



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2020 – 08:01 pm BST

PDB ID : 1FE1
Title : CRYSTAL STRUCTURE PHOTOSYSTEM II
Authors : Zouni, A.; Witt, H.-T.; Kern, J.; Fromme, P.; Krauss, N.; Saenger, W.; Orth, P.
Deposited on : 2000-07-20
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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)
Xtrriage (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

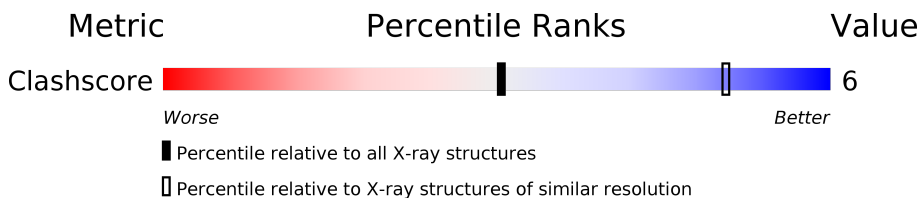
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

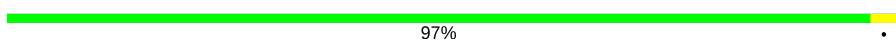


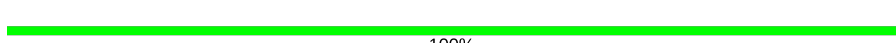
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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




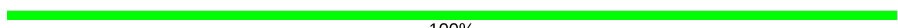




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 100%
4	M	155	 100%
5	E	40	 100%
5	N	40	 100%

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	175	X	-	-	-
12	CLA	A	176	X	-	-	-
12	CLA	A	177	X	-	-	-
12	CLA	A	179	X	-	-	-
12	CLA	B	177	X	-	-	-
12	CLA	B	179	X	-	-	-
12	CLA	C	157	X	-	-	-
12	CLA	C	158	X	-	-	-
12	CLA	C	159	X	-	-	-
12	CLA	C	160	X	-	-	-
12	CLA	C	161	X	-	-	-
12	CLA	C	162	X	-	-	-
12	CLA	C	163	X	-	-	-
12	CLA	C	164	X	-	-	-
12	CLA	C	165	X	-	-	-
12	CLA	C	166	X	-	-	-
12	CLA	C	167	X	-	-	-
12	CLA	C	168	X	-	-	-
12	CLA	D	156	X	-	-	-
12	CLA	D	157	X	-	-	-
12	CLA	D	158	X	-	-	-
12	CLA	D	159	X	-	-	-
12	CLA	D	160	X	-	-	-

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 4328 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBA).

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

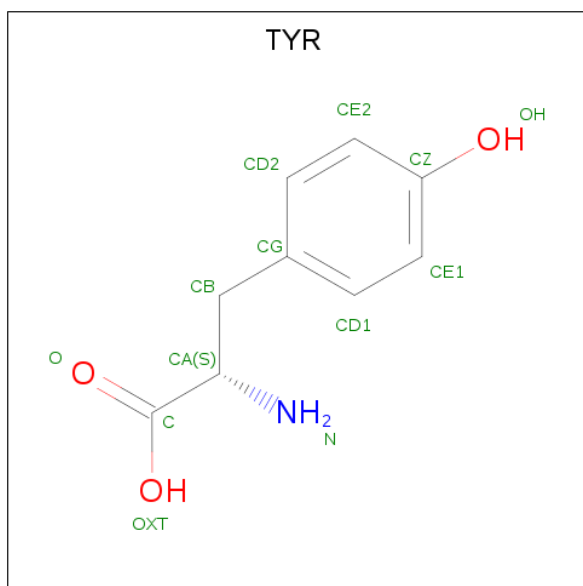
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	J	4	Total Mn 4 4	0	0

Continued on next page...

Continued from previous page...

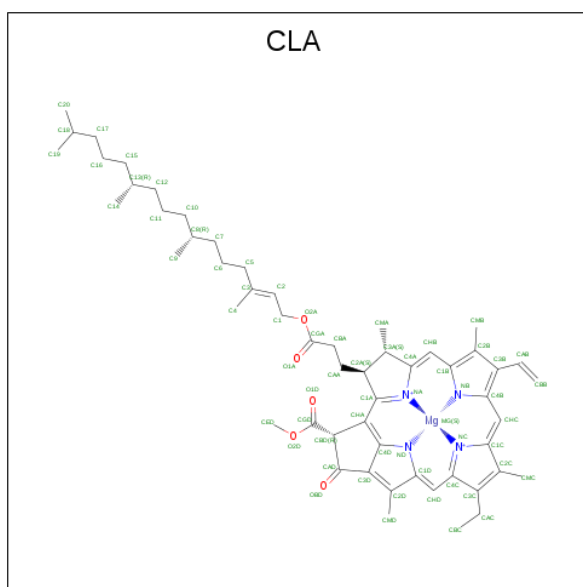
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	Mn	0	0
			4	4		

- Molecule 11 is TYROSINE (three-letter code: TYR) (formula: C₉H₁₁NO₃).



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

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

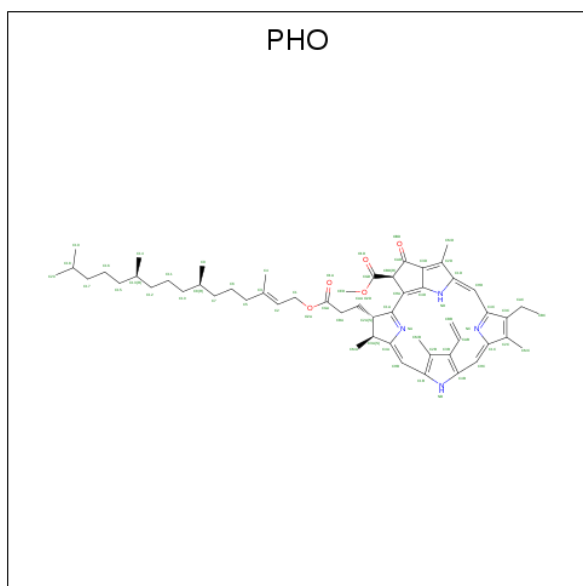
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	J	1	Total 25	C 20	Mg 1	N 4	0	0
12	K	1	Total 25	C 20	Mg 1	N 4	0	0
12	K	1	Total 25	C 20	Mg 1	N 4	0	0
12	L	1	Total 25	C 20	Mg 1	N 4	0	0
12	L	1	Total 25	C 20	Mg 1	N 4	0	0
12	L	1	Total 25	C 20	Mg 1	N 4	0	0
12	L	1	Total 25	C 20	Mg 1	N 4	0	0
12	L	1	Total 25	C 20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

Continued on next page...

Continued from previous page...

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

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



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

Continued on next page...

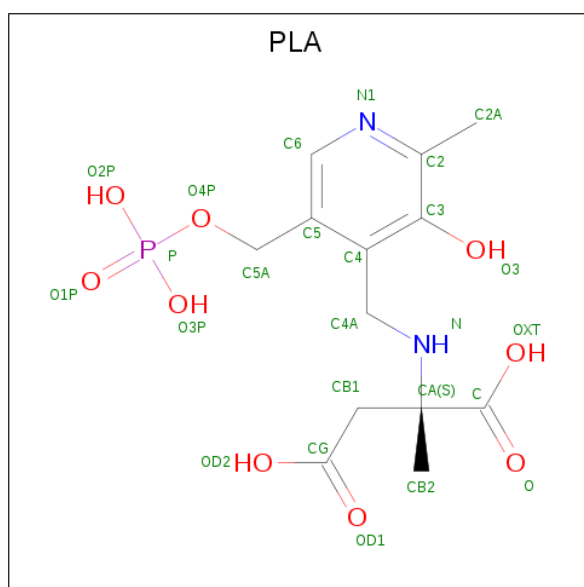
Continued from previous page...

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

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

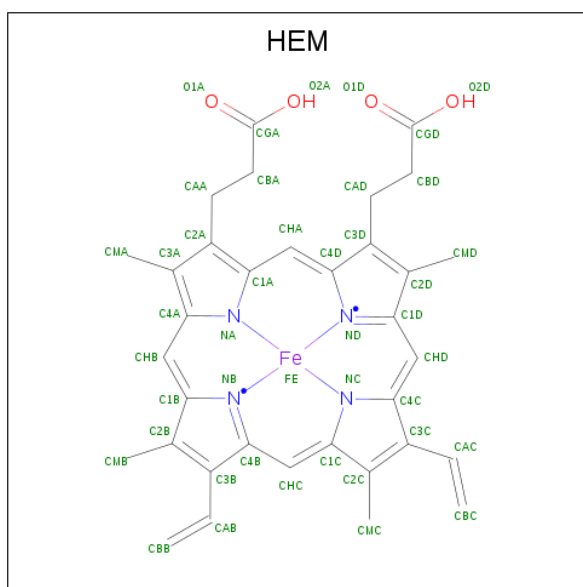
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	Fe		0	0
			1	1			
14	K	1	Total	Fe		0	0
			1	1			

- Molecule 15 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-2-METHYL-SUCCINIC ACID (three-letter code: PLA) (formula: C₁₃H₁₉N₂O₉P).



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

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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

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

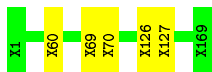
3 Residue-property plots [i](#)

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

Note EDS was not executed.

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

Chain A:  97%



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

Chain J:  97%



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

Chain B:  97%



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

Chain K:  97%



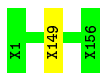
- Molecule 3: PROTEIN (PHOTOSYSTEM II: SUBUNIT PSBC)

Chain C:  99%



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

Chain L:  99%



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

Chain D:  100%

There are no outlier residues recorded for this chain.

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

Chain M:  100%

There are no outlier residues recorded for this chain.

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

Chain E:  100%

There are no outlier residues recorded for this chain.

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

Chain N:  100%

There are no outlier residues recorded for this chain.

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

Chain F:  100%

There are no outlier residues recorded for this chain.

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

Chain O:  100%

There are no outlier residues recorded for this chain.

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

Chain G:  100%

There are no outlier residues recorded for this chain.

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

Chain P:  100%

There are no outlier residues recorded for this chain.

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

Chain H:  100%

There are no outlier residues recorded for this chain.

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

Chain Q:  100%

There are no outlier residues recorded for this chain.

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

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PROTEIN (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	4328	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	169	0	0	4	0
1	J	169	0	0	4	0
2	B	174	0	0	4	0
2	K	174	0	0	4	0
3	C	156	0	0	2	0
3	L	156	0	0	2	0
4	D	155	0	0	0	0
4	M	155	0	0	0	0
5	E	40	0	0	0	0
5	N	40	0	0	0	0
6	F	30	0	0	0	0
6	O	30	0	0	0	0
7	G	312	0	0	0	0
7	P	312	0	0	0	0
8	H	115	0	0	0	0
8	Q	115	0	0	0	0

Continued on next page...

Continued from previous page...

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 26 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:UNK:CA	2:B:53:UNK:CA	1.88	1.49
1:A:60:UNK:CA	2:B:131:UNK:CA	1.95	1.45
1:J:60:UNK:CA	2:K:131:UNK:CA	1.95	1.44
3:L:149:UNK:CA	12:L:166:CLA:C2A	2.23	1.17

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	M	163	-	22,32,73	2.66	6 (27%)	26,54,113	2.95	8 (30%)
16	HEM	I	88	-	12,32,50	3.17	2 (16%)	23,54,82	3.69	11 (47%)
12	CLA	L	160	-	22,32,73	2.65	6 (27%)	26,54,113	2.99	8 (30%)
12	CLA	C	162	-	22,32,73	2.69	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	K	177	-	22,32,73	2.68	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	C	163	-	22,32,73	2.66	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	D	161	-	22,32,73	2.68	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	J	177	-	22,32,73	2.64	6 (27%)	26,54,113	3.01	8 (30%)
12	CLA	D	160	-	22,32,73	2.65	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	D	165	-	22,32,73	2.66	6 (27%)	26,54,113	2.96	8 (30%)
13	PHO	A	178	-	18,28,69	1.15	0	7,40,99	1.83	3 (42%)
12	CLA	D	164	-	22,32,73	2.65	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	B	177	-	22,32,73	2.67	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	J	175	-	22,32,73	2.66	6 (27%)	26,54,113	2.99	8 (30%)
12	CLA	M	161	-	22,32,73	2.66	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	C	165	-	22,32,73	2.67	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	C	168	-	22,32,73	2.66	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	C	157	-	22,32,73	2.69	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	C	161	-	22,32,73	2.65	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	C	159	-	22,32,73	2.66	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	G	313	-	22,32,73	2.65	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	L	165	-	22,32,73	2.66	6 (27%)	26,54,113	2.97	8 (30%)
13	PHO	B	178	-	18,28,69	1.15	0	7,40,99	1.83	3 (42%)
12	CLA	L	164	-	22,32,73	2.66	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	D	157	-	22,32,73	2.68	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	A	179	-	22,32,73	2.67	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	C	164	-	22,32,73	2.66	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	L	157	-	22,32,73	2.68	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	M	162	-	22,32,73	2.66	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	B	179	-	22,32,73	2.67	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	P	313	-	22,32,73	2.66	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	L	162	-	22,32,73	2.69	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	M	166	-	22,32,73	2.69	6 (27%)	26,54,113	2.97	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	M	159	-	22,32,73	2.67	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	L	166	-	22,32,73	2.67	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	M	157	-	22,32,73	2.69	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	M	158	-	22,32,73	2.68	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	C	166	-	22,32,73	2.67	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	D	162	-	22,32,73	2.65	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	D	168	-	22,32,73	2.66	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	M	160	-	22,32,73	2.67	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	C	158	-	22,32,73	2.67	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	L	168	-	22,32,73	2.64	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	M	164	-	22,32,73	2.66	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	L	163	-	22,32,73	2.67	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	M	165	-	22,32,73	2.67	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	A	177	-	22,32,73	2.65	6 (27%)	26,54,113	3.00	8 (30%)
12	CLA	C	160	-	22,32,73	2.64	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	L	158	-	22,32,73	2.66	6 (27%)	26,54,113	2.98	8 (30%)
13	PHO	K	178	-	18,28,69	1.15	0	7,40,99	1.81	3 (42%)
12	CLA	L	159	-	22,32,73	2.64	6 (27%)	26,54,113	2.99	8 (30%)
15	PLA	B	180	-	6,6,25	2.92	6 (100%)	6,6,37	0.89	0
16	HEM	R	88	-	12,32,50	3.17	2 (16%)	23,54,82	3.69	11 (47%)
12	CLA	J	176	-	22,32,73	2.69	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	J	179	-	22,32,73	2.67	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	M	168	-	22,32,73	2.66	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	C	167	-	22,32,73	2.65	6 (27%)	26,54,113	2.95	8 (30%)
16	HEM	F	31	-	12,32,50	3.16	2 (16%)	23,54,82	3.66	11 (47%)
12	CLA	D	166	-	22,32,73	2.69	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	M	156	-	22,32,73	2.69	6 (27%)	26,54,113	2.96	8 (30%)
16	HEM	O	58	-	12,32,50	3.17	2 (16%)	23,54,82	3.65	11 (47%)
12	CLA	L	161	-	22,32,73	2.66	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	L	167	-	22,32,73	2.65	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	A	176	-	22,32,73	2.69	6 (27%)	26,54,113	2.98	8 (30%)
12	CLA	K	179	-	22,32,73	2.67	6 (27%)	26,54,113	2.97	8 (30%)
12	CLA	A	175	-	22,32,73	2.64	6 (27%)	26,54,113	2.99	8 (30%)
12	CLA	D	163	-	22,32,73	2.66	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	M	167	-	22,32,73	2.68	6 (27%)	26,54,113	2.97	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	D	167	-	22,32,73	2.68	6 (27%)	26,54,113	2.96	8 (30%)
12	CLA	D	159	-	22,32,73	2.66	6 (27%)	26,54,113	2.95	8 (30%)
12	CLA	D	158	-	22,32,73	2.68	6 (27%)	26,54,113	2.98	8 (30%)
13	PHO	J	178	-	18,28,69	1.15	0	7,40,99	1.82	3 (42%)
12	CLA	D	156	-	22,32,73	2.69	6 (27%)	26,54,113	2.95	8 (30%)
15	PLA	K	180	-	6,6,25	2.92	6 (100%)	6,6,37	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	D	157	-	3/3/7/25	-	-
12	CLA	A	179	-	3/3/7/25	-	-
12	CLA	C	164	-	3/3/7/25	-	-
12	CLA	L	157	-	3/3/7/25	-	-
12	CLA	M	162	-	3/3/7/25	-	-
12	CLA	B	179	-	3/3/7/25	-	-
12	CLA	L	162	-	3/3/7/25	-	-
12	CLA	M	166	-	3/3/7/25	-	-
12	CLA	M	159	-	3/3/7/25	-	-
12	CLA	L	166	-	3/3/7/25	-	-
12	CLA	M	157	-	3/3/7/25	-	-
12	CLA	M	158	-	3/3/7/25	-	-
12	CLA	C	166	-	3/3/7/25	-	-
12	CLA	D	162	-	3/3/7/25	-	-
12	CLA	D	168	-	3/3/7/25	-	-
13	PHO	B	178	-	-	0/8/34/103	0/4/5/6
12	CLA	M	160	-	3/3/7/25	-	-
12	CLA	C	158	-	3/3/7/25	-	-
12	CLA	L	168	-	3/3/7/25	-	-
12	CLA	M	164	-	3/3/7/25	-	-
12	CLA	L	163	-	3/3/7/25	-	-
12	CLA	M	165	-	3/3/7/25	-	-
12	CLA	A	177	-	3/3/7/25	-	-
12	CLA	C	160	-	3/3/7/25	-	-
12	CLA	L	158	-	3/3/7/25	-	-
13	PHO	K	178	-	-	0/8/34/103	0/4/5/6
12	CLA	L	159	-	3/3/7/25	-	-
15	PLA	B	180	-	-	-	0/1/1/1
12	CLA	J	176	-	3/3/7/25	-	-
12	CLA	J	179	-	3/3/7/25	-	-
12	CLA	M	168	-	3/3/7/25	-	-
12	CLA	C	167	-	3/3/7/25	-	-
13	PHO	A	178	-	-	0/8/34/103	0/4/5/6
12	CLA	D	166	-	3/3/7/25	-	-
12	CLA	M	156	-	3/3/7/25	-	-

Continued on next page...

Continued from previous page...

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

The worst 5 of 404 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	162	CLA	CHB-C4A	7.71	1.40	1.34
12	L	162	CLA	CHB-C4A	7.70	1.40	1.34
12	M	156	CLA	CHB-C4A	7.66	1.40	1.34
12	M	160	CLA	CHB-C4A	7.65	1.40	1.34
12	D	156	CLA	CHB-C4A	7.63	1.40	1.34

The worst 5 of 568 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	R	88	HEM	C3D-C4D-ND	10.20	116.33	108.27
16	I	88	HEM	C3D-C4D-ND	10.17	116.30	108.27
16	F	31	HEM	C3D-C4D-ND	10.07	116.23	108.27
16	O	58	HEM	C3D-C4D-ND	10.04	116.20	108.27
12	J	177	CLA	C2D-C3D-C4D	-8.84	98.68	106.30

5 of 192 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	L	160	CLA	NC
12	L	160	CLA	ND
12	L	160	CLA	NA
12	D	161	CLA	NC
12	D	161	CLA	ND

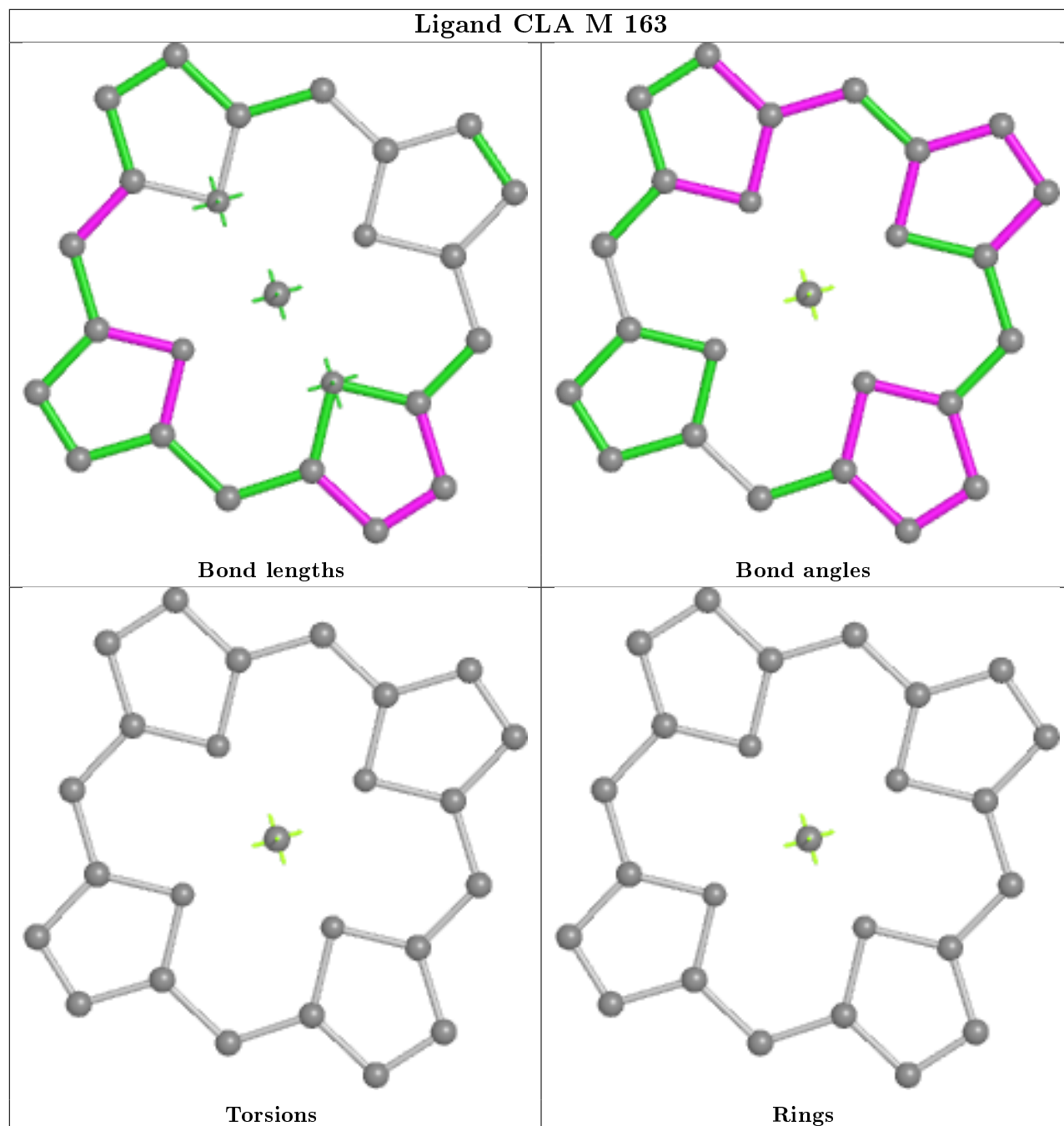
There are no torsion outliers.

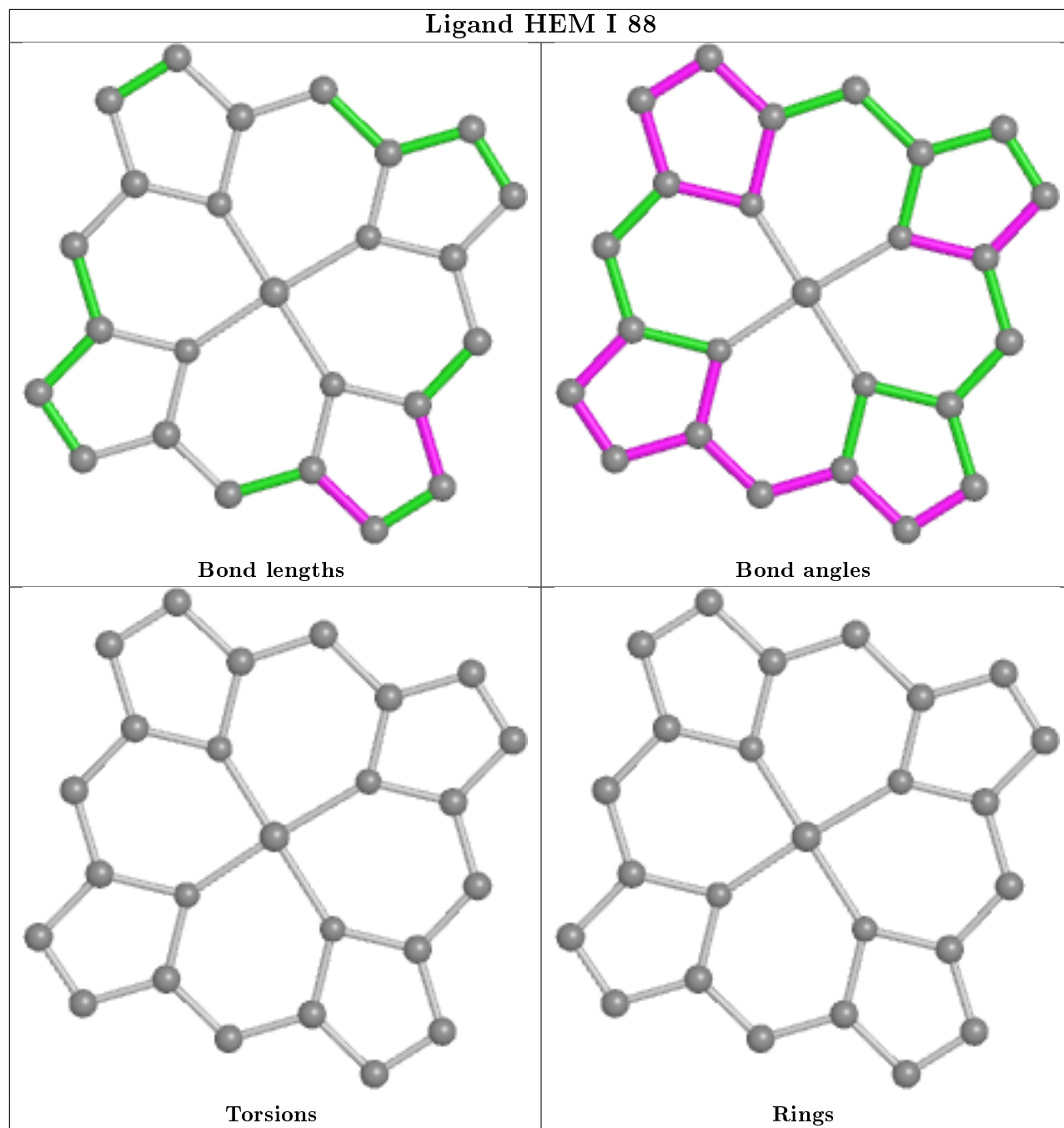
There are no ring outliers.

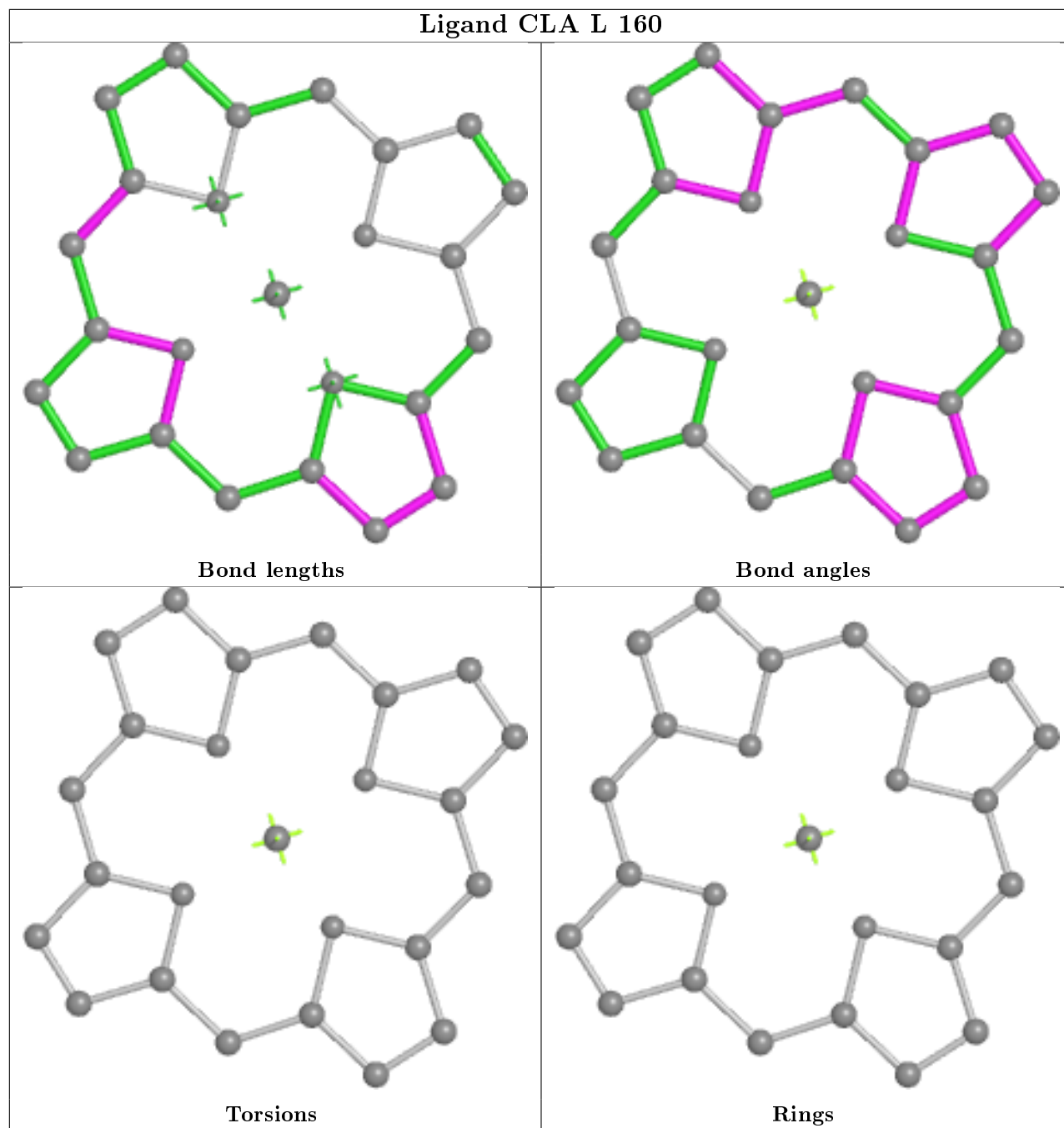
6 monomers are involved in 16 short contacts:

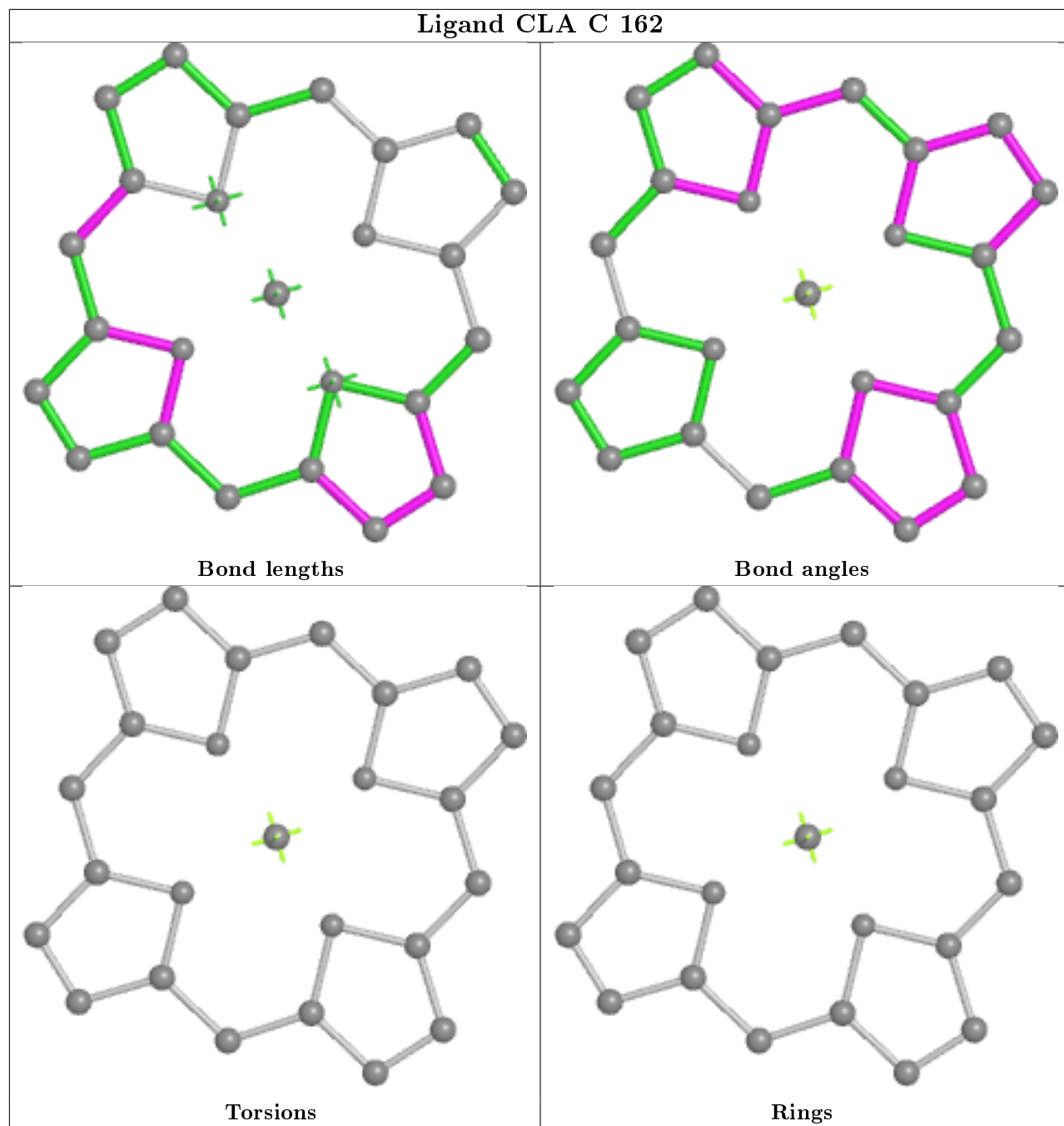
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	162	CLA	6	0
12	M	159	CLA	6	0
12	L	166	CLA	2	0
12	C	166	CLA	2	0
12	D	162	CLA	6	0
12	D	159	CLA	6	0

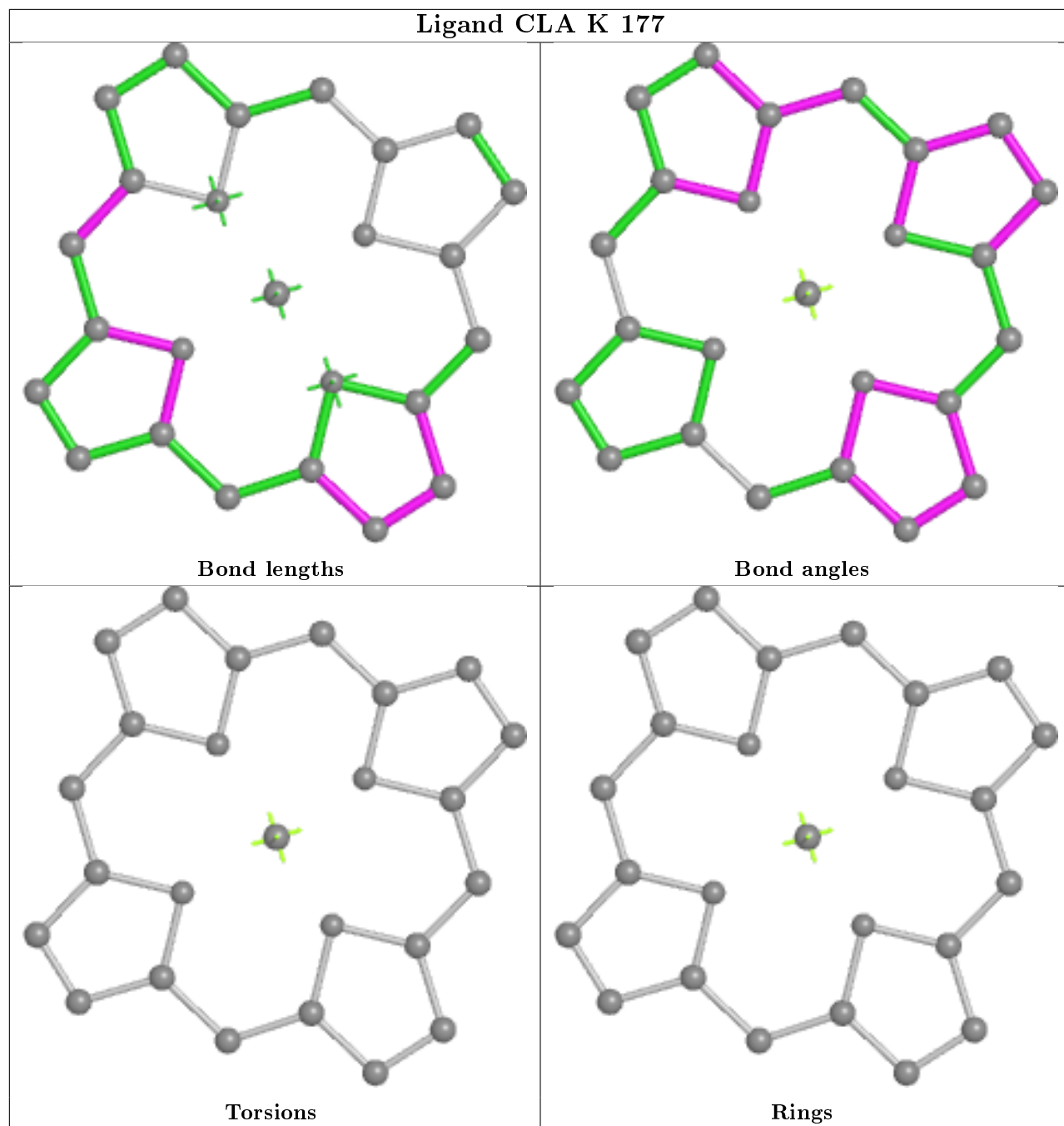
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

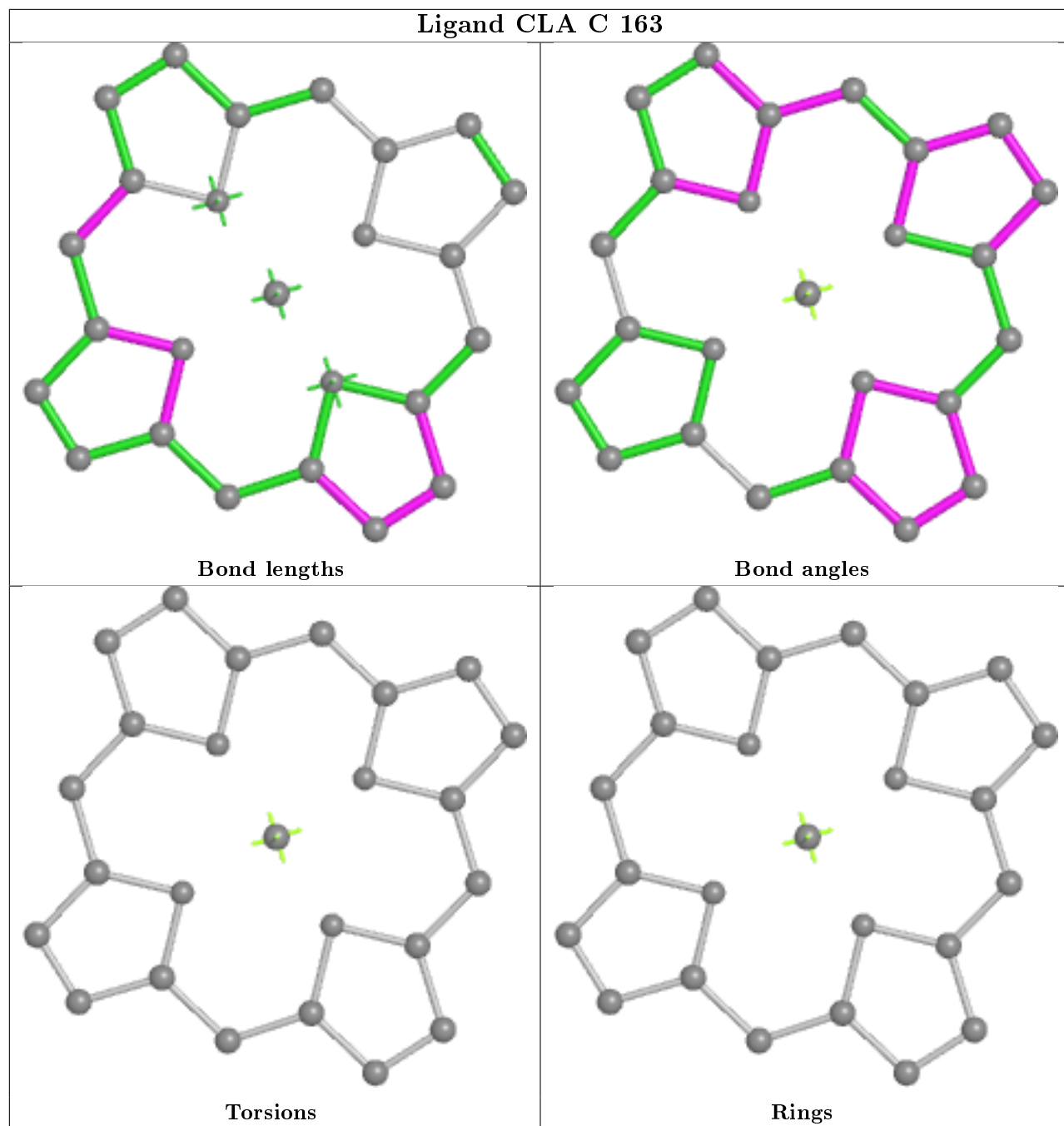


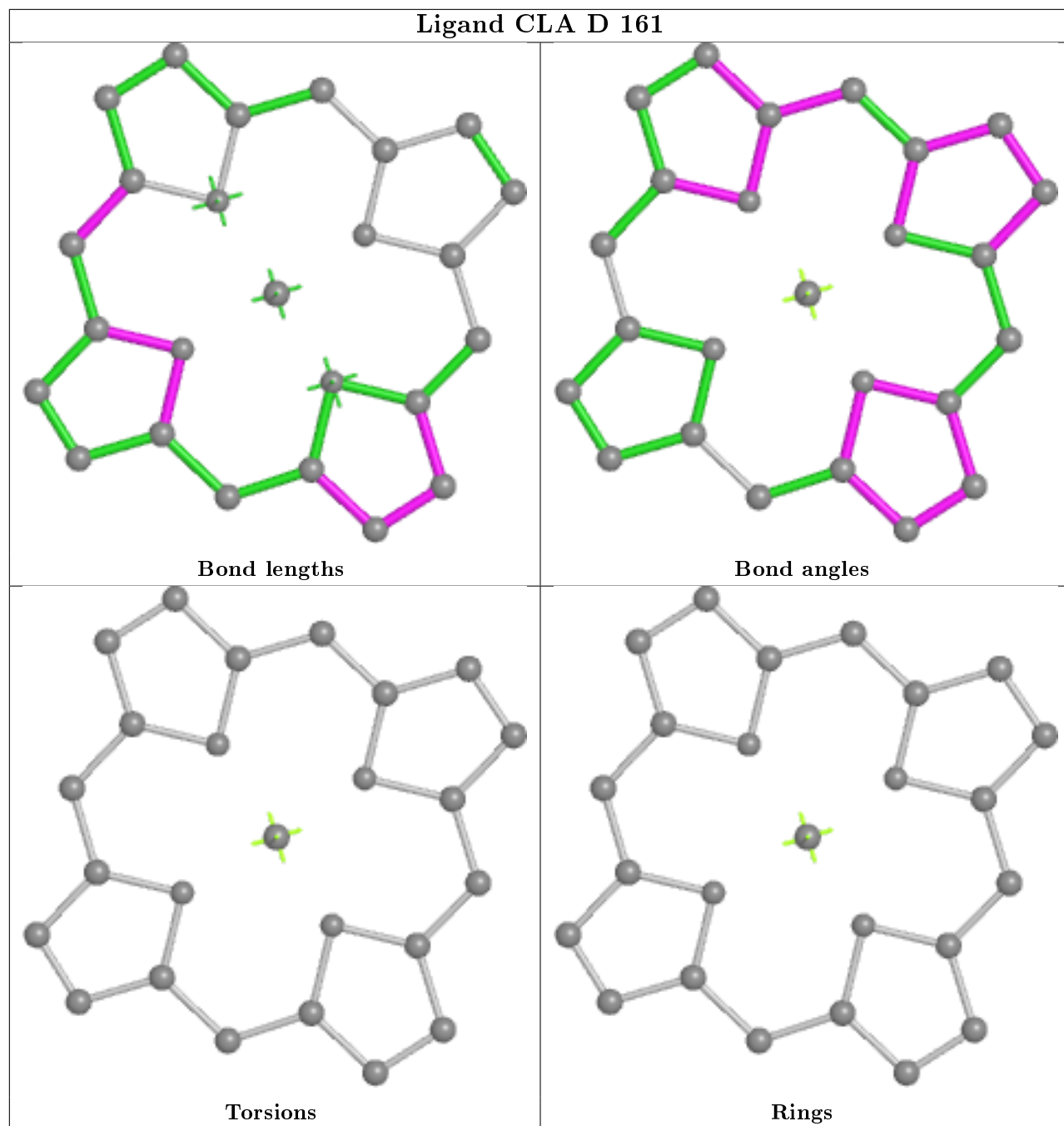


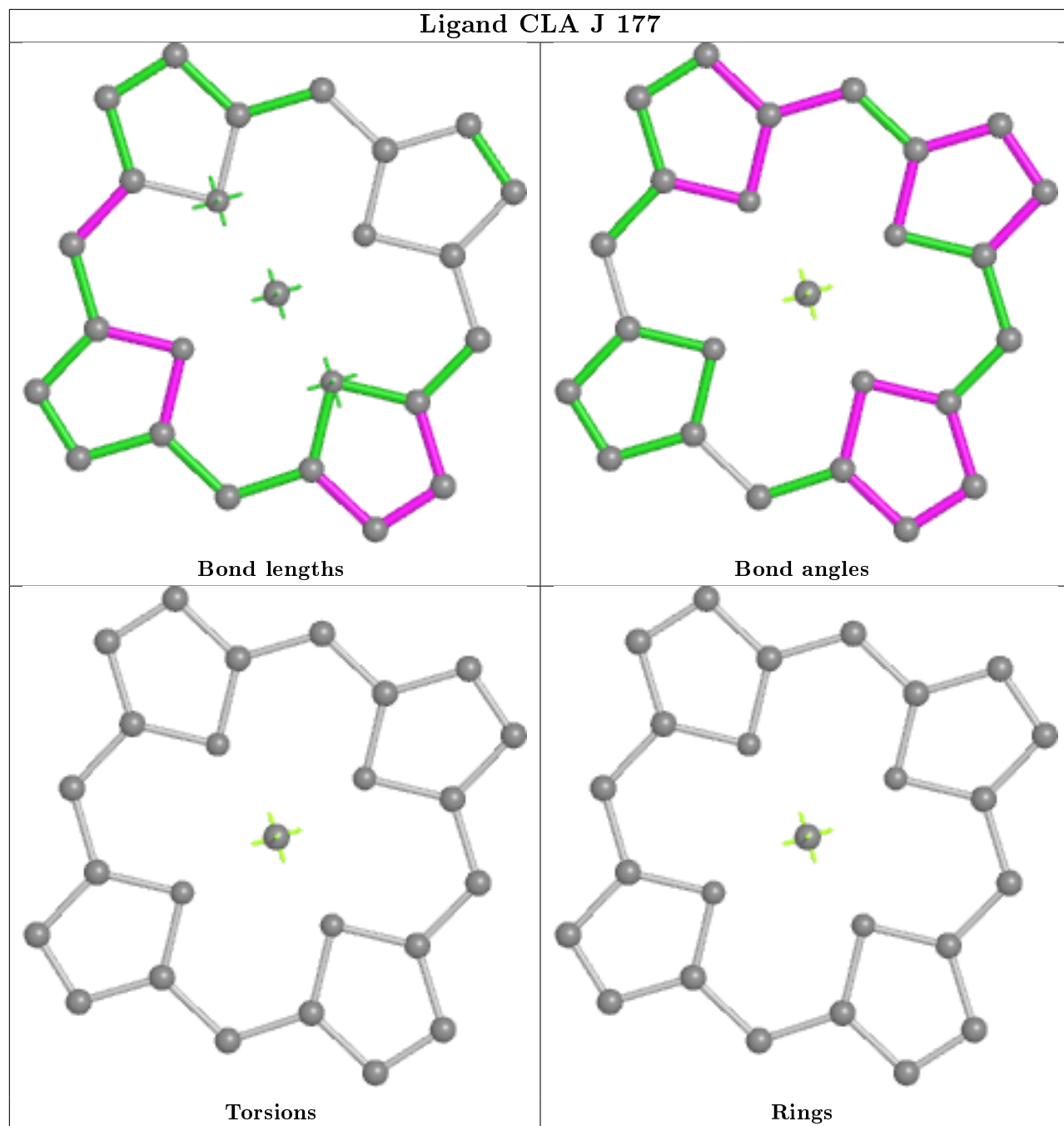


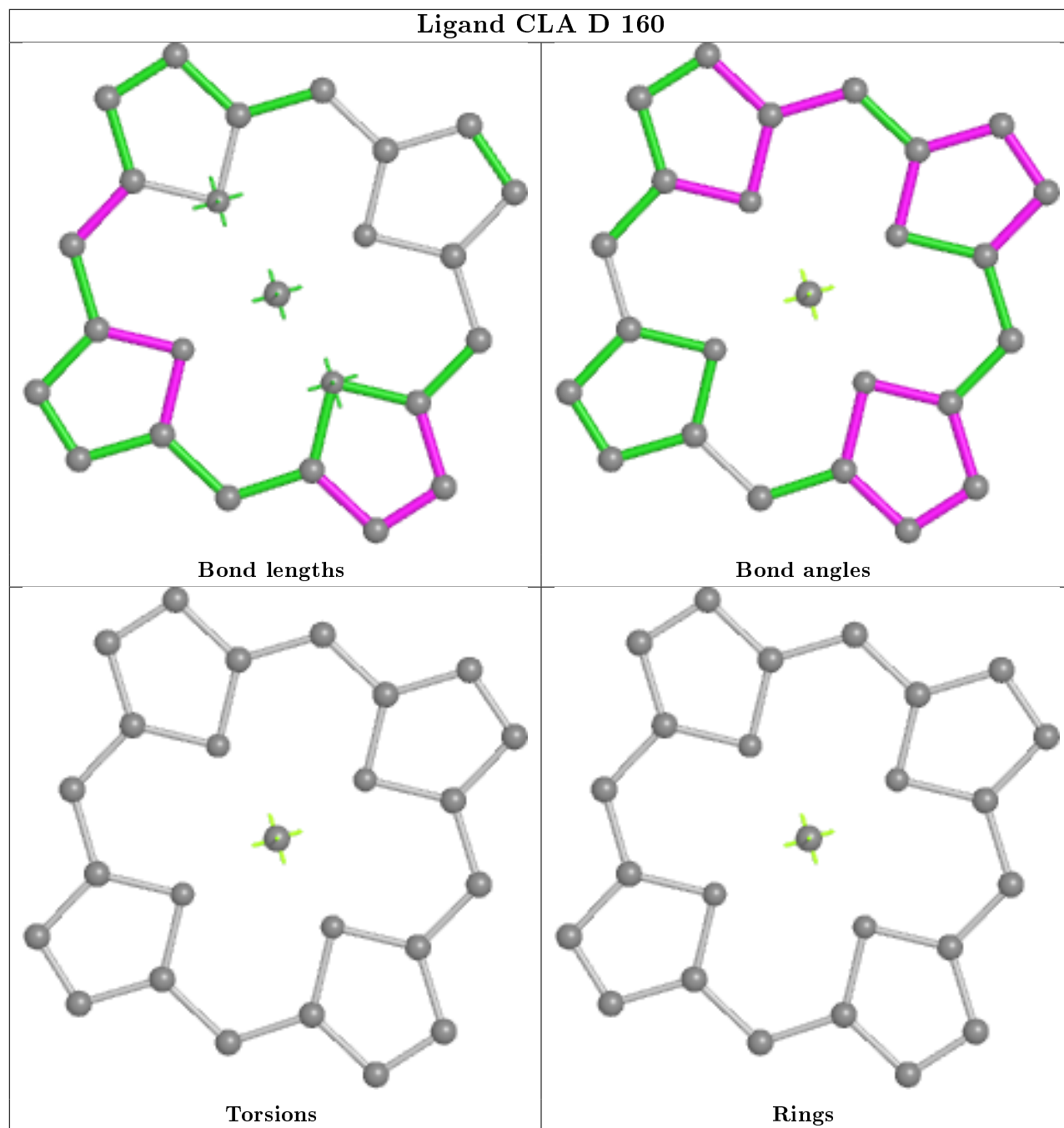


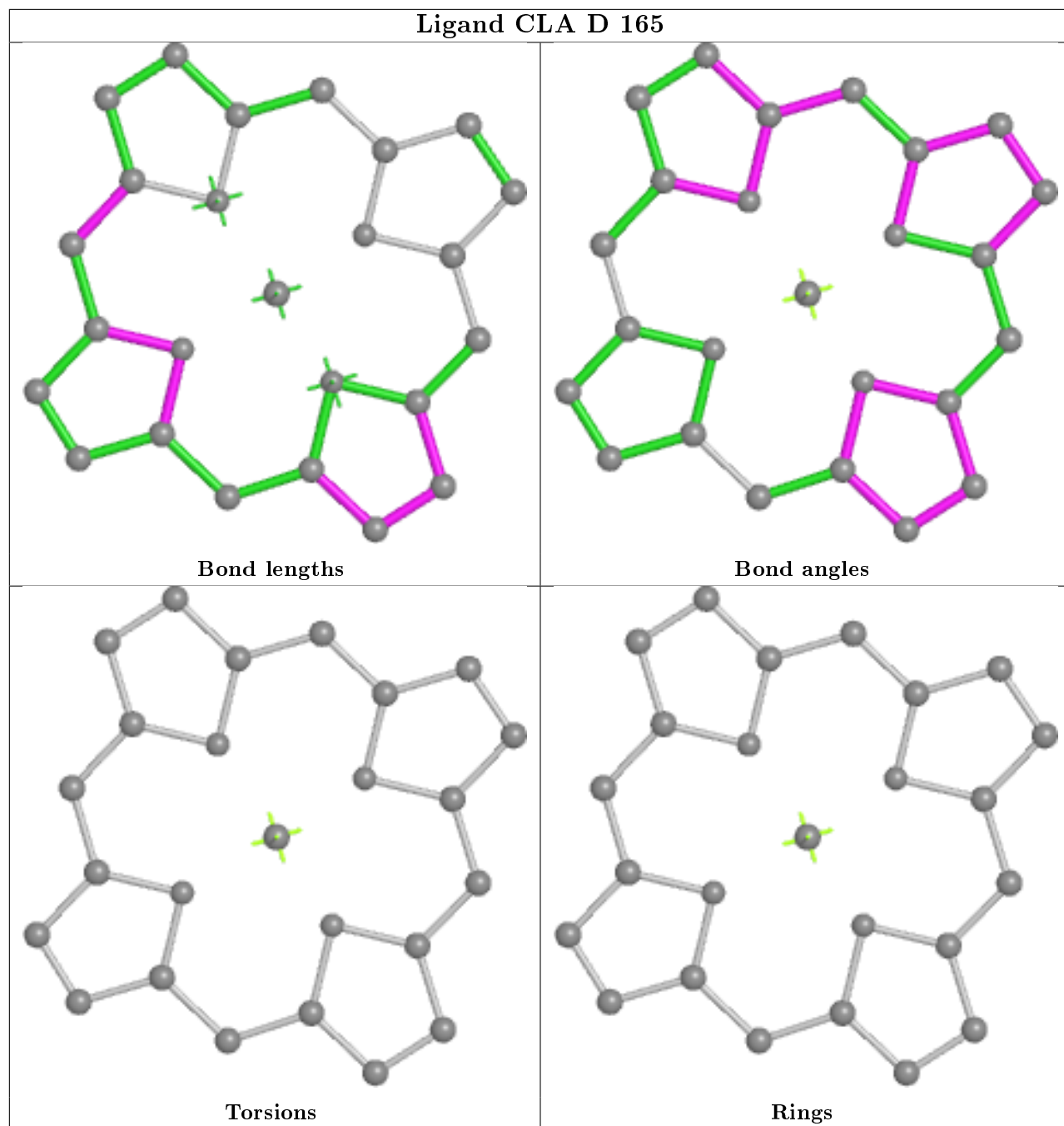


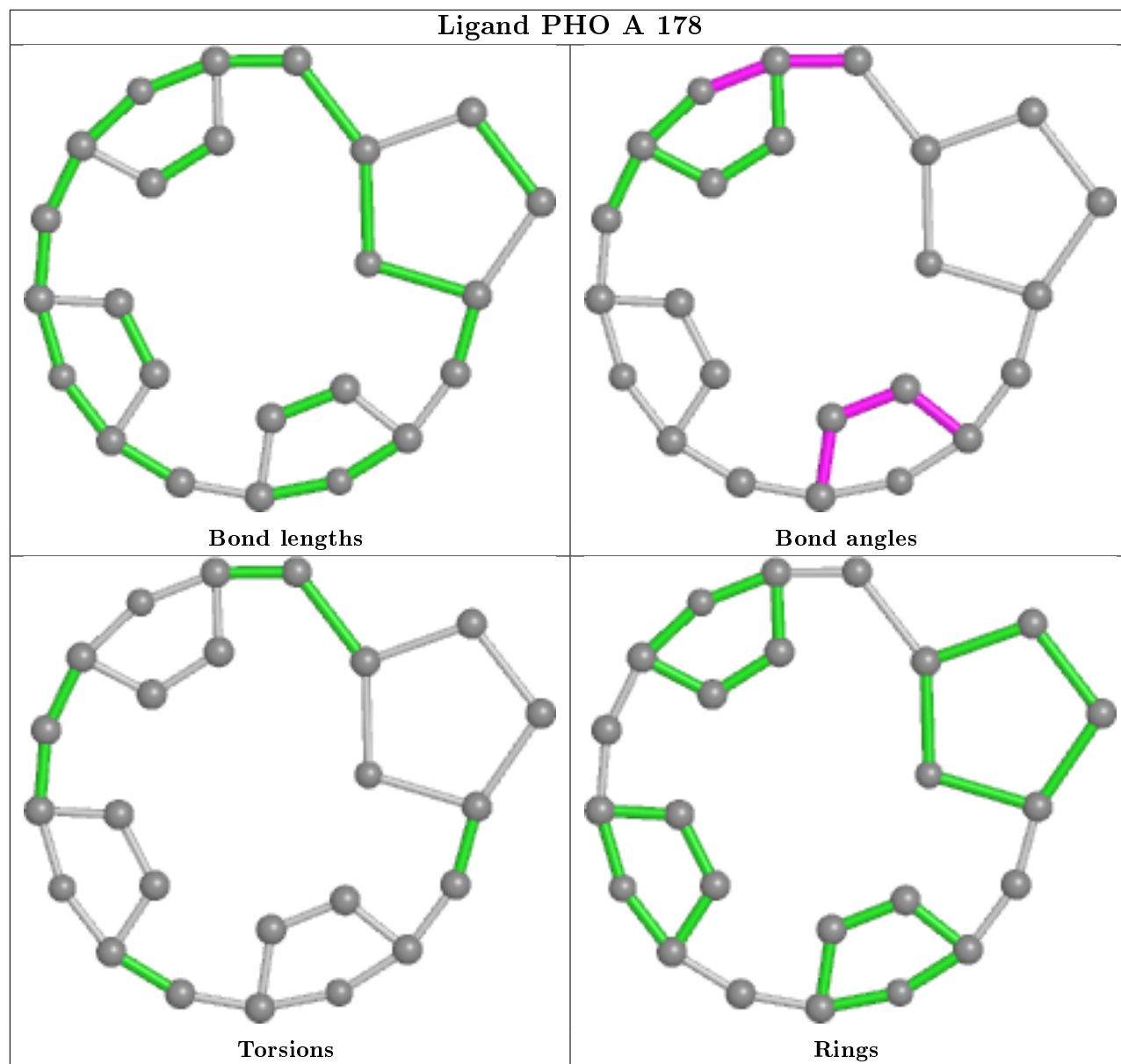


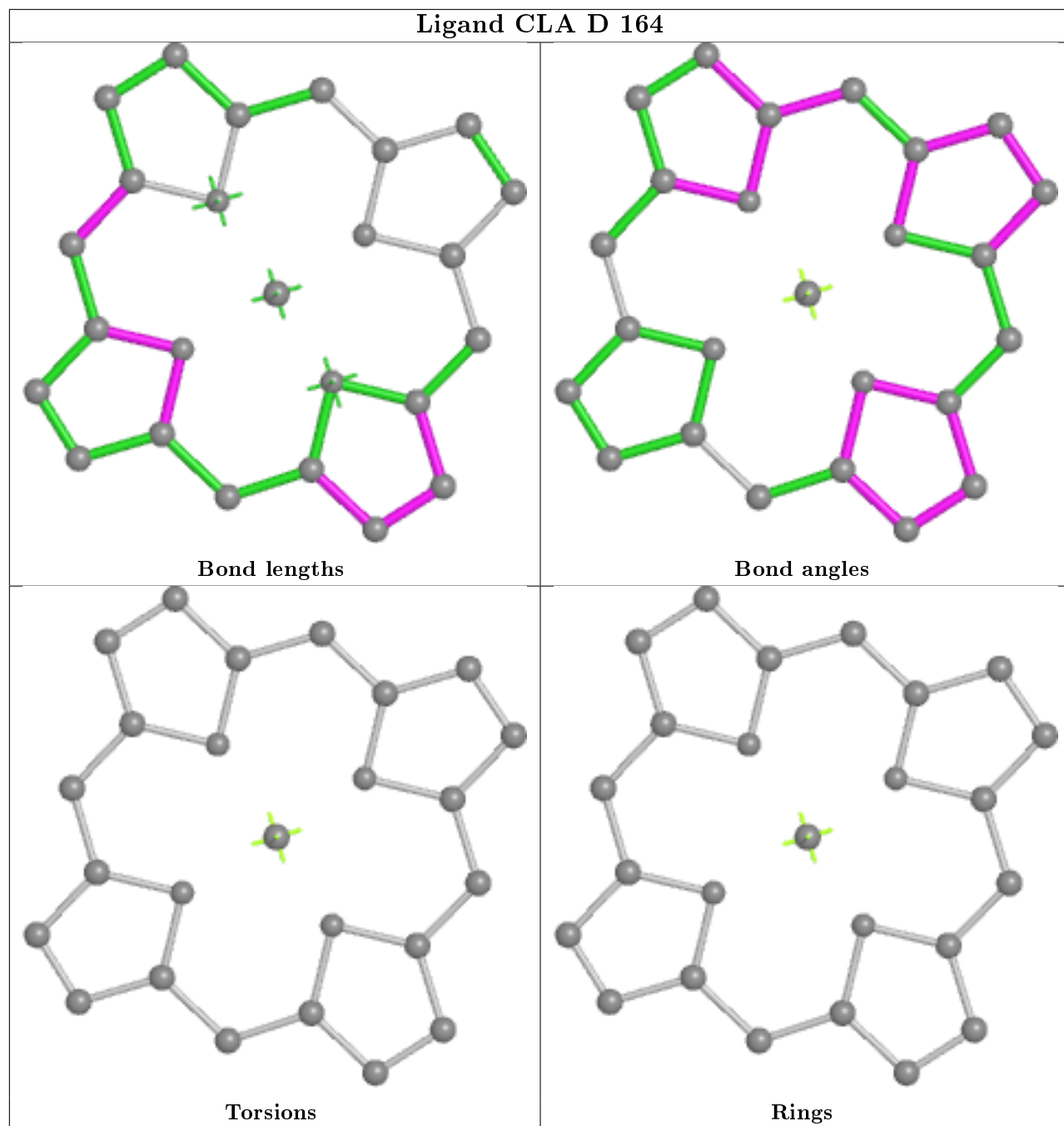


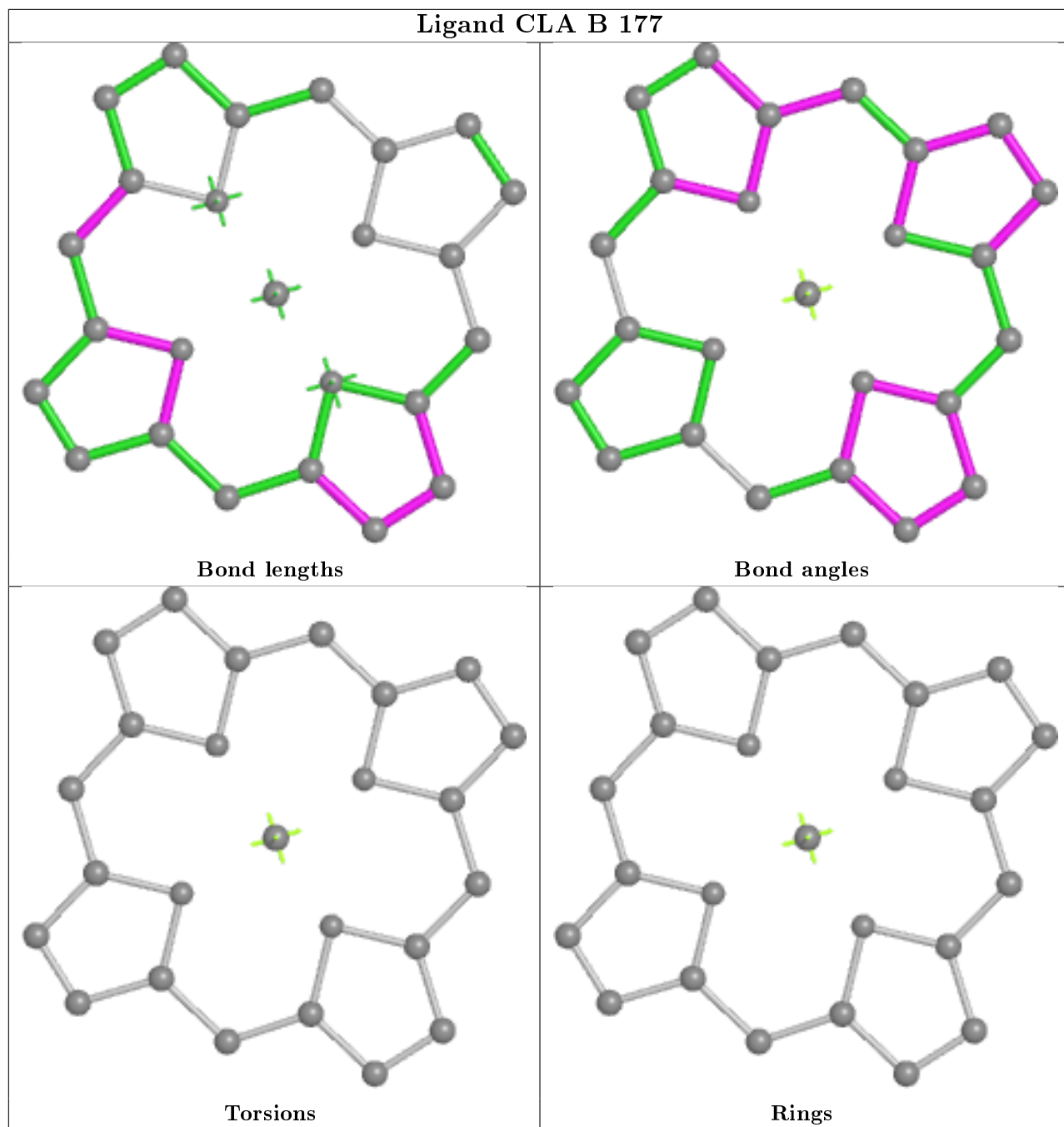


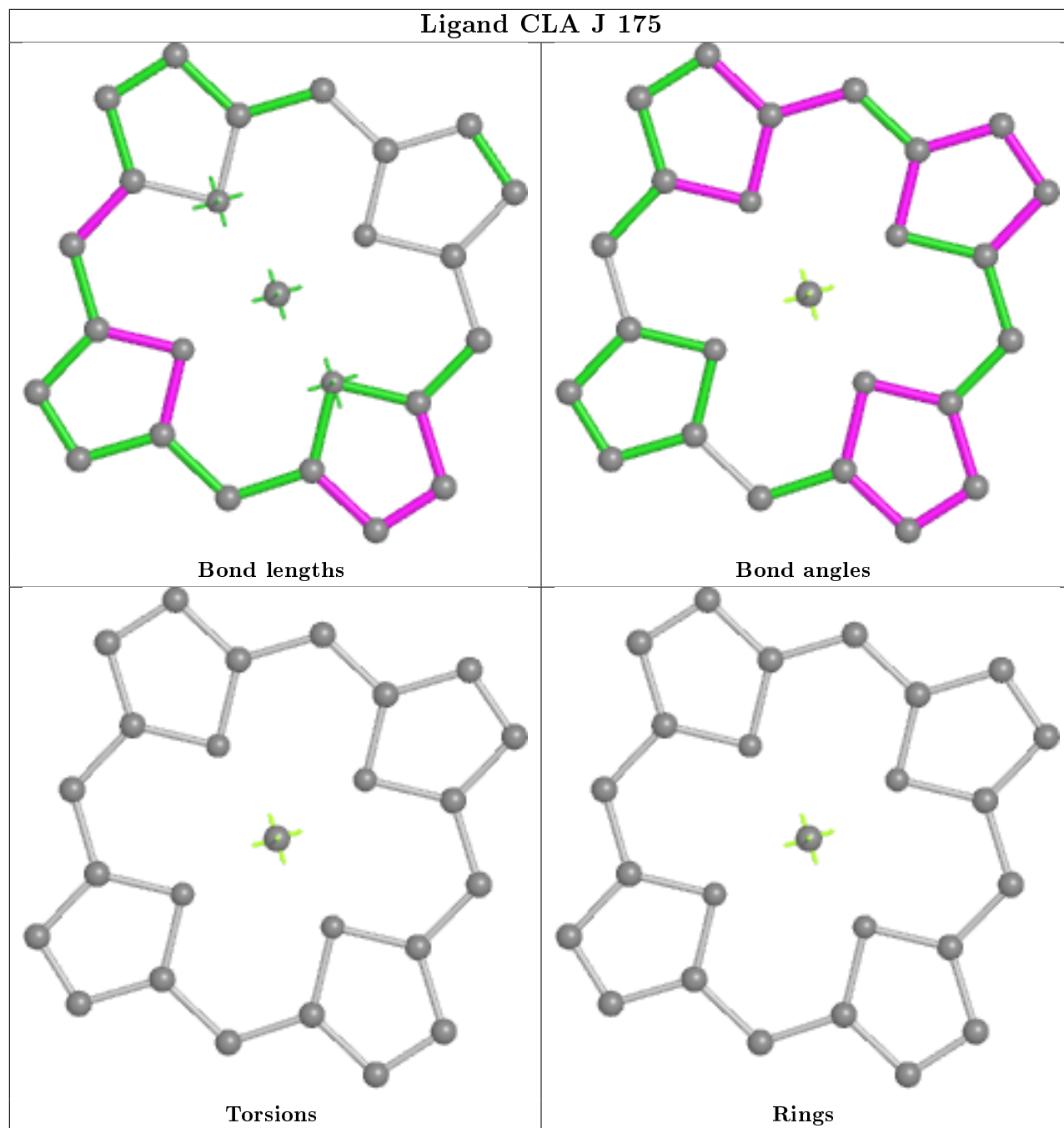


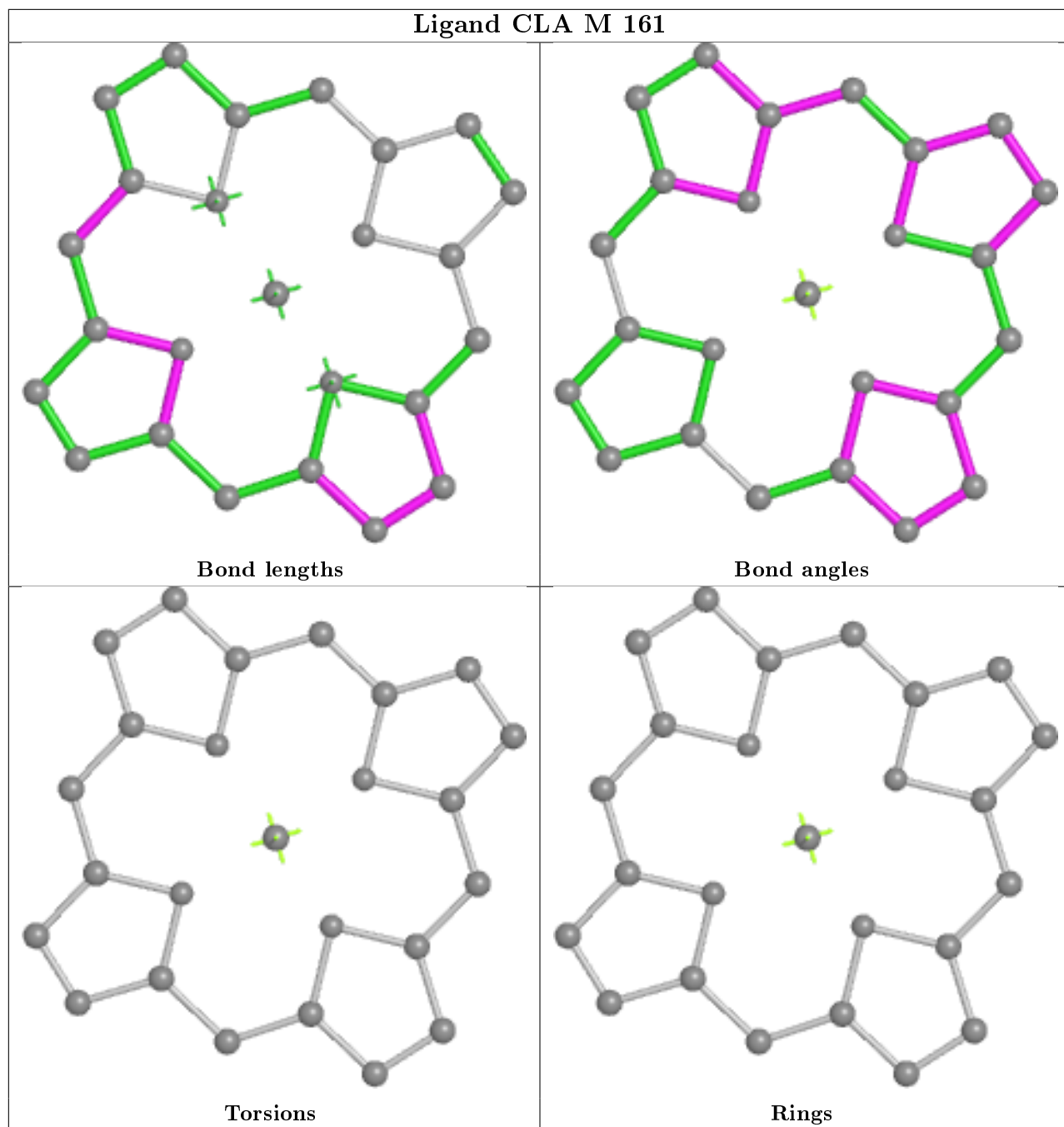


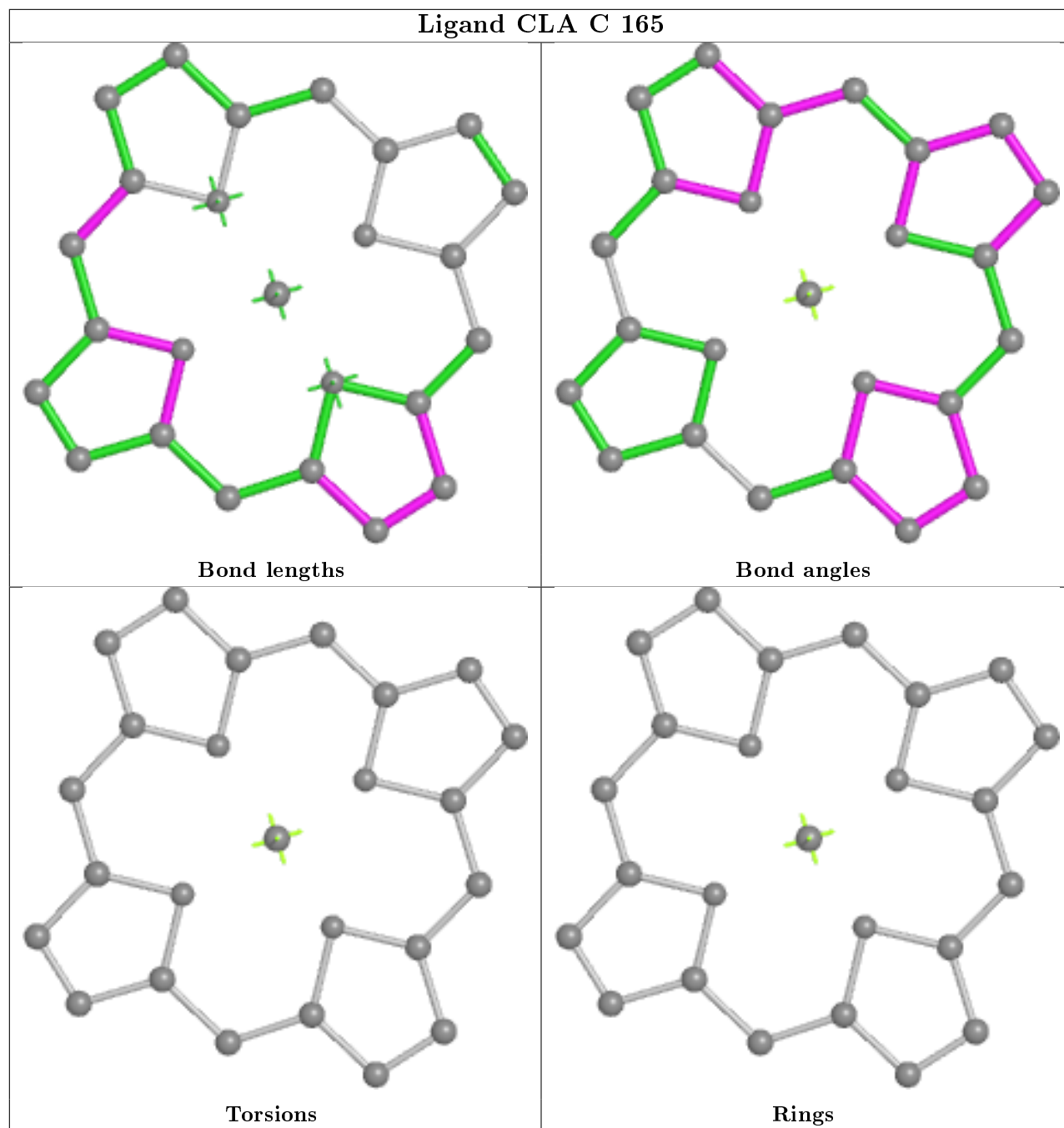


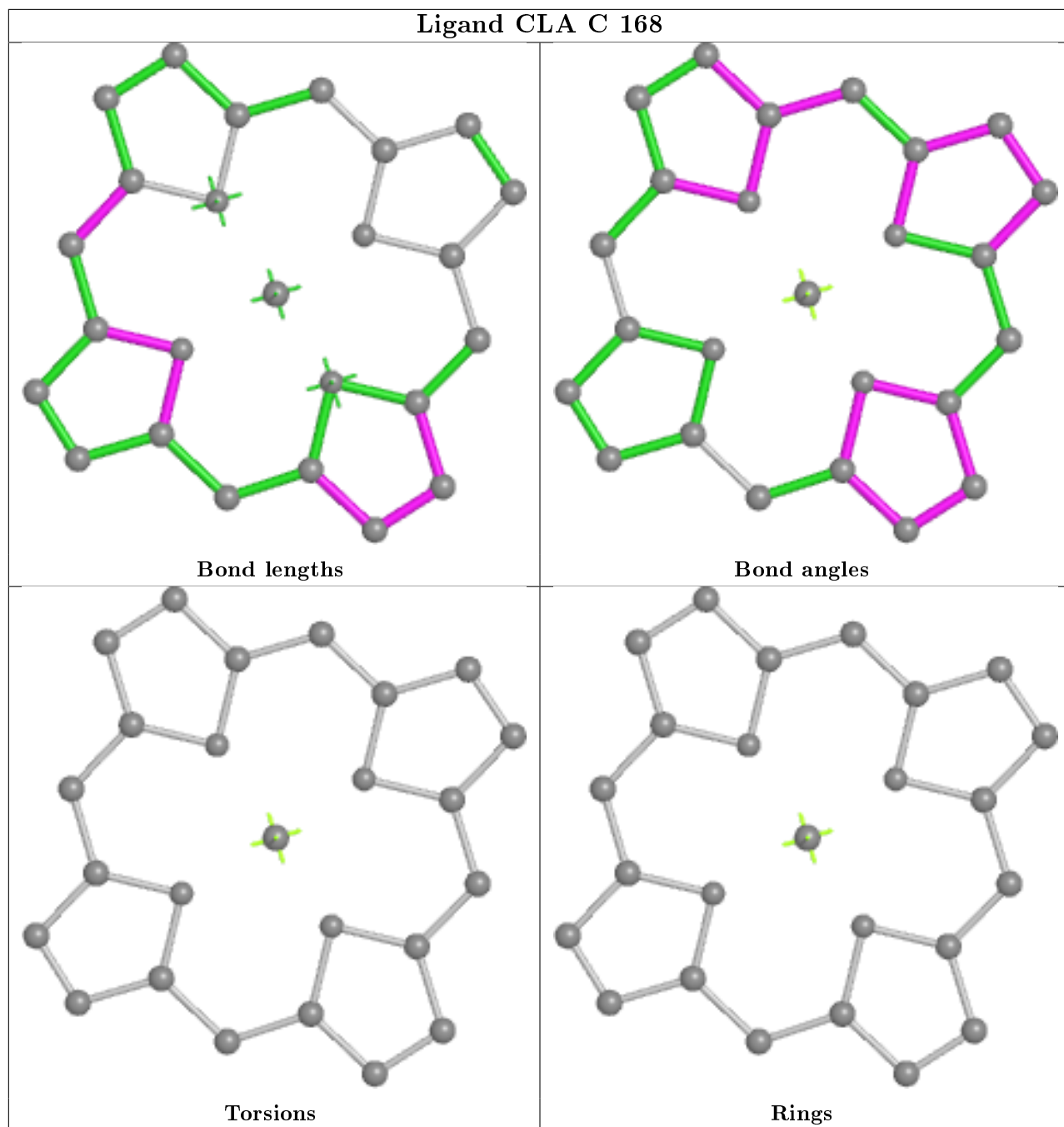


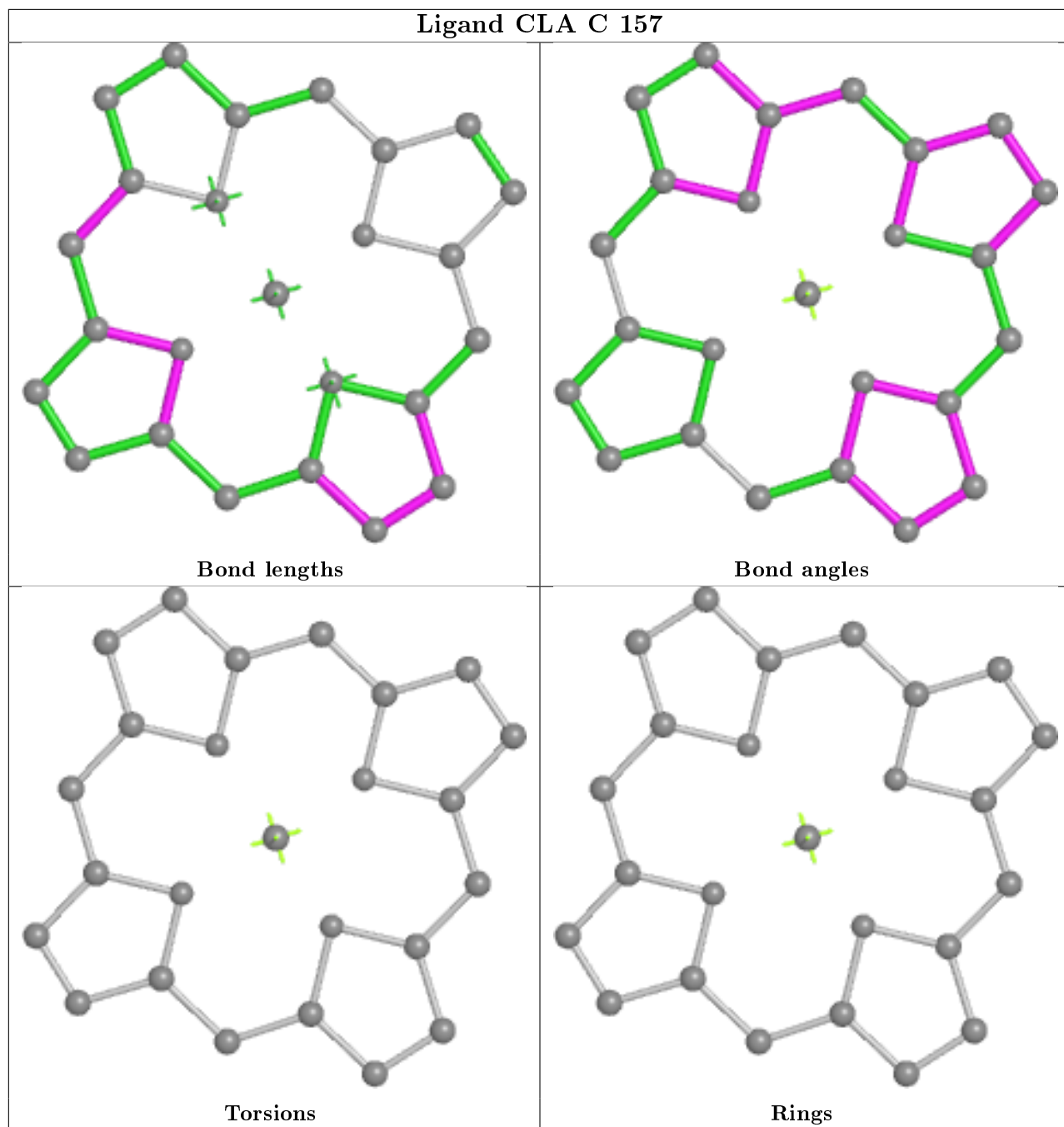


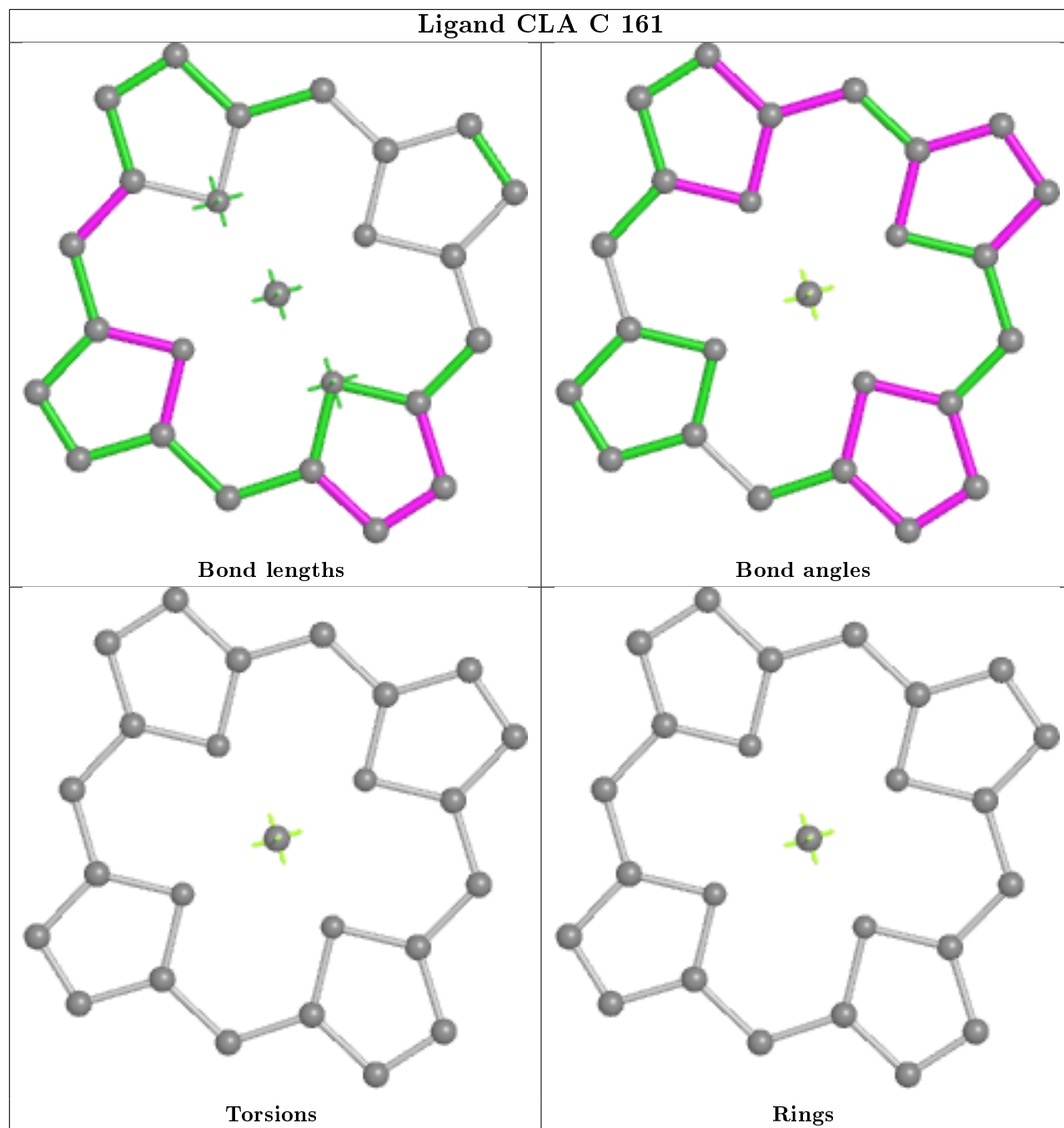


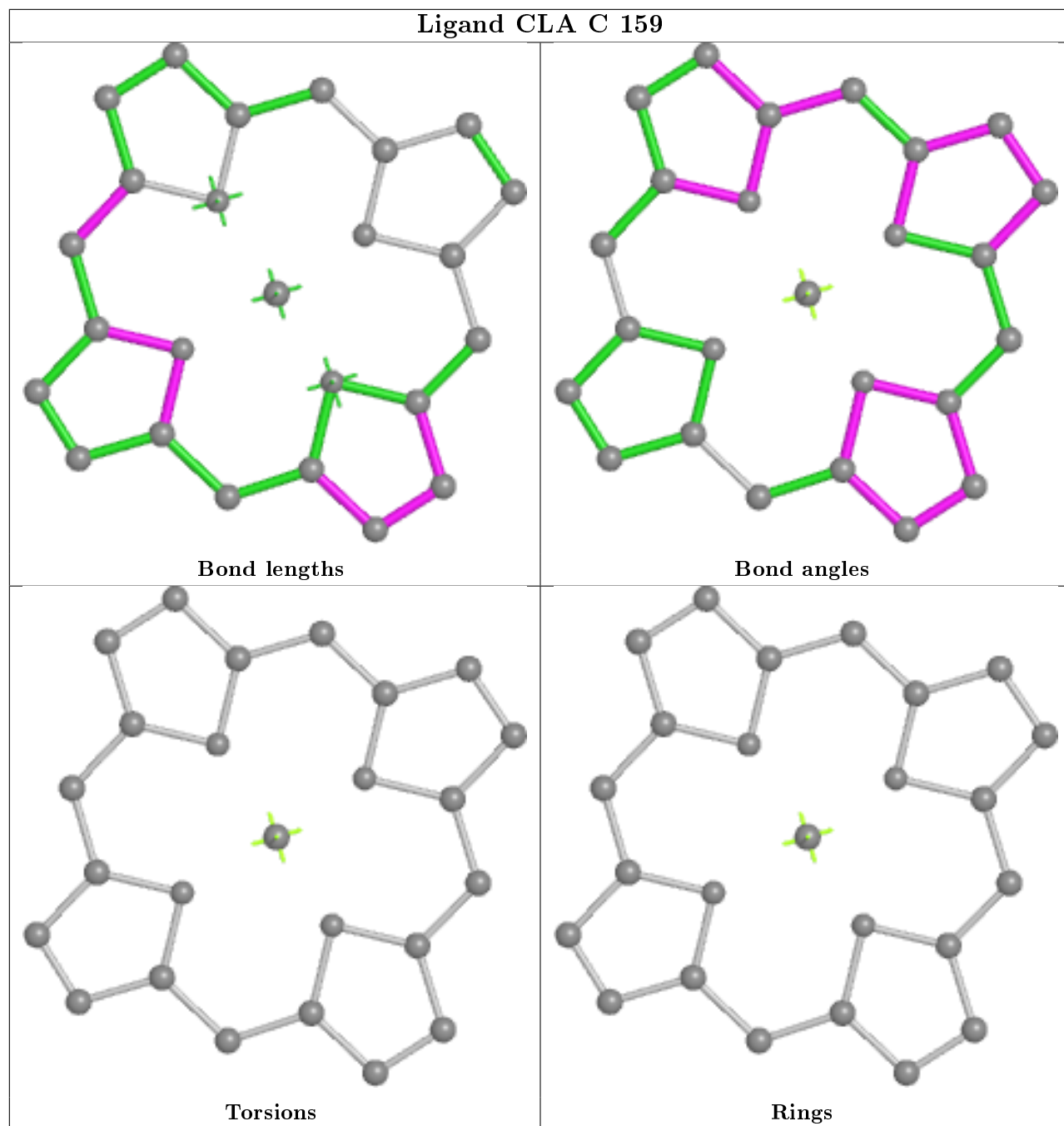


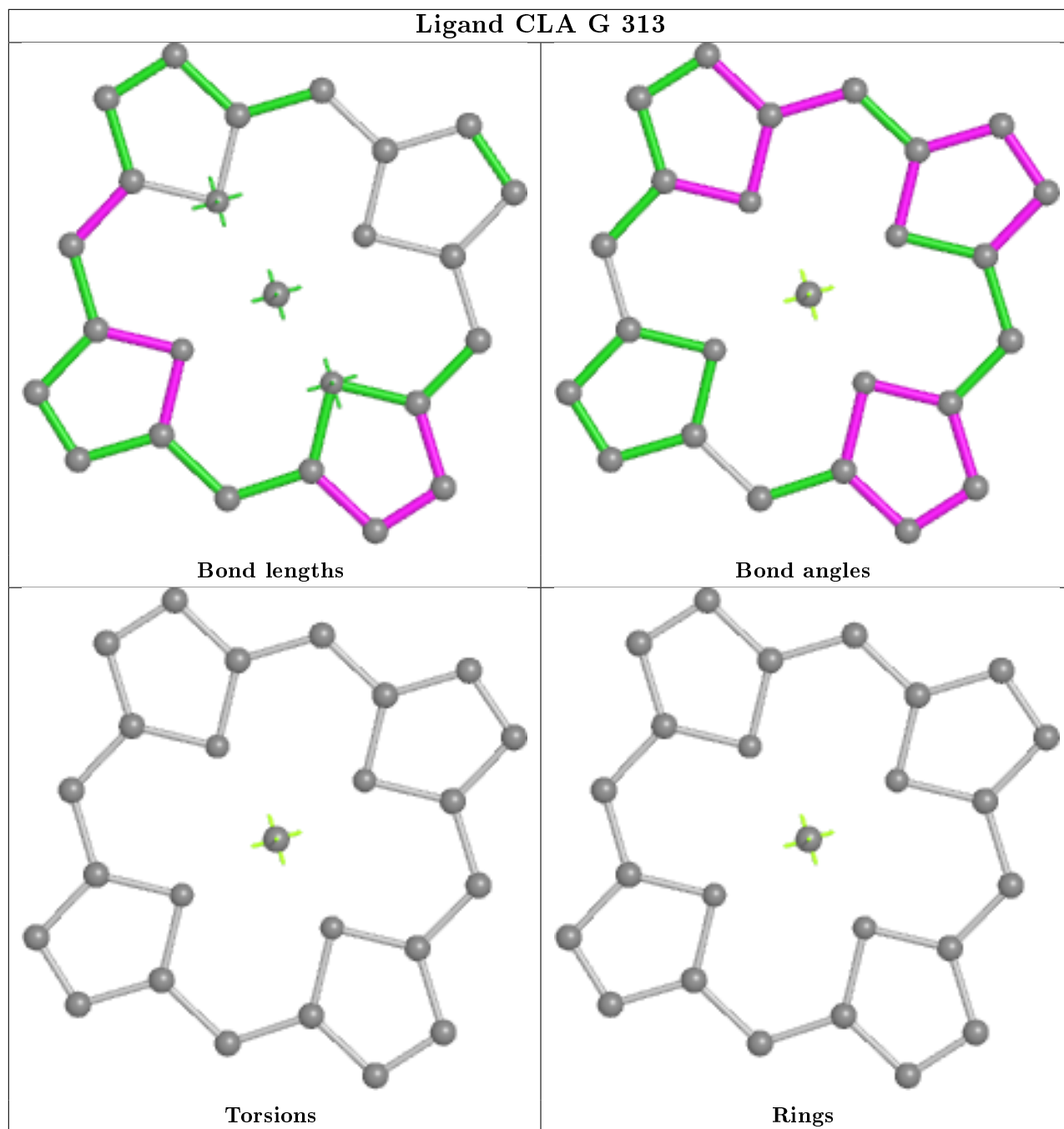


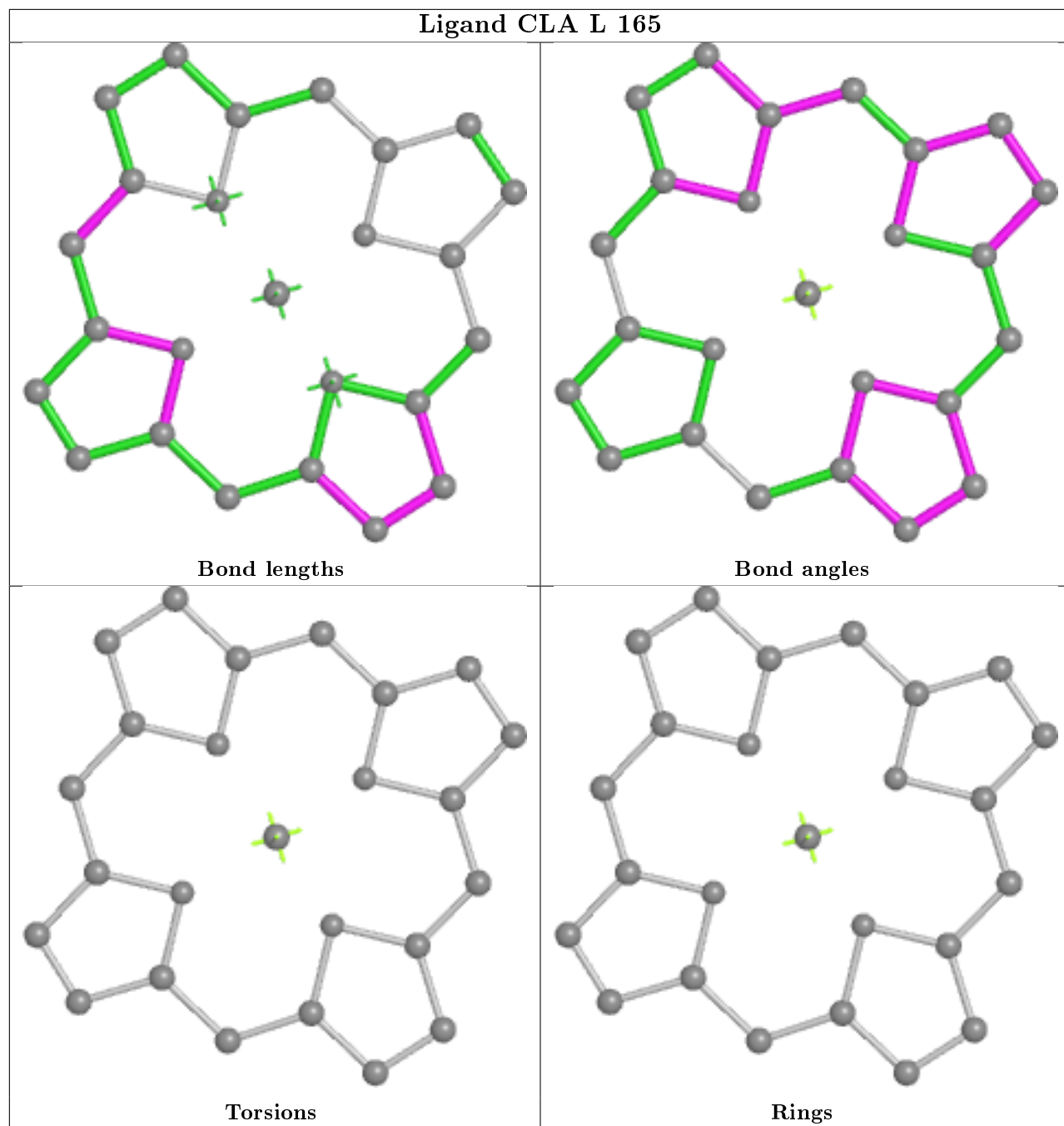


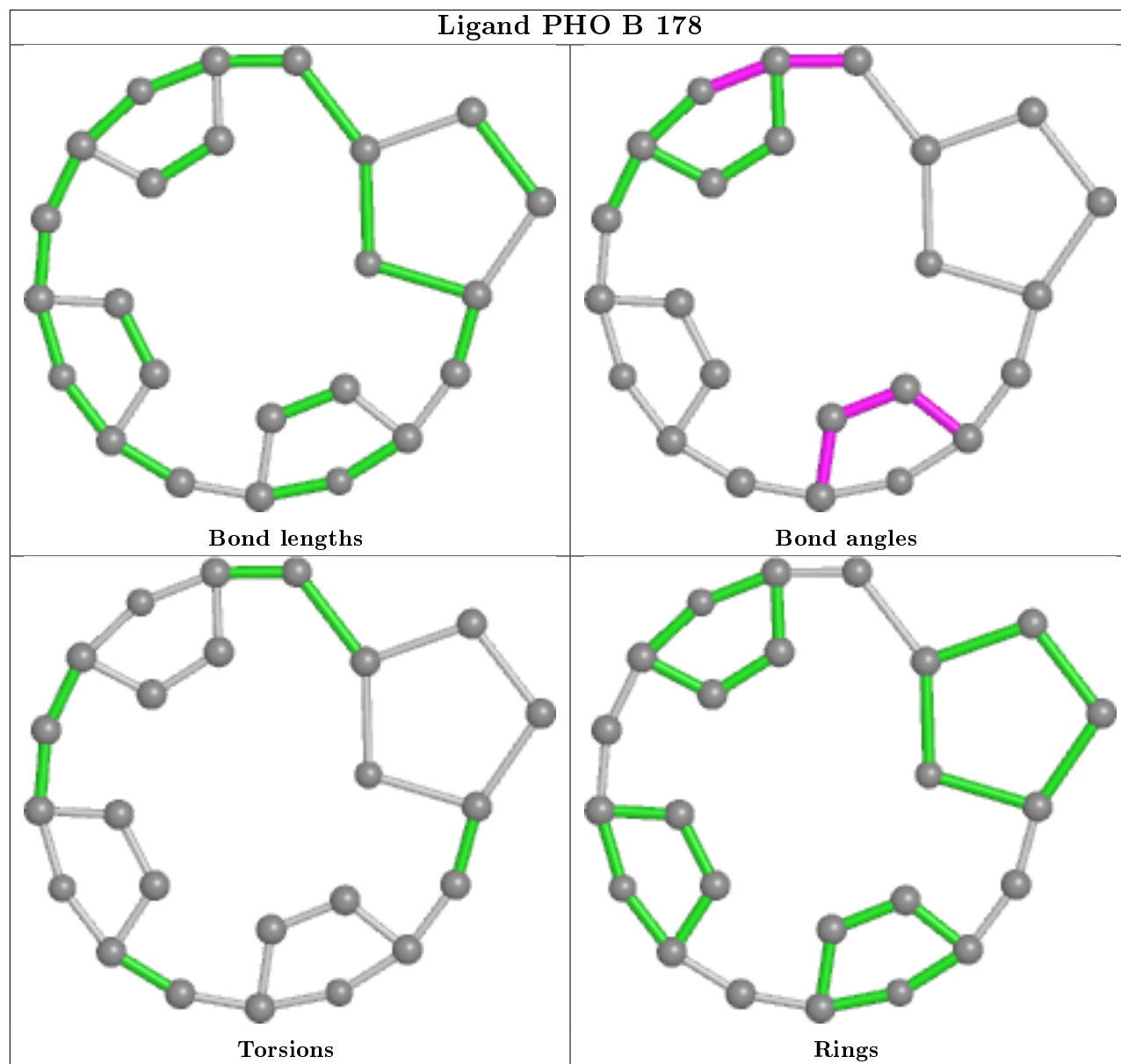


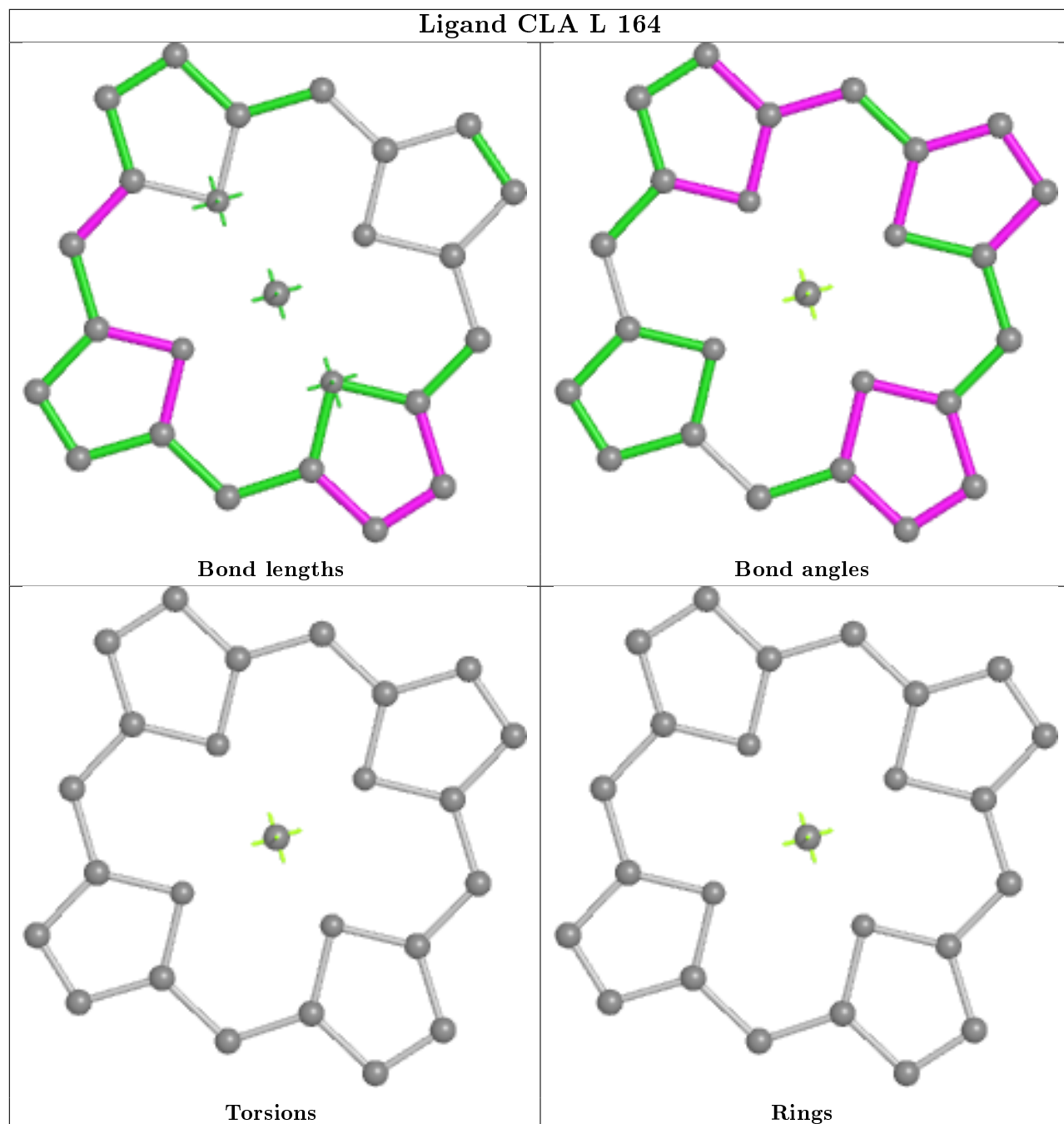


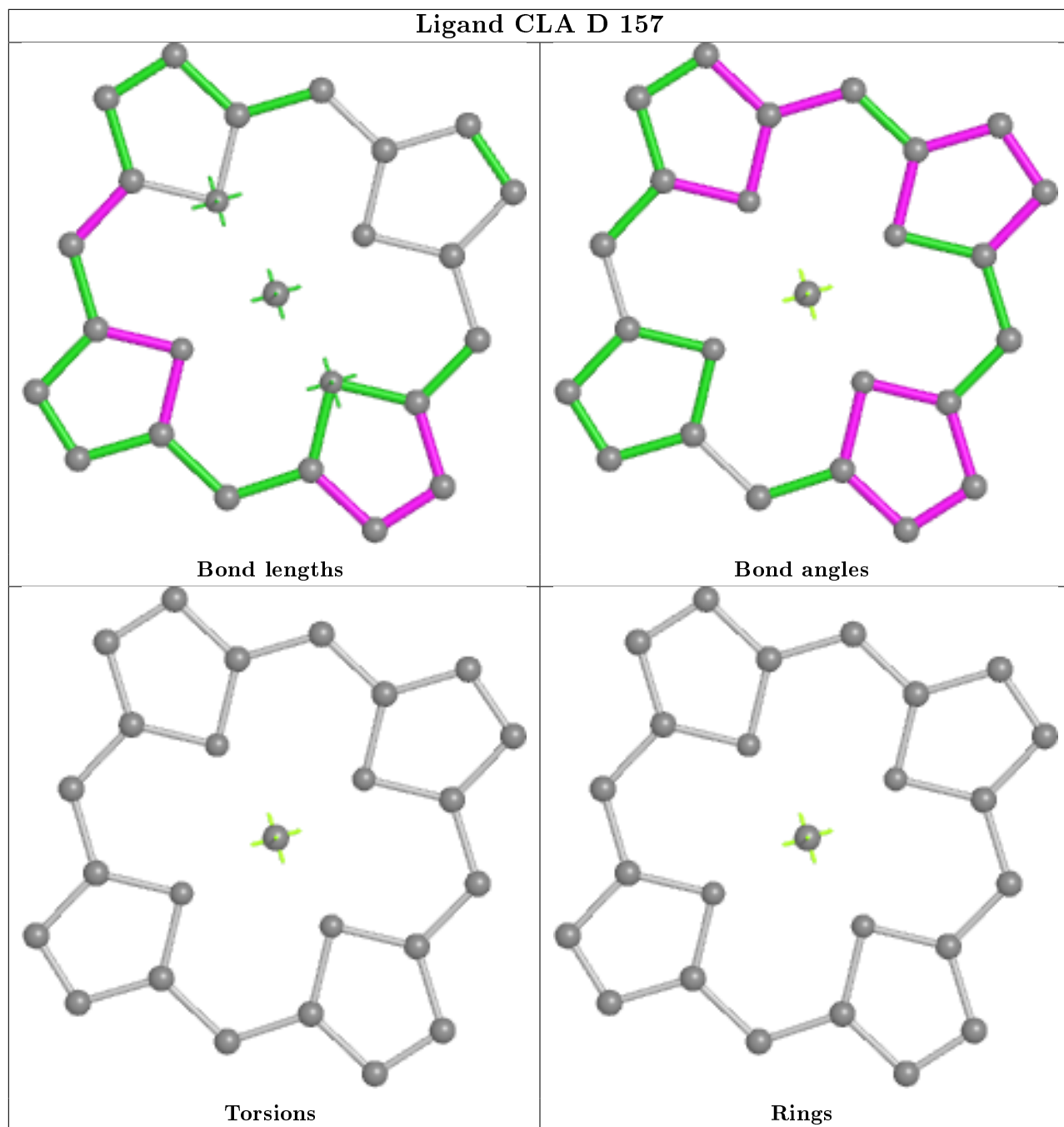


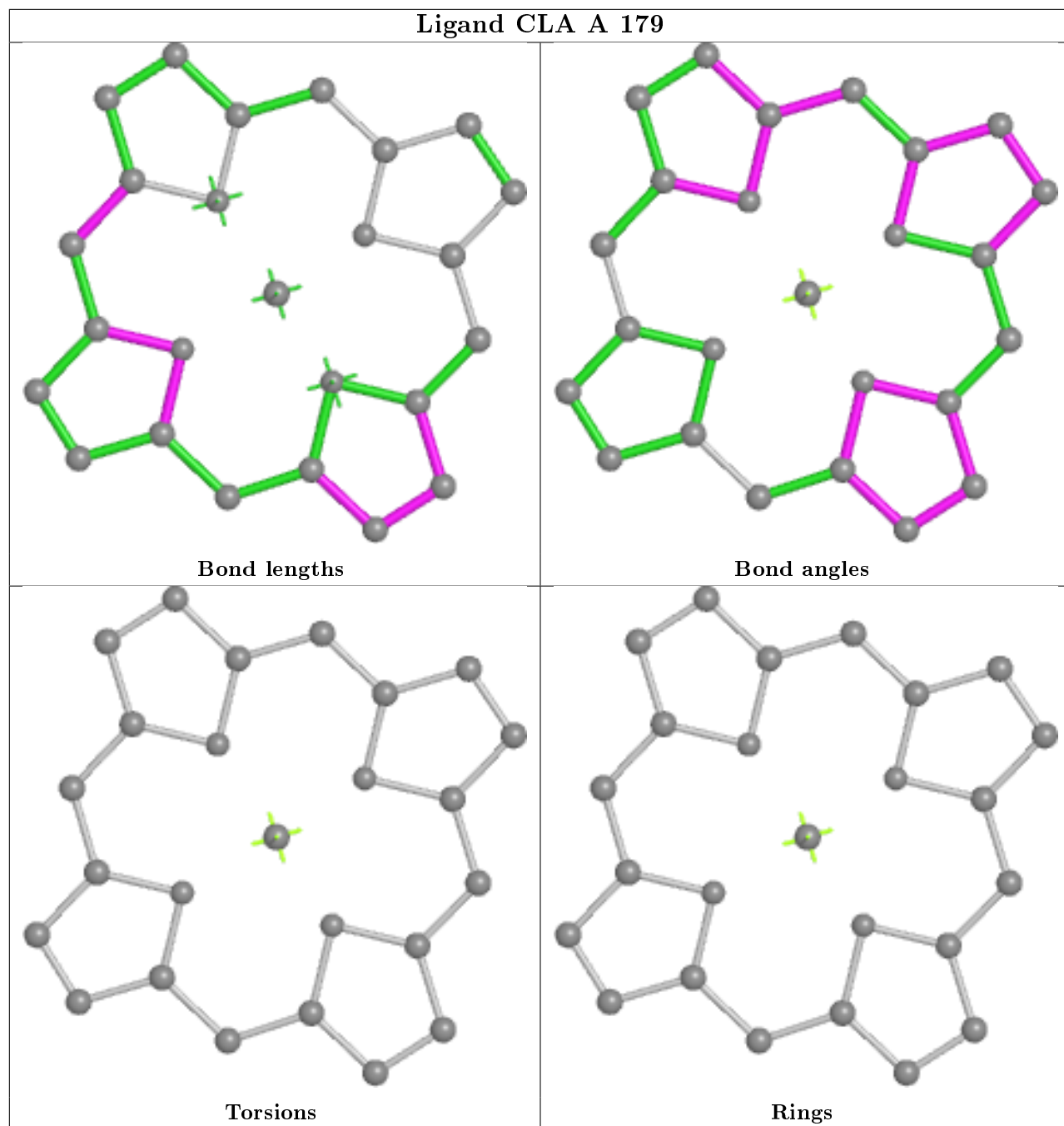


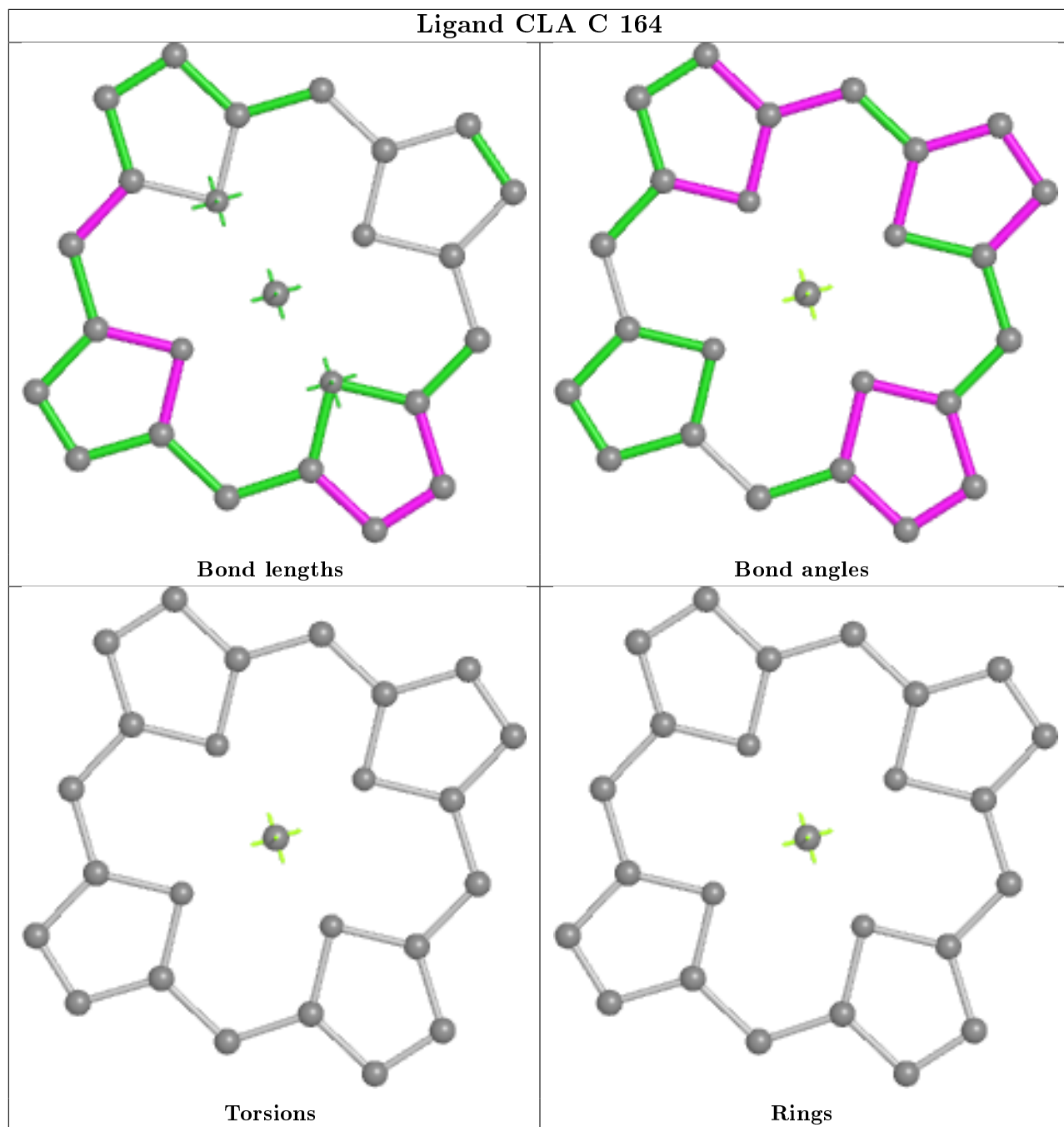


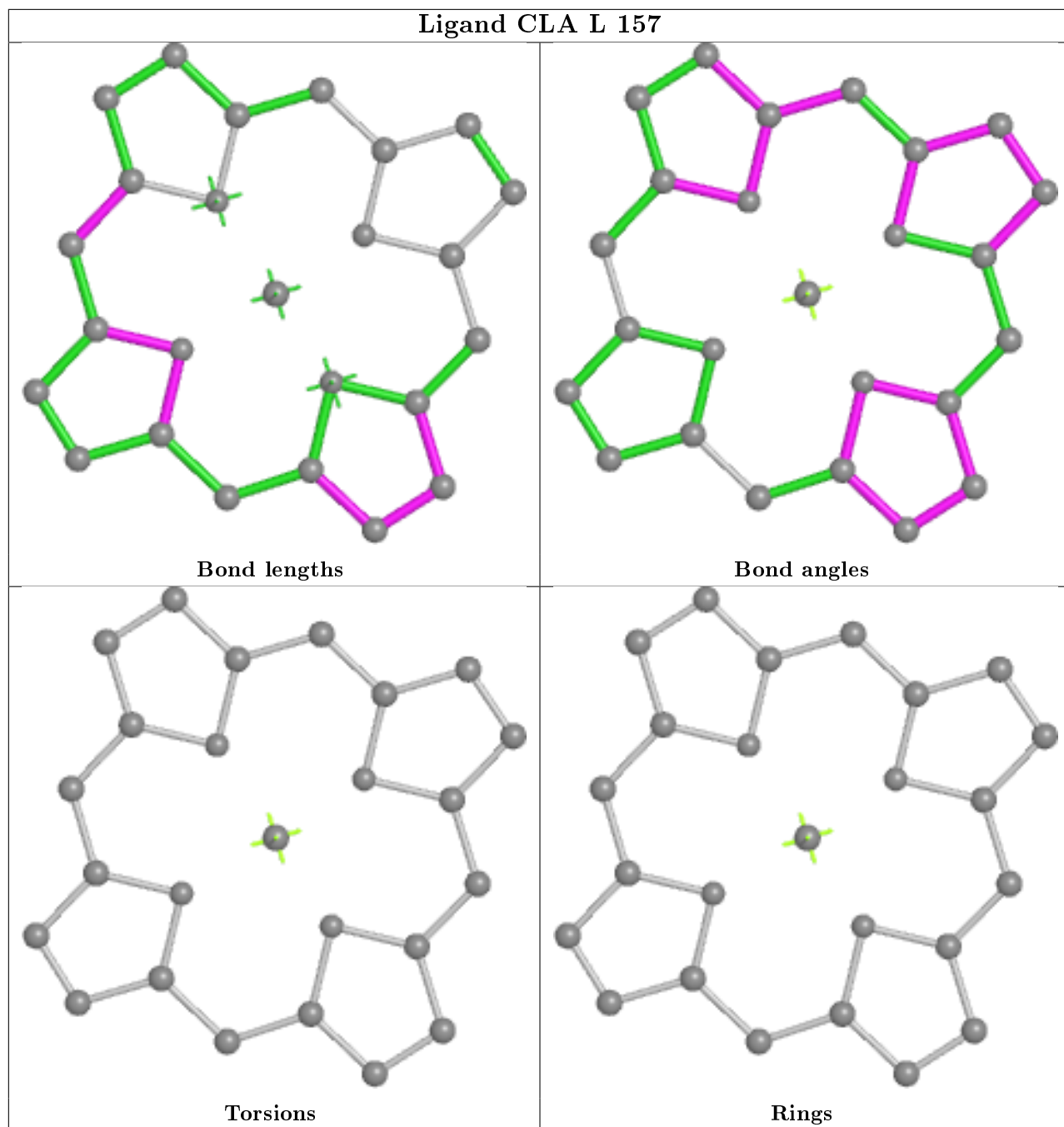


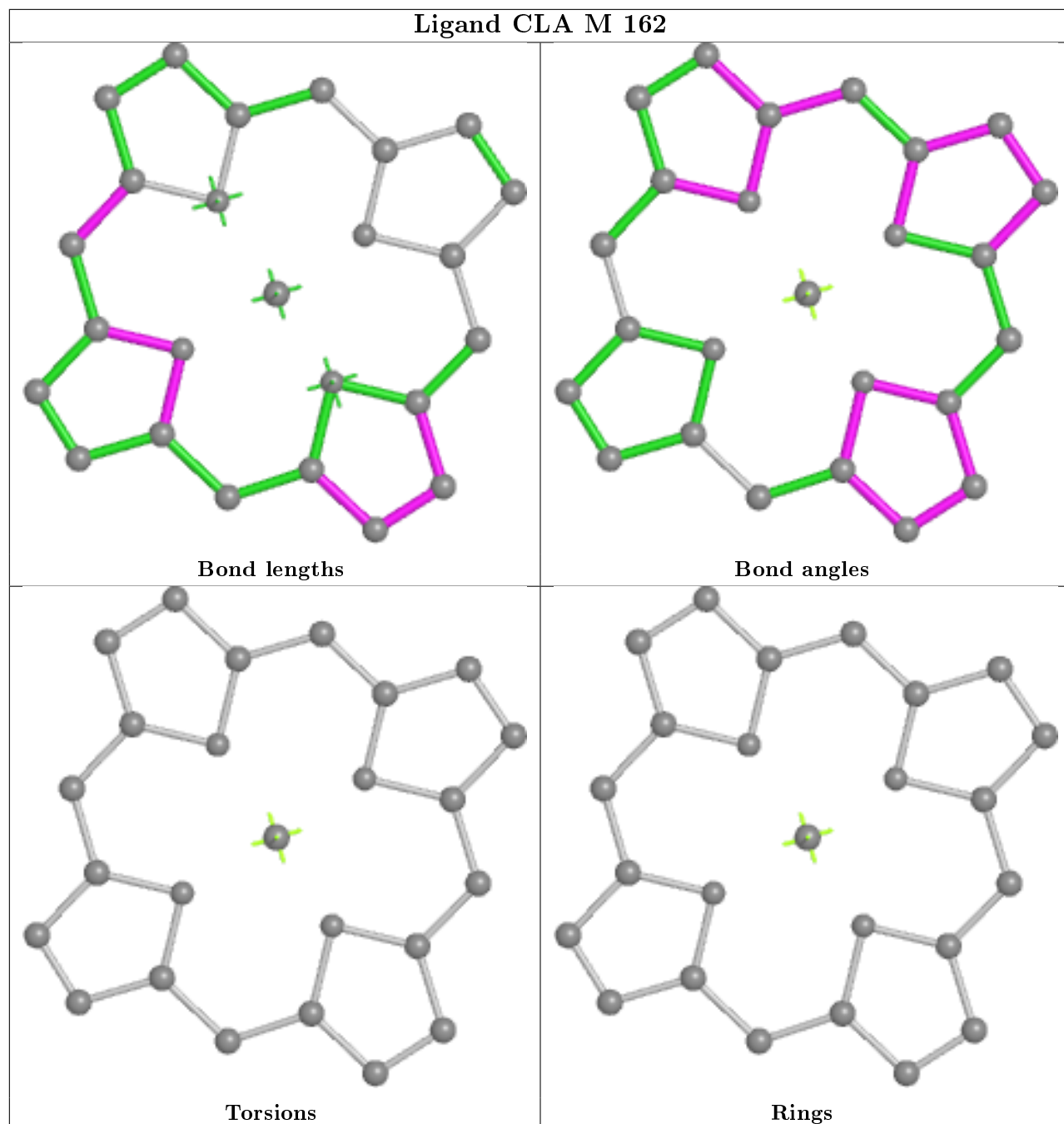


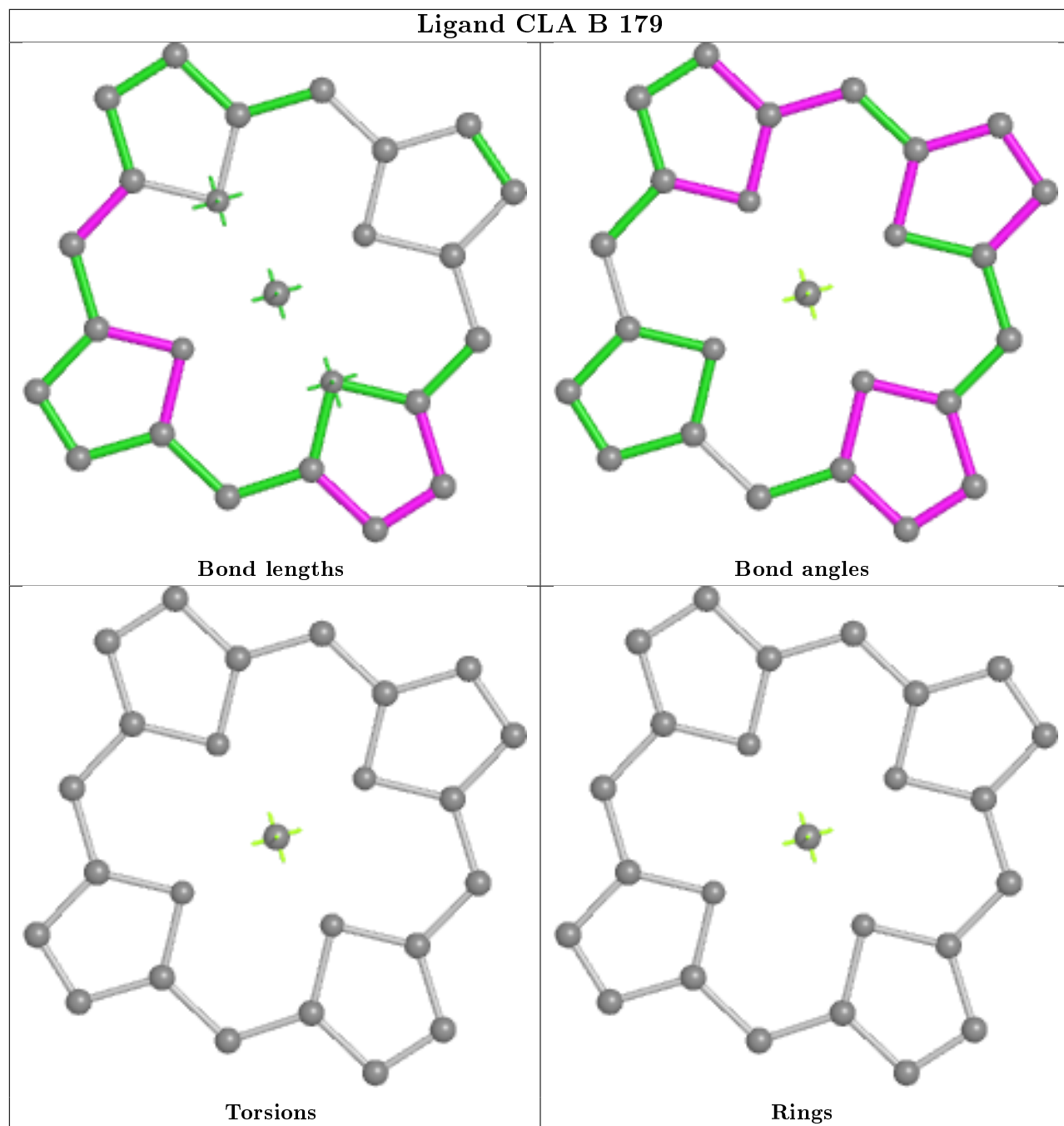


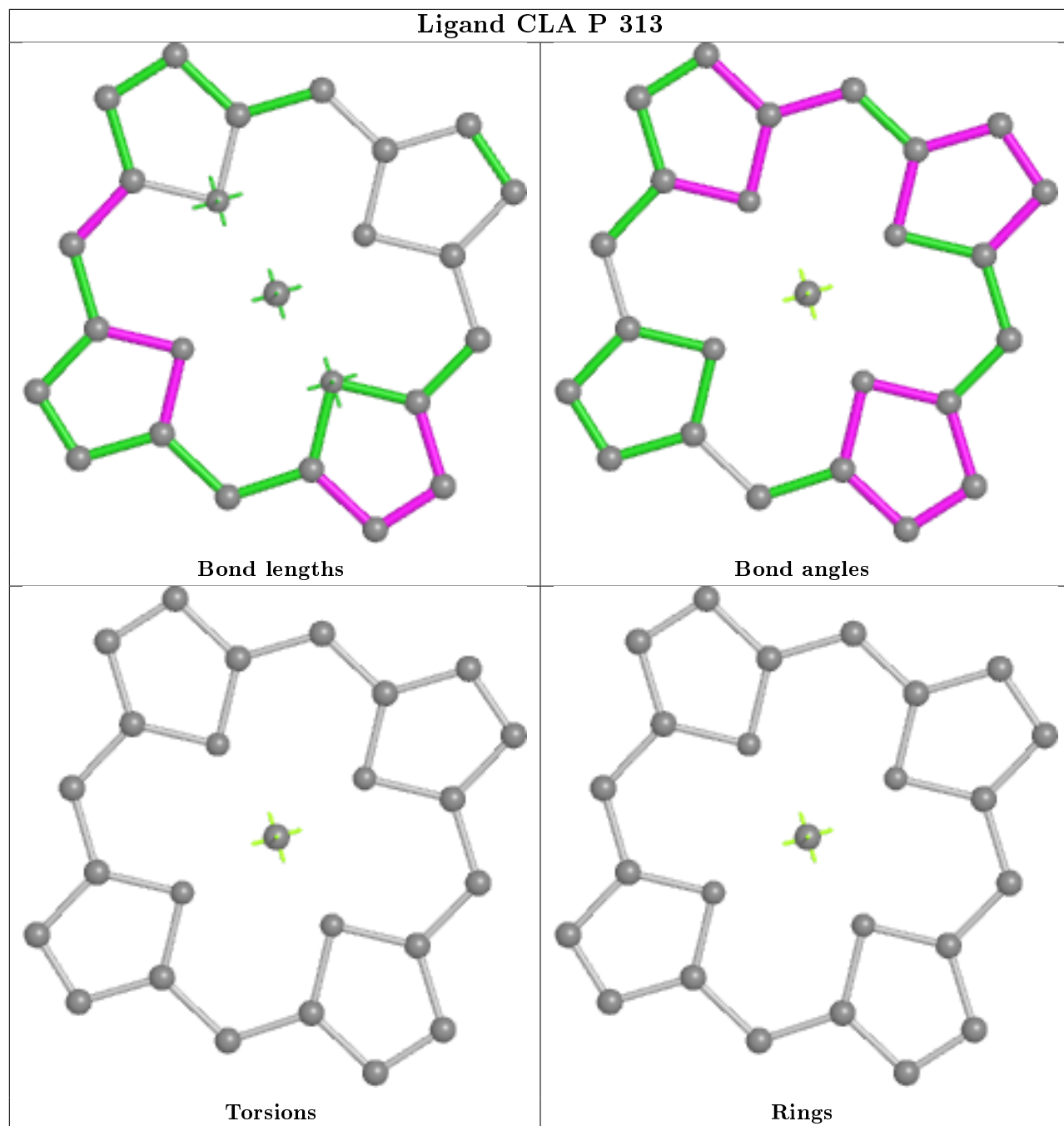


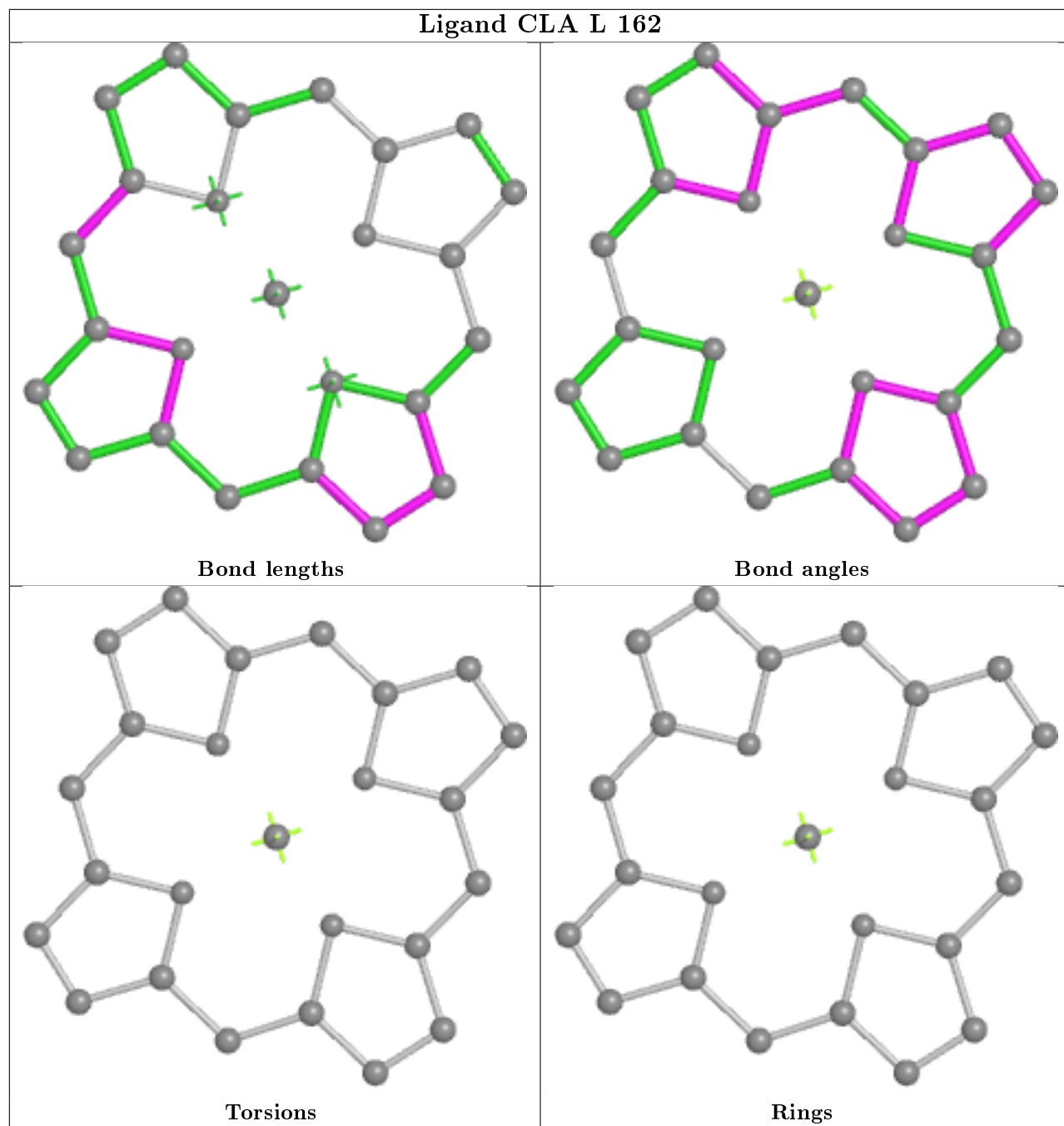


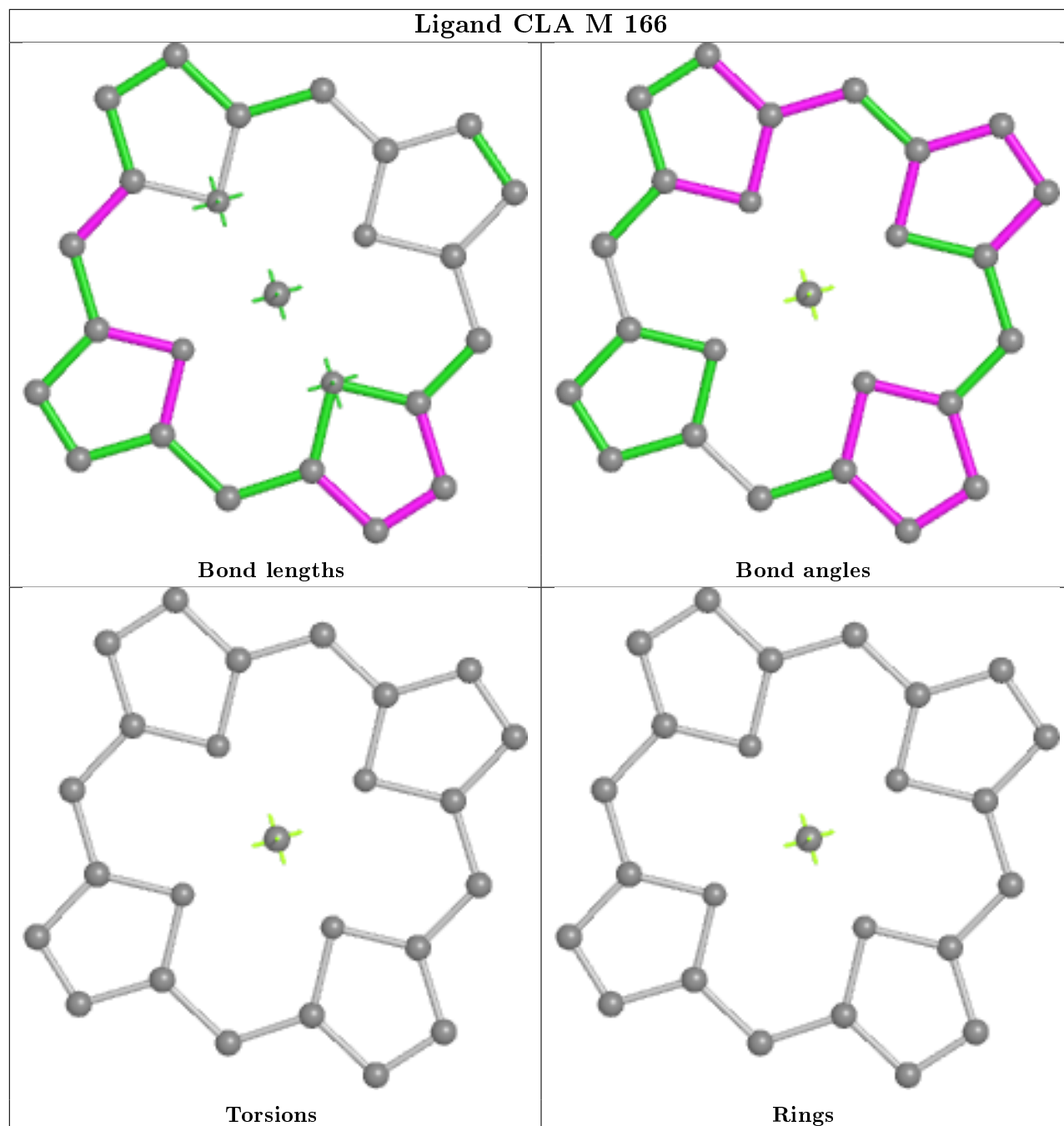


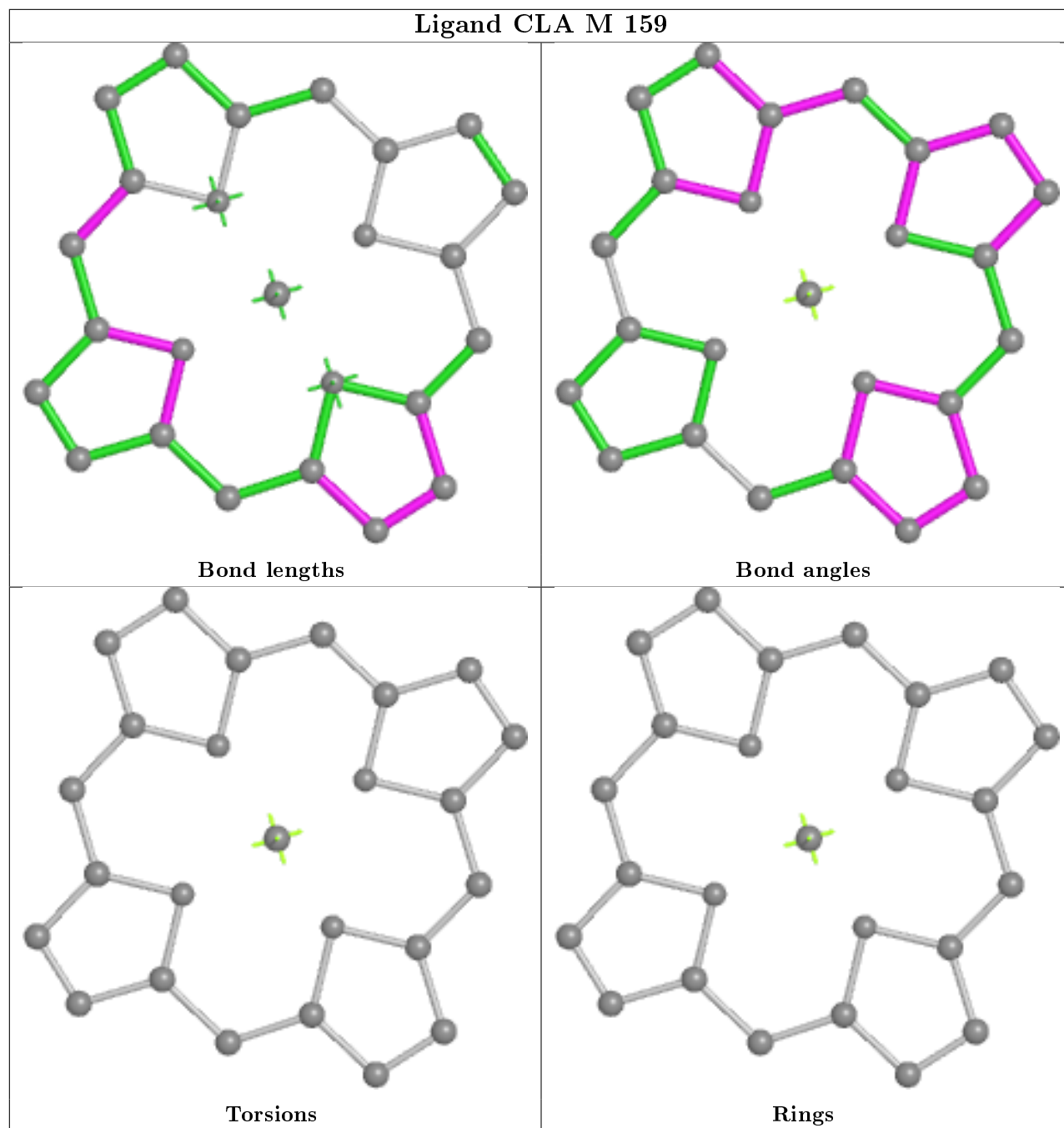


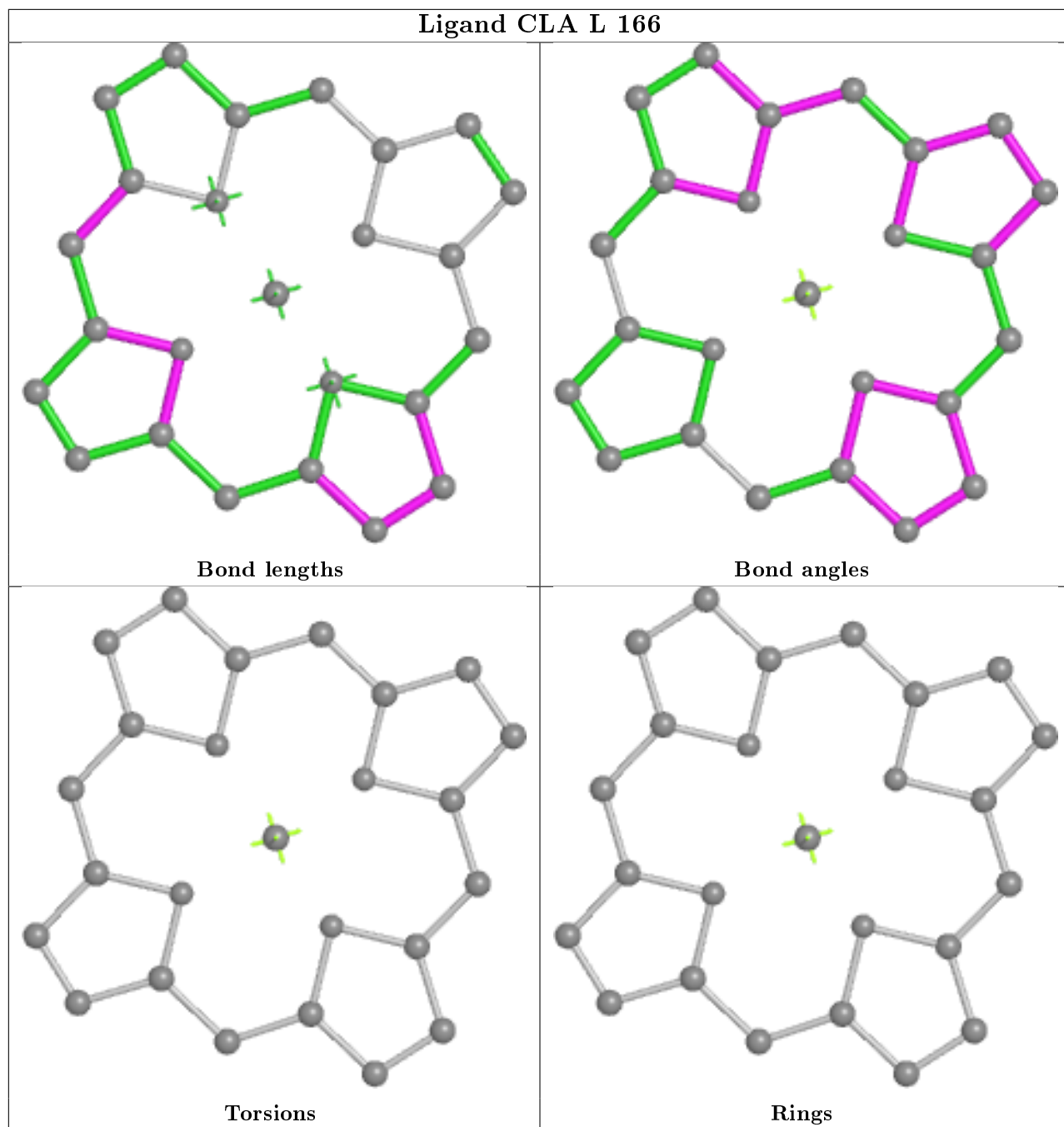


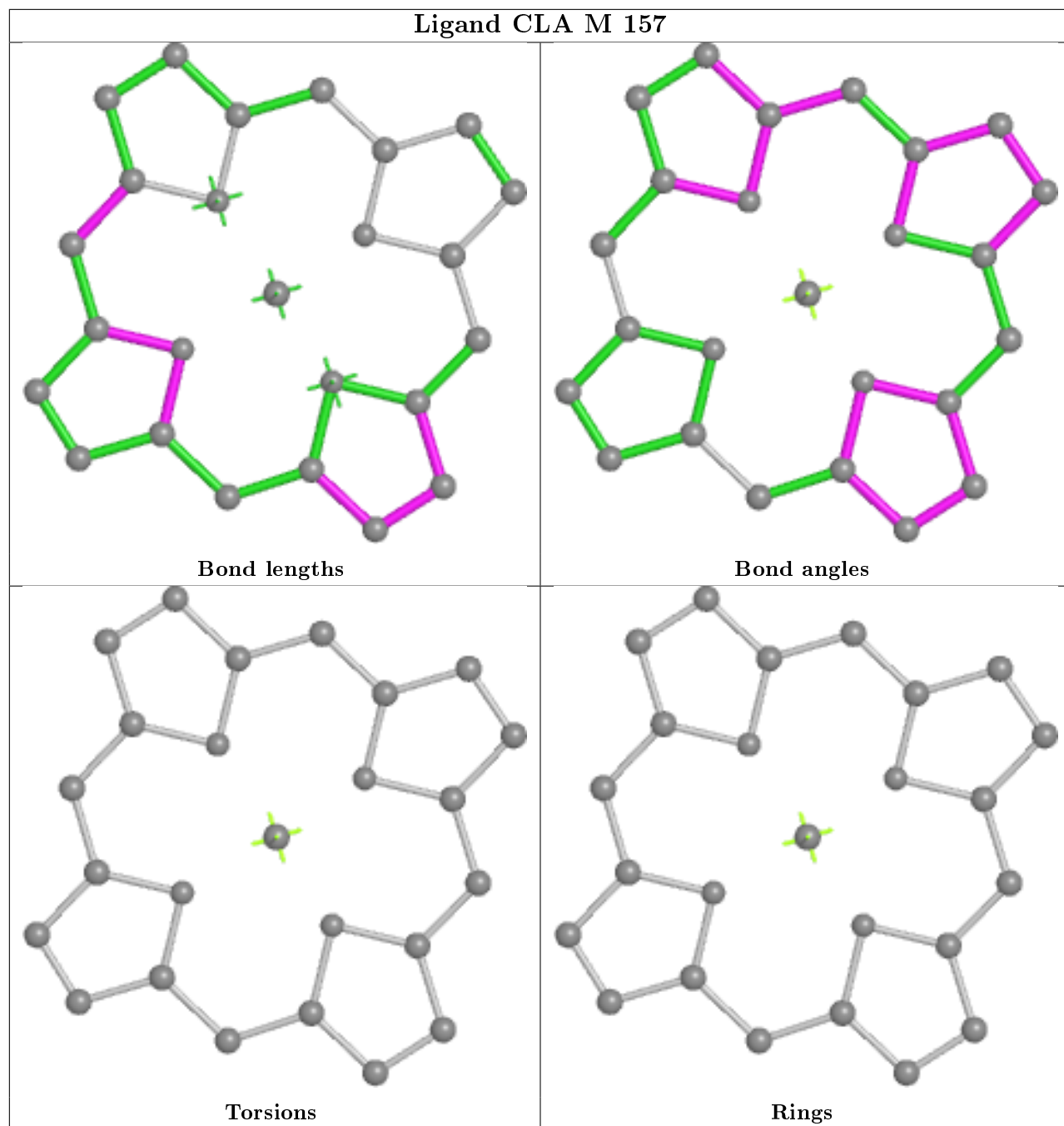


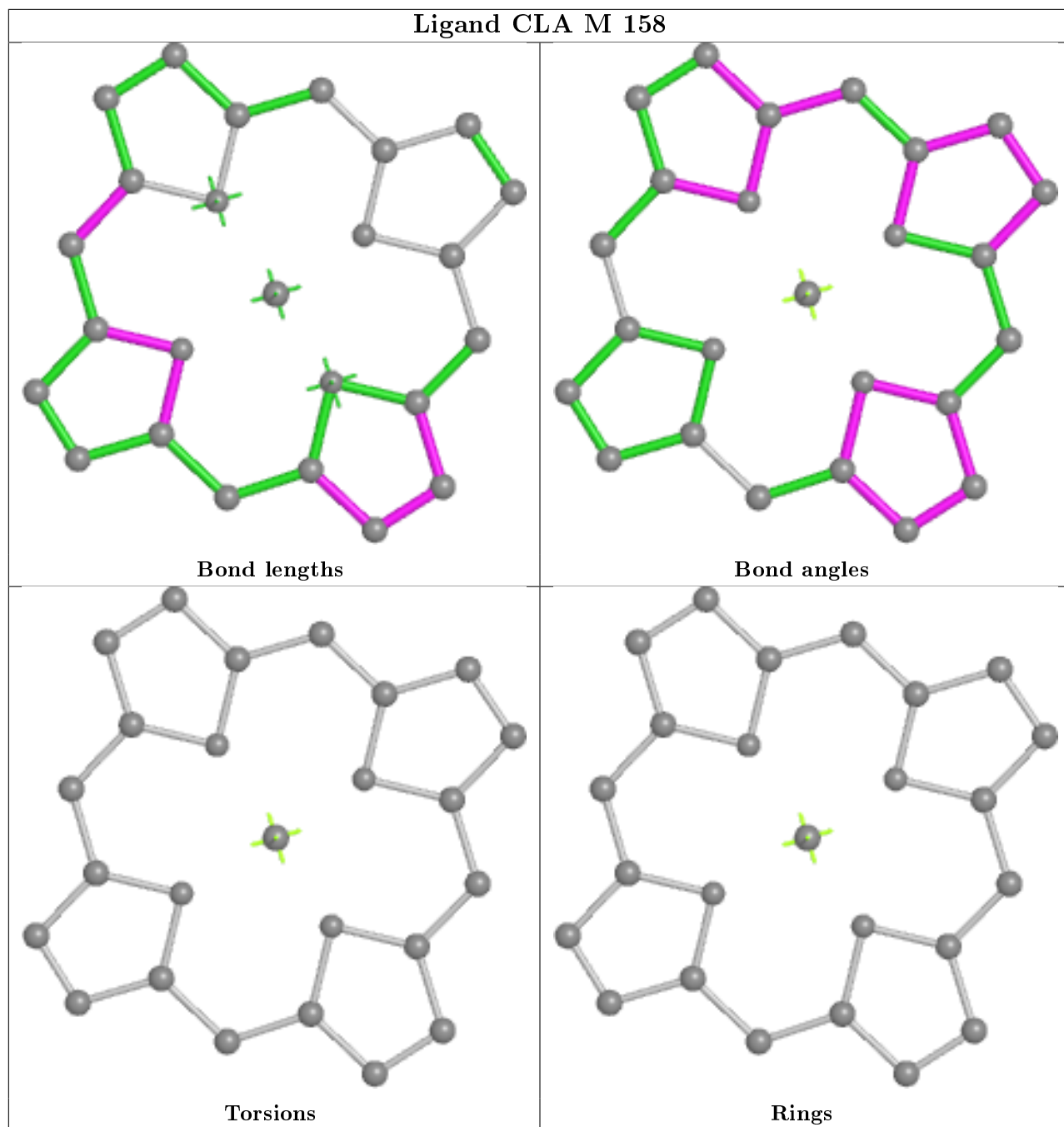


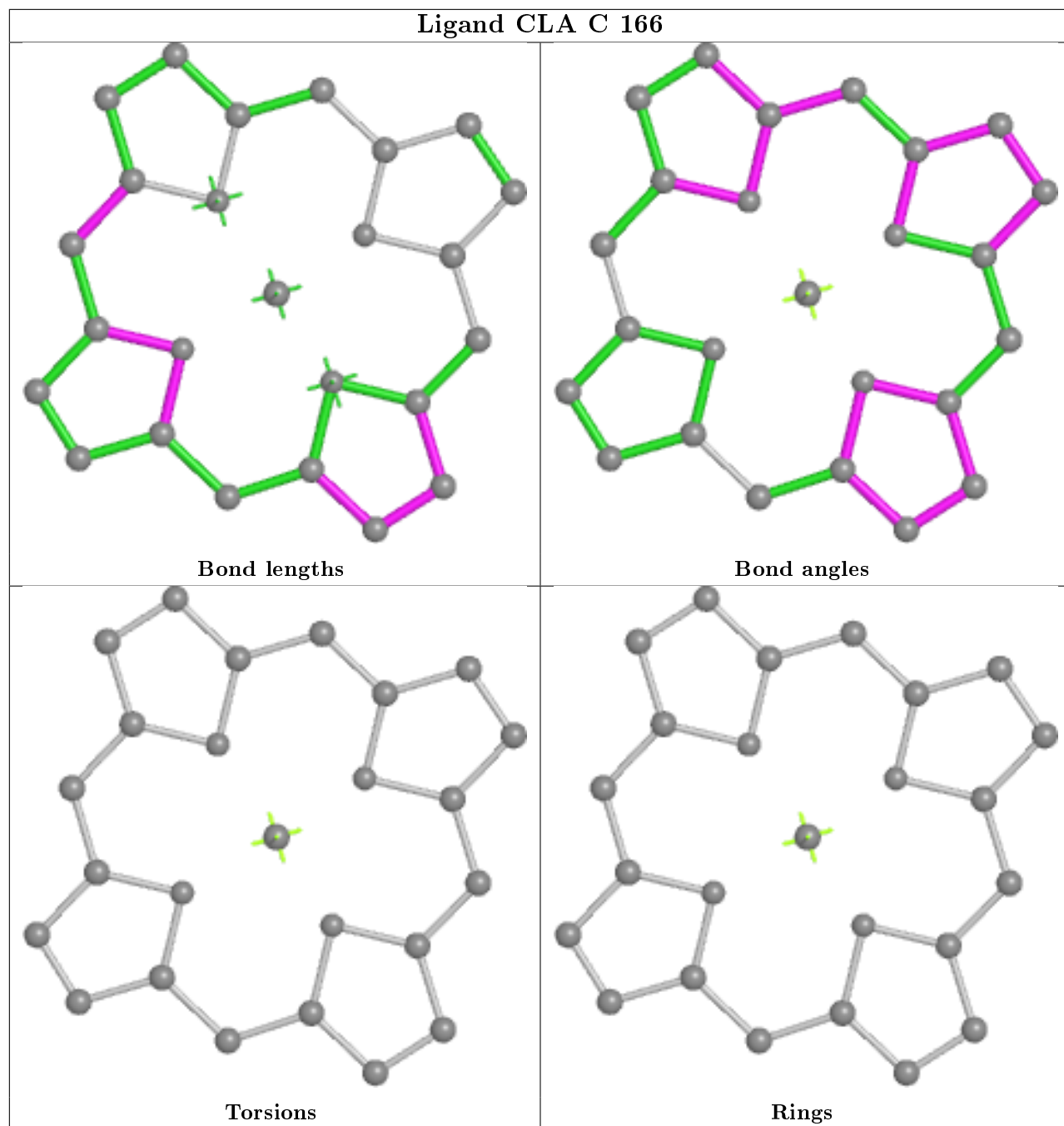


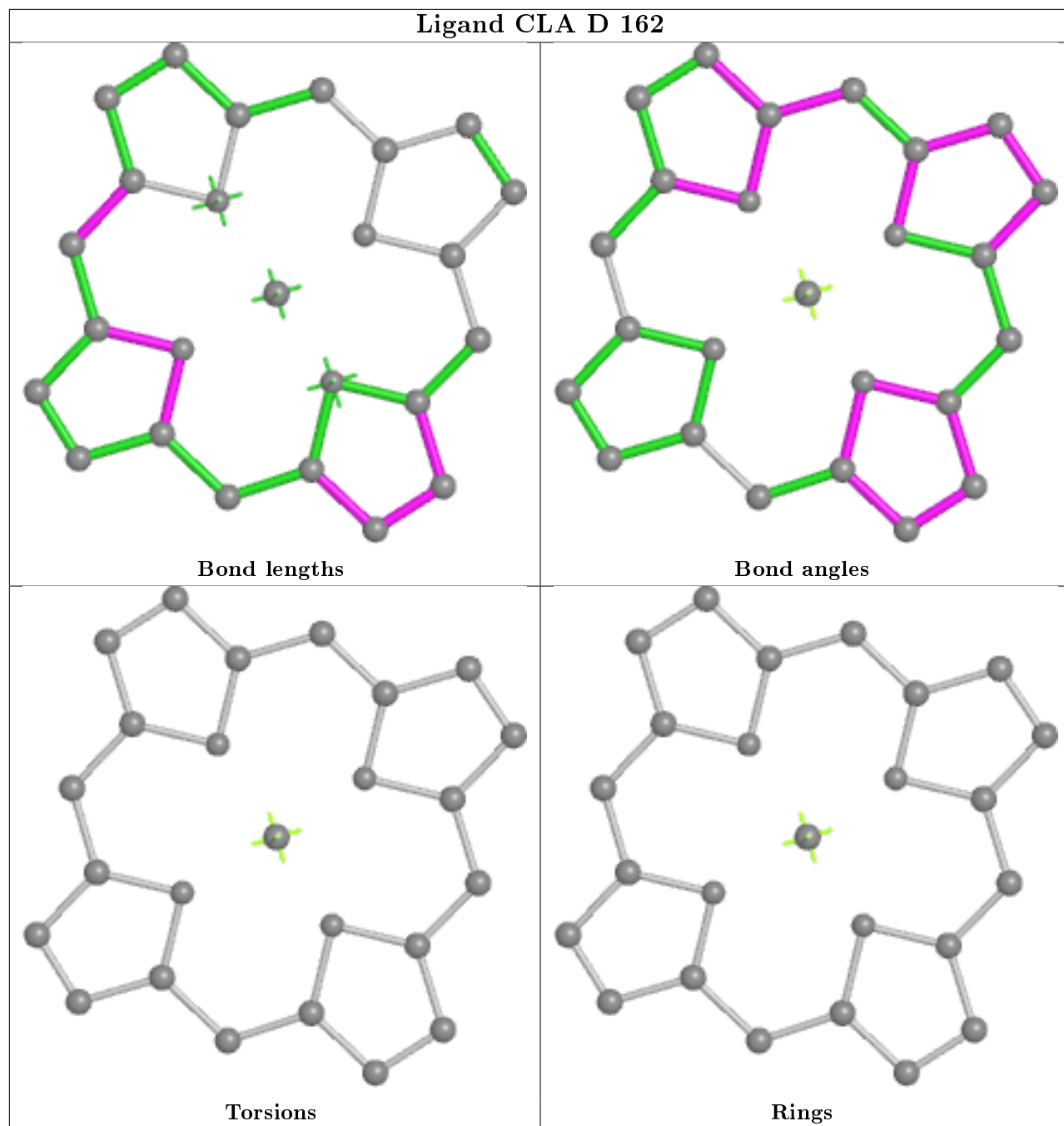


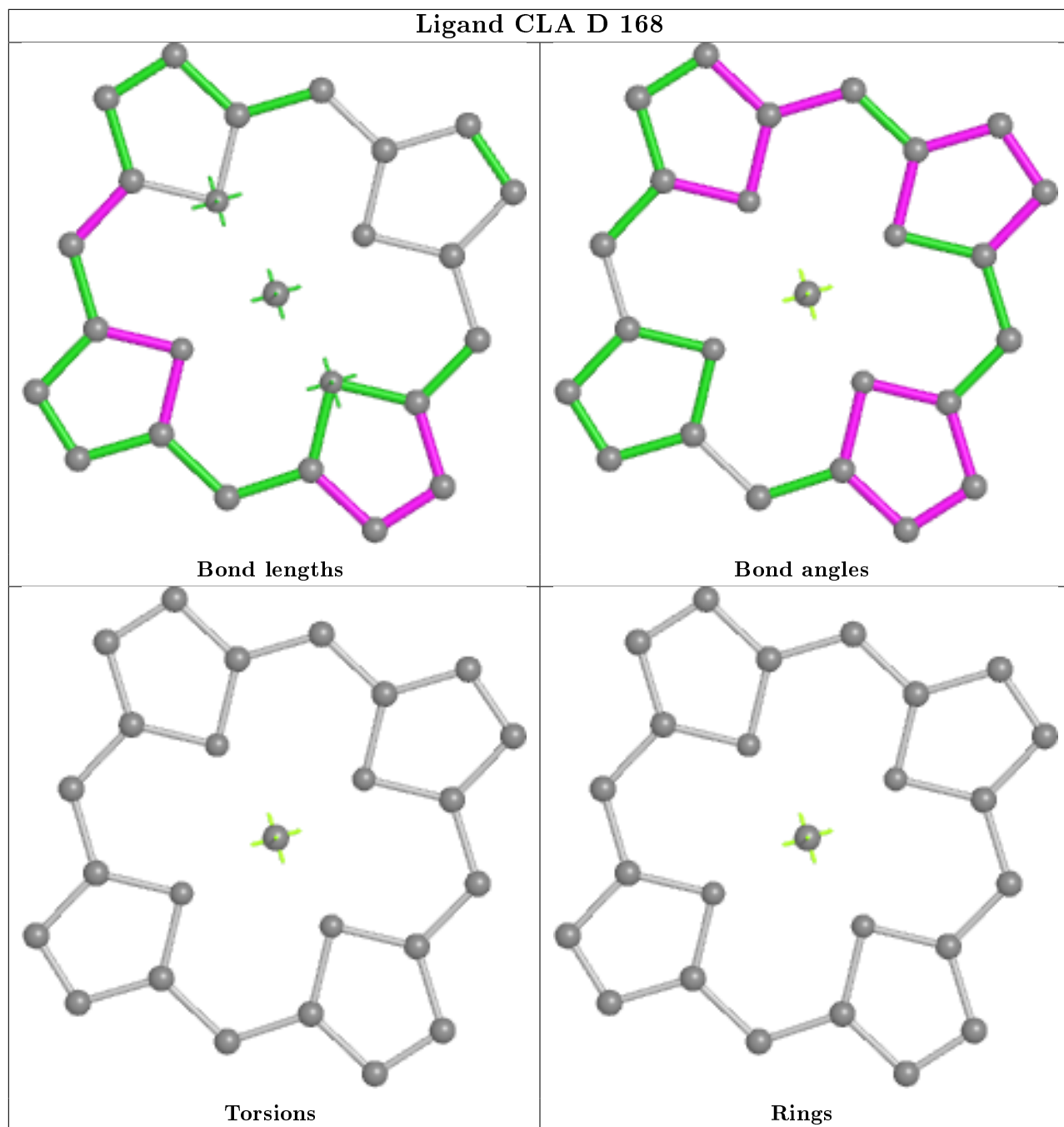


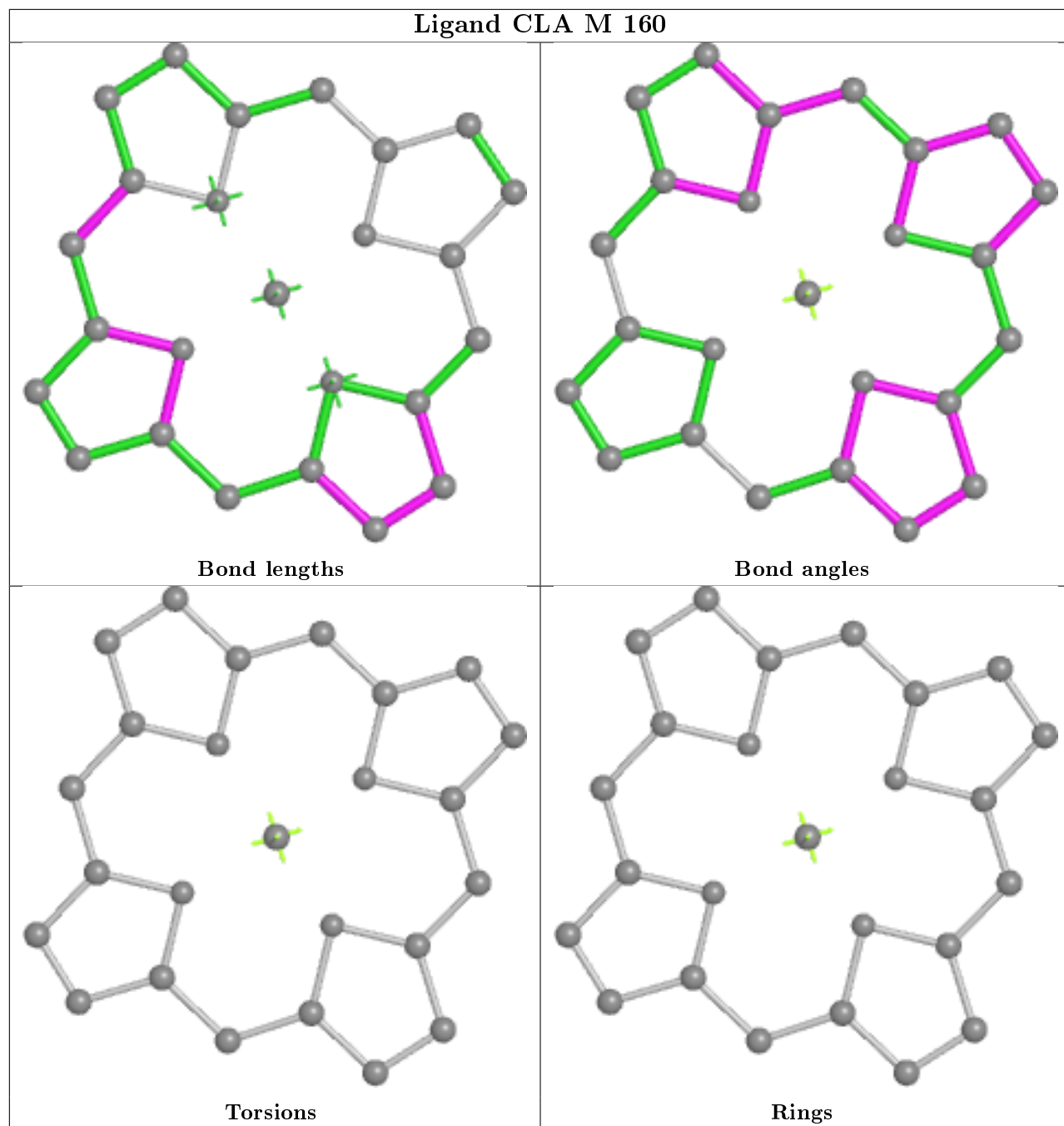


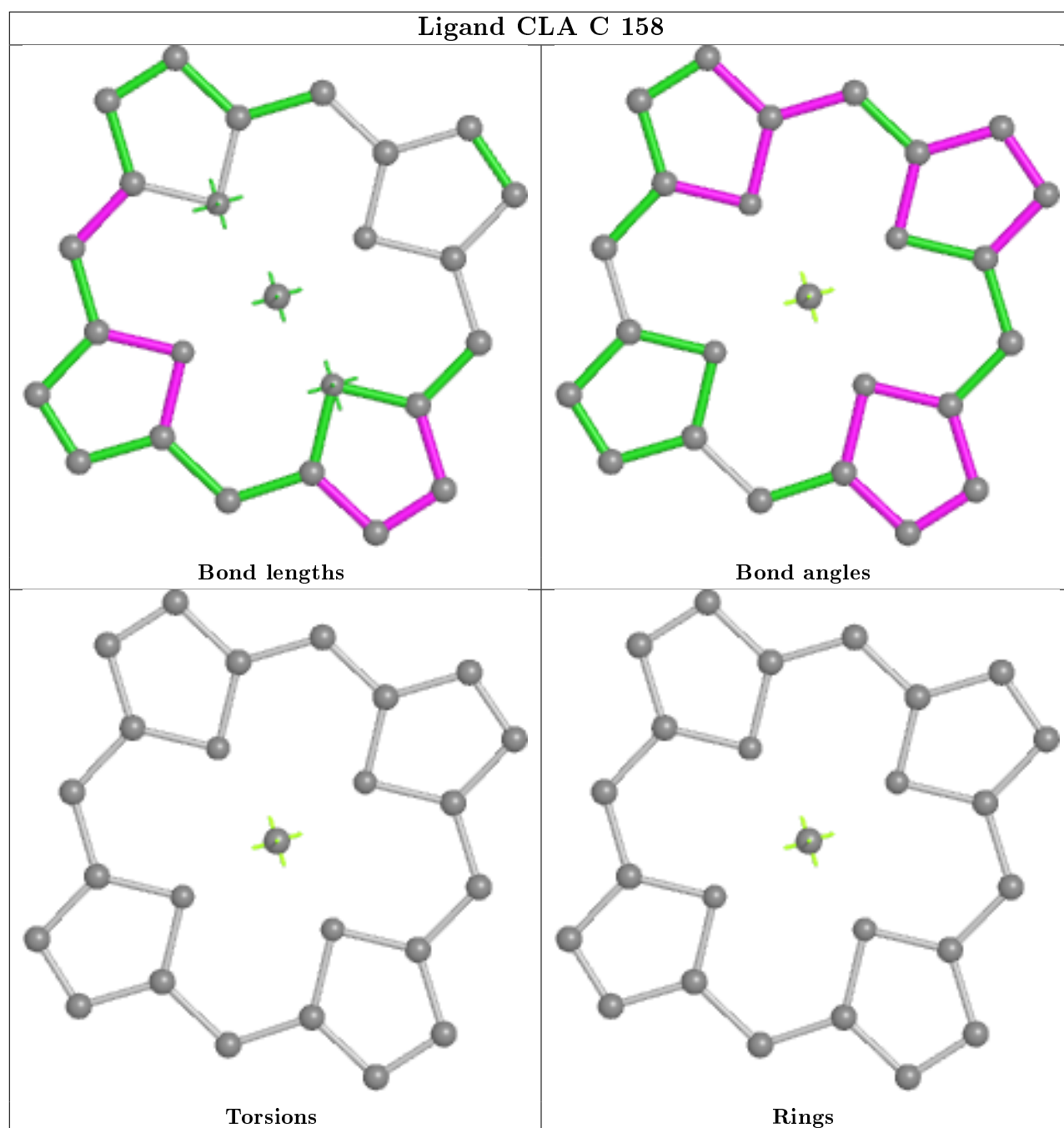


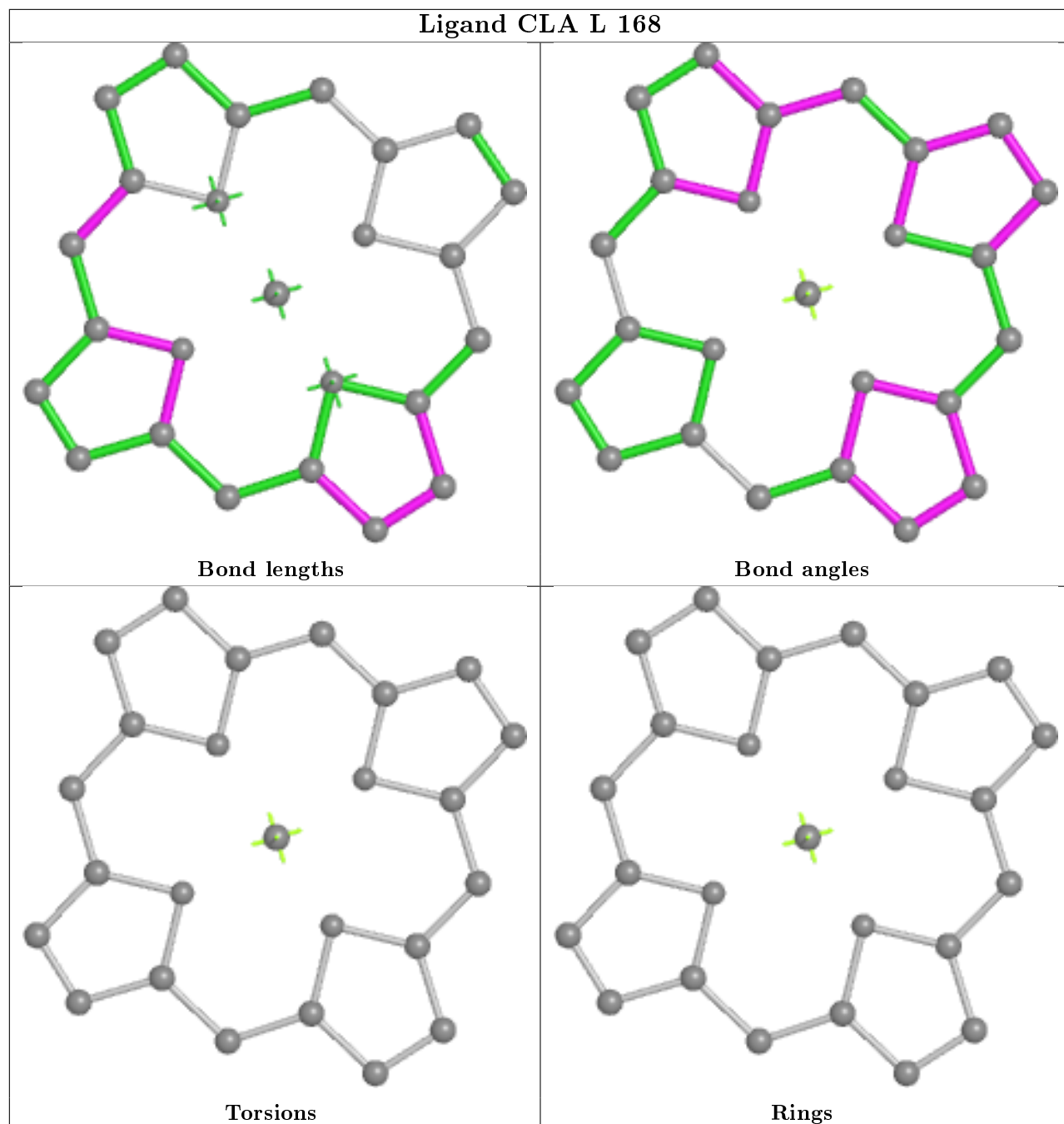


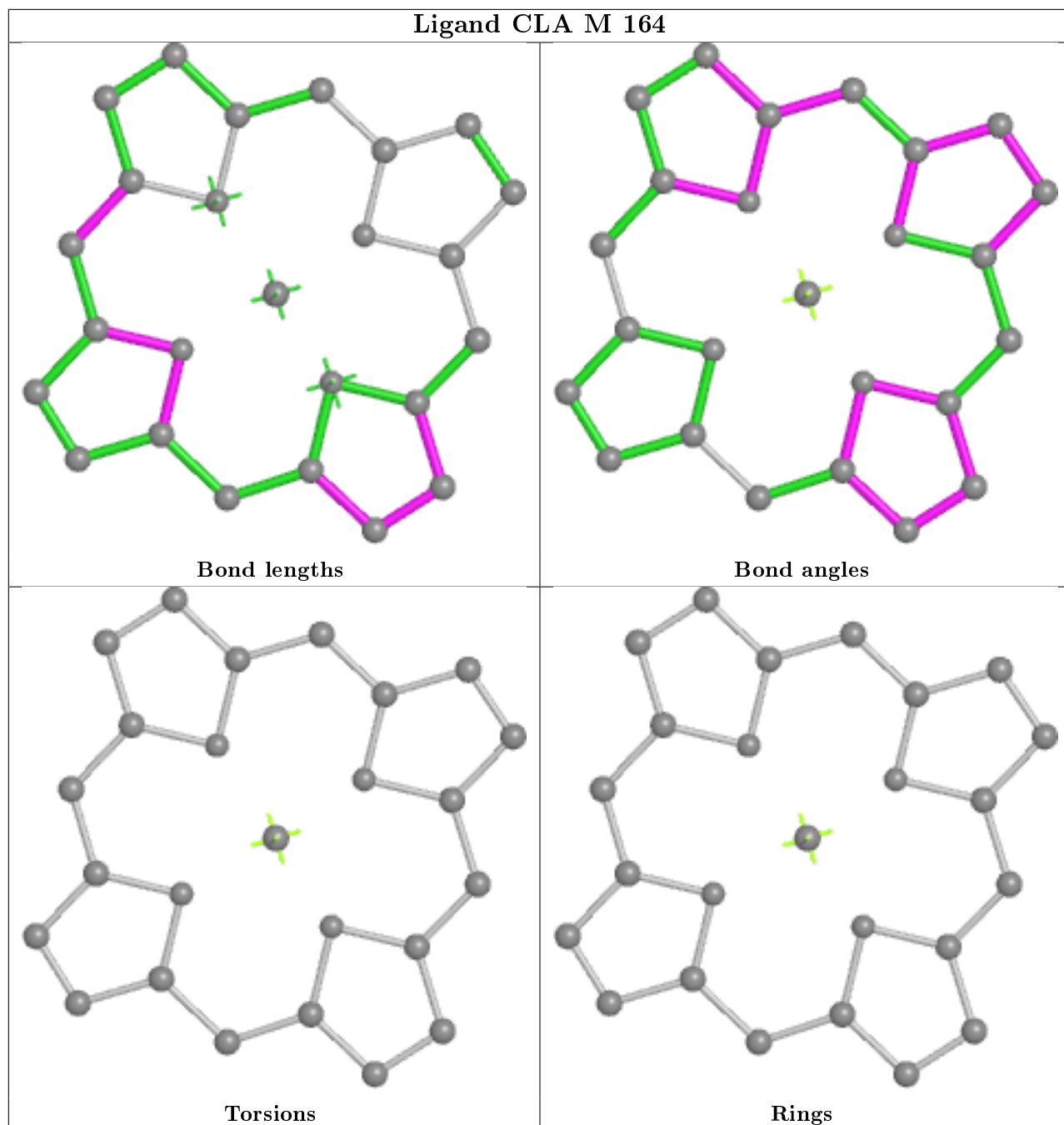




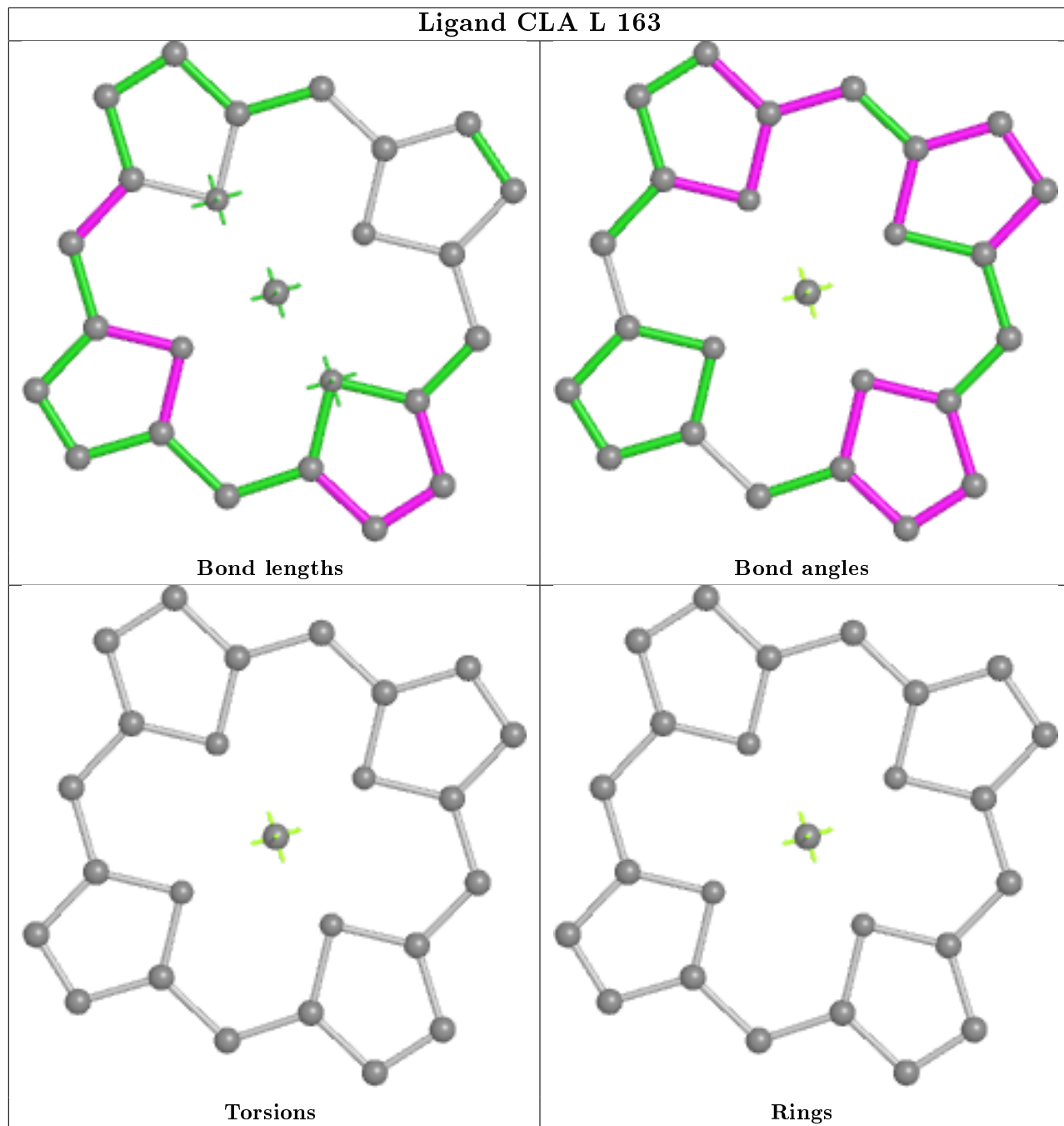


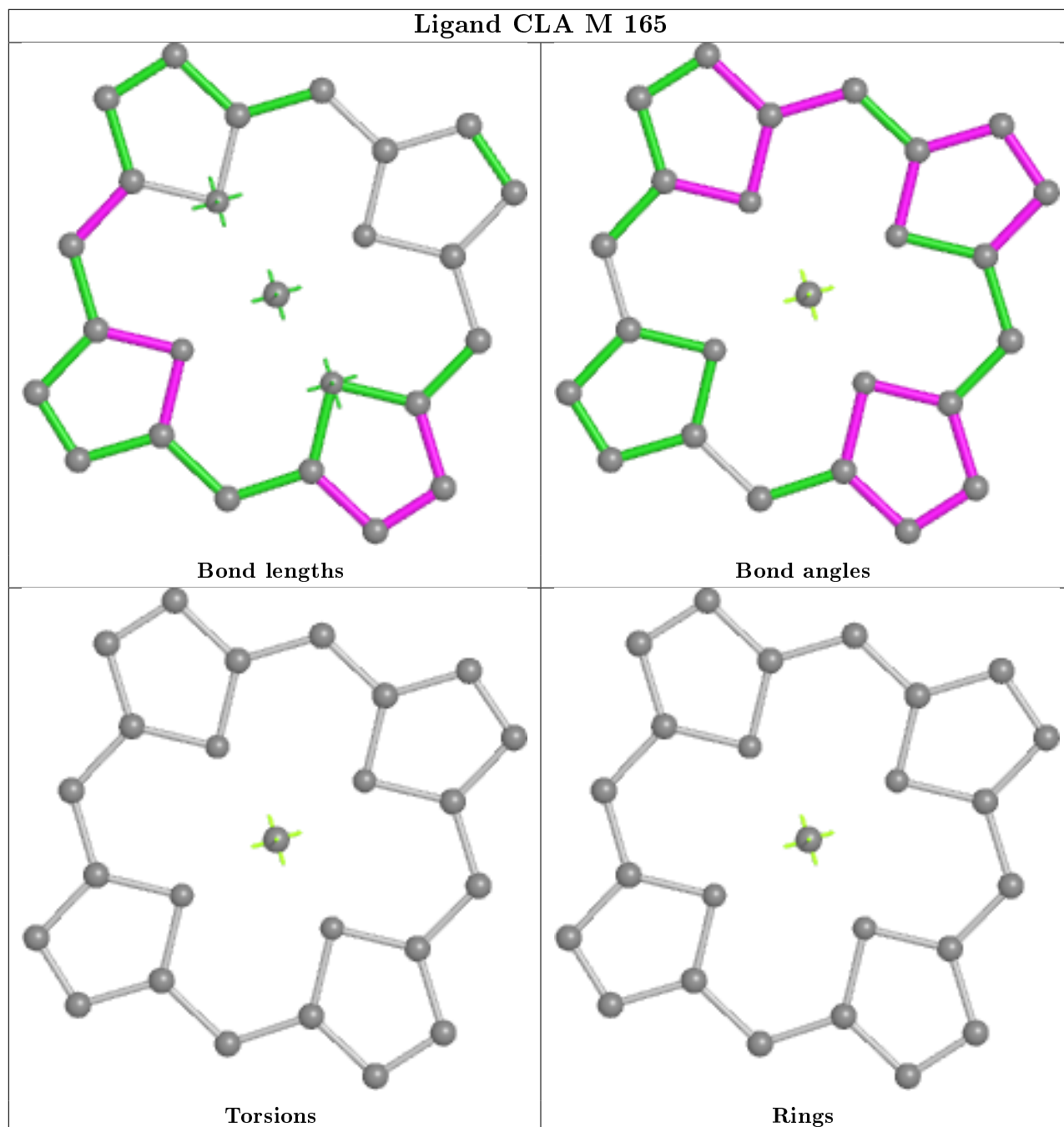


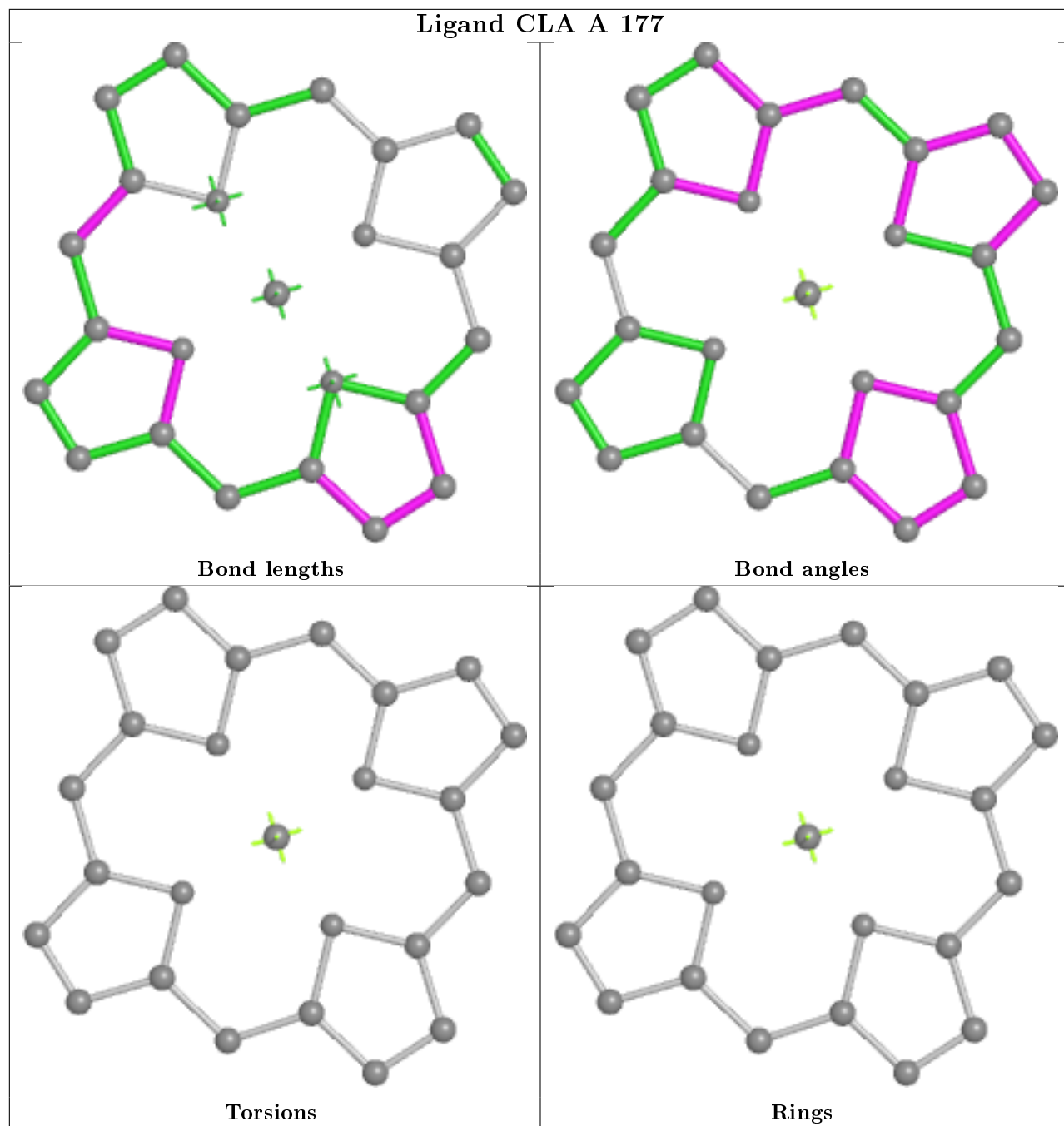


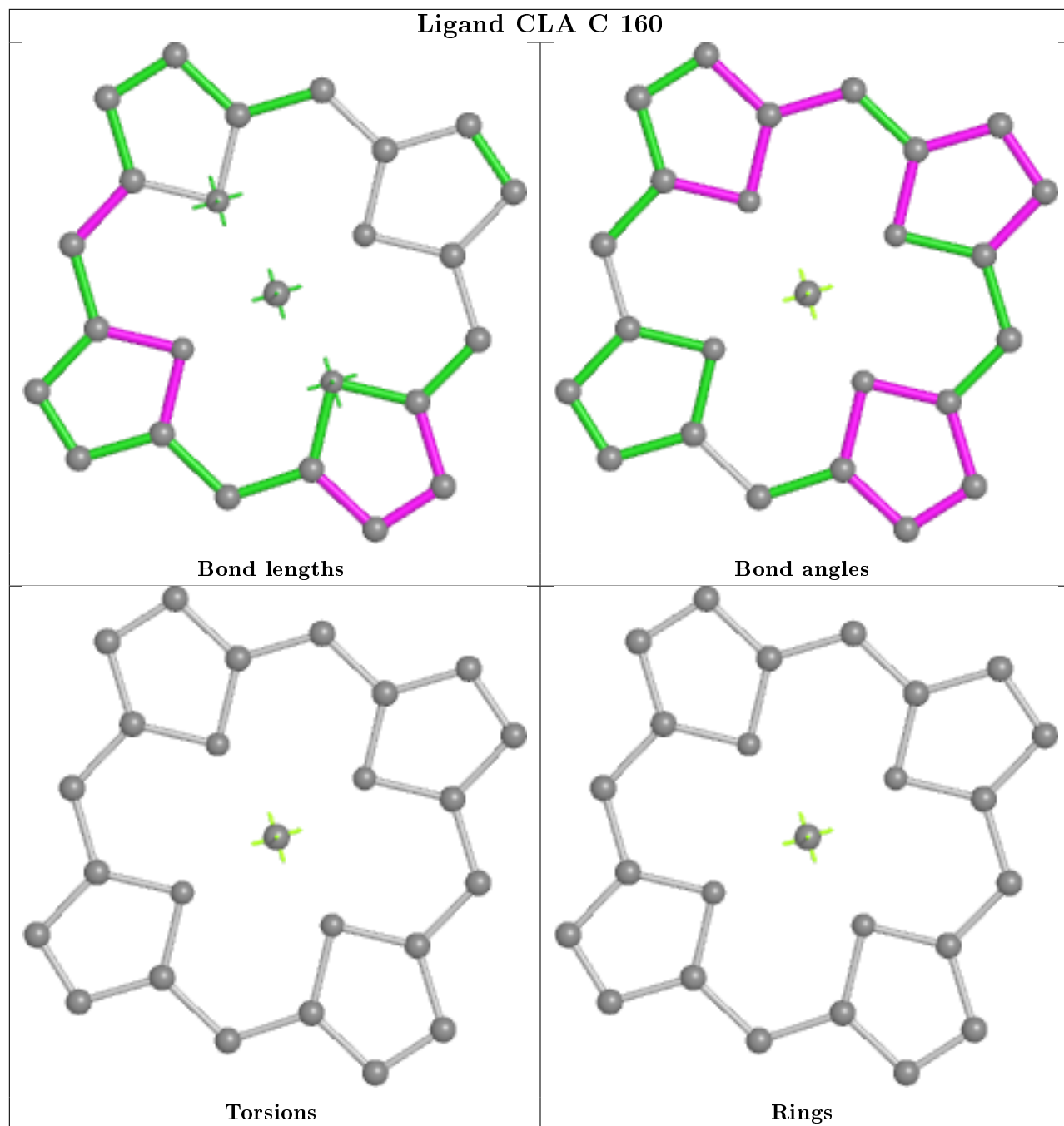


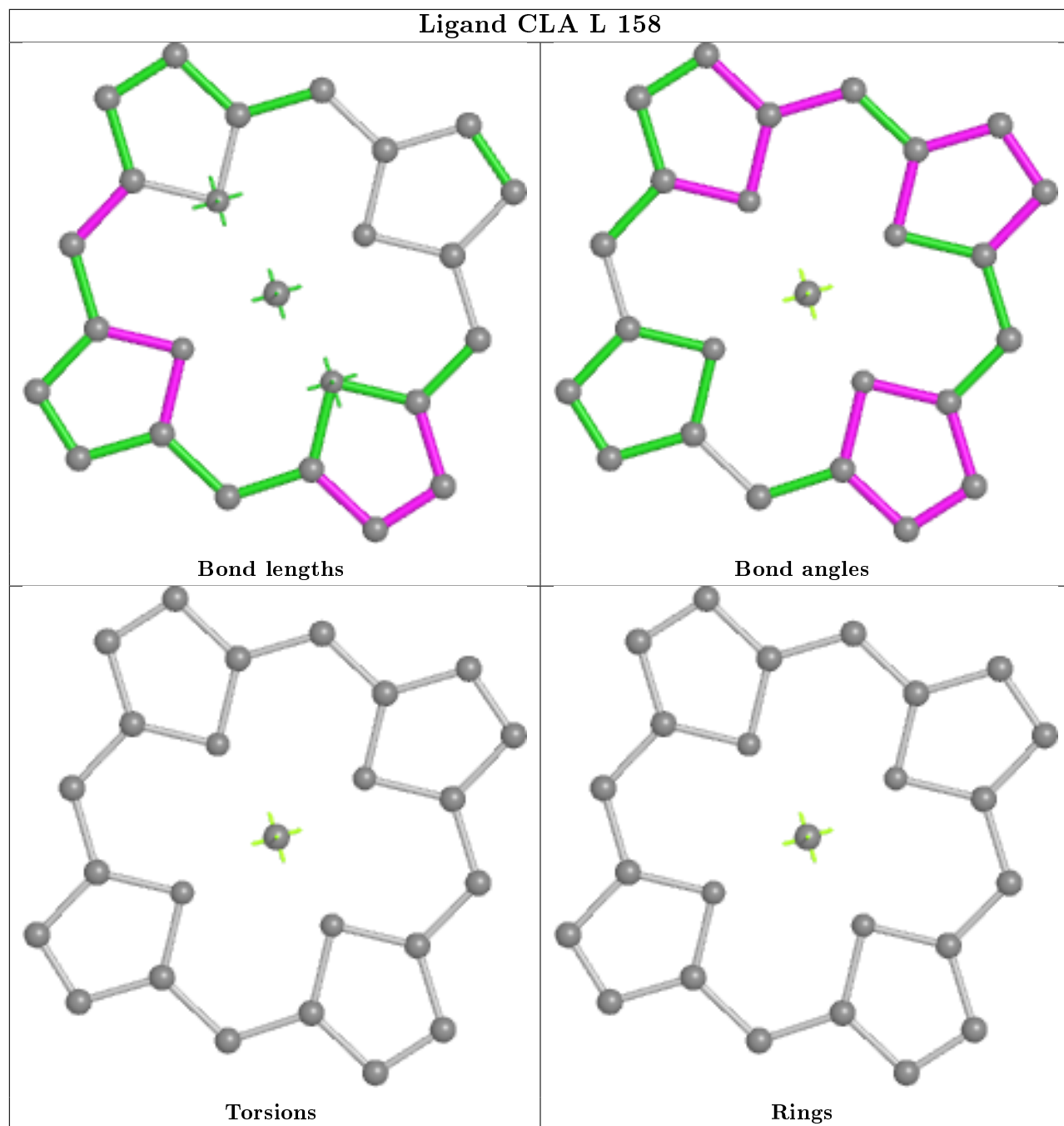
Ligand CLA L 163

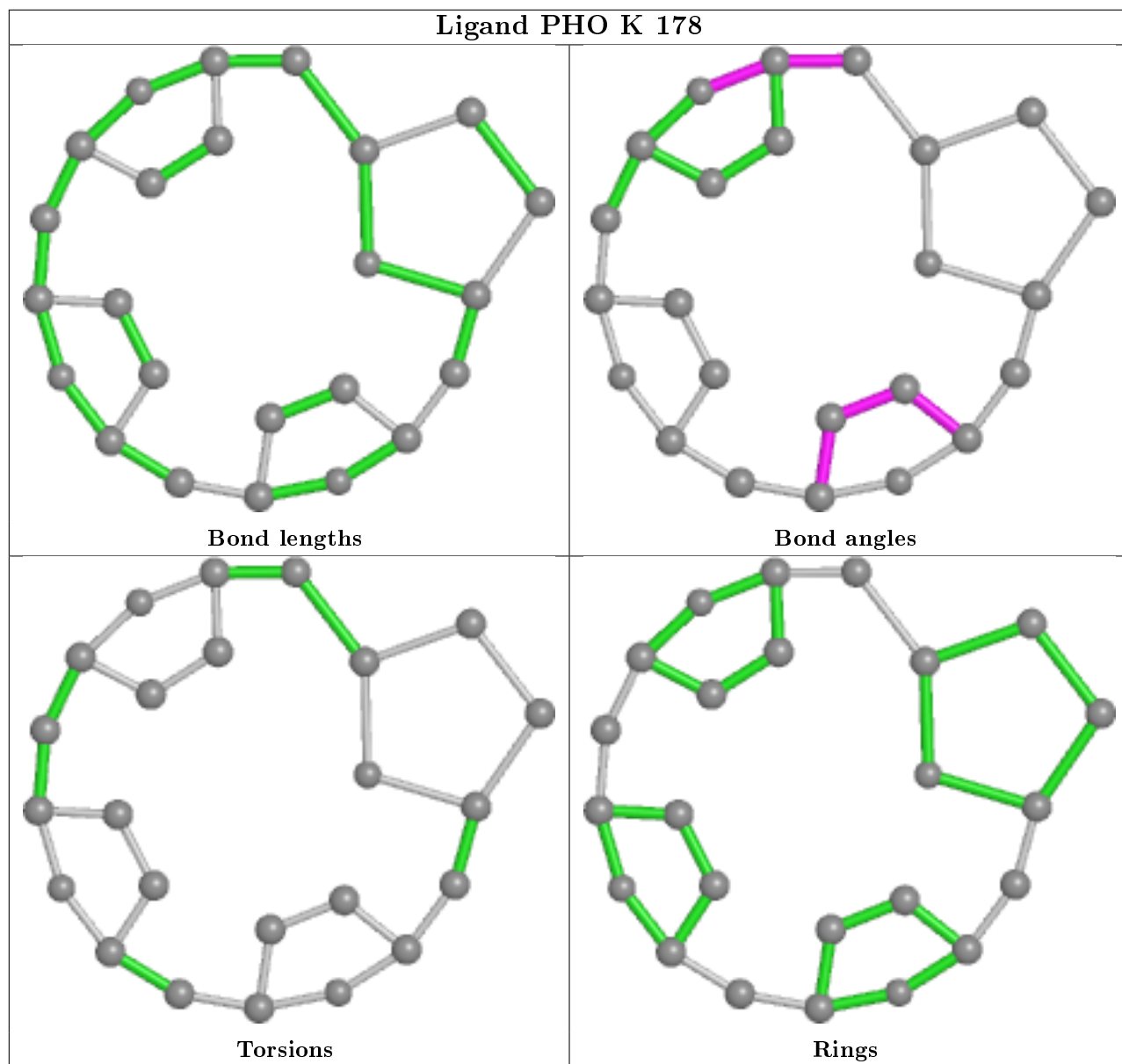


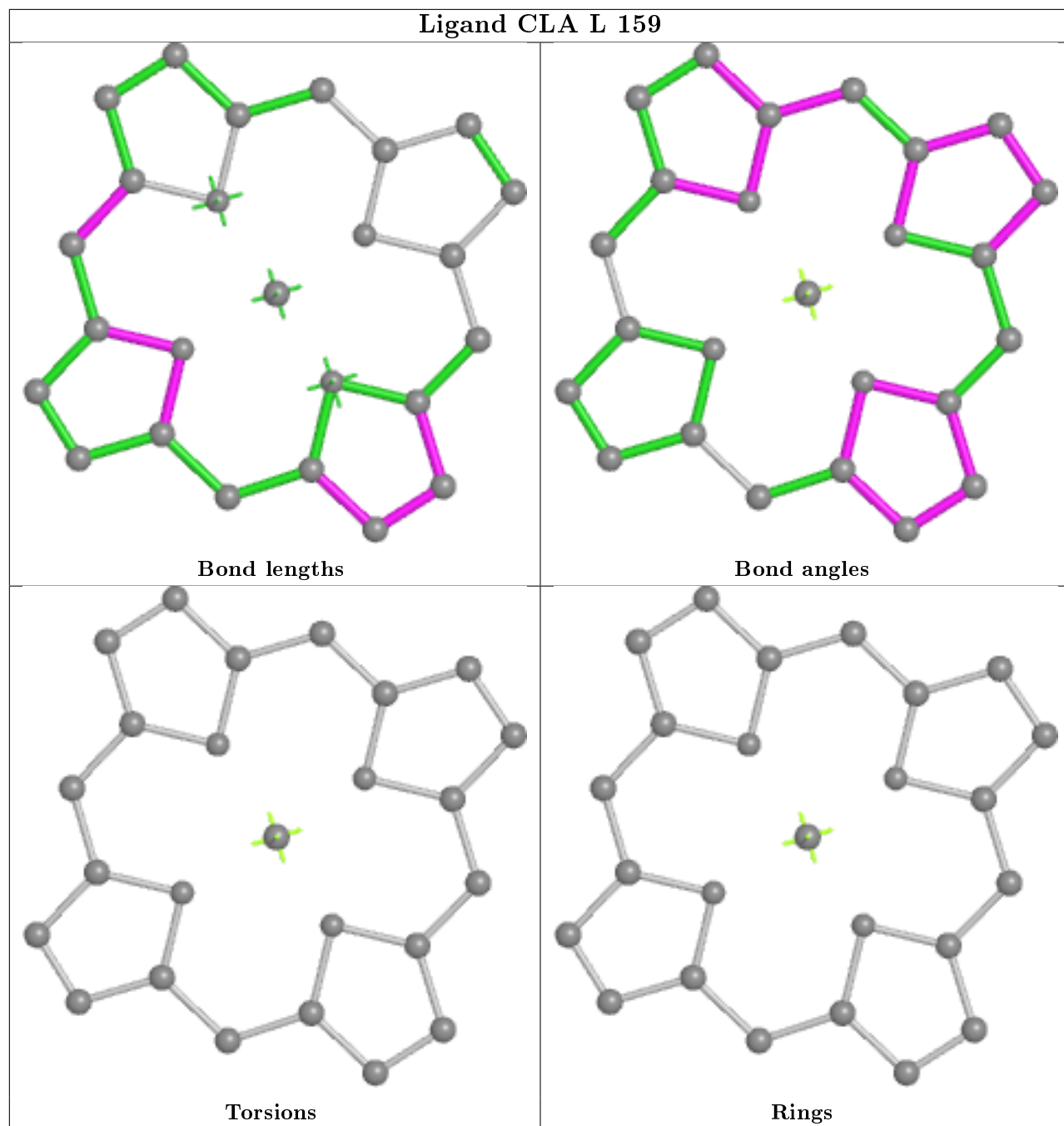


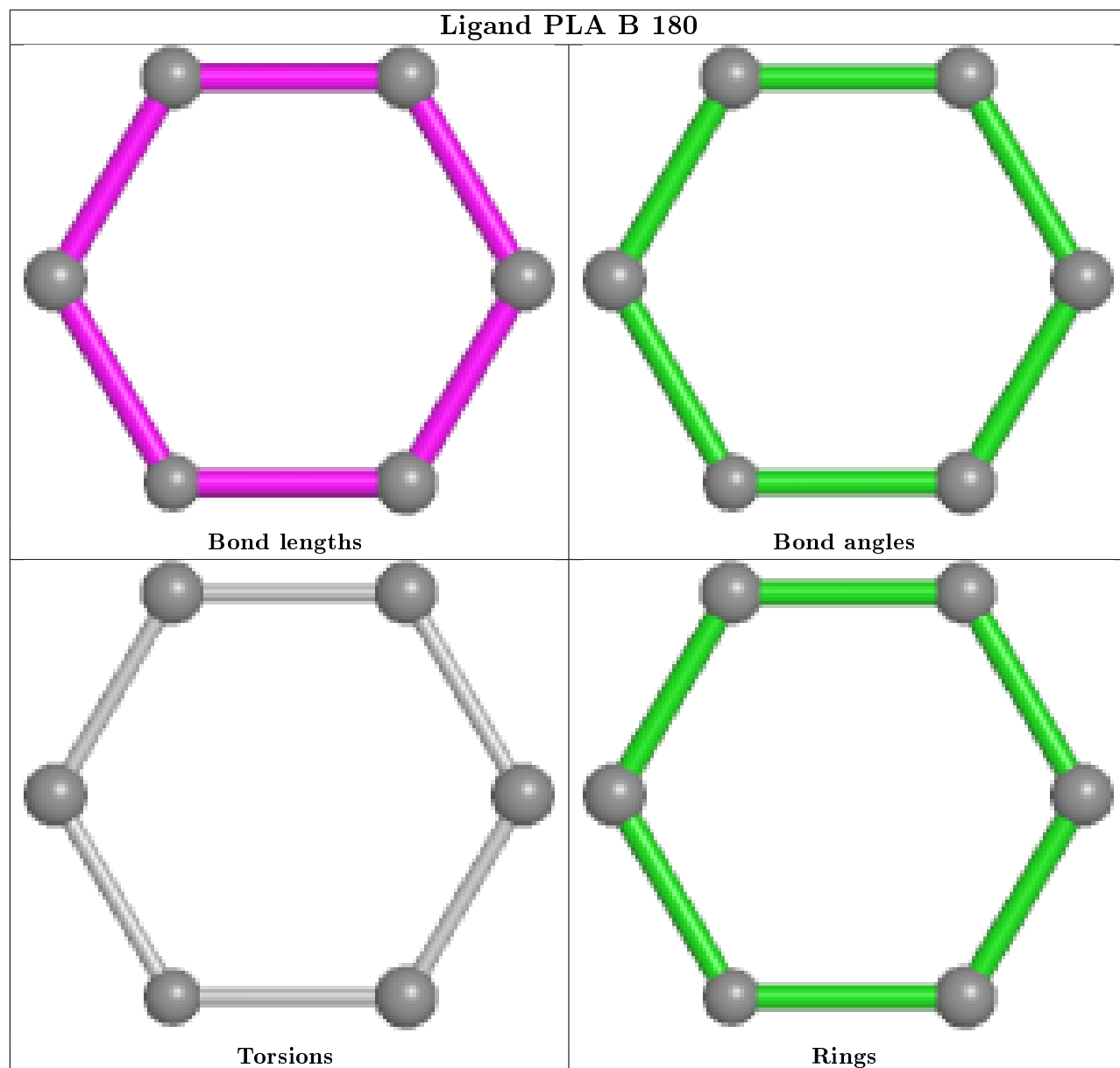




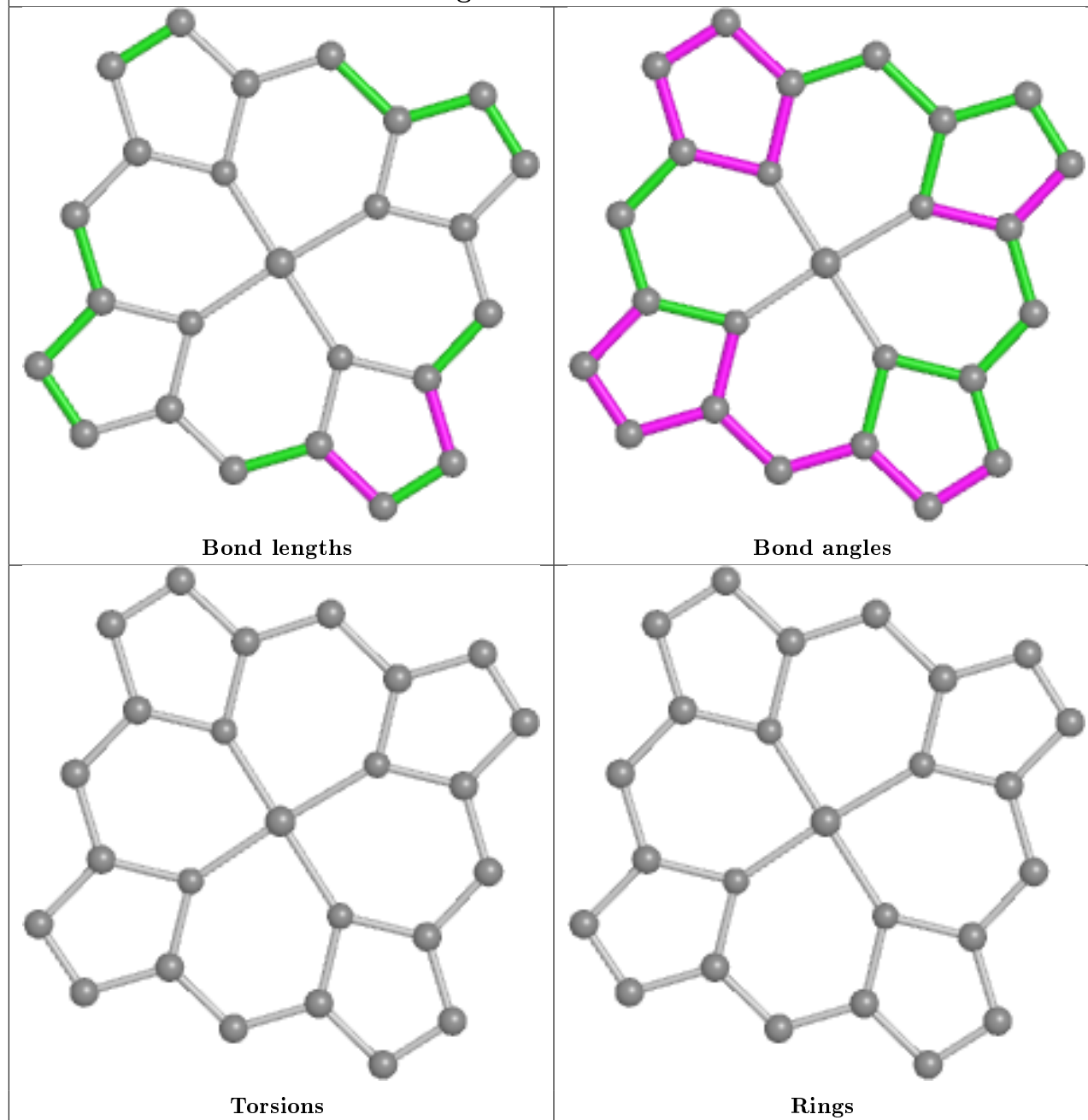


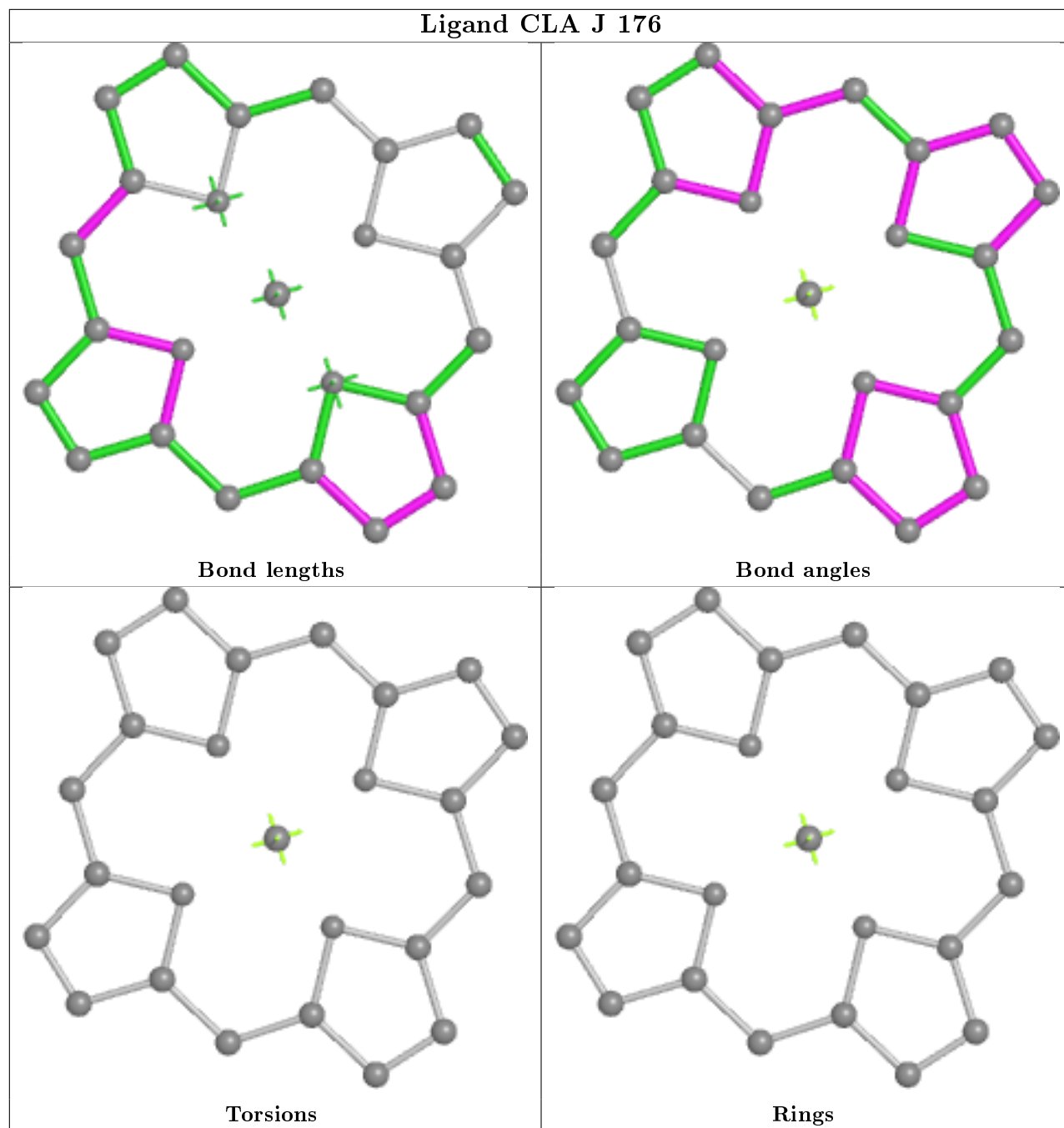


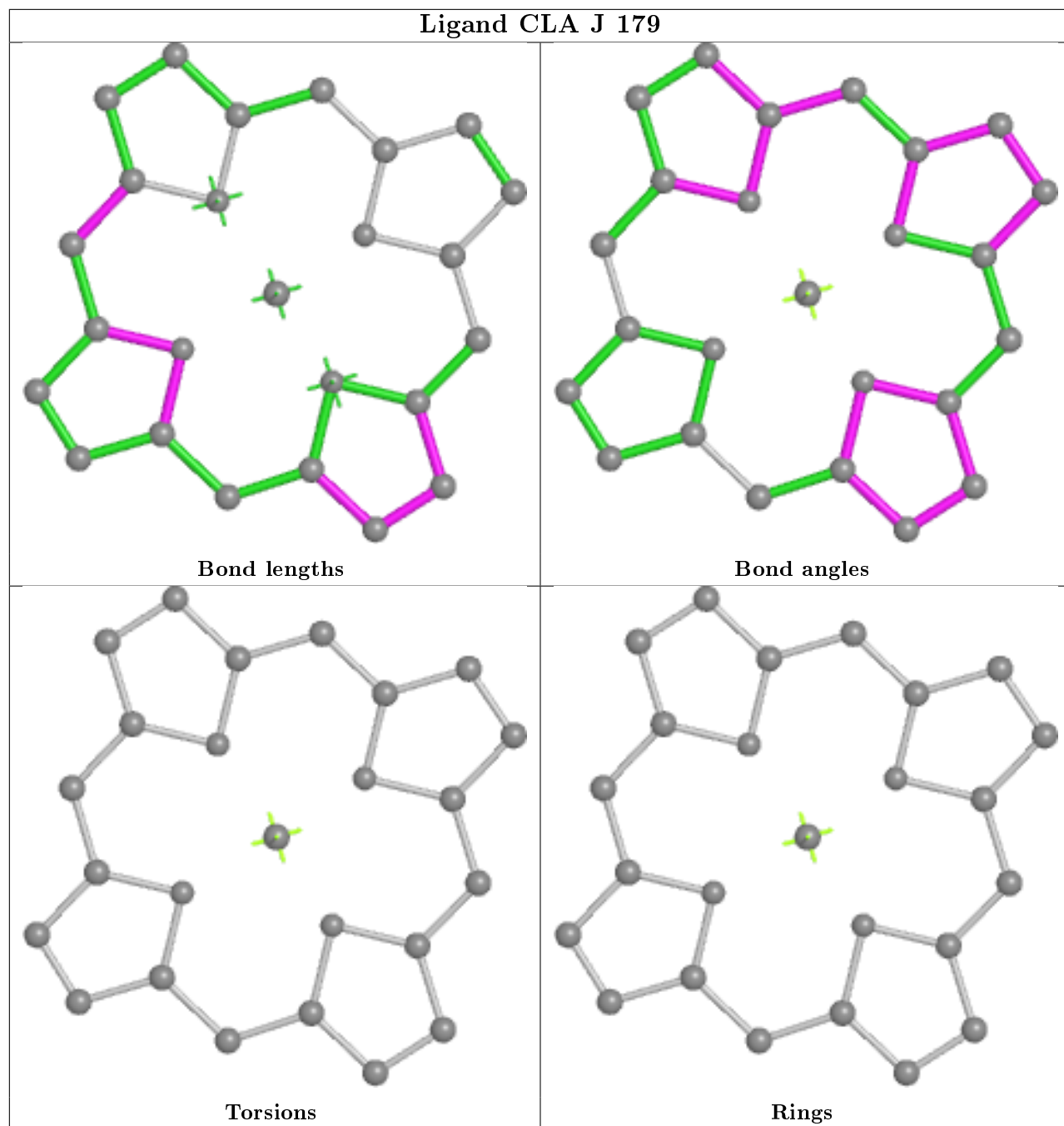


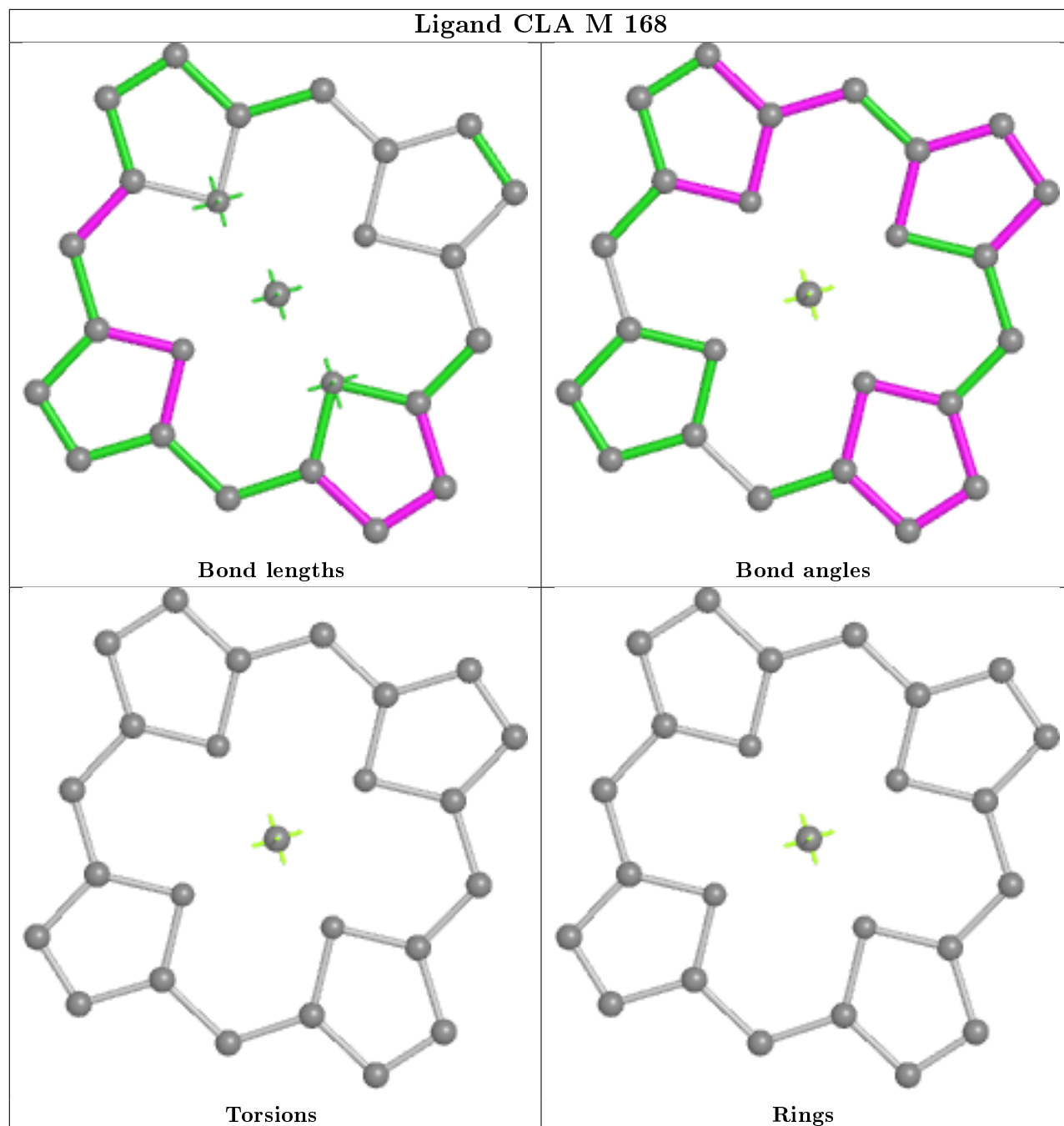


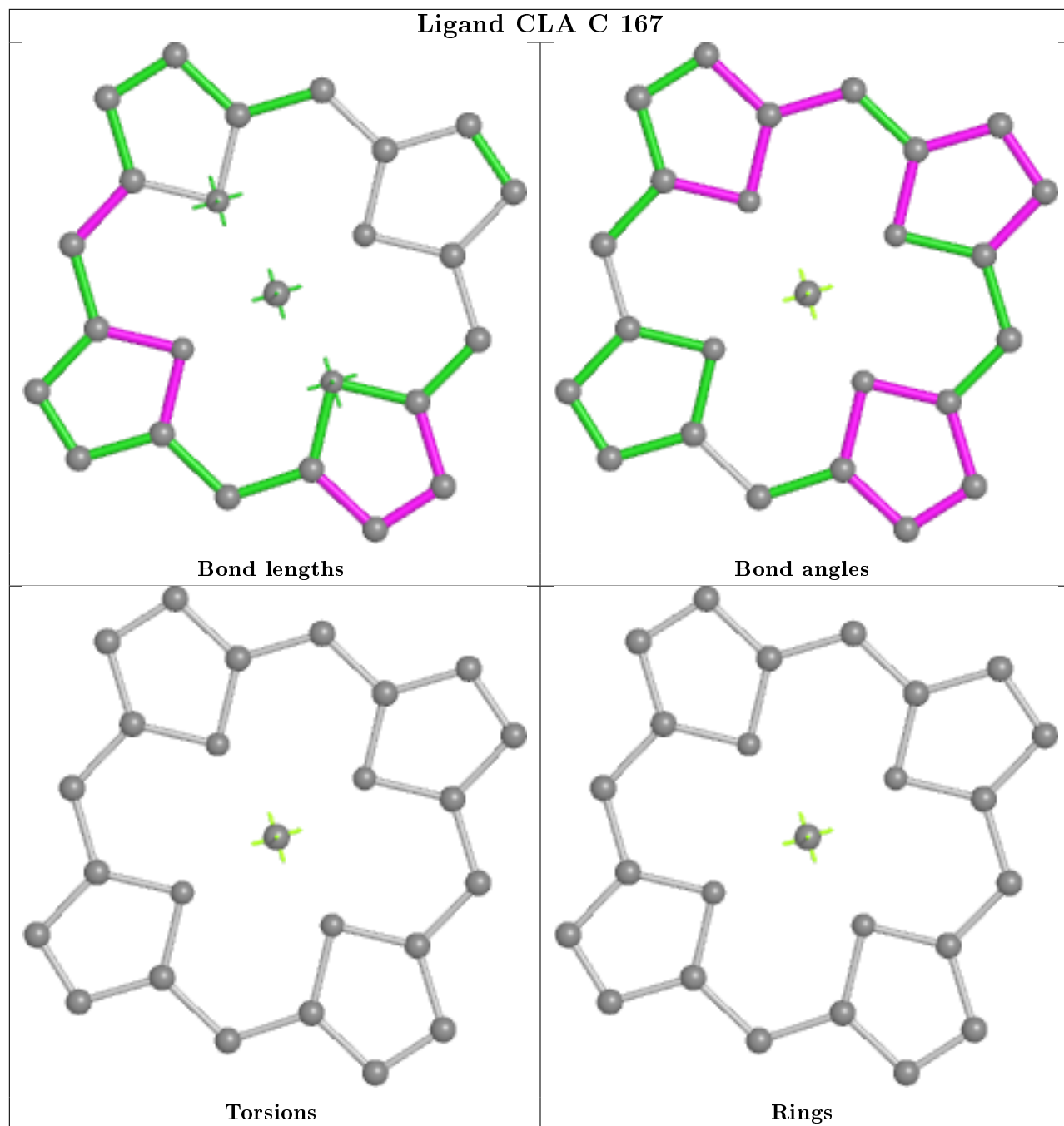
Ligand HEM R 88



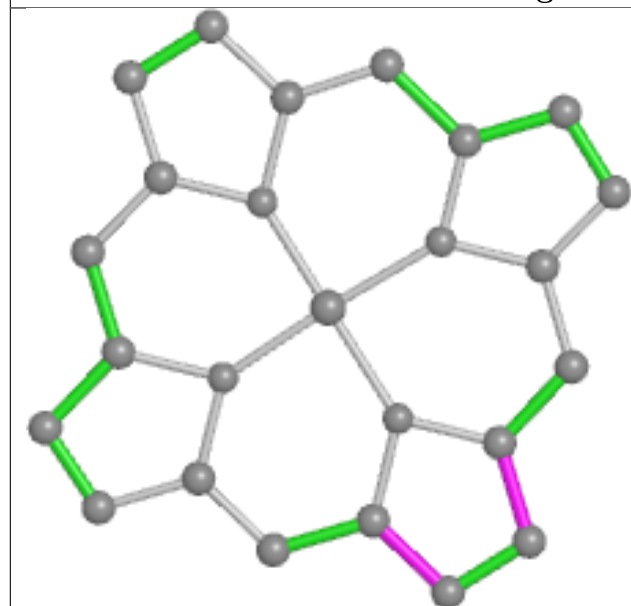




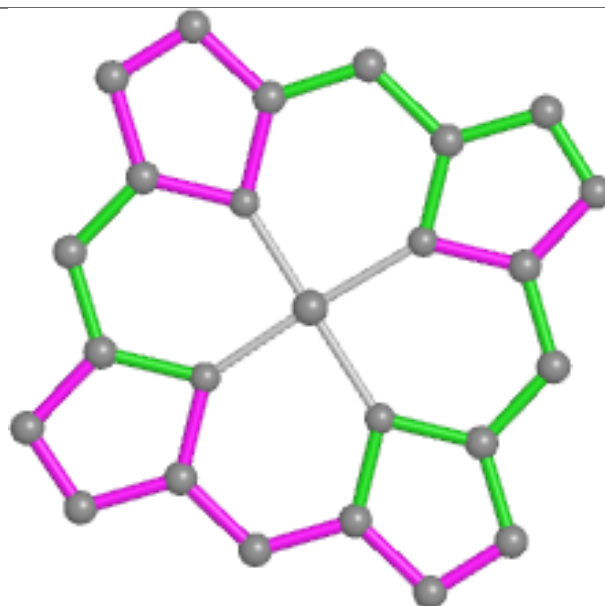




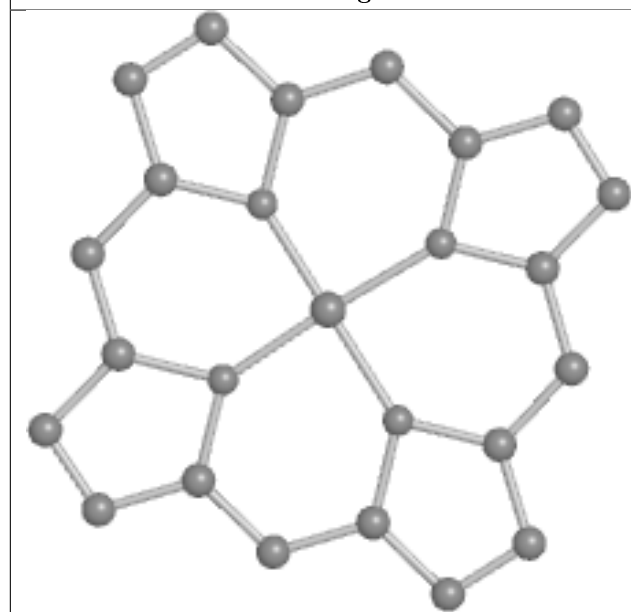
Ligand HEM F 31



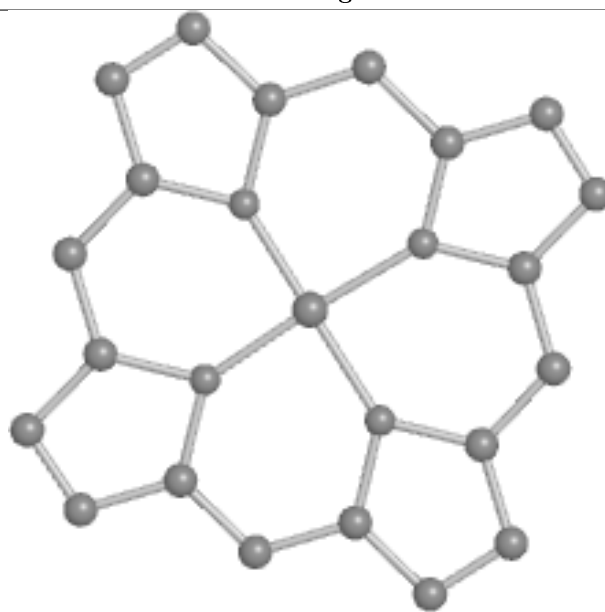
Bond lengths



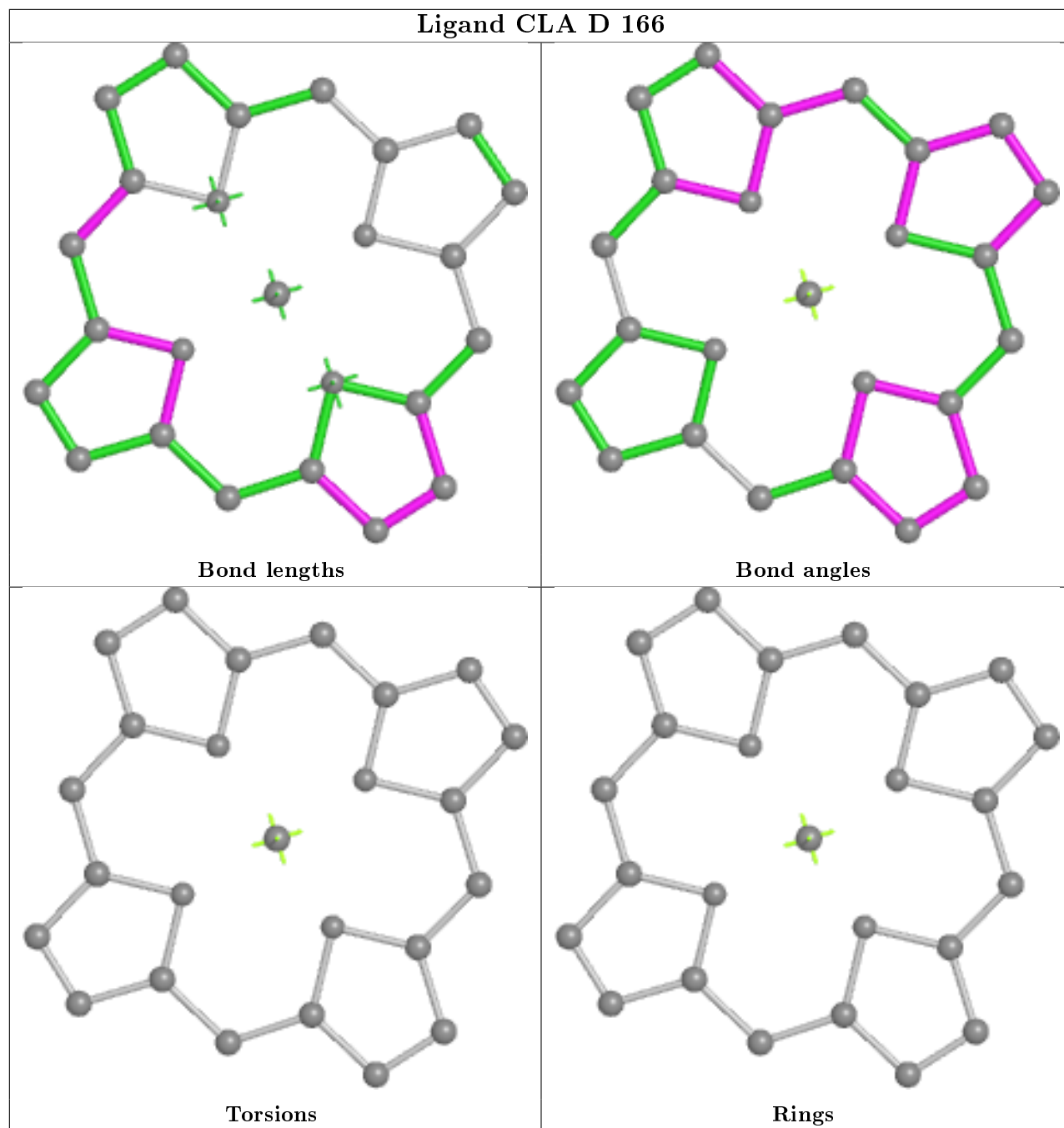
Bond angles

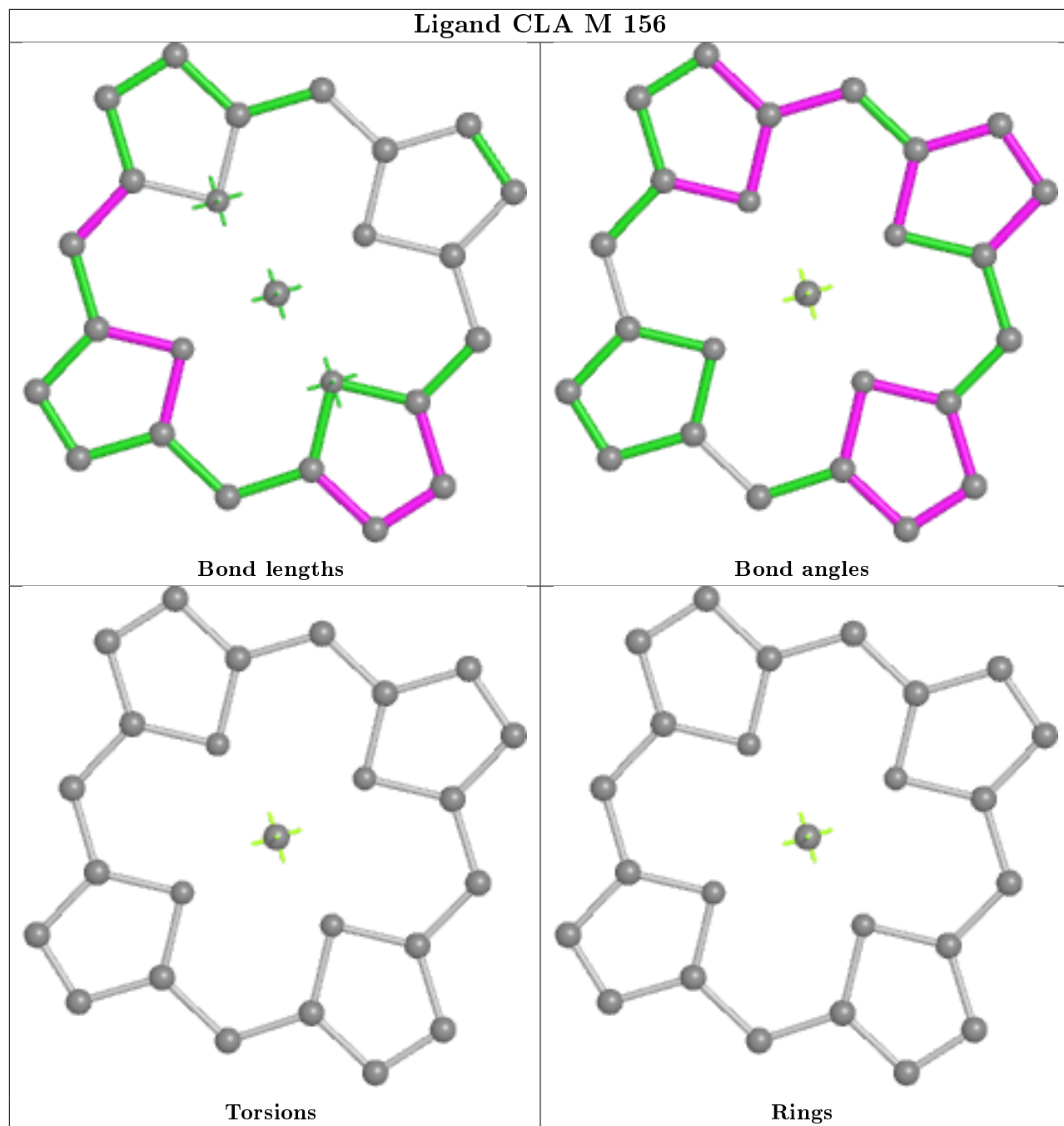


Torsions

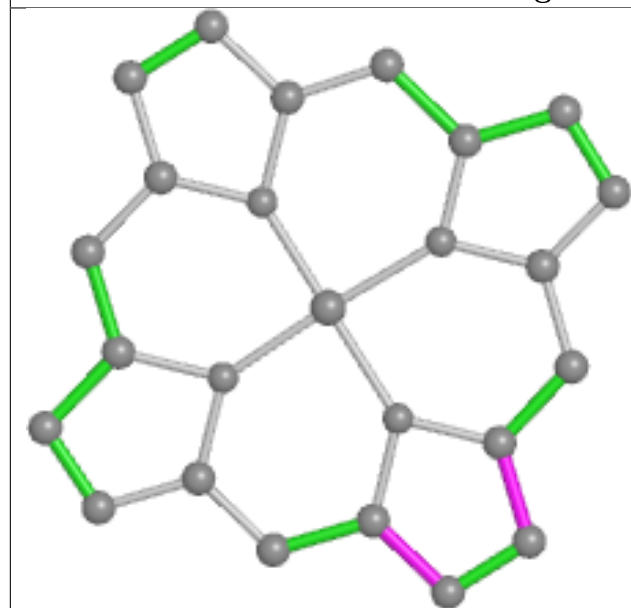


Rings

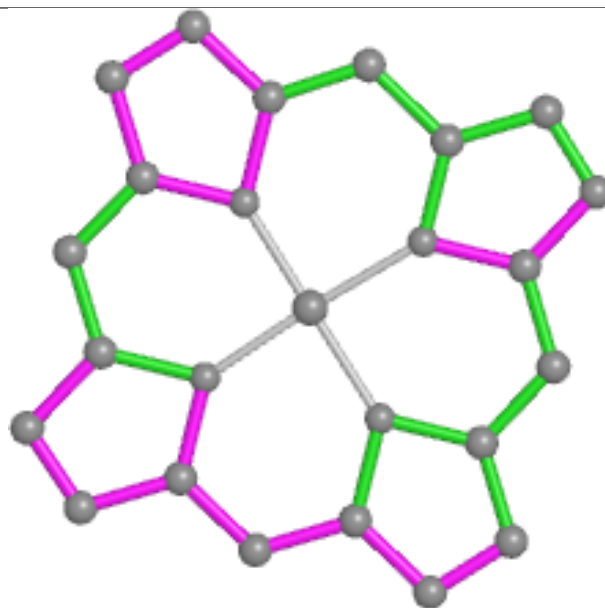




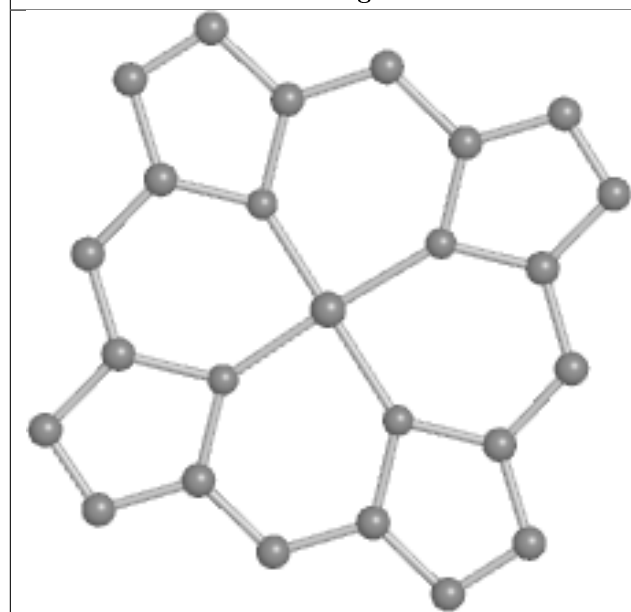
Ligand HEM O 58



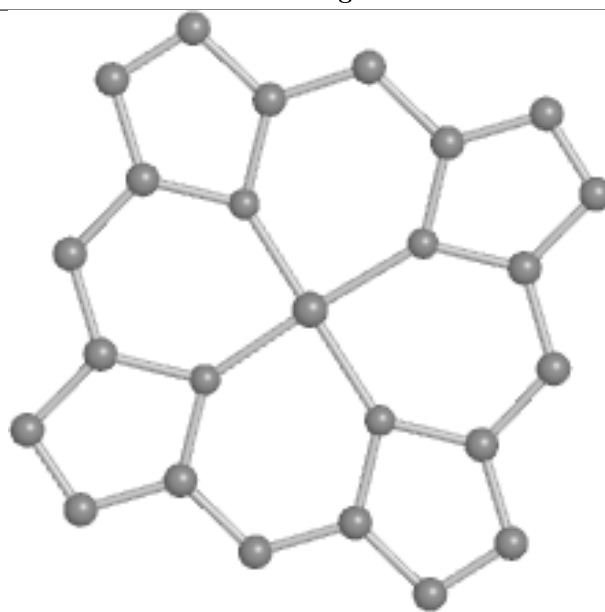
Bond lengths



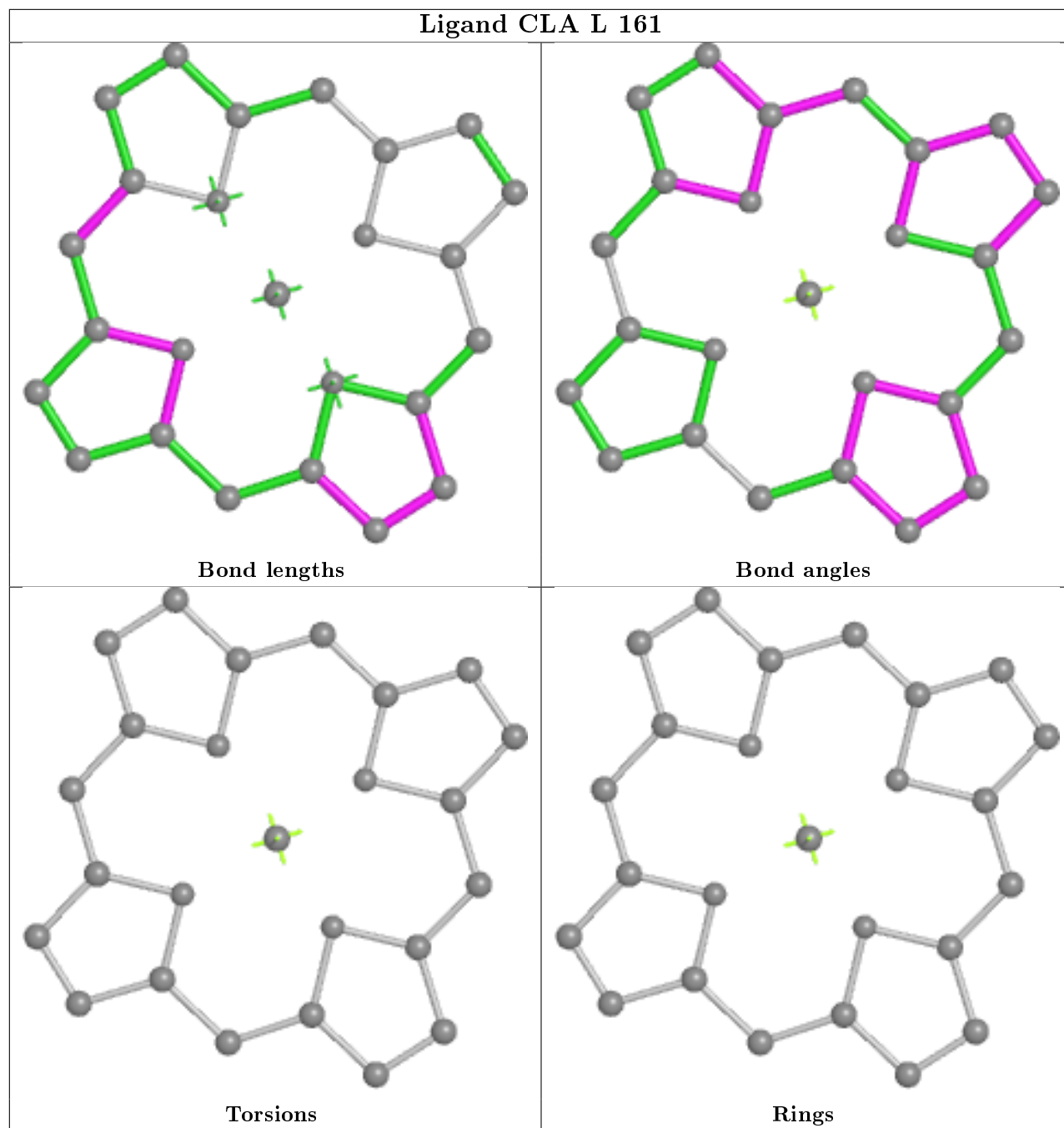
Bond angles

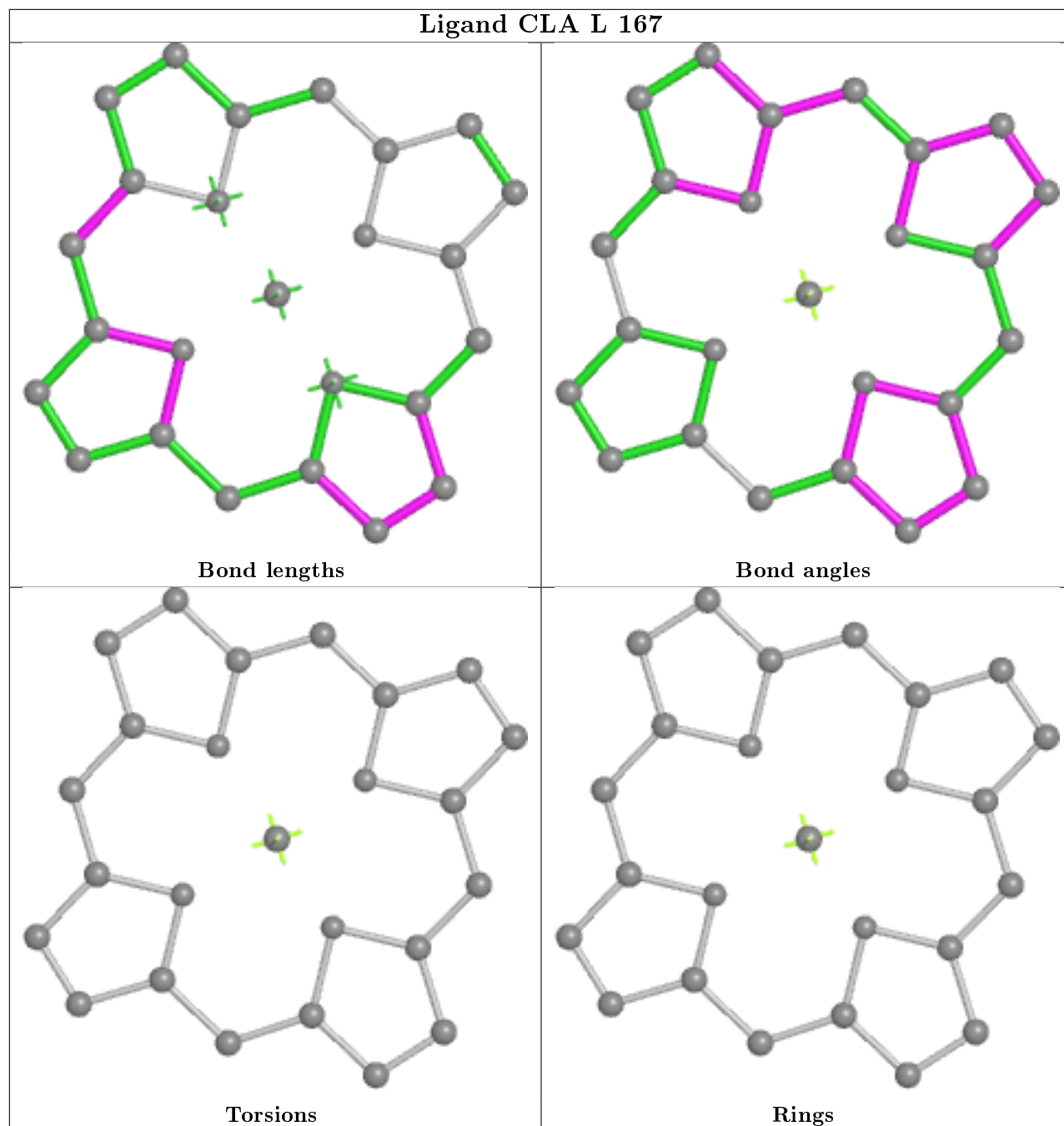


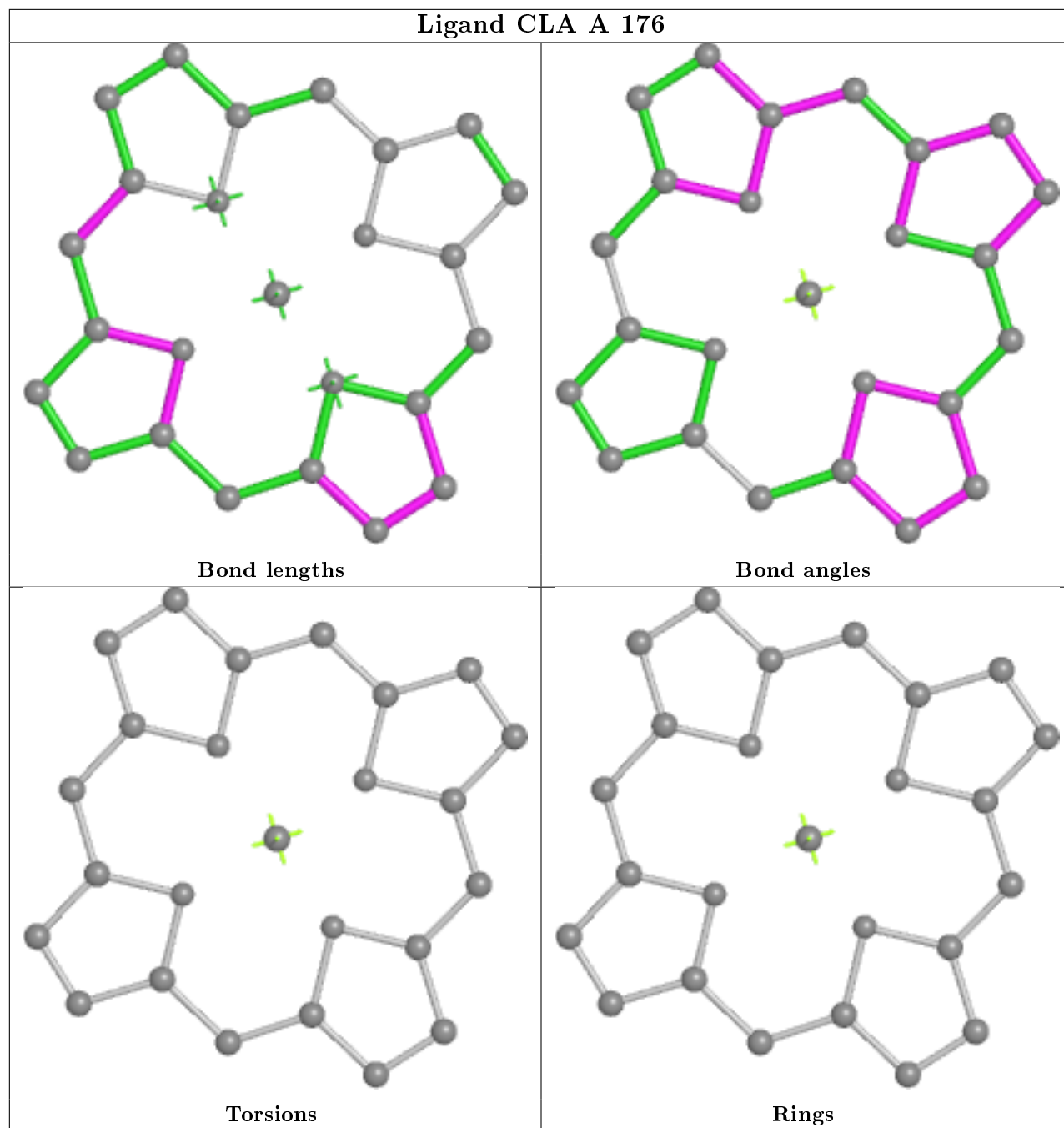
Torsions

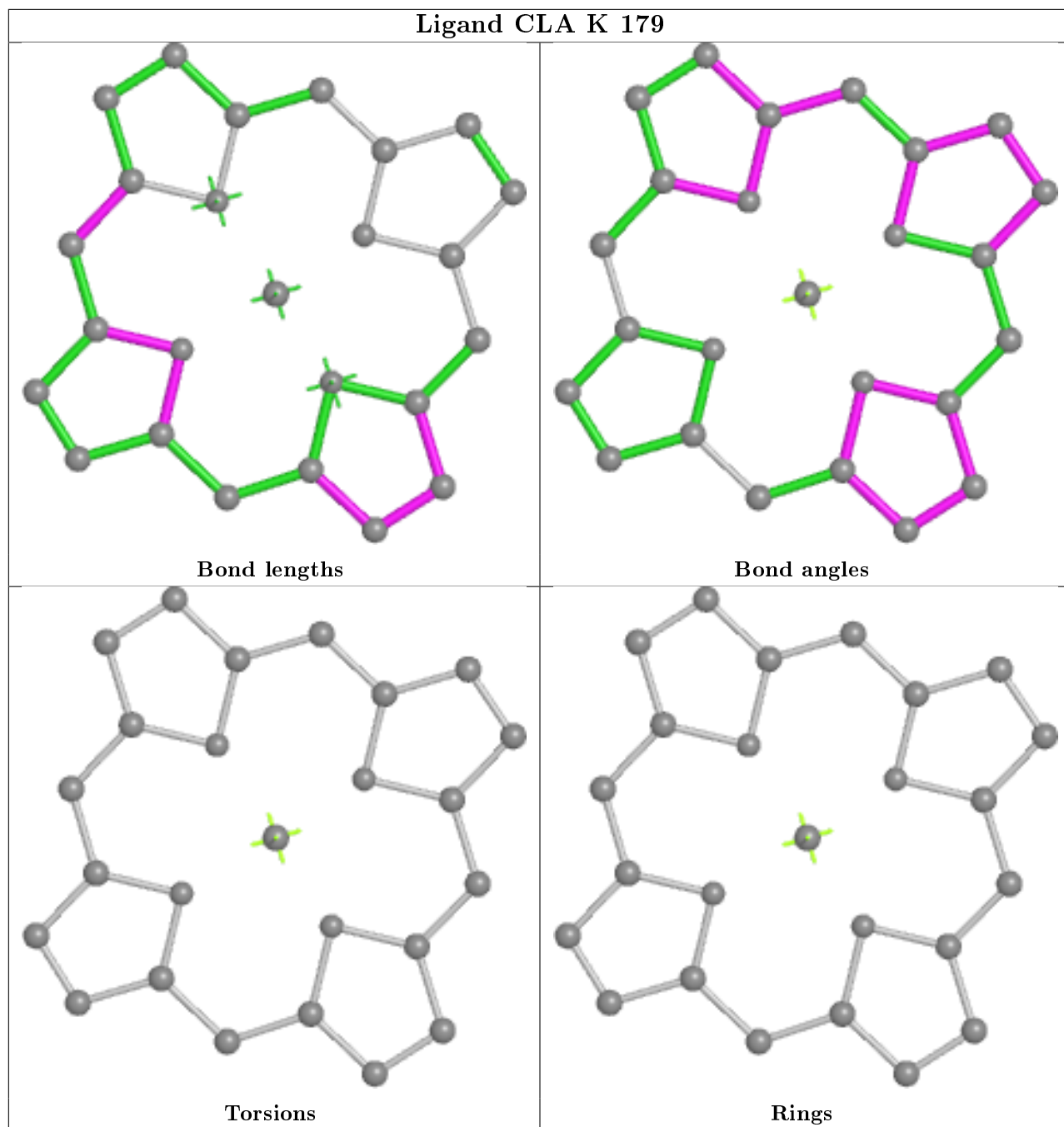


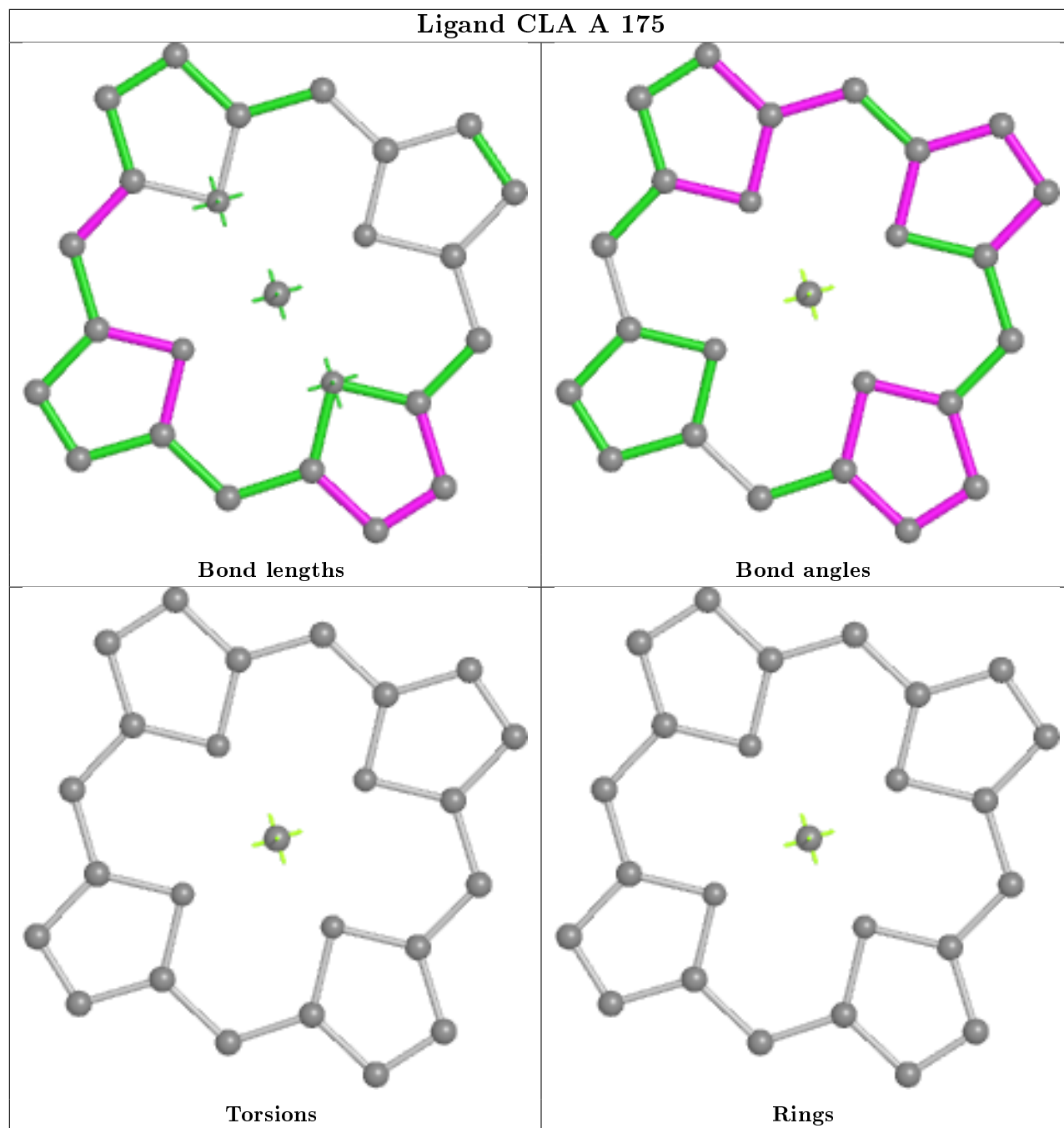
Rings

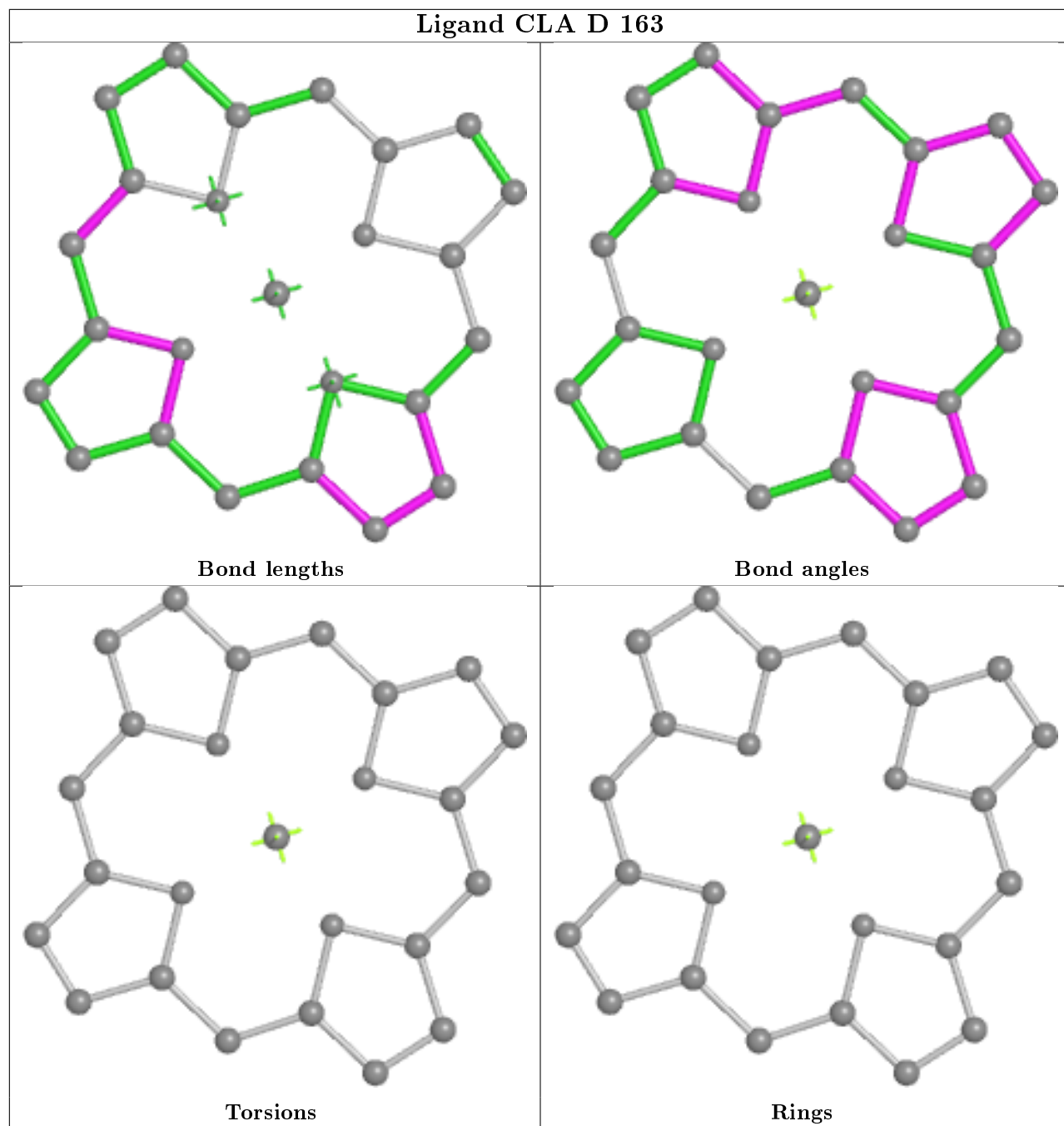


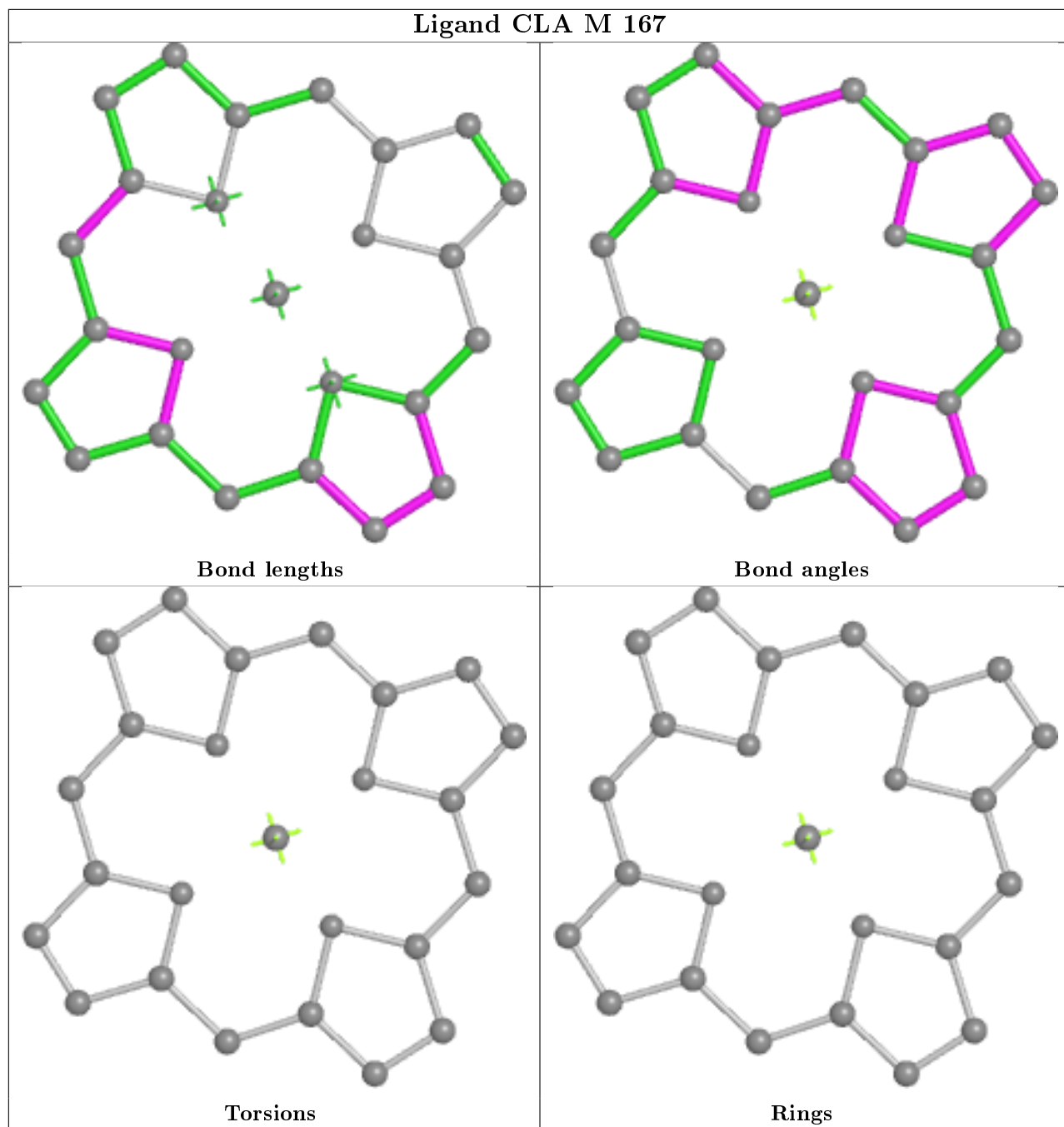


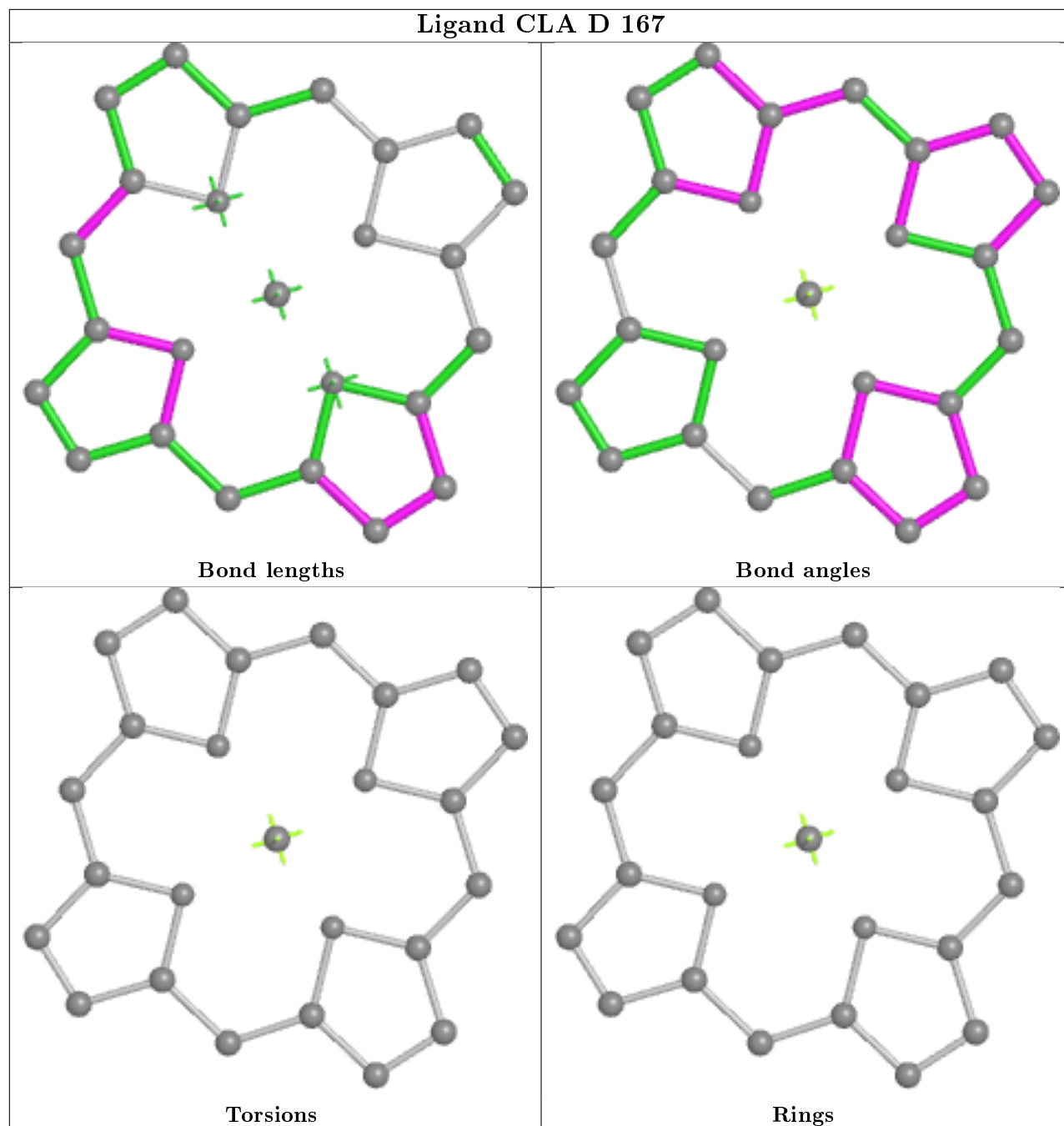


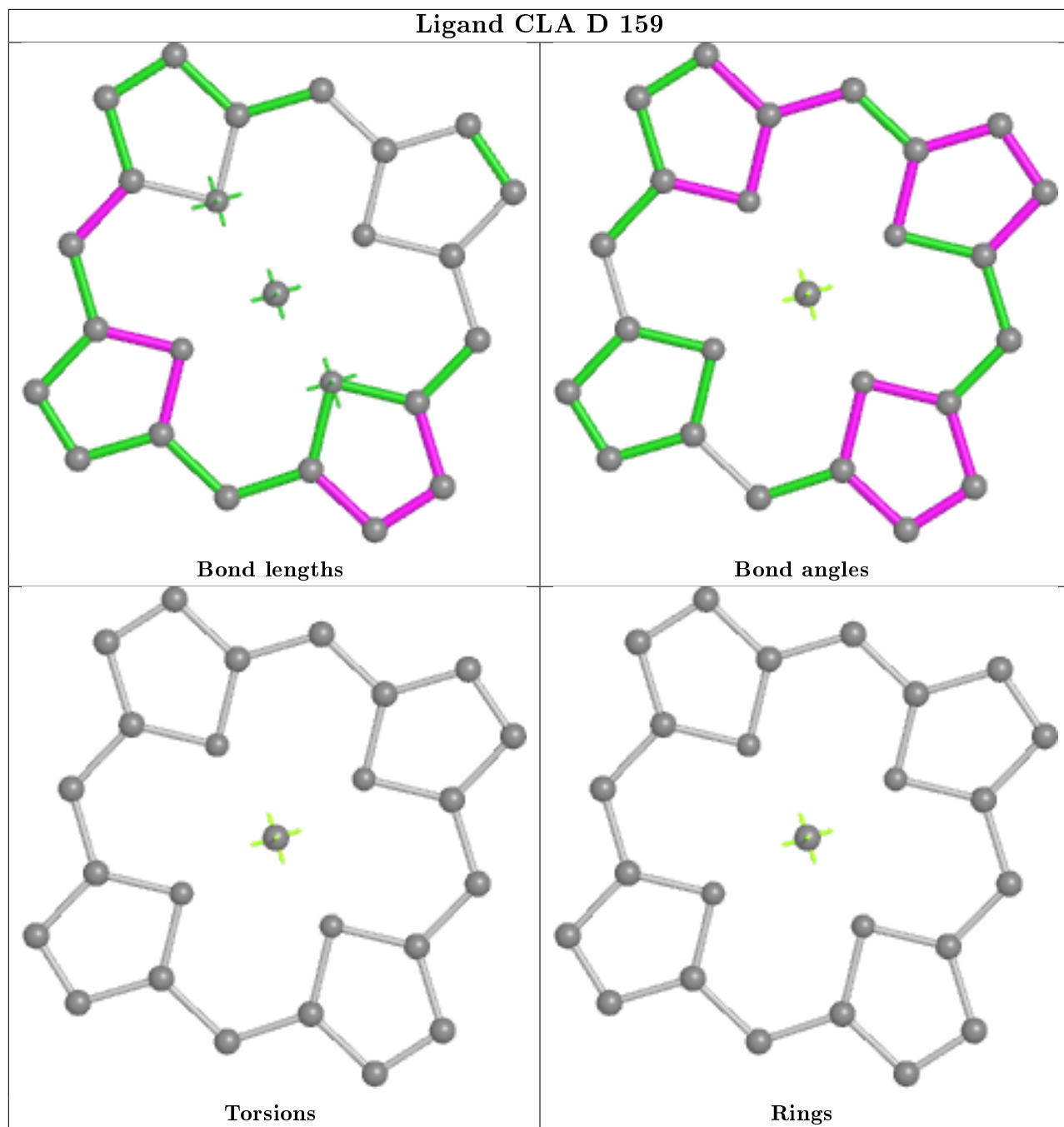


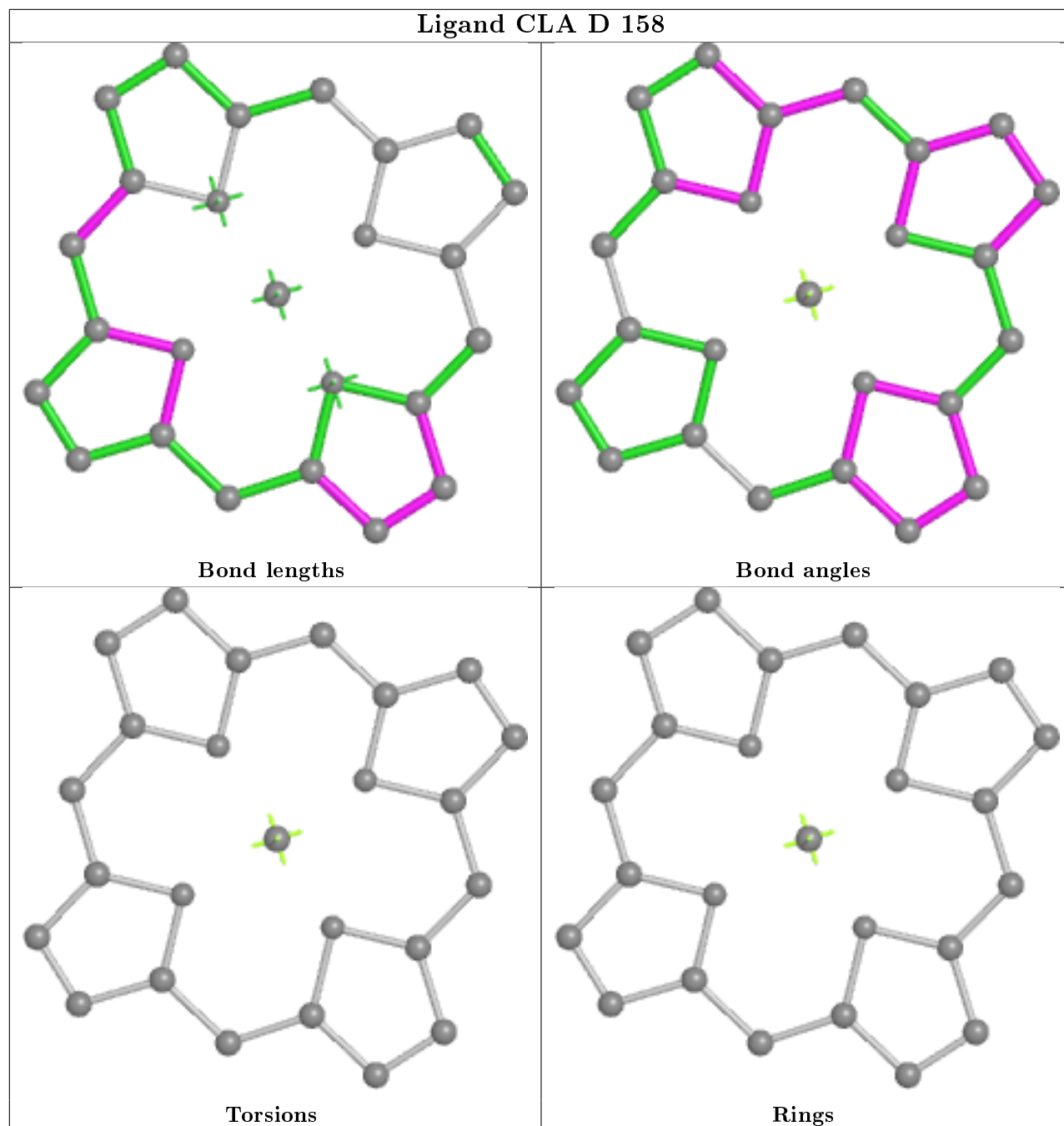


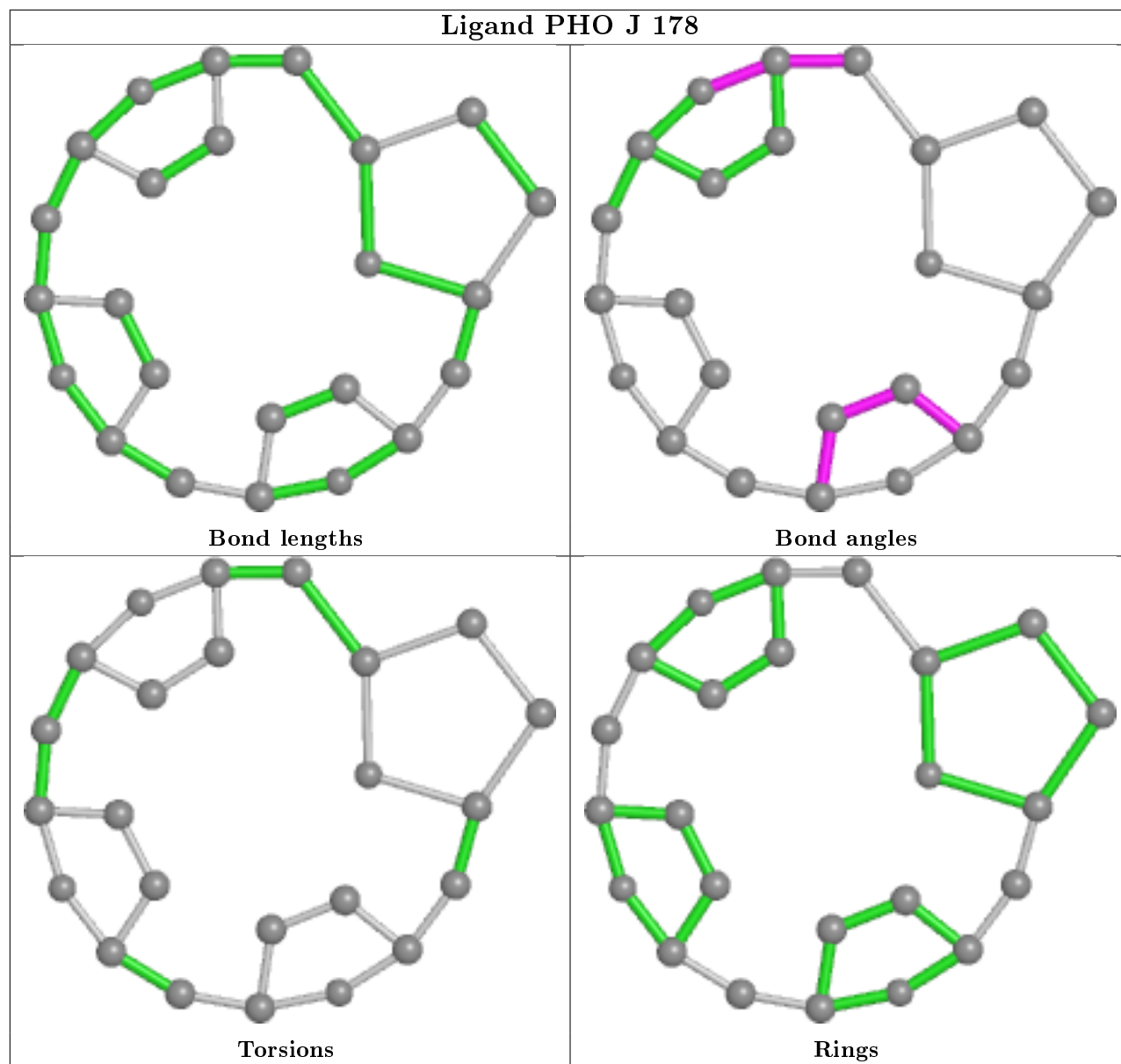


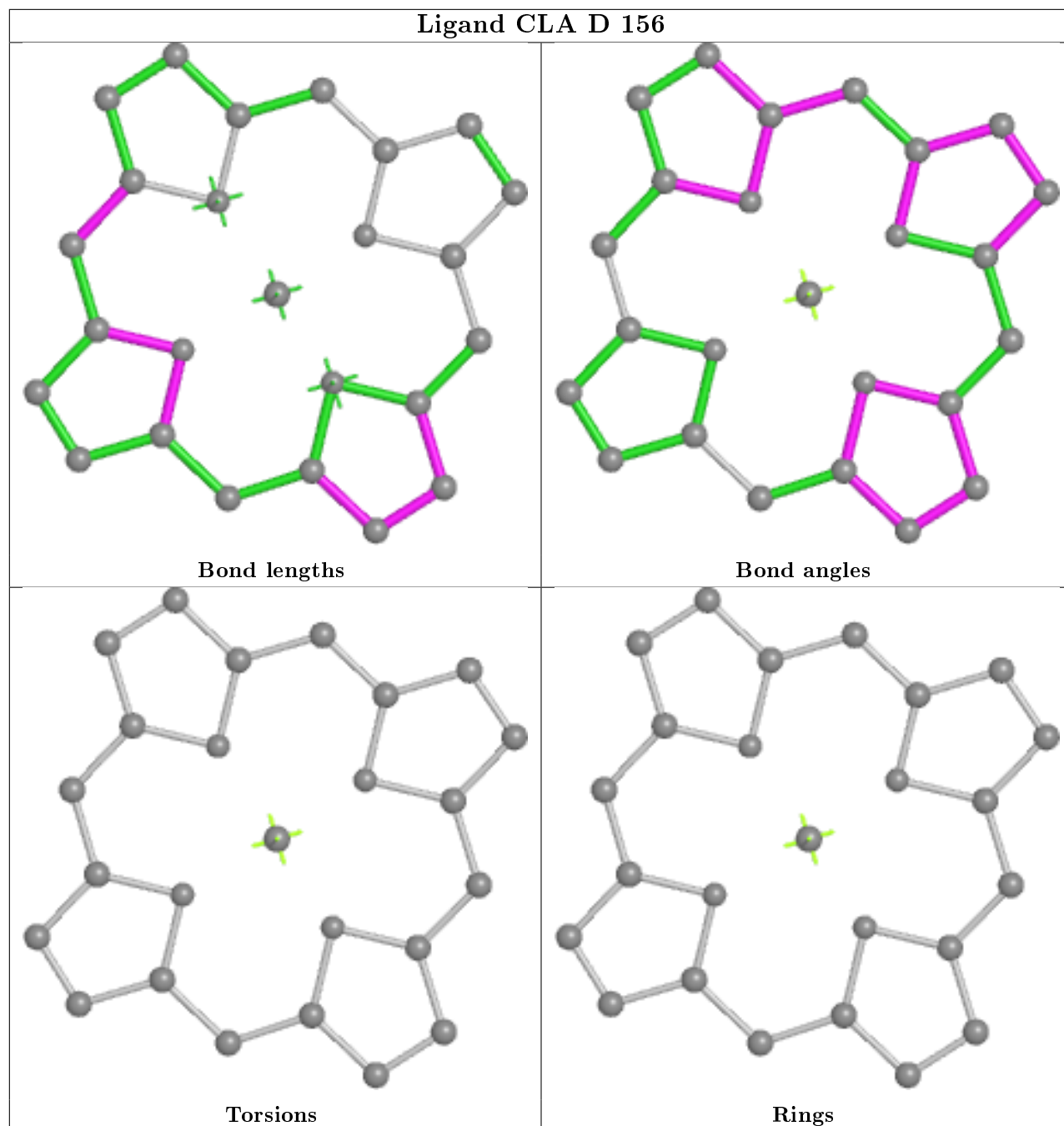


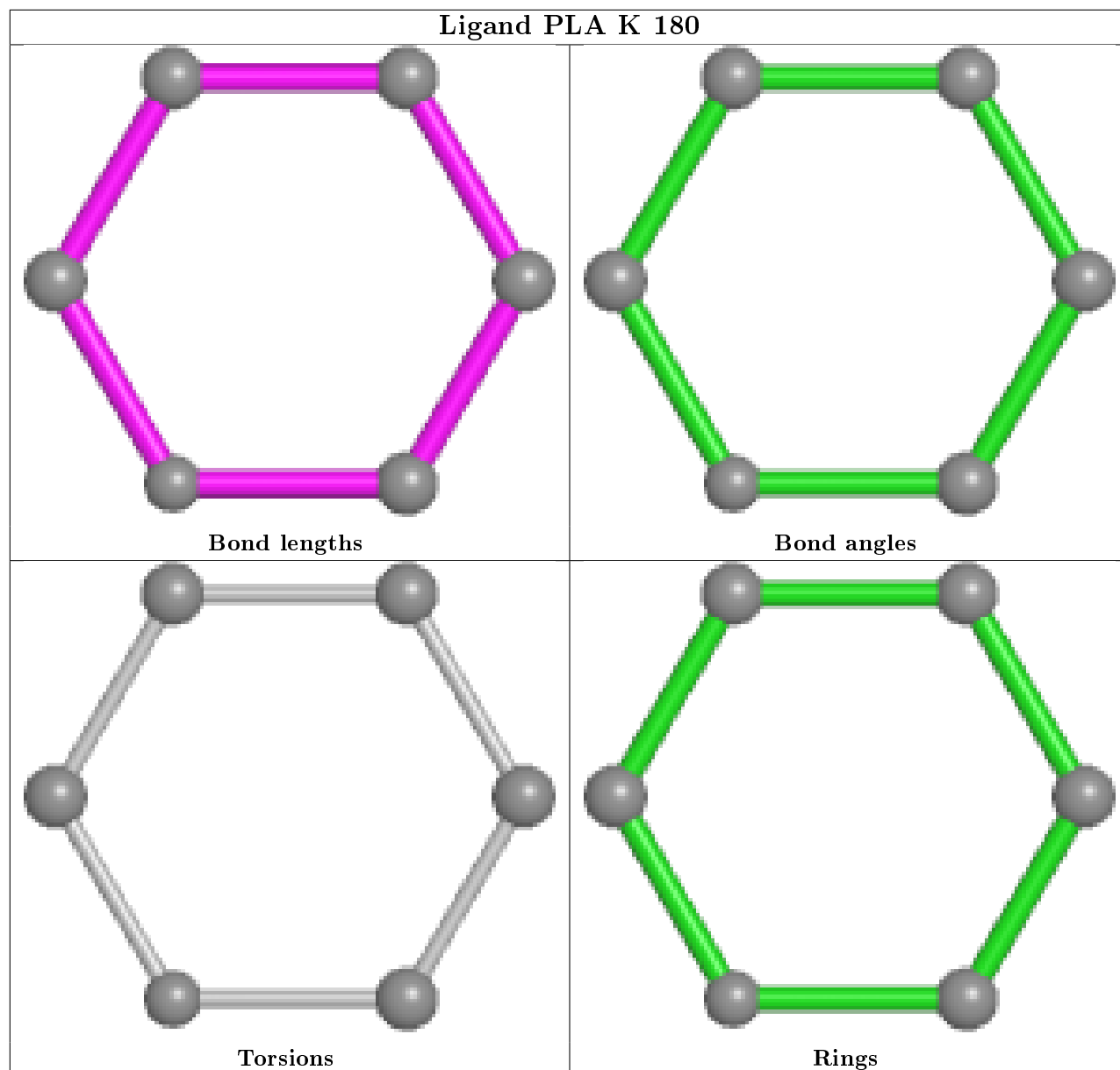












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.