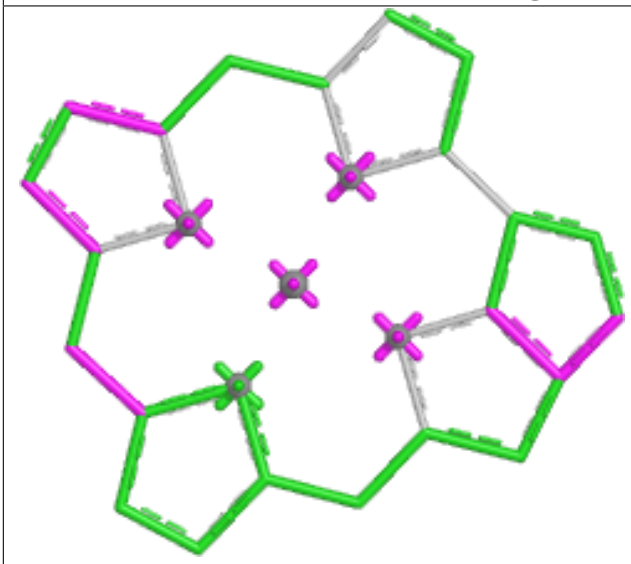


Torsions

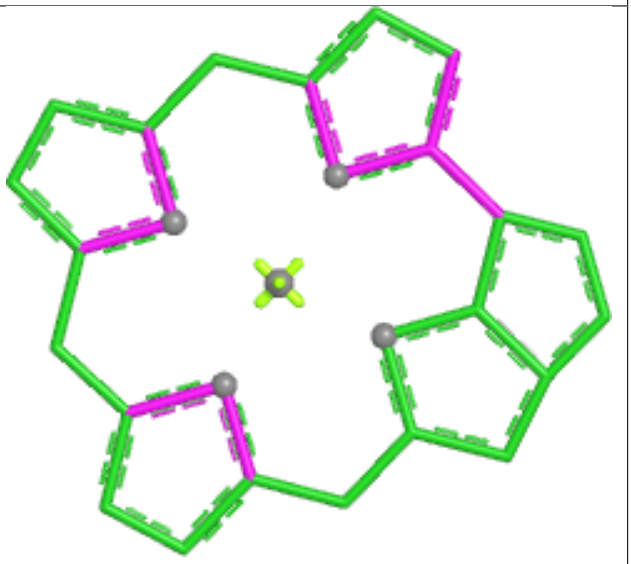


Rings

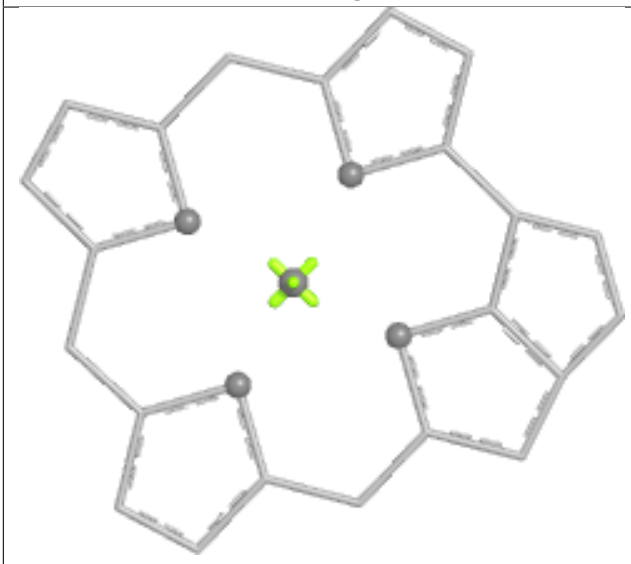
Ligand CLA L 160



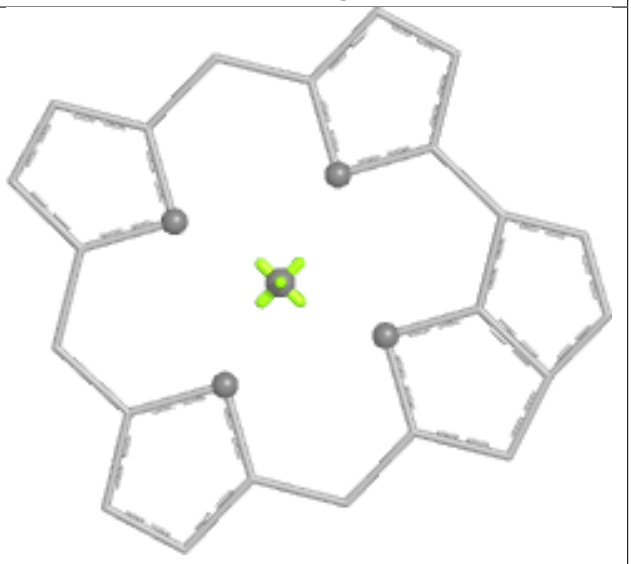
Bond lengths



Bond angles

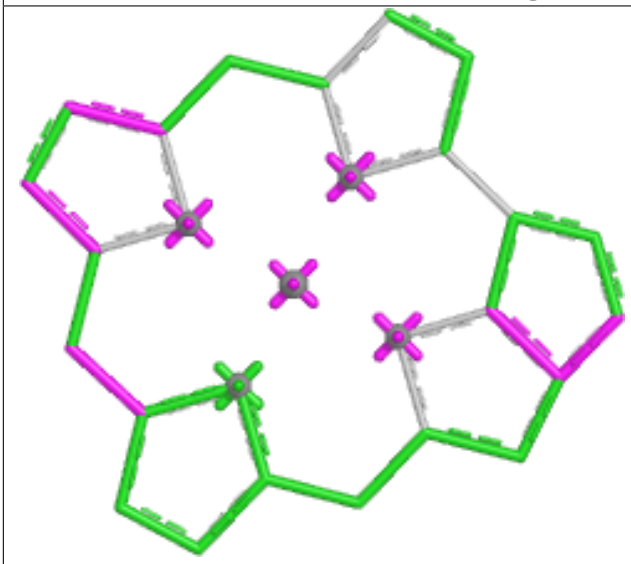


Torsions

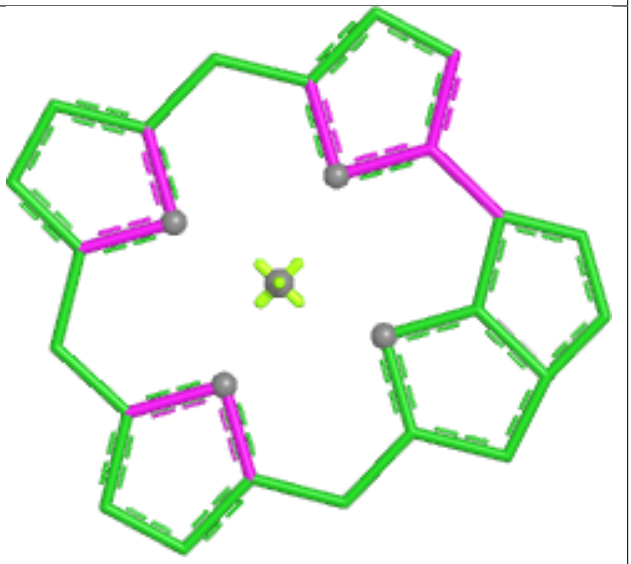


Rings

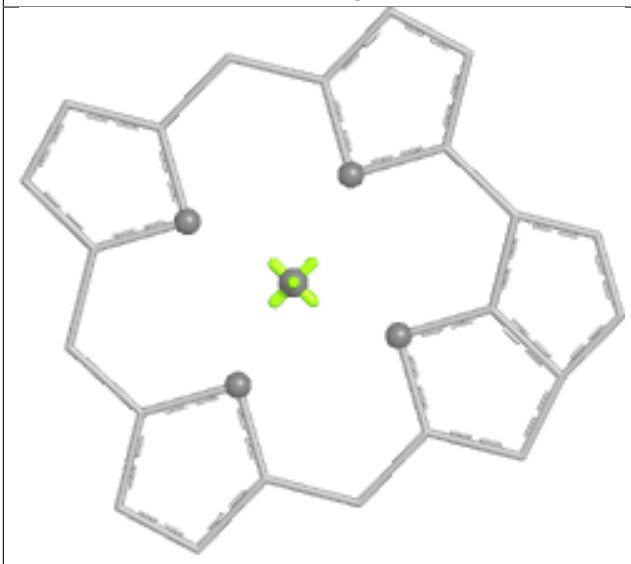
Ligand CLA C 162



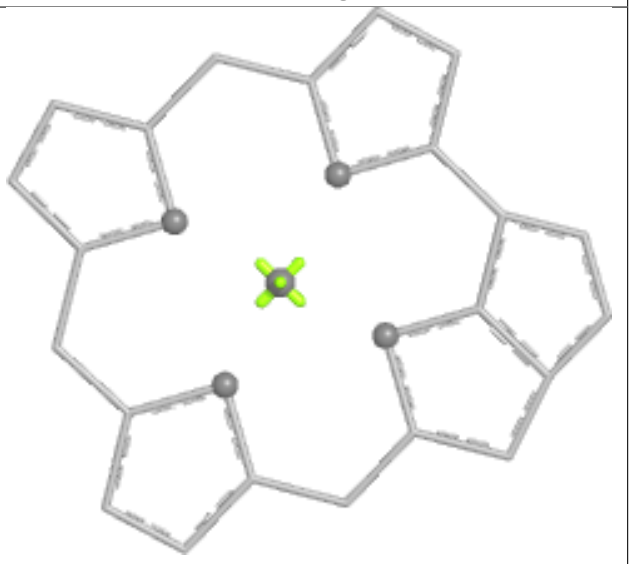
Bond lengths



Bond angles

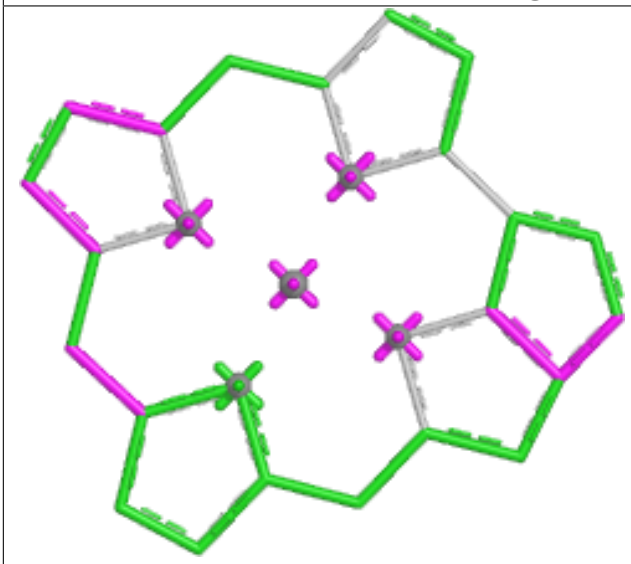


Torsions

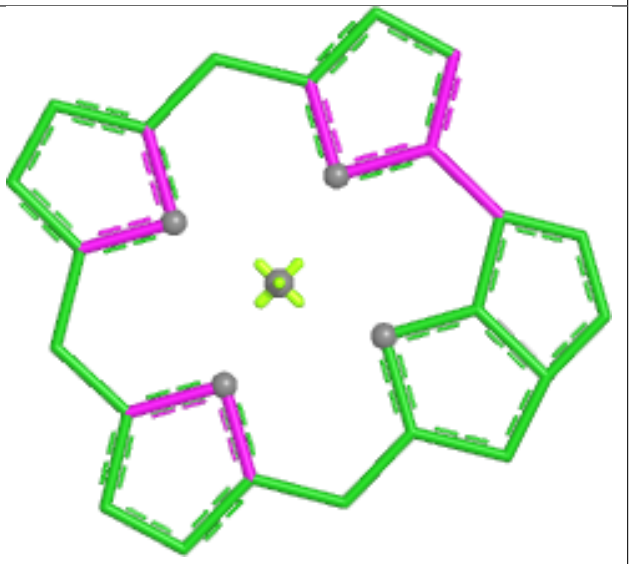


Rings

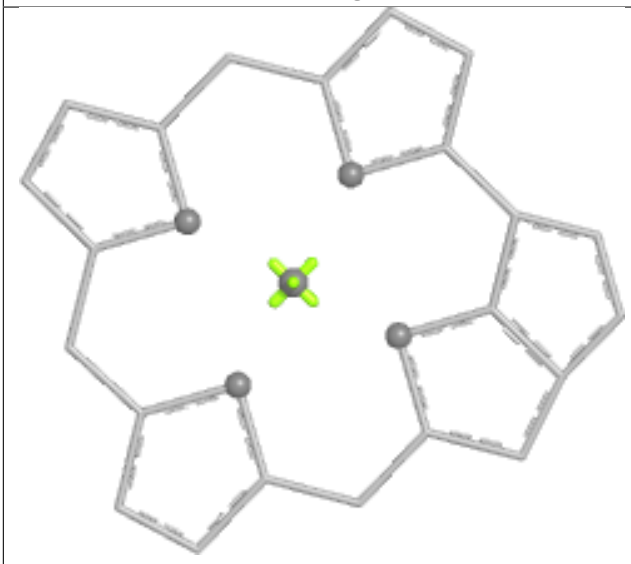
Ligand CLA L 166



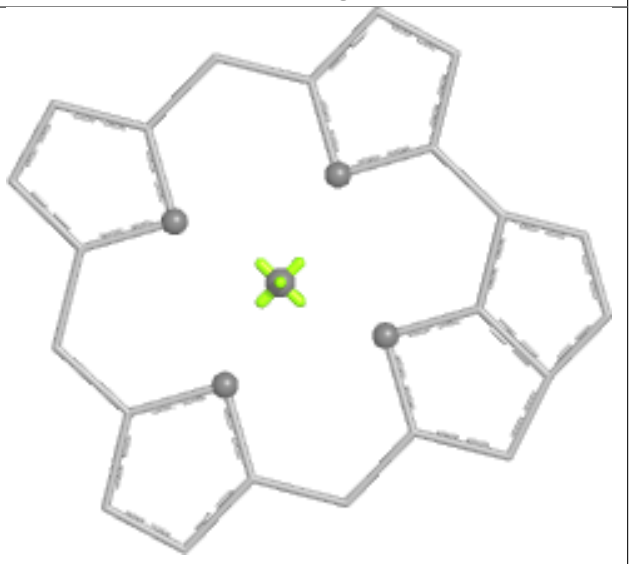
Bond lengths



Bond angles

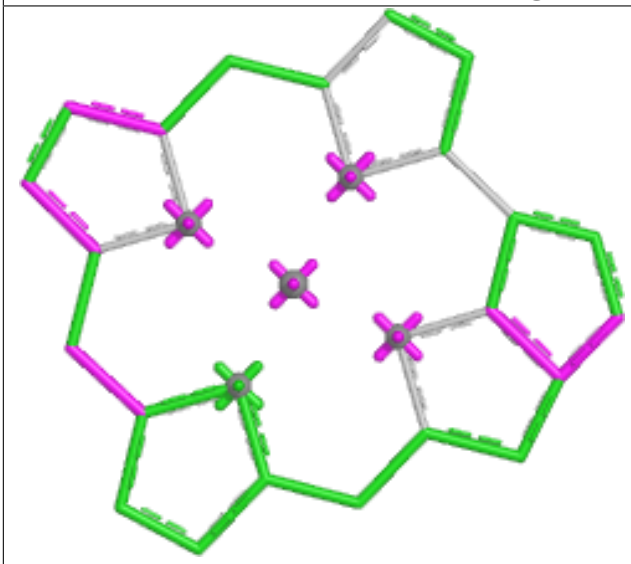


Torsions

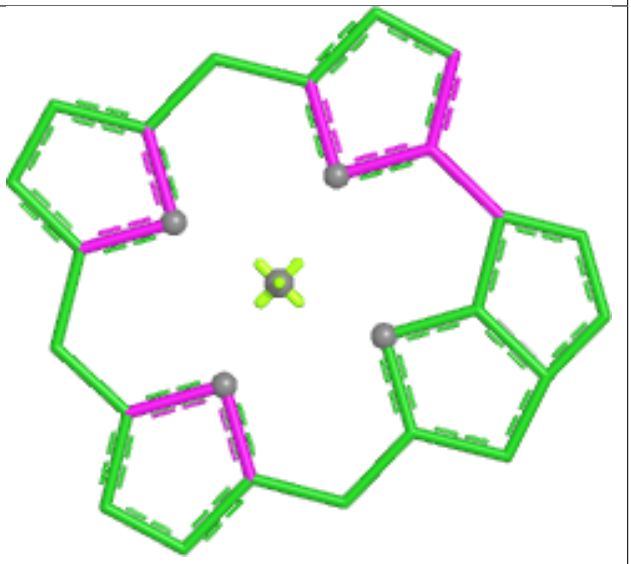


Rings

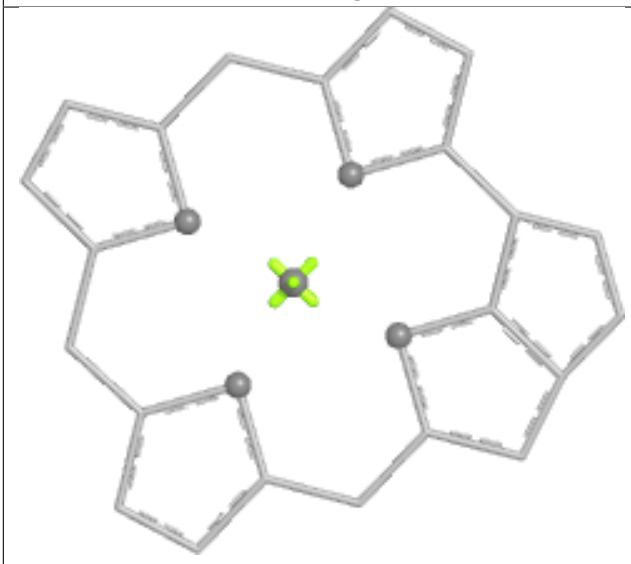
Ligand CLA J 175



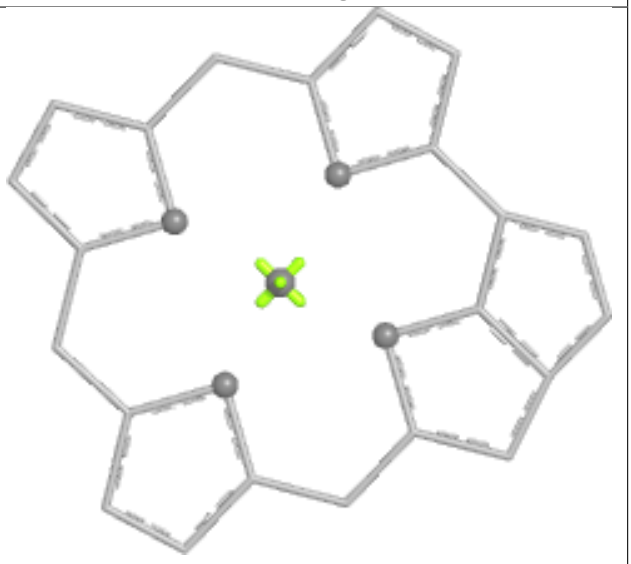
Bond lengths



Bond angles

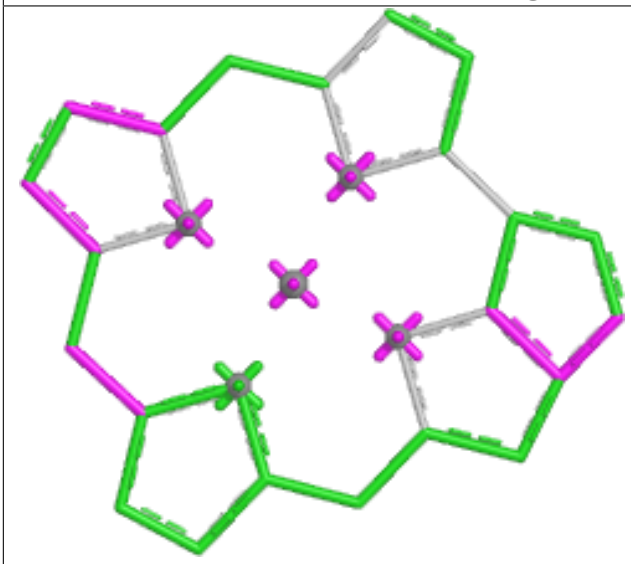


Torsions

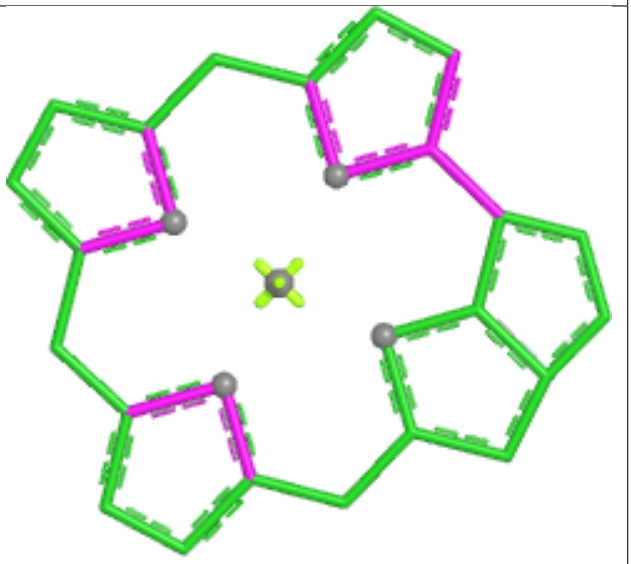


Rings

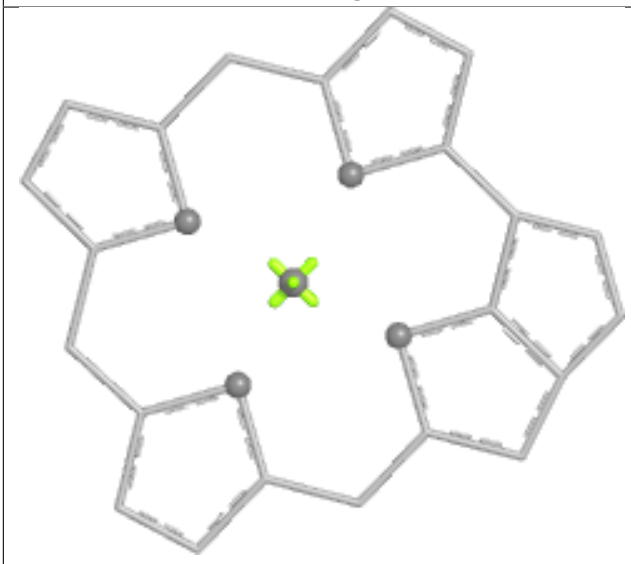
Ligand CLA C 161



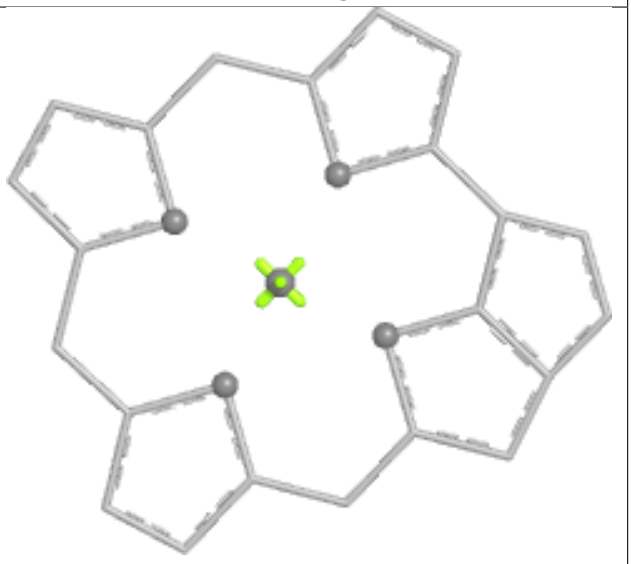
Bond lengths



Bond angles

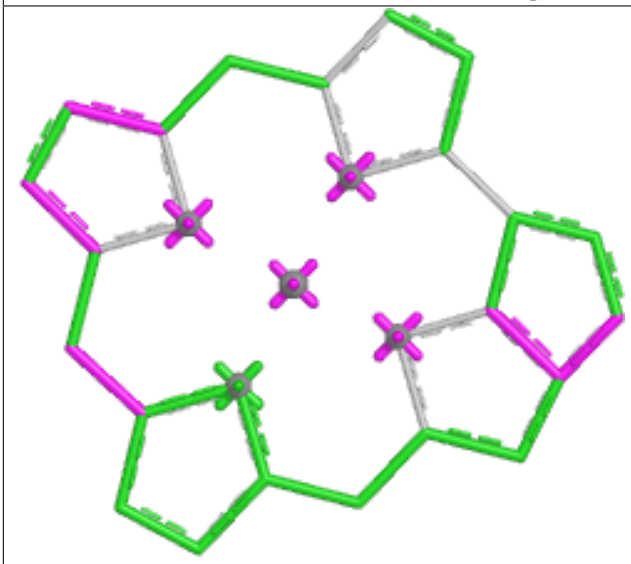


Torsions

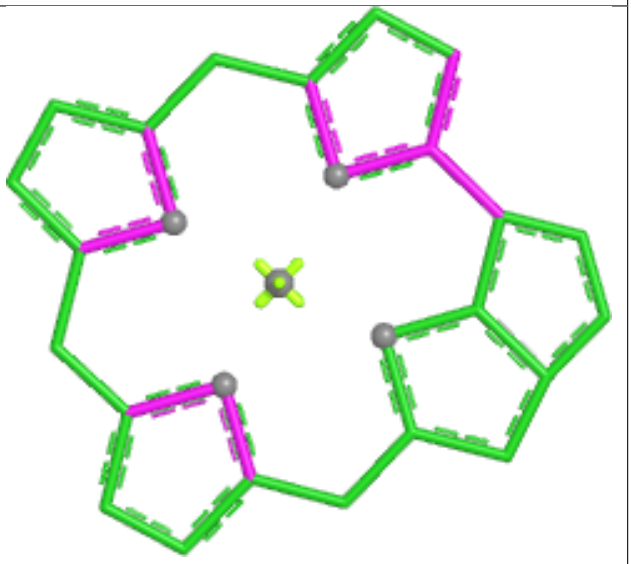


Rings

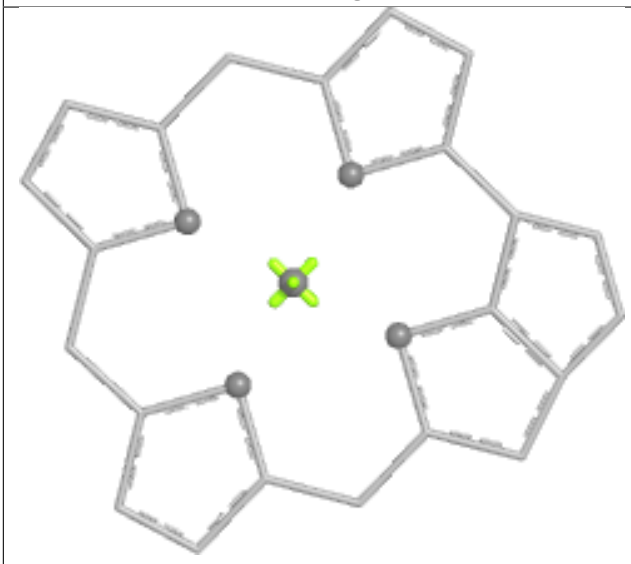
Ligand CLA C 166



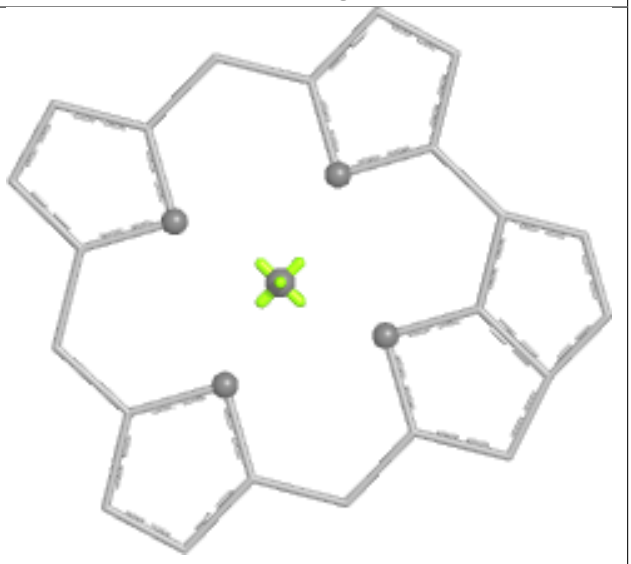
Bond lengths



Bond angles

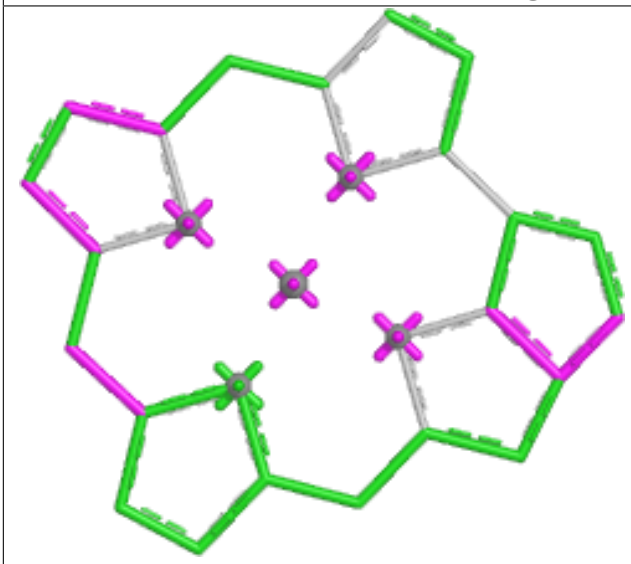


Torsions

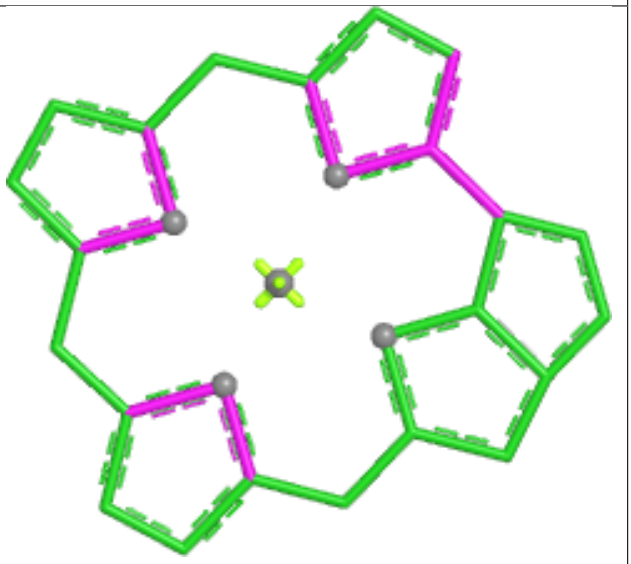


Rings

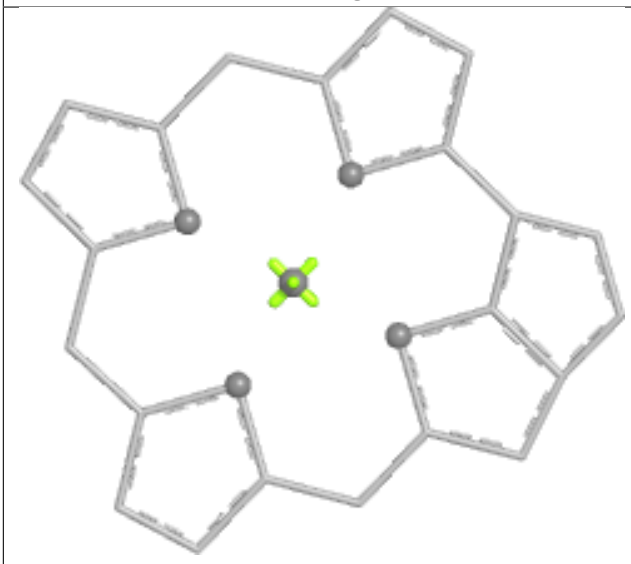
Ligand CLA B 178



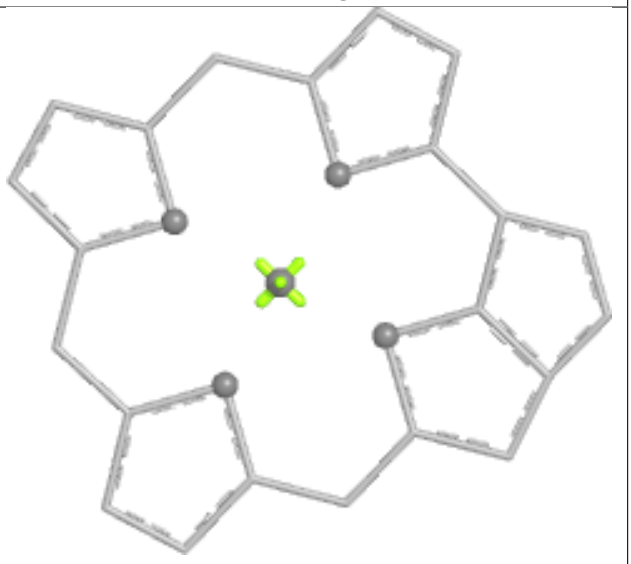
Bond lengths



Bond angles

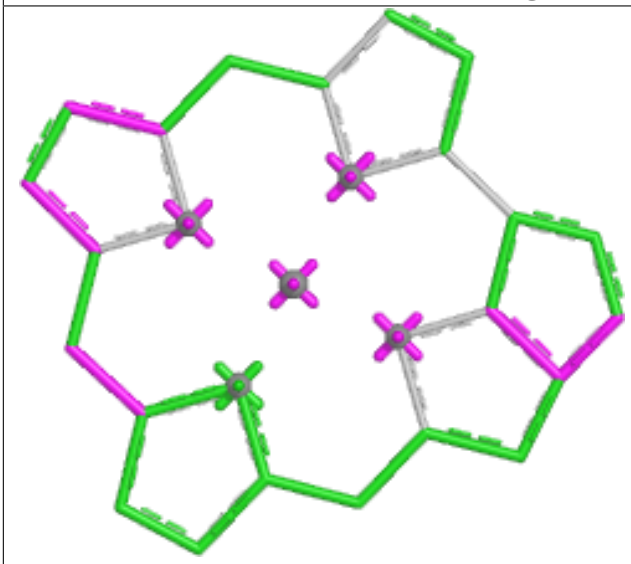


Torsions

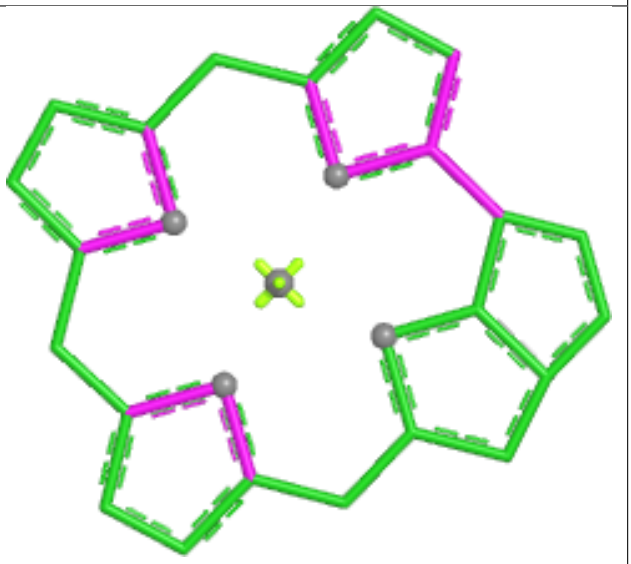


Rings

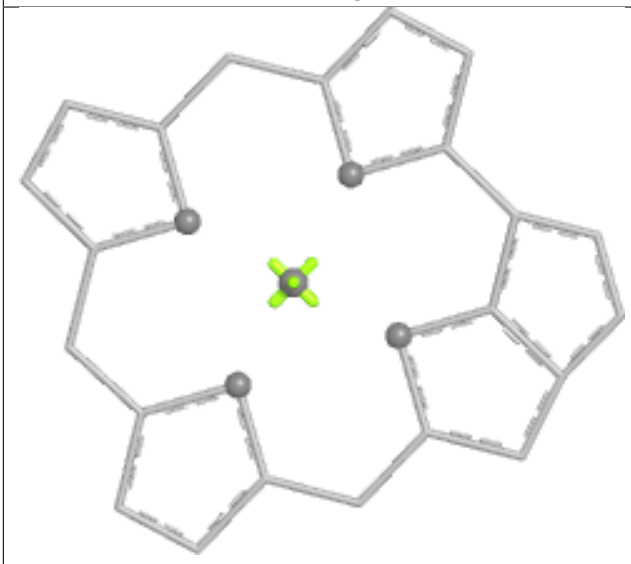
Ligand CLA D 158



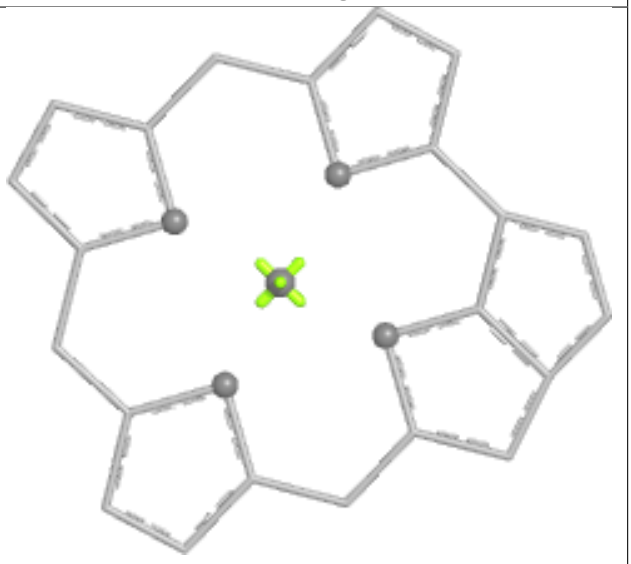
Bond lengths



Bond angles

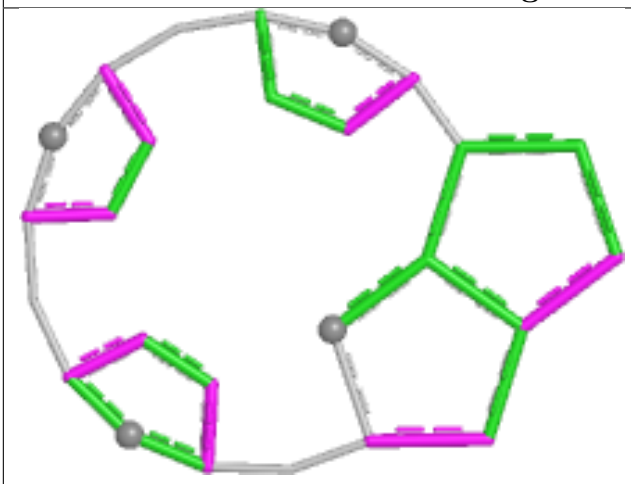


Torsions

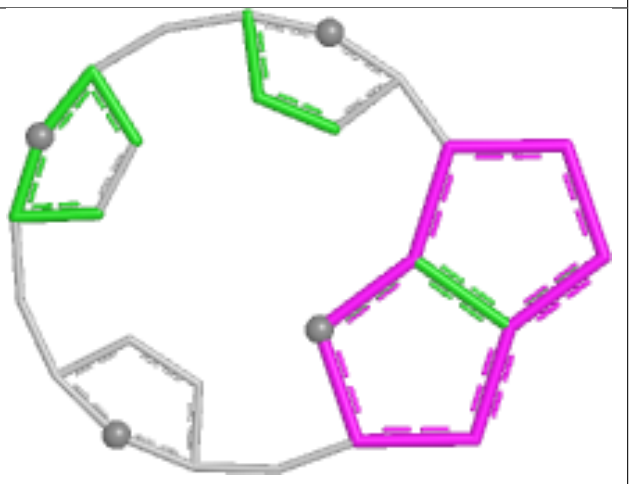


Rings

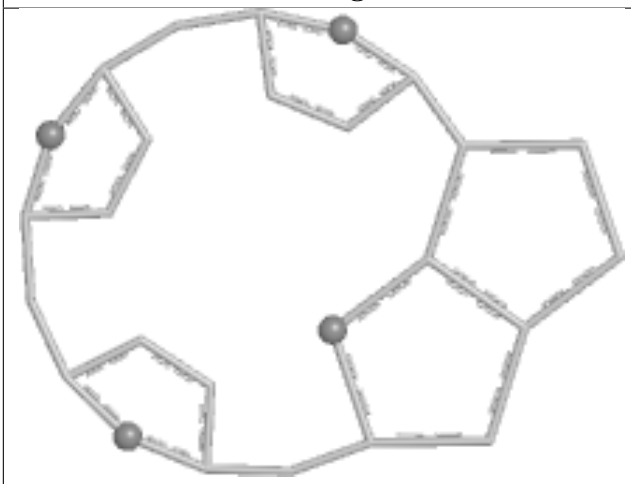
Ligand PHO A 177



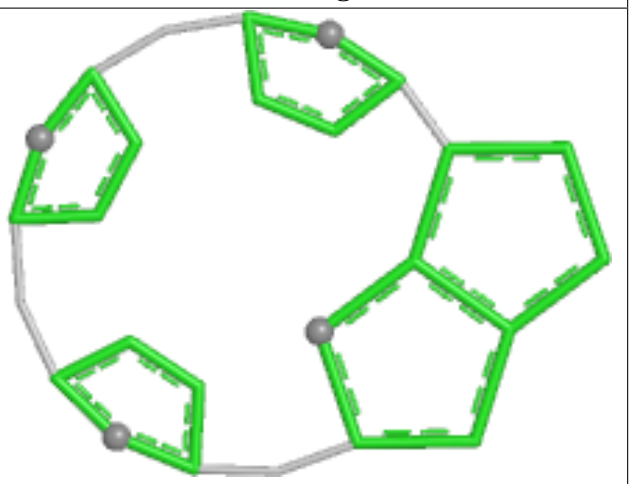
Bond lengths



Bond angles

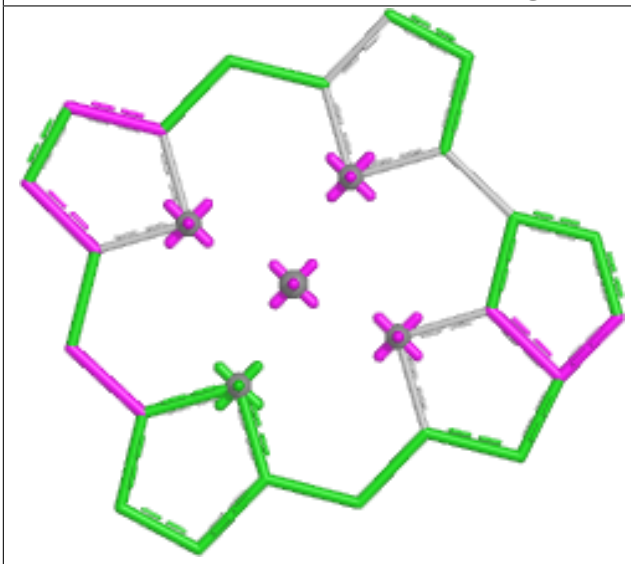


Torsions

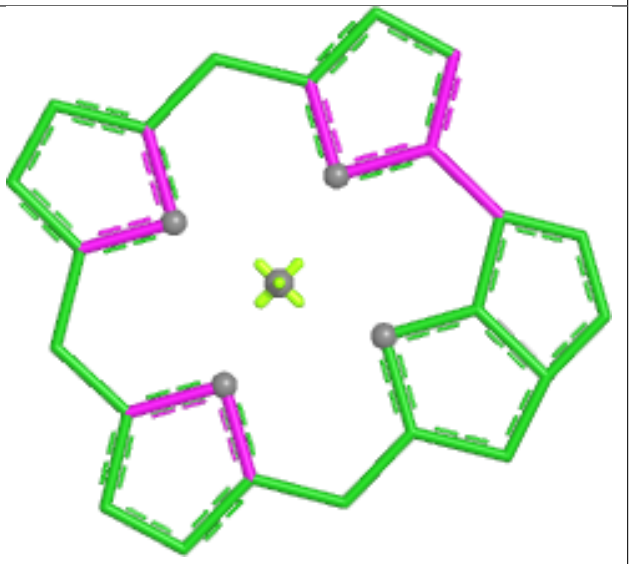


Rings

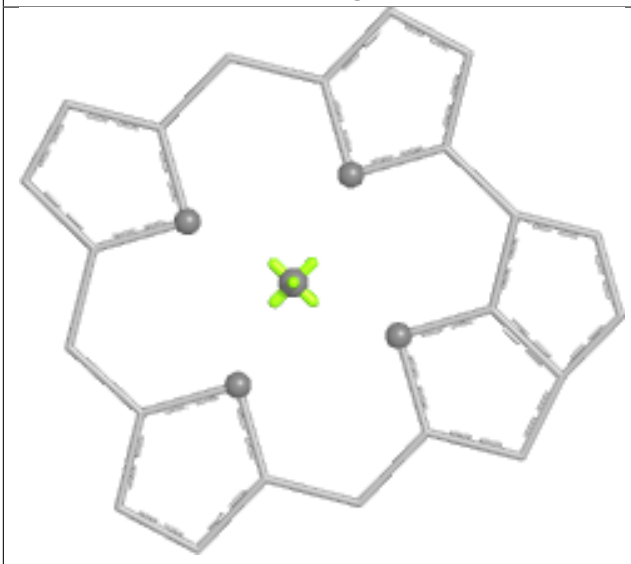
Ligand CLA C 159



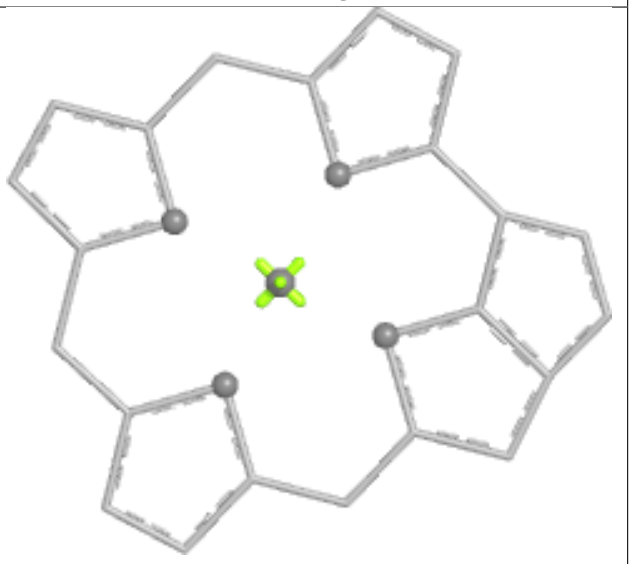
Bond lengths



Bond angles

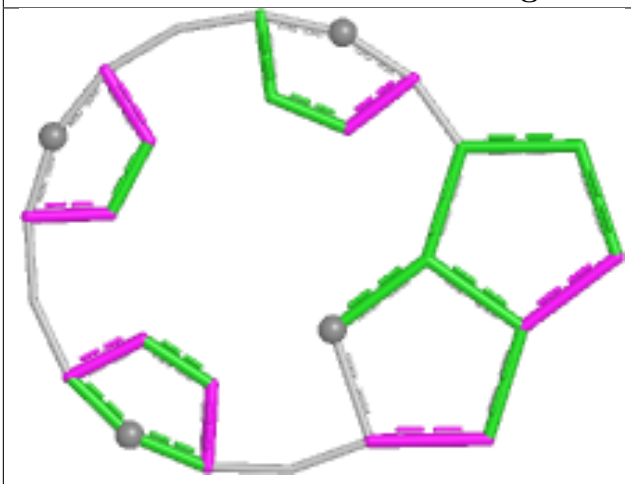


Torsions

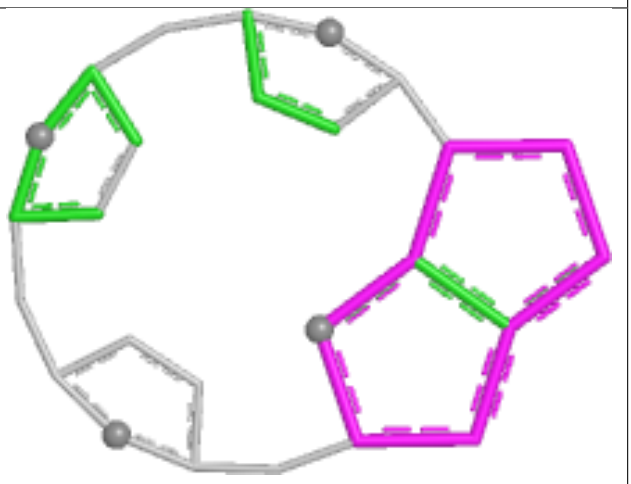


Rings

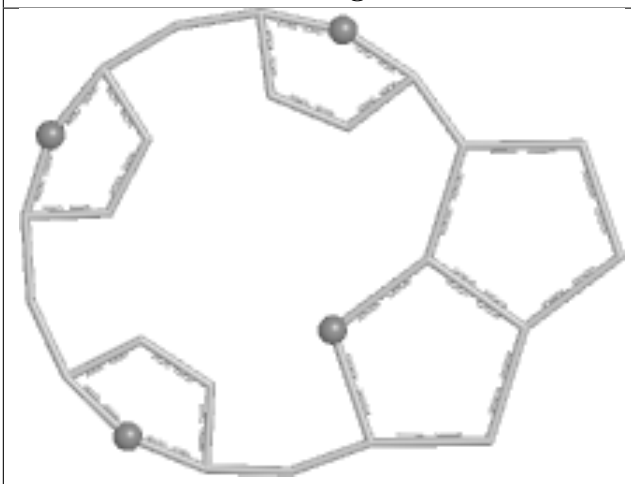
Ligand PHO K 177



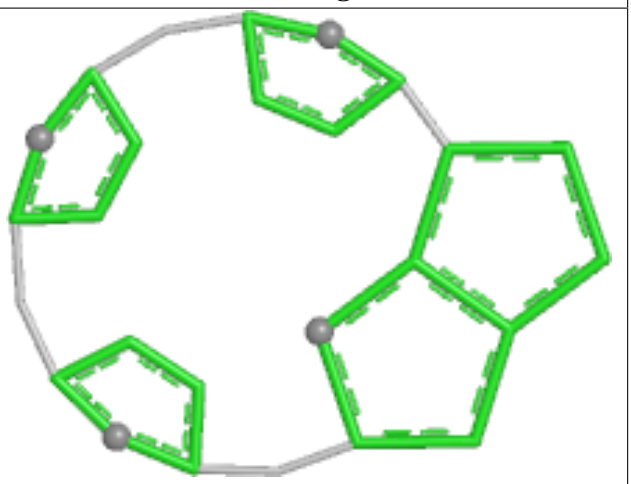
Bond lengths



Bond angles

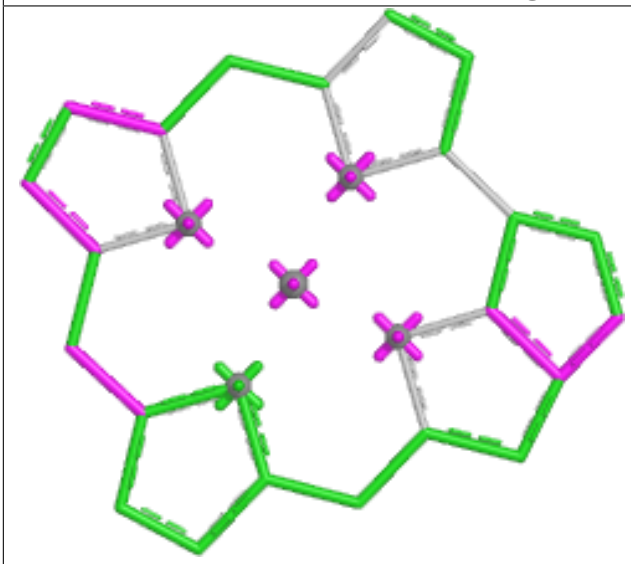


Torsions

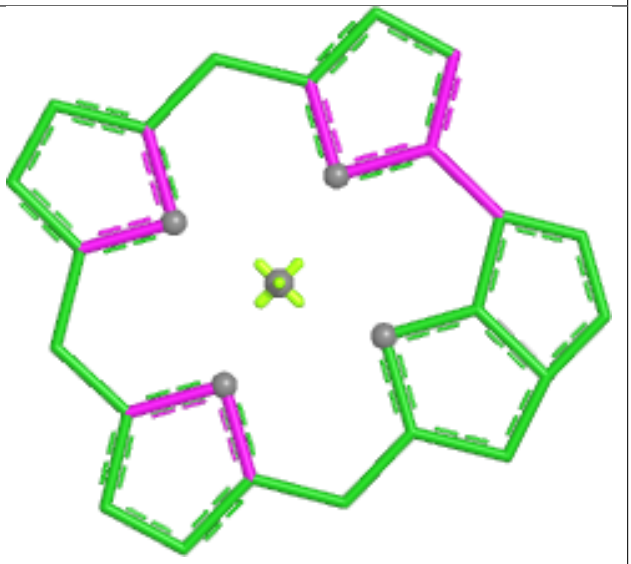


Rings

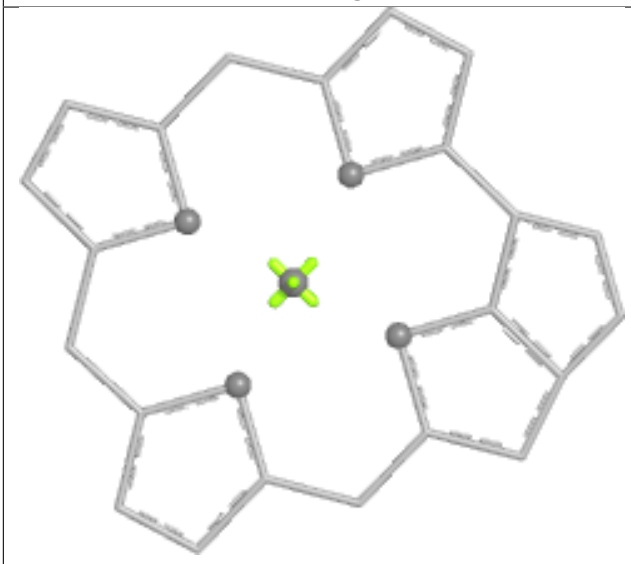
Ligand CLA A 179



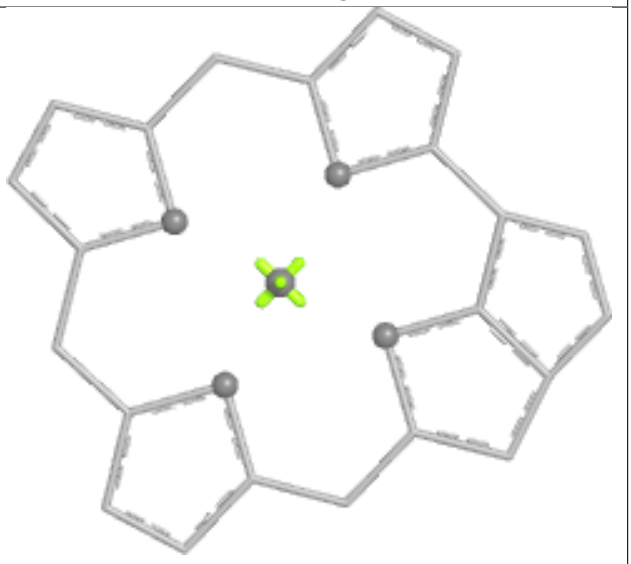
Bond lengths



Bond angles

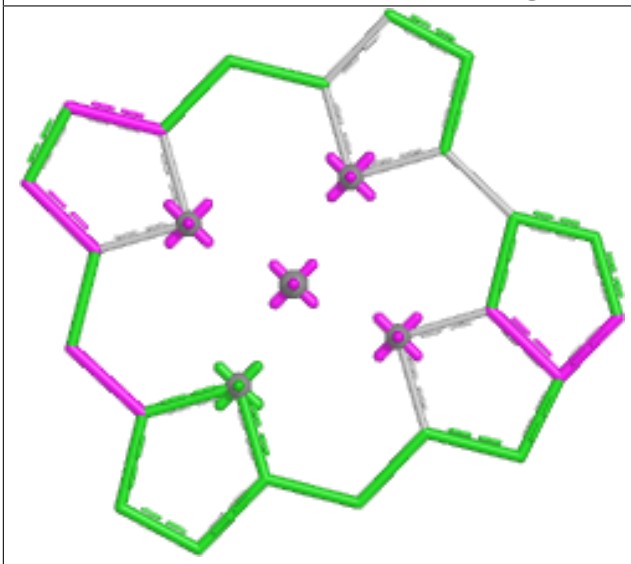


Torsions

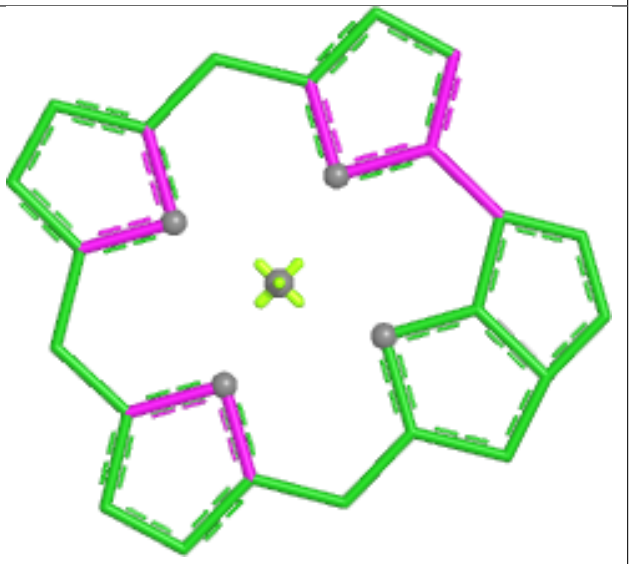


Rings

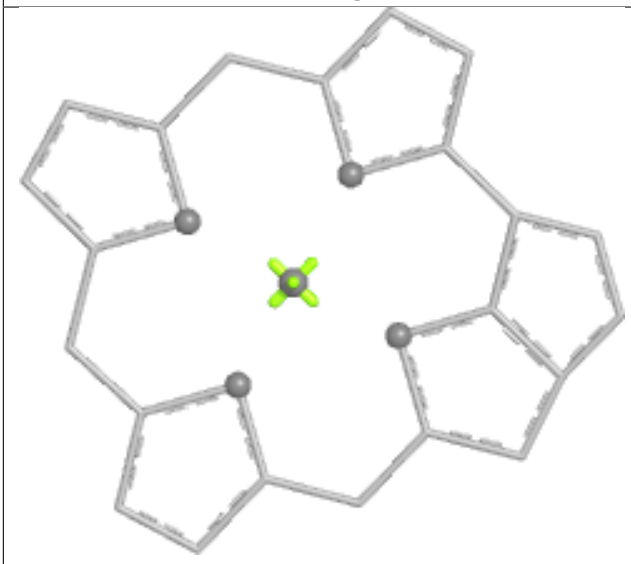
Ligand CLA D 170



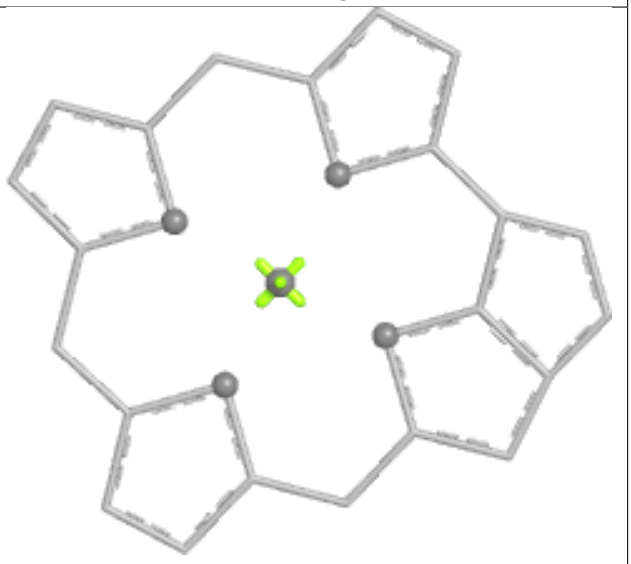
Bond lengths



Bond angles

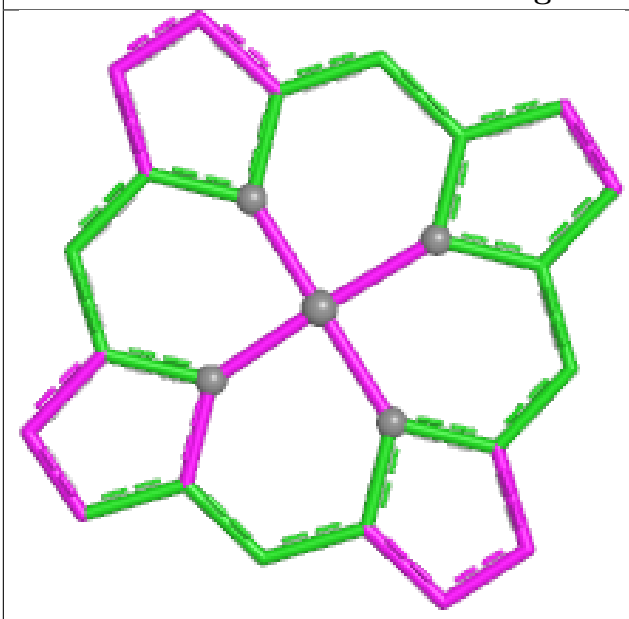


Torsions

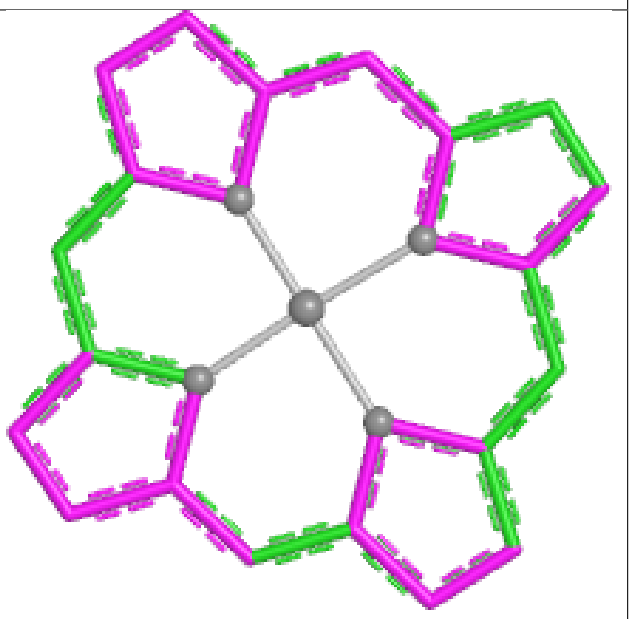


Rings

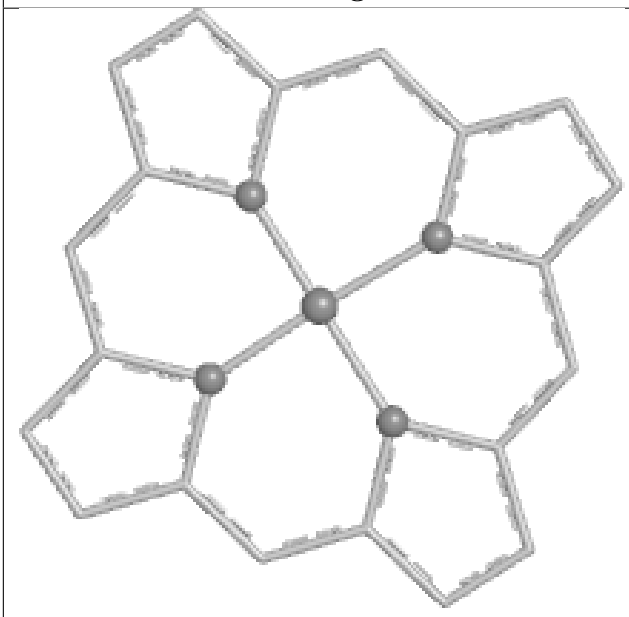
Ligand HEM I 88



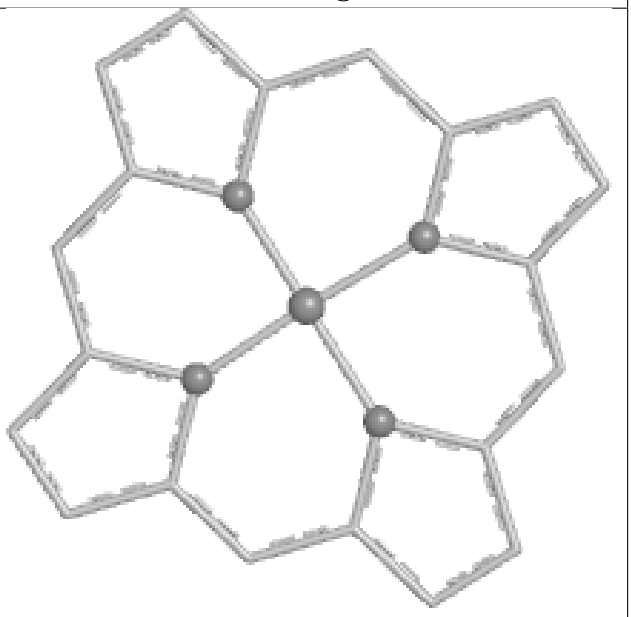
Bond lengths



Bond angles

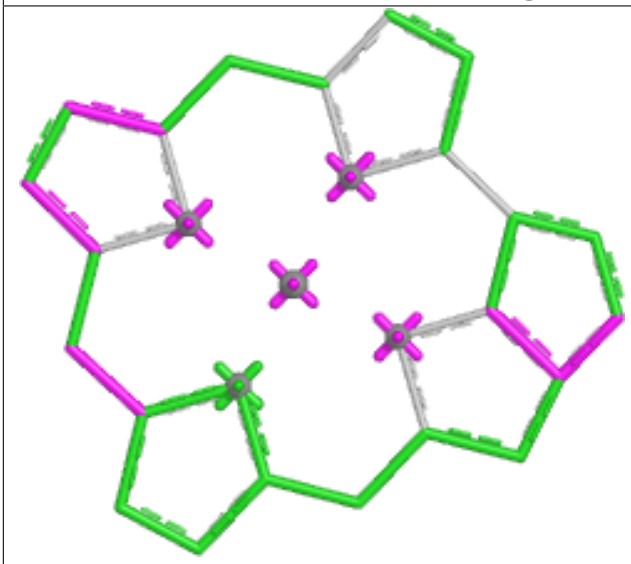


Torsions

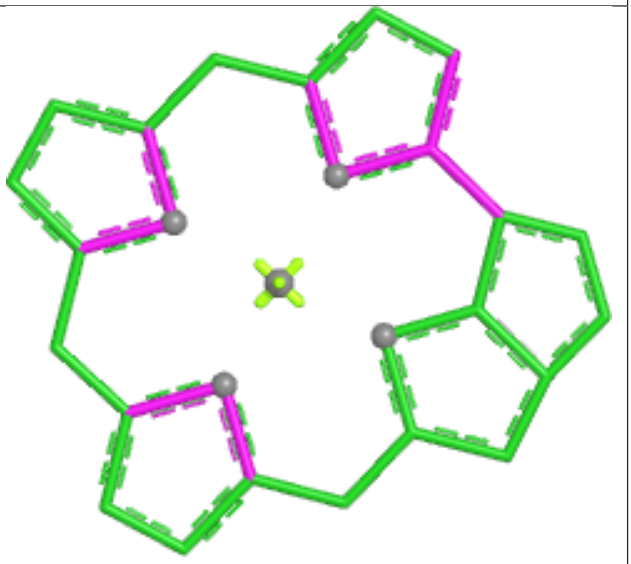


Rings

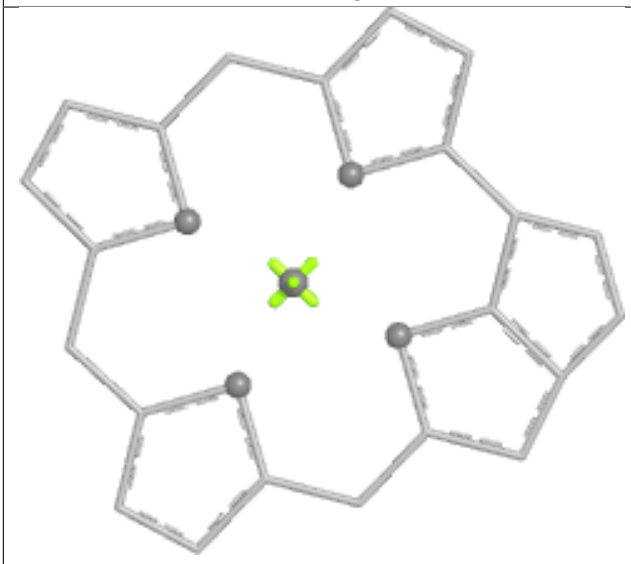
Ligand CLA M 158



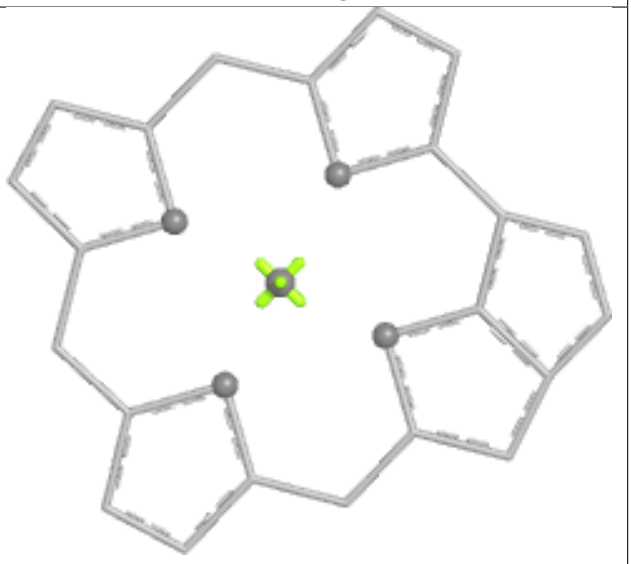
Bond lengths



Bond angles

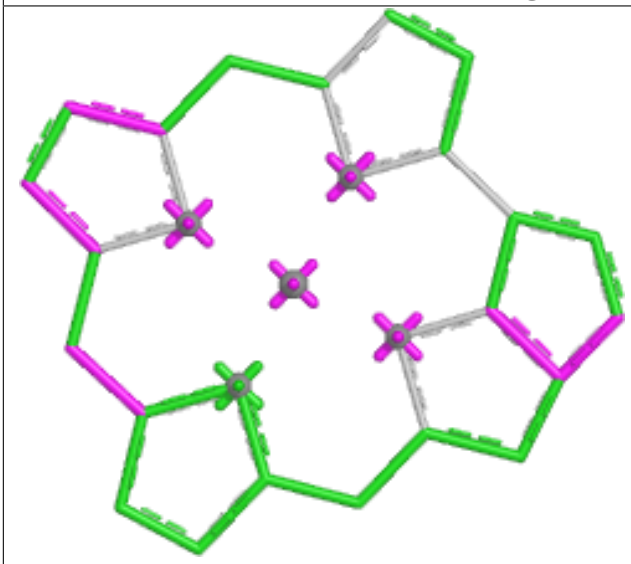


Torsions

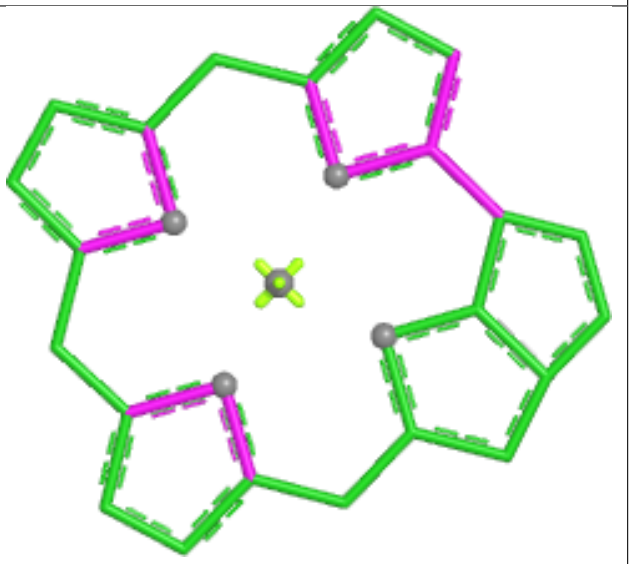


Rings

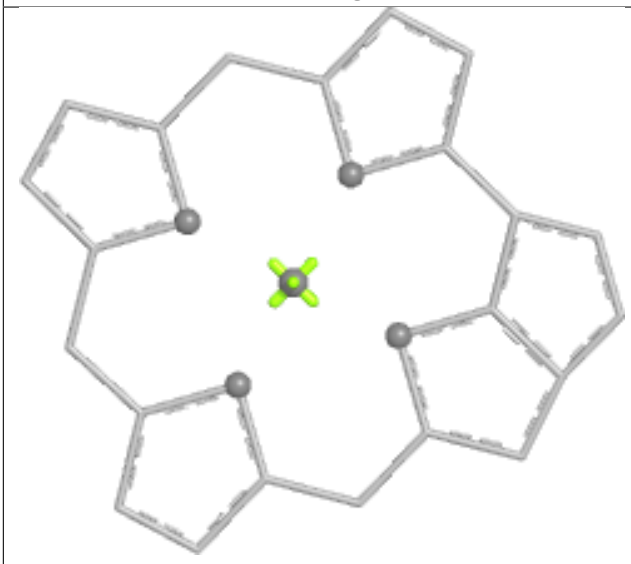
Ligand CLA D 162



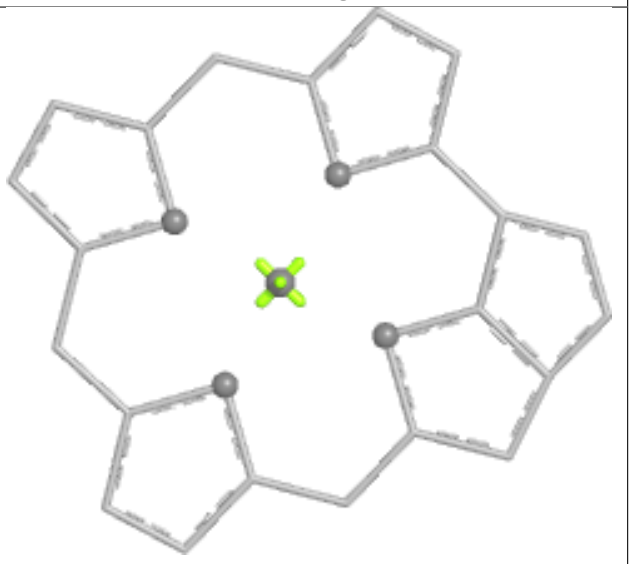
Bond lengths



Bond angles

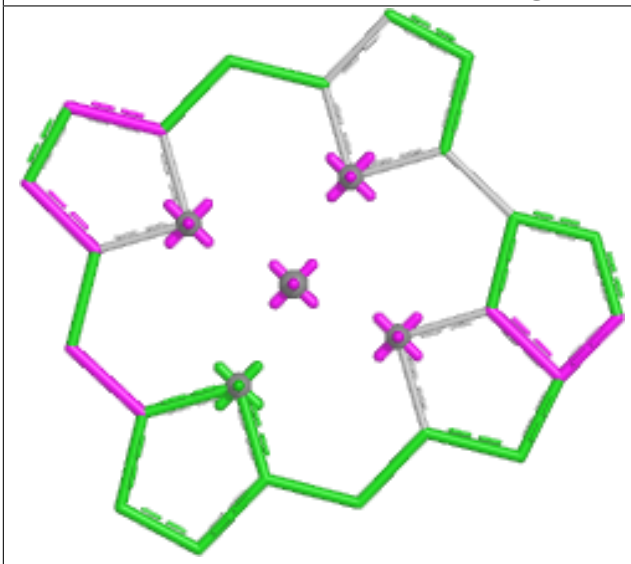


Torsions

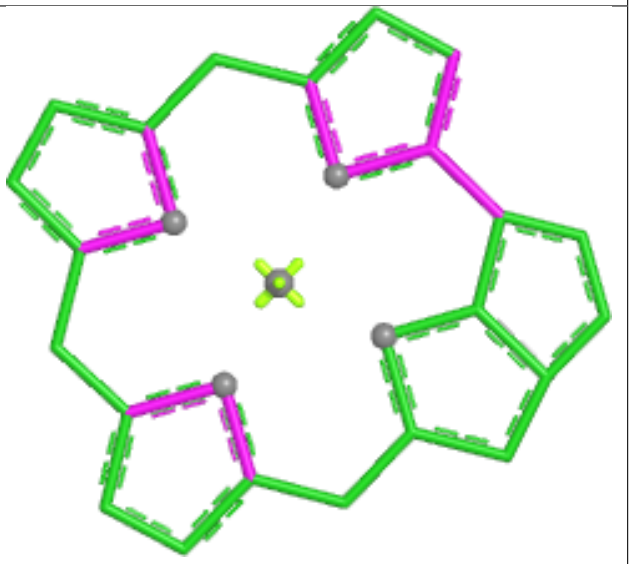


Rings

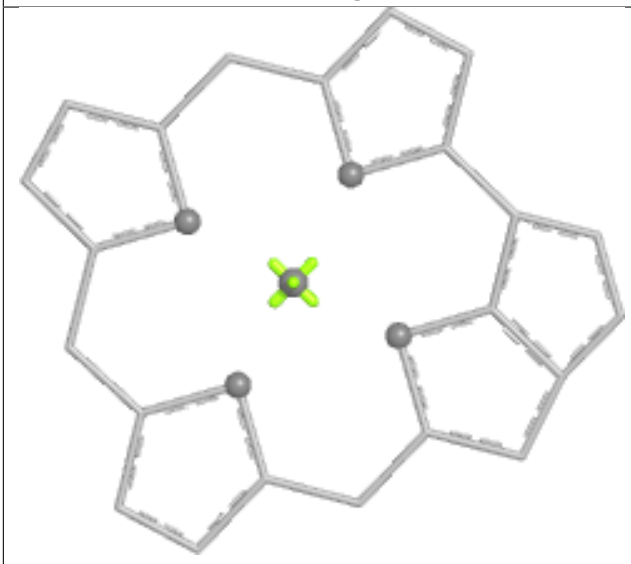
Ligand CLA J 176



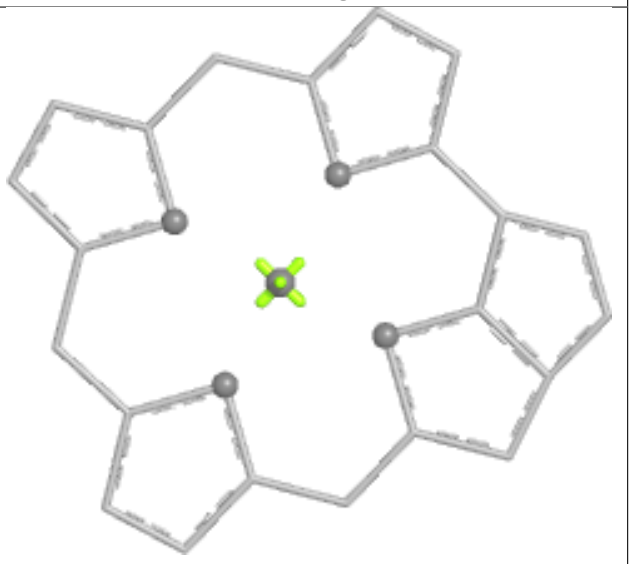
Bond lengths



Bond angles

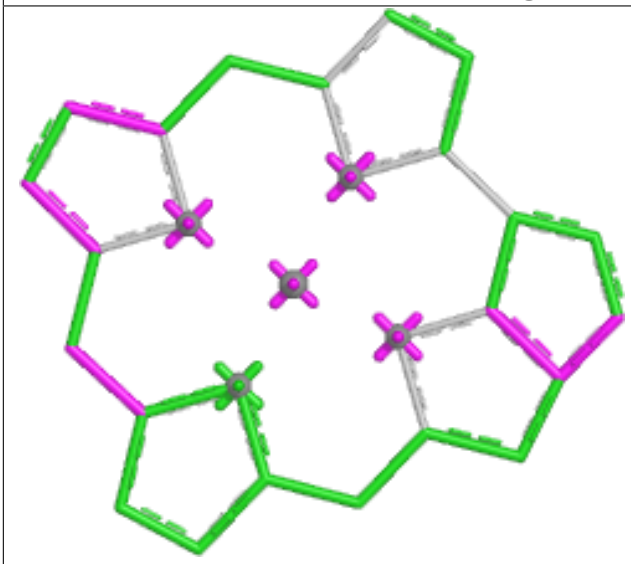


Torsions

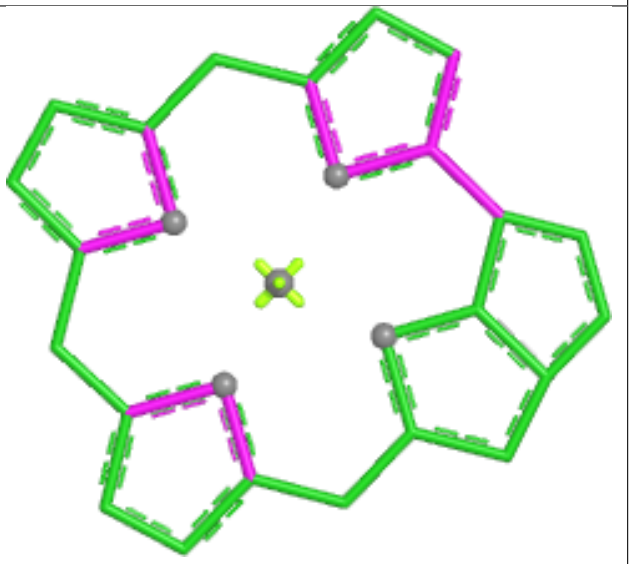


Rings

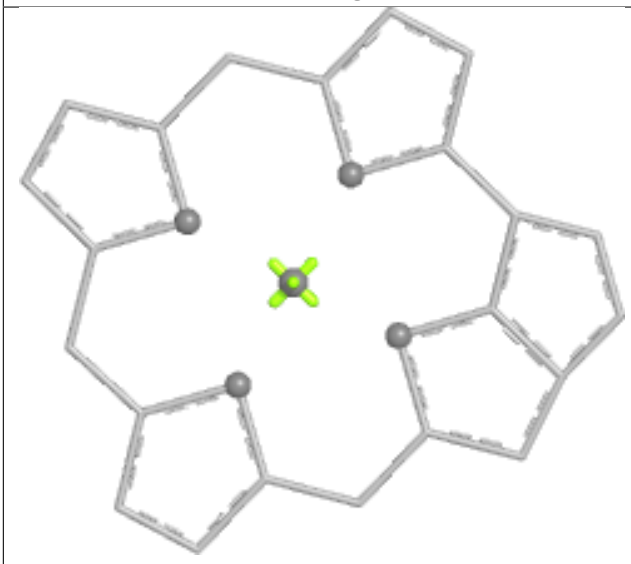
Ligand CLA M 167



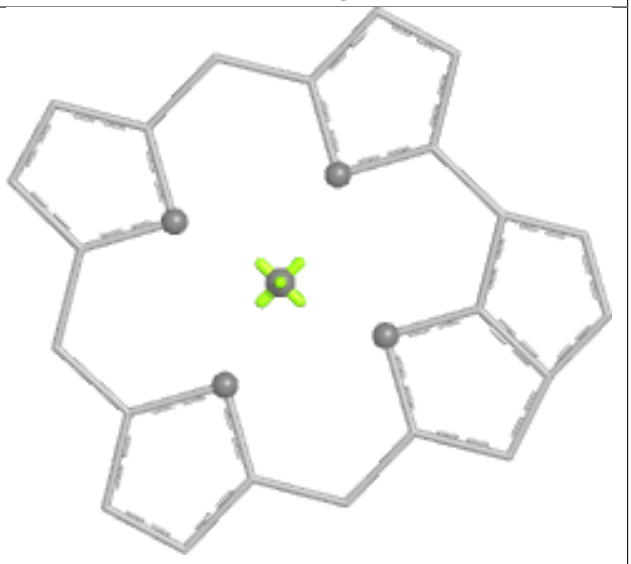
Bond lengths



Bond angles

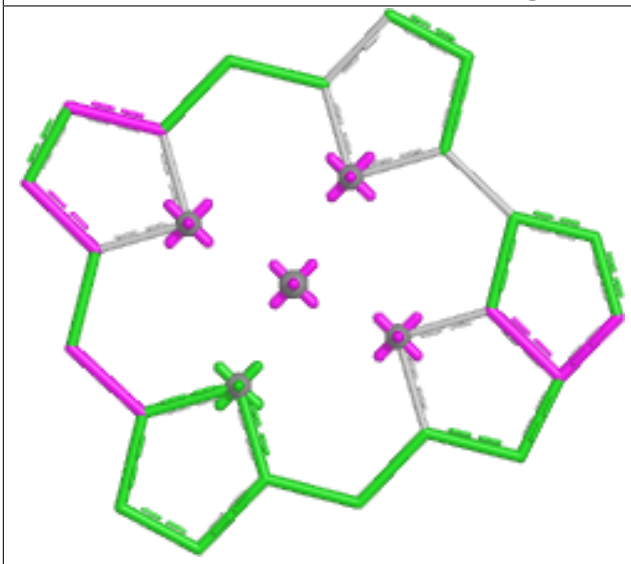


Torsions

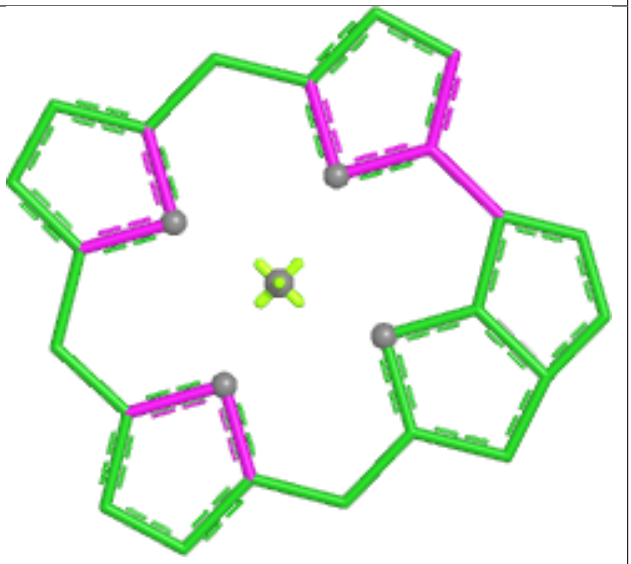


Rings

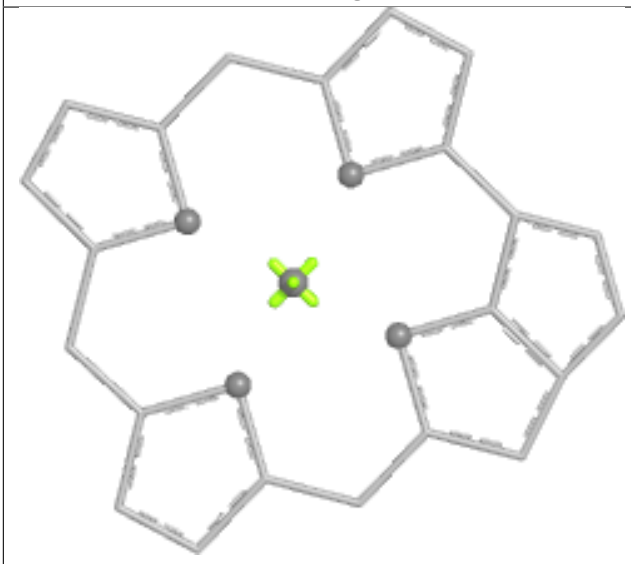
Ligand CLA A 178



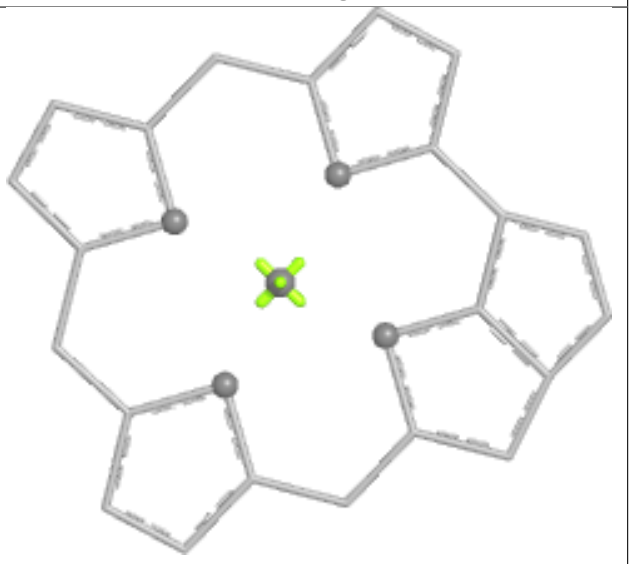
Bond lengths



Bond angles

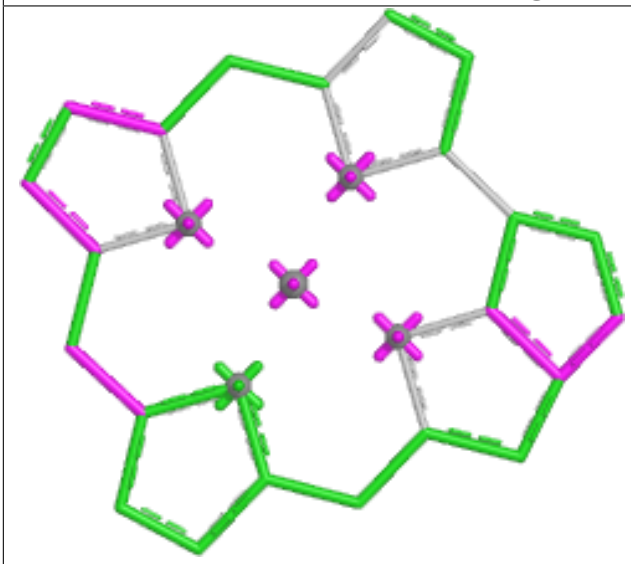


Torsions

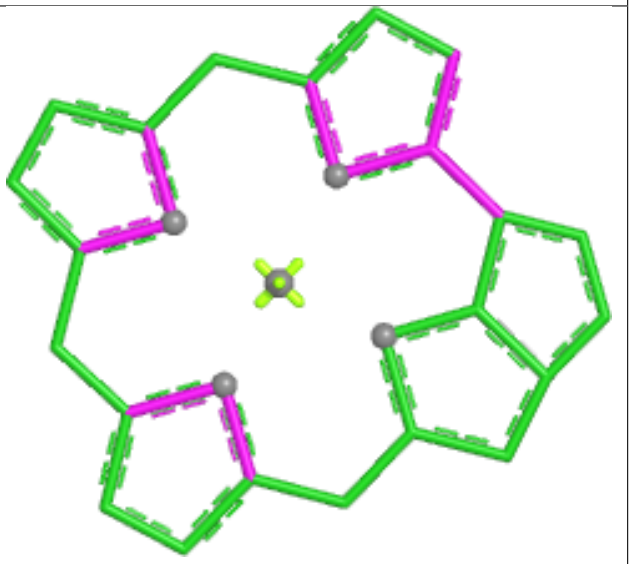


Rings

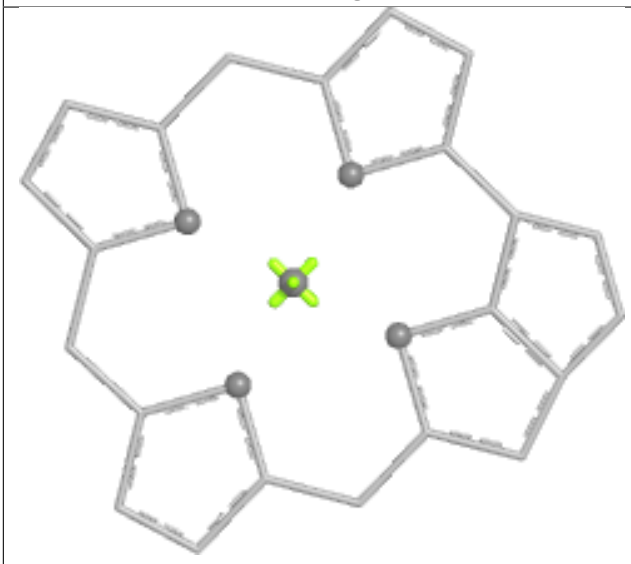
Ligand CLA J 178



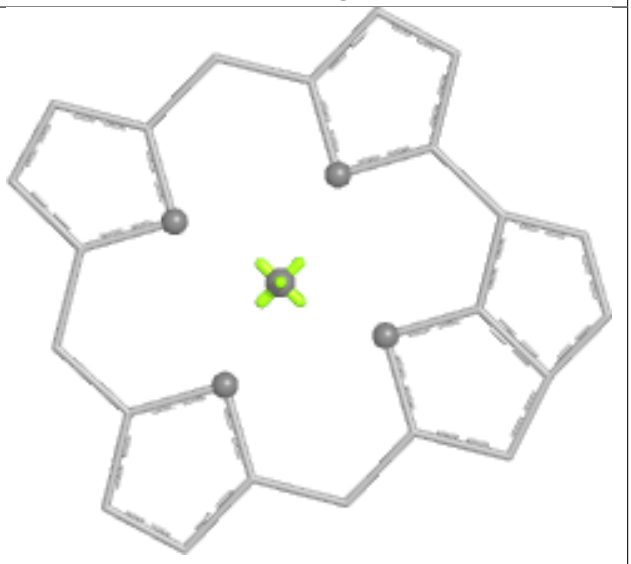
Bond lengths



Bond angles

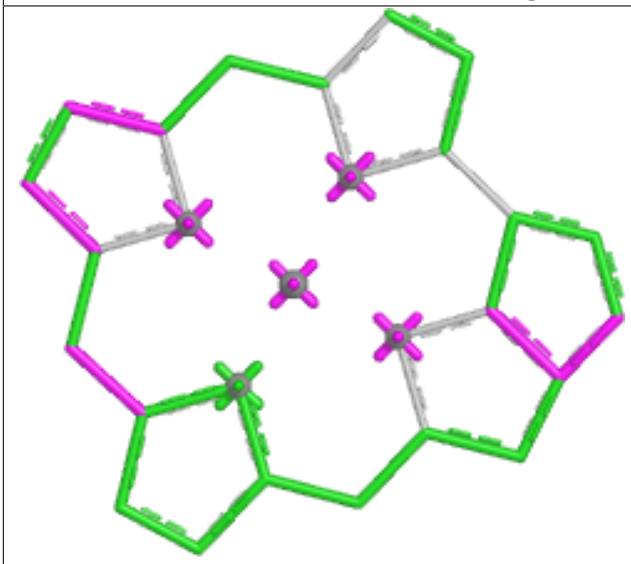


Torsions

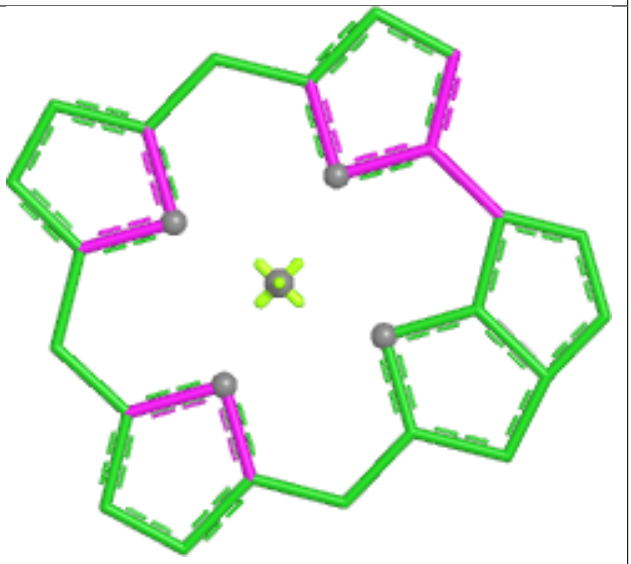


Rings

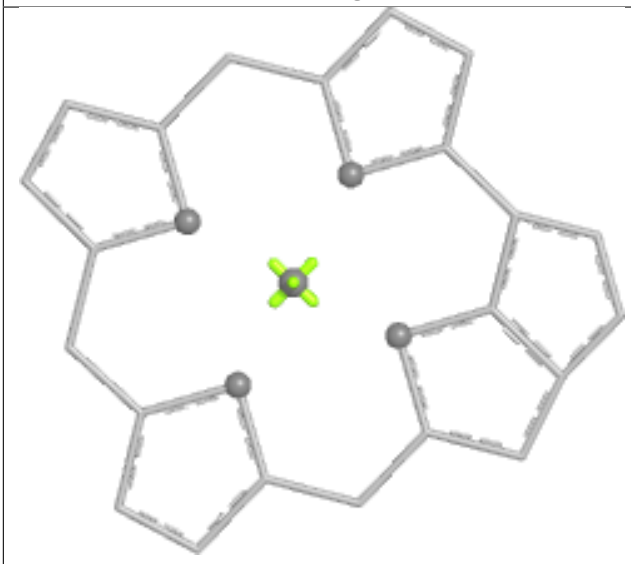
Ligand CLA K 178



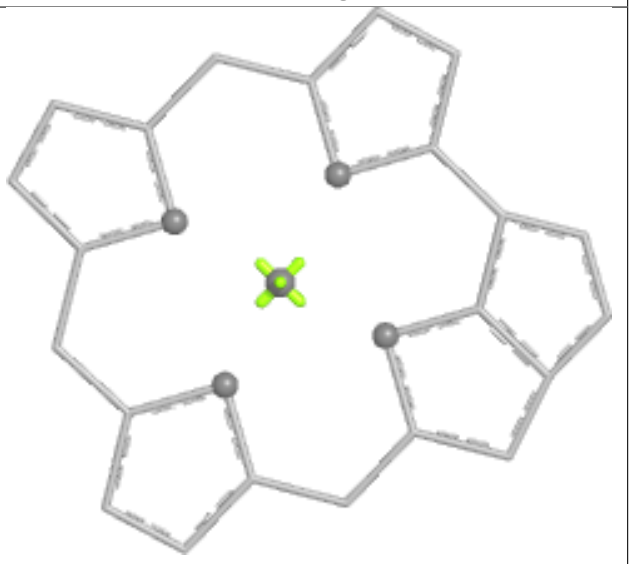
Bond lengths



Bond angles

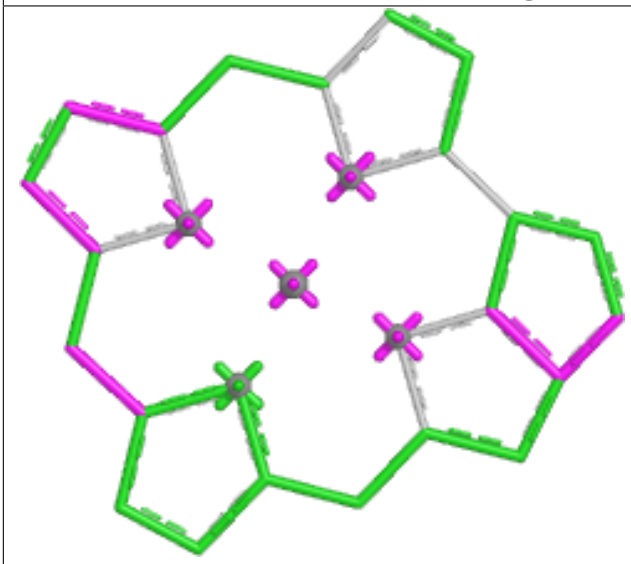


Torsions

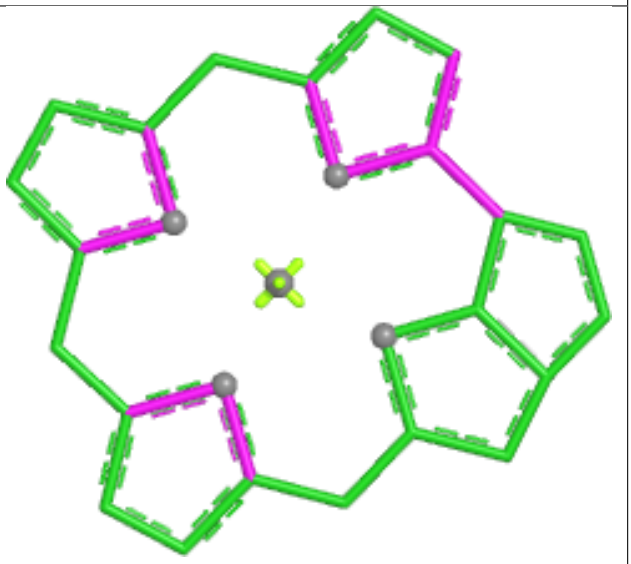


Rings

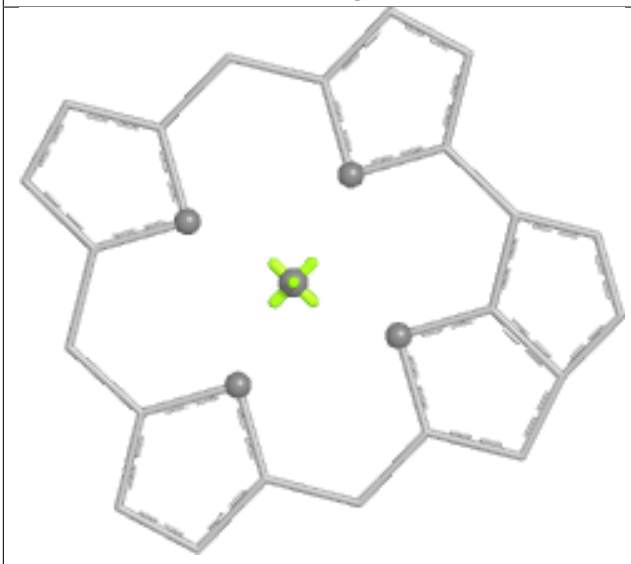
Ligand CLA M 156



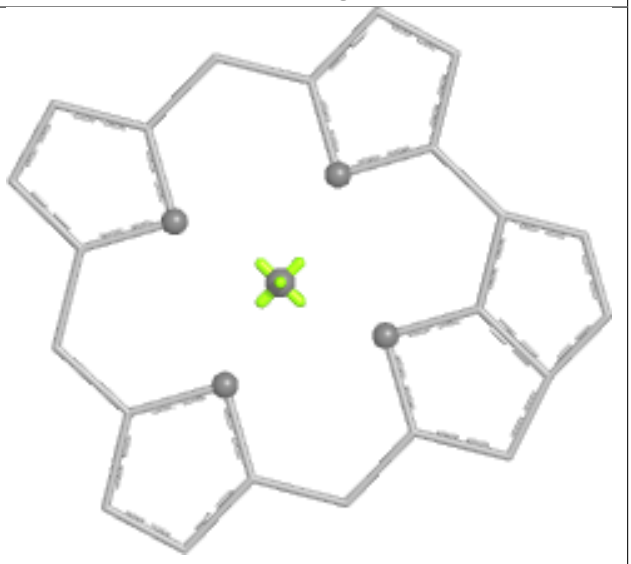
Bond lengths



Bond angles

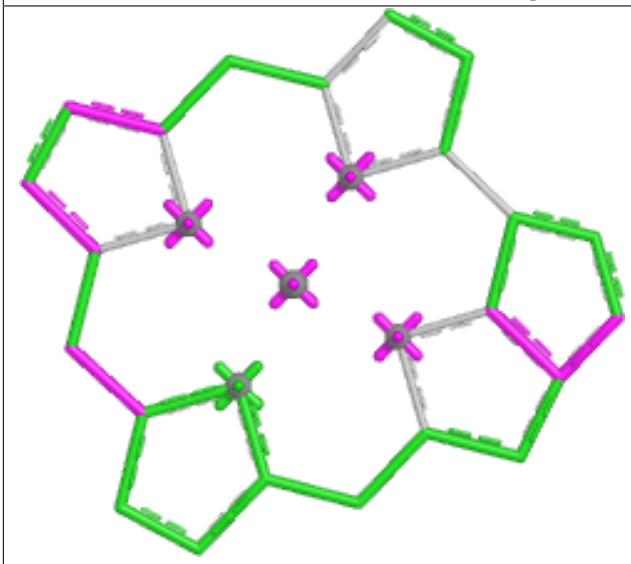


Torsions

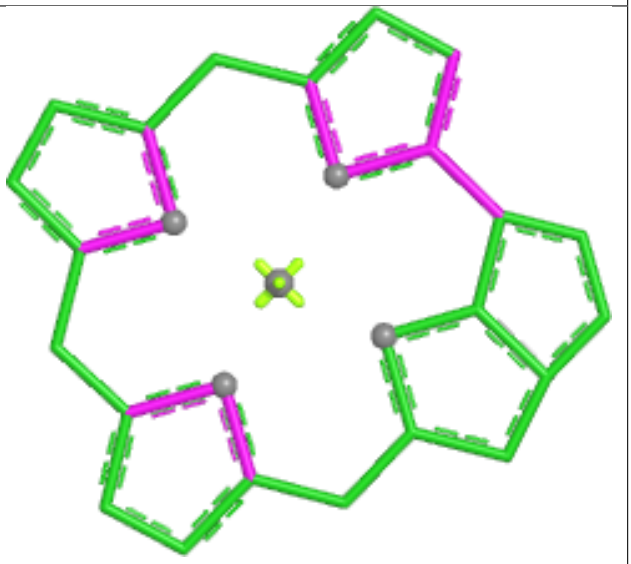


Rings

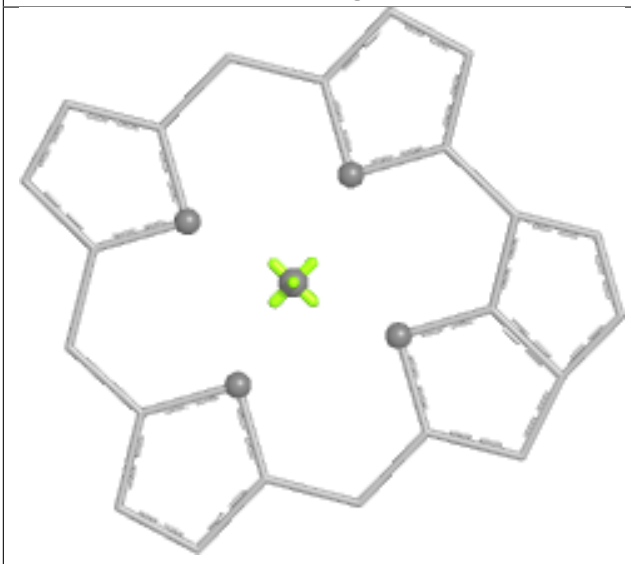
Ligand CLA C 160



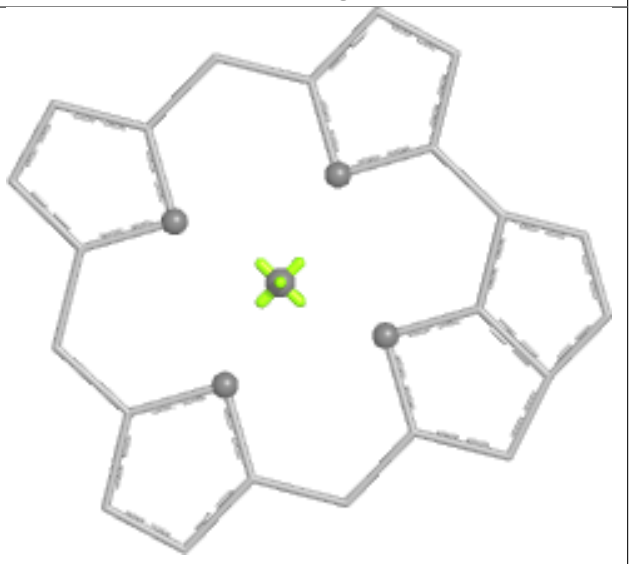
Bond lengths



Bond angles

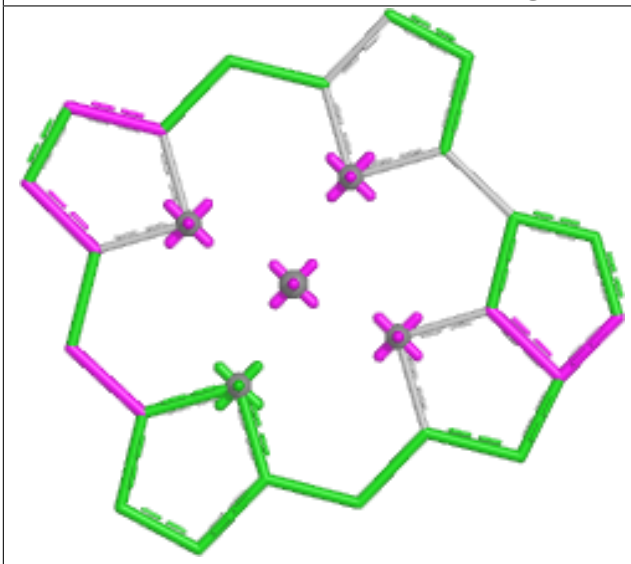


Torsions

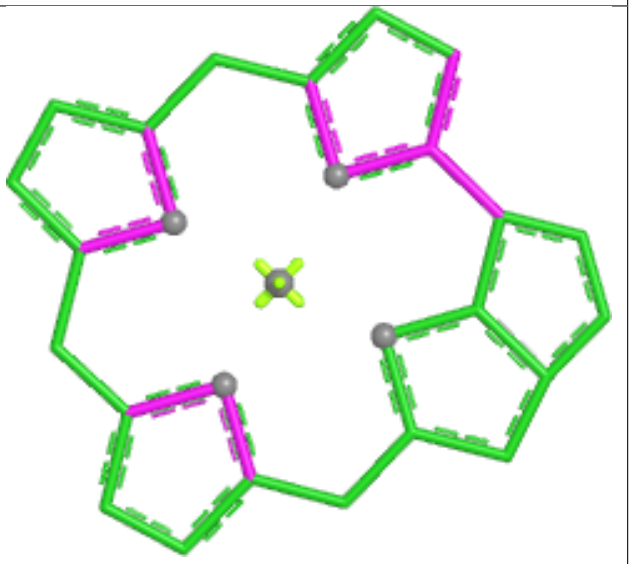


Rings

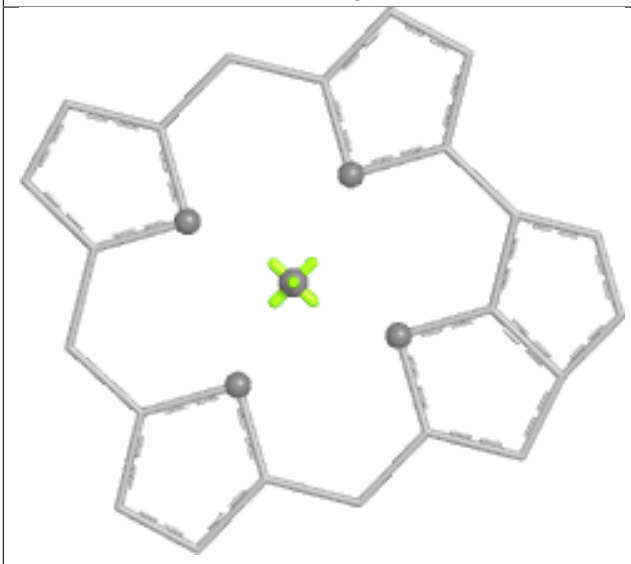
Ligand CLA C 157



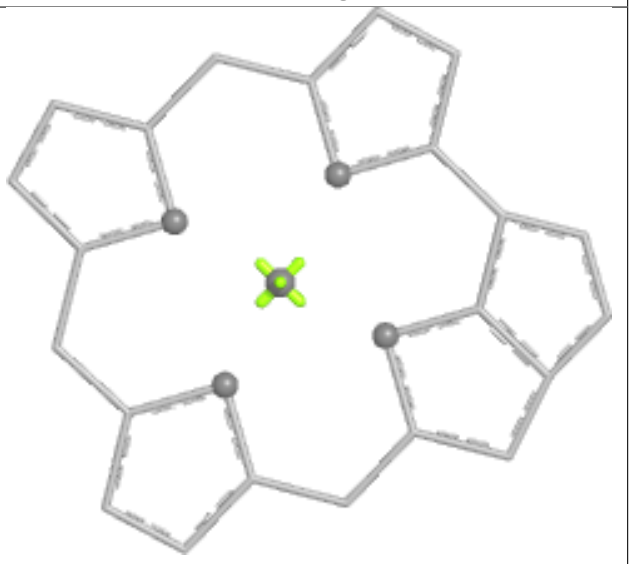
Bond lengths



Bond angles

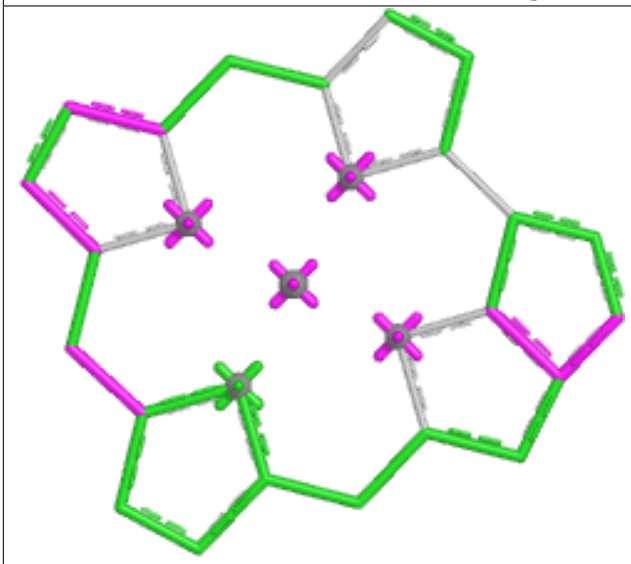


Torsions

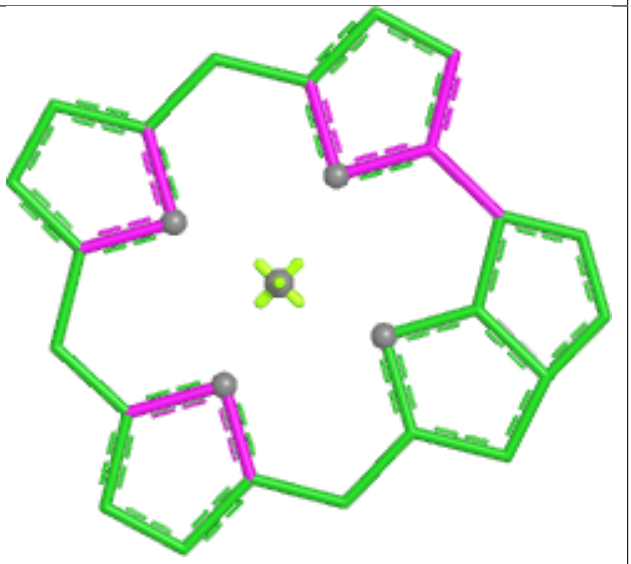


Rings

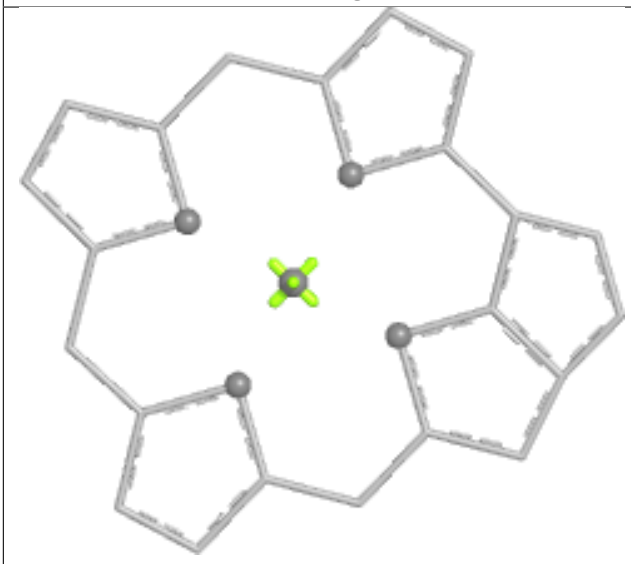
Ligand CLA P 313



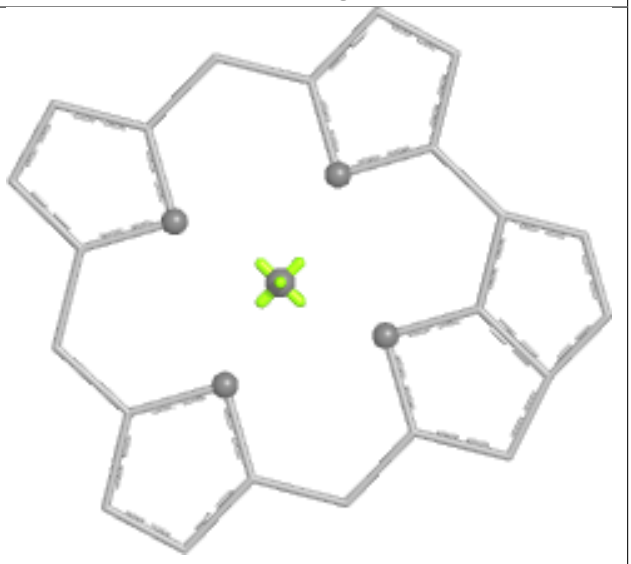
Bond lengths



Bond angles

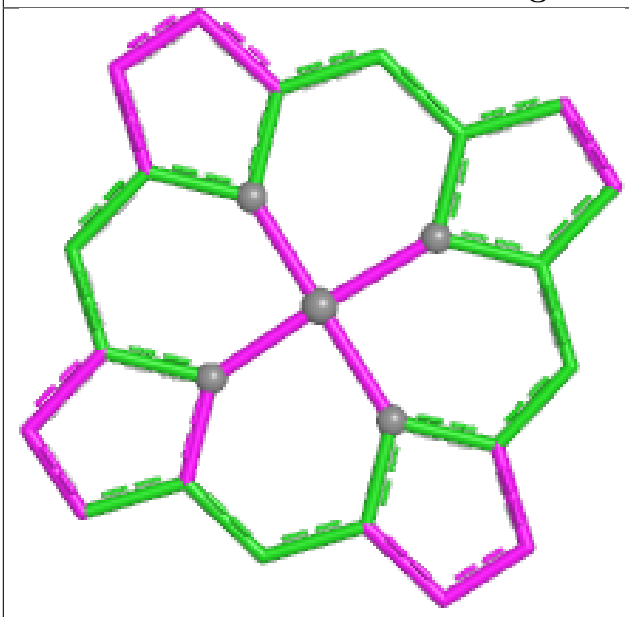


Torsions

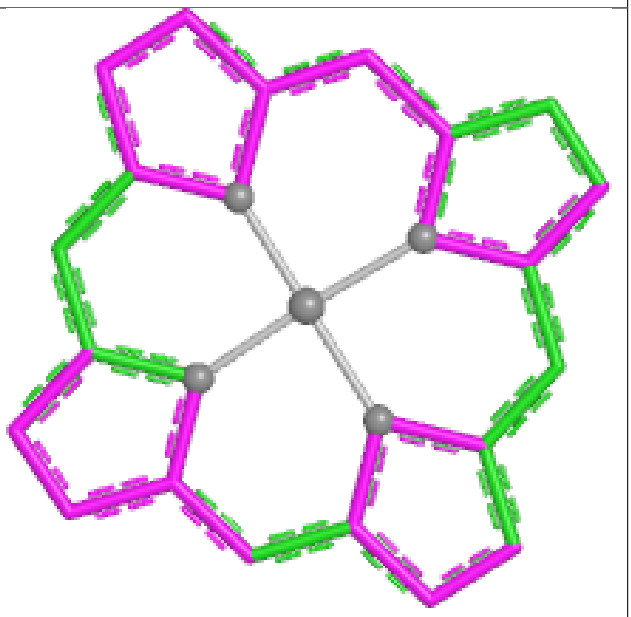


Rings

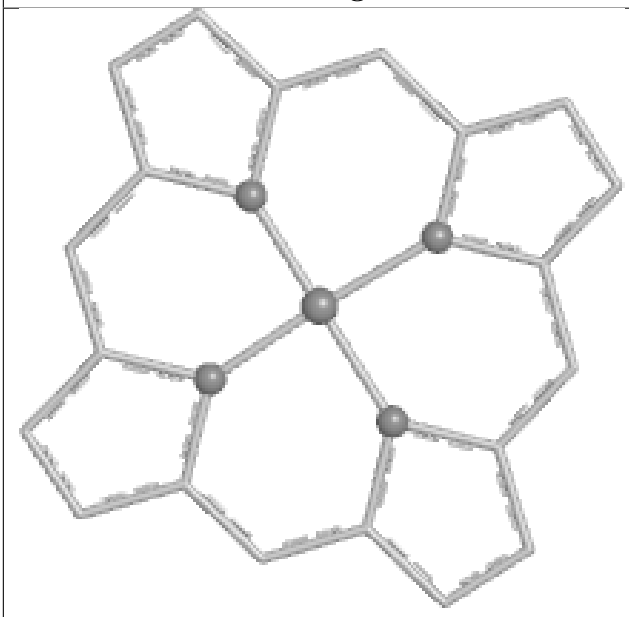
Ligand HEM F 50



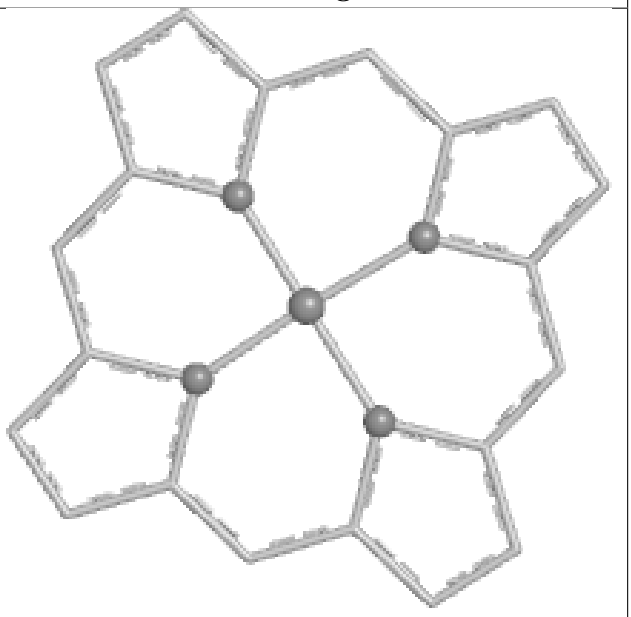
Bond lengths



Bond angles

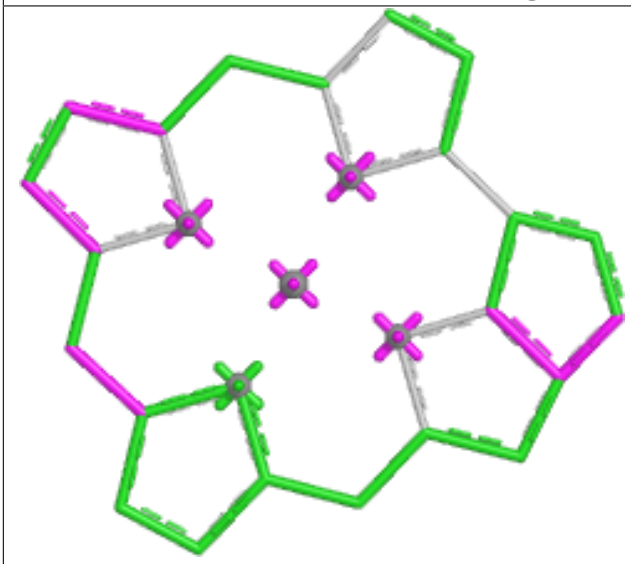


Torsions

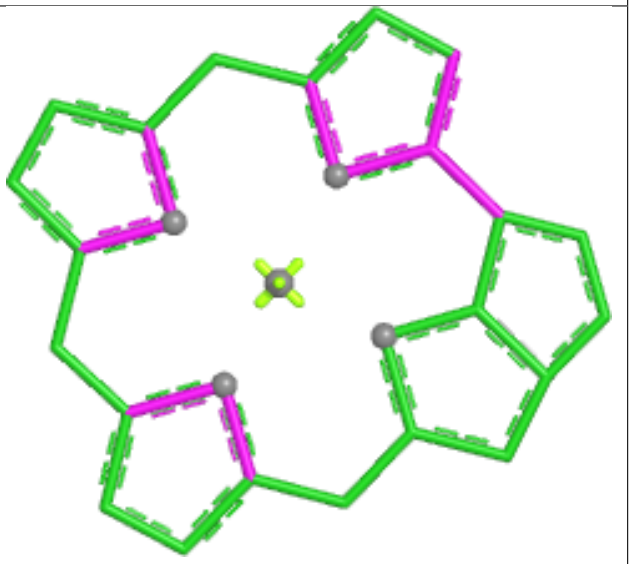


Rings

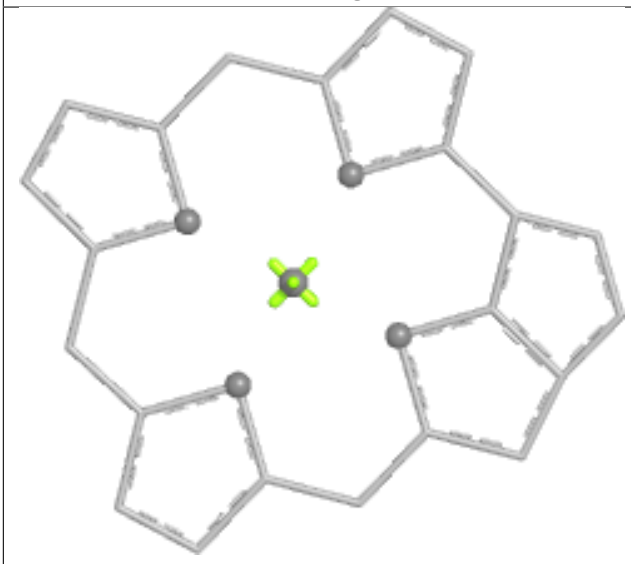
Ligand CLA D 156



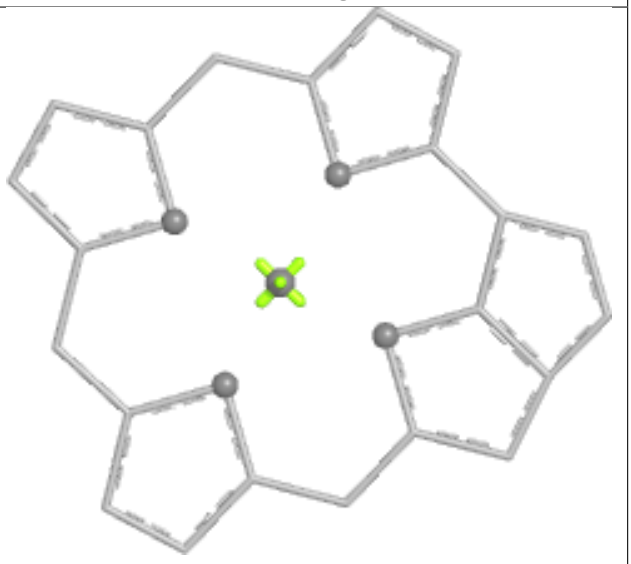
Bond lengths



Bond angles

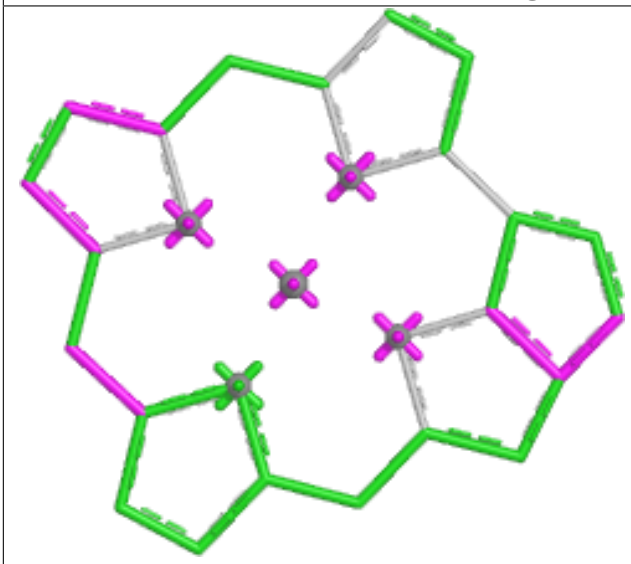


Torsions

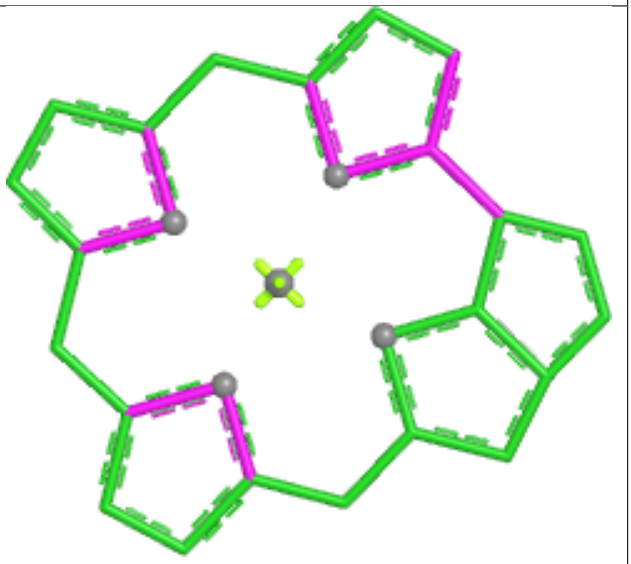


Rings

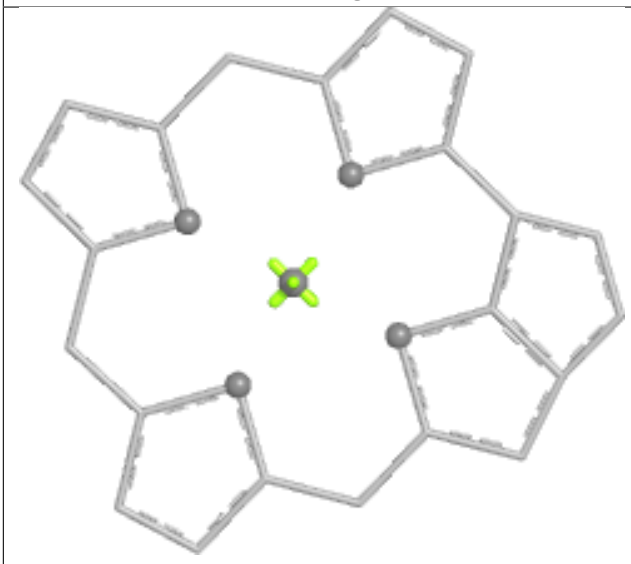
Ligand CLA A 176



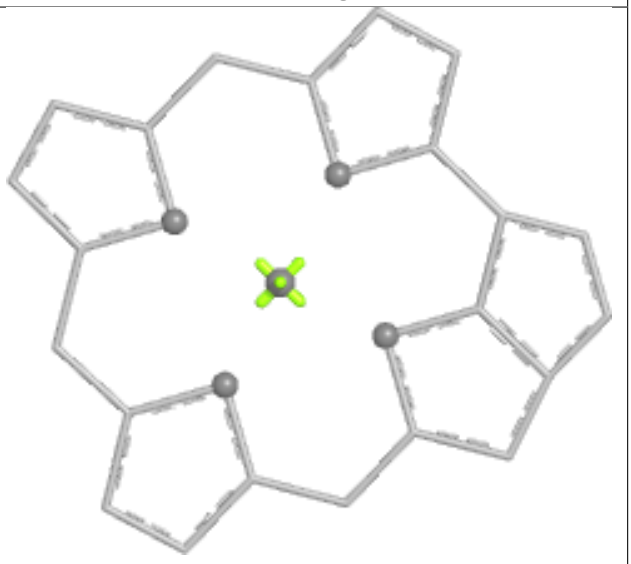
Bond lengths



Bond angles

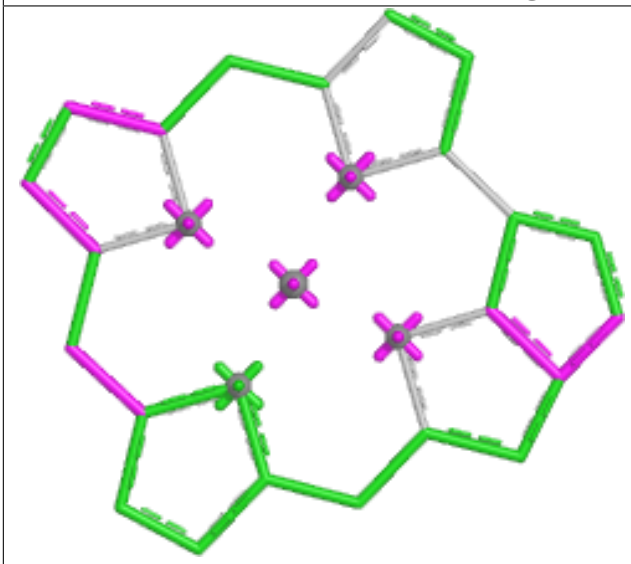


Torsions

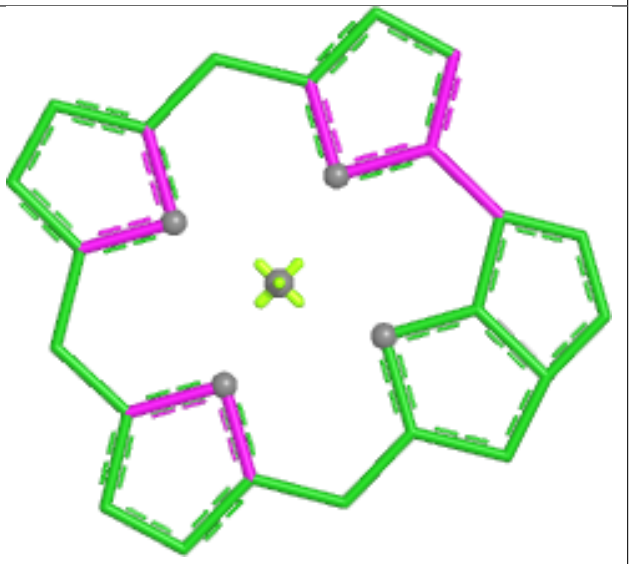


Rings

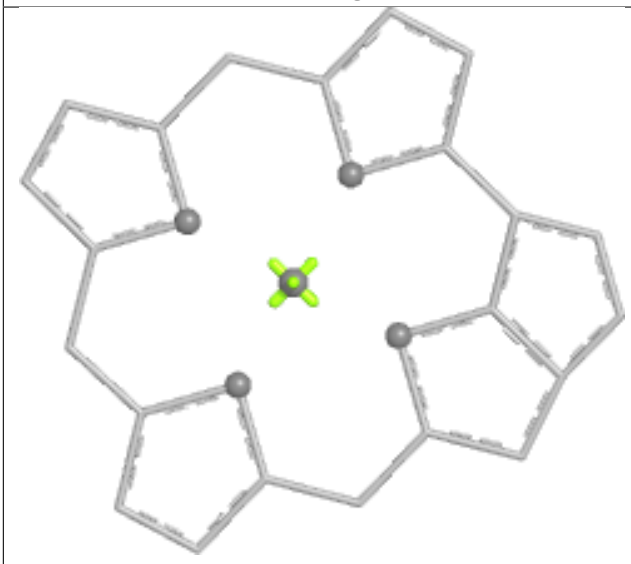
Ligand CLA D 165



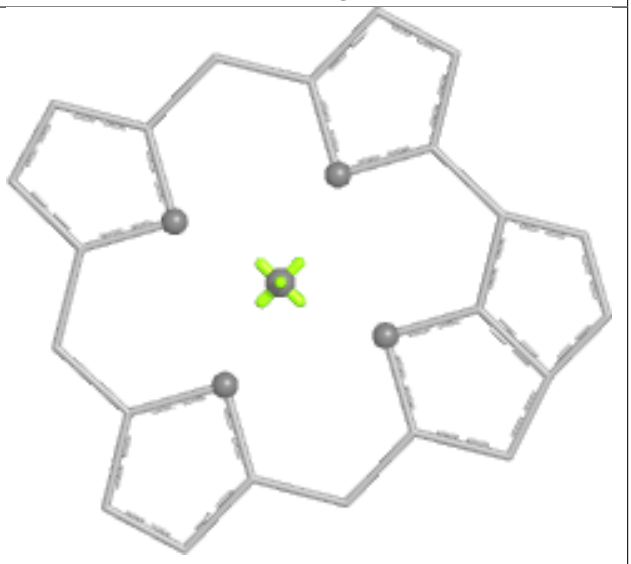
Bond lengths



Bond angles

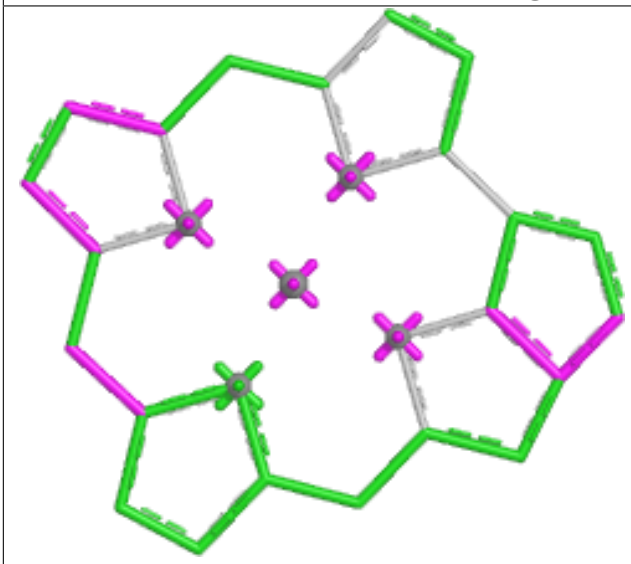


Torsions

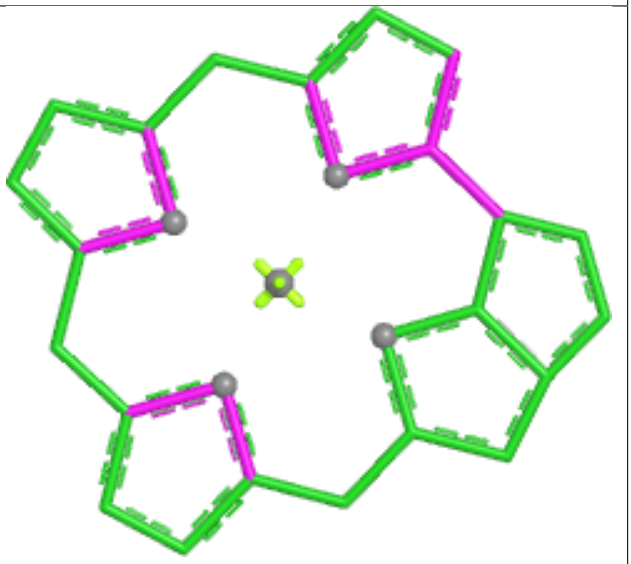


Rings

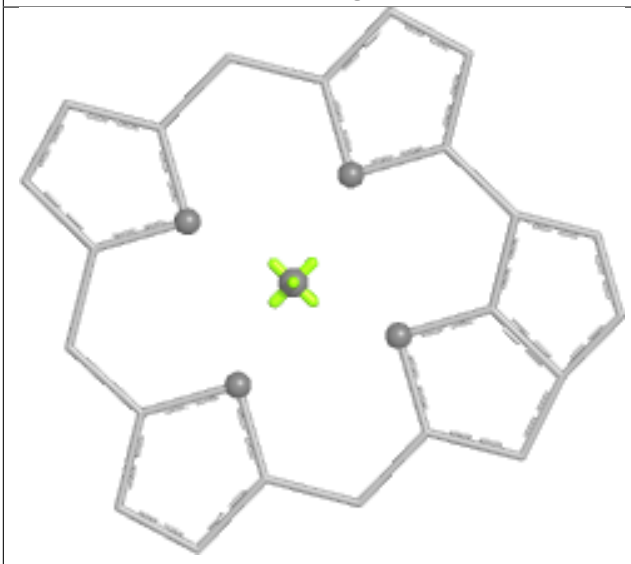
Ligand CLA L 167



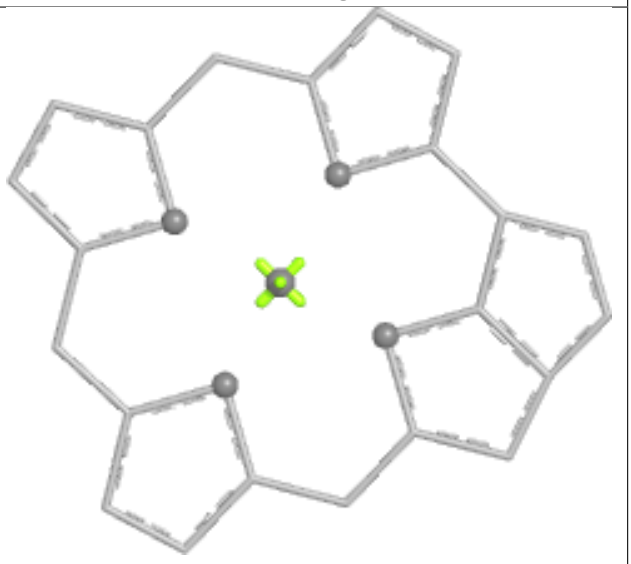
Bond lengths



Bond angles

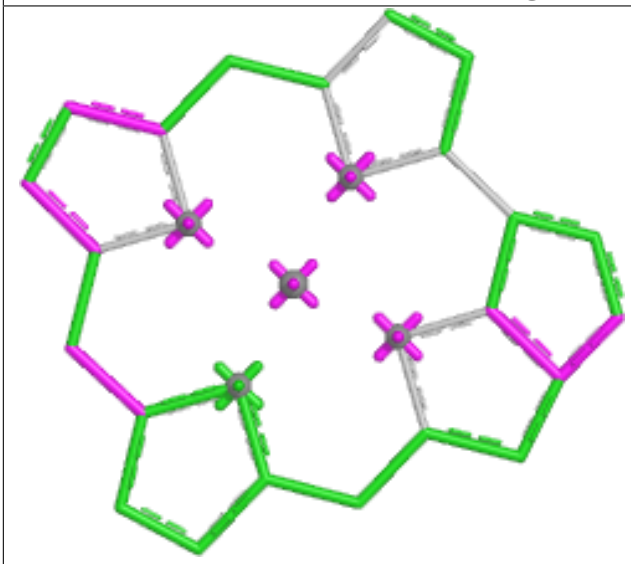


Torsions

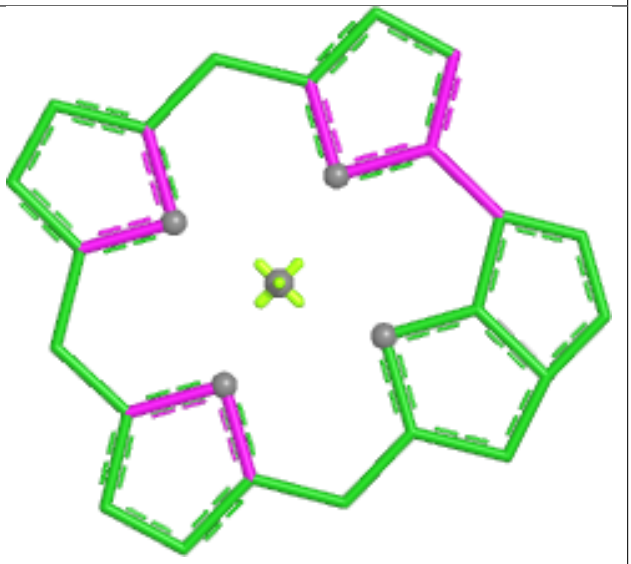


Rings

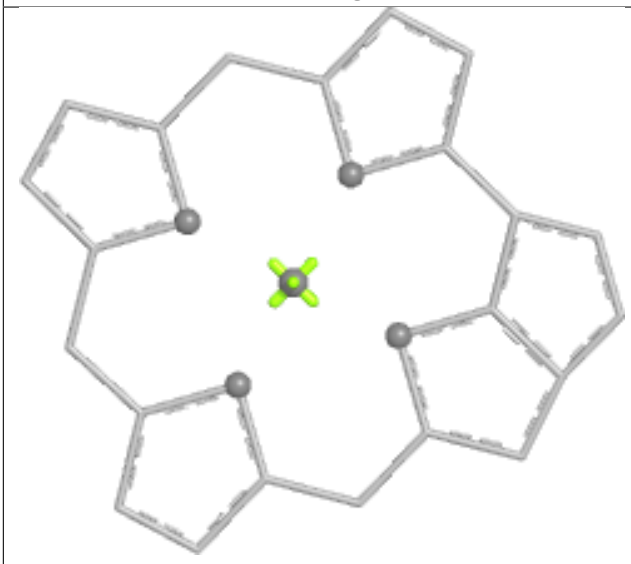
Ligand CLA D 163



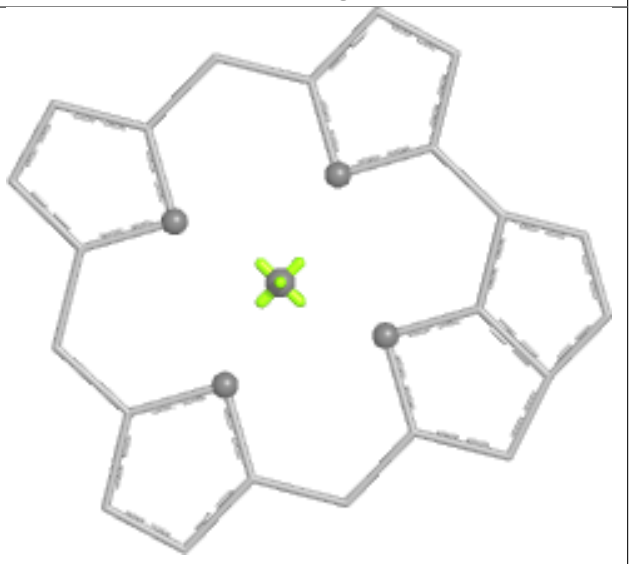
Bond lengths



Bond angles

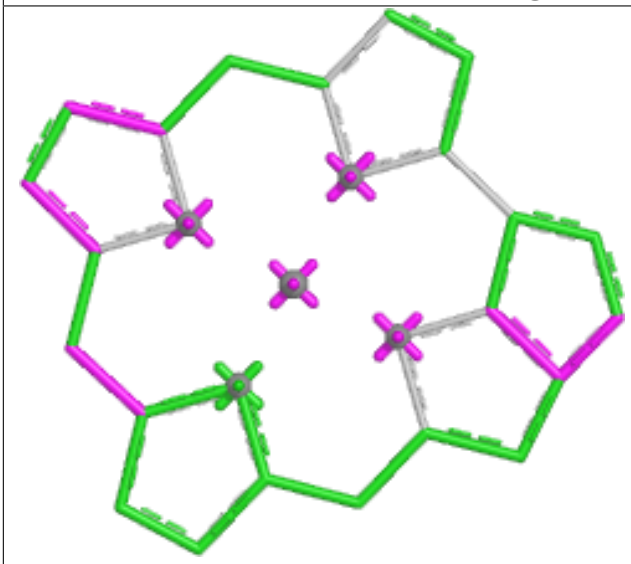


Torsions

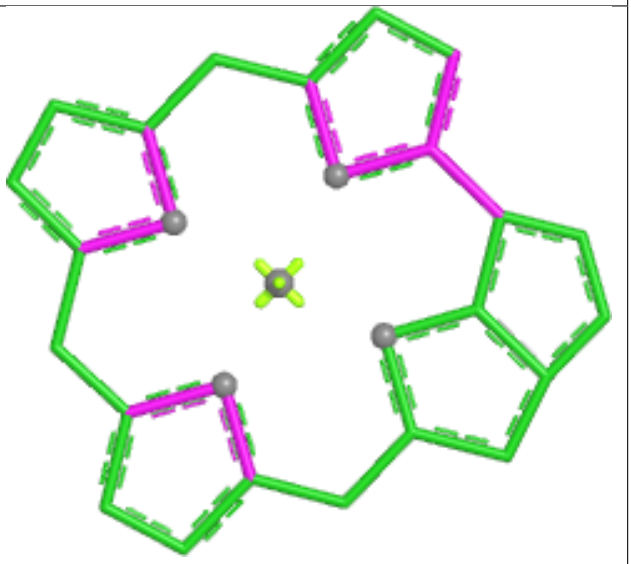


Rings

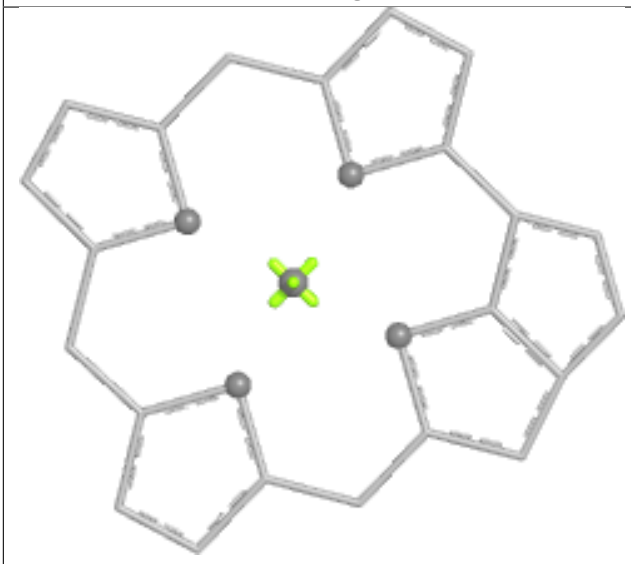
Ligand CLA L 165



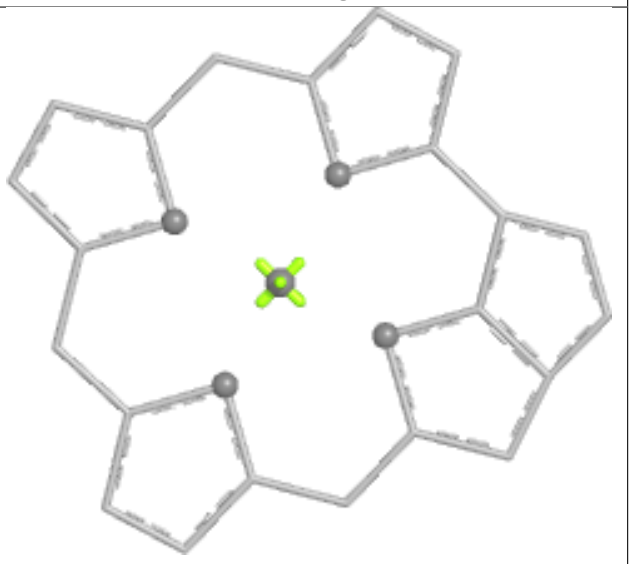
Bond lengths



Bond angles

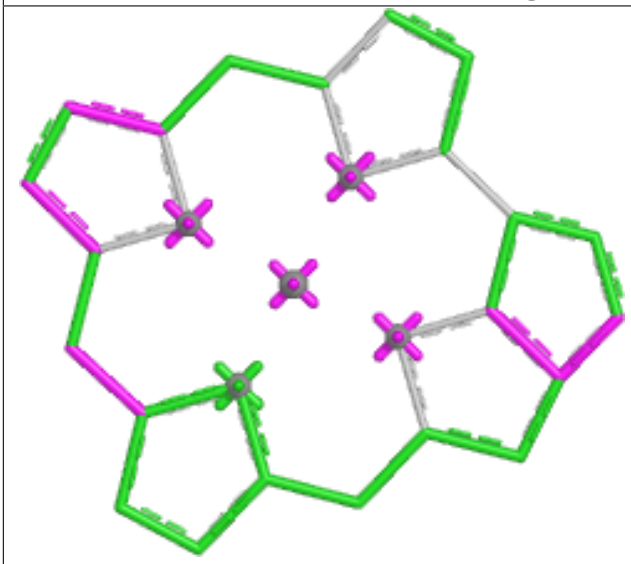


Torsions

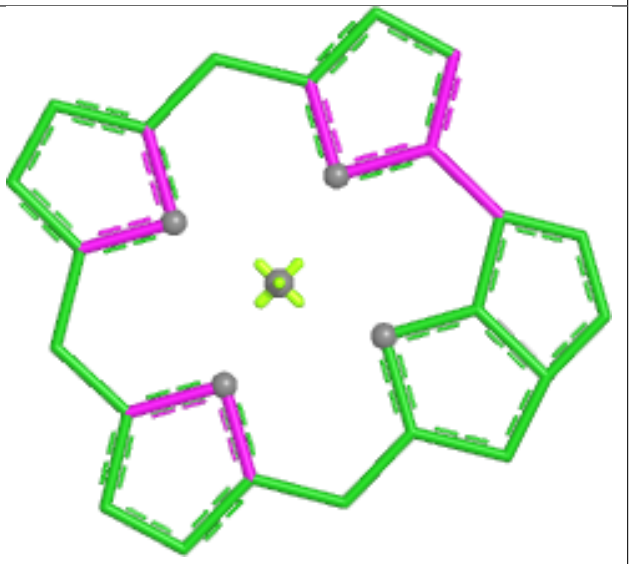


Rings

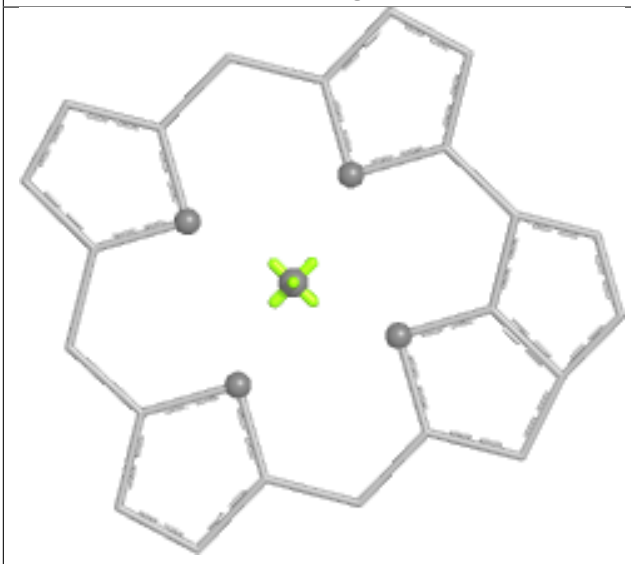
Ligand CLA K 176



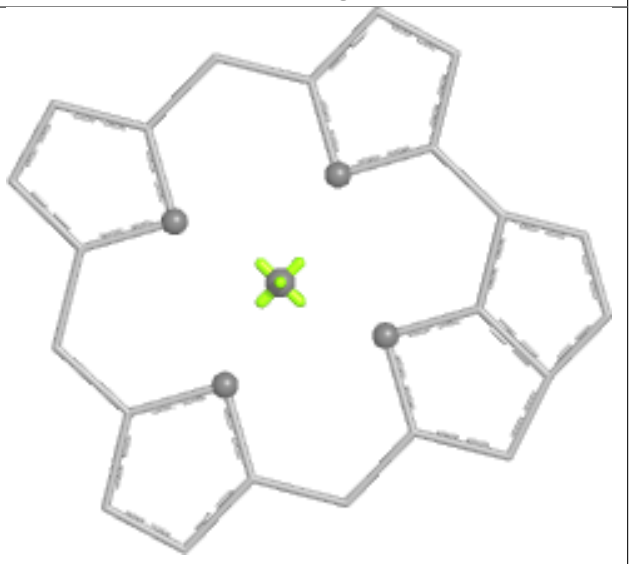
Bond lengths



Bond angles

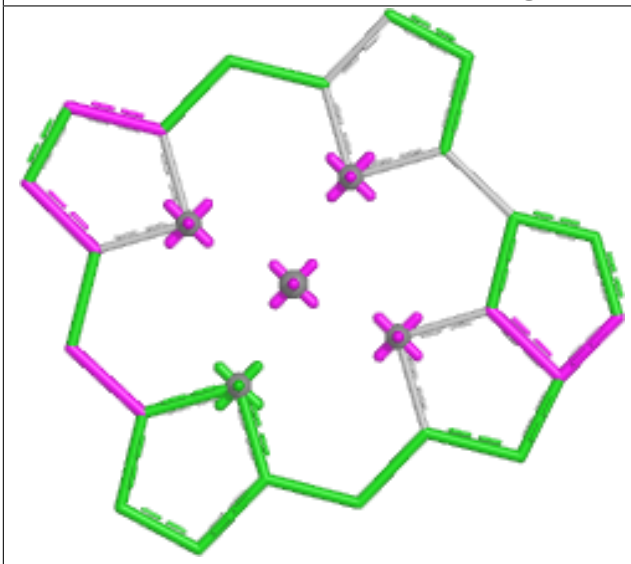


Torsions

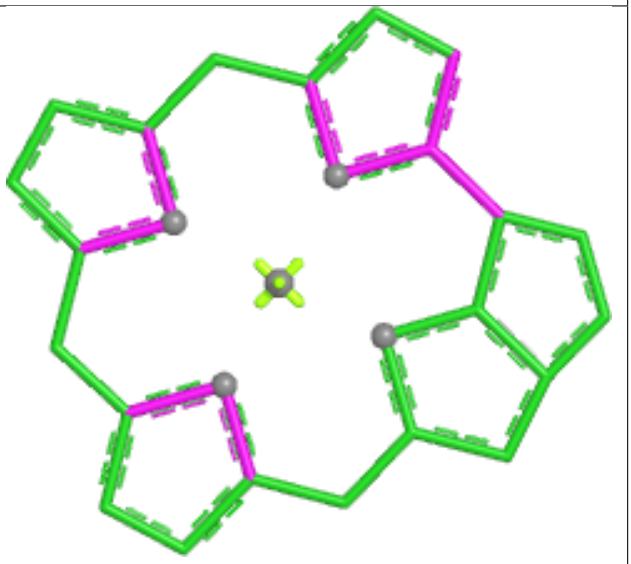


Rings

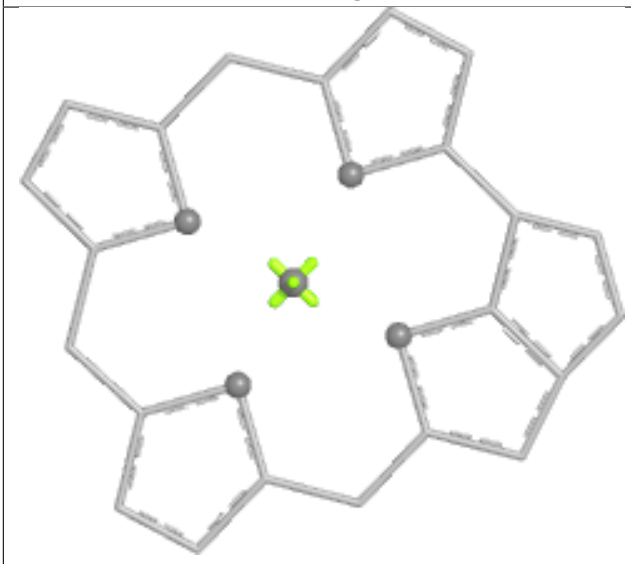
Ligand CLA M 161



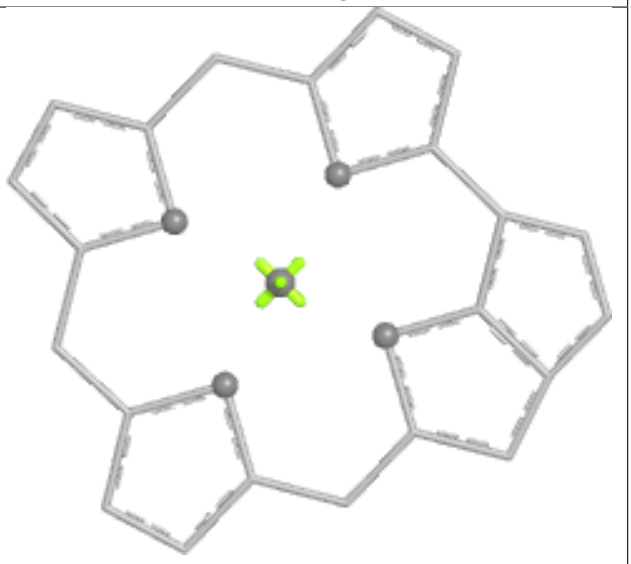
Bond lengths



Bond angles

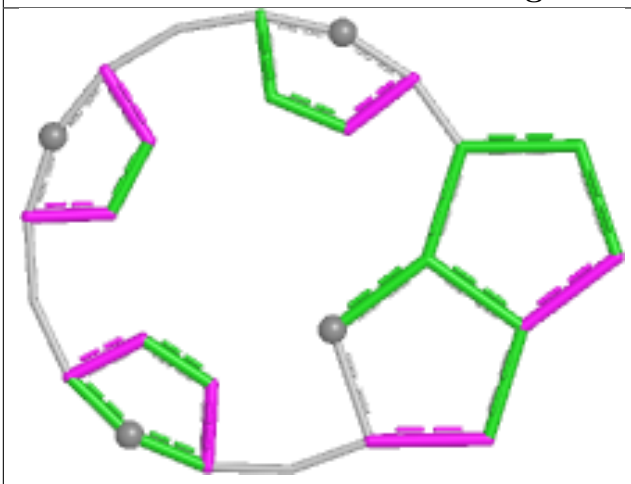


Torsions

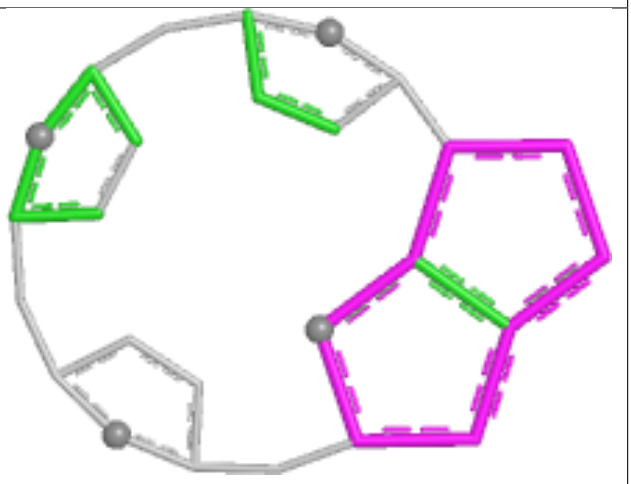


Rings

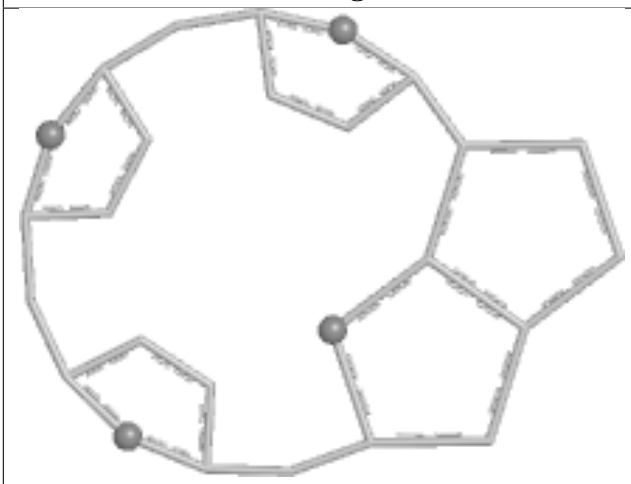
Ligand PHO J 177



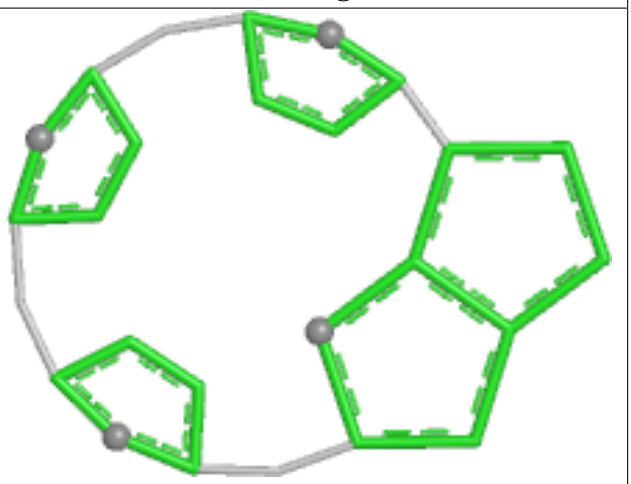
Bond lengths



Bond angles

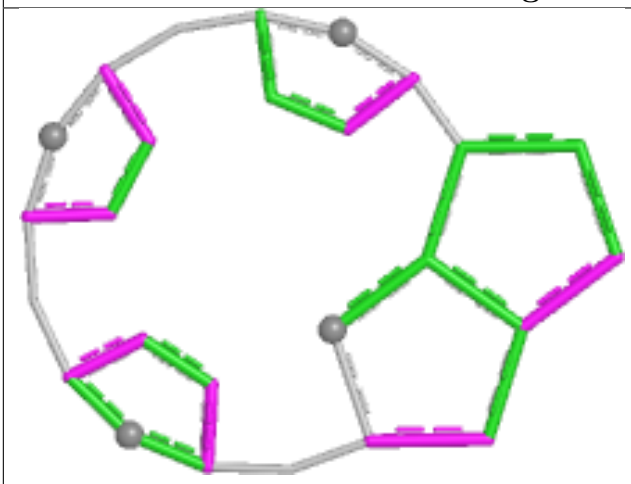


Torsions

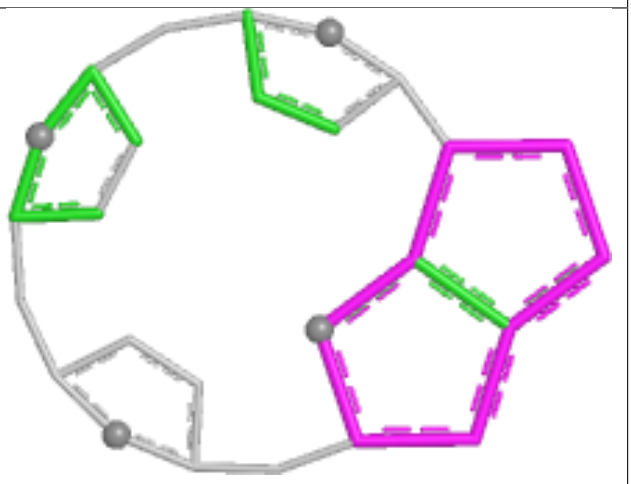


Rings

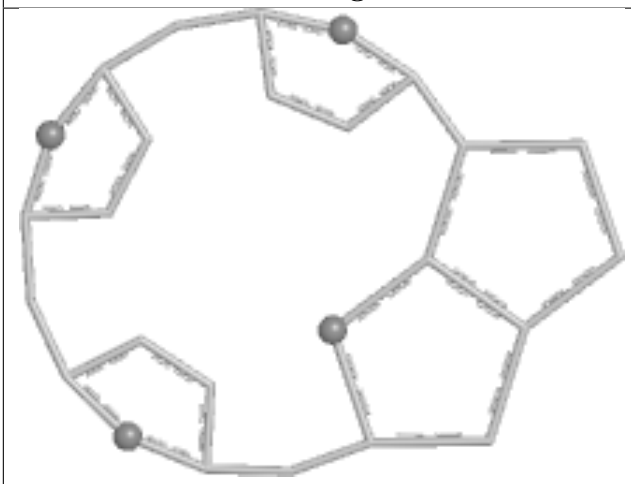
Ligand PHO B 177



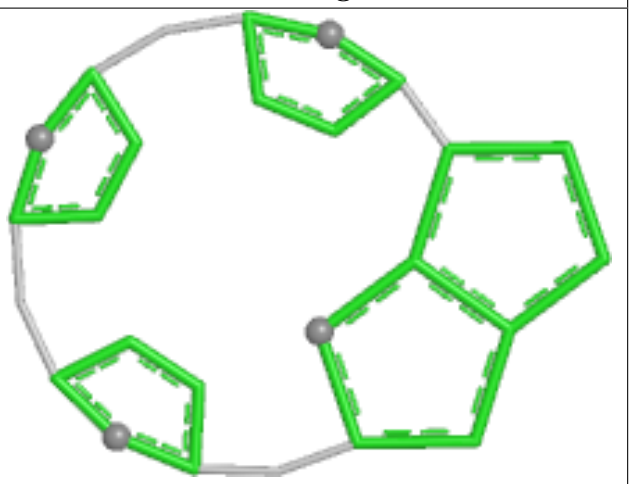
Bond lengths



Bond angles

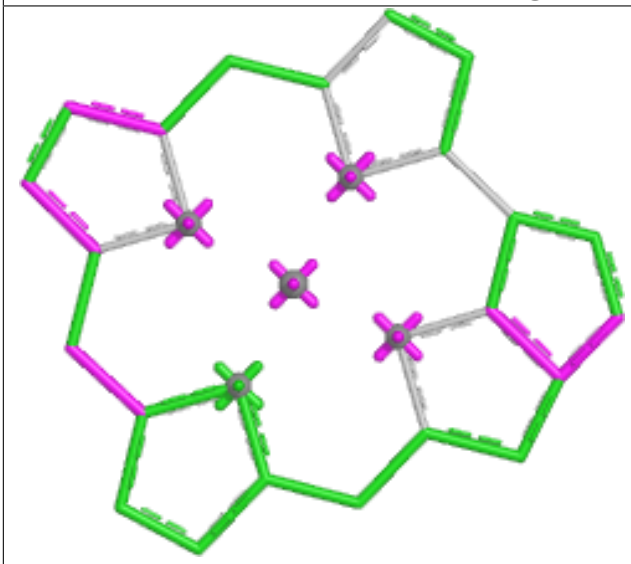


Torsions

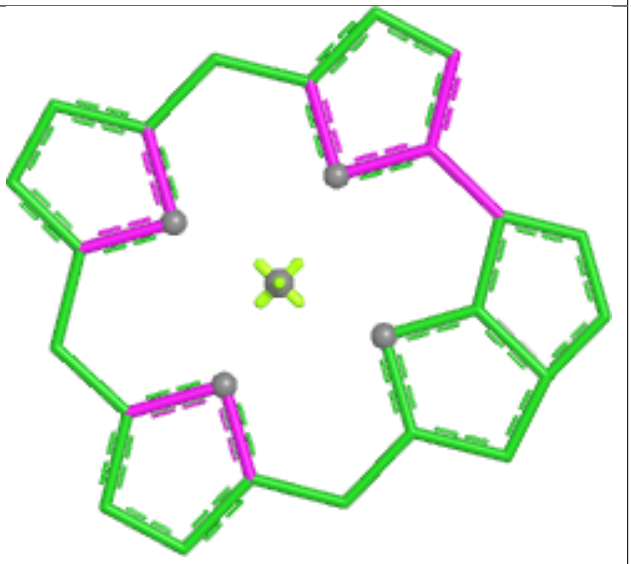


Rings

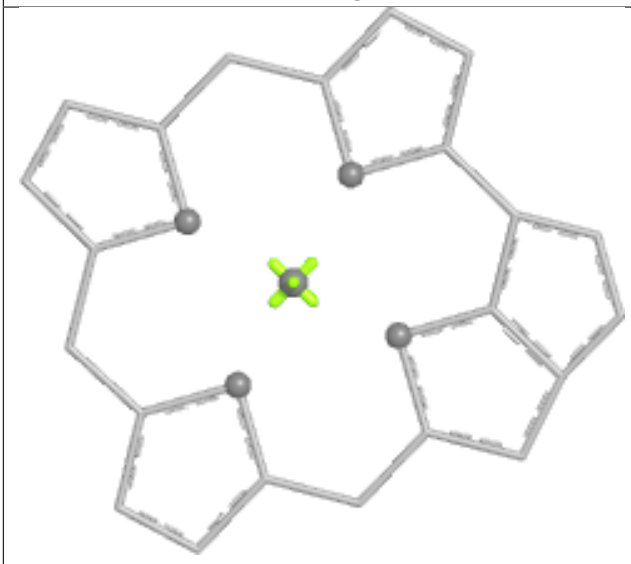
Ligand CLA L 158



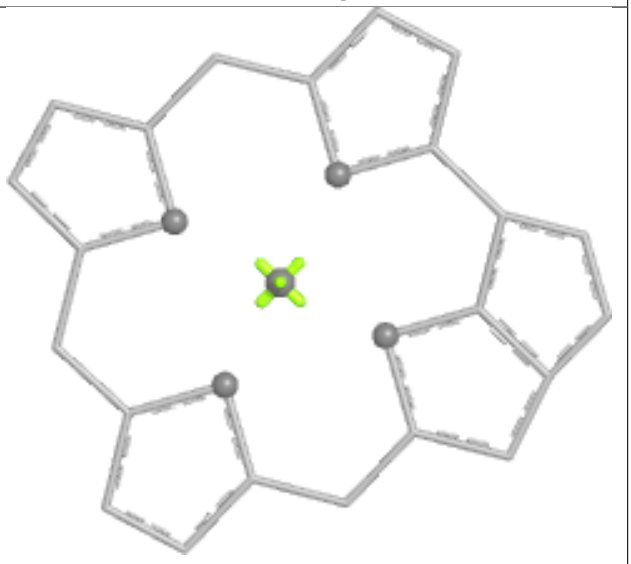
Bond lengths



Bond angles

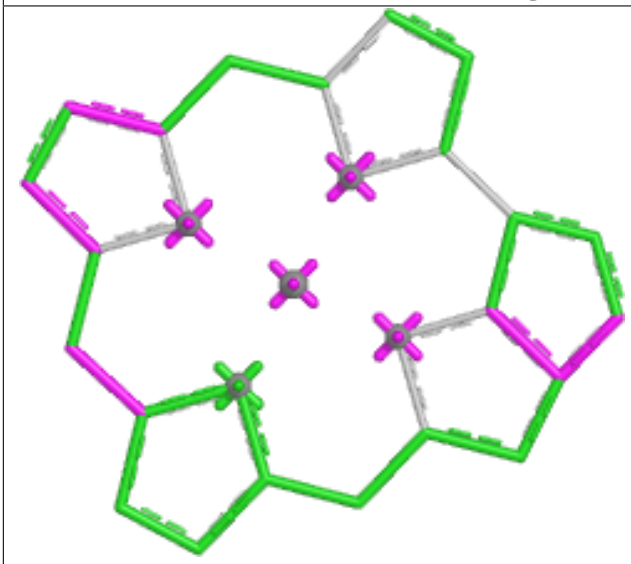


Torsions

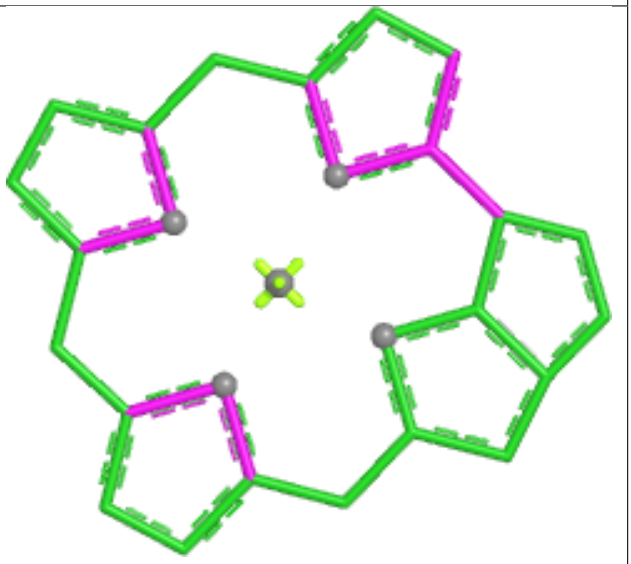


Rings

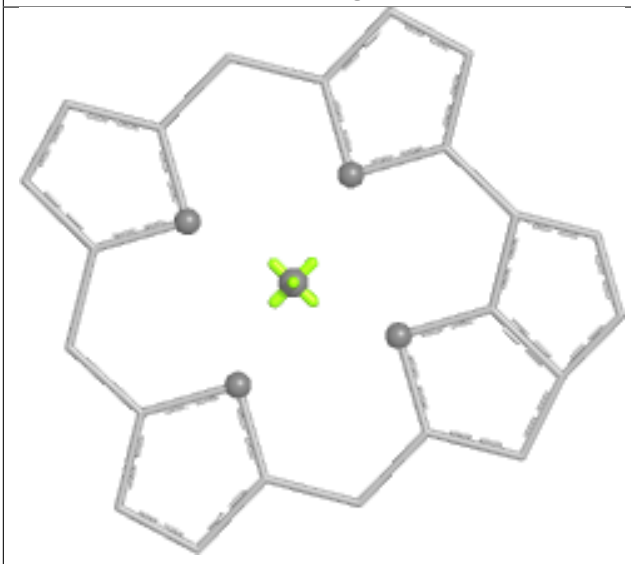
Ligand CLA C 158



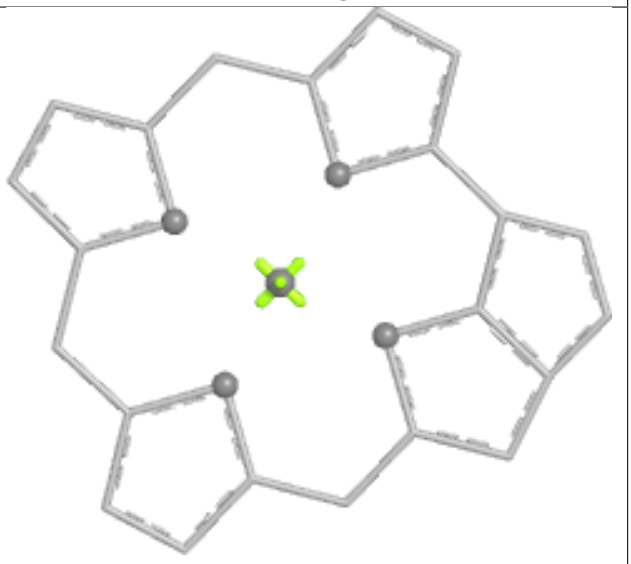
Bond lengths



Bond angles

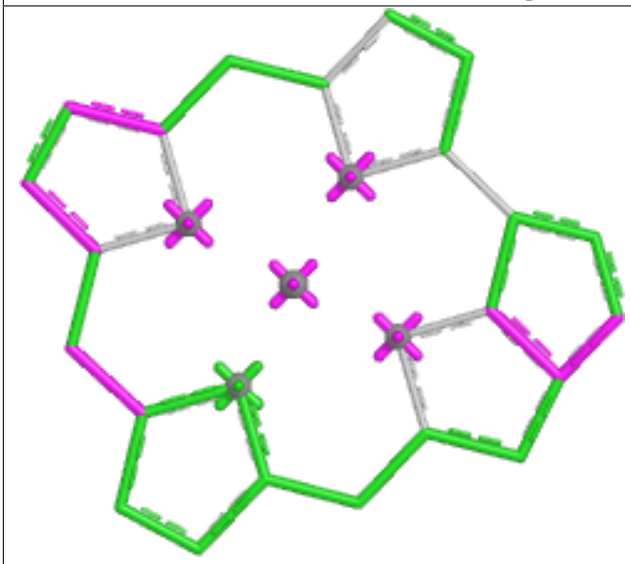


Torsions

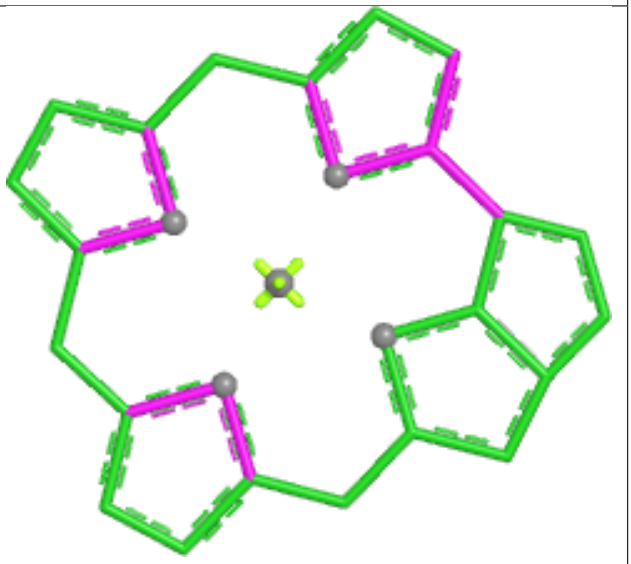


Rings

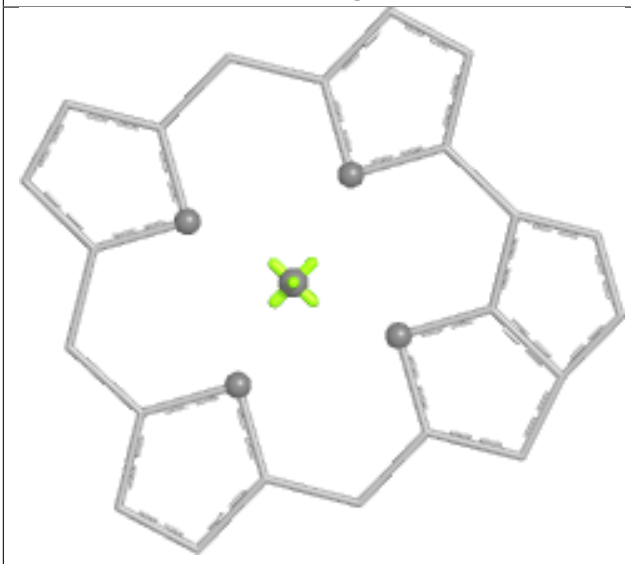
Ligand CLA M 165



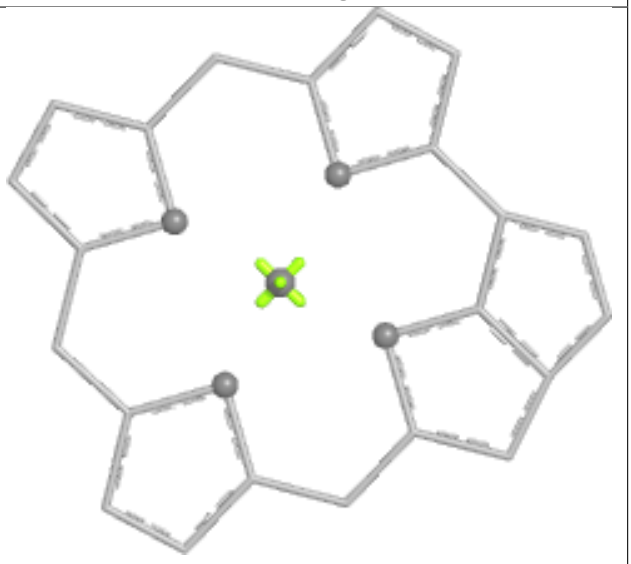
Bond lengths



Bond angles

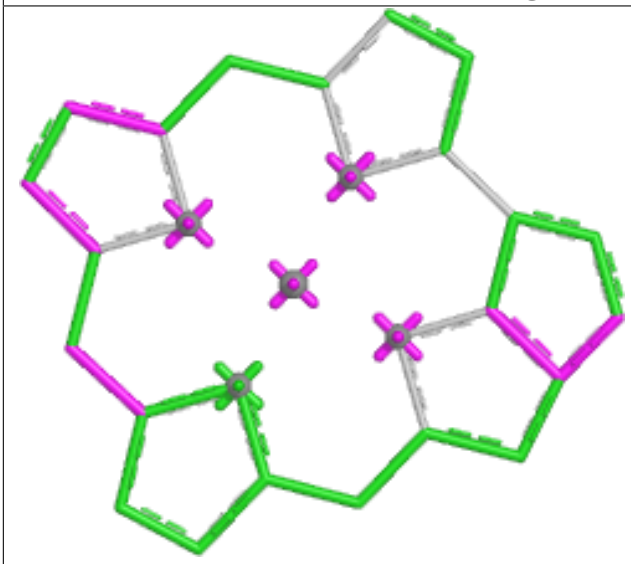


Torsions

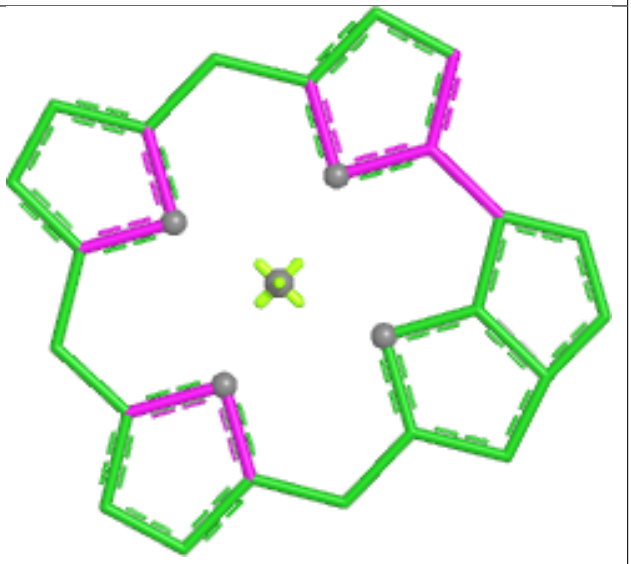


Rings

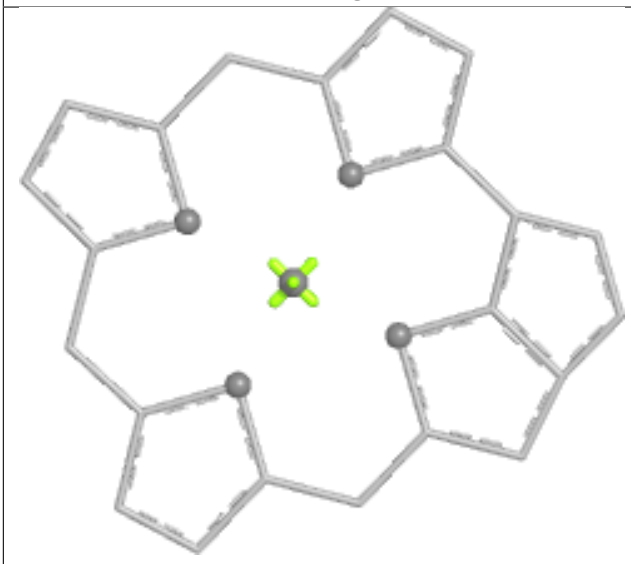
Ligand CLA D 160



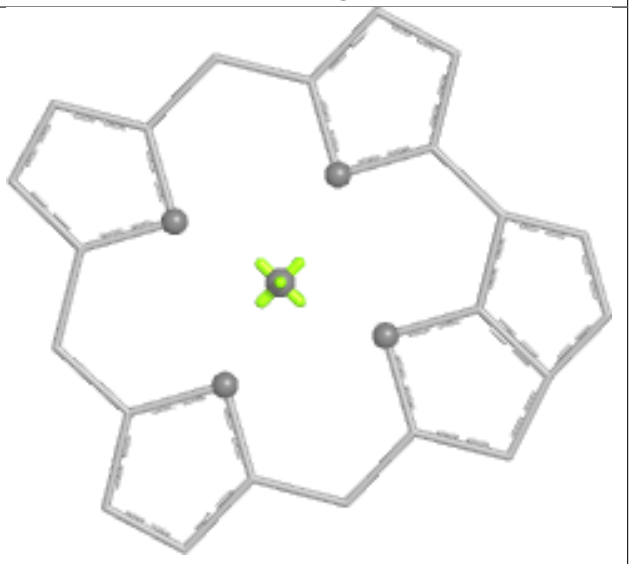
Bond lengths



Bond angles

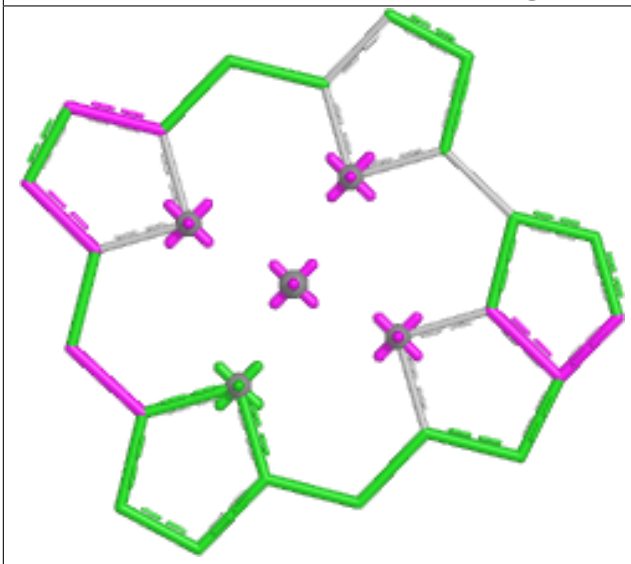


Torsions

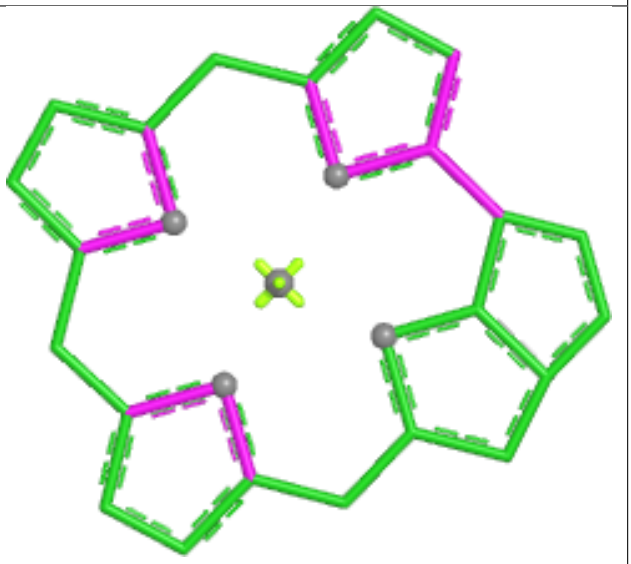


Rings

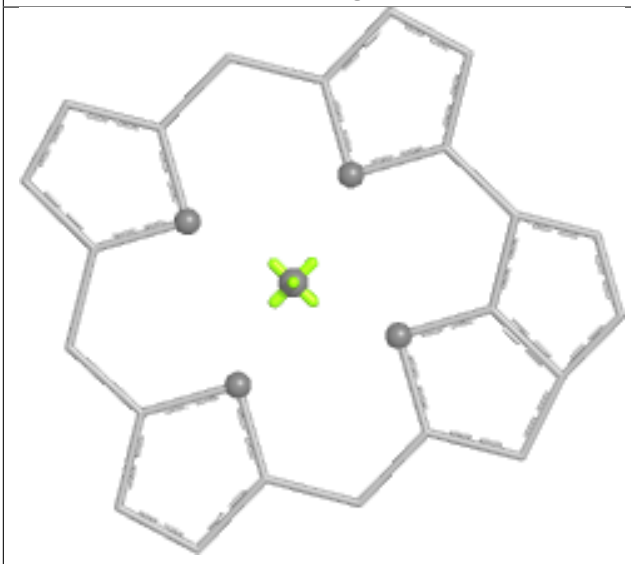
Ligand CLA D 157



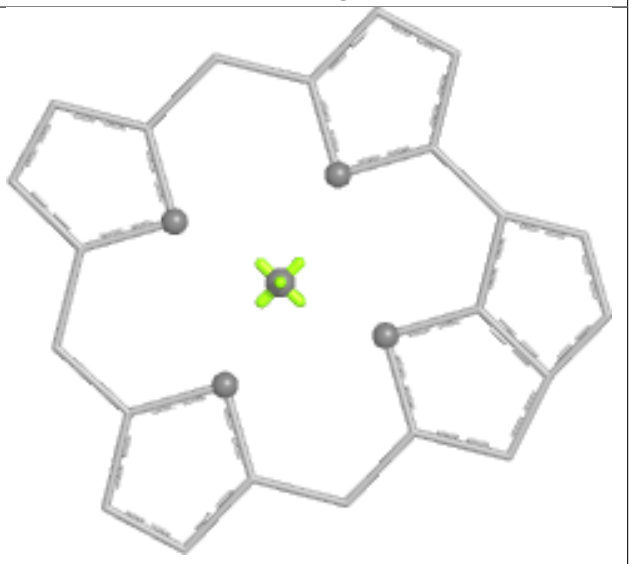
Bond lengths



Bond angles

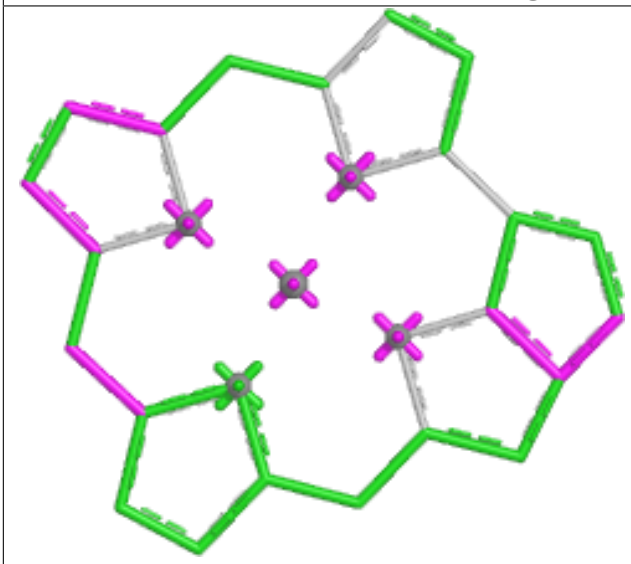


Torsions

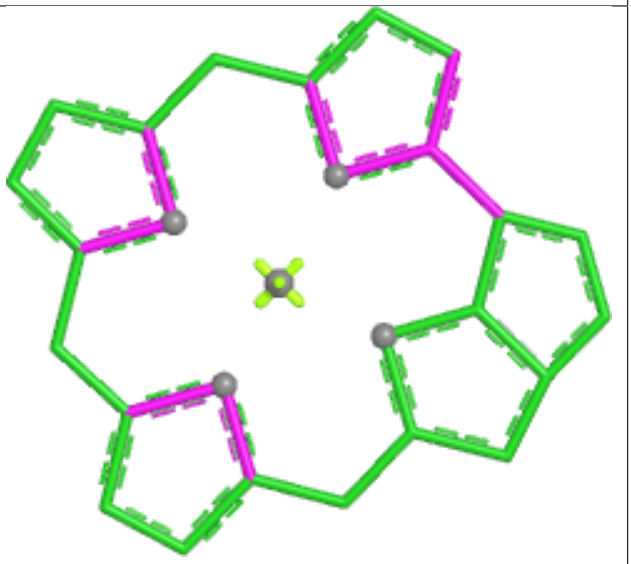


Rings

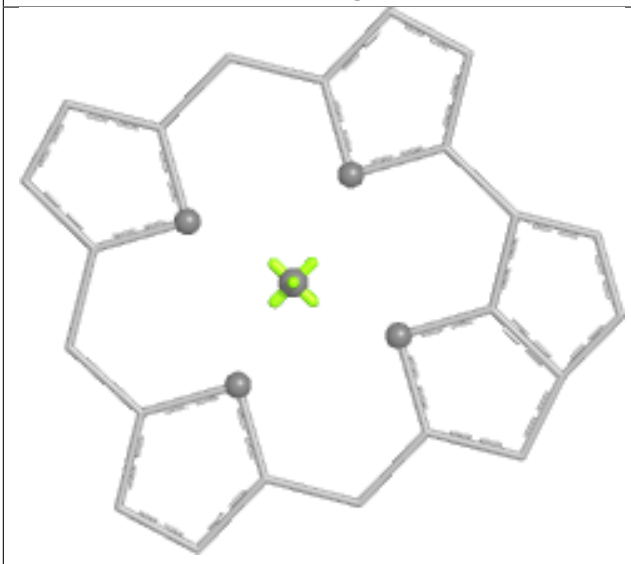
Ligand CLA C 163



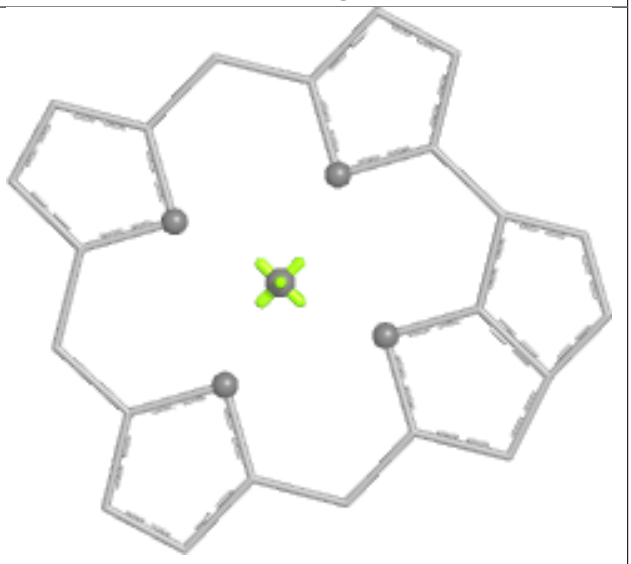
Bond lengths



Bond angles

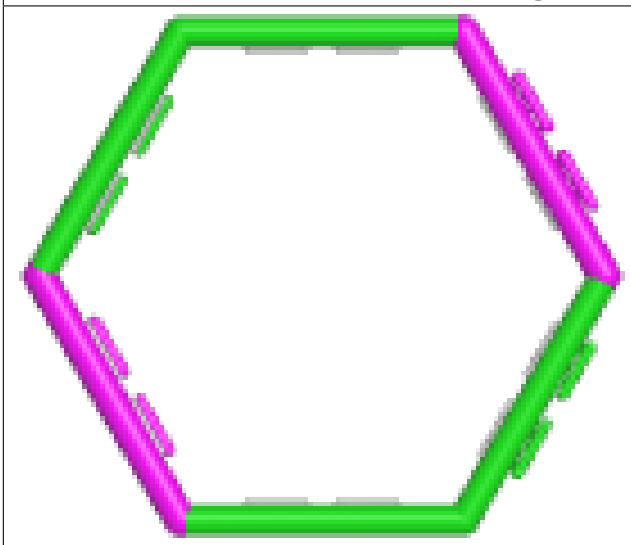


Torsions

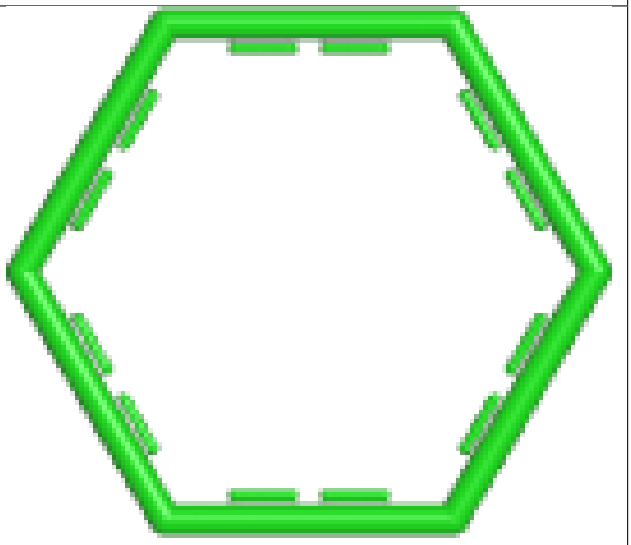


Rings

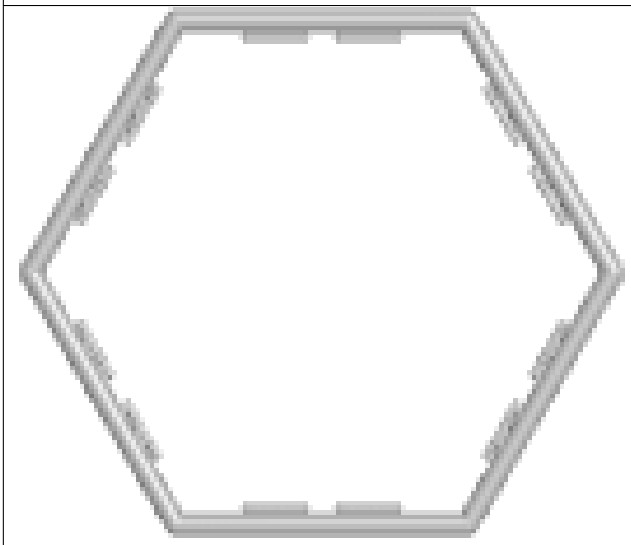
Ligand PL9 B 179



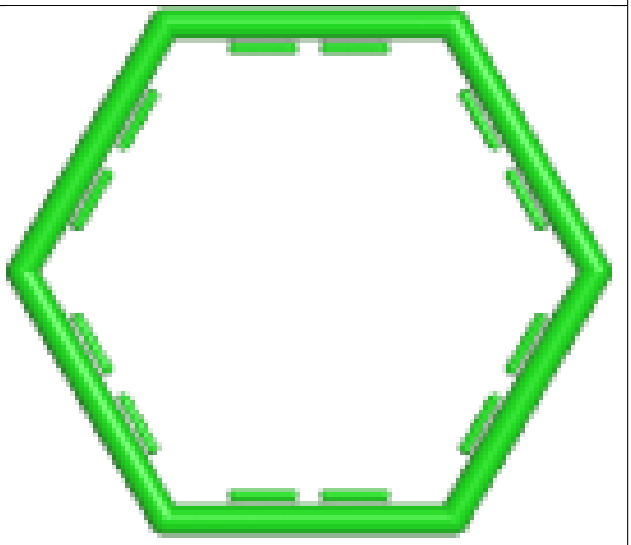
Bond lengths



Bond angles

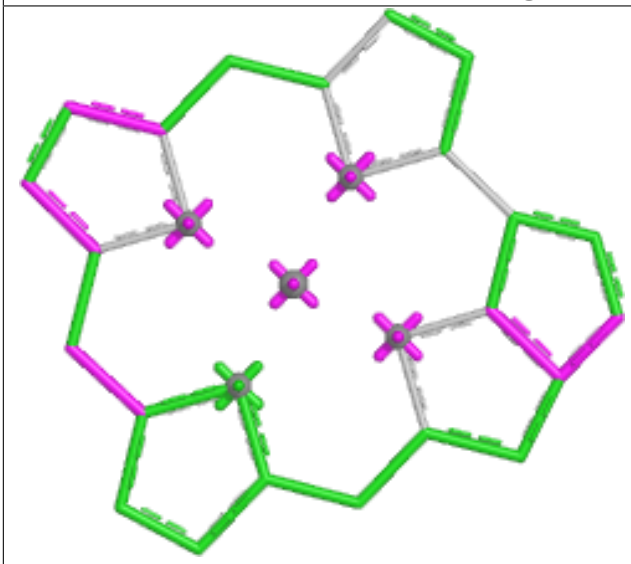


Torsions

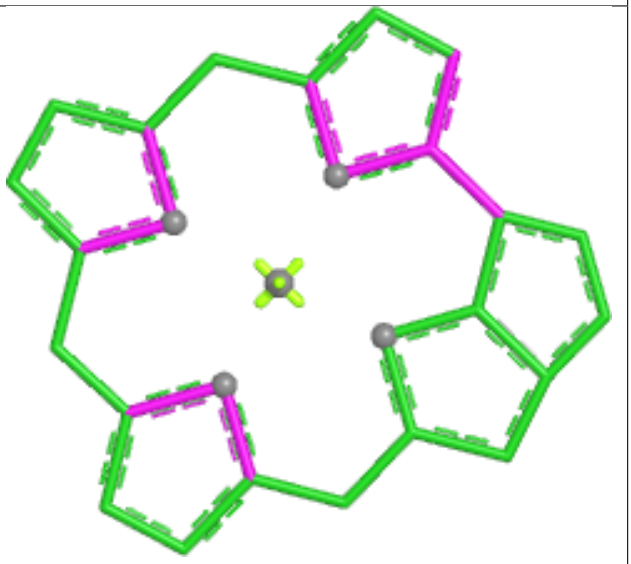


Rings

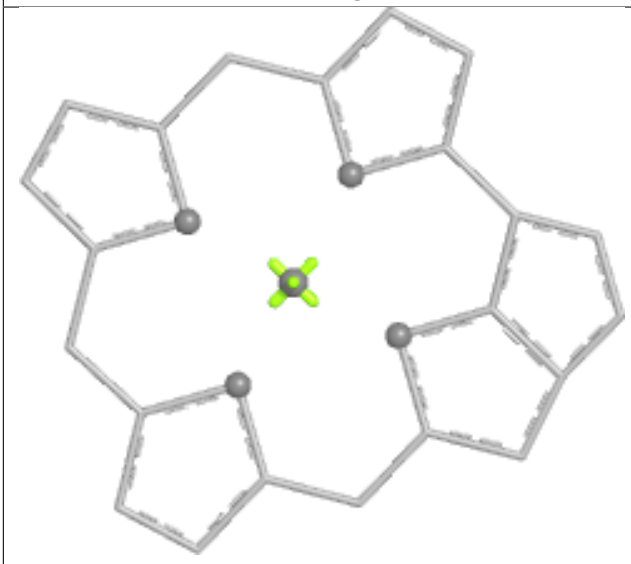
Ligand CLA M 162



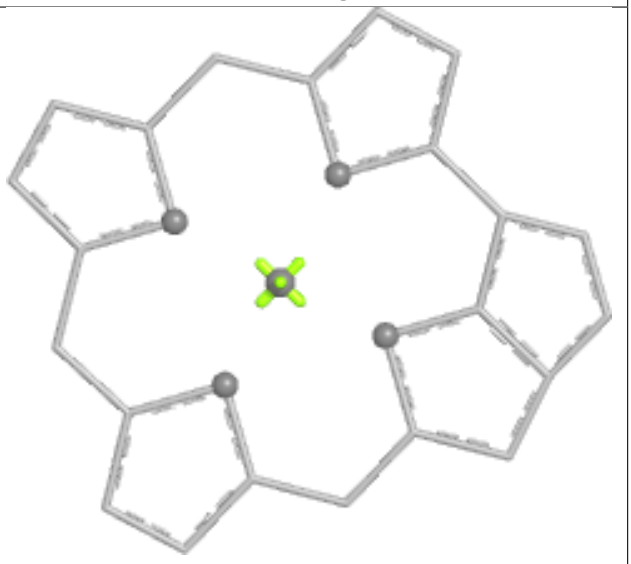
Bond lengths



Bond angles

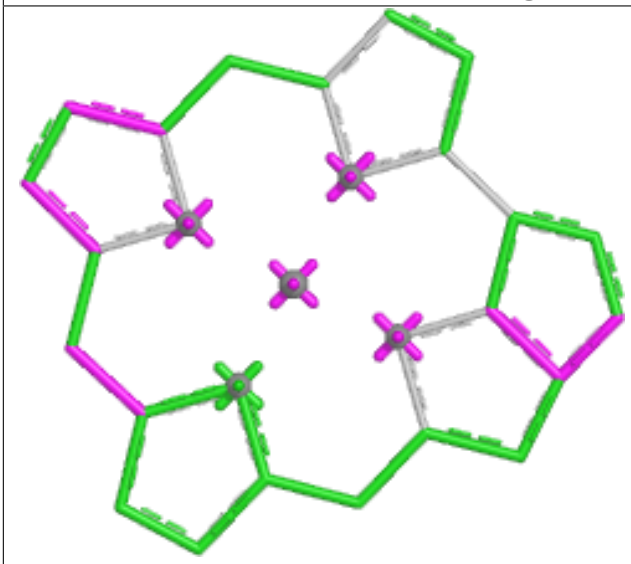


Torsions

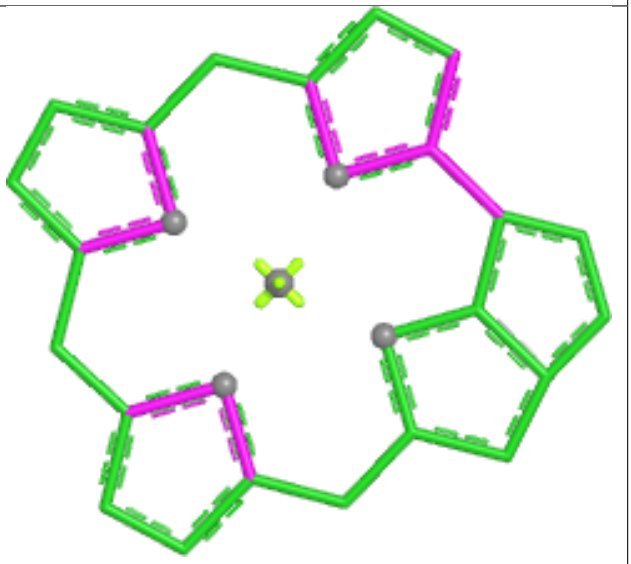


Rings

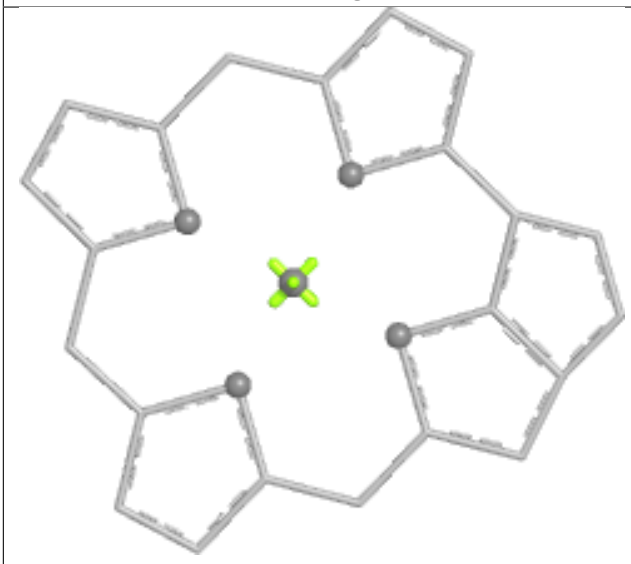
Ligand CLA M 163



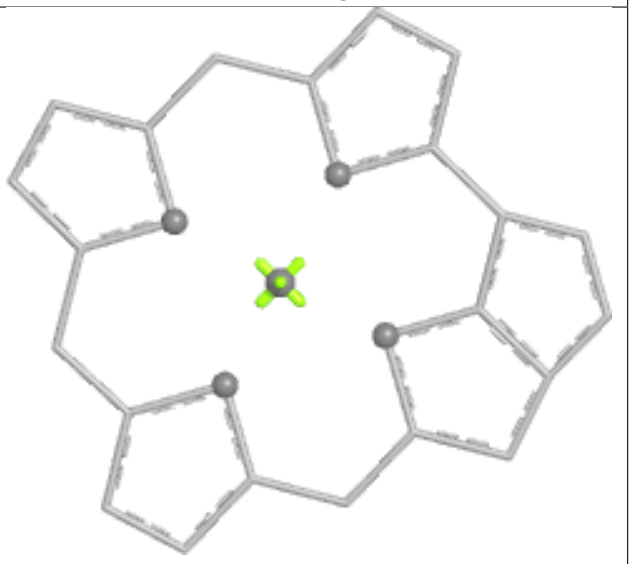
Bond lengths



Bond angles

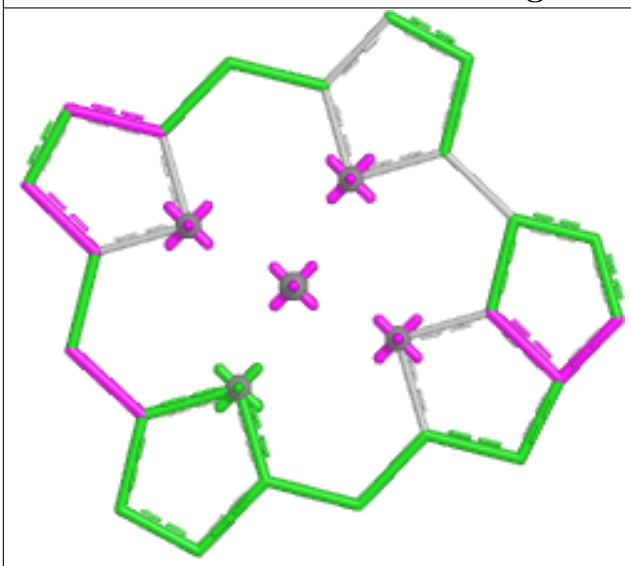


Torsions

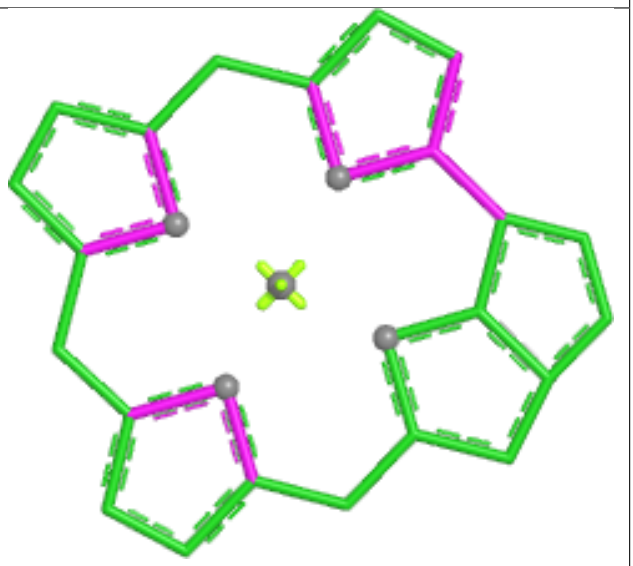


Rings

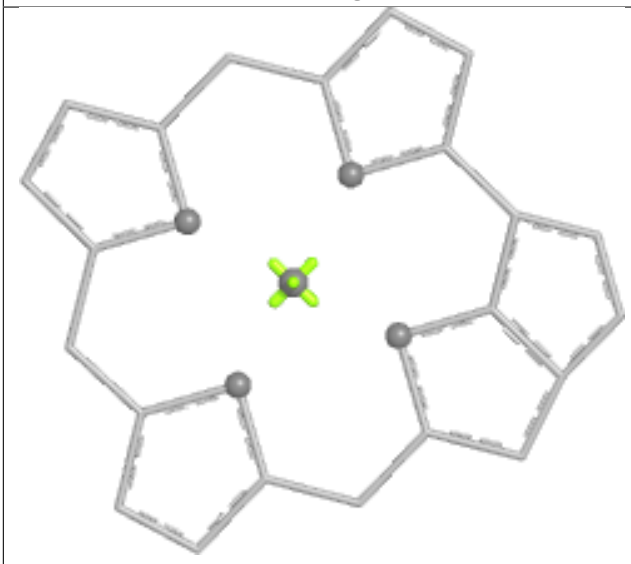
Ligand CLA L 161



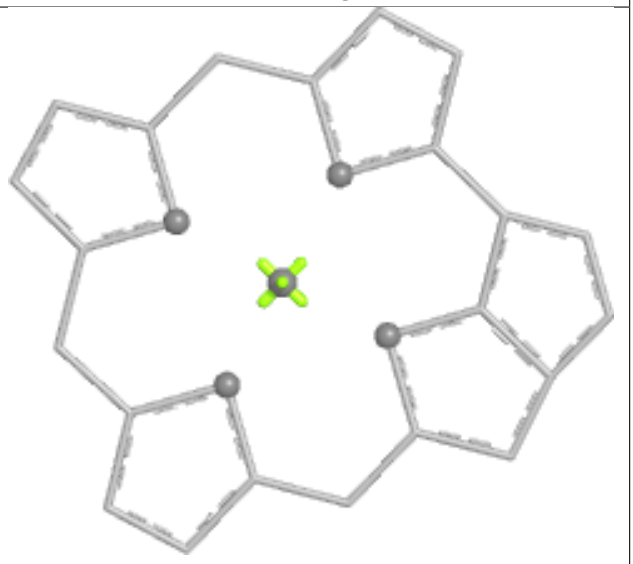
Bond lengths



Bond angles

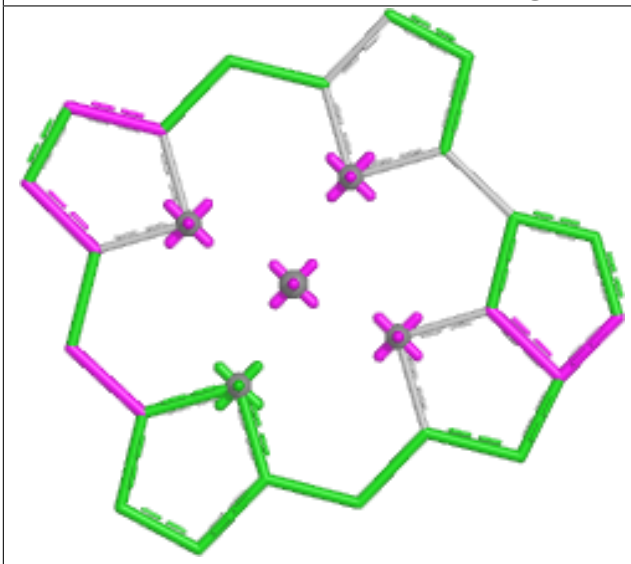


Torsions

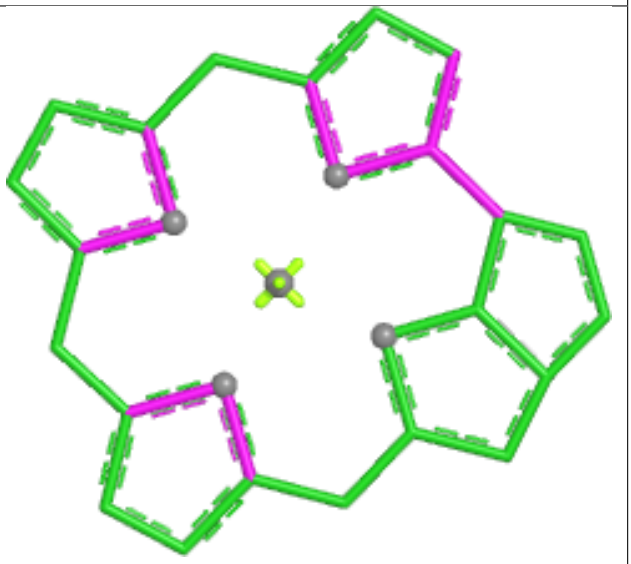


Rings

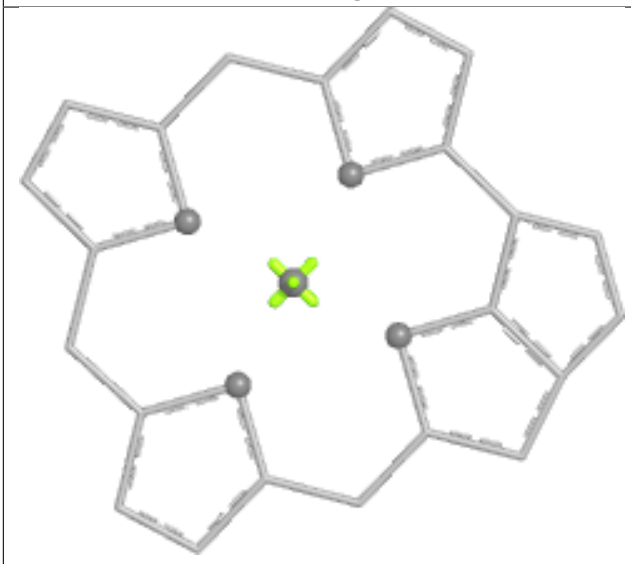
Ligand CLA L 162



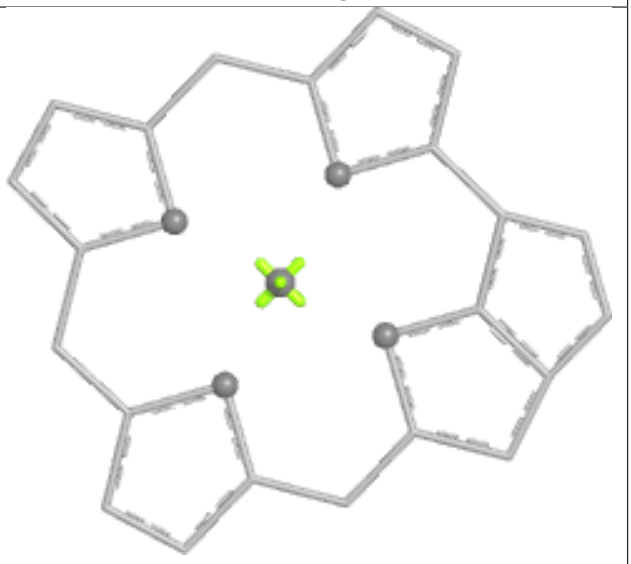
Bond lengths



Bond angles

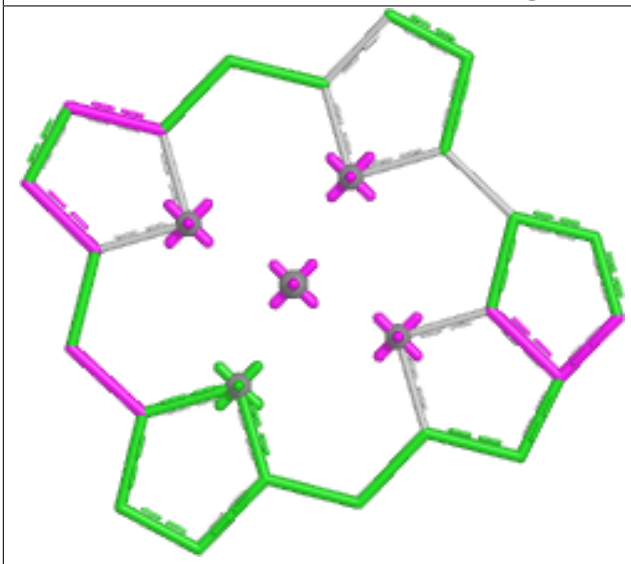


Torsions

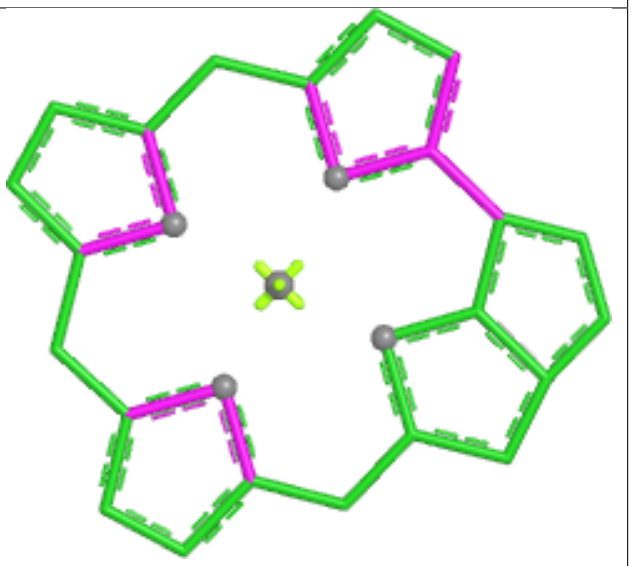


Rings

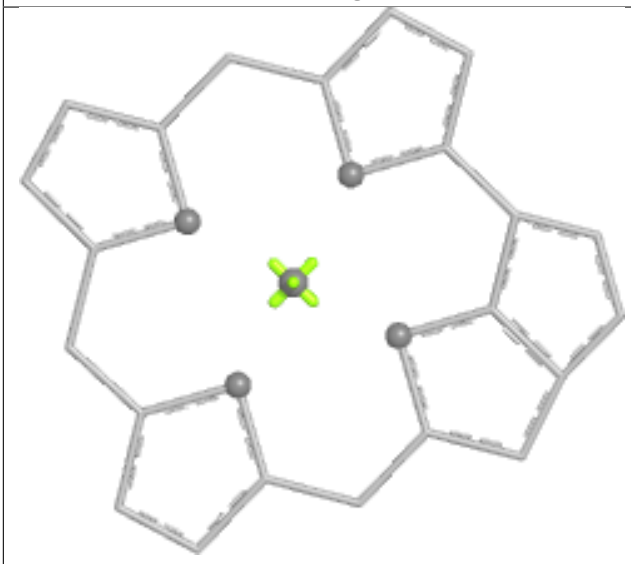
Ligand CLA D 164



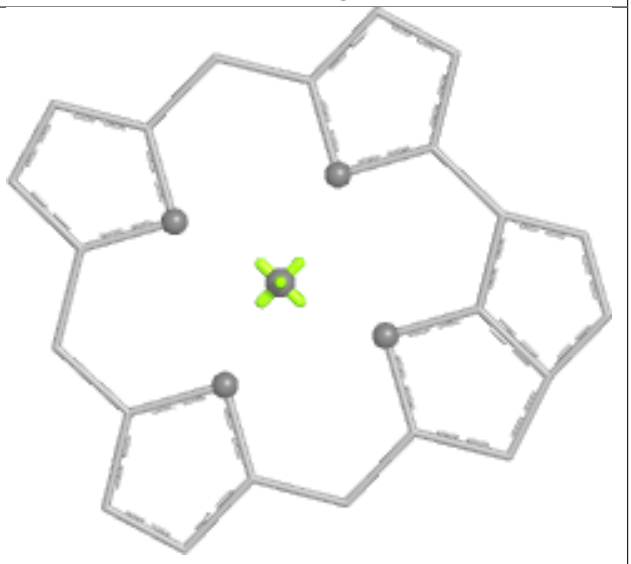
Bond lengths



Bond angles

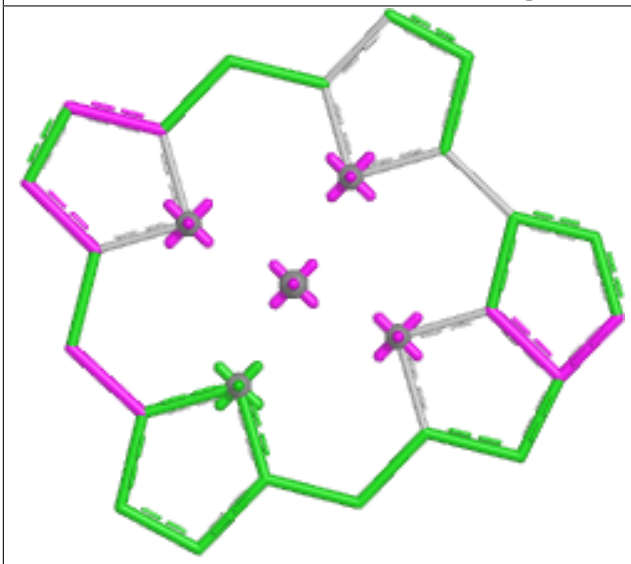


Torsions

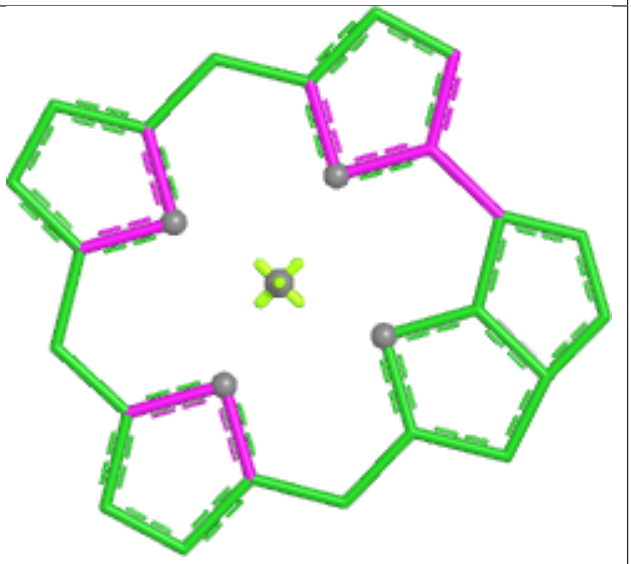


Rings

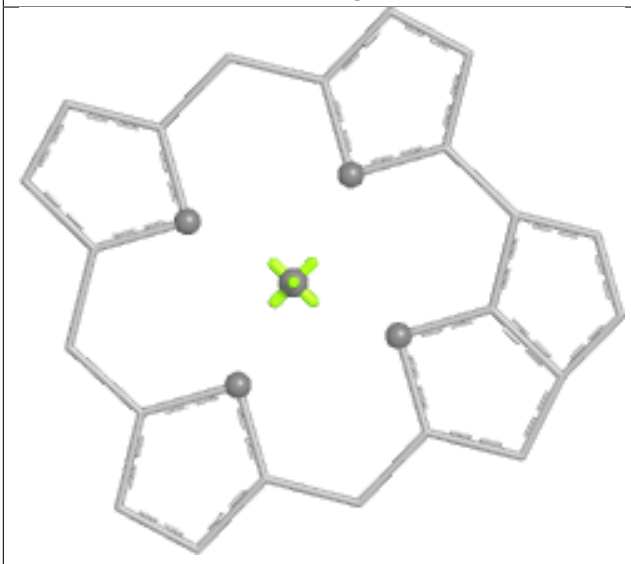
Ligand CLA M 166



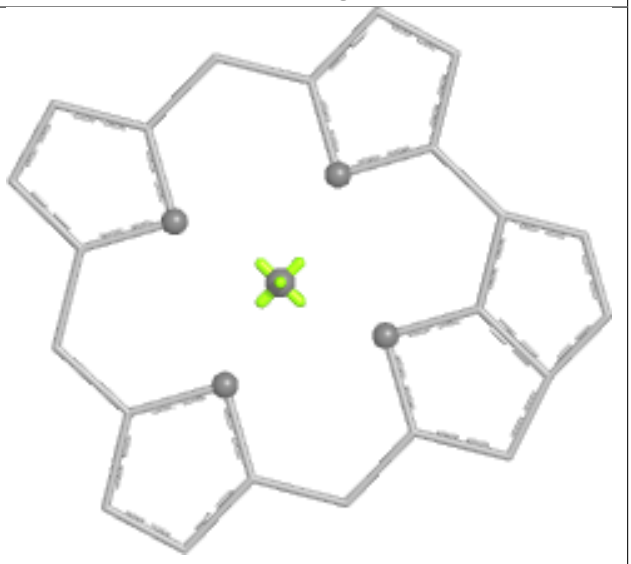
Bond lengths



Bond angles

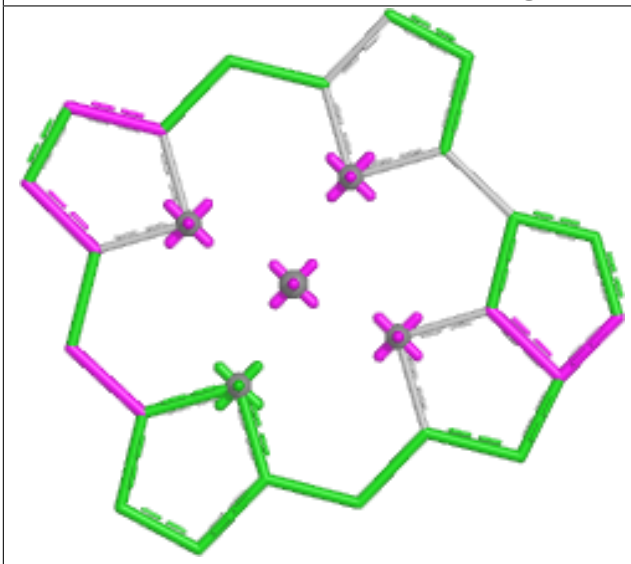


Torsions

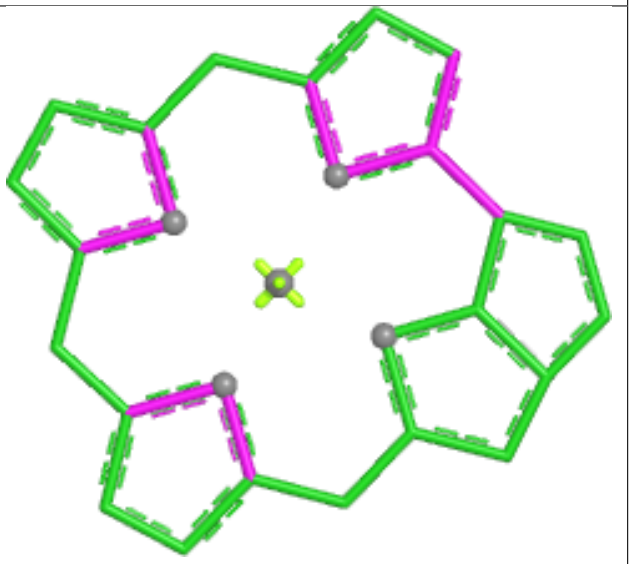


Rings

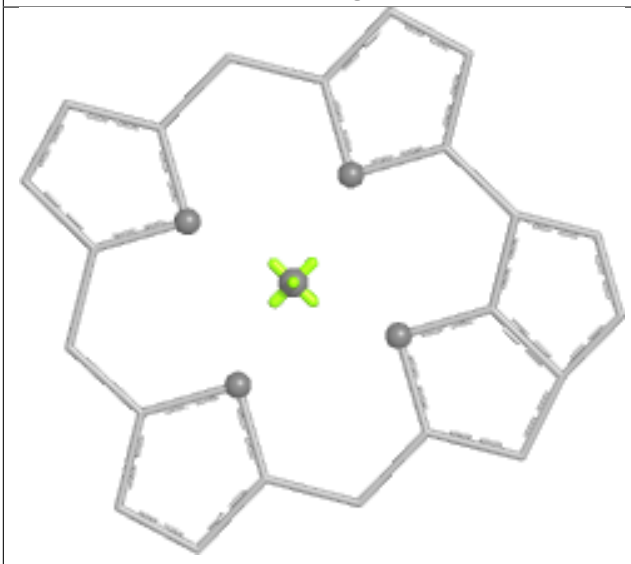
Ligand CLA M 168



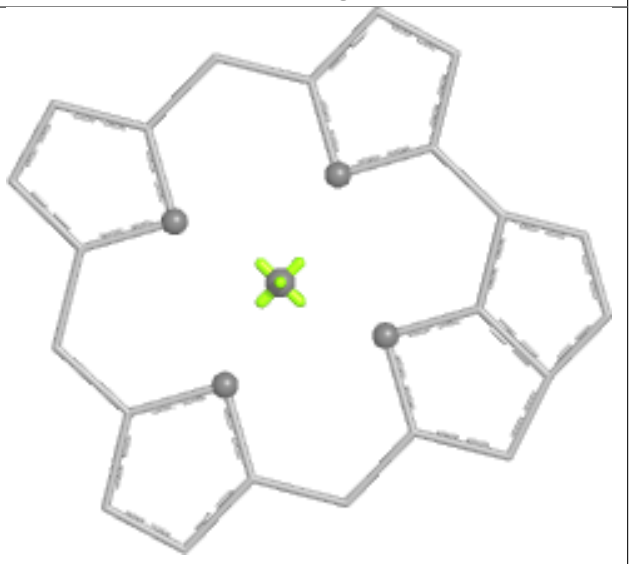
Bond lengths



Bond angles

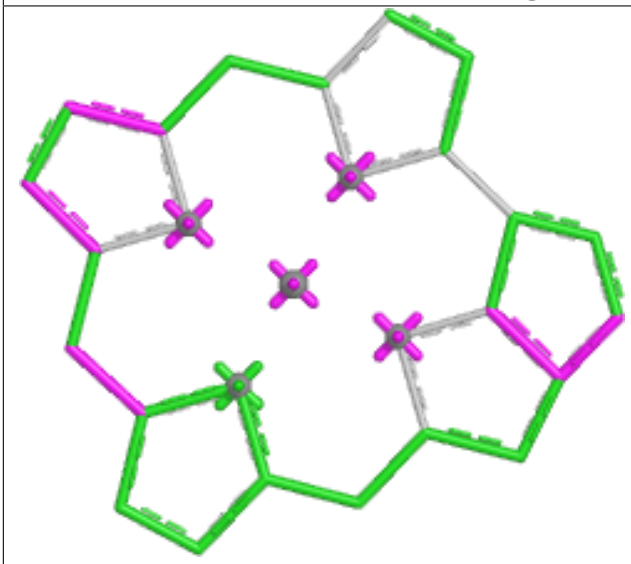


Torsions

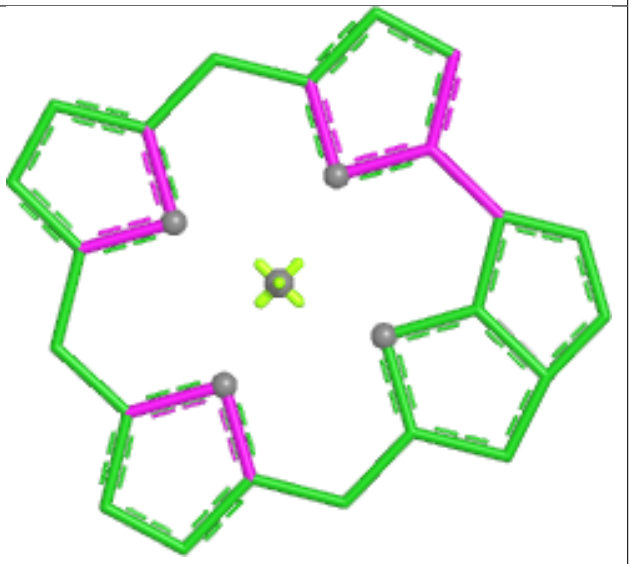


Rings

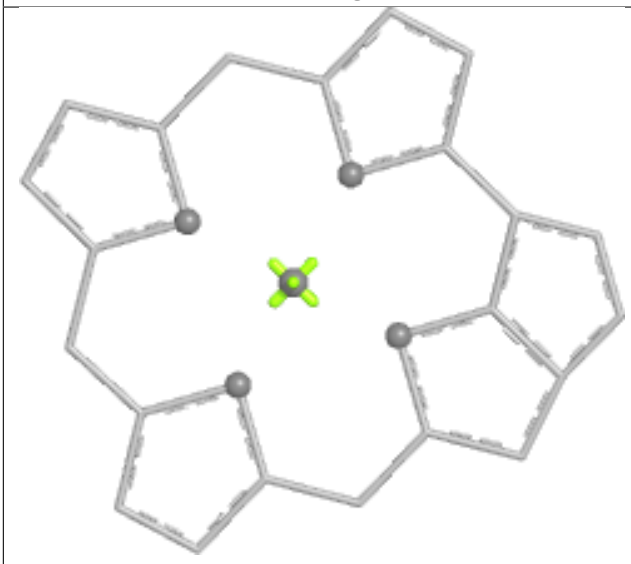
Ligand CLA D 167



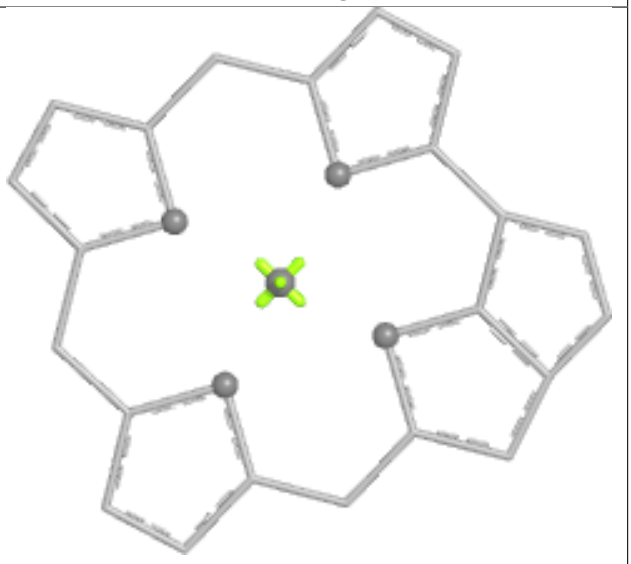
Bond lengths



Bond angles

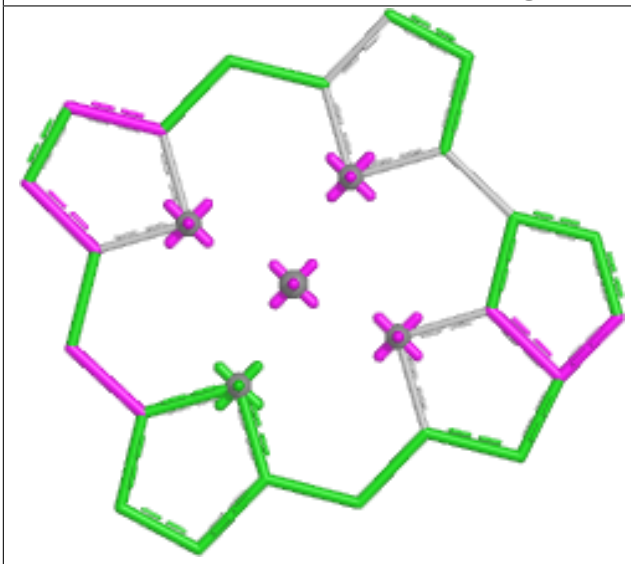


Torsions

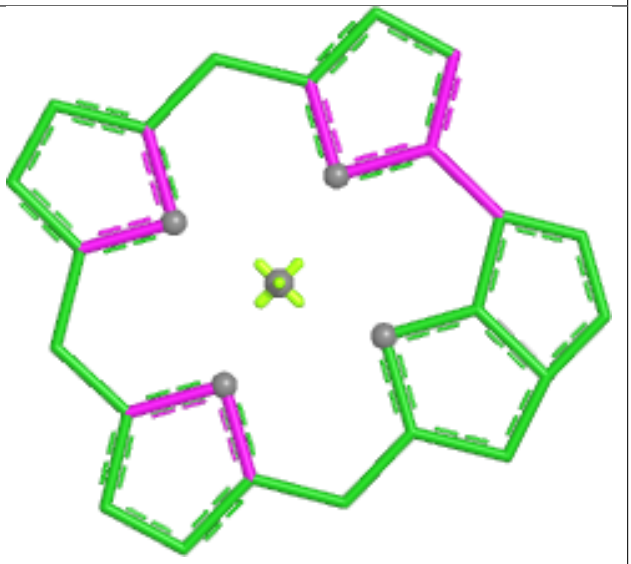


Rings

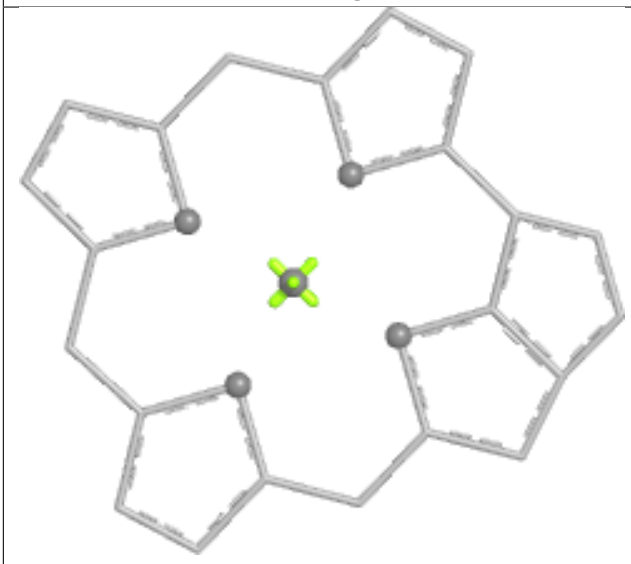
Ligand CLA M 170



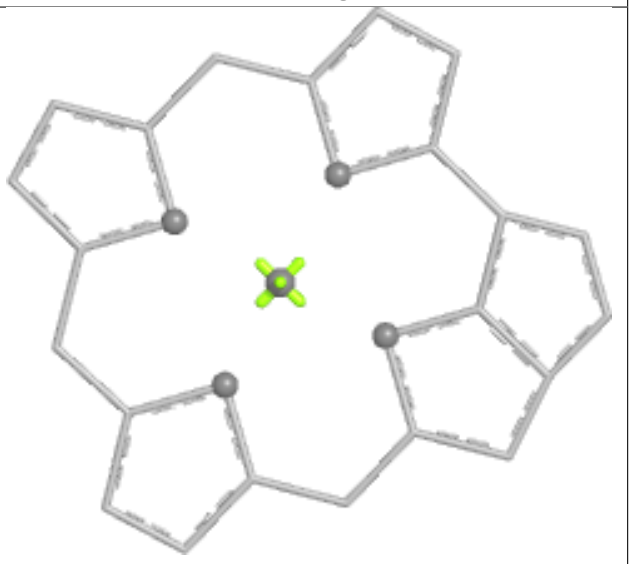
Bond lengths



Bond angles

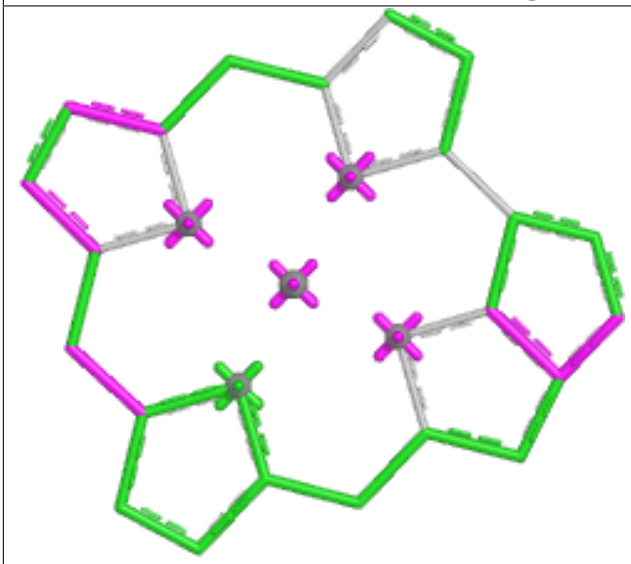


Torsions

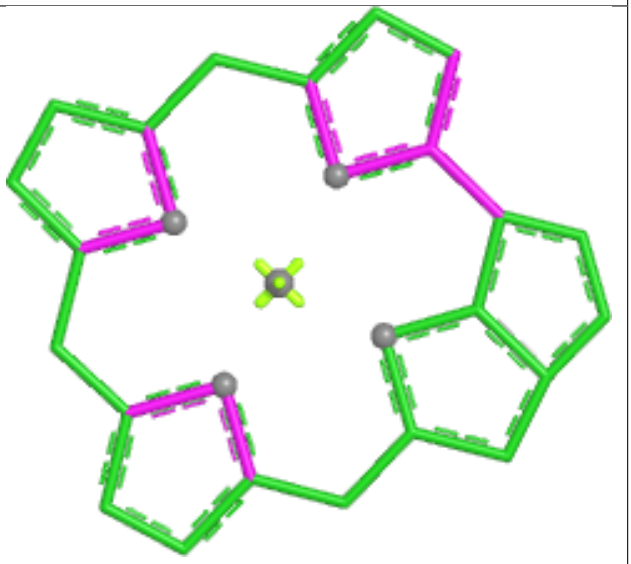


Rings

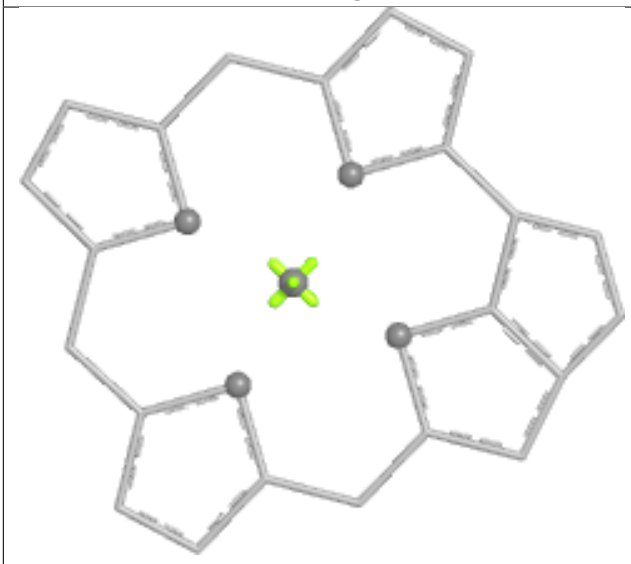
Ligand CLA D 161



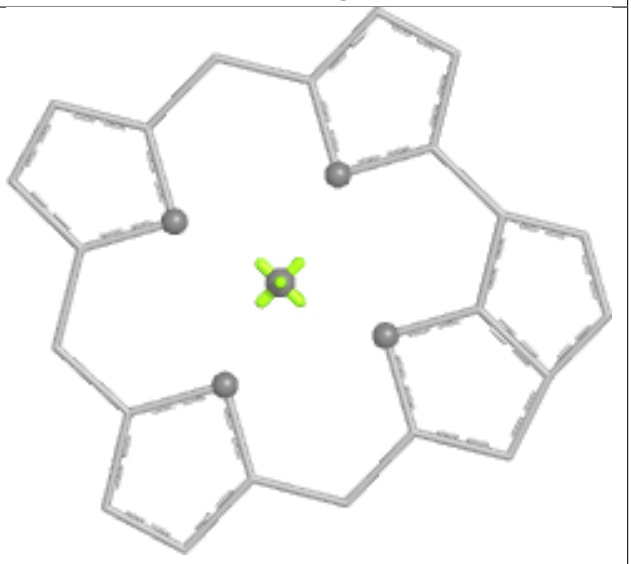
Bond lengths



Bond angles

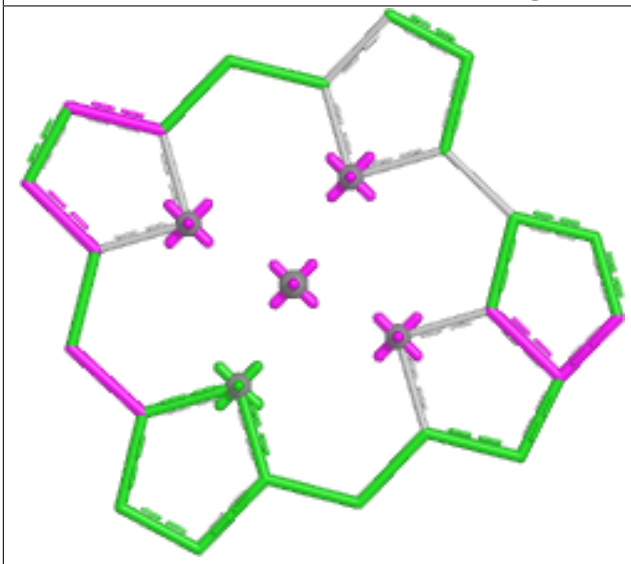


Torsions

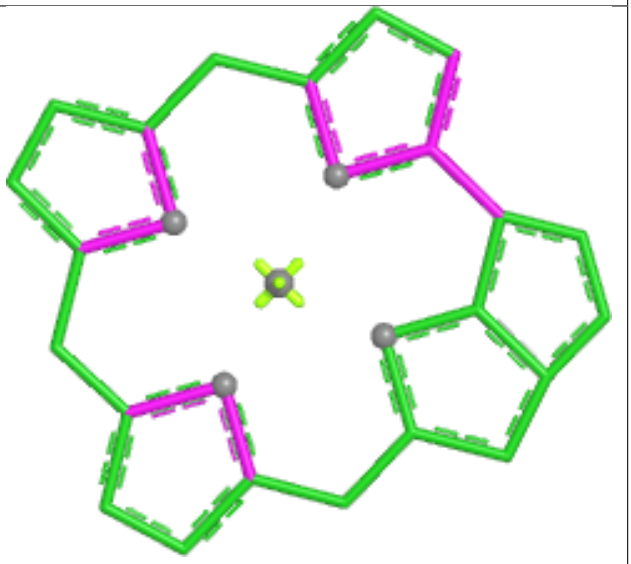


Rings

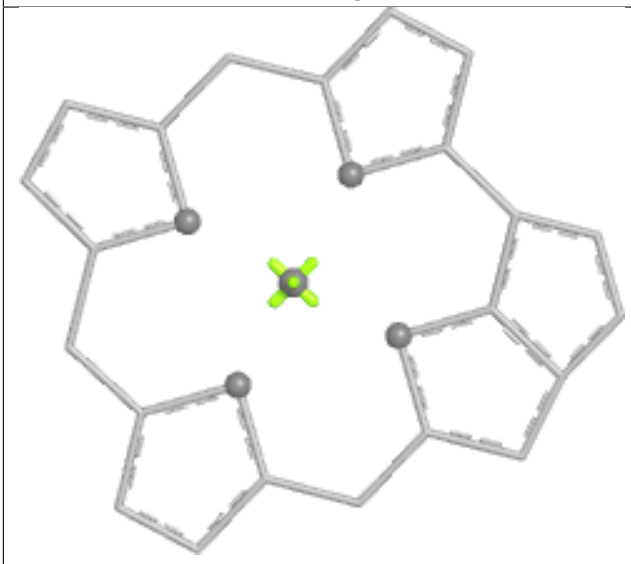
Ligand CLA L 157



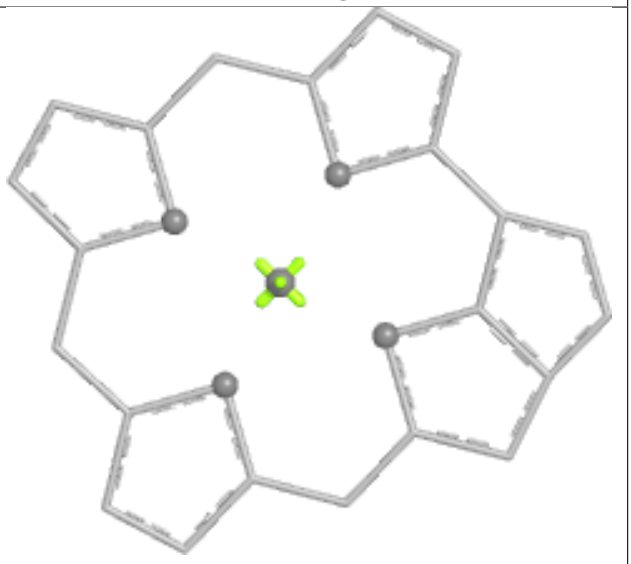
Bond lengths



Bond angles

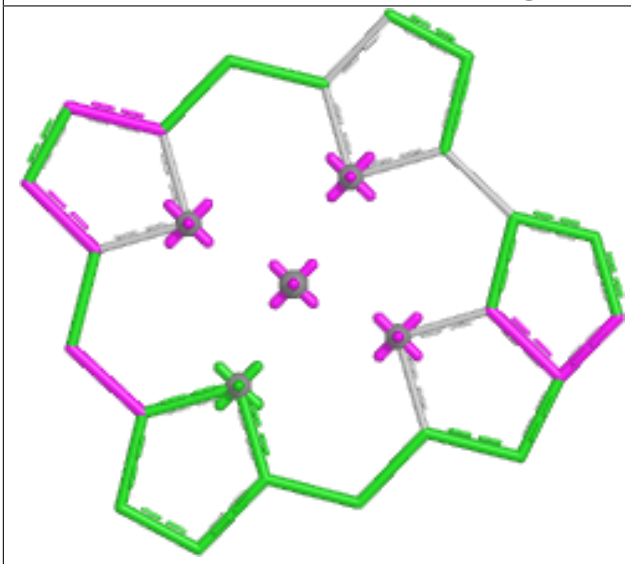


Torsions

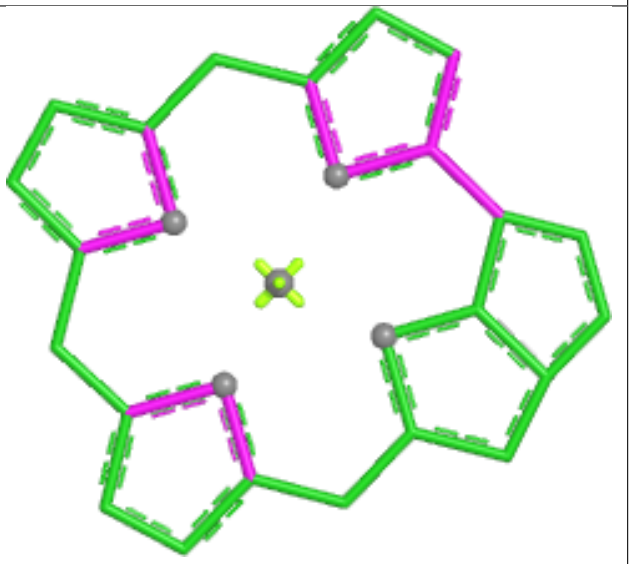


Rings

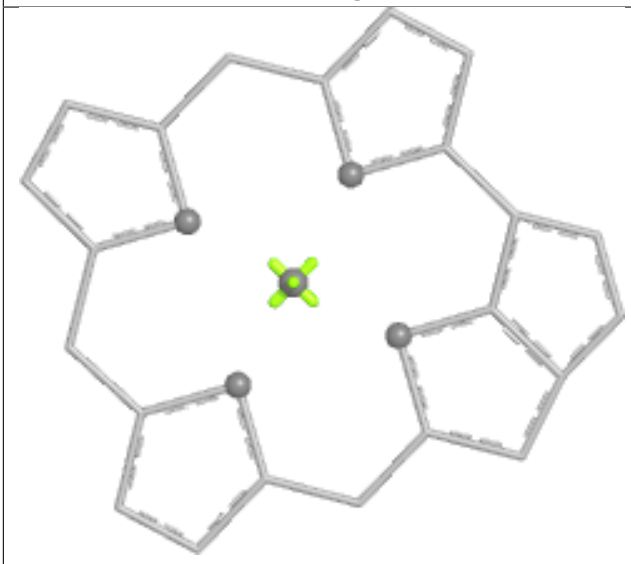
Ligand CLA M 169



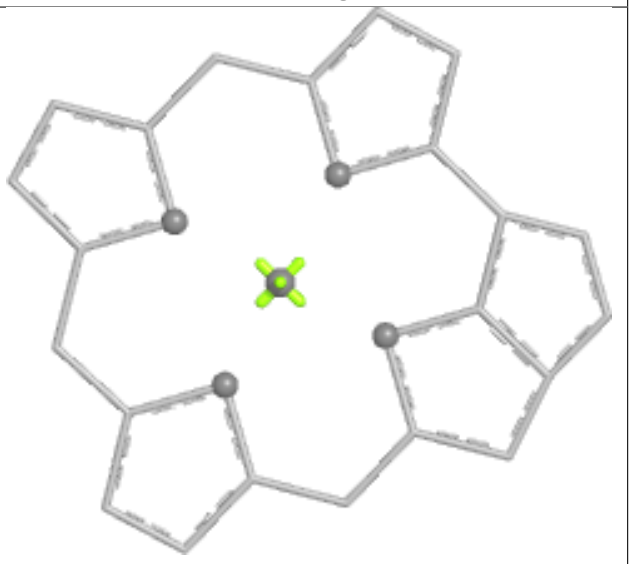
Bond lengths



Bond angles

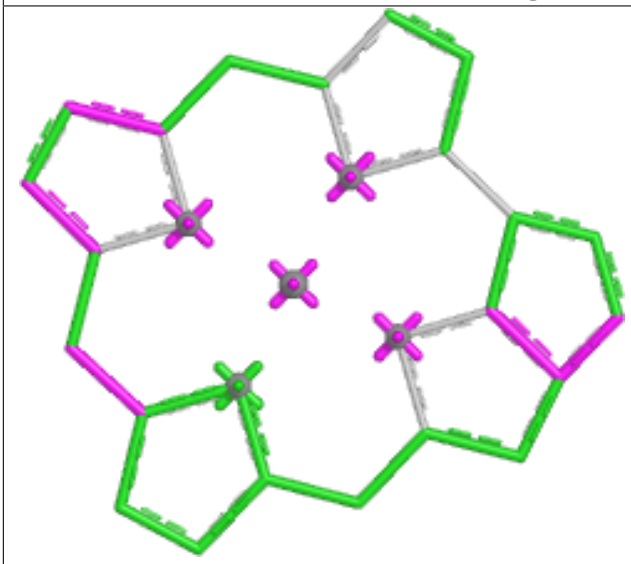


Torsions

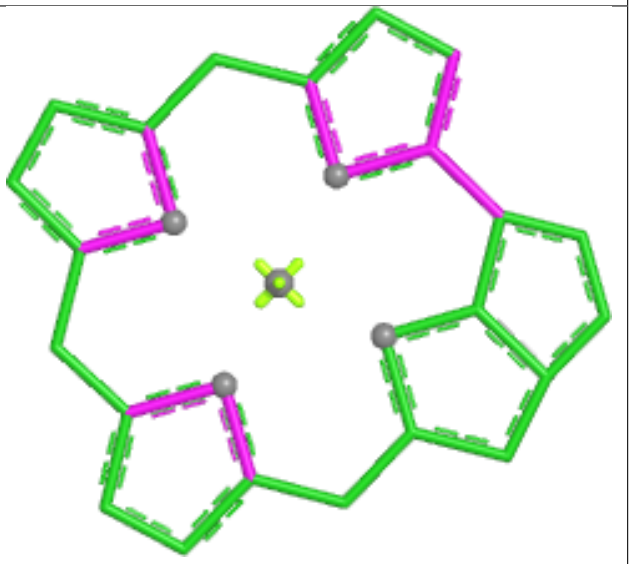


Rings

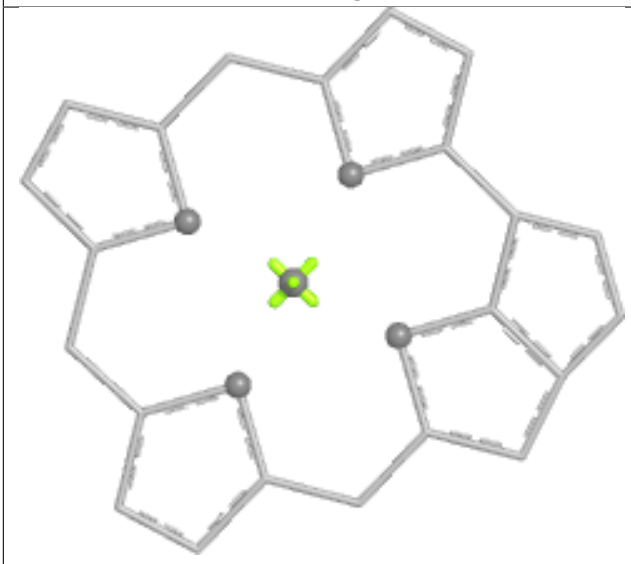
Ligand CLA C 167



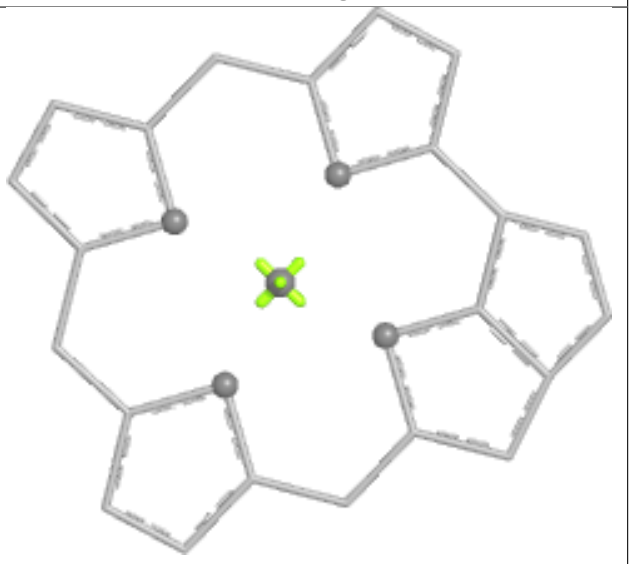
Bond lengths



Bond angles

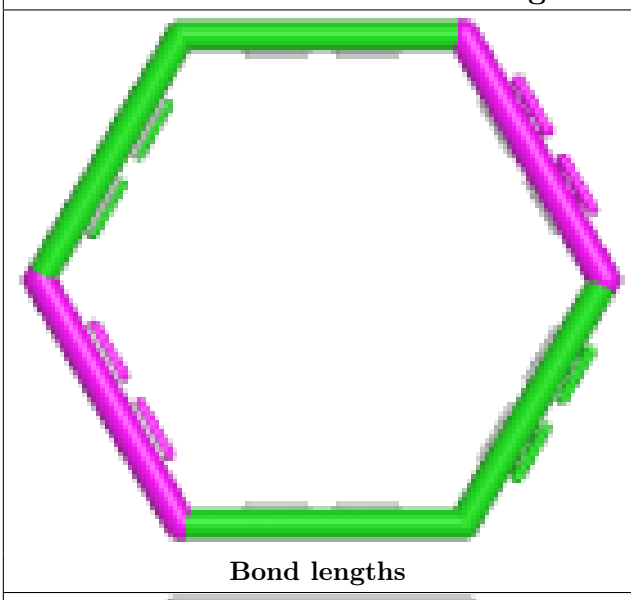


Torsions

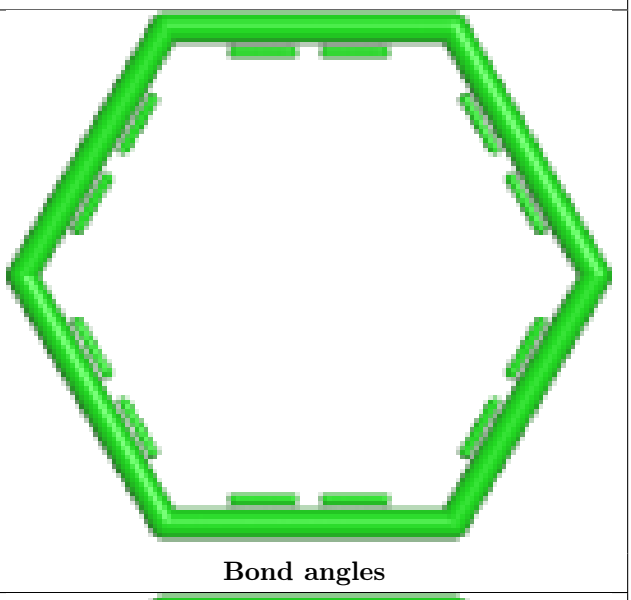


Rings

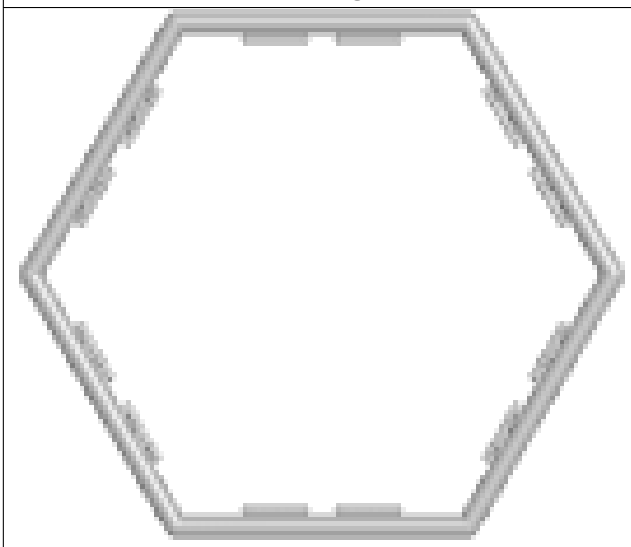
Ligand PL9 K 179



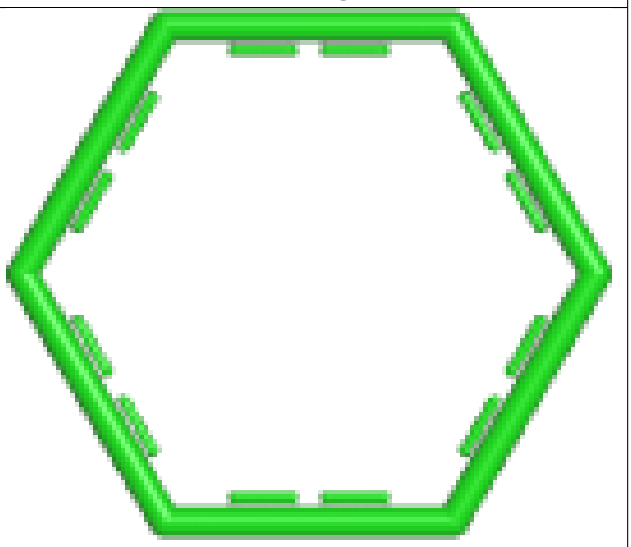
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.