



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:14 am BST

PDB ID : 1ILX
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

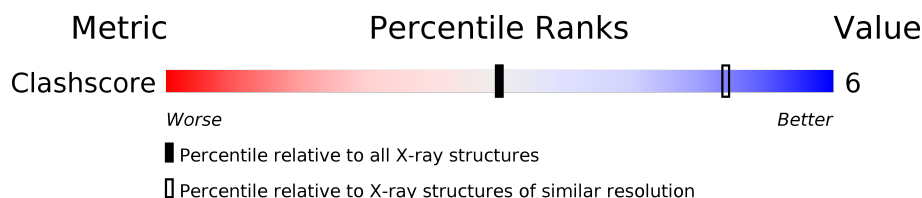
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

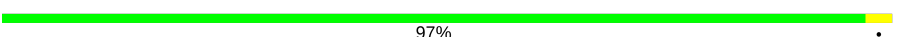




Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1288 (4.00-3.60)









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

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%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	A	174	X	-	-	-
11	CLA	A	175	X	-	-	-
11	CLA	A	176	X	-	-	-
11	CLA	A	178	X	-	-	-
11	CLA	A	179	X	-	-	-
11	CLA	B	176	X	-	-	-
11	CLA	B	178	X	-	-	-
11	CLA	C	157	X	-	-	-
11	CLA	C	158	X	-	-	-
11	CLA	C	159	X	-	-	-
11	CLA	C	160	X	-	-	-
11	CLA	C	161	X	-	-	-
11	CLA	C	162	X	-	-	-
11	CLA	C	163	X	-	-	-
11	CLA	C	164	X	-	-	-
11	CLA	C	165	X	-	-	-
11	CLA	C	166	X	-	-	-
11	CLA	C	167	X	-	-	-
11	CLA	C	168	X	-	-	-
11	CLA	D	156	X	-	-	-
11	CLA	D	157	X	-	-	-
11	CLA	D	158	X	-	-	-
11	CLA	D	159	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	D	160	X	-	-	-
11	CLA	D	161	X	-	-	-
11	CLA	D	162	X	-	-	-
11	CLA	D	163	X	-	-	-
11	CLA	D	164	X	-	-	-
11	CLA	D	165	X	-	-	-
11	CLA	D	166	X	-	-	-
11	CLA	D	167	X	-	-	-
11	CLA	D	168	X	-	-	-
11	CLA	D	169	X	-	-	-
11	CLA	D	170	X	-	-	-
11	CLA	G	313	X	-	-	-
11	CLA	J	174	X	-	-	-
11	CLA	J	175	X	-	-	-
11	CLA	J	176	X	-	-	-
11	CLA	J	178	X	-	-	-
11	CLA	J	179	X	-	-	-
11	CLA	K	176	X	-	-	-
11	CLA	K	178	X	-	-	-
11	CLA	L	157	X	-	-	-
11	CLA	L	158	X	-	-	-
11	CLA	L	159	X	-	-	-
11	CLA	L	160	X	-	-	-
11	CLA	L	161	X	-	-	-
11	CLA	L	162	X	-	-	-
11	CLA	L	163	X	-	-	-
11	CLA	L	164	X	-	-	-
11	CLA	L	165	X	-	-	-
11	CLA	L	166	X	-	-	-
11	CLA	L	167	X	-	-	-
11	CLA	L	168	X	-	-	-
11	CLA	M	156	X	-	-	-
11	CLA	M	157	X	-	-	-
11	CLA	M	158	X	-	-	-
11	CLA	M	159	X	-	-	-
11	CLA	M	160	X	-	-	-
11	CLA	M	161	X	-	-	-
11	CLA	M	162	X	-	-	-
11	CLA	M	163	X	-	-	-
11	CLA	M	164	X	-	-	-
11	CLA	M	165	X	-	-	-
11	CLA	M	166	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	M	167	X	-	-	-
11	CLA	M	168	X	-	-	-
11	CLA	M	169	X	-	-	-
11	CLA	M	170	X	-	-	-
11	CLA	P	313	X	-	-	-

2 Entry composition

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 (three-letter code: MN) (formula: Mn).

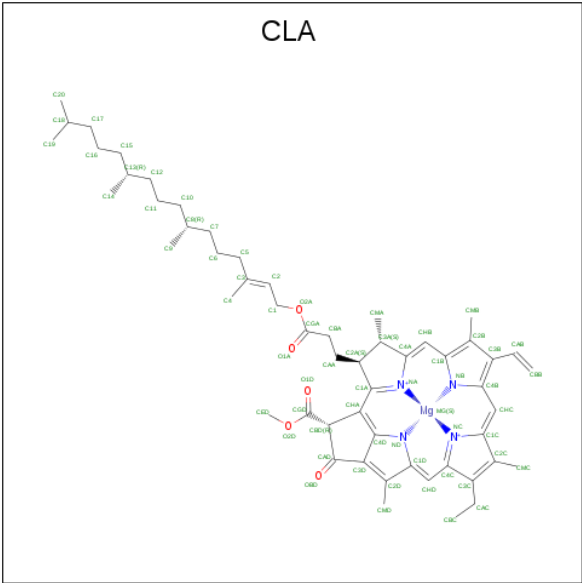
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	J	4	Total Mn 4 4	0	0

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

- Molecule 11 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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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	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		

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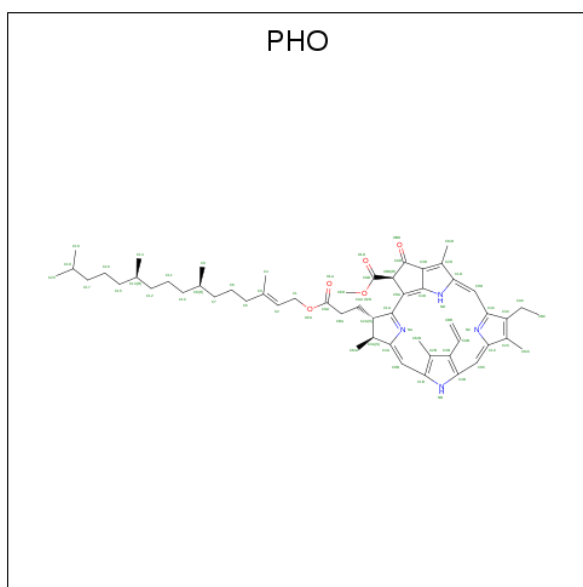
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	D	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	G	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	J	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	J	1	Total	C	Mg	N	0	0
			27	22	1	4		
11	J	1	Total	C	Mg	N	0	0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

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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	P	1	Total	C	Mg	N	0	0
			27	22	1	4		

- Molecule 12 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).

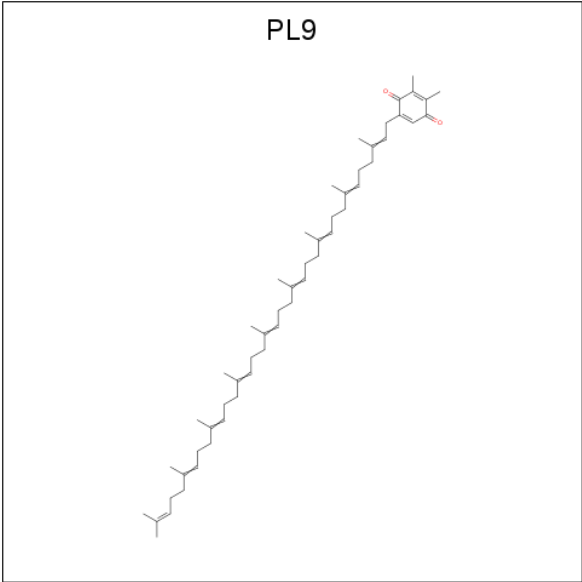


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	N	0	0
			26	22	4		
12	B	1	Total	C	N	0	0
			26	22	4		
12	J	1	Total	C	N	0	0
			26	22	4		
12	K	1	Total	C	N	0	0
			26	22	4		

- Molecule 13 is FE (III) ION (three-letter code: FE) (formula: Fe).

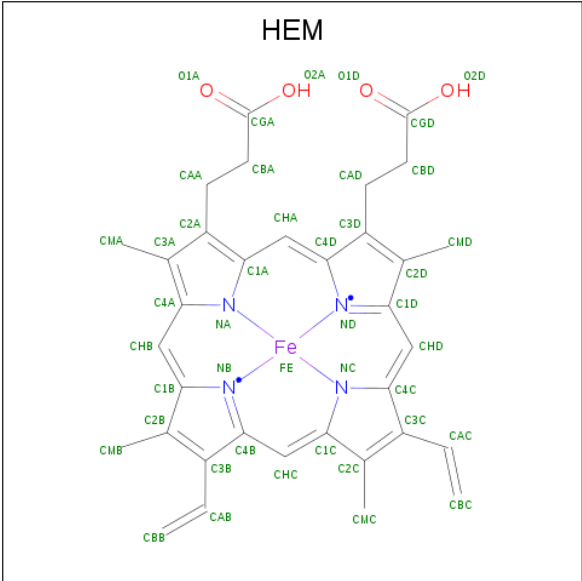
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	Fe	0	0
			1	1		
13	K	1	Total	Fe	0	0
			1	1		

- 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 (three-letter code: PL9) (formula: C₅₃H₈₀O₂).



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

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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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 (three-letter code: 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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: PHOTOSYSTEM II: SUBUNIT PSBA

Chain A:  97%



- Molecule 1: PHOTOSYSTEM II: SUBUNIT PSBA

Chain J:  97%



- Molecule 2: PHOTOSYSTEM II: SUBUNIT PSBD

Chain B:  97%



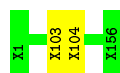
- Molecule 2: PHOTOSYSTEM II: SUBUNIT PSBD

Chain K:  97%



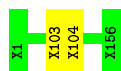
- Molecule 3: PHOTOSYSTEM II: SUBUNIT PSBC

Chain C:  99%



- Molecule 3: PHOTOSYSTEM II: SUBUNIT PSBC

Chain L:  99%



- Molecule 4: PHOTOSYSTEM II: SUBUNIT PSBB

Chain D:  99%



- Molecule 4: PHOTOSYSTEM II: SUBUNIT PSBB

Chain M:  99%



- Molecule 5: PHOTOSYSTEM II: SUBUNIT PSBE

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: PHOTOSYSTEM II: SUBUNIT PSBE

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: PHOTOSYSTEM II: SUBUNIT PSBF

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: PHOTOSYSTEM II: SUBUNIT PSBF

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: PHOTOSYSTEM II: SUBUNIT UNKNOWN

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: PHOTOSYSTEM II: SUBUNIT UNKNOWN

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PHOTOSYSTEM II: SUBUNIT PSBO

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PHOTOSYSTEM II: SUBUNIT PSBO

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PHOTOSYSTEM II: SUBUNIT PSBV

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PHOTOSYSTEM II: SUBUNIT PSBV

Chain R:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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: PHO, MN, CLA, PL9, CD, FE, HEM

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	169	0	0	4	0
1	J	169	0	0	4	0
2	B	174	0	0	4	0
2	K	174	0	0	4	0
3	C	156	0	0	2	0
3	L	156	0	0	2	0
4	D	155	0	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	87	0	0	0	0
9	R	87	0	0	0	0
10	A	4	0	0	0	0
10	J	4	0	0	0	0
11	A	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

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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 [i](#)

5.3.1 Protein backbone [i](#)

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

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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$
15	HEM	I	88	-	12,32,50	3.17	2 (16%)	23,54,82	3.69	11 (47%)
11	CLA	M	159	-	23,35,73	3.16	8 (34%)	26,60,113	2.65	6 (23%)
11	CLA	C	163	-	23,35,73	3.15	8 (34%)	26,60,113	2.65	6 (23%)
11	CLA	M	158	-	23,35,73	3.15	8 (34%)	26,60,113	2.61	6 (23%)
11	CLA	A	174	-	23,35,73	3.15	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	C	162	-	23,35,73	3.16	8 (34%)	26,60,113	2.62	6 (23%)
11	CLA	J	175	-	23,35,73	3.16	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	B	176	-	23,35,73	3.14	8 (34%)	26,60,113	2.61	6 (23%)
11	CLA	C	166	-	23,35,73	3.15	8 (34%)	26,60,113	2.62	6 (23%)
11	CLA	G	313	-	23,35,73	3.16	8 (34%)	26,60,113	2.63	6 (23%)
12	PHO	B	177	-	30,31,69	1.39	4 (13%)	34,46,99	0.94	1 (2%)
14	PL9	K	179	-	6,6,55	2.44	2 (33%)	6,6,69	1.03	0
11	CLA	C	159	-	23,35,73	3.17	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	A	176	-	23,35,73	3.14	8 (34%)	26,60,113	2.62	6 (23%)
11	CLA	A	178	-	23,35,73	3.17	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	J	179	-	23,35,73	3.17	8 (34%)	26,60,113	2.61	6 (23%)
11	CLA	M	170	-	23,35,73	3.15	8 (34%)	26,60,113	2.62	6 (23%)
11	CLA	K	178	-	23,35,73	3.14	8 (34%)	26,60,113	2.59	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	D	160	-	23,35,73	3.18	8 (34%)	26,60,113	2.65	6 (23%)
11	CLA	M	157	-	23,35,73	3.15	8 (34%)	26,60,113	2.62	6 (23%)
11	CLA	D	161	-	23,35,73	3.15	8 (34%)	26,60,113	2.64	6 (23%)
15	HEM	F	50	-	12,32,50	3.16	2 (16%)	23,54,82	3.66	11 (47%)
11	CLA	L	162	-	23,35,73	3.16	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	L	165	-	23,35,73	3.14	8 (34%)	26,60,113	2.65	6 (23%)
11	CLA	M	162	-	23,35,73	3.16	8 (34%)	26,60,113	2.61	6 (23%)
12	PHO	A	177	-	30,31,69	1.39	4 (13%)	34,46,99	0.94	1 (2%)
14	PL9	B	179	-	6,6,55	2.45	2 (33%)	6,6,69	1.03	0
11	CLA	J	174	-	23,35,73	3.14	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	L	167	-	23,35,73	3.18	8 (34%)	26,60,113	2.62	6 (23%)
11	CLA	K	176	-	23,35,73	3.13	8 (34%)	26,60,113	2.61	6 (23%)
11	CLA	C	157	-	23,35,73	3.15	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	A	175	-	23,35,73	3.15	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	D	158	-	23,35,73	3.15	8 (34%)	26,60,113	2.65	6 (23%)
11	CLA	D	167	-	23,35,73	3.16	8 (34%)	26,60,113	2.62	6 (23%)
11	CLA	M	156	-	23,35,73	3.16	8 (34%)	26,60,113	2.66	6 (23%)
11	CLA	M	169	-	23,35,73	3.14	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	D	163	-	23,35,73	3.16	8 (34%)	26,60,113	2.65	6 (23%)
15	HEM	R	91	-	12,32,50	3.17	2 (16%)	23,54,82	3.69	11 (47%)
11	CLA	M	168	-	23,35,73	3.19	8 (34%)	26,60,113	2.66	6 (23%)
11	CLA	C	160	-	23,35,73	3.14	8 (34%)	26,60,113	2.61	6 (23%)
15	HEM	O	90	-	12,32,50	3.17	2 (16%)	23,54,82	3.65	11 (47%)
11	CLA	J	178	-	23,35,73	3.17	8 (34%)	26,60,113	2.65	6 (23%)
11	CLA	P	313	-	23,35,73	3.16	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	M	161	-	23,35,73	3.16	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	L	159	-	23,35,73	3.16	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	A	179	-	23,35,73	3.17	8 (34%)	26,60,113	2.61	6 (23%)
11	CLA	L	158	-	23,35,73	3.13	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	D	168	-	23,35,73	3.18	8 (34%)	26,60,113	2.65	6 (23%)
11	CLA	D	166	-	23,35,73	3.15	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	D	169	-	23,35,73	3.14	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	D	159	-	23,35,73	3.16	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	L	168	-	23,35,73	3.16	8 (34%)	26,60,113	2.67	6 (23%)
11	CLA	D	156	-	23,35,73	3.16	8 (34%)	26,60,113	2.65	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	M	160	-	23,35,73	3.17	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	C	167	-	23,35,73	3.17	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	B	178	-	23,35,73	3.14	8 (34%)	26,60,113	2.61	6 (23%)
12	PHO	K	177	-	30,31,69	1.39	4 (13%)	34,46,99	0.93	1 (2%)
11	CLA	C	164	-	23,35,73	3.16	8 (34%)	26,60,113	2.61	6 (23%)
11	CLA	D	164	-	23,35,73	3.14	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	M	165	-	23,35,73	3.16	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	M	163	-	23,35,73	3.18	8 (34%)	26,60,113	2.65	6 (23%)
12	PHO	J	177	-	30,31,69	1.40	4 (13%)	34,46,99	0.95	1 (2%)
11	CLA	D	165	-	23,35,73	3.16	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	J	176	-	23,35,73	3.15	8 (34%)	26,60,113	2.61	6 (23%)
11	CLA	L	166	-	23,35,73	3.17	8 (34%)	26,60,113	2.60	6 (23%)
11	CLA	L	160	-	23,35,73	3.14	8 (34%)	26,60,113	2.62	6 (23%)
11	CLA	C	158	-	23,35,73	3.14	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	D	170	-	23,35,73	3.16	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	D	162	-	23,35,73	3.16	8 (34%)	26,60,113	2.61	6 (23%)
11	CLA	L	157	-	23,35,73	3.14	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	M	164	-	23,35,73	3.15	8 (34%)	26,60,113	2.65	6 (23%)
11	CLA	M	167	-	23,35,73	3.15	8 (34%)	26,60,113	2.61	6 (23%)
11	CLA	C	161	-	23,35,73	3.15	8 (34%)	26,60,113	2.63	6 (23%)
11	CLA	M	166	-	23,35,73	3.15	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	L	164	-	23,35,73	3.17	8 (34%)	26,60,113	2.61	6 (23%)
11	CLA	C	168	-	23,35,73	3.15	8 (34%)	26,60,113	2.66	6 (23%)
11	CLA	C	165	-	23,35,73	3.15	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	L	161	-	23,35,73	3.14	8 (34%)	26,60,113	2.64	6 (23%)
11	CLA	D	157	-	23,35,73	3.15	8 (34%)	26,60,113	2.62	6 (23%)
11	CLA	L	163	-	23,35,73	3.14	8 (34%)	26,60,113	2.64	6 (23%)

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
11	CLA	M	159	-	3/3/8/25	-	-
11	CLA	C	163	-	3/3/8/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	M	158	-	3/3/8/25	-	-
11	CLA	A	174	-	3/3/8/25	-	-
11	CLA	C	162	-	3/3/8/25	-	-
11	CLA	J	175	-	3/3/8/25	-	-
11	CLA	B	176	-	3/3/8/25	-	-
11	CLA	C	166	-	3/3/8/25	-	-
11	CLA	G	313	-	3/3/8/25	-	-
11	CLA	D	165	-	3/3/8/25	-	-
11	CLA	M	161	-	3/3/8/25	-	-
11	CLA	C	159	-	3/3/8/25	-	-
12	PHO	J	177	-	-	0/14/43/103	0/5/6/6
11	CLA	A	176	-	3/3/8/25	-	-
11	CLA	A	178	-	3/3/8/25	-	-
11	CLA	J	179	-	3/3/8/25	-	-
11	CLA	M	170	-	3/3/8/25	-	-
11	CLA	K	178	-	3/3/8/25	-	-
11	CLA	D	160	-	3/3/8/25	-	-
11	CLA	M	157	-	3/3/8/25	-	-
11	CLA	D	161	-	3/3/8/25	-	-
11	CLA	D	157	-	3/3/8/25	-	-
11	CLA	M	162	-	3/3/8/25	-	-
12	PHO	A	177	-	-	0/14/43/103	0/5/6/6
14	PL9	B	179	-	-	-	0/1/1/1
11	CLA	J	174	-	3/3/8/25	-	-
11	CLA	L	167	-	3/3/8/25	-	-
11	CLA	K	176	-	3/3/8/25	-	-
11	CLA	C	157	-	3/3/8/25	-	-
12	PHO	B	177	-	-	0/14/43/103	0/5/6/6
11	CLA	A	175	-	3/3/8/25	-	-
11	CLA	D	158	-	3/3/8/25	-	-
11	CLA	D	167	-	3/3/8/25	-	-
11	CLA	M	156	-	3/3/8/25	-	-
11	CLA	M	169	-	3/3/8/25	-	-
11	CLA	D	163	-	3/3/8/25	-	-
11	CLA	M	167	-	3/3/8/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	M	168	-	3/3/8/25	-	-
11	CLA	C	160	-	3/3/8/25	-	-
11	CLA	J	178	-	3/3/8/25	-	-
11	CLA	P	313	-	3/3/8/25	-	-
14	PL9	K	179	-	-	-	0/1/1/1
11	CLA	L	159	-	3/3/8/25	-	-
11	CLA	A	179	-	3/3/8/25	-	-
11	CLA	L	158	-	3/3/8/25	-	-
11	CLA	D	168	-	3/3/8/25	-	-
11	CLA	D	166	-	3/3/8/25	-	-
11	CLA	D	169	-	3/3/8/25	-	-
11	CLA	D	159	-	3/3/8/25	-	-
11	CLA	L	168	-	3/3/8/25	-	-
11	CLA	D	156	-	3/3/8/25	-	-
11	CLA	M	160	-	3/3/8/25	-	-
11	CLA	C	167	-	3/3/8/25	-	-
11	CLA	B	178	-	3/3/8/25	-	-
12	PHO	K	177	-	-	0/14/43/103	0/5/6/6
11	CLA	C	164	-	3/3/8/25	-	-
11	CLA	D	164	-	3/3/8/25	-	-
11	CLA	M	165	-	3/3/8/25	-	-
11	CLA	M	163	-	3/3/8/25	-	-
11	CLA	L	165	-	3/3/8/25	-	-
11	CLA	J	176	-	3/3/8/25	-	-
11	CLA	L	166	-	3/3/8/25	-	-
11	CLA	L	160	-	3/3/8/25	-	-
11	CLA	C	158	-	3/3/8/25	-	-
11	CLA	D	170	-	3/3/8/25	-	-
11	CLA	D	162	-	3/3/8/25	-	-
11	CLA	L	157	-	3/3/8/25	-	-
11	CLA	M	164	-	3/3/8/25	-	-
11	CLA	C	161	-	3/3/8/25	-	-
11	CLA	M	166	-	3/3/8/25	-	-
11	CLA	L	164	-	3/3/8/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	C	168	-	3/3/8/25	-	-
11	CLA	C	165	-	3/3/8/25	-	-
11	CLA	L	161	-	3/3/8/25	-	-
11	CLA	L	162	-	3/3/8/25	-	-
11	CLA	L	163	-	3/3/8/25	-	-

All (588) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	168	CLA	CHB-C4A	8.88	1.41	1.34
11	A	179	CLA	CHB-C4A	8.83	1.41	1.34
11	J	179	CLA	CHB-C4A	8.80	1.41	1.34
11	D	168	CLA	CHB-C4A	8.80	1.41	1.34
11	D	160	CLA	CHB-C4A	8.74	1.41	1.34
11	C	162	CLA	CHB-C4A	8.74	1.41	1.34
11	C	164	CLA	CHB-C4A	8.72	1.41	1.34
11	L	164	CLA	CHB-C4A	8.71	1.41	1.34
11	L	162	CLA	CHB-C4A	8.71	1.41	1.34
11	C	159	CLA	CHB-C4A	8.70	1.41	1.34
11	M	160	CLA	CHB-C4A	8.70	1.41	1.34
11	L	167	CLA	CHB-C4A	8.70	1.41	1.34
11	P	313	CLA	CHB-C4A	8.70	1.41	1.34
11	C	167	CLA	CHB-C4A	8.69	1.41	1.34
11	D	170	CLA	CHB-C4A	8.68	1.41	1.34
11	M	163	CLA	CHB-C4A	8.67	1.41	1.34
11	B	176	CLA	CHB-C4A	8.66	1.41	1.34
11	A	178	CLA	CHB-C4A	8.66	1.41	1.34
11	D	159	CLA	CHB-C4A	8.66	1.41	1.34
11	L	166	CLA	CHB-C4A	8.65	1.41	1.34
11	C	157	CLA	CHB-C4A	8.65	1.41	1.34
11	D	167	CLA	CHB-C4A	8.65	1.41	1.34
11	D	156	CLA	CHB-C4A	8.64	1.41	1.34
11	M	165	CLA	CHB-C4A	8.64	1.41	1.34
11	M	161	CLA	CHB-C4A	8.63	1.41	1.34
11	G	313	CLA	CHB-C4A	8.63	1.41	1.34
11	B	178	CLA	CHB-C4A	8.63	1.41	1.34
11	J	178	CLA	CHB-C4A	8.63	1.41	1.34
11	M	162	CLA	CHB-C4A	8.63	1.41	1.34
11	D	162	CLA	CHB-C4A	8.63	1.41	1.34
11	D	157	CLA	CHB-C4A	8.62	1.41	1.34
11	D	163	CLA	CHB-C4A	8.62	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	163	CLA	CHB-C4A	8.62	1.41	1.34
11	D	165	CLA	CHB-C4A	8.62	1.41	1.34
11	K	176	CLA	CHB-C4A	8.61	1.41	1.34
11	L	159	CLA	CHB-C4A	8.61	1.41	1.34
11	M	170	CLA	CHB-C4A	8.61	1.41	1.34
11	M	156	CLA	CHB-C4A	8.61	1.41	1.34
11	L	157	CLA	CHB-C4A	8.61	1.41	1.34
11	K	178	CLA	CHB-C4A	8.60	1.41	1.34
11	M	164	CLA	CHB-C4A	8.60	1.41	1.34
11	J	176	CLA	CHB-C4A	8.60	1.41	1.34
11	M	158	CLA	CHB-C4A	8.59	1.41	1.34
11	M	167	CLA	CHB-C4A	8.59	1.41	1.34
11	C	166	CLA	CHB-C4A	8.59	1.41	1.34
11	D	164	CLA	CHB-C4A	8.59	1.41	1.34
11	A	176	CLA	CHB-C4A	8.58	1.41	1.34
11	D	169	CLA	CHB-C4A	8.58	1.41	1.34
11	L	163	CLA	CHB-C4A	8.58	1.41	1.34
11	C	161	CLA	CHB-C4A	8.58	1.41	1.34
11	C	160	CLA	CHB-C4A	8.57	1.41	1.34
11	J	175	CLA	CHB-C4A	8.57	1.41	1.34
11	D	166	CLA	CHB-C4A	8.57	1.41	1.34
11	L	160	CLA	CHB-C4A	8.57	1.41	1.34
11	L	168	CLA	CHB-C4A	8.57	1.41	1.34
11	D	158	CLA	CHB-C4A	8.56	1.41	1.34
11	M	157	CLA	CHB-C4A	8.55	1.41	1.34
11	A	175	CLA	CHB-C4A	8.55	1.41	1.34
11	M	166	CLA	CHB-C4A	8.55	1.41	1.34
11	M	159	CLA	CHB-C4A	8.54	1.41	1.34
11	M	169	CLA	CHB-C4A	8.54	1.41	1.34
11	D	161	CLA	CHB-C4A	8.54	1.41	1.34
11	C	165	CLA	CHB-C4A	8.54	1.41	1.34
11	C	158	CLA	CHB-C4A	8.53	1.41	1.34
11	J	174	CLA	CHB-C4A	8.52	1.41	1.34
11	L	161	CLA	CHB-C4A	8.52	1.41	1.34
11	C	168	CLA	CHB-C4A	8.51	1.41	1.34
11	L	165	CLA	CHB-C4A	8.50	1.41	1.34
11	A	174	CLA	CHB-C4A	8.50	1.41	1.34
11	L	158	CLA	CHB-C4A	8.48	1.41	1.34
15	R	91	HEM	C2A-C1A	7.38	1.52	1.39
15	I	88	HEM	C2A-C1A	7.36	1.52	1.39
15	O	90	HEM	C2A-C1A	7.35	1.52	1.39
15	F	50	HEM	C2A-C1A	7.35	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	90	HEM	C3A-C4A	6.85	1.52	1.39
15	R	91	HEM	C3A-C4A	6.82	1.51	1.39
15	I	88	HEM	C3A-C4A	6.82	1.51	1.39
15	F	50	HEM	C3A-C4A	6.81	1.51	1.39
11	J	179	CLA	CAD-C3D	-5.85	1.42	1.51
11	A	174	CLA	CAD-C3D	-5.79	1.42	1.51
11	L	157	CLA	CAD-C3D	-5.79	1.42	1.51
11	C	167	CLA	CAD-C3D	-5.78	1.42	1.51
11	A	179	CLA	CAD-C3D	-5.77	1.42	1.51
11	C	168	CLA	CAD-C3D	-5.76	1.42	1.51
11	J	174	CLA	CAD-C3D	-5.76	1.42	1.51
11	L	167	CLA	CAD-C3D	-5.76	1.42	1.51
11	J	178	CLA	CAD-C3D	-5.76	1.42	1.51
11	M	163	CLA	CAD-C3D	-5.75	1.42	1.51
11	D	170	CLA	CAD-C3D	-5.75	1.42	1.51
11	L	168	CLA	CAD-C3D	-5.75	1.42	1.51
11	G	313	CLA	CAD-C3D	-5.75	1.42	1.51
11	B	178	CLA	CAD-C3D	-5.74	1.42	1.51
11	M	170	CLA	CAD-C3D	-5.74	1.42	1.51
11	C	157	CLA	CAD-C3D	-5.74	1.42	1.51
11	M	162	CLA	CAD-C3D	-5.74	1.42	1.51
11	C	165	CLA	CAD-C3D	-5.74	1.42	1.51
11	D	159	CLA	CAD-C3D	-5.74	1.42	1.51
11	M	165	CLA	CAD-C3D	-5.74	1.42	1.51
11	M	159	CLA	CAD-C3D	-5.74	1.42	1.51
11	D	167	CLA	CAD-C3D	-5.74	1.42	1.51
11	P	313	CLA	CAD-C3D	-5.74	1.42	1.51
11	A	178	CLA	CAD-C3D	-5.73	1.42	1.51
11	D	165	CLA	CAD-C3D	-5.73	1.42	1.51
11	L	166	CLA	CAD-C3D	-5.73	1.42	1.51
11	M	167	CLA	CAD-C3D	-5.73	1.42	1.51
11	L	160	CLA	CAD-C3D	-5.73	1.42	1.51
11	D	163	CLA	CAD-C3D	-5.73	1.42	1.51
11	J	175	CLA	CAD-C3D	-5.73	1.42	1.51
11	M	166	CLA	CAD-C3D	-5.73	1.42	1.51
11	L	165	CLA	CAD-C3D	-5.72	1.42	1.51
11	D	168	CLA	CAD-C3D	-5.72	1.42	1.51
11	C	158	CLA	CAD-C3D	-5.72	1.42	1.51
11	M	158	CLA	CAD-C3D	-5.71	1.42	1.51
11	D	166	CLA	CAD-C3D	-5.71	1.42	1.51
11	K	178	CLA	CAD-C3D	-5.71	1.42	1.51
11	D	158	CLA	CAD-C3D	-5.71	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	176	CLA	CAD-C3D	-5.71	1.42	1.51
11	M	156	CLA	CAD-C3D	-5.71	1.42	1.51
11	D	156	CLA	CAD-C3D	-5.71	1.42	1.51
11	M	168	CLA	CAD-C3D	-5.70	1.42	1.51
11	A	175	CLA	CAD-C3D	-5.70	1.42	1.51
11	C	164	CLA	CAD-C3D	-5.70	1.42	1.51
11	C	160	CLA	CAD-C3D	-5.70	1.42	1.51
11	L	158	CLA	CAD-C3D	-5.70	1.42	1.51
11	L	159	CLA	CAD-C3D	-5.70	1.42	1.51
11	C	161	CLA	CAD-C3D	-5.70	1.42	1.51
11	D	161	CLA	CAD-C3D	-5.69	1.42	1.51
11	D	162	CLA	CAD-C3D	-5.69	1.42	1.51
11	D	160	CLA	CAD-C3D	-5.69	1.42	1.51
11	D	169	CLA	CAD-C3D	-5.69	1.42	1.51
11	M	161	CLA	CAD-C3D	-5.68	1.42	1.51
11	C	166	CLA	CAD-C3D	-5.68	1.42	1.51
11	M	160	CLA	CAD-C3D	-5.68	1.42	1.51
11	C	159	CLA	CAD-C3D	-5.67	1.42	1.51
11	A	176	CLA	CAD-C3D	-5.67	1.42	1.51
11	L	164	CLA	CAD-C3D	-5.67	1.42	1.51
11	C	162	CLA	CAD-C3D	-5.67	1.42	1.51
11	L	161	CLA	CAD-C3D	-5.67	1.42	1.51
11	B	176	CLA	CAD-C3D	-5.67	1.42	1.51
11	C	163	CLA	CAD-C3D	-5.67	1.42	1.51
11	M	169	CLA	CAD-C3D	-5.65	1.42	1.51
11	D	164	CLA	CAD-C3D	-5.64	1.42	1.51
11	L	162	CLA	CAD-C3D	-5.64	1.42	1.51
11	L	163	CLA	CAD-C3D	-5.64	1.42	1.51
11	M	164	CLA	CAD-C3D	-5.64	1.42	1.51
11	K	176	CLA	CAD-C3D	-5.63	1.42	1.51
11	M	157	CLA	CAD-C3D	-5.61	1.42	1.51
11	D	157	CLA	CAD-C3D	-5.60	1.42	1.51
11	L	167	CLA	C3B-C4B	4.95	1.48	1.39
11	M	163	CLA	C3B-C4B	4.95	1.48	1.39
11	M	160	CLA	C3B-C4B	4.94	1.48	1.39
11	D	160	CLA	C3B-C4B	4.93	1.48	1.39
11	D	165	CLA	C3B-C4B	4.93	1.48	1.39
11	M	165	CLA	C3B-C4B	4.93	1.48	1.39
11	A	175	CLA	C3B-C4B	4.93	1.48	1.39
11	D	170	CLA	C3B-C4B	4.92	1.48	1.39
11	C	167	CLA	C3B-C4B	4.92	1.48	1.39
11	D	163	CLA	C3B-C4B	4.92	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	159	CLA	C3B-C4B	4.92	1.48	1.39
11	M	156	CLA	C3B-C4B	4.92	1.48	1.39
11	J	175	CLA	C3B-C4B	4.92	1.48	1.39
11	C	159	CLA	C3B-C4B	4.91	1.48	1.39
11	D	164	CLA	C3B-C4B	4.91	1.48	1.39
11	C	166	CLA	C3B-C4B	4.91	1.48	1.39
11	M	170	CLA	C3B-C4B	4.90	1.48	1.39
11	L	166	CLA	C3B-C4B	4.90	1.48	1.39
11	M	164	CLA	C3B-C4B	4.90	1.48	1.39
11	K	178	CLA	C3B-C4B	4.90	1.48	1.39
11	L	157	CLA	C3B-C4B	4.89	1.48	1.39
11	B	178	CLA	C3B-C4B	4.89	1.48	1.39
11	A	179	CLA	C3B-C4B	4.89	1.48	1.39
11	L	162	CLA	C3B-C4B	4.89	1.48	1.39
11	M	169	CLA	C3B-C4B	4.89	1.48	1.39
11	M	166	CLA	C3B-C4B	4.89	1.48	1.39
11	M	159	CLA	C3B-C4B	4.89	1.48	1.39
11	C	157	CLA	C3B-C4B	4.89	1.48	1.39
11	D	161	CLA	C3B-C4B	4.88	1.48	1.39
11	M	162	CLA	C3B-C4B	4.88	1.48	1.39
11	M	161	CLA	C3B-C4B	4.88	1.48	1.39
11	D	158	CLA	C3B-C4B	4.88	1.48	1.39
11	J	179	CLA	C3B-C4B	4.88	1.48	1.39
11	A	174	CLA	C3B-C4B	4.88	1.48	1.39
11	D	162	CLA	C3B-C4B	4.88	1.48	1.39
11	D	166	CLA	C3B-C4B	4.88	1.48	1.39
11	D	167	CLA	C3B-C4B	4.88	1.48	1.39
11	D	156	CLA	C3B-C4B	4.87	1.48	1.39
11	C	158	CLA	C3B-C4B	4.87	1.48	1.39
11	C	163	CLA	C3B-C4B	4.87	1.48	1.39
11	L	168	CLA	C3B-C4B	4.87	1.48	1.39
11	L	164	CLA	C3B-C4B	4.87	1.48	1.39
11	C	161	CLA	C3B-C4B	4.87	1.48	1.39
11	C	162	CLA	C3B-C4B	4.87	1.48	1.39
11	J	176	CLA	C3B-C4B	4.87	1.48	1.39
11	L	161	CLA	C3B-C4B	4.87	1.48	1.39
11	M	157	CLA	C3B-C4B	4.86	1.48	1.39
11	C	168	CLA	C3B-C4B	4.86	1.48	1.39
11	P	313	CLA	C3B-C4B	4.86	1.48	1.39
11	M	167	CLA	C3B-C4B	4.86	1.48	1.39
11	C	165	CLA	C3B-C4B	4.86	1.48	1.39
11	A	176	CLA	C3B-C4B	4.86	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	313	CLA	C3B-C4B	4.86	1.48	1.39
11	M	158	CLA	C3B-C4B	4.85	1.48	1.39
11	D	169	CLA	C3B-C4B	4.85	1.48	1.39
11	D	159	CLA	C3B-C4B	4.85	1.48	1.39
11	J	174	CLA	C3B-C4B	4.85	1.48	1.39
11	D	157	CLA	C3B-C4B	4.85	1.48	1.39
11	L	163	CLA	C3B-C4B	4.85	1.48	1.39
11	C	164	CLA	C3B-C4B	4.85	1.48	1.39
11	L	158	CLA	C3B-C4B	4.85	1.48	1.39
11	J	178	CLA	C3B-C4B	4.84	1.48	1.39
11	A	178	CLA	C3B-C4B	4.84	1.48	1.39
11	M	169	CLA	MG-NA	4.84	2.17	2.06
11	M	168	CLA	C3B-C4B	4.84	1.48	1.39
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	165	CLA	C3B-C4B	4.83	1.48	1.39
11	L	168	CLA	MG-NA	4.83	2.17	2.06
11	D	168	CLA	C3B-C4B	4.83	1.48	1.39
11	M	164	CLA	MG-NA	4.83	2.17	2.06
11	B	176	CLA	C3B-C4B	4.82	1.48	1.39
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
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	M	158	CLA	MG-NA	4.80	2.17	2.06
11	D	163	CLA	MG-NA	4.80	2.17	2.06
11	M	167	CLA	MG-NA	4.80	2.17	2.06
11	J	175	CLA	MG-NA	4.80	2.17	2.06
11	C	157	CLA	MG-NA	4.80	2.17	2.06
11	D	166	CLA	MG-NA	4.80	2.17	2.06
11	C	160	CLA	C3B-C4B	4.80	1.48	1.39
11	D	158	CLA	MG-NA	4.79	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	L	160	CLA	C3B-C4B	4.79	1.48	1.39
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	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	L	159	CLA	MG-NA	4.78	2.17	2.06
11	D	156	CLA	MG-NA	4.78	2.17	2.06
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	A	175	CLA	MG-NA	4.77	2.17	2.06
11	L	160	CLA	MG-NA	4.77	2.17	2.06
11	L	158	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	K	176	CLA	C3B-C4B	4.77	1.48	1.39
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	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	L	167	CLA	MG-NA	4.76	2.17	2.06
11	M	161	CLA	MG-NA	4.76	2.17	2.06
11	L	166	CLA	MG-NA	4.75	2.17	2.06
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	K	176	CLA	MG-NA	4.75	2.17	2.06
11	J	176	CLA	MG-NA	4.75	2.17	2.06
11	M	162	CLA	MG-NA	4.75	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	176	CLA	MG-NA	4.74	2.17	2.06
11	C	160	CLA	MG-NA	4.74	2.17	2.06
11	B	178	CLA	MG-NA	4.72	2.17	2.06
11	K	178	CLA	MG-NA	4.70	2.17	2.06
11	L	167	CLA	C1B-CHB	-4.54	1.34	1.43
14	B	179	PL9	C6-C5	4.53	1.46	1.32
11	M	168	CLA	C1B-CHB	-4.53	1.34	1.43
11	M	160	CLA	C1B-CHB	-4.52	1.34	1.43
14	K	179	PL9	C6-C5	4.52	1.46	1.32
11	L	164	CLA	C1B-CHB	-4.52	1.34	1.43
11	M	159	CLA	C1B-CHB	-4.52	1.34	1.43
11	C	167	CLA	C1B-CHB	-4.51	1.34	1.43
11	D	162	CLA	C1B-CHB	-4.51	1.34	1.43
11	D	160	CLA	C1B-CHB	-4.51	1.34	1.43
11	C	164	CLA	C1B-CHB	-4.50	1.34	1.43
11	D	165	CLA	C1B-CHB	-4.50	1.34	1.43
11	M	163	CLA	C1B-CHB	-4.50	1.34	1.43
11	C	163	CLA	C1B-CHB	-4.50	1.34	1.43
11	D	157	CLA	C1B-CHB	-4.50	1.34	1.43
11	D	159	CLA	C1B-CHB	-4.50	1.34	1.43
11	G	313	CLA	C1B-CHB	-4.50	1.34	1.43
11	M	166	CLA	C1B-CHB	-4.49	1.34	1.43
11	M	164	CLA	C1B-CHB	-4.49	1.34	1.43
11	M	162	CLA	C1B-CHB	-4.49	1.34	1.43
11	D	168	CLA	C1B-CHB	-4.49	1.34	1.43
11	C	162	CLA	C1B-CHB	-4.49	1.34	1.43
11	C	159	CLA	C1B-CHB	-4.49	1.34	1.43
11	D	156	CLA	C1B-CHB	-4.49	1.34	1.43
11	J	178	CLA	C1B-CHB	-4.48	1.34	1.43
11	J	176	CLA	C1B-CHB	-4.48	1.34	1.43
11	D	163	CLA	C1B-CHB	-4.48	1.34	1.43
11	M	161	CLA	C1B-CHB	-4.48	1.34	1.43
11	M	157	CLA	C1B-CHB	-4.48	1.34	1.43
11	A	178	CLA	C1B-CHB	-4.48	1.34	1.43
11	M	165	CLA	C1B-CHB	-4.48	1.34	1.43
11	L	162	CLA	C1B-CHB	-4.47	1.34	1.43
11	C	168	CLA	C1B-CHB	-4.47	1.34	1.43
11	D	166	CLA	C1B-CHB	-4.47	1.34	1.43
11	J	175	CLA	C1B-CHB	-4.47	1.34	1.43
11	L	166	CLA	C1B-CHB	-4.47	1.34	1.43
11	A	176	CLA	C1B-CHB	-4.47	1.34	1.43
11	M	156	CLA	C1B-CHB	-4.47	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	176	CLA	C1B-CHB	-4.47	1.34	1.43
11	L	161	CLA	C1B-CHB	-4.46	1.34	1.43
11	D	164	CLA	C1B-CHB	-4.46	1.34	1.43
11	L	163	CLA	C1B-CHB	-4.46	1.34	1.43
11	K	178	CLA	C1B-CHB	-4.46	1.34	1.43
11	D	158	CLA	C1B-CHB	-4.46	1.34	1.43
11	L	168	CLA	C1B-CHB	-4.46	1.34	1.43
11	A	175	CLA	C1B-CHB	-4.46	1.34	1.43
11	C	165	CLA	C1B-CHB	-4.46	1.34	1.43
11	D	161	CLA	C1B-CHB	-4.46	1.34	1.43
11	L	159	CLA	C1B-CHB	-4.46	1.34	1.43
11	B	178	CLA	C1B-CHB	-4.46	1.34	1.43
11	D	169	CLA	C1B-CHB	-4.46	1.34	1.43
11	P	313	CLA	C1B-CHB	-4.46	1.34	1.43
11	C	166	CLA	C1B-CHB	-4.46	1.34	1.43
11	D	170	CLA	C1B-CHB	-4.45	1.34	1.43
11	B	176	CLA	C1B-CHB	-4.45	1.34	1.43
11	A	174	CLA	C1B-CHB	-4.45	1.34	1.43
11	L	165	CLA	C1B-CHB	-4.45	1.34	1.43
11	D	167	CLA	C1B-CHB	-4.45	1.34	1.43
11	M	158	CLA	C1B-CHB	-4.45	1.34	1.43
11	M	169	CLA	C1B-CHB	-4.44	1.34	1.43
11	C	160	CLA	C1B-CHB	-4.44	1.34	1.43
11	L	160	CLA	C1B-CHB	-4.44	1.34	1.43
11	C	161	CLA	C1B-CHB	-4.44	1.34	1.43
11	M	167	CLA	C1B-CHB	-4.44	1.34	1.43
11	C	158	CLA	C1B-CHB	-4.43	1.34	1.43
11	C	157	CLA	C1B-CHB	-4.43	1.35	1.43
11	J	174	CLA	C1B-CHB	-4.43	1.35	1.43
11	A	179	CLA	C1B-CHB	-4.42	1.35	1.43
11	M	170	CLA	C1B-CHB	-4.42	1.35	1.43
11	L	158	CLA	C1B-CHB	-4.42	1.35	1.43
11	L	157	CLA	C1B-CHB	-4.42	1.35	1.43
11	J	179	CLA	C1B-CHB	-4.37	1.35	1.43
12	K	177	PHO	CAD-C3D	-4.36	1.42	1.50
12	J	177	PHO	CAD-C3D	-4.36	1.42	1.50
12	A	177	PHO	CAD-C3D	-4.36	1.42	1.50
12	B	177	PHO	CAD-C3D	-4.35	1.42	1.50
11	M	159	CLA	C4B-NB	3.71	1.38	1.35
11	M	157	CLA	C4B-NB	3.69	1.38	1.35
11	L	165	CLA	C4B-NB	3.67	1.38	1.35
11	L	167	CLA	C4B-NB	3.66	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	160	CLA	C2B-C1B	3.66	1.46	1.39
11	D	159	CLA	C4B-NB	3.66	1.38	1.35
11	J	178	CLA	C2B-C1B	3.66	1.46	1.39
11	L	164	CLA	C2B-C1B	3.66	1.46	1.39
11	L	167	CLA	C2B-C1B	3.65	1.46	1.39
11	C	165	CLA	C4B-NB	3.65	1.38	1.35
11	M	166	CLA	C2B-C1B	3.65	1.46	1.39
11	L	164	CLA	C4B-NB	3.65	1.38	1.35
11	C	164	CLA	C2B-C1B	3.65	1.46	1.39
11	M	156	CLA	C2B-C1B	3.64	1.46	1.39
14	B	179	PL9	C3-C2	3.64	1.43	1.32
14	K	179	PL9	C3-C2	3.64	1.43	1.32
11	M	158	CLA	C4B-NB	3.64	1.38	1.35
11	D	157	CLA	C4B-NB	3.64	1.38	1.35
11	M	156	CLA	C4B-NB	3.64	1.38	1.35
11	M	164	CLA	C2B-C1B	3.64	1.46	1.39
11	D	156	CLA	C4B-NB	3.64	1.38	1.35
11	L	168	CLA	C4B-NB	3.64	1.38	1.35
11	D	160	CLA	C2B-C1B	3.64	1.46	1.39
11	B	176	CLA	C2B-C1B	3.64	1.46	1.39
11	L	165	CLA	C2B-C1B	3.64	1.46	1.39
11	K	176	CLA	C2B-C1B	3.64	1.46	1.39
11	D	158	CLA	C2B-C1B	3.64	1.46	1.39
11	K	178	CLA	C2B-C1B	3.63	1.46	1.39
11	J	178	CLA	C4B-NB	3.63	1.38	1.35
11	L	166	CLA	C2B-C1B	3.63	1.46	1.39
11	C	165	CLA	C2B-C1B	3.63	1.46	1.39
11	M	161	CLA	C2B-C1B	3.63	1.46	1.39
11	C	167	CLA	C2B-C1B	3.63	1.46	1.39
11	L	161	CLA	C2B-C1B	3.63	1.46	1.39
11	C	161	CLA	C2B-C1B	3.63	1.46	1.39
11	M	162	CLA	C2B-C1B	3.63	1.46	1.39
11	D	156	CLA	C2B-C1B	3.62	1.46	1.39
11	A	178	CLA	C2B-C1B	3.62	1.46	1.39
11	D	159	CLA	C2B-C1B	3.62	1.46	1.39
11	G	313	CLA	C2B-C1B	3.62	1.46	1.39
11	M	158	CLA	C2B-C1B	3.62	1.46	1.39
11	B	178	CLA	C2B-C1B	3.62	1.46	1.39
11	C	168	CLA	C4B-NB	3.62	1.38	1.35
11	L	168	CLA	C2B-C1B	3.62	1.46	1.39
11	L	162	CLA	C2B-C1B	3.62	1.46	1.39
11	L	161	CLA	C4B-NB	3.62	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	178	CLA	C4B-NB	3.62	1.38	1.35
11	D	164	CLA	C2B-C1B	3.62	1.46	1.39
11	D	161	CLA	C2B-C1B	3.62	1.46	1.39
11	P	313	CLA	C2B-C1B	3.62	1.46	1.39
11	C	163	CLA	C2B-C1B	3.61	1.46	1.39
11	M	170	CLA	C2B-C1B	3.61	1.46	1.39
11	M	157	CLA	C2B-C1B	3.61	1.46	1.39
11	C	166	CLA	C2B-C1B	3.61	1.46	1.39
11	D	169	CLA	C2B-C1B	3.61	1.46	1.39
11	M	163	CLA	C4B-NB	3.61	1.38	1.35
11	L	163	CLA	C4B-NB	3.61	1.38	1.35
11	C	164	CLA	C4B-NB	3.61	1.38	1.35
11	D	165	CLA	C2B-C1B	3.61	1.46	1.39
11	D	161	CLA	C4B-NB	3.61	1.38	1.35
11	D	166	CLA	C2B-C1B	3.60	1.46	1.39
11	M	169	CLA	C2B-C1B	3.60	1.46	1.39
11	C	162	CLA	C2B-C1B	3.60	1.46	1.39
11	D	163	CLA	C2B-C1B	3.60	1.46	1.39
11	L	159	CLA	C2B-C1B	3.60	1.46	1.39
11	D	162	CLA	C2B-C1B	3.60	1.46	1.39
11	M	159	CLA	C2B-C1B	3.60	1.46	1.39
11	M	167	CLA	C2B-C1B	3.60	1.46	1.39
11	L	166	CLA	C4B-NB	3.60	1.38	1.35
11	D	167	CLA	C4B-NB	3.60	1.38	1.35
11	C	167	CLA	C4B-NB	3.60	1.38	1.35
11	C	158	CLA	C2B-C1B	3.60	1.46	1.39
11	D	157	CLA	C2B-C1B	3.60	1.46	1.39
11	M	161	CLA	C4B-NB	3.60	1.38	1.35
11	D	158	CLA	C4B-NB	3.60	1.38	1.35
11	C	160	CLA	C2B-C1B	3.60	1.46	1.39
11	J	175	CLA	C2B-C1B	3.60	1.46	1.39
11	M	165	CLA	C2B-C1B	3.59	1.46	1.39
11	C	163	CLA	C4B-NB	3.59	1.38	1.35
11	L	162	CLA	C4B-NB	3.59	1.38	1.35
11	D	167	CLA	C2B-C1B	3.59	1.46	1.39
11	L	160	CLA	C2B-C1B	3.59	1.46	1.39
11	C	168	CLA	C2B-C1B	3.59	1.46	1.39
11	L	163	CLA	C2B-C1B	3.59	1.46	1.39
11	C	159	CLA	C2B-C1B	3.59	1.46	1.39
11	L	158	CLA	C2B-C1B	3.59	1.46	1.39
11	J	179	CLA	C2B-C1B	3.58	1.46	1.39
11	A	175	CLA	C2B-C1B	3.58	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	163	CLA	C2B-C1B	3.58	1.46	1.39
11	C	166	CLA	C4B-NB	3.58	1.38	1.35
11	J	176	CLA	C2B-C1B	3.58	1.46	1.39
11	M	170	CLA	C4B-NB	3.58	1.38	1.35
11	A	174	CLA	C2B-C1B	3.58	1.46	1.39
11	C	158	CLA	C4B-NB	3.58	1.38	1.35
11	D	170	CLA	C2B-C1B	3.58	1.46	1.39
11	J	176	CLA	C4B-NB	3.58	1.38	1.35
11	C	161	CLA	C4B-NB	3.58	1.38	1.35
11	G	313	CLA	C4B-NB	3.57	1.38	1.35
11	D	168	CLA	C4B-NB	3.57	1.38	1.35
11	D	168	CLA	C2B-C1B	3.57	1.46	1.39
11	D	163	CLA	C4B-NB	3.57	1.38	1.35
11	C	162	CLA	C4B-NB	3.57	1.38	1.35
11	A	179	CLA	C2B-C1B	3.57	1.46	1.39
11	C	160	CLA	C4B-NB	3.56	1.38	1.35
11	L	158	CLA	C4B-NB	3.56	1.38	1.35
11	P	313	CLA	C4B-NB	3.56	1.38	1.35
11	A	176	CLA	C2B-C1B	3.56	1.46	1.39
11	J	174	CLA	C4B-NB	3.55	1.38	1.35
11	M	168	CLA	C2B-C1B	3.55	1.46	1.39
11	A	176	CLA	C4B-NB	3.55	1.38	1.35
11	J	174	CLA	C2B-C1B	3.55	1.46	1.39
11	C	157	CLA	C2B-C1B	3.55	1.46	1.39
11	L	159	CLA	C4B-NB	3.55	1.38	1.35
11	D	162	CLA	C4B-NB	3.54	1.38	1.35
11	C	159	CLA	C4B-NB	3.54	1.38	1.35
11	C	157	CLA	C4B-NB	3.54	1.38	1.35
11	L	157	CLA	C4B-NB	3.54	1.38	1.35
11	M	167	CLA	C4B-NB	3.53	1.38	1.35
11	L	157	CLA	C2B-C1B	3.53	1.46	1.39
11	J	175	CLA	C4B-NB	3.53	1.38	1.35
11	J	179	CLA	C4B-NB	3.53	1.38	1.35
11	M	162	CLA	C4B-NB	3.53	1.38	1.35
11	A	179	CLA	C4B-NB	3.52	1.38	1.35
11	D	160	CLA	C4B-NB	3.52	1.38	1.35
11	A	175	CLA	C4B-NB	3.51	1.38	1.35
11	D	170	CLA	C4B-NB	3.51	1.38	1.35
11	L	160	CLA	C4B-NB	3.51	1.38	1.35
11	M	160	CLA	C4B-NB	3.50	1.38	1.35
11	M	169	CLA	C4B-NB	3.50	1.38	1.35
11	D	165	CLA	C4B-NB	3.49	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	174	CLA	C4B-NB	3.49	1.38	1.35
11	M	165	CLA	C4B-NB	3.49	1.38	1.35
11	M	168	CLA	C4B-NB	3.49	1.38	1.35
11	D	169	CLA	C4B-NB	3.49	1.38	1.35
11	D	164	CLA	C4B-NB	3.48	1.38	1.35
11	D	166	CLA	C4B-NB	3.47	1.38	1.35
11	M	164	CLA	C4B-NB	3.46	1.38	1.35
11	B	178	CLA	C4B-NB	3.44	1.38	1.35
11	K	178	CLA	C4B-NB	3.43	1.38	1.35
11	K	176	CLA	C4B-NB	3.42	1.38	1.35
11	M	166	CLA	C4B-NB	3.42	1.38	1.35
11	B	176	CLA	C4B-NB	3.36	1.38	1.35
11	M	163	CLA	C1B-NB	3.13	1.38	1.35
11	L	159	CLA	C1B-NB	3.09	1.38	1.35
11	C	159	CLA	C1B-NB	3.08	1.38	1.35
11	M	166	CLA	C1B-NB	3.07	1.37	1.35
11	M	169	CLA	C1B-NB	3.06	1.37	1.35
11	M	165	CLA	C1B-NB	3.05	1.37	1.35
11	L	166	CLA	C1B-NB	3.03	1.37	1.35
11	J	176	CLA	C1B-NB	3.02	1.37	1.35
11	D	162	CLA	C1B-NB	3.02	1.37	1.35
11	M	161	CLA	C1B-NB	3.01	1.37	1.35
11	P	313	CLA	C1B-NB	3.01	1.37	1.35
11	M	157	CLA	C1B-NB	3.01	1.37	1.35
11	D	166	CLA	C1B-NB	3.00	1.37	1.35
11	G	313	CLA	C1B-NB	3.00	1.37	1.35
11	M	167	CLA	C1B-NB	2.99	1.37	1.35
11	A	178	CLA	C1B-NB	2.99	1.37	1.35
11	D	163	CLA	C1B-NB	2.99	1.37	1.35
11	K	176	CLA	C1B-NB	2.99	1.37	1.35
11	D	169	CLA	C1B-NB	2.99	1.37	1.35
11	D	165	CLA	C1B-NB	2.99	1.37	1.35
11	D	157	CLA	C1B-NB	2.99	1.37	1.35
11	D	167	CLA	C1B-NB	2.98	1.37	1.35
11	L	160	CLA	C1B-NB	2.98	1.37	1.35
11	A	174	CLA	C1B-NB	2.98	1.37	1.35
11	A	176	CLA	C1B-NB	2.97	1.37	1.35
11	M	168	CLA	C1B-NB	2.97	1.37	1.35
11	D	161	CLA	C1B-NB	2.97	1.37	1.35
11	J	178	CLA	C1B-NB	2.96	1.37	1.35
11	J	174	CLA	C1B-NB	2.95	1.37	1.35
11	M	162	CLA	C1B-NB	2.95	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	156	CLA	C1B-NB	2.94	1.37	1.35
11	C	166	CLA	C1B-NB	2.93	1.37	1.35
11	C	162	CLA	C1B-NB	2.93	1.37	1.35
11	D	160	CLA	C1B-NB	2.93	1.37	1.35
11	L	162	CLA	C1B-NB	2.93	1.37	1.35
11	D	170	CLA	C1B-NB	2.93	1.37	1.35
11	L	168	CLA	C1B-NB	2.92	1.37	1.35
11	C	168	CLA	C1B-NB	2.91	1.37	1.35
11	C	163	CLA	C1B-NB	2.91	1.37	1.35
11	D	156	CLA	C1B-NB	2.91	1.37	1.35
11	D	158	CLA	C1B-NB	2.90	1.37	1.35
11	M	160	CLA	C1B-NB	2.90	1.37	1.35
11	B	176	CLA	C1B-NB	2.90	1.37	1.35
11	D	168	CLA	C1B-NB	2.90	1.37	1.35
11	L	167	CLA	C1B-NB	2.89	1.37	1.35
11	C	165	CLA	C1B-NB	2.89	1.37	1.35
11	A	175	CLA	C1B-NB	2.89	1.37	1.35
11	C	157	CLA	C1B-NB	2.89	1.37	1.35
11	J	175	CLA	C1B-NB	2.89	1.37	1.35
11	C	160	CLA	C1B-NB	2.87	1.37	1.35
11	L	161	CLA	C1B-NB	2.86	1.37	1.35
11	B	178	CLA	C1B-NB	2.86	1.37	1.35
11	L	165	CLA	C1B-NB	2.86	1.37	1.35
11	M	159	CLA	C1B-NB	2.86	1.37	1.35
11	L	157	CLA	C1B-NB	2.86	1.37	1.35
11	M	164	CLA	C1B-NB	2.85	1.37	1.35
11	D	159	CLA	C1B-NB	2.85	1.37	1.35
11	L	163	CLA	C1B-NB	2.85	1.37	1.35
11	C	161	CLA	C1B-NB	2.84	1.37	1.35
11	C	167	CLA	C1B-NB	2.83	1.37	1.35
11	M	158	CLA	C1B-NB	2.83	1.37	1.35
11	M	170	CLA	C1B-NB	2.83	1.37	1.35
11	D	164	CLA	C1B-NB	2.83	1.37	1.35
11	C	158	CLA	C1B-NB	2.82	1.37	1.35
11	K	178	CLA	C1B-NB	2.82	1.37	1.35
11	L	164	CLA	C1B-NB	2.82	1.37	1.35
11	L	158	CLA	C1B-NB	2.81	1.37	1.35
11	C	164	CLA	C1B-NB	2.78	1.37	1.35
11	A	179	CLA	C1B-NB	2.76	1.37	1.35
11	J	179	CLA	C1B-NB	2.68	1.37	1.35
12	K	177	PHO	C4D-CHA	-2.52	1.38	1.45
12	J	177	PHO	C4D-CHA	-2.51	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	177	PHO	C4D-CHA	-2.50	1.39	1.45
12	A	177	PHO	C4D-CHA	-2.50	1.39	1.45
12	B	177	PHO	C4D-C3D	-2.35	1.39	1.45
12	K	177	PHO	C4D-C3D	-2.34	1.39	1.45
12	J	177	PHO	C4D-C3D	-2.33	1.39	1.45
12	A	177	PHO	C4D-C3D	-2.32	1.39	1.45
12	B	177	PHO	C1D-ND	-2.32	1.33	1.38
12	A	177	PHO	C1D-ND	-2.31	1.33	1.38
12	K	177	PHO	C1D-ND	-2.30	1.33	1.38
12	J	177	PHO	C1D-ND	-2.29	1.33	1.38

All (468) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	168	CLA	C4A-NA-C1A	10.50	111.42	106.71
11	M	164	CLA	C4A-NA-C1A	10.48	111.42	106.71
11	M	168	CLA	C4A-NA-C1A	10.48	111.42	106.71
11	M	169	CLA	C4A-NA-C1A	10.45	111.40	106.71
11	D	163	CLA	C4A-NA-C1A	10.45	111.40	106.71
11	C	168	CLA	C4A-NA-C1A	10.44	111.40	106.71
11	M	156	CLA	C4A-NA-C1A	10.43	111.40	106.71
11	M	159	CLA	C4A-NA-C1A	10.43	111.40	106.71
11	D	168	CLA	C4A-NA-C1A	10.43	111.39	106.71
11	D	169	CLA	C4A-NA-C1A	10.43	111.39	106.71
11	M	166	CLA	C4A-NA-C1A	10.43	111.39	106.71
11	D	166	CLA	C4A-NA-C1A	10.41	111.39	106.71
11	D	158	CLA	C4A-NA-C1A	10.41	111.39	106.71
11	C	163	CLA	C4A-NA-C1A	10.40	111.38	106.71
11	L	165	CLA	C4A-NA-C1A	10.40	111.38	106.71
11	J	178	CLA	C4A-NA-C1A	10.39	111.38	106.71
11	M	163	CLA	C4A-NA-C1A	10.39	111.38	106.71
11	D	164	CLA	C4A-NA-C1A	10.39	111.38	106.71
11	D	160	CLA	C4A-NA-C1A	10.38	111.37	106.71
11	D	156	CLA	C4A-NA-C1A	10.37	111.37	106.71
11	A	175	CLA	C4A-NA-C1A	10.37	111.37	106.71
11	J	175	CLA	C4A-NA-C1A	10.37	111.37	106.71
11	D	161	CLA	C4A-NA-C1A	10.37	111.37	106.71
11	M	160	CLA	C4A-NA-C1A	10.35	111.36	106.71
11	L	163	CLA	C4A-NA-C1A	10.35	111.36	106.71
11	A	174	CLA	C4A-NA-C1A	10.35	111.36	106.71
11	L	161	CLA	C4A-NA-C1A	10.35	111.36	106.71
11	M	157	CLA	C4A-NA-C1A	10.35	111.36	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	J	174	CLA	C4A-NA-C1A	10.35	111.36	106.71
11	L	162	CLA	C4A-NA-C1A	10.35	111.36	106.71
11	M	170	CLA	C4A-NA-C1A	10.34	111.36	106.71
11	C	165	CLA	C4A-NA-C1A	10.34	111.35	106.71
11	C	161	CLA	C4A-NA-C1A	10.33	111.35	106.71
11	L	157	CLA	C4A-NA-C1A	10.33	111.35	106.71
11	A	178	CLA	C4A-NA-C1A	10.33	111.35	106.71
11	L	159	CLA	C4A-NA-C1A	10.33	111.35	106.71
11	D	170	CLA	C4A-NA-C1A	10.33	111.35	106.71
11	D	157	CLA	C4A-NA-C1A	10.32	111.34	106.71
11	C	157	CLA	C4A-NA-C1A	10.31	111.34	106.71
11	D	159	CLA	C4A-NA-C1A	10.31	111.34	106.71
11	P	313	CLA	C4A-NA-C1A	10.30	111.34	106.71
11	L	158	CLA	C4A-NA-C1A	10.30	111.34	106.71
11	M	161	CLA	C4A-NA-C1A	10.30	111.34	106.71
11	C	158	CLA	C4A-NA-C1A	10.30	111.34	106.71
11	C	167	CLA	C4A-NA-C1A	10.30	111.34	106.71
11	C	159	CLA	C4A-NA-C1A	10.29	111.33	106.71
11	M	165	CLA	C4A-NA-C1A	10.29	111.33	106.71
11	G	313	CLA	C4A-NA-C1A	10.28	111.33	106.71
11	D	165	CLA	C4A-NA-C1A	10.28	111.33	106.71
11	C	166	CLA	C4A-NA-C1A	10.27	111.33	106.71
11	C	162	CLA	C4A-NA-C1A	10.27	111.32	106.71
11	M	167	CLA	C4A-NA-C1A	10.26	111.32	106.71
11	M	158	CLA	C4A-NA-C1A	10.25	111.31	106.71
11	D	167	CLA	C4A-NA-C1A	10.25	111.31	106.71
11	D	162	CLA	C4A-NA-C1A	10.25	111.31	106.71
11	L	160	CLA	C4A-NA-C1A	10.24	111.31	106.71
11	L	164	CLA	C4A-NA-C1A	10.24	111.31	106.71
11	C	160	CLA	C4A-NA-C1A	10.24	111.31	106.71
11	L	167	CLA	C4A-NA-C1A	10.23	111.30	106.71
11	C	164	CLA	C4A-NA-C1A	10.22	111.30	106.71
11	A	176	CLA	C4A-NA-C1A	10.22	111.30	106.71
11	K	176	CLA	C4A-NA-C1A	10.21	111.29	106.71
11	M	162	CLA	C4A-NA-C1A	10.20	111.29	106.71
11	B	176	CLA	C4A-NA-C1A	10.20	111.29	106.71
15	R	91	HEM	C3D-C4D-ND	10.20	116.33	108.27
11	J	176	CLA	C4A-NA-C1A	10.19	111.29	106.71
15	I	88	HEM	C3D-C4D-ND	10.17	116.30	108.27
11	B	178	CLA	C4A-NA-C1A	10.16	111.27	106.71
11	L	166	CLA	C4A-NA-C1A	10.14	111.27	106.71
11	A	179	CLA	C4A-NA-C1A	10.14	111.27	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	178	CLA	C4A-NA-C1A	10.11	111.25	106.71
11	J	179	CLA	C4A-NA-C1A	10.10	111.25	106.71
15	F	50	HEM	C3D-C4D-ND	10.07	116.23	108.27
15	O	90	HEM	C3D-C4D-ND	10.04	116.20	108.27
15	I	88	HEM	C2D-C3D-C4D	-8.73	98.78	106.30
15	R	91	HEM	C2D-C3D-C4D	-8.72	98.79	106.30
15	F	50	HEM	C2D-C3D-C4D	-8.62	98.87	106.30
15	O	90	HEM	C2D-C3D-C4D	-8.58	98.91	106.30
15	R	91	HEM	C3D-C2D-C1D	5.98	111.41	106.29
15	I	88	HEM	C3D-C2D-C1D	5.97	111.40	106.29
15	F	50	HEM	C3D-C2D-C1D	5.81	111.26	106.29
15	O	90	HEM	C3D-C2D-C1D	5.77	111.23	106.29
11	J	179	CLA	CAD-C3D-C2D	5.04	144.95	132.79
11	D	170	CLA	CAD-C3D-C2D	5.04	144.95	132.79
11	M	170	CLA	CAD-C3D-C2D	5.04	144.94	132.79
11	M	163	CLA	CAD-C3D-C2D	5.03	144.93	132.79
11	M	160	CLA	CAD-C3D-C2D	5.03	144.92	132.79
11	A	179	CLA	CAD-C3D-C2D	5.03	144.91	132.79
11	M	165	CLA	CAD-C3D-C2D	5.02	144.91	132.79
11	D	165	CLA	CAD-C3D-C2D	5.02	144.91	132.79
11	P	313	CLA	CAD-C3D-C2D	5.02	144.90	132.79
11	C	168	CLA	CAD-C3D-C2D	5.02	144.89	132.79
11	A	174	CLA	CAD-C3D-C2D	5.02	144.89	132.79
11	C	165	CLA	CAD-C3D-C2D	5.02	144.89	132.79
11	D	163	CLA	CAD-C3D-C2D	5.02	144.89	132.79
11	C	163	CLA	CAD-C3D-C2D	5.01	144.88	132.79
11	D	156	CLA	CAD-C3D-C2D	5.01	144.88	132.79
11	L	157	CLA	CAD-C3D-C2D	5.01	144.88	132.79
11	C	157	CLA	CAD-C3D-C2D	5.01	144.88	132.79
11	L	168	CLA	CAD-C3D-C2D	5.01	144.88	132.79
11	L	163	CLA	CAD-C3D-C2D	5.01	144.88	132.79
11	D	160	CLA	CAD-C3D-C2D	5.01	144.88	132.79
11	L	167	CLA	CAD-C3D-C2D	5.01	144.88	132.79
11	L	161	CLA	CAD-C3D-C2D	5.01	144.87	132.79
11	G	313	CLA	CAD-C3D-C2D	5.01	144.87	132.79
11	M	156	CLA	CAD-C3D-C2D	5.01	144.87	132.79
11	D	168	CLA	CAD-C3D-C2D	5.01	144.87	132.79
11	J	178	CLA	CAD-C3D-C2D	5.01	144.87	132.79
11	M	167	CLA	CAD-C3D-C2D	5.01	144.87	132.79
11	D	167	CLA	CAD-C3D-C2D	5.00	144.86	132.79
11	L	165	CLA	CAD-C3D-C2D	5.00	144.86	132.79
11	J	176	CLA	CAD-C3D-C2D	5.00	144.86	132.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	161	CLA	CAD-C3D-C2D	5.00	144.85	132.79
11	D	169	CLA	CAD-C3D-C2D	5.00	144.85	132.79
11	J	174	CLA	CAD-C3D-C2D	5.00	144.85	132.79
11	A	176	CLA	CAD-C3D-C2D	5.00	144.85	132.79
11	D	166	CLA	CAD-C3D-C2D	5.00	144.85	132.79
11	A	178	CLA	CAD-C3D-C2D	5.00	144.85	132.79
11	M	168	CLA	CAD-C3D-C2D	5.00	144.85	132.79
11	D	157	CLA	CAD-C3D-C2D	5.00	144.85	132.79
11	B	176	CLA	CAD-C3D-C2D	5.00	144.85	132.79
11	M	169	CLA	CAD-C3D-C2D	5.00	144.85	132.79
11	C	167	CLA	CAD-C3D-C2D	5.00	144.85	132.79
11	C	161	CLA	CAD-C3D-C2D	5.00	144.84	132.79
11	M	162	CLA	CAD-C3D-C2D	5.00	144.84	132.79
11	M	164	CLA	CAD-C3D-C2D	5.00	144.84	132.79
11	C	162	CLA	CAD-C3D-C2D	4.99	144.84	132.79
11	M	161	CLA	CAD-C3D-C2D	4.99	144.84	132.79
11	M	166	CLA	CAD-C3D-C2D	4.99	144.84	132.79
11	B	178	CLA	CAD-C3D-C2D	4.99	144.83	132.79
11	C	158	CLA	CAD-C3D-C2D	4.99	144.83	132.79
11	M	157	CLA	CAD-C3D-C2D	4.99	144.83	132.79
11	L	159	CLA	CAD-C3D-C2D	4.99	144.83	132.79
11	D	159	CLA	CAD-C3D-C2D	4.99	144.82	132.79
11	L	160	CLA	CAD-C3D-C2D	4.99	144.82	132.79
11	D	164	CLA	CAD-C3D-C2D	4.99	144.82	132.79
11	K	176	CLA	CAD-C3D-C2D	4.99	144.82	132.79
11	D	158	CLA	CAD-C3D-C2D	4.99	144.82	132.79
11	M	158	CLA	CAD-C3D-C2D	4.98	144.81	132.79
11	K	178	CLA	CAD-C3D-C2D	4.98	144.81	132.79
11	J	175	CLA	CAD-C3D-C2D	4.98	144.81	132.79
11	C	159	CLA	CAD-C3D-C2D	4.98	144.80	132.79
11	A	175	CLA	CAD-C3D-C2D	4.98	144.80	132.79
11	D	162	CLA	CAD-C3D-C2D	4.98	144.80	132.79
11	L	162	CLA	CAD-C3D-C2D	4.98	144.80	132.79
11	M	159	CLA	CAD-C3D-C2D	4.98	144.80	132.79
11	C	166	CLA	CAD-C3D-C2D	4.98	144.80	132.79
11	C	160	CLA	CAD-C3D-C2D	4.98	144.80	132.79
11	L	158	CLA	CAD-C3D-C2D	4.97	144.79	132.79
11	C	164	CLA	CAD-C3D-C2D	4.97	144.77	132.79
11	L	166	CLA	CAD-C3D-C2D	4.96	144.76	132.79
11	L	164	CLA	CAD-C3D-C2D	4.96	144.75	132.79
15	F	50	HEM	C2C-C1C-NC	4.67	111.96	108.27
15	O	90	HEM	C2C-C1C-NC	4.66	111.95	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
15	R	91	HEM	C2C-C1C-NC	4.63	111.92	108.27
15	I	88	HEM	C2C-C1C-NC	4.63	111.92	108.27
11	L	167	CLA	CBD-CAD-C3D	4.10	107.28	104.34
11	J	179	CLA	CBD-CAD-C3D	4.08	107.27	104.34
11	A	174	CLA	CBD-CAD-C3D	4.06	107.25	104.34
11	C	168	CLA	CBD-CAD-C3D	4.05	107.25	104.34
11	C	167	CLA	CBD-CAD-C3D	4.05	107.24	104.34
11	A	179	CLA	CBD-CAD-C3D	4.05	107.24	104.34
11	M	156	CLA	CBD-CAD-C3D	4.04	107.24	104.34
11	M	163	CLA	CBD-CAD-C3D	4.04	107.24	104.34
11	L	165	CLA	CBD-CAD-C3D	4.04	107.23	104.34
11	M	161	CLA	CBD-CAD-C3D	4.04	107.23	104.34
11	M	160	CLA	CBD-CAD-C3D	4.04	107.23	104.34
11	D	170	CLA	CBD-CAD-C3D	4.04	107.23	104.34
11	L	157	CLA	CBD-CAD-C3D	4.04	107.23	104.34
11	C	165	CLA	CBD-CAD-C3D	4.03	107.23	104.34
11	L	168	CLA	CBD-CAD-C3D	4.03	107.23	104.34
11	D	161	CLA	CBD-CAD-C3D	4.03	107.23	104.34
11	D	156	CLA	CBD-CAD-C3D	4.03	107.22	104.34
11	D	160	CLA	CBD-CAD-C3D	4.02	107.22	104.34
11	D	165	CLA	CBD-CAD-C3D	4.02	107.22	104.34
11	M	165	CLA	CBD-CAD-C3D	4.02	107.22	104.34
11	J	174	CLA	CBD-CAD-C3D	4.02	107.22	104.34
11	G	313	CLA	CBD-CAD-C3D	4.02	107.22	104.34
11	M	170	CLA	CBD-CAD-C3D	4.02	107.22	104.34
11	C	157	CLA	CBD-CAD-C3D	4.02	107.22	104.34
11	D	168	CLA	CBD-CAD-C3D	4.01	107.22	104.34
11	C	161	CLA	CBD-CAD-C3D	4.01	107.21	104.34
11	M	168	CLA	CBD-CAD-C3D	4.01	107.21	104.34
11	L	163	CLA	CBD-CAD-C3D	4.00	107.21	104.34
11	D	163	CLA	CBD-CAD-C3D	4.00	107.20	104.34
11	C	163	CLA	CBD-CAD-C3D	3.99	107.20	104.34
11	L	162	CLA	CBD-CAD-C3D	3.99	107.20	104.34
11	M	167	CLA	CBD-CAD-C3D	3.99	107.20	104.34
11	J	178	CLA	CBD-CAD-C3D	3.99	107.20	104.34
11	A	178	CLA	CBD-CAD-C3D	3.99	107.20	104.34
11	D	167	CLA	CBD-CAD-C3D	3.99	107.20	104.34
11	P	313	CLA	CBD-CAD-C3D	3.99	107.20	104.34
11	A	175	CLA	CBD-CAD-C3D	3.98	107.19	104.34
11	C	162	CLA	CBD-CAD-C3D	3.97	107.19	104.34
11	L	161	CLA	CBD-CAD-C3D	3.97	107.19	104.34
11	L	160	CLA	CBD-CAD-C3D	3.97	107.19	104.34

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	D	169	CLA	CBD-CAD-C3D	3.97	107.18	104.34
11	D	159	CLA	CBD-CAD-C3D	3.96	107.18	104.34
11	D	166	CLA	CBD-CAD-C3D	3.96	107.18	104.34
11	J	175	CLA	CBD-CAD-C3D	3.96	107.18	104.34
11	C	166	CLA	CBD-CAD-C3D	3.95	107.17	104.34
11	M	166	CLA	CBD-CAD-C3D	3.95	107.17	104.34
11	A	176	CLA	CBD-CAD-C3D	3.95	107.17	104.34
11	M	158	CLA	CBD-CAD-C3D	3.95	107.17	104.34
11	D	158	CLA	CBD-CAD-C3D	3.94	107.17	104.34
11	B	178	CLA	CBD-CAD-C3D	3.94	107.17	104.34
11	C	158	CLA	CBD-CAD-C3D	3.94	107.17	104.34
11	B	176	CLA	CBD-CAD-C3D	3.94	107.16	104.34
11	M	159	CLA	CBD-CAD-C3D	3.94	107.16	104.34
11	D	157	CLA	CBD-CAD-C3D	3.94	107.16	104.34
11	D	164	CLA	CBD-CAD-C3D	3.93	107.16	104.34
11	C	160	CLA	CBD-CAD-C3D	3.92	107.15	104.34
11	L	158	CLA	CBD-CAD-C3D	3.92	107.15	104.34
11	L	166	CLA	CBD-CAD-C3D	3.92	107.15	104.34
11	M	169	CLA	CBD-CAD-C3D	3.91	107.14	104.34
11	M	162	CLA	CBD-CAD-C3D	3.91	107.14	104.34
11	M	164	CLA	CBD-CAD-C3D	3.91	107.14	104.34
11	K	178	CLA	CBD-CAD-C3D	3.90	107.14	104.34
11	J	176	CLA	CBD-CAD-C3D	3.90	107.14	104.34
15	F	50	HEM	C2B-C1B-NB	3.90	111.35	108.27
11	M	157	CLA	CBD-CAD-C3D	3.90	107.14	104.34
11	K	176	CLA	CBD-CAD-C3D	3.90	107.13	104.34
11	C	159	CLA	CBD-CAD-C3D	3.89	107.13	104.34
11	L	159	CLA	CBD-CAD-C3D	3.89	107.13	104.34
15	I	88	HEM	C2B-C1B-NB	3.88	111.33	108.27
15	R	91	HEM	C2B-C1B-NB	3.87	111.33	108.27
15	O	90	HEM	C2B-C1B-NB	3.87	111.33	108.27
11	D	162	CLA	CBD-CAD-C3D	3.87	107.11	104.34
11	C	164	CLA	CBD-CAD-C3D	3.85	107.10	104.34
11	L	164	CLA	CBD-CAD-C3D	3.84	107.09	104.34
15	R	91	HEM	C3C-C4C-NC	3.68	111.18	108.27
15	I	88	HEM	C3C-C4C-NC	3.63	111.13	108.27
15	F	50	HEM	C3C-C4C-NC	3.62	111.13	108.27
15	O	90	HEM	C3C-C4C-NC	3.61	111.13	108.27
15	F	50	HEM	C4C-NC-C1C	3.47	108.40	105.79
15	I	88	HEM	C4C-NC-C1C	3.45	108.39	105.79
15	O	90	HEM	C4C-NC-C1C	3.45	108.39	105.79
15	R	91	HEM	C4C-NC-C1C	3.42	108.36	105.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	159	CLA	C1C-NC-C4C	3.30	108.19	106.71
11	A	178	CLA	C1C-NC-C4C	3.28	108.18	106.71
11	B	178	CLA	C1C-NC-C4C	3.27	108.18	106.71
11	A	179	CLA	C1C-NC-C4C	3.27	108.18	106.71
11	J	178	CLA	C1C-NC-C4C	3.27	108.18	106.71
12	J	177	PHO	CBD-CHA-C1A	3.27	131.18	124.52
12	K	177	PHO	CBD-CHA-C1A	3.26	131.18	124.52
11	J	179	CLA	C1C-NC-C4C	3.26	108.17	106.71
12	A	177	PHO	CBD-CHA-C1A	3.26	131.17	124.52
11	J	176	CLA	C1C-NC-C4C	3.26	108.17	106.71
12	B	177	PHO	CBD-CHA-C1A	3.26	131.17	124.52
11	C	167	CLA	C1C-NC-C4C	3.26	108.17	106.71
11	L	157	CLA	C1C-NC-C4C	3.25	108.17	106.71
11	L	168	CLA	C1C-NC-C4C	3.25	108.17	106.71
11	C	168	CLA	C1C-NC-C4C	3.24	108.16	106.71
11	C	165	CLA	C1C-NC-C4C	3.24	108.16	106.71
11	L	163	CLA	C1C-NC-C4C	3.24	108.16	106.71
11	K	176	CLA	C1C-NC-C4C	3.23	108.16	106.71
11	L	159	CLA	C1C-NC-C4C	3.23	108.16	106.71
11	L	160	CLA	C1C-NC-C4C	3.23	108.16	106.71
11	A	176	CLA	C1C-NC-C4C	3.23	108.16	106.71
11	L	158	CLA	C1C-NC-C4C	3.23	108.16	106.71
11	C	163	CLA	C1C-NC-C4C	3.23	108.16	106.71
11	C	164	CLA	C1C-NC-C4C	3.23	108.16	106.71
11	D	158	CLA	C1C-NC-C4C	3.23	108.16	106.71
11	B	176	CLA	C1C-NC-C4C	3.22	108.15	106.71
11	M	168	CLA	C1C-NC-C4C	3.22	108.15	106.71
11	A	175	CLA	C1C-NC-C4C	3.22	108.15	106.71
11	L	164	CLA	C1C-NC-C4C	3.20	108.15	106.71
11	D	162	CLA	C1C-NC-C4C	3.20	108.14	106.71
11	C	157	CLA	C1C-NC-C4C	3.20	108.14	106.71
11	K	178	CLA	C1C-NC-C4C	3.20	108.14	106.71
11	L	165	CLA	C1C-NC-C4C	3.20	108.14	106.71
11	D	164	CLA	C1C-NC-C4C	3.20	108.14	106.71
11	P	313	CLA	C1C-NC-C4C	3.20	108.14	106.71
11	D	165	CLA	C1C-NC-C4C	3.19	108.14	106.71
11	J	175	CLA	C1C-NC-C4C	3.19	108.14	106.71
11	M	162	CLA	C1C-NC-C4C	3.18	108.14	106.71
11	D	163	CLA	C1C-NC-C4C	3.17	108.13	106.71
11	D	160	CLA	C1C-NC-C4C	3.16	108.13	106.71
11	M	159	CLA	C1C-NC-C4C	3.15	108.12	106.71
11	L	161	CLA	C1C-NC-C4C	3.15	108.12	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	160	CLA	C1C-NC-C4C	3.15	108.12	106.71
11	C	158	CLA	C1C-NC-C4C	3.15	108.12	106.71
11	L	162	CLA	C1C-NC-C4C	3.15	108.12	106.71
11	M	165	CLA	C1C-NC-C4C	3.15	108.12	106.71
11	M	156	CLA	C1C-NC-C4C	3.15	108.12	106.71
11	D	168	CLA	C1C-NC-C4C	3.15	108.12	106.71
11	D	159	CLA	C1C-NC-C4C	3.13	108.11	106.71
11	D	156	CLA	C1C-NC-C4C	3.13	108.11	106.71
11	D	169	CLA	C1C-NC-C4C	3.13	108.11	106.71
11	C	161	CLA	C1C-NC-C4C	3.13	108.11	106.71
11	M	164	CLA	C1C-NC-C4C	3.13	108.11	106.71
11	G	313	CLA	C1C-NC-C4C	3.13	108.11	106.71
11	D	161	CLA	C1C-NC-C4C	3.13	108.11	106.71
11	L	167	CLA	C1C-NC-C4C	3.13	108.11	106.71
11	M	163	CLA	C1C-NC-C4C	3.11	108.10	106.71
11	D	166	CLA	C1C-NC-C4C	3.11	108.10	106.71
11	M	169	CLA	C1C-NC-C4C	3.10	108.10	106.71
11	L	166	CLA	C1C-NC-C4C	3.10	108.10	106.71
11	C	162	CLA	C1C-NC-C4C	3.09	108.09	106.71
11	C	166	CLA	C1C-NC-C4C	3.09	108.09	106.71
11	C	160	CLA	C1C-NC-C4C	3.08	108.09	106.71
11	M	158	CLA	C1C-NC-C4C	3.07	108.09	106.71
11	J	174	CLA	C1C-NC-C4C	3.07	108.09	106.71
11	D	167	CLA	C1C-NC-C4C	3.07	108.09	106.71
11	M	161	CLA	C1C-NC-C4C	3.05	108.08	106.71
11	M	166	CLA	C1C-NC-C4C	3.05	108.08	106.71
11	A	174	CLA	C1C-NC-C4C	3.05	108.08	106.71
11	D	170	CLA	C1C-NC-C4C	3.05	108.08	106.71
11	M	167	CLA	C1C-NC-C4C	3.04	108.07	106.71
11	D	157	CLA	C1C-NC-C4C	3.00	108.05	106.71
11	M	157	CLA	C1C-NC-C4C	2.98	108.04	106.71
11	M	170	CLA	C1C-NC-C4C	2.94	108.03	106.71
15	F	50	HEM	C3C-C2C-C1C	-2.56	104.10	106.30
15	R	91	HEM	C3C-C2C-C1C	-2.54	104.11	106.30
15	O	90	HEM	C3C-C2C-C1C	-2.54	104.12	106.30
15	I	88	HEM	C3C-C2C-C1C	-2.52	104.13	106.30
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	M	159	CLA	C2A-C1A-CHA	2.49	126.58	122.71
11	A	174	CLA	C2A-C1A-CHA	2.49	126.58	122.71
11	C	164	CLA	C2A-C1A-CHA	2.49	126.57	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	D	167	CLA	C2A-C1A-CHA	2.47	126.53	122.71
11	A	176	CLA	C2A-C1A-CHA	2.47	126.53	122.71
11	M	162	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	L	164	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	B	178	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	J	175	CLA	C2A-C1A-CHA	2.46	126.53	122.71
11	D	165	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	169	CLA	C2A-C1A-CHA	2.46	126.52	122.71
11	M	166	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
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	163	CLA	C2A-C1A-CHA	2.45	126.51	122.71
11	L	162	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	M	167	CLA	C2A-C1A-CHA	2.45	126.51	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	168	CLA	C2A-C1A-CHA	2.45	126.51	122.71
11	C	167	CLA	C2A-C1A-CHA	2.45	126.50	122.71
11	M	163	CLA	C2A-C1A-CHA	2.45	126.50	122.71
11	D	158	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	K	176	CLA	C2A-C1A-CHA	2.43	126.48	122.71
11	J	179	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
11	L	160	CLA	C2A-C1A-CHA	2.41	126.44	122.71
11	J	175	CLA	C3B-C4B-NB	-2.31	108.08	110.11
11	L	167	CLA	C3B-C4B-NB	-2.30	108.09	110.11
11	M	156	CLA	C3B-C4B-NB	-2.30	108.09	110.11
11	L	162	CLA	C3B-C4B-NB	-2.29	108.10	110.11
11	A	175	CLA	C3B-C4B-NB	-2.28	108.10	110.11
11	C	167	CLA	C3B-C4B-NB	-2.28	108.11	110.11
11	M	168	CLA	C3B-C4B-NB	-2.28	108.11	110.11
11	D	157	CLA	C3B-C4B-NB	-2.27	108.11	110.11
11	M	164	CLA	C3B-C4B-NB	-2.27	108.11	110.11
11	L	161	CLA	C3B-C4B-NB	-2.27	108.11	110.11
11	L	158	CLA	C3B-C4B-NB	-2.27	108.11	110.11
11	D	156	CLA	C3B-C4B-NB	-2.27	108.12	110.11
11	L	157	CLA	C3B-C4B-NB	-2.27	108.12	110.11
11	D	160	CLA	C3B-C4B-NB	-2.27	108.12	110.11
11	M	159	CLA	C3B-C4B-NB	-2.26	108.12	110.11
11	M	157	CLA	C3B-C4B-NB	-2.26	108.12	110.11
11	C	157	CLA	C3B-C4B-NB	-2.26	108.12	110.11
11	C	158	CLA	C3B-C4B-NB	-2.26	108.13	110.11
11	M	161	CLA	C3B-C4B-NB	-2.25	108.13	110.11
11	C	164	CLA	C3B-C4B-NB	-2.25	108.13	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	D	168	CLA	C3B-C4B-NB	-2.25	108.13	110.11
11	L	164	CLA	C3B-C4B-NB	-2.25	108.13	110.11
11	D	161	CLA	C3B-C4B-NB	-2.25	108.13	110.11
11	C	162	CLA	C3B-C4B-NB	-2.25	108.13	110.11
11	J	176	CLA	C3B-C4B-NB	-2.25	108.13	110.11
11	C	161	CLA	C3B-C4B-NB	-2.25	108.14	110.11
11	D	159	CLA	C3B-C4B-NB	-2.25	108.14	110.11
11	C	163	CLA	C3B-C4B-NB	-2.24	108.14	110.11
11	M	162	CLA	C3B-C4B-NB	-2.24	108.14	110.11
15	F	50	HEM	C3A-C2A-C1A	-2.24	104.37	106.29
11	A	176	CLA	C3B-C4B-NB	-2.24	108.14	110.11
11	D	158	CLA	C3B-C4B-NB	-2.24	108.14	110.11
11	A	179	CLA	C3B-C4B-NB	-2.24	108.14	110.11
11	D	164	CLA	C3B-C4B-NB	-2.23	108.15	110.11
11	M	163	CLA	C3B-C4B-NB	-2.23	108.15	110.11
11	C	165	CLA	C3B-C4B-NB	-2.23	108.15	110.11
11	L	159	CLA	C3B-C4B-NB	-2.23	108.15	110.11
11	J	179	CLA	C3B-C4B-NB	-2.23	108.15	110.11
11	D	163	CLA	C3B-C4B-NB	-2.23	108.15	110.11
15	R	91	HEM	C3A-C2A-C1A	-2.23	104.38	106.29
11	C	166	CLA	C3B-C4B-NB	-2.22	108.16	110.11
11	L	163	CLA	C3B-C4B-NB	-2.22	108.16	110.11
11	M	158	CLA	C3B-C4B-NB	-2.22	108.16	110.11
15	I	88	HEM	C3A-C2A-C1A	-2.22	104.39	106.29
11	M	160	CLA	C3B-C4B-NB	-2.22	108.16	110.11
11	L	166	CLA	C3B-C4B-NB	-2.22	108.16	110.11
11	D	162	CLA	C3B-C4B-NB	-2.22	108.16	110.11
11	P	313	CLA	C3B-C4B-NB	-2.22	108.16	110.11
15	O	90	HEM	C3A-C2A-C1A	-2.21	104.39	106.29
11	A	178	CLA	C3B-C4B-NB	-2.20	108.17	110.11
11	L	165	CLA	C3B-C4B-NB	-2.20	108.17	110.11
11	D	165	CLA	C3B-C4B-NB	-2.20	108.17	110.11
11	D	170	CLA	C3B-C4B-NB	-2.20	108.17	110.11
11	G	313	CLA	C3B-C4B-NB	-2.20	108.18	110.11
11	C	159	CLA	C3B-C4B-NB	-2.20	108.18	110.11
11	C	160	CLA	C3B-C4B-NB	-2.20	108.18	110.11
11	M	170	CLA	C3B-C4B-NB	-2.20	108.18	110.11
11	K	178	CLA	C3B-C4B-NB	-2.20	108.18	110.11
15	F	50	HEM	C2C-C3C-C4C	-2.20	104.41	106.30
11	C	168	CLA	C3B-C4B-NB	-2.20	108.18	110.11
11	B	178	CLA	C3B-C4B-NB	-2.19	108.18	110.11
15	O	90	HEM	C2C-C3C-C4C	-2.19	104.41	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	R	91	HEM	C2C-C3C-C4C	-2.19	104.41	106.30
11	D	166	CLA	C3B-C4B-NB	-2.19	108.19	110.11
11	J	178	CLA	C3B-C4B-NB	-2.19	108.19	110.11
15	I	88	HEM	C2C-C3C-C4C	-2.19	104.42	106.30
11	L	168	CLA	C3B-C4B-NB	-2.18	108.19	110.11
11	M	166	CLA	C3B-C4B-NB	-2.18	108.19	110.11
11	L	160	CLA	C3B-C4B-NB	-2.18	108.20	110.11
11	D	167	CLA	C3B-C4B-NB	-2.17	108.20	110.11
11	J	174	CLA	C3B-C4B-NB	-2.17	108.20	110.11
11	M	169	CLA	C3B-C4B-NB	-2.17	108.20	110.11
11	B	176	CLA	C3B-C4B-NB	-2.17	108.20	110.11
11	M	167	CLA	C3B-C4B-NB	-2.16	108.21	110.11
11	A	174	CLA	C3B-C4B-NB	-2.16	108.21	110.11
11	D	169	CLA	C3B-C4B-NB	-2.16	108.21	110.11
11	M	165	CLA	C3B-C4B-NB	-2.15	108.22	110.11
11	K	176	CLA	C3B-C4B-NB	-2.13	108.23	110.11
15	F	50	HEM	C4D-CHA-C1A	-2.06	126.47	129.64
15	I	88	HEM	C4D-CHA-C1A	-2.05	126.48	129.64
15	R	91	HEM	C4D-CHA-C1A	-2.03	126.51	129.64
15	O	90	HEM	C4D-CHA-C1A	-2.03	126.52	129.64

All (210) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	C	163	CLA	NC
11	C	163	CLA	ND
11	C	163	CLA	NA
11	C	166	CLA	NC
11	C	166	CLA	ND
11	C	166	CLA	NA
11	M	159	CLA	NC
11	M	159	CLA	ND
11	M	159	CLA	NA
11	C	159	CLA	NC
11	C	159	CLA	ND
11	C	159	CLA	NA
11	D	160	CLA	NC
11	D	160	CLA	ND
11	D	160	CLA	NA
11	K	176	CLA	NC
11	K	176	CLA	ND
11	K	176	CLA	NA

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Mol	Chain	Res	Type	Atom
11	A	175	CLA	NC
11	A	175	CLA	ND
11	A	175	CLA	NA
11	D	164	CLA	NC
11	D	164	CLA	ND
11	D	164	CLA	NA
11	M	169	CLA	NC
11	M	169	CLA	ND
11	M	169	CLA	NA
11	L	161	CLA	NC
11	L	161	CLA	ND
11	L	161	CLA	NA
11	C	160	CLA	NC
11	C	160	CLA	ND
11	C	160	CLA	NA
11	L	159	CLA	NC
11	L	159	CLA	ND
11	L	159	CLA	NA
11	D	159	CLA	NC
11	D	159	CLA	ND
11	D	159	CLA	NA
11	D	156	CLA	NC
11	D	156	CLA	ND
11	D	156	CLA	NA
11	M	160	CLA	NC
11	M	160	CLA	ND
11	M	160	CLA	NA
11	M	158	CLA	NC
11	M	158	CLA	ND
11	M	158	CLA	NA
11	C	164	CLA	NC
11	C	164	CLA	ND
11	C	164	CLA	NA
11	L	166	CLA	NC
11	L	166	CLA	ND
11	L	166	CLA	NA
11	D	162	CLA	NC
11	D	162	CLA	ND
11	D	162	CLA	NA
11	K	178	CLA	NC
11	K	178	CLA	ND
11	K	178	CLA	NA

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Mol	Chain	Res	Type	Atom
11	J	175	CLA	NC
11	J	175	CLA	ND
11	J	175	CLA	NA
11	A	178	CLA	NC
11	A	178	CLA	ND
11	A	178	CLA	NA
11	M	162	CLA	NC
11	M	162	CLA	ND
11	M	162	CLA	NA
11	L	167	CLA	NC
11	L	167	CLA	ND
11	L	167	CLA	NA
11	C	157	CLA	NC
11	C	157	CLA	ND
11	C	157	CLA	NA
11	D	167	CLA	NC
11	D	167	CLA	ND
11	D	167	CLA	NA
11	L	160	CLA	NC
11	L	160	CLA	ND
11	L	160	CLA	NA
11	M	167	CLA	NC
11	M	167	CLA	ND
11	M	167	CLA	NA
11	D	166	CLA	NC
11	D	166	CLA	ND
11	D	166	CLA	NA
11	D	169	CLA	NC
11	D	169	CLA	ND
11	D	169	CLA	NA
11	M	161	CLA	NC
11	M	161	CLA	ND
11	M	161	CLA	NA
11	L	163	CLA	NC
11	L	163	CLA	ND
11	L	163	CLA	NA
11	M	163	CLA	NC
11	M	163	CLA	ND
11	M	163	CLA	NA
11	C	158	CLA	NC
11	C	158	CLA	ND
11	C	158	CLA	NA

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Mol	Chain	Res	Type	Atom
11	D	158	CLA	NC
11	D	158	CLA	ND
11	D	158	CLA	NA
11	L	164	CLA	NC
11	L	164	CLA	ND
11	L	164	CLA	NA
11	C	168	CLA	NC
11	C	168	CLA	ND
11	C	168	CLA	NA
11	L	165	CLA	NC
11	L	165	CLA	ND
11	L	165	CLA	NA
11	D	165	CLA	NC
11	D	165	CLA	ND
11	D	165	CLA	NA
11	C	162	CLA	NC
11	C	162	CLA	ND
11	C	162	CLA	NA
11	J	174	CLA	NC
11	J	174	CLA	ND
11	J	174	CLA	NA
11	G	313	CLA	NC
11	G	313	CLA	ND
11	G	313	CLA	NA
11	A	176	CLA	NC
11	A	176	CLA	ND
11	A	176	CLA	NA
11	M	170	CLA	NC
11	M	170	CLA	ND
11	M	170	CLA	NA
11	M	157	CLA	NC
11	M	157	CLA	ND
11	M	157	CLA	NA
11	D	161	CLA	NC
11	D	161	CLA	ND
11	D	161	CLA	NA
11	D	157	CLA	NC
11	D	157	CLA	ND
11	D	157	CLA	NA
11	J	178	CLA	NC
11	J	178	CLA	ND
11	J	178	CLA	NA

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Mol	Chain	Res	Type	Atom
11	L	158	CLA	NC
11	L	158	CLA	ND
11	L	158	CLA	NA
11	D	168	CLA	NC
11	D	168	CLA	ND
11	D	168	CLA	NA
11	L	168	CLA	NC
11	L	168	CLA	ND
11	L	168	CLA	NA
11	B	178	CLA	NC
11	B	178	CLA	ND
11	B	178	CLA	NA
11	J	176	CLA	NC
11	J	176	CLA	ND
11	J	176	CLA	NA
11	C	161	CLA	NC
11	C	161	CLA	ND
11	C	161	CLA	NA
11	M	166	CLA	NC
11	M	166	CLA	ND
11	M	166	CLA	NA
11	D	170	CLA	NC
11	D	170	CLA	ND
11	D	170	CLA	NA
11	A	174	CLA	NC
11	A	174	CLA	ND
11	A	174	CLA	NA
11	C	167	CLA	NC
11	C	167	CLA	ND
11	C	167	CLA	NA
11	B	176	CLA	NC
11	B	176	CLA	ND
11	B	176	CLA	NA
11	J	179	CLA	NC
11	J	179	CLA	ND
11	J	179	CLA	NA
11	L	162	CLA	NC
11	L	162	CLA	ND
11	L	162	CLA	NA
11	M	164	CLA	NC
11	M	164	CLA	ND
11	M	164	CLA	NA

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Mol	Chain	Res	Type	Atom
11	M	156	CLA	NC
11	M	156	CLA	ND
11	M	156	CLA	NA
11	D	163	CLA	NC
11	D	163	CLA	ND
11	D	163	CLA	NA
11	M	168	CLA	NC
11	M	168	CLA	ND
11	M	168	CLA	NA
11	P	313	CLA	NC
11	P	313	CLA	ND
11	P	313	CLA	NA
11	A	179	CLA	NC
11	A	179	CLA	ND
11	A	179	CLA	NA
11	M	165	CLA	NC
11	M	165	CLA	ND
11	M	165	CLA	NA
11	L	157	CLA	NC
11	L	157	CLA	ND
11	L	157	CLA	NA
11	C	165	CLA	NC
11	C	165	CLA	ND
11	C	165	CLA	NA

There are no torsion outliers.

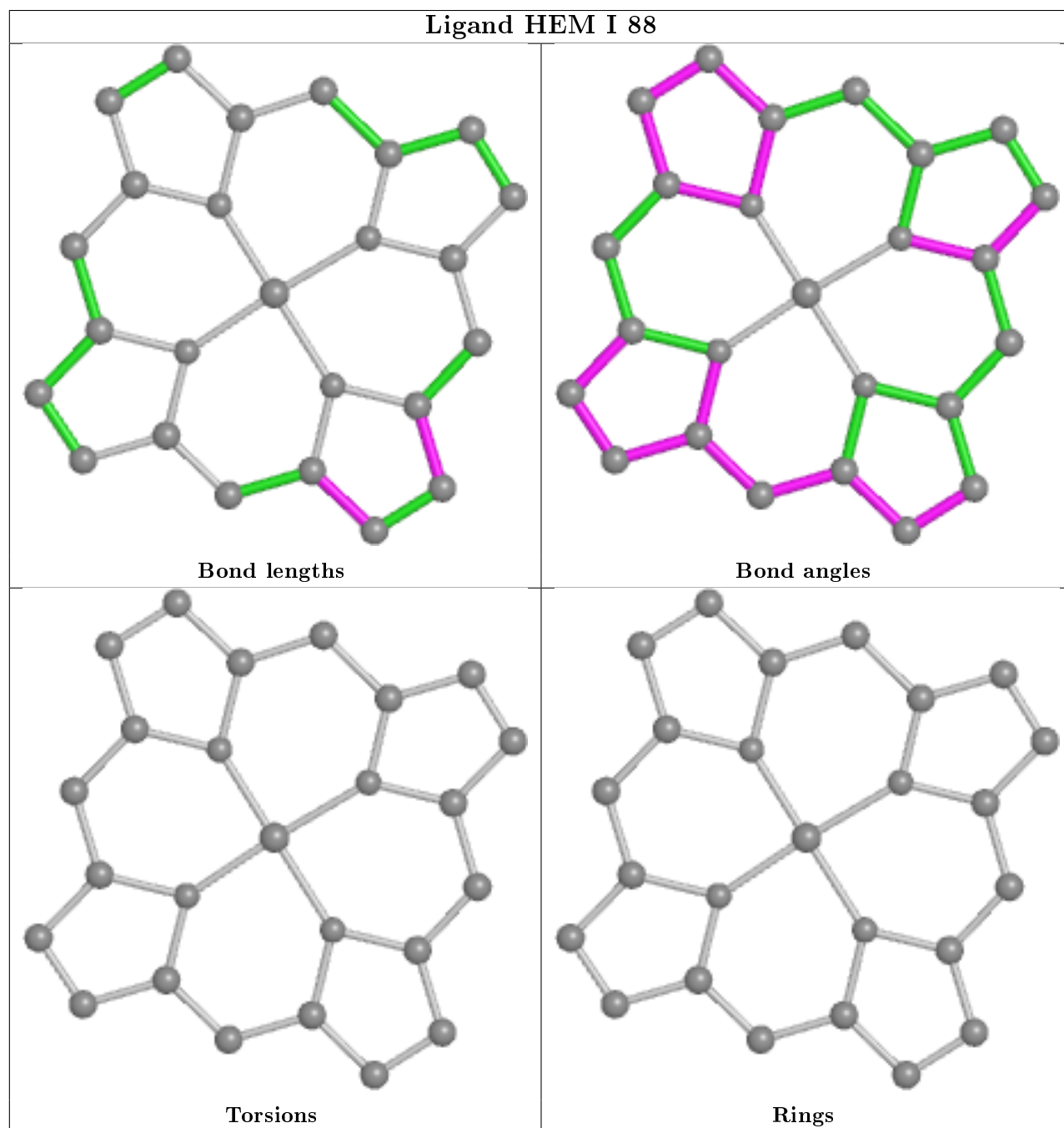
There are no ring outliers.

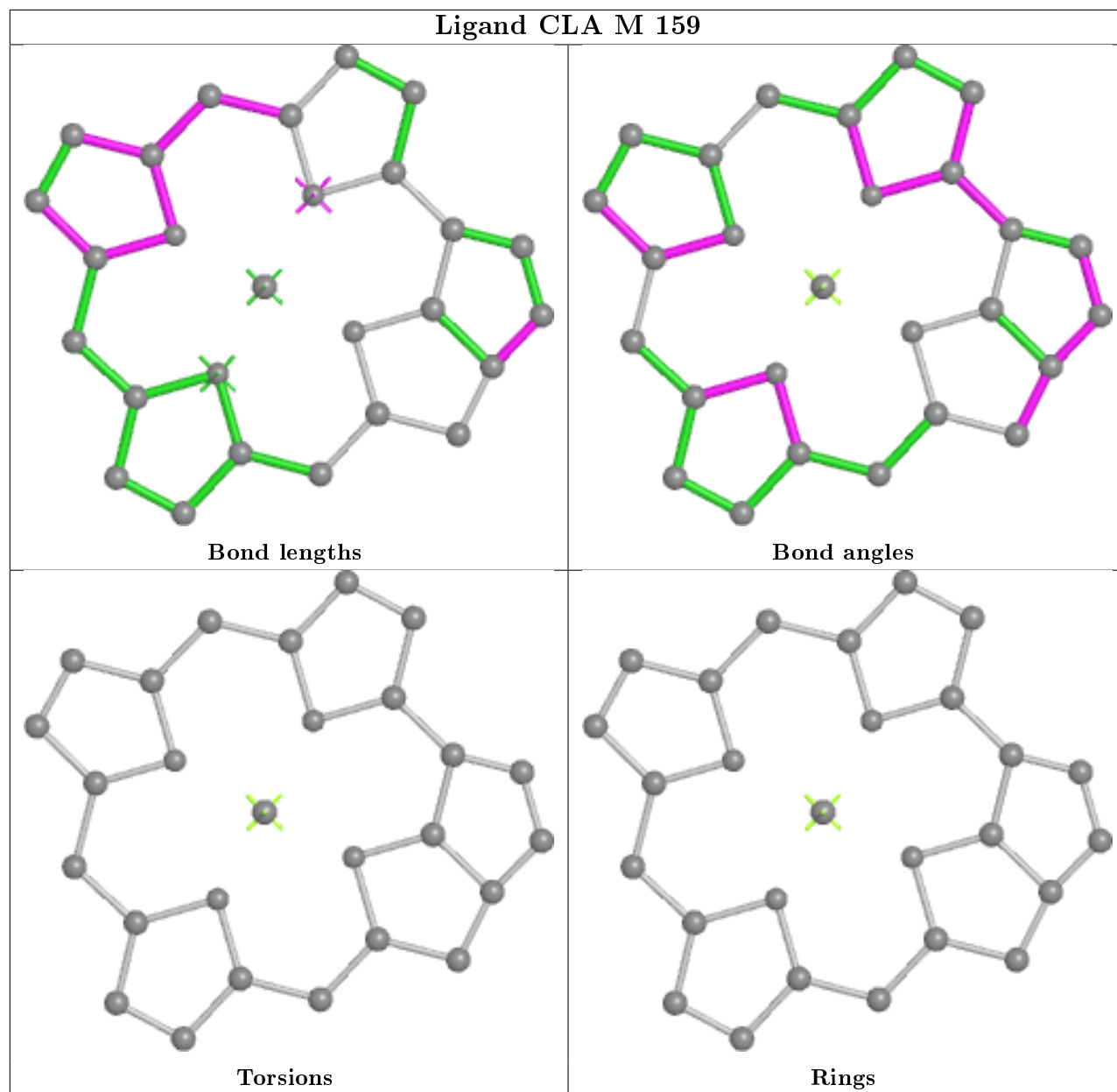
8 monomers are involved in 18 short contacts:

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

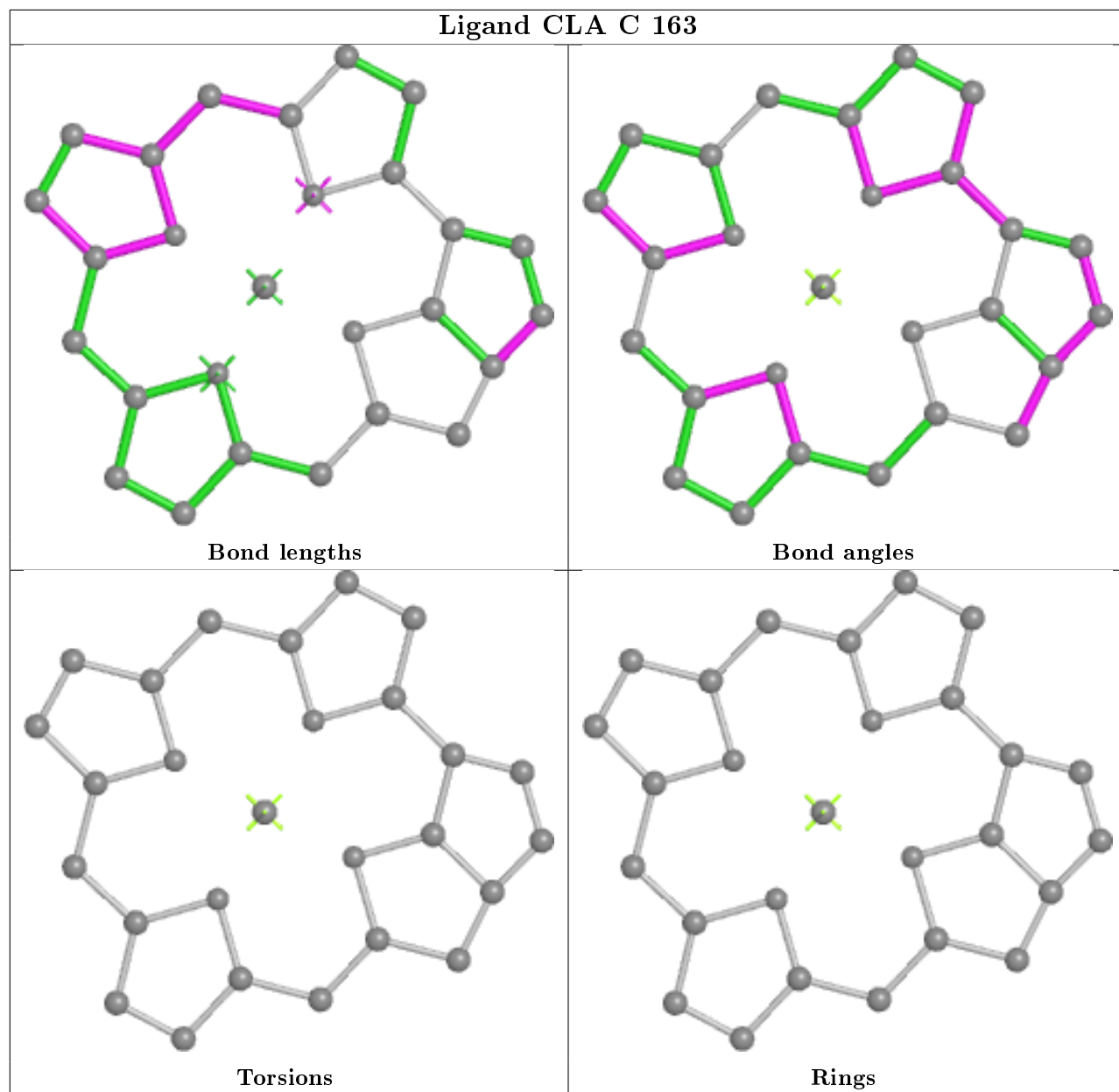
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

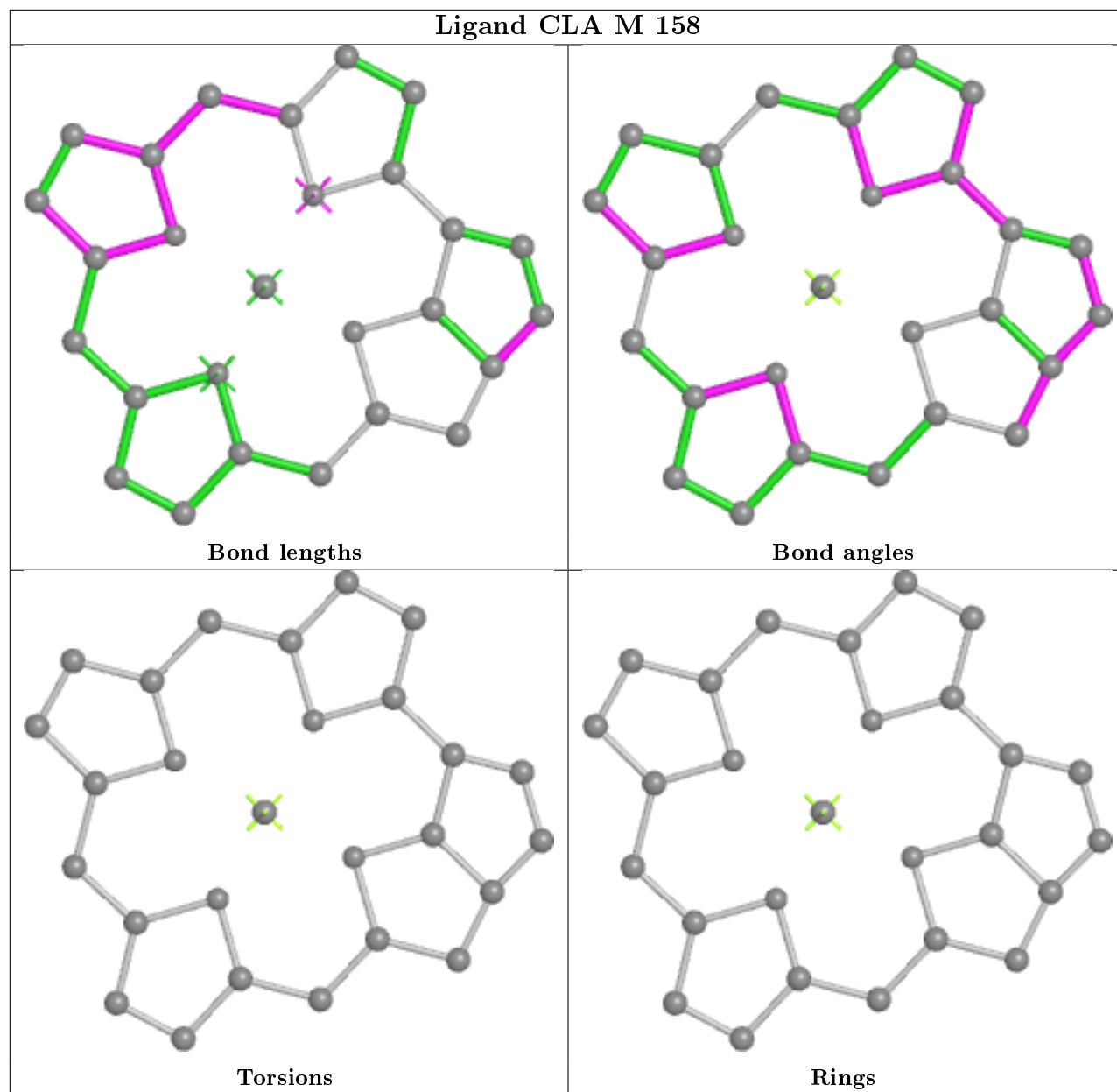
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



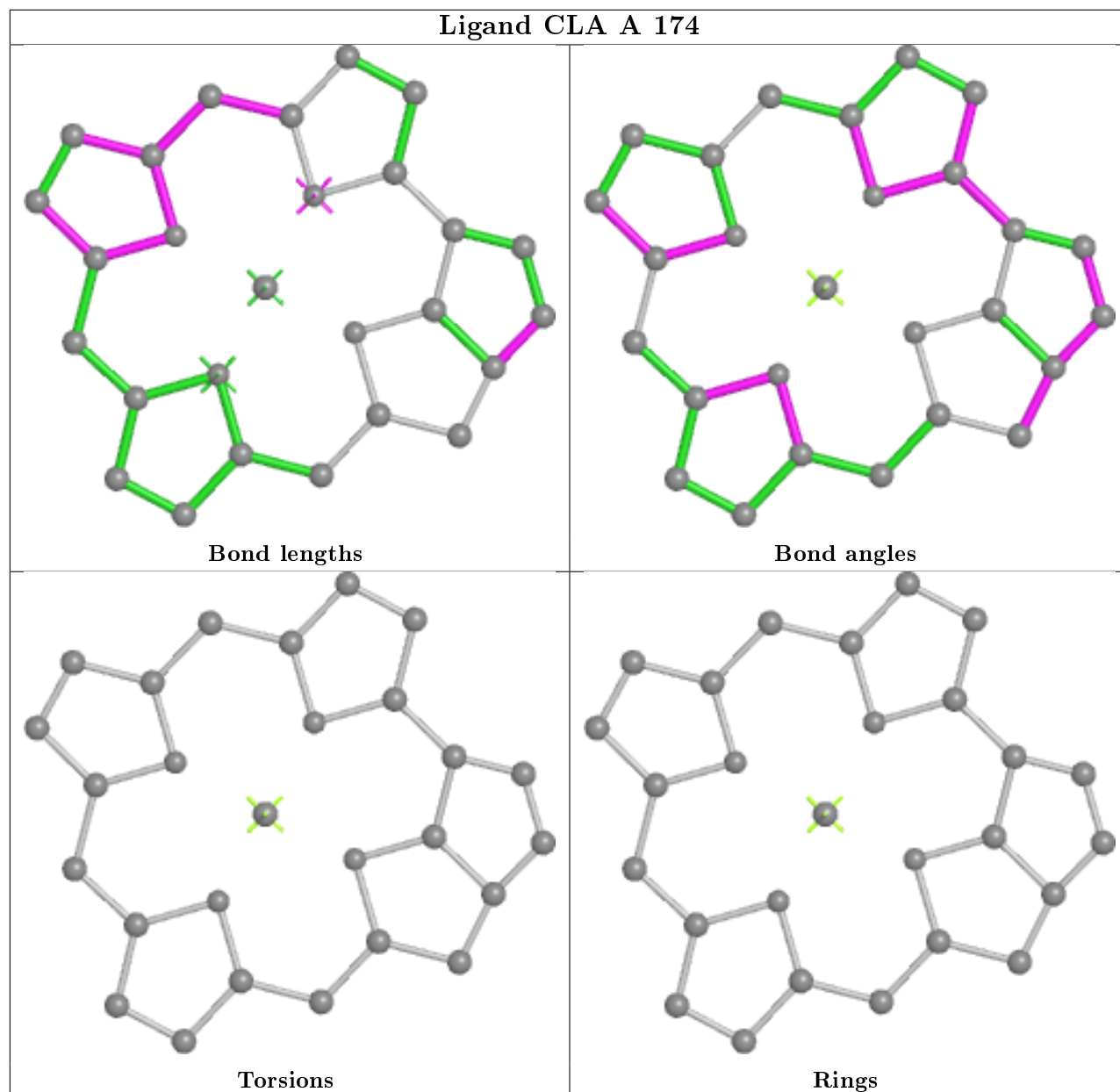


Ligand CLA C 163

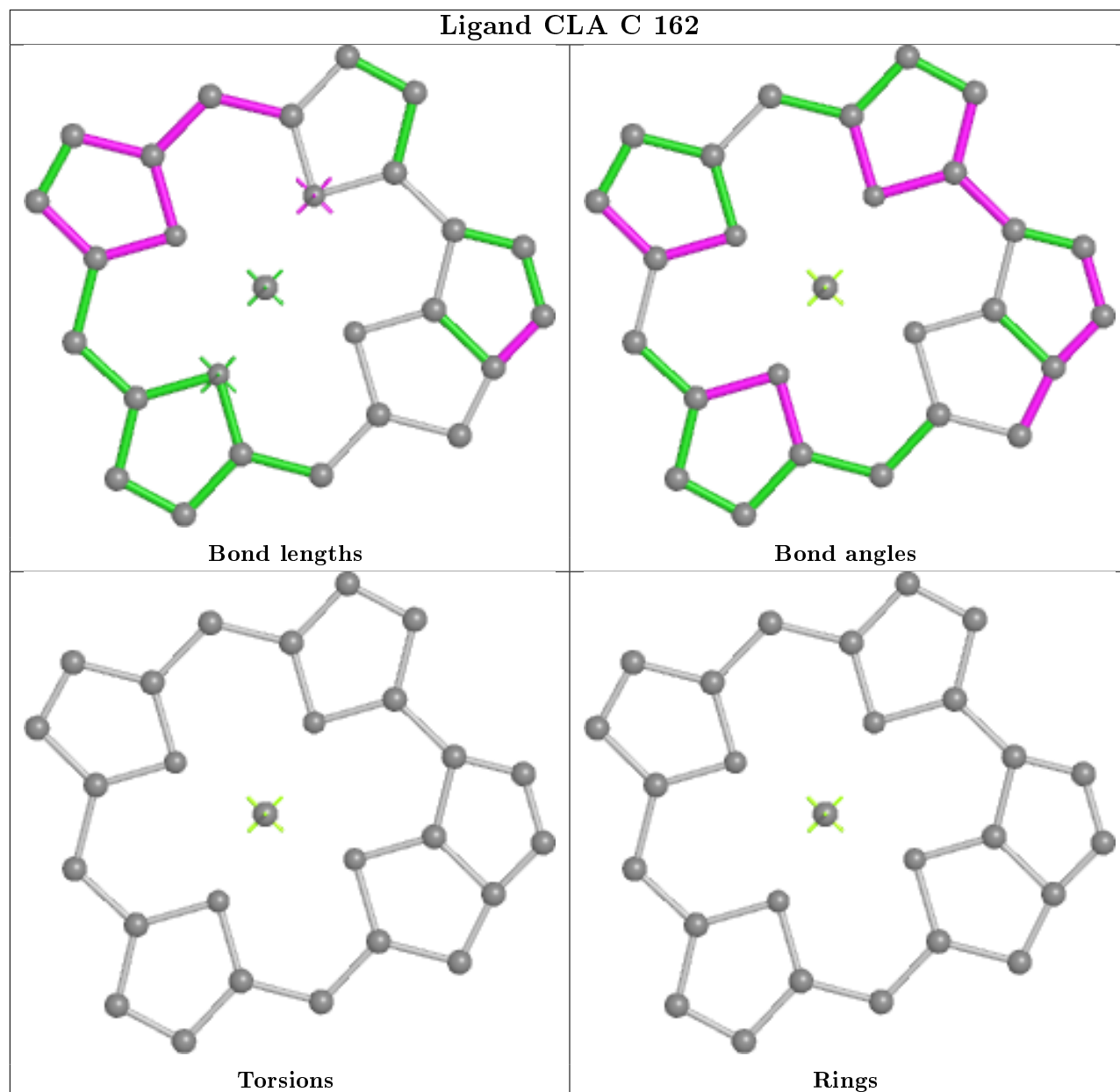




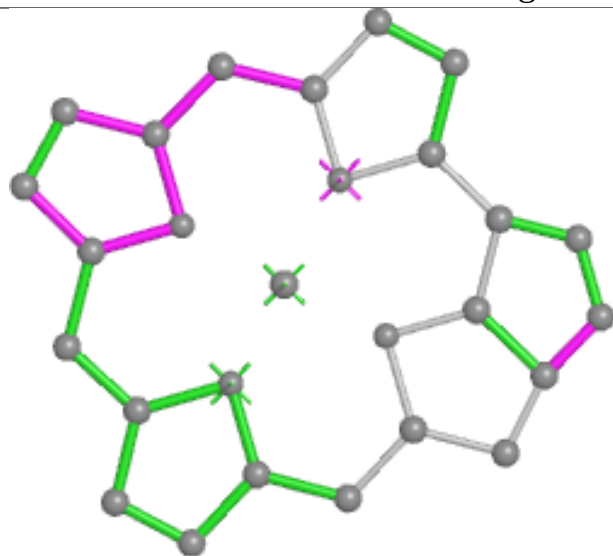
Ligand CLA A 174



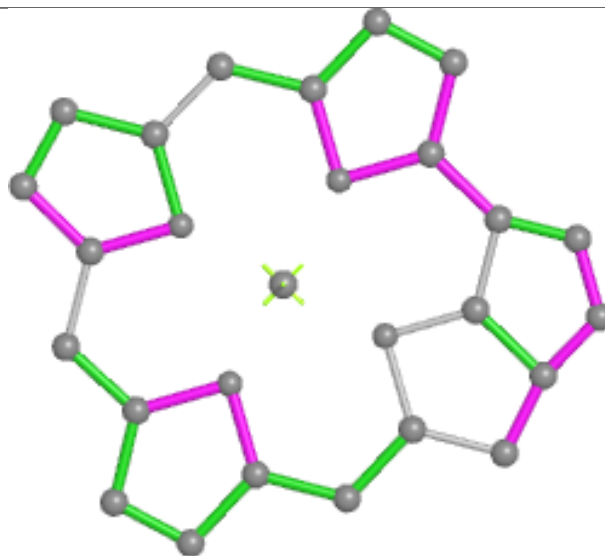
Ligand CLA C 162



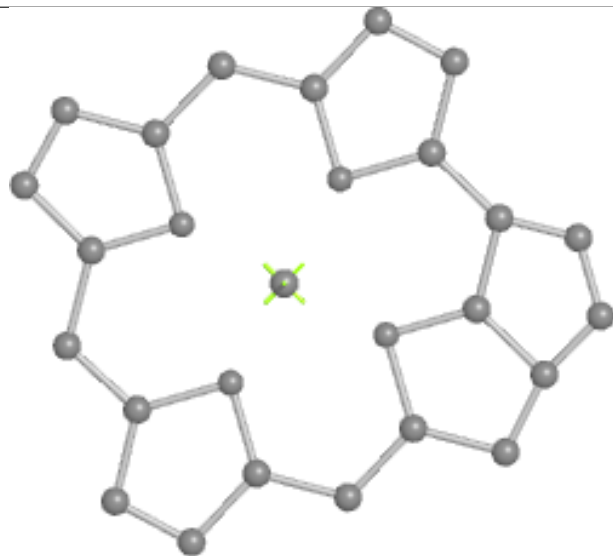
Ligand CLA J 175



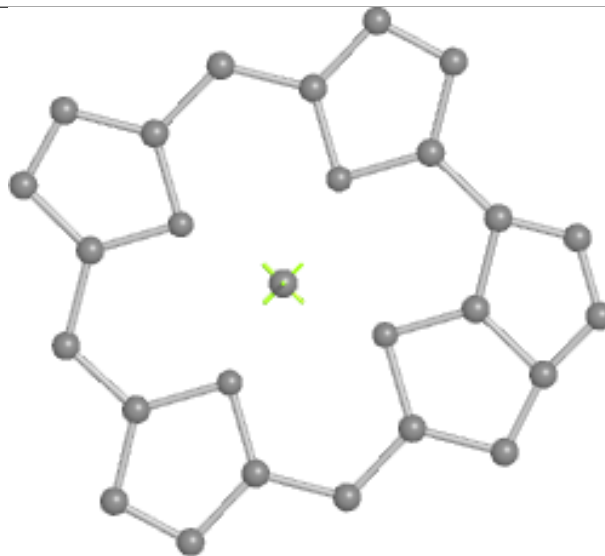
Bond lengths



Bond angles

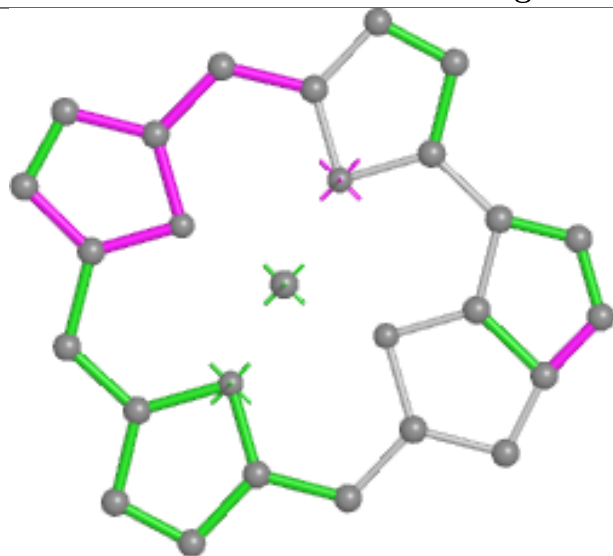


Torsions

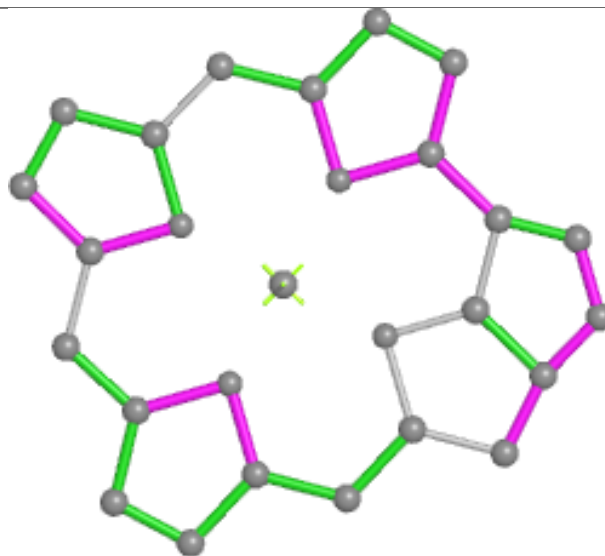


Rings

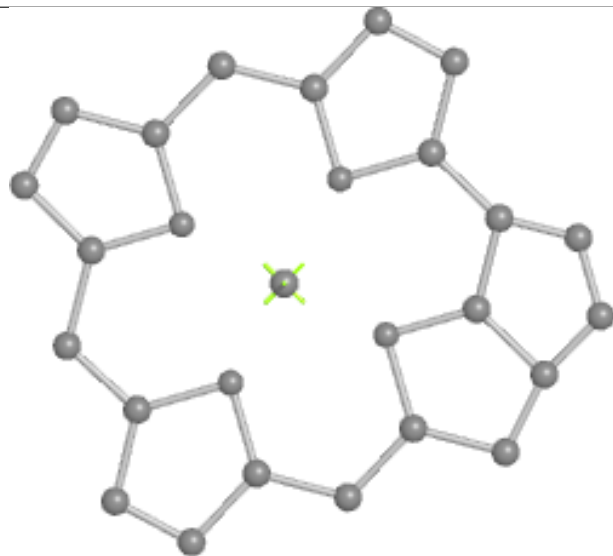
Ligand CLA B 176



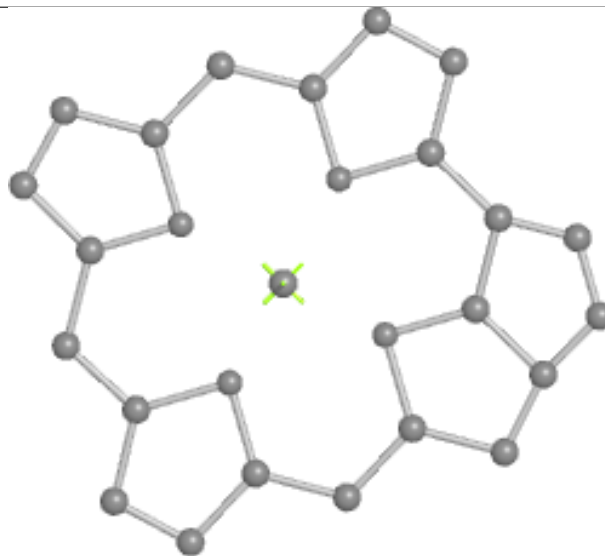
Bond lengths



Bond angles

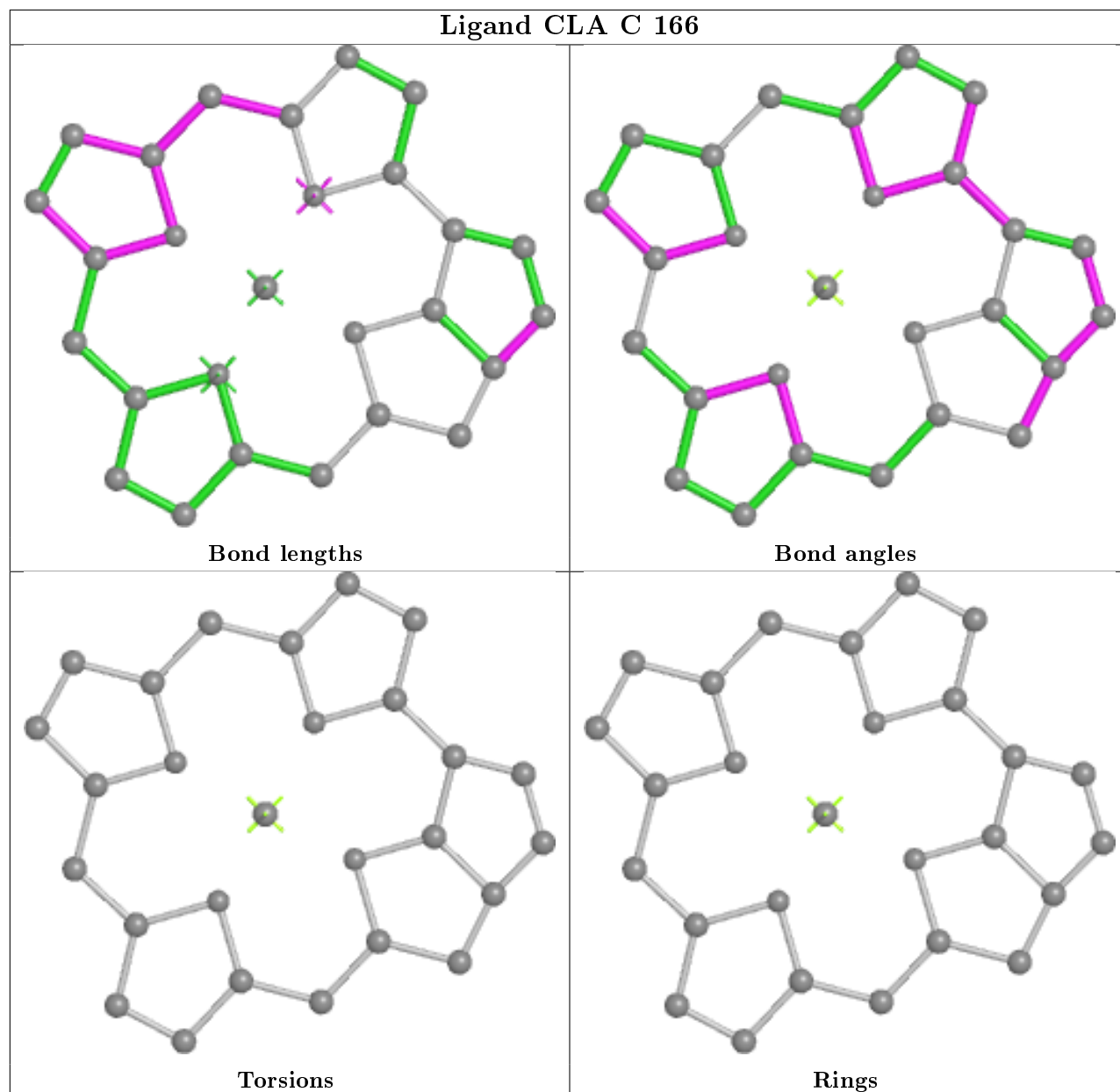


Torsions

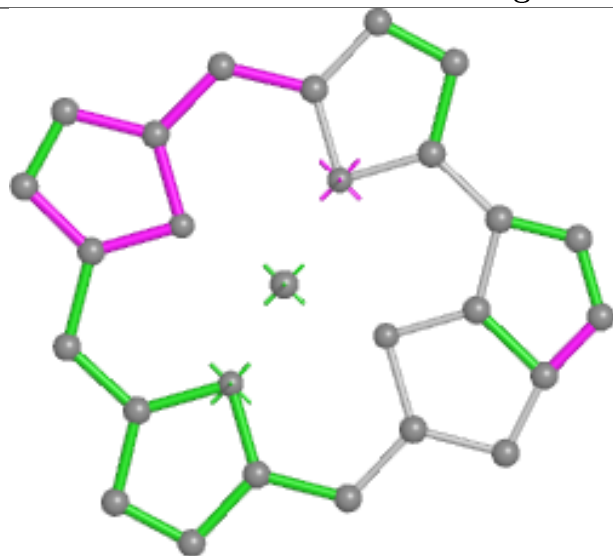


Rings

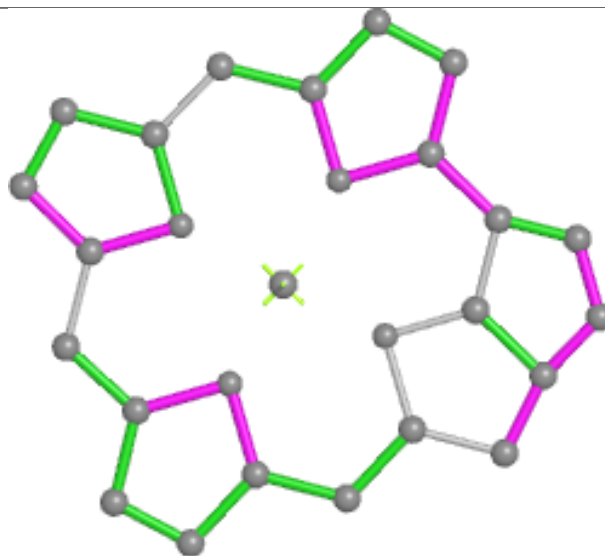
Ligand CLA C 166



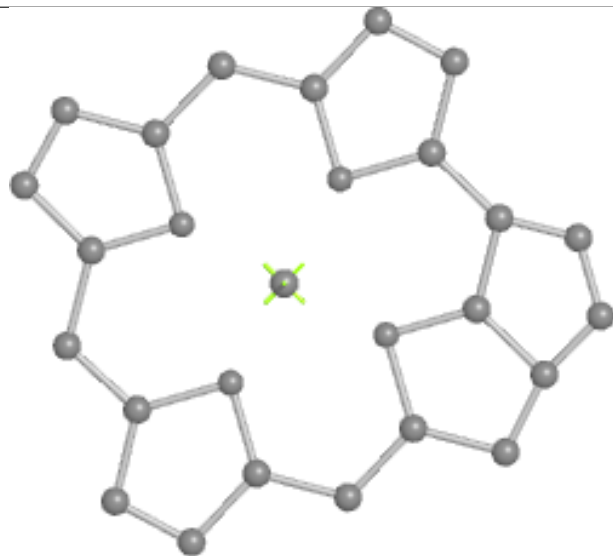
Ligand CLA G 313



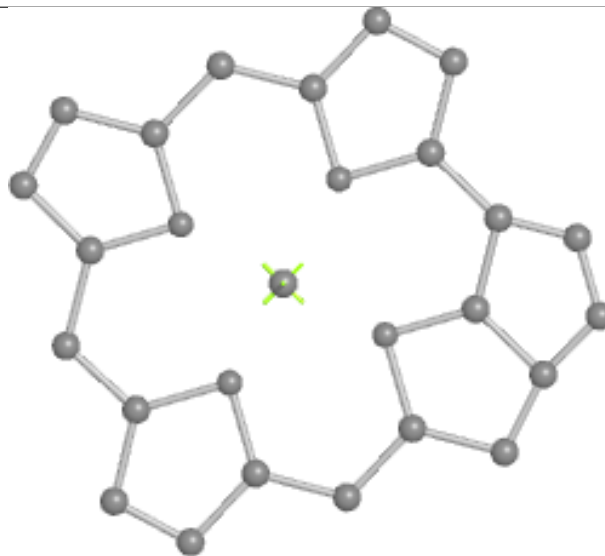
Bond lengths



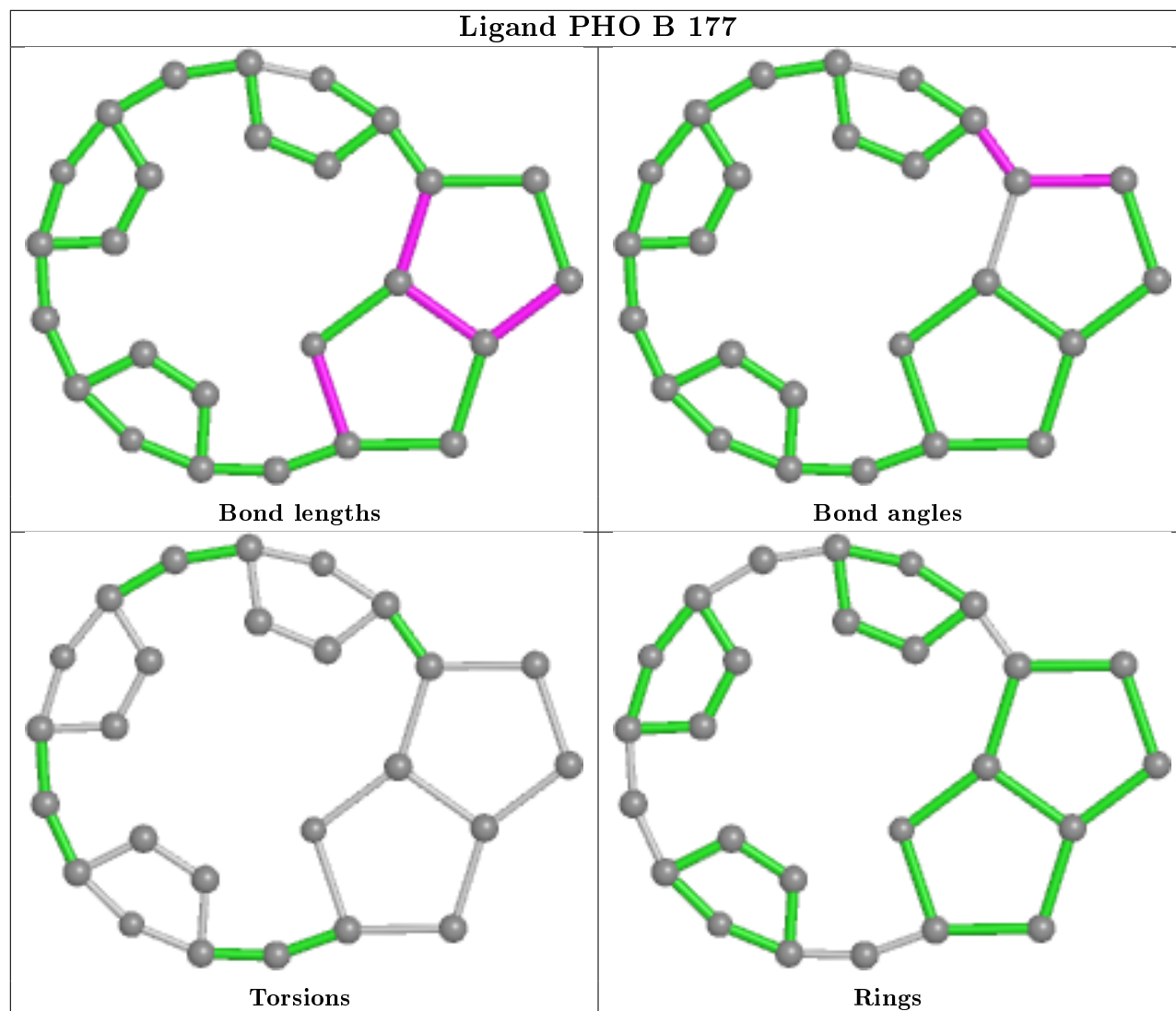
Bond angles

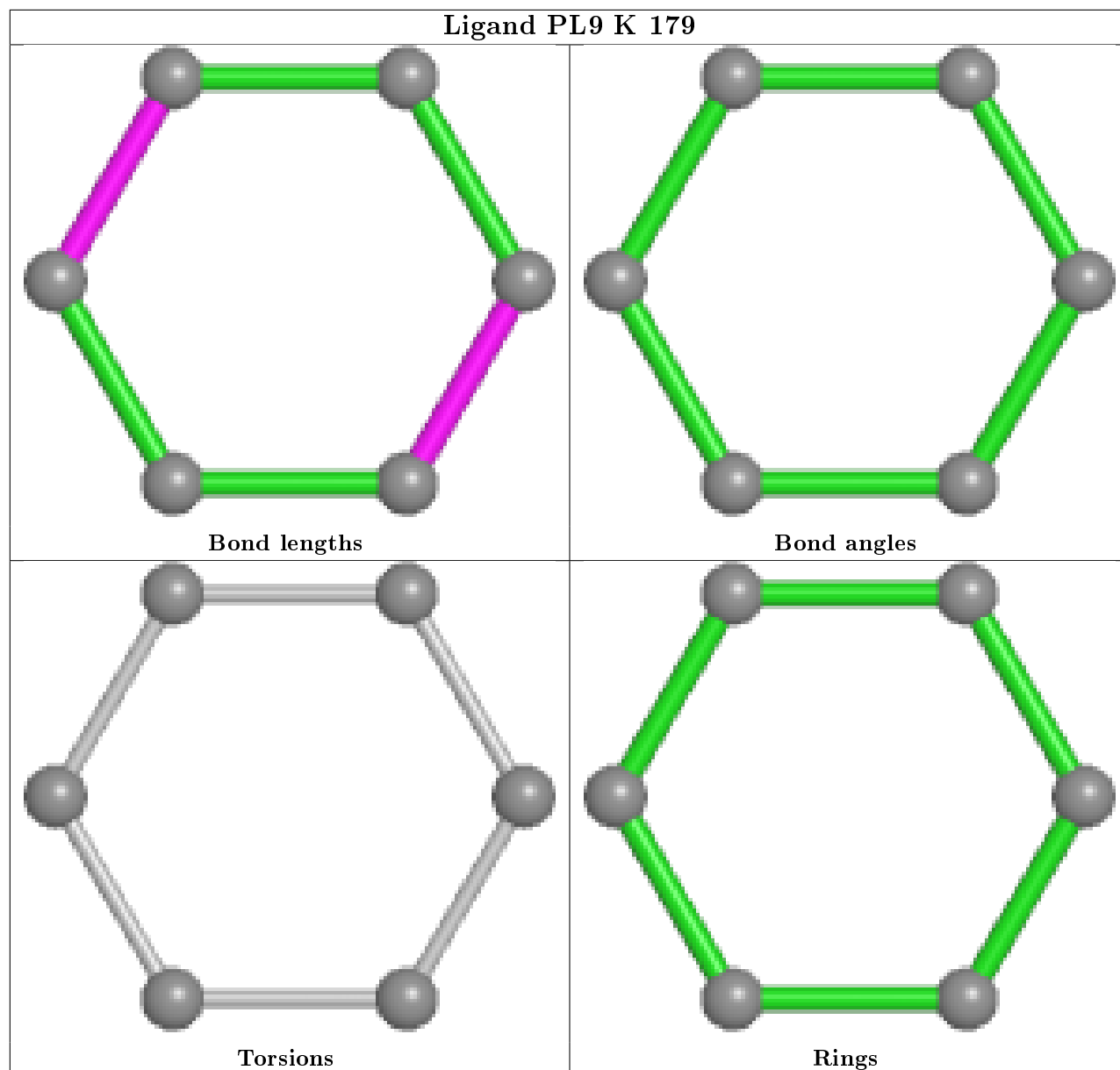


Torsions

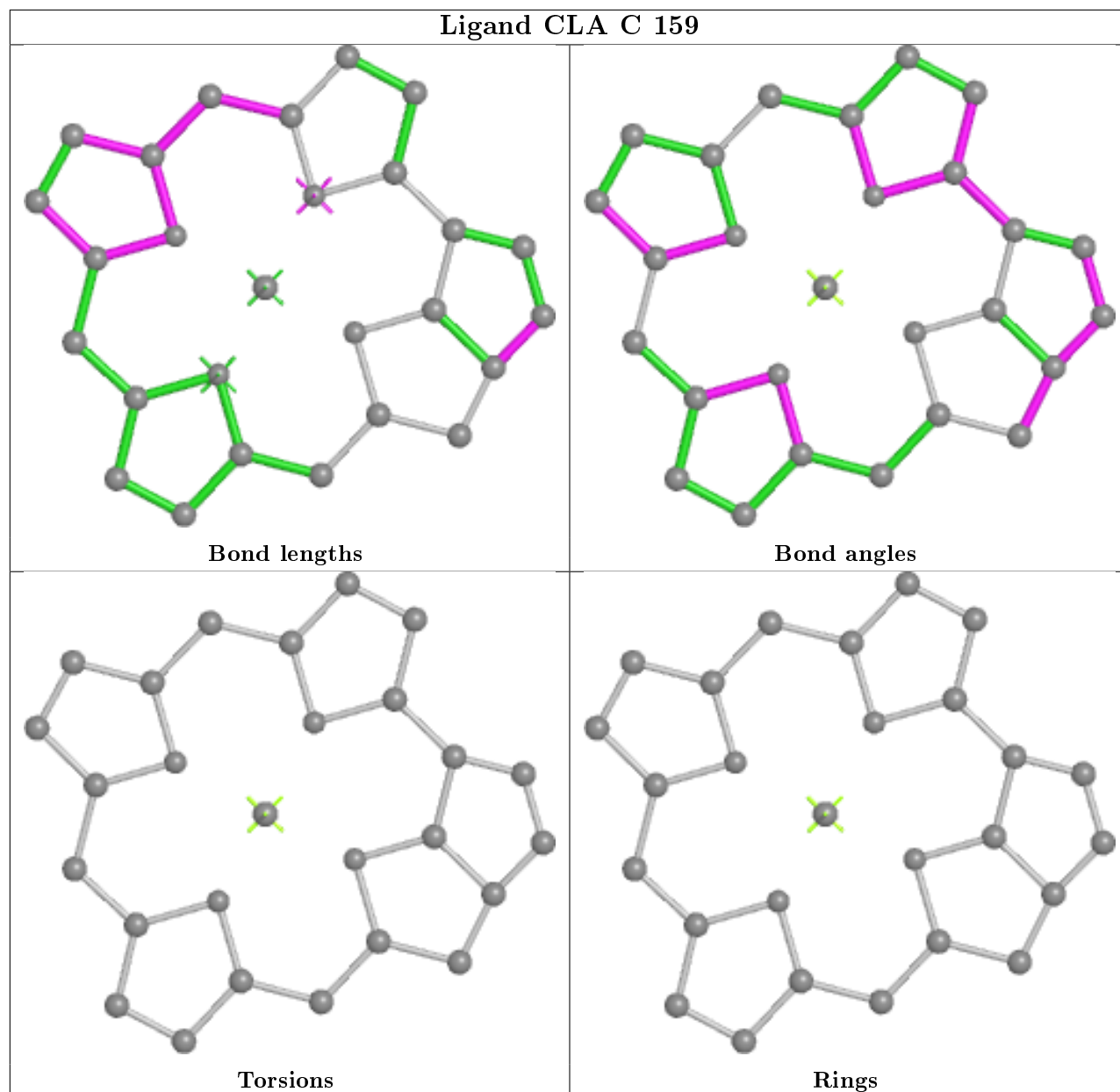


Rings

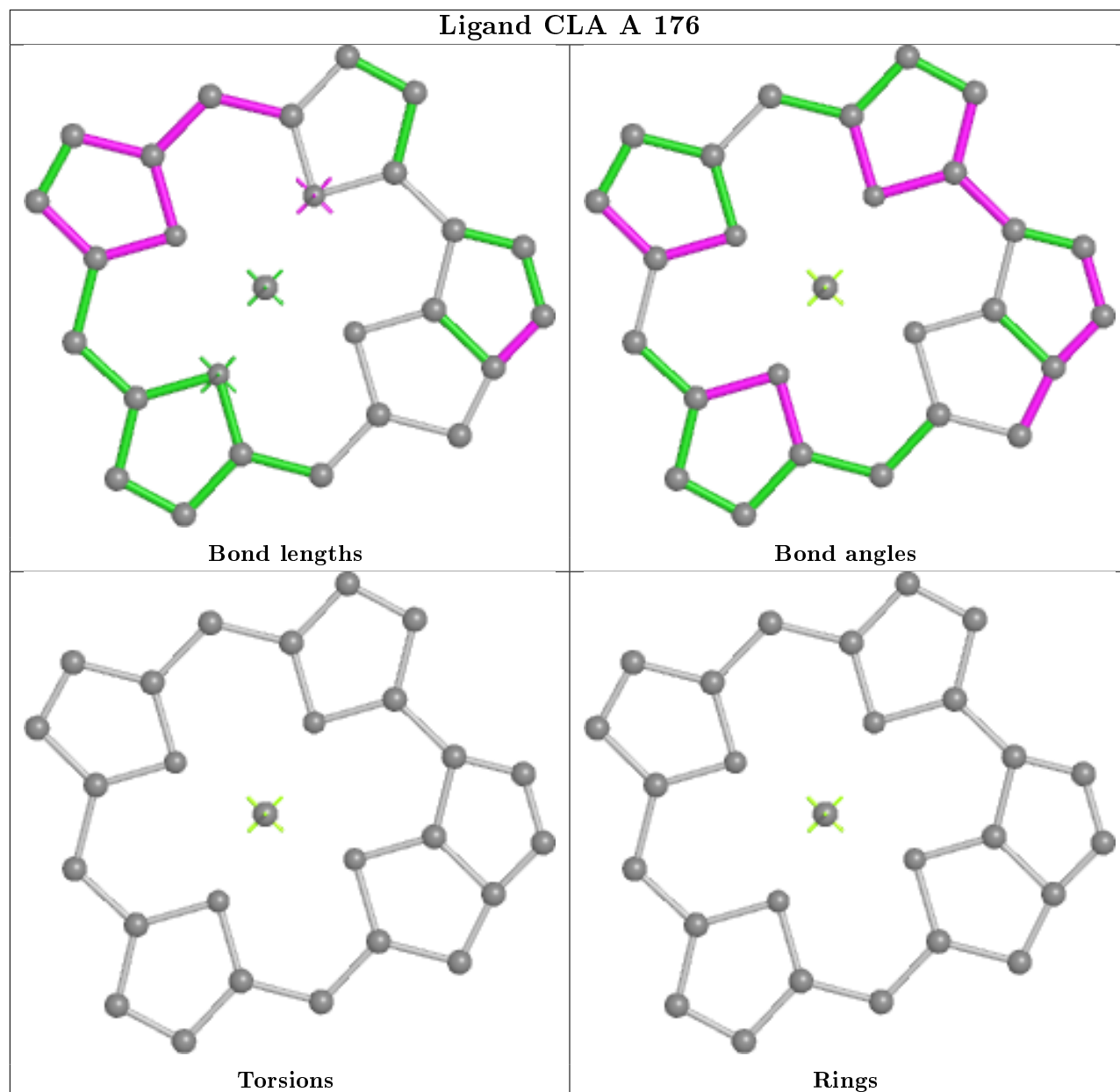




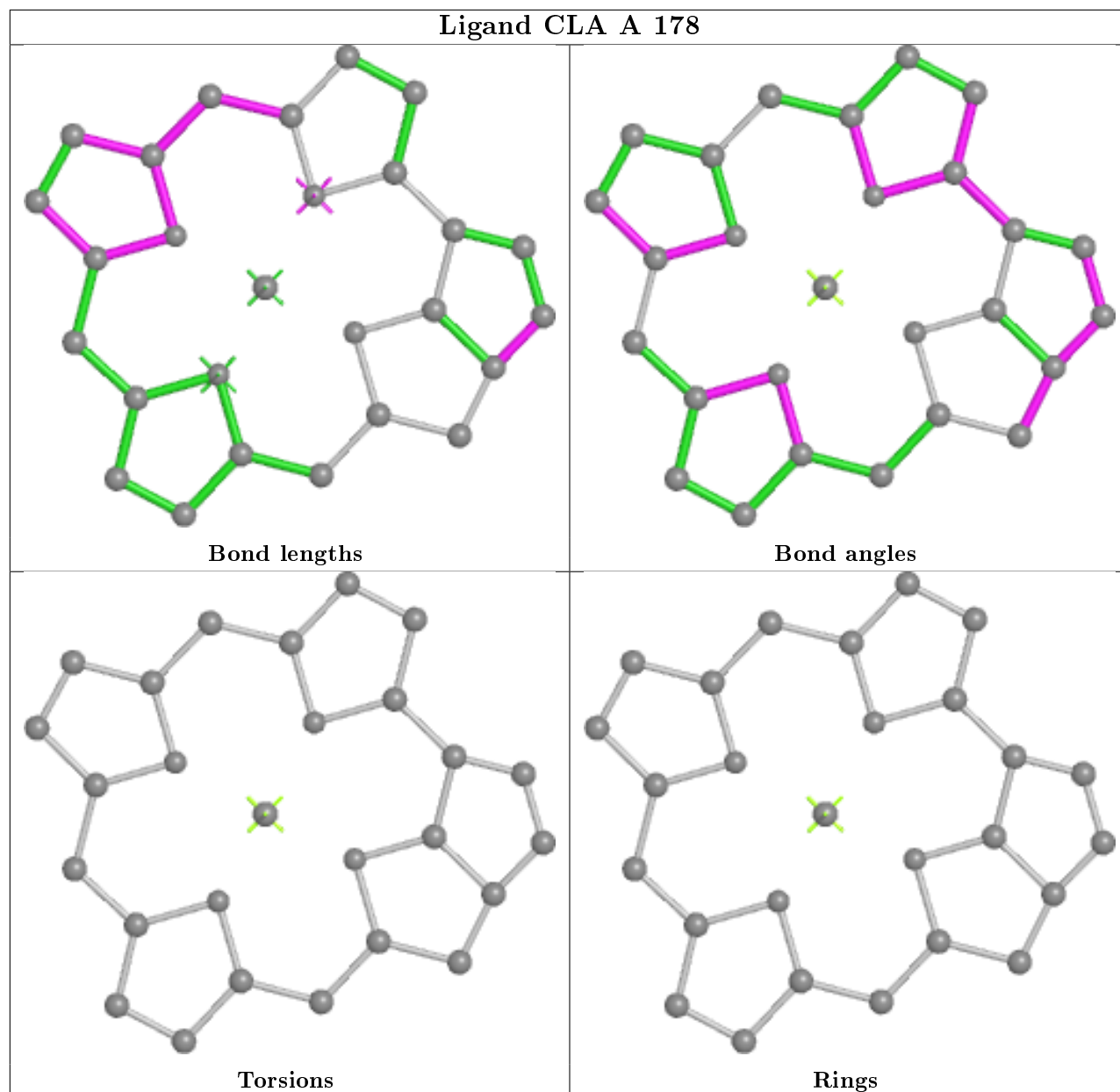
Ligand CLA C 159



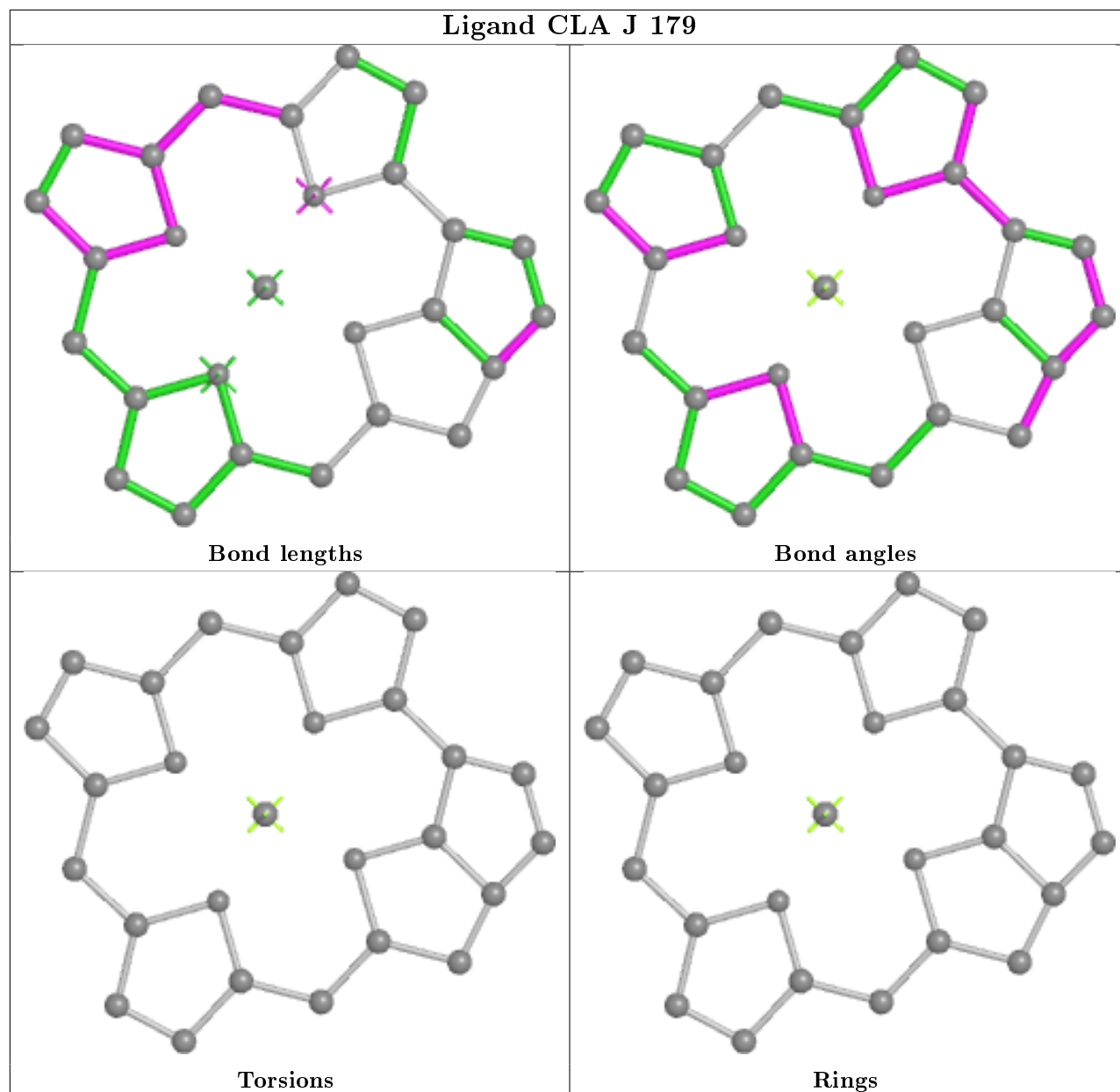
Ligand CLA A 176

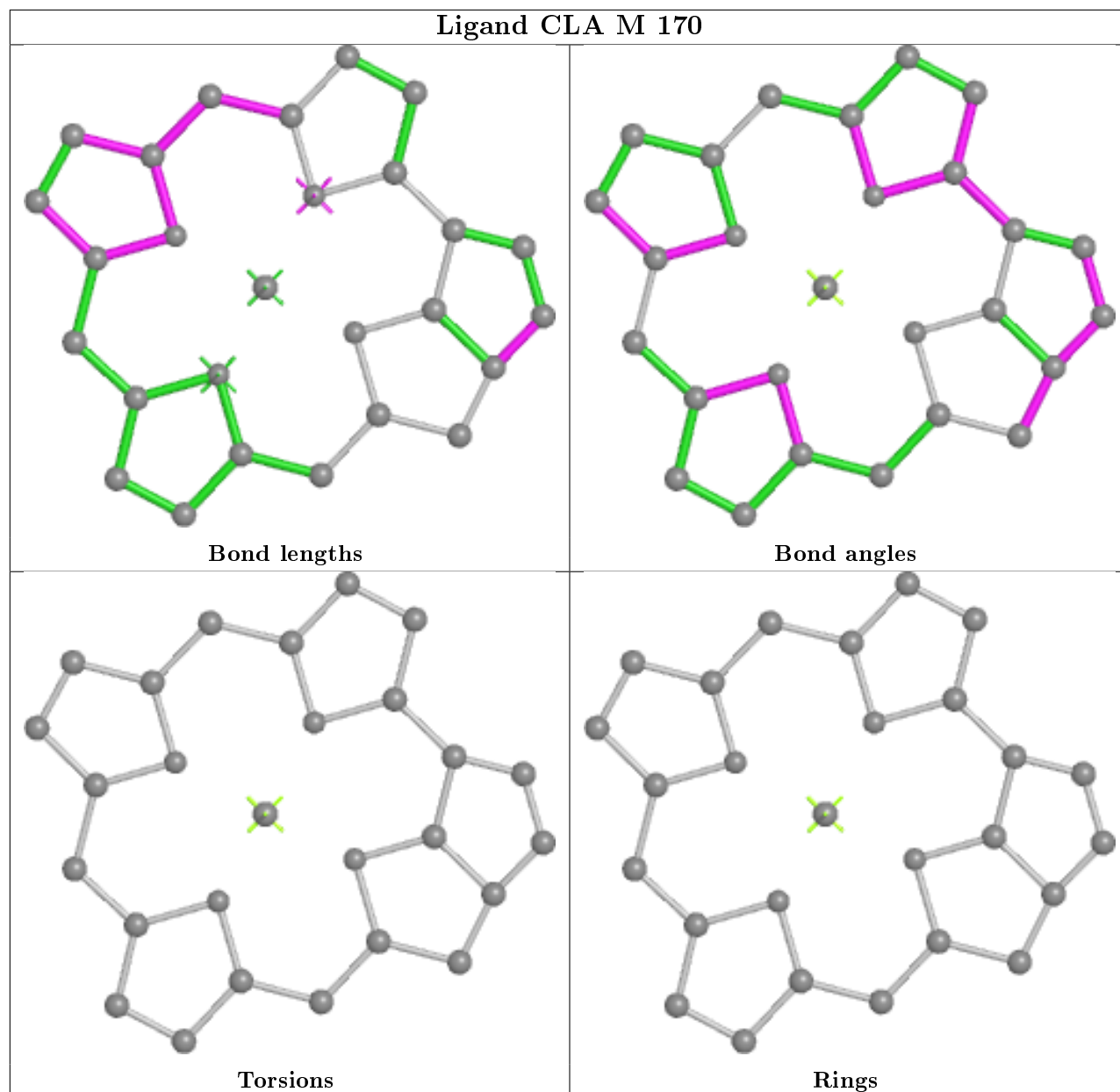


Ligand CLA A 178

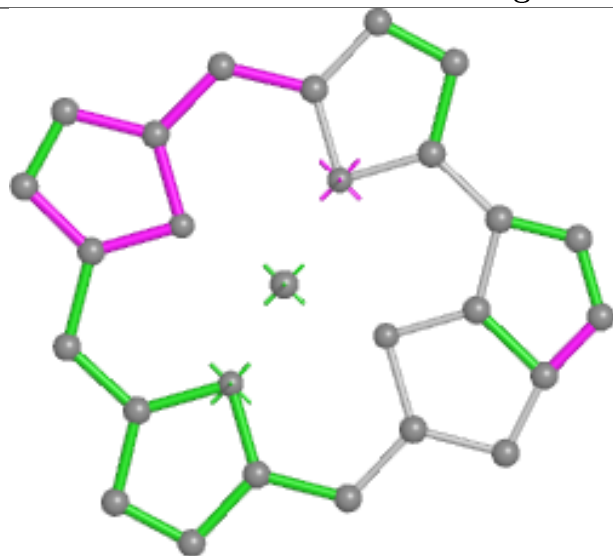


Ligand CLA J 179

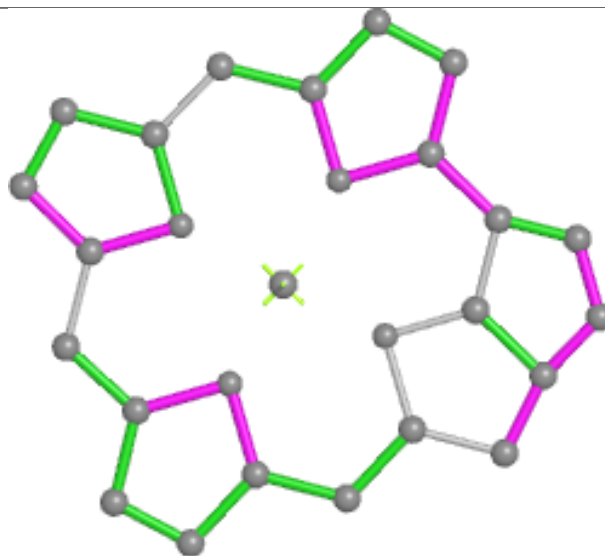




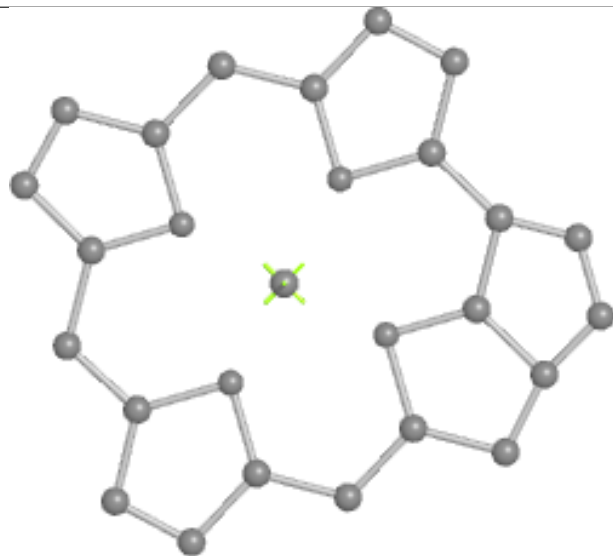
Ligand CLA K 178



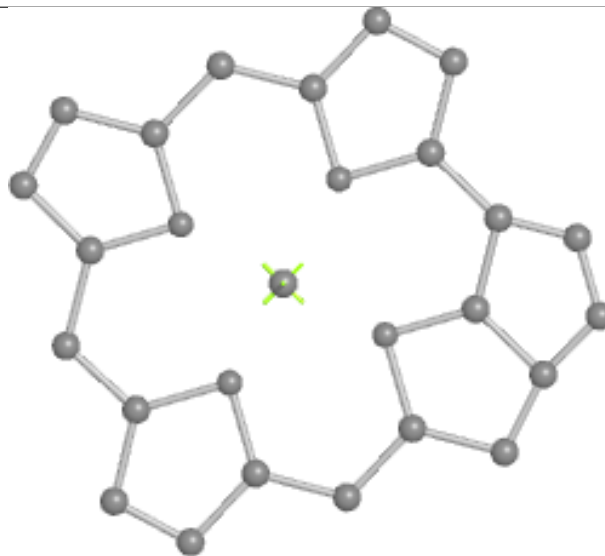
Bond lengths



Bond angles

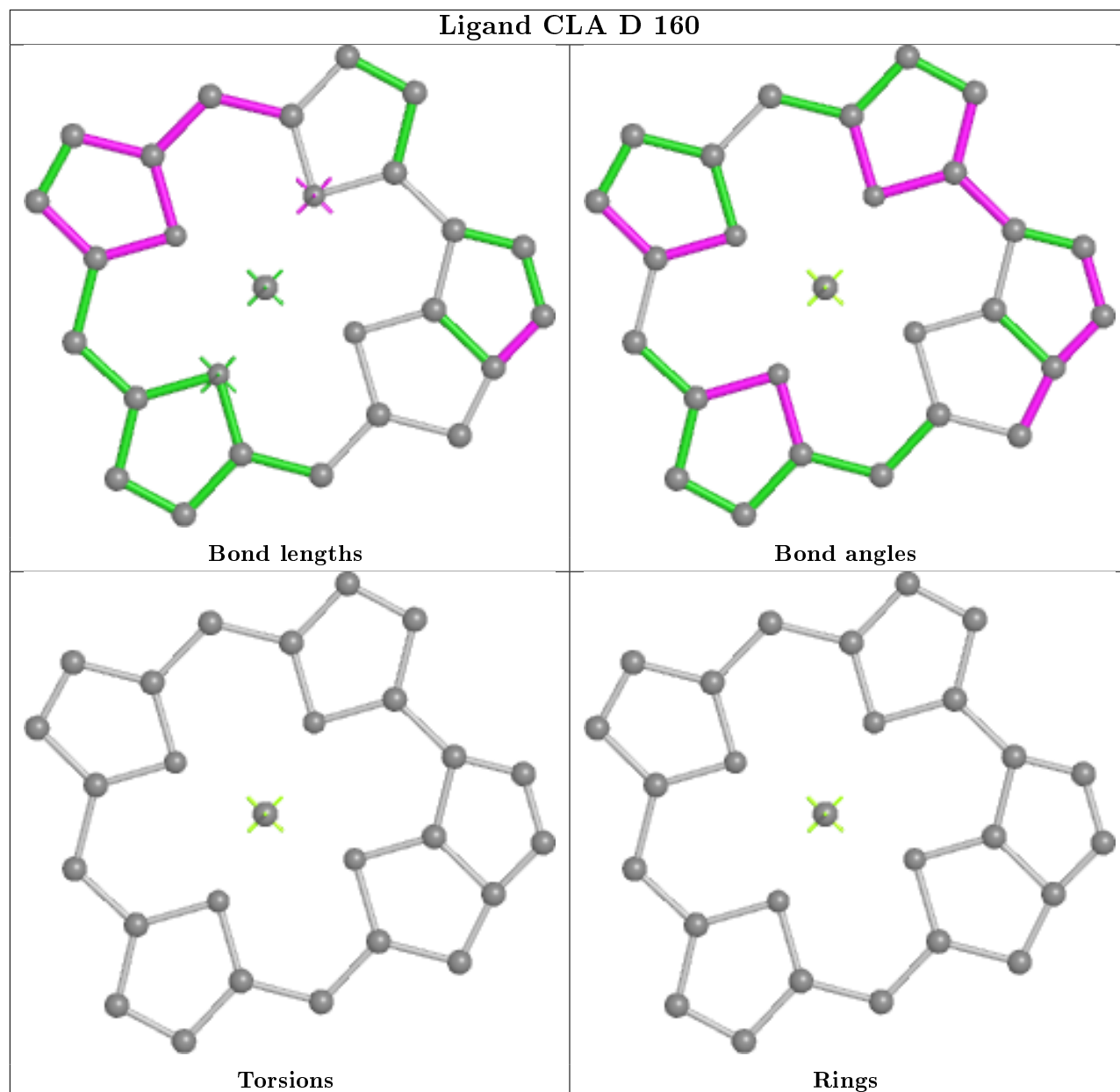


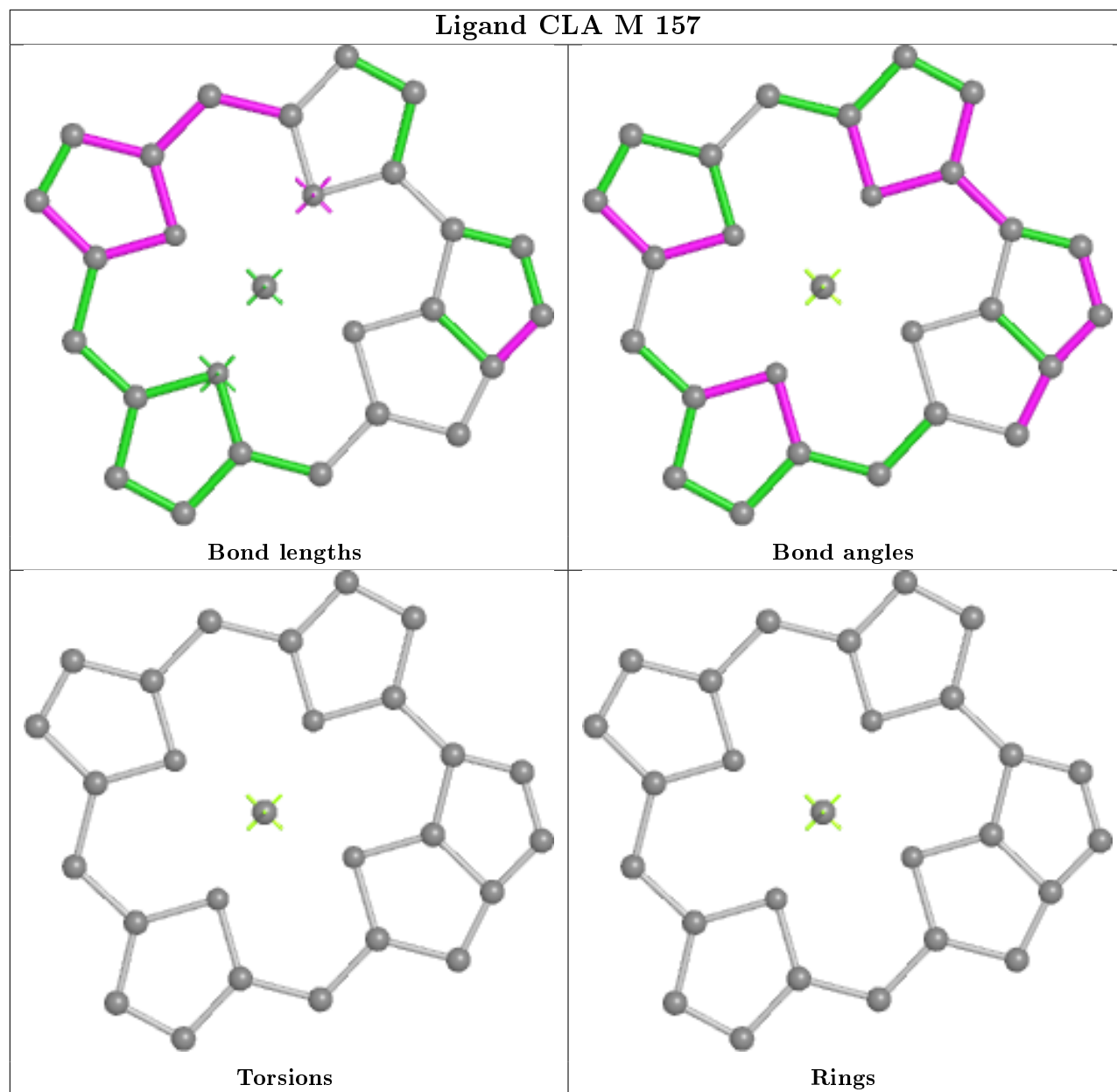
Torsions



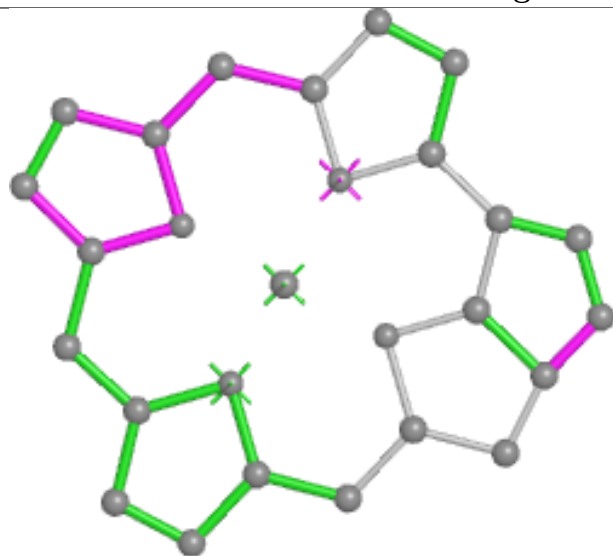
Rings

Ligand CLA D 160

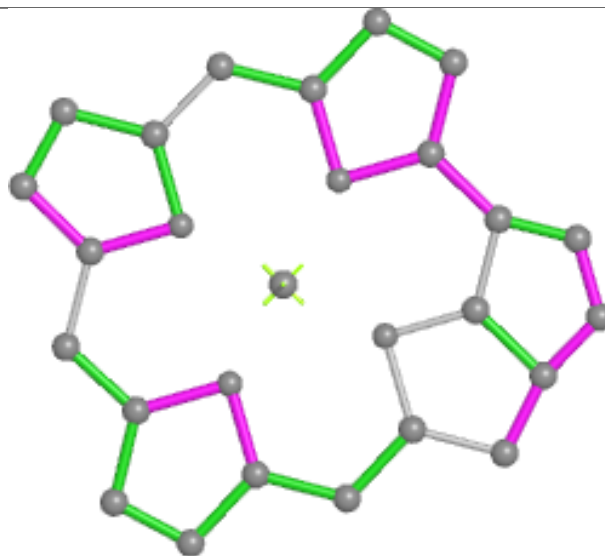




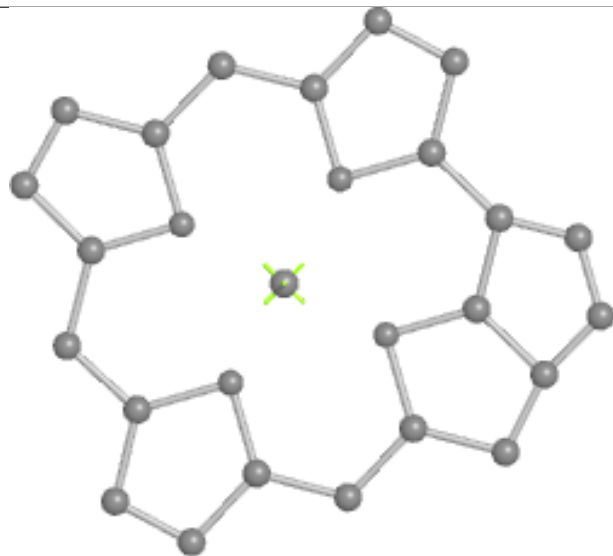
Ligand CLA D 161



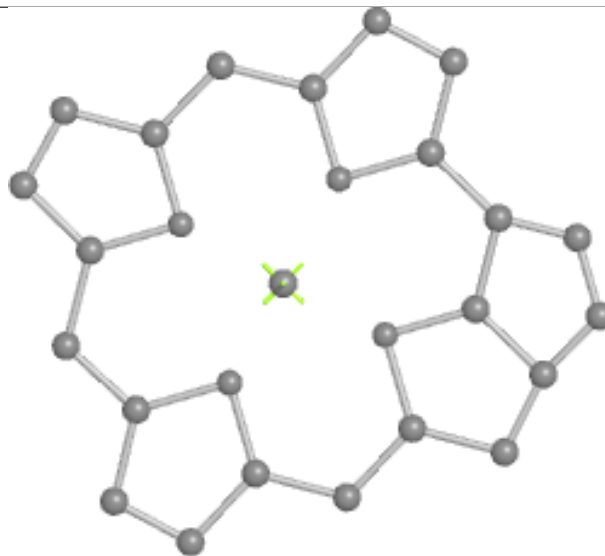
Bond lengths



Bond angles

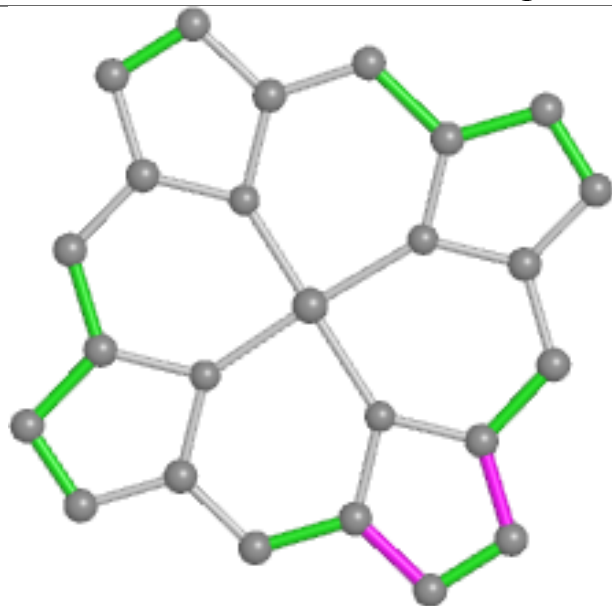


Torsions

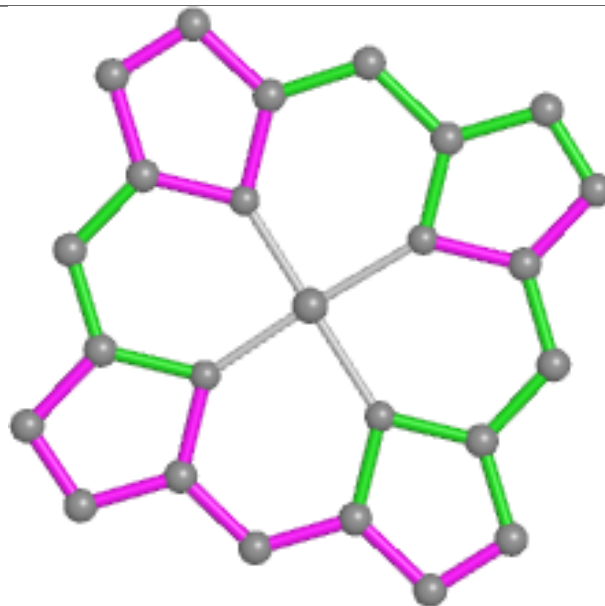


Rings

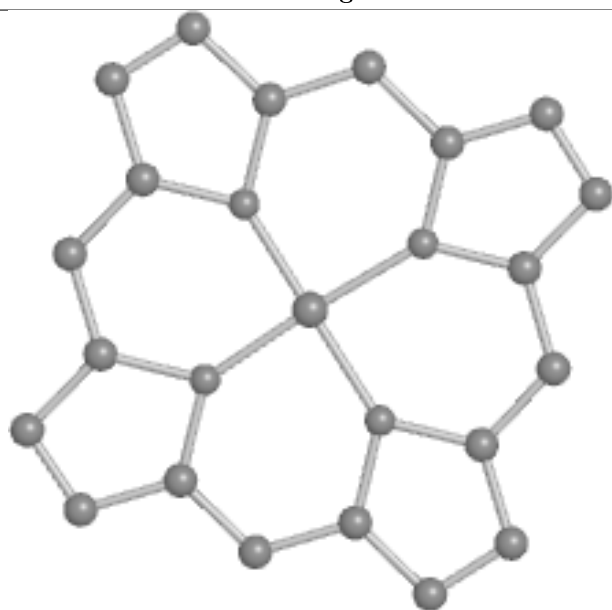
Ligand HEM F 50



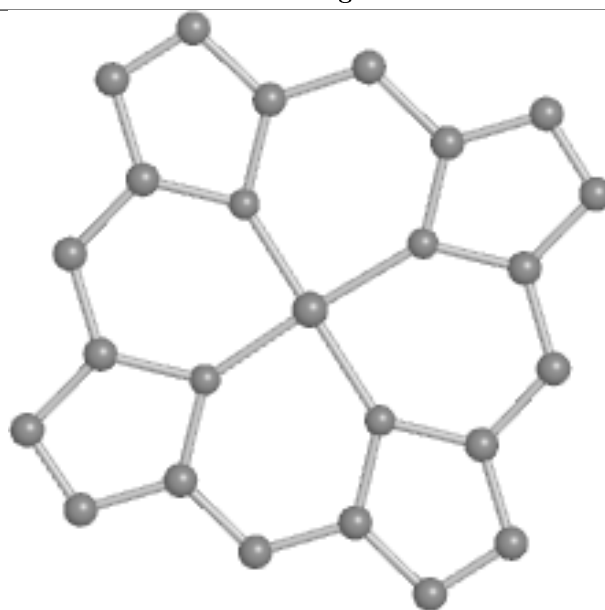
Bond lengths



Bond angles

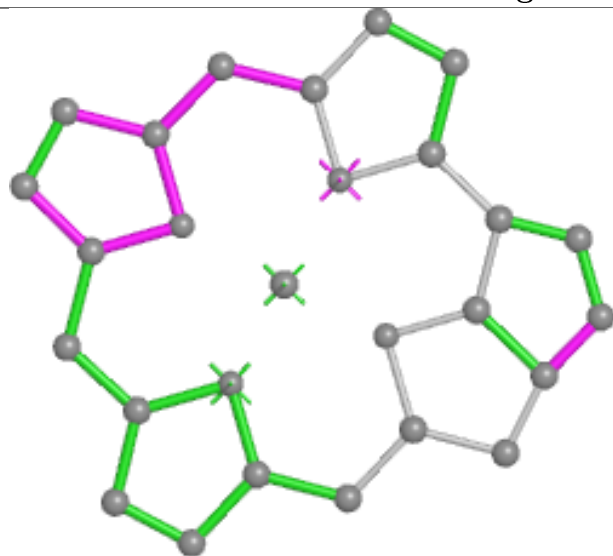


Torsions

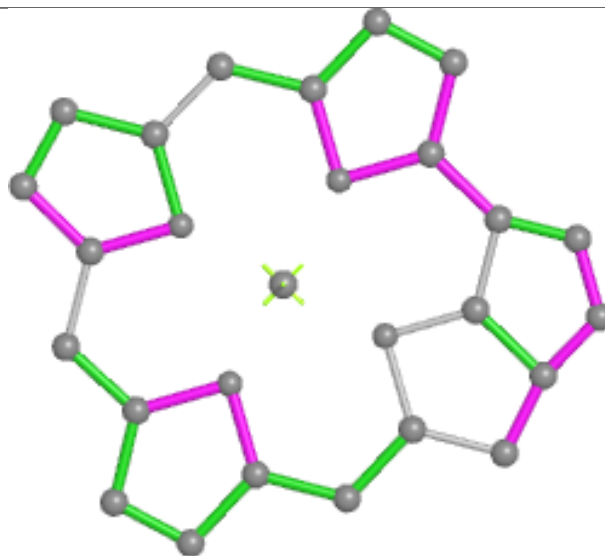


Rings

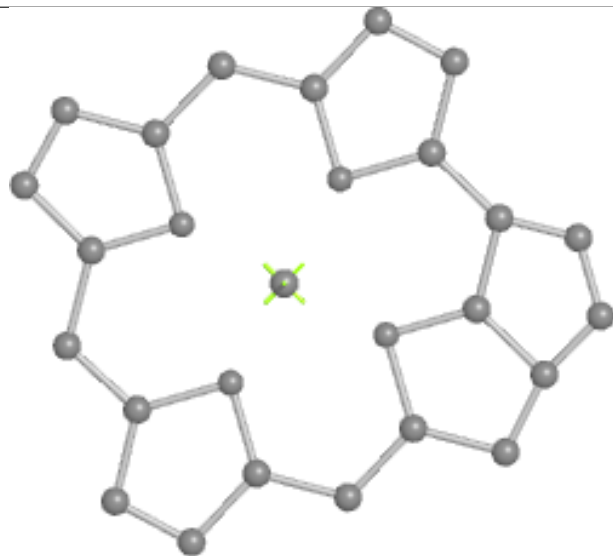
Ligand CLA L 162



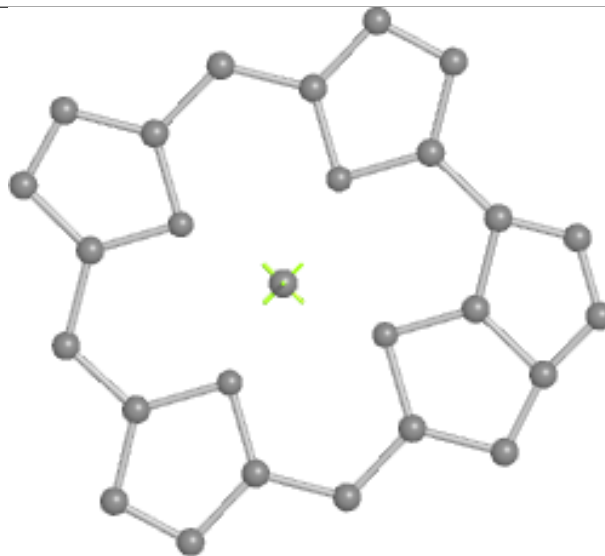
Bond lengths



Bond angles

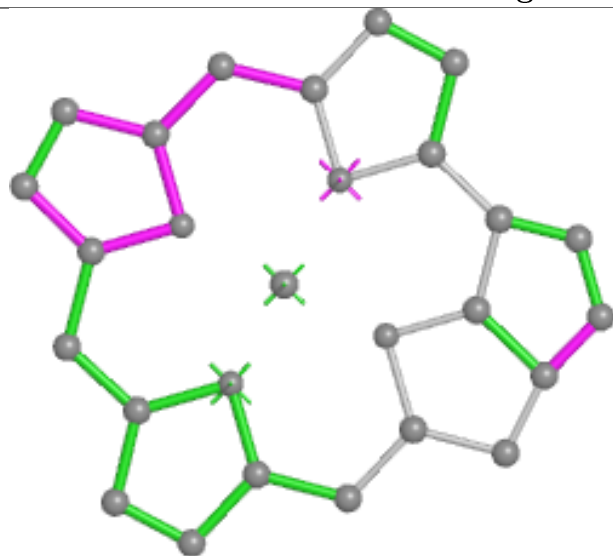


Torsions

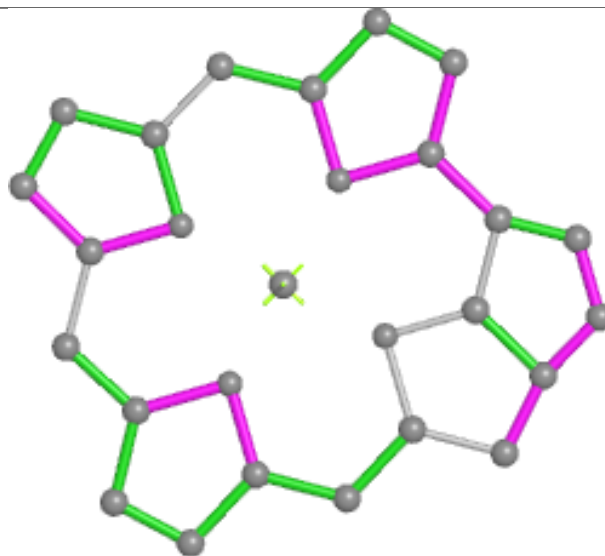


Rings

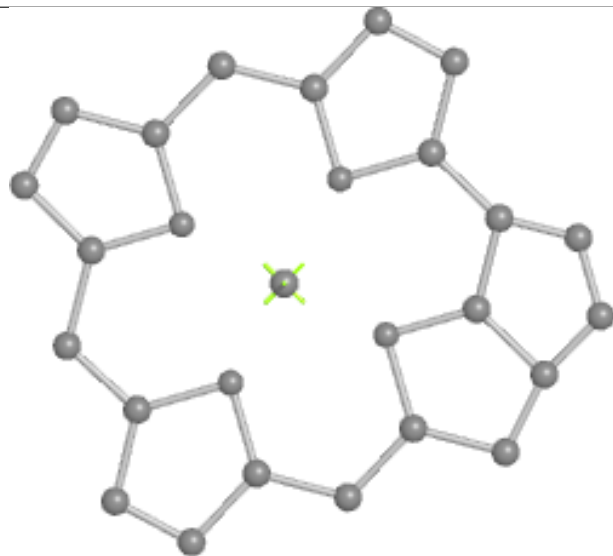
Ligand CLA L 165



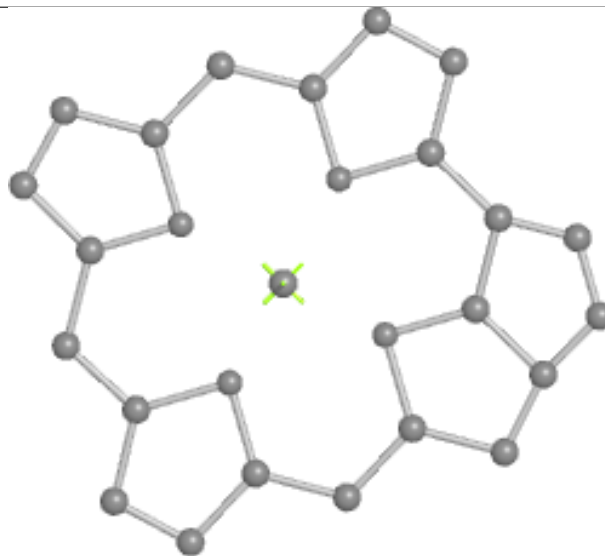
Bond lengths



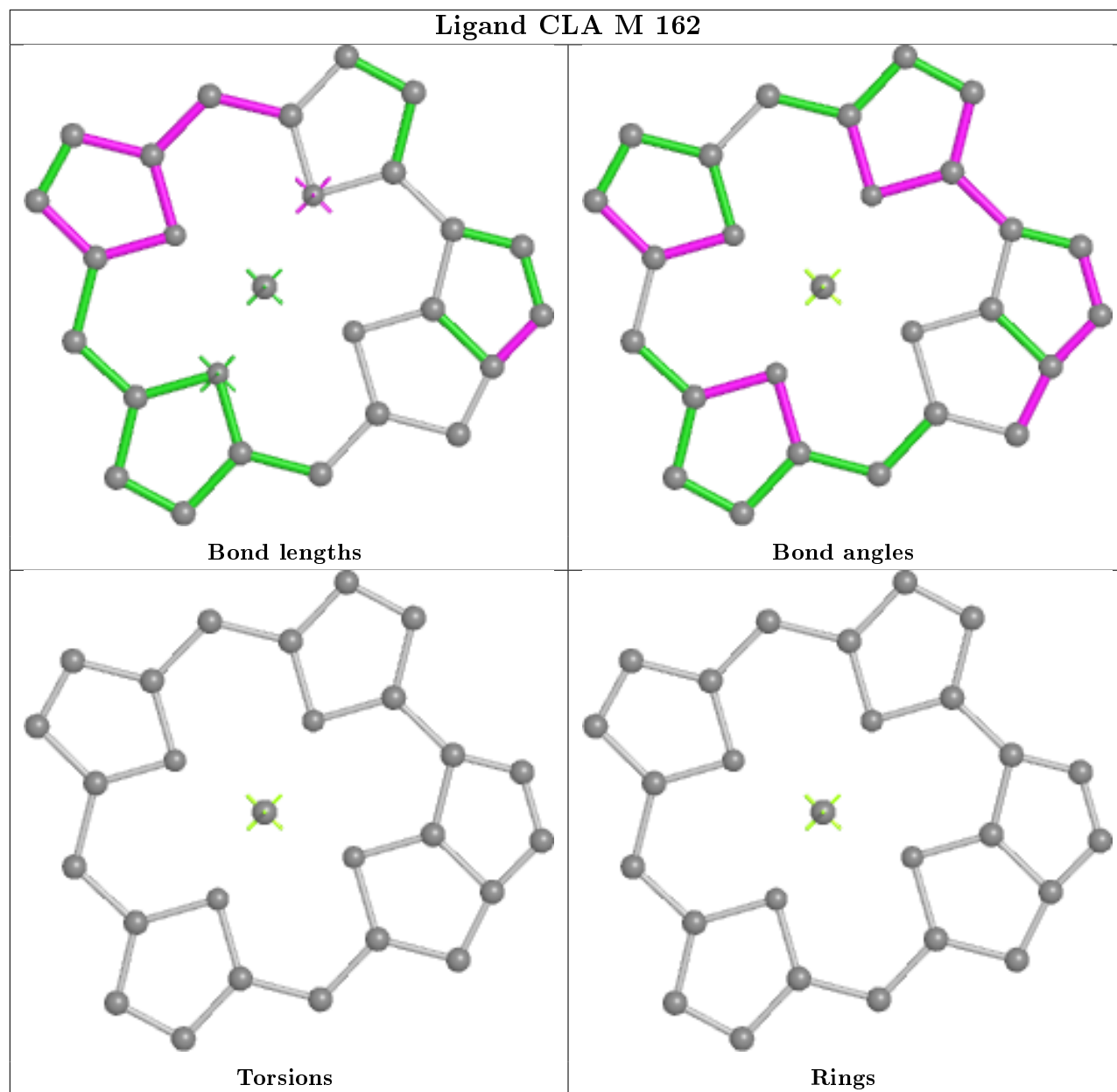
Bond angles

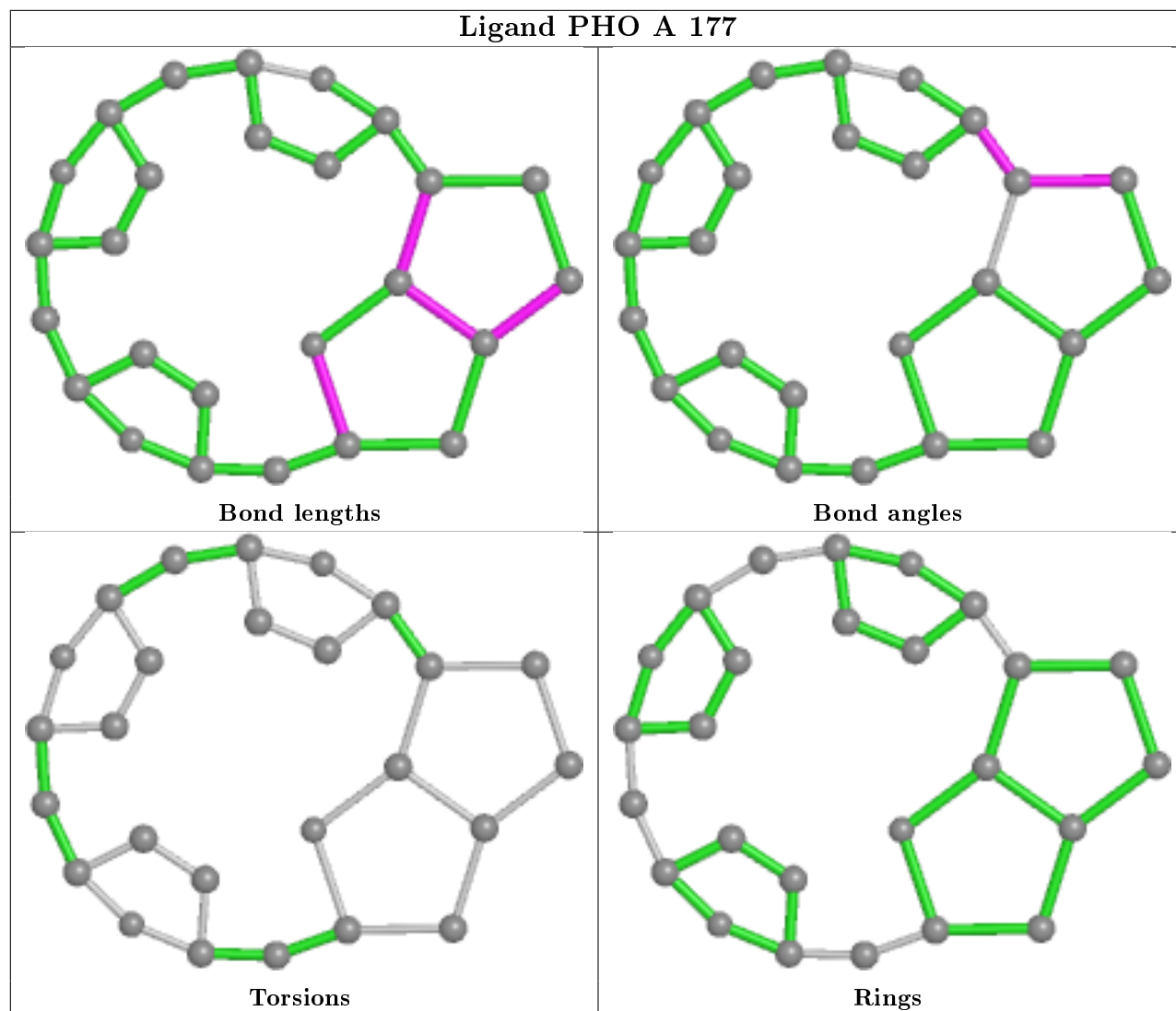


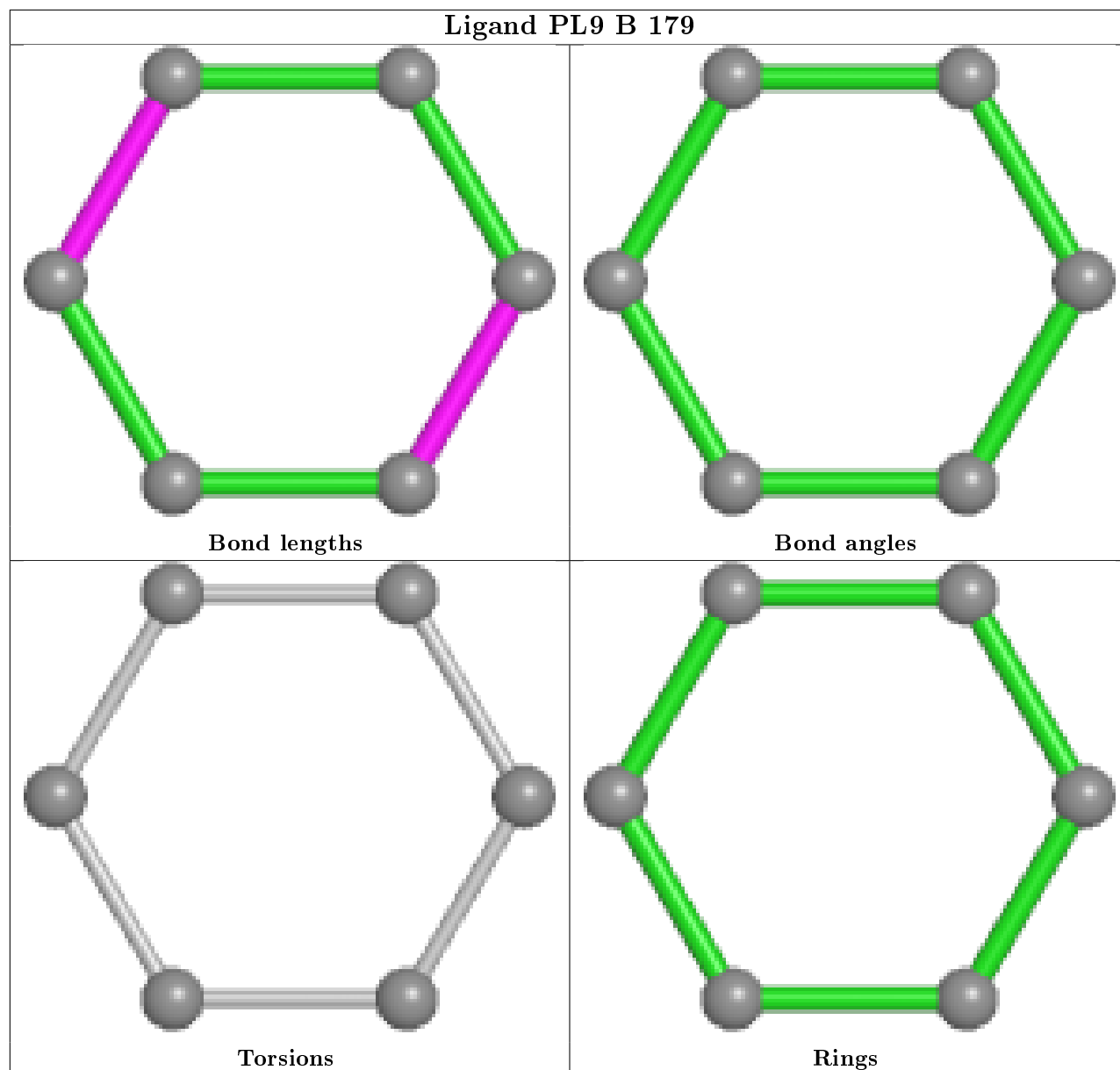
Torsions



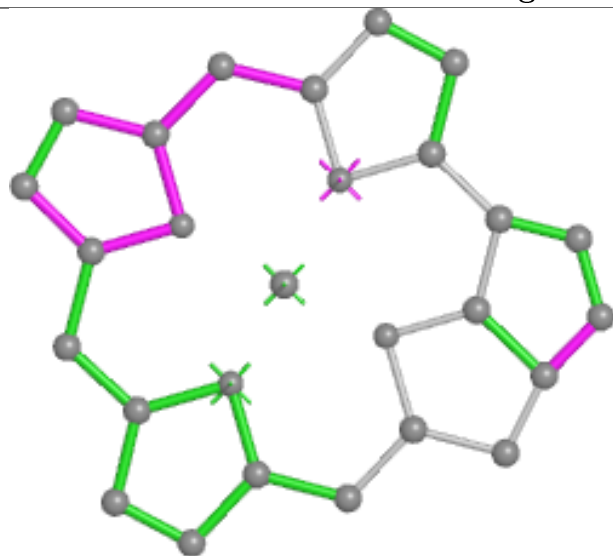
Rings



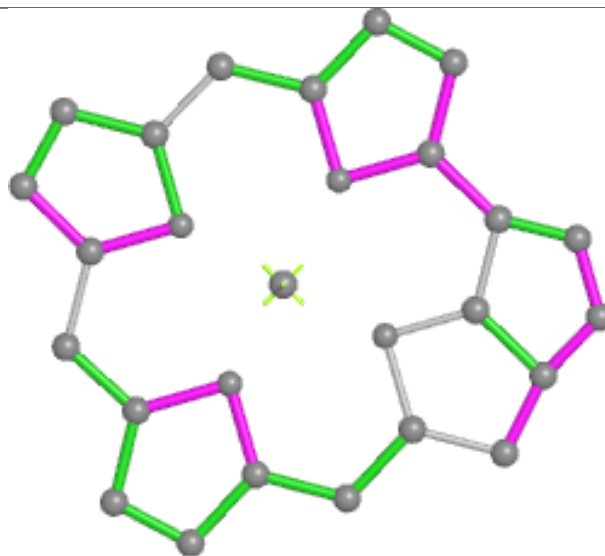




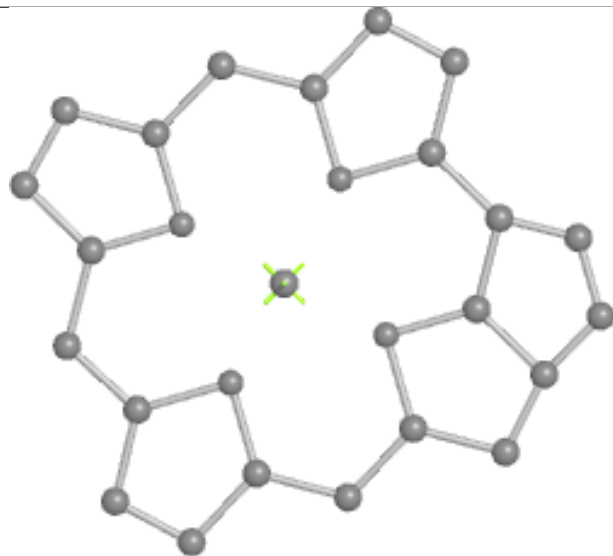
Ligand CLA J 174



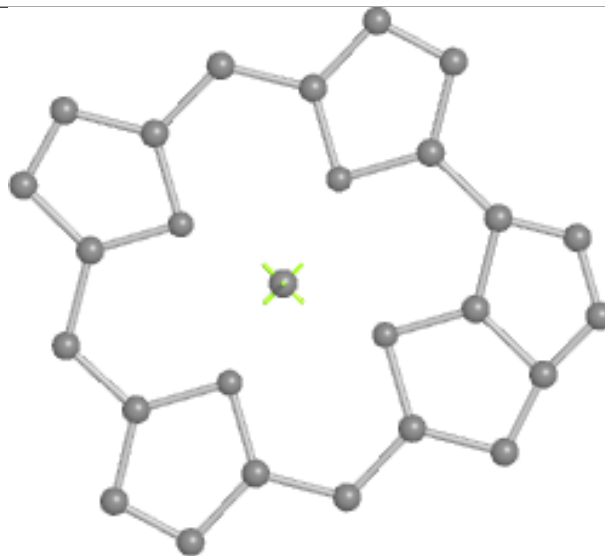
Bond lengths



Bond angles

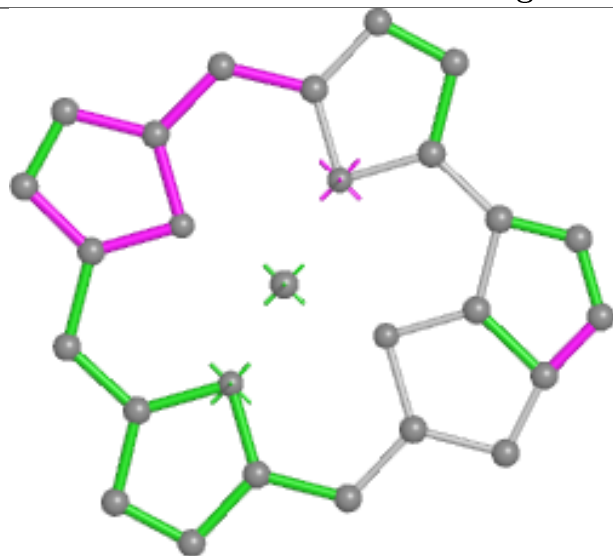


Torsions

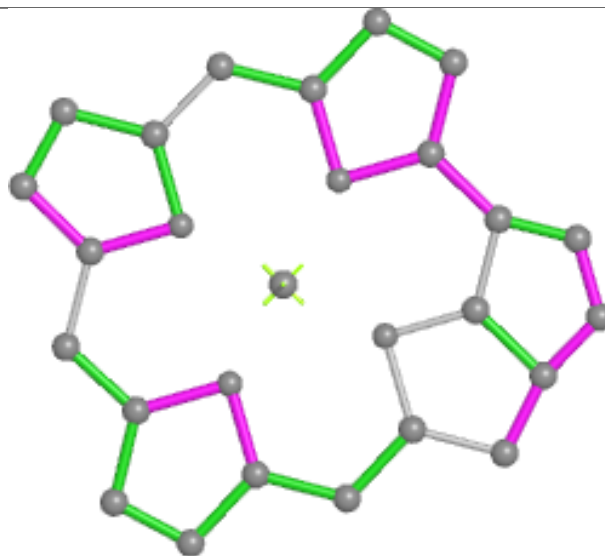


Rings

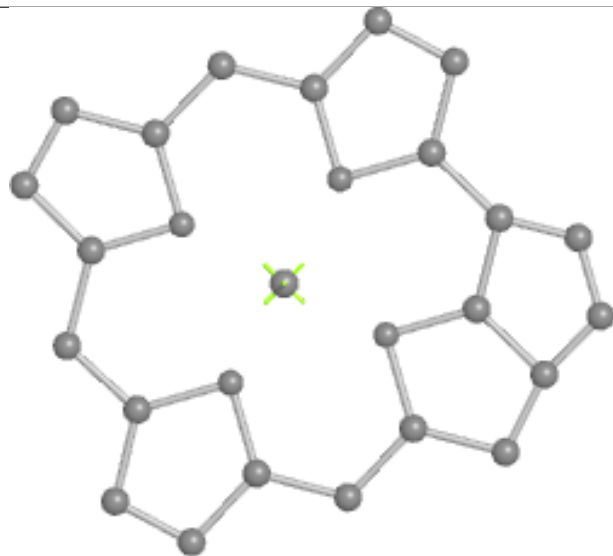
Ligand CLA L 167



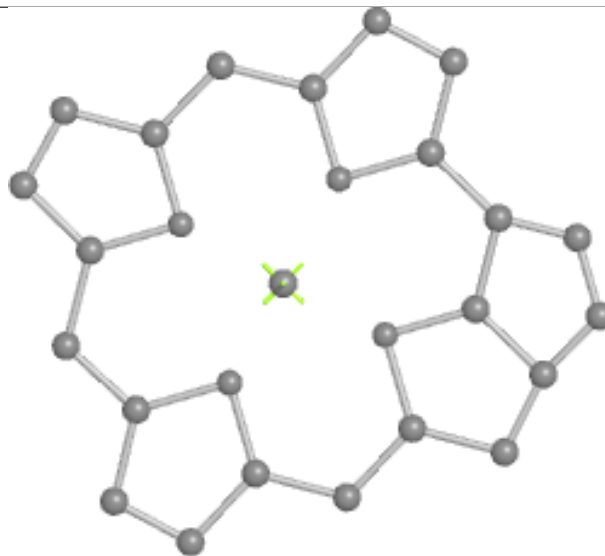
Bond lengths



Bond angles

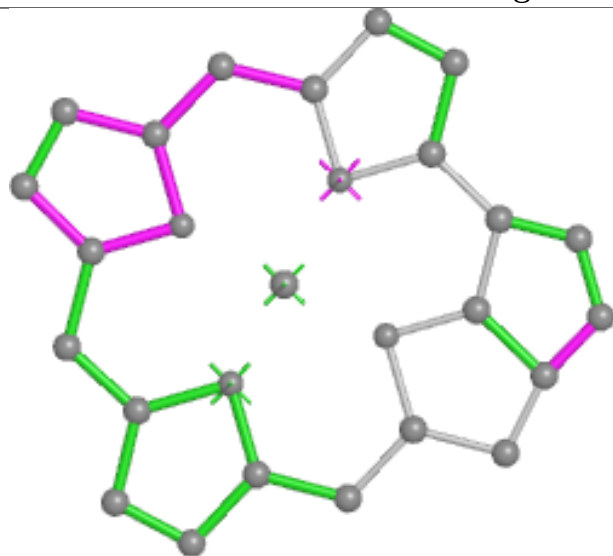


Torsions

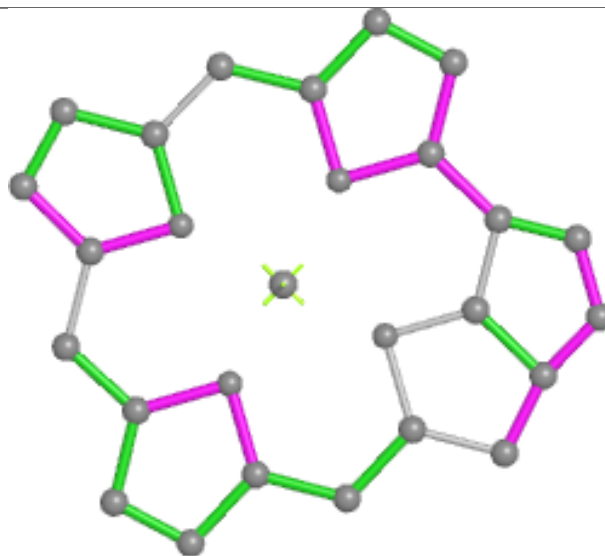


Rings

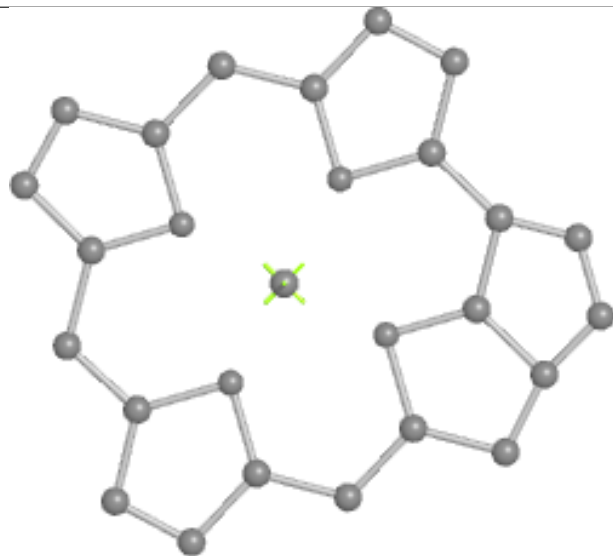
Ligand CLA K 176



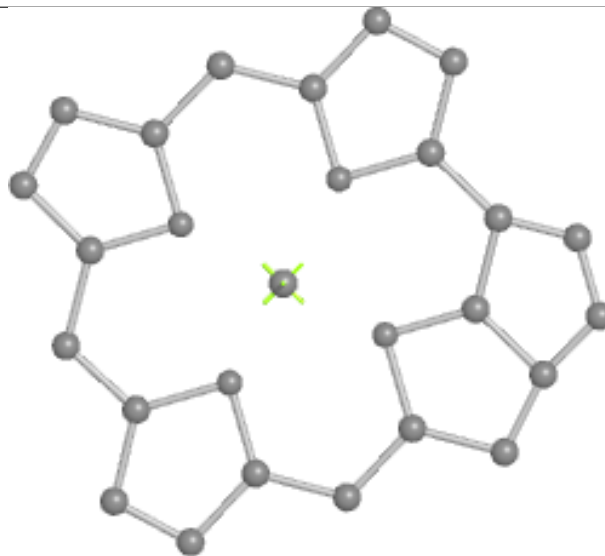
Bond lengths



Bond angles

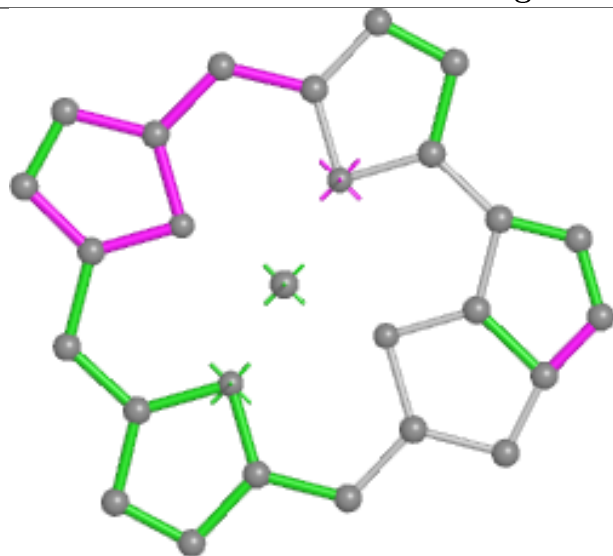


Torsions

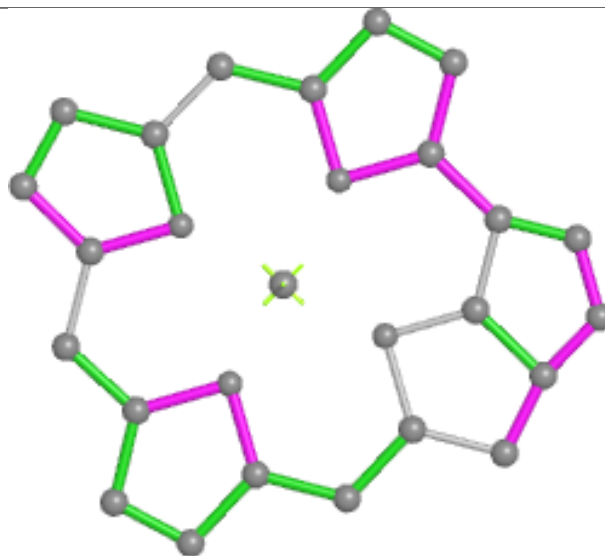


Rings

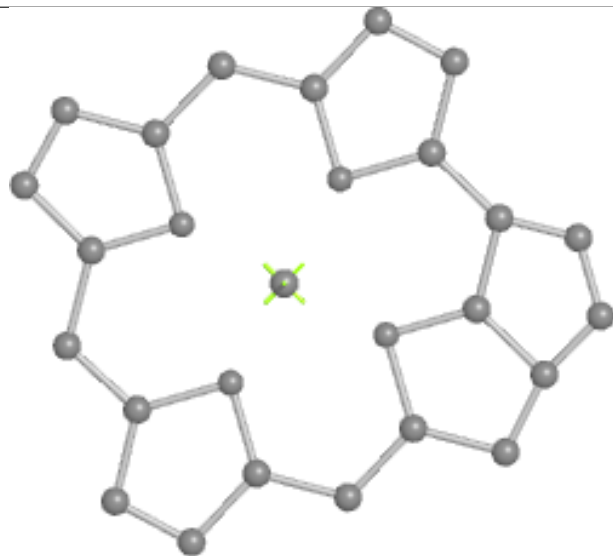
Ligand CLA C 157



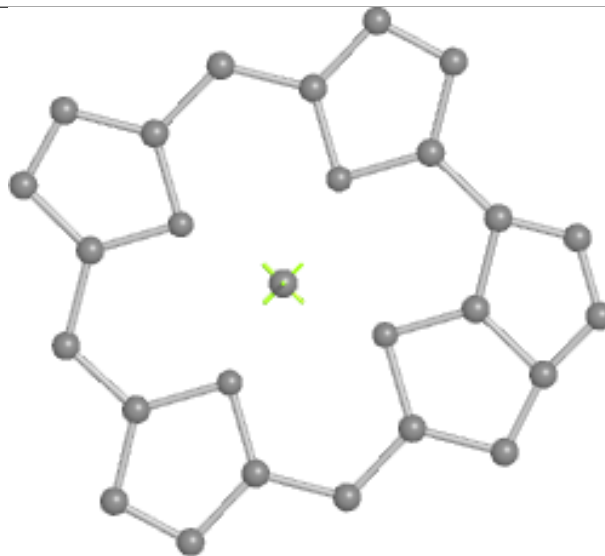
Bond lengths



Bond angles

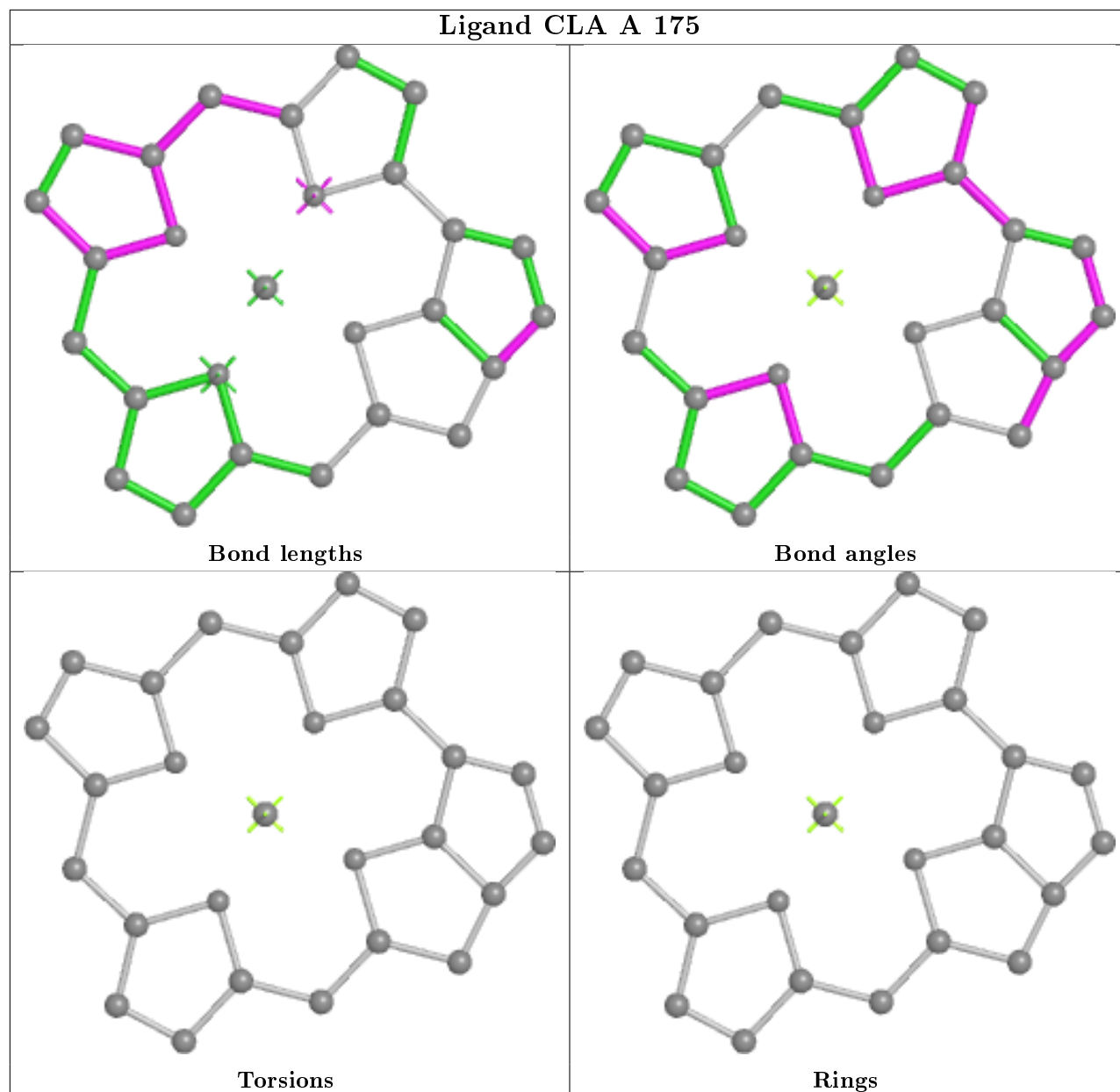


Torsions

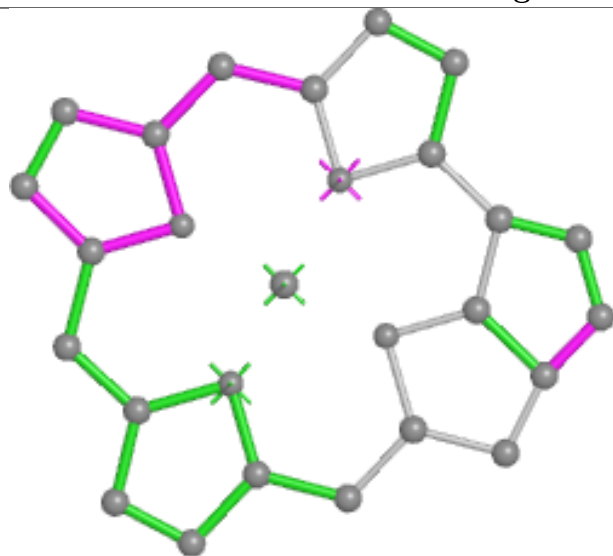


Rings

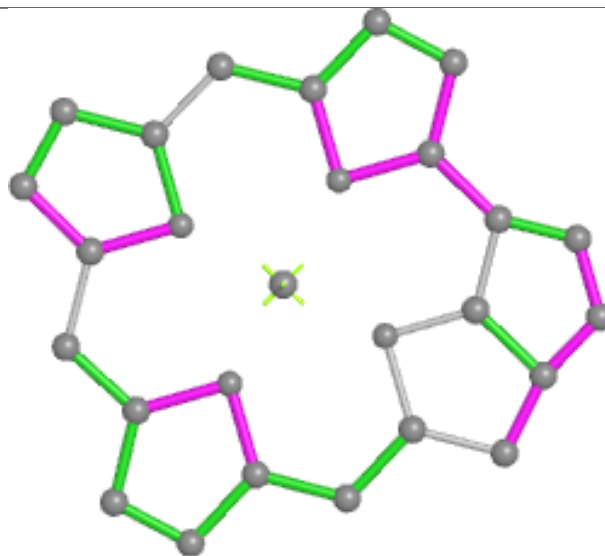
Ligand CLA A 175



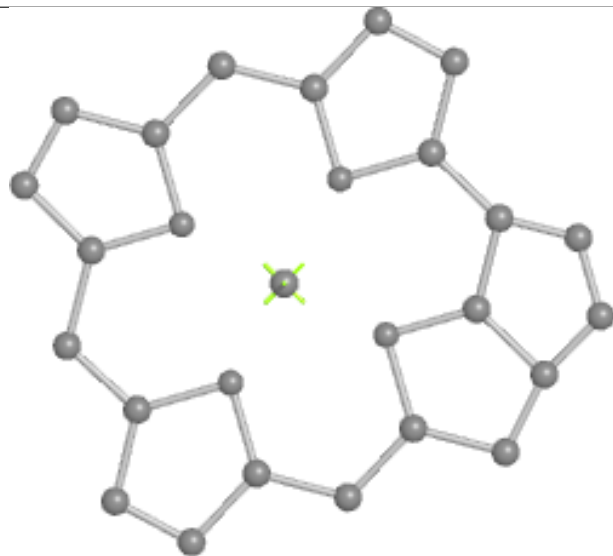
Ligand CLA D 158



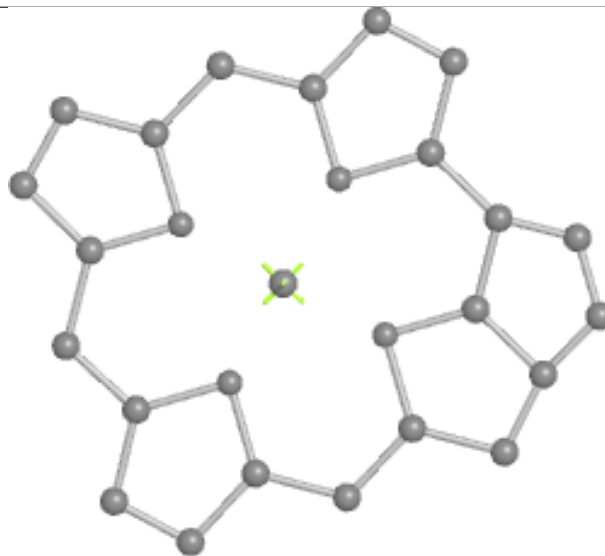
Bond lengths



Bond angles

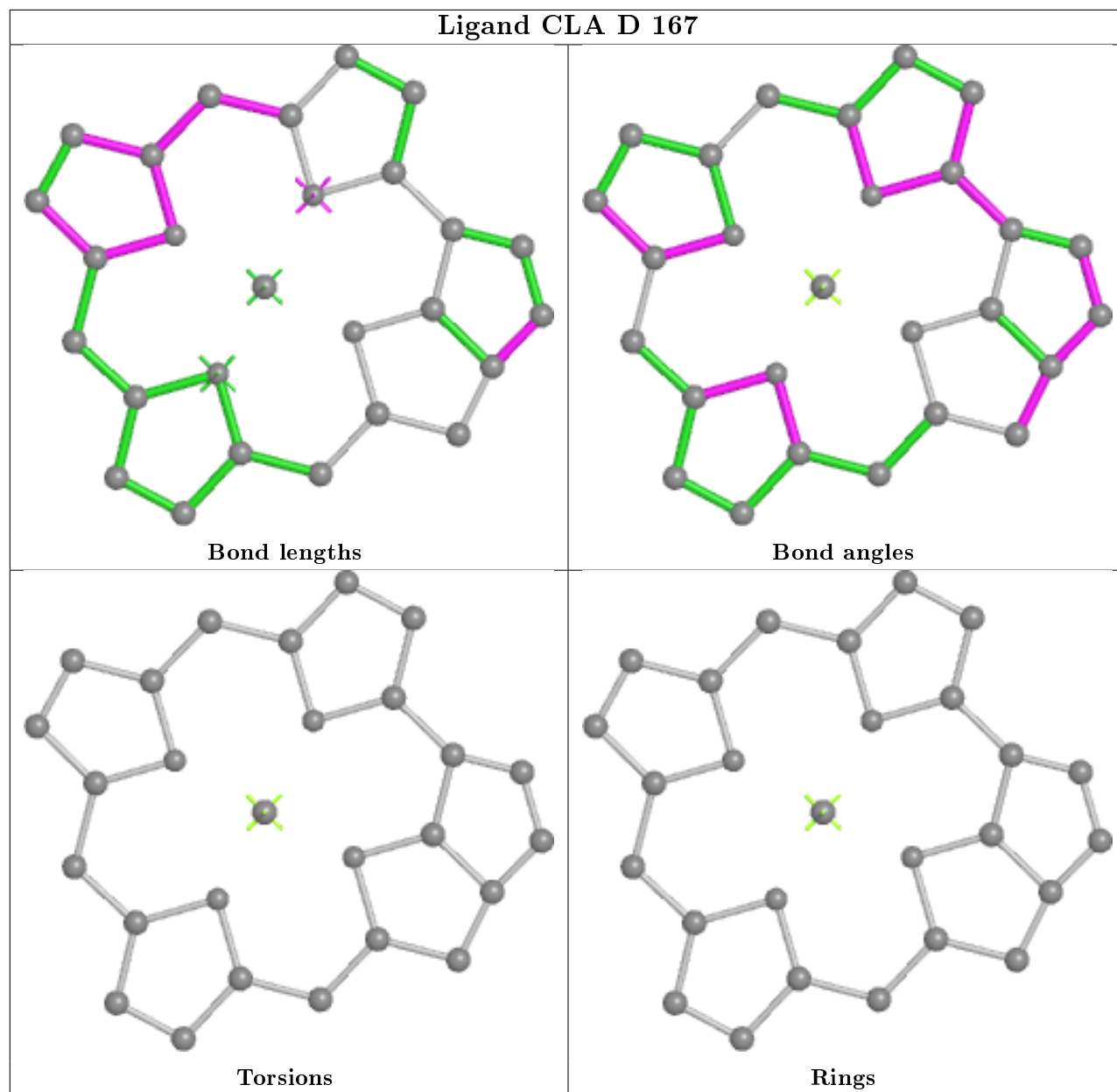


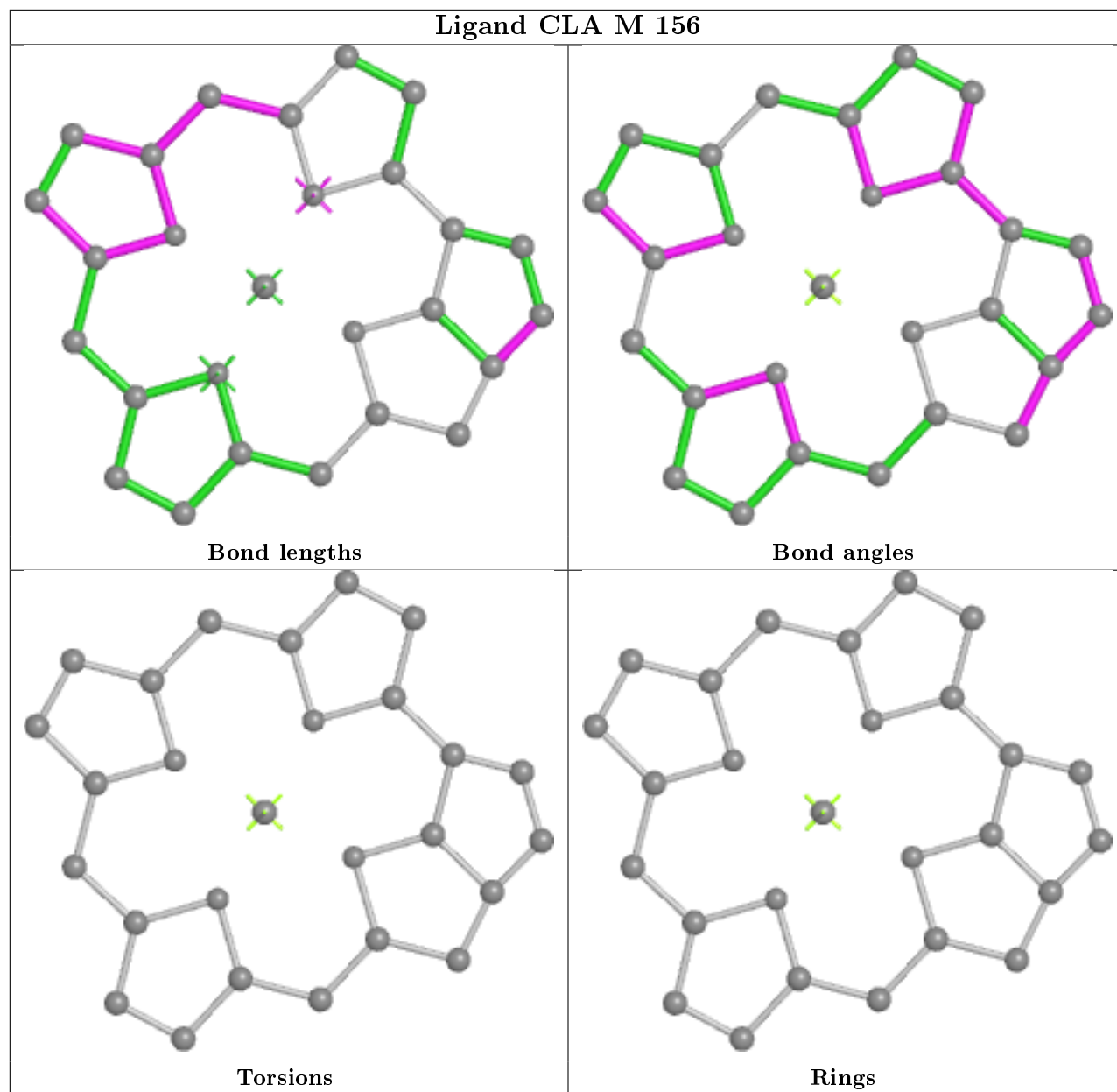
Torsions

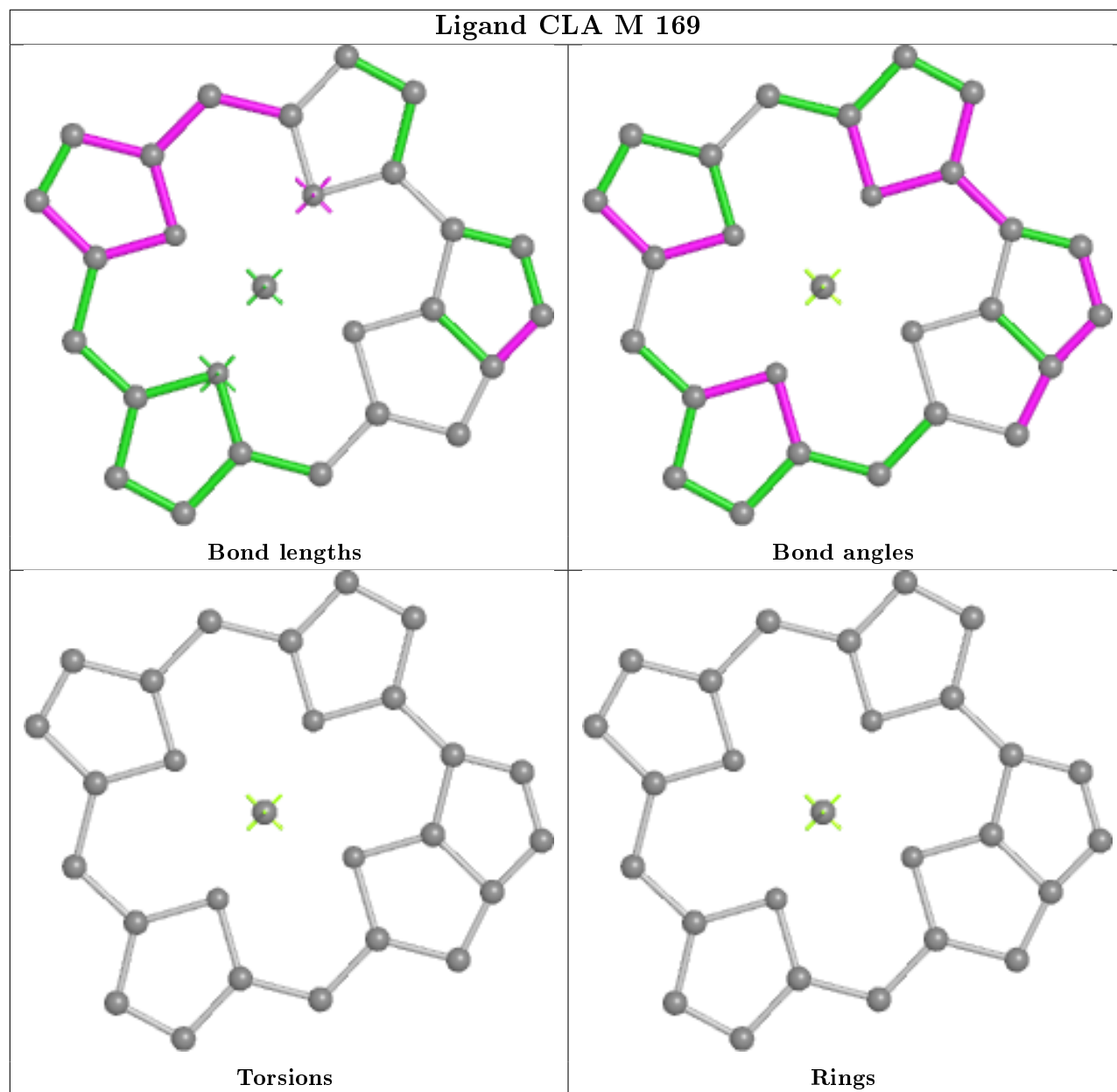


Rings

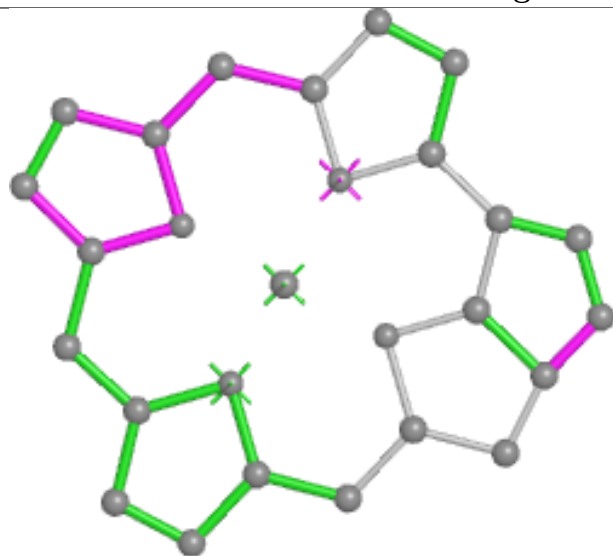
Ligand CLA D 167



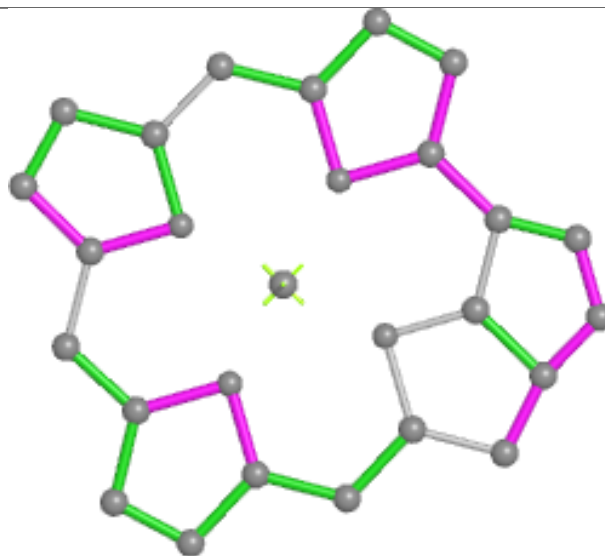




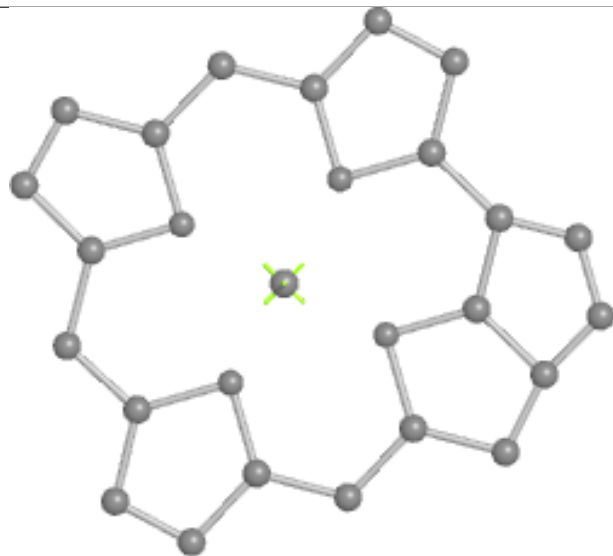
Ligand CLA D 163



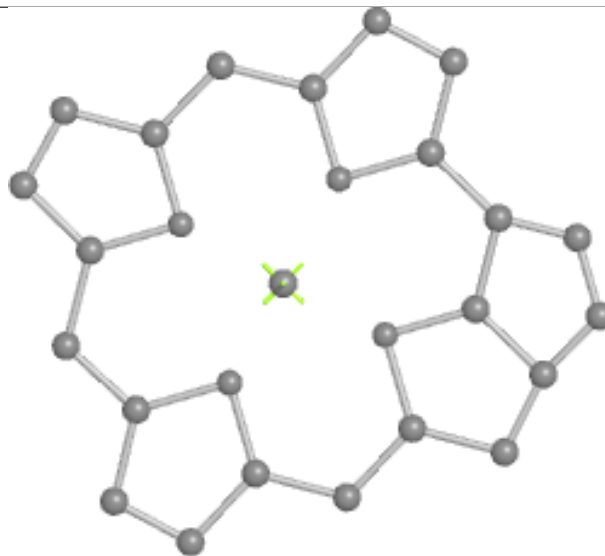
Bond lengths



Bond angles

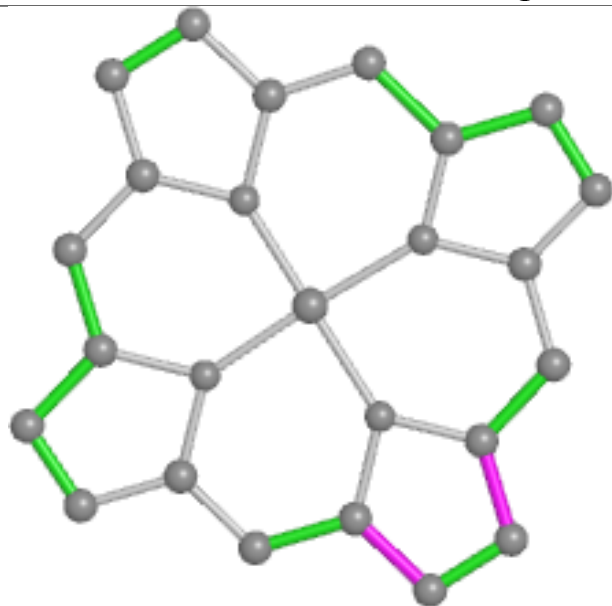


Torsions

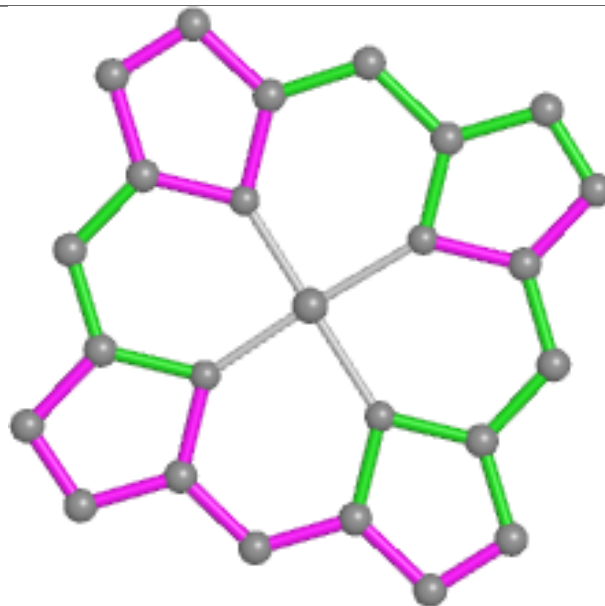


Rings

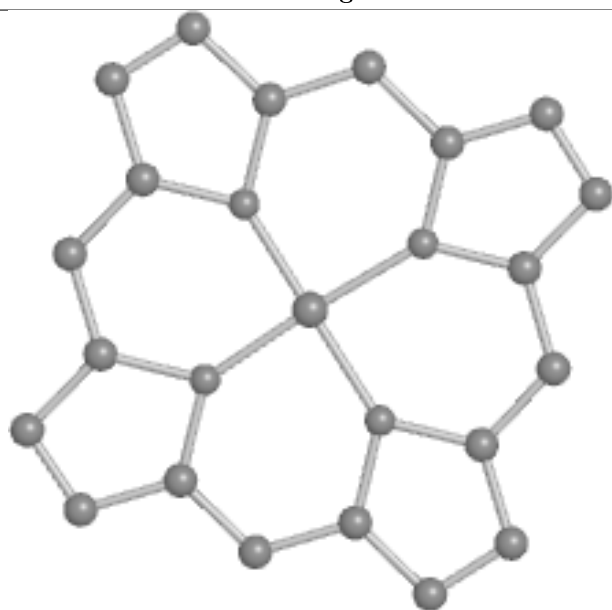
Ligand HEM R 91



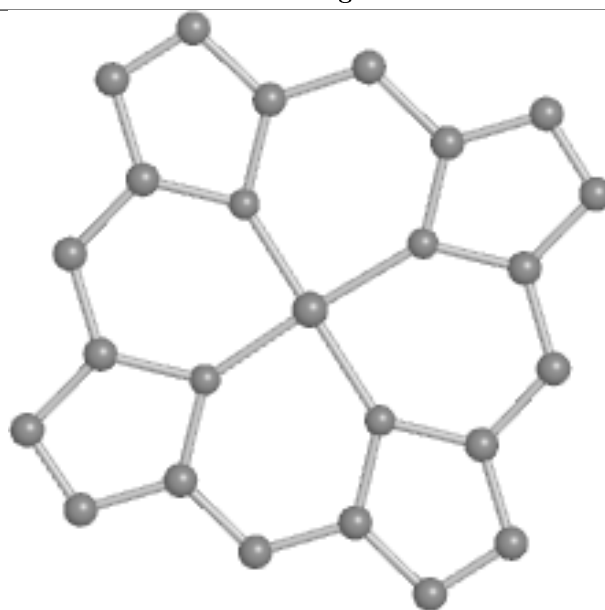
Bond lengths



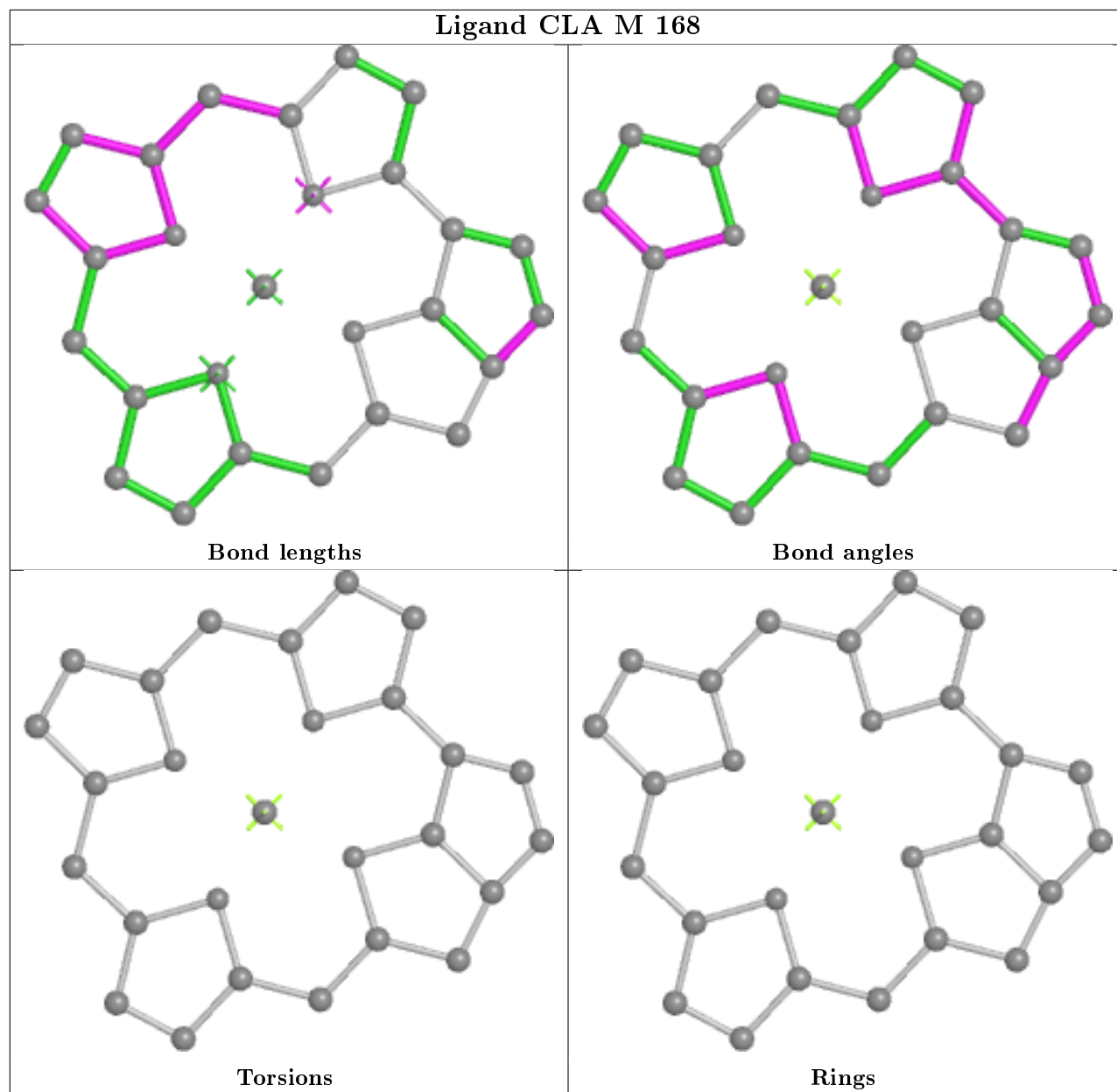
Bond angles



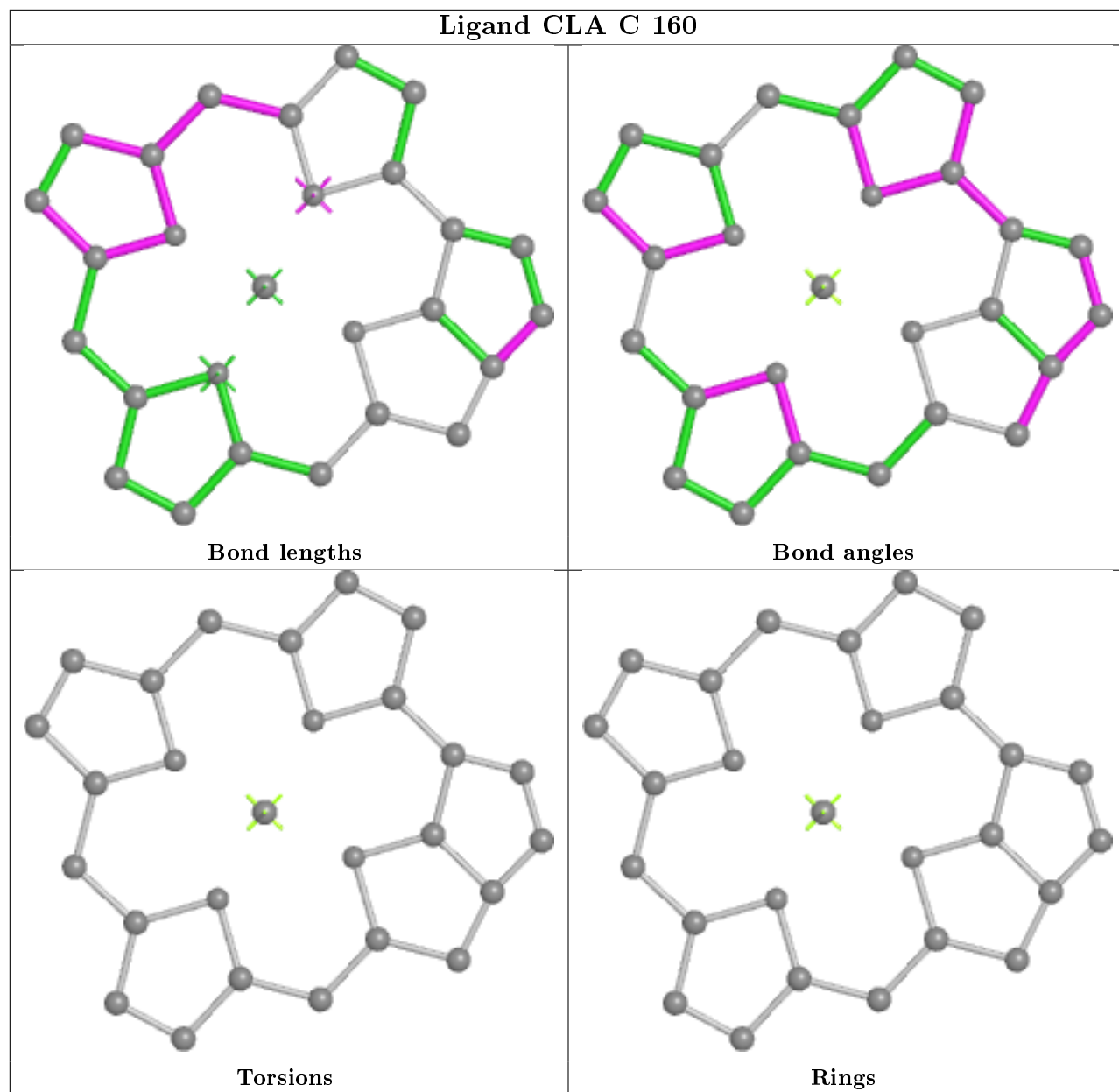
Torsions



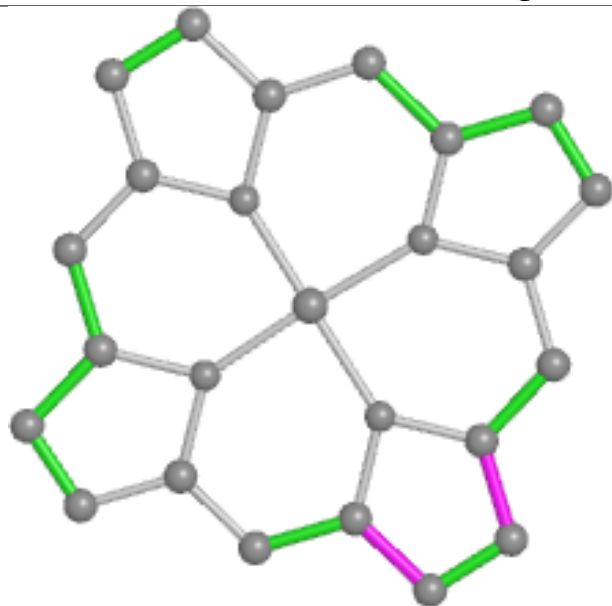
Rings



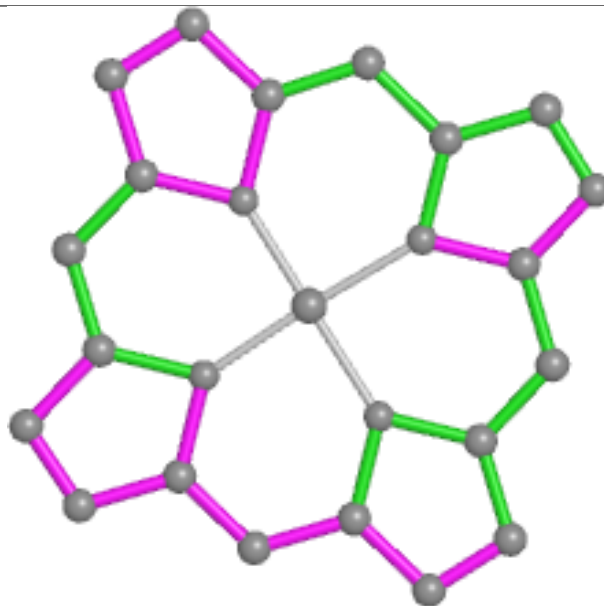
Ligand CLA C 160



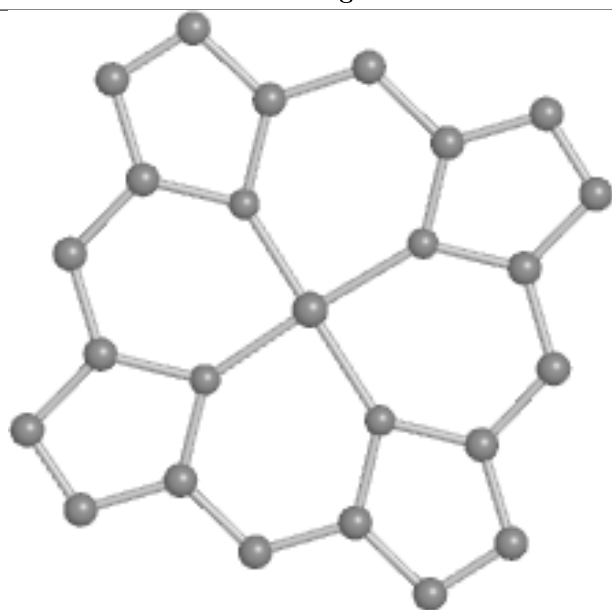
Ligand HEM O 90



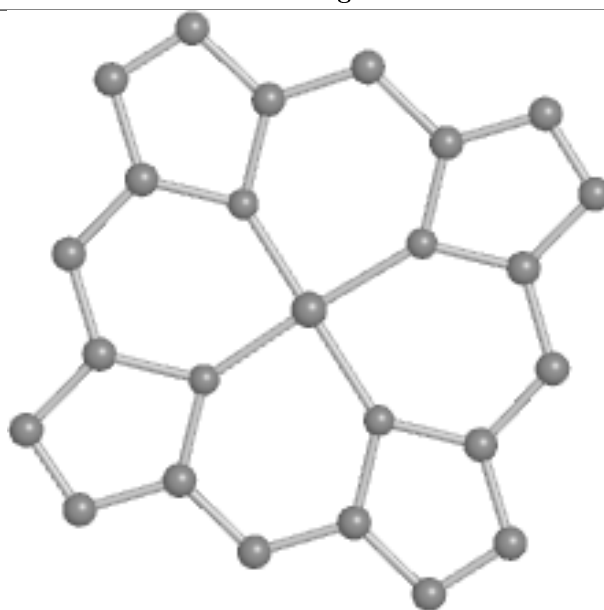
Bond lengths



Bond angles

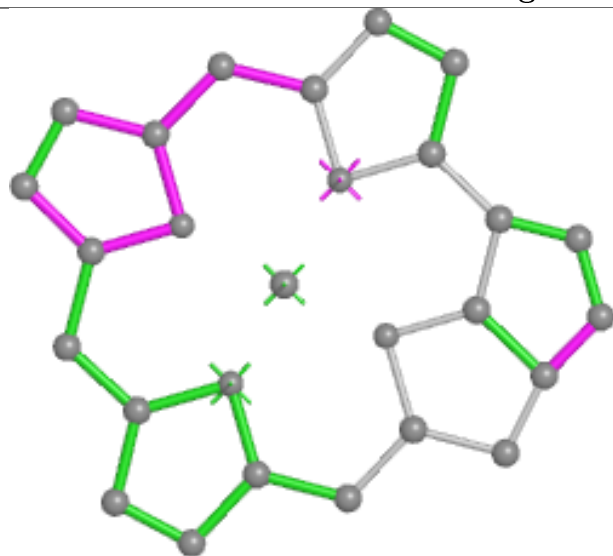


Torsions

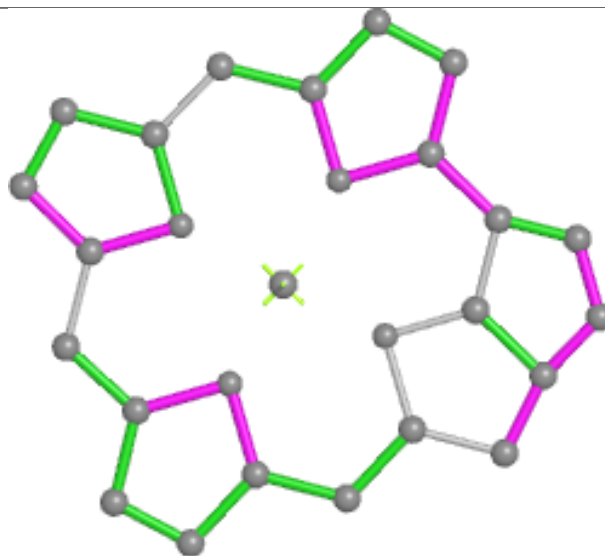


Rings

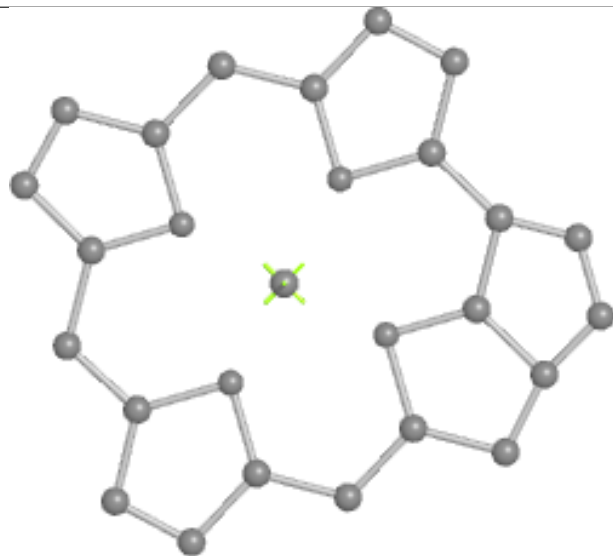
Ligand CLA J 178



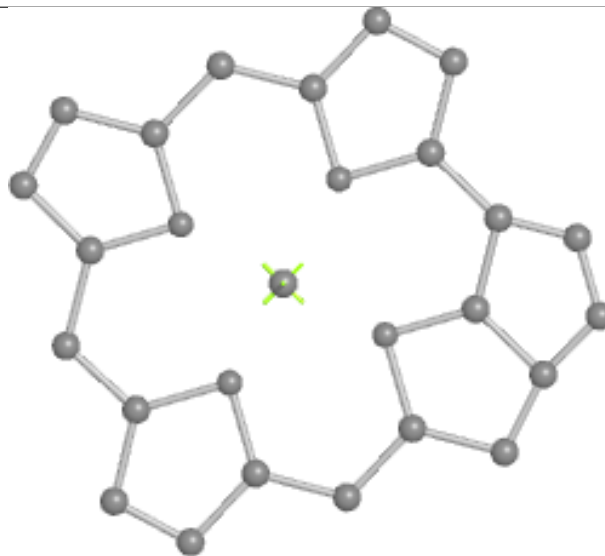
Bond lengths



Bond angles

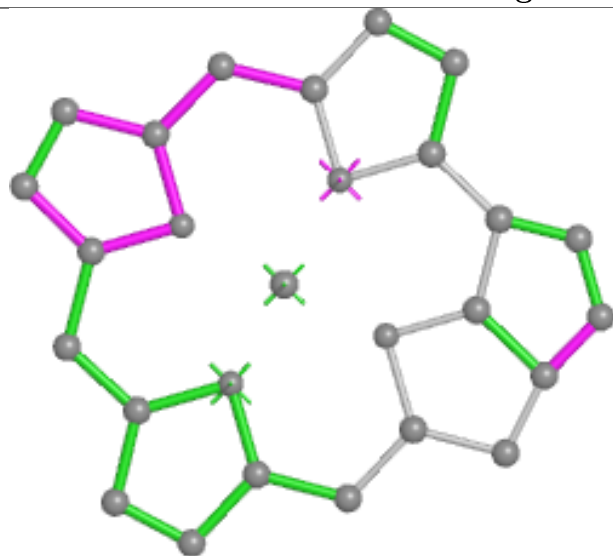


Torsions

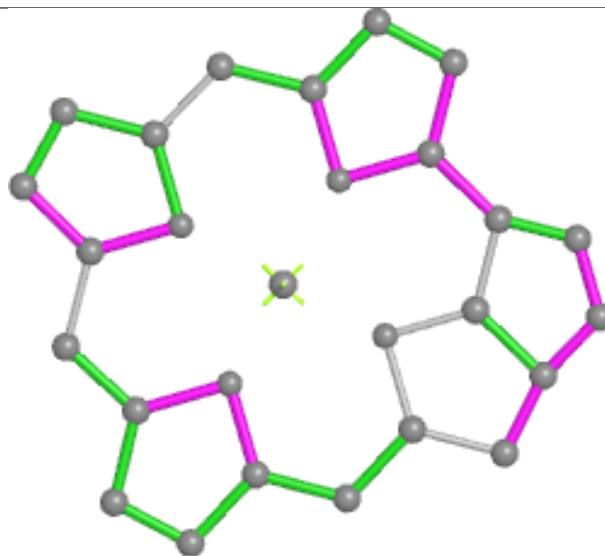


Rings

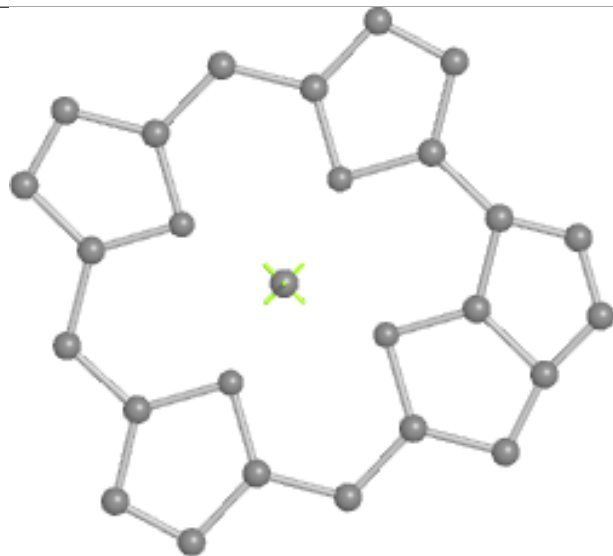
Ligand CLA P 313



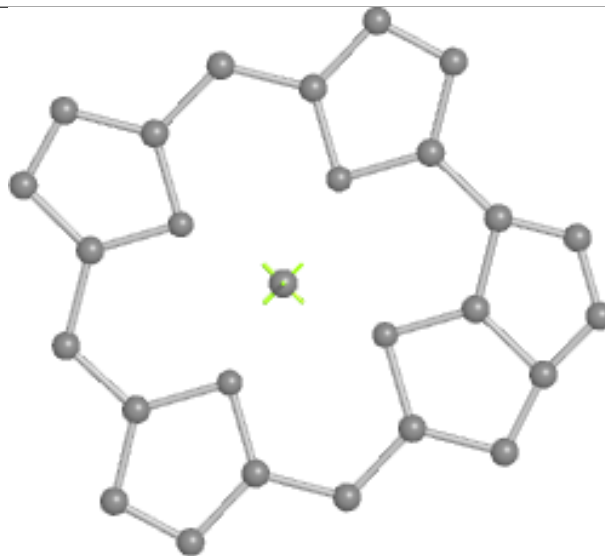
Bond lengths



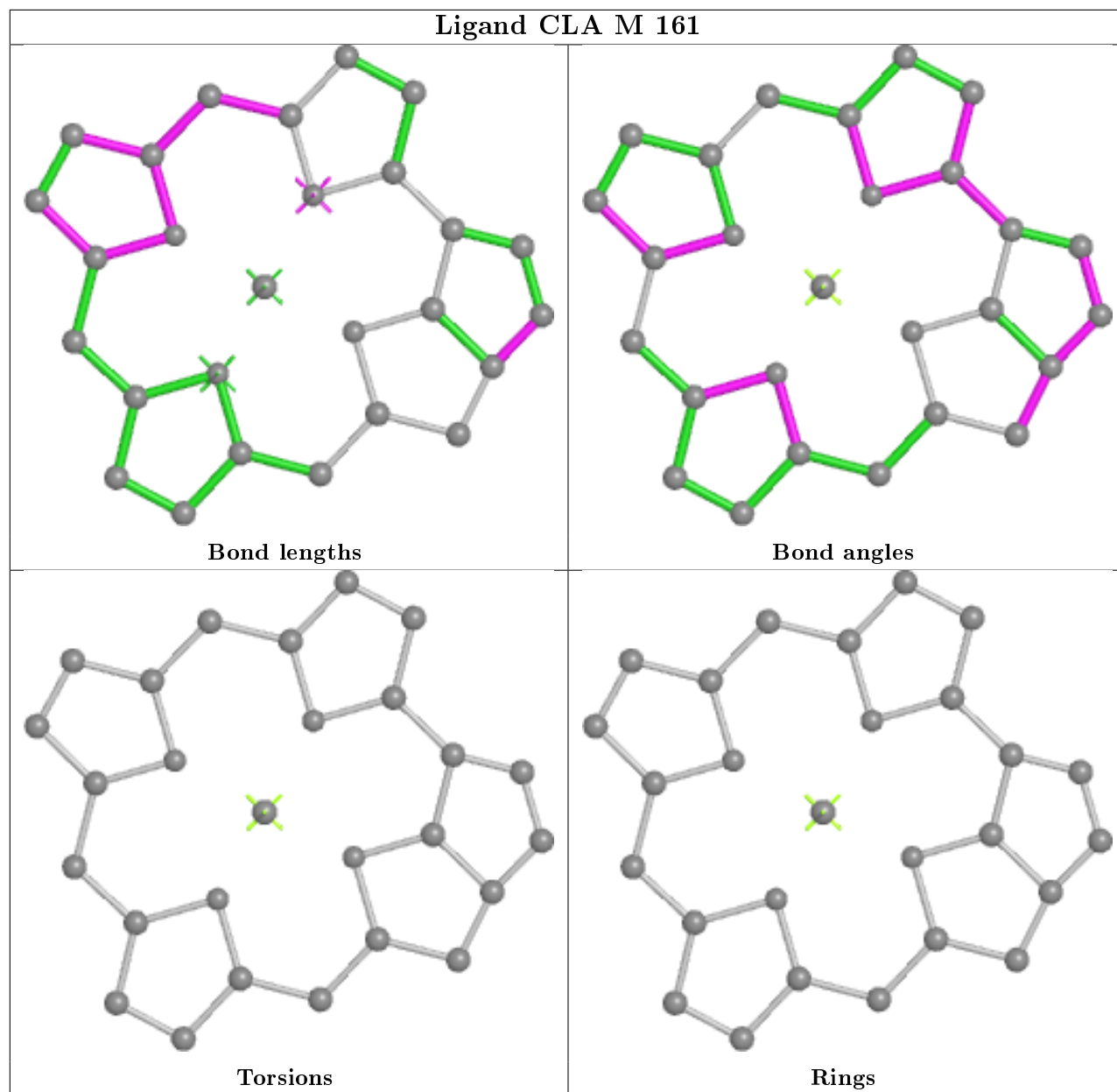
Bond angles



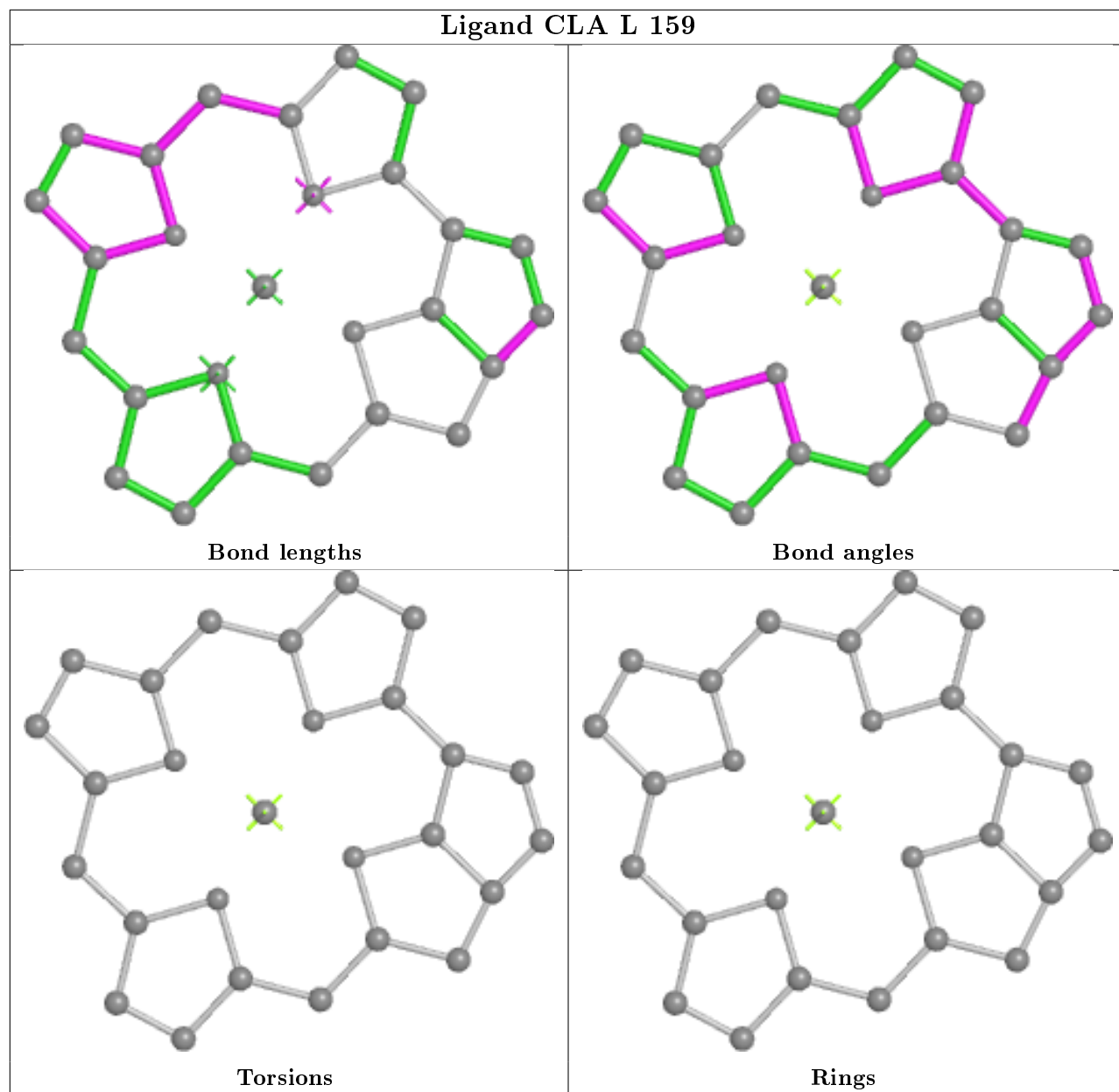
Torsions



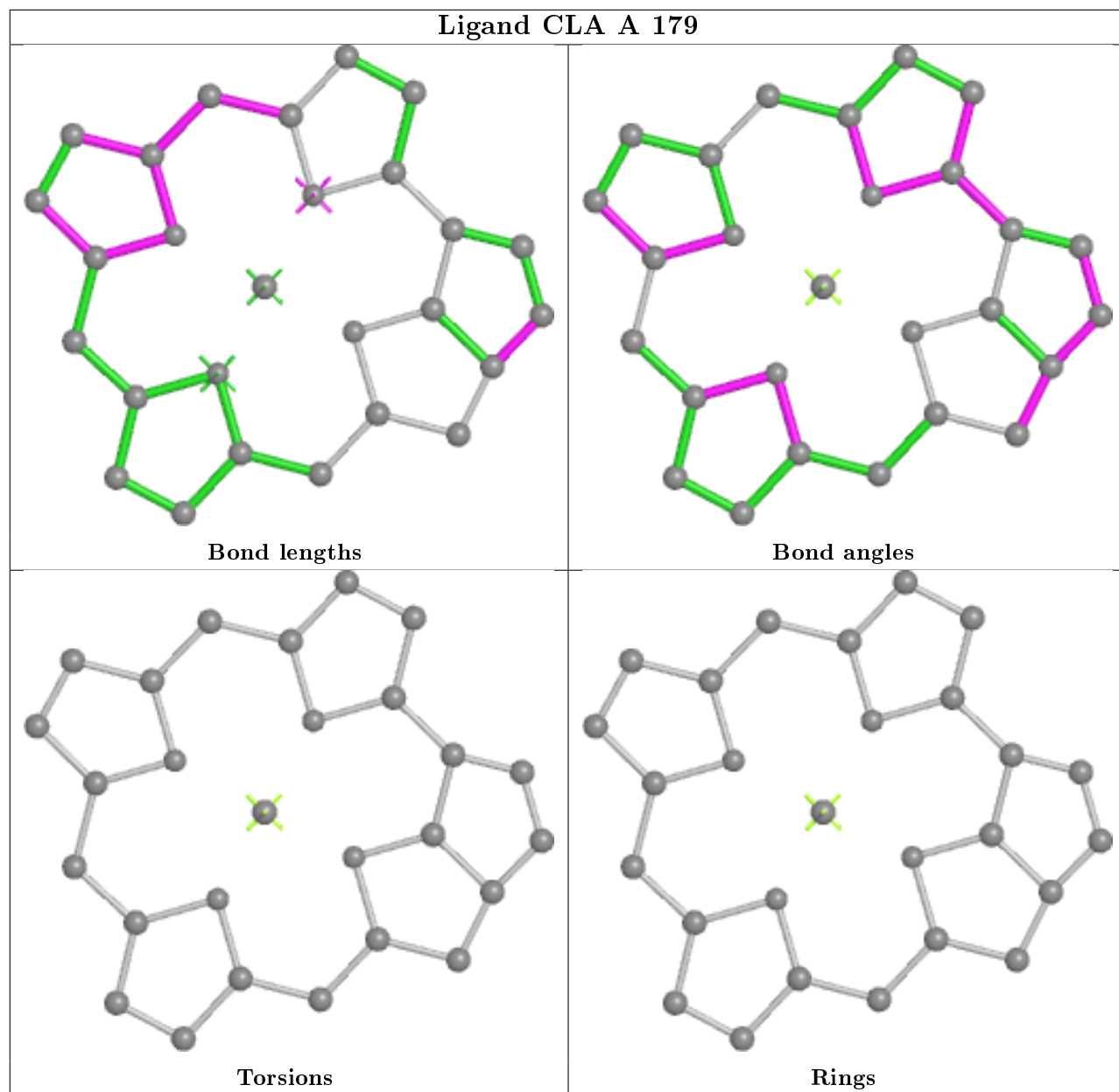
Rings



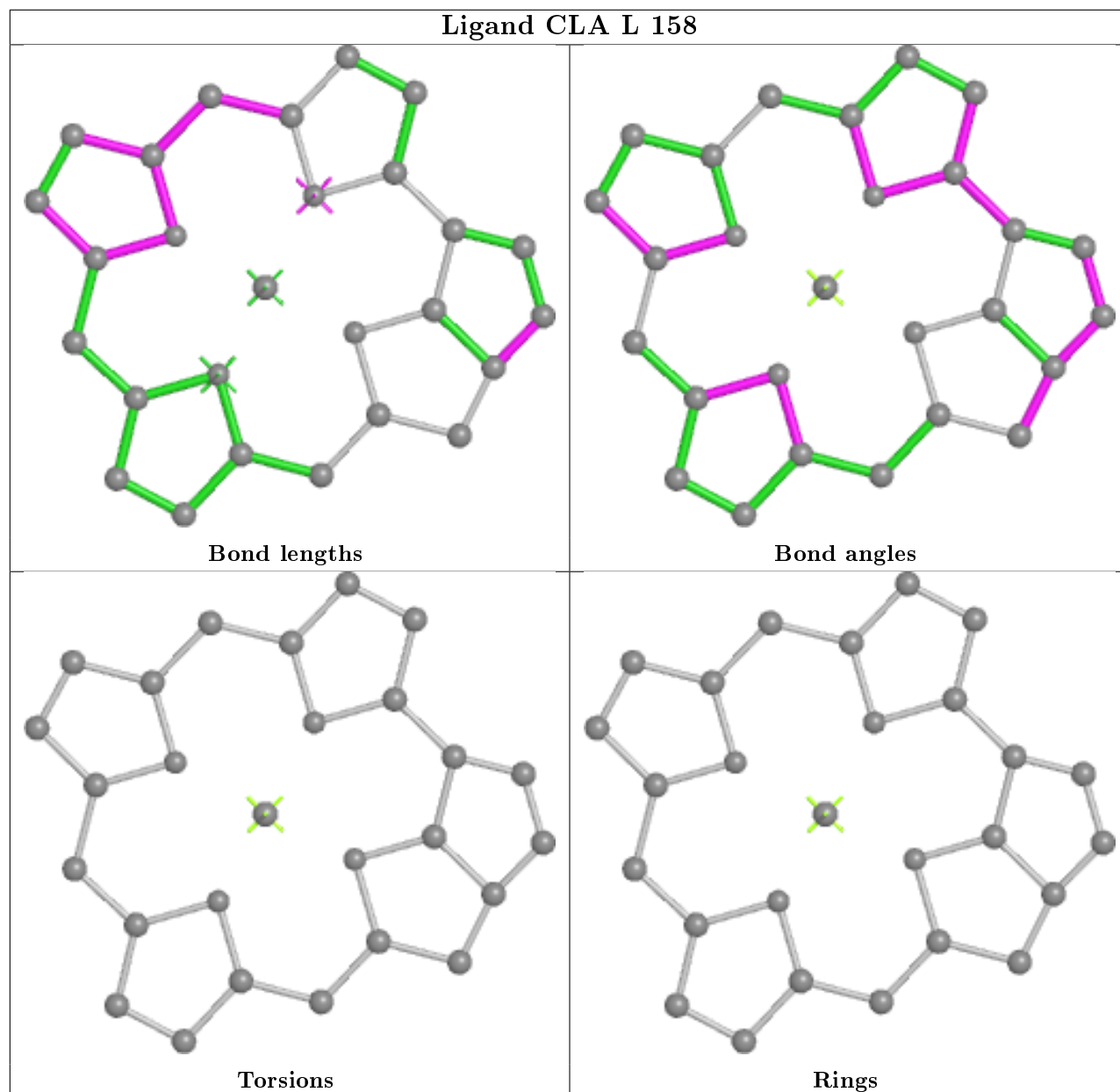
Ligand CLA L 159



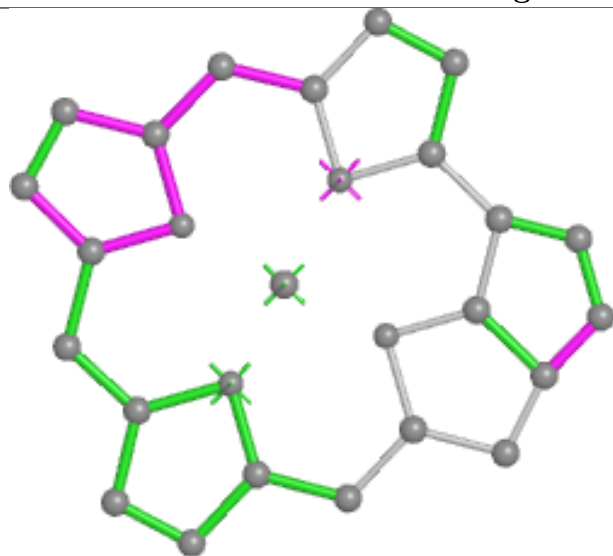
Ligand CLA A 179



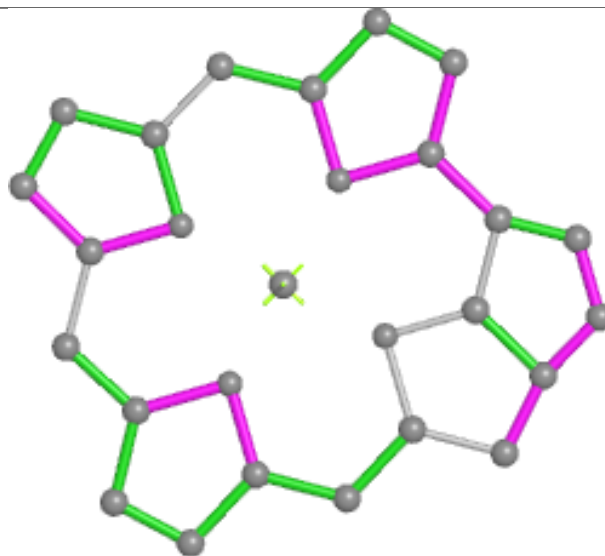
Ligand CLA L 158



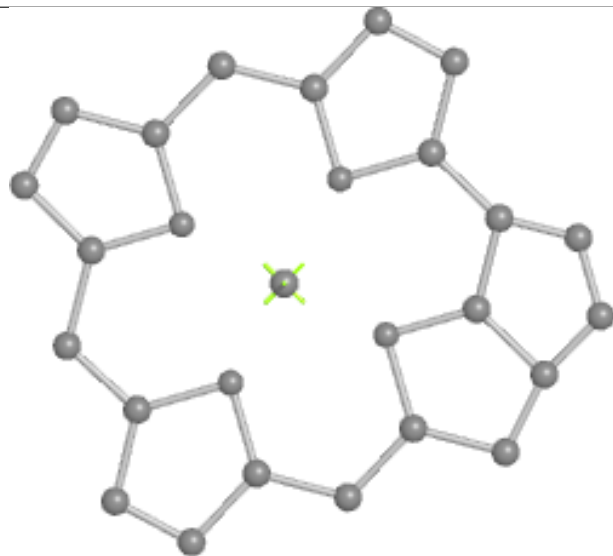
Ligand CLA D 168



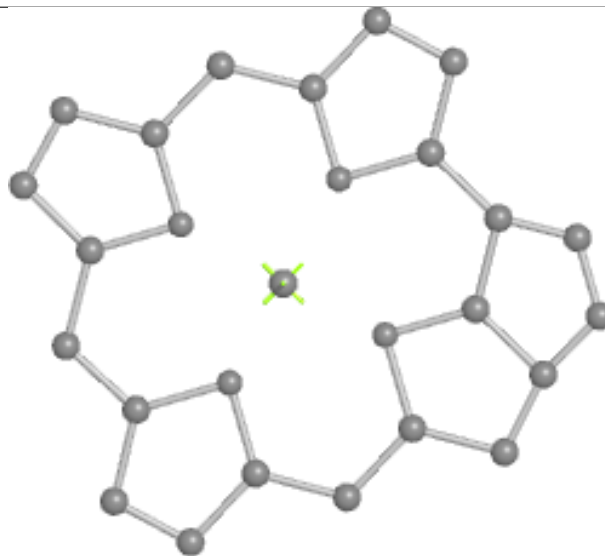
Bond lengths



Bond angles

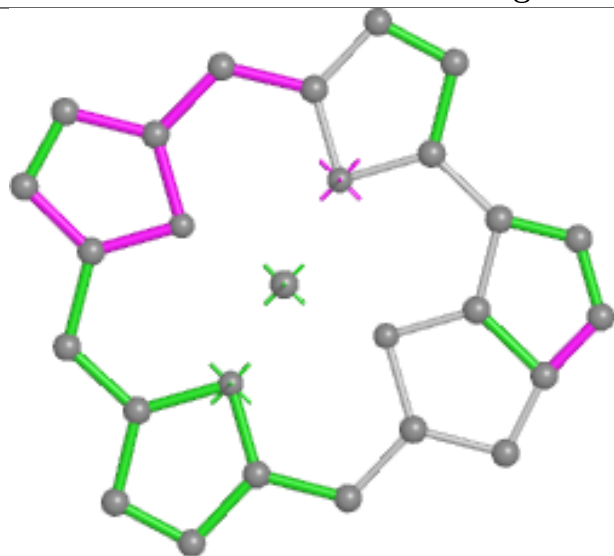


Torsions

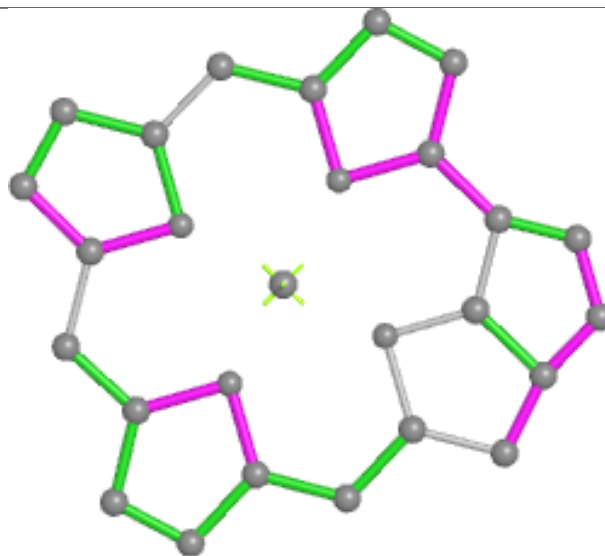


Rings

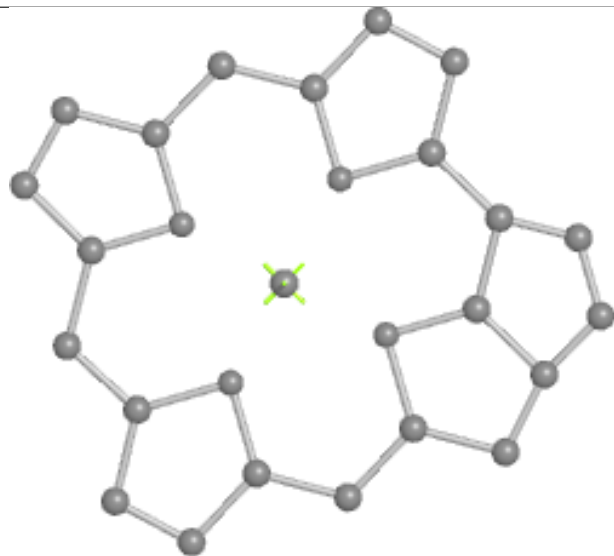
Ligand CLA D 166



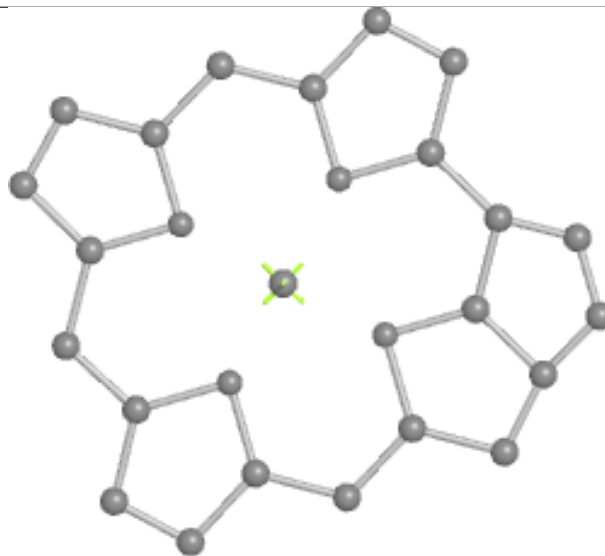
Bond lengths



Bond angles

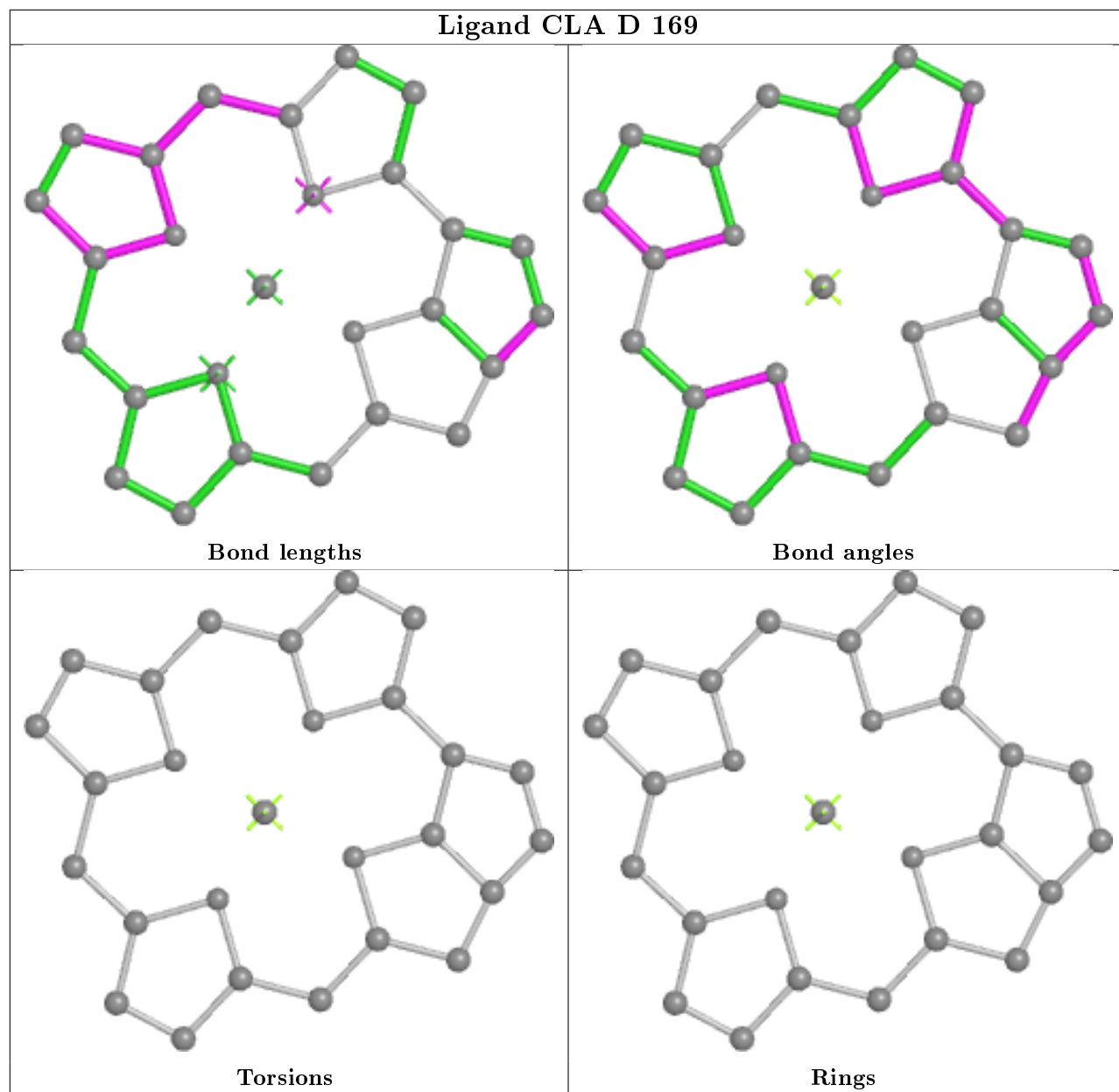


Torsions

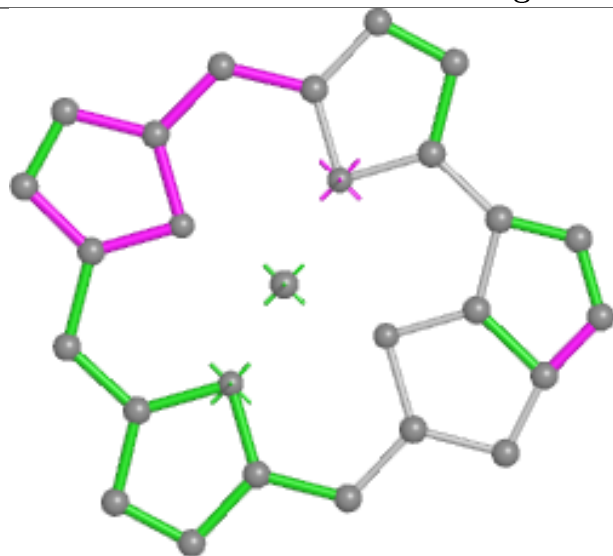


Rings

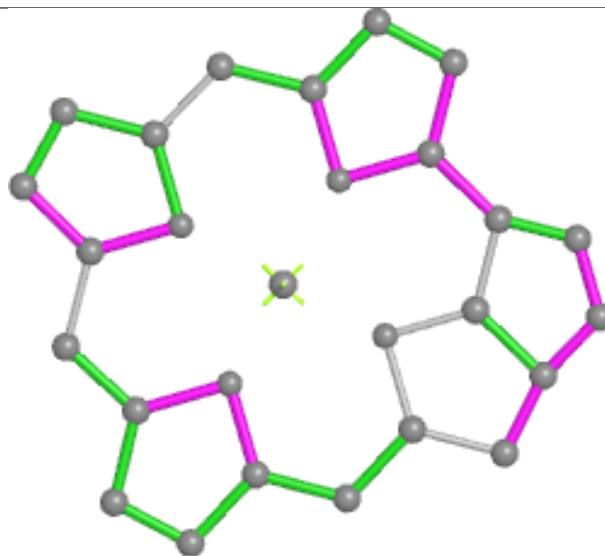
Ligand CLA D 169



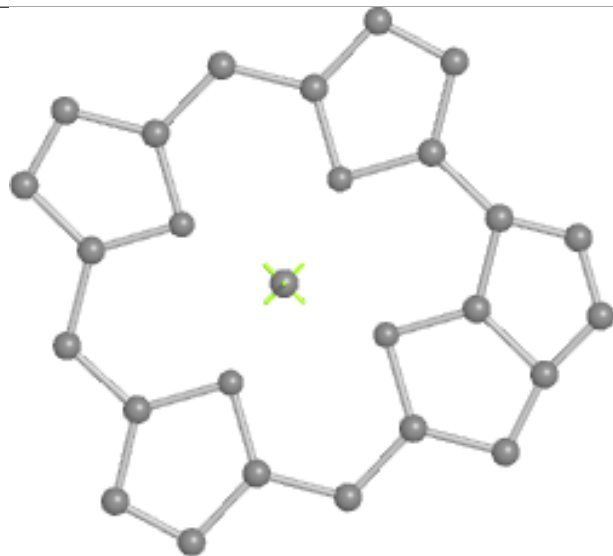
Ligand CLA D 159



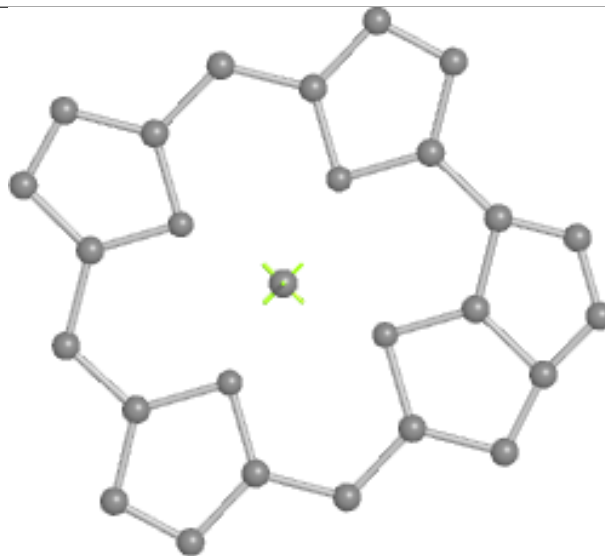
Bond lengths



Bond angles

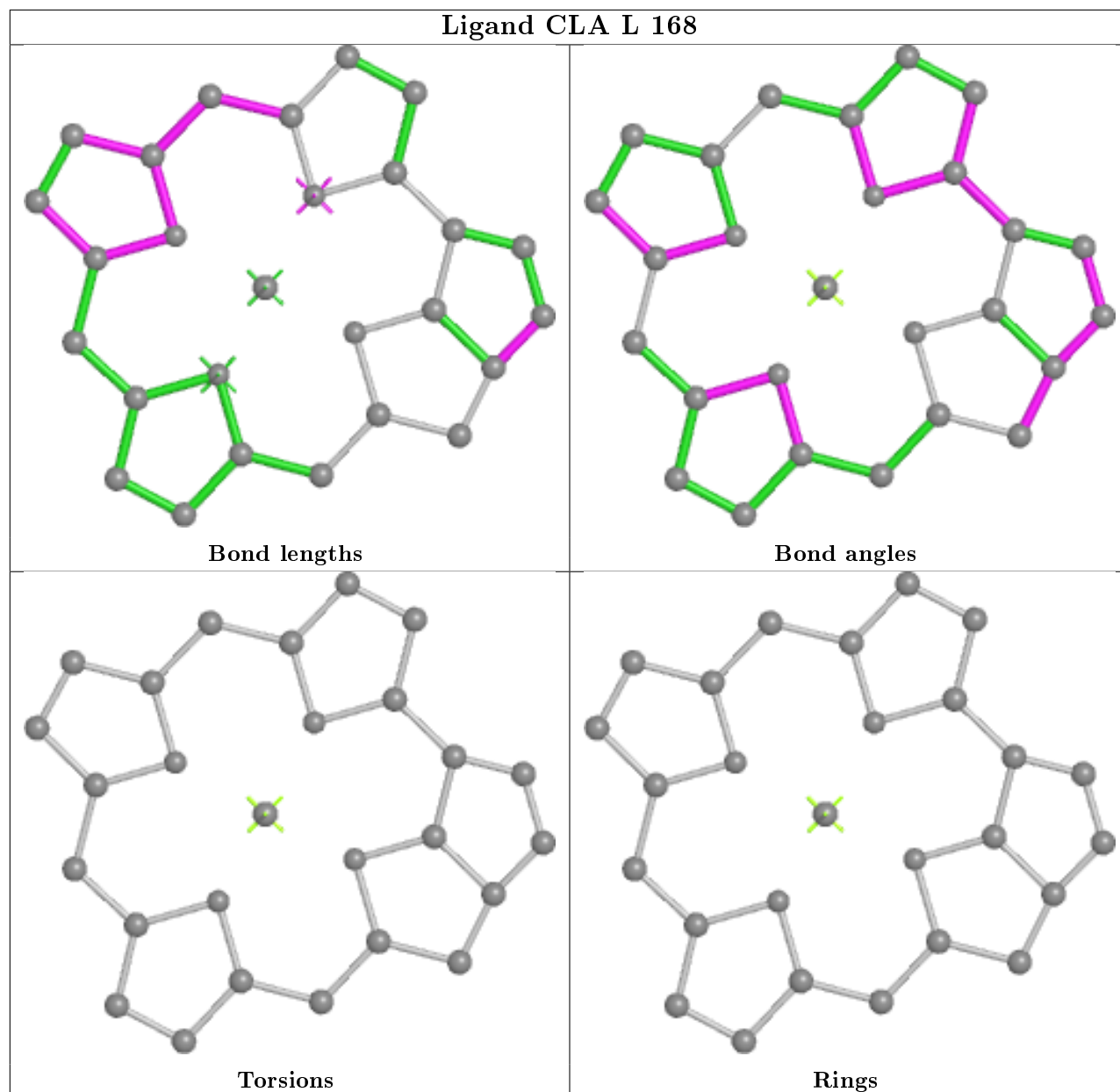


Torsions

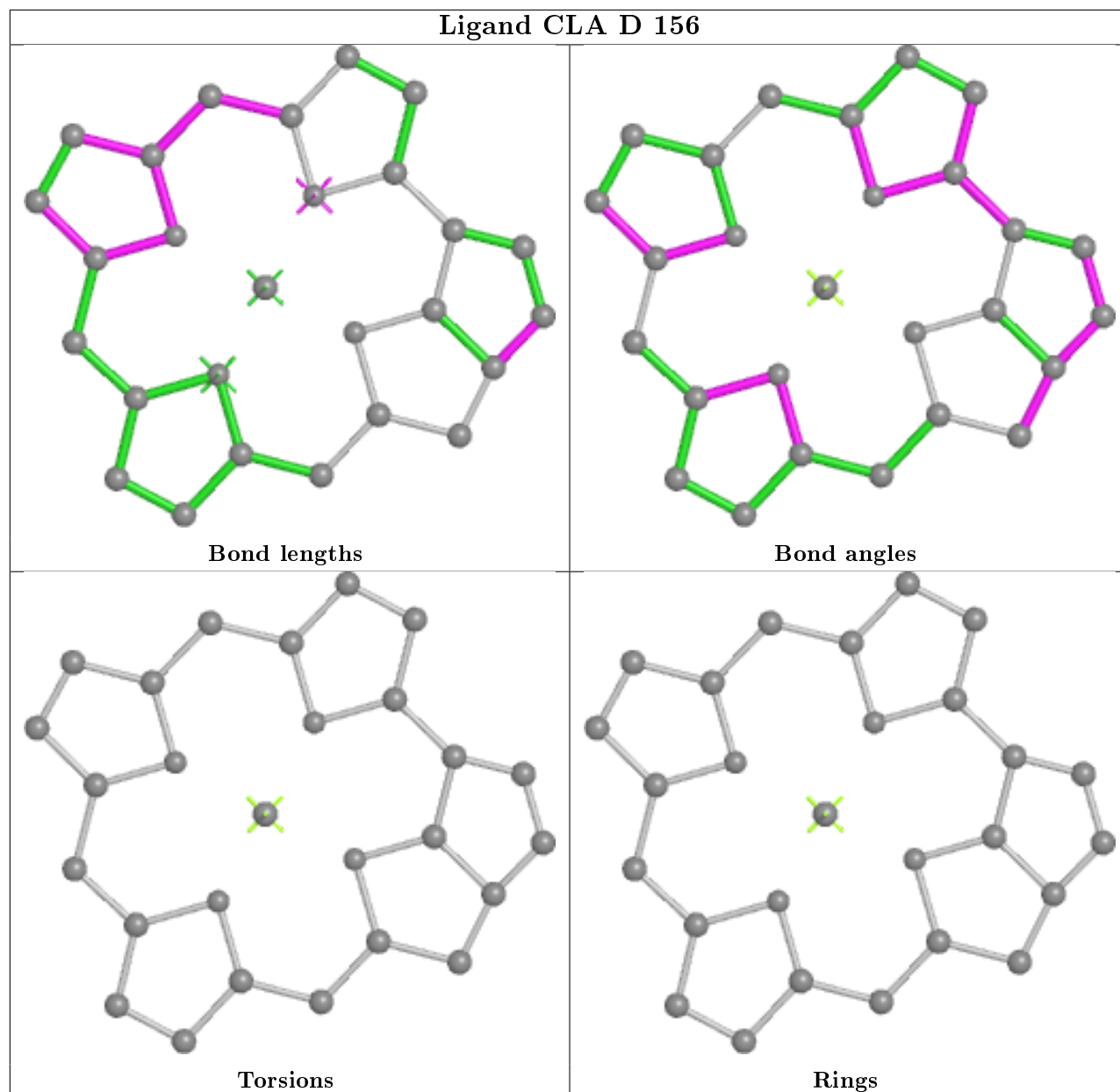


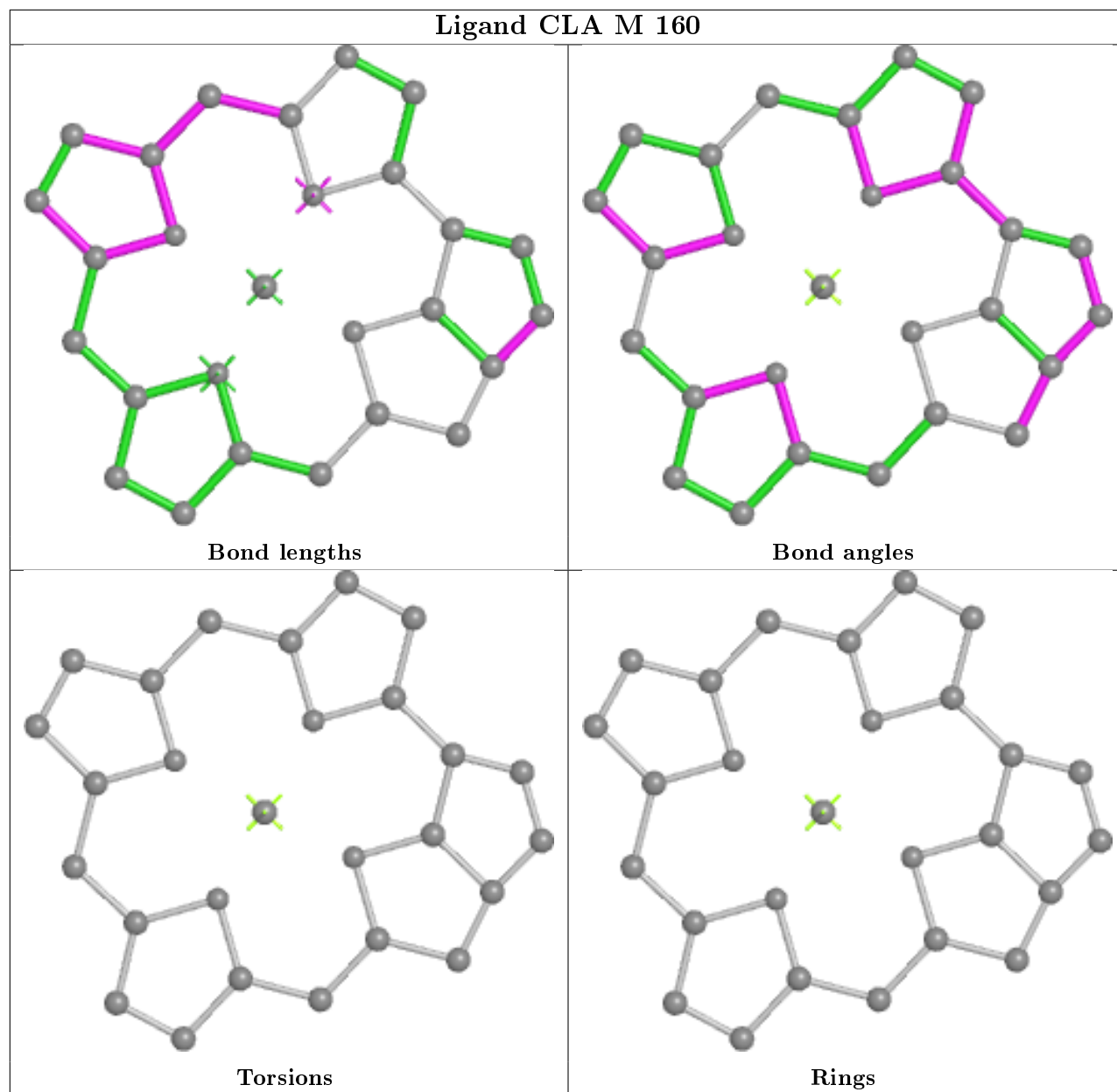
Rings

Ligand CLA L 168

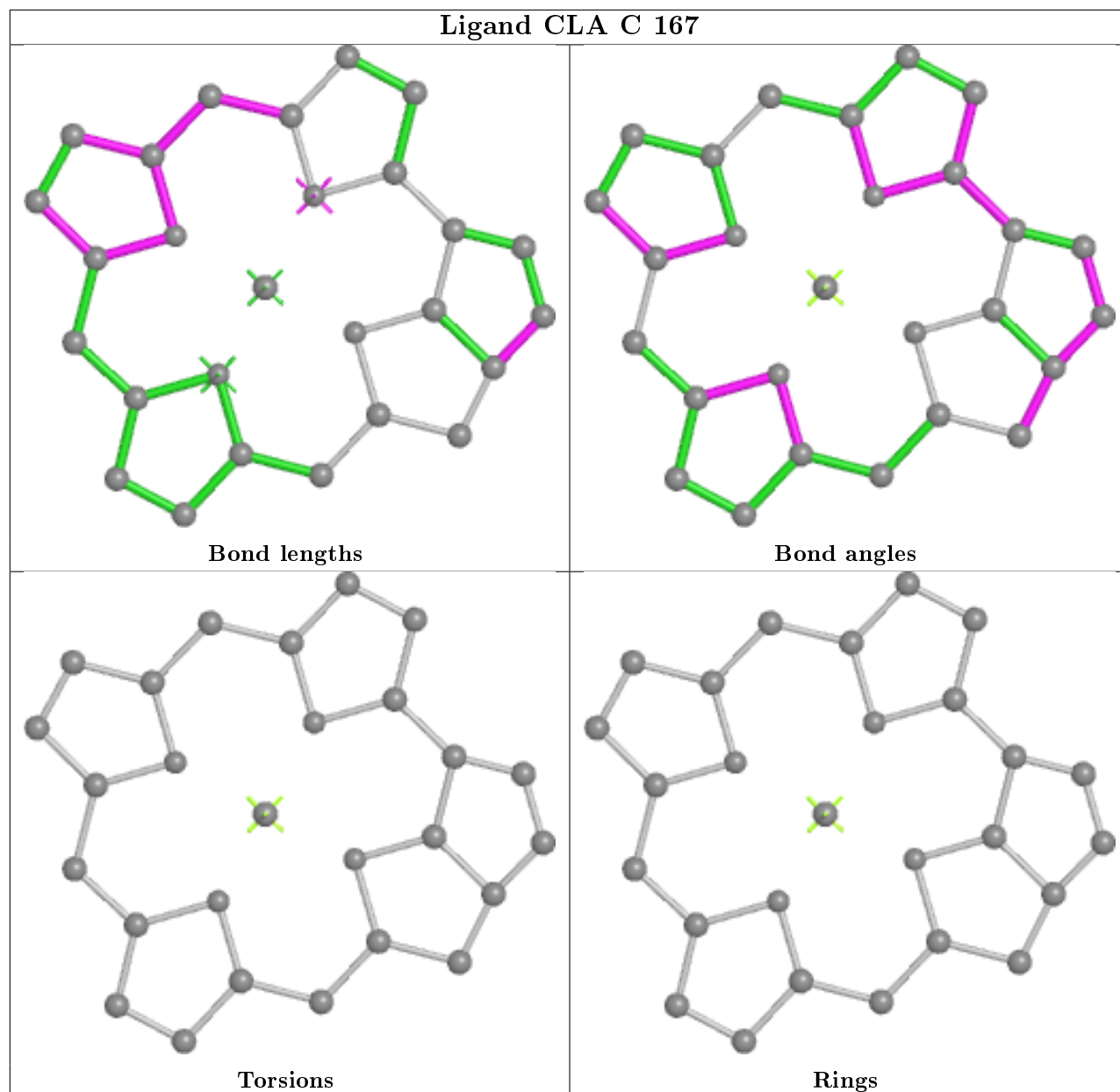


Ligand CLA D 156

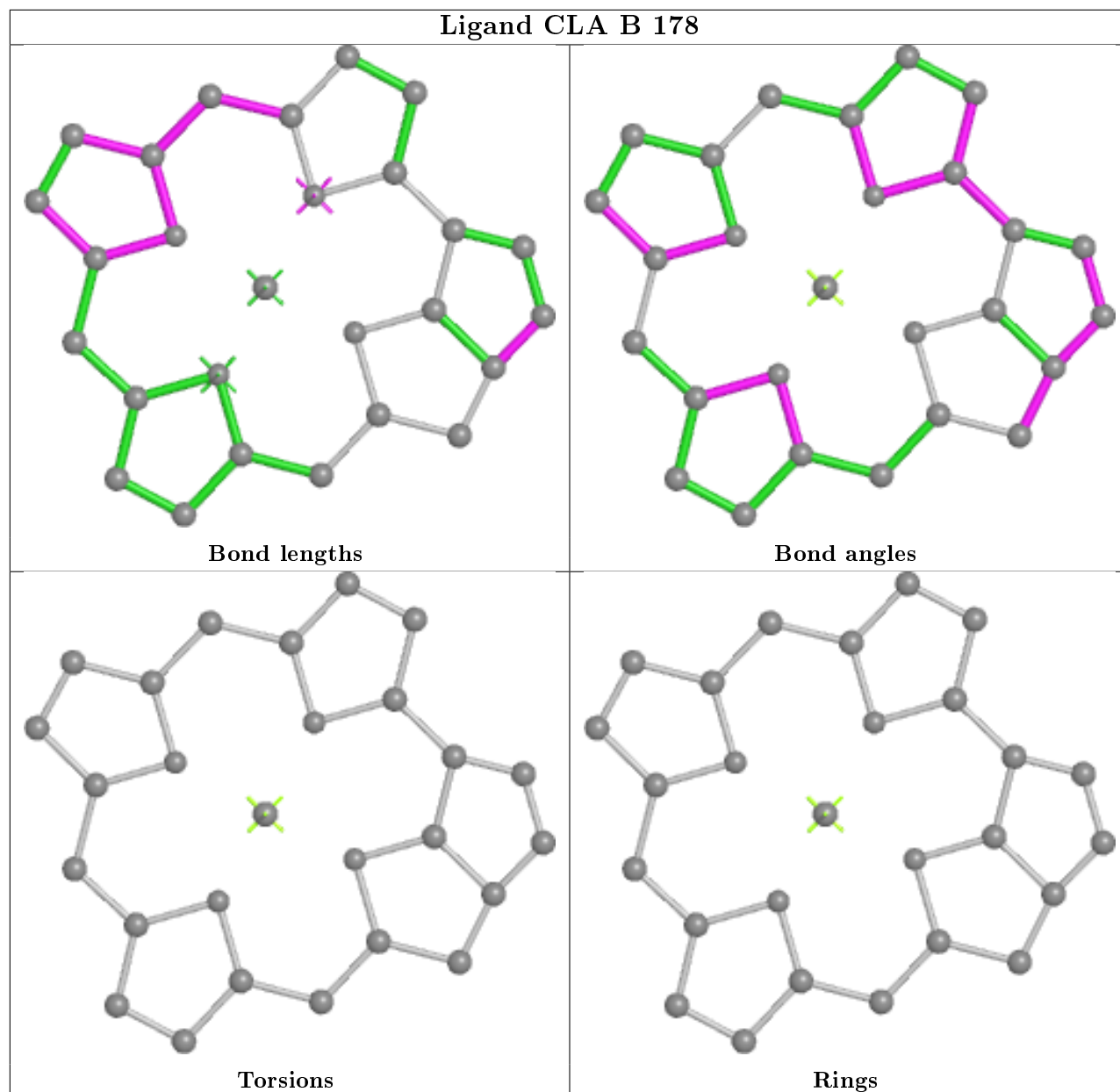


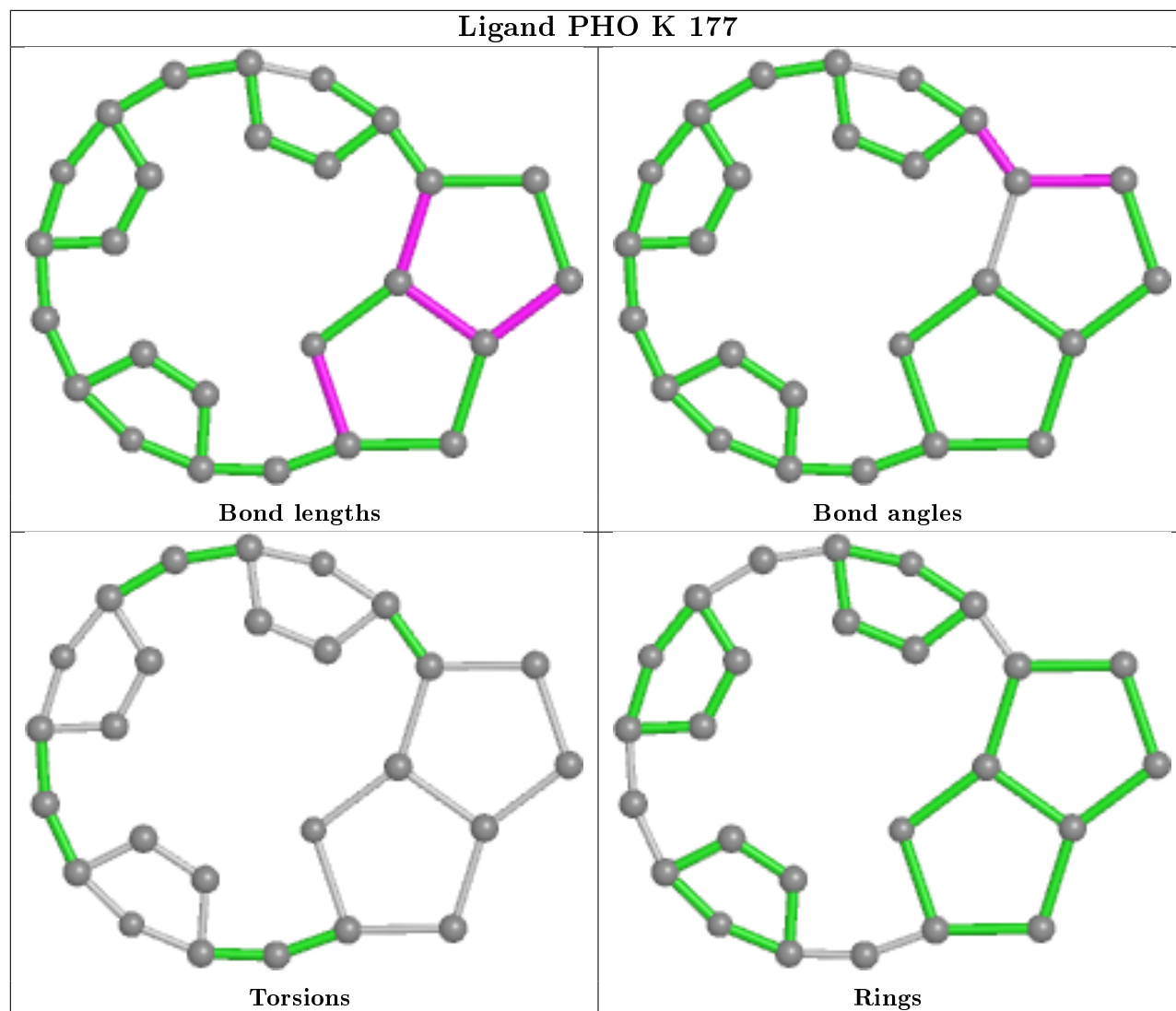


Ligand CLA C 167

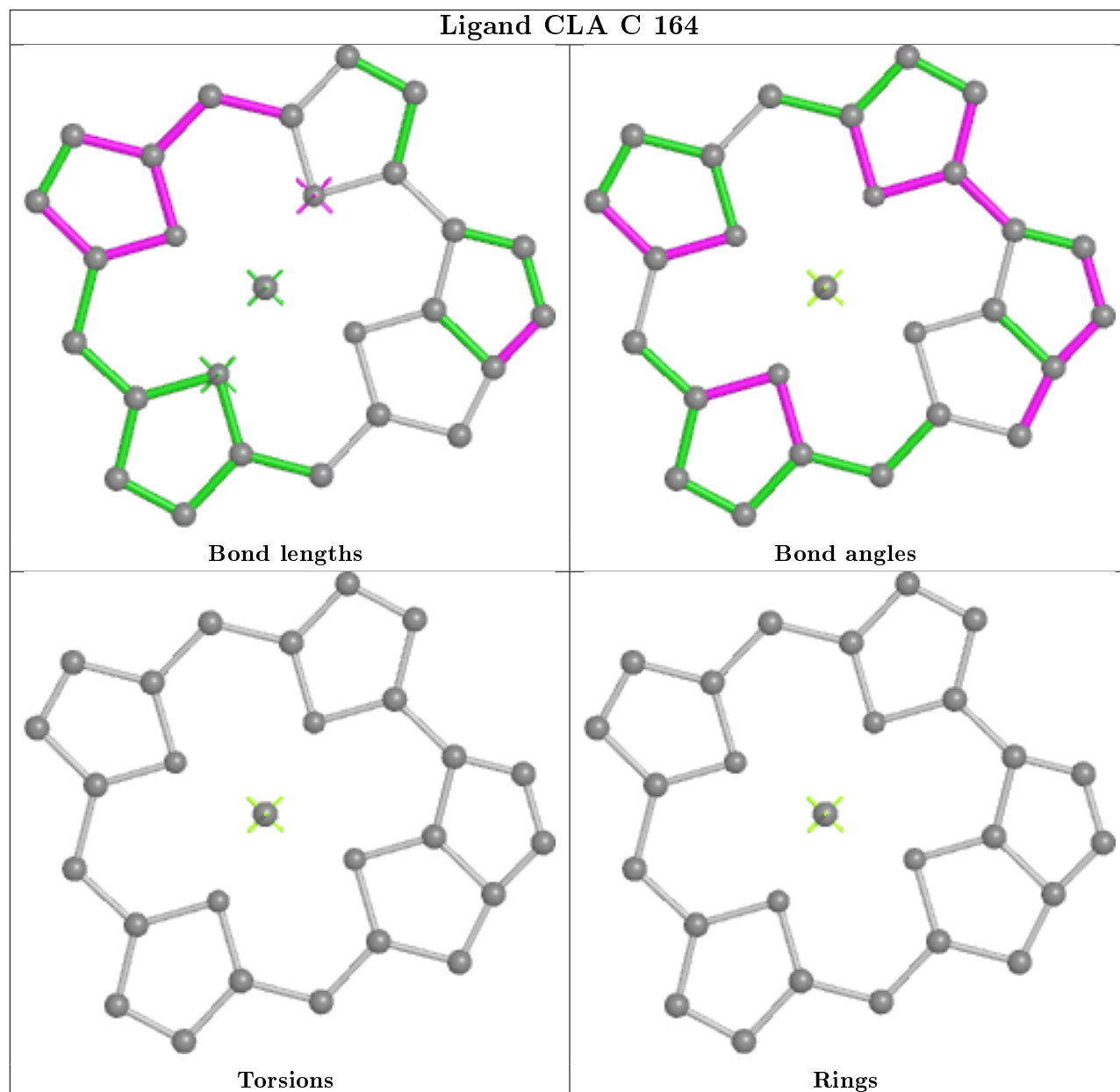


Ligand CLA B 178

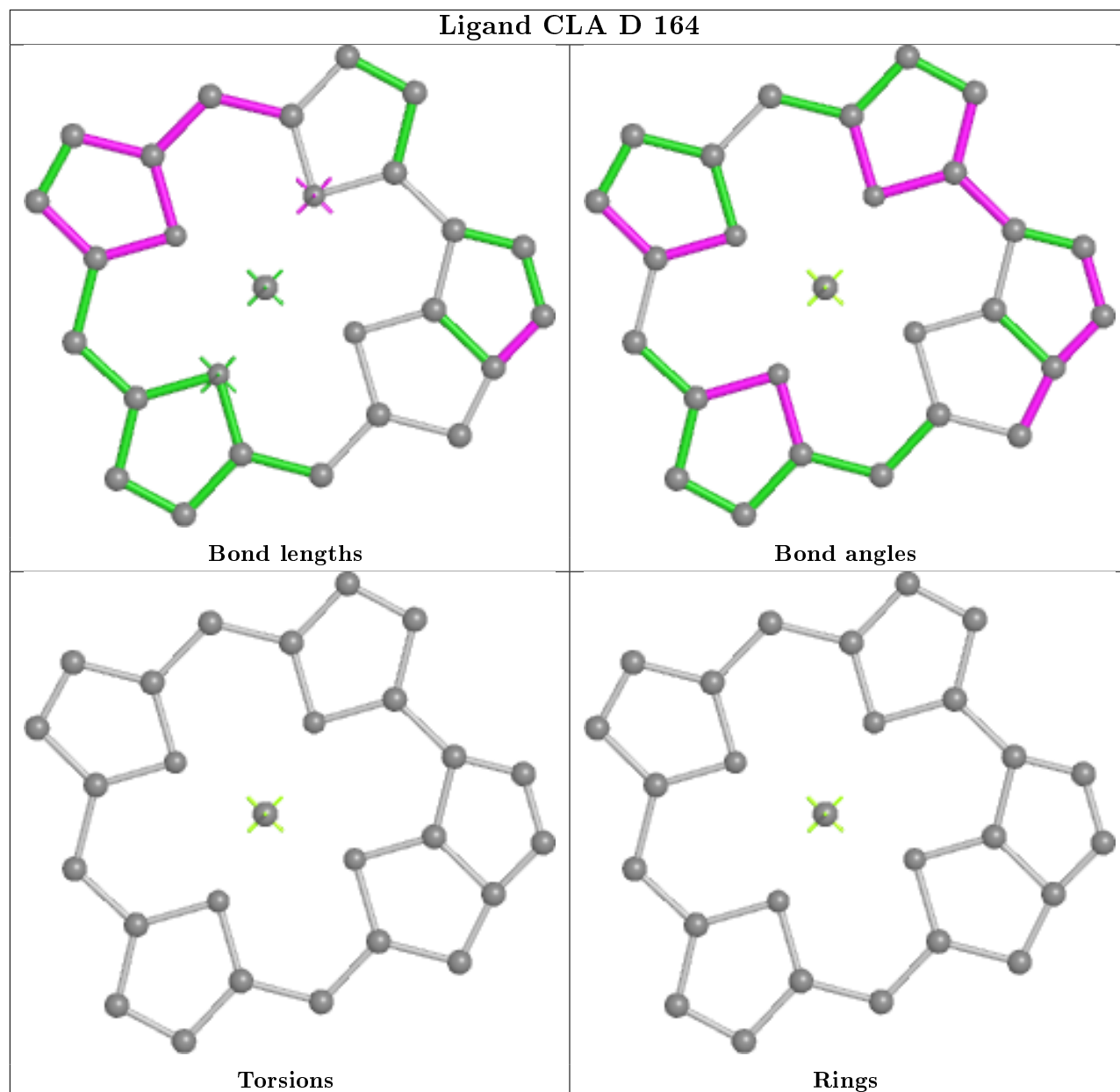


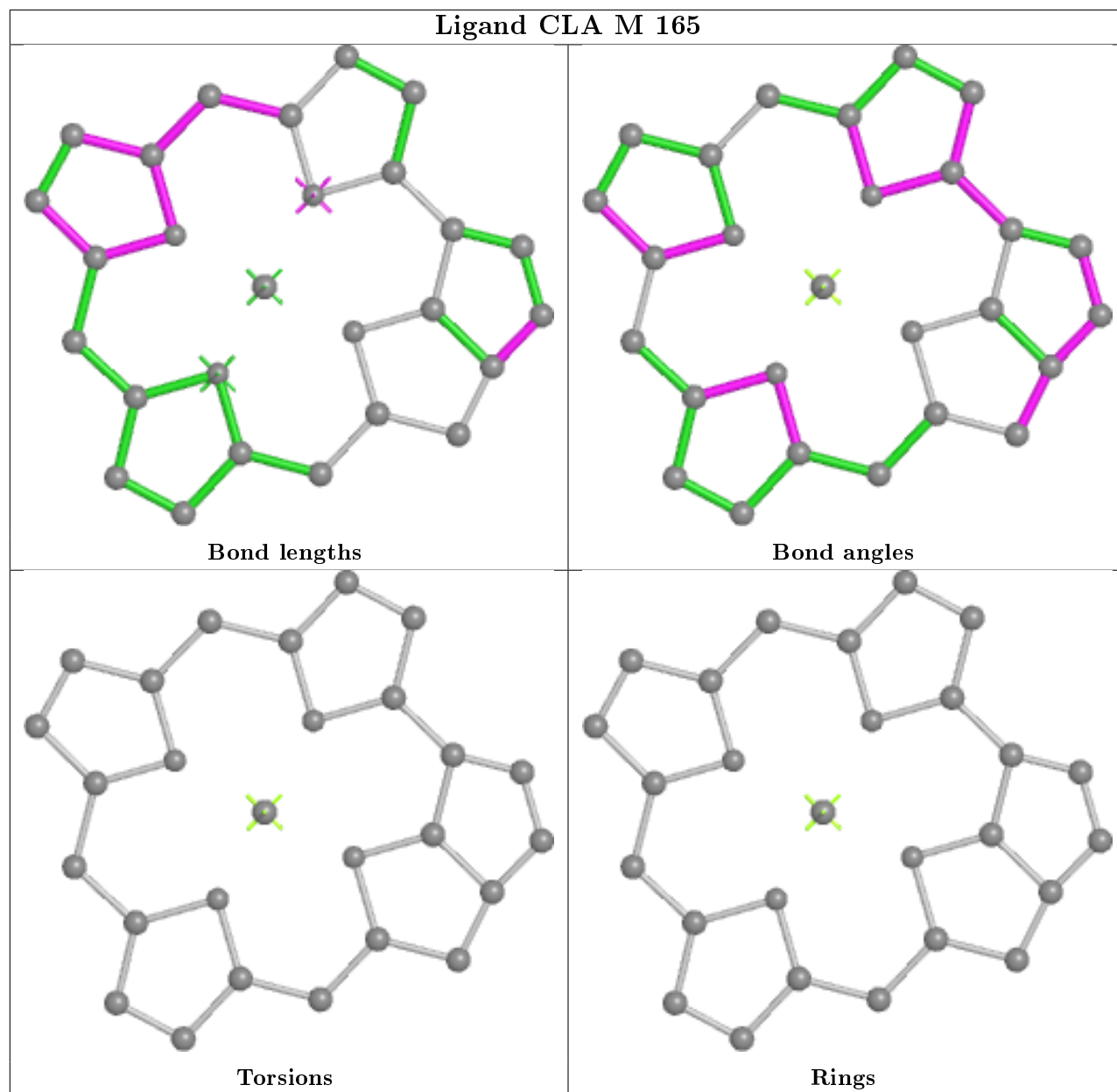


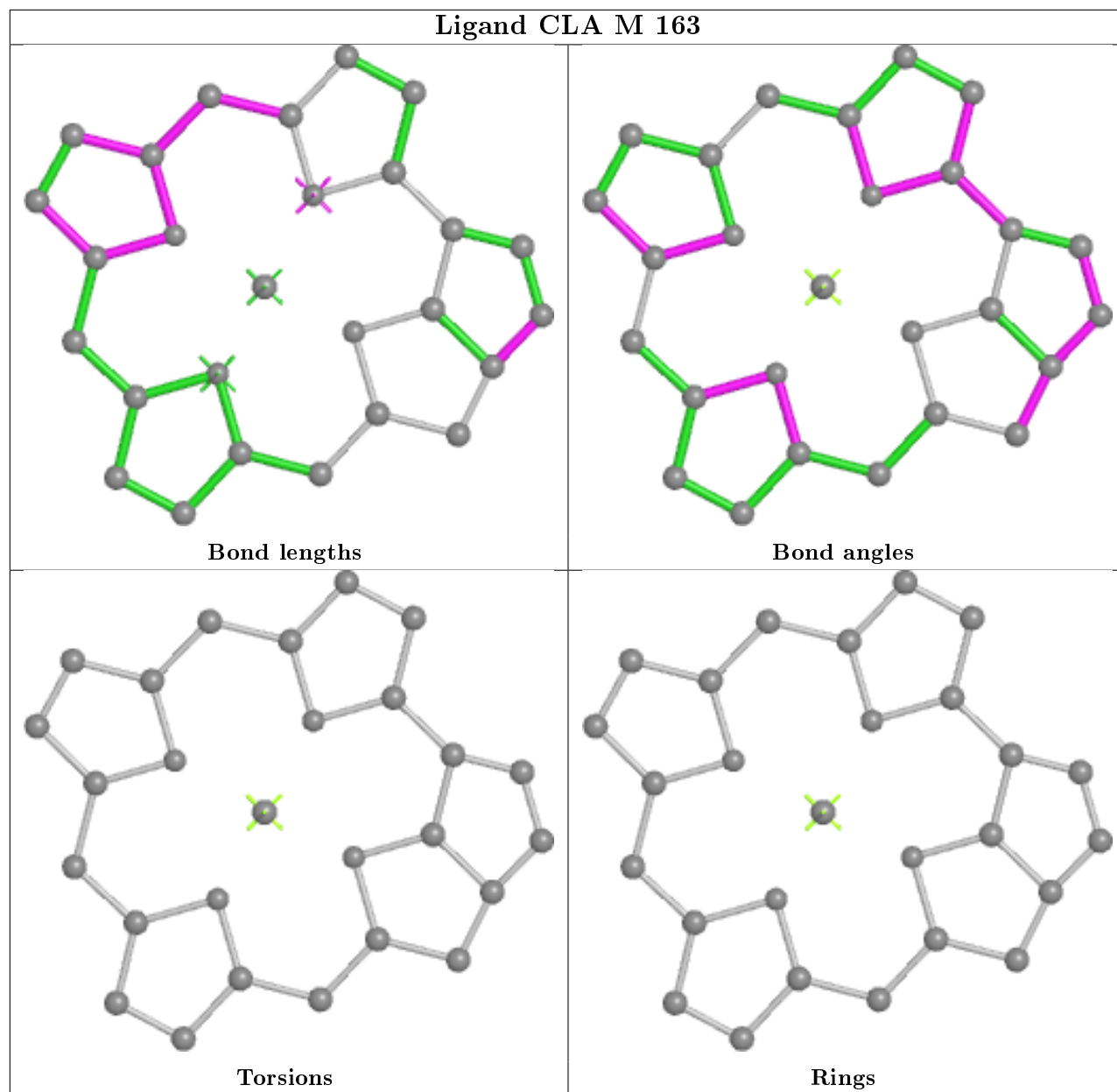
Ligand CLA C 164



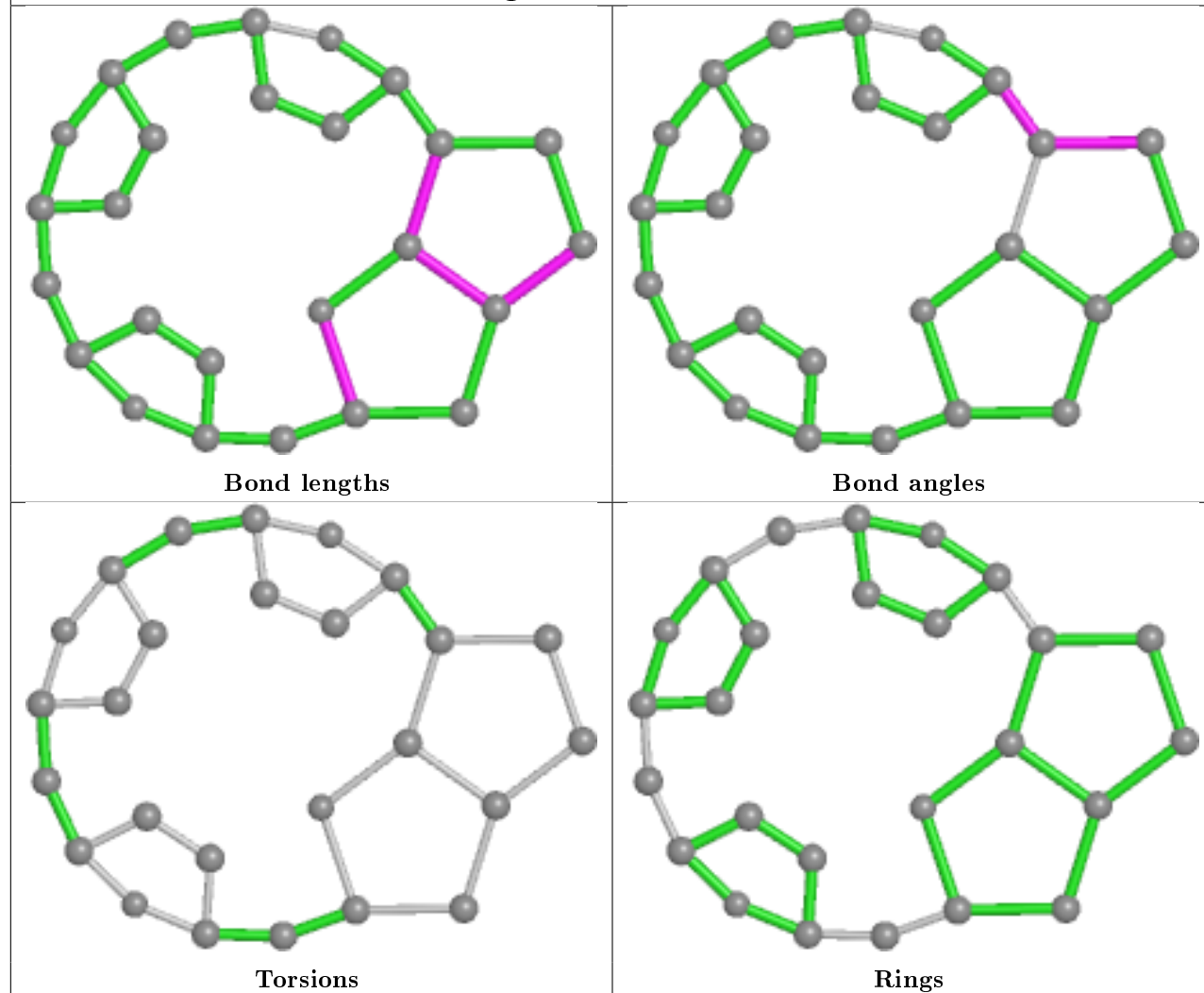
Ligand CLA D 164



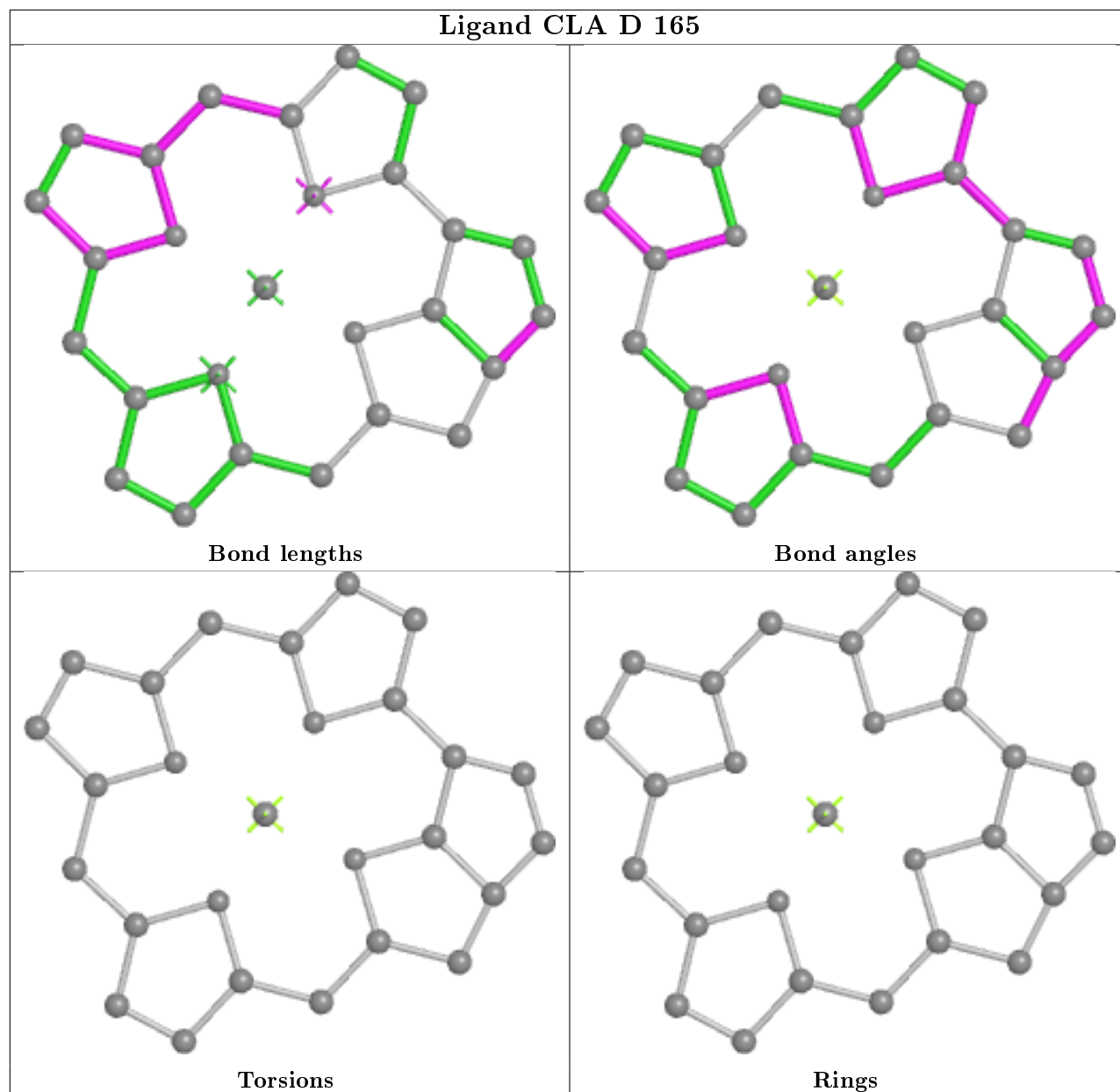




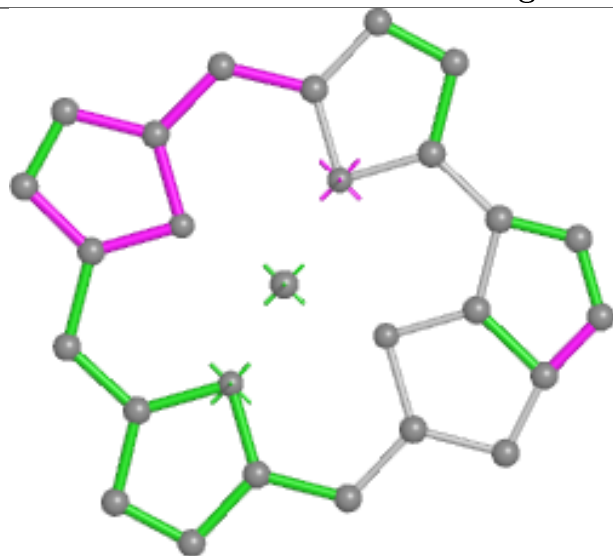
Ligand PHO J 177



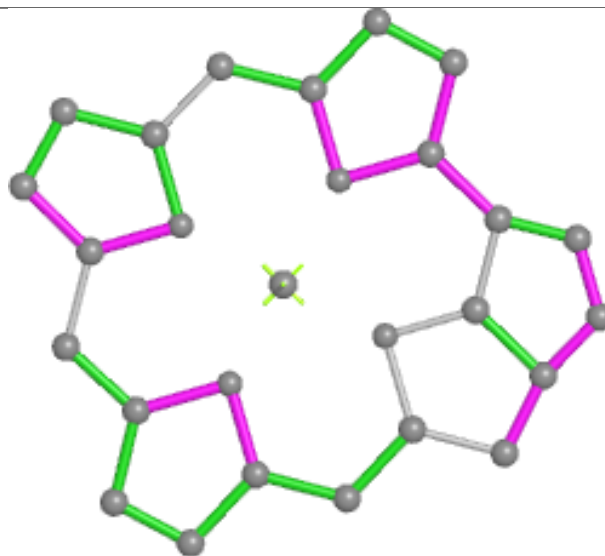
Ligand CLA D 165



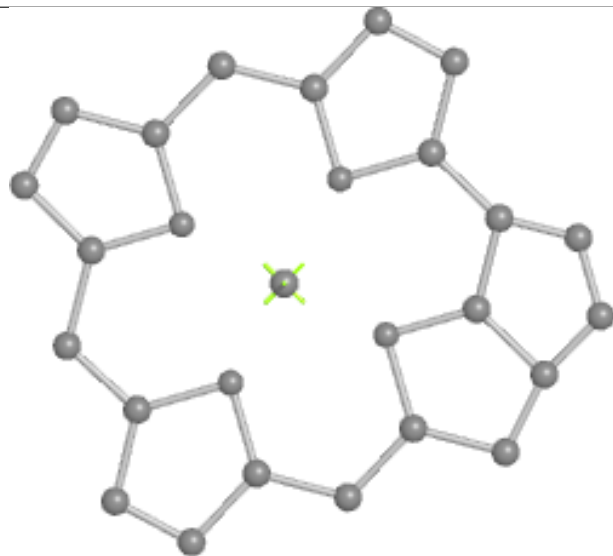
Ligand CLA J 176



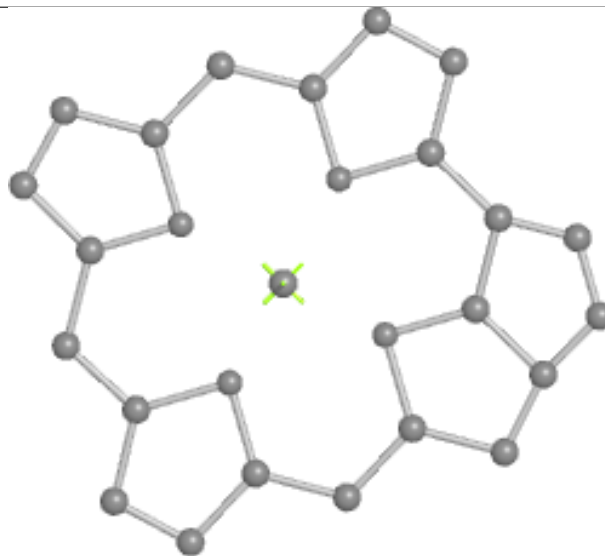
Bond lengths



Bond angles

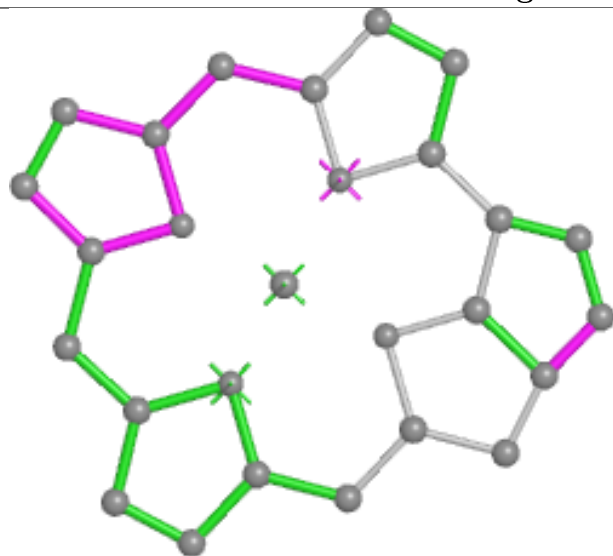


Torsions

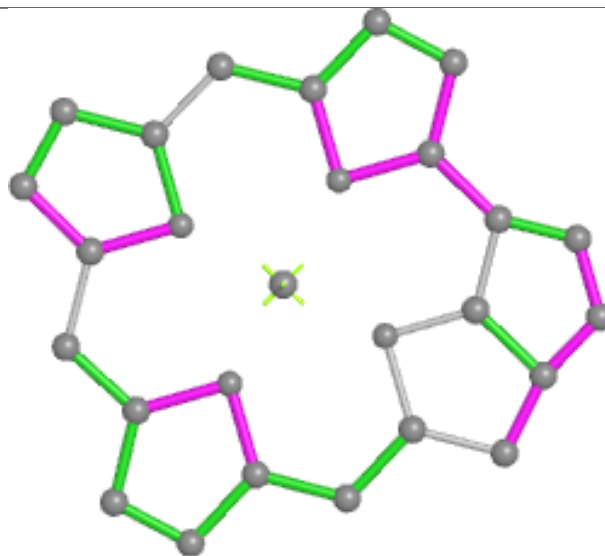


Rings

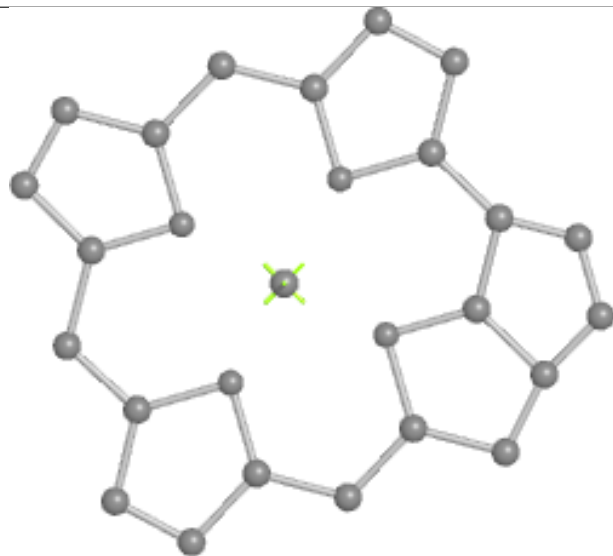
Ligand CLA L 166



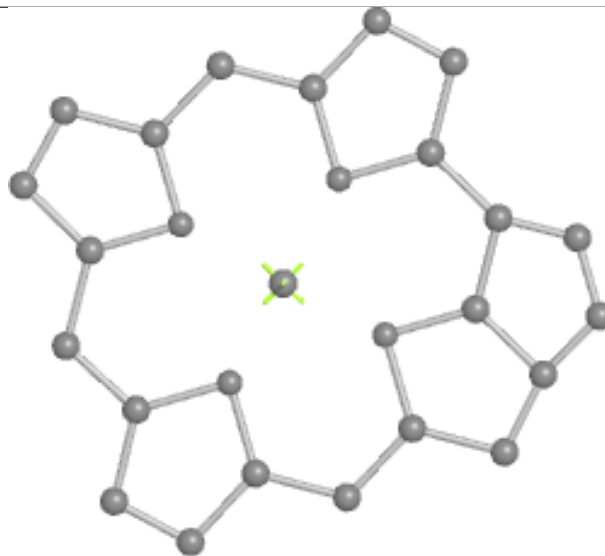
Bond lengths



Bond angles

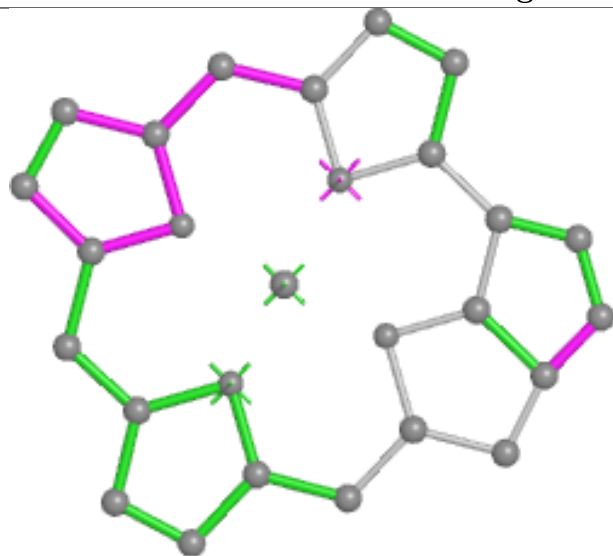


Torsions

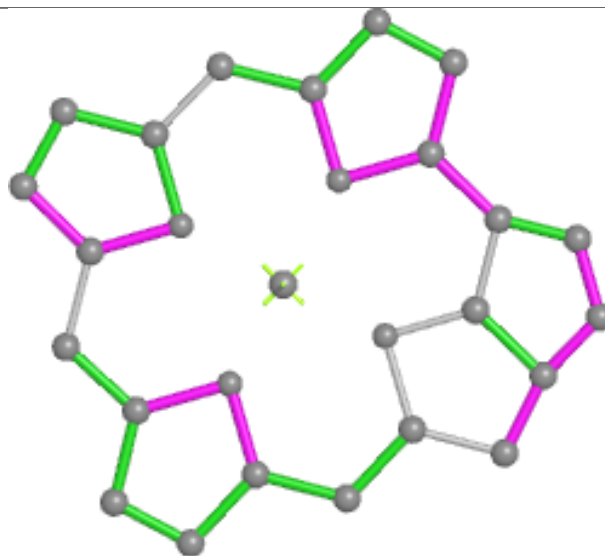


Rings

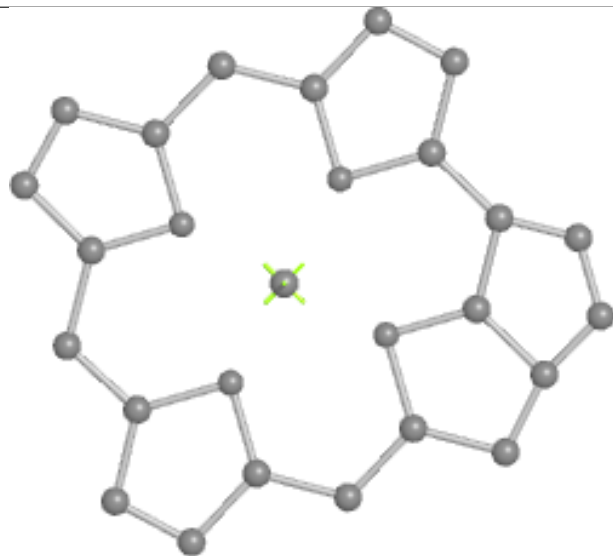
Ligand CLA L 160



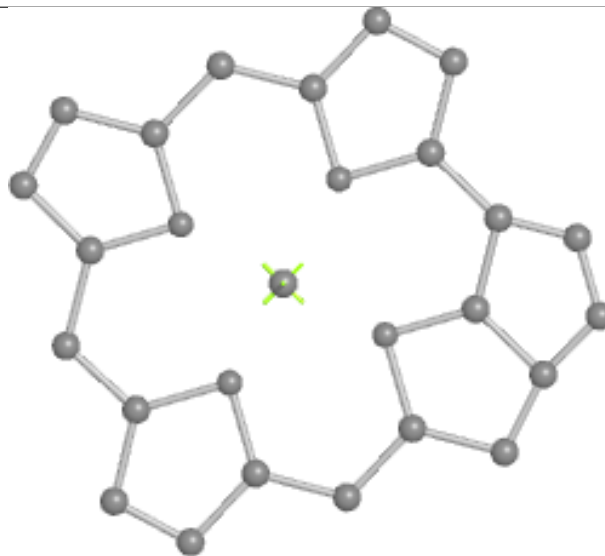
Bond lengths



Bond angles

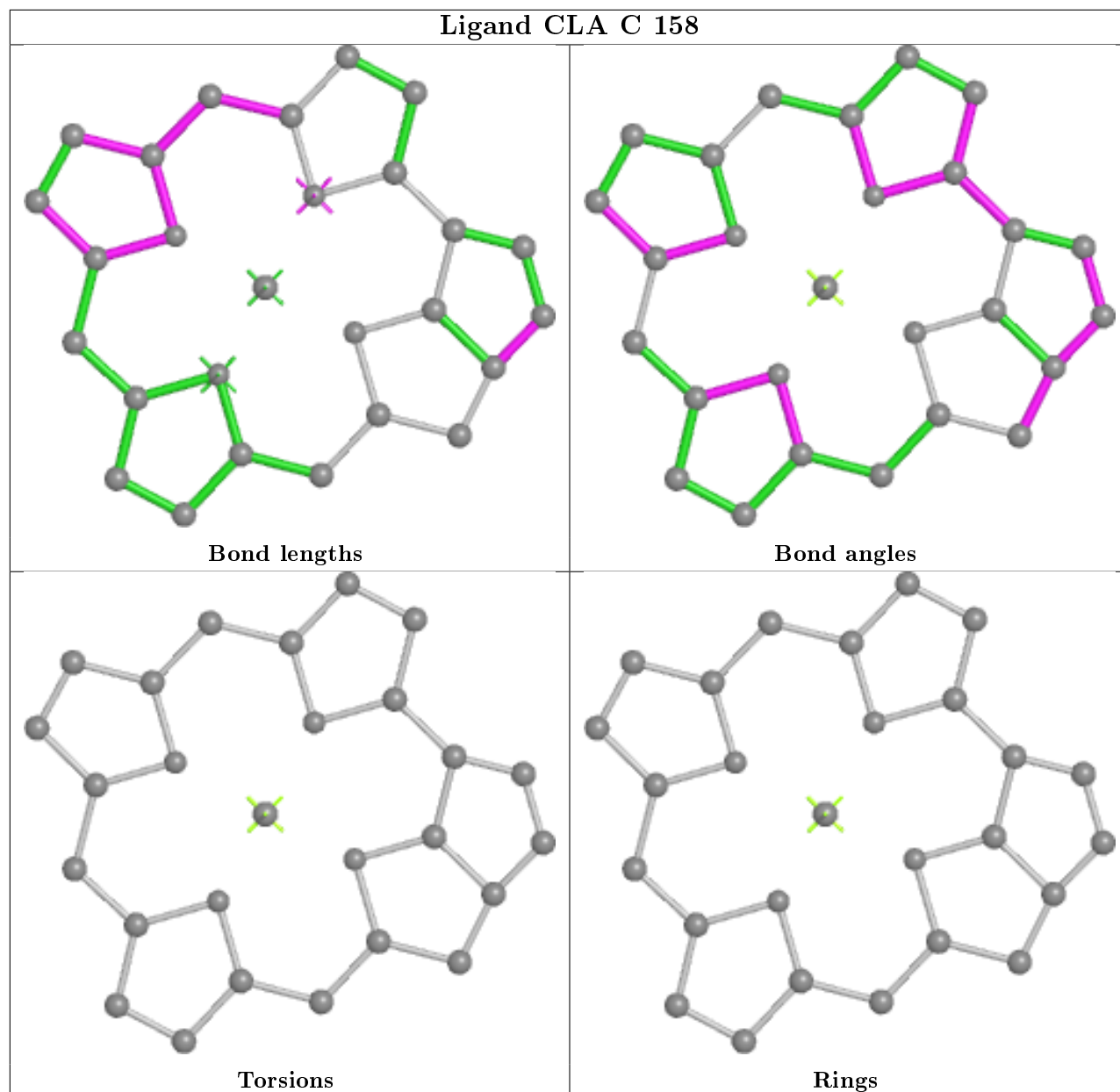


Torsions

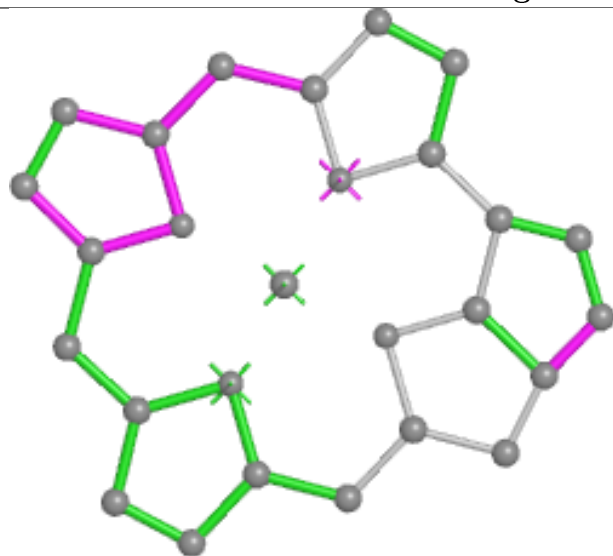


Rings

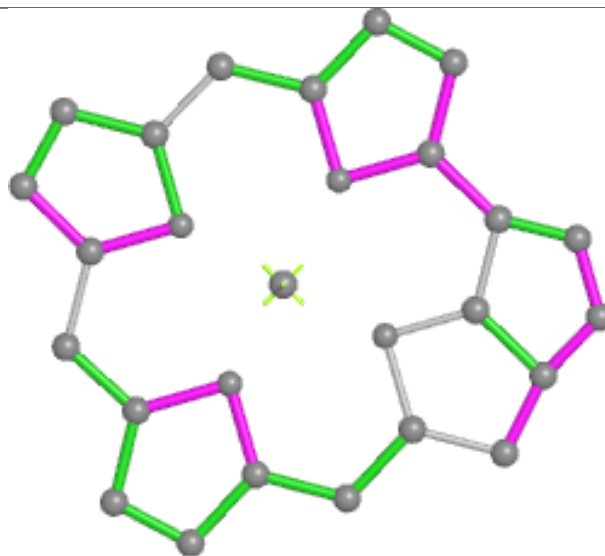
Ligand CLA C 158



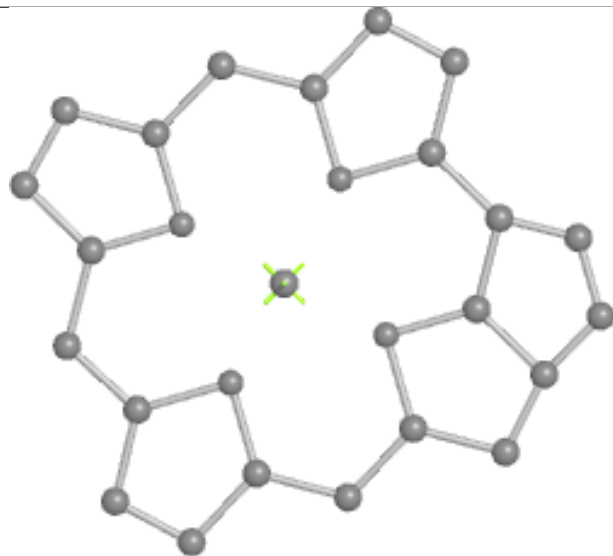
Ligand CLA D 170



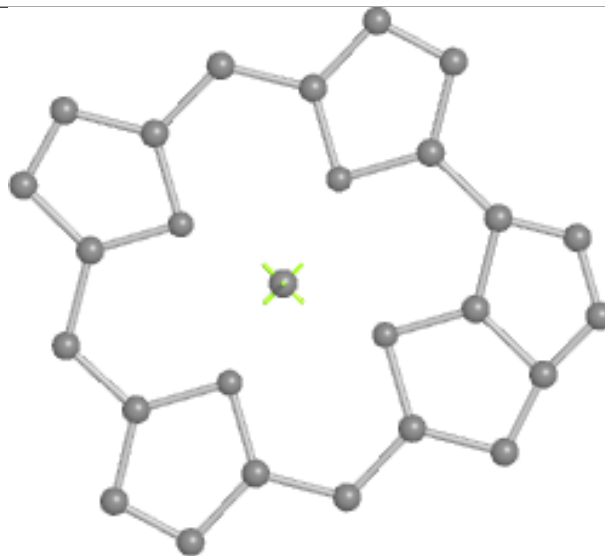
Bond lengths



Bond angles

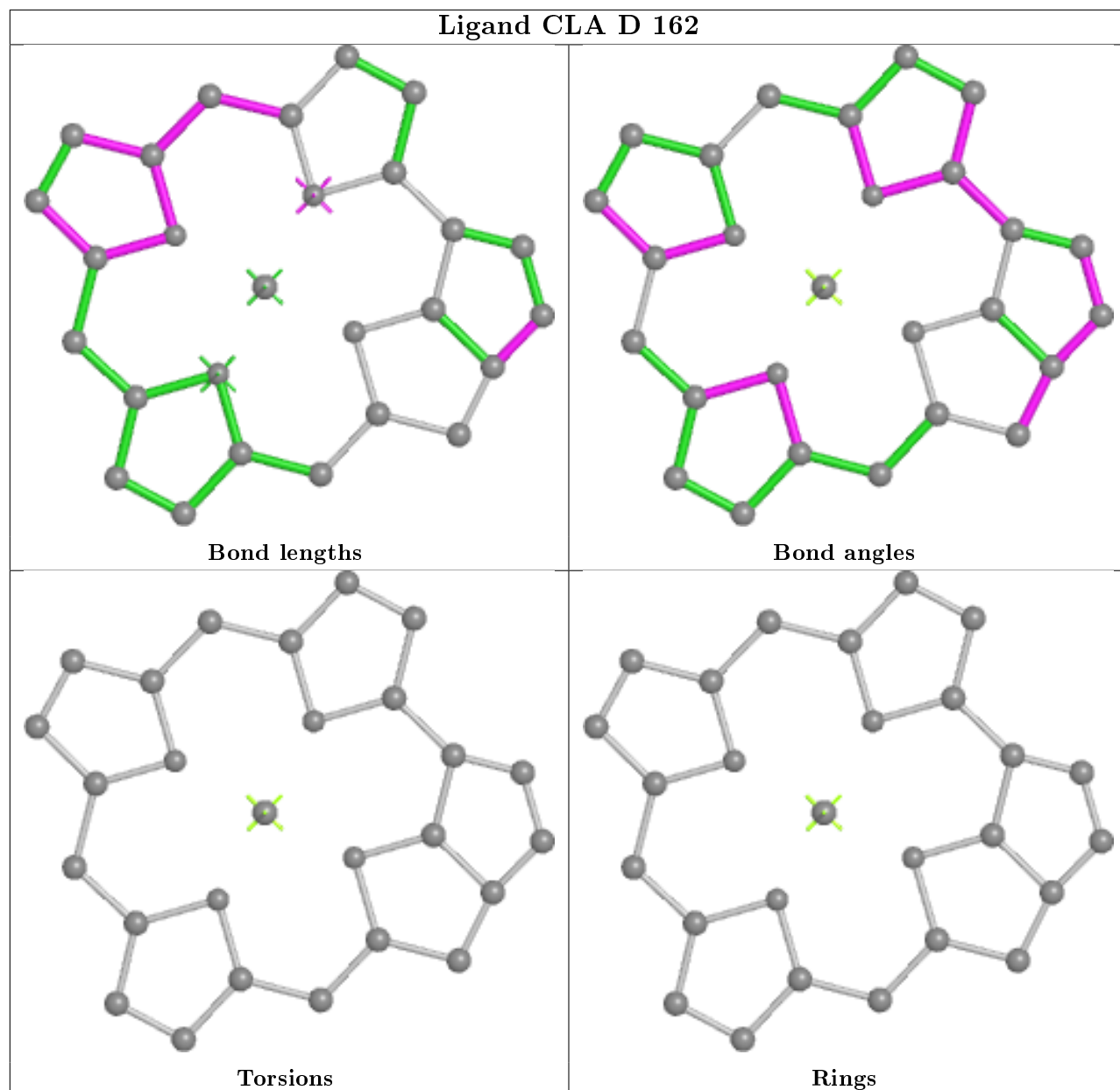


Torsions

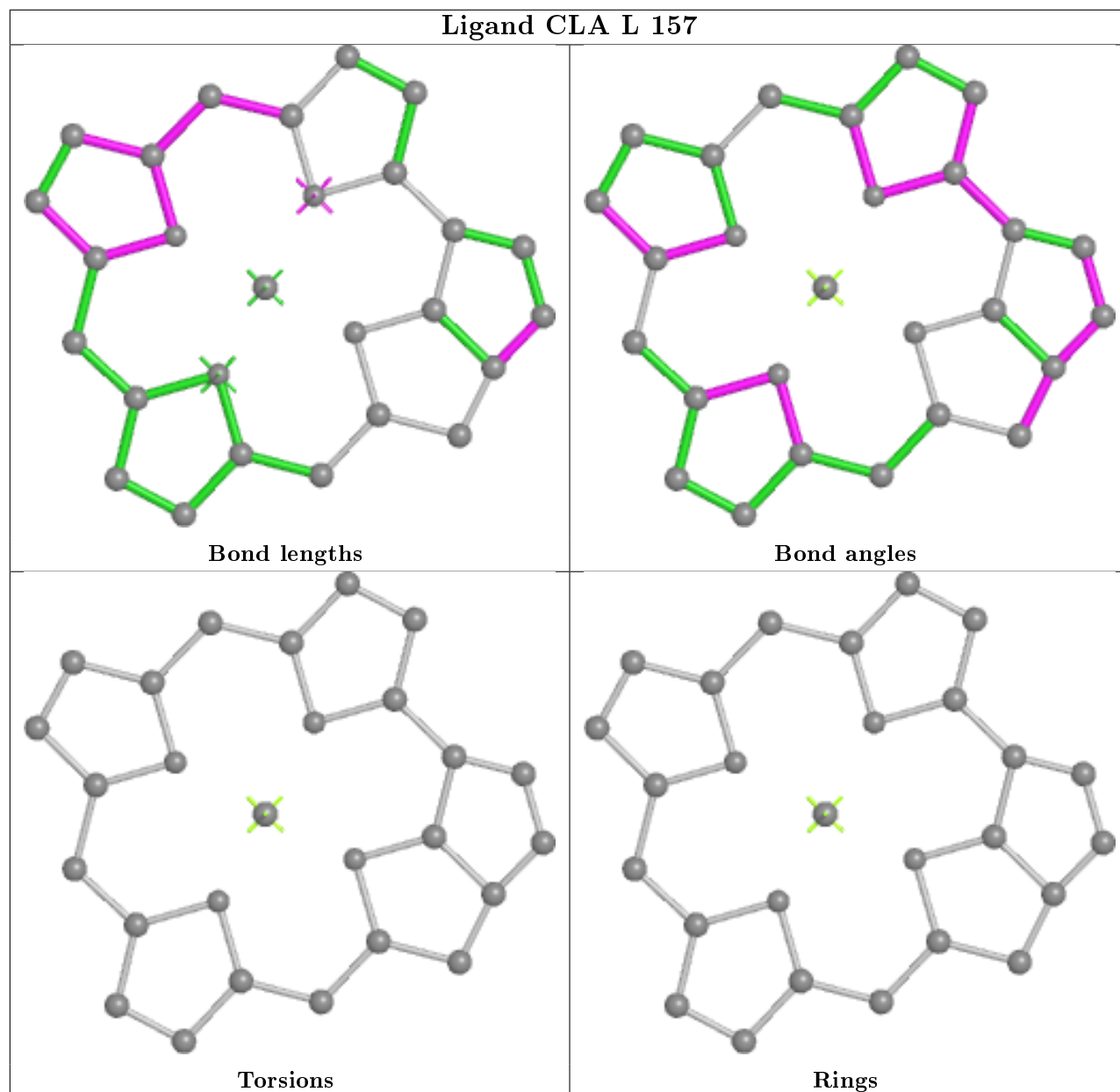


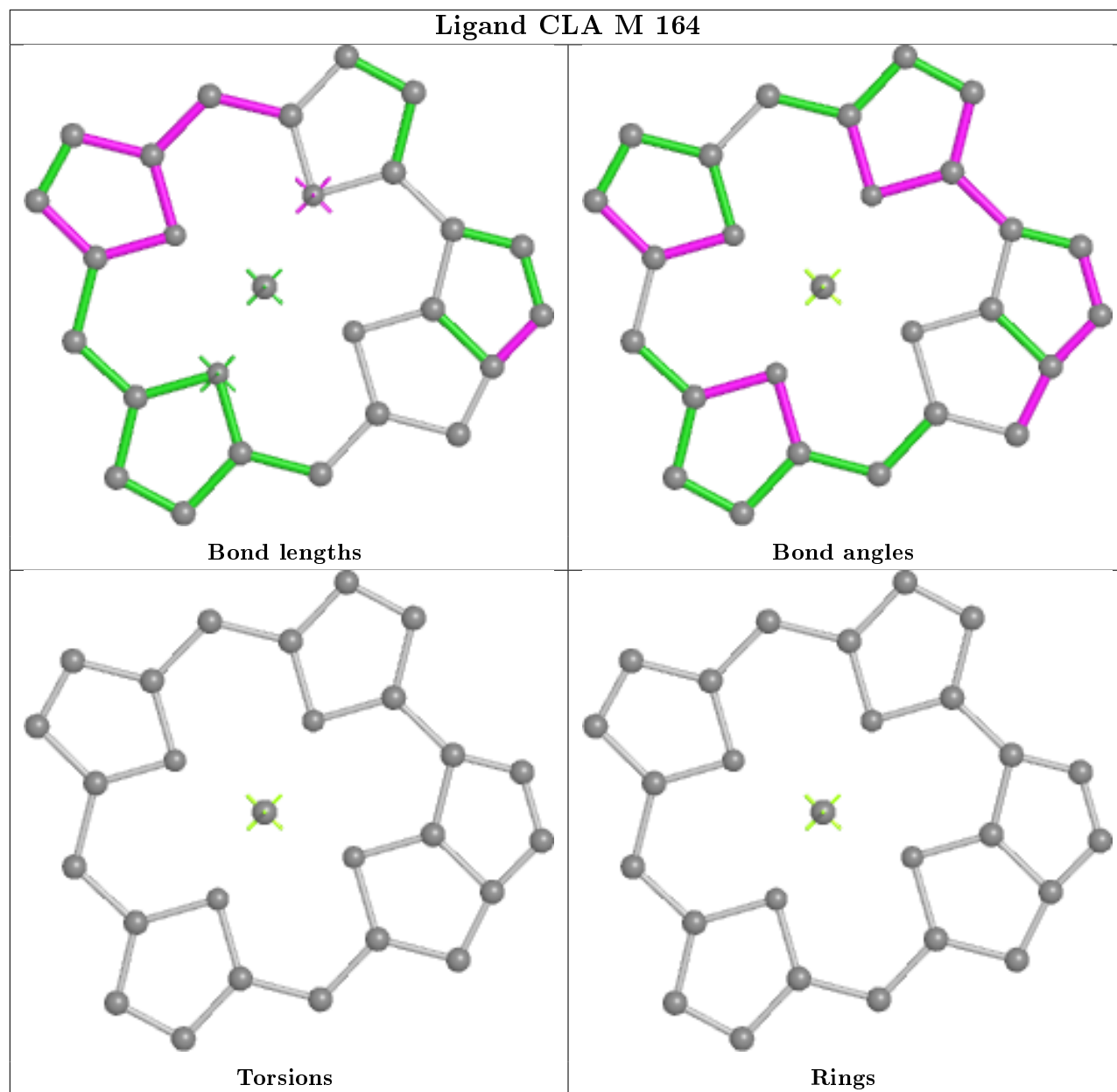
Rings

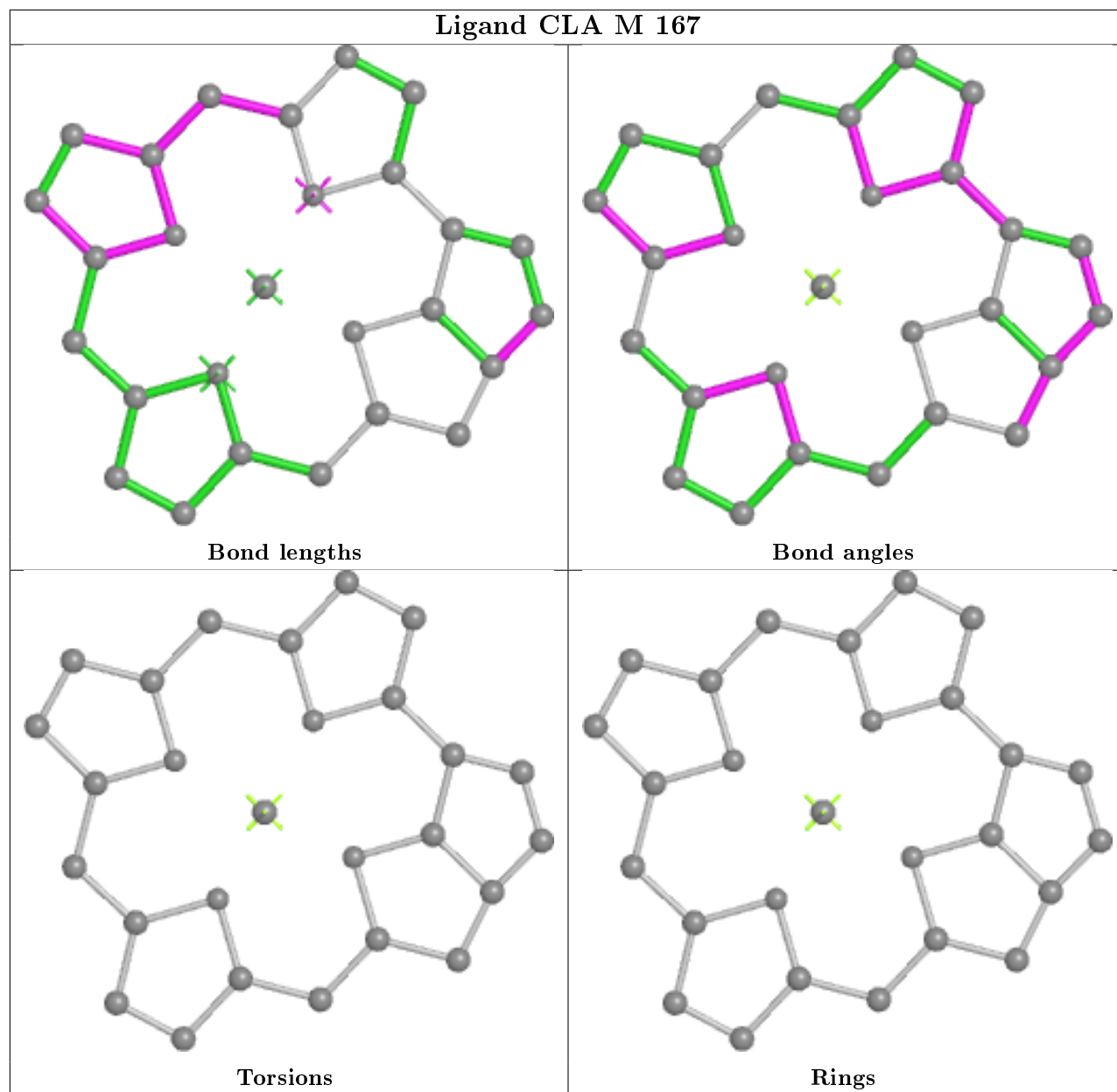
Ligand CLA D 162



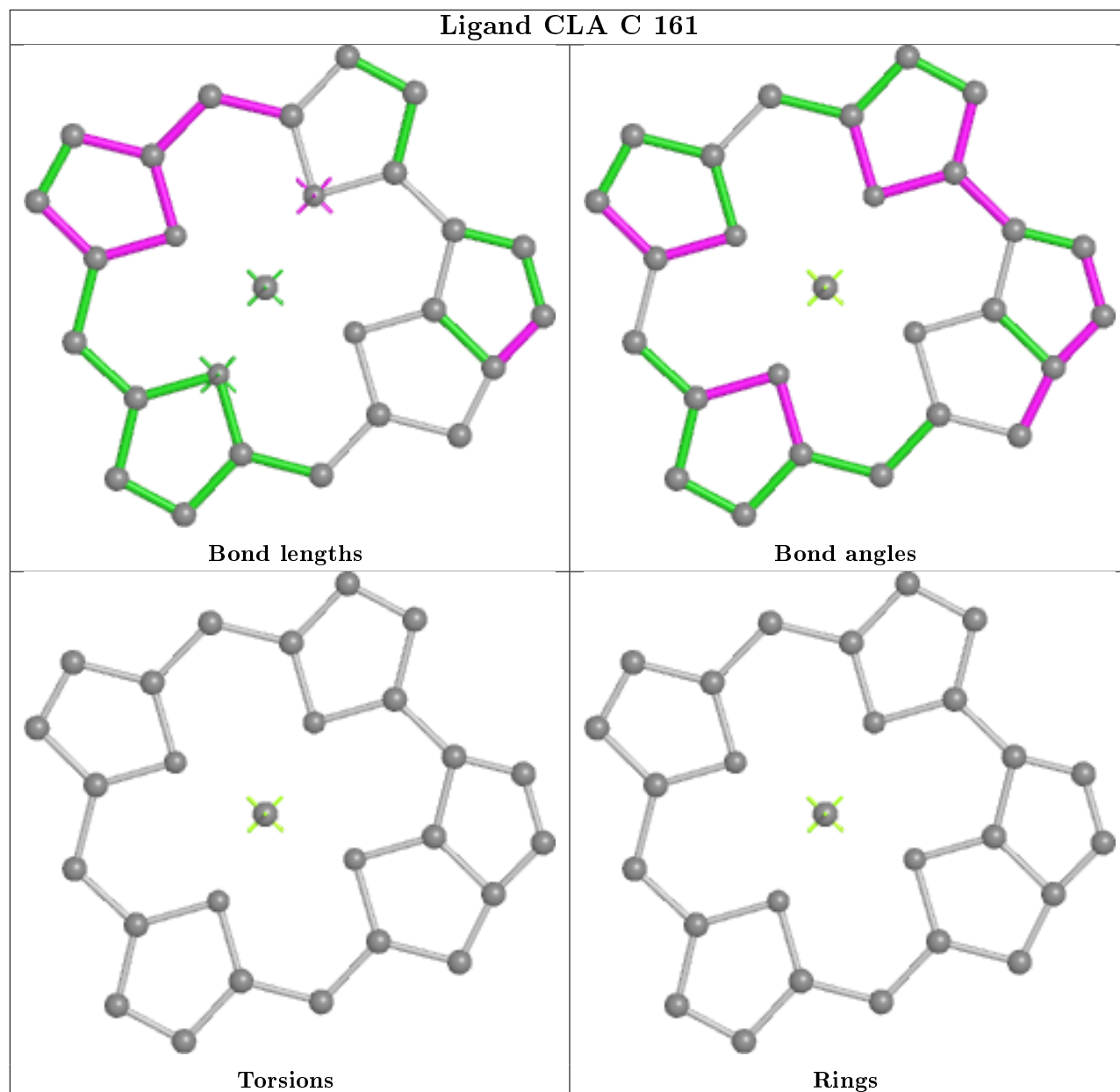
Ligand CLA L 157

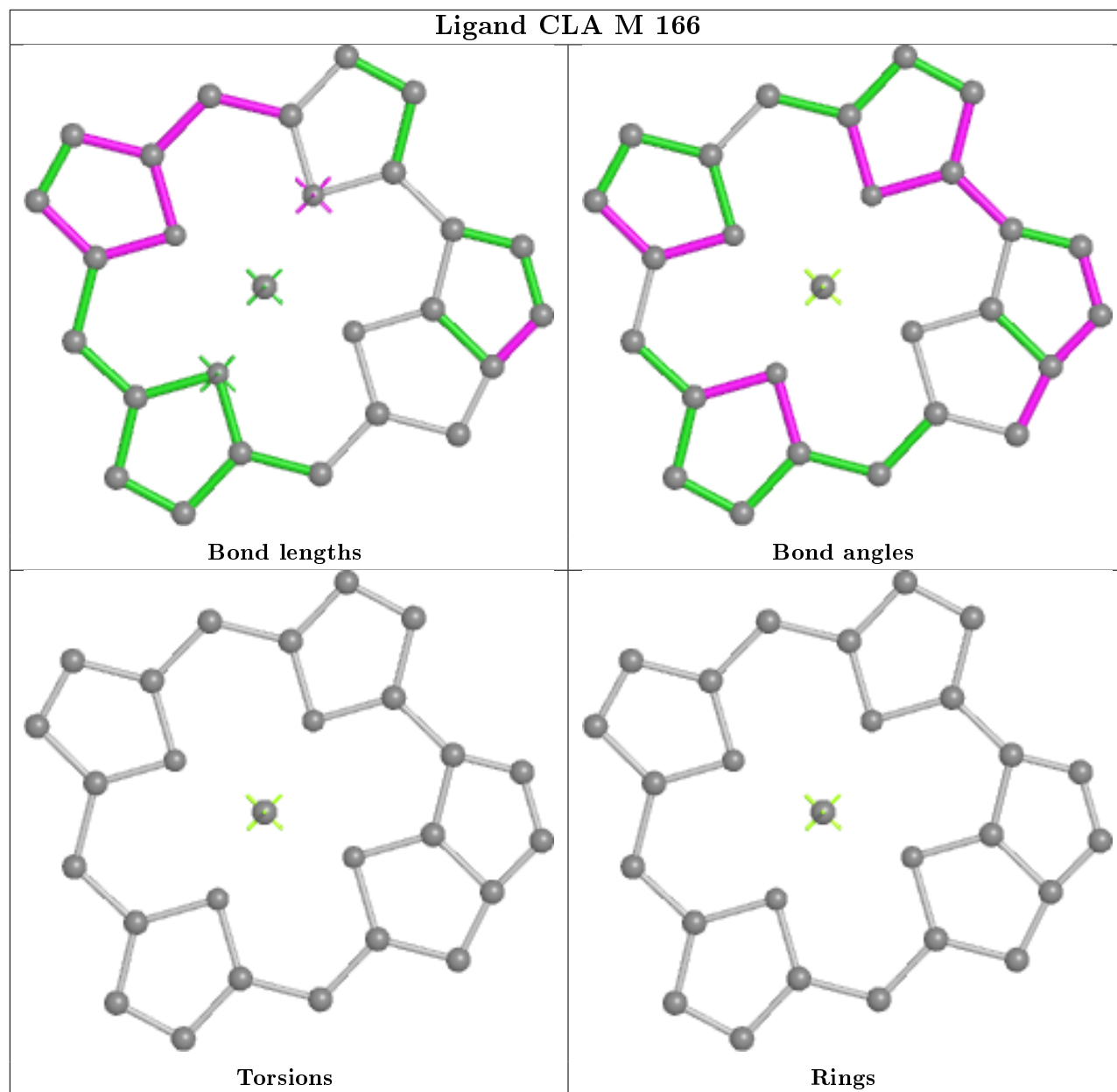




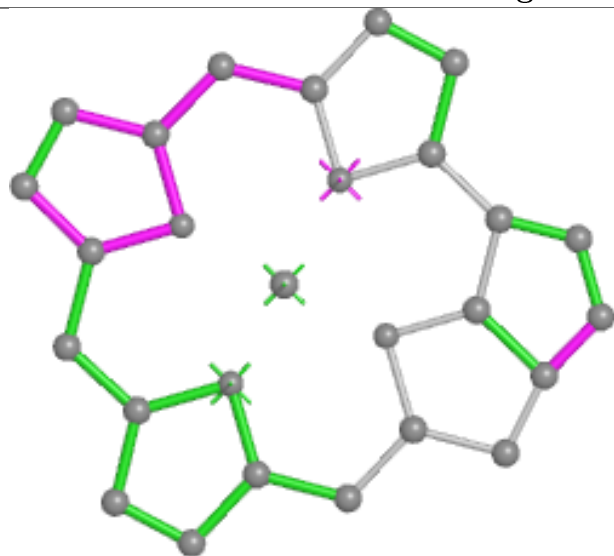


Ligand CLA C 161

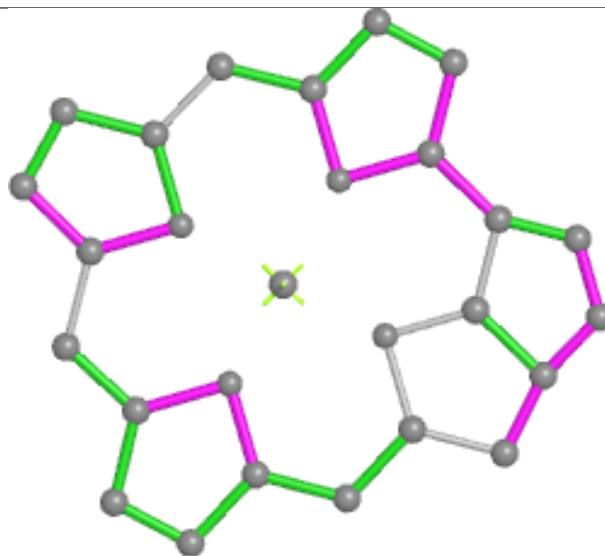




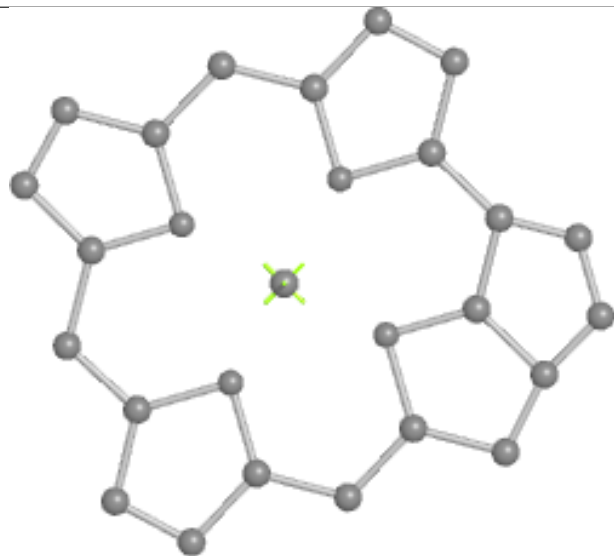
Ligand CLA L 164



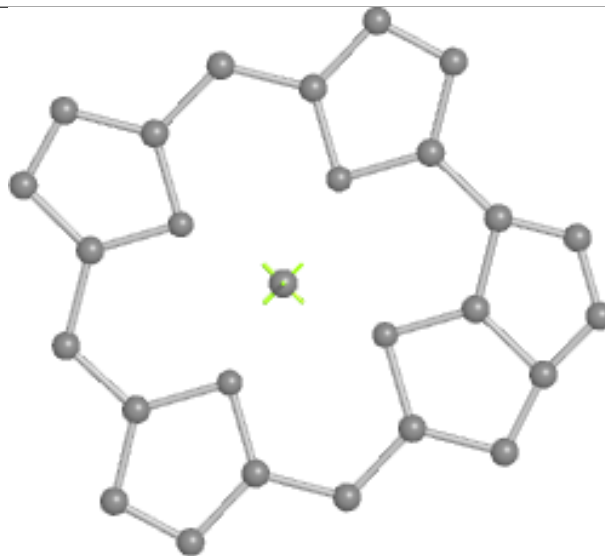
Bond lengths



Bond angles

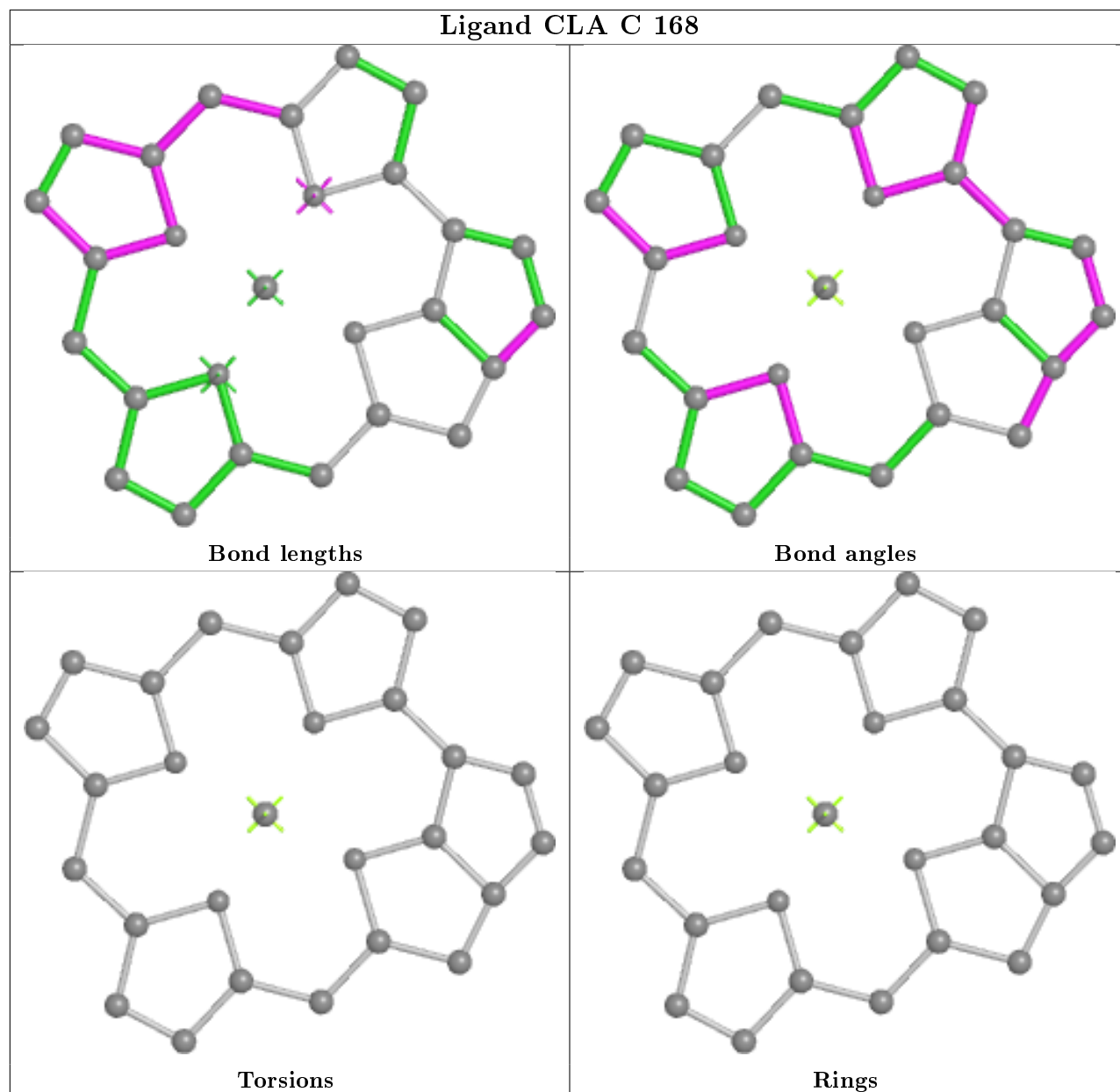


Torsions

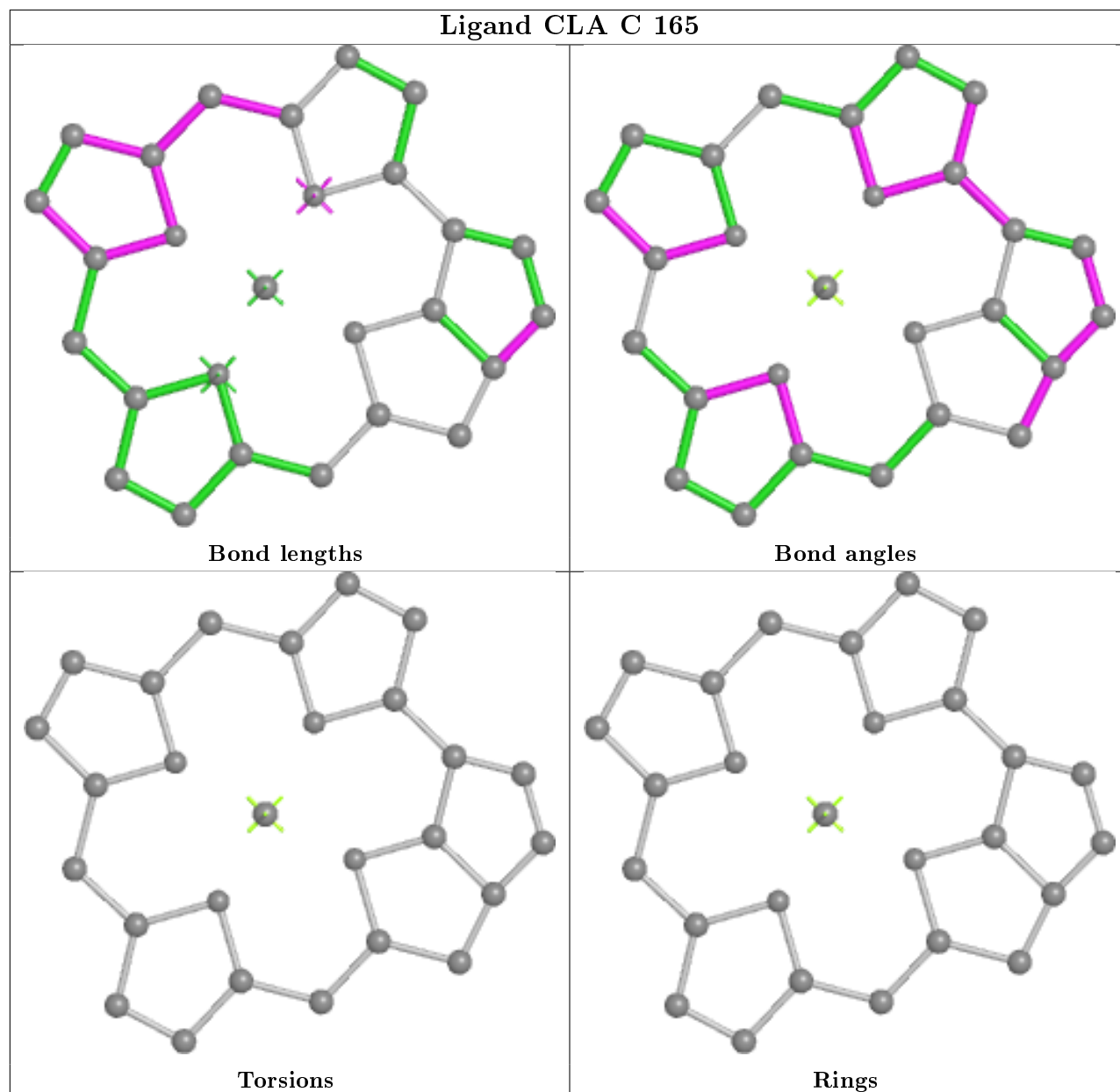


Rings

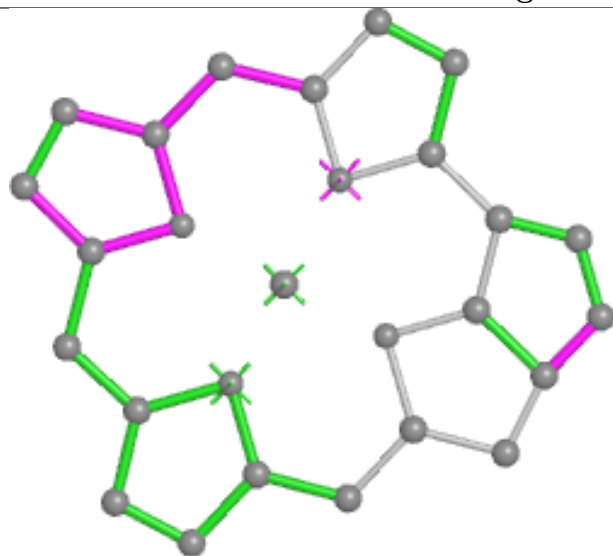
Ligand CLA C 168



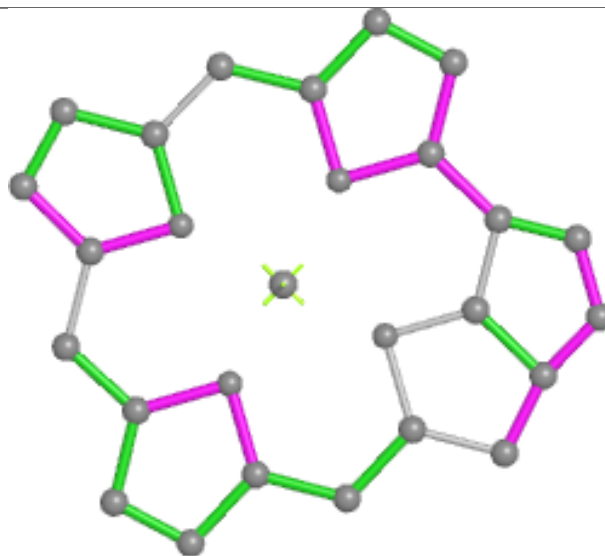
Ligand CLA C 165



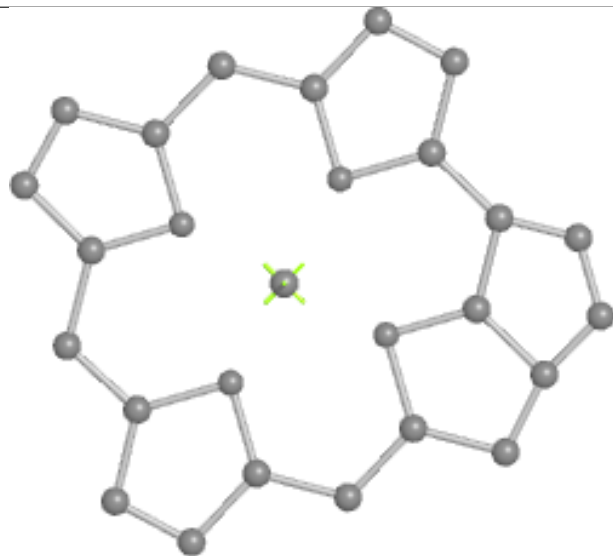
Ligand CLA L 161



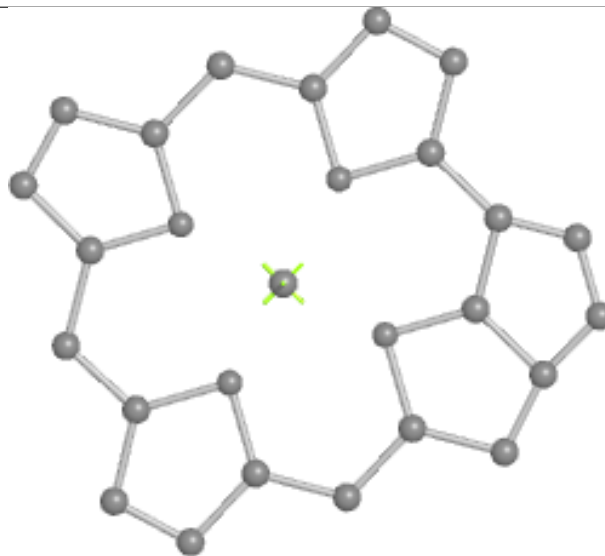
Bond lengths



Bond angles

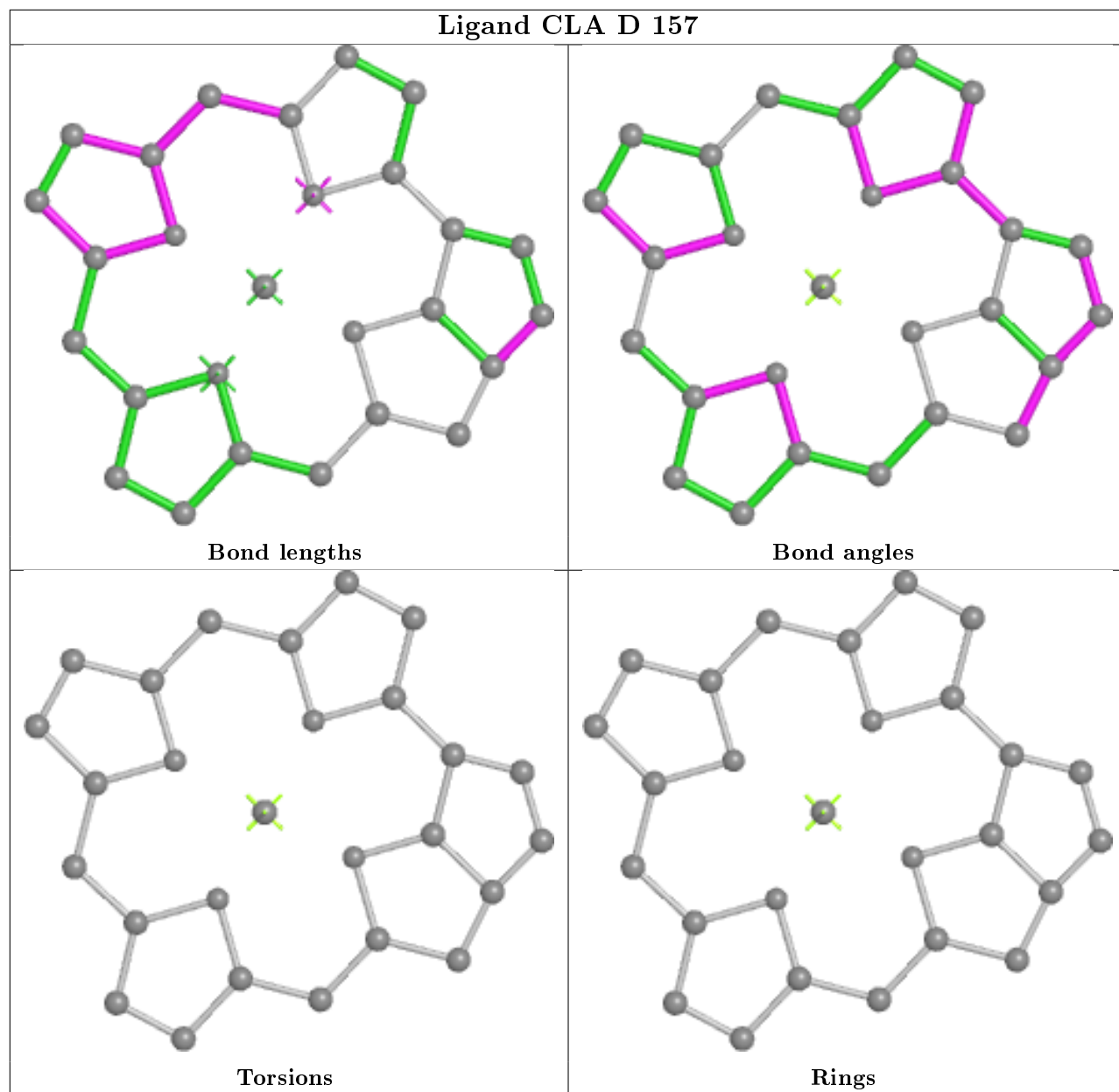


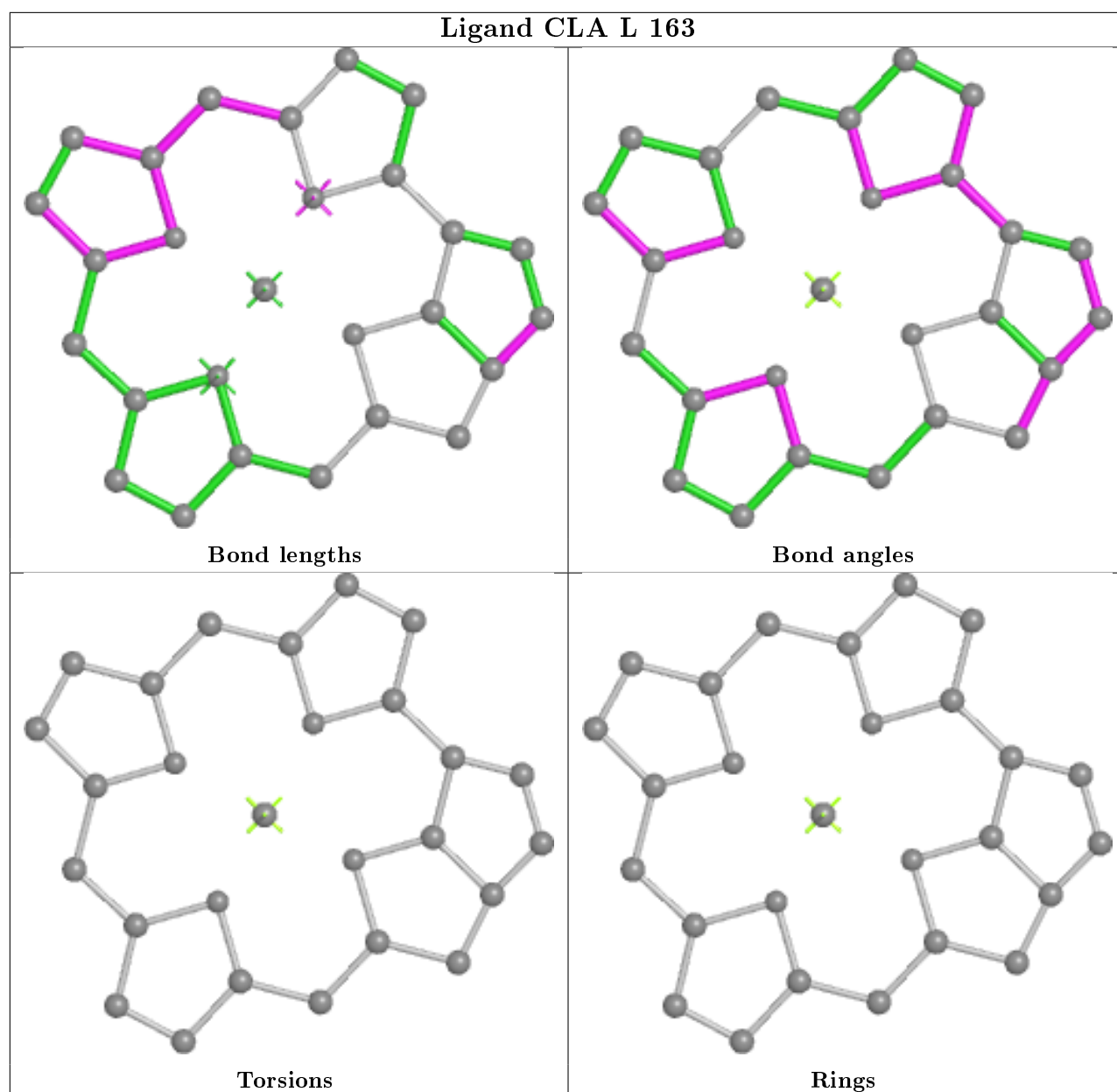
Torsions



Rings

Ligand CLA D 157





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.